

**Supplementary Table 1 Using the TCSMP database, 118 candidate compounds were selected**

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<b>Mol ID</b>	<b>Molecule Name</b>
MOL0028	
79	Diop
MOL0004	
49	Stigmasterol
MOL0003	
58	beta-sitosterol
MOL0036	
48	Inermin
MOL0004	
22	kaempferol
MOL0044	
92	Chrysanthemaxanthin
MOL0053	
08	Aposiopalamine
MOL0053	
14	Celabenzine
MOL0053	
17	Deoxyharringtonine
MOL0053	
18	Dianthramine
MOL0053	
20	arachidonate

MOL0053  
21 Frutinone A  
MOL0053  
44 ginsenoside rh2  
MOL0053  
48 Ginsenoside-Rh4\_qt  
MOL0053  
56 Girinimbin  
MOL0053  
57 Gomisin B  
MOL0053  
60 malkangunin  
MOL0053  
76 Panaxadiol  
MOL0053  
84 suchilactone  
MOL0053  
99 alexandrin\_qt  
MOL0054  
01 ginsenoside Rg5\_qt  
MOL0007  
87 Fumarine  
MOL0003  
59 sitosterol

MOL0000  
20 12-senecioid-2E,8E,10E-atractylentriol  
MOL0000  
21 14-acetyl-12-senecioid-2E,8E,10E-atractylentriol  
MOL0000  
22 14-acetyl-12-senecioid-2E,8Z,10E-atractylentriol  
MOL0000  
28  $\alpha$ -Amyrin  
MOL0000 (3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2R,5S)-5-propan-2-yl]octan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol  
33  
MOL0000  
49 3 $\beta$ -acetoxyatractylone  
MOL0000  
72 8 $\beta$ -ethoxy atractylenolide III  
MOL0014  
84 Inermine  
MOL0017  
92 DFV  
MOL0023  
11 Glycyrol  
MOL0002  
39 Jaranol  
MOL0025  
65 Medicarpin

MOL0003  
54 isorhamnetin  
MOL0036  
56 Lupiwighteone  
MOL0038  
96 7-Methoxy-2-methyl isoflavone  
MOL0003  
92 formononetin  
MOL0004  
17 Calycosin  
MOL0043  
28 naringenin  
MOL0048  
05 (2S)-2-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]-8,8-dimethyl-2,3-dihydropyrano[2,3-f]chromen-4-one  
MOL0048  
06 euchrenone  
MOL0048  
08 glyasperin B  
MOL0048  
10 glyasperin F  
MOL0048  
11 Glyasperin C  
MOL0048  
14 Isotrifoliol

MOL0048  
15 (E)-1-(2,4-dihydroxyphenyl)-3-(2,2-dimethylchromen-6-yl)prop-2-en-1-one  
MOL0048  
20 kanzonols W  
MOL0048  
24 (2S)-6-(2,4-dihydroxyphenyl)-2-(2-hydroxypropan-2-yl)-4-methoxy-2,3-dihydrofuro[3,2-g]chromen-7-one  
MOL0048  
27 Semilicoisoflavone B  
MOL0048  
28 Glepidotin A  
MOL0048  
33 Phaseolinisoflavan  
MOL0048  
35 Glypallichalcone  
MOL0048  
38 8-(6-hydroxy-2-benzofuranyl)-2,2-dimethyl-5-chromenol  
MOL0048  
41 Licochalcone B  
MOL0048  
48 licochalcone G  
MOL0048  
49 3-(2,4-dihydroxyphenyl)-8-(1,1-dimethylprop-2-enyl)-7-hydroxy-5-methoxy-coumarin  
MOL0048  
55 Licoricone

MOL0048  
56 Gancaonin A  
MOL0048  
57 Gancaonin B  
MOL0048  
60 licorice glycoside E  
MOL0048  
63 3-(3,4-dihydroxyphenyl)-5,7-dihydroxy-8-(3-methylbut-2-enyl)chromone  
MOL0048  
64 5,7-dihydroxy-3-(4-methoxyphenyl)-8-(3-methylbut-2-enyl)chromone  
MOL0048  
66 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-(3-methylbut-2-enyl)chromone  
MOL0048  
79 Glycyrin  
MOL0048  
82 Licocoumarone  
MOL0048  
83 Licoisoflavone  
MOL0048  
84 Licoisoflavone B  
MOL0048  
85 licoisoflavanone  
MOL0048  
91 shinpterocarpin

MOL0048  
98 (E)-3-[3,4-dihydroxy-5-(3-methylbut-2-enyl)phenyl]-1-(2,4-dihydroxyphenyl)prop-2-en-1-one  
MOL0049  
03 liquiritin  
MOL0049  
04 licopyranocoumarin  
MOL0049  
05 3,22-Dihydroxy-11-oxo-delta(12)-oleanene-27-alpha-methoxycarbonyl-29-oic acid  
MOL0049  
07 Glyzaglabrin  
MOL0049  
08 Glabridin  
MOL0049  
10 Glabranin  
MOL0049  
11 Glabrene  
MOL0049  
12 Glabrone  
MOL0049  
13 1,3-dihydroxy-9-methoxy-6-benzofurano[3,2-c]chromenone  
MOL0049  
14 1,3-dihydroxy-8,9-dimethoxy-6-benzofurano[3,2-c]chromenone  
MOL0049  
15 Eurycarpin A

MOL0049  
17 glycyroside  
MOL0049  
24 (-)-Medicocarpin  
MOL0049  
35 Sigmoidin-B  
MOL0049  
41 (2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one  
MOL0049  
45 (2S)-7-hydroxy-2-(4-hydroxyphenyl)-8-(3-methylbut-2-enyl)chroman-4-one  
MOL0049  
48 Isoglycyrol  
MOL0049  
49 Isolicoflavonol  
MOL0049  
57 HMO  
MOL0049  
59 1-Methoxyphaseollidin  
MOL0049  
61 Quercetin der.  
MOL0049  
66 3'-Hydroxy-4'-O-Methylglabridin  
MOL0004  
97 licochalcone a



MOL0049

74 3'-Methoxyglabridin

MOL0049

78 2-[(3R)-8,8-dimethyl-3,4-dihydro-2H-pyrano[6,5-f]chromen-3-yl]-5-methoxyphenol

MOL0049

80 Inflacoumarin A

MOL0049

85 icos-5-enoic acid

MOL0049

88 Kanzonol F

MOL0049

89 6-prenylated eriodictyol

MOL0049

90 7,2',4'-trihydroxy-5-methoxy-3-arylcoumarin

MOL0049

91 7-Acetoxy-2-methylisoflavone

MOL0049

93 8-prenylated eriodictyol

MOL0049

96 gadelaidic acid

MOL0005

00 Vestitol

MOL0050

00 Gancaonin G

MOL0050  
01 Gancaonin H  
MOL0050  
03 Licoagrocarpin  
MOL0050  
07 Glyasperins M  
MOL0050  
08 Glycyrrhiza flavonol A  
MOL0050  
12 Licoagroisoflavone  
MOL0050  
13 18 $\alpha$ -hydroxyglycyrrhetic acid  
MOL0050  
16 Odoratin  
MOL0050  
17 Phaseol  
MOL0050  
18 Xambioona  
MOL0050  
20 dehydroglyasperins C  
MOL0000  
98 quercetin

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