

Supporting Information

Non-volatile natural products in plant glandular trichomes: chemistry, biological activities and biosynthesis

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Table S1. Names and sources of sesquiterpenoids 1-158.

No.	Names	Species	Family	Ref.
1	Glandulone A	<i>Helianthus annuus</i>	Asteraceae	1
2	Glandulone C	<i>H. annuus</i>	Asteraceae	1
3	Glandulone B	<i>H. annuus</i>	Asteraceae	1
4	Glandulone D	<i>H. annuus</i>	Asteraceae	2
5	Glandulone E	<i>H. annuus</i>	Asteraceae	2
6	Glandulone F	<i>H. annuus</i>	Asteraceae	2
7	Helibisabonol A	<i>H. annuus</i>	Asteraceae	2
8	Helibisabonol C	<i>H. annuus</i>	Asteraceae	2
9	Heliannuol A	<i>H. annuus</i>	Asteraceae	2
10	Heliannuol D	<i>H. annuus</i>	Asteraceae	2
11	Tomentosin	<i>Scalesia</i> sp.	Asteraceae	3
12	4-Dihydrotomentosin	<i>Scalesia</i> sp.	Asteraceae	3
13	Ivalbin	<i>Helianthus stuebelii</i>	Asteraceae	4
14	11 α ,13-Dihydro-4H-tomentosin	<i>Viguiera acutifolia</i> , <i>H. stuebelii</i> , <i>H. sagasteguii</i>	Asteraceae	4
15	Xanthatin	<i>Xanthium strumarium</i>	Asteraceae	5
16	Xanthinosin	<i>X. strumarium</i>	Asteraceae	5
17	8- <i>epi</i> -Xanthatin	<i>X. strumarium</i>	Asteraceae	5
18	Xanthumin	<i>X. strumarium</i>	Asteraceae	5
19	Carabrone	<i>Scalesia</i> sp.	Asteraceae	3
20	4-Dihydrocarabrone	<i>Scalesia</i> sp.	Asteraceae	3
21	4,11,13-Trihydrocarabrone	<i>V. acutifolia</i> , <i>H. sagasteguii</i>	Asteraceae	4
22	Umbellifolide	<i>Artemisia umbelliformis</i>	Asteraceae	6
23	8 β -Angeloyloxy-9 β ,14-dihydroxy-1(10),4(5)-trans,trans-germacradienolide	<i>Blainvillea rhomboidea</i>	Asteraceae	7
24	8 β -Angeloyloxy-9 β -hydroxy-ovatifolin	<i>B. rhomboidea</i>	Asteraceae	7
25	8 β -Tigloyloxy-grazielia acid	<i>B. rhomboidea</i>	Asteraceae	7
26	8 β ,14-Dihydroxy costunolide	<i>Helianthus tuberosus</i>	Asteraceae	8
27	Desacetyleupaserrin	<i>H. tuberosus</i>	Asteraceae	8
28	Mollisorin B 2'S,3'S stereoisomer	<i>H. tuberosus</i>	Asteraceae	8
29	8 β -(4'-Hydroxy)tiglinoyloxy-ovatifolin	<i>V. radula</i>	Asteraceae	9

30	2'S,3'S-Epang-8 β - Epoxyangeloyloxy- ovatifolin	<i>V. radula</i>	Asteraceae	9
31	2'R,3'R-Epang-9 β - Epoxyangeloyloxy- ovatifolin	<i>V. radula</i>	Asteraceae	9
32	2 α -Hydroxy-9 β -O- methylbutanoyl- 1(10),4,11(13)- germacatrien, 6 α ,12-olide	<i>V. quinqueremis</i>	Asteraceae	10
33	2 α -Hydroxy-9 β -O-angeloyl- 1(10),4,11(13)- germacatrien, 6 α ,12-olide	<i>V. quinqueremis</i>	Asteraceae	10
34	2 α ,3 β -Dihydroxy-8 β - methacryloyloxy-germacra- 1(10),4,11(13)-trien-6 α ,12- olide	<i>V. gardneri</i>	Asteraceae	11
35	Cnicin	<i>Centaurea maculosa</i>	Asteraceae	12
36	Haagenolide	<i>H. annuus</i>	Asteraceae	13
37	Tagitinin C	<i>Tithonia diversifolia</i>	Asteraceae	14
38	Tagitinin C methylbutyrate	<i>T. diversifolia</i>	Asteraceae	14
39	15-Hydroxy-3- Dehydrodesoxyfruticin	<i>H. annuus, V. quinqueremis</i>	Asteraceae	10
40	15-Hydroxy-3- dehydrodesoxy-2',3'- dihydrotifruticin	<i>V. quinqueremis</i>	Asteraceae	10
41	1 α ,10 β ,15-Trihydroxy- 3 α -8 β -O-methylbutanoyl- 4,11(13)- germacradien,6 α ,12-olide	<i>V. quinqueremis</i>	Asteraceae	10
42	8 β -Angeloyloxy-9 β - hydroxy-14- α - acanthospermolide	<i>B. rhomboidea</i>	Asteraceae	7
43	8 β -Angeloyloxy-14- α - acanthospermolide	<i>B. rhomboidea</i>	Asteraceae	7
44	8 β -Hydroxy-9 β - angeloyloxy-14- α - acanthospermolide	<i>B. rhomboidea</i>	Asteraceae	7
45	8 β -Hydroxy-9 α - angeloyloxy-14- α - acanthospermolide	<i>B. rhomboidea</i>	Asteraceae	7
46	8 β -Tigloyloxy-14- α -	<i>B. rhomboidea</i>	Asteraceae	7

	acanthospermolide			
47	8 β -Senecioyloxy-14-oxo- acanthospermolide	<i>B. rhomboidea</i>	Asteraceae	7
48	Uvedalin	<i>Smallanthus sonchifolius</i>	Asteraceae	15
49	Enhydrin	<i>S. sonchifolius</i>	Asteraceae	15
50	8,9-Epoxy-14-oxo- 1(10)Z,4(5)E,7(11)- germacatrien-6,12-olide	<i>B. rhomboidea</i>	Asteraceae	7
51	1 β ,2 α -Epoxy tagitinic C	<i>T. diversifolia</i>	Asteraceae	14
52	Parthenolide	<i>Tanacetum parthenium</i>	Asteraceae	16
53	Tithifolin epoxyangelate, 14-acetoxy	<i>H. tuberosus</i>	Asteraceae	8
54	3 β -O-Acetyl-8 β - epoxyangeloyloxy-tithifolin	<i>V. puruana</i>	Asteraceae	17
55	8 β -Angeloyloxy-14- hydroxy-tithifolin	<i>V. radula</i>	Asteraceae	9
56	Argophyllin A	<i>H. annuus</i>	Asteraceae	18
57	Argophyllin B	<i>H. annuus</i>	Asteraceae	18
58	Erioflorin	<i>Viguiera eriophora</i> ssp. <i>Eriophora</i> , <i>V. puruana</i>	Asteraceae	17
59	Acetylerioflorin	<i>V. eriophora</i> ssp. <i>eriphora</i>	Asteraceae	17
60	Acetylleptocarpin	<i>V. puruana</i> , <i>V. radula</i>	Asteraceae	9
61	3 β -Ethoxy-leptocarpin	<i>V. puruana</i>	Asteraceae	17
62	Heliangine	<i>V. puruana</i>	Asteraceae	17
63	1 β ,10 α -Epoxy-3 β -hydroxy- 8 β -(2'R,3'R)- epoxyangeloyloxy- heliangolide	<i>V. puruana</i>	Asteraceae	17
64	1 β ,10 α -Epoxy-3 β -acetoxy- 8 β -(2'R,3'R)- epoxyangeloyloxy- heliangolide	<i>V. puruana</i>	Asteraceae	17
65	1 β ,10 α -Epoxy-3 β - isobutyrate-8 β -(2'R,3'R)- epoxyangeloyloxy- heliangolide	<i>V. puruana</i>	Asteraceae	17
66	3 β -(2'-Methylbutanoyloxy)- 8 β -epoxyangeloyloxy- leptocarpin	<i>V. puruana</i>	Asteraceae	17
67	1 β ,10 α -Epoxy-3 β - isovalerate-8 β -(2'R,3'R)- epoxyangeloyloxy-	<i>V. puruana</i>	Asteraceae	17

	heliangolide			
68	3 β -O-Acetyl-8 β -sarracinyloxy-leptocarpin	<i>V. puruana</i>	Asteraceae	17
69	Rotundin	<i>V. radula</i>	Asteraceae	9
70	Tagitinin E	<i>H. tuberosus</i> , <i>T. diversifolia</i>	Asteraceae	8, 14
71	Leptocarpin	<i>H. tuberosus</i> , <i>V. eriophora</i> ssp. <i>Eriophora</i> , <i>V. radula</i>	Asteraceae	8, 9
72	14-Hydroxy-leptocarpin	<i>H. tuberosus</i> , <i>V. radula</i>	Asteraceae	8, 9
73	1-O-Methyl-4,5-dihydroniveusin A	<i>H. annuus</i>	Asteraceae	18, 19
74	4,5-Dihydro-niveusin A-methylbutyrate (enol)	<i>H. annuus</i>	Asteraceae	13
75	1,2-Anhydrido-4,5-dihydroniveusin A	<i>H. annuus</i> , <i>V. quinquereimis</i>	Asteraceae	18
76	Niveusin C	<i>H. annuus</i> , <i>H. stubelii</i> , <i>V. acutifolia</i>	Asteraceae	4, 18
77	Tagitinin F	<i>T. diversifolia</i>	Asteraceae	14
78	3 α ,15-Dihydroxy-3,10-epoxy-8 β -O-methylbutanoyl-1,4,11(13)-germacatrien,6 α ,12-olide	<i>V. quinquereimis</i> , <i>T. diversifolia</i>	Asteraceae	10
79	2 β -Methoxydesoxy-tagitinin	<i>T. diversifolia</i>	Asteraceae	14
80	8 β -Angeloyloxy-viguilenin	<i>V. radula</i>	Asteraceae	9
81	Tagitinin A	<i>T. diversifolia</i>	Asteraceae	14
82	3-O-Methyltirobundin	<i>T. diversifolia</i>	Asteraceae	14
83	Tirobundin	<i>T. diversifolia</i>	Asteraceae	14
84	1-O-Methyl-4,5-dihydroniveusin A	<i>H. annuus</i>	Asteraceae	18
85	Atripliciolide tiglata	<i>V. radula</i>	Asteraceae	9
86	Budlein A	<i>H. tuberosus</i> , <i>V. eriophora</i> ssp. <i>Eriophora</i> , <i>V. quinquereimis</i>	Asteraceae	8, 17
87	Budlein A tiglata	<i>H. tuberosus</i>	Asteraceae	8
88	Budlein A 2-methylbutyrate	<i>H. tuberosus</i> , <i>V. quinquereimis</i>	Asteraceae	8, 10
89	Budlein A isobutyrate	<i>H. tuberosus</i>	Asteraceae	8
90	Budlein A methylacrylate	<i>H. tuberosus</i>	Asteraceae	8
91	Budlein A isovalerate	<i>V. acutifolia</i> , <i>H. stubelii</i> , <i>H. sagasteguii</i>	Asteraceae	4
92	Atripliciolide 2-methylbutyrate	<i>V. acutifolia</i> , <i>H. stubelii</i> , <i>H. sagasteguii</i>	Asteraceae	4
93	4,15-iso-Budlein A isobutyrate	<i>H. tuberosus</i>	Asteraceae	8
94	4,15-iso-Atripliciolide	<i>H. tuberosus</i>	Asteraceae	8

	isobutyrate			
95	4,15-iso-Atripliciolide methylacrylate	<i>H. tuberosus</i>	Asteraceae	8
96	4,15-iso-Atripliciolide tiglate	<i>H. tuberosus</i>	Asteraceae	8
97	4,15-iso-Atripliciolide angelate	<i>H. tuberosus</i>	Asteraceae	8
98	3-Hydroxy atripliciolide tiglate	<i>H. tuberosus</i>	Asteraceae	8
99	Ladibranolide	<i>V. radula</i>	Asteraceae	9
100	17,18-Dehydro-viguiepinin	<i>V. eriophora</i> ssp. <i>eriophora</i>	Asteraceae	17
101	Calaxin	<i>V. eriophora</i> ssp. <i>eriophora</i>	Asteraceae	17
102	1-Keto-3,10-epoxy-11a-methoxymethyl-8-O-methacryloyl-15-hydroxy-2,4-germacradiene, 6,12-olide	<i>V. eriophora</i> ssp. <i>eriophora</i>	Asteraceae	17
103	1-Keto-3,10-epoxy-8-O-methacryloyl-4,15-dihydroxy-5-acetoxy-2,11-germacradiene, 6,12-olide	<i>V. eriophora</i> ssp. <i>eriophora</i>	Asteraceae	17
104	Niveusin A isobutyrate	<i>H. sagasteguii</i>	Asteraceae	4
105	Niveusin A 2-methylbutyrate	<i>V. acutifolia</i> , <i>H. sagasteguii</i> , <i>V. quinquereimis</i>	Asteraceae	4, 10
106	Niveusin B isobutyrate	<i>V. acutifolia</i> , <i>H. stubelii</i> , <i>H. sagasteguii</i>	Asteraceae	4
107	Niveusin B	<i>V. acutifolia</i> , <i>H. stubelii</i> , <i>H. sagasteguii</i> , <i>H. annuus</i> , <i>V. quinquereimis</i>	Asteraceae	10
108	Niveusin B 2-methylbutyrate	<i>V. quinquereimis</i>	Asteraceae	10
109	1 α ,3 α ,15-Trihydroxy-3,10-epoxy-8-O-methacryloyl-4,11-germacradiene,6,12-olide	<i>V. eriophora</i> ssp. <i>Eriophora</i>	Asteraceae	17
110	Niveusin A	<i>V. quinquereimis</i>	Asteraceae	10
111	1 α -Methoxy-3 α ,15-dihydroxy-3,10-epoxy-8 β -O-methylbutanoyl-4,11(13)-germacradien,6 α ,12-olide	<i>V. quinquereimis</i>	Asteraceae	10
112	1 α -Methoxy-3 α ,15-dihydroxy-3,10-epoxy-8 β -	<i>V. quinquereimis</i>	Asteraceae	10

	<i>O</i> -angeloyl-4,11(13)- germacradien,6 α ,12-olide			
113	1 β -Methoxy-3 α -hydroxy- 3,10 β -4,5 α -diepoxy-8 β - isobutyroyloxy-germacra- 11(13)-en-6 α ,12-olide	<i>T. diversifolia</i>	Asteraceae	14
114	Prevernocistifolide-8- <i>O</i> - isobutyrate	<i>Vernonia galamensis</i> ssp. <i>galamensis</i> var. <i>ethiopica</i>	Asteraceae	20
115	8 α -Acetoxy-10 α -hydroxy- 13- <i>O</i> -methylhirsutinolide	<i>Chrysolaena</i> spp.	Asteraceae	21
116	8 α ,13-Diacetoxy-10 α - hydroxy-hirsutinolide	<i>Chrysolaena</i> spp.	Asteraceae	21
117	-	<i>Chrysolaena</i> spp.	Asteraceae	21
118	4- <i>Oxo</i> -8 β -isobutyroyloxy- 3,4-secoguaia-11(13)-en- 6 α ,12,10 α ,3-diolide	<i>T. diversifolia</i>	Asteraceae	14
119	Artemisinin	<i>Artemisia annua</i>	Asteraceae	22
120	Artemisitene	<i>A. annua</i>	Asteraceae	22
121	2-Methoxy-calamenene-14- carboxylic acid	<i>Heterotheca subaxillaris</i>	Asteraceae	23
122	2-Acetoxy-calamenene-14- carboxylic acid	<i>H. subaxillaris</i>	Asteraceae	23
123	2-Hydroxy-calamenene-14- carboxylic acid	<i>H. subaxillaris</i>	Asteraceae	23
124	2-Hydroxy-calamenene-14- ol	<i>H. subaxillaris</i>	Asteraceae	23
125	2-Methoxy-14- calamenenone	<i>H. subaxillaris</i>	Asteraceae	23
126	2-Hydroxy-14- calamenenone	<i>H. subaxillaris</i>	Asteraceae	23
127	7,8-Dehydro-2-hydroxy- calamenene-14-ol	<i>H. subaxillaris</i>	Asteraceae	23
128	Gerin	<i>Geraea viscida</i>	Asteraceae	24
129	5-Desoxy-5- hydroperoxytelekin	<i>A. umbelliformis</i>	Asteraceae	6
130	5-Desoxy-5-hydroperoxy- 5-epitelekin	<i>A. umbelliformis</i>	Asteraceae	6
131	1 α ,2-Dihydroxy-pinnatifidin	<i>H. tuberosus</i>	Asteraceae	8
132	3- <i>Oxo</i> -isoalantolactone	<i>Scalesia</i> spp.	Asteraceae	3
133	Pinnatifidin	<i>Scalesia</i> spp.	Asteraceae	3
134	8 β -2,3-Epoxyangeloyloxy- balchanin	<i>V. puruana</i>	Asteraceae	17

135	Parthenin	<i>Parthenium hysterophorus</i>	Asteraceae	25
136	Ambrosin	<i>P. hysterophorus</i>	Asteraceae	25
137	Cumambrin A	<i>A. nova</i>	Asteraceae	26
138	Cumambrin B	<i>A. nova</i>	Asteraceae	26
139	Zaluzanin C	<i>Scalesia stewartii</i>	Asteraceae	3
140	15-Hydroxyzaluzanin C	<i>Sca. stewartii</i>	Asteraceae	3
141	15-Hydroxy-11,13-dihydrozaluzanin C	<i>Sca. stewartii</i>	Asteraceae	3
142	Scalesin	<i>Sca. stewartii</i>	Asteraceae	3
143	8 β -Angeloyloxy-14-oxo-4 β ,9 β -dihydroxy-guaia-11(13)-en-6,12-olide	<i>B. rhomboidea</i>	Asteraceae	7
144	9 β -Angeloyloxy-14-oxo,4 β ,8 β -dihydroxy-guaia-11(13)-en-6,12-olide	<i>B. rhomboidea</i>	Asteraceae	7
145	2-One-8 β -methacryloyloxy-guaia-1(10),3,11(13)-trien-6 α ,12-olide	<i>V. gardneri</i>	Asteraceae	11
146	2-One-8 β -tigloyloxy-guaia-1(10),3,11(13)-trien-6 α ,12-olide	<i>V. gardneri</i>	Asteraceae	11
147	2-One-8 β -methacryloyloxy-10 β -hydroxy-guaia-3,11(13)-dien-6 α ,12-olide	<i>V. gardneri</i>	Asteraceae	11
148	2-One-8 β -methacryloyloxy-10 α -hydroxy-guaia-3,11(13)-dien-6 α ,12-olide	<i>V. gardneri</i>	Asteraceae	11
149	2-One-8 β -methacryloyloxy-guaia-3,10(14),11(13)-trien-6 α ,12-olide	<i>V. gardneri</i>	Asteraceae	11
150	3-Hydroxy-8 β -isobutyryloxydehydroleucodin	<i>T. diversifolia</i>	Asteraceae	14
151	4 β ,10 α -Dihydroxy-3-oxo-8 β -isobutyryloxyguaia-11(13)-en-12,6 α -olide	<i>T. diversifolia</i>	Asteraceae	14
152	8 β -Angeloyloxy-9 β -hydroxy-guaia-11(13)-en-6(12),4(14)-diolide	<i>B. rhomboidea</i>	Asteraceae	7
153	8 β -Angeloyloxy-9 β -hydroxy-guaia-13-methoxy-6(12),4(14)-diolide	<i>B. rhomboidea</i>	Asteraceae	7

154	(-)-epi- α -Bisabolol 6-deoxy- β -D-gulopyranodide	<i>Brillantaisia owariensis</i>	Acanthaceae	27
155	2-O-(6'-O-Malonyl- β -D-glucopyranosyl), 12-O-(β -D-glucopyranosyl)-campherenane-2-endo,12-diol	<i>Solanum habrochaites</i>	Solanaceae	28
156	12-O-(6'-O-Malonyl- β -D-glucopyranosyl)-campherenane-2-endo,12-diol	<i>S. habrochaites</i>	Solanaceae	28
157	2,12-Bis-O-(β -D-glucopyranosyl)-campherenane-2-endo,12-diol	<i>S. habrochaites</i>	Solanaceae	28
158	12-O-(6''-O-Acetyl- β -D-glucopyranosyl-(1 \rightarrow 2)- β -D-glucopyranosyl)-campherenane-2-endo,12-diol	<i>S. habrochaites</i>	Solanaceae	28

Table S2. Names and sources of diterpenoids 159-192.

No.	Names	Species	Family	Ref.
159	α -4,8,13-Duvatriene-1,3-diol (DVT)	<i>Nicotiana tabacum</i>	Solanaceae	29
160	β -4,8,13-Duvatriene-1,3-diol	<i>N. tabacum</i>	Solanaceae	29
161	α -4,8,13-Duvatriene-ol	<i>N. tabacum</i>	Solanaceae	29
162	β -4,8,13-Duvatriene-ol	<i>N. tabacum</i>	Solanaceae	29
163	(1 <i>S</i> ,2 <i>E</i> ,4 <i>R</i> ,6 <i>R</i> ,7 <i>E</i> ,11 <i>E</i>)-2,7,11-Cembratriene-4,6-diol (CBT-diol)	<i>N. tabacum</i>	Solanaceae	30
164	(1 <i>S</i> ,2 <i>E</i> ,4 <i>S</i> ,6 <i>R</i> ,7 <i>E</i> ,11 <i>E</i>)-2,7,11-Cembratriene-4,6-diol	<i>N. tabacum</i>	Solanaceae	30
165	(-)-Kolavenol	<i>Salvia divinorum</i>	Lamiaceae	31
166	<i>cis</i> -Abienol	<i>N. tabacum</i>	Solanaceae	32
167	15-Hydroxy abienol	<i>N. tabacum</i>	Solanaceae	32
168	(-)-Sclareol	<i>Salvia sclarea</i>	Lamiaceae	33
169	Paraguhenryisin A	<i>Paragutzlaffia henryi</i>	Acanthaceae	34
170	Paraguhenryisin B	<i>P. henryi</i>	Acanthaceae	34
171	Paraguhenryisin C	<i>P. henryi</i>	Acanthaceae	34
172	Paraguhenryisin D	<i>P. henryi</i>	Acanthaceae	34

173	Physacoztomatin	<i>P. henryi</i>	Acanthaceae	34
174	Leoheterin	<i>Leonurus japonicus</i>	Lamiaceae	35
175	Galeopsin	<i>L. japonicus</i>	Lamiaceae	35
176	Vitexilactone	<i>Vitex agnus-castus</i>	Lamiaceae	36
177	Seguiniilactone A	<i>Colquhounia seguinii</i>	Lamiaceae	37
178	Seguiniilactone B	<i>C. seguinii</i>	Lamiaceae	37
179	Seguiniilactone C	<i>C. seguinii</i>	Lamiaceae	37
180	(-)-Hardwickiic acid	<i>S. divinorum</i>	Lamiaceae	31
181	Salvianduline D	<i>Salvia blepharophylla</i>	Lamiaceae	38
182	Salvinorin A	<i>S. divinorum</i>	Lamiaceae	39
183	Salvinorin B	<i>S. divinorum</i>	Lamiaceae	39
184	Salvinorin C	<i>S. divinorum</i>	Lamiaceae	39
185	Salvinorin D	<i>S. divinorum</i>	Lamiaceae	39
186	Carnosic acid	<i>Rosmarinus officinalis</i>	Lamiaceae	40
187	Carnosol	<i>R. officinalis</i>	Lamiaceae	40
188	<i>ent</i> -Kaurenoic acid	<i>T. diversifolia</i> , <i>M.</i> <i>tomentosa</i> , <i>P.</i> <i>sonchifolia</i> , <i>P.</i> <i>cheiranthifolium</i> , <i>P. vira</i> <i>vira</i> , <i>P. robustum</i>	Asteraceae	14, 41
189	Grandiflorenic acid	<i>Montanoa tomentosa</i>	Asteraceae	41
190	<i>ent</i> -Kaur-16-en-19-oic acid 15-angeloyloxy ester	<i>Polymnia sonchifolia</i>	Asteraceae	42
191	18-Angeloyloxy- <i>ent</i> -kaur-16-en-19-oic acid	<i>P. sonchifolia</i>	Asteraceae	42
192	15-Angeloyloxy-16,17-epoxy-19-kauronic acid	<i>P. sonchifolia</i>	Asteraceae	42

Table S3. Names and sources of sesterterpenoids 193-200.

No.	Names	Species	Family	Ref.
193	Leucosceptroid A	<i>Leucosceptrum canum</i>	Lamiaceae	43
194	Leucosceptroid B	<i>L. canum</i>	Lamiaceae	43
195	11- β H-Leucosceptroid B	<i>L. canum</i>	Lamiaceae	44
196	Leucosceptroid J	<i>L. canum</i>	Lamiaceae	44
197	Leucosceptroid I	<i>L. canum</i>	Lamiaceae	44
198	Colquhounoid A	<i>Colquhounia coccinea</i> var. <i>mollis</i>	Lamiaceae	45
199	Colquhounoid B	<i>C. coccinea</i> var. <i>mollis</i>	Lamiaceae	45
200	Colquhounoid C	<i>C. coccinea</i> var. <i>mollis</i>	Lamiaceae	45

Table S4. Names and sources of triterpenoids 201-222.

No.	Names	Species	Family	Ref.
201	Ursolic acid	<i>Salvia</i> <i>blepharophylla</i>	Lamiaceae	38
202	α -Amyrin	<i>S. blepharophylla</i>	Lamiaceae	38
203	(2 α ,20S)-2,20-Dihydroxydammar-24-en-3-one	<i>Cerasus</i> <i>yedoensis</i>	Rosaceae	46
204	(20S)-20-Hydroxydammar-24-en-3-one	<i>C. yedoensis</i>	Rosaceae	46
205	Betulafolienetriol	<i>Proboscidea</i> <i>louisiana</i>	Martyniaceae	47
206	Probosciderol A	<i>P. louisiana</i>	Martyniaceae	47
207	Probosciderol B	<i>P. louisiana</i>	Martyniaceae	47
208	Probosciderol C	<i>P. louisiana</i>	Martyniaceae	47
209	Probosciderol D	<i>P. louisiana</i>	Martyniaceae	47
210	Probosciderol F	<i>P. louisiana</i>	Martyniaceae	47
211	Probosciderol E	<i>P. louisiana</i>	Martyniaceae	47
212	Probosciderol G	<i>P. louisiana</i>	Martyniaceae	47
213	Probosciderol H	<i>P. louisiana</i>	Martyniaceae	47
214	Probosciderol I	<i>P. louisiana</i>	Martyniaceae	47
215	Probosciderol L	<i>P. louisiana</i>	Martyniaceae	47
216	Probosciderol J	<i>P. louisiana</i>	Martyniaceae	47
217	Probosciderol K	<i>P. louisiana</i>	Martyniaceae	47
218	Betulatrierpene C 3-acetate	<i>Ibicella lutea</i>	Martyniaceae	47
219	24- <i>epi</i> -Polacandrin 1,3-diacetate	<i>I. lutea</i>	Martyniaceae	47
220	Betulatrierpene C	<i>I. lutea</i>	Martyniaceae	47
221	24- <i>epi</i> -Polacandrin 3-acetate	<i>I. lutea</i>	Martyniaceae	47
222	Papyriferic acid	<i>B. neoalaskana</i> , <i>B. pendula</i>	Betulaceae	48

Table S5. Names and sources of meroterpenoids 223-232.

No.	Names	Species	Family	Ref.
223	Δ^9 -Tetrahydrocannabinolic acid (THCA)	<i>Cannabis sativa</i>	Cannabaceae	49
224	Δ^9 -Tetrahydrocannabinol (Δ^9 -THC)	<i>C. sativa</i>	Cannabaceae	49
225	Cannabidiolic acid (CBDA)	<i>C. sativa</i>	Cannabaceae	49
226	Cannabidiol (CBD)	<i>C. sativa</i>	Cannabaceae	49
227	Cannabigerolic acid (CBGA)	<i>C. sativa</i>	Cannabaceae	49
228	Cannabigerol (CBG)	<i>C. sativa</i>	Cannabaceae	49
229	Cannabichromenic acid (CBCA)	<i>C. sativa</i>	Cannabaceae	49
230	Cannabichromene (CBC)	<i>C. sativa</i>	Cannabaceae	49

231	Cannabinol (CBN)	<i>C. sativa</i>	Cannabaceae	49
232	Vedelianin	<i>Macaranga vedeliana</i>	Euphorbiaceae	50

Table S6. Names and sources of simple phenolics 233-284.

No.	Names	Species	Family	Ref.
233	Geranylgeranylhydroquinone	<i>Phacelia minor</i> , <i>P. parryi</i>	Hydrophyllaceae	51
234	1-Oxofarnesylhydroquinone(= 2-Farnesoyl-hydroquinone)	<i>P. minor</i> , <i>P. parryi</i> , <i>P. campanularia</i>	Hydrophyllaceae	51
235	5-Farnesoyl-1,2,4-trihydroxybenzene	<i>P. campanularia</i>	Hydrophyllaceae	52
236	Geranylhydroquinone	<i>P. crenulata</i>	Hydrophyllaceae	53
237	3-Geranyl-2,5-dihydroxyphenyl acetate	<i>P. ixodes</i>	Hydrophyllaceae	54
238	2-Geranyl-4-hydroxyphenyl acetate	<i>P. ixodes</i>	Hydrophyllaceae	54
239	2,4-Dihydroxy-6-geranylphenyl acetate	<i>P. pedicellata</i>	Hydrophyllaceae	52
240	Geranylbenzoquinone	<i>P. ixodes</i>	Hydrophyllaceae	54
241	2-Geranyl-6-hydroxy-4-methoxyphenyl acetate	<i>P. ixodes</i>	Hydrophyllaceae	54
242	6-Hydroxy-2-methyl-2-(4-methyl-3-pentenyl)-chromene	<i>P. ixodes</i>	Hydrophyllaceae	54
243	6-Farnesyl-1,2,4-trihydroxybenzene	<i>P. campanularia</i>	Hydrophyllaceae	52
244	5-Farnesyl-1,2,4-trihydroxybenzene	<i>P. campanularia</i>	Hydrophyllaceae	52
245	3-Farnesyl-4-hydroxybenzoic acid	<i>P. pedicellata</i>	Hydrophyllaceae	52
246	6 <i>E</i> -Turriculoic acid A	<i>Turricula parryi</i>	Hydrophyllaceae	55
247	6 <i>E</i> -Turriculoic acid B	<i>T. parryi</i>	Hydrophyllaceae	55
248	Turriculoic acid C	<i>T. parryi</i>	Hydrophyllaceae	55
249	Turriculol F	<i>T. parryi</i>	Hydrophyllaceae	55
250	6 <i>Z</i> -Turriculoic acid A	<i>T. parryi</i>	Hydrophyllaceae	55
251	6 <i>Z</i> -Turriculoic acid B	<i>T. parryi</i>	Hydrophyllaceae	55
252	Turriculoic acid D	<i>T. parryi</i>	Hydrophyllaceae	55
253	Turriculol E	<i>T. parryi</i>	Hydrophyllaceae	55
254	3-Farnesyl-4-hydroxybenzoic acid	<i>T. parryi</i> , <i>P. pedicellata</i>	Hydrophyllaceae	55
255	6-[(<i>Z</i>)-10'-Pentadecenyl]salicylic acid	<i>Pelargonium hortorum</i>	Geraniaceae	56, 57

256	6-[(Z)-12'-Heptadecenyl]salicylic acid	<i>P. hortorum</i>	Geraniaceae	56, 57
257	Romanicardic acid	<i>P. hortorum</i>	Geraniaceae	56
258	Geranicardic acid	<i>P. hortorum</i>	Geraniaceae	56
259	22:0 Anacardic acid	<i>P. hortorum</i>	Geraniaceae	58, 59
260	24:0 Anacardic acid	<i>P. hortorum</i>	Geraniaceae	58, 59
261	Primin	<i>Primula obconica</i>	Primulaceae	60
262	Aspidinol B	<i>Dryopteris villarii</i>	Pteridaceae	61
263	4-Hydroxy-3-(2,3-dihydroxy-3-methylbutyl)-benzoic acid methyl ester	<i>Eriodictyon sessilifolium</i>	Hydrophyllaceae	62
264	Methyl-2-(1-hydroxy-1-methylethyl)-2,3-dihydrobenzofuran-5-carboxylate	<i>E. sessilifolium</i>	Hydrophyllaceae	62
265	2,2-Dimethyl-3-hydroxychroman-6-carboxylic acid methyl ester	<i>E. sessilifolium</i>	Hydrophyllaceae	62
266	2,3-Dihydro-12,13-dihydroxy euparin	<i>Heliunthus stuebelii</i>	Asteraceae	4
267	2,3-Dehydro-2-[2-propanyl-1-ol] tremeton	<i>H. stuebelii</i>	Asteraceae	4
268	2,3-Dehydro-2-[2-propanyl-3-ol]-tremeton	<i>V. acutifolia</i> , <i>H. stuebelii</i> , <i>H. sagasteguii</i>	Asteraceae	4
269	2,3-Dehydro-2-[2-propanyl-2,3-epoxi-1-ol]-tremeton	<i>H. stuebelii</i>	Asteraceae	4
270	5-Hydroxy-2,3,4-trimethoxy-9,10-dihydrophenanthrene	<i>E. nigrum</i>	Empetraceae	63
271	4,5-Dihydroxy-2,3-dimethoxy-9,10-dihydrophenanthrene	<i>E. nigrum</i>	Empetraceae	63
272	Humulone (α -bitter acid)	<i>Humulus lupulus</i>	Cannabaceae	64
273	Lupulone (β -bitter acid)	<i>H. lupulus</i>	Cannabaceae	64
274	Para-aspidin AA	<i>Dryopteris arguta</i>	Pteridaceae	61
275	Desaspidin AA	<i>D. arguta</i>	Pteridaceae	61
276	Desaspidin AP	<i>D. arguta</i>	Pteridaceae	61
277	Desaspidin AB	<i>D. arguta</i>	Pteridaceae	61
278	Desaspidin PB	<i>D. arguta</i>	Pteridaceae	61
279	Albaspidin AA	<i>D. villarii</i>	Pteridaceae	61
280	Albaspidin AP	<i>D. villarii</i>	Pteridaceae	61
281	Albaspidin PP	<i>D. villarii</i>	Pteridaceae	61
282	Albaspidin AB	<i>D. villarii</i>	Pteridaceae	61

283	Albaspidin PB	<i>D. villarii</i>	Pteridaceae	61
284	Albaspidin BB	<i>D. villarii</i>	Pteridaceae	61

Table S7. Names and sources of flavonoids 285-341.

No.	Names	Species	Family	Ref.
285	Naringenin	<i>Scalesia baurii</i> ssp. <i>Hopkinsii</i> , <i>Betula</i> spp.	Asteraceae, Betulaceae	3, 65
286	6-Methoxynaringenin	<i>S. baurii</i> ssp. <i>hopkinsii</i>	Asteraceae	3
287	2,3-Dihydro-5,7,4'-trihydroxy-3,6-dimethoxy-flavonol	<i>Scalesia stewartii</i>	Asteraceae	3
288	(2 <i>R</i> ,3 <i>R</i>)-2,3-Dihydro-5,7,4'-trihydroxy-6-methoxyflavonol	<i>Sca. stewartii</i>	Asteraceae	3
289	Nevadensin	<i>Helianthus annuus</i>	Asteraceae	2
290	Desmethoxysudachitin	<i>H. annuus</i>	Asteraceae	2
291	5,7,3'-Trihydroxy-6,8,4'-trimethoxyflavone	<i>H. annuus</i>	Asteraceae	2
292	Xanthomicrol	<i>H. annuus</i>	Asteraceae	2
293	Gardenin B	<i>H. annuus</i>	Asteraceae	2
294	Sideritiflavone	<i>H. annuus</i>	Asteraceae	2
295	Methylsudachitin	<i>H. annuus</i>	Asteraceae	2
296	5-Deoxy-flavenone	<i>H. annuus</i>	Asteraceae	2
297	Hispidulin	<i>H. angustifolius</i> , <i>H. floridanus</i> , <i>H. simulans</i> , <i>T. diversifolia</i> , <i>Heterotheca subaxillaris</i>	Asteraceae	66
298	Nepetin	<i>H. angustifolius</i> , <i>H. floridanus</i> , <i>H. simulans</i>	Asteraceae	66
299	Jaceosidin	<i>H. angustifolius</i> , <i>H. floridanus</i> , <i>H. simulans</i>	Asteraceae	66
300	Hymenoxin	<i>H. angustifolius</i> , <i>H. floridanus</i> , <i>H. simulans</i>	Asteraceae	66
301	Chrysin	<i>Lychnophora ericoides</i>	Asteraceae	67
302	Pinocembrin	<i>Pseudognaphalium robustum</i> , <i>L. ericoides</i>	Asteraceae	67, 68
303	Pinostrobin	<i>L. ericoides</i>	Asteraceae	67
304	Pinobanksin	<i>L. ericoides</i>	Asteraceae	67
305	3- <i>O</i> -Acetylpinobanksin	<i>L. ericoides</i>	Asteraceae	67
306	Artemetin	<i>Laggera pterodonta</i>	Asteraceae	69
307	5-Hydroxy-3,4',6,7-tetramethoxyflavone	<i>L. pterodonta</i>	Asteraceae	69
308	Casticin	<i>L. pterodonta</i>	Asteraceae	69

309	Penduletin	<i>L. pterodonta</i>	Asteraceae	69
310	Eupatilin	<i>A. umbelliformis</i>	Asteraceae	6
311	Apigenin	<i>Betula</i> spp.	Betulaceae	65
312	Kaempferol	<i>Betula</i> spp.	Betulaceae	65
313	Acacetin	<i>Betula</i> spp.	Betulaceae	65
314	Centaureidin	<i>Heterotheca subaxillaris</i>	Asteraceae	23
315	Pectolarigenin	<i>H. subaxillaris</i>	Asteraceae	23
316	Sorbifolin	<i>H. subaxillaris</i>	Asteraceae	23
317	Nuchensin	<i>S. blepharophylla</i>	Lamiaceae	38
318	Pedalitin	<i>S. blepharophylla</i>	Lamiaceae	38
319	6-Geranyl-5,7-dihydroxy-3',4'-dimethoxyflavanone	<i>Paulownia tomentosa</i>	Scrophulariaceae	70
320	6-Geranyl-3',5,7-trihydroxy-4'-methoxyflavanone	<i>P. tomentosa</i>	Scrophulariaceae	70
321	6-Geranyl-4',5,7-trihydroxy-3',5'-dimethoxyflavanone	<i>P. tomentosa</i>	Scrophulariaceae	70
322	6-Geranyl-4',5,5',7-tetrahydroxy-3'-methoxyflavanone	<i>P. tomentosa</i>	Scrophulariaceae	70
323	6-Geranyl-4',5,7-trihydroxy-3'-methoxyflavanone	<i>P. tomentosa</i>	Scrophulariaceae	70
324	Diplacone	<i>P. tomentosa</i>	Scrophulariaceae	70
325	3,4',5,5',7-Pentahydroxy-3'-methoxy-6-(3-methyl-2-butenyl)flavanone	<i>P. tomentosa</i>	Scrophulariaceae	70
326	6-Geranyl-3,3',5,7-tetrahydroxy-4'-methoxyflavanone	<i>P. tomentosa</i>	Scrophulariaceae	70
327	6-Geranyl-3,4',5,7-tetrahydroxy-3'-methoxyflavane	<i>P. tomentosa</i>	Scrophulariaceae	70
328	Diplacol	<i>P. tomentosa</i>	Scrophulariaceae	70
329	4',5,5',7-Tetrahydroxy-6-[6-hydroxy-3,7-dimethyl-2(<i>E</i>),7-octadienyl]-3'-methoxyflavanone	<i>P. tomentosa</i>	Scrophulariaceae	70
330	3',4',5,7-tetrahydroxy-6-[6-hydroxy-3,7-dimethyl-2(<i>E</i>),7-octadienyl]flavanone	<i>P. tomentosa</i>	Scrophulariaceae	70
331	3,3',4',5,7-Pentahydroxy-6-[6-hydroxy-3,7-dimethyl-2(<i>E</i>),7-octadienyl]flavanone	<i>P. tomentosa</i>	Scrophulariaceae	70
332	3,3',4',5,7-Pentahydroxy-6-[7-hydroxy-3,7-dimethyl-2(<i>E</i>)-octenyl]flavanone	<i>P. tomentosa</i>	Scrophulariaceae	70
333	3',4',5,7-Pentahydroxy-6-[7-	<i>P. tomentosa</i>	Scrophulariaceae	70

	hydroxy-3,7-dimethyl-2(<i>E</i>)- octenyl]flavanone			
334	Xanthohumol	<i>H. lupulus</i>	Cannabaceae	64
335	2',4'-Dihydroxychalcone	<i>Empetrum nigrum</i>	Empetraceae	63
336	2'-Hydroxy-4'-methoxychalcone	<i>E. nigrum</i>	Empetraceae	63
337	2',4'-Dihydroxydihydrochalcone	<i>E. nigrum</i>	Empetraceae	63
338	4'-Hydroxy-2'-methoxy- dihydrochalcone	<i>E. nigrum</i>	Empetraceae	63
339	2'-Hydroxy-4'-methoxy- dihydrochalcone	<i>E. nigrum</i>	Empetraceae	63
340	2',4'-Dihydroxy-6'-methoxy- dihydrochalcone	<i>E. nigrum</i>	Empetraceae	63
341	2'-Hydroxy-4',6'-dimethoxy- dihydrochalcone	<i>E. nigrum</i>	Empetraceae	63

Table S8. Names and sources of acylsugars 342-416.

No.	Names	Species	Family	Ref.
342	6 <i>S</i> -(6- <i>O</i> -Acetyl- β -D- glucopyranosyloxy)octadecanoic acid	<i>Ibicella lutea</i>	Martyniaceae	47
343	6 <i>S</i> -(6- <i>O</i> -Acetyl- β -D- glucopyranosyloxy)eicosanoic acid	<i>I. lutea</i>	Martyniaceae	47
344	6 <i>S</i> -(6- <i>O</i> -Acetyl- β -D- glucopyranosyloxy)docosanoic acid	<i>I. lutea</i>	Martyniaceae	47
345	6 <i>S</i> -(β -D- Glucopyranosyloxy)octadecanoic acid	<i>I. lutea</i>	Martyniaceae	47
346	6 <i>S</i> -(β -D- Glucopyranosyloxy)eicosanoic acid	<i>I. lutea</i>	Martyniaceae	47
347	6 <i>S</i> -(β -D- Glucopyranosyloxy)docosanoic acid	<i>I. lutea</i>	Martyniaceae	47
348	8 <i>S</i> -(6- <i>O</i> -Acetyl- β -D- glucopyranosyloxy)eicosanoic acid	<i>Proboscidea louisiana</i>	Martyniaceae	47
349	8 <i>S</i> -(6- <i>O</i> -Acetyl- β -D- glucopyranosyloxy)docosanoic acid	<i>P. louisiana</i>	Martyniaceae	47

350	8 <i>S</i> -(β -D-Glucopyranosyloxy)icosanoic acid	<i>P. louisiana</i>	Martyniaceae	47
351	8 <i>S</i> -(β -D-Glucopyranosyloxy)docosanoic acid	<i>P. louisiana</i>	Martyniaceae	47
352	2- <i>O</i> -Acetyl-3- <i>O</i> -isobutyryl-4- <i>O</i> -isocaprylglucopyranose	<i>Solanum</i> spp.	Solanaceae	71
353	3'- <i>O</i> -Hexanoyl glucose	<i>Datura wrightii</i>	Solanaceae	72
354-359	Tri- <i>O</i> -acyl- α -D-glucopyranosyl- β -D-fructofuranosides	<i>Nicotiana attenuata</i>	Solanaceae	73
360-364	Tri- <i>O</i> -acyl- α -D-glucopyranosyl-(<i>O</i> -acetyl)- β -D-fructofuranosides	<i>N. attenuata</i>	Solanaceae	73
365-368	(<i>O</i> -Acetyl-tri- <i>O</i> -acyl)- α -D-glucopyranosyl-(<i>O</i> -Acetyl)- β -D-fructofuranosides	<i>N. attenuata</i>	Solanaceae	73
369	3,4-Di- <i>O</i> -isobutyryl-6- <i>O</i> -caprylsucrose	<i>Solanum berthaultii</i>	Solanaceae	74
370	6- <i>O</i> -Capryl-3,3',4-tri- <i>O</i> -isobutyrylsucrose	<i>S. berthaultii</i>	Solanaceae	75
371	6- <i>O</i> -Capryl-3'- <i>O</i> -isobutyryl-3,4-di- <i>O</i> -(2-methylbutyryl)sucrose	<i>S. berthaultii</i>	Solanaceae	75
372	2- <i>O</i> -Acetyl-3'- <i>O</i> -hexanoyl-3,4-di- <i>O</i> -isobutyrylsucrose	<i>S. neocurdenusii</i>	Solanaceae	76
373	2- <i>O</i> -Acetyl-3',4-di- <i>O</i> -hexanoyl-3- <i>O</i> -isobutyrylsucrose	<i>S. neocurdenusii</i>	Solanaceae	76
374	2- <i>O</i> -Acetyl-3'- <i>O</i> -decanoyl-3,4-di- <i>O</i> -isobutyrylsucrose	<i>S. neocurdenusii</i>	Solanaceae	76
375	2,4,1'-Tri- <i>O</i> -(3-methylbutyryl)-3- <i>O</i> -(2-methylbutyryl)sucrose	<i>Lycopersicon hirsutum</i>	Solanaceae	77
376	2- <i>O</i> -Acetyl-3- <i>O</i> -isobutyryl-3'- <i>O</i> -isodecanoyl-4- <i>O</i> -(3-methylbutyryl)-sucrose	<i>L. typicum</i>	Solanaceae	78
377	2-Acetyl-3,4-di- <i>O</i> -isobutyryl-3'- <i>O</i> -isodecanoyl sucrose	<i>L. typicum</i>	Solanaceae	78
378	2- <i>O</i> -Acetyl-4,3'-di- <i>O</i> -(3-methylbutyryl)-3- <i>O</i> -(2-methylbutyryl)sucrose	<i>L. typicum</i>	Solanaceae	78
379	2- <i>O</i> -Acetyl-3,4,3'-tri- <i>O</i> -isobutyrylsucrose	<i>L. typicum</i>	Solanaceae	78
380	1',6'-Diacyl-2,3,4,6-tetra(3-methyl valerianyl)-sucrose	<i>Salpichroa organifolia</i>	Solanaceae	79

381	2-Acetyl-1-{3-[3,4-di- <i>O</i> -acetyl- β -D-glucopyranosyl-(1 \rightarrow 3)-2- <i>O</i> -acetyl- α -L-rhamnopyranosyloxy]octadecanoyl}- <i>sn</i> -glycerol	<i>Cerasus yedoensis</i>	Rosaceae	46
382	Pelargoside A1	<i>Erodium pelargoniflorum</i>	Geraniaceae	80
383	Pelargoside B1	<i>E. pelargoniflorum</i>	Geraniaceae	80
384	Pelargoside A2	<i>E. pelargoniflorum</i>	Geraniaceae	80
385	Pelargoside A3	<i>E. pelargoniflorum</i>	Geraniaceae	80
386	Pelargoside A4	<i>E. pelargoniflorum</i>	Geraniaceae	80
387	Pelargoside B2	<i>E. pelargoniflorum</i>	Geraniaceae	80
388	Pelargoside B3	<i>E. pelargoniflorum</i>	Geraniaceae	80
389	Pelargoside B4	<i>E. pelargoniflorum</i>	Geraniaceae	80
390	Caroliniaside A	<i>E. pelargoniflorum</i>	Geraniaceae	81
391	Caroliniaside B	<i>E. pelargoniflorum</i>	Geraniaceae	81
392	Caroliniaside C	<i>E. pelargoniflorum</i>	Geraniaceae	81
393	Gallicaside A	<i>Silene gallica</i>	Caryophyllaceae	82
394	Gallicaside C	<i>S. gallica</i>	Caryophyllaceae	82
395	Gallicaside F	<i>S. gallica</i>	Caryophyllaceae	82
396	Gallicaside I	<i>S. gallica</i>	Caryophyllaceae	82
397	Gallicaside B	<i>S. gallica</i>	Caryophyllaceae	82
398	Gallicaside D	<i>S. gallica</i>	Caryophyllaceae	82
399	Gallicaside E	<i>S. gallica</i>	Caryophyllaceae	82
400	Gallicaside G	<i>S. gallica</i>	Caryophyllaceae	82
401	Gallicaside H	<i>S. gallica</i>	Caryophyllaceae	82
402	Gallicaside J	<i>S. gallica</i>	Caryophyllaceae	82
403	Glomeraside A	<i>Cerastium glomeratum</i>	Caryophyllaceae	83
404	Glomeraside D	<i>C. glomeratum</i>	Caryophyllaceae	83
405	Glomeraside F	<i>C. glomeratum</i>	Caryophyllaceae	83
406	Glomeraside I	<i>C. glomeratum</i>	Caryophyllaceae	83
407	Glomeraside K	<i>C. glomeratum</i>	Caryophyllaceae	83
408	Glomeraside M	<i>C. glomeratum</i>	Caryophyllaceae	83
409	Glomeraside B	<i>C. glomeratum</i>	Caryophyllaceae	83
410	Glomeraside E	<i>C. glomeratum</i>	Caryophyllaceae	83
411	Glomeraside G	<i>C. glomeratum</i>	Caryophyllaceae	83
412	Glomeraside J	<i>C. glomeratum</i>	Caryophyllaceae	83
413	Glomeraside L	<i>C. glomeratum</i>	Caryophyllaceae	83
414	Glomeraside N	<i>C. glomeratum</i>	Caryophyllaceae	83
411	Glomeraside C	<i>C. glomeratum</i>	Caryophyllaceae	83
416	Glomeraside H	<i>C. glomeratum</i>	Caryophyllaceae	83

Table S9. Names and sources of glycerides 417-483.

No.	Names	Species	Family	Ref.
417		<i>Ceratotheca triloba</i>	Pedaliaceae	84
418	1- <i>O</i> -Acetyl-2- <i>O</i> -[(<i>R</i>)-(3-acetyloxyoctadecanoyl)-3- <i>O</i> -malonylglycerol	<i>C. triloba</i>	Pedaliaceae	84
419-422		<i>C. triloba</i>	Pedaliaceae	84
423	1- <i>O</i> -Acetyl-2- <i>O</i> -[(<i>R</i>)-3-acetyloxyicosanoyl]-3- <i>O</i> -malonylglycerol	<i>C. triloba</i>	Pedaliaceae	84
424-425		<i>C. triloba</i>	Pedaliaceae	84
426-430	2- <i>O</i> -[(3 <i>R</i> ,6 <i>S</i>)-3,6-Diacetyloxyfattyacyl]glycerols	<i>Ibicella lutea</i> , <i>Proboscidea louisiana</i>	Martyniaceae	47
431-435	2- <i>O</i> -[(3 <i>R</i>)-3-Acetyloxyfattyacyl]glycerols	<i>I. lutea</i> , <i>P. louisiana</i>	Martyniaceae	47
436-440	2- <i>O</i> -[(3 <i>R</i> ,6 <i>S</i>)-3,6-Diacetyloxyfattyacyl]glycerols	<i>I. lutea</i> , <i>P. louisiana</i>	Martyniaceae	47
441-445	2- <i>O</i> -[(3 <i>R</i>)-3-Acetyloxyfattyacyl]glycerols	<i>I. lutea</i> , <i>P. louisiana</i>	Martyniaceae	47
446-449	2- <i>O</i> -[(3 <i>R</i> ,6 <i>S</i>)-3,6-Diacetyloxyfattyacyl]glycerols	<i>I. lutea</i> , <i>P. louisiana</i>	Martyniaceae	47
450	1- <i>O</i> -Acetyl-3- <i>O</i> -[(<i>R</i>)-3-Hydroxytetradecanoyl]glycerol	<i>Verbascum blattaria</i> <i>f. erubescens</i>	Scrophulariaceae	85
451	1- <i>O</i> -Acetyl-3- <i>O</i> -[(<i>R</i>)-3-Hydroxyhexadecanoyl]glycerol	<i>V. blattaria f.</i> <i>erubescens</i>	Scrophulariaceae	85
452	2- <i>O</i> -(3-Hydroxytetradecanoyl)glycerol	<i>V. blattaria f.</i> <i>erubescens</i>	Scrophulariaceae	85
453	2- <i>O</i> -(3-Hydroxyhexadecanoyl)glycerol	<i>V. blattaria f.</i> <i>erubescens</i>	Scrophulariaceae	85
454	1,3-di- <i>O</i> -Acetyl-2- <i>O</i> -[(3 <i>R</i> ,6 <i>S</i>)-3-(acetyloxy)-6-hydroxyeicosanoyl]glycerol	<i>Paulownia tomentosa</i>	Scrophulariaceae	86, 87
455	2- <i>O</i> -[(3 <i>R</i>)-3-(Acetyloxy)octadecanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
456	2- <i>O</i> -[(3 <i>R</i>)-3-(Acetyloxy)eicosanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
457	1- <i>O</i> -Acetyl-2- <i>O</i> -[(3 <i>R</i>)-3-(acetyloxy)octadecanoyl]- <i>sn</i> -	<i>P. tomentosa</i>	Scrophulariaceae	86, 87

	glycerol			
458	1- <i>O</i> -Acetyl-2- <i>O</i> -[(3R)-3-(acetyloxy)eicosanoyl]- <i>sn</i> -glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
459	1- <i>O</i> -Acetyl-2- <i>O</i> -[(3R,7R)-3,7-bis(acetyloxy)octadecanoyl]- <i>sn</i> -glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
460	1- <i>O</i> -Acetyl-2- <i>O</i> -[(3R,6S)-3,6-bis(acetyloxy)eicosanoyl]- <i>sn</i> -glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
461	1- <i>O</i> -Acetyl-2- <i>O</i> -[(3R,7R)-3,7-bis(acetyloxy)eicosanoyl]- <i>sn</i> -glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
462	1- <i>O</i> -Acetyl-2- <i>O</i> -[(3R,6S)-3-(acetyloxy)-6-hydroxyoctadecanoyl]- <i>sn</i> -glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
463	1- <i>O</i> -Acetyl-2- <i>O</i> -[(3R,6S)-3-(acetyloxy)-6-hydroxyeicosanoyl]- <i>sn</i> -glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
464	1- <i>O</i> -Acetyl-2- <i>O</i> -[(3R,8R)-3,8-bis(acetyloxy)eicosanoyl]- <i>sn</i> -glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
465	1- <i>O</i> -Acetyl-2- <i>O</i> -[(3R,9R)-3,9-bis(acetyloxy)eicosanoyl]- <i>sn</i> -glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
466	1- <i>O</i> -Acetyl-2- <i>O</i> -[(3R,8R)-3-(acetyloxy)-8-hydroxyeicosanoyl]- <i>sn</i> -glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
467	1- <i>O</i> -Acetyl-2- <i>O</i> -[(3R,9R)-3-(acetyloxy)-9-hydroxyeicosanoyl]- <i>sn</i> -glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
468	2- <i>O</i> -[(3R,7R)-3,7-bis(Acetyloxy)octadecanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
469	2- <i>O</i> -[(3R,8R)-3,8-bis-(Acetyloxy)octadecanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
470	2- <i>O</i> -[(3R,8R)-3,8-bis(Acetyloxy)eicosanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
471	2- <i>O</i> -[(3R,6S)-3-(Acetyloxy)-6-hydroxyoctadecanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
472	2- <i>O</i> -[(3R,8R)-3-(Acetyloxy)-8-hydroxyoctadecanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87

473	2- <i>O</i> -[(3R,6S)-3-(Acetyloxy)-6-hydroxyeicosanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
474	2- <i>O</i> -[(3R,8R)-3-(Acetyloxy)-8-hydroxyeicosanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
475	2- <i>O</i> -[(3R,9R)-3,9-bis(Acetyloxy)eicosanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
476	2- <i>O</i> -[(3R,7R)-3-(Acetyloxy)-7-hydroxyoctadecanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
477	2- <i>O</i> -[(3R,9R)-3-(Acetyloxy)-9-hydroxyoctadecanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
478	2- <i>O</i> -[(3R,7R)-3-(Acetyloxy)-7-hydroxyeicosanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
479	2- <i>O</i> -[(3R,9R)-3-(Acetyloxy)-9-hydroxyeicosanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
480	2- <i>O</i> -[(3R,6S)-3,6-Dihydroxyeicosanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
481	2- <i>O</i> -[(3R,8R)-3,8-Dihydroxyeicosanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
482	2- <i>O</i> -[(3R,7R)-3,7-Dihydroxyeicosanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87
483	2- <i>O</i> -[(3R,9R)-3,9-Dihydroxyeicosanoyl]glycerol	<i>P. tomentosa</i>	Scrophulariaceae	86, 87

Table S10. Names and sources of alkaloids 484-489.

No.	Names	Species	Family	Ref.
484	<i>N</i> -Hydroxydodecanoic acid normicotine	<i>Nicotiana repanda</i>	Solanaceae	88
485	<i>N</i> -Hydroxy-tridecanoic acid normicotine	<i>N. repanda</i>	Solanaceae	88
486	<i>N</i> -Hydroxytetradecanoic acid normicotine	<i>N. repanda</i>	Solanaceae	88
487	<i>N</i> -Hydroxypentanoic acid normicotine	<i>N. repanda</i>	Solanaceae	88
488	<i>N</i> -Undecanoic acid normicotine	<i>N. repanda</i>	Solanaceae	88
489	<i>N</i> -Dodecanoic acid normicotine	<i>N. repanda</i>	Solanaceae	88

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