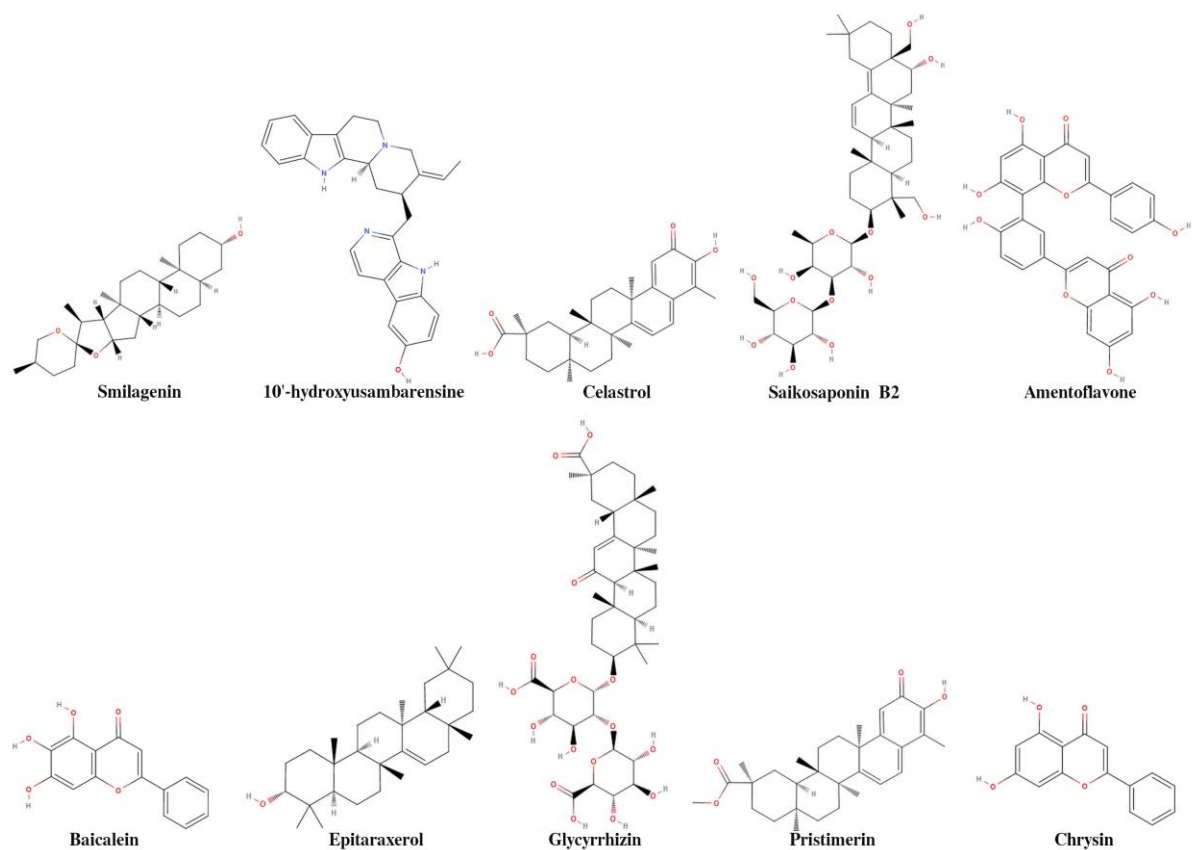


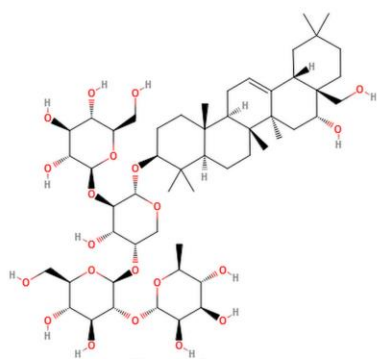
Partitioning pattern of natural products based on molecular properties descriptors possessing a drug-likeness property - Chemometric approach

Supplementary Information

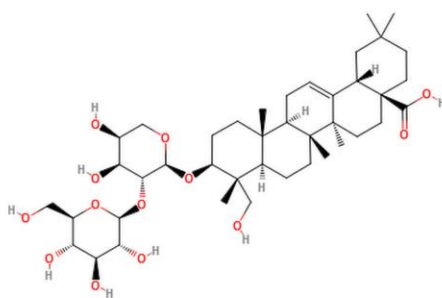
Figure S1

Tables S1 and S2

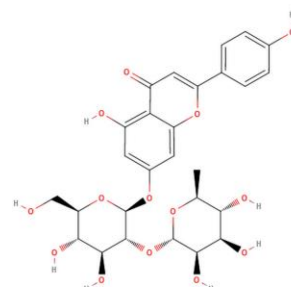




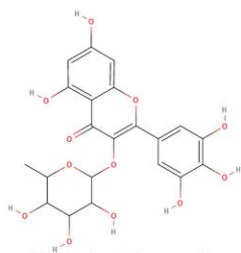
Ardisia saponin



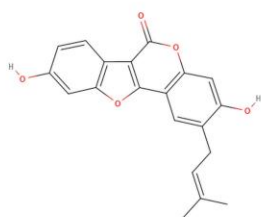
Akebia saponin c



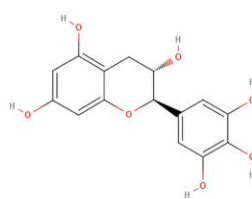
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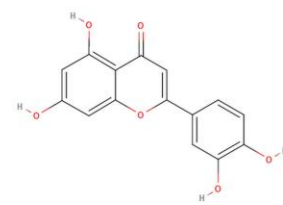
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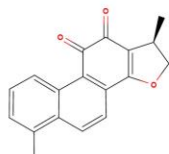
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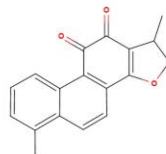
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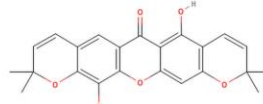
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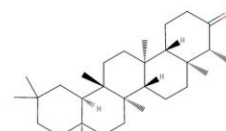
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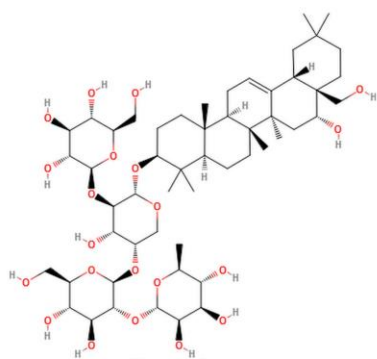
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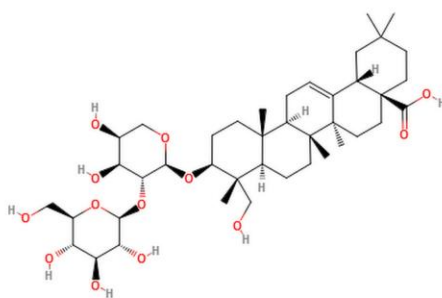
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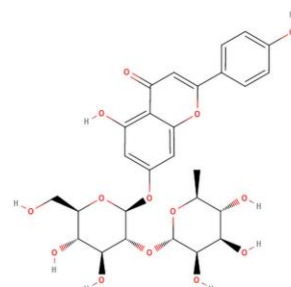
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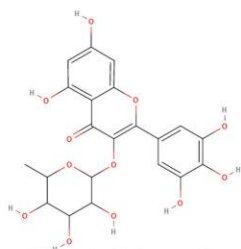
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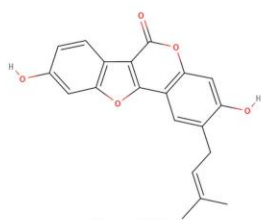
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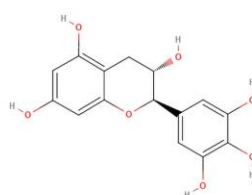
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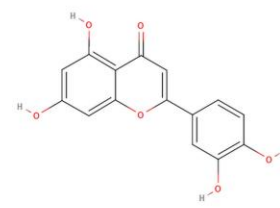
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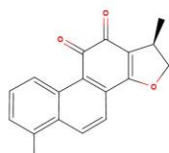
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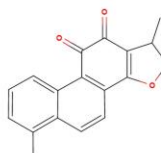
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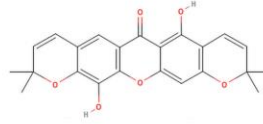
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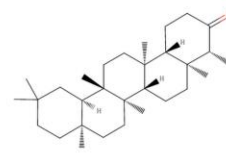
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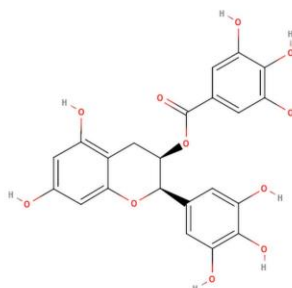
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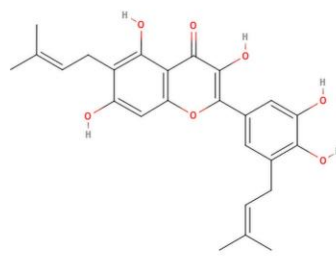
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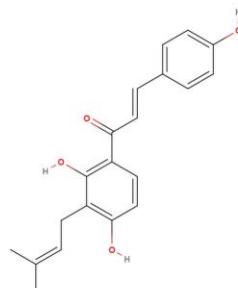
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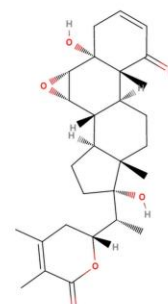
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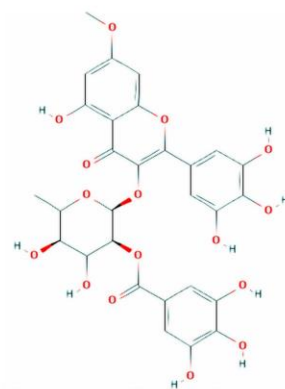
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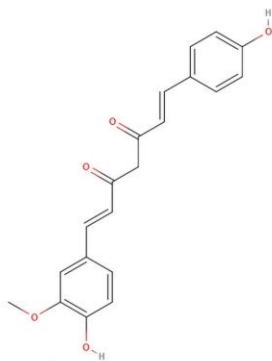
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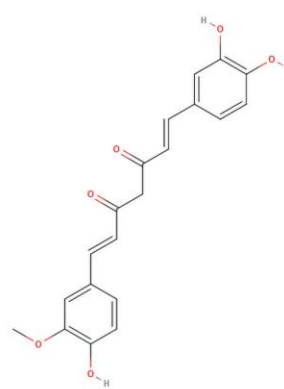
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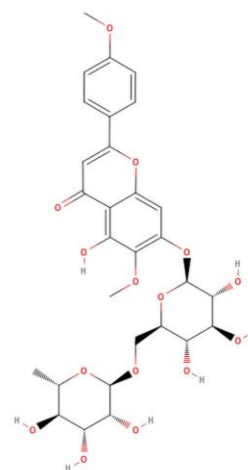
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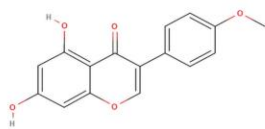
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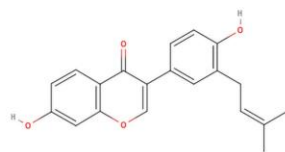
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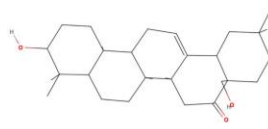
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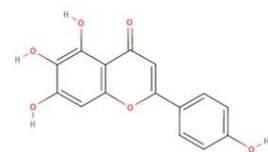
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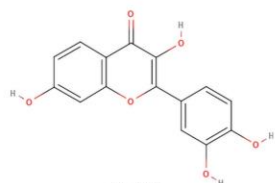
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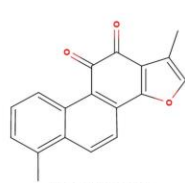
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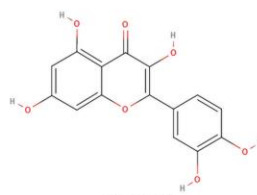
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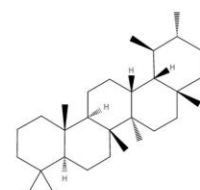
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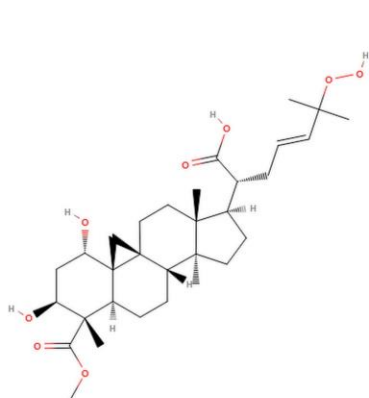
Tanshinone i



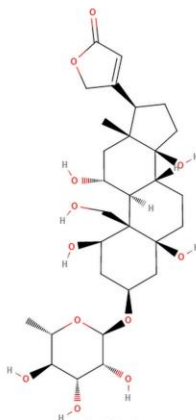
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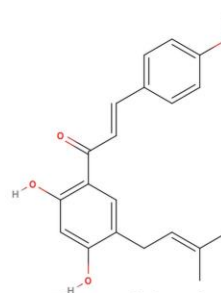
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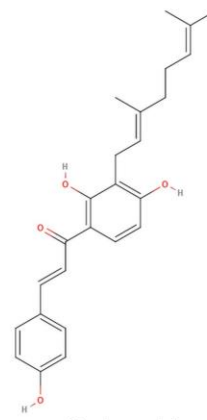
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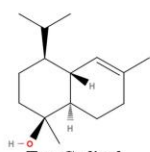
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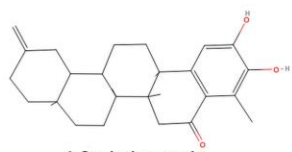
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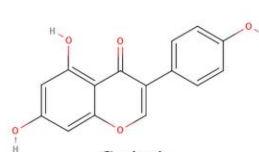
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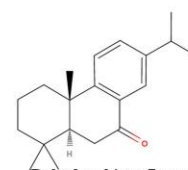
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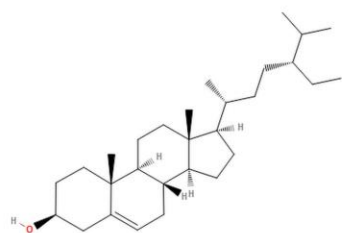
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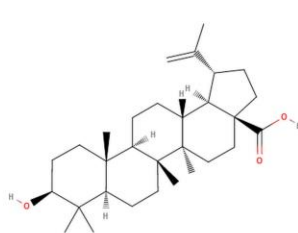
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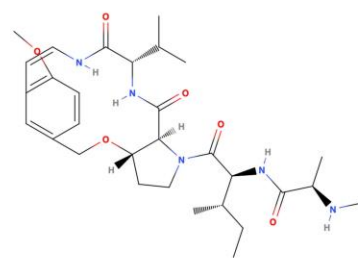
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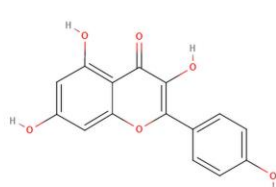
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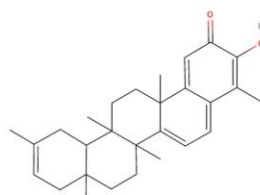
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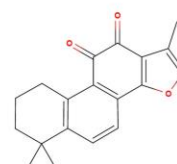
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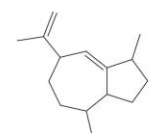
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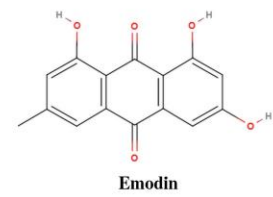
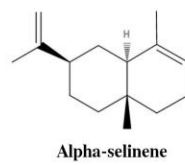
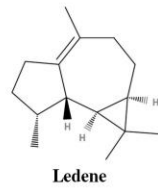
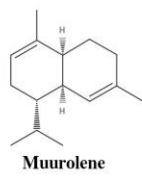
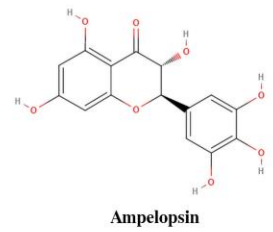
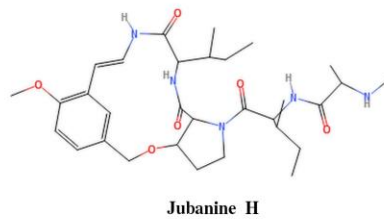
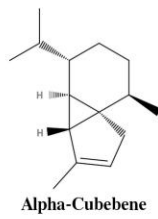
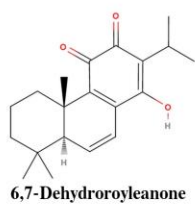
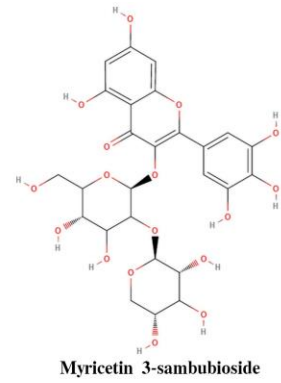
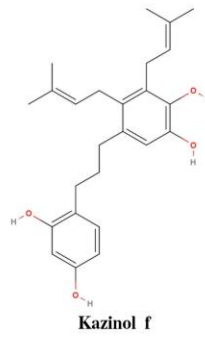
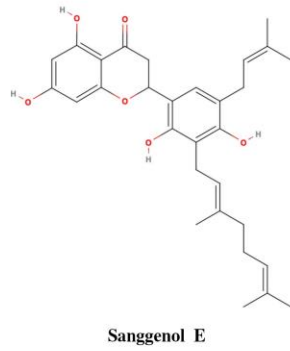
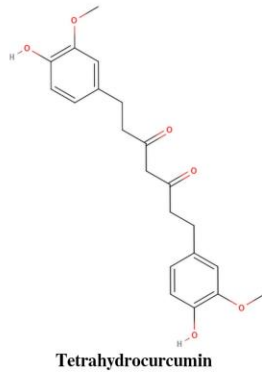
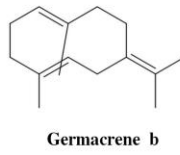
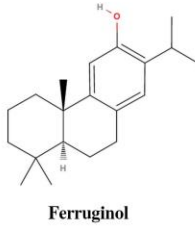
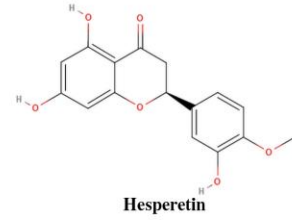
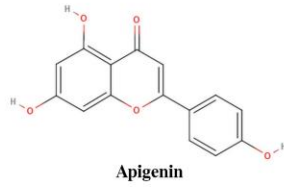
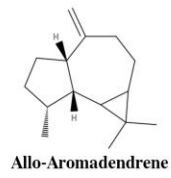
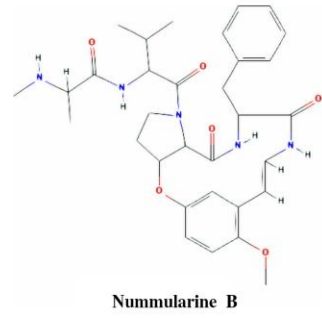
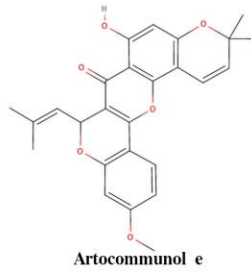
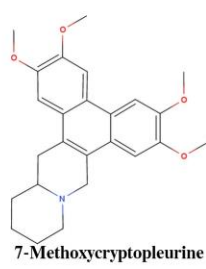
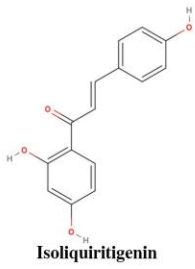
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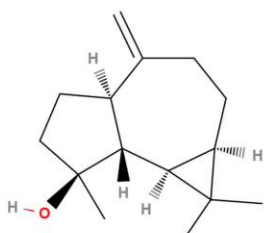


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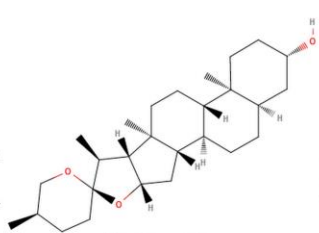


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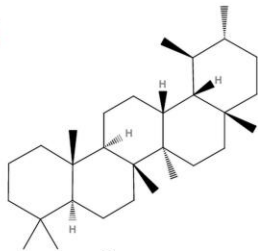




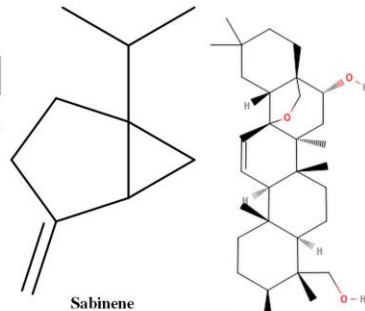
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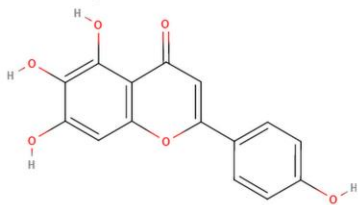
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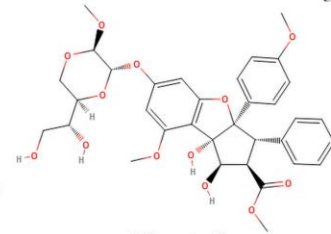
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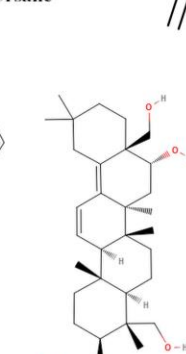
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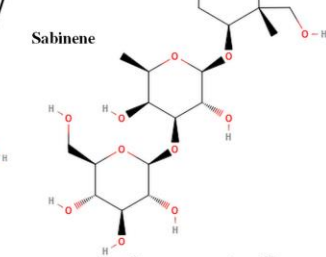
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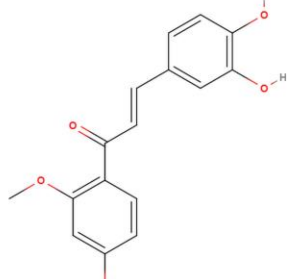
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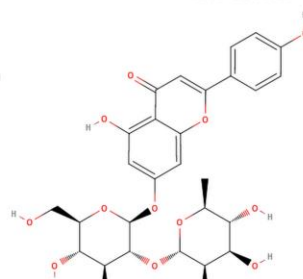
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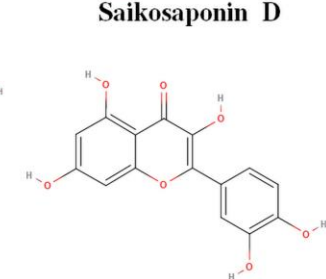
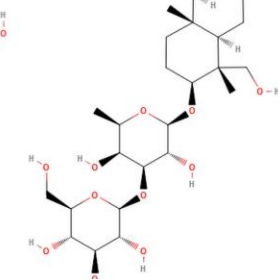
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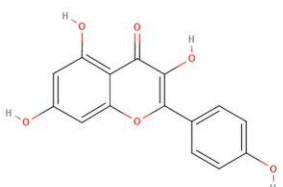
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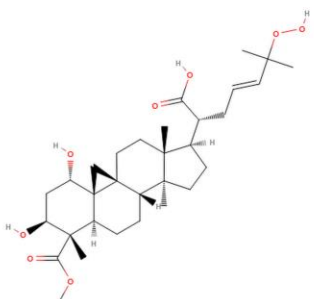
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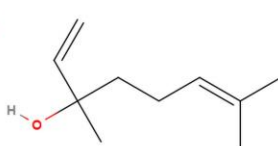
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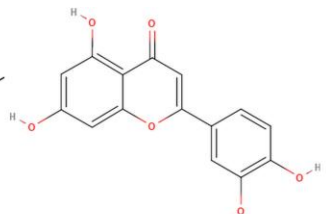
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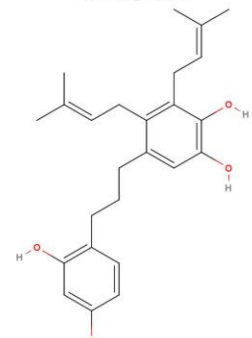
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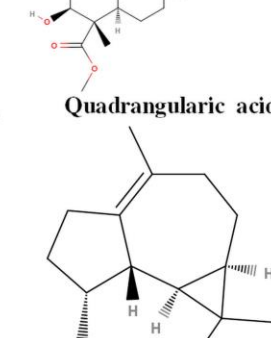
Linalool



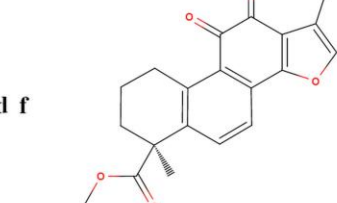
Luteolin



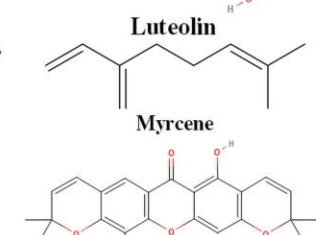
Kazinol F



Ledene



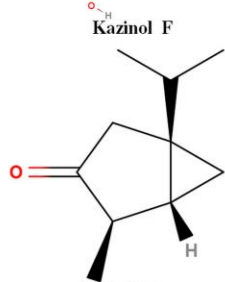
Methyl tanshinonate



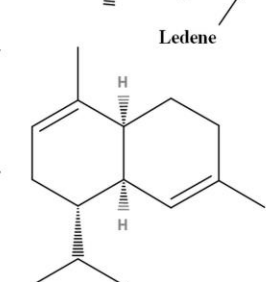
Myrcene



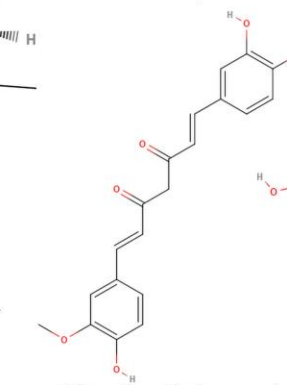
Pyranojacareubin



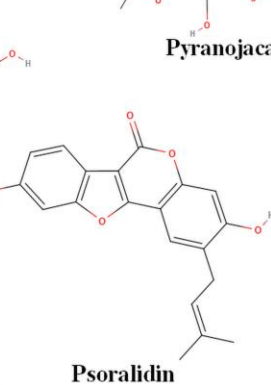
L-Thujone



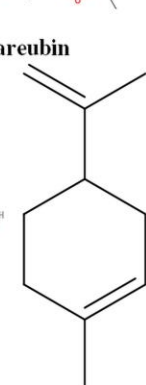
Muurolene



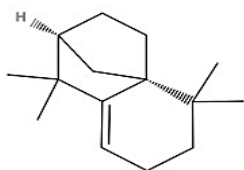
Monodemethylcurcumin



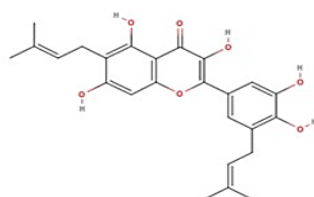
Psoralidin



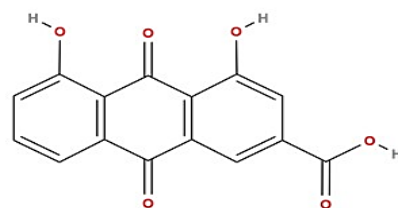
Limonene



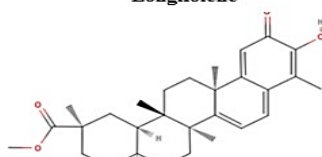
Longifolene



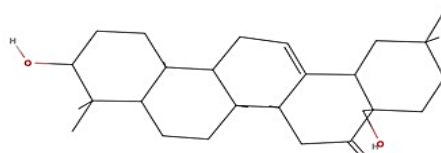
Pavyriflavonol A



Rhein



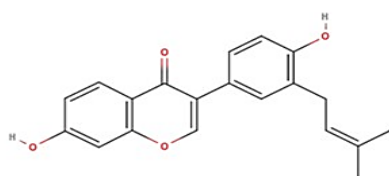
Pristimerin



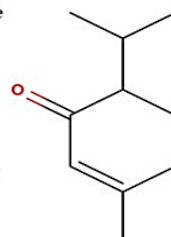
Schimperinone



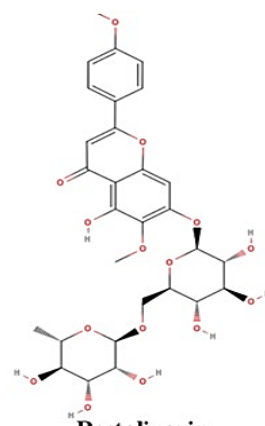
Pinocarvone



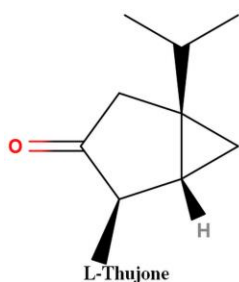
Neobavaisoflavone



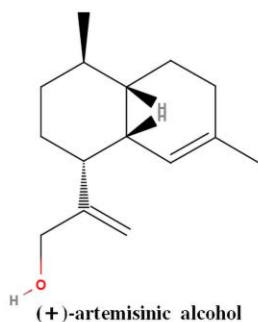
Piperitone



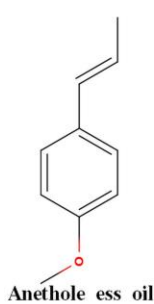
Pectolinarin



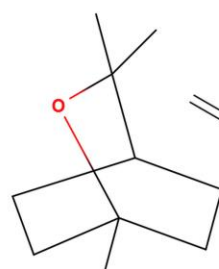
L-Thujone



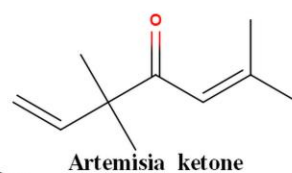
(+)-artemisinic alcohol



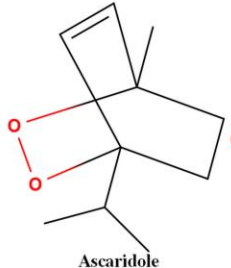
Anethole ess oil



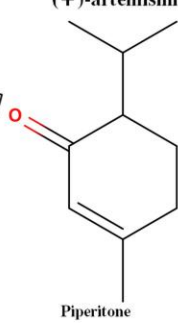
1,8-Cineole



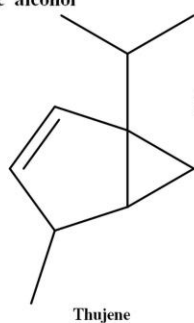
Artemisia ketone



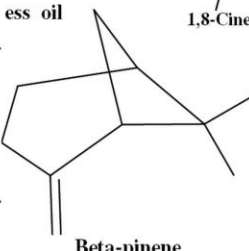
Ascaridole



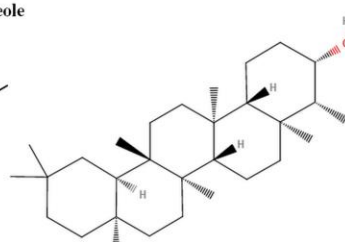
Piperitone



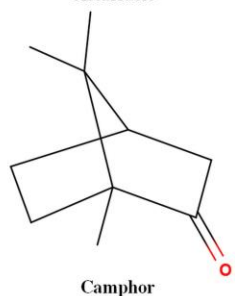
Thujene



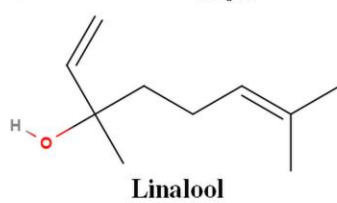
Beta-pinene



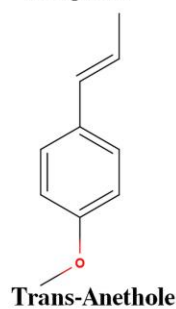
3-beta-Friedelanol



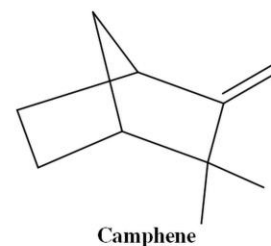
Camphor



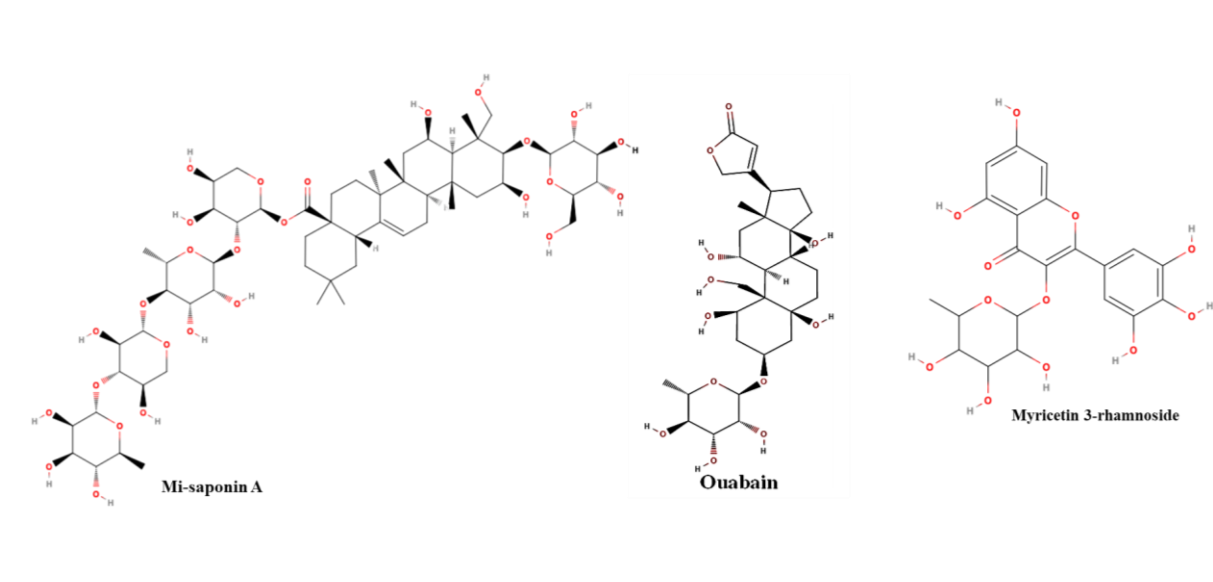
Linalool



Trans-Anethole



Camphene



Members of Cluster Number 1 and 2 with Distances from Respective Cluster Center Cluster contains

Table S1

Members of Cluster Number 1 and Distances from Respective Cluster Center Cluster contains 41 cases	
	Distance
7	0.855639 6-Oxoisoiguesterin
12	0.781140 Akebia saponin c
18	0.823507 Amentoflavone
23	1.007173 Ardisia Saponin
26	0.771381 Artocommunol e
30	1.122738 Beta-Sitosterol
32	1.194801 Betulinic acid
42	1.073424 Celastrol
48	1.086486 cyclamine
54	1.053580 Epigallocatechin gallate
55	1.204444 Epitaraxerol
60	1.354408 Friedelin
62	1.053580 Gallocatechin gallate
66	0.952781 Ginsenoside C
67	0.909883 Ginsenoside rb1
68	1.021728 Ginsenoside RG1
69	0.790489 Glycyrrhizin
72	0.926111 Iguesterin

77	1.071891 Jubanine G
78	0.803373 Jubanine H
88	1.394115 Mi-saponin a
92	1.134754 Myricetin 3-(4''-Galloylrhamnoside)
93	1.118380 Myricetin 3-Neohesperidoside
94	1.106600 Myricetin 3-Sambubioside
95	1.097532 Myricetin 3'-Rhamnoside
97	1.098568 Nummularine B
98	0.706861 Ouabain
100	0.879584 Pectolinarin
103	1.033050 Pristimerin
106	0.992617 Quadrangularic acid f
109	1.471622 Rhoifolin
111	0.815626 Ursane
112	0.775833 Saikosaponin B2
113	0.946317 Saikosaponin C
114	0.749987 Saikosaponin D
115	1.448341 Sanggenol E
116	1.065983 Saponin Pk
118	0.896917 Schimperinone
120	0.674960 Silvestrol
121	1.012564 Smilagenin
123	2.352550 Tannic acid

Table S2

Members of Cluster Number 2 and Distances from Respective Cluster Center Cluster contains 94 cases	
	Distance
1 (+)-artemisinic alcohol	0.693823
2(E)-caryophyllene	0.558627
3 1-Cyclopentyl-2-propen-1-ol	0.565627
4 1,8-Cineole	0.905901
5 3-α-Friedelanol,mol2	0.761464
6 4-Terpinyol acetate	0.896593
8 6,7-dehydroroyleanone	0.797484
9 7-Methoxycryptopleurine	0.811668
10 10'-hydroxyusambarensine	1.140652

11 12-Deoxy-6,7-Dehydroroleanone	0.867073
13 Allo-Aromadendrene	0.565990
14 Alpha-Bisabolol	1.075422
15 Alpha-Cubebene	0.550212
16 Alpha-pinene	0.703466
17 Alpha-selinene	0.548782
19 Ampelopsin	0.944002
20 Anethole_ess_oil	0.786739
21 APA	1.250938
22 Apigenin	0.568685
24 Artemisia alcohol	0.689683
25 Artemisia ketone	0.789960
27 Ascaridole	0.688435
28 Baicalein	0.631071
29 Beta-pinene	1.153202
31 Beta-Thujone	0.841120
33 Bicyclgermacrene	0.560492
34 Biochanin a	0.733838
35 Blancoxanthone	0.720251
36 Brousochalcone b	0.642362
37 Camazulene	0.812865
38 Camphene	0.824153
39 Camphor	0.738321
40 Carvacrol	0.581619
41 Caryophyllene oxide	0.760308
43 Chrysin_phyto	0.605913
44 Cis-anethole	0.786739
45 Citronellyl acetate	0.846896
46 Cryptojaponol	0.802626
47 Curcumin	0.550596
49 Dehydroabieta-7-one	0.950712
50 Demethoxycurcumin	0.650381
51 Dihydrotanshinone i	0.506505
52 Dihydrotanshinone	0.506505
53 Emodin_phyto	0.575585
56 Eugenol	1.041811

57 Ferruginol	0.882911
58 Fisetin	0.565612
59 Formononetin	0.806121
61 Gallic acid	0.785742
63 Gamma-Gurjunene	0.663955
64 Genistein	0.567518
65 Germacrene b	0.887756
70 Guaiol	0.666568
71 Hesperetin	0.606806
73 Isobavachalcone	0.734125
74 Isoledene	0.600361
75 Isoliquiritigenin	0.852302
76 Isopinocampone	0.778907
79 Kaempferol	0.595013
80 Kazinol F	1.020229
81 L-Thujone	0.841120
82 Ledene	0.567677
83 Limonene	0.589909
84 Linalool	0.690567
85 Longifolen	0.583677
86 Luteolin	0.562967
87 Methyl tanshinonate	0.547521
89 Monodemethylcurcumin	0.557514
90 Muurolene	0.550252
91 Myrcene	0.611121
96 Neobavaisoflavone	1.053613
99 Papyriflavonol A	1.067758
101 Pinocarvone	1.092367
102 Piperitone	1.065338
104 Psoralidin	1.092933
105 Pyranojacareubin	0.625930
107 Quercetin	0.714347
108 Rhein_phyto	0.466111
110 Sabinene	0.771419
117 Sappanchalcone	0.648372
119 Scutellarein	0.557173

122 Spathulenol	0.453896
124 Tanshinone i	0.506493
125 Tanshinone iia	0.612395
126 Tanshinone IIb	0.897818
127 Tau-Cadinol	0.597733
128 Taxifolin	0.613332
129 Terpinen-4-ol	0.691491
130 Tetrahydrocurcumin	0.774661
131 Thujene	0.647612
132 Trans-anethole	0.786739
133 Viridiflorol	0.913397
134 Withanone	0.808455
135 Xanthoangelol	0.931500