FOODINTEGRITY
Ensuring the Integrity of the European food chain

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Deliverable 14.3 Validation of the tool-kit containing chemical, metabolomic and genetic markers of product integrity using commercial foods.

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Deliverable 14.3 Validation of chemical and metabolomic markers of product integrity and stability along processing.

1 Description of Deliverable

This deliverable reports the use of the tool-kit developed, using chemical, metabolomic and genetic markers, to assess the integrity of complex commercial foods containing nutritive seeds (chia, flaxseed and sesame).

Different markers were evaluated by different methods at three different laboratories (MPIMP, CONICET-ICYTAC and CONICET-IGEVET). Previous results (deliverable 14.1) demonstrated that seeds can be differentiated by a set of chemical markers, which can be used to prevent fraud at any food industry using these seeds within their products, and by consumers acquiring these seeds for their own nutrition. In addition, a method to track the authenticity of the seeds by means of genetic markers was developed. Different extraction methods were used to purify DNA from the seed and food samples, including homemade and commercial kits, in order to improve DNA quality and quantity. A Real Time Melting Curve Genotyping method was designed to distinguish the presence of chia, sesame and flax seed in complex foods, showing that it is possible to identify the three species by its melting temperatures. Thus, genetic markers were also useful to identify t nutritive seeds as raw materials. The Deliverable 14.2 shows how these three independent methods (genetic, metabolomic and target chemical profiling) can be used to verify the presence of these nutritive seeds in lab-scale bakery products, affording good results in the identification of the presence of such seeds (alone or mixed) in a complex food. Furthermore, deliverable 14.2 also shows that DNA, metabolic and chemical markers were stable to the bakery process, including high temperature in the oven. Thus, the tool-kit constituted by a combination of three independent methods looks useful to verify the food integrity of lab-scale foods, detecting seeds to a limit close to 5% of the global composition of the food (5% of seeds combined with other ingredients necessary to produce a baked cookie, for instance).

Current work validates the use of previous chemical/ metabolomic and genetic markers using commercial bakery products, containing different amounts of individual seeds or a mixture with different proportions of seeds. Thus, the main goal of this deliverable was verifying the usefulness of developed markers to check for the presence of nutritive seeds in commercial baked foods (real life food products).

2 Achievement of the Deliverable 14.3:

2.1 Sampling.

Commercial samples were acquired at different supermarkets and bakery shops at the city of Córdoba (Argentina) and distributed to other participants to be tested for the presence of nutritive seeds (chia, flax and sesame) as claimed in the food-label. Samples consisted of:

Sample ID.		
A	CHA C:	**chía** crackers
B	ACL:	sweet cookies with **chia** and **flax**
C	ASAG: salted cookies with **sesame**	
D	GRA L:	salted cookies with **flax**
E	GRA S:	sweet cookies with **sesame**, sunflower, etc.
F	GRI SLC:	crackers with **sesame**, **flax** and **chia**
G	MASA CLA:	pasta with **chia**, **flax** and amaranth
H	PAN ATCL:	bread with **chia, flax, sesame** and oats

In addition to commercial samples, we included two lab-samples (**lab mix 10** and **lab mix 20**), containing a mix of **chia, sesame**, **flax** (10% and 20% of a mix of seeds at equal parts, ca. 3.33% or 6.66% each seed, respectively).

2.2 Use of target compounds (polyphenols) to verify the presence of chia, flax and sesame seeds in commercial bakery products:

The method used to extract and analyze polyphenols in both raw seeds and bakery products has been previously described (see Deliverable 14.2 and related SOP). Table 2.2shows target compounds (µg compound / Kg product) used to discriminate between both lab and commercial samples containing nutritive seeds. From Table 2.2 we can see that Rosmarinic acid and Salviaflaside I enable a clear identification of chia seeds in commercial samples. Considering the relative amount of these compounds in lab-sample 10, we can see that all commercial samples containing chia gave a positive identification, with an amount of chia seeds close or above 3,3% (based on the comparison with lab-sample 10). On the other hand, Eriodictyol o-glucoside is a good marker on the presence of flax in both lab- and commercial samples. In this case, positive identification in lab-samples was possible when 7% flax was present; thus, commercial samples positively identified as containing flax could have ca. 7% of this seed. In the case of sesame, the presence of sesamolinol diglucoside I and sesaminol triglucoside allow the positive identification of sesame contained in both lab- and commercial samples at levels close to 7%.

Although the sensitivity of this method is not high (seeds can be detected when ranging 3,5% to 7% in a commercial sample), it can be improved using a more selective MS/MS spectrometer (e.g. triple quadrupole) for measuring target compounds, which could lower the

detection limit to values close or below 1% of a given seed in commercial samples. So far, this method could be used as a good confirmatory tool within the tool-kit, enabling the assessment of chia, flax and/ or sesame seeds in bakery product, which can be extensive to other complex foods. Furthermore, this method could be fitted to evaluate other highly nutritive components in complex foods, which is out of the scope of the WP14 proposal.

Table 2.2-T1: Identification of nutritive seeds in bakery products by target markers (polyphenols). Values expressed in µg compound / Kg product

Seed Declared	**Chia/Flaxseed/ Sesame**	**Chia/Flaxseed/ Sesame**	**Chia**	**Chia/ Flaxseed**	**Chia/Flaxseed/ Sesame**	**Chia/ Flaxseed**	**Sesame**	**Flaxseed**	**Sesame**	**Chia/Flaxseed/ Sesame**
Sample ID / Target Marker	**Lab Mix 20**	**Lab Mix 10**	**A**	**B**	**F**	**G**	**C**	**D**	**E**	**H**
Chia/Flaxseed										
Quinic acid	19,6 ± 0,64	17,01 ± 0,51	9,66 ± 1,69	19,43 ± 0,48	27,02 ± 3,4	13,39 ± 0,67	14,22 ± 3,96	17,7 ± 1,94	10,63 ± 0,65	14,21 ± 0,39
Chia										
Rosmarinic acid	16,01 ± 2,25	7,7 ± 1,48	10,61 ± 0,42	16,74 ± 1,82	15,48 ± 0,59	13,26 ± 1,44				12,79 ± 0,69
Dashenshu						9,18 ± 7,96				
Salvianolic acid E/B/L	<LOQ	<LOD		3,91 ± 0,13	3 ± 0,18	2,57 ± 2,24				
Salviaflaside I	36,09 ± 3,44	17,04 ± 3,74	33,25 ± 2,32	45,35 ± 0,81	51,87 ± 2,72	30,08 ± 2,62				43,35 ± 1,41
Salviaflaside II	9,01 ± 0,37	<LOD	9,62 ± 1,11	7,7 ± 0,31	5,93 ± 0,89					5,24 ± 0,78
Flaxseed										
Eriodictyol hexoside	0,39 ± 0,19	<LOD		0,61 ± 0,04	**0,47 ± 0,07**			1,49 ± 0,19		0,07 ± 0,13
Nortrachelogenin					3,8 ± 2,31			5,44 ± 0,2		3,61 ± 0,53
Quercetin di hexoside	2,09 0,02			10 ± 1,09	10,2 ± 0,02	2,76 ± 0,67	16,7 ± 2,79	16,7 ± 2,79		6,48 ± 0,03
Ferulic acid				129,43 ± 23,44		70,27 ± 8,75		411,35 ± 59,92		166,39 ± 111,78
Sesame										
Matairesinol dihexoside	1,89 ± 0,15	<LOQ			0,99 ± 0,19				4,39 ± 0,38	
7-hydroxymatairesinol					3,25 ± 0,21				11 ± 0,38	
Sesaminol trihexoside	0,76 ± 0,18	<LOQ			11,91 ± 1,43		1,71 ± 0,3		3,56 ± 0,07	0,72 ± 0,15
Matairesinol/Pinoresinol									2,18 ± 0,48	
Sesamolinol dihexoside I	1,66 ± 0,4	<LOQ			3,08 ± 0,31				1,79 ± 0,24	0,27 ± 0,46
Sesaminol dihexoside II	9,22 ± 1,73	2,78 ± 0,66			2,85 ± 0,38		1,58 ± 0,05		3,59 ± 0,38	3,55 ± 0,33
Sesaminol dihexoside III	2,47 ± 0,12	<LOQ			3,61 ± 0,35		0,1 ± 0,09		1,31 ± 0,17	

2.3 Use of non-target method (metabolomic) to verify the presence of chia, flax and sesame seeds in commercial bakery products:

In the following we describe the properties and use of metabolic markers that were selected by non-targeted metabolomics and data mining by machine learning, e.g. random forest analyses in combination with statistical approaches as was described previously (Deliverable 14.2). Marker searches were performed using non-processed seeds and experimental wheat cookies with additions of either defatted chia, linseed (flax), or sesame seed flour or whole seeds. We selected 15 potential seed markers of non-processed seeds (M01-M15) and 16 potential seed markers of seed additions to wheat cookies (C01-C16). Two markers of non-processed and processed seeds were identical, namely M09/C14 and M10/C15, yet non-identified compounds. The remaining makers of processed seeds were either general indicators of seed additions, similar to quinic acid that was detected by our metabolite targeted approaches (paragraph 2.2) or, as was discussed previously, likely chemical breakdown products of more complex metabolites, e.g. 4-hydroxybenzaldehyde, tyrosol, or succinic acid monomethylester.

The methods used to extract, analyze and data-mine metabolic fractions of non-processed seeds or cookies with or without added seeds have been described previously (Deliverable 14.2 and related SOP). The same analytical and datamining methods were applied to analyze off-the-shelf bakery products with different combinations of added seeds, namely crackers with either chia, linseed, or sesame seeds, breadsticks with 2.5 % chia, 6.5 % linseeds, and 7.5 % sesame or oat bread with chia and linseeds. In agreement with non-targeted metabolomics approaches we did not measure exact concentrations of compound but the relative changes of normalized compound abundance, for example relative to a reference material (see Deliverable 14.2 and related SOP). We found that each seed specific marker may have a food processing background that we detected, for example, in reference wheat cookies without any seed material or without additions of the respective single seed type. Because exact background controls or each off-the-shelf food material was not available we selected background levels of marker abundance from the measurements of experimental cookie material. These background levels were subtracted prior to the scoring/ verification of the presence or absence (n.d.) of chia, flax and sesame seeds in commercial off-the-shelf bakery products (Table 2.3-T1). As was discussed previously (Deliverable 14.2), some of the markers may not be fully seed type specific because we applied machine learning to marker discovery. In short, machine learning may select combinations of markers that may allow error-free classification but that are not fully specific when used alone. We took this fact into regard by reporting the false presence, i.e. a false positive call (f.p.), in cases of not full specific marker properties (Table 2.3-T1).

Table 2.3-T1: Qualitative assessment of nutritive seeds in bakery products by markers that were identified by non-targeted metabolomics and datamining. Markers are identified by selected mass features from non-targeted metabolomics and, if identified, by metabolite name. Non-identified metabolites are characterized by mass spectra and retention indices, see appended Supplemental File.

Mass feature	Metabolite Name	Detectability in wheat cookies (% of added defatted seed flour)			Wheat cookies with whole seeds				Crackers			Breadsticks	Oat Bread
		Chia	Linseed	Sesame	Chia	Linseed	Sesame	Chia/ Linseed/ Sesame	Chia	Linseed	Sesame	Chia/ Linseed/ Sesame	Chia/ Linseed
Chia/Linseed/Sesame													
C16_POL_2091.88_218	*myo*-Inositol	≥ 5%	≥ 5%	≥ 5%	√	√	√	√	√	√	√	√	√
C07_POL_2960.17_433	Galactinol	≥ 5%	≥ 5%	n.d.	n.d.	√	√	√	√	√	√	√	√
C05_POL_1684.05_103	Pentitol	≥ 10%	≥ 10%	≥ 5%	n.d.	√	√	√	√	√	√	√	√
Chia													
C04_POL_1497.34_208	4-Hydroxybenzaldehyde	≥ 5%	n.d.	≥ 20%	√			√	√			√	√
C13_POL_1571.41_179	Tyrosol	≥ 10%	n.d.	n.d.	n.d.			n.d.	√			√	√
M06_POL_2051.73_267	Catechollactic acid	≥ 20%	n.d.	n.d.	n.d.			n.d.	√			√	√
M13_POL_3398.47_396	Rosmarinic acid, trans-	≥ 10%	n.d.	n.d.	√			n.d.	√			√	n.d.
C12_POL_1805.65_265	Methylinositol	≥ 5%	n.d.	n.d.	n.d.			n.d.	√			n.d.	√
C09_POL_3426.44_272	Trisaccharide	≥ 10%	n.d.	n.d.	√		f.p.	√	√		f.p.	√	√
Linseed													
C10_POL_1335.52_97	-	n.d.	≥ 5%	n.d.		√		√		√		√	√
C14|M09_POL_3028.18_204	-	n.d.	≥ 5%	n.d.		√		√		√		√	√
C01_POL_1175.17_189	Succinic acid monomethylester	n.d.	≥ 5%	n.d.		√		√		√		n.d.	√
C02_POL_1379.8_141	-	n.d.	≥ 5%	n.d.		√		√		n.d.		n.d.	n.d.
C15|M10_POL_3025.02_84	-	n.d.	≥ 5%	n.d.		√		√		n.d.		n.d.	n.d.
M04_POL_2004.69_333	Saccharic acid	n.d.	≥ 15%	n.d.		n.d.		n.d.		√		√	√
M01_POL_1626.8_292	Tartaric acid	n.d.	≥ 15%	n.d.		n.d.		n.d.		√		√	√
C08_POL_3345.95_129	Raffinose	n.d.	≥ 10%	n.d.		√		n.d.		√	f.p.	√	√
Sesame													
M07_POL_2215.54_247	-	n.d.	n.d.	≥ 5%			√	n.d.			√	√	
M05_POL_2045.39_285	-	n.d.	n.d.	≥ 10%			n.d.	n.d.			√	√	

Oat bread: commercial sample H

Bread sticks: commercial sample F

Crackers with chia: commercial sample A

Crackers with sesame: commercial sample C

Crackers with flaxseed: Commercial sample D

n.d., not detected (above background)

f.p., false positive

Eight of the 15 potential seed markers of non-processed seeds (M01-M15) were found to be useful to verify the presence of chia, linseed and sesame seeds in off-the-shelf bakery products. None of these markers caused a false positive call. The other markers were not detected. Of the 16 potential markers of processed seeds (C01-C16) we found 13 to be useful markers. Most of these markers may act as single compounds. As was discussed above, two of these compounds, raffinose (C08) and a trisaccharide (C09) caused false positive calls but can be used in combination. In the following we will discuss the marker compound in regard to their marker properties as general or seed specific markers.

General markers of seed addition. These markers, myo-inositol (C16), a pentitol (C05) and galactinol (C07), are likely highly ubiquitous metabolites that are present in many seed materials. These markers may be useful to monitor the normalcy of a seed addition but - lacking specificity - cannot be used alone to verify the presence of chia, flax and sesame seeds in commercial bakery products. Nevertheless, monitoring normalcy by as many as possible specific and non-specific markers will make falsifications increasingly difficult.

Markers of chia seeds. Rosmarinic acid (M13), in agreement with our metabolite targeted analyses (Table 2.2-T1-T2) and the biosynthetic precursor chatechollactic acid (M06) that we added by our non-targeted approach can be used as chia markers in processed food (Table 2.2-T1). The concentrations are, however, low and require addition of at least 10 % or 20 % of defatted seed flour to be directly detected without further compound targeted chemical enrichment, e.g. by solid phase extraction methods. 4-Hydroxybenzaldehyde (C04), tyrosol (C13), a methylinositol (C12), and a trisaccharide (C09) may serve to build a computational model that detects even lower amounts of added chia seeds.

Markers of Linseeds. As was indicated by our random Forest models, linseeds are best detectable but may also serve as an example that different food processing may alter the relative abundance of seed specific markers. Markers C10 and C14/M09 are apparently useful to detect linseeds correctly in all analyzed processed food material. In contrast, Succinic acid methylester cannot be used in breadsticks, while the markers C02 and C15/M10 are only useful in wheat cookies with added seed material. Additional markers tartaric acid (M04), saccharic acid (M01) and raffinose (C08) may serve as additional markers of linseed normalcy but are limited to certain processed food materials and as likely more ubiquitous metabolites must be carefully controlled for false positive calls in other processed food or when other seed material may be present.

Markers of sesame. We found only two useful markers of sesame seeds using the non-targeted approach, M05 and M07. These markers are useful in breadsticks and crackers and in wheat cookies with added seed flour. Whole seed additions however are difficult to diagnose.

Conclusion. Non-targeted and targeted approaches allow efficient marker searches and verification in processed food materials. The two sets of markers reported in this and the previous section complements each other. While the targeted markers of linseeds (flax) are few (Table 2.2-T2T1) more markers can be obtained from Table 2.3-T1. Inversely, more sesame markers were found by targeted approaches. The combination of both the markers found by targeted and non-targeted approaches will allow for a highly accurate diagnosis of chia, linseed and sesame seed to processed food materials. Our Analyses also indicate the caveats. Specific food processing may alter the abundance of markers from non-processed seeds in respective food or may alter chemical reactions that form breakdown products. In conclusion, obviously we need to extend the range of added seed material so as to avoid false positive calls in the presence of other seed types. In addition each new food processing method must be thoroughly assessed, because the processing conditions may alter the stability of markers from non-processed materials and inversely alter the respective breakdown products. Nevertheless, specifically the breakdown products may not only indicated the nature of the added food ingredient but may also indicate or even validate the method of food processing.

Finally, we suggest that not yet identified metabolic markers that can be characterized and archived according to their analytical properties, e.g. mass spectra and retention indices may be useful as marker substance. For this reason we add to this report an appendix that lists the chemo-physical properties of all non-targeted markers for future study that may want to build on our current report.

2.4 Use of DNA-based methods to verify the presence of chia, flax and sesame seeds in commercial bakery products:

We used a High Resolution Melting real time Post PCR (HRM) analyses to verify the presence of chia, flax and sesame in different commercial bakery products. Furthermore, experimental lab made cookies were used as control know samples. The method carried out was described in previous deliverables and SOP. In addition to the samples obtained by CONICET-ICYTAC, different commercial products were obtained from local stores.

The HRM post PCR analysis method has proven to be effective in verifying the presence of nutritive seeds in bakery products, including those undergoing physical chemical complex processes. The samples analysed that contained a single species reached the expected Melting temperature, and could be satisfactorily identified with the composition described by the manufacturer. On the other hand, when samples containing the three target species in this study, it was only possible to detect one of them (Table 2.4.1, samples Lyv, MUELCS and F).

In addition, The HRM post PCR results were confirmed through an End Point PCR using specie specific primers to evaluate Chia (*Salvia hispanica*), Sesame (*Sesame indicus*) and Flax (*Linum usitatissimum*) species identification in food containing seeds.

			HRM POST PCR Analysis		
Sample ID	Description	Procedence	Chia (1 peak at 78.2 ± 0.2)	Sesame (1 peak 79.3 ± 0.2)	Flax (1 peak at 80.5 ± 0.2)
GUEL1	sweet cookies containig flax	commercial			*
GUES2	sweet cookies containig sesame	commercial		*	
GUEC	sweet cookies containig chia	commercial	*		
Chia Egle	cookies containig chia	commercial	*		
BOS	cereal bar with sesame	commercial		*	
LYV	cereal bar with flax, sesame, chia and sunflower	commercial		*	
GUEACL	sweet cookies with oat, chia and flax	commercial	*		*
E (ASAG)	sweet cookies containig oat, sesame, sunflower and amaranth	commercial		*	
MUELCS	baked dough with flax, sesame and chia	commercial			*
PUEATCL	bread with oat, wheat, chia and flax	commercial	*		*
F (GRI SLC)	breadsticks with Chia flax and sesame	commercial		*	
A (CHA C)	salted cookies with chia	commercial	*		
D (GRA L)	salted cokies with flax	commercial			*
C (GRA S)	salted cokies with sesame	commercial		*	
GRS20	cookies with 20% sesame residue	lab made		*	
GRL20	cookies with 20% flax residue	lab made			*
GRC20	cookies with 20% chia residue	lab made	*		
GC5/17	control cookie	lab made	no amplification		
GC7/17	control cookie	lab made	no amplification		
GSS20	cookies containig 20% sesame seeds	lab made		*	
GSC20	cookies containig 20% chia seeds	lab made	*		
GSL20	cookies containig 20% flax seeds	lab made			*
GM3020	cookies containig a mixture of sesame, chia and flax (20% each)	lab made	*	*	

In conclusion, the HRM analysis can discriminate between the Chia, Flax and Sesame species individually and its presence in experimental and commercial complex food matrix. However, the method cannot be appropriated in matrix food containing a mixture in different proportion of the three species in simultaneous. Whereas, EP PCR, is simple and cost effective alternative approach to the HRM analysis, especially for those samples that has mixtures of more than two different species. Target NGS assays are carried out in order to contribute to the knowledge of different techniques in the agro food integrity.

3. Conclusion and proposal for future work:

- ✓ We have **three independent methods** to verify the presence of chia, flax and sesame **seeds in complex foods** (GC-MS+ Machine Learning / LC-MS+ Chemometrics / RT-PCR of rbcl ribosome gene). These three methods perform quite well with cookies and other bakery products.
- ✓ Identification of metabolic markers is possible considering the complexity of chemical reactions during food processing, especially baking (non-target vs. target analysis).
- ✓ Combination of metabolic markers (non-target) with other molecular (genetic) and target markers brings better results to fully identify the presence of nutritive seeds in baked products (complex food).
- ✓ **Integrating three independent methods into a "tool kit**" enable both screening and confirmatory methods, mainly non-target methods for screening and target methods for confirmatory issues (quantitative levels could be necessary for regulatory purposes).
- ✓ This tool-kit should enable **detection of frauds** in foods containing these nutritive seeds, also **improving the nutritional information to consumers on the presence of bioactive compounds** in such foods.

Further work is necessary to improve the selectivity of DNA-based method as Tm used in the tool-kit are quite close for three studied seeds, affording some difficulty to clearly establish the presence of a particular seed when mixed with others. NGS (next generation sequencing) looks as a promising method to overcome this difficulty, which development is out of the scope of the proposal developed by WP14. However, we strongly recommend further research on NGS to improve the selectivity and sensitivity of DNA based methods to identify highly nutritive components in complex foods. Also at metabolic level additional work appears to be necessary. Markers detected by non-targeted approaches can be adopted as targets and chemical enrichment technologies can be applied so as to optimise the loss of sensitivity that is caused by dilution of added ingredients or by chemical instability of marker compounds. Obviously the specificity and selectivity of the current marker set should be enhanced by adding more type of added seed types such as quinoa or amaranth. In addition, more methods of food processing should be explored to assess the further application range of our current marker set beyond bakery products. Finally, we currently only applied with random forest algorithms only one type of machine learning tool to establish models that allow diagnoses of seed additions to bakery products. Exploration of additional machine leaning tool may enhance our diagnostic capabilities and result in additional combinatorial markers that will further support our current marker set when added ingredients and processing methods will be integrated.

Appendix (Supplemental file of Marker mass spectra and retention indices).

```
Name: C01_POL_1175.17_189
Synon: Metabolite name: Monomethyl succinate
Synon:  Analyte  name:  M001706_A117010-101-xxx_NA_1,168.56_PRED_VAR5_ALK_Succinic  acid
methylester (1TMS)
Synon: Analyte name: Monomethyl succinate, trimethylsilyl ester
Synon: RI: 1175 iu
Synon: Formula: C8H16O4Si
Synon: MW: 204 Exact Mass: 204.081785 CAS#: 86827-76-1
DB#: 54
Num Peaks: 295
73 387; 75 304; 76 19; 79 21; 89 999;
90 64; 91 31; 93 3; 94 1; 101 3;
105 35; 106 2; 107 5; 108 2; 109 1;
110 1; 114 68; 115 49; 121 1; 122 2;
123 5; 128 2; 129 101; 130 2; 133 1;
145 2; 153 2; 156 3; 157 17; 158 4;
162 2; 168 3; 169 11; 172 5; 173 60;
174 27; 175 5; 176 1; 182 2; 187 1;
189 205; 190 26; 191 10; 192 3; 196 1;
198 2; 202 1; 203 1; 206 2; 207 2;
210 2; 211 1; 212 1; 216 2; 217 7;
218 3; 219 2; 220 2; 222 5; 223 3;
224 1; 228 3; 229 2; 230 2; 231 3;
232 2; 235 3; 236 1; 237 3; 238 3;
239 2; 240 1; 242 2; 244 2; 245 1;
246 4; 248 2; 249 1; 251 4; 252 1;
253 1; 254 1; 256 1; 257 1; 259 2;
261 2; 262 1; 263 2; 264 1; 265 1;
266 5; 267 2; 268 3; 269 3; 270 3;
271 10; 272 4; 273 4; 274 3; 275 1;
276 1; 277 2; 278 2; 279 1; 280 1;
281 1; 282 2; 283 1; 284 6; 285 2;
286 2; 287 1; 288 1; 289 5; 290 4;
292 3; 294 1; 295 2; 297 3; 298 1;
300 2; 301 2; 302 3; 304 5; 305 4;
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369 3; 370 3; 371 3; 372 3; 373 3;
375 4; 379 3; 380 2; 381 1; 382 2;
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390 3; 392 3; 393 4; 395 3; 397 2;
399 1; 400 3; 402 3; 403 3; 404 1;
405 2; 406 3; 408 3; 409 5; 410 1;
413 2; 414 1; 415 3; 416 3; 417 2;
418 2; 421 1; 423 1; 424 1; 427 2;
428 4; 429 1; 430 2; 432 3; 435 2;
436 2; 437 4; 439 4; 440 1; 442 1;
443 1; 445 2; 447 3; 448 2; 449 1;
450 2; 453 2; 456 3; 458 2; 460 2;
461 2; 462 2; 463 2; 464 2; 466 1;
474 3; 478 1; 479 1; 480 1; 482 3;
483 2; 484 3; 487 1; 488 3; 493 2;
494 1; 497 4; 498 1; 499 1; 501 2;
503 3; 504 3; 505 2; 508 1; 509 1;
512 4; 513 5; 515 1; 517 1; 519 2;
520 2; 525 1; 527 4; 528 3; 530 1;
531 1; 532 1; 534 4; 536 1; 541 2;
542 1; 543 1; 544 2; 545 2; 547 2;
552 1; 554 3; 557 3; 558 3; 560 2;
563 2; 566 1; 568 1; 569 3; 573 3;
574 1; 577 1; 586 1; 590 2; 591 2;

Name: C02_POL_1379.80_141
Synon: Metabolite name: non-identified
Synon: RI: 1380 iu
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DB#: 48
Num Peaks: 107
70 4; 72 13; 73 555; 74 45; 75 509;
76 30; 77 30; 81 12; 83 272; 84 2;
85 330; 86 11; 87 35; 89 999; 90 75;
91 40; 93 2; 97 4; 99 3; 101 30;
105 296; 106 6; 107 13; 109 158; 110 1;
111 8; 112 13; 113 123; 114 2; 115 72;
116 25; 121 119; 122 49; 131 5; 139 4;
140 8; 141 621; 142 24; 143 58; 153 2;
157 38; 170 6; 173 189; 174 26; 175 4;
183 16; 189 118; 190 3; 199 19; 200 1;
203 1; 205 21; 206 3; 212 1; 215 128;
216 32; 217 31; 220 16; 226 4; 240 8;
243 2; 244 1; 247 52; 248 10; 253 13;
255 12; 260 1; 265 11; 266 1; 280 10;
288 5; 296 16; 297 6; 300 3; 306 10;
311 3; 312 4; 315 11; 318 7; 329 5;
331 5; 335 24; 336 25; 342 2; 346 2;
348 1; 355 3; 362 6; 364 5; 367 7;
392 4; 399 1; 402 2; 414 1; 426 8;
441 1; 453 7; 471 4; 478 14; 481 4;
486 2; 488 7; 494 5; 523 6; 545 1;
556 1; 590 2;

Name: C04_POL_1497.34_208
Synon: Metabolite name: 4-Hydroxybenzaldehyde
Synon: Analyte name: M001447_A150014-101-xxx_NA_1,493.64_PRED_VAR5_ALK_4-Hydroxybenzaldehyde
(1MeOX) (1TMS) MP
Synon: Analyte name: 4-Hydroxybenzaldehyde (1MeOX) (1TMS)
Synon: RI: 1497 iu
Synon: Formula: C11H17NO2Si
Synon: MW: 223 Exact Mass: 223,10286
DB#: 86
Num Peaks: 77
76 24; 88 68; 89 107; 90 121; 91 343;
92 96; 93 98; 94 154; 102 54; 104 129;
107 64; 108 85; 109 13; 120 71; 121 82;
122 33; 123 69; 132 25; 135 208; 136 89;
137 54; 138 28; 150 217; 151 99; 152 75;
158 50; 159 37; 160 90; 162 54; 163 17;
164 46; 165 104; 166 98; 167 71; 171 5;
172 32; 173 27; 174 24; 176 882; 177 640;
178 206; 180 36; 181 70; 185 37; 186 31;
187 35; 188 7; 190 17; 192 150; 193 93;
194 73; 195 78; 196 61; 197 49; 198 27;
199 47; 200 57; 201 15; 202 44; 203 28;
204 46; 205 38; 206 47; 207 30; 208 778;
209 146; 210 28; 211 53; 215 47; 216 87;
220 22; 222 34; 223 999; 224 199; 225 104;
226 19; 227 4;

Name: C05_POL_1684.05_103
Synon: Metabolite name: non-identified
Synon: Analyte name: M000000_A170001-101-xxx_NA_1,688.90_PRED_VAR5_ALK_NA170001 (classified
unknown)
Synon: Note: similar to pentitol (5TMS)
Synon: RI: 1684 iu
DB#: 9
Num Peaks: 137
70 2; 71 1; 72 17; 73 999; 74 85;
75 69; 76 3; 77 2; 81 9; 82 1;
83 4; 84 1; 85 2; 86 1; 87 5;
88 4; 89 23; 90 2; 91 1; 97 1;
98 1; 99 2; 100 1; 101 21; 102 3;
103 295; 104 30; 105 13; 106 1; 111 2;
113 4; 114 1; 115 5; 116 10; 117 100;
118 10; 119 8; 120 1; 127 1; 128 1;
129 123; 130 16; 131 27; 132 3; 133 54;
134 7; 135 4; 137 1; 141 1; 142 1;
143 8; 144 1; 145 3; 146 1; 147 253;
148 44; 149 28; 150 3; 151 1; 153 1;
155 3; 156 1; 157 18; 158 2; 159 2;
160 2; 161 3; 163 3; 164 1; 165 1;
169 1; 170 1; 171 2; 172 1; 173 1;
175 5; 176 1; 177 4; 178 1; 179 1;
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187 1; 189 42; 190 9; 191 29; 192 5;
193 2; 201 1; 203 16; 204 46; 205 104;
206 22; 207 11; 208 1; 215 1; 216 1;
217 263; 218 68; 219 29; 220 4; 221 6;
222 1; 223 1; 229 5; 230 1; 231 1;
242 1; 243 18; 244 4; 245 2; 246 1;
247 1; 277 13; 278 4; 279 2; 280 1;
291 3; 292 1; 293 1; 305 2; 306 5;
307 50; 308 14; 309 6; 310 1; 317 5;
318 3; 319 42; 320 11; 321 5; 322 1;
332 4; 333 2; 334 1; 395 1; 407 1;
422 1; 423 1;

Name: C06A_POL_2210.58_337
Synon: Metabolite name: Linoleic acid
Synon: Analyte name: M000488_A221003-101-xxx_NA_2,209.91_TRUE_VAR5_ALK_Octadecadienoic acid,
9,12-(Z,Z)- (1TMS)
Synon: Analyte name: 9,12-Octadecadienoic acid (Z,Z)-, TMS derivative
Synon: RI: 2211 iu
Synon: Formula: C21H40O2Si
Synon: MW: 352 Exact Mass: 352.279757 CAS#: 56259-07-5
DB#: 11
Num Peaks: 210
70 29; 71 15; 72 21; 73 772; 74 99;
75 999; 76 41; 77 167; 78 60; 79 334;
80 275; 81 617; 82 287; 83 139; 85 18;
87 6; 88 13; 89 53; 90 6; 91 109;
92 35; 93 209; 94 163; 95 385; 96 185;
97 87; 99 20; 100 2; 101 12; 102 8;
103 16; 104 4; 105 71; 106 25; 107 136;
108 85; 109 132; 110 120; 111 60; 115 6;
116 27; 117 112; 118 25; 119 23; 120 21;
121 146; 122 70; 123 75; 124 50; 125 30;
126 5; 128 5; 129 169; 130 15; 131 105;
132 31; 133 24; 134 17; 135 134; 136 109;
137 31; 138 20; 139 29; 141 12; 142 3;
143 12; 144 5; 145 29; 146 6; 147 39;
148 13; 149 78; 150 142; 151 25; 152 7;
153 7; 154 6; 155 15; 156 9; 157 23;
159 27; 160 4; 161 8; 162 2; 163 33;
164 60; 171 17; 172 7; 173 28; 175 6;
177 15; 178 67; 179 15; 180 4; 183 15;
187 11; 189 6; 191 18; 192 5; 193 5;
200 7; 201 13; 202 6; 204 20; 205 10;
206 2; 208 7; 209 2; 210 1; 211 1;
214 1; 215 14; 216 2; 217 9; 218 8;
219 8; 220 44; 221 2; 224 1; 225 4;
226 3; 227 8; 228 1; 229 9; 231 1;
232 2; 233 1; 234 9; 235 3; 239 4;
240 1; 241 1; 242 1; 243 9; 244 2;
247 2; 248 1; 249 1; 251 2; 254 1;
255 4; 259 1; 262 93; 263 17; 272 3;
276 1; 282 1; 285 1; 290 1; 296 3;
304 1; 310 2; 313 1; 315 1; 320 1;
327 1; 336 9; 337 80; 338 31; 343 2;
350 1; 352 6; 362 2; 364 2; 366 1;
368 2; 369 2; 371 1; 374 1; 377 1;
378 1; 380 1; 381 1; 383 1; 385 1;
393 1; 394 1; 396 1; 404 1; 407 1;
413 1; 414 1; 415 1; 417 1; 420 1;
421 1; 429 1; 433 1; 435 1; 437 5;
438 1; 451 1; 453 1; 456 1; 458 1;
471 1; 476 1; 504 1; 511 1; 535 1;
547 1; 563 1; 567 1; 568 1; 572 1;
580 1; 594 1; 595 1; 598 1; 600 1;

Name: C06B_POL_2215.16_339
Synon: Metabolite name: Oleic Acid
Synon: Analyte name: M000486_A222001-101-xxx_NA_2,221.65_TRUE_VAR5_ALK_Octadecenoic acid, 9-
(Z)- (1TMS)
Synon: Analyte name: Oleic Acid, (Z)-, TMS derivative
Synon: RI: 2215 iu
Synon: Formula: C21H42O2Si
Synon: MW: 354 Exact Mass: 354.295406 CAS#: 21556-26-3
DB#: 14
Num Peaks: 314
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70 50; 71 33; 72 50; 73 841; 74 88;
75 999; 76 77; 77 80; 78 20; 79 119;
80 58; 81 269; 82 136; 83 165; 84 193;
85 41; 86 14; 87 10; 88 10; 89 30;
90 8; 91 41; 92 17; 93 75; 94 45;
95 179; 96 229; 97 146; 98 159; 99 38;
100 3; 101 12; 102 1; 104 2; 105 34;
106 10; 107 36; 108 22; 109 95; 110 92;
111 73; 112 28; 113 6; 114 2; 115 7;
116 63; 117 585; 118 65; 119 53; 120 13;
121 54; 122 18; 123 70; 124 46; 125 27;
126 6; 127 7; 128 6; 129 432; 130 65;
131 105; 132 121; 133 50; 134 28; 135 38;
136 21; 137 43; 138 30; 139 15; 140 2;
141 7; 142 8; 143 34; 144 4; 145 180;
146 28; 147 23; 148 15; 149 21; 150 22;
151 28; 152 31; 153 8; 154 2; 155 21;
156 6; 157 19; 158 4; 159 20; 160 2;
161 6; 162 4; 163 4; 164 12; 165 15;
166 20; 167 9; 168 6; 169 15; 170 6;
171 29; 172 14; 173 11; 174 6; 175 6;
176 3; 177 2; 178 6; 179 7; 180 34;
181 5; 182 2; 183 19; 184 5; 185 51;
186 11; 187 13; 188 7; 189 5; 190 4;
191 5; 193 4; 194 4; 195 4; 197 4;
198 1; 199 60; 200 7; 201 15; 202 1;
203 5; 204 3; 206 4; 207 5; 208 3;
209 2; 210 2; 211 6; 212 1; 213 9;
215 4; 216 1; 219 7; 220 10; 221 8;
222 32; 223 7; 225 4; 227 11; 228 3;
229 2; 230 1; 234 4; 235 6; 236 6;
239 3; 240 2; 241 9; 242 3; 243 3;
244 1; 245 2; 246 1; 248 1; 249 2;
251 1; 253 3; 254 1; 255 5; 256 2;
257 7; 258 2; 260 1; 262 4; 263 2;
264 28; 265 5; 266 1; 269 1; 271 3;
272 3; 273 2; 275 1; 277 1; 278 1;
279 1; 280 2; 282 1; 285 1; 292 2;
294 2; 295 4; 296 2; 297 1; 298 1;
299 3; 300 2; 302 1; 303 1; 304 1;
305 1; 306 2; 307 2; 308 1; 311 1;
315 1; 316 1; 317 1; 318 2; 319 1;
320 2; 321 3; 322 2; 323 1; 325 2;
326 1; 327 1; 328 1; 329 1; 330 3;
332 1; 333 2; 334 1; 336 3; 337 12;
338 14; 339 115; 340 37; 341 8; 342 4;
343 1; 345 1; 349 1; 352 4; 353 3;
354 7; 355 3; 356 3; 358 1; 359 1;
360 3; 361 5; 364 2; 367 1; 368 2;
370 1; 373 1; 374 2; 376 1; 379 1;
381 1; 382 1; 383 1; 384 1; 392 1;
395 1; 399 1; 400 1; 402 1; 404 1;
405 1; 407 1; 409 1; 410 1; 411 1;
413 1; 414 1; 423 1; 428 1; 429 1;
436 1; 438 1; 439 1; 444 1; 452 1;
454 1; 455 1; 457 1; 458 1; 459 1;
462 1; 464 1; 469 1; 473 1; 474 1;
484 1; 488 1; 489 1; 491 1; 495 1;
499 1; 511 1; 515 1; 517 1; 523 1;
531 1; 532 1; 535 1; 538 1; 541 1;
551 1; 554 1; 555 1; 556 1; 558 1;
559 1; 561 1; 566 1; 575 1; 578 1;
582 1; 585 1; 591 1; 593 1;

Name: C07_POL_2960.08_433
Synon: Metabolite name: Galactinol
Synon: Analyte name: M000673_A299002-101-xxx_NA_2,966.29_TRUE_VAR5_ALK_Galactinol (9TMS)
Synon: Analyte name: Galactinol, nonakis(trimethylsilyl) ether
Synon: RI: 2960 iu
Synon: Formula: C39H94O11Si9
Synon: MW: 990 Exact Mass: 990.471954
DB#: 18
Num Peaks: 198
70 2; 71 2; 72 9; 73 999; 74 83;
75 69; 76 3; 77 3; 79 1; 81 20;
82 2; 83 4; 84 1; 85 4; 86 1;
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87 4; 88 1; 89 5; 90 1; 91 1;
95 1; 97 3; 98 1; 99 4; 100 1;
101 12; 102 3; 103 155; 104 16; 105 7;
106 1; 109 5; 111 3; 112 1; 113 6;
114 1; 115 4; 116 6; 117 20; 118 2;
119 3; 125 1; 126 1; 127 4; 128 1;
129 146; 130 20; 131 24; 132 3; 133 35;
134 5; 135 3; 139 2; 140 1; 141 3;
142 4; 143 25; 144 3; 145 5; 146 1;
147 225; 148 36; 149 26; 150 2; 151 2;
153 3; 154 1; 155 11; 156 3; 157 14;
158 2; 159 2; 160 1; 161 4; 162 1;
163 3; 164 1; 167 1; 169 39; 170 6;
171 4; 173 4; 174 1; 175 3; 177 5;
178 1; 179 1; 181 1; 183 1; 185 1;
187 1; 189 19; 190 9; 191 171; 192 32;
193 16; 194 1; 195 1; 199 1; 201 2;
202 1; 203 9; 204 640; 205 128; 206 55;
207 11; 208 2; 215 3; 216 2; 217 207;
218 51; 219 23; 220 3; 221 14; 222 3;
223 1; 227 2; 228 1; 229 6; 230 19;
231 10; 232 3; 233 3; 234 1; 235 1;
239 1; 241 2; 242 1; 243 23; 244 6;
245 7; 246 2; 247 1; 255 2; 256 1;
257 2; 258 1; 259 2; 263 1; 265 9;
266 2; 267 1; 270 1; 271 16; 272 4;
273 2; 274 1; 278 1; 279 1; 289 1;
290 1; 291 7; 292 1; 293 7; 294 2;
295 1; 303 1; 304 6; 305 35; 306 14;
307 6; 308 1; 317 3; 318 11; 319 14;
320 5; 321 2; 330 1; 331 5; 332 3;
333 1; 342 1; 343 15; 344 5; 345 4;
346 1; 347 1; 359 2; 360 3; 361 31;
362 12; 363 5; 364 1; 393 1; 419 1;
420 1; 432 3; 433 25; 434 11; 435 6;
436 2; 437 1; 451 1; 507 1; 508 1;
523 1; 524 1; 539 1;

Name: C08_POL_3345.95_129
Synon: Metabolite name: Raffinose
Synon: Analyte name: M000049_A337002-101-xxx_NA_3,350.64_TRUE_VAR5_ALK_Raffinose (11TMS)
Synon: Analyte name: Raffinose (11TMS)
Synon: RI: 3346 iu
Synon: Formula: C51H120O16Si11
Synon: MW: 1296 Exact Mass: 1296.60383
DB#: 8
Num Peaks: 234
70 2; 71 4; 72 9; 73 999; 74 79;
75 78; 76 5; 77 4; 78 1; 80 1;
81 30; 82 2; 83 7; 84 1; 85 9;
86 1; 87 4; 88 4; 89 11; 91 2;
92 1; 95 1; 96 1; 97 4; 98 2;
99 4; 101 17; 102 6; 103 155; 104 16;
105 8; 106 1; 107 1; 109 11; 111 4;
112 1; 113 7; 114 1; 115 8; 116 8;
117 43; 118 3; 119 3; 124 1; 125 1;
126 1; 127 4; 128 2; 129 175; 130 24;
131 26; 132 2; 133 34; 134 4; 135 3;
137 1; 139 4; 140 1; 141 7; 142 6;
143 26; 144 3; 145 6; 146 2; 147 161;
148 28; 149 23; 150 2; 151 2; 152 1;
153 4; 154 1; 155 24; 156 4; 157 27;
158 3; 159 2; 161 4; 163 5; 165 1;
167 1; 169 125; 170 16; 171 13; 172 2;
173 3; 175 4; 177 4; 179 1; 181 2;
182 1; 183 7; 185 2; 187 1; 188 1;
189 26; 190 6; 191 53; 192 9; 193 5;
195 1; 197 2; 198 1; 199 4; 200 2;
201 2; 202 1; 203 13; 204 169; 205 49;
206 15; 207 8; 210 1; 211 1; 213 1;
214 1; 215 6; 216 2; 217 183; 218 50;
219 21; 220 4; 221 8; 222 2; 223 1;
227 3; 228 1; 229 9; 230 14; 231 11;
232 2; 233 2; 234 1; 235 1; 236 1;
240 1; 241 2; 242 2; 243 48; 244 12;
245 12; 246 4; 247 3; 248 1; 249 1;
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250 1; 252 1; 254 1; 255 1; 257 11;
258 3; 259 5; 260 1; 261 1; 264 1;
265 1; 269 1; 270 2; 271 50; 272 12;
273 7; 274 1; 276 1; 277 2; 279 1;
282 1; 285 1; 289 3; 290 2; 291 5;
292 2; 293 2; 294 1; 295 1; 301 1;
303 1; 304 2; 305 6; 306 4; 307 2;
313 1; 317 3; 318 2; 319 15; 320 7;
321 3; 322 1; 323 1; 326 1; 327 1;
328 1; 330 1; 331 6; 332 4; 333 4;
334 1; 335 1; 336 1; 337 1; 338 1;
345 2; 347 1; 348 1; 349 1; 352 1;
353 1; 360 18; 361 229; 362 86; 363 46;
364 9; 365 4; 366 1; 368 1; 376 1;
378 1; 391 1; 414 1; 423 1; 435 1;
436 5; 437 37; 438 17; 439 8; 440 2;
447 1; 450 4; 451 23; 452 11; 453 4;
469 1; 560 1; 593 1; 594 1;

Name: C09_POL_3426.44_272
Synon: Metabolite name: non-identified
Synon: Note: similar to melezitose (11TMS)
Synon: RI: 3426 iu
DB#: 11
Num Peaks: 247
70 4; 71 4; 72 8; 73 999; 74 90;
75 101; 76 5; 77 8; 78 1; 79 1;
80 1; 81 28; 82 2; 83 7; 84 1;
85 8; 86 1; 87 4; 88 5; 89 11;
90 1; 91 1; 94 1; 95 2; 97 6;
98 1; 99 6; 100 1; 101 17; 102 4;
103 179; 104 18; 105 8; 107 1; 109 13;
110 1; 111 4; 112 1; 113 7; 114 1;
115 7; 116 6; 117 43; 118 5; 119 5;
125 1; 127 5; 128 2; 129 190; 130 27;
131 29; 132 2; 133 39; 134 5; 135 2;
137 1; 139 4; 140 2; 141 4; 142 7;
143 30; 144 3; 145 8; 146 1; 147 174;
148 29; 149 25; 150 3; 151 1; 153 5;
154 1; 155 30; 156 5; 157 33; 158 4;
159 3; 161 5; 163 4; 167 2; 168 1;
169 145; 170 20; 171 12; 172 2; 173 6;
174 1; 175 3; 177 4; 181 3; 182 2;
183 8; 184 2; 185 2; 187 2; 189 30;
190 7; 191 68; 192 10; 193 6; 195 2;
197 2; 199 6; 200 1; 201 2; 202 2;
203 11; 204 253; 205 67; 206 20; 207 9;
208 1; 209 1; 215 5; 216 3; 217 186;
218 49; 219 21; 220 4; 221 7; 222 2;
223 2; 227 3; 228 2; 229 10; 230 25;
231 18; 232 6; 233 6; 234 1; 235 1;
236 1; 240 1; 241 4; 242 1; 243 51;
244 13; 245 12; 246 2; 247 8; 248 2;
249 1; 251 1; 255 2; 256 1; 257 6;
258 2; 259 5; 260 1; 261 1; 263 1;
265 1; 267 1; 269 1; 270 3; 271 90;
272 21; 273 12; 274 2; 275 2; 277 1;
278 1; 279 1; 280 1; 282 1; 283 1;
285 1; 287 1; 288 1; 289 2; 290 1;
291 6; 292 3; 293 3; 294 1; 301 1;
303 1; 304 2; 305 7; 306 4; 307 3;
308 1; 317 5; 318 3; 319 15; 320 7;
321 2; 322 1; 324 1; 329 1; 330 1;
331 11; 332 5; 333 3; 334 1; 335 1;
336 1; 339 1; 344 1; 345 3; 346 2;
347 1; 348 1; 349 1; 350 1; 351 1;
352 1; 359 1; 360 16; 361 225; 362 92;
363 46; 364 9; 365 3; 372 1; 374 1;
375 1; 377 1; 393 2; 394 1; 407 1;
434 1; 438 1; 450 2; 451 9; 452 4;
453 1; 454 1; 462 1; 472 1; 482 1;
487 1; 489 1; 490 1; 500 1; 521 1;
523 1; 532 1; 541 1; 542 1; 559 1;
561 1; 569 1; 570 1; 576 1; 577 1;
581 1; 600 1;
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Name: C10_POL_1335.52_97
Synon: Metabolite name: non-identified
Synon: Note: similar to itaconic acid (2TMS)
Synon: RI: 1336 iu
DB#: 59
Num Peaks: 212
70 22; 72 12; 73 523; 75 128; 81 7;
82 10; 83 5; 86 5; 87 3; 89 7;
90 2; 97 999; 98 64; 99 10; 100 9;
103 7; 112 4; 113 4; 118 1; 127 3;
128 2; 130 5; 131 29; 133 21; 135 1;
137 4; 139 2; 141 3; 142 1; 143 9;
144 5; 147 470; 148 67; 149 35; 151 2;
155 6; 156 1; 157 8; 158 2; 161 2;
164 4; 170 25; 171 1; 173 8; 174 5;
178 2; 184 2; 185 6; 190 1; 193 1;
195 1; 199 12; 200 6; 201 3; 205 3;
214 11; 215 13; 216 5; 220 1; 223 1;
230 7; 231 2; 236 2; 240 1; 245 2;
256 3; 257 7; 259 12; 260 7; 271 1;
273 7; 275 4; 277 1; 283 1; 286 1;
288 4; 290 4; 294 1; 296 2; 302 7;
304 1; 313 4; 315 1; 321 3; 330 3;
332 1; 341 2; 343 2; 344 5; 348 1;
354 3; 355 1; 365 3; 367 5; 372 4;
373 1; 374 3; 376 1; 377 3; 379 9;
381 3; 387 2; 389 1; 396 7; 399 3;
400 6; 401 8; 404 1; 407 3; 408 1;
410 8; 412 2; 416 3; 417 3; 418 2;
419 3; 421 5; 422 3; 423 3; 424 2;
425 4; 427 2; 429 8; 430 3; 432 3;
436 7; 443 1; 444 2; 445 1; 446 7;
447 3; 450 1; 452 6; 453 1; 457 1;
462 6; 463 1; 465 8; 467 4; 470 2;
471 5; 474 5; 475 3; 476 4; 477 2;
478 1; 479 2; 482 1; 487 4; 489 2;
490 1; 494 1; 497 2; 498 1; 499 2;
501 5; 502 4; 505 3; 507 1; 509 2;
512 3; 513 2; 514 6; 516 3; 517 2;
518 8; 519 4; 520 3; 522 5; 523 6;
525 4; 526 6; 528 5; 530 6; 533 8;
539 4; 541 1; 543 1; 545 6; 547 1;
548 4; 549 7; 551 2; 552 6; 559 3;
560 2; 561 1; 562 1; 563 1; 565 2;
566 1; 569 3; 570 2; 573 2; 575 1;
576 2; 577 3; 581 1; 583 1; 585 1;
586 1; 587 5; 588 5; 589 2; 590 7;
591 2; 592 1; 594 3; 595 2; 596 3;
597 4; 598 1;

Name: C12_POL_1813.26_433
Synon: Metabolite name: non-identified
Synon: Note: similar to pinitol (5TMS)
Synon: RI: 1813 iu
DB#: 7
Num Peaks: 188
70 2; 71 41; 72 14; 73 999; 74 88;
75 86; 76 4; 77 3; 81 12; 82 2;
83 4; 84 2; 85 6; 86 1; 87 3;
88 1; 89 87; 90 5; 91 4; 95 1;
97 1; 98 1; 99 5; 100 1; 101 9;
102 3; 103 139; 104 12; 105 8; 109 2;
111 4; 113 3; 114 1; 115 4; 116 11;
117 18; 118 2; 119 7; 120 1; 121 1;
125 1; 126 1; 127 3; 128 1; 129 84;
130 9; 131 27; 132 3; 133 131; 134 14;
135 7; 139 1; 141 1; 142 4; 143 15;
144 3; 145 5; 146 5; 147 197; 148 34;
149 21; 150 2; 151 1; 153 1; 155 3;
156 2; 157 8; 158 1; 159 71; 160 8;
161 6; 162 1; 163 21; 164 3; 165 1;
167 1; 169 2; 170 1; 171 1; 172 2;
173 20; 174 3; 175 3; 177 16; 178 2;
179 1; 183 1; 184 1; 185 2; 186 1;
187 1; 189 9; 190 5; 191 101; 192 15;
193 7; 194 1; 197 1; 198 1; 199 1;
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201 2; 202 1; 203 4; 204 31; 205 23;
206 5; 207 45; 208 7; 209 3; 213 1;
215 2; 216 1; 217 143; 218 30; 219 12;
220 1; 221 8; 222 1; 223 1; 228 1;
230 4; 231 5; 232 1; 233 14; 234 2;
235 2; 243 5; 244 1; 245 4; 246 2;
247 39; 248 6; 249 2; 255 1; 259 2;
260 109; 261 24; 262 8; 263 3; 264 1;
265 13; 266 3; 267 1; 271 2; 277 2;
278 1; 285 2; 291 2; 292 1; 293 2;
304 2; 305 34; 306 9; 307 9; 308 2;
309 1; 317 3; 318 54; 319 16; 320 7;
321 1; 331 1; 335 2; 336 1; 342 1;
343 14; 344 5; 345 4; 346 1; 359 2;
361 2; 367 2; 368 1; 373 1; 374 8;
375 5; 376 2; 377 1; 417 1; 418 1;
432 5; 433 6; 434 3; 435 1; 448 1;
449 6; 450 3; 451 2;

Name: C13_POL_1571.41_179
Synon: Metabolite name: Tyrosol
Synon:   Analyte   name:   M000852_A157014-101-xxx_NA_1,575.25_TRUE_VAR5_ALK_Ethanol,   2-(4-
hydroxyphenyl)- (2TMS)
Synon: Analyte name: Tyrosol, 2TMS derivative
Synon: RI: 1571 iu
Synon: Formula: C14H26O2Si2
Synon: MW: 282 Exact Mass: 282.147133 CAS#: 321884-10-0
DB#: 39
Num Peaks: 403
73 901; 74 73; 75 100; 76 9; 77 46;
78 20; 79 4; 80 5; 81 8; 82 29;
83 3; 84 8; 86 5; 88 2; 89 36;
90 12; 91 43; 92 5; 93 4; 95 1;
97 7; 98 2; 102 2; 103 214; 104 21;
105 24; 106 1; 108 2; 109 7; 113 3;
114 4; 115 13; 117 32; 118 6; 119 6;
121 14; 122 11; 123 4; 126 42; 127 6;
128 6; 132 5; 135 17; 136 2; 137 2;
138 2; 140 1; 141 2; 142 4; 143 8;
144 2; 145 3; 146 7; 151 11; 152 3;
153 3; 154 4; 155 3; 156 28; 161 16;
162 5; 163 13; 164 8; 166 4; 167 3;
168 3; 169 7; 170 7; 171 3; 174 9;
175 7; 176 2; 177 21; 178 9; 179 999;
180 137; 181 39; 182 9; 184 4; 185 4;
186 5; 187 3; 188 6; 189 7; 191 5;
192 3; 193 81; 194 15; 195 6; 198 18;
199 3; 200 1; 201 4; 202 2; 208 1;
210 3; 211 2; 212 2; 213 2; 214 3;
216 1; 220 2; 224 2; 225 2; 227 1;
228 1; 229 4; 232 1; 235 5; 236 5;
237 2; 238 1; 239 1; 240 4; 242 1;
243 3; 244 2; 245 5; 250 2; 252 2;
253 6; 254 7; 255 1; 256 2; 257 3;
258 4; 259 2; 260 3; 261 4; 262 4;
263 4; 264 4; 265 4; 266 1; 267 52;
268 16; 269 9; 271 7; 272 3; 273 2;
274 5; 275 5; 276 3; 277 4; 278 1;
279 2; 280 5; 281 4; 282 70; 283 24;
284 7; 285 4; 286 2; 287 3; 288 5;
289 6; 290 1; 291 3; 293 5; 294 2;
295 4; 296 3; 297 6; 298 2; 299 2;
300 5; 301 3; 302 5; 303 4; 304 8;
305 5; 306 6; 307 2; 308 4; 309 2;
310 4; 312 3; 313 1; 314 3; 315 7;
316 1; 317 2; 318 3; 319 1; 320 1;
323 3; 327 3; 328 4; 329 5; 330 3;
331 2; 332 5; 333 3; 334 4; 335 2;
336 4; 337 2; 338 2; 339 2; 340 2;
341 2; 342 3; 343 3; 344 2; 346 3;
348 2; 352 4; 353 2; 354 3; 355 5;
356 2; 357 1; 359 6; 360 5; 361 6;
362 6; 363 6; 364 4; 369 3; 371 3;
372 1; 374 2; 375 2; 376 3; 377 3;
378 4; 379 4; 380 5; 381 4; 382 1;
383 2; 384 8; 385 3; 386 2; 387 3;
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388 1; 389 5; 390 4; 391 2; 392 3;
393 5; 394 2; 395 6; 396 2; 398 1;
399 1; 400 2; 401 1; 402 3; 403 1;
404 3; 405 4; 406 2; 407 3; 408 2;
409 1; 411 3; 412 2; 413 4; 414 4;
415 5; 416 5; 417 2; 418 2; 419 6;
421 4; 422 2; 424 3; 425 5; 426 4;
427 4; 428 3; 430 2; 431 1; 433 1;
434 3; 435 2; 436 2; 437 1; 438 6;
439 6; 440 2; 441 3; 442 3; 443 3;
444 4; 445 3; 446 2; 447 2; 448 4;
449 1; 450 1; 451 4; 453 1; 454 2;
455 1; 457 5; 458 1; 459 2; 461 3;
462 1; 464 6; 465 5; 466 7; 467 4;
469 3; 470 2; 471 3; 472 5; 474 1;
475 2; 476 2; 477 6; 478 4; 479 2;
480 4; 481 4; 483 3; 484 1; 486 3;
487 1; 488 7; 489 2; 490 4; 491 1;
492 4; 493 3; 494 8; 495 3; 496 3;
499 1; 503 1; 504 4; 507 1; 508 1;
510 1; 511 1; 514 1; 515 2; 516 2;
517 5; 519 1; 520 2; 521 1; 522 1;
523 5; 525 3; 527 1; 528 1; 529 3;
531 1; 532 1; 533 2; 534 3; 535 1;
536 1; 538 2; 539 2; 540 3; 541 2;
542 4; 545 4; 546 1; 548 4; 549 2;
550 3; 552 4; 553 5; 554 3; 556 3;
557 1; 558 3; 559 2; 560 2; 561 2;
562 4; 563 5; 564 1; 565 1; 567 3;
570 2; 571 1; 572 1; 573 6; 574 3;
575 1; 577 3; 579 2; 580 3; 583 1;
584 2; 585 1; 586 2; 587 5; 588 2;
589 7; 590 1; 591 3; 592 1; 593 3;
594 2; 595 5; 596 2;

Name: C14_POL_2970.13_84
Synon: Metabolite name: non-identified
Synon: Note: also identified as M09
Synon: RI: 2970 iu
DB#: 21
Num Peaks: 221
70 4; 71 6; 72 10; 73 999; 74 82;
75 95; 76 6; 77 5; 79 2; 80 1;
81 21; 82 2; 83 5; 84 13; 85 13;
86 2; 87 5; 88 1; 89 11; 90 1;
91 1; 94 1; 95 2; 97 5; 98 1;
99 6; 100 4; 101 31; 102 5; 103 107;
104 10; 105 6; 107 1; 109 7; 110 1;
111 3; 112 1; 113 8; 114 2; 115 10;
116 13; 117 51; 118 5; 119 8; 120 1;
121 1; 125 1; 126 1; 127 5; 128 1;
129 149; 130 21; 131 32; 132 4; 133 32;
134 4; 135 3; 136 1; 139 2; 140 3;
141 13; 142 5; 143 28; 144 3; 145 12;
146 1; 147 147; 148 25; 149 22; 150 2;
151 2; 152 1; 153 2; 154 2; 155 12;
156 2; 157 19; 158 3; 159 4; 160 1;
161 4; 162 1; 163 3; 164 1; 167 2;
168 1; 169 33; 170 5; 171 8; 172 13;
173 21; 174 5; 175 4; 176 1; 177 4;
178 1; 179 1; 181 1; 182 1; 183 4;
184 1; 185 2; 186 4; 187 2; 188 1;
189 31; 190 7; 191 38; 192 6; 193 3;
195 1; 197 1; 199 6; 200 2; 201 2;
202 1; 203 11; 204 652; 205 131; 206 60;
207 10; 208 2; 214 1; 215 3; 216 2;
217 100; 218 31; 219 13; 220 3; 221 4;
222 1; 223 1; 227 1; 228 1; 229 3;
230 3; 231 9; 232 2; 233 3; 234 1;
239 1; 240 1; 241 1; 242 2; 243 18;
244 4; 245 5; 246 2; 247 3; 248 1;
255 1; 256 1; 257 3; 258 1; 259 2;
260 1; 261 1; 263 1; 265 1; 266 1;
270 1; 271 14; 272 4; 273 5; 274 1;
275 1; 282 1; 287 1; 289 2; 290 1;
291 3; 292 1; 293 1; 298 1; 300 1;

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303 1; 304 1; 305 8; 306 3; 307 2;
314 1; 317 4; 318 2; 319 4; 320 1;
321 1; 331 3; 332 3; 333 3; 334 1;
345 1; 346 1; 347 1; 356 2; 357 1;
359 1; 360 2; 361 29; 362 11; 363 6;
364 2; 365 1; 388 2; 389 1; 435 1;
437 1; 445 2; 446 15; 447 7; 448 3;
449 1; 451 1; 462 1; 505 1; 506 3;
507 1; 508 1; 563 1; 564 4; 565 3;
566 1;

Name: C15_POL_3025.02_84
Synon: Metabolite name: non-identified
Synon: Note: also identified as M10
Synon: RI: 3025 iu
DB#: 5
Num Peaks: 191
70 4; 71 6; 72 30; 73 999; 74 85;
75 98; 76 6; 77 4; 79 1; 80 1;
81 21; 82 17; 83 6; 84 11; 85 10;
86 1; 87 3; 88 1; 89 9; 91 1;
94 1; 95 1; 97 6; 98 1; 99 6;
100 3; 101 29; 102 4; 103 109; 104 10;
105 5; 109 7; 111 3; 112 1; 113 7;
114 1; 115 8; 116 13; 117 53; 118 4;
119 8; 120 1; 125 1; 126 1; 127 5;
128 1; 129 155; 130 21; 131 26; 132 3;
133 32; 134 4; 135 3; 139 1; 140 4;
141 3; 142 4; 143 27; 144 3; 145 15;
146 2; 147 146; 148 24; 149 22; 150 2;
151 2; 153 2; 154 6; 155 19; 156 3;
157 20; 158 3; 159 4; 161 4; 163 3;
164 1; 167 1; 168 1; 169 32; 170 5;
171 8; 172 12; 173 10; 174 3; 175 4;
177 4; 178 1; 181 1; 183 4; 184 1;
185 1; 187 10; 188 2; 189 32; 190 7;
191 37; 192 5; 193 2; 194 1; 195 1;
197 1; 199 6; 200 5; 201 2; 202 1;
203 10; 204 654; 205 136; 206 62; 207 9;
208 2; 213 1; 214 1; 215 3; 216 1;
217 101; 218 28; 219 11; 220 2; 221 3;
222 1; 227 1; 228 1; 229 3; 230 3;
231 8; 232 2; 233 3; 241 1; 242 2;
243 16; 244 4; 245 4; 246 2; 247 3;
255 1; 256 1; 257 2; 258 1; 259 2;
261 1; 263 1; 271 14; 272 3; 273 4;
274 1; 275 1; 280 1; 282 1; 286 1;
287 1; 288 1; 289 2; 291 2; 292 1;
293 1; 304 1; 305 7; 306 2; 307 1;
314 1; 317 4; 318 2; 319 3; 320 1;
331 3; 332 3; 333 2; 345 1; 360 2;
361 29; 362 10; 363 6; 364 1; 365 1;
370 1; 388 1; 459 2; 460 13; 461 6;
462 3; 463 1; 505 1; 506 3; 507 1;
508 1; 577 1; 578 4; 579 2; 580 1;
581 1;

Name: C16_POL_2091.88_218
Synon: Metabolite name: myo-Inositol
Synon: Analyte name: M000060_A209002-101-xxx_NA_2,080.20_TRUE_VAR5_ALK_Inositol, myo- (6TMS)
Synon: Analyte name: myo-Inositol (6TMS)
Synon: RI: 2092 iu
Synon: Formula: C24H60O6Si6
Synon: MW: 612 Exact Mass: 612.30055 CAS#: 2582-79-8
DB#: 15
Num Peaks: 146
70 1; 71 1; 72 11; 73 999; 74 81;
75 58; 76 2; 77 2; 79 1; 81 8;
82 1; 83 4; 84 1; 85 3; 86 1;
87 3; 88 1; 89 1; 99 2; 101 6;
102 2; 103 80; 104 8; 105 4; 109 2;
111 3; 113 3; 115 3; 116 3; 117 7;
118 1; 119 3; 125 1; 126 1; 127 3;
128 1; 129 83; 130 9; 131 27; 132 3;
133 61; 134 8; 135 5; 136 1; 139 1;
140 1; 141 2; 142 1; 143 20; 144 2;
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145 2; 146 1; 147 267; 148 43; 149 27;
150 2; 151 1; 153 1; 155 1; 156 1;
157 6; 158 1; 159 2; 161 6; 162 1;
163 1; 169 1; 173 1; 175 2; 176 1;
177 7; 178 1; 179 1; 181 1; 189 9;
190 6; 191 134; 192 27; 193 12; 194 1;
201 1; 203 4; 204 51; 205 14; 206 4;
207 6; 208 1; 209 1; 215 2; 216 2;
217 216; 218 47; 219 21; 220 2; 221 23;
222 4; 223 2; 229 1; 230 3; 231 2;
243 5; 244 1; 245 1; 264 1; 265 41;
266 8; 267 4; 268 1; 271 1; 291 10;
292 3; 293 4; 294 1; 303 1; 304 7;
305 138; 306 46; 307 24; 308 4; 309 1;
317 5; 318 73; 319 35; 320 13; 321 3;
322 1; 343 2; 344 1; 345 1; 366 1;
367 8; 368 3; 369 1; 392 1; 393 4;
394 1; 395 1; 419 1; 431 1; 432 11;
433 8; 434 4; 435 1; 507 2; 508 1;
509 1;

Name: M01_POL_1625.4_423
Synon: Seed: Linseed
Synon: Metabolite name: Tartaric acid
Synon: Analyte name: M000575_A164006-101-xxx_NA_1,628.94_TRUE_VAR5_ALK_Tartaric acid (4TMS)
Synon: Analyte name: Tartaric acid, 4TMS derivative
Synon: Formula: C16H38O6Si4
Synon: MW: 438 Exact Mass: 438.174545 CAS#: 18602-86-3
Synon: RI: 1625 iu
DB#: 79
Num Peaks: 122
70 3; 71 4; 72 16; 73 999; 74 81;
75 51; 76 2; 77 1; 83 1; 84 1;
85 3; 87 4; 88 1; 89 1; 99 5;
101 4; 102 50; 103 19; 104 4; 105 3;
113 1; 115 6; 116 2; 117 12; 118 1;
119 4; 120 1; 127 1; 129 1; 130 22;
131 19; 132 4; 133 33; 134 5; 135 3;
142 1; 143 41; 144 6; 145 3; 147 255;
148 38; 149 22; 150 3; 151 1; 157 1;
159 1; 161 2; 163 5; 164 1; 165 1;
171 12; 172 2; 173 2; 175 16; 176 3;
177 4; 178 1; 185 1; 189 89; 190 17;
191 17; 193 1; 204 6; 205 3; 206 1;
207 6; 208 1; 209 1; 215 1; 217 16;
219 74; 220 13; 221 29; 222 7; 223 3;
224 1; 231 4; 232 1; 233 1; 245 1;
259 1; 261 1; 263 9; 264 2; 265 1;
277 10; 278 4; 279 4; 280 1; 291 5;
292 119; 293 33; 294 16; 295 3; 296 1;
304 2; 305 27; 306 10; 307 5; 308 1;
321 6; 322 2; 323 1; 332 1; 333 17;
334 6; 335 3; 336 1; 351 5; 352 2;
353 1; 367 4; 368 2; 369 1; 395 1;
396 1; 422 4; 423 25; 424 10; 425 5;
426 1; 438 1;

Name: M02_POL_1837.1_171
Synon: Seed: Sesame
Synon: Metabolite name: non-identified
Synon: RI: 1837 iu
DB#: 76
Num Peaks: 206
70 2; 71 3; 72 17; 73 999; 74 86;
75 180; 76 11; 77 21; 78 3; 79 25;
80 3; 81 29; 82 6; 83 10; 84 1;
85 8; 87 4; 88 1; 89 4; 90 1;
91 20; 92 2; 93 8; 94 1; 95 6;
96 1; 97 11; 98 2; 99 8; 101 17;
102 2; 103 56; 104 5; 105 35; 106 5;
107 39; 108 3; 109 6; 110 2; 111 8;
112 2; 113 4; 114 2; 115 14; 116 6;
117 36; 118 3; 119 8; 120 1; 121 7;
122 1; 123 12; 124 2; 125 3; 126 1;
127 9; 128 1; 129 15; 130 14; 131 22;
132 6; 133 75; 134 7; 135 6; 136 1;
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137 2; 138 1; 139 2; 140 1; 141 14;
142 5; 143 23; 144 2; 145 2; 147 224;
148 39; 149 40; 150 4; 151 7; 152 2;
153 3; 154 2; 155 31; 156 8; 157 43;
158 4; 159 3; 161 2; 162 1; 163 8;
164 1; 165 4; 166 1; 167 6; 168 8;
169 26; 170 4; 171 84; 172 9; 173 4;
175 1; 177 3; 178 1; 179 12; 180 15;
181 40; 182 8; 183 6; 184 1; 185 1;
189 2; 191 20; 192 2; 193 3; 194 17;
195 58; 196 11; 197 7; 198 1; 199 1;
201 1; 202 9; 203 2; 204 1; 205 3;
207 7; 208 1; 209 4; 210 1; 211 1;
213 1; 215 2; 216 1; 217 39; 218 6;
219 3; 221 8; 222 14; 223 39; 224 7;
225 3; 228 1; 229 3; 230 2; 231 103;
232 23; 233 7; 234 1; 239 1; 240 4;
241 2; 242 1; 243 2; 244 3; 245 3;
246 10; 247 9; 248 2; 249 1; 253 1;
255 2; 256 1; 257 4; 258 1; 259 2;
260 1; 261 22; 262 4; 263 2; 268 2;
269 4; 270 2; 271 4; 272 15; 273 5;
274 1; 283 1; 284 12; 285 27; 286 9;
287 3; 296 1; 297 11; 298 3; 299 5;
300 1; 301 1; 311 5; 312 102; 313 27;
314 8; 315 2; 319 1; 333 2; 334 1;
347 1; 359 1; 360 1; 361 1; 387 3;
388 1; 389 1; 401 1; 402 2; 403 1;
404 1;

Name: M03_POL_1946.26_306
Synon: Seed: Linseed
Synon: Metabolite name: non-identified
Synon: Note: similar to gluconic acid (6TMS)
Synon: RI: 1946 iu
DB#: 88
Num Peaks: 165
72 7; 73 999; 74 81; 75 51; 76 2;
81 2; 83 10; 84 1; 85 2; 87 4;
88 2; 89 14; 90 1; 97 4; 99 3;
101 13; 102 20; 103 104; 104 11; 105 4;
107 1; 111 1; 113 3; 115 4; 116 3;
117 64; 118 6; 119 5; 127 2; 129 70;
130 22; 131 29; 132 4; 133 48; 134 6;
135 4; 141 2; 142 1; 143 40; 144 4;
145 4; 146 1; 147 334; 148 53; 149 36;
150 3; 151 1; 153 2; 155 1; 157 45;
158 5; 159 3; 161 2; 163 3; 169 7;
170 1; 171 9; 172 1; 173 2; 175 5;
176 1; 177 2; 185 1; 187 1; 189 43;
190 11; 191 26; 192 4; 193 1; 197 3;
201 2; 202 1; 203 4; 204 36; 205 99;
206 23; 207 15; 208 2; 209 1; 215 2;
216 1; 217 77; 218 18; 219 16; 220 5;
221 19; 222 4; 223 2; 227 1; 229 16;
230 3; 231 5; 232 1; 233 1; 241 1;
243 2; 244 1; 245 7; 246 1; 247 1;
257 1; 259 2; 260 1; 261 1; 263 1;
265 1; 269 2; 271 1; 277 9; 278 3;
279 2; 290 1; 291 11; 292 86; 293 29;
294 13; 295 2; 304 2; 305 35; 306 11;
307 10; 308 2; 309 1; 315 1; 316 1;
317 1; 318 4; 319 62; 320 20; 321 10;
322 2; 323 1; 330 1; 331 8; 332 8;
333 83; 334 30; 335 13; 336 2; 343 1;
344 1; 345 3; 346 1; 358 1; 359 12;
360 3; 361 1; 379 1; 389 1; 393 1;
394 1; 405 1; 406 1; 407 1; 421 1;
422 1; 423 5; 424 2; 425 1; 432 1;
433 8; 434 3; 435 5; 436 2; 437 1;

Name: M04_POL_2003.15_333
Synon: Seed: Linseed
Synon: Metabolite name: Saccharic acid
Synon: Analyte name: M000093_A201001-101-xxx_NA_2,000.79_TRUE_VAR5_ALK_Saccharic acid (6TMS)
Synon: Analyte name: Galactaric acid, 6TMS derivative
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Synon: Formula: C24H58O8Si6
Synon: MW: 642 Exact Mass: 642.274727 CAS#: 38165-96-7
Synon: RI: 2003 iu
DB#: 68
Num Peaks: 166
70 2; 71 3; 72 13; 73 999; 74 82;
75 57; 76 3; 77 2; 81 1; 83 5;
84 2; 85 5; 86 1; 87 5; 88 1;
89 2; 95 2; 97 1; 98 1; 99 6;
100 1; 101 8; 102 23; 103 28; 104 4;
105 3; 111 2; 113 3; 114 1; 115 4;
116 3; 117 9; 118 1; 119 4; 125 1;
127 4; 128 1; 129 13; 130 9; 131 16;
132 4; 133 27; 134 4; 135 3; 141 2;
142 1; 143 53; 144 7; 145 5; 146 1;
147 201; 148 30; 149 18; 150 2; 151 1;
155 1; 156 1; 157 3; 159 2; 161 3;
163 3; 169 2; 171 17; 172 3; 173 3;
175 4; 176 1; 177 2; 183 2; 185 1;
187 1; 189 36; 190 8; 191 15; 192 3;
193 2; 201 2; 203 2; 204 12; 205 5;
206 2; 207 6; 208 1; 209 1; 211 1;
215 2; 217 26; 218 5; 219 12; 220 4;
221 18; 222 5; 223 3; 224 1; 229 4;
230 1; 231 4; 232 1; 233 1; 243 1;
245 6; 246 2; 247 1; 249 1; 257 3;
258 1; 259 1; 261 1; 263 1; 265 1;
277 12; 278 4; 279 3; 280 1; 291 4;
292 43; 293 13; 294 6; 295 1; 303 1;
304 1; 305 16; 306 5; 307 3; 308 1;
317 1; 318 1; 319 1; 320 1; 321 2;
322 1; 331 1; 332 1; 333 99; 334 25;
335 9; 336 2; 345 3; 346 1; 347 1;
373 9; 374 4; 375 2; 379 3; 380 1;
381 1; 393 3; 394 1; 395 1; 419 5;
420 2; 421 1; 422 1; 423 8; 424 4;
425 2; 435 4; 436 2; 437 1; 447 4;
448 2; 449 1; 493 1; 509 2; 510 1;
537 1;

Name: M05_POL_2045.05_231
Synon: Seed: Sesame
Synon: Metabolite name: non-identified
Synon: RI: 2045 iu
DB#: 145
Num Peaks: 289
70 3; 71 9; 72 21; 73 999; 74 77;
75 317; 76 24; 77 27; 78 3; 79 17;
80 2; 81 31; 82 5; 83 24; 84 5;
85 11; 86 2; 87 5; 88 2; 89 79;
90 7; 91 19; 92 2; 93 10; 94 1;
95 33; 96 3; 97 17; 98 9; 99 11;
101 13; 102 2; 103 53; 104 7; 105 53;
106 5; 107 9; 108 2; 109 17; 110 2;
111 15; 112 4; 113 4; 114 1; 115 17;
116 17; 117 197; 118 22; 119 26; 120 4;
121 17; 122 1; 123 15; 124 2; 125 5;
126 2; 127 6; 128 2; 129 101; 130 21;
131 67; 132 87; 133 82; 134 13; 135 14;
136 2; 137 5; 138 1; 139 15; 140 2;
141 13; 142 4; 143 57; 144 9; 145 57;
146 7; 147 180; 148 34; 149 47; 150 5;
151 7; 152 2; 153 10; 154 3; 155 7;
156 5; 157 24; 158 3; 159 43; 160 9;
161 24; 162 3; 163 30; 164 4; 165 10;
166 2; 167 17; 168 8; 169 29; 170 5;
171 10; 172 2; 173 4; 174 1; 175 3;
176 16; 177 10; 178 2; 179 9; 180 3;
181 8; 182 2; 183 11; 184 2; 185 9;
186 2; 187 5; 188 1; 189 2; 190 3;
191 56; 192 7; 193 14; 194 4; 195 12;
196 5; 197 13; 198 2; 199 9; 200 2;
201 13; 202 7; 203 2; 204 1; 205 8;
206 2; 207 15; 208 4; 209 9; 210 1;
211 2; 212 1; 213 7; 214 2; 215 4;
216 1; 217 57; 218 11; 219 6; 220 2;
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221 21; 222 4; 223 7; 224 2; 225 4;
226 1; 227 5; 228 1; 229 19; 230 4;
231 90; 232 24; 233 10; 234 2; 235 1;
236 2; 237 8; 238 3; 239 14; 240 11;
241 12; 242 3; 243 6; 244 3; 245 5;
246 8; 247 17; 248 6; 249 25; 250 4;
251 5; 252 5; 253 13; 254 3; 255 3;
256 1; 257 9; 258 3; 259 2; 260 1;
261 1; 265 3; 266 1; 267 3; 268 1;
269 6; 270 2; 271 4; 272 1; 273 2;
274 1; 279 1; 280 12; 281 15; 282 3;
283 5; 284 12; 285 112; 286 36; 287 15;
288 3; 289 1; 295 3; 296 1; 297 2;
298 2; 299 2; 300 1; 301 1; 303 1;
305 3; 306 1; 307 1; 308 1; 309 1;
310 3; 311 4; 312 5; 313 52; 314 13;
315 4; 316 1; 317 1; 318 1; 319 3;
320 1; 321 1; 323 3; 324 1; 325 2;
326 2; 327 3; 328 4; 329 2; 330 4;
331 2; 332 1; 333 4; 334 2; 335 1;
337 1; 338 6; 339 5; 340 2; 341 1;
342 3; 343 6; 344 2; 345 1; 346 1;
354 1; 355 4; 356 1; 357 2; 358 1;
359 1; 369 2; 370 22; 371 5; 372 2;
373 3; 374 1; 375 3; 376 1; 386 1;
387 1; 391 1; 403 1; 413 1; 430 1;
444 2; 445 13; 446 5; 447 2; 448 1;
460 1; 534 1; 535 3; 536 1;

Name: M06_POL_2051.2_267
Synon: Seed: Chia
Synon: Metabolite name: Catechollactic acid
Synon: Analyte name: Trimethylsilylcatechollactatetris(trimethylsilyl) ether
Synon: Formula: C21H42O5Si4
Synon: MW: 486 Exact Mass: 486.21093 CAS#: 68595-72-2
Synon: RI: 2051 iu
DB#: 71
Num Peaks: 118
70 2; 71 2; 72 9; 73 999; 74 87;
75 67; 76 3; 77 8; 78 2; 82 4;
83 1; 84 1; 87 2; 88 2; 89 3;
91 5; 93 1; 95 1; 97 1; 99 1;
101 1; 102 4; 103 6; 104 3; 105 7;
109 1; 115 6; 116 2; 117 9; 118 1;
119 5; 120 1; 121 1; 129 3; 130 1;
131 16; 132 2; 133 23; 134 2; 135 4;
136 1; 137 1; 145 1; 147 128; 148 17;
149 25; 150 3; 151 2; 159 1; 160 1;
161 3; 162 1; 163 4; 164 1; 165 1;
175 2; 177 4; 178 1; 179 168; 180 20;
181 6; 189 1; 191 18; 192 4; 193 5;
194 1; 195 1; 204 1; 205 3; 207 21;
208 3; 209 2; 219 24; 220 3; 221 3;
223 3; 224 1; 233 1; 235 1; 237 1;
249 3; 250 1; 251 2; 263 1; 265 8;
266 7; 267 299; 268 79; 269 25; 270 3;
279 2; 280 1; 281 4; 282 1; 292 4;
293 4; 294 1; 307 1; 309 1; 353 1;
355 1; 368 1; 369 1; 381 4; 382 1;
395 5; 396 38; 397 12; 398 5; 399 1;
443 1; 444 1; 471 2; 472 1; 485 1;
486 5; 487 2; 488 1;

Name: M07_POL_2209.11_109
Synon: Seed: Sesame
Synon: Metabolite name: non-identified
Synon: RI: 2209 iu
DB#: 128
Num Peaks: 355
72 14; 73 999; 74 80; 75 88; 76 5;
77 4; 79 3; 80 1; 81 11; 82 1;
83 14; 87 3; 88 1; 89 59; 90 5;
91 11; 92 2; 93 4; 95 18; 96 1;
97 23; 98 2; 99 5; 101 7; 102 2;
103 62; 104 6; 105 11; 106 1; 107 4;
108 2; 109 21; 110 1; 111 7; 112 1;
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113 4; 114 2; 115 7; 116 4; 117 29;
118 3; 119 17; 120 2; 121 6; 123 9;
124 1; 125 4; 126 1; 127 4; 128 1;
129 25; 130 7; 131 25; 132 3; 133 56;
134 8; 135 12; 136 2; 137 6; 138 1;
139 9; 140 1; 141 20; 142 4; 143 35;
144 4; 145 6; 146 2; 147 293; 148 47;
149 41; 150 5; 151 10; 152 1; 153 5;
154 2; 155 6; 156 11; 157 31; 158 4;
159 44; 160 15; 161 9; 162 1; 163 26;
164 4; 165 6; 166 2; 167 13; 168 3;
169 37; 170 8; 171 5; 172 1; 173 3;
175 5; 176 2; 177 5; 178 1; 179 6;
180 2; 181 7; 182 3; 183 14; 184 3;
185 5; 186 1; 187 3; 188 1; 189 5;
190 1; 191 27; 192 5; 193 20; 194 4;
195 7; 196 3; 197 13; 198 2; 199 4;
200 2; 201 3; 202 11; 203 8; 204 16;
205 32; 206 7; 207 15; 208 3; 209 8;
210 2; 211 5; 212 5; 213 13; 214 2;
215 5; 216 1; 217 20; 218 285; 219 64;
220 29; 221 21; 222 4; 223 4; 224 1;
225 4; 226 1; 227 5; 228 1; 229 3;
230 4; 231 57; 232 12; 233 6; 234 1;
235 4; 236 1; 237 5; 238 1; 239 5;
240 38; 241 13; 242 3; 243 9; 244 3;
245 19; 246 113; 247 169; 248 46; 249 18;
250 4; 251 12; 252 3; 253 5; 254 2;
255 6; 256 2; 257 20; 258 14; 259 14;
260 4; 261 1; 263 1; 264 1; 265 5;
266 1; 267 4; 268 1; 269 3; 270 3;
271 7; 272 2; 273 5; 274 2; 275 1;
277 1; 278 6; 279 19; 280 4; 281 7;
282 2; 283 6; 284 3; 285 3; 286 5;
287 4; 288 2; 289 3; 290 1; 291 1;
293 1; 294 1; 295 2; 296 1; 297 3;
298 5; 299 5; 300 2; 301 3; 302 3;
303 2; 304 1; 305 2; 306 1; 307 2;
308 2; 309 11; 310 4; 311 4; 312 1;
313 2; 314 1; 315 4; 316 1; 317 2;
318 2; 319 15; 320 4; 321 2; 322 1;
323 2; 324 2; 325 6; 326 3; 327 4;
328 2; 329 4; 330 40; 331 15; 332 5;
333 2; 334 2; 335 1; 336 3; 337 7;
338 2; 339 2; 340 4; 341 5; 342 2;
343 2; 344 1; 345 1; 346 1; 347 1;
348 1; 352 1; 353 5; 354 2; 355 5;
356 2; 357 2; 358 1; 359 1; 360 1;
362 1; 363 2; 364 1; 367 3; 368 28;
369 23; 370 7; 371 3; 372 3; 373 16;
374 6; 375 3; 376 1; 377 1; 383 1;
384 1; 385 1; 386 1; 387 1; 388 1;
389 1; 390 1; 391 1; 392 2; 393 1;
398 1; 399 2; 400 1; 401 1; 402 1;
403 2; 404 2; 405 2; 406 1; 411 1;
412 1; 413 1; 414 1; 415 1; 416 1;
417 1; 418 1; 419 2; 420 8; 421 3;
422 1; 423 1; 426 1; 427 2; 428 1;
429 1; 430 1; 431 2; 432 1; 433 1;
442 1; 443 7; 444 3; 445 2; 446 1;
447 1; 457 2; 458 9; 459 4; 460 2;
461 1; 473 1; 501 1; 503 1; 504 1;
505 1; 506 1; 507 1; 532 1; 533 2;
534 1; 535 1; 547 1; 548 1; 549 1;

Name: M08_POL_2409.48_204
Synon: Seed: Sesame
Synon: Metabolite name: non-identified
Synon: RI: 2409 iu
DB#: 132
Num Peaks: 155
70 2; 71 16; 72 15; 73 999; 74 89;
75 147; 76 8; 77 6; 81 8; 82 2;
83 5; 84 1; 85 5; 86 1; 87 4;
88 2; 89 8; 90 1; 91 2; 94 1;
95 1; 97 2; 98 1; 99 10; 101 19;
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102 3; 103 84; 104 6; 105 3; 109 3;
111 3; 113 6; 114 1; 115 7; 116 10;
117 42; 118 3; 119 5; 125 1; 127 3;
128 1; 129 138; 130 15; 131 25; 132 3;
133 39; 134 4; 135 3; 139 1; 141 2;
142 1; 143 38; 144 28; 145 19; 146 3;
147 199; 148 33; 149 31; 150 3; 151 2;
153 2; 154 1; 155 7; 156 1; 157 12;
158 2; 159 2; 160 1; 161 2; 163 12;
164 2; 169 38; 170 4; 171 5; 172 1;
173 4; 175 2; 177 2; 183 2; 185 1;
187 1; 189 22; 190 5; 191 36; 192 5;
193 3; 197 1; 199 2; 201 1; 202 1;
203 8; 204 423; 205 99; 206 38; 207 6;
208 1; 215 1; 216 1; 217 79; 218 21;
219 8; 220 1; 221 5; 222 1; 223 1;
227 1; 229 3; 230 2; 231 10; 232 3;
233 6; 234 2; 235 1; 241 1; 242 1;
243 13; 244 3; 245 5; 246 1; 247 2;
257 1; 258 1; 259 2; 260 1; 261 17;
262 3; 263 2; 265 1; 271 11; 272 2;
273 2; 291 3; 292 1; 293 1; 305 4;
306 5; 307 2; 308 1; 319 2; 321 1;
331 2; 332 1; 333 1; 334 1; 335 2;
345 1; 360 5; 361 61; 362 16; 363 7;
364 1; 379 3; 380 1; 381 1; 451 1;

Name: M09_POL_2978.07_360
Synon: Seed: Linseed
Synon: Metabolite name: non-identified
Synon: Note: also identified as C14
Synon: RI: 2978 iu
DB#: 104
Num Peaks: 253
70 4; 71 6; 72 10; 73 999; 74 77;
75 67; 76 4; 77 3; 79 1; 81 17;
82 2; 83 5; 84 7; 85 13; 86 2;
87 4; 88 2; 89 9; 90 1; 91 2;
94 1; 95 1; 97 5; 98 1; 99 5;
100 4; 101 23; 102 4; 103 104; 104 10;
105 5; 109 5; 110 1; 111 3; 112 1;
113 7; 114 2; 115 8; 116 9; 117 37;
118 4; 119 6; 120 1; 125 1; 126 1;
127 4; 128 1; 129 119; 130 15; 131 22;
132 4; 133 16; 134 3; 135 2; 139 1;
140 4; 141 15; 142 6; 143 18; 144 3;
145 11; 146 2; 147 109; 148 16; 149 12;
150 2; 151 1; 153 1; 154 1; 155 7;
156 2; 157 12; 158 3; 159 3; 160 1;
161 4; 162 1; 163 3; 164 1; 167 1;
168 1; 169 18; 170 4; 171 6; 172 9;
173 15; 174 4; 175 3; 176 1; 177 3;
181 1; 183 2; 184 1; 185 1; 186 4;
187 2; 188 1; 189 12; 190 4; 191 19;
192 4; 193 2; 195 1; 197 1; 198 1;
199 6; 200 2; 201 2; 202 1; 203 7;
204 500; 205 83; 206 30; 207 4; 208 1;
214 1; 215 4; 216 1; 217 95; 218 25;
219 12; 220 2; 221 4; 222 1; 223 1;
226 1; 227 1; 228 1; 229 5; 230 4;
231 11; 232 3; 233 5; 234 1; 235 1;
238 1; 239 1; 240 1; 241 2; 242 5;
243 22; 244 7; 245 8; 246 3; 247 6;
248 1; 249 1; 255 1; 256 1; 257 5;
258 1; 259 4; 260 1; 261 1; 263 1;
265 1; 266 3; 267 1; 268 1; 269 1;
270 1; 271 19; 272 8; 273 8; 274 2;
275 1; 277 1; 278 1; 279 1; 282 1;
285 1; 286 1; 287 1; 288 1; 289 4;
290 1; 291 5; 292 2; 293 1; 298 2;
299 1; 300 1; 301 1; 302 1; 303 1;
304 2; 305 14; 306 5; 307 3; 308 1;
313 1; 314 2; 315 1; 316 1; 317 9;
318 4; 319 7; 320 2; 321 1; 329 1;
330 1; 331 7; 332 7; 333 4; 334 1;
335 1; 345 3; 346 1; 347 1; 356 4;
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357 1; 358 1; 359 1; 360 3; 361 39;
362 13; 363 10; 364 3; 365 1; 372 1;
379 1; 388 4; 389 1; 390 1; 393 1;
403 1; 405 1; 406 1; 407 2; 408 1;
430 1; 431 1; 432 1; 433 1; 435 1;
445 4; 446 33; 447 13; 448 6; 449 1;
462 2; 463 1; 505 1; 506 8; 507 4;
508 3; 509 1; 562 1; 563 4; 564 17;
565 8; 566 4; 567 1;

Name: M10_POL_3032.18_172
Synon: Seed: Linseed
Synon: Metabolite name: non-identified
Synon: Note: also identified as C15
Synon: RI: 3032 iu
DB#: 107
Num Peaks: 236
70 3; 71 6; 72 19; 73 999; 74 81;
75 69; 76 4; 77 3; 79 1; 80 1;
81 17; 82 28; 83 6; 84 6; 85 11;
86 1; 87 4; 88 1; 89 9; 90 1;
91 2; 94 1; 95 1; 97 6; 98 1;
99 5; 100 4; 101 22; 102 4; 103 109;
104 11; 105 5; 109 7; 110 1; 111 3;
112 1; 113 8; 114 2; 115 6; 116 11;
117 40; 118 5; 119 8; 120 1; 125 1;
126 1; 127 4; 128 2; 129 132; 130 17;
131 18; 132 3; 133 17; 134 3; 135 2;
136 1; 139 1; 140 6; 141 3; 142 4;
143 16; 144 3; 145 15; 146 2; 147 112;
148 17; 149 13; 150 2; 151 1; 153 2;
154 8; 155 16; 156 3; 157 14; 158 3;
159 3; 160 1; 161 4; 162 1; 163 3;
167 1; 169 18; 170 4; 171 7; 172 10;
173 9; 174 3; 175 3; 176 1; 177 3;
178 1; 181 1; 183 3; 184 1; 185 1;
187 10; 188 2; 189 13; 190 5; 191 20;
192 4; 193 2; 195 1; 197 1; 198 1;
199 5; 200 5; 201 2; 202 1; 203 7;
204 477; 205 89; 206 36; 207 5; 208 1;
213 1; 214 1; 215 3; 216 1; 217 83;
218 22; 219 11; 220 2; 221 4; 222 1;
223 1; 226 1; 227 1; 228 1; 229 4;
230 4; 231 10; 232 2; 233 4; 234 1;
235 1; 241 1; 242 2; 243 16; 244 6;
245 6; 246 2; 247 5; 248 1; 254 1;
255 1; 256 2; 257 3; 258 1; 259 3;
260 1; 261 1; 263 1; 265 1; 270 1;
271 16; 272 5; 273 6; 274 1; 275 1;
279 1; 280 1; 282 1; 286 1; 287 1;
288 1; 289 3; 290 1; 291 4; 292 1;
293 1; 298 1; 300 1; 301 1; 303 1;
304 2; 305 13; 306 4; 307 2; 308 1;
314 1; 315 1; 316 1; 317 9; 318 3;
319 6; 320 1; 321 1; 328 1; 330 1;
331 6; 332 5; 333 3; 334 1; 335 1;
344 1; 345 2; 346 1; 347 1; 359 1;
360 4; 361 32; 362 12; 363 9; 364 2;
365 1; 370 3; 371 1; 372 1; 379 1;
388 3; 389 1; 390 1; 405 1; 406 1;
407 2; 408 1; 435 1; 444 1; 459 5;
460 26; 461 12; 462 7; 463 2; 464 1;
505 2; 506 8; 507 3; 508 2; 509 1;
576 1; 577 4; 578 13; 579 7; 580 3;
581 1;

Name: M11_POL_3145.68_205
Synon: Seed: Linseed
Synon: Metabolite name: non-identified
Synon: RI: 3146 iu
DB#: 109
Num Peaks: 181
70 5; 71 3; 72 10; 73 999; 74 87;
75 144; 76 8; 77 7; 79 8; 80 1;
81 16; 82 1; 83 3; 84 3; 85 7;
86 1; 87 3; 88 2; 89 9; 90 1;
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91 17; 92 1; 93 3; 94 1; 97 3;
99 4; 100 2; 101 21; 102 4; 103 97;
104 9; 105 11; 106 2; 107 2; 109 4;
111 5; 112 1; 113 6; 114 1; 115 8;
116 16; 117 50; 118 6; 119 8; 120 1;
121 1; 125 1; 126 1; 127 3; 128 3;
129 129; 130 76; 131 28; 132 10; 133 50;
134 4; 135 3; 137 1; 139 2; 141 4;
142 17; 143 24; 144 4; 145 6; 146 5;
147 161; 148 20; 149 17; 150 1; 151 1;
153 3; 155 13; 156 2; 157 14; 158 21;
159 18; 160 3; 161 4; 162 1; 163 2;
164 1; 168 1; 169 35; 170 4; 171 4;
173 4; 174 2; 175 7; 176 1; 177 2;
179 1; 182 4; 183 3; 186 1; 187 1;
189 21; 190 3; 191 26; 192 3; 195 1;
196 1; 199 3; 200 1; 201 1; 203 4;
204 391; 205 67; 206 22; 207 5; 214 1;
215 1; 216 1; 217 88; 218 16; 219 8;
221 2; 223 1; 229 2; 230 2; 231 6;
232 8; 233 5; 238 1; 242 1; 243 11;
244 2; 245 1; 246 1; 248 1; 249 1;
255 1; 257 1; 259 3; 260 1; 264 1;
265 4; 266 1; 267 1; 270 2; 271 12;
272 4; 273 2; 281 1; 285 1; 286 1;
287 1; 289 2; 291 1; 305 4; 308 1;
310 1; 317 2; 318 1; 319 3; 320 1;
321 1; 331 1; 332 2; 356 1; 361 27;
362 8; 363 2; 364 2; 370 1; 391 1;
393 1; 414 1; 422 1; 458 1; 460 1;
466 1; 467 1; 489 1; 523 1; 538 1;
539 2; 540 1; 548 1; 586 1; 591 1;
593 1;

Name: M12_POL_3210.66_179
Synon: Seed: Chia
Synon: Metabolite name: Rosmarinic acid, cis-
Synon: Analyte name: M001162_A340009-101-xxx_NA_3,400.96_TRUE_VAR5_ALK_Rosmarinic acid (5TMS)
Synon: Analyte name: Rosmarinic acid, 5O-TMS
Synon: Formula: C33H56O8Si5
Synon: MW: 720 Exact Mass: 720.28215
Synon: RI: 3211 iu
DB#: 69
Num Peaks: 159
70 1; 72 8; 73 999; 74 90; 75 80;
76 5; 77 8; 78 1; 82 2; 83 3;
86 1; 87 2; 88 9; 89 10; 90 1;
91 3; 95 1; 99 1; 101 1; 102 5;
103 4; 104 2; 105 4; 107 1; 109 1;
114 1; 115 10; 116 3; 117 13; 118 1;
119 3; 121 1; 128 2; 129 2; 130 1;
131 8; 132 1; 133 12; 134 1; 135 9;
136 1; 137 3; 139 1; 141 2; 142 1;
143 2; 145 4; 147 16; 148 2; 149 8;
150 1; 151 2; 156 1; 157 1; 159 1;
160 3; 161 5; 162 2; 163 9; 164 2;
165 1; 166 1; 169 1; 171 1; 173 1;
174 1; 175 5; 176 1; 177 4; 178 1;
179 109; 180 13; 181 4; 182 1; 185 1;
186 1; 187 1; 189 2; 190 3; 191 72;
192 15; 193 8; 194 1; 195 1; 201 1;
203 4; 207 3; 208 1; 209 1; 210 1;
216 1; 217 2; 218 2; 219 170; 220 29;
221 8; 222 1; 223 2; 231 1; 232 1;
233 4; 234 1; 235 2; 236 3; 237 1;
247 1; 248 1; 249 13; 250 3; 251 2;
252 1; 261 1; 263 1; 264 1; 265 5;
266 2; 267 24; 268 5; 269 2; 277 2;
278 1; 279 6; 280 4; 281 2; 282 1;
289 1; 290 1; 291 5; 292 6; 293 12;
294 3; 295 1; 296 1; 297 1; 305 2;
306 2; 307 27; 308 9; 309 7; 310 1;
323 3; 324 56; 325 12; 326 4; 327 1;
337 1; 360 1; 361 1; 380 1; 381 9;
382 5; 383 3; 394 1; 395 19; 396 144;
397 58; 398 28; 399 6; 400 2;
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Name: M13_POL_3399.31_396
Synon: Seed: Chia
Synon: Metabolite name: Rosmarinic acid, trans-
Synon: Analyte name: M001162_A340009-101-xxx_NA_3,400.96_TRUE_VAR5_ALK_Rosmarinic acid (5TMS)
Synon: Analyte name: Rosmarinic acid, 5O-TMS
Synon: Formula: C33H56O8Si5
Synon: MW: 720 Exact Mass: 720.28215
Synon: RI: 3399 iu
DB#: 70
Num Peaks: 170
70 1; 71 1; 72 9; 73 999; 74 83;
75 74; 76 5; 77 8; 78 1; 79 1;
82 2; 83 4; 84 1; 85 1; 86 1;
87 2; 88 12; 89 14; 90 1; 91 4;
93 1; 95 1; 99 1; 101 1; 102 6;
103 7; 104 2; 105 6; 106 1; 107 1;
109 2; 110 1; 115 14; 116 4; 117 20;
118 2; 119 5; 120 1; 121 1; 123 1;
127 1; 128 2; 129 6; 130 1; 131 11;
132 2; 133 16; 134 2; 135 12; 136 2;
137 3; 139 1; 141 2; 142 1; 143 2;
144 1; 145 5; 146 1; 147 25; 148 5;
149 11; 150 1; 151 1; 157 1; 159 1;
160 4; 161 7; 162 2; 163 11; 164 2;
165 1; 166 1; 173 1; 174 1; 175 7;
176 1; 177 5; 178 1; 179 100; 180 17;
181 5; 182 1; 185 1; 187 1; 188 1;
189 3; 190 4; 191 79; 192 21; 193 10;
194 1; 195 1; 201 1; 203 6; 204 2;
205 4; 206 1; 207 4; 208 1; 209 2;
216 1; 217 4; 218 3; 219 201; 220 39;
221 13; 222 1; 223 2; 231 1; 232 1;
233 6; 234 1; 235 2; 236 3; 237 2;
247 1; 248 1; 249 20; 250 4; 251 2;
252 1; 261 1; 263 2; 264 1; 265 7;
266 2; 267 29; 268 6; 269 2; 277 2;
278 1; 279 9; 280 7; 281 3; 282 1;
289 1; 290 1; 291 5; 292 8; 293 19;
294 5; 295 2; 296 1; 305 3; 306 3;
307 44; 308 16; 309 14; 310 3; 311 1;
323 3; 324 47; 325 13; 326 4; 327 1;
338 1; 339 1; 360 1; 380 2; 381 16;
382 7; 383 3; 384 1; 394 1; 395 25;
396 195; 397 73; 398 39; 399 9; 400 2;

Name: M14_SOL_1392.44_210
Synon: Seed: Sesame
Synon: Metabolite name: Sesamol
Synon: Analyte name: Sesamol, TMS derivative
Synon: Formula: C10H14O3Si
Synon: MW: 210 Exact Mass: 210.07122 CAS#: 17903-26-3
Synon: RI: 1392 iu
DB#: 159
Num Peaks: 206
70 91; 76 25; 77 211; 78 6; 79 190;
80 12; 81 1; 82 15; 83 185; 90 1;
93 1; 94 14; 97 242; 99 2; 101 1;
106 4; 107 29; 109 66; 110 1; 111 13;
113 2; 116 6; 117 2; 121 67; 122 36;
123 1; 124 1; 136 1; 137 654; 138 93;
139 6; 147 1; 151 7; 152 2; 155 19;
160 12; 165 993; 166 93; 167 148; 168 5;
169 77; 171 16; 172 3; 179 1; 182 40;
183 23; 189 1; 195 753; 196 77; 197 8;
204 7; 210 999; 211 166; 212 14; 217 7;
218 5; 219 2; 220 1; 234 3; 236 21;
237 23; 239 14; 240 12; 249 14; 250 2;
251 3; 252 10; 263 11; 264 4; 265 13;
269 2; 275 16; 276 4; 279 3; 285 2;
286 24; 289 4; 290 16; 293 2; 298 5;
300 4; 305 21; 306 6; 307 2; 308 6;
309 4; 311 2; 313 1; 314 1; 317 1;
319 2; 322 2; 326 5; 329 10; 331 1;
337 1; 340 1; 341 2; 347 9; 348 1;
353 3; 357 1; 358 9; 362 5; 364 7;
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366 3; 367 5; 369 2; 370 2; 371 8;
372 1; 373 19; 382 3; 384 1; 390 7;
391 4; 393 1; 395 3; 396 10; 398 1;
399 1; 402 1; 403 3; 407 13; 409 2;
413 7; 417 1; 418 5; 421 1; 425 2;
429 3; 430 1; 432 5; 434 1; 435 2;
436 3; 440 6; 442 3; 443 4; 448 2;
450 2; 454 1; 456 1; 457 1; 459 7;
460 1; 465 2; 470 3; 471 1; 472 7;
473 1; 474 2; 475 7; 477 1; 478 1;
481 4; 483 2; 484 1; 485 1; 490 1;
491 1; 492 1; 494 8; 497 8; 498 5;
501 2; 506 2; 508 3; 511 1; 512 1;
514 3; 516 2; 520 6; 521 2; 525 3;
527 3; 531 3; 532 1; 533 2; 534 1;
538 4; 539 1; 541 6; 545 1; 548 1;
549 3; 552 1; 557 5; 558 7; 559 1;
561 2; 563 3; 564 1; 570 2; 571 3;
572 1; 574 1; 575 5; 580 1; 585 6;
586 2; 589 1; 596 7; 598 1; 599 11;
600 2;

Name: M15_SOL_2614.79_335
Synon: Seed: Chia
Synon: Metabolite name: non-identified
Synon: RI: 2615 iu
DB#: 147
Num Peaks: 268
70 4; 71 6; 72 14; 73 999; 74 86;
75 75; 76 5; 77 3; 79 1; 80 2;
81 1; 82 8; 83 4; 84 2; 85 5;
86 1; 87 3; 88 3; 89 34; 90 3;
91 2; 94 1; 95 2; 96 1; 97 1;
98 2; 99 4; 100 27; 101 15; 102 4;
103 111; 104 12; 105 9; 106 1; 107 1;
110 1; 111 3; 112 3; 113 4; 114 3;
115 4; 116 7; 117 57; 118 6; 119 5;
120 1; 123 1; 124 1; 125 1; 126 6;
127 9; 128 3; 129 34; 130 6; 131 14;
132 3; 133 34; 134 5; 135 4; 136 1;
138 5; 139 1; 140 2; 141 3; 142 17;
143 34; 144 7; 145 7; 146 2; 147 208;
148 35; 149 23; 150 3; 151 2; 152 1;
153 1; 154 1; 155 1; 156 2; 157 6;
158 11; 159 5; 160 3; 161 10; 162 2;
163 6; 164 1; 165 1; 166 1; 167 1;
168 5; 169 36; 170 7; 171 5; 172 2;
173 45; 174 72; 175 20; 176 5; 177 3;
178 1; 180 1; 181 1; 182 1; 183 1;
184 2; 185 4; 186 3; 187 3; 188 1;
189 18; 190 6; 191 16; 192 3; 193 2;
196 1; 197 1; 198 4; 199 2; 200 2;
201 2; 202 2; 203 3; 204 49; 205 113;
206 25; 207 13; 208 2; 209 1; 213 1;
214 2; 215 4; 216 3; 217 175; 218 40;
219 19; 220 4; 221 7; 222 2; 223 1;
227 1; 228 1; 229 4; 230 3; 231 5;
232 2; 233 17; 234 6; 235 3; 236 1;
240 1; 241 2; 242 2; 243 7; 244 6;
245 7; 246 15; 247 6; 248 2; 249 1;
255 1; 256 3; 257 18; 258 6; 259 9;
260 4; 261 5; 262 2; 263 2; 264 1;
265 1; 271 1; 272 1; 273 1; 274 9;
275 4; 276 2; 277 8; 278 4; 279 3;
280 1; 285 6; 286 2; 287 2; 288 10;
289 6; 290 2; 291 6; 292 10; 293 3;
294 2; 301 1; 303 1; 304 1; 305 17;
306 7; 307 45; 308 13; 309 7; 310 1;
316 1; 317 2; 318 2; 319 4; 320 2;
321 2; 322 1; 324 2; 330 1; 331 7;
332 4; 333 25; 334 9; 335 6; 336 2;
337 1; 345 2; 346 2; 347 3; 348 2;
349 3; 350 1; 351 1; 358 1; 359 3;
360 1; 361 1; 362 1; 374 3; 375 55;
376 19; 377 11; 378 18; 379 6; 380 3;
381 1; 390 1; 391 4; 392 2; 393 1;
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394 1; 395 1; 406 1; 407 1; 419 1;
421 1; 422 1; 423 2; 424 1; 435 2;
436 1; 437 1; 448 1; 449 3; 450 1;
451 1; 452 1; 465 1; 466 1; 467 2;
468 1; 469 1; 539 1; 593 1; 594 2;
595 2; 596 1; 597 1;
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