UPLC-ESI-HRMS/MS conditions for untargeted metabolomic analysis

The analysis was performed on an ultra-high-performance liquid chromatography system (Acquity UPLC I Class, Waters, USA) coupled to electrospray ionization source-single quadrupole-time of flight mass spectrometer (Q-TOF; Synapt G2 Si, Waters, USA). The separation was carried out in an Acquity BEH column (2.1 mm x 50 mm, 1.7 μ m, C18, Waters, USA). The column oven and sample manager temperatures were 40 °C and 15 °C, respectively. The flow rate was 300 μ L/min, and 5 μ L of each sample was injected into the UPLC-ESI-HRMS system in triplicate. The mobile phase consisted of water (A) and acetonitrile (B), both acidified with formic acid (0.1% v/v), and the elution gradient conditions were as follows:

Time (min)	% A	% B
0	99	1
13	20	80
14	20	80
15	99	1
20	99	1

The detection was carried out in both positive and negative ionization modes with the following parameters:

Parameter	Value
Capillary voltage	3 kV
Capillary temperature	100 °C
Desolvatation gas flow (N₂)	600 L/h
Desolvatation gas temperature	200 °C
Sampling cone voltage	40 V
Source offset voltage	80 V
Nebulizer pressure	6.5 Bar

The mass spectra were acquired in a mass-to-charge ratio range of 50-1200 Da and a scan time of 0.5 s [function 1 (low collision energy) = 6 V; function 2 (high collision energy) = 10-30 V]. The real-time mass exact correction was done with the reference peptide Leucine-enkephalin ([M+H]⁺=556.2771; ([M-H]⁻=554.2615). Data management was carried out with MassLynx (V. 4.1, Waters, USA) and Progenesis QI (V 3.0, Waters, UK).

UPLC-ESI-MS/MS conditions for phenolics-targeted metabolomic analysis

The analysis was performed on an ultra-high-performance liquid chromatography system (1290 Infinity series, Agilent Technologies, USA) coupled to an electrospray ionization source-triple quadrupole mass spectrometer (QqQ; 6460, Agilent Technologies, USA). The separation was carried out in an Acquity BEH column (2.1 mm x 50 mm, 1.7 μ m, C18, Waters, USA). The temperature for the column oven was 40 °C. The flow rate was 300 μ L/min, and 2 μ L of each sample was injected into the UPLC-ESI-MS system in triplicate. The mobile phase consisted of water (A) and acetonitrile (B), both acidified with formic acid (0.1% v/v), and the elution gradient conditions were as follows:

Time (min)	A (%)	B (%)
0	99	1
30	50	50
35	1	99
39	1	99
40	99	1
45	99	1

The detection was carried out in both positive and negative ionization modes based on the analyte, with the following parameters:

Parameter	Value
Gas temperature	300° C
Gas flow	5 L/min
Nebulizer pression	45 psi
Sheath Gas Temp	250 ° C
Sheath Gas Flow	11 L/min
Capillary voltage (positive and negative)	3.5 kV
Nozzle voltage (positive and negative)	500 V

The protocol used was a dynamic MRM (Multiple Reaction Monitoring). The conditions for each compound are described in the following table:

	dl	/IRM transiti	on	Mass sp	ectrometric co	nditions	Quantification conditions			
Compound	Precurso r ion	Fragmen t ion	Retentio n time	Collisio n energy	Fragmento r	Polarity	Quantifica- tion range (µM)	Regression type	R²	
Shikimic acid	173.1	111.1	0.54	10	100	Negativ e	0.5 - 19	Quadratic	0.97	
Gallic acid	169.0	125.2	1.35	10	100	Negativ e	0.5 - 19	Quadratic	0.99	
L-Phenylalanine	166.1	131.0	2.23	10	100	Positive	0.5 - 19	Quadratic	0.99	
Protocatechuic acid	153.0	109.1	2.54	10	100	Negativ e	0.5 - 19	Quadratic	0.99	
Gentisic acid	153.0	109.0	3.79	10	100	Negativ e	0.5 - 19	Quadratic	0.98	
4-Hydroxybenzoic acid	137.1	92.8	3.83	10	100	Negativ e	0.5 - 19	Quadratic	0.99	
(-)- Epigallocatechin	305.1	125.0	4.62	20	140	Negativ e	0.5 - 19	Quadratic	0.99	
4- Hydroxyphenylacet ic acid	107.1	77.0	4.94	20	140	Positive	0.5 - 19	Quadratic	0.99	
(+)-Catechin	291.0	138.9	4.96	10	100	Positive	0.25 - 19	Quadratic	0.99	
Vanillic acid	169.0	93.0	5.17	10	100	Positive	0.5 - 19	Quadratic	0.99	
Chlorogenic acid	355.1	163.0	5.23	10	100	Positive	0.25 - 19	Quadratic	0.99	

Caffeic acid	181.0	163.0	5.31	10	100	Positive	0.25 - 19	Quadratic	0.99
Malvin	655.1	331.1	5.63	40	100	Positive	0.5 - 19	Quadratic	0.99
Kuromanin	449.0	286.9	6.07	30	100	Positive	0.25 - 19	Quadratic	0.99
Procyanidin B2	577.1	425.1	6.21	10	100	Negativ	0.5 - 19	Quadratic	0.99
L'oronionin	E0E 2	287.1	6.57	20	100	Positive	0.125 10	Oundratia	0.00
Keracyanin	595.2		6.57	20	100		0.125 - 19	Quadratic	0.99
Vanillin	153.0	124.9	6.65	10	100	Positive	0.25 - 19	Quadratic	0.99
(-)-Epicatechin	291.0	138.8	6.79	10	100	Positive	0.5 - 19	Quadratic	0.99
Mangiferin	423.0	302.8	6.90	10	100	Positive	0.5 - 19	Quadratic	0.99
4-Coumaric acid	165.0	147.0	7.15	10	100	Positive	0.5 - 19	Quadratic	0.99
(-)-Gallocatechin gallate	458.9	139.0	7.57	20	80	Positive	0.5 - 19	Quadratic	0.98
Umbelliferone	163.0	107.0	7.65	30	100	Positive	0.5 - 19	Quadratic	0.99
Scopoletin	193.0	133.0	8.30	10	100	Positive	0.5 - 19	Quadratic	0.99
	193.0	133.0	0.30	10	100	FUSITIVE	0.5 - 19	Quadratic	0.99
Quercetin 3,4-di-O- glucoside	627.0	302.9	8.40	10	100	Positive	0.5 - 19	Quadratic	0.98
Ferulic acid	195.1	145.0	8.53	20	100	Positive	0.5 – 19	Quadratic	0.99
3-Coumaric acid	165.05	147.04	8.96	10	100	Positive	0.5 - 19	Quadratic	0.99
Sinapic acid	225.1	207.1	8.97	10	100	Positive	0.25 - 19	Quadratic	0.99
Ellagic acid	300.5	145.0	9.25	30	170	Negativ e	0.5 - 19	Quadratic	0.97
Salicylic acid	137.0	93	9.51	10	100	Negativ e	0.5 - 19	Quadratic	0.98
Myricitrin	465.0	318.9	9.61	10	100	Positive	0.5 – 19	Quadratic	0.99
Epicatechin gallate	443.1	123.0	9.65	10	100	Positive	0.5 - 19	Quadratic	0.99
Quercetin 3-D-	465.0	302.9	9.82	10	100	Positive	0.5 - 19	Quadratic	0.99
galactoside Rutin	611.0	302.9	9.92	10	100	Positive	0.5 - 19	Quadratic	0.97
Quercetin 3-								,	
glucoside	465.0	303.0	10.13	10	100	Positive	0.5 - 19	Quadratic	0.99
Luteolin 7-O- glucoside	449.0	287.0	10.44	10	100	Positive	0.5 – 19	Quadratic	0.98
p-Anisic acid	153.1	109.0	10.8	5	120	Positive	0.25 - 19	Quadratic	0.99
Penta-O-galloyl-B- D-glucose	771.1	153.0	11.30	20	100	Positive	0.25 - 19	Quadratic	0.99
Kaemperol 3-O- glucoside	449.0	286.9	11.47	10	100	Positive	0.5 - 19	Quadratic	0.98
Quercitrin	449.1	303.1	11.54	10	100	Positive	0.5 - 19	Quadratic	0.99
2,4-Dimethoxy-6- methylbenzoic acid	197.0	179.0	11.62	5	80	Positive	0.25 - 19	Quadratic	0.99
Myricetin	317.0	179.0	11.70	10	100	Negativ e	0.5 - 19	Quadratic	0.96
Naringin	273.0	153.0	12.09	10	120	Positive	0.5 - 19	Quadratic	0.99
trans-Resveratrol	229.1	135.0	12.29	10	100	Positive	0.125 - 19	Quadratic	0.99
	361.1	163.0	12.54	10	100	Positive	0.25 - 19	-	0.99
Rosmarinic acid	301.1	103.0	12.54	10	100		0.25 - 19	Quadratic	0.99
Hesperidin	609.1	301.1	12.66	20	100	Negativ e	0.5 - 19	Quadratic	0.99
Secoisolariciresinol	363.2	137.1	12.82	20	100	Positive	0.5 - 19	Quadratic	0.99
Phloridzin	435.0	272.9	13.02	10	100	Negativ e	0.5 - 19	Quadratic	0.99
trans-Cinnamic acid	149.1	131.0	14.42	10	100	Positive	0.25 - 19	Quadratic	0.99
Quercetin	301	151	14.67	20	100	Negativ e	0.125 - 19	Quadratic	0.99
Luteolin	285	151	14.75	20	100	Negativ	0.5 - 19	Quadratic	0.99
	187.0		14.78		100	Positivo		Oundratia	0.00
Psoralen Angeliein		131.1		20	100	Positive Positive	0.5 - 19	Quadratic	0.99
Angelicin	187.0	131.1	15.54	20		Negativ	0.25 - 19	Quadratic	0.99
Naringenin	271.0 271.0	151 153.0	16.47	10 30	100	e Positive	0.5 - 19 0.25 - 19	Quadratic	0.99
Apigenin			16.86			Negativ		Quadratic	
Kaempferol	285	151	17.27	10	100	e	0.5 - 19	Quadratic	0.98
Hesperetin	303.1	177.1	17.7	20	100	Positive	0.25 - 19	Quadratic	0.99
Podophyllotoxin	415.1	397.1	18.8	10	100	Positive	0.25 - 19	Quadratic	0.99
Methyl cinnamate	163.1	131.0	21.34	6	100	Positive	0.25 - 19	Quadratic	0.99
Chrysin	255.1	153.0	22.6	40	100	Positive	0.25 - 19	Quadratic	0.99
Nordihydroguaiaret									
ic acid Kaempferide	303.0 299	193.1 284	22.81	10 20	100	Positive Positive	0.5 - 19 0.5 - 19	Quadratic Quadratic	0.93
·						Negativ			
Emodin	269.0	225.0	27.26	20	150	e	0.5 - 19	Quadratic	0.99
Chrysophanol	255.1	153.0	30.98	40	100	Positive	0.5 - 19	Quadratic	0.98

The retention time variation allowed for the search of the compounds was 2 min in each case. The cell accelerator voltage was 7 V for each compound. If the concentration of some compounds was higher than the linearity range, dilutions were made.

Metabolic pathways identified in Sida species

*The Mummichog algorithm, the KEGG database, and the *Gossypium hirsutum* (upland cotton, Malvaceae) library were used for metabolic pathway analysis. For genus-level identification, the total rt-*m/z* data matrix was used in both ionization modes (ESI+ and ESI-). For species analysis, spectrometric features with analytical signal intensity equal to zero were removed for each case. FDR= False Discovery Rate.

Genus level

Pathway*	Total	Expected	Hits	P value	-LOG ₁₀ (<i>P</i>)	Holm adj	FDR	Impact
Flavonoid biosynthesis	53	11.207	38	9.88E-16	15.005	9.19E-14	9.19E-14	0.62232
Steroid biosynthesis	44	9.3042	30	1.10E-11	10.958	1.01E-09	5.12E-10	0.77902
Flavone and flavonol biosynthesis	15	3.1719	14	3.43E-09	8.4647	3.12E-07	1.06E-07	0.74999
Phenylpropanoid biosynthesis	35	7.4011	19	1.32E-05	4.8789	1.19E-03	2.77E-04	0.62385
Galactose metabolism	27	5.7094	16	1.49E-05	4.8267	1.33E-03	2.77E-04	0.8154
alpha-Linolenic acid metabolism	28	5.9209	16	2.82E-05	4.5503	2.48E-03	4.37E-04	0.74319
Brassinosteroid biosynthesis	24	5.075	14	6.75E-05	4.1709	5.87E-03	8.96E-04	0.69964
Biosynthesis of various plant secondary metabolites	26	5.498	14	2.18E-04	3.6607	1.88E-02	2.54E-03	0.625
Isoflavonoid biosynthesis	14	2.9604	8	3.32E-03	2.4786	2.82E-01	3.43E-02	0
Phenylalanine metabolism	12	2.5375	7	5.24E-03	2.2806	4.40E-01	4.87E-02	0.76923
Ubiquinone and other terpenoid-quinone biosynthesis	48	10.15	18	6.19E-03	2.2086	5.13E-01	5.23E-02	0.40665
Cutin, suberine and wax biosynthesis	16	3.3834	8	9.55E-03	2.0201	7.83E-01	7.40E-02	0.1818
Isoquinoline alkaloid biosynthesis	6	1.2688	4	0.0205	1.6881	1.00E+00	1.45E-01	0.64705
Tyrosine metabolism	18	3.8063	8	0.0218	1.661	1.00E+00	1.45E-01	0.5919
Starch and sucrose metabolism	22	4.6521	9	0.0274	1.5621	1.00E+00	1.63E-01	0.53553
Carotenoid biosynthesis	44	9.3042	15	0.0304	1.5178	1.00E+00	1.63E-01	0.10345
Linoleic acid metabolism	4	0.84584	3	0.0316	1.5	1.00E+00	1.63E-01	1
Monoterpenoid biosynthesis	4	0.84584	3	0.0316	1.5	1.00E+00	1.63E-01	0

S. hyssopifolia

Pathway*	Total	Expected	Hits	Raw p	-LOG ₁₀ (P)	Holm adj	FDR	Impact
Flavonoid biosynthesis	53	9.9782	36	1.70E-15	14.77	1.58E-13	1.58E-13	0.61732
Steroid biosynthesis	44	8.2838	30	4.15E-13	12.382	3.81E-11	1.93E-11	0.77902
Flavone and flavonol biosynthesis	15	2.824	12	4.27E-07	6.3693	3.89E-05	1.32E-05	0.74999
Galactose metabolism	27	5.0832	16	2.97E-06	5.5277	0.00026705	6.90E-05	0.8154
alpha-Linolenic acid metabolism	28	5.2715	16	5.76E-06	5.2398	0.00051237	0.00010708	0.74319

Phenylpropanoid biosynthesis	35	6.5894	18	1.09E-05	4.963	0.00095834	0.0001688	0.62385
Brassinosteroid biosynthesis	24	4.5184	14	1.66E-05	4.7788	0.001448	0.00022112	0.69964
Biosynthesis of various plant secondary metabolites	26	4.895	14	5.68E-05	4.2459	0.0048821	0.00065993	0.625
Phenylalanine metabolism	12	2.2592	7	0.0026013	2.5848	0.22111	0.02688	0.76923
Ubiquinone and other terpenoid-quinone biosynthesis	48	9.0368	17	0.0043421	2.3623	0.36473	0.038341	0.39522
Cutin, suberine and wax biosynthesis	16	3.0123	8	0.004535	2.3434	0.37641	0.038341	0.1818
Starch and sucrose metabolism	22	4.1419	9	0.013077	1.8835	1	0.10135	0.53553
Linoleic acid metabolism	4	0.75307	3	0.022754	1.6429	1	0.16278	1
Phenylalanine, tyrosine and tryptophan biosynthesis	22	4.1419	8	0.039733	1.4009	1	0.26394	0.2002

S. glabra

Pathway*	Total	Expected	Hits	Raw p	-LOG ₁₀ (P)	Holm adjust	FDR	Impact
Flavonoid biosynthesis	53	10.448	38	7.46E-17	16.127	6.94E-15	6.94E-15	0.62232
Flavone and flavonol biosynthesis	15	2.957	14	1.28E-09	8.8936	1.18E-07	5.94E-08	0.74999
Phenylpropanoid biosynthesis	35	6.8997	19	4.37E-06	5.3591	0.00039801	0.00013151	0.62385
Galactose metabolism	27	5.3226	16	5.66E-06	5.2475	0.00050906	0.00013151	0.8154
alpha-Linolenic acid metabolism	28	5.5198	16	1.09E-05	4.964	0.00096694	0.00020208	0.74319
Brassinosteroid biosynthesis	24	4.7312	13	0.00016191	3.7907	0.014248	0.0025097	0.69964
Biosynthesis of various plant secondary metabolites	26	5.1255	12	0.0018705	2.728	0.16273	0.024851	0.5
Steroid biosynthesis	44	8.6739	17	0.0024951	2.6029	0.21458	0.029006	0.29963
Phenylalanine metabolism	12	2.3656	7	0.0034406	2.4634	0.29245	0.035552	0.76923
Cutin, suberine and wax biosynthesis	16	3.1542	8	0.0061112	2.2139	0.51334	0.056834	0.1818
Ubiquinone and other terpenoid-quinone biosynthesis	48	9.4625	17	0.0071217	2.1474	0.5911	0.060211	0.40665
Isoflavonoid biosynthesis	14	2.7599	7	0.01036	1.9846	0.84952	0.08029	0
Tyrosine metabolism	18	3.5484	8	0.014387	1.842	1	0.10292	0.5919
Isoquinoline alkaloid biosynthesis	6	1.1828	4	0.015892	1.7988	1	0.10557	0.64705
Starch and sucrose metabolism	22	4.337	9	0.017626	1.7539	1	0.10928	0.53553
Linoleic acid metabolism	4	0.78854	3	0.025934	1.5861	1	0.14187	1
Monoterpenoid biosynthesis	4	0.78854	3	0.025934	1.5861	1	0.14187	0
Carotenoid biosynthesis	44	8.6739	14	0.036824	1.4339	1	0.19026	0.10005

S. rhombifolia

Pathway*	Total	Expected	Hits	Raw p	-LOG ₁₀ (P)	Holm adj	FDR	Impact
Flavonoid biosynthesis	53	10.014	36	1.93E-15	14.715	1.79E-13	1.79E-13	0.6075
Flavone and flavonol biosynthesis	15	2.8342	14	7.02E-10	9.1535	6.46E-08	3.27E-08	0.74999
Steroid biosynthesis	44	8.3138	22	2.12E-06	5.6728	0.0001933	6.59E-05	0.48314

Galactose metabolism	27	5.1016	16	3.12E-06	5.5055	0.00028101	7.26E-05	0.8154
alpha-Linolenic acid metabolism	28	5.2906	15	3.44E-05	4.4633	0.0030627	0.00064007	0.74319
Phenylpropanoid biosynthesis	35	6.6132	17	5.33E-05	4.2731	0.0046923	0.00078709	0.55148
Biosynthesis of various plant secondary metabolites	26	4.9127	14	5.92E-05	4.2274	0.0051541	0.00078709	0.625
Brassinosteroid biosynthesis	24	4.5348	11	0.0021725	2.663	0.18683	0.025255	0.67766
Phenylalanine metabolism	12	2.2674	7	0.0026593	2.5752	0.22604	0.02748	0.76923
Cutin, suberine and wax biosynthesis	16	3.0232	8	0.0046433	2.3332	0.39004	0.043182	0.1818
Isoflavonoid biosynthesis	14	2.6453	7	0.0081409	2.0893	0.6757	0.068828	0
Tyrosine metabolism	18	3.4011	8	0.011114	1.9541	0.91136	0.0804	0.5919
Ubiquinone and other terpenoid-quinone biosynthesis	48	9.0696	16	0.011239	1.9493	0.91136	0.0804	0.40665
Starch and sucrose metabolism	22	4.1569	9	0.013391	1.8732	1	0.084369	0.53553
Isoquinoline alkaloid biosynthesis	6	1.1337	4	0.013608	1.8662	1	0.084369	0.64705
Linoleic acid metabolism	4	0.7558	3	0.02299	1.6385	1	0.12577	1
Monoterpenoid biosynthesis	4	0.7558	3	0.02299	1.6385	1	0.12577	0
Carotenoid biosynthesis	44	8.3138	14	0.026253	1.5808	1	0.13564	0.10345
Biosynthesis of unsaturated fatty acids	22	4.1569	8	0.040516	1.3924	1	0.19832	0

Compound names corresponding to the PubChem Compound Identifier (CID) number of tentatively annotated metabolites based on LC-MS untargeted metabolomics (MetaScope, Progenesis QI, Waters)

CID (PubChem Compound Identifier)	Name
126	4-Hydroxybenzaldehyde
127	4-Hydroxyphenylacetic acid
135	4-Hydroxybenzoic acid
179	Acetoin
180	Acetone
190	Adenine
240	Benzaldehyde
244	Benzyl Alcohol
263	1-Butanol
311	Citric Acid
322	3-(4-Hydroxyphenyl)acrylic acid
323	Coumarin
338	Salicylic Acid
341	Digallic Acid
370	Gallic Acid
379	Octanoic Acid
525	Malic Acid
798	Indole
996	Phenol
1054	Pyridoxine
1110	Succinic Acid
1140	Toluene
1174	Uracil
1183	Vanillin
1203	2-(3,4-Dihydroxyphenyl)chroman-3,5,7-triol
1249	Flavan-3,3',4',5,5',7-hexol
2214	Acetovanillone
2371	9-Hydroxy-5a,5b,8,8,11a-pentamethyl-1-prop-1-en-2-yl-1,2,3,4,5,6,7,7a,9,10,11,11b,12,13,13a,13b-hexadecahydrocyclopenta[a]chrysene-3a-carboxylic acid
2518	3,4-Dihydroxy cinnamic acid
2682	Cetyl Alcohol

3314	Eugenol
3469	Gentisic Acid
3503	Gossypol
3931	9,12-Octadecadienoic Acid
5099	alpha-((3-(3,4-Dihydroxyphenyl)-1-oxo-2-propen-1-yl)oxy)-3,4-dihydroxybenzenepropanoic acid
5202	Serotonin
5204	1,3-Benzodioxole, 5,5'-(tetrahydro-1H,3H-furo(3,4-c)furan-1,4-diyl)bis-, (1S-(1alpha,3aalpha,4alpha,6aalpha))-
5281	Stearic Acid
5429	Theobromine
5570	Trigonelline
5793	D-Glucose D-Glucose
5951	Serine
5960	Aspartic Acid
5988	Sucrose
6029	Uridine
6054	Phenylethyl Alcohol
6057	Tyrosine
6185	Strophanthidin
6274	Histidine
6287	Valine
6734	Acenaphthene
7017	2-Phenylphenol
7146	2-Phenylpropanal
7237	O-Xylene
7302	gamma-Butyrolactone
7361	Furfuryl alcohol
7362	Furfural
7438	Carveol
7478	p-Anisic acid
7500	Ethylbenzene
7654	Phenethyl acetate
7966	Cyclohexanol
7967	Cyclohexanone
8080	3,4-dihydro-2H-pyran
8103	1-Hexanol
8130	Heptanal
8158	Nonanoic Acid

8180	Undecanoic Acid
8215	Behenic Acid
8299	Hydroxyacetone
8417	Scoparone
8842	beta-Citronellol, (+-)-
10256	Indole-3-Carboxaldehyde
10393	Tyrosol
10394	Phloretic acid
10400	Cycloheptanone
10416	Malvalic acid
10457	Suberic acid
10465	Heptadecanoic acid
10494	Oleanolic Acid
10582	Myrtenol
10680	Flavone
10743	Sinapic acid
10748	7-Methoxycoumarin
11142	Beta-Phellandrene
12020	1-Penten-3-Ol
12088	4-Formylbenzoic acid
12097	5-Methylfurfural
12580	4-Propylphenol
12756	4-Hexanolide
12777	Delta-Octalactone
13250	Ethyl gallate
13642	4'-Ethylacetophenone
13849	Pentadecanoic Acid
14079	2-Acetylpyrrole
14091	1-Methyl-2-propylbenzene
14296	Ligustrazine
14340	Dihydroferulic Acid
15294	Methyl 4-Formylbenzoate
16275	Cyclohexanecarboxaldehyde
16441	Perillaldehyde
16900	Oct-2-enal
17166	Non-2-enal
19212	Ecdysone

19309	Furaneol
19844	Methyl Vanillate
21742	Mansonone C
22238	Crotyl mercaptan
23485	(3S,5S,10S,13R,14S,17R)-3-[(2R,5S)-6-[[(3R,6S)-4,6-dihydroxy-2-methyloxan-3-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl]oxy-5,14-dihydroxy-13-methyl-17-(5-oxo-2H-furan-3-yl)-2,3,4,6,7,8,9,11,12,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-10-carbaldehyde
25310	L-Rhamnose
28516	Mellein
28619	Precocene I
31242	4-Ethylphenol
31265	Ethyl hexanoate
32033	3,5-Dimethyl-1,2,4-trithiolane
33931	2-ethyl-4-hydroxy-5-methyl-3(2H)-furanone
34645	Cyclohexanone, 5-methyl-2-(1-methylethenyl)-
35698	8-Nonynoic acid
60961	Adenosine
61130	Myrtenal
61370	Hex-4-en-1-ol
62465	4-Ethylguaiacol
65064	Epigallocatechin Gallate
65373	Secoisolariciresinol
68262	2,6-Dimethoxyquinone
71567	D-Phenylalanine
72732	alpha-Lapachone
73193	Tormentic acid
73207	Xanthomicrol
73641	Arjunolic Acid
75142	3-Hydroxy-1-(4-hydroxy-3,5-dimethoxyphenyl)-1-propanone
75324	1,3,7,9-Tetramethyluric acid
78603	o-Phenethylbenzoic acid
82143	Cryptolepine
86052	2,5,8-Trimethyl-2-(4,8,12-trimethyltridecyl)-6-chromanol
92794	Prunin
94225	Taraxerol acetate
100151	(2R,3R)-3-(4-hydroxy-3-methoxyphenyl)-2-(hydroxymethyl)-5-methoxy-2,3-dihydropyrano[3,2-h][1,4]benzodioxin-9-one
100332	Loliolide
101536	Ethyl 2-hydroxy-2-methylbutyrate
102430	2-Hydroxytetracosanoic acid

107526	(2R,3S,4R,5R)-2,3,4,5,6-pentahydroxyhexanal
107557	3-(3,4-Dimethoxyphenyl)-2-propenal
107876	Procyanidin
107905	Epicatechin Gallate
112720	2-aminoethyl Acetate
114776	Isoorientin
117769	Heptadecaenoic acid
119205	Matairesinol
119216	2-Propenal, 3-(4-hydroxy-3,5-dimethoxyphenyl)-
123908	1,2-Dihydroxypropane-1,2,3-tricarboxylic acid
125213	N-feruloyltyramine; Moupinamide
128853	Flavylium, 3,3',4',5,5',7-hexahydroxy-
133372	10-Hydroxyoctadec-2-enoic acid
133551	(1R,3aS,5aR,5bR,7aR,9S,11aR,11bR,13aR,13bR)-9-[3-(3,4-dihydroxyphenyl)prop-2-enoyloxy]-5a,5b,8,8,11a-pentamethyl-1-prop-1-en-2-yl-1,2,3,4,5,6,7,7a,9,10,11,11b,12,13,13a,13b-hexadecahydrocyclopenta[a]chrysene-3a-carboxylic acid
135191	D-Xylose
139711	Ethane, 1,1-bis(ethylthio)-
151202	3-O-Acetyloleanolic acid
155022	2-Hydroxy-7-methoxycadalene
156741	Raimondal
159055	Camphor (synthetic)
160510	1-methyl-3H,4H,9H-pyrido(3,4-b)indole
161355	Dhurrin
162350	Isovitexin
165559	delphinidin 3-O-beta-D-glucoside betaine
178034	Cryptolepinone
181681	Medioresinol
186775	Melosatin A
193484	2-Hydroxydocosanoic acid
231324	1-(Furan-2-yl)-2-methylpropan-1-one
258412	Strophanthidol
286498	Corosin
328066	2-Hydroxy-7-methoxy-6-methyl-5,8-dioxo-4-propan-2-ylnaphthalene-1-carbaldehyde
348502	Guaiacol propionate
373912	3,8-Dimethyl-1,2-naphthoquinone
375713	7-(8-Formyl-1,7-dihydroxy-5-isopropyl-6-methoxy-3-methyl-2-naphthyl)-2,8-dihydroxy-4-isopropyl-3-methoxy-6-methyl-naphthalene-1-carbaldehyde
384679	Dihydrodehydrodiconiferyl alcohol
417052	6-Methoxyharmalan

439242	Raffinose
439246	Naringenin
439341	Amylodextrin
439514	Scopolin
439944	2-Carboxy-D-arabinitol
440265	4-Hydroxy-3,5,5-trimethyl-4-(3-oxo-1-butenyl)-2-cyclohexen-1-one
440735	Eriodictyol
440833	Leucocianidol
440835	Leucodelphidin
441574	(S)-4-Nonanolide
441644	(5S)-5-heptyloxolan-2-one
441667	Cyanidin 3-glucoside
441765	Malvin
441772	Pelargonin
441833	2beta,3beta,3beta,14,20,22R,25-Heptahydroxycholest-7-en-6-one
442101	Cichoriin
442396	(S)-2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-6,8-dimethyl-4-benzopyrone
442849	Cichorine
444539	Cinnamic Acid
444899	Arachidonic Acid
446066	Phosphatidic Acids
447791	(1r)-2-(Phosphonooxy)-1-[(Tridecanoyloxy)methyl]ethyl Pentadecanoate
479957	[(1R,3aS,5aR,5bR,7aR,9S,11aR,11bR,13aR,13bR)-3a-(hydroxymethyl)-5a,5b,8,8,11a-pentamethyl-1-prop-1-en-2-yl- 1,2,3,4,5,6,7,7a,9,10,11,11b,12,13,13a,13b-hexadecahydrocyclopenta[a]chrysen-9-yl] acetate
518900	Benzeneacetic acid, 4-hydroxy-, methyl ester
520684	CID 520684
521790	2-Hydroxy-3-pentanone
522636	Gibberellins
525578	4-Isopropylcyclohexene
538953	3-Buten-2-one, 4-(4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-, (3E)-
539381	6-(3-Hydroxybut-1-enyl)-1,5,5-trimethyl-7-oxabicyclo[4.1.0]heptan-3-ol
540124	4-Methyl-2-phenylpent-2-enal
546377	Octanethioic acid, S-methyl ester
576026	5-Methyl-2-phenylhex-2-enal
608115	7-Hydroxycadalene
632128	2-(3-Hydroxy-4-methoxyphenyl)-3,5,7-trimethoxy-4H-chromen-4-one
636543	Erythro-canabisine H
636576	6-Hydroxy-5-isopropyl-3,8-dimethyl-chromen-2-one

637139	Boehmenan K
637239	4-[(1R,2S,3S)-2,3-bis(hydroxymethyl)-6,7-dimethoxy-1,2,3,4-tetrahydronaphthalen-1-yl]-2-methoxyphenol
638014	beta-lonone
667639	Piceatannol
1548883	cis-Ferulic acid
1549026	Geranyl acetate
1549095	Coniferyl Alcohol
1551480	(2Z,6E)-Farnesyl acetate
1711945	Farnesyl acetone
1742210	beta-Caryophyllene oxide
1794427	Chlorogenic Acid
2723872	D-Fructose
3015413	6-Hydro xy-2,6-dimethyl-2,7-octadienoic acid
3083616	Fraxidin
3084131	Paulownin
3084463	1-Palmitoyl-sn-glycerol
3702506	4-Oxoniobenzoate
4486984	(+)-7-epi-Syringaresinol 4'-glucoside
5274621	Demethylcarolignan E
5274625	(4aS,6aR,6bR,10S,12aR,14bS)-6a-[[(E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxymethyl]-10-[(E)-3-(4-hydroxy-3-methoxy-phenyl)prop-2-enoyl]oxy-2,2,6b,9,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid
5274626	(4aS,6aR,6bR,10S,12aR,14bS)-6a-[(E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]-10-hydroxy-2,2,6b,9,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid
5280343	Quercetin
5280379	Gibberellin A1
5280435	Phytol
5280442	Acacetin
5280443	Apigenin
5280445	Luteolin
5280460	Scopoletin
5280536	4-Hydroxy-3-methoxycinnamaldehyde
5280607	Gibberellin A8
5280637	Luteolin 7-O-glucoside
5280647	Gossypetin
5280863	Kaempferol
5280934	Linolenic Acid
5280953	Harmine
5281115	alpha-Eleostearic acid

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5281119	Myristoleic Acid
5281128	(-)-Vernolic acid
5281319	Cucurbitacin E
5281321	Cucurbitacin I
5281416	Esculetin
5281426	Umbelliferone
5281578	Adouetine Y
5281601	Apigenin 7,4'-dimethyl ether
5281607	Chrysin
5281612	Diosmetin
5281614	Fisetin
5281647	Mangiferin
5281676	Oxyayanin A
5281702	Tricin
5281984	Gibberellin A9
5282102	Astragalin
5283446	Linoleic monoethanolamide
5315831	6"-O-Acetylgenistin
5316673	Afzelin
5317025	Linarin
5318717	Juglanin
5318761	Kaempferol 3-neohesperidoside
5319474	6-Methoxy-7,8-methylenedioxycoumarin
5320006	9-Hydroxy-alpha-lapachone
5320254	[2-hydroxy-3-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypropyl] (9Z,12Z)-octadeca-9,12-dienoate
5320686	Tiliroside
5320834	Quercetin 3-gentiobioside
5386960	4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-(4-hydroxyphenyl)-3,6,8-trimethoxy-
5459840	20-Hydroxyecdysone
5460372	Gibberellin A44
5460657	Gibberellin A17
5466138	Flindulatin
5468749	Kaempferol 3,7,4'-trimethyl ether
5487855	Dillenetin
5488575	4H-1-Benzopyran-4-one, 3-((6-deoxy-alpha-L-mannopyranosyl)oxy)-5,7-dihydroxy-
5490334	Hibifolin
5491693	Kaempferol 4'-glucoside
2401030	Nacripieroi 4 - giacosiae

6436348	Germacrone
6441104	Arvenin I
6450144	Myriceron caffeoyl ester
6452262	Pyrrolo(2,1-b)quinazoline-3,7-diol, 1,2,3,9-tetrahydro-, (R)-
6602508	Stigmasterol glucoside
6973640	(+)-Isoborneol
7156991	ethyl (2R)-2-methylbutanoate
9561835	10-Hydroxystearic Acid
9930500	(2S,3R)-3-hydroxy-3-methoxycarbonyl-5-oxooxolane-2-carboxylic acid
9978316	(4S)-4-hydroxy-3,5,5-trimethyl-4-[(E)-3-oxo-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybut-1-enyl]cyclohex-2-en-1-one
10015552	2-Hydroxy-6-(hydroxymethyl)-7,8-dimethoxynaphthalene-1-carbaldehyde
10023166	Corchoionoside A
10105245	5-Hydroxy-11-methoxy-10-methyl-2-oxatricyclo[6.3.1.04,12]dodeca-1(11),4,6,8(12),9-pentaen-3-one
10176654	Methyl cis-ferulate
10187514	6"-O-Malonylisoquercitrin
10252339	Quercetin 3-arabinoside
10255859	Methyl oleanolate acetate
10262028	trans-4-Hydroxymellein
10308838	N-(E)-Caffeoyl-L-tyrosine
10317980	Corchoionoside C
10371536	Quercetin 3-O-robinobioside
10403282	Cuscuta propenamide 1
10413856	3-[3,4-dimethoxy-5-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-5-hydroxy-7-methoxychromen-4-one
10439806	9,9'-Di-O-(E)-feruloylsecoisolariciresinol
10465398	9-hydroxyundec-10-enoic Acid
10472650	Vavain
10508776	(2S)-3-[3-hydroxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-2-[(E)-3-[3-hydroxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]prop-2-enoyl]oxypropanoic acid
10538510	11-Methoxyquindoline
10582821	Ethyl thiobutyrate
10603919	[(3S,4R,4aR,6aR,6bS,8aS,12aS,14aR,14bR)-3-hydroxy-8a-(hydroxymethyl)-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicen-4-yl]methyl (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate
10630882	(3S,4S,5R)-3-Amino-4,5-dimethyloxolan-2-one
10652163	corchorusoside C
10720349	(2S)-3-(4-hydroxyphenyl)-2-[(E)-3-[3-hydroxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]prop-2-enoyl]oxypropanoic acid
10723382	Card-20(22)-enolide, 3-[(2,6-dideoxy-4-O-I(2)-D-glucopyranosyl-I(2)-D-ribo-hexopyranosyl)oxy]-11,14,19-trihydroxy-, (3I(2),5I(2),11I+/-)-
10813969	Isoquercitin
10815866	(2S)-3-(3,4-dihydroxyphenyl)-2-[(E)-3-[3-hydroxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]prop-2-enoyl]oxypropanoic acid

10912308	(5R,8R)-5-hydroxy-3,8-dimethyl-5-propan-2-yl-7,8-dihydronaphthalene-1,2,6-trione
10922890	(2R,3S)-2,6-dihydroxy-3,8-dimethyl-5-propan-2-yl-3,4-dihydro-2H-naphthalen-1-one
10969116	5,9,11-Trimethoxy-10-methyl-7-propan-2-yl-2-oxatricyclo[6.3.1.04,12]dodeca-1(11),4,6,8(12),9-pentaen-3-one
11060391	20-Hydroxyecdysone 20,22-acetonide
11061627	7-[(2S,3R,4R,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxy-3-[(2S,3R,4R,5R,6R)-3,4-dihydroxy-6-(hydroxymethyl)-5-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)chromen-4-one
11063054	Methyl Dec-9-ynoate
11072668	7-[(2S,3R,4R,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-3-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6- [[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxan-2-yl]oxychromen-4-one
11079623	5-Hydroxyauranetin
11167374	10-Hydroxy-6a-(hydroxymethyl)-2,2,6b,9,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid
11194416	4-Hydroxyisoleucine
11227946	(2R)-N-[(Z,2S,3S,4R)-3,4-dihydroxy-1-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoctadec-8-en-2-yl]-2-hydroxyhexadecanamide
11250133	Procyanidin B1
11276243	4-Hydroxy-3-[(4-hydroxyphenyl)methyl]benzaldehyde
11276313	2,8-Dihydroxy-7-methoxy-6-methyl-naphthalene-1-carbaldehyde
11277992	(4S,10R)-10-hydroxy-4,8,12-trimethyl-10-(2-oxopropyl)-2-oxatricyclo[7.3.1.05,13]trideca-1(12),5(13),6,8-tetraen-11-one
11354754	(4aS,6aR,6aR,6bR,8aR,10S,12aR,14bS)-6a-[[(E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxymethyl]-10-[(E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxy-2,2,6b,9,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid
11464176	Cleomiscosin C
11623832	Hildegardiol
11692717	(1R,3aS,5aS,5bR,7aR,9S,11aR,11bR,13aR,13bR)-5a-(benzoyloxymethyl)-9-hydroxy-5b,8,8,11a-tetramethyl-1-prop-1-en-2-yl-1,2,3,4,5,6,7,7a,9,10,11,11b,12,13,13a,13b-hexadecahydrocyclopenta[a]chrysene-3a-carboxylic acid
11953803	6-methoxy-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-3,4-dihydrochromen-2-one
11968644	(2S,3S,4S,5R,6S)-6-[5,7-dihydroxy-2-(4-methoxyphenyl)-4-oxochromen-8-yl]oxy-3,4,5-trihydroxyoxane-2-carboxylic acid
12303930	Corchoroside A
12305415	Lespedin;Lespenephryl
12313704	Oleanonic acid
12681283	(2R)-2-benzamido-3-(4-hydroxy-3-methoxyphenyl)propanoic acid
12695575	4-Hydroxy-2-methoxybenzoic acid
12799212	4,5-Dimethyl-3-hydroxy-2,5-dihydro-2-furanone, (-)-
13197868	2-Butyl-4-methylfuran
13245586	Isorhamnetin 3-galactoside
13871877	Chrysoeriol-7-O-beta-D-glucoside
13915427	4-Butyl-2,6-dimethoxyphenol
13918554	2-Methyl-3-Oxy-5-Methoxy-p-Chinon
13988634	2-(3,4-Dihydroxyphenyl)-8-((6-O-beta-D-glucopyranosyl-beta-D-glucopyranosyl)oxy)-5,7-dihydroxy-4H-1-benzopyran-4-one
14009683	2-Methoxy-6-propylphenol
14035324	Kaempferol-3-O-glucoside-7-O-rhamnoside

14055737	24-Hydroxytormentic acid
14187088	Glucodistylin
14311156	3-[[6-[5,7-Dihydroxy-2-(3,4,5-trihydroxyphenyl)chromenylium-3-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methoxy]-3-oxopropanoic acid
14311160	3-[[6-[2-(3,4-Dihydroxy-5-methoxyphenyl)-5,7-dihydroxychromenylium-3-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methoxy]-3-oxopropanoic acid
14311167	3-[[6-[5,7-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)chromenylium-3-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methoxy]-3-oxopropanoic acid
14332450	ISOSCUTELLAREIN 8-O-beta-D-GLUCURONIDE
14376672	Turkesterone
14484636	Betulalbuside A
14681438	Dihydrodehydroconiferyl alcohol 4-O-glucoside
14704521	Phenylethyl primeveroside
14707301	(1R,3aS,5aS,5bR,7aR,9S,11aR,11bR,13aR,13bR)-9-hydroxy-5a-(hydroxymethyl)-5b,8,8,11a-tetramethyl-1-prop-1-en-2-yl-1,2,3,4,5,6,7,7a,9,10,11,11b,12,13,13a,13b-hexadecahydrocyclopenta[a]chrysene-3a-carboxylic acid
14887603	beta-D-Glucopyranosiduronic acid, 2-(3,4-dihydroxyphenyl)-3-(beta-D-glucopyranosyloxy)-5,7-dihydroxy-4-oxo-4H-1-benzopyran-8-yl
14887605	Hypolaetin 8-glucuronide
14887607	5,7-Dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4-oxo-4H-1-benzopyran-8-yl beta-D-glucopyranosiduronic acid
15289454	5,8-Dihydroxy-7,4'-dimethoxyflavone
15559735	Hibiscetin
15560128	Augustic Acid
15645217	1-Ethyl-2-methylnaphthalene
15767724	Myriceric acid B
16077448	(2R,3R)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2S,3S,4S,5S,6R)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-chroman-4-one
16093748	Cucurbitacin b 2-sulfate
21120946	AKOS040753028
21579640	Arvenin III
21722016	Quercetin 3-(6-methylglucuronide)
21763831	3,7,8-trimethoxy-2-methyl-5-(5-phenylpentyl)-1H-quinolin-4-one
21881649	(2R,3R,4R)-4-[(2R,3R)-2-(3,5-dihydroxy-4-methoxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-(4-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,5,7-triol
22236717	2,3-Di-sec-butylphenol
23642717	Bombamalone C
23658567	N-Caffeoyl-L-aspartic acid
23815394	(-)-Lariciresinol
24796850	3-[(1R,2R,4aR,4bS,5S,6aR,7R,12aR)-2-[(2R)-1,2-dihydroxypropan-2-yl]-5,7-dihydroxy-1,4a,4b,6a,9,9-hexamethyl-3,4,5,6,7,8,10,12a-octahydro-2H-chrysen-1-yl]propanoic acid
24796851	3-[(1R,2R,4aR,4bS,5S,6aR,7S,10aR,12aR)-2-[(2R)-1,2-dihydroxypropan-2-yl]-5,7-dihydroxy-1,4a,4b,6a,9,9-hexamethyl-3,4,5,6,7,8,10,10a,12,12a-decahydro-2H-chrysen-1-yl]propanoic acid
24982202	Glochidioboside
25021697	(2R,3S,4R,5R)-2,3,4,5-tetrahydroxy-6-oxohexanoic acid
26339717	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2S,3S,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxychromen-4-one
42608087	Naringenin 5,7-dimethyl ether 4'-O-xylosyl-(1->4)-arabinoside

Hypolaetin 8-O-beta-D-glucoside Gossypetin 3-O-sulfate Gossypetin	4-enyl]-
## ## ## ## ## ## ## ## ## ## ## ## ##	
hydroxy-2-(4-hydroxypheny)-4-oxochromen-7-yloxy-3.4,5-trihydroxyoxane-2-carboxylate	
Ad592130)ху-5-
44566588 Vavain 3'-O-beta-d-glucoside 44566911 Isoscutellarein 8-O-beta-D-glucuronide 6"-methyl ester 44577733 (3R)-8-hydroxy-3-methyl-1-oxo-3,4-dihydroisochromene-5-carbaldehyde 44578390 rel-(3S,3aR,6S,6aS)-3,6-Bis(4-hydroxy-3-methoxyphenyl)tetrahydrofuro[3,4-c]furan-1(3H)-one 44631546 Vcbhabvpyykijs-xrgyyrrgsa- 45273405 Gardenolic Acid B 46181828 procyanidin B2 3-O-gallate 49831447 (+)-Boehmenan X 49831491 (-)-(7'S,8'S)-threo-carolignan X 49831493 (-)-(7'S,8'S)-threo-carolignan Y 49842399 quercetin-3-O-glucoside-7-O-rhamnoside 53420248 3-O-p-Coumaroylquinicacid 53429614 5-Methyl furfur-2-al 54005211 3-Dodecenedioic acid 54355075 Heptadecadienic acid	(an-2-
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44577733 (3R)-8-hydroxy-3-methyl-1-oxo-3,4-dihydroisochromene-5-carbaldehyde 44578390 rel-(3S,3aR,6S,6aS)-3,6-Bis(4-hydroxy-3-methoxyphenyl)tetrahydrofturo[3,4-c]furan-1(3H)-one 44631546 Vcbhabvpyyfxjs-xrgyyrrgsa- 45273405 Gardenolic Acid B 46181828 procyanidin B2 3-O-gallate 49831447 (+)-Boehmenan X 49831491 (-)-(7'S,8'S)-threo-carolignan X 49831493 (-)-(7'S,8'S)-threo-carolignan Y 49842399 quercetin-3-O-glucoside-7-O-rhamnoside 53420248 3-O-p-Coumaroylquinicacid 53429614 5-Methyl furfur-2-al 54005211 3-Dodecenedioic acid 54355075 Heptadecadlenic acid	
44578390 rel-(3S,3aR,6S,6aS)-3,6-Bis(4-hydroxy-3-methoxyphenyl)tetrahydrofuro[3,4-c]furan-1(3H)-one 44631546 Vcbhabvpyyfxjs-xrgyyrrgsa- 45273405 Gardenolic Acid B 46181828 procyanidin B2 3-O-gallate 49831447 (+)-Boehmenan X 49831491 (-)-(7'S,8'S)-threo-carolignan X 49831493 (-)-(7'S,8'S)-threo-carolignan Y 49842399 quercetin-3-O-glucoside-7-O-rhamnoside 53420248 3-O-p-Coumaroylquinicacid 53429614 5-Methyl furfur-2-al 54005211 3-Dodecenedioic acid Heptadecadienic acid	
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57006309 Oct-6-en-4-ol	
57172986 18,18,18-Trihydroxyoctadecanoic acid	
57402770 (8S,9R,10R,13R,14S,16R,17R)-2,16-dihydroxy-4,4,9,13,14-pentamethyl-17-[(2R,5S)-2,5,6-trihydroxy-6-methyl-3-oxoheptan-2-yl]-8,10,12,15,16, hexahydro-7H-cyclopenta[a]phenanthrene-3,11-dione	16,17-
69634125 Forsythoside E	
71359328 Methyl 9,12,13-trihydroxyoctadec-10-enoate	
71403936 2,3-Dihydroxyoctadec-2-enoic acid	
71438848 3-methyl-6-[[2-(2-methylbut-3-en-2-yl)-5-(3-methylbut-2-enyl)-1H-indol-3-yl]methylidene]piperazine-2,5-dione	
72730313 2-Hepta-3,5-dienyl-3,6-dihydroxy-5-(3-methylbut-2-enyl)benzaldehyde	
72730314 2-Hept-5-enyl-3,6-dihydroxy-5-(3-methylbut-2-enyl)benzaldehyde	
72730315 2,5-Dihydroxy-3-(3-methyl-2-butenyl)-6-heptenyl-benzaldehyde	
72751004 1-(3-Hydroxybut-1-en-1-yl)-2,6,6-trimethylcyclohexane-1,2,4-triol	
73172655 6-hydroxy-2-(3-hydroxybut-1-enyl)-7-(3-methylbut-2-enyl)-3,4-dihydro-2H-chromene-5-carbaldehyde	
73323377 [6-[2-(3,4-Dihydroxyphenyl)ethoxy]-3,5-dihydroxy-4-(3,4,5-trihydroxy-6-methyloxan-2-yl)oxyoxan-2-yl]methyl 3-(3,4-dihydroxyphenyl)prop-2-eno	noate
73821792 (2S,5R,9S)-9-Acetyl-9-hydroxy-2,7,8-trimethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)-1-oxaspiro[4.4]non-7-en-6-one	
74977035 Delphinidin 3-O-sambubioside	

74070075	7 [2 F Dibudrous 6 method 4 [2 4 F tribudrous 6 /budrous method) over 2 ullous over 2 ullous 2 F dibudrous 2 (4 budrous phonol observer) 4 one
74978075	7-[3,5-Dihydroxy-6-methyl-4-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxyo-3,5-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one
75069340	5-Hydroxy-6-(3-methylbut-2-enyl)-2-(pent-1-enyl) benzofuran-4-carbaldehyde
78162875	5,6,11,12,13-Pentahydroxy-4,14-dimethyl-16-oxo-8,17-dioxatetracyclo[7.7.1.02,7.010,15]heptadeca-2(7),3,5,10,12,14-hexaene-3-carbaldehyde
85091334	Corchorusoside B
85524814	Methyl 10-oxo-11-octadecynoate
85664554	12-Hydroxyheptadec-9-enoic acid
90657201	Kaempferide 7-glucoside
92863445	[(2R)-2,3-dihydroxypropyl] icosanoate
100914108	[(3S,5R)-5-[(1S)-1-[(1S,3R,6S,8R,11S,12S,14S,15R,16R)-14-hydroxy-7,7,12,16-tetramethyl-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-15-pentacyclo[9.7.0.01,3.03,8.012,16]octadecanyl]ethyl]-2,2-dimethyloxolan-3-yl] acetate
100935400	[3-(3,4-dihydroxyphenyl)-1-methoxy-1-oxopropan-2-yl] 11-[(E)-3-[3-(3,4-dihydroxyphenyl)-1-methoxy-1-oxopropan-2-yl]oxy-3-oxoprop-1-enyl]-1,4,5-trihydroxy-14-oxotetracyclo[8.3.1.02,7.08,13]tetradeca-2,4,6,11-tetraene-9-carboxylate
100953140	Card-20(22)-enolide, 3-[(2,6-dideoxy-I(2)-D-xylo-hexopyranosyl)oxy]-14-hydroxy-, (3I(2),5I(2))-
100955863	methyl (2S)-3-hydroxy-2-(4-hydroxy-3-methoxyphenyl)propanoate
100967916	(4aS,6aR,6aR,6bR,8aR,10S,12aR,14bS)-10-hydroxy-6a-[[(Z)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]oxymethyl]-2,2,6b,9,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid
101114357	3-[(2R,3S)-2-(4-hydroxy-3-methoxyphenyl)-3-(hydroxymethyl)-7-methoxy-2,3-dihydro-1-benzofuran-5-yl]propyl (E)-3-(4-hydroxy-3-methoxyphenyl)prop- 2-enoate
101114359	3-[4-[(1R,2S)-1,3-dihydroxy-1-(4-hydroxy-3-methoxyphenyl)propan-2-yl]oxy-3-methoxyphenyl]propyl (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate
101114360	3-[(2R,3S)-2-(4-hydroxy-3,5-dimethoxyphenyl)-3-[((E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]oxymethyl]-7-methoxy-2,3-dihydro-1-benzofuran-5-yl]propyl (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate
101114361	3-[4-[(1S,2S)-1-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-[(E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]oxypropan-2-yl]oxy-3,5-dimethoxyphenyl]propyl (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate
101182982	(2S,3R,4R,5R,6S)-2-[(2R,3S,4R,5R,6R)-4,5-dihydroxy-6-[[(1S,3R,6S,8R,11S,12S,14S,15R,16R)-14-hydroxy-15-[(1S)-1-[(2R,4S)-4-hydroxy-5,5-dimethyloxolan-2-yl]ethyl]-7,7,12,16-tetramethyl-6-pentacyclo[9.7.0.01,3.03,8.012,16]octadecanyl]oxy]-2-(hydroxymethyl)oxan-3-yl]oxy-6-methyloxane-3,4,5-triol
101182983	(2R,3R,4S,5S,6R)-2-[(2R,3R,4S,5R,6R)-3,5-dihydroxy-2-[[(1S,3R,6S,8R,11S,12S,14S,15R,16R)-14-hydroxy-15-[(1S)-1-[(2R,4S)-4-hydroxy-5,5-dimethyloxolan-2-yl]ethyl]-7,7,12,16-tetramethyl-6-pentacyclo[9.7.0.01,3.03,8.012,16]octadecanyl]oxy]-6-(hydroxymethyl)oxan-4-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol
101204053	(2S,3R,4S,5S,6R)-2-(3,8-dimethylnaphthalen-2-yl)oxy-6-(hydroxymethyl)oxane-3,4,5-triol
101204054	(E)-3-[(2R,3S)-2-(4-hydroxy-3-methoxyphenyl)-3-(hydroxymethyl)-7-methoxy-2,3-dihydro-1-benzofuran-5-yl]-N-[2-(4-hydroxyphenyl)ethyl]prop-2-enamide
101248984	(3S,5R,6S,8R,9R,10R,13R,14R,16R,17R)-17-[(Z,2S)-2,7-dihydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,16-triol
101262727	Grossamide
101286273	3-[(3S,5R,8R,9S,10S,13R,14S,17R)-14-hydroxy-3-[(2R,4R,5S,6R)-4-hydroxy-6-methyl-5-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-10,13-dimethyl-1,2,3,4,5,6,7,8,9,11,12,15,16,17-tetradecahydrocyclopenta[a]phenanthren-17-yl]-2H-furan-5-one
101607227	(2R,3R,4R,4aR,6aR,6bS,8aR,12R,12aS,14aR,14bR)-2,3-dihydroxy-4,6a,6b,11,12,14b-hexamethyl-2,3,4a,5,6,7,8,9,12,12a,14,14a-dodecahydro-1H-picene-4,8a-dicarboxylic acid
101836179	(5R,7R,8S,10S)-8-hydroxy-10-methyl-7-propan-2-yl-5-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-2-oxatricyclo[6.3.1.04,12]dodeca-1(12),3-dien-11-one
101836180	(5R,7S,8R,10S)-7-[2-[(2S,3R,4S,5S,6R)-6-[[(2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl]oxypropan-2-yl]-5-hydroxy-10-methyl-2-oxatricyclo[6.3.1.04,12]dodeca-1(12),3-dien-11-one
101928607	(1S,4S)-7-hydroxy-1,6-dimethyl-4-propan-2-yl-3,4-dihydro-1H-naphthalen-2-one
102239783	6-Hydroxy-3,3,11-trimethyl-9,10-dioxo-2-oxatricyclo[6.3.1.04,12]dodeca-1(11),4,6,8(12)-tetraene-7-carbaldehyde
118110362	Syringyl propanol
118716647	(5R)-2-(hydroxymethyl)-1,3-dimethoxy-5-octyl-5,6,7,8-tetrahydroquinolin-4-one

118855455	(3S)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)-2,3-dihydrochromen-4-one
122382587	(3aR,4S,5S)-4-hydroxy-7-methoxy-1,5,8-trimethyl-4,5-dihydro-3aH-benzo[e][1]benzofuran-2-one
124222280	beta-D-Glucopyranoside, 2-(3-hydroxy-4-methoxyphenyl)ethyl 3-O-(6-deoxy-alpha-L-mannopyranosyl)-, 6-[3-(4-hydroxy-3-methoxyphenyl)-2-propenoate], (E)-
124708157	(2S,3R)-5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[(2R,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-2,3-dihydrochromen-4-one
129686415	Quindolinone
129819530	9-Hydroxyheptadecenoic acid
129847920	Methyl (e)-11-methoxy-9-oxo-10-nonadecenoate
129881889	3,3'-Methylenebis(4,6-dihydroxycoumarin)
132596278	3-[4-[(1R,2R)-1-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-[(E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]oxypropan-2-yl]oxy-3-methoxyphenyl]propyl (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate
132966232	(5S)-3-methoxy-2-methyl-5-(5-phenylpentyl)-1,5,6,7-tetrahydroquinoline-4,8-dione
132990894	Psif(b2-1a)[Gal(a1-6)D-ldo(a1-6)]Glc
134781708	(6S,7aR)-2-[(2E,4E,6E,8E,10E,12E,14E)-15-[(6S,7aR)-6-hydroxy-4,4,7a-trimethyl-2,5,6,7-tetrahydro-1-benzofuran-2-yl]-6,11-dimethylhexadeca-2,4,6,8,10,12,14-heptaen-2-yl]-4,4,7a-trimethyl-2,5,6,7-tetrahydro-1-benzofuran-6-ol
135542082	Malvone A
135596557	1,2-Naphthalenedione, 7,8-dihydroxy-3-methyl-5-(1-methylethyl)-
136085678	6-Hydroxyharman
137185909	Gossyrubilone
139031043	(2S)-5,7-dihydroxy-2-[4-[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-2,3-dihydrochromen-4-one
154497005	(2S,3S,4R,5S,6S)-6-[2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4-oxochromen-3-yl]oxy-3,4,5-trihydroxyoxane-2-carboxylic acid
154505258	6-Methoxy-1-propylcyclohexa-2,4-dien-1-ol
160557896	(1S)-1,7-dihydroxy-1-methyl-4-propan-2-ylnaphthalen-2-one
162653491	(1R,12S)-5-methoxy-12-(2-methoxyphenyl)-6-methyl-14-oxa-7-azatetracyclo[10.2.2.02,11.03,8]hexadeca-2(11),3(8),5,9-tetraen-4-one
162659502	(1S,12R,13S)-5,13-dimethoxy-12-(2-methoxyphenyl)-6-methyl-14-oxa-7-azatetracyclo[10.2.2.02,11.03,8]hexadeca-2(11),3(8),5,9-tetraen-4-one
162820576	(3R)-8-hydroxy-6,7-dimethoxy-3,5-dimethyl-3,4-dihydroisochromen-1-one
162821381	(2S,4aS,6aR,7R,10aS,12S,12aS)-7-(4-hydroxy-6-methylheptan-2-yl)-4a,6a-dimethyl-1,2,3,4,6,7,8,9,10,10a,10b,11,12,12a-tetradecahydrochrysene-2,12-diol
162842866	(1R,3S,5S,6R,7S,8R,10R,12S,13R,14R)-7-[(2R,3R,4S,5S,6S)-6-carboxy-3,4,5-trihydroxyoxan-2-yl]oxy-6,13,14-trihydroxy-12-methyl-2,4,9,11-tetraoxatricyclo[8.4.0.03,8]tetradecane-5-carboxylic acid
162844792	(4R,5S,8R,9S,10S,13R,14S,17R)-17-[(2R,5R)-5-hydroxy-6-methylhept-6-en-2-yl]-4,5,9,13,14-pentamethyl-1,2,4,6,7,8,10,11,12,15,16,17-dodecahydrocyclopenta[a]phenanthren-3-one
162847751	(2R,3R)-2-(dimethylamino)-N-[(3S,4S,7S,10E)-7-ethyl-5,8-dioxo-3-propan-2-yl-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-1(14),10,12,15-tetraen-4-yl]-3-hydroxy-4-methylpentanamide
162849047	methyl (2S,3S,4R,5R,6S)-6-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxochromen-8-yl]-3,4,5-trihydroxyoxane-2-carboxylate
162851990	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[(2R,3R,4R,5S)-3,4,5-trihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxychromen-4-one
162853228	1-[2-(4-Hydroxy-3-methoxyphenyl)-3-(hydroxymethyl)-7-methoxy-2,3-dihydro-1-benzofuran-5-yl]ethanone
162866484	[(2R,3S,4S,5R,6S)-3,4,5-trihydroxy-6-[[6-hydroxy-10-(hydroxymethyl)-7-[(2S)-1-hydroxypropan-2-yl]-2-oxatricyclo[6.3.1.04,12]dodeca-1(11),4,6,8(12),9-pentaen-5-yl]oxy]oxan-2-yl]methyl hydrogen sulfate
162882460	[(2R,3S,4S,5R,6S)-3,4,5-trihydroxy-6-[[6-hydroxy-7-[(2S)-1-hydroxypropan-2-yl]-10-methyl-2-oxatricyclo[6.3.1.04,12]dodeca-1(11),4,6,8(12),9-pentaen-5-yl]oxy]oxan-2-yl]methyl hydrogen sulfate
162883937	(2S,3R,4R,5R,6S)-2-[[(1S,2R,3R)-7-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-(hydroxymethyl)-6-methoxy-1,2,3,4-tetrahydronaphthalen-2-yl]methoxy]-6-methyloxane-3,4,5-triol
162887298	(2S,3R)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2S,3R,4S,5S)-3,4,5-trihydroxyoxan-2-yl]oxy-2,3-dihydrochromen-4-one

162887874	(2S,3R)-3-[(2S,3R,4R,5R)-5-[(1R)-1,2-dihydroxyethyl]-3,4-dihydroxyoxolan-2-yl]oxy-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-2,3-dihydroxhromen-4-one-2-yl]oxy-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-2,3-dihydroxyethyl]-3,4-dihydroxyoxolan-2-yl]oxy-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-2,3-dihydroxyethyl]-3,4-dihydroxyoxolan-2-yl]oxy-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-2,3-dihydroxy-2,3-dihydroxyethyl]-3,4-dihydroxyoxolan-2-yl]oxy-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-2,3-dihyd
162904343	(2R,3S)-5-[(2S,3R,4R,5S,6R)-3,4-dihydroxy-6-(hydroxymethyl)-5-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-3,7-dihydroxy-2-phenyl-2,3-dihydrochromen-4-one
162912427	(2S,3R,4R,5R,6S)-2-[(2S,3R,4S,5S,6R)-2-[4-[(3S,3aS,6S,6aS)-3-(4-hydroxy-3-methoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan-6-yl]-2-methoxyphenoxy]-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy-6-methyloxane-3,4,5-triol
162913355	3-[3-[(2S,3R,4S,5S,6R)-6-[[(2R,3S,4R,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl]oxy-4,5-dimethoxyphenyl]-5-hydroxy-7-methoxychromen-4-one
162915878	(2R,3S)-3-(hydroxymethyl)-7-methoxy-2-[3-methoxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-2,3-dihydro-1-benzofuran-5-carboxylic acid
162917701	5,6,7,8-tetrahydroxy-2-(4-hydroxyphenyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one
162919119	3-[(3S,8R,9S,10R,13R,14S,17R)-14-hydroxy-10,13-dimethyl-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy-1,2,3,6,7,8,9,11,12,15,16,17-dodecahydrocyclopenta[a]phenanthren-17-yl]-2H-furan-5-one
162933403	methyl (2S,3S,4R,5R,6S)-6-[5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4-oxochromen-8-yl]-3,4,5-trihydroxyoxane-2-carboxylate
162939299	3-[3-[(2S,3R,4S,5S,6R)-6-[[(2S,3R,4R,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]methoxymethyl]-3,4,5-trihydroxyoxan-2-yl]oxy-4,5-dimethoxyphenyl]-5-hydroxy-7-methoxychromen-4-one
162945016	(2R,3R,4S,5R,6R)-2-[[(3S,4R,4aS,6aR,6bS,8S,8aS,12aR,14aR,14bR)-8-hydroxy-4,8a-bis(hydroxymethyl)-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicen-3-yl]oxy]-6-(hydroxymethyl)oxane-3,4,5-triol
162952341	(8S,8aR)-3,8-dimethyl-5-propan-2-yl-1,7,8,8a-tetrahydroazulene-2,6-dione
162953603	(1R,3S,5S,6R,7S,8R,10R,12S,13R,14R)-6,7,13,14-tetrahydroxy-12-methyl-2,4,9,11-tetraoxatricyclo[8.4.0.03,8]tetradecane-5-carboxylic acid
162957279	(3R)-3-methyl-3,4-dihydro-1,2-benzodioxine-5-carbaldehyde
162957786	(2R,3R,4S,5R,6R)-2-[[(1S,2S,4S,5R,8R,9R,10S,13S,14R,17S,18S)-2-hydroxy-9-(hydroxymethyl)-4,5,9,13,20,20-hexamethyl-24-oxahexacyclo[15.5.2.01,18.04,17.05,14.08,13]tetracos-15-en-10-yl]oxy]-6-(hydroxymethyl)oxane-3,4,5-triol
162961573	(Z,9R)-9-hydroxyoctadec-11-enoic acid
162961650	3-[(3R,8R,9S,10R,13R,14R,17R)-3-[(2R,4R,5S,6R)-4,5-dihydroxy-6-methyloxan-2-yl]oxy-14-hydroxy-10,13-dimethyl-1,2,3,6,7,8,9,11,12,15,16,17-dodecahydrocyclopenta[a]phenanthren-17-yl]-2H-furan-5-one
162962930	(3S)-3-hydroxy-3,10,10,13-tetramethyl-6,11-dioxatetracyclo[7.6.1.02,7.012,16]hexadeca-1(16),2(7),4,8,12-pentaene-14,15-dione
162966990	GalA(a1-4)aldehydo-Gal
162969771	(2S,3S,4R,5R,6S)-2-[[(3S,5R,8R,9R,10R,12R,13R,14S,17R)-3,12-dihydroxy-4,4,8,10-tetramethyl-17-[(2S,5S)-2-methyl-5-[2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypropan-2-yl]oxylan-2-yl]-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-14-yl]methoxy]-6-(hydroxymethyl)oxane-3,4,5-triol
162971414	2-Methyl-6-[[3,4,5-trihydroxy-6-[2-(3-hydroxy-4-methoxyphenyl)ethoxy]oxan-2-yl]methoxy]oxane-3,4,5-triol
162972958	2-(3,4-dihydroxyphenyl)-5-hydroxy-7-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy-3-[(2S,3R,4S,5R)-3,4,5-trihydroxyoxan-2-yl]oxychromen-4-one
162978216	(1R,2R,5R,6S,7S,10S,14R,15R,16S,21R)-6,7,16-trihydroxy-1,2,5,8,8,15,20,20-octamethyl-19-oxapentacyclo[12.9.0.02,11.05,10.015,21]tricos-11-ene-18,23-dione
162985801	GalA(a1-2)aldehydo-Qui
162999405	1-[3-(Hydroxymethyl)-7-methoxy-2-[3-methoxy-4-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-2,3-dihydro-1-benzofuran-5-yl]ethanone
163003716	[5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4-oxochromen-8-yl] (2S,3S,4S,5R,6R)-3,4,5,6-tetrahydroxyoxane-2-carboxylate
163004460	3-[(1R,2R,4R,4aR,4bR,5S,6aR,7S,10aR,12aR)-2-[(2R)-1,2-dihydroxypropan-2-yl]-4,5,7-trihydroxy-1,4a,4b,6a,9,9-hexamethyl-3,4,5,6,7,8,10,10a,12,12a-decahydro-2H-chrysen-1-yl]propanoic acid
163004735	(2R,3R,4S,5R,6R)-2-[[(3S,4aS,6aR,6bS,8S,8aS,12aR,14aS,14bR)-8-hydroxy-8a-(hydroxymethyl)-4,4,6a,6b,11,11,14b-heptamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicen-3-yl]oxy]-6-(hydroxymethyl)oxane-3,4,5-triol
163017122	2-[(1R)-3-methyl-1-[4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-1-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxynaphthalen-2-yl]but-2-enyl]naphthalene-1,4-dione
163020497	5,7,8-trihydroxy-3-[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-2-(3,4,5-trihydroxyphenyl)chromen-4-one
163033482	(3R,3aS,6R,6aS)-3,6-bis(2,6-dimethoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan
163034124	8-[(2S,3R,4R,5R)-5-[(1R)-1,2-dihydroxyethyl]-3,4-dihydroxyoxolan-2-yl]oxy-5,7-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one
163034978	2,6,10,14-Tetramethylhexadeca-6,10,15-triene-2,3,9,14-tetrol

163035053	[2-Hydroxy-2-(4-hydroxy-3-methoxy-5-oxooxolan-2-yl)ethyl] 3-(4-hydroxyphenyl)prop-2-enoate
163040205	(2S,3R,4S,5R,6R)-2-[(3S,4R,5S,6S)-6-[[(2R,3S)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-methoxy-3,4-dihydro-2H-chromen-3-yl]oxy]-4,5-dihydroxyoxan-3-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol
163047490	7-hydroxy-6-[(2S)-2-hydroxy-3-methylbut-3-enoxy]chromen-2-one
163051559	(2S,3R,4S,5S,6R)-2-[(2R,3R,4S,5R,6R)-2-[[(3S,4aR,6aR,6bS,8S,8aS,12aR,14aR,14bR)-8-hydroxy-8a-(hydroxymethyl)-4,4,6a,6b,11,11,14b-heptamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicen-3-yl]oxy]-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol
163051662	butyl (2R,3R,4R,5S,6R)-6-[5,7-dihydroxy-2-(4-methoxyphenyl)-4-oxochromen-8-yl]oxy-3,4,5-trihydroxyoxane-2-carboxylate
163057526	2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-8-[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxychromen-4-one
163062115	(2S,10S,11S,15R)-2,11,24-trihydroxy-10-[(E)-3-hydroxy-3-methylbut-1-enyl]-13-methyl-19-[(2R,3S,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexacyclo[14.8.0.02,11.03,8.010,15.018,23]tetracosa-1(16),3,5,7,13,17,19,21,23-nonaen-9-one
163069155	(6R,8S,8aR)-6-hydroxy-3,8-dimethyl-5-propan-2-yl-6,7,8,8a-tetrahydro-1H-azulen-2-one
163106470	(2S,3S,4S,5S,6S)-6-[2-(3,4-dihydroxyphenyl)-5,7,8-trihydroxy-4-oxochromen-3-yl]oxy-3,4,5-trihydroxyoxane-2-carboxylic acid
163106804	(2S,3S,4S,5R,6S)-6-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxochromen-8-yl]oxy-3,4-dihydroxy-5-sulfooxyoxane-2-carboxylic acid
163189360	(2S)-2-(dimethylamino)-3-methyl-N-[(3S,4R,7R,10Z)-7-(2-methylpropyl)-5,8-dioxo-3-phenyl-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-1(14),10,12,15-tetraen-4-yl]butanamide
163189932	10-Methylidene-9-oxooctadecanoic acid
163190248	[(2E,6S)-6-hydroxy-2,6-dimethylocta-2,7-dienoyl] 5-[(2S,3R,4S,5S,6R)-3-[(2S,3S,4S)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-2-hydroxybenzoate
163190709	3-methoxy-2-methyl-6-[(11S)-11-[(2S,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxydodecyl]-1H-pyridin-4-one
163191065	(2S)-2-(dimethylamino)-N-[(3R,4R,7R,10Z)-7-[(4-hydroxyphenyl)methyl]-5,8-dioxo-3-propan-2-yl-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-1(14),10,12,15-tetraen-4-yl]-3-methylbutanamide
163191530	(5S)-3-methoxy-2-methyl-8-methylidene-5-octyl-1,5,6,7-tetrahydroquinolin-4-one
163192296	10-Oxooctadec-11-ynoic acid
163192547	8-Oxooctadec-9-ynoic acid
163193559	methyl (2S,3S,4S,5R,6S)-6-[5,7-dihydroxy-2-(4-methoxyphenyl)-4-oxochromen-8-yl]oxy-3,4,5-trihydroxyoxane-2-carboxylate
163195750	2-Butyl-4-ethenylfuran
163195778	2-Cyclohexa-1,3-dien-1-yl-4-methylpentan-1-ol
163195811	9-Methylidene-8-oxoheptadecanoic acid

Tentative chemical annotations in *Sida* species based on LC-MS untargeted metabolomics (MetaScope, Progenesis QI, Waters)

Retention time	Exact mass	CID	Adducts	Formula	Score	Fragmentation Score	Mass Error (ppm)
2.81	123.0446	126	M+H	C7H6O2	55.1	85.4	4.5
4.38	135.0439	127	M+H-H2O	C8H8O3	44.2	30.8	-0.8
4.98	121.0288	135	M+H-H2O	C7H6O3	42.5	23.8	2.8
1.23	133.0499	179	M+FA-H	C4H8O2	38.5	6.22	-7.9
21.95	81.0316	180	M+Na	C3H6O	37.2	0	9.5
1.27	136.0622	190	M+H	C5H5N5	58.3	95.4	2.9
3.65	89.0378	240	M+H-H2O	C7H6O	55.9	94.6	-6.9
5.44	91.0546	244	M+H-H2O	C7H8O	49.3	57.7	3.2
17.91	57.0692	263	M+H-H2O	C4H10O	35.3	0	-9.7
0.53	191.0189	311	M-H	C6H8O7	39.8	9.97	-4.5
4.3	147.0443	322	M+H-H2O	C9H8O3	45.1	33.9	1.2
2.44	188.0709	323	M+ACN+H	C9H6O2	49.7	55.6	1.9
2.83	183.0288	338	M+FA-H	C7H6O3	40.1	10.2	-7.7
4.28	305.0292	341	M+H-H2O	C14H10O9	44.1	33.2	0.1
4.08	153.0186	370	M+H-H2O	C7H6O5	43.8	26.4	2.1
10.16	109.1017	379	M+H-2H2O	C8H16O2	55.4	89.6	3.3
2.04	115.003	525	M-H2O-H	C4H6O5	47.3	47.8	-5.3
2.44	118.0655	798	M+H	C8H7N	45.7	37	3.1
4.08	95.0496	996	M+H	C6H6O	41.1	17.7	5
2.96	134.0603	1054	M+H-2H2O	C8H11NO3	38.7	0	1.3
1	117.0184	1110	M-H	C4H6O4	54.7	86.6	-8.1
8.49	93.0698	1140	M+H	C7H8	55.3	84.7	-0.6
0.97	113.0347	1174	M+H	C4H4N2O2	38.6	0	1.3
3.9	151.0394	1183	M-H	C8H8O3	46.2	45.2	-4.7
2.81	291.0865	1203	M+H	C15H14O6	41	15.8	0.8
5.24	271.0592	1249	M+H-2H2O	C15H14O7	42.6	24.2	-3
5.26	167.0703	2214	M+H	C9H10O3	41.9	14.7	0.4
12.4	501.3579	2371	M+FA-H	C30H48O3	45.7	43.1	-1.4

2.39	163.0396	2518	M+H-H2O	C9H8O4	53.2	80.4	3.5
19.18	284.295	2682	M+ACN+H	C16H34O	38.9	2.29	0.7
5.44	163.0759	3314	M-H	C10H12O2	41.1	17	-3.2
4.08	137.0238	3469	M+H-H2O	C7H6O4	43.5	22.4	3
3.45	553.1647	3503	M+CI	C30H30O8	35.8	0	2.4
17.99	280.2403	3931	M+H-2H2O, M+H- H2O, M+Na	C18H32O2	51.5	66.2	0.3
4.48	341.0653	5099	M-H2O-H	C18H16O8	40.5	12.3	-3.8
8.01	199.0856	5202	M+Na	C10H12N2O	40.3	21.3	7.9
9.34	335.0921	5204	M-H2O-H	C20H18O6	35.6	0	-1.2
20.73	283.2635	5281	M-H	C18H36O2	43.8	36.2	-2.5
7.36	203.0522	5429	M+Na	C7H8N4O2	39.8	19	-9.8
2.72	136.0396	5570	M-H	C7H7NO2	38.9	3.03	-5.5
0.53	203.0527	5793	M+Na	C6H12O6	51.9	65.2	0.3
1.32	150.0413	5951	M+FA-H	C3H7NO3	50.1	60.8	4.7
3.64	132.0293	5960	M-H	C4H7NO4	40.9	17.4	-6.6
3.24	323.0981	5988	M-H2O-H	C12H22O11	40.4	17.6	-0.9
0.97	267.0584	6029	M+Na	C9H12N2O6	37.4	0	-1.6
12.75	105.0698	6054	M+H-H2O	C8H10O	44.4	30.9	-0.4
1.03	182.0821	6057	M+H	C9H11NO3	40.2	17.1	5.1
6.31	369.205	6185	M+H-2H2O	C23H32O6	54	76.4	-2.6
3.09	136.0513	6274	M-H2O-H	C6H9N3O2	43.5	21.4	-2.2
0.51	118.0868	6287	M+H	C5H11NO2	56.1	88.4	4.9
15.72	196.112	6734	M+ACN+H	C12H10	37.4	0	-0.7
4.91	203.1072	7017	M+CH3OH+H	C12H10O	37.9	0	3.2
7.89	117.0697	7146	M+H-H2O	C9H10O	41.9	20.5	-1.3
8.49	107.0852	7237	M+H	C8H10	56.6	95.5	-3.4
6.4	85.0288	7302	M-H	C4H6O2	52.7	77	-7.7
20.21	81.0332	7361	M+H-H2O	C5H6O2	38.1	0	-3.3
1.23	97.0285	7362	M+H	C5H4O2	47.7	44.9	0.5
11.54	135.1163	7438	M+H-H2O	C10H16O	54.2	85.1	-3.1
3.92	175.0373	7478	M+Na	C8H8O3	44.4	36.7	4.9
15.7	107.0861	7500	M+H	C8H10	46.4	44.6	5.2
20.61	165.0902	7654	M+H	C10H12O2	40.4	14	-4.7
17.62	83.0856	7966	M+H-H2O	C6H12O	42.7	21	0.9
5.97	81.0696	7967	M+H-H2O	C6H10O	53.1	75.6	-2.9
7.9	83.0494	8080	M-H	C5H8O	39.5	13.8	-9.9
17.91	85.1014	8103	M+H-H2O	C6H14O	38.8	3.5	2.3

16.88	97.1015	8130	M+H-H2O	C7H14O	42.9	25.5	2.8
12.15	123.1171	8158	M+H-2H2O	C9H18O2	52.5	74.3	1.5
16.84	151.1484	8180	M+H-2H2O	C11H22O2	46.9	47.7	1.3
17.99	339.3265	8215	M-H	C22H44O2	36.9	0	-1.1
4.9	73.0288	8299	M-H	C3H6O2	37.2	0	-9.3
5.89	207.0652	8417	M+H	C11H10O4	44.4	34.5	0.3
11.18	198.1859	8842	M+ACN+H	C10H20O	36.9	0	4.2
5.43	190.0503	10256	M+FA-H	C9H7NO	39.9	14.9	-4.8
6.12	121.0652	10393	M+H-H2O	C8H10O2	43.1	23.3	3.1
3.44	147.0443	10394	M-H2O-H	C9H10O3	38.1	6.51	-5.3
13.31	95.086	10400	M+H-H2O	C7H12O	46.6	43.7	4.3
16.81	313.2742	10416	M+CH3OH+H	C18H32O2	52.2	72.2	1.5
22.61	139.0757	10457	M+H-2H2O	C8H14O4	40.3	13.1	2.1
12.39	315.2536	10465	M+FA-H	C17H34O2	41.1	21.5	-1.9
12.24	501.3588	10494	M+FA-H	C30H48O3	44.8	44.4	0.6
9.26	197.1175	10582	M+FA-H	C10H16O	48.9	56	-5.4
8.49	267.0662	10680	M+FA-H	C15H10O2	39.5	7.32	-0.2
11.16	247.0598	10743	M+Na	C11H12O5	41.5	21.3	9.6
4.32	209.0809	10748	M+CH3OH+H	C10H8O3	46.9	37.6	0.2
16.83	137.1329	11142	M+H	C10H16	47.9	50.8	3.2
4.88	69.0701	12020	M+H-H2O	C5H10O	42.5	21	2.4
2.54	195.0287	12088	M+FA-H	C8H6O3	37	2.54	-7.8
4.08	93.0339	12097	M+H-H2O	C6H6O2	44.6	34	3.5
7.89	119.0856	12580	M+H-H2O	C9H12O	45	34.9	0.5
16.83	97.0652	12756	M+H-H2O	C6H10O2	41.6	19.1	3.6
8.21	107.0859	12777	M+H-2H2O	C8H14O2	55.9	91.1	2.3
5.15	179.034	13250	M-H2O-H	C9H10O5	49	57.8	-4.9
11.54	181.1223	13642	M+CH3OH+H	C10H12O	43.5	28	0
8.71	287.2221	13849	M+FA-H	C15H30O2	46	34.9	-2.7
7.3	144.0212	14079	M+Cl	C6H7NO	36.6	0	-9
20.23	134.1093	14091	M+H, M+Na	C10H14	45.1	35.6	-2
2.52	178.1341	14296	M+ACN+H	C8H12N2	47.3	40.5	1.7
5.34	161.0598	14340	M+H-2H2O	C10H12O4	47.8	42.3	0.4
4.05	147.0445	15294	M+H-H2O	C9H8O3	47.1	48.5	2.5
16.81	95.086	16275	M+H-H2O	C7H12O	44.8	32.4	4.5
12.67	133.1012	16441	M+H-H2O	C10H14O	54.4	83	0.3
16.83	109.1018	16900	M+H-H2O	C8H14O	47	46	4.8

8.59	185.1174	17166	M+FA-H	C9H16O	47.7	53.4	-6.7
6.2	464.3138	19212	M+H-2H2O, M+H- H2O, M+H, M+Na	C27H44O6	53.9	70.6	0.1
0.53	128.0464	19309	M-H2O-H, M-H	C6H8O3	43.5	37.5	-7.5
2.81	147.0445	19844	M+H-2H2O	C9H10O4	40.9	15.4	2.6
5.34	251.1047	21742	M+Na	C15H16O2	37.7	6.36	2.1
24.58	53.0206	22238	M+H-2H2O	C4H8S	37.6	0	-2.4
6.39	741.3332	23485	M+FA-H	C35H52O14	44.3	29.7	-1
4.4	129.055	25310	M+H-2H2O	C6H12O5	42.5	22.4	2.2
4.08	161.06	28516	M+H-H2O	C10H10O3	45.3	39.1	1.5
5.74	173.0959	28619	M+H-H2O	C12H14O2	42.3	25.4	-0.8
6	123.0808	31242	M+H	C8H10O	43.7	30.5	3
5.71	109.1014	31265	M+H-2H2O	C8H16O2	45.5	37.9	1.5
18	185.0117	32033	M+CH3OH+H	C4H8S3	35.5	0	-3.9
2.81	123.0441	33931	M-H2O-H	C7H10O3	45	34.2	-7.5
18.27	135.1175	34645	M+H-H2O	C10H16O	45.8	35.1	4.4
12.02	119.0859	35698	M+H-2H2O	C9H14O2	56.8	96.6	2.2
1.27	268.104	60961	M+H	C10H13N5O4	53.1	66.3	0
6.22	133.1018	61130	M+H-H2O	C10H14O	48.2	56.7	4.4
12.67	83.0858	61370	M+H-H2O	C6H12O	54.8	84.3	3
1.83	133.065	62465	M-H2O-H	C9H12O2	44.1	32.5	-6.1
4.41	481.0767	65064	M+Na	C22H18O11	41.6	22.1	5.6
11.16	327.159	65373	M+H-2H2O	C20H26O6	42.6	24.5	-0.3
4.98	133.0287	68262	M+H-2H2O	C8H8O4	44.6	34.5	1.8
2.91	164.0712	71567	M-H	C9H11NO2	41.7	14.8	-3.2
3.37	287.0926	72732	M+FA-H	C15H14O3	39.3	12.8	0.3
13.31	453.3371	73193	M+H-2H2O	C30H48O5	48.3	59	1.6
4.45	367.0821	73207	M+Na	C18H16O7	43	32.4	9.5
11.21	488.3503	73641	M+H-2H2O, M+Na	C30H48O5	43.7	22.8	0.3
3.09	195.0655	75142	M-H	C10H12O4	41.1	13.4	-4.2
4.12	259.0605	75324	M+CI	C9H12N4O3	37.6	0	0.8
4.88	191.0837	78603	M+H-2H2O	C15H14O2	36.7	5.79	-8.1
3.62	255.0893	82143	M+Na	C16H12N2	44.7	30.4	0.3
20.61	461.3627	86052	M+FA-H	C28H48O2	39.6	14.2	-2.3
6.64	415.1024	92794	M-H2O-H	C21H22O10	42.6	25.3	-2.4
17.94	510.4301	94225	M+ACN+H	C32H52O2	39.9	6.42	-1
6.75	387.1082	100151	M+H	C20H18O8	41.2	16.6	2
4.81	179.1066	100332	M+H-H2O	C11H16O3	40.4	14.5	-0.4

7.91	127.0758	101536	M-H2O-H	C7H14O3	40.3	14.9	-4.6
20.38	383.3529	102430	M-H	C24H48O3	44	35.6	-0.5
5.44	161.0448	107526	M-H2O-H	C6H12O6	41.1	13.3	-4.1
5.34	175.0754	107557	M+H-H2O	C11H12O3	43	27	0
2	593.1295	107876	M-H	C30H26O13	37.6	8.48	-0.9
4.65	441.0819	107905	M-H	C22H18O10	41.4	19.7	-1.7
10.18	126.053	112720	M+Na	C4H9NO2	37.9	0	4.4
4.4	448.1007	114776	M-H2O-H, M-H	C21H20O11	50.7	58.2	0.4
15.7	233.2265	117769	M+H-2H2O	C17H32O2	44.7	41.7	0.6
12.44	323.1271	119205	M+H-2H2O	C20H22O6	44.5	28.3	-1.8
7.66	191.0711	119216	M+H-H2O	C11H12O4	42.7	30.1	3.8
3.99	242.9929	123908	M+CI	C6H8O8	36.4	9.63	7.4
6.11	314.1389	125213	M+H	C18H19NO4	41.3	11.7	0.6
9.92	284.0317	128853	M-H2O-H	C15H11O7+	36.8	3.97	-3.1
14.62	297.243	133372	M-H	C18H34O3	45.8	45.9	-1.9
15.67	617.3847	133551	M-H	C39H54O6	44.6	29.8	-0.2
3.25	149.0449	135191	M-H	C5H10O5	42.2	17.6	-4
4.68	185.0237	139711	M+CI	C6H14S2	35.9	0	4.3
17.6	531.4073	151202	M+CH3OH+H	C32H50O4	37.7	0	5.8
13.98	277.1794	155022	M+CH3OH+H	C16H20O2	37.3	0	-1.6
6.17	335.1158	156741	M+FA-H	C16H18O5	36.1	0	7.5
5.84	135.1169	159055	M+H-H2O	C10H16O	48.3	53	0.6
8.01	185.1073	160510	M+H	C12H12N2	49.5	60.3	-0.1
2.44	334.0896	161355	M+Na	C14H17NO7	40.9	9.65	-0.5
4.93	431.0971	162350	M-H	C21H20O10	43.6	36.8	-3.1
4.08	465.1034	165559	M+H	C21H20O12	50.6	57.7	1.4
5.61	249.1022	178034	M+H	C16H12N2O	51.9	61.2	-0.3
5.28	353.1394	181681	M+H-2H2O	C21H24O7	40.4	10.4	2.8
19.03	353.1632	186775	M-	C21H23NO4	39.9	14.2	-0.2
18.69	355.3212	193484	M-H	C22H44O3	44.7	30	-1.5
12.68	121.0648	231324	M+H-H2O	C8H10O2	46.8	43	0.2
4.86	371.2224	258412	M+H-2H2O	C23H34O6	52.8	71.4	1.8
13.5	499.306	286498	M-H2O-H	C30H46O7	44.2	46	-1
5.44	330.1345	328066	M+ACN+H	C16H16O5	42.5	22.2	3.1
1.83	161.0598	348502	M-H2O-H	C10H12O3	46.6	40.7	-5.5
4.98	167.0505	373912	M-H2O-H	C12H10O2	41.6	22.5	1.5
6.85	511.2117	375713	M+H-2H2O	C32H34O8	37.7	2.4	0.4

5.34	325.1431	384679	M+H-2H2O	C20H24O6	40.8	16.4	-1
4.78	249.0792	417052	M+CI	C13H14N2O	38.6	1.34	-3.6
0.53	527.1586	439242	M+Na	C18H32O16	50.8	59.4	0.7
5.26	273.0761	439246	M+H	C15H12O5	42.4	17.1	1.4
0.53	365.1057	439341	M+Na	C12H22O11	47	39.1	0.7
3.45	377.0838	439514	M+Na	C16H18O9	41.4	20.1	-1.5
3.73	231.0286	439944	M+CI	C6H12O7	42.3	20.4	4.6
5.74	187.1122	440265	M+H-2H2O	C13H18O3	47.1	43.6	2.2
7.22	269.0448	440735	M-H2O-H	C15H12O6	44.5	41.7	-2.6
4.98	329.0654	440833	M+Na	C15H14O7	47.9	59	7.3
4.51	345.0602	440835	M+Na	C15H14O8	47.9	49.8	6.6
12.67	137.0966	441574	M-H2O-H	C9H16O2	55.8	93.4	-3.8
12.15	149.1332	441644	M+H-2H2O	C11H20O2	46.4	48.2	3.7
4.41	450.1117	441667	M+H	C21H21O11+	49.5	64.5	-8.7
3.04	655.1875	441765	M-	C29H35O17+	33.9	0.345	-0.7
3.25	595.1664	441772	M-	C27H31O15+	44.1	23.5	-0.7
6.29	461.2897	441833	M+H-2H2O	C27H44O8	52.7	66.9	-0.2
2.69	385.0764	442101	M+FA-H	C15H16O9	43.8	28	-3.5
5.34	281.0816	442396	M-H2O-H	C17H16O5	41.5	21.5	-1.1
2.96	174.0552	442849	M-H2O-H	C10H11NO3	44.6	32.4	-4.2
2.71	148.0516	444539	M-H, M+FA-H	C9H8O2	40.7	14.4	-5.4
21.67	337.2718	444899	M+CH3OH+H	C20H32O2	38.2	0.745	-6.4
4.86	683.4372	446066	M+CI	C35H69O8P	33.4	0	-8.1
16.78	575.4121	447791	M+H-H2O	C31H61O8P	37.2	0.0029	8.3
16.81	526.4301	479957	M+ACN+H	C32H52O3	35.1	3.74	9.6
7.68	167.0707	518900	M+H	C9H10O3	44.1	33.1	2.3
15.7	173.1329	520684	M+H-2H2O	C13H20O2	49.9	61.1	1.9
11.86	103.0751	521790	M+H	C5H10O2	38.3	0	-2.2
6.05	311.1273	522636	M+H-2H2O	C19H22O6	42.7	27.7	-1.4
17.62	125.133	525578	M+H	C9H16	42.8	28.5	4.5
6.19	191.1432	538953	M+H-H2O	C13H20O2	42.8	28.7	0.9
10.16	225.1487	539381	M-H	C13H22O3	53.1	84.2	-4
4.86	175.1112	540124	M+H	C12H14O	42.2	23.4	-3.1
5.43	209.0785	546377	M+Cl	C9H18OS	36.1	0	7.3
19.05	221.1536	576026	M+CH3OH+H	C13H16O	40.8	9.37	0.2
4.86	214.1358	608115	M+H-H2O, M+H, M+Na	C15H18O	44.8	27.3	0
6.85	339.0871	632128	M-H2O-H	C19H18O7	46.9	42.1	-0.9

6.17	510.2129	636543	M+H	C28H31NO8	40	13.6	1.4
5.31	277.1068	636576	M+FA-H	C14H16O3	38.4	13.3	-5.8
1.33	715.1908	637139	M+CI	C39H36O11	33.5	0	-6.4
19.03	355.1576	637239	M-H2O-H	C21H26O6	37.1	4.75	6.8
13.71	175.1488	638014	M+H-H2O	C13H20O	49.1	63.1	3.4
7.73	243.0653	667639	M-H	C14H12O4	38.4	7.48	-3.8
8.19	177.0544	1548883	M+H-H2O	C10H10O4	54.5	84.8	-1
16.84	161.1327	1549026	M+H-2H2O	C12H20O2	44.5	36.8	1.4
11.21	163.076	1549095	M+H-H2O	C10H12O3	49.2	61.2	3.8
9.95	309.2064	1551480	M+FA-H	C17H28O2	41.3	23.3	-2.9
16.63	262.2296	1711945	M+H-H2O, M+H	C18H30O	47.7	49.9	-0.3
13.86	203.1792	1742210	M+H-H2O	C15H24O	51	67.4	-1
2.87	377.0847	1794427	M+Na	C16H18O9	44.8	27	1.2
6.87	161.0451	2723872	M-H2O-H	C6H12O6	50.1	61.1	-2.4
13.27	149.0969	3015413	M+H-2H2O	C10H16O3	42.3	27.5	4.2
4.08	187.0396	3083616	M+H-2H2O	C11H10O5	40	6.84	2.9
7.63	415.1031	3084131	M+FA-H	C20H18O7	43.5	23.8	-1
12.48	353.2689	3084463	M+Na	C19H38O4	45.5	40.1	8.1
2.81	139.0394	3702506	M+H	C7H6O3	46.8	40.4	3
5.91	545.1989	4486984	M+H-2H2O	C28H36O13	40.3	21.4	-4.9
10.38	715.2391	5274621	M-H	C39H40O13	36.1	5.04	-0.7
16.64	775.4257	5274625	M+H-2H2O	C49H62O10	37.2	8	6.4
12.04	649.3746	5274626	M+FA-H	C38H52O6	46.2	54.4	0.1
4.08	302.0428	5280343	M+H-H2O, M+H	C15H10O7	50.6	54.4	0.4
4.63	329.1385	5280379	M-H2O-H	C19H24O6	41.8	17.3	-2.6
21.1	338.3422	5280435	M+ACN+H	C20H40O	38.8	0.719	1.4
7.89	267.0669	5280442	M+H-H2O	C16H12O5	35.5	1.33	6
5.86	315.0496	5280443	M+FA-H	C15H10O5	43	31.9	-5.4
7.4	285.0395	5280445	M-H	C15H10O6	43.8	31	-3.2
2.97	191.0338	5280460	M-H	C10H8O4	49.4	58.8	-6.3
2.39	223.0602	5280536	M+FA-H	C10H10O3	43.6	38.4	-5.6
3.95	364.1492	5280607	M-H2O-H, M+FA-H	C19H24O7	36.5	1.65	-8.4
6.04	429.0828	5280637	M-H2O-H	C21H20O11	47.3	46.6	0.1
4.08	299.0186	5280647	M-H2O-H	C15H10O8	43.9	40.2	-3.4
4.98	287.0553	5280863	M+H	C15H10O6	50.5	54.1	1
16.83	320.2585	5280934	M+ACN+H	C18H30O2	49.5	66.3	0.3
6.44	235.0862	5280953	M+Na	C13H12N2O	40.3	14	9.6

15.7	278.2249	5281115	M+H-2H2O, M+H- H2O, M+H	C18H30O2	49.9	54.7	1.1
13.71	191.1801	5281119	M+H-2H2O	C14H26O2	45.7	46.8	3
14.91	296.2351	5281128	M+H-H2O, M+Na	C18H32O3	40.9	23.3	-0.1
5.79	589.3359	5281319	M+CH3OH+H	C32H44O8	39.2	12.6	-2.1
14.26	537.2823	5281321	M+Na	C30H42O7	36.3	0.0151	0
3.68	179.0337	5281416	M+H	C9H6O4	42.1	21.7	-0.9
2.87	162.0321	5281426	M+H-H2O, M+H	C9H6O3	48.2	46.9	2.2
4.75	569.3158	5281578	M+H	C34H40N4O4	42.6	32.7	6.2
5.96	279.066	5281601	M-H2O-H	C17H14O5	42.7	18.1	-1
4.42	299.0552	5281607	M+FA-H	C15H10O4	46.8	45.7	-3.8
9.92	301.0704	5281612	M+H	C16H12O6	48.8	46.3	-1
3.05	287.0552	5281614	M+H	C15H10O6	41.6	17.4	0.5
3.77	423.0908	5281647	M+H	C19H18O11	41	15.6	-3.4
3.93	325.0704	5281676	M+H-2H2O	C18H16O8	50	62.7	-0.6
4.41	353.0649	5281702	M+Na	C17H14O7	52.1	67.4	5.1
4.86	281.1542	5281984	M+H-2H2O	C19H24O4	42.4	22.3	1.9
6.79	448.1004	5282102	M-H2O-H, M-H	C21H20O11	53.2	78.1	-0.4
15.57	323.2828	5283446	M+H, M+Na	C20H37NO2	42.8	23.7	1.3
5.54	519.115	5315831	M+FA-H	C23H22O11	41.8	17.1	1.3
4.73	477.1037	5316673	M+FA-H	C21H20O10	41.6	16.5	-0.4
3.62	575.1709	5317025	M+H-H2O	C28H32O14	39	7.4	-8.4
4.98	418.0919	5318717	M+H-2H2O, M+H- H2O, M+H	C20H18O10	47.6	57.3	4.5
4.86	594.1578	5318761	M-H, M+Cl	C27H30O15	40.8	6.62	-1.2
4.23	203.0341	5319474	M+H-H2O	C11H8O5	45.6	41.8	1.1
13.98	239.0738	5320006	M-H2O-H	C15H14O4	47.4	58.9	9.5
5.74	539.3196	5320254	M+Na	C27H48O9	42.3	21.9	1.1
6.79	594.1374	5320686	M+H, M+Na	C30H26O13	43.6	19.1	0
4.53	609.1458	5320834	M+H-H2O	C27H30O17	42	13.9	1.2
5.52	341.0666	5386960	M-H2O-H	C18H16O8	43	27.5	-0.2
4.86	480.3095	5459840	M+H-2H2O, M+H- H2O, M+H	C27H44O7	54.2	74	1.7
6.29	329.1756	5460372	M+H-H2O	C20H26O5	48.7	52.1	2.4
11.23	343.1535	5460657	M+H-2H2O	C20H26O7	42.5	35.2	-1.3
5.72	339.087	5466138	M-H2O-H	C19H18O7	43.4	24.4	-1.2
5.34	309.0759	5468749	M-H2O-H	C18H16O6	43	22.1	-3
4.47	313.0704	5487855	M+H-H2O	C17H14O7	40.8	23	-0.7
2.79	323.0736	5488575	M+H-H2O	C15H16O9	43.3	26.8	-7.6

3.52	495.0763	5490334	M+H	C21H18O14	41.3	31.2	-1.2
3.93	471.0905	5491693	M+Na	C21H20O11	51.7	61.5	1.5
13.71	201.1637	6436348	M+H-H2O	C15H22O	56.4	89.3	-0.5
4.58	755.3469	6441104	M+CI	C38H56O13	35.2	0.0837	7.4
1.38	597.3581	6450144	M+H-2H2O	C39H52O7	35.4	0	1
2.44	203.0817	6452262	M-H	C11H12N2O2	37.7	0.214	-4.2
20.46	619.4218	6602508	M+FA-H	C35H58O6	35.4	4.99	0.5
14.81	153.1279	6973640	M-H	C10H18O	54.9	87.8	-4
7.91	95.0859	7156991	M+H-2H2O	C7H14O2	42.6	24.5	2.9
18.27	265.2522	9561835	M+H-2H2O	C18H36O3	42.7	23.1	-1.2
0.77	203.018	9930500	M-H	C7H8O7	37.3	2.19	-8.3
3.11	423.1635	9978316	M+Na	C19H28O9	44.9	47.8	2.3
6.55	307.0813	10015552	M+FA-H	C14H14O5	40.1	7.57	-4
5.34	411.1985	10023166	M+Na	C19H32O8	40.1	21.9	-1.1
4.98	230.0581	10105245	M+H-H2O, M+H	C13H10O4	41.2	9.45	0.7
4.48	209.0811	10176654	M+H	C11H12O4	44.4	25.2	1.1
4.41	551.103	10187514	M+H	C24H22O15	43.4	31.6	-0.3
4.51	434.0851	10252339	M+H-2H2O, M+H- H2O, M+H	C20H18O11	51	61.7	0.5
20.06	513.3893	10255859	M+H	C33H52O4	35.6	0	-8.8
9.2	177.0543	10262028	M+H-H2O	C10H10O4	54.2	84	-1.7
1.38	343.1029	10308838	M-	C18H17NO6	41.7	22.3	-9.4
3.52	409.1835	10317980	M+Na	C19H30O8	40.7	10.7	0.4
4.4	610.154	10371536	M+H, M+Na	C27H30O16	49.5	50.2	1
6.11	312.1233	10403282	M-H	C18H19NO4	45.9	36.5	-2.8
5.44	551.1399	10413856	M+FA-H	C24H26O12	40.1	13.2	-1.4
11.08	759.2658	10439806	M+FA-H	C40H42O12	42.3	36.1	0
4.6	233.1728	10465398	M+CH3OH+H	C11H20O3	37.2	0	-9.8
6.64	367.0812	10472650	M+Na	C18H16O7	38.1	4.06	6.8
5.41	729.1882	10508776	M+FA-H	C30H36O18	42	19.2	-0.3
5.36	231.091	10538510	M+H-H2O	C16H12N2O	43.3	44.3	-2.7
4.1	132.0605	10582821	M+H-H2O, M+H, M+Na	C6H12OS	38	4.24	-2.7
18.49	601.3893	10603919	M-H2O-H	C39H56O6	36.1	12.6	-1
1.12	174.0762	10630882	M+FA-H	C6H11NO2	36.9	0	-7.4
5.81	647.3392	10652163	M+H-2H2O	C35H54O13	42.4	42.9	-4.9
7.05	551.1401	10720349	M+FA-H	C24H26O12	40.6	7.13	-1
12.48	698.3494	10723382	M+H, M+Na	C35H54O14	42.9	19.9	-2.7
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4.55	463.0873	10813969	M-H	C21H20O12	51.6	62	-2
4.14	567.1349	10815866	M+FA-H	C24H26O13	42.1	18	-1.2
22.48	297.0875	10912308	M+CI	C15H18O4	42.4	31.5	-9.2
6.2	248.1413	10922890	M+H-H2O, M+H	C15H20O3	47.1	37.5	0.2
6.59	339.1227	10969116	M+Na	C18H20O5	42.1	26.6	7.7
10.64	501.3216	11060391	M-H2O-H	C30H48O7	52.4	70.9	-1
3.9	741.1878	11061627	M-H	C32H38O20	43.4	22.9	-0.8
13.3	147.1173	11063054	M+H-2H2O	C11H18O2	51.5	72.5	2.9
3.92	743.2028	11072668	M+H	C32H38O20	46	41.8	-0.1
11.18	353.1017	11079623	M+H-2H2O	C20H20O8	44.4	30.9	-0.6
9.67	517.3533	11167374	M+FA-H	C30H48O4	52.3	80.9	-0.4
2.19	146.0815	11194416	M-H	C6H13NO3	37.8	1.86	-4.9
22.15	731.5546	11227946	M-H, M+FA-H	C40H77NO10	44	33.8	-0.1
2.63	577.1348	11250133	M-H	C30H26O12	40.8	10.6	-0.6
5.64	273.0757	11276243	M+FA-H	C14H12O3	39.4	17.3	-5
6.55	213.0548	11276313	M-H2O-H	C13H12O4	43.6	30.4	-3.9
5.48	323.1278	11277992	M+Na	C18H20O4	40.1	17.2	8.2
16.13	745.4141	11354754	M+H-2H2O	C48H60O9	43	29.5	5.4
6.64	416.1105	11464176	M+H-H2O, M+H, M+Na	C21H20O9	43.4	18.6	-0.6
5.85	349.1258	11623832	M+CH3OH+H	C17H16O6	37.4	1.58	-7.5
19.56	618.4143	11692717	M+ACN+H	C37H52O5	37.8	0.00195	-1.7
3.39	379.1003	11953803	M+Na	C16H20O9	40	11.3	0.9
6.95	477.1021	11968644	M+H	C22H20O12	36.4	6.99	-1.3
13.99	579.2837	12303930	M+FA-H	C29H42O9	42.7	24.3	4.9
6.55	601.1539	12305415	M+Na	C27H30O14	41.4	24.3	1.9
13.35	454.3446	12313704	M+H-H2O, M+H	C30H46O3	42.8	26.6	-0.3
4.2	314.1025	12681283	M-H	C17H17NO5	36.2	0.295	-2.7
2.79	151.0382	12695575	M+H-H2O	C8H8O4	47.1	50.3	-4.8
2.19	109.0288	12799212	M-H2O-H	C6H8O3	55.3	86.1	-5.8
12.77	121.1017	13197868	M+H-H2O	C9H14O	52.6	75.1	3.6
3.02	511.1427	13245586	M+CH3OH+H	C22H22O12	39.4	8.63	-4.1
6.52	461.1084	13871877	M-H	C22H22O11	44	32.8	-1.2
7.78	255.1226	13915427	M+FA-H	C12H18O3	36.2	0	-5.5
3.68	133.0286	13918554	M+H-2H2O	C8H8O4	45.5	38.1	1.3
4.68	591.1336	13988634	M+H-2H2O	C27H30O17	38.1	3.7	-1.3
3.57	131.0851	14009683	M+H-2H2O	C10H14O2	41.4	20.6	-2.4
4.45	575.1403	14035324	M-H2O-H	C27H30O15	41.5	17.6	-0.6

6.29	469.3315	14055737	M+H-2H2O	C30H48O6	52.2	73.9	0.5
4.07	449.1085	14187088	M+H-H2O	C21H22O12	52.8	66.3	1.3
4.68	532.0892	14311156	M-H2O-H	C24H23O15+	37.4	15	6.1
4.48	565.1194	14311160	M-	C25H25O15+	40.1	3.39	-0.9
4.96	549.1243	14311167	M-	C25H25O14+	40.7	6.21	-1.2
4.55	461.0722	14332450	M-H	C21H18O12	53.1	73.3	-0.9
4.91	496.305	14376672	M+H, M+Na	C27H44O8	46.2	35.7	2.8
6.33	355.1724	14484636	M+Na	C16H28O7	40.1	9.55	-0.8
4.68	545.2008	14681438	M+Na	C26H34O11	42.5	22.7	2.7
3.12	439.1576	14704521	M+Na	C19H28O10	42.1	21.9	0.2
17.89	453.3372	14707301	M-H2O-H	C30H48O4	38	4.62	-0.5
2.79	639.1224	14887603	M+H-H2O	C27H28O19	38.1	9	4.8
2.89	459.0562	14887605	M-H2O-H	C21H18O13	44	35.9	-1.5
3.99	473.0766	14887607	M-H2O-H	C22H20O13	42.3	32	8.1
3.93	314.0777	15289454	M+H-H2O, M+CH3OH+H	C17H14O6	42.7	29.3	-4.2
1.41	367.0639	15559735	M+CH3OH+H	C15H10O9	49.1	69.3	-6.3
13.71	472.3559	15560128	M+H-2H2O, M+H- H2O, M+Na	C30H48O4	50	58.7	1.3
20.23	170.1092	15645217	M+H, M+Na	C13H14	41.2	17.5	-2.4
12.96	657.3765	15767724	M+Na	C39H54O7	42.9	20.7	0.5
5.26	433.114	16077448	M+H-H2O	C21H22O11	40.2	9.85	2.3
18.8	639.2818	16093748	M+H	C32H46O11S	43.1	32.8	-2.5
14.81	677.4012	21120946	M+FA-H	C40H56O6	35.2	7.01	-7.4
16.13	701.3457	21579640	M+Na	C36H54O12	36.6	14	-7.5
6.52	491.0862	21722016	M-H	C22H20O13	48	56.5	6.2
6.35	395.2106	21763831	M-	C24H29NO4	35	0	1
6.8	637.1559	21881649	M+FA-H	C31H28O12	36.8	2.7	-0.6
13.86	189.1637	22236717	M+H-H2O	C14H22O	42.6	27.6	-0.3
4.43	259.0969	23642717	M-H	C15H16O4	37.3	5.59	-2.5
6	295.0702	23658567	M-	C13H13NO7	41.5	12.8	1.6
5.76	405.1525	23815394	M+FA-H	C20H24O6	41.4	24.5	-8.3
10.12	504.3444	24796850	M-H, M+FA-H	C30H48O6	55.4	89.6	-1.4
18.5	489.3569	24796851	M+H-H2O	C30H50O6	41.9	24.4	-1
4.63	521.2023	24982202	M-H	C26H34O11	38.4	4.99	-1.1
3.29	229.0131	25021697	M+CI	C6H10O7	41.3	16.8	5.4
3.37	447.0923	26339717	M-H	C21H20O11	44.2	30.2	-2.1
5.44	547.1817	42608087	M+H-H2O	C27H32O13	38.5	0.28	1.2
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8.79	527.3359	44178847	M+CH3OH+H	C31H42O5	36	0	-1.6
2.79	445.0752	44258591	M-H2O-H	C21H20O12	44.1	32.1	-5.2
1.4	396.9851	44260032	M-H	C15H10O11S	37.9	4.43	-5.1
4.48	845.177	44552029	M+FA-H	C37H36O20	37.7	0.869	-1.5
4.23	619.1271	44552030	M-H2O-H	C28H30O17	44.3	33.3	-5.2
12.2	293.2112	44559173	M+H-2H2O	C18H32O5	55.4	95.8	0.1
4.56	537.124	44566588	M+FA-H	C23H24O12	46.3	43.6	-2.1
3.05	477.1014	44566911	M+H	C22H20O12	42.1	28	-2.8
6.14	207.0656	44577733	M+H	C11H10O4	45.2	36.2	2
4.18	373.1285	44578390	M+H	C20H20O7	39.2	1.33	0.8
9.59	257.0811	44631546	M-H2O-H	C15H16O5	43	34.4	-2.8
10.12	486.3346	45273405	M+H-2H2O, M+Na	C30H46O5	37.6	0	0.1
3.22	711.1387	46181828	M-H2O-H	C37H30O16	36.5	0.699	4.4
11.08	727.2397	49831447	M+FA-H	C39H38O11	40.4	14	0.1
10.99	700.2524	49831491	M+H-H2O, M+Na	C39H40O12	40.3	7.03	0.7
11.16	697.2653	49831493	M+H-H2O	C40H42O12	50.8	69.3	1.4
3.37	610.1544	49842399	M+H, M+Na	C27H30O16	40.6	14.8	1.7
5.01	383.0981	53420248	M+FA-H	C16H18O8	40.4	5.11	-0.7
7.89	91.0546	53429614	M+H-2H2O	C7H10O2	48.6	50.8	2.6
8.04	251.1254	54005211	M+Na	C12H20O4	38.5	0	0.2
11.97	311.222	54355075	M+FA-H	C17H30O2	47.2	43.6	-2.8
17.99	111.117	57006309	M+H-H2O	C8H16O	44.5	32.6	1.3
16.03	297.24	57172986	M+H-2H2O	C18H36O5	46	54.4	-7.2
14.29	555.2933	57402770	M+Na	C30H44O8	38.3	9.26	0.9
6.35	461.1652	69634125	M-H	C20H30O12	42.7	23.4	-2.7
10.16	367.2451	71359328	M+Na	C19H36O5	39.3	0.318	-1.1
11.51	337.2354	71403936	M+Na	C18H34O4	39	1.6	1.3
4.55	436.2236	71438848	M+FA-H	C24H29N3O2	39.1	0.57	-1.5
10.56	333.2039	72730313	M+CH3OH+H	C19H24O3	55.5	97.5	-7.2
6.04	303.1949	72730314	M+H	C19H26O3	46.8	40.4	-1.8
4.86	302.1878	72730315	M+H-2H2O, M+H- H2O, M+H, M+Na	C19H26O3	48.9	49.8	-1.3
5.37	209.1532	72751004	M+H-2H2O	C13H24O4	40.1	16.5	-1.5
6.29	299.1639	73172655	M+H-H2O	C19H24O4	42.3	24.2	-0.8
2.72	625.2103	73323377	M+H	C29H36O15	39.2	13.3	-3.8
19.11	462.3712	73821792	M+H-2H2O, M+Na	C29H50O4	38.6	0.00689	0.5
4.62	597.1449	74977035	M-	C26H29O16+	44	23.8	-2
4.45	595.1664	74978075	M+H	C27H30O15	44	28.8	1.2

12.74	298.1595	75069340	M-H, M+Cl	C19H22O3	36.9	0	8.8
0.9	419.0634	78162875	M+FA-H	C18H14O9	39.3	6.03	3.8
13.31	647.3407	85091334	M+H-2H2O	C35H54O13	48.8	66.4	-2.8
5.97	331.2251	85524814	M+Na	C19H32O3	40	8.56	2.3
9.46	329.2326	85664554	M+FA-H	C17H32O3	53.4	79.9	-2.6
4.93	445.1097	90657201	M+H-H2O	C22H22O11	49	64.6	-7
14.58	428.373	92863445	M+ACN+H	C23H46O4	38.5	0	-1
7.91	701.4206	100914108	M+Na	C38H62O10	39.7	17.2	-4.3
2.94	727.1721	100935400	M-H2O-H	C38H34O16	34.2	0.284	7
5.71	487.3028	100953140	M+H-H2O	C29H44O7	51.3	74.3	-5.2
6.62	191.0707	100955863	M+H-2H2O	C11H14O5	48.8	58.3	1.7
16.13	647.3957	100967916	M-H	C40H56O7	40.2	9.82	0.5
11.21	519.2022	101114357	M+H-H2O	C30H32O9	40.1	12.3	1.6
9.2	553.2072	101114359	M-H	C30H34O10	45.5	35.8	-1.3
6.11	775.2928	101114360	M+CH3OH+H	C41H42O13	36	3.93	-4.3
11.08	783.2627	101114361	M+Na	C41H44O14	46.9	54.9	0.5
15.28	815.5121	101182982	M+CH3OH+H	C42H70O13	40.4	24.6	-3.8
16.83	781.4725	101182983	M+H-H2O	C42H70O14	40.8	11.7	-1
7.23	315.1257	101204053	M-H2O-H	C18H22O6	37.1	10.7	5.5
7.38	472.1761	101204054	M-H2O-H	C28H29NO7	40.5	13.5	-0.9
11.69	473.3625	101248984	M-H2O-H	C30H52O5	37.5	0	-2.2
8.51	647.2345	101262727	M+Na	C36H36N2O8	44.6	45.1	-3.1
5.81	649.3523	101286273	M+H-H2O	C35H54O12	45	61.8	-8.9
9.98	499.3063	101607227	M-H	C30H44O6	43	27.3	-0.5
9.2	425.1839	101836179	M-H	C21H30O9	37.3	0.075	5.2
17.89	541.2249	101836180	M+H-H2O	C26H38O13	48	55.2	-5.5
6.2	233.1531	101928607	M+H	C15H20O2	47.8	46.8	-2.2
9.92	271.0604	102239783	M-H	C15H12O5	43.7	38.2	-3
4.86	209.1165	118110362	M+H-H2O	C12H18O4	39.8	6.46	-3.1
7.18	334.237	118716647	M+H-H2O	C20H33NO4	42.8	27.3	-1.8
4.12	287.0555	118855455	M-H	C15H12O6	40.6	14.2	-2.3
5.11	309.092	122382587	M+Cl	C16H18O4	37.3	2.33	7.8
5.13	635.2303	124222280	M+H-H2O	C31H40O15	41.6	24.8	-4.9
4.43	431.0969	124708157	M-H2O-H	C21H22O11	40.4	12.5	-3.2
5.63	232.0634	129686415	M-	C15H8N2O	38.9	1.06	-3.6
9.19	329.2315	129819530	M+FA-H	C17H32O3	41.2	27	-6.3
16.88	354.2774	129847920	M+H-H2O, M+H, M+Na	C21H38O4	40.6	8.45	1.2

4.51	369.0608	129881889	M+H	C19H12O8	37.5	8.85	0.8
11.21	730.2631	132596278	M+H-H2O, M+Na	C40H42O13	49.7	50.4	0.8
14.66	353.1998	132966232	M-	C22H27NO3	38.2	0	0.5
0.53	689.2107	132990894	M+Na	C24H42O21	48.1	48.5	-0.5
20.19	623.4097	134781708	M+Na	C40H56O4	42.4	33	4.4
4.12	217.0507	135542082	M+H-H2O	C12H10O5	45.1	36	4.8
2.81	246.0881	135596557	M-H2O-H, M-H	C14H14O4	41.8	16	-4.5
2.61	201.1017	136085678	M+H	C12H12N2O	55.6	94.2	-2.9
16	378.1495	137185909	M+CI	C20H25NO4	34.3	0.0898	4.9
6.64	435.126	139031043	M+H	C21H22O10	43.5	32.5	-5.8
2.66	523.0715	154497005	M+FA-H	C21H18O13	50.9	63.3	-3.1
7.91	133.1012	154505258	M+H-2H2O	C10H16O2	46	40.9	0.1
4.86	197.0954	160557896	M+H-2H2O	C14H16O3	46.2	45.3	-2.8
17.99	377.1633	162653491	M-	C23H23NO4	40.2	6.49	0.1
16.81	407.1757	162659502	M-	C24H25NO5	37.6	0.764	4.7
6.68	217.0862	162820576	M+H-2H2O	C13H16O5	40.9	20	1.2
20.97	415.3565	162821381	M+H-H2O	C28H48O3	36.4	0	-1.3
13.42	463.1042	162842866	M+H-2H2O	C18H26O16	36.5	1.13	-8.1
24.69	487.3794	162844792	M+FA-H	C30H50O2	43.2	21.9	0.2
6	530.3326	162847751	M+ACN+H	C26H40N4O5	47.6	45.4	-2.2
3.57	443.0998	162849047	M+H-H2O	C22H20O11	37	3.97	5.5
4.4	465.1028	162851990	M+H	C21H20O12	48.7	46.5	0.1
4.84	344.1253	162853228	M-H, M+FA-H	C19H20O6	38.8	0.973	-1.9
0.57	499.0864	162866484	M-H2O-H	C21H26O13S	33.3	0.536	-10
24.09	467.0998	162882460	M+H-2H2O	C21H26O12S	36.8	0	-1.6
6.5	505.2078	162883937	M-H	C26H34O10	40.9	11.1	-0.3
3.95	469.132	162887298	M+CH3OH+H	C20H20O11	41.1	16	-4.7
5.17	489.1006	162887874	M+Na	C21H22O12	40.7	9.53	0.6
3.27	596.1737	162904343	M+H-2H2O, M+H, M+Na	C27H32O15	41.7	23.5	-0.6
14.97	689.2442	162912427	M+Na	C32H42O15	36.5	3.53	4
4.36	621.1803	162913355	M+H-H2O	C29H34O16	36.3	0.264	-1.7
6.6	507.15	162915878	M-H	C24H28O12	38.6	10	-1.6
5.01	515.0592	162917701	M+CI	C21H20O13	46	49.2	-1.3
6.22	517.2773	162919119	M-H	C29H42O8	40.5	30	-6.5
5.41	489.1031	162933403	M-H	C23H22O12	44	26.8	-1.4
4.47	697.198	162939299	M+FA-H	C30H36O16	37	0.0711	-0.9
21.43	671.3902	162945016	M+Cl	C36H60O9	39.3	12.3	-4.6

5.37	232.1461	162952341	M+H-H2O, M+H	C15H20O2	44.3	33.3	-1
4.6	357.0608	162953603	M+CI	C12H18O10	44.2	35.7	4.2
4.4	159.0442	162957279	M-H2O-H	C10H10O3	44	37.2	-5.5
10.35	679.4059	162957786	M+FA-H	C36H58O9	49.3	66.3	-0.6
10.31	343.2486	162961573	M+FA-H	C18H34O3	45.4	32.5	-1.3
15.29	483.2724	162961650	M-H2O-H	C29H42O7	41	20.9	-5.6
0.51	277.0888	162962930	M+H-2H2O	C18H16O5	40.2	30	9.2
0.55	337.0767	162966990	M-H2O-H	C12H20O12	42.4	24.7	-2.6
23.21	851.4625	162969771	M+Cl	C42H72O15	34.4	0.93	7.4
6.45	476.1933	162971414	M+H-2H2O, M+Na	C21H32O12	37	0.495	8.3
4.55	581.151	162972958	M+H	C26H28O15	40.2	8.56	1.6
6.02	525.3156	162978216	M+Na	C30H46O6	46.9	58.2	-6.1
3.44	375.0689	162985801	M+Cl	C12H20O11	41.7	16	-3.3
5.28	507.1843	162999405	M+H	C25H30O11	38.3	4.15	-3.5
5.87	493.0976	163003716	M+H	C22H20O13	40.8	7.68	-0.2
15.34	522.3552	163004460	M+H-H2O, M+H	C30H50O7	37.2	3.71	-1
21.37	619.4216	163004735	M-H	C36H60O8	42.4	20.3	0.2
4.58	689.2297	163017122	M-H2O-H	C37H40O14	34.4	0.271	8
2.66	496.0859	163020497	M+H-H2O, M+H, M+Na	C21H20O14	42.8	21.6	1.1
6.34	421.1441	163033482	M+CI	C22H26O6	37.8	0.162	4.5
3.37	449.1074	163034124	M+H	C21H20O11	45.3	34.4	-1
13.3	305.2471	163034978	M+H-2H2O	C20H36O4	52.6	71.6	-1.3
3.45	361.0895	163035053	M+Na	C16H18O8	42.4	21	0.4
4.32	613.1767	163040205	M-H	C27H34O16	40.4	6.67	-1.1
3.59	295.1168	163047490	M+CH3OH+H	C14H14O5	39.1	5.92	-3.1
16.73	805.4753	163051559	M+Na	C42H70O13	37.7	11.1	5.7
4.43	577.1554	163051662	M+FA-H	C26H28O12	40.7	18.1	-1.6
1.47	509.0895	163057526	M+FA-H	C21H20O12	46.5	47.8	-9
6.75	627.2282	163062115	M-H2O-H	C36H38O11	32.1	0	7.1
4.86	199.1476	163069155	M+H-2H2O	C15H22O2	46.2	44	-2.4
4.28	477.0676	163106470	M+H-H2O	C21H18O14	41.9	30.5	2.4
2.15	541.0255	163106804	M-H	C21H18O15S	36.5	3.2	-7.1
16.7	555.2783	163189360	M+CI	C30H40N4O4	36.3	0.0557	7.5
21.67	333.2408	163189932	M+Na	C19H34O3	45.2	38.3	2.5
5.77	637.2099	163190248	M+Na	C28H38O15	39.2	4.36	-0.7
4.89	508.2874	163190709	M+Na	C25H43NO8	38.3	16.1	-1.3
19.31	559.2881	163191065	M+Na	C30H40N4O5	39.9	8.44	-1.9

18.45	282.2217	163191530	M+H-2H2O	C20H31NO2	42.7	16.9	0.4
12.65	277.2163	163192296	M+H-H2O	C18H30O3	53.6	75.4	0.4
11.82	259.2059	163192547	M+H-2H2O	C18H30O3	49.9	69.4	1
5.23	489.1032	163193559	M-H	C23H22O12	41.1	18	-1.3
5.79	195.102	163195750	M+FA-H	C10H14O	38.4	8.06	-4.6
17.99	163.1477	163195778	M+H-H2O	C12H20O	48.1	55.4	-2.1
17.46	341.2328	163195811	M+FA-H	C18H32O3	49.5	63.6	-1.9

Supporting Information 6

Fold-change values and statistical significance of molecular features detected in Sida species methanolic extracts. The tables summarizes the results of a comparative untargeted metabolomic analysis performed using MetaboAnalyst 6.0. Fold-change values (log_2 scale) and p-values are reported. Statistical significance was assessed using an unpaired Student's t-test to compare two experimental groups. These results correspond to the data visualized in the volcano plots shown in the main manuscript (Figure 4D-F), and highlight metabolites with differential accumulation between groups.

S. hyssopifolia vs. S. glabra (Fig. 4D)

CID	FC	Log₂(FC)	P value	-LOG ₁₀ (P)
73193	80394	16.295	1.31E-05	4.884
11060391	5977	12.545	4.41E-08	7.3557
163106804	800.1	9.644	1.40E-09	8.853
163106470	736.27	9.5241	0.00054466	3.2639
338	467.9	8.8701	7.19E-08	7.143
44178847	404.78	8.661	0.034385	1.4636
163020497	310.77	8.2797	3.81E-05	4.4195
162887874	271.77	8.0862	2.88E-05	4.5411
25021697	250.42	7.9682	1.03E-06	5.9863
439944	169.68	7.4067	1.45E-07	6.8376
14055737	163.44	7.3526	0.00016677	3.7779
62465	156.71	7.2919	1.16E-06	5.9358
133551	138.24	7.111	1.91E-07	6.719
14187088	104.51	6.7076	9.38E-06	5.0276
45273405	96.427	6.5914	0.02134	1.6708
5491693	95.758	6.5813	1.45E-06	5.8385
44260032	92.351	6.5291	3.08E-05	4.5113
15559735	88.067	6.4605	0.00032868	3.4832
123908	83.113	6.377	9.17E-06	5.0376
5274626	81.274	6.3447	0.00012509	3.9028
100967916	78.413	6.293	3.53E-07	6.4528
107876	72.937	6.1886	5.43E-06	5.2651
12313704	50.442	5.6565	0.00022186	3.6539
75324	49.388	5.6261	2.96E-06	5.5293
5281676	45.824	5.518	0.0002798	3.5531
44566911	41.074	5.3601	6.52E-05	4.1856
348502	35.529	5.1509	5.99E-06	5.2224
73207	35.142	5.1351	0.0013624	2.8657
5487855	34.601	5.1128	0.00028838	3.54
6436348	33.544	5.068	0.00040601	3.3915
5319474	33.427	5.0629	0.00044349	3.3531
65064	33.051	5.0466	0.00015476	3.8103
11250133	31.472	4.976	8.79E-06	5.0559
15560128	28.64	4.84	0.0001286	3.8908
9930500	27.944	4.8045	5.41E-06	5.2668
90657201	27.749	4.7944	0.00028005	3.5528
5281119	26.95	4.7522	0.0097279	2.012
10603919	26.858	4.7473	1.06E-05	4.9728

15767724	25.052	4.6469	0.00054143	3.2665
135596557	23.917	4.58	2.70E-07	6.5683
5281702	22.658	4.5019	0.00019417	3.7118
118855455	22.008	4.46	2.65E-06	5.5769
1203	21.732	4.4417	0.00043667	3.3598
162999405	20.808	4.3791	0.00065134	3.1862
33931	19.422	4.2796	4.07E-05	4.3904
341	15.444	3.949	0.00026235	3.5811
286498	15.4	3.9448	0.00063249	3.1989
162953603	14.244	3.8323	3.72E-06	5.43
22236717	11.962	3.5804	0.0043987	2.3567
124708157	11.183	3.4832	8.63E-08	7.064
13871877	10.72	3.4222	0.00023886	3.6219
5490334	10.719	3.422	0.031064	1.5077
3702506	10.559	3.4003	0.00094194	3.026
19309	10.505	3.393	0.00027119	3.5667
154497005	10.299	3.3644	0.0003147	3.5021
163189360	9.8783	3.3043	0.014322	1.844
638014	9.313	3.2192	0.0029353	2.5324
1742210	7.7304	2.9505	0.00039119	3.4076
126	7.1204	2.832	0.0020033	2.6983
101607227	6.8459	2.7752	1.13E-05	4.9469
162957786	6.5559	2.7128	4.44E-06	5.3525
107905	6.3594	2.6689	2.05E-06	5.6881
24796850	6.1334	2.6167	1.04E-06	5.9826
101248984	6.0456	2.5959	1.09E-06	5.9644
11167374	5.8725	2.554	9.84E-07	6.0072
2371	5.817	2.5403	1.04E-06	5.9814
114776	5.7924	2.5342	8.09E-06	5.092
10494	5.758	2.5256	2.80E-07	6.553
5316673	5.6377	2.4951	2.95E-05	4.5308
162883937	5.4638	2.4499	4.75E-06	5.3232
162915878	4.2369	2.083	0.000938	3.0278
5281607	4.1712	2.0605	0.00047632	3.3221
44258591	3.6936	1.885	5.25E-05	4.2798
5280637	3.2579	1.704	0.00056255	3.2498
10308838	3.1258	1.6442	0.00015451	3.811
11276243	2.7652	1.4674	0.042787	1.3687
162917701	2.5688	1.3611	9.80E-06	5.009
162350	2.5132	1.3295	0.0013903	2.8569
163193559	2.3797	1.2508	0.00086085	3.0651
14707301	2.3417	1.2276	0.012535	1.9019
5280460	2.0454	1.0324	0.0056573	2.2474
439242	2.0175	1.0126	0.022662	1.6447
444539	0.48124	-1.0552	0.010674	1.9717
11354754	0.40975	-1.2872	0.04377	1.3588
1110	0.40564	-1.3017	0.00464	2.3335
5281321	0.34938	-1.5171	0.012233	1.9125
0201021	J.0-300	1.01,1	0.012200	1.5125

14704521	0.32618	-1.6163	0.021979	1.658
14311156	0.32274	-1.6316	0.029739	1.5267
5280443	0.31911	-1.6479	0.021737	1.6628
10723382	0.31041	-1.6877	0.048878	1.3109
132966232	0.29446	-1.7639	0.00036217	3.4411
447791	0.29193	-1.7763	0.0059346	2.2266
311	0.27761	-1.8488	2.66E-05	4.5759
162659502	0.26148	-1.9352	2.47E-05	4.6069
5793	0.25582	-1.9668	0.0055313	2.2572
21881649	0.24569	-2.0251	0.0055978	2.252
439341	0.22847	-2.1299	0.0053254	2.2736
5099	0.22366	-2.1606	0.0001203	3.9197
101536	0.2177	-2.1996	0.014123	1.8501
10400	0.19326	-2.3714	0.02967	1.5277
179	0.18888	-2.4045	0.0051817	2.2855
7438	0.18459	-2.4376	0.035499	1.4498
6441104	0.18118	-2.4645	4.22E-08	7.3752
8299	0.18117	-2.4646	0.030534	1.5152
440735	0.17157	-2.5431	3.90E-06	5.4088
163195811	0.16929	-2.5624	0.00048125	3.3176
163191530	0.16866	-2.5679	0.016943	1.771
162933403	0.15925	-2.6506	0.000154	3.8125
163034124	0.15756	-2.6661	0.027136	1.5665
3314	0.15724	-2.6689	4.41E-05	4.3551
5280379	0.15721	-2.6692	9.92E-06	5.0033
441644	0.15719	-2.6694	0.024733	1.6067
163062115	0.15592	-2.6811	0.0010371	2.9842
75069340	0.15522	-2.6876	0.00017186	3.7648
5281601	0.1548	-2.6916	5.14E-05	4.2892
632128	0.15356	-2.7031	0.00015846	3.8001
14332450	0.15231	-2.7149	1.89E-05	4.7228
82143	0.15163	-2.7213	2.48E-05	4.6053
23815394	0.15022	-2.7348	0.012395	1.9068
101182983	0.14898	-2.7468	0.0071499	2.1457
5281	0.14692	-2.7669	0.002712	2.5667
10015552	0.14692	-2.7669	0.0041332	2.3837
162919119	0.14564	-2.7795	6.77E-05	4.1695
10439806	0.14467	-2.7892	0.0017347	2.7608
163195750	0.14273	-2.8086	2.23E-05	4.6522
10582	0.13769	-2.8605	0.00021453	3.6685
44631546	0.13703	-2.8674	0.00048819	3.3114
7302	0.13578	-2.8807	0.0003892	3.4098
12097	0.13505	-2.8884	0.044215	1.3544
163004735	0.1348	-2.8911	0.017758	1.7506
163033482	0.13336	-2.9066	0.005108	2.2917
322	0.13287	-2.9119	0.0022261	2.6525
5988	0.1327	-2.9138	8.13E-05	4.0902
163017122	0.132	-2.9214	0.00035537	3.4493
7156991	0.13168	-2.9249	0.027396	1.5623

100953140	0.12888	-2.9559	0.00044228	3.3543
258412	0.12743	-2.9722	0.00059181	3.2278
5274621	0.12678	-2.9796	0.00066131	3.1796
102239783	0.12503	-2.9997	0.0003423	3.4656
21763831	0.12482	-3.002	0.0020993	2.6779
8103	0.12373	-3.0147	0.024907	1.6037
163069155	0.12355	-3.0168	0.0031826	2.4972
128853	0.12298	-3.0235	0.00027025	3.5682
5459840	0.12296	-3.0237	0.00073862	3.1316
14376672	0.12239	-3.0304	0.00092948	3.0318
11276313	0.12115	-3.0451	0.00010032	3.9986
7966	0.12064	-3.0512	0.0061752	2.2094
10813969	0.12062	-3.0515	1.27E-06	5.896
5320686	0.11678	-3.0981	0.001706	2.768
14296	0.11646	-3.102	0.005751	2.2403
10630882	0.11376	-3.1359	0.00026266	3.5806
5951	0.11369	-3.1368	5.36E-05	4.271
31265	0.11286	-3.1473	0.0029872	2.5247
441833	0.11166	-3.1628	0.0020052	2.6978
5280536	0.11165	-3.1629	0.00025395	3.5953
7237	0.11148	-3.1651	0.047863	1.32
442396	0.10977	-3.1875	0.00031478	3.502
101204053	0.10966	-3.1889	0.00045455	3.3424
102430	0.10902	-3.1973	0.00236	2.6271
72730315	0.109	-3.1975	0.0019571	2.7084
5460372	0.10877	-3.2007	0.0041701	2.3799
440835	0.10852	-3.204	0.0020857	2.6807
73323377	0.10845	-3.2049	0.0027026	2.5682
44577733	0.1068	-3.227	0.0053027	2.2755
44552030	0.10664	-3.2292	8.92E-05	4.0495
65373	0.10653	-3.2306	0.0030892	2.5102
12799212	0.10637	-3.2328	0.001834	2.7366
540124	0.10619	-3.2352	0.0014895	2.827
7017	0.10605	-3.2371	0.0063743	2.1956
12020	0.10504	-3.251	0.0022271	2.6523
139031043	0.10418	-3.2629	0.0043709	2.3594
14079	0.10381	-3.268	0.001985	2.7022
13915427	0.10289	-3.2808	0.00036749	3.4348
11277992	0.10242	-3.2875	0.0073741	2.1323
162945016	0.10223	-3.2902	0.0026741	2.5728
181681	0.102	-3.2934	0.0053872	2.2686
125213	0.10161	-3.2989	0.0032241	2.4916
178034	0.10149	-3.3005	0.0026297	2.5801
5960	0.10124	-3.3042	0.0011858	2.926
263	0.1007	-3.3119	0.017644	1.7534
6029	0.098814	-3.3391	0.0023452	2.6298
446066	0.098448	-3.3445	0.00085233	3.0694
10393	0.098403	-3.3452	0.0061819	2.2089
10582821	0.09813	-3.3492	0.0060833	2.2159

31242	0.098032	-3.3506	0.0061984	2.2077
162847751	0.097936	-3.352	0.0034324	2.4644
10256	0.097704	-3.3554	0.00087373	3.0586
525	0.097558	-3.3576	0.0034402	2.4634
5320254	0.097305	-3.3613	0.005574	2.2538
10743	0.09688	-3.3677	0.0031514	2.5015
57172986	0.09686	-3.368	0.0064532	2.1902
119205	0.096674	-3.3707	0.0082171	2.0853
440265	0.0966	-3.3718	0.0027494	2.5608
1249	0.095082	-3.3947	0.004868	2.3127
5281612	0.094835	-3.3984	0.0034425	2.4631
162952341	0.094509	-3.4034	0.006099	2.2147
9978316	0.094286	-3.4068	0.0058485	2.233
26339717	0.093023	-3.4263	5.49E-05	4.2601
5280953	0.092974	-3.427	0.0038172	2.4183
24796851	0.091477	-3.4504	0.0026344	2.5793
5280442	0.091077	-3.4568	0.0067316	2.1719
7362	0.091026	-3.4576	0.023799	1.6234
154505258	0.09075	-3.462	0.0064634	2.1895
5281984	0.090487	-3.4662	0.0034783	2.4586
101262727	0.090293	-3.4692	0.0080365	2.0949
10652163	0.09002	-3.4736	0.0068365	2.1652
439246	0.089617	-3.4801	0.0078086	2.1074
49831491	0.089346	-3.4845	0.0052053	2.2836
92863445	0.089089	-3.4886	0.024891	1.604
636576	0.088341	-3.5008	0.00080531	3.094
5318717	0.088178	-3.5034	0.0046616	2.3315
13988634	0.087816	-3.5094	0.0019941	2.7003
375713	0.087782	-3.5099	0.0035788	2.4463
12305415	0.087384	-3.5165	0.0052266	2.2818
163003716	0.087083	-3.5215	0.0047898	2.3197
10922890	0.086354	-3.5336	0.0027903	2.5543
100332	0.085934	-3.5406	0.003953	2.4031
42608087	0.085826	-3.5424	0.0029651	2.528
73172655	0.085471	-3.5484	0.0087349	2.0587
74978075	0.085237	-3.5524	0.006541	2.1844
129881889	0.084413	-3.5664	0.0048035	2.3184
85524814	0.084346	-3.5675	0.0059782	2.2234
118110362	0.082266	-3.6036	0.0028843	2.54
16900	0.082115	-3.6062	0.00096634	3.0149
11194416	0.082054	-3.6073	0.0013044	2.8846
25310	0.081055	-3.625	0.010254	1.9891
10187514	0.080797	-3.6296	0.0051024	2.2922
11072668	0.079857	-3.6464	0.016581	1.7804
21722016	0.079745	-3.6485	0.00024955	3.6028
636543	0.079487	-3.6531	0.0091921	2.0366
637239	0.079023	-3.6616	3.57E-05	4.4479
12088	0.078794	-3.6658	0.0012598	2.8997
14340	0.07878	-3.666	0.016731	1.7765

13849	0.078257	-3.6756	0.00046262	3.3348
155022	0.077501	-3.6896	0.0045841	2.3387
10413856	0.077443	-3.6907	9.82E-05	4.008
162849047	0.07735	-3.6925	0.0061133	2.2137
16275	0.076727	-3.7041	0.0010097	2.9958
49831493	0.076674	-3.7051	0.0086026	2.0654
7478	0.076471	-3.7089	0.01691	1.7719
12580	0.075136	-3.7343	0.0086633	2.0623
118716647	0.075062	-3.7358	0.0078806	2.1034
17166	0.074837	-3.7401	0.0011168	2.952
10969116	0.074648	-3.7438	0.011072	1.9558
107557	0.073526	-3.7656	0.0079049	2.1021
163190709	0.073189	-3.7722	0.0055048	2.2593
101114361	0.072324	-3.7894	0.009477	2.0233
5317025	0.072259	-3.7907	0.0012739	2.8949
129847920	0.070616	-3.8239	0.0022303	2.6516
384679	0.070456	-3.8271	0.0072691	2.1385
6057	0.068874	-3.8599	0.010049	1.9979
85091334	0.068603	-3.8656	0.01022	1.9905
133372	0.066082	-3.9196	0.00012952	3.8877
44578390	0.06607	-3.9199	0.018763	1.7267
135542082	0.065775	-3.9263	0.011285	1.9475
162842866	0.064273	-3.9596	0.023935	1.621
129819530	0.063452	-3.9782	0.00020563	3.6869
54355075	0.062009	-4.0114	4.62E-05	4.3358
2214	0.061522	-4.0228	0.01066	1.9723
163047490	0.061414	-4.0253	0.010995	1.9588
539381	0.060607	-4.0444	0.00078657	3.1043
72730313	0.060109	-4.0563	0.014702	1.8326
44566588	0.058512	-4.0951	1.42E-05	4.8484
162978216	0.058388	-4.0982	0.019708	1.7054
5281578	0.058182	-4.1033	0.01231	1.9098
28619	0.058038	-4.1069	0.0070209	2.1536
163195778	0.05802	-4.1073	0.0038957	2.4094
163191065	0.056498	-4.1457	0.0040584	2.3916
162961573	0.055681	-4.1667	2.97E-05	4.5276
520684	0.055439	-4.173	0.0054341	2.2649
49842399	0.05528	-4.1771	0.013831	1.8592
163190248	0.053699	-4.219	0.0064824	2.1883
10262028	0.05369	-4.2192	0.010579	1.9756
2682	0.053549	-4.223	0.029055	1.5368
13918554	0.052433	-4.2534	0.015339	1.8142
100151	0.050549	-4.3062	0.0065944	2.1808
101286273	0.050389	-4.3108	0.011704	1.9317
441765	0.050085	-4.3195	0.0092804	2.0324
162985801	0.04955	-4.335	1.46E-05	4.8355
71438848	0.049352	-4.3407	0.0036782	2.4344
135191	0.048809	-4.3567	5.12E-05	4.2906
1174	0.048276	-4.3725	0.0073082	2.1362

996	0.048149	-4.3764	0.015747	1.8028
479957	0.047972	-4.3817	0.004877	2.3118
72751004	0.047378	-4.3996	0.015297	1.8154
8130	0.046304	-4.4327	0.0020068	2.6975
35698	0.04565	-4.4532	0.014261	1.8459
78603	0.045336	-4.4632	0.0051169	2.291
119216	0.045052	-4.4723	0.0079257	2.101
10720349	0.044163	-4.501	3.53E-05	4.4524
11953803	0.043793	-4.5132	0.0040194	2.3958
518900	0.043674	-4.5171	0.019391	1.7124
328066	0.043454	-4.5244	0.024299	1.6144
163051662	0.042789	-4.5466	0.00066198	3.1792
1549095	0.041807	-4.5801	0.016809	1.7745
5281416	0.041478	-4.5915	0.0085837	2.0663
11079623	0.040814	-4.6148	0.033093	1.4803
101836179	0.04019	-4.637	0.0032309	2.4907
101836180	0.039263	-4.6707	0.00066072	3.18
13250	0.038938	-4.6827	0.00015423	3.8118
6973640	0.038625	-4.6943	0.0022642	2.6451
7967	0.038607	-4.695	0.023247	1.6336
14887603	0.038394	-4.703	0.00061505	3.2111
24982202	0.037822	-4.7246	5.09E-05	4.2931
442101	0.037671	-4.7304	0.00011288	3.9474
190	0.037311	-4.7442	0.0016633	2.779
1183	0.03723	-4.7474	0.00012826	3.8919
78162875	0.037069	-4.7536	0.00099583	3.0018
1711945	0.036772	-4.7653	0.0024923	2.6034
1140	0.036302	-4.7838	0.015275	1.816
71403936	0.035876	-4.8009	0.0035251	2.4528
525578	0.035613	-4.8114	0.010678	1.9715
3015413	0.035462	-4.8176	0.0063243	2.199
163057526	0.034983	-4.8372	0.0064505	2.1904
8417	0.034743	-4.8471	0.0073193	2.1355
32033	0.0344	-4.8614	2.62E-05	4.5813
6274	0.034288	-4.8662	0.00040086	3.397
23642717	0.033475	-4.9008	0.00015074	3.8218
10680	0.032908	-4.9254	2.79E-05	4.5548
156741	0.032893	-4.9261	0.028932	1.5386
3931	0.032489	-4.9439	0.00031975	3.4952
5570	0.032482	-4.9442	7.40E-05	4.1306
124222280	0.032449	-4.9457	0.035617	1.4483
34645	0.03186	-4.9721	0.011631	1.9344
23658567	0.031186	-5.003	0.00020618	3.6858
5320006	0.031107	-5.0066	6.56E-05	4.183
373912	0.030911	-5.0157	0.0037962	2.4207
10465398	0.030515	-5.0343	0.0015414	2.8121
5281115	0.030507	-5.0347	0.00068436	3.1647
3083616	0.030475	-5.0362	0.008919	2.0497
100914108	0.029939	-5.0618	0.0078016	2.1078

6054	0.029628	-5.0769	0.010282	1.9879
53429614	0.029294	-5.0932	0.0042917	2.3674
107526	0.02865	-5.1253	2.23E-06	5.652
5280647	0.027949	-5.161	1.07E-06	5.9701
5429	0.027349	-5.1924	0.010572	1.9758
12756	0.027344	-5.1926	0.0018378	2.7357
163051559	0.027268	-5.1967	0.00045234	3.3445
117769	0.026895	-5.2165	0.021322	1.6712
165559	0.026836	-5.2197	0.00057883	3.2374
2723872	0.026462	-5.24	5.71E-05	4.2437
74977035	0.026368	-5.2451	1.73E-05	4.7623
10508776	0.026303	-5.2486	4.67E-05	4.3308
54005211	0.024076	-5.3763	0.012405	1.9064
162851990	0.023994	-5.3812	0.00075585	3.1216
6450144	0.023812	-5.3922	0.0019973	2.6996
100955863	0.023575	-5.4066	0.033113	1.48
186775	0.022805	-5.4545	1.42E-05	4.8463
538953	0.022511	-5.4732	0.013042	1.8846
14681438	0.022345	-5.4839	0.00054978	3.2598
22238	0.02219	-5.4939	0.028982	1.5379
100935400	0.022066	-5.5021	8.56E-05	4.0677
1549026	0.022022	-5.5049	0.00074685	3.1268
7500	0.021835	-5.5172	0.00063143	3.1997
160510	0.02114	-5.5639	0.011298	1.947
441574	0.020759	-5.5901	1.45E-05	4.8385
13197868	0.020324	-5.6207	0.0016123	2.7926
5460657	0.018732	-5.7383	0.04154	1.3815
5318761	0.018628	-5.7464	6.68E-06	5.1749
162653491	0.018016	-5.7946	5.31E-06	5.2751
7654	0.017655	-5.8238	0.0050274	2.2987
92794	0.017245	-5.8577	0.00017796	3.7497
163040205	0.017067	-5.8727	7.20E-06	5.143
637139	0.016613	-5.9115	1.63E-05	4.7883
11227946	0.016025	-5.9635	0.00020388	3.6906
231324	0.014948	-6.0639	0.023548	1.628
28516	0.01491	-6.0676	0.0024777	2.6059
14035324	0.013761	-6.1833	5.08E-06	5.2942
522636	0.013684	-6.1914	0.016831	1.7739
193484	0.013336	-6.2285	6.40E-06	5.194
8180	0.013155	-6.2482	0.0018434	2.7344
5468749	0.012929	-6.2732	3.84E-06	5.4161
137185909	0.012804	-6.2873	0.0011154	2.9526
576026	0.012364	-6.3377	0.029799	1.5258
60961	0.011944	-6.3876	0.00095351	3.0207
163192296	0.01189	-6.3941	0.0005632	3.2493
5280863	0.011129	-6.4896	0.00045061	3.3462
21579640	0.010434	-6.5826	0.0012207	2.9134
46181828	0.010153	-6.622	1.82E-06	5.7407
10255859	0.010097	-6.6299	0.00079945	3.0972

5281128	0.0092451	-6.7571	0.0010771	2.9677
12681283	0.0092183	-6.7613	6.59E-05	4.1812
10912308	0.0092012	-6.764	5.35E-06	5.2713
1548883	0.0089699	-6.8007	0.027718	1.5572
162904343	0.0087733	-6.8327	0.0017628	2.7538
5466138	0.0087418	-6.8378	1.81E-05	4.7428
163034978	0.0086929	-6.8459	0.0044909	2.3477
71359328	0.0084269	-6.8908	0.00055698	3.2542
11142	0.0083699	-6.9006	0.00018828	3.7252
162972958	0.0082344	-6.9241	0.00038049	3.4197
101928607	0.008049	-6.957	0.00029967	3.5234
6185	0.0075424	-7.0508	0.00034325	3.4644
5280607	0.0074821	-7.0623	1.74E-05	4.7591
5488575	0.0074054	-7.0772	0.00040437	3.3932
546377	0.0071776	-7.1223	2.02E-05	4.6943
132596278	0.0071226	-7.1334	0.00010701	3.9706
3084131	0.0070948	-7.139	0.00011801	3.9281
14311160	0.0068268	-7.1946	1.57E-06	5.8039
162844792	0.0065618	-7.2517	0.049719	1.3035
6287	0.0062967	-7.3112	0.0010587	2.9752
101182982	0.0062016	-7.3331	0.00067913	3.168
14311167	0.0058115	-7.4269	5.31E-07	6.2751
44552029	0.0057888	-7.4325	0.00078751	3.1037
162971414	0.0056754	-7.4611	0.00019425	3.7116
75142	0.0055345	-7.4973	1.35E-05	4.8703
5283446	0.005515	-7.5024	0.0011857	2.926
3469	0.0052193	-7.5819	0.00042133	3.3754
10252339	0.0051173	-7.6104	0.00030077	3.5218
122382587	0.0047155	-7.7284	1.74E-05	4.759
10538510	0.004639	-7.752	0.0033746	2.4718
73821792	0.0044772	-7.8032	0.0010715	2.97
3503	0.0042271	-7.8861	2.29E-06	5.6393
135	0.0042136	-7.8907	0.00075416	3.1225
44559173	0.0041078	-7.9274	0.0008749	3.058
5280445	0.0039725	-7.9758	6.56E-06	5.1829
1551480	0.0038813	-8.0093	6.94E-05	4.1589
101114360	0.003777	-8.0485	0.00014302	3.8446
162853228	0.0036607	-8.0937	3.27E-05	4.4859
162939299	0.0034217	-8.1911	3.13E-05	4.5046
16077448	0.0030485	-8.3577	0.0022994	2.6384
608115	0.002916	-8.4218	0.00015502	3.8096
5320834	0.0027199	-8.5222	0.00013249	3.8778
53420248	0.0022087	-8.8226	0.0001236	3.908
23485	0.0021276	-8.8765	7.00E-05	4.1546
14484636	0.0020584	-8.9243	9.59E-05	4.0181
160557896	0.0017033	-9.1974	0.00018759	3.7268
10371536	0.0016475	-9.2455	9.99E-05	4.0006
10815866	0.0016195	-9.2703	8.53E-06	5.069
11623832	0.0014752	-9.4049	7.17E-05	4.1445

5280343	0.0013061	-9.5806	0.00012432	3.9055
101114357	0.0011011	-9.8268	0.00034243	3.4654
162887298	0.001021	-9.9357	7.43E-05	4.1292
129686415	0.00096328	-10.02	2.49E-07	6.6042
11464176	0.00095422	-10.033	0.00011782	3.9288
5281647	0.00094583	-10.046	0.00055582	3.2551
10472650	0.00092743	-10.074	0.00029477	3.5305
94225	0.00082883	-10.237	0.00070706	3.1505
13245586	0.00080918	-10.271	0.0010282	2.9879
49831447	0.00052884	-10.885	2.97E-06	5.5272
72732	0.00037684	-11.374	4.32E-06	5.3646
441772	0.00035261	-11.47	5.38E-06	5.2693
101204054	0.00031747	-11.621	2.96E-05	4.5291
11061627	0.00031046	-11.653	4.20E-06	5.3772
10176654	0.00018563	-12.395	0.00017515	3.7566
21742	9.60E-05	-13.346	0.047284	1.3253
101114359	6.14E-05	-13.99	2.84E-06	5.5467
10105245	3.83E-05	-14.674	0.0011851	2.9262
19212	3.69E-05	-14.726	7.25E-05	4.1395
10748	2.49E-05	-15.295	0.00053576	3.271
10403282	1.05E-05	-16.545	2.93E-07	6.5329

S. hyssopifolia vs. S. rhombifolia (Fig. 4E)

CID	FC	Log₂(FC)	P value	-LOG ₁₀ (P)
21722016	314180	18.261	0.0000334	4.4768
135596557	12779	13.641	5.59E-10	9.2525
163106804	3554.3	11.795	0.0000000293	8.5329
11060391	2072.6	11.017	0.00000315	6.5019
338	1049.4	10.035	0.0000000464	8.3336
348502	931.4	9.8633	0.000000288	7.5411
162953603	621.93	9.2806	0.000000305	7.5152
15560128	557.64	9.1232	0.0000144	4.8428
439944	534.36	9.0617	7.28E-10	9.138
45273405	363.86	8.5072	0.021165	1.6744
12313704	348.13	8.4435	0.00013779	3.8608
5491693	262.24	8.0347	0.00000141	6.8518
133551	257.36	8.0077	0.000000535	7.2713
25021697	241.72	7.9172	0.00000249	5.6043
100967916	197.87	7.6284	0.00000341	6.4671
5280460	177.15	7.4688	0.00000183	6.7371
90657201	170.61	7.4146	0.00000285	5.5455
100935400	167.79	7.3906	0.0006721	3.1726
139711	153.42	7.2614	0.0010001	3
162999405	152.57	7.2534	0.00018328	3.7369
13871877	136.04	7.0878	0.0000128	4.8931
11276243	115.16	6.8475	0.00000175	6.7565
10023166	111.9	6.806	0.0080542	2.094
10394	94.119	6.5564	0.00010584	3.9754
123908	81.558	6.3498	0.0000233	4.6329
10603919	76.824	6.2635	0.0000952	5.0215
286498	75.74	6.243	0.00024444	3.6118
5316673	75.688	6.242	0.000000599	7.2223

5274626	72.024	6.1704	0.00019407	3.712
5280443	70.878	6.1473	0.0034379	2.4637
5281607	67.956	6.0865	0.0000139	5.8556
114776	65.447	6.0323	0.00000315	6.5015
5281614	60.026	5.9075	0.0006417	3.1927
162915878	52.935	5.7262	0.0000154	4.8133
132990894	52.176	5.7053	0.00076496	3.1164
44258591	48.518	5.6004	0.0000408	5.3888
5386960	48.176	5.5902	0.0038392	2.4158
15767724	45.465	5.5067	0.00032116	3.4933
5315831	43.834	5.454	0.0000362	4.4418
163034124	34.414	5.1049	0.023758	1.6242
124708157	29.555	4.8853	0.00000201	6.6965
162985801	27.306	4.7711	0.0017169	2.7653
163193559	27.064	4.7583	0.0000138	4.8611
5281119	26.95	4.7522	0.017992	1.7449
71567	25.72	4.6848	0.00013804	3.86
163106470	25.345	4.6636	0.0048203	2.3169
163189360	24.328	4.6046	0.0068932	2.1616
15294	22.953	4.5206	0.0055481	2.2559
9930500	22.865	4.5151	0.0000588	5.2308
44566588	22.622	4.4996	0.00026936	3.5697
107905	22.017	4.4605	0.0000103	5.9855
240	20.338	4.3461	0.0000358	4.4459
14887607	19.485	4.2843	0.010842	1.9649
5490334	17.136	4.099	0.019554	1.7088
15289454	16.256	4.0229	0.0010984	2.9592
162883937	15.987	3.9988	0.0000099	5.0043
5280637	15.641	3.9673	0.0000386	4.4138
439242	15.299	3.9353	0.00000391	6.4073
10308838	14.153	3.823	0.0000646	5.1895
162350	13.811	3.7878	0.0000145	4.8401
4486984	12.701	3.6669	0.0069157	2.1602
14055737	12.564	3.6512	0.0022593	2.646
73207	12.264	3.6164	0.0066013	2.1804
638014	12.218	3.6109	0.0016708	2.7771
22236717	11.962	3.5804	0.010111	1.9952
15559735	11.486	3.5218	0.003541	2.4509
14332450	11.291	3.4971	0.0017636	2.7536
5487855	11.158	3.4801	0.00124	2.9066
6436348	10.545	3.3985	0.0021524	2.6671
5319474	10.184	3.3482	0.0018247	2.7388
440833	9.7112	3.2797	0.00085401	3.0685
441667	9.4332	3.2377	0.0026552	2.5759
163020497	9.378	3.2293	0.00080454	3.0945
44178847	9.3572	3.2261	0.048902	1.3107
1794427	9.3535	3.2255	0.00086004	3.0655
49842399	9.1791	3.1984	0.049143	1.3085
162851990	8.9201	3.1571	0.0001979	3.7036
162887874	8.7622	3.1313	0.000584	3.2336
65064	8.7232	3.1249	0.00082017	3.0861
14311156	8.7124	3.1231	0.00061389	3.2119
5281426	8.6598	3.1143	0.00064469	3.1907
44566911	8.4075	3.0717	0.00038815	3.411
73193	8.3718	3.0655	0.0011935	2.9232
5281702	7.9874	2.9977	0.00020049	3.6979
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5281676	7.7743	2.9587	0.00026681	3.5738
341	7.7561	2.9553	0.00014991	3.8242
44260032	7.7507	2.9543	0.00017201	3.7644
1742210	7.7304	2.9505	0.00086954	3.0607
74977035	7.5889	2.9239	0.0061986	2.2077
1203	7.578	2.9218	0.00032726	3.4851
126	7.5744	2.9211	0.00037848	3.422
370	7.4157	2.8906	0.0000644	4.1913
3702506	6.9028	2.7872	0.0000888	4.0514
10439806	6.8981	2.7862	0.00013152	3.881
101607227	6.8459	2.7752	0.0000238	4.624
162933403	6.6268	2.7283	0.00012584	3.9002
14887605	6.6074	2.7241	0.0016517	2.7821
162917701	6.5927	2.7209	0.00000225	5.6485
162957786	6.5559	2.7128	0.00000919	5.0366
19309	6.526	2.7062	0.00006919	3.7785
14187088	6.4561	2.6907	0.00016033	4.2049
165559	6.3634	2.6698	0.005206	1.5985
	6.1652			
75324 62465	6.1652	2.6242 2.6177	0.0000564 0.0000212	5.2489 4.6747
		-		
24796850	6.1334	2.6167	0.00000215	5.6674
154497005	6.0469	2.5962	0.00000186	5.7305
101248984	6.0456	2.5959	0.00000228	5.643
11167374	5.8725	2.554	0.00000211	5.6753
2371	5.817	2.5403	0.00000222	5.6533
10494	5.758	2.5256	0.00000592	6.228
11250133	5.6143	2.4891	0.00000166	6.7802
33931	5.5866	2.482	0.00000676	6.1703
107876	5.5062	2.461	0.00000177	6.7512
10813969	5.4329	2.4417	0.0000291	4.5355
118855455	5.3342	2.4153	0.000000989	7.005
19844	5.3157	2.4103	0.0011032	2.9573
163035053	5.0795	2.3447	0.029152	1.5353
14887603	4.6085	2.2043	0.012847	1.8912
442396	4.222	2.0779	0.029802	1.5258
14707301	3.9196	1.9707	0.00053684	3.2702
162966990	3.9085	1.9666	0.0000159	4.7997
69634125	3.6948	1.8855	0.030489	1.5159
5099	3.4074	1.7687	0.0042409	2.3725
5280647	3.0577	1.6124	0.028167	1.5503
14704521	2.3345	1.2231	0.010371	1.9842
75069340	0.45565	-1.134	0.013495	1.8698
162961650	0.43749	-1.1927	0.015017	1.8234
1110	0.42348	-1.2396	0.003674	2.4349
10015552	0.34335	-1.5422	0.024059	1.6187
163191530	0.31156	-1.6824	0.034832	1.458
5318761	0.28692	-1.8013	0.0052769	2.2776
16093748	0.27188	-1.8789	0.020252	1.6935
57006309	0.25774	-1.956	0.014054	1.8522
7966	0.25427	-1.9756	0.024339	1.6137
322	0.25271	-1.9844	0.017112	1.7667
7146	0.23798	-2.0711	0.024459	1.6116
444899	0.23712	-2.0763	0.03528	1.4525
162659502	0.23689	-2.0777	0.0000761	4.1184
163195811	0.23211	-2.1071	0.0090732	2.0422
14296	0.22532	-2.1499	0.0032517	2.4879
•	•	•	•	

23815394	0.22183	-2.1725	0.03186	1.4967
7362	0.21458	-2.2204	0.017332	1.7611
24796851	0.21141	-2.2419	0.029905	1.5243
10400	0.2107	-2.2468	0.026758	1.5725
10416	0.20578	-2.2808	0.048095	1.3179
5280442	0.19532	-2.3561	0.035239	1.453
112720	0.19226	-2.3789	0.021348	ID
100332	0.19195	-2.3812	0.0059599	21722016
101536	0.19076	-2.3902	0.0024964	135596557
5280863	0.18815	-2.4101	0.018833	163106804
5281	0.18669	-2.4213	0.00021932	11060391
101928607	0.17914	-2.4808	0.023044	338
13250	0.17258	-2.5347	0.0050644	348502
101836179	0.16181	-2.6276	0.0000883	162953603
155022	0.16149	-2.6305	0.029341	15560128
12020	0.16072	-2.6374	0.0000312	439944
5429	0.15597	-2.6807	0.035186	45273405
100953140	0.15149	-2.7227	0.045776	12313704
258412	0.14975	-2.7393	0.0001307	5491693
163189932	0.14707	-2.7654	0.018814	133551
82143	0.14597	-2.7763	0.00014358	25021697
5459840	0.14596	-2.7764	0.00033916	100967916
162962930	0.14178	-2.8183	0.0011526	5280460
162961573	0.14145	-2.8217	0.0018717	90657201
14376672	0.14054	-2.831	0.00034424	100935400
10582	0.13733	-2.8643	0.0012961	139711
133372	0.13729	-2.8647	0.0023507	162999405
231324	0.13656	-2.8723	0.00056048	13871877
163004735	0.13468	-2.8924	0.0000416	11276243
10723382	0.13057	-2.9371	0.0012625	10023166
11276313	0.12958	-2.948	0.00091474	10394
21763831	0.12915	-2.9529	0.00032827	123908
162919119	0.12802	-2.9655	0.00099388	10603919
520684	0.12743	-2.9722	0.0019361	286498
72730315	0.12717	-2.9751	0.0026037	5316673
576026	0.12668	-2.9808	0.0026965	5274626
162945016	0.12666	-2.9809	0.0014476	5280443
12303930	0.12661	-2.9816	0.0013014	5281607
193484	0.12646	-2.9832	0.00074555	114776
139031043	0.12442	-3.0067	0.0084323	5281614
5320686	0.12119	-3.0447	0.0029517	162915878
6029	0.12111	-3.0456	0.0020469	132990894
637239	0.11897	-3.0714	0.0000431	44258591
21881649	0.1177	-3.0868	0.0031411	5386960
178034	0.11631	-3.104	0.0019902	15767724
163191065	0.11518	-3.118	0.0037064	5315831
5488575	0.11443	-3.1274	0.012506	163034124
118110362	0.11354	-3.1387	0.0017768	124708157
101836180	0.11056	-3.1771	0.0061151	162985801
31265	0.10844	-3.205	0.00616	163193559
5988	0.10755	-3.217	0.0032333	5281119
5280343	0.10705	-3.2236	0.0033422	71567
6734	0.1068	-3.2269	0.0052066	163106470
8130	0.10305	-3.2786	0.0002418	163189360
162912427	0.10299	-3.2795	0.0080256	15294
14311160	0.10272	-3.2832	0.00067698	9930500
	1 0.202.2	1 0.2002	1 2.0000.000	1 333333

5960	0.099659	-3.3269	0.0013617	44566588
1054	0.096347	-3.3756	0.0030006	107905
440735	0.094633	-3.4015	0.0013062	240
32033	0.093479	-3.4192	0.041936	14887607
16900	0.093461	-3.4195	0.00012557	5490334
34645	0.092192	-3.4392	0.0074469	15289454
5280953	0.091176	-3.4552	0.0062763	162883937
16275	0.089599	-3.4804	0.00010857	5280637
540124	0.089477	-3.4823	0.0020272	439242
3084463	0.088569	-3.4971	0.0033943	10308838
160510	0.086376	-3.5332	0.0249	162350
117769	0.084468	-3.5654	0.0043002	4486984
92794	0.084352	-3.5674	0.015851	14055737
539381	0.083672	-3.5791	0.0084698	73207
54355075	0.083663	-3.5793	0.0004030	638014
5280934	0.080306	-3.6384	0.0030859	22236717
5951	0.076445	-3.7094	0.0030839	15559735
71438848	0.076316	-3.7119	0.01616	14332450
5281984	0.076308	-3.712	0.0067075	5487855
53429614	0.074784	-3.7411	0.035989	6436348
12305415	0.074068	-3.755	0.010054	5319474
5281416	0.072493	-3.786	0.014509	440833
163069155	0.070717	-3.8218	0.0090839	441667
17166	0.068992	-3.8574	0.0033821	163020497
136085678	0.068503	-3.8677	0.018065	44178847
129819530	0.068496	-3.8678	0.00053843	1794427
637139	0.067473	-3.8896	0.0017908	49842399
10680	0.067011	-3.8995	0.00035181	162851990
3931	0.06577	-3.9264	0.00081161	162887874
7654	0.065552	-3.9312	0.0029545	65064
118716647	0.064757	-3.9488	0.0075617	14311156
5317025	0.064666	-3.9508	0.00012207	5281426
525	0.062481	-4.0004	0.015173	44566911
6054	0.062292	-4.0048	0.019899	73193
8215	0.061684	-4.019	0.016207	5281702
5204	0.058841	-4.087	0.018803	5281676
162849047	0.057472	-4.121	0.011699	341
132596278	0.057463	-4.1212	0.0082266	44260032
6450144	0.05705	-4.1316	0.0096332	1742210
163017122	0.055203	-4.1791	0.039832	74977035
21120946	0.054834	-4.1888	0.0046302	1203
190	0.05308	-4.2357	0.00069928	126
7017	0.051265	-4.2859	0.021732	370
9561835	0.049781	-4.3283	0.042497	3702506
162971414	0.049522	-4.3358	0.016198	10439806
16441	0.046939	-4.4131	0.020237	101607227
1549026	0.046848	-4.4159	0.0019786	162933403
5280607	0.046459	-4.4279	0.005696	14887605
10720349	0.045722	-4.451	0.00033788	162917701
71359328	0.044012	-4.506	0.0092721	162957786
162952341	0.041254	-4.5993	0.011724	19309
72730313	0.041068	-4.6058	0.039917	14187088
12756	0.040226	-4.6357	0.002859	165559
163051559	0.040016	-4.6433	0.0043791	75324
2214	0.040004	-4.6437	0.040309	62465
162887298	0.039611	-4.6579	0.012253	24796850
	1	1.33.3	1	

23658567	0.039237	-4.6716	0.0010651	154497005
23485	0.03776	-4.727	0.026933	101248984
75142	0.03742	-4.7401	0.00027637	11167374
13197868	0.036712	-4.7676	0.0041058	2371
5570	0.036238	-4.7863	0.00026373	10494
5281128	0.035223	-4.8274	0.0076855	11250133
14311167	0.033835	-4.8853	0.00025546	33931
186775	0.032583	-4.9397	0.00015576	107876
10912308	0.030285	-5.0452	0.000294	10813969
154505258	0.029324	-5.0918	0.01669	118855455
78603	0.02745	-5.1871	0.045229	19844
162653491	0.026773	-5.2231	0.0000562	163035053
14091	0.025903	-5.2708	0.00088524	14887603
134781708	0.024097	-5.375	0.0012942	442396
5281115	0.023761	-5.3952	0.00045686	14707301
101114357	0.022798	-5.4549	0.019174	162966990
163051662	0.022692	-5.4617	0.0098888	69634125
10465398	0.0217	-5.5262	0.0000304	5099
11227946	0.02153	-5.5375	0.00057857	5280647
8180	0.021373	-5.548	0.00014477	14704521
11061627	0.020576	-5.6029	0.0075229	75069340
7500	0.019334	-5.6927	0.00054737	162961650
60961	0.017306	-5.8526	0.00044277	1110
6287	0.01687	-5.8894	0.0000393	10015552
162939299	0.016048	-5.9615	0.0015781	163191530
163192296	0.014496	-6.1082	0.0016315	5318761
5283446	0.013912	-6.1675	0.0081067	16093748
5280445	0.013782	-6.1811	0.00026081	57006309
122382587	0.013003	-6.265	0.0032571	7966
13849	0.010663	-6.5513	0.00014126	322
11464176	0.009852	-6.6654	0.0010515	7146
11142	0.0098232	-6.6696	0.00011092	444899
3503	0.0092383	-6.7582	0.00052779	162659502
44559173	0.0091676	-6.7692	0.0042418	163195811
49831447	0.0087756	-6.8323	0.0005342	14296
608115	0.0086431	-6.8542	0.00049366	23815394
15645217	0.0086332	-6.8559	0.0002627	3.5805
160557896	0.0083636	-6.9017	0.00086254	3.0642
10815866	0.008153	-6.9385	0.0003874	3.4118
163190709	0.008124	-6.9436	0.014652	1.8341
162853228	0.0072681	-7.1042	0.00014104	3.8507
3084131	0.0065905	-7.2454	0.00087287	3.0591
1551480	0.0060405	-7.3711	0.0057278	2.242
6973640	0.0057738	-7.4363	0.0000103	4.9872
441772	0.0057275	-7.4479	0.00050522	3.2965
10538510	0.0056286	-7.473	0.020349	1.6914
546377	0.005066	-7.6249	0.0000164	4.7855
442849	0.0044808	-7.802	0.0000399	4.3995
14484636	0.0040817	-7.9366	0.00018585	3.7308
137185909	0.0032408	-8.2695	0.0000675	4.1704
129686415	0.0031848	-8.2946	0.0000115	4.9404
73821792	0.0031019	-8.3326	0.00068556	3.164
11623832	0.0014799	-9.4003	0.0000536	4.271
19212	0.00079154	-10.303	0.002516	2.5993
163034978	0.00059674	-10.711	0.00082802	3.082
101114359	0.00052123	-10.906	0.00059852	3.2229
	0.00002120		1.0000002	0.2220

53420248	0.00049518	-10.98	0.00010924	3.9616
10403282	0.0000856	-13.512	0.00018826	3.7252

S. rhombifolia vs. S. glabra (Fig. 4F)

CID	FC	Log₂(FC)	P value	-LOG ₁₀ (P)
5204	92.647	6.5337	0.0024437	2.6119
442849	39.484	5.3032	0.0000637	4.196
21120946	23.422	4.5498	0.0016631	2.7791
163034978	14.567	3.8647	0.0025601	2.5917
576026	14.266	3.8346	0.0020718	2.6836
1054	10.379	3.3756	0.0013069	2.8838
162912427	7.9521	2.9913	0.0084071	2.0754
71438848	7.3558	2.8789	0.021391	1.6698
13849	7.3392	2.8756	0.00082179	3.0852
6973640	6.6897	2.7419	0.00062191	3.2063
162962930	5.8923	2.5588	0.0041584	2.3811
12303930	5.5965	2.4845	0.0016206	2.7903
5988	5.5199	2.4646	0.0045453	2.3424
53420248	4.4603	2.1571	0.0048665	2.3128
162969771	3.9966	1.9988	0.048049	1.3183
137185909	3.9508	1.9822	0.0085901	2.066
162945016	3.4365	1.7809	0.014434	1.8406
10723382	2.3774	1.2494	0.04134	1.3836
10680	0.49108	-1.026	0.013146	1.8812
133372	0.48134	-1.0549	0.034056	1.4678
162866484	0.47051	-1.0877	0.00084672	3.0723
10582	0.46154	-1.1155	0.030028	1.5225
5282102	0.45981	-1.1209	0.015602	1.8068
3503	0.45756	-1.128	0.022329	1.6511
10015552	0.42789	-1.2247	0.013771	1.861
258412	0.42597	-1.2312	0.026634	1.5746
447791	0.42462	-1.2358	0.032709	1.4853
5459840	0.41272	-1.2768	0.030776	1.5118
162961573	0.39365	-1.345	0.012114	1.9167
162917701	0.38964	-1.3598	0.00074096	3.1302
311	0.38723	-1.3687	0.0034911	2.457
32033	0.38456	-1.3787	0.021591	1.6657
124708157	0.37837	-1.4021	0.0080618	2.0936
162966990	0.36724	-1.4452	0.0011882	2.9251
122382587	0.36265	-1.4634	0.024156	1.617
162919119	0.35576	-1.491	0.0050402	2.2976
101836180	0.35513	-1.4936	0.026387	1.5786
5320686	0.3454	-1.5337	0.037088	1.4308

5793	0.34288	-1.5442	0.011701	1.9318
162883937	0.34177	-1.5489	0.0089158	2.0498
75069340	0.34066	-1.5536	0.0043251	2.364
608115	0.33738	-1.5675	0.041532	1.3816
441574	0.3254	-1.6197	0.037371	1.4275
10912308	0.30382	-1.7187	0.0014922	2.8262
129686415	0.30247	-1.7251	0.00033579	3.4739
72730315	0.30185	-1.7281	0.027802	1.5559
23642717	0.29982	-1.7378	0.029577	1.529
163033482	0.29637	-1.7545	0.01755	1.7557
107905	0.28885	-1.7916	0.0045885	2.3383
5280445	0.28823	-1.7947	0.0031175	2.5062
439341	0.28106	-1.8311	0.0091332	2.0394
444539	0.28064	-1.8332	0.0037256	2.4288
163069155	0.25915	-1.9482	0.028938	1.5385
102430	0.25531	-1.9697	0.014604	1.8355
637139	0.24622	-2.022	0.0017212	2.7642
129847920	0.23833	-2.069	0.01421	1.8474
13250	0.22563	-2.148	0.0010173	2.9925
163106804	0.22511	-2.1513	0.014568	1.8366
10308838	0.22087	-2.1788	0.0044981	2.347
11354754	0.2205	-2.1811	0.0058918	2.2298
162939299	0.21322	-2.2296	0.0045531	2.3417
5274625	0.21256	-2.2341	0.01359	1.8668
5280637	0.20829	-2.2633	0.0088616	2.0525
57172986	0.20773	-2.2672	0.038369	1.416
92794	0.20444	-2.2902	0.0053027	2.2755
160557896	0.20366	-2.2958	0.015375	1.8132
5280953	0.20244	-2.3044	0.021137	1.675
540124	0.20112	-2.3139	0.0084203	2.0747
10815866	0.19863	-2.3318	0.0015959	2.797
75324	0.19605	-2.3507	0.028358	1.5473
11953803	0.19498	-2.3586	0.03664	1.436
5320006	0.19459	-2.3615	0.0069406	2.1586
71359328	0.19147	-2.3848	0.021861	1.6603
5281984	0.18877	-2.4053	0.018447	1.7341
101836179	0.18832	-2.4088	0.026759	1.5725
323	0.18697	-2.4191	0.03283	1.4837
162350	0.18197	-2.4582	0.0047858	2.32
6441104	0.18118	-2.4645	0.000000422	7.3752
21763831	0.17676	-2.5002	0.0051292	2.29
11692717	0.17541	-2.5112	0.018638	1.7296
8103	0.17371	-2.5253	0.04092	1.3881
14311167	0.17176	-2.5415	0.00013701	3.8633

10508776	0.16817	-2.572	0.011293	1.9472
163017122	0.16254	-2.6212	0.0046742	2.3303
5280607	0.16105	-2.6344	0.00051246	3.2903
69634125	0.15839	-2.6585	0.0005966	3.2243
12088	0.1578	-2.6638	0.00016963	3.7705
163195750	0.15596	-2.6808	0.005585	2.253
44552029	0.15447	-2.6946	0.023769	1.624
2214	0.15263	-2.7119	0.041496	1.382
162849047	0.15258	-2.7123	0.022205	1.6536
7017	0.15104	-2.727	0.018263	1.7384
14376672	0.14973	-2.7395	0.0017887	2.7475
75142	0.1479	-2.7573	0.00011719	3.9311
44552030	0.14539	-2.782	0.00070117	3.1542
178034	0.14499	-2.786	0.00625	2.2041
31265	0.14002	-2.8363	0.0064126	2.193
14704521	0.13972	-2.8394	0.0027276	2.5642
100953140	0.13673	-2.8706	0.0029347	2.5324
798	0.13534	-2.8853	0.031206	1.5058
12097	0.13505	-2.8884	0.044215	1.3544
107526	0.13309	-2.9095	0.0018606	2.7303
12799212	0.13251	-2.9158	0.00086224	3.0644
439242	0.13187	-2.9228	0.0022599	2.6459
479957	0.12849	-2.9603	0.018188	1.7402
11194416	0.12757	-2.9706	0.0054669	2.2623
1711945	0.12611	-2.9872	0.014639	1.8345
102239783	0.12503	-2.9997	0.0003423	3.4656
5280536	0.12412	-3.0102	0.00020623	3.6857
132596278	0.12395	-3.0122	0.0020429	2.6897
128853	0.12298	-3.0235	0.00027025	3.5682
5466138	0.12273	-3.0265	0.001813	2.7416
10403282	0.1222	-3.0327	0.0000943	4.0256
636576	0.12122	-3.0443	0.0074199	2.1296
162952341	0.11909	-3.0699	0.012437	1.9053
101114359	0.11789	-3.0845	0.00040412	3.3935
162971414	0.1146	-3.1253	0.0048223	2.3167
163057526	0.1138	-3.1355	0.026665	1.5741
370	0.11276	-3.1486	0.002665	2.5743
78162875	0.11211	-3.1571	0.0078163	2.107
101182982	0.11199	-3.1585	0.012678	1.897
101204053	0.10966	-3.1889	0.00045455	3.3424
5460372	0.10877	-3.2007	0.0041701	2.3799
440835	0.10852	-3.204	0.0020857	2.6807
5320834	0.10813	-3.2091	0.0019068	2.7197
1183	0.10683	-3.2267	0.0027563	2.5597

5468749	0.10561	-3.2432	0.0010847	2.9647
193484	0.10545	-3.2453	0.00011718	3.9311
10630882	0.1051	-3.2501	0.0024258	2.6152
440833	0.10215	-3.2912	0.0024687	2.6075
1794427	0.1019	-3.2948	0.0031467	2.5021
5281426	0.1016	-3.2991	0.004817	2.3172
5280379	0.10012	-3.3202	0.0017431	2.7587
10582821	0.09813	-3.3492	0.0060833	2.2159
162851990	0.097881	-3.3528	0.0032745	2.4849
162957279	0.097734	-3.355	0.0077478	2.1108
10256	0.097704	-3.3554	0.00087373	3.0586
162972958	0.097479	-3.3588	0.0021816	2.6612
11464176	0.096855	-3.368	0.0028032	2.5523
440265	0.0966	-3.3718	0.0027494	2.5608
14681438	0.0928	-3.4297	0.0054522	2.2634
101204054	0.09213	-3.4402	0.0025847	2.5876
10439806	0.091998	-3.4422	0.00065743	3.1821
5281647	0.091782	-3.4457	0.0081456	2.0891
4486984	0.091283	-3.4535	0.017694	1.7522
28619	0.089773	-3.4776	0.015493	1.8099
114776	0.088504	-3.4981	0.00033718	3.4721
163193559	0.087928	-3.5075	0.00085385	3.0686
14311156	0.087611	-3.5127	0.0013432	2.8719
996	0.085669	-3.5451	0.029373	1.5321
73172655	0.085471	-3.5484	0.0087349	2.0587
129881889	0.084413	-3.5664	0.0048035	2.3184
25310	0.081055	-3.625	0.010254	1.9891
10187514	0.080797	-3.6296	0.0051024	2.2922
440735	0.080645	-3.6323	0.0000133	4.8766
162915878	0.08004	-3.6431	0.0067766	2.169
21579640	0.080002	-3.6438	0.009028	2.0444
11072668	0.079857	-3.6464	0.016581	1.7804
9978316	0.079739	-3.6486	0.0068513	2.1642
13871877	0.0788	-3.6657	0.011986	1.9213
14340	0.07878	-3.666	0.016731	1.7765
72732	0.078703	-3.6674	0.0013944	2.8556
85524814	0.078503	-3.6711	0.0070184	2.1538
49831493	0.076674	-3.7051	0.0086026	2.0654
44258591	0.076129	-3.7154	0.00060209	3.2203
5316673	0.074486	-3.7469	0.00052344	3.2811
10652163	0.073937	-3.7576	0.0067199	2.1726
107557	0.073526	-3.7656	0.0079049	2.1021
101114361	0.072324	-3.7894	0.009477	2.0233
2723872	0.069278	-3.8515	0.00019897	3.7012

441667	0.068282	-3.8724	0.014281	1.8453
118855455	0.068223	-3.8736	0.0014779	2.8304
44577733	0.067902	-3.8804	0.0039505	2.4034
14311160	0.066462	-3.9113	0.0000141	4.851
5099	0.065638	-3.9293	0.0000428	4.3685
341	0.06503	-3.9427	0.01842	1.7347
5318761	0.064925	-3.9451	0.0000406	4.3914
5488575	0.064713	-3.9498	0.0023026	2.6378
162842866	0.064273	-3.9596	0.023935	1.621
15289454	0.063788	-3.9706	0.033367	1.4767
11250133	0.063308	-3.9815	0.014804	1.8296
441772	0.061564	-4.0218	0.000123	3.9101
163047490	0.061414	-4.0253	0.010995	1.9588
5281607	0.061381	-4.0261	0.0021235	2.673
3314	0.060418	-4.0489	0.00034798	3.4585
49831447	0.060263	-4.0526	0.0000733	4.1346
126	0.059557	-4.0696	0.010879	1.9634
5280863	0.05915	-4.0795	0.0019037	2.7204
49842399	0.058804	-4.0879	0.013222	1.8787
8299	0.057074	-4.131	0.043144	1.3651
23485	0.056345	-4.1496	0.00096428	3.0158
14079	0.055264	-4.1775	0.0013938	2.8558
10105245	0.054632	-4.1941	0.013667	1.8643
5281578	0.053709	-4.2187	0.011309	1.9466
163190248	0.053699	-4.219	0.0064824	2.1883
10262028	0.05369	-4.2192	0.010579	1.9756
15560128	0.051359	-4.2832	0.040662	1.3908
14887605	0.049691	-4.3309	0.00017862	3.7481
163035053	0.048866	-4.355	0.0097144	2.0126
15294	0.048711	-4.3596	0.012534	1.9019
101114357	0.048299	-4.3719	0.0030959	2.5092
3083616	0.047525	-4.3952	0.012457	1.9046
72751004	0.047378	-4.3996	0.015297	1.8154
19212	0.046628	-4.4227	0.0010865	2.964
135191	0.046571	-4.4244	0.00038411	3.4155
119216	0.045052	-4.4723	0.0079257	2.101
101928607	0.044242	-4.4984	0.0011454	2.941
10413856	0.043948	-4.5081	0.00015631	3.806
163190709	0.043941	-4.5083	0.0044539	2.3513
518900	0.043674	-4.5171	0.019391	1.7124
101286273	0.043514	-4.5224	0.010633	1.9733
328066	0.043454	-4.5244	0.024299	1.6144
10743	0.043028	-4.5386	0.0016105	2.793
373912	0.041915	-4.5764	0.0045106	2.3458

632128	0.041904	-4.5768	0.00012484	3.9036
162978216	0.041811	-4.58	0.014616	1.8352
11079623	0.040814	-4.6148	0.033093	1.4803
8417	0.039623	-4.6575	0.008566	2.0672
7967	0.038607	-4.695	0.023247	1.6336
348502	0.038146	-4.7123	0.0073262	2.1351
24982202	0.038118	-4.7134	0.0000137	4.8644
11277992	0.036935	-4.7589	0.0027017	2.5684
163040205	0.036775	-4.7651	0.00021396	3.6697
26339717	0.036301	-4.7839	0.0000664	4.1779
522636	0.035822	-4.803	0.029223	1.5343
154497005	0.035609	-4.8116	0.010669	1.9719
442101	0.035421	-4.8193	0.00036029	3.4434
7302	0.034922	-4.8397	0.00015275	3.816
14187088	0.034897	-4.8407	0.039379	1.4047
10922890	0.034551	-4.8551	0.001642	2.7846
132990894	0.034225	-4.8688	0.0032298	2.4908
1549095	0.033901	-4.8825	0.014111	1.8504
135	0.033201	-4.9126	0.0027536	2.5601
101114360	0.033136	-4.9155	0.000677	3.1694
33931	0.031882	-4.9711	0.0085244	2.0693
10969116	0.031057	-5.0089	0.005274	2.2779
5318717	0.028776	-5.119	0.0017979	2.7452
71567	0.028043	-5.1562	0.00045871	3.3385
101262727	0.02776	-5.1708	0.0026525	2.5764
5281614	0.027471	-5.1859	0.0046291	2.3345
5386960	0.026567	-5.2342	0.00052457	3.2802
442396	0.025999	-5.2654	0.00025743	3.5893
125213	0.025986	-5.2661	0.0012089	2.9176
162887298	0.025777	-5.2778	0.00042556	3.371
28516	0.025672	-5.2837	0.0036562	2.437
3702506	0.024044	-5.3782	0.021929	1.659
162933403	0.024031	-5.379	0.0000175	4.7561
44578390	0.023013	-5.4414	0.0076575	2.1159
162953603	0.022903	-5.4483	0.00020301	3.6925
11276243	0.022887	-5.4493	0.021702	1.6635
119205	0.022734	-5.459	0.0020916	2.6795
538953	0.022511	-5.4732	0.013042	1.8846
10472650	0.022473	-5.4757	0.0012572	2.9006
10813969	0.022202	-5.4932	0.00000633	6.1983
85091334	0.022018	-5.5051	0.0035285	2.4524
10748	0.021435	-5.5439	0.0031679	2.4992
10394	0.021076	-5.5682	0.00059653	3.2244
46181828	0.021045	-5.5703	0.000016	4.7967

1548883	0.020115	-5.6356	0.038015	1.42
5460657	0.018732	-5.7383	0.04154	1.3815
5281601	0.018173	-5.7821	0.00010177	3.9924
100151	0.017385	-5.846	0.0029792	2.5259
11061627	0.015088	-6.0504	0.0000279	4.5539
42608087	0.014381	-6.1197	0.0006485	3.1881
181681	0.014376	-6.1202	0.00090968	3.0411
124222280	0.014371	-6.1207	0.020859	1.6807
5315831	0.014208	-6.1371	0.00018528	3.7322
14332450	0.01349	-6.212	0.0000311	4.5077
65373	0.013378	-6.224	0.00051427	3.2888
7478	0.013111	-6.253	0.0035946	2.4444
5280343	0.0122	-6.357	0.00030897	3.5101
5280460	0.011546	-6.4364	0.0000226	4.6467
44631546	0.011177	-6.4833	0.0000503	4.2981
5274621	0.010746	-6.54	0.0000758	4.1205
5280647	0.010472	-6.5773	0.0000199	5.7022
139711	0.010465	-6.5782	0.036151	1.4419
6274	0.010106	-6.6286	0.0000829	4.0816
12681283	0.0097847	-6.6753	0.0000748	4.1261
162904343	0.0097499	-6.6804	0.0018192	2.7401
439514	0.0094405	-6.7269	0.025812	1.5882
14887603	0.009265	-6.754	0.00023038	3.6376
441833	0.0091313	-6.775	0.00023839	3.6227
1249	0.0090673	-6.7851	0.00068367	3.1652
73323377	0.0087765	-6.8321	0.00030566	3.5148
49831491	0.0086508	-6.8529	0.00083282	3.0795
14035324	0.0082007	-6.93	0.0000884	5.0536
240	0.008119	-6.9445	0.0057337	2.2416
439246	0.007927	-6.979	0.0011259	2.9485
10252339	0.0078832	-6.987	0.00037886	3.4215
74978075	0.0078001	-7.0023	0.00099532	3.002
375713	0.0076288	-7.0343	0.00052248	3.2819
31242	0.0050448	-7.631	0.00062737	3.2025
94225	0.0049168	-7.6681	0.0011906	2.9242
636543	0.0048092	-7.7	0.0012594	2.8999
10255859	0.004658	-7.7461	0.00044615	3.3505
163034124	0.0045783	-7.771	0.0007621	3.118
5280443	0.0045022	-7.7951	0.0000214	4.6686
165559	0.0042173	-7.8895	0.00017352	3.7606
10393	0.0040977	-7.931	0.00058844	3.2303
384679	0.0036195	-8.11	0.0010276	2.9882
3469	0.0035932	-8.1205	0.00035605	3.4485
74977035	0.0034745	-8.169	0.00000645	5.1906

0.0024227			
0.0034327	-8.1864	0.00027065	3.5676
0.0033513	-8.2211	0.00014012	3.8535
0.0032237	-8.277	0.0020483	2.6886
0.0029307	-8.4146	0.0013877	2.8577
0.0025865	-8.5948	0.0000503	5.2981
0.0024151	-8.6937	0.00029883	3.5246
0.0018717	-9.0615	0.0000212	4.6727
0.0018146	-9.1061	0.0000108	5.9663
0.0016253	-9.2651	0.00023998	3.6198
0.0010252	-9.9299	0.00013552	3.868
0.00064172	-10.606	0.00031182	3.5061
0.00054959	-10.829	0.00017783	3.75
0.0004706	-11.053	0.00093499	3.0292
0.00039942	-11.29	0.00028895	3.5392
0.0001315	-12.893	0.0000126	4.8997
0.0000254	-15.262	0.00082789	3.082
0.000000254	-21.91	0.0000691	5.1606
	0.0032237 0.0029307 0.0025865 0.0024151 0.0018717 0.0018146 0.0016253 0.0010252 0.00064172 0.00054959 0.00039942 0.0001315 0.0000254	0.0032237 -8.277 0.0029307 -8.4146 0.0025865 -8.5948 0.0024151 -8.6937 0.0018717 -9.0615 0.0018146 -9.1061 0.0016253 -9.2651 0.0010252 -9.9299 0.00064172 -10.606 0.00054959 -10.829 0.0004706 -11.053 0.00039942 -11.29 0.0001315 -12.893 0.0000254 -15.262	0.0032237 -8.277 0.0020483 0.0029307 -8.4146 0.0013877 0.0025865 -8.5948 0.00000503 0.0024151 -8.6937 0.00029883 0.0018717 -9.0615 0.0000212 0.0018146 -9.1061 0.00000108 0.0016253 -9.2651 0.00023998 0.0010252 -9.9299 0.00013552 0.00064172 -10.606 0.00031182 0.00054959 -10.829 0.00017783 0.0004706 -11.053 0.00093499 0.00039942 -11.29 0.00028895 0.0001315 -12.893 0.0000126 0.0000254 -15.262 0.00082789

Supporting information 7

Hierarchical clustering heatmap showing the relative concentration of phenolic compounds across the different *Sida* species. Data were processed and visualized using MetaboAnalyst 6.0 (generated using the Euclidean and Ward methods for distance estimation and as a clustering algorithm, respectively). Each row represents a phenolic compound, while columns correspond to technical replicates of each species. The color gradient reflects normalized and scaled intensities (red: higher abundance; blue: lower abundance), highlighting species-specific metabolic profiles and clustering patterns.

