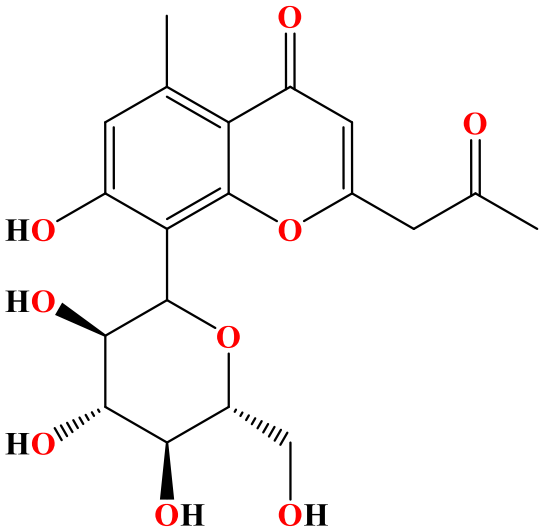
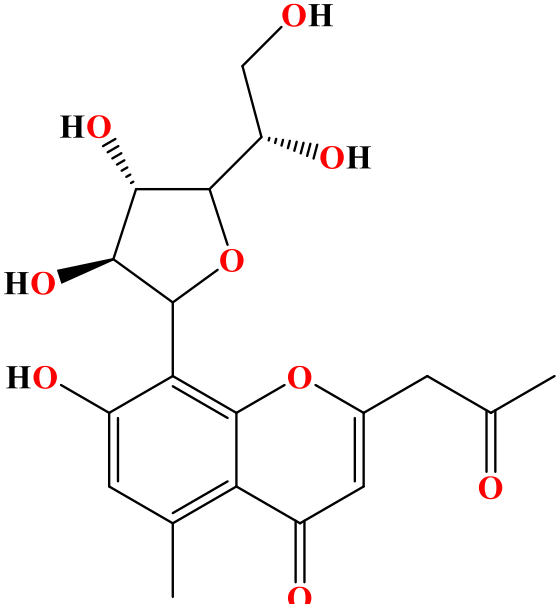
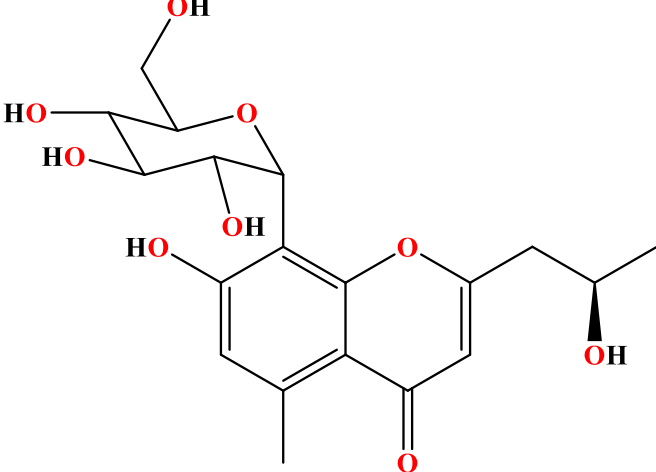
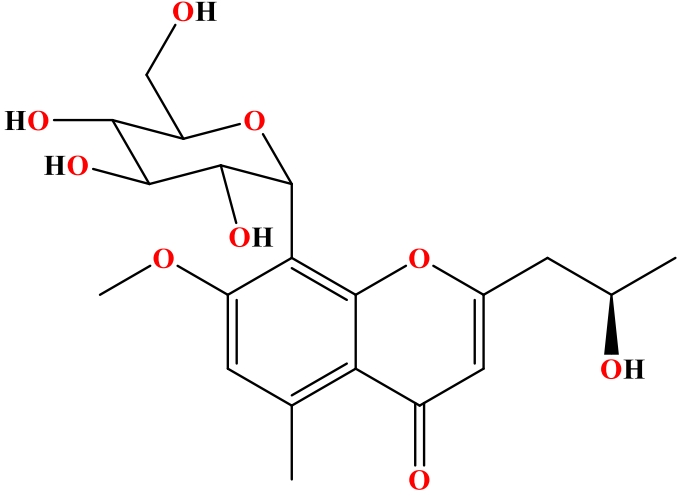
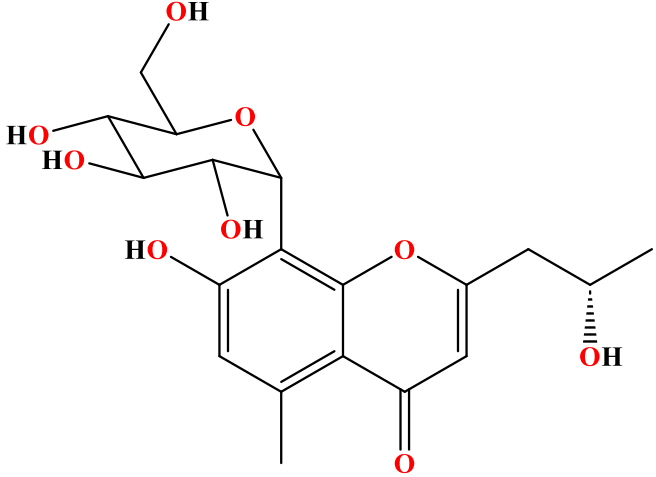
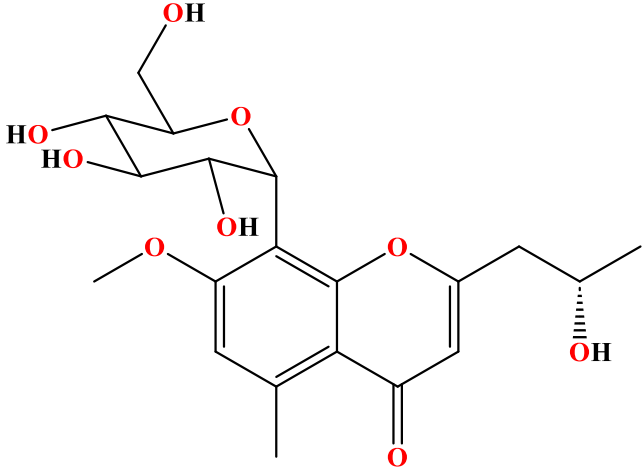
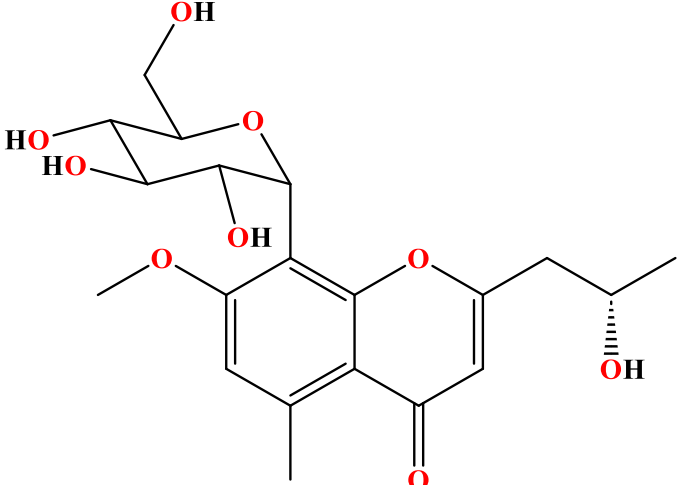
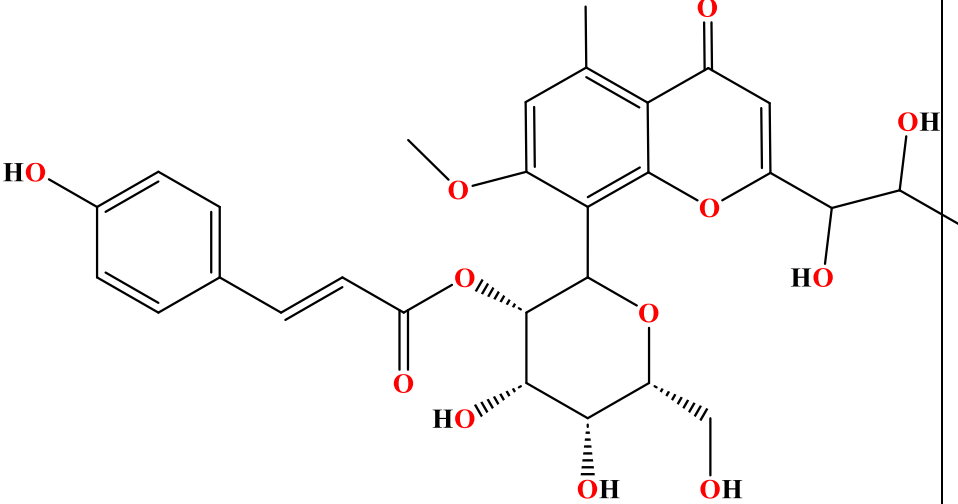
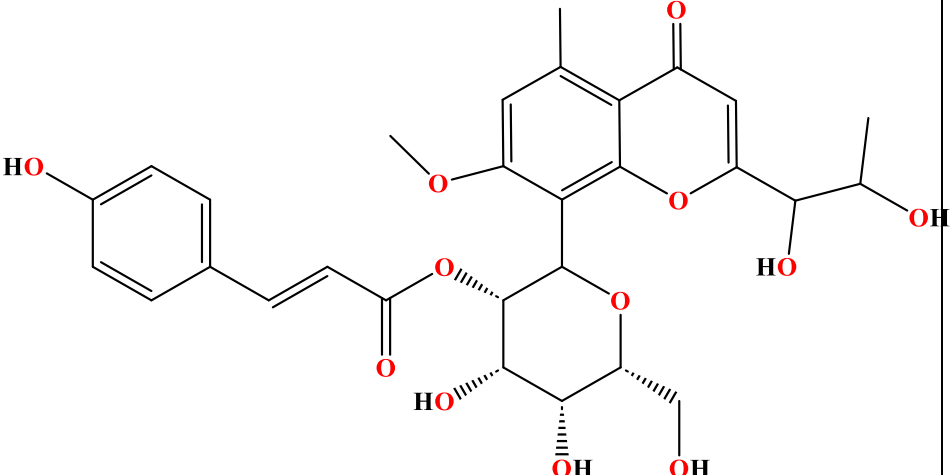
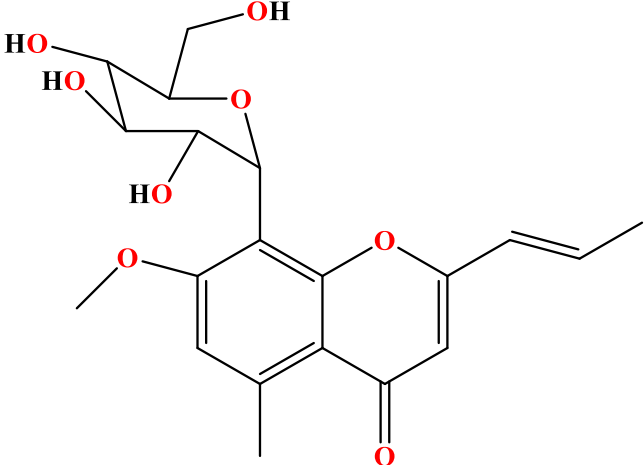
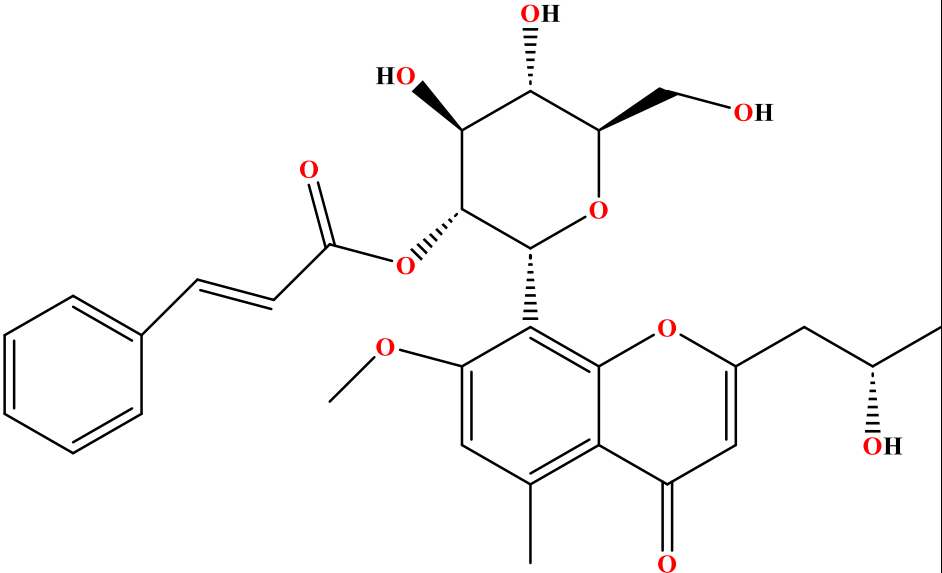
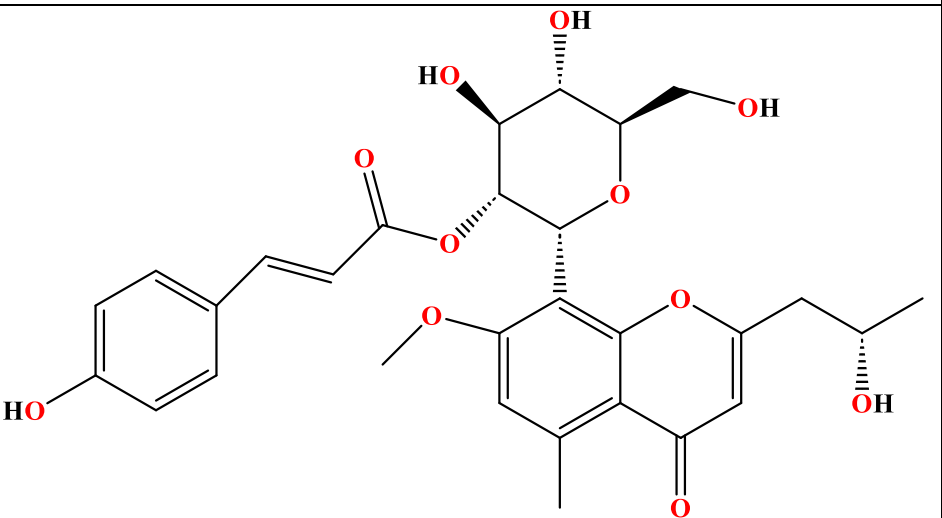


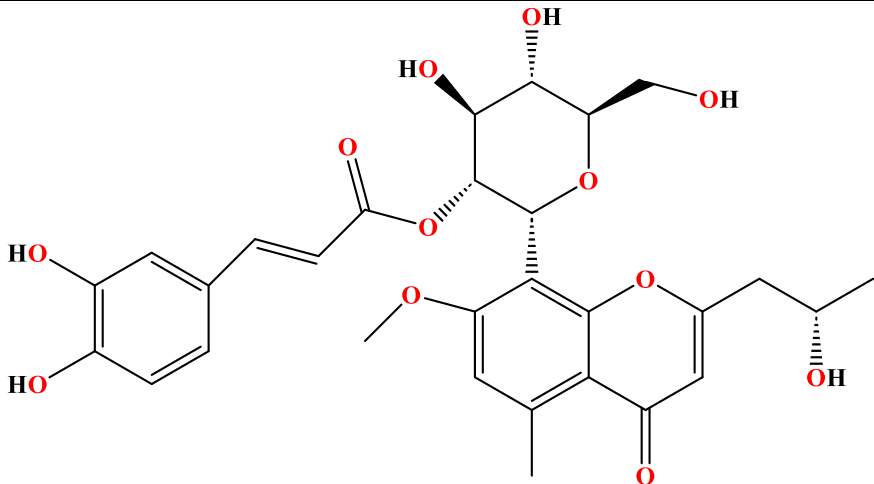
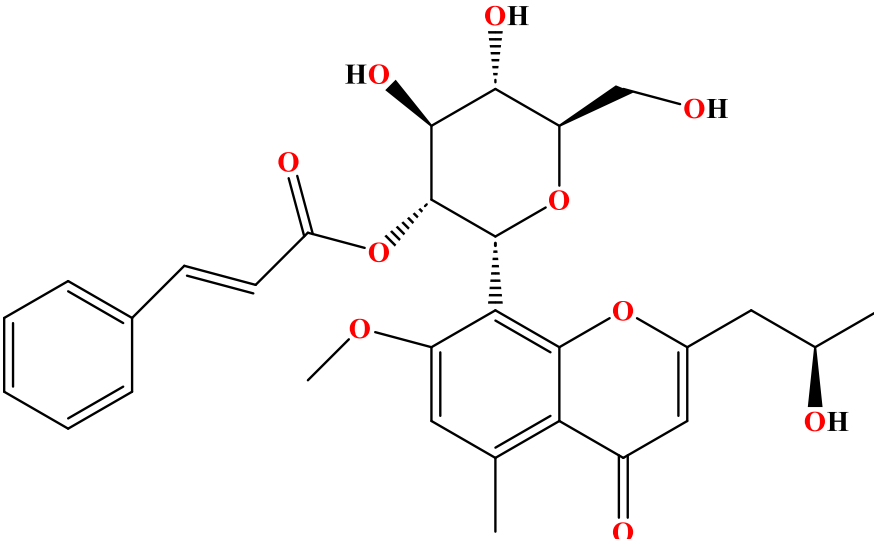
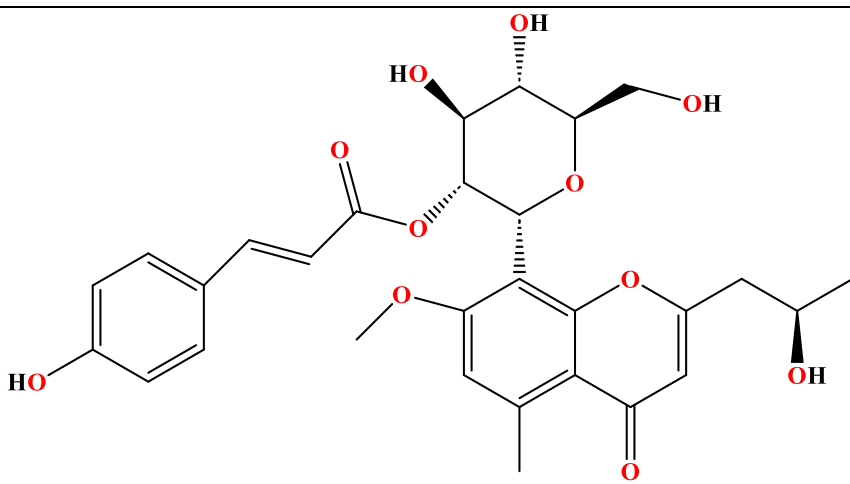
Table S1: Chemical structures, IUPAC names and 2D structure of aloe vera-derived compounds evaluated as inhibitors in atopic dermatitis therapeutics.

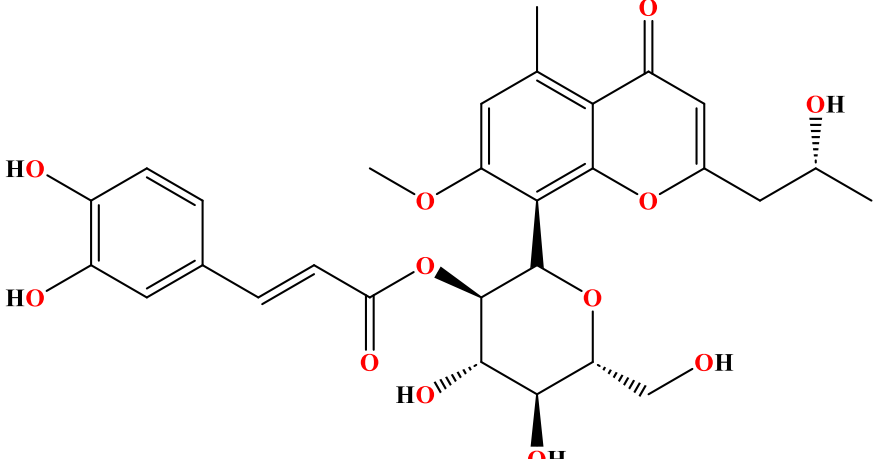
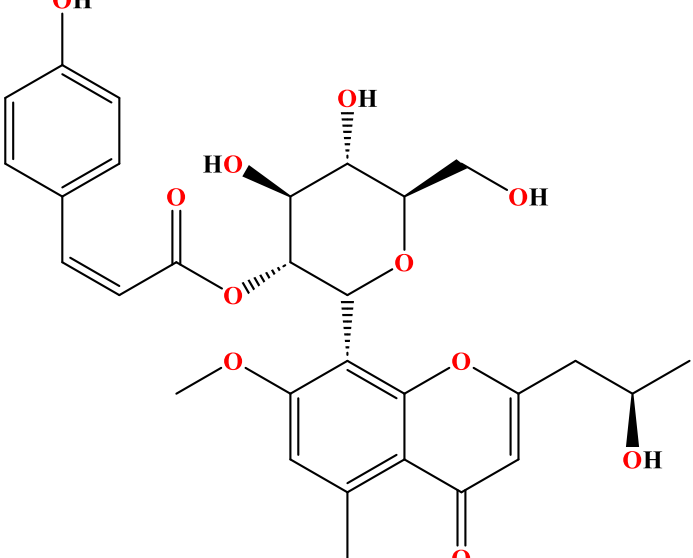
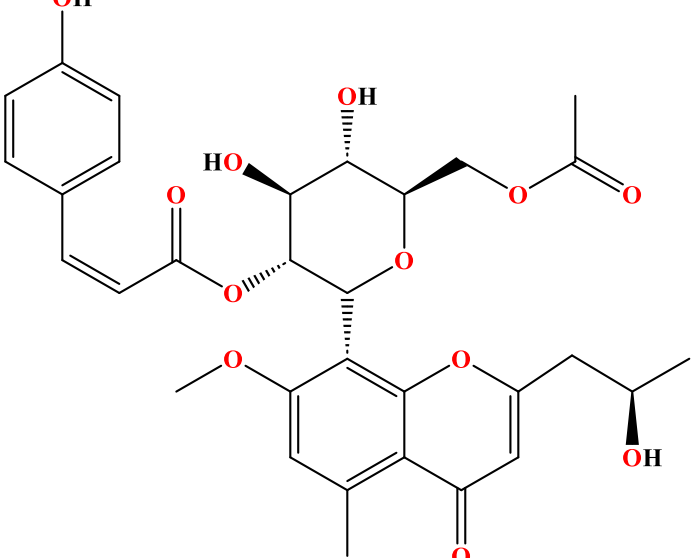
ID	IUPAC names	2D structure
M1	Aloesin	 The structure of Aloesin consists of a chromone core. At position 2, there is a 3-acetylpropyl side chain. At position 3, there is a hydroxyl group. At position 4, there is a glucose moiety attached via its C1. The glucose ring has hydroxyl groups at C2 (wedge), C3 (dash), C4 (wedge), and C6 (dash).
M2	Neoaloesin A	 The structure of Neoaloesin A features a chromone core. At position 2, there is a 3-acetylpropyl side chain. At position 3, there is a hydroxyl group. At position 4, there is a ribose moiety attached via its C1. The ribose ring has hydroxyl groups at C2 (wedge), C3 (dash), and C4 (wedge).
M3	8-C-glucosyl-(R)-aloesol	 The structure of 8-C-glucosyl-(R)-aloesol shows a chromone core. At position 2, there is a 1-hydroxyethyl side chain. At position 3, there is a hydroxyl group. At position 8, there is a glucose moiety attached via its C1. The glucose ring is in a chair conformation with hydroxyl groups at C2 (wedge), C3 (wedge), and C4 (wedge).

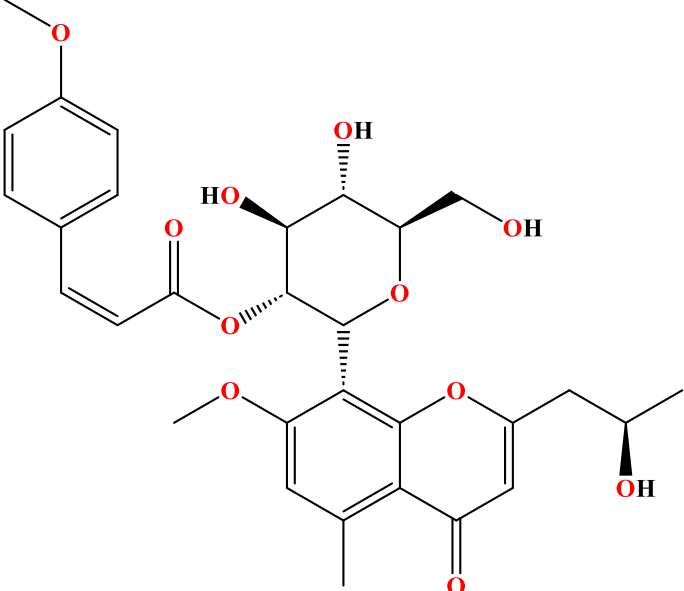
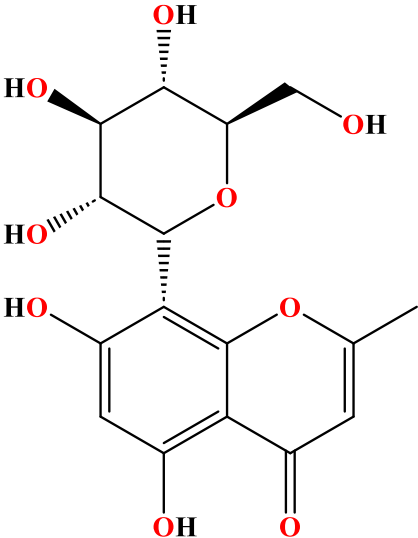
M4	8-C-glucosyl-7-methoxy-(R)-aloesol	
M5	8-C-glucosyl-(S)-aloesol	
M6	8-C-glucosyl-7-methoxy-(S)-aloesol	

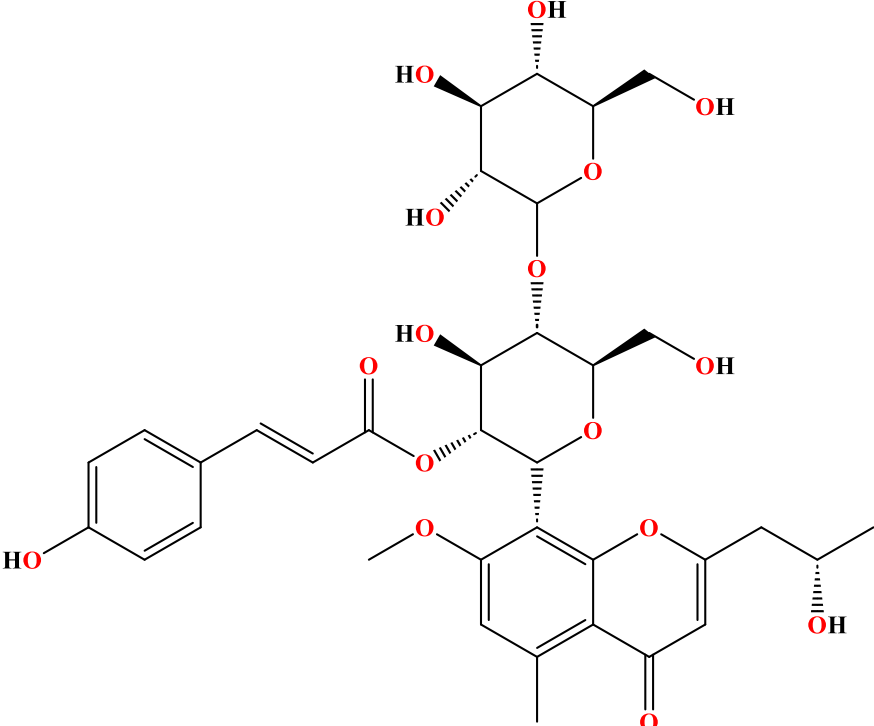
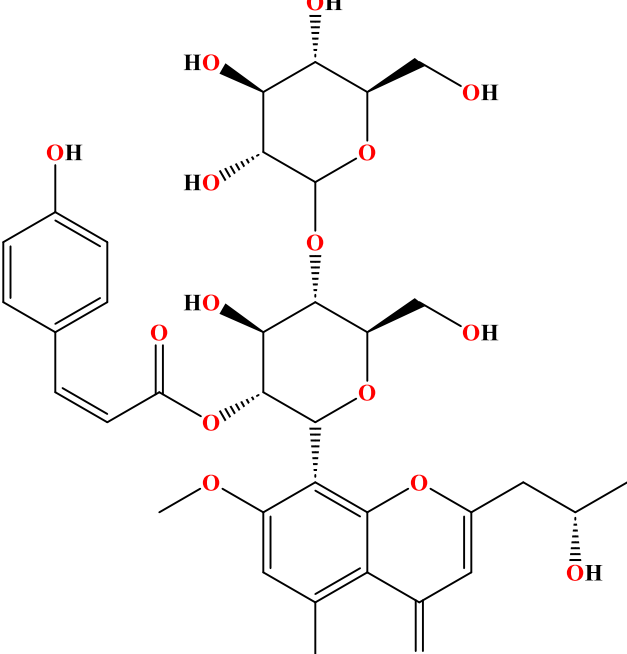
M7	8-C-glucosyl-7-O-methylaloediol	
M8	8-glucosyl-(2'-O-cinnamoyl)-7-O-methylaloediol A	
M9	8-glucosyl-(2'-O-cinnamoyl)-7-O-methylaloediol B	

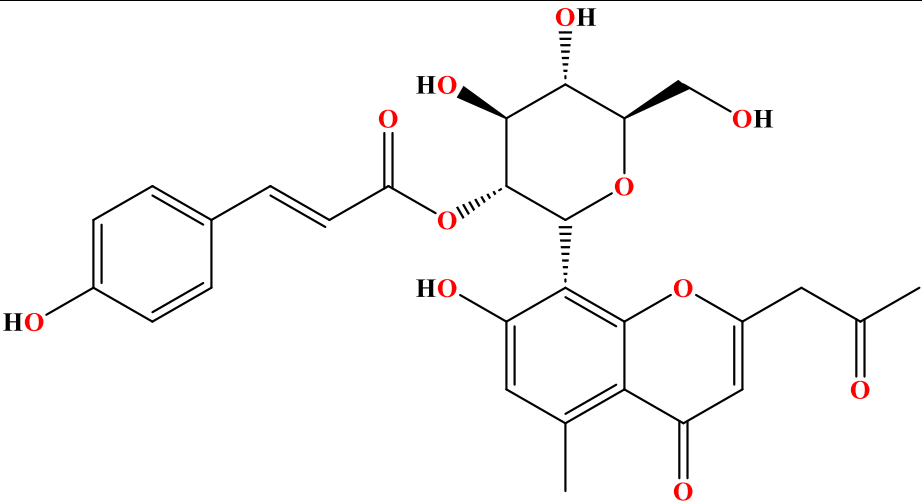
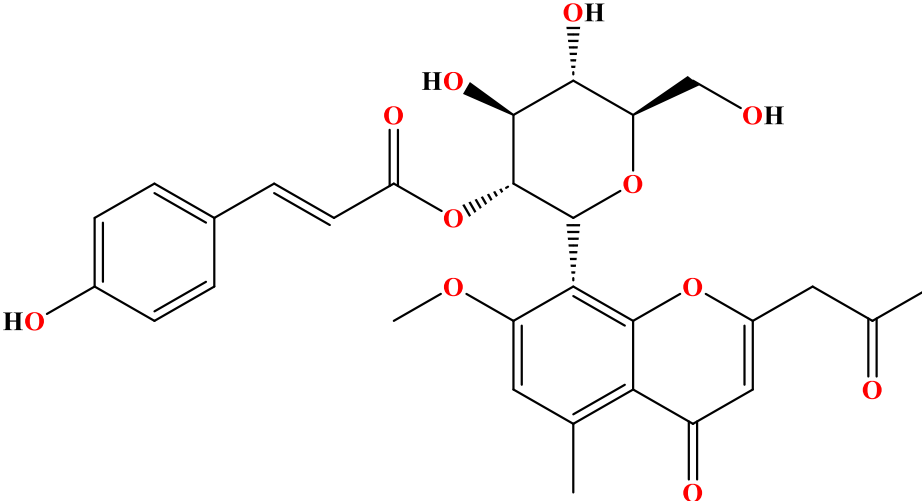
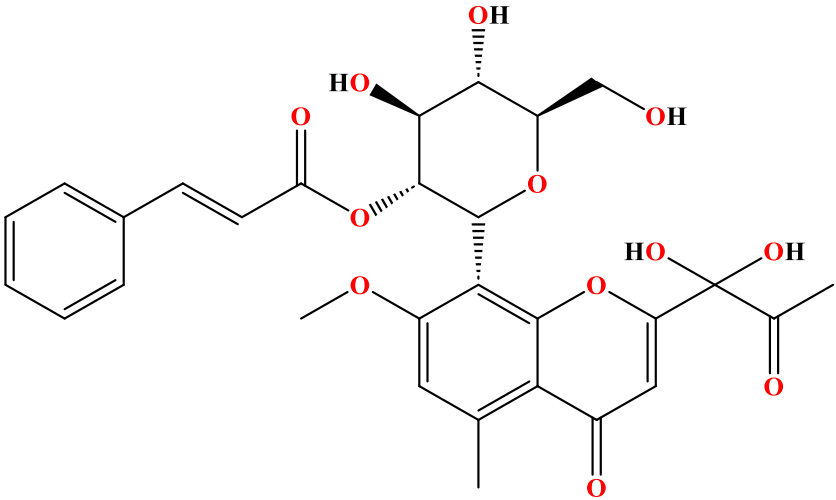
M10	C-2'-decoumaroyl- aloeresin G	
M11	Aloeresin E	
M12	Isoaloeresin D	

M13	Iso-rabaichromone	 The structure of Iso-rabaichromone features a 7-methoxy-5-methylchromone core. At the 2-position, it is substituted with a (R)-2-hydroxypropyl group (shown with a wedge bond to the hydroxyl group) and an 8-(3,4-dihydroxybenzylidene)acrylate group (shown with a dashed bond to the ester oxygen). The glucose moiety is attached at the 8-position via an ester linkage, with its anomeric carbon at C-1' and hydroxyl groups at C-2' (wedge), C-3' (dashed), and C-6' (wedge).
M14	8-[C-β-D-[2-O-(E)-cinnamoyl] glucopyranosyl]-2-[(R)-2-hydroxypropyl]-7-methoxy-5-methylchromone	 This structure is similar to Iso-rabaichromone but the benzene ring of the side chain is unsubstituted. It consists of a 7-methoxy-5-methylchromone core with a (R)-2-hydroxypropyl group at C-2 (wedge bond) and a 8-(3,4-dihydroxybenzylidene)acrylate group at C-8 (dashed bond to the ester oxygen). The glucose moiety is attached at C-8 via an ester linkage, with hydroxyl groups at C-2' (wedge), C-3' (dashed), and C-6' (wedge).
M15	Aloeresin D	 The structure of Aloeresin D features a 7-methoxy-5-methylchromone core. At the 2-position, it is substituted with a (R)-2-hydroxypropyl group (shown with a wedge bond to the hydroxyl group) and an 8-(4-hydroxybenzylidene)acrylate group (shown with a dashed bond to the ester oxygen). The glucose moiety is attached at the 8-position via an ester linkage, with its anomeric carbon at C-1' and hydroxyl groups at C-2' (wedge), C-3' (dashed), and C-6' (wedge).

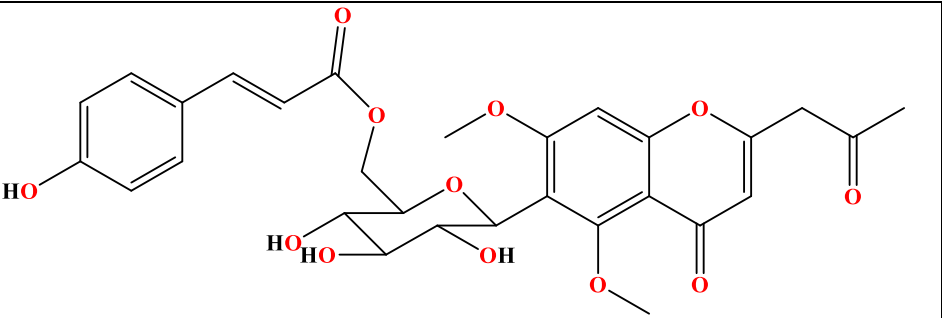
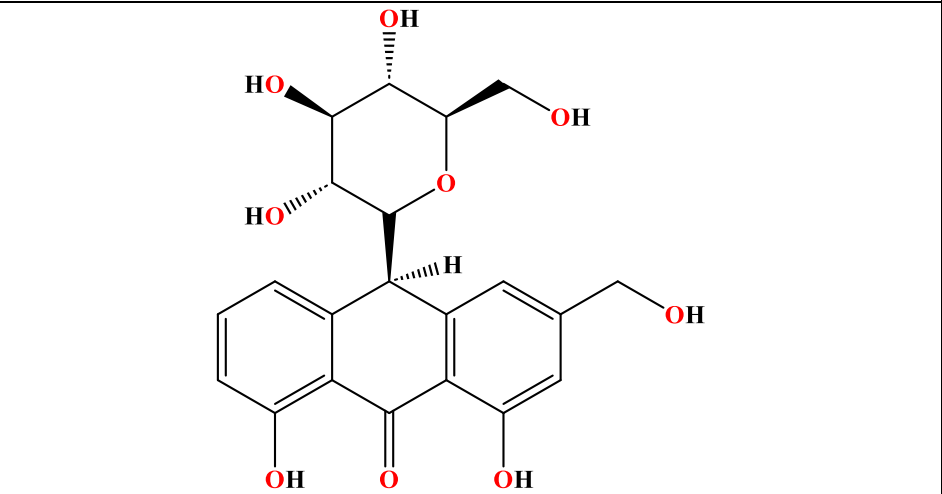
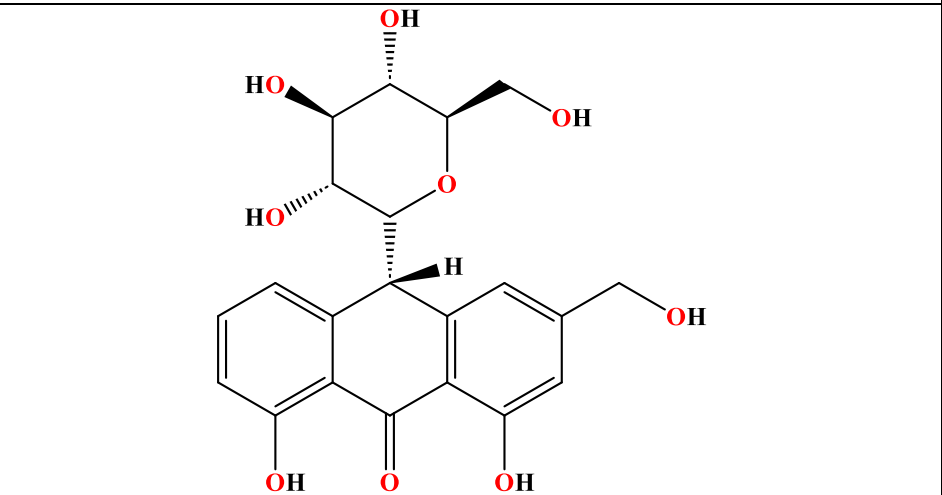
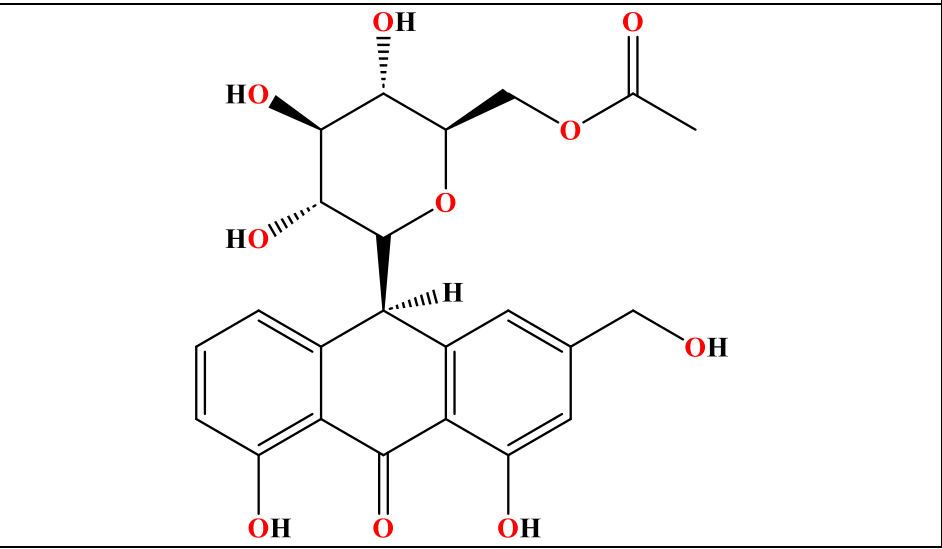
M16	Rabaichromone	 The chemical structure of Rabaichromone features a central pyranose ring. At the C1 position, there is a p-coumaroyl group (a benzene ring with two adjacent hydroxyl groups at the 3 and 4 positions, connected via a trans-vinyl group to a carbonyl group, which is esterified to the C1 of the pyranose). At the C2 position, there is a 6-methoxy-8-(1-hydroxyethyl)-2,4-dimethylchromone moiety. The pyranose ring also has hydroxyl groups at C3 (dashed), C4 (wedged), and C5 (dashed).
M17	Allo-aloeresin D	 The chemical structure of Allo-aloeresin D consists of a central pyranose ring. At the C1 position, it has a p-coumaroyl group. At the C2 position, it is linked to a 6-methoxy-8-(1-hydroxyethyl)-2,4-dimethylchromone moiety. The pyranose ring has hydroxyl groups at C3 (wedged), C4 (dashed), and C6 (wedged).
M18	Aloeresin K	 The chemical structure of Aloeresin K is similar to Allo-aloeresin D, with a central pyranose ring, a p-coumaroyl group at C1, and a 6-methoxy-8-(1-hydroxyethyl)-2,4-dimethylchromone moiety at C2. However, the pyranose ring has a different stereochemistry: hydroxyl groups at C3 (wedged), C4 (wedged), and C6 (wedged).

M19	Aloeresin J	 The chemical structure of Aloeresin J is a complex molecule. It features a central chromone core. At the 8-position of the chromone, there is a glucose moiety attached via a glycosidic bond. The glucose ring has several hydroxyl groups: a dashed OH at C2, a wedged OH at C3, a dashed OH at C4, and a wedged CH2OH group at C6. At the 3-position of the chromone, there is a side chain consisting of a methoxy group, a double bond, and a carboxylic acid group. The carboxylic acid group is further substituted with a 4-methoxyphenyl group.
M20	8-C-glucosyl-noreugenin	 The chemical structure of 8-C-glucosyl-noreugenin is a chromone derivative. It features a central chromone core. At the 8-position of the chromone, there is a glucose moiety attached via a glycosidic bond. The glucose ring has several hydroxyl groups: a dashed OH at C2, a wedged OH at C3, a dashed OH at C4, and a wedged CH2OH group at C6. The chromone core has a hydroxyl group at the 6-position and a methyl group at the 7-position.

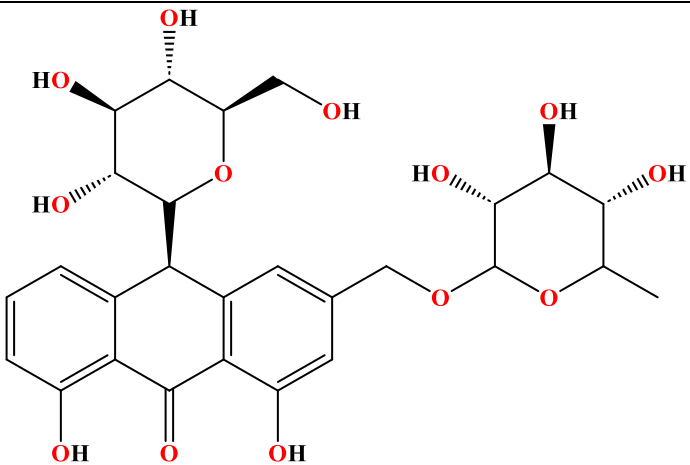
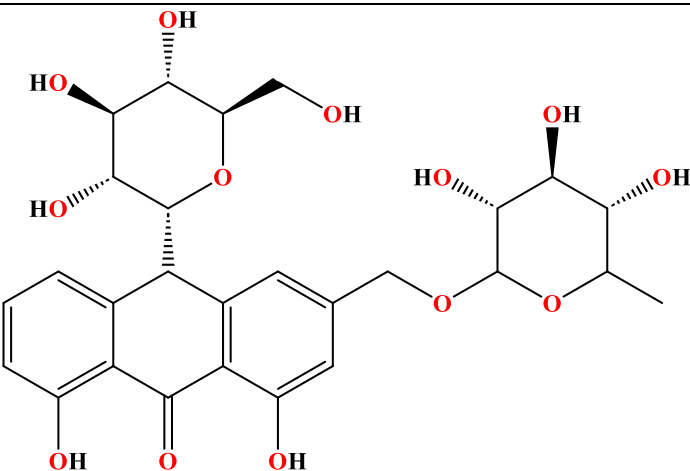
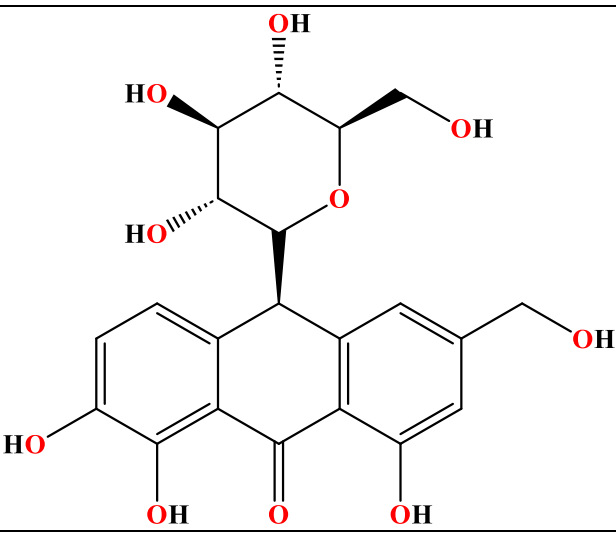
M21	4'-O-glucosyl- isoaloeresin DI	
M22	4'-O-glucosyl- isoaloeresin DII	

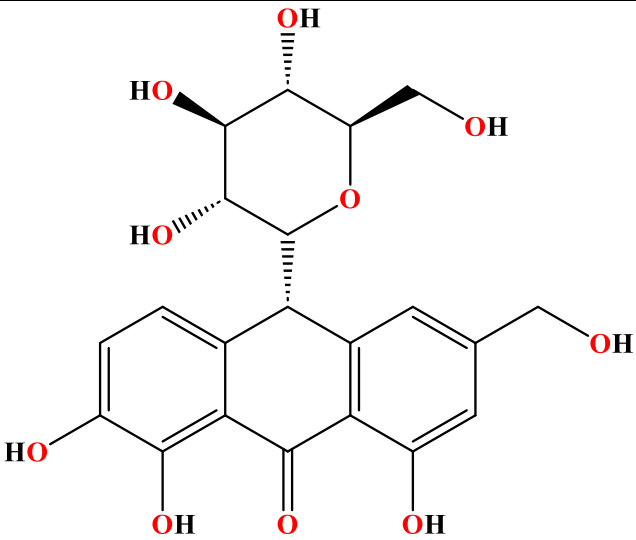
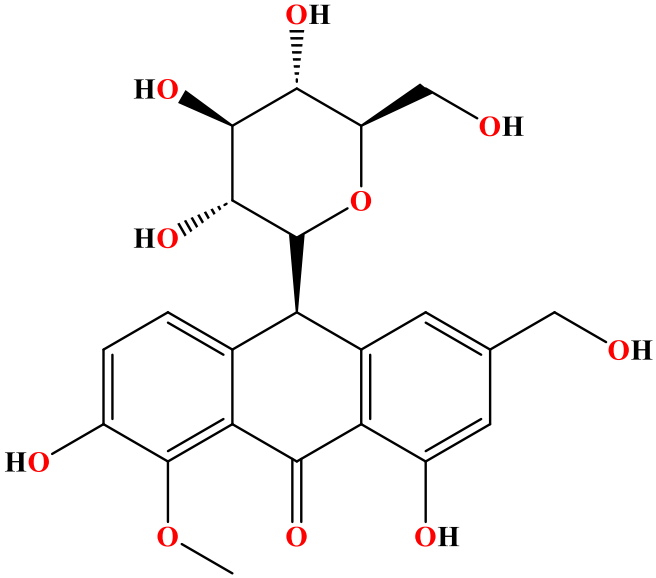
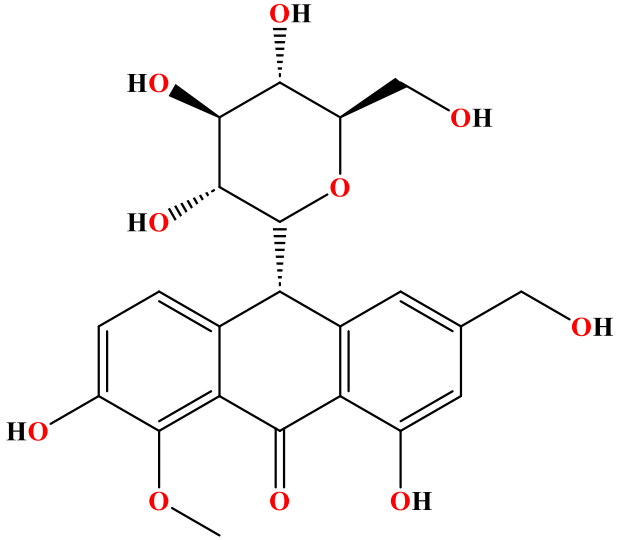
M23	Aloeresin A	 The chemical structure of Aloeresin A consists of a 4-hydroxybenzyl group attached to a (Z)-cinnamoyl moiety, which is esterified to a pyranose ring. The pyranose ring has a hydroxyl group at C2 (dashed), a hydroxymethyl group at C3 (wedged), and a hydroxyl group at C4 (dashed). This pyranose is linked at its C1 position to the C7 position of a chromone core. The chromone core has a methyl group at C6, a carbonyl group at C4, and a 2-acetyl-2-hydroxyethyl side chain at C2.
M24	7-O-methyl-aloesresin A	 The chemical structure of 7-O-methyl-aloesresin A is identical to Aloeresin A, except for the presence of a methoxy group at the C7 position of the chromone core, instead of the hydroxyl group.
M25	9-dihydroxyl-2'-O-(Z)-cinnamoyl-7-methoxy-aloesin	 The chemical structure of 9-dihydroxyl-2'-O-(Z)-cinnamoyl-7-methoxy-aloesin features a (Z)-cinnamoyl group attached to a pyranose ring. The pyranose ring has a hydroxyl group at C2 (dashed), a hydroxymethyl group at C3 (wedged), and a hydroxyl group at C4 (dashed). This pyranose is linked at its C1 position to the C7 position of a chromone core. The chromone core has a methyl group at C6, a carbonyl group at C4, and a 2,2-dihydroxy-2-methylpropyl side chain at C2. Additionally, there is a methoxy group at the C9 position of the chromone core.

M26	6'-O-coumaroyl-aloesin	
M27	7-methoxy-6'-O-coumaroyl-aloesin	
M28	Aloeveraside B	

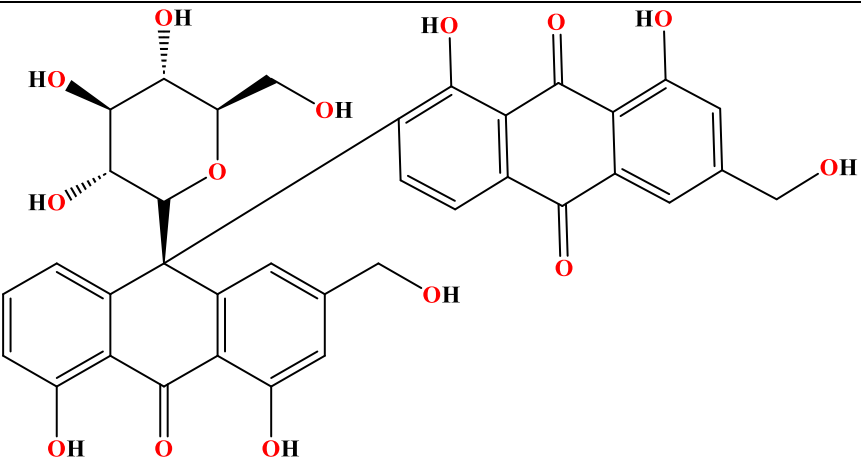
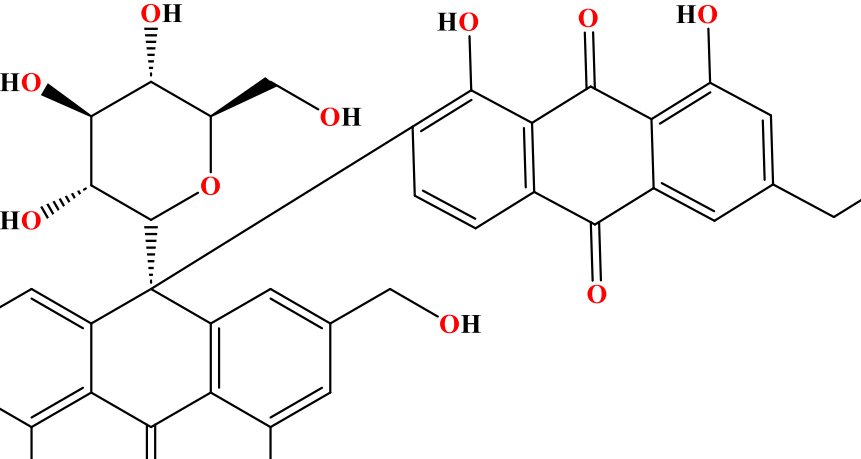
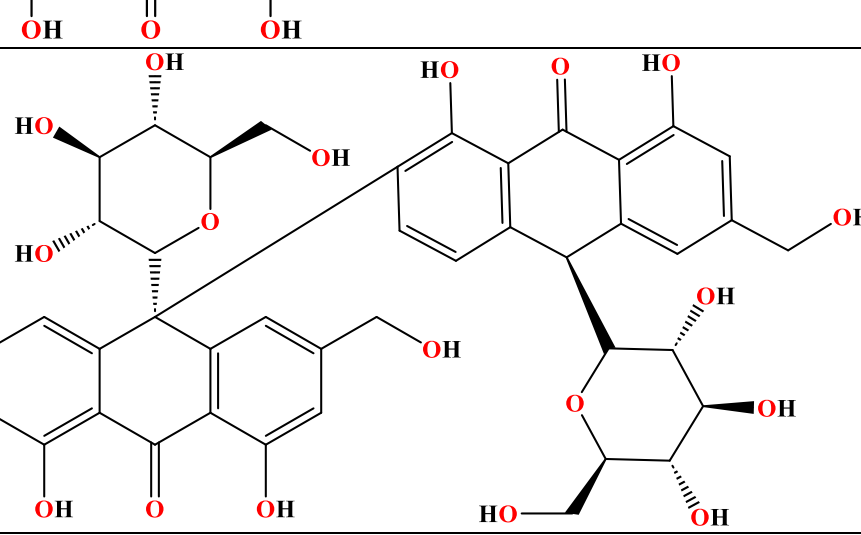
M29	Aloeveraside A	
M30	Aloin A	
M31	Aloin B	
M32	6'-O-acetyl-aloin A	

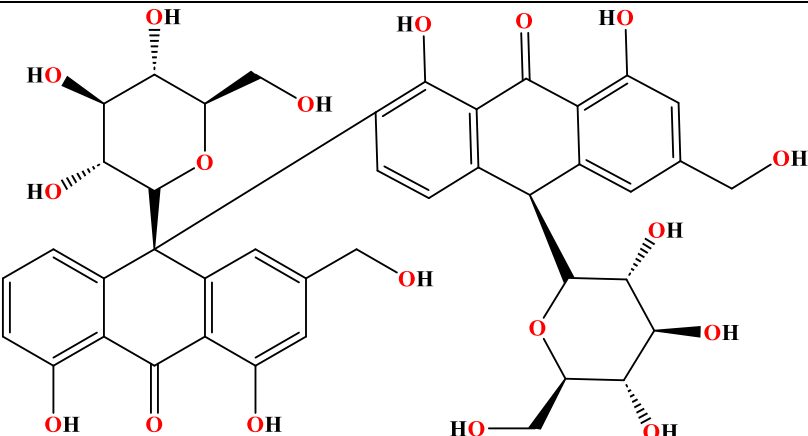
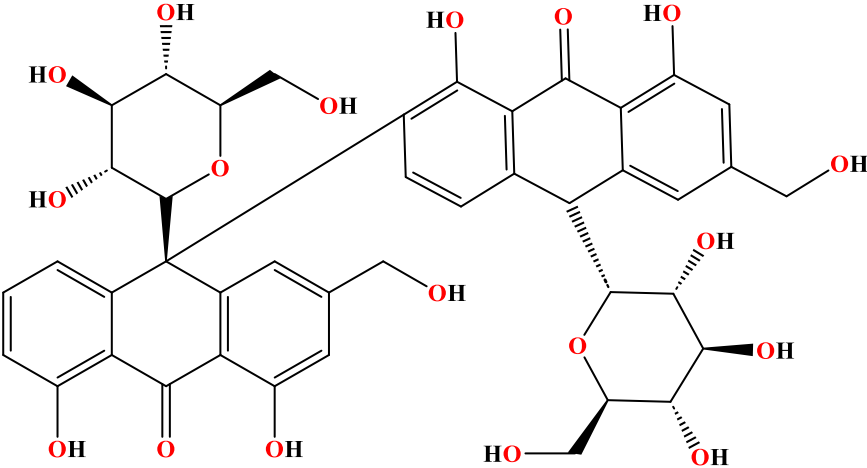
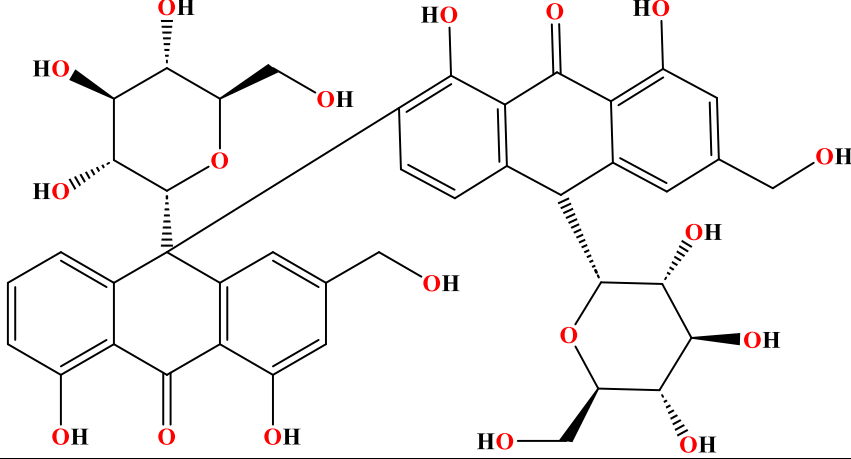
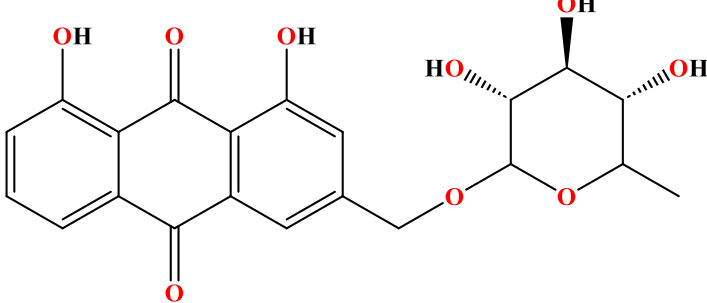
M33	6'-O-acetyl-aloin B	
M34	10-hydroxyaloin A	
M35	10-hydroxyaloin B	

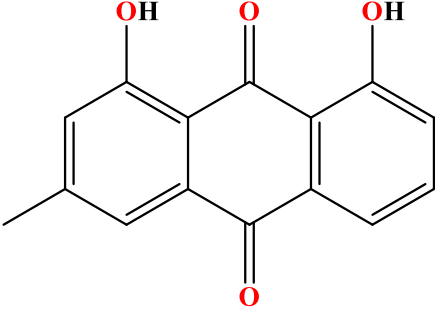
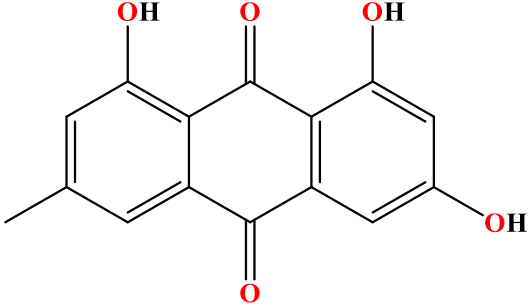
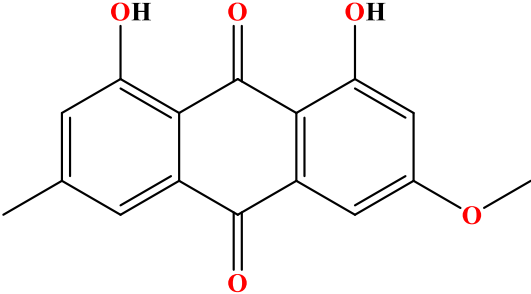
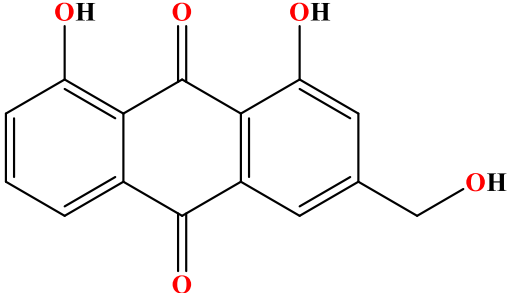
M36	Aloinoside A	 The chemical structure of Aloinoside A features a central anthraquinone core. The anthraquinone has hydroxyl groups at positions 1, 3, and 8, and a carbonyl group at position 9. At position 4, there is a glycosidic linkage to a glucose molecule. The glucose is in its cyclic form, with hydroxyl groups at positions 2, 3, and 6. At position 7, there is another glycosidic linkage to a second glucose molecule. This second glucose is also in its cyclic form, with hydroxyl groups at positions 2, 3, and 6.
M37	Aloinoside B	 The chemical structure of Aloinoside B is identical to Aloinoside A. It consists of an anthraquinone core with hydroxyl groups at positions 1, 3, and 8, and a carbonyl group at position 9. It has a glucose molecule attached at position 4 and another glucose molecule attached at position 7, both in their cyclic forms with hydroxyl groups at positions 2, 3, and 6.
M38	7-hydroxyaloin A	 The chemical structure of 7-hydroxyaloin A features a central anthraquinone core. The anthraquinone has hydroxyl groups at positions 1, 3, and 8, and a carbonyl group at position 9. At position 4, there is a glycosidic linkage to a glucose molecule. The glucose is in its cyclic form, with hydroxyl groups at positions 2, 3, and 6. At position 7, there is a hydroxyl group instead of a glycosidic linkage.

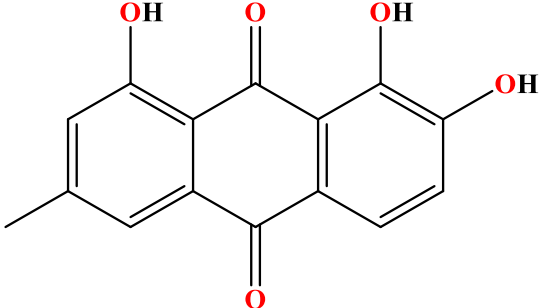
M39	7-hydroxyaloin B	
M40	7-hydroxy-8-O-methylaloin A	
M41	7-hydroxy-8-O-methylaloin B	

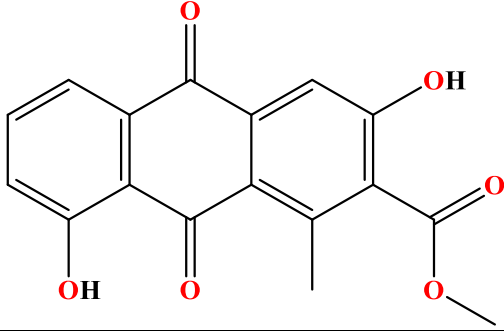
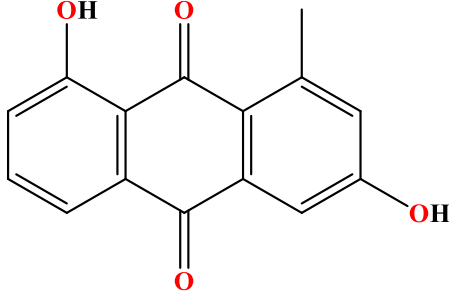
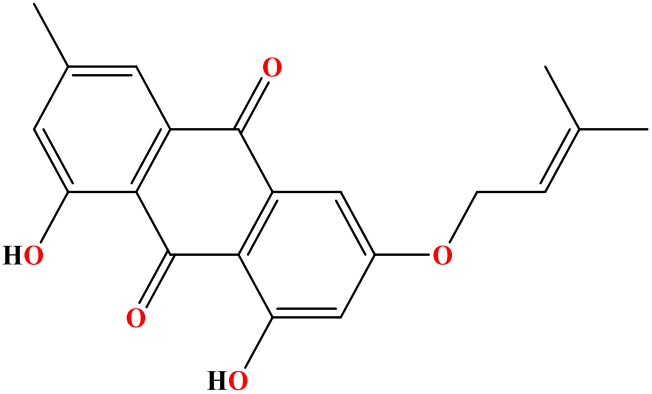
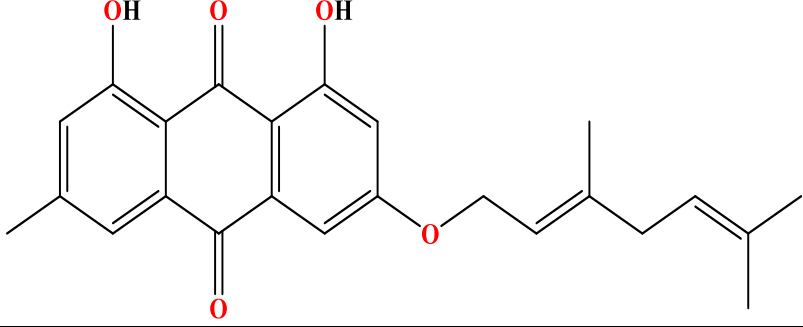
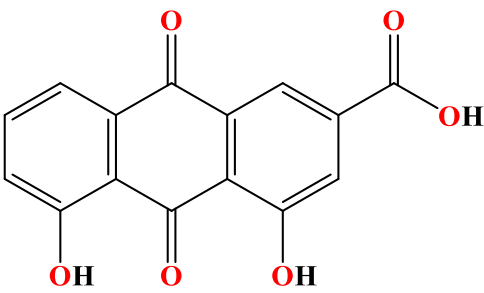
M42	6'-malonylnataloin A	
M43	6'-malonylnataloin B	
M44	Homonataloside B	

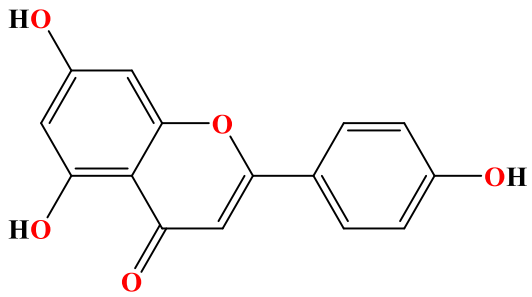
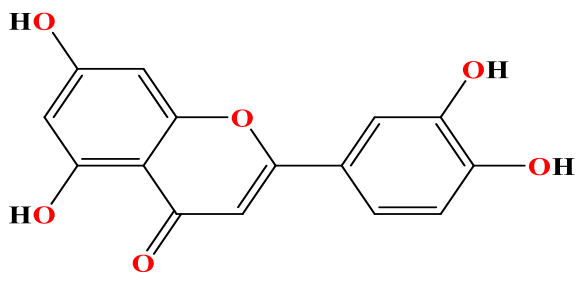
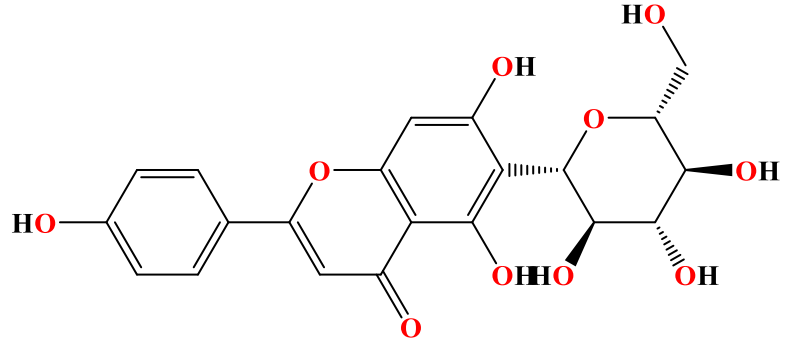
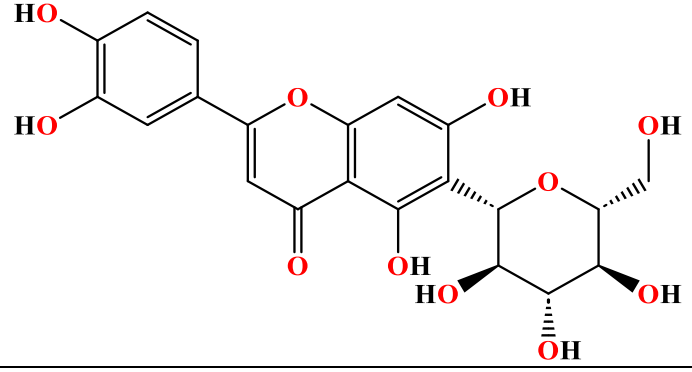
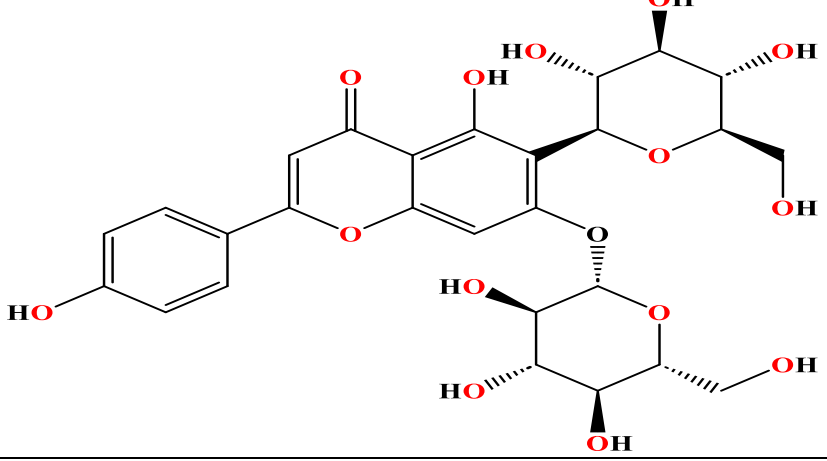
M45	Elgonica dimer A	 Chemical structure of Elgonica dimer A. It consists of two 3,5,6-trihydroxy-2,4-dioxocyclohexa-1,4-diene units linked by a central ether bridge. The left unit has a hydroxyl group at C3 (dashed), a hydroxyl group at C4 (wedged), and a hydroxyl group at C6 (wedged). The right unit has a hydroxyl group at C3 (wedged), a hydroxyl group at C4 (wedged), and a hydroxyl group at C6 (wedged). The central ether bridge connects the C1 of the left unit to the C1 of the right unit.
M46	Elgonica dimer B	 Chemical structure of Elgonica dimer B. It consists of two 3,5,6-trihydroxy-2,4-dioxocyclohexa-1,4-diene units linked by a central ether bridge. The left unit has a hydroxyl group at C3 (dashed), a hydroxyl group at C4 (wedged), and a hydroxyl group at C6 (wedged). The right unit has a hydroxyl group at C3 (wedged), a hydroxyl group at C4 (wedged), and a hydroxyl group at C6 (wedged). The central ether bridge connects the C1 of the left unit to the C1 of the right unit.
M47	Aloindimer A	 Chemical structure of Aloindimer A. It consists of two 3,5,6-trihydroxy-2,4-dioxocyclohexa-1,4-diene units linked by a central ether bridge. The left unit has a hydroxyl group at C3 (dashed), a hydroxyl group at C4 (wedged), and a hydroxyl group at C6 (wedged). The right unit has a hydroxyl group at C3 (wedged), a hydroxyl group at C4 (wedged), and a hydroxyl group at C6 (wedged). The central ether bridge connects the C1 of the left unit to the C1 of the right unit.

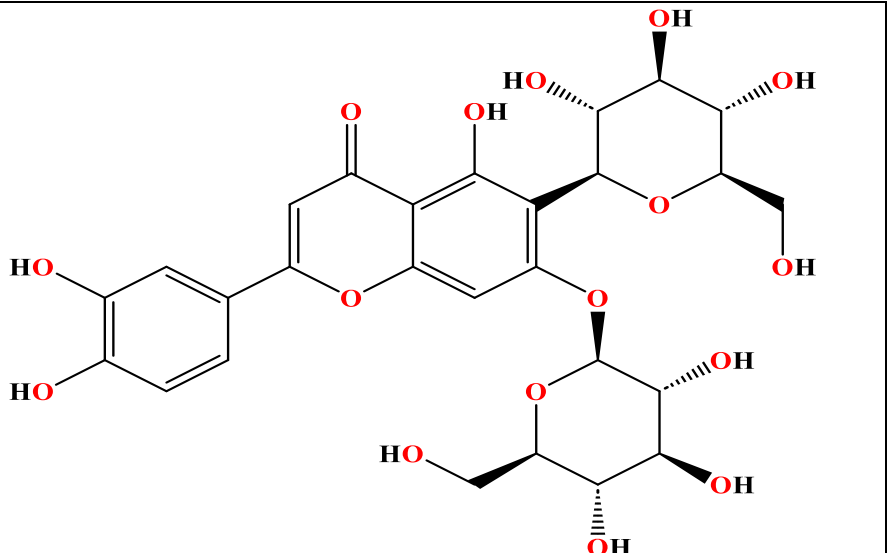
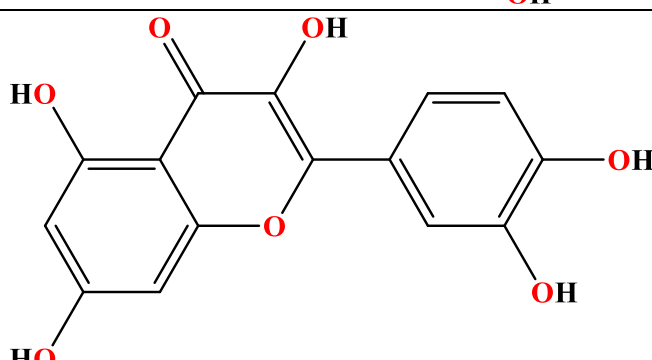
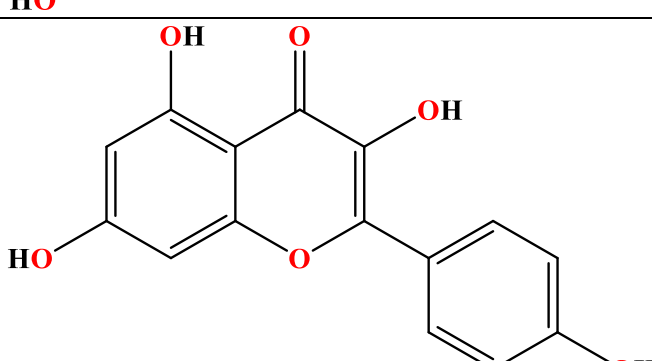
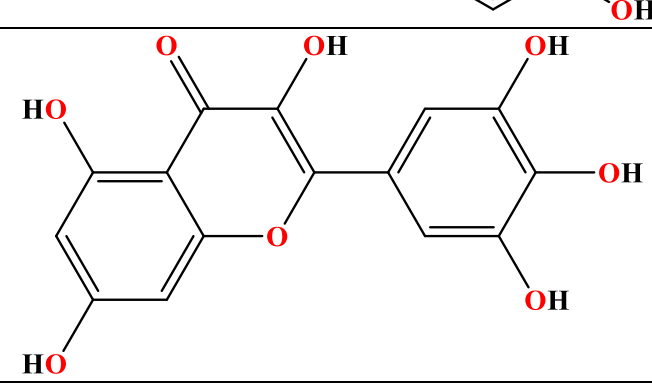
M48	Aloindimer B	
M49	Aloindimer C	
M50	Aloindimer D	
M51	Aloe-emodin-11-O-rhamnoside	

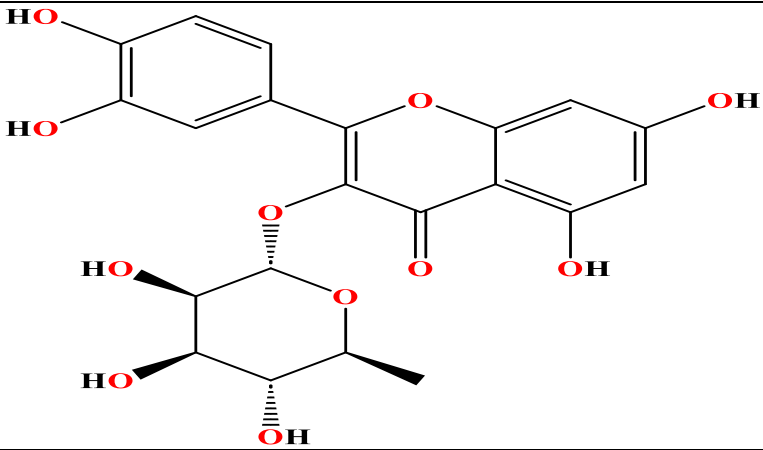
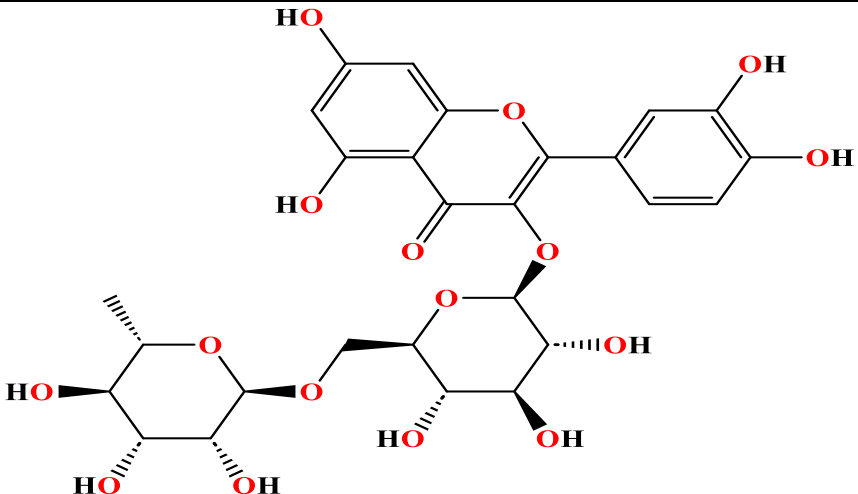
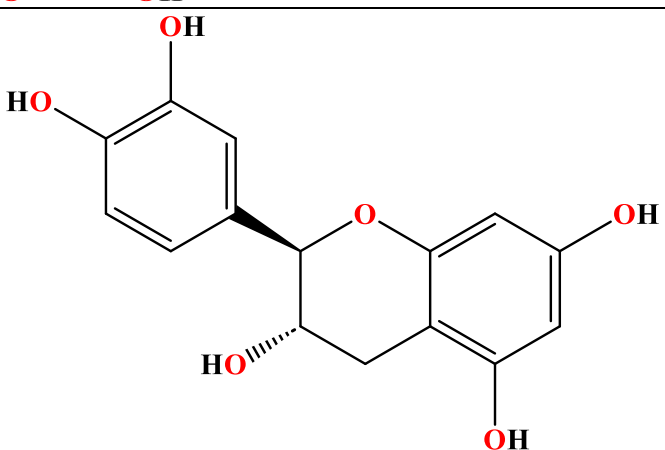
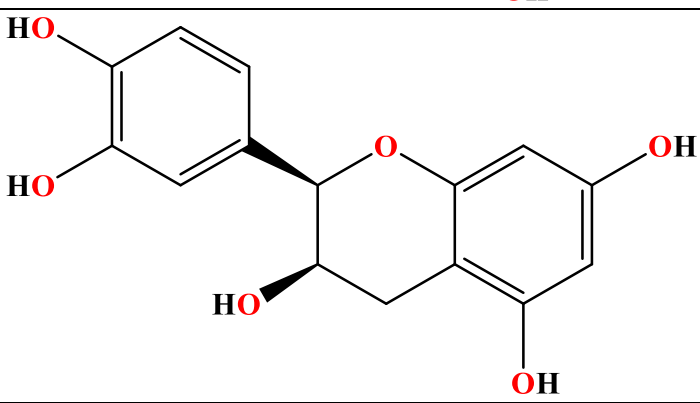
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M53	Emodin	
M54	Physcione	
M55	Aloe-emodin	

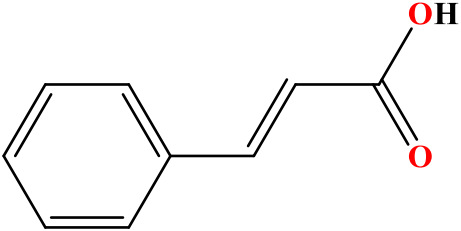
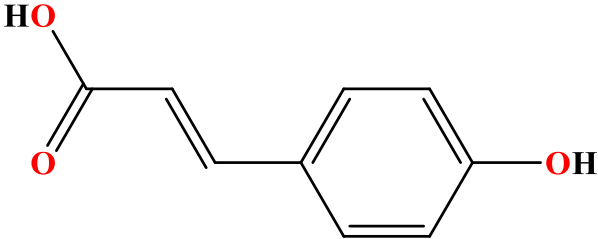
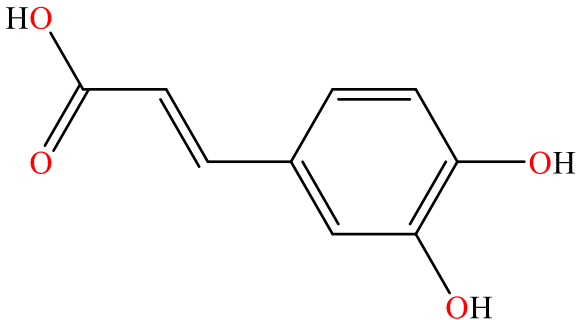
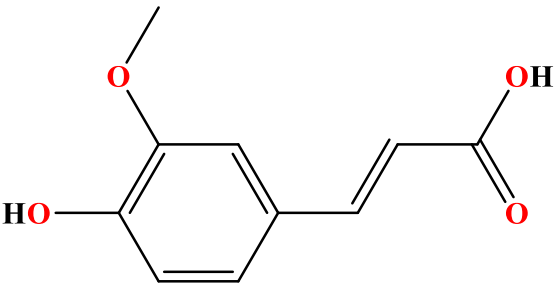
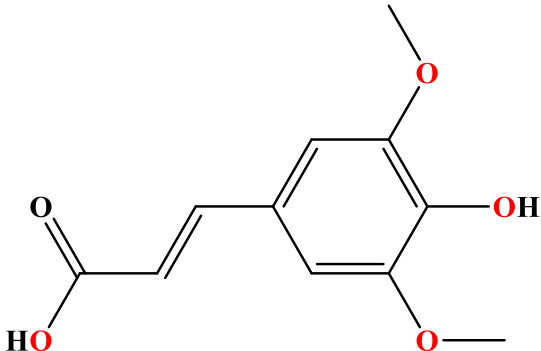
M56	Nataloe-emodin	
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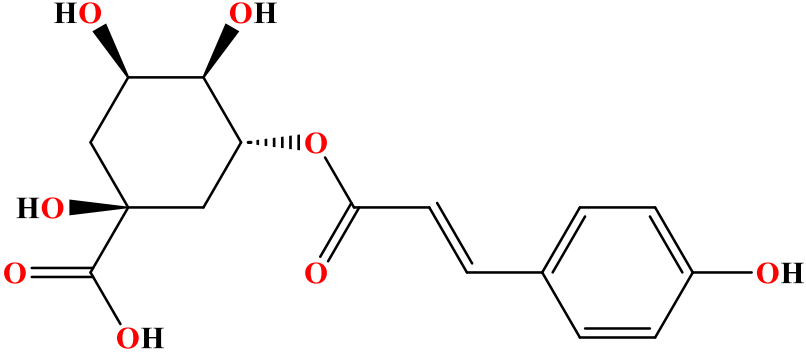
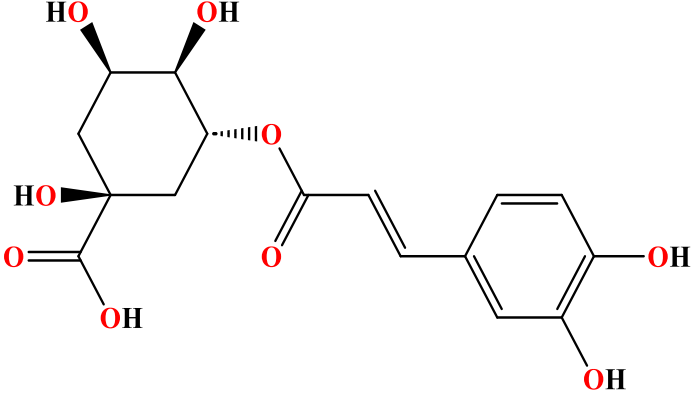
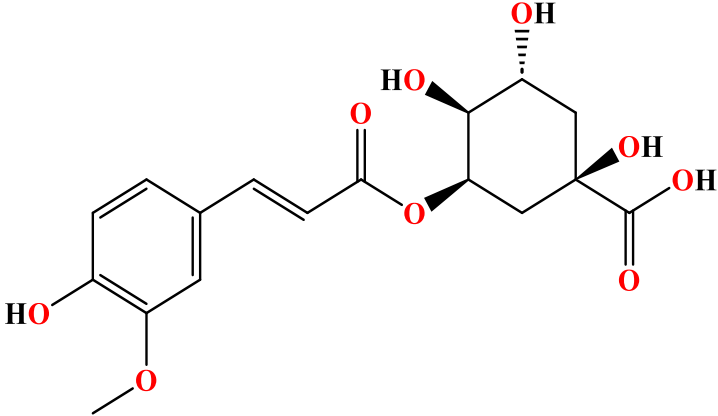
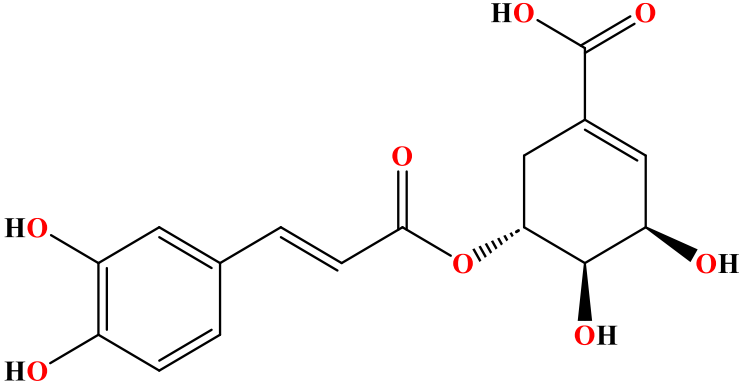
M57	Aloesaponarin I	
M58	Aloesaponarin II	
M59	Madagascine	
M60	3-Geranyloxyemodin	
M61	Rhein	

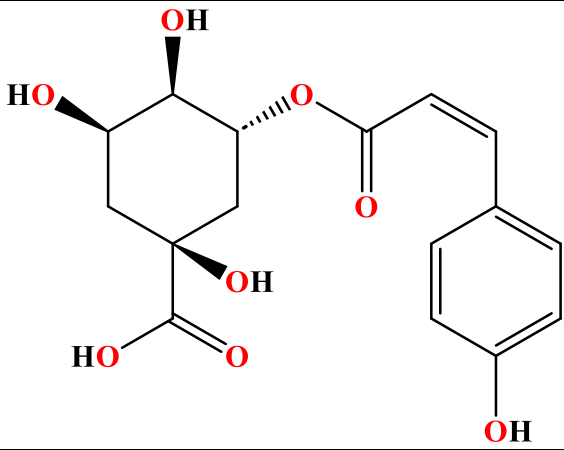
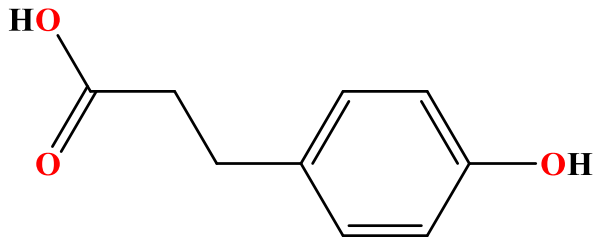
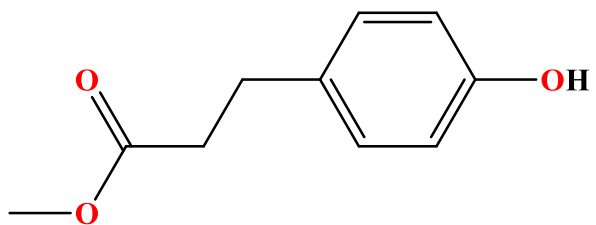
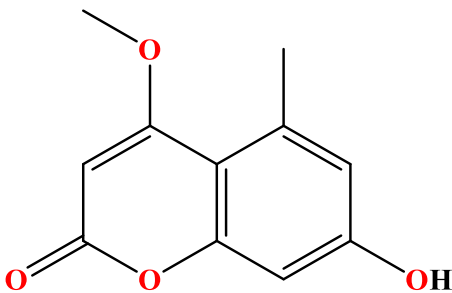
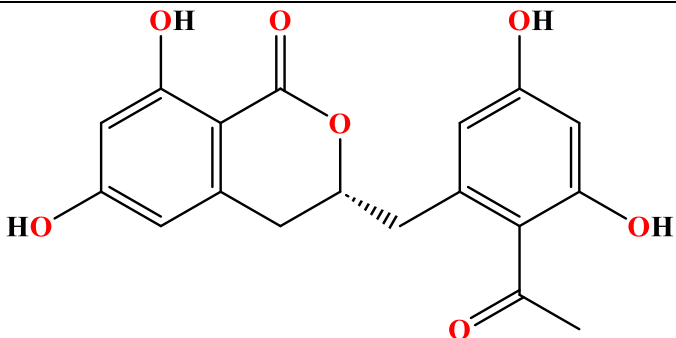
M62	Apigenin	
M63	Luteolin	
M64	Isovitexin	
M65	Isoorientin	
M66	Saponarin	

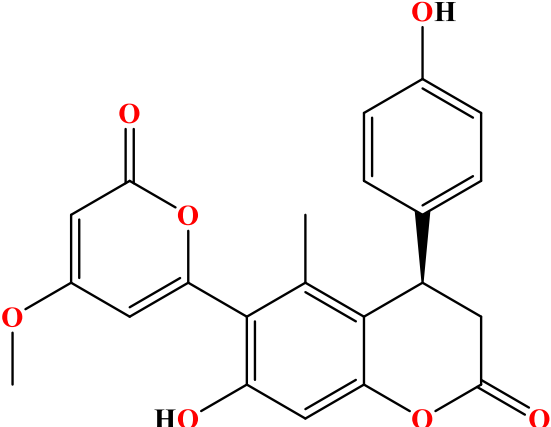
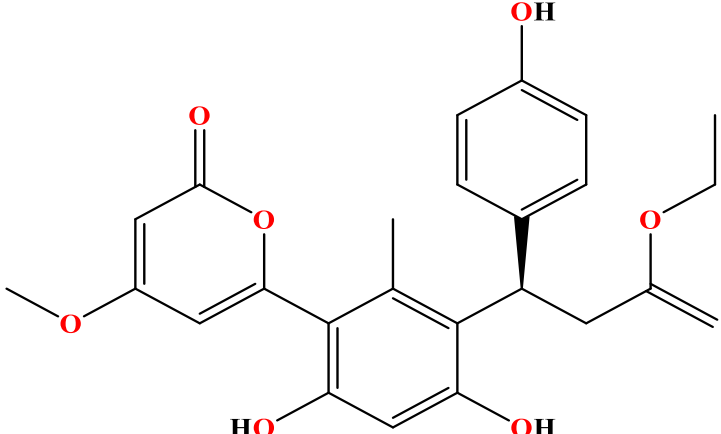
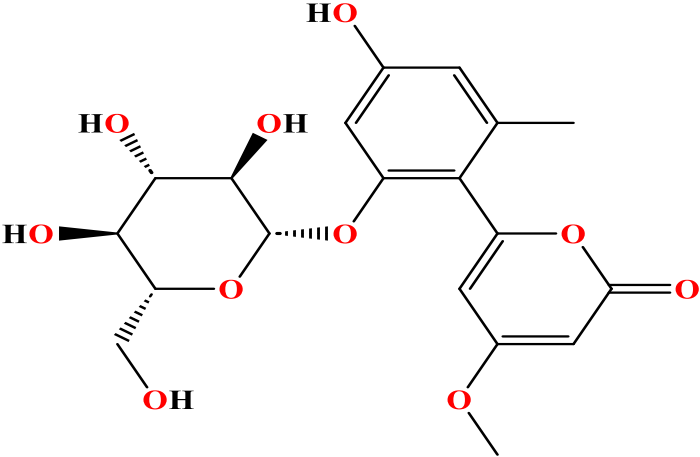
M67	Lutonarin	 The chemical structure of Lutonarin is a complex polyphenolic compound. It features a central chromone core. At the 2-position of the chromone, there is a 3,4-dihydroxyphenyl group. At the 3-position, there is a hydroxyl group. At the 4-position, there is a 3,4,5-trihydroxyphenyl group. At the 7-position, there is a 3,4,5-trihydroxyphenyl group. The structure is highly symmetrical and contains multiple hydroxyl groups.
M68	Quercetin	 The chemical structure of Quercetin is a flavonoid. It consists of a chromone core with a 3,4,5-trihydroxyphenyl group at the 2-position and a 3,4-dihydroxyphenyl group at the 3-position. The structure is highly symmetrical and contains multiple hydroxyl groups.
M69	Kaempferol	 The chemical structure of Kaempferol is a flavonoid. It consists of a chromone core with a 3,4,5-trihydroxyphenyl group at the 2-position and a 3,4-dihydroxyphenyl group at the 3-position. The structure is highly symmetrical and contains multiple hydroxyl groups.
M70	Myricetin	 The chemical structure of Myricetin is a flavonoid. It consists of a chromone core with a 3,4,5-trihydroxyphenyl group at the 2-position and a 3,4-dihydroxyphenyl group at the 3-position. The structure is highly symmetrical and contains multiple hydroxyl groups.

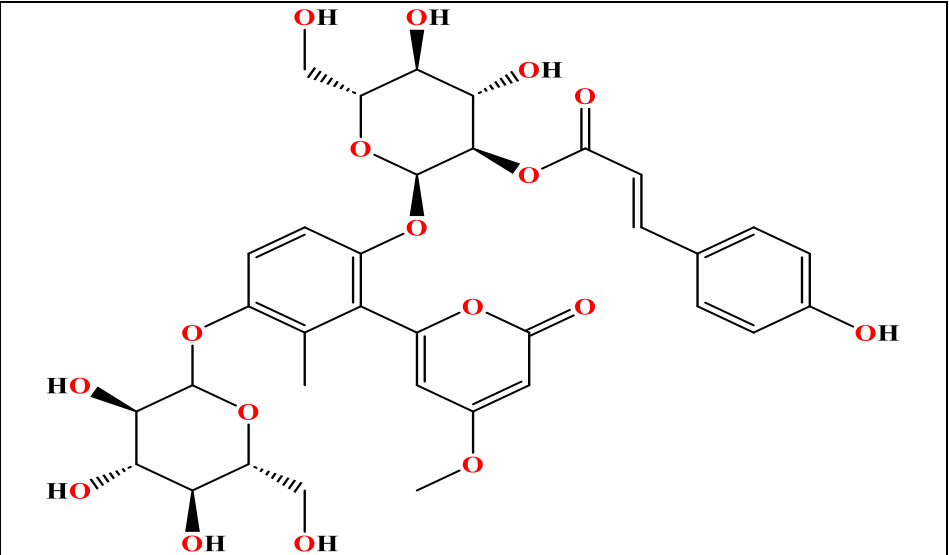
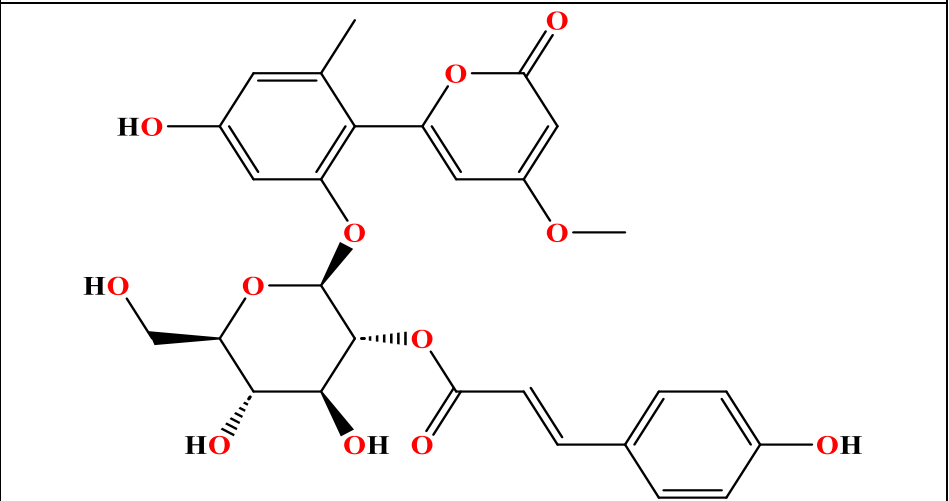
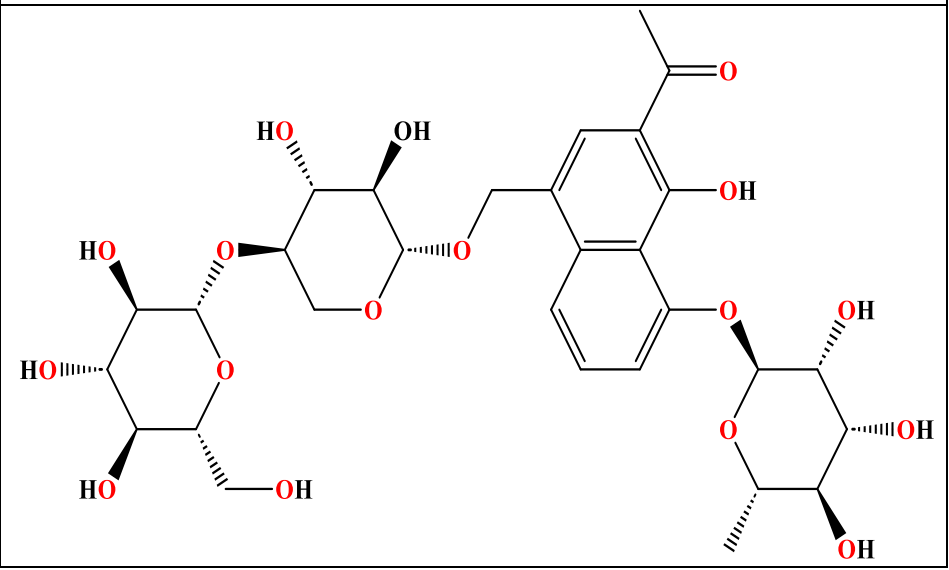
M71	Quercitrin	 The chemical structure of Quercitrin consists of a quercetin aglycone linked to a rhamnoside sugar. The quercetin part features a central chromone ring with hydroxyl groups at positions 2, 3, 6, and 7. A 3,4,5-trihydroxyphenyl group is attached at position 4. The rhamnoside sugar is a six-membered ring with hydroxyl groups at positions 1, 2, 3, and 6, and a methyl group at position 5. The linkage is an O-glycosidic bond at the 3-position of the quercetin.
M72	Rutin	 The chemical structure of Rutin is a flavonoid glycoside. It features a quercetin aglycone linked to a rutinose sugar. The quercetin part is identical to the one in Quercitrin. The rutinose sugar is a disaccharide composed of a glucose unit and a rhamnose unit. The glucose unit is linked to the quercetin at its 1-position, and the rhamnose unit is linked to the glucose at its 6-position. The rutinose sugar has multiple hydroxyl groups and a methyl group.
M73	Catechin	 The chemical structure of Catechin is a flavan-3-ol. It consists of a chromane ring system. The A-ring has a hydroxyl group at position 5 and a hydroxyl group at position 2. The B-ring has hydroxyl groups at positions 2 and 6. The C-ring has a hydroxyl group at position 3 and a hydroxyl group at position 4. The D-ring has a hydroxyl group at position 1 and a hydroxyl group at position 2.
M74	Epicatechin	 The chemical structure of Epicatechin is a flavan-3-ol, similar to Catechin but with a different stereochemistry at the 2-position of the D-ring. It consists of a chromane ring system. The A-ring has a hydroxyl group at position 5 and a hydroxyl group at position 2. The B-ring has hydroxyl groups at positions 2 and 6. The C-ring has a hydroxyl group at position 3 and a hydroxyl group at position 4. The D-ring has a hydroxyl group at position 1 and a hydroxyl group at position 2.

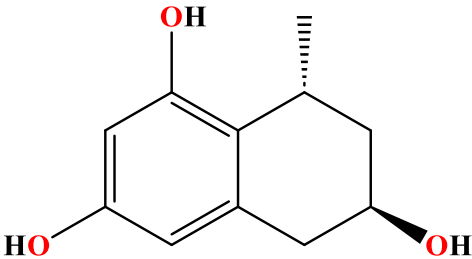
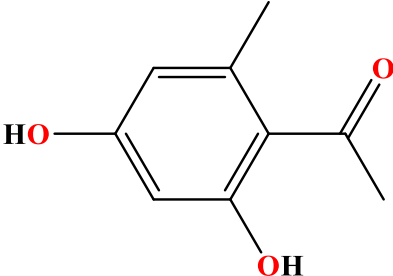
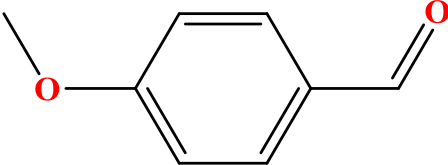
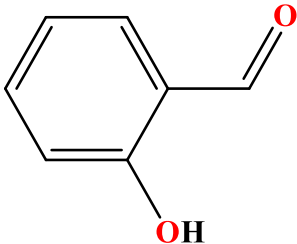
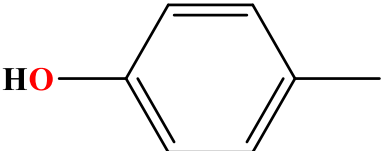
M75	Cinnamic acid	
M76	P-coumaric	
M77	Caffeic acid	
M78	Ferulic acid	
M79	Sinapic acid	

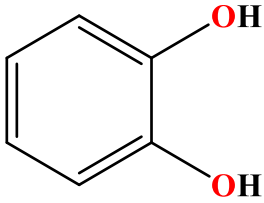
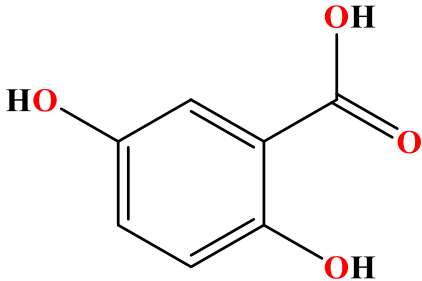
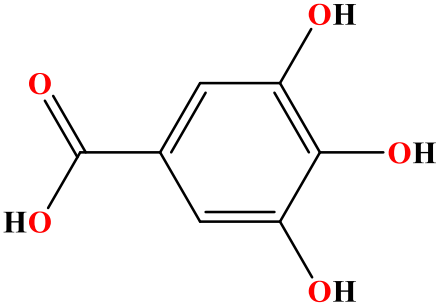
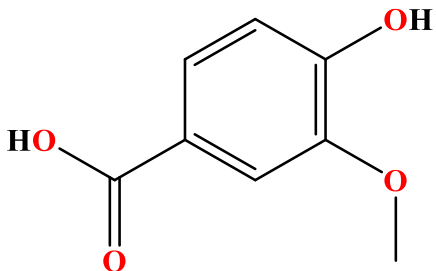
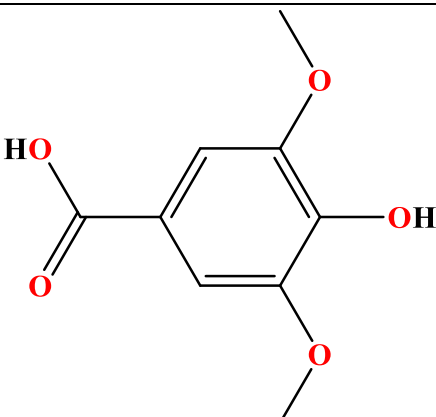
M80	5-p-coumaroylquinic	
M81	Chlorogenic	
M82	5-feruloylquinic	
M83	Caffeoylshikimic	

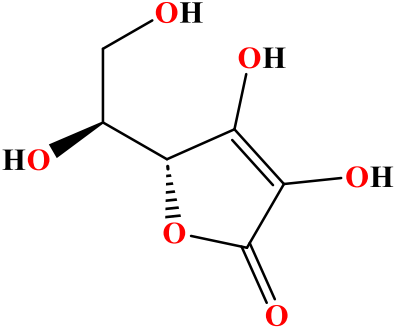
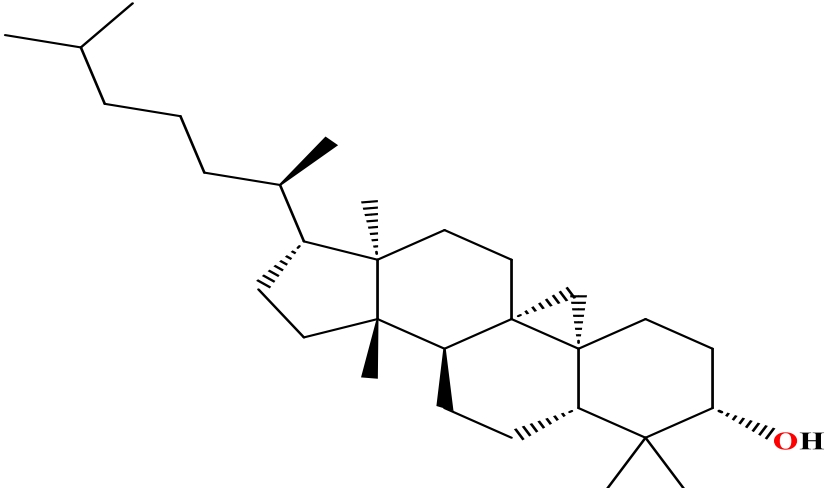
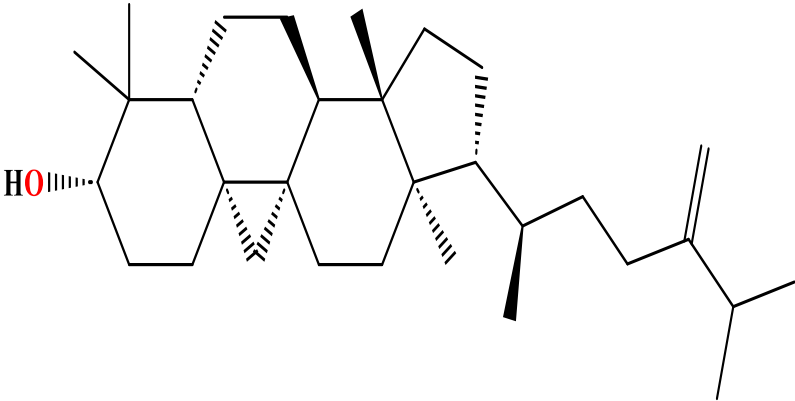
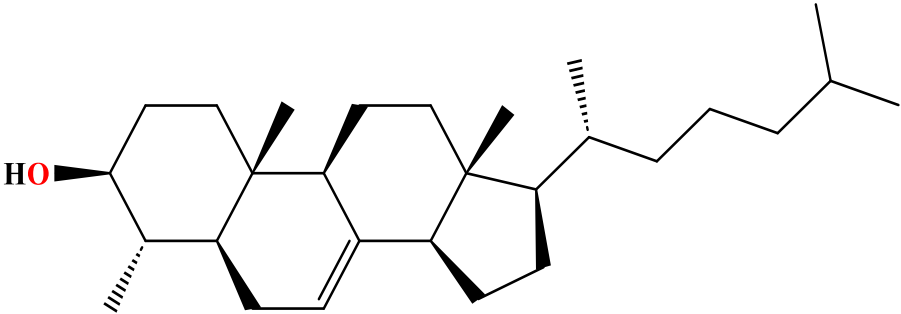
M84	5-p-cis-coumaroylquinic	 The structure shows a cyclohexane ring with a carboxylic acid group at position 1 (HO-C=O), a hydroxyl group at position 2 (OH), and a hydroxyl group at position 3 (OH). At position 5, there is a p-cis-coumaroyl group attached via an ester linkage (-O-C(=O)-CH=CH-C6H4-OH).
M85	3-(4-hydroxyphenyl) propanoic acid	 The structure shows a propanoic acid chain (HO-C(=O)-CH2-CH2-) attached to a 4-hydroxyphenyl ring (C6H4-OH) at the 3-position.
M86	Methyl 3-(4-hydroxyphenyl) propionate	 The structure shows a methyl propionate chain (CH3-O-C(=O)-CH2-CH2-) attached to a 4-hydroxyphenyl ring (C6H4-OH) at the 3-position.
M87	7-demethylsiderin	 The structure shows a naphthalene-like core with a lactone ring fused at positions 1 and 2. There is a methoxy group (-OCH3) at position 7 and a hydroxyl group (-OH) at position 4.
M88	Feralolide	 The structure shows a complex molecule with a central lactone ring fused to two benzene rings. The left benzene ring has hydroxyl groups at positions 1 and 3. The right benzene ring has hydroxyl groups at positions 1 and 3, and an acetyl group (-C(=O)CH3) at position 4. The central lactone ring has a hydroxyl group at position 2 and a methyl group at position 3.

M89	Dihydrocoumarin	 The structure shows a coumarin core with a methoxy group at C6, a hydroxyl group at C7, and a 4-hydroxyphenyl group at C2. The pyrone ring has a carbonyl at C4 and a methoxy group at C5.
M90	Dihydrocoumarin ethyl ester	 The structure is similar to M89 but features an ethyl ester group at C3 instead of a hydroxyl group. The pyrone ring has a carbonyl at C4 and a methoxy group at C5.
M91	Aloenin A	 The structure shows a coumarin core with a methoxy group at C6, a hydroxyl group at C7, and a 4-hydroxyphenyl group at C2. The pyrone ring has a carbonyl at C4 and a methoxy group at C5. The structure also includes a sugar moiety attached to the coumarin core via an ether linkage.

M92	Aloenin B	 The chemical structure of Aloenin B features a central benzene ring substituted with a methoxy group, a coumarin-3-yl group, and a 4-hydroxyphenyl group. This central ring is linked via an ether bond to a 2,6-dihydroxyphenyl group, which is further connected to a 2,4,6-trihydroxyphenyl group. The structure also includes a 4-hydroxyphenyl group connected to a 3-hydroxy-2-methoxyphenyl group, which is linked to a 2,4,6-trihydroxyphenyl group.
M93	P-coumaroyl aloenin	 The chemical structure of P-coumaroyl aloenin consists of a central benzene ring substituted with a methoxy group, a coumarin-3-yl group, and a 4-hydroxyphenyl group. This central ring is linked via an ether bond to a 2,6-dihydroxyphenyl group, which is further connected to a 2,4,6-trihydroxyphenyl group. The structure also includes a 4-hydroxyphenyl group connected to a 3-hydroxy-2-methoxyphenyl group, which is linked to a 2,4,6-trihydroxyphenyl group.
M94	Aloveroside A	 The chemical structure of Aloveroside A is a complex molecule featuring a central benzene ring substituted with a methoxy group, a coumarin-3-yl group, and a 4-hydroxyphenyl group. This central ring is linked via an ether bond to a 2,6-dihydroxyphenyl group, which is further connected to a 2,4,6-trihydroxyphenyl group. The structure also includes a 4-hydroxyphenyl group connected to a 3-hydroxy-2-methoxyphenyl group, which is linked to a 2,4,6-trihydroxyphenyl group.

M95	Feroxidin	
M96	1-(2,4-dihydroxy-6-methylphenyl) ethanone	
M97	P-anisaldehyde	
M98	Salicylaldehyde	
M99	P-cresol	

M100	Pyrocatechol	
M101	Gentisic acid	
M102	Gallic acid	
M103	Vanillic acid	
M104	Syringic acid	

M105	Ascorbic acid	
M106	Cycloartanol	
M107	24-methylene-cycloartanol	
M108	Lophenol	

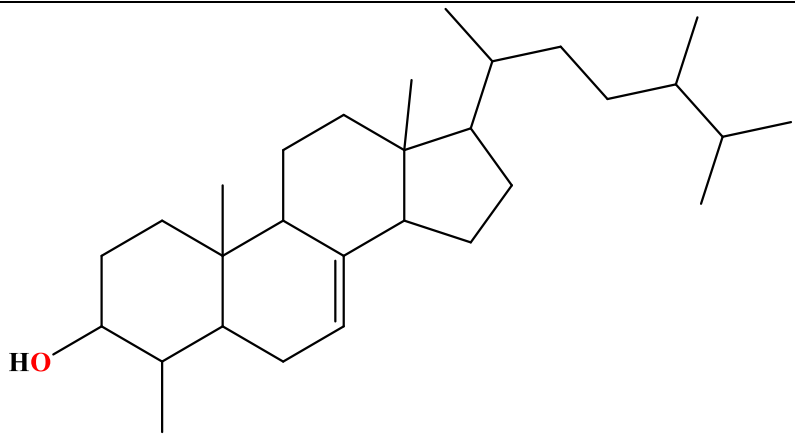
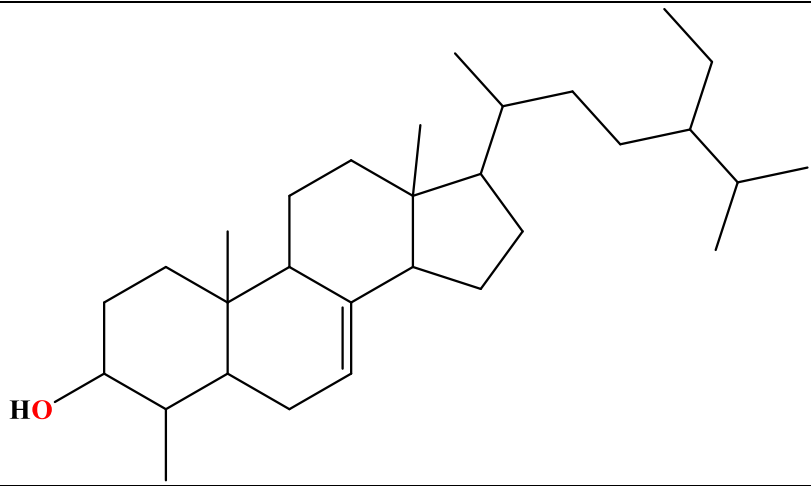
M109	24-methyl-lophenol	 The chemical structure of 24-methyl-lophenol is a complex polycyclic molecule. It features a central core with a double bond in one of the rings. A hydroxyl group (HO) is attached to one of the rings. A methyl group is attached to the 24th carbon of the side chain. The side chain is a branched alkyl group.
M110	24-ethyl-lophenol	 The chemical structure of 24-ethyl-lophenol is similar to 24-methyl-lophenol, but the methyl group at the 24th carbon is replaced by an ethyl group. The rest of the structure, including the hydroxyl group and the branched side chain, remains the same.

Table S2: Molecular docking scores of aloe vera-derived compounds against target proteins in atopic dermatitis

ID	5EH1	5mj3	4RG2	2BDF	3O96	1NME
M1	-6,6	-6.1	-7.3	-7.8	-8.4	-6.3
M2	-6,5	-6.4	-6.5	-8.3	-10.3	-7.3
M3	-7,2	-6.3	-7.4	-8.4	-8.9	-6.6
M4	-6,4	-5.9	-6.5	-8.0	-9.1	-6.6
M5	-7	-6.2	-7.4	-8.1	-8.5	-6.5
M6	-6,2	-6.2	-6.6	-7.9	-9.3	-6.7
M7	-7,1	-6.2	-6.7	-8.4	-9.2	-7.1
M8	-7,3	-7.4	-7.3	-9.1	-9.0	-7.9
M9	-8,3	-7.7	-7.7	-9.0	-8.8	-8.1
M10	-6,9	-6.0	-6.4	-8.5	-10.5	-6.5
M11	-7,1	-7.1	-7.0	-7.7	-8.8	-7.6
M12	-7,1	-6.6	-7.1	-8.1	-8.3	-8.0
M13	-7,1	-6.5	-7.4	-7.9	-8.7	-8.4
M14	-7,1	-6.9	-7.3	-7.9	-8.4	-7.1
M15	-7,1	-6.6	-7.5	-8.3	-8.4	-7.7
M16	-7,2	-6.5	-7.4	-8.0	-9.6	-7.6
M17	-7,1	-6.3	-6.8	-8.4	-7.5	-6.9
M18	-6,7	-6.8	-6.8	-7.3	-7.7	-7.3
M19	-6,5	-6.3	-7.0	-8.4	-8.2	-7.1
M20	-6,8	-5.8	-7.1	-7.7	-9.8	-6.3
M21	-7	-7.8	-7.9	-8.9	-8.6	-8.4
M22	-7,2	-7.4	-7.5	-8.5	-8.5	-7.9
M23	-6,9	-7.1	-7.5	-7.7	-7.9	-7.6
M24	-6,8	-6.6	-6.9	-8.0	-7.9	-7.3
M25	-7,5	-7.2	-7.5	-7.2	-8.8	-7.3
M26	-7,2	-7.1	-7.3	-8.7	-9.0	-7.5
M27	-7,3	-6.8	-6.9	-9.1	-7.8	-7.8
M28	-7,6	-6.4	-6.6	-7.6	-9.0	-8.0
M29	-7,1	-6.2	-6.6	-7.4	-7.8	-7.7
M30	-7,2	-6.9	-7.2	-8.0	-9.0	-7.4
M31	-7,2	-6.5	-7.0	-7.1	-8.2	-7.0
M32	-7,2	-6.5	-6.9	-7.3	-8.1	-7.1
M33	-7	-7.1	-6.9	-8.2	-8.4	-7.1
M34	-6,9	-6.0	-7.2	-8.6	-8.1	-7.5
M35	-7,8	-7.0	-6.8	-8.0	-7.9	-7.0
M36	-8,2	-7.0	-7.7	-8.2	-9.5	-8.3
M37	-7,9	-7.3	-8.1	-8.6	-7.9	-9.3
M38	-7,3	-6.6	-7.4	-8.2	-8.1	-7.5
M39	-7,6	-6.6	-6.9	-7.5	-8.2	-7.0
M40	-6,8	-6.3	-7.3	-8.1	-7.6	-7.3
M41	-7,5	-6.5	-6.7	-7.2	-7.4	-7.0
M42	-7,5	-7.1	-7.3	-8.4	-8.2	-7.6
M43	-7	-6.6	-7.0	-9.1	-7.7	-7.6
M44	-7,3	-7.2	-7.8	-8.7	-8.9	-7.9
M45	-8,4	-8.6	-9.3	-9.9	-9.7	-8.5

M46	-8,4	-7.9	-9.5	-10.2	-9.2	-8.6
M47	-9,1	-7.8	-8.0	-9.8	-9.3	-8.9
M48	-9,4	-7.7	-8.9	-9.5	-9.4	-9.4
M49	-9,4	-7.7	-8.9	-9.5	-9.4	-9.4
M50	-9,4	-7.7	-8.9	-9.5	-9.4	-9.4
M51	-7,8	-6.8	-7.8	-9.7	-11.5	-8.1
M52	-7,1	-6.5	-7.5	-9.0	-10.3	-6.9
M53	-7	-6.7	-7.6	-9.0	-10.4	-6.7
M54	-7	-6.8	-7.2	-9.0	-10.2	-6.6
M55	-6,5	-6.4	-7.3	-8.8	-10.3	-6.7
M56	-7	-6.7	-7.1	-8.9	-10.2	-6.9
M57	-6,4	-7.1	-7.3	-9.0	-10.3	-6.7
M58	-6,4	-6.5	-7.9	-9.1	-10.3	-6.9
M59	-7,3	-7.4	-7.5	-9.8	-10.5	-7.4
M60	-6,8	-6.8	-8.1	-9.8	-10.5	-7.8
M61	-6,6	-6.8	-7.6	-9.1	-10.4	-7.0
M62	-6,9	-6.5	-7.0	-8.3	-9.5	-7.1
M63	-6,9	-6.4	-6.8	-8.5	-9.8	-7.4
M64	-7,8	-7.7	-7.6	-8.8	-10.6	-8.1
M65	-8,3	-6.6	-7.4	-8.6	-11.0	-8.1
M66	-7,6	-7.1	-7.4	-9.3	-9.1	-8.6
M67	-8,2	-8.2	-8.3	-9.5	-9.9	-8.8
M68	-8.1	-7.9	-8.2	-8.5	-8.2	-8
M69	-8	-7.6	-8.3	-8.1	-8.4	-7.9
M70	-7,1	-6.0	-6.5	-8.6	-9.6	-7.6
M71	-7,4	-7.0	-7.1	-8.9	-10.7	-7.0
M72	-7,7	-6.9	-7.2	-8.0	-9.5	-8.0
M73	-7	-6.0	-7.3	-8.3	-9.6	-7.7
M74	-6,6	-6.5	-7.1	-8.2	-9.0	-7.2
M75	-5	-4.7	-6.3	-5.9	-6.5	-5.4
M76	-5,6	-4.7	-5.8	-6.0	-6.8	-6.1
M77	-5,7	-5.0	-5.6	-6.3	-6.9	-6.1
M78	-5,8	-4.7	-5.8	-6.2	-6.9	-6.1
M79	-5,6	-4.9	-5.4	-6.1	-6.7	-5.4
M80	-6,8	-6.5	-7.0	-7.5	-10.4	-6.9
M81	-6,8	-6.0	-6.9	-7.6	-9.9	-7.1
M82	-6,9	-6.2	-7.0	-8.8	-8.5	-7.0
M83	-7,1	-6.7	-6.8	-8.2	-9.2	-7.1
M84	-6,3	-6.4	-6.0	-7.5	-9.7	-6.3
M85	-5,4	-5.0	-6.0	-6.1	-6.6	-5.9
M86	-4,9	-5.0	-5.8	-6.0	-6.4	-5.2
M87	-5,5	-5.3	-6.5	-7.1	-7.8	-5.7
M88	-7,2	-7.0	-7.2	-8.1	-10.2	-6.9
M89	-7,1	-7.1	-7.6	-8.4	-10.0	-7.1
M90	-6,5	-6.0	-6.3	-7.5	-6.9	-7.0
M91	-7,1	-6.2	-7.3	-8.0	-9.5	-7.2
M92	-7,2	-7.0	-7.4	-8.3	-8.8	-9.0
M93	-7,5	-7.5	-7.7	-8.1	-8.0	-7.8

M94	-8,4	-9.1	-7.3	-9.2	-9.3	-8.5
M95	-5,5	-5.1	-6.8	-7.1	-7.5	-5.7
M96	-4,9	-4.6	-5.6	-5.9	-6.4	-5.0
M97	-4,4	-4.4	-5.8	-5.1	-5.7	-4.7
M98	-4,6	-4.4	-5.2	-5.2	-5.4	-4.6
M99	-4,5	-4.1	-5.1	-4.9	-5.6	-4.7
M100	-4,4	-4.2	-4.8	-4.7	-5.5	-4.3
M101	-4,8	-4.7	-5.7	-5.6	-6.0	-5.0
M102	-4,7	-4.9	-5.8	-5.6	-6.0	-5.0
M103	-4,9	-4.6	-5.8	-5.7	-6.0	-5.3
M104	-4,8	-4.5	-5.6	-5.7	-6.2	-4.9
M105	-4,8	-4.6	-4.9	-5.4	-5.3	-4.8
M106	-6,8	-6.8	-7.1	-7.8	-10.9	-6.9
M107	-7,4	-7.2	-7.8	-7.6	-11.5	-8.0
M108	-6,5	-7.2	-7.9	-8.2	-10.6	-7.3
M109	-6,8	-7.1	-6.7	-8.0	-10.4	-7.9
M110	-6,1	-7.1	-6.8	-7.3	-8.6	-7.8
Natif ligand	-5,7	-2,9	-7,3	-9,4	-9,6	-5,1
Reference	-8	-7,2	-6,1	-6,8	-9,4	-6,7