

## Supplementary Materials

# Exploring African medicinal plants for potential anti-diabetic compounds with the DIA-DB inverse virtual screening web server.

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**Table S1.** SMILES notations of all compounds evaluated in the study

Compound name	SMILES
(+)-Toddanol	<chem>C=C(C)[C@@H](Cc1c(cc2c(ccc(=O)o2)c1OC)OC)O</chem>
[7]-Paradol	<chem>CCCCCCCC(=O)CCc1ccc(c1)OC)O</chem>
1,10,5-Germacrodien-4-ol	<chem>CC(C)[C@@H]1CC/C(=C\CC[C@@](C)/C=C\1)O)/C</chem>
1,2-Epoxysecoisochlorogenic acid	<chem>CC(=O)OC1C[C@@]2(C(CC[C@]3(C)C[C@H](C[C@]23O)c2ccc(=O)oc2)[C@]2(C)C1=C[C@H]([C@H]1[C@@H]2O1)O)O</chem>
1,3,6,8-Tetrahydroxy-2,5-dimethoxyanthrone	<chem>COC1=C(C2C(C=C1O)Oc1c(cc(c1OC)O)O)C2=O)O</chem>
1,5-Dicaffeoylquinic acid	<chem>C1C(C(C(CC1(C(=O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)OC(=O)C=CC3=CC(=C(C=C3)O)O)O)O</chem>
1,5-Dihydroxy-3-methylanthraquinone	<chem>Cc1cc2c(c1)OC(=O)c1ccc(cc1C2=O)O</chem>
1,8-Cineole	<chem>CC1(C)C2CC[C@@](C)(CC2)O1</chem>
10-Deoxyeucommiol	<chem>OCC[C@@H]1C(CO)=C(C)C[C@H]1O</chem>
10-Hydroxyakagerine	<chem>C/C=C(/C=O)\[C@@H]1C[C@H]2c3c(CCN2C)c2cc(ccc2n3[C@H](C1)O)O</chem>
12B-Hydroxysecoisochlorogenic acid	<chem>CC(=O)O[C@@H]1C[C@@]2([C@H](CC(=O)[C@]3(C)[C@H](CC[C@]23O)C2=COC(=O)OC2)[C@@]2(C)CC[C@@H](C=C12)O)O</chem>
12-Hydroxydaphnetoxin	<chem>C=C(C)[C@]12[C@@H](C(C)[C@]34C5C=C(C)C(=O)[C@]5([C@@H]([C@]5(CO)[C@H]([C@H]3[C@H]1OC(c1cccc1)(O2)O4)O5)O)O)O</chem>
12-O-Palmitoyl-13-O-acetyl-16-hydroxyphorbol	<chem>CCCCCCCCCCCCCCCC(=O)O[C@@H]1[C@@H](C)[C@]2([C@@H](CC=C(C[C@]3([C@H]2C=C(C)C3=O)O)CO)[C@@H]2[C@@](C)(CO)[C@]12OC(=O)C)O</chem>
15-Acetoxy-14-hydroxycostundide	<chem>C=C1[C@@H]2CC/C(=C\CC/C(=C\[C@H]2OC1=O)/COC(=O)C)/CO</chem>
15B-Hydroxygomphoside	<chem>C[C@@H]1C[C@H]([C@@]2(C[C@@H]3C[C@@]4(C)C(CC[C@@H]5C4CC[C@]4(C)[C@H](C[C@H]([C@]54O)O)C4=CC(=O)OC4)C[C@H]3C[C@@H]2O1)O)O</chem>
15-Oxo-kaurenoic acid	<chem>C=C1[C@@H]2CC[C@H]3[C@]4(C)CCC[C@](C)([C@H]4CC[C@]3(C2)C1=O)C(=O)O</chem>
16B-Formylxybovogenin A	<chem>C[C@@]12CCC3C(CC[C@H]4C[C@H](CC[C@]34CO)O)[C@]2(C[C@@H]([C@@H]1c1ccc(=O)oc1)OC=O)O</chem>
19-Deoxyuscharin	<chem>C[C@@H]1CC2([C@]3([C@@H](O1)O[C@@H]1C[C@@H]4CC[C@@H]5C(CC[C@]6(C)C(CC[C@]56O)C5=CC(=O)OC5)[C@@]4(C)C[C@H]1O3)O)N=CCS2</chem>
19-Hydroxyglaucolide A	<chem>C=C(CO)C(=O)OC1CC(C)(OC(C)=O)C(=O)CCC3(C)OC3C2OC(=O)C(COC(C)=O)=C12</chem>
1B,3B-Dihydroxy-5,16-pregnadien-20-one	<chem>CC(=O)C1=CCC2C3CC=C4C[C@H](C[C@H]([C@]4(C)C3CC[C@]12C)O)O</chem>
1-Hydroxydimethylanthraquinone	<chem>Cc1cc2c(c1)OC(=O)c1cccc1C2=O</chem>
2-(1-Hydroxyethyl)naphtho[2,3-b]furan-4,9-dione	<chem>C=C(C)c2cc3C(=O)c1cccc1C(=O)c3o2</chem>
24-Ethylcholest-5-en-3B-ol	<chem>CC(=CCC[C@@H](C)[C@H]1CC[C@@]2(C)[C@@H]3CC[C@H]4C(C)(C)[C@H](CC[C@@]54C[C@]35CC[C@]12C)O)C</chem>
2-Hydroxy-4-methoxybenzaldehyde	<chem>COC1=CC(=C(C=C1)C=O)O</chem>
2-Hydroxygenistein	<chem>C1=CC(=C(C=C1O)O)C2=COC3=CC(=CC(=C3C2=O)O)O</chem>
2-Methoxyfuranodiene	<chem>CC1=CCC2=C(CCC(=CC(C1)OC)C)OC=C2C</chem>

2-Methyl-6,3-methyl-2-butenylbenzo-1,4-quinone	<chem>CC(=CCC1=CC(=O)C=C(C)C1=O)C</chem>
2-Undecanone	<chem>CCCCCCCCC(=O)C</chem>
2 $\alpha$ ,3 $\alpha$ ,23-Trihydroxyurs-12-en-28-oic acid	<chem>C[C@@H]1CC[C@@]2(CC[C@]3(C)C(=CC[C@@H]4[C@@]5(C)C[C@@H](O)[C@@H](O)[C@@](C)(CO)[C@@H]5CC[C@@]34C)[C@@H]2[C@H]1C)C(=O)O</chem>
2 $\alpha$ ,3 $\alpha$ -Dihydroxyurs-12-en-28-oic acid	<chem>C[C@H]1[C@@H]([C@@H]2[C@@](CC[C@@]3(C2=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(C[C@H]([C@H]([C@]5(C)C)O)O)C)C)(CC1)C(=O)O)C</chem>
2 $\alpha$ ,3 $\beta$ -Dihydroxyurs-12-en-18-oic acid	<chem>C[C@H]1[C@@H]([C@@H]2[C@@](CC[C@@]3(C2=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(C[C@H]([C@H]([C@]5(C)C)O)O)C)C)(CC1)C(=O)O)C</chem>
2 $\alpha$ ,3 $\beta$ -Dihydroxyurs-12-en-28-oic acid	<chem>CC1CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C(C5(C)C)O)O)C)C)C2C1C)C(=O)OC6C(C(C(C(O6)CO)O)O)O</chem>
2 $\alpha$ -Hydroxyursolic acid	<chem>C[C@@H]1CC[C@@]2(CC[C@]3(C)C(=CC[C@@H]4[C@@]5(C)C[C@H]([C@@H](C(C)(C)[C@@H]5CC[C@@]34C)O)O)[C@@H]2[C@H]1C)C(=O)O</chem>
3-(2'-hydroxyethyl)-5-(2"-hydroxypropyl)-dihydrofuran-2(3H)-one	<chem>OC(C)CC1CC(CCO)C(=O)O1</chem>
3,3,4,5,5-Pentahydroxystilbene	<chem>C(=C\c1cc(c(c(c1)O)O)O)/c1cc(cc(c1)O)O</chem>
3,3,4-Dihydroxyphenyl-1,2-propane diol	<chem>c1cc(c(cc1CC(CO)O)O)O</chem>
3,8,11-Heptadecadienylcatechol	<chem>CCCCC/C=C\C/C=C\CCCCCcc1cccc(c1O)O</chem>
3,9-Dihydroeucomnalin	<chem>Oc1ccc(cc1)CC2COc3cc(O)c(OC)c(O)c3C2=O</chem>
3-Acetoxybrachylaenolide	<chem>C=C1[C@@H]2CC[C@@]3(C)C=C[C@H](C(=C)C3[C@H]2OC1=O)OC(=O)C</chem>
3-Acetylnerbowdine	<chem>CC(=O)O[C@@H]1C[C@@H]2[C@@]3(CCN2Cc2c3cc3c(c2OC)OCO3)[C@@H](C1)O</chem>
3B,24-Dihydroxyurs-12-en-28-oic acid	<chem>C[C@@H]1CC[C@@]2(CC[C@]3(C(=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(CC[C@@H]([C@]5(C)CO)O)C)C)[C@@H]2[C@H]1C)C(=O)O</chem>
3B-Hydroxynorerythrosumamine	<chem>O=C(OCCNC)\C=C3/CCC2C([C@@H](O)C(=O)C1[C@]2(C)CC[C@H](O)[C@]1(C)C(=O)OC)[C@H]3C</chem>
3B-Hydroxynorerythrosumamine- $\beta$ -D-glucopyranosyl	<chem>O=C(OCCNC)\C=C1/CCC3C([C@H]1C)[C@@H](O)C(=O)C4[C@](C)([C@@H](OC2OC(CO)C(O)C(O)C2O)CC[C@]34C)C(=O)OC</chem>
3-Coumaric acid	<chem>c1cc(ccc1/C=C/C(=O)O)O</chem>
3-Epioleanolic acid	<chem>CC1(C)CCC2(CC[C@]3(C)C(=CCC4[C@@]5(C)CC[C@H](C(C)(C)C5CC[C@@]34C)O)C2C1)C(=O)O</chem>
3-Hydroxy-4-methoxy-3-methyloxidole	<chem>CC1(c2c(cccc2OC)NC1=O)O</chem>
3-Hydroxyheterodendrin	<chem>CC(C)([C@@H](C#N)OC1C(C(C(CO)O1)O)O)O</chem>
3-Oxo-20,24-dammaradien-26-ol	<chem>C/C(=C\CCC(=O)[C@H]1CC[C@]2(C)[C@@H]1CCC1[C@@]3(C)CCC(=O)C(C)(C)C3CC[C@@]21C)/CO</chem>
3-O- $\alpha$ -D-galactopyranosyl-L-arabinose	<chem>C(C1[C@H](C([C@H]([C@H](O1)O)[C@H]1[C@H](COC([C@H]1O)O)O)O)O)O</chem>
3-O- $\beta$ -D-Glucopyranosyl rosmarinic acid	<chem>c1cc(c(cc1/C=C/C(=O)O)[C@@H](Cc1ccc(c(c1)OCC(C(C(C(=O)O)O)O)O)O)C(=O)O)O)O</chem>
3-O- $\beta$ -L-arabinopyranosyl-L-arabinose	<chem>O[C@H]2CO[C@H](O)[C@@H](O)C2O[C@H]1OC[C@H](O)C(O)[C@@H]1O</chem>
4,5-Hydroxy-5,16-nonadecenyl-2-cyclohexen-1-one	<chem>CC/C=C/CCCCCCCCCCCCC[C@@H]1CC(=O)C=C[C@@H]1O</chem>

4,5 $\alpha$ -Epoxy-6 $\alpha$ -hydroxy-1(10)- E-11(13)-germacradien-12,8 $\alpha$ -olide	<chem>C/C1=C/CC[C@@]2(C)[C@@H]([C@H]([C@@H]3C(=C)C(=O)O[C@H]3C1)O)O2</chem>
411-Eudesmonediol	<chem>CC(C)([C@@H]1CC[C@@]2(C)CCC[C@](C)(C2C1)O)O</chem>
4-Deoxy-13-O-phenylacetyl-12-O-tiloylphorbol	<chem>C/C=C(/C)\C(=O)OC1[C@@H](C)[C@@]2([C@@H]3C=C(C)C(=O)C3CC(=C[C@H]2[C@@H]2C(C)(C)[C@]12OC(=O)CC1CCCC1)CO)O</chem>
4-Hydroxyacetophenone	<chem>CC(=O)c1ccc(cc1)O</chem>
4-Hydroxymethylanthrixianone	<chem>C=C1C[C@]23C=CC4=C(CO)C(=O)CC[C@@]4(C)[C@@H]3CC[C@H]1C2</chem>
4-Hydroxyphenyl-N-methylaziridine	<chem>CN1CC1c1ccc(cc1)O</chem>
4-Methoxy-1-Methyl-2,1H-quinolinone	<chem>Cn1c2cccc(c2ccc1=O)OC</chem>
4-Methoxy-1-methyl-2-quinolone	<chem>Cn1c2cccc2c(cc1=O)OC</chem>
4-O-Ethylgallic acid	<chem>C(CO)c1c(cc(cc1O)C(=O)O)O</chem>
4-O-Methylpyridoxine	<chem>Cc1c(c(COC)c(cn1)CO)O</chem>
4 $\alpha$ ,18-Epoxyafricanin	<chem>C[C@@H]1CC(=O)[C@]2(COC(=O)C)[C@H](CCC(=O)[C@@]32CO3)[C@]21C[C@@H](c1ccoc1)OC2=O</chem>
5,6,7-Trimethoxycoumarin	<chem>COc1cc2c(ccc(=O)o2)c(c1OC)OC</chem>
5,7,4-Trihydroxy-3,6-dimethylmethoxyflavone	<chem>COc1c(cc2c(c1O)c(=O)c(c(c1cccc(c1)O)o2)OC)O</chem>
5,7,8-Trimethoxycoumarin	<chem>COc1cc(c(c2c1ccc(=O)o2)OC)OC</chem>
5,7-Dihydroxy-6-methoxy-3(4-hydroxybenzyl)chroman-4-one	<chem>c1cc(c(cc1CC1COc2cc(c(c2C1=O)O)O)O)O</chem>
5-Caffeoylquinic acid	<chem>C1C(C(C(CC1(C(=O)O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)O)O</chem>
5-Chloropropacin	<chem>CC1C(OC2=C(O1)C3=C(C=CC(=O)O3)C(=C2OC)C1)C4=CC(=C(C=C4)O)OC</chem>
5-Hydroxyaloin A	<chem>C1=CC(=C2C(=C1O)C(C3=CC(=CC(=C3C2=O)O)CO)C4C(C(C(C(O4)CO)O)O)O)O</chem>
5-Hydroxyhexamethoxyflavanol	<chem>COc1cc(cc(c1OC)OC)c1c(c(=O)c2c(c(c(c2o1)OC)OC)OC)O)O</chem>
5-Hydroxyindole-3-acetic acid	<chem>c1cc2c(cc1O)c(CC(=O)O)c[nH]2</chem>
5-Hydroxytryptophan	<chem>c1cc2c(cc1O)c(CC(C(=O)O)N)c[nH]2</chem>
5-Methoxysuberenon	<chem>CC(=O)/C=C/c1c(cc2OC(=O)C=Cc2c1OC)OC</chem>
5-O-Acetyl-4-O-methylpyridoxine	<chem>Cc1c(c(COC)c(cn1)COC(=O)C)O</chem>
5 $\alpha$ -Hydroxy-10B-hydroprintzionic acid	<chem>C[C@@H]1CC[C@]2(CC(=CCC[C@@H]2[C@@]1(C)CCc1ccoc1)C(=O)O)O</chem>
6-(2-Hydroxy-3-methoxy-3-methylbutyl)-5,7-dimethoxycoumarin	<chem>CC(C)(OC)C(O)Cc1c(cc2OC(=O)C=Cc2c1OC)OC</chem>
6-(3-Chloro-2-hydroxy-3-methylbutyl)-5,7-dimethoxycoumarin	<chem>CC(C)(Cl)C(O)Cc1c(cc2OC(=O)C=Cc2c1OC)OC</chem>
6,7-Dihydro-6,7-ocimenediol	<chem>CC(C)(O)C(O)C\C=C(/C)C=C</chem>
6-Formyllimetin	<chem>COc1cc2OC(=O)C=Cc2c(OC)c1C=O</chem>
6-Gingerol	<chem>CCCCC[C@@H](CC(=O)CCc1ccc(c(c1)OC)O)O</chem>

6-Hydroxy-5,7-dimethoxycoumarin-8-sulfate	<chem>COc1c2ccc(=O)oc2c(c1O)OC)S</chem>
6-Methyldiosgenin	<chem>C[C@H]6C2C(CC3C4CC(C)=C1C[C@@H](O)CC[C@]1(C)C4CC[C@]23C)O[C@@]56CCC(C)CO5</chem>
6-Paradol	<chem>CCCCCCCC(=O)CCC1=CC(=C(C=C1)O)OC</chem>
6-Shogaol	<chem>CCCCC=CC(=O)CCC1=CC(=C(C=C1)O)OC</chem>
7-Hydroxy-10-deoxyeucommiol	<chem>CC1=C(CO)[C@@H](CCO)[C@H](O)[C@@H]1O</chem>
7-Hydroxy-4-6-dimethoxypropacin	<chem>COc1cc(cc(OC)c1O)[C@H]2Oc3c(O[C@@H]2C)c4OC(=O)C=Cc4cc3OC</chem>
7-Hydroxyeucommic acid	<chem>OCC1=C(CO)[C@@H](CC(=O)O)[C@H](O)[C@@H]1O</chem>
7-hydroxyviteoid II	<chem>O=C1OCC[C@@H]2C1=C(CO)[C@@H](O)[C@H]2O</chem>
7-Methyljuglone	<chem>Cc1cc2c(c1O)C(=O)C=C(C2=O)O</chem>
8-(3,3-Dimethylallyl)-6,7-dimethoxycoumarin	<chem>CC(=CCc1c2c(ccc(=O)o2)cc(c1OC)OC)C</chem>
8,(14),15-Isopyrimidine-7,18-diol	<chem>C=C[C@@]1(C)CCC2C(=C1)[C@@H](CC1[C@@](C)(CCC[C@]21C)CO)O</chem>
8-Formyllymettin	<chem>COc2cc(OC)c(C=O)c1OC(=O)C=Cc12</chem>
8-Hydroxypinoresinol	<chem>COC1=C(C=CC(=C1)C2C3COC(C3(CO2)O)C4=CC(=C(C=C4)O)OC)O</chem>
9-Geranyl-a-terpineol	<chem>CC(=CCC/C(=C/CCC(C)(C1CC=C(C)CC1)O)/C)C</chem>
9Z-Octadec- 9-enamide	<chem>CCCCCCCC/C=C\CCCCCCCC(=O)N</chem>
Abrine	<chem>CN[C@@H](Cc1c[nH]c2cccc12)C(=O)O</chem>
Acacic acid	<chem>CC1(C)C[C@H]2C3=CCC4[C@@]5(C)CC[C@@H](C(C)(C)C5CC[C@@]4(C)[C@]3(C)C[C@H]([C@]2(C[C@@H]1O)C(=O)O)O)O</chem>
Acalyphin	<chem>CN1C(=O)C=C(C(C#N)(C1O)OC1C(C(C(CO)O1)O)O)OC</chem>
Acetylcaranine	<chem>CC(=O)OC1CC=C2CCN3Cc4cc5c(cc4[C@H]1[C@@H]23)OCO5</chem>
Acolongifloroside K	<chem>CC1C(C(C(C(O1)OC2CC(C3(C4C(CCC3(C2)O)C5(CCC(C5(CC4O)C)C6=CC(=O)OC6)O)CO)O)O)O)O</chem>
Acorenone	<chem>CC(C)[C@@H]1CC[C@H](C)C21CC=C(C)C(=O)C2</chem>
Acovenoside A	<chem>CC1C(C(C(C(O1)OC2CC3CCC4C(C3(C(C2)O)C)CCC5(C4(CCC5C6=CC(=O)OC6)O)C)O)OC)O</chem>
Adiantone	<chem>CC1(C)CCC[C@@H]2C3CC[C@@H]4[C@@]5(C)CC[C@H](COC)[C@@H]5CC[C@@]4(C)[C@@H]3CCC12</chem>
Africanol	<chem>CC1CCC2C1(CC(CC3C2(C3)C)(C)C)O</chem>
Afromosin	<chem>COC1=CC=C(C=C1)C2=COC3=CC(=C(C=C3C2=O)OC)O</chem>
Afroside	<chem>C[C@@H]1C[C@H]([C@]2([C@@H](O1)O[C@@H]1C[C@@H]3CCC4C(CCC5[C@H](C[C@H]([C@]45O)O)C4=CC(=O)OC4)C3C[C@H]1O2)O)O.CC.CC</chem>
Agapanthagenin	<chem>CC1CCC2(C(C)C3C(CC4C5CC[C@]6(C[C@H]([C@@H](C[C@]6(C)C5CC[C@]34C)O)O)O)O2)OC1</chem>
Ajmalicine	<chem>CC1[C@H]2CN3CCc4c5cccc5[nH]c4[C@@H]3C[C@@H]2C(=CO1)C(=O)OC</chem>
Ajmaline	<chem>CCC1C2CC3C4C5(CC(C2C5O)N3C1O)C6=CC=CC=C6N4C</chem>
Ajugol	<chem>CC1(CC(C2C1C(OC=C2)OC3C(C(C(C(O3)CO)O)O)O)O)O</chem>
Akuammine	<chem>CC=C1CN2CCC34C5=C(C=CC(=C5)O)N(C36C2CC1C4(CO6)C(=O)OC)C</chem>

Allantoin	<chem>C(N)ON[C@@H]1C(=O)NC(=O)N1</chem>
Alliin	<chem>C=CCS(=O)CC(C(=O)O)N</chem>
Allopurinol	<chem>c1c2c(ncnc2O)[nH]n1</chem>
Allouzarin	<chem>CC12CCC(CC1CCC3C2CCC4(C)C(CCC34O)C5=CC(=O)OC5)OC6OC(CO)C(O)C(O)C6OC7OC(CO)C(O)C(O)C7O</chem>
Alloxysmalorin	<chem>CC12CCC(CC1=CCC3C2CCC4(C)C(CCC34O)C5=CC(=O)OC5)OC6OC(CO)C(O)C(O)C6OC7OC(CO)C(O)C(O)C7O</chem>
Aloe-emodin anthrone	<chem>c1cc2c(c(c1)O)C(=O)c1c(cc(cc1O)CO)C2=O</chem>
Aloenin	<chem>Cc1cc(cc(c1c1cc(cc(=O)o1)OC)O)OCC(C(C(C(C=O)O)O)O)O</chem>
Aloeresin A	<chem>CC1=CC(=C(C2=C1C(=O)C=C(O2)CC(=O)C)C3C(C(C(C(O3)CO)O)O)OC(=O)C=CC4=CC=C(C=C4)O)O</chem>
Aloeresin B	<chem>CC1=CC(=C(C2=C1C(=O)C=C(O2)CC(=O)C)C3C(C(C(C(O3)CO)O)O)O)O</chem>
Aloesin	<chem>Cc1cc(c(c2c1C(=O)CC(CC(=O)C)O2)O)OCC(C(C(C(C=O)O)O)O)O</chem>
Aloin A	<chem>c1cc2c(c(c1)O)C(=O)c1c(cc(cc1O)CO)[C@H]2O)OCC(C(C(C(CO)O)O)O)O</chem>
Aloinoside A	<chem>C[C@H]1[C@@H]([C@H]([C@H]([C@H](OCc2cc3[C@H](c4cccc(c4C(=O)c3c(c2)O)O)[C@H]2[C@@H]([C@H]([C@H]([C@@H](CO)O2)O)O)O1)O)O)O</chem>
Aloinoside B	<chem>CC1C(C(C(C(OCc2cc3C(c4cccc(c4C(=O)c3c(c2)O)O)C2C(C(C(C(CO)O2)O)O)O1)O)O)O</chem>
Ambelline	<chem>CO[C@H]1C=CC23c4cc5c(c(c4CN(C[C@@H]3O)[C@@H]2C1)OC)OCO5</chem>
Amentoflavone	<chem>c1cc(ccc1c1cc(=O)c2c(cc(c(c3cc(ccc3O)c3cc(=O)c4c(cc(cc4o3)O)O)c2o1)O)O)O</chem>
Amritoside	<chem>C1=C2C3=C(C(=C1O)O)OC(=O)C4=CC(=C(C(=C43)OC2=O)O)OC5C(C(C(C(O5)COC6C(C(C(C(O6)CO)O)O)O)O)O)O</chem>
Amygladin	<chem>c1ccc(cc1)C(C#N)OC1C(C(C(C(COC2C(C(C(C(CO)O2)O)O)O1)O)O)O</chem>
Anabasin	<chem>c1cc(cnc1)[C@@H]1CCCN1</chem>
Anemonin	<chem>C1=CC2(CC3(C=CC(=O)O3)C2)OC1=O</chem>
Anethole	<chem>C/C=C/c1ccc(cc1)OC</chem>
Angustine	<chem>C=CC1=C2C=C3C4=C(CCN3C(=O)C2=CN=C1)C5=CC=CC=C5N4</chem>
Angustoline	<chem>CC(C1=C2C=C3C4=C(CCN3C(=O)C2=CN=C1)C5=CC=CC=C5N4)O</chem>
Anolignan B	<chem>C=C(Cc1ccc(cc1)O)C(=C)Cc1ccc(cc1)O</chem>
Antidesmone	<chem>Cc1nc(O)c2c(c1OC)[C@H](CCC2=O)CCCCCCCC</chem>
Aphloiol	<chem>c1c2c(cc(c1O)O)oc1cc(c(c1c2=O)O)C1C(C(C(C(CO)O1)O)O)O</chem>
Apigenin	<chem>c1cc(ccc1c1cc(=O)c2c(cc(cc2o1)O)O)O</chem>
Apigenin dimethylether	<chem>COc1ccc(cc1)C1CC(=O)c2c(cc(cc2O1)OC)O</chem>
Arachidic acid	<chem>CCCCCCCCCCCCCCCCCCCC(=O)O</chem>
Arbutin	<chem>c1cc(ccc1O)OCC(C(C(C(C=O)O)O)O)O</chem>
Arcinine	<chem>CC1C2CN3CCC4=C(C3CC2C(=CO1)C(=O)OC)NC5=C4C=C(C=C5)OC</chem>
Arjunglucoside	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C(C5(C)CO)O)O)C)C)C2C1O)C)C(=O)OC6C(C(C(C(O6)CO)O)O)O)C</chem>

Arjunolic acid	<chem>CC1(C)CC[C@@]2(CC[C@]3(C)C(=CCC4[C@@]5(C)C[C@H]([C@@H]([C@@](C)(CO)C5CC[C@@]34C)O)O)[C@]2(C)C1)C(=O)O</chem>
Arnottianamide	<chem>CN(C=O)c1c(ccc2cc3c(cc12)OCO3)c1ccc(c(c1O)OC)OC</chem>
Arteglasin A	<chem>CC1=C2C[C@@H]3[C@](C)(C2[C@@H]2[C@H](C(=C)C(=O)O2)[C@H](C1)OC(=O)C)O3</chem>
Artemisyl acetate	<chem>CC(=CC(C(C)(C)C=C)OC(=O)C)C</chem>
Arvenin I	<chem>CC(=O)OC(C)(C)/C=C/C(=O)[C@@](C)([C@H]1[C@@H](C[C@@]2(C)[C@@H]3CC=C4[C@@H](C[C@@H](C(=O)C4(C)C)O[C@H]4[C@@H]([C@H]([C@@H]([C@@H](CO)O4)O)O)O)[C@]3(C)C(=O)C[C@]12C)O)O</chem>
Arvenin II	<chem>CC(=O)OC(C)(C)CCC(=O)[C@@](C)([C@H]1[C@@H](C[C@@]2(C)[C@@H]3CC=C4[C@@H](C[C@@H](C(=O)C4(C)C)O[C@H]4[C@@H]([C@H]([C@@H]([C@@H](CO)O4)O)O)O)[C@]3(C)C(=O)C[C@]12C)O)O</chem>
Ascaricin	<chem>C=CCc1cc2c(cc1OC)OCO2</chem>
Ascaridole	<chem>CC(C)C12C=CC(C)(CC1)OO2</chem>
Asiatic acid	<chem>C[C@@H]1CCC2(CC[C@]3(C)C(=CCC4[C@@]5(C)C[C@H]([C@@H]([C@@](C)(CO)C5CC[C@@]34C)O)O)[C@@H]2[C@H]1C)C(=O)O</chem>
Asiaticoside	<chem>CC1CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C(C5(C)CO)O)O)C)C)C2C1C)C)C(=O)OC6C(C(C(C(O6)COC7C(C(C(C(O7)CO)OC8C(C(C(C(O8)C)O)O)O)O)O)O)O)O</chem>
Aspalathin	<chem>c1cc(c(cc1CCC1c2c(cc(c(c2O[H-J]O1)OCC(C(C(C(CO)O)O)O)O)O)O)O)O</chem>
Aspirin	<chem>CC(=O)Oc1ccccc1C(=O)O</chem>
Atractyloside	<chem>CC(C)CC(=O)OC1C(C(C(OC1OC2CC(C3CCC45CC(CCC4C3(C2)C)C(=C)C5O)C(=O)O)CO)OS(=O)(=O)O)OS(=O)(=O)O</chem>
Atraric acid	<chem>Cc1cc(c(C)c(c1C(=O)OC)O)O</chem>
Atropine	<chem>CN1[C@H]2CCC1CC(C2)OC(=O)[C@H](CO)c1ccccc1</chem>
Autumnariniol	<chem>Cc2cc(O)c(OC)c3OC(=O)c1c(cccc1O)c23</chem>
Autumnariol	<chem>Cc1cc(cc2c1c1cccc(c1c(=O)o2)O)O</chem>
Avenasterol	<chem>C/C=C(/CC[C@@H](C)[C@H]1CC[C@H]2C3=CC[C@H]4C[C@H](CC[C@]4(C)C3CC[C@]12C)O)\C(C)C</chem>
Avicine	<chem>C[n+]1cc2cc3c(cc2c2ccc4cc5c(cc4c12)OCO5)OCO3</chem>
Aviprin	<chem>CC(C)(C[C@@H](O)Oc1c2ccc(=O)oc2cc2c1cco2)O</chem>
Balagyptin	<chem>CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3CCC4(C5CCC6(C(C5CC=C4C3)CC(C6C(C)O)O)C)C)OC7C(C(C(C(O7)C)O)O)O)O)O)O)O</chem>
Balanitin 4	<chem>CC1CCC2(C(C3C(O2)CC4C3(CCC5C4CC=C6C5(CCC(C6)OC7C(C(C(C(O7)CO)OC8C(C(C(C(O8)CO)O)OC9C(C(C(C(O9)CO)O)O)O)O)OC2C(C(C(C(O2)C)O)O)O)C)C)OC1</chem>
Balanitin 6	<chem>CC1CCC2(C(C3C(O2)CC4C3(CCC5C4CC=C6C5(CCC(C6)OC7C(C(C(C(O7)CO)OC8C(C(C(C(O8)CO)O)O)O)OC9C(C(C(C(O9)C)O)O)O)C)C)OC1</chem>
Balanitin 7	<chem>CC1CCC2(C(C3C(O2)CC4C3(CCC5C4CC=C6C5(CCC(C6)OC7C(C(C(C(O7)CO)OC8C(C(C(C(O8)CO)O)OC9C(C(C(C(O9)O)O)O)O)OC2C(C(C(C(O2)C)O)O)O)C)C)OC1</chem>

Balanitine 1	<chem>OC%10C(O)C(O)C(C)OC%10OC9C(O)C(O)C(CO)OC9OC2C(O)C(OC1OC(C)C(O)C(O)C1O)C(OC2CO)OC7CC8=CC3C(CCC4(C)C6C(CC34)OC5(CCC(C)CO5)C6C)C8(C)CC7</chem>
balanitine 2	<chem>OC9C(O)C(O)C(C)OC9OC8C(O)C(O)C(CO)OC8OC1C(O)C(O)C(OC1CO)OC6CC7=CCC2C(CCC3(C)C5C(CC23)OC4(CCC(C)CO4)C5C)C7(C)CC6</chem>
balanitine 3	<chem>CC%10C2C(CC3C4CC=C1CC(CCC1(C)C4CCC23C)OC8OC(CO)C(O)C(OC6OC(COC5OCC(O)C(O)C5O)C(O)C(O)C6O)C8OC7OC(C)C(O)C(O)C7O)OC9%10CCC(C)CO9</chem>
Balanitoside	<chem>CC1C2C(CC3C2(CCC4C3CC=C5C4(CCC(C5)OC6C(C(C(C(O6)CO)OC7C(C(C(C(O7)CO)O)O)O)OC8C(C(C(C(O8)C)O)O)O)C)OC1(CCC(C)COC9C(C(C(C(O9)CO)O)O)O)O</chem>
Ballotenol	<chem>C[C@@H]1C(=O)[C@H](C2C(C)C)CCC[C@]2(C)[C@]1(CCc1ccoc1)O)O</chem>
Barringenol A	<chem>CC1(C)C[C@H]2C3=CCC4[C@@]5(C)CC[C@H](C(C)(C)C5CC[C@@]4(C)[C@]3(C)[C@H]([C@H]([C@@]2(CO)[C@H](C1)O)O)O)O</chem>
Bauerenol	<chem>CC1CCC2(CCC3(C4=CCC5C(C(CCC5(C4CCC3(C2C1C)C)C)O)(C)C)C)C</chem>
Behenic acid	<chem>CCCCCCCCCCCCCCCCCCCCCCCC(=O)O</chem>
Benzo[c]phenanthridine	<chem>c1ccc2c(c1)ccc1c3ccccc3cnc21</chem>
Benzoic acid	<chem>C1=CC=C(C=C1)C(=O)O</chem>
Berberine	<chem>COc1ccc2cc3c4cc5c(cc4CC[n+]3cc2c1OC)OCO5</chem>
Bergapten	<chem>COc1c2ccc(=O)oc2cc2c1cco2</chem>
Berulide	<chem>CCCCC/C=C/C/C=C/CCCCCCCC(=O)OCC(COC(=O)CCCCCCC/C=C/C/C=C/C/CCCC)OC(=O)CCCCCCCCCCCCCCC</chem>
Betain	<chem>C[N+](C)(C)CC(=O)[O-]</chem>
Betulinic acid	<chem>C=C(C)C1CC[C@@]2(CC[C@]3(C)[C@H](CCC4[C@@]5(C)CC[C@H](C(C)(C)[C@H]5CC[C@@]34C)O)[C@H]12)C(=O)O</chem>
Biochanin A	<chem>COC1=CC=C(C=C1)C2=COC3=CC(=CC(=C3C2=O)O)O</chem>
Bisabolene	<chem>CC(=CCC/C(=C/1\CC=C(C)CC1)/C)C</chem>
Biscryptolepine	<chem>CN2c1cccc1C(=C3N=C4C=CC=CC4=C23)C7=C6N=C5CC=CCC5=C6N(C)c8cccc78</chem>
Borneol	<chem>CC1(C)C2CC[C@]1(C)[C@H](C2)O</chem>
Bovogenin A	<chem>C[C@@]12CCC3[C@@H](CC[C@H]4C[C@H](CC[C@]34CO)O)[C@]2(CC[C@H]1c1ccc(=O)oc1)O</chem>
Bovoside A	<chem>CC1C(C(C(C(O1)O)[C@H]1CC[C@@]2(CO)[C@@H](CCC3C2CC[C@]2(C)[C@H](CC[C@]32O)c2ccc(=O)oc2)C1)O)OC)O</chem>
Brassinolide	<chem>CC(C)C(C)C(C(C)C1CCC2C1(CCC3C2COC(=O)C4C3(CC(C(C4)O)O)C)O)O</chem>
Brunfelsamidine	<chem>c1c[nH]cc1C(=N)N</chem>
Bulbispermine	<chem>C1=CC23c4cc5c(cc4CN(CC3O)[C@H]2C[C@H]1O)OCO5</chem>
Buphanamine	<chem>COC1=C2CN3CCC4(C3CC=CC4O)C2=CC5=C1OCO5</chem>
Buphanidrine	<chem>CO[C@H]1C=C[C@@]23CCN(Cc4c2cc2c(c4OC)OCO2)[C@@H]3C1</chem>
Buphanisin	<chem>COC1CC2C3(CCN2CC4=CC5=C(C=C43)OCO5)C=C1</chem>



Butyric acid	<chem>CCCC(=O)O</chem>
Caespitin	<chem>CC(=CCc1c(cc(c(C(=O)CCC(C)C)c1O)O)O)C</chem>
Caffeic acid	<chem>c1cc(c(cc1/C=C/C(=O)O)O)O</chem>
Caffeine	<chem>Cn1cnc2c1c(=O)n(C)c(=O)n2C</chem>
Cajanol	<chem>COC1=CC(=C2C(=C1)OCC(C2=O)C3=C(C=C(C=C3)O)OC)O</chem>
Cajaquinone	<chem>CC1=C(C=C2C(=C1)C(=O)C3=CC(=CC(=C3C2=O)OC)O)O</chem>
Calcium oxalate	<chem>C(=O)(C(=O)[O-])[O-].[Ca+2]</chem>
Calycosin	<chem>COC1=C(C=C(C=C1)C2=COCC3=C(C2=O)C=CC(=C3)O)O</chem>
Campesterol	<chem>CC(C)[C@H](C)CC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@H](CC[C@]4(C)[C@H]3CC[C@]12C)O</chem>
Camphene	<chem>C=C1C2CCC(C2)C1(C)C</chem>
Camphor	<chem>CC1(C)C2CCC1(C)C(=O)C2</chem>
Canavanine	<chem>CC(CCONC(=N)N)N</chem>
Cannabidiol	<chem>CCCCCCC1=CC(=C(C(=C1)O)C2C=C(CCC2C(=C)C)C)O</chem>
Capsaicin	<chem>CC(C)/C=C/CCCCCC(=O)NCc1ccc(c(c1)OC)O</chem>
Caranine	<chem>C1CN2CC3=CC4=C(C=C3C5C2C1=CCC5O)OCO4</chem>
Carapanaubine	<chem>CC1C2CN3CCC4(C3CC2C(=CO1)C(=O)OC)C5=CC(=C(C=C5NC4=O)OC)OC</chem>
Carboxyparquin	<chem>CC(C)CC(=O)OC1C(OC2C[C@@]3(C)C4CC[C@@H]5C[C@@]4(CC[C@@H]3C(C2)(C(=O)O)C(=O)O)C(C5=C)O)OC(CO)C(C1(CO)O)OC1C(C(=O)C(=O)O1)OCO</chem>
Cardanol	<chem>CCCCCC/C=C\CCCCCCCc1ccc(c1)O</chem>
Carene	<chem>CC1=CCC2C(C1)C2(C)C</chem>
Carnasol	<chem>CC(C)c1cc2[C@@H]3CC4C(C)(C)CCC[C@@]4(c2c(c1O)O)C(=O)O3</chem>
Carpusin	<chem>COC1=C2C(=CC(=C1)O)OC(C2=O)(CC3=CC=C(C=C3)O)O</chem>
Carvone	<chem>C=C(C)C1CC=C(C)C(=O)C1</chem>
Caryophyllene	<chem>C/C/1=C/CCC(=C)[C@@H]2CC(C)(C)[C@H]2CC1</chem>
Cassaine	<chem>C[C@H]1/C(=C/C(=O)OCCNC)/CC[C@H]2[C@H]1C(=O)C[C@H]1C(C)(C)[C@H](CC[C@]21C)O</chem>
Castalagin	<chem>C1C2C(C3C4C(C5=C(C(=C(C(=C5(=O)O4)C6=C(C(=C(C(=C6(=O)O3)C7=C(C(=C(C=C7(=O)O2)O)O)O)O)O)O)O)OC(=O)C8=CC(=C(C(=C8C9=C(C(=C(C=C9(=O)O1)O)O)O)O)O)O)O</chem>
Catechin	<chem>c1cc(c(cc1C1=C(Cc2c(cc(cc2O1)O)O)O)O)O)O</chem>
Catharanthine	<chem>CCC1=CC2CN3CCc4c5cccc5[nH]c4[C@@]2(COC)C13</chem>
Cathinone	<chem>C[C@@H](C(=O)c1cccc1)N</chem>
Celastrin	<chem>CC1CCC(C2(C13C(C(C2OC(=O)C4=CC=CC=C4)OC(=O)C)C(O3)(C)C)OC(=O)C)COC(=O)C)OC(=O)C</chem>
Centelloside	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CC(C5C4(CC(C(C5(C)CO)O)O)C)O)C)C2C1)C)C(=O)OC6C(C(C(C(O6)COC7C(C(C(C(O7)CO)O)O)O)O)O)O)C</chem>

Chelerythrine	<chem>C[n+]1cc2c(ccc(c2OC)OC)c2ccc3cc4c(cc3c12)OCO4</chem>
Chironioside	<chem>O=C1OCCC2(O)C(C=C)C(OC=C12)OC4OC(COC3OCC(O)C(O)C3O)C(O)C(O)C4O</chem>
Chlerythrine-Ψ-cyanide	<chem>COc2ccc1c3ccc4cc5OCOc5cc4c3N(C)C(C#N)c1c2OC</chem>
Chlorogenic acid	<chem>c1cc(c(cc1/C=C/C(=O)OC1CC(CC(C1O)O)(C(=O)O)O)O)O</chem>
Christyoside	<chem>CC1C(C(C(C(O1)O)[C@H]1CC[C@@]2(CO)[C@@H](CCCC3C2CC[C@]2(C)[C@H](CC[C@]32O)C2=CC(=O)OC2)C1)O)O</chem>
Chrysanthenyl acetate	<chem>CC1=CCC2C(C1C2(C)C)OC(=O)C</chem>
Chrysophonein	<chem>Cc1cc2c(c(c1)OCC(C(C(C(=O)O)O)O)O)C(=O)c1c(cccc1O)C2=O</chem>
Chrysophonol	<chem>Cc1cc2c(c(c1)O)C(=O)c1c(cccc1O)C2=O</chem>
Cineole	<chem>CC1(C)C2CCC(C)(CC2)O1</chem>
Cinnamaldehyde	<chem>C1=CC=C(C=C1)C=CC=O</chem>
cis-Allocimene	<chem>CC=C(C)C=CC=C(C)C</chem>
Cissacapine	<chem>CN1CCc2cc(c3c4c2[C@H]1Cc1ccc2c(c1)COc1c(cc5CCN(C)[C@H](Cc6ccc(c(c6)CO3)O4)c5c1O2)OC)OC</chem>
Cissampreine	<chem>CN1CCc2cc(c(c3c2[C@H]1Cc1ccc(cc1)COc1c(cc2CCN=C(Cc4ccc(cc4)O3)c2c1O)OC)OC)OC</chem>
Citral	<chem>CC(=CCCC(=CC=O)C)C</chem>
Citric acid	<chem>C(C(=O)O)C(CC(=O)O)(C(=O)O)O</chem>
Citronellol	<chem>CC(=CCC[C@@H](C)CCO)C</chem>
Cliviamartine	<chem>CCOC(=O)C1=C(N=C(C(=C1)C(=O)OC2CC3CCN(C3C4C2OC(=O)C5=CC6=C(C=C45)OCO6)C)C)C</chem>
Cliviasine	<chem>CN4CCC5CC(O)C3OC(=O)c2cc1OCOc1cc2C3C45</chem>
Clividine	<chem>CN1CCC2C1C3c4cc5c(cc4C(=O)OC3C(C2)O)OCO5</chem>
Clivimine	<chem>CC1=C(C=C(C(=N1)C)C(=O)OC2CC3CCN(C3C4C2OC(=O)C5=CC6=C(C=C45)OCO6)C)C(=O)OC7CC8CCN(C8C9C7OC(=O)C1=CC2=C(C=C91)OCO2)C</chem>
Clivonine	<chem>CN1CCC2C1C3C(C(C2)O)OC(=O)C4=CC5=C(C=C34)OCO5</chem>
Cnicin	<chem>C/C1=C/CC/C(=C\[C@@H]2C(C(=C)C(=O)O2)[C@H](C1)O OCC(=C)C(CO)O)/CO</chem>
Coccinine	<chem>CO[C@@H]1C=C2[C@H]3CN(Cc4cc5c(cc34)OCO5)[C@]2(C[C@@H]1O)N</chem>
Colchicine	<chem>CC(=O)N[C@H]1CCc2cc(c(c2c2ccc(c(=O)cc12)OC)OC)OC</chem>
Colosolic acid	<chem>CC1CCC2(CCC3(C)C(=CCC4C5(C)CC(C(C(C)C)C5CCC34C)O)O)C2C1C)C(=O)O</chem>
Combretastatin A	<chem>COc1ccc(/C=C\c2cc(c(c2)OC)OC)OC)cc1O</chem>
Combretin A	<chem>O=C(O)[C@@]1(C)C2CCC4[C@@]3(C[C@]23CC[C@@H]1O)CC[C@]5(C)C(C[C@H](O)[C@@]45C)C(C)CCC(=C)C(C)C</chem>
Combretin B	<chem>CC(C)C(=C)CCC(C)C2C[C@H](O)[C@@]3(C)C4CCC6[C@@](C)([C@H](OC1OCC(O)C(O)C1O)CC[C@@]65CC45CC[C@]23C)C(=O)O</chem>
Coniceine	<chem>CCCC1=NCCCC1</chem>
Coniine	<chem>CCC[C@H]1CCCCN1</chem>

Conyscabraic-acid	<chem>C[C@@H]1CC[C@H]2C[C@@]3(C=C[C@@H]3[C@@H]2[C@@]1(C)CCc1ccoc1)C(=O)O</chem>
Cornustannin A	<chem>c1c(cc(c(c1O)O)O)C(=O)OC1[C@@H]2C(COC(=O)c3cc(c(c(c3c3c(cc(c(c3O)O)O)C(=O)O2)O)O)O)[C@H](C1OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O</chem>
Corsoleic acid	<chem>C[C@@H]1CC[C@@]2(CC[C@]3(C)C(=CC[C@@H]4[C@@]5(C)C[C@H]([C@@H](C(C)(C)[C@@H]5CC[C@@]34C)O)O)[C@@H]2[C@H]1C)C(=O)O</chem>
Cotyledoside	<chem>CC1C([C@]2([C@H]([C@@H](O1)O)[C@@H]1C[C@@H]3C[C@H]4[C@@]5(C)CC[C@]6(C)[C@H](CC[C@]56O)c5ccc(=O)oc5)[C@@]3(C)C[C@H]1O2)O4)O)OC)O</chem>
Coumurrayin	<chem>CC(=CCc1c(cc(c2ccc(=O)oc12)OC)OC)C</chem>
Crinamine	<chem>CO[C@H]1C=C[C@]23c4cc5c(cc4CN(CC3O)C2C1)OCO5</chem>
Crinasiadine	<chem>C1OC2=C(O1)C=C3C(=C2)C4=CC=CC=C4NC3=O</chem>
Crinasiatine	<chem>C1C(OC2=C(O1)C=C3C4=CC=CC=C4NC(=O)C3=C2)CC5=CC=C(C=C5)O</chem>
Crinine	<chem>C1CN2CC3=CC4=C(C=C3C15C2CC(C=C5)O)OCO4</chem>
Crotofoline A	<chem>C=C1CCC2C(=C(C)C(=O)O2)[C@@H]2[C@@H]1C1=C(C[C@@]2(C)O)C[C@](C)(C1=O)O</chem>
Crotonin	<chem>C[C@@H]1CC(=O)C[C@H]2[C@@H]1CC[C@@H](C)[C@@]12CC(c2ccoc2)OC1=O</chem>
Cryptogenin	<chem>CC(CCC(=O)C(C)C1C(=O)CC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)CO</chem>
cryptoheptine	<chem>OC=1C=C4C(N=C2C=CC=CC=12)c3ccccc3N4C</chem>
Cryptolepine	<chem>CN1C2=CC=CC=C2C=C3C1=C4C=CC=CC4=N3</chem>
Cryptomisrine	<chem>C1=CC=C2C(=C1)C3=NC4=CC=CC=C4C(=C3N2)C(=O)C5=C6C(=NC7=CC=CC=C75)C8=CC=CC=C8N6</chem>
Cryptoquindoline	<chem>CN7C1=C8C=CC=CC8=NC1=C(n4c2ccccc2c3nc5ccccc5cc34)c6ccccc67</chem>
Cryptospirolepine	<chem>CN2c1ccccc1C57C(On3c5c2c4ccccc34)n9c6c(N(C)c8ccccc8C=C67)c%10ccccc9%10</chem>
Cucurbitacin B	<chem>CC(=O)OC(C)(C)/C=C/C(=O)[C@@](C)(C1[C@@H](C[C@@]2(C)C3CC=C4C(C[C@@H](C(=O)C4(C)C)O)[C@]3(C)C(=O)C[C@]12C)O)O</chem>
Cuminic aldehyde	<chem>CC(C)c1ccc(cc1)C=O</chem>
Cuminol	<chem>CC(C)c1ccc(cc1)CO</chem>
Curcanoleic acid	<chem>C(=C(\ CC(=O)O)/C(=O)O)\ C(=O)O</chem>
Curcumin	<chem>COc1cc(/C=C/C(=O)CC(=O)/C=C/c2ccc(c(c2)OC)O)ccc1O</chem>
Curcuson A	<chem>CC1CC2=C(C1=O)C3C(C=C(C2=O)C)C(CCC3=C)C(=C)C</chem>
Curcuson C	<chem>C=C(C)[C@@H]1CCC(=C)C2C1C=CCC1=C2C(=O)C(C)(C1)O</chem>
Cyanidin	<chem>c1cc(c(cc1c1c(cc2c(cc(cc2[O+]1)O)O)O)O)O)O</chem>
Cycasin	<chem>C/[N+](=N\COC1C(C(C(C(CO)O1)O)O)O)/[O-]</chem>
Cyclamin	<chem>CC1(C2CCC3(C(C2(CCC1OC4C(C(C(CO4)OC5C(C(C(C(O5)CO)O)OC6C(C(C(C(O6)CO)O)O)OC7C(C(C(CO7)O)O)O)OC8C(C(C(C(O8)CO)O)O)O)C)CCC91C3(CC(C2(C9CC(CC2)(C)C=O)CO1)O)C)C</chem>
Cycloartenol	<chem>CC(CCC=C(C)C)C1CCC2(C1(CCC34C2CCC5C3(C4)CCC(C5(C)C)O)C)C</chem>
Cymene	<chem>CC(C)c1ccc(C)cc1</chem>

Cynafoside B	<chem>CC(=O)[C@H]1CC[C@@]2(C3CC[C@H]4C[C@H](CC[C@]4(C)C3[C@@H]([C@H]([C@]12C)OC(=O)C1CCCC1)OC(=O)C)OC1CC(C(C(C)O1)OC1CC(C(C(C)O1)OC1CC(C(C(C)O1)OC1C(C(C(C(CO)O1)O)O)OC)OC)O)O</chem>
Cynafoside H	<chem>CC(=O)C4CCC5(O)C2CCC1CC(CCC1(C)C2C(OC(C)=O)C(OC(=O)c3ccccc3)C45C)OC%10OC(C)C(OC9OC(C)C(OC8OC(C)C(OC7OC(CO)C(OC6OC(CO)C(O)C(O)C6O)C(O)C7O)C(OC)C8)C(OC)C9)C(OC)C%10</chem>
Cytisine	<chem>c1cc2[C@H]3C[C@@H](CNC3)Cn2c(=O)c1</chem>
D-Amphetamine	<chem>C[C@@H](Cc1ccccc1)N</chem>
Daucosterol	<chem>CC[C@H](CC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@H](CC[C@]4(C)[C@H]3CC[C@]12C)O[C@H]1[C@@H]([C@H]([C@@H]([C@@H](CO)O1)O)O)C(C)C</chem>
Deacetyldesformoakumamiline	<chem>O=C(OC)C5C2CC3C4=Nc1cccc1C45CCN3C/C2=C\C</chem>
Deguelin	<chem>CC1(C)C=Cc2c(ccc3C(=O)[C@H]4c5cc(c(cc5OC[C@H]4Oc23)OC)OC)O1</chem>
Dehydrofalcariinol	<chem>C=CCCCC/C=C/C/C=C/C=C/C(C=C)O</chem>
Delphinidin	<chem>c1c(cc(c(c1O)O)O)c1c(cc2c(cc(cc2[o+]1)O)O)O</chem>
Deltonin	<chem>C[C@@H]1CC[C@@]2([C@@H](C)[C@H]3[C@H](C[C@H]4[C@@H]5CC=C6C[C@H](CC[C@]6(C)[C@H]5CC[C@]34C)O[C@H]3[C@@H]([C@H]([C@@H]([C@@H](CO)O3)O)[C@H]3[C@@H]([C@H]([C@@H]([C@@H](CO)O3)O)O)O)O)[C@H]3[C@@H]([C@@H]([C@H]([C@H](C)O3)O)O)O)O2)OC1</chem>
Deltoside	<chem>C[C@H](CC[C@@]1(O)O[C@H]2C[C@H]3[C@@H]4CC=C5C[C@H](CC[C@]5(C)[C@H]4CC[C@]3(C)[C@H]2[C@@H]1C)O[C@@H]1O[C@H](CO)[C@@H](O[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@H](O)[C@H]1O[C@@H]1O[C@@H](C)[C@H](O)[C@@H](O)[C@H]1O)CO[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O</chem>
Deoxyloganin	<chem>CC1CCC2C1C(OC=C2C(=O)OC)OC3C(C(C(C(O3)CO)O)O)O</chem>
Des-N-methylchelerythrine	<chem>COC1=C(C2=CN=C3C=C2C=C1)C=CC4=CC5=C(C=C43)OCO5)OC</chem>
Dhurrin	<chem>c1cc(ccc1[C@@H](C#N)OC1C(C(C(C(CO)O1)O)O)O)O</chem>
Dicoumarol	<chem>c1ccc2c(c1)c(c(Cc1c(c3ccccc3oc1=O)O)c(=O)o2)O</chem>
Dicrotaline	<chem>C[C@@]1(CC(=O)OCC2=CCN3CC[C@H]([C@@H]23)OC(=O)C1)O</chem>
Digallic acid	<chem>c1c(cc(c(c1O)O)OC(=O)c1cc(c(c(c1)O)O)O)C(=O)O</chem>
Digitoxin	<chem>CC1C(C(CC(O1)OC1C(C)OC(CC1O)OC1C(C)OC(CC1O)O)[C@H]1CC[C@@]2(C)[C@H](CCC3C2CC[C@]2(C)[C@H](C[C@]32O)C2=CC(=O)OC2)C1)O)O</chem>
Dihydrosanguinarine	<chem>CN1Cc2c(ccc3c2OCO3)c2ccc3cc4c(cc3c12)OCO4</chem>
Dioscin	<chem>C[C@@H]1CC[C@@]2([C@@H](C)[C@H]3[C@H](C[C@H]4[C@@H]5CC=C6C[C@H](CC[C@]6(C)[C@H]5CC[C@]34C)O[C@H]3[C@@H]([C@H]([C@@H]([C@@H](CO)O3)O)[C@H]3[C@@H]([C@@H]([C@H]([C@H](C)O3)O)O)O)O)O)[C@H]3[C@@H]([C@@H]([C@H]([C@H](C)O3)O)O)O)O2)OC1</chem>
Dioscorine	<chem>CC1=CC(=O)O[C@@]2(C1)C[C@H]1CC[C@@H]2CN1C</chem>
Diosgenin	<chem>C[C@@H]1CC[C@@]2([C@@H](C)C3C(CC4C5CC=C6CC(CC[C@]6(C)C5CC[C@]34C)O)O2)OC1</chem>
Diosmetin	<chem>COC1=C(C=C(C=C1)C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O</chem>

Diosmin	<chem>C[C@@H]1[C@H]([C@@H]([C@@H]([C@@H](OCC(C(C(CO)c2ccc3c(=O)cc(c4ccc(c(c4)O)OC)oc3c2)O)O)O)O)O)O)O)O</chem>
Diosphenol	<chem>O</chem>
Diospyrin	<chem>CC(C)C1=C(C(=O)C(C)CC1)O</chem>
Docosanol	<chem>Cc1cc2c(c(c1)O)C(=O)C=C(c1c(C)cc3C(=O)C=CC(=O)c3c1O)C2=O</chem>
Docosyl ferulate	<chem>CCCCCCCCCCCCCCCCCCCCCO</chem>
Dodonic acid	<chem>CCCCCCCCCCCCCCCCCCCCCOC(=O)/C=C/c1ccc(c(c1)OC)O</chem>
Dregeana 4	<chem>C[C@@H]1C[C@H]([C@]2(C)C(=CCC[C@@H]2[C@@]1(C)CCc1ccoc1)C(=O)O)O</chem>
Dregeanin	<chem>CC(CC)C(OC(C)=O)C(=O)O[C@@H]3CC4[C@@]5(C)C(CC(=O)O[C@](C)(CO)C5C[C@@H](OC(=O)C(O)C(C)C)[C@@]4(C)C2=CC[C@@H](c1ccoc1)[C@@]23C)OC(C)=O</chem>
Durantocide I	<chem>CCC(C)C(C(=O)O[C@H]1[C@@H](C(C(=C)[C@@]23[C@@H](C[C@@H](c4ccoc4)[C@]12C)O3)[C@]1(C)C2CC(=O)O[C@]2(C)COC(=O)C[C@@H]1OC(=O)C)OC(=O)C)OC(=O)C</chem>
Durantocide II	<chem>C[C@@]1([C@H](C[C@@]2(C(=CO[C@H](C12)OC1C(C(C(CO)O1)O)O)O)C(=O)OC)O)OC(=O)/C=C/c1cccc1)O</chem>
Durantocide III	<chem>CC1(C(CC2(C1C(OC=C2C(=O)OC)OC3C(C(C(C(O3)CO)O)O)O)OC(=O)C=CC4=CC=C(C=C4)OC)O</chem>
Eburnamonine	<chem>COc1ccc(cc1OC)/C=C/C(=O)OC4CC3(O)C(=COC(OC2OC(CO)C(O)C(O)C2O)C3C4(C)O)C(=O)OC</chem>
Ekebergin	<chem>CC[C@]12CCCN3CCc4c5cccc5n(C(=O)C1)c4[C@H]23</chem>
Elaeocyanidin	<chem>CC(C)CC(=O)O[C@H]1[C@H](C(C)(C)[C@H](CCC(=O)OC)[C@@]2(C)[C@H]3CC[C@@]4(C)[C@H](c5ccoc5)OC(=O)[C@H]([C@@]4(C3=C)O)[C@@H]12)OC(=O)C)O</chem>
Elemanolide	<chem>CC1(C)c2c(cc(c(c2O)OC)O)C2C(Cc3c(cc(cc3O2)O)O)O)O1</chem>
Ellagic acid	<chem>CC(=C)C1C2C(C(CC1(C)C=C)OC(=O)C)C(=C)C(=O)O2</chem>
Embelin	<chem>c1c2c3c4c(cc(c(c4oc2=O)O)O)c(=O)oc3c(c1O)O</chem>
Ent-16-Kauren-18-oic-acid	<chem>CCCCCCCCCCCCC1=C(C(=O)C=C(C1=O)O)O</chem>
Ent-16-Kauren-19-oic-acid	<chem>C=C1C[C@]23CC[C@@H]4[C@](C)(CCC[C@@]4(C)[C@@H]3CC[C@H]1C2)CC(=O)O</chem>
Entagenic-acid	<chem>C=C1C[C@]23CCC4[C@@](C)(CCC[C@@]4(C)C(=O)O)C3CC[C@H]1C2</chem>
Epicatechin	<chem>CC1(C)CC[C@]2([C@@H](C1)C1=CCC3[C@@]4(C)CC[C@@H](C(C)(C)C4CC[C@@]3(C)[C@]1(C)[C@H]([C@H]2O)O)O)C(=O)O</chem>
Epifriedelinol	<chem>c1cc(c(cc1[C@@H]1[C@@H](Cc2c(cc(cc2O1)O)O)O)O)O</chem>
Epigallocatechin	<chem>CC3(C)C[C@H]4[C@]5(C)CC[C@]2(C)[C@H](CC[C@@]1(C)[C@H]2CC[C@H](O)[C@@H]1C)[C@@]5(C)CC[C@@]4(C)C3</chem>
Epigallocatechin gallate	<chem>c1c(cc(c(c1O)O)O)C1C(Cc2c(cc(cc2O1)O)O)O)OC(=O)c1cc(c(c1)O)O</chem>
Epimaslinic acid	<chem>c1c(cc(c(c1O)O)O)C1C(Cc2c(cc(cc2O1)O)O)O)OC(=O)c1cc(c(c1)O)O</chem>
Erectene	<chem>CC1(C)CC[C@@]2(CC[C@]3(C)C(=CC[C@@H]4[C@@]5(C)C[C@H]([C@H](C(C)(C)[C@@H]5CC[C@@]34C)O)O)[C@@H]2C1)C(=O)O</chem>
Ergine	<chem>CC/C=C\C/C=C/C/CCCCCCCCCCCCCCC</chem>
	<chem>[CH][C@@]12Cc3c[nH]c4cccc(C1=C[C@H](CN2C)C(=O)N)c34</chem>

Ergoline	<chem>c1cc2[C@H]3CCCN[C@@H]3Cc3c[nH]c(c1)c23</chem>
Eroidictyol	<chem>C1C(OC2=CC(=CC(=C2C1=O)O)O)C3=CC(=C(C=C3)O)O</chem>
Erysotrine	<chem>COC1C=CC2=CCN3CCc4cc(c(cc4[C@]23C1)OC)OC</chem>
Erysovine	<chem>CO[C@H]1C=CC2=CCN3CCc4cc(c(cc4[C@]23C1)OC)OC</chem>
Erythraline	<chem>CO[C@H]1C=CC2=CCN3CCc4cc5c(cc4[C@]23C1)OCO5</chem>
Erythropleine	<chem>C[C@H]1/C(=C/C(=O)OCCNC)/CCC2C1[C@H](CC1[C@]2(C)CCC[C@]1(C)C(=O)OC)O</chem>
Erythrophylic-acid	<chem>CC(=CCCC(CO)[C@H]1CC[C@@]2(C)C3CCC4C(C)(C)C(=O)C=C[C@]54C[C@@]35C=C[C@]12C)C</chem>
Ethyl octanoate	<chem>CCOCCCCCCC(=O)C</chem>
Eucomnaline	<chem>COc1c(cc2c(C(=O)/C(=C/c3ccc(cc3)O)/CO2)c1O)O</chem>
Eucoesterol	<chem>CCC(=O)[C@@H]1C[C@@H](C)[C@]2(CC(=O)[C@@]3(C)C4=C(CC[C@]23C)[C@@]2(C)CC[C@@H]([C@](C)(CO)C2CC4)O)O1</chem>
Eugenol	<chem>C=CCc1ccc(c(c1)OC)O</chem>
Falcarinol	<chem>CCCCCCC/C=C\C/C=C/C=C/[C@@H](C=C)O</chem>
Febuxostat	<chem>CC(C)COc1ccc(cc1C#N)c1nc(C)c(C(=O)O)s1</chem>
Fenchone	<chem>CC1(C)[C@@H]2CC[C@@](C)(C2)C1=O</chem>
Ferullic-acid	<chem>COc1cc(ccc1O)/C=C/C(=O)O</chem>
Flemichapparin C	<chem>COC1=CC2=C(C=C1)C3=C(C4=CC5=C(C=C4O3)OCO5)C(=O)O2</chem>
Formononetin	<chem>COC1=CC=C(C=C1)C2=COC3=C(C2=O)C=CC(=C3)O</chem>
Friedelin	<chem>C[C@H]1C(=O)CCC2[C@]1(C)CCC1[C@@]2(C)CC[C@@]2(C)[C@@H]3CC(C)(C)CC[C@]3(C)CC[C@]12C</chem>
Fructose	<chem>C([C@@H]1[C@@H](C([C@@](CO)(O)O1)O)O)O</chem>
Frutinone A	<chem>c1ccc2c(c1)c(=O)c1c(c3ccccc3oc1=O)o2</chem>
Fujikinetin	<chem>COC1=C(C=C2C(=C1)C(=O)C(=CO2)C3=CC4=C(C=C3)OCO4)O</chem>
Fumaric acid	<chem>C(=C\C(=O)O)/C(=O)O</chem>
Furanodiene	<chem>CC=1Cc2occ(C)c2CC=C(C)CCC=1C</chem>
Furanoeudesma-1-3-diene	<chem>CC2=CC=CC1Cc3occ(C)c3CC12</chem>
Gaboroquinone A	<chem>CC(=O)C1=C(C=C(C(=C1OC)C2=C3C(=C(C=C2CO)O)C(=O)C4=C(C3=O)C=CC=C4O)O)O</chem>
Gaboroquinone B	<chem>CC(=O)C1=C(C=C(C(=C1O)C2=C3C(=C(C=C2CO)O)C(=O)C4=C(C3=O)C=CC=C4O)O)OC</chem>
Galathamine	<chem>CN1CCC23C=CC(CC2OC4=C(C=CC(=C34)C1)OC)O</chem>
Gallic acid	<chem>c1c(cc(c(c1O)O)O)C(=O)O</chem>
Gallocatechin	<chem>c1c(cc(c(c1O)O)O)[C@@H]1[C@H](Cc2c(cc(cc2O1)O)O)O</chem>
Garcifuran B	<chem>COC1=CC(=CC(=C1O)O)C2=CC3=C(C=C2)OC=C3</chem>
Garcinia biflavonoid 1	<chem>C1=CC(=CC=C1C2C(C(=O)C3=C(C=C(C=C3O2)O)O)C4=C(C=C(C5=C4OC(C(C5=O)O)C6=CC=C(C=C6)O)O)O)O</chem>
Garcinia biflavonoid 2	<chem>C1=CC(=CC=C1C2C(C(=O)C3=C(C=C(C=C3O2)O)O)C4=C(C=C(C5=C4OC(C(C5=O)O)C6=CC(=C(C=C6)O)O)O)O)O</chem>

Geissoschizine	<chem>CC=C1CN2CCC3=C(C2CC1C(C=O)C(=O)OC)NC4=CC=CC=C34</chem>
Geissoschizol	<chem>CC=C1CN2CCC3=C(C2CC1CCO)NC4=CC=CC=C34</chem>
Gelsemicine	<chem>CC[C@@H]1[C@@H]2C[C@@H]3[C@]4(C[C@@H]([C@H]2CO3)N1)c1ccc(cc1N(C4=O)OC)OC</chem>
Genistein	<chem>c1cc(cc(c1)O)c1coc2cc(cc(c2c1=O)O)O</chem>
Gentiopicroside	<chem>C=C[C@@H]1C2=CCOC(=O)C2=CO[C@H]1OCC(C(C(C(CO)O)O)O)O</chem>
Geraniin	<chem>c1c(cc(c(c1O)O)O)OC(=O)[C@H]1C2C3[C@H](C(COC(=O)c4cc(c(c(c4c4c(cc(c(c4O)O)O)C(=O)O3)O)O)O)O1)OC(=O)C1=CC(=O)[C@]3(C(C1c1c(cc(c(c1O3)O)O)C(=O)O2)(O)O)O</chem>
Geraniol	<chem>CC(=CCC/C(=C/CO)/C)C</chem>
Germacrene B	<chem>CC(=C1CC/C(=C/CC/C(=C/C1)/C)/C)C</chem>
Germacrene D	<chem>CC(C)C1/C=C\C(=C)CC/C=C(/C)\CC1</chem>
Gingerdione	<chem>CCCCC(=O)CC(=O)CCC1=CC(=C(C=C1)O)OC</chem>
Gitogenin	<chem>C[C@@H]1CC[C@@]2([C@@H](C)[C@H]3[C@H](C[C@H]4[C@@H]5CC[C@H]6C[C@H]([C@@H](C[C@]6(C)[C@H]5CC[C@]34C)O)O)O2)OC1</chem>
Glaucolide A	<chem>CC(=O)OC1=C2[C@@H](C[C@@](C)(C(=O)CC[C@@]3(C)[C@@H]([C@@H]2OC1=O)O3)OC(=O)C)O</chem>
Glaziovine	<chem>CN1CCc2cc(c(c3c2[C@@H]1CC13C=CC(=O)C=C1)O)OC</chem>
Glucose	<chem>C(C1[C@H]([C@@H](C([C@H](O)O1)O)O)O)O</chem>
Glycyrrhizin	<chem>CC1(C)C2CC[C@]3(C)C(C(=O)C=C4[C@@H]5C[C@](C)(CC[C@]5(C)CC[C@@]34C)C(=O)O)[C@@]2(C)CC[C@@H]1OC1C(C(C(C(C(=O)O)O1)O)O)OC1C(C(C(C(C(=O)O)O1)O)O)O</chem>
Gnidicin	<chem>CC1C(C2(C3C4C1(C5C=C(C(=O)C5(C(C6(C4O6)CO)O)O)C)OC(O3)(O2)C7=CC=CC=C7)C(=C)C)OC(=O)C=CC8=CC=CC=C8</chem>
Gnidilatin	<chem>CCCCCCCCC12OC3C4C5C(O5)(C(C6(C(C4(O1)C(C(C3(O2)C(=O)C)OC(=O)C7=CC=CC=C7)C)C=C(C6=O)C)O)O)C O</chem>
Gniditrin	<chem>CCCC=CC=CC=CC(=O)OC1C(C23C4C=C(C(=O)C4(C(C5(C(C2C6C1(OC(O6)(O3)C7=CC=CC=C7)C(=C)C)O5)CO)O)O)C)C</chem>
Gomphoside	<chem>O=C1C=C(CO1)[C@H]7CC[C@@]3(O)C7CCC2C4C[C@H]5O[C@@]6(O)[C@H](O)C[C@@H](C)O[C@H]6O[C@@H]5C[C@@H]4CCC23</chem>
Gossypetin	<chem>C1=CC(=C(C=C1C2=C(C(=O)C3=C(O2)C(=C(C=C3O)O)O)O)O)O</chem>
Grayanotoxin I	<chem>CC(=O)O[C@@H]1[C@H]2CCC3[C@](C)([C@@H]4C[C@@H](C(C)(C)[C@]4([C@@H](C[C@@]13CC2(C)O)O)O)O)O</chem>
Grevillol	<chem>CCCCCCCCCCCCc1cc(cc(c1)O)O</chem>
Guaijaverin	<chem>Oc1ccc(cc1O)C=3Oc4cc(O)cc(O)c4C(=O)C=3OC2OC[C@H](O)[C@H](O)[C@H]2O</chem>
Harman	<chem>Cc1c2c(ccn1)c1cccc1[nH]2</chem>
Harpagide	<chem>C[C@@]1(C[C@H]([C@@]2(C=CO[C@H]([C@H]12)OCC(C(C(C(C=O)O)O)O)O)O)O)O</chem>
Harpagoside	<chem>C[C@@]1(C[C@H]([C@@]2(C=CO[C@H]([C@H]12)OCC(C(C(C(C=O)O)O)O)O)O)O)OC(=O)/C=C\c1cccc1</chem>
Harunganin	<chem>CC1=C(C2=CC3=C(C(=CC(=O)C3(CC=C(C)C)CC=C(C)C)O)C(=C2C(=C1)O)O)CC=C(C)C</chem>

Harunganol B	<chem>C/C(C)=C\Cc2c1Cc3c(C(=O)c1c(O)c(C\C=C(/C)C)c2C)c(O)cc(O)c3C\C=C(/C)C</chem>
Harunmadagascarin A	<chem>CC1=CC2=CC3=C(C(=C2C(=C1)O)O)C(=O)C4=C(C3(CC=C(C)C)CC=C(C)C)OC(C=C4)(C)C</chem>
Harunmadagascarin B	<chem>C/C(C)=C\Cc2(C\C=C(/C)C)C=4OC(C)(C)C=CC=4C(=O)c1c(O)c3c(cc12)c(C\C=C(/C)C)c(C)cc3O</chem>
Hautriwaic acid	<chem>C[C@@H]1CC[C@@]2(CO)C(=CCC[C@@H]2[C@@]1(C)CCc1ccoc1)C(=O)O</chem>
Heamanthamine	<chem>C1=CC23c4cc5c(cc4CN(C[C@H]3O)[C@H]2C[C@@H]1ON)OCO5</chem>
Heamanthidine	<chem>C1=CC23c4cc5c(cc4C(N(C[C@H]3O)[C@H]2C[C@@H]1ON)O)OCO5</chem>
Hederagenin	<chem>CC1(C)CC[C@@]2(CC[C@]3(C)C(=CCC4[C@@]5(C)CC[C@@H]([C@@](C)(CO)C5CC[C@@]34C)O)C2C1)C(=O)O</chem>
Helichrysetin	<chem>COc1cc(cc(c1C(=O))/C=C/C1C=CC(C=C1)O)O)O</chem>
Helinudichromene quinone	<chem>CC(=CCCC1(C)C=Cc2c(c(=O)c(C(=O)C(C)C)o2)OC)O1)C</chem>
Heliosupine	<chem>C/C=C(/C)\C(=O)O[C@H]1CCN2CC=C(COC(=O)[C@@]([C@@H](C)O)(C(C)(C)O)O)C12</chem>
hellebrigenin	<chem>CC12CCC3C(C1(CCC2C4=COC(=O)C=C4)O)CCC5(C3(CCC(C5)O)C=O)O</chem>
Hellebrigenin-3-acetate	<chem>CC(=O)OC1CCC2(C3CCC4(C(CCC4(C3CCC2(C1)O)O)C5=COC(=O)C=C5)C)C=O</chem>
Henningsiine	<chem>C[C@@H]1[C@@H]2CN3CC[C@@]45c6cccc6N(C(=O)CO)[C@H]5C(=CO1)[C@H]2C[C@H]34</chem>
Hesperidin	<chem>COc1ccc(cc1O)[C@@H]1CC(=O)c2c(cc(cc2O1)OCC(C(C(C(=O)O)O)O)O)O)O</chem>
Hesperitin	<chem>COC1=C(C=C(C=C1)C2CC(=O)C3=C(C=C(C=C3O2)O)O)O</chem>
Hibiscetin	<chem>C1=C(C=C(C(=C1)O)O)C2=C(C(=O)C3=C(O2)C(=C(C=C3O)O)O)O</chem>
Hibiscin	<chem>C1C(C(C(C(O1)OC2C(C(C(OC2OC3=C([O+]=C4C=C(C=C(C4=C3)O)O)C5=CC(=C(C(=C5)O)O)O)CO)O)O)O)O)O</chem>
Hibiscitrin	<chem>C1=C(C=C(C(=C1)O)O)C2=C(C(=O)C3=C(O2)C(=C(C=C3O)O)O)OC4C(C(C(C(O4)CO)O)O)O</chem>
Hibiscus acid	<chem>C(C(=O)O)C(C(C(=O)O)O)(C(=O)O)O</chem>
Hippeastrine	<chem>CN1CCC2=C[C@@H]([C@@H]3[C@@H](c4cc5c(cc4C(=O)O3)OCO5)[C@H]12)O</chem>
Hircinol	<chem>COc1cc(cc2CCc3cccc(c3c12)O)O</chem>
Hispanolone	<chem>C[C@@H]1C(=O)CC2C(C)CCC[C@]2(C)[C@]1(CCc1ccoc1)O</chem>
Histamine	<chem>C(CN)c1c[nH]cn1</chem>
Hordenine	<chem>CN(C)CCc1ccc(cc1)O</chem>
Humulene	<chem>C/C/1=C\Cc2C(=C/CC(C)(C)/C=C/C1)/C</chem>
Hydroxyvernolide	<chem>C=C1C2C(CC34C(O3)CCC(=CC2OC1=O)COC4O)OC(=O)C(=C)CO</chem>
Hyoscine	<chem>CN1[C@@H]2CC(CC1[C@@H]1[C@H]2O1)OC(=O)[C@H](CO)c1cccc1</chem>
Hyoscyamine	<chem>CN1C2CCC1CC(C2)OC(=O)[C@H](CO)c1cccc1</chem>
Hyperforin	<chem>CC(=CCCC1(C)C(CC=C(C)C)CC2(CC=C(C)C)C(=O)C(=C(C1(C(=O)C(C)C)C2=O)O)CC=C(C)C)C</chem>
Hypericin	<chem>CC1=CC(=C2C3=C1C4=C5C(=C(C=C4)O)C(=O)C6=C(C=C(C7=C6C5=C3C8=C7C(=CC(=C8C2=O)O)O)O)O)O</chem>
Hyperin	<chem>C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)OC4C(C(C(C(O4)CO)O)O)O)O)[O-]</chem>
Hyperoside	<chem>c1cc(c(cc1c1c(c(=O)c2c(cc(cc2o1)O)O)OCC(C(C(C(=O)O)O)O)O)O)O</chem>
hypoxoside	<chem>C1=CC(=C(C=C1C=CCC#CC2=CC(=C(C=C2)OC3C(C(C(C(O3)CO)O)O)O)O)OC4C(C(C(C(O4)CO)O)O)O</chem>



Ibogaine	<chem>CCC1CC2CC3C1N(C2)CCC4=C3NC5=C4C=C(C=C5)OC</chem>
Ibogamine	<chem>CC[C@H]1C[C@H]2C[C@@H]3[C@H]1N(C2)CCC4=C3NC5=CC=CC=C45</chem>
Iboxygaine	<chem>C[C@@H]([C@@H]1C[C@@H]2C[C@H]3c4c(CCN(C2)[C@@H]13)c1cc(ccc1[nH]4)OC)O</chem>
Ibozol	<chem>CC(C)[C@]1(CCC2=C(C1)[C@H](CC1C(C)(C)CCC[C@]21C)O)O</chem>
Icterogenin	<chem>CC=C(C)C(=O)OC1CC(CC2C1(CCC3(C2=CCC4C3(CCC5C4(CCC(=O)C5(C)CO)C)C)C(=O)O)(C)C</chem>
Ilexoside A	<chem>C[C@@H]1CC[C@@]2(CC[C@]3(C)C(=CCC4[C@@]5(C)CC[C@@H](C(C)(C)C5CC[C@@]34C)O[C@H]3[C@@H]([C@H]([C@@H](CO)O3)O)O)C2=C1C)C(=O)O</chem>
Indole-3-acetyl aspartic acid	<chem>c1ccc2c(c1)c(CC(=N[C@@H](CC(=O)O)C(=O)O)c[nH]2</chem>
Ingenol	<chem>CC1=CC23[C@H](C)CC4C(C(C=C(CO)[C@H]([C@@]3([C@H]1O)O)O)C2=O)C4(C)C</chem>
Insularine	<chem>CN1CCc2cc(c3c4c2[C@H]1Cc1ccc(cc1)Oc1c2c(CCN(C)[C@@H]2Cc2ccc(c(c2)CO3)O4)cc(c1OC)OC)OC</chem>
Integerrimine	<chem>CC=C1CC(C(C(=O)OCC2=CCN3C2C(CC3)OC1=O)(C)O)C</chem>
Integriquinoline	<chem>Oc1ccc2c(c1)C(=CC(=O)N2C)OC</chem>
Ipsdienone	<chem>C=CC(=C)CC(=O)C=C(C)C</chem>
Isocryptolepine	<chem>CN1C=C2C3=CC=CC=C3N=C2C4=CC=CC=C41</chem>
Isoeugenitol	<chem>Cc1cc(=O)c2c(cc(c(C)c2o1)O)O</chem>
Isofucosterol	<chem>C/C=C/CC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@H](CC[C@]4(C)[C@H]3CC[C@]12C)O)\C(C)C</chem>
Isofuranogermacrene	<chem>CC1=COC2=C1CC(C(C2)(C)C=C)C(=C)C</chem>
Isokigelinol	<chem>Oc3cc4C(=O)C2=CC1=C(C)CCC1=C(C)C2(C)C(=O)c4cc3</chem>
Isomethone	<chem>CC(C)[C@H]1CC[C@@H](C)C(C)C1=O</chem>
Isoorientin	<chem>c1cc(c(cc1c1cc(=O)c2c(cc(c(c2O)[C@H]2[C@@H]([C@H]([C@@H]([C@@H](CO)O2)O)O)O)O)O)O)O)O</chem>
Isopimpinellin	<chem>COc1c2ccc(=O)oc2c(c2c1cco2)OC</chem>
Isopinnatal	<chem>CC12CCC3C1C=C4C(=O)C5=C(C=CC(=C5)O)C(=O)C4(C3(C)C=O)O2</chem>
Isopolygodial	<chem>CC1(C)CCC[C@]2(C)[C@H](C=O)C(=CC[C@@H]12)C=O</chem>
Isoquercetin	<chem>C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)OC4C(C(C(C(O4)CO)O)O)O)O)O</chem>
Isoreserpiline	<chem>C[C@H]1[C@@H]2CN3CCc4c5cc(c(cc5[nH]c4[C@@H]3[C@@H]2C(=CO1)C(=O)OC)OC)OC</chem>
Isoreserpine	<chem>COC1C(CC2CN3CCC4=C(C3CC2C1C(=O)OC)NC5=C4C=CC(=C5)OC)OC(=O)C6=CC(=C(C(=C6)OC)OC)OC</chem>
Isorhamnetin	<chem>COC1=C(C=CC(=C1)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O</chem>
Isosakuranetin	<chem>COc1ccc(cc1)[C@@H]1CC(=O)c2c(cc(cc2O1)O)O</chem>
Isovanillin	<chem>COC1=C(C=C(C=C1)C=O)O</chem>
Isovitexin	<chem>C1=CC(=CC=C1C2=CC(=O)C3=C(C(=C(C=C3O2)O)C4C(C(C(C(O4)CO)O)O)O)O)O</chem>
Ivangustin	<chem>CC1=C2CCC3C(=C)C(=O)O[C@@H]3C[C@@]2(C)[C@@H](CC1)O</chem>
Jiofuran	<chem>C1=C2[C@H]([C@@H]([C@@H](C2=CO1)O)O)CCO</chem>
Jioglutolide	<chem>CC1(CC(C2C1COC(=O)C2)O)O</chem>

Kaempferol	<chem>c1cc(ccc1c1c(c(=O)c2c(cc(cc2o1)O)O)O)O</chem>
kaempferol-3-glucoside	<chem>C1=CC(=CC=C1C2=C(C(=O)C3=C(O2)C=C(C=C3[O-])O)OC4C(C(C(C(O4)CO)O)O)O)O</chem>
kaempferol-3-o-(6'-malonyl-glucoside)	<chem>C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)OC4C(C(C(C(O4)COC(=O)CC(=O)O)O)O)O)O</chem>
kaempferol-3-O-rhamnoglucoside	<chem>OC6C(O)C(O)C(CO)OC6OC1C(O)C(OC(C)C1O)OCC5OC(OC=2C(=O)c4c(O)cc(O)cc4OC=2c3ccc(O)cc3)C(O)C(O)C5O</chem>
Kauran-16 $\alpha$ -ol	<chem>CC4(C)CCCC1(C)C4CCC32CC(CCC12)C(C)(O)C3</chem>
Kigelin	<chem>C[C@@H]1Cc2cc(c(c2C(=O)O1)O)OC)OC</chem>
Kigelinol	<chem>CC1=C2C=C3C(=O)C4=C(C=C(C=C4)O)C(=O)C3(C=C2CC1)C)O</chem>
Kigelinone	<chem>CC(C1=CC2=C(O1)C(=O)C3=C(C2=O)C=CC=C3O)O</chem>
Knipholone	<chem>CC(=O)c1c(cc(c2c(cc(c3c2C(=O)c2cccc(c2C3=O)O)O)CO)c1O)O)CO</chem>
Kokusaginine	<chem>COC1=C(C=C2C(=C1)C(=C3C=COC3=N2)OC)OC</chem>
Kolaflavanone	<chem>COC1=C(C=C(C=C1)C2C(C(=O)C3=C(O2)C(=C(C=C3O)O)C4C(OC5=CC(=CC(=C5C4=O)O)O)C6=CC=C(C=C6)O)O)O</chem>
Kolanone	<chem>CC(=CCCC(=CCC1(C(=O)C(=C(C(=C(C2=CC=CC=C2)O)C1=O)O)CC=C(C)C)CC=C(C)C)C</chem>
Kraussianin	<chem>CCCCCCCC(=O)O[C@H]1[C@@H](C)[C@@H]2[C@H](C)CCCCC[C@H](C34[C@@H](C)[C@@]56[C@@H](C7[C@](CO)([C@H]([C@]1([C@@H]25)O)O)O7)[C@@H]1C3(C(=C)C)OC4(O1)O6)O</chem>
Lactucin	<chem>CC1=C2C(=O)C=C(CO)[C@@H]2[C@@H]2C(C(=C)C(=O)O2)[C@H](C1)O</chem>
Lanceotoxin A	<chem>C[C@@H]([C@@H]([C@H]([C@H](C(=O)O[C@H]1CC[C@]2(CO)C3CC[C@]4(C)[C@H](CC[C@@]4(C3CC[C@@]2(C1)OC(=O)C)O)c1ccc(=O)oc1)O)O)O</chem>
Lanceotoxin B	<chem>CC1C(C(C(O1)O[C@H]1CC[C@]2(CO)C3CC[C@]4(C)[C@H](CC[C@@]4(C3CC[C@@]2(C1)OC(=O)C)O)c1ccc(=O)oc1)O)O</chem>
Lantadene A	<chem>C/C=C(/C)\C(=O)O[C@@H]1CC(C)(C)C[C@H]2C3=CC[C@@H]4[C@@]5(C)CCC(=O)C(C)(C)[C@@H]5CC[C@@]4(C)[C@]3(C)CC[C@@]12C(=O)O</chem>
Lantadene B	<chem>CC(=CC(=O)OC1CC(CC2C1(CCC3(C2=CCC4C3(CCC5C4(CCC(=O)C5(C)C)C)C)C(=O)O)(C)C)C</chem>
Lapachol	<chem>CC(=CCC1=C(C(=O)c2cccc2C1=O)O)C</chem>
Lasiosperman	<chem>CC(CCCc1ccoc1)Cc1cc(C)co1</chem>
Lauric acid	<chem>CCCCCCCCCCCC(=O)O</chem>
L-Djenkolic acid	<chem>C([C@@H](C(=O)O)N)SC5CC(C(=O)O)N</chem>
Lemmatoxin	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)OC6C(C(C(C(O6)CO)OC7C(C(C(C(O7)CO)O)O)OC8C(C(C(C(O8)CO)O)O)O)O)C)C)C2C1)C)C(=O)O)C</chem>
Leucocyanidin	<chem>C1=CC(=C(C=C1C2C(C(C3=C(C=C(C=C3O2)O)O)O)O)O)O</chem>
Leurosidine	<chem>CCC1(CC2CC(C3=C(CCN(C2)C1)C4=CC=CC=C4N3)(C5=C(C=C6C(=C5)C78CCN9C7C(C=CC9)(C(C(C8N6C)(C(=O)O)C)O)OC(=O)C)CC)OC)C(=O)OC)O</chem>
Leurosine	<chem>CCC12CN3CCC4=C(C(CC(C3)C1O2)(C5=C(C=C6C(=C5)C78CCN9C7C(C=CC9)(C(C(C8N6C)(C(=O)OC)O)OC(=O)C)CC)OC)C(=O)OC)NC1=CC=CC=C41</chem>

Lignoceric acid	<chem>CCCCCCCCCCCCCCCCCCCCCCCC(=O)O</chem>
Ligustroside	<chem>C/C=C/1\[C@H](CC(=O)OCCc2ccc(cc2)O)C(=CO[C@H]1OC1C(C(C(C(CO)O1)O)O)OC(=O)OC</chem>
Limonene	<chem>C=C(C)C1CC=C(C)CC1</chem>
Linalool	<chem>C=C[C@](C)(CCC=C(C)C)O</chem>
Linamarin	<chem>CC(C)(C#N)OC1C(C(C(C(CO)O1)O)O)O</chem>
Lindestrene	<chem>C=C1CC=CC2(C)Cc3occ(C)c3CC12</chem>
Liquiritin	<chem>c1cc(ccc1[C@@H]1CC(=O)c2ccc(cc2O1)O)OCC(C(C(C(C=O)O)O)O)O</chem>
Lithospermic acid	<chem>C1=CC(=C(C=C1CC(C(=O)O)OC(=O)C=CC2=C3C(C(OC3=C(C=C2)O)C4=CC(=C(C=C4)O)O)C(=O)O)O)O</chem>
L-Mimosine	<chem>c1cn(C[C@@H](C(=O)O)N)cc(c1=O)O</chem>
Lochnerine	<chem>CC=C1CN2C3CC1C(C2CC4=C3NC5=C4C=C(C=C5)OC)CO</chem>
Loganin	<chem>CC1C(CC2C1C(OC=C2C(=O)OC)OC3C(C(C(C(O3)CO)O)O)O)O</chem>
Longistylin A	<chem>CC(=CCC1=C(C=C(C=C1OC)C=CC2=CC=CC=C2)O)C</chem>
Longistylin C	<chem>CC(=CCC1=C(C=C(C=C1C=CC2=CC=CC=C2)O)OC)C</chem>
L-Quebrachitol	<chem>COC1C(C(C(C(C1O)O)O)O)O</chem>
Lupanine	<chem>C1CCN2C[C@@H]3C[C@H](CN4[C@@H]3CCCC4=O)[C@@H]2C1</chem>
Lupeol	<chem>CC(=C)C1CCC2(C1C3CCC4C5(CCC(C(C5CCC4(C3(CC2)C)C)(C)C)O)C)C</chem>
Luteolin	<chem>C1=CC(=C(C=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O)O</chem>
Luteolin-4-rutinoside	<chem>Oc1cc(O)cc2OC(CC(=O)c12)c5ccc(OC4O[C@H](COC3C[C@H](C)[C@@H](O)[C@H](O)[C@H]3O)[C@@H](O)[C@H](O)[C@H]4O)c(O)c5</chem>
Luteolin-7-glucoside	<chem>C1=CC(=C(C=C1C2=CC(=O)C3=C(C=C(C=C3O2)OC4C(C(C(C(O4)CO)O)O)O)O)O)O</chem>
Luteolin-7-rutinoside	<chem>CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=CC(=C4C(=C3)OC(=CC4=O)C5=CC(=C(C=C5)O)O)O)O)O)O)O)O</chem>
Lycorine	<chem>C1CN2Cc3cc4c(cc3[C@H]3[C@H]2C1=C[C@@H]([C@H]3O)O)OCO4</chem>
Macowine	<chem>COc1cc2c(cc1O)CN1CC[C@@]32C=C[C@@H](C[C@@H]13)O</chem>
Macrozamin	<chem>C/[N+] (=N \ CO[C@H]1C([C@H]([C@@H](C(CO[C@H]2[C@@H](C([C@@H](CO2)O)O)O1)O)O)/[O-]</chem>
Madecassic acid	<chem>C[C@@H]1CCC2(CC[C@]3(C)C(=CCC4[C@@]5(C)C[C@H]([C@@H]([C@@](C)(CO)C5[C@@H](C[C@@]34C)O)O)[C@H]2[C@H]1C)C(=O)O</chem>
Maleic acid	<chem>C(=C \ C(=O)O) \ C(=O)O</chem>
Malic acid	<chem>C(C(C(=O)O)O)C(=O)O</chem>
Malinic acid	<chem>C(=C \ CC(=O)O) / C(=O)O \ C(=O)O</chem>
Malvidin	<chem>COC1=CC(=CC(=C1O)OC)C2=C(C=C3C(=CC(=CC3=[O+])2)O)O</chem>
Mangiferin	<chem>c1c2c(cc(c1O)O)oc1cc(c(c1c2=O)O)OCC(C(C(C(CO)O)O)O)O</chem>
Mannitol	<chem>C(C(C(C(C(CO)O)O)O)O)O</chem>
Marasmicin	<chem>CSCSS(=O)CSC</chem>

Marrubiin	<chem>C[C@@H]1C[C@@H]2[C@H]3[C@](C)(CCC[C@]3(C)[C@]1(CCC1C=CO1)O)C(=O)O2</chem>
Maslinic acid	<chem>CC1(C)CC[C@@]2(CC[C@]3(C)C(=CC[C@@H]4[C@@]5(C)C[C@H]([C@@H](C(C)(C)[C@@H]5CC[C@@]34C)O)O)[C@@H]2C1)C(=O)O</chem>
Medicagol	<chem>C1OC2=C(O1)C=C3C(=C2)C4=C(O3)C5=C(C=C(C=C5)O)OC4=O</chem>
Melianol	<chem>CC1(C)[C@@H]2CC=C3[C@H](CC[C@@]4(C)[C@@H](CC[C@]34C)[C@@H]3C[C@H]([C@H]4C(C)(C)O4)O[C@H]3O)[C@@]2(C)CC[C@@H]1O</chem>
Melianthugenin	<chem>CC(=O)O[C@H]1C[C@]2(CO)C3CC[C@]4(C)C[C@H](C[C@@]4([C@@H]3CC[C@@]2(C[C@H]1OC(=O)C)OC(=O)C)O)c1ccc(=O)oc1</chem>
Melianthusigenin	<chem>CC(=O)OCC12C7CC6CC1(CCC3C2CCC4(C)C(CCC34O)c5ccc(=O)oc5)OC(C)(O6)O7</chem>
Meliatoxin A1	<chem>CCC(C)C(=O)OC1C2(C)C3CC(C4(C)C(C(=O)CC5(C)C(CC6C45O6)c4ccoc4)C3(CO1)C(C(C2OC(=O)C)OC(=O)C)O)O</chem>
Meliatoxin A2	<chem>CC(C)C(=O)OC1C2(C)C3CC(C4(C)C(C(=O)CC5(C)C(CC6C45O6)c4ccoc4)C3(CO1)C(C(C2OC(=O)C)OC(=O)C)O)O</chem>
Meliatoxin B1	<chem>CCC(C)C(=O)OC1C2(C)C3CC(C4(C)C5CC(=O)C(c6ccoc6)C5(C)CC(=O)C4C3(CO1)C(C(C2OC(=O)C)OC(=O)C)O)O</chem>
Meliatoxin B2	<chem>CC(C)C(=O)OC1C2(C)C3CC(C4(C)C5CC(=O)C(c6ccoc6)C5(C)CC(=O)C4C3(CO1)C(C(C2OC(=O)C)OC(=O)C)O)O</chem>
Melissic acid	<chem>CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)O</chem>
Mellitoxin	<chem>C=C(C)C1([C@@H]2C(=O)O[C@H]1[C@H]([C@@]1(C)[C@@]3(CO3)[C@H]3[C@@H]([C@@]21O)O3)O)O</chem>
Menthol	<chem>CC(C)[C@@H]1CC[C@@H](C)C[C@H]1O</chem>
Menthone	<chem>CC(C)[C@@H]1CC[C@@H](C)CC1=O</chem>
Mesembranol	<chem>CN1CCC2(CCC(CC12)O)c1ccc(c(c1)OC)OC</chem>
Mesembrenone	<chem>CN1CCC2(C=CC(=O)CC12)c1ccc(c(c1)OC)OC</chem>
Mesembrine	<chem>CN1CCC2(CCC(=O)CC12)c1ccc(c(c1)OC)OC</chem>
Mesquitol	<chem>c1cc(c(cc1[C@H]1[C@@H](Cc2ccc(c(c2O1)O)O)O)O)O</chem>
Methyl salicylate	<chem>COC(=O)c1ccccc1O</chem>
Methylasparagine	<chem>CNC(=O)CC(C(=O)O)N</chem>
Methylazoxymethanol	<chem>C/[N+](=N/CO)/[O-]</chem>
Methylnonyl ketone	<chem>CCCCCCCCCCCCOC</chem>
Monofluoroacetic acid	<chem>C(C(=O)O)F</chem>
Montanine	<chem>CO[C@H]1C=C2[C@H]3CN(Cc4cc5c(cc34)OCO5)[C@H]2C[C@@H]1O</chem>
Moringine	<chem>C1=CC=C(C=C1)CN</chem>
Moringyne	<chem>CC1=CC=CC(C)=C1C(=O)OC1OC(CO)C(O)C1O</chem>
Mucronine D	<chem>CCC(C)C1C(=O)N/C=C/c2ccc(cc2)OC2CCN(C2C(=O)N1)C(=O)C(CC(C)C)NC(=O)C(Cc1ccccc1)N(C)C</chem>
Mukaadial	<chem>CC1(C)CCC[C@@]2(C)[C@H]1[C@H](C=C(C=O)[C@@]2(C=O)O)O</chem>
Muzigadial	<chem>CC1CCC2(C(C1=C)CC=C(C2(C=O)O)C=O)C</chem>
Myrcene	<chem>C=CC(=C)CCC=C(C)C</chem>

Myricetin	<chem>c1cc(c(c1c1coc2cc(cc2c1=O)O)O)O)O</chem>
Myristic acid	<chem>CCCCCCCCCCCCC(=O)O</chem>
Naringenin	<chem>c1cc(ccc1C1CC(=O)c2c(cc(cc2O1)O)O)O</chem>
Nauclefidine	<chem>O=CC3=CC=C2c4nc1cccc1c4CCN2C3=O</chem>
Nauclefine	<chem>CC(=O)C1=C2C=C3C4=C(CCN3C(=O)C2=CN=C1)C5=CC=CC=C5N4</chem>
Neocryptolepine	<chem>CN1C2=CC=CC=C2C=C3C1=NC4=CC=CC=C43</chem>
Neral	<chem>CC(=CCC/C(=C\C=O)/C)C</chem>
N-Hentriacontane	<chem>CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC</chem>
Niazimicin	<chem>CCOC(=S)NCC1=CC=C(C=C1)OC2C(C(C(O2)C)O)O</chem>
Niazinin A	<chem>CC1C(C(C(O1)OC2=CC=C(C=C2)CNC(=S)OC)O)O</chem>
Niazinin B	<chem>COC(=S)NCC1=CC=C(OC2OC(C)C(O)C(O)C2O)C=C1</chem>
Nicotine	<chem>CN1CCC[C@H]1c1ccnc1</chem>
N-Methylconiine	<chem>CCC[C@H]1CCCCN1C</chem>
N-methylflindersine	<chem>CC1(C)C=Cc2c(c3cccc3n(C)c2=O)O1</chem>
N-Nonacosane	<chem>CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC</chem>
Norajmaline	<chem>CCC1C2CC3C4C5(CC(C2C5O)N3C1O)C6=CC=CC=C6N4</chem>
Norharman	<chem>c1ccc2c(c1)c1ccncc1[nH]2</chem>
Norhyoscine	<chem>c1ccc(cc1)[C@@H](CO)C(=O)OC1CC2C3C(C(C1)N2)O3</chem>
Nothofagin	<chem>c1cc(ccc1CCC1c2c(cc(cc2O[H-]O1)O)O)O</chem>
N-trans-Feruloyltyramine	<chem>COc1cc(ccc1O)/C=C/C(=O)NCCc1ccc(cc1)O</chem>
N-trans-Tetracosyl ferulate	<chem>Oc1ccc(cc1OC)/C=C/C(=O)OCCCCCCCCCCCCCCCCCCCCCCCCCCCC</chem>
Nudicauline	<chem>CCN1C[C@@]2(CCC(C34[C@@H]5C[C@@H]6[C@H](C[C@@]([C@H]5[C@H]6OC(=O)C)(C([C@@H]([C@H]23)OC)[C@H]14)O)OC)OC)COC(=O)c1cccc1N1C(=O)C[C@H](C)C1=O</chem>
Nymanina 1	<chem>CC(CC)C(O)C(=O)O[C@H]2[C@H](OC=O)C(C(=C)[C@@]3(O)C(=O)C[C@@H](c1ccoc1)[C@]23C)[C@]4(C)[C@@H](CC(=O)OC)[C@]5(C)COC(O)(C[C@@H]4OC(C)=O)O5</chem>
Obebioside	<chem>CC1C(C(C(C(O1)O)[C@H]1CC[C@@]2(C)[C@H](CCC3C2CC[C@]2(C)[C@@H](C4=CC(=O)OC4)[C@H](C[C@]32O)OC(=O)CC(=O)C(=O)O)C1)O)OC1C(C(C(C(O)O)O)O)O</chem>
Ocubullenone	<chem>C=CCC12CC34C(=CC(=C)C23CC1c1cc(c2c(c1)OCO2)OC)OCO4</chem>
Oleacein	<chem>C/C=C(/C=O)\C(CC=O)CC(=O)OCCc1ccc(c1)O)O</chem>
Oleandrin	<chem>CC1C(C(CC(O1)O)[C@H]1CC[C@@]2(C)[C@H](CCC3C2CC[C@]2(C)[C@@H](C4=CC(=O)OC4)[C@H](C[C@]32O)OC(=O)C)C1)OC)O</chem>
Oleanoglycotoxin	<chem>CC1(C)CC[C@@]2(CC[C@]3(C)C(=CCC4[C@@]5(C)CC[C@@H](C(C)(C)C5CC[C@@]34C)OC3C(C(C(C(O)O3)O)OC3(C(C(C(O)O3)O)O)OC3C(C(C(C(O)O3)O)O)O)C2C1)C(=O)O</chem>
Oleanolic acid	<chem>CC1(C)CCC2(CC[C@]3(C)C(=CCC4[C@@]5(C)CC[C@@H](C(C)(C)[C@@H]5CC[C@@]34C)O)[C@@H]2C1)C(=O)O</chem>

Oleanolic-3-acetate	<chem>CC(=O)OC1CCC2(C)C(CCC3(C)C2CC=C2C4CC(C)(C)CCC4(CCC32C)C(=O)O)C1(C)C</chem>
Oleuropein	<chem>C/C=C/1\[C@H](CC(=O)OCCc2ccc(c2)O)O)C(=CC[C@H]1OCC(C(C(C(=O)O)O)O)O)C(=O)OC</chem>
Olivil	<chem>COC1=C(C=CC(=C1)CC2(COC(C2CO)C3=CC(=C(C=C3)O)OC)O)O</chem>
Orbicuside A	<chem>C[C@H]1C[C@H]2[C@H]3[C@@H](O1)O[C@@H]1CC4C[C@H]5[C@@]6(C(CC(=O)[C@]7(C)[C@H](CC[C@]67O)c6ccc(=O)oc6)[C@@]4(C)C[C@]1(O2)O3)O5</chem>
Orientin	<chem>c1cc(c(cc1c1cc(=O)c2c(cc(c2o1)[C@H]1[C@@H]([C@H]([C@@H]([C@@H](CO)O1)O)O)O)O)O)O)O</chem>
Osmitopsin	<chem>CC1=C2[C@@H]3[C@H](CC[C@@H](C)[C@@]2(C)CC1)C(=C)C(=O)O3</chem>
Ouabain	<chem>C[C@@]12C[C@H](C3[C@@H](CC[C@@]4(C[C@H](CC([C@]34CO)O)OCC(C(C(C(=O)O)O)O)O)[C@]2(CC[C@@H]1C1=CC(=O)OC1)O)O</chem>
Ouratea-proanthocyanidin A	<chem>COc1c(cc(cc1O)[C@@H]1[C@H](Cc2c(cc(c3c4c(cc(cc4O[C@H](c4ccc(cc4)O)[C@@H]3O)O)O)c2O1)O)O)O)O</chem>
Oxalic acid	<chem>C(=O)(C(=O)O)O</chem>
Oxyavicine	<chem>Cn1c2c(ccc3cc4c(cc23)OCO4)c2cc3c(cc2c1=O)OCO3</chem>
Oxychelerythrine	<chem>Cn1c2c(ccc3cc4c(cc23)OCO4)c2ccc(c2c1=O)OC)OC</chem>
Oxypurinol	<chem>c1c2c([nH]c(=O)[nH]c2=O)[nH]n1</chem>
P57	<chem>C/C=C(\C)/C(=O)O[C@H]1CC2C(CC=C3C[C@H](CC[C@]23C)O[C@H]2C[C@@H]([C@@H]([C@@H](C)O2)O[C@H]2C[C@@H]([C@@H]([C@@H](C)O2)O[C@H]2[C@@H]([C@H]([C@@H]([C@@H](C)O2)O)OC)O)OC)OC)[C@]2(CC[C@H](C(=O)C)[C@@]12C)O</chem>
Palmitic acid	<chem>CCCCCCCCCCCCCCCC(=O)O</chem>
Palustrine	<chem>CC[C@@H]([C@@H]1CC=C[C@@H]2CC(=O)NCCCCNCCCN12)O</chem>
Parquin	<chem>CC(C)CC(=O)OC1C(OC2C[C@H]([C@H]3CC[C@@]45C[C@@H](CCC4[C@]3(C)C2)C(=C)C5O)C(=O)O)OC(CO)C(C1(C)O)O)OC1C(C(=O)C(=O)O1)OCO</chem>
p-Coumaric acid	<chem>C1=CC(=CC=C1C=CC(=O)O)O</chem>
p-Cymene	<chem>CC(C)c1ccc(C)cc1</chem>
Peddiea Factor A1	<chem>CCC/C=C/C=C/C=C/C12O[C@@H]3[C@@H]4[C@H]5[C@@](CO)([C@H]([C@]6(C(C=C(C)C6=O)[C@]4(C(C)[C@H]([C@]3(C(=C)C)O1)O)O2)O)O)O5</chem>
Pelletierine	<chem>CC(=O)C[C@H]1CCCCN1</chem>
Pentacosane	<chem>CCCCCCCCCCCCCCCCCCCCCCCCCCCC</chem>
Pentalongin	<chem>c1ccc2c(c1)C(=O)C1=C(COC=C1)C2=O</chem>
Pentatriacontane	<chem>CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC</chem>
Perforatin A	<chem>Cc1cc(=O)c2c(cc3c(C=CC(C)(C)O3)c2o1)OC</chem>
Persin	<chem>CCCCC/C=C\C/C=C\C CCCCCC(=O)C[C@H](COC(=O)C)O</chem>
Pescaproside A	<chem>CCCCCCCCCCCC(=O)OC1C(C(C(OC1OC2C(OC(C(C2O)O)OC3C(C(C(OC3OC(CCCCC)CCCCCCCC(=O)OC)C)O)O)C)OC4C(C(C(C(O4)C)O)O)OC5C(C(C(C(O5)C)O)O)O</chem>

Pescaproside B	<chem>CCCCCCCCCCCC(=O)O[C@@H]1[C@@H]([C@H]([C@H](C)O[C@H]1O[C@H]1[C@H](C)O[C@H]([C@@H]([C@@H]1O)O)O)[C@@H]1[C@H]([C@H]([C@@H](C)O[C@H]1O[C@@H](CCCC)CCCCCCCCC(=O)OC)O)O)[C@H]1[C@@H]([C@@H]([C@H]([C@H](C)O1)O)O)O)[C@H]1[C@@H]([C@@H]([C@H]([C@H](C)O1)O)O)O)O</chem>
Pescaproside E	<chem>CCCCCCCCCCCC(=O)O[C@@H]1[C@@H]([C@H]([C@H](C)O[C@H]1O[C@H]1[C@H](C)O[C@H]([C@@H]([C@@H]1O)O)O)[C@@H]1[C@H]([C@H]([C@@H](C)O[C@H]1O[C@@H](CCCC)CCCCCCCCC(=O)OC)O)O)[C@H]1[C@@H]([C@@H]([C@H]([C@H](C)O1)O)O)O)O)[C@H]1[C@@H]([C@@H]([C@H]([C@H](C)O1)O)O)O)O</chem>
Petunidine	<chem>COC1=CC(=CC(=C1O)O)C2=C(C=C3C(=CC(=CC3=[O+])2)O)O</chem>
Phytic acid	<chem>C1(C(C(C(C(C1OP(=O)(O)O)OP(=O)(O)O)OP(=O)(O)O)OP(=O)(O)O)OP(=O)(O)O)OP(=O)(O)O)OP(=O)(O)O</chem>
Picrinine	<chem>CC=C1CN2C3CC1C(C45C3(NC6=CC=CC=C64)OC2C5)C(=O)OC</chem>
Pinitol	<chem>C[C@@H]1C([C@@H](C(C([C@@H]1O)O)O)O)O</chem>
Pinoembrine	<chem>c1ccc(cc1)C1CC(=O)c2c(cc(cc2O1)O)O</chem>
Pinoresinol	<chem>COC1=C(C=CC(=C1)C2C3COC(C3CO2)C4=CC(=C(C=C4)O)OC)O</chem>
Pinostrobin	<chem>COC1=CC(=C2C(=O)CC(OC2=C1)C3=CC=CC=C3)O</chem>
Platyphylline	<chem>C/C=C\1/C[C@@H](C)C[C@](C)(C(=O)OCC2CCN3CC[C@H]([C@@H]23)OC1=O)O</chem>
Plumbagin	<chem>CC1=CC(=O)c2c(cccc2O)C1=O</chem>
Polygodial	<chem>CC1(C)CCC[C@]2(C)[C@@H](C=O)C(=CC[C@@H]12)C=O</chem>
Potassium nitrate	<chem>[K]N(=O)[O-]</chem>
Potassium nitrite	<chem>[K]N(=O)=O</chem>
Powelline	<chem>COC1=C2CN3CCC4(C3CC(C=C4)O)C2=CC5=C1OCO5</chem>
Pratorimine	<chem>COc1cc2c(cc1O)c1cccc3CCn(c13)c2=O</chem>
Pratorinine	<chem>Oc3cc4c2cccc1ccn(c12)C(=O)c4cc3OC</chem>
Premarrubin	<chem>C[C@@H]1C[C@@H]2[C@H]3[C@](C)(CCC[C@]3(C)[C@]31CCC1(C=COC1)O3)C(=O)O2</chem>
Presenegenin	<chem>CC1(C)CC[C@@]2(CCC3(CO)C(=CCC4[C@@]5(C)C[C@@H]([C@@H]([C@](C)(C5CC[C@@]34C)C(=O)O)O)[C@@H]2C1)C(=O)O</chem>
Primin	<chem>CCCCC1=CC(=O)C=C(C1=O)OC</chem>
Proacacipetalin	<chem>C=C(C)[C@@H](C#N)OC1C(C(C(CO)O1)O)O</chem>
Procumbide	<chem>C[C@@]12[C@H]3[C@@H](OC=C[C@]3([C@H]([C@@H]1O2)O)O)OCC(C(C(C(C=O)O)O)O)O</chem>
Procyanidin C1	<chem>c1cc(c(cc1[C@@H]1C(Cc2c(cc(c(C3c4c(cc(c(C5c6c(cc(cc6O[C@H](c6ccc(c(c6)O)O)C5O)O)O)c4O[C@H](c4ccc(c(c4)O)O)C3O)O)O)c2O1)O)O)O)O</chem>
Propacin	<chem>Oc1ccc(cc1OC)[C@H]2Oc3c(O[C@@H]2C)c4OC(=O)C=Cc4cc3OC</chem>
Proscillardin A	<chem>CC1C(C(C(C(O1)O)[C@H]1CC[C@@]2(C)C(=C1)CCC1C2CC[C@]2(C)[C@H](CC[C@]12O)c1ccc(=O)oc1)O)O</chem>
Protoanemonin	<chem>C=C1C=CC(=O)O1</chem>
Protocatechuic acid	<chem>c1cc(c(cc1C(=O)O)O)O</chem>
Protopine	<chem>CN1CCC2=CC3=C(C=C2C(=O)CC4=C(C1)C5=C(C=C4)OCO5)OCO3</chem>

Prunasin	<chem>c1ccc(cc1)[C@H](C#N)OC1C(C(C(CO)O1)O)O</chem>
Pseudobaptigen	<chem>Oc3cc4OC=C(c1ccc2OCOc2c1)C(=O)c4cc3</chem>
Psoralen	<chem>c1cc(=O)oc2cc3c(cco3)cc12</chem>
Ptaquiloside	<chem>C[C@@H]1C[C@]2(C=C(C)C3(CC3)[C@](C)([C@@H]2C1=O)O)OC1[C@H]([C@H](C(C(CO)O1)O)O)O</chem>
Ptearoxylone	<chem>Cc1cc(=O)c2c(cc3c(C=CC(=O)CO3)c2O)o1</chem>
pterygospermin	<chem>C1=CC=C(C=C1)CN2C(=S)OC23C=CC4(C=C3)N(C(=S)O4)CC5=CC=CC=C5</chem>
Pulegone	<chem>CC(=C1CC[C@@H](C)CC1=O)C</chem>
Punicalagin	<chem>C1C2C(C3C(C(O2)O)OC(=O)C4=CC(=C(C(=C4C5=C(C(=C(C=C5C(=O)O3)O)O)O)O)OC(=O)C6=CC(=C(C(=C6C7=CC(C(=C8C9=C7C(=O)OC2=C(C(=C(C3=C(C(=C(C=C3C(=O)O1)O)O)O)C(=C92)C(=O)O8)O)O)O)O)O)O)O)C(=C67)C(=O)O5)O)O)O)O)O</chem>
Punicalin	<chem>C1C2C(C(C(C(O2)O)O)O)OC(=O)C3=CC(=C(C(=C3C4=C(C(=C5C6=C4C(=O)OC7=C(C(=C(C8=C(C(=C(C=C8C(=O)O1)O)O)O)C(=C67)C(=O)O5)O)O)O)O)O)O</chem>
Punicic acid	<chem>CCCC/C=C\C=C\C=C/C/CCCCCCCC(=O)O</chem>
Pyrethrin I	<chem>C=C/C=C\CC1=C(C)[C@H](CC1=O)OC(=O)[C@@H]1[C@@H](C=C(C)C)C1(C)C</chem>
Pyrethrin II	<chem>C=C/C=C\CC1=C(C)[C@H](CC1=O)OC(=O)[C@@H]1[C@@H](/C=C(\C)/C(=O)OC)C1(C)C</chem>
Pyridoxine	<chem>Cc1c(c(CO)c(m1)CO)O</chem>
Pyrogallol	<chem>c1cc(c(c1)O)O</chem>
Quercetin	<chem>c1cc(c(cc1c1c(c(=O)c2c(cc(cc2o1)O)O)O)O)O</chem>
Quercetin-3,7-diglucoside	<chem>C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)OC4C(C(C(C(O4)CO)O)O)O)OC5C(C(C(C(O5)CO)O)O)O)O)O)O</chem>
Quercetin-3-glucoside	<chem>C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)OC4C(C(C(C(O4)CO)O)O)O)[O-]</chem>
Quercetin-3-O-(6'-malonyl-glucoside)	<chem>C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)OC4C(C(C(C(O4)COC(=O)CC(=O)O)O)O)O)O)O</chem>
Quercetin-7 O-β-D-xylopyranoside	<chem>c1cc(c(cc1c1c(c(=O)c2c(cc(cc2o1)O)O)O)O)O)O</chem>
Quercitrin	<chem>CC1C(C(C(C(O1)OC2=C(OC3=CC(=CC(=C3C2=O)O)O)C4=CC(=C(C=C4)O)O)O)O)O</chem>
Quindoline	<chem>C1=CC=C2C(=C1)C=C3C(=N2)C4=CC=CC=C4N3</chem>
Ranunculin	<chem>C1=CC(=O)O[C@H]1COC1C(C(C(CO)O1)O)O</chem>
Rauvoxin	<chem>O=C(OC)C3=CO[C@@H](C)[C@@H]4[C@H]6N5CCC1(c2cc(OC)c(OC)cc2NC1=O)C56C[C@H]34</chem>
Rauvoxinin	<chem>O=C(OC)C3=CC(C)[C@@H](C)[C@@H]4CN5CCC1(c2cc(OC)c(OC)cc2NC1=O)C5C[C@H]34</chem>
Reserpine acid	<chem>COC1C(CC2CN3CCC4=C(C3CC2C1C(=O)O)NC5=C4C=CC(=C5)OC)O.Cl</chem>
Reserpiline	<chem>CC1C2CN3CCC4=C(C3CC2C(=CO1)C(=O)OC)NC5=CC(=C(C=C45)OC)OC</chem>
Reserpine	<chem>COc1cc(cc(c1OC)OC)C(=O)O[C@@H]1C[C@@H]2CN3CCc4c5cccc5[nH]c4[C@H]3C[C@@H]2[C@@H]([C@H]1OC)C(=O)OC</chem>
Reservatrol	<chem>C(=C\c1cc(cc(c1)O)O)/c1ccc(cc1)O</chem>
Resveratrol-3-O-β-rutinoside	<chem>Oc1ccc(cc1)/C=C/c2cc(cc(O)c2)O[C@@H]4O[C@H](COC3O[C@@H](C)[C@H](O)[C@@H](O)[C@H]3O)[C@@H](O)[C@H]4O</chem>



Retrorsine	<chem>C/C=C\1/C[C@@H](C)[C@](CO)(C(=O)OCC2=CCN3CC[C@H]([C@@H]23)OC1=O)O</chem>
Rhinocerotoic acid	<chem>C/C(=C\C(=O)O)/CCC1=C(C)C(=O)C[C@H]2C(C)(C)CCC[C@]12C</chem>
Ricinine	<chem>Cn1ccc(c(C#N)c1=O)OC</chem>
Ricinoleic acid	<chem>CCCCCCC(C/C=C\CCCCCCCC(=O)O)O</chem>
Rohituka 3	<chem>CCC(C)C(C(=O)OC1C2C(C(=C)C3(C1(C(C3=O)C4=COC=C4)C)O)C5(C6CC(=O)OCC6(OC(=O)CC5O2)C)C)O</chem>
Rooperol	<chem>C(/C=C/c1ccc(c(c1)O)O)C#Cc1ccc(c(c1)O)O</chem>
Rosmarinic acid	<chem>c1cc(c(cc1/C=C/C(=O)O[C@@H](Cc1ccc(c(c1)O)O)C(=O)O)O)O</chem>
Rotenone	<chem>C=C(C)[C@H]1Cc2c(ccc3C(=O)[C@H]4c5cc(c(cc5OC[C@H]4Oc23)OC)OC)O1</chem>
Rubiadin	<chem>Cc1c(cc2c(c1O)C(=O)c1cccc1C2=O)O</chem>
Rubiadin xyloglucoside	<chem>O=C4c3cc(OC2OC(CO)C(O)C2OC1OCC(O)C(O)C1O)c(C)c(O)c3C(=O)c5cccc45</chem>
Ruscogenin-(25S)-form	<chem>C[C@@H]1CC[C@@]2([C@H](C)[C@H]3[C@H](CC4C5CC=C6C[C@H](C[C@H]([C@]6(C)C5CC[C@]34C)O)O)2)OC1</chem>
Rutaretin	<chem>CC(C)(C1CC2=C(O1)C(=C3C(=C2)C=CC(=O)O3)O)O</chem>
Rutin	<chem>CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C=C5)O)O)O)O)O)O)O</chem>
Sabinene	<chem>CC(C)[C@@]12CCC(=C)[C@H]2C1</chem>
Sakurasosaponin	<chem>O[C@H]%11[C@@H](O)[C@@H](O)C(C)OC%11O[C@H]%10[C@@H](O)[C@@H](O)C(C)OC%10O[C@H]9[C@@H](O)[C@@H](O)C(CO)OC9O[C@@H]2[C@H](OC1OC(CO)[C@@H](O)[C@H](O)[C@@H]1O)C(OC(C(=O)O)[C@H]2O)O[C@H]8CC[C@@]7(C)C(CC[C@]6(C)C7CC[C@]35OCC4(CC[C@@](C)(C)CC34)[C@H](O)C[C@]56C)[C@]8(C)C</chem>
Salicin	<chem>c1ccc(c(c1)CO)OCC(C(C(C(=O)O)O)O)O</chem>
Salicortin	<chem>c1ccc(c(c1)COC(=O)C1(C=CCCC1=O)O)OCC(C(C(C(=O)O)O)O)O</chem>
Salicylic acid	<chem>c1ccc(c(c1)C(=O)O)O</chem>
Salutarisolid	<chem>CC1CC[C@@]2(C)C(CC=C3C(=O)OC[C@]23O)C1=C</chem>
Sanguinarine	<chem>C[n+]1cc2c(ccc3c2OCO3)c2ccc3cc4c(cc3c12)OCO4</chem>
Sanjoinine A	<chem>CC(C)CC1C(=O)N/C=C\c2ccc(cc2)OC(C(C)C)C(C(=O)N1)NC(=O)C(Cc1cccc1)N(C)C</chem>
Santin	<chem>COc1ccc(cc1)c1c(c(=O)c2cc(c(cc2o1)CO)OC)OC</chem>
Saponin C	<chem>CC1CC[C@@]2([C@@H](C)C3C(CC4C5CC=C6C[C@H](C[C@H]([C@]6(C)C5CC[C@]34C)OC3C(C(C(C(OC(=O)C)O3)O)O)OC3C(C(C(C(C)O3)O)O)O)O2)OC1</chem>
sarcovimiside B	<chem>C[C@H]1[C@@H]([C@@H](C[C@@H](O1)O[C@@H]1[C@@H](C)O[C@H](C[C@@H]1OC)O[C@@H]1[C@@H](C)O[C@H](C[C@@H]1O)O[C@H]1CC[C@]2(C)[C@@H](C[C@H]([C@@]3(C)C(=O)CC[C@]3([C@H](C)OC(=O)c3cccc3)O)OC(=O)c3cccc3)C(=O)C=C[C@@]2(C1)O)OC)O</chem>
Sauveoline	<chem>CN1CCC2=CC(=C(C3=C2C1CC4=C3C(=C(C=C4)O)O)OC)OC</chem>
Sceleratine	<chem>CC1C(C(C(=O)OC2CCN3C2C(=CC3)COC(=O)C1(C)O)(CO)O)C</chem>
Scillaren A	<chem>CC1[C@@H](C([C@@H]([C@@H](O1)OC1CC[C@@]2(C)C(=C1)CCC1C2CC[C@]2(C)[C@H](CC[C@]12O)c1ccc(=O)oc1)O)O[C@H]1C([C@H]([C@H](C(CO)O1)O)O)O</chem>
Scillarenin	<chem>C[C@]12CC[C@@H](C=C1CCC1C2CC[C@]2(C)[C@H](CC[C@]12O)c1ccc(=O)oc1)O</chem>

Scopolamine	<chem>CN1C2CC(CC1C1C2O1)OC(=O)[C@H](CO)c1ccccc1</chem>
Scopoletin	<chem>COc1cc2ccc(=O)oc2cc1O</chem>
secologanin	<chem>COC(=O)C1=CO[C@H]([C@@H]([C@@H]1CC=O)C=C)O[C@H]2[C@@H]([C@H]([C@@H]([C@H](O2)CO)O)O)O</chem>
Securinine	<chem>C1CCN2[C@H]3C=CCC4=CC(=O)O[C@]4(C3)[C@H]2C1</chem>
Senecionine	<chem>C/C=C \ 1/C[C@@H](C)C[C@](C)(C(=O)OCC2=CCN3CC[C@H]([C@@H]23)OC1=O)O</chem>
Sennoside A	<chem>c1cc2C(c3cc(ccc3C(=O)c2c(c1)OCC(C(C(C(C(=O)O)O)O)O)C(=O)O)C1c2cccc(c2C(=O)c2c1cc(cc2O)C(=O)O)OCC(C(C(C(=O)O)O)O)O</chem>
Sericic acid	<chem>CC1(C)CC[C@@]2(CC[C@]3(C)C(=CCC4[C@@]5(C)C[C@H]([C@@H]([C@](C)(CO)C5CC[C@@]34C)O)O)[C@@H]2C1)C(=O)O</chem>
Sericoside	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C(C5(C)CO)O)O)C)C)C2C1O)C)C(=O)OC6C(C(C(C(O6)CO)O)O)O)C</chem>
Serpenticine	<chem>O=C(OC)C3=CO[C@H](C)[C@H]4C[n+]5cccc1c(nc2cc(OC)ccc12)c5C[C@H]34</chem>
serpentine	<chem>CC1C2CN3C=CC4=C5C=CC=CC5=NC4=C3CC2C(=CO1)C(=O)OC</chem>
Sesbanimide A	<chem>C=C1CO[C@]([C@@H]1C)([C@@H]1[C@H]([C@H](C2CC(=O)NC(=O)C2)OCO1)O)O</chem>
Sesbanimide B	<chem>C=C1COC(C1C)(C1C(C(C2CC(=NC(=O)C2)O)OCO1)O)O</chem>
Sesbanimide C	<chem>C=C1COC(C1C)(C(C(CC1CC(=NC(=O)C1)O)O)OC)O</chem>
Siphonochilone	<chem>CC1C=CC(=O)C2(C)Cc3c(CC12)c(C)co3</chem>
Sitosterol-3-glucoside	<chem>CC[C@H](CC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@H](CC[C@]4(C)[C@H]3CC[C@]12C)O[C@H]1[C@@H]([C@H]([C@@H]([C@@H](CO)O1)O)O)C(C)C</chem>
Sivasinolide	<chem>CC1=CC[C@H]([C@]2(C)C[C@H]3[C@@H](C(=C)C(=O)O3)[C@@H](C12)O)O</chem>
Skimmianine	<chem>COc1ccc2c(c1OC)nc1c(cco1)c2OC</chem>
Sodium ent knipholone 6-O-sulfate	<chem>CC(=O)c1c(cc(c2c(cc(c3c2C(=O)c2cccc(c2C3=O)O)O)CO)c1OS(O)(O)O[Na])O)C=O</chem>
Solanine	<chem>C[C@H]1CC[C@@H]2C(C)C3C(CC4C5CC=C6C[C@H](CC[C@]6(C)C5CC[C@]34C)OC3C(C(C(C(CO)O3)O)OC3C(C(C(C(CO)O3)O)O)OC3C(C(C(C(C)O3)O)O)O)N2C1</chem>
Solanocapsine	<chem>C[C@@H]1C[C@]2([C@@H]([C@@H](C)C3C(CC4C5CC[C@H]6C[C@H](CC[C@]6(C)C5CC[C@]34C)N)O2)NC1)O</chem>
Solasodine	<chem>C[C@@H]1CC[C@@]2([C@@H](C)[C@H]3[C@H](CC4C5CC=C6C[C@H](CC[C@]6(C)C5CC[C@]34C)O)O2)NC1</chem>
Solasonine	<chem>CC1CCC2(C(C3C(O2)CC4C3(CCC5C4CC=C6C5(CCC(C6)OC7C(C(C(C(O7)CO)O)OC8C(C(C(C(O8)CO)O)O)O)OC9C(C(C(C(O9)C)O)O)O)C)C)NC1</chem>
Sophoracoumestan B	<chem>COC1=C(C=CC2=C1OC(=O)C3=C2OC4=CC5=C(C=C43)OCO5)O</chem>
Sophoricoside	<chem>C1=CC(=CC=C1C2=COC3=CC(=CC(=C3C2=O)O)O)OC4C(C(C(C(O4)CO)O)O)O</chem>
Sparteine	<chem>C=C1CCC[C@@H]2[C@H]3C[C@H](CN12)[C@@H]1CCCCN1C3</chem>
Spathulenol	<chem>C=C1CC[C@@H]2[C@H]([C@H]3[C@H]1CC[C@]3(C)O)C2(C)C</chem>
Stachenol	<chem>CC1(C)C2CC[C@]34C=C[C@@](C)(CC[C@H]4[C@]2(C)CC[C@@H]1O)C3</chem>
Stachenone	<chem>CC1(C)C2CC[C@]34C=C[C@@](C)(CC[C@H]4[C@]2(C)CCC1=O)C3</chem>
Stachydrine	<chem>C[N+]1(C)CCC[C@@H]1C(=O)O</chem>

Stearic acid	<chem>Cn1c(cnc(c1=O)NC(=N)N)CO</chem>
Sterol	<chem>C1CC2CCC3C4CCC(CC4CCC3C2C1)O</chem>
Stigmast-4-en-3-one	<chem>CCC(CCC(C)C1CCC2C1(CCC3C2CCC4=CC(=O)CCC34C)C)C(C)C</chem>
Stigmasterol	<chem>CCC(C=CC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C</chem>
Stizolamine	<chem>CN1C(=CN=C(C1=O)N=C(N)N)CO</chem>
Stoloniferin III	<chem>CCCCCCCCC(=O)O[C@@H]1[C@@H]([C@H]([C@H](C)O[C@H]1O[C@H]1[C@H](C)O[C@@H]2[C@@H]([C@@H]1O C(=O)CCCCCCCC[C@H](CCCC)O[C@H]1[C@@H]([C@H]([C@H]([C@@H](C)O1)O)O)O2)O)O[C@H]1[C@@H]([C@ @H]([C@H]([C@H](C)O1)OC(=O)[C@@H](C)CC)O)O)O[C@H]1[C@@H]([C@@H]([C@H]([C@H](C)O1)O)O)O</chem>
Stricosamine	<chem>C=CC1C2CC3C4=C(CCN3C(=O)C2=COC1OC5C(C(C(C(O5)CO)O)O)O)C6=CC=CC=C6N4</chem>
Strictosidine	<chem>COC(=O)C1=COC(C(C1CC2C3=C(CCN2)C4=CC=CC=C4N3)C=C)OC5C(C(C(C(O5)CO)O)O)O</chem>
Strogoside	<chem>CC1C(C(C(C(O1)OC2CC(C34C5C(CCC3(C2)O)C6(CCC(C6(CC5OC4=O)C)C7=CC(=O)OC7)O)O)O)O)O</chem>
Strophanthidin	<chem>C[C@@]12CCC3C(CC[C@@]4(C[C@H](CC[C@]34CO)O)O)[C@]2(CC[C@@H]1C1=CC(=O)OC1)O</chem>
Strychnine	<chem>c1ccc2c(c1)[C@]13CCN4CC5=CCO[C@H]6CC(=O)N2[C@H]3[C@H]6[C@H]5C[C@@H]14</chem>
Succinic acid	<chem>C(CC(=O)O)C(=O)O</chem>
Sucrose	<chem>C(C1[C@H](C([C@H]([C@H](O1)O[C@]1(CO)C([C@H]([C@@H](CO)O1)O)O)O)O)O)O</chem>
Sutherlandioside B	<chem>C[C@H](CCC(C(C)C)OCC(C(C(C(=O)O)O)O)O)[C@H]1CC[C@@]2(C)C3C(CC4C(C)C)[C@@H](CC(=O)[C@]54C[C@@]35CC[C@]12C)O)O</chem>
Sweroside	<chem>C=CC1C2CCOC(=O)C2=COC1OC3C(C(C(C(O3)CO)O)O)O</chem>
Swertiamarine	<chem>C=C[C@H]1[C@@H](OC=C2C(=O)OCC[C@@]12O)O[C@H]1[C@@H]([C@H]([C@@H]([C@@H](CO)O1)O)O)O</chem>
Symphytine	<chem>C/C=C(\C)/C(=O)O[C@@H]1CCN2CC=C([C@H]12)OC(=O)[C@@](C(C)C)([C@H](C)O)O</chem>
Synaptoleptis factor K1	<chem>CCCCCCCCCCCCC/C=C/C12O[C@@H]3C4[C@H]5[C@@](CO)([C@H]([C@]6([C@@H](C=C(C)C6=O)[C@]4([C@H](C)C[C@]3(C=C)C)O1)O2)O)O)O5</chem>
Synaptoleptis factor K7	<chem>C=C(C)[C@]12C[C@@H](C)[C@@]34[C@@H]5[C@H]1OC(/C=C/CCCCCCCCCCCCC1[C@H](C)C(=O)[C@@]([C@@H]([C@]6(CO)[C@H]5O6)O)([C@]31C)O)(O2)O4</chem>
Syringic acid	<chem>COC1=CC(=CC(=C1O)OC)C(=O)O</chem>
Tabersonine	<chem>CC[C@]12C=CCN3CC[C@@]4(c5cccc5NC4=C(C1)C(=O)OC)[C@H]23</chem>
Taraxerol	<chem>CC1(CCC2(CC=C3C4(CCC5C(C(CCC5(C4CCC3(C2C1)C)C)O)(C)C)C)C)C</chem>
Tartaric acid	<chem>C(C(C(=O)O)O)(C(=O)O)O</chem>
Tatridin A	<chem>C/C1=C/[C@H]([C@@H]2C(=C)C(=O)O[C@H]2/C=C(/C)\[C@H](CC1)O)O</chem>
Taxine A	<chem>CC1=C2[C@H](C(=O)[C@@]3(C)C/C(=C\[C@@H](C(C[C@@H]1OC(=O)C)C2(C)C)OC(=O)C)/[C@H](C[C@@H]3O)OC(=O)[C@@H]([C@H](C1CCCC1)N(C)C)O)O</chem>
Tephrosin	<chem>CC1(C)C=Cc2c(ccc3c2O[C@@H]2COc4cc(c(cc4[C@@]2(C3=O)O)OC)OC)O1</chem>
Terminoic acid	<chem>O=C(O)[C@]4(C)CC[C@]5(C)CC[C@]3(C)C(=CCC2[C@@]3(C)CCC1[C@]2(C)C[C@@H](O)[C@H](O)C1(C)C)C5[C@@H]4O</chem>

Terpinen-4-ol	<chem>CC(C)C1(CC=C(C)CC1)O</chem>
Terpineol	<chem>CC1=CCC(CC1)C(C)(C)O</chem>
Terpinolene	<chem>CC(=C1CC=C(C)CC1)C</chem>
Tetracoson-1-ol	<chem>CCCCCCCCCCCCCCCCCCCCCCCCCO</chem>
Tetrahydroalstonine	<chem>CC1C2CN3CCC4=C(C3CC2C(=CO1)C(=O)OC)NC5=CC=CC=C45</chem>
Tetrahydrocannabinol	<chem>CCCCC1c1cc(c2C3C=C(C)CC[C@H]3C(C)(C)Oc2c1)O</chem>
Tetrahydroxyflavanone	<chem>c1cc2C(=O)C[C@@H](c3cc(c(cc3O)O)O)Oc2cc1O</chem>
Tetraphylline	<chem>C1=C[C@@](C[C@@H]1O)(C#N)OC1C(C(C(C(CO)O1)O)O)O</chem>
Teutrifidin	<chem>C[C@@H]1[C@H](C(=O)[C@]2(COC(=O)C)[C@H](CCC(=O)[C@@]32CO3)[C@]21C[C@@H](c1ccoc1)OC2=O)O</chem>
Thesinine	<chem>C1C[C@@H]2[C@@H](CCN2C1)COC(=O)/C=C/c1ccc(cc1)O</chem>
Thesiuside	<chem>CC(=O)O[C@@]12CCC3C(CC[C@]4(C)[C@H](CC[C@]34O)c3ccc(=O)oc3)[C@]2(CC[C@@H](C1)OC1C(C(C(C(CO)O1)O)O)CO</chem>
Thevetin A	<chem>C[C@H]1[C@@H]([C@H]([C@@H]([C@@H](O1)O[C@H]1CC[C@@]2(C=O)[C@H](CC[C@@H]3[C@@H]2CC[C@]2(C)[C@H](CC[C@]32O)C2=CC(=O)OC2)C1)O)OC)O[C@H]1[C@@H]([C@H]([C@@H]([C@@H](CO[C@H]2[C@@H]([C@H]([C@@H]([C@@H](CO)O2)O)O)O)O1)O)O)O</chem>
Thevetin B	<chem>CC1C(C(C(C(O1)O[C@H]1CC[C@@]2(C)[C@H](CCC3C2CC[C@]2(C)[C@H](CC[C@]32O)C2=CC(=O)OC2)C1)O)OC)O</chem>
Thiamine	<chem>C1C(C(C(C(COC2C(C(C(C(CO)O2)O)O)O)O1)O)O)O)O</chem>
Thrichilin A	<chem>CC1=C(SC=[N+]1CC2=CN=C(N=C2N)C)CCO</chem>
Toddaculin	<chem>CCC(C)C(=O)OC1C2(C)C3C[C@H]([C@]4(C)C(C(=O)[C@H]([C@@]5(C)[C@@H](C[C@@H]6[C@]45O6)c4ccoc4)O)[C@@]3(CO1)[C@H]([C@H]([C@H]2OC(=O)C)OC(=O)C)O)O</chem>
Toddalenol	<chem>CC(=CCc1c(cc2c(ccc(=O)o2)c1OC)OC)C</chem>
Toddalenone	<chem>CC(C)(O)/C=C/c1c(cc2OC(=O)C=Cc2c1OC)OC</chem>
Toddalolactone	<chem>CC(=O)/C=C/c1c(cc(c2ccc(=O)oc12)OC)OC</chem>
Toddalolactone	<chem>CC(C)(C(Cc1c(cc2c(ccc(=O)o2)c1OC)OC)O)O</chem>
Toddalosin	<chem>CC1=C[C@H](c2c(cc(c3ccc(=O)oc23)OC)OC)[C@@H]([C@H](c2c(cc(c3ccc(=O)oc23)OC)OC)O)C(C)(C)C1</chem>
Toddasin	<chem>CC1(CCC=CC1c1c(cc(c2ccc(=O)oc12)OC)OC)/C=C/c1c(cc(c2ccc(=O)oc12)OC)OC</chem>
Tortuosamine	<chem>CNCC[C@@]1(CCc2c(cccn2)C1)c1ccc(c(c1)OC)OC</chem>
Trachelogenin	<chem>COC1=C(C=C(C=C1)CC2COC(=O)C2(CC3=CC(=C(C=C3)O)OC)O)OC</chem>
Trans-Pinocarveol	<chem>C=C1C2CC(CC1O)C2(C)C</chem>
Trans-p-Mentha-1-7-8-dien-2-ol	<chem>C=C(C)[C@@H]1CCC(=C)[C@H](C1)O</chem>
TR-B	<chem>CCC(C)C(O)C(=O)OC2C(OC=O)C(C(=O)C3(O)C(=O)CC(c1ccoc1)C23C)C4(C)C(CC(=O)OC5(C)COC(=O)CC45)OC(C)=O</chem>
Trehalose	<chem>C([C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)O[C@@H]1[C@@H]([C@H]([C@@H]([C@@H]([C@@H](CO)O1)O)O)O)O)O)O)O)O</chem>
Triacontane	<chem>CCCCCCCCCCCCCCCCCCCCCCCCCCCCCC</chem>

Trimethylamine	CN(C)C
Tutin	C=C(C)[C@H]1[C@@H]2C(=O)O[C@H]1[C@H]([C@@]1(C)[C@@]3(CO3)[C@H]3[C@@H]([C@@]21O)O3)O
Tyledoside C	C[C@@H]1CC([C@]2([C@@H](O1)O)[C@@H]1CC3C[C@H]4[C@@]5(C([C@@H](C(=O)[C@]6(C)[C@H](CC[C@]56O)c5ccc(=O)oc5)O)[C@@]3(C)C[C@H]1O2)O4)O)OC(=O)C
Typhaphtalide	c1ccc(cc1)CC1c2cccc(c2C(=O)O1)O
Typharin	c1ccc(cc1)/C=C/C1Cc2cccc(c2C(=O)O1)O
Typhasterol	CC[C@H](C)[C@H]([C@@H]([C@@H](C)[C@H]1CCC2[C@]1(C)CCC1[C@@]3(C)CC[C@H](C[C@@H]3C(=O)C[C@@]21C)O)O)O
Tyramine	c1cc(ccc1CCN)O
Ulopterol	CC(C)([C@@H](Cc1cc2ccc(=O)oc2cc1OC)O)O
Umckalin	COc1c2ccc(=O)oc2cc(c1OC)O
Umtatin	C=C(C)C1Cc2c(cc3c(c(=O)cc(CO)o3)c2O)O1
Umuravumbolide	CCCCC(/C=C\C1CC=CC(=O)O1)OC(=O)C
Undulatine	COC1CC2C3(CCN2CC4=C(C5=C(C=C43)OCO5)OC)C6C1O6
Uric acid	c12c([nH]c(=O)[nH]2)[nH]c(=O)[nH]c1=O
Ursolic acid	C[C@@H]1CC[C@@]2(CC[C@]3(C)C(=CCC4[C@@]5(C)CC[C@@H](C(C)(C)C5CC[C@@]34C)O)C2[C@H]1C)C(=O)O
Urushiol component	CCCCC/C=C\CCCCCCc1cccc(c1O)O
Urushiol III	CCC/C=C/C/C=C/C(CCCCCCc1cccc(c1O)O)
Uzarigenin	C[C@]12CC[C@@H](C[C@@H]1CC[C@@H]1[C@@H]2CC[C@]2(C)[C@H](CC[C@]12O)C1=CC(=O)OC1)O
Uzarin	C[C@]12CCC(C[C@@H]1CCC1C2CC[C@]2(C)[C@H](CC[C@]12O)C1=CC(=O)OC1)OCC(C(C(C(COCC(C(C(C(=O)O)O)O)O)O)O)O)O)O
Valeranone	CC(C)[C@@H]1CC[C@]2(C)CCCC(=O)[C@]2(C)C1
Valerenic acid	C[C@@H]1CC[C@@H](/C=C\C)/C(=O)O)C2=C(C)CC[C@H]12
Valtrate	CC(C)CC(=O)O[C@H]1C=C2C(=CO[C@H]([C@@H]2[C@]21CO2)OC(=O)CC(C)C)COC(=O)C
Vanillic acid	COC1=C(C=CC(=C1)C(=O)O)O
Vellosimine	CC=C1CN2C3CC1C(C2CC4=C3NC5=CC=CC=C45)C=O
Venusol	c1cc(ccc1/C=C\1/C(=O)OC2C(C(C(CO)OC2O1)O)O)O
vermeeric acid	C(=C(\CC(=O)O)/C(=O)O)\C(=O)O
Vermeerin	C[C@@H]1C[C@H]2[C@H](C[C@]3(C)COC(=O)C[C@@H]13)C(=C)C(=O)O2
verminoside	C1=COC(C2C1C(C3C2(O3)CO)OC(=O)C=CC4=CC(=C(C=C4)O)O)OC5C(C(C(C(O5)CO)O)O)O
Vernodalin	C=CC12CC(C3C(C1C(=C)C(=O)OC2)OC(=O)C3=C)OC(=O)C(=C)CO
Vernodalol	COC(=O)C(=C)C1C(CC2(COC(=O)C(=C)C2C1O)C=C)OC(=O)C(=C)CO
Vernolepin	C=CC12CC(C3C(C1C(=C)C(=O)OC2)OC(=O)C3=C)O

Vernolide	<chem>CC(=C)C(=O)OC1CC23C(O2)CCC(=CC4C1C(=C)C(=O)O4)COC3O</chem>
Vernomydin	<chem>CC(C)C(=O)O[C@H]2C[C@]14O[C@@H]4CCC(COC1O)=C[C@H]3OC(=O)C(=C)[C@H]23</chem>
Vernonioside A1	<chem>CC(C)[C@]1(O[C@H]1C)[C@H]2OC(=O)C([C@@H]2)C3C(O)C[C@H]4C5=CC[C@H]6CC(CC[C@]6(C)C5=CC[C@]34C)O[C@@H]7O[C@H](CO)[C@@H](O)[C@H](O)[C@H]7O</chem>
Vernonioside A3	<chem>CC(C)[C@]1(O[C@H]1C)[C@H]2OC(=O)C([C@@H]2)C3C(=O)C[C@H]4C5=CC[C@H]6CC(CC[C@]6(C)C5=CC[C@]34C)O[C@@H]7O[C@H](CO)[C@@H](O)[C@H](O)[C@H]7O</chem>
Vernonioside B1	<chem>CC(C)[C@]1(O[C@H]1C)[C@H]2OC(=O)C([C@@H]2O)C3CC[C@H]4C5=CC[C@H]6CC(CC[C@]6(C)C5=CC[C@]34C)O[C@@H]7O[C@H](CO)[C@@H](O)[C@H](O)[C@H]7O</chem>
Vernonioside B2	<chem>OC7C(O)C(O)C(CO)O[C@H]7OC1CC[C@]2(C)C3=CC[C@]4(C)C([C@H](O)C[C@H]4C3=CC[C@H]2C1)[C@@H]6[C@H](O)O[C@H]5[C@@H]6O[C@](C)(OC)[C@]5(O)C(C)C</chem>
Vernonioside B3	<chem>CC(C)[C@]1(O[C@H]1C)[C@H]2OC(=O)[C@H]([C@@H]2)[C@H]3C(OC(C)=O)C[C@H]4C5=CC[C@H]6CC(CC[C@]6(C)C5=CC[C@]34C)O[C@@H]7O[C@H](CO)[C@@H](O)[C@H](O)[C@H]7O</chem>
Vinblastine	<chem>CC[C@@]1(C[C@@H]2C[C@](c3cc4c(cc3OC)N(C)[C@@H]3[C@@]54CCN4CC=C[C@](CC)([C@@H]54)[C@H]([C@]3(C(=O)OC)O)OC(=O)C)(c3c(CCN(C2)C1)c1cccc1[nH]3)C(=O)OC)O</chem>
Vinburnine	<chem>CCC12CCCN3C1C4=C(CC3)C5=CC=CC=C5N4C(=O)C2</chem>
Vincamine	<chem>CC[C@]12CCCN3CCc4c5cccc5n(c4[C@H]23)[C@](C1)(C(=O)OC)O</chem>
Vincristine	<chem>CC[C@@]1(C[C@@H]2C[C@](c3cc4c(cc3OC)N(CO)[C@@H]3[C@@]54CCN4CC=C[C@](CC)(C54)[C@H]([C@]3(C(=O)OC)O)OC(=O)C)(c3c(CCN(C2)C1)c1cccc1[nH]3)C(=O)OC)O</chem>
Vindoline	<chem>CCC12C=CCN3C1C4(CC3)C(C(C2OC(=O)C)(C(=O)OC)O)N(C5=C4C=CC(=C5)OC)C</chem>
Viscolin	<chem>COc1cc(c(c(c1CCc1ccc(c(c1)OC)O)OC)OC)O</chem>
Viscumside A	<chem>COc1cc(ccc1O)[C@@H]1CC(=O)c2c(cc(cc2O1)OCC(C(C(C(=O)O)O)O)O)O</chem>
Vitexin	<chem>C1=CC(=CC=C1C2=CC(=O)C3=C(O2)C(=C(C=C3O)O)C4C(C(C(C(O4)CO)O)O)O)O</chem>
Voacamidine	<chem>CCC1CC2CC3(C1N(C2)CCC4=C3NC5=C4C(=C(C=C5)OC)C6CC7C(C(CC8=C6NC9=CC=CC=C89)N(CC7=CC)C)C(=O)OC)C(=O)OC</chem>
Voacamine	<chem>CCC1CC2CC3(C1N(C2)CCC4=C3NC5=CC(=C(C=C45)OC)C6CC7C(C(CC8=C6NC9=CC=CC=C89)N(CC7=CC)C)C(=O)OC)C(=O)OC</chem>
Voacangine	<chem>CCC1CC2CC3(C1N(C2)CCC4=C3NC5=C4C(=C(C=C5)OC)C(=O)OC</chem>
Voacorine	<chem>CC=C1CN(C2CC3=C(C(CC1C2C(=O)OC)C4=C(C=C5C6=C(C7(CC8CC(C7N(C8)CC6)C(C)O)C(=O)OC)NC5=C4)OC)N(C9=CC=CC=C39)C</chem>
Voacristine	<chem>C[C@@H]([C@H]1C[C@@H]2C[C@]3(c4c(CCN(C2)[C@@H]13)c1cc(ccc1[nH]4)OC)C(=O)OC)O</chem>
Voaphylline	<chem>CC[C@]12CCc3c(CCN(C[C@@H]4[C@H]2O4)C1)c1cccc1[nH]3</chem>
Vobtusine	<chem>COC1=CC=CC2=C1N3CC4(CC5C3(C26CCN7C6C8(C5)CCOC8CC7)O)CN9CCC12C9C3(C4OCC3)CC(=C1NC1=CC=CC=C21)C(=O)OC</chem>
Vomifoliol	<chem>OC1(CCC(C)O)C(C)=CC(=O)CC1(C)C</chem>
Warburganal	<chem>CC1(C)CCC[C@@]2(C)C1CC=C(CO)[C@@]2(CO)O</chem>

Warfarin	<chem>CC(=O)CC(C1CCCCC1)c1c(c2ccccc2oc1=O)O</chem>
Wighteone	<chem>CC(=CCc1c(cc2c(c1O)c(=O)c(co2)c1ccc(cc1)O)O)C</chem>
Withaferin A	<chem>CC1=C(CO)C(=O)OC[C@H]1[C@@H](C)C1CCC2C3C[C@@H]4[C@@]5([C@H](C=CC(=O)[C@]5(C)C3CC[C@]12C)O)O4</chem>
Withasomnine	<chem>c1ccc(cc1)c1cc2CCcn2n1</chem>
Xanthine	<chem>c1[nH]c2c(n1)[nH]c(=O)[nH]c2=O</chem>
Xanthinin	<chem>CC1CC2C(CC=C1C(CC(=O)C)OC(=O)C)C(=C)C(=O)O2</chem>
Xanthotoxin	<chem>COc1c2c(cco2)cc2ccc(=O)oc12</chem>
Xylopic acid	<chem>CC(=O)OC1C(=C)C2CCC3C1(C2)CCC4C3(CCCC4(C)C(=O)O)C</chem>
Xysmalorin	<chem>C[C@]12CCCC(C1=CCC1C2CC[C@]2(C)[C@H](CC[C@]12O)C1=CC(=O)OC1)OCC(C(C(C(COCC(C(C(C(C=O)O)O)O)O)O)O)O)O</chem>
Yamogenin	<chem>CC1CCC2(C(C3C(O2)CC4C3(CCC5C4CC=C6C5(CCC(C6)O)C)C)C)OC1</chem>
Yohimbine	<chem>COC(=O)C1C(CCC2C1CC3C4=C(CCN3C2)C5=CC=CC=C5N4)O</chem>
Yomogi alcohol	<chem>CC(C)(C=C)C=CC(C)(C)O</chem>
$\alpha$ -Amyrin	<chem>CC1CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)O)C)C)C2C1)C)C</chem>
$\alpha$ -Amyrin acetate	<chem>CC1CCC2(C)CCC3(C)C(=CCC4C5(C)CCC(C(C)(C)C5CCC34C)OC(=O)C)C2C1C</chem>
$\alpha$ -cadinol	<chem>CC1=CC2C(CCC(C2CC1)(C)O)C(C)C</chem>
$\alpha$ -caryophyllene	<chem>C/C1=C\CC/C(=C/CC(C)(C)/C=C/C1)/C</chem>
$\alpha$ -Fenchol	<chem>CC1(C)[C@@H]2CC[C@@](C)(C2)C1O</chem>
$\alpha$ -Humulene	<chem>C/C1=C/CC/C(=C\CC(C)(C)/C=C\C1)/C</chem>
$\alpha$ -Linolenic acid	<chem>CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)O</chem>
$\alpha$ -phellandrene	<chem>CC(C)C1C=CC(=CC1)C</chem>
$\alpha$ -pinene	<chem>CC1=CCC2CC1C2(C)C</chem>
$\alpha$ -spinasterol	<chem>CCC(C=CC(C)C1CCC2C1(CCC3C2=CCC4C3(CCC(C4)O)C)C)C(C)C</chem>
$\alpha$ -Terpinene	<chem>CC1=CCC(=CC1)C(C)C</chem>
$\alpha$ -Terpineol	<chem>CC1C=CC(CC1)C(C)(C)O</chem>
$\alpha$ -Thujone	<chem>CC(C)[C@]12CC2[C@@H](C)C(=O)C1</chem>
$\alpha$ -Zingiberene	<chem>CC(=CCC[C@H](C)[C@@H]1C=CC(=CC1)C)C</chem>
$\beta$ -Amyrin	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)O)C)C)C2C1)C)C)C</chem>
$\beta$ -Amyrin acetate	<chem>CC(=O)OC1CCC2(C)C(CCC3(C)C2CC=C2C4CC(C)(C)CCC4(C)CCC32C)C1(C)C</chem>
$\beta$ -Asarone	<chem>CC=CC1=CC(=C(C=C1OC)OC)OC</chem>
$\beta$ -Caryophyllene	<chem>C/C1=C\CCC(=C)[C@H]2CC(C)(C)[C@@H]2CC1</chem>
$\beta$ -Damascenone	<chem>C/C=C/C(=O)C1=C(C)C=CCC1(C)C</chem>

$\beta$ -Glochidone	<chem>C=C(C)[C@@H]1CC[C@]2(C)CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)C=CC(=O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12</chem>
$\beta$ -Methylglucoside	<chem>CO[C@H]1[C@@H](C([C@H](C(CO)O1)O)O)O</chem>
$\beta$ -Ocimene	<chem>C=C/C(=C\C=C(C)C)/C</chem>
$\beta$ -Phyllandrene	<chem>CC(C)C1C=CC(=C)CC1</chem>
$\beta$ -Pinene	<chem>C=C1CCC2CC1C2(C)C</chem>
$\beta$ -Sitosterol	<chem>CCC(CCC(C)C1CCC2C3CC=C4C[C@H](CC[C@]4(C)C3CC[C@]12C)O)C(C)C</chem>
$\beta$ -Terpinene	<chem>CC(C)C1=CCC(=C)CC1</chem>
$\beta$ -Thujone	<chem>CC(C)[C@]12CC2[C@H](C)C(=O)C1</chem>
$\beta$ -Yohimbine	<chem>COC(=O)[C@H]1[C@@H](CC[C@@H]2[C@@H]1C[C@H]3c4c(c5cccc5[nH]4)CCN3C2)O</chem>
$\gamma$ -Diosphenol	<chem>CC(C)C1=C(C(=C)C(C)CC1)O</chem>
$\gamma$ -Terpinene	<chem>CC1=CCC(=CC1)C(C)C</chem>
$\delta$ -7-Avenasterol	<chem>CC=C(CCC(C)C1CCC2C1(CCC3C2=CCC4C3(CCC(C4)O)C)C)C(C)C</chem>
$\delta$ -Camphor	<chem>CC1(C2CCC1(C(=O)C2)C)C</chem>
$\epsilon$ -phytol	<chem>CC(C)CCC[C@@H](C)CCC[C@@H](C)CCCC(\C)=C\CO</chem>

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**Table S2.** Assigned numerical identity of the predicted active compounds, their plant sources and predicted targets.

Number	Compound	Plant	Predicted targets (docking score in kcal/mol)
1	1,2-Epoxyascillirosidin	<i>Homeria Pallida</i>	PPARD (-9.5)
2	1,5-Dicaffeoylquinic acid	<i>Vernonia amygdalina</i>	DPP4 (-9.2); GCK (-9.1); PPARD (-9.3); PPARG (-9.1)
3	10-Hydroxyakagerine	<i>Strychnos spinosa</i>	PPARD (-9.1)
4	12-B-hydroxyascillirosidin	<i>Drimia robusta</i>	DPP4 (-9.0); HSD11B1 (-9.3)
5	12-Hydroxydaphnetoxin	<i>Gnidia kraussiana</i>	PPARD (-10.8)
6	15-Oxo-kaurenoic acid	<i>Xylopiya aethiopia</i>	HSD11B1 (-9.5); PPARD (-9.9); PPARG (-9.4)
7	16-B-Formyloxybovogenin A	<i>Moraea polystachya</i>	DPP4 (-9.1); HSD11B1 (-9.3); PPARD (-9.1); PPARG (-9.8)
8	1-Hydroxydimethylanthraquinone	<i>Danais fragrans</i>	AKR1B1 (-9.00); PPARD (-9.0); RBP4 (-10.1)
9	2-(1-Hydroxyethyl)naphtho[2,3-b]furan-4,9-dione	<i>Kigelia africana</i>	AKR1B1 (-9.6); FFAR1 (-9.2); RBP4 (-9.6)
10	2a,3b-Dihydroxyurs-12-en-18-oic acid	<i>Prunus africana</i>	AMY2A (-9.5); PYGL (-9.2)
11	Esculentic acid	<i>Prunus africana</i>	AMY2A (-9.0); HSD11B1 (-9.1)
12	3-Epicorosolic acid	<i>Prunus africana</i>	AMY2A (-9.6); PYGL (-9.3)
13	2-Hydroxygenistein	<i>Cajanus cajan</i>	AKR1B1 (-9.1)
14	3,3,4,5,5-Pentahydroxystilbene	<i>Schotia Brachypetala</i>	FFAR1 (-9.4)
15	3,8,11-Heptadecadienyl catechol	<i>Smodingium argutum</i>	AKR1B1 (-9.2); RBP4 (-9.0)
16	3-Acetylnerbowdine	<i>Boophane disticha</i>	RBP4 (-9.0)
17	3-Epioleanolic acid	<i>Melianthus Comosus, Prunus africana</i>	DPP4 (-10.4); HSD11B1 (-10.2)
18	3-Oxo-20,24-dammaradien-26-ol	<i>Rapanea melanophloeos</i>	AMY2A (-9.1); HSD11B1 (-9.9); PPARD (-9.9); PPARG (-9.1)
19	3,9-Dihydroeucomnalin	<i>Eucommis autumnalis</i>	AKR1B1 (-9.1)
20	19-Deoxyuscharin	<i>Asclepias fruticosa</i>	DPP4 (-9.5); GCK (-9.7); PPARG (-10.4); PDK2 (-9.8)
21	4-Deoxy-13-O-phenylacetyl-12-O-tigloylphorbol	<i>Synadenium grantii</i>	PPARD (-10.2)
22	Umtatin	<i>Ptaeroxylon obliquum</i>	RBP4 (-9.1)
23	5-Chloropropacin	<i>Mondia whitei</i>	HSD11B1 (-9.9); PPARD (-10.0); PPARG (-9.2)
24	6-Methyldiosgenin	<i>Balanites aegyptiacus</i>	AMY2A (-9.1); PPARD (-9.5); PPARG (-10.4)
25	7-Hydroxy-4-6-dimethoxypropacin	<i>Mondia whitei</i>	HSD11B1 (-9.5); PPARG (-9.1)

26	8,(14),15-Isopimaradiene-7,18-diol	<i>Tetradenia Riparia</i>	HSD11B1 (-9.0); PPARD (-9.2)
27	8-Hydroxypinoresinol	<i>Olea europaea, Strophanthus gratus</i>	AKR1B1 (-9.1); GCK (-9.1); HSD11B1 (-9.0); PPARG (-9.0)
28	Alpha-Humulene	<i>Aframomum melegueta, Helichrysum Species</i>	RBP4 (-9.1)
29	Alpha-linolenic acid	<i>Adansonia digitata, Cajanus cajan</i>	AKR1B1 (-9.3); FFAR1 (-9.4); RBP4 (-10.0); RXRA (-9.4)
30	Acetylcaranine	<i>Amaryllis belladonna, Crinum bulbispermum</i>	AKR1B1 (-9.5); RBP4 (-10.7)
31	Acolongifloroside K	<i>Acokanthera oppositifolia, Strophanthus gratus</i>	AMY2A (-9.3)
32	Acovenoside A	<i>Acokanthera oppositifolia</i>	AMY2A (-9.6); DPP4 (-9.8); HSD11B1 (-9.5)
33	Adiantone	<i>Adiantum species</i>	GCK (-10.6); NR5A2 (-9.4); PPARD (-10.0); PPARG (-9.1)
34	Afrormosin	<i>Cyclopia spp</i>	AKR1B1 (-9.6)
35	Afroside	<i>Asclepias fruticosa</i>	DPP4 (-10.2); PPARD (-9.3); PTPN9 (-9.6); PYGL (-9.1)
36	Agapanthagenin	<i>Agapanthus Africanus</i>	AMY2A (-9.1); HSD11B1 (-9.3); PPARD (-9.0)
37	Ajmalicine	<i>Catharanthus roseus, Rauwolfia caffra</i>	GCK (-9.0); HSD11B1 (-9.6); PPARD (10.1)
38	Ajmaline	<i>Rauwolfia caffra, Rauwolfia vomitoria</i>	HSD11B1 (-9.4); PPARD (-9.8)
39	Akuammine	<i>Catharanthus roseus</i>	PPARD (-9.0)
40	Allouzarin	<i>Xysmalobium undulatum</i>	AMY2A (-9.2); DDP4 (-9.4); PDK2 (-9.3); PPARD (-9.2)
41	Alloxysmalorin	<i>Xysmalobium undulatum</i>	AMY2A (-9.5); DPP4 (-9.6); PYGL (-9.1)
42	Aloe-emodin anthrone	<i>Aloe ferox</i>	HSD11B1 (-9.1); RBP4 (-9.4)
43	Aloeresin A	<i>Aloe ferox</i>	AKR1B1 (-9.3); GCK (-9.8); HSD11B1 (-9.4); PPARD (-10.6); PPARG (-9.1)
44	Aloinoside A	<i>Aloe ferox</i>	AMY2A (-9.2); DPP4 (-9.4); HSD11B1 (-10.4)
45	Aloinoside B	<i>Aloe ferox</i>	AMY2A (-9.2); DPP4 (-9.4); HSD11B1 (-10.5)
46	Alpha-amyrin	<i>Artemisia afra, Euphorbia hirta, Impomoea pes-caprae ssp. Brasiliensis</i>	AMY2A (-9.5); HSD11B1 (-9.6); PTPn9 (-9.0)
47	Alpha-amyrin acetate	<i>Impomoea pes-caprae ssp. Brasiliensis</i>	HSD11B1 (-10.8)
48	Alpha-spinasterol	<i>Ravanela madagascariensis</i>	AKR1B1 (-9.0); HSD11B1 (-10.5); PPARD (-10.3)

49	Amentoflavone	<i>Xerophyta retinervis</i>	AMY2A (-10.4); DPP4 (-10.4); GCK (-10.0); HSD11B1 (-10.5); INSR (-10.0); MGAM (-9.8); NR5A2 (-9.0); PDK2 (-9.3); PPARA (-10.5); PPARD (-11.0); PPARG (-10.8); PYGL (-10.0)
50	Amritoside	<i>Psidium guajava</i>	AMY2A (-9.1); DPP4 (-10.4); HSD11B1 (-10.4); PPARD (-10.4); PPARG (-9.9)
51	Amygdalin	<i>Brabejum Stellatifolium, Prunus africana, Prunus Laurocerasus</i>	HSD11B1 (-9.3)
52	Angustine	<i>Nauclea latifolia</i>	AKR1B1 (-10.5); AMY2A (-9.1); DPP4 (-10.5); GCK (-9.4); HSD11B1 (-9.9); PPARD (-9.7); PPARG (-9.6)
53	Angustoline	<i>Nauclea latifolia</i>	AKR1B1 (-10.6); GCK (-10.5); HSD11B1 (-10.1); PPARD (-9.8); PPARG (-10.0)
54	Anolignan B	<i>Terminalia sericea</i>	AKR1B1 (-10.3); FFAR1 (-10.5); RBP4 (-9.1); RXR1 (-9.5)
55	Apigenin	<i>Cajanus cajan</i>	AKR1B1 (-9.1); HSD11B1 (-9.0); RBP4 (-9.9); RXRA (-9.1)
56	Apigenin dimethylether	<i>Rhus undulata</i>	HSD11B1 (-9.0); RBP4 (-10.0)
57	Arjunglucoside	<i>Terminalia sericea</i>	AMY2A (-9.3); DPP4 (-9.4)
58	Arjunolic acid	<i>Syzygium Cordatum</i>	AMY2A (-9.2)
59	Arnottianamide	<i>Toddalia asiatica</i>	HSD11B1 (-9.1)
60	Arvenin I	<i>Anagallis arvensis</i>	DPP4 (-9.0)
61	Arvenin II	<i>Anagallis arvensis</i>	DPP4 (-9.1)
62	Asiatic acid	<i>Centella asiatica</i>	AMY2A (-9.6); DPP4 (-9.4); HSD11B1 (-9.0)
63	Asiaticoside	<i>Centella asiatica</i>	AMY2A (-9.3); DPP4 (-9.6); PPARG (-9.9)
64	Aspalathin	<i>Aspalathus linearis</i>	AKR1B1 (-9.0); HSD11B1 (-9.2)
65	Autumnariniol	<i>Eucomnis autumnnalis</i>	RBP4 (-9.0)
66	Autumnariol	<i>Eucomis autumnnalis</i>	RBP4 (-9.0)
67	Avenasterol	<i>Adansonia digitata</i>	AKR1B1 (-10.3); HSD11B1 (-9.9); NR5A2 (-9.0); PPARD (-9.1); PPARG (-9.3); RXRA (-9.4)

68	Avicine	<i>Toddalia asiatica</i>	AKR1B1 (-10.6); AMY2A (-9.5); DPP4 (-9.9); GCK (-10.6); HSD11B1 (-10.4); INSR (-9.5); PPARG (-9.3); PPARG (-10.0); RXRA (-9.4)
69	Aviprin	<i>Ficus Salicifolia</i>	RBP4 (-9.4)
70	Beta-sitosterol	<i>Acacia karroo, Adansonia digitata, Centella asiatica, Dodonaea Angustifolia, Euphorbia hirta, Harpagophytum procumbens, Hypoxis hemerocallidea, Kigelia africana, Prunus africana, Ravenala madagascariensis, Syzygium Cordatum</i>	HSD11B1 (-9.1); PPARG (-10.1)
71	Balagyptin	<i>Balanites aegyptiacus</i>	AMY2A (-10.0); DPP4 (-9.9); HSD11B1 (-10.0); PPARG (-11.2)
72	Balanitin 1	<i>Balanites aegyptiacus</i>	AMY2A (-9.4); DPP4 (-10.5)
73	Balanitin 2	<i>Balanites aegyptiacus</i>	AMY2A (-9.3); DPP4 (-10.2); PPARG (-11.4)
74	Balanitin 3	<i>Balanites aegyptiacus</i>	AMY2A (-9.8); DPP4 (-10.0); GCK (-9.1); PPARG (-9.4); PPARG (-10.0); PDK2 (-9.4)
75	Balanitin 4	<i>Balanites aegyptiacus</i>	AMY2A (-9.9); DPP4 (-10.2); INSR (-9.8); PYGL (-9.2)
76	Balanitin 6	<i>Balanites aegyptiacus</i>	AMY2A (-9.0); DPP4 (-10.3)
77	Balanitin 7	<i>Balanites aegyptiacus</i>	DPP4 (-10.2)
78	Balanitoside	<i>Balanites aegyptiacus</i>	AMY2A (-9.0); DPP4 (-9.9); INSR (-9.1)
79	Bauerenol	<i>Adansonia digitata</i>	AMY2A (-9.3); HSD11B1 (-10.1); PPARG (-9.2)
80	Benzo[c]phenanthridine	<i>Toddalia asiatica</i>	AKR1B1 (-10.9); GCK (-9.0); PPARG (-9.2); PPARG (-9.5); RBP4 (-11.0); RXRA (-9.5)
81	Berberine	<i>Argemone Ochroleuca</i>	AKR1B1 (-9.1); HSD11B1 (-9.3); PPARG (-9.0)
82	Beta-amyrin	<i>Artemisia afra, Euphorbia hirta, Impomoea pes-caprae ssp. Brasiliensis</i>	AMY2A (-9.7); HSD11B1 (-9.7); PTPN9 (-9.0)
83	Beta-amyrin acetate	<i>Impomoea pes-caprae ssp. Brasiliensis</i>	AMY2A (-9.8)
84	Beta-glochidone	<i>Impomoea pes-caprae ssp. Brasiliensis</i>	AMY2A (-10.8); DPP4 (-9.6); HSD11B1 (-11.2); PTPN9 (-9.0)
85	Betulinic acid	<i>Adansonia digitata, Cajanus cajan, Harungana madagascariensis</i>	AMY2A (-9.1); PTPN9 (-9.3)
86	Biochanin A	<i>Cajanus cajan</i>	AKR1B1 (-9.2); FFAR1 (-9.2)

87	bisabolene	<i>Xylopiia aethiopica</i>	AKR1B1 (-9.1)
88	biscryptolepine	<i>Cryptolepis sanguinolenta</i>	AMY2A (-10.5); DPP4 (-10.5); FFAR1 (-9.1); GCK (-9.9); INSR (-9.2); PDK2 (-9.7); PPARA (-11.4); PPARD (-9.2); PPARG (-11.5)
89	Bovogenin A	<i>Bowiea volubilis</i>	HSD11B1 (-10.2); PPARD (-9.8); PPARG (-10.1)
90	Bovoside A	<i>Bowiea volubilis</i>	AMY2A (-9.2); PPARD (-9.7); PPARG (-9.0)
91	brassinolide	<i>Catharanthus roseus</i>	AKR1B1 (-9.8); HSD11B1 (-10.2); PPARD (-9.4); PPARG (-9.3)
92	Bulbispermine	<i>Crinum bulbispermum</i>	HSD11B1 (-9.0)
93	Buphanisin	<i>Boophane disticha</i>	AKR1B1 (-9.4); GCK (-9.3)
94	Cajaquinone	<i>Cajanus cajan</i>	RBP4 (-9.4)
95	Calycosin	<i>Cyclopia spp</i>	AKR1B1 (-9.4); FFAR1 (-9.0)
96	Campesterol	<i>Adansonia digitata, Euphorbia Hirta, Prunus africana</i>	AKR1B1 (-9.5); AMY2A (-9.1); DPP4 (-9.4); FFAR1 (-9.2); HSD11B1 (-11.0); MGAM (-9.0); PPARD (-9.7); PPARG (-9.9)
97	Caranine	<i>Amaryllis belladonna</i>	RBP4 (-9.7)
98	Carapanaubine	<i>Rauvolfia vomitoria</i>	PPARD (-9.4)
99	Castalagin	<i>Quercus robur</i>	AMY2A (-9.0); DPP4 (-10.4); PDK2 (-9.0); PYGL (-9.1)
100	Catechin	<i>Adansonia digitata, Combretum micranthum, Pelargonium sidoides, Prunus africana, Sclerocarya birrea, Typha capensis</i>	AKR1B1 (-9.0); HSD11B1 (-9.5); RBP4 (-9.3)
101	Celastrin	<i>Gunnera perpensa</i>	PPARD (-9.9)
102	Centelloside	<i>Centella asiatica</i>	AMY2A (-9.3); DPP4 (-9.9)
103	Chelerythrine	<i>Toddalia asiatica</i>	AKR1B1 (-9.5); DPP4 (-9.0); GCK (-9.1); HSD11B1 (-9.4); PPARG (-9.0)
104	Chironioside	<i>Chironia baccifera</i>	HSD11B1 (-9.6)
105	Chelerythrine-psi-cyanide	<i>Toddalia asiatica</i>	HSD11B1 (-9.2); PPARD (-9.1)
106	Chlorogenic acid	<i>Euphorbia hirta, Moringa oleifera, Scabiosa columbaria, Trichilia emetica, Vernonia amygdalina</i>	AKR1B1 (-9.1)
107	Christyoside	<i>Strophanthus speciosus</i>	PPARD (-10.1)
108	Chrysophonein	<i>Rumex lanceolatus</i>	PPARG (-9.1)

109	Chrysophonol	<i>Bulbine frutescens, Harungana madagascariensis, Rumex lanceolatus</i>	RBP4 (-9.8)
110	Cissacapine	<i>Cissampelos capensis</i>	AMY2A (-11.0); DPP4 (-10.1); NR5A2 (-9.1); PYGL (-9.1)
111	Cissampreine	<i>Cissampelos capensis</i>	AMY2A (-9.6); DPP4 (-9.6)
112	Cliviamartine	<i>Clivia miniata</i>	AKR1B1 (-9.4); AMY2A (-9.1); DPP4 (-10.1); GCK (-10.9); HSD11B1 (-10.1); NR5A2 (-9.3); PPARA (-9.4); PPARD (-11.2); PPARG (-9.8)
113	Cliviasine	<i>Clivia miniata</i>	HSD11B1 (-9.2); PPARG (-9.2)
114	Clividine	<i>Clivia miniata</i>	HSD11B1 (-9.2); PPARG (-9.0)
115	Clivimine	<i>Clivia miniata</i>	AKR1B1 (-11.1); AMY2A (-11.5); DPP4 (-11.7); FFAR1 (-10.0); GCK (-11.5); INSR (-9.6); MGAM (-9.1); NR5A2 (-12.2); PDK2 (-11.5); PPARA (-9.3); PPARD (-13.7); PPARG (-12.9); PYGL (-10.5); RXRA (-10.1)
116	Clivonine	<i>Clivia miniata</i>	GCK (-9.0); HSD11B1 (-9.5); RBP4 (-10.1)
117	Combretin A	<i>Combretum micranthum</i>	GCK (-9.2); HSD11B1 (-9.6); PPARD (-9.5)
118	Combretin B	<i>Combretum micranthum</i>	DPP4 (-9.2)
119	Cornustannin 2	<i>Curtisia dentata</i>	AMY2A (-9.9); DPP4 (-10.8); PDK2 (-9.4)
120	Corosolic acid	<i>Prunus africana</i>	AMY2A (-9.2); DPP4 (-9.9); HSD11B1 (-9.7); PDK2 (-9.1); PTPN9 (-9.0)
121	Cotyledoside	<i>Tylecodon wallichii</i>	AMY2A (-9.4); DPP4 (-9.5); PTPN9 (-9.5)
122	Crinamine	<i>Crinum bulbispermum, Crinum macowanii</i>	GCK (-9.4)
123	Crinasiadine	<i>Crinum bulbispermum</i>	AKR1B1 (-9.5); RBP4 (-9.9)
124	Crinasiatine	<i>Crinum bulbispermum</i>	AKR1B1 (-10.8); AMY2A (-9.0); DPP4 (-9.8); FFAR1 (-9.9); GCK (-10.0); HSD11B1 (-11.0); PPARA (-10.9); PPARD (-10.6); PPARG (-10.9)
125	Crotofolin A	<i>Croton Gratissimus</i>	AMY2A (-9.2); HSD11B1 (-9.9); PPARD (-9.3)
126	Crotonin	<i>Croton Gratissimus</i>	PPARD (-9.4)
127	Cryptogenin	<i>Balanites maughami</i>	AMY2A (-9.0); HSD11B1 (-10.0); PPARD (-9.8); RBP4 (-10.0)

128	Cryptoheptine	<i>Cryptolepis sanguinolenta</i>	GCK (-9.3); HSD11B1 (-9.1); RBP4 (-10.3)
129	Cryptolepine	<i>Cryptolepis sanguinolenta</i>	PPARG (-9.3); RBP4 (-10.1)
130	Cryptomisrine	<i>Cryptolepis sanguinolenta</i>	AKR1B1 (-11.1); AMY2A (-11.3); DPP4 (-11.7); FFAR1 (-9.3); GCK (-13.0); HSD11B1 (-12.8); INSR (10.8); MGAM (-10.0); NR5A2 (-11.5); PDK2 (-10.2); PPARA (-9.5); PPARD (-14.3); PPARG (-11.7); PTPN9 (-10.0); PYGL (-10.5)
131	Cryptoquindoline	<i>Cryptolepis sanguinolenta</i>	AKR1B1 (-9.8); AMY2A (-11.4); DPP4 (-11.2); FFAR1 (-9.3); GCK (-11.1); HSD11B1 (-12.0); INSR (-10.6); MGAM (-10.0); NR5A2 (-10.0); PDK2 (-10.1); PPARA (-11.3); PPARD (-11.2); PPARG (-11.9); PYGL (-9.1); RXRA (-9.5)
132	Cryptospirolepine	<i>Cryptolepis sanguinolenta</i>	AMY2A (-10.8); DPP4 (-11.8); FFAR1 (-9.5); GCK (-12.4); INSR (-10.9); MGAM (-9.7); PDK2 (-9.6); PPARD (-9.2); PTPN9 (-10.2); PYGL (- 10.2)
133	Cucurbitacin B	<i>Cucumis africanus</i>	HSD11B1 (-9.0); PPARD (-9.1); PPARG (-9.8)
134	Curcuson A	<i>Jatropha curcas</i>	AKR1B1 (-9.6); GCK (-9.7); PPARD (-9.7); RBP4 (-10.0); RXRA (-9.1)
135	Curcuson C	<i>Jatropha curcas</i>	AKR1B1 (-9.6); RBP4 (-9.7)
136	Cyanidin	<i>Rhoicissus tridentata</i>	AKR1B1 (-9.1); HSD11B1 (-9.5); RBP4 (-9.2)
137	Cyclamin	<i>Cyclamen Persicum</i>	AMY2A (-9.0); DPP4 (-10.9)
138	Cycloartenol	<i>Ravanela madagascariensis</i>	AMY2A (-9.7); FFAR1 (-9.3); GCK (-9.7); HSD11B1 (-11.1); PPARD (-9.7); PPARG (-9.7)
139	Cynafoside B	<i>Cynanchum africanum</i>	PDK2 (-9.4); PPARG (-9.3)
140	Daucosterol	<i>Prunus africana</i>	DPP4 (-9.5); HSD11B1 (-10.2); PPARD (-9.8); PPARG (-9.9)
141	Deacetyldesformoakuummilin	<i>Rauvolfia vomitoria</i>	HSD11B1 (-9.1); PPARD (-9.0)
142	Deguelin	<i>Mundulea sericea</i>	AKR1B1 (-9.5); AMY2A (-9.0); DPP4 (-9.7); HSD11B1 (-10.5); PPARD (-9.6); PPARG (-10.6)
143	Delphinidin	<i>Hibiscus sabdariffa, Rhoicissus tridentata, Syzygium Cordatum</i>	AKR1B1 (-9.0); HSD11B1 (-9.6); RBP4 (-9.1)

144	Delta-7-avenasterol	<i>Ravanela madagascariensis</i>	HSD11B1 (-10.7); PPARD (-10.4)
145	Deltonin	<i>Dioscorea dregeana</i>	AMY2A (-9.6); DPP4 (-10.5)
146	Deltoside	<i>Dioscorea dregeana</i>	DPP4 (-9.0)
147	Des-N-methylchelerythrine	<i>Toddalia asiatica</i>	AKR1B1 (-9.4); HSD11B1 (-9.4); PPARG (-9.4)
148	Dicoumarol	<i>Melilotus alba</i>	AKR1B1 (-11.5); DPP4 (-9.4); GCK (-10.1); HSD11B1 (-9.5); PPARD (9.6); PPARG (-10.4); RBP4 (-9.1); RXRA (-9.8)
149	Digallic acid	<i>Quercus robur</i>	AKR1B1 (-9.2)
150	Digitoxin	<i>Digitalis purpurea</i>	AMY2A (-10.7); DPP4 (-9.7); GCK (-10.3); PPARD (-9.0); PPARG (-9.8); PTPN9 (-9.8); PYGL (-9.0)
151	Dihydrosanguinarine	<i>Eschscholzia californica</i>	AKR1B1 (-10.6); DPP4 (-9.2); GCK (-9.5); HSD11B1 (-10.3); INSR (-9.2); PPARD (-9.7); PPARG (-9.8)
152	Dioscin	<i>Dioscorea dregeana</i>	AMY2A (-9.9); DPP4 (-10.3)
153	Diosgenin	<i>Balanites aegyptiavus, Balanites maughamii, Dioscorea dregeana</i>	AKR1B1 (-9.5); NR5A2 (-9.0); PPARD (-12.0)
154	Diosmetin	<i>Agathosma betulina</i>	AKR1B1 (-9.1); HSD11B1 (-9.1); RBP4 (-9.5); RXRA (-9.0)
155	Diosmin	<i>Agathosma betulina</i>	GCK (-9.0); HSD11B1 (-9.3); PPARD (-9.2); PPARG (-9.4)
156	Diospyrin	<i>Euclea undulata</i>	AKR1B1 (-9.4); AMY2A (-9.7); DPP4 (-10.4); FFAR1 (-9.0); HSD11B1 (-10.5); MR5A2 (-9.2); PPARD (-10.4); PPARG (-10.4)
157	Durantoside I	<i>Duranta erecta</i>	PPARD (-9.3)
158	Durantoside II	<i>Duranta erecta</i>	DPP4 (-9.4); HSD11B1 (-9.6); MGAM (-9.2); PPARD (-9.1); PPARG (-9.5)
159	Durantoside III	<i>Duranta erecta</i>	PPARD (-9.3); PPARG (-9.2)
160	Eburnamonine	<i>Vinca minor</i>	AKR1B1 (-9.4); HSD11B1 (-9.2); PPARD (-9.3); RBP4 (-9.4)
161	Elaeocyanidin	<i>Cassine transvaalensis</i>	HSD11B1 (-9.3); PPARG (-9.1)
162	Ent-16-Kauren-18-oic-acid	<i>Aster bakeranus</i>	AMY2A (-9.0); HSD11B1 (-9.1)



163	Ent-16-Kauren-19-oic-acid	<i>Aster bakeranus</i>	HSD11B1 (-9.4); PPARD (-9.4)
164	Epicatechin	<i>Acacia karroo, Harungana madagascariensis, Prunus africana</i>	AKR1B1 (-9.2); RBP4 (-9.3)
165	Epifriedelinol	<i>Syzygium cordatum</i>	HSD11B1 (-11.4)
166	Epimaslinic acid	<i>Prunus africana</i>	AMY2A (-9.7); DPP4 (-9.0)
167	Ergine	<i>Ipomoea purpurea</i>	HSD11B1 (-9.2); RBP4 (-9.4)
168	Eriodictyol	<i>Cyclopia spp</i>	HSD11B1 (-9.2); RBP4 (-9.5)
169	Erythraline	<i>Erythrina caffra, Erythrina lysistemon</i>	AKR1B1 (-9.0); GCK (-9.8); RBP4 (-9.0)
170	Erythrophleine	<i>Erythrophleum lasianthum</i>	AKR1B1 (-9.0); HSD11B1 (-9.4)
171	Eucosterol	<i>Eucomis autumnnalis</i>	DPP4 (-9.3); PPARD (-9.7)
172	Flemichapparin C	<i>Cyclopia spp</i>	AKR1B1 (-10.0); DPP4 (-9.1); GCK (-9.2); HSD11B1 (-9.3); PPARD (-9.2); RBP4 (-9.4)
173	Formononetin	<i>Cyclopia spp</i>	AKR1B1 (-9.4)
174	Friedelin	<i>Adansonia digitata, Artemisia afra, Aster bakeranus, Euphorbia hirta, Harungana madagascariensis, Prunus africana, Syzygium Cordatum</i>	AMY2A (-9.2); DPP4 (-9.8); HSD11B1 (-10.5); NR5A2 (-9.6); PPARD (-9.5); PYGL (-9.0)
175	Frutinone A	<i>Polygala fruticosa</i>	AKR1B1 (-9.5); GCK (-9.4); HSD11B1 (-9.1); PPARD (-9.6); PPARG (-9.5); RBP4 (-10.5); RXRA (-9.0)
176	Fujikinetin	<i>Cyclopia spp</i>	AKR1B1 (-10.2); FFAR1 (-9.0); PPARG (-9.0); RBP4 (-9.8)
177	Furanoeudesma-1,3-diene	<i>Commiphora myrrha</i>	RBP4 (-9.0)
178	Gaboroquinone A	<i>Bulbine frutescens</i>	AMY2A (-9.0)
179	Gaboroquinone B	<i>Bulbine frutescens</i>	HSD11B1 (-9.1); PPARD (-9.40)
180	Galanthamine	<i>Crinum bulbispermum</i>	AKR1B1 (-9.1)
181	Gallocatechin	<i>Pelargonium sidoides</i>	HSD11B1 (-9.2); RBP4 (-9.0)
182	Garcifuran B	<i>Garcinia kola</i>	AKR1B1 (-9.4); RBP4 (-9.6)
183	Garcinia biflavonoid 1	<i>Garcinia kola</i>	AKR1B1 (-9.2); AMY2A (-9.2); DPP4 (-9.0); MGAM (-9.1); PPARD (-10.9)
184	Garcinia biflavonoid 2	<i>Garcinia kola</i>	AKR1B1 (-9.3); AMY2A (-9.1); DPP4 (-9.1); MGAM (-9.3); PPARD (-10.7); PYGL (-9.1)

185	Geissoschizine	<i>Rauvolfia vomitoria</i>	PPARD (-9.1)
186	Geissoschizol	<i>Rauvolfia vomitoria</i>	PPARD (-9.1)
187	Gelsemicine	<i>Gelsemium sempervirens</i>	HSD11B1 (-9.3); PPARG (-9.2)
188	Genistein	<i>Cajanus cajan</i>	AKR1B1 (-9.2); HSD11B1 (-9.0); RBP4 (-9.9)
189	Geraniin	<i>Geranium Incanum</i>	AMY2A (-9.0); DPP4 (-10.9); PDK2 (-10.1); PTPN9 (-9.3)
190	Gitogenin	<i>Tribulus terrestris</i>	AMY2A (-9.4); HSD11B1 (-9.4)
191	Glycyrrhizin	<i>Abrus Precatorius, Glycyrrhiza glabra</i>	AMY2A (-9.6); DPP4 (-10.2); PTPN9 (-9.6); PYGL (-9.4)
192	Gnidicin	<i>Gnidia kraussiana</i>	DPP4 (-10.4); FFAR1 (-9.3); GCK (-9.1); MGAM (-9.7); PDK2 (-9.7); PPARD (-12.7); PPARG (-9.3); PYGL (-9.6)
193	Gnidilatin	<i>Gnidia kraussiana</i>	DPP4 (-9.4); PPARD (-10.8)
194	Gniditrin	<i>Gnidia kraussiana</i>	AMY2A (-9.6); FFAR1 (-9.4); PPARD (-9.5)
195	Gomphoside	<i>Asclepias fruticosa</i>	AKR1B1 (-9.8); AMY2A (-10.7); DPP4 (-9.3); GCK (-10.6); KSD11B1 (-11.2); NR5A2 (-10.4); PPARG (-10.3); PTPN9 (-9.8)
196	Gossypetin	<i>Hibiscus sabdariffa</i>	HSD11B1 (-9.7); RBP4 (-9.4)
197	Grayanotoxin I	<i>Rhododendron indicum</i>	HSD11B1 (-9.4)
198	Guajaverin	<i>Psidium guajava</i>	PPARG (-9.3)
199	Harman	<i>Tribulus terrestris</i>	AKR1B1 (-9.1)
200	Harpagoside	<i>Harpagophytum procumbens</i>	HSD11B1 (-9.0)
201	Harunganin	<i>Harungana madagascariensis</i>	AKR1B1 (-9.7); GCK (-9.1); PPARD (-10.3)
202	Harunganol B	<i>Harungana madagascariensis</i>	AKR1B1 (-11.7); DPP4 (-9.1); GCK (-9.5); HSD11B1 (-9.7); PPARD (-9.8); PPARG (-9.1)
203	Harunmadagascarin A	<i>Harungana madagascariensis</i>	AKR1B1 (-10.5); AMY2A (-9.4); DPP4 (-10.0); GCK (-9.2); HSD11B1 (-10.8); PPARD (-11.0); PPARG (-9.0)
203	Harunmadagascarin B	<i>Harungana madagascariensis</i>	AMY2A (-9.0); DPP4 (-9.0); GCK (-9.3); HSD11B1 (-9.6); PPARD (-11.2); PPARG (-9.5)
205	Hautriwaic acid	<i>Dodonaea Angustifolia</i>	AKR1B1 (-9.3)
206	Haemanthamine	<i>Scadoxus puniceus</i>	AKR1B1 (-9.5); GCK (-9.2)

207	Haemanthidine	<i>Scadoxus puniceus</i>	AKR1B1 (-9.1)
208	Hederagenin	<i>Hedera helix</i>	DPP4 (-9.8); PTPN9 (-9.0)
209	Helichrysetin	<i>Helichrysum Species</i>	FFAR1 (-9.8)
210	Hellebrigenin	<i>Kalanchoe lanceolata</i>	PPARD (-9.3)
211	Hellebrigenin-3-acetate	<i>Melianthus comosus</i>	AMY2A (-9.0); GCK (-9.7); HSD11B1 (-9.6); PPARD (-9.3)
212	Henningsiine	<i>Strychnos henningsii</i>	AMY2A (-9.1); HSD11B1 (-9.6); PPARD (-10.0); PPARG (-9.0)
213	Hesperitin	<i>Cyclopia spp</i>	FFAR1 (-9.0); HSD11B1 (-9.2); RBP4 (-9.3)
214	Hibiscetin	<i>Hibiscus sabdariffa</i>	HSD11B1 (-9.7); RBP4 (-9.3)
215	Hibiscin	<i>Hibiscus sabdariffa</i>	HSD11B1 (-10.2)
216	Hibiscitrin	<i>Hibiscus sabdariffa</i>	HSD11B1 (-9.5); PPARG (-9.0)
217	Hippeastrine	<i>Clivia miniata, Crinum bulbispermum</i>	AKR1B1 (-10.9); HSD11B1 (-9.3)
218	Hircinol	<i>Dioscorea dregeana</i>	RBP4 (-9.1)
219	Hydroxyveranolide	<i>Vernonia colorata</i>	HSD11B1 (-9.1); PPARD (-9.1)
220	Hyoscyamine	<i>Datura stramonium</i>	AKR1B1 (-9.0)
221	Hyperforin	<i>Hypericum perforatum</i>	PPARD (-11.1)
222	Hypericin	<i>Harungana madagascariensis, Hypericum aethiopicum, Hypericum perforatum</i>	AMY2A (-11.1); DPP4 (-10.7); GCK (-9.7); INSR (-10.5); MGAM (-9.8); NR5A2 (-10.0); PPARD (-9.3); PPARG (-9.3); PTPN9 (-9.7)
223	Hyperin	<i>Hypericum perforatum</i>	AKR1B1 (-9.0); PPARD (-9.3)
224	Hypoxoside	<i>Hypoxis hemerocallidea</i>	DPP4 (-9.1); PPARG (-9.0)
225	Ibogaine	<i>Voacanga africana</i>	HD11B1 (-9.1); PPARD (-9.0)
226	Ibogamine	<i>Voacanga africana</i>	HSD11B1 (-9.1); PPARD (-9.3); RBP4 (-10.6); RXRA (-9.3)
227	Iboxygaine	<i>Voacanga africana</i>	HSD11B1 (-9.4); PPARD (-9.0)
228	Ibozol	<i>Tetradenia Riparia</i>	GCK (-9.7)
229	Icterogenin	<i>Lippia Rhenmannii</i>	DPP4 (-9.1)
230	Indole-3-acetyl aspartic acid	<i>Griffonia simplicifolia</i>	AKR1B1 (-9.0)
231	Ingenol	<i>Euphorbia hirta, Euphorbia ingens</i>	PPARD (-9.4)
232	Ingenol triacetate	<i>Euphorbia hirta</i>	PPARD (-9.1)

233	Insularine	<i>Cissampelos capensis</i>	AMY2A (-9.0); DPP4 (-9.4); MGAM (-9.1); PPARG (-9.1); PYGL (-9.1)
234	Integerrimine	<i>Lotononis laxa</i>	HSD11B1 (-9.1); PPARD (-9.3)
235	Isocryptolepine	<i>Cryptolepis sanguinolenta</i>	RBP4 (-9.9); RXRA (-9.0)
236	Isofucosterol	<i>Adansonia digitata</i>	AKR1B1 (-10.9); HSD11B1 (-10.3); PPARG (-9.0)
237	Isokigelinol	<i>Kigelia africana</i>	AMY2A (-9.6); GCK (-9.1); HSD11B1 (-10.1); NR5A2 (-9.0); PPARD (-9.6)
238	Isoorientin	<i>Aspalathus linearis</i>	AKR1B1 (-9.8); AMY2A (-9.0); DPP4 (-9.4); HSD11B1 (-9.9); PPARG (-10.2)
239	Isopinnatal	<i>Kigelia africana</i>	NR5A2 (-9.3); PPARD (-9.6)
240	Isoquercetin	<i>Centella asiatica, Impomoea pes-caprae ssp. Brasiliensis, Moringa oleifera</i>	AKR1B1 (-9.0); PPARD (-9.3)
241	Isoreserpiline	<i>Rauwolfia vomitoria</i>	PPARD (-9.1)
242	Isoreserpine	<i>Rauwolfia vomitoria</i>	GCK (-9.3)
243	Isorhamnetin	<i>Cajanus cajan</i>	HSD11B1 (-9.1); RBP4 (-9.2)
244	Isosakuranetin	<i>Cyclopia spp</i>	HSD11B1 (-9.0); RBP4 (-9.8)
245	Isovitexin	<i>Combretum micranthum</i>	DPP4 (-9.5); HSD11B1 (-9.6); PPARG (-10.0)
246	Ivangustine	<i>Eriocephalus africanus</i>	RBP4 (-9.9)
247	Kaempferol	<i>Euphorbia hirta, Harpephyllum Caffrum, Moringa oleifera, Rauwolfia vomitoria</i>	HSD11B1 (-9.0); RBP4 (-9.5)
248	Kaempferol-3-glucoside	<i>Moringa oleifera</i>	AKR1B1 (-9.3); HSD11B1 (-9.3); PPARD (-9.6)
249	Kaempferol-3-o-(6'-malonyl-glucoside)	<i>Moringa oleifera</i>	DPP4 (-9.1); HSD11B1 (-9.8); PPARD (-9.1); PPARG (-9.0)
250	Kaempferol-3-O-rhamnoglucoside	<i>Danais fragrans</i>	DPP4 (-10.0); HSD11B1 (-9.0); PPARD (-9.4); PPARG (-9.4)
251	Kauran-16a-ol	<i>Xylopiya aethiopica</i>	HSD11B1 (-9.4)
252	Kigelinol	<i>Kigelia africana</i>	HSD11B1 (-9.1); PPARD (-9.4)
253	Kigelinone	<i>Kigelia africana</i>	AKR1B1 (-9.1); RBP4 (-9.4)
254	Knipholone	<i>Bulbine frutescens, Bulbine natalensis</i>	AKR1B1 (-9.7); HSD11B1 (-9.8); PPARD (-9.2); PPARG (-9.5)
255	Kolaflavanone	<i>Garcinia kola</i>	AMY2A (-9.0); DPP4 (-9.2); MGAM (-9.0); PPARD (-10.9)

256	Kolanone	<i>Garcinia kola</i>	AKR1B1 (-11.5); GCK (-10.3); HSD11B1 (-9.4); PPARD (-10.0); PPARG (-9.8)
257	Lactucin	<i>Chicorium intybus</i>	RBP4 (-9.4)
258	Lanceotoxin A	<i>Kalanchoe lanceolata</i>	PPARD (-9.1)
259	Lantadene A	<i>Lantana camara, Lippia Rehmannii</i>	AMY2A (-9.0); DPP4 (-9.5); HSD11B1 (-9.6); INSR (-9.0)
260	Lantadene B	<i>Lantana camara</i>	PTPN9 (-9.0)
261	Lapachol	<i>Kigelia africana</i>	AKR1B1 (-9.2)
262	Lemmatoxin	<i>Phytolacca dodecandra</i>	DPP4 (-10.3)
263	Leucocyanidin	<i>Euphorbia hirta</i>	RBP4 (-9.2)
264	Leurosidine	<i>Catharanthus roseus</i>	DPP4 (-9.0)
265	Leurosine	<i>Catharanthus roseus</i>	DPP4 (-9.1)
266	Ligustroside	<i>Ligustrum lucidum</i>	HSD11B1 (-9.3); PPARG (-9.4)
267	Liquiritin	<i>Glycyrrhiza glabra</i>	FFAR1 (-9.1); HSD11B1 (-9.1); PPARG (-9.0)
268	Lithospermic acid	<i>Echium vulgare</i>	AKR1B1 (-9.0); DPP4 (-9.0); GCK (-9.4); HSD11B1 (-9.6); PPARD (-9.8); PPARG (-11.0); PYGL (-9.0)
269	Lochnerine	<i>Catharanthus roseus</i>	DPP4 (-9.5); PPARD (-9.0)
270	Longistylin A	<i>Cajanus cajan</i>	AKR1B1 (-9.6); DPP4 (-9.0); FFAR1 (-9.8); GCK (-9.0); PPARG (-9.0)
271	Longistylin C	<i>Cajanus cajan</i>	AKR1B1 (-10.0); PPARD (-9.3); RBP4 (-9.8); RXRA (-9.5)
272	Lupeol	<i>Catharanthus roseus</i>	HSD11B1 (-9.8); PPARD (-9.8)
273	Luteolin	<i>Kigelia africana, Vernonia amygdalina</i>	AKR1B1 (-9.2); HSD11B1 (-9.5); RBP4 (-10.0); RXRA (-9.2)
274	Luteolin-4-rutinoside	<i>Vernonia amygdalina</i>	AMY2A (-9.4); DPP4 (-9.9); FFAR1 (-9.1); HSD11B1 (-9.8); PPARD (-10.4); PPARG (-10.1)
275	Luteolin-7-glucoside	<i>Vernonia amygdalina</i>	DPP4 (-9.3); HSD11B1 (-9.6); PPARD (-9.6); PPARG (-10.0)
276	Luteolin-7-rutinoside	<i>Vernonia amygdalina</i>	AKR1B1 (-9.1); AMY2A (-9.7); DPP4 (-10.5); GCK (-9.8); HSD11B1 (-9.8); INSR (-9.4); PPARD (-9.8); PPARG (-11.4); PTPN9 (-9.8); PYGL (-9.4)

277	Lycorine	<i>Amaryllis belladonna</i> , <i>Clivia miniata</i> , <i>Crinum bulbispermum</i> , <i>Crinum macowanii</i>	AKR1B1 (-9.0); HSD11B1 (-9.1); RBP4 (-9.7)
278	Madecassic acid	<i>Centella asiatica</i>	AMY2A (-9.1); DPP4 (-9.1); HSD11B1 (-9.1)
279	Maslinic acid	<i>Prunus africana</i>	AMY2A (-9.7); DPP4 (-9.0)
280	Medicagol	<i>Cyclopia spp</i>	AKR1B1 (-9.4); GCK (-9.5); HSD11B1 (-9.4); PPARD (-9.4); PPARG (-9.4); RBP4 (-10.1)
281	Melianol	<i>Melia azedarach</i>	AMY2A (-9.3); DPP4 (-9.2); HSD11B1 (-9.0); PTPN9 (-9.1); PYGL (-9.0)
282	Melianthugenin	<i>Bersama lucens</i> , <i>Melianthus comsus</i>	AKR1B1 (-9.8); AMY2A (-9.5); DPP4 (-9.1); GCK (-9.0); HSD11B1 (-9.6); PDK2 (-9.1); PPARD (- 10.3); PPARG (-10.3)
283	Meliatoxin B1	<i>Melia azedarach</i>	AKR1B1 (-10.1); DPP4 (-9.7)
284	Meliatoxin B2	<i>Melia azedarach</i>	AKR1B1 (-10.3); DPP4 (-10.0)
285	Mucronine D	<i>Ziziphus mucronata</i>	AMY2A (-9.1); DPP4 (-11.4); GCK (-10.3); HSD11B1 (-10.3); NR5A2 (-10.0); PPARD (-10.0); PPARG (-10.3)
286	Naringenin	<i>Cyclopia spp.</i>	HSD11B1 (-9.0); RBP4 (-9.8)
287	Nauclefidine	<i>Nauclea latifolia</i>	AKR1B1 (-10.1); HSD11B1 (-9.0); RBP4 (-10.0)
288	Nauclefine	<i>Nauclea latifolia</i>	AKR1B1 (-9.3); GCK (-10.5); HSD11B1 (-10.2); PPARD (-9.9); PPARG (-10.50); PTPN9 (-9.0); PYGL (-9.0)
289	Neocryptolepine	<i>Cryptolepis sanguinolenta</i>	AKR1B1 (-9.6); PPARD (-9.1); RBP4 (-10.3); RXRA (-9.5)
290	N-methylflindersine	<i>Toddalia asiatica</i>	AKR1B1 (-9.2); RBP4 (-9.5)
291	Norajmaline	<i>Rauwolfia vomitoria</i>	HSD11B1 (-9.1); PPARD (-9.6)
292	Nothofagin	<i>Aspalathus linearis</i>	AKR1B1 (-9.8); FFAR1 (9.7); RXRA (-9.0)
293	Nudicauline	<i>Delphinium grandiflorum</i>	AMY2A (-9.0); DPP4 (-9.8); PPARD (-10.3)
294	Obebioside	<i>Adenium multiflorum</i>	DPP4 (-9.8); PTPN9 (-9.2)
295	Ocubullenone	<i>Ocotea bullata</i>	AKR1B1 (-9.5)
296	Oleacein	<i>Olea europaea</i>	AKR1B1 (-9.1); FFAR1 (-9.1)
297	Oleandrin	<i>Nerium oleander</i>	HSD11B1 (-9.9); PPARD (-9.0)
298	Oleanoglycotoxin	<i>Phytolacca dodecandra</i>	DPP4 (-9.7)

299	Oleanolic acid	<i>Ligustrum lucidum, Melianthus comosus, Prunus africana</i>	DPP4 (-9.6); HSD11B1 (-10.7)
300	Oleanolic-3-acetate	<i>Prunus africana</i>	AMY2A (-9.1)
301	Oleuropein	<i>Ligustrum lucidum, Olea europaea</i>	HSD11B1 (-9.0)
302	Orbicuside A	<i>Cotyledon orbiculata</i>	AMY2A (-10.9); DPP4 (-9.3); PTPN9 (-9.7); PYGL (-9.3)
303	Orientin	<i>Aspalathus linearis</i>	HSD11B1 (-9.5)
304	Ouabain	<i>Acokanthera oppositifolia, Strophanthus gratus</i>	HSD11B1 (-9.9)
305	Ouratea proanthocyanidin A	<i>Cassine transvaalensis</i>	AMY2A (-9.4); PPARD (-9.1)
306	Oxyavicine	<i>Toddalia asiatica</i>	AKR1B1 (-10.0); AMY2A (-9.8); DPP4 (-9.5); GCK (-10.1); HSD11B1 (-10.6); INSR (-9.2); PPARD (-9.7); PPARG (-10.3); RXRA (-9.2)
307	Oxychelerythrine	<i>Toddalia asiatica</i>	AKR1B1 (-9.3); AMY2A (-9.1); HSD11B1 (-9.9); PPARG (-9.4)
308	P57 compound	<i>Hoodia gordonii</i>	DDP4 (-10.2); PPARG (-9.3)
309	Palmitic acid	<i>Hibiscus sabdariffa</i>	RBP4 (-9.1)
310	Parquin	<i>Cestrum laevigatum</i>	DPP4 (-9.2)
311	Peddiea Factor A1	<i>Peddiea africana</i>	PPARD (-9.5); PTPN9 (-9.1)
312	Petunidine	<i>Catharanthus roseus</i>	AKR1B1 (-9.0); HSD11B1 (-9.4); RBP4 (-9.0)
313	Picrinine	<i>Rauvolfia vomitoria</i>	AMY2A (-9.1); HSD11B1 (-9.4); PPARD (-9.6); PPARG -9.0)
314	Pinocembrin	<i>Tarchonanthus camphoratus</i>	FFAR1 (-9.0); RBP4 (-9.6)
315	Pinoresinol	<i>Strophanthus gratus</i>	AKR1B1 (-9.2); HSD11B1 (-9.0); PPARG (-9.0)
316	Pinostrobin	<i>Cajanus cajan</i>	RBP4 (-9.5)
317	Platyphylline	<i>Senecio serratuloides</i>	HSD11B1 (-9.4); PPARD (-9.3)
318	Plumbagin	<i>Plumbago auriculata</i>	FFAR1 (-9.1)
319	Pratorimine	<i>Crinum bulbispermum, Crinum macowanii</i>	AKR1B1 (-9.0); RBP4 (-10.0)
320	Premarrubiin	<i>Leonotis leonurus</i>	HSD11B1 (-9.9); NR5A2 (-9.1); PPARD (-9.7)
321	Presenegenin	<i>Polygala fruticosa, Securidaca longipedunculata</i>	HSD11B1 (-10.1)
322	Procyanidin C1	<i>Sclerocarya birrea</i>	AMY2A (-10.0); DPP4 (-10.7); GCK (-9.9); MGAM (-9.9); PYGL (-10.8)

323	Propacin	<i>Mondia whitei</i>	AMY2A (-9.0); HSD11B1 (-9.7); PPARD (-9.2); PPARG (-9.4)
324	Proscillaridin A	<i>Drimia robusta, Scilla natalensis</i>	AKR1B1 (-10.0); AMY2A (-9.3); DPP4 (-10.2); HSD11B1 (-10.7); PPARD (-10.0)
325	Protopine	<i>Argemone ochoroleuca</i>	HSD11B1 (-10.1); IMSR (-9.1); PPARD (-10.4)
326	Pseudobaptigen	<i>Cyclopia spp</i>	AKR1B1 (-10.3); DPP4 (-9.1); FFAR1 (-10.0); HSD11B1 (-9.1); RBP4 (-9.8)
327	Pterygospermin	<i>Moringa oleifera</i>	AKR1B1 (-11.9); AMY2A (-9.0); DPP4 (-9.8); GCK (-11.1); HSD11B1 (-9.9); INSR (-9.2); NR5A2 (-9.8); (PPARD (-11.6); PPARG (-9.5); RXRA (-9.0)
328	Punicalagin	<i>Punica granatum</i>	DPP4 (-11.3); MGAM (-9.3); PYGL (-10.3)
329	Punicalin	<i>Punica Granatum</i>	AMY2A (-10.8); DPP4 (-10.5); PTPN9 (-10.1); PYGL (-10.5)
330	Pyrethrin I	<i>Chrysanthemum cinerariifolium</i>	AKR1B1 (-9.7); GCK (-9.5); PPARD (-9.0); PPARG (-9.1); RXRA (-9.3)
331	Quercetin	<i>Acacia karroo, Aspalathus linearis, Cajanus cajan, Euphorbia hirta, Harungana madagascariensis, Kigelia africana, Moringa oleifera, Pelargonium sidoides, Psidium guajava, Rauwolfia vomitoria</i>	HSD11B1 (-9.6); RBP4 (-9.6)
332	Quercetin-7-O-B-D-xylopyranoside	<i>Adansonia digitata</i>	HSD11B1 (-9.2); PPARG (-9.2)
333	Quercetin-3,7-diglucoside	<i>Agathosma betulina</i>	DPP4 (-9.0); HSD11B1 (-9.4); PPARD (-10.3); PPARG (-9.8)
334	Quercetin-3-o-(6'-malonyl-glucoside)	<i>Moringa oleifera</i>	HSD11B1 (-9.8); PPARD (-9.2); PPARG (-9.2)
335	Quercitrin	<i>Danais fragrans, Euphorbia hirta, Thesium hystrix</i>	AKR1B1 (-9.3); HSD11B1 (-9.2); PPARD (-9.5); PPARG (-9.2)
336	Quindoline	<i>Cryptolepis sanguinolenta</i>	AKR1B1 (-9.5); RBP4 (-9.7); RXRA (-10.1)
337	Rauvoxin	<i>Rauwolfia vomitoria</i>	PPARD (-9.4)
338	Rauvoxinin	<i>Rauwolfia vomitoria</i>	PPARD (-9.4)
339	Reserpinic acid	<i>Rauwolfia vomitoria</i>	PPARD (-9.0); PPARG (-9.3)
340	Reserpine	<i>Catharanthus roseus, Rauwolfia caffra, Rauwolfia, vomitoria</i>	DPP4 (-9.0); PPARD (-9.4); PPARG (-9.8)



341	Resveratrol	<i>Terminalia sericea</i>	AKR1B1 (-9.0); FFAR1 (-9.6)
342	Resveratrol-3-O-B-rutinoside	<i>Terminalia sericea</i>	DPP4 (-9.6); FFAR1 (-9.0); GCK (-9.3); HSD11B1 (-9.9); PPARD (-9.1); PPARG (-10.2); PYGL (-9.5)
343	Retrorsine	<i>Crotalaria spartioides, Senecio retrorsus</i>	HSD11B1 (-9.3)
344	Rhinocerotoic acid	<i>Elytropappus rhinoceotis</i>	HSD11B1 (-9.2); RBP4 (-9.9)
345	Rohituka 3	<i>Trichilia emetica</i>	PYGL (-9.3)
346	Rooperol	<i>Hypoxis hemerocallidea</i>	AKR1B1 (-9.7); FFAR1 (-9.4); GCK (-9.6); RXRA (-9.3)
347	Rotenone	<i>Mundulea sericea</i>	AKR1B1 (-9.6); GCK (-10.1)
348	Rubiadin	<i>Danais fragrans</i>	RBP4 (-9.9)
349	Rubiadin xyloglucoside	<i>Danais fragrans</i>	AMY2A (-9.0); DPP4 (-9.8); HSD11B1 (-11.0); PPARD (-9.4); PPARG (-9.9); PTPN9 (-9.1); PYGL (-9.1)
350	Ruscogenin-(25S)-form	<i>Sansiviera hyacinthoides</i>	AMY2A (-10.1); DPP4 (-9.0); NR5A2 (-9.2)
351	Rutaretin	<i>Ruta graveolens</i>	AKR1B1 (-9.1); RBP4 (-9.0)
352	Rutin	<i>Acacia senegal, Agathosma betulina, Hypericum perforatum, Ruta graveolens</i>	DPP4 (-9.4); GCK (-9.2); HSD11B1 (-10.2); PPARD (-10.1); PPARG (-9.7); PTPN9 (-9.4)
353	Sakurasosaponin	<i>Rapanea melanphloeos</i>	AMY2A (-9.3); DPP4 (-9.8)
354	Sanguinarine	<i>Argemone ochroleuca, Fumaria officinalis, Zanthoxylum capense</i>	AKR1B1 (-10.3); AMY2A (-9.3); GCK (-9.5); HSD11B1 (-10.1); INSR (-9.2); PPARD (-10.1); PPARG (-9.9); RBP4 (-9.7)
355	Sanjoinine A	<i>Ziziphus mucronata</i>	PPARD (-11.7)
356	Sarcovimisine B	<i>Sarcostemma viminale</i>	AKR1B1 (-10.8); AMY2A (-10.0); DPP4 (-10.1); GCK (-10.3); PDK2 (-9.8); PPARD (-9.1); PPARG (-9.2)
357	Scillaren A	<i>Urginea maritima, Urginea sanguinea</i>	AMY2A (-9.3); DPP4 (-10.6); NR5A2 (-9.4); PPARD (-9.6); PTPN9 (-9.0)
358	Scillarenin	<i>Urginea maritima</i>	AKR1B1 (-10.3); DPP4 (-9.3); GCK (-10.2); HSD11B1 (-10.0); PPARD (-9.5); PPARG (-10.0)
359	Senecionine	<i>Lotononis laxa, Senecio serratuloides</i>	HSD11B1 (-10.3); PPARD (-9.4)
360	Sericic acid	<i>Terminalia sericea</i>	AMY2A (-9.7); HSD11B1 (-10.9)

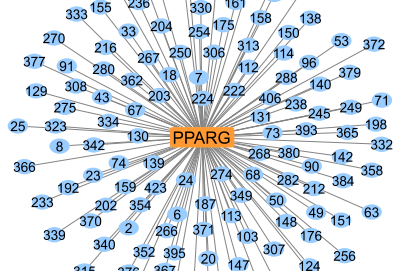
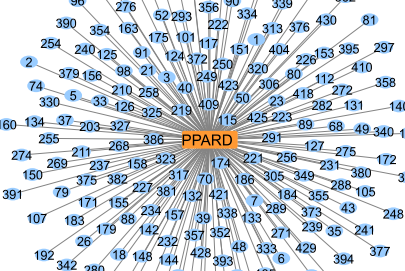
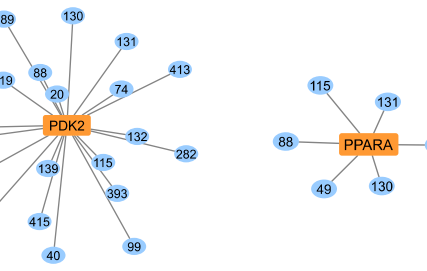
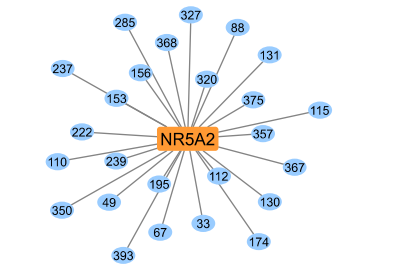
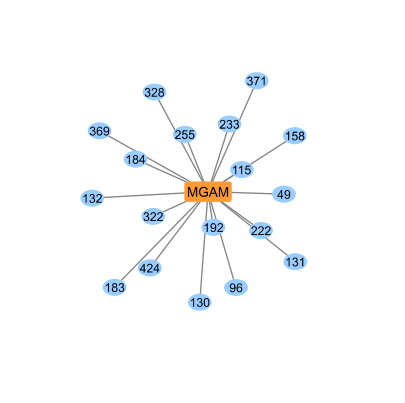
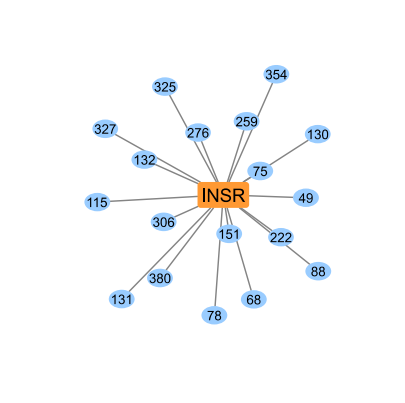
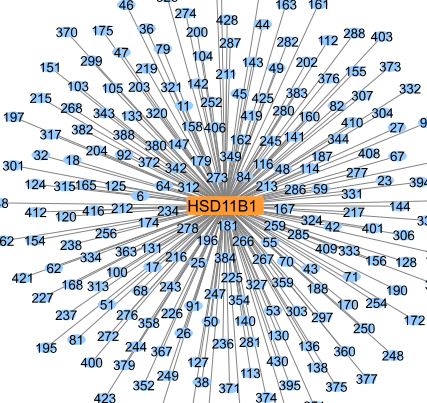
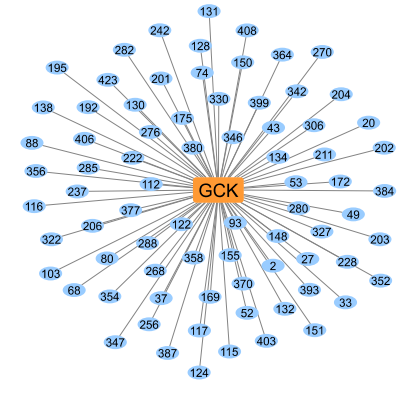
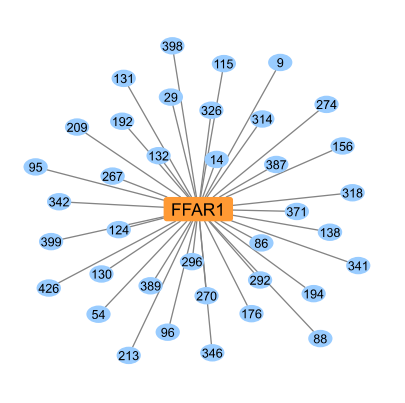
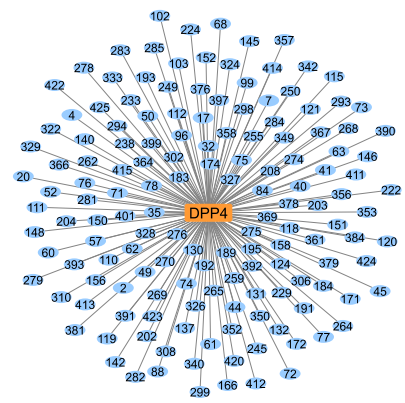
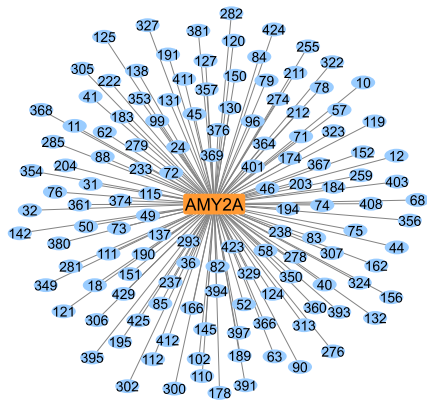
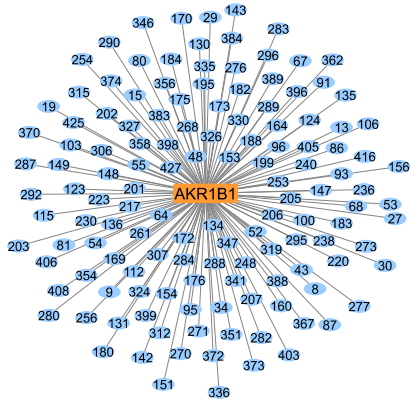
361	Sericoside	<i>Terminalia sericea</i>	AMY2A (-9.3); DPP4 (-9.3)
362	Serpenticine	<i>Rauvolfia vomitoria</i>	AKR1B1 (-9.2); HSD11B1 (-9.7); PPARD (-9.4); PPARG (-9.2)
363	Serpentine	<i>Catharanthus roseus, Rauvolfia vomitoria</i>	HSD11B1 (-9.7); PPARD (-9.6)
364	Sitosterol-3-glucoside	<i>Pelargonium sidoides</i>	AMY2A (-9.4); DPP4 (-9.2); GCK (-9.2); PPARD (-9.1)
365	Sodium-en- knipholone-6-O-sulfate	<i>Bulbine frutescens</i>	PPARG (-9.1)
366	Solanine	<i>Solanum incanum, Solanum tuberosum</i>	AMY2A (-9.5); DPP4 (-9.6); PPARG (-9.5)
367	Solanocapsine	<i>Solanum pseudocapsicum</i>	AKR1B1 (-9.6); AMY2A (-9.4); DPP4 (-10.2); HSD11B1 (-10.5); NR5A2 (-9.1); PPARG (-9.1)
368	Solasodine	<i>Solanum incanum, Solanum nigrum</i>	AMY2A (-9.7); NR5A2 (-9.4)
369	Solasonine	<i>Solanum incanum</i>	AMY2A (-9.1); DPP4 (-11.0); MGAM (-9.9); PYGL (-9.7)
370	Sophoracoumestan B	<i>Cyclopia spp</i>	AKR1B1 (-9.7); GCK (-9.1); HSD11B1 (-9.5); PPARG (-9.2); RBP4 (-10.7)
371	Sophoricoside	<i>Styphnolobium Japonicum</i>	FFAR1 (-10.2); HSD11B1 (-10.1); MGAM (-9.0); PPARD (-9.3); PPARG (-9.9)
372	Stachenol	<i>Spirostachys africana</i>	AKR1B1 (-9.0); HSD11B1 (-9.3); PPARD (-9.7); PPARG (-9.7); RXRA (-9.1)
373	Stachenone	<i>Spirostachys africana</i>	AKR1B1 (-9.0); HSD11B1 (-9.3); PPARD (-9.6)
374	Stigmast-4-en-3-one	<i>Prunus africana</i>	AKR1B1 (-9.2); AMY2A (-9.4); HSD11B1 (-10.5); PPARD (-9.7)
375	Stigmasterol	<i>Dodonaea angustifolia, Harpagophytum procumbens, Kigelia africana, Ravenala madagascariensis</i>	HSD11B1 (-10.0); NR5A2 (-9.0); PPARD (-10.5)
376	Strictosamine	<i>Nauclea latifolia</i>	AMY2A (-9.0); DPP4 (-9.4); HSD11B1 (-9.9); PPARD (-9.3); PPARG (-10.7)
377	Strictosidine	<i>Nauclea latifolia</i>	GCK (-9.9); HSD11B1 (-10.8); PPARD (-9.3); PPARG (-9.7)
378	Strogoside	<i>Strophanthus gratus</i>	DPP4 (-9.4); PPARD (-9.4); PTPN9 (-9.0)
379	Strophantidin	<i>Strophanthus gratus</i>	DPP4 (-9.4); HSD11B1 (-9.6); PPARD (-9.1); PPARG (-9.8)

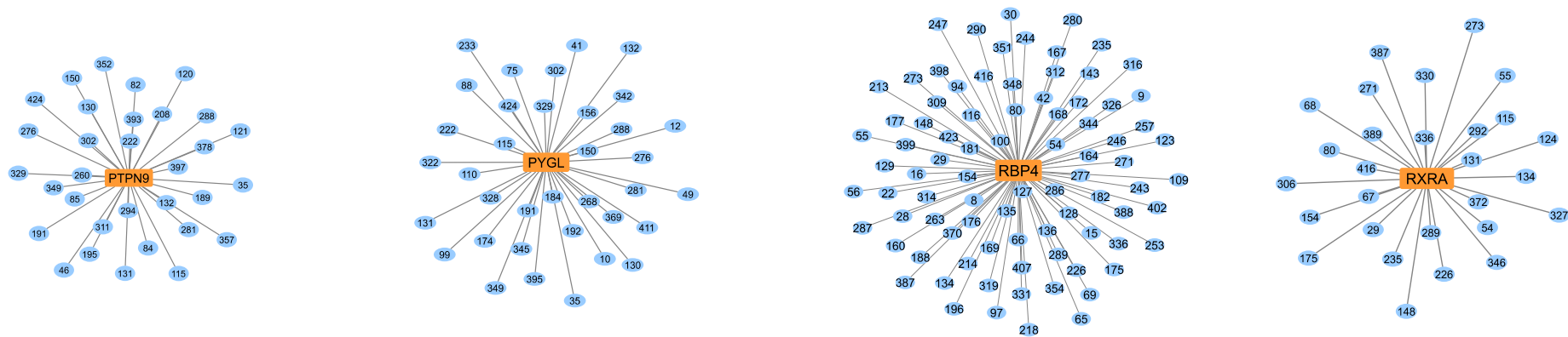
380	Strychnine	<i>Strychnos henningsii, Strychnos spinosa</i>	AMY2A (-9.5); GCK (-9.4); HSD11B1 (-10.2); INSR (-9.1); PPARD (-10.0); PPARG (-9.4)
381	Synaptolepis factor K1	<i>Synaptolepis kirkii</i>	AMY2A (-10.0); DPP4 (-10.1); PPARD (-10.7)
382	Synaptolepis factor K7	<i>Synaptolepis kirkii</i>	HSD11B1 (-9.3); PPARD (-9.5)
383	Taraxerol	<i>Euphorbia hirta</i>	AKR1B1 (-9.2); HSD11B1 (-10.8)
384	Tephrosin	<i>Mundulea sericea</i>	AKR1B1 (-10.0); DPP4 (-9.1); GCK (-9.6); HSD11B1 (-10.0); PPARG (-9.3)
385	Terminoic acid	<i>Terminalia sericea</i>	PPARD (-9.1)
386	Tetrahydroalstonine	<i>Catharanthus roseus</i>	PPARD (-9.7)
387	Tetrahydrocannabinol	<i>Cannabis sativa</i>	FFAR1 (-9.1); GCK (-9.2); RBP4 (-9.5); RXRA (-9.2)
388	Tetrahydroxyflavanone	<i>Lansea acida</i>	AKR1B1 (-9.0); HSD11B1 (-9.2); RBP4 (-9.4)
389	Thesinine	<i>Borago officinalis, Thesium minkwitzianum</i>	AKR1B1 (-9.3); FFAR1 (-9.7); RXRA (-9.2)
390	Thevetin A	<i>Thevetia peruviana</i>	DPP4 (-9.2); PPARD (-9.5); PPARG (-9.6)
391	Thevetin B	<i>Thevetia peruviana</i>	AMY2A (-10.1); DPP4 (-9.8); PPARD (-9.1); PPARG (-9.5)
392	Trichilin A	<i>Trichilia emetica</i>	DPP4 (-9.3)
393	Tinyatoxin	<i>Euphorbia hirta</i>	AMY2A (-9.7); DPP4 (-10.2); GCK (9.4); NR5A2 (-9.2); PDK2 (-9.1); PPARD (-10.9); PPARG (-9.4); PTPN9 (-9.0)
394	Toddalosis	<i>Toddalia asiatica</i>	AMY2A (-9.5); HSD11B1 (-9.3); PPARD (-9.9)
395	Toddasin	<i>Toddalia asiatica</i>	AMY2A (-9.9); HSD11B1 (-9.1); PPARD (-9.6); PPARG (-10.1); PYGL (-9.1)
396	Trachelogenin	<i>Cnicus benedictus</i>	AKR1B1 (-9.2)
397	Tyledoside C	<i>Cotyledon orbiculata</i>	AMY2A (-9.1); DPP4 (-9.1); PTPN9 (-9.6)
398	Typhaphtalide	<i>Typha capensis</i>	AKR1B1 (-9.1); FFAR1 (-10.1); RBP4 (-9.6)
399	Typharin	<i>Typha capensis</i>	AKR1B1 (-10.2); DPP4 (-9.5); FFAR1 (-11.6); GCK (-9.4); PPARD (-9.2); RBP4 (-9.6)
400	Typhasterol	<i>Typha capensis</i>	HSD11B1 (-9.3); PPARD (-9.4)
401	Ursolic acid	<i>Catharanthus roseus, Ligustrum lucidum, Prunus africana, Rauwolfia vomitoria</i>	AMY2A (-9.5); DPP4 (-9.8); HSD11B1 (-11.5); PPARG (-9.4)
402	Urushiol III	<i>Hyaenanche globosa</i>	RBP4 (-9.1)

403	Uzarigenin	<i>Xysmalobium undulatum</i>	AKR1B1 (-9.2); AMY2A (-9.1); GCK (-9.0); HSD11B1 (-10.3); PPARD (-9.6); PPARG (-9.1)
404	Uzarin	<i>Xysmalobium undulatum</i>	PPARD (-10.3)
405	Valerenic acid	<i>Valeriana capensis</i>	AKR1B1 (-9.0)
406	Vellosimine	<i>Rauvolfia vomitoria</i>	AKR1B1 (-9.8); GCK (-9.2); HSD11B1 (-9.8); PPARD (-9.0); PPARG (-9.0)
407	Vermeerin	<i>Geigeria ornativa</i>	RBP4 (-9.8)
408	Verminoside	<i>Kigelia africana</i>	AKR1B1 (-9.4); AMY2A (-9.0); GCK (-9.5); HSD11B1 (-9.9)
409	Vernolide	<i>Vernonia amygdalina, Vernonia colorata</i>	HSD11B1 (-9.6); PPARD (-9.3)
410	Vernomygdin	<i>Vernonia amygdalina</i>	HSD11B1 (-9.6); PPARD (-9.4)
411	Vernonioside A1	<i>Vernonia amygdalina</i>	AMY2A (-9.0); DPP4 (-9.6); PPARD (-9.6); PYGL (-9.4)
412	Vernonioside A3	<i>Vernonia amygdalina</i>	AMY2A (-9.7); DPP4 (-10.7); HSD11B1 (-10.5)
413	Vernonioside B1	<i>Vernonia amygdalina</i>	DPP4 (-9.9); PDK2 (-9.6)
414	Vernonioside B2	<i>Vernonia amygdalina</i>	DPP4 (-10.2)
415	Vernonioside B3	<i>Vernonia amygdalina</i>	DPP4 (-9.8); PDK2 (-9.7)
416	Vinburnine	<i>Voacanga africana</i>	AKR1B1 (-9.6); HSD11B1 (-9.1); PPARD (-9.3); PPARG (-9.4); RBP4 (-10.7); RXRA (-9.3)
417	Vincamine	<i>Vinca minor</i>	PPARD (-9.1)
418	Vindoline	<i>Catharanthus roseus</i>	PPARD (-9.2)
419	Vitexin	<i>Combretum micranthum</i>	HSD11B1 (-9.1)
420	Voacamine	<i>Voacanga africana</i>	DPP4 (-9.4)
421	Voacangine	<i>Voacanga africana</i>	HSD11B1 (-9.3); PPARD (-9.3)
422	Voacorine	<i>Voacanga africana</i>	DPP4 (-9.3)
423	Voaphylline	<i>Voacanga africana</i>	AMY2A (-9); DPP4 (-9.6); GCK (-9.1); HSD11B1 (-9.3); PPARD (-9.1); PPARG (-9.8); RBP4 (-9.2)
424	Vobtusine	<i>Voacanga africana</i>	AMY2A (-9.7); DPP4 (-10.0); MGAM (-9.5); PTPN9 (-9.5); PYGL (-9.1)
425	Withaferin A	<i>Withania somnifera</i>	AKR1B1 (-9.3); AMY2A (-9.6); DPP4 (-9.5); HSD11B1 (-11.3); PPARD (-10.1)
426	Withasomnine	<i>Withania somnifera</i>	FFAR1 (-9.1)

427	Xanthinin	<i>Xanthium strumarium</i>	AKR1B1 (-9.1)
428	Xylopic acid	<i>Xylopia aethiopica</i>	HSD11B1 (-9.2); PPARD (-9.5)
429	Yamogenin	<i>Balanites aegyptiacus</i>	AMY2A (-10.0); PPARD (-11.3)
430	Yohimbine	<i>Catharanthus roseus</i>	HSD11B1 (-9.6); PPARD (-9.0)

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**Figure S1.** Individual predicted active compound-protein target networks. Compounds are represented by their assigned numerical value as in Table S2.

Table S3. Plants having scientific anti-diabetic evidence and evidence of traditional use only identified by virtual screening and their predicted bioactive compounds.

<b>Plant name</b>	<b>Family</b>	<b>Compounds</b>
<b>Plants with scientific evidence</b>		
<i>Abrus Precatorius</i>	Fabaceae	<b>Glycyrrhizin</b> <sup>191</sup>
<i>Acacia karroo</i>	Fabaceae	<b>Beta-sitosterol</b> <sup>70</sup> , <b>epicatechin</b> <sup>164</sup> , <b>quercetin</b> <sup>331</sup>
<i>Acacia senegal</i> *	Fabaceae	<b>Quercetin</b> <sup>331</sup>
<i>Adansonia digitata</i>	Malvaceae	<b>Alpha-Linolenic acid</b> <sup>29</sup> , <b>avenasterol</b> <sup>67</sup> , <b>bauerenol</b> <sup>79</sup> , <b>betulinic acid</b> <sup>85</sup> , <b>beta-sitosterol</b> <sup>70</sup> , <b>campesterol</b> <sup>96</sup> , <b>catechin</b> <sup>100</sup> , <b>friedelin</b> <sup>174</sup> , <b>isofucosterol</b> <sup>236</sup> , <b>quercetin-7-O-B-D-xylopyranoside</b> <sup>332</sup>
<i>Adiantum capillus-veneris</i>	Pteridaceae	Adiantone <sup>33</sup>
<i>Aframomum melegueta</i>	Zingiberaceae	alpha-Humulene <sup>28</sup>
<i>Agathosma betulina</i>	Rutaceae	<b>Diosmetin</b> <sup>154</sup> , <b>diosmin</b> <sup>155</sup> , <b>quercetin-3,7-diglucoside</b> <sup>333</sup> , <b>rutin</b> <sup>352</sup>
<i>Aloe ferox</i>	Asphodelaceae	<b>Aloe-emodin anthrone</b> <sup>42</sup> , <b>aloesin A</b> <sup>43</sup> , <b>aloinoside A</b> <sup>44</sup> , <b>aloinoside B</b> <sup>45</sup>
<i>Artemisia Afra</i> *	Asteraceae	<b>Alpha-amyrin</b> <sup>46</sup> , <b>beta-amyrin</b> <sup>82</sup> , <b>friedelin</b> <sup>174</sup>
<i>Aspalathus linearis</i>	Fabaceae	<b>Aspalathin</b> <sup>64</sup> , <b>isorientin</b> <sup>238</sup> , <b>nothofagin</b> <sup>292</sup> , <b>orientin</b> <sup>303</sup> , <b>quercetin</b> <sup>331</sup>
<i>Balanites aegyptiacus</i> *	Zygophyllaceae	<b>Balagypsin</b> <sup>71</sup> , <b>balanitins 1</b> <sup>72</sup> , <b>2</b> <sup>73</sup> , <b>3</b> <sup>74</sup> , <b>4</b> <sup>75</sup> , <b>6</b> <sup>76</sup> , <b>7</b> <sup>77</sup> , <b>balanitoside</b> <sup>78</sup> , <b>diosgenin</b> <sup>153</sup> , <b>6-methyldiosgenin</b> <sup>24</sup> , <b>yamogenin</b> <sup>429</sup>
<i>Borago officinalis</i>	Boraginaceae	Thesinine <sup>389</sup>
<i>Bulbine frutescens</i> *	Asphodelaceae	<b>Chrysophonol</b> <sup>109</sup> , <b>gaboroquinone A</b> <sup>178</sup> , <b>gaboroquinone B</b> <sup>179</sup> , <b>knipholone</b> <sup>254</sup> , <b>Sodium ent knipholone-6-O-sulfate</b> <sup>365</sup>
<i>Cajanus cajan</i> *	Fabaceae	<b>Alpha-Linolenic acid</b> <sup>29</sup> , <b>apigenin</b> <sup>55</sup> , <b>betulinic acid</b> <sup>85</sup> , <b>biochanin A</b> <sup>86</sup> , <b>cajaquinone</b> <sup>94</sup> , <b>genistein</b> <sup>188</sup> , <b>2-hydroxygenistein</b> <sup>13</sup> , <b>isorhamnetin</b> <sup>243</sup> , <b>longistylin A</b> <sup>270</sup> , <b>longistylin C</b> <sup>271</sup> , <b>pinostrobin</b> <sup>316</sup> , <b>quercetin</b> <sup>331</sup>
<i>Cannabis sativa</i>	Cannabaceae	<b>Tetrahydrocannabinol</b> <sup>387</sup>
<i>Cassine transvaalensis</i>	Celastraceae	<b>Elaeocyanidin</b> <sup>161</sup> , <b>ouratea proanthocyanidin A</b> <sup>305</sup>
<i>Catharanthus roseus</i> *	Apocynaceae	<b>Ajmalicine</b> <sup>37</sup> , <b>akuammine</b> <sup>39</sup> , <b>brassinolide</b> <sup>91</sup> , <b>leurosidine</b> <sup>264</sup> , <b>leurosine</b> <sup>265</sup> , <b>lochnerine</b> <sup>269</sup> , <b>lupeol</b> <sup>272</sup> , <b>petunidine</b> <sup>312</sup> , <b>reserpine</b> <sup>340</sup> , <b>serpentine</b> <sup>363</sup> , <b>tetrahydroalstonine</b> <sup>386</sup> , <b>ursolic acid</b> <sup>401</sup> , <b>vindoline</b> <sup>418</sup> , <b>yohimbine</b> <sup>430</sup>
<i>Centella asiatica</i>	Apiaceae	<b>Asiatic acid</b> <sup>62</sup> , <b>asiaticoside</b> <sup>63</sup> , <b>beta-sitosterol</b> <sup>70</sup> , <b>centelloside</b> <sup>102</sup> , <b>isoquercetin</b> <sup>240</sup> , <b>madecassic acid</b> <sup>278</sup>
<i>Chironia baccifera</i>	Gentianaceae	<b>Chironioside</b> <sup>104</sup>
<i>Cichorium intybus</i>	Asteraceae	<b>Lactucin</b> <sup>257</sup>
<i>Cissampelos capensis</i>	Menispermaceae	<b>Cissacapine</b> <sup>110</sup> , <b>cissampreine</b> <sup>111</sup> , <b>insularine</b> <sup>233</sup>
<i>Cnicus benedictus</i> *	Asteraceae	<b>Trachelogenin</b> <sup>296</sup>
<i>Combretum micranthum</i>	Combretaceae	<b>Catechin</b> <sup>100</sup> , <b>combretin A</b> <sup>117</sup> , <b>combretin B</b> <sup>118</sup> , <b>isovitexin</b> <sup>245</sup> , <b>vitexin</b> <sup>419</sup>



<i>Commiphora myrrha</i> *	Burseraceae	Furanoeudesma-1-3-diene <sup>177</sup>
<i>Cryptolepis sanguinolenta</i> *	Apocynaceae	Biscryptolepine <sup>88</sup> , cryptoheptine <sup>128</sup> , <b>cryptolepine</b> <sup>129</sup> , cryptomisine <sup>130</sup> , cryptoquindoline <sup>131</sup> , cryptospirolepine <sup>132</sup> , isocryptolepine <sup>235</sup> , neocryptolepine <sup>289</sup> , quindoline <sup>336</sup>
<i>Curtisia dentata</i>	Curtisiaceae	<b>Cornustannin-2</b> <sup>119</sup>
<i>Cyclopia intermedia</i>	Fabaceae	<b>Afromosin</b> <sup>34</sup> , calycosin <sup>95</sup> , <b>eriodictyol</b> <sup>168</sup> , flemmichapparin C <sup>172</sup> , <b>formononetin</b> <sup>173</sup> , fujikinetin <sup>176</sup> , <b>hesperitin</b> <sup>213</sup> , isosakuranetin <sup>244</sup> , medicagol <sup>280</sup> , <b>naringenin</b> <sup>286</sup> , pseudobaptigen <sup>26</sup> , sophoracoumestan B <sup>370</sup>
<i>Duranta erecta</i>	Verbenaceae	Durantosides I <sup>157</sup> , II <sup>158</sup> , III <sup>159</sup>
<i>Echium vulgare</i>	Boraginaceae	Lithospermic acid <sup>268</sup>
<i>Euclea undulata</i>	Ebenaceae	Diospyrin <sup>156</sup>
<i>Euphorbia hirta</i> *	Euphorbiaceae	<b>Alpha-amyrin</b> <sup>46</sup> , <b>beta-amyrin</b> <sup>82</sup> , <b>beta-sitosterol</b> <sup>70</sup> , <b>campesterol</b> <sup>96</sup> , <b>chlorogenic acid</b> <sup>106</sup> , <b>friedelin</b> <sup>174</sup> , ingenol <sup>231</sup> , ingenol triacetate <sup>232</sup> , <b>kaempferol</b> <sup>247</sup> , <b>leucocyanidin</b> <sup>263</sup> , <b>quercetin</b> <sup>331</sup> , <b>quercitrin</b> <sup>335</sup> , <b>taraxerol</b> <sup>383</sup> , tinyatoxin <sup>393</sup>
<i>Garcinia kola</i> *	Clusiaceae	Garcifuran B <sup>182</sup> , <b>garcinia biflavonoid 1</b> <sup>183</sup> , <b>garcinia biflavonoid 2</b> <sup>184</sup> , <b>kolaflavanone</b> <sup>255</sup> , kolanone <sup>256</sup>
<i>Glycyrrhiza glabra</i>	Fabaceae	<b>Glycyrrhizin</b> <sup>191</sup> , liquiritin <sup>267</sup>
<i>Gunnera perperna</i>	Gunneraceae	Celastrin <sup>101</sup>
<i>Harpagophytum procumbens</i>	Pedaliaceae	<b>Beta-sitosterol</b> <sup>70</sup> , <b>harpagoside</b> <sup>200</sup> , <b>stigmasterol</b> <sup>375</sup>
<i>Harpephyllum caffrum</i>	Anacardiaceae	<b>Kaempferol</b> <sup>247</sup>
<i>Harungana madagascariensis</i>	Hypericaceae	<b>Betulinic acid</b> <sup>85</sup> , <b>chrysophonol</b> <sup>109</sup> , <b>epicatechin</b> <sup>164</sup> , <b>friedelin</b> <sup>174</sup> , <b>harunganin</b> <sup>201</sup> , <b>harunganol B</b> <sup>202</sup> , harunmadagascarin A <sup>203</sup> , harunmadagascarin B <sup>204</sup> , hypericin <sup>222</sup> , <b>quercetin</b> <sup>331</sup>
<i>Hedera helix</i>	Araliaceae	<b>Hederagenin</b> <sup>208</sup>
<i>Helichrysum species</i>	Asteraceae	Alpha-humulene <sup>28</sup> , <b>helichrysetin</b> <sup>209</sup>
<i>Hibiscus sabdariffa</i> *	Malvaceae	<b>Delphinidin</b> <sup>143</sup> , gossypetin <sup>196</sup> , hibiscetin <sup>214</sup> , hibiscin <sup>215</sup> , hibiscitrin <sup>216</sup> , <b>palmitic acid</b> <sup>309</sup>
<i>Hoodia gordonii</i> *	Apocynaceae	<b>P57 compound</b> <sup>308</sup>
<i>Hypericum perforatum</i>	Hypericaceae	<b>Hyperforin</b> <sup>221</sup> , hypericin <sup>222</sup> , <b>hyperin</b> <sup>223</sup> , <b>rutin</b> <sup>352</sup>
<i>Hypoxis hemerocallidea</i>	Hypoxidaceae	<b>Beta-sitosterol</b> <sup>70</sup> , hypoxoside <sup>224</sup> , rooperol <sup>346</sup>
<i>Ipomoea pes-caprae</i> ssp. <i>Brasiliensis</i>	Convolvulaceae	<b>Alpha-amyrin</b> <sup>46</sup> , <b>alpha-amyrin acetate</b> <sup>47</sup> , <b>beta-amyrin</b> <sup>82</sup> , beta-amyrin acetate <sup>83</sup> , beta-glochidone <sup>84</sup> , <b>isoquercetin</b> <sup>240</sup>
<i>Jatropha curcas</i>	Euphorbiaceae	Curcusion A <sup>134</sup> , curcusion C <sup>135</sup>
<i>Kigelia africana</i>	Bignoniaceae	<b>Beta-sitosterol</b> <sup>70</sup> , 2-(1-hydroxyethyl)naphtho[2,3-beta]furan-4,9-dione <sup>9</sup> , isokigelinol <sup>237</sup> , isopinnatal <sup>239</sup> , kigelinol <sup>252</sup> , kigelinone <sup>253</sup> , <b>lapachol</b> <sup>261</sup> , <b>luteolin</b> <sup>273</sup> , <b>quercetin</b> <sup>331</sup> , <b>stigmasterol</b> <sup>375</sup> , <b>verminoside</b> <sup>408</sup>
<i>Lantana camara</i>	Verbenaceae	Lantadene A <sup>259</sup> , lantadene B <sup>260</sup>
<i>Leonotis leonurus</i>	Lamiaceae	Premarrubin <sup>320</sup>

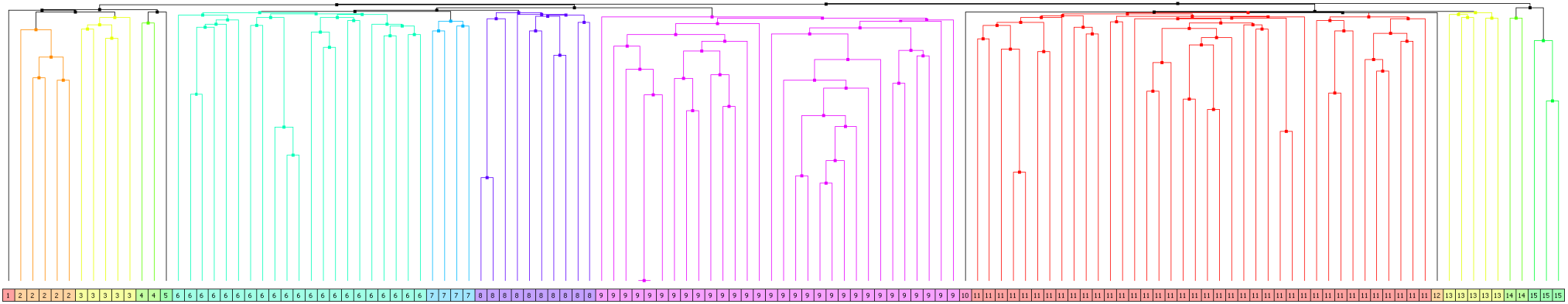
<i>Ligustrum lucidum</i>	Oleaceae	Ligstroside <sup>266</sup> , <b>oleanolic acid</b> <sup>299</sup> , <b>oleuropein</b> <sup>301</sup> , <b>ursolic acid</b> <sup>401</sup>
<i>Melia azedarach</i>	Meliaceae	Melianol <sup>281</sup> , meliatoxin B1 <sup>283</sup> , meliatoxin B2 <sup>284</sup>
<i>Moringa oleifera</i>	Moringaceae	<b>Chlorogenic acid</b> <sup>106</sup> , <b>isoquercetin</b> <sup>240</sup> , <b>kaempferol</b> <sup>247</sup> , <b>kaempferol-3-glucoside</b> <sup>248</sup> , kaempferol-3-o-(6'-malonyl-glucoside) <sup>249</sup> , pterygospermin <sup>327</sup> , <b>quercetin</b> <sup>331</sup> , quercetin-3-o-(6'-malonyl-glucoside) <sup>334</sup>
<i>Nauclea latifolia</i> *	Rutaceae	Angustine <sup>52</sup> , angustoline <sup>53</sup> , nauclefidine <sup>287</sup> , nauclefine <sup>288</sup> , strictosamine <sup>376</sup> , strictosidine <sup>377</sup>
<i>Nerium oleander</i>	Apocynaceae	Oleandrin <sup>297</sup>
<i>Olea europaea</i> *	Oleaceae	<b>8-Hydroxypinoresinol</b> <sup>27</sup> , oleacein <sup>296</sup> , <b>oleanolic acid</b> <sup>299</sup> , <b>oleuropein</b> <sup>301</sup>
<i>Prunus africana</i>	Rosaceae	<b>Amygdalin</b> <sup>51</sup> , <b>beta-sitosterol</b> <sup>70</sup> , <b>campesterol</b> <sup>96</sup> , <b>catechin</b> <sup>100</sup> , <b>corosolic acid</b> <sup>120</sup> , <b>daucosterol</b> <sup>140</sup> , <b>epicatechin</b> <sup>164</sup> , <b>3-epicorosolic acid</b> <sup>71</sup> , <b>epimaslinic acid</b> <sup>166</sup> , esculentic acid <sup>11</sup> , <b>friedelin</b> <sup>174</sup> , <b>maslinic acid</b> <sup>279</sup> , <b>oleanolic acid</b> <sup>299</sup> , oleanolic-3-acetate <sup>300</sup> , <b>stigmast-4-en-3-one</b> <sup>374</sup> , <b>ursolic acid</b> <sup>401</sup>
<i>Prunus laurocerasus</i>	Rosaceae	<b>Amygdalin</b> <sup>51</sup>
<i>Psidium guajava</i> *	Myrtaceae	Amritoside <sup>50</sup> , guajaverin <sup>198</sup> , <b>quercetin</b> <sup>331</sup>
<i>Punica granatum</i> *	Lythraceae	<b>Punicalagin</b> <sup>328</sup> , <b>punicalin</b> <sup>329</sup>
<i>Rauvolfia caffra</i>	Apocynaceae	Ajmalicine <sup>37</sup> , ajmaline <sup>38</sup> , reserpine <sup>340</sup>
<i>Rauvolfia vomitoria</i>	Apocynaceae	Ajmaline <sup>38</sup> , carapanaubine <sup>98</sup> , desacetyl-desformoakuammilin <sup>141</sup> , geissoschizine <sup>185</sup> , geissoschizol <sup>186</sup> , isoreserpiline <sup>241</sup> , isoreserpine <sup>242</sup> , <b>kaempferol</b> <sup>247</sup> , norajmaline <sup>291</sup> , picrinine <sup>313</sup> , <b>quercetin</b> <sup>331</sup> , rauvoxin <sup>337</sup> , rauvoxinin <sup>338</sup> , reserpic acid <sup>339</sup> , reserpine <sup>340</sup> , serpenticine <sup>362</sup> , serpentine <sup>363</sup> , <b>ursolic acid</b> <sup>401</sup> , vellosimine <sup>406</sup>
<i>Ravenala madagascariensis</i> *	Strelitziaceae	<b>Alpha-spinasterol</b> <sup>48</sup> , <b>beta-sitosterol</b> <sup>70</sup> , cycloartenol <sup>138</sup> , delta-7-avenasterol <sup>144</sup> , <b>stigmasterol</b> <sup>375</sup>
<i>Rhoicissus tridentata</i>	Vitaceae	<b>Cyanidin</b> <sup>136</sup> , <b>delphinidin</b> <sup>143</sup>
<i>Ruta graveolens</i>	Rutaceae	Rutaretin <sup>351</sup> , <b>rutin</b> <sup>352</sup>
<i>Sclerocarya birrea</i> *	Anacardiaceae	<b>Catechin</b> <sup>100</sup> , <b>procyanidin C1</b> <sup>322</sup>
<i>Securidaca longipedunculata</i>	Polygalaceae	Presenegenin <sup>321</sup>
<i>Solanum incanum</i>	Solanaceae	Solanine <sup>366</sup> , solasodine <sup>368</sup> , solasonine <sup>369</sup>
<i>Solanum nigrum</i>	Solanaceae	Solasonine <sup>369</sup>
<i>Strophanthus gratus</i>	Apocynaceae	Acolongifloroside K <sup>31</sup> , <b>8-hydroxypinoresinol</b> <sup>27</sup> , ouabain <sup>304</sup> , <b>pinoresinol</b> <sup>315</sup> , strogoside <sup>378</sup> , strophathidin <sup>379</sup>
<i>Strychnos henningsii</i>	Loganiaceae	Henningsiine <sup>212</sup> , strychnine <sup>380</sup>
<i>Styphnolobium japonicum</i>	Fabaceae	<b>Sophoricoside</b> <sup>371</sup>
<i>Syzygium cordatum</i>	Myrtaceae	<b>Arjunolic acid</b> , <b>beta-sitosterol</b> <sup>70</sup> , <b>delphinidin</b> <sup>143</sup> , epifriedelinol <sup>165</sup> , <b>friedelin</b> <sup>174</sup> , <b>oleanolic acid</b> <sup>299</sup>
<i>Tarchonanthus camphoratus</i>	Asteraceae	Pinocebrin <sup>314</sup>
<i>Terminalia sericea</i> *	Combretaceae	Anolignan B <sup>54</sup> , <b>arjunglucoside</b> <sup>57</sup> , <b>resveratrol</b> <sup>341</sup> , resveratrol-3-o-b-rutinoside <sup>342</sup> , sericic acid <sup>360</sup> , sericoside <sup>361</sup> , terminoic acid <sup>385</sup>

<i>Toddalia asiatica</i>	Rutaceae	Arnottianamide <sup>59</sup> , avicine <sup>68</sup> , benzo[c]phenanthridine <sup>80</sup> , <b>chelerythrine</b> <sup>103</sup> , chelerythrine-psi-cyanide <sup>105</sup> , des-N-methylchelerythrine <sup>147</sup> , N-methylflindersine <sup>290</sup> , oxyavicine <sup>306</sup> , oxychelerythrine <sup>307</sup> , toddalasin <sup>394</sup> , toddasin <sup>395</sup>
<i>Tribulus terrestris</i>	Zygophyllaceae	<b>Gitogenin</b> <sup>190</sup> , harman <sup>199</sup>
<i>Trichilia emetica</i>	Meliaceae	<b>Chlorogenic acid</b> <sup>106</sup> , rohituka 3 <sup>345</sup> , trichilin A <sup>392</sup>
<i>Vernonia amygdalina</i> *	Asteraceae	<b>Chlorogenic acid</b> <sup>106</sup> , <b>1,5-dicaffeoylquinic acid</b> <sup>2</sup> , <b>luteolin</b> <sup>273</sup> , luteolin-4-rutinoside <sup>274</sup> , <b>luteolin-7-glucoside</b> <sup>275</sup> , <b>luteolin-7-rutinoside</b> <sup>276</sup> , vernolide <sup>409</sup> , vernomygdin, <sup>410</sup> vernoniosides A1 <sup>411</sup> , A3 <sup>412</sup> , B1 <sup>413</sup> , B2 <sup>414</sup> , B3 <sup>415</sup>
<i>Vernonia colorata</i> *	Asteraceae	Hydroxyvernolide <sup>219</sup> , vernolide <sup>409</sup>
<i>Withania somnifera</i>	Solanaceae	<b>Withaferin A</b> <sup>425</sup> , withasomnine <sup>426</sup>
<i>Xanthium strumarium</i>	Asteraceae	Xanthinin <sup>427</sup>
<i>Xylopia aethiopica</i>	Annonaceae	Bisabolene <sup>87</sup> , kauran-16- $\alpha$ -ol <sup>251</sup> , 15-oxo-kaurenoic acid <sup>6</sup> , xylopic acid <sup>428</sup>
<i>Ziziphus mucronata</i>	Rhamnaceae	Mucronine D <sup>285</sup> , sanjoinine A <sup>355</sup>

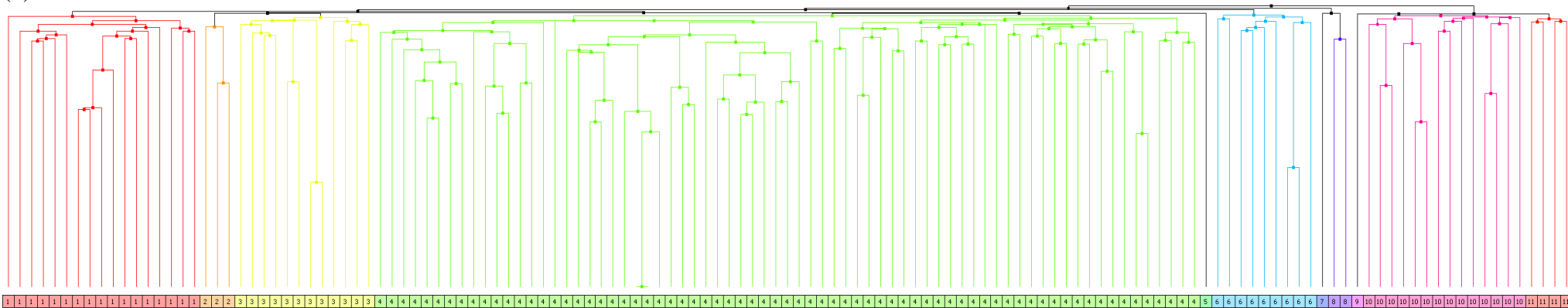
#### **Plants with traditional use but lack of scientific evidence**

<i>Argemone ochroleuca</i>	Papaveraceae	<b>Berberine</b> <sup>81</sup> , <b>protopine</b> <sup>325</sup> , <b>sanguinarine</b> <sup>354</sup>
<i>Bulbine natalensis</i> *	Asphodelaceae	Knipholone <sup>254</sup>
<i>Elytropappus rhinocerotis</i>	Asteraceae	Rhinocerotinoic acid <sup>344</sup>
<i>Fumaria officinalis</i>	Papaveraceae	<b>Sanguinarine</b> <sup>354</sup>
<i>Gelsemium sempervirens</i>	Gelsemiaceae	Gelsemicine <sup>187</sup>
<i>Lannea acida</i>	Anacardiaceae	Tetrahydroxyflavanone <sup>388</sup>
<i>Mondia whitei</i>	Apocynaceae	5-Chloropropacin <sup>23</sup> , 7-hydroxy-4,6-dimethoxypropacin <sup>25</sup> , propacin <sup>323</sup>
<i>Rumex lanceolatus</i>	Polygalaceae	Chrysophonein <sup>108</sup> , <b>chrysophonol</b> <sup>109</sup>
<i>Solanum tuberosum</i>	Solanaceae	Solanine <sup>366</sup>
<i>Strychnos spinosa</i>	Loganiaceae	10-Hydroxyakagerine <sup>3</sup> , strychnine <sup>380</sup>
<i>Voacanga africana</i>	Apocynaceae	Ibogaine <sup>225</sup> , ibogamine <sup>226</sup> , iboxygaine <sup>227</sup> , vinburnine <sup>416</sup> , voacamine <sup>420</sup> , voacangine <sup>421</sup> , voacordine <sup>422</sup> , voaphylline <sup>423</sup> , vobtusine <sup>424</sup>
<i>Xysmalobium undulatum</i>	Apocynaceae	Allouzarin <sup>40</sup> , alloxysmalorin <sup>41</sup> , uzarigenin <sup>403</sup> , uzarin <sup>404</sup>

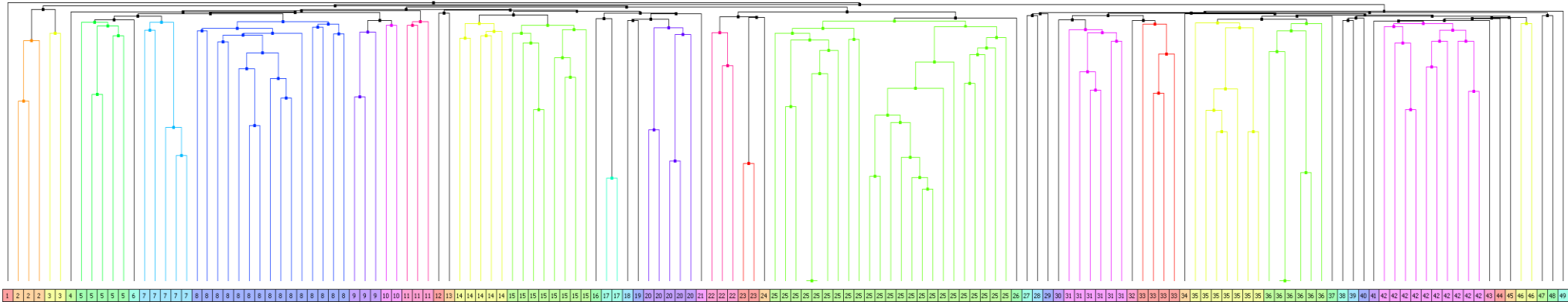
\* These plants were noted in the source books African Herbal Pharmacopoeia (Brendler et al., 2010) and Medicinal Plants of South Africa (Van Wyk, 1997) as having anti-diabetic properties. The numbers 1-430 serves as the identification of each compound in Figure 1. All compounds in bold are compounds identified with some previous literature on their potential anti-diabetic activity.



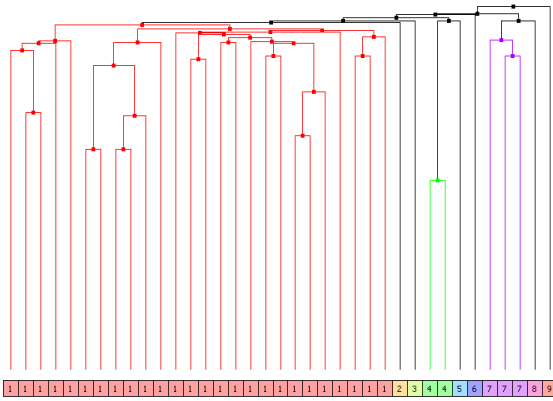
(a)



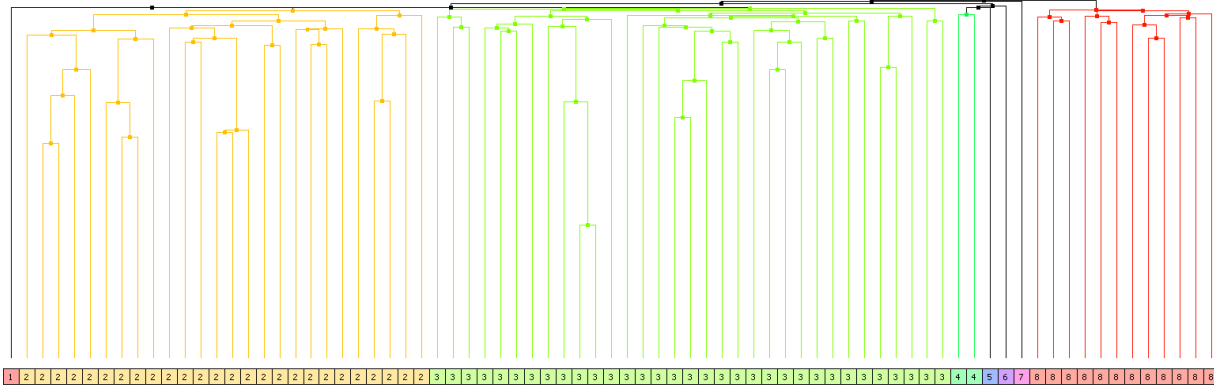
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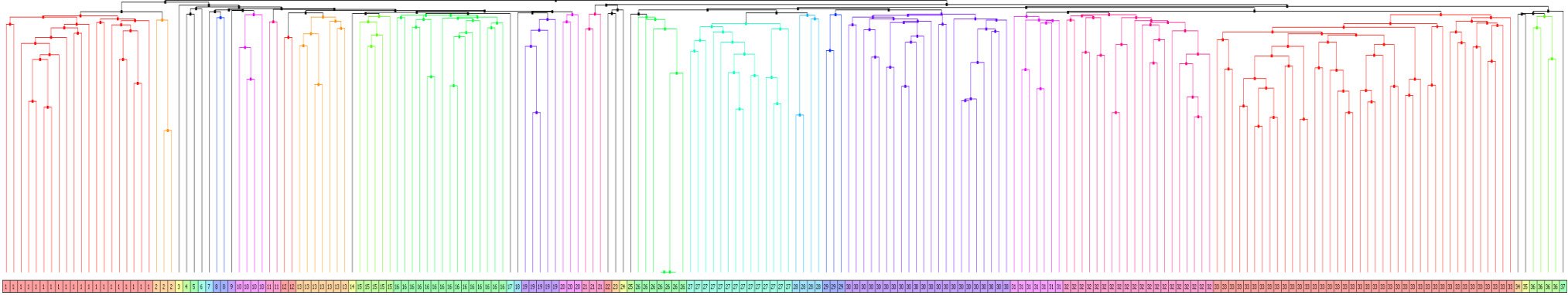
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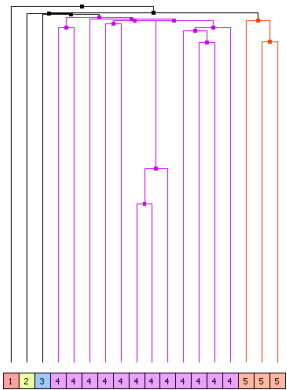
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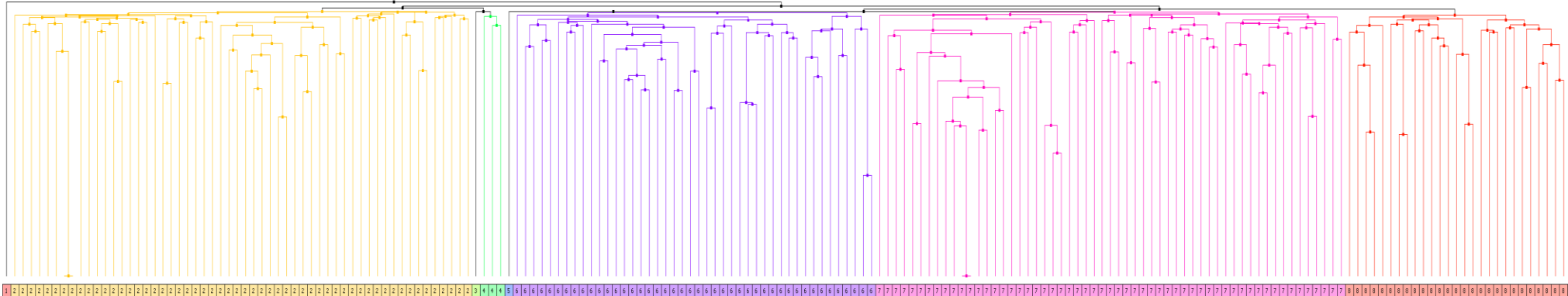
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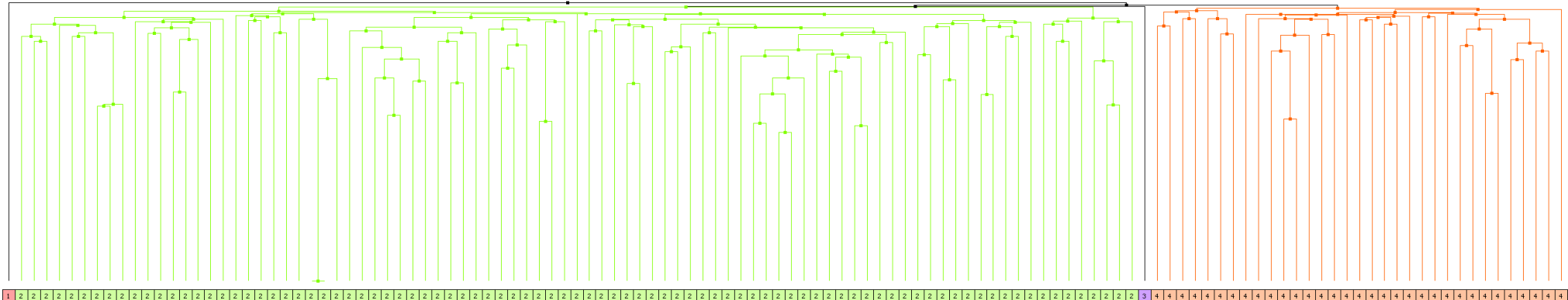
(f)



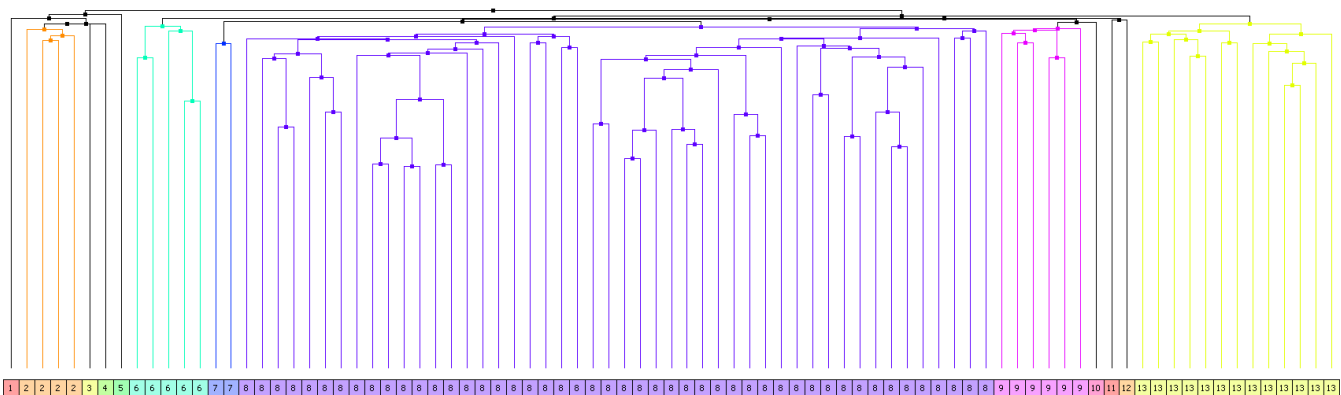
**(g)**



**(h)**



**(i)**



(j)

**Figure S2.** Dendrograms of hierarchical clustering analysis for (a) AKR1B1; (b) AMY2A; (c) DPP4; (d) FFAR1; (e) GCK; (f) HSD11B1; (g) MGAM; (h) PPARD; (i) PPARG; (j) RBP4. No clustering of compounds was found for six of the protein target-compound groups namely INSR, NR5A2, PDK2, PPARA, PTPN9, PYGL and RXRA.