AOAC INTERNATIONAL

INTERNATIONAL STAKEHOLDER PANEL ON ALTERNATIVE METHODS (ISPAM)

Food Allergen Working Group Chair Information/Documentation for Presentation

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AOAC INTERNATIONAL
BYLAWS

As Amended September 26, 2010

ARTICLE I
Name

The name by which this Association shall be known is "AOAC INTERNATIONAL" (hereinafter referred to as the "Association").[1]

ARTICLE II
Purpose

The primary purpose of the Association is to promote methods validation and quality measurements in the analytical sciences.

ARTICLE III
Membership

Section 1. Types of Membership

There shall be three (3) types of membership in the Association: Individual Members, Sustaining Member Organizations, and Organizational Affiliates.

A. Individual Members

There shall be four (4) categories of Individual Members in the Association: Members, Retired Members, Student Members, and Honorary Members.

B. Sustaining Member Organizations

There shall be one (1) category of Sustaining Member Organizations.

C. Organizational Affiliate

There shall be one (1) category of Organizational Affiliate.

Section 2. Qualifications for Membership

A. Individual Members

[1] Members

Qualifications for Members shall be a degree in science, or equivalent as approved by the Board of Directors, and interest in supporting and furthering the purpose and goals of the Association. Such scientists shall be eligible for membership provided they are engaged, or have been engaged, directly or indirectly, in a field relevant to the purpose of the Association.

[2] Retired Members

[1] AOAC INTERNATIONAL was incorporated in the District of Columbia on January 20, 1932, as the Association of Official Agricultural Chemists. On November 10, 1965, the name of the corporation was changed to the Association of Official Analytical Chemists, and on September 12, 1991, the current name was adopted.

A current Member who is no longer actively engaged, directly or indirectly, in a field relevant to the purpose of the Association but who has served the Association as a Member for at least ten (10) years shall be eligible for Retired Member status upon written request and payment of the annual Retired Member dues. Any special benefits accorded Retired Members shall be determined by the Executive Director.

[3] Student Members

Any full-time student working toward an undergraduate or graduate degree in the areas of chemistry, microbiology, food science or other related science shall be eligible for Student Membership in AOAC INTERNATIONAL.

[4] Honorary Members

Honorary Members shall be persons recognized for their substantial contribution toward the achievement of the objectives of the Association. They shall be nominated by the Board of Directors and may be elected by a two-thirds vote of the Individual Members voting.

B. Sustaining Member Organizations

A Sustaining Member Organization shall be any agency of a local, state, provincial, national, or international government; a university, college, or academic department; or any firm, business, or organization with an interest in supporting and furthering the purpose of the Association. Every Sustaining Member Organization must have a designated representative(s). All such Sustaining Member Organization representatives must meet the qualifications for Members and become Individual Members with all the rights and privileges thereof.

C. Organizational Affiliate

An Organizational Affiliate Organization shall be any agency of a local, state, provincial, national, or international government; a university, college, or academic department; or any firm, business, or organization with an interest in supporting and furthering the purpose of the Association. Every Organizational Affiliate must have a designated representative(s). All such Organizational Affiliate representatives must meet the qualifications for Members and become Individual Members with all the rights and privileges thereof.

Section 3. Application for Membership

Applications or requests for membership shall be submitted to the Association's headquarters office. Membership shall become effective upon approval of the application or request, payment of any required membership dues, entry on the membership rolls, and assignment of a member number.

Section 4. Expulsion

The Board of Directors, at any duly called meeting of the Board, by a two-thirds vote of those holding office, may terminate the membership of any member who in its judgment has violated the Bylaws or has been guilty of conduct detrimental to the best interests of the Association. Any member convicted of a felony is subject to immediate expulsion from the Association. Expulsion of a member by the Board of Directors shall be final and shall cancel all rights, interest, or privileges of such member in the services or resources of the Association. Any member, for whom expulsion is proposed, for reasons other than conviction of a felony, shall be entitled to not less than 60 days advance notice of the charges, the date upon which a hearing will be scheduled, and the right to present evidence in defense. The date and place of any such hearing, if held other than at the headquarters or annual meeting site of the Association, must be reasonable with respect to the location of any individual so charged.

Section 5. Dues, Membership Year, and Waivers

A. Annual dues for membership in the Association shall be fixed by the Board of Directors, subject to approval by the majority of the Individual Members voting by ballot by any of the following means (whichever is deemed appropriate by the Board at the time): mail, telephone call, telegram, cablegram, electronic mail or other means of electronic or telephonic transmission.

B. Honorary Members of the Association shall be exempt from payment of dues and annual meeting registration fees.

C. The membership year and the delinquency date shall be determined by the Board of Directors.

D. The authority to grant waivers of membership dues rests with Executive Director.

E. Student Member dues shall be one-third of regular Member dues, rounded up to the nearest $5.00 increment.

Section 6. Members in Good Standing; Rights and Privileges

All Individual Members who maintain their membership by payment of dues as required under these Bylaws and who otherwise qualify shall be considered in good standing and entitled to full privileges of membership.

ARTICLE IV
Officers

Section 1. Elected Officers

The elected officers of the Association shall be Individual Members and shall consist of a President, President-Elect, Secretary, Treasurer, and Immediate Past President.

A. President

The President shall be the principal elected officer of the Association, shall preside at meetings of the Association and of the Board of Directors and of the Executive Committee, and shall be a member ex-officio, with right to vote, of all committees except the Nominating Committee. He or she shall also, at the annual meeting of the Association and at such other times as he or she shall deem proper, communicate to the Association or the Board of Directors such matters and make such suggestions as may in his or her opinion tend to promote the welfare and further the purpose of the Association and shall perform such other

duties as are necessarily incident to the office of President or as may be prescribed by the Board of Directors.

B. President-Elect

In the absence of the President, or in the event of the President's inability or refusal to act, the President-Elect shall perform the duties of the President, and, when so acting, shall have all the powers of and be subject to all the restrictions upon the President. The President-Elect shall perform such other duties as from time to time may be assigned to him or her by the President or by the Board of Directors.

C. Secretary

The Secretary shall give notice of all meetings of the Association, keep a record of all proceedings, attest documents, and, in general, perform such other duties as are usual of the office of Secretary and such other duties as may be assigned by the President or by the Board of Directors.

D. Treasurer

The Treasurer shall be responsible for the funds and securities of the Association; serve as financial officer of the organization and as Chairperson of the Finance Committee; manage the Board of Director's review of and action related to the Board of Director's financial responsibilities; serve as the chief Board liaison in overseeing and reviewing the annual audit, and in general, perform such other duties as are usual of the office of Treasurer and such other duties as may be assigned by the President or by the Board of Directors.

E. Immediate Past President

The Immediate Past President shall serve as advisor to the President and Directors and perform such other duties as may be assigned from time to time by the President or by the Board of Directors.

Section 2. Appointed Officers

The appointed officers shall include the Executive Director and such other appointed officers as may be designated by the Board of Directors from time to time.

A. Executive Director

The day-to-day administration and management of the Association's offices shall be vested in a salaried manager employed or appointed by, and directly responsible to, the Board of Directors. This manager shall have the title of Executive Director with responsibility for the management and direction of all operations, programs, activities, and affairs of the Association, as approved or delegated by the Board of Directors. The Executive Director shall have direct responsibility for employment and termination of employment and the determination of compensation for staff members within the budgetary framework determined by the Board of Directors. The Executive Director functions as the chief operating officer of the Association within the guidelines established by the policies and procedures of the Board of Directors and, as necessary, with the concurrence of the President. The Executive Director shall have such other duties as may be prescribed by the Board.

B. Other Appointed Officers

Other appointed officers shall have such duties as may be prescribed by the Board.

ARTICLE V
Nominations, Elections, Terms, and Appointments to the Board of Directors

Section 1. Nominating Committee

The Nominating Committee shall annually recommend to the Board of Directors a slate of Individual Members as potential nominees for the elected positions where vacancies will occur. The Nominating Committee shall consist of five (5) members who shall be three (3) immediate Past Presidents, as available, and two (2) Individual Members-at-Large of the Association. If three Past Presidents are not available to serve, other Individual Members-at-Large shall be appointed by the President to the extent necessary to form the five (5)-member committee.

Section 2. Elections and Terms of Office

The President-Elect, the Secretary, Treasurer, and the Directors of the Board of Directors shall be elected by a majority of Individual Members voting, from a slate of nominees recommended annually by the Board of Directors.

Terms of office for all Officers and Directors shall begin with the adjournment of the annual meeting following their election and shall end with the adjournment of the annual meeting occurring nearest the expiration of their term. The six (6) Directors shall be elected to staggered three-year terms with two Directors elected to full three-year terms each year, but not to more than two (2), consecutive, three-year terms. Appointment or election to fill an unexpired term shall not affect the eligibility of a person to subsequently be elected to two (2) full terms. The Secretary shall be elected to a one-year term and may be re-elected to successive one-year terms. The Treasurer shall be elected for a one-year term and may be re-elected to successive one-year terms. The President-Elect shall be elected to a one-year term; whereupon the current President-Elect shall become President and the current President shall become the Immediate Past President, each serving a one-year term.

Section 3. Appointments

Directors-at-Large are appointed by the Board in accordance with Article VI, Section 2. Directors-at-Large are appointed for one (1) year terms, renewable at the discretion of the elected Board.

ARTICLE VI
Board of Directors

Section 1. Composition

The Board of Directors shall consist of eleven (11) elected members to include the President, President-Elect, Secretary, Treasurer, Immediate Past President, six (6) Directors, and up to three (3) appointed Directors-at-Large, all of whom shall be Individual Members of the Association. The elected Board shall reflect the makeup of the Association membership and shall not be dominated by any single interest.

Section 2. Powers and Duties

The Board of Directors shall provide supervision, control, and direction of the affairs of the Association, shall determine the Association's policies or changes therein within the limits of the Bylaws, shall actively prosecute

its purpose, and shall have discretion in the disbursement of its funds. It may adopt such rules and procedures for the conduct of its business as shall be deemed advisable, and may, in the execution of the powers granted, appoint such agents as it may consider necessary. The Board of Directors may appoint up to three (3) Directors-at-Large, if, in their opinion, such appointments advance the purpose of the Association. Directors-at-Large shall be accorded the same voting privileges as elected Directors.

Section 3. Meetings

Except that the Board shall have a regular meeting at the time and place of the annual meeting, the Board shall meet, in person or via telephone conference call, upon call of the President at such times and places as he or she may designate within the policies adopted by the Board, and shall be called to meet upon demand of a majority of its members. Notice of all meetings of the Board of Directors shall be sent by any of the following means (whichever is deemed appropriate by the President at the time): mail, telephone call, telegram, cablegram, electronic mail or other means of electronic or telephonic transmission to each member of the Board at his or her last recorded address or number at least fourteen (14) days in advance of in-person meetings or forty-eight (48) hours in advance of conference call meetings.

Section 4. Quorum

A quorum for any meeting of the Board is six (6) Board members elected in accordance with Article V (1). Any less number may: (1) set a time to adjourn, (2) adjourn, (3) recess, or (4) take measures to obtain a quorum.

Section 5. Absence

Any member of the Board of Directors unable to attend a meeting of the Board shall notify the President and state the reason for his or her absence. If a member of the Board is absent from two (2) consecutive meetings, he or she may be removed by a two-thirds vote of the Board Members then in office.

Section 6. Compensation

Members of the Board of Directors, as such, shall not receive any compensation for their services as Board members, but the Board may, by resolution under policies it may adopt, authorize reimbursement of expenses incurred in the performance of members' duties. Such authorization may prescribe conditions and procedures for approval and payment of such expenses. Nothing herein shall preclude a Board member from serving the Association in any other capacity and receiving compensation for such services, if compensation is customarily paid for such services.

Section 7. Resignation or Removal

Any member of the Board may resign at any time by giving written notice to the President, Secretary, Treasurer, or to the Board of Directors. Such resignation shall take effect at the time specified therein, or, if no time is specified, at the time of acceptance thereof as determined by the President or the Board.

Any member of the Board may be removed by a three-fourths vote of the Board members then in office and present at any regular or special meeting of the Board.

Section 8. Vacancies: Members of the Board

If a vacancy should occur in the membership of the elected Board of Directors, any Past President may be appointed by action of the remaining members of the Board to temporarily fill such vacancy until the next

regularly scheduled election. At the next regularly scheduled election nominations will be presented to fill the vacancy for the unexpired portion of the term remaining.

Section 9. Vacancies: President and Other Officers

If the office of the President shall become vacant, the President-Elect shall thereupon become President of the Association for the unexpired term, followed by his or her duly elected term. In the event the office of President becomes vacant at a time when the office of President-Elect is also vacant, the Presidency shall be filled for the remainder of the term by the action of the Board of Directors. If any other officer position shall become vacant, the office may be filled for the remainder of the term by action of the Board.

ARTICLE VII
Committees

Section 1. Committee Formation

The Board of Directors shall form and adopt terms of reference for such standing or special boards, committees, subcommittees, task forces, or task groups as may be required by these Bylaws or as the Board may determine necessary to carry out the affairs of the Association.

Section 2. Committee Appointments

Subject to the requirements of these Bylaws and the specific terms of reference adopted by the Board, the President shall make the appointments to fill the vacancies occurring in the Association's standing or special boards, committees, subcommittees, task forces, or task groups.

ARTICLE VIII
Official Methods of Analysis

The Board of Directors (BoD) is empowered to develop written policies and procedures for the study, adoption, and change in status of the Official Methods of Analysis of AOAC INTERNATIONAL. Implementation of the policies and procedures shall be delegated to an Official Methods Board (OMB).

Section 1. Composition of the Official Methods Board

The Official Methods Board shall consist of a chair and a vice chair, and members who are recommended by the chair. The chair, vice chair and members are appointed by the President of AOAC INTERNATIONAL. The OMB shall be composed of members representing a balance of government, industry, and academia as appropriate to the scope of the group and shall not be dominated by any single interest.

Section 2. Purpose of the Official Methods Board

The OMB shall serve the Association in a scientific and advisory capacity on methods and the process of their adoption. The OMB shall be responsible for implementation of procedures adopted by the BoD, according to the principles in section 3 below.

Section 3. Principles of the Official Methods Program

A. Adequate records of technical data, discussions, and decisions on the study, adoption, and change of status of Official Methods of Analysis shall be maintained for a reasonable time.

B. Timely notice of proposed method studies, adoption, or change in status shall be published in an Association publication that is circulated to the members.

C. Opportunity shall be provided for materially interested parties to submit input during method study and adoption procedures and to submit comments on the adoption, use of, or change in status of specific methods.

D. Methods submitted to the OMB for inclusion in the OMA shall be thoroughly studied, scientifically reviewed, and available in published form prior to adoption as Final Action by the OMB.

E. The OMB shall adopt methods as Final Action.

ARTICLE IX
Meetings

Section 1. Annual Meeting

The annual business meeting of the Association shall be held at the time and place decided by the Board of Directors. A special meeting of the entire Association may be called by the Board of Directors; announcement thereof shall be made at least thirty (30) days prior to the time of said meeting.

Section 2. Quorum

One hundred Individual Members who are present in person or by proxy and entitled to vote shall constitute a quorum at any meeting of the Association which is duly called pursuant to the provisions of these Bylaws.

ARTICLE X
Voting

Section 1. Voting by Ballot

By direction of the Board of Directors, unless otherwise required by these Bylaws or conducted under alternative procedures established under these Bylaws, voting on any matter, including the election of officers and directors, the election of Honorary Members, amendment of the Bylaws, and the approval of dues, may be conducted by ballot of the voting membership by any of the following means (whichever is deemed appropriate at the time): mail, telephone call, telegram, cablegram, electronic mail or other means of electronic or telephonic transmission, and the question(s) thus presented shall be determined according to the votes received, provided in each case votes of at least five (5) percent of the voting membership shall be received. Any and all action taken in pursuance of a vote by any of the means indicated above (whichever the Board deemed appropriate at the time)

in each case shall be binding upon the Association in the same manner as would be action taken at a duly called meeting and shall become effective, unless otherwise provided for in these Bylaws or otherwise stated in the ballot, on the day following certification of the vote.

Section 2. Voting by Proxy

At any duly called meeting of Individual Members, a member-of-record, as determined thirty (30) days prior to any meeting and who is entitled to vote, may vote by proxy executed in writing by the Individual Member or his or her duly authorized attorney-in-fact. No proxy shall be valid for more than eleven (11) months after the date of its execution unless otherwise provided in the proxy.

ARTICLE XI
Earnings and Assets

Section 1. Non-Profit Status

A. Regardless of any provision of the Bylaws which may be construed otherwise:

[1] No part of the net earnings of the Association shall under any circumstances inure to the benefit of any member or individual.

[2] The Association shall not be operated for a private profit.

B. On lawful dissolution of the Association and after settlement of all just obligations of the Association, the Board of Directors shall distribute all remaining assets of the Association to one (1) or more organizations selected by the Board of Directors which have been held exempt from Federal Income Tax as organizations described in section 501(c)(3) of the Internal Revenue Code of 1954.

Section 2. Political Activities

A. No substantial part of the Association's activities shall consist of carrying on propaganda or otherwise attempting to influence local, state, or national legislation. All activities of the Association shall be determined by the Board of Directors.

B. The Association shall not participate or intervene in any manner in any campaign on behalf of any candidate for a political office.

ARTICLE XII
Sections

Section 1. Sections

The Board of Directors shall set geographic limits and grant authority to groups of Individual Members of the Association residing or working in the same geographical areas for the establishment of Sections.

Section 2. Purpose of Sections

The purpose of Sections shall be to promote and further the purpose of the Association.

Section 3. Membership in Sections

Individuals interested in the purpose of the Section shall be eligible for Section membership. Only Individual Members of the Association shall be eligible for election to the Executive Committee of the Section.

Section 4. Bylaws of Sections

Subject to approval of the Board of Directors, each Section shall adopt, for its own governance, bylaws not inconsistent with these Bylaws.

Section 5. Dissolution of Sections

When any Section shall cease to function as a Section for a period of more than one year, or if its membership shall be less than ten (10) Individual Members of the Association for a period of one (1) year, the Board of Directors may terminate the existence of such Section.

Section 6. Actions of Sections

No act of a Section or its members shall be considered an act of the Association unless expressly authorized, ratified, or affirmed by the Board of Directors.

ARTICLE XIII
Technical Divisions

Section 1. Purpose

Technical Divisions shall represent communities of interest within the Association which have the purpose of furthering the purpose of the Association through the development of the analytical sciences either in a commodity-based or scientific discipline-based field. Their activities shall not duplicate the organizational structure nor conflict with the policies or procedures for the adoption of official methods of analysis by the Association.

Section 2. Creation, Combination, Discontinuance, or Change

Technical Divisions may be created, existing Technical Divisions may be combined or discontinued, or the name of a Technical Division may be changed under policies and procedures adopted by the Board of Directors. Each Technical Division shall adopt bylaws not inconsistent with these Bylaws. The jurisdiction of each Technical Division shall be described in its bylaws. No act of any Technical Division or its members shall be considered an act of the Association unless expressly authorized, ratified, or affirmed by the Board of Directors.

ARTICLE XIV
Indemnification

The Association shall have the power to pay, by indemnity, reimbursement, or otherwise, to or for the use of any person designated by resolution of the Board of Directors who was or is a party or is threatened to be made a party to any threatened, pending, or completed action, suit, or proceeding, whether civil, criminal, administrative, or investigative (other than an action by or on behalf of the Association), by reason of the fact he or she is or was a director, officer, committee member, employee or agent of the Association, or was serving as such for another at the request of the Association, against expenses (including legal, accounting, witness and other), judgments, fines, and amounts paid in settlement so long as such person was not found by a court of competent jurisdiction to have been willfully negligent of the interests of the Association or such person had reasonable cause to believe that his or her conduct was lawful.

ARTICLE XV
Parliamentary Authority

The rules contained in the current edition of *Robert's Rules of Order Newly Revised* shall govern the Association in all cases in which they are applicable and in which they are not inconsistent with these Bylaws or any special rules of order the Association may adopt.

ARTICLE XVI
Amendments to the Bylaws

These Bylaws may be amended, repealed, or altered, in whole or in part, by a three-fourths vote: (a) of the Individual Members at any annual business or duly called special meeting of the Association, provided notice of any amendment proposed for consideration shall be sent by any of the following means (whichever may be deemed appropriate at the time): mail, telephone call, telegram, cablegram, electronic mail or other means of electronic or telephonic transmission to the last recorded address or number of each Individual Member at least thirty (30) days prior to the date of the meeting; or (b) by approval of the Individual Members through ballot sent by any means indicated above in accordance with the provisions of Article X, Voting.

All proposed amendments of these Bylaws shall be presented in writing to the Board of Directors. The Board shall present the proposals to the Association membership, with recommendations. All amendments to the Bylaws, unless otherwise stated, will become effective at the adjournment of the meeting where action is taken or on the day following the certification of a vote by mail ballot.

AOAC INTERNATIONAL
POLICY ON THE USE OF THE
ASSOCIATION NAME, INITIALS,
IDENTIFYING INSIGNIA, LETTERHEAD, AND BUSINESS CARDS

Introduction

The following policy and guidelines for the use of the name, initials, and other identifying insignia of AOAC INTERNATIONAL have been developed in order to protect the reputation, image, legal integrity and property of the Association.

The name of the Association, as stated in its bylaws, is "AOAC INTERNATIONAL". The Association is also known by its initials, AOAC, and by its logo, illustrated below, which incorporates the Association name and a representation of a microscope, book, and flask. The AOAC logo is owned by the Association and is registered with the U.S. Patent and Trademark Office.

The full Association insignia, illustrated below, is comprised of the logo and the tagline, "The Scientific Association Dedicated to Analytical Excellence," shown below. The typeface used is Largo. The AOAC tagline is owned by the Association and is registered with the U.S. Patent and Trademark office.

The Scientific Association Dedicated to Analytical Excellence®

Policy

Policy on the use of the Association's name and logo is established by the AOAC Board of Directors as follows:

> "The Board approves and encourages reference to the Association by name, either as AOAC INTERNATIONAL or as AOAC; or reference to our registered trademark, AOAC®, in appropriate settings to describe our programs, products, etc., in scientific literature and other instances so long as the reference is fair, accurate, complete and truthful and does not indicate or imply unauthorized endorsement of any kind.
>
> The insignia (logo) of AOAC INTERNATIONAL is a registered trade and service mark and shall not be reproduced or used by any person or organization other than the Association, its elected and appointed officers, sections, or committees, without the prior written permission of the Association. Those authorized to use the AOAC INTERNATIONAL insignia shall use it only for the purposes for which permission has been specifically granted.
>
> The name and insignia of the Association shall not be used by any person or organization in any way which indicates, tends to indicate, or implies AOAC official endorsement of any product, service, program, company, organization, event or person, endorsement of which, has not been authorized by the Association, or which suggests that membership in the Association is available to any organization."

The Executive Director, in accordance with the above stated policy, is authorized to process, approve, fix rules, and make available materials containing the Association name and insignia.

It should be noted that neither the Association's name nor its insignia nor part of its insignia may be incorporated into any personal, company, organization, or any other stationery other than that of the Association; nor may any statement be included in the printed portion of such stationery which states or implies that an individual, company, or other organization is a Member of the Association.

Instructions

1. Reproduction or use of the Association name or insignia requires prior approval by the Executive Director or his designate.

2. Association insignia should not be altered in any manner without approval of the Executive Director or his designate, except to be enlarged or reduced in their entirety.

3. Artwork for reproducing the Association name or insignia, including those incorporating approved alterations, will be provided on request to those authorized to use them (make such requests to the AOAC Marketing Department). Examples of the types of alterations that would be approved are inclusion of a section name in or the addition of an officer's name and address to the letterhead insignia.

4. When the Association name is used without other text as a heading, it should, when possible, be set in the Largo typeface.

5. Although other colors may be used, AOAC blue, PMS 287, is the preferred color when printing the AOAC insignia, especially in formal and official documents. It is, of course, often necessary and acceptable to reproduce the insignia in black.

6. Do not print one part of the logo or insignia in one color and other parts in another color.

7. The letterhead of AOAC INTERNATIONAL shall not be used by any person or organization other than the Association, its elected and appointed officers, staff, sections, or committees; except by special permission.

   Correspondence of AOAC official business should be conducted using AOAC letterhead. However, those authorized to use AOAC letterhead shall use it for official AOAC business only.

   Copies of all correspondence using AOAC letterhead or conducting AOAC official business, whether on AOAC letterhead or not, must be sent to the appropriate office at AOAC headquarters.

8. AOAC INTERNATIONAL business cards shall not be used by any person or organization other than the Association, its staff, and elected officials, except by special permission.

   Those authorized to use AOAC business cards shall use them for official AOAC business only and shall not represent themselves as having authority to bind the Association beyond that authorized.

Sanctions

1. Upon learning of any violation of the above policy, the Executive Director or a designate will notify the individual or organization that they are in violation of AOAC policy and will ask them to refrain from further misuse of the AOAC name or insignia.

2. If the misuse is by an Individual Member or Sustaining Member of the Association, and the misuse continues after notification, the Board of Directors will take appropriate action.

3. If continued misuse is by a nonmember of the Association or if a member continues misuse in spite of notification and Board action, ultimately, the Association will take legal action to protect its property, legal integrity, reputation, and image.

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Adopted by the AOAC Board of Directors: September 24, 1989
Revised: June 13, 1991; February 26, 1992; March 21, 1995; October 1996

AOAC INTERNATIONAL
ANTITRUST POLICY
STATEMENT AND GUIDELINES

Introduction

It is the policy of AOAC INTERNATIONAL (AOAC) and its members to comply strictly with all laws applicable to AOAC activities. Because AOAC activities frequently involve cooperative undertakings and meetings where competitors may be present, it is important to emphasize the on_going commitment of our members and the Association to full compliance with national and other antitrust laws. This statement is a reminder of that commitment and should be used as a general guide for AOAC and related individual activities and meetings.

Responsibility for Antitrust Compliance

The Association's structure is fashioned and its programs are carried out in conformance with antitrust standards. However, an equal responsibility for antitrust compliance __ which includes avoidance of even an appearance of improper activity __ belongs to the individual. Even the appearance of improper activity must be avoided because the courts have taken the position that actual proof of misconduct is not required under the law. All that is required is whether misconduct can be inferred from the individual's activities.

Employers and AOAC depend on individual good judgment to avoid all discussions and activities which may involve improper subject matter and improper procedures. AOAC staff members work conscientiously to avoid subject matter or discussion which may have unintended implications, and counsel for the Association can provide guidance with regard to these matters. It is important for the individual to realize, however, that the competitive significance of a particular conduct or communication probably is evident only to the individual who is directly involved in such matters.

Antitrust Guidelines

In general, the U.S. antitrust laws seek to preserve a free, competitive economy and trade in the United States and in commerce with foreign countries. Laws in other countries have similar objectives. Competitors (including individuals) may not restrain competition among themselves with reference to the price, quality, or distribution of their products, and they may not act in concert to restrict the competitive capabilities or opportunities of competitors, suppliers, or customers.

Although the Justice Department and Federal Trade Commission generally enforce the U.S. antitrust laws, private parties can bring their own lawsuits.

Penalties for violating the U.S. and other antitrust laws are severe: corporations are subject to heavy fines and injunctive decrees, and may have to pay substantial damage judgments to injured competitors, suppliers, or customers. Individuals are subject to criminal prosecution, and will be punished by fines and imprisonment.
Under current U.S. federal sentencing guidelines, individuals found guilty of bid rigging, price fixing, or market allocation must be sent to jail for at least 4 to 10 months and must pay substantial minimum fines.

Since the individual has an important responsibility in ensuring antitrust compliance in AOAC activities, everyone should read and heed the following guidelines.

1. Don't make any effort to bring about or prevent the standardization of any method or product for the purpose or intent of preventing the manufacture or sale of any method or product not conforming to a specified standard.

2. Don't discuss with competitors your own or the competitors' prices, or anything that might affect prices such as costs, discounts, terms of sale, distribution, volume of production, profit margins, territories, or customers.

3. Don't make announcements or statements at AOAC functions, outside leased exhibit space, about your own prices or those of competitors.

4. Don't disclose to others at meetings or otherwise any competitively sensitive information.

5. Don't attempt to use the Association to restrict the economic activities of any firm or any individual.

6. Don't stay at a meeting where any such price or anti_competitive talk occurs.

7. Do conduct all AOAC business meetings in accordance with AOAC rules. These rules require that an AOAC staff member be present or available, the meeting be conducted by a knowledgeable chair, the agenda be followed, and minutes be kept.

8. Do confer with counsel before raising any topic or making any statement with competitive ramifications.

9. Do send copies of meeting minutes and all AOAC_related correspondence to the staff member involved in the activity.

10. Do alert the AOAC staff to any inaccuracies in proposed or existing methods and statements issued, or to be issued, by AOAC and to any conduct not in conformance with these guidelines.

Conclusion

Compliance with these guidelines involves not only avoidance of antitrust violations, but avoidance of any behavior which might be so construed. Bear in mind, however, that the above antitrust laws are stated in general terms, and that this statement is not a summary of applicable laws. It is intended only to highlight and emphasize the principal antitrust standards which are relevant to AOAC programs. You must, therefore, seek the guidance of either AOAC counsel or your own counsel if antitrust questions arise.

* * * * *

Adopted by the AOAC Board of Directors: September 24, 1989
Revised: March 11, 1991
Revised October 1996

AOAC INTERNATIONAL

POLICY AND PROCEDURES ON

VOLUNTEER CONFLICT OF INTEREST

Statement of Policy

While it is not the intention of AOAC INTERNATIONAL (AOAC) to restrict the personal, professional, or proprietary activities of AOAC members nor to preclude or restrict participation in Association affairs solely by reason of such activities, it is the sense of AOAC that conflicts of interest or even the appearance of conflicts of interest on the part of AOAC volunteers should be avoided. Where this is not possible or practical under the circumstances, there shall be written disclosure by the volunteers of actual or potential conflicts of interest in order to ensure the credibility and integrity of AOAC. Such written disclosure shall be made to any individual or group within the Association which is reviewing a recommendation which the volunteer had a part in formulating and in which the volunteer has a material interest causing an actual or potential conflict of interest.

AOAC requires disclosure of actual or potential conflicts of interest as a condition of active participation in the business of the Association. The burden of disclosure of conflicts of interest or the appearance of conflicts of interest falls upon the volunteer.

A disclosed conflict of interest will not in itself bar an AOAC member from participation in Association activities, but a three-fourths majority of the AOAC group reviewing the issue presenting the conflict must concur by secret ballot that the volunteer's continued participation is necessary and will not unreasonably jeopardize the integrity of the decision-making process.

Employees of AOAC are governed by the provision of the AOAC policy on conflict of interest by staff. If that policy is in disagreement with or mute on matters covered by this policy, the provisions of this policy shall prevail and apply to staff as well.

Illustrations of Conflicts of Interest

1. A volunteer who is serving as a committee member or referee engaged in the evaluation of a method or device; who is also an employee of or receiving a fee from the firm which is manufacturing or distributing the method or device or is an employee of or receiving a fee from a competing firm.

2. A volunteer who is requested to evaluate a proposed method or a related collaborative study in which data are presented that appear detrimental (or favorable) to a product distributed or a position supported by the volunteer's employer.

3. A referee who is conducting a study and evaluating the results of an instrument, a kit, or a piece of equipment which will be provided gratis by the manufacturer or distributor to one or more of the participating laboratories, including his or her own laboratory, at the conclusion of the study.

4. Sponsorship of a collaborative study by an interest (which may include the referee) which stands to profit from the results; such sponsorship usually involving the privilege granted by the investigator to permit the sponsor to review and comment upon the results prior to AOAC evaluation.

5. A volunteer asked to review a manuscript submitted for publication when the manuscript contains information which is critical of a proprietary or other interest of the reviewer.

The foregoing are intended as illustrative and should not be interpreted to be all-inclusive examples of conflicts of interest AOAC volunteers may find themselves involved in.

Do's and Don'ts

Do avoid the appearance as well as the fact of a conflict of interest.

Do make written disclosure of any material interest which may constitute a conflict of interest or the appearance of a conflict of interest.

Do not accept payment or gifts for services rendered as a volunteer of the Association without disclosing such payment or gifts.

Do not vote on any issue before an AOAC decision-making body where you have the appearance of or an actual conflict of interest regarding the recommendation or decision before that body.

Do not participate in an AOAC decision-making body without written disclosure of actual or potential conflicts of interest in the issues before that body.

Do not accept a position of responsibility as an AOAC volunteer, without disclosure, where the discharge of the accepted responsibility will be or may appear to be influenced by proprietary or other conflicting interests.

Procedures

Each volunteer elected or appointed to an AOAC position of responsibility shall be sent, at the time of election or appointment, a copy of this policy and shall be advised of the requirement to adhere to the provisions herein as a condition for active participation in the business of the Association. Each volunteer, at the time of his or her election or appointment, shall indicate, in writing, on a form provided for this purpose by AOAC, that he or she has read and accepts this policy.

Each year, at the spring meeting of the AOAC Board of Directors, the Executive Director shall submit a report certifying the requirements of this policy have been met; including the names and positions of any elected or appointed volunteers who have not at that time indicated in writing that they have accepted the policy.

Anyone with knowledge of specific instances in which the provisions of this policy have not been complied with shall report these instances to the Board of Directors, via the Office of the Executive Director, as soon as discovered.

* * * * * *

Adopted: March 2, 1989
Revised: March 28, 1990
Revised: October 1996

AOAC INTERNATIONAL
STAKHOLDER PANEL WORKING GROUP TERMS OF REFERENCE

I. NAME: ISPAM WORKING GROUP ON FODD ALLERGEN ASSAYS

REPORTS TO CONSENSUS GROUP: INTERNATIONAL STAKEHOLDER PANEL ON ALTERNATIVE METHODOLOGY (ISPAM)

II. MISSION:
Working groups are formed to develop and recommend standard method performance requirements for prioritized food allergens to the stakeholder panel, review available methodology, identify expertise and specific tasks designated by the stakeholder panel. They are *recommending* bodies which report its recommendations to the stakeholder panel for consideration. The working is used to accomplish tasks that are too detailed and/or complex for a large body to complete efficiently.

III. RESPONSIBILITIES:
The working group will meet either in person and via teleconference, web conferencing or by other means of communication. All communication and meetings of the working group must be facilitated through AOAC staff. The working group's tasks will include developing standard method performance requirements (SMPRs), review of methodology, identifying expertise and other as may be requested by the ISPAM chair. Working groups are not required to vote, but to show general consensus for its recommendations. The groups should meet to discuss their objectives and complete their assigned tasks. Individuals on the working groups may be tasked with their own action items and responsibilities. More than one meeting and one round of communication may be required to complete the working group's tasks. All working group participants are expected to contribute and are expected to have completed the SMPR Education Session. AOAC staff must document all working group deliberations.

The chair of the working group will moderate the working group meetings, assist in scheduling the meetings, and report the working group's recommendation back to ISPAM. AOAC will work with working group chairs to formulate the working group's recommendation into motions for ISPAM's consideration.

IV. COMPOSITION AND ORGANIZATION:
In order for a working group to complete its assigned task efficiently, working groups will consist of on average 15-20 appropriate experts and thought leaders from a variety of pertinent perspectives. Perspectives include industry, government, academia, NGOs, and regional sectors. Industry includes contract research organizations and laboratories, raw materials, reference materials, method developers, and technology providers. Working group members must be members of ISPAM with the approval of the working group and stakeholder panel chair. The working group chair will be appointed by the Chair of ISPAM.

These groups are established within AOAC policies and procedures and are administered by AOAC. All members are considered volunteers and must participate in a SMPR Education Session. AOAC INTERNATIONAL requires a concise statement of your expertise to maintain participation on this working group.

V. STAFF LIASON:
AOAC will assign staff to facilitate the work of the working group

VI. TERMS OF REVIEW:
This document will be reviewed periodically by the ISPAM Chair though completion of the working group's tasks.

VII. DATE ESTABLISHED
June 15, 2016

VIII. DATES REVISED

AOAC INTERNATIONAL
Fitness for Purpose Statement Guideline

A description of the minimum performance characteristics required by an analytical method to detect or measure an analytes or analytes. A Fitness for Purpose statement must clearly identify the:

1) analyte or class of analytes
2) analytical range
3) matrix or matrixes
4) types of test samples (powder, liquid, raw food, sprays, etc.)
5) regulatory requirements (if any)
6) time-to-signal (sample preparation to analytical results)
7) type of analysts (trained chemists or microbiologist, first responder, field hand)

A Fitness for Purpose statement may also provide additional information about the analytical requirements that materially affects the types of methods that can be used. . For example, will the method be used in a laboratory under controlled conditions or will the method by used in the field. A Fitness for Purpose statement should describe whether qualified methods will be screening or confirmatory techniques, and/or intended to be used as reference methods for dispute resolution

A Fitness for Purpose statement should be no longer than one paragraph.

Version 2
6/21/10

Appendix F: Guidelines for Standard Method Performance Requirements

Contents

Introduction to Standard Method Performance Requirements

Standard method performance requirements (SMPRs) are a unique and novel concept for the analytical methods community. SMPRs are voluntary consensus standards, developed by stakeholders, that prescribe the minimum analytical performance requirements for classes of analytical methods. In the past, analytical methods were evaluated and the results compared to a "gold standard" method, or if a gold standard method did not exist, then reviewers would decide retrospectively if the analytical performance was acceptable. Frequently, method developers concentrated on the process of evaluating the performance parameters of a method, and rarely set acceptance criteria. However, as the *Eurachem Guide* points out: " . . . the judgment of method suitability for its intended use is equally important . . ." (1) to the evaluation process.

International Voluntary Consensus Standards

An SMPR is a form of an international, voluntary consensus standard. A standard is an agreed, repeatable way of doing something that is published as document that contains a technical specification or other precise criteria designed to be used consistently as a rule, guideline, or definition. SMPRs are a *consensus* standards developed by stakeholders in a very controlled process that ensures that users, research organizations, government departments, and consumers work together to create a standard that meets the demands of the analytical community and technology. SMPRs are also *voluntary* standards. AOAC cannot, and does not, impose the use of SMPRs. Users are free to use SMPRs as they see fit. AOAC is very careful to include participants from as many regions of the world as possible so that SMPRs are accepted as *international* standards.

Guidance for Standard Method Performance Requirements

Commonly known as the "SMPR Guidelines." The first version of the SMPR Guidelines were drafted in 2010 in response to the increasing use and popularity of SMPRs as a vehicle to describe the analytical requirements of a method. Several early "acceptance criteria" documents were prepared for publication in late 2009, but the format of the acceptance criteria documents diverged significantly from one another in basic format. AOAC realized that a guidance document was needed to promote uniformity.

An early version of the SMPR Guidelines were used for a project to define the analytical requirements for endocrine disruptors in potable water. The guidelines proved to be extremely useful in guiding the work of the experts and resulted in uniform SMPRs. Subsequent versions of the SMPR Guidelines were used in the Stakeholder Panel for Infant Formula and Adult Nutritionals (SPIFAN) project with very positive results. The SMPR Guidelines are now published for the first time in the *Journal of AOAC INTERNATIONAL* and *Official Methods of Analysis*.

Users of the guidelines are advised that they are: (*1*) a *guidance* document, not a statute that users must conform to; and (*2*) a "living" document that is regularly updated, so users should check the AOAC website for the latest version before using these guidelines.

The SMPR Guidelines are intended to provide basic information for working groups assigned to prepare SMPRs. The guidelines consist of the standard format of an SMPR, followed by a series of informative tables and annexes.

SMPR Format

The general format for an SMPR is provided in *Annex A*.

Each SMPR is identified by a unique SMPR number consisting of the year followed by a sequential identification number (YYYY.XXX). An SMPR number is assigned when the standard is approved. By convention, the SMPR number indicates the year a standard is approved (as opposed to the year the standard is initiated). For example, SMPR 2010.003 indicates the third SMPR adopted in 2010.

The SMPR number is followed by a method name that must include the analyte(s), matrix(es), and analytical technique (unless the SMPR is truly intended to be independent of the analytical technology). The method name may also refer to a "common" name (e.g., "Kjeldahl" method).

The SMPR number and method name are followed by the name of the stakeholder panel or expert review panel that approved the SMPR, and the approval and effective dates.

Information about method requirements is itemized into nine categories: (*1*) intended use; (*2*) applicability; (*3*) analytical technique; (*4*) definitions; (*5*) method performance requirements; (*6*) system suitability; (*7*) reference materials; (*8*) validation guidance; and (*9*) maximum time-to-determination.

An SMPR for qualitative and/or identification methods may include up to three additional annexes: (*1*) inclusivity/selectivity panel; (*2*) exclusivity/cross-reactivity panel; and (*3*) environmental material panels. These annexes not required.

Informative tables.—The SMPR Guidelines contain seven informative tables that represent the distilled knowledge of many years of method evaluation, and are intended as guidance for SMPR working groups. The informative tables are not necessarily AOAC

policy. SMPR working groups are expected to apply their expertise in the development of SMPRs.

Table A1: Performance Requirements. Provides recommended performance parameters to be included into an SMPR. Table A1 is organized by five method classifications: (*1*) main component quantitative methods; (*2*) trace or contaminant quantitative methods; (*3*) main component qualitative methods; (*4*) trace or contaminant quantitative methods; and (*5*) identification methods. The table is designed to accommodate both microbiological and chemical methods. Alternate microbiological/chemical terms are provided for equivalent concepts.

Table A2: Recommended Definitions. Provides definitions for standard terms in the SMPR Guidelines. AOAC relies on *The International Vocabulary of Metrology Basic and General Concepts and Associated Terms* (VIM) and the International Organization for Standadization (ISO) for definition of terms not included in Table A2.

Table A3: Recommendations for Evaluation. Provides general guidance for evaluation of performance parameters. More detailed evaluation guidance can be found in *Appendix D, Guidelines for Collaborative Study Procedures to Validate Characteristics of a Method of Analysis* (2); *Appendix I, Guidelines for Validation of Biological Threat Agent Methods and/or Procedures* (3); *Appendix K, AOAC Guidelines for Single-Laboratory Validation of Chemical Methods for Dietary Supplements and Botanicals* (4); Codex Alimentarius Codex Procedure Manual (5); and ISO Standard 5725-1-1994 (6).

Table A4: Expected Precision (Repeatability) as a Function of Analyte Concentration. The precision of a method is the closeness of agreement between independent test results obtained under stipulated conditions. Precision is usually expressed in terms of imprecision and computed as a relative standard deviation (RSD) of the test results. The imprecision of a method increases as the concentration of the analyte decreases. This table provides target RSDs for a range of analyte concentrations.

Table A5: Expected Recovery as a Function of Analyte Concentration. Recovery is defined as the ratio of the observed mean test result to the true value. The range of the acceptable mean recovery expands as the concentration of the analyte decreases. This table provides target mean recovery ranges for analyte concentrations from 1 ppb to 100%.

Table A6: Predicted Relative Standard Deviation of Reproducibility ($PRSD_R$). This table provides the calculated $PRSD_R$ using the Horwitz formula:

$$PRSD_R = 2C^{-0.15}$$

where C is expressed as a mass fraction.

Table A7: POD and Number of Test Portions. This table provides the calculated probability of detection (POD) for given sample sizes and events (detections). A method developer can use this table to determine the number of analyses required to obtain a specific POD.

Informative annexes.—The SMPR Guidelines contain informative annexes on the topics of classification of methods, POD model, HorRat values, reference materials, and method accuracy and review. As with the informative tables, these annexes are intended to provide guidance and information to the working groups.

Initiation of an SMPR

See Figure 1 for a schematic flowchart diagram of the SMPR development process.

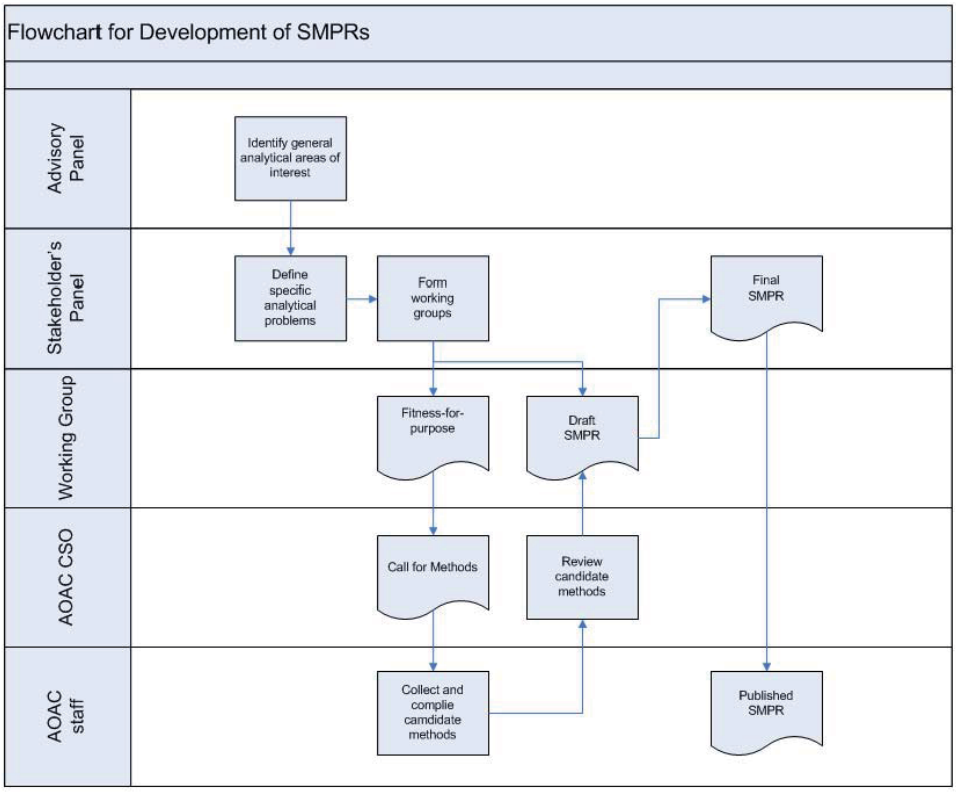


Figure 1. Schematic flowchart diagram of the SMPR development process.

Advisory panels.—Most commonly, an SMPR is created in response to an analytical need identified by an advisory panel. Advisory panels normally consist of sponsors and key stakeholders who have organized to address analytical problems. Usually, the advisory panel identifies general analytical problems, such as the need to update analytical methods for determination of nutrients in infant formula. An advisory panel, with the input of appropriate subject matter experts, also prioritizes the specific analytical problems within the general topic. This panel is critical in planning for the stakeholder panel meeting.

Stakeholder panels.—After an advisory panel has identified a general analytical problem, AOAC announces the standards development activity, identifies stakeholders, and organizes a stakeholder panel. Membership on a stakeholder panel is open to anyone materially affected by the proposed standard. AOAC recruits scientists to participate on stakeholder panels on the basis of their expertise with the analytical problem identified by the advisory panel. Experts are recruited from academia, government, nongovernmental organizations (such as ISO), industry, contract research organizations, method developers, and instrument/equipment manufacturers. AOAC employs a representative voting panel model to ensure balance with regards to stakeholder perspective, and to ensure that no particular stakeholder perspective dominates the proceedings of the stakeholder panel. All stakeholder candidates are reviewed by the AOAC Chief Scientific Officer (CSO) for relevant qualifications, and again by the Official Methods Board to ensure that the stakeholder panel is balanced and all stakeholders are fairly represented.

Stakeholder panels are extremely important as they serve several functions: (*1*) identify specific analytical topics within the general analytical problem described by the advisory panel; (*2*) form working groups to address the specific analytical topics; (*3*) identify additional subject matter experts needed for the working groups; (*4*) provide oversight of the SMPR development; and (*5*) formally adopt SMPRs originally drafted by working groups.

Working groups.—Working groups are formed by the stakeholder panel when a specific analytical topic has been identified. The primary purpose of a working group is to draft an SMPR. Working groups may also be formed to make general recommendations, such as developing a common definition to be used by multiple working groups. For example, SPIFAN formed a working group to create a definition for "infant formula" that could be shared and used by all of the SPIFAN working groups.

The process of drafting an SMPR usually requires several months, and several meetings and conference calls. An SMPR drafted by a working group is presented to a stakeholder panel. A stakeholder panel may revise, amend, or adopt a proposed SMPR on behalf of AOAC.

Fitness-for-Purpose Statement and Call for Methods

One of the first steps in organizing a project is creating a fitness-for-purpose statement. In AOAC, the fitness-for-purpose statement is a very general description of the methods needed. It is the responsibility of a working group chair to draft a fitness-for-purpose statement. A working group chair is also asked to prepare a presentation with background information about the analyte, matrix, and the nature of the analytical problem. A working group chair presents the background information and proposes a draft fitness-for-purpose statement to the presiding stakeholder panel. The stakeholder panel is asked to endorse the fitness-for-purpose statement.

The AOAC CSO prepares a call for methods based on the stakeholder panel-approved fitness-for-purpose statement. The call for methods is posted on the AOAC website and/or e-mailed to the AOAC membership and other known interested parties. AOAC staff collects and compiles candidate methods submitted in response to the call for methods. The CSO reviews and categorizes the methods.

Creating an SMPR

Starting the process of developing an SMPR can be a daunting challenge. In fact, drafting an SMPR should be a daunting challenge because the advisory panel has specifically identified an analytical problem that has yet to be resolved. Completing an SMPR can be a very rewarding experience because working group members will have worked with their colleagues through a tangle of problems and reached a consensus where before there were only questions.

It is advisable to have some representative candidate methods available for reference when a working group starts to develop an SMPR. These methods may have been submitted in response to the call for methods, or may be known to a working group member. In any case, whatever the origin of the method, candidate methods may assist working group members to determine reasonable performance requirements to be specified in the SMPR. The performance capabilities of exisiting analytical methodologies is a common question facing a working group.

Normally, a working chair and/or the AOAC CSO prepares a draft SMPR. A draft SMPR greatly facilitates the process and provides the working group with a structure from which to work.

Working group members are advised to first consider the "intended use" and "maximum time-to-determination" sections as this will greatly affect expectations for candidate methods. For example, methods intended to be used for surveillance probably need to be quick but do not require a great deal of precision, and false-positive results might be more tolerable. Whereas methods intended to be used for dispute resolution will require better accuracy, precision, and reproducibility, but time to determination is not as important.

Once a working group has agreed on the intended use of candidate methods, then it can begin to define the applicability of candidate methods. The applicability section of the SMPR is one of the most important, and sometimes most difficult, sections of the SMPR. The analyte(s) and matrixes must be explicitly identified. For chemical analytes, International Union of Pure and Applied Chemistry (IUPAC) nomenclature and/or Chemical Abstracts Service (CAS) registry numbers should be specified. Matrixes should be clearly identified including the form of the matrix such as raw, cooked, tablets, powders, etc. The nature of the matrix may affect the specific analyte. It may be advantageous to fully identify and describe the matrix before determining the specific analyte(s). It is not uncommon for working groups to revise the initial definition of the analyte(s) after the matrix(es) has been better defined.

Table 1. Example of method performance table for a single analyte

Analytical range	7.0–382.6 µg/mL	
Limit of quantitation (LOQ)	≤7.0 µg/mL	
Repeatability (RSD_r)	<10 µg/mL	≤8%
	≥10 µg/mL	≤6%

Table 2. Example of method performance table for multiple analytes

	Analyte 1		Analyte 2		Analyte 3	
Analytical range	10–20 µg/mL		100–200 µg/mL		200–500 µg/mL	
Limit of quantitation (LOQ)	≤10 µg/mL		≤100 µg/mL		≤200 µg/mL	
Repeatability (RSD_r)	<10 µg/mL	≤8%	<10 µg/mL	≤8%	<200 µg/mL	≤10%
	≥10 µg/mL	≤6%	≥10 µg/mL	≤6%	≥200 µg/mL	≤8%

For projects with multiple analytes, for example, vitamins A, D, E, and K in infant formula, it may be useful to organize a separate working group to fully describe the matrix(es) so that a common description of the matrix(es) can be applied to all of the analytes.

For single analyte SMPRs, it is most common to organize the method performance requirements into a table with 2–3 columns as illustrated in Table 1. For multiple analyte SMPRs, it is often convenient to present the requirements in an expanded table with analytes forming additional columns as illustrated in Table 2.

Once the intended use, analytical techniques, and method performance requirements have been determined, then a working group can proceed to consider the quality control parameters, such as the minimum validation requirements, system suitability procedures, and reference materials (if available). It is not uncommon that an appropriate reference material is not available. *Annex F* of the SMPR Guidelines provides comprehensive guidance for the development and use of in-house reference materials.

Most working groups are able to prepare a consensus SMPR in about 3 months.

Open Comment Period

Once a working group has produced a draft standard, AOAC opens a comment period for the standard. The comment period provides an opportunity for other stakeholders to state their perspective on the draft SMPR. All collected comments are reviewed by the AOAC CSO and the working group chair, and the comments are reconciled. If there are significant changes required to the draft standard as a result of the comments, the working group is convened to discuss and any unresolved issues will be presented for discussion at the stakeholder panel meeting.

Submission of Draft SMPRs to the Stakeholder Panel

Stakeholder panels meet several times a year at various locations. The working group chair (or designee) presents a draft SMPR to the stakeholder panel for review and discussion. A working group chair is expected to be able to explain the conclusions of the working group, discuss comments received, and to answer questions from the stakeholder panel. The members of the stakeholder panel may revise, amend, approve, or defer a decision on the proposed SMPR. A super majority of 2/3 or more of those voting is required to adopt an SMPR as an AOAC voluntary consensus standard.

Publication

Adopted SMPRs are prepared for publication by AOAC staff, and are published in the *Journal of AOAC INTERNATIONAL* and in the AOAC *Official Methods of Analysis*℠ compendium. Often, the AOAC CSO and working group chair prepare a companion article to introduce an SMPR and describe the analytical issues considered and resolved by the SMPR. An SMPR is usually published within 6 months of adoption.

Conclusion

SMPRs are a unique and novel concept for the analytical methods community. SMPRs are voluntary, consensus standards developed by stakeholders that prescribe the minimum analytical performance requirements for classes of analytical methods. The SMPR Guidelines provide a structure for working groups to use as they develop an SMPR. The guidelines have been employed in several AOAC projects and have been proven to be very useful. The guidelines are not a statute that users must conform to; they are a "living" document that is regularly updated, so users should check the AOAC website for the latest version before using the guidelines.

References

(1) Eurachem, *The Fitness for Purpose of Analytical Methods: A Laboratory Guide to Method Validation and Related Topics, Validation*, http://www.eurachem.org/guides/pdf/valid.pdf, posted December 1998, accessed March 2012

(2) *Guidelines for Collaborative Study Procedures to Validate Characteristics of a Method of Analysis* (2012) *Official Methods of Analysis, Appendix D*, AOAC INTERNATIONAL, Gaithersburg, MD

(3) *AOAC INTERNATIONAL Methods Committee Guidelines for Validation of Biological Threat Agent Methods and/or Procedures* (2012) *Official Methods of Analysis,* 19th Ed., *Appendix I, Calculation of CPOD and dCPOD Values from Qualitative Method Collaborative Study Data*, AOAC INTERNATIONAL, Gaithersburg, MD

(4) *AOAC Guidelines for Single-Laboratory Validation of Chemical Methods for Dietary Supplements and Botanicals* (2012) *Official Methods of Analysis*, 19th Ed., *Appendix K*, AOAC INTERNATIONAL, Gaithersburg, MD

(5) Codex Alimentarius Codex Procedure Manual

(6) International Organization for Standardization, Geneva, Switzlerland

ANNEX A
Format of a
Standard Method Performance Requirement

AOAC SMPR YYYY.XXX
(YYYY = Year; XXX = sequential identification number)

Method Name: Must include the analyte(s), matrix(es), and analytical technique [unless the standard method performance requirement (SMPR) is truly intended to be independent of the analytical technology]. The method name may refer to a "common" name (e.g., "Kjeldahl" method).

Approved By: Name of stakeholder panel or expert review panel

Final Version Date: Date

Effective Date: Date

1. Intended Use: Additional information about the method and conditions for use.

2. Applicability: List matrixes if more than one. Provide details on matrix such as specific species for biological analytes, or International Union of Pure and Applied Chemistry (IUPAC) nomenclature and Chemical Abstracts Service (CAS) registry number for chemical analytes. Specify the form of the matrix such as raw, cooked, tablets, powders, etc.

3. Analytical Technique: Provide a detailed description of the analytical technique if the SMPR is to apply to a specific analytical technique; or state that the SMPR applies to any method that meets the method performance requirements.

4. Definitions: List and define terms used in the performance parameter table (*see* Table A2 for list of standard terms).

5. Method Performance Requirements: List the performance parameters and acceptance criteria appropriate for each method/analyte/matrix. *See* Table A1 for appropriate performance requirements.

If more than one analyte/matrix, and if acceptance criteria differ for analyte/matrix combinations then organize a table listing each analyte/matrix combination and its minimum acceptance criteria for each performance criteria.

6. System Suitability Tests and/or Analytical Quality Control: Describe minimum system controls and QC procedures.

7. Reference Material(s): Identify the appropriate reference materials if they exist, or state that reference materials are not available. Refer to *Annex E* (*AOAC Method Accuracy Review*) for instructions on the use of reference materials in evaluations.

8. Validation Guidance: Recommendations for type of evaluation or validation program such as single-laboratory validation (SLV), *Official Methods of Analysis*℠ (OMA), or *Performance Tested Methods*℠ (PTM).

9. Maximum Time-to-Determination: Maximum allowable time to complete an analysis starting from the test portion preparation to final determination or measurement.

Annex I: Inclusivity/Selectivity Panel. Recommended for qualitative and identification method SMPRs.

Annex II: Exclusivity/Cross-Reactivity Panel. Recommended for qualitative and identification method SMPRs.

Annex III: Environmental Materials Panel. Recommended for qualitative and identification method SMPRs.

Table A1. Performance requirements

Classifications of methods[a]				
Quantitative method		Qualitative method		
Main component[b]	Trace or contaminant[c]	Main component[b]	Trace or contaminant[c]	Identification method
Parameter				
Single-laboratory validation				
Applicable range	Applicable range	Inclusivity/selectivity	Inclusivity/selectivity	Inclusivity/selectivity
Bias[d]	Bias[d]	Exclusivity/cross-reactivity	Exclusivity/cross-reactivity	Exclusivity/cross-reactivity
Precision	Precision	Environmental interference	Environmental interference	Environmental interference
Recovery	Recovery	Laboratory variance	Laboratory variance	
Limit of quantitation (LOQ)	LOQ			
		Probability of detection (POD)[e]	POD at AMDL[f]	Probability of identification (POI)
Reproducibility				
RSD_R or target measurement uncertainty	RSD_R or target measurement uncertainty	POD (0)	POD (0)	POI (c)
		POD (c)	POD (c)	
		Laboratory POD[g]	Laboratory POD[g]	Laboratory POI

[a] *See Annex B* for additional information on classification of methods.

[b] ≥100 g/kg.

[c] <100 g/kg.

[d] If a reference material is available.

[e] At a critical level.

[f] AMDL = Acceptable minimum detection level.

[g] LPOD = CPOD.

Table A2. Recommended definitions

Bias	Difference between the expectation of the test results and an accepted reference value. Bias is the total systematic error as contrasted to random error. There may be one or more systematic error components contributing to the bias.
Environmental interference	Ability of the assay to detect target organism in the presence of environmental substances and to be free of cross reaction from environmental substances.
Exclusivity	Strains or isolates or variants of the target agent(s) that the method must not detect.
Inclusivity	Strains or isolates or variants of the target agent(s) that the method can detect.
Laboratory probability of detection (POD)	Overall fractional response (mean POD = CPOD) for the method calculated from the pooled POD_j responses of the individual laboratories (j = 1, 2, ..., L).[a] *See Annex C*.
Limit of quantitation (LOQ)	Minimum concentration or mass of analyte in a given matrix that can be reported as a quantitative result.
POD (0)	Probability of the method giving a (+) response when the sample is truly without analyte.
POD (c)	Probability of the method giving a (–) response when the sample is truly without analyte.
POD	Proportion of positive analytical outcomes for a qualitative method for a given matrix at a given analyte level or concentration. Consult *Annex C* for a full explanation.
Probability of identification (POI)	Expected or observed fraction of test portions at a given concentration that gives positive result when tested at a given concentration. Consult *Probability of Identification (POI): A Statistical Model for the Validation of Qualitative Botanical Identification Methods*.[c]
Precision (repeatability)	Closeness of agreement between independent test results obtained under stipulated conditions. The measure of precision is usually expressed in terms of imprecision and computed as a standard deviation of the test results.[d]
Recovery	Fraction or percentage of the analyte that is recovered when the test sample is analyzed using the entire method. There are two types of recovery: (*1*) Total recovery based on recovery of the native plus added analyte, and (*2*) marginal recovery based only on the added analyte (the native analyte is subtracted from both the numerator and denominator).[e]
Repeatability	Precision under repeatability conditions.
Repeatability conditions	Conditions where independent test results are obtained with the same method on identical test items in the same laboratory by the same operator using the same equipment within short intervals of time.
Reproducibility	Precision under reproducibility conditions.
Reproducibility conditions	Conditions where independent test results are obtained with the same method on identical test items in different laboratories with different operators using different equipment.
Relative standard deviation (RSD)	$RSD = s_i \times 100/\bar{x}$
Standard deviation (s_i)	$s_i = [\Sigma(x_i - \bar{x})^2/n]^{0.5}$

[a] *AOAC INTERNATIONAL Methods Committee Guidelines for Validation of Biological Threat Agent Methods and/or Procedures* (*Calculation of CPOD and dCPOD Values from Qualitative Method Collaborative Study Data*), *J. AOAC Int*. **94**, 1359(2011) and *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., *Appendix I*.

[b] *International Vocabulary of Metrology (VIM)—Basic and General Concepts and Associated Terms* (2008) JCGM 200:2008, Joint Committee for Guides in Metrology (JCGM), www.bipm.org

[c] LaBudde, R.A., & Harnly, J.M. (2012) *J. AOAC Int*. **95**, 273–285.

[d] ISO 5725-1-1994.

[e] *Official Methods of Analysis* (2012) *Appendix D* (*Guidelines for Collaborative Study Procedures to Validate Characteristics of a Method of Analysis*), AOAC INTERNATIONAL, Gaithersburg, MD.

Table A3. Recommendations for evaluation

Bias (if a reference material is available)	A minimum of five replicate analyses of a Certified Reference Material.[a]
Environmental interference	Analyze test portions containing a specified concentration of one environmental materials panel member. Materials may be pooled. Consult with AOAC statistician.
Exclusivity/cross-reactivity	Analyze one test portion containing a specified concentration of one exclusivity panel member. More replicates can be used. Consult with AOAC statistician.
Inclusivity/selectivity	Analyze one test portion containing a specified concentration of one inclusivity panel member. More replicates can be used. Consult with AOAC statistician.
Limit of quantitation (LOQ)	Estimate the LOQ = average (blank) + 10 × s_0 (blank). Measure blank samples with analyte at the estimated LOQ. Calculate the mean average and standard deviation of the results. Guidance[b]: For ML ≥ 100 ppm (0.1 mg/kg): LOD = ML × 1/5. For ML < 100 ppm (0.1 mg/kg): LOD = ML × 2/5.
Measurement uncertainty	Use ISO 21748: *Guidance for the use of repeatability, reproducibility, and trueness estimates in measurement uncertainty estimation to analyze data collected for bias, repeatability, and intermediate precision to estimate measurement uncertainty*.
POD(0)	Use data from collaborative study.
POD (c)	
Repeatability	Prepare and homogenize three unknown samples at different concentrations to represent the full, claimed range of the method. Analyze each unknown sample by the candidate method seven times, beginning each analysis from weighing out the test portion through to final result with no additional replication (unless stated to do so in the method). All of the analyses for one unknown sample should be performed within as short a period of time as is allowed by the method. The second and third unknowns may be analyzed in another short time period. Repeat for each claimed matrix.
Probability of detection (POD)	Determine the desired POD at a critical concentration. Consult with Table A7 to determine the number of test portions required to demonstrate the desired POD.
Probability of identification (POI)	Consult *Probability of Identification (POI): A Statistical Model for the Validation of Qualitative Botanical Identification Methods*[c].
Recovery	Determined from spiked blanks or samples with at least seven independent analyses per concentration level at a minimum of three concentration levels covering the analytical range. Independent means at least at different times. If no confirmed (natural) blank is available, the average inherent (naturally containing) level of the analyte should be determined on at least seven independent replicates. Marginal % recovery = $(C_f - C_u) \times 100/C_A$ Total % recovery = $100(C_f)/(C_u + C_A)$ where C_f = concentration of fortified samples, C_u = concentration of unfortified samples, and C_A = concentration of analyte added to the test sample.[d] Usually total recovery is used unless the native analyte is present in amounts greater than about 10% of the amount added, in which case use the method of addition.[e]
Reproducibility (collaborative or interlaboratory study)	Quantitative methods: Recruit 10–12 collaborators; must have eight valid data sets; two blind duplicate replicates at five concentrations for each analyte/matrix combination to each collaborator.
	Qualitative methods: Recruit 12–15 collaborators; must have 10 valid data sets; six replicates at five concentrations for each analyte/matrix combination to each collaborator.

[a] *Guidance for Industry for Bioanalytical Method Validation* (May 2001) U.S. Department of Health and Human Services, U.S. Food and Drug Administration, Center for Drug Evaluation and Research (CDER), Center for Veterinary Medicine (CVM).

[b] Codex Alimentarius Codex Procedure Manual.

[c] LaBudde, R.A., & Harnly, J.M. (2012) *J. AOAC Int.* **95**, 273–285.

[d] *Guidelines for Collaborative Study Procedures to Validate Characteristics of a Method of Analysis* (2012) *Official Methods of Analysis*, 19th Ed., *Appendix D,* AOAC INTERNATIONAL, Gaithersburg, MD.

[e] *AOAC Guidelines for Single-Laboratory Validation of Chemical Methods for Dietary Supplements and Botanicals* (2012) *Official Methods of Analysis*, 19th Ed., *Appendix K*, AOAC INTERNATIONAL, Gaithersburg, MD.

Table A4. Expected precision (repeatability) as a function of analyte concentration[a]

Analyte, %	Analyte ratio	Unit	RSD, %
100	1	100%	1.3
10	10^{-1}	10%	1.9
1	10^{-2}	1%	2.7
0.01	10^{-3}	0.1%	3.7
0.001	10^{-4}	100 ppm (mg/kg)	5.3
0.0001	10^{-5}	10 ppm (mg/kg)	7.3
0.00001	10^{-6}	1 ppm (mg/kg)	11
0.000001	10^{-7}	100 ppb (µg/kg)	15
0.0000001	10^{-8}	10 ppb (µg/kg)	21
0.00000001	10^{-9}	1 ppb (µg/kg)	30

[a] Table excerpted from *AOAC Peer-Verified Methods Program, Manual on Policies and Procedures* (1998) AOAC INTERNATIONAL, Gaithersburg, MD.

The precision of a method is the closeness of agreement between independent test results obtained under stipulated conditions. Precision is usually expressed in terms of imprecision and computed as a relative standard deviation of the test results. The imprecision of a method increases as the concentration of the analyte decreases. This table provides targets RSDs for a range of analyte concentrations.

Table A5. Expected recovery as a function of analyte concentration[a]

Analyte, %	Analyte ratio	Unit	Mean recovery, %
100	1	100%	98–102
10	10^{-1}	10%	98–102
1	10^{-2}	1%	97–103
0.01	10^{-3}	0.1%	95–105
0.001	10^{-4}	100 ppm	90–107
0.0001	10^{-5}	10 ppm	80–110
0.00001	10^{-6}	1 ppm	80–110
0.000001	10^{-7}	100 ppb	80–110
0.0000001	10^{-8}	10 ppb	60–115
0.00000001	10^{-9}	1 ppb	40–120

[a] Table excerpted from *AOAC Peer-Verified Methods Program, Manual on Policies and Procedures* (1998) AOAC INTERNATIONAL, Gaithersburg, MD.

Recovery is defined as the ratio of the observed mean test result to the true value. The range of the acceptable mean recovery expands as the concentration of the analyte decreases. This table provides target mean recovery ranges for analyte concentrations from 100% to 1 ppb.

Table A6. Predicted relative standard deviation of reproducibility ($PRSD_R$)[a]

Concentration (C)	Mass fraction (C)	$PRSD_R$, %
100%	1.0	2
1%	0.01	4
0.01%	0.0001	8
1 ppm	0.000001	16
10 ppb	0.00000001	32
1 ppb	0.000000001	45

[a] Table excerpted from *Definitions and Calculations of HorRat Values from Intralaboratory Data*, HorRat for SLV.doc, 2004-01-18, AOAC INTERNATIONAL, Gaithersburg, MD.

Predicted relative standard deviation = $PRSD_R$. Reproducibility relative standard deviation calculated from the Horwitz formula:

$$PRSD_R = 2C^{-0.15}, \text{ where C is expressed as a mass fraction}$$

This table provides the calculated $PRSD_R$ for a range of concentrations. *See Annex D* for additional information.

Table A7. POD and number of test portions[a,b]

	Sample size required for proportion						
Assume	1. Binary outcome (occur/not occur). 2. Constant probability rho of event occurring. 3. Independent trials (e.g., simple random sample). 4. Fixed number of trials (*N*)						
Inference	95% Confidence interval lies entirely at or above specified minimum rho						
Desired	Sample size *N* needed						
Minimum probability rho, %	Sample size (*N*)	Minimum No. events (*x*)	Maximum No. nonevents (*y*)	1-Sided lower confidence limit on rho[c], %	Expected lower confidence limit on rho, %	Expected upper confidence limit on rho, %	Effective AOQL[d] rho, %
50	3	3	0	52.6	43.8	100.0	71.9
50	10	8	2	54.1	49.0	94.3	71.7
50	20	14	6	51.6	48.1	85.5	66.8
50	40	26	14	52.0	49.5	77.9	63.7
50	80	48	32	50.8	49.0	70.0	59.5
55	4	4	0	59.7	51.0	100.0	75.5
55	10	9	1	65.2	59.6	100.0	79.8
55	20	15	5	56.8	53.1	88.8	71.0
55	40	28	12	57.1	54.6	81.9	68.2
55	80	52	28	55.9	54.1	74.5	64.3
60	5	5	0	64.9	56.5	100.0	78.3
60	10	9	1	65.2	59.6	100.0	79.8
60	20	16	4	62.2	58.4	91.9	75.2
60	40	30	10	62.4	59.8	85.8	72.8
60	80	56	24	61.0	59.2	78.9	69.1
65	6	6	0	68.9	61.0	100.0	80.5
65	10	9	1	65.2	59.6	100.0	79.8
65	20	17	3	67.8	64.0	94.8	79.4
65	40	31	9	65.1	62.5	87.7	75.1
65	80	59	21	65.0	63.2	82.1	72.7
70	7	7	0	72.1	64.6	100.0	82.3
70	10	10	0	78.7	72.2	100.0	86.1
70	20	18	2	73.8	69.9	97.2	83.6
70	40	33	7	70.7	68.0	91.3	79.7
70	80	63	17	70.4	68.6	86.3	77.4
75	9	9	0	76.9	70.1	100.0	85.0
75	10	10	0	78.7	72.2	100.0	86.1
75	20	19	1	80.4	76.4	100.0	88.2
75	40	35	5	76.5	73.9	94.5	84.2
75	80	67	13	75.9	74.2	90.3	82.2
80	11	11	0	80.3	74.1	100.0	87.1
80	20	19	1	80.4	76.4	100.0	88.2
80	40	37	3	82.7	80.1	97.4	88.8
80	80	70	10	80.2	78.5	93.1	85.8
85	20	20	0	88.1	83.9	100.0	91.9
85	40	38	2	86.0	83.5	98.6	91.1
85	80	74	6	86.1	84.6	96.5	90.6
90	40	40	0	93.7	91.2	100.0	95.6
90	60	58	2	90.4	88.6	99.1	93.9
90	80	77	3	91.0	89.5	98.7	94.1
95	60	60	0	95.7	94.0	100.0	97.0
95	80	80	0	96.7	95.4	100.0	97.7
95	90	89	1	95.2	94.0	100.0	97.0
95	96	95	1	95.5	94.3	100.0	97.2
98	130	130	0	98.0	97.1	100.0	98.6
98	240	239	1	98.2	97.7	100.0	98.8
99	280	280	0	99.0	98.6	100.0	99.3
99	480	479	1	99.1	98.8	100.0	99.4

[a] Table excerpted from Technical Report TR308, *Sampling plans to verify the proportion of an event exceeds or falls below a specified value*, LaBudde, R. (June 4, 2010) (not published). The table was produced as part of an informative report for the Working Group for Validation of Identity Methods for Botanical Raw Materials commissioned by the AOAC INTERNATIONAL Presidential Task Force on Dietary Supplements. The project was funded by the Office of Dietary Supplements, National Institutes of Health.

[b]

[c] Based on modified Wilson score 1-sided confidence interval.

[d] AOQL = Average outgoing quality level.

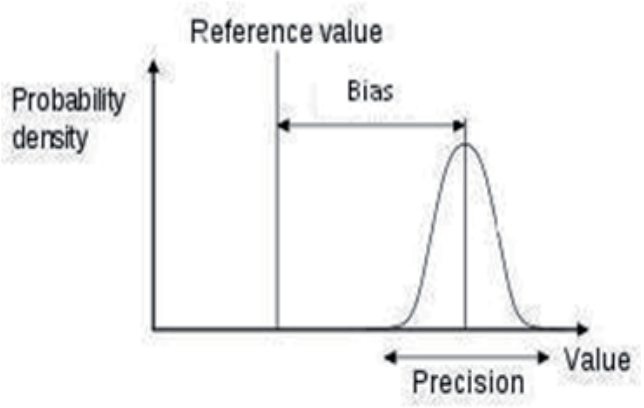


Figure A1. Relationship between precision versus bias (trueness). Trueness is reported as bias. Bias is defined as the difference between the test results and an accepted reference value.

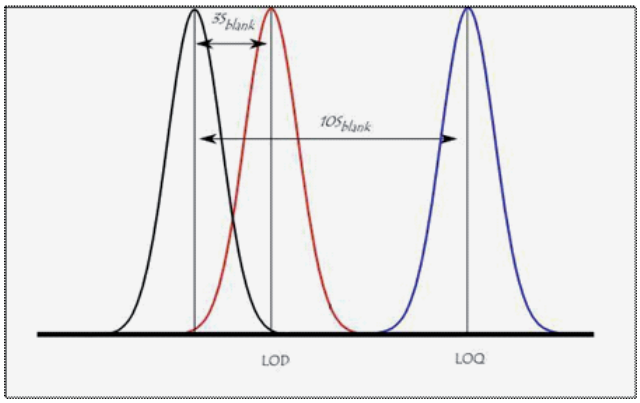


Figure A2. Relationship between LOD and LOQ. LOD is defined as the lowest quantity of a substance that can be distinguished from the absence of that substance (a blank value) within a stated confidence limit. LOQ is the level above which quantitative results may be obtained with a stated degree of confidence.

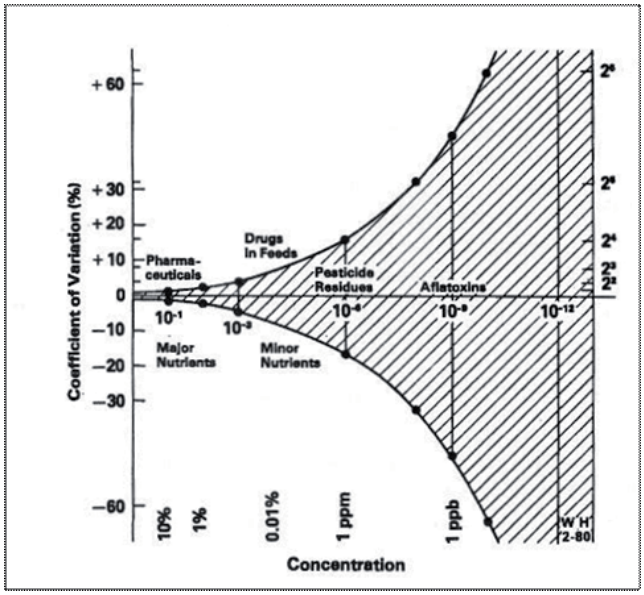


Figure A3. Horwitz Curve, illustrating the exponential increase in the coefficient of variation as the concentration of the analyte decreases [*J. AOAC Int*. 89, 1095(2006)].

ANNEX B
Classification of Methods

The following guidance may be used to determine which performance parameters in Table A1 apply to different classifications of methods. AOAC INTERNATIONAL does not recognize the term "semiquantitative" as a method classification. Methods that have been self-identified as semiquantitative will be classified into one of the following five types:

Type I: Quantitative Methods

Characteristics: Generates a continuous number as a result.

Recommendation: Use performance requirements specified for quantitative method (main or trace component). Use recovery range and maximum precision variation in Tables A4 and A5.

In some cases and for some purposes, methods with less accuracy and precision than recommended in Tables A4 and A5 may be acceptable. Method developers should consult with the appropriate method committee to determine if the recommendations in Tables A4 and A5 do or do not apply to their method.

Type II: Methods that Report Ranges

Characteristics: Generates a "range" indicator such as 0, low, moderate, and high.

Recommendation: Use performance requirements specified for qualitative methods (main component). Specify a range of POD for each range "range" indicator.

Type III: Methods with Cutoff Values

Characteristics: Method may generate a continuous number as an interim result (such as a CT value for a PCR method), which is not reported but converted to a qualitative result (presence/ absence) with the use of a cutoff value.

Recommendation: Use performance requirements specified for qualitative methods.

Type IV: Qualitative Methods

Characteristics: Method of analysis whose response is either the presence or absence of the analyte detected either directly or indirectly in a specified test portion.

Recommendation: Use performance requirements specified for qualitative methods.

Type V: Identification Methods

Characteristics: Method of analysis whose purpose is to determine the identity of an analyte.

Recommendation: Use performance requirements specified for identification methods.

ANNEX C
Understanding the POD Model

Excerpted from AOAC INTERNATIONAL Methods Committee Guidelines for Validation of Biological Threat Agent Methods and/or Procedures, J. AOAC Int. ***94****, 1359(2011) and Official Methods of Analysis of AOAC INTERNATIONAL (2012) 19th Ed., Appendix I.*

The Probability of Detection (POD) model is a way of characterizing the performance of a qualitative (binary) method. A binary qualitative method is one that gives a result as one of two possible outcomes, either positive or negative, presence/absence, or +/–.

The single parameter of interest is the POD, which is defined as the probability at a given concentration of obtaining a positive response by the detection method. POD is assumed to be dependent on concentration, and generally, the probability of a positive response will increase as concentration increases.

For example, at very low concentration, the expectation is that the method will not be sensitive to the analyte, and at very high concentration, a high probability of obtaining a positive response is desired. The goal of method validation is to characterize how method response transitions from low concentration/low response to high concentration/high response.

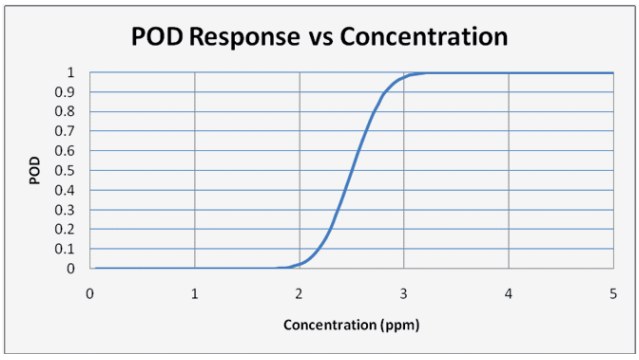


Figure C1. Theoretical POD curve for a qualitative detection method.

POD is always considered to be dependent upon analyte concentration. The POD curve is a graphical representation of method performance, where the probability is plotted as a function of concentration (*see*, for example, Figure C1).

The POD model is designed to allow an objective description of method response without consideration to an a priori expectation of the probabilities at given concentrations. The model is general enough to allow comparisons to any theoretical probability function.

The POD model is also designed to allow for an independent description of method response without consideration to the response of a reference method. The model is general enough to allow for comparisons between reference and candidate method responses, if desired.

Older validation models have used the terms "sensitivity," "specificity," "false positive," and "false negative" to describe method performance. The POD model incorporates all of the performance concepts of these systems into a single parameter, POD.

For example, false positive has been defined by some models as the probability of a positive response, given the sample is truly negative (concentration = 0). The equivalent point on the POD curve for this performance characteristic is the value of the curve at Conc = 0.

Similarly, false negative has sometimes been defined as the probability of a negative response when the sample is truly positive (concentration >0). In the POD curve, this would always be specific to a given sample concentration, but would be represented as the distance from the POD curve to the POD = 1 horizontal top axis at all concentrations except C = 0.

The POD model incorporates all these method characteristics into a single parameter, which is always assumed to vary by concentration. In other models, the terms "false positive," "false negative," "sensitivity," and "specificity" have been defined in a variety of ways, usually not conditional on concentration. For these reasons, these terms are obsolete under this model (*see* Table C1).

The terms "sensitivity," "specificity," "false positive," and "false negative" are obsolete under the POD model (*see* Figure C2).

Table C1. Terminology

Traditional terminology	Concept	POD equivalent	Comment
False positive	Probability of the method giving a (+) response when the sample is truly without analyte	POD(0) POD at conc = 0	POD curve value at conc = 0; "*Y*-intercept" of the POD curve
Specificity	Probability of the method giving a (-) response when the sample is truly without analyte	1-POD(0)	Distance along the POD axis from POD = 1 to the POD curve value
False negative (at a given concentration)	Probability of a (–) response at a given concentration	1-POD(c)	Distance from the POD curve to the POD = 1 "top axis" in the vertical direction
Sensitivity (at a given concentration)	Probability of a (+) response at a given concentration	POD(c)	Value of the POD curve at any given concentration
True negative	A sample that contains no analyte	C = 0	Point on concentration axis where c = 0
True positive	A sample that contains analyte at some positive concentration	C > 0	Range of concentration where c > 0

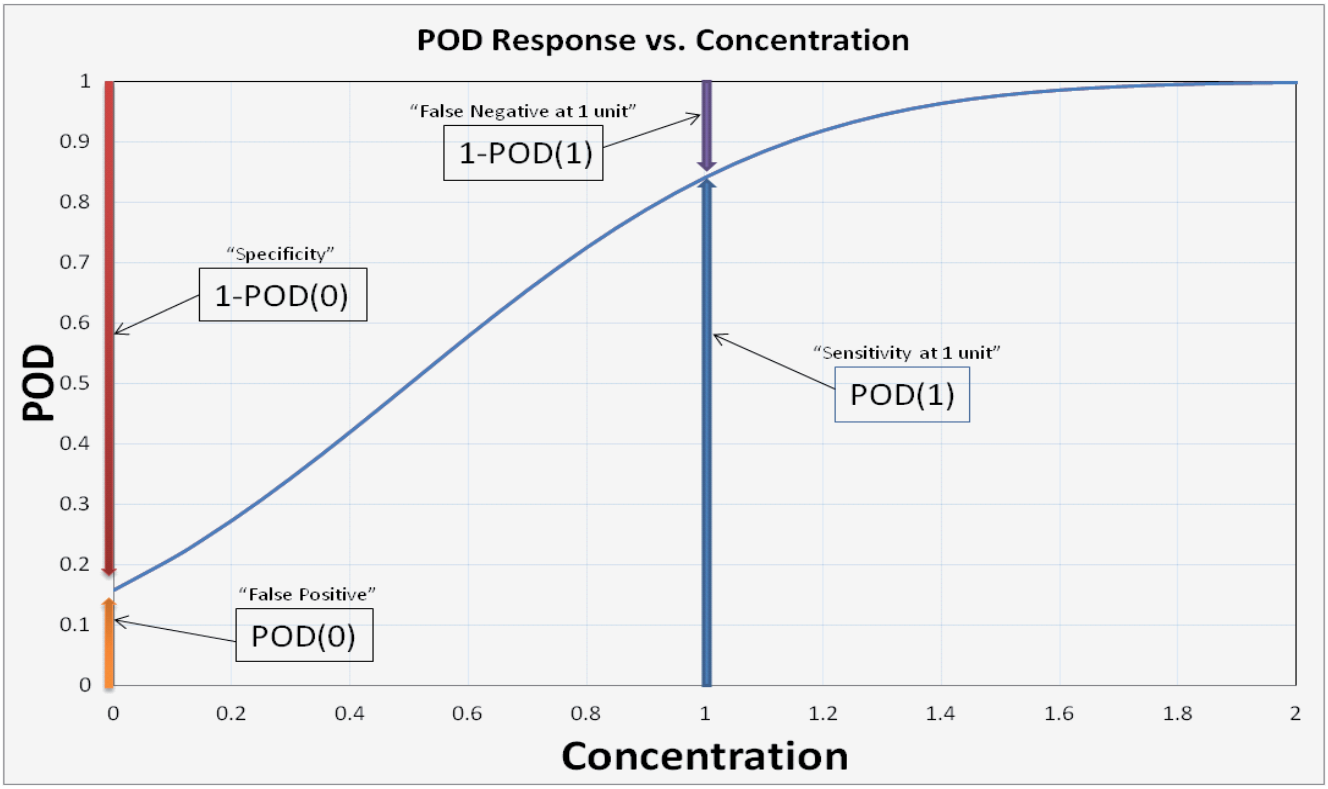


Figure C2. Comparison of POD model terminology to other obsolete terms.

ANNEX D
Definitions and Calculations of HorRat Values from Intralaboratory Data

Excerpted from Definitions and Calculations of HorRat Values from Intralaboratory Data, AOAC INTERNATIONAL, HorRat for SLV.doc, 2004-01-18.

1. Definitions

1.1 Replicate Data

Data developed under common conditions in the same laboratory: simultaneous performance, or, if necessary to obtain sufficient values, same series, same analyst, same day. Such data provides "repeatability statistical parameters."

1.2 Pooled Data

Replicate data developed in the same laboratory under different conditions but considered sufficiently similar that, for the purpose of statistical analysis, they may be considered together. These may include different runs, different instruments, different analysts, and different days.

1.3 Average

0 = Sum of the individual values, x_i, divided by the number of individual values, *n*.

$$0 = (\Sigma\, x_i)/n$$

1.4 Standard Deviation

$$s_i = [\Sigma(x_i - (\bar{x})^2/n]^{0.5}$$

1.5 Relative Standard Deviation

$$RSD = s_i \times 100/\bar{x}$$

1.5.1 Repeatability Relative Standard Deviation [RSD(r) or RSD_r]

The relative standard deviation calculated from within-laboratory data.

1.5.2 Reproducibility Relative Standard Deviation [RSD(R) or RSD_R]

The relative standard deviation calculated from among-laboratory data.

Table D1. Predicted relative standard deviations

Concentration (C)	Mass fraction (C)	$PRSD_R$, %
100%	1.0	2
1%	0.01	4
0.01%	0.0001	8
1 ppm	0.000001	16
10 ppb	0.00000001	32
1 ppb	0.000000001	45

1.6 Mass Fraction

Concentration, C, expressed as a decimal fraction. For calculating and reporting statistical parameters, data may be expressed in any convenient units (e.g., %, ppm, ppb, mg/g, µg/g; µg/kg; µg/L, µg/µL, etc.). For reporting HorRat values, data must be reported as a mass fraction where the units of the numerator and denominator are the same: e.g., for 100% (pure materials), the mass fraction C = 1.00; for 1 µg/g (ppm), C = 0.000001 = (E-6). *See* Table D1 for other examples.

1.7 Predicted Relative Standard Deviation [PRSD(R) or $PRSD_R$]

The reproducibility relative standard deviation calculated from the Horwitz formula:

$$PRSD(R) = 2C^{-0.15}$$

where C is expressed as a mass fraction. *See* Table D1.

In spreadsheet notation: PRSD(R) = 2 * C ^(–0.15).

1.8 HorRat Value

The ratio of the reproducibility relative standard deviation calculated from the data to the PRSD(R) calculated from the Horwitz formula:

$$HorRat = RSD(R)/PRSD(R)$$

To differentiate the usual HorRat value calculated from reproducibility data from the HorRat value calculated from repeatability data, attach an R for the former and an r for the latter. But note that the denominator always uses the PRSD(R) calculated from reproducibility data because this parameter is more predictable than the parameter calculated from repeatability data:

$$HorRat(R) = RSD_R/PRSD(R)$$

$$HorRat(r) = RSD_r/PRSD(R)$$

Some expected, predicted relative standard deviations are given in Table D1.

2 *Acceptable HorRat Values*

2.1 For Interlaboratory Studies

HorRat(R): The original data developed from interlaboratory (among-laboratory) studies assigned a HorRat value of 1.0 with limits of acceptability of 0.5 to 2.0. The corresponding within-laboratory relative standard deviations were found to be typically 1/2 to 2/3 the among-laboratory relative standard deviations.

Table D2. Predicted relative standard deviations

Concentration (C)	$PRSD_R$, %	$PRSD_r$, %
100%	2	1
1%	4	2
0.01%	8	4
1 ppm	16	8
10 ppb	32	16
1 ppb	45	22

2.1.1 Limitations

HorRat values do not apply to method-defined (empirical) analytes (moisture, ash, fiber, carbohydrates by difference, etc.), physical properties or physical methods (pH, viscosity, drained weight, etc.), and ill-defined analytes (polymers, products of enzyme reactions).

2.2 For Intralaboratory Studies

2.2.1 Repeatability

Within-laboratory acceptable predicted target values for repeatability are given in Table D2 at 1/2 of PRSD(R), which represents the best case.

2.2.2 HorRat(r)

Based on experience and for the purpose of exploring the extrapolation of HorRat values to SLV studies, take as the minimum acceptability 1/2 of the lower limit ($0.5 \times 0.5 \approx 0.3$) and as the maximum acceptability 2/3 of the upper limit ($0.67 \times 2.0 \approx 1.3$).

Calculate HorRat(r) from the SLV data:

$$HorRat(r) = RSD(r)/PRSD(R)$$

Acceptable HorRat(r) values are 0.3–1.3. Values at the extremes must be interpreted with caution. With a series of low values, check for unreported averaging or prior knowledge of the analyte content; with a series of high values, check for method deficiencies such as unrestricted times, temperatures, masses, volumes, and concentrations; unrecognized impurities (detergent residues on glassware, peroxides in ether); incomplete extractions and transfers and uncontrolled parameters in specific instrumental techniques.

2.3 Other Limitations and Extrapolations

The HorRat value is a very rough but useful summary of the precision in analytical chemistry. It overestimates the precision at the extremes, predicting more variability than observed at the high end of the scale (C > ca 0.1; i.e., >10%) and at the low end of the scale (C < E-8; i.e., 10 ng/g; 10 ppb).

ANNEX E
AOAC Method Accuracy Review

Accuracy of Method Based on Reference Material

Reference material (RM) used.—The use of RMs should be seen as integral to the process of method development, validation, and performance evaluation. RMs are not the only component of a quality system, but correct use of RMs is essential to appropriate quality management. RMs with or without assigned quantity values can be used for measurement precision control, whereas only RMs with assigned quantity values can be used for calibration or measurement trueness control. Method development and validation for matrices within the scope of the method is done to characterize attributes such as recovery, selectivity, "trueness" (accuracy, bias), precision (repeatability and reproducibility), uncertainty estimation, ruggedness, LOQ or LOD, and dynamic range. RMs should be chosen that are fit-for-purpose. When certified reference materials (CRMs) are available with matrices that match the method scope, much of the work involved in method development has already been completed, and that work is documented through the certificate. RMs with analyte values in the range of test samples, as well as "blank" matrix RMs, with values below or near detection limits, are needed.

Availability of RM.—Consideration needs to be given to the future availability of the chosen RM. Well-documented methods that cannot be verified in the future due to lack of material may lose credibility or be seen as inferior.

Fit to method scope.—Natural matrix CRMs provide the greatest assurance that the method is capable of producing accurate results for that matrix. When selecting an RM to perform a method validation, analysts should consider the method to material fit. An example of a good fit would be a method for specified organic molecules in infant formula and using an infant formula or powder milk RM. A poor fit would be a method for specified organic molecules in infant formula and using a sediment material.

Stability.—Providing a stable RM can be challenging where analytes are biologically active, easily oxidized, or interactive with other components of the matrix. CRM producers provide assurance of material stability, as well as homogeneity.CRMs are accompanied by a certificate that includes the following key criteria:

(*1*) Assigned values with measurement uncertainty and metrological traceability
(*2*) Homogeneity
(*3*) Stability, with the expiration date for the certificate
(*4*) Storage requirements
(*5*) Information on intended use
(*6*) Identity of matrix

For some RMs, such as botanical RMs, the source and/or authenticity can be a very important piece of information that should be included with the certificate. Even under ideal storage conditions, many analytes have some rate of change. Recertification may be done by the supplier, and a certificate reissued with a different expiration date and with certain analyte data updated or removed.

Definition of CRM.—Refer to the AOAC TDRM document for definitions from ISO Guide 30, Amd. 1 (2008), http://www.aoac.org/divisions/References.pdf.

Information on source of RM is available.—It is the responsibility of the material producer to provide reliable authentication of the RM and make a clear statement in the accompanying documentation. This should be an as detailed listing as possible, including handling of ingredients, identification of plant materials as completely as feasible (species, type, subtype, growing region), etc. This is comparable to other required information on an RM for judging its suitability for a specific application purpose (e.g., containing how much of the targeted analyte, stabilized by adding acid—therefore not suited for certain parameters/procedures, etc.).

Separate RM used for calibration and validation.—A single RM cannot be used for both calibration and validation of results in the same measurement procedure.

Blank RM used where appropriate.—Blank matrix RMs are useful for ensuring performance at or near the detection limits. These are particularly useful for routine quality control in methods measuring, for instance, trace levels of allergens, mycotoxins, or drug residues.

Storage requirements were maintained.—Method developers should maintain good documentation showing that the RM producer's recommended storage conditions were followed.

Cost.—The cost of ongoing method checks should be considered. Daily use of CRMs can be cost prohibitive. Monthly or quarterly analysis of these materials may be an option.

Concentration of analyte fits intended method.—Concentration of the analyte of interest is appropriate for standard method performance requirements (SMPRs).

Uncertainty available.—Every measurement result has an uncertainty associated with it, and the individual contributions toward the combined uncertainty arise from multiple sources. Achieving the target measurement uncertainty set by the customer for his/her problem of interest is often one of the criteria used in selecting a method for a given application. Estimation of measurement uncertainty can be accomplished by different approaches, but the use of RMs greatly facilitates this part of a method validation.

Demonstration of Method Accuracy when No Reference Material Is Available

If an RM is not available, how is accuracy demonstrated?

There are many analytes for which a CRM with a suitable matrix is not available. This leaves the analyst with few options. For some methods, there may be proficiency testing programs that include a matrix of interest for the analyte. Proficiency testing allows an analyst to compare results with results from other laboratories, which may or may not be using similar methods. Spiking is another technique that may be used. When alternative methods are available, results may be compared between the different methods. These alternatives do not provide the same level of assurance that is gained through the use of a CRM.

Spike recovery.—In the absence of an available CRM, one technique that is sometimes used for assessing performance is the spiking of a matrix RM with a known quantity of the analyte. When this method is used, it cannot be assumed that the analyte is bound in the same way as it would be in a natural matrix. Nevertheless, a certified blank RM would be the preferred choice for constructing a spiked material.

When preparing reference solutions, the pure standards must be completely soluble in the solvent. For insoluble materials in a liquid suspension or for powdered forms of dry materials, validation is required to demonstrate that the analyte is homogeneously distributed and that the response of the detection system to the analyte is not affected by the matrix or preparation technique. When a matrix material is selected for spiking, it should be reasonably

The document, *AOAC Method Accuracy Review*, was prepared by the AOAC Technical Division on Reference Materials (TDRM) and approved by the AOAC Official Methods Board in June 2012.

characterized to determine that it is sufficiently representative of the matrix of interest. Spiked samples must be carried through all steps of the method. Many analytes are bound in a natural matrix and whether the spiked analyte will behave the same as the analyte in a natural matrix is unknown.

Other.—Use of a substitute RM involves the replacement of the CRM with an alternative matrix RM matching the matrix of interest as close as possible based on technical knowledge.

ANNEX F
Development and Use of In-House Reference Materials

The use of reference materials is a vital part of any analytical quality assurance program. However, you may have questions about their creation and use. The purpose of this document is to help answer many of these questions.

- What is a reference material?
- Why use reference materials?
- What certified reference materials are currently available?
- Why use an in-house reference material?
- How do I create an in-house reference material?
- How do I use the data from an in-house reference material?

What Is a Reference Material?

The International Organization for Standardization (ISO) defines a reference material as a "material or substance one or more of whose property values are sufficiently homogeneous and well established to be used for the calibration of an apparatus, the assessment of a measurement method, or for assigning values to materials" (1). In plain English, natural-matrix reference materials, such as those you might prepare for use in-house, can be used to validate an analytical method or for quality assurance while you're using your method to analyze your samples. (Natural-matrix materials are not generally used as calibrants because of the increased uncertainty that this would add to an analysis.) The assigned values for the target analytes of an in-house reference material can be used to establish the precision of your analytical method and, if used in conjunction with a CRM, to establish the accuracy of your method.

ISO defines a certified reference material (CRM) as a "reference material, accompanied by a certificate, one or more of whose property values are certified by a procedure which establishes traceability to an accurate realization of the unit in which the property values are expressed, and for which each certified value is accompanied by an uncertainty at a stated level of confidence" (1).

Why Use Reference Materials?

Certified reference materials can be used across the entire scope of an analytical method and can provide traceability of results to the International System of Units (SI). During method development, CRMs can be used to optimize your method. During method validation, they can be used to ensure that your method is capable of producing the "right" answer, and to determine how close your result is to that answer. During routine use, they can be used to determine within-day and between-day repeatability, and so demonstrate that your method is in control and is producing accurate results every time it is used.

Natural-matrix reference materials should mimic the real samples that will be analyzed with a method. They should behave just as your samples would during a procedure, so if you obtain accurate and precise values for your reference material, you should obtain accurate and precise values for your samples as well.

What Certified Reference Materials Are Currently Available?

CRMs are available from a number of sources, including (but not limited to):

- American Association of Cereal Chemists (AACC)
- American Oil Chemists Society (AOCS)
- International Atomic Energy Agency (IAEA)
- Institute for Reference Materials and Measurements (IRMM)
- LGC Promochem
- National Institute of Standards and Technology (NIST)
- National Research Council Canada (NRC Canada)
- UK Food Analysis Proficiency Assessment Program (FAPAS)

A number of websites provide general overviews and catalogs of producers' and distributors' reference materials:

http://www.aocs.org/tech/crm/
http://www.comar.bam.de
http://www.erm-crm.org
http://www.iaea.org/oregrammeslaqcs
http://www.aaccnet.org/checksample
http://www.irmm·ire.be/mrm.html
http://www.lgcpromochem.com
http://www.naweb.iaea.org/nahu/nmrm/
http://www.nist.gov/srm
http://www.fapas.com/index. cfm
http://www.virm.net.

Because new reference materials are produced regularly, it is important to check these websites to determine what is currently available.

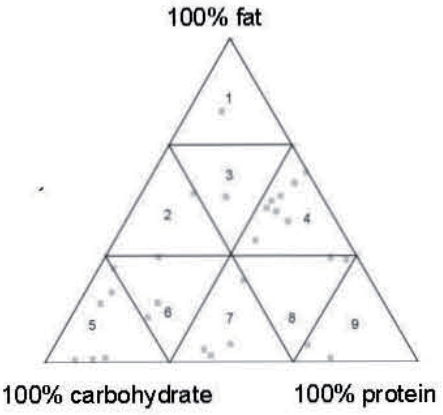
Why Use an In-House Reference Material?

There are many benefits to the use of a CRM. CRMs have been prepared to be homogeneous and, if stored under the proper conditions, stable. You are provided with a certified value as well as the statistical data for theconcentration of your analyte; this is about as close as you can come to knowing the true value of the concentration of the analyte. The material has been tested by experienced analysts in leading laboratories, so you have the security of knowing that your method is generating values similar to those generated in other competent laboratories. The CRMs from the sources mentioned above are nationally and/or internationally recognized, so when you obtain acceptable results for a CRM using your analytical method, you give credibility to your methodology and traceability to your results.

But there are some drawbacks associated with CRMs. Unfortunately, many analyte/matrix combinations are not currently available. When testing food products for nutrient content, for example, a laboratory can be asked to analyze anything that might be found in a kitchen or grocery store. Reference materials that represent all of the types of foods that need to be tested are not available, and most CRMs are certified for a limited number of analytes. It is important to match the reference material matrix to your sample matrix. (Food examples dominate the discussion below, but the same processes apply to the development of in-house RMs in other areas of analytical chemistry.)

To demonstrate the applicability of an analytical method to a wide variety of food matrices, AOAC INTERNATIONAL's Task

Excerpted from *Development and Use of In-House Reference Materials*, Rev. 2, 2009. Copyright 2005 by the AOAC Technical Division on Reference Materials (TDRM).



Force on Methods for Nutrition Labeling developed a triangle partitioned into sectors in which foods are placed based on their protein, fat, and carbohydrate content (2, 3). Since ash does not have a great impact on the performance of an analytical method for organic-material foods, and water can be added or removed, it can be assumed that the behavior of an analytical method is determined to large extent by the relative proportions of these proximates. AOAC INTERNATIONAL anticipated that one or two foods in a given sector would be representative of other foods in that sector and therefore would be useful for method assessment. Similarly, one or two reference materials in a given sector (or near each other in adjacent sectors) should be useful for quality assurance for analyses involving the other foods in the sector. The positions of many of the food-matrix CRMs from the sources listed above are shown in the triangle and are provided in the list.

These food-matrix reference materials are spread through all sectors of the triangle, thereby making it likely that you can find an appropriate CRM to match to your samples. Ultimately, however, the routine use of a CRM can be cost prohibitive, and is not really the purpose of CRMs. For example, in order to use NIST's Standard Reference Material (SRM) 2387 Peanut Butter for all mandatory nutrition labeling analyses, you could buy one sales unit (three jars, each containing 170 g material) for $649 (2009 price). If you charge your customer about $1000 for analysis of all mandatory nutrients in a test material, the control material would account for more than 60% of your fees. Therefore, many laboratories have found it more cost-effective to create in-house reference materials for routine quality control and characterize them in conjunction with the analysis of a CRM (4). You can prepare larger quantities of a reference material by preparing it in-house, and you have more flexibility in the types of matrices you can use. There are not many limitations on what can be purchased.

How Do I Create an In-House Reference Material?

There are basically three steps to preparing an in-house reference material: selection (including consideration of homogeneity and stability), preparation, and characterization. Additional guidance through these steps can be provided from TDRM as well as in ISO Guides 34 (5) and 35 (6).

References

(1) JCGM 200:2008, *International vocabulary of metrology—Basic and general concepts and associated terms (VIM)*, International Bureau of Weights and Measures (www.bipm.org)

Sector	RM No.	Matrix
	NIST 1563	Coconut oil
1	NIST 3274	Fatty acids in botanical oils
1	NIST 3276	Carrot extract in oil
1	LGC 7104	Sterilized cream
2	NIST 2384	Baking chocolate
3	NIST 2387	Peanut butter
4	NIST 1546	Meat homogenate
4	LGC 7106	Processed cheese
4	LGC 7000	Beef/pork meat
4	LGC 7150	Processed meat
4	LGC 7151	Processed meat
4	LGC 7152	Processed meat
4	SMRD 2000	Fresh meat
4	LGC 7101	Mackerel paste
4	LGC QC1001	Meat paste 1
4	LGC QC1004	Fish paste 1
5	BCR-382	Wleat flour
5	BCR-381	Rye flour
5	LGC 7103	Sweet digestive biscuit
5	LGC 7107	Madeira cake
5	LGC QC1002	Flour 1
6	NIST 1544	Fatty acids
6	NIST 1548a	Typical diet
6	NIST 1849	Infant/adult nutritional formula
6	LGC 7105	Rice pudding
7	LGC 7001	Pork meat
7	NIST 1566b	Oyster tissue
7	NIST 1570a	Spinach leaves
7	NIST 2385	Spinach
8	NIST 1946	Lake trout
8	LGC 7176	Canned pet food
9	NIST 1974a	Mussel tissue
9	NIST 3244	Protein powder

(2) Wolf, W.R., & Andrews, K.W. (1995) *Fresenius' J. Anal. Chem.* **352**, 73–76

(3) Wolf, W.R. (1993) *Methods of Analysis for Nutrition Labeling*, D.R. Sullivan & D.E. Carpenter (Eds), AOAC INTERNATIONAL, Gaithersburg, MD

(4) European Reference Materials (2005) *Comparison of a Measurement Result with the Certified Value*, Application Note 1

(5) *ISO Guide 34 General Requirements for the Competence of Reference Material Producers* (2009) 2nd, International Organization for Standardization, Geneva, Switzerland

(6) *Guide 35 Certification of Reference Materials—General and Statistical Principles* (2006) International Organization for Standardization, Geneva, Switzerland

For more information about the AOAC Technical Division on Reference Materials, visit http://aoac.org/divisions/tdrm.

STAKEHOLDER PANEL ON STRATEGIC FOOD ANALYTICAL METHODS (SPSFAM)

Background & Fitness for Purpose

Allergens Screening Working Group

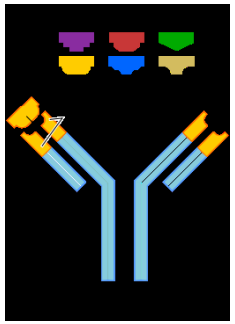
Presented by Vincent Paez & Hua-Fen Liu, SCIEX

Los Angeles

September 27, 2015

Background

- What are allergens?
  - Complex mix of chemicals including proteins and sulfites that induce an adverse response in the body
- What are the adverse responses (allergenic reactions)?
  - Due to binding of the allergen's proteins to immunoglobulin (IG), a Y-shaped protein in the body, releasing a histamine.
  - Inflammation resulting in hives, irritation in the skin/eyes, shortness of breath, swelling, etc.
  - Sensitivities to allergens vary from person to person.

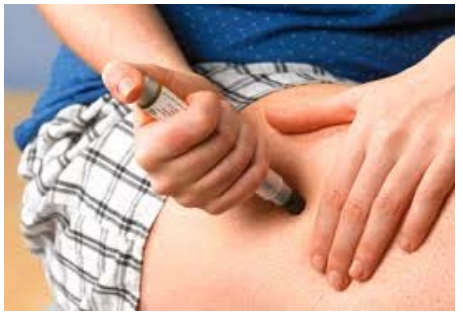


- What are the major sources of these allergens?
  - Wheat, peanut, tree nuts, eggs, milk, soya, fish, shellfish, and sulfites, sesame seeds, mustard, and celery.

Significance

- Over 150 million people worldwide suffer from a food allergy. Around 1-4 % of the overall population and 5-7 % of infants suffer from food allergies.
  - Food allergy statistics in North America:
    - ~8% of children
    - 3.7% of adults
    - … and rising

- The cure?
  - There is none! The only solution is to avoid consumption of the allergen.
  - Deal with anaphylaxis in a reactive way (epinephrine injection)



Significance

- Recalls – allergens are the single largest cause of food recalls.

- Business – $10B gluten-free food market.

- As a result, accurate food labeling for allergens is extremely important and requires analysis.

General Analytical Needs

- Detection of the most popular allergens at around 10ppm in a given food sample in a cost effective manner.
- A screening technique that can cover the most important allergens.
- High confidence analysis with minimal-to-no false positives and false negatives.

Challenges

- Current ELISA methods appear to be cost-effective, but they result in some false positives and false negatives.

- ELISA kits can detect only one allergen at a time.

- ELISA kits have served the industry very well with good sensitivity and cost-effectiveness…but there is a better way…LC/MS/MS.

Challenges

- ELISA kits oftentimes are used by technicians who are not experienced at LC/MS/MS.
- Allergens are present in many matrices.

- Method development to determine allergen proteins is time consuming.
- Most food testing labs are used to using LC/MS/MS for small molecule contaminant testing.
- Sample preparation for allergens (protein digestion) is significantly different from current sample prep methods (LLE, QuEChERS, SPE, etc)

Challenges

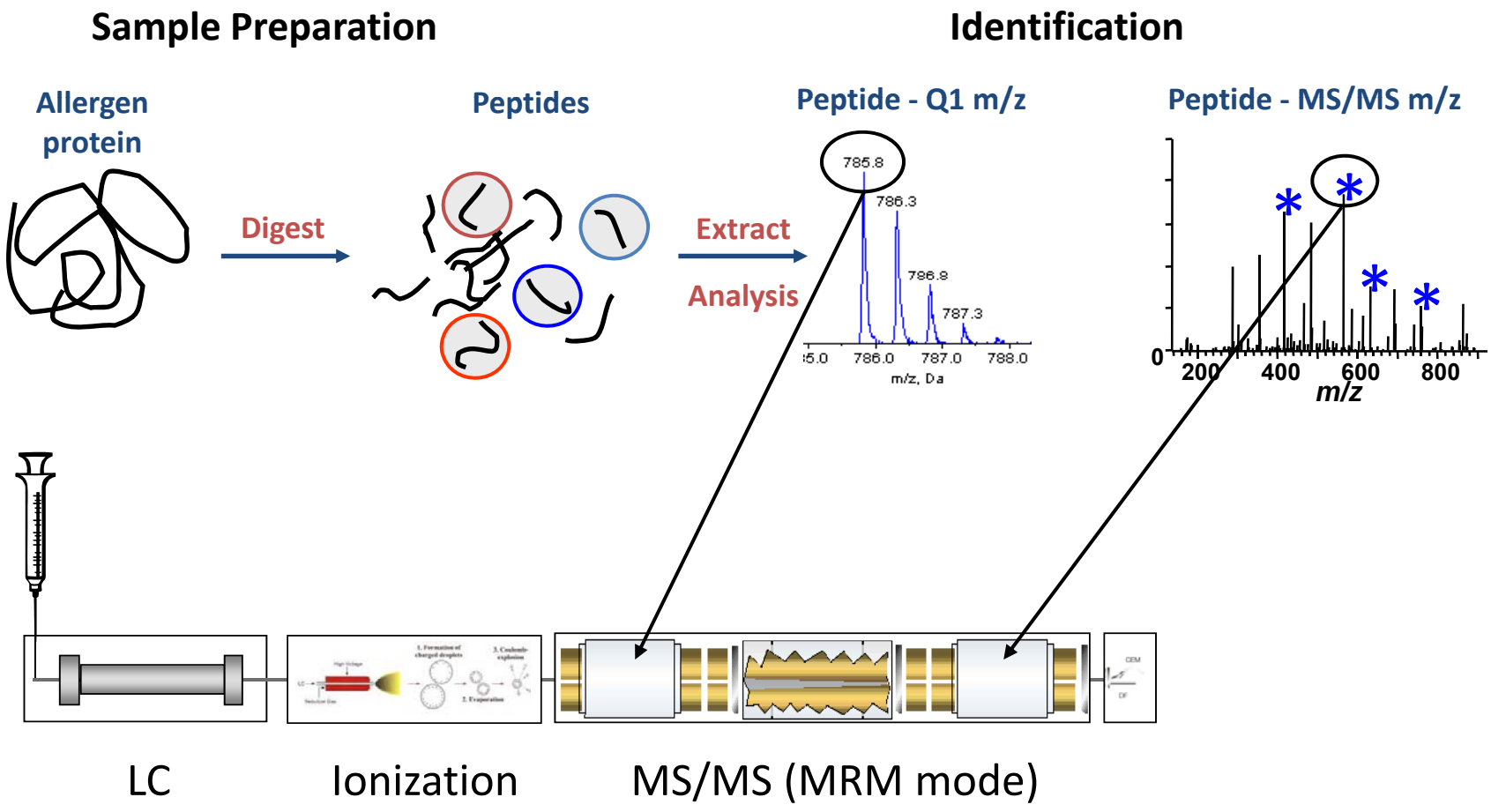
- Unique protein and peptide selections with different digestion conditions
  - Perform protein ID for allergens: Trypsin; chymotrypsin; species selected based on the list highlighted by The Codex Alimentarius.
  - Search against database and select unique proteins/peptides.

Goal:

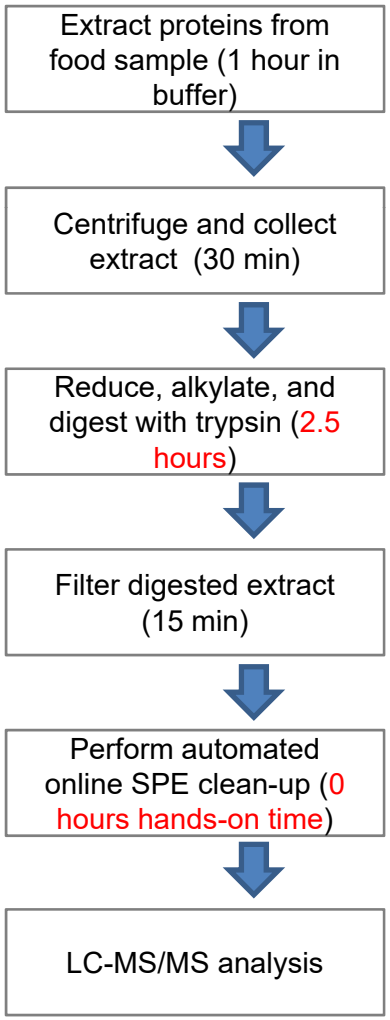
- Detection of two proteins each species (if available), 3-4 peptides each protein, and 3-4 MRM transitions each peptide.
- MRM transition selections with consideration on sensitivity and few/no interferences from the food matrix.
- MRM transition selections made with consideration of potential modification during food processing (cooking, baking, fermenting etc.)and storage (i.e. MRMs must be detectable in raw and processed food)
- Sample clean up: lipids removal
  - Try different solvents (ex. hexane, etc)
- Protein extraction and digestion optimization
  - Try different denature conditions: (ex. heat, urea, OGS, guanidine).
  - Final combined mixture of denature reagent.
  - Must be simple for sample preparation and easy to reproduce.

Existing methods

LC/MS/MS method to target allergen peptides



Existing LC/MS/MS Methods



- Revision of the sample preparation utilizing automated online SPE
- Total sample preparation time down to 4.5 hours
- Results achieved through modification:
  - Prep-time reduced by 4x
  - Sensitivity improved by 2-4x
  - LC-MS/MS run time reduced by nearly 2x
- Addition of more allergens (milk, egg, peanut, treenuts, gluten, sesame, mustard)

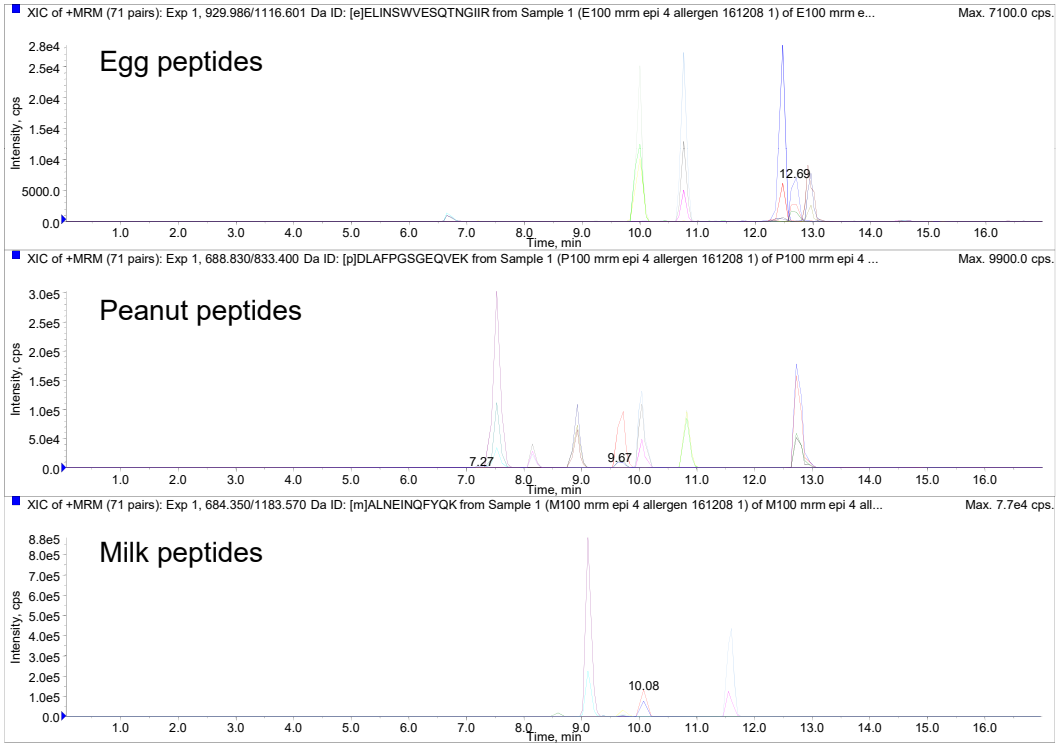
Regulatory Guidance / Issues

- **Food Allergen Labeling and Consumer Protection Act of 2004.**
  - Labeling requires the word “Contains” followed by the name of the major food allergen – for example, “Contains milk, wheat” – or a parenthetical statement in the list of ingredients – for example, “albumin (egg)”

- **Regulation (EU) No 1169/2011**
  - on the provision of food information to consumers entered into application on **13 December 2014**. The obligation to provide nutrition information will apply from **13 December 2016**.

Fitness for Purpose

- Benefits of LC-MS/MS:
  - Improved throughput through multiplexing
  - Multiple allergens in one injection
  - Multiple fragments for each allergen detected
  - More confidence for fewer false positive or false negative results



Multi-allergen analysis

Fitness for Purpose

- The LC/MS/MS method must be able to screen peptides of at least five of the big eight allergens (peanut, tree nuts, soy, egg, and milk).
- The levels of detection must be at the highest 10 ppm for the allergen.
- Each peptide should be unique for the allergen marker protein
- Each peptide should not be modified in processing and preparation

QUESTIONS??

AOAC INTERNATIONAL STAKEHOLDER PANEL ON STRATEGIC FOOD ANALYTICAL METHODS (SPSFAM)

Vincent Paez, SCIEX
Allergens Working Group
March 14, 2016

Gaithersburg, Maryland

Fitness for Purpose

- Mass spectrometry based method or methods able to detect and/or quantify peanut, tree nuts, soy, egg, gluten, shellfish, fish and milk allergens in selected finished products and ingredients.

- Each allergen should be uniquely identified.

Allergens Working Group Members

Vincent Paez, SCIEX
Brad Barrett, Gerstel
Melanie Downs, University of Nebraska
Christophe Fuerer, Nestlé
Gregory Hostetler, Perrigo
Erik Konings, Nestlé
Markus Lacorn, R-Biopharm
John Lawry, Covance
Huafen Liu, SCIEX
Eric Marceau, CFIA
Katerina Mastovska, Covance
Lisa Monteroso, 3M
Christina Parker, FDA
Melissa Phillips, NIST
Bert Popping, Mérieux NutriSciences
Scott Radcliffe, Romer Labs
Andre Schreiber, SCIEX
Jeffrey Shippar, Covance
Darryl Sullivan, Covance
John Szpykla, Mérieux NutriSciences
Jeff Turner, Sigma-Aldrich
Bryan Wirthwine, Q Laboratories
Jason Wubben, ADM
Sudhakar Yadlapalli, First Source Labs

Allergens Working Group
Work to Date

- 2 teleconferences, including one ½ day telecon (November 2015 – December 2015)

- 1 SMPR Drafted

- Public comment period (January 8, 2016 – February 5, 2016)

- SMPRs made ready for SPDS review and approval

Allergen Working Group Topics for Discussion

1. Nature of Analyte

The precise nature of the analyte has not been resolved. Working Group members have discussed peptides, proteins, and commodities.

Allergens are regulated by the FDA and EU as the whole allergen (i.e., peanuts) and products thereof.

The draft SMPR specifies mass spectrometry as the analytical technique, and presumably methods will detect/measure the peaks associated with certain peptides. However, the exact peptide is left up to the method developer. Methods may differ as to the peptide and fragmentation methods. Therefore the exact ratio of peptide to whole commodity may differ. It should be left up to the method develop to: 1) decide which peptide and fragmentation method; and 2) determine the appropriate conversion factor. The AOAC Expert Review Panel will review the method developer's proposed conversion factors as part of the method review.

RECOMMENDATION: PPM OF ALLERGEN PER COMMODITY.

WORKING GROUP DECISION: **AGREED.**

2. Commutability

It was suggested that reference materials should be commutable. The term "commutability" was first used to describe the ability of a reference or control material to have interassay properties comparable to the properties demonstrated by authentic clinical samples when measured by more than one analytical method.

Commutability is not an AOAC requirement for evaluation of methods.

While commutability would seem ideal, it may not be practical. A commutable allergen reference material would require that a reference material provider demonstrate that equivalent results are obtained using a variety of techniques, or example ELISA. Lateral flow, LC-MS, MALDI-TOF-MS, and PCR. It would seem unlikely that many, if any, reference materials would be characterized by multiple techniques, and just as unlikely that equivalent results would be demonstrated.

RECOMMENDATION: DO NOT REQUIRE COMMUTABILITY OF REFERENCE MATERIALS.

WORKING GROUP DECISION: **AGREED.**

ADDITIONAL: COATES TO REACH OUT TO DAIRY COMMUNITY TO IDENTIFY ADDITIONAL REFERENCE MATERIALS USED BY THE INDUSTRY.

3. VITAL reference doses

3.1 Voluntary Incidental Trace Allergen Labeling (VITAL) is a project of the Allergen Bureau based in Australia/New Zealand. There is also an EU-VITAL. VITAL is a voluntary consensus project to establish maximum levels of allergens for safe consumption by individuals with food allergies.

The maximum allergen concentrations are calculated using the specification provided by the commenter for a 200 g serving size of food.

	serving size (g)	converted to kg	mg/kg
hazel nut	200	0.2	3.2
milk	200	0.2	15.2
peanut	200	0.2	4
whole egg	200	0.2	1.2

As the commenter noted, the maximum permissible concentration of allergens are all below the proposed LOQ in the SMPR.

While the VITAL concentrations are not binding, they are based on scientific studies.

RECOMMENDATION: LOQ AND RANGES CONSISTENT WITH THE VITAL WOULD SEEM TO BE A BENEFIT FOR INTERNATIONAL TRADE, AND THEREFORE A GOOD REASON TO REVISE THE SMPR.

WORKING GROUP DECISION: VITAL IS NOT AN INTERNATIONALLY RECOGNIZED STANDARD. **AGREED NOT REVISE THE SMPR.**

3.2 VITAL values are based on amount of protein per service size. Therefore, the definition of the food allergens as “food commodities” without mentioning the protein content will establish a non-comparability between results obtained by an LC-MS/MS method and VITAL values.

Method developers can provide conversion factors in their methods for peptide to protein to “whole” allergen.

RECOMMENDATION: NO CHANGE RECOMMENDED.

WORKING GROUP DECISION: AGREED WITH RECIMMENDATION. **NO CHANGE RECOMMENDED.**

AOAC SPSFAM ALLERGENS DRAFT SMPR - COMMENTS on ALLERGENS SMPR FINAL

Item	Line Numbers (If Applicable)	Comment	Proposed Change(s)	Response
1	139 (table 2)	Chocolate is an important matrix for peanut, hazelnut and milk.	Chocolate should be included into the list of priority allergens. If chocolate is a known problem than the applicability should clearly state that chocolate is not possible to measure using the validated method.	**No change.** Chocolate is an optional matrix to be tested for candidate method that claim to work in chocolate.
2	56-65	Should the precision data obtained over the whole analytical range? Number of levels?	Describe the validation of precision in a more precise way e.g. include number of levels and replicates	**Additional reference** to Appendix D and F are added
3	116 (table 1)	By definition the analytical range can only start with an LoQ. MDL only gives a yes or no.		**No change recommended.** The comment is true but there is not any prohibition against the LOQ = MDL.
4		After validation, LC-MS/MS methods will be used for comparison with ELISA results. An commercial ELISA is (often) calibrated to the whole allergenic food while LC-MS/MS is calibrated to peptides. Is comparability established via reference materials? (again: traceability of LC-MS/MS to these RMs is mandatory!)	Discuss traceability and comparability to ELISA results (note: this SMPR discuss a possible reference method for cGMP compliance!)	**No change.** The working group did not agree to tie LC-MS/MS results to ELISA results.
5	96	NIST SRM 2387 is not pure peanut but a mixture of roasted peanut, sugar, partially hydrogenated vegetables oils and salt. See NIST certificate: protein content is given but not peanut content.	Discuss suitability of this SRM in the working group and give conversion factor	**No change.** That's will be left up to the methode developer.
6	92	NIST SRM 1549 is superseded by NIST 1549a	Delete NIST SRM 1549	**Agree. Replace NIST SRM 1549 wuth 1549a.**
7	85	NIST 8445 is a whole egg powder with a given protein content. How should a method developer trace it to whole egg without conversion factor?	Discuss traceability in the working group and discuss a conversion factor	**Working Group agreed that all results to be "reported as ppm of the target allergen in food commodity".**
8	67	Recovery: What kind of samples is required? Spiked or incurred? For ELISA incurred is preferred.	We should follow the guideline for ELISA which prefer incurred	**Add a reference to Appendix M: Validation Procedures for Quantitative Food Allergen ELISA Methods.** Appendix M does mandate the use of incurred samples. AOAC policy allows for both kinds of samples. Method developer discretion.
9	67	Recovery: How should a method developer determine this parameter? By spiking with reference materials or peptides or a different material. One should remember that it is not allowed to use a reference material for calibration AND spiking! If peptides are used for calibration, how was traceability established?	Discuss in the working group and remember to solve the traceability problem	**No change recommended.** Method development issue not SMPR issue.
10	62	Since reproducibility determination is only possible by a collaborative study, an intra-laboratory reproducibility should be defined to ease single-lab validations at the beginning	Inlcude a new clause after repeatability and describe the validation to be done	**No change.** All previous SMPRs used RSDR and RSDr.

11	50	MDL: How should a method developer estimate this parameter? By using blank matrices or blank matrices spiked with reference materials/peptides? How many replicates? We have very clear guidelines for allergen determination by ELISA-why not for "Reference methods for cGMP compliance"?	Discuss in the working group maybe follow ELISA guidelines	**Reference to Appendix M: Validation Procedures for Quantitative Food Allergen ELISA Methods added to SMPR.** SMPR will also refer to FDA and/or EPA definition for MDL.
12	46	LoQ: How should a method developer determine or even estimate this parameter? By using reference materials or peptide solutions or blank matrices or blank matrices spiked with reference materials/peptides? How many replicates? We have very clear guidelines for allergen determination by ELISA-why not for "Reference methods for cGMP compliance"?	Discuss in the working group maybe follow ELISA guidelines	**Reference to Appendix M: Validation Procedures for Quantitative Food Allergen ELISA Methods added to SMPR.**
13	46-69	LoQ, MDL, recovery and precision data need to be determined for every claimed matrix	include a sentence for each parameter that explains the parameter-specific validation	**Line 108 of version revised** to recommend "LOQ, MDL, recovery and precision" data for every claimed matrix.
14	116 (table 1)	By taking the latest published VITAL reference doses C18(Food Chem. Toxicol. 63: 9-17, 2014) it is obvious that the MDLs/LoQs in table 1 are not sufficient when a food is analyzed that is consumed in a service size of more than 50 g. Lower MDL/LoQ appropriately to the following table. Note: C19 Hazelnut: Reference dose as protein: 0.1 mg; Reference dose as allergenic food: 0.64 mg; Minimum concentration to be quantified when consuming 50 g food: 12.8 mg/kg and for 200 g 3.2 mg/kg. Milk: Reference dose as protein: 0.1 mg; Reference dose as allergenic food: 3.03 mg; Minimum concentration to be quantified when consuming 50 g food: 60.6 mg/kg and for 200 g 15.2 mg/kg. Peanut: Reference dose as protein: 0.2 mg; Reference dose as allergenic food: 0.8 mg; Minimum concentration to be quantified when consuming 50 g food: 16 mg/kg and for 200 g 4 mg/kg. Whole egg: Reference dose as protein: 0.03 mg; Reference dose as allergenic food: 0.25 mg; Minimum concentration to be quantified when consuming 50 g food: 4.8 mg/kg and for 200 g 1.2 mg/kg.	Change MDLs/LoQ in table 1 according to the VITAL values and calculations given under comments. Discuss in the working group	**No change.** Working Group discussed on 3/3/2016. There are multiple VITALs with different maximum permissiable concentrations. The Working Group consensus is that none of the VITALs are international concensusn standards, and declined to reset the LOQs or MDLs based on VITALmaximum permissiable concentrations.
15		How should a method developer prove that the selected peptides are not "too" specific e.g. a sequence is used that is not present in every commercially available peanut or hazelnut variety. On the opposite, if the selected peptides are not specific enough, near botanical relatives are detected which are maybe not allergenic or regulated (see prunus mahaleb example).	At minimum a chapter describing the known specificities/selectivities should be provided. (Note: Unknown occurrence of peptides that are not from a allergenic source will always occur in the future, see also prunus mahaleb)	**No change.** The working group did not agree.
16		What are the minimum performance criteria for peptide selection?	Include criteria for peptide selection or give reference	**No change.** The working group did not agree.
17		VITAL values are based on amount of protein per service size. Therefore, the definition of the food allergens as "food commodities" without mentioning the protein content will establish a non-comparability between results obtained by an LC-MS/MS method and VITAL values.	Include some guidance for the user or let the method developer describe his way of establishing traceability to VITAL values	**No change.** Working Group discussed on 3/3/2016. There are multiple VITALs with different maximum permissiable concentrations. The Working Group consensus is that none of the VITALs are international concensusn standards, and declined to reset the LOQs or MDLs based on VITALmaximum permissiable concentrations. AND E25
18	9	collaborative test: It should be critically checked if Appendix D is sufficient in the case where LESS than 8 participants (and/or LC-MS/MS machines) are available. Is this still collaborative or forbidden at all?	discuss in the working group	**No change.** AOAC policy not a working group decision.
19	3	The title is unclear	change to "…selected food allergens"	**Change title to "…selected food allergens."**
20	9	This means a method comparison between the original method (checked by an ERP) and this method transferred to another lab. Are there any guidelines for this case? What is the minimum required number of measurements to be sure that both methods are comparable?	Include minimum requirements for verification	**No change.** Method comparision is not a verification requirement.

21		Hazelnuts and peanut are not defined in sense of their variety while milk and egg are not defined in sense of their origin	A method developer should validate the differences between different varieties of hazelnuts and peanuts in sense of traceability and measurement uncertainty. A method developer should validate different species that deliver milk (cow, goat, sheeo etc.); same for egg. Maybe an in-silico analysis of peptide sequences is sufficient.	**Species names were added to the SMPR. The working group group did not agree to requireing different varieties.**
22		The term "allergen" is not defined	The SMPR should contain a clarifying chapter or clause that explains that the term “allergen” is used in an analytical and not immunological way. “Allergen” could also mean a specific protein from hazelnut that differs between regions and varieties.	**No change recomended.** Although the term "allergen" itself is not defined, the identification of food allergens types in the SMPR provides all of the needed information for method developers. No definition were found that weren't circular. i.e., an allergen is a molecule causes an allergic reaction.
23		A general problem of this SMPR is traceability of results. In detail, an LC-MS/MS user prepared peptide solutions on a weight by weight basis and uses reference materials also on a weight by weight basis. Are these reference materials of a higher order in the calibration hierarchy or are the peptides of higher level? Furthermore, how should we re-calculate to the “analyte” which is for example “milk”. There is no conversion factor to re-calculate from “weight whole milk powder from NIST” to “milk”. Even more problematic is the recalculation from “peak area of a specific milk peptide” to “milk”.	At a minimum, each validation report should contain a chapter that clearly describes how the validation manager solved this fundamental problem for each allergen or describes the limitations of quantitative results.	Working Group agreed that all results to be "reported as ppm of the target allergen in food commodity".
24		I have developed a sign system for the 14 allergens which, according to the European Union, must be indicated in food packagings. It has being the work of 7 months for my final grade in Graphic Design.	Implement your standard regulation by applying the sign system for the allergens (eggs, milk, nuts, peanuts, celery, sesame, mustard, sulphites, fish, crustaceans, mollusks, gluten, lupin and soy). It would help to the interpretation of the ingredients independently from the country where people live or the language that they speak. Thank you	**No change.** Irrelevant

Motion

- Move to accept the Standard Method Performance Requirements for selected allergens as presented.

DRAFT AOAC Allergen SMPR Version 5; March 10, 2016.

Detection and Quantitation of Selected Food Allergens

Intended Use: Reference method for cGMP compliance.

1. **Purpose:** AOAC SMPRs describe the minimum recommended performance characteristics to be used during the evaluation of a method. The evaluation may be an on-site verification, a single-laboratory validation, or a multi-site collaborative study. SMPRs are written and adopted by AOAC Stakeholder Panels composed of representatives from the industry, regulatory organizations, contract laboratories, test kit manufacturers, and academic institutions. AOAC SMPRs are used by AOAC Expert Review Panels in their evaluation of validation study data for method being considered for *Performance Tested Methods* or AOAC *Official Methods of Analysis*, and can be used as acceptance criteria for verification at user laboratories.

2. **Applicability**:
Detection and quantitation of egg, milk, peanut, and hazelnut food allergens in finished food products and ingredients. Method(s) shall uniquely identify each allergen.

3. **Analytical Technique**:
Mass spectrometry based methods.

4. **Definitions**:

Food Allergens

Hazelnut

Any of the nuts deriving from species of the genus *Corylus*, especially the nuts of the species *Corylus avellana* (the common hazel tree). ~~It is also known as cobnut or filbert nut according to species. For the purposes of this SMPR, includes both raw and processed nuts.~~

Milk

For the purposes of this SMPR: "milk" refers to pasteurized whole cow's (*Bos Taurus*) milk~~,~~ and shall contain not less than 8 1/4 percent milk solids not fat and not less than 3 1/4 percent milkfat.[1]

Peanut

The seed of the *Arachis hypogaea* plant. For the purposes of this SMPR, includes both raw and roasted peanuts.

[1] Code of Federal Regulations; Title 21 - Food and Drugs, § 131.110. Other internationally recognized definition may be applied.

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Whole Egg

A combination of pasteurized ~~[~~chicken~~]~~ (*Gallus gallus domesticus*) egg whites and egg yolks from the same production batch blended together in their entirety, in natural proportions.[2]

Limit of Quantitation (LOQ)

The minimum concentration or mass of analyte in a given matrix that can be reported as a quantitative result. LOQ = average (blank) + 10 * s0 (blank).*

Method detection limit (MDL)

Method detection limit (MDL) is the minimum concentration of a substance than can be measured and reported with 99% confidence that the analyte concentration is greater than zero. It is determined from analysis of a sample in a given matrix containing the analyte.[3]

The minimum concentration of a substance that can be measured (detected) and reported with 99% confidence that the analyte concentration is greater than zero and is determined from analysis of a sample in a given matrix containing the analyte using at least two ion MS/MS transitions. See 4 (a) of 40 CFR Part 136, Appendix B to Part 136 - Definition and Procedure for the Determination of the Method Detection Limit-Revision.[4]

Repeatability

Variation arising when all efforts are made to keep conditions constant by using the same instrument and operator and repeating during a short time period. Expressed as the repeatability standard deviation (SD_r); or % repeatability relative standard deviation (%RSD_r).*

Reproducibility

The standard deviation or relative standard deviation calculated from among-laboratory data. Expressed as the reproducibility standard deviation (SD_R); or % reproducibility relative standard deviation (% RSD_R).*

Recovery

The fraction or percentage of spiked analyte that is recovered when the test sample is analyzed using the entire method.**

5. **Method Performance Requirements**:

See table 1.

[2] Introduction to Egg Products, USDA Food Safety and Inspection Service, website: http://www.fsis.usda.gov/wps/wcm/connect/c5c85914-5055-4f09-8098-1a179a1c6e14/EPT_Introduction.pdf?MOD=AJPERES, accessed 12/15/2015.

* See Table A3 in Appendix F: *Guidelines for Standard Method Performance Requirements* for additional guidance.

** See Spiking method in Appendix M in the Official Methods of Analysis.

[3] Volume II - Methods, Method Verification and Validation ORA-LAB.5.4.5; DOCUMENT NO.: IV-02; VERSION NO.:1.7; Section 2 – Microbiology; EFFECTIVE DATE: 10-01-03; REVISED: 08-25-14; WEBSITE: http://www.fda.gov/ScienceResearch/FieldScience/ucm171877.htm, ACCESSED: Feb. 22, 16.

[4] 40 CFR Part 136, Appendix B to Part 136 - Definition and Procedure for the Determination of the Method Detection Limit-Revision (link)

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6. **System suitability tests and/or analytical quality control:**
Suitable methods will include blank check samples, and check standards at the lowest point and midrange point of the analytical range.

7. **Potential Reference Material(s):**

Whole Egg
- NIST 8445
- LGC SAL-RSM-5 (Check for characterization level)

Nonfat Milk Powder
- ~~NIST SRM 1549 (nonfat milk powder)~~
- NIST SRM 1549a (whole milk powder)

Peanut
- NIST SRM 2387 (peanut butter)
- LGC FAL-RFM1017-XXX

Hazelnut
- ~~No known reference material available.~~
- LGC FAL-RFM1015-50 or FAL-RFM1015-50Â or FAL-RFM1015-5

Additional materials can be found at the LGC and FAPAS websites
LGC = http://www.lgcstandards.com/HK/en/search/?q=allergen:relevance:category:CEFP_77243
FAPAS = http://fapas.com/quality-control-materials/Available-quality-control-materials.cfm

Refer to Annex F: *Development and Use of In-House Reference Materials* in Appendix F: *Guidelines for Standard Method Performance Requirements*, 19th Edition of the AOAC INTERNATIONAL Official Methods of Analysis (2012). Available at: http://www.eoma.aoac.org/app_f.pdf

NIST = National Institute for Standards and Technology.
LGC = formerly the UK *Laboratory of the Government Chemist*, now simply "LGC Standards".
FAPAS = formerly the *Food Analysis Performance Assessment Scheme* in the UK, now simply "FAPAS".

8. **Validation Guidance**:

Method developers shall submit LOQ, MDL, recovery and precision data ~~evaluating~~ for the matrices in Table 2.

Appendix D: Guidelines for Collaborative Study Procedures To Validate Characteristics of a Method of Analysis; 19th Edition of the AOAC INTERNATIONAL Official Methods of Analysis (2012). Available at: http://www.eoma.aoac.org/app_d.pdf

Appendix F: Guidelines for Standard Method Performance Requirements; 19th Edition of the AOAC INTERNATIONAL Official Methods of Analysis (2012). Available at: http://www.eoma.aoac.org/app_f.pdf

9. **Maximum Time-To-Result:** None

Table 1: Method performance requirements.

Parameter	Target allergen			
	whole egg	milk	peanut	hazelnut
Analytical Range (ppm)	~~10-1000~~	~~10-1000~~	~~10-1000~~	~~10-1000~~
LOQ (ppm*)	5	10	10	10
MDL (ppm*)	~~10~~ 1.65	~~10~~3	~~10~~3	~~10~~3
Recovery (%)	60-120%	60-120%	60-120%	60-120%
% RSD_r	≤20 %	≤20 %	≤20 %	≤20 %
% RSD_R	≤ 30%	≤ 30%	≤ 30%	≤ 30%
* Reported as ppm of the target allergen in food commodity, i.e., 25 ppm of "whole egg" in cookies. Definitions for LOQ and MDL provided in section 4.				

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Table 2: Priority Allergen/Matrix Combinations

whole egg	cookies bread dough salad dressing wine
milk	cookies, baked goods infant formula wine dark chocolate (optional matrix for methods that claim a chocolate matrix)
peanut	cookies ice cream breakfast cereal milk chocolate (optional matrix for methods that claim a chocolate matrix)
hazelnut	cookies ice cream breakfast cereal milk chocolate (optional matrix for methods that claim a chocolate matrix)

Table A3. Recommendations for evaluation

Bias (if a reference material is available)	A minimum of five replicate analyses of a Certified Reference Material.[a]
Environmental interference	Analyze test portions containing a specified concentration of one environmental materials panel member. Materials may be pooled. Consult with AOAC statistician.
Exclusivity/cross-reactivity	Analyze one test portion containing a specified concentration of one exclusivity panel member. More replicates can be used. Consult with AOAC statistician.
Inclusivity/selectivity	Analyze one test portion containing a specified concentration of one inclusivity panel member. More replicates can be used. Consult with AOAC statistician.
Limit of quantitation (LOQ)	Estimate the LOQ = average (blank) + 10 × s_b (blank). Measure blank samples with analyte at the estimated LOQ. Calculate the mean average and standard deviation of the results. Guidance[b]: For ML ≥ 100 ppm (0.1 mg/kg): LOD = ML × 1/5. For ML < 100 ppm (0.1 mg/kg): LOD = ML × 2/5.
Measurement uncertainty	Use ISO 21748: *Guidance for the use of repeatability, reproducibility, and trueness estimates in measurement uncertainty estimation to analyze data collected for bias, repeatability, and intermediate precision to estimate measurement uncertainty.*
POD(0)	Use data from collaborative study.
POD (c)	
Repeatability	Prepare and homogenize three unknown samples at different concentrations to represent the full, claimed range of the method. Analyze each unknown sample by the candidate method seven times, beginning each analysis from weighing out the test portion through to final result with no additional replication (unless stated to do so in the method). All of the analyses for one unknown sample should be performed within as short a period of time as is allowed by the method. The second and third unknowns may be analyzed in another short time period. Repeat for each claimed matrix.
Probability of detection (POD)	Determine the desired POD at a critical concentration. Consult with Table A7 to determine the number of test portions required to demonstrate the desired POD.
Probability of identification (POI)	Consult *Probability of Identification (POI): A Statistical Model for the Validation of Qualitative Botanical Identification Methods*[c].
Recovery	Determined from spiked blanks or samples with at least seven independent analyses per concentration level at a minimum of three concentration levels covering the analytical range. Independent means at least at different times. If no confirmed (natural) blank is available, the average inherent (naturally containing) level of the analyte should be determined on at least seven independent replicates. Marginal % recovery = $(C_f - C_u) \times 100/C_A$ Total % recovery = $100(C_f)/(C_u + C_A)$ where C_f = concentration of fortified samples, C_u = concentration of unfortified samples, and C_A = concentration of analyte added to the test sample.[d] Usually total recovery is used unless the native analyte is present in amounts greater than about 10% of the amount added, in which case use the method of addition.[e]
Reproducibility (collaborative or interlaboratory study)	Quantitative methods: Recruit 10–12 collaborators; must have eight valid data sets; two blind duplicate replicates at five concentrations for each analyte/matrix combination to each collaborator.
	Qualitative methods: Recruit 12–15 collaborators; must have 10 valid data sets; six replicates at five concentrations for each analyte/matrix combination to each collaborator.

[a] *Guidance for Industry for Bioanalytical Method Validation* (May 2001) U.S. Department of Health and Human Services, U.S. Food and Drug Administration, Center for Drug Evaluation and Research (CDER), Center for Veterinary Medicine (CVM).

[b] Codex Alimentarius Codex Procedure Manual.

[c] LaBudde, R.A., & Harnly, J.M. (2012) *J. AOAC Int.* **95**, 273–285.

[d] *Guidelines for Collaborative Study Procedures to Validate Characteristics of a Method of Analysis* (2012) *Official Methods of Analysis*, 19th Ed., *Appendix D*, AOAC INTERNATIONAL, Gaithersburg, MD.

[e] *AOAC Guidelines for Single-Laboratory Validation of Chemical Methods for Dietary Supplements and Botanicals* (2012) *Official Methods of Analysis*, 19th Ed., *Appendix K*, AOAC INTERNATIONAL, Gaithersburg, MD.

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40 CFR Part 136, Appendix B to Part 136 - Definition and Procedure for the Determination of the Method Detection Limit-Revision

analyte between one and five times the estimated detection limit.

If the measured level of analyte is greater than five times the estimated detection limit, there are two options.

(1) Obtain another sample with a lower level of analyte in the same matrix if possible.

(2) The sample may be used as is for determining the method detection limit if the analyte level does not exceed 10 times the MDL of the analyte in reagent water. The variance of the analytical method changes as the analyte concentration increases from the MDL, hence the MDL determined under these circumstances may not truly reflect method variance at lower analyte concentrations.

4. (a) Take a minimum of seven aliquots of the sample to be used to calculate the method detection limit and process each through the entire analytical method. Make all computations according to the defined method with final results in the method reporting units. If a blank measurement is required to calculate the measured level of analyte, obtain a separate blank measurement for each sample aliquot analyzed. The average blank measurement is subtracted from the respective sample measurements.

(b) It may be economically and technically desirable to evaluate the estimated method detection limit before proceeding with 4a. This will: (1) Prevent repeating this entire procedure when the costs of analyses are high and (2) insure that the procedure is being conducted at the correct concentration. It is quite possible that an inflated MDL will be calculated from data obtained at many times the real MDL even though the level of analyte is less than five times the calculated method detection limit. To insure that the estimate of the method detection limit is a good estimate, it is necessary to determine that a lower concentration of analyte will not result in a significantly lower method detection limit. Take two aliquots of the sample to be used to calculate the method detection limit and process each through the entire method, including blank measurements as described above in 4a. Evaluate these data:

(1) If these measurements indicate the sample is in desirable range for determination of the MDL, take five additional aliquots and proceed. Use all seven measurements for calculation of the MDL.

(2) If these measurements indicate the sample is not in correct range, reestimate the MDL, obtain new sample as in 3 and repeat either 4a or 4b.

5. Calculate the variance (S^2) and standard deviation (S) of the replicate measurements, as follows:

(http://ecfr.gpoaccess.gov/graphics/ec15no91.208.gif)

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Stakeholder Panel on Dietary Supplements

Working Group on PDE5 Inhibitors

Chair, Katerina Mastovska

Friday, March 21, 2014
Hilton Washington, North
Gaithersburg, Maryland USA

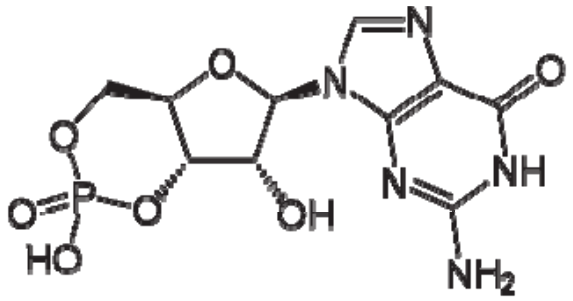
Outline

- Technical background
- Analytical challenges
- Current analytical methods and techniques
- Fitness for purpose statement
- Questions for SPDS discussion

Phosphodiesterase Type 5 (PDE5) Inhibitors

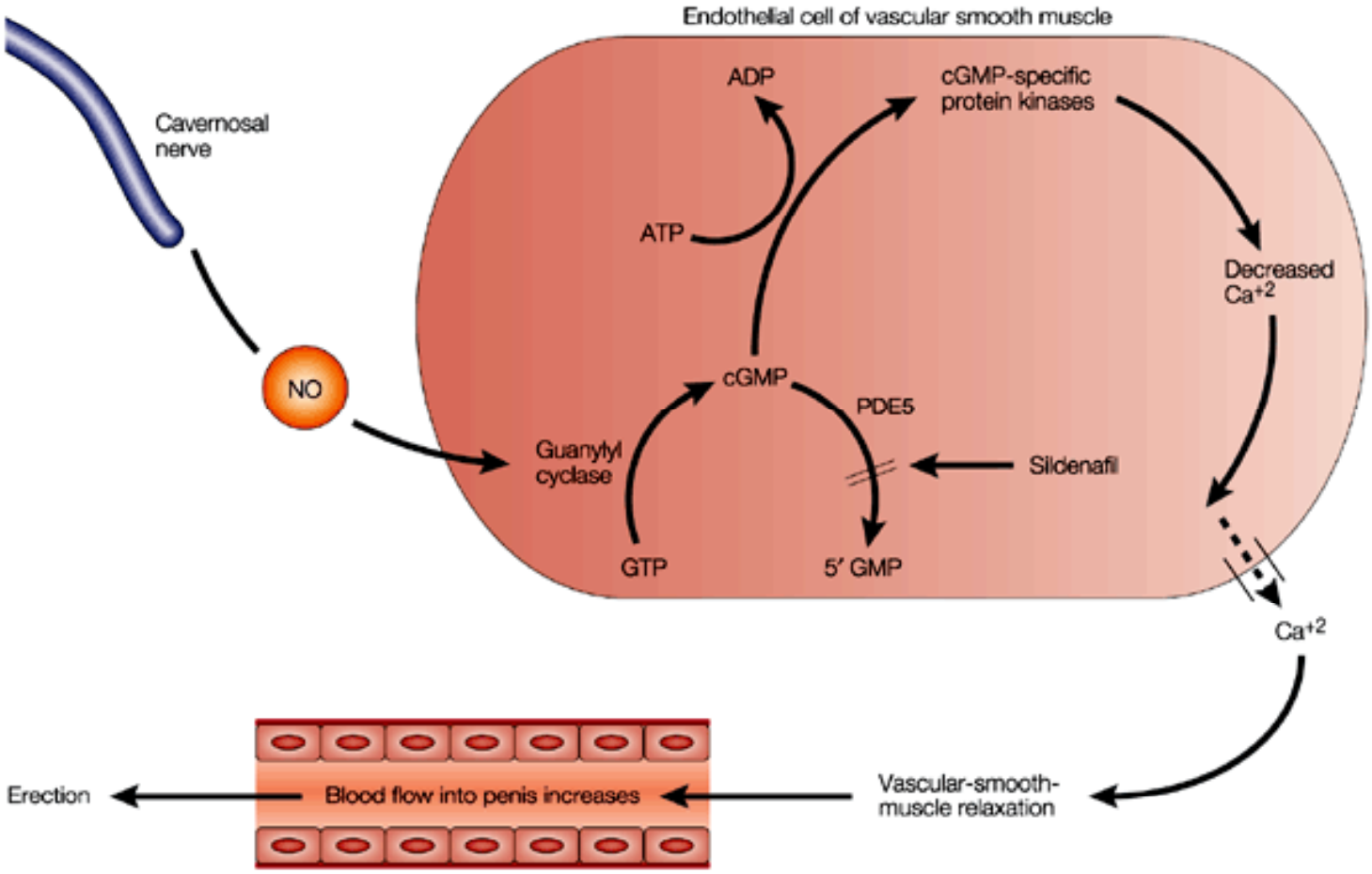
- Used in the treatment of erectile dysfunction (ED) and also explored for the treatment of pulmonary hypertension
- Block degradative action of PDE5 on cyclic guanosine monophosphate (cGMP) in smooth muscle cells lining the blood vessels supplying the corpus cavernosum of the penis (and arterial walls within the lungs)

cGMP



- cGMP – second messenger which relaxes smooth muscle tissues, leading to the increased blood flow in blood vessels

PDE5 Inhibitors – Mechanism of Action



Nature Reviews | Drug Discovery

Approved PDE5 Inhibitor Drugs

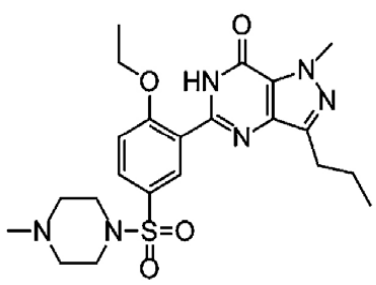
In the US:

- **Sildenafil** (Viagra®, Pfizer, 1998)
- **Tadalafil** (Cialis®, Elli Lilly, 2003)
- **Vardenafil** (Levitra®, Bayer, 2003)
- **Avanafil** (Stendra®, Vivus, 2012)

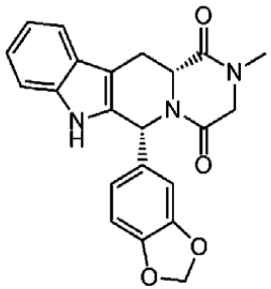
Other countries:

- **Udenafil** (Zydena®,Dong-A Pharmaceutical Co. Ltd) in South Korea and Malaysia
- **Mirodenafil** (Mvix®, SK Chemicals Life Science) in South Korea
- **Lodenafil carbonate** (Helleva®, Cristália Produtos Químicos e Farmacêuticos) in Brazil

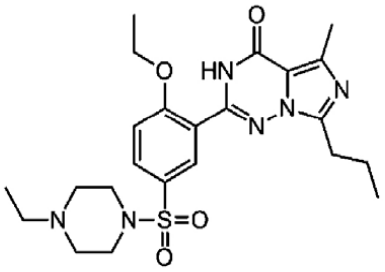
Approved PDE5 Inhibitor Drugs



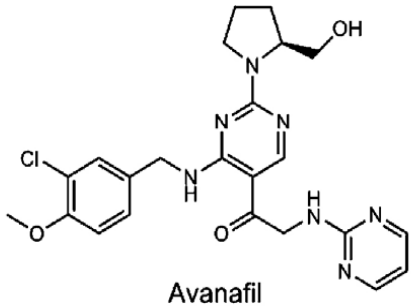
Sildenafil



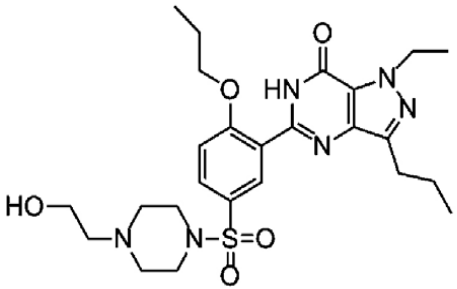
Tadalafil



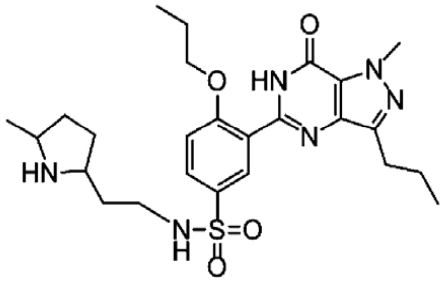
Vardenafil



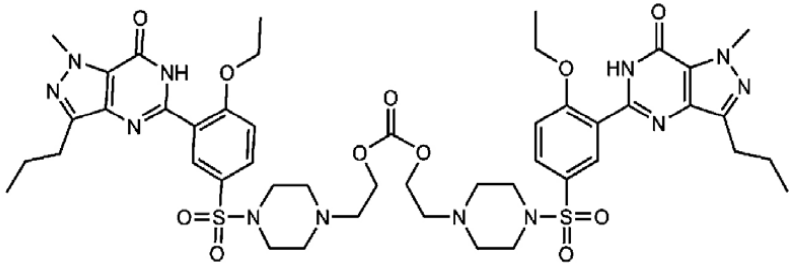
Avanafil



Mitrodenafil



Udenafil



Lodenafil carbonate

Patel *et al.* , *J. Pharm. Biomed. Anal*. 87 (2014) 176– 190

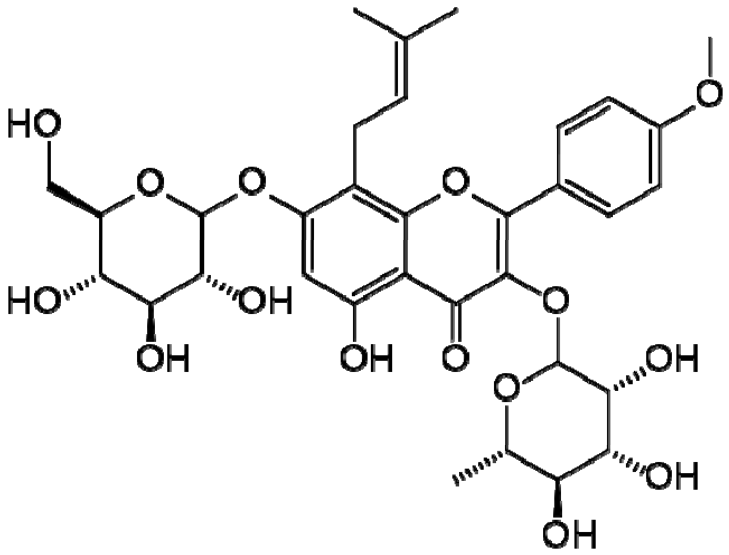
Adverse PDE5 Inhibitor Drug Side-Effects

- Nausea
- Headache
- Abdominal pain
- Back pain
- Photosensitivity
- Abnormal vision
- Eye pain
- Sudden hearing loss
- Hypotension
- Face edema
- Joint and muscle pain
- Nasal congestion
- Palpitation
- Tachycardia
- Rash
- Itch
- Priapism
- Heart attack
- Life-threatening drug interactions (*e.g.* with nitrates and cardiac antiarrhythmic drugs)

Natural PDE5 Inhibitors

Icariin

- Active component of *Epimedium* extracts (horny goat weed, yin yang huo, barrenwort, bishop's hat, fairy wings, rowdy lamb herb, randy beef grass)



Natural PDE5 Inhibitors

Icariin

- Weak PDE5 inhibitor (studied synthetic derivatives showed similar PDE5 activity as sildenafil but better specificity)
- Demonstrated to increase production of bioactive nitric oxide and mimic effects of testosterone
- Used as an aphrodisiac and ED treatment in traditional Chinese medicine
- Potential to treat osteoporosis

Examples of other herbal drugs and dietary supplements used for sexual enhancement

- ***Tribulus terrestris***
  - claimed to increase natural testosterone levels

- ***Turnera diffusa* (damiana)**
  - aphrodisiac

Plant photos: Wikipedia

Examples of other herbal drugs and dietary supplements used for sexual enhancement

- ***Ptychopetalum*** (**Muira Puama**)
  - "potency wood" root and bark used traditional remedies in South America
- ***Pausinystalia yohimbe*** (**Yohimbe**)
  - bark of an African tree used as aphrodisiac and ED remedy
- ***Lepidium meyenii (Maca)***
- ***Ginseng***
- ***Gingko***
- ***Saw palmetto***

Hidden Risks of Erectile Dysfunction "Treatments" Sold Online

Men looking online for "dietary supplements" to treat erectile dysfunction (ED) or enhance their sexual performance should beware: these products may contain prescription drugs or other undisclosed ingredients that can be harmful.

"The number of these problematic products available on the Internet appears to be increasing," says Michael Levy, director of the Food and Drug Administration's (FDA) Division of New Drugs and Labeling Compliance. The division is part of the Office of Compliance (OOC) in the agency's Center for Drug Evaluation and Research (CDER).

Many consumers perceive these products as completely safe because they are often sold with labeling, suggesting that they are all-natural alternatives to prescription drug products that have been approved by FDA for treating ED.

But these products may be laced with potentially hazardous ingredients that aren't noted on the label.

Since 2004, FDA has become aware of several such "dietary supplements" (see sidebar for list).

Viagra Ingredient Found

Working with other FDA components, the division's Internet and Health Fraud Team led an Internet survey in which more than one-third of purchased "dietary supplements" claiming to spur sexual enhancement or treat ED contained undisclosed prescription drug ingredients or similar substances.

Six of the 17 products contained sildenafil (the active ingredient in Viagra) or a substance similar to either sildenafil or vardenafil. Vardenafil is the active ingredient in Levitra, another FDA-approved prescription drug that treats ED.

Mark Hirsch, a medical team Leader in CDER's Division of Reproductive and Urologic Products, says this undisclosed presence of prescription drug ingredients—and similar compounds known as analogs of the drugs—can lead to serious side effects in users.

Dangerous Interactions

"These products may interact in dangerous ways with drugs that a consumer is already taking," Hirsch says. For example, taking sildenafil in addition to certain prescription drugs containing nitrates may lower blood pressure to an unsafe level.

People with diabetes, high blood pressure, high cholesterol,

Online Products to Avoid

Since 2004, FDA has identified several products sold online as so-called "dietary supplements" for treating erectile dysfunction and enhancing sexual performance. These products have contained potentially harmful, undeclared ingredients. Included among them are

- Actra-Rx
- Actra-Sx
- Libidus
- Nasutra
- Neophase
- Vigor-25
- Yilishen
- Zimaxx
- 4EVERON
- Liviro3
- Lycium Barbarum L.
- Adam Free
- Rhino V Max
- V.Max
- True Man
- Energy Max
- HS Joy of Love
- NaturalUp
- Blue Steel
- Erextra
- Super Shangai
- Strong Testis
- Shangai Ultra
- Shangai Ultra X
- Lady Shangai
- Shangai Regular, also marketed as Shangai Chaojimengnan
- Hero
- Naturalë Super Plus
- Xiadafil VIP tablets (Lots 6K029 and 6K209-SEI only)

FDA Consumer Health Information
www.fda.gov/consumer

Magic Power Coffee: **POTENTIALLY DANGEROUS** Not Magical

Consumers should not use an instant coffee being sold online as a dietary supplement for sexual enhancement, warns the Food and Drug Administration (FDA).

The product, Magic Power Coffee, contains a potentially dangerous ingredient. The product is sold in a two-serving box as well as in a carton that contains six two-serving boxes.

FDA's lab analysis determined that Magic Power Coffee contains a chemical similar to the active ingredient in the prescription drug Viagra to treat erectile dysfunction. The chemical may interact with prescription drugs known as nitrates, including nitroglycerin, and cause dangerously low blood pressure.

Although Magic Power Coffee is labeled as an "all natural dietary supplement," it can cause serious harm. Sexual enhancement products that claim to work as well as prescription products are likely to expose consumers to unpredictable risks and the potential for injury or even death.

Advice for Consumers

1. Stop using Magic Power Coffee immediately.
2. If you have experienced any bad side effects from Magic Power Coffee or any sexual enhancement products, talk to a health care professional.
3. Report any side effects with the use of any sexual enhancement products to FDA's MedWatch Adverse Event Reporting Program either online, by regular mail, by fax, or by phone.
   - Online (*www.fda.gov/MedWatch/*)
   - Regular Mail: Use postage-paid, pre-addressed FDA form 3500 (*www.accessdata.fda.gov/scripts/medwatch/*)
   - Fax: 1-800-FDA-0178
   - Phone: 1-800-332-1088

Photo of actual product.

Find this and other Consumer Updates at *www.fda.gov/ForConsumers/ConsumerUpdates*

Sign up for free e-mail subscriptions at *www.fda.gov/consumer/consumerenews.html*

Sildenafil analog

determined by the FDA!

Adulteration of Dietary Supplements with Synthetic PDE5 Inhibitors

- ***Serious problem***
  - Potential serious adverse (even lethal) health affects
  - Adulteration with approved drugs but also their unapproved analogs (unknown toxicological effects)
  - High incidence of adulteration

Campbell *et al*., *J. Sex. Med.* 10 (2013) 1842-1849:
- **81%** out of 91 tested **herbal products adulterated** with synthetic PDE5 inhibitors and their analogs

SHORT COMMUNICATION

Drug Saf 2009; 32 (12): 1141-1146
0114-5916/09/0012-1141/$49.95/0

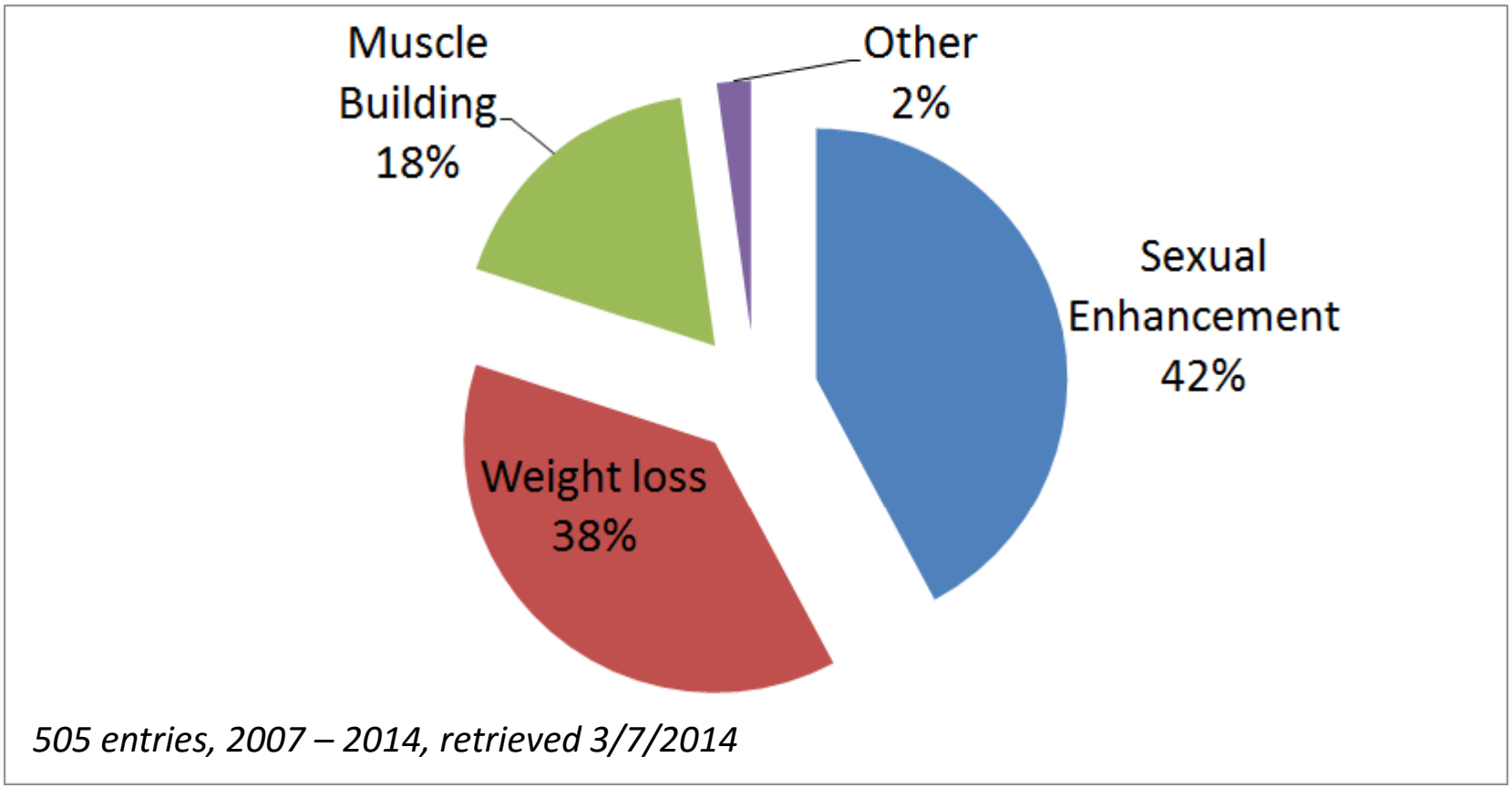
Safety and Quality Assessment of 175 Illegal Sexual Enhancement Products Seized in Red-Light Districts in Singapore

Min-Yong Low,[1,2] *Yun Zeng*,[1] *Lin Li*,[2] *Xiao-Wei Ge*,[1] *Ruth Lee*,[3] *Bosco-Chen Bloodworth*[1] and *Hwee-Ling Koh*[2]

1 Applied Sciences Group, Pharmaceutical Division, Health Sciences Authority, Singapore
2 Department of Pharmacy, Faculty of Science, National University of Singapore, Singapore
3 Health Products Regulation Group, Enforcement Division, Health Sciences Authority, Singapore

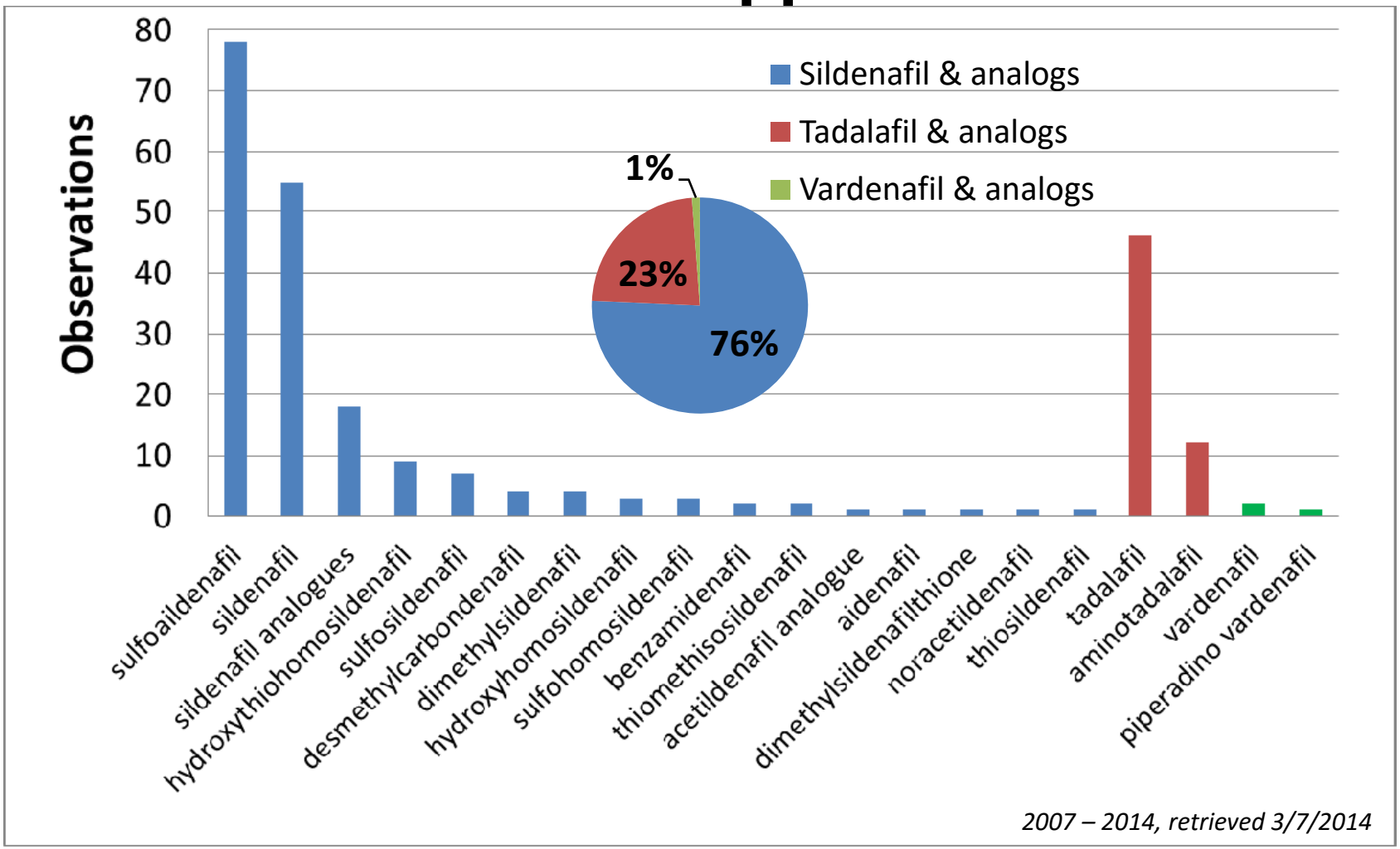
77% of the products contained synthetic drugs and their analogs

FDA-CDER Tainted Supplement Database

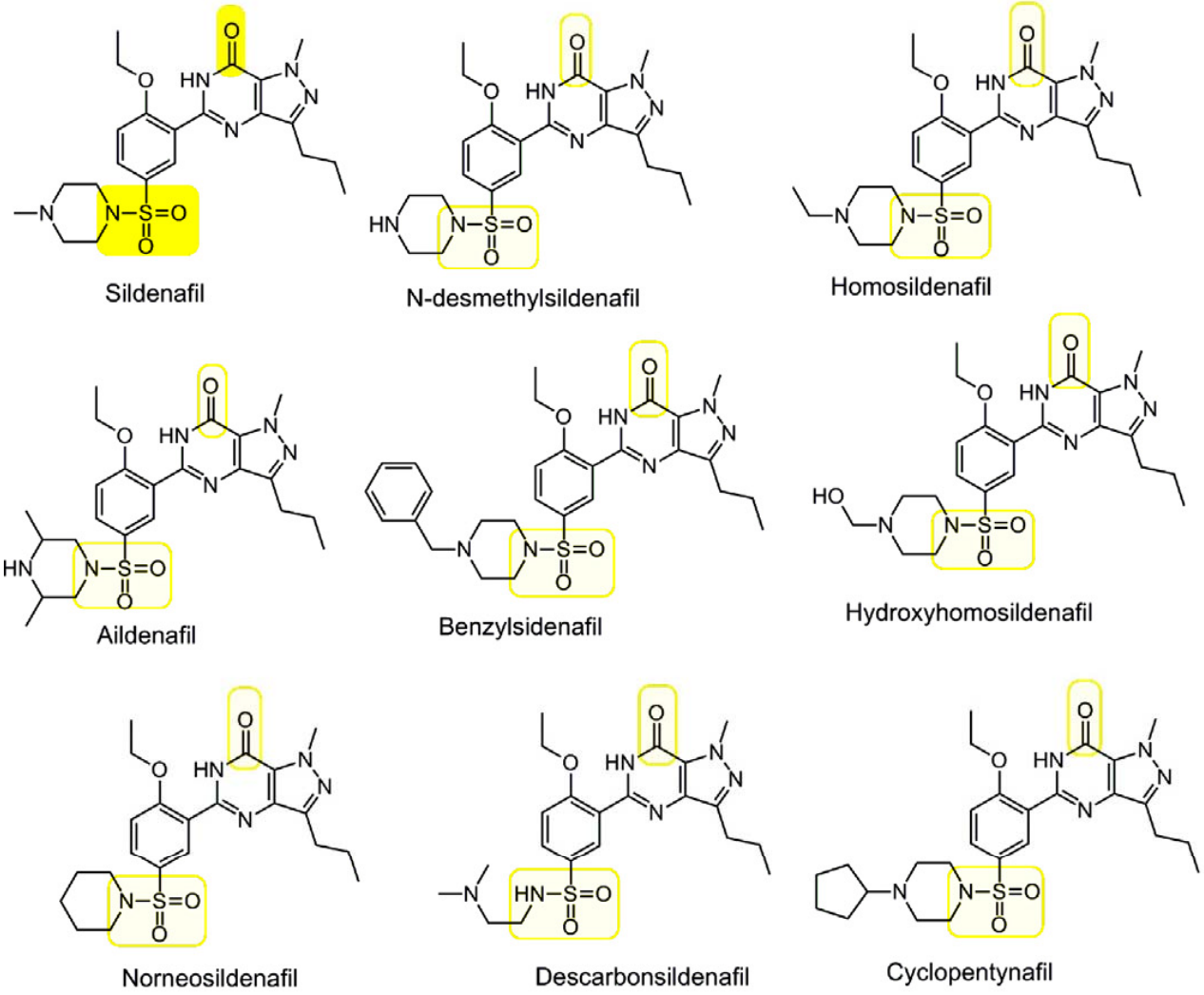


505 entries, 2007 – 2014, retrieved 3/7/2014

FDA-CDER Tainted Supplement Database

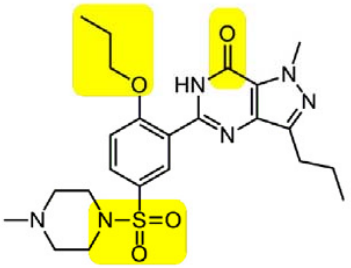


Sildenafil Analog Examples

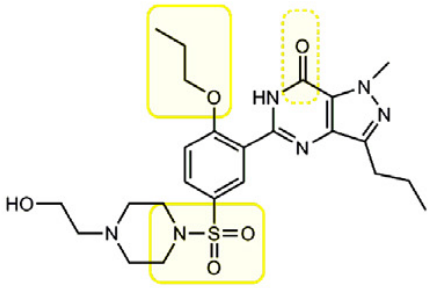


Patel *et al.* ,
J. Pharm. Biomed. Anal.
87 (2014) 176– 190

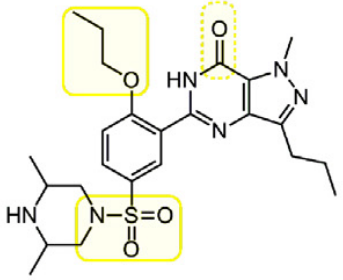
Sildenafil Analog Examples



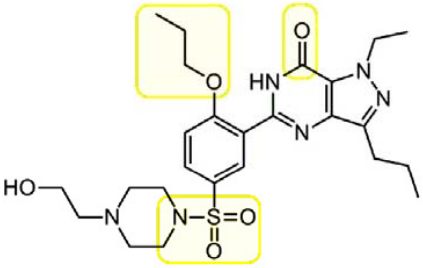
Propoxyphenyl sildenafil



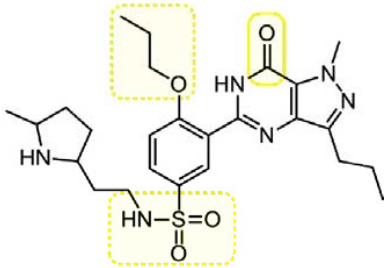
Propoxyphenyl hydroxyhomosildenafil



Propoxyphenyl aildenafil



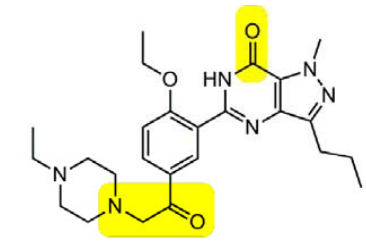
Mirodenafil



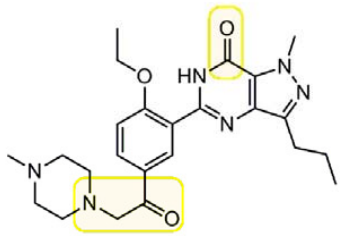
Udenafil

Patel *et al.* ,
J. Pharm. Biomed. Anal.
87 (2014) 176– 190

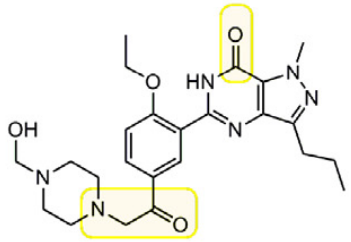
Sildenafil Analog Examples



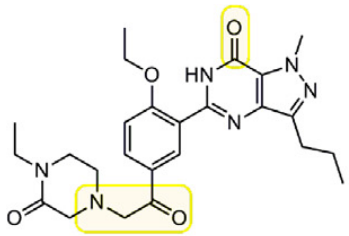
Acetildenafil



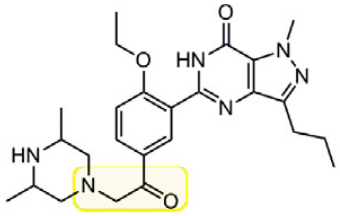
Noracetildenafil



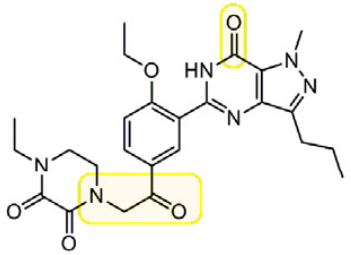
Hydroxyacetildenafil



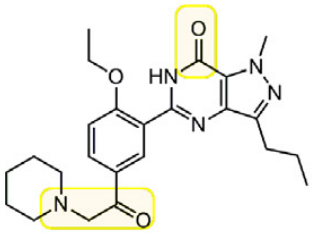
Oxohongdenafil



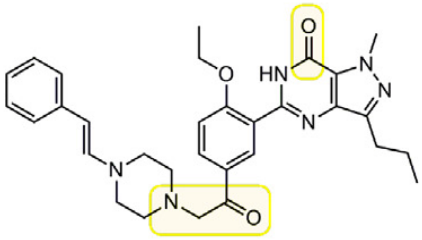
Dimethylacetildenafil



Dioxoacetildenafil



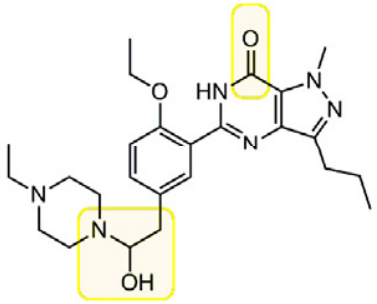
Piperidino acetildenafil



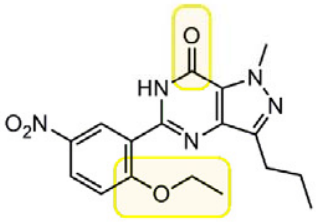
Cinnamyldenafil

Patel *et al.* ,
J. Pharm. Biomed. Anal.
87 (2014) 176– 190

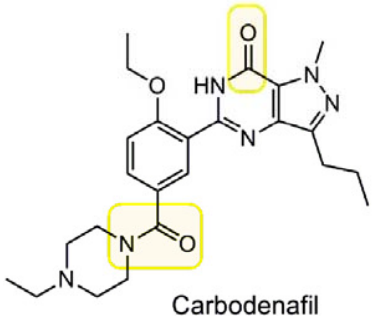
Sildenafil Analog Examples



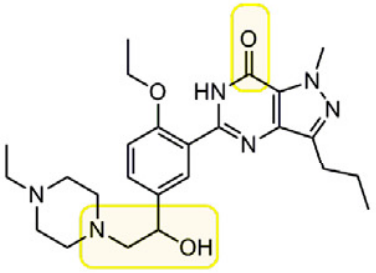
Isopiperazinonafil



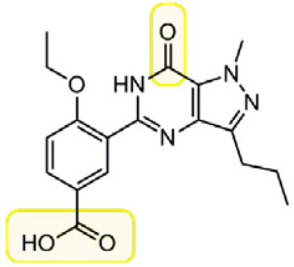
Nitrodenafil



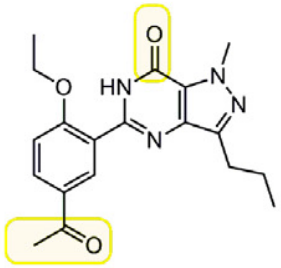
Carbodenafil



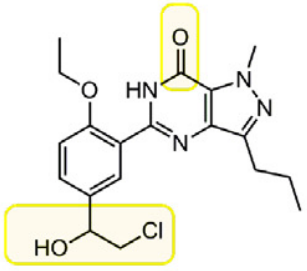
Dihydroacetildenafil
Piperazinonafil



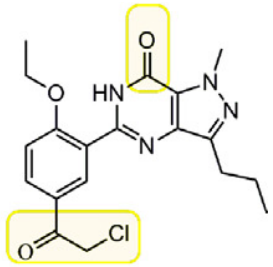
Acetil acid



Gendenafil



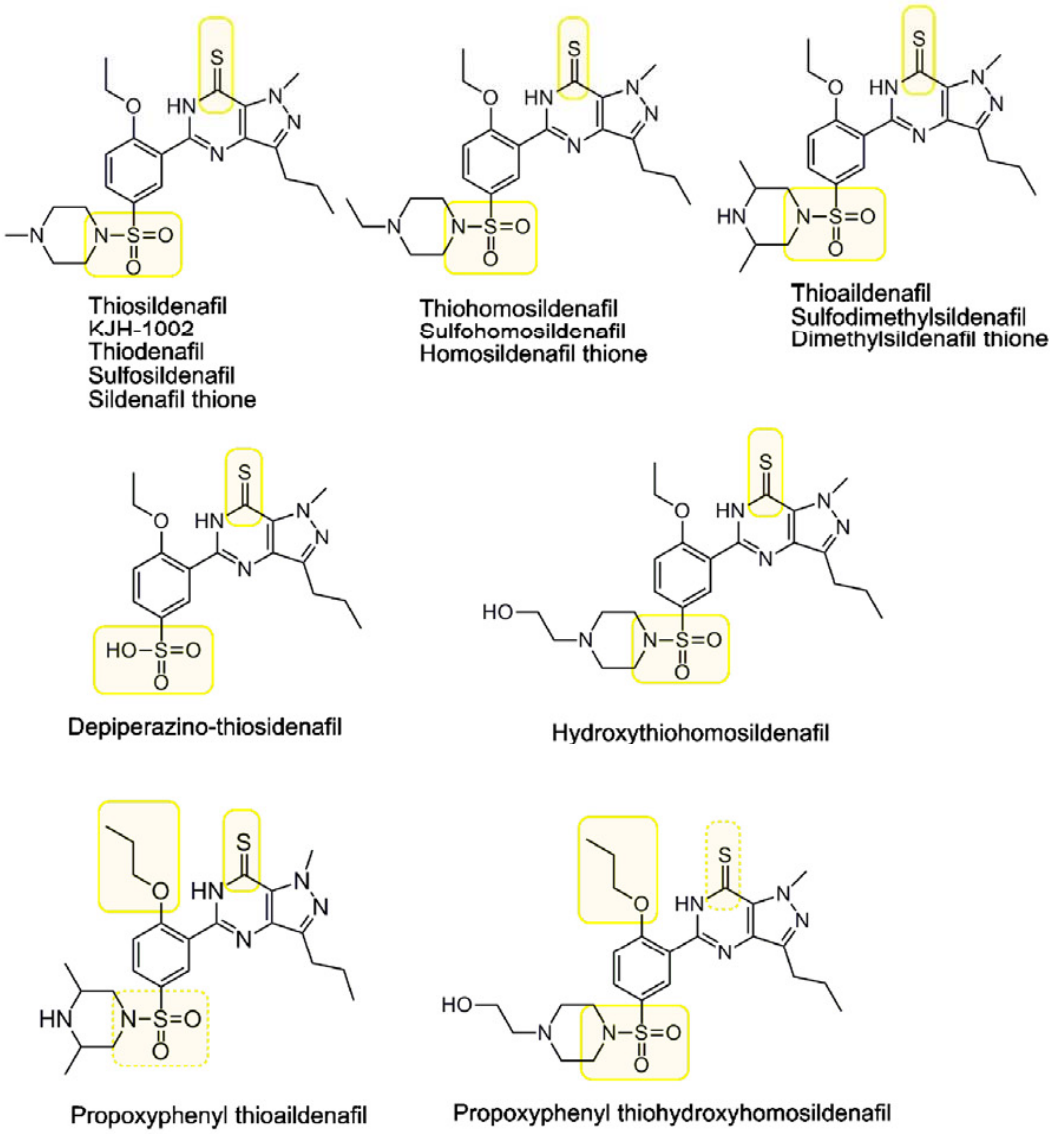
Hydroxychlorodenafil



Chlorodenafil

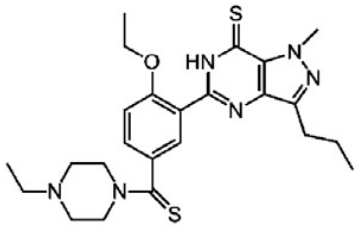
Patel *et al.* ,
J. Pharm. Biomed. Anal.
87 (2014) 176– 190

Sildenafil Analog Examples

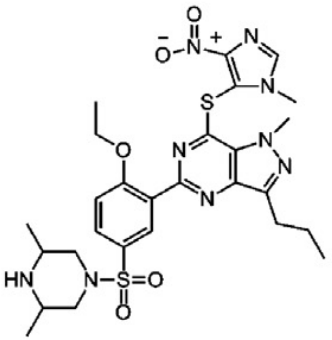


Patel *et al.* ,
J. Pharm. Biomed. Anal.
87 (2014) 176– 190

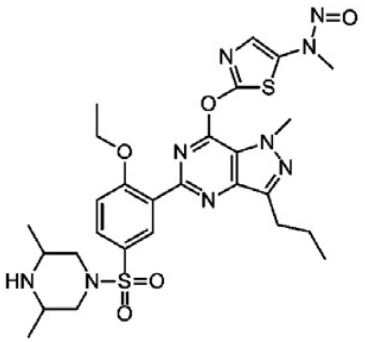
Sildenafil Analog Examples



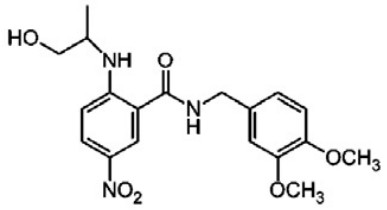
Dithio-desmethyl-carbodenafil



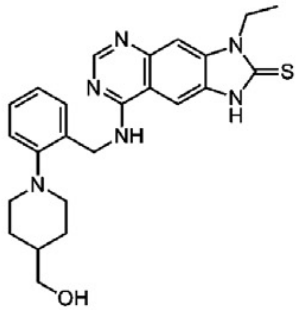
Muta-prodenafil



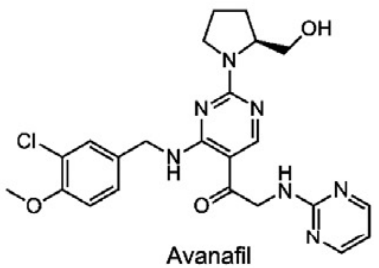
Nitroso-prodenafil



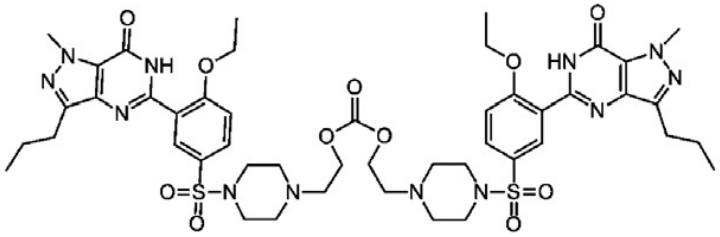
Benzamidenafil
Xanthoanthrafil



KF31327
Thioquinapiperifil



Avanafil



Lodenafil carbonate

Patel *et al.* ,
J. Pharm. Biomed. Anal.
87 (2014) 176– 190

Analytical Challenges:

- Number of potential synthetic PDE5 inhibitors:
  - more than 100 known analogs
  - more than 50 analogs reported as adulterants
- Availability of reference standards
- Inventiveness of adulterators:
  - exotic analogs
  - mixtures of analogs
  - embedding of adulterants into capsule walls
- Complex and variable dietary supplement matrices

Techniques in Current PDE5 Inhibitor Analysis

- Mass spectrometry (mostly LC-MS)
- (U)HPLC-UV/DAD
- Spectrofluorometry
- TLC/HPTLC
- Bioassay based on PDE5 inhibition
- ELISA
- Molecular spectroscopy (NMR, NIR, Raman)

Bioassay Based on PDE5 Inhibition

- Screening based on the common mode of action of PDE5 inhibitors
- Bioassays developed for screening of suitable drug candidates to detect their inhibition activity

Examples:

- *PDE Glo™ (Promega) - homogenous bioluminescent cAMP-PDE/cGMP-PDE assay*
- *PDE5A Assay Kit (BPS Bioscience) – fluorescence-based cGMP-PDE5A assay*

Enzyme-Linked Immunosorbent Assay (ELISA)

- Monoclonal antibodies specific to a common structure
- Potential for a group-specific screening

Examples:

- *Guo et al., Development of an immunoassay for rapid screening of **vardenafil and its potential analogues** in herbal products based on a group specific monoclonal antibody, Anal. Chim. Acta 658 (2010) 197–203*
- *Song et al., Development of enzyme-linked immunosorbent assay for rapid determination of **sildenafil** in adulterated functional foods, Food Agric. Immunol. 23 (2012) 338–351*

Thin Layer Chromatography (TLC)

- Screening and preliminary identification limited to known analogs with reference standards
- Cheap, fast but not very sensitive
- HPTLC can improve sensitivity (densitometric analysis of spots can be used for quantitation)

Examples:

- *Cai et al., J. Liquid Chromatogr. Relat. Technol. 33 (2010) 1287–1306 (8 compounds)*
- *Abourashed et al., J. Planar Chromatogr. Mod. TLC 18 (2005) 372–376 (sildenafil)*
- *Reddy et al., J. Planar Chromatogr. Mod. TLC 19 (2006) 427–431 (sildenafil)*

Spectrofluorometry

- Measurement based on excitation and emission maxima of known PDE5 inhibitors
- Potential for screening and (semi-) quantitation
- Sensitivity and linearity can be improved by addition of surfactants (demonstrated for sildenafil)

Examples:

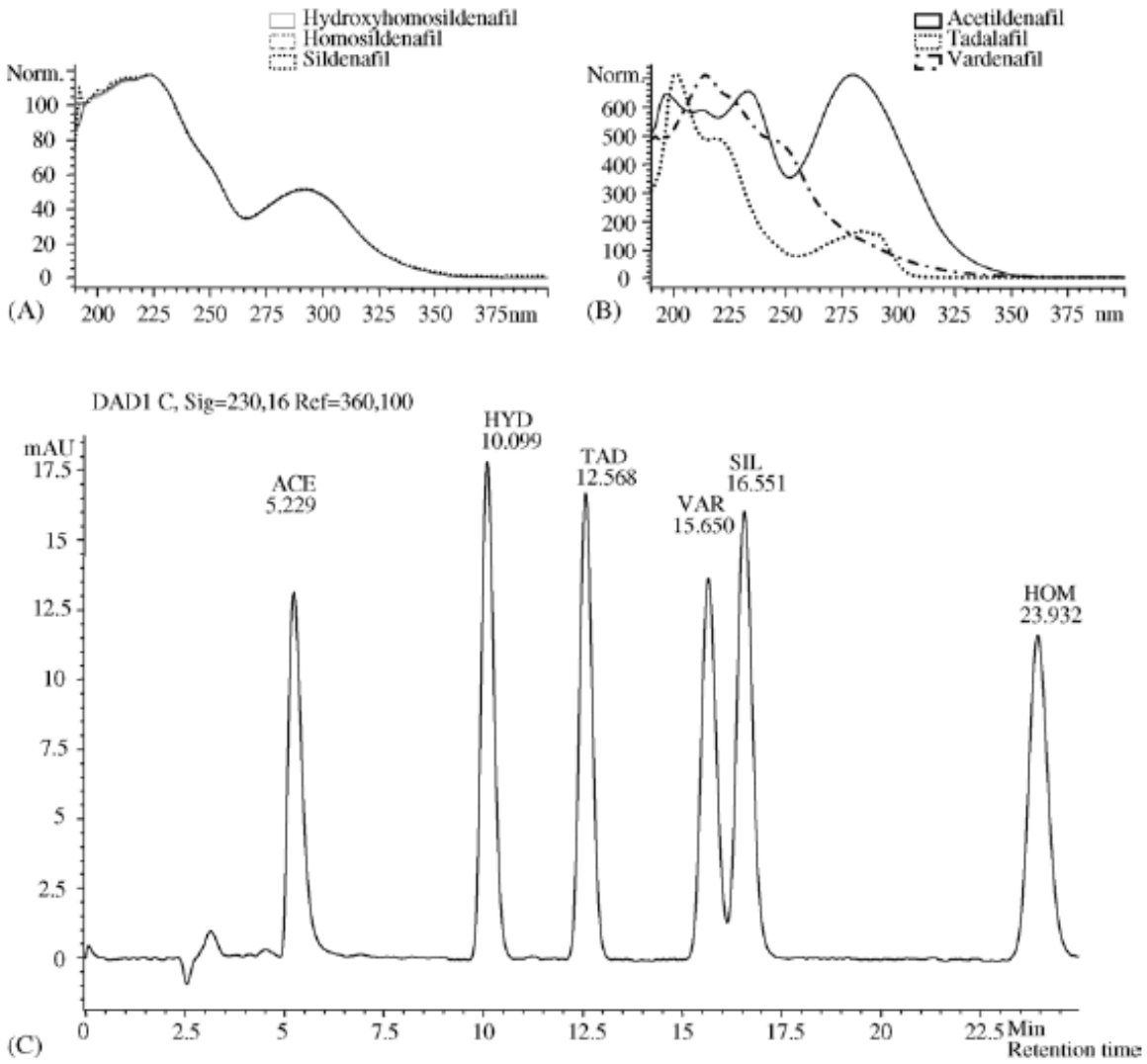
- *Wang et al., Anal. Methods 2 (2010) 519–524*
- *Anumolu et al., Asian J. Pharm. Clin. Res. 6 (2013)326-329*

(U)HPLC-UV/DAD

- Screening/quantitation of known adulterants
- Detection of structurally similar compounds
- Limited identification
- Possibility to combine with LC-MS for improved screening and identification

Examples:

- *Zou et al., J. Chromatogr. A 1104 (2006) 113–122*
  (6 compounds)
- *Sacré et al., J. Chromatogr. A 1218 (2011) 6439–6447*
  (8 compounds)
- *Sakamoto et al., J. AOAC Int. 95 (2012) 1048-1052*
  (novel analog identification)


Hydroxyhomosildenafil
Homosildenafil
Sildenafil
Norm.
100
80
60
40
20
0
(A)
200 225 250 275 300 325 350 375nm
Acetildenafil
Tadalafil
Vardenafil
Norm.
600
500
400
300
200
100
0
(B)
200 225 250 275 300 325 350 375 nm
DAD1 C, Sig=230,16 Ref=360,100
mAU
17.5
15
12.5
10
7.5
5
2.5
0
ACE
5.229
HYD
10.099
TAD
12.568
VAR
15.650
SIL
16.551
HOM
23.932
0 2.5 5 7.5 10 12.5 15 17.5 20 22.5 Min
Retention time
(C)

Nuclear Magnetic Resonance (NMR)

- Powerful for structure elucidation
- Technological advances (new NMR experiments and data processing tools) improved sensitivity and enabled measurements in solutions
- Diffusion ordered spectroscopy (DOSY) NMR
  - separation based on diffusion coefficients, allowing fingerprinting of active ingredients and excipients
- Potential for screening, identification, and quantitation of adulterants

Examples:

- Balayssac et al., J. Pharm. Biomed. Anal. 50 (2009) 602–612.

- Silva et al., Magn. Reson. Chem. 51 (2013) 169-176

Mass Spectrometry (MS)

- Direct MS without chromatographic separation (Ambient MS or Flow-Injection MS)
- GC-MS – limited use for identification
- LC-MS – prevalent technique for PDE5 inhibitors

<u>Benefits of MS:</u>

- Sensitivity
- Selectivity – tandem MS (MS/MS) and accurate mass-high resolution (AM/HR) MS and MS/MS
- Structure-based identification/confirmation
- Can be combined with UV or fluorescence detection
- Suitable for both targeted and non-targeted analysis

Targeted MS Analysis

- Analyte-specific conditions for data acquisition and/or data analysis
- Typically SIM or MS/MS (MRM) analysis
- Known chromatographic behavior (retention times) and MS data (MS or MS/MS spectra and ion ratios)
- Screening of known adulterants
- Quantitative analysis for compounds with reference standards

Example:

- *Lee et al., J. Pharm. Biomed. Anal. 83 (2013) 171– 178*
  (38 PDE5 inhibitors)

Non-Targeted MS Analysis

- Analyte-specific conditions not used for data acquisition
- Full-scan MS analysis (precursor ion and/or all-ion fragmentation)
- Increased selectivity using AM/HR MS(-MS)
- Data-dependent experiments with ion trap or hybrid instruments (Q-Trap, Q-TOF, Q-Exactive) based on known or predicted structures or common (characteristic) MS fragments
- Screening of known and unknown adulterants

Examples:

- *H.M. Lee & B.J. Lee, Food Addit. Contam. 28 (2011) 396–407*
- *Shi et al., J. Chromatogr. A (doi: 10.1016/j.chroma.2013.12.030)*

Fitness For Purpose Statements

(1) Screening Method

(2) Identification/Confirmation Method

Fitness For Purpose Statement

“Screening Method”

The method must be able to screen known and unknown (unexpected) PDE5 inhibitors in various dietary supplement matrices.

Questions for SPDS Discussion

"Screening Method"

- Time-to-signal requirement?
- Limit of detection?
- Rate of false negatives and false positives?
- Lab-based or field-based?
- Cost of analysis?

Fitness For Purpose Statement

“Identification/Confirmation Method”

The method must be able to identify known and unknown (unexpected) PDE5 inhibitors in various dietary supplement matrices.
Ideally, the method should combine targeted and non-targeted approaches, with the ability to quantitate PDE5 inhibitors for which reference standards are available.

Questions for SPDS Discussion

“Identification/Confirmation Method”

- Limit of identification?
- Identification criteria?
- Limit of quantitation?
- List of analytes for the targeted approach?
- Time-to-signal requirement?

QUESTIONS

Katerina Mastovska, Ph.D.
Covance Laboratories
Nutritional Chemistry and Food Safety
katerina.mastovska@covance.com

AOAC INTERNATIONAL STAKEHOLDER PANEL ON DIETARY SUPPLEMENTS

Katerina Mastovska, Covance Laboratories
PDE5 Inhibitors Working Group Chair

September 5, 2014

Boca Raton Resort, Boca Raton, Florida

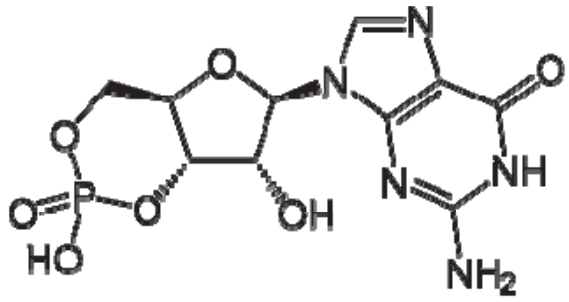
Technical Background

- What are PDE5 inhibitors?
- Why are they an issue in dietary supplements?
- What are the analytical challenges?

Phosphodiesterase Type 5 (PDE5) Inhibitors

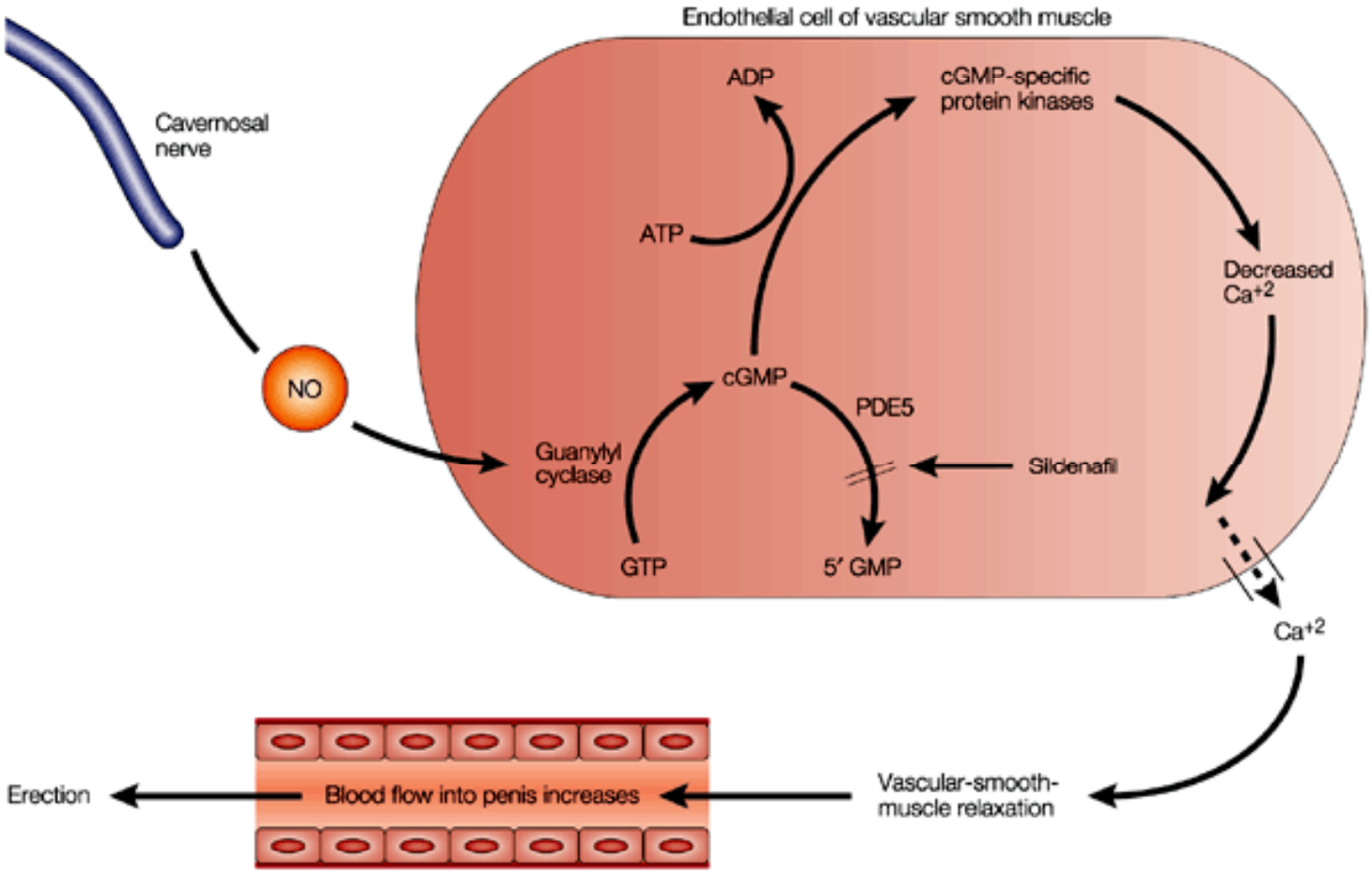
- Used in the treatment of erectile dysfunction (ED) and also explored for the treatment of pulmonary hypertension
- Block degradative action of PDE5 on cyclic guanosine monophosphate (cGMP) in smooth muscle cells lining the blood vessels supplying the corpus cavernosum of the penis (and arterial walls within the lungs)

cGMP



- cGMP = second messenger relaxing smooth muscle tissues, leading to the increased blood flow in blood vessels

PDE5 Inhibitors – Mechanism of Action



Approved PDE5 Inhibitor Drugs

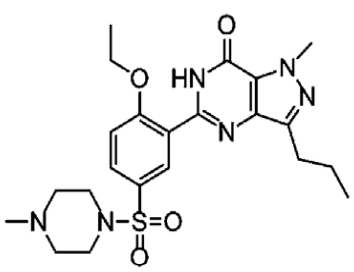
In the US:

- **Sildenafil** (Viagra®, Pfizer, 1998)
- **Tadalafil** (Cialis®, Elli Lilly, 2003)
- **Vardenafil** (Levitra®, Bayer, 2003)
- **Avanafil** (Stendra®, Vivus, 2012)

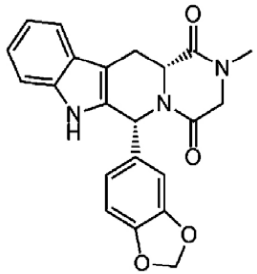
Other countries:

- **Udenafil** (Zydena®, Dong-A Pharmaceutical Co. Ltd) in South Korea and Malaysia
- **Mirodenafil** (Mvix®, SK Chemicals Life Science) in South Korea
- **Lodenafil carbonate** (Helleva®, Cristália Produtos Químicos e Farmacêuticos) in Brazil

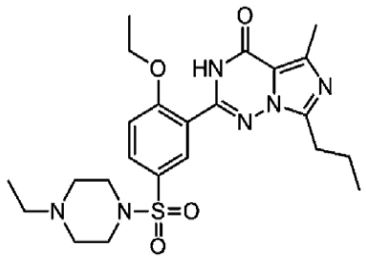
Approved PDE5 Inhibitor Drugs



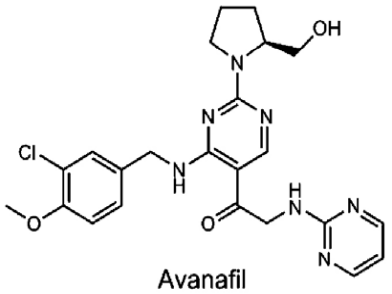
Sildenafil



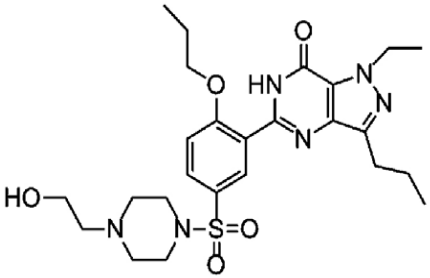
Tadalafil



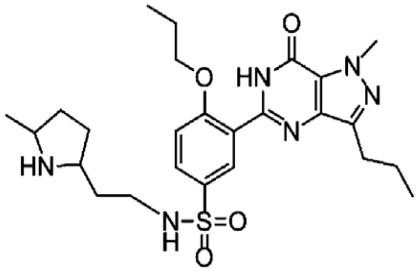
Vardenafil



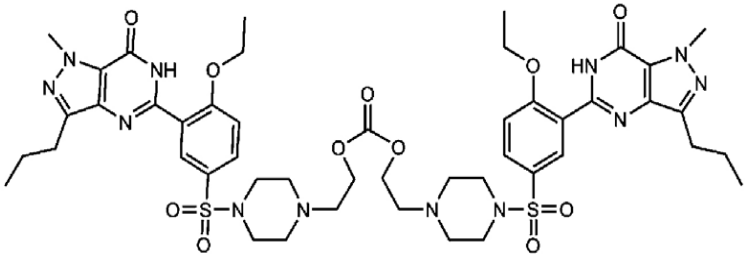
Avanafil



Mitrodenafil



Udenafil



Lodenafil carbonate

Patel *et al.* , *J. Pharm. Biomed. Anal.* 87 (2014) 176– 190

Adverse PDE5 Inhibitor Drug Side-Effects

- Nausea
- Headache
- Abdominal pain
- Back pain
- Photosensitivity
- Abnormal vision
- Eye pain
- Sudden hearing loss
- Hypotension
- Face edema
- Joint and muscle pain
- Nasal congestion
- Palpitation
- Tachycardia
- Rash
- Itch
- Priapism
- Heart attack
- Life-threatening drug interactions (*e.g.* with nitrates and cardiac antiarrhythmic drugs)

Adulteration of Dietary Supplements with Synthetic PDE5 Inhibitors

FDA Consumer Health Information
www.fda.gov/consumer

www.fda.gov/consumer/update/erectiledysfunction010408.html

Hidden Risks of Erectile Dysfunction "Treatments" Sold Online

Men looking online for "dietary supplements" to treat erectile dysfunction (ED) or enhance their sexual performance should beware: these products may contain prescription drugs or other undisclosed ingredients that can be harmful.

"The number of these problematic products available on the Internet appears to be increasing," says Michael Levy, director of the Food and Drug Administration's (FDA) Division of New Drugs and Labeling Compliance. The division is part of the Office of Compliance (OOC) in the agency's Center for Drug Evaluation and Research (CDER).

Many consumers perceive these products as completely safe because they are often sold with labeling, suggesting that they are all-natural alternatives to prescription drug products that have been approved by FDA for treating ED.

But these products may be laced with potentially hazardous ingredients that aren't noted on the label.

Since 2004, FDA has become aware of several such "dietary supplements" (see sidebar for list).

Viagra Ingredient Found

Working with other FDA components, the division's Internet and Health Fraud Team led an Internet survey in which more than one-third of purchased "dietary supplements" claiming to spur sexual enhancement or treat ED contained undisclosed prescription drug ingredients or similar substances.

Six of the 17 products contained sildenafil (the active ingredient in Viagra) or a substance similar to either sildenafil or vardenafil. Vardenafil is the active ingredient in Levitra, another FDA-approved prescription drug that treats ED.

Mark Hirsch, a medical team Leader in CDER's Division of Reproductive and Urologic Products, says this undisclosed presence of prescription drug ingredients—and similar compounds known as analogs of the drugs—can lead to serious side effects in users.

Dangerous Interactions

"These products may interact in dangerous ways with drugs that a consumer is already taking," Hirsch says. For example, taking sildenafil in addition to certain prescription drugs containing nitrates may lower blood pressure to an unsafe level.

People with diabetes, high blood pressure, high cholesterol,

Online Products to Avoid

Since 2004, FDA has identified several products sold online as so-called "dietary supplements" for treating erectile dysfunction and enhancing sexual performance. These products have contained potentially harmful, undeclared ingredients. Included among them are

- Actra-Rx
- Actra-Sx
- Libidus
- Nasutra
- Neophase
- Vigor-25
- Yilishen
- Zimaxx
- 4EVERON
- Liviro3
- Lycium Barbarum L.
- Adam Free
- Rhino V Max
- V.Max
- True Man
- Energy Max
- HS Joy of Love
- NaturalUp
- Blue Steel
- Erextra
- Super Shangai
- Strong Testis
- Shangai Ultra
- Shangai Ultra X
- Lady Shangai
- Shangai Regular, also marketed as Shangai Chaojimengnan
- Hero
- Naturalë Super Plus
- Xiadafil VIP tablets (Lots 6K029 and 6K209-SEI only)

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Adulteration of Dietary Supplements with Synthetic PDE5 Inhibitors

- ***Serious problem***
  - Potential serious adverse (even lethal) health affects
  - Adulteration with approved drugs but also their unapproved analogs (unknown toxicological effects)
  - High incidence of adulteration

Campbell *et al*., *J. Sex. Med.* 10 (2013) 1842-1849:
- **81%** out of 91 tested **herbal products adulterated** with synthetic PDE5 inhibitors and their analogs

Adulteration of Dietary Supplements with Synthetic PDE5 Inhibitors

SHORT COMMUNICATION

Drug Saf 2009; 32 (12): 1141-1146
0114-5916/09/0012-1141/$49.95/0

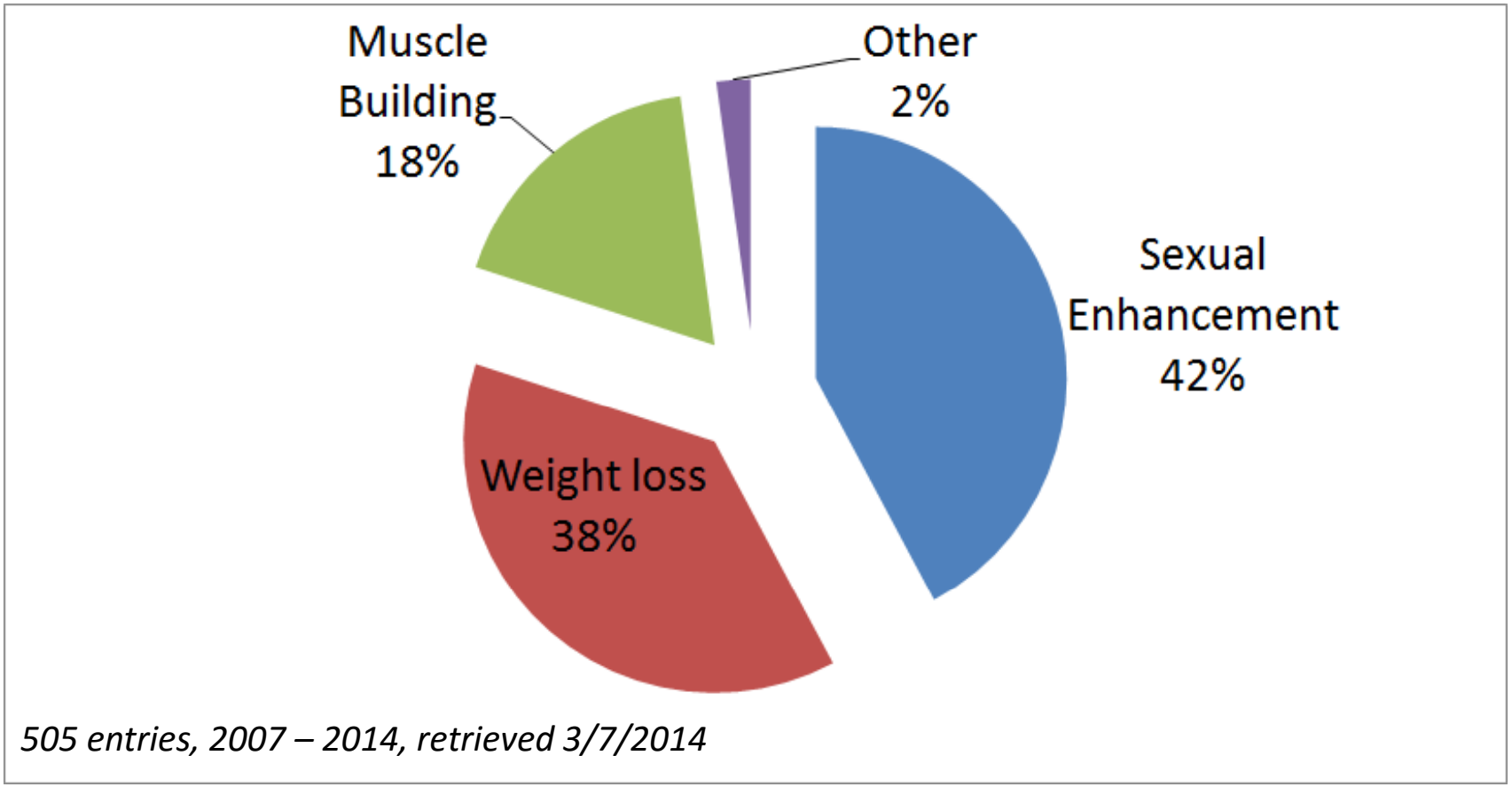
Safety and Quality Assessment of 175 Illegal Sexual Enhancement Products Seized in Red-Light Districts in Singapore

Min-Yong Low,[1,2] *Yun Zeng,*[1] *Lin Li,*[2] *Xiao-Wei Ge,*[1] *Ruth Lee,*[3] *Bosco-Chen Bloodworth*[1] and *Hwee-Ling Koh*[2]

1 Applied Sciences Group, Pharmaceutical Division, Health Sciences Authority, Singapore
2 Department of Pharmacy, Faculty of Science, National University of Singapore, Singapore
3 Health Products Regulation Group, Enforcement Division, Health Sciences Authority, Singapore

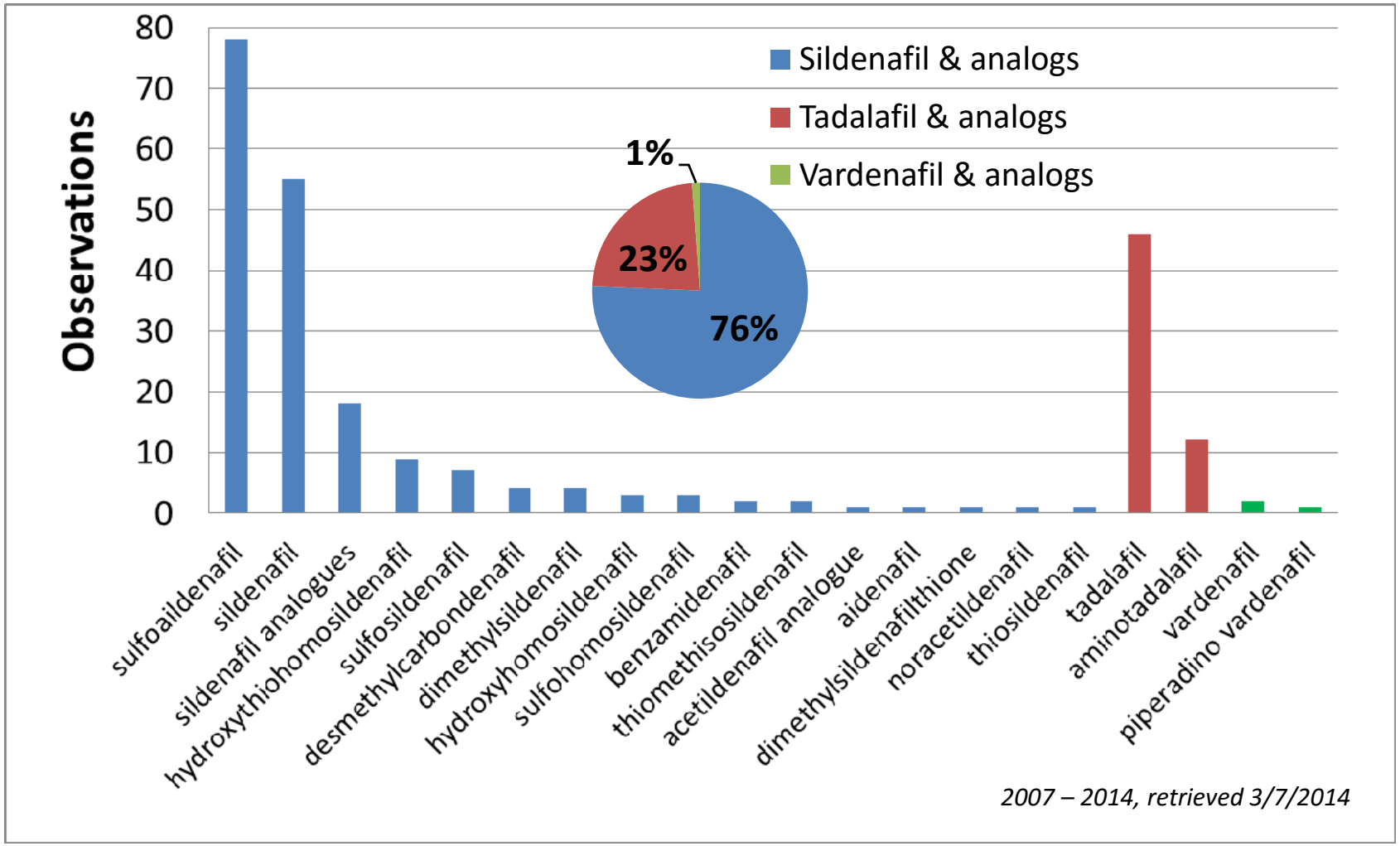
77% of the products contained synthetic drugs and their analogs

FDA-CDER Tainted Supplement Database



505 entries, 2007 – 2014, retrieved 3/7/2014

FDA-CDER Tainted Supplement Database



Analytical Challenges

- Number of potential synthetic PDE5 inhibitors:
  - more than 100 known analogs
  - more than 50 analogs reported as adulterants
- Availability of reference standards
- Inventiveness of adulterators:
  - exotic analogs
  - mixtures of analogs
  - embedding of adulterants into capsule walls
- Complex and variable dietary supplement matrices

Fitness for Purpose

(1) Screening Method

(2) Identification/Determination Method

Fitness for Purpose

“Screening Method”

The method must be able to screen known and unknown (unexpected) PDE5 inhibitors in various dietary supplement matrices.

Fitness for Purpose

“Identification/Determination Method”

The method must be able to identify known and unknown (unexpected) PDE5 inhibitors in various dietary supplement matrices. Ideally, the method should combine targeted and non-targeted approaches, with the ability to quantitate PDE5 inhibitors for which reference standards are available.

PDE5 Inhibitors Working Group: Members

- Katerina Mastovska, Covance (Chair)
- Anton Bzhelyansky, USP
- Teresa Cain, FDA
- Jana Hildreth, Blaze Science Industries
- David Kennedy, Phenomenex
- James Neal-Kababick, Flora Research
- Melissa Phillips, NIST
- Steve Royce, Agilent
- John Travis, NSF International
- Lukas Vaclavik, FDA
- Jerry Zweigenbaum, Agilent
- Joe Betz, NIH
- Anatoly Chlenov, PerkinElmer
- John Edwards, Process NMR
- Todd Koch, Pfizer
- Alexander Krynitsky, FDA
- Stephen Lock, AB SCIEX
- Elisa Nickum, FDA
- Catherine Rimmer, NIST
- Brian Schaneberg, Starbucks
- Olga Shimelis, Supelco
- Garrett Zielinski, Covance

PDE5 Inhibitors Working Group: Work to Date

- 8 teleconferences (May 2014 – July 2014)
- 3 SMPRs Drafted
  - Screening Method for PDE5 Inhibitors
  - Identification of PDE5 Inhibitors
  - Determination of PDE5 Inhibitors
- 30 day public comment period
  (July 25, 2014 – August 25, 2014)
- SMPRs made ready for SPDS review and approval

SMPRs Key Points: Target Compound Panel

- Acetaminotadalafil
- Acetildenafil
- Avanafil
- Homosildenafil
- Hydroxyacetildenafil
- Hydroxyhomosildenafil
- Hydroxythiohomosildenafil
- Lodenafil carbonate
- Mirodenafil
- Propoxyphenyl hydroxyhomosildenafil
- Sildenafil
- Tadalafil
- Thiohomosildenafil
- Udenafil
- Vardenafil

SMPRs Key Points: Matrices

- Tablets
- Capsules (both the content and the capsule shells)
- Softgels
- Gelcaps
- Liquids
- Powders
- Extracts

SMPR Key Points: Screening Method

- **Intended Use**: Routine surveillance of dietary ingredients and products by a trained technician.
- **Applicability**: Qualitative assay for PDE5 inhibitors in dietary ingredients and supplements.
- **Maximum Time-To-Result:** 1 hour
- **Non-Target Compound Panel:** Shall be developed for the selectivity study based on the used analytical technique.

SMPR Key Points: Screening Method

	Parameter	Parameter Requirements	Target Test Concentration	Minimum Acceptable Results
Single Laboratory Validation	POD @ low concentration	Minimum of 33 replicates per matrix type, spiked at or below the designated low level target test conc.	100 ppm	90% POD[§]
	POD @ high concentration	Minimum of 5 replicates per matrix type spiked at 10x the designated low level target test conc.	10 x low conc.	100% correct analyses are expected per matrix type
	POD @ zero concentration	Minimum of 5 replicates per matrix type.	0 ppm	

[§] 95% confidence interval

SMPR Key Points: Screening Method

	Parameter	Parameter Requirements	Target Test Concentration	Minimum Acceptable Results
Multi -Laboratory Validation	LPOD	Use Appendix N: ISPAM Guidelines for Validation of Qualitative Binary Chemistry Methods.	low concentration	≥ 0.85§
			10 x low conc.	≥ 0.95§
	$LPOD_{(0)}$		0 ppm	≤ 0.05§
§ 95% confidence interval				

SMPR Key Points: Screening Method

Selectivity Study:

	Parameter	Parameter Requirements	Final Test Conc.	Minimum Acceptable Results
Single Laboratory Validation	Target	Test each target compound listed in Annex II at the final test concentration.	Low concentration	100% positive results**
	Non-target	Test each non-target panel compound at the final test concentration or at the highest expected matrix concentration in the case of naturally occurring matrix components. A list of potential non-target compounds for immunoassays is provided in Annex III.	10 x low conc.	≥95% negative results

**100% correct analyses are expected. Some aberrations may be acceptable if the aberrations are investigated, and acceptable explanations can be determined and communicated to method users.

SMPR Key Points: Identification Method

- **Intended Use**: Reference method for dispute resolution.
- **Applicability**: Identification of PDE5 inhibitors in dietary ingredients and supplements.
- **Identification Method:** A method that is capable of identifying the PDE5 inhibitors listed in Annex II and providing at least class identification of other PDE5 inhibitors based on their structural similarity to the compounds listed in Annex II . The identification should be done using technique-specific, generally acceptable criteria, such as those given in 2002/657/EC.
- **Maximum Time-To-Result:** No maximum time.

SMPR Key Points: Identification Method

	Parameter	Parameter Requirements	Target Test Concentration	Minimum Acceptable Results
Single Laboratory Validation	POI @ low concentration	Minimum of 33 replicates representing all target compounds in Annex II and all matrix types listed in Annex III, spiked at or below the designated low level target test conc.	100 ppm	90% POI[§] of the pooled data for all target compounds and matrices
	POI @ high concentration	Minimum of 5 replicates per matrix type spiked at 10x the designated low level target test conc.	10 x low conc.	100% correct analyses are expected
	POI @ zero concentration	Minimum of 5 replicates per matrix type.	0 ppm	

[§] 95% confidence interval

SMPR Key Points: Screening Method

	Parameter	Parameter Requirements	Target Test Concentration	Minimum Acceptable Results
Multi -Laboratory Validation	LPOI	Use Appendix N: ISPAM Guidelines for Validation of Qualitative Binary Chemistry Methods.	low concentration	≥ 0.85§
			10 x low conc.	≥ 0.95§
	$LPOI_{(0)}$		0 ppm	≤ 0.05§
§ 95% confidence interval				

SMPR Key Points: Determination Method

- **Intended Use**: Reference method for dispute resolution.
- **Applicability**: Quantitative method for PDE5 inhibitors in dietary ingredients and supplements for use in testing laboratories by trained technicians.
- **Maximum Time-To-Result:** No maximum time.

SMPR Key Points: Determination Method

Single Laboratory Validation	Analytical range	50 - 200 ppm
	Limit of Quantitation (LOQ)	≤ 50 ppm
	Repeatability (RSD_r)	≤ 20%
	Recovery	70% to 120% of mean spiked recovery over the analytical range
Multi-Lab Validation	Reproducibility (RSD_R)	≤ 30%

Motion

- Move to accept the Standard Method Performance Requirements for *Screening Method for PDE5 Inhibitors* as presented.

Discussion?

Motion

- Move to accept the Standard Method Performance Requirements for *Identification of PDE5 Inhibitors* as presented.

Discussion?

Motion

- Move to accept the Standard Method Performance Requirements for *Determination of PDE5 Inhibitors* as presented.

Discussion?

AOAC SPIFAN Stakeholder Meeting

Iodine

Saturday, September 17th, 2011

New Orleans, LA

Iodine

Darryl Sullivan
Director of Scientific and Regulatory Affairs
Covance Laboratories
darryl.sullivan@covance.com

Background and History

- Iodine was discovered by Courtois in 1811
- Iodine is a chemical element with the symbol I and atomic number 53
- Iodine like many other halogens occurs primarily as a diatomic molecule I_2
- Iodine is a relatively rare element in nature, ranking 47^{th} in abundance

Background and History

- Iodine is essential in humans for the synthesis of thyroid hormones
- Thyroid hormones regulate physiological processes such as growth, development, metabolism, and reproductive functions
- Due to it’s rarity, iodine deficiency affects as many as 2 billion people worldwide

Background and History

- Iodine deficiency in mothers can lead to increased rates of abortion, prenatal death, infant mortality, and babies being born with central nervous system defects
- Iodine deficiency in infants may cause mild decreases in intellectual performance to severe mental retardation

Iodine Chemistry

- Iodine under standard conditions is a bluish back solid.

Iodine Chemistry

- Iodine in a gas phase shows a violet color which is the origin of the name (Greek)

Iodine Chemistry

- Elemental iodine is readily soluble in most organic solvents, but only slightly soluble in water
- Potassium iodide, the most common form of iodine in nutrition, is highly water soluble

Iodine Recommended Daily Allowances (RDA)

- Adolescents and adults 150 mcg/day
- Pregnant women 220 mcg/day
- Lactating women 290 mcg/day

Iodine Recommended Daily Allowances (RDA)

- Infants (0-6 months) 110 mcg/day
- Infants (7-12 months) 130 mcg/day
- Children (1-3 years) 90 mcg/day
- Children (3-13 years) 90-120 mcg/day

Regulations (Iodine content)

Regulating Entity	Regulation		
	Units	Minimum	Maximum
Australia/ New Zealand	mcg/100 kcal	15	42
China	mcg/100 kcal	18	58.6
CODEX	mcg/100 kcal	20	50

Regulations (Iodine content)

Regulating Entity	Regulation		
	Units	Minimum	Maximum
European Union	mcg/100 kcal	(20)	50
Thailand	mcg/100 kcal	10	50
United States	mcg/100 kcal	(15)	(50)

Calculated Range for Infant Formula

- Minimum = 100 μg/100 mL
- Maximum = 500 μg/100 mL

Analysis of Iodine – Sample Digestion

- Direct analysis
- Dry ashing procedures
- Open vessel ashing with acids
- Open vessel ashing with base
- Microwave oven for above

Analysis of Iodine – Detection

- Titration methods
- Catalytic colorimetric reactions
- Ion specific electrodes
- Atomic Absorption (flame and furnace)

Analysis of Iodine – Detection

- X-ray fluorescence
- HPLC, GC, IC
- Neutron Activation
- ICP – MS

Analysis of Iodine – Precautions

- Losses of iodine during digestion
- Laboratory contamination
- Absorption of iodine into glass
- Background readings (ICP-MS)
- Interferences

Analysis of Iodine – ICP-MS

- Sample digestion using acid and tetramethyl ammonium hydroxide (TMAH)
- Sample digestion using base

Official Methods for Iodine

- **AOAC 992.22 – HPLC EC Detection**
  - **Requires use of a membrane filter to remove protein and insoluble material**
  - **Chromatography is challenging**

Official Methods for Iodine

- **AOAC 992.24 – Ion Specific Electrode**
  - **Very simple method to set up and use**
  - **Suffers from a number of interferences**

Official Methods for Iodine

- **EN 15111:2007 – ICP-MS**
  - **Method used microwave digestion and TMAH extraction**
  - **Not collaboratively studied on infant formula or adult nutrtionals**

Fitness for Purpose

Iodine Working Group

Fitness for Purpose Statement

- An analytical method to determine the level of total iodine in infant formula and adult nutritionals, as defined by AOAC SPIFAN, in concentration ranges from 5 mcg/100 mL to 1000 mcg/100 mL. Time to signal should be <12 hours. The method need to be capable of dispute resolution.

Questions?

The Scientific Association Dedicated to Analytical Excellence®

Approval of SMPR for: Iodine

Darryl Sullivan

Covance Laboratories

Las Vegas, Nevada USA

September 29, 2012

The Scientific Association Dedicated to Analytical Excellence®

Agenda

- **Review**
  - Draft SMPR
  - Comments / Responses
- **Motion to Adopt SMPR**

Analyte Definition

- **Description of the analyte: Total Iodine**
- **Rationale: All forms of iodine are available and need to be considered in the analysis**
- **Implications: An effective digestion must be part of the analytical methodology**

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Method Performance Requirements:

Analytical range	5 - 1000*	
Limit of Quantitation (LOQ)	≤ 5 *	
Repeatability (RSD_r)	5 - 1000*	≤ 8%
Recovery	90% to 110% of mean spiked recovery over the range of the assay.	
Reproducibility (RSD_R)	5 - 1000*	≤ 15%
Concentrations apply to: a) 'ready-to-feed" liquids "as is"; b) re-constituted powders (25 g into 200 g of water); and c) liquid concentrates diluted 1:1 by weight.		
* mcg /100 g reconstituted final product.		

Specific Performance Claims

- **Analytical range: 5-1000 mcg/100 g reconstituted**
- **LOD: N/A**
- **LOQ: ≤ 5 mcg/100 g reconstituted**

Specific Performance Claims

- **Repeatability: ≤ 8%**
- **Recovery: 90% - 110%**
- **Reproducibility: ≤ 15%**

The Scientific Association Dedicated to Analytical Excellence®

Stakeholder Comments

Draft SMPR's were posted on AOAC web-site for Stakeholder comments

Two comments were received for the Draft SMPR.

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Stakeholder Comment #1

<u>Comment</u> – should the precision be differentiated at different concentrations of the analyte to be consistent with other SMPR's

<u>Response</u> – the precision is consistent with the SMPR's for other trace elements (Se, Cr, Mo)

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Stakeholder Comment #2

<u>Comment</u> – should the time to result be specified at 12 hours, or list no specified time to result

<u>Response</u> – the time to result is consistent with the SMPR's for other trace elements (Se, Cr, Mo) which listed an 8 hour time to results

The Scientific Association Dedicated to Analytical Excellence®

Motion for Approval

I move to approve the SMPR for Iodine.


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Questions??

AOAC SMPR 2016.002

Standard Method Performance Requirements (SMPRs®) for Detection and Quantitation of Selected Food Allergens

Intended Use: Reference method for cGMP compliance

1 Purpose

AOAC SMPRs describe the minimum recommended performance characteristics to be used during the evaluation of a method. The evaluation may be an on-site verification, a single-laboratory validation, or a multi-site collaborative study. SMPRs are written and adopted by AOAC stakeholder panels composed of representatives from the industry, regulatory organizations, contract laboratories, test kit manufacturers, and academic institutions. AOAC SMPRs are used by AOAC expert review panels in their evaluation of validation study data for method being considered for *Performance Tested Methods*℠ or AOAC *Official Methods of Analysis*℠, and can be used as acceptance criteria for verification at user laboratories.

2 Applicability

Detection and quantitation of egg, milk, peanut, and hazelnut food allergens in finished food products and ingredients. Method(s) shall uniquely identify each allergen.

3 Analytical Technique

Mass spectrometry-based methods.

4 Definitions

Food allergens:

Hazelnut.—Any of the nuts deriving from species of the genus *Corylus*, especially the nuts of the species *Corylus avellana* (the common hazel tree).

Milk.—For the purposes of this SMPR, "milk" refers to pasteurized whole cow's (*Bos Taurus*) milk, and shall contain not less than 8 1/4% milk solids not fat and not less than 3 1/4% milkfat [*Code of Federal Regulations*, Title 21-Food and Drugs, § 131.110. Other internationally recognized definition may be applied.]

Peanut.—The seed of the *Arachis hypogaea* plant. For the purposes of this SMPR, includes both raw and roasted peanuts.

Whole egg.—A combination of pasteurized chicken (*Gallus gallus domesticus*) egg whites and egg yolks from the same production batch blended together in their entirety, in natural proportions [Introduction to Egg Products, U.S. Department of Agriculture-Food Safety and Inspection Service, http://www.fsis.usda.gov/wps/wcm/connect/c5c85914-5055-4f09-8098-1a179a1c6e14/EPT_Introduction.pdf?MOD=AJPERES, accessed 12/15/2015].

Method quantitation limit (MQL).—The minimum concentration or mass of analyte in a given matrix that can be reported as a quantitative result. MQL = average (blank) + 10 * s0 (blank) [*see* Table A3 in Appendix F: *Guidelines for Standard Method Performance Requirements*, *Official Methods of Analysis* (2016) 20th Ed., AOAC INTERNATIONAL, Rockville, MD, USA (http://www.eoma.aoac.org/app_f.pdf)].

Method detection limit (MDL).—The minimum concentration of a substance than can be measured and reported with 99% confidence that the analyte concentration is greater than zero. It is determined from analysis of a sample in a given matrix containing the analyte [Volume II—*Methods, Method Verification and Validation* ORA-LAB.5.4.5; Document No. IV-02; Version No.: 1.7; Section 2–*Microbiology*; Effective date: 10/01/03; Revised: 08/25/14; http://www.fda.gov/ScienceResearch/FieldScience/ucm171877.htm, accessed February 22, 2016].

Repeatability.—Variation arising when all efforts are made to keep conditions constant by using the same instrument and operator and repeating during a short time period. Expressed as the repeatability standard deviation (SD_r); or % repeatability relative standard deviation (%RSD_r) [*see* Table A3 in Appendix F: *Guidelines for Standard Method Performance Requirements*, *Official Methods of Analysis* (2016) 20th Ed., AOAC INTERNATIONAL, Rockville, MD, USA (http://www.eoma.aoac.org/app_f.pdf)].

Reproducibility.—The standard deviation or relative standard deviation calculated from among-laboratory data. Expressed as the reproducibility standard deviation (SD_R); or % reproducibility relative standard deviation (%RSD_R) [*see* Table A3 in Appendix F: *Guidelines for Standard Method Performance Requirements*, *Official Methods of Analysis* (2016) 20th Ed., AOAC INTERNATIONAL, Rockville, MD, USA (http://www.eoma.aoac.org/app_f.pdf)].

Recovery.—The fraction or percentage of spiked analyte that is recovered when the test sample is analyzed using the entire method [*see* spiking method in Appendix M: *Validation Procedures for Quantitative Food Allergen ELISA Methods: Community Guidance and Best Practices* (2016) 20th Ed., AOAC INTERNATIONAL, Rockville, MD, USA (http://www.eoma.aoac.org/app_m.pdf)].

Table 1. Method performance requirements

	Target allergen			
Parameter	Whole egg	Milk	Peanut	Hazelnut
Analytical range, ppm	10–1000	10–1000	10–1000	10–1000
MQL[a], ppm[b]	≤5	≤10	≤10	≤10
MDL[a], ppm[b]	≤1.65	≤3	≤3	≤3
Recovery, %	60–120	60–120	60–120	60–120
RSD_r, %	≤20	≤20	≤20	≤20
RSD_R, %	≤30	≤30	≤30	≤30

[a] Definitions for MQL and MDL provided in section 4.
[b] Reported as ppm of the target allergen in food commodity, i.e., 25 ppm of "whole egg" in cookies.

5 Method Performance Requirements

See Table 1.

6 System Suitability Tests and/or Analytical Quality Control

Suitable methods will include blank check samples, and check standards at the lowest point and midrange point of the analytical range.

7 Examples of Appropriate Reference Material(s)

Whole egg:
NIST 8445
LGC SAL-RSM-5 (check for characterization level)

Peanut:
NIST SRM 2387 (peanut butter)
LGC FAL-RFM1017-XXX

Hazelnut:
LGC FAL-RFM1015-50 or FAL-RFM1015-50Â or FAL-RFM1015-5

Additional materials can be found at the LGC and FAPAS websites:
LGC = http://www.lgcstandards.com/HK/en/search/?q=allergen:relevance:category:CEFP_77243
FAPAS = http://fapas.com/quality-control-materials/Available-quality-control-materials.cfm

Refer to Annex F: *Development and Use of In-House Reference Materials* in Appendix F: *Guidelines for Standard Method Performance Requirements*, *Official Methods of Analysis* (2016) 20th Ed., AOAC INTERNATIONAL, Rockville, MD, USA (http://www.eoma.aoac.org/app_f.pdf).

NIST = National Institute of Standards and Technology

LGC = Formerly the UK Laboratory of the Government Chemist, now simply "LGC Standards"

FAPAS = Formerly the Food Analysis Performance Assessment Scheme in the United Kingdom, now simply "FAPAS"

8 Validation Guidance

Method developers shall submit LOQ, MDL, recovery and precision data for the matrices in Table 2.

Appendix D: *Guidelines for Collaborative Study Procedures to Validate Characteristics of a Method of Analysis*, *Official Methods of Analysis* (2016) 20th Ed., AOAC INTERNATIONAL, Rockville, MD, USA (http://www.eoma.aoac.org/app_d.pdf)

Table 2. Priority allergen/matrix combinations

Whole egg	Cookies Bread Dough Salad dressing Wine
Milk	Cookies, baked goods Infant formula Wine Dark chocolate (optional matrix for methods that claim a chocolate matrix)
Peanut	Cookies Ice cream Breakfast cereal Milk chocolate (optional matrix for methods that claim a chocolate matrix)
Hazelnut	Cookies Ice cream Breakfast cereal Milk chocolate (optional matrix for methods that claim a chocolate matrix)

Appendix F: *Guidelines for Standard Method Performance Requirements*, *Official Methods of Analysis* (2016) 20th Ed., AOAC INTERNATIONAL, Rockville, MD, USA (http://www.eoma.aoac.org/app_f.pdf)

9 Maximum Time-to-Result

None.

Approved by AOAC Stakeholder Panel on Strategic Food Analytical Methods (SPSFAM). Final Version Date: March 31, 2016. Effective Date: March 31, 2016.

AOAC SMPR 2014.010

Standard Method Performance Requirements for Identification of Phosphodiesterase Type 5 (PDE5) Inhibitors in Dietary Ingredients and Supplements

Intended Use: Reference Method for Dispute Resolution or Routine Use

1 Purpose

AOAC *Standard Method Performance Requirements*SM (SMPRs) describe the minimum recommended performance characteristics to be used during the evaluation of a method. The evaluation may be an on-site verification, a single-laboratory validation, or a multi-site collaborative study. SMPRs are written and adopted by AOAC stakeholder panels composed of representatives from industry, regulatory organizations, contract laboratories, test kit manufacturers, and academic institutions. AOAC SMPRs are used by AOAC expert review panels in their evaluation of validation study data for method being considered for *Performance Tested Methods*SM or AOAC *Official Methods of Analysis*SM, and can be used as acceptance criteria for verification at user laboratories. [Refer to Appendix F: *Guidelines for Standard Method Performance Requirements*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA.]

2 Applicability

Identification of phosphodiesterase type 5 (PDE5) inhibitors (as listed in Annex I) in dietary ingredients and supplements.

3 Analytical Technique

Any analytical technique(s) that identifies the analytes of interest and meets the following method performance requirements is/are acceptable.

4 Definitions

Dietary ingredients.—A vitamin; a mineral; an herb or other botanical; an amino acid; a dietary substance for use by man to supplement the diet by increasing total dietary intake; or a concentrate, metabolite, constituent, extract, or combination of any of the above dietary ingredients. {United States Federal Food Drug and Cosmetic Act §201(ff) [U.S.C. 321 (ff)]}

Dietary supplements.—A product intended for ingestion that contains a "dietary ingredient" intended to add further nutritional value to (supplement) the diet. Dietary supplements may be found in many forms such as tablets, capsules, softgels, gelcaps, liquids, or powders.

Identification method.—A method that is capable of identifying the PDE5 inhibitors listed in Annex I and providing at least class identification of other PDE5 inhibitors based on their structural similarity to the compounds listed in Annex I. A *Supplemental List of Known PDE5 Inhibitors* provides an overview of currently known PDE5 inhibitors, for which analytical standards are available in the majority of cases. The identification should be done using technique-specific, generally acceptable criteria, such as those given in the European Commission Decision 2002/657/EC.

Interference control.—A control designed to confirm that a test matrix does not interfere with the assay's ability to detect target compounds.

Probability of identification (POI).—The proportion of positive analytical outcomes for an identification method for a given matrix at a given analyte level or concentration.

PDE5 inhibitors.—For the purposes of this SMPR: PDE5 inhibitors are defined as avanafil, lodenafil carbonate, mirodenafil, sildenafill, tadalafil, udenafil, or vardenafil; or any of their analogs. Refer to the *Supplemental List of Known PDE5 Inhibitors*.

5 Method Performance Requirements

See Table 1.

Table 1. Method performance requirements

Type of study	Study	Parameter	Parameter requirements	Target test concn	Minimum acceptable results
Single-laboratory validation	Matrix study	POI at low concn	Minimum of 33 replicates representing all target compounds in Annex I and ideally all matrix types listed in Annex II, spiked at or below the designated low level target test concentration	100 ppm	90% POI[a] of the pooled data for all target compounds and matrixes
		POI at high concn	Minimum of five replicates per matrix type spiked at 10× the designated low level target test concentration	10× low concn	100% correct analyses are expected[b]
		POI at 0 concn	Minimum of five replicates per matrix type	0 ppm	
Multi-laboratory validation	Matrix study[c]	LPOI	Use Appendix N: *ISPAM Guidelines for Validation of Qualitative Binary Chemistry Methods*	Low concn	≥0.85[a]
				10× low concn	≥0.95[a]
		$LPOI_{(0)}$		0 ppm	≤0.05[a]

[a] 95% confidence interval.
[b] 100% correct analyses are expected. Some aberrations may be acceptable if the aberrations are investigated, and acceptable explanations can be determined and communicated to method users.
[c] Multi-laboratory validation matrix study (LPOI and $LPOI_{(0)}$) are not required for First Action *Official Methods of Analysis* approval.

6 System Suitability Tests and/or Analytical Quality Control

The controls listed in Annex III shall be embedded in assays as appropriate. Interference controls shall be used for method verification for each new matrix.

7 Reference Material(s)

Refer to Annex F: *Development and Use of In-House Reference Materials* in Appendix F: *Guidelines for Standard Method Performance Requirements*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA (http://www.eoma.aoac.org/app_f.pdf)

ISO Guide 34:2009 *General requirements for the competence of reference material producers*

8 Validation Guidance

All target compounds in Annex I and ideally in all matrixes in Annex II shall be evaluated.

Appendix D: *Guidelines for Collaborative Study Procedures to Validate Characteristics of a Method of Analysis*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA (http://www.eoma.aoac.org/app_d.pdf)

Appendix K: *Guidelines for Dietary Supplements and Botanicals*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA (http://www.eoma.aoac.org/app_k.pdf). Also at: *J. AOAC Int.* (2012) **95**, 268; DOI: 10.5740/jaoacint.11-447.

Appendix N: *ISPAM Guidelines for Validation of Qualitative Binary Chemistry Methods*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA (http://www.eoma.aoac.org/app_n.pdf)

European Commission Decision 2002/657/EC of 12 August 2002 implementing Council Directive 96/23/EC concerning the performance of analytical methods and the interpretation of results (http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2002:221:0008:0036:EN:PDF)

9 Maximum Time-to-Result

No maximum time.

Approved by Stakeholder Panel on Dietary Supplements (SPDS). Final Version Date: September 5, 2014. Effective Date: October 16, 2014.

AOAC SMPR 2014.011

Standard Method Performance Requirements for Determination of Phosphodiesterase Type 5 (PDE5) Inhibitors in Dietary Ingredients and Supplements

Intended Use: Reference Method for Dispute Resolution or Routine Use

1 Purpose

AOAC *Standard Method Performance Requirements*SM (SMPRs) describe the minimum recommended performance characteristics to be used during the evaluation of a method. The evaluation may be an on-site verification, a single-laboratory validation, or a multi-site collaborative study. SMPRs are written and adopted by AOAC stakeholder panels composed of representatives from industry, regulatory organizations, contract laboratories, test kit manufacturers, and academic institutions. AOAC SMPRs are used by AOAC expert review panels in their evaluation of validation study data for method being considered for *Performance Tested Methods*SM or AOAC *Official Methods of Analysis*SM, and can be used as acceptance criteria for verification at user laboratories. [Refer to Appendix F: *Guidelines for Standard Method Performance Requirements*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA.]

2 Applicability

Quantitative method for phosphodiesterase type 5 (PDE5) in dietary ingredients and supplements for use in testing laboratories by trained technicians.

3 Analytical Technique

Any analytical technique(s) that measures the analytes of interest and meets the following method performance requirements is/are acceptable.

4 Definitions

Dietary ingredients.—A vitamin; a mineral; an herb or other botanical; an amino acid; a dietary substance for use by man to supplement the diet by increasing total dietary intake; or a concentrate, metabolite, constituent, extract, or combination of any of the above dietary ingredients. {United States Federal Food Drug and Cosmetic Act §201(ff) [U.S.C. 321 (ff)]}

Dietary supplements.—A product intended for ingestion that contains a "dietary ingredient" intended to add further nutritional value to (supplement) the diet. Dietary supplements may be found in many forms such as tablets, capsules, softgels, gelcaps, liquids, or powders.

Limit of quantitation (LOQ).—The minimum concentration or mass of analyte in a given matrix that can be reported as a quantitative result.

PDE5 inhibitors.—For the purposes of this SMPR: PDE5 inhibitors are defined as avanafil, lodenafil carbonate, mirodenafil, sildenafill, tadalafil, udenafil, or vardenafil; or any of their analogs. Refer to the *Supplemental List of Known PDE5 Inhibitors*.

Quantitative method.—Method of analysis which response is the amount of the analyte measured either directly (enumeration in a mass or a volume), or indirectly (color, absorbance, impedance, etc.) in a certain amount of sample.

Repeatability.—Variation arising when all efforts are made to keep conditions constant by using the same instrument and operator and repeating during a short time period. Expressed as the repeatability standard deviation (SD_r); or % repeatability relative standard deviation (%RSD_r).

Reproducibility.—The standard deviation or relative standard deviation calculated from among-laboratory data. Expressed as the reproducibility standard deviation (SD_R); or % reproducibility relative standard deviation (%RSD_R).

Recovery.—The fraction or percentage of spiked analyte that is recovered when the test sample is analyzed using the entire method.

Table 1. Method performance requirements

Type of study	Parameter	Minimum acceptable criteria
Single-laboratory validation	Analytical range	50–500 000 ppm
	Limit of quantitation (LOQ)	≤50 ppm
	Repeatability (RSD_r)	≤20%
	Recovery	70 to 120% of mean spiked recovery over the analytical range
Multi-laboratory validation	Reproducibility (RSD_R)	≤30%

5 Method Performance Requirements

See Table 1.

6 System Suitability Tests and/or Analytical Quality Control

Suitable methods will include blank check samples, and check standards at the lowest point and midrange point of the analytical range.

7 Reference Material(s)

Refer to Annex F: *Development and Use of In-House Reference Materials* in Appendix F: *Guidelines for Standard Method Performance Requirements*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA (http://www.eoma.aoac.org/app_f.pdf)

ISO Guide 34:2009 *General requirements for the competence of reference material producers*

8 Validation Guidance

All target compounds in Annex I and ideally in all matrices in Annex II shall be evaluated.

Appendix D: *Guidelines for Collaborative Study Procedures to Validate Characteristics of a Method of Analysis*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA (http://www.eoma.aoac.org/app_d.pdf)

Appendix F: *Guidelines for Standard Method Performance Requirements*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA (http://www.eoma.aoac.org/app_f.pdf)

Appendix K: *Guidelines for Dietary Supplements and Botanicals*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012)

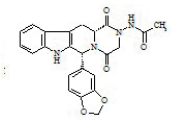
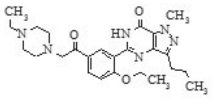
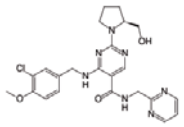
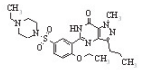
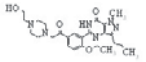
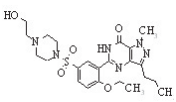
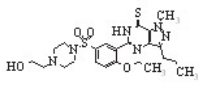
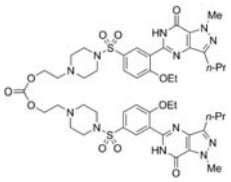
19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA (http://www.eoma.aoac.org/app_k.pdf)

8 Maximum Time-to-Result

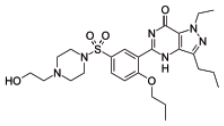
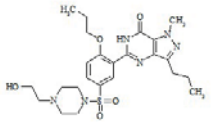
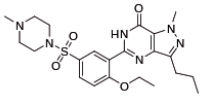
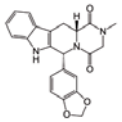
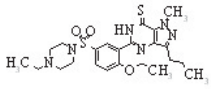
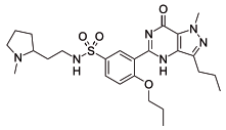
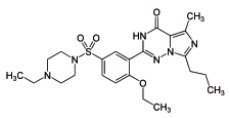
No maximum time.

Approved by Stakeholder Panel on Dietary Supplements (SPDS). Final Version Date: September 5, 2014. Effective Date: October 16, 2014.

ANNEX I
Target Compound Panel

Analyte	CAS No.	Formula	Structure
Acetaminotadalafil	1446144-71-3	$C_{23}H_{20}N_4O_5$	
Acetildenafil	831217-01-7	$C_{25}H_{34}N_6O_3$	
Avanafil (sold under the brand names *Stendra* and *Spedra*)	330784-47-9	$C_{23}H_{26}ClN_7O_3$	
Homosildenafil	642928-07-2	$C_{23}H_{32}N_6O_4S$	
Hydroxyacetildenafil	147676-56-0	$C_{25}H_{34}N_6O_4$	
Hydroxyhomosildenafil	139755-85-4	$C_{23}H_{32}N_6O_5S$	
Hydroxythiohomosildenafil	479073-82-0	$C_{23}H_{32}N_6O_4S_2$	
Lodenafil carbonate (sold under the brand name *Helleva* in Brazil)	398507-55-6	$C_{43}H_{54}N_{12}O_9S_2$	

ANNEX I
Target Compound Panel (*continued*)

Analyte	CAS No.	Formula	Structure
Mirodenafil (sold under the trade name of *Mvix*.)	862189-95-5	$C_{26}H_{37}N_5O_5S$	
Propoxyphenyl hydroxyhomosildenafil	139755-87-6	$C_{24}H_{34}N_6O_5S$	
Sildenafil (sold under the brand names *Viagra* and *Revatio*, and other various brand names)	139755-83-2	$C_{22}H_{30}N_6O_4S$	
Tadalafil (sold under the brand names *Cialis* and *Adcirca*)	171596-29-5	$C_{22}H_{19}N_3O_4$	
Thiohomosildenafil	479073-80-8	$C_{23}H_{32}N_6O_3S_2$	
Udenafil (sold under the brand name *Zydena*)	268203-93-6	$C_{25}H_{36}N_6O_4S$	
Vardenafil (sold under the brand names *Levitra*, *Staxyn*, and *Vivanza*)	224785-90-4	$C_{23}H_{32}N_6O_4S$	

ANNEX II
Matrixes

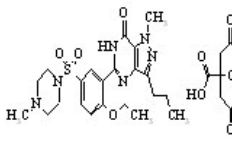
Tablets
Capsules (both the content and the capsule shells)
Softgels
Gelcaps
Liquids
Powders
Extracts

Supplemental List of Known PDE5 Inhibitors (as of July 2014)

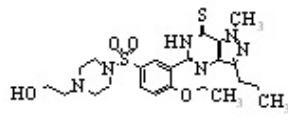
1. **Standards available from Cachesyn http://www.cachesyn.com/ which include the majority of characterized PDE-5i analogues and all of the parent drugs including catalog numbers. (Some structure images not available)**

Sildenafil Related Compounds (commercial standards available) – includes deuterated standards.

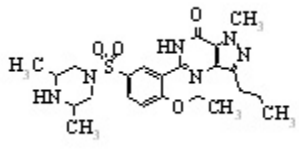
Sildenafil citrate
CAS No. 171599-83-0
C22H30N6O4S.C6H8O7 M.W. 474.59 192.13
CSTS061



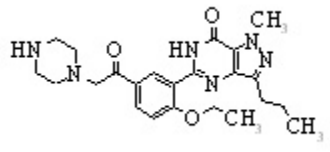
Hydroxythiohomosildenafil
C23H32N6O4S2 M.W. 520.68
CSTS0611



Dimethyl Sildenafil
C23H32N6O4S M.W. 488.61
CSTS0612



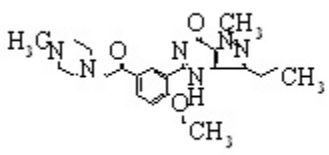
N-Desmethyl Acetildenafil
C23H30N6O3 M.W. 438.53
CSTS0613



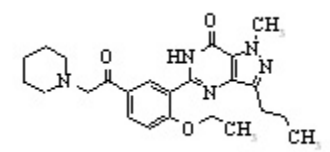
Hydroxyacetildenafil
C25H34N6O4 M.W. 482.59
CSTS0614

Nor-acetildenafil
CAS No. 949091-37-7
C24H32N6O3 M.W. 452.56
CSTS0615

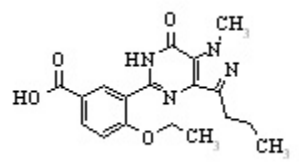
Nor-acetildenafil
CAS No. 949091-37-7
C24H32N6O3 M.W. 452.56
CSTS0615



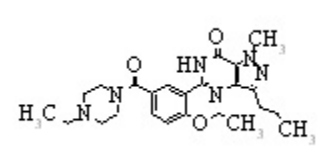
Piperiacetildenafil
C24H31N5O3 M.W. 437.55
CSTS0616



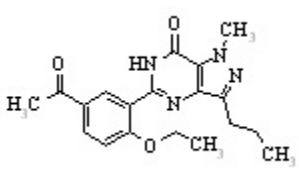
Acetil Acid
C18H20N4O4 M.W. 356.38
CSTS0617



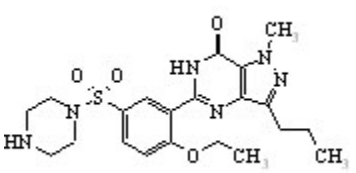
Carbodenafil
C24H32N6O3 M.W. 452.56
CSTS0618



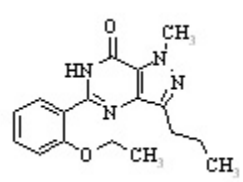
Gendenafil
C19H22N4O3 M.W. 354.41
CSTS0619



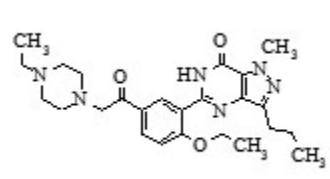
N-Desmethyl Sildenafil
CAS No. 139755-82-1
C21H38N6O4S M.W. 460.56
CSTS062



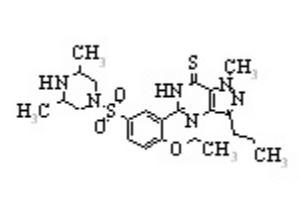
Imidazosagatriazinone
C17H20N4O2 M.W. 312.37
CSTS0620



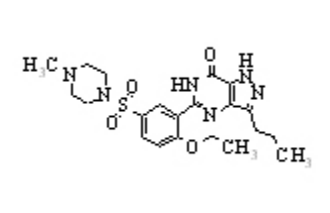
Acetildenafil (Hongdenafil)
C25H34N6O3 M.W. 466.59
CSTS0621



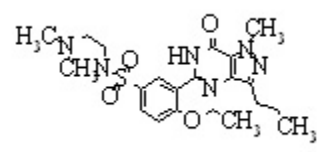
Thiodimethyl Sildenafil (Dimethylthiosildenafil)
C23H32N6O3S2 M.W. 504.68
CSTS0622



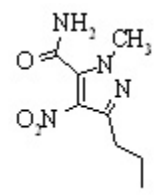
Pyrazole N-desmethyl sildenafil
C21H28N6O4S M.W. 460.56
CSTS0623



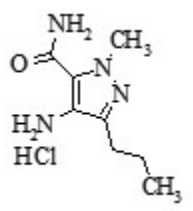
PDE-5 Inhibitor (Sildenafil Related Compound)
C21H30N6O M.W. 462.5
CSTS0624



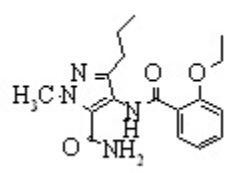
Sildenafil amide
C8H12N4O3 M.W. 212.21
CSTS0625



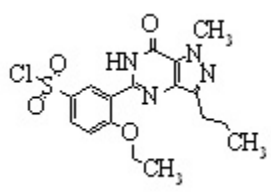
Sildenafil Amine HCl
C8H14N4O.HCl M.W. 182.23 36.46
CSTS0626



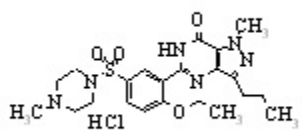
Sildenafil coupled
C17H22N4O3 M.W. 330.39
CSTS0627



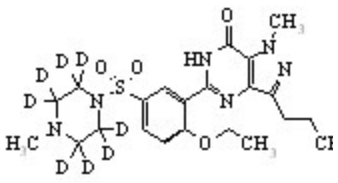
Sildenafil chlorosulfonyl
C17H19ClN4O4S M.W. 410.88
CSTS0628



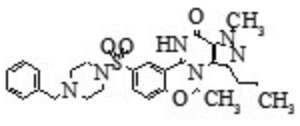
Sildenafil HCl
C22H30N6O4S.HCl M.W. 474.59 36.46
CSTS0629



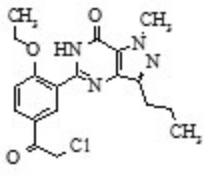
Sildenafil-d8
CAS No. 171599-83-0(non-d)
C22H22D8N6O4S M.W. 482.63
CSTS063



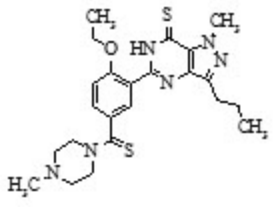
Benzyl Sildenafil
C28H34N6O4S M.W. 550.68
CSTS0631



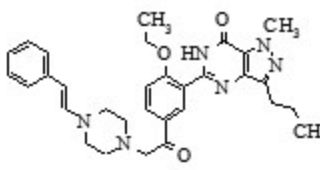
Chlorodenafil
CAS No. N/A
C19H21ClN4O3 M.W. 388.86
CSTS0633



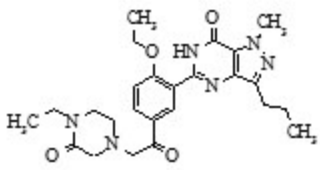
Dithio-desmethyl-carbodenafil
CAS No. N/A
C23H30N6OS2 M.W. 470.66
CSTS0635



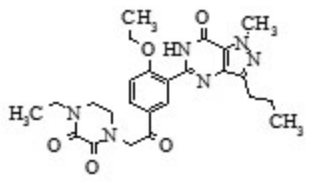
Cinnamyldenafil
CAS No. N/A
C31H36N6O3 M.W. 540.67
CSTS0637



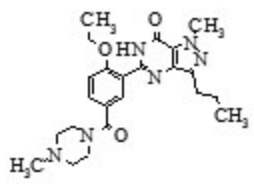
Oxohongdenafil
CAS No. N/A
C25H32N6O4 M.W. 480.57
CSTS0639



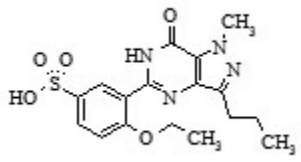
Dioxohongdenafil
CAS No. N/A
C25H30N6O5 M.W. 494.56
CSTS0640



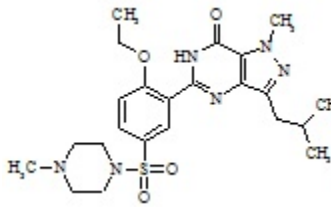
Desmethyl Carbodenafil
C23H30N6O3 M.W. 438.53
CSTS0642



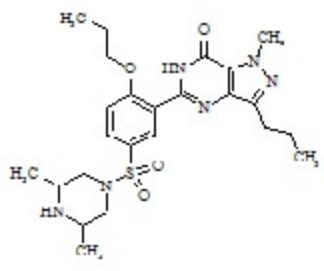
Demethylpiperazinyl Sildenafil Sulfonic Acid
C17H20N4O5S M.W. 392.44
CSTS0644



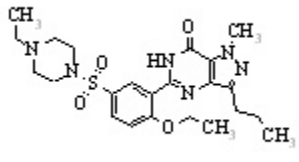
Sildenafil Impurity A (Isobutyl Sildenafil)
CAS No. N/A
C23H32N6O4S M.W. 488.61
CSTS0646



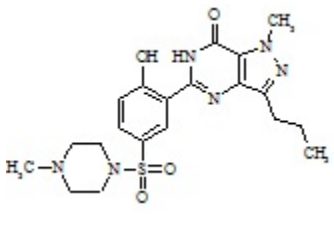
Propoxyphenyl Sildenafil
CAS No. 877777-10-1
C23H32N6O4S M.W. 488.61
CSTS0648



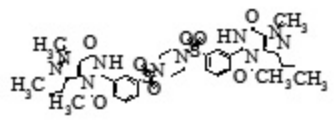
Homosildenafil
C23H32N6O4S M.W. 488.61
CSTS065



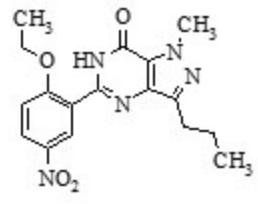
O-Desethyl Sildenafil (Sildenafil Impurity C)
CAS No. N/A
C20H26N6O4S M.W. 446.53
CSTS0651



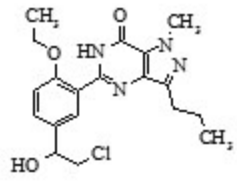
Sildenafil Dimer Impurity
C38H46N10O8S2 M.W. 834.98
CSTS0630



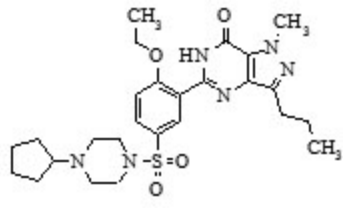
Nitrodenafil
CAS No. N/A
C17H19N5O4 M.W. 357.37
CSTS0632



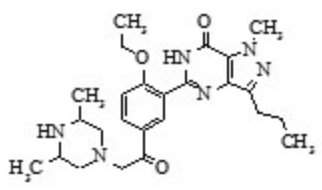
Hydroxychlorodenafil
CAS No. N/A
C19H23ClN4O3 M.W. 390.87
CSTS0634



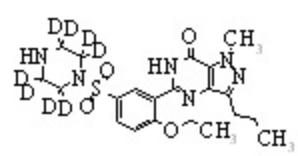
Cyclopentynafil
CAS No. N/A
C26H36N6O4S M.W. 528.68
CSTS0636



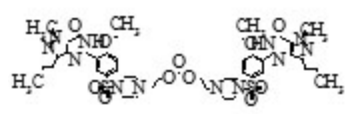
Dimethylacetildenafil
CAS No. N/A
C25H34N6O3 M.W. 466.59
CSTS0638



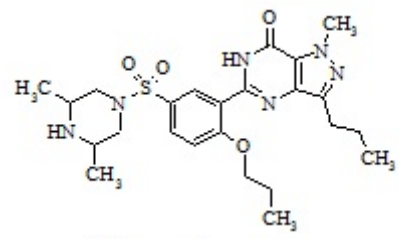
N-Desmethyl sildenafil-d8
CAS No. 139755-82-1 (non-d)
C21H20N6O4SD8 M.W. 468.61
CSTS064



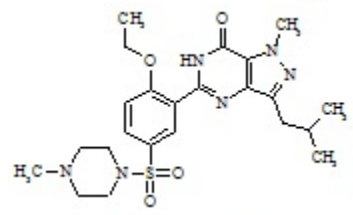
Lodenafilcarbonate
CAS No. N/A
C47H62N12O11S2 M.W. 1035.22
CSTS0641



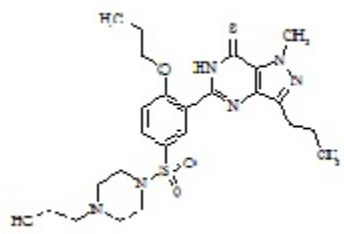
Sildenafil analogue
C24H34N6O4S M.W. 502.64
CSTS0643



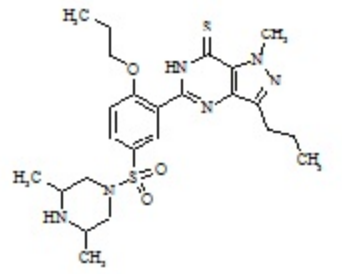
Nitroso-prodenafil
CAS No. N/A
C27H35N9O5S2 M.W. 629.77
CSTS0645



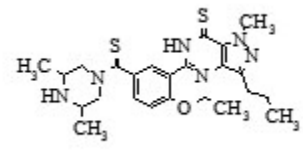
Sildenafil Analogue I
CAS No. N/A
C24H34N6O4S2 M.W. 534.70
CSTS0647



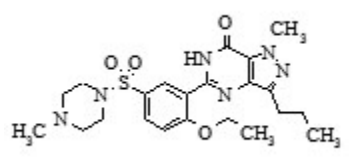
Sildenafil Analogue III
CAS No. N/A
C24H34N6O3S2 M.W. 518.70
CSTS0649



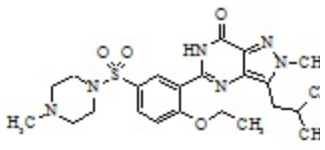
Sildenafil Related Compound
C24H32N6OS2 M.W. 484.69
CSTS0650



Sildenafil
C22H30N6O4S M.W. 474.59
CSTS0652



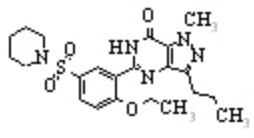
Sildenafil Impurity A Related Compound (Isomer of Isobutyl Sildenafil)
C23H32N6O4S M.W. 488.61
CSTS0653



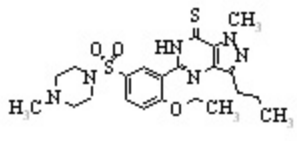
Sildenafil N-Oxide
C22H30N6O5S M.W. 490.59
CSTS0655

no image of structure available

Norneosildenafil
C22H29N5O4S M.W. 459.57
CSTS066



Thiosildenafil
C22H30N6O3S2 M.W. 490.65
CSTS068



Sildenafil Impurity ((1-methyl-4-Nitro -3-n-propyl pyrazole-5- carboxylic acid)
C8H11N3O4 M.W. 213.19
CSTS0654

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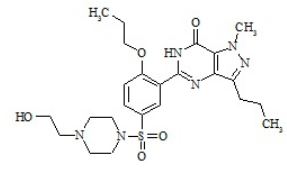
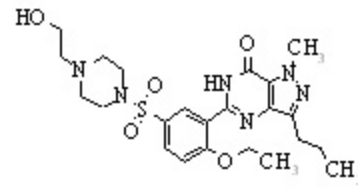
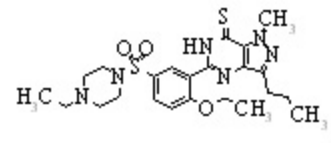
Propoxyphenyl-Hydroxyhomosildenafil
CAS No. N/A
C24H34N6O5S M.W. 518.64
CSTS0656



Hydroxyhomosildenafil
C23H32N6O5S M.W. 504.61
CSTS067

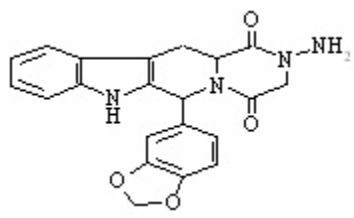


Thiohomosildenafil
C23H32N6O3S2 M.W. 504.68
CSTS069

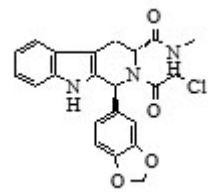


Tadalafil Related Compounds (commercial standards available) – includes deuterated standards.

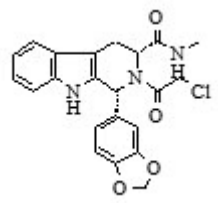
Aminotadalafil
C21H18N4O4 M.W. 390.40
CSTT101



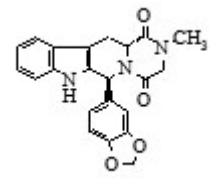
Tadalafil Impurity C
CAS No. NA
C22H20ClN3O4 M.W. 425.88
CSTT1010



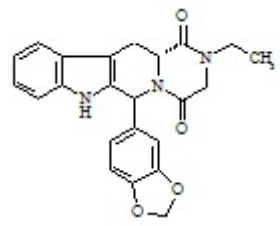
Tadalafil Impurity D
CAS No. NA
C22H20ClN3O4 M.W. 425.88
CSTT1011



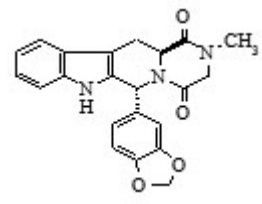
Tadalafil Impurity E
C22H19N3O4 M.W. 389.41
CSTT1012



N-Ethyl Tadalafil
CAS No. N/A
C23H21N3O4 M.W. 403.44
CSTT1013



6R,12S-Tadalafil
C22H19N3O4 M.W. 389.41
CSTT1014



Tadalafil Hydroxylactam Impurity
C22H19N3O6 M.W. 421.41
CSTT1015

no image of structure available

Tadalafil Aminohemiketal Impurity
C22H19N3O6 M.W. 421.41
CSTT1016

no image of structure available

Tadalafil Spiro-urethane Impurity
C21H18N3O6 M.W. 408.39
CSTT1017

no image of structure available

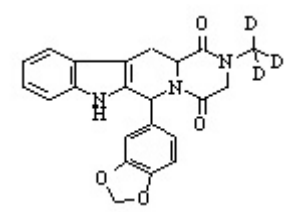
Tadalafil Hydroxyquinoline Impurity
C22H17N3O5 M.W. 403.40
CSTT1018

no image of structure available

Tadalafil Ketolactam Impurity
C22H21N3O6 M.W. 423.43
CSTT1019

no image of structure available

Tadalafil-d3
C22H16N3O4D3 M.W. 392.43
CSTT102



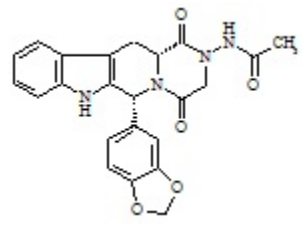
Tadalafil Spiro-oxindole Impurity
C22H19N3O5 M.W. 405.41
CSTT1020

no image of structure available

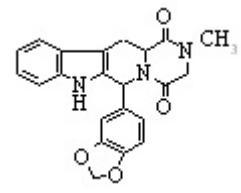
Tadalafil Impurity B (6S,12aS)
C22H19N3O4 M.W. 389.41
CSTT1021

no image of structure available

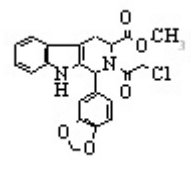
Acetaminotadalafil
CAS No. N/A
C23H20N4O5 M.W. 432.44
CSTT1022



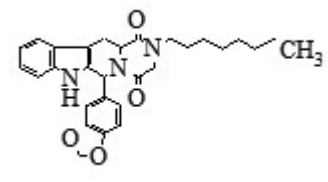
Tadalafil
C22H19N3O4 M.W. 389.41
CSTT103



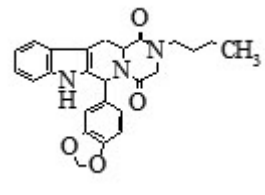
Chloropretadalafil
C22H19ClN2O5 M.W. 426.86
CSTT104



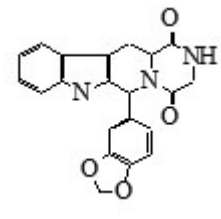
N-Octyl-nortadalafil
C29H33N3O4 M.W. 487.60
CSTT105



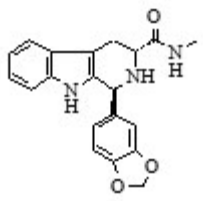
N-Butyl Tadalafil
C25H25N3O4 M.W. 431.50
CSTT106



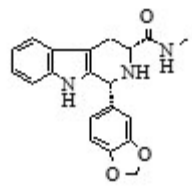
Nortadalafil
C21H17N3O4 M.W. 375.39
CSTT107



Tadalafil Impurity A
CAS No. NA
C20H19N3O3 M.W. 349.39
CSTT108

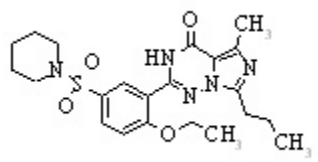


Tadalafil Impurity B
CAS No. NA
C20H19N3O3 M.W. 349.39
CSTT109



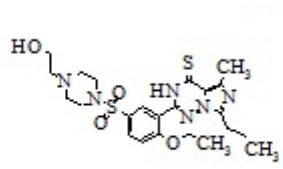
Vardenafil Related Compounds (commercial standards available) – includes deuterated standards.

Pseudovardenafil
C22H29N5O4S
M.W. 459.57
CSTV051

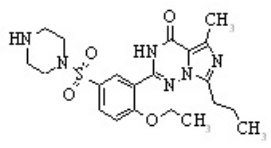


no image of structure available

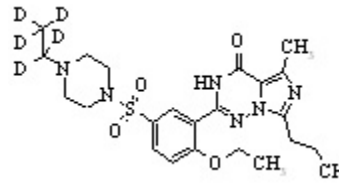
Hydroxythio Vardenafil
C23H32N6O4S2 M.W. 520.68
CSTV0510



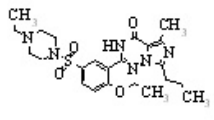
N-Desethyl Vardenafil
C21H28N6O4S M.W. 460.56
CSTV052



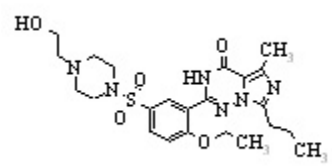
Vardenafil-d5
C23H27N6O4SD5 M.W. 493.64
CSTV053



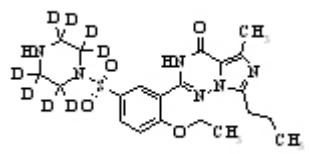
Vardenafil HCl
CAS No. 224785-90-4
C23H32N6O4S M.W. 488.61
CSTV054



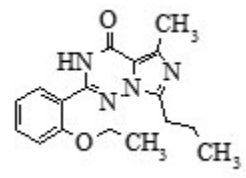
Hydroxy Vardenafil
C23H32N6O5S M.W. 504.61
CSTV055



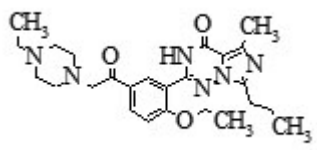
N-Desethyl Vardenafil-d8
CAS No. V-052
C21H28N6O4S M.W. 460.56
CSTV056



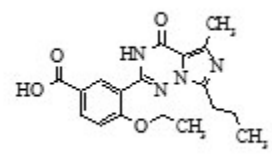
2-(2-Ethoxyphenyl)-5-methyl-7-propyl-3H-imidazo[5,1-f][1,2,4]triazin-4-one
C17H20N4O2 M.W. 312.37
CSTV057



Acetylvardenafil
C25H34N6O3 M.W. 466.59
CSTV058

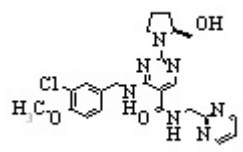


Norneovardenafil
CAS No. N/A
C18H20N4O4 M.W. 356.38
CSTV059

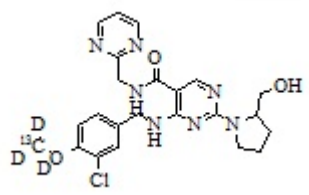


Avanafil Related Compounds (commercial standards available) – includes deuterated standards.

Avanafil
CAS No. 330784-47-9
C23H26ClN7O3 M.W. 483.96
CSTA291

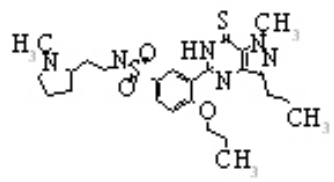


Avanafil-13CD3
C22H23ClN7O313CD3 M.W. 487.97
CSTA292



Udenafil

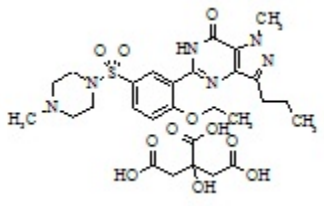
Udenafil
CAS No. 268203-93-6
C25H36N6O4S M.W. 516.67
CSTU031



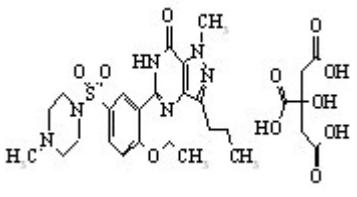
2. **Standards available from TLC Pharmachem http://www.tlcpharmachem.com which include the majority of characterized PDE-5i analogues and all of the parent drugs including catalog numbers. (Some structure images not available)**

Sildenafil Related Compounds (commercial standards available) – includes deuterated standards.

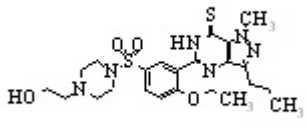
Sildenafil Citrate
CAS No. 171599-83-0
C22H30N6O4S. C6H8O7 M.W. 474.59
192.13
PF-0017



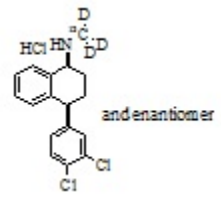
Sildenafil citrate
CAS No. 171599-83-0
C22H30N6O4S.C6H8O7 M.W. 474.59
192.13
S-061



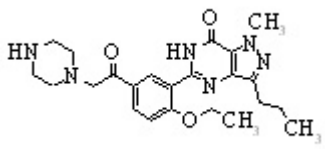
Hydroxythiohomosildenafil
C23H32N6O4S2 M.W. 520.68
S-0611



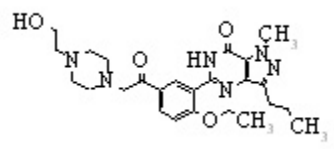
Dimethyl Sildenafil
CAS No. 1416130-63-6
C23H32N6O4S M.W. 488.61
S-0612



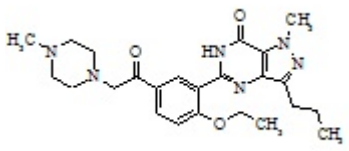
N-Desmethyl Acetildenafil
C23H30N6O3 M.W. 438.53
S-0613



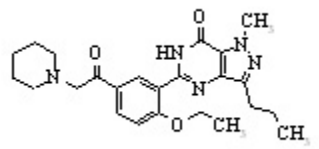
Hydroxyacetildenafil
C25H34N6O4 M.W. 482.59
S-0614



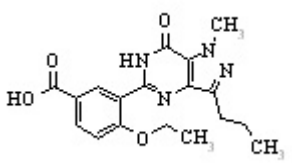
Nor-acetildenafil
CAS No. 949091-38-7
C24H32N6O3 M.W. 452.56
S-0615



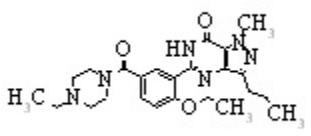
Piperiacetildenafil
C24H31N5O3 M.W. 437.55
S-0616



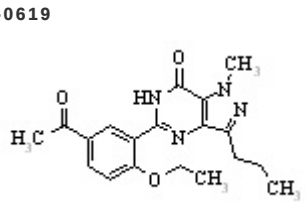
Acetil Acid
C18H20N4O4 M.W. 356.38
S-0617



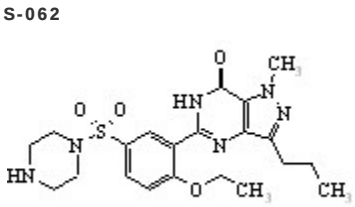
Carbodenafil
C24H32N6O3 M.W. 452.56
S-0618



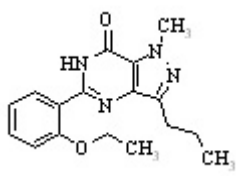
Gendenafil
CAS No. 147676-66-2
C19H22N4O3 M.W. 354.41
S-0619



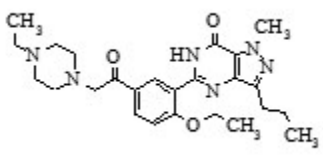
N-Desmethyl Sildenafil
CAS No. 139755-82-1
C21H28N6O4S M.W. 460.56
S-062



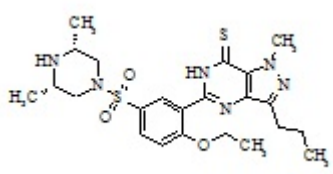
Imidazosagatriazinone
C17H20N4O2 M.W. 312.37
S-0620



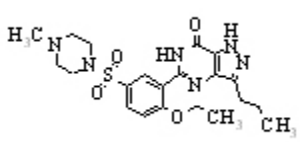
Acetildenafil (Hongdenafil)
CAS No. 831217-01-7
C25H34N6O3 M.W. 466.59
S-0621



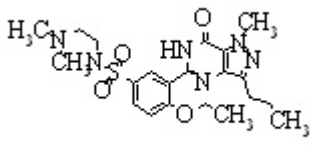
Thiodimethyl Sildenafil (Thioaildenafill, Sulfoaildenafil)
CAS No. 856190-47-1
C23H32N6O3S2 M.W. 504.68
S-0622



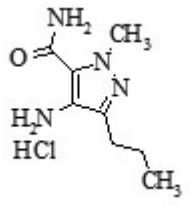
Pyrazole N-desmethyl sildenafil
C21H28N6O4S M.W. 460.56
S-0623



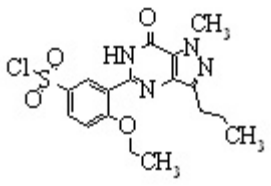
PDE-5 Inhibitor (Sildenafil Related Compound)
C21H30N6O4S M.W. 462.58
S-0624



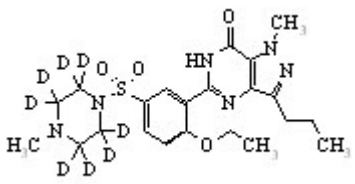
Sildenafil Amine HCl
C8H14N4O.HCl M.W. 182.23 36.46
S-0626



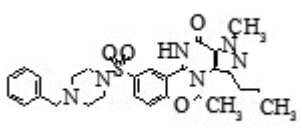
Sildenafil chlorosulfonyl
CAS No. 139756-22-2
C17H19ClN4O4S M.W. 410.88
S-0628



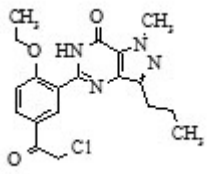
Sildenafil-d8
CAS No. 171599-83-0(non-d)
C22H22D8N6O4S M.W. 482.63
S-063



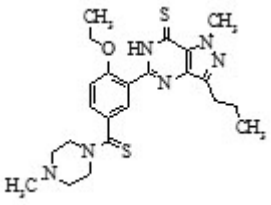
Benzyl Sildenafil
C28H34N6O4S M.W. 550.68
S-0631



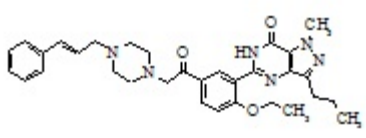
Chlorodenafil
CAS No. N/A
C19H21ClN4O3 M.W. 388.86
S-0633



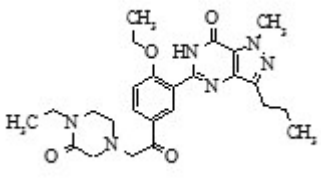
Dithio-desmethyl-carbodenafil
CAS No. N/A
C23H30N6OS2 M.W. 470.66
S-0635



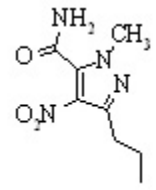
Cinnamyldenafil
CAS No. N/A
C32H38N6O3 M.W. 554.70
S-0637



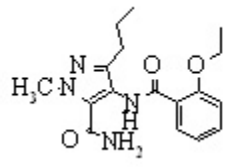
Oxohongdenafil
CAS No. N/A
C25H32N6O4 M.W. 480.57
S-0639



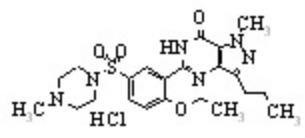
Sildenafil amide
C8H12N4O3 M.W. 212.21
S-0625



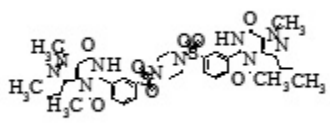
Sildenafil coupled
C17H22N4O3 M.W. 330.39
S-0627



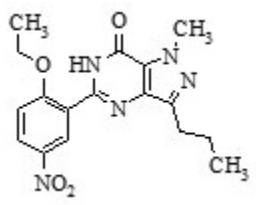
Sildenafil HCl
C22H30N6O4S.HCl M.W. 474.59 36.46
S-0629



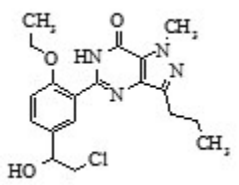
Sildenafil Dimer Impurity
C38H46N10O8S2 M.W. 834.98
S-0630



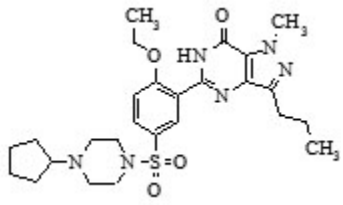
Nitrodenafil
CAS No. N/A
C17H19N5O4 M.W. 357.37
S-0632



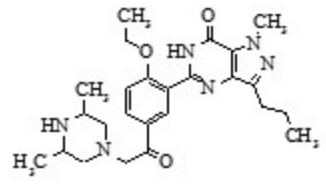
Hydroxychlorodenafil
CAS No. N/A
C19H23ClN4O3 M.W. 390.87
S-0634



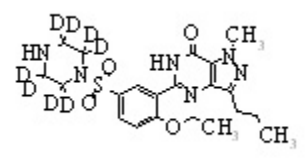
Cyclopentynafil
CAS No. N/A
C26H36N6O4S M.W. 528.68
S-0636



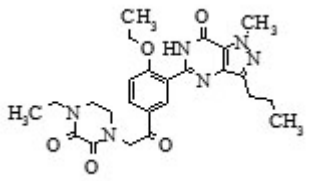
Dimethylacetildenafil
CAS No. N/A
C25H34N6O3 M.W. 466.59
S-0638



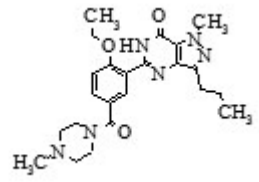
N-Desmethyl sildenafil-d8
CAS No. 1185168-06-2
C21H20N6O4SD8 M.W. 468.61
S-064



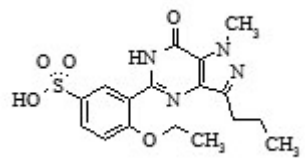
Dioxohongdenafil
CAS No. N/A
C25H30N6O5 M.W. 494.56
S-0640



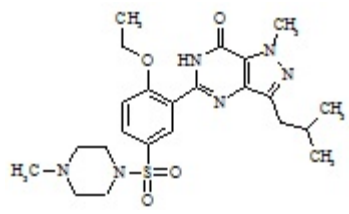
Desmethyl Carbodenafil
C23H30N6O3 M.W. 438.53
S-0642



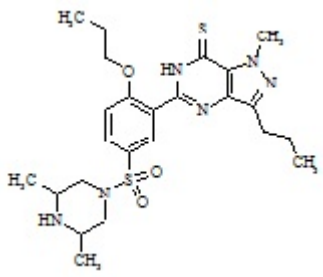
Demethylpiperazinyl Sildenafil Sulfonic Acid
C17H20N4O5S M.W. 392.44
S-0644



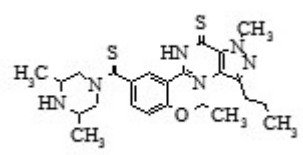
Sildenafil Impurity A (Isobutyl Sildenafil)
CAS No. 1391053-95-4
C23H32N6O4S M.W. 488.61
S-0646



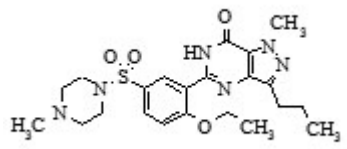
Sildenafil Analogue III
CAS No. N/A
C24H34N6O3S2 M.W. 518.70
S-0649



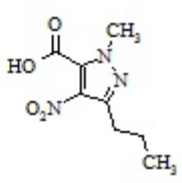
Sildenafil Related Compound
C24H32N6OS2 M.W. 484.69
S-0650



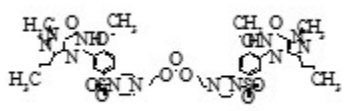
Sildenafil
C22H30N6O4S M.W. 474.59
S-0652



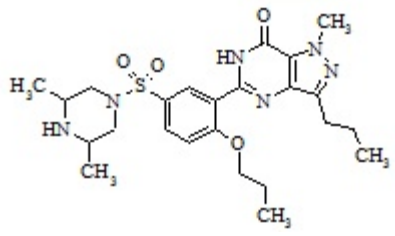
Sildenafil Impurity ((1-methyl-4-Nitro -3-n-propyl pyrazole-5- carboxylic acid)
C8H11N3O4 M.W. 213.19
S-0654



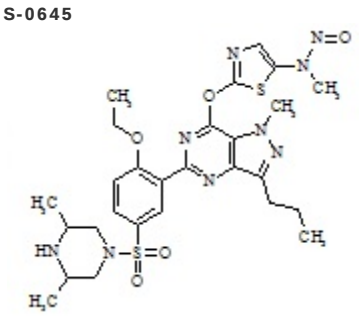
Lodenafilcarbonate
CAS No. N/A
C47H62N12O11S2 M.W. 1035.22
S-0641



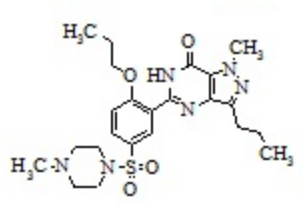
Sildenafil analogue
C24H34N6O4S M.W. 502.64
S-0643



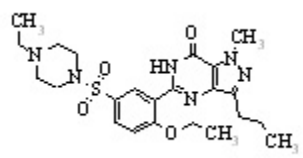
Nitroso-prodenafil
CAS No. N/A
C27H35N9O5S2 M.W. 629.77
S-0645



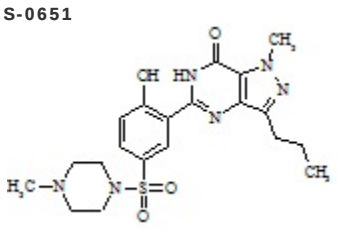
Propoxyphenyl Sildenafil
CAS No. 877777-10-1
C23H32N6O4S M.W. 488.61
S-0648



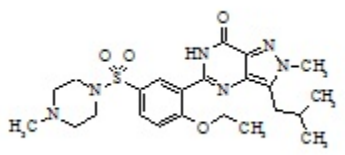
Homosildenafil
CAS No. 642928-07-2
C23H32N6O4S M.W. 488.61
S-065



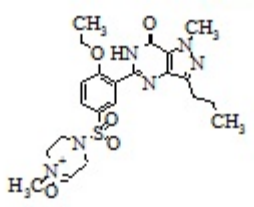
O-Desethyl Sildenafil (Sildenafil Impurity C)
CAS No. N/A
C20H26N6O4S M.W. 446.53
S-0651



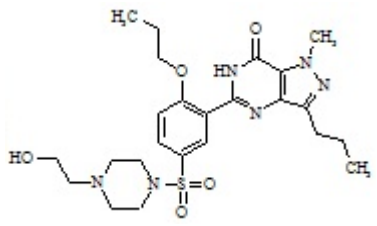
Sildenafil Impurity A Related Compound (Isomer of Isobutyl Sildenafil)
C23H32N6O4S M.W. 488.61
S-0653



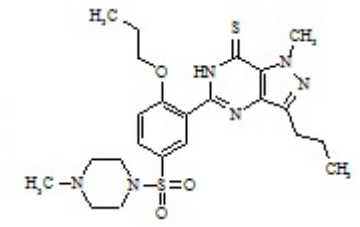
Sildenafil N-Oxide
C22H30N6O5S M.W. 490.59
S-0655



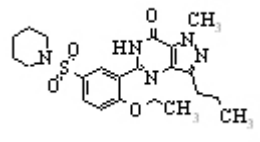
Propoxyphenyl-Hydroxyhomosildenafil
CAS No. N/A
C24H34N6O5S M.W. 518.64
S-0656



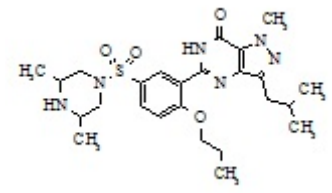
Propoxyphenyl-Thiosildenafil
CAS No. N/A
C23H32N6O3S2 M.W. 504.68
S-0658



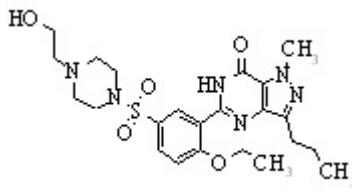
Norneosildenafil
C22H29N5O4S M.W. 459.57
S-066



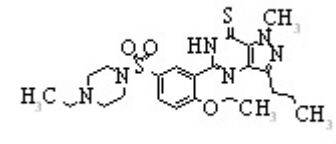
Sildenafil Related Compound 2
C25H36N6O4S M.W. 516.67
S-0661



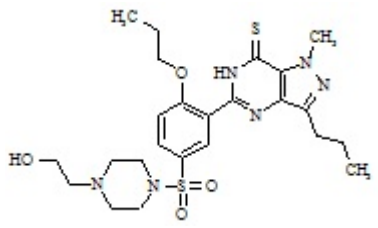
Hydroxyhomosildenafil
C23H32N6O5S M.W. 504.61
S-067



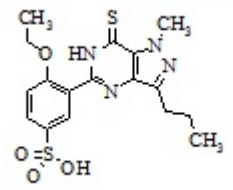
Thiohomosildenafil
C23H32N6O3S2 M.W. 504.68
S-069



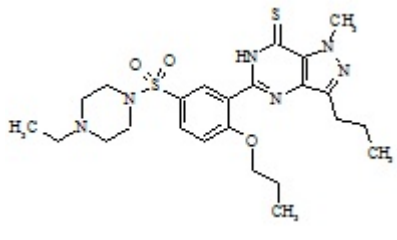
Sildenafil Analogue I (Propoxyphenyl-Thiohydroxyhomosildenafil)
CAS No. 479073-90-0
C24H34N6O4S2 M.W. 534.70
S-0657



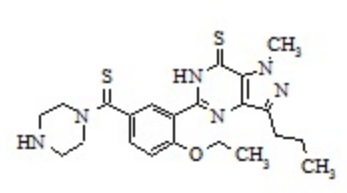
Depiperazinothiosildenafil
C17H20N4O4S2 M.W. 408.50
S-0659



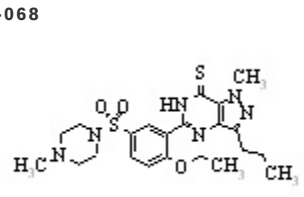
Propoxyphenyl Thiohomosidenafil
CAS No. 479073-88-6
C24H34N6O3S2 M.W. 518.70
S-0660



Dithio-Desethyl-Carbodenafil
CAS No. N/A
C22H28N6OS2 M.W. 456.64
S-0662

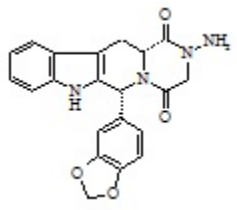


Thiosildenafil
CAS No. 479073-79-5
C22H30N6O3S2 M.W. 490.65
S-068

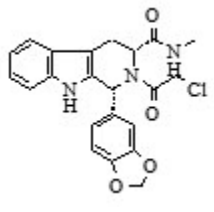


Tadalafil Related Compounds (commercial standards available) – includes deuterated standards.

Aminotadalafil
CAS No. 385769-84-6
C21H18N4O4 M.W. 390.40
T-101



Tadalafil Impurity D
CAS No. NA
C22H20ClN3O4 M.W. 425.88
T-1011



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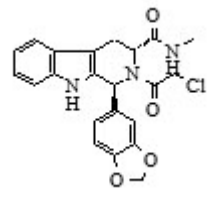
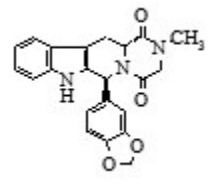
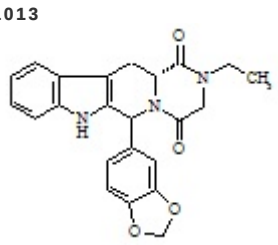
CAS No. NA
C22H20ClN3O4 M.W. 425.88
T-1010



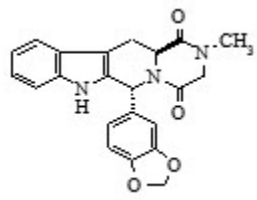
Tadalafil Impurity E (6S, 12R)
CAS No. 171596-28-4
C22H19N3O4 M.W. 389.41
T-1012



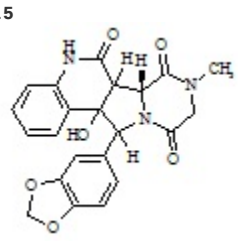
N-Ethyl Tadalafil
CAS No. N/A
C23H21N3O4 M.W. 403.44
T-1013



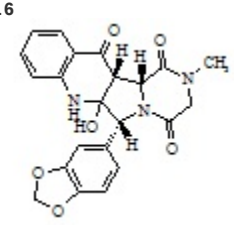
6R,12S-Tadalafil
CAS No. 171596-27-3
C22H19N3O4 M.W. 389.41
T-1014



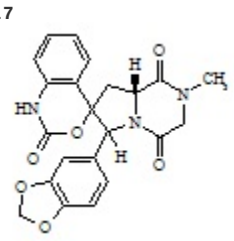
Tadalafil Hydroxylactam Impurity
C22H19N3O6 M.W. 421.41
T-1015



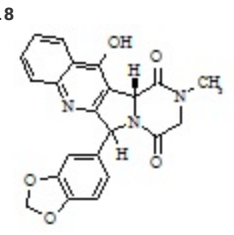
Tadalafil Aminohemiketal Impurity
C22H19N3O6 M.W. 421.41
T-1016



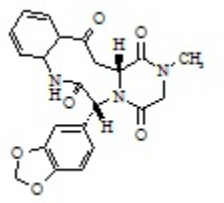
Tadalafil Spiro-urethane Impurity
C22H19N3O6 M.W. 421.41
T-1017



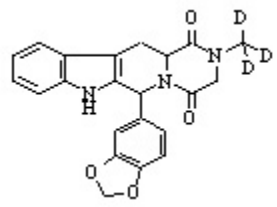
Tadalafil Hydroxyquinoline Impurity
C22H17N3O5 M.W. 403.40
T-1018



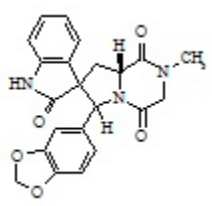
Tadalafil Ketolactam Impurity
CAS No. 1346605-38-6
C22H19N3O6 M.W. 421.41
T-1019



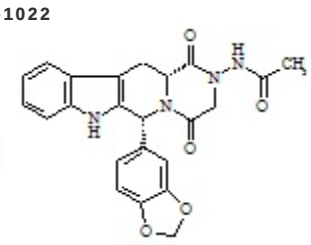
Tadalafil-d3
CAS No. 960226-55-5
C22H16N3O4D3 M.W. 392.43
T-102



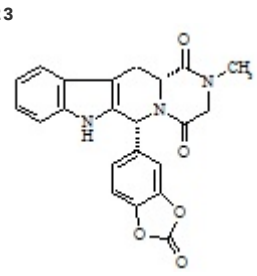
Tadalafil Spiro-oxindole Impurity
C22H19N3O5 M.W. 405.41
T-1020



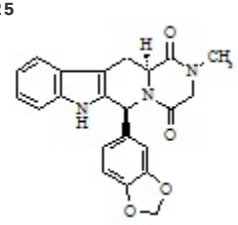
Acetaminotadalafil
CAS No. N/A
C23H20N4O5 M.W. 432.44
T-1022



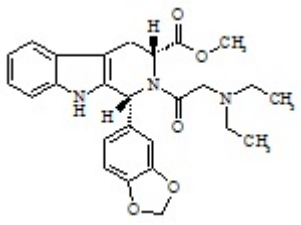
Tadalafil Oxo Impurity
CAS No. 1346602-17-2
C22H17N3O5 M.W. 403.40
T-1023



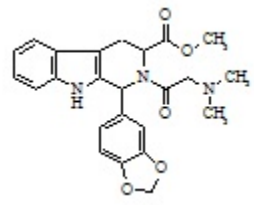
Tadalafil EP Impurity B (ent-tadalafil)
CAS No. 629652-72-8
C22H19N3O4 M.W. 389.41
T-1025



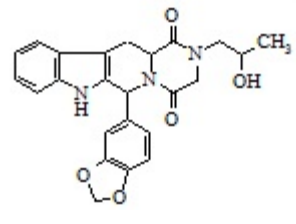
Tadalafil Related Compound
CAS No. N/A
C26H29N3O5 M.W. 463.54
T-1027



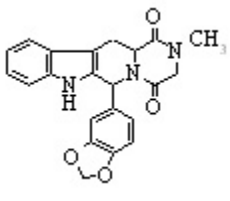
Tadalafil Related Compound 2
C24H25N3O5 M.W. 435.48
T-1028



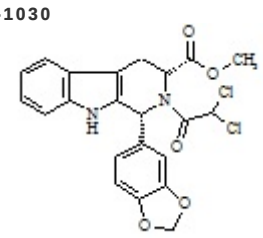
2-Hydroxypropylnortadalafil
C24H23N3O5 M.W. 433.47
T-1029



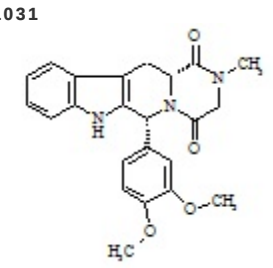
Tadalafil
CAS No. 171596-29-5
C22H19N3O4 M.W. 389.41
T-103



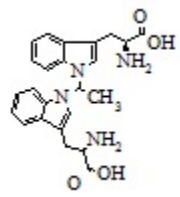
Tadalafil Dichloro Impurity
CAS No. N/A
C22H18Cl2N2O5 M.W. 461.31
T-1030



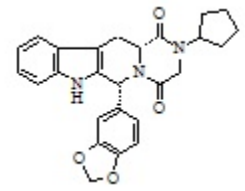
Tadalafil Dimethoxy Impurity
CAS No. 1356345-67-9
C23H23N3O4 M.W. 405.46
T-1031



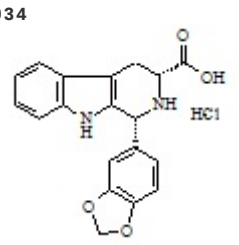
Tadalafil Impurity (1,1 Œ-ethylidenebistryptophan)
C24H26N4O4 M.W. 434.50
T-1032



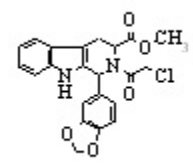
Tadalafil Related Impurity 1
CAS No. N/A
C26H25N3O4 M.W. 443.51
T-1033



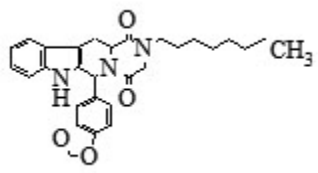
Tadalafil Acid Impurity
CAS No. N/A
C19H16N2O4 HCl M.W. 336.35 36.46
T-1034



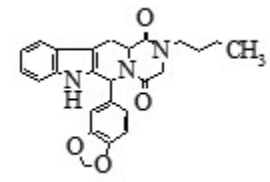
Chloropretadalafil
C22H19ClN2O5 M.W. 426.86
T-104



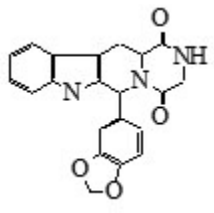
N-Octyl-nortadalafil
C29H33N3O4 M.W. 487.60
T-105



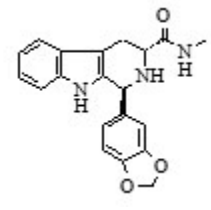
N-Butyl Tadalafil
C25H25N3O4 M.W. 431.50
T-106



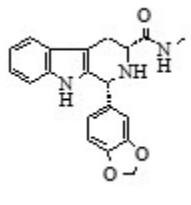
Nortadalafil
C21H17N3O4 M.W. 375.39
T-107



Tadalafil Impurity A
CAS No. NA
C20H19N3O3 M.W. 349.39
T-108

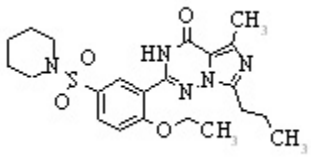


Tadalafil Impurity B
CAS No. NA
C20H19N3O3 M.W. 349.39
T-109

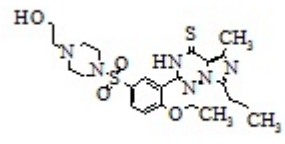


Vardenafil Related Compounds (commercial standards available) – includes deuterated standards.

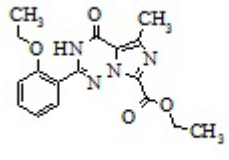
Pseudovardenafil
CAS No. 224788-34-5
C22H29N5O4S M.W. 459.57
V-051



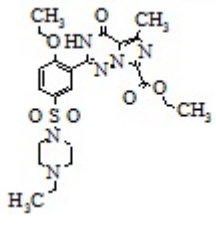
Hydroxythio Vardenafil
C23H32N6O4S2 M.W. 520.68
V-0510



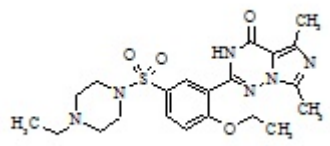
Vardenafil Impurity 1
CAS No. 1417529-67-9
C17H18N4O4 M.W. 342.36
V-0511



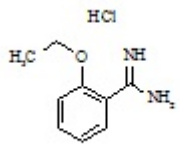
Vardenafil Impurity 2
CAS No. 1417529-69-1
C23H30N6O6S M.W. 518.60
V-0512



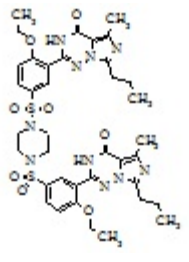
Vardenafil Impurity 3
C21H28N6O4S M.W. 460.56
V-0513



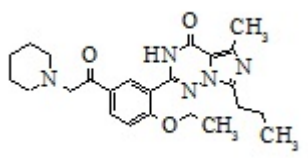
Vardenafil Impurity (2-Ethoxy Benzamidine Hydrochloride)
CAS No. 18637-00-8
C9H12N2O HCl M.W. 164.21 36.46
V-0515



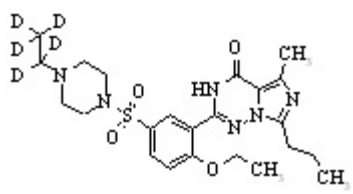
Vardenafil Dimer
C38H46N10O8S2 M.W. 834.98
V-0517



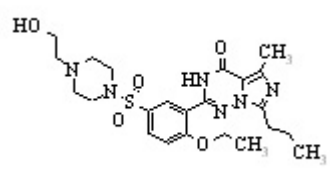
Vardenafil Acetyl Analogue
CAS No. N/A
C24H31N5O3 M.W. 437.55
V-0519



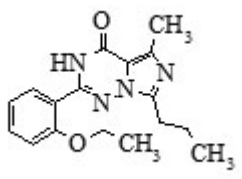
Vardenafil-d5
C23H27N6O4SD5 M.W. 493.64
V-053



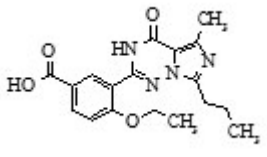
Hydroxy Vardenafil
C23H32N6O5S M.W. 504.61
V-055



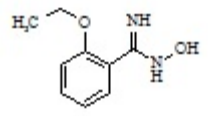
2-(2-Ethoxyphenyl)-5-methyl-7-propyl-3H-imidazo[5,1-f][1,2,4]triazin-4-one
C17H20N4O2 M.W. 312.37
V-057



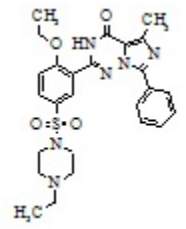
Norneovardenafil
CAS No. N/A
C18H20N4O4 M.W. 356.38
V-059



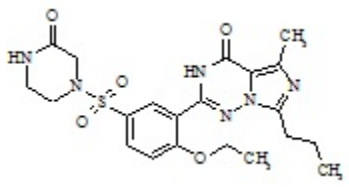
Vardenafil Impurity (2-Ethoxy-N-Hydroxy Benzamidine)
CAS No. 879-57-2
C9H12N2O2 M.W. 180.21
V-0514



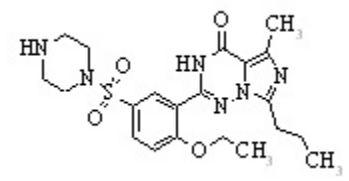
Vardenafil Benzoyl Impurity
C26H30N6O4S M.W. 522.63
V-0516



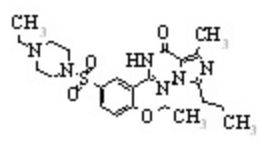
Vardenafil Oxopiperazine
C21H26N6O5S M.W. 474.54
V-0518



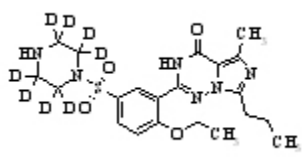
N-Desethyl Vardenafil
CAS No. 448184-46-1
C21H28N6O4S M.W. 460.56
V-052



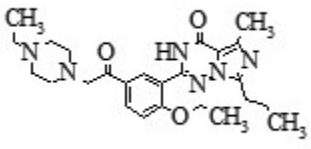
Vardenafil HCl
CAS No. 224785-90-4
C23H32N6O4S M.W. 488.61
V-054



N-Desethyl Vardenafil-d8
CAS No. 448184-46-1 (Unlabelled)
C21H28N6O4S M.W. 460.56
V-056

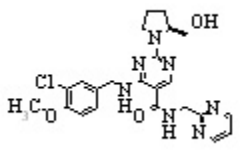


Acetylvardenafil
C25H34N6O3 M.W. 466.59
V-058

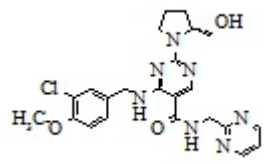


Avanafil Related Compounds (commercial standards available) – includes deuterated standards.

Avanafil
CAS No. 330784-47-9
C23H26ClN7O3 M.W. 483.96
A-291

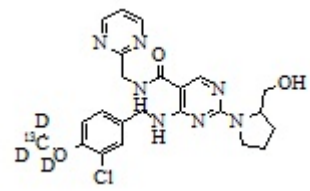


Avanafil Impurity 8 (R-Avanafil)
CAS No. N/A
C23H26ClN7O3 M.W. 483.96
A-2910

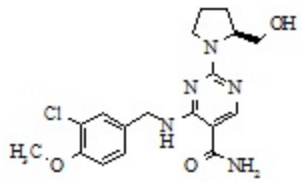


Avanafil Impurity 9
C18H17ClN6O3 M.W. 400.83
A-2911

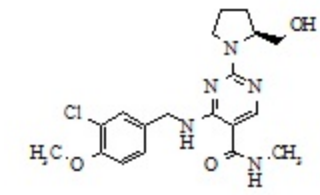
Avanafil-13CD3
C22H23ClN7O313CD3 M.W. 487.97
A-292



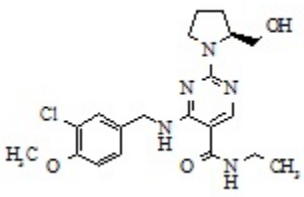
Avanafil impurity 1
C18H22ClN5O3 M.W. 391.86
A-293



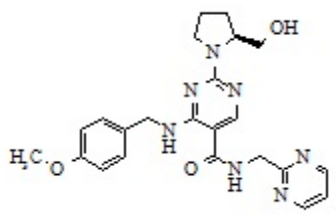
Avanafil impurity 2
C19H24ClN5O3 M.W. 405.89
A-294



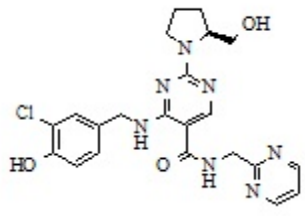
Avanafil impurity 3
C20H26ClN5O3 M.W. 419.91
A-295



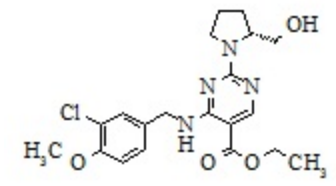
Avanafil impurity 4
C23H27N7O3 M.W. 449.52
A-296



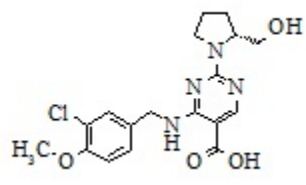
Avanafil impurity 5
C22H24ClN7O3 M.W. 469.93
A-297



Avanafil Impurity 6
CAS No. N/A
C20H25ClN4O4 M.W. 420.90
A-298

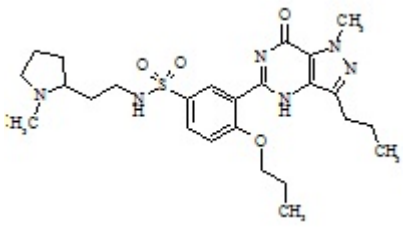


Avanafil Impurity 7
CAS No. N/A
C18H21ClN4O4 M.W. 392.85
A-299

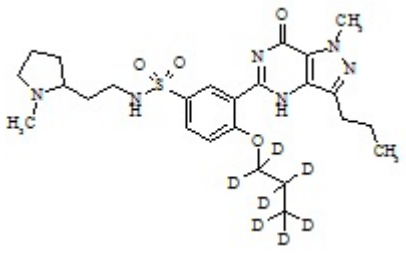


Udenafil Related Compounds (commercial standards available) – includes deuterated standards.

Udenafil
CAS No. 268203-93-6
C25H36N6O4S M.W. 516.67
U-031

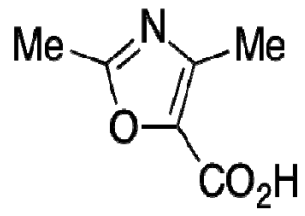


Udenafil-d7
CAS No. N/A
C25H29N6O4SD7 M.W. 523.71
U-032



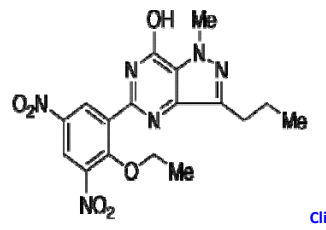
3. **Standards available from Toronto Research Chemicals http://www.trc-canada.com/ which include the majority of characterized PDE-5i analogues and all of the parent drugs including catalog numbers. (Some structure images not available) NOTE: Includes some compounds that are discontinued from TRC.**

Sildenafil Related Compounds (commercial standards available) – includes deuterated standards.



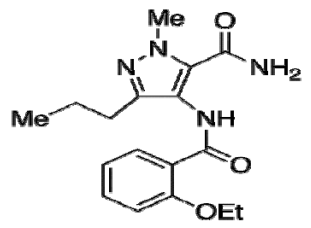
Click on image to enlarge

Catalogue #: D476330
Chemical Name: 2,4-Dimethyl-5-oxazolecarboxylic Acid
CAS Number: 2510-37-4
Mol. Formula: C6H7NO3
Synsynonyms: 2,4-Dimethyl-1,3-oxazole-5-carboxylic Acid; 2,4-Dimethyloxazole-5-carboxylic Acid; 5-Carboxy-2,4-dimethyloxazole



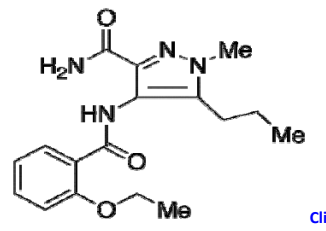
Click on image to enlarge

Catalogue #: D479775
Chemical Name: Dinitrodenafil
CAS Number:
Mol. Formula: C17H18N6O6
Synonyms: 5-(2-Ethoxy-3,5-dinitrophenyl)-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



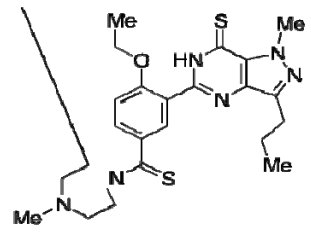
Click on image to enlarge

Catalogue #: E891000
Chemical Name: 4-(2-Ethoxybenzamido)-1-methyl-3-n-propylpyrazole-5-carboxamide
CAS Number: 139756-03-9
Mol. Formula: C17H22N4O3
Synonyms: 4-[(2-Ethoxybenzoyl)amino]-1-methyl-3-propyl-1H-pyrazole-5-carboxamide;



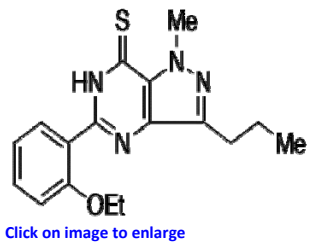
Click on image to enlarge

Catalogue #: E891010
Chemical Name: 4-[(2-Ethoxybenzoyl)amino]-1-methyl-5-propyl-1H-pyrazole-3-carboxamide
CAS Number: 501120-38-3
Mol. Formula: C17H22N4O3
Synonyms: 4-(2-Ethoxybenzamido)-1-methyl-5-propyl-1H-pyrazole-3-carboxamide



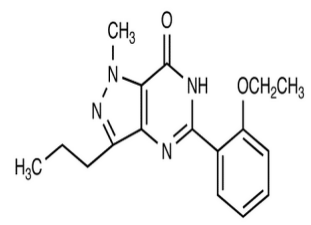
Click on image to enlarge

Catalogue #: E892530
Chemical Name: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)thioxomethyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyr
CAS Number: 1333233-46-7
Mol. Formula: C23H30N6OS2
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)thioxomethyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-Pyrazolo[4,3-d]pyrimidine-7-thione; Dithiodesmethylcarbodenafil



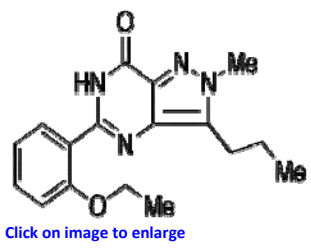
Click on image to enlarge

Catalogue #: E892710
Chemical Name: 5-(2-Ethoxyphenyl)-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione
CAS Number: 479074-06-1
Mol. Formula: C17H20N4OS
Synonyms: 5-(2-Ethoxyphenyl)-1,4-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione



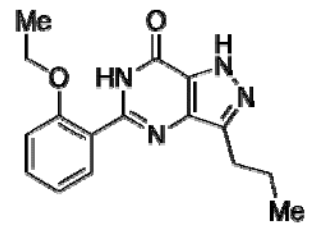
Click on image to enlarge

Catalogue #: E892725
Chemical Name: 5-(2-Ethoxyphenyl)-1-methyl-3-n-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 139756-21-1
Mol. Formula: C17H20N4O2
Synonyms: UK 088800; “Imidazosagatriazinone”



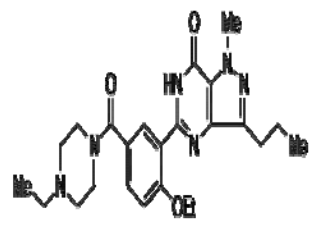
Click on image to enlarge

Catalogue #: E892730
Chemical Name: 5-(2-Ethoxyphenyl)-2,6-dihydro-2-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 501120-40-7
Mol. Formula: C17H20N4O2
Synonyms:



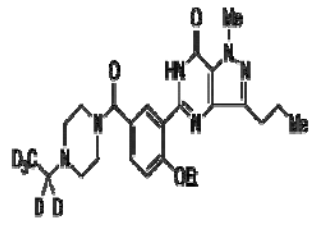
Click on image to enlarge

Catalogue #: E892765
Chemical Name: 5-(2-Ethoxyphenyl)-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 139756-30-2
Mol. Formula: C16H18N4O2
Synonyms: 5-(2-Ethoxyphenyl)-1,6-dihydro-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Des(4-methylpiperazin-1-ylsulfonyl) Desmethyl**sildenafil**



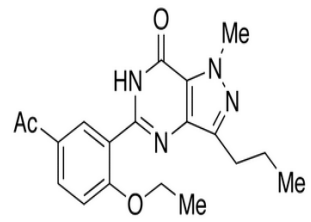
Click on image to enlarge

Catalogue #: F685400
Chemical Name: Fondenafil
CAS Number: 944241-52-5
Mol. Formula: C24H32N6O3
Synonyms: 5-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)carbonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Carbodenafil;



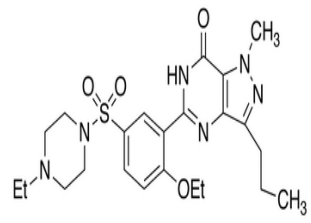
Click on image to enlarge

Catalogue #: F685402
Chemical Name: Fondenafil-d5
CAS Number:
Mol. Formula: C24H27D5N6O3
Synonyms: 5-[2-Ethoxy-5-[(4-ethyl-d5-1-piperazinyl)carbonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



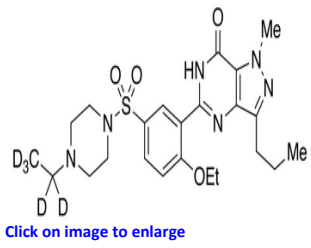
Click on image to enlarge

Catalogue #: G349960
Chemical Name: Gendenafil
CAS Number: 147676-66-2
Mol. Formula: C19H22N4O3
Synonyms: 5-(5-Acetyl-2-ethoxyphenyl)-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; 5-(5-Acetyl-2-ethoxyphenyl)-1-methyl-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one



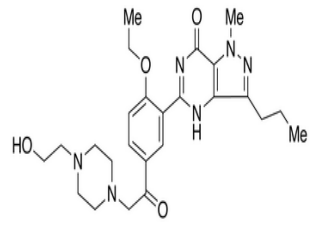
Click on image to enlarge

Catalogue #: H615150
Chemical Name: Homo Sildenafil
CAS Number: 642928-07-2
Mol. Formula: C23H32N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



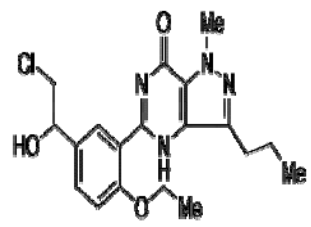
Click on image to enlarge

Catalogue #: H615152
Chemical Name: Homo Sildenafil-d5
CAS Number:
Mol. Formula: C23H27D5N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-(ethyl-d5)-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



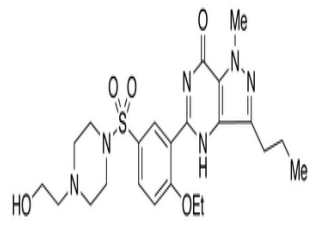
Click on image to enlarge

Chemical Name: Hydroxy Acetildenafil
CAS Number: 147676-56-0
Mol. Formula: C25H34N6O4
Synonyms: 5-[2-Ethoxy-5-[2-[4-(2-hydroxyethyl)-1-piperazinyl]acetyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Hydroxyhongdenafil;



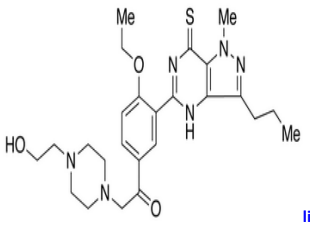
Click on image to enlarge

Catalogue #: H825115
Chemical Name: Hydroxy Chlorodenafil
CAS Number: 1391054-00-4
Mol. Formula: C19H23ClN4O3
Synonyms: 5-[5-(2-Chloro-1-hydroxyethyl)-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one



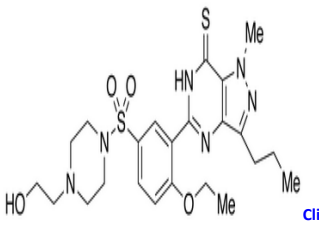
Click on image to enlarge

Catalogue #: H942840
Chemical Name: Hydroxyhomo Sildenafil
CAS Number: 139755-85-4
Mol. Formula: C23H32N6O5S
Synonyms: 5-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Lodenafil



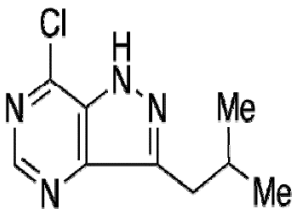
lick on image to enlarge

Catalogue #: H963100
Chemical Name: Hydroxythio Acetildenafil
CAS Number: 1159977-47-5
Mol. Formula: C25H34N6O3S
Synonyms: 5-[2-Ethoxy-5-[2-[4-(2-hydroxyethyl)-1-piperazinyl]acetyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-7-thio-pyrazolo[4,3-d]pyrimidine; 1-[3-(6,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]-2-[4-(2-hydroxyethyl)-1-piperazinyl]ethanone;



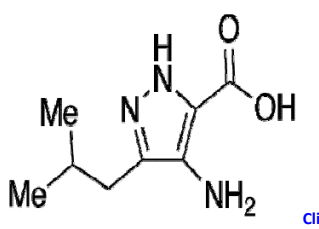
Click on image to enlarge

Catalogue #: H963150
Chemical Name: Hydroxythiohomo Sildenafil
CAS Number: 479073-82-0
Mol. Formula: C23H32N6O4S2
Synonyms: 5-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 4-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazineethanol



Click on image to enlarge

Catalogue #: I780530
Chemical Name: 3-Isobutyl-7-chloro-pyrazolo[4,3-d]pyrimidine
CAS Number:
Mol. Formula: C9H11ClN4
Synonyms: 3-Isobutyl-7-chloro-1H-pyrazolo[4,3-d]pyrimidine;



Click on image to enlarge

Catalogue #: I780615
Chemical Name: 5-(2-Isobutyl)-4-amino-1H-pyrazole-3-carboxylic Acid
CAS Number: 1093415-88-3
Mol. Formula: C8H13N3O2
Synonyms: 4-Amino-5-(2-methylpropyl)-1H-pyrazole-3-carboxylic Acid

no image of structure available

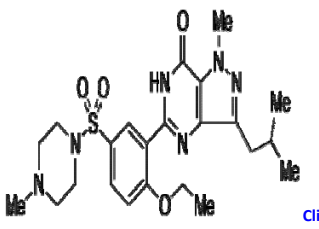
Catalogue #: I780620
Chemical Name: 3-Isobutylpyrazolo[4,3-d]pyrimidine
CAS Number:
Mol. Formula: C9H12N4
Synonyms: 3-Isobutyl-1H-pyrazolo[4,3-d]pyrimidine;

no image of structure available

Catalogue #: I780625
Chemical Name: 5-Isobutyl-4-nitro-1H-pyrazole-3-carboxylic Acid
CAS Number: 222729-55-7
Mol. Formula: C8H11N3O4
Synonyms: 5-(2-Methylpropyl)-4-nitro-1H-pyrazole-3-carboxylic Acid;

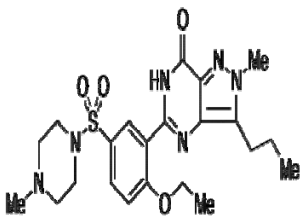
no image of structure available

Catalogue #: I780630
Chemical Name: 5-Isobutyl-1H-pyrazole-3-carboxylic Acid
CAS Number: 92933-49-8
Mol. Formula: C8H12N2O2
Synonyms: 5-(2-Methylpropyl)-1H-pyrazole-3-carboxylic Acid;



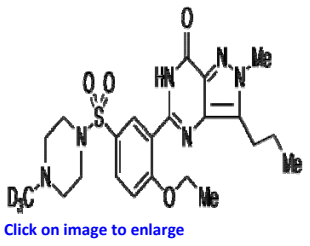
Click on image to enlarge

Catalogue #: I780650
Chemical Name: Isobutyl Sildenafil
CAS Number: 1391053-95-4
Mol. Formula: C23H32N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-(2-methylpropyl)-7H-pyrazolo[4,3-d]pyrimidin-7-one;



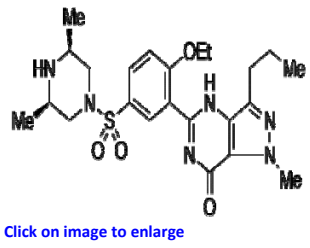
Click on image to enlarge

Catalogue #: I900800
Chemical Name: Iso Sildenafil
CAS Number: 253178-46-0
Mol. Formula: C22H30N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-2,6-dihydro-2-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; 1-[[3-(4,7-Dihydro-2-methyl-7-oxo-3-propyl-2H- pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine;



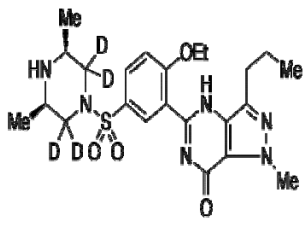
Click on image to enlarge

Catalogue #: I900802
Chemical Name: Iso Sildenafil-d3
CAS Number:
Mol. Formula: C22H27D3N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-(methyl-d3)-1-piperazinyl)sulfonyl]phenyl]-2,6-dihydro-2-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; 1-[[3-(4,7-Dihydro-2-methyl-7-oxo-3- propyl-2H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-(methyl-d3)piperazine;



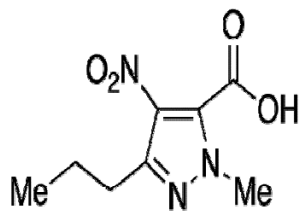
Click on image to enlarge

Catalogue #: M225935
Chemical Name: Methiso**sildenafil**
CAS Number: 496835-35-9
Mol. Formula: C23H32N6O4S
Synonyms: rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Aildenafil; Dimethyl**sildenafil**



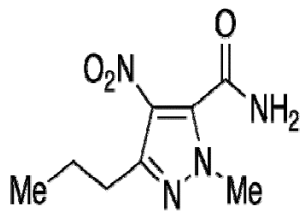
Click on image to enlarge

Catalogue #: M225937
Chemical Name: Methiso**sildenafil**-d4
CAS Number:
Mol. Formula: C23H28D4N6O4S
Synonyms: rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl-d4]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Aildenafil-d4;



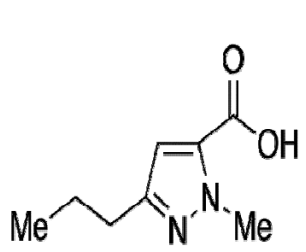
Click on image to enlarge

Catalogue #: M320530
Chemical Name: 1-Methyl-4-nitro-3-propyl-1H-pyrazole-5-carboxylic Acid
CAS Number: 139756-00-6
Mol. Formula: C8H11N3O4
Synonyms: 1-Methyl-4-nitro-3-propylpyrazole-5-carboxylic Acid



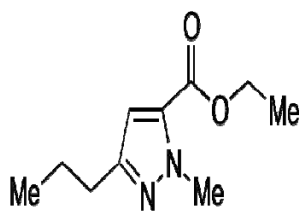
Click on image to enlarge

Catalogue #: M320535
Chemical Name: 1-Methyl-4-nitro-3-propylpyrazole-5-carboxamide
CAS Number: 139756-01-7
Mol. Formula: C8H12N4O3
Synonyms: 1-Methyl-4-nitro-3-propyl-1H-pyrazole-5-carboxamide



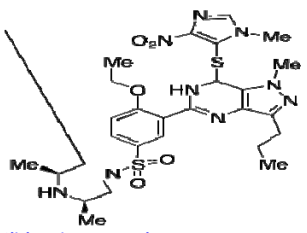
Click on image to enlarge

Catalogue #: M320655
Chemical Name: 1-Methyl-3-propyl-1H-pyrazole-5-carboxylic Acid
CAS Number: 139755-99-0
Mol. Formula: C8H12N2O2
Synonyms: 1-Methyl-3-propylpyrazole-5-carboxylic Acid; 2-Methyl-5-propyl-2H-pyrazole-3-carboxylic Acid



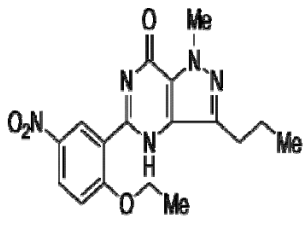
Click on image to enlarge

Catalogue #: M320775
Chemical Name: 1-Methyl-3-propyl-1H-pyrazole-5-carboxylic Acid Ethyl Ester
CAS Number: 133261-07-1
Mol. Formula: C10H16N2O2
Synonyms: 1-Methyl-3-propylpyrazole-5-carboxylic Acid Ethyl Ester; Ethyl 1-Methyl-3-propyl-1H-pyrazole-5-carboxylate; Ethyl 1-Methyl-3-propylpyrazole-5-carboxylate;



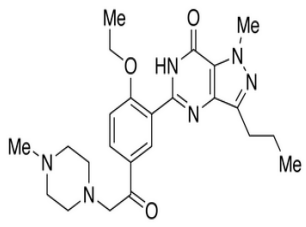
Click on image to enlarge

Catalogue #: M820000
Chemical Name: Mutaprodenafil
CAS Number: 138577-30-1
Mol. Formula: C27H37N9O5S2
Synonyms: rel-5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1-methyl-7-[(1-methyl-4-nitro-1H-imidazol-5-yl)thio]-3-propyl-1H-pyrazolo[4,3-d]pyrimidine



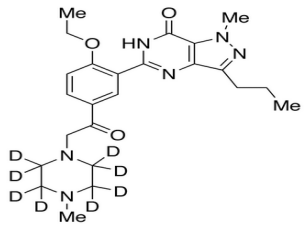
Click on image to enlarge

Catalogue #: N493770
Chemical Name: Nitrodenafil
CAS Number: 147676-99-1
Mol. Formula: C17H19N5O4
Synonyms: 5-(2-Ethoxy-5-nitrophenyl)-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



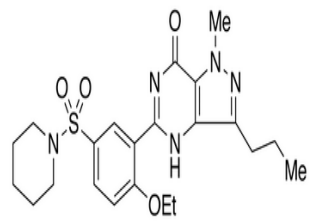
Click on image to enlarge

Catalogue #: N660500
Chemical Name: Nor Acetildenafil
CAS Number: 949091-38-7
Mol. Formula: C24H32N6O3
Synonyms: 5-[2-Ethoxy-5-[2-(4-methyl-1-piperazinyl)acetyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



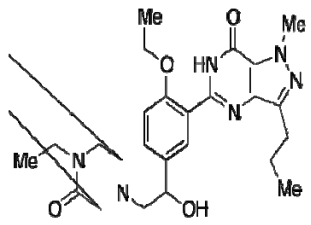
Click on image to enlarge

Catalogue #: N660502
Chemical Name: Nor Acetildenafil-d8
CAS Number: 1185117-07-0
Mol. Formula: C24H24D8N6O3
Synonyms: 5-[2-Ethoxy-5-[2-(4-methyl-1-piperazinyl-d8)acetyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



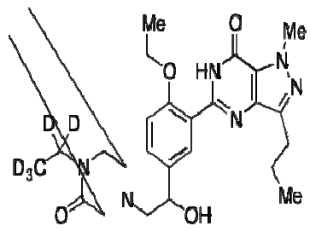
Click on image to enlarge

Catalogue #: N824300
Chemical Name: Norneo Sildenafil
CAS Number: 371959-09-0
Mol. Formula: C22H29N5O4S
Synonyms: 5-[2-Ethoxy-5-(1-piperidinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; 1-[[3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]piperidine;



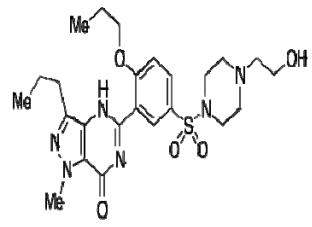
Click on image to enlarge

Catalogue #: P480470
Chemical Name: Piperazonifil
CAS Number: 1335201-04-1
Mol. Formula: C25H34N6O4
Synonyms: 5-[2-Ethoxy-5-[2-(4-ethyl-3-oxo-1-piperazinyl)-1-hydroxyethyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one,



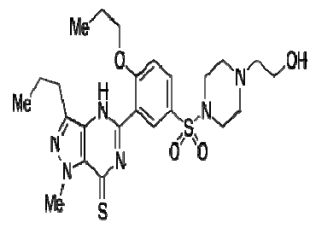
Click on image to enlarge

Catalogue #: P480472
Chemical Name: Piperazonifil-d5
CAS Number:
Mol. Formula: C25H29D5N6O4
Synonyms: 5-[2-Ethoxy-5-[2-(4-ethyl-3-oxo-1-piperazinyl)-1-hydroxyethyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one-d5



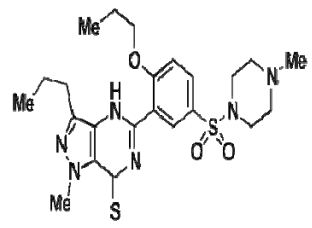
Click on image to enlarge

Catalogue #: P831600
Chemical Name: Propoxyphenyl Homohydroxy**sildenafil**
CAS Number: 139755-87-6
Mol. Formula: C24H34N6O5S
Synonyms: 5-[5-[4-(2-Hydroxyethyl)piperazinylsulfonyl]-2-propoxyphenyl]-1-methyl-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one; 4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-1-Piperazineethanol



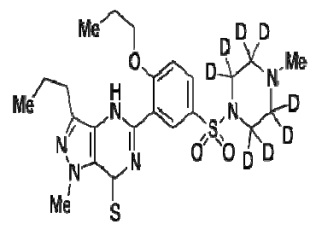
Click on image to enlarge

Catalogue #: P831630
Chemical Name: Propoxyphenyl-thiohydroxyhomosildenafil
CAS Number: 479073-90-0
Mol. Formula: C24H34N6O4S2
Synonyms: 1,6-dihydro-5-[5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1-methyl-3-propyl-7H-Pyrazolo[4,3-d]pyrimidine-7-thione; 4-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-1-Piperazineethanol; 5-(5-((4-(2-hydroxyethyl)piperazin-1-yl)sulfonyl)-2-propoxyphenyl)-1-methyl-3-propyl-1H-pyrazolo[4,3-d]pyrimidine-7(4H)-thione



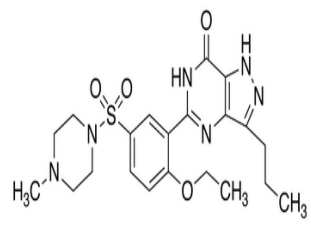
Click on image to enlarge

Catalogue #: P831635
Chemical Name: Propoxyphenyl Thio**sildenafil**
CAS Number: 479073-87-5
Mol. Formula: C23H32N6O3S2
Synonyms: 1,6-Dihydro-1-methyl-5-[5-[(4-methyl-1-piperazinyl)sulfonyl]-2-propoxyphenyl]-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-4-methyl-piperazine; rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione



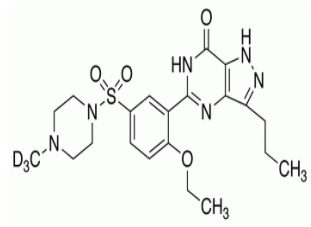
Click on image to enlarge

Catalogue #: P831637
Chemical Name: Propoxyphenyl-thio**sildenafil**-d8
CAS Number:
Mol. Formula: C23H24D8N6O3S2
Synonyms: 1,6-Dihydro-1-methyl-5-[5-[(4-methyl-1-piperazinyl)sulfonyl]-2-propoxyphenyl]-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione-d8; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-4-methyl-piperazine-d8; rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione-d8



Click on image to enlarge

Catalogue #: P842800
Chemical Name: Pyrazole N-Demethyl Sildenafil
CAS Number: 139755-95-6
Mol. Formula: C21H28N6O4S
Synonyms: 1-[[3-(4,7-Dihydroxy-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methyl-piperazine; Desmethyl**sildenafil**;



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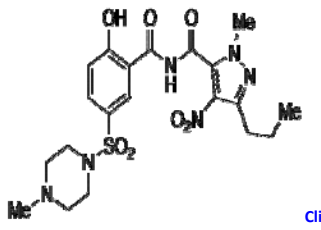
Catalogue #: P842802
Chemical Name: Pyrazole N-Demethyl Sildenafil-d3
CAS Number:
Mol. Formula: C21H25D3N6O4S
Synonyms: 1-[[3-(4,7-Dihydroxy-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl-4- ethoxyphenyl]sulfonyl]-4-(methyl-d3)piperazine; Desmethyl**sildenafil**-d3;



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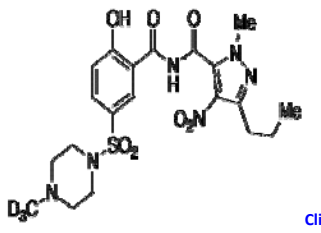
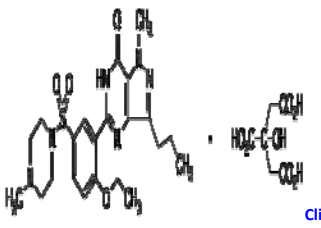
Catalogue #: P846500
Chemical Name: Pyrazolosalicyloyl Imide
CAS Number:
Mol. Formula: C20H26N6O7S
Synonyms: N-[2-Hydroxy-5-[(4-methyl-1-piperazinyl)sulfonyl]benzoyl]-1-methyl-4-nitro-3-n-propyl-1H-pyrazol-5-carboxamide; Pyrazolosalicylimide



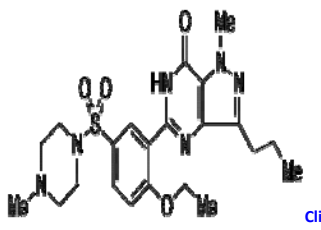
Click on image to enlarge

Catalogue #: P846502
Chemical Name: Pyrazolosalicyloyl Imide-d3
CAS Number:
Mol. Formula: C20H23D3N6O7S
Synonyms: N-[2-Hydroxy-5-[(4-methyl-1-piperazinyl)sulfonyl]benzoyl]-1-methyl-4-nitro-3-n-propyl-1H-pyrazol-5-carboxamide-d3; Pyrazolosalicylimide-d3



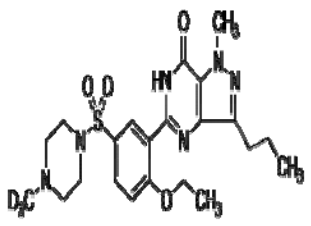
Click on image to enlarge

Catalogue #: S435000
Chemical Name: Sildenafil Citrate
CAS Number: 171599-83-0
Mol. Formula: C28H38N6O11S
Synonyms: 1-[[3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine Citrate;



Click on image to enlarge

Catalogue #: S435001
Chemical Name: Sildenafil
CAS Number: 139755-83-2
Mol. Formula: C22H30N6O4S
Synonyms: 1-[[3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine; 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;

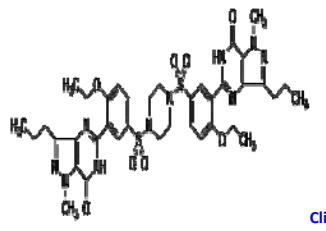


Click on image to enlarge

Catalogue #: S435002
Chemical Name: Sildenafil-d3
CAS Number: 1126745-90-1
Mol. Formula: C22H27D3N6O4S
Synonyms: 1-[[3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine-d3; 5-[2-Ethoxy-5-[[4-(methyl-d3)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;

no image of structure available

Catalogue #: S435003
Chemical Name: Sildenafil-d8
CAS Number: 951385-68-5
Mol. Formula: C22H22D8N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl-2,2,3,3,5,5,6,6-d8)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; BDD 10402;

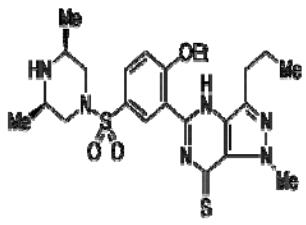


Click on image to enlarge

Catalogue #: S435020
Chemical Name: Sildenafil Dimer Impurity
CAS Number:
Mol. Formula: C38H46N10O8S2
Synonyms:

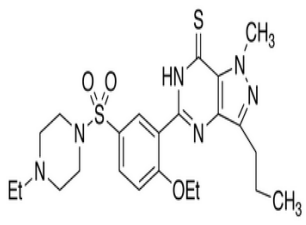
no image of structure available

Catalogue #: S435035
Chemical Name: Sildenafil N-Oxide
CAS Number: 1094598-75-0
Mol. Formula: C22H30N6O5S
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-4-oxido-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



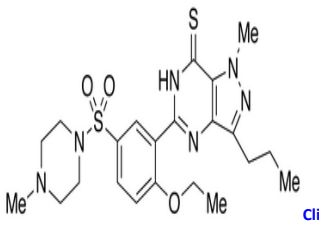
Click on image to enlarge

Catalogue #: T344365
Chemical Name: Thioaildenafil
CAS Number: 856190-47-1
Mol. Formula: C23H32N6O3S2
Synonyms: (3R,5S)-rel-1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-3,5-dimethyl-piperazine; Sulfoaildenafil;



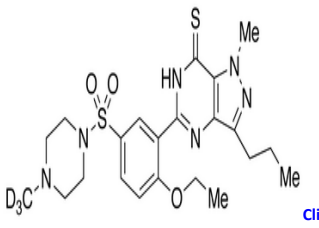
Click on image to enlarge

Catalogue #: T344470
Chemical Name: Thiohomo Sildenafil
CAS Number: 479073-80-8
Mol. Formula: C23H32N6O3S2
Synonyms: 5-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-ethyl-piperazine



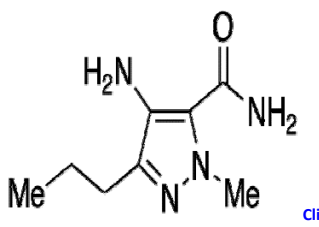
Click on image to enlarge

Catalogue #: T371500
Chemical Name: Thio**sildenafil**
CAS Number: 479073-79-5
Mol. Formula: C22H30N6O3S2
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo- 1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine;



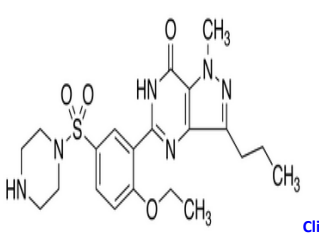
Click on image to enlarge

Catalogue #: T371502
Chemical Name: Thio**sildenafil**-d3
CAS Number:
Mol. Formula: C22H27D3N6O3S2
Synonyms: 5-[2-Ethoxy-5-[(4-(methyl-d3)-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl -7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-(methyl-d3)piperazine;



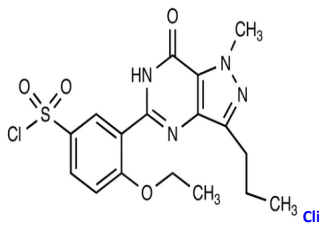
Click on image to enlarge

Catalogue #: A617415
Chemical Name: 4-Amino-1-methyl-3-propyl-1H-pyrazole-5-carboxamide
CAS Number: 139756-02-8
Mol. Formula: C8H14N4O
Synonyms: 4-Amino-2-methyl-5-propyl-2H-pyrazole-3-carboxamide;



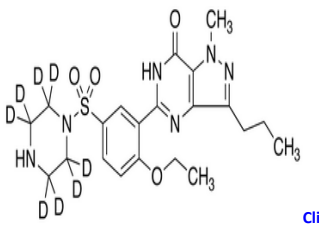
Click on image to enlarge

Catalogue #: D292200
Chemical Name: N-Desmethyl Sildenafil
CAS Number: 139755-82-1
Mol. Formula: C21H28N6O4S
Synonyms: 5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Desmethyl**sildenafil**; UK 103320;



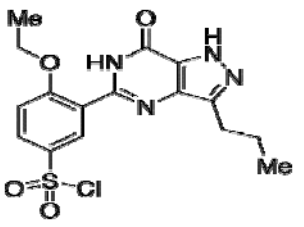
Click on image to enlarge

Catalogue #: C380005
Chemical Name: 5-(5-Chlorosulfonyl-2-ethoxyphenyl)-1-methyl-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 139756-22-2
Mol. Formula: C17H19ClN4O4S
Synonyms: 3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxy-benzenesulfonyl Chloride;



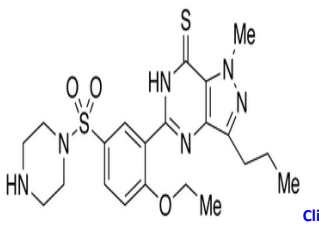
Click on image to enlarge

Catalogue #: D292202
Chemical Name: N-Desmethyl Sildenafil-d8
CAS Number:
Mol. Formula: C21H20D8N6O4S
Synonyms: 5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one-d8; Desmethyl**sildenafil**-d8; UK 103320-d8;



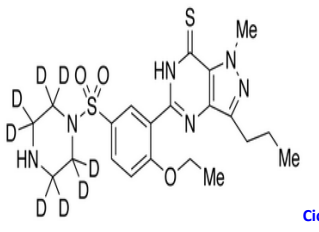
Click on image to enlarge

Catalogue #: C383500
Chemical Name: 5-(5-Chlorosulfonyl-2-ethoxyphenyl)-3-propyl-1,6-dihydro -7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 139756-31-3
Mol. Formula: C16H17ClN4O4S
Synonyms: 3-(6,7-Dihydro-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxybenzenesulfonyl Chloride; Des-4-methylpiperazine Desmethyl**sildenafil** Chloride;



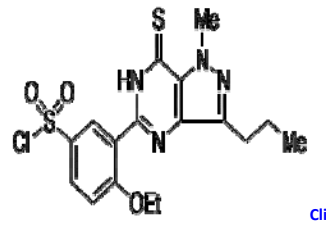
Click on image to enlarge

Catalogue #: D294350
Chemical Name: Desmethyl Thio**sildenafil**
CAS Number: 479073-86-4
Mol. Formula: C21H28N6O3S2
Synonyms: 5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl- 7H-pyrazolo[4,3-d]pyrimidine-7-thione;



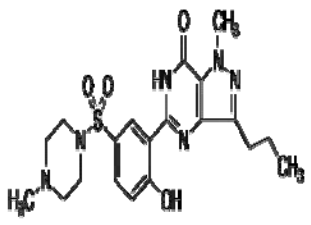
Cick on image to enlarge

Catalogue #: D294352
Chemical Name: Desmethyl Thio**sildenafil**-d8
CAS Number: 1215321-44-0
Mol. Formula: C21H20D8N6O3S2
Synonyms: 5-[2-Ethoxy-5-(1-piperazinyl-d8-sulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl- 7H-pyrazolo[4,3-d]pyrimidine-7-thione;



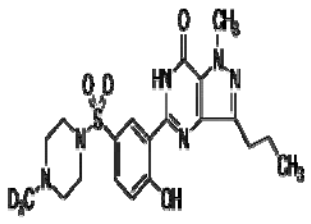
Click on image to enlarge

Catalogue #: D449445
Chemical Name: 3-(6,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxy-benzenesulfonyl Chloride
CAS Number: 479074-07-2
Mol. Formula: C17H19ClN4O3S2
Synonyms:



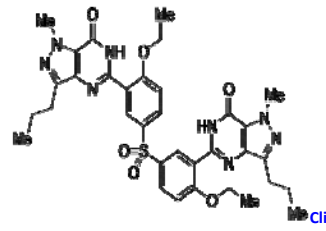
Click on image to enlarge

Chemical Name: Desethyl Sildenafil
CAS Number: 139755-91-2
Mol. Formula: C20H26N6O4S
Synonyms: 5-[2-Hydroxy-5-(4-methylpiperazinylsulphonyl)phenyl]1-methyl-3-n-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyramidin-7-one; 5-[2-Hydroxy-5-[[4-(methyl)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



Click on image to enlarge

Catalogue #: D289602
Chemical Name: Desethyl Sildenafil-d3
CAS Number: 1346603-75-5
Mol. Formula: C20H23D3N6O4S
Synonyms: 5-[2-Hydroxy-5-(4-methyl-d3-piperazinylsulphonyl)phenyl]1-methyl-3-n-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyramidin-7-one; 5-[2-Hydroxy-5-[[4-(methyl-d3)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;

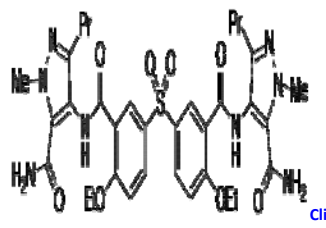


Click on image to enlarge

Catalogue #: D231215
Chemical Name: De(methypiperazinyl) Sildenafil Dimer Impurity
CAS Number: 1346603-48-2
Mol. Formula: C34H38N8O6S
Synonyms: 5-[2-Ethoxy-5-[4-[4-ethoxy-3-(1-methyl-7-oxo-3-propyl-4,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-yl)phenyl]sulfonyl]phenyl]-1-methyl-3-n-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one;

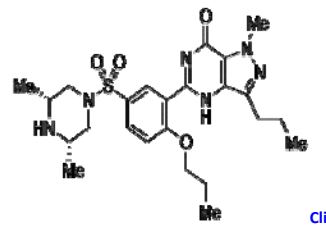
no image of structure available

Catalogue #: D231235
Chemical Name: Demethylpiperazinyl Sildenafil Sulfonic Acid
CAS Number:
Mol. Formula: C17H20N4O5S
Synonyms: 3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxybenzenesulfonic Acid;



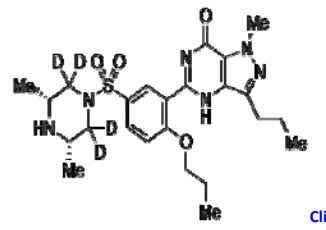
Click on image to enlarge

Catalogue #: A603070
Chemical Name: 3-[[[5-Aminocarbonyl-1-methyl-3-propyl-1H-pyrazol-4-yl]amino]carbonyl]-4-ethoxy-benzenesulfonyl Dimer
CAS Number:
Mol. Formula: C34H42N8O8S
Synonyms: 3,3'-Sulfonyl Bis[(4-Ethoxy-3-(6,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo-pyrimidin-5-yl)benzene)



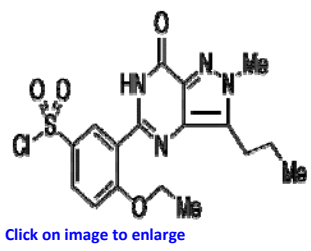
Click on image to enlarge

Catalogue #: D289495
Chemical Name: O-Desethyl-O-propyl Methiso**sildenafil**
CAS Number: 1391053-82-9
Mol. Formula: C24H34N6O4S
Synonyms: rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



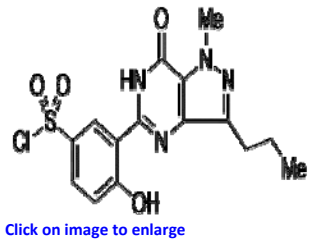
Click on image to enlarge

Catalogue #: D289497
Chemical Name: O-Desethyl-O-propyl Methiso**sildenafil**-d4
CAS Number:
Mol. Formula: C24H30D4N6O4S
Synonyms: rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one-d4;



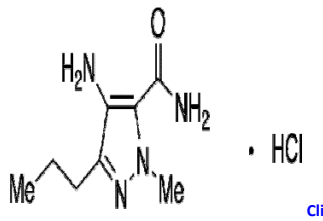
Click on image to enlarge

Catalogue #: D231290
Chemical Name: Demethylpiperazinyl Iso Sildenafil Sulfonyl Chloride
CAS Number: 501120-42-9
Mol. Formula: C17H19ClN4O4S
Synonyms: 3-(6,7-Dihydro-2-methyl-7-oxo-3-propyl-2H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxy-benzenesulfonyl Chloride



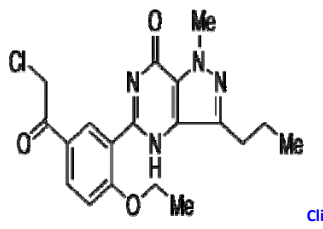
Click on image to enlarge

Catalogue #: D231300
Chemical Name: Demethylpiperazinyl Desethyl Sildenafil Sulfonyl Chloride
CAS Number: 139756-27-7
Mol. Formula: C15H15ClN4O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-hydroxy-benzenesulfonyl Chloride; 5-(5-Chlorosulfonyl-2-hydroxyphenyl)-1-methyl-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one



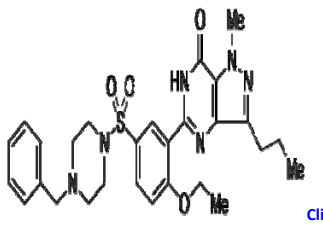
Click on image to enlarge

Catalogue #: A617420
Chemical Name: 4-Amino-1-methyl-3-propyl-1H-pyrazole-5-carboxamide Hydrochloride
CAS Number: 247584-10-7
Mol. Formula: C8H15ClN4O
Synonyms: 4-Amino-2-methyl-5-propyl-2H-pyrazole-3-carboxamide Hydrochloride;



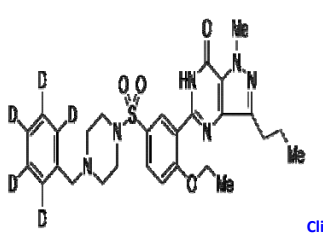
Click on image to enlarge

Catalogue #: C365535
Chemical Name: Chlorodenafil
CAS Number: 1058653-74-9
Mol. Formula: C19H21ClN4O3
Synonyms: 5-[5-(2-Chloroacetyl)-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



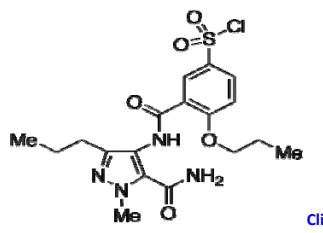
Click on image to enlarge

Catalogue #: D292205
Chemical Name: N-Desmethyl-N-benzyl Sildenafil
CAS Number:
Mol. Formula: C28H34N6O4S
Synonyms: 5-[2-Ethoxy-5-(1-benzyl-1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Benzyl Sildenafil;



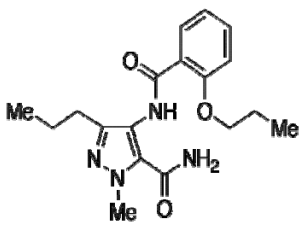
Click on image to enlarge

Catalogue #: D292207
Chemical Name: N-Desmethyl-N-benzyl Sildenafil-d5
CAS Number:
Mol. Formula: C28H29D5N6O4S
Synonyms: 5-[2-Ethoxy-5-(1-(benzyl-d5)-1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Benzyl Sildenafil-d5;



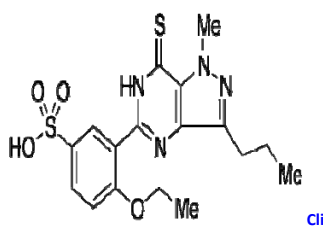
Click on image to enlarge

Catalogue #: A603110
Chemical Name: 3-[[[5-(Aminocarbonyl)-1-methyl-3-propyl-1H-pyrazol-4-yl]amino]carbonyl]-4-propoxy-benzenesulfonyl Chloride
CAS Number: 374776-34-8
Mol. Formula: C18H23ClN4O5S
Synonyms:



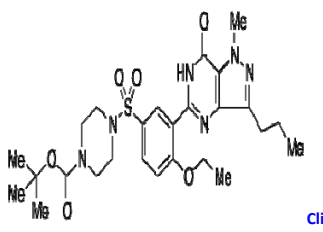
Click on image to enlarge

Catalogue #: A603105
Chemical Name: 3-[[[5-(Aminocarbonyl)-1-methyl-3-propyl-1H-pyrazol-4-yl]amino]carbonyl]-4-propoxybenzene
CAS Number: 139756-04-0
Mol. Formula: C18H24N4O3
Synonyms: 1-Methyl-4-(2-propoxybenzamido)-3-propylpyrazole-5-carboxamide; 1-Methyl-4-[(2-propoxybenzoyl)amino]-3-propyl-1H-pyrazole-5-carboxamide



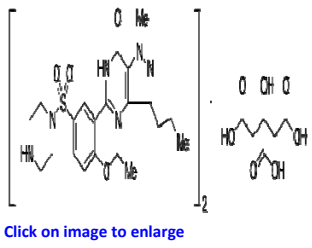
Click on image to enlarge

Catalogue #: D231260
Chemical Name: Demethylpiperazinyl 7-Desoxo 7-Thioxo**sildenafil** Sulfonic Acid
CAS Number: 1353018-10-6
Mol. Formula: C17H20N4O4S2
Synonyms: 4-Ethoxy-3-(1-methyl-3-propyl-7-thioxo-6,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-yl)benzenesulfonic Acid



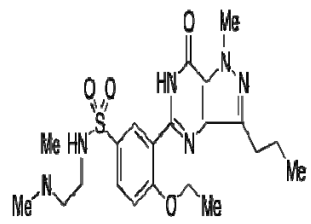
Click on image to enlarge

Catalogue #: D292245
Chemical Name: N-(Desmethyl)-tert-butyl Acetate Sildenafil
CAS Number: 398507-63-6
Mol. Formula: C26H36N6O6S
Synonyms: tert-Butyl 4-((4-Ethoxy-3-(1-methyl-7-oxo-3-propyl-6,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-yl)phenyl)sulfonyl)piperazine-1-carboxylate; 4-[[3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazinecarboxylic Acid 1,1-Dimethylethyl Ester



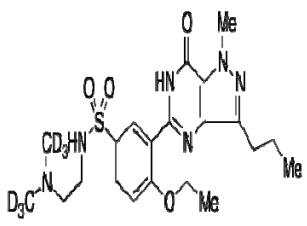
Click on image to enlarge

Catalogue #: D292201
Chemical Name: N-Desmethyl Sildenafil Hemicitrate
CAS Number:
Mol. Formula: C48H64N12O15S2
Synonyms: 5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one Hemicitrate; Desmethyl**sildenafil** Hemicitrate; UK 103320 Hemicitrate



Click on image to enlarge

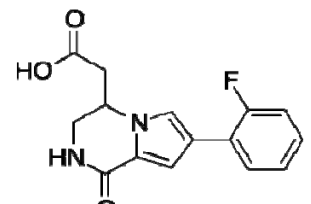
Catalogue #: D289520
Chemical Name: Descarbon**sildenafil**
CAS Number: 1393816-99-3
Mol. Formula: C21H30N6O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-N-[2-(dimethylamino)ethyl]-4-ethoxy-benzenesulfonamide



Click on image to enlarge

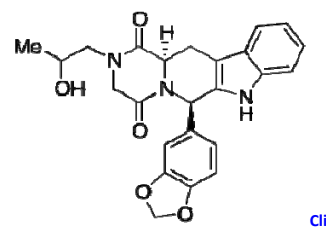
Catalogue #: D289522
Chemical Name: Descarbon**sildenafil**-d6
CAS Number:
Mol. Formula: C21H24D6N6O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-N-[2-(dimethyl-d6-amino)ethyl]-4-ethoxy-benzenesulfonamide

Tadalafil Related Compounds (commercial standards available) – includes deuterated standards.



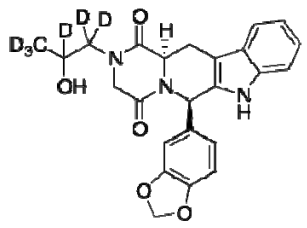
Click on image to enlarge

Catalogue #: F595590
Chemical Name: 7-(2-Fluorophenyl)-1,2,3,4-tetrahydro-1-oxo-pyrrolo[1,2-a]pyrazine-4-acetic Acid
CAS Number: 1170575-17-3
Mol. Formula: C15H13FN2O3
Synonyms:



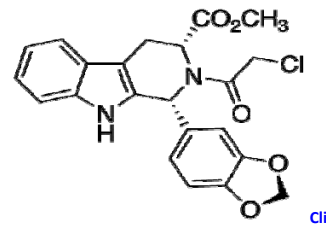
Click on image to enlarge

Catalogue #: H952705
Chemical Name: 2-Hydroxypropyl Nor**tadalafil**
CAS Number: 1353020-85-5
Mol. Formula: C24H23N3O5
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(2-hydroxypropyl)-pyrazino[1&#65533;,2&#65533;:1,6]pyrido[3,4-b]indole-1,4-dione;



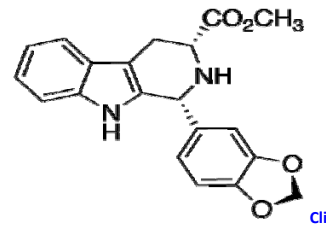
Click on image to enlarge

Catalogue #: H952707
Chemical Name: 2-Hydroxypropyl-d6 Nor**tadalafil**
CAS Number:
Mol. Formula: C24H17D6N3O5
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(2-hydroxypropyl)-pyrazino[1&#65533;,2&#65533;:1,6]pyrido[3,4-b]indole-1,4-dione-d6;



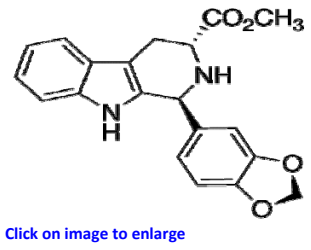
Click on image to enlarge

Catalogue #: M330125
Chemical Name: (1R,3R)-Methyl-1,2,3,4-tetrahydro-2-chloroacetyl-1-(3,4-methylenedioxyphenyl)-9H-pyrido[3,4-b]indole-3-carboxylate (Chloropre**tadalafil**)
CAS Number: 171489-59-1
Mol. Formula: C22H19ClN2O5
Synonyms: (1R,3R)-1-(1,3-Benzodioxol-5-yl)-2-(2-chloroacetyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester;



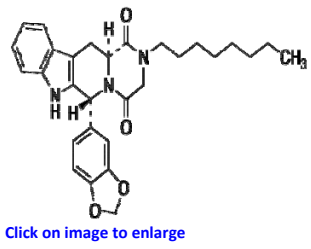
Click on image to enlarge

Catalogue #: M330150
Chemical Name: (1R,3R)-Methyl-1,2,3,4-tetrahydro-1-(3,4-methylenedioxyphenyl)-9H-pyrido[3,4-b]indole-3-carboxylate
CAS Number: 171596-41-1
Mol. Formula: C20H18N2O4
Synonyms: (1R,3R)-1-(1,3-Benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester;



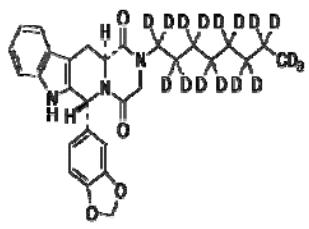
Click on image to enlarge

Catalogue #: M330155
Chemical Name: (1S,3R)-Methyl-1,2,3,4-tetrahydro-1-(3,4-methylenedioxyphenyl)-9H-pyrido[3,4-b]indole-3-carboxylate
CAS Number: 171596-42-2
Mol. Formula: C20H18N2O4
Synonyms: (1S,3R)-1-(1,3-Benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester;



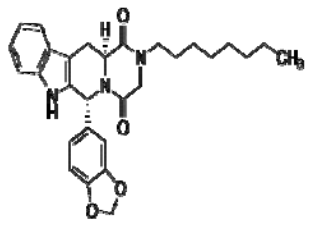
Click on image to enlarge

Catalogue #: O241350
Chemical Name: N-Octyl Nor**tadalafil**
CAS Number: 1173706-35-8
Mol. Formula: C29H33N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-octylpyrazino[1&#65533;,2&#65533;:1,6]pyrido[3,4-b]indole-1,4-dione;



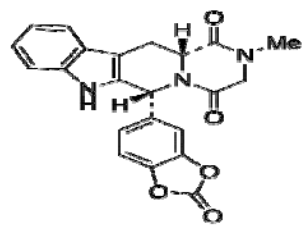
Click on image to enlarge

Catalogue #: O241352
Chemical Name: N-Octyl Nor**tadalafil**-d17
CAS Number:
Mol. Formula: C29H16D17N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(octyl-d17)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



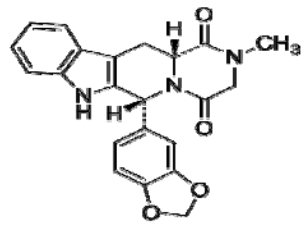
Click on image to enlarge

Catalogue #: O241360
Chemical Name: N-Octyl cis-Nor**tadalafil**
CAS Number:
Mol. Formula: C29H33N3O4
Synonyms: (6R,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-octylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



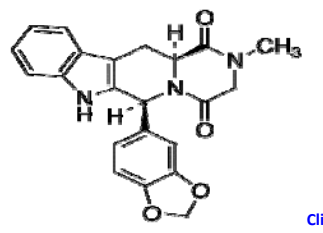
Click on image to enlarge

Catalogue #: O870430
Chemical Name: 2'-Oxo Tadalafil
CAS Number:
Mol. Formula: C22H17N3O5
Synonyms: (6R,12aR)-6-(2-Oxo-1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; 2'-Keto Tadalafil;



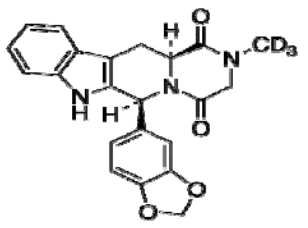
Click on image

Catalogue #: T004500
Chemical Name: Tadalafil
CAS Number: 171596-29-5
Mol. Formula: C22H19N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; Cialis; GF 196960; IC 351; ICOS 351; Tildenafil; UK 336017;



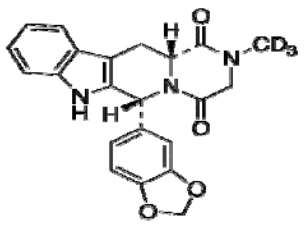
Click on image to enlarge

Catalogue #: T004505
Chemical Name: ent-Tadalafil
CAS Number: 629652-72-8
Mol. Formula: C22H19N3O4
Synonyms: (6S,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methyl-pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; L-Tadalafil; L-Tildenafil;



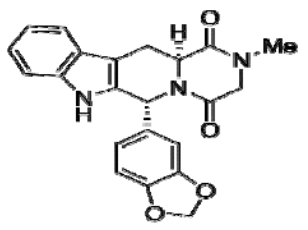
Click on image to enlarge

Catalogue #: T004507
Chemical Name: ent-Tadalafil-d3
CAS Number:
Mol. Formula: C22H16D3N3O4
Synonyms: (6S,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(methyl-d3)-pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; L-Tadalafil-d3; L-Tildenafil-d3;



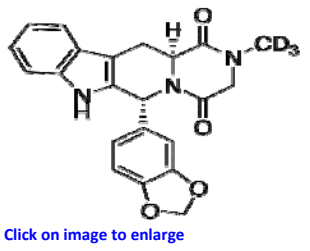
Click on image to enlarge

Catalogue #: T004510
Chemical Name: Tadalafil-d3
CAS Number: 960226-55-5
Mol. Formula: C22H16D3N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; Cialis-d3; GF 196960-d3; IC 351-d3; ICOS 351-d3; Tildenafil-d3; UK 336017-d3;



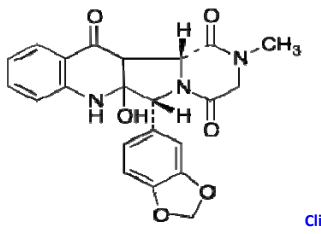
Click on image to enlarge

Catalogue #: T004520
Chemical Name: cis-Tadalafil
CAS Number: 171596-27-3
Mol. Formula: C22H19N3O4
Synonyms: (6R,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R-cis)-6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a- hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



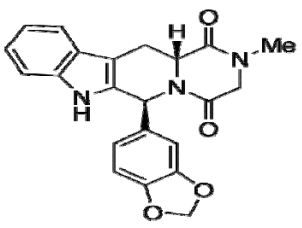
Click on image to enlarge

Catalogue #: T004522
Chemical Name: cis-Tadalafil-d3
CAS Number:
Mol. Formula: C22H16D3N3O4
Synonyms: (6R,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R-cis)-6-(1,3-benzodioxol-5-yl)- 2,3,6,7,12,12a-hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



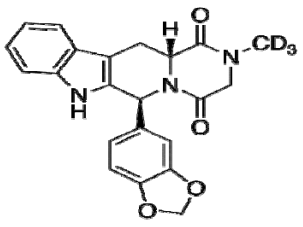
Click on image to enlarge

Catalogue #: T004525
Chemical Name: Tadalafil Hydroxypiperidone
CAS Number:
Mol. Formula: C22H19N3O6
Synonyms: Tadalafil Impurity



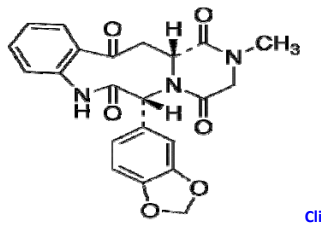
Click on image to enlarge

Catalogue #: T004530
Chemical Name: cis-ent-Tadalafil
CAS Number: 171596-28-4
Mol. Formula: C22H19N3O4
Synonyms: (6S,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6S-cis)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a- hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



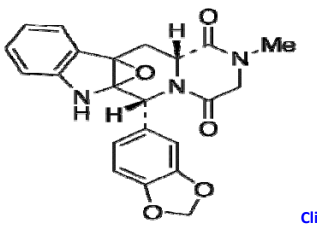
Click on image to enlarge

Catalogue #: T004532
Chemical Name: cis-ent-Tadalafil-d3
CAS Number:
Mol. Formula: C22H16D3N3O4
Synonyms: 6S,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6S-cis)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a- hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



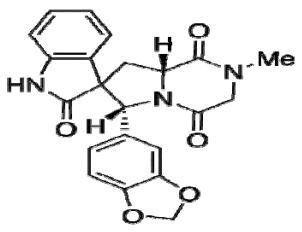
Click on image to enlarge

Catalogue #: T004535
Chemical Name: Tadalafil Ketolactam
CAS Number: 1346605-38-6
Mol. Formula: C22H19N3O6
Synonyms: (6R,14aR)-rel-6-(1,3-Benzodioxol-5-yl)-2,3,14,14a-tetrahydro-2-methylpyrazino[1,2-d][1,4]benzodiazonine-1,4,7,13(6H,8H)-tetrone;



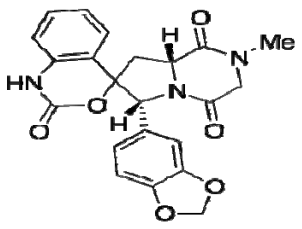
Click on image to enlarge

Catalogue #: T004540
Chemical Name: Tadalafil Epoxide Discontinued
CAS Number:
Mol. Formula: C22H19N3O5
Synonyms: Epoxy Tadalafil;



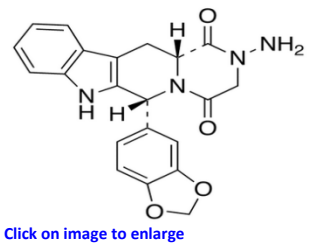
Click on image to enlarge

Catalogue #: T004550
Chemical Name: Tadalafil Spiro-oxindole
CAS Number:
Mol. Formula: C22H19N3O5
Synonyms: Tadalafil Impurity



Click on image to enlarge

Catalogue #: T004555
Chemical Name: Tadalafil Spiro-2-keto-1,3-oxazine
CAS Number:
Mol. Formula: C22H19N3O6
Synonyms: Tadalafil Impurity



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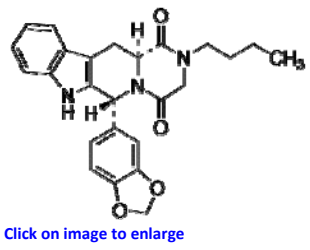
Catalogue #: A629550
Chemical Name: Amino Tadalafil
CAS Number: 385769-84-6
Mol. Formula: C21H18N4O4
Synonyms: (6R,12aR)-2-Amino-6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



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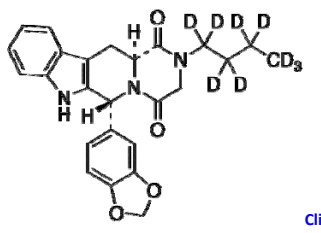
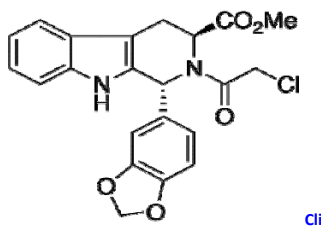
Catalogue #: B693585
Chemical Name: N-Butyl Nor**tadalafil**
CAS Number: 171596-31-9
Mol. Formula: C25H25N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2-butyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



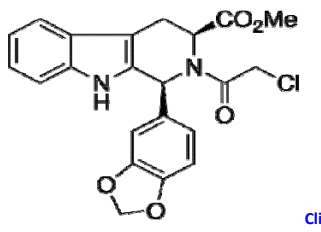
Click on image to enlarge

Catalogue #: B693587
Chemical Name: N-Butyl Nor**tadalafil**-d9
CAS Number:
Mol. Formula: C25H16D9N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2-(butyl-d9)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



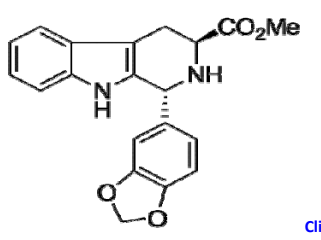
Click on image to enlarge

Catalogue #: B200000
Chemical Name: (1R,3S)-1-(1,3-Benzodioxol-5-yl)-2-(2-chloroacetyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester
CAS Number: 629652-44-4
Mol. Formula: C22H19ClN2O5
Synonyms:



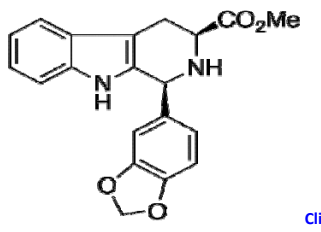
Click on image to enlarge

Catalogue #: B200005
Chemical Name: (1S,3S)-1-(1,3-Benzodioxol-5-yl)-2-(2-chloroacetyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester
CAS Number: 629652-42-2
Mol. Formula: C22H19ClN2O5
Synonyms:



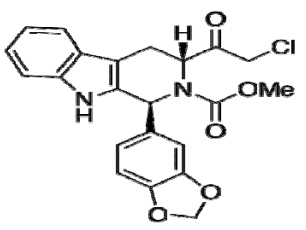
Click on image to enlarge

Catalogue #: B200025
Chemical Name: (1R,3S)-1-(1,3-Benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester
CAS Number: 171596-44-4
Mol. Formula: C20H18N2O4
Synonyms:



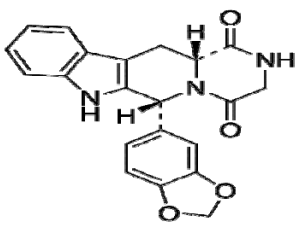
Click on image to enlarge

Catalogue #: B200020
Chemical Name: (1S,3S)-1-(1,3-Benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester
CAS Number: 171596-43-3
Mol. Formula: C20H18N2O4
Synonyms: (1S-cis)-1-(1,3-benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester



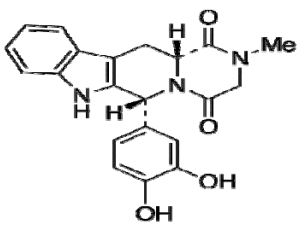
Click on image to enlarge

Catalogue #: B121700
Chemical Name: (1S,3R)-1-Benzo[1,3]dioxol-5-yl-2-(2-chloro-acetyl)-2,3,4,9-tetrahydro-1H-b-carboline-3-carboxylic Acid Methyl Ester
CAS Number: 629652-40-0
Mol. Formula: C22H19ClN2O5
Synonyms: (1S,3R)-1-(1,3-Benzodioxol-5-yl)-2-(2-chloroacetyl)-2,3,4,9-tetrahydro1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester; (1S,3R)-1-(1,3-Benzodioxol-5-yl)-2-(chloroacetyl)-2,3,4,9-tetrahydro1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester;



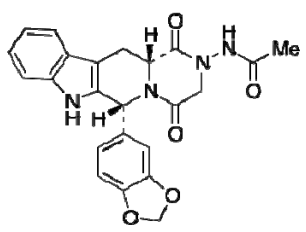
Click on image to enlarge

Catalogue #: D293800
Chemical Name: N-Desmethyl Tadalafil
CAS Number: 171596-36-4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R-trans)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; Nor**tadalafil**



Click on image to enlarge

Catalogue #: D291990
Chemical Name: Desmethylene Tadalafil
CAS Number: 171489-03-5
Mol. Formula: C21H19N3O4
Synonyms: (6R,12aR)-6-(3,4-dihydroxyphenyl)-2,3,6,7,12,12a-hexahydro-2-methyl-pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R,trans)-6-(3,4-dihydroxyphenyl)-2,3,6,7,12,12a-hexahydro-2-methyl-pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;

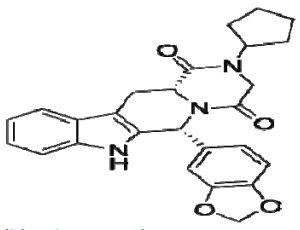


Click on image to enlarge

Catalogue #: A161250
Chemical Name: Acetamino**tadalafil**
CAS Number: 1446144-71-3
Mol. Formula: C23H20N4O5
Synonyms: N-[(6R,12aR)-6-(1,3-Benzodioxol-5-yl)-3,4,6,7,12,12a-hexahydro-1,4-dioxopyrazino[1,2:1,6]pyrido[3,4-b]indol-2(1H)-yl]-acetamide;

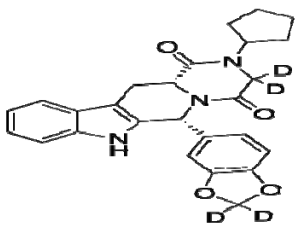
no image of structure available

Catalogue #: D293805
Chemical Name: N-Desmethyl ent-Tadalafil
CAS Number: 929100-66-3
Mol. Formula: C21H17N3O4
Synonyms: (6R,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione



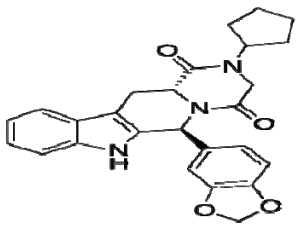
Click on image to enlarge

Catalogue #: B199000
Chemical Name: N-Desmethyl-N-cyclopentyl Tadalafil
CAS Number: 171596-32-0
Mol. Formula: C26H25N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2-cyclopentyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R-trans)-6-(1,3-Benzodioxol-5-yl)-2-cyclopentyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione



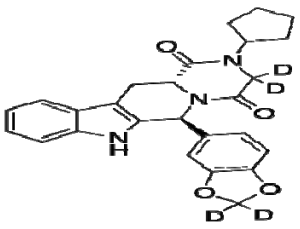
Click on image to enlarge

Catalogue #: B199002
Chemical Name: N-Desmethyl-N-cyclopentyl Tadalafil-D4
CAS Number:
Mol. Formula: C26H21D4N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2-cyclopentyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione-D4; (6R-trans)-6-(1,3-Benzodioxol-5-yl)-2-cyclopentyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione-D4



Click on image to enlarge

Catalogue #: B199005
Chemical Name: N-Desmethyl-N-cyclopentyl cis-ent-Tadalafil
CAS Number:
Mol. Formula: C26H25N3O4
Synonyms:



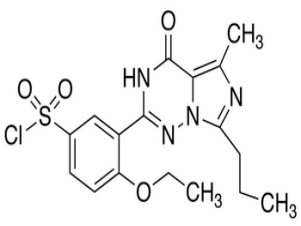
Click on image to enlarge

Catalogue #: B199007
Chemical Name: N-Desmethyl-N-cyclopentyl cis-ent-Tadalafil-D4
CAS Number:
Mol. Formula: C26H21D4N3O4
Synonyms:

Vardenafil Related Compounds (commercial standards available) – includes deuterated standards.

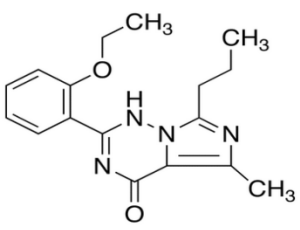
no image of structure available

Chemical Name: 2-Ethoxybenzamidine Hydrochloride
CAS Number: 18637-00-8
Mol. Formula: C9H13ClN2O
Synonyms: 2-Ethoxybenzenecarboximidamide Hydrochloride; o-Ethoxybenzamidine Monohydrochloride; 2-Ethoxybenzenecarboximidamide Monohydrochloride



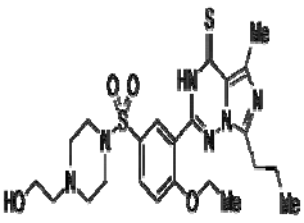
Click on image to enlarge

Catalogue #: E892500
Chemical Name: 4-Ethoxy-3-(5-methyl-4-oxo-7-propyl-3,4-dihydro-imidazo[5,1-f][1,2,4]-triazin-2-yl)benzene-sulfonyl Chloride
CAS Number: 224789-26-8
Mol. Formula: C17H19ClN4O4S
Synonyms: 3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxy-benzenesulfonyl Chloride;



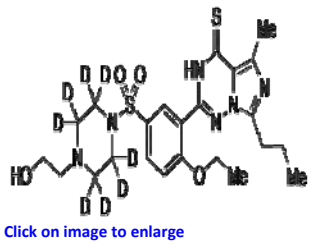
Click on image to enlarge

Catalogue #: E892745
Chemical Name: 2-(2-Ethoxyphenyl)-5-methyl-7-propyl-3H-imidazo[5,1-f][1,2,4]triazin-4-one
CAS Number: 224789-21-3
Mol. Formula: C17H20N4O2
Synonyms: 2-(2-Ethoxyphenyl)-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one;



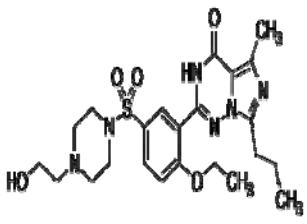
Click on image to enlarge

Catalogue #: H963400
Chemical Name: Hydroxythio**vardenafil**
CAS Number: 912576-30-8
Mol. Formula: C23H32N6O4S2
Synonyms: 2-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazine-4(1H)-thione; 4-[[3-(1,4-Dihydro-5-methyl-7-propyl-4-thioxoimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazineethanol;



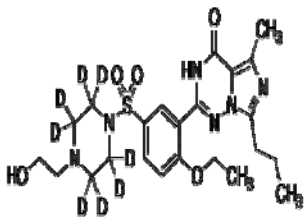
Click on image to enlarge

Catalogue #: H963402
Chemical Name: Hydroxythio**vardenafil**-d8
CAS Number:
Mol. Formula: C23H24D8N6O4S2
Synonyms: 2-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazine-4(1H)-thione-d8; 4-[[3-(1,4-Dihydro-5-methyl-7-propyl-4-thioxoimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazineethanol-d8;



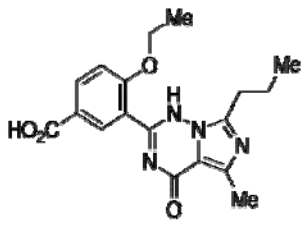
Click on image to enlarge

Catalogue #: H995300
Chemical Name: Hydroxy Vardenafil
CAS Number: 224785-98-2
Mol. Formula: C23H32N6O5S
Synonyms: 2-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazin-4(1H)-one; 4-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo [5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazineethanol;



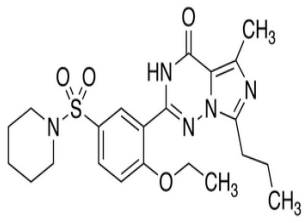
Click on image to enlarge

Catalogue #: H995302
Chemical Name: Hydroxy Vardenafil-d8
CAS Number:
Mol. Formula: C23H24D8N6O5S
Synonyms: 2-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-(piperazinyl-d8)]sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazin-4(1H)-one; 4-[[3-(1,4-Dihydro-5-methyl-4-oxo-7- propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-1-(piperazine-d8)ethanol;



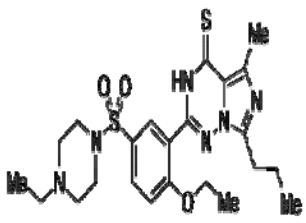
Click on image to enlarge

Chemical Name: Norneo Vardenafil
CAS Number: 358390-39-3
Mol. Formula: C18H20N4O4
Synonyms: 3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxybenzoic Acid;



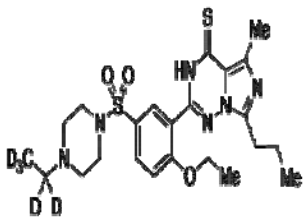
Click on image to enlarge

Catalogue #: P839615
Chemical Name: Pseudo Vardenafil
CAS Number: 224788-34-5
Mol. Formula: C22H29N5O4S
Synonyms: 2-[2-Ethoxy-5-(1-piperidinylsulfonyl)phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazin-4(1H)-one; Piperidenafil; Pseudo**vardenafil**;



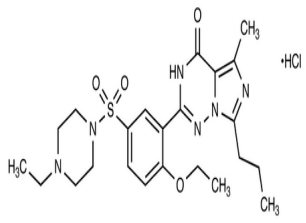
Click on image to enlarge

Catalogue #: T384250
Chemical Name: Thio**vardenafil**
CAS Number: 912576-24-0
Mol. Formula: C23H32N6O3S2
Synonyms: 2-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazine-4(1H)-thione; 1-[[3-(1,4-Dihydro-5-methyl-7-propyl-4-thioxoimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-4-ethylpiperazine;



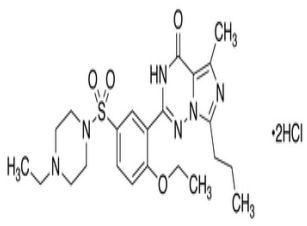
Click on image to enlarge

Catalogue #: T384252
Chemical Name: Thio**vardenafil**-d5
CAS Number:
Mol. Formula: C23H27D5N6O3S2
Synonyms: 2-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazine-4(1H)-thione-d5; 1-[[3-(1,4-Dihydro-5-methyl-7-propyl-4-thioxoimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-4-ethylpiperazine-d5;



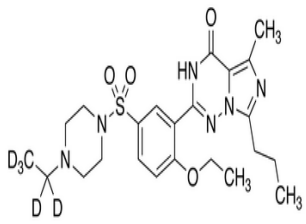
Click on image to enlarge

Catalogue #: V098000
Chemical Name: Vardenafil, Hydrochloride Salt Discontinued See V098001
CAS Number: 224785-91-5
Mol. Formula: C23H33ClN6O4S
Synonyms: Levitra, Valdenafil



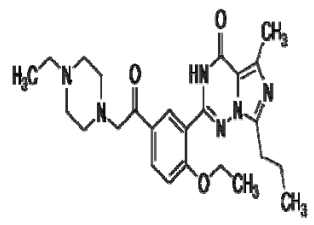
Click on image to enlarge

Catalogue #: V098001
Chemical Name: Vardenafil Dihydrochloride Salt
CAS Number: 224789-15-5
Mol. Formula: C23H34Cl2N6O4S
Synonyms: 1-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-4-ethyl-piperazine;Levitra; Nuviva;



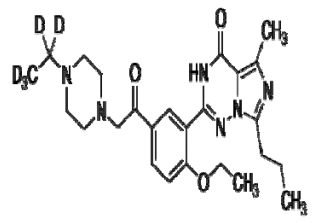
Click on image to enlarge

Catalogue #: V098002
Chemical Name: Vardenafil-d5
CAS Number: 1189685-70-8
Mol. Formula: C23H27D5N6O4S
Synonyms: 1-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-4-(ethyl-d5)-piperazine; Levitra-d5; Nuviva-d5;



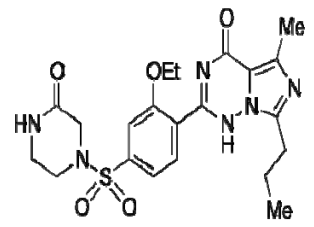
Click on image to enlarge

Catalogue #: V098015
Chemical Name: Vardenafil Acetyl Analogue
CAS Number: 1261351-28-3
Mol. Formula: C25H34N6O3
Synonyms: 2-[2-Ethoxy-5-[2-(4-ethyl-1-piperazinyl)acetyl]phenyl]-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one;



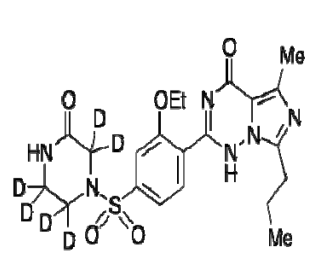
Click on image to enlarge

Catalogue #: V098017
Chemical Name: Vardenafil Acetyl-d5 Analogue
CAS Number: 1330171-51-1
Mol. Formula: C25H29D5N6O3
Synonyms: 2-[2-Ethoxy-5-[2-(4-(ethyl-d5)-1-piperazinyl)acetyl]phenyl]-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one;



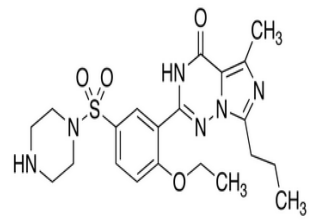
Click on image to enlarge

Catalogue #: V098030
Chemical Name: Vardenafil Oxopiperazine (Impurity)
CAS Number: 448184-58-5
Mol. Formula: C21H26N6O5S
Synonyms: 2-[2-Ethoxy-5-[(3-oxo-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one; 4-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-piperazinone



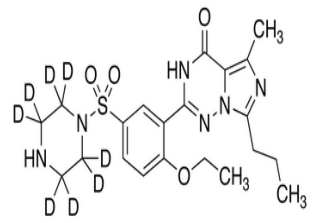
Click on image to enlarge

Catalogue #: V098032
Chemical Name: Vardenafil Oxopiperazine-D6 (Impurity)
CAS Number:
Mol. Formula: C21H20D6N6O5S
Synonyms: 2-[2-Ethoxy-5-[(3-oxo-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one-D6; 4-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-piperazinone-D6



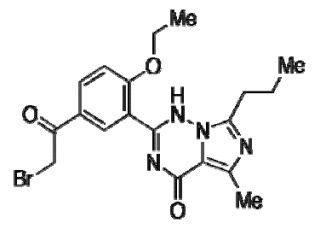
Click on image to enlarge

Catalogue #: D289950
Chemical Name: N-Desethyl Vardenafil
CAS Number: 448184-46-1
Mol. Formula: C21H28N6O4S
Synonyms: 1-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-piperazine;



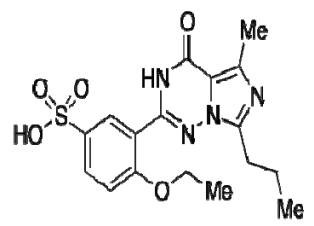
Click on image to enlarge

Catalogue #: D289952
Chemical Name: N-Desethyl Vardenafil-d8
CAS Number:
Mol. Formula: C21H20D8N6O4S
Synonyms: 1-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-piperazine-d8;



Click on image to enlarge

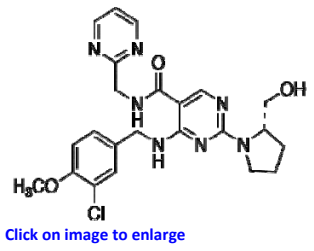
Catalogue #: D220200
Chemical Name: 1-Decarboxyl-1-(bromoacetyl) Norneo**vardenafil**
CAS Number: 358388-58-6
Mol. Formula: C19H21BrN4O3
Synonyms: 2-[5-(Bromoacetyl)-2-ethoxyphenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazin-4(1H)-one;



Click on image to enlarge

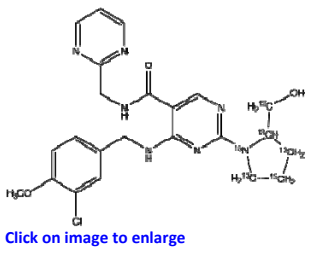
Catalogue #: D453410
Chemical Name: 3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxybenzenesulfonic Acid
CAS Number: 437717-43-6
Mol. Formula: C17H20N4O5S
Synonyms:

Avanafil Related Compounds (commercial standards available) – includes deuterated standards.



Click on image to enlarge

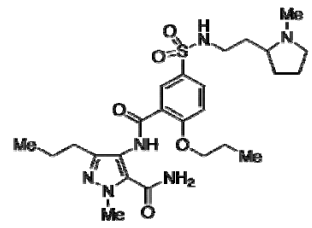
Catalogue #: A794670
Chemical Name: Avanafil
CAS Number: 330784-47-9
Mol. Formula: C23H26ClN7O3
Synonyms: (S)-2-(2-Hydroxymethyl-1-pyrrolidinyl)-4-(3-chloro-4-methoxybenzylamino)-5-[(2-pyrimidinylmethyl)carbamoyl]pyrimidine; 4-[[(3-Chloro-4-methoxyphenyl)methyl] amino]-2-[(2S)-2-(hydroxymethyl)-1-pyrrolidinyl]-N-(2-pyrimidinylmethyl)-5-pyrimidinecarboxamide; TA 1790;



Click on image to enlarge

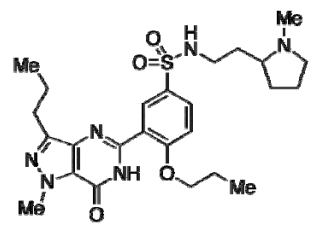
Catalogue #: A794672
Chemical Name: Avanafil-13C5,15N
CAS Number:
Mol. Formula: C1813C5H26ClN615NO3
Synonyms: (S)-2-(2-Hydroxymethyl-1-pyrrolidinyl)-4-(3-chloro-4-methoxybenzylamino)-5-[(2-pyrimidinylmethyl)carbamoyl]pyrimidine-13C5,15N; 4-[[(3-Chloro-4-methoxyphenyl)methyl] amino]-2-[(2S)-2-(hydroxymethyl)-1-pyrrolidinyl]-N-(2-pyrimidinylmethyl)-5-pyrimidinecarboxamide-13C5,15N; TA 1790-13C5,15N;

Udenafil Related Compounds (commercial standards available) – includes deuterated standards.



Click on image to enlarge

Catalogue #: M320180
Chemical Name: 1-Methyl-4-[[5-[[[2-(1-methyl-2-pyrrolidinyl)ethyl]amino]sulfonyl]-2-propoxybenzoyl]amino]-3-propyl-1H-pyrazole-5-carboxamide
CAS Number: 382592-28-1
Mol. Formula: C25H38N6O5S
Synonyms:



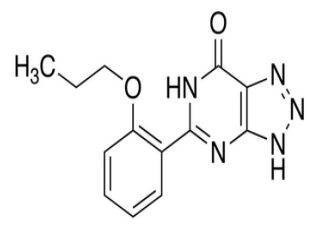
Click on image to enlarge

Catalogue #: U250500
Chemical Name: Udenafil
CAS Number: 268203-93-6
Mol. Formula: C25H36N6O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-N-[2-(1-methyl-2-pyrrolidinyl)ethyl]-4-propoxybenzenesulfonamide; DA 8159; Zydena;

no image of structure available

Catalogue #: U250502
Chemical Name: Udenafil-d7
CAS Number: 1175992-76-3
Mol. Formula: C25H29D7N6O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-N-[2-(1-methyl-2-pyrrolidinyl)ethyl]-4-(propoxy-d7)benzenesulfonamide; DA 8159-d7; Zydena-d7;

Zaprinast

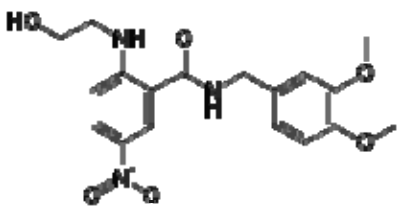


Click on image to enlarge

Catalogue #: Z150000
Chemical Name: Zaprinast
CAS Number: 37762-06-4
Mol. Formula: C13H13N5O2
Synonyms: 3,6-dihydro-5-(2-propoxyphenyl)-7H-1,2,3-triazolo[4,5-d]pyrimidin-7-one; 1,4-Dihydro-5-[2-propoxyphenyl]-7H-1,2,3-triazolo[4,5-d]pyrimidine-7-one; 8-Aza-2-(2-propoxyphenyl)-6-purinone; M&B 22,948;

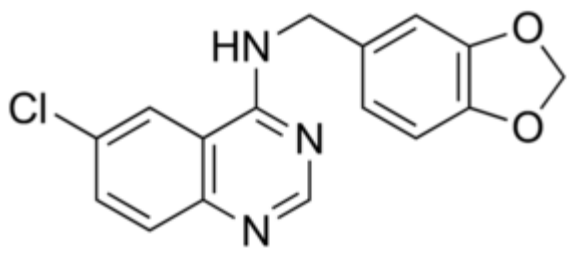
4. Additional Items for Consideration Web Based Search Data

Benzamidenafil
IUPAC name: N-[(3,4-Dimethoxyphenyl)methyl]-2-(1-hydroxypropan-2-ylamino)-5-nitrobenzamide
Other names: Xanthoanthrafil
CAS number: 1020251-53-

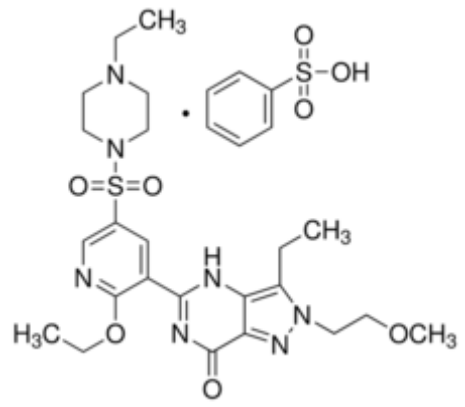


5. Additional Items for Consideration Novel PDE-5 inhibitors from SIAL

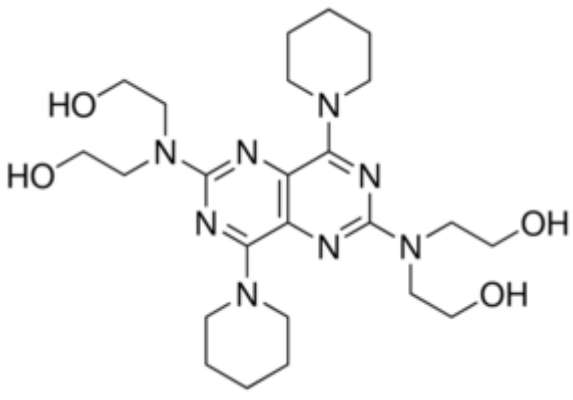
MBCQ
SML0439 SIGMA
≥98% (HPLC)
Synonym: 4-((3,4-Methylenedioxybenzyl)amino)-6-chloroquinazoline
CAS Number 150450-53-6
Empirical Formula (Hill Notation) $C_{16}H_{12}ClN_3O_2$
Molecular Weight 313.74
MDL number MFCD00673946



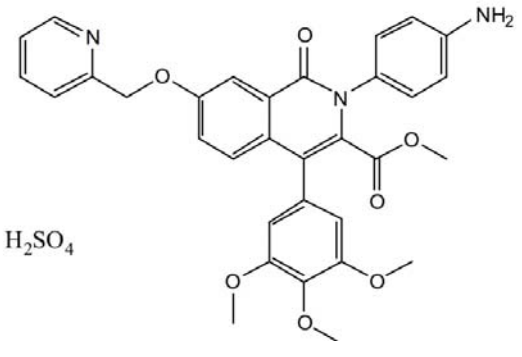
Gisadenafil besylate salt
≥98% (HPLC)
PZ0172 SIGMA
Synonym: 5-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]-3-pyridinyl]-3-ethyl-2,6-dihydro-2-(2-methoxyethyl)-7H-pyrazolo[4,3-d]pyrimidin-7-one benzenesulfonate besylate salt, UK 369003-26, UK 369003
CAS Number 334827-98-4
Empirical Formula (Hill Notation) $C_{23}H_{33}N_7O_5S \cdot C_6H_6O_3S$
Molecular Weight 677.79
MDL number MFCD18384964



Dipyridamole
≥98% (TLC), powder
D9766 SIGMA
CAS Number 58-32-2
Empirical Formula (Hill Notation) $C_{24}H_{40}N_8O_4$
Molecular Weight 504.63
EC Number 200-374-7
MDL number MFCD00010555
PubChem Substance ID 24277705
No Longer Offered by SIAL but published and possibly produced in Japan



Product Number T7692
Cas #: 212500-03-3
Synonyms: Methyl-(2-(4-aminophenyl)-1,2-dihydro-1-oxo-7-(2-pyridinylmethoxy)-4-(3,4,5-trimethoxyphenyl))-3-isoquinoline carboxylic acid, sulfate salt
Molecular Formula: C32H29N3O7·H2SO4



The isoquinolone derivative, T-1032, is a potent, selective inhibitor of cyclic GMP-specific phosphodiesterase (PDE5). In studies of PDE isoenzymes isolated from canine tissues, T-1032 was a competitive inhibitor of cyclic GMP hydrolysis by PDE5 at nanomolar concentrations (IC50 1.0 nM, Ki = 1.2 nM).

6. Additional Information

There are a significant number of lead compounds being researched which depart from the classic sildenafil pyrazolopyrimidinone template. These compounds number into the thousands and are likely to appear in greater number over time as research publications and patent literature show more detail on particular structures and their synthesis.

AOAC SMPR 2014.012

Standard Method Performance Requirements for Screening Method for Phosphodiesterase Type 5 (PDE5) Inhibitors in Dietary Ingredients and Supplements

Intended Use: Routine Surveillance of Dietary Ingredients and Products

1 Purpose

AOAC *Standard Method Performance Requirements*SM (SMPRs) describe the minimum recommended performance characteristics to be used during the evaluation of a method. The evaluation may be an on-site verification, a single-laboratory validation, or a multi-site collaborative study. SMPRs are written and adopted by AOAC stakeholder panels composed of representatives from industry, regulatory organizations, contract laboratories, test kit manufacturers, and academic institutions. AOAC SMPRs are used by AOAC expert review panels in their evaluation of validation study data for method being considered for *Performance Tested Methods*SM or AOAC *Official Methods of Analysis*SM, and can be used as acceptance criteria for verification at user laboratories. [Refer to Appendix F: *Guidelines for Standard Method Performance Requirements*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA.]

2 Applicability

Qualitative assay for phosphodiesterase type 5 (PDE5) inhibitors in dietary ingredients and supplements.

3 Analytical Technique

Any analytical technique(s) that detects the analytes of interest and meets the following method performance requirements is/are acceptable.

4 Definitions

Dietary ingredients.—A vitamin; a mineral; an herb or other botanical; an amino acid; a dietary substance for use by man to supplement the diet by increasing total dietary intake; or a concentrate, metabolite, constituent, extract, or combination of any of the above dietary ingredients. {United States Federal Food Drug and Cosmetic Act §201(ff) [U.S.C. 321 (ff)]}

Dietary supplements.—A product intended for ingestion that contains a "dietary ingredient" intended to add further nutritional value to (supplement) the diet. Dietary supplements may be found in many forms such as tablets, capsules, softgels, gelcaps, liquids, or powders.

Interference control.—A control designed to confirm that a test matrix does not interfere with the assay's ability to detect target compounds.

Probability of detection (POD).—The proportion of positive analytical outcomes for a qualitative method for a given matrix at a given analyte level or concentration. [Appendix H: *Probability of Detection (POD) as a Statistical Model for the Validation of Qualitative Methods, Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA (http://www.eoma.aoac.org/app_h.pdf)]

Laboratory probability of detection (LPOD).—The POD value obtained from combining all valid collaborator data sets for a method for a given matrix at a given analyte level or concentration [Appendix H: *Probability of Detection (POD) as a Statistical Model for the Validation of Qualitative Methods, Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, Maryland, USA (http://www.eoma.aoac.org/app_h.pdf)].

Qualitative assay.—A method of analysis with two possible outcomes.

PDE5 inhibitors.—For the purposes of this SMPR: PDE5 inhibitors are defined as avanafil, lodenafil carbonate, mirodenafil, sildenafill, tadalafil, udenafil, or vardenafil; or any of their analogs. Refer to the *Supplemental List of Known PDE5 Inhibitors*.

Selectivity study.—A study designed to demonstrate that a candidate method does not detect nontarget compounds, and at the same time, demonstrate a candidate method's ability to detect the different types of PDE5 inhibitors (as a minimum the target panel provided in Annex I).

5 Method Performance Requirements

See Tables 1 and 2.

6 System Suitability Tests and/or Analytical Quality Control

The controls listed in Annex III shall be embedded in assays as appropriate. Interference controls should be used for method verification for each new matrix.

7 Reference Material(s)

Refer to Annex F: *Development and Use of In-House Reference Materials* in Appendix F: *Guidelines for Standard Method Performance Requirements, Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA (http://www.eoma.aoac.org/app_f.pdf)

ISO Guide 34:2009 *General requirements for the competence of reference material producers*

8 Validation Guidance

All claimed matrices shall be evaluated (see Annex IV for matrices relevant to the detection of PDE5 inhibitors.) Minimum matrices for validation study shall include at least one raw ingredient, such as Epimedium herbal extract and/or powder, and at least one finished product, such as capsules (both the content and the capsule shell).

Appendix D: *Guidelines for Collaborative Study Procedures to Validate Characteristics of a Method of Analysis*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA (http://www.eoma.aoac.org/app_d.pdf)

Appendix K: *Guidelines for Dietary Supplements and Botanicals*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA (http://www.eoma.aoac.org/app_k.pdf)

Appendix N*: ISPAM Guidelines for Validation of Qualitative Binary Chemistry Methods*, *Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, MD, USA (http://www.eoma.aoac.org/app_n.pdf)

9 Maximum Time-to-Result

1 hour.

Approved by Stakeholder Panel on Dietary Supplements (SPDS). Final Version Date: September 5, 2014. Effective Date: October 16, 2014.

Table 1. Matrix-dependent criteria

Type of study	Parameter	Parameter requirements	Target test concn	Minimum acceptable results
Single laboratory validation	POD at low concn	Minimum of 33 replicates per matrix type, spiked at or below the designated low level target test concentration	100 ppm	90% POD[a]
	POD at high concn	Minimum of five replicates per matrix type spiked at 10× the designated low level target test concentration	10× low concn	100% correct analyses are expected per matrix type[b]
	POD at 0 concn	Minimum of five replicates per matrix type	0 ppm	
Multi-laboratory validation	LPOD[c]	Use Appendix N: *ISPAM Guidelines for Validation of Qualitative Binary Chemistry Methods*	Low concn	≥0.85[a]
			10× low concn	≥0.95[a]
	$LPOD_{(0)}$[c]		0 ppm	≤0.05[a]

a 95% confidence interval.

b 100% correct analyses are expected. Some aberrations may be acceptable if the aberrations are investigated, and acceptable explanations can be determined and communicated to method users.

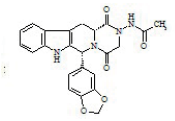
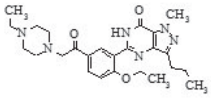
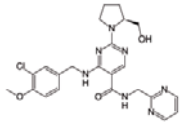
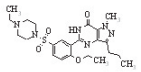
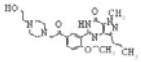
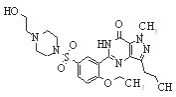
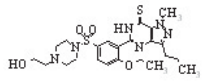
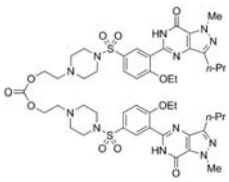
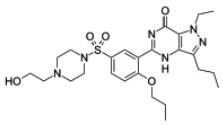
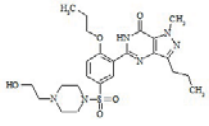
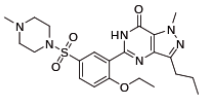
c LPOD = Laboratory probability of detection. The POD value obtained from combining all valid collaborator data sets for a method for a given matrix at a given analyte level or concentration [Appendix H: *Probability of Detection (POD) as a Statistical Model for the Validation of Qualitative Methods, Official Methods of Analysis of AOAC INTERNATIONAL* (2012) 19th Ed., AOAC INTERNATIONAL, Gaithersburg, Maryland, USA]. LPOD and $LPOD_{(0)}$ are not required for single-laboratory validations.

Table 2. Selectivity study

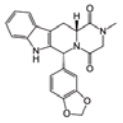
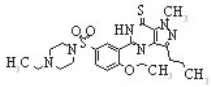
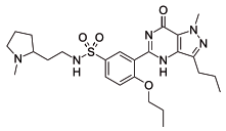
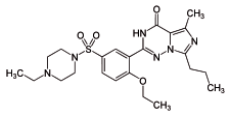
Type of study	Parameter	Parameter requirements	Final test concn	Minimum acceptable results
Single laboratory validation	Target	Test each target compound listed in Annex I at the final test concentration	Low concn	100% positive results[a]
	Nontarget	Test each nontarget panel compound at the final test concentration or at the highest expected matrix concentration in the case of naturally occurring matrix components. A list of potential nontarget compounds for immunoassays is provided in Annex II.	10× low concn	≥95% negative results

a 100% correct analyses are expected. Some aberrations may be acceptable if the aberrations are investigated, and acceptable explanations can be determined and communicated to method users.

ANNEX I
Target Compound Panel

Analyte	CAS No.	Formula	Structure
Acetaminotadalafil	1446144-71-3	$C_{23}H_{20}N_4O_5$	
Acetildenafil	831217-01-7	$C_{25}H_{34}N_6O_3$	
Avanafil (sold under the brand names *Stendra* and *Spedra*)	330784-47-9	$C_{23}H_{26}ClN_7O_3$	
Homosildenafil	642928-07-2	$C_{23}H_{32}N_6O_4S$	
Hydroxyacetildenafil	147676-56-0	$C_{25}H_{34}N_6O_4$	
Hydroxyhomosildenafil	139755-85-4	$C_{23}H_{32}N_6O_5S$	
Hydroxythiohomosildenafil	479073-82-0	$C_{23}H_{32}N_6O_4S_2$	
Lodenafil carbonate (sold under the brand name *Helleva* in Brazil)	398507-55-6	$C_{43}H_{54}N_{12}O_9S_2$	
Mirodenafil (sold under the trade name of *Mvix*.)	862189-95-5	$C_{26}H_{37}N_5O_5S$	
Propoxyphenyl hydroxyhomosildenafil	139755-87-6	$C_{24}H_{34}N_6O_5S$	
Sildenafil (sold under the brand names *Viagra* and *Revatio*, and other various brand names)	139755-83-2	$C_{22}H_{30}N_6O_4S$	

ANNEX I
Target Compound Panel (*continued*)

Analyte	CAS No.	Formula	Structure
Tadalafil (sold under the brand names *Cialis* and *Adcirca*)	171596-29-5	$C_{22}H_{19}N_3O_4$	
Thiohomosildenafil	479073-80-8	$C_{23}H_{32}N_6O_3S_2$	
Udenafil (sold under the brand name *Zydena*)	268203-93-6	$C_{25}H_{36}N_6O_4S$	
Vardenafil (sold under the brand names *Levitra*, *Staxyn*, and *Vivanza*)	224785-90-4	$C_{23}H_{32}N_6O_4S$	

ANNEX II
Nontarget Panel

A suitable nontarget panel shall be selected based on the analytical technique.

For nonbioassays: It is expected that an appropriate nontarget panel will be developed for the selectivity study in Table 2 of the method performance requirements.

For a bioassay based on PDE5 inhibitors: Natural components/matrices with PDE5 inhibition activity shall be evaluated, such as extracts/powders of *Tribulus terrestris, Cnidium monieri, Morinda officinalis, Cuscuta chinensis,* and *Epimedium koreanum.*

For immunoassay, structurally similar compounds should be tested, such as the following examples of compounds that are subcomponents of PDE5 inhibitors, which are provided for illustration purposes:

2-Pyrimidinecarboxamide, 5-pyrimidinecarboxamide, benzenesulfonyl, piperazin, piperazinyl, piperazinylphenolate, 3,6,7,12,12a-hexahydro-2-methyl-pyrazino [1′,2′:1,6] pyrido[3,4-b]indole-1,4-dione, benzenesulfonamide

ANNEX III
Controls

Control	Description	Implementation	Acceptance criteria
Positive control	Designed to demonstrate an appropriate test response. This positive control should be included at a low but easily detectable concentration, and should monitor the performance of the entire assay. The purpose of using a low concentration of positive control is to avoid contamination of the test sample and/or instrument.	Single use per sample (or sample set) run	Success: Control detected at expected levels Failure: Control not detected or at levels below expected
Negative Control	Designed to demonstrate that the assay itself does not produce a positive detection in the absence of target compounds. The purpose of this control is to rule out contamination in the assay or test.	Single use per sample (or sample set) run	Success: No detections made Failure: Detections made
Interference Control	Designed to specifically address the impact of a sample or sample matrix on the assay's ability to detect target compounds	Single use per sample run	Success: Control detected at expected levels Failure: Control not detected or at levels below expected

ANNEX IV
Matrixes

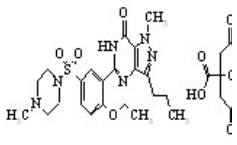
Tablets
Capsules (both the content and the capsule shells)
Softgels
Gelcaps
Liquids
Powders
Extracts

Supplemental List of Known PDE5 Inhibitors (as of July 2014)

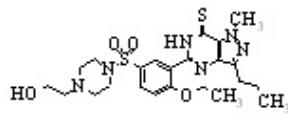
1. **Standards available from Cachesyn http://www.cachesyn.com/ which include the majority of characterized PDE-5i analogues and all of the parent drugs including catalog numbers. (Some structure images not available)**

Sildenafil Related Compounds (commercial standards available) – includes deuterated standards.

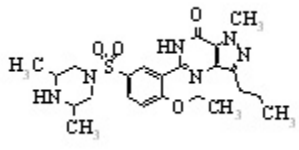
Sildenafil citrate
CAS No. 171599-83-0
C22H30N6O4S.C6H8O7 M.W. 474.59 192.13
CSTS061



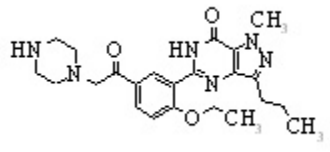
Hydroxythiohomosildenafil
C23H32N6O4S2 M.W. 520.68
CSTS0611



Dimethyl Sildenafil
C23H32N6O4S M.W. 488.61
CSTS0612



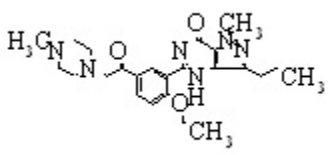
N-Desmethyl Acetildenafil
C23H30N6O3 M.W. 438.53
CSTS0613



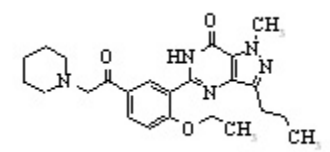
Hydroxyacetildenafil
C25H34N6O4 M.W. 482.59
CSTS0614

Nor-acetildenafil
CAS No. 949091-37-7
C24H32N6O3 M.W. 452.56
CSTS0615

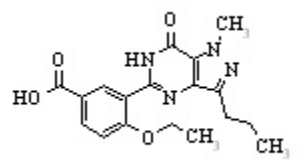
Nor-acetildenafil
CAS No. 949091-37-7
C24H32N6O3 M.W. 452.56
CSTS0615



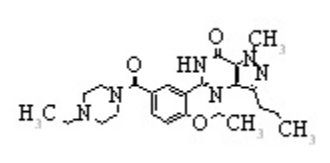
Piperiacetildenafil
C24H31N5O3 M.W. 437.55
CSTS0616



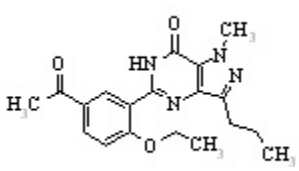
Acetil Acid
C18H20N4O4 M.W. 356.38
CSTS0617



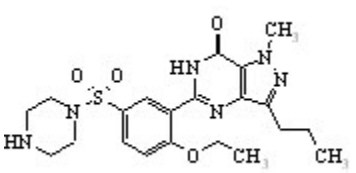
Carbodenafil
C24H32N6O3 M.W. 452.56
CSTS0618



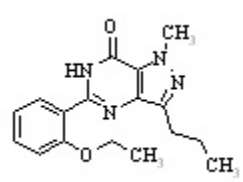
Gendenafil
C19H22N4O3 M.W. 354.41
CSTS0619



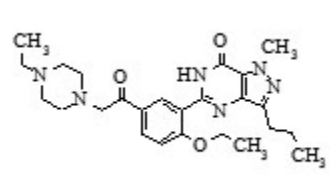
N-Desmethyl Sildenafil
CAS No. 139755-82-1
C21H38N6O4S M.W. 460.56
CSTS062



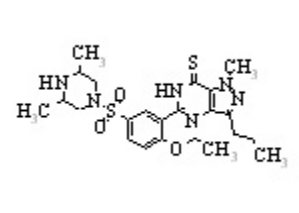
Imidazosagatriazinone
C17H20N4O2 M.W. 312.37
CSTS0620



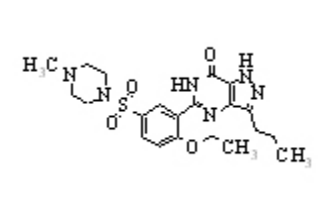
Acetildenafil (Hongdenafil)
C25H34N6O3 M.W. 466.59
CSTS0621



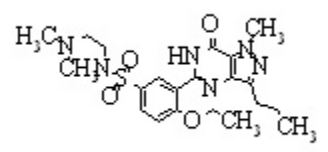
Thiodimethyl Sildenafil (Dimethylthiosildenafil)
C23H32N6O3S2 M.W. 504.68
CSTS0622



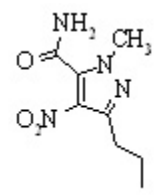
Pyrazole N-desmethyl sildenafil
C21H28N6O4S M.W. 460.56
CSTS0623



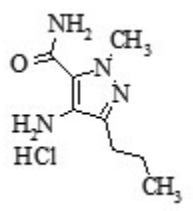
PDE-5 Inhibitor (Sildenafil Related Compound)
C21H30N6O M.W. 462.5
CSTS0624



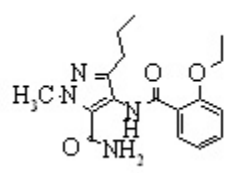
Sildenafil amide
C8H12N4O3 M.W. 212.21
CSTS0625



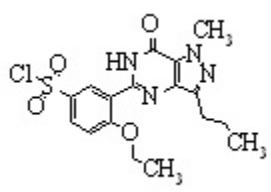
Sildenafil Amine HCl
C8H14N4O.HCl M.W. 182.23 36.46
CSTS0626



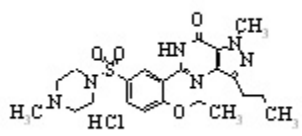
Sildenafil coupled
C17H22N4O3 M.W. 330.39
CSTS0627



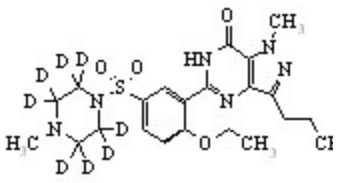
Sildenafil chlorosulfonyl
C17H19ClN4O4S M.W. 410.88
CSTS0628



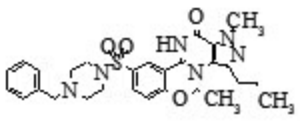
Sildenafil HCl
C22H30N6O4S.HCl M.W. 474.59 36.46
CSTS0629



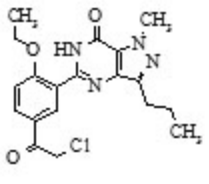
Sildenafil-d8
CAS No. 171599-83-0(non-d)
C22H22D8N6O4S M.W. 482.63
CSTS063



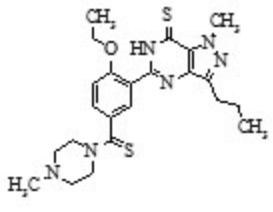
Benzyl Sildenafil
C28H34N6O4S M.W. 550.68
CSTS0631



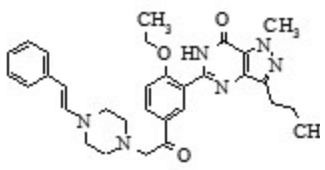
Chlorodenafil
CAS No. N/A
C19H21ClN4O3 M.W. 388.86
CSTS0633



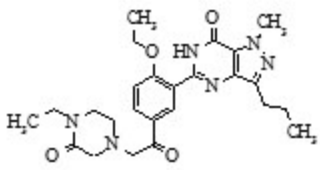
Dithio-desmethyl-carbodenafil
CAS No. N/A
C23H30N6OS2 M.W. 470.66
CSTS0635



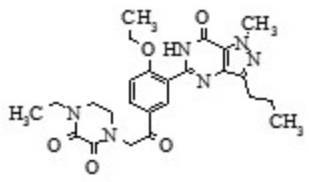
Cinnamyldenafil
CAS No. N/A
C31H36N6O3 M.W. 540.67
CSTS0637



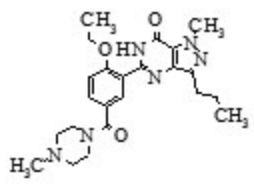
Oxohongdenafil
CAS No. N/A
C25H32N6O4 M.W. 480.57
CSTS0639



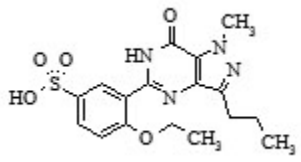
Dioxohongdenafil
CAS No. N/A
C25H30N6O5 M.W. 494.56
CSTS0640



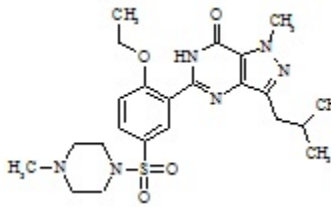
Desmethyl Carbodenafil
C23H30N6O3 M.W. 438.53
CSTS0642



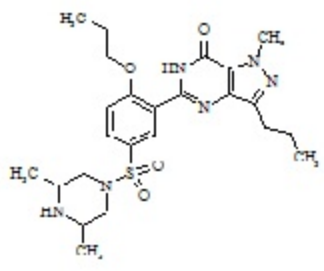
Demethylpiperazinyl Sildenafil Sulfonic Acid
C17H20N4O5S M.W. 392.44
CSTS0644



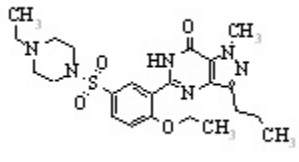
Sildenafil Impurity A (Isobutyl Sildenafil)
CAS No. N/A
C23H32N6O4S M.W. 488.61
CSTS0646



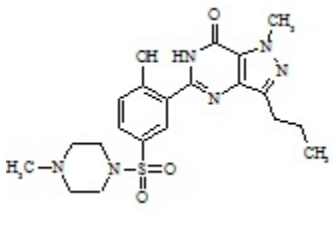
Propoxyphenyl Sildenafil
CAS No. 877777-10-1
C23H32N6O4S M.W. 488.61
CSTS0648



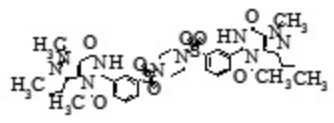
Homosildenafil
C23H32N6O4S M.W. 488.61
CSTS065



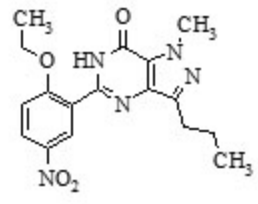
O-Desethyl Sildenafil (Sildenafil Impurity C)
CAS No. N/A
C20H26N6O4S M.W. 446.53
CSTS0651



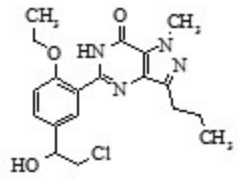
Sildenafil Dimer Impurity
C38H46N10O8S2 M.W. 834.98
CSTS0630



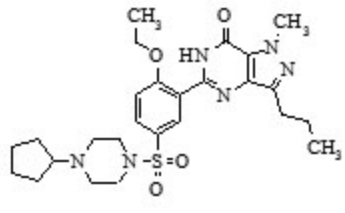
Nitrodenafil
CAS No. N/A
C17H19N5O4 M.W. 357.37
CSTS0632



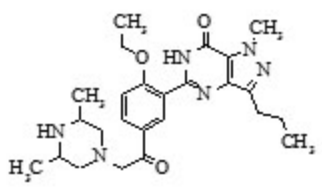
Hydroxychlorodenafil
CAS No. N/A
C19H23ClN4O3 M.W. 390.87
CSTS0634



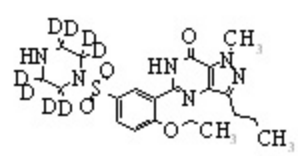
Cyclopentynafil
CAS No. N/A
C26H36N6O4S M.W. 528.68
CSTS0636



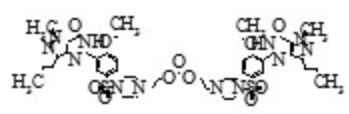
Dimethylacetildenafil
CAS No. N/A
C25H34N6O3 M.W. 466.59
CSTS0638



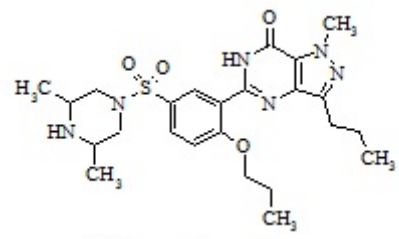
N-Desmethyl sildenafil-d8
CAS No. 139755-82-1 (non-d)
C21H20N6O4SD8 M.W. 468.61
CSTS064



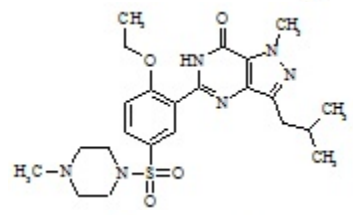
Lodenafilcarbonate
CAS No. N/A
C47H62N12O11S2 M.W. 1035.22
CSTS0641



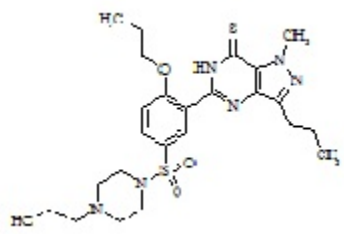
Sildenafil analogue
C24H34N6O4S M.W. 502.64
CSTS0643



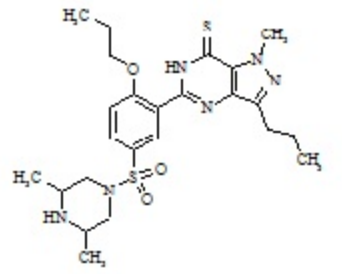
Nitroso-prodenafil
CAS No. N/A
C27H35N9O5S2 M.W. 629.77
CSTS0645



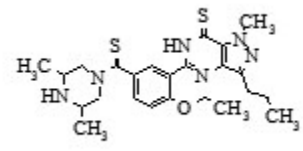
Sildenafil Analogue I
CAS No. N/A
C24H34N6O4S2 M.W. 534.70
CSTS0647



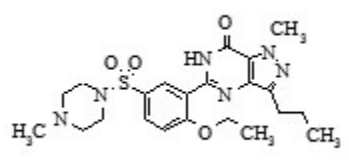
Sildenafil Analogue III
CAS No. N/A
C24H34N6O3S2 M.W. 518.70
CSTS0649



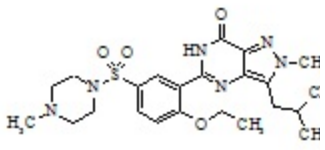
Sildenafil Related Compound
C24H32N6OS2 M.W. 484.69
CSTS0650



Sildenafil
C22H30N6O4S M.W. 474.59
CSTS0652



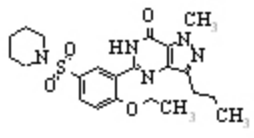
Sildenafil Impurity A Related Compound (Isomer of Isobutyl Sildenafil)
C23H32N6O4S M.W. 488.61
CSTS0653



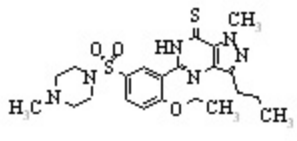
Sildenafil N-Oxide
C22H30N6O5S M.W. 490.59
CSTS0655

no image of structure available

Norneosildenafil
C22H29N5O4S M.W. 459.57
CSTS066



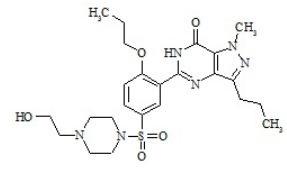
Thiosildenafil
C22H30N6O3S2 M.W. 490.65
CSTS068



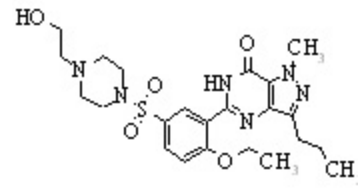
Sildenafil Impurity ((1-methyl-4-Nitro -3-n-propyl pyrazole-5- carboxylic acid)
C8H11N3O4 M.W. 213.19
CSTS0654

no image of structure available

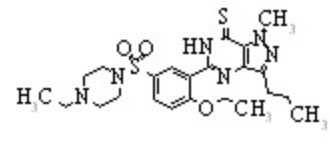
Propoxyphenyl-Hydroxyhomosildenafil
CAS No. N/A
C24H34N6O5S M.W. 518.64
CSTS0656



Hydroxyhomosildenafil
C23H32N6O5S M.W. 504.61
CSTS067

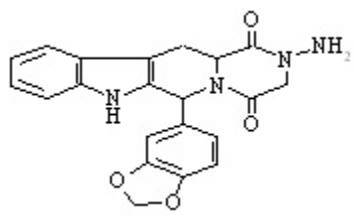


Thiohomosildenafil
C23H32N6O3S2 M.W. 504.68
CSTS069

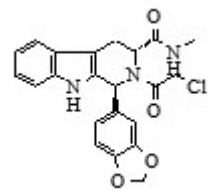


Tadalafil Related Compounds (commercial standards available) – includes deuterated standards.

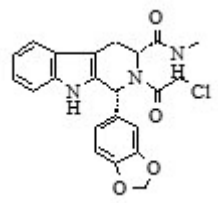
Aminotadalafil
C21H18N4O4 M.W. 390.40
CSTT101



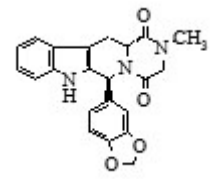
Tadalafil Impurity C
CAS No. NA
C22H20ClN3O4 M.W. 425.88
CSTT1010



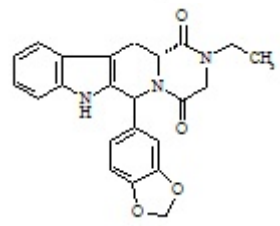
Tadalafil Impurity D
CAS No. NA
C22H20ClN3O4 M.W. 425.88
CSTT1011



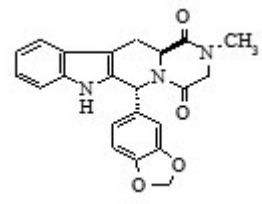
Tadalafil Impurity E
C22H19N3O4 M.W. 389.41
CSTT1012



N-Ethyl Tadalafil
CAS No. N/A
C23H21N3O4 M.W. 403.44
CSTT1013



6R,12S-Tadalafil
C22H19N3O4 M.W. 389.41
CSTT1014



Tadalafil Hydroxylactam Impurity
C22H19N3O6 M.W. 421.41
CSTT1015

no image of structure available

Tadalafil Aminohemiketal Impurity
C22H19N3O6 M.W. 421.41
CSTT1016

no image of structure available

Tadalafil Spiro-urethane Impurity
C21H18N3O6 M.W. 408.39
CSTT1017

no image of structure available

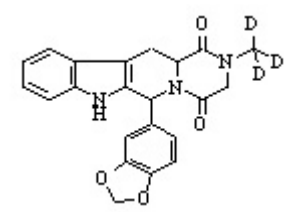
Tadalafil Hydroxyquinoline Impurity
C22H17N3O5 M.W. 403.40
CSTT1018

no image of structure available

Tadalafil Ketolactam Impurity
C22H21N3O6 M.W. 423.43
CSTT1019

no image of structure available

Tadalafil-d3
C22H16N3O4D3 M.W. 392.43
CSTT102



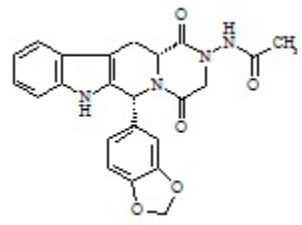
Tadalafil Spiro-oxindole Impurity
C22H19N3O5 M.W. 405.41
CSTT1020

no image of structure available

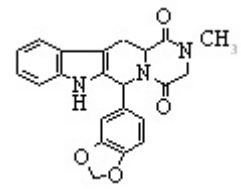
Tadalafil Impurity B (6S,12aS)
C22H19N3O4 M.W. 389.41
CSTT1021

no image of structure available

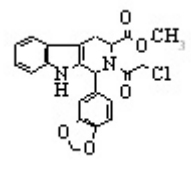
Acetaminotadalafil
CAS No. N/A
C23H20N4O5 M.W. 432.44
CSTT1022



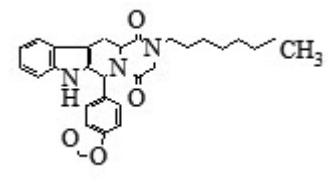
Tadalafil
C22H19N3O4 M.W. 389.41
CSTT103



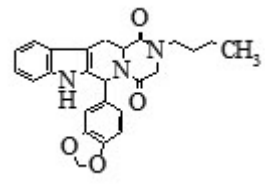
Chloropretadalafil
C22H19ClN2O5 M.W. 426.86
CSTT104



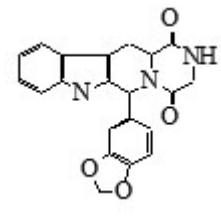
N-Octyl-nortadalafil
C29H33N3O4 M.W. 487.60
CSTT105



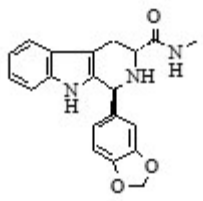
N-Butyl Tadalafil
C25H25N3O4 M.W. 431.50
CSTT106



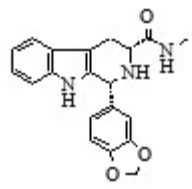
Nortadalafil
C21H17N3O4 M.W. 375.39
CSTT107



Tadalafil Impurity A
CAS No. NA
C20H19N3O3 M.W. 349.39
CSTT108

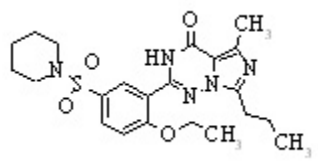


Tadalafil Impurity B
CAS No. NA
C20H19N3O3 M.W. 349.39
CSTT109



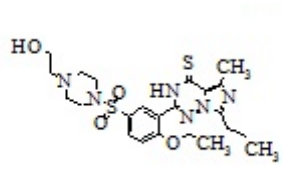
Vardenafil Related Compounds (commercial standards available) – includes deuterated standards.

Pseudovardenafil
C22H29N5O4S
M.W. 459.57
CSTV051

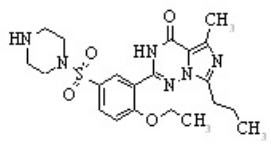


no image of structure available

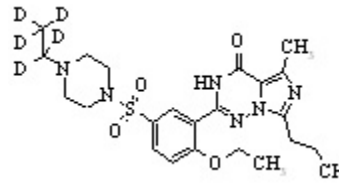
Hydroxythio Vardenafil
C23H32N6O4S2 M.W. 520.68
CSTV0510



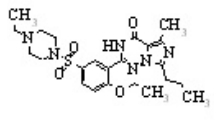
N-Desethyl Vardenafil
C21H28N6O4S M.W. 460.56
CSTV052



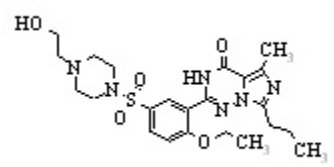
Vardenafil-d5
C23H27N6O4SD5 M.W. 493.64
CSTV053



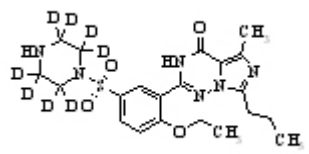
Vardenafil HCl
CAS No. 224785-90-4
C23H32N6O4S M.W. 488.61
CSTV054



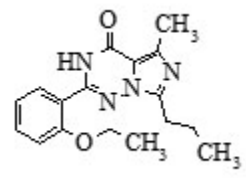
Hydroxy Vardenafil
C23H32N6O5S M.W. 504.61
CSTV055



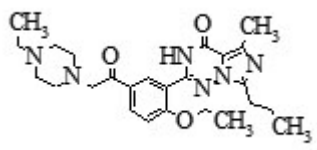
N-Desethyl Vardenafil-d8
CAS No. V-052
C21H28N6O4S M.W. 460.56
CSTV056



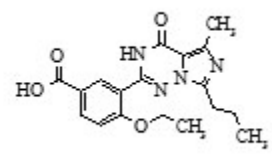
2-(2-Ethoxyphenyl)-5-methyl-7-propyl-3H-imidazo[5,1-f][1,2,4]triazin-4-one
C17H20N4O2 M.W. 312.37
CSTV057



Acetylvardenafil
C25H34N6O3 M.W. 466.59
CSTV058

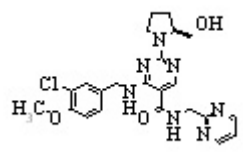


Norneovardenafil
CAS No. N/A
C18H20N4O4 M.W. 356.38
CSTV059

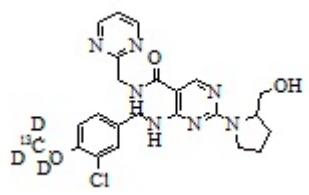


Avanafil Related Compounds (commercial standards available) – includes deuterated standards.

Avanafil
CAS No. 330784-47-9
C23H26ClN7O3 M.W. 483.96
CSTA291

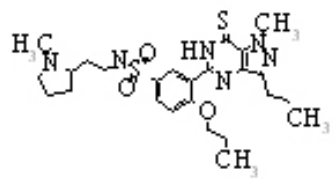


Avanafil-13CD3
C22H23ClN7O313CD3 M.W. 487.97
CSTA292



Udenafil

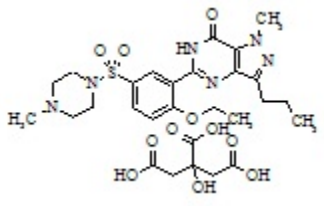
Udenafil
CAS No. 268203-93-6
C25H36N6O4S M.W. 516.67
CSTU031



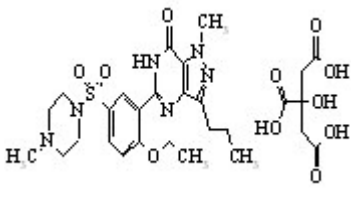
2. **Standards available from TLC Pharmachem http://www.tlcpharmachem.com which include the majority of characterized PDE-5i analogues and all of the parent drugs including catalog numbers. (Some structure images not available)**

Sildenafil Related Compounds (commercial standards available) – includes deuterated standards.

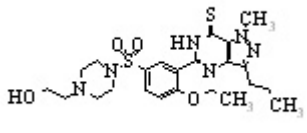
Sildenafil Citrate
CAS No. 171599-83-0
C22H30N6O4S. C6H8O7 M.W. 474.59
192.13
PF-0017



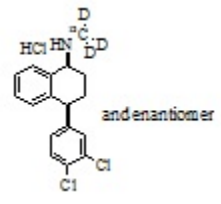
Sildenafil citrate
CAS No. 171599-83-0
C22H30N6O4S.C6H8O7 M.W. 474.59
192.13
S-061



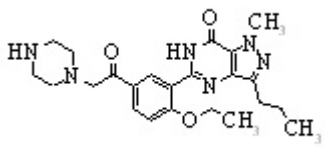
Hydroxythiohomosildenafil
C23H32N6O4S2 M.W. 520.68
S-0611



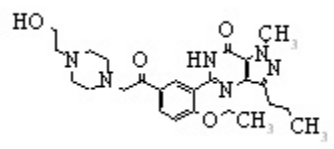
Dimethyl Sildenafil
CAS No. 1416130-63-6
C23H32N6O4S M.W. 488.61
S-0612



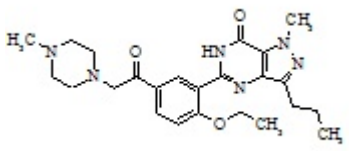
N-Desmethyl Acetildenafil
C23H30N6O3 M.W. 438.53
S-0613



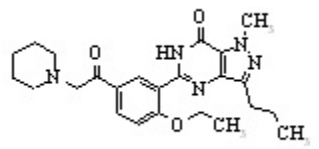
Hydroxyacetildenafil
C25H34N6O4 M.W. 482.59
S-0614



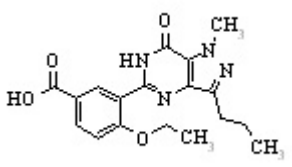
Nor-acetildenafil
CAS No. 949091-38-7
C24H32N6O3 M.W. 452.56
S-0615



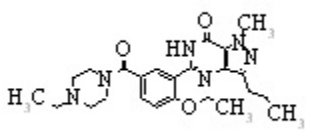
Piperiacetildenafil
C24H31N5O3 M.W. 437.55
S-0616



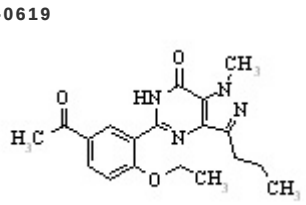
Acetil Acid
C18H20N4O4 M.W. 356.38
S-0617



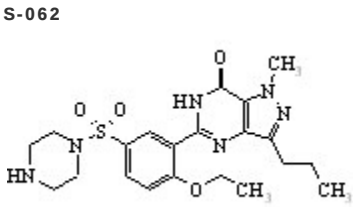
Carbodenafil
C24H32N6O3 M.W. 452.56
S-0618



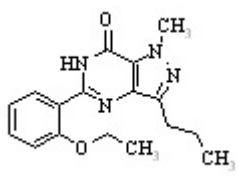
Gendenafil
CAS No. 147676-66-2
C19H22N4O3 M.W. 354.41
S-0619



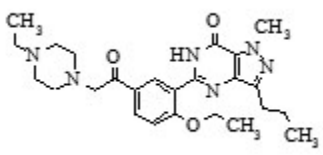
N-Desmethyl Sildenafil
CAS No. 139755-82-1
C21H28N6O4S M.W. 460.56
S-062



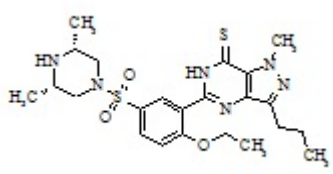
Imidazosagatriazinone
C17H20N4O2 M.W. 312.37
S-0620



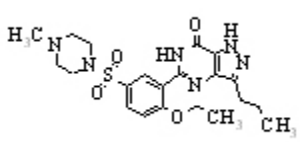
Acetildenafil (Hongdenafil)
CAS No. 831217-01-7
C25H34N6O3 M.W. 466.59
S-0621



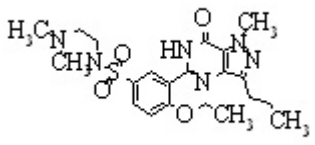
Thiodimethyl Sildenafil (Thioaildenafill, Sulfoaildenafil)
CAS No. 856190-47-1
C23H32N6O3S2 M.W. 504.68
S-0622



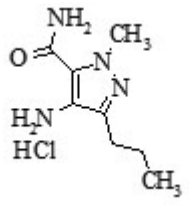
Pyrazole N-desmethyl sildenafil
C21H28N6O4S M.W. 460.56
S-0623



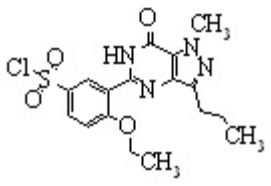
PDE-5 Inhibitor (Sildenafil Related Compound)
C21H30N6O4S M.W. 462.58
S-0624



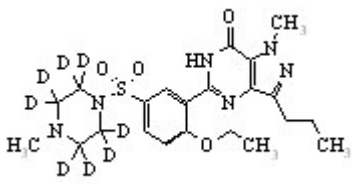
Sildenafil Amine HCl
C8H14N4O.HCl M.W. 182.23 36.46
S-0626



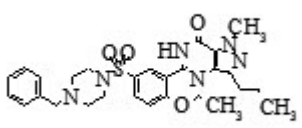
Sildenafil chlorosulfonyl
CAS No. 139756-22-2
C17H19ClN4O4S M.W. 410.88
S-0628



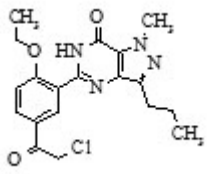
Sildenafil-d8
CAS No. 171599-83-0(non-d)
C22H22D8N6O4S M.W. 482.63
S-063



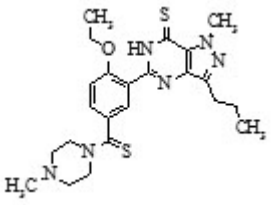
Benzyl Sildenafil
C28H34N6O4S M.W. 550.68
S-0631



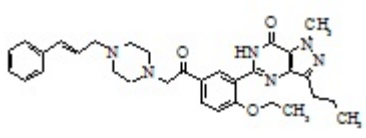
Chlorodenafil
CAS No. N/A
C19H21ClN4O3 M.W. 388.86
S-0633



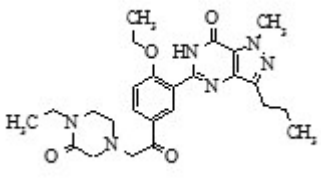
Dithio-desmethyl-carbodenafil
CAS No. N/A
C23H30N6OS2 M.W. 470.66
S-0635



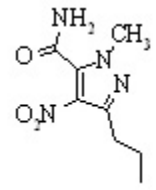
Cinnamyldenafil
CAS No. N/A
C32H38N6O3 M.W. 554.70
S-0637



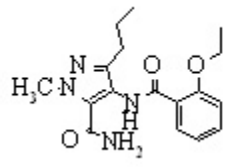
Oxohongdenafil
CAS No. N/A
C25H32N6O4 M.W. 480.57
S-0639



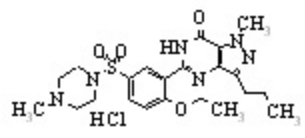
Sildenafil amide
C8H12N4O3 M.W. 212.21
S-0625



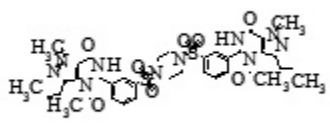
Sildenafil coupled
C17H22N4O3 M.W. 330.39
S-0627



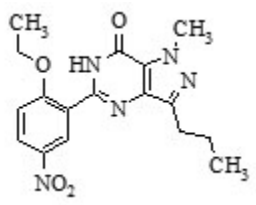
Sildenafil HCl
C22H30N6O4S.HCl M.W. 474.59 36.46
S-0629



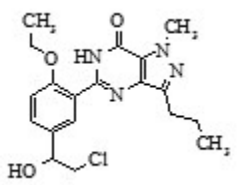
Sildenafil Dimer Impurity
C38H46N10O8S2 M.W. 834.98
S-0630



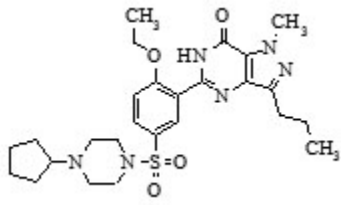
Nitrodenafil
CAS No. N/A
C17H19N5O4 M.W. 357.37
S-0632



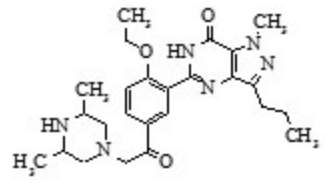
Hydroxychlorodenafil
CAS No. N/A
C19H23ClN4O3 M.W. 390.87
S-0634



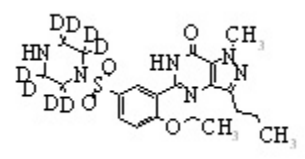
Cyclopentynafil
CAS No. N/A
C26H36N6O4S M.W. 528.68
S-0636



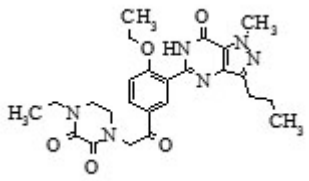
Dimethylacetildenafil
CAS No. N/A
C25H34N6O3 M.W. 466.59
S-0638



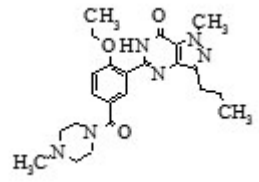
N-Desmethyl sildenafil-d8
CAS No. 1185168-06-2
C21H20N6O4SD8 M.W. 468.61
S-064



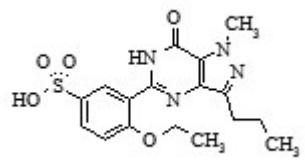
Dioxohongdenafil
CAS No. N/A
C25H30N6O5 M.W. 494.56
S-0640



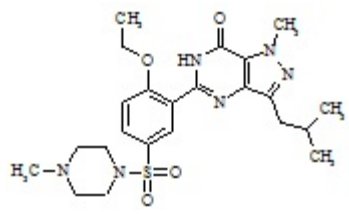
Desmethyl Carbodenafil
C23H30N6O3 M.W. 438.53
S-0642



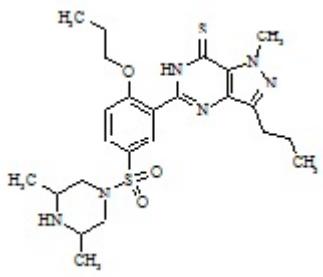
Demethylpiperazinyl Sildenafil Sulfonic Acid
C17H20N4O5S M.W. 392.44
S-0644



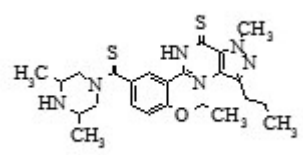
Sildenafil Impurity A (Isobutyl Sildenafil)
CAS No. 1391053-95-4
C23H32N6O4S M.W. 488.61
S-0646



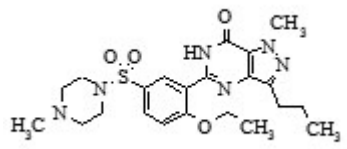
Sildenafil Analogue III
CAS No. N/A
C24H34N6O3S2 M.W. 518.70
S-0649



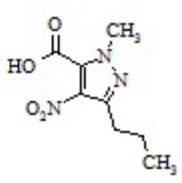
Sildenafil Related Compound
C24H32N6OS2 M.W. 484.69
S-0650



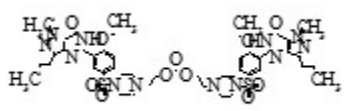
Sildenafil
C22H30N6O4S M.W. 474.59
S-0652



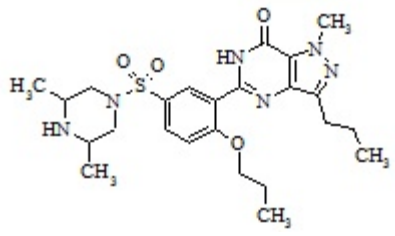
Sildenafil Impurity ((1-methyl-4-Nitro -3-n-propyl pyrazole-5- carboxylic acid)
C8H11N3O4 M.W. 213.19
S-0654



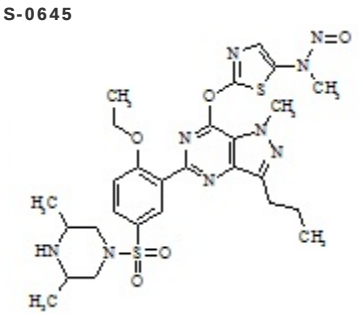
Lodenafilcarbonate
CAS No. N/A
C47H62N12O11S2 M.W. 1035.22
S-0641



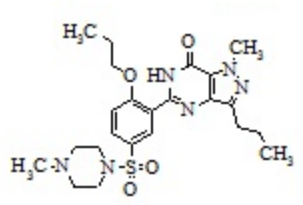
Sildenafil analogue
C24H34N6O4S M.W. 502.64
S-0643



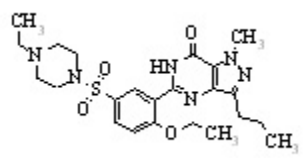
Nitroso-prodenafil
CAS No. N/A
C27H35N9O5S2 M.W. 629.77
S-0645



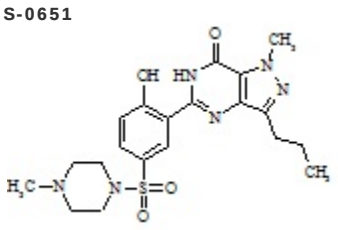
Propoxyphenyl Sildenafil
CAS No. 877777-10-1
C23H32N6O4S M.W. 488.61
S-0648



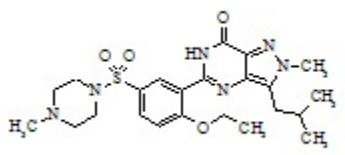
Homosildenafil
CAS No. 642928-07-2
C23H32N6O4S M.W. 488.61
S-065



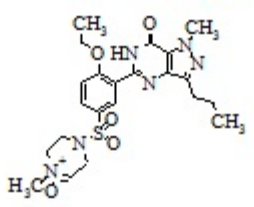
O-Desethyl Sildenafil (Sildenafil Impurity C)
CAS No. N/A
C20H26N6O4S M.W. 446.53
S-0651



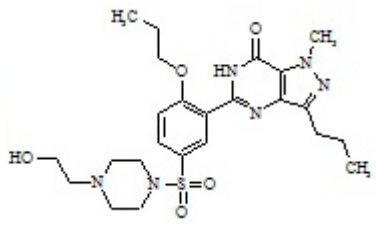
Sildenafil Impurity A Related Compound (Isomer of Isobutyl Sildenafil)
C23H32N6O4S M.W. 488.61
S-0653



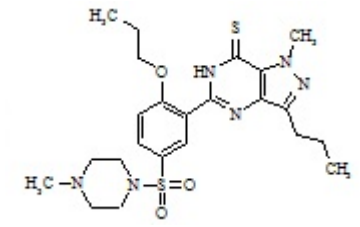
Sildenafil N-Oxide
C22H30N6O5S M.W. 490.59
S-0655



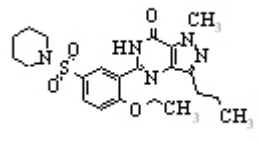
Propoxyphenyl-Hydroxyhomosildenafil
CAS No. N/A
C24H34N6O5S M.W. 518.64
S-0656



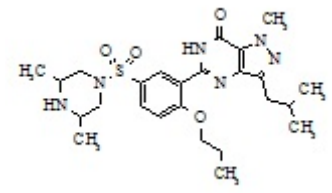
Propoxyphenyl-Thiosildenafil
CAS No. N/A
C23H32N6O3S2 M.W. 504.68
S-0658



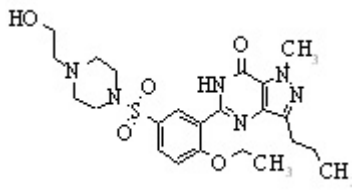
Norneosildenafil
C22H29N5O4S M.W. 459.57
S-066



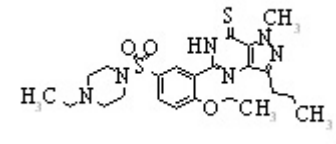
Sildenafil Related Compound 2
C25H36N6O4S M.W. 516.67
S-0661



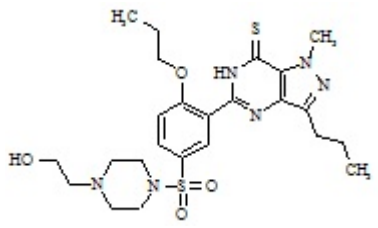
Hydroxyhomosildenafil
C23H32N6O5S M.W. 504.61
S-067



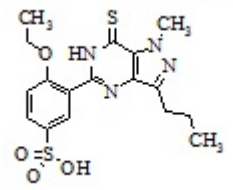
Thiohomosildenafil
C23H32N6O3S2 M.W. 504.68
S-069



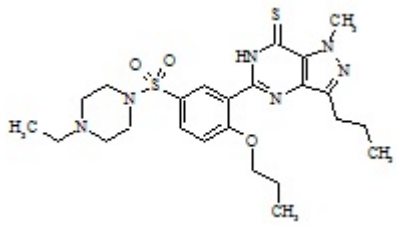
Sildenafil Analogue I (Propoxyphenyl-Thiohydroxyhomosildenafil)
CAS No. 479073-90-0
C24H34N6O4S2 M.W. 534.70
S-0657



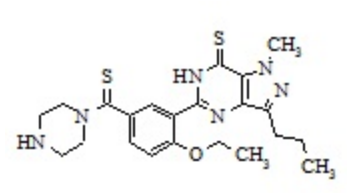
Depiperazinothiosildenafil
C17H20N4O4S2 M.W. 408.50
S-0659



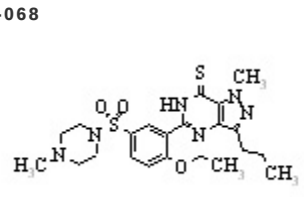
Propoxyphenyl Thiohomosidenafil
CAS No. 479073-88-6
C24H34N6O3S2 M.W. 518.70
S-0660



Dithio-Desethyl-Carbodenafil
CAS No. N/A
C22H28N6OS2 M.W. 456.64
S-0662

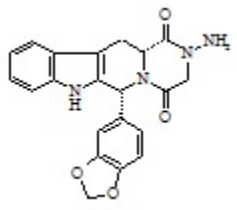


Thiosildenafil
CAS No. 479073-79-5
C22H30N6O3S2 M.W. 490.65
S-068

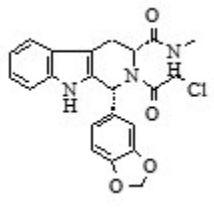


Tadalafil Related Compounds (commercial standards available) – includes deuterated standards.

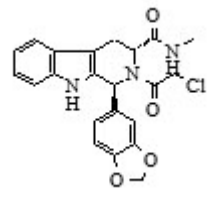
Aminotadalafil
CAS No. 385769-84-6
C21H18N4O4 M.W. 390.40
T-101



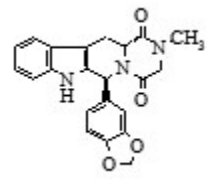
Tadalafil Impurity D
CAS No. NA
C22H20ClN3O4 M.W. 425.88
T-1011



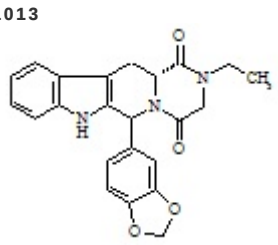
Tadalafil Impurity C
CAS No. NA
C22H20ClN3O4 M.W. 425.88
T-1010



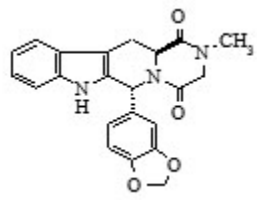
Tadalafil Impurity E (6S, 12R)
CAS No. 171596-28-4
C22H19N3O4 M.W. 389.41
T-1012



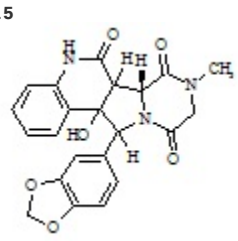
N-Ethyl Tadalafil
CAS No. N/A
C23H21N3O4 M.W. 403.44
T-1013



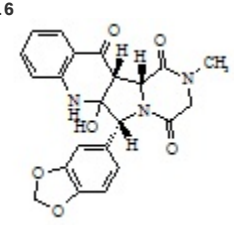
6R,12S-Tadalafil
CAS No. 171596-27-3
C22H19N3O4 M.W. 389.41
T-1014



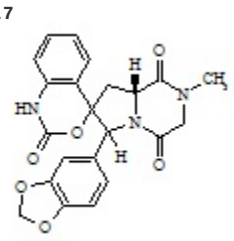
Tadalafil Hydroxylactam Impurity
C22H19N3O6 M.W. 421.41
T-1015



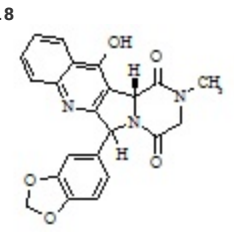
Tadalafil Aminohemiketal Impurity
C22H19N3O6 M.W. 421.41
T-1016



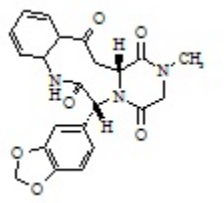
Tadalafil Spiro-urethane Impurity
C22H19N3O6 M.W. 421.41
T-1017



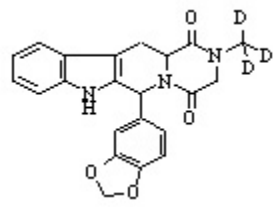
Tadalafil Hydroxyquinoline Impurity
C22H17N3O5 M.W. 403.40
T-1018



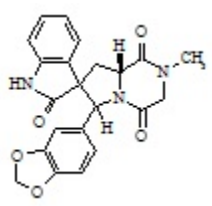
Tadalafil Ketolactam Impurity
CAS No. 1346605-38-6
C22H19N3O6 M.W. 421.41
T-1019



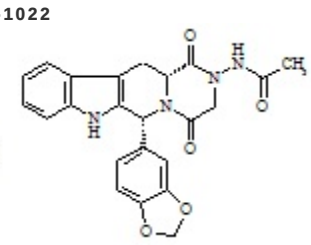
Tadalafil-d3
CAS No. 960226-55-5
C22H16N3O4D3 M.W. 392.43
T-102



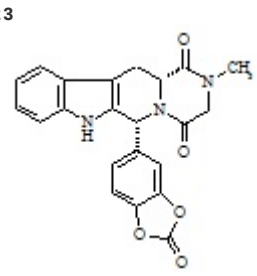
Tadalafil Spiro-oxindole Impurity
C22H19N3O5 M.W. 405.41
T-1020



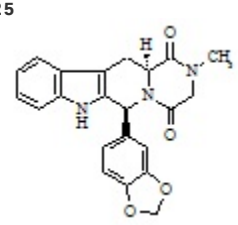
Acetaminotadalafil
CAS No. N/A
C23H20N4O5 M.W. 432.44
T-1022



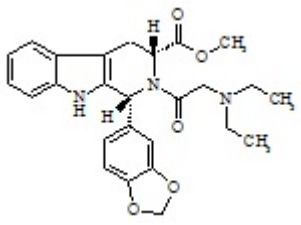
Tadalafil Oxo Impurity
CAS No. 1346602-17-2
C22H17N3O5 M.W. 403.40
T-1023



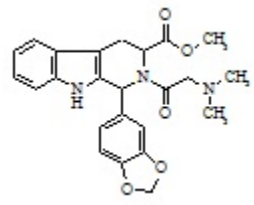
Tadalafil EP Impurity B (ent-tadalafil)
CAS No. 629652-72-8
C22H19N3O4 M.W. 389.41
T-1025



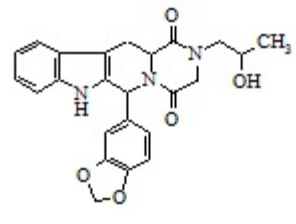
Tadalafil Related Compound
CAS No. N/A
C26H29N3O5 M.W. 463.54
T-1027



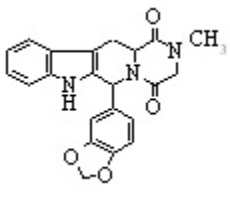
Tadalafil Related Compound 2
C24H25N3O5 M.W. 435.48
T-1028



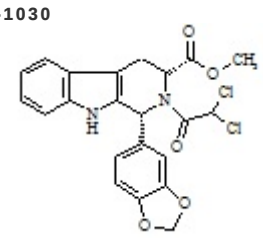
2-Hydroxypropylnortadalafil
C24H23N3O5 M.W. 433.47
T-1029



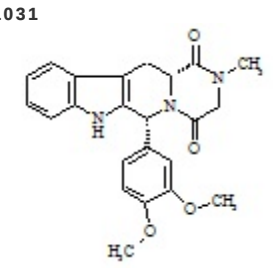
Tadalafil
CAS No. 171596-29-5
C22H19N3O4 M.W. 389.41
T-103



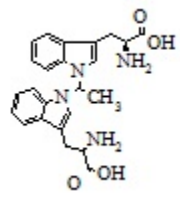
Tadalafil Dichloro Impurity
CAS No. N/A
C22H18Cl2N2O5 M.W. 461.31
T-1030



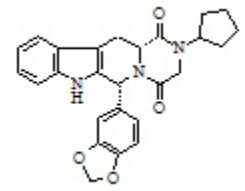
Tadalafil Dimethoxy Impurity
CAS No. 1356345-67-9
C23H23N3O4 M.W. 405.46
T-1031



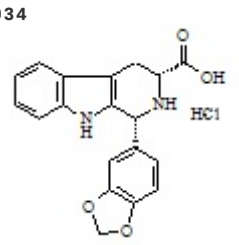
Tadalafil Impurity (1,1 Œ-ethylidenebistryptophan)
C24H26N4O4 M.W. 434.50
T-1032



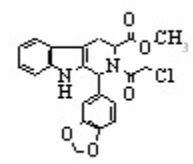
Tadalafil Related Impurity 1
CAS No. N/A
C26H25N3O4 M.W. 443.51
T-1033



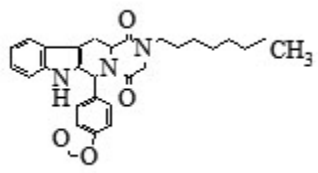
Tadalafil Acid Impurity
CAS No. N/A
C19H16N2O4 HCl M.W. 336.35 36.46
T-1034



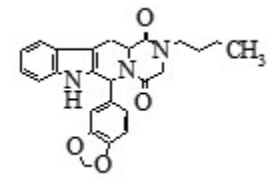
Chloropretadalafil
C22H19ClN2O5 M.W. 426.86
T-104



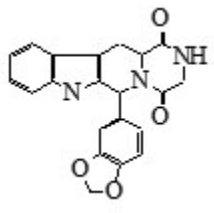
N-Octyl-nortadalafil
C29H33N3O4 M.W. 487.60
T-105



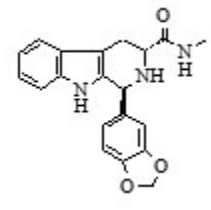
N-Butyl Tadalafil
C25H25N3O4 M.W. 431.50
T-106



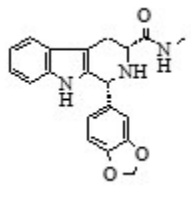
Nortadalafil
C21H17N3O4 M.W. 375.39
T-107



Tadalafil Impurity A
CAS No. NA
C20H19N3O3 M.W. 349.39
T-108

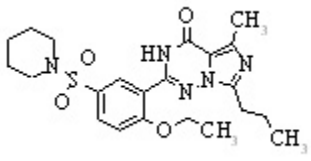


Tadalafil Impurity B
CAS No. NA
C20H19N3O3 M.W. 349.39
T-109

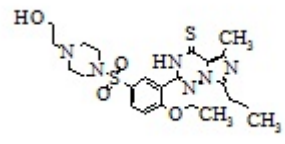


Vardenafil Related Compounds (commercial standards available) – includes deuterated standards.

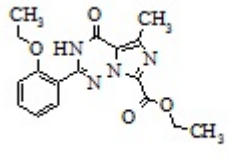
Pseudovardenafil
CAS No. 224788-34-5
C22H29N5O4S M.W. 459.57
V-051



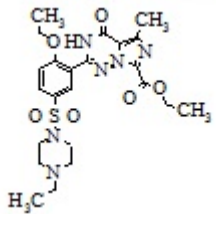
Hydroxythio Vardenafil
C23H32N6O4S2 M.W. 520.68
V-0510



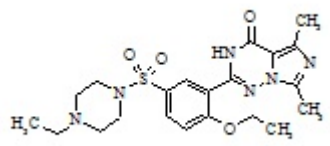
Vardenafil Impurity 1
CAS No. 1417529-67-9
C17H18N4O4 M.W. 342.36
V-0511



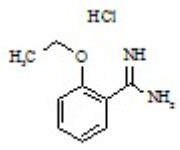
Vardenafil Impurity 2
CAS No. 1417529-69-1
C23H30N6O6S M.W. 518.60
V-0512



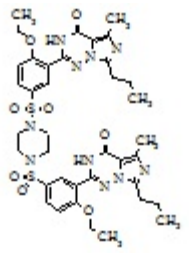
Vardenafil Impurity 3
C21H28N6O4S M.W. 460.56
V-0513



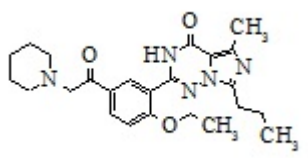
Vardenafil Impurity (2-Ethoxy Benzamidine Hydrochloride)
CAS No. 18637-00-8
C9H12N2O HCl M.W. 164.21 36.46
V-0515



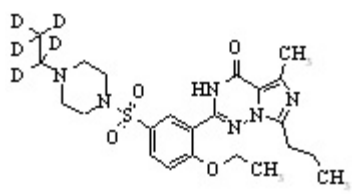
Vardenafil Dimer
C38H46N10O8S2 M.W. 834.98
V-0517



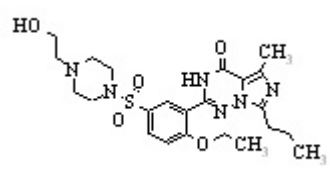
Vardenafil Acetyl Analogue
CAS No. N/A
C24H31N5O3 M.W. 437.55
V-0519



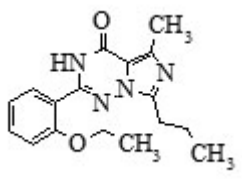
Vardenafil-d5
C23H27N6O4SD5 M.W. 493.64
V-053



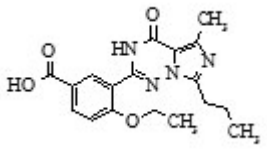
Hydroxy Vardenafil
C23H32N6O5S M.W. 504.61
V-055



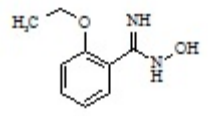
2-(2-Ethoxyphenyl)-5-methyl-7-propyl-3H-imidazo[5,1-f][1,2,4]triazin-4-one
C17H20N4O2 M.W. 312.37
V-057



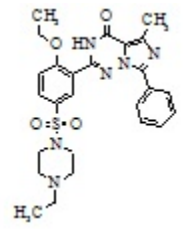
Norneovardenafil
CAS No. N/A
C18H20N4O4 M.W. 356.38
V-059



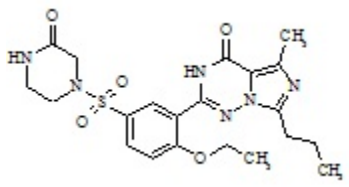
Vardenafil Impurity (2-Ethoxy-N-Hydroxy Benzamidine)
CAS No. 879-57-2
C9H12N2O2 M.W. 180.21
V-0514



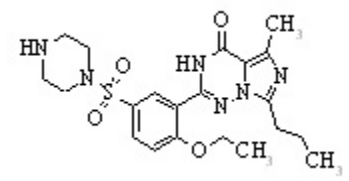
Vardenafil Benzoyl Impurity
C26H30N6O4S M.W. 522.63
V-0516



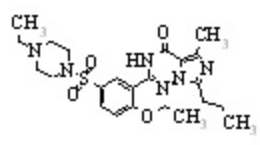
Vardenafil Oxopiperazine
C21H26N6O5S M.W. 474.54
V-0518



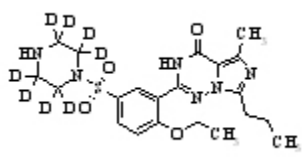
N-Desethyl Vardenafil
CAS No. 448184-46-1
C21H28N6O4S M.W. 460.56
V-052



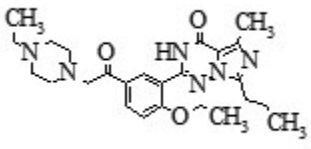
Vardenafil HCl
CAS No. 224785-90-4
C23H32N6O4S M.W. 488.61
V-054



N-Desethyl Vardenafil-d8
CAS No. 448184-46-1 (Unlabelled)
C21H28N6O4S M.W. 460.56
V-056

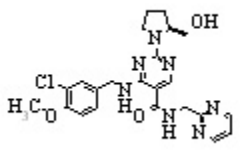


Acetylvardenafil
C25H34N6O3 M.W. 466.59
V-058

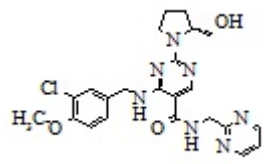


Avanafil Related Compounds (commercial standards available) – includes deuterated standards.

Avanafil
CAS No. 330784-47-9
C23H26ClN7O3 M.W. 483.96
A-291

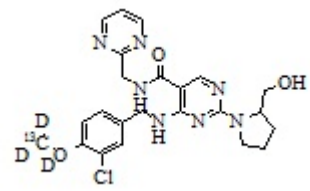


Avanafil Impurity 8 (R-Avanafil)
CAS No. N/A
C23H26ClN7O3 M.W. 483.96
A-2910

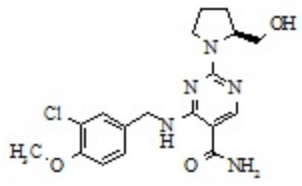


Avanafil Impurity 9
C18H17ClN6O3 M.W. 400.83
A-2911

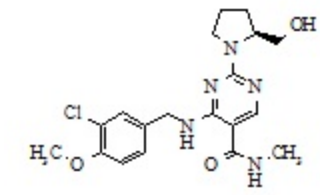
Avanafil-13CD3
C22H23ClN7O313CD3 M.W. 487.97
A-292



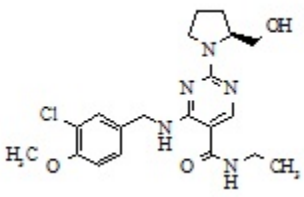
Avanafil impurity 1
C18H22ClN5O3 M.W. 391.86
A-293



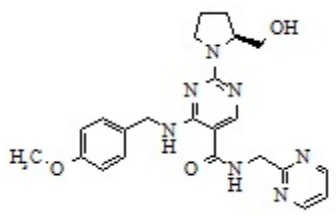
Avanafil impurity 2
C19H24ClN5O3 M.W. 405.89
A-294



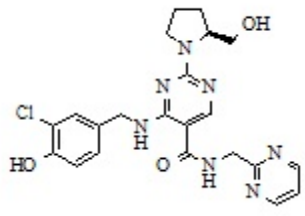
Avanafil impurity 3
C20H26ClN5O3 M.W. 419.91
A-295



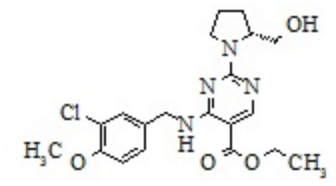
Avanafil impurity 4
C23H27N7O3 M.W. 449.52
A-296



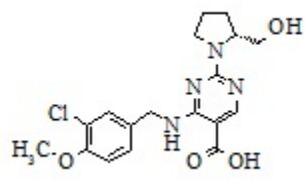
Avanafil impurity 5
C22H24ClN7O3 M.W. 469.93
A-297



Avanafil Impurity 6
CAS No. N/A
C20H25ClN4O4 M.W. 420.90
A-298

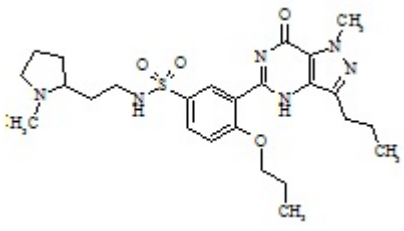


Avanafil Impurity 7
CAS No. N/A
C18H21ClN4O4 M.W. 392.85
A-299

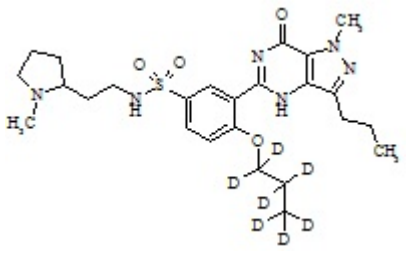


Udenafil Related Compounds (commercial standards available) – includes deuterated standards.

Udenafil
CAS No. 268203-93-6
C25H36N6O4S M.W. 516.67
U-031

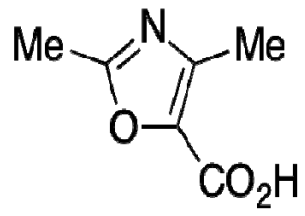


Udenafil-d7
CAS No. N/A
C25H29N6O4SD7 M.W. 523.71
U-032



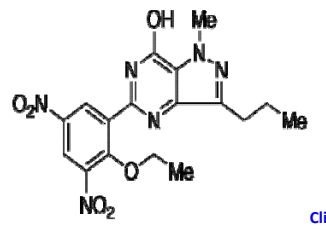
3. **Standards available from Toronto Research Chemicals http://www.trc-canada.com/ which include the majority of characterized PDE-5i analogues and all of the parent drugs including catalog numbers. (Some structure images not available) NOTE: Includes some compounds that are discontinued from TRC.**

Sildenafil Related Compounds (commercial standards available) – includes deuterated standards.



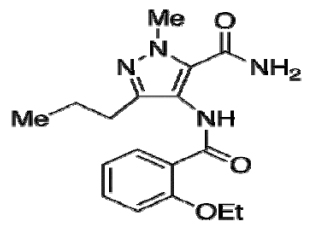
Click on image to enlarge

Catalogue #: D476330
Chemical Name: 2,4-Dimethyl-5-oxazolecarboxylic Acid
CAS Number: 2510-37-4
Mol. Formula: C6H7NO3
Synsynonyms: 2,4-Dimethyl-1,3-oxazole-5-carboxylic Acid; 2,4-Dimethyloxazole-5-carboxylic Acid; 5-Carboxy-2,4-dimethyloxazole



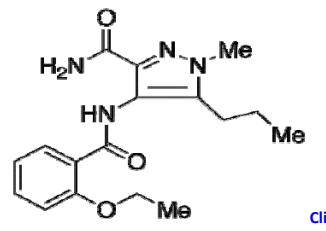
Click on image to enlarge

Catalogue #: D479775
Chemical Name: Dinitrodenafil
CAS Number:
Mol. Formula: C17H18N6O6
Synonyms: 5-(2-Ethoxy-3,5-dinitrophenyl)-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



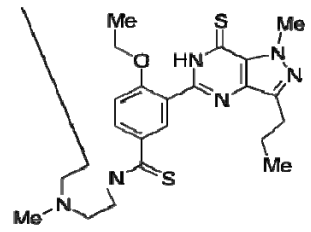
Click on image to enlarge

Catalogue #: E891000
Chemical Name: 4-(2-Ethoxybenzamido)-1-methyl-3-n-propylpyrazole-5-carboxamide
CAS Number: 139756-03-9
Mol. Formula: C17H22N4O3
Synonyms: 4-[(2-Ethoxybenzoyl)amino]-1-methyl-3-propyl-1H-pyrazole-5-carboxamide;



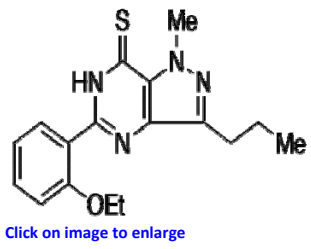
Click on image to enlarge

Catalogue #: E891010
Chemical Name: 4-[(2-Ethoxybenzoyl)amino]-1-methyl-5-propyl-1H-pyrazole-3-carboxamide
CAS Number: 501120-38-3
Mol. Formula: C17H22N4O3
Synonyms: 4-(2-Ethoxybenzamido)-1-methyl-5-propyl-1H-pyrazole-3-carboxamide



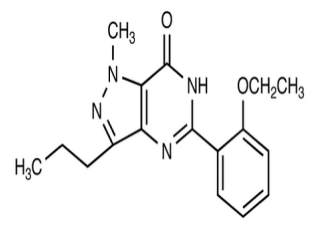
Click on image to enlarge

Catalogue #: E892530
Chemical Name: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)thioxomethyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyr
CAS Number: 1333233-46-7
Mol. Formula: C23H30N6OS2
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)thioxomethyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-Pyrazolo[4,3-d]pyrimidine-7-thione; Dithiodesmethylcarbodenafil



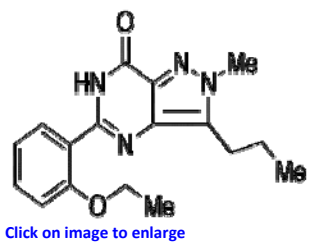
Click on image to enlarge

Catalogue #: E892710
Chemical Name: 5-(2-Ethoxyphenyl)-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione
CAS Number: 479074-06-1
Mol. Formula: C17H20N4OS
Synonyms: 5-(2-Ethoxyphenyl)-1,4-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione



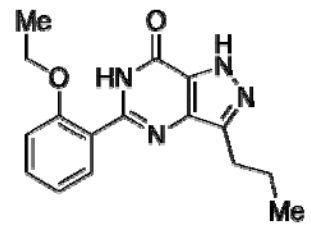
Click on image to enlarge

Catalogue #: E892725
Chemical Name: 5-(2-Ethoxyphenyl)-1-methyl-3-n-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 139756-21-1
Mol. Formula: C17H20N4O2
Synonyms: UK 088800; “Imidazosagatriazinone”



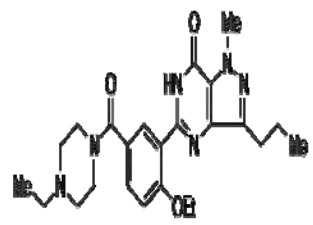
Click on image to enlarge

Catalogue #: E892730
Chemical Name: 5-(2-Ethoxyphenyl)-2,6-dihydro-2-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 501120-40-7
Mol. Formula: C17H20N4O2
Synonyms:



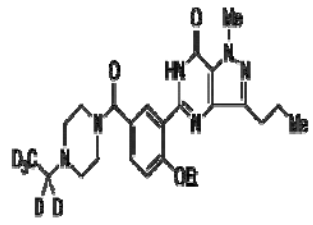
Click on image to enlarge

Catalogue #: E892765
Chemical Name: 5-(2-Ethoxyphenyl)-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 139756-30-2
Mol. Formula: C16H18N4O2
Synonyms: 5-(2-Ethoxyphenyl)-1,6-dihydro-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Des(4-methylpiperazin-1-ylsulfonyl) Desmethyl**sildenafil**



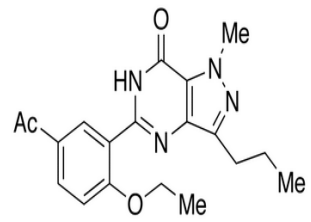
Click on image to enlarge

Catalogue #: F685400
Chemical Name: Fondenafil
CAS Number: 944241-52-5
Mol. Formula: C24H32N6O3
Synonyms: 5-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)carbonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Carbodenafil;



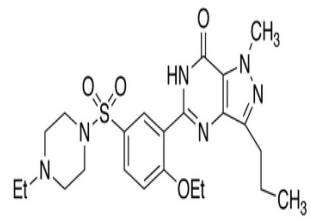
Click on image to enlarge

Catalogue #: F685402
Chemical Name: Fondenafil-d5
CAS Number:
Mol. Formula: C24H27D5N6O3
Synonyms: 5-[2-Ethoxy-5-[(4-ethyl-d5-1-piperazinyl)carbonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



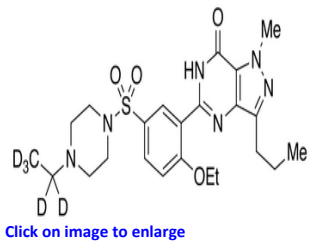
Click on image to enlarge

Catalogue #: G349960
Chemical Name: Gendenafil
CAS Number: 147676-66-2
Mol. Formula: C19H22N4O3
Synonyms: 5-(5-Acetyl-2-ethoxyphenyl)-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; 5-(5-Acetyl-2-ethoxyphenyl)-1-methyl-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one



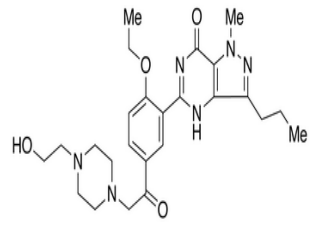
Click on image to enlarge

Catalogue #: H615150
Chemical Name: Homo Sildenafil
CAS Number: 642928-07-2
Mol. Formula: C23H32N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



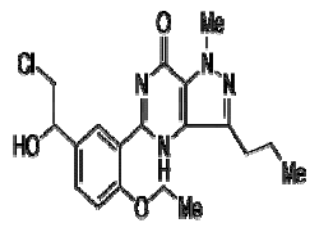
Click on image to enlarge

Catalogue #: H615152
Chemical Name: Homo Sildenafil-d5
CAS Number:
Mol. Formula: C23H27D5N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-(ethyl-d5)-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



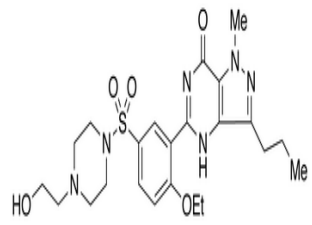
Click on image to enlarge

Chemical Name: Hydroxy Acetildenafil
CAS Number: 147676-56-0
Mol. Formula: C25H34N6O4
Synonyms: 5-[2-Ethoxy-5-[2-[4-(2-hydroxyethyl)-1-piperazinyl]acetyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Hydroxyhongdenafil;



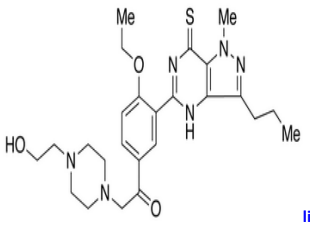
Click on image to enlarge

Catalogue #: H825115
Chemical Name: Hydroxy Chlorodenafil
CAS Number: 1391054-00-4
Mol. Formula: C19H23ClN4O3
Synonyms: 5-[5-(2-Chloro-1-hydroxyethyl)-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one



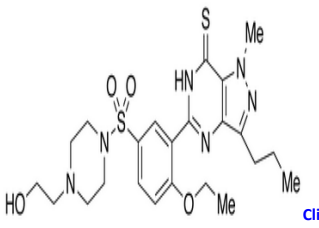
Click on image to enlarge

Catalogue #: H942840
Chemical Name: Hydroxyhomo Sildenafil
CAS Number: 139755-85-4
Mol. Formula: C23H32N6O5S
Synonyms: 5-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Lodenafil



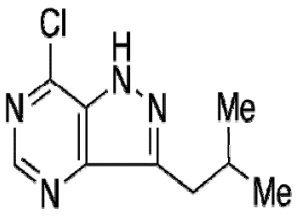
lick on image to enlarge

Catalogue #: H963100
Chemical Name: Hydroxythio Acetildenafil
CAS Number: 1159977-47-5
Mol. Formula: C25H34N6O3S
Synonyms: 5-[2-Ethoxy-5-[2-[4-(2-hydroxyethyl)-1-piperazinyl]acetyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-7-thio-pyrazolo[4,3-d]pyrimidine; 1-[3-(6,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]-2-[4-(2-hydroxyethyl)-1-piperazinyl]ethanone;



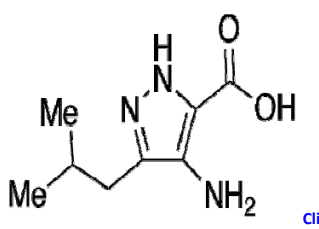
Click on image to enlarge

Catalogue #: H963150
Chemical Name: Hydroxythiohomo Sildenafil
CAS Number: 479073-82-0
Mol. Formula: C23H32N6O4S2
Synonyms: 5-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 4-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazineethanol



Click on image to enlarge

Catalogue #: I780530
Chemical Name: 3-Isobutyl-7-chloro-pyrazolo[4,3-d]pyrimidine
CAS Number:
Mol. Formula: C9H11ClN4
Synonyms: 3-Isobutyl-7-chloro-1H-pyrazolo[4,3-d]pyrimidine;



Click on image to enlarge

Catalogue #: I780615
Chemical Name: 5-(2-Isobutyl)-4-amino-1H-pyrazole-3-carboxylic Acid
CAS Number: 1093415-88-3
Mol. Formula: C8H13N3O2
Synonyms: 4-Amino-5-(2-methylpropyl)-1H-pyrazole-3-carboxylic Acid

no image of structure available

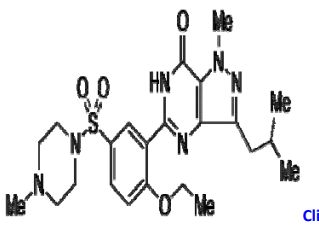
Catalogue #: I780620
Chemical Name: 3-Isobutylpyrazolo[4,3-d]pyrimidine
CAS Number:
Mol. Formula: C9H12N4
Synonyms: 3-Isobutyl-1H-pyrazolo[4,3-d]pyrimidine;

no image of structure available

Catalogue #: I780625
Chemical Name: 5-Isobutyl-4-nitro-1H-pyrazole-3-carboxylic Acid
CAS Number: 222729-55-7
Mol. Formula: C8H11N3O4
Synonyms: 5-(2-Methylpropyl)-4-nitro-1H-pyrazole-3-carboxylic Acid;

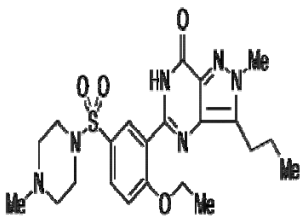
no image of structure available

Catalogue #: I780630
Chemical Name: 5-Isobutyl-1H-pyrazole-3-carboxylic Acid
CAS Number: 92933-49-8
Mol. Formula: C8H12N2O2
Synonyms: 5-(2-Methylpropyl)-1H-pyrazole-3-carboxylic Acid;



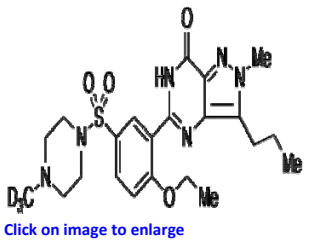
Click on image to enlarge

Catalogue #: I780650
Chemical Name: Isobutyl Sildenafil
CAS Number: 1391053-95-4
Mol. Formula: C23H32N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-(2-methylpropyl)-7H-pyrazolo[4,3-d]pyrimidin-7-one;



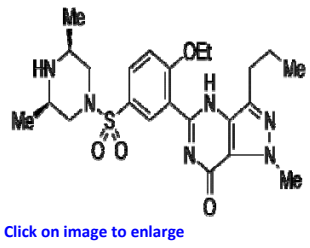
Click on image to enlarge

Catalogue #: I900800
Chemical Name: Iso Sildenafil
CAS Number: 253178-46-0
Mol. Formula: C22H30N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-2,6-dihydro-2-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; 1-[[3-(4,7-Dihydro-2-methyl-7-oxo-3-propyl-2H- pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine;



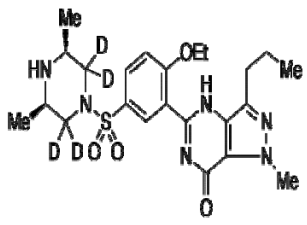
Click on image to enlarge

Catalogue #: I900802
Chemical Name: Iso Sildenafil-d3
CAS Number:
Mol. Formula: C22H27D3N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-(methyl-d3)-1-piperazinyl)sulfonyl]phenyl]-2,6-dihydro-2-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; 1-[[3-(4,7-Dihydro-2-methyl-7-oxo-3- propyl-2H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-(methyl-d3)piperazine;



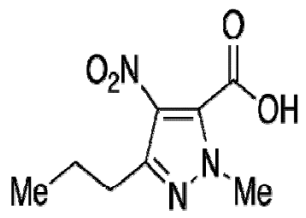
Click on image to enlarge

Catalogue #: M225935
Chemical Name: Methiso**sildenafil**
CAS Number: 496835-35-9
Mol. Formula: C23H32N6O4S
Synonyms: rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Aildenafil; Dimethyl**sildenafil**



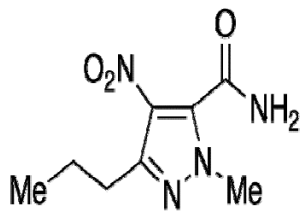
Click on image to enlarge

Catalogue #: M225937
Chemical Name: Methiso**sildenafil**-d4
CAS Number:
Mol. Formula: C23H28D4N6O4S
Synonyms: rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl-d4]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Aildenafil-d4;



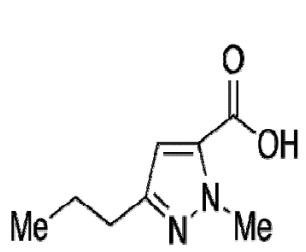
Click on image to enlarge

Catalogue #: M320530
Chemical Name: 1-Methyl-4-nitro-3-propyl-1H-pyrazole-5-carboxylic Acid
CAS Number: 139756-00-6
Mol. Formula: C8H11N3O4
Synonyms: 1-Methyl-4-nitro-3-propylpyrazole-5-carboxylic Acid



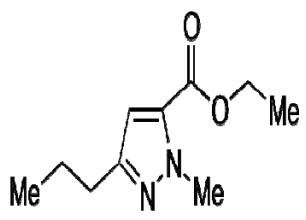
Click on image to enlarge

Catalogue #: M320535
Chemical Name: 1-Methyl-4-nitro-3-propylpyrazole-5-carboxamide
CAS Number: 139756-01-7
Mol. Formula: C8H12N4O3
Synonyms: 1-Methyl-4-nitro-3-propyl-1H-pyrazole-5-carboxamide



Click on image to enlarge

Catalogue #: M320655
Chemical Name: 1-Methyl-3-propyl-1H-pyrazole-5-carboxylic Acid
CAS Number: 139755-99-0
Mol. Formula: C8H12N2O2
Synonyms: 1-Methyl-3-propylpyrazole-5-carboxylic Acid; 2-Methyl-5-propyl-2H-pyrazole-3-carboxylic Acid



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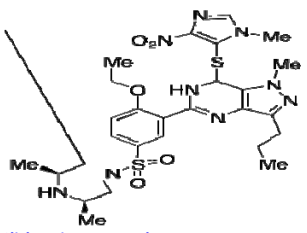
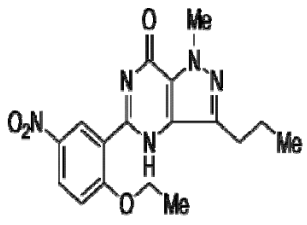
Catalogue #: M320775
Chemical Name: 1-Methyl-3-propyl-1H-pyrazole-5-carboxylic Acid Ethyl Ester
CAS Number: 133261-07-1
Mol. Formula: C10H16N2O2
Synonyms: 1-Methyl-3-propylpyrazole-5-carboxylic Acid Ethyl Ester; Ethyl 1-Methyl-3-propyl-1H-pyrazole-5-carboxylate; Ethyl 1-Methyl-3-propylpyrazole-5-carboxylate;



Click on image to enlarge

Catalogue #: M820000
Chemical Name: Mutaprodenafil
CAS Number: 138577-30-1
Mol. Formula: C27H37N9O5S2
Synonyms: rel-5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1-methyl-7-[(1-methyl-4-nitro-1H-imidazol-5-yl)thio]-3-propyl-1H-pyrazolo[4,3-d]pyrimidine



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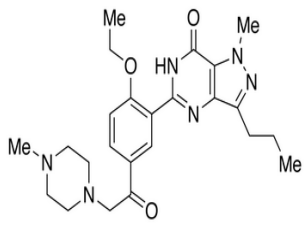
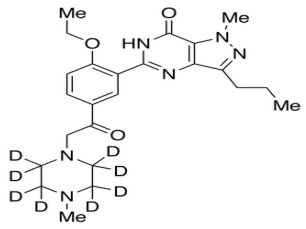
Catalogue #: N493770
Chemical Name: Nitrodenafil
CAS Number: 147676-99-1
Mol. Formula: C17H19N5O4
Synonyms: 5-(2-Ethoxy-5-nitrophenyl)-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



Click on image to enlarge

Catalogue #: N660500
Chemical Name: Nor Acetildenafil
CAS Number: 949091-38-7
Mol. Formula: C24H32N6O3
Synonyms: 5-[2-Ethoxy-5-[2-(4-methyl-1-piperazinyl)acetyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



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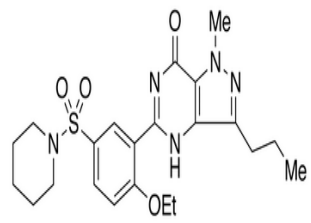
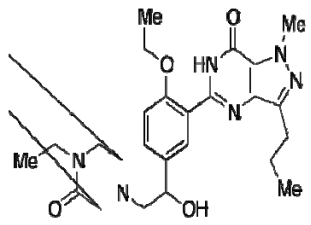
Catalogue #: N660502
Chemical Name: Nor Acetildenafil-d8
CAS Number: 1185117-07-0
Mol. Formula: C24H24D8N6O3
Synonyms: 5-[2-Ethoxy-5-[2-(4-methyl-1-piperazinyl-d8)acetyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



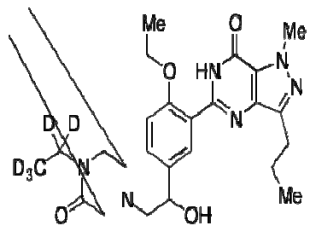
Click on image to enlarge

Catalogue #: N824300
Chemical Name: Norneo Sildenafil
CAS Number: 371959-09-0
Mol. Formula: C22H29N5O4S
Synonyms: 5-[2-Ethoxy-5-(1-piperidinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; 1-[[3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]piperidine;



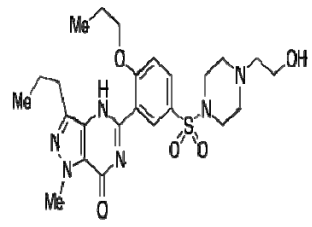
Click on image to enlarge

Catalogue #: P480470
Chemical Name: Piperazonifil
CAS Number: 1335201-04-1
Mol. Formula: C25H34N6O4
Synonyms: 5-[2-Ethoxy-5-[2-(4-ethyl-3-oxo-1-piperazinyl)-1-hydroxyethyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one,



Click on image to enlarge

Catalogue #: P480472
Chemical Name: Piperazonifil-d5
CAS Number:
Mol. Formula: C25H29D5N6O4
Synonyms: 5-[2-Ethoxy-5-[2-(4-ethyl-3-oxo-1-piperazinyl)-1-hydroxyethyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one-d5



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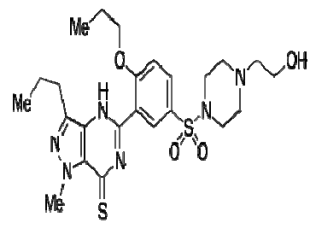
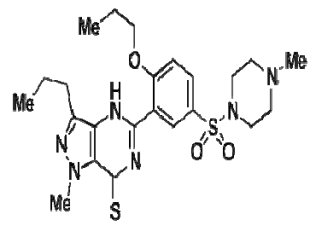
Catalogue #: P831600
Chemical Name: Propoxyphenyl Homohydroxy**sildenafil**
CAS Number: 139755-87-6
Mol. Formula: C24H34N6O5S
Synonyms: 5-[5-[4-(2-Hydroxyethyl)piperazinylsulfonyl]-2-propoxyphenyl]-1-methyl-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one; 4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-1-Piperazineethanol



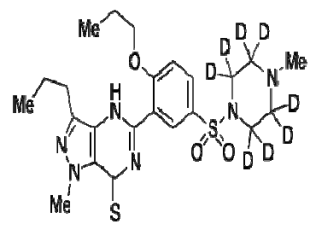
Click on image to enlarge

Catalogue #: P831630
Chemical Name: Propoxyphenyl-thiohydroxyhomosildenafil
CAS Number: 479073-90-0
Mol. Formula: C24H34N6O4S2
Synonyms: 1,6-dihydro-5-[5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1-methyl-3-propyl-7H-Pyrazolo[4,3-d]pyrimidine-7-thione; 4-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-1-Piperazineethanol; 5-(5-((4-(2-hydroxyethyl)piperazin-1-yl)sulfonyl)-2-propoxyphenyl)-1-methyl-3-propyl-1H-pyrazolo[4,3-d]pyrimidine-7(4H)-thione



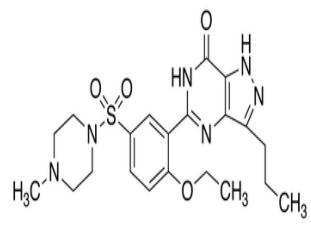
Click on image to enlarge

Catalogue #: P831635
Chemical Name: Propoxyphenyl Thio**sildenafil**
CAS Number: 479073-87-5
Mol. Formula: C23H32N6O3S2
Synonyms: 1,6-Dihydro-1-methyl-5-[5-[(4-methyl-1-piperazinyl)sulfonyl]-2-propoxyphenyl]-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-4-methyl-piperazine; rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione



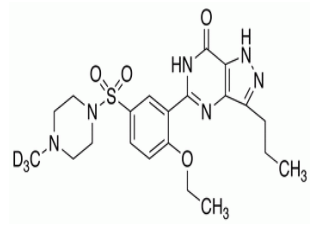
Click on image to enlarge

Catalogue #: P831637
Chemical Name: Propoxyphenyl-thio**sildenafil**-d8
CAS Number:
Mol. Formula: C23H24D8N6O3S2
Synonyms: 1,6-Dihydro-1-methyl-5-[5-[(4-methyl-1-piperazinyl)sulfonyl]-2-propoxyphenyl]-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione-d8; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-4-methyl-piperazine-d8; rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione-d8



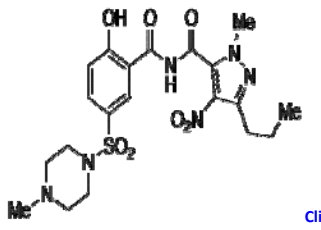
Click on image to enlarge

Catalogue #: P842800
Chemical Name: Pyrazole N-Demethyl Sildenafil
CAS Number: 139755-95-6
Mol. Formula: C21H28N6O4S
Synonyms: 1-[[3-(4,7-Dihydroxy-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methyl-piperazine; Desmethyl**sildenafil**;



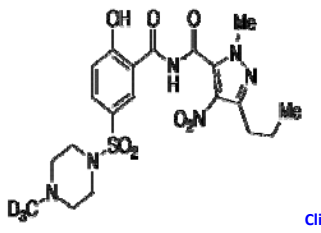
Click on image to enlarge

Catalogue #: P842802
Chemical Name: Pyrazole N-Demethyl Sildenafil-d3
CAS Number:
Mol. Formula: C21H25D3N6O4S
Synonyms: 1-[[3-(4,7-Dihydroxy-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl-4- ethoxyphenyl]sulfonyl]-4-(methyl-d3)piperazine; Desmethyl**sildenafil**-d3;



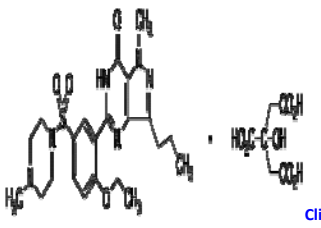
Click on image to enlarge

Catalogue #: P846500
Chemical Name: Pyrazolosalicyloyl Imide
CAS Number:
Mol. Formula: C20H26N6O7S
Synonyms: N-[2-Hydroxy-5-[(4-methyl-1-piperazinyl)sulfonyl]benzoyl]-1-methyl-4-nitro-3-n-propyl-1H-pyrazol-5-carboxamide; Pyrazolosalicylimide



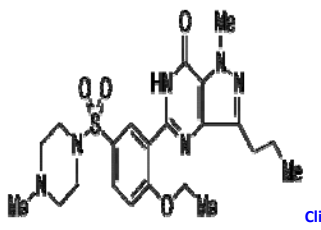
Click on image to enlarge

Catalogue #: P846502
Chemical Name: Pyrazolosalicyloyl Imide-d3
CAS Number:
Mol. Formula: C20H23D3N6O7S
Synonyms: N-[2-Hydroxy-5-[(4-methyl-1-piperazinyl)sulfonyl]benzoyl]-1-methyl-4-nitro-3-n-propyl-1H-pyrazol-5-carboxamide-d3; Pyrazolosalicylimide-d3



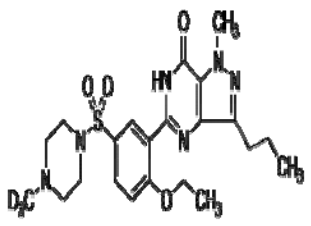
Click on image to enlarge

Catalogue #: S435000
Chemical Name: Sildenafil Citrate
CAS Number: 171599-83-0
Mol. Formula: C28H38N6O11S
Synonyms: 1-[[3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine Citrate;



Click on image to enlarge

Catalogue #: S435001
Chemical Name: Sildenafil
CAS Number: 139755-83-2
Mol. Formula: C22H30N6O4S
Synonyms: 1-[[3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine; 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;

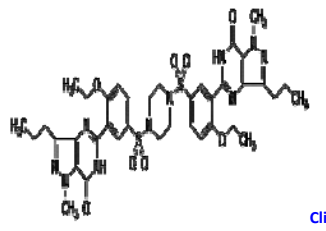


Click on image to enlarge

Catalogue #: S435002
Chemical Name: Sildenafil-d3
CAS Number: 1126745-90-1
Mol. Formula: C22H27D3N6O4S
Synonyms: 1-[[3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine-d3; 5-[2-Ethoxy-5-[[4-(methyl-d3)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;

no image of structure available

Catalogue #: S435003
Chemical Name: Sildenafil-d8
CAS Number: 951385-68-5
Mol. Formula: C22H22D8N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl-2,2,3,3,5,5,6,6-d8)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; BDD 10402;

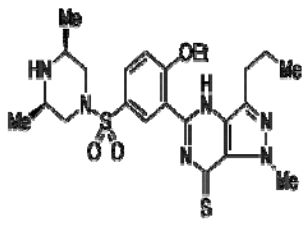


Click on image to enlarge

Catalogue #: S435020
Chemical Name: Sildenafil Dimer Impurity
CAS Number:
Mol. Formula: C38H46N10O8S2
Synonyms:

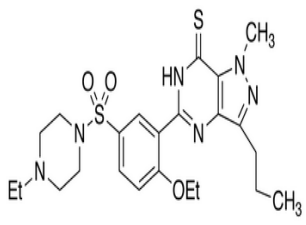
no image of structure available

Catalogue #: S435035
Chemical Name: Sildenafil N-Oxide
CAS Number: 1094598-75-0
Mol. Formula: C22H30N6O5S
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-4-oxido-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



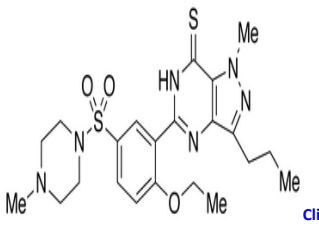
Click on image to enlarge

Catalogue #: T344365
Chemical Name: Thioaildenafil
CAS Number: 856190-47-1
Mol. Formula: C23H32N6O3S2
Synonyms: (3R,5S)-rel-1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-3,5-dimethyl-piperazine; Sulfoaildenafil;



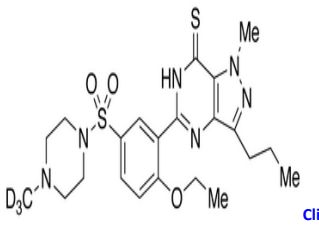
Click on image to enlarge

Catalogue #: T344470
Chemical Name: Thiohomo Sildenafil
CAS Number: 479073-80-8
Mol. Formula: C23H32N6O3S2
Synonyms: 5-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-ethyl-piperazine



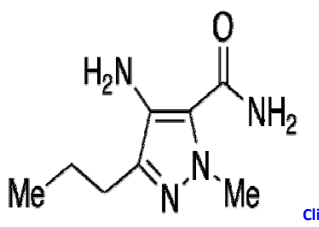
Click on image to enlarge

Catalogue #: T371500
Chemical Name: Thio**sildenafil**
CAS Number: 479073-79-5
Mol. Formula: C22H30N6O3S2
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo- 1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine;



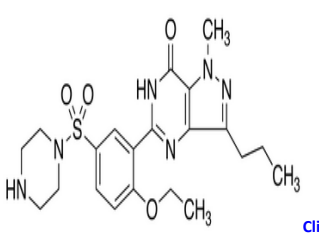
Click on image to enlarge

Catalogue #: T371502
Chemical Name: Thio**sildenafil**-d3
CAS Number:
Mol. Formula: C22H27D3N6O3S2
Synonyms: 5-[2-Ethoxy-5-[(4-(methyl-d3)-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl -7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-(methyl-d3)piperazine;



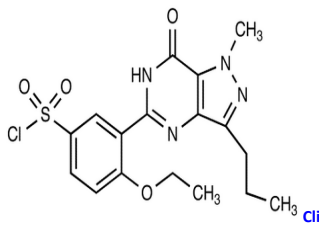
Click on image to enlarge

Catalogue #: A617415
Chemical Name: 4-Amino-1-methyl-3-propyl-1H-pyrazole-5-carboxamide
CAS Number: 139756-02-8
Mol. Formula: C8H14N4O
Synonyms: 4-Amino-2-methyl-5-propyl-2H-pyrazole-3-carboxamide;



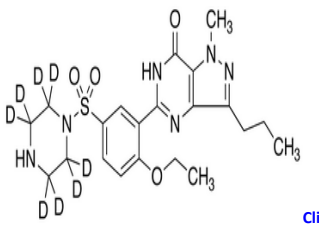
Click on image to enlarge

Catalogue #: D292200
Chemical Name: N-Desmethyl Sildenafil
CAS Number: 139755-82-1
Mol. Formula: C21H28N6O4S
Synonyms: 5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Desmethyl**sildenafil**; UK 103320;



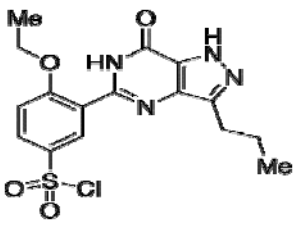
Click on image to enlarge

Catalogue #: C380005
Chemical Name: 5-(5-Chlorosulfonyl-2-ethoxyphenyl)-1-methyl-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 139756-22-2
Mol. Formula: C17H19ClN4O4S
Synonyms: 3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxy-benzenesulfonyl Chloride;



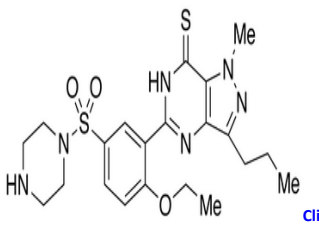
Click on image to enlarge

Catalogue #: D292202
Chemical Name: N-Desmethyl Sildenafil-d8
CAS Number:
Mol. Formula: C21H20D8N6O4S
Synonyms: 5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one-d8; Desmethyl**sildenafil**-d8; UK 103320-d8;



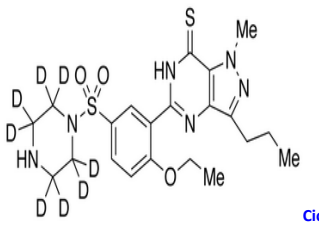
Click on image to enlarge

Catalogue #: C383500
Chemical Name: 5-(5-Chlorosulfonyl-2-ethoxyphenyl)-3-propyl-1,6-dihydro -7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 139756-31-3
Mol. Formula: C16H17ClN4O4S
Synonyms: 3-(6,7-Dihydro-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxybenzenesulfonyl Chloride; Des-4-methylpiperazine Desmethyl**sildenafil** Chloride;



Click on image to enlarge

Catalogue #: D294350
Chemical Name: Desmethyl Thio**sildenafil**
CAS Number: 479073-86-4
Mol. Formula: C21H28N6O3S2
Synonyms: 5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl- 7H-pyrazolo[4,3-d]pyrimidine-7-thione;



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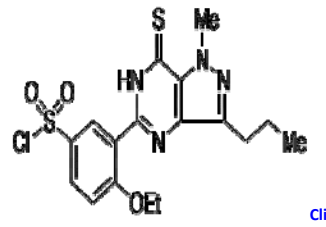
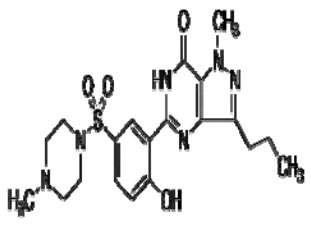
Catalogue #: D294352
Chemical Name: Desmethyl Thio**sildenafil**-d8
CAS Number: 1215321-44-0
Mol. Formula: C21H20D8N6O3S2
Synonyms: 5-[2-Ethoxy-5-(1-piperazinyl-d8-sulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl- 7H-pyrazolo[4,3-d]pyrimidine-7-thione;



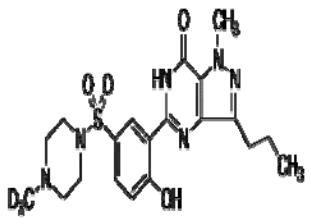
Click on image to enlarge

Catalogue #: D449445
Chemical Name: 3-(6,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxy-benzenesulfonyl Chloride
CAS Number: 479074-07-2
Mol. Formula: C17H19ClN4O3S2
Synonyms:



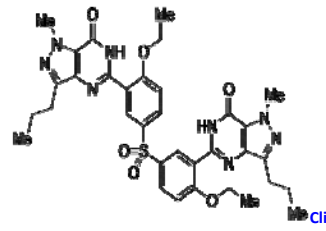
Click on image to enlarge

Chemical Name: Desethyl Sildenafil
CAS Number: 139755-91-2
Mol. Formula: C20H26N6O4S
Synonyms: 5-[2-Hydroxy-5-(4-methylpiperazinylsulphonyl)phenyl]1-methyl-3-n-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyramidin-7-one; 5-[2-Hydroxy-5-[[4-(methyl)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



Click on image to enlarge

Catalogue #: D289602
Chemical Name: Desethyl Sildenafil-d3
CAS Number: 1346603-75-5
Mol. Formula: C20H23D3N6O4S
Synonyms: 5-[2-Hydroxy-5-(4-methyl-d3-piperazinylsulphonyl)phenyl]1-methyl-3-n-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyramidin-7-one; 5-[2-Hydroxy-5-[[4-(methyl-d3)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



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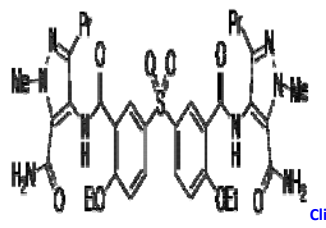
Catalogue #: D231215
Chemical Name: De(methypiperazinyl) Sildenafil Dimer Impurity
CAS Number: 1346603-48-2
Mol. Formula: C34H38N8O6S
Synonyms: 5-[2-Ethoxy-5-[4-[4-ethoxy-3-(1-methyl-7-oxo-3-propyl-4,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-yl)phenyl]sulfonyl]phenyl]-1-methyl-3-n-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one;

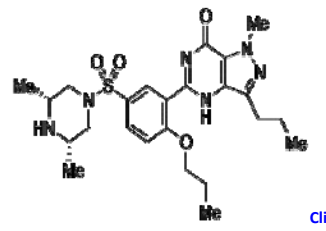
no image of structure available

Catalogue #: D231235
Chemical Name: Demethylpiperazinyl Sildenafil Sulfonic Acid
CAS Number:
Mol. Formula: C17H20N4O5S
Synonyms: 3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxybenzenesulfonic Acid;



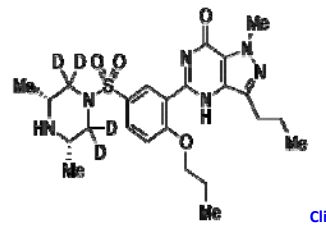
Click on image to enlarge

Catalogue #: A603070
Chemical Name: 3-[[[5-Aminocarbonyl-1-methyl-3-propyl-1H-pyrazol-4-yl]amino]carbonyl]-4-ethoxy-benzenesulfonyl Dimer
CAS Number:
Mol. Formula: C34H42N8O8S
Synonyms: 3,3'-Sulfonyl Bis[(4-Ethoxy-3-(6,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo-pyrimidin-5-yl)benzene)



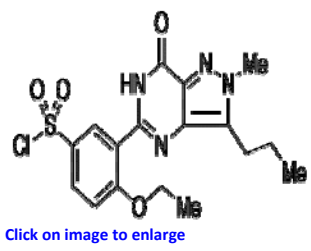
Click on image to enlarge

Catalogue #: D289495
Chemical Name: O-Desethyl-O-propyl Methiso**sildenafil**
CAS Number: 1391053-82-9
Mol. Formula: C24H34N6O4S
Synonyms: rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



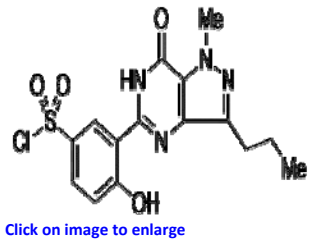
Click on image to enlarge

Catalogue #: D289497
Chemical Name: O-Desethyl-O-propyl Methiso**sildenafil**-d4
CAS Number:
Mol. Formula: C24H30D4N6O4S
Synonyms: rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one-d4;



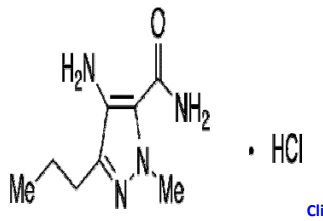
Click on image to enlarge

Catalogue #: D231290
Chemical Name: Demethylpiperazinyl Iso Sildenafil Sulfonyl Chloride
CAS Number: 501120-42-9
Mol. Formula: C17H19ClN4O4S
Synonyms: 3-(6,7-Dihydro-2-methyl-7-oxo-3-propyl-2H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxy-benzenesulfonyl Chloride



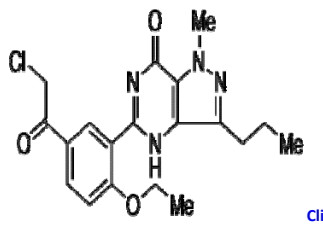
Click on image to enlarge

Catalogue #: D231300
Chemical Name: Demethylpiperazinyl Desethyl Sildenafil Sulfonyl Chloride
CAS Number: 139756-27-7
Mol. Formula: C15H15ClN4O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-hydroxy-benzenesulfonyl Chloride; 5-(5-Chlorosulfonyl-2-hydroxyphenyl)-1-methyl-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one



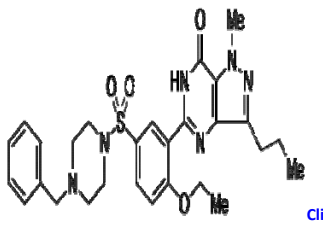
Click on image to enlarge

Catalogue #: A617420
Chemical Name: 4-Amino-1-methyl-3-propyl-1H-pyrazole-5-carboxamide Hydrochloride
CAS Number: 247584-10-7
Mol. Formula: C8H15ClN4O
Synonyms: 4-Amino-2-methyl-5-propyl-2H-pyrazole-3-carboxamide Hydrochloride;



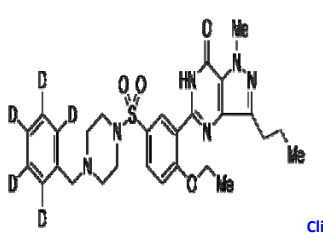
Click on image to enlarge

Catalogue #: C365535
Chemical Name: Chlorodenafil
CAS Number: 1058653-74-9
Mol. Formula: C19H21ClN4O3
Synonyms: 5-[5-(2-Chloroacetyl)-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



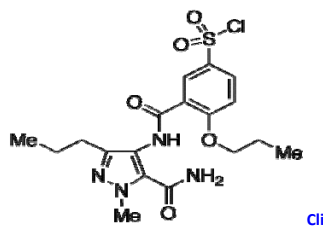
Click on image to enlarge

Catalogue #: D292205
Chemical Name: N-Desmethyl-N-benzyl Sildenafil
CAS Number:
Mol. Formula: C28H34N6O4S
Synonyms: 5-[2-Ethoxy-5-(1-benzyl-1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Benzyl Sildenafil;



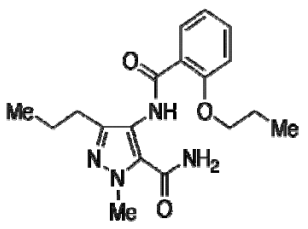
Click on image to enlarge

Catalogue #: D292207
Chemical Name: N-Desmethyl-N-benzyl Sildenafil-d5
CAS Number:
Mol. Formula: C28H29D5N6O4S
Synonyms: 5-[2-Ethoxy-5-(1-(benzyl-d5)-1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Benzyl Sildenafil-d5;



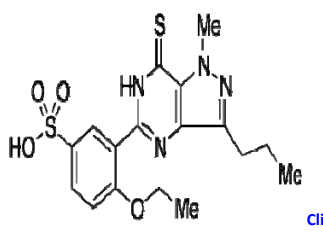
Click on image to enlarge

Catalogue #: A603110
Chemical Name: 3-[[[5-(Aminocarbonyl)-1-methyl-3-propyl-1H-pyrazol-4-yl]amino]carbonyl]-4-propoxy-benzenesulfonyl Chloride
CAS Number: 374776-34-8
Mol. Formula: C18H23ClN4O5S
Synonyms:



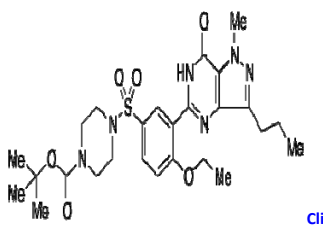
Click on image to enlarge

Catalogue #: A603105
Chemical Name: 3-[[[5-(Aminocarbonyl)-1-methyl-3-propyl-1H-pyrazol-4-yl]amino]carbonyl]-4-propoxybenzene
CAS Number: 139756-04-0
Mol. Formula: C18H24N4O3
Synonyms: 1-Methyl-4-(2-propoxybenzamido)-3-propylpyrazole-5-carboxamide; 1-Methyl-4-[(2-propoxybenzoyl)amino]-3-propyl-1H-pyrazole-5-carboxamide



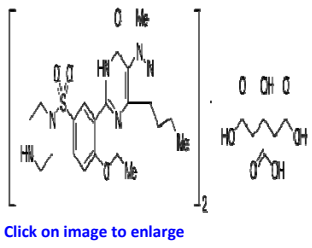
Click on image to enlarge

Catalogue #: D231260
Chemical Name: Demethylpiperazinyl 7-Desoxo 7-Thioxo**sildenafil** Sulfonic Acid
CAS Number: 1353018-10-6
Mol. Formula: C17H20N4O4S2
Synonyms: 4-Ethoxy-3-(1-methyl-3-propyl-7-thioxo-6,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-yl)benzenesulfonic Acid



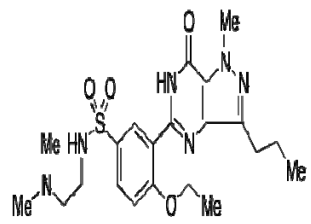
Click on image to enlarge

Catalogue #: D292245
Chemical Name: N-(Desmethyl)-tert-butyl Acetate Sildenafil
CAS Number: 398507-63-6
Mol. Formula: C26H36N6O6S
Synonyms: tert-Butyl 4-((4-Ethoxy-3-(1-methyl-7-oxo-3-propyl-6,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-yl)phenyl)sulfonyl)piperazine-1-carboxylate; 4-[[3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazinecarboxylic Acid 1,1-Dimethylethyl Ester



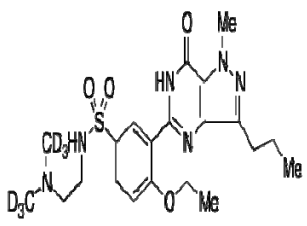
Click on image to enlarge

Catalogue #: D292201
Chemical Name: N-Desmethyl Sildenafil Hemicitrate
CAS Number:
Mol. Formula: C48H64N12O15S2
Synonyms: 5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one Hemicitrate; Desmethyl**sildenafil** Hemicitrate; UK 103320 Hemicitrate



Click on image to enlarge

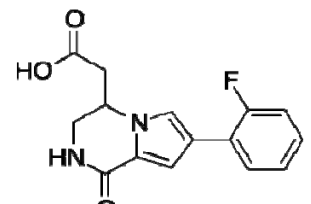
Catalogue #: D289520
Chemical Name: Descarbon**sildenafil**
CAS Number: 1393816-99-3
Mol. Formula: C21H30N6O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-N-[2-(dimethylamino)ethyl]-4-ethoxy-benzenesulfonamide



Click on image to enlarge

Catalogue #: D289522
Chemical Name: Descarbon**sildenafil**-d6
CAS Number:
Mol. Formula: C21H24D6N6O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-N-[2-(dimethyl-d6-amino)ethyl]-4-ethoxy-benzenesulfonamide

Tadalafil Related Compounds (commercial standards available) – includes deuterated standards.



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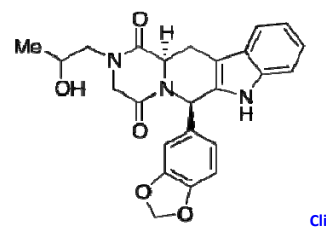
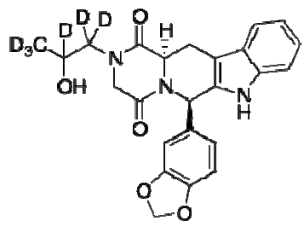
Catalogue #: F595590
Chemical Name: 7-(2-Fluorophenyl)-1,2,3,4-tetrahydro-1-oxo-pyrrolo[1,2-a]pyrazine-4-acetic Acid
CAS Number: 1170575-17-3
Mol. Formula: C15H13FN2O3
Synonyms:



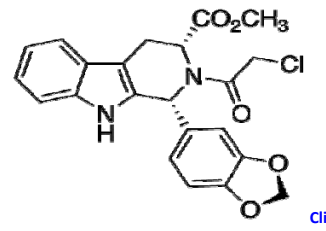
Click on image to enlarge

Catalogue #: H952705
Chemical Name: 2-Hydroxypropyl Nor**tadalafil**
CAS Number: 1353020-85-5
Mol. Formula: C24H23N3O5
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(2-hydroxypropyl)-pyrazino[1&#65533;,2&#65533;:1,6]pyrido[3,4-b]indole-1,4-dione;



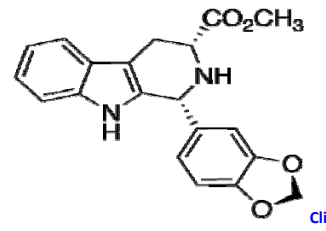
Click on image to enlarge

Catalogue #: H952707
Chemical Name: 2-Hydroxypropyl-d6 Nor**tadalafil**
CAS Number:
Mol. Formula: C24H17D6N3O5
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(2-hydroxypropyl)-pyrazino[1&#65533;,2&#65533;:1,6]pyrido[3,4-b]indole-1,4-dione-d6;



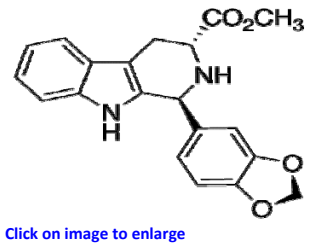
Click on image to enlarge

Catalogue #: M330125
Chemical Name: (1R,3R)-Methyl-1,2,3,4-tetrahydro-2-chloroacetyl-1-(3,4-methylenedioxyphenyl)-9H-pyrido[3,4-b]indole-3-carboxylate (Chloropre**tadalafil**)
CAS Number: 171489-59-1
Mol. Formula: C22H19ClN2O5
Synonyms: (1R,3R)-1-(1,3-Benzodioxol-5-yl)-2-(2-chloroacetyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester;



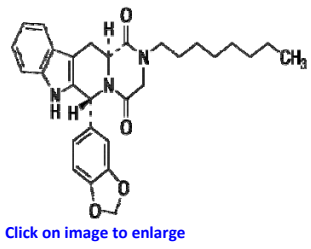
Click on image to enlarge

Catalogue #: M330150
Chemical Name: (1R,3R)-Methyl-1,2,3,4-tetrahydro-1-(3,4-methylenedioxyphenyl)-9H-pyrido[3,4-b]indole-3-carboxylate
CAS Number: 171596-41-1
Mol. Formula: C20H18N2O4
Synonyms: (1R,3R)-1-(1,3-Benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester;



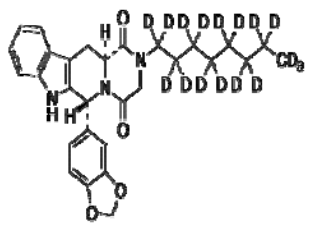
Click on image to enlarge

Catalogue #: M330155
Chemical Name: (1S,3R)-Methyl-1,2,3,4-tetrahydro-1-(3,4-methylenedioxyphenyl)-9H-pyrido[3,4-b]indole-3-carboxylate
CAS Number: 171596-42-2
Mol. Formula: C20H18N2O4
Synonyms: (1S,3R)-1-(1,3-Benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester;



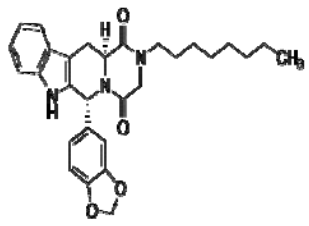
Click on image to enlarge

Catalogue #: O241350
Chemical Name: N-Octyl Nor**tadalafil**
CAS Number: 1173706-35-8
Mol. Formula: C29H33N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-octylpyrazino[1&#65533;,2&#65533;:1,6]pyrido[3,4-b]indole-1,4-dione;



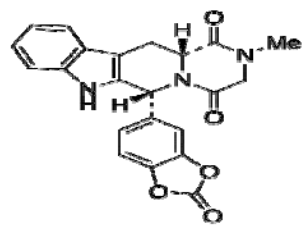
Click on image to enlarge

Catalogue #: O241352
Chemical Name: N-Octyl Nor**tadalafil**-d17
CAS Number:
Mol. Formula: C29H16D17N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(octyl-d17)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



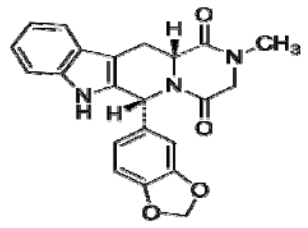
Click on image to enlarge

Catalogue #: O241360
Chemical Name: N-Octyl cis-Nor**tadalafil**
CAS Number:
Mol. Formula: C29H33N3O4
Synonyms: (6R,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-octylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



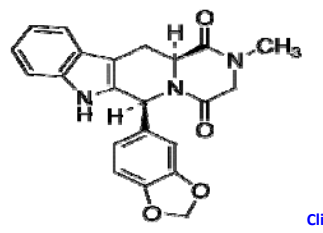
Click on image to enlarge

Catalogue #: O870430
Chemical Name: 2'-Oxo Tadalafil
CAS Number:
Mol. Formula: C22H17N3O5
Synonyms: (6R,12aR)-6-(2-Oxo-1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; 2'-Keto Tadalafil;



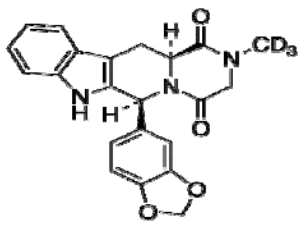
Click on image

Catalogue #: T004500
Chemical Name: Tadalafil
CAS Number: 171596-29-5
Mol. Formula: C22H19N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; Cialis; GF 196960; IC 351; ICOS 351; Tildenafil; UK 336017;



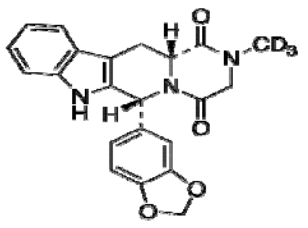
Click on image to enlarge

Catalogue #: T004505
Chemical Name: ent-Tadalafil
CAS Number: 629652-72-8
Mol. Formula: C22H19N3O4
Synonyms: (6S,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methyl-pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; L-Tadalafil; L-Tildenafil;



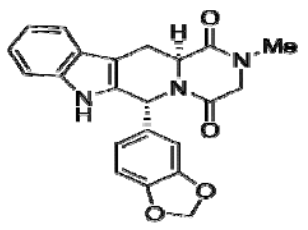
Click on image to enlarge

Catalogue #: T004507
Chemical Name: ent-Tadalafil-d3
CAS Number:
Mol. Formula: C22H16D3N3O4
Synonyms: (6S,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(methyl-d3)-pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; L-Tadalafil-d3; L-Tildenafil-d3;



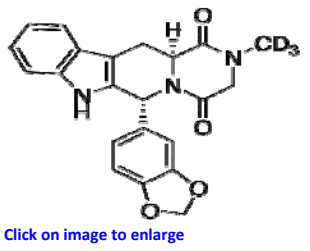
Click on image to enlarge

Catalogue #: T004510
Chemical Name: Tadalafil-d3
CAS Number: 960226-55-5
Mol. Formula: C22H16D3N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; Cialis-d3; GF 196960-d3; IC 351-d3; ICOS 351-d3; Tildenafil-d3; UK 336017-d3;



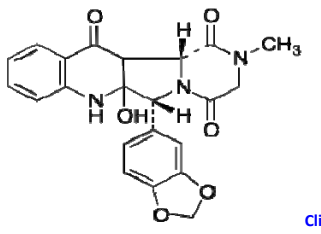
Click on image to enlarge

Catalogue #: T004520
Chemical Name: cis-Tadalafil
CAS Number: 171596-27-3
Mol. Formula: C22H19N3O4
Synonyms: (6R,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R-cis)-6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a- hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



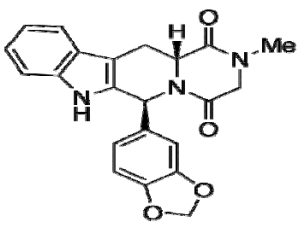
Click on image to enlarge

Catalogue #: T004522
Chemical Name: cis-Tadalafil-d3
CAS Number:
Mol. Formula: C22H16D3N3O4
Synonyms: (6R,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R-cis)-6-(1,3-benzodioxol-5-yl)- 2,3,6,7,12,12a-hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



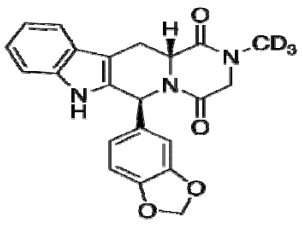
Click on image to enlarge

Catalogue #: T004525
Chemical Name: Tadalafil Hydroxypiperidone
CAS Number:
Mol. Formula: C22H19N3O6
Synonyms: Tadalafil Impurity



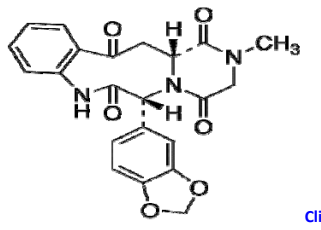
Click on image to enlarge

Catalogue #: T004530
Chemical Name: cis-ent-Tadalafil
CAS Number: 171596-28-4
Mol. Formula: C22H19N3O4
Synonyms: (6S,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6S-cis)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a- hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



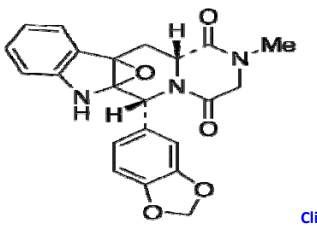
Click on image to enlarge

Catalogue #: T004532
Chemical Name: cis-ent-Tadalafil-d3
CAS Number:
Mol. Formula: C22H16D3N3O4
Synonyms: 6S,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6S-cis)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a- hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



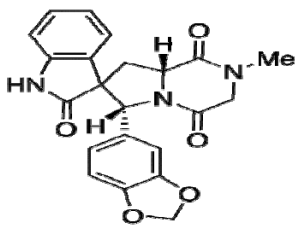
Click on image to enlarge

Catalogue #: T004535
Chemical Name: Tadalafil Ketolactam
CAS Number: 1346605-38-6
Mol. Formula: C22H19N3O6
Synonyms: (6R,14aR)-rel-6-(1,3-Benzodioxol-5-yl)-2,3,14,14a-tetrahydro-2-methylpyrazino[1,2-d][1,4]benzodiazonine-1,4,7,13(6H,8H)-tetrone;



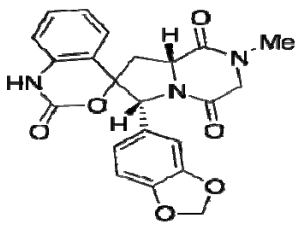
Click on image to enlarge

Catalogue #: T004540
Chemical Name: Tadalafil Epoxide Discontinued
CAS Number:
Mol. Formula: C22H19N3O5
Synonyms: Epoxy Tadalafil;



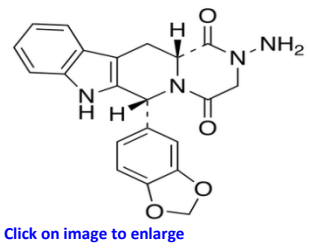
Click on image to enlarge

Catalogue #: T004550
Chemical Name: Tadalafil Spiro-oxindole
CAS Number:
Mol. Formula: C22H19N3O5
Synonyms: Tadalafil Impurity



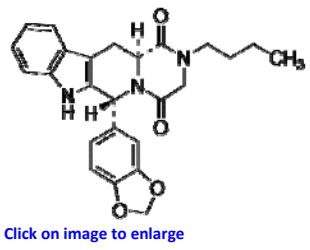
Click on image to enlarge

Catalogue #: T004555
Chemical Name: Tadalafil Spiro-2-keto-1,3-oxazine
CAS Number:
Mol. Formula: C22H19N3O6
Synonyms: Tadalafil Impurity



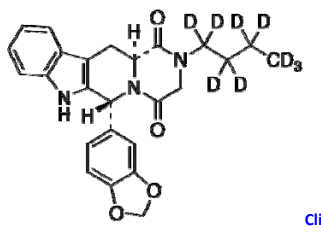
Click on image to enlarge

Catalogue #: A629550
Chemical Name: Amino Tadalafil
CAS Number: 385769-84-6
Mol. Formula: C21H18N4O4
Synonyms: (6R,12aR)-2-Amino-6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



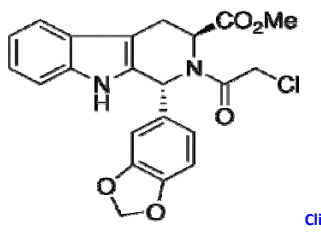
Click on image to enlarge

Catalogue #: B693585
Chemical Name: N-Butyl Nor**tadalafil**
CAS Number: 171596-31-9
Mol. Formula: C25H25N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2-butyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



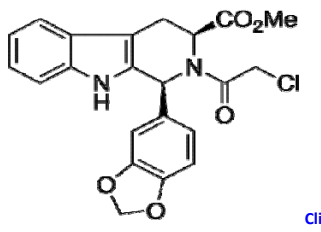
Click on image to enlarge

Catalogue #: B693587
Chemical Name: N-Butyl Nor**tadalafil**-d9
CAS Number:
Mol. Formula: C25H16D9N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2-(butyl-d9)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



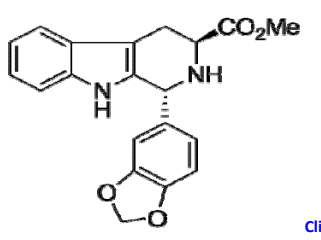
Click on image to enlarge

Catalogue #: B200000
Chemical Name: (1R,3S)-1-(1,3-Benzodioxol-5-yl)-2-(2-chloroacetyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester
CAS Number: 629652-44-4
Mol. Formula: C22H19ClN2O5
Synonyms:



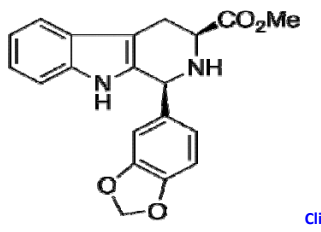
Click on image to enlarge

Catalogue #: B200005
Chemical Name: (1S,3S)-1-(1,3-Benzodioxol-5-yl)-2-(2-chloroacetyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester
CAS Number: 629652-42-2
Mol. Formula: C22H19ClN2O5
Synonyms:



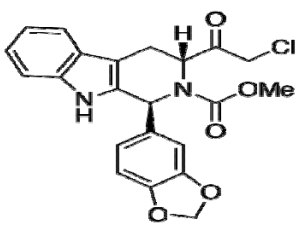
Click on image to enlarge

Catalogue #: B200025
Chemical Name: (1R,3S)-1-(1,3-Benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester
CAS Number: 171596-44-4
Mol. Formula: C20H18N2O4
Synonyms:



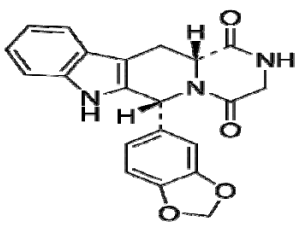
Click on image to enlarge

Catalogue #: B200020
Chemical Name: (1S,3S)-1-(1,3-Benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester
CAS Number: 171596-43-3
Mol. Formula: C20H18N2O4
Synonyms: (1S-cis)-1-(1,3-benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester



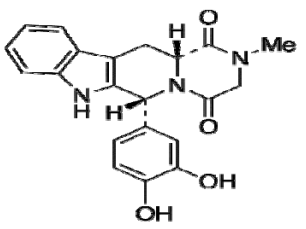
Click on image to enlarge

Catalogue #: B121700
Chemical Name: (1S,3R)-1-Benzo[1,3]dioxol-5-yl-2-(2-chloro-acetyl)-2,3,4,9-tetrahydro-1H-b-carboline-3-carboxylic Acid Methyl Ester
CAS Number: 629652-40-0
Mol. Formula: C22H19ClN2O5
Synonyms: (1S,3R)-1-(1,3-Benzodioxol-5-yl)-2-(2-chloroacetyl)-2,3,4,9-tetrahydro1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester; (1S,3R)-1-(1,3-Benzodioxol-5-yl)-2-(chloroacetyl)-2,3,4,9-tetrahydro1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester;



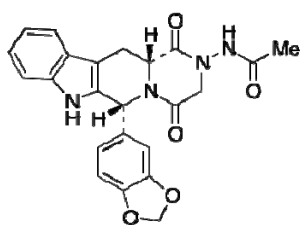
Click on image to enlarge

Catalogue #: D293800
Chemical Name: N-Desmethyl Tadalafil
CAS Number: 171596-36-4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R-trans)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; Nor**tadalafil**



Click on image to enlarge

Catalogue #: D291990
Chemical Name: Desmethylene Tadalafil
CAS Number: 171489-03-5
Mol. Formula: C21H19N3O4
Synonyms: (6R,12aR)-6-(3,4-dihydroxyphenyl)-2,3,6,7,12,12a-hexahydro-2-methyl-pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R,trans)-6-(3,4-dihydroxyphenyl)-2,3,6,7,12,12a-hexahydro-2-methyl-pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;

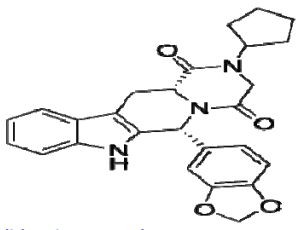


Click on image to enlarge

Catalogue #: A161250
Chemical Name: Acetamino**tadalafil**
CAS Number: 1446144-71-3
Mol. Formula: C23H20N4O5
Synonyms: N-[(6R,12aR)-6-(1,3-Benzodioxol-5-yl)-3,4,6,7,12,12a-hexahydro-1,4-dioxopyrazino[1,2:1,6]pyrido[3,4-b]indol-2(1H)-yl]-acetamide;

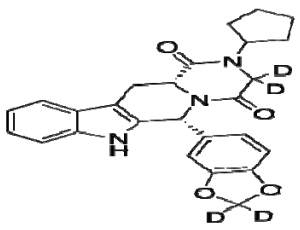
no image of structure available

Catalogue #: D293805
Chemical Name: N-Desmethyl ent-Tadalafil
CAS Number: 929100-66-3
Mol. Formula: C21H17N3O4
Synonyms: (6R,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione



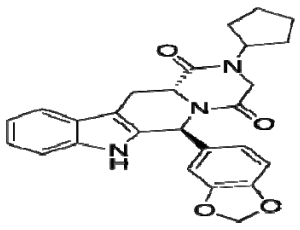
Click on image to enlarge

Catalogue #: B199000
Chemical Name: N-Desmethyl-N-cyclopentyl Tadalafil
CAS Number: 171596-32-0
Mol. Formula: C26H25N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2-cyclopentyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R-trans)-6-(1,3-Benzodioxol-5-yl)-2-cyclopentyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione



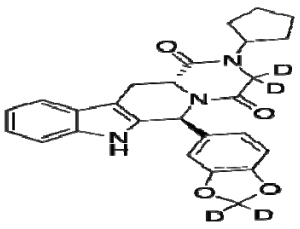
Click on image to enlarge

Catalogue #: B199002
Chemical Name: N-Desmethyl-N-cyclopentyl Tadalafil-D4
CAS Number:
Mol. Formula: C26H21D4N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2-cyclopentyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione-D4; (6R-trans)-6-(1,3-Benzodioxol-5-yl)-2-cyclopentyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione-D4



Click on image to enlarge

Catalogue #: B199005
Chemical Name: N-Desmethyl-N-cyclopentyl cis-ent-Tadalafil
CAS Number:
Mol. Formula: C26H25N3O4
Synonyms:



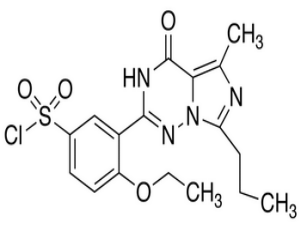
Click on image to enlarge

Catalogue #: B199007
Chemical Name: N-Desmethyl-N-cyclopentyl cis-ent-Tadalafil-D4
CAS Number:
Mol. Formula: C26H21D4N3O4
Synonyms:

Vardenafil Related Compounds (commercial standards available) – includes deuterated standards.

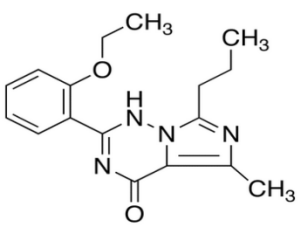
no image of structure available

Chemical Name: 2-Ethoxybenzamidine Hydrochloride
CAS Number: 18637-00-8
Mol. Formula: C9H13ClN2O
Synonyms: 2-Ethoxybenzenecarboximidamide Hydrochloride; o-Ethoxybenzamidine Monohydrochloride; 2-Ethoxybenzenecarboximidamide Monohydrochloride



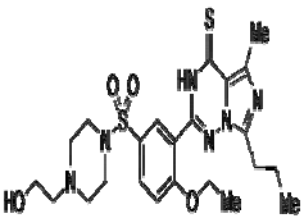
Click on image to enlarge

Catalogue #: E892500
Chemical Name: 4-Ethoxy-3-(5-methyl-4-oxo-7-propyl-3,4-dihydro-imidazo[5,1-f][1,2,4]-triazin-2-yl)benzene-sulfonyl Chloride
CAS Number: 224789-26-8
Mol. Formula: C17H19ClN4O4S
Synonyms: 3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxy-benzenesulfonyl Chloride;



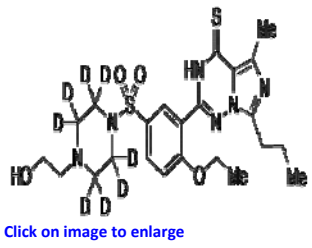
Click on image to enlarge

Catalogue #: E892745
Chemical Name: 2-(2-Ethoxyphenyl)-5-methyl-7-propyl-3H-imidazo[5,1-f][1,2,4]triazin-4-one
CAS Number: 224789-21-3
Mol. Formula: C17H20N4O2
Synonyms: 2-(2-Ethoxyphenyl)-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one;



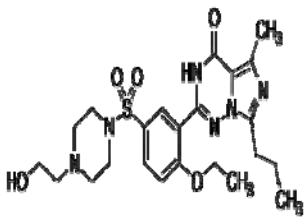
Click on image to enlarge

Catalogue #: H963400
Chemical Name: Hydroxythio**vardenafil**
CAS Number: 912576-30-8
Mol. Formula: C23H32N6O4S2
Synonyms: 2-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazine-4(1H)-thione; 4-[[3-(1,4-Dihydro-5-methyl-7-propyl-4-thioxoimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazineethanol;



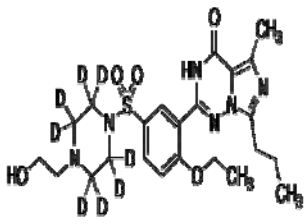
Click on image to enlarge

Catalogue #: H963402
Chemical Name: Hydroxythio**vardenafil**-d8
CAS Number:
Mol. Formula: C23H24D8N6O4S2
Synonyms: 2-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazine-4(1H)-thione-d8; 4-[[3-(1,4-Dihydro-5-methyl-7-propyl-4-thioxoimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazineethanol-d8;



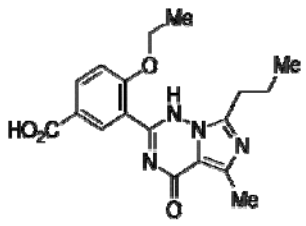
Click on image to enlarge

Catalogue #: H995300
Chemical Name: Hydroxy Vardenafil
CAS Number: 224785-98-2
Mol. Formula: C23H32N6O5S
Synonyms: 2-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazin-4(1H)-one; 4-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo [5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazineethanol;



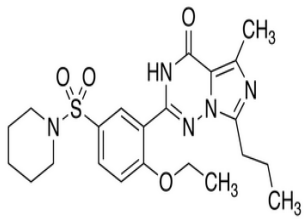
Click on image to enlarge

Catalogue #: H995302
Chemical Name: Hydroxy Vardenafil-d8
CAS Number:
Mol. Formula: C23H24D8N6O5S
Synonyms: 2-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-(piperazinyl-d8)]sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazin-4(1H)-one; 4-[[3-(1,4-Dihydro-5-methyl-4-oxo-7- propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-1-(piperazine-d8)ethanol;



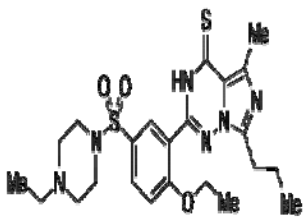
Click on image to enlarge

Chemical Name: Norneo Vardenafil
CAS Number: 358390-39-3
Mol. Formula: C18H20N4O4
Synonyms: 3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxybenzoic Acid;



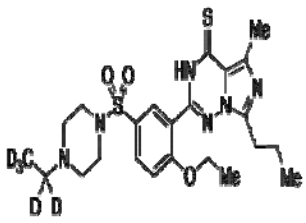
Click on image to enlarge

Catalogue #: P839615
Chemical Name: Pseudo Vardenafil
CAS Number: 224788-34-5
Mol. Formula: C22H29N5O4S
Synonyms: 2-[2-Ethoxy-5-(1-piperidinylsulfonyl)phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazin-4(1H)-one; Piperidenafil; Pseudo**vardenafil**;



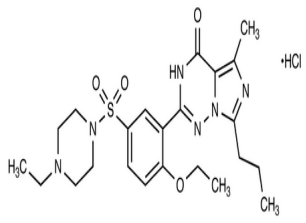
Click on image to enlarge

Catalogue #: T384250
Chemical Name: Thio**vardenafil**
CAS Number: 912576-24-0
Mol. Formula: C23H32N6O3S2
Synonyms: 2-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazine-4(1H)-thione; 1-[[3-(1,4-Dihydro-5-methyl-7-propyl-4-thioxoimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-4-ethylpiperazine;



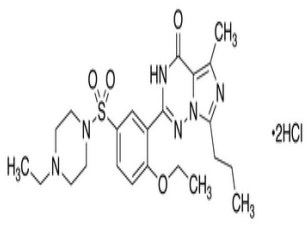
Click on image to enlarge

Catalogue #: T384252
Chemical Name: Thio**vardenafil**-d5
CAS Number:
Mol. Formula: C23H27D5N6O3S2
Synonyms: 2-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazine-4(1H)-thione-d5; 1-[[3-(1,4-Dihydro-5-methyl-7-propyl-4-thioxoimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-4-ethylpiperazine-d5;



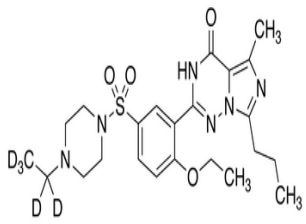
Click on image to enlarge

Catalogue #: V098000
Chemical Name: Vardenafil, Hydrochloride Salt Discontinued See V098001
CAS Number: 224785-91-5
Mol. Formula: C23H33ClN6O4S
Synonyms: Levitra, Valdenafil



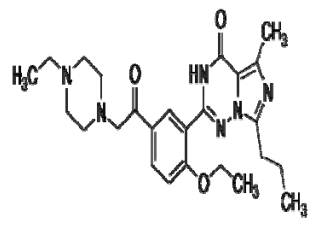
Click on image to enlarge

Catalogue #: V098001
Chemical Name: Vardenafil Dihydrochloride Salt
CAS Number: 224789-15-5
Mol. Formula: C23H34Cl2N6O4S
Synonyms: 1-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-4-ethyl-piperazine;Levitra; Nuviva;



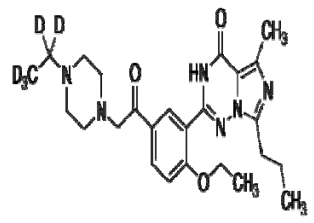
Click on image to enlarge

Catalogue #: V098002
Chemical Name: Vardenafil-d5
CAS Number: 1189685-70-8
Mol. Formula: C23H27D5N6O4S
Synonyms: 1-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-4-(ethyl-d5)-piperazine; Levitra-d5; Nuviva-d5;



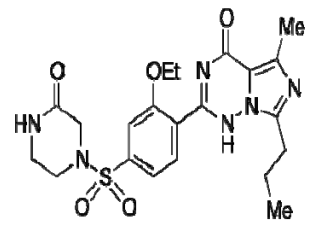
Click on image to enlarge

Catalogue #: V098015
Chemical Name: Vardenafil Acetyl Analogue
CAS Number: 1261351-28-3
Mol. Formula: C25H34N6O3
Synonyms: 2-[2-Ethoxy-5-[2-(4-ethyl-1-piperazinyl)acetyl]phenyl]-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one;



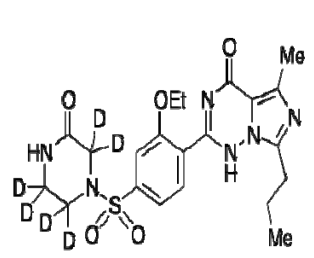
Click on image to enlarge

Catalogue #: V098017
Chemical Name: Vardenafil Acetyl-d5 Analogue
CAS Number: 1330171-51-1
Mol. Formula: C25H29D5N6O3
Synonyms: 2-[2-Ethoxy-5-[2-(4-(ethyl-d5)-1-piperazinyl)acetyl]phenyl]-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one;



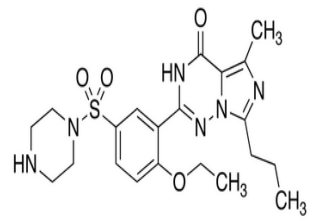
Click on image to enlarge

Catalogue #: V098030
Chemical Name: Vardenafil Oxopiperazine (Impurity)
CAS Number: 448184-58-5
Mol. Formula: C21H26N6O5S
Synonyms: 2-[2-Ethoxy-5-[(3-oxo-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one; 4-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-piperazinone



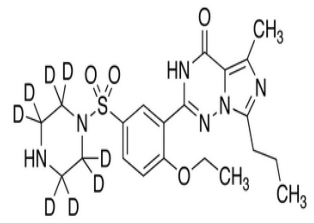
Click on image to enlarge

Catalogue #: V098032
Chemical Name: Vardenafil Oxopiperazine-D6 (Impurity)
CAS Number:
Mol. Formula: C21H20D6N6O5S
Synonyms: 2-[2-Ethoxy-5-[(3-oxo-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one-D6; 4-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-piperazinone-D6



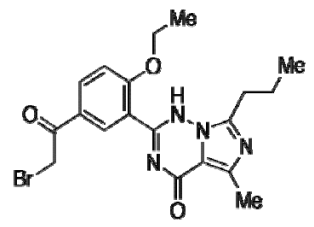
Click on image to enlarge

Catalogue #: D289950
Chemical Name: N-Desethyl Vardenafil
CAS Number: 448184-46-1
Mol. Formula: C21H28N6O4S
Synonyms: 1-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-piperazine;



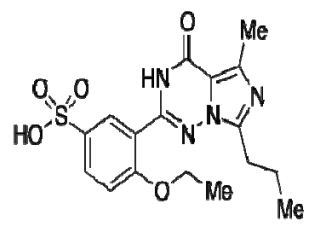
Click on image to enlarge

Catalogue #: D289952
Chemical Name: N-Desethyl Vardenafil-d8
CAS Number:
Mol. Formula: C21H20D8N6O4S
Synonyms: 1-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-piperazine-d8;



Click on image to enlarge

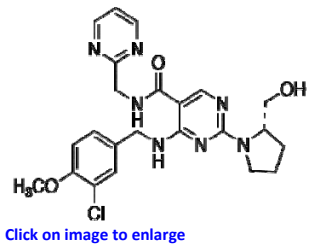
Catalogue #: D220200
Chemical Name: 1-Decarboxyl-1-(bromoacetyl) Norneo**vardenafil**
CAS Number: 358388-58-6
Mol. Formula: C19H21BrN4O3
Synonyms: 2-[5-(Bromoacetyl)-2-ethoxyphenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazin-4(1H)-one;



Click on image to enlarge

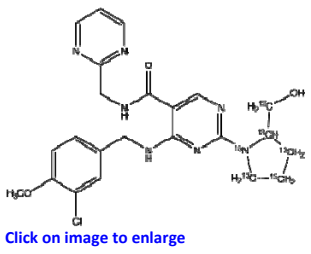
Catalogue #: D453410
Chemical Name: 3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxybenzenesulfonic Acid
CAS Number: 437717-43-6
Mol. Formula: C17H20N4O5S
Synonyms:

Avanafil Related Compounds (commercial standards available) – includes deuterated standards.



Click on image to enlarge

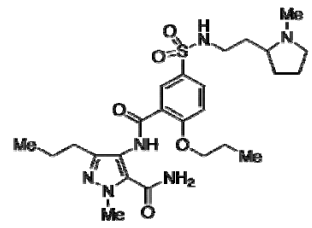
Catalogue #: A794670
Chemical Name: Avanafil
CAS Number: 330784-47-9
Mol. Formula: C23H26ClN7O3
Synonyms: (S)-2-(2-Hydroxymethyl-1-pyrrolidinyl)-4-(3-chloro-4-methoxybenzylamino)-5-[(2-pyrimidinylmethyl)carbamoyl]pyrimidine; 4-[[(3-Chloro-4-methoxyphenyl)methyl] amino]-2-[(2S)-2-(hydroxymethyl)-1-pyrrolidinyl]-N-(2-pyrimidinylmethyl)-5-pyrimidinecarboxamide; TA 1790;



Click on image to enlarge

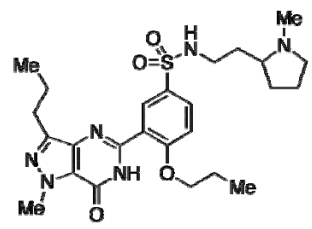
Catalogue #: A794672
Chemical Name: Avanafil-13C5,15N
CAS Number:
Mol. Formula: C1813C5H26ClN615NO3
Synonyms: (S)-2-(2-Hydroxymethyl-1-pyrrolidinyl)-4-(3-chloro-4-methoxybenzylamino)-5-[(2-pyrimidinylmethyl)carbamoyl]pyrimidine-13C5,15N; 4-[[(3-Chloro-4-methoxyphenyl)methyl] amino]-2-[(2S)-2-(hydroxymethyl)-1-pyrrolidinyl]-N-(2-pyrimidinylmethyl)-5-pyrimidinecarboxamide-13C5,15N; TA 1790-13C5,15N;

Udenafil Related Compounds (commercial standards available) – includes deuterated standards.



Click on image to enlarge

Catalogue #: M320180
Chemical Name: 1-Methyl-4-[[5-[[[2-(1-methyl-2-pyrrolidinyl)ethyl]amino]sulfonyl]-2-propoxybenzoyl]amino]-3-propyl-1H-pyrazole-5-carboxamide
CAS Number: 382592-28-1
Mol. Formula: C25H38N6O5S
Synonyms:



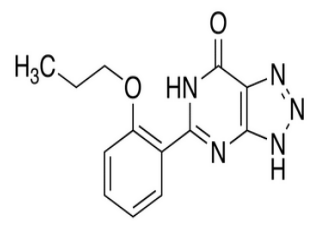
Click on image to enlarge

Catalogue #: U250500
Chemical Name: Udenafil
CAS Number: 268203-93-6
Mol. Formula: C25H36N6O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-N-[2-(1-methyl-2-pyrrolidinyl)ethyl]-4-propoxybenzenesulfonamide; DA 8159; Zydena;

no image of structure available

Catalogue #: U250502
Chemical Name: Udenafil-d7
CAS Number: 1175992-76-3
Mol. Formula: C25H29D7N6O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-N-[2-(1-methyl-2-pyrrolidinyl)ethyl]-4-(propoxy-d7)benzenesulfonamide; DA 8159-d7; Zydena-d7;

Zaprinast

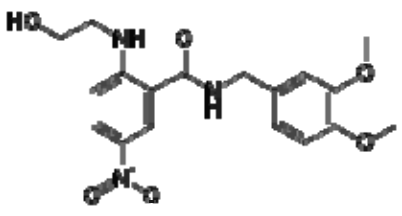


Click on image to enlarge

Catalogue #: Z150000
Chemical Name: Zaprinast
CAS Number: 37762-06-4
Mol. Formula: C13H13N5O2
Synonyms: 3,6-dihydro-5-(2-propoxyphenyl)-7H-1,2,3-triazolo[4,5-d]pyrimidin-7-one; 1,4-Dihydro-5-[2-propoxyphenyl]-7H-1,2,3-triazolo[4,5-d]pyrimidine-7-one; 8-Aza-2-(2-propoxyphenyl)-6-purinone; M&B 22,948;

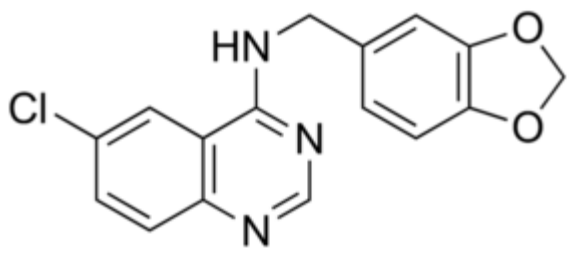
4. Additional Items for Consideration Web Based Search Data

Benzamidenafil
IUPAC name: N-[(3,4-Dimethoxyphenyl)methyl]-2-(1-hydroxypropan-2-ylamino)-5-nitrobenzamide
Other names: Xanthoanthrafil
CAS number: 1020251-53-

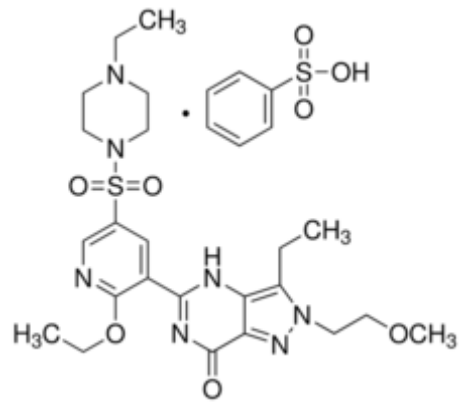


5. Additional Items for Consideration Novel PDE-5 inhibitors from SIAL

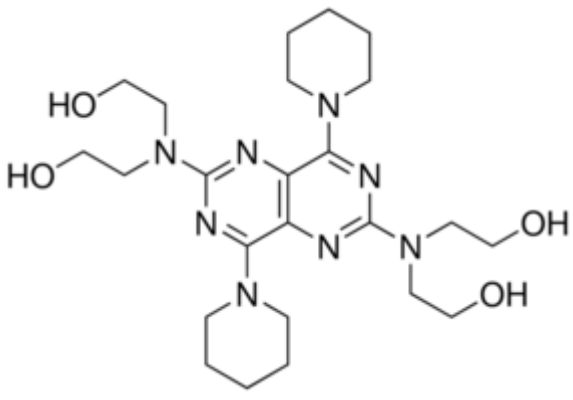
MBCQ
SML0439 SIGMA
≥98% (HPLC)
Synonym: 4-((3,4-Methylenedioxybenzyl)amino)-6-chloroquinazoline
CAS Number 150450-53-6
Empirical Formula (Hill Notation) $C_{16}H_{12}ClN_3O_2$
Molecular Weight 313.74
MDL number MFCD00673946



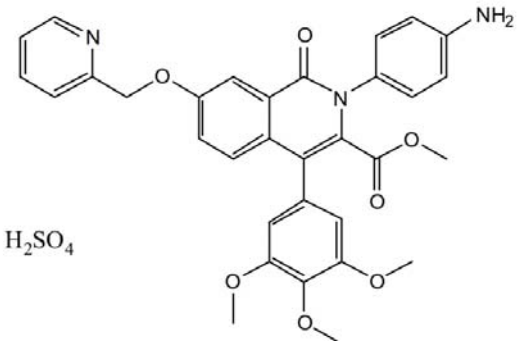
Gisadenafil besylate salt
≥98% (HPLC)
PZ0172 SIGMA
Synonym: 5-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]-3-pyridinyl]-3-ethyl-2,6-dihydro-2-(2-methoxyethyl)-7H-pyrazolo[4,3-d]pyrimidin-7-one benzenesulfonate besylate salt, UK 369003-26, UK 369003
CAS Number 334827-98-4
Empirical Formula (Hill Notation) $C_{23}H_{33}N_7O_5S \cdot C_6H_6O_3S$
Molecular Weight 677.79
MDL number MFCD18384964



Dipyridamole
≥98% (TLC), powder
D9766 SIGMA
CAS Number 58-32-2
Empirical Formula (Hill Notation) $C_{24}H_{40}N_8O_4$
Molecular Weight 504.63
EC Number 200-374-7
MDL number MFCD00010555
PubChem Substance ID 24277705
No Longer Offered by SIAL but published and possibly produced in Japan



Product Number T7692
Cas #: 212500-03-3
Synonyms: Methyl-(2-(4-aminophenyl)-1,2-dihydro-1-oxo-7-(2-pyridinylmethoxy)-4-(3,4,5-trimethoxyphenyl))-3-isoquinoline carboxylic acid, sulfate salt
Molecular Formula: C32H29N3O7·H2SO4



The isoquinolone derivative, T-1032, is a potent, selective inhibitor of cyclic GMP-specific phosphodiesterase (PDE5). In studies of PDE isoenzymes isolated from canine tissues, T-1032 was a competitive inhibitor of cyclic GMP hydrolysis by PDE5 at nanomolar concentrations (IC50 1.0 nM, Ki = 1.2 nM).

6. Additional Information

There are a significant number of lead compounds being researched which depart from the classic sildenafil pyrazolopyrimidinone template. These compounds number into the thousands and are likely to appear in greater number over time as research publications and patent literature show more detail on particular structures and their synthesis.

AOAC SMPR 2012.008

Standard Method Performance Requirements for Iodine in Infant Formula and Adult/Pediatric Nutritional Formula

Intended Use: Global dispute resolution method

1 Applicability

Determination of total iodine in all forms of infant, adult, and/or pediatric formula (powders, ready-to-feed liquids, and liquid concentrates).

2 Analytical Technique

Any analytical technique that meets the following method performance requirements is acceptable.

3 Definitions

Adult/pediatric formula.—Nutritionally complete, specially formulated food, consumed in liquid form, which may constitute the sole source of nourishment [AOAC Stakeholder Panel on Infant Formula and Adult Nutritionals (SPIFAN); 2010], made from any combination of milk, soy, rice, whey, hydrolyzed protein, starch, and amino acids, with and without intact protein.

Infant formula.—Breast-milk substitute specially manufactured to satisfy, by itself, the nutritional requirements of infants during the first months of life up to the introduction of appropriate complementary feeding (Codex Standard 72–1981), made from any combination of milk, soy, rice, whey, hydrolyzed protein, starch, and amino acids, with and without intact protein.

Limit of detection (LOD).—The minimum concentration or mass of analyte that can be detected in a given matrix with no greater than 5% false-positive risk and 5% false-negative risk.

Iodine.—CAS No. 7553-56-2.

Limit of quantitation (LOQ).—The minimum concentration or mass of analyte in a given matrix that can be reported as a quantitative result.

Reproducibility.—The standard deviation or relative standard deviation calculated from among-laboratory data. Expressed as the reproducibility standard deviation (SD_R); or % reproducibility relative standard deviation (%RSD_R).

Repeatability.—Variation arising when all efforts are made to keep conditions constant by using the same instrument and operator, and repeating during a short time period. Expressed as the repeatability standard deviation (SD_r); or % repeatability relative standard deviation (%RSD_r).

Recovery.—The fraction or percentage of spiked analyte that is recovered when the test sample is analyzed using the entire method.

Table 1. Method performance requirements[a]

Analytical range	5–1000[b]	
Limit of quantitation (LOQ)	≤5[b]	
Repeatability (RSD_r)	5–1000[b]	≤8%
Recovery	90 to 110% of mean spiked recovery over the range of the assay	
Reproducibility (RSD_R)	5–1000[b]	≤15%

[a] Concentrations apply to: (*1*) "ready-to-feed" liquids "as is"; (*2*) reconstituted powders (25 g into 200 g water); and (*3*) liquid concentrates diluted 1:1 by weight.

[b] mcg/100 g reconstituted final product.

5 System Suitability Tests and/or Analytical Quality Control

Suitable methods will include blank check samples, and check standards at the lowest point and midrange point of the analytical range.

6 Reference Material(s)

NIST Standard Reference Material® (SRM) 1849a Infant/Adult Nutritional Formula, or equivalent. The SRM is a milk-based, hybrid infant/adult nutritional powder prepared by a manufacturer of infant formula and adult nutritional products. A unit of SRM 1849a consists of 10 packets, each containing approximately 10 g of material. Certified value of NIST SRM 1849a is 1.29 ± 0.11 mg/kg as iodine.

7 Validation Guidance

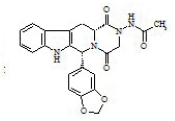
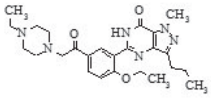
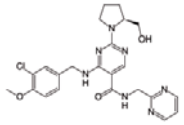
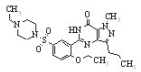
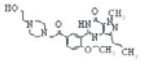
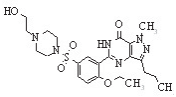
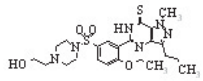
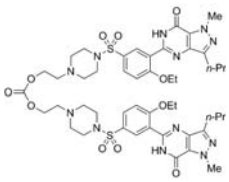
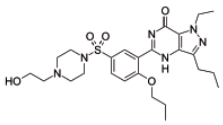
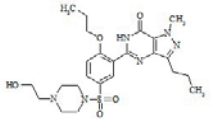
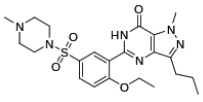
Recommended level of validation: *Official Methods of Analysis*℠.

8 Maximum Time-to-Result

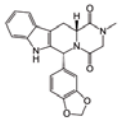
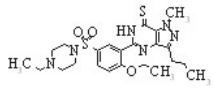
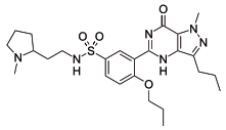
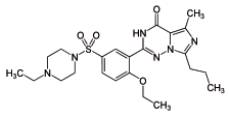
Time to determine must be 12 h or less.

Approved by the AOAC Stakeholder Panel on Infant Formula and Adult Nutritionals (SPIFAN) on September 29, 2012. Final Version Date: September 29, 2012.

ANNEX I
Target Compound Panel

Analyte	CAS No.	Formula	Structure
Acetaminotadalafil	1446144-71-3	$C_{23}H_{20}N_4O_5$	
Acetildenafil	831217-01-7	$C_{25}H_{34}N_6O_3$	
Avanafil (sold under the brand names *Stendra* and *Spedra*)	330784-47-9	$C_{23}H_{26}ClN_7O_3$	
Homosildenafil	642928-07-2	$C_{23}H_{32}N_6O_4S$	
Hydroxyacetildenafil	147676-56-0	$C_{25}H_{34}N_6O_4$	
Hydroxyhomosildenafil	139755-85-4	$C_{23}H_{32}N_6O_5S$	
Hydroxythiohomosildenafil	479073-82-0	$C_{23}H_{32}N_6O_4S_2$	
Lodenafil carbonate (sold under the brand name *Helleva* in Brazil)	398507-55-6	$C_{43}H_{54}N_{12}O_9S_2$	
Mirodenafil (sold under the trade name of *Mvix*.)	862189-95-5	$C_{26}H_{37}N_5O_5S$	
Propoxyphenyl hydroxyhomosildenafil	139755-87-6	$C_{24}H_{34}N_6O_5S$	
Sildenafil (sold under the brand names *Viagra* and *Revatio*, and other various brand names)	139755-83-2	$C_{22}H_{30}N_6O_4S$	

ANNEX I
Target Compound Panel (*continued*)

Analyte	CAS No.	Formula	Structure
Tadalafil (sold under the brand names *Cialis* and *Adcirca*)	171596-29-5	$C_{22}H_{19}N_3O_4$	
Thiohomosildenafil	479073-80-8	$C_{23}H_{32}N_6O_3S_2$	
Udenafil (sold under the brand name *Zydena*)	268203-93-6	$C_{25}H_{36}N_6O_4S$	
Vardenafil (sold under the brand names *Levitra*, *Staxyn*, and *Vivanza*)	224785-90-4	$C_{23}H_{32}N_6O_4S$	

ANNEX II
Matrixes

Tablets
Capsules (both the content and the capsule shells)
Softgels
Gelcaps
Liquids
Powders
Extracts

ANNEX III
Controls

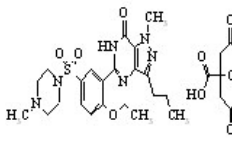
Control	Description	Implementation	Acceptance criteria
Positive	Designed to demonstrate an appropriate test response. This positive control should be included at a low but easily detectable concentration, and should monitor the performance of the entire assay. The purpose of using a low concentration of positive control is to avoid contamination of the test sample and/or instrument.	Single use per sample (or sample set) run	Success: Control detected at expected levels Failure: Control not detected or at levels below expected
Negative	Designed to demonstrate that the assay itself does not produce a positive detection in the absence of target compounds. The purpose of this control is to rule out contamination in the assay or test.	Single use per sample (or sample set) run	Success: No detections made Failure: Detections made
Interference	Designed to specifically address the impact of a sample or sample matrix on the assay's ability to detect target compounds	Single use per sample run	Success: Control detected at expected levels Failure: Control not detected or at levels below expected

Supplemental List of Known PDE5 Inhibitors (as of July 2014)

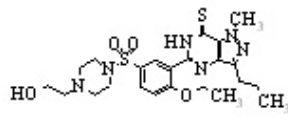
1. **Standards available from Cachesyn http://www.cachesyn.com/ which include the majority of characterized PDE-5i analogues and all of the parent drugs including catalog numbers. (Some structure images not available)**

Sildenafil Related Compounds (commercial standards available) – includes deuterated standards.

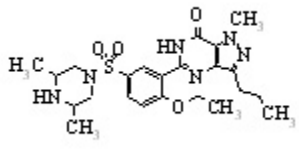
Sildenafil citrate
CAS No. 171599-83-0
C22H30N6O4S.C6H8O7 M.W. 474.59 192.13
CSTS061



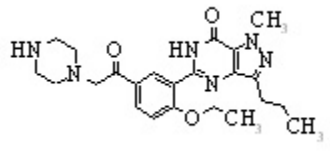
Hydroxythiohomosildenafil
C23H32N6O4S2 M.W. 520.68
CSTS0611



Dimethyl Sildenafil
C23H32N6O4S M.W. 488.61
CSTS0612



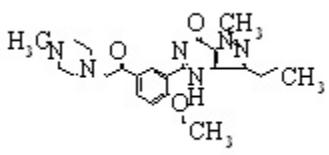
N-Desmethyl Acetildenafil
C23H30N6O3 M.W. 438.53
CSTS0613



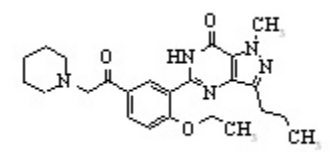
Hydroxyacetildenafil
C25H34N6O4 M.W. 482.59
CSTS0614

Nor-acetildenafil
CAS No. 949091-37-7
C24H32N6O3 M.W. 452.56
CSTS0615

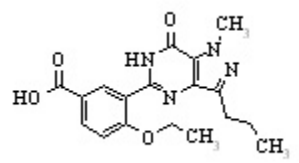
Nor-acetildenafil
CAS No. 949091-37-7
C24H32N6O3 M.W. 452.56
CSTS0615



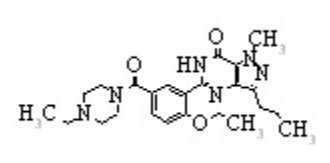
Piperiacetildenafil
C24H31N5O3 M.W. 437.55
CSTS0616



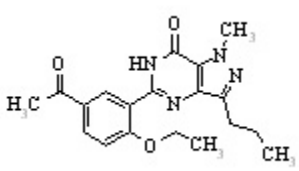
Acetil Acid
C18H20N4O4 M.W. 356.38
CSTS0617



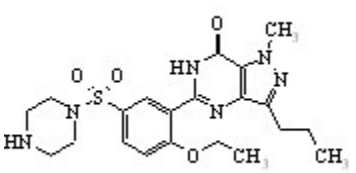
Carbodenafil
C24H32N6O3 M.W. 452.56
CSTS0618



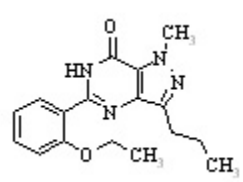
Gendenafil
C19H22N4O3 M.W. 354.41
CSTS0619



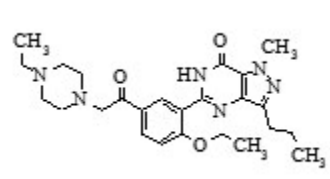
N-Desmethyl Sildenafil
CAS No. 139755-82-1
C21H38N6O4S M.W. 460.56
CSTS062



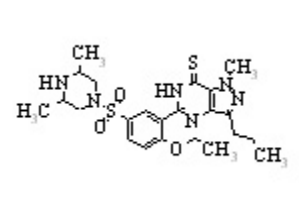
Imidazosagatriazinone
C17H20N4O2 M.W. 312.37
CSTS0620



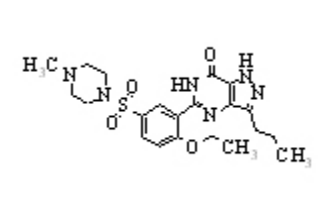
Acetildenafil (Hongdenafil)
C25H34N6O3 M.W. 466.59
CSTS0621



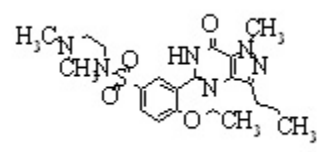
Thiodimethyl Sildenafil (Dimethylthiosildenafil)
C23H32N6O3S2 M.W. 504.68
CSTS0622



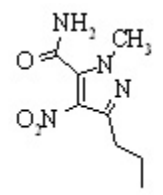
Pyrazole N-desmethyl sildenafil
C21H28N6O4S M.W. 460.56
CSTS0623



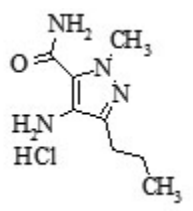
PDE-5 Inhibitor (Sildenafil Related Compound)
C21H30N6O M.W. 462.5
CSTS0624



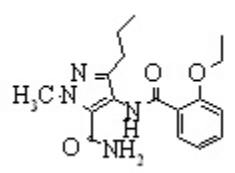
Sildenafil amide
C8H12N4O3 M.W. 212.21
CSTS0625



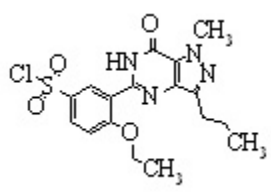
Sildenafil Amine HCl
C8H14N4O.HCl M.W. 182.23 36.46
CSTS0626



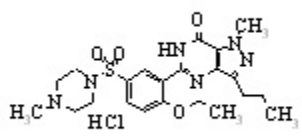
Sildenafil coupled
C17H22N4O3 M.W. 330.39
CSTS0627



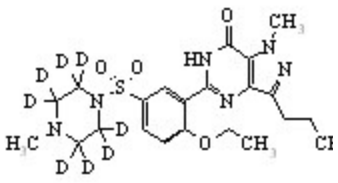
Sildenafil chlorosulfonyl
C17H19ClN4O4S M.W. 410.88
CSTS0628



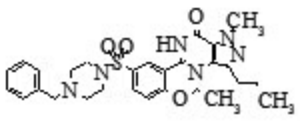
Sildenafil HCl
C22H30N6O4S.HCl M.W. 474.59 36.46
CSTS0629



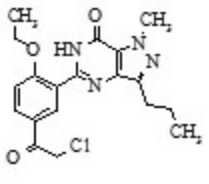
Sildenafil-d8
CAS No. 171599-83-0(non-d)
C22H22D8N6O4S M.W. 482.63
CSTS063



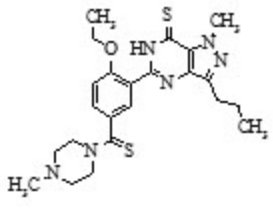
Benzyl Sildenafil
C28H34N6O4S M.W. 550.68
CSTS0631



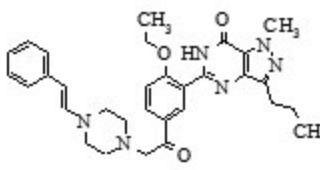
Chlorodenafil
CAS No. N/A
C19H21ClN4O3 M.W. 388.86
CSTS0633



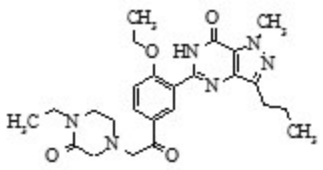
Dithio-desmethyl-carbodenafil
CAS No. N/A
C23H30N6OS2 M.W. 470.66
CSTS0635



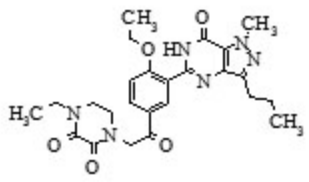
Cinnamyldenafil
CAS No. N/A
C31H36N6O3 M.W. 540.67
CSTS0637



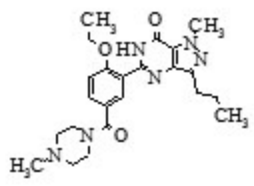
Oxohongdenafil
CAS No. N/A
C25H32N6O4 M.W. 480.57
CSTS0639



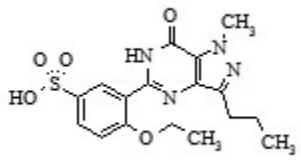
Dioxohongdenafil
CAS No. N/A
C25H30N6O5 M.W. 494.56
CSTS0640



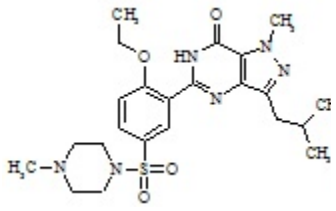
Desmethyl Carbodenafil
C23H30N6O3 M.W. 438.53
CSTS0642



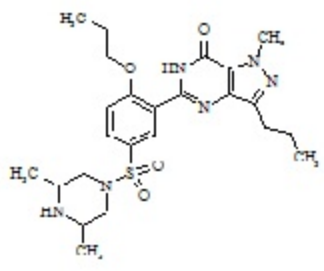
Demethylpiperazinyl Sildenafil Sulfonic Acid
C17H20N4O5S M.W. 392.44
CSTS0644



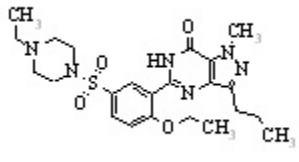
Sildenafil Impurity A (Isobutyl Sildenafil)
CAS No. N/A
C23H32N6O4S M.W. 488.61
CSTS0646



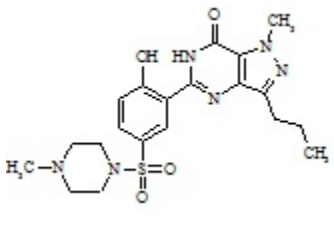
Propoxyphenyl Sildenafil
CAS No. 877777-10-1
C23H32N6O4S M.W. 488.61
CSTS0648



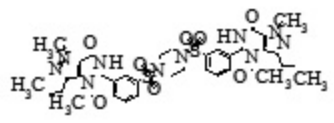
Homosildenafil
C23H32N6O4S M.W. 488.61
CSTS065



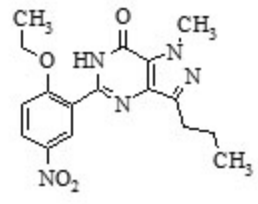
O-Desethyl Sildenafil (Sildenafil Impurity C)
CAS No. N/A
C20H26N6O4S M.W. 446.53
CSTS0651



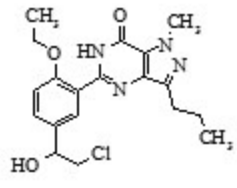
Sildenafil Dimer Impurity
C38H46N10O8S2 M.W. 834.98
CSTS0630



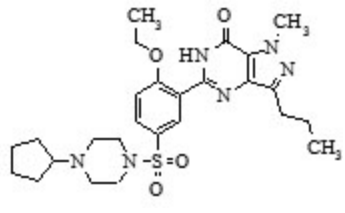
Nitrodenafil
CAS No. N/A
C17H19N5O4 M.W. 357.37
CSTS0632



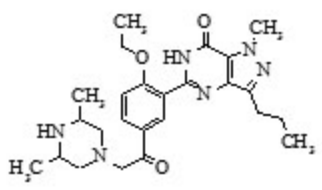
Hydroxychlorodenafil
CAS No. N/A
C19H23ClN4O3 M.W. 390.87
CSTS0634



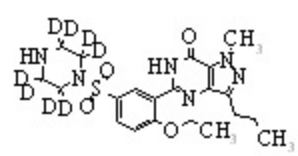
Cyclopentynafil
CAS No. N/A
C26H36N6O4S M.W. 528.68
CSTS0636



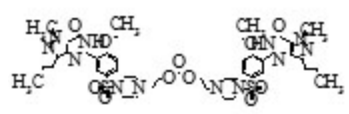
Dimethylacetildenafil
CAS No. N/A
C25H34N6O3 M.W. 466.59
CSTS0638



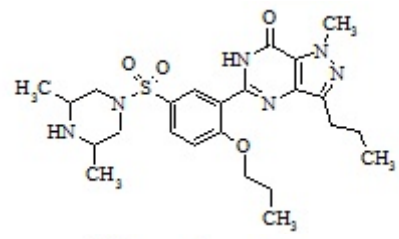
N-Desmethyl sildenafil-d8
CAS No. 139755-82-1 (non-d)
C21H20N6O4SD8 M.W. 468.61
CSTS064



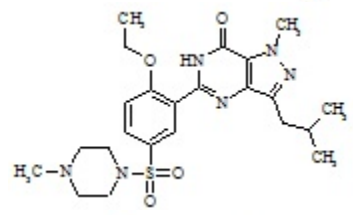
Lodenafilcarbonate
CAS No. N/A
C47H62N12O11S2 M.W. 1035.22
CSTS0641



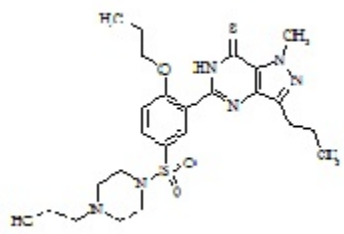
Sildenafil analogue
C24H34N6O4S M.W. 502.64
CSTS0643



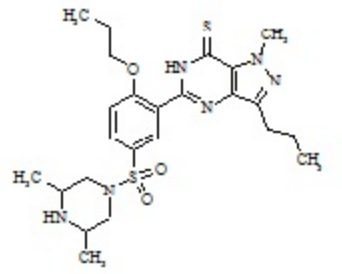
Nitroso-prodenafil
CAS No. N/A
C27H35N9O5S2 M.W. 629.77
CSTS0645



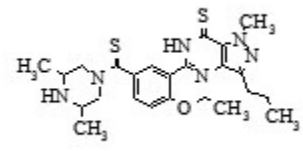
Sildenafil Analogue I
CAS No. N/A
C24H34N6O4S2 M.W. 534.70
CSTS0647



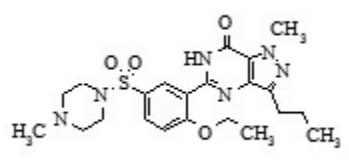
Sildenafil Analogue III
CAS No. N/A
C24H34N6O3S2 M.W. 518.70
CSTS0649



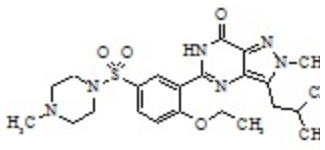
Sildenafil Related Compound
C24H32N6OS2 M.W. 484.69
CSTS0650



Sildenafil
C22H30N6O4S M.W. 474.59
CSTS0652



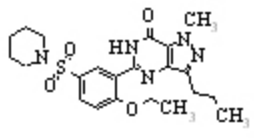
Sildenafil Impurity A Related Compound (Isomer of Isobutyl Sildenafil)
C23H32N6O4S M.W. 488.61
CSTS0653



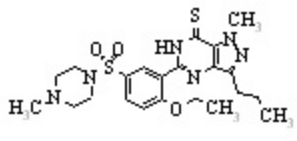
Sildenafil N-Oxide
C22H30N6O5S M.W. 490.59
CSTS0655

no image of structure available

Norneosildenafil
C22H29N5O4S M.W. 459.57
CSTS066



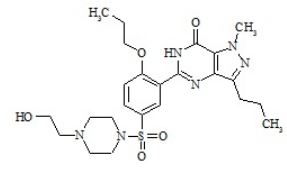
Thiosildenafil
C22H30N6O3S2 M.W. 490.65
CSTS068



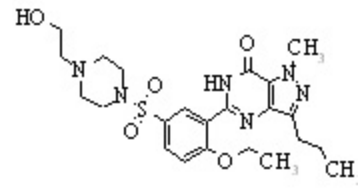
Sildenafil Impurity ((1-methyl-4-Nitro -3-n-propyl pyrazole-5- carboxylic acid)
C8H11N3O4 M.W. 213.19
CSTS0654

no image of structure available

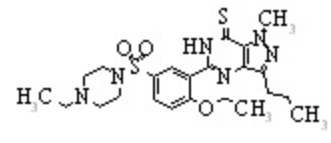
Propoxyphenyl-Hydroxyhomosildenafil
CAS No. N/A
C24H34N6O5S M.W. 518.64
CSTS0656



Hydroxyhomosildenafil
C23H32N6O5S M.W. 504.61
CSTS067

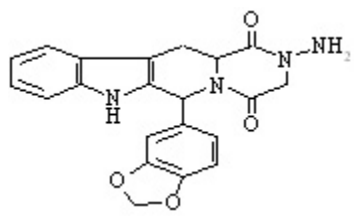


Thiohomosildenafil
C23H32N6O3S2 M.W. 504.68
CSTS069

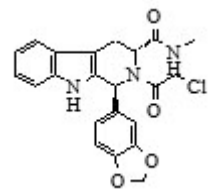


Tadalafil Related Compounds (commercial standards available) – includes deuterated standards.

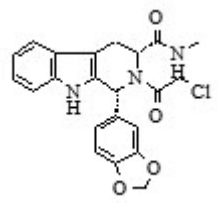
Aminotadalafil
C21H18N4O4 M.W. 390.40
CSTT101



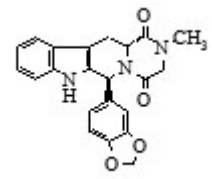
Tadalafil Impurity C
CAS No. NA
C22H20ClN3O4 M.W. 425.88
CSTT1010



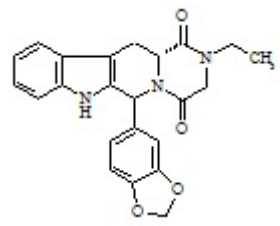
Tadalafil Impurity D
CAS No. NA
C22H20ClN3O4 M.W. 425.88
CSTT1011



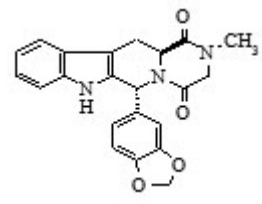
Tadalafil Impurity E
C22H19N3O4 M.W. 389.41
CSTT1012



N-Ethyl Tadalafil
CAS No. N/A
C23H21N3O4 M.W. 403.44
CSTT1013



6R,12S-Tadalafil
C22H19N3O4 M.W. 389.41
CSTT1014



Tadalafil Hydroxylactam Impurity
C22H19N3O6 M.W. 421.41
CSTT1015

no image of structure available

Tadalafil Aminohemiketal Impurity
C22H19N3O6 M.W. 421.41
CSTT1016

no image of structure available

Tadalafil Spiro-urethane Impurity
C21H18N3O6 M.W. 408.39
CSTT1017

no image of structure available

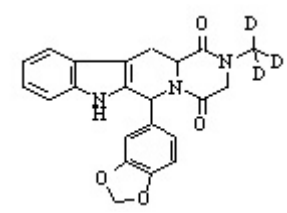
Tadalafil Hydroxyquinoline Impurity
C22H17N3O5 M.W. 403.40
CSTT1018

no image of structure available

Tadalafil Ketolactam Impurity
C22H21N3O6 M.W. 423.43
CSTT1019

no image of structure available

Tadalafil-d3
C22H16N3O4D3 M.W. 392.43
CSTT102



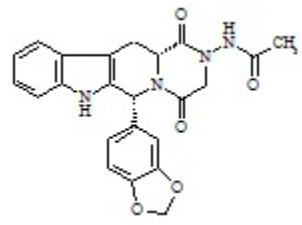
Tadalafil Spiro-oxindole Impurity
C22H19N3O5 M.W. 405.41
CSTT1020

no image of structure available

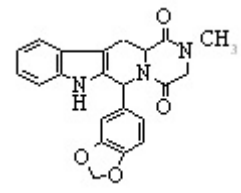
Tadalafil Impurity B (6S,12aS)
C22H19N3O4 M.W. 389.41
CSTT1021

no image of structure available

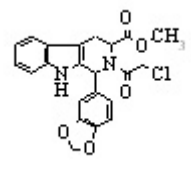
Acetaminotadalafil
CAS No. N/A
C23H20N4O5 M.W. 432.44
CSTT1022



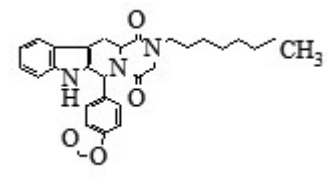
Tadalafil
C22H19N3O4 M.W. 389.41
CSTT103



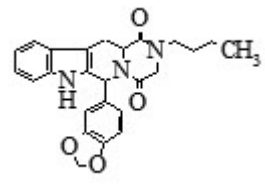
Chloropretadalafil
C22H19ClN2O5 M.W. 426.86
CSTT104



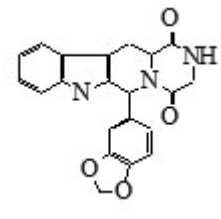
N-Octyl-nortadalafil
C29H33N3O4 M.W. 487.60
CSTT105



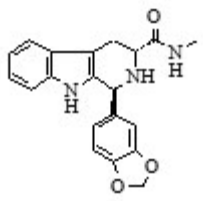
N-Butyl Tadalafil
C25H25N3O4 M.W. 431.50
CSTT106



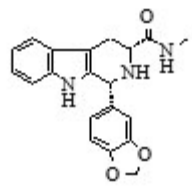
Nortadalafil
C21H17N3O4 M.W. 375.39
CSTT107



Tadalafil Impurity A
CAS No. NA
C20H19N3O3 M.W. 349.39
CSTT108

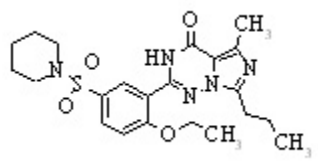


Tadalafil Impurity B
CAS No. NA
C20H19N3O3 M.W. 349.39
CSTT109



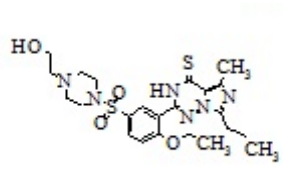
Vardenafil Related Compounds (commercial standards available) – includes deuterated standards.

Pseudovardenafil
C22H29N5O4S
M.W. 459.57
CSTV051

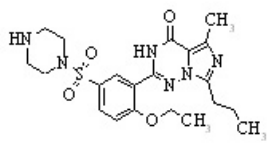


no image of structure available

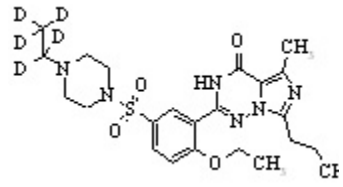
Hydroxythio Vardenafil
C23H32N6O4S2 M.W. 520.68
CSTV0510



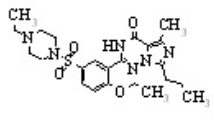
N-Desethyl Vardenafil
C21H28N6O4S M.W. 460.56
CSTV052



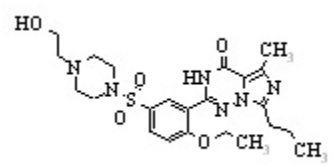
Vardenafil-d5
C23H27N6O4SD5 M.W. 493.64
CSTV053



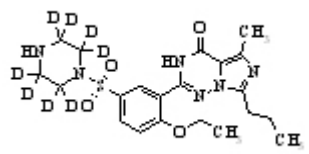
Vardenafil HCl
CAS No. 224785-90-4
C23H32N6O4S M.W. 488.61
CSTV054



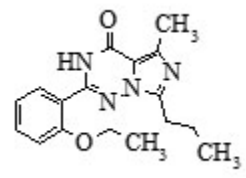
Hydroxy Vardenafil
C23H32N6O5S M.W. 504.61
CSTV055



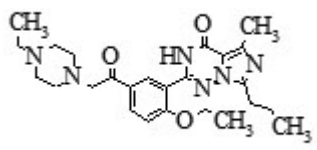
N-Desethyl Vardenafil-d8
CAS No. V-052
C21H28N6O4S M.W. 460.56
CSTV056



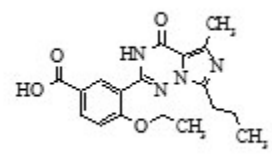
2-(2-Ethoxyphenyl)-5-methyl-7-propyl-3H-imidazo[5,1-f][1,2,4]triazin-4-one
C17H20N4O2 M.W. 312.37
CSTV057



Acetylvardenafil
C25H34N6O3 M.W. 466.59
CSTV058

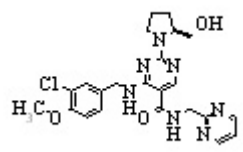


Norneovardenafil
CAS No. N/A
C18H20N4O4 M.W. 356.38
CSTV059

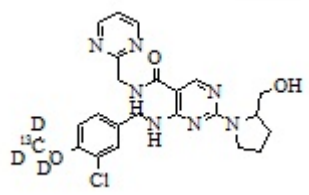


Avanafil Related Compounds (commercial standards available) – includes deuterated standards.

Avanafil
CAS No. 330784-47-9
C23H26ClN7O3 M.W. 483.96
CSTA291

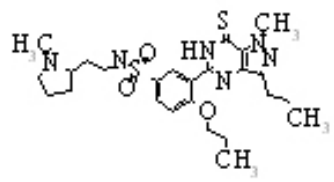


Avanafil-13CD3
C22H23ClN7O313CD3 M.W. 487.97
CSTA292



Udenafil

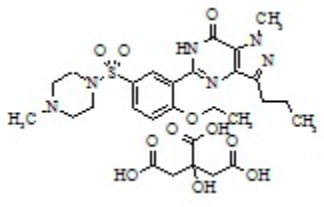
Udenafil
CAS No. 268203-93-6
C25H36N6O4S M.W. 516.67
CSTU031



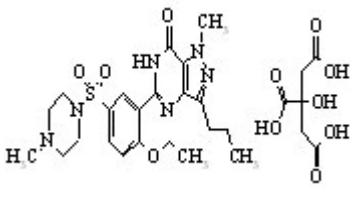
2. **Standards available from TLC Pharmachem http://www.tlcpharmachem.com which include the majority of characterized PDE-5i analogues and all of the parent drugs including catalog numbers. (Some structure images not available)**

Sildenafil Related Compounds (commercial standards available) – includes deuterated standards.

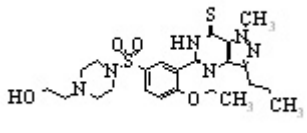
Sildenafil Citrate
CAS No. 171599-83-0
C22H30N6O4S. C6H8O7 M.W. 474.59
192.13
PF-0017



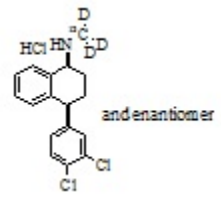
Sildenafil citrate
CAS No. 171599-83-0
C22H30N6O4S.C6H8O7 M.W. 474.59
192.13
S-061



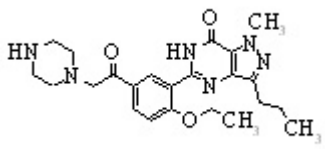
Hydroxythiohomosildenafil
C23H32N6O4S2 M.W. 520.68
S-0611



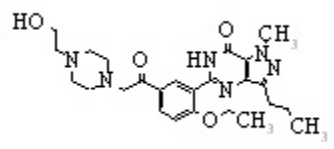
Dimethyl Sildenafil
CAS No. 1416130-63-6
C23H32N6O4S M.W. 488.61
S-0612



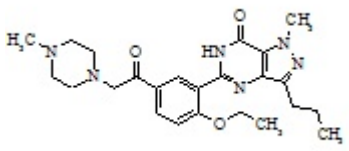
N-Desmethyl Acetildenafil
C23H30N6O3 M.W. 438.53
S-0613



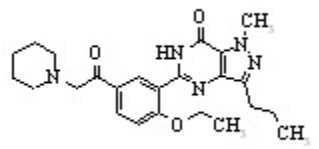
Hydroxyacetildenafil
C25H34N6O4 M.W. 482.59
S-0614



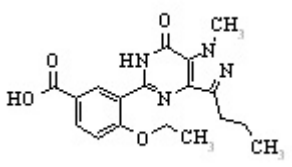
Nor-acetildenafil
CAS No. 949091-38-7
C24H32N6O3 M.W. 452.56
S-0615



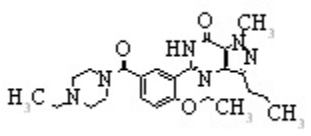
Piperiacetildenafil
C24H31N5O3 M.W. 437.55
S-0616



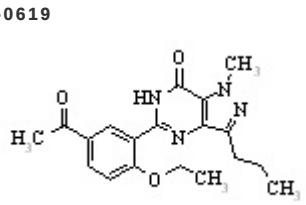
Acetil Acid
C18H20N4O4 M.W. 356.38
S-0617



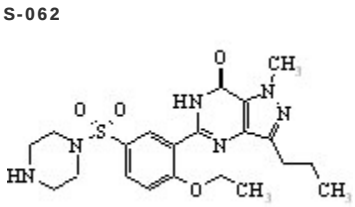
Carbodenafil
C24H32N6O3 M.W. 452.56
S-0618



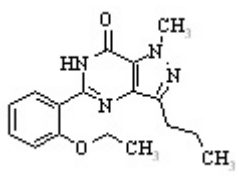
Gendenafil
CAS No. 147676-66-2
C19H22N4O3 M.W. 354.41
S-0619



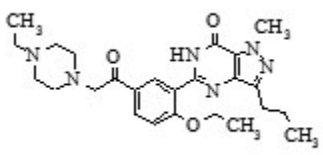
N-Desmethyl Sildenafil
CAS No. 139755-82-1
C21H28N6O4S M.W. 460.56
S-062



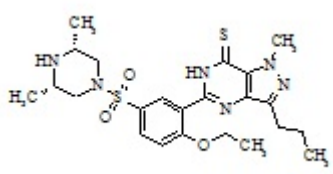
Imidazosagatriazinone
C17H20N4O2 M.W. 312.37
S-0620



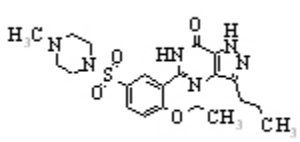
Acetildenafil (Hongdenafil)
CAS No. 831217-01-7
C25H34N6O3 M.W. 466.59
S-0621



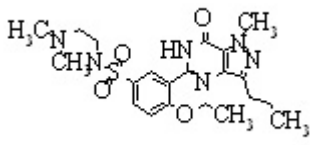
Thiodimethyl Sildenafil (Thioaildenafill, Sulfoaildenafil)
CAS No. 856190-47-1
C23H32N6O3S2 M.W. 504.68
S-0622



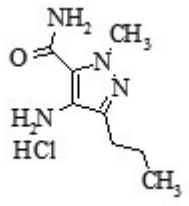
Pyrazole N-desmethyl sildenafil
C21H28N6O4S M.W. 460.56
S-0623



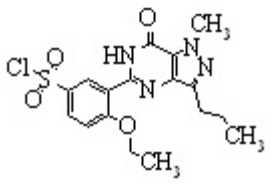
PDE-5 Inhibitor (Sildenafil Related Compound)
C21H30N6O4S M.W. 462.58
S-0624



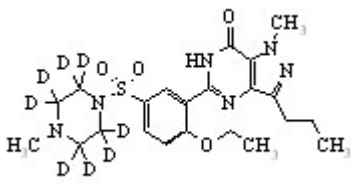
Sildenafil Amine HCl
C8H14N4O.HCl M.W. 182.23 36.46
S-0626



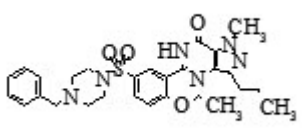
Sildenafil chlorosulfonyl
CAS No. 139756-22-2
C17H19ClN4O4S M.W. 410.88
S-0628



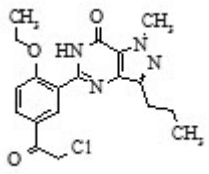
Sildenafil-d8
CAS No. 171599-83-0(non-d)
C22H22D8N6O4S M.W. 482.63
S-063



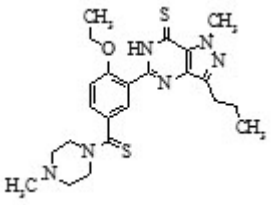
Benzyl Sildenafil
C28H34N6O4S M.W. 550.68
S-0631



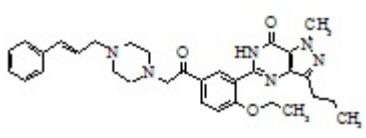
Chlorodenafil
CAS No. N/A
C19H21ClN4O3 M.W. 388.86
S-0633



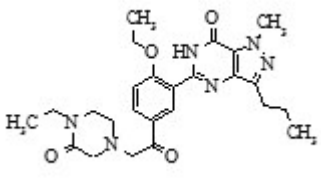
Dithio-desmethyl-carbodenafil
CAS No. N/A
C23H30N6OS2 M.W. 470.66
S-0635



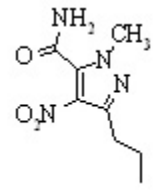
Cinnamyldenafil
CAS No. N/A
C32H38N6O3 M.W. 554.70
S-0637



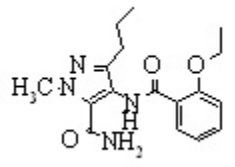
Oxohongdenafil
CAS No. N/A
C25H32N6O4 M.W. 480.57
S-0639



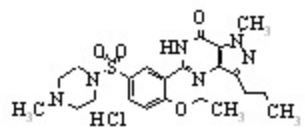
Sildenafil amide
C8H12N4O3 M.W. 212.21
S-0625



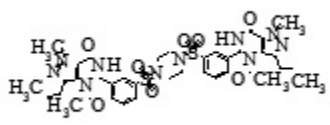
Sildenafil coupled
C17H22N4O3 M.W. 330.39
S-0627



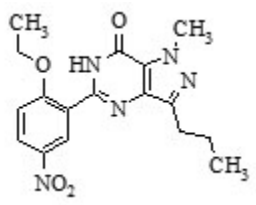
Sildenafil HCl
C22H30N6O4S.HCl M.W. 474.59 36.46
S-0629



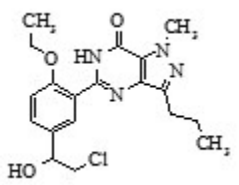
Sildenafil Dimer Impurity
C38H46N10O8S2 M.W. 834.98
S-0630



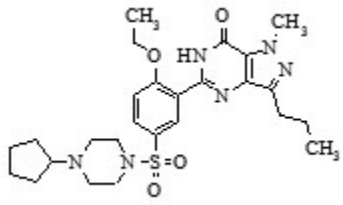
Nitrodenafil
CAS No. N/A
C17H19N5O4 M.W. 357.37
S-0632



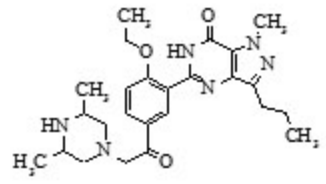
Hydroxychlorodenafil
CAS No. N/A
C19H23ClN4O3 M.W. 390.87
S-0634



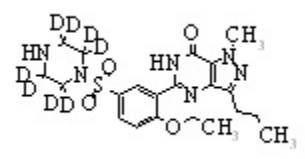
Cyclopentynafil
CAS No. N/A
C26H36N6O4S M.W. 528.68
S-0636



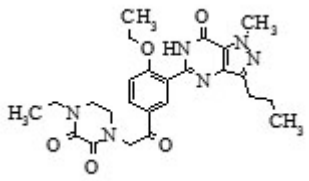
Dimethylacetildenafil
CAS No. N/A
C25H34N6O3 M.W. 466.59
S-0638



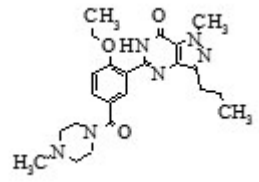
N-Desmethyl sildenafil-d8
CAS No. 1185168-06-2
C21H20N6O4SD8 M.W. 468.61
S-064



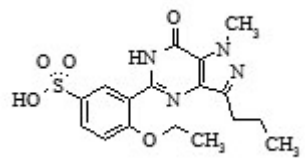
Dioxohongdenafil
CAS No. N/A
C25H30N6O5 M.W. 494.56
S-0640



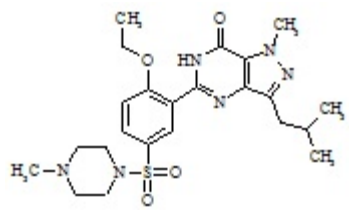
Desmethyl Carbodenafil
C23H30N6O3 M.W. 438.53
S-0642



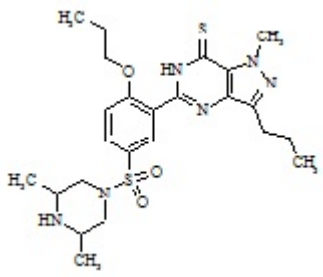
Demethylpiperazinyl Sildenafil Sulfonic Acid
C17H20N4O5S M.W. 392.44
S-0644



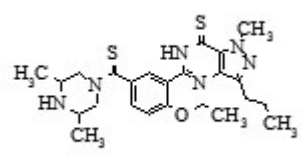
Sildenafil Impurity A (Isobutyl Sildenafil)
CAS No. 1391053-95-4
C23H32N6O4S M.W. 488.61
S-0646



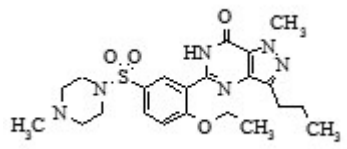
Sildenafil Analogue III
CAS No. N/A
C24H34N6O3S2 M.W. 518.70
S-0649



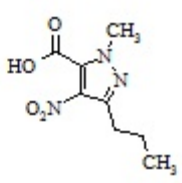
Sildenafil Related Compound
C24H32N6OS2 M.W. 484.69
S-0650



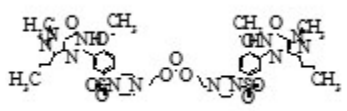
Sildenafil
C22H30N6O4S M.W. 474.59
S-0652



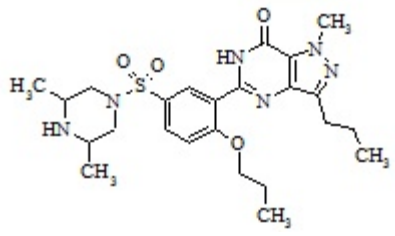
Sildenafil Impurity ((1-methyl-4-Nitro -3-n-propyl pyrazole-5- carboxylic acid)
C8H11N3O4 M.W. 213.19
S-0654



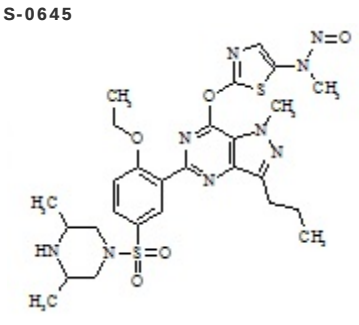
Lodenafilcarbonate
CAS No. N/A
C47H62N12O11S2 M.W. 1035.22
S-0641



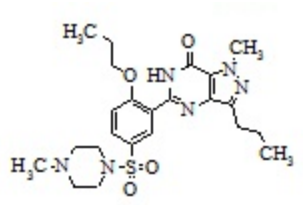
Sildenafil analogue
C24H34N6O4S M.W. 502.64
S-0643



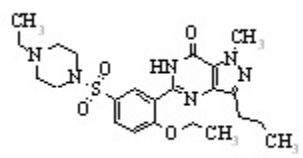
Nitroso-prodenafil
CAS No. N/A
C27H35N9O5S2 M.W. 629.77
S-0645



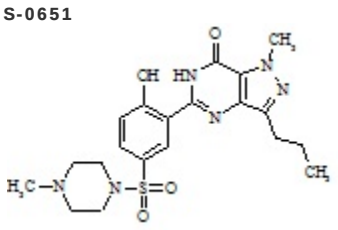
Propoxyphenyl Sildenafil
CAS No. 877777-10-1
C23H32N6O4S M.W. 488.61
S-0648



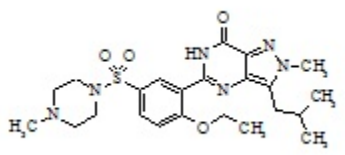
Homosildenafil
CAS No. 642928-07-2
C23H32N6O4S M.W. 488.61
S-065



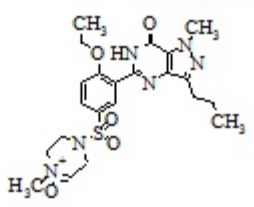
O-Desethyl Sildenafil (Sildenafil Impurity C)
CAS No. N/A
C20H26N6O4S M.W. 446.53
S-0651



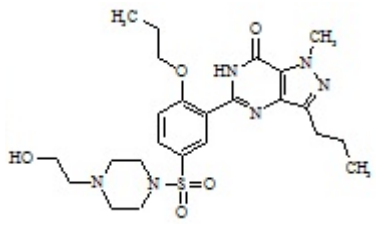
Sildenafil Impurity A Related Compound (Isomer of Isobutyl Sildenafil)
C23H32N6O4S M.W. 488.61
S-0653



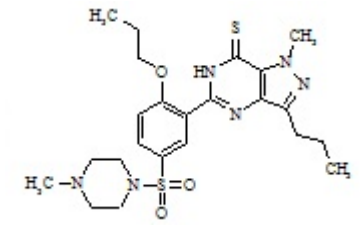
Sildenafil N-Oxide
C22H30N6O5S M.W. 490.59
S-0655



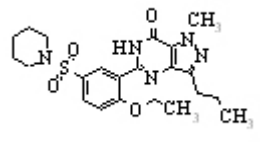
Propoxyphenyl-Hydroxyhomosildenafil
CAS No. N/A
C24H34N6O5S M.W. 518.64
S-0656



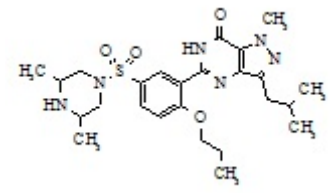
Propoxyphenyl-Thiosildenafil
CAS No. N/A
C23H32N6O3S2 M.W. 504.68
S-0658



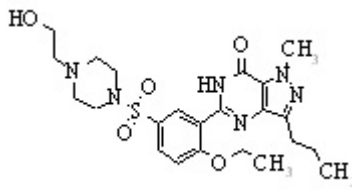
Norneosildenafil
C22H29N5O4S M.W. 459.57
S-066



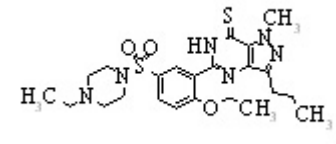
Sildenafil Related Compound 2
C25H36N6O4S M.W. 516.67
S-0661



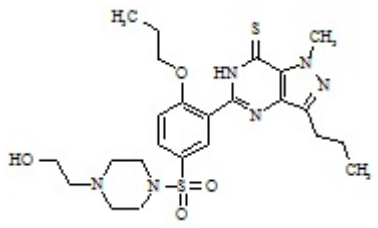
Hydroxyhomosildenafil
C23H32N6O5S M.W. 504.61
S-067



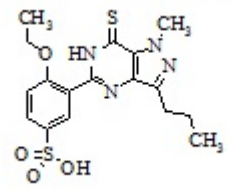
Thiohomosildenafil
C23H32N6O3S2 M.W. 504.68
S-069



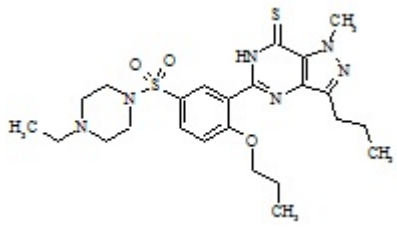
Sildenafil Analogue I (Propoxyphenyl-Thiohydroxyhomosildenafil)
CAS No. 479073-90-0
C24H34N6O4S2 M.W. 534.70
S-0657



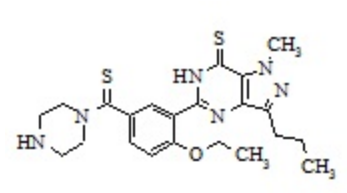
Depiperazinothiosildenafil
C17H20N4O4S2 M.W. 408.50
S-0659



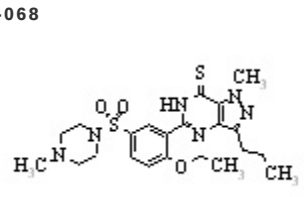
Propoxyphenyl Thiohomosidenafil
CAS No. 479073-88-6
C24H34N6O3S2 M.W. 518.70
S-0660



Dithio-Desethyl-Carbodenafil
CAS No. N/A
C22H28N6OS2 M.W. 456.64
S-0662

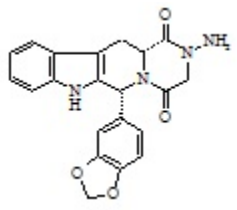


Thiosildenafil
CAS No. 479073-79-5
C22H30N6O3S2 M.W. 490.65
S-068

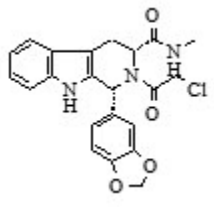


Tadalafil Related Compounds (commercial standards available) – includes deuterated standards.

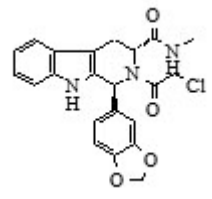
Aminotadalafil
CAS No. 385769-84-6
C21H18N4O4 M.W. 390.40
T-101



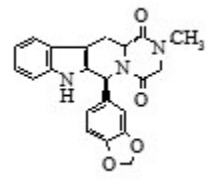
Tadalafil Impurity D
CAS No. NA
C22H20ClN3O4 M.W. 425.88
T-1011



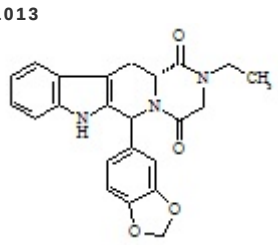
Tadalafil Impurity C
CAS No. NA
C22H20ClN3O4 M.W. 425.88
T-1010



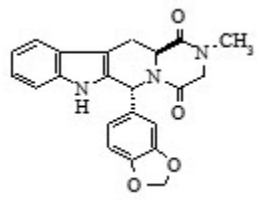
Tadalafil Impurity E (6S, 12R)
CAS No. 171596-28-4
C22H19N3O4 M.W. 389.41
T-1012



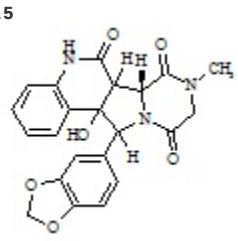
N-Ethyl Tadalafil
CAS No. N/A
C23H21N3O4 M.W. 403.44
T-1013



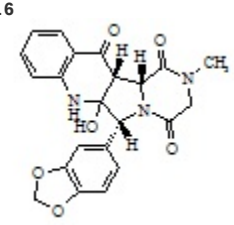
6R,12S-Tadalafil
CAS No. 171596-27-3
C22H19N3O4 M.W. 389.41
T-1014



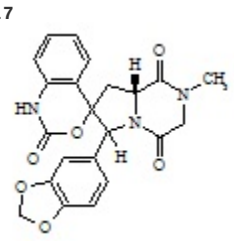
Tadalafil Hydroxylactam Impurity
C22H19N3O6 M.W. 421.41
T-1015



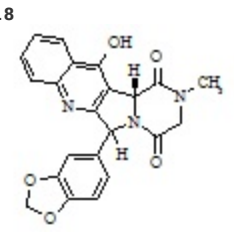
Tadalafil Aminohemiketal Impurity
C22H19N3O6 M.W. 421.41
T-1016



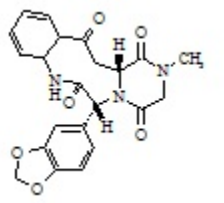
Tadalafil Spiro-urethane Impurity
C22H19N3O6 M.W. 421.41
T-1017



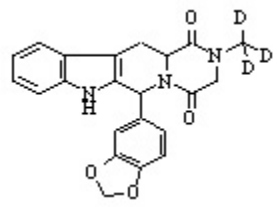
Tadalafil Hydroxyquinoline Impurity
C22H17N3O5 M.W. 403.40
T-1018



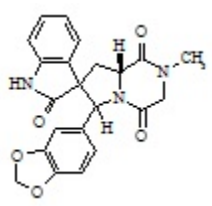
Tadalafil Ketolactam Impurity
CAS No. 1346605-38-6
C22H19N3O6 M.W. 421.41
T-1019



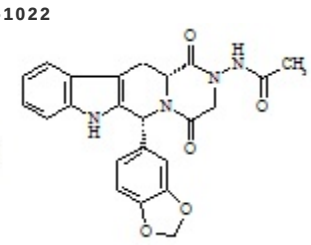
Tadalafil-d3
CAS No. 960226-55-5
C22H16N3O4D3 M.W. 392.43
T-102



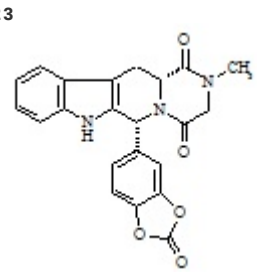
Tadalafil Spiro-oxindole Impurity
C22H19N3O5 M.W. 405.41
T-1020



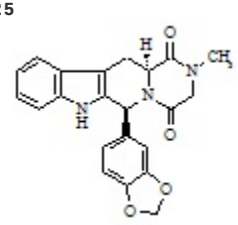
Acetaminotadalafil
CAS No. N/A
C23H20N4O5 M.W. 432.44
T-1022



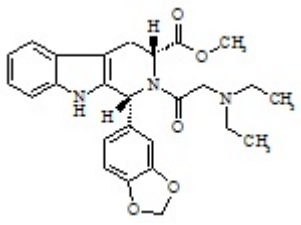
Tadalafil Oxo Impurity
CAS No. 1346602-17-2
C22H17N3O5 M.W. 403.40
T-1023



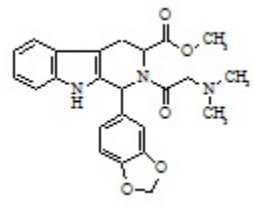
Tadalafil EP Impurity B (ent-tadalafil)
CAS No. 629652-72-8
C22H19N3O4 M.W. 389.41
T-1025



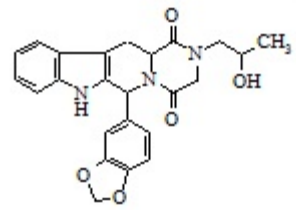
Tadalafil Related Compound
CAS No. N/A
C26H29N3O5 M.W. 463.54
T-1027



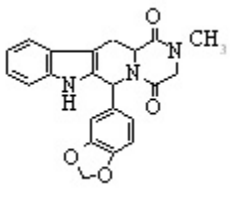
Tadalafil Related Compound 2
C24H25N3O5 M.W. 435.48
T-1028



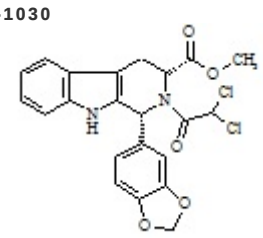
2-Hydroxypropylnortadalafil
C24H23N3O5 M.W. 433.47
T-1029



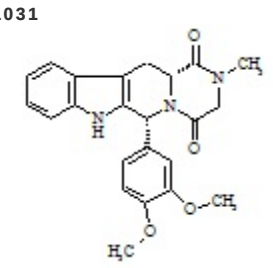
Tadalafil
CAS No. 171596-29-5
C22H19N3O4 M.W. 389.41
T-103



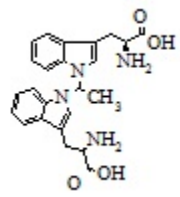
Tadalafil Dichloro Impurity
CAS No. N/A
C22H18Cl2N2O5 M.W. 461.31
T-1030



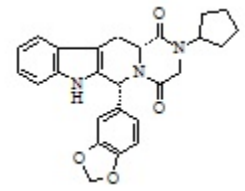
Tadalafil Dimethoxy Impurity
CAS No. 1356345-67-9
C23H23N3O4 M.W. 405.46
T-1031



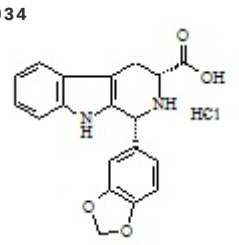
Tadalafil Impurity (1,1 Œ-ethylidenebistryptophan)
C24H26N4O4 M.W. 434.50
T-1032



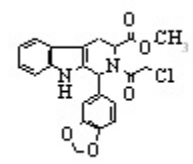
Tadalafil Related Impurity 1
CAS No. N/A
C26H25N3O4 M.W. 443.51
T-1033



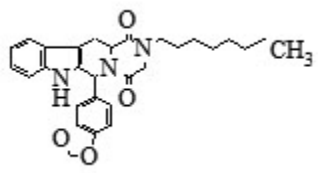
Tadalafil Acid Impurity
CAS No. N/A
C19H16N2O4 HCl M.W. 336.35 36.46
T-1034



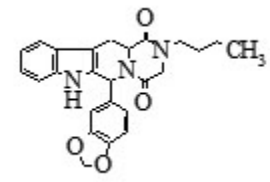
Chloropretadalafil
C22H19ClN2O5 M.W. 426.86
T-104



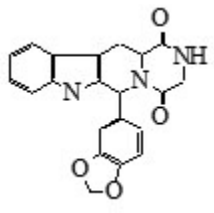
N-Octyl-nortadalafil
C29H33N3O4 M.W. 487.60
T-105



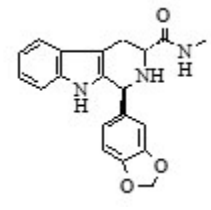
N-Butyl Tadalafil
C25H25N3O4 M.W. 431.50
T-106



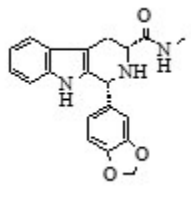
Nortadalafil
C21H17N3O4 M.W. 375.39
T-107



Tadalafil Impurity A
CAS No. NA
C20H19N3O3 M.W. 349.39
T-108

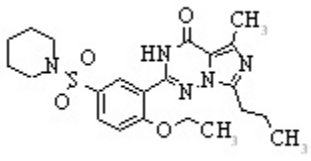


Tadalafil Impurity B
CAS No. NA
C20H19N3O3 M.W. 349.39
T-109

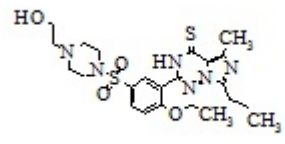


Vardenafil Related Compounds (commercial standards available) – includes deuterated standards.

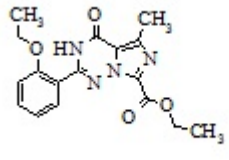
Pseudovardenafil
CAS No. 224788-34-5
C22H29N5O4S M.W. 459.57
V-051



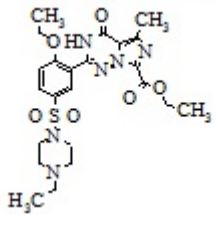
Hydroxythio Vardenafil
C23H32N6O4S2 M.W. 520.68
V-0510



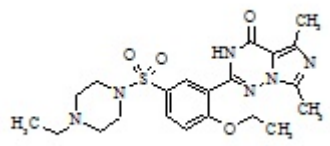
Vardenafil Impurity 1
CAS No. 1417529-67-9
C17H18N4O4 M.W. 342.36
V-0511



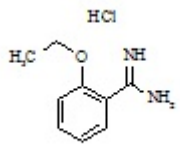
Vardenafil Impurity 2
CAS No. 1417529-69-1
C23H30N6O6S M.W. 518.60
V-0512



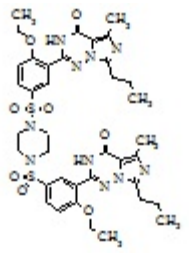
Vardenafil Impurity 3
C21H28N6O4S M.W. 460.56
V-0513



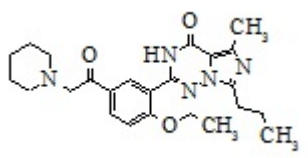
Vardenafil Impurity (2-Ethoxy Benzamidine Hydrochloride)
CAS No. 18637-00-8
C9H12N2O HCl M.W. 164.21 36.46
V-0515



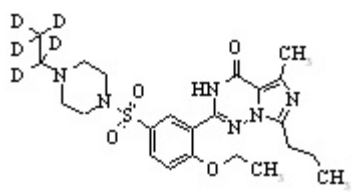
Vardenafil Dimer
C38H46N10O8S2 M.W. 834.98
V-0517



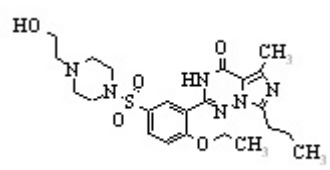
Vardenafil Acetyl Analogue
CAS No. N/A
C24H31N5O3 M.W. 437.55
V-0519



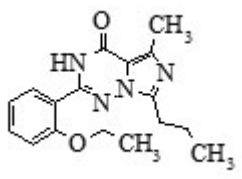
Vardenafil-d5
C23H27N6O4SD5 M.W. 493.64
V-053



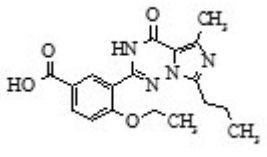
Hydroxy Vardenafil
C23H32N6O5S M.W. 504.61
V-055



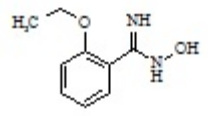
2-(2-Ethoxyphenyl)-5-methyl-7-propyl-3H-imidazo[5,1-f][1,2,4]triazin-4-one
C17H20N4O2 M.W. 312.37
V-057



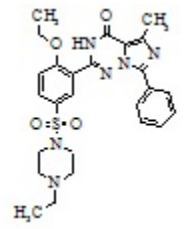
Norneovardenafil
CAS No. N/A
C18H20N4O4 M.W. 356.38
V-059



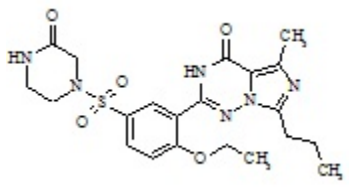
Vardenafil Impurity (2-Ethoxy-N-Hydroxy Benzamidine)
CAS No. 879-57-2
C9H12N2O2 M.W. 180.21
V-0514



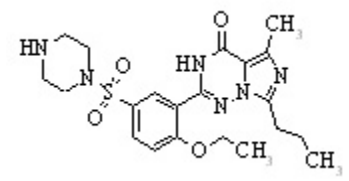
Vardenafil Benzoyl Impurity
C26H30N6O4S M.W. 522.63
V-0516



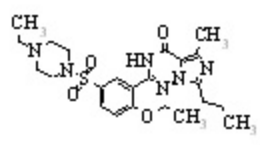
Vardenafil Oxopiperazine
C21H26N6O5S M.W. 474.54
V-0518



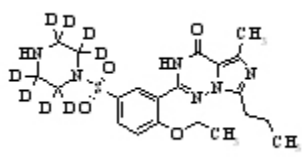
N-Desethyl Vardenafil
CAS No. 448184-46-1
C21H28N6O4S M.W. 460.56
V-052



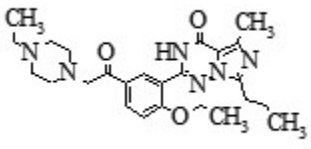
Vardenafil HCl
CAS No. 224785-90-4
C23H32N6O4S M.W. 488.61
V-054



N-Desethyl Vardenafil-d8
CAS No. 448184-46-1 (Unlabelled)
C21H28N6O4S M.W. 460.56
V-056

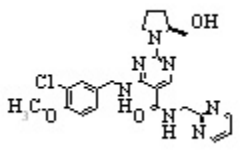


Acetylvardenafil
C25H34N6O3 M.W. 466.59
V-058

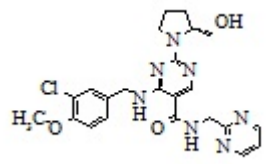


Avanafil Related Compounds (commercial standards available) – includes deuterated standards.

Avanafil
CAS No. 330784-47-9
C23H26ClN7O3 M.W. 483.96
A-291

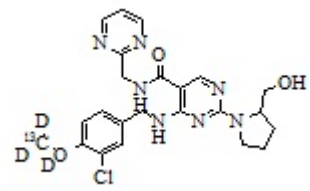


Avanafil Impurity 8 (R-Avanafil)
CAS No. N/A
C23H26ClN7O3 M.W. 483.96
A-2910

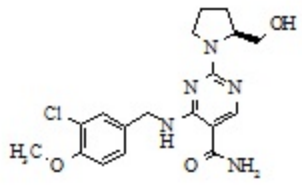


Avanafil Impurity 9
C18H17ClN6O3 M.W. 400.83
A-2911

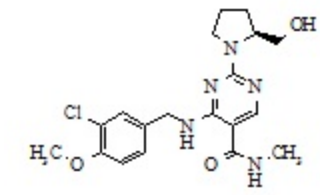
Avanafil-13CD3
C22H23ClN7O313CD3 M.W. 487.97
A-292



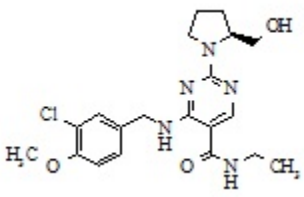
Avanafil impurity 1
C18H22ClN5O3 M.W. 391.86
A-293



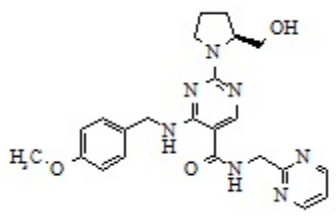
Avanafil impurity 2
C19H24ClN5O3 M.W. 405.89
A-294



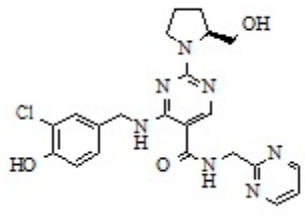
Avanafil impurity 3
C20H26ClN5O3 M.W. 419.91
A-295



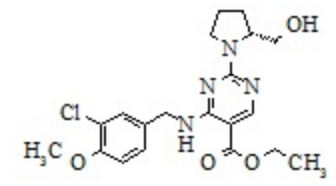
Avanafil impurity 4
C23H27N7O3 M.W. 449.52
A-296



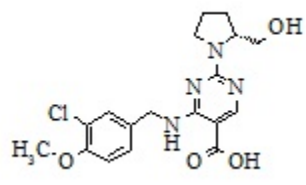
Avanafil impurity 5
C22H24ClN7O3 M.W. 469.93
A-297



Avanafil Impurity 6
CAS No. N/A
C20H25ClN4O4 M.W. 420.90
A-298

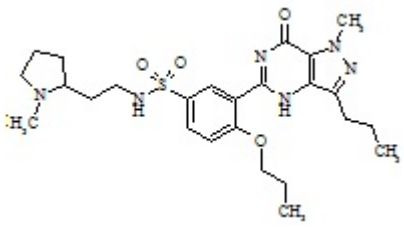


Avanafil Impurity 7
CAS No. N/A
C18H21ClN4O4 M.W. 392.85
A-299

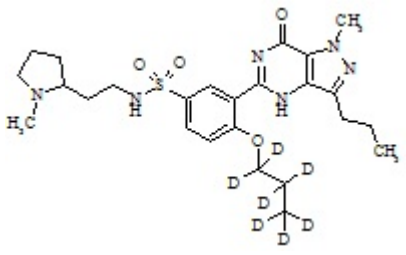


Udenafil Related Compounds (commercial standards available) – includes deuterated standards.

Udenafil
CAS No. 268203-93-6
C25H36N6O4S M.W. 516.67
U-031

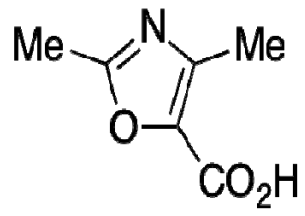


Udenafil-d7
CAS No. N/A
C25H29N6O4SD7 M.W. 523.71
U-032



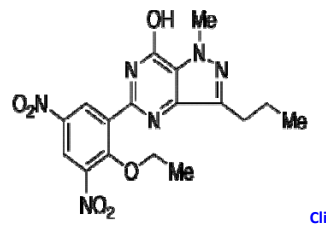
3. **Standards available from Toronto Research Chemicals http://www.trc-canada.com/ which include the majority of characterized PDE-5i analogues and all of the parent drugs including catalog numbers. (Some structure images not available) NOTE: Includes some compounds that are discontinued from TRC.**

Sildenafil Related Compounds (commercial standards available) – includes deuterated standards.



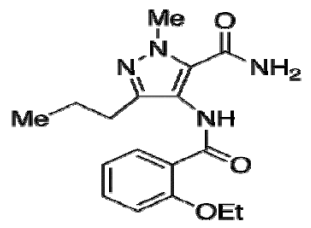
Click on image to enlarge

Catalogue #: D476330
Chemical Name: 2,4-Dimethyl-5-oxazolecarboxylic Acid
CAS Number: 2510-37-4
Mol. Formula: C6H7NO3
Synsynonyms: 2,4-Dimethyl-1,3-oxazole-5-carboxylic Acid; 2,4-Dimethyloxazole-5-carboxylic Acid; 5-Carboxy-2,4-dimethyloxazole



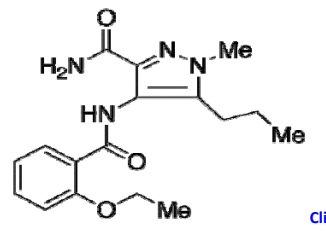
Click on image to enlarge

Catalogue #: D479775
Chemical Name: Dinitrodenafil
CAS Number:
Mol. Formula: C17H18N6O6
Synonyms: 5-(2-Ethoxy-3,5-dinitrophenyl)-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



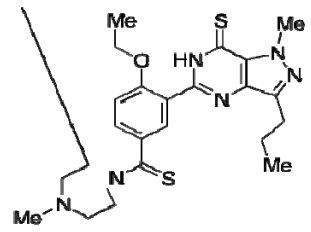
Click on image to enlarge

Catalogue #: E891000
Chemical Name: 4-(2-Ethoxybenzamido)-1-methyl-3-n-propylpyrazole-5-carboxamide
CAS Number: 139756-03-9
Mol. Formula: C17H22N4O3
Synonyms: 4-[(2-Ethoxybenzoyl)amino]-1-methyl-3-propyl-1H-pyrazole-5-carboxamide;



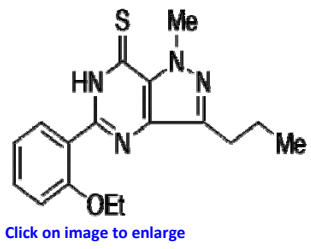
Click on image to enlarge

Catalogue #: E891010
Chemical Name: 4-[(2-Ethoxybenzoyl)amino]-1-methyl-5-propyl-1H-pyrazole-3-carboxamide
CAS Number: 501120-38-3
Mol. Formula: C17H22N4O3
Synonyms: 4-(2-Ethoxybenzamido)-1-methyl-5-propyl-1H-pyrazole-3-carboxamide



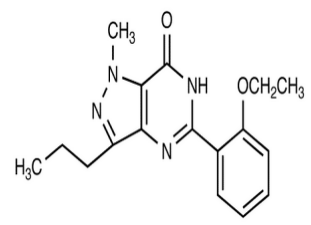
Click on image to enlarge

Catalogue #: E892530
Chemical Name: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)thioxomethyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyr
CAS Number: 1333233-46-7
Mol. Formula: C23H30N6OS2
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)thioxomethyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-Pyrazolo[4,3-d]pyrimidine-7-thione; Dithiodesmethylcarbodenafil



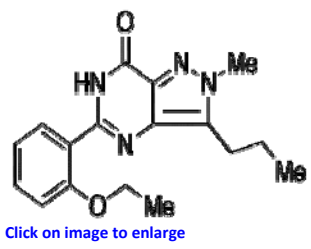
Click on image to enlarge

Catalogue #: E892710
Chemical Name: 5-(2-Ethoxyphenyl)-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione
CAS Number: 479074-06-1
Mol. Formula: C17H20N4OS
Synonyms: 5-(2-Ethoxyphenyl)-1,4-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione



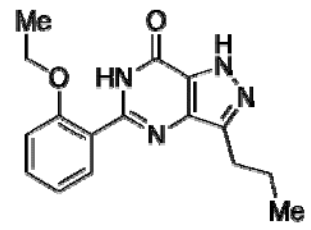
Click on image to enlarge

Catalogue #: E892725
Chemical Name: 5-(2-Ethoxyphenyl)-1-methyl-3-n-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 139756-21-1
Mol. Formula: C17H20N4O2
Synonyms: UK 088800; “Imidazosagatriazinone”



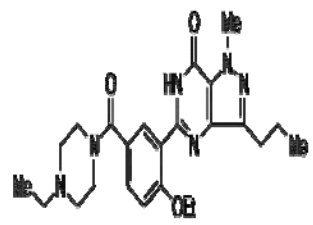
Click on image to enlarge

Catalogue #: E892730
Chemical Name: 5-(2-Ethoxyphenyl)-2,6-dihydro-2-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 501120-40-7
Mol. Formula: C17H20N4O2
Synonyms:



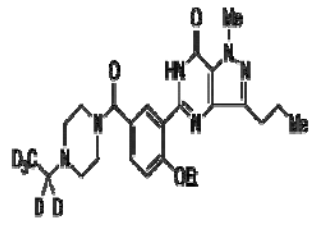
Click on image to enlarge

Catalogue #: E892765
Chemical Name: 5-(2-Ethoxyphenyl)-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 139756-30-2
Mol. Formula: C16H18N4O2
Synonyms: 5-(2-Ethoxyphenyl)-1,6-dihydro-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Des(4-methylpiperazin-1-ylsulfonyl) Desmethyl**sildenafil**



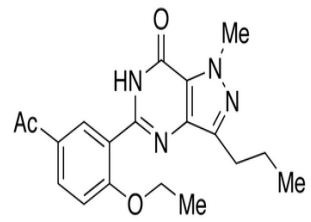
Click on image to enlarge

Catalogue #: F685400
Chemical Name: Fondenafil
CAS Number: 944241-52-5
Mol. Formula: C24H32N6O3
Synonyms: 5-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)carbonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Carbodenafil;



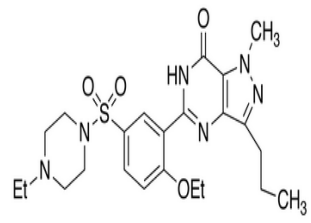
Click on image to enlarge

Catalogue #: F685402
Chemical Name: Fondenafil-d5
CAS Number:
Mol. Formula: C24H27D5N6O3
Synonyms: 5-[2-Ethoxy-5-[(4-ethyl-d5-1-piperazinyl)carbonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



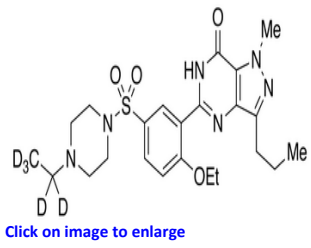
Click on image to enlarge

Catalogue #: G349960
Chemical Name: Gendenafil
CAS Number: 147676-66-2
Mol. Formula: C19H22N4O3
Synonyms: 5-(5-Acetyl-2-ethoxyphenyl)-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; 5-(5-Acetyl-2-ethoxyphenyl)-1-methyl-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one



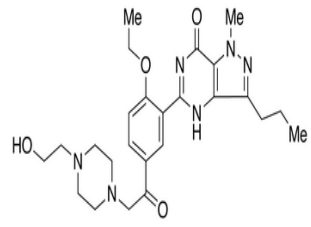
Click on image to enlarge

Catalogue #: H615150
Chemical Name: Homo Sildenafil
CAS Number: 642928-07-2
Mol. Formula: C23H32N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



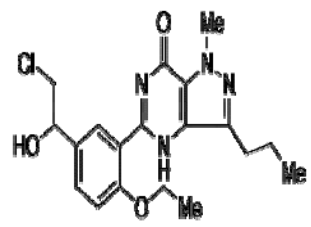
Click on image to enlarge

Catalogue #: H615152
Chemical Name: Homo Sildenafil-d5
CAS Number:
Mol. Formula: C23H27D5N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-(ethyl-d5)-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



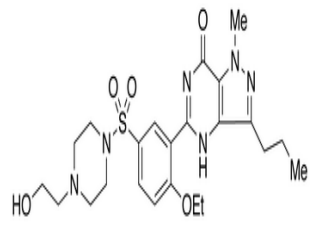
Click on image to enlarge

Chemical Name: Hydroxy Acetildenafil
CAS Number: 147676-56-0
Mol. Formula: C25H34N6O4
Synonyms: 5-[2-Ethoxy-5-[2-[4-(2-hydroxyethyl)-1-piperazinyl]acetyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Hydroxyhongdenafil;



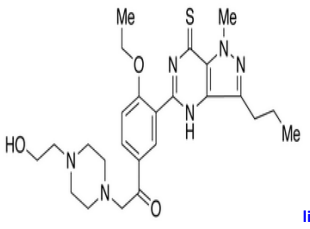
Click on image to enlarge

Catalogue #: H825115
Chemical Name: Hydroxy Chlorodenafil
CAS Number: 1391054-00-4
Mol. Formula: C19H23ClN4O3
Synonyms: 5-[5-(2-Chloro-1-hydroxyethyl)-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one



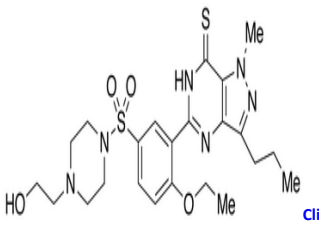
Click on image to enlarge

Catalogue #: H942840
Chemical Name: Hydroxyhomo Sildenafil
CAS Number: 139755-85-4
Mol. Formula: C23H32N6O5S
Synonyms: 5-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Lodenafil



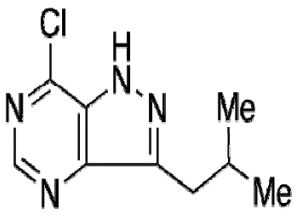
lick on image to enlarge

Catalogue #: H963100
Chemical Name: Hydroxythio Acetildenafil
CAS Number: 1159977-47-5
Mol. Formula: C25H34N6O3S
Synonyms: 5-[2-Ethoxy-5-[2-[4-(2-hydroxyethyl)-1-piperazinyl]acetyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-7-thio-pyrazolo[4,3-d]pyrimidine; 1-[3-(6,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]-2-[4-(2-hydroxyethyl)-1-piperazinyl]ethanone;



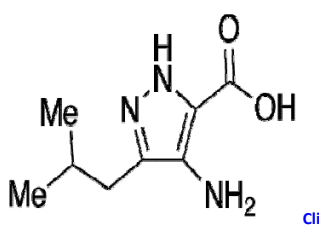
Click on image to enlarge

Catalogue #: H963150
Chemical Name: Hydroxythiohomo Sildenafil
CAS Number: 479073-82-0
Mol. Formula: C23H32N6O4S2
Synonyms: 5-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 4-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazineethanol



Click on image to enlarge

Catalogue #: I780530
Chemical Name: 3-Isobutyl-7-chloro-pyrazolo[4,3-d]pyrimidine
CAS Number:
Mol. Formula: C9H11ClN4
Synonyms: 3-Isobutyl-7-chloro-1H-pyrazolo[4,3-d]pyrimidine;



Click on image to enlarge

Catalogue #: I780615
Chemical Name: 5-(2-Isobutyl)-4-amino-1H-pyrazole-3-carboxylic Acid
CAS Number: 1093415-88-3
Mol. Formula: C8H13N3O2
Synonyms: 4-Amino-5-(2-methylpropyl)-1H-pyrazole-3-carboxylic Acid

no image of structure available

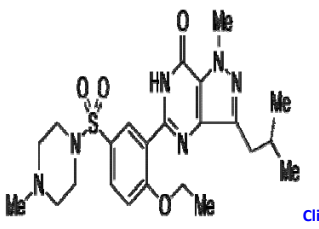
Catalogue #: I780620
Chemical Name: 3-Isobutylpyrazolo[4,3-d]pyrimidine
CAS Number:
Mol. Formula: C9H12N4
Synonyms: 3-Isobutyl-1H-pyrazolo[4,3-d]pyrimidine;

no image of structure available

Catalogue #: I780625
Chemical Name: 5-Isobutyl-4-nitro-1H-pyrazole-3-carboxylic Acid
CAS Number: 222729-55-7
Mol. Formula: C8H11N3O4
Synonyms: 5-(2-Methylpropyl)-4-nitro-1H-pyrazole-3-carboxylic Acid;

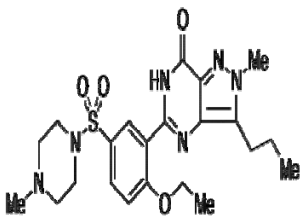
no image of structure available

Catalogue #: I780630
Chemical Name: 5-Isobutyl-1H-pyrazole-3-carboxylic Acid
CAS Number: 92933-49-8
Mol. Formula: C8H12N2O2
Synonyms: 5-(2-Methylpropyl)-1H-pyrazole-3-carboxylic Acid;



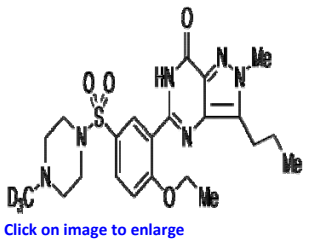
Click on image to enlarge

Catalogue #: I780650
Chemical Name: Isobutyl Sildenafil
CAS Number: 1391053-95-4
Mol. Formula: C23H32N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-(2-methylpropyl)-7H-pyrazolo[4,3-d]pyrimidin-7-one;



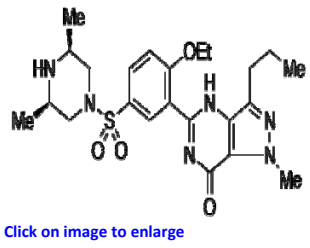
Click on image to enlarge

Catalogue #: I900800
Chemical Name: Iso Sildenafil
CAS Number: 253178-46-0
Mol. Formula: C22H30N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-2,6-dihydro-2-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; 1-[[3-(4,7-Dihydro-2-methyl-7-oxo-3-propyl-2H- pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine;



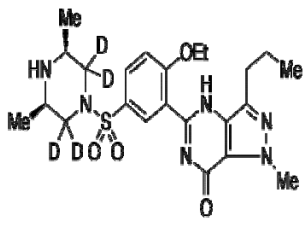
Click on image to enlarge

Catalogue #: I900802
Chemical Name: Iso Sildenafil-d3
CAS Number:
Mol. Formula: C22H27D3N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-(methyl-d3)-1-piperazinyl)sulfonyl]phenyl]-2,6-dihydro-2-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; 1-[[3-(4,7-Dihydro-2-methyl-7-oxo-3- propyl-2H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-(methyl-d3)piperazine;



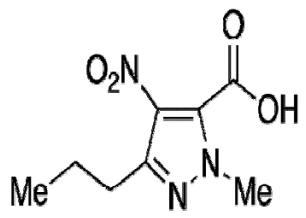
Click on image to enlarge

Catalogue #: M225935
Chemical Name: Methiso**sildenafil**
CAS Number: 496835-35-9
Mol. Formula: C23H32N6O4S
Synonyms: rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Aildenafil; Dimethyl**sildenafil**



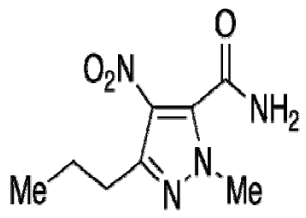
Click on image to enlarge

Catalogue #: M225937
Chemical Name: Methiso**sildenafil**-d4
CAS Number:
Mol. Formula: C23H28D4N6O4S
Synonyms: rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl-d4]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Aildenafil-d4;



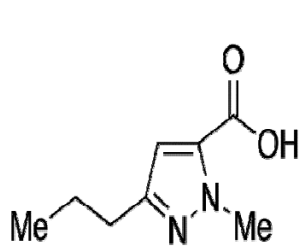
Click on image to enlarge

Catalogue #: M320530
Chemical Name: 1-Methyl-4-nitro-3-propyl-1H-pyrazole-5-carboxylic Acid
CAS Number: 139756-00-6
Mol. Formula: C8H11N3O4
Synonyms: 1-Methyl-4-nitro-3-propylpyrazole-5-carboxylic Acid



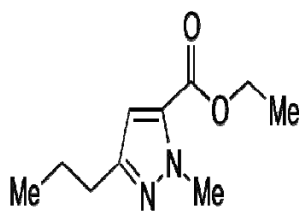
Click on image to enlarge

Catalogue #: M320535
Chemical Name: 1-Methyl-4-nitro-3-propylpyrazole-5-carboxamide
CAS Number: 139756-01-7
Mol. Formula: C8H12N4O3
Synonyms: 1-Methyl-4-nitro-3-propyl-1H-pyrazole-5-carboxamide



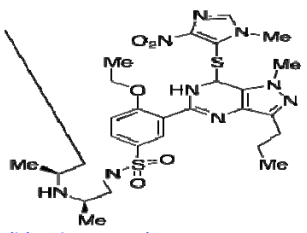
Click on image to enlarge

Catalogue #: M320655
Chemical Name: 1-Methyl-3-propyl-1H-pyrazole-5-carboxylic Acid
CAS Number: 139755-99-0
Mol. Formula: C8H12N2O2
Synonyms: 1-Methyl-3-propylpyrazole-5-carboxylic Acid; 2-Methyl-5-propyl-2H-pyrazole-3-carboxylic Acid



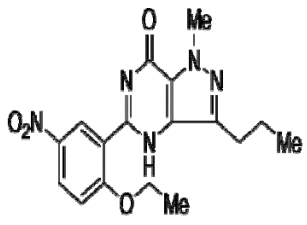
Click on image to enlarge

Catalogue #: M320775
Chemical Name: 1-Methyl-3-propyl-1H-pyrazole-5-carboxylic Acid Ethyl Ester
CAS Number: 133261-07-1
Mol. Formula: C10H16N2O2
Synonyms: 1-Methyl-3-propylpyrazole-5-carboxylic Acid Ethyl Ester; Ethyl 1-Methyl-3-propyl-1H-pyrazole-5-carboxylate; Ethyl 1-Methyl-3-propylpyrazole-5-carboxylate;



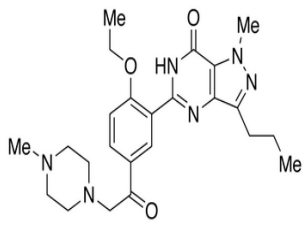
Click on image to enlarge

Catalogue #: M820000
Chemical Name: Mutaprodenafil
CAS Number: 138577-30-1
Mol. Formula: C27H37N9O5S2
Synonyms: rel-5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1-methyl-7-[(1-methyl-4-nitro-1H-imidazol-5-yl)thio]-3-propyl-1H-pyrazolo[4,3-d]pyrimidine



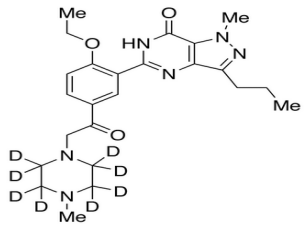
Click on image to enlarge

Catalogue #: N493770
Chemical Name: Nitrodenafil
CAS Number: 147676-99-1
Mol. Formula: C17H19N5O4
Synonyms: 5-(2-Ethoxy-5-nitrophenyl)-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



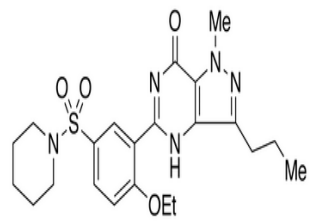
Click on image to enlarge

Catalogue #: N660500
Chemical Name: Nor Acetildenafil
CAS Number: 949091-38-7
Mol. Formula: C24H32N6O3
Synonyms: 5-[2-Ethoxy-5-[2-(4-methyl-1-piperazinyl)acetyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



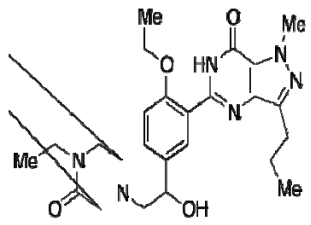
Click on image to enlarge

Catalogue #: N660502
Chemical Name: Nor Acetildenafil-d8
CAS Number: 1185117-07-0
Mol. Formula: C24H24D8N6O3
Synonyms: 5-[2-Ethoxy-5-[2-(4-methyl-1-piperazinyl-d8)acetyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



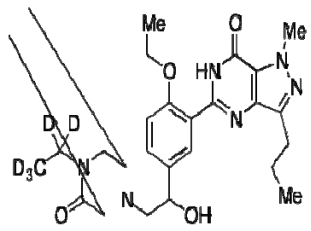
Click on image to enlarge

Catalogue #: N824300
Chemical Name: Norneo Sildenafil
CAS Number: 371959-09-0
Mol. Formula: C22H29N5O4S
Synonyms: 5-[2-Ethoxy-5-(1-piperidinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; 1-[[3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]piperidine;



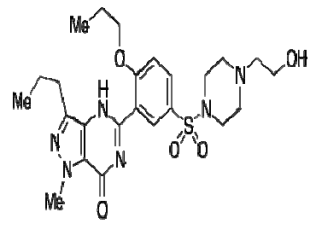
Click on image to enlarge

Catalogue #: P480470
Chemical Name: Piperazonifil
CAS Number: 1335201-04-1
Mol. Formula: C25H34N6O4
Synonyms: 5-[2-Ethoxy-5-[2-(4-ethyl-3-oxo-1-piperazinyl)-1-hydroxyethyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one,



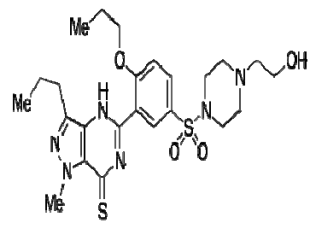
Click on image to enlarge

Catalogue #: P480472
Chemical Name: Piperazonifil-d5
CAS Number:
Mol. Formula: C25H29D5N6O4
Synonyms: 5-[2-Ethoxy-5-[2-(4-ethyl-3-oxo-1-piperazinyl)-1-hydroxyethyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one-d5



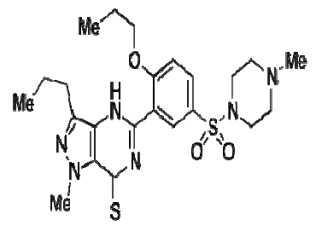
Click on image to enlarge

Catalogue #: P831600
Chemical Name: Propoxyphenyl Homohydroxy**sildenafil**
CAS Number: 139755-87-6
Mol. Formula: C24H34N6O5S
Synonyms: 5-[5-[4-(2-Hydroxyethyl)piperazinylsulfonyl]-2-propoxyphenyl]-1-methyl-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one; 4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-1-Piperazineethanol



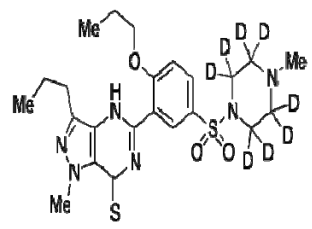
Click on image to enlarge

Catalogue #: P831630
Chemical Name: Propoxyphenyl-thiohydroxyhomosildenafil
CAS Number: 479073-90-0
Mol. Formula: C24H34N6O4S2
Synonyms: 1,6-dihydro-5-[5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1-methyl-3-propyl-7H-Pyrazolo[4,3-d]pyrimidine-7-thione; 4-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-1-Piperazineethanol; 5-(5-((4-(2-hydroxyethyl)piperazin-1-yl)sulfonyl)-2-propoxyphenyl)-1-methyl-3-propyl-1H-pyrazolo[4,3-d]pyrimidine-7(4H)-thione



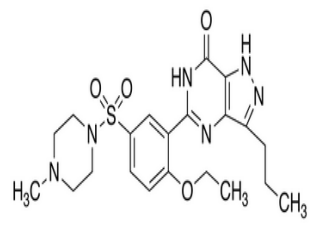
Click on image to enlarge

Catalogue #: P831635
Chemical Name: Propoxyphenyl Thio**sildenafil**
CAS Number: 479073-87-5
Mol. Formula: C23H32N6O3S2
Synonyms: 1,6-Dihydro-1-methyl-5-[5-[(4-methyl-1-piperazinyl)sulfonyl]-2-propoxyphenyl]-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-4-methyl-piperazine; rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione



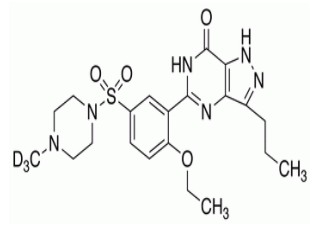
Click on image to enlarge

Catalogue #: P831637
Chemical Name: Propoxyphenyl-thio**sildenafil**-d8
CAS Number:
Mol. Formula: C23H24D8N6O3S2
Synonyms: 1,6-Dihydro-1-methyl-5-[5-[(4-methyl-1-piperazinyl)sulfonyl]-2-propoxyphenyl]-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione-d8; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-4-methyl-piperazine-d8; rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione-d8



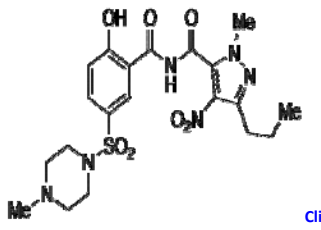
Click on image to enlarge

Catalogue #: P842800
Chemical Name: Pyrazole N-Demethyl Sildenafil
CAS Number: 139755-95-6
Mol. Formula: C21H28N6O4S
Synonyms: 1-[[3-(4,7-Dihydroxy-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methyl-piperazine; Desmethyl**sildenafil**;



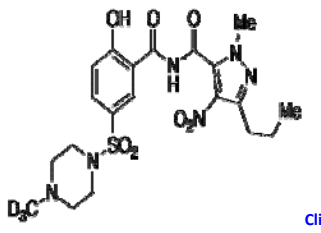
Click on image to enlarge

Catalogue #: P842802
Chemical Name: Pyrazole N-Demethyl Sildenafil-d3
CAS Number:
Mol. Formula: C21H25D3N6O4S
Synonyms: 1-[[3-(4,7-Dihydroxy-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl-4- ethoxyphenyl]sulfonyl]-4-(methyl-d3)piperazine; Desmethyl**sildenafil**-d3;



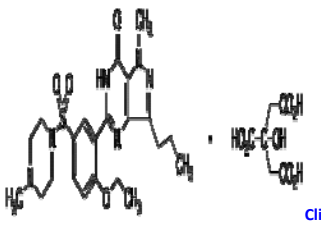
Click on image to enlarge

Catalogue #: P846500
Chemical Name: Pyrazolosalicyloyl Imide
CAS Number:
Mol. Formula: C20H26N6O7S
Synonyms: N-[2-Hydroxy-5-[(4-methyl-1-piperazinyl)sulfonyl]benzoyl]-1-methyl-4-nitro-3-n-propyl-1H-pyrazol-5-carboxamide; Pyrazolosalicylimide



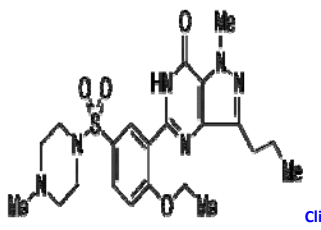
Click on image to enlarge

Catalogue #: P846502
Chemical Name: Pyrazolosalicyloyl Imide-d3
CAS Number:
Mol. Formula: C20H23D3N6O7S
Synonyms: N-[2-Hydroxy-5-[(4-methyl-1-piperazinyl)sulfonyl]benzoyl]-1-methyl-4-nitro-3-n-propyl-1H-pyrazol-5-carboxamide-d3; Pyrazolosalicylimide-d3



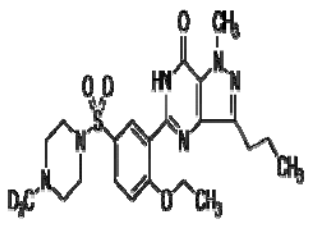
Click on image to enlarge

Catalogue #: S435000
Chemical Name: Sildenafil Citrate
CAS Number: 171599-83-0
Mol. Formula: C28H38N6O11S
Synonyms: 1-[[3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine Citrate;



Click on image to enlarge

Catalogue #: S435001
Chemical Name: Sildenafil
CAS Number: 139755-83-2
Mol. Formula: C22H30N6O4S
Synonyms: 1-[[3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine; 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;

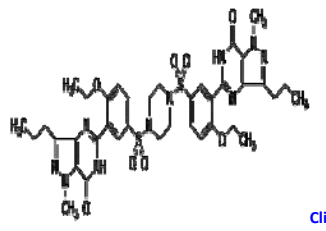


Click on image to enlarge

Catalogue #: S435002
Chemical Name: Sildenafil-d3
CAS Number: 1126745-90-1
Mol. Formula: C22H27D3N6O4S
Synonyms: 1-[[3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine-d3; 5-[2-Ethoxy-5-[[4-(methyl-d3)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;

no image of structure available

Catalogue #: S435003
Chemical Name: Sildenafil-d8
CAS Number: 951385-68-5
Mol. Formula: C22H22D8N6O4S
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl-2,2,3,3,5,5,6,6-d8)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; BDD 10402;

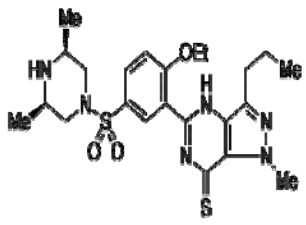


Click on image to enlarge

Catalogue #: S435020
Chemical Name: Sildenafil Dimer Impurity
CAS Number:
Mol. Formula: C38H46N10O8S2
Synonyms:

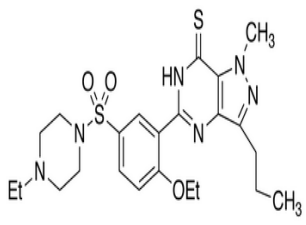
no image of structure available

Catalogue #: S435035
Chemical Name: Sildenafil N-Oxide
CAS Number: 1094598-75-0
Mol. Formula: C22H30N6O5S
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-4-oxido-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



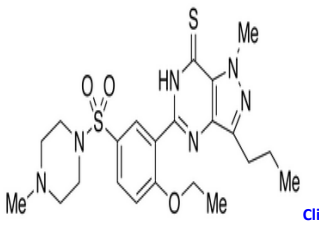
Click on image to enlarge

Catalogue #: T344365
Chemical Name: Thioaildenafil
CAS Number: 856190-47-1
Mol. Formula: C23H32N6O3S2
Synonyms: (3R,5S)-rel-1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-3,5-dimethyl-piperazine; Sulfoaildenafil;



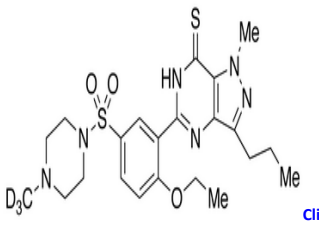
Click on image to enlarge

Catalogue #: T344470
Chemical Name: Thiohomo Sildenafil
CAS Number: 479073-80-8
Mol. Formula: C23H32N6O3S2
Synonyms: 5-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-ethyl-piperazine



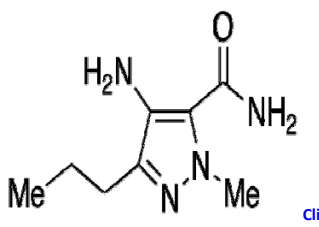
Click on image to enlarge

Catalogue #: T371500
Chemical Name: Thio**sildenafil**
CAS Number: 479073-79-5
Mol. Formula: C22H30N6O3S2
Synonyms: 5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl-7-thioxo- 1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine;



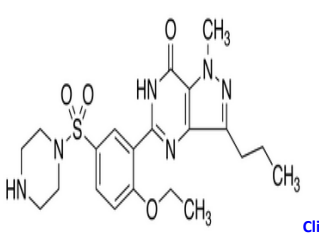
Click on image to enlarge

Catalogue #: T371502
Chemical Name: Thio**sildenafil**-d3
CAS Number:
Mol. Formula: C22H27D3N6O3S2
Synonyms: 5-[2-Ethoxy-5-[(4-(methyl-d3)-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione; 1-[[3-(4,7-Dihydro-1-methyl-3-propyl -7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-(methyl-d3)piperazine;



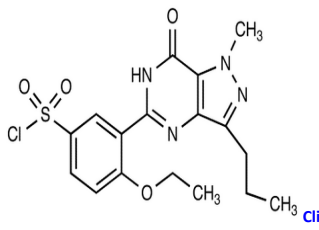
Click on image to enlarge

Catalogue #: A617415
Chemical Name: 4-Amino-1-methyl-3-propyl-1H-pyrazole-5-carboxamide
CAS Number: 139756-02-8
Mol. Formula: C8H14N4O
Synonyms: 4-Amino-2-methyl-5-propyl-2H-pyrazole-3-carboxamide;



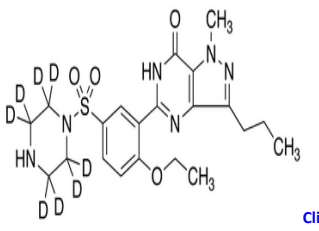
Click on image to enlarge

Catalogue #: D292200
Chemical Name: N-Desmethyl Sildenafil
CAS Number: 139755-82-1
Mol. Formula: C21H28N6O4S
Synonyms: 5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Desmethyl**sildenafil**; UK 103320;



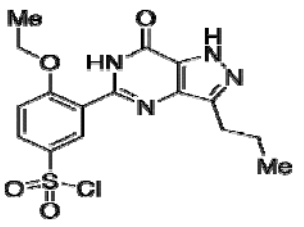
Click on image to enlarge

Catalogue #: C380005
Chemical Name: 5-(5-Chlorosulfonyl-2-ethoxyphenyl)-1-methyl-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 139756-22-2
Mol. Formula: C17H19ClN4O4S
Synonyms: 3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxy-benzenesulfonyl Chloride;



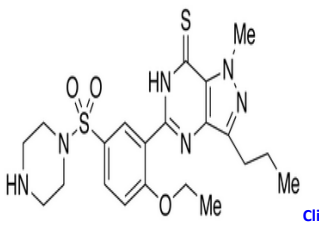
Click on image to enlarge

Catalogue #: D292202
Chemical Name: N-Desmethyl Sildenafil-d8
CAS Number:
Mol. Formula: C21H20D8N6O4S
Synonyms: 5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one-d8; Desmethyl**sildenafil**-d8; UK 103320-d8;



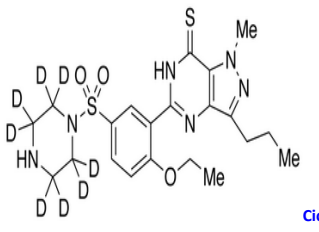
Click on image to enlarge

Catalogue #: C383500
Chemical Name: 5-(5-Chlorosulfonyl-2-ethoxyphenyl)-3-propyl-1,6-dihydro -7H-pyrazolo[4,3-d]pyrimidin-7-one
CAS Number: 139756-31-3
Mol. Formula: C16H17ClN4O4S
Synonyms: 3-(6,7-Dihydro-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxybenzenesulfonyl Chloride; Des-4-methylpiperazine Desmethyl**sildenafil** Chloride;



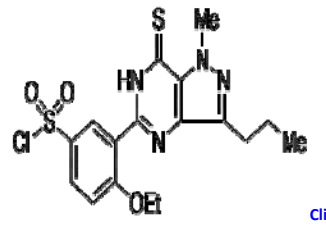
Click on image to enlarge

Catalogue #: D294350
Chemical Name: Desmethyl Thio**sildenafil**
CAS Number: 479073-86-4
Mol. Formula: C21H28N6O3S2
Synonyms: 5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl- 7H-pyrazolo[4,3-d]pyrimidine-7-thione;



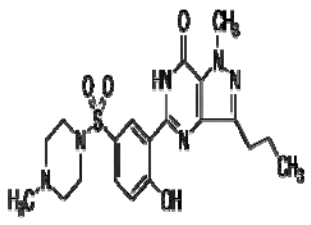
Cick on image to enlarge

Catalogue #: D294352
Chemical Name: Desmethyl Thio**sildenafil**-d8
CAS Number: 1215321-44-0
Mol. Formula: C21H20D8N6O3S2
Synonyms: 5-[2-Ethoxy-5-(1-piperazinyl-d8-sulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl- 7H-pyrazolo[4,3-d]pyrimidine-7-thione;



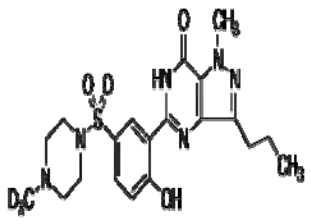
Click on image to enlarge

Catalogue #: D449445
Chemical Name: 3-(6,7-Dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxy-benzenesulfonyl Chloride
CAS Number: 479074-07-2
Mol. Formula: C17H19ClN4O3S2
Synonyms:



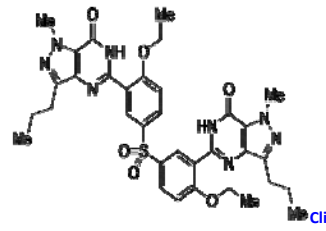
Click on image to enlarge

Chemical Name: Desethyl Sildenafil
CAS Number: 139755-91-2
Mol. Formula: C20H26N6O4S
Synonyms: 5-[2-Hydroxy-5-(4-methylpiperazinylsulphonyl)phenyl]1-methyl-3-n-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyramidin-7-one; 5-[2-Hydroxy-5-[[4-(methyl)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



Click on image to enlarge

Catalogue #: D289602
Chemical Name: Desethyl Sildenafil-d3
CAS Number: 1346603-75-5
Mol. Formula: C20H23D3N6O4S
Synonyms: 5-[2-Hydroxy-5-(4-methyl-d3-piperazinylsulphonyl)phenyl]1-methyl-3-n-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyramidin-7-one; 5-[2-Hydroxy-5-[[4-(methyl-d3)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;

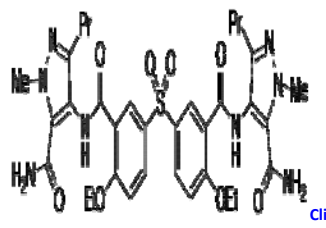


Click on image to enlarge

Catalogue #: D231215
Chemical Name: De(methypiperazinyl) Sildenafil Dimer Impurity
CAS Number: 1346603-48-2
Mol. Formula: C34H38N8O6S
Synonyms: 5-[2-Ethoxy-5-[4-[4-ethoxy-3-(1-methyl-7-oxo-3-propyl-4,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-yl)phenyl]sulfonyl]phenyl]-1-methyl-3-n-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one;

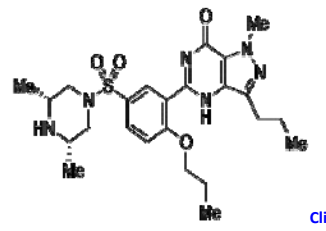
no image of structure available

Catalogue #: D231235
Chemical Name: Demethylpiperazinyl Sildenafil Sulfonic Acid
CAS Number:
Mol. Formula: C17H20N4O5S
Synonyms: 3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxybenzenesulfonic Acid;



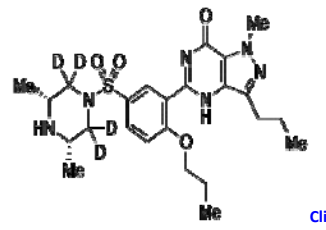
Click on image to enlarge

Catalogue #: A603070
Chemical Name: 3-[[[5-Aminocarbonyl-1-methyl-3-propyl-1H-pyrazol-4-yl]amino]carbonyl]-4-ethoxy-benzenesulfonyl Dimer
CAS Number:
Mol. Formula: C34H42N8O8S
Synonyms: 3,3'-Sulfonyl Bis[(4-Ethoxy-3-(6,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo-pyrimidin-5-yl)benzene)



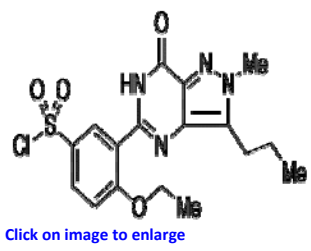
Click on image to enlarge

Catalogue #: D289495
Chemical Name: O-Desethyl-O-propyl Methiso**sildenafil**
CAS Number: 1391053-82-9
Mol. Formula: C24H34N6O4S
Synonyms: rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



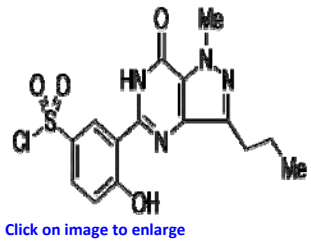
Click on image to enlarge

Catalogue #: D289497
Chemical Name: O-Desethyl-O-propyl Methiso**sildenafil**-d4
CAS Number:
Mol. Formula: C24H30D4N6O4S
Synonyms: rel-5-[5-[[(3R,5S)-3,5-Dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one-d4;



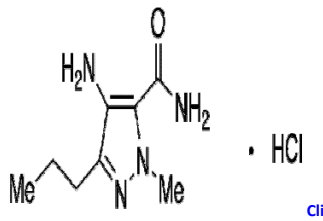
Click on image to enlarge

Catalogue #: D231290
Chemical Name: Demethylpiperazinyl Iso Sildenafil Sulfonyl Chloride
CAS Number: 501120-42-9
Mol. Formula: C17H19ClN4O4S
Synonyms: 3-(6,7-Dihydro-2-methyl-7-oxo-3-propyl-2H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxy-benzenesulfonyl Chloride



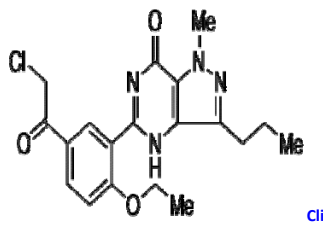
Click on image to enlarge

Catalogue #: D231300
Chemical Name: Demethylpiperazinyl Desethyl Sildenafil Sulfonyl Chloride
CAS Number: 139756-27-7
Mol. Formula: C15H15ClN4O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-hydroxy-benzenesulfonyl Chloride; 5-(5-Chlorosulfonyl-2-hydroxyphenyl)-1-methyl-3-propyl-1,6-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one



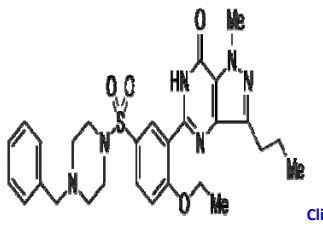
Click on image to enlarge

Catalogue #: A617420
Chemical Name: 4-Amino-1-methyl-3-propyl-1H-pyrazole-5-carboxamide Hydrochloride
CAS Number: 247584-10-7
Mol. Formula: C8H15ClN4O
Synonyms: 4-Amino-2-methyl-5-propyl-2H-pyrazole-3-carboxamide Hydrochloride;



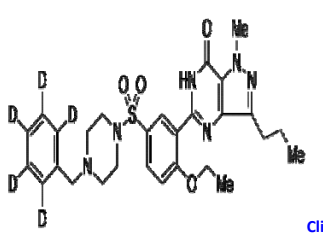
Click on image to enlarge

Catalogue #: C365535
Chemical Name: Chlorodenafil
CAS Number: 1058653-74-9
Mol. Formula: C19H21ClN4O3
Synonyms: 5-[5-(2-Chloroacetyl)-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one;



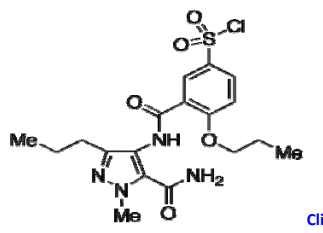
Click on image to enlarge

Catalogue #: D292205
Chemical Name: N-Desmethyl-N-benzyl Sildenafil
CAS Number:
Mol. Formula: C28H34N6O4S
Synonyms: 5-[2-Ethoxy-5-(1-benzyl-1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Benzyl Sildenafil;



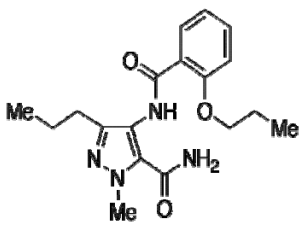
Click on image to enlarge

Catalogue #: D292207
Chemical Name: N-Desmethyl-N-benzyl Sildenafil-d5
CAS Number:
Mol. Formula: C28H29D5N6O4S
Synonyms: 5-[2-Ethoxy-5-(1-(benzyl-d5)-1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Benzyl Sildenafil-d5;



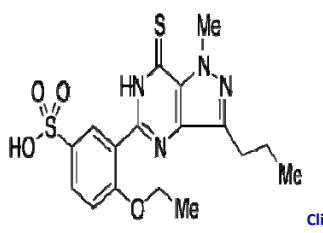
Click on image to enlarge

Catalogue #: A603110
Chemical Name: 3-[[[5-(Aminocarbonyl)-1-methyl-3-propyl-1H-pyrazol-4-yl]amino]carbonyl]-4-propoxy-benzenesulfonyl Chloride
CAS Number: 374776-34-8
Mol. Formula: C18H23ClN4O5S
Synonyms:



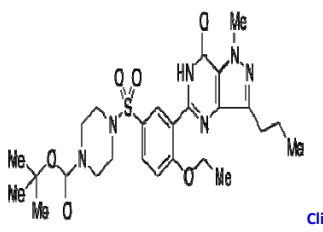
Click on image to enlarge

Catalogue #: A603105
Chemical Name: 3-[[[5-(Aminocarbonyl)-1-methyl-3-propyl-1H-pyrazol-4-yl]amino]carbonyl]-4-propoxybenzene
CAS Number: 139756-04-0
Mol. Formula: C18H24N4O3
Synonyms: 1-Methyl-4-(2-propoxybenzamido)-3-propylpyrazole-5-carboxamide; 1-Methyl-4-[(2-propoxybenzoyl)amino]-3-propyl-1H-pyrazole-5-carboxamide



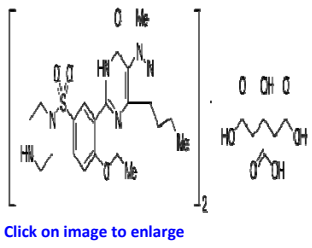
Click on image to enlarge

Catalogue #: D231260
Chemical Name: Demethylpiperazinyl 7-Desoxo 7-Thioxo**sildenafil** Sulfonic Acid
CAS Number: 1353018-10-6
Mol. Formula: C17H20N4O4S2
Synonyms: 4-Ethoxy-3-(1-methyl-3-propyl-7-thioxo-6,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-yl)benzenesulfonic Acid



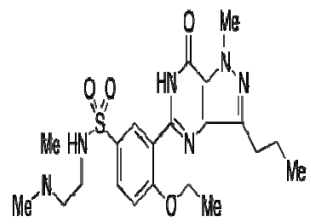
Click on image to enlarge

Catalogue #: D292245
Chemical Name: N-(Desmethyl)-tert-butyl Acetate Sildenafil
CAS Number: 398507-63-6
Mol. Formula: C26H36N6O6S
Synonyms: tert-Butyl 4-((4-Ethoxy-3-(1-methyl-7-oxo-3-propyl-6,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-yl)phenyl)sulfonyl)piperazine-1-carboxylate; 4-[[3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazinecarboxylic Acid 1,1-Dimethylethyl Ester



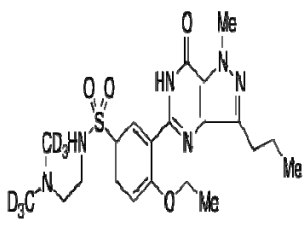
Click on image to enlarge

Catalogue #: D292201
Chemical Name: N-Desmethyl Sildenafil Hemicitrate
CAS Number:
Mol. Formula: C48H64N12O15S2
Synonyms: 5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one Hemicitrate; Desmethyl**sildenafil** Hemicitrate; UK 103320 Hemicitrate



Click on image to enlarge

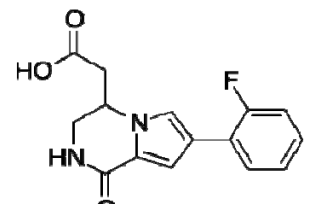
Catalogue #: D289520
Chemical Name: Descarbon**sildenafil**
CAS Number: 1393816-99-3
Mol. Formula: C21H30N6O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-N-[2-(dimethylamino)ethyl]-4-ethoxy-benzenesulfonamide



Click on image to enlarge

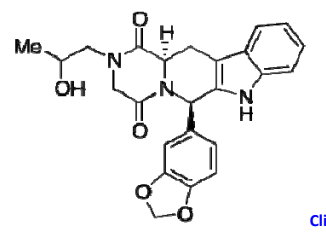
Catalogue #: D289522
Chemical Name: Descarbon**sildenafil**-d6
CAS Number:
Mol. Formula: C21H24D6N6O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-N-[2-(dimethyl-d6-amino)ethyl]-4-ethoxy-benzenesulfonamide

Tadalafil Related Compounds (commercial standards available) – includes deuterated standards.



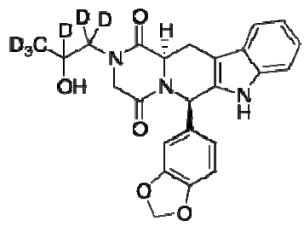
Click on image to enlarge

Catalogue #: F595590
Chemical Name: 7-(2-Fluorophenyl)-1,2,3,4-tetrahydro-1-oxo-pyrrolo[1,2-a]pyrazine-4-acetic Acid
CAS Number: 1170575-17-3
Mol. Formula: C15H13FN2O3
Synonyms:



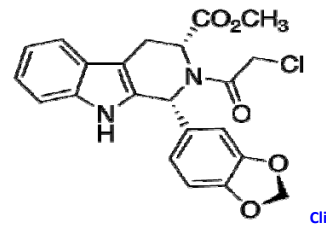
Click on image to enlarge

Catalogue #: H952705
Chemical Name: 2-Hydroxypropyl Nor**tadalafil**
CAS Number: 1353020-85-5
Mol. Formula: C24H23N3O5
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(2-hydroxypropyl)-pyrazino[1&#65533;,2&#65533;:1,6]pyrido[3,4-b]indole-1,4-dione;



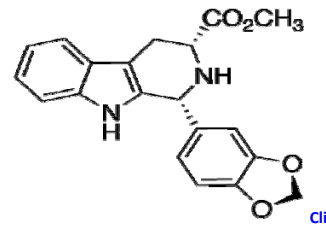
Click on image to enlarge

Catalogue #: H952707
Chemical Name: 2-Hydroxypropyl-d6 Nor**tadalafil**
CAS Number:
Mol. Formula: C24H17D6N3O5
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(2-hydroxypropyl)-pyrazino[1&#65533;,2&#65533;:1,6]pyrido[3,4-b]indole-1,4-dione-d6;



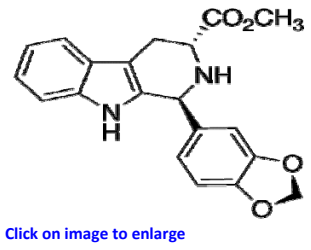
Click on image to enlarge

Catalogue #: M330125
Chemical Name: (1R,3R)-Methyl-1,2,3,4-tetrahydro-2-chloroacetyl-1-(3,4-methylenedioxyphenyl)-9H-pyrido[3,4-b]indole-3-carboxylate (Chloropre**tadalafil**)
CAS Number: 171489-59-1
Mol. Formula: C22H19ClN2O5
Synonyms: (1R,3R)-1-(1,3-Benzodioxol-5-yl)-2-(2-chloroacetyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester;



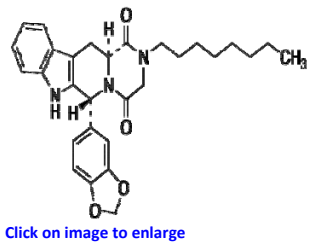
Click on image to enlarge

Catalogue #: M330150
Chemical Name: (1R,3R)-Methyl-1,2,3,4-tetrahydro-1-(3,4-methylenedioxyphenyl)-9H-pyrido[3,4-b]indole-3-carboxylate
CAS Number: 171596-41-1
Mol. Formula: C20H18N2O4
Synonyms: (1R,3R)-1-(1,3-Benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester;



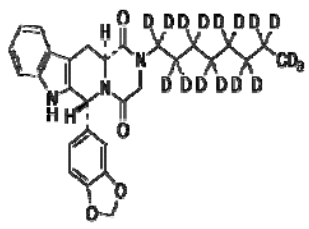
Click on image to enlarge

Catalogue #: M330155
Chemical Name: (1S,3R)-Methyl-1,2,3,4-tetrahydro-1-(3,4-methylenedioxyphenyl)-9H-pyrido[3,4-b]indole-3-carboxylate
CAS Number: 171596-42-2
Mol. Formula: C20H18N2O4
Synonyms: (1S,3R)-1-(1,3-Benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester;



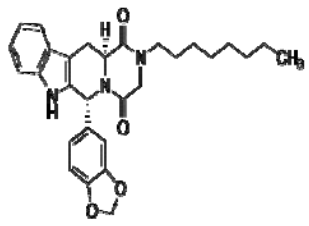
Click on image to enlarge

Catalogue #: O241350
Chemical Name: N-Octyl Nor**tadalafil**
CAS Number: 1173706-35-8
Mol. Formula: C29H33N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-octylpyrazino[1&#65533;,2&#65533;:1,6]pyrido[3,4-b]indole-1,4-dione;



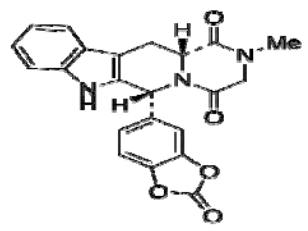
Click on image to enlarge

Catalogue #: O241352
Chemical Name: N-Octyl Nor**tadalafil**-d17
CAS Number:
Mol. Formula: C29H16D17N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(octyl-d17)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



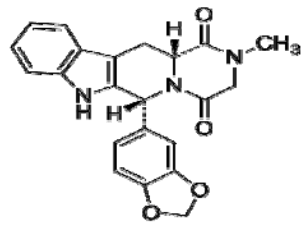
Click on image to enlarge

Catalogue #: O241360
Chemical Name: N-Octyl cis-Nor**tadalafil**
CAS Number:
Mol. Formula: C29H33N3O4
Synonyms: (6R,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-octylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



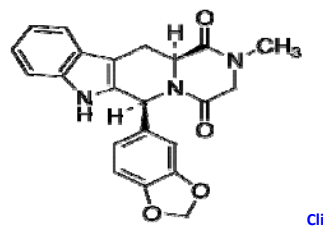
Click on image to enlarge

Catalogue #: O870430
Chemical Name: 2'-Oxo Tadalafil
CAS Number:
Mol. Formula: C22H17N3O5
Synonyms: (6R,12aR)-6-(2-Oxo-1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; 2'-Keto Tadalafil;



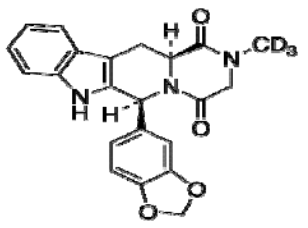
Click on image

Catalogue #: T004500
Chemical Name: Tadalafil
CAS Number: 171596-29-5
Mol. Formula: C22H19N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; Cialis; GF 196960; IC 351; ICOS 351; Tildenafil; UK 336017;



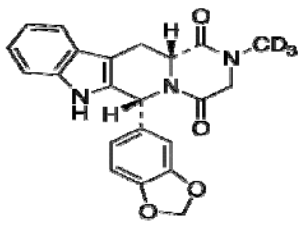
Click on image to enlarge

Catalogue #: T004505
Chemical Name: ent-Tadalafil
CAS Number: 629652-72-8
Mol. Formula: C22H19N3O4
Synonyms: (6S,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methyl-pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; L-Tadalafil; L-Tildenafil;



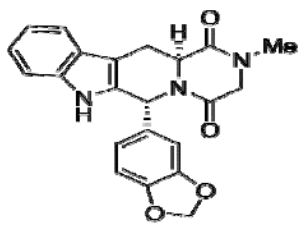
Click on image to enlarge

Catalogue #: T004507
Chemical Name: ent-Tadalafil-d3
CAS Number:
Mol. Formula: C22H16D3N3O4
Synonyms: (6S,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(methyl-d3)-pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; L-Tadalafil-d3; L-Tildenafil-d3;



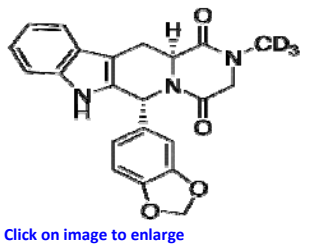
Click on image to enlarge

Catalogue #: T004510
Chemical Name: Tadalafil-d3
CAS Number: 960226-55-5
Mol. Formula: C22H16D3N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; Cialis-d3; GF 196960-d3; IC 351-d3; ICOS 351-d3; Tildenafil-d3; UK 336017-d3;



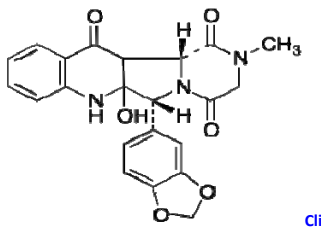
Click on image to enlarge

Catalogue #: T004520
Chemical Name: cis-Tadalafil
CAS Number: 171596-27-3
Mol. Formula: C22H19N3O4
Synonyms: (6R,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R-cis)-6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a- hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



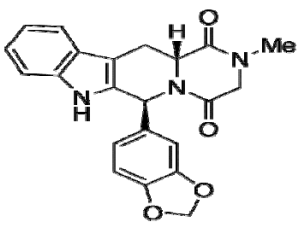
Click on image to enlarge

Catalogue #: T004522
Chemical Name: cis-Tadalafil-d3
CAS Number:
Mol. Formula: C22H16D3N3O4
Synonyms: (6R,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R-cis)-6-(1,3-benzodioxol-5-yl)- 2,3,6,7,12,12a-hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



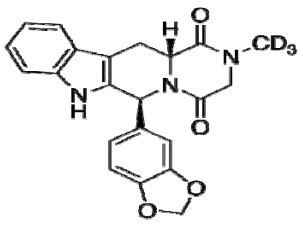
Click on image to enlarge

Catalogue #: T004525
Chemical Name: Tadalafil Hydroxypiperidone
CAS Number:
Mol. Formula: C22H19N3O6
Synonyms: Tadalafil Impurity



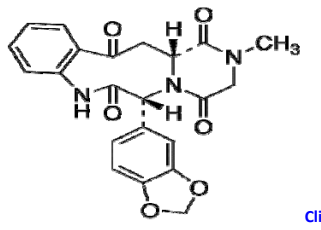
Click on image to enlarge

Catalogue #: T004530
Chemical Name: cis-ent-Tadalafil
CAS Number: 171596-28-4
Mol. Formula: C22H19N3O4
Synonyms: (6S,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6S-cis)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a- hexahydro-2-methylpyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



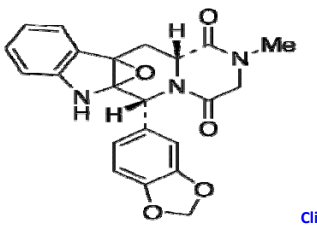
Click on image to enlarge

Catalogue #: T004532
Chemical Name: cis-ent-Tadalafil-d3
CAS Number:
Mol. Formula: C22H16D3N3O4
Synonyms: 6S,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6S-cis)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a- hexahydro-2-(methyl-d3)pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



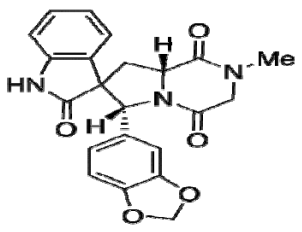
Click on image to enlarge

Catalogue #: T004535
Chemical Name: Tadalafil Ketolactam
CAS Number: 1346605-38-6
Mol. Formula: C22H19N3O6
Synonyms: (6R,14aR)-rel-6-(1,3-Benzodioxol-5-yl)-2,3,14,14a-tetrahydro-2-methylpyrazino[1,2-d][1,4]benzodiazonine-1,4,7,13(6H,8H)-tetrone;



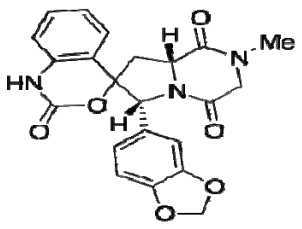
Click on image to enlarge

Catalogue #: T004540
Chemical Name: Tadalafil Epoxide Discontinued
CAS Number:
Mol. Formula: C22H19N3O5
Synonyms: Epoxy Tadalafil;



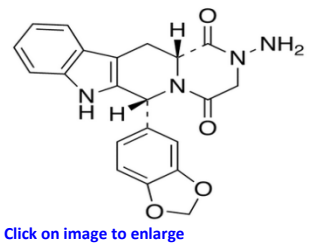
Click on image to enlarge

Catalogue #: T004550
Chemical Name: Tadalafil Spiro-oxindole
CAS Number:
Mol. Formula: C22H19N3O5
Synonyms: Tadalafil Impurity



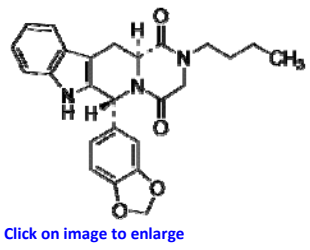
Click on image to enlarge

Catalogue #: T004555
Chemical Name: Tadalafil Spiro-2-keto-1,3-oxazine
CAS Number:
Mol. Formula: C22H19N3O6
Synonyms: Tadalafil Impurity



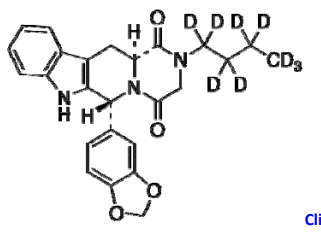
Click on image to enlarge

Catalogue #: A629550
Chemical Name: Amino Tadalafil
CAS Number: 385769-84-6
Mol. Formula: C21H18N4O4
Synonyms: (6R,12aR)-2-Amino-6-(1,3-benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



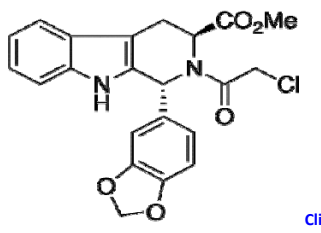
Click on image to enlarge

Catalogue #: B693585
Chemical Name: N-Butyl Nor**tadalafil**
CAS Number: 171596-31-9
Mol. Formula: C25H25N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2-butyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



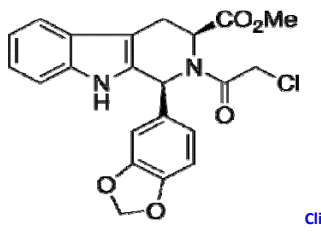
Click on image to enlarge

Catalogue #: B693587
Chemical Name: N-Butyl Nor**tadalafil**-d9
CAS Number:
Mol. Formula: C25H16D9N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2-(butyl-d9)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;



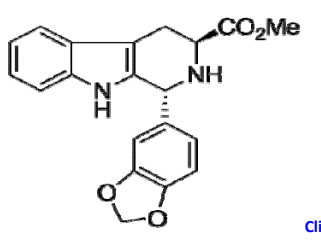
Click on image to enlarge

Catalogue #: B200000
Chemical Name: (1R,3S)-1-(1,3-Benzodioxol-5-yl)-2-(2-chloroacetyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester
CAS Number: 629652-44-4
Mol. Formula: C22H19ClN2O5
Synonyms:



Click on image to enlarge

Catalogue #: B200005
Chemical Name: (1S,3S)-1-(1,3-Benzodioxol-5-yl)-2-(2-chloroacetyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester
CAS Number: 629652-42-2
Mol. Formula: C22H19ClN2O5
Synonyms:



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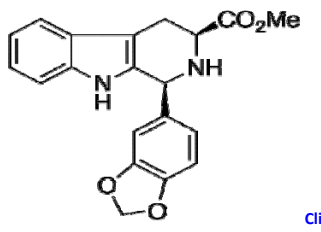
Catalogue #: B200025
Chemical Name: (1R,3S)-1-(1,3-Benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester
CAS Number: 171596-44-4
Mol. Formula: C20H18N2O4
Synonyms:



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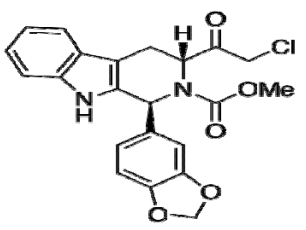
Catalogue #: B200020
Chemical Name: (1S,3S)-1-(1,3-Benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester
CAS Number: 171596-43-3
Mol. Formula: C20H18N2O4
Synonyms: (1S-cis)-1-(1,3-benzodioxol-5-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester



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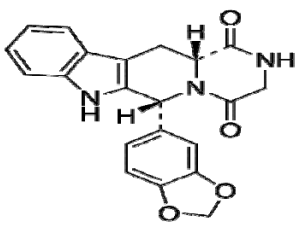
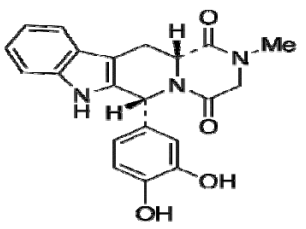
Catalogue #: B121700
Chemical Name: (1S,3R)-1-Benzo[1,3]dioxol-5-yl-2-(2-chloro-acetyl)-2,3,4,9-tetrahydro-1H-b-carboline-3-carboxylic Acid Methyl Ester
CAS Number: 629652-40-0
Mol. Formula: C22H19ClN2O5
Synonyms: (1S,3R)-1-(1,3-Benzodioxol-5-yl)-2-(2-chloroacetyl)-2,3,4,9-tetrahydro1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester; (1S,3R)-1-(1,3-Benzodioxol-5-yl)-2-(chloroacetyl)-2,3,4,9-tetrahydro1H-pyrido[3,4-b]indole-3-carboxylic Acid Methyl Ester;



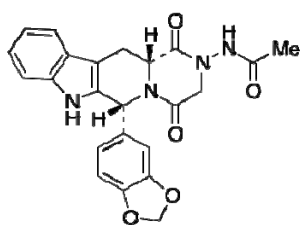
Click on image to enlarge

Catalogue #: D293800
Chemical Name: N-Desmethyl Tadalafil
CAS Number: 171596-36-4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R-trans)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; Nor**tadalafil**



Click on image to enlarge

Catalogue #: D291990
Chemical Name: Desmethylene Tadalafil
CAS Number: 171489-03-5
Mol. Formula: C21H19N3O4
Synonyms: (6R,12aR)-6-(3,4-dihydroxyphenyl)-2,3,6,7,12,12a-hexahydro-2-methyl-pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R,trans)-6-(3,4-dihydroxyphenyl)-2,3,6,7,12,12a-hexahydro-2-methyl-pyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione;

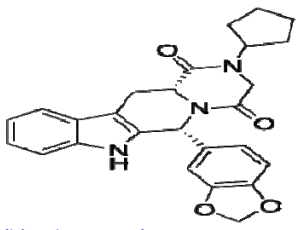


Click on image to enlarge

Catalogue #: A161250
Chemical Name: Acetamino**tadalafil**
CAS Number: 1446144-71-3
Mol. Formula: C23H20N4O5
Synonyms: N-[(6R,12aR)-6-(1,3-Benzodioxol-5-yl)-3,4,6,7,12,12a-hexahydro-1,4-dioxopyrazino[1,2:1,6]pyrido[3,4-b]indol-2(1H)-yl]-acetamide;

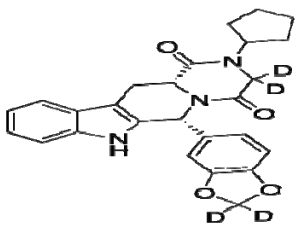
no image of structure available

Catalogue #: D293805
Chemical Name: N-Desmethyl ent-Tadalafil
CAS Number: 929100-66-3
Mol. Formula: C21H17N3O4
Synonyms: (6R,12aS)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione



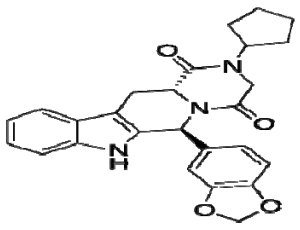
Click on image to enlarge

Catalogue #: B199000
Chemical Name: N-Desmethyl-N-cyclopentyl Tadalafil
CAS Number: 171596-32-0
Mol. Formula: C26H25N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2-cyclopentyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione; (6R-trans)-6-(1,3-Benzodioxol-5-yl)-2-cyclopentyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione



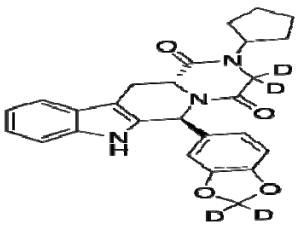
Click on image to enlarge

Catalogue #: B199002
Chemical Name: N-Desmethyl-N-cyclopentyl Tadalafil-D4
CAS Number:
Mol. Formula: C26H21D4N3O4
Synonyms: (6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2-cyclopentyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione-D4; (6R-trans)-6-(1,3-Benzodioxol-5-yl)-2-cyclopentyl-2,3,6,7,12,12a-hexahydropyrazino[1,2:1,6]pyrido[3,4-b]indole-1,4-dione-D4



Click on image to enlarge

Catalogue #: B199005
Chemical Name: N-Desmethyl-N-cyclopentyl cis-ent-Tadalafil
CAS Number:
Mol. Formula: C26H25N3O4
Synonyms:



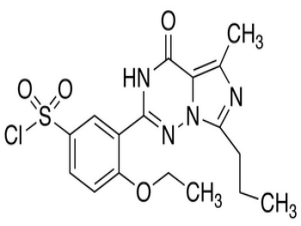
Click on image to enlarge

Catalogue #: B199007
Chemical Name: N-Desmethyl-N-cyclopentyl cis-ent-Tadalafil-D4
CAS Number:
Mol. Formula: C26H21D4N3O4
Synonyms:

Vardenafil Related Compounds (commercial standards available) – includes deuterated standards.

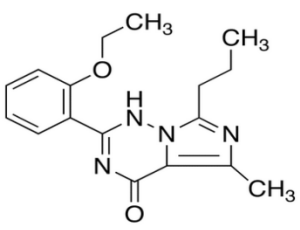
no image of structure available

Chemical Name: 2-Ethoxybenzamidine Hydrochloride
CAS Number: 18637-00-8
Mol. Formula: C9H13ClN2O
Synonyms: 2-Ethoxybenzenecarboximidamide Hydrochloride; o-Ethoxybenzamidine Monohydrochloride; 2-Ethoxybenzenecarboximidamide Monohydrochloride



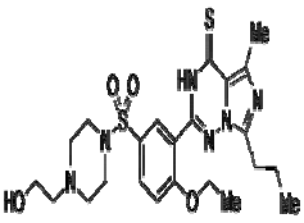
Click on image to enlarge

Catalogue #: E892500
Chemical Name: 4-Ethoxy-3-(5-methyl-4-oxo-7-propyl-3,4-dihydro-imidazo[5,1-f][1,2,4]-triazin-2-yl)benzene-sulfonyl Chloride
CAS Number: 224789-26-8
Mol. Formula: C17H19ClN4O4S
Synonyms: 3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxy-benzenesulfonyl Chloride;



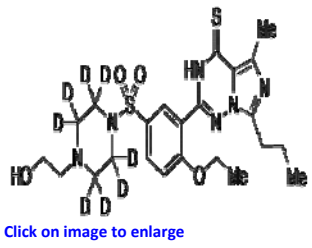
Click on image to enlarge

Catalogue #: E892745
Chemical Name: 2-(2-Ethoxyphenyl)-5-methyl-7-propyl-3H-imidazo[5,1-f][1,2,4]triazin-4-one
CAS Number: 224789-21-3
Mol. Formula: C17H20N4O2
Synonyms: 2-(2-Ethoxyphenyl)-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one;



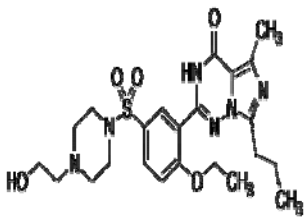
Click on image to enlarge

Catalogue #: H963400
Chemical Name: Hydroxythio**vardenafil**
CAS Number: 912576-30-8
Mol. Formula: C23H32N6O4S2
Synonyms: 2-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazine-4(1H)-thione; 4-[[3-(1,4-Dihydro-5-methyl-7-propyl-4-thioxoimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazineethanol;



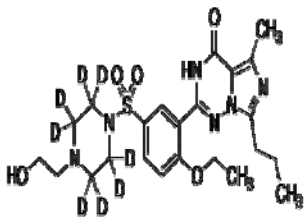
Click on image to enlarge

Catalogue #: H963402
Chemical Name: Hydroxythio**vardenafil**-d8
CAS Number:
Mol. Formula: C23H24D8N6O4S2
Synonyms: 2-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazine-4(1H)-thione-d8; 4-[[3-(1,4-Dihydro-5-methyl-7-propyl-4-thioxoimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazineethanol-d8;



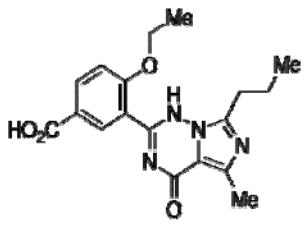
Click on image to enlarge

Catalogue #: H995300
Chemical Name: Hydroxy Vardenafil
CAS Number: 224785-98-2
Mol. Formula: C23H32N6O5S
Synonyms: 2-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-piperazinyl]sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazin-4(1H)-one; 4-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo [5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-1-piperazineethanol;



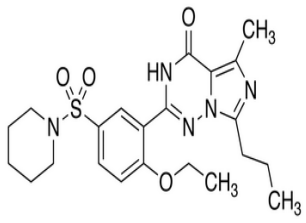
Click on image to enlarge

Catalogue #: H995302
Chemical Name: Hydroxy Vardenafil-d8
CAS Number:
Mol. Formula: C23H24D8N6O5S
Synonyms: 2-[2-Ethoxy-5-[[4-(2-hydroxyethyl)-1-(piperazinyl-d8)]sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazin-4(1H)-one; 4-[[3-(1,4-Dihydro-5-methyl-4-oxo-7- propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-1-(piperazine-d8)ethanol;



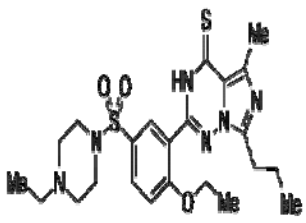
Click on image to enlarge

Chemical Name: Norneo Vardenafil
CAS Number: 358390-39-3
Mol. Formula: C18H20N4O4
Synonyms: 3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxybenzoic Acid;



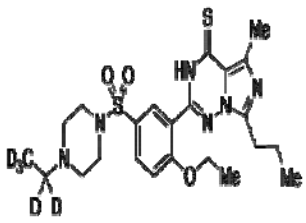
Click on image to enlarge

Catalogue #: P839615
Chemical Name: Pseudo Vardenafil
CAS Number: 224788-34-5
Mol. Formula: C22H29N5O4S
Synonyms: 2-[2-Ethoxy-5-(1-piperidinylsulfonyl)phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazin-4(1H)-one; Piperidenafil; Pseudo**vardenafil**;



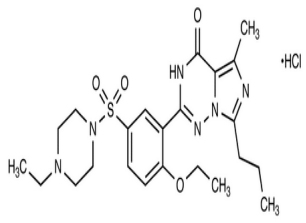
Click on image to enlarge

Catalogue #: T384250
Chemical Name: Thio**vardenafil**
CAS Number: 912576-24-0
Mol. Formula: C23H32N6O3S2
Synonyms: 2-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazine-4(1H)-thione; 1-[[3-(1,4-Dihydro-5-methyl-7-propyl-4-thioxoimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-4-ethylpiperazine;



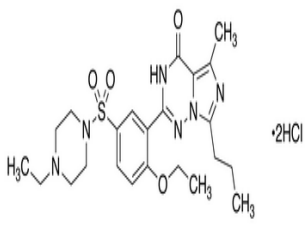
Click on image to enlarge

Catalogue #: T384252
Chemical Name: Thio**vardenafil**-d5
CAS Number:
Mol. Formula: C23H27D5N6O3S2
Synonyms: 2-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazine-4(1H)-thione-d5; 1-[[3-(1,4-Dihydro-5-methyl-7-propyl-4-thioxoimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-4-ethylpiperazine-d5;



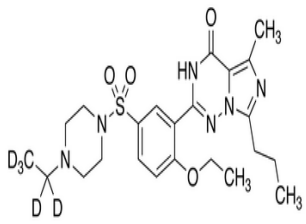
Click on image to enlarge

Catalogue #: V098000
Chemical Name: Vardenafil, Hydrochloride Salt Discontinued See V098001
CAS Number: 224785-91-5
Mol. Formula: C23H33ClN6O4S
Synonyms: Levitra, Valdenafil



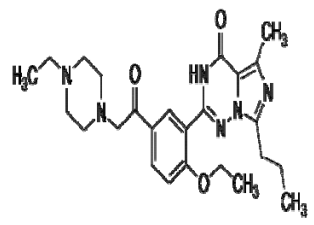
Click on image to enlarge

Catalogue #: V098001
Chemical Name: Vardenafil Dihydrochloride Salt
CAS Number: 224789-15-5
Mol. Formula: C23H34Cl2N6O4S
Synonyms: 1-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-4-ethyl-piperazine;Levitra; Nuviva;



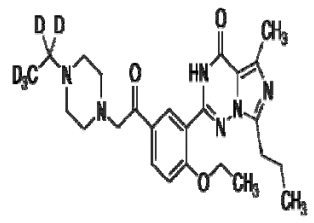
Click on image to enlarge

Catalogue #: V098002
Chemical Name: Vardenafil-d5
CAS Number: 1189685-70-8
Mol. Formula: C23H27D5N6O4S
Synonyms: 1-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-4-(ethyl-d5)-piperazine; Levitra-d5; Nuviva-d5;



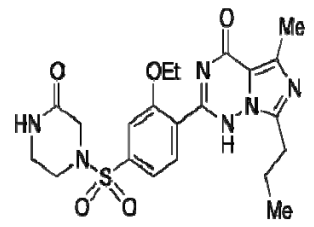
Click on image to enlarge

Catalogue #: V098015
Chemical Name: Vardenafil Acetyl Analogue
CAS Number: 1261351-28-3
Mol. Formula: C25H34N6O3
Synonyms: 2-[2-Ethoxy-5-[2-(4-ethyl-1-piperazinyl)acetyl]phenyl]-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one;



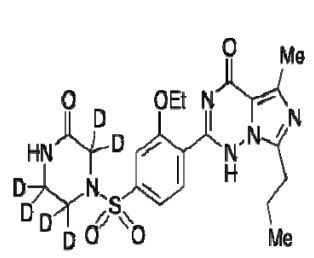
Click on image to enlarge

Catalogue #: V098017
Chemical Name: Vardenafil Acetyl-d5 Analogue
CAS Number: 1330171-51-1
Mol. Formula: C25H29D5N6O3
Synonyms: 2-[2-Ethoxy-5-[2-(4-(ethyl-d5)-1-piperazinyl)acetyl]phenyl]-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one;



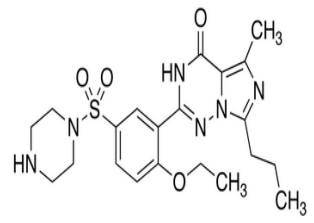
Click on image to enlarge

Catalogue #: V098030
Chemical Name: Vardenafil Oxopiperazine (Impurity)
CAS Number: 448184-58-5
Mol. Formula: C21H26N6O5S
Synonyms: 2-[2-Ethoxy-5-[(3-oxo-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one; 4-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-piperazinone



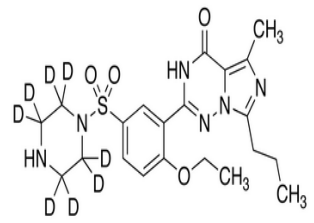
Click on image to enlarge

Catalogue #: V098032
Chemical Name: Vardenafil Oxopiperazine-D6 (Impurity)
CAS Number:
Mol. Formula: C21H20D6N6O5S
Synonyms: 2-[2-Ethoxy-5-[(3-oxo-1-piperazinyl)sulfonyl]phenyl]-5-methyl-7-propyl-imidazo[5,1-f][1,2,4]triazin-4(1H)-one-D6; 4-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-piperazinone-D6



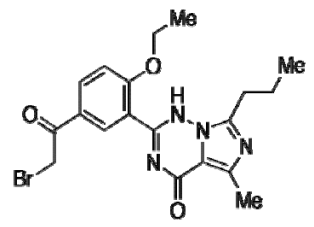
Click on image to enlarge

Catalogue #: D289950
Chemical Name: N-Desethyl Vardenafil
CAS Number: 448184-46-1
Mol. Formula: C21H28N6O4S
Synonyms: 1-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-piperazine;



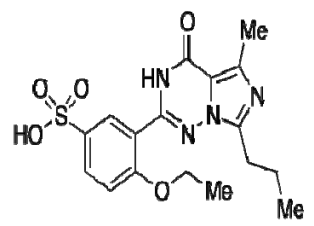
Click on image to enlarge

Catalogue #: D289952
Chemical Name: N-Desethyl Vardenafil-d8
CAS Number:
Mol. Formula: C21H20D8N6O4S
Synonyms: 1-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-piperazine-d8;



Click on image to enlarge

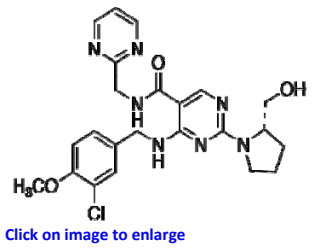
Catalogue #: D220200
Chemical Name: 1-Decarboxyl-1-(bromoacetyl) Norneo**vardenafil**
CAS Number: 358388-58-6
Mol. Formula: C19H21BrN4O3
Synonyms: 2-[5-(Bromoacetyl)-2-ethoxyphenyl]-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazin-4(1H)-one;



Click on image to enlarge

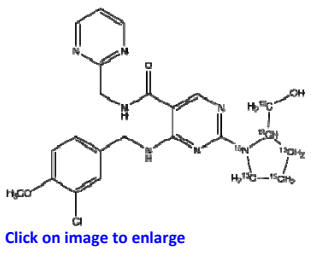
Catalogue #: D453410
Chemical Name: 3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxybenzenesulfonic Acid
CAS Number: 437717-43-6
Mol. Formula: C17H20N4O5S
Synonyms:

Avanafil Related Compounds (commercial standards available) – includes deuterated standards.



Click on image to enlarge

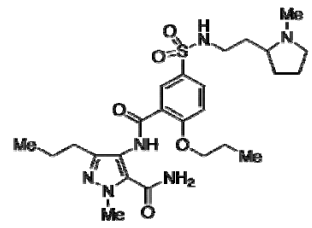
Catalogue #: A794670
Chemical Name: Avanafil
CAS Number: 330784-47-9
Mol. Formula: C23H26ClN7O3
Synonyms: (S)-2-(2-Hydroxymethyl-1-pyrrolidinyl)-4-(3-chloro-4-methoxybenzylamino)-5-[(2-pyrimidinylmethyl)carbamoyl]pyrimidine; 4-[[(3-Chloro-4-methoxyphenyl)methyl] amino]-2-[(2S)-2-(hydroxymethyl)-1-pyrrolidinyl]-N-(2-pyrimidinylmethyl)-5-pyrimidinecarboxamide; TA 1790;



Click on image to enlarge

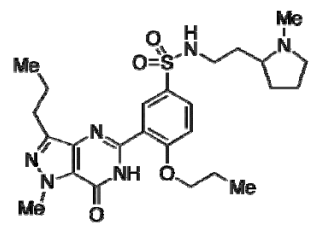
Catalogue #: A794672
Chemical Name: Avanafil-13C5,15N
CAS Number:
Mol. Formula: C1813C5H26ClN615NO3
Synonyms: (S)-2-(2-Hydroxymethyl-1-pyrrolidinyl)-4-(3-chloro-4-methoxybenzylamino)-5-[(2-pyrimidinylmethyl)carbamoyl]pyrimidine-13C5,15N; 4-[[(3-Chloro-4-methoxyphenyl)methyl] amino]-2-[(2S)-2-(hydroxymethyl)-1-pyrrolidinyl]-N-(2-pyrimidinylmethyl)-5-pyrimidinecarboxamide-13C5,15N; TA 1790-13C5,15N;

Udenafil Related Compounds (commercial standards available) – includes deuterated standards.



Click on image to enlarge

Catalogue #: M320180
Chemical Name: 1-Methyl-4-[[5-[[[2-(1-methyl-2-pyrrolidinyl)ethyl]amino]sulfonyl]-2-propoxybenzoyl]amino]-3-propyl-1H-pyrazole-5-carboxamide
CAS Number: 382592-28-1
Mol. Formula: C25H38N6O5S
Synonyms:



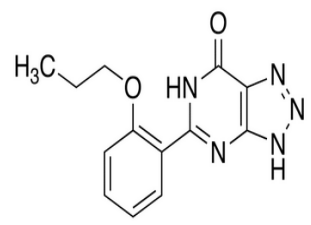
Click on image to enlarge

Catalogue #: U250500
Chemical Name: Udenafil
CAS Number: 268203-93-6
Mol. Formula: C25H36N6O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-N-[2-(1-methyl-2-pyrrolidinyl)ethyl]-4-propoxybenzenesulfonamide; DA 8159; Zydena;

no image of structure available

Catalogue #: U250502
Chemical Name: Udenafil-d7
CAS Number: 1175992-76-3
Mol. Formula: C25H29D7N6O4S
Synonyms: 3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-N-[2-(1-methyl-2-pyrrolidinyl)ethyl]-4-(propoxy-d7)benzenesulfonamide; DA 8159-d7; Zydena-d7;

Zaprinast

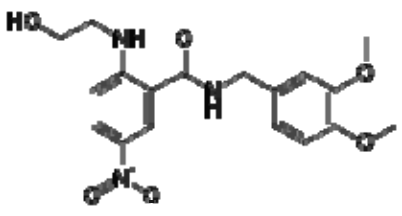


Click on image to enlarge

Catalogue #: Z150000
Chemical Name: Zaprinast
CAS Number: 37762-06-4
Mol. Formula: C13H13N5O2
Synonyms: 3,6-dihydro-5-(2-propoxyphenyl)-7H-1,2,3-triazolo[4,5-d]pyrimidin-7-one; 1,4-Dihydro-5-[2-propoxyphenyl]-7H-1,2,3-triazolo[4,5-d]pyrimidine-7-one; 8-Aza-2-(2-propoxyphenyl)-6-purinone; M&B 22,948;

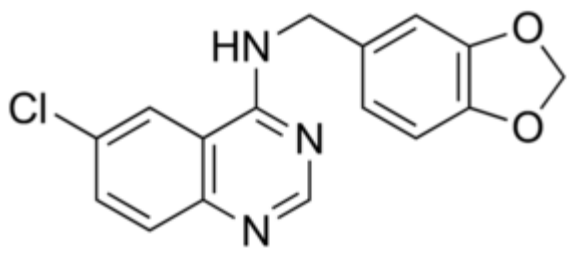
4. Additional Items for Consideration Web Based Search Data

Benzamidenafil
IUPAC name: N-[(3,4-Dimethoxyphenyl)methyl]-2-(1-hydroxypropan-2-ylamino)-5-nitrobenzamide
Other names: Xanthoanthrafil
CAS number: 1020251-53-

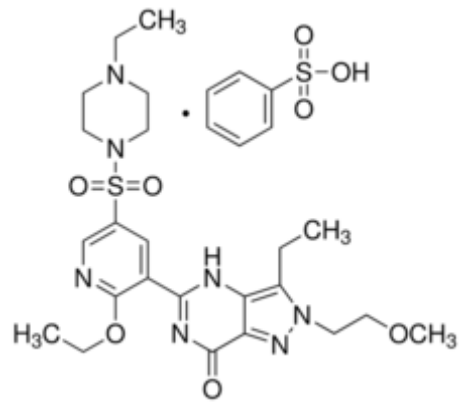


5. Additional Items for Consideration Novel PDE-5 inhibitors from SIAL

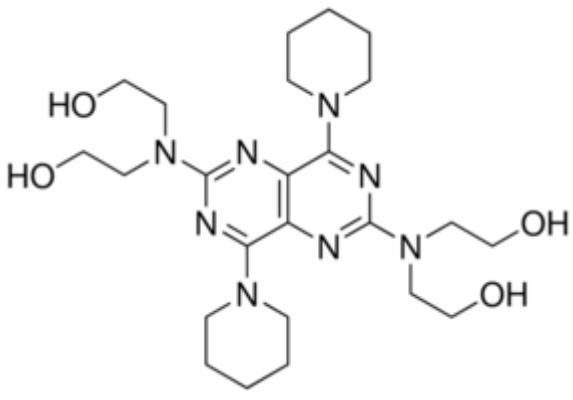
MBCQ
SML0439 SIGMA
≥98% (HPLC)
Synonym: 4-((3,4-Methylenedioxybenzyl)amino)-6-chloroquinazoline
CAS Number 150450-53-6
Empirical Formula (Hill Notation) $C_{16}H_{12}ClN_3O_2$
Molecular Weight 313.74
MDL number MFCD00673946



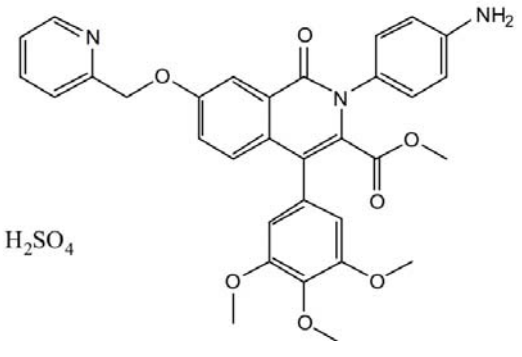
Gisadenafil besylate salt
≥98% (HPLC)
PZ0172 SIGMA
Synonym: 5-[2-Ethoxy-5-[(4-ethyl-1-piperazinyl)sulfonyl]-3-pyridinyl]-3-ethyl-2,6-dihydro-2-(2-methoxyethyl)-7H-pyrazolo[4,3-d]pyrimidin-7-one benzenesulfonate besylate salt, UK 369003-26, UK 369003
CAS Number 334827-98-4
Empirical Formula (Hill Notation) $C_{23}H_{33}N_7O_5S \cdot C_6H_6O_3S$
Molecular Weight 677.79
MDL number MFCD18384964



Dipyridamole
≥98% (TLC), powder
D9766 SIGMA
CAS Number 58-32-2
Empirical Formula (Hill Notation) $C_{24}H_{40}N_8O_4$
Molecular Weight 504.63
EC Number 200-374-7
MDL number MFCD00010555
PubChem Substance ID 24277705
No Longer Offered by SIAL but published and possibly produced in Japan



Product Number T7692
Cas #: 212500-03-3
Synonyms: Methyl-(2-(4-aminophenyl)-1,2-dihydro-1-oxo-7-(2-pyridinylmethoxy)-4-(3,4,5-trimethoxyphenyl))-3-isoquinoline carboxylic acid, sulfate salt
Molecular Formula: C32H29N3O7·H2SO4



The isoquinolone derivative, T-1032, is a potent, selective inhibitor of cyclic GMP-specific phosphodiesterase (PDE5). In studies of PDE isoenzymes isolated from canine tissues, T-1032 was a competitive inhibitor of cyclic GMP hydrolysis by PDE5 at nanomolar concentrations (IC50 1.0 nM, Ki = 1.2 nM).

6. Additional Information

There are a significant number of lead compounds being researched which depart from the classic sildenafil pyrazolopyrimidinone template. These compounds number into the thousands and are likely to appear in greater number over time as research publications and patent literature show more detail on particular structures and their synthesis.

AOAC SMPR 2011.008

Standard Method Performance Requirements for Nucleotides in Infant Formula and Adult/Pediatric Nutritional Formula

Intended Use: Global Dispute Resolution Method

1 Applicability

Determination of nucleotides in all forms of infant, adult, and/or pediatric formula (powders, ready-to-feed liquids, and liquid concentrates). For the purpose of this SMPR, nucleotides are defined as adenosine 5′-monophosphate (CAS 61-19-8), cytidine 5′-monophosphate (CAS 63-37-6), guanosine 5′-monophosphate (CAS 85-32-5), inosine 5′-monophosphate (CAS 131-99-7), and uridine 5′-monophosphate (CAS 58-97-9). It would also be desirable to measure the corresponding nucleosides: adenosine (CAS 58-61-7), cytidine (CAS 65-46-3), guanosine (CAS 118-00-3), inosine (CAS 58-63-9), and uridine (CAS 58-96-8).

2 Analytical Technique

Any analytical technique that meets the following method performance requirements is acceptable.

3 Definitions

*Adult/pediatric formul*a.—Nutritionally complete, specially formulated food, consumed in liquid form, which may constitute the sole source of nourishment (AOAC SPIFAN, 2010), made from any combination of milk, soy, rice, whey, hydrolyzed protein, starch, and amino acids, with and without intact protein.

Infant formula.—Breast-milk substitute specially manufactured to satisfy, by itself, the nutritional requirements of infants during the first months of life up to the introduction of appropriate complementary feeding (Codex Standard 72-1981), made from any combination of milk, soy, rice, whey, hydrolyzed protein, starch, and amino acids, with and without intact protein.

Limit of detection (LOD).—The minimum concentration or mass of analyte that can be detected in a given matrix with no greater than 5% false-positive risk and 5% false-negative risk.

Limit of quantitation (LOQ).—The minimum concentration or mass of analyte in a given matrix that can be reported as a quantitative result.

Repeatability.—Variation arising when all efforts are made to keep conditions constant by using the same instrument and operator, and repeating during a short time period. Expressed as the repeatability standard deviation (SD_r), or % repeatability relative standard deviation ($\%RSD_r$).

Reproducibility.—The SD or RSD calculated from among-laboratory data; expressed as the reproducibility standard deviation (SD_R), or % reproducibility relative standard deviation ($\%RSD_R$).

Recovery.—The fraction or percentage of spiked analyte that is recovered when the test sample is analyzed using the entire method.

Table 1. Method performance requirements[a]

Analytical range	0.02–3.5[b]	
	0.31–22.3[c]	
Limit of detection (LOD)	≤0.006[b]	
Limit of quantitation (LOQ)	≤0.02[b]	
Repeatability (RSD_r)	0.02	≤10%
	0.1	≤8%
	1	≤6%
	5	
Recovery	90–110% of mean spiked recovery over the range of the assay	
Reproducibility (RSD_R)	0.02	≤20%
	0.1	≤16%
	1	≤11%
	5	

[a] Concentrations apply to: (*1*) "ready-to-feed" liquids, "as is"; (*2*) reconstituted powders (25 g into 200 g water); and (*3*) liquid concentrates diluted 1:1 by weight.

[b] mg/100 mL individual nucleotide results reported.

[c] mg/100 mL aggregate of all five nucleotide results reported.

4 Method Performance Requirements

See Table 1.

5 System Suitability Tests and/or Analytical Quality Control

Suitable methods will include blanks and quality control check samples.

6 Reference Material(s)

National Institute of Standards and Technology (NIST) Standard Reference Material (SRM) 1849 Infant/Adult Nutritional Formula. The SRM is a milk-based, hybrid infant/adult nutritional powder prepared by a manufacturer of infant formula and adult nutritional products. A unit of SRM 1849 consists of 10 packets, each containing approximately 10 g of material. Reference values are given as 106 (±5) mg/kg for adenosine 5′-monophosphate; 305 (±5) mg/kg for cytidine 5′-monophosphate; 147 (±38) mg/kg for guanosine 5′-monophosphate; and 148 (±8) mg/kg for uridine 5′-monophosphate.

7 Validation Guidance

Recommended level of validation: *Official Methods of Analysis*[SM].

8 Maximum Time-to-Signal

No maximum time.

Approved by Stakeholder Panel on Infant Formula and Adult Nutritionals (SPIFAN). Final Version Date: September 17, 2011. Effective Date: September 20, 2011.