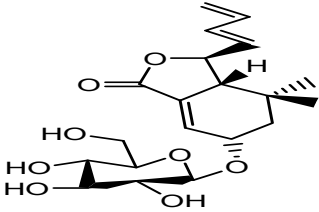
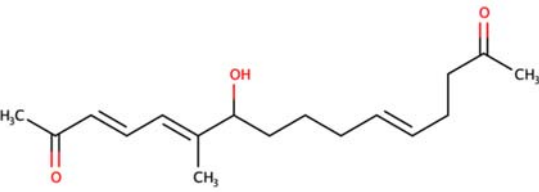
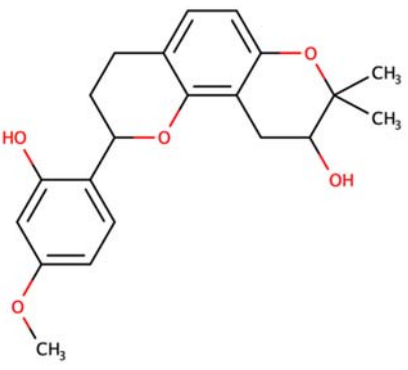


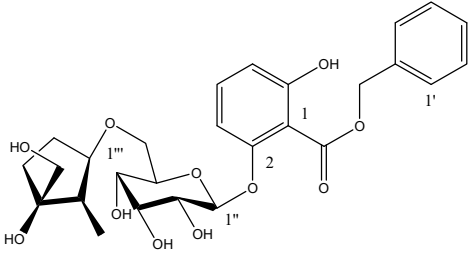
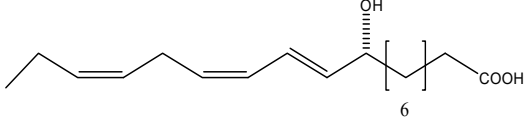
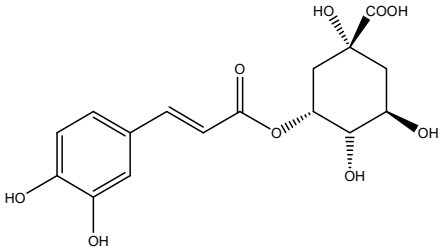
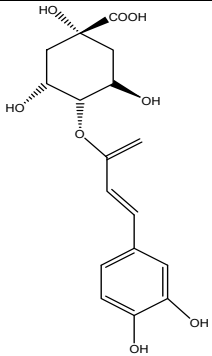
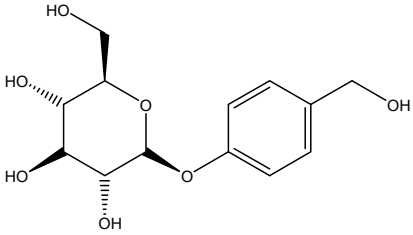
**Pharmacoinformatics-based Identification of Transmembrane Protease
Serine-2 Inhibitors from *Morus Alba* as SARS-CoV-2 cell entry Inhibitors**

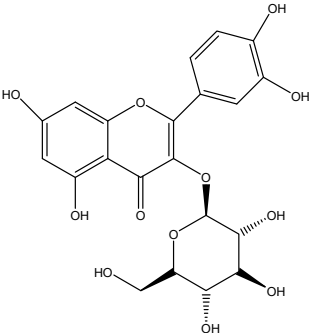
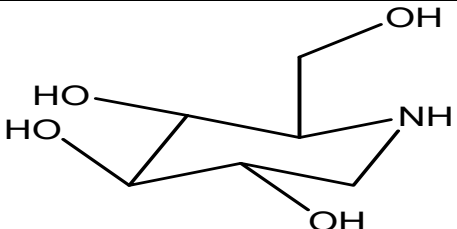
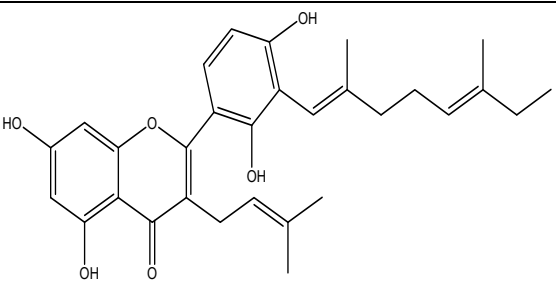
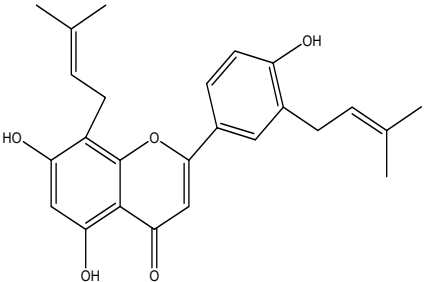
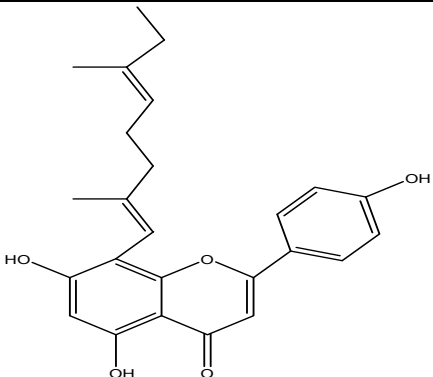
Anshul Shakya, Rupesh V. Chikhale, Hans Raj Bhat, Fatmah Ali Asmary, Tahani Mazyad Almutairi, Surajit Kumar Ghosh¹ Hassna Mohammed Alhajri, Siham A. Alissa, Md Ataul Islam

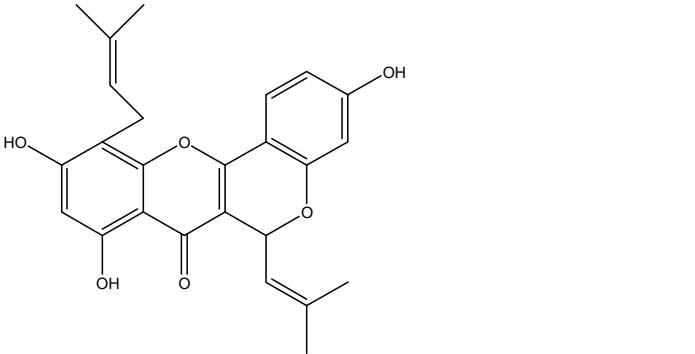
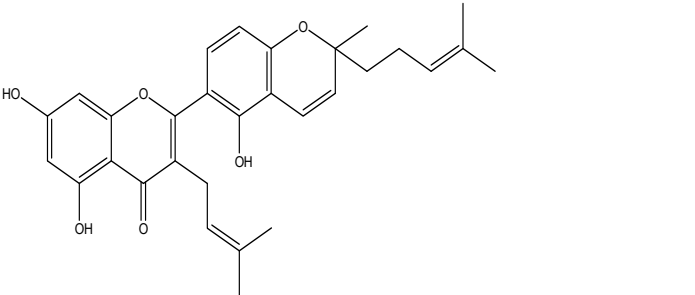
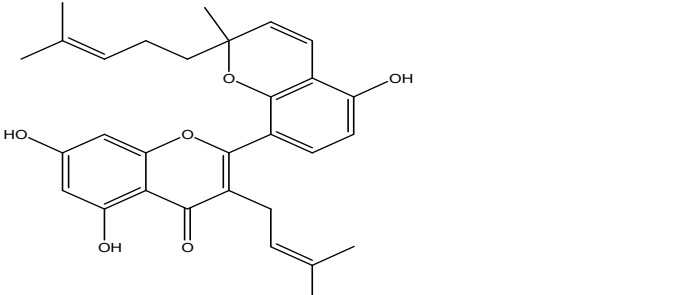
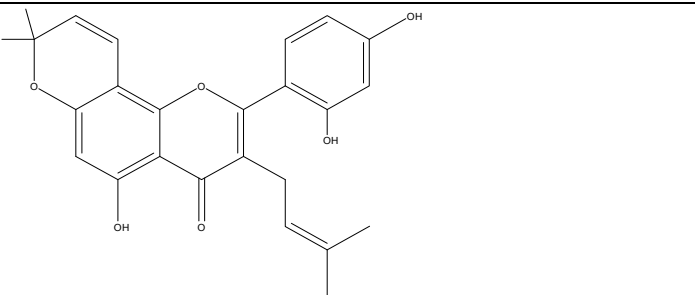
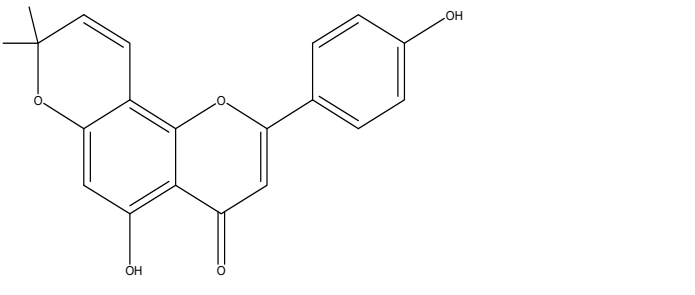
Supplementary data

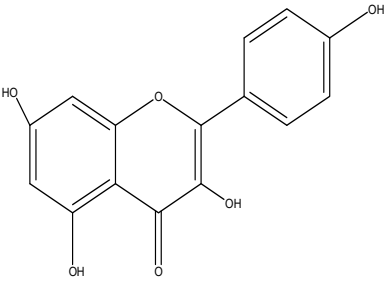
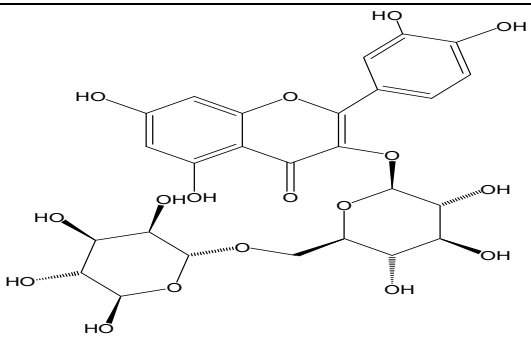
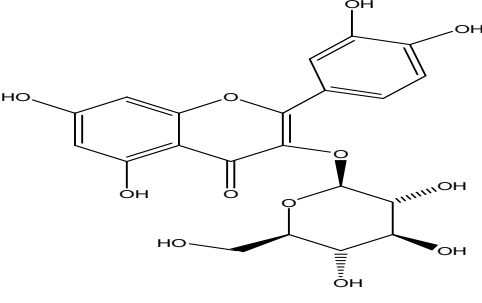
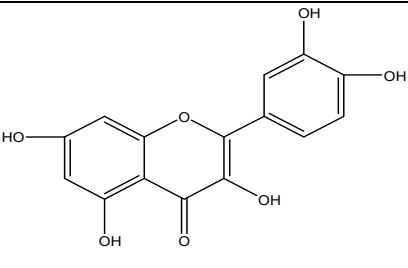
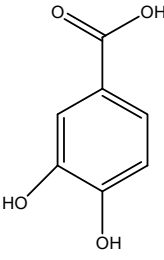
Table S1: Structures of phytoconstituents reported to be present in *M. alba* Linn.

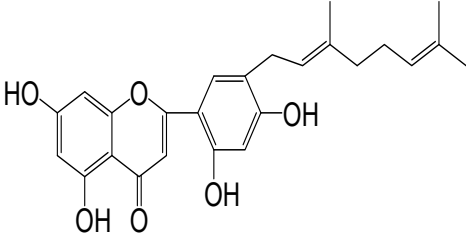
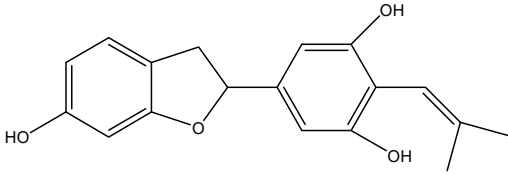
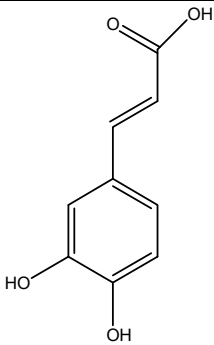
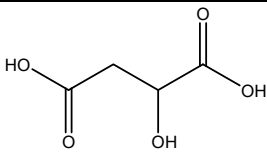
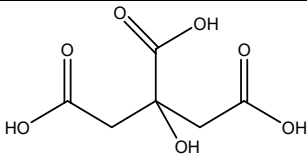
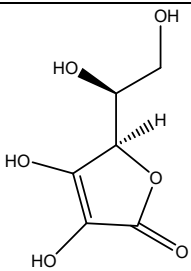
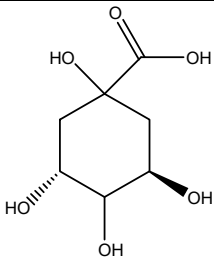
S. No.	Code	Structure	Name
1.	11		Moralsin
2.	12		(3E,5E,10Z)-7-hydroxy-6, 10-dimethyl-pentadecatrien-2,14-dione
3.	13		2'-Hydroxy-4'-methoxyl-2H-(2''', 2'''-dimethyl-3'''-hydroxy)-pyran-(5''',6''':8,7)-flavane

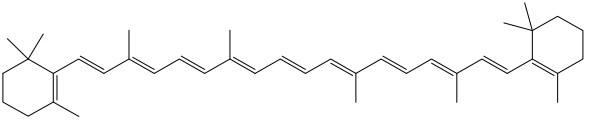
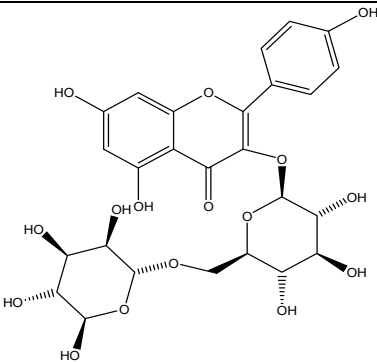
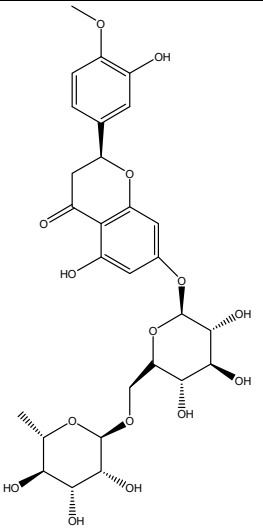
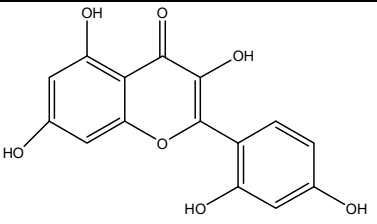
4.	14		Benzyl 2-O-[[β -D-apiofuranosyl(1 \rightarrow 6)- β -D-glucopyranosyl]-2,6-dihydroxybenzoate
5.	15		(9R)-Hydroxy-(10E,12Z,15Z)-octadecatrienoic acid
6.	16		3-O-caffeoylquinic acid/ Chlorogenic acid
7.	17		4-O-caffeoylquinic acid/ Cryptochlorogenic acid
8.	18		Gastrodin

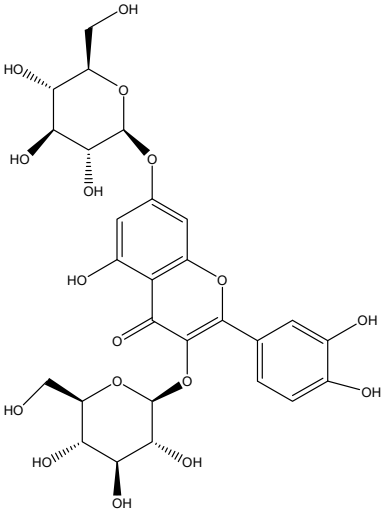
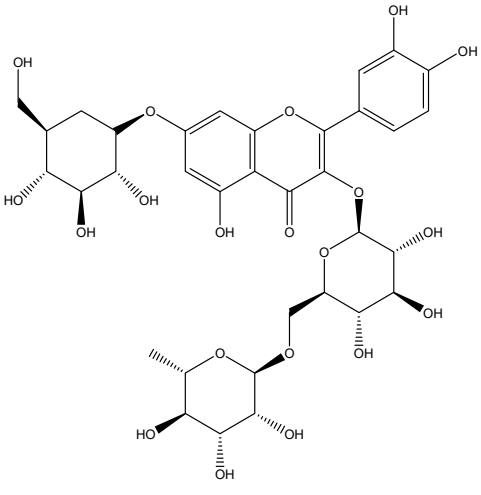
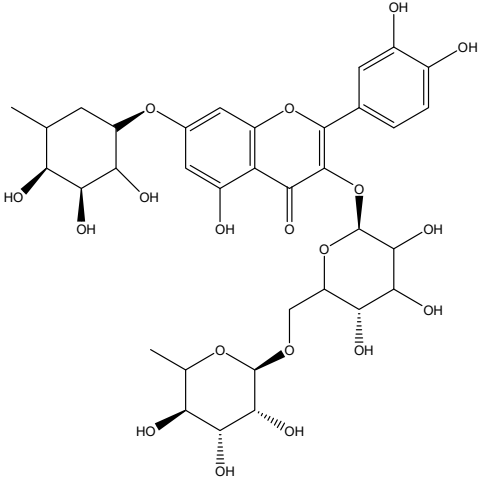
9.	19	 <p>The structure shows a flavonol core (quercetin) with a glucose molecule attached to the 3-position of the C-ring. The glucose is in its cyclic pyranose form, with hydroxyl groups at the 2, 3, 4, and 6 positions. The quercetin core has hydroxyl groups at the 2, 3, 5, and 7 positions.</p>	Quercetin 3-O-glucoside/Isoquercetin
10.	110	 <p>The structure shows a bicyclic imino-sugar, 1-Deoxynojirimycin, in its chair conformation. It features a piperidine ring fused to a five-membered ring. Hydroxyl groups are attached to the 2, 3, and 4 positions, and an amino group is attached to the 1 position.</p>	1-Deoxynojirimycin
11.	111	 <p>The structure shows a flavone core with a geranyl chain at the 3' position and a prenyl chain at the 3 position. The flavone core has hydroxyl groups at the 2', 4', 5, and 7 positions.</p>	3'-geranyl-3-prenyl-2',4',5,7-tetrahydroxyflavone
12.	112	 <p>The structure shows a flavone core with prenyl chains at the 3' and 8 positions. The flavone core has hydroxyl groups at the 4', 5, and 7 positions.</p>	3',8-diprenyl-4',5,7-trihydroxyflavone
13.	113	 <p>The structure shows a flavone core with a geranyl chain at the 8 position. The flavone core has hydroxyl groups at the 5 and 7 positions.</p>	8-geranylapigenin

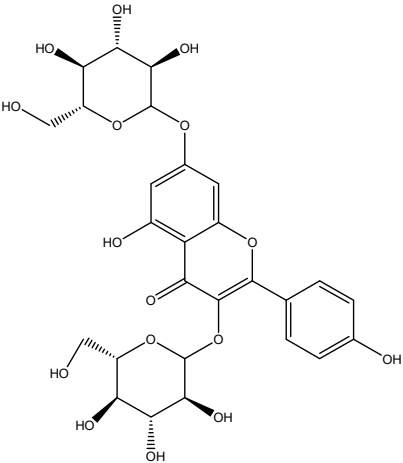
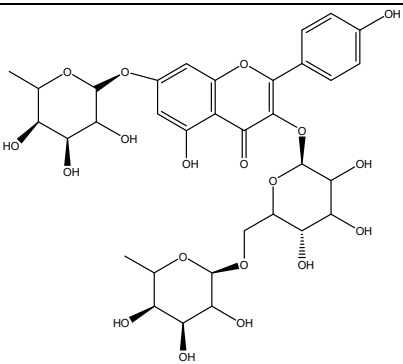
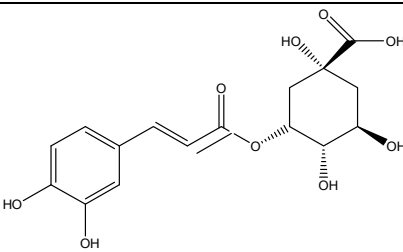
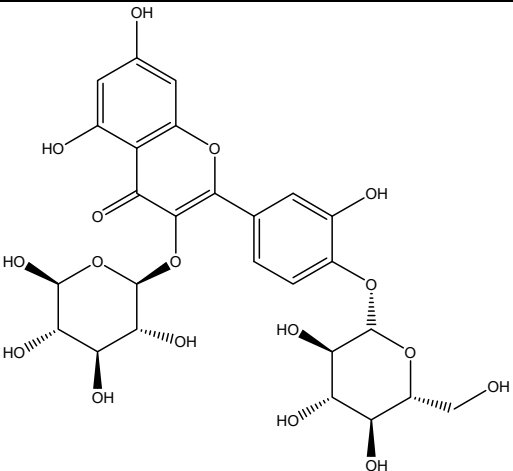
14.	114		Cyclomulberri n
15.	115		Sanggenon J
16.	116		Sanggenon K
17.	117		Morusin
18.	118		Atalantoflavon e

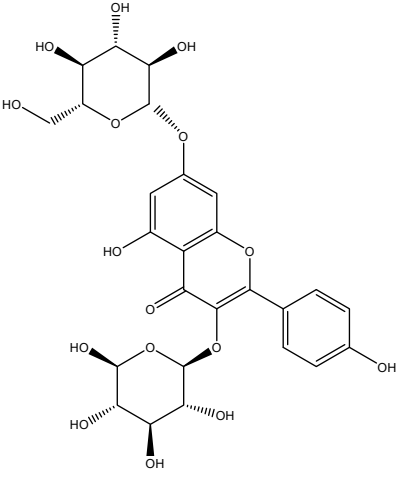
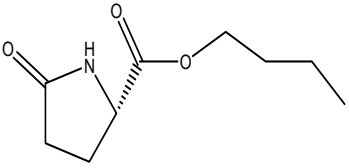
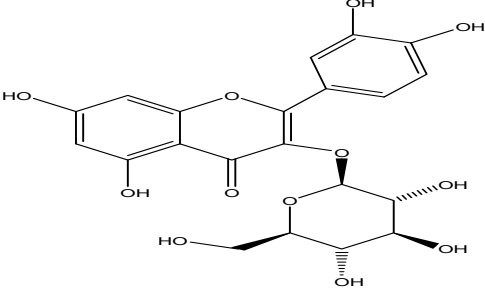
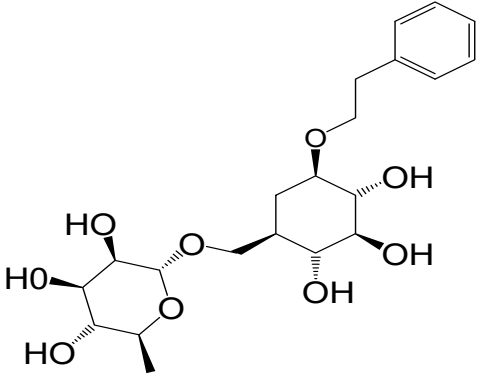
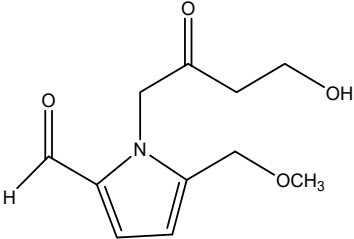
19.	119		Kaempferol
20.	120		Quercetin 3-O-rutinoside/ Rutin
21.	121		Kaempferol 3-O-D-glucoside/ Astragalin
22.	122		Quercetin
23.	123		Dihydroxybenzoic acid/ Protocatechuic acid

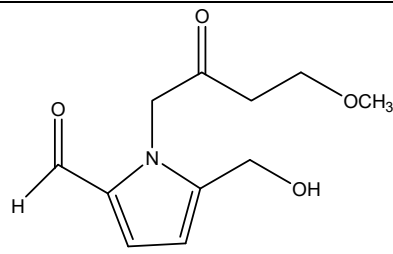
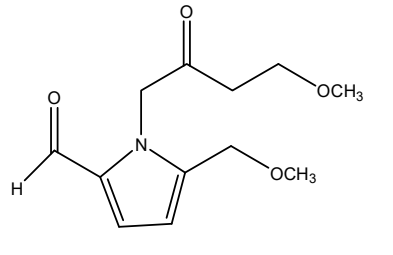
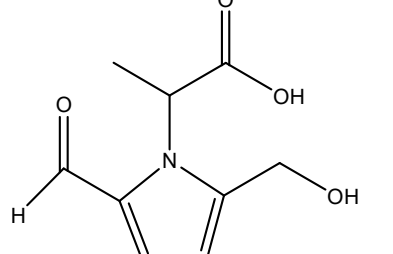
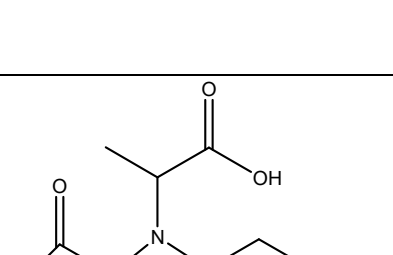
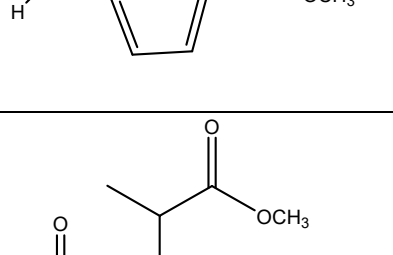
24.	124		Kuwanon S
25.	125		Moracin C
26.	126		Caffeic acid
27.	127		Malic acid
28.	128		Citric acid
29.	129		Ascorbic acid/ Vitamin C
30.	130		Quinic acid

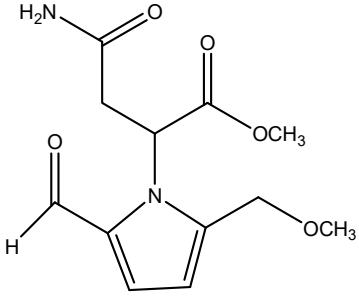
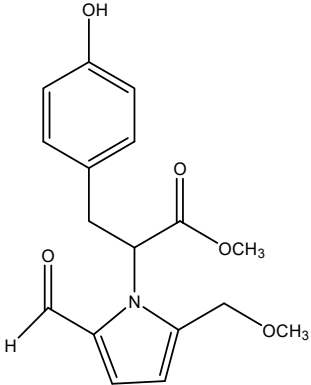
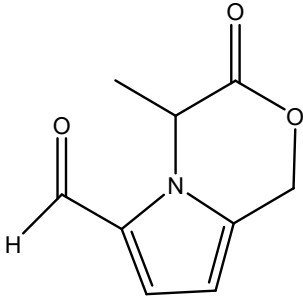
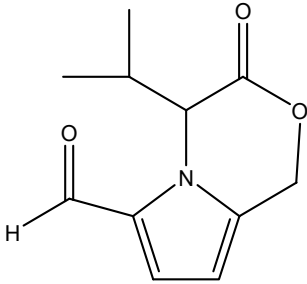
31.	I31		β- carotene
32.	I32		Kaempferol 3- O-D- rutinoside/ Nicotiflorin
33.	I33		Hesperidin
34.	I34		Morin

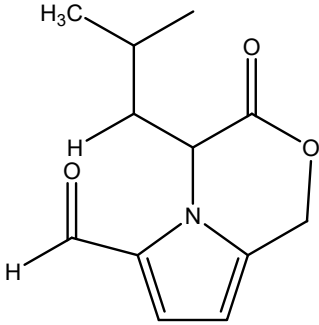
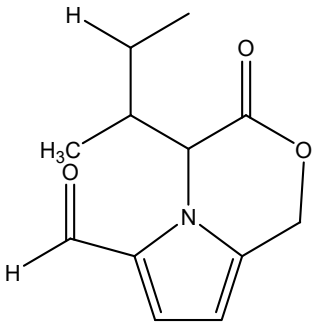
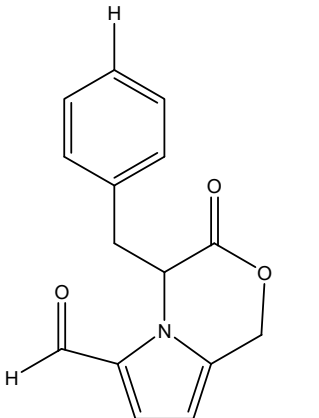
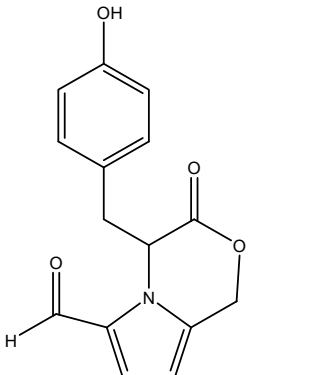
35.	135		Quercetin 3,7-di-O-glucoside
36.	136		Quercetin 3-O-rutinoside-7-O-glucoside/ Morkotin A
37.	137		Quercetin 3-O-rutinoside-7-O-rhamnoside/ Morkotin B

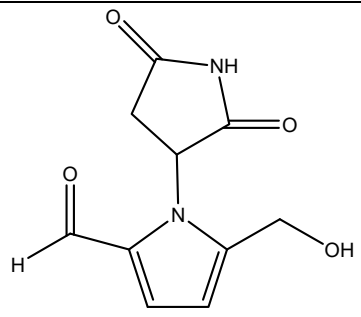
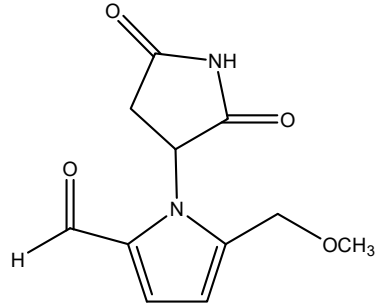
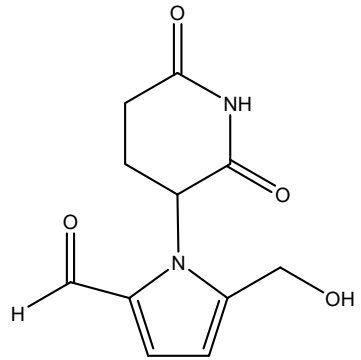
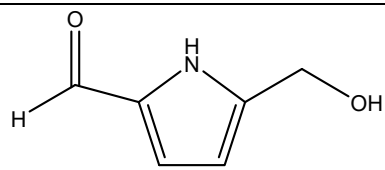
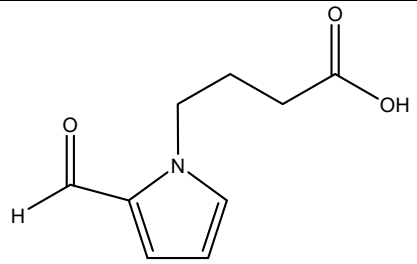
38.	138		Kaempferol 3,7, di- O-glucoside
39.	139		Kaempferol 3-O-rutinoside 7-O-rhamnoside/ Moragrol B
40.	140		5-caffeoylquinic acid/ Neochlorogenic acid
41.	141		Quercetin-di-hexoside

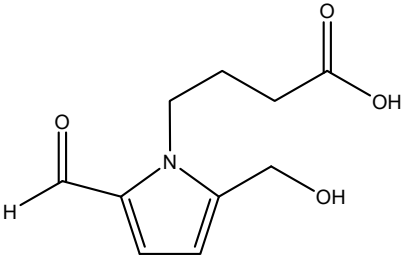
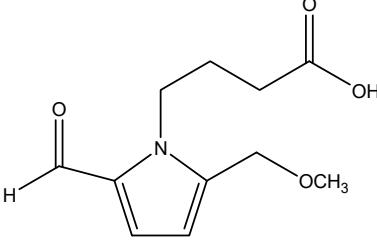
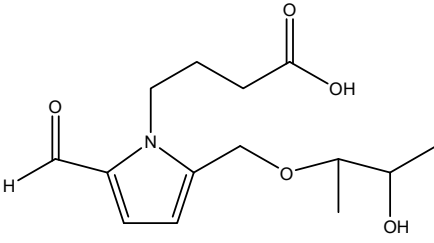
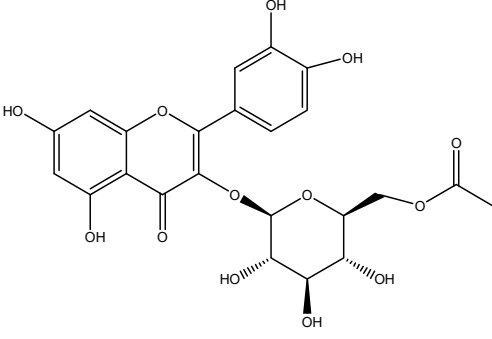
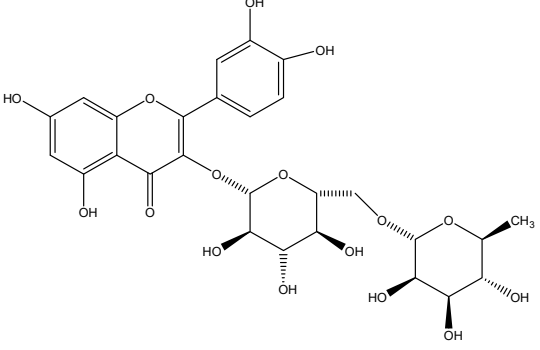
42.	142		Kaempferol- di-hexoside
43.	f1		Butyl pyroglutamate
44.	f2		Kaempferol3- O-D- glucoside/Astr agalgin
45.	f5		2-phenylethyl D-rutinoside
46.	f6		4-[formyl-5 (methoxymeth yl)-1H-pyrrol- 1-yl]butanoate

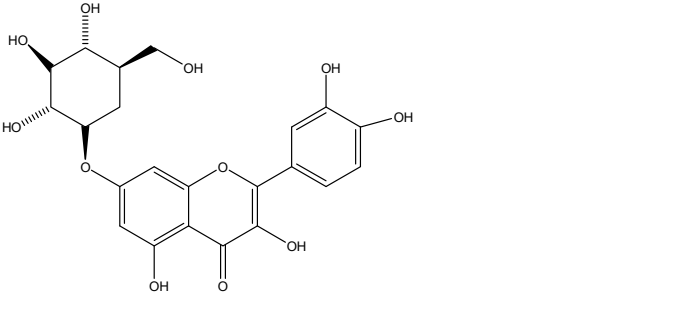
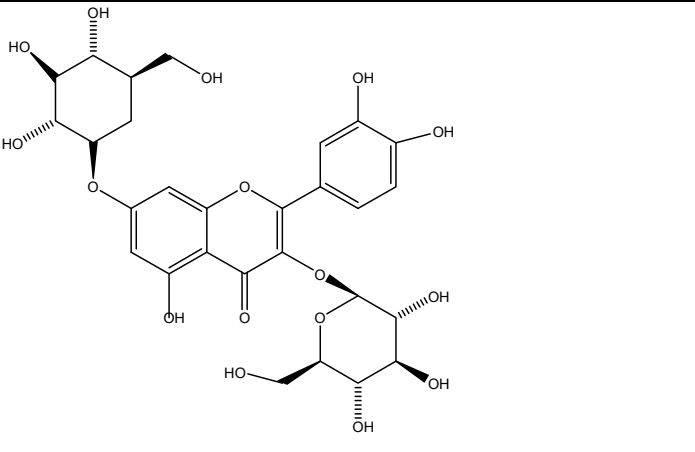
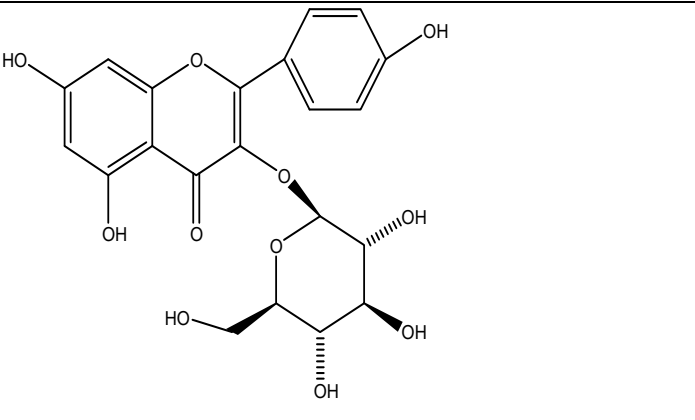
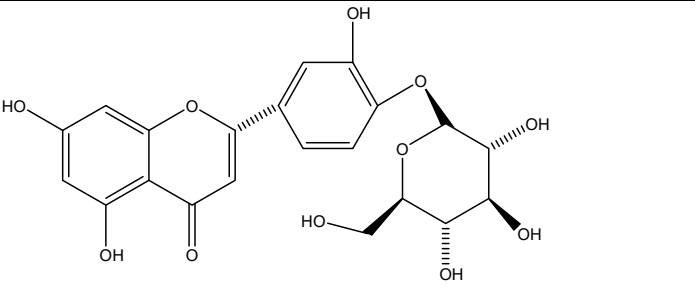
47.	f7		4-[formyl-5-(hydroxymethyl)-1H-pyrrol-1-yl]butanoate
48.	f8		4-[formyl-5-(methoxymethyl)-1H-pyrrol-1-yl]butanoic acid
49.	f9		[2-formyl-5-(hydroxymethyl)-1H-pyrrol-1-yl]propanoic acid/ morrole B
50.	f10		2[2-formyl-(methoxymethyl)-1H-pyrrol-1-yl]propanoic acid/ morrole C
51.	f11		Methyl 2-[2-formyl-5-(methoxymethyl)-1H-pyrrol-1-yl]propanoate

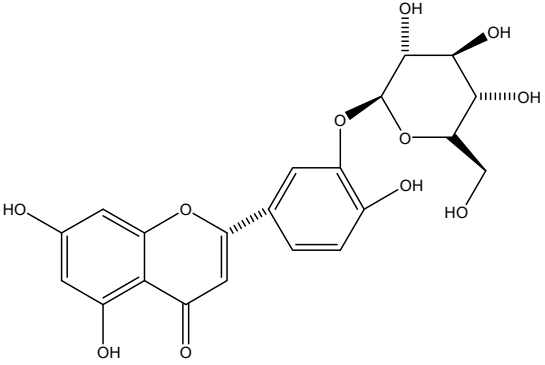
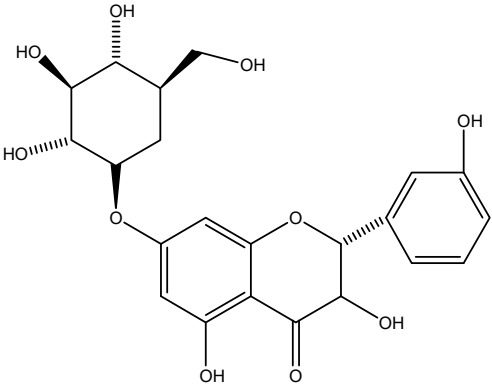
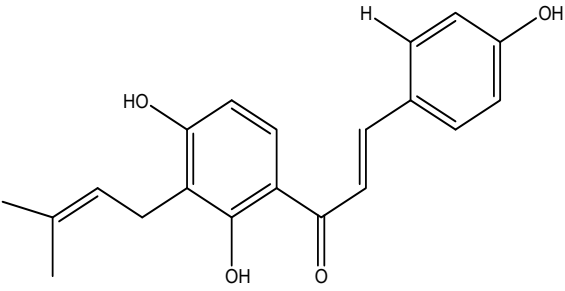
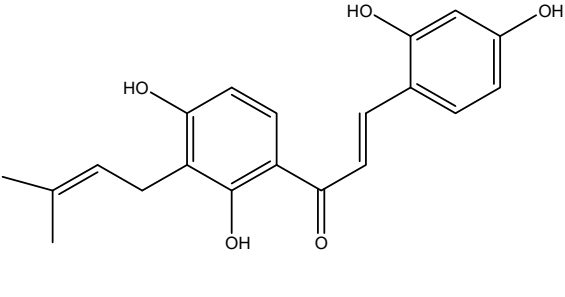
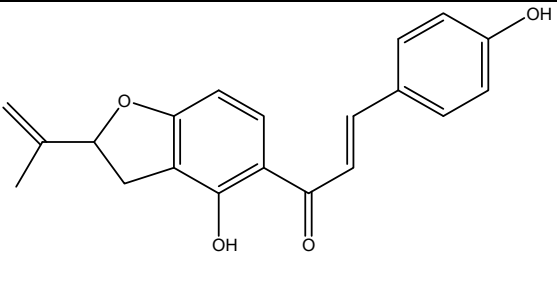
52.	f12	 <p>The structure shows a pyrrole ring with a formyl group (-CHO) at position 2, a methoxymethyl group (-CH₂OCH₃) at position 5, and a 2-amino-4-oxobutanoate side chain (-CH₂-CH(NH₂)-C(=O)-OCH₃) attached to the nitrogen atom.</p>	4-amino-2-[2-formyl-5-(methoxymethyl)-1H-pyrrol-1-yl]-4-oxobutanoate/ morrole E
53.	f13	 <p>The structure shows a pyrrole ring with a formyl group (-CHO) at position 2, a methoxymethyl group (-CH₂OCH₃) at position 5, and a 2-(4-hydroxyphenyl)propanoate side chain (-CH₂-CH₂-C(=O)-OCH₃) attached to the nitrogen atom.</p>	Methyl 2-[2-formyl-5-(methoxymethyl)-1H-pyrrol-1-yl]-3-(4-hydroxyphenyl)propanoate
54.	f14	 <p>The structure shows a pyrrole ring with a formyl group (-CHO) at position 2, a methyl group (-CH₃) at position 3, and a 5-hydroxymethyl-2-propionyl lactone side chain (-CH₂-CH₂-C(=O)-O-CH₂-) attached to the nitrogen atom.</p>	2-(5-hydroxymethyl-2-formylpyrrole-1-yl)propionic acid lactone
55.	f15	 <p>The structure shows a pyrrole ring with a formyl group (-CHO) at position 2, a methyl group (-CH₃) at position 3, and a 5-hydroxymethyl-2-isovaleryl lactone side chain (-CH₂-CH₂-C(=O)-O-CH₂-) attached to the nitrogen atom.</p>	2-(5-hydroxymethyl-2-formylpyrrole-1-yl)isovaleric acid lactone

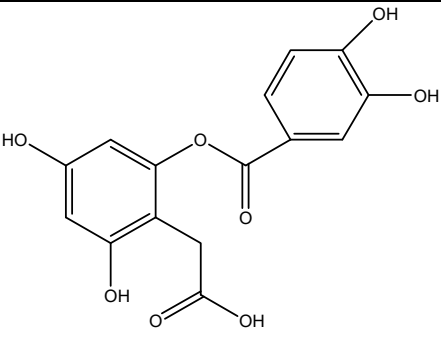
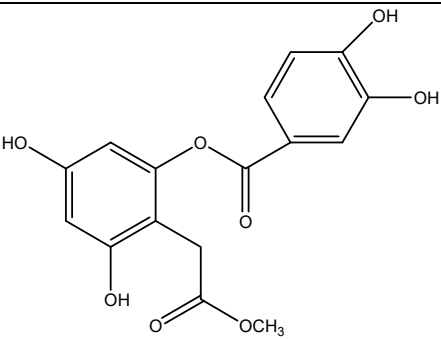
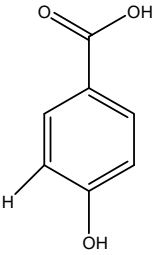
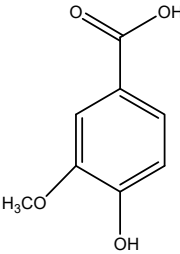
56.	f16		2-(5-hydroxymethyl-2-formylpyrrol-1-yl)isocaproic acid lactone
57.	f17		2-(5'-hydroxymethyl-2'-formylpyrrol-1'-yl)-3-phenylpropionic acid lactone
58.	f18		2-[2-formyl-5-(hydroxymethyl)-1-pyrrolyl]-3-methylpentanoic acid lactone
59.	f19		2-(5'-hydroxymethyl-2'-formylpyrrol-1'-yl)-3-(4-hydroxyphenyl)propionic acid lactone

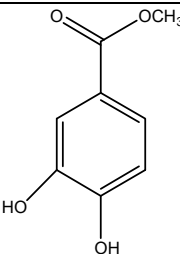
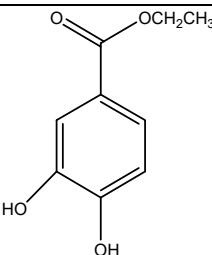
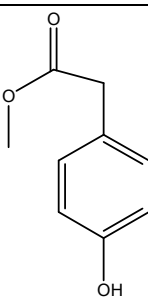
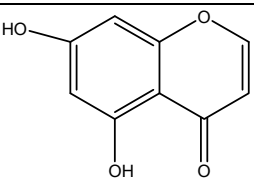
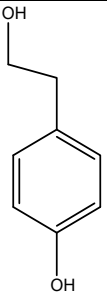
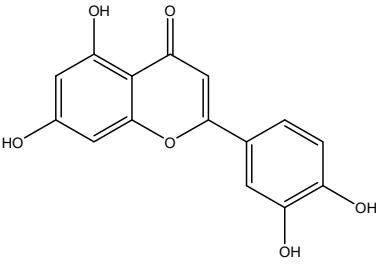
60.	f20		2-(5-hydroxymethyl-20',5'-dioxo-2',3',4',5'-tetrahydro-1'H-1,3'-bipyrrole)carbaldehyde
61.	f21		Morrole G
62.	f22		1-(2,6-dioxopiperidin-3-yl)-5-(hydroxymethyl)-1H-pyrrole-2-carbaldehyde/ morrole H
63.	f23		5-(hydroxymethyl)-1H-pyrrole-2-carboxaldehyde
64.	f24		2-formyl-1H-pyrrole-1-butanoic acid

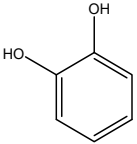
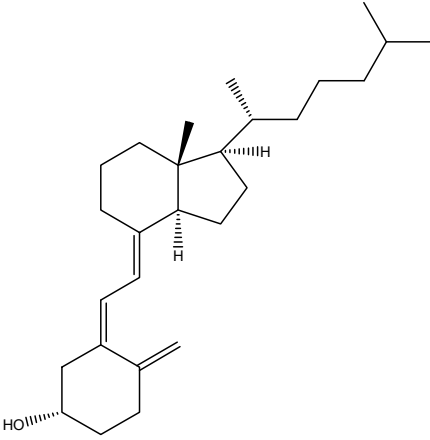
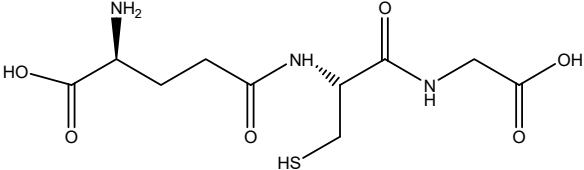
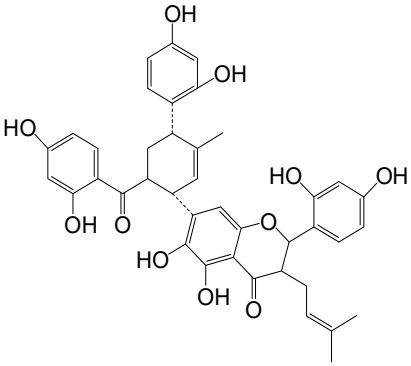
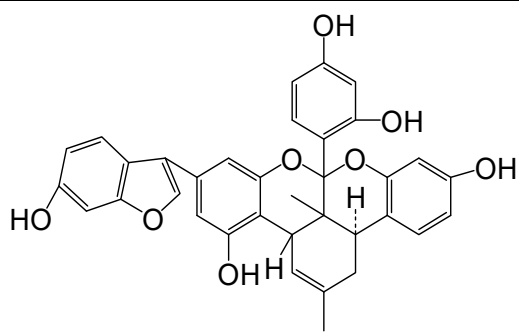
65.	f25		2-formyl-5-(hydroxymethyl)-1H-pyrrole-1-butanoic acid
66.	f26		2-formyl-5-(methoxymethyl)-1H-pyrrole-1-butanoic acid
67.	f27		MorroleA
68.	f29		Quercetin 3-O-(6''-O-acetyl)-beta-D-glucopyranoside
69.	f30		Quercetin 3-O-beta-D-rutinoside

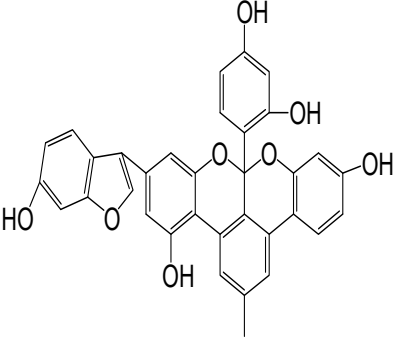
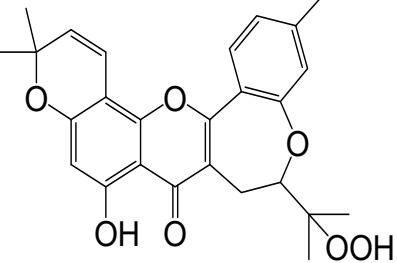
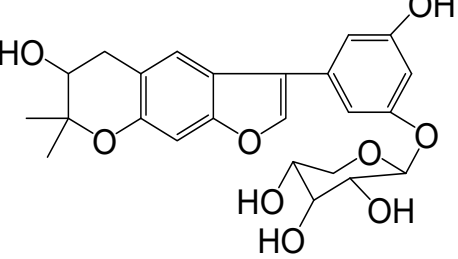
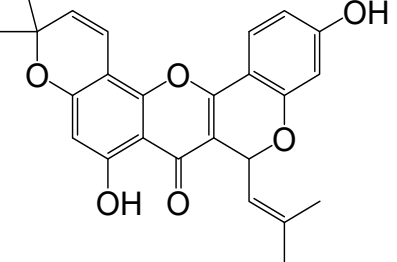
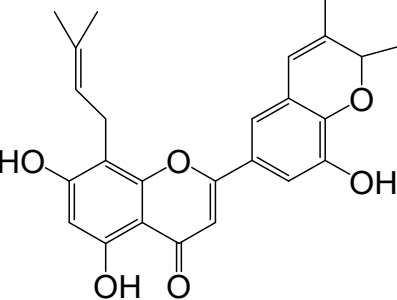
70.	f31		Quercetin 7-O- β -D-glucopyranoside
71.	f32		Quercetin 3,7-di-O- β -D-glucopyranoside
72.	f33		Kaempferol 3-O- β -D-glucopyranoside
73.	f34		5,7,3'-trihydroxyflavanone-4'-O- β -D-glucopyranoside

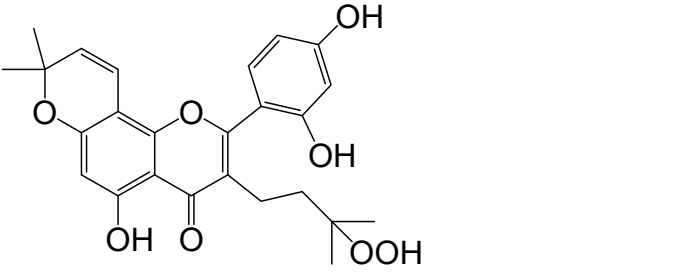
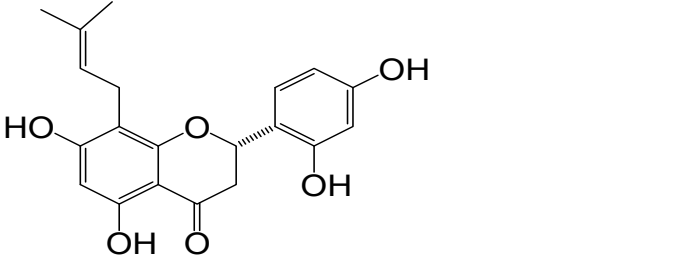
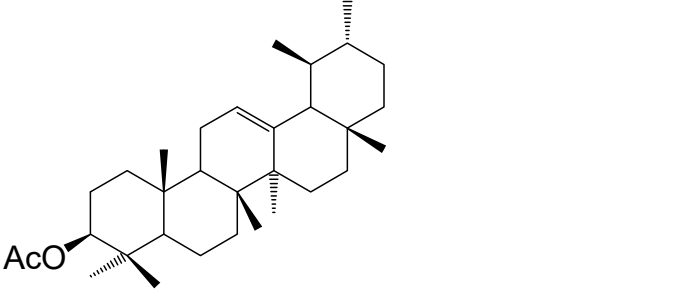
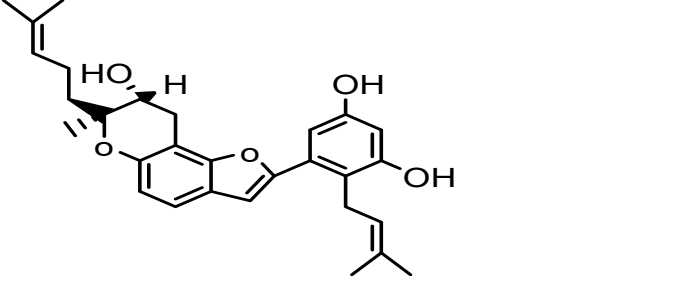
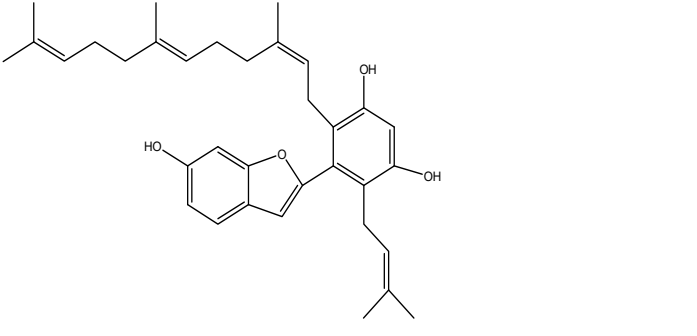
74.	f35		5,7,4'-trihydroxy - flavanone - 3' - O - β - D - glucopyranoside
75.	f36		Dihydrokaempferol 7-O- β -D-glucopyranoside
76.	f37		Isobavachalcone
77.	f38		2,4,2',4',tetrahydroxy-3'-(3-methyl-2-butenyl) - chalcone / morachalcone
78.	f39		(2E)-1-[2,3-dihydro-4-hydroxy-2-(1-methylethenyl)-5-benzofuranyl]-

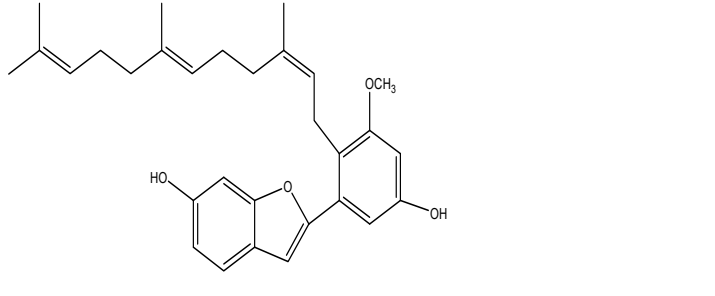
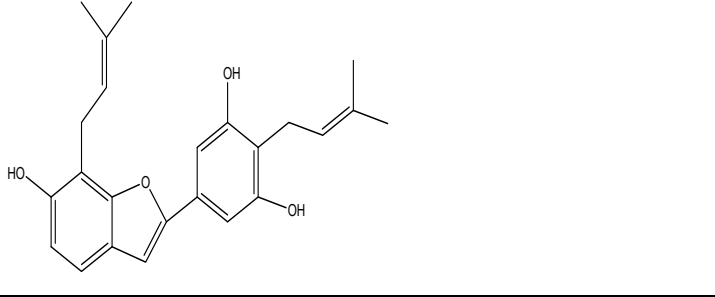
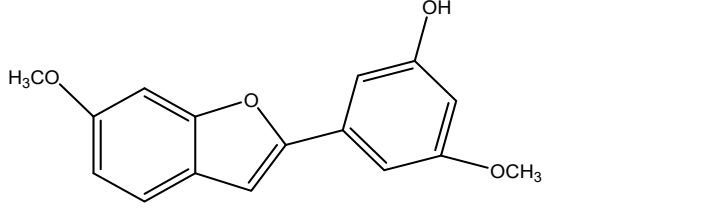
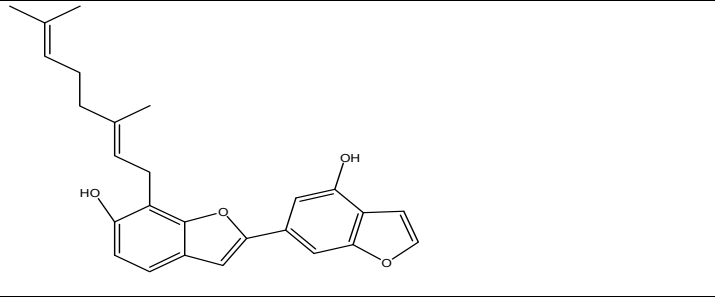
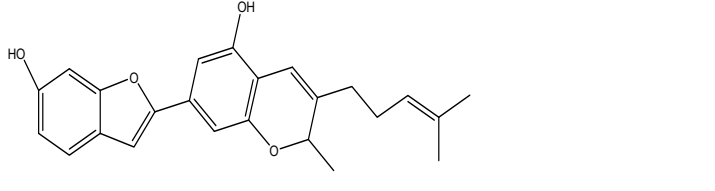
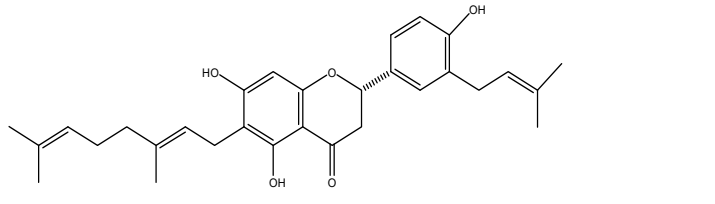
			3-(4-hydroxyphenyl) - 1-propanone
79.	f40		2-O-(3,4-dihydroxybenzoyl)-2,4,6-trihydroxyphenylacetic acid
80.	f41		2-O-(3,4-dihydroxybenzoyl)-2,4,6-trihydroxyphenyl methyl acetate/ jaboticabin
81.	f42		p-hydroxybenzoic acid
82.	f44		3-methoxy-4-hydroxybenzoic acid/ vanillic acid

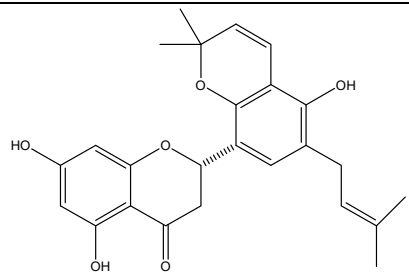
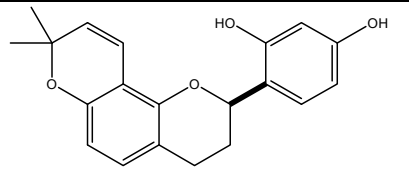
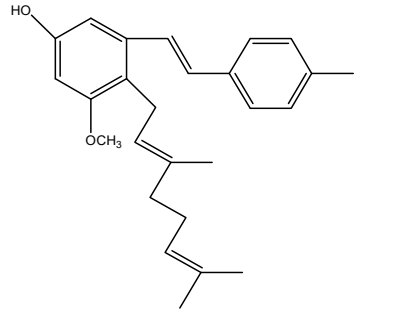
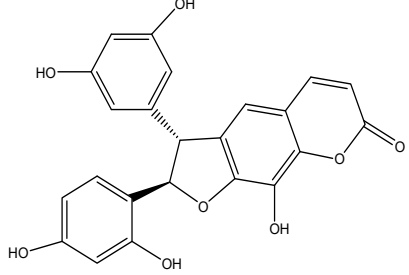
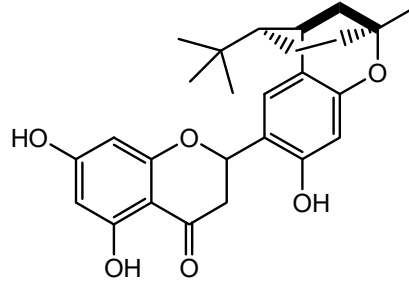
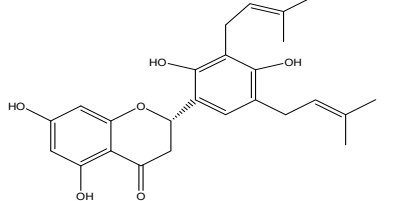
83.	f45		Protocatechuic acid methyl ester
84.	f46		Protocatechuic acid ethyl ester
85.	f47		4-hydroxyphenyl acetic acid methyl ester
86.	f48		5,7-dihydroxychromone
87.	f49		2-(4-hydroxyphenyl)ethanol/ tyrosol
88.	f57		Leuteolin

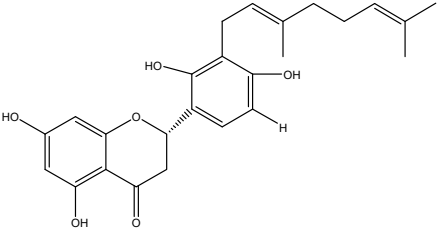
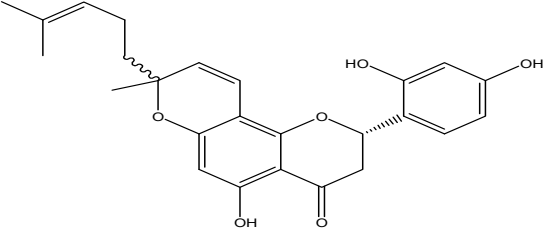
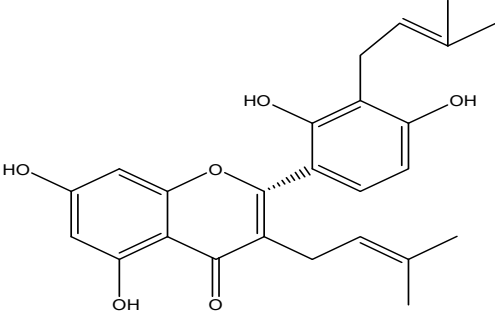
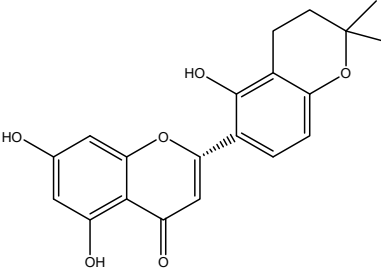
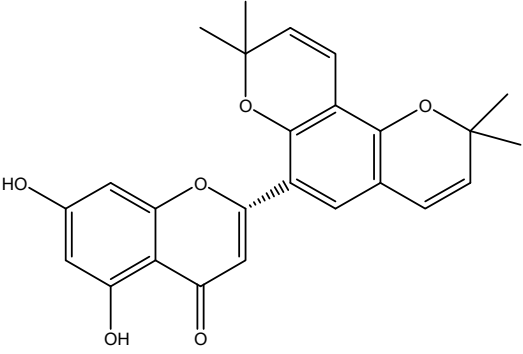
89.	f58		Pyrocatechol
90.	f60		Cholecalciferol / Vitamin D
91.	f61		Glutathione
92.	r1		Kuwanon G
93.	r2		Mulberrofuran G

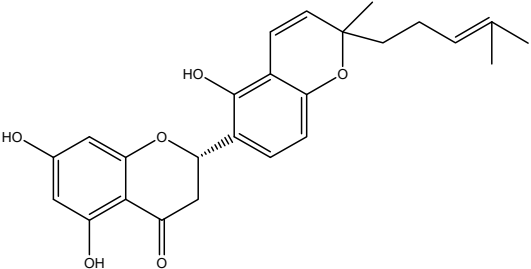
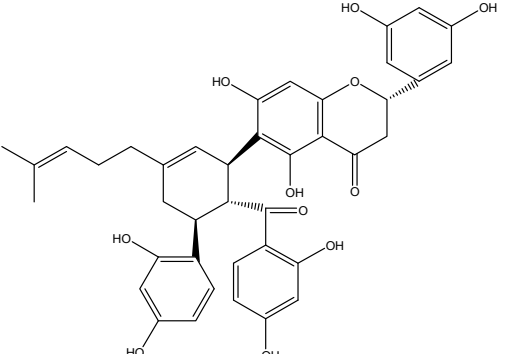
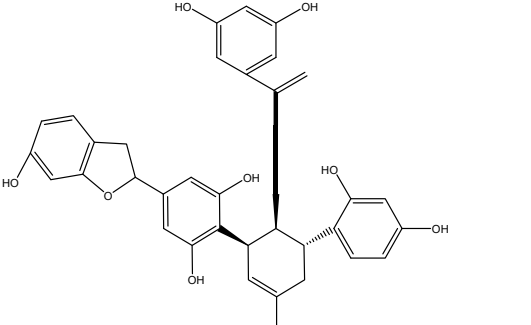
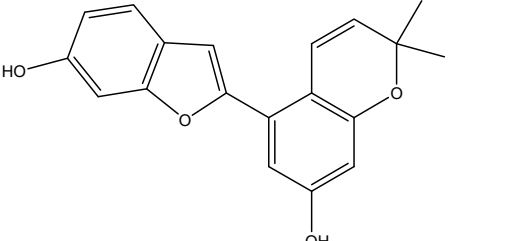
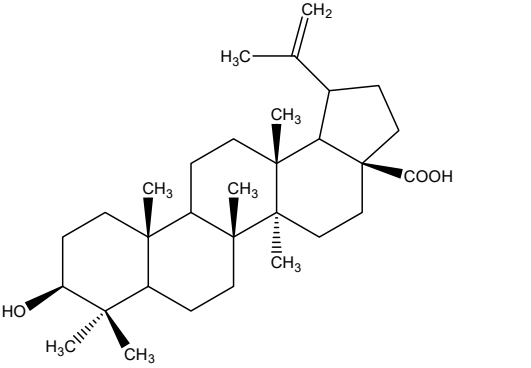
94.	r3		Albanol B
95.	r4		Moralbanone
96.	r6		Mulberroside C
97.	r7		Cyclomorusin
98.	r8		Eudraflavone B hydroperoxide

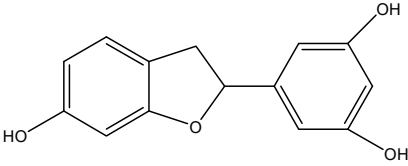
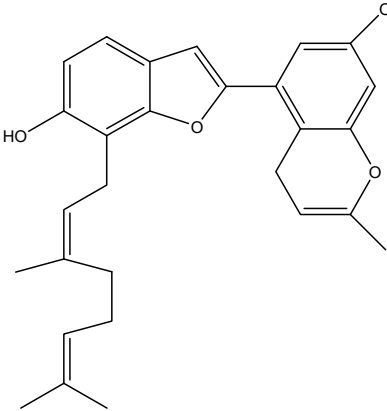
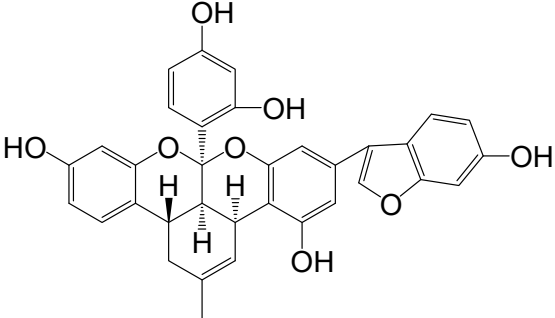
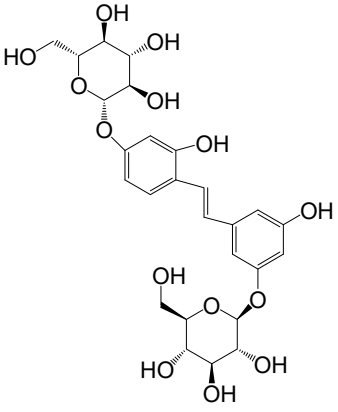
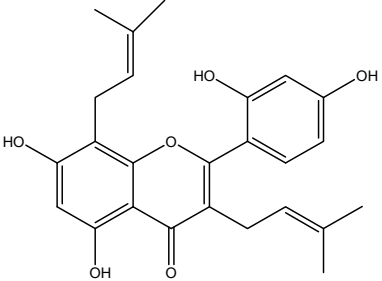
99.	r9		Oxydihydromorusin
100.	r10		Leachianone G
101.	r11		α -acetyl-amyryn
102.	r12		Morusalfuran A
103.	r13		Morusalfuran B

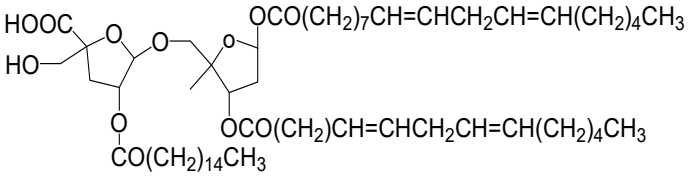
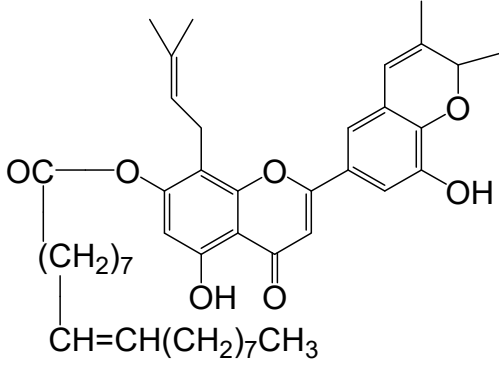
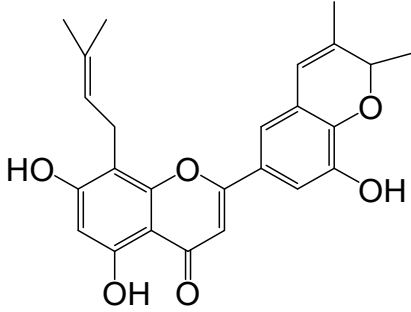
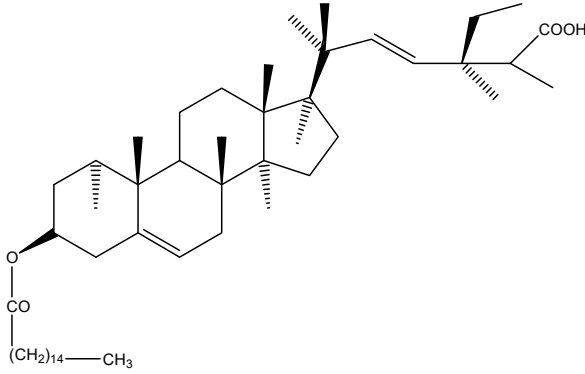
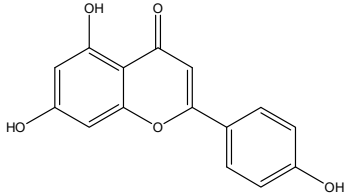
104.	r14		Morusalfuran C
105.	r15		Morusalfuran D
106.	r16		Morusalfuran E
107.	r17		Morusalfuran F
108.	r18		Morusalfuran G
109.	r19		Morusalno A

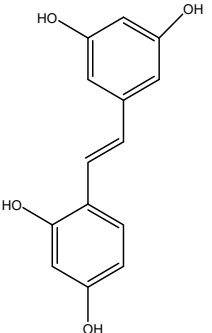
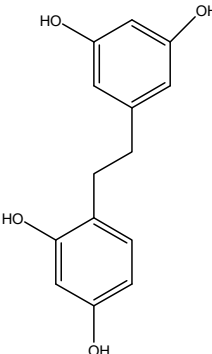
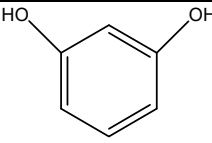
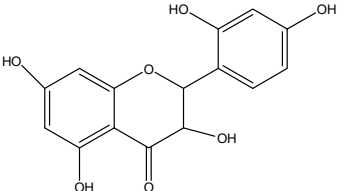
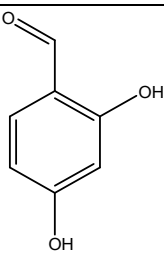
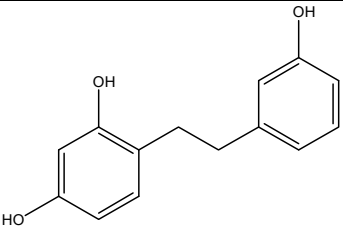
110.	r20		Morusalno B
111.	r21		Morusalno C
112.	r22		Morusibene A
113.	r23		Morescoumarin A
114.	r24		Morflavanone A
115.	r25		Sanggenol Q

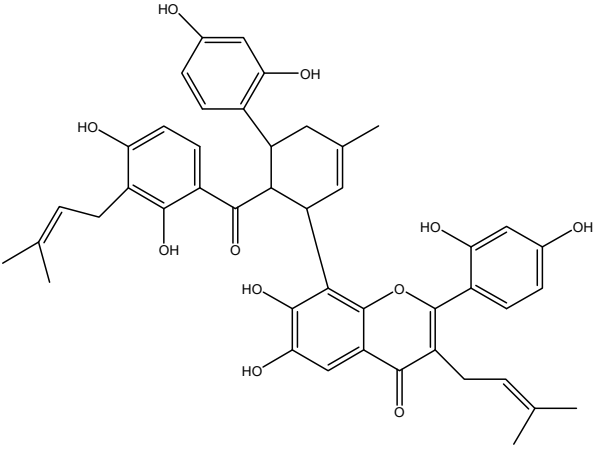
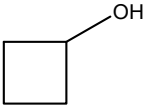
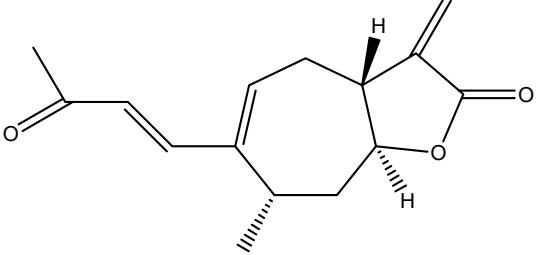
116.	r26		Sanggenol A
117.	r27		Sanggenol L
118.	r28		Kuwanon T
119.	r29		Sanggenon F
120.	r30		Sanggenol O

121.	r31	 <p>The structure of Sanggenon N consists of a chromane core. The chromane ring has a hydroxyl group at the 6-position and a carbonyl group at the 8-position. The 2-position is substituted with a 3,4-dihydro-2H-benzopyran ring, which has a hydroxyl group at the 6-position and a prenyl chain at the 3-position.</p>	Sanggenon N
122.	r32	 <p>The structure of Sanggenon G is a complex polycyclic molecule. It features a chromane core with a hydroxyl group at the 6-position and a carbonyl group at the 8-position. The 2-position is substituted with a 3,4-dihydro-2H-benzopyran ring, which has a hydroxyl group at the 6-position and a prenyl chain at the 3-position. The 3-position of the chromane core is also substituted with a 3,4-dihydro-2H-benzopyran ring, which has a hydroxyl group at the 6-position and a prenyl chain at the 3-position. The 3-position of this second benzopyran ring is substituted with a 3,4-dihydro-2H-benzopyran ring, which has a hydroxyl group at the 6-position and a prenyl chain at the 3-position.</p>	Sanggenon G
123.	r33	 <p>The structure of Mulberrofuran C is a complex polycyclic molecule. It features a chromane core with a hydroxyl group at the 6-position and a carbonyl group at the 8-position. The 2-position is substituted with a 3,4-dihydro-2H-benzopyran ring, which has a hydroxyl group at the 6-position and a prenyl chain at the 3-position. The 3-position of the chromane core is also substituted with a 3,4-dihydro-2H-benzopyran ring, which has a hydroxyl group at the 6-position and a prenyl chain at the 3-position. The 3-position of this second benzopyran ring is substituted with a 3,4-dihydro-2H-benzopyran ring, which has a hydroxyl group at the 6-position and a prenyl chain at the 3-position.</p>	Mulberrofuran C
124.	r34	 <p>The structure of Moracin E consists of a chromane core. The chromane ring has a hydroxyl group at the 6-position and a carbonyl group at the 8-position. The 2-position is substituted with a 3,4-dihydro-2H-benzopyran ring, which has a hydroxyl group at the 6-position and a prenyl chain at the 3-position.</p>	Moracin E
125.	r35	 <p>The structure of Betulinic acid is a complex polycyclic molecule. It features a chromane core with a hydroxyl group at the 6-position and a carbonyl group at the 8-position. The 2-position is substituted with a 3,4-dihydro-2H-benzopyran ring, which has a hydroxyl group at the 6-position and a prenyl chain at the 3-position. The 3-position of the chromane core is also substituted with a 3,4-dihydro-2H-benzopyran ring, which has a hydroxyl group at the 6-position and a prenyl chain at the 3-position. The 3-position of this second benzopyran ring is substituted with a 3,4-dihydro-2H-benzopyran ring, which has a hydroxyl group at the 6-position and a prenyl chain at the 3-position.</p>	Betulinic acid

126.	r37		Moracin M
127.	r39		Mulberrofuran D
128.	r40		Albanol A
129.	r41		Mulberroside A
130.	r43		Kuwanon C

131.	b1		Linoleoyldiglycose
132.	b2		Morusflavonyl palmitate
133.	b3		Morusflavone
134.	b4		Albosteroid
135.	b8		Apigenin

136.	b9		Oxyresveratrol
137.	b10		Dihydroxyresveratrol
138.	b13		Resorcinol
139.	b14		trans-dihydromorin
140.	b15		2,4-dihydroxybenzaldehyde
141.	b16		2,3,3'-trihydroxydihydrostilbene

142.	b17		Kuwanon H
143.	b20		Cyclobutanol
144.	b21		Xanthatin

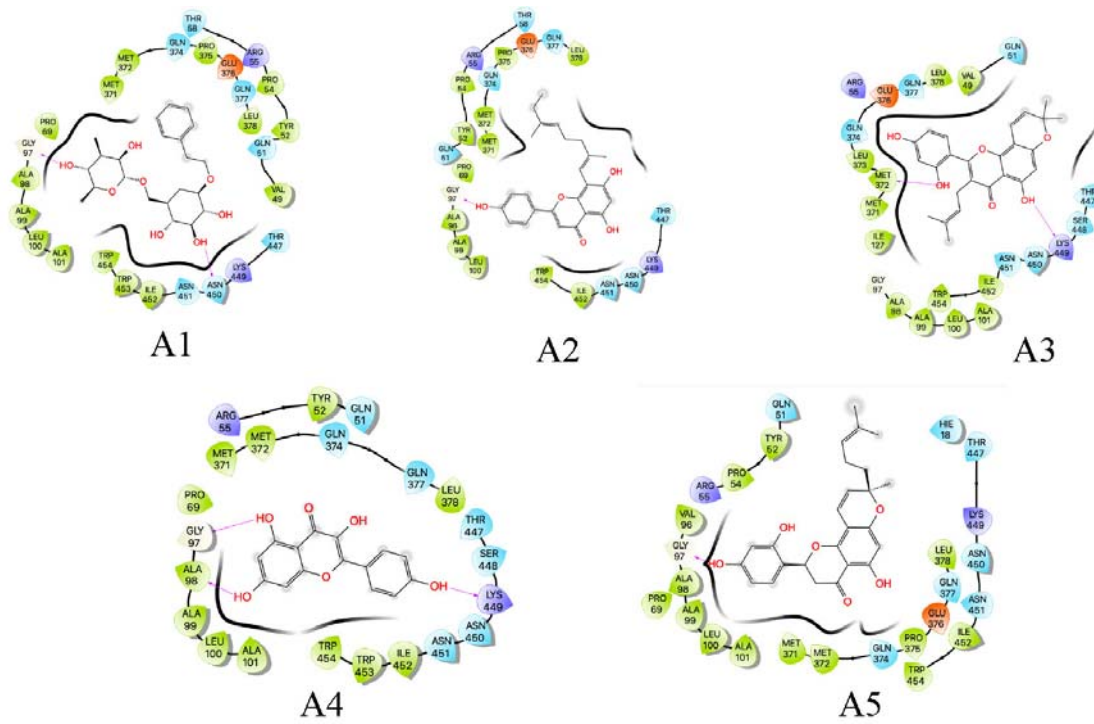


Figure S1. Presence of amino acids in close proximity of the proposed TMPRSS2 modulators