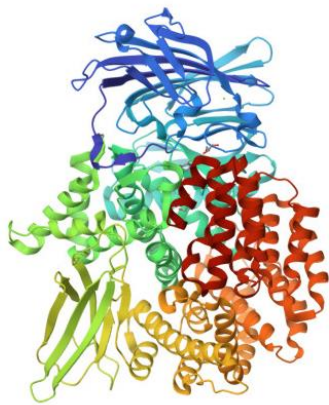
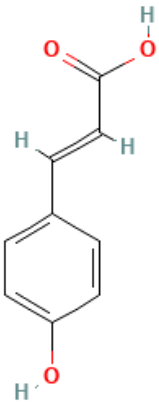
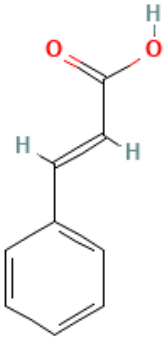


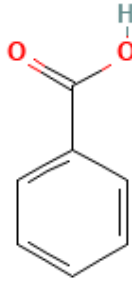
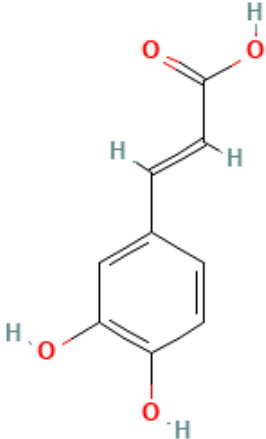
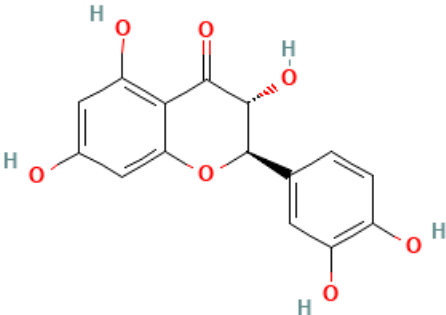
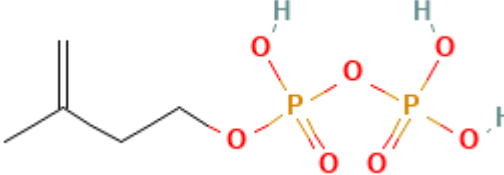
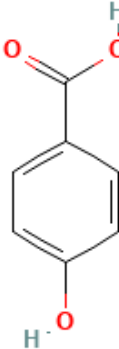
LAMPIRAN

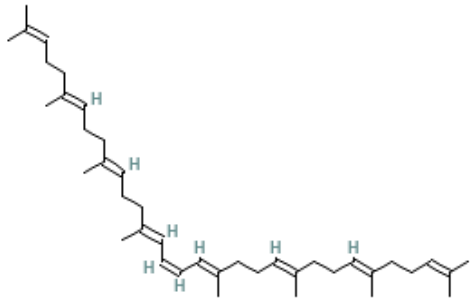
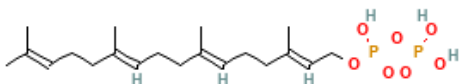
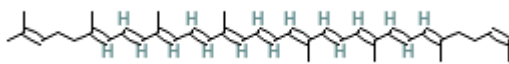
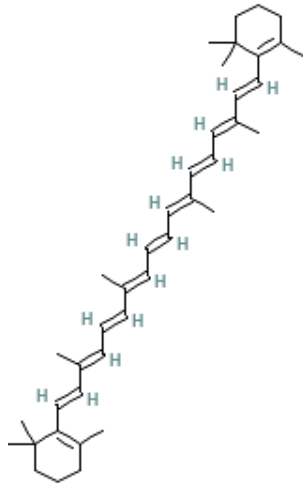
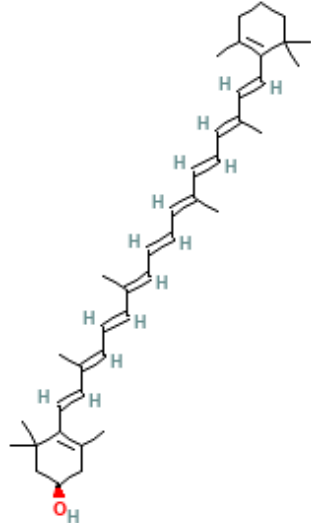
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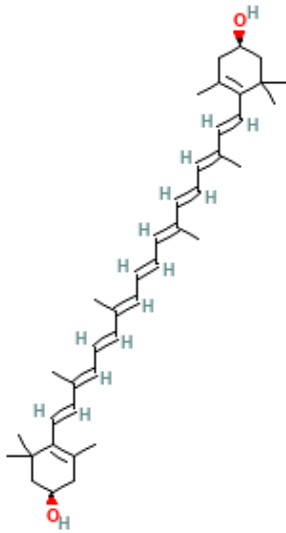
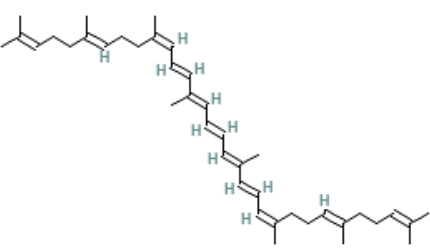
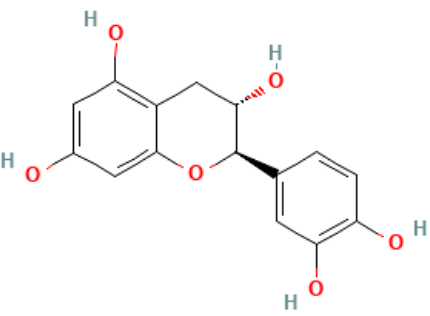
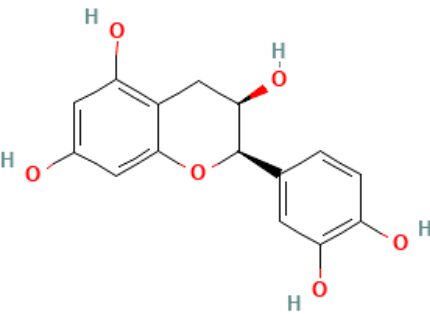
Plasmodium falciparum M1 alanyl aminopeptidase (PfA-M1)	
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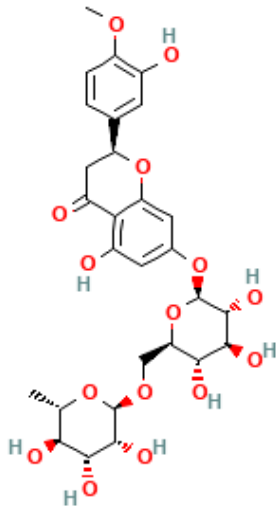
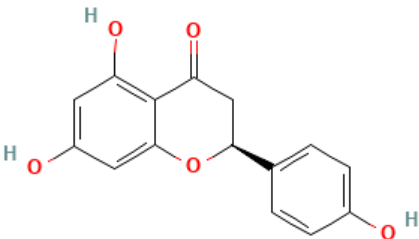
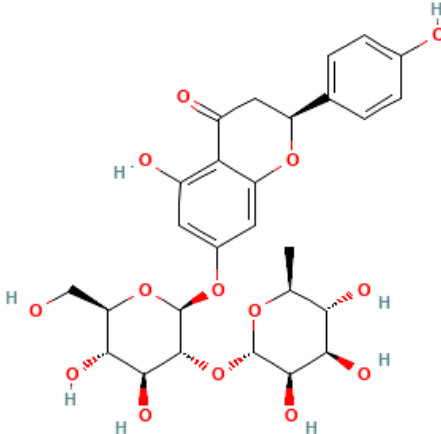
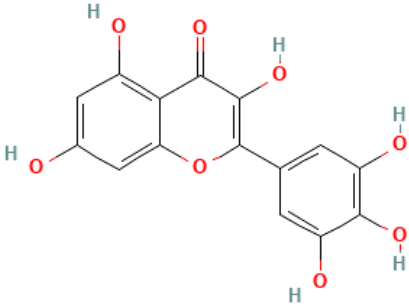
Lampiran 2 Senyawa Pare (*Momordica charantia* L.)

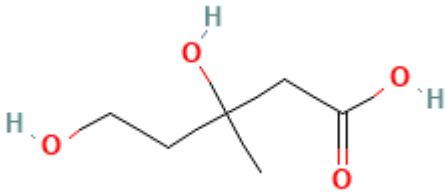
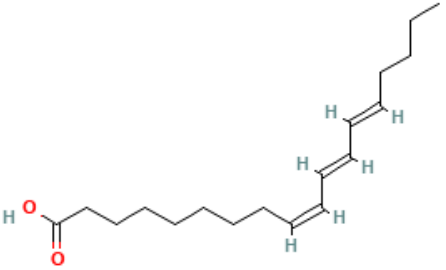
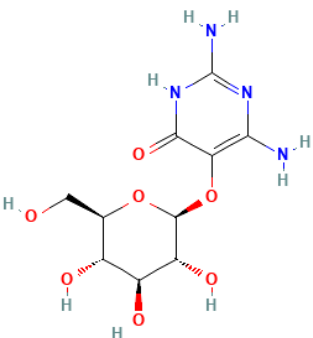
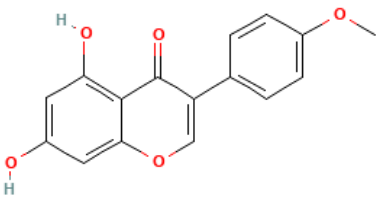
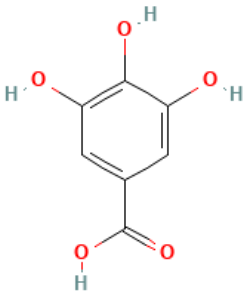
No	Nama IUPAC	Gambar
1	(<i>E</i>)-3-(4-hydroxyphenyl)prop-2-enoic acid	
2	(<i>E</i>)-3-phenylprop-2-enoic acid	

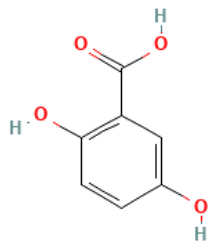
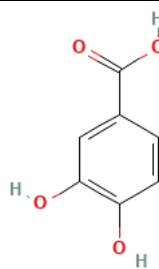
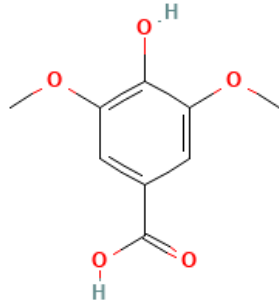
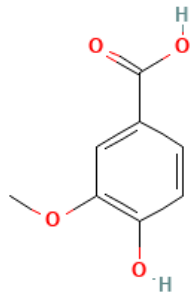
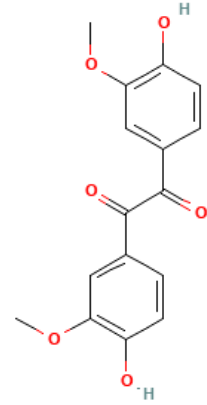
3	benzoic acid	
4	(E)-3-(3,4-dihydroxyphenyl)prop-2-enoic acid	
5	(2R,3R)-2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-2,3-dihydrochromen-4-one	
6	3-methylbut-3-enyl phosphono hydrogen phosphate	
7	4-hydroxybenzoic acid	

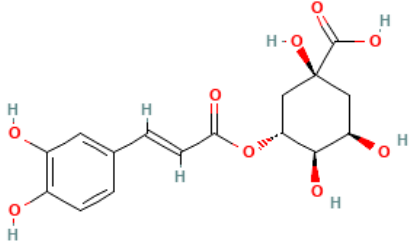
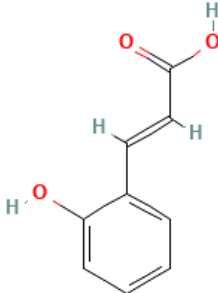
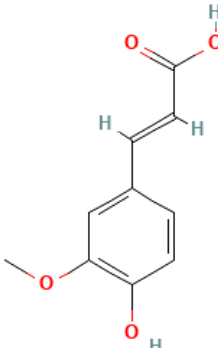
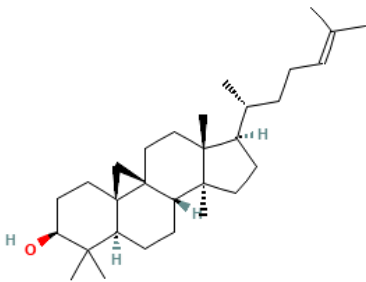
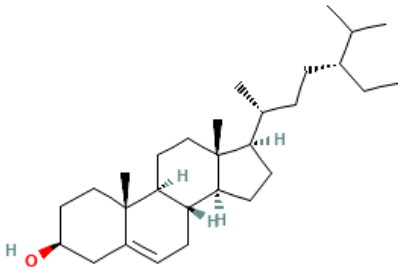
8	(6E,10E,14E,16Z,18E,22E,26E)-2,6,10,14,19,23,27,31-octamethyldotriaconta-2,6,10,14,16,18,22,26,30-nonaene	
9	phosphono [(2E,6E,10E)-3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraenyl] hydrogen phosphate	
10	(6E,8E,10E,12E,14E,16E,18E,20E,22E,24E,26E)-2,6,10,14,19,23,27,31-octamethyldotriaconta-2,6,8,10,12,14,16,18,20,22,24,26,30-tridecaene	
11	1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene	
12	(1R)-3,5,5-trimethyl-4-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol	

13	(1 <i>R</i>)-4-[(1 <i>E</i> ,3 <i>E</i> ,5 <i>E</i> ,7 <i>E</i> ,9 <i>E</i> ,11 <i>E</i> ,13 <i>E</i> ,15 <i>E</i> ,17 <i>E</i>)-18-[(4 <i>R</i>)-4-hydroxy-2,6,6-trimethylcyclohexen-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaenyl]-3,5,5-trimethylcyclohex-3-en-1-ol	
14	(6 <i>E</i> ,10 <i>Z</i> ,12 <i>E</i> ,14 <i>E</i> ,16 <i>E</i> ,18 <i>E</i> ,20 <i>E</i> ,22 <i>Z</i> ,26 <i>E</i>)-2,6,10,14,19,23,27,31-octamethyldotriaconta-2,6,10,12,14,16,18,20,22,26,30-undecaene	
15	(2 <i>R</i> ,3 <i>S</i>)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-2 <i>H</i> -chromene-3,5,7-triol	
16	(2 <i>R</i> ,3 <i>R</i>)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-2 <i>H</i> -chromene-3,5,7-triol	

17	(2 <i>S</i>)-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-7-[(2 <i>S</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-[(2 <i>R</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>S</i>)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxy-2,3-dihydrochromen-4-one	
18	(2 <i>S</i>)-5,7-dihydroxy-2-(4-hydroxyphenyl)-2,3-dihydrochromen-4-one	
19	(2 <i>S</i>)-7-[(2 <i>S</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2 <i>S</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>S</i>)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-2,3-dihydrochromen-4-one	
20	3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)chromen-4-one	

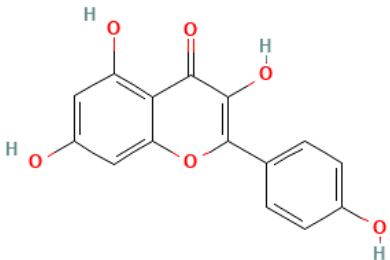
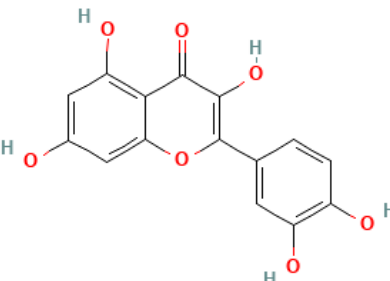
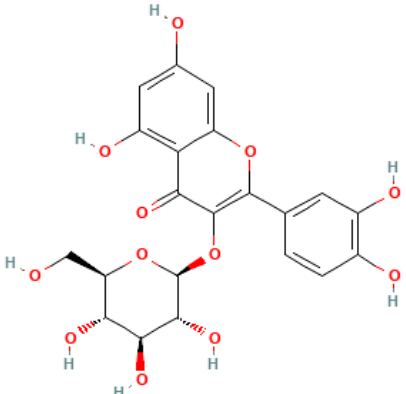
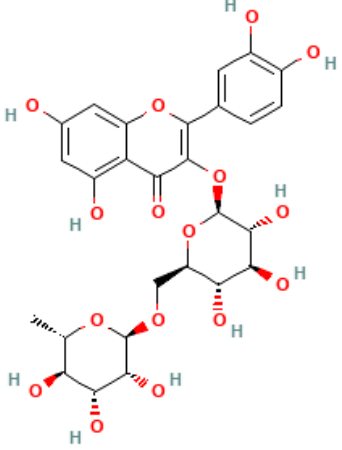
21	3,5-dihydroxy-3-methylpentanoic acid	
22	(9Z,11E,13E)-octadeca-9,11,13-trienoic acid	
23	2,4-diamino-5-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-1H-pyrimidin-6-one	
24	5,7-dihydroxy-3-(4-methoxyphenyl)chromen-4-one	
25	3,4,5-trihydroxybenzoic acid	

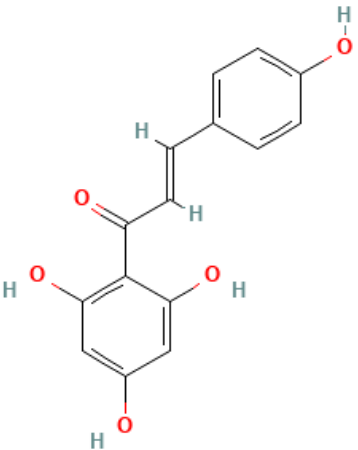
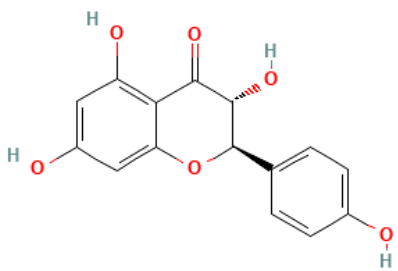
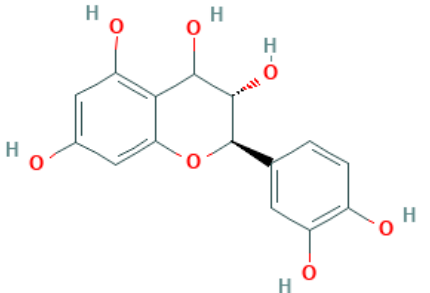
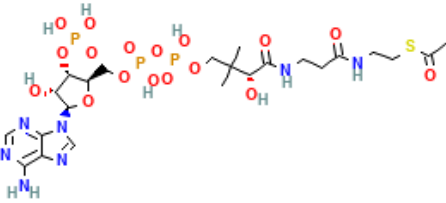
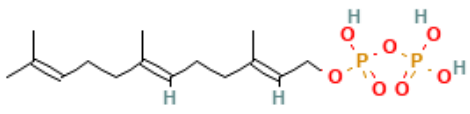
26	2,5-dihydroxybenzoic acid	
27	3,4-dihydroxybenzoic acid	
28	4-hydroxy-3,5-dimethoxybenzoic acid	
29	4-hydroxy-3-methoxybenzoic acid	
30	1,2-bis(4-hydroxy-3-methoxyphenyl)ethane-1,2-dione	

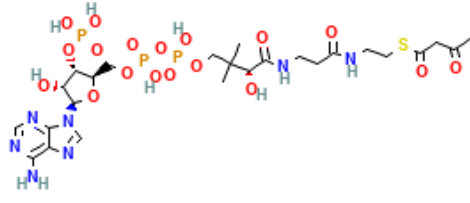
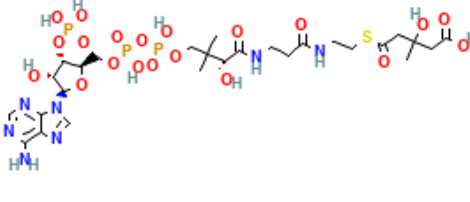
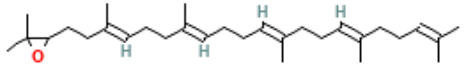
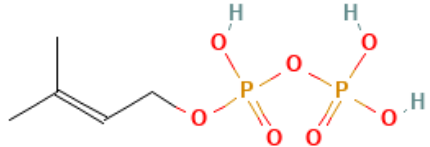
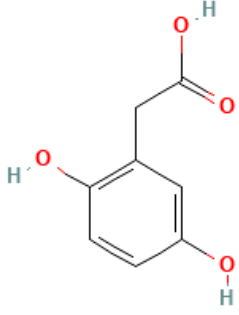
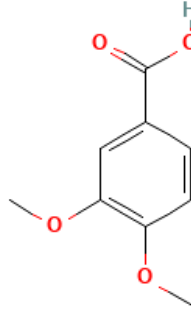
31	(1 <i>S</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>R</i>)-3-[(<i>E</i>)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy-1,4,5-trihydroxycyclohexane-1-carboxylic acid	
32	(<i>E</i>)-3-(2-hydroxyphenyl)prop-2-enoic acid	
33	(<i>E</i>)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid	
34	(1 <i>S</i> ,3 <i>R</i> ,6 <i>S</i> ,8 <i>R</i> ,11 <i>S</i> ,12 <i>S</i> ,15 <i>R</i> ,16 <i>R</i>)-7,7,12,16-tetramethyl-15-[(2 <i>R</i>)-6-methylhept-5-en-2-yl]pentacyclo[9.7.0.0 ^{1,3} .0 ^{3,8} .0 ^{12,16}]octadecan-6-ol	
35	(3 <i>S</i> ,8 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-17-[(2 <i>R</i> ,5 <i>R</i>)-5-ethyl-6-methylheptan-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-3-ol	

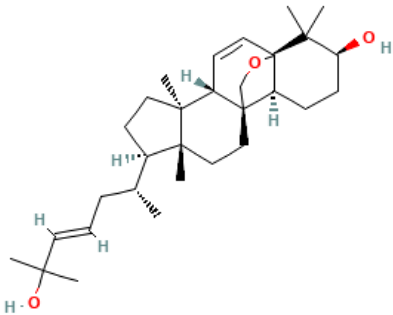
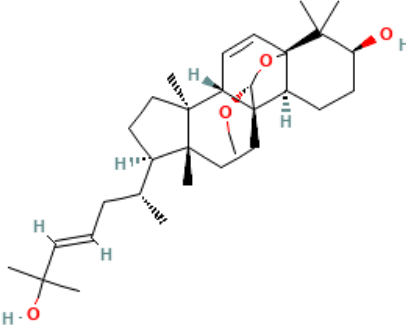
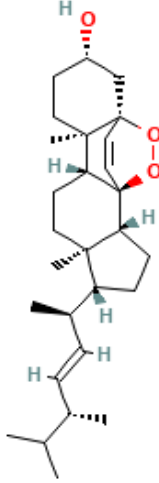
36	(3 <i>S</i> ,8 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-17-[(<i>E</i> ,2 <i>R</i> ,5 <i>S</i>)-5-ethyl-6-methylhept-3-en-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-3-ol	
37	[(<i>E</i> ,6 <i>R</i>)-6-[(8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,16 <i>R</i> ,17 <i>R</i>)-2,16-dihydroxy-4,4,9,13,14-pentamethyl-3,11-dioxo-8,10,12,15,16,17-hexahydro-7 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-17-yl]-6-hydroxy-2-methyl-5-oxohept-3-en-2-yl] acetate	
38	(2 <i>S</i> ,3 <i>S</i> ,8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,16 <i>R</i> ,17 <i>R</i>)-17-[(<i>E</i> ,2 <i>R</i>)-2,6-dihydroxy-6-methyl-3-oxohept-4-en-2-yl]-2,3,16-trihydroxy-4,4,9,13,14-pentamethyl-1,2,3,7,8,10,12,15,16,17-decahydrocyclopenta[<i>a</i>]phenanthren-11-one	
39	(3 <i>S</i> ,4 <i>aR</i> ,6 <i>aR</i> ,6 <i>bS</i> ,8 <i>aR</i> ,12 <i>aR</i> ,14 <i>aR</i> ,14 <i>bR</i>)-4,4,6 <i>a</i> ,6 <i>b</i> ,8 <i>a</i> ,11,11,14 <i>b</i> -octamethyl-1,2,3,4 <i>a</i> ,5,6,7,8,9,10,12,12 <i>a</i> ,14,14 <i>a</i> -tetradecahydricen-3-ol	
40	(6 <i>E</i> ,10 <i>E</i> ,14 <i>E</i> ,18 <i>E</i>)-2,6,10,15,19,23-hexamethyltetracos-2,6,10,14,18,22-hexaene	

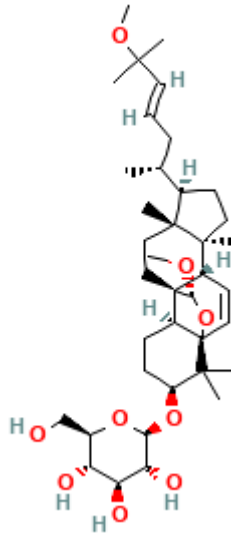
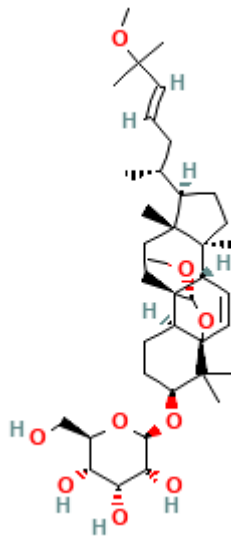
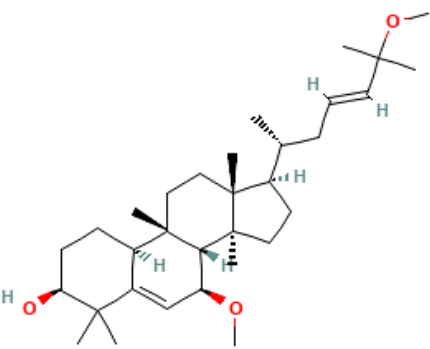
41	(1R,3S,6S)-6-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4R)-4-hydroxy-2,6,6-trimethylcyclohexen-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaenyl]-1,5,5-trimethyl-7-oxabicyclo[4.1.0]heptan-3-ol	
42	1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene	
43	(1R)-4-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1R,4R)-4-hydroxy-2,6,6-trimethylcyclohex-2-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaenyl]-3,5,5-trimethylcyclohex-3-en-1-ol	
44	(1R,3S,6S)-6-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4S,6R)-4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]heptan-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaenyl]-1,5,5-trimethyl-7-oxabicyclo[4.1.0]heptan-3-ol	

45	3,5,7-trihydroxy-2-(4-hydroxyphenyl)chromen-4-one	
46	2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxychromen-4-one	
47	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2 <i>S</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	
48	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2 <i>S</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-[(2 <i>R</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>S</i>)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxychromen-4-one	

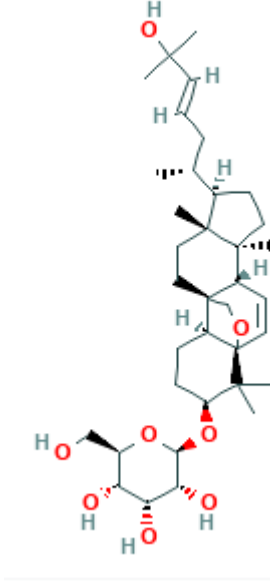
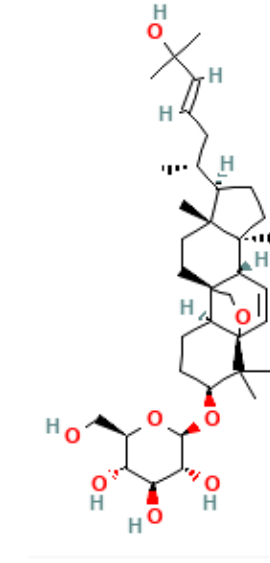
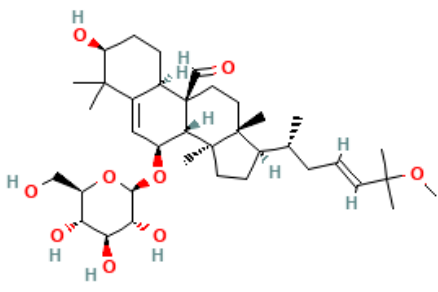
49	(<i>E</i>)-3-(4-hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)prop-2-en-1-one	
50	(2 <i>R</i> ,3 <i>R</i>)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)-2,3-dihydrochromen-4-one	
51	(2 <i>R</i> ,3 <i>S</i>)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-2 <i>H</i> -chromene-3,4,5,7-tetrol	
52	<i>S</i> -[2-[3-[[[(2 <i>R</i>)-4-[[[(2 <i>R</i> ,3 <i>S</i> ,4 <i>R</i> ,5 <i>R</i>)-5-(6-aminopurin-9-yl)-4-hydroxy-3-phosphonooxyoxolan-2-yl]methoxy-hydroxyphosphoryl]oxy-hydroxyphosphoryl]oxy-2-hydroxy-3,3-dimethylbutanoyl]amino]propanoylamino]ethyl] ethanethioate	
53	phosphono [(2 <i>E</i> ,6 <i>E</i>)-3,7,11-trimethyldodeca-2,6,10-trienyl] hydrogen phosphate	

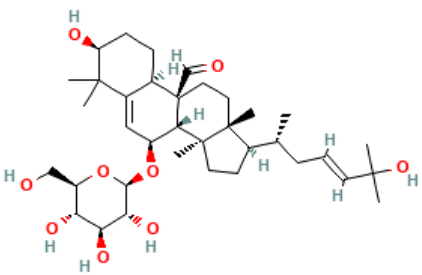
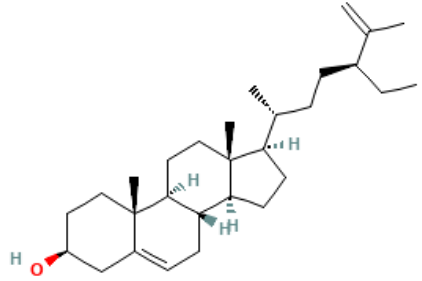
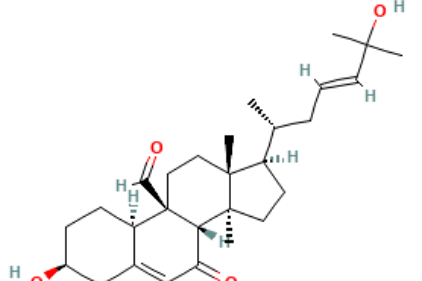
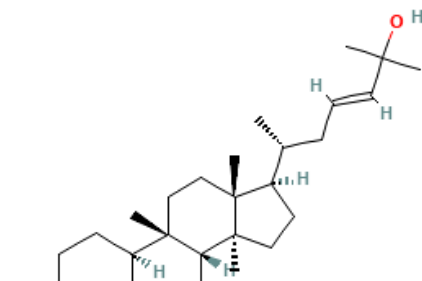
54	S-[2-[3-[[<i>(2R)</i> -4-[[[<i>(2R,3S,4R,5R)</i>]-5-(6-aminopurin-9-yl)-4-hydroxy-3-phosphonooxyoxolan-2-yl]methoxy-hydroxyphosphoryl]oxy-hydroxyphosphoryl]oxy-2-hydroxy-3,3-dimethylbutanoyl]amino]propanoylamino]ethyl 3-oxobutanethioate	
55	5-[2-[3-[[<i>(2R)</i> -4-[[[<i>(2R,3S,4R,5R)</i>]-5-(6-aminopurin-9-yl)-4-hydroxy-3-phosphonooxyoxolan-2-yl]methoxy-hydroxyphosphoryl]oxy-hydroxyphosphoryl]oxy-2-hydroxy-3,3-dimethylbutanoyl]amino]propanoylamino]ethylsulfanyl]-3-hydroxy-3-methyl-5-oxopentanoic acid	
56	2,2-dimethyl-3-[(3 <i>E</i> ,7 <i>E</i> ,11 <i>E</i> ,15 <i>E</i>)-3,7,12,16,20-pentamethylhenicosa-3,7,11,15,19-pentaenyl]oxirane	
57	3-methylbut-2-enyl phosphono hydrogen phosphate	
58	2-(2,5-dihydroxyphenyl)acetic acid	
59	3,4-dimethoxybenzoic acid	

60	(1 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,8 <i>R</i> ,9 <i>R</i> ,12 <i>S</i> ,13 <i>S</i> ,16 <i>S</i>)-8-[(<i>E</i> ,2 <i>R</i>)-6-hydroxy-6-methylhept-4-en-2-yl]-5,9,17,17-tetramethyl-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-ol	
61	(1 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,8 <i>R</i> ,9 <i>R</i> ,12 <i>S</i> ,13 <i>S</i> ,16 <i>S</i> ,19 <i>R</i>)-8-[(<i>E</i> ,2 <i>R</i>)-6-hydroxy-6-methylhept-4-en-2-yl]-19-methoxy-5,9,17,17-tetramethyl-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-ol	
62	(1 <i>S</i> ,2 <i>R</i> ,5 <i>R</i> ,6 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>S</i> ,15 <i>S</i>)-5-[(<i>E</i> ,2 <i>R</i> ,5 <i>R</i>)-5,6-dimethylhept-3-en-2-yl]-6,10-dimethyl-16,17-dioxapentacyclo[13.2.2.0 ^{1,9} .0 ^{2,6} .0 ^{10,15}]nonadec-18-en-13-ol	

63	(2 <i>R</i> ,3 <i>S</i> ,4 <i>S</i> ,5 <i>R</i> ,6 <i>R</i>)-2-(hydroxymethyl)-6-[[<i>(</i> 1 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,8 <i>R</i> ,9 <i>R</i> ,12 <i>S</i> ,13 <i>S</i> ,16 <i>S</i> ,19 <i>R</i> <i>)</i> -19-methoxy-8-[(<i>E</i> ,2 <i>R</i>)-6-methoxy-6-methylhept-4-en-2-yl]-5,9,17,17-tetramethyl-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-yl]oxy]oxane-3,4,5-triol	
64	(2 <i>R</i> ,3 <i>S</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>R</i>)-2-(hydroxymethyl)-6-[[<i>(</i> 1 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,8 <i>R</i> ,9 <i>R</i> ,12 <i>S</i> ,13 <i>S</i> ,16 <i>S</i> ,19 <i>R</i> <i>)</i> -19-methoxy-8-[(<i>E</i> ,2 <i>R</i>)-6-methoxy-6-methylhept-4-en-2-yl]-5,9,17,17-tetramethyl-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-yl]oxy]oxane-3,4,5-triol	
65	(3 <i>S</i> ,7 <i>S</i> ,8 <i>R</i> ,9 <i>S</i> ,10 <i>S</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-7-methoxy-17-[(<i>E</i> ,2 <i>R</i>)-6-methoxy-6-methylhept-4-en-2-yl]-4,4,9,13,14-pentamethyl-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-3-ol	

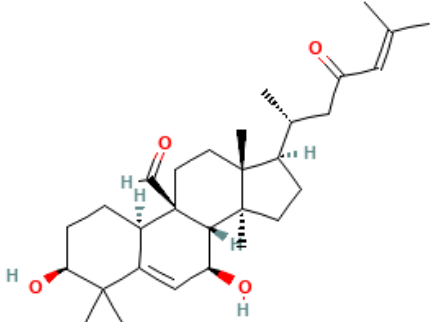
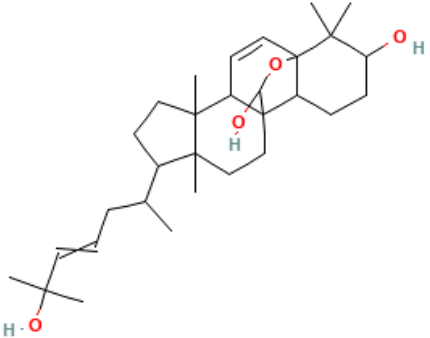
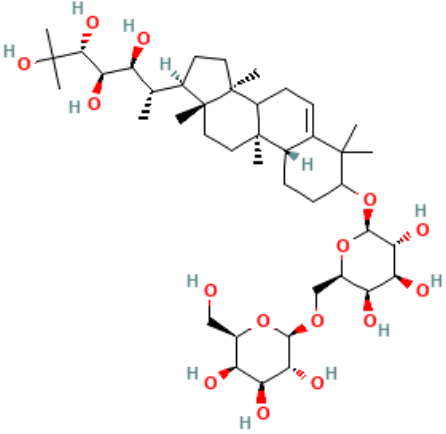
66	(3S,7S,8R,9S,10S,13R,14S,17R)-17-[(E,2R)-6-hydroxy-6-methylhept-4-en-2-yl]-7-methoxy-4,4,9,13,14-pentamethyl-2,3,7,8,10,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-3-ol	
67	(2R,3S,4R,5R,6R)-2-(hydroxymethyl)-6-[[[(3S,7S,9S,13R,14S)-17-[(2S)-3-hydroxy-6-methyl-4-[(2R,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhept-5-en-2-yl]-7-methoxy-4,4,9,13,14-pentamethyl-2,3,7,8,10,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-3-yl]oxy]oxane-3,4,5-triol	
68	(2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[[[(1R,4S,5S,8R,9R,12S,13S,16S)-8-[(E,2R)-6-methoxy-6-methylhept-4-en-2-yl]-5,9,17,17-tetramethyl-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-yl]oxy]oxane-3,4,5-triol	
69	(2R,3S,4R,5R,6R)-2-(hydroxymethyl)-6-[[[(1R,4S,5S,8R,9R,12S,13S,16S)-8-[(E,2R)-6-methoxy-6-methylhept-4-en-2-yl]-5,9,17,17-tetramethyl-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-yl]oxy]oxane-3,4,5-triol	

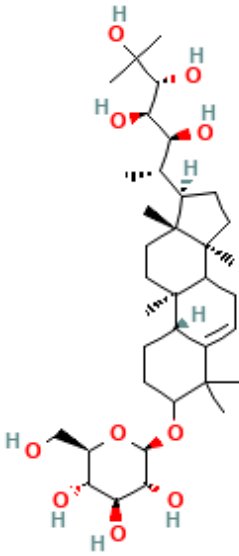
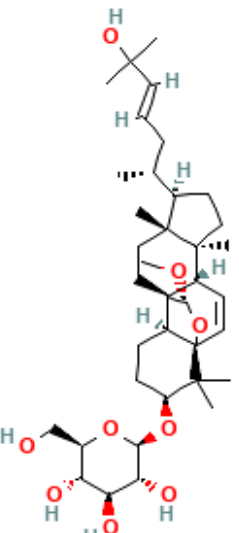
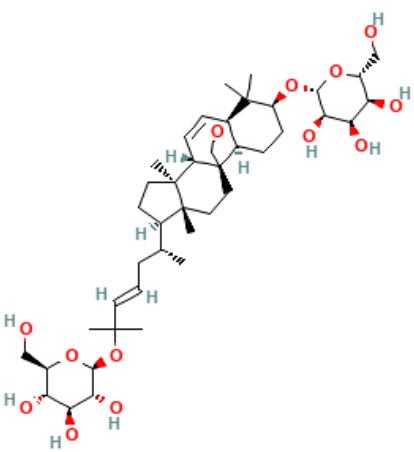
70		
71	(2<i>R</i>,3<i>S</i>,4<i>S</i>,5<i>R</i>,6<i>R</i>)-2-(hydroxymethyl)-6-[[[(1<i>R</i>,4<i>S</i>,5<i>S</i>,8<i>R</i>,9<i>R</i>,12<i>S</i>,13<i>S</i>,16<i>S</i>)-8-[(<i>E</i>,2<i>R</i>)-6-hydroxy-6-methylhept-4-en-2-yl]-5,9,17,17-tetramethyl-18-oxapentacyclo[10.5.2.0^{1,13}.0^{4,12}.0^{5,9}]nonadec-2-en-16-yl]oxy]oxane-3,4,5-triol	
72	(3<i>S</i>,7<i>S</i>,8<i>S</i>,9<i>R</i>,10<i>R</i>,13<i>R</i>,14<i>S</i>,17<i>R</i>)-3-hydroxy-17-[(<i>E</i>,2<i>R</i>)-6-methoxy-6-methylhept-4-en-2-yl]-4,4,13,14-tetramethyl-7-[(2<i>R</i>,3<i>R</i>,4<i>S</i>,5<i>S</i>,6<i>R</i>)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-2,3,7,8,10,11,12,15,16,17-decahydro-1<i>H</i>-cyclopenta[<i>a</i>]phenanthrene-9-carbaldehyde	

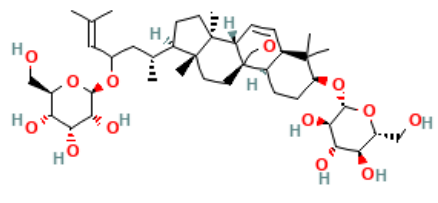
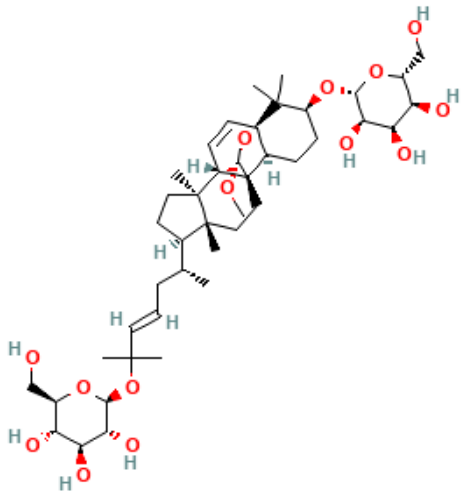
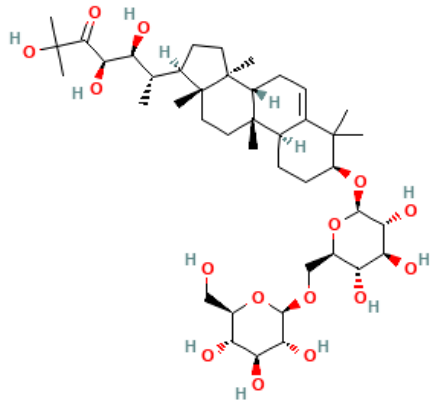
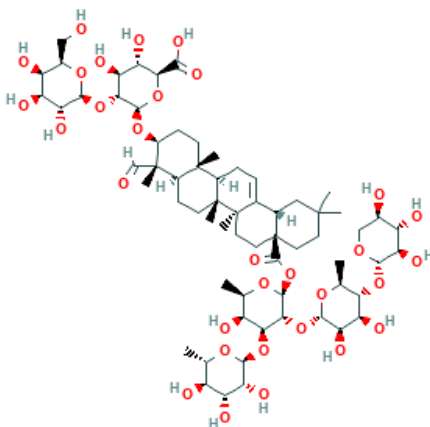
73	(3 <i>S</i> ,7 <i>S</i> ,8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-3-hydroxy-17-[(<i>E</i> ,2 <i>R</i>)-6-hydroxy-6-methylhept-4-en-2-yl]-4,4,13,14-tetramethyl-7-[(2 <i>R</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthrene-9-carbaldehyde	
74	(3 <i>S</i> ,8 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-17-[(2 <i>R</i> ,5 <i>S</i>)-5-ethyl-6-methylhept-6-en-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-3-ol	
75	(3 <i>S</i> ,8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-3-hydroxy-17-[(<i>E</i> ,2 <i>R</i>)-6-hydroxy-6-methylhept-4-en-2-yl]-4,4,13,14-tetramethyl-7-oxo-1,2,3,8,10,11,12,15,16,17-decahydrocyclopenta[<i>a</i>]phenanthrene-9-carbaldehyde	
76	(3 <i>S</i> ,8 <i>R</i> ,9 <i>S</i> ,10 <i>S</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-3-hydroxy-17-[(<i>E</i> ,2 <i>R</i>)-6-hydroxy-6-methylhept-4-en-2-yl]-4,4,9,13,14-pentamethyl-1,2,3,8,10,11,12,15,16,17-decahydrocyclopenta[<i>a</i>]phenanthren-7-one	

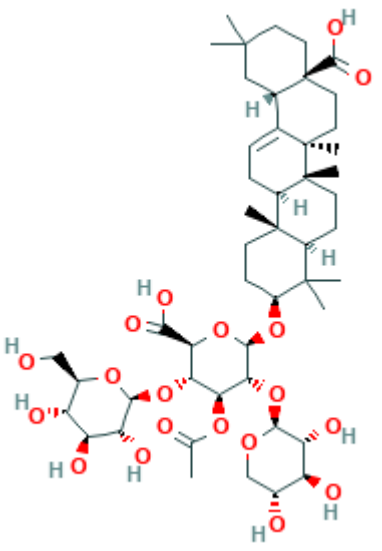
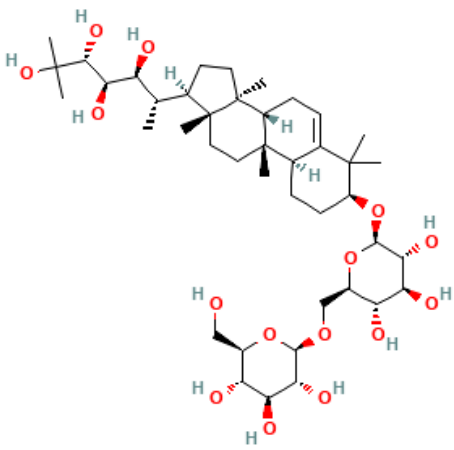
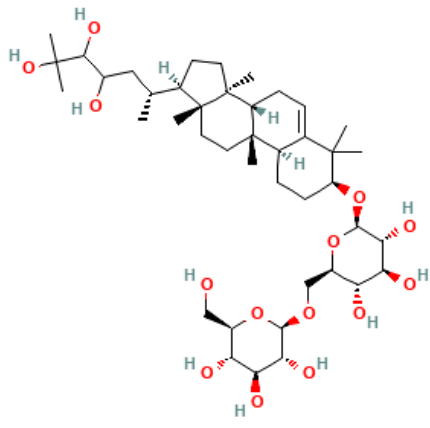
77	(3 <i>S</i> ,8 <i>R</i> ,9 <i>S</i> ,10 <i>S</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-3-hydroxy-4,4,9,13,14-pentamethyl-17-[(2 <i>R</i>)-4-oxopentan-2-yl]-1,2,3,8,10,11,12,15,16,17-decahydrocyclopenta[<i>a</i>]phenanthren-7-one	
78	(1 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,8 <i>R</i> ,9 <i>R</i> ,12 <i>S</i> ,13 <i>S</i> ,16 <i>S</i> ,19 <i>R</i>)-19-methoxy-8-[(<i>E</i> ,2 <i>R</i>)-6-methoxy-6-methylhept-4-en-2-yl]-5,9,17,17-tetramethyl-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-ol	
79	(3 <i>S</i> ,7 <i>S</i> ,8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-3,7-dihydroxy-17-[(2 <i>R</i>)-4-hydroxy-6-methylhept-5-en-2-yl]-4,4,13,14-tetramethyl-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthrene-9-carbaldehyde	
80	(1 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,8 <i>R</i> ,9 <i>R</i> ,12 <i>S</i> ,13 <i>S</i> ,16 <i>S</i>)-16-hydroxy-8-[(<i>E</i> ,2 <i>R</i>)-6-hydroxy-6-methylhept-4-en-2-yl]-5,9,17,17-tetramethyl-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-19-one	

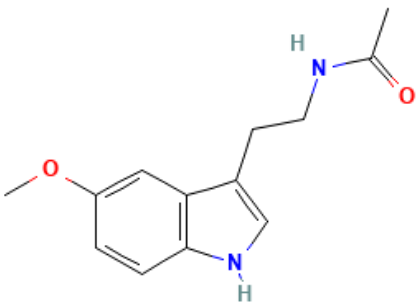
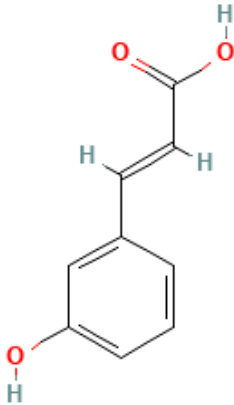
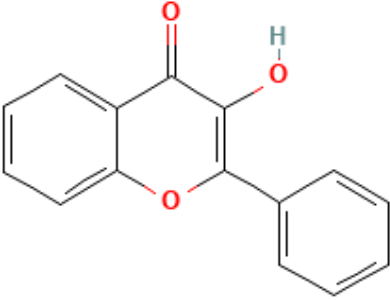
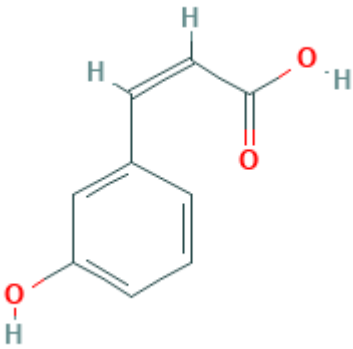
81	(1 <i>R</i> ,2 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>S</i> ,12 <i>S</i> ,15 <i>R</i> ,16 <i>R</i>)-6,6,12,16-tetramethyl-15-[(2 <i>R</i>)-6-methyl-4-oxohept-5-en-2-yl]-5,10-dioxo-8-oxapentacyclo[9.7.0.0 ^{2,7} .0 ^{7,9} .0 ^{12,16}]octadecane-1-carbaldehyde	
82	(1 <i>R</i> ,2 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>S</i> ,12 <i>S</i> ,15 <i>R</i> ,16 <i>R</i>)-15-[(2 <i>R</i>)-6-hydroxy-6-methyl-4-oxoheptan-2-yl]-6,6,12,16-tetramethyl-5,10-dioxo-8-oxapentacyclo[9.7.0.0 ^{2,7} .0 ^{7,9} .0 ^{12,16}]octadecane-1-carbaldehyde	
83	(8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-17-[(2 <i>R</i>)-6-hydroxy-6-methyl-4-oxoheptan-2-yl]-4,4,13,14-tetramethyl-3,7-dioxo-2,8,10,11,12,15,16,17-octahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthrene-9-carbaldehyde	
84	(3 <i>S</i> ,7 <i>S</i> ,8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-3,7-dihydroxy-4,4,13,14-tetramethyl-17-[(2 <i>R</i> ,4 <i>E</i>)-6-methylhepta-4,6-dien-2-yl]-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthrene-9-carbaldehyde	

85	(3 <i>S</i> ,7 <i>S</i> ,8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-3,7-dihydroxy-4,4,13,14-tetramethyl-17-[(2 <i>R</i>)-6-methyl-4-oxohept-5-en-2-yl]-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthrene-9-carbaldehyde	
86	8-(6-hydroxy-6-methylhept-4-en-2-yl)-5,9,17,17-tetramethyl-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-ene-16,19-diol	
87	(3 <i>R</i> ,4 <i>R</i> ,5 <i>S</i> ,6 <i>S</i>)-2-methyl-6-[(9 <i>S</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-4,4,9,13,14-pentamethyl-3-[(2 <i>R</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>R</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-[(2 <i>R</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>R</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxan-2-yl]oxymethyl]oxan-2-yl]oxy-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-17-yl]heptane-2,3,4,5-tetrol	

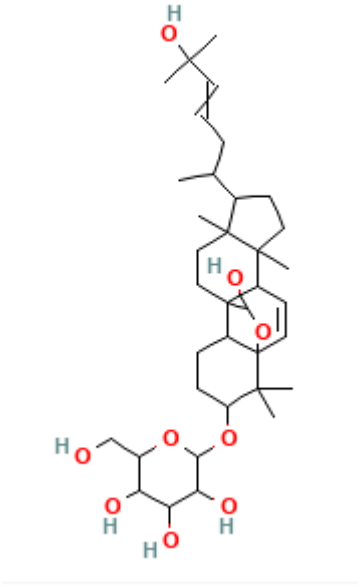
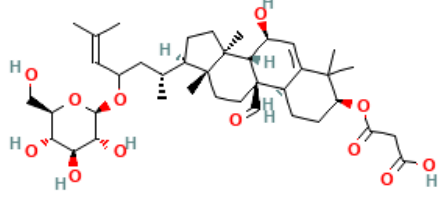
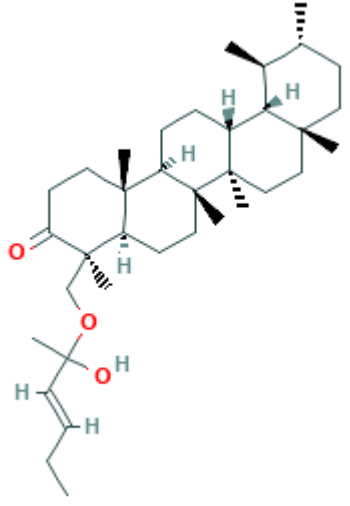
88	(3 <i>R</i> ,4 <i>R</i> ,5 <i>S</i> ,6 <i>S</i>)-2-methyl-6-[(9 <i>S</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-4,4,9,13,14-pentamethyl-3-[(2 <i>R</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-17-yl]heptane-2,3,4,5-tetrol	
89	(2 <i>R</i> ,3 <i>S</i> ,4 <i>S</i> ,5 <i>R</i> ,6 <i>R</i>)-2-(hydroxymethyl)-6-[[1 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,8 <i>R</i> ,9 <i>R</i> ,12 <i>S</i> ,13 <i>S</i> ,16 <i>S</i> ,19 <i>R</i>)-8-[(<i>E</i> ,2 <i>R</i>)-6-hydroxy-6-methylhept-4-en-2-yl]-19-methoxy-5,9,17,17-tetramethyl-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-yl]oxy]oxane-3,4,5-triol	
90	(2 <i>R</i> ,3 <i>S</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>R</i>)-2-(hydroxymethyl)-6-[[1 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,8 <i>R</i> ,9 <i>R</i> ,12 <i>S</i> ,13 <i>S</i> ,16 <i>S</i>)-5,9,17,17-tetramethyl-8-[(<i>E</i> ,2 <i>R</i>)-6-methyl-6-[(2 <i>S</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhept-4-en-2-yl]-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-yl]oxy]oxane-3,4,5-triol	

91	(2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[[[(1R,4S,5S,8R,9R,12S,13S,16S)-5,9,17,17-tetramethyl-8-[(2R)-6-methyl-4-[(2R,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhept-5-en-2-yl]-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-yl]oxy]oxane-3,4,5-triol	
92	(2R,3S,4R,5R,6R)-2-(hydroxymethyl)-6-[[[(1R,4S,5S,8R,9R,12S,13S,16S,19R)-19-methoxy-5,9,17,17-tetramethyl-8-[(E,2R)-6-methyl-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhept-4-en-2-yl]-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-yl]oxy]oxane-3,4,5-triol	
93	(4R,5S,6S)-2,4,5-trihydroxy-2-methyl-6-[(3S,8R,9R,10S,13R,14S,17R)-4,4,9,13,14-pentamethyl-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxan-2-yl]oxy-2,3,7,8,10,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-17-yl]heptan-3-one	
94	(2S,3S,4S,5R,6R)-6-[[[(3S,4S,4aR,6aR,6bS,8aS,12aS,14aR,14bR)-8a-[(2S,3R,4S,5S,6R)-3-[(2S,3R,4S,5R,6S)-3,4-dihydroxy-6-methyl-5-[(2S,3R,4S,5R)-3,4,5-trihydroxyoxan-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-6-methyl-4-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxycarbonyl-4-formyl-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicen-3-yl]oxy]-3,4-dihydroxy-5-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-2-carboxylic acid	

95	(2 <i>S</i> ,3 <i>S</i> ,4 <i>S</i> ,5 <i>R</i> ,6 <i>R</i>)-6-[[<i>(3S,4aR,6aR,6bS,8aS,12aS,14aR,14bR)</i> -8 <i>a</i> -carboxy-4,4,6 <i>a</i> ,6 <i>b</i> ,11,11,14 <i>b</i> -heptamethyl-1,2,3,4 <i>a</i> ,5,6,7,8,9,10,12,12 <i>a</i> ,14,14 <i>a</i> -tetradecahdropicen-3-yl]oxy]-4-acetyloxy-3-[[<i>(2S,3R,4S,5S,6R)</i> -3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]-5-[[<i>(2S,3R,4S,5R)</i> -3,4,5-trihydroxyoxan-2-yl]oxy]oxane-2-carboxylic acid	
96	(3 <i>R</i> ,4 <i>R</i> ,5 <i>S</i> ,6 <i>S</i>)-2-methyl-6-[[<i>(3S,8R,9R,10S,13R,14S,17R)</i> -4,4,9,13,14-pentamethyl-3-[[<i>(2R,3R,4S,5S,6R)</i> -3,4,5-trihydroxy-6-[[<i>(2R,3R,4S,5S,6R)</i> -3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxan-2-yl]oxy-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-17-yl]heptane-2,3,4,5-tetrol	
97	(2 <i>R</i> ,3 <i>S</i> ,4 <i>S</i> ,5 <i>R</i> ,6 <i>R</i>)-2-(hydroxymethyl)-6-[[<i>(2R,3S,4S,5R,6R)</i> -3,4,5-trihydroxy-6-[[<i>(3S,8R,9R,10S,13R,14S,17R)</i> -4,4,9,13,14-pentamethyl-17-[[<i>(2R)</i> -4,5,6-trihydroxy-6-methylheptan-2-yl]-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-3-yl]oxy]oxan-2-yl]methoxy]oxane-3,4,5-triol	

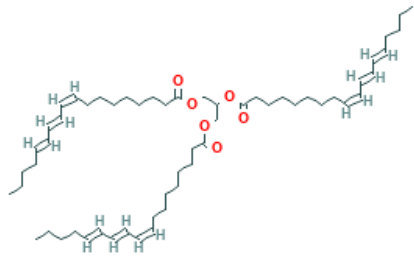
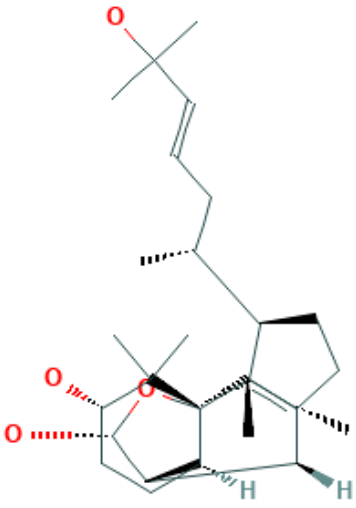
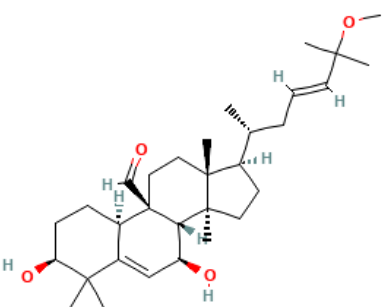
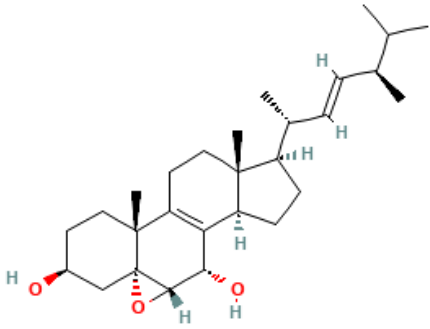
98	<i>N</i> -[2-(5-methoxy-1 <i>H</i> -indol-3-yl)ethyl]acetamide	
99	(<i>E</i>)-3-(3-hydroxyphenyl)prop-2-enoic acid	
100	3-hydroxy-2-phenylchromen-4-one	
101	(<i>Z</i>)-3-(3-hydroxyphenyl)prop-2-enoic acid	

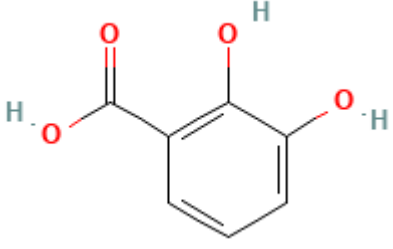
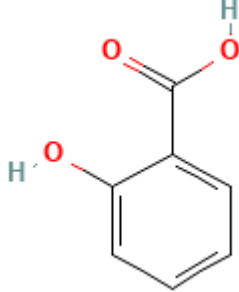
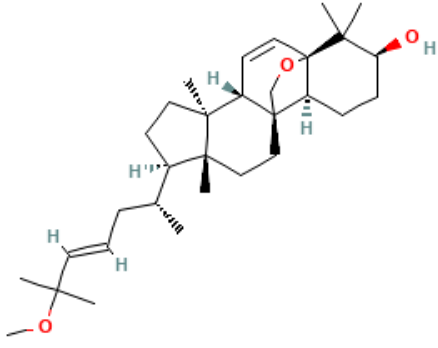
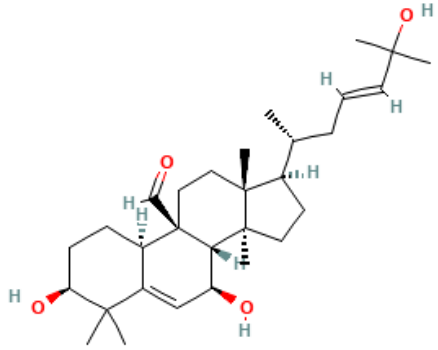
102	(3 <i>S</i> ,8 <i>R</i> ,9 <i>R</i> ,10 <i>S</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-4,4,9,13,14-pentamethyl-17-[(2 <i>R</i>)-6-methylhept-5-en-2-yl]-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-3-ol	
103	(1 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,8 <i>R</i> ,9 <i>R</i> ,12 <i>S</i> ,13 <i>S</i> ,16 <i>S</i>)-5,9,17,17-tetramethyl-8-[(2 <i>R</i> ,4 <i>E</i>)-6-methylhepta-4,6-dien-2-yl]-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-ene-16,19-diol	
104	(3 <i>S</i> ,7 <i>S</i> ,8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-3-hydroxy-4,4,13,14-tetramethyl-17-[(2 <i>R</i> ,4 <i>E</i>)-6-methylhepta-4,6-dien-2-yl]-7-[(2 <i>R</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthrene-9-carbaldehyde	
105	(1 <i>S</i> ,4 <i>S</i> ,5 <i>R</i> ,8 <i>R</i> ,13 <i>S</i> ,14 <i>R</i> ,17 <i>S</i> ,18 <i>R</i> ,19 <i>S</i> ,20 <i>R</i>)-4,5,9,9,13,19,20-heptamethyl-24-oxahexacyclo[15.5.2.0 ^{1,18} .0 ^{4,17} .0 ^{5,14} .0 ^{8,13}]tetracos-15-en-10-one	

106	2-[[19-hydroxy-8-(6-hydroxy-6-methylhept-4-en-2-yl)-5,9,17,17-tetramethyl-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-yl]oxy]-6-(hydroxymethyl)oxane-3,4,5-triol	
107	3-[[[(3S,7S,8S,9R,10R,13R,14S,17R)-9-formyl-7-hydroxy-4,4,13,14-tetramethyl-17-[(2R)-6-methyl-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhept-5-en-2-yl]-2,3,7,8,10,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-3-yl]oxy]-3-oxopropanoic acid	
118	(4S,4aR,6aR,6aR,6bR,8aR,11R,12S,12aS,14aR,14bR)-4-[[[(E)-2-hydroxyhex-3-en-2-yl]oxymethyl]-4,6a,6b,8a,11,12,14b-heptamethyl-1,2,4a,5,6,6a,7,8,9,10,11,12,12a,13,14,14a-hexadecahydricen-3-one	

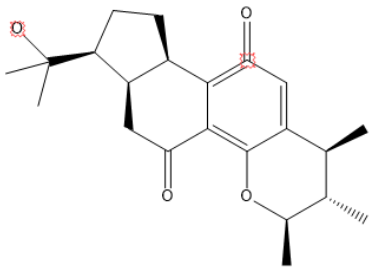
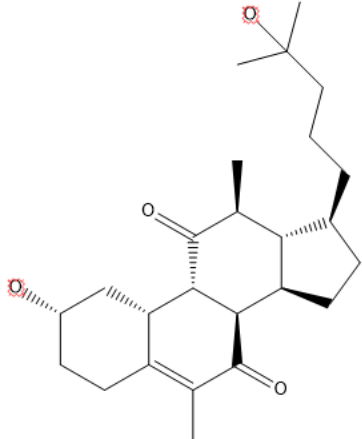
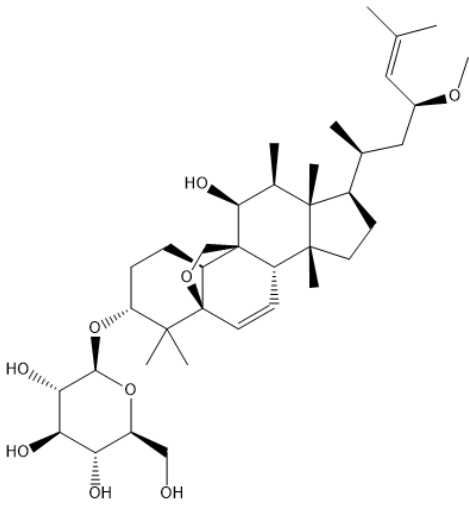
109	(3 <i>S</i> ,8 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> ,13 <i>R</i> ,17 <i>R</i>)-17-[(2 <i>R</i> ,5 <i>R</i>)-5-ethyl-6-methylheptan-2-yl]-3-hydroxy-10,13-dimethyl-1,2,3,4,7,8,9,11,12,17-decahydrocyclopenta[<i>a</i>]phenanthren-16-one	
110	5-[8,10-dihydroxy-11-(hydroxymethyl)-4,7-dimethyltridecyl]-6-ethyl-4-hydroxy-4,5-dimethylcyclohex-2-en-1-one	
111	(2 <i>R</i>)- <i>N</i> -[(<i>E</i> ,2 <i>S</i> ,3 <i>S</i> ,4 <i>R</i>)-3,4-dihydroxy-1-[(2 <i>R</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoctadec-8-en-2-yl]-2-hydroxytetracosanamide	
112	6-[3-[3,4-dihydroxy-6-[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]-5-(3,4,5-trihydroxyoxan-2-yl)oxyoxan-2-yl]oxy-4,4,9,13,14-pentamethyl-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-17-yl]-2-methylheptane-2,3,4,5-tetrol	

113	2-[[6-[[17-(3,4-dihydroxy-6-methylhept-5-en-2-yl)-4,4,9,13,14-pentamethyl-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-3-yl]oxy]-3,4,5-trihydroxyoxan-2-yl]methoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	
114	2-[4,4,9,13,14-pentamethyl-3-[3,4,5-trihydroxy-6-[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxan-2-yl]oxy-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-17-yl]propanal	
115	(3 <i>S</i> ,7 <i>S</i> ,8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-3-hydroxy-17-[(2 <i>R</i> ,4 <i>R</i>)-4-hydroxy-6-methylhept-5-en-2-yl]-4,4,13,14-tetramethyl-7-[(2 <i>R</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthrene-9-carbaldehyde	
116	(3 <i>S</i> ,7 <i>S</i> ,8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-3,7-dihydroxy-4,4,13,14-tetramethyl-17-[(2 <i>R</i>)-6-methyl-4-[(2 <i>R</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhept-5-en-2-yl]-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthrene-9-carbaldehyde	

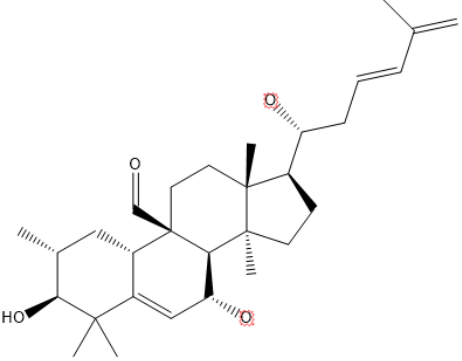
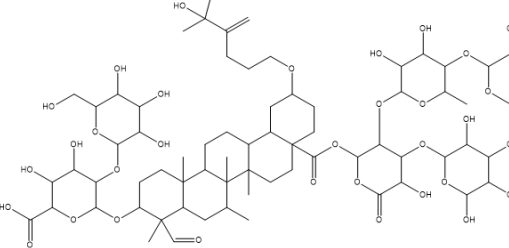
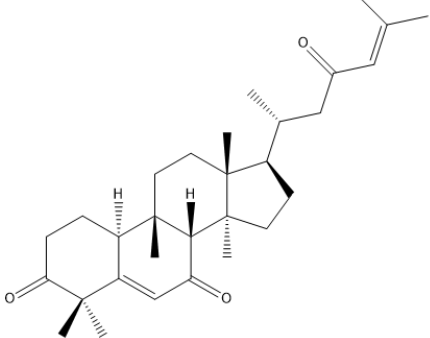
117	2,3-bis[[<i>(9Z,11E,13E)</i> -octadeca-9,11,13-trienoyl]oxy]propyl <i>(9Z,11E,13E)</i> -octadeca-9,11,13-trienoate	
118		
119	(3 <i>S</i> ,7 <i>S</i> ,8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-3,7-dihydroxy-17-[(<i>E</i> ,2 <i>R</i>)-6-methoxy-6-methylhept-4-en-2-yl]-4,4,13,14-tetramethyl-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthrene-9-carbaldehyde	
120	(2 <i>R</i> ,5 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>S</i> ,12 <i>R</i> ,15 <i>R</i> ,16 <i>R</i>)-15-[(<i>E</i> ,2 <i>R</i> ,5 <i>R</i>)-5,6-dimethylhept-3-en-2-yl]-2,16-dimethyl-8-oxapentacyclo[9.7.0.0 ^{2,7} .0 ^{7,9} .0 ^{12,16}]octadec-1(11)-ene-5,10-diol	

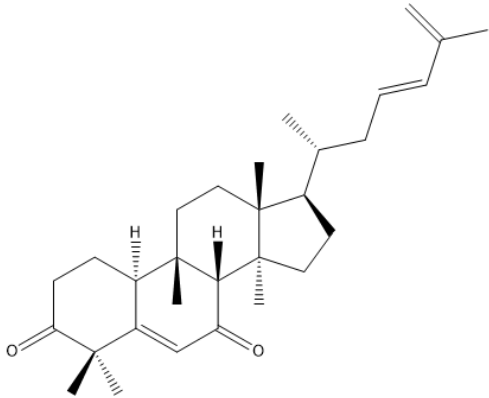
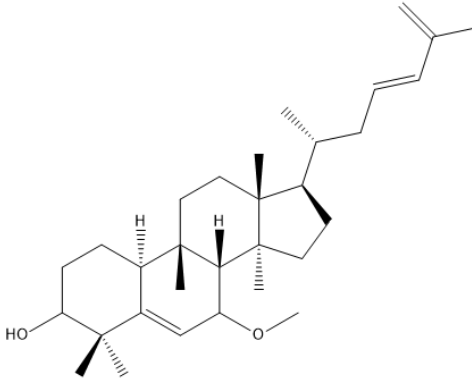
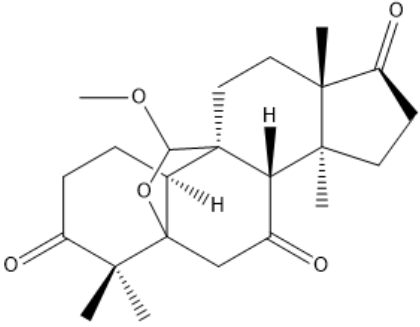
121	2,3-dihydroxybenzoic acid	
122	2-hydroxybenzoic acid	
123	(1 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,8 <i>R</i> ,9 <i>R</i> ,12 <i>S</i> ,13 <i>S</i> ,16 <i>S</i>)-8-[(<i>E</i> ,2 <i>R</i>)-6-methoxy-6-methylhept-4-en-2-yl]-5,9,17,17-tetramethyl-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-ol	
124	(3 <i>S</i> ,7 <i>S</i> ,8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-3,7-dihydroxy-17-[(<i>E</i> ,2 <i>R</i>)-6-hydroxy-6-methylhept-4-en-2-yl]-4,4,13,14-tetramethyl-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthrene-9-carbaldehyde	

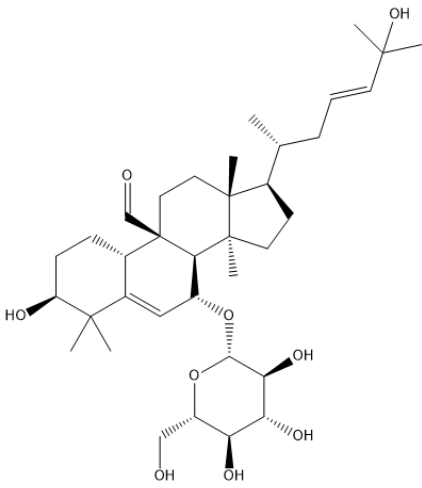
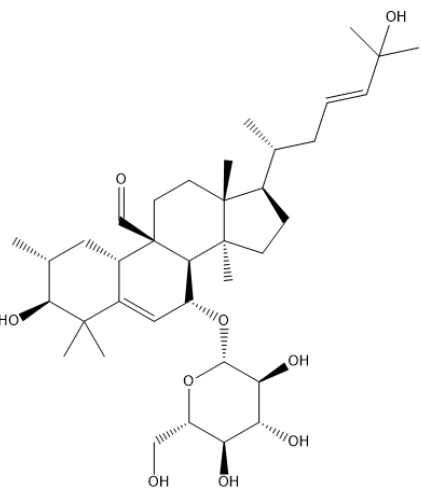
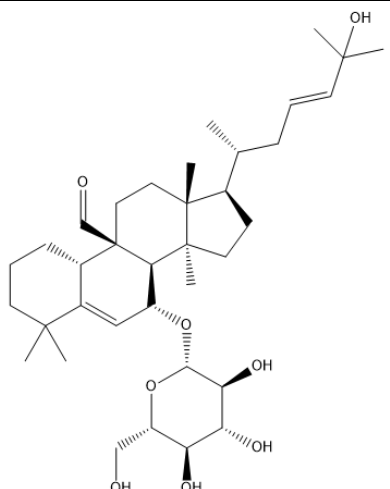
125	(3 <i>S</i> ,7 <i>S</i> ,8 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-3-hydroxy-7-methoxy-17-[(<i>E</i> ,2 <i>R</i>)-6-methoxy-6-methylhept-4-en-2-yl]-4,4,13,14-tetramethyl-2,3,7,8,10,11,12,15,16,17-decahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthrene-9-carbaldehyde	
126	(4 <i>aR</i> ,6 <i>aR</i> ,6 <i>aS</i> ,6 <i>bS</i> ,8 <i>aS</i> ,11 <i>R</i> ,12 <i>S</i> ,12 <i>aR</i> ,14 <i>aR</i> ,14 <i>bS</i>)-6 <i>a</i> -hydroxy-8 <i>a</i> -(methoxymethyl)-4,4,6 <i>a</i> ,6 <i>b</i> ,11,12,14 <i>b</i> -heptamethyl-2,4 <i>a</i> ,5,6,7,8,9,10,11,12,12 <i>a</i> ,14 <i>a</i> -dodecahydro-1 <i>H</i> -picen-3-one	
127	(2 <i>R</i> ,3 <i>S</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>R</i>)-2-(hydroxymethyl)-6-[[[(1 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,8 <i>R</i> ,9 <i>R</i> ,12 <i>S</i> ,13 <i>S</i> ,16 <i>S</i>)-5,9,17,17-tetramethyl-8-[(2 <i>R</i> ,4 <i>R</i> ,5 <i>S</i>)-4,5,6-trihydroxy-6-methylheptan-2-yl]-18-oxapentacyclo[10.5.2.0 ^{1,13} .0 ^{4,12} .0 ^{5,9}]nonadec-2-en-16-yl]oxy]oxane-3,4,5-triol	

128	7-(2-(11-oxidanyl)propan-2-yl)-1,2,3-trimethyl-2,3,6,6a,7,8,9,9a-octahydro-10l5-indeno[4,5-h]chromene-5,10(1H)-dione	
129	6,12-dimethyl-17-(4-methyl-4-(11-oxidanyl)pentyl)-2-(11-oxidanyl)-1,3,4,8,9,10,12,13,14,15,16,17-dodecahydro-7H-cyclopenta[a]phenanthrene-7,11(2H)-dione	
130	2-((11-hydroxy-17-(4-methoxy-6-methylhept-5-en-2-yl)-4,4,12,13,14-pentamethyl-1,3,4,8,10,11,12,13,14,15,16,17-dodecahydro-2H-5,9-(epoxymethano)cyclopenta[a]phenanthren-3-yl)oxy)-6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol	

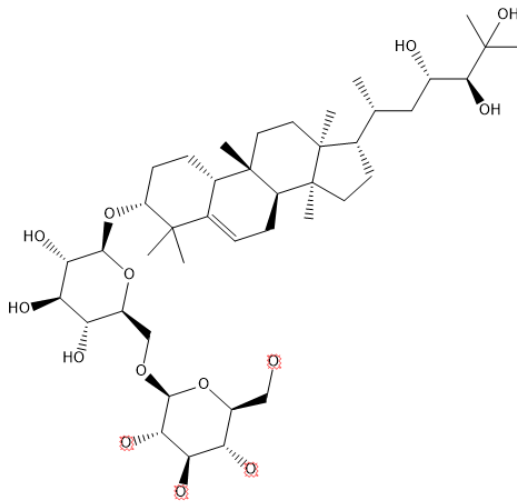
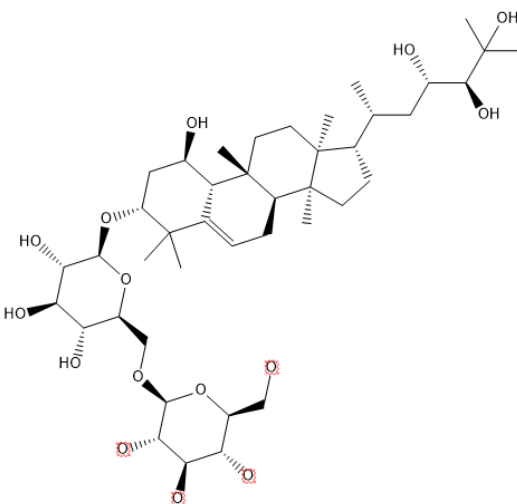
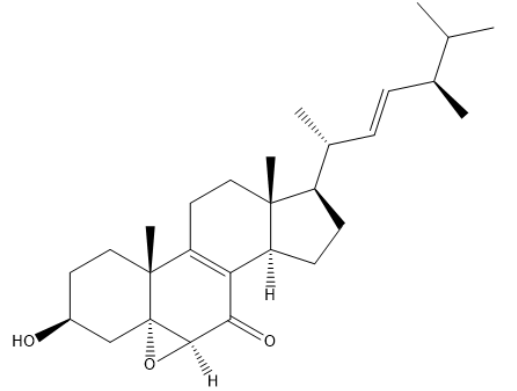
131	7-(2-(11-oxidanyl)propan-2-yl)-1,2,3-trimethyl-2,3,6,6a,7,8,9,9a-octahydro-10l5-indeno[4,5-h]chromene-5,10(1H)-dione	
132	(E)-2,4,4,13,14-pentamethyl-17-(5-methyl-1-(11-oxidanyl)hexa-3,5-dien-1-yl)-7-(11-oxidanyl)-3-oxo-1,2,3,4,7,8,10,11,12,13,14,15,16,17-tetradecahydro-9H-cyclopenta[a]phenanthrene-9-carbaldehyde	
133	(E)-9-(hydroxymethyl)-13,14-dimethyl-17-(5-methyl-1-(11-oxidanyl)hexa-3,5-dien-1-yl)-7-(11-oxidanyl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol	
134	(E)-(6,7,13,14-tetramethyl-17-(5-methyl-1-(11-oxidanyl)hexa-3,5-dien-1-yl)-2,3,4-tri(11-oxidanyl)hexadecahydro-9H-cyclopenta[a]phenanthren-9-yl)methanol	

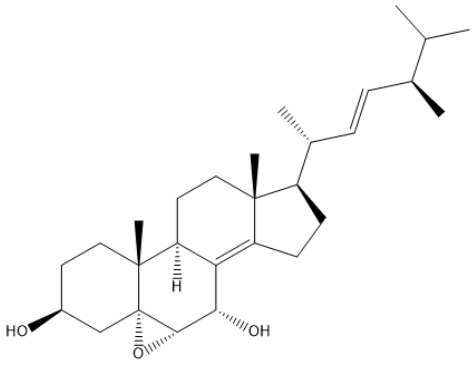
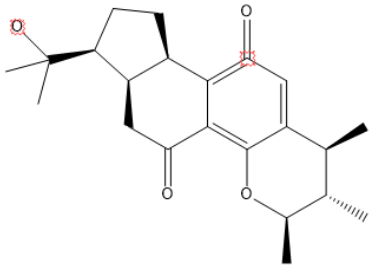
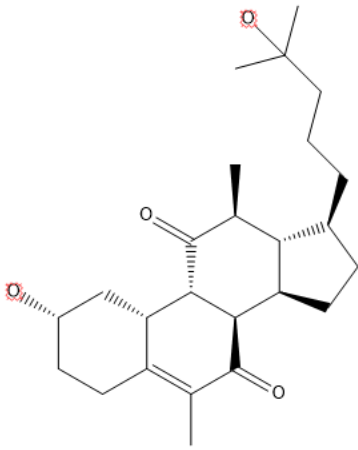
135	(E)-3-hydroxy-2,4,4,13,14-pentamethyl-17-(5-methyl-1-(11-oxidanyl)hexa-3,5-dien-1-yl)-7-(11-oxidanyl)-1,2,3,4,7,8,10,11,12,13,14,15,16,17-tetradecahydro-9H-cyclopenta[a]phenanthrene-9-carbaldehyde	
136	6-(((8a-(((3-((3,4-dihydroxy-6-methyl-5-((3,4,5-trihydroxytetrahydro-2H-pyran-2-yl)oxy)tetrahydro-2H-pyran-2-yl)oxy)-5-hydroxy-6-oxo-4-((3,4,5,6-tetrahydroxytetrahydro-2H-pyran-2-yl)oxy)tetrahydro-2H-pyran-2-yl)oxy)carbonyl)-4-formyl-11-((5-hydroxy-5-methyl-4-methylenehexyl)oxy)-4,6,6a,6b,14b-pentamethyldocosahydripicen-3-yl)oxy)-3,4-dihydroxy-5-((3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)tetrahydro-2H-pyran-2-carboxylic acid	
137	Cucurbita-5,24-diene-3,7,23-trione	

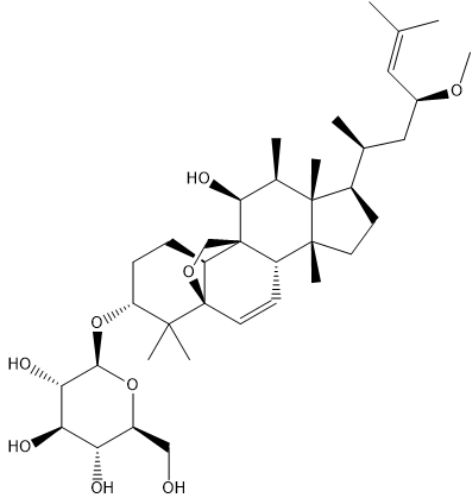
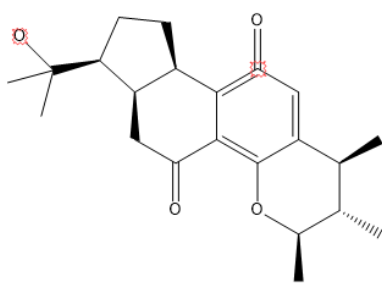
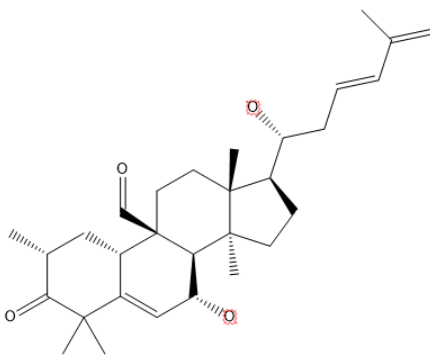
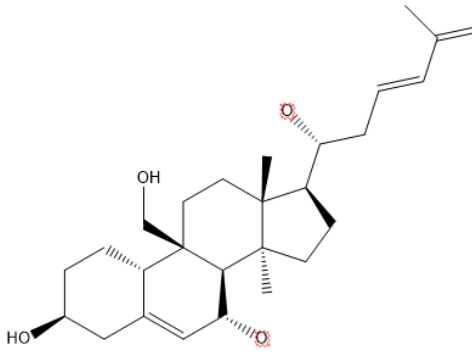
138	Cucurbita-5,23,25-triene-3,7-dione	
139	7-Methoxycucurbita-5,23,25-trien-3-ol	
140	5,19-Epoxy-19-methoxy-20,21,22,23,24,25,26,27-octanorcucurbitane-3,7,17-trione	

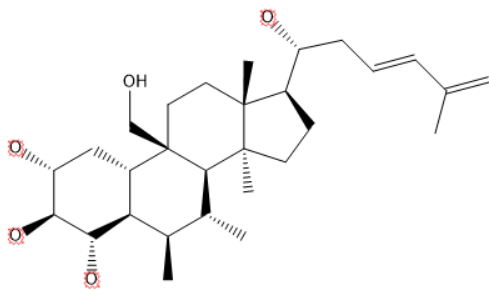
141	(E)-3-hydroxy-17-(6-hydroxy-6-methylhept-4-en-2-yl)-4,4,13,14-tetramethyl-7-((3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)-1,2,3,4,7,8,10,11,12,13,14,15,16,17-tetradecahydro-9H-cyclopenta[a]phenanthrene-9-carbaldehyde	
142	(E)-3-hydroxy-17-(6-hydroxy-6-methylhept-4-en-2-yl)-2,4,4,13,14-pentamethyl-7-((3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)-1,2,3,4,7,8,10,11,12,13,14,15,16,17-tetradecahydro-9H-cyclopenta[a]phenanthrene-9-carbaldehyde	
143	(E)-17-(6-hydroxy-6-methylhept-4-en-2-yl)-4,4,13,14-tetramethyl-7-((3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)-1,2,3,4,7,8,10,11,12,13,14,15,16,17-tetradecahydro-9H-cyclopenta[a]phenanthrene-9-carbaldehyde	

144	20,21,22,23,24,25,26,27-Octanorcucurbit-5-ene-3,7,17-trione	
145	20,21,22,23,24,25,26,27-Octanorcucurbit-5-ene-3,7,16-trione	
146	(8R,9S,10S,13S,14S)-6-hydroxy-2,4,4,9,11,12,13,14-octamethyl-1,8,9,10,11,12,13,14,15,17-decahydro-3H-cyclopenta[a]phenanthrene-3,7,16(2H,4H)-trione	
147	(E)-1,3-dihydroxy-17-(2-hydroxy-5-methoxy-5-methyl-1-(11-oxidanyl)hex-3-en-1-yl)-7-((6-(hydroxymethyl)-3,4,5-trimethoxytetrahydro-2H-pyran-2-yl)oxy)-2-methoxy-4,4,13,14,15,16-hexamethyl-12-(11-oxidanyl)-1,2,3,4,7,8,10,11,12,13,14,15,16,17-tetradecahydro-9H-cyclopenta[a]phenanthrene-9-carbaldehyde	

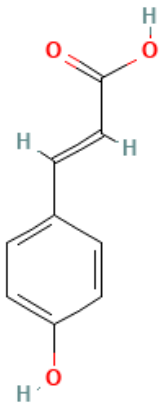
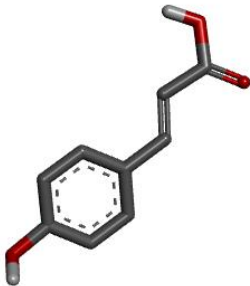
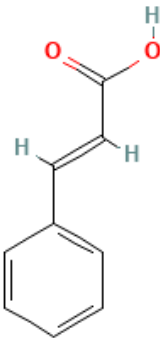
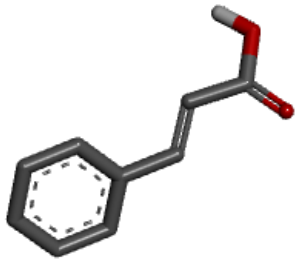
148	2-(((6-((11-oxidanyl)methyl)-3,4,5-tri(11-oxidanyl)tetrahydro-2H-pyran-2-yl)oxy)methyl)-6-((4,4,9,13,14-pentamethyl-17-(4,5,6-trihydroxy-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl)oxy)tetrahydro-2H-pyran-3,4,5-triol	
149	2-(((6-((11-oxidanyl)methyl)-3,4,5-tri(11-oxidanyl)tetrahydro-2H-pyran-2-yl)oxy)methyl)-6-((1-hydroxy-4,4,9,13,14-pentamethyl-17-(4,5,6-trihydroxy-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl)oxy)tetrahydro-2H-pyran-3,4,5-triol	
150	(3beta,5alpha,6alpha,22E)-5,6-Epoxy-3-hydroxyergosta-8,22-dien-7-one	

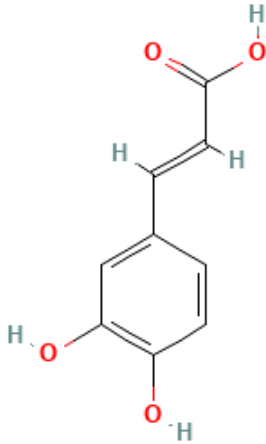
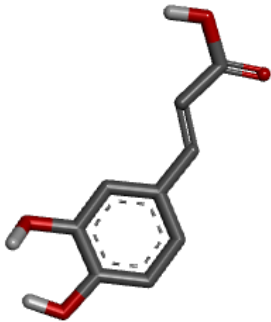
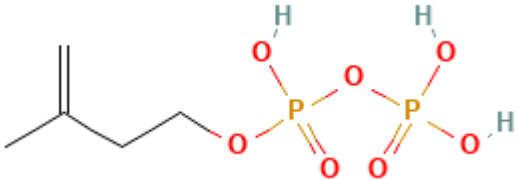
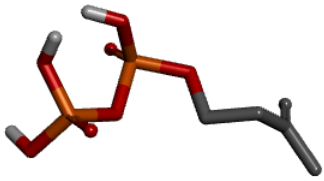
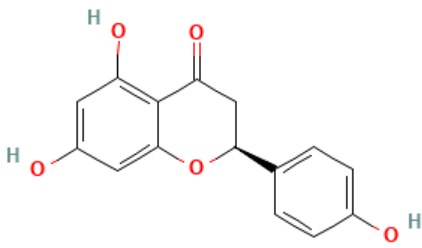
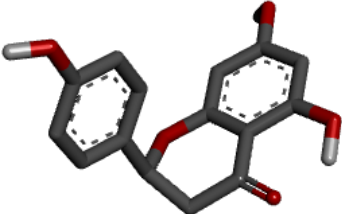
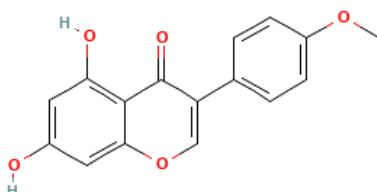
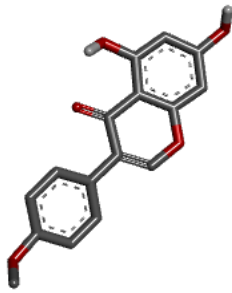
151	5alpha,6alpha-Epoxyergosta-8(14),22-diene-3beta,7alpha-diol	
152	7-(2-(11-oxidanyl)propan-2-yl)-1,2,3-trimethyl-2,3,6,6a,7,8,9,9a-octahydro-10l5-indeno[4,5-h]chromene-5,10(1H)-dione	
153	6,12-dimethyl-17-(4-methyl-4-(11-oxidanyl)pentyl)-2-(11-oxidanyl)-1,3,4,8,9,10,12,13,14,15,16,17-dodecahydro-7H-cyclopenta[a]phenanthrene-7,11(2H)-dione	

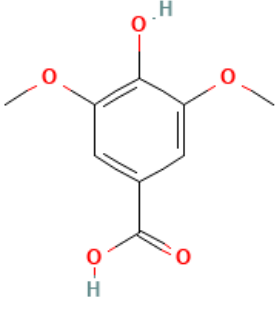
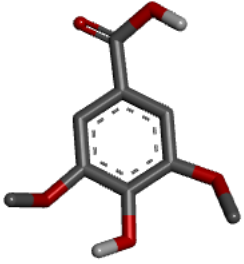
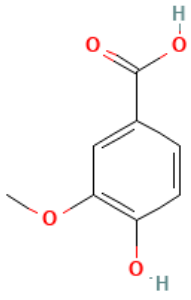
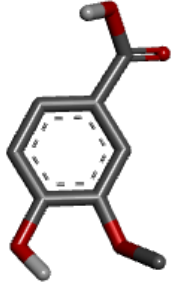
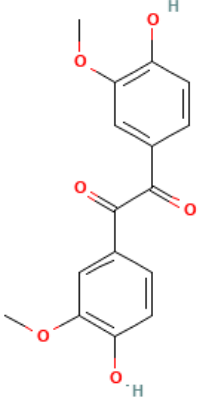
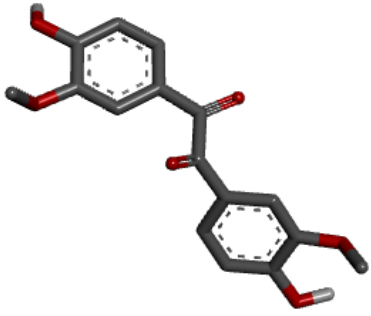
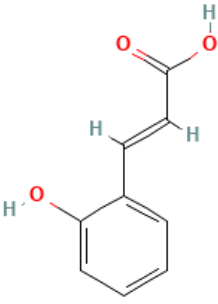
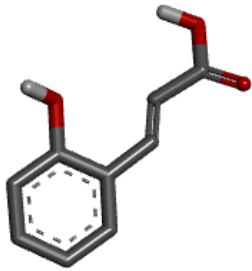
154	2-((11-hydroxy-17-(4-methoxy-6-methylhept-5-en-2-yl)-4,4,12,13,14-pentamethyl-1,3,4,8,10,11,12,13,14,15,16,17-dodecahydro-2H-5,9-(epoxymethano)cyclopenta[a]phenanthren-3-yl)oxy)-6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol	
155	7-(2-(11-oxidanyl)propan-2-yl)-1,2,3-trimethyl-2,3,6,6a,7,8,9,9a-octahydro-10l5-indeno[4,5-h]chromene-5,10(1H)-dione	
156	(E)-2,4,4,13,14-pentamethyl-17-(5-methyl-1-(11-oxidanyl)hexa-3,5-dien-1-yl)-7-(11-oxidanyl)-3-oxo-1,2,3,4,7,8,10,11,12,13,14,15,16,17-tetradecahydro-9H-cyclopenta[a]phenanthrene-9-carbaldehyde	
157	(E)-9-(hydroxymethyl)-13,14-dimethyl-17-(5-methyl-1-(11-oxidanyl)hexa-3,5-dien-1-yl)-7-(11-oxidanyl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol	

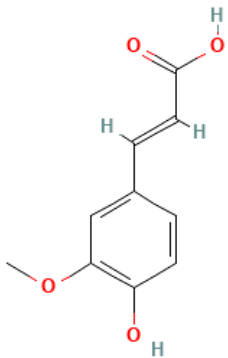
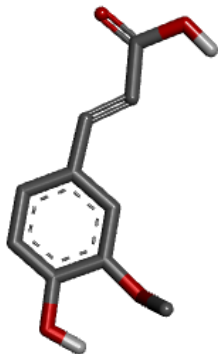
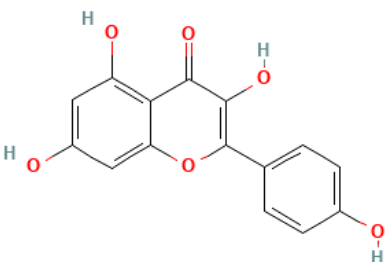
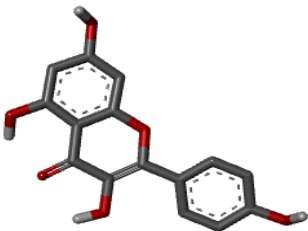
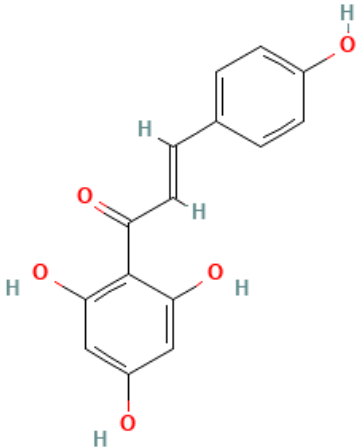
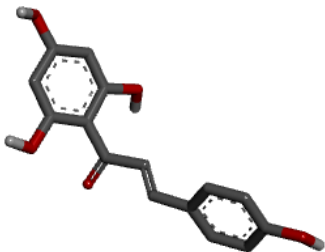
158	(E)-(6,7,13,14-tetramethyl-17-(5-methyl-1-(11-oxidanyl)hexa-3,5-dien-1-yl)-2,3,4-tri(11-oxidanyl)hexadecahydro-9H-cyclopenta[a]phenanthren-9-yl)methanol	
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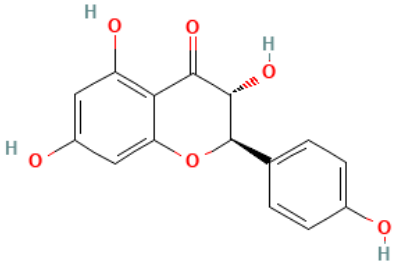
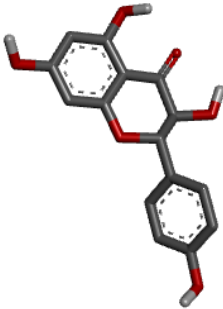
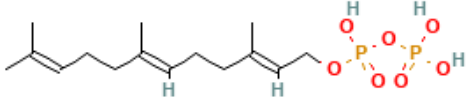
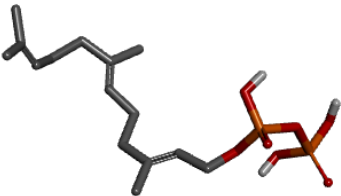
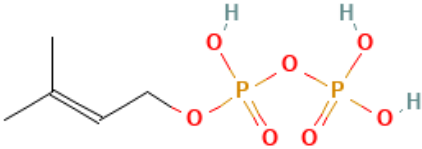
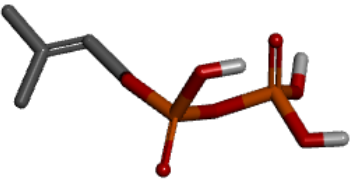
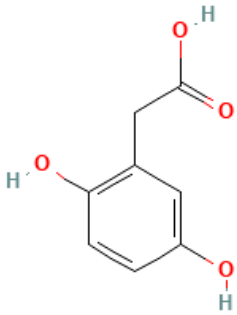
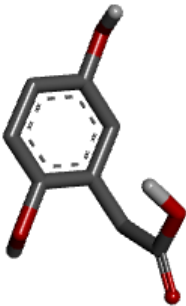
Lampiran 3 Pemodelan struktur ligan

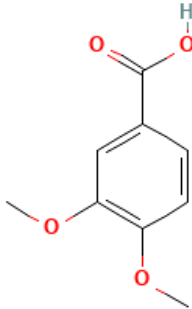
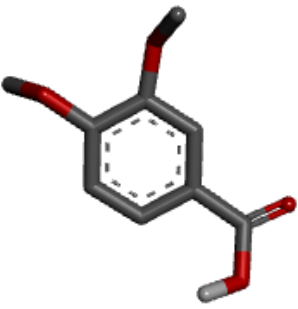
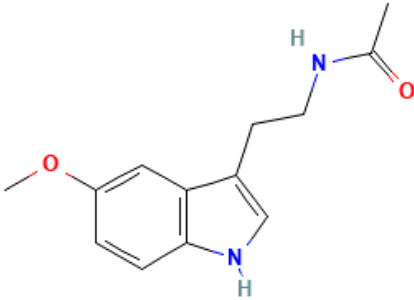
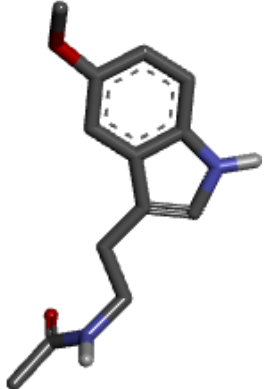
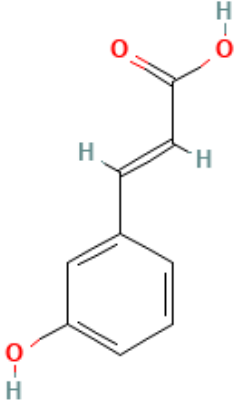
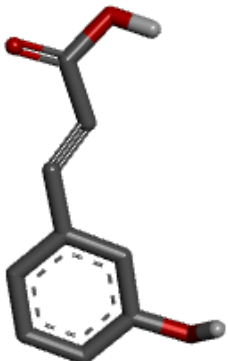
Kode Ligan	Senyawa 2D	Senyawa 3D
LU 1		
LU 2		

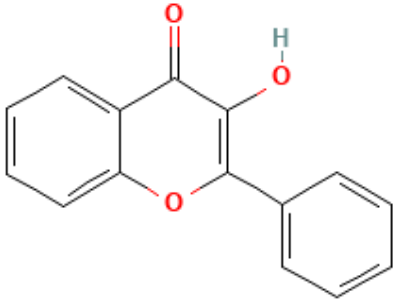
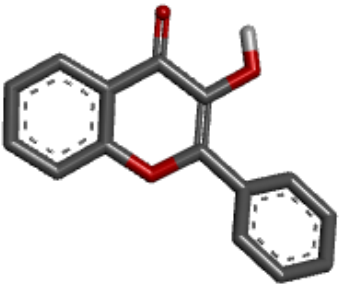
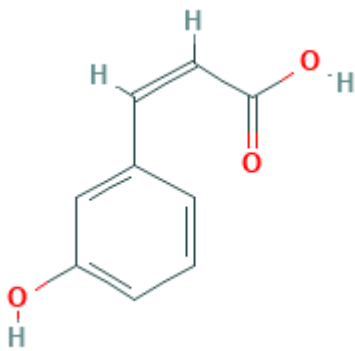
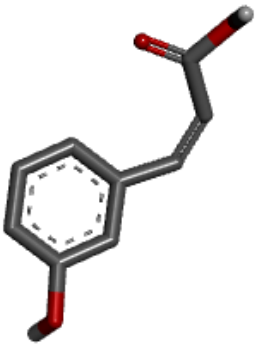
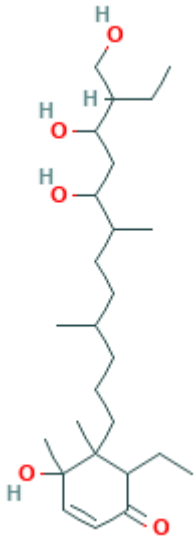
LU 4		
LU 6		
LU 18		
LU 24		

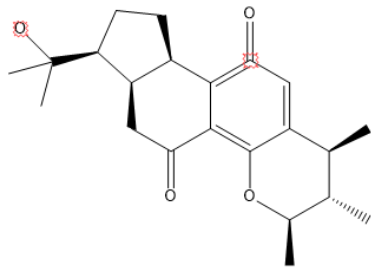
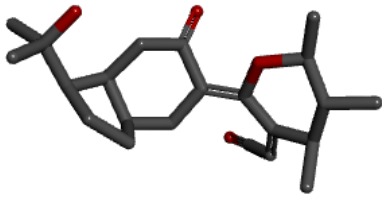
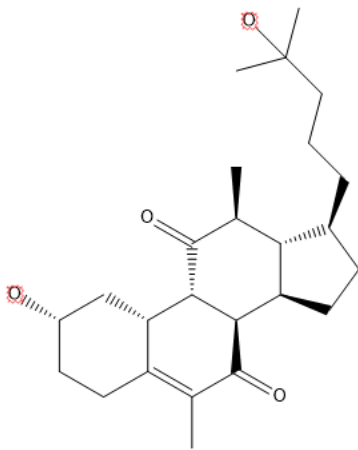
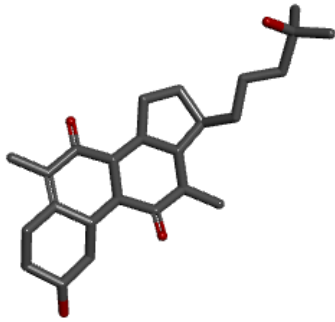
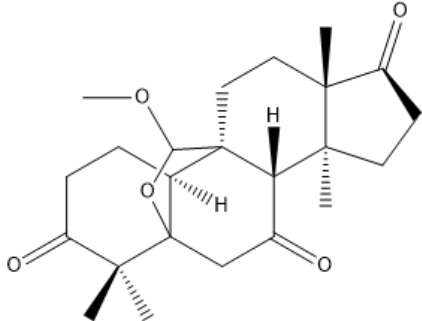
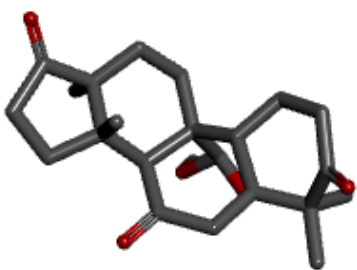
LU 28	 Chemical structure of 3,5-dimethoxybenzoic acid, showing a benzene ring with a carboxylic acid group at position 1 and methoxy groups at positions 3 and 5.	 3D ball-and-stick model of 3,5-dimethoxybenzoic acid, showing the spatial arrangement of atoms.
LU 29	 Chemical structure of 3-methoxybenzoic acid, showing a benzene ring with a carboxylic acid group at position 1 and a methoxy group at position 3.	 3D ball-and-stick model of 3-methoxybenzoic acid, showing the spatial arrangement of atoms.
LU 30	 Chemical structure of 3,3'-dimethoxy-4,4'-dicarboxybenzophenone, showing two benzene rings connected by a carbonyl group, with methoxy groups at positions 3 and 3' and carboxylic acid groups at positions 4 and 4'.	 3D ball-and-stick model of 3,3'-dimethoxy-4,4'-dicarboxybenzophenone, showing the spatial arrangement of atoms.
LU 32	 Chemical structure of 2-hydroxy-3-oxo-3-phenylprop-2-enoic acid, showing a benzene ring attached to a prop-2-enoic acid chain with a hydroxyl group at position 2.	 3D ball-and-stick model of 2-hydroxy-3-oxo-3-phenylprop-2-enoic acid, showing the spatial arrangement of atoms.

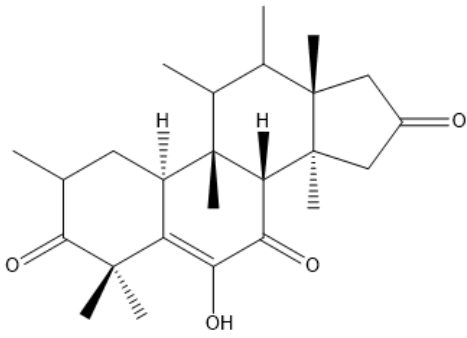
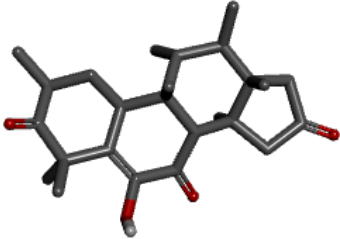
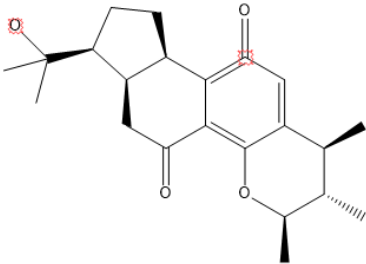
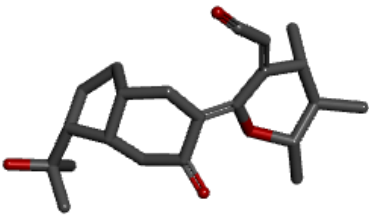
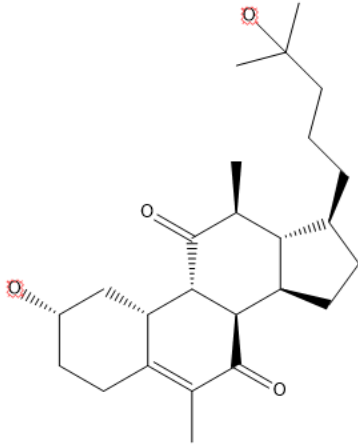
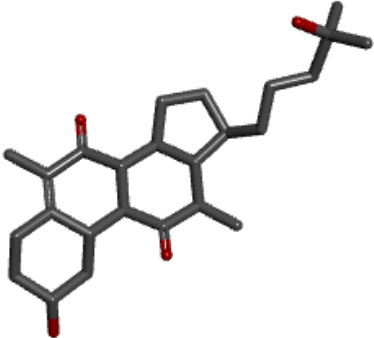
LU 33	 <chem>COc1ccc(cc1C(=O)c2ccccc2)C=O</chem>	
LU 45	 <chem>O=C1C(=O)C(=O)C(=O)C1=Cc2ccc(O)cc2</chem>	
LU 49	 <chem>O=C1C(=O)C(=O)C(=O)C1=Cc2ccc(O)cc2</chem>	

LU 50		
LU 53		
LU 57		
LU 58		

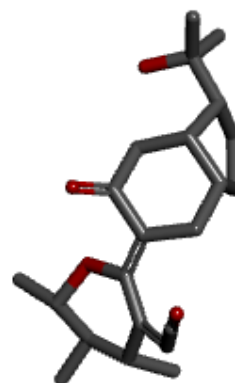
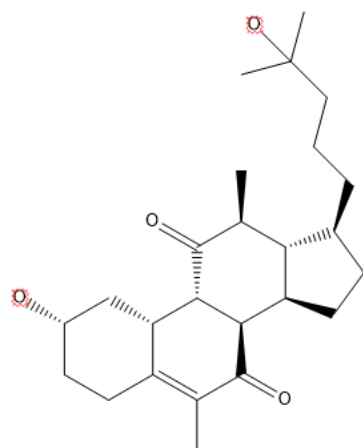
LU 59	 Chemical structure of 3,5-dimethoxybenzoic acid, showing a benzene ring with a carboxylic acid group at position 1 and methoxy groups at positions 3 and 5.	 3D ball-and-stick model of 3,5-dimethoxybenzoic acid, showing the spatial arrangement of atoms.
LU 98	 Chemical structure of 1-(4-methoxyphenyl)-2-(2-(acetamidoethyl))indole, showing an indole ring system with a 4-methoxyphenyl group at position 1 and a 2-(acetamidoethyl) group at position 2.	 3D ball-and-stick model of 1-(4-methoxyphenyl)-2-(2-(acetamidoethyl))indole, showing the spatial arrangement of atoms.
LU 99	 Chemical structure of 4-hydroxybenzaldehyde, showing a benzene ring with a hydroxyl group at position 1 and an aldehyde group at position 4.	 3D ball-and-stick model of 4-hydroxybenzaldehyde, showing the spatial arrangement of atoms.

LU 100	 2D chemical structure of 2-phenyl-4-hydroxy-1,4-dihydro-2H-chromene-3-one. It features a benzene ring fused to a six-membered ring containing an oxygen atom, a carbonyl group, and a phenyl substituent, with a hydroxyl group at the 4-position.	 3D ball-and-stick model of 2-phenyl-4-hydroxy-1,4-dihydro-2H-chromene-3-one, showing the spatial arrangement of atoms and the relative orientation of the fused rings and substituents.
LU 101	 2D chemical structure of 4-hydroxy-3-(4-hydroxyphenyl)acrylaldehyde. It consists of a central carbon-carbon double bond with an aldehyde group and a hydroxyl group on one carbon, and a 4-hydroxyphenyl group on the other carbon.	 3D ball-and-stick model of 4-hydroxy-3-(4-hydroxyphenyl)acrylaldehyde, illustrating the conformation of the molecule in three dimensions.
LU 110	 2D chemical structure of a complex branched molecule. It features a central carbon chain with multiple hydroxyl groups, a ketone group, and a cyclohexene ring system, along with various alkyl substituents.	 3D ball-and-stick model of the complex branched molecule, showing the spatial arrangement of the various functional groups and the ring system.

LU 128	 2D chemical structure of LU 128, a complex polycyclic molecule featuring a central benzene ring fused to a six-membered ring containing an oxygen atom and a carbonyl group. It also includes a five-membered ring with a carbonyl group and a quaternary carbon atom bonded to two methyl groups and a hydrogen atom.	 3D ball-and-stick model of LU 128, showing the spatial arrangement of atoms and the overall shape of the molecule.
LU 129	 2D chemical structure of LU 129, a complex polycyclic molecule featuring a central benzene ring fused to a six-membered ring containing a carbonyl group and a quaternary carbon atom bonded to a methyl group and a hydrogen atom. It also includes a five-membered ring with a carbonyl group and a quaternary carbon atom bonded to two methyl groups and a hydrogen atom.	 3D ball-and-stick model of LU 129, showing the spatial arrangement of atoms and the overall shape of the molecule.
LU 140	 2D chemical structure of LU 140, a complex polycyclic molecule featuring a central benzene ring fused to a six-membered ring containing a carbonyl group and a quaternary carbon atom bonded to a methyl group and a hydrogen atom. It also includes a five-membered ring with a carbonyl group and a quaternary carbon atom bonded to two methyl groups and a hydrogen atom.	 3D ball-and-stick model of LU 140, showing the spatial arrangement of atoms and the overall shape of the molecule.

LU 146	 2D chemical structure of LU 146, a complex polycyclic molecule featuring multiple fused rings, a hydroxyl group (OH), and several carbonyl groups (C=O). Stereochemistry is indicated with wedges and dashes.	 3D ball-and-stick model of LU 146, showing the spatial arrangement of atoms and the overall molecular shape.
LU 152	 2D chemical structure of LU 152, a complex polycyclic molecule featuring multiple fused rings, a carbonyl group (C=O), and a hydroxyl group (OH). Stereochemistry is indicated with wedges and dashes.	 3D ball-and-stick model of LU 152, showing the spatial arrangement of atoms and the overall molecular shape.
LU 153	 2D chemical structure of LU 153, a complex polycyclic molecule featuring multiple fused rings, a carbonyl group (C=O), and a hydroxyl group (OH). Stereochemistry is indicated with wedges and dashes.	 3D ball-and-stick model of LU 153, showing the spatial arrangement of atoms and the overall molecular shape.

LU 155



Lampiran 4 Ikatan hidrogen bond

Kode Ligan	Acceptor	DonorH	Donor	Frac	Okupansi (%)
LIG	LIG 890	GLN 122 HE22	GLN 122 NE2	0,0062	0,62
	LIG 890	GLY 265 H	GLY 265 N	0,0052	0,52
	LIG 890	ALA 266 H	ALA 266 N	0,0036	0,36
	LIG 890	THR 126 H	THR 126 N	0,0021	0,21
	LIG 890	ALA 125 H	ALA 125 N	0,001	0,1
	LIG 890	THR 126 HG1	THR 126 OG1	0,0005	0,05
	LIG 890	ASN 878 HD21	ASN 878 ND2	0,0004	0,04
	LIG 890	GLN 122 HE22	GLN 122 NE2	0,0003	0,03
	LIG 890	LYS 323 HZ3	LYS 323 NZ	0,0003	0,03
	LIG 890	GLU 268 H	GLU 268 N	0,0002	0,02
	LIG 890	LYS 323 HZ2	LYS 323 NZ	0,0001	0,01
	LIG 890	THR 110 HG1	THR 110 OG1	0,0001	0,01
	LIG 890	GLN 122 HE21	GLN 122 NE2	0,0001	0,01
	LIG 890	THR 842 HG1	THR 842 OG1	0	0
	LIG 890	THR 842 HG1	THR 842 OG1	0	0
	LIG 890	LYS 323 HZ1	LYS 323 NZ	0	0
	LIG 890	ASN 878 HD21	ASN 878 ND2	0	0
	LIG 890	GLN 843 HE22	GLN 843 NE2	0	0
	LIG 890	ARG 130 HE	ARG 130 NE	0	0
	LIG 890	GLN 843 HE22	GLN 843 NE2	0	0
	LIG 890	ASN 878 HD22	ASN 878 ND2	0	0
	LIG 890	TYR 385 HH	TYR 385 OH	0	0
	LIG 890	TYR 380 HH	TYR 380 OH	0	0
	LIG 890	ARG 130 HE	ARG 130 NE	0	0
S53	S53 890	GLN 843 HE21	GLN 843 NE2	0,0115	1,15
	S53 890	ASN 878 HD21	ASN 878 ND2	0,0037	0,37
	S53 890	ASN 378 HD22	ASN 378 ND2	0,001	0,1
	S53 890	TYR 882 HH	TYR 882 OH	0,0008	0,08
	S53 890	ASN 378 HD21	ASN 378 ND2	0,0007	0,07
	S53 890	LYS 849 HZ2	LYS 849 NZ	0,0006	0,06
	S53 890	LYS 849 HZ3	LYS 849 NZ	0,0005	0,05
	S53 890	LYS 849 HZ1	LYS 849 NZ	0,0004	0,04
	S53 890	ASN 378 HD22	ASN 378 ND2	0,0003	0,03
	S53 890	ALA 266 H	ALA 266 N	0,0003	0,03
	S53 890	TYR 882 HH	TYR 882 OH	0,0003	0,03
	S53 890	ARG 885 HE	ARG 885 NE	0,0003	0,03
	S53 890	ASN 276 HD22	ASN 276 ND2	0,0002	0,02
	S53 890	THR 382 H	THR 382 N	0,0002	0,02
	S53 890	THR 382 H	THR 382 N	0,0002	0,02
	S53 890	ASN 878 HD22	ASN 878 ND2	0,0001	0,01
	S53 890	ARG 885 HH21	ARG 885 NH2	0,0001	0,01
	S53 890	ASN 278 HD21	ASN 278 ND2	0,0001	0,01
	S53 890	GLN 843 HE22	GLN 843 NE2	0,0001	0,01
	S53 890	ASN 378 HD22	ASN 378 ND2	0,0001	0,01
	S53 890	THR 381 HG1	THR 381 OG1	0,0001	0,01
	S53 890	ARG 885 HH22	ARG 885 NH2	0,0001	0,01

	S53 890	THR 842 HG1	THR 842 OG1	0,0001	0,01
	S53 890	ASN 263 HD21	ASN 263 ND2	0,0001	0,01
	S53 890	ARG 885 HH22	ARG 885 NH2	0,0001	0,01
	S53 890	GLN 843 HE21	GLN 843 NE2	0,0001	0,01
	S53 890	TYR 380 HH	TYR 380 OH	0	0
	S53 890	GLY 265 H	GLY 265 N	0	0
	S53 890	ARG 885 HH12	ARG 885 NH1	0	0
	S53 890	THR 381 HG1	THR 381 OG1	0	0
	S53 890	ARG 885 HH12	ARG 885 NH1	0	0
	S53 890	ARG 802 HH12	ARG 802 NH1	0	0
	S53 890	ASN 263 HD22	ASN 263 ND2	0	0
	S53 890	ASN 378 HD21	ASN 378 ND2	0	0
	S53 890	ARG 294 HH22	ARG 294 NH2	0	0
	S53 890	TYR 882 HH	TYR 882 OH	0	0
	S53 890	ARG 885 HH11	ARG 885 NH1	0	0
S29	S29 890	GLN 766 HE22	GLN 766 NE2	0,0118	1,18
	S29 890	THR 382 H	THR 382 N	0,0066	0,66
	S29 890	GLY 265 H	GLY 265 N	0,0031	0,31
	S29 890	GLN 843 HE21	GLN 843 NE2	0,0013	0,13
	S29 890	ASN 810 HD21	ASN 810 ND2	0,0012	0,12
	S29 890	GLN 843 HE22	GLN 843 NE2	0,0005	0,05
	S29 890	LYS 849 HZ1	LYS 849 NZ	0,0002	0,02
	S29 890	TYR 882 HH	TYR 882 OH	0,0002	0,02
	S29 890	LYS 849 HZ3	LYS 849 NZ	0,0002	0,02
	S29 890	LYS 849 HZ2	LYS 849 NZ	0,0001	0,01
	S29 890	THR 382 H	THR 382 N	0,0001	0,01
	S29 890	GLN 766 HE21	GLN 766 NE2	0,0001	0,01
	S29 890	GLN 843 HE22	GLN 843 NE2	0,0001	0,01
	S29 890	ARG 294 HH21	ARG 294 NH2	0,0001	0,01
	S29 890	TYR 385 HH	TYR 385 OH	0	0
	S29 890	GLN 843 HE21	GLN 843 NE2	0	0
	S29 890	LYS 770 HZ3	LYS 770 NZ	0	0
	S29 890	GLN 843 HE22	GLN 843 NE2	0	0
	S29 890	LYS 770 HZ1	LYS 770 NZ	0	0
	S29 890	ARG 802 HH12	ARG 802 NH1	0	0
	S29 890	TYR 385 HH	TYR 385 OH	0	0
	S29 890	ARG 802 HH12	ARG 802 NH1	0	0
	S29 890	ARG 802 HE	ARG 802 NE	0	0
	S29 890	ARG 294 HH12	ARG 294 NH1	0	0
S52	S52 890	GLN 843 HE22	GLN 843 NE2	0,0182	1,82
	S52 890	ASN 810 HD21	ASN 810 ND2	0,006	0,6
	S52 890	ASN 810 HD22	ASN 810 ND2	0,0019	0,19
	S52 890	GLN 843 HE22	GLN 843 NE2	0,0016	0,16
	S52 890	ARG 774 HH21	ARG 774 NH2	0,001	0,1
	S52 890	ARG 774 HH22	ARG 774 NH2	0,0007	0,07
	S52 890	GLN 766 HE21	GLN 766 NE2	0,0005	0,05
	S52 890	ARG 774 HH12	ARG 774 NH1	0,0003	0,03
	S52 890	GLN 766 HE22	GLN 766 NE2	0,0002	0,02
	S52 890	SER 279 HG	SER 279 OG	0,0001	0,01
	S52 890	ARG 774 HH11	ARG 774 NH1	0,0001	0,01

	S52 890	LYS 770 HZ3	LYS 770 NZ	0,0001	0,01
	S52 890	ARG 774 HE	ARG 774 NE	0	0
	S52 890	ASN 278 HD21	ASN 278 ND2	0	0
	S52 890	LYS 770 HZ1	LYS 770 NZ	0	0
	S52 890	GLN 766 HE22	GLN 766 NE2	0	0
	S52 890	LYS 770 HZ3	LYS 770 NZ	0	0
	S52 890	LYS 770 HZ2	LYS 770 NZ	0	0
	S52 890	GLY 265 H	GLY 265 N	0	0
	S52 890	ARG 294 HH21	ARG 294 NH2	0	0
	S52 890	GLY 265 H	GLY 265 N	0	0
	S52 890	LYS 770 HZ1	LYS 770 NZ	0	0
	S52 890	ARG 802 HE	ARG 802 NE	0	0

Lampiran 5 Optimasi geometri

No.	Kode Ligan	Optimasi Geometri				
		HOMO		LO		Gap Energi
1	LU1	-0,23522	43	-0,06229	44	-0,17293
2	LU2	-0,25901	39	-0,06249	40	-0,19652
3	LU4	-0,22799	47	-0,07402	48	-0,15397
4	LU6	-0,26857	64	-0,08936	65	-0,17921
5	LU18	-0,22591	71	-0,06494	72	-0,16097
6	LU24	-0,20544	74	-0,05089	75	-0,15455
7	LU28	-0,22414	52	-0,05149	53	-0,17265
8	LU29	-0,23471	44	-0,05407	45	-0,18064
9	LU30	-0,21917	79	-0,09062	80	-0,12855
10	LU32	-0,23437	43	-0,07457	44	-0,1598
11	LU33	-0,21874	51	-0,07286	52	-0,14588
12	LU45	-0,21164	74	-0,05846	75	-0,15318
13	LU49	-0,21583	71	-0,07965	72	-0,13618
14	LU50	-0,23308	75	-0,06922	76	-0,16386
15	LU53	-0,22346	102	-0,08308	103	-0,14038
16	LU57	-0,27482	64	-0,08593	65	-0,18889
17	LU58	-0,23075	44	-0,02832	45	-0,20243
18	LU59	-0,22283	48	-0,04948	49	-0,17335
19	LU98	-0,19744	62	-0,00807	63	-0,18937
20	LU99	-0,24108	43	-0,07941	44	-0,16167
21	LU100	-0,2217	62	-0,07129	63	-0,15041
22	LU101	-0,2319	43	-0,07913	44	-0,15277
23	LU110	-0,23537	122	-0,06347	123	-0,1719
24	LU128	-0,16595	97	-0,14233	98	-0,02362
25	LU129	-0,21223	109	-0,20379	110	-0,00844
26	LU133	-0,20313	117	-0,07051	118	-0,13262
27	LU140	-0,23079	105	-0,02449	106	-0,2063
28	LU146	-0,23363	93	-0,07407	94	-0,15956
29	LU152	-0,16707	93	-0,14328	94	-0,02379
30	LU153	-0,21223	109	-0,20379	110	-0,00844
31	LU155	-0,16595	97	-0,14233	98	-0,02362

Lampiran 6 Penambatan molekul

Kode Ligan	Nilai Ki	Binding Energi	Interaksi Ikatan
LU153	0.01381	- 10.72	ALA461, LYS1044, TYR1077, VAL459, TYR580, MET1034
LU129	0.01442	- 10.70	GLY460, ALA461, LYS1044, TYR1077, VAL459, TYR580, MET1034
LU152	0.05593	- 9.89	ARG489, PHE457, VAL459, MET462, HIS496, TYR575, TYR580, MET1034, ZN1101
8EX3	0.06113	- 9.84	ASN458, ALA461, GLU463, GLU497, TYR580, GLU319, ALA320, TYR575, MET1034, VAL459, MET462, GLU572, ZN1101
LU133	0.06445	- 9.81	
LU128	0.13175	- 9.39	ARG489, TYR580, VAL459M HIS496
LU153	0.01381	- 10.72	ALA461, LYS1044, TYR1077, VAL459, TYR580, MET1034
LU155	0.13190	- 9.39	ARG489, TYR580, VAL459M HIS496
LU146	0.22438	- 9.07	THR577, THR1037, GLU1041, VAL459, MET1034, ASP581
LU140	0.56533	- 8.52	GLN1038, VAL459, TYR1077, GLU1041
LU45	1.03	- 8.17	TYR308, ASN458, GLU463, MET1034, VAL459, MET462, PHE457, GLU319, GLN317, ZN1101
LU49	1.37	- 8.00	GLU572, ASN458, GLU463, GLU497, TYR580, MET1034, GLN317, GLU519, VAL459, TYR575
LU50	1.80	- 7.84	LEU304, GLU319, ASN458, GLU497, ALA461, TYR580, VAL459, MET462, MET1034, PHE457
LU30	2.18	- 7.72	ALA320, GLU319, GLY460, GLU497, GLN317, TYR580, VAL459, TYR575, MET1034
LU18	2.23	- 7.71	LEU304, GLU319, GLU463, ASN458, MET462, VAL459, MET1034, PHE457, TYR575
LU24	2.63	- 7.61	GLU463, GLU497, TYR580, MET462, GLU519, VAL459, TYR575
LU100	3.49	- 7.45	MET1034, ALA461, TYR580, MET462, GLU319, VAL459, HIS496, TYR575, ZN1101
LU98	4.04	- 7.36	GLU463, TYR580, GLU319, MET462, LEU304, TYR308, GLN317, VAL459, MET1034, PHE457, TYR575
LU110	5.41	- 7.18	ARG489, GLU554, THR557, ALA461, VAL459, TYR575, LYS1044
LU53	29.10	- 6.19	ARG489, ASN471, ASN473, SER474, LYS965, GLY460, VAL459, MET462, VAL493, HIS496, HIS500, ARG997
LU33	84.90	- 5.55	LEU304, VAL459, GLU319, TYR575, MET1034
LU4	99.56	- 5.46	GLU572, LEU304, VAL459, ASN458, GLU319, TYR575, MET1034
LU1	108.38	- 5.41	LEU304, VAL459, GLU319, TYR575, MET1034
LU101	118.01	- 5.36	ARG489, GLY460, GLU463, TYR580, VAL459, ZN1101
LU32	118.31	- 5.36	MET1034, LEU304, VAL459, ASN458, PHE457, TYR575
LU99	135.27	- 5.28	LEU304, VAL459, GLU319, PHE457, TYR575, MET1034
LU58	145.08	- 5.24	ALA461, GLY460, GLU463, GLU497, TYR580, GLU519
LU2	178.50	- 5.11	LEU304, ASN458, VAL459, PHE457, GLN317, TYR575, MET1034
LU59	462.03	- 4.55	LEU304, ASN458, VAL459, PHE457, GLN317, GLU319, MET1034
LU29	538.34	- 4.46	ALA461, GLY460, GLU319, TYR580, VAL459, GLU519

LU28	810.87	- 4.22	LEU304, ASN458, VAL459, PHE457, GLN317, GLU319, GLU572, MET1034
LU6	1230	- 3.97	ARG997, ASN473, ASN994, LEU1001, PRO1002, ARG489, LYS965
LU57	188000	- 3.72	ARG997, ASN473, ASN994, LEU1001, PRO1002, LYS965

Lampiran 7 Hasil turnitin

Skripsi_Zulfan Rodia Akbar_201FF03189		
ORIGINALITY REPORT		
11%	11%	10%
SIMILARITY INDEX	INTERNET SOURCES	PUBLICATIONS
		9%
		STUDENT PAPERS
PRIMARY SOURCES		
1	repository.bku.ac.id Internet Source	2%
2	www.scfbio-iitd.res.in Internet Source	2%
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8	cb.imsc.res.in Internet Source	1%
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10	Hanine Almubayedh, Rizwan Ahmad. "Ethnopharmacological uses, phytochemistry, biological activities of Debregeasia salicifolia: A review", Journal of Ethnopharmacology, 2019 Publication	1%

Lampiran 8 Lembar bimbingan

No. Dok. 02.04.00FRM-03IAKD-SPM



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KARTU BIMBINGAN TUGAS AKHIR I/TUGAS AKHIR II

Pembimbing Utama	: Ennis Erawati, M. Si				
Nama Mahasiswa	: Zulfan Rodia Akbar				
NPM	: 2017F03189				
Bidang Ilmu	: AFKM				

No	Hari/Tanggal	Waktu	Tempat	Materi	Paraf Dosen
1	25/05/2024	10.00	Lab. kimia	Konfirmasi penemuan yang akan diteliti	
2	02/06/2024	16.00	LPPM	Konfirmasi hasil wawancara yang diteliti	
3	22/06/2024	11.00	Lab. kimia	Penemuan yang akan diteliti pada Ety MD	
4	06/05/2024	11.00	Lab. kimia	Menyusun skripsi tentang kendala pada senyawa	
5	27/05/2024	09.00	Kampus	Laporan kemajuan	
6	02/06/2024	15.30	Kampus	Pembahasan	
7	25/06/2024	10.00	Kampus	Hasil MD senyawa 1	
8	11/06/2024	14.00	Kampus	Hasil MD senyawa 2 & 3 TTO Hal. Persetujuan	
9					
10					
11					
12					
13					
14					
15					
16					

Catatan: Kartu ini harus diisi setiap kali melakukan bimbingan dan harus diisi oleh dosen pembimbing

No. Dok. 02.04.00FRM-03IAKD-SPM



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KARTU BIMBINGAN TUGAS AKHIR I/TUGAS AKHIR II

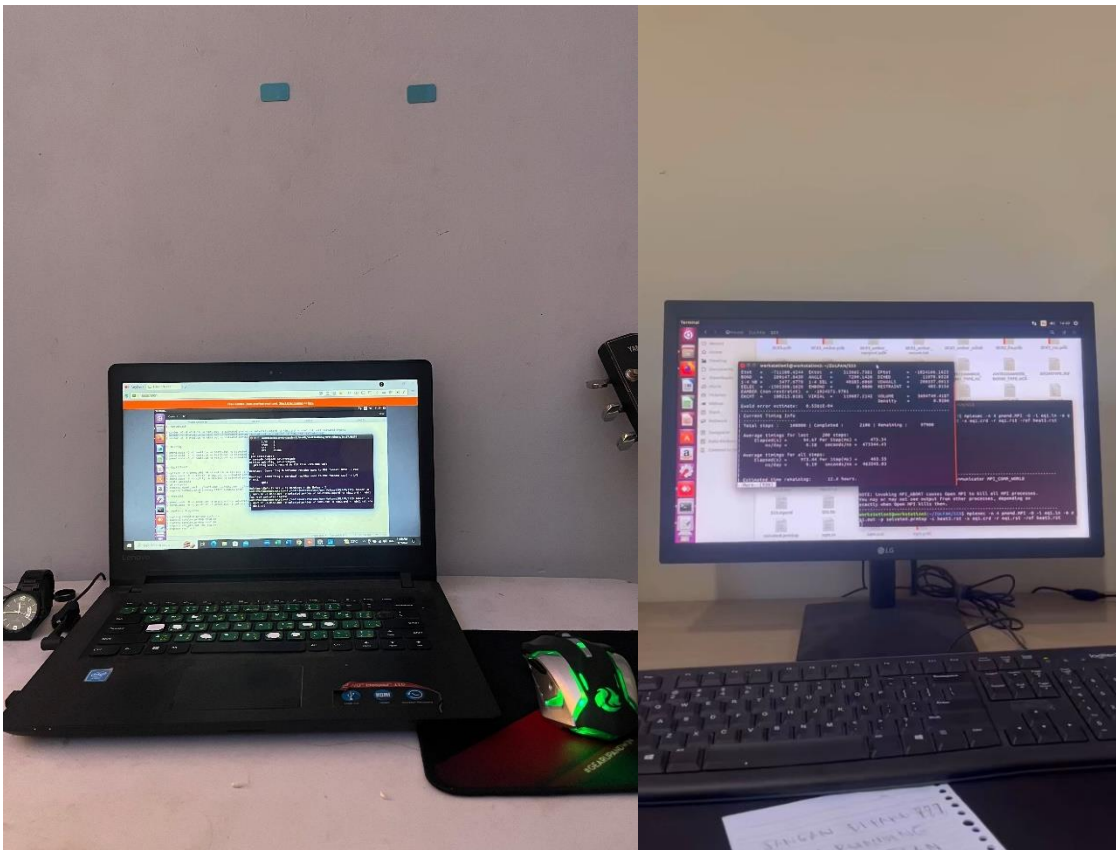
Pembimbing Seta	: Anne Yulianti, M. Si				
Nama Mahasiswa	: Zulfan Rodia Akbar				
NPM	: 2017F03189				
Bidang Ilmu	: AFKM				

No	Hari/Tanggal	Waktu	Tempat	Materi	Paraf Dosen
1	27/05/2024		WA	Konfirmasi: senyawa yang akan diteliti	
2	5/06/2024		"	Konfirmasi hasil wawancara yang diteliti	
3	23/06/2024		"	Tahap MD	
4	10/05/2024		"	Kendala senyawa	
5	29/05/2024		"	Laporan kemajuan	
6	22/06/2024		"	Pembahasan	
7	24/06/2024		"	Hasil MD senyawa 1	
8	13/07/2024		Kampus	Hasil MD senyawa 2 dan 3 TTO Hal. Persetujuan	
9					
10					
11					
12					
13					
14					
15					
16					
17					

Catatan: Kartu ini harus diisi setiap kali melakukan bimbingan dan harus diisi oleh dosen pembimbing

022 7830 765, 022 7830 768
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Lampiran 9 Dokumentasi penelitian



Lampiran 10 CV



ZULFAN RODIA AKBAR

Quality Control (QC)

Alamat : Dusun Tegalwaru, RT/RW 004/002, Desa Tegalwaru, Kec. Cilamaya Wetan,
Kab. Karawang
Kode Pos : 41386
Nomor HP : 085778859250
E-mail : razulfan02@gmail.com

PROFIL PRIBADI

Lulusan S1 Jurusan Farmasi, memiliki skill di bidang industri khususnya di bagian Quality Control (QC). Saya mampu mengoperasikan *Software Microsoft Office*. Selain aktif di kampus sebagai Ketua Organisasi *SM Project*, saya juga memiliki pengalaman sebagai *Data Entry* di sebuah Instansi Kesehatan (Puskesmas). Sedang mencari peluang kerja di bidang industri untuk mengaplikasikan dan juga mengasah kemampuan yang saya miliki.

KEAHLIAN

- Public Speaking
- Event Handle
- Communicating in English
- Desain Grafis
- Microsoft Office
- Leadership
- Work in Team

RIWAYAT PENDIDIKAN

SEKOLAH MENENGAH ATAS (SMA)	2017-2020
SMA NU Kaplongan, Indramayu	
PERGURUAN TINGGI	2020 - 2024
Universitas Bhakti Kencana	
Sarjana Farmasi	
Indeks Prestasi Kumulatif (IPK): 3,16	

RIWAYAT ORGANISASI

ORGANISASI PESANTREN DARUL MA'ARIF (OPDM)	2018 - 2019
• Ketua bagian keamanan	
PANGGUNG GEMBIRA	2018 - 2019
• Ketua pelaksana	
ANGGOTA PENGIBAR BENDERA MERAH PUTIH	2018 - 2019
• Pasukan 8	
ORGANISASI SYMPHONY MUSIK PROJECT (SM PROJECT)	2022 - 2023
• Ketua umum	
PANITIA RAPAT KERJA NASIONAL ISMAFARSI	2022 - 2023
• Anggota Publikasi, Dekorasi dan Dokumentasi	
PENGABDIAN MASYARAKAT DOSEN	2022
• Panitia pelaksana (Pemberian edukasi kesehatan melalui penggunaan media pembelajaran dalam upaya peningkatan kesehatan)	

PELATIHAN

LATIHAN KEPEMIMPINAN 1 ISMAFARSI	2020
LATIHAN KEPEMIMPINAN MANAGERIAL MAHASISWA FARMASI	2020
BMS Global Softskills Development	2020
BMS Global Softskills Development	2023