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AOAC Candidate Method #CIN-01

Identification of Selected *Cinnamomum* spp.Bark in Dietary Supplement Raw Materials and/or Finished Products - Gas Chromatography with Flame Ionization Detection After Hydrodistillation

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- RESUBMISSION 7/7 Notes:
  Attached please find the updated MIDI Cinnamon Method.

  The major changes are:

  - Addition of C. ramulus to the species identification.
  - Alternative automated peak naming using MIDI Sherlock software.
  - Alternative pattern matching species identification using MIDI Sherlock software.

Identification of Selected *Cinnamomum* spp. Bark in Dietary Supplement Raw Materials and/or Finished Products

Gas Chromatography with Flame Ionization Detection After Hydrodistillation

A. Principle

Volatile oils from *Cinnamomum* spp. are extracted into toluene using hydrodistillation.The volatile oil extract is then analyzed by gas chromatography-flame ionization detection (GC-FID). The *Cinnamomum* spp. are identified using a series of predetermined tests (hierarchical decision tree) and comparison of these results to known species. Interference compounds from potentially cross-reactive substances are excluded from the calculations. Analysis can be done manually, or automatically using MIDI, Inc.'s Sherlock Supplement Analysis software package.

B. Materials

Authenticated samples of *Cinnamomum burmannii, C. cassia, C. loureirii,* and *C. verum* were obtained from The Technical Innovation Center & McCormick Science Institute (Hunt Valley, MD USA). *C. ramulus, Cinnamomum* spp. from spices and supplement products (hard-shell capsules) were obtained from commercial suppliers. Descriptions of the *Cinnamomum* spp. products used in this study are presented in **Table 1**. In cases where different brands had identical composition and label claims, the number of brands tested is indicated.

C. Apparatus

(a) *GC system.*—Agilent Series 7890B (Agilent Technologies, Inc., Wilmington, DE, USA), flame ionization detector (FID), automatic liquid sampler, injector, controller, sampler tray, and ChemStation software (B.04.03 or higher), or equivalent.

(b) *Optional analysis software.*—MIDI Sherlock Software version 6.3 or higher (MIDI, Inc., Newark, DE, USA) with Supplement Analysis Package.

(c) *Operating conditions.*—Injector 150°C, split ratio 100:1, injecting 0.2 µL. Detector 250°C. Oven temperature ramp: 60°C to 200°C at 7°C/min; 200°C to 300°C at 60°C/min; 300°C for 1 min. GC run time: 22.7 min. Gases: H_2 carrier gas and N_2 makeup gas (both 99.999+% pure); air, industrial grade, dry, <1 THC. Environmental: gas chromatograph needs to operate within temperatures of 10°–40°C (50°–104°F) and 20–80% relative humidity.

(d) *GC Capillary column*.—Agilent J&W Ultra II, 25 m 0.20 mm × 0.33 µm film thickness with (5%)-diphenyl-(95%)- dimethylsiloxane, or equivalent.

(e) *Syringe*.—10 µL straight, 23 gauge fixed needle (Agilent Technologies, or equivalent).

(f) *Injection port liners*.—Microbial ID, Inc. (Newark, DE, USA), or equivalent. Must contain silanized wool.

(g) *Autosampler vials*.—2 mL, 12x32mm, screw cap vials and caps with PTFE/Silicone/PTFE septa.

(h) *Pasteur pipettes*.—5 in. and 9 in. disposable.

(i) *Volumetric pipettes*.— Various sizes.

(j) *Volumetric flask*.—500 mL, glass.

(k) *13 x 100 mm glass tubes with PTFE-lined caps.*

(l) *Round-bottom flasks*.—500 mL, standard taper joint No.: 24/40.

(m) *Liebig condenser*.—Model 2400-400 (Corning, Inc., Corning, NY, USA), or equivalent.

(n) *Volatile oil trap*.— 5 mL Clevenger style, outer 24/40 and inner 24/40 standard taper joints.

(o) *Regulated heating mantle.*

(p) *Analytical lab balance*.— ± 0.1 mg.

(q) *Vortex mixer.*

(r) *Silicone pump tubing.*

(s) *Boiling chips.*

(t) *Cork ring support*.— For 500 mL round-bottom flask.

(u) *Weighing paper.*

(v) *Powder funnel.*

(w) *Glass cleaning brush.*

Table 1. Materials.

Material No.	Type	Composition	Claim	No. Brands
1	Authenticated	*Cinnamonum burmannii*	Pure	
2	Authenticated	*C. cassia*	Pure	
3	Authenticated	*C. loureirii*	Pure	
4	Authenticated	*C. verum*	Pure	
5	Commercial Bark	*C. ramulus*	Pure	
6	Capsules	*C. cassia* Bark	500 mg/capsule	5
7	Capsules	*C. verum* Bark	750 mg/capsule	
8	Capsules	*C. verum* Bark	600 mg/capsule	
9	Spice	*C. burmannii*	3% Oil, Organic	
10	Spice	*C. cassia*	3.75-4% Oil	
11	Spice	*C. burmannii*	Pure	
12	Spice	*C. loureirii*	Pure	2
13	Spice	*C. verum*	Pure, Organic	3

D. Reagents

(Note: Chemicals from any supplier meeting the specifications may be used.)

(a) *Toluene*.—Optima grade, or equivalent.

(b) *Hexanes*.—HPLC grade.

(c) *Methanol*.—HPLC grade.

(d) *Acetone*.—ACS grade

(e) *Sodium sulfate*.—ACS grade, anhydrous.

(f) *Deionized (DI) water*

(g) *Reference standards*.—See **Table 2**. Purities were obtained from the supplier's certificate of analysis. These purities were determined by gas chromatography. No independent confirmation of purity was confirmed.

E. Preparation of Test Solutions

Note: All steps must be followed exactly as described. Any deviation may result in an incorrect match. The calibration standard may be used for a manual-based identification approach or in conjunction with the Sherlock Supplement analysis software (MIDI, Inc.). If using the manual approach, response values are taken from the Agilent ChemStation software using the area of each peak. If using the Sherlock analysis software, use the response value listed on the Sherlock report.

(a) *Preparation of standard solution*.—Accurately weigh 10.00g of each of the alkane compounds listed in **Table 2** and transfer to a 500 mL volumetric flask. Add 250 mL HPLC-grade hexane and mix. This is the stock instrument calibration solution.

(b) *Instrument calibration solution*.—Dilute 1.0 mL of the stock instrument calibration solution with 9.0 mL hexane (10-fold dilution). This is the working instrument calibration solution. Fill a GC autosampler vial with the instrument calibration solution and cap.

(c) *Preparation of instrument negative control*.—Fill a 2 mL autosampler vial with HPLC grade hexane.

(d) *Sample test solutions* .—Accurately weigh 2.0 g of *Cinnamomum* spp. raw material, spice or capsules (inner contents) into a 500 mL round-bottom flask. Add 250 mL DI water.

(e) *Hydrodistillation setup*.— Add several boiling chips to the 500 mL round-bottom flask. To the Clevenger trap, add 5-6 mL DI water and 2 mL toluene. Connect the 500 mL flask and the Clevenger trap to the Liebig condenser.

(f) *Cooling water*.—Connect the Liebig condenser to a cooling water source via the pump tubing and maintain cool water flow through the outer jacket of the condenser.

(g) *Heating step*.—Use a regulated heating mantle to bring the flask solution to boiling. Turn down the heat to medium and boil for 2 hrs. Turn off heat and cool.

(h) *Volatile oil collection step*.—Remove the Clevenger trap from the condenser setup and aspirate and retain the top toluene layer. Include any emulsion layer, but avoid dipping the pipette into the bottom aqueous layer.

(i) *Drying step*.—Transfer the toluene layer to a 13 x 100 mm glass tube. Add approximately 1 mL of anhydrous sodium sulfate and cap. Vortex briefly. Transfer liquid to another 13 x 100 mm glass tube. If the liquid is visibly cloudy, add an additional 1 mL of anhydrous sodium sulfate, cap and vortex again. Repeat as needed. Once clear, transfer the liquid contents to a GC autosampler vial for analysis.

Table 2. Reference standards.

Name	Supplier
Decane, ReagentPlus®, >=99%	Sigma-Aldrich, No. D901
Dodecane, ReagentPlus®, >=99%	Sigma-Aldrich, No. D221104
Tetradecane, 99%+	Sigma-Aldrich, No. 172456
Hexadecane, ReagentPlus®, >=99%	Sigma-Aldrich, No. H6703
Octadecane, 99%	Sigma-Aldrich, No. O652

F. System Suitability

Note: Several tests must pass before samples can be processed. Complete a Performance Qualification (PQ) for each batch of samples by executing a calibration standard run, negative reagent control, negative process control and a positive process control.

(a) *Calibration standard*.—The system calibration standard must be run prior to processing samples (see Section E).

Manual. The retention times for each of the five alkane compounds must be determined in order to determine the Equivalent Carbon Lengths (ECLs) of eluted unknown compounds. The ECL value for each compound is derived as a function of its elution time in relation to the five alkanes from the system calibration standard.

All peaks must be manually determined based on ECL ranges using the following formula:

$$ECLpk = ECL_{A1} + (RT_{pk} - RT_{A1}) \times (ECL_{A2} - ECL_{A1}) / (RT_{A2} - RT_{A1})$$

where pk is the peak in question, A1 is the alkane immediately before the peak, and A2 is the alkane immediately after the peak. (See example in section G (b).)

Record the retention time and response for each alkane in the calibration standard for use in these calculations.

Automatic. The Sherlock software will run the calibration standard as part of the batch and determine the retention times as well as the Equivalent Carbon Lengths (ECLs) for each peak. The Calibration Standard is said to pass if no error message is listed and the calibration report indicates *Good Peak Matching*.

(b) *Negative reagent control*.—HPLC-grade hexane. If the negative reagent control response >= 1% of the calibration report response, steps must be taken to remove the contamination in the instrument. If the negative reagent control response < 1% of the calibration standard response, proceed to the next step.

(c) *Negative process control*.—Follow the steps in Section E, but do not include any sample to the 500 mL round-bottom flask. If the negative process control response >= 3% of the calibration report response, the distillation setup must be re-cleaned to remove the contamination. If the negative process control response < 3% of the calibration standard response, proceed to the next step.

(d) *Positive process control*.—Follow the steps in Section E, using a known sample of *C. verum* (National Center for Natural Products Research, University of Mississippi, Oxford, MS, USA) to the 500 mL round-bottom flask. If the sample is identified as *C. verum*, according to the steps in Sections G and H, proceed with processing the sample batch.

G. Determination of the Predominance of Cinnamomum spp.

(a) *Sample concentration*.—Evaluate the largest peak in the range C_{10} to C_{18} (Decane to Octadecane).
Manual. If the response of the largest peak in the Agilent ChemStation software is larger than 1,200 then dilute the sample to bring the peak into the range 300 – 1,200.
Automatic. If the Sherlock response of the largest peak is larger than 2,400,000 dilute to the range 600,000 – 2,400,000.

Note: The chromatogram must integrate all peaks with responses at least 1/500 the size of the *Trans-cinnamaldehyde* (heretofore, ***t-cinn***). That is, if the t-cinn has response of 850, all peaks with response greater than 1.7 must be integrated.

Manual (b) – (e).

(b) *Trans-Cinnamaldehyde (t-cinn) peak*.—The chromatogram of the potential *Cinnamomum* spp. sample must have, as the largest peak between C10 and C18, the t-cinn peak eluting at ECL 12.790 ± 0.050. To calculate ECL, see Section F.

Example: if the retention times of Dodecane and Tetradecane are 9.133 and 12.865 minutes respectively, a peak at 10.612 would have ECL: 12.000 + (10.612-9.133)*(14-12)/(12.865-9.133) which equals 12.793 and would meet the criteria for the t-cinn peak.

(c) *Methoxycinnamaldehyde (OMCA) peak*.—Following the same procedure shown in step b, determine if there is a OMCA peak at ECL 15.397 ± 0.030. (If more than one peak is present in this ECL range, select the largest peak.)

(d) *Coumarin peak*.—Following the same procedure shown in step b, determine if there is a coumarin peak at ECL 14.473 ± 0.050. (If more than one peak is present in this ECL range, select the largest peak.)

(e) *Copaene peak*.—Following the same procedure shown in step b, determine if there is a copaene peak at ECL 13.857 ± 0.050. (If more than one peak is present in this ECL range, select the largest peak.)

Automatic (b) – (e).
Sherlock will automatically name each of the other peaks listed in sections (b) through (e) if found in the sample.

(f) *Cinnamomun spp. positive*.— **Manual and Automatic**. A sample is deemed to have cinnamon predominantly present if the following three criteria are met:

1. The response of t-cinn peak is greater than 70% of the sum of the responses of all integrated peaks between ECL 10.000 and ECL 18.000 (Decane and Octadecane), including the t-cinn peak itself.
2. The copaene peak is present.
3. The sum of the responses of the OMCA, coumarin and copaene peaks is at least 2% the response of the t-cinn peak.

H. Determination of Cinnamomum spp.

(Note: Proceed to this section only if the sample passes the requirements in Section G.)

(a) *Peak determination*.

Manual Peak Determination. —Following the same procedure as described in Section G, determine the presence and response of the following peaks:

1. Linalool at ECL 10.990 ± 0.050
2. 1,8 Cineole at ECL 10.3580 ± 0.050
3. t-cinn at ECL 12.79 ± 0.050 (see section G)
4. Copaene peak at ECL 13.857 ± 0.050 (see section G)
5. Trans-caryophyllene at 14.326 ± 0.050
6. Coumarin at ECL 14.473 ± 0.050 (see section G)
7. Cinnamyl acetate at 14.494 ± 0.050
8. Alpha-curcumene at 14.915 ± 0.050
9. Calamenene at ECL 15.337 ± 0.030
10. OMCA at ECL 15.397 ± 0.030 (see section G)
11. Benzyl benzoate at 17.756 ± 0.050

Note that not all peaks will be present for any specific sample. For each of the compounds above, determine the ratio of the response of the compound to the response of t-cinn, and multiply by 10,000 for convenience in display.

> *Example*: if the response of t-cinn is 825 and that of OMCA is 9.94, then the recorded value for OMCA will be 10000*9.94/825 = 120.5.

Automatic Peak Determination. The Sherlock software will determine the presence and size of the peaks needed for further analysis. The Sherlock software will further calculate the ratios to t-cinn of designated compounds.

(a) *Cinnamomum determination*.

Manual Species Determination using Decision Tables.

Cinnamomum spp. raw materials and spices.—Fill in **Table 3**. To determine whether a sample matches one of the *Cinnamomum* spp. listed, it must match at least **9 out of 10** of the criteria.

Cinnamomum spp. capsules.—Fill in **Table 4**. To determine whether a sample matches one of the *Cinnamomum* spp. listed, it must match at least **6 out of 7** of the criteria.

Automatic Species Determination using Pattern Recognition. Given the Sherlock Cinnamon Library from the Supplement Analysis Package, the Sherlock software will determine a *Similarity Index* for the sample when compared to the library entries. Similarity Index is a value between 0.000 and 1.000 calculated based on the variance and covariance of the named compounds, with 1.000 being a perfect match. If the top match is greater than 0.500 with no secondary match within 0.100 of the top match, the sample is determined to match that species of *Cinnamomum*. (See example in Appendix B.)

Table 3: *Cinnamomum* spp. Calculation for Raw Materials and Spices

Compound	10000 * resp / t-cinn resp	Test	Result (+/-)	*C. cassia*	*C. burmanniii*	*C. verum*	*C. ramulus*	*C. loureirii*
Linalool		>50		-	-	+	-	-
1,8 Cineole		>50		-	+	-	-	-
Copaene		>200		-	-	-	-	+
Trans-caryophyllene		>100		-	-	+	-	-
Coumarin		>100		-	+	-	+	+
Cinnamyl acetate		>50		-	-	+	-	-
Alpha-curcumene		>25		+	-	-	-	-
OMCA		>100		+	-	+	+	+
OMCA (big)		>750		-	-	-	+	-
Benzyl benzoate		>100		-	-	+	-	-
Number of matches →								

Table 4: *Cinnamomum* spp. Calculation for Capsules

				***Cinnamomum* spp. Criteria**	
Compound	10000 * resp / t-cinn resp	Test	Result (+/-)	*C. cassia*	*C. verum*
Linalool		>25		-	+
1,8 Cineole		>50		+	-
Copaene		>50		+	-
Coumarin		>100		+	-
Calemenene		>50		+	-
OMCA		>100		-	+
Benzyl benzoate		>100		-	+
Number of matches →					

Appendix A: Example of Calculation using Sherlock Supplement Analysis Package

A.1 Calibration Standard

RT	Response	ECL	Peak Name	Percent
5.3492	347671	10.0000	Decane	14.35
9.1329	343888	12.0000	Dodecane	14.19
12.8653	344523	14.0000	Tetradecane	14.22
16.2757	342837	16.0000	Hexadecane	14.15
19.3614	341950	18.0000	Octadecane	14.11
22.1689	358107	20.0000	Eicosane	14.78
24.7378	344550	22.0000	Docosane	14.22

Profile Comment: Good peak matching. Peak position matching error (RMS) is 0.0001.

A.2 Sample Analysis

RT	Response	ECL	Peak Name	Percent
10.6103	1.592E+6	12.7900	Trans-cinnamaldehyde (t-cinn)	87.84
12.5965	26481	13.8545	Copaene	1.46
13.4166	2497	14.3221	Trans-caryophyllene	0.14
13.6705	4249	14.4711	Coumarin	0.23
14.4170	5432	14.9093	Alpha-curcumene	0.30
15.2160	66740	15.3783	Methoxycinnamaldehyde(OMCA)	3.68

The t-cinn peak is in the acceptable range (response < 2.4E6) as per section G (a).
The t-cinn peak is over 70% of the total peaks as per section G (f) 1.
The Copaene peak is presence as per section G (f) 2.
The sum of responses for OMCA, Coumarin and Copaene is 97,470 which is 6.1% of the t-cinn peak, over the 2% required in section G (f) 3.

This sample may proceed to analysis in section H.

A.3 Transformed Sample Analysis

Response	Peak Name
166	Copaene/Cinnald
16	Trans-caryophyllene/Cinnald
27	Coumarin/Cinnald
34	Alpha-curcumene/Cinnald
419	OMCA/Cinnald

These values can be directly entered into Table 3:

Application of Table 3 to Sample Analysis

Compound	10000 * resp / t-cinn resp	Test	Result (+/-)	*C. cassia*	*C. burmanniii*	*C. verum*	*C. ramulus*	*C. loureirii*
Linalool	0	>50	-	-	-	+	-	-
1,8 Cineole	0	>50	-	-	+	-	-	-
Copaene	166	>200	-	-	-	-	-	+
Trans-caryophyllene	16	>100	-	-	-	+	-	-
Coumarin	27	>100	-	-	+	-	+	+
Cinnamyl acetate	0	>50	-	-	-	+	-	-
Alpha-curcumene	34	>25	+	+	-	-	-	-
OMCA	419	>100	+	+	-	+	+	+
OMCA (big)	419	>750	-	-	-	-	+	-
Benzyl benzoate	0	>100	-	-	-	+	-	-
			Number of matches →	10	6	5	6	7

A.4 Final Determination

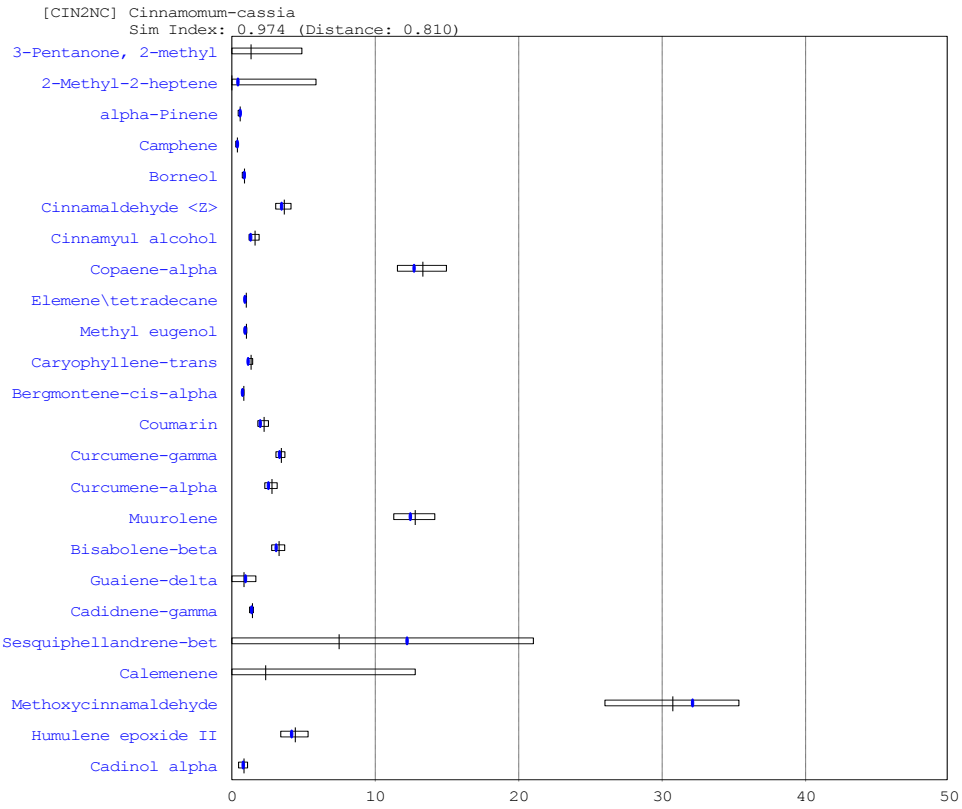
The sample matches 10/10 against *C. cassia*.

The sample is deemed to be a positive for *C. cassia*.

Appendix B: Example of Determination using Sherlock Supplement Analysis Pattern Recognition

The same sample as in Appendix A can be automatically identified using the Sherlock Cinnamon Library from the Supplement Analysis Package.

The result is determined by comparison to the model (feature chart) for *C. cassia* developed by the software from known samples of *C. cassia*.



Note: Sherlock software uses many more compounds than the manual technique to make its determination. The t-cinn compound is not used in pattern recognition due to its overwhelming size.

The final result is described by the Similarity Index metric.

Library	Sim Index	Entry Name
CINLIB 1.00	0.974	Cinnamomum-cassia

Since the top match is above 0.500 and no other secondary match is found, this is considered to be a determination of *C. cassia*.

The sample is deemed to be a positive for *C. cassia*.

ID_Only	Seq_Fname	Index	ID_Nbr	Name	Cassia	Verum	
SD-CAPSULE-C_CASSIA-286	E163125.CRT	6	11766	Cassia	7	0	
SD-CAPSULE-C_CASSIA-288	E163125.CRT	7	11767	Cassia	6	1	
SD-CAPSULE-C_CASSIA-281	E163085.CRT	4	1494	Cassia	6	1	
SD-CAPSULE-C_CASSIA-286	E163085.CRT	2	1499	Cassia	7	0	
SD-CAPSULE-C_CASSIA-286	E163085.CRT	9	1499	Cassia	7	0	
SD-CAPSULE-C_CASSIA-288	E163085.CRT	11	1501	Cassia	6	1	
SD-CAPSULE-C_CASSIA-289	E163085.CRT	12	1502	Cassia	7	0	
SD-CAPSULE-C_CASSIA-287	E163085.CRT	3	1500	Cassia	7	0	
SD-CAPSULE-C_CASSIA-287	E163085.CRT	10	1500	Cassia	7	0	
SD-CAPSULE-C_CASSIA-281	E163075.CRT	3	1494	Cassia	6	1	
SD-CAPSULE-C_CASSIA-281	E163075.CRT	10	1494	Cassia	6	1	
SD-CAPSULE-C_VERUM-291	E163115.CRT	8	1522	Verum	0	7	
SD-CAPSULE-C_VERUM-291	E163135.CRT	8	1522	Verum	0	7	
SD-CAPSULE-C_VERUM-290	E163115.CRT	6	1520	Verum	0	7	
SD-CAPSULE-C_VERUM-290	E163135.CRT	6	1520	Verum	0	7	

ID_Only	002: Cineole/Cinnald	003: Linalool/Cinnald	004: cis/Cinnald	005: Copaene/Cinnald	006: Caryophy/Cinnald	007: Coumarin/Cinnald	010: OMCA/Cinnald	012: Benzyl/Cinnald	013: Calemenene/Cinnald
SD-CAPSULE-C_CASSIA-286	83.7	7.8	179.2	145.1	63.9	190.9	12.6		129.0
SD-CAPSULE-C_CASSIA-288	17.4		156.8	90.2	49.3	163.9	11.6		102.1
SD-CAPSULE-C_CASSIA-281	19.9	4.1	78.7	144.3	43.0	178.1	11.3		100.4
SD-CAPSULE-C_CASSIA-286	85.0	8.0	50.5	142.8	64.6	197.0	15.0		132.5
SD-CAPSULE-C_CASSIA-286	85.7	7.9	54.0	142.1	64.3	195.0	14.8		130.6
SD-CAPSULE-C_CASSIA-288	18.7		46.4	89.1	49.9	175.9	13.8		105.1
SD-CAPSULE-C_CASSIA-289	74.4	11.4	56.1	148.4	47.5	192.8	12.0		128.4
SD-CAPSULE-C_CASSIA-287	122.8	5.9	51.9	210.5	77.7	201.0	15.6		148.5
SD-CAPSULE-C_CASSIA-287	122.3	6.2	54.9	210.1	78.0	203.0	16.4		150.8
SD-CAPSULE-C_CASSIA-281	19.0	4.0	58.1	140.6	41.7	181.6	11.0		97.4
SD-CAPSULE-C_CASSIA-281	19.7	4.1	61.0	139.5	41.1	178.4	10.9		95.4
SD-CAPSULE-C_VERUM-291		72.7	64.9	12.4	109.6		240.6	292.0	
SD-CAPSULE-C_VERUM-291		72.0	87.0	12.3	109.2		234.9	288.9	
SD-CAPSULE-C_VERUM-290		63.6	91.7		80.2		239.7	298.3	
SD-CAPSULE-C_VERUM-290		63.0	125.4		81.2		235.0	296.5	

ID_Only	Seq_Fname	Index	ID_Nbr	Name	Cassia	Burmannii	Verum	Loureirii	
SD-C. BURMANNII-284	E163085.CRT	7	1497	Burmannii	6	8	3	7	
SD-C_BURMANNII-270	E163064.CRT	2	1486	Burmannii	5	9	2	6	
SD-C_BURMANNII-270	E163106.CRT	2	1508	Burmannii	5	9	2	6	
SD-C_BURMANNII-270	E163106.CRT	3	1509	Burmannii	5	9	2	6	
SD-C_BURMANNII-270	E163125.CRT	2	11762	Burmannii	5	9	2	6	
SD-C_BURMANNII-270	E163247.CRT	4	1590	Burmannii	5	9	2	6	
SD-C_BURMANNII-284	E163075.CRT	12	1497	Burmannii	6	8	3	7	
SD-C_BURMANNII-278	E163064.CRT	10	1491	Burmannii	6	8	3	5	
SD-C_CASSIA-273	E163056.CRT	9	1484	Cassia	9	5	4	6	
SD-C_CASSIA-273	E163064.CRT	8	1489	Cassia	9	5	4	6	
SD-C_CASSIA-273	E163106.CRT	7	1513	Cassia	9	5	4	6	
SD-C_CASSIA-273	E163125.CRT	5	11765	Cassia	9	5	4	6	
SD-C_CASSIA-277	E163056.CRT	7	1482	Cassia	8	4	3	7	
SD-C_LOUREIROI-271	E163064.CRT	9	1487	Loureirii	6	6	3	9	
SD-C_LOUREIROI-271	E163106.CRT	5	1511	Loureirii	6	6	3	9	
SD-C_LOUREIROI-271	E163125.CRT	3	11763	Loureirii	6	6	3	9	
SD-C_LOUREIROI-271	E163253.CRT	4	1595	Loureirii	6	6	3	9	
SD-C_LOUREIROI-279	E163064.CRT	11	1492	Loureirii	6	6	3	9	
SD-C_LOUREIROI-275	E163064.CRT	4	1480	Loureirii	5	5	4	8	
SD-C_VERUM-272	E163056.CRT	8	1483	Verum	4	2	9	3	
SD-C_VERUM-272	E163064.CRT	7	1488	Verum	4	2	9	3	
SD-C_VERUM-272	E163106.CRT	6	1512	Verum	4	2	9	3	
SD-C_VERUM-272	E163125.CRT	4	11764	Verum	4	2	9	3	
SD-C_VERUM-280	E163075.CRT	2	1493	Verum	4	2	9	3	
SD-C_VERUM-276	E163056.CRT	6	1481	Verum	4	2	9	3	

ID_Only	001: Limonene/Cinnald	002: Cineole/Cinnald	003: Linalool/Cinnald	004: cis/Cinnald	005: Copaene/Cinnald	006: Caryophy/Cinnald	007: Coumarin/Cinnald	008: Cinnacet/Cinnald	009: Curcumene/Cinnald	010: OMCA/Cinnald	012: Benzyl/Cinnald
SD-C. BURMANNII-284		38.7		57.0	115.9	45.1	106.0	24.3		14.1	
SD-C_BURMANNII-270	49.1	106.5	21.0	60.5	178.8	76.6	147.0	21.2		9.5	
SD-C_BURMANNII-270	52.5	121.7	22.6	54.0	146.4	64.1	114.3	25.0		7.9	
SD-C_BURMANNII-270	55.3	129.8		54.6	149.3	64.7	117.8				
SD-C_BURMANNII-270	53.0	123.4	22.9	75.4	146.9	64.8	102.8	23.7			
SD-C_BURMANNII-270	45.6	111.2	21.7	51.6	108.0	47.3	117.4	21.3		6.8	
SD-C_BURMANNII-284	3.2	37.4	3.2	40.3	114.2	44.8	106.0	24.1		14.0	
SD-C_BURMANNII-278	3.5	55.8	4.2	38.9	174.5	66.4	97.1	16.7		16.2	
SD-C_CASSIA-273				45.5	163.8	17.4	30.5		34.0	428.9	
SD-C_CASSIA-273				47.9	178.7	19.3	26.4		36.1	382.9	
SD-C_CASSIA-273				46.1	166.3	15.7	26.7		34.1	419.2	
SD-C_CASSIA-273				60.7	169.2	16.9	20.2		33.4	414.3	
SD-C_CASSIA-277				51.7	697.6	36.5	32.5	17.3	51.3	501.5	4.3
SD-C_LOUREIROI-271				56.0	384.4	19.1	139.1	36.0	12.9	177.8	
SD-C_LOUREIROI-271				44.0	364.9	17.8	101.3	21.0		152.1	
SD-C_LOUREIROI-271				57.4	367.4	18.0	114.8			143.5	
SD-C_LOUREIROI-271				37.6	317.7	15.3	121.2	16.3	11.2	139.7	
SD-C_LOUREIROI-279		2.1		41.5	400.2	16.2	115.4		13.4	138.2	
SD-C_LOUREIROI-275	8.4			63.4	704.1	36.5	108.0	52.1	16.4	182.9	
SD-C_VERUM-272			111.2	66.4	92.6	185.8		65.4		307.7	291.5
SD-C_VERUM-272			114.3	68.7	94.8	189.4		63.0		293.9	293.6
SD-C_VERUM-272			117.0	66.7	97.6	193.1		65.0		278.5	312.6
SD-C_VERUM-272			116.3	83.3	99.1	192.1		60.8	14.7	265.4	282.7
SD-C_VERUM-280	10.7		101.1	64.9	36.6	262.3		512.2	5.0	256.1	284.8
SD-C_VERUM-276	19.0		105.5	63.1	20.4	194.6		442.5	6.6	248.8	333.3