Supporting Information

In silico screening of phenylethanoid glycosides, a class of pharmacologically active compounds as natural inhibitors of SARS-CoV-2 proteases

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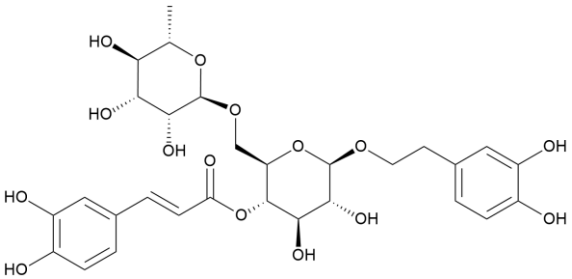
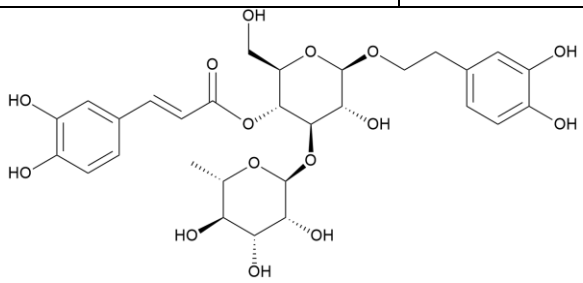
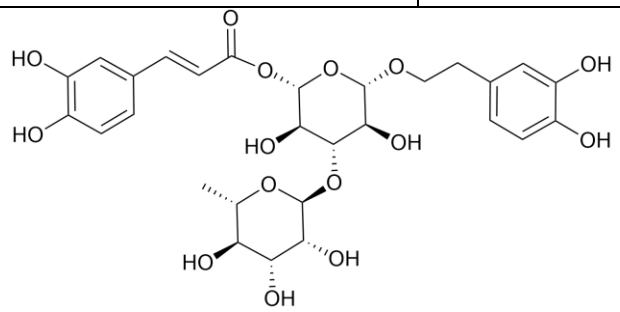
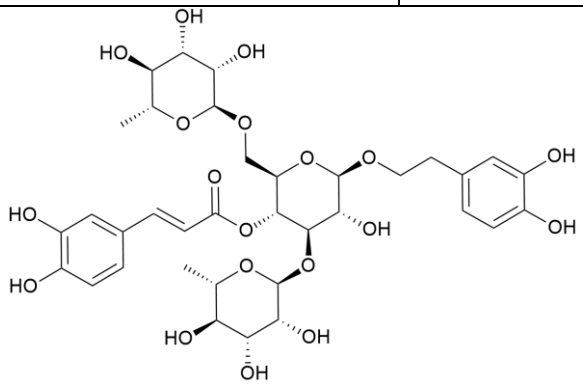
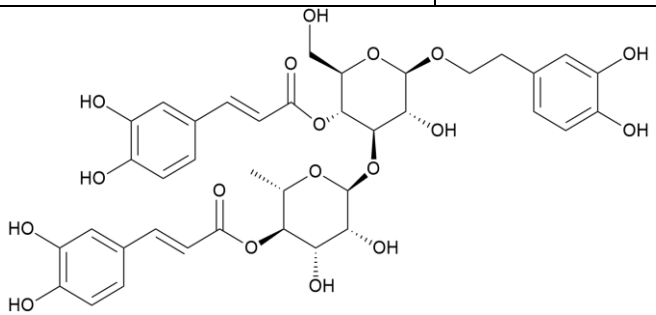
Figure Summary

Table Summary

Table S1: Phenylethanoid glycoside dataset based in the four review manuscripts published between 1994 and 2020 (26, 27, 28, 31). In the first row of the table are displayed the code numbers PG which were given for *in silico* analyses, followed by the trivial names (when available) in the second row. In the third row, the compounds numbers in the original references are given, together with their molecular weight. The numbering of PGs is not always continuous because duplicates were eliminated after all structures were drawn. In the original articles, some cis and trans caffeoyl derivatives received the same numbering but were considered here as different substances (examples: PG_287-1 and PG_287-2; PG343-1 and PG_343-2; PG_359-1 and PG_359-2).

Code	Compound	Reference	Molecular Weight (Da)
PG_001	Forsythoside A (or Forsythiaside or Forsythoside)	(compound 76) – (27) (compound 124) – (31)	626.606
			
Code	Compound	Reference	Molecular Weight (Da)
PG_002	Verbascoside (or acteoside or orobanchin)	(compound 41) – (27) (compound 121) – (31)	624.59
			
Code	Compound	Reference	Molecular Weight (Da)
PG_003	Isoverbascoside (or Isoacteoside)	(compound 54) – (27) (compound 121) –	610.563

		(31)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_004	Poliumoside (Magnolidin)	(compound 128) – (27)	770.731 Da
			
Code	Compound	Reference	Molecular Weight (Da)
PG_005	Lippiarubelloside A	(compound 42) – (26)	786.733
			
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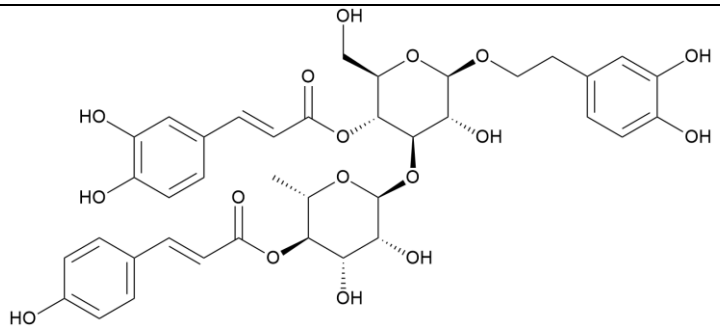
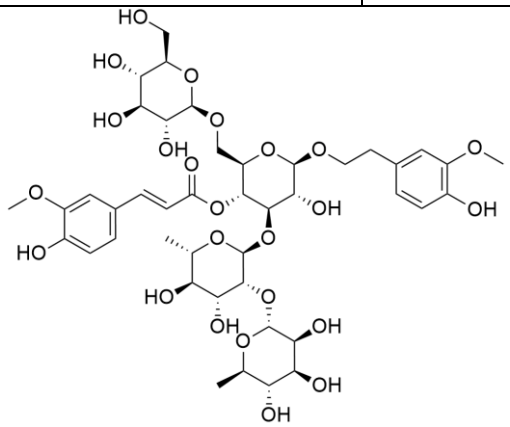
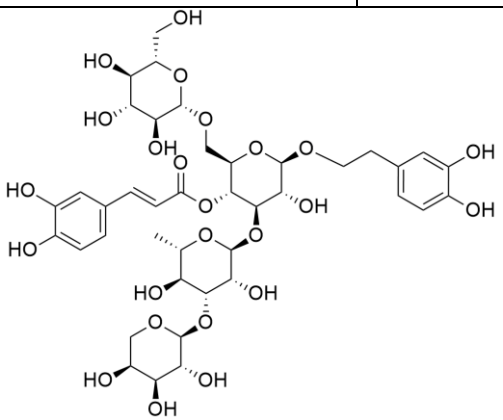
PG_006	Lippiarubelloside B	(compound 43) – (26)	772.75



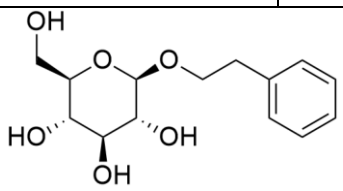
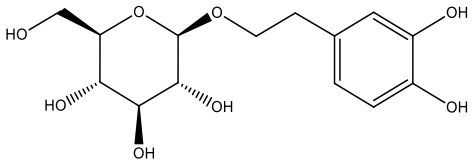
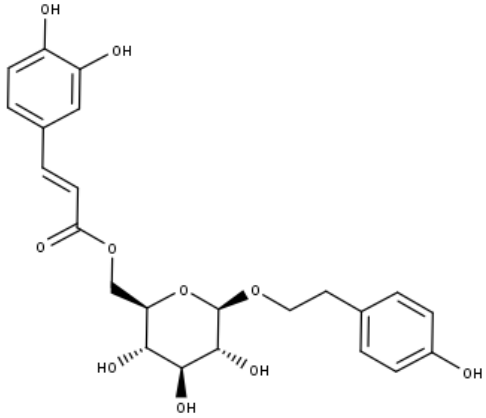
Code	Compound	Reference	Molecular Weight (Da)
PG_007	Physocalycoside	(compound 46) – (28)	962.941

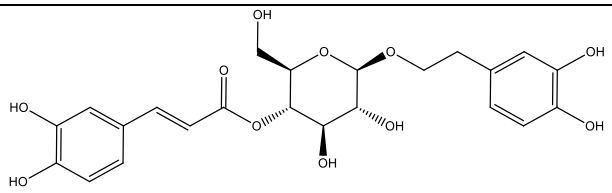
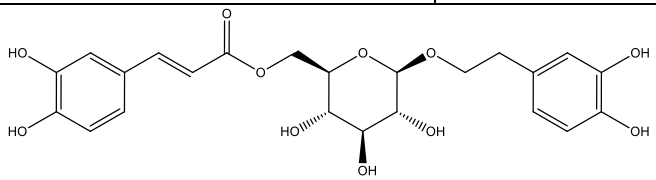
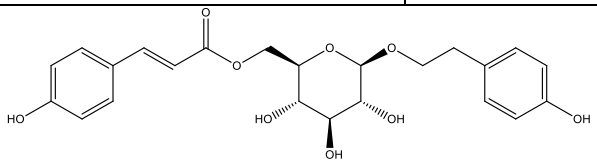
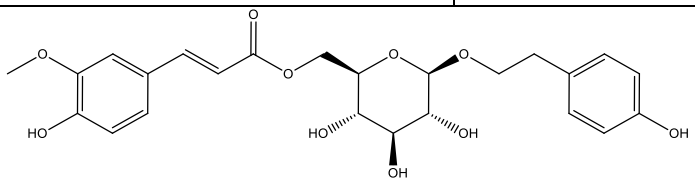
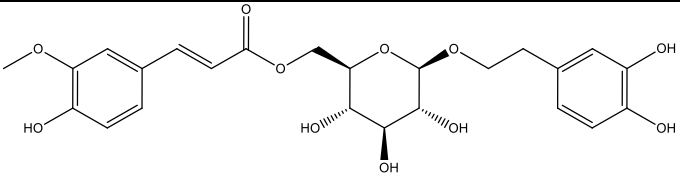


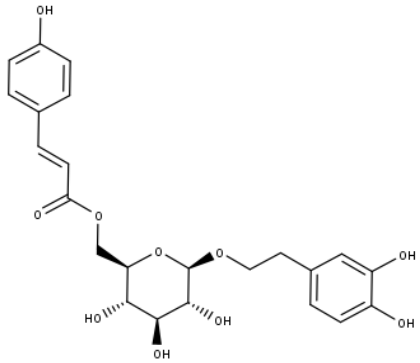
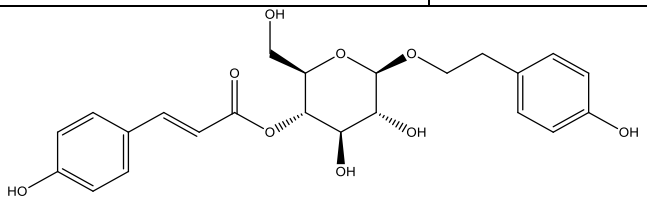
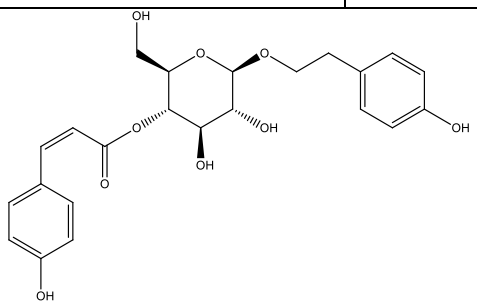
Code	Compound	Reference	Molecular Weight (Da)
PG_008	Velutinoside I	(compound 36) – (28)	920.861

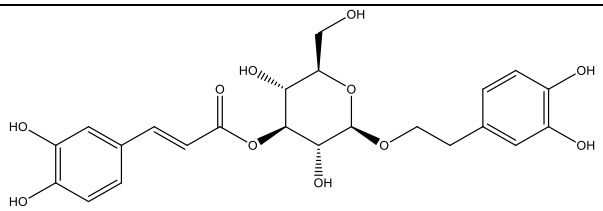


Code	Compound	Reference	Molecular Weight (Da)

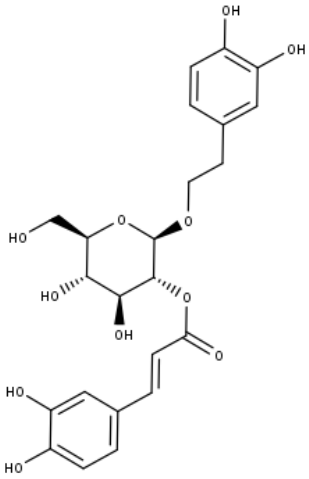
PG_009	β-Phenethyl-β-D-glycopyranoside	(compound 1) – (27)	284.307
			
Code	Compound	Reference	Molecular Weight (Da)
PG_010	β-3,4-Dihydroxyphenethyl-β-d-glucopyranoside	(compound 2) – (27)	316.305
			
Code	Compound	Reference	Molecular Weight (Da)
PG_011	β-4-hydroxyphenethyl-6'-O-caffeoyl-β-D-glucopyranoside	(compound 3) – (27)	462.449
			
Code	Compound	Reference	Molecular Weight (Da)
PG_012	Calceolariside A (Calceorioside A / desrhamnosyl acteoside)	(compound 4) – (27) (compound127) – (31)	478.448

			
Code	Compound	Reference	Molecular Weight (Da)
PG_013	Calceolariside B	(compound 5) – (27)	480.464
			
Code	Compound	Reference	Molecular Weight (Da)
PG_014	Eutigoside A	(compound 6) – (27)	446.45
			
Code	Compound	Reference	Molecular Weight (Da)
PG_015	Grayanoside A	(compound 7) – (27)	476.476
			
Code	Compound	Reference	Molecular Weight (Da)
PG_016	Grayanoside B (Osmanthuside E)	(compound 8) – (27)	492.475
			
Code	Compound	Reference	Molecular

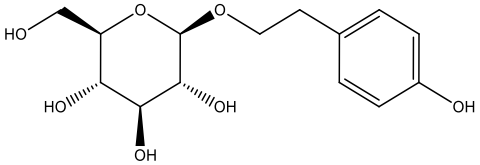
			Weight (Da)
PG_017	Neosyringalide	(compound 9) – (27)	462.449
			
Code	Compound	Reference	Molecular Weight (Da)
PG_018	Osmanthuside A	(compound 10) – (27)	446.45
			
Code	Compound	Reference	Molecular Weight (Da)
PG_019	Osmanthuside C	(compound 11) – (27)	446.45
			
Code	Compound	Reference	Molecular Weight (Da)
PG_020	Plantainoside A	(compound 12) – (27)	478.448



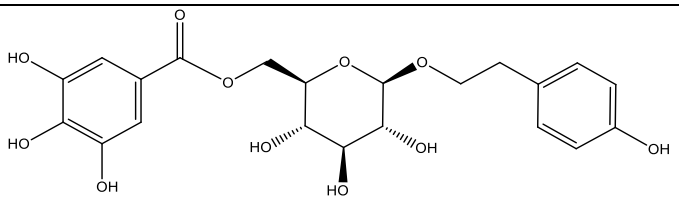
Code	Compound	Reference	Molecular Weight (Da)
PG_021	Plantainoside B	(compound 13) – (27)	478.448



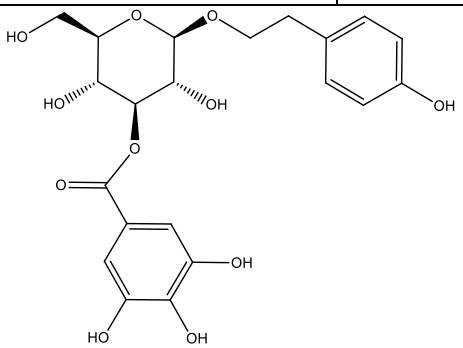
Code	Compound	Reference	Molecular Weight (Da)
PG_022	Salidroside (Rhodioloside)	(compound 14) – (27) (compound123) – (31)	300.306



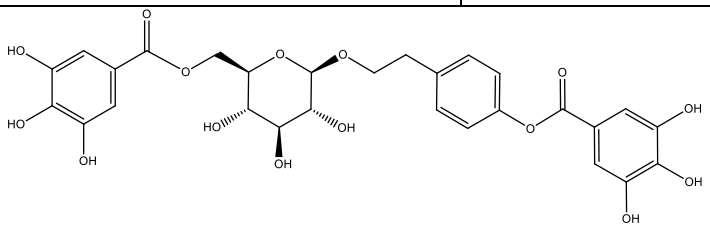
Code	Compound	Reference	Molecular Weight (Da)
PG_023	6'-O-Galloyl salidroside	(compound 15) – (27)	452.411



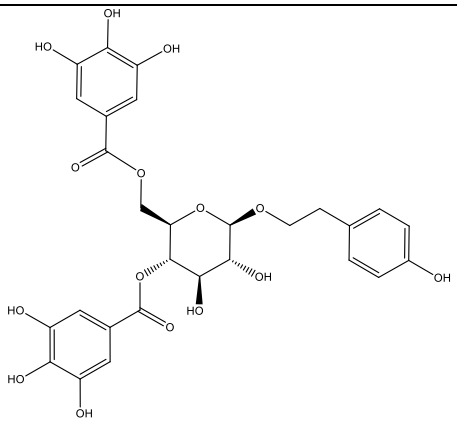
Code	Compound	Reference	Molecular Weight (Da)
PG_024	3'-O-Galloyl salidroside	(compound 16) – (27)	454.426



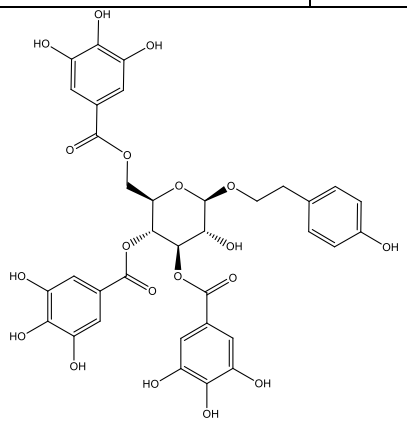
Code	Compound	Reference	Molecular Weight (Da)
PG_025	4,6'-Di-O-galloyl salidroside	(compound 17) – (27)	604.515



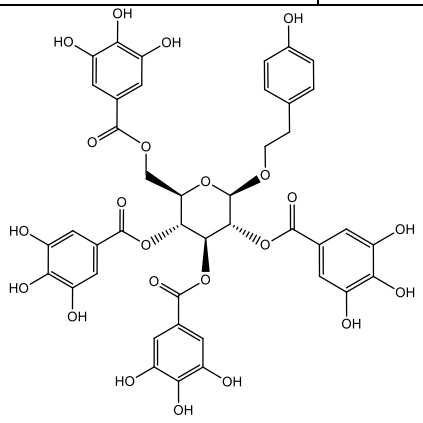
Code	Compound	Reference	Molecular Weight (Da)
PG_026	4',6'-Di-O-galloyl salidroside	(compound 18) – (27)	604.515



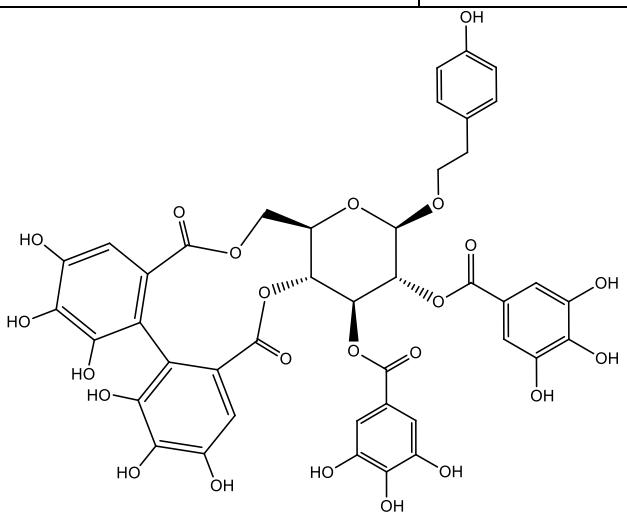
Code	Compound	Reference	Molecular Weight (Da)
PG_027	3',4',6'-Tri-O-galloyl salidroside	(compound 19) – (27)	756.62



Code	Compound	Reference	Molecular Weight (Da)
PG_028	2',3',4',6'- Treta-O-galloyl salidroside	(compound 20) – (27)	908.725



Code	Compound	Reference	Molecular Weight (Da)

PG_029	2',3'- di- O- galloyl- 4',6'-(S)- hexahydroxydiphenoyl salidroside	(compound 21) – (27)	906.709
			
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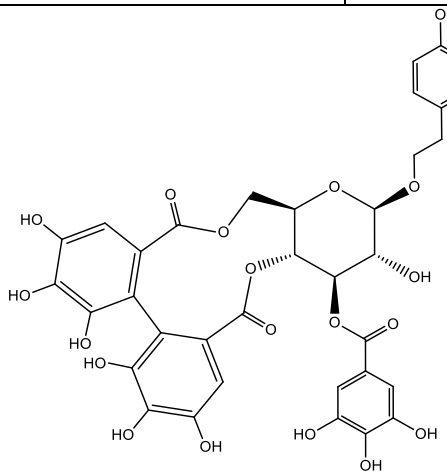
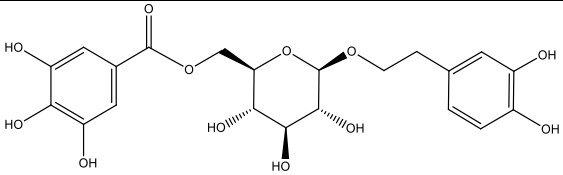
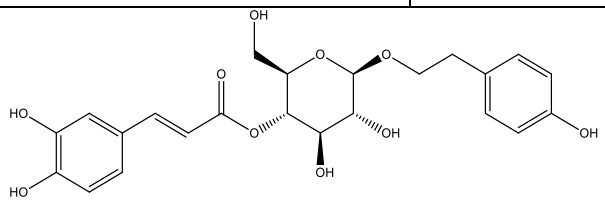
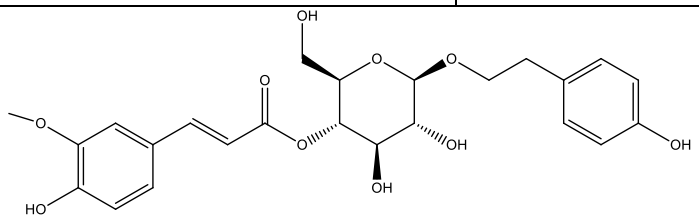
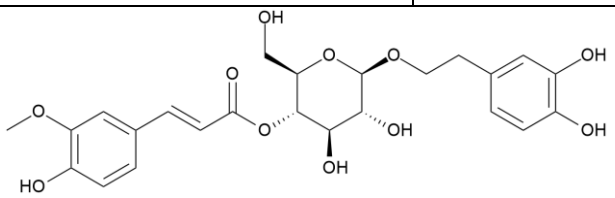
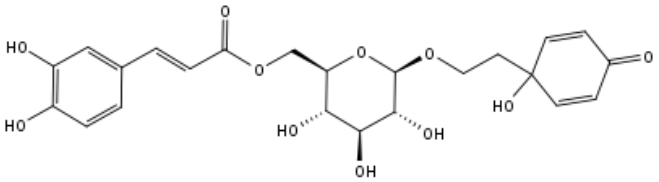
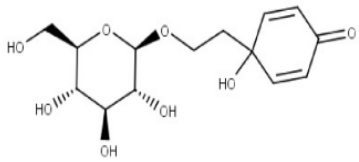
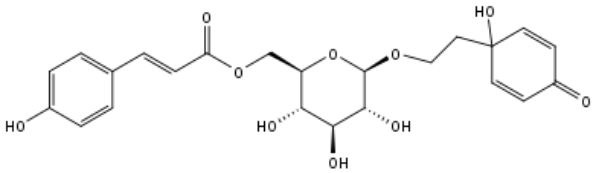
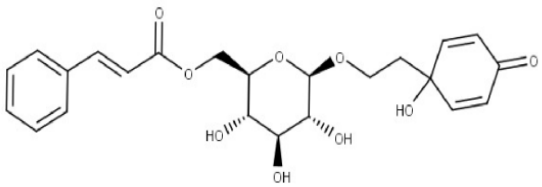
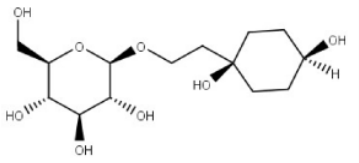
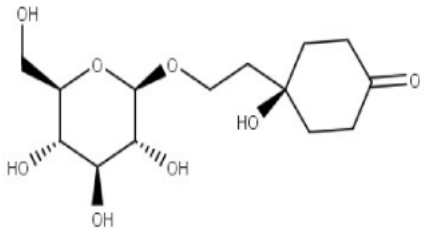
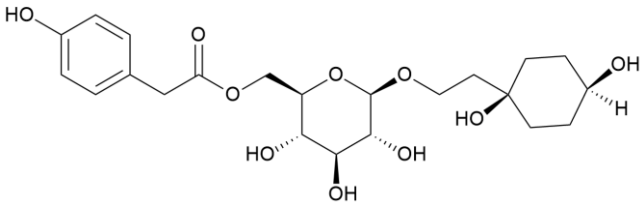
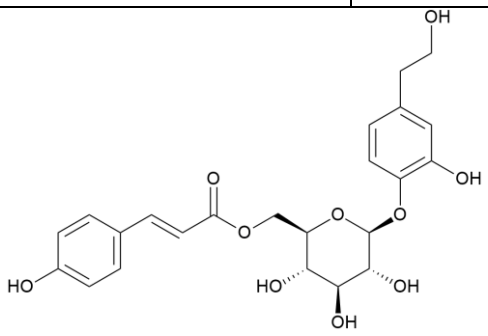
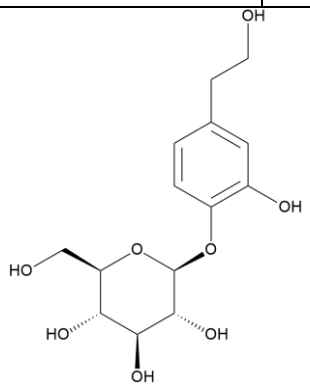
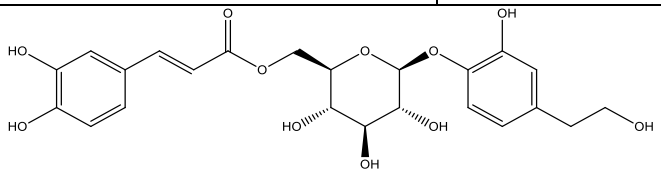
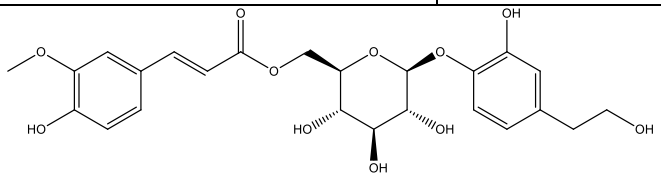
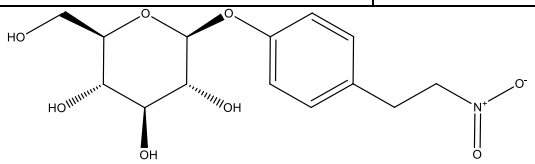
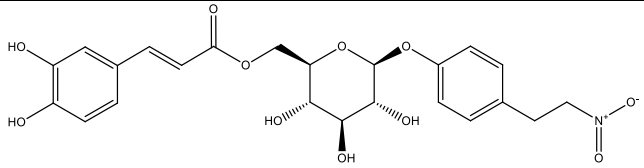
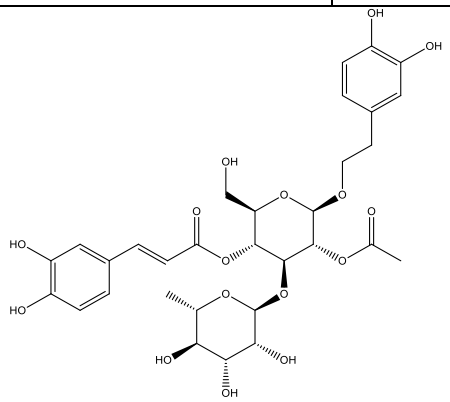
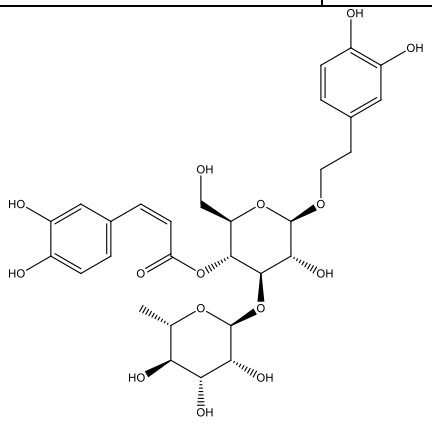
PG_030	3'-O-Galloyl-4',6'-(S)- hexahydroxydiphenoyl salidroside	(compound 22) – (27)	754.604
			
Code	Compound	Reference	Molecular Weight (Da)
PG_031	β-3,4-Dihydroyphenethyl-β-D-(6'- O-galloyl)-glucopyranoside	(compound 23) – (27)	468.41
			
Code	Compound	Reference	Molecular Weight (Da)

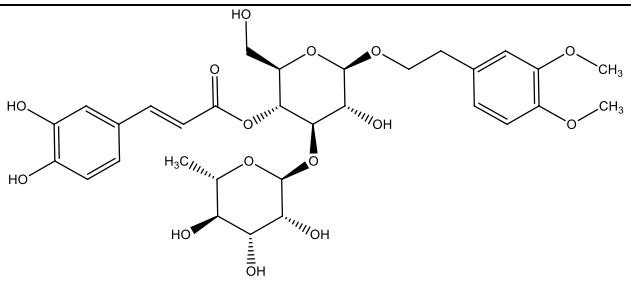
PG_032	Syringalide A	(24) – Jimenez et al., 1994	462.449
			
Code	Compound	Reference	Molecular Weight (Da)
PG_033	Syringalide B	(compound 25) – (27)	476.476
			
Code	Compound	Reference	Molecular Weight (Da)
PG_034	Syringalide C	(compound 26) – (27)	492.475
			
Code	Compound	Reference	Molecular Weight (Da)
PG_035	Calceolarioside D	(compound 27) – (27)	478.448
			
Code	Compound	Reference	Molecular Weight (Da)

PG_036	Cornoside	(compound 28) – (27)	316.305
			
Code	Compound	Reference	Molecular Weight (Da)
PG_037	Eutigoside B	(compound 29) – (27)	462.449
			
Code	Compound	Reference	Molecular Weight (Da)
PG_038	Eutigoside C	(compound 30) – (27)	446.45
			
Code	Compound	Reference	Molecular Weight (Da)
PG_039	Rengyoside A	(compound 31) – (27)	322.352
			

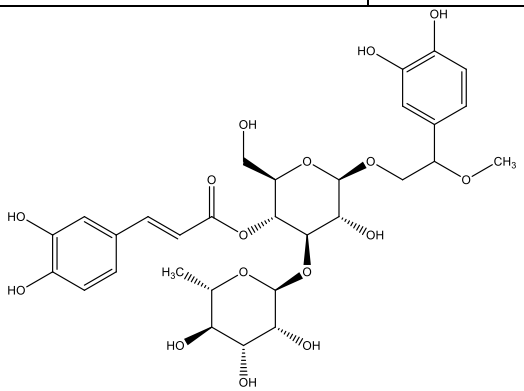
Code	Compound	Reference	Molecular Weight (Da)
PG_040	Rengyoside B	(compound 32) – (27)	320.337
			
Code	Compound	Reference	Molecular Weight (Da)
PG_041	Rengyoside C	(compound 33) – (27)	456.486
			
Code	Compound	Reference	Molecular Weight (Da)
PG_042	Ibotanolide	(compound 34) – (27)	462.449
			
Code	Compound	Reference	Molecular Weight (Da)

PG_043	De-*p*-coumaroyl ibotanolide	(compound 35) – (27)	316.305
			
Code	Compound	Reference	Molecular Weight (Da)
PG_044	Ibotanolide B	(compound 36) – (27)	478.448
			
Code	Compound	Reference	Molecular Weight (Da)
PG_045	Ibotanolide C	(compound 36) – (27)	492.475
			
Code	Compound	Reference	Molecular Weight (Da)
PG_046	Thalictoside	(compound 38) – (27)	329.304
			
Code	Compound	Reference	Molecular Weight (Da)
PG_047	6'-O-caffeoyl thalictoside	(compound 39) –	491.448

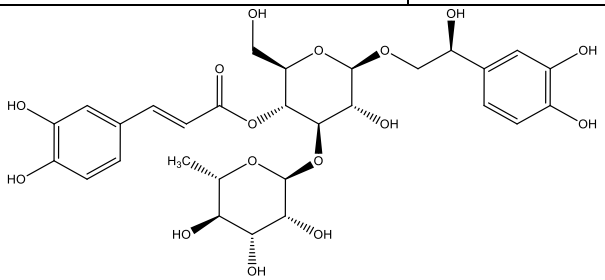
		(27)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_048	2'-O-acetyl acteoside	(compound 40) – (27)	668.643
			
Code	Compound	Reference	Molecular Weight (Da)
PG_049	Acteoside (Z isomer)	(compound 42) – (27)	624.59
			
Code	Compound	Reference	Molecular Weight (Da)
PG_050	Brachyonoside	(compound 43) – (27)	652.644



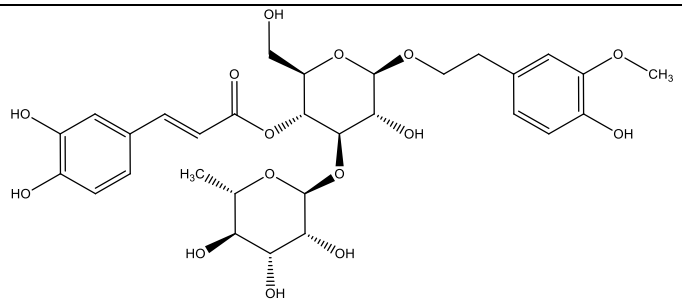
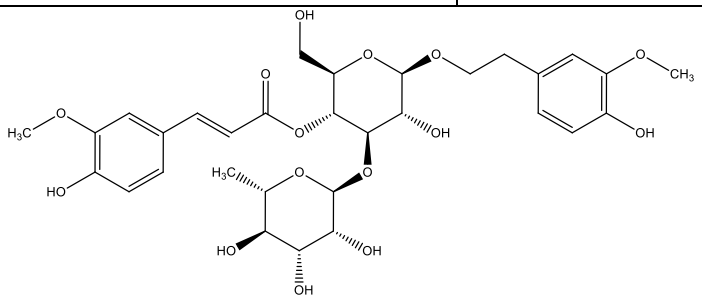
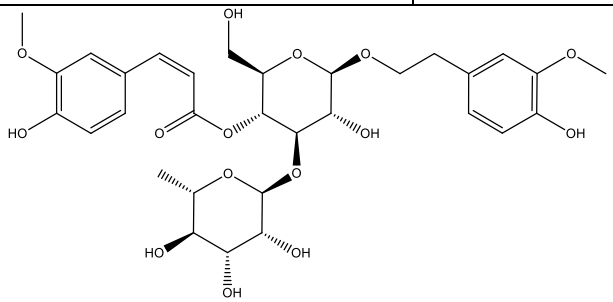
Code	Compound	Reference	Molecular Weight (Da)
PG_051	Campneoside I	(compound 44) – (27)	656.632

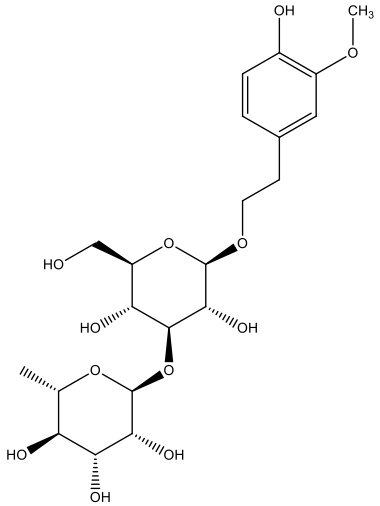


Code	Compound	Reference	Molecular Weight (Da)
PG_052	Campneoside II (β-hydroxy-acteoside)	(compound 45) – (27)	640.589

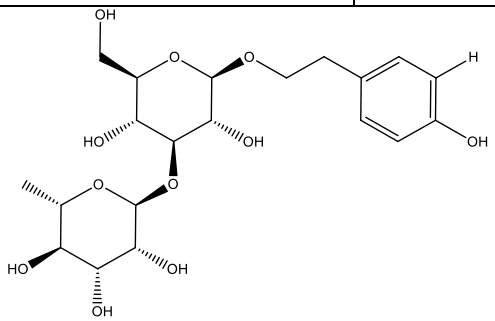


Code	Compound	Reference	Molecular Weight (Da)
PG_053	Cistanoside C	(compound 46) – (27)	638.617

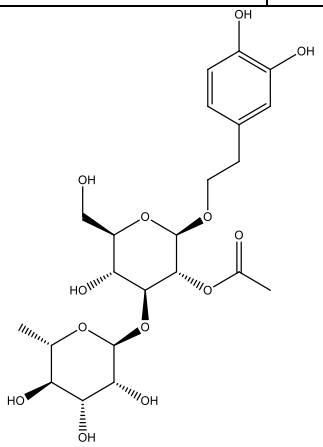
			
Code	Compound	Reference	Molecular Weight (Da)
PG_054	Cistanoside D (*E* isomer)	(compound 47) – (27)	652.644
			
Code	Compound	Reference	Molecular Weight (Da)
PG_055	Cistanoside D (*Z* isomer)	(compound 48) – (27)	654.659
			
Code	Compound	Reference	Molecular Weight (Da)
PG_056	Cistanoside E	(compound 49) – (27)	476.473



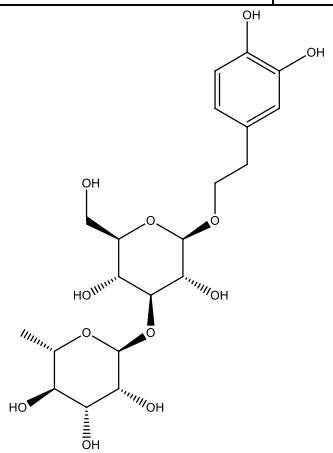
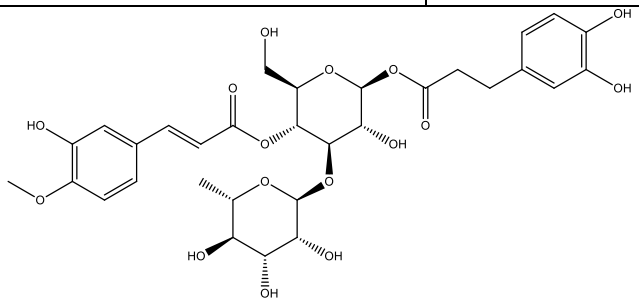
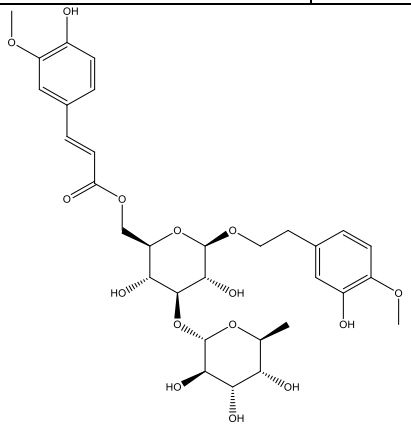
Code	Compound	Reference	Molecular Weight (Da)
PG_057	Cistanoside G	(compound 50) – (27)	446.447

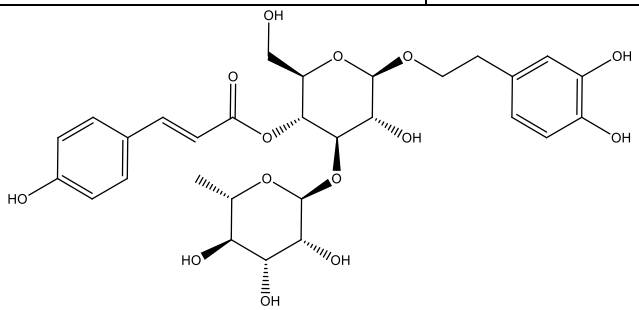
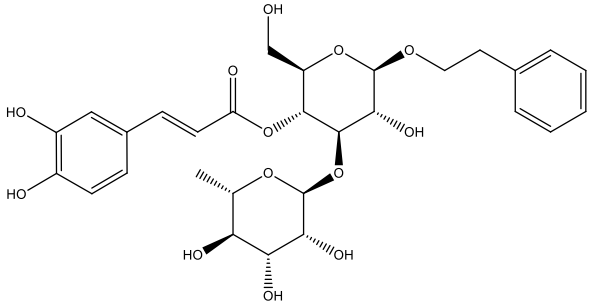
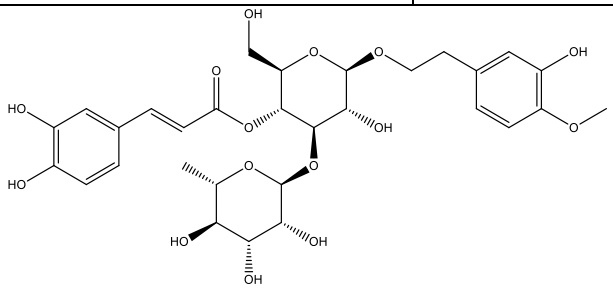


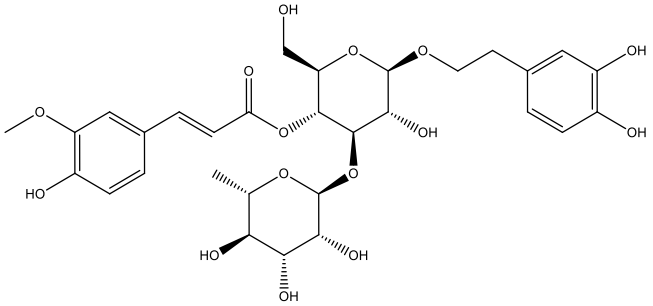
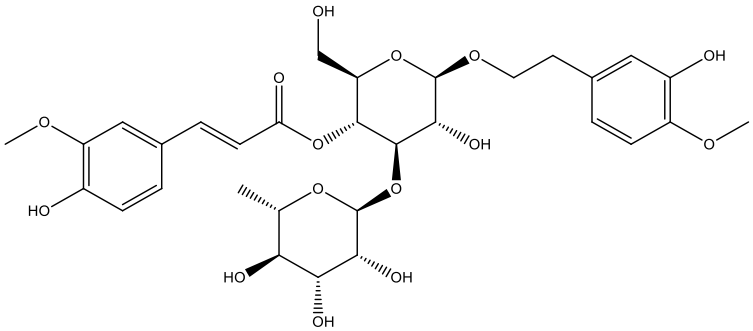
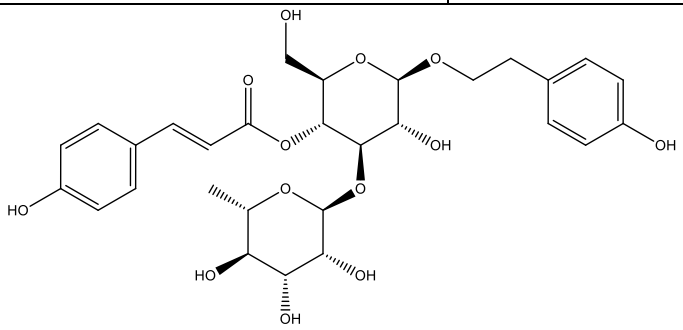
Code	Compound	Reference	Molecular Weight (Da)
PG_058	Cistanoside H	(compound 51) – (27)	504.483

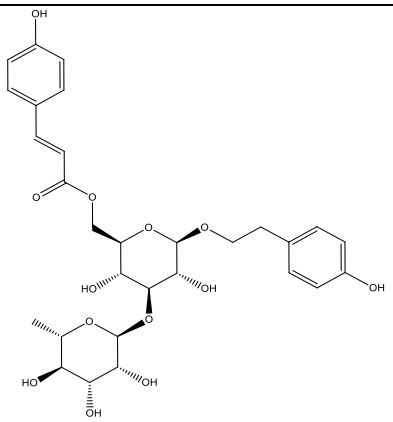


Code	Compound	Reference	Molecular Weight (Da)

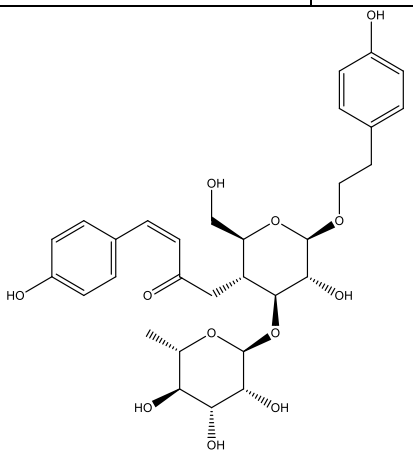
PG_059	Decaffeoylacteoside	(compound 52) – (27) (compound 134) – (31)	462.446
			
Code	Compound	Reference	Molecular Weight (Da)
PG_060	Eukovoside	(compound 53) – (27)	638.617
			
Code	Compound	Reference	Molecular Weight (Da)
PG_061	Isomartynoside	(compound 55) – (27)	652.644
			
Code	Compound	Reference	Molecular

			Weight (Da)
PG_062	3'-α- L- rhamnopyranosyl isosyringalide (or Lipedoside A-I)	(compound 56) – (27) (compound 5) – (26)	608.591
			
Code	Compound	Reference	Molecular Weight (Da)
PG_063	Jionoside C	(compound 57) – (27)	592.592
			
Code	Compound	Reference	Molecular Weight (Da)
PG_064	Jionoside D	(compound 58) – (27)	638.617
			
Code	Compound	Reference	Molecular Weight (Da)
PG_065	Leucosceptoside A	(compound 59) – (27) (compound	638.617

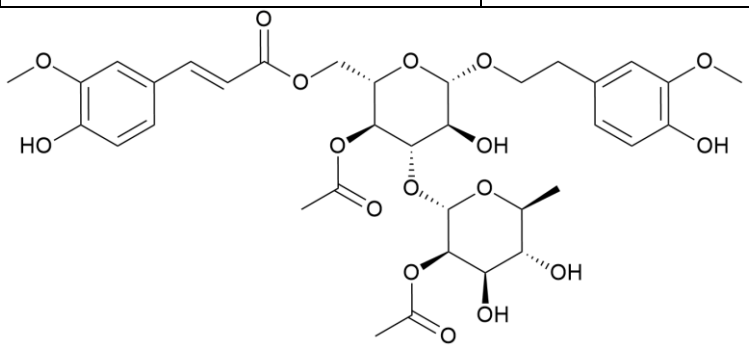
		119) – (31)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_066	Martynoside	(compound 60) – (27) (compound 74) – (28)	652.644
			
Code	Compound	Reference	Molecular Weight (Da)
PG_067	Osmanthuside B	(compound 61) – (27)	592.592
			
Code	Compound	Reference	Molecular Weight (Da)
PG_068	Osmanthuside B6	(compound 62) – (27)	592.592



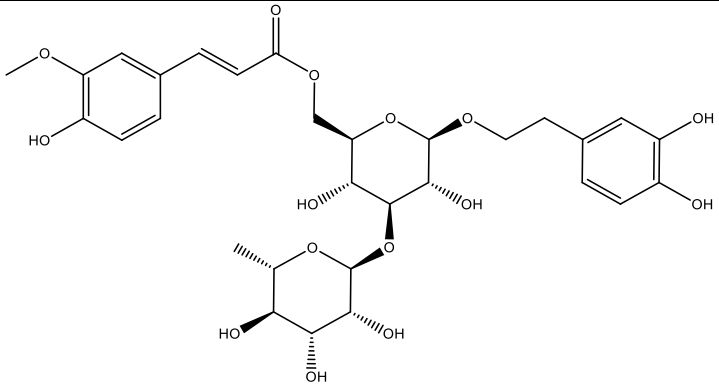
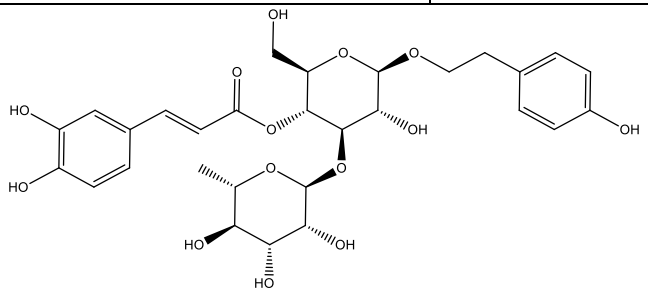
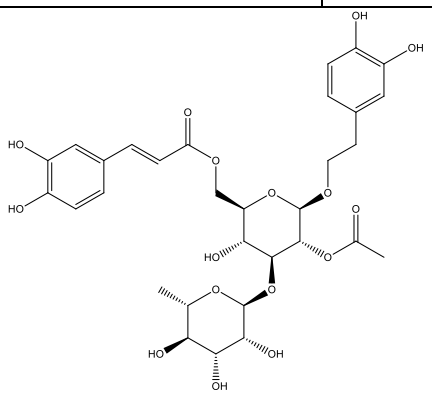
Code	Compound	Reference	Molecular Weight (Da)
PG_069	Osmanthuside D	(compound 63) – (27)	592.592

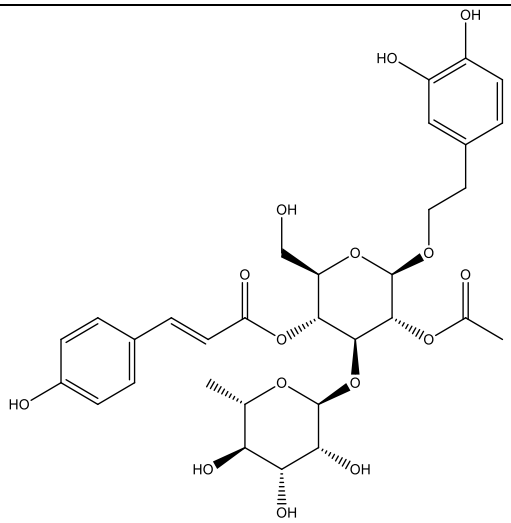


Code	Compound	Reference	Molecular Weight (Da)
PG_070	Pedicularioside E 2"-O-acetyl rhamnoside	(compound 64) – (27)	738.733

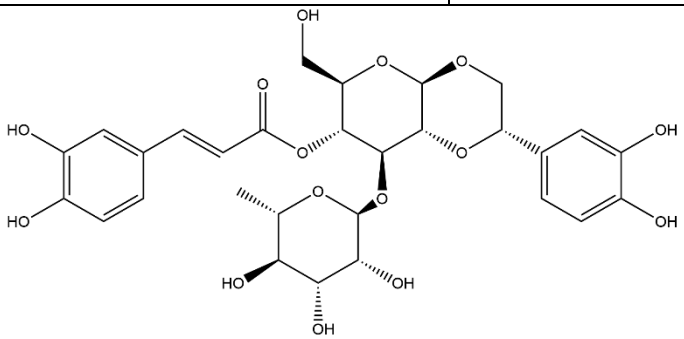


Code	Compound	Reference	Molecular Weight (Da)
PG_071	Plantainoside C	(compound 65) –	638.617

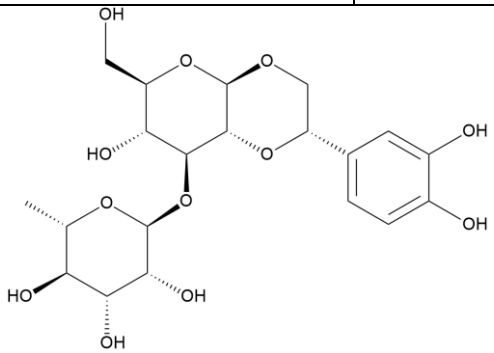
		(27)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_072	3'-α-L-rhamnopyranosyl syringalide A	(compound 66) – (27)	608.591
			
Code	Compound	Reference	Molecular Weight (Da)
PG_073	Tubuloside B	(compound 67) – (27) (compound 139) – (31)	666.627
			
Code	Compound	Reference	Molecular Weight (Da)
PG_074	Tubuloside E	(compound 68) – (27)	650.628



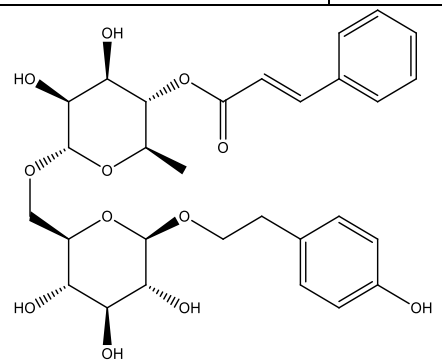
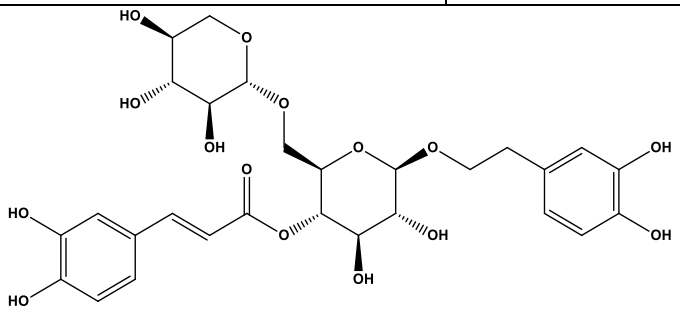
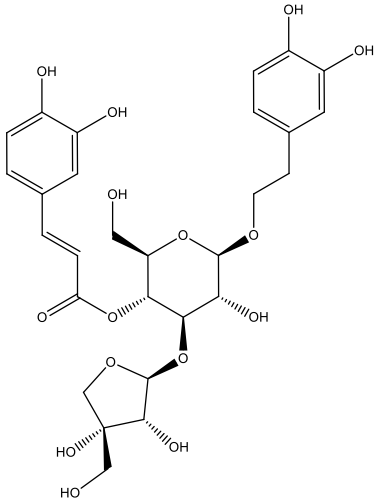
Code	Compound	Reference	Molecular Weight (Da)
PG_075	Crenatoside	(compound 69) – (27)	622.574

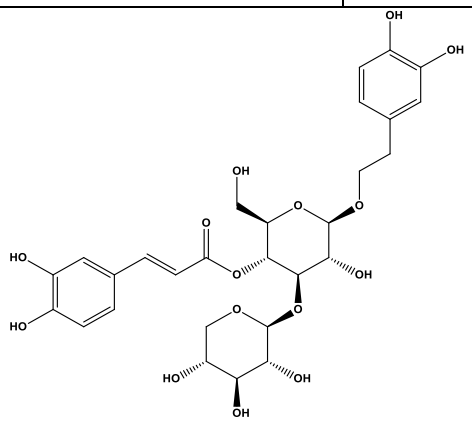
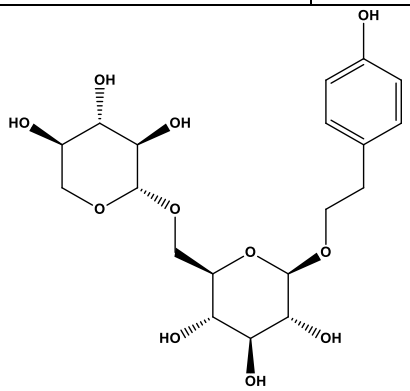
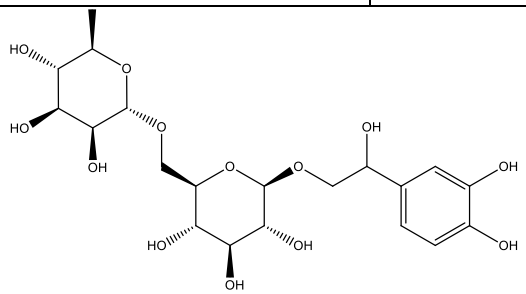


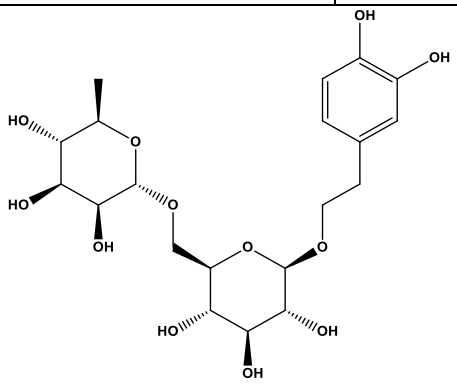
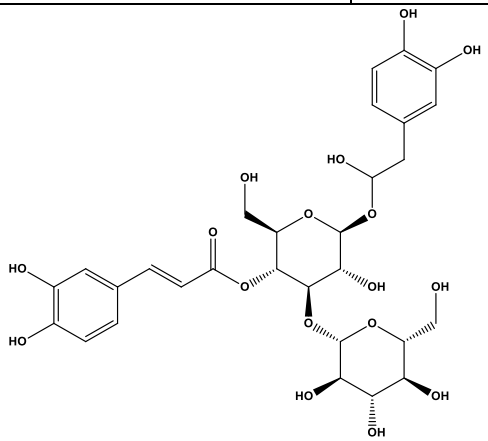
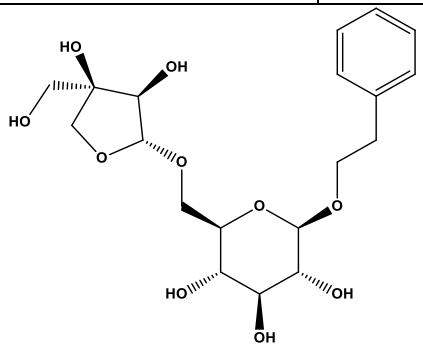
Code	Compound	Reference	Molecular Weight (Da)
PG_076	Decaffeoyl crenatoside	(compound 70) – (27)	460.43

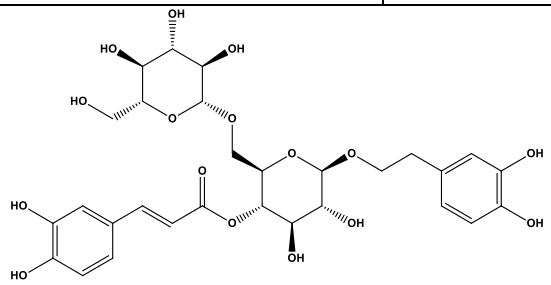
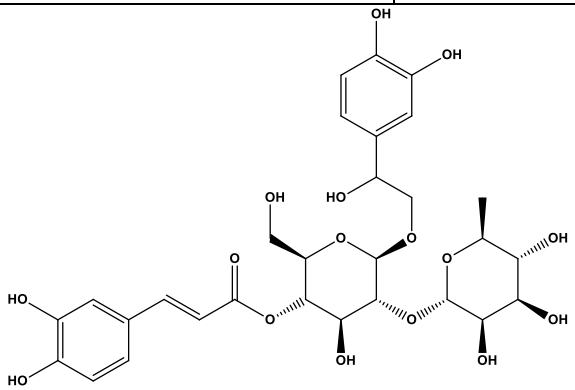
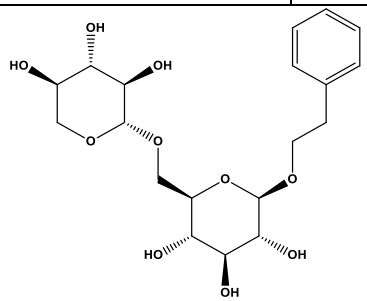


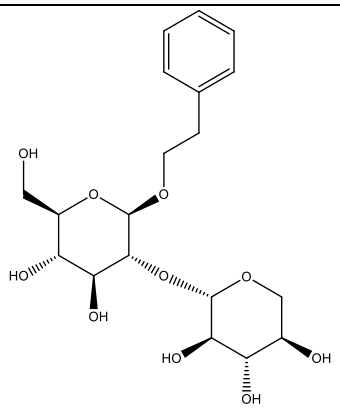
Code	Compound	Reference	Molecular Weight (Da)
PG_077	4-cinnamoyl	(compound 71) –	576.593

	desxyloxylmussatioside	(27)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_078	Calceolarioside C	(compound 72) – (27)	610.563
			
Code	Compound	Reference	Molecular Weight (Da)
PG_079	Calceolarioside E	(compound 73) – (27)	610.563
			
Code	Compound	Reference	Molecular Weight (Da)

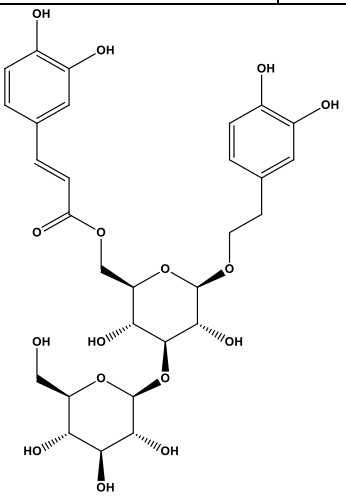
PG_080	Conandroside	(compound 74) – (27)	610.563
			
Code	Compound	Reference	Molecular Weight (Da)
PG_081	Cuchiloside	(compound 75) – (27)	432.42
			
Code	Compound	Reference	Molecular Weight (Da)
PG_082	Forsythoside D	(compound 77) – (27)	478.445
			
Code	Compound	Reference	Molecular Weight (Da)
PG_083	Forsythoside E	(compound 78) –	462.446

		(27)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_084	Hellicoside	(compound 79) – (27)	656.588
			
Code	Compound	Reference	Molecular Weight (Da)
PG_085	Icariside D1	(compound 80) – (27)	416.421
			
Code	Compound	Reference	Molecular Weight (Da)
PG_086	Lugrandoside	(compound 81) –	640.589

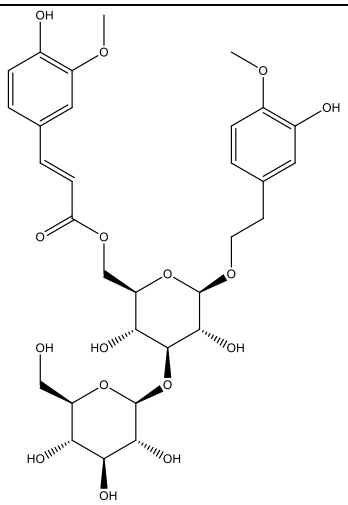
		(27)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_087	Orobanchoside	(compound 82) – (27)	640.589
			
Code	Compound	Reference	Molecular Weight (Da)
PG_088	β-Phenethyl-O-β-D-xylopyranosyl (1"-->6')- β-D-glucopyranoside	(compound 83) – (27)	416.421
			
Code	Compound	Reference	Molecular Weight (Da)
PG_089	β-Phenethyl-O-β-D-xylopyranosyl (1"-->2')- β-D-glucopyranoside	(compound 84) – (27)	416.421



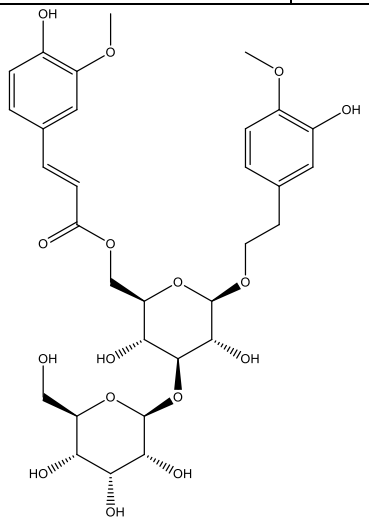
Code	Compound	Reference	Molecular Weight (Da)
PG_090	Plantainoside D	(compound 85) – (27)	640.589



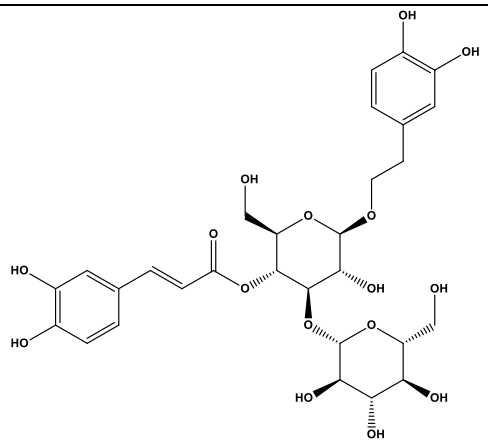
Code	Compound	Reference	Molecular Weight (Da)
PG_091	Plantainoside E	(compound 86) – (27)	668.643



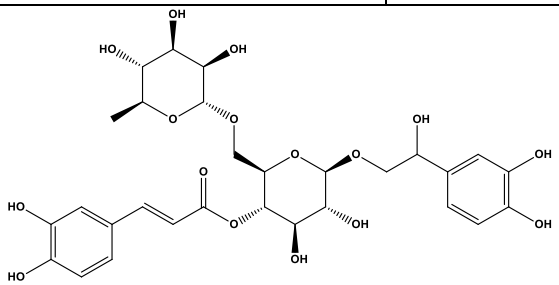
Code	Compound	Reference	Molecular Weight (Da)
PG_092	Plantainoside F	(compound 87) – (27)	668.643



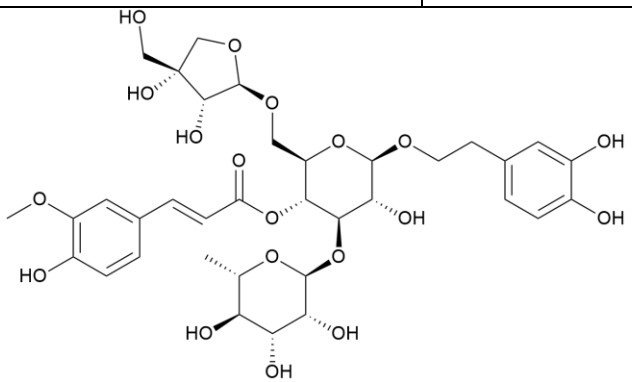
Code	Compound	Reference	Molecular Weight (Da)
PG_093	Purpureaside A (or Plantamajoside)	(compound 88) – (27) (compound 138) – (31)	640.589



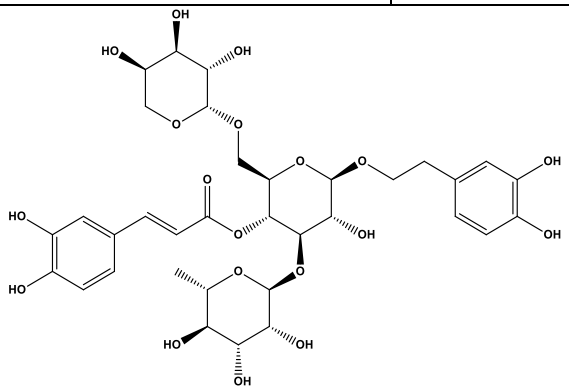
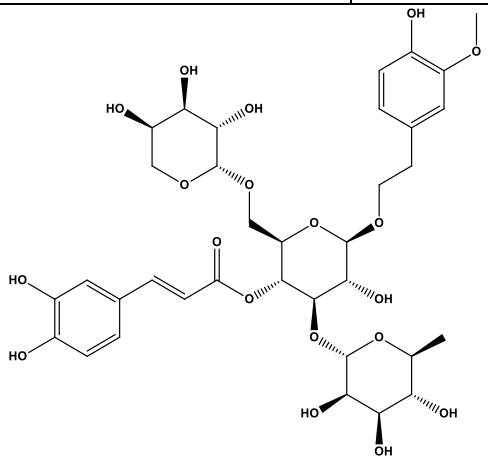
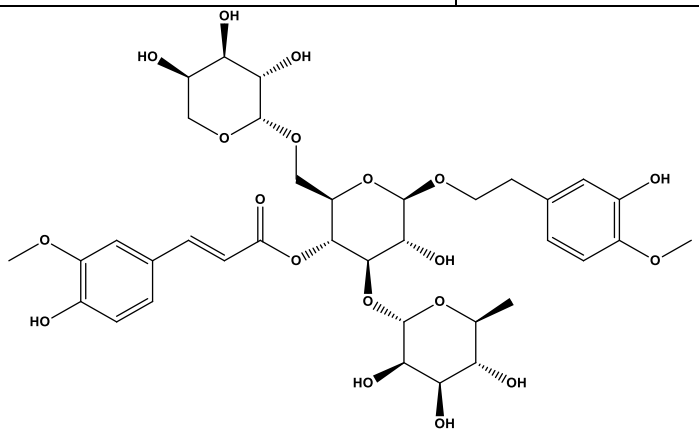
Code	Compound	Reference	Molecular Weight (Da)
PG_094	Suspensaside (or Forsythoside C)	(compound 89) – (27)	640.589

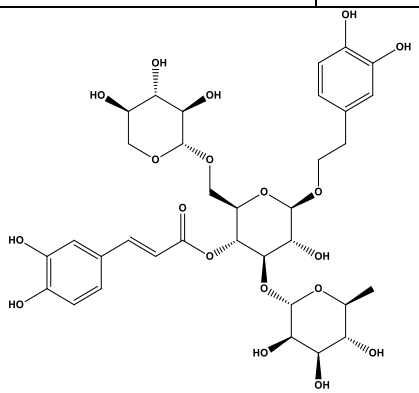
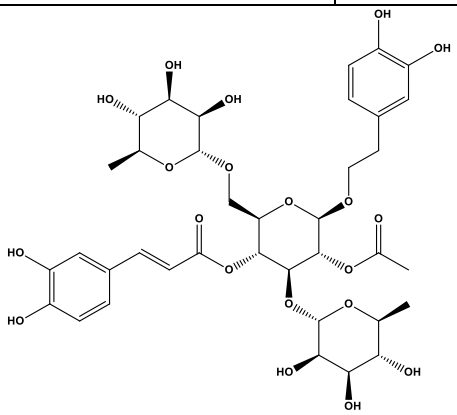


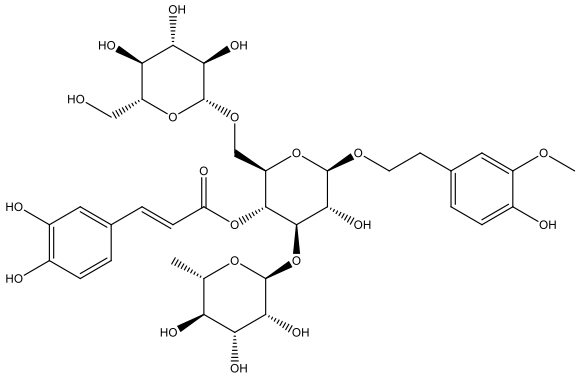
Code	Compound	Reference	Molecular Weight (Da)
PG_095	Alyssonoside	(compound 90) – (27) (compound 129) – (31)	798.785



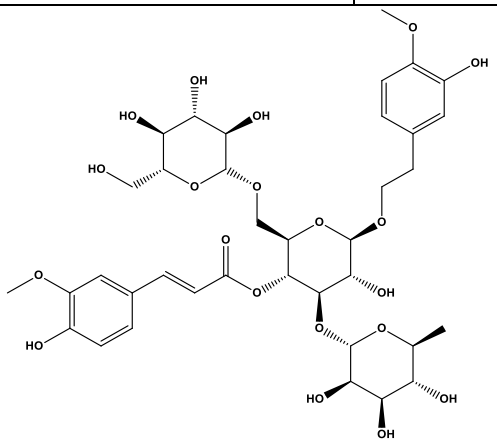
Code	Compound	Reference	Molecular Weight (Da)
PG_096	Angoroside A	(compound 91) –	756.704

		(27)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_097	Angoroside B	(compound 92) – (27)	770.731
			
Code	Compound	Reference	Molecular Weight (Da)
PG_098	Angoroside C	(compound 93) – (27)	786.774
			

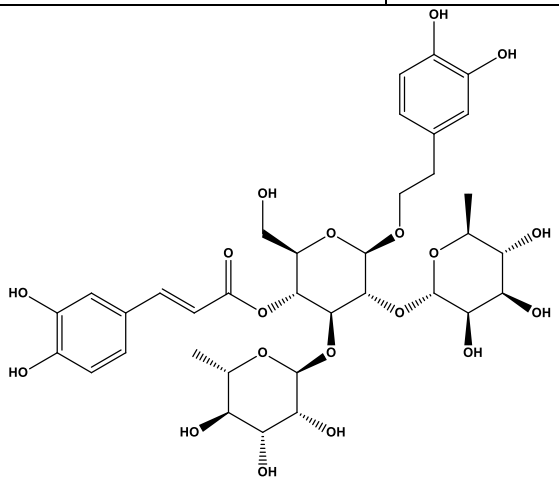
Code	Compound	Reference	Molecular Weight (Da)
PG_099	Arenarioside (or Arenariside)	(compound 94) – (27) (compound 122) – (31)	758.72
			
Code	Compound	Reference	Molecular Weight (Da)
PG_100	Brandioside (or 2'-O-Acetyl poliumoside)	(compound 95) – (27) (compound 130) – (31)	812.768
			
Code	Compound	Reference	Molecular Weight (Da)
PG_101	Cistanoside A	(compound 96) – (27)	800.757



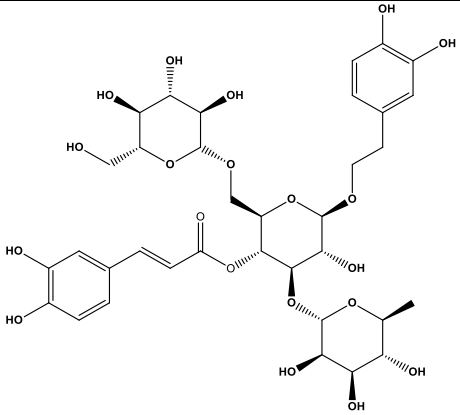
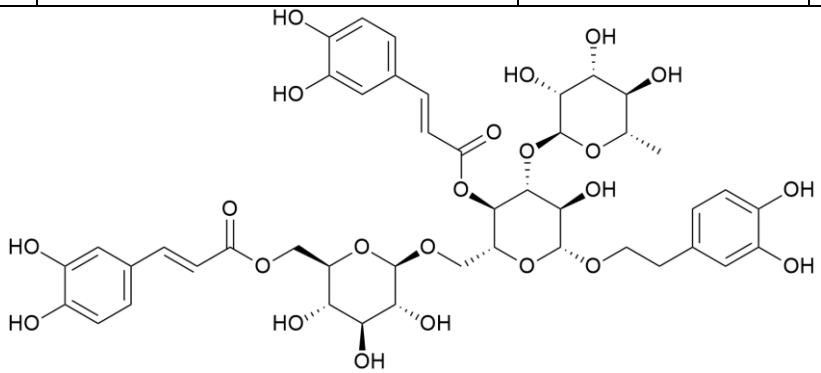
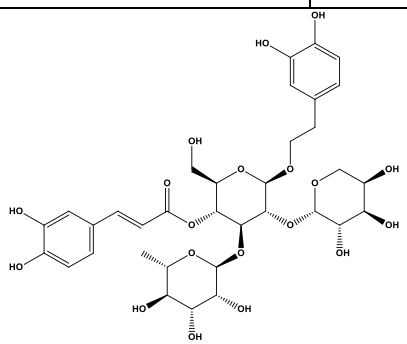
Code	Compound	Reference	Molecular Weight (Da)
PG_102	Cistanoside B	(compound 97) – (27)	814.784

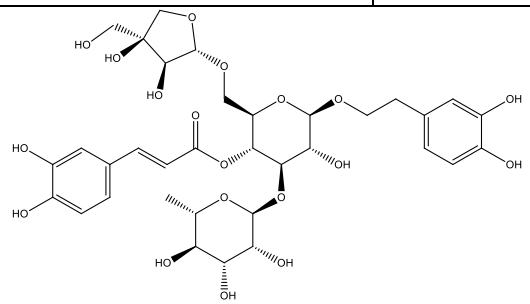
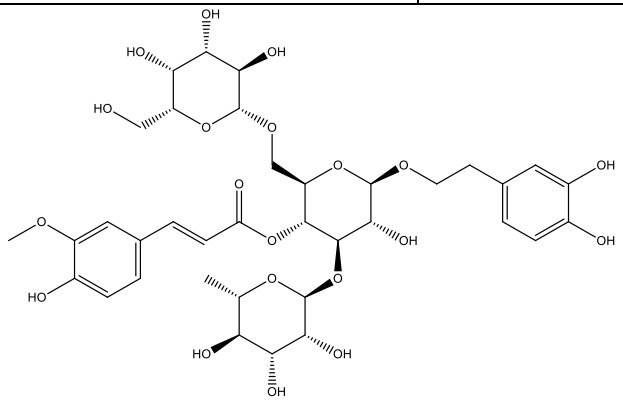
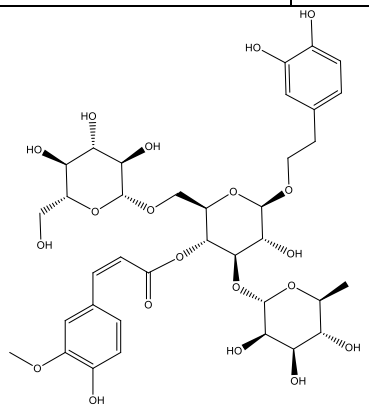


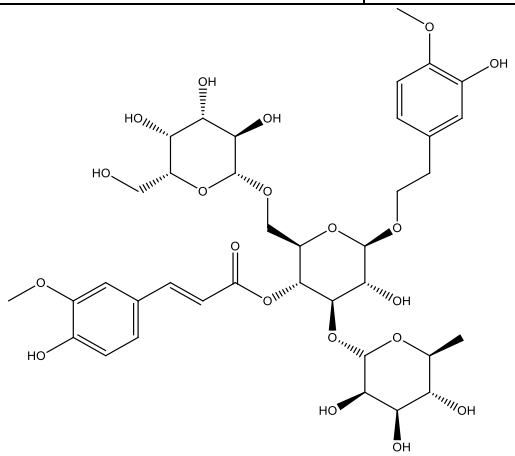
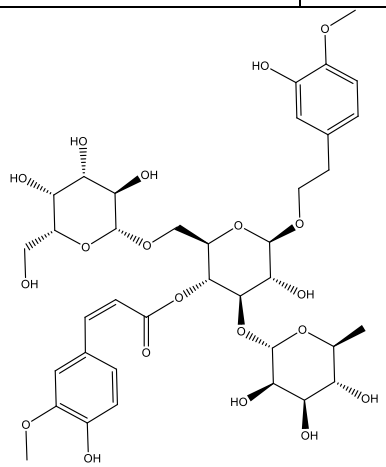
Code	Compound	Reference	Molecular Weight (Da)
PG_103	Crassifolioside	(compound 98) – (27)	772.747

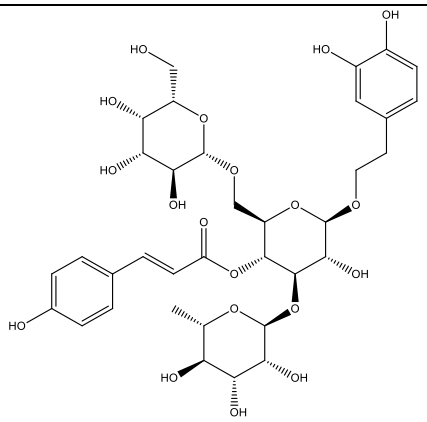


Code	Compound	Reference	Molecular

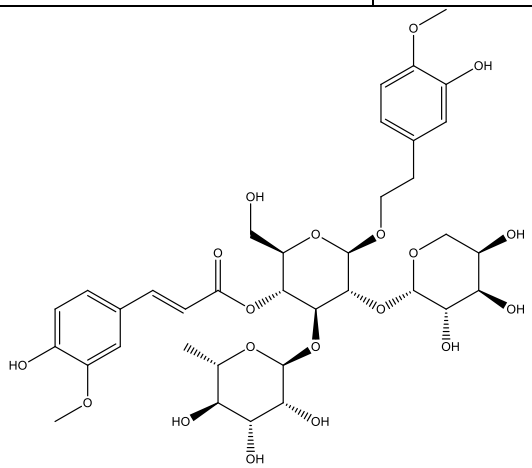
			Weight (Da)
PG_104	Echinacoside	(compound 99) – (27) (compound 117) – (31)	786.73
			
Code	Compound	Reference	Molecular Weight (Da)
PG_105	6'''-O-caffeoyl echinacoside	(compound 100) – (27)	948.874
			
Code	Compound	Reference	Molecular Weight (Da)
PG_106	Ehrenoside	(compound 101) – (27)	756.704
			
Code	Compound	Reference	Molecular

			Weight (Da)
PG_107	Forsythoside B	(compound 102) – (27) (compound 125) – (31)	756.704
			
Code	Compound	Reference	Molecular Weight (Da)
PG_108	Jionoside A1	(compound 103) – (27)	800.757
			
Code	Compound	Reference	Molecular Weight (Da)
PG_109	Jionoside A2	(compound 104) – (27)	800.757
			
Code	Compound	Reference	Molecular

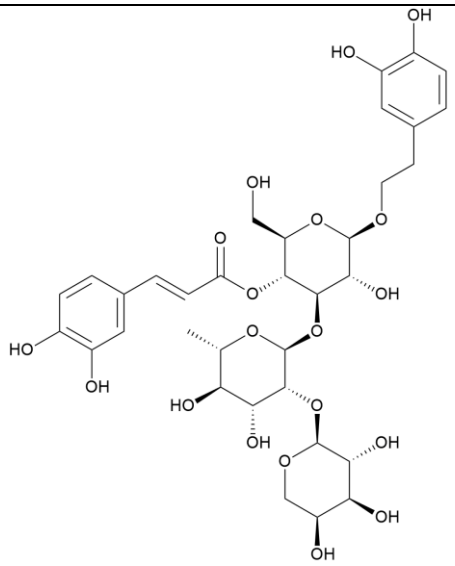
			Weight (Da)
PG_110	Jionoside B1	(compound 105) – (27)	814.784
			
Code	Compound	Reference	Molecular Weight (Da)
PG_111	Jionoside B2	(compound 106) – (27)	814.784
			
Code	Compound	Reference	Molecular Weight (Da)
PG_112	Jionoside E	(compound 107) – (27)	770.731



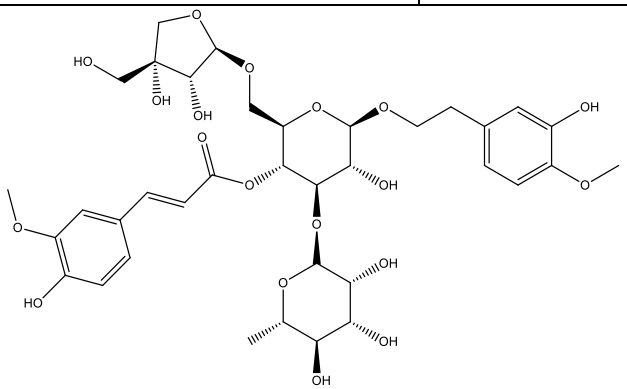
Code	Compound	Reference	Molecular Weight (Da)
PG_113	Lagotoside	(compound 108) – (27)	784.758



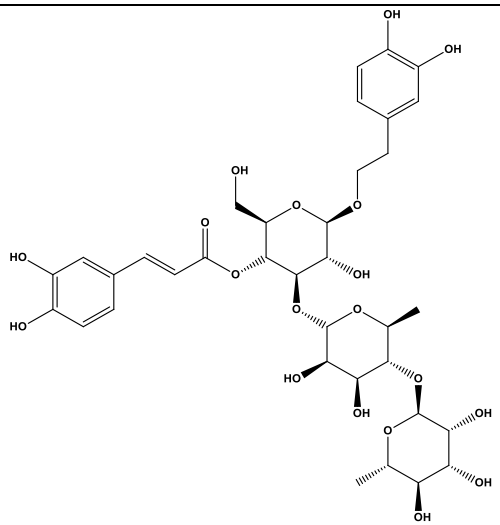
Code	Compound	Reference	Molecular Weight (Da)
PG_114	Lavandulifolioside Arb (1'''-->2'') Rha (or Stachyoside A or Stachyoside B)	(compound 109) – (27)	624.59



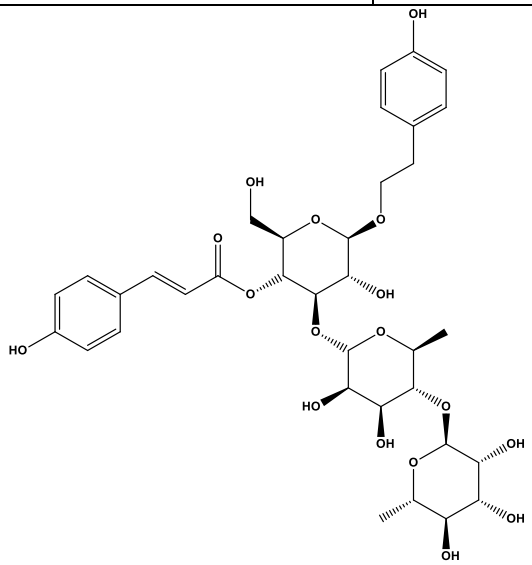
Code	Compound	Reference	Molecular Weight (Da)
PG_115	Leucosceptoside B	(compound 110) – (27) (compound 126) – (31)	784.758



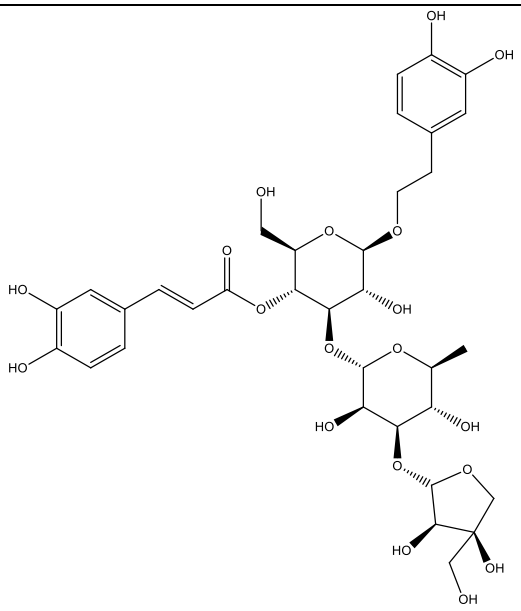
Code	Compound	Reference	Molecular Weight (Da)
PG_116	Ligupurpuroside A Rha(1'''-->4'') Rha	(compound 111) – (27)	770.731



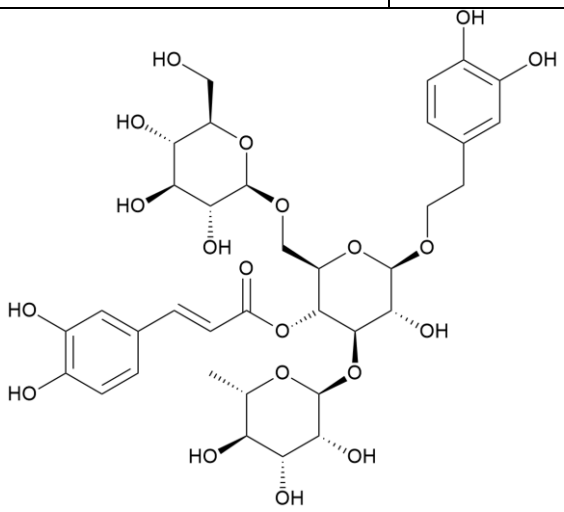
Code	Compound	Reference	Molecular Weight (Da)
PG_117	Ligupurpuroside B Rha(1'''-->4'') Rha	(compound 112) – (27)	740.749



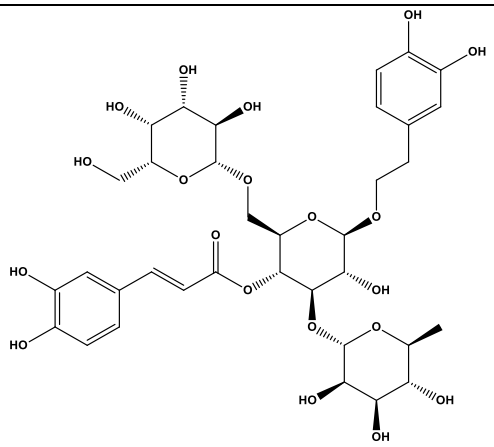
Code	Compound	Reference	Molecular Weight (Da)
PG_118	Myricoside Api (1'''-->3'') Rha	(compound 113) – (27)	756.704



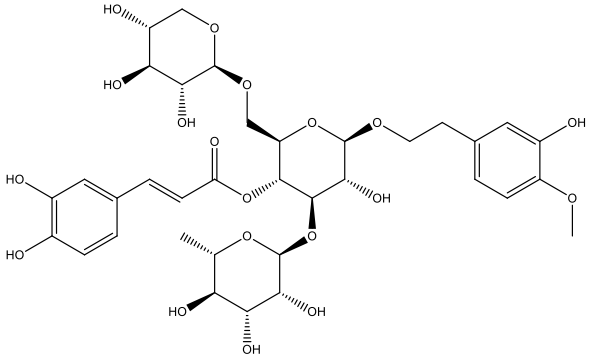
Code	Compound	Reference	Molecular Weight (Da)
PG_119	Neoacteoside	(compound 114) – (27)	786.73



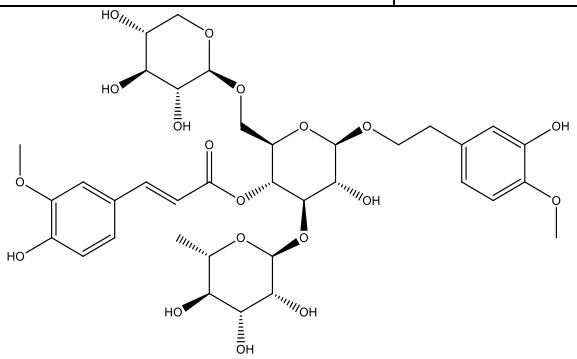
Code	Compound	Reference	Molecular Weight (Da)
PG_120	Purpureaside C	(compound 115) – (27)	788.746



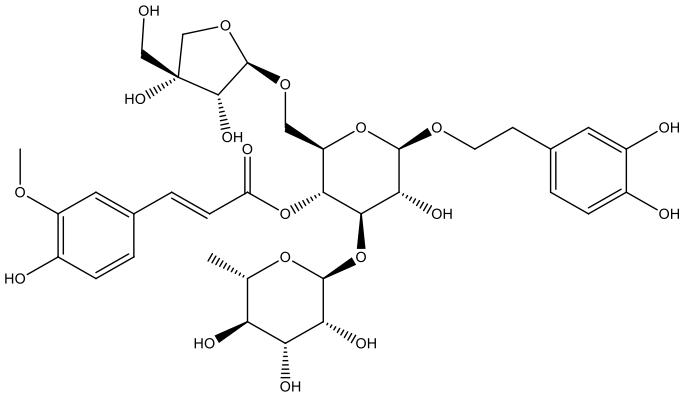
Code	Compound	Reference	Molecular Weight (Da)
PG_121	NO TRIVIAL NAME	(compound 116) – (27)	772.747



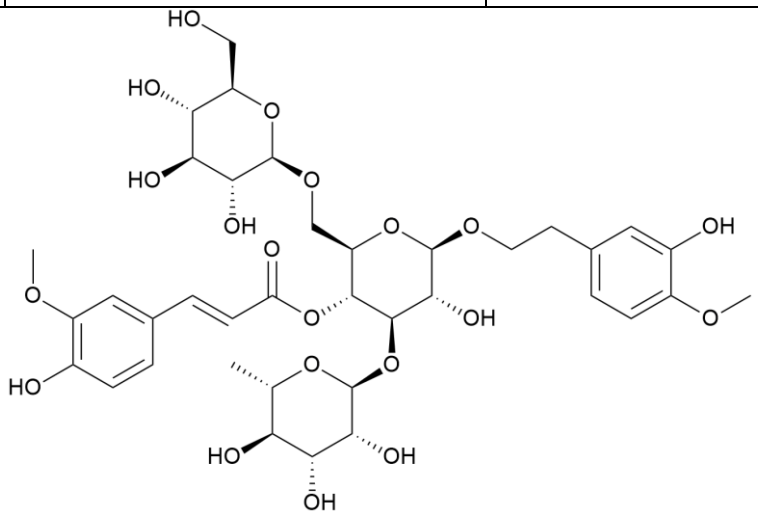
Code	Compound	Reference	Molecular Weight (Da)
PG_122	NO TRIVIAL NAME	(compound 117) – (27)	784.758



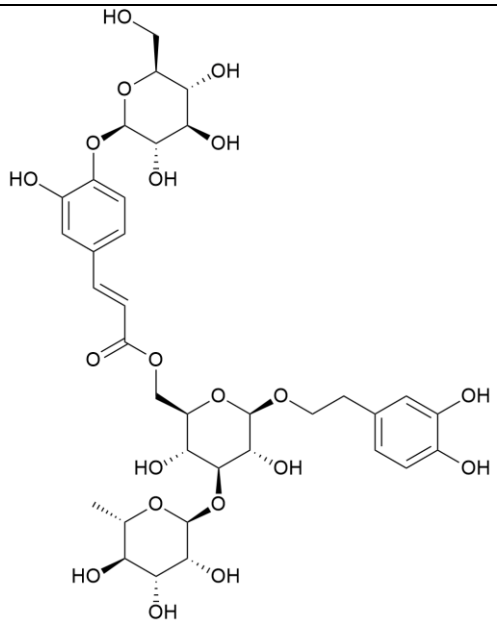
Code	Compound	Reference	Molecular Weight (Da)
PG_123	NO TRIVIAL NAME	(compound 118) – (27)	770.731



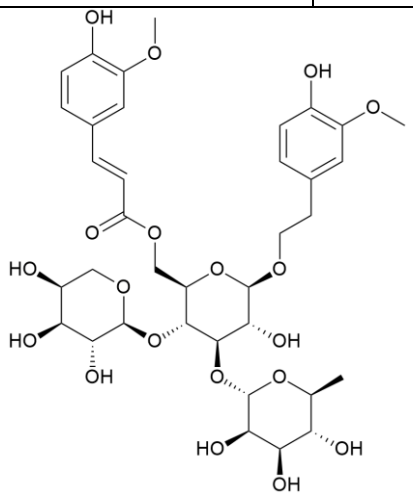
Code	Compound	Reference	Molecular Weight (Da)
PG_124	NO TRIVIAL NAME	(compound 119) – (27)	814.784



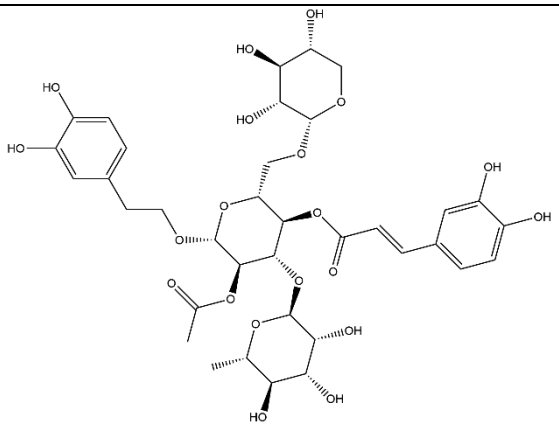
Code	Compound	Reference	Molecular Weight (Da)
PG_125	NO TRIVIAL NAME	(compound 120) – (27)	786.73



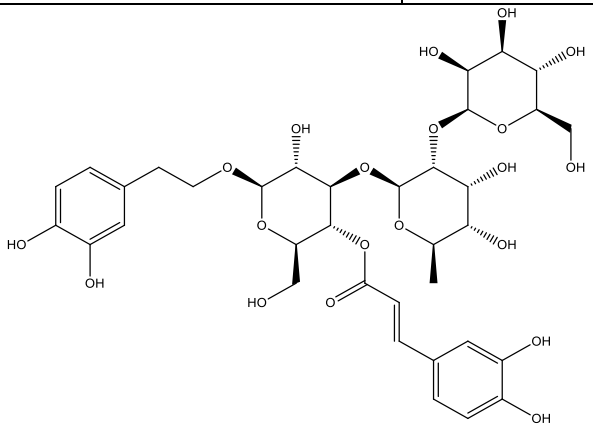
Code	Compound	Reference	Molecular Weight (Da)
PG_126	Pedicularioside I	(compound 121) – (27)	784.758



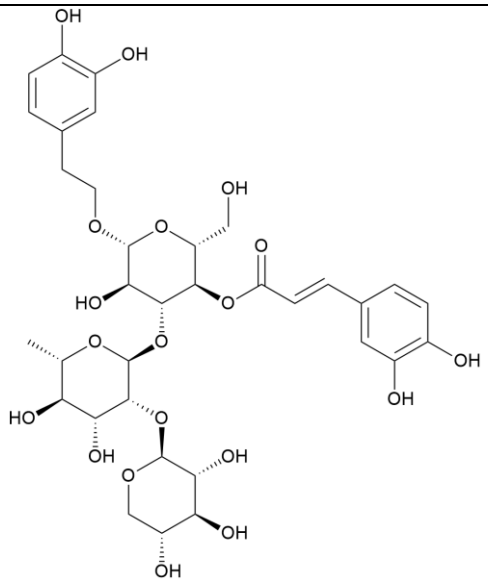
Code	Compound	Reference	Molecular Weight (Da)
PG_127	Pheliposide	(compound 122) – (27)	800.757



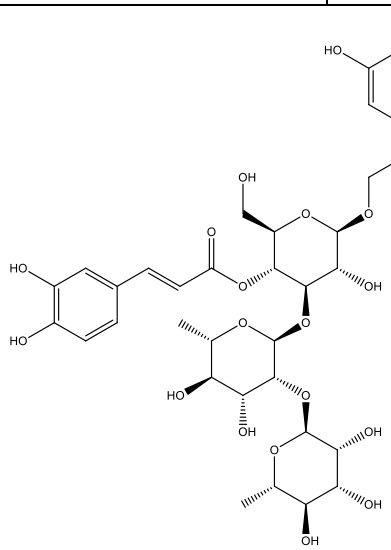
Code	Compound	Reference	Molecular Weight (Da)
PG_128	Phlinoside A Glc (1""-->2") Rha	(compound 123) – (27)	786.73



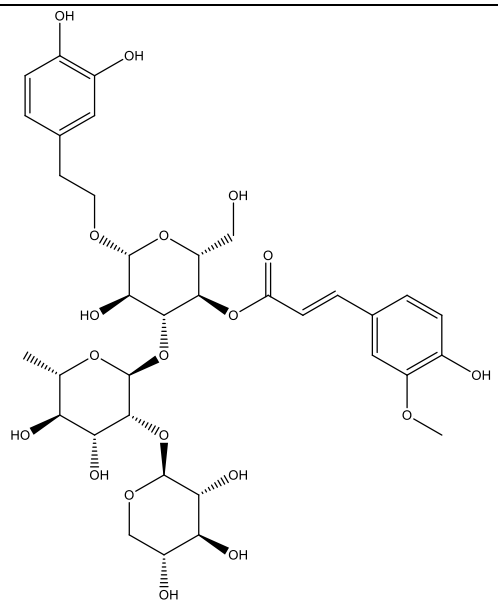
Code	Compound	Reference	Molecular Weight (Da)
PG_129	Phlinoside B xyl (1"'-->2") Rha	(compound 124) – (27)	756.704



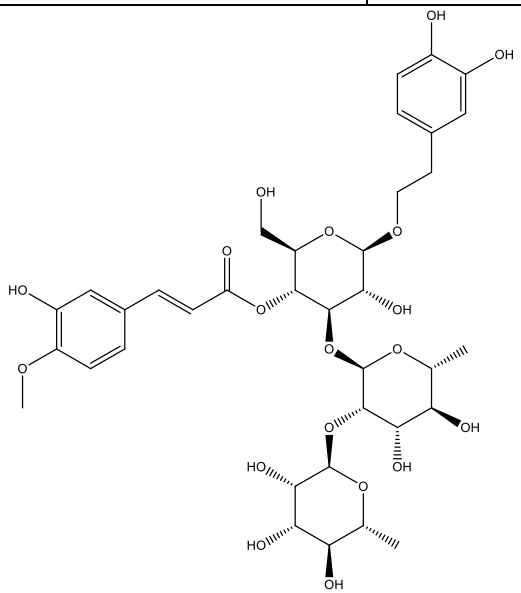
Code	Compound	Reference	Molecular Weight (Da)
PG_130	Phlinoside C Rha(1'''--> 2'') Rha	(compound 122) – (27)	770.731



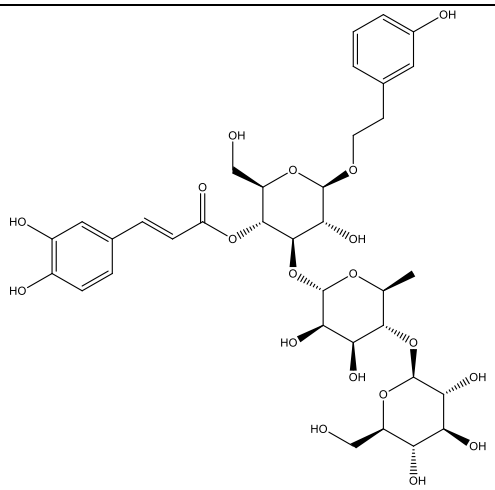
Code	Compound	Reference	Molecular Weight (Da)
PG_131	Phlinoside D Xyl(1'''--> 2'') Rha	(compound 126) – (27)	770.731



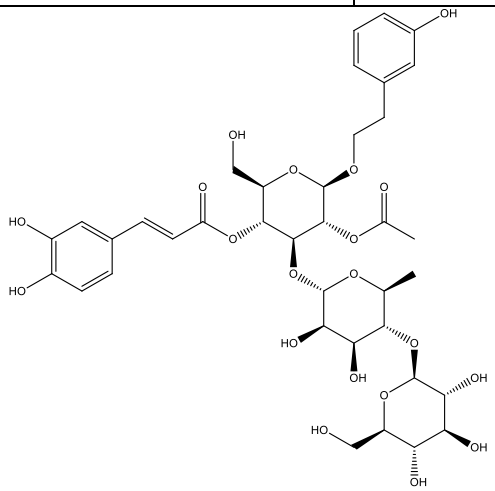
Code	Compound	Reference	Molecular Weight (Da)
PG_132	Phlinoside E Rha(1'''--> 2'') Rha	(compound 127) – (27)	784.758



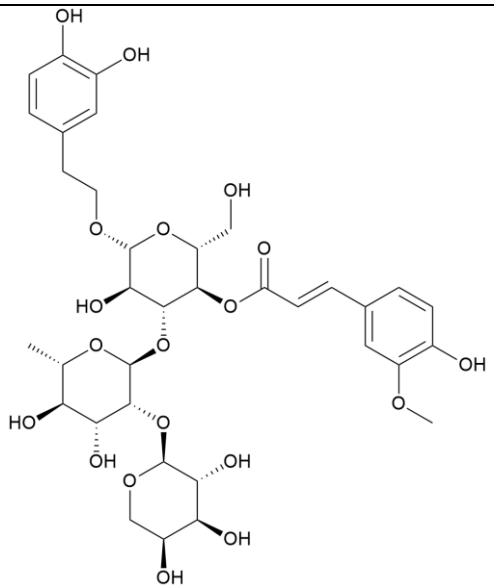
Code	Compound	Reference	Molecular Weight (Da)
PG_133	Rossicaside A Glc (1'''-->4'') Rha	(compound 129) – (27)	772.747



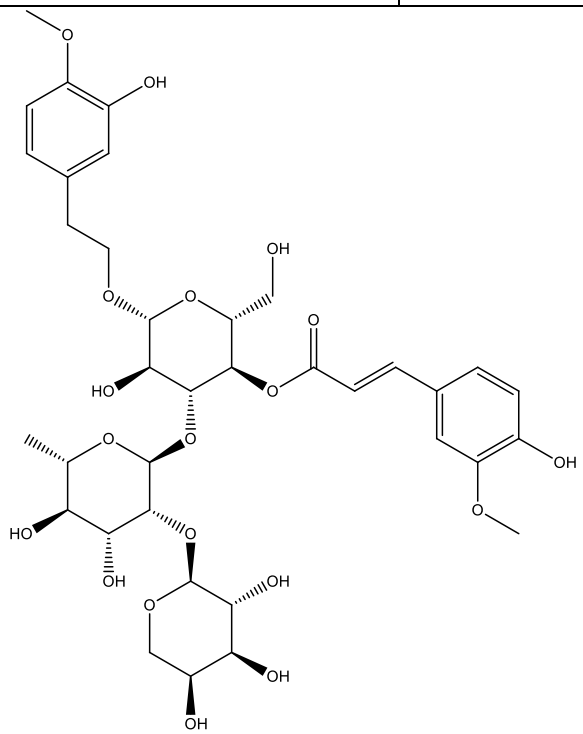
Code	Compound	Reference	Molecular Weight (Da)
PG_134	2'-O-acetyl rossicaside A Glc (1'''-->4") Rha	(compound 130) – (27)	814.784



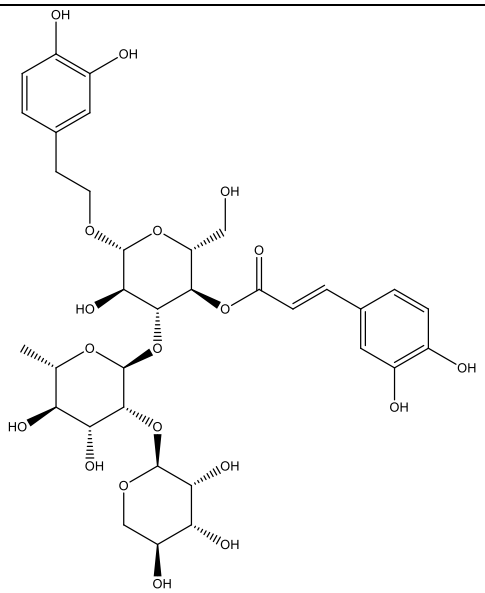
Code	Compound	Reference	Molecular Weight (Da)
PG_135	Stachysoside C Arb (1'''-->2") Rha (or Stachysoside B or Leonoside A)	(compound 131) – (27)	770.731



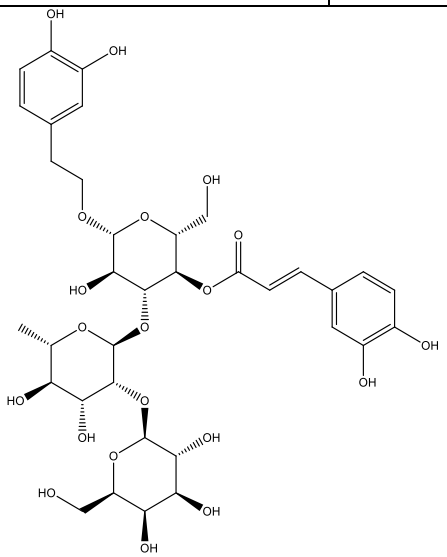
Code	Compound	Reference	Molecular Weight (Da)
PG_136	Stachysoside D Arb (1'''-->2'') Rha (or leonoside B)	(compound 132) – (27)	784.758



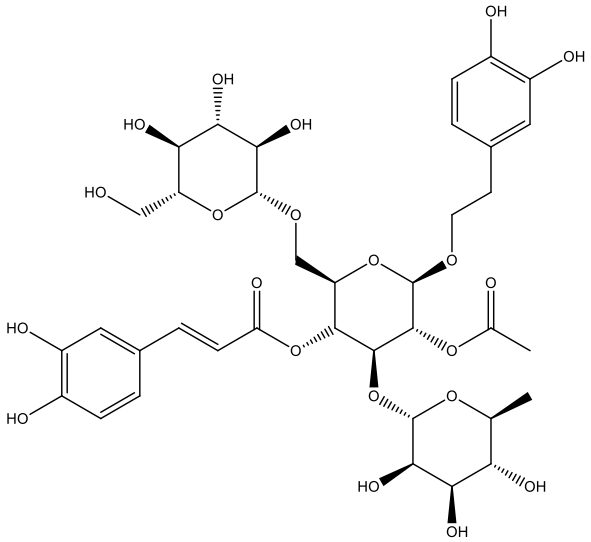
Code	Compound	Reference	Molecular Weight (Da)
PG_137	Teucrioside Lyx (1'''-->2'') Rha	(compound 133) – (27) (compound 135) – (31)	756.704



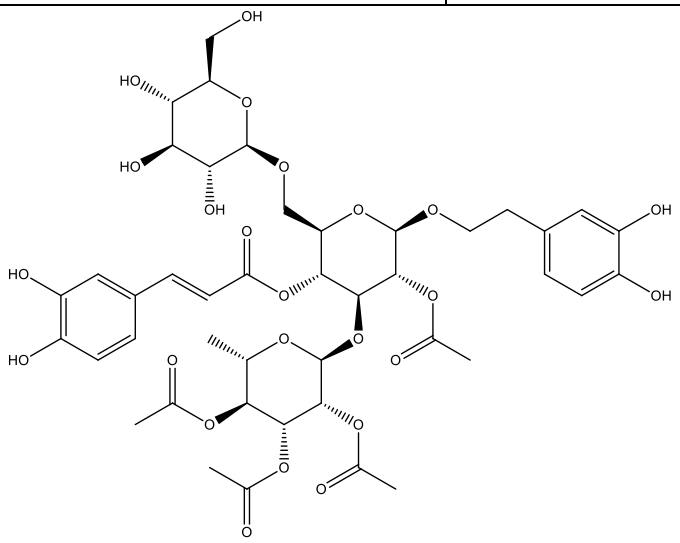
Code	Compound	Reference	Molecular Weight (Da)
PG_138	Teupolioside Glt (1'''-->2'') Rha (or Lamiusides A or Lamiuside A)	(compound 134) – (27) (compound 10) – (28) (compound 136) – (31)	786.73



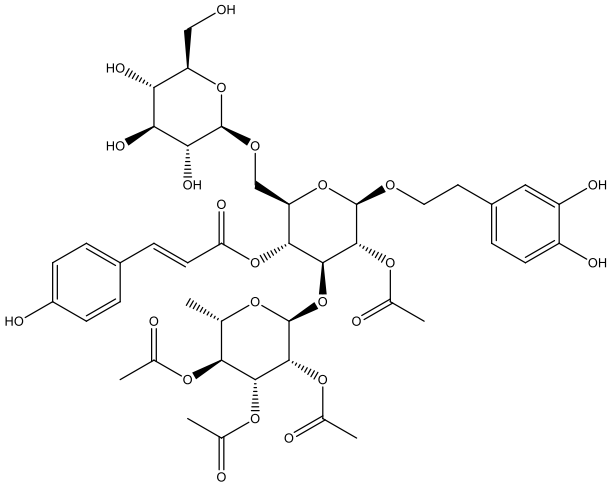
Code	Compound	Reference	Molecular Weight (Da)
PG_139	Tubuloside A	(compound 135) – (27)	828.767



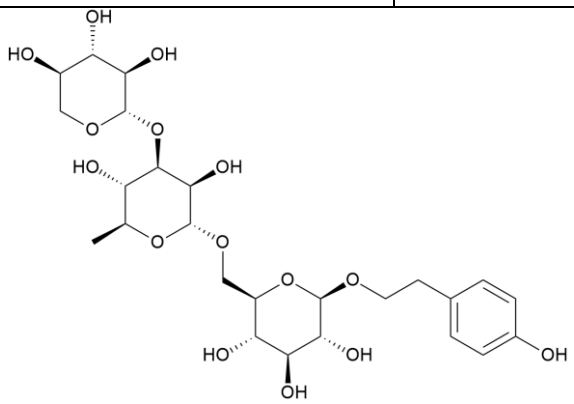
Code	Compound	Reference	Molecular Weight (Da)
PG_140	Tubuloside C 2",3",4"-tri-O-acetylrhamnoside	(compound 136) – (27)	956.894



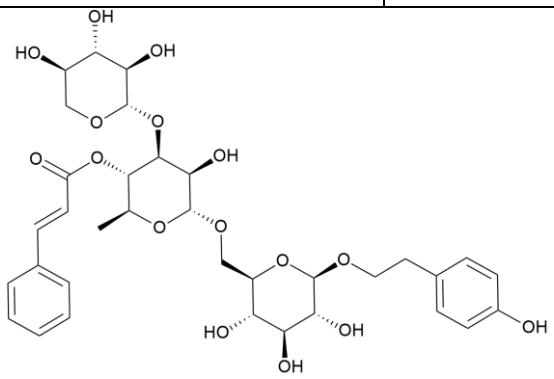
Code	Compound	Reference	Molecular Weight (Da)
PG_141	Tubuloside D 2",3",4"-tri-O-acetylrhamnoside	(compound 137) – (27)	940.895



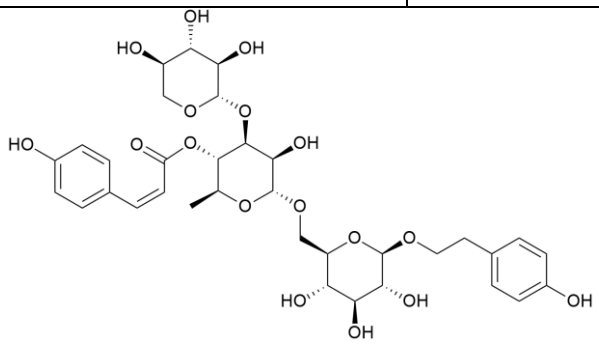
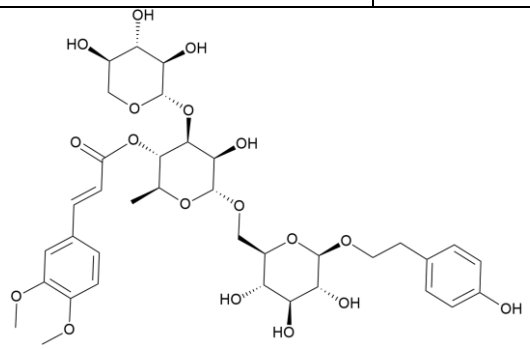
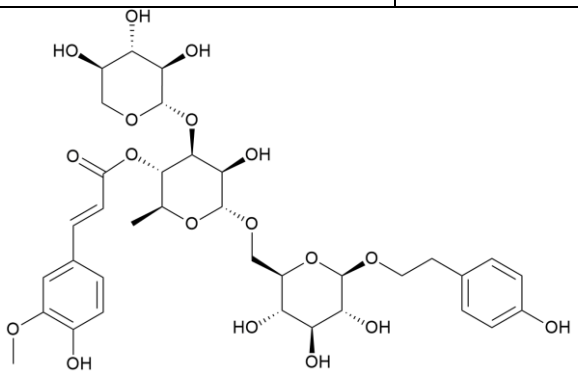
Code	Compound	Reference	Molecular Weight (Da)
PG_142	Mussatioside	(compound 138) – (27)	578.562

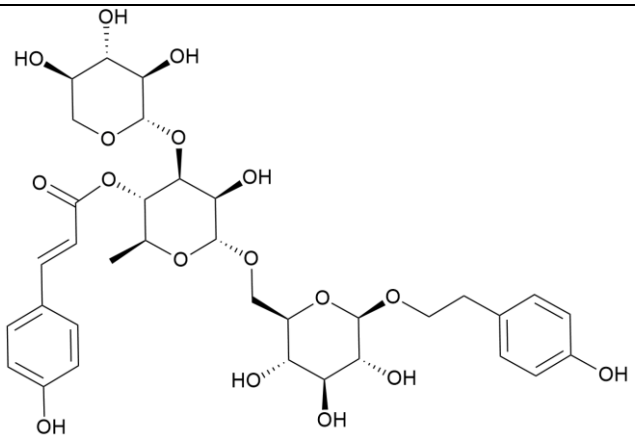


Code	Compound	Reference	Molecular Weight (Da)
PG_143	4-cinnamoyl mussatioside (or mussatioside I)	(compound 139) – (27)	708.707

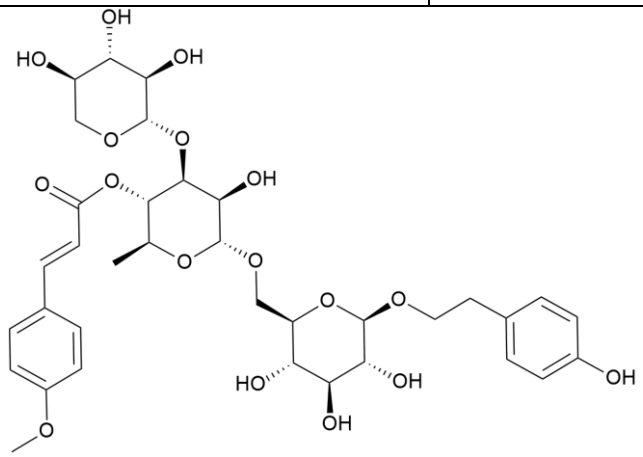


Code	Compound	Reference	Molecular Weight (Da)

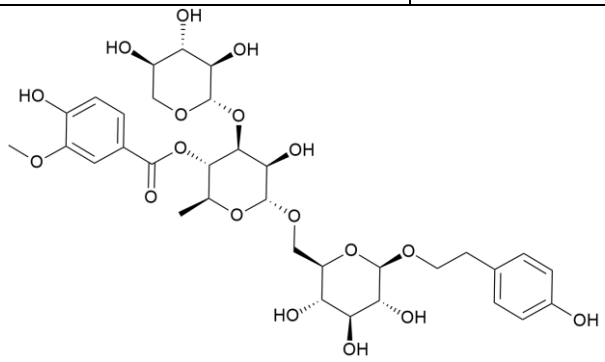
PG_144	4-cis-p-coumaroyl mussatioside	(compound 140) – (27)	724.706
			
Code	Compound	Reference	Molecular Weight (Da)
PG_145	4-dimethylcaffeoyl mussatioside (or mussatioside II)	(compound 141) – (27)	768.759
			
Code	Compound	Reference	Molecular Weight (Da)
PG_146	4-feruloyl mussatioside	(compound 142) – (27)	754.732
			
Code	Compound	Reference	Molecular Weight (Da)
PG_147	4-p-coumaroyl mussatioside	(compound 143) – (27)	724.706



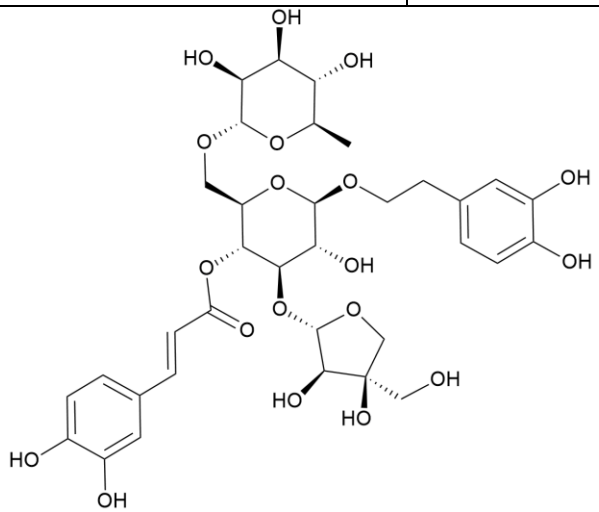
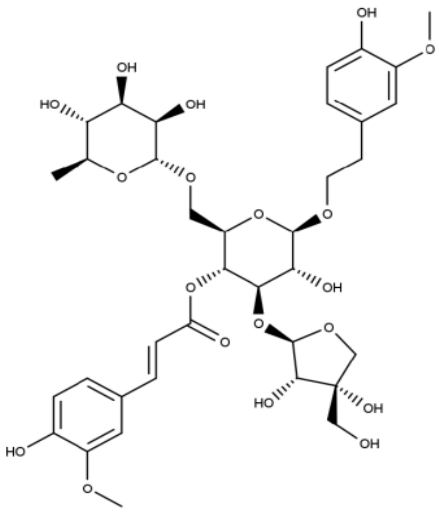
Code	Compound	Reference	Molecular Weight (Da)
PG_148	4-p-methoxycinnamoyl mussatioside (or mussatioside III)	(compound 144) – (27)	740.749

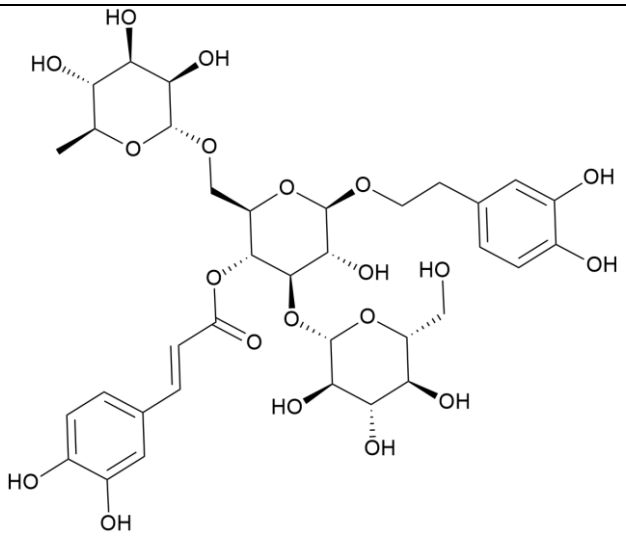


Code	Compound	Reference	Molecular Weight (Da)
PG_149	4-vanilloyl mussatioside	(compound 145) – (27)	728.694

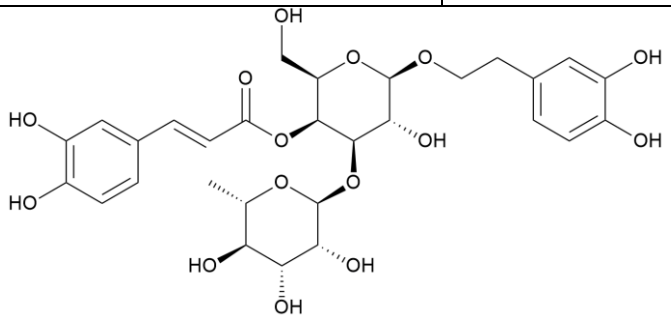


Code	Compound	Reference	Molecular

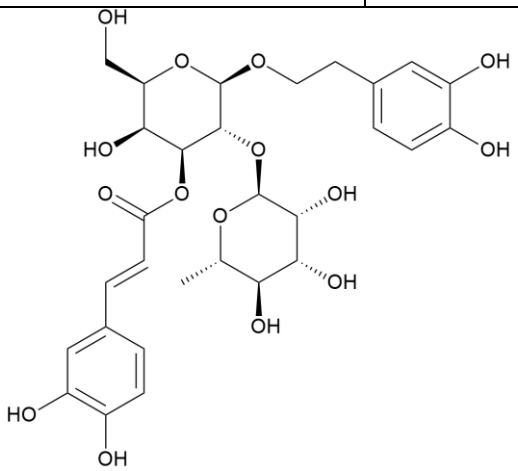
			Weight (Da)
PG_150	Pedicularioside A	(compound 146) – (27) (compound 118) – (31)	756.704
			
Code	Compound	Reference	Molecular Weight (Da)
PG_151	Pedicularioside H	(compound 147) – (27)	784.758
			
Code	Compound	Reference	Molecular Weight (Da)
PG_152	Purpureaside B	(compound 148) – (27)	786.73



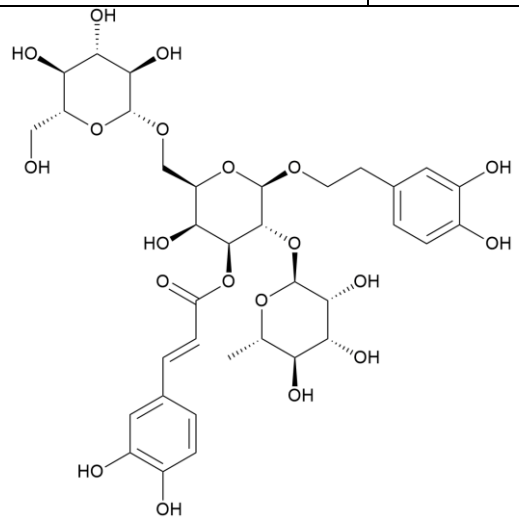
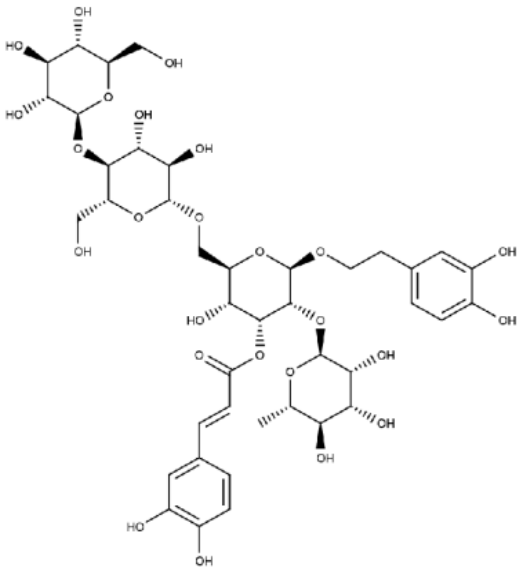
Code	Compound	Reference	Molecular Weight (Da)
PG_153	Pedicularioside G	(compound 149) – (27)	624.59

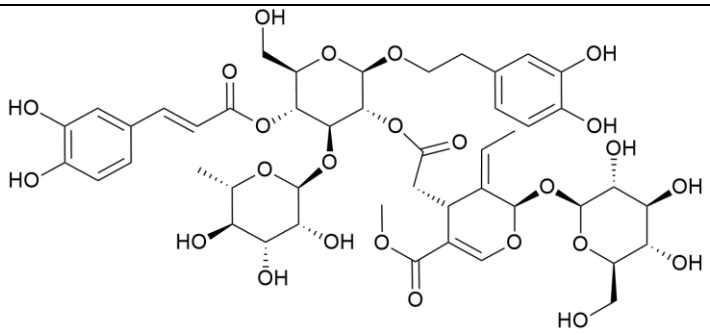


Code	Compound	Reference	Molecular Weight (Da)
PG_154	Mangnoloside A	(compound 150) – (27)	626.606

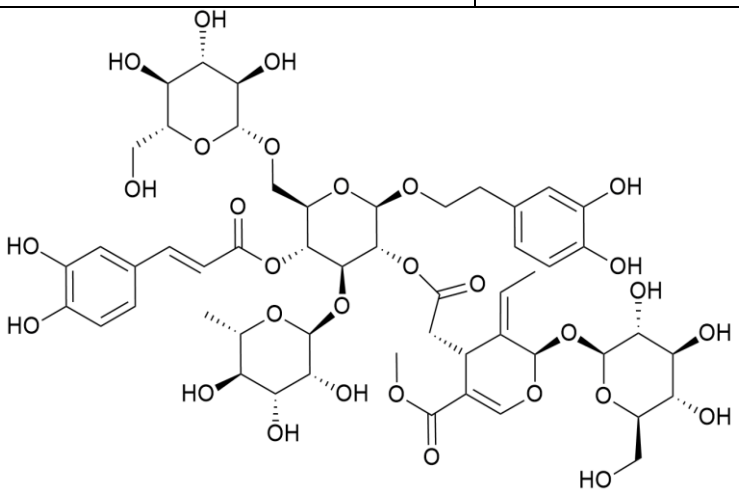


Code	Compound	Reference	Molecular

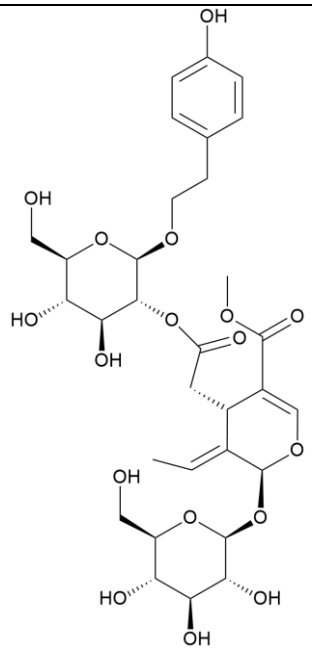
			Weight (Da)
PG_155	Magnoloside B	(compound 151) – (27)	786.73
			
Code	Compound	Reference	Molecular Weight (Da)
PG_156	Magnoloside C	(compound 152) – (27)	948.871
			
Code	Compound	Reference	Molecular Weight (Da)
PG_157	Oleoacteoside	(compound 153) – (27)	1014.97



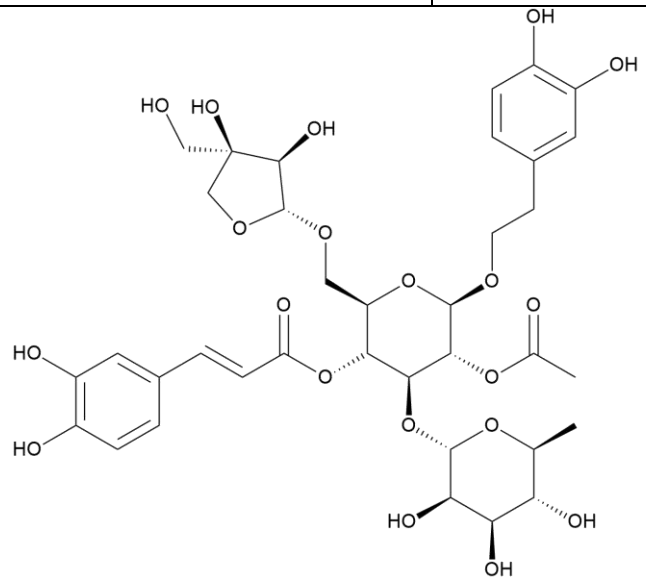
Code	Compound	Reference	Molecular Weight (Da)
PG_158	Oleoechinacoside	(compound 154) – (27)	1175.1



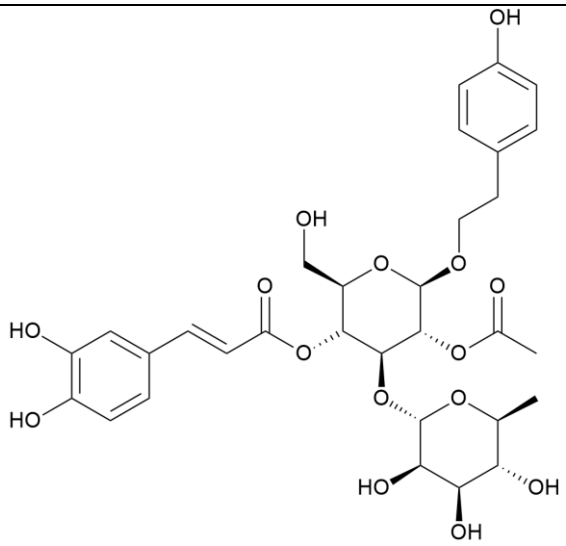
Code	Compound	Reference	Molecular Weight (Da)
PG_159	Nuzhenide	(compound 155) – (27)	686.657



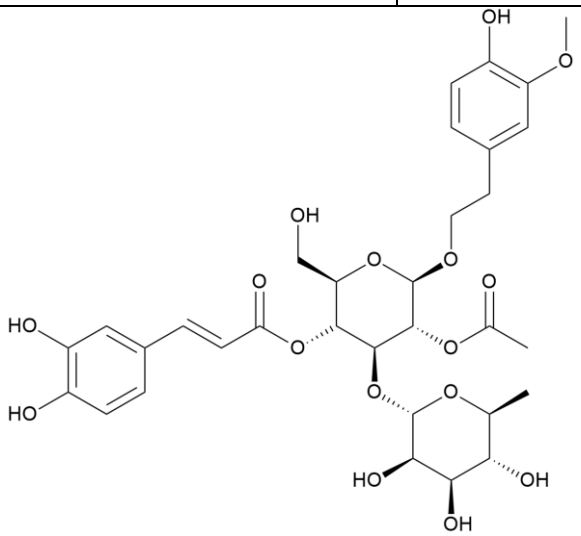
Code	Compound	Reference	Molecular Weight (Da)
PG_160	Acetyl forsythoside B	(compound 1) – (28)	800.757



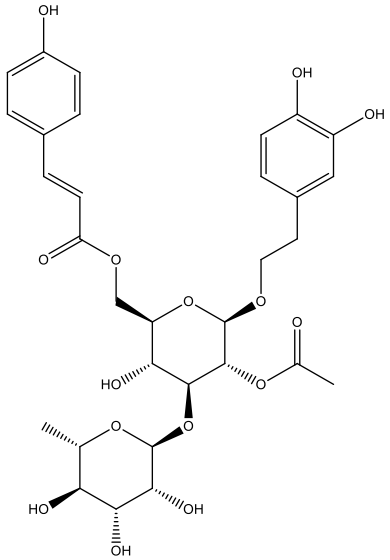
Code	Compound	Reference	Molecular Weight (Da)
PG_161	Salsasides D	(compound 2) – (28)	650.628



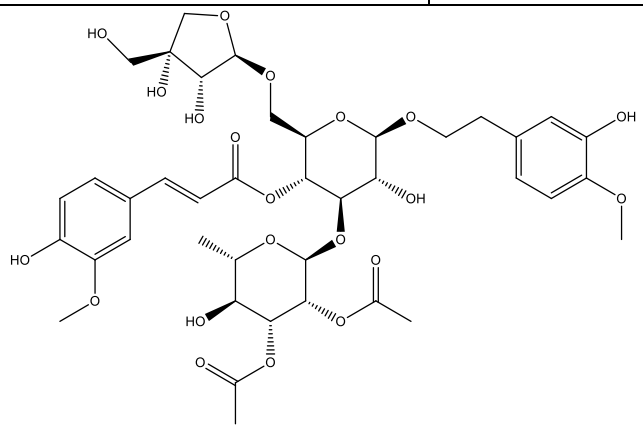
Code	Compound	Reference	Molecular Weight (Da)
PG_162	Salsasides E	(compound 3) – (28)	680.654



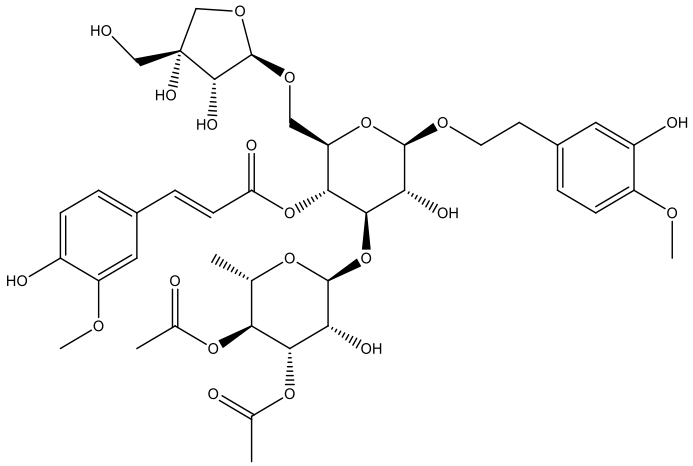
Code	Compound	Reference	Molecular Weight (Da)
PG_163	Salsasides F	(compound 4) – (28)	650.628



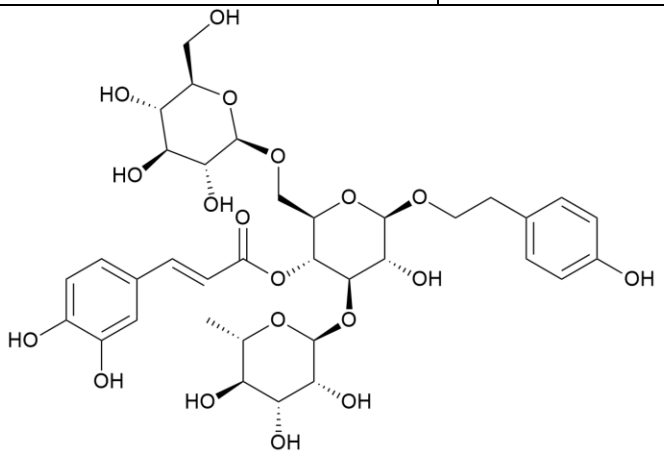
Code	Compound	Reference	Molecular Weight (Da)
PG_164	2’’’,3’’’-Diacetyl-O-betonyoside	(compound 5) – (28) (compound 74) – (31)	868.832



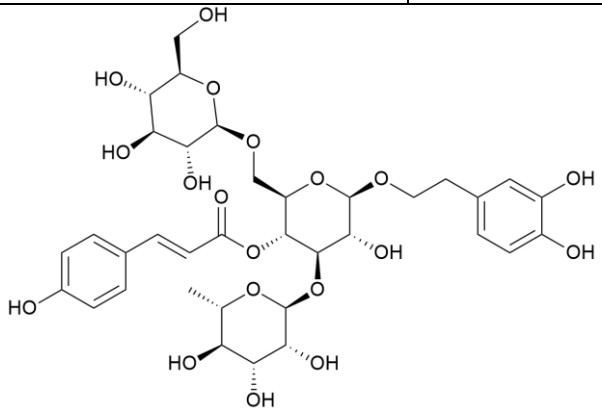
Code	Compound	Reference	Molecular Weight (Da)
PG_165	3’’’,4’’’-Diacetyl-O-betonyoside	(compound 6) – (28) (compound 75) – (31)	868832

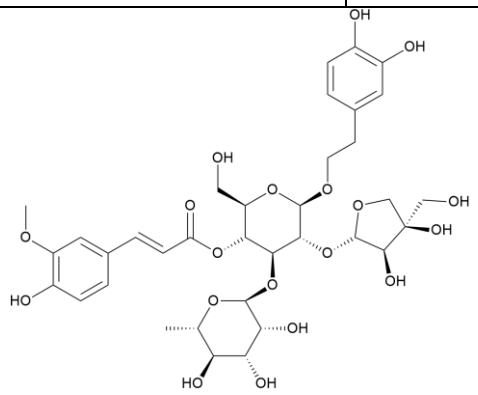
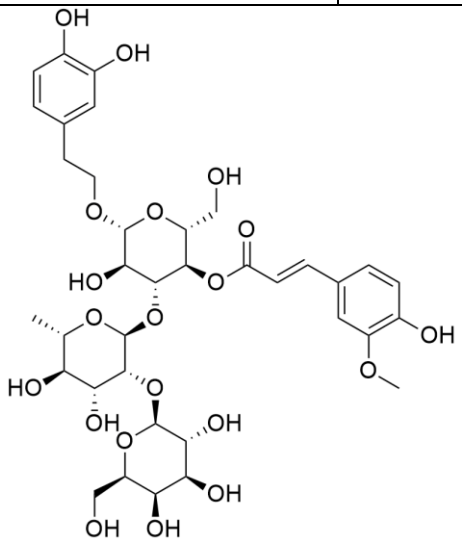


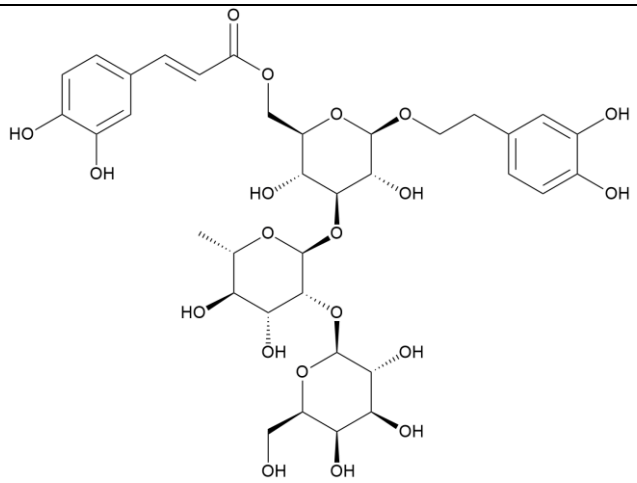
Code	Compound	Reference	Molecular Weight (Da)
PG_166	Cistantubulosides A	(compound 7) – (28)	770.731



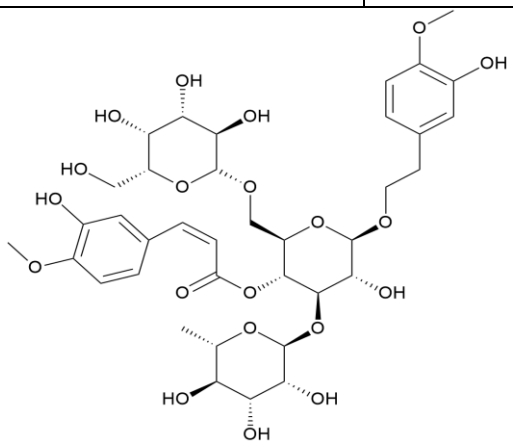
Code	Compound	Reference	Molecular Weight (Da)
PG_167	Cistantubulosides B1/B2	(compound 8) – (28)	770.731



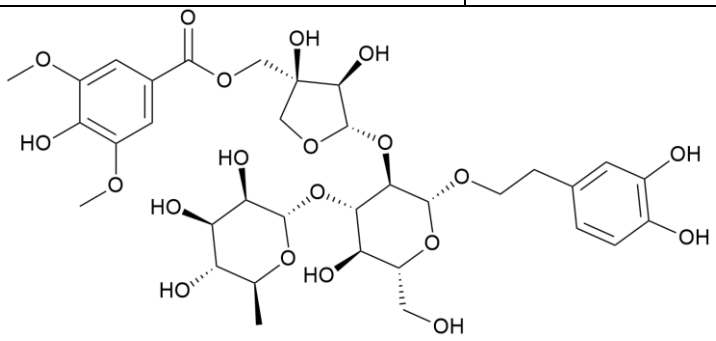
Code	Compound	Reference	Molecular Weight (Da)
PG_168	Dolichandroside	(compound 9) – (28)	772.747
			
Code	Compound	Reference	Molecular Weight (Da)
PG_169	Lamiusides B	(compound 11) – (28)	802.773
			
Code	Compound	Reference	Molecular Weight (Da)
PG_170	Lamiusides C	(compound 12) – (28)	786.73



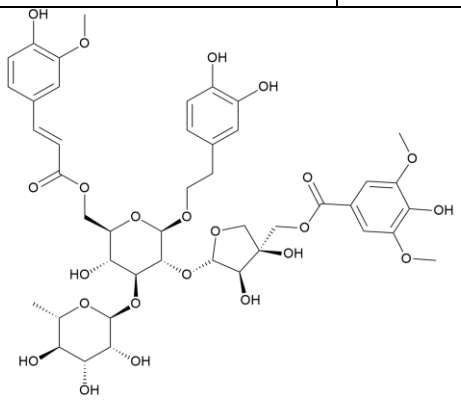
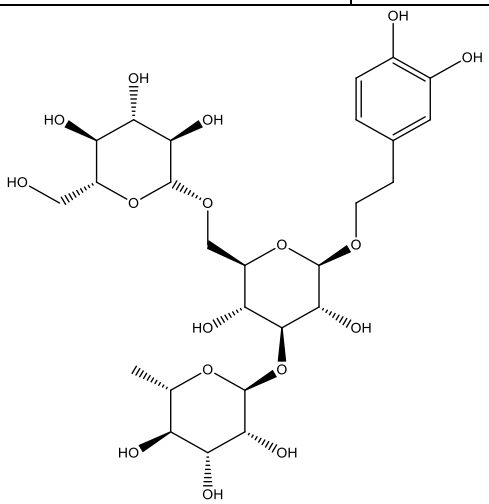
Code	Compound	Reference	Molecular Weight (Da)
PG_171	Lamiusides E	(compound 13) – (28)	814.784

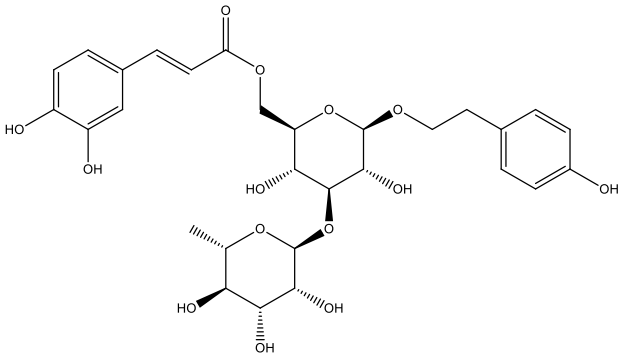


Code	Compound	Reference	Molecular Weight (Da)
PG_172	Newbouldioside A	(compound 14) – (28)	774.719

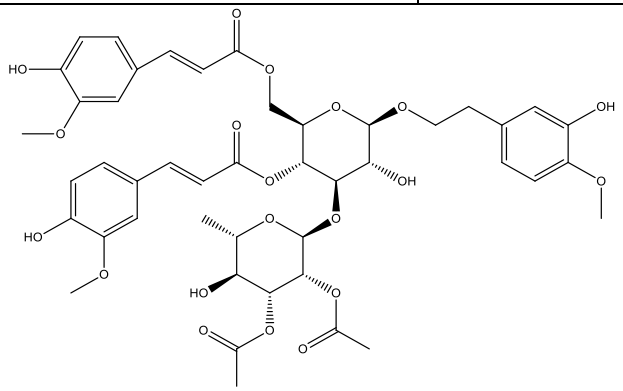


Code	Compound	Reference	Molecular Weight (Da)

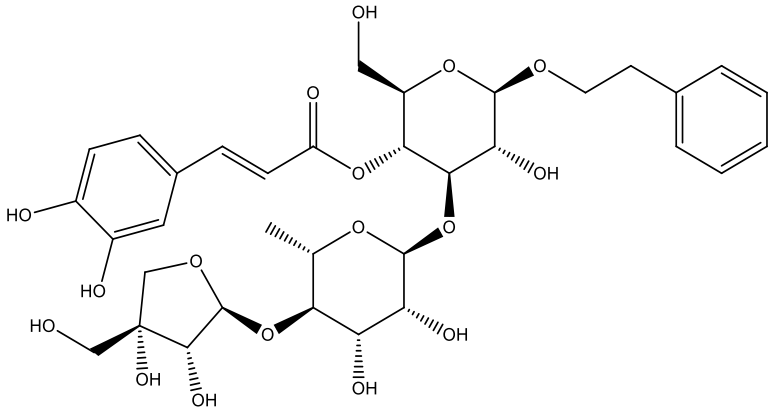
PG_173	Newbouldioside B	(compound 15) – (28)	952.906
			
Code	Compound	Reference	Molecular Weight (Da)
PG_174	Kankanosides F	(compound 16) – (28)	624.587
			
Code	Compound	Reference	Molecular Weight (Da)
PG_175	Kankanosides G	(compound 17) – (28)	608.591



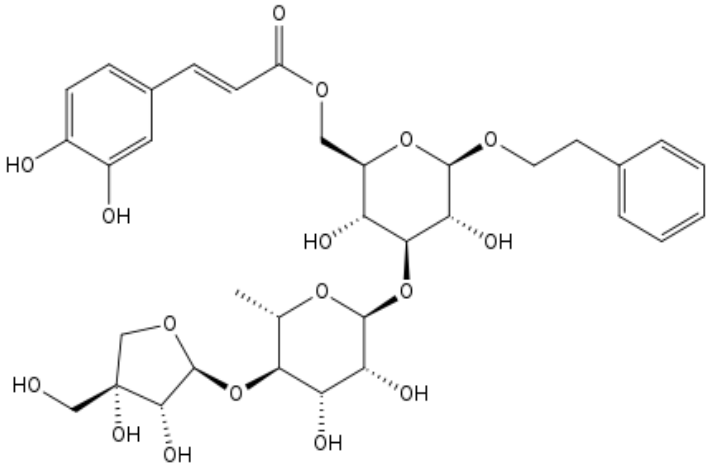
Code	Compound	Reference	Molecular Weight (Da)
PG_176	Trichotomoside	(compound 18) – (28)	914.904



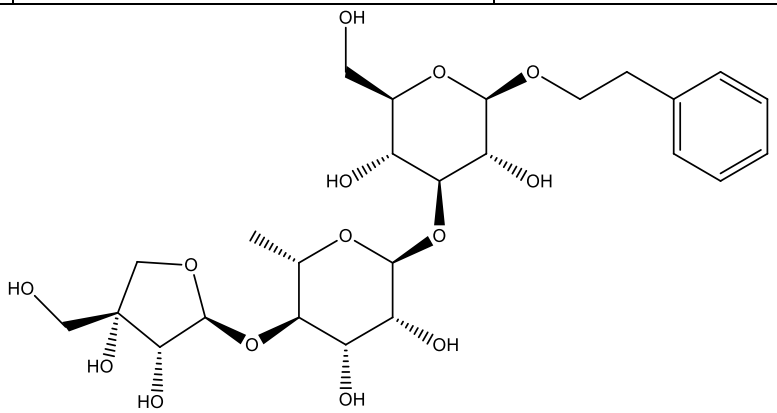
Code	Compound	Reference	Molecular Weight (Da)
PG_177	Picfeosides A	(compound 19) – (28)	726.722



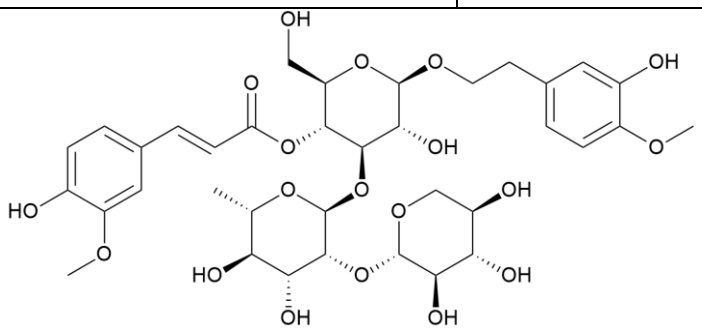
Code	Compound	Reference	Molecular Weight (Da)
PG_178	Picfeosides B	(compound 20) – (28)	724.706



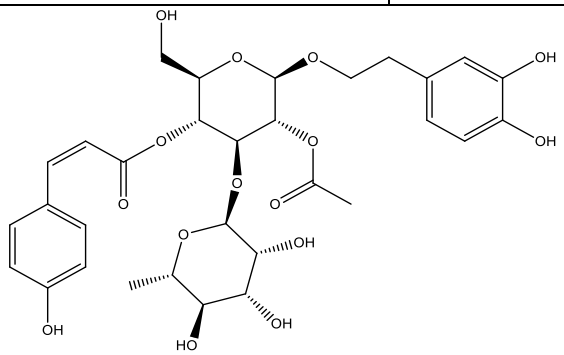
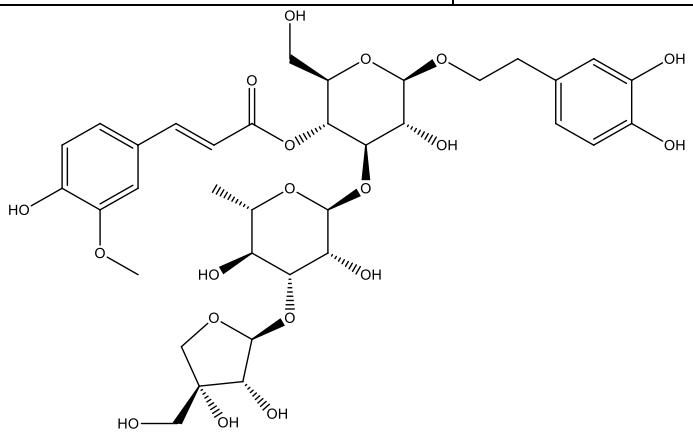
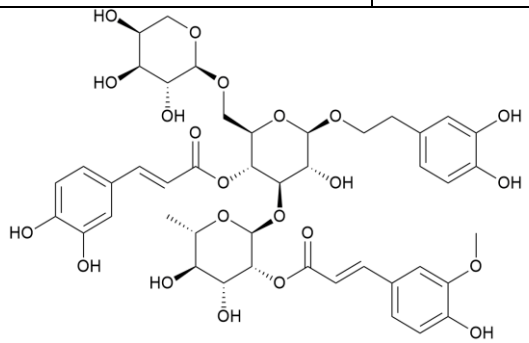
Code	Compound	Reference	Molecular Weight (Da)
PG_179	Picfeosides C	(compound 21) – (28)	562.563

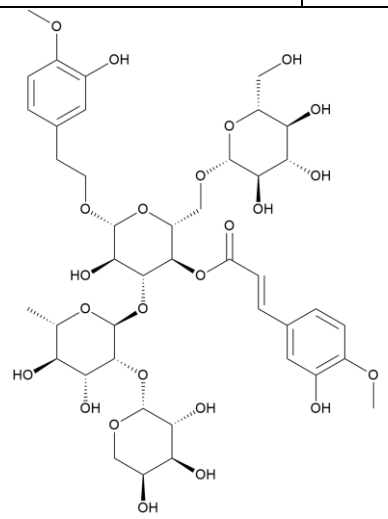
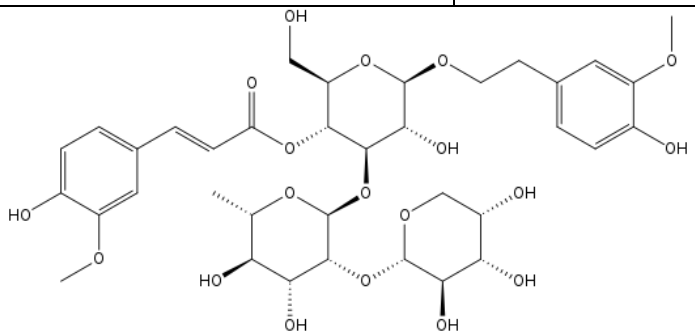


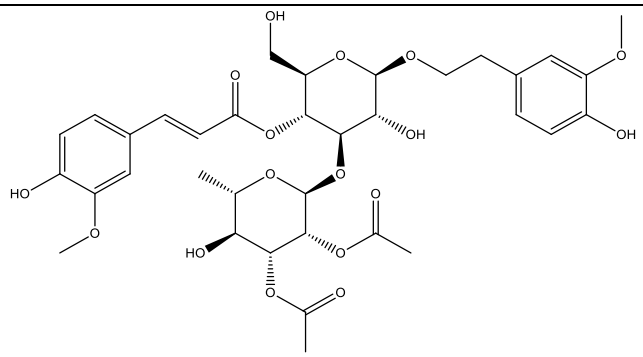
Code	Compound	Reference	Molecular Weight (Da)
PG_180	Phlinoside F	(compound 22) – (28)	768.759



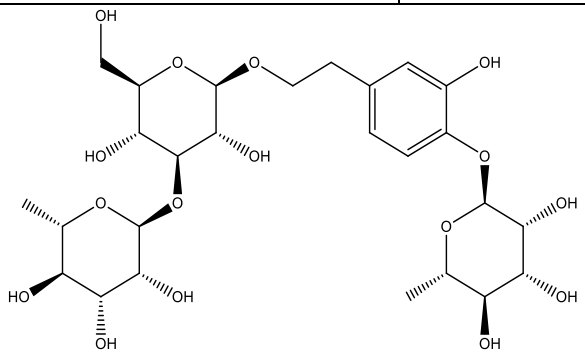
Code	Compound	Reference	Molecular Weight (Da)

PG_181	Z-tubuloside E	(compound 23) – (28)	650.628
			
Code	Compound	Reference	Molecular Weight (Da)
PG_182	Myricoside - 3""-O-methylether	(compound 24) – (28)	770.731
			
Code	Compound	Reference	Molecular Weight (Da)
PG_183	Buddleoside A	(compound 25) – (28)	934.891
			
Code	Compound	Reference	Molecular Weight (Da)

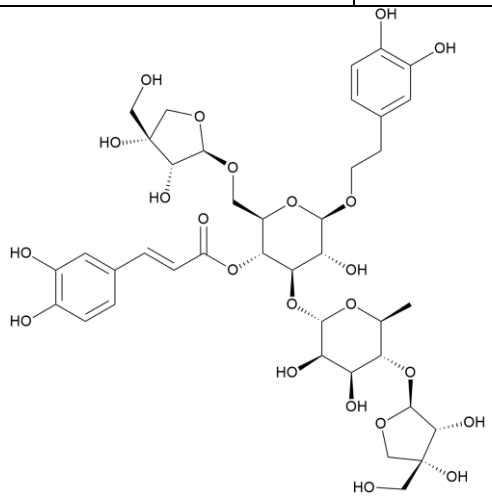
PG_184	Velutinoside III	(compound 26) – (28)	948.914
			
Code	Compound	Reference	Molecular Weight (Da)
PG_185	Velutinoside IVIV	(compound 27) – (28)	784.758
			
Code	Compound	Reference	Molecular Weight (Da)
PG_186	2-(3-Methoxy-4-hydroxyphenyl)ethyl-O- 2",3"-diacetyl-α-L-rhamnopyranosyl (1--> 3)-4-O-(E)-feruloyl-β-D-glucopyranoside	(compound 28) – (28)	736.717



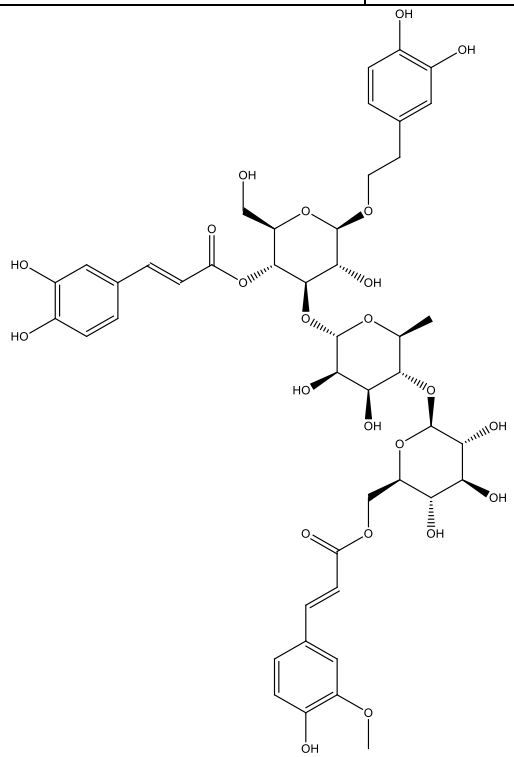
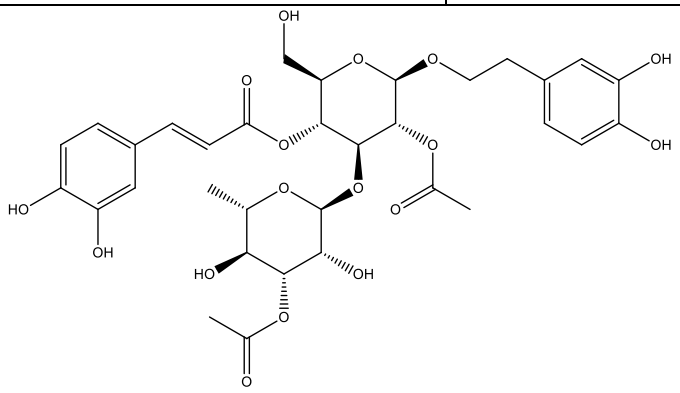
Code	Compound	Reference	Molecular Weight (Da)
PG_187	4-O-α-L-Rhamnopyranosylcistanoside E	(compound 29) – (28)	608.588

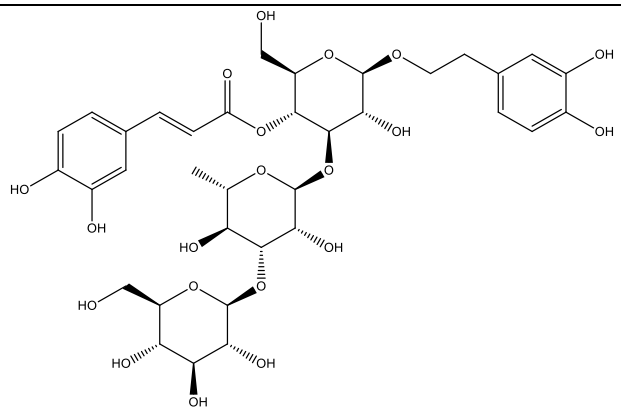


Code	Compound	Reference	Molecular Weight (Da)
PG_188	Lunariifolioside	(compound 30) – (28)	888.819

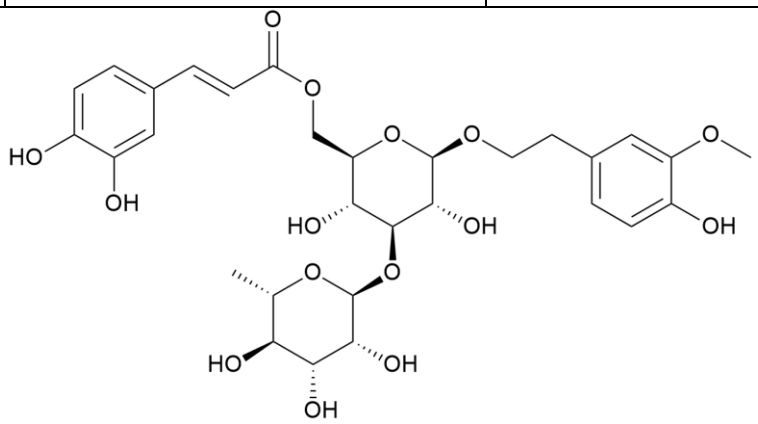


Code	Compound	Reference	Molecular Weight (Da)

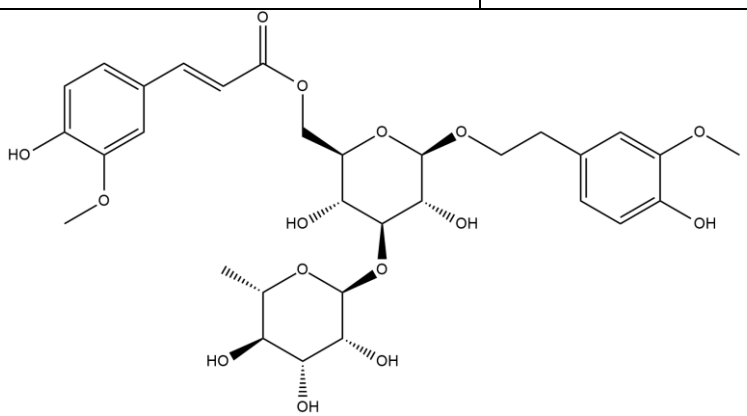
PG_189	Globusintenoside	(compound 31) – (28)	962.901
			
Code	Compound	Reference	Molecular Weight (Da)
PG_190	2",3'''-Diacetyl acteoside	(compound 32) – (28)	710.679
			
Code	Compound	Reference	Molecular Weight (Da)
PG_191	Caerulescenoside	(compound 33) – (28)	788.746



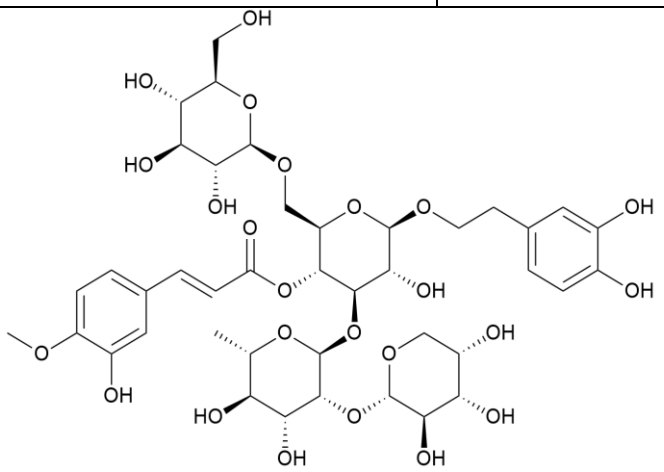
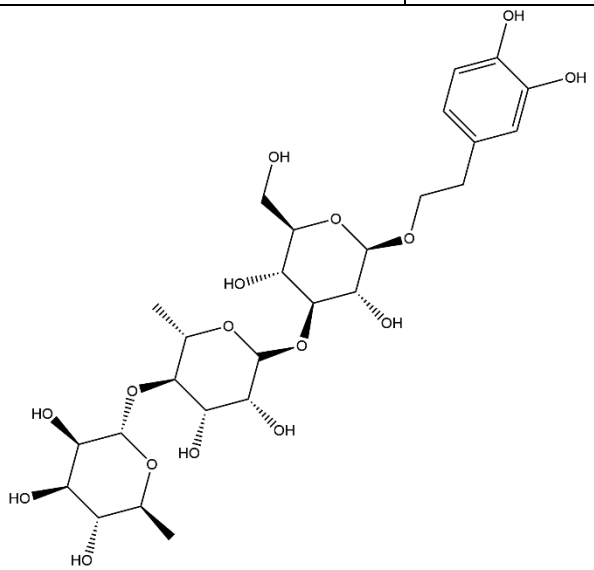
Code	Compound	Reference	Molecular Weight (Da)
PG_192	Isocistanoside C	(compound 34) – (28)	638.617

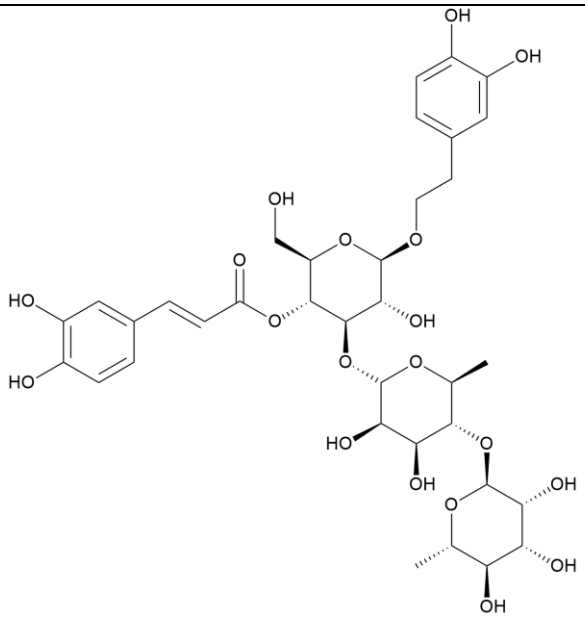


Code	Compound	Reference	Molecular Weight (Da)
PG_193	Epimeridinoside A	(compound 35) – (28)	652.644

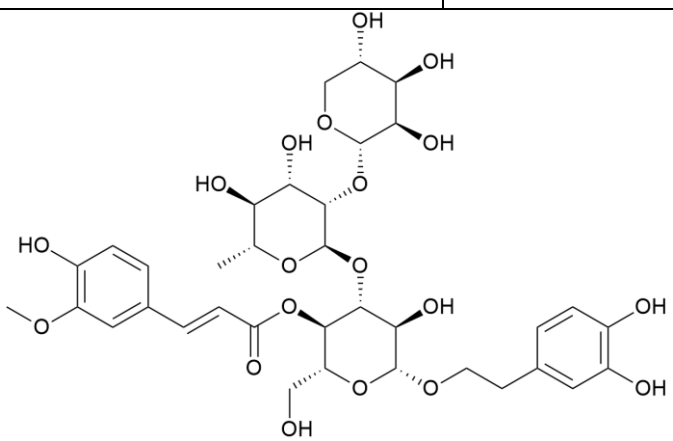


Code	Compound	Reference	Molecular Weight (Da)

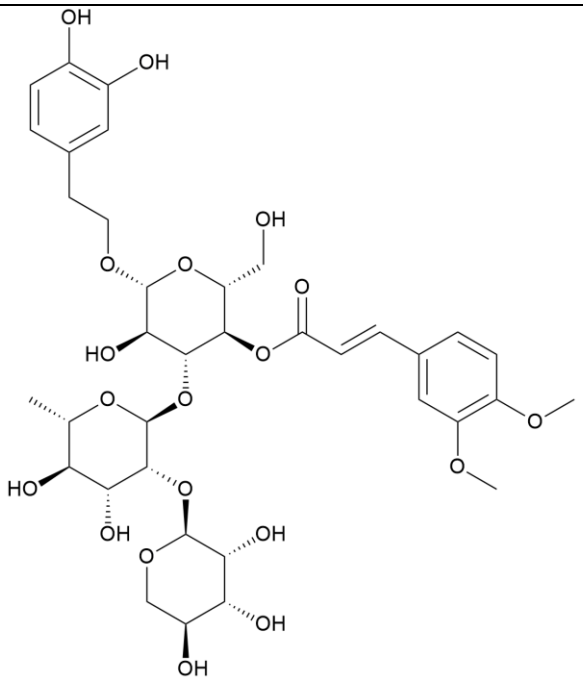
PG_194	Velutinosides II	(compound 37) – (28)	934.888
			
Code	Compound	Reference	Molecular Weight (Da)
PG_195	Ligurobustosides M	(compound 38) – (28)	608.588
			
Code	Compound	Reference	Molecular Weight (Da)
PG_196	Ligurobustosides N	(compound 39) – (28)	770.731



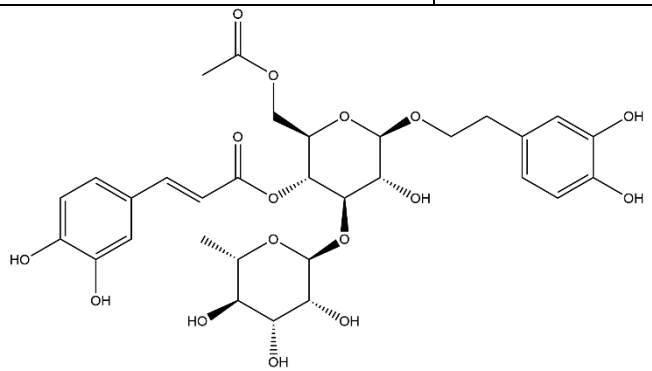
Code	Compound	Reference	Molecular Weight (Da)
PG_197	Teucrioside-3""-O-methylether	(compound 40) – (28)	770.731



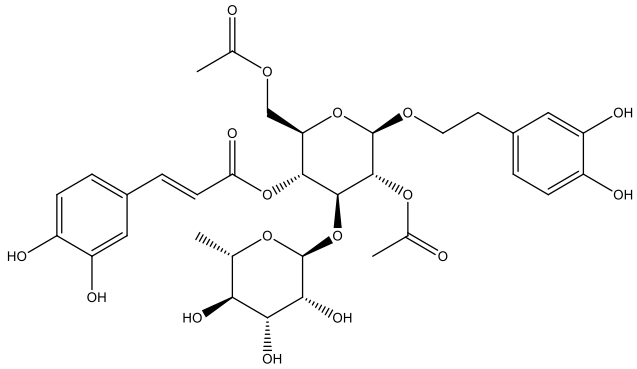
Code	Compound	Reference	Molecular Weight (Da)
PG_ 198	Teucrioside-3"",4""-O-dimethylether	(compound 41) – (28)	786.774



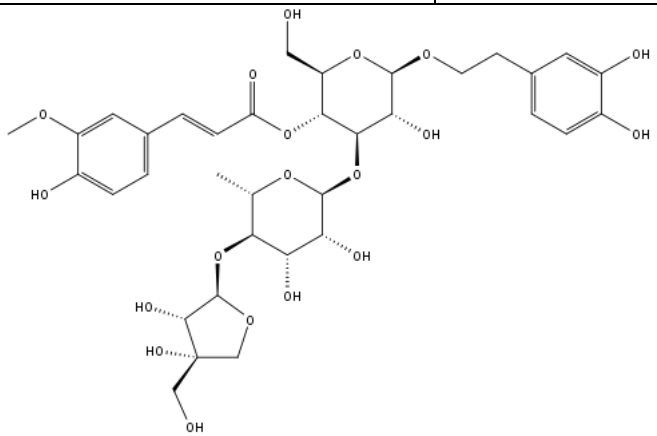
Code	Compound	Reference	Molecular Weight (Da)
PG_199	6'-O-acetylacteoside (or 6'-O-verbascoside)	(compound 42) – (28)	666.627



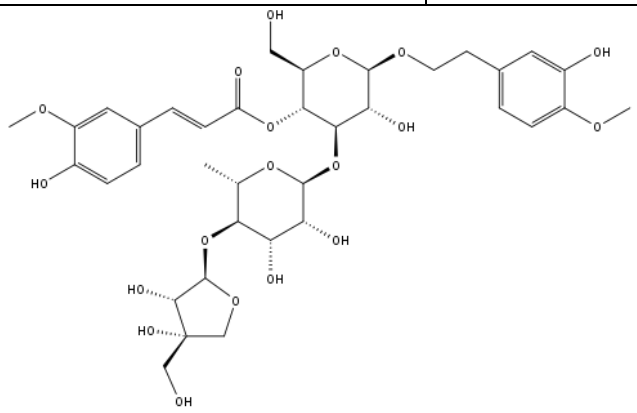
Code	Compound	Reference	Molecular Weight (Da)
PG_200	2'-O, 6'-O-Diacetylacteoside	(compound 43) – (28)	708.664



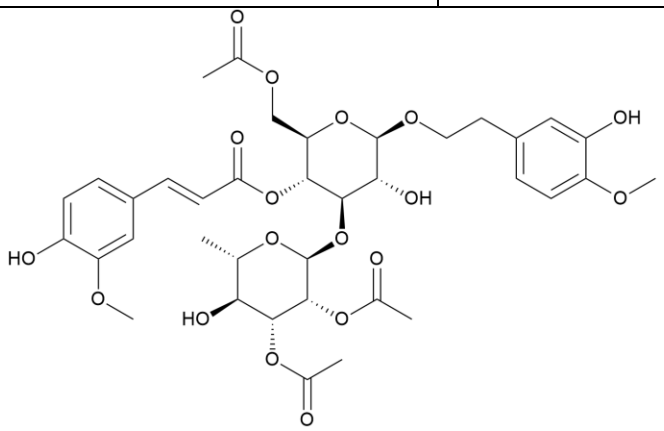
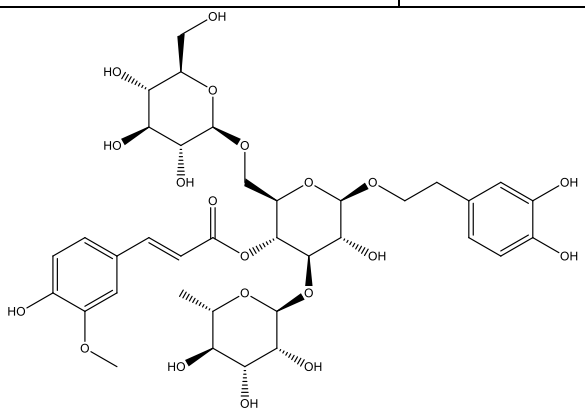
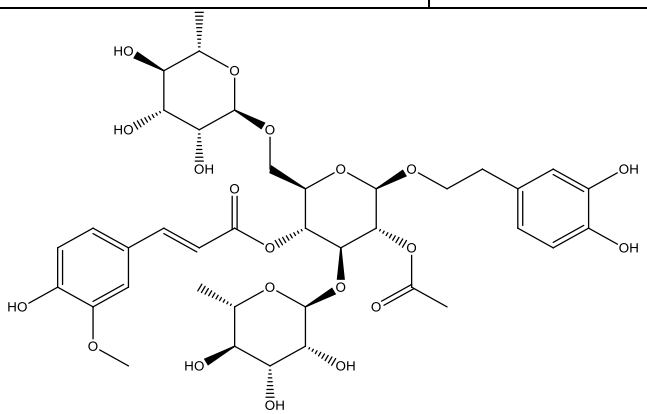
Code	Compound	Reference	Molecular Weight (Da)
PG_201	Integrifoliosides A	(compound 44) – (28)	770.731

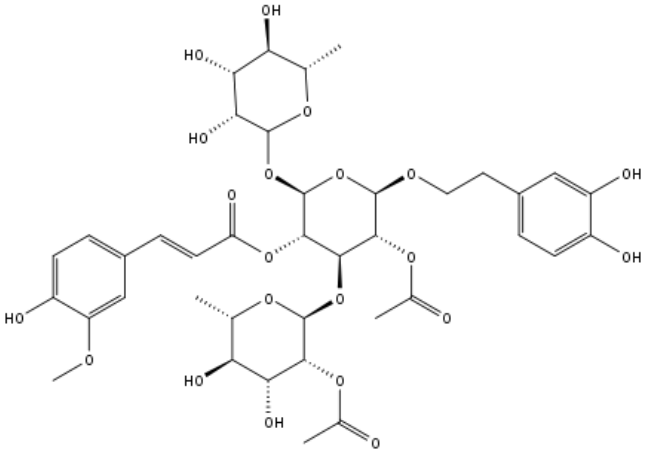
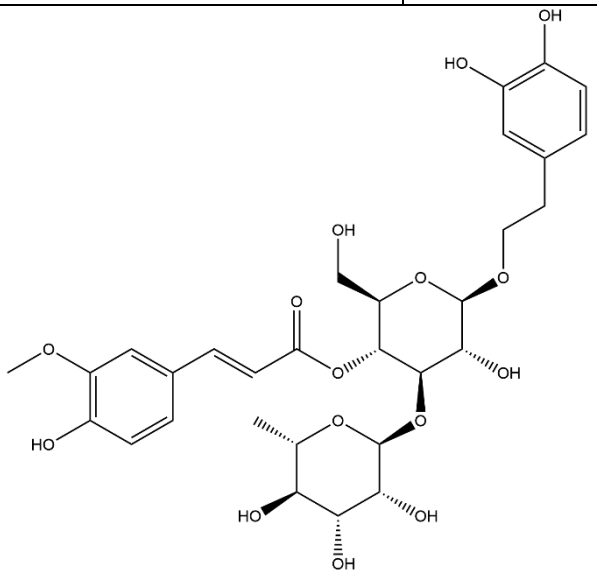


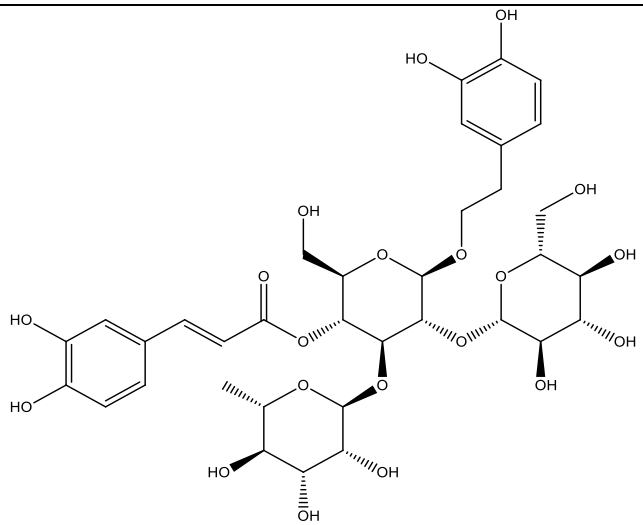
Code	Compound	Reference	Molecular Weight (Da)
PG_202	Integrifoliosides B	(compound 45) – (28)	784.758



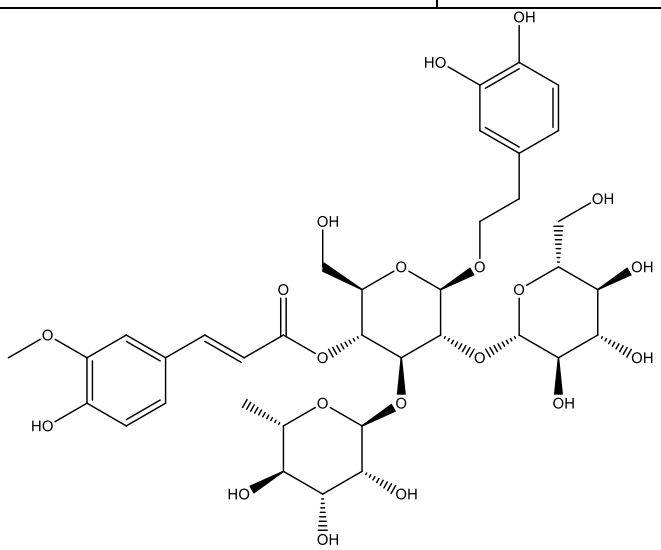
Code	Compound	Reference	Molecular Weight (Da)

PG_203	Wiedemannioside B	(compound 47) – (28)	778.798
			
Code	Compound	Reference	Molecular Weight (Da)
PG_204	Wiedemannioside C	(compound 48) – (28)	800.757
			
Code	Compound	Reference	Molecular Weight (Da)
PG_205	Wiedemannioside D	(compound 49) – (28)	826.795
			

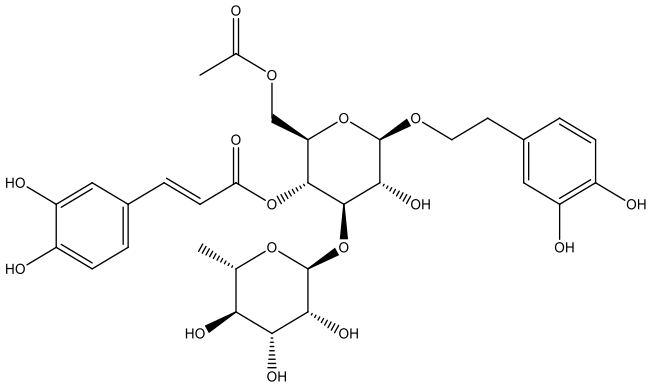
Code	Compound	Reference	Molecular Weight (Da)
PG_206	Wiedemannioside E	(compound 50) – (28)	856.821
			
Code	Compound	Reference	Molecular Weight (Da)
PG_207	Verpectoside A	(compound 51) – (28)	638.617
			
Code	Compound	Reference	Molecular Weight (Da)
PG_208	Verpectoside B	(compound 52) – (28)	786.73



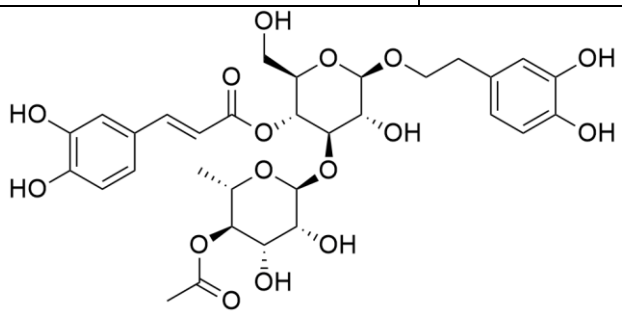
Code	Compound	Reference	Molecular Weight (Da)
PG_209	Verpectoside C	(compound 53) – (28)	800.757



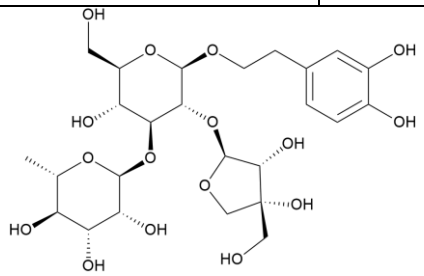
Code	Compound	Reference	Molecular Weight (Da)
PG_210	6"-O-Acetylverbascoside	(compound 54) – (28)	668.643



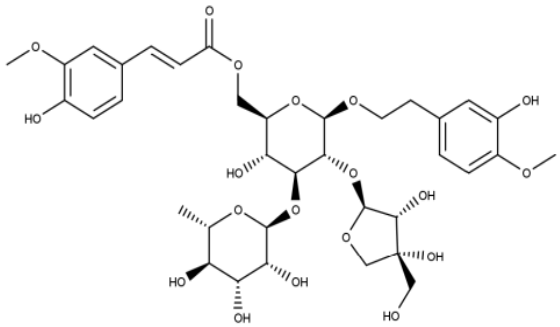
Code	Compound	Reference	Molecular Weight (Da)
PG_211	4'''-O-Acetylverbascoside	(compound 55) – (28)	666.627



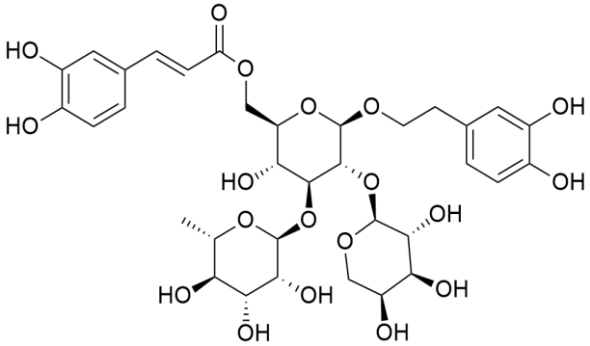
Code	Compound	Reference	Molecular Weight (Da)
PG_212	Markhamioside A	(compound 56) – (28)	594.561



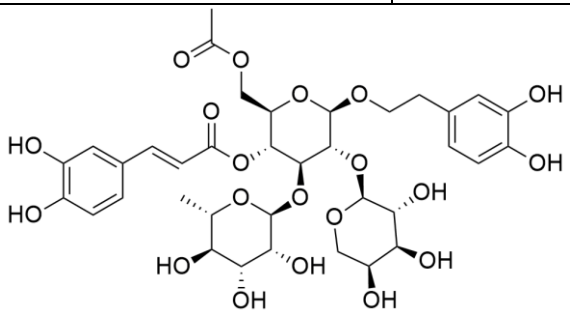
Code	Compound	Reference	Molecular Weight (Da)
PG_213	Markhamioside B	(compound 57) – (28)	784.758



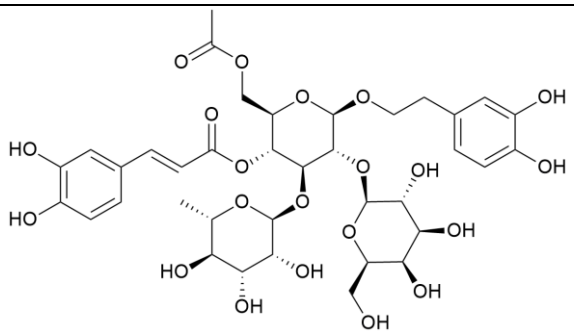
Code	Compound	Reference	Molecular Weight (Da)
PG_214	Markhamioside C	(compound 58) – (28)	756.704



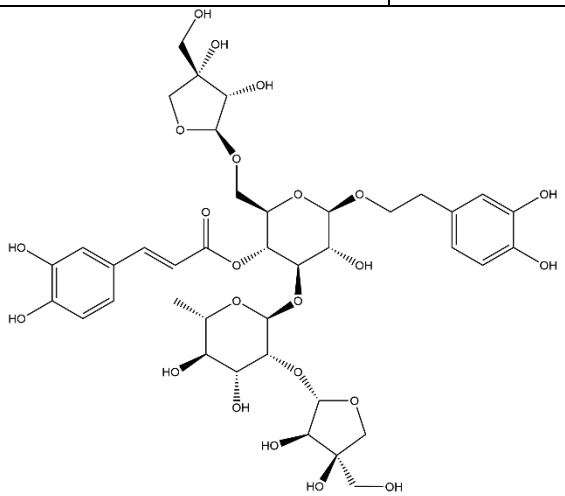
Code	Compound	Reference	Molecular Weight (Da)
PG_215	Markhamioside D	(compound 59) – (28)	798.741



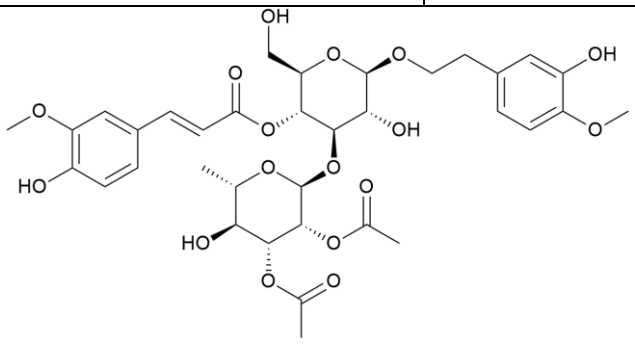
Code	Compound	Reference	Molecular Weight (Da)
PG_216	Markhamioside E	(compound 60) – (28)	828.767



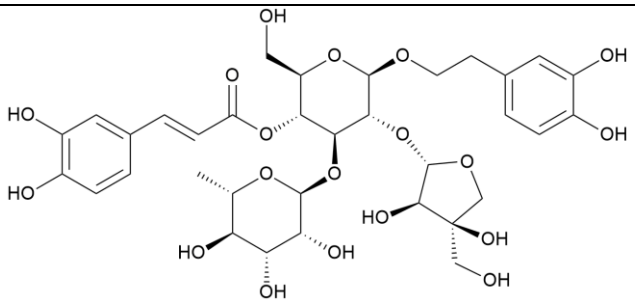
Code	Compound	Reference	Molecular Weight (Da)
PG_217	Marruboside	(compound 61) – (28)	888.819



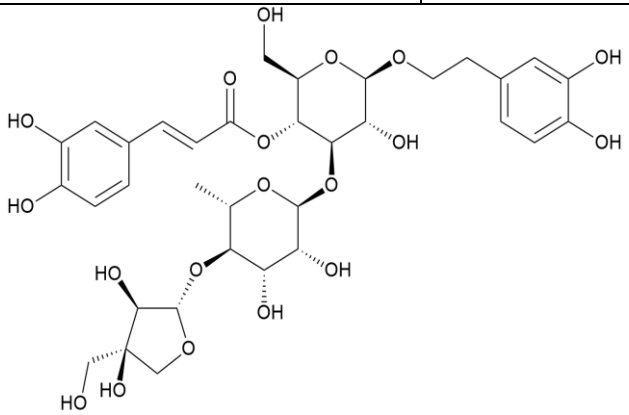
Code	Compound	Reference	Molecular Weight (Da)
PG_218	2",3"-Di-O-acetyl martynoside	(compound 62) – (28)	736.717



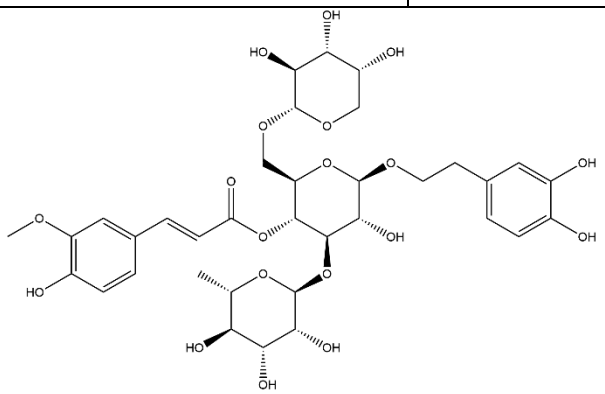
Code	Compound	Reference	Molecular Weight (Da)
PG_219	2"-O-β-Apiosylverbascoside	(compound 63) – (28)	758.72



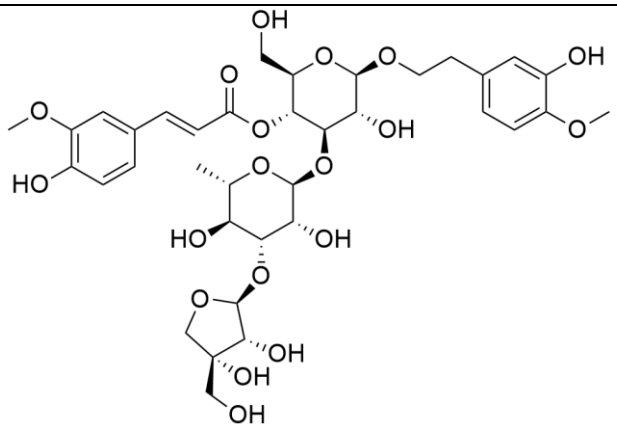
Code	Compound	Reference	Molecular Weight (Da)
PG_220	Samioside	(compound 64) – (28)	756.704



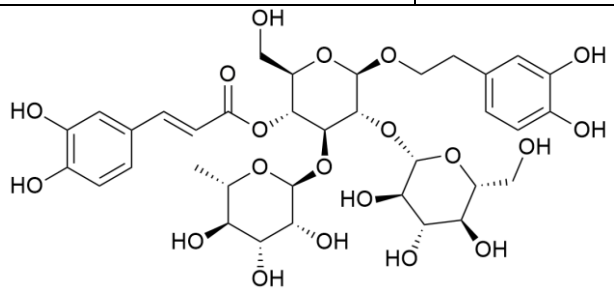
Code	Compound	Reference	Molecular Weight (Da)
PG_221	Angoroside D	(compound 65) – (28)	770.731



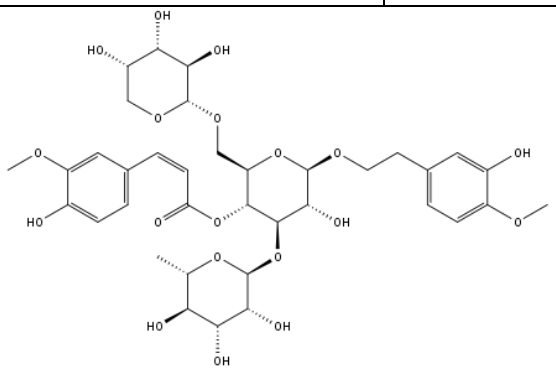
Code	Compound	Reference	Molecular Weight (Da)
PG_222	Serratumoside A	(compound 66) – (28)	784.758



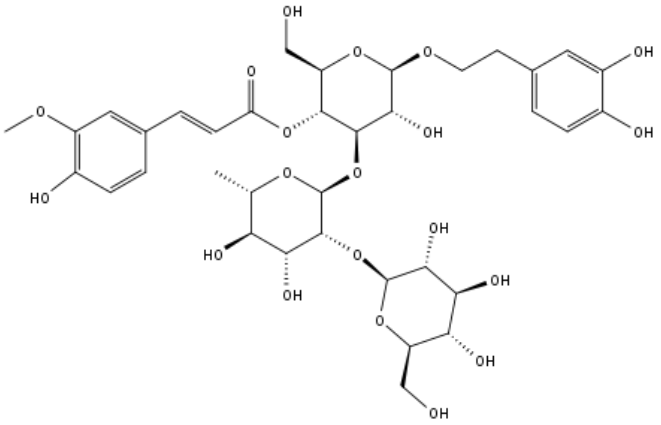
Code	Compound	Reference	Molecular Weight (Da)
PG_223	Crassoside	(compound 67) – (28)	788.746



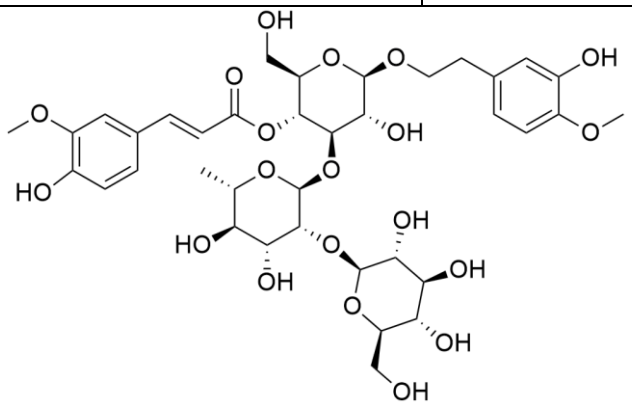
Code	Compound	Reference	Molecular Weight (Da)
PG_224	Isoangoroside C	(compound 68) – (28)	784.758



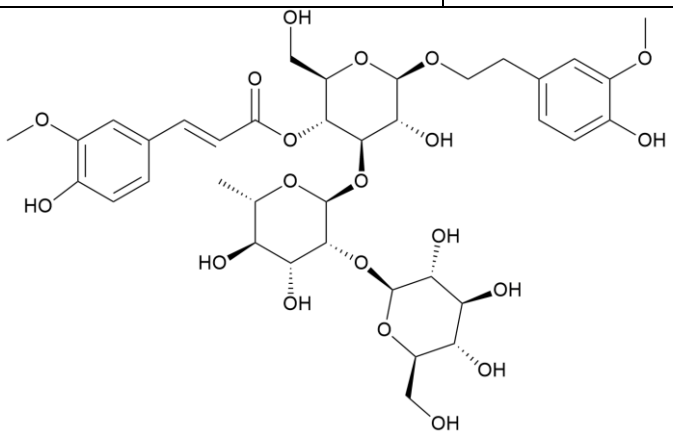
Code	Compound	Reference	Molecular Weight (Da)
PG_225	Incanoside C	(compound 69) – (28)	800.757



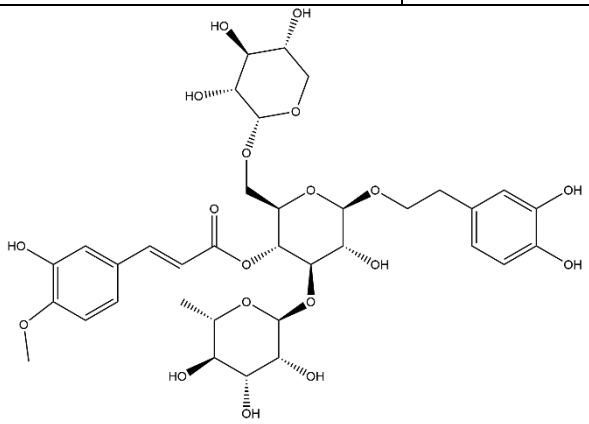
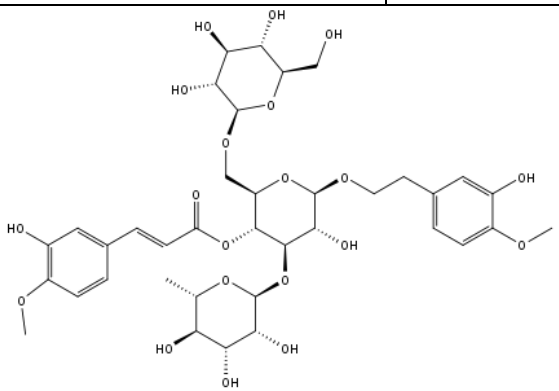
Code	Compound	Reference	Molecular Weight (Da)
PG_226	Incanoside D	(compound 70) – (28)	814.784

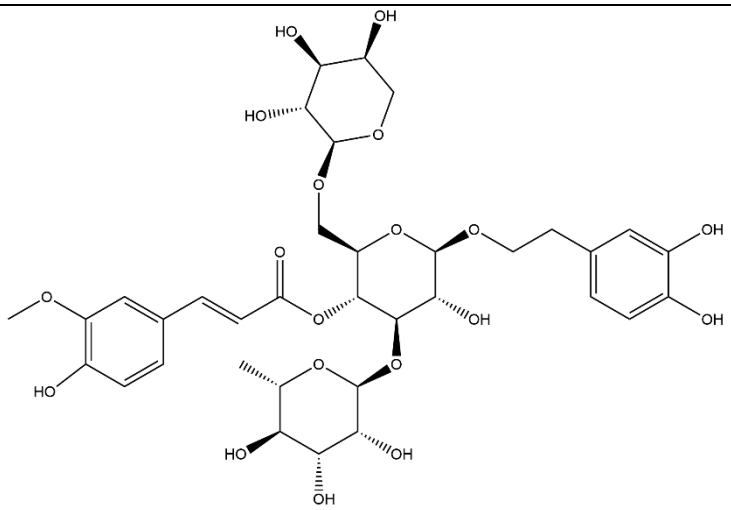


Code	Compound	Reference	Molecular Weight (Da)
PG_227	Incanoside E	(compound 71) – (28)	814.784

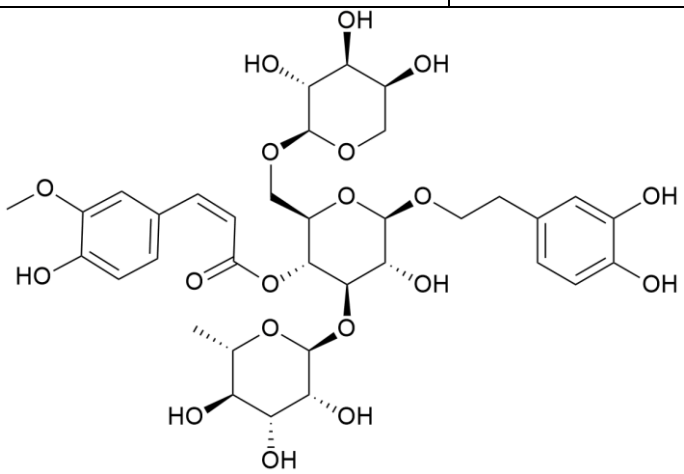


Code	Compound	Reference	Molecular Weight (Da)

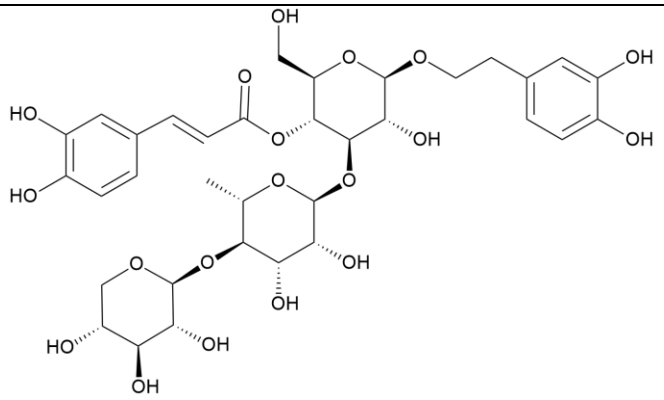
PG_228	β-(3,4-dihydroxyphenyl)-ethyl-O-α- L-rhamnopyranosyl(1-->3)-β-D-[β- D-xylopyranosyl(1-->6)]-(4-O-iso- ferulyl)glucopyranoside	(compound 72) – (28)	770.731
			
Code	Compound	Reference	Molecular Weight (Da)
PG_229	β-(3-hydroxy-4-methoxyphenyl)-ethyl- O-α-L-rhamnopyranosyl(1-->3)- β-D-[β- D-glucopyranosyl(1-->6)]- (4-O-isoferulyl) glucopyranoside	(compound 73) – (28)	814.784
			
Code	Compound	Reference	Molecular Weight (Da)
PG_230	Scrophuloside B1	(compound 75) – (28)	770.731



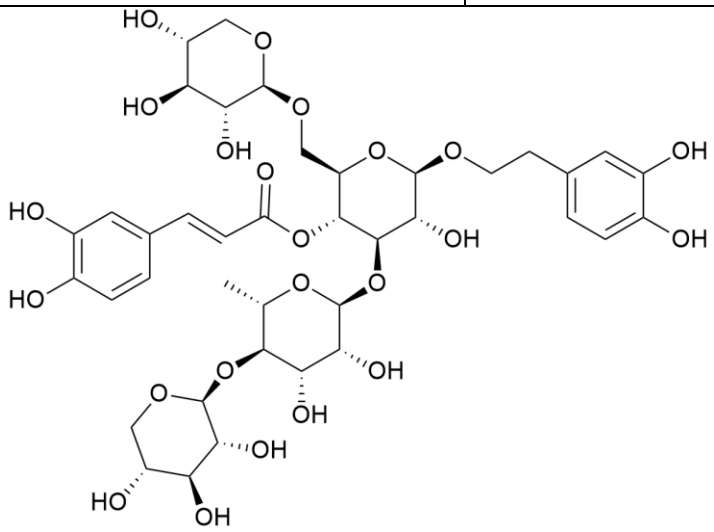
Code	Compound	Reference	Molecular Weight (Da)
PG_231	Scrophuloside B2	(compound 76) – (28)	770.731



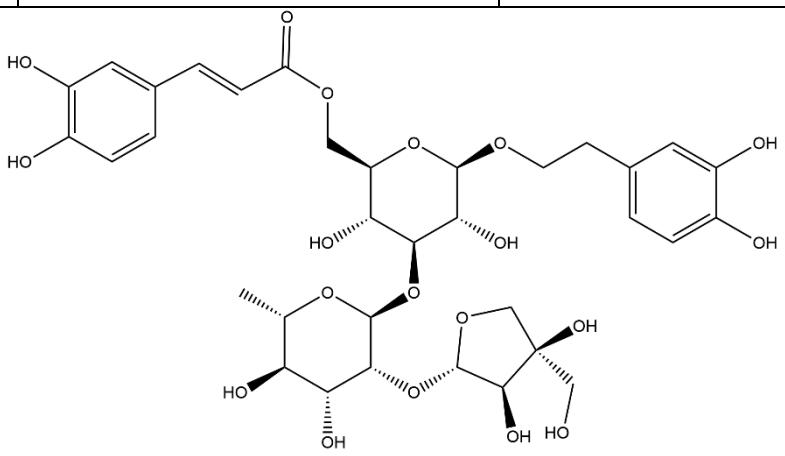
Code	Compound	Reference	Molecular Weight (Da)
PG_232	Trichosanthoside A	(compound 77) – (28)	756.704

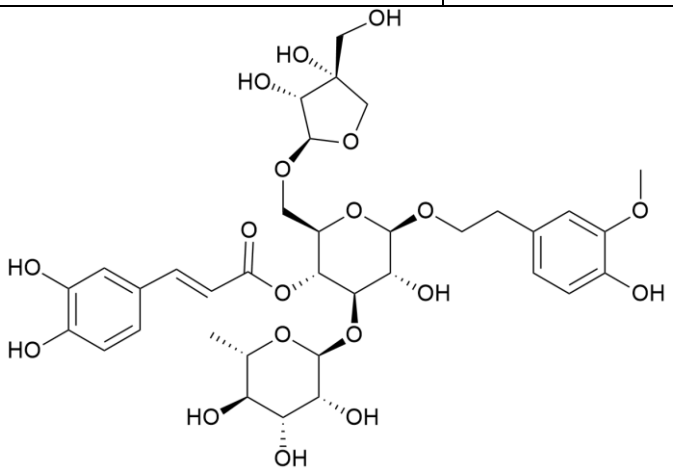
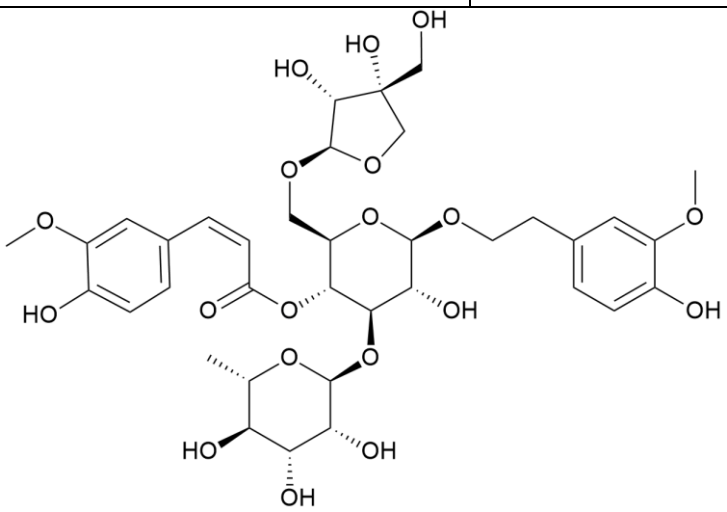


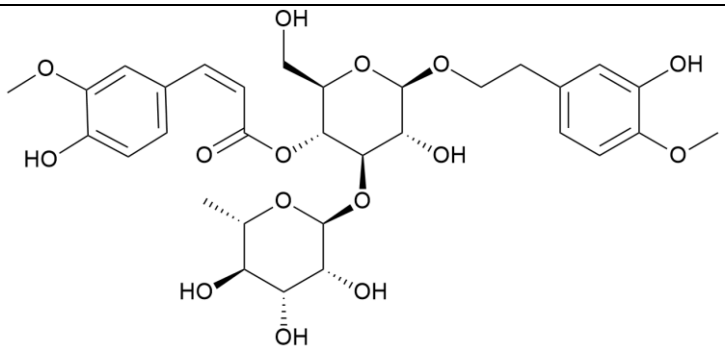
Code	Compound	Reference	Molecular Weight (Da)
PG_233	Trichosanthoside B	(compound 78) – (28)	888.819



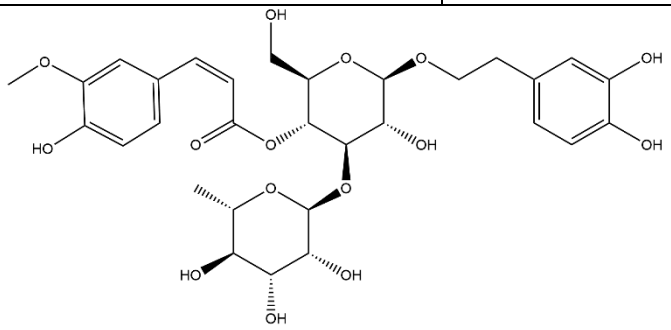
Code	Compound	Reference	Molecular Weight (Da)
PG_234	Isobetonyoside F	(compound 79) – (28)	756.704



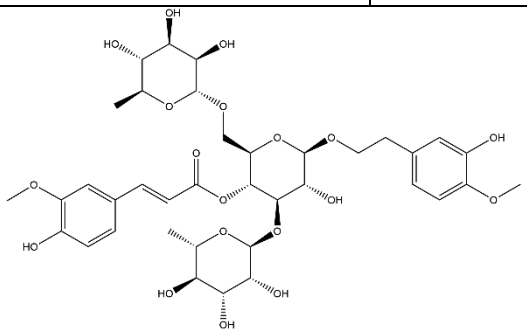
Code	Compound	Reference	Molecular Weight (Da)
PG_235	6'-β-D-Apiofuranosyl cistanoside C	(compound 80) – (28)	770.731
			
Code	Compound	Reference	Molecular Weight (Da)
PG_236	Cis-lamiophlomiside A	(compound 81) – (28)	784.758
			
Code	Compound	Reference	Molecular Weight (Da)
PG_237	Cis-martynoside	(compound 82) – (28)	652.644



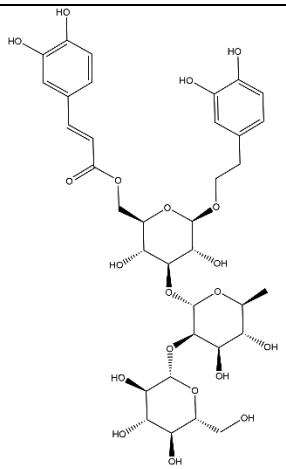
Code	Compound	Reference	Molecular Weight (Da)
PG_238	Cis-leucosceptoside A	(compound 83) – (28)	638.617



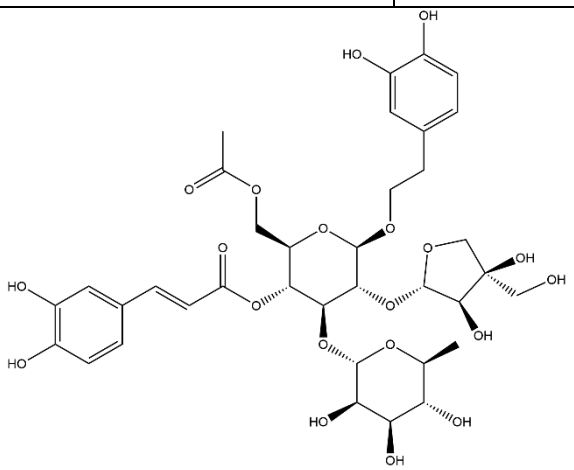
Code	Compound	Reference	Molecular Weight (Da)
PG_239	Ferruginoside C	(compound 84) – (28)	798.785



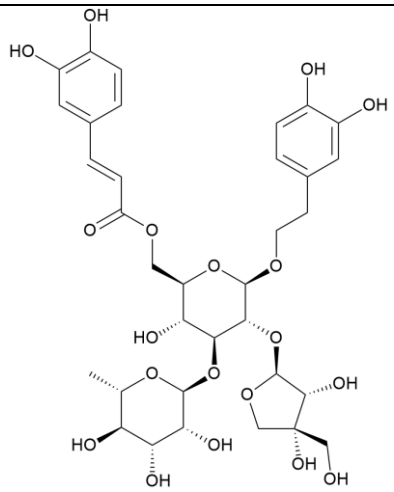
Code	Compound	Reference	Molecular Weight (Da)
PG_240	Incanoside	(compound 85) – (28)	786.73



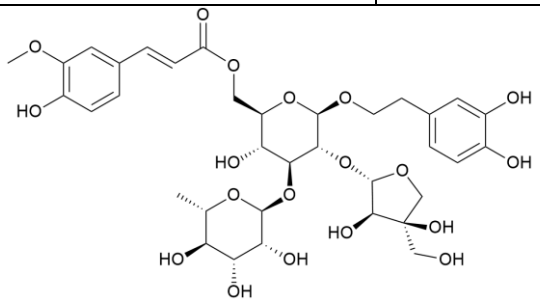
Code	Compound	Reference	Molecular Weight (Da)
PG_241	Luteoside A	(compound 86) – (28)	798.741



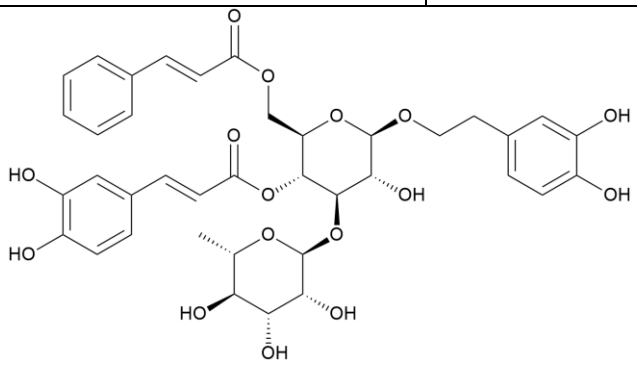
Code	Compound	Reference	Molecular Weight (Da)
PG_242	Luteoside B	(compound 87) – (28)	756.704



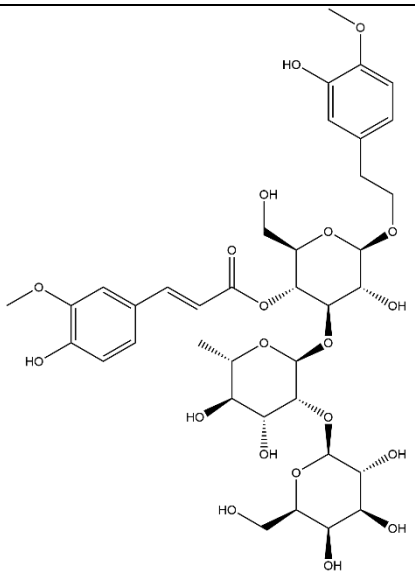
Code	Compound	Reference	Molecular Weight (Da)
PG_243	Luteoside C	(compound 88) – (28)	770.731



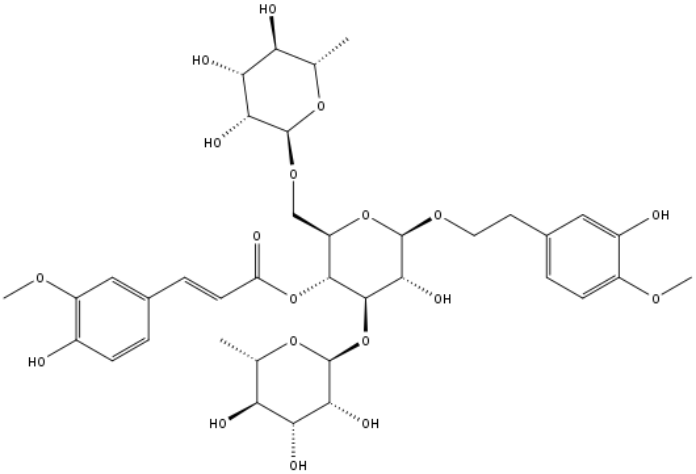
Code	Compound	Reference	Molecular Weight (Da)
PG_244	6'-O-(E)-Cinnamoylverbascoside	(compound 89) – (28)	754.735



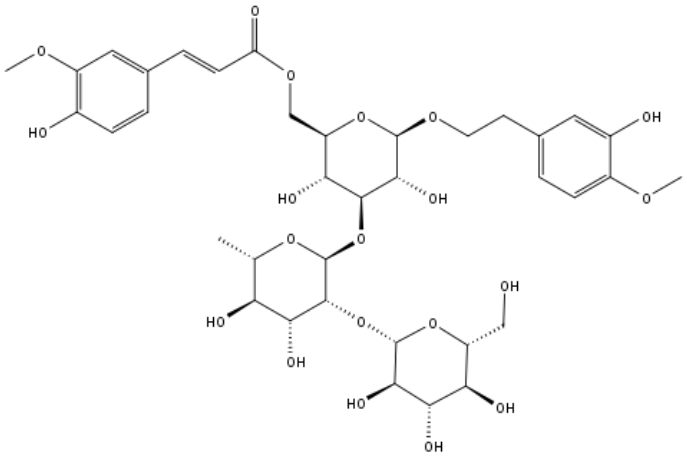
Code	Compound	Reference	Molecular Weight (Da)
PG_245	Galactosylmartynoside	(compound 90) – (28)	814.784



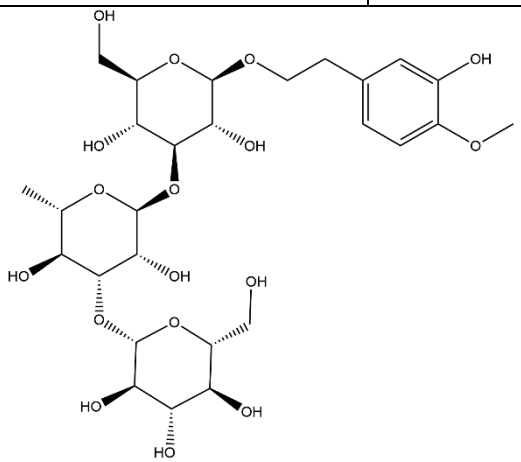
Code	Compound	Reference	Molecular Weight (Da)
PG_246	2-(3-Hydroxy-4-methoxyphenyl)-ethyl-O-(α-L-rhamnosyl)-(1--> 3)-O-(α-L-rhamnosyl)-(1-->6)-4-O-E- feruloyl-β-D-glucopyranoside	(compound 91) – (28)	798.785



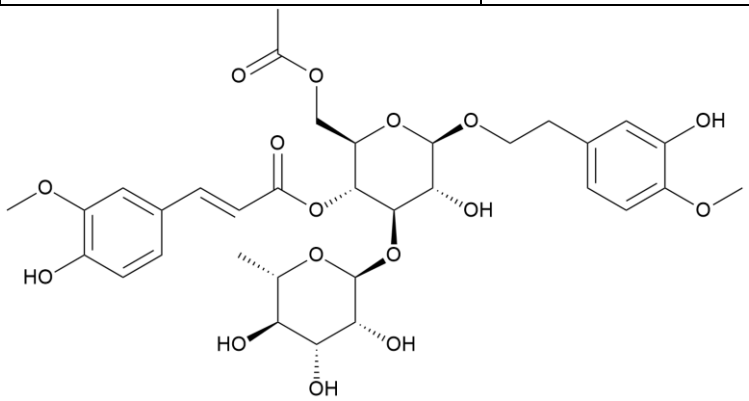
Code	Compound	Reference	Molecular Weight (Da)
PG_247	Incanoside A	(compound 92) – (28)	814.784



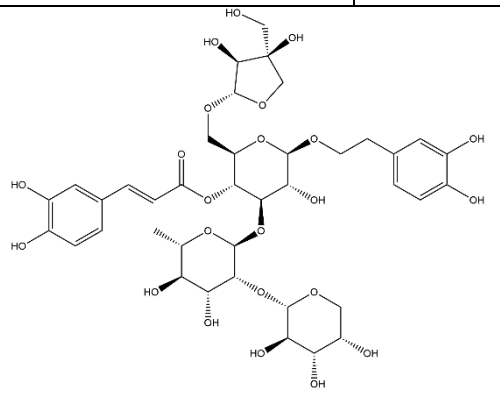
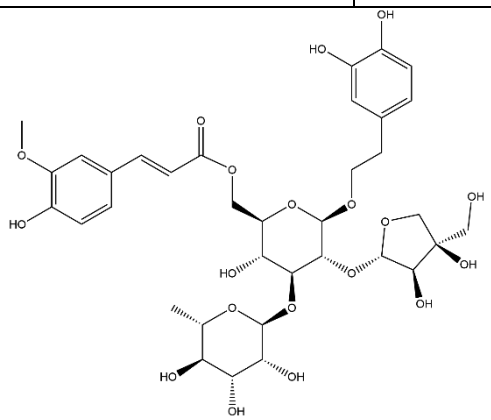
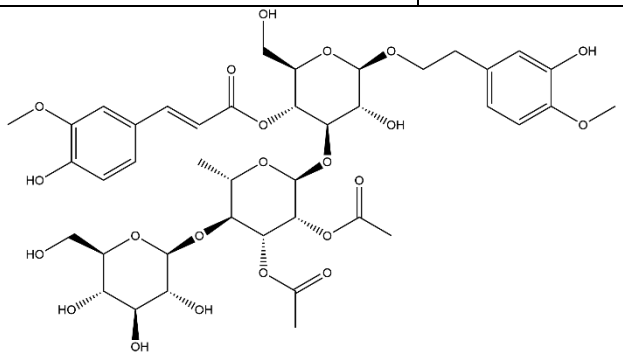
Code	Compound	Reference	Molecular Weight (Da)
PG_248	Incanoside B	(compound 93) – (28)	638.613

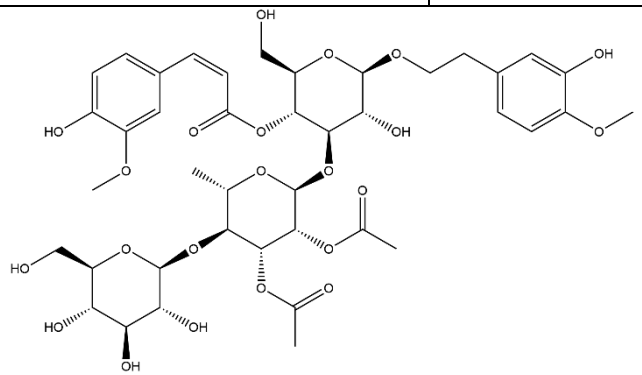
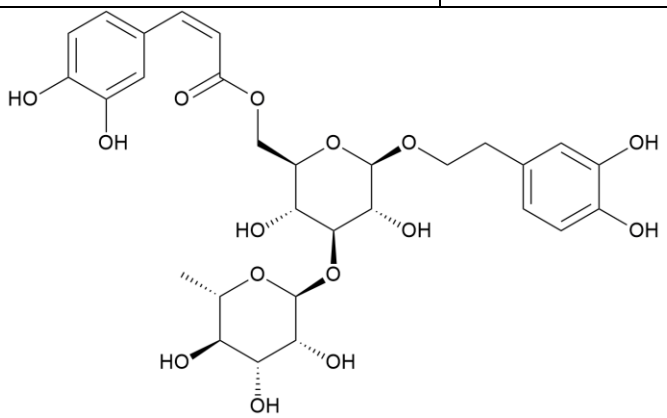
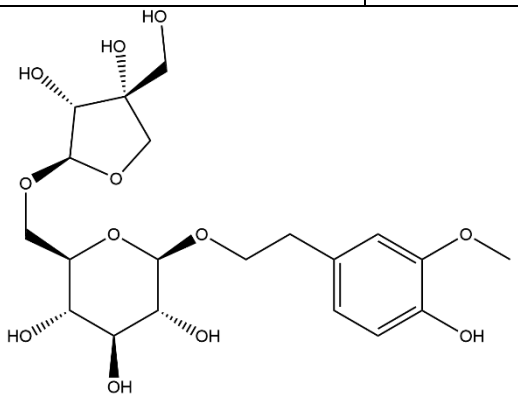


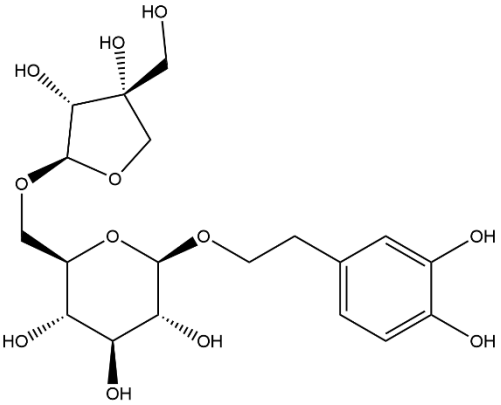
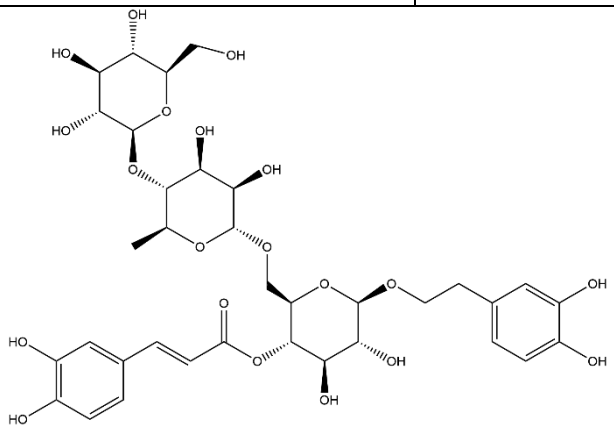
Code	Compound	Reference	Molecular Weight (Da)
PG_249	6'-O-Acetyl-martynoside	(compound 94) – (28)	694.68

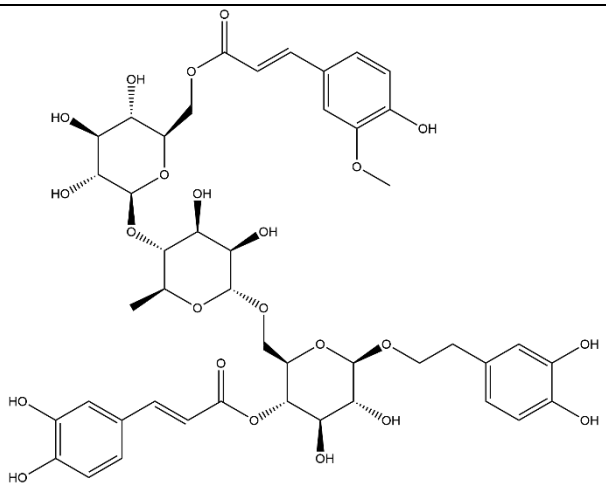


Code	Compound	Reference	Molecular

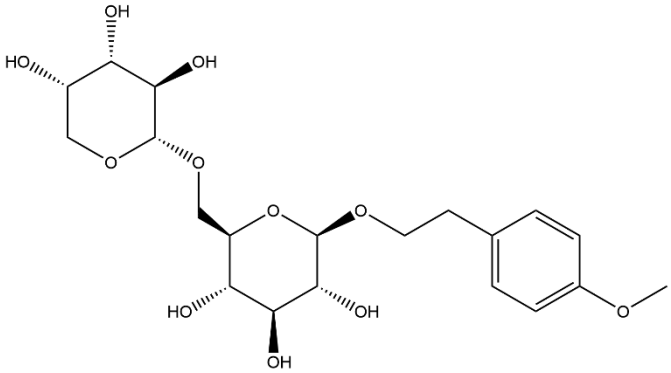
			Weight (Da)
PG_250	Ballotetroside	(compound 95) – (28)	890.835
			
Code	Compound	Reference	Molecular Weight (Da)
PG_251	Newbouldioside	(compound 96) – (28)	772.747
			
Code	Compound	Reference	Molecular Weight (Da)
PG_252	Premnethanosides A (trans)	(compound 97) – (28)	898.858
			
Code	Compound	Reference	Molecular

			Weight (Da)
PG_253	Premnethanosides A (cis)	(compound 98) – (28)	900.874
			
Code	Compound	Reference	Molecular Weight (Da)
PG_254	cis-isoverbascoside	(compound 99) – (28)	624.59
			
Code	Compound	Reference	Molecular Weight (Da)
PG_255	2-(4-Hydroxy-3-methoxyphenyl) ethanol 1-*O*-[*β*-D-apiofuranosyl-(1→6)-*β*-D- glucopyranoside]	(compound 100) – (28)	462.446
			

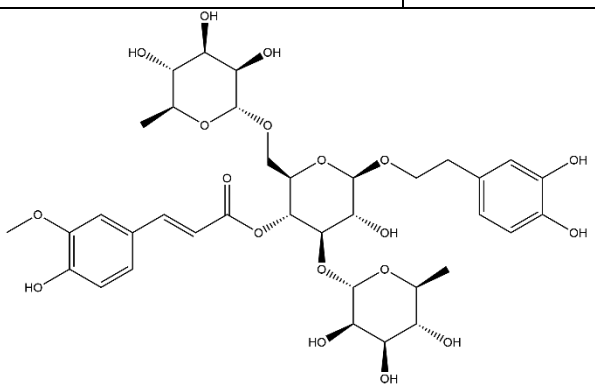
Code	Compound	Reference	Molecular Weight (Da)
PG_256	2-(3,4-Dihydroxyphenyl) ethanol 1-*O*-[*β*-D-apiofuranosyl-(1→6)-*β*-D-glucopyranoside]	(compound 101) – (28)	448.419
			
Code	Compound	Reference	Molecular Weight (Da)
PG_257	Turrilliosides A	(compound 102) – (28)	786.73
			
Code	Compound	Reference	Molecular Weight (Da)
PG_258	Turrilliosides B	(compound 103) – (28)	962.901



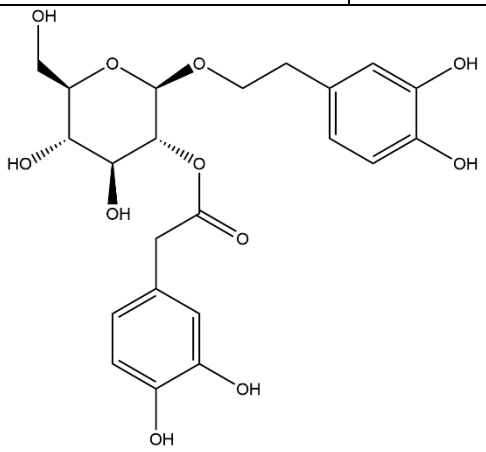
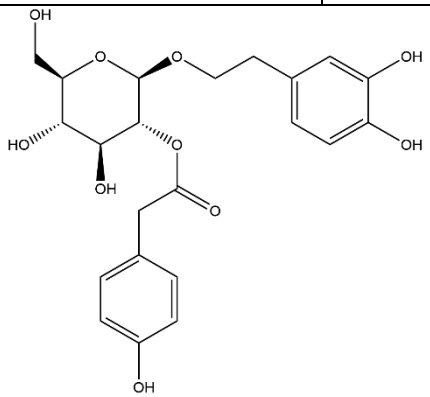
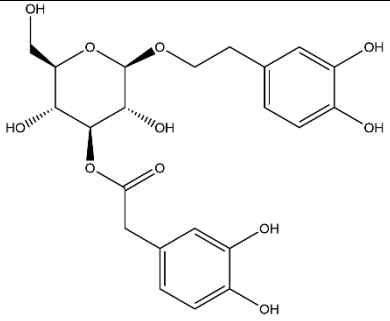
Code	Compound	Reference	Molecular Weight (Da)
PG_259	Mongrhoside	(compound 104) – (28)	446.447

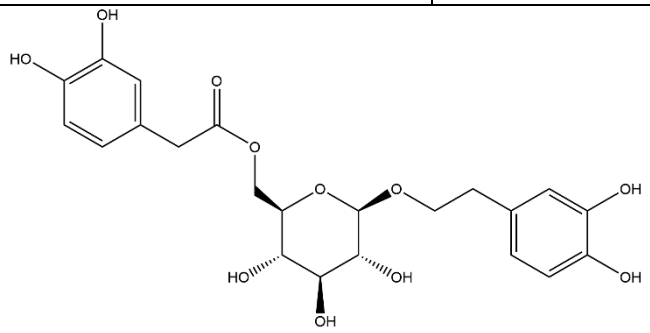
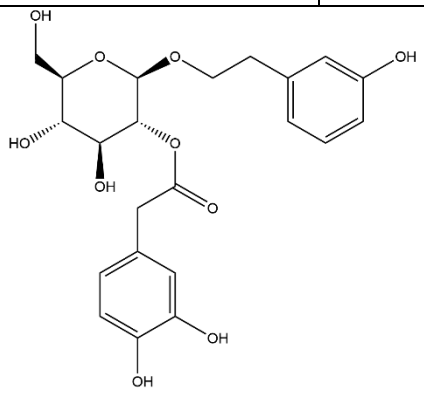
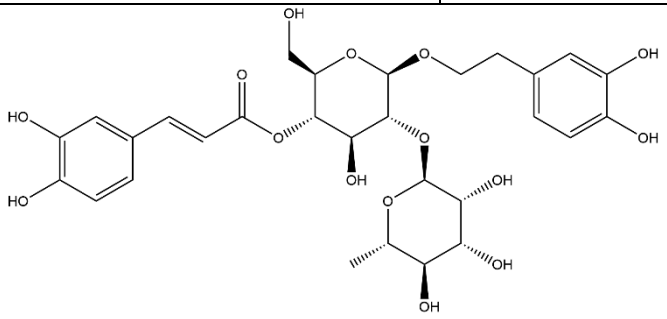


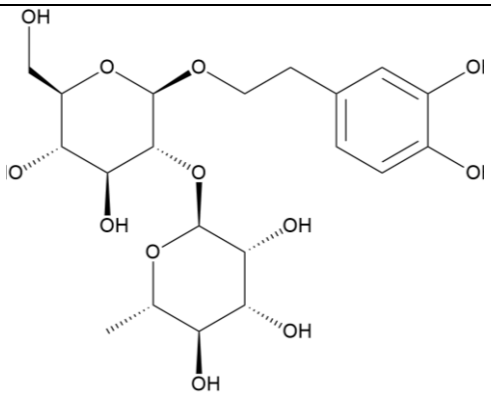
Code	Compound	Reference	Molecular Weight (Da)
PG_260	3-*O*-Methylpoliumoside	(compound 105) – (28)	784.758



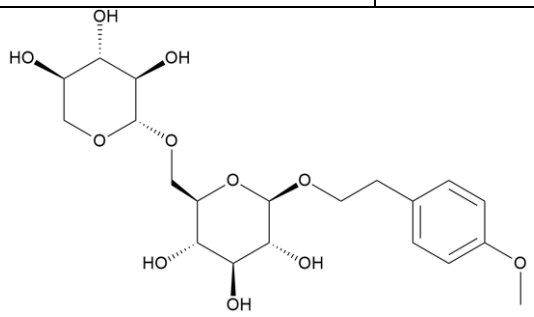
Code	Compound	Reference	Molecular Weight (Da)

PG_261	Ternstrosides A	(compound 106) – (28)	466.437
			
Code	Compound	Reference	Molecular Weight (Da)
PG_262	Ternstrosides B	(compound 107) – (28)	450.43
			
Code	Compound	Reference	Molecular Weight (Da)
PG_263	Ternstrosides C	(compound 108) – (28)	466.437
			
Code	Compound	Reference	Molecular Weight (Da)

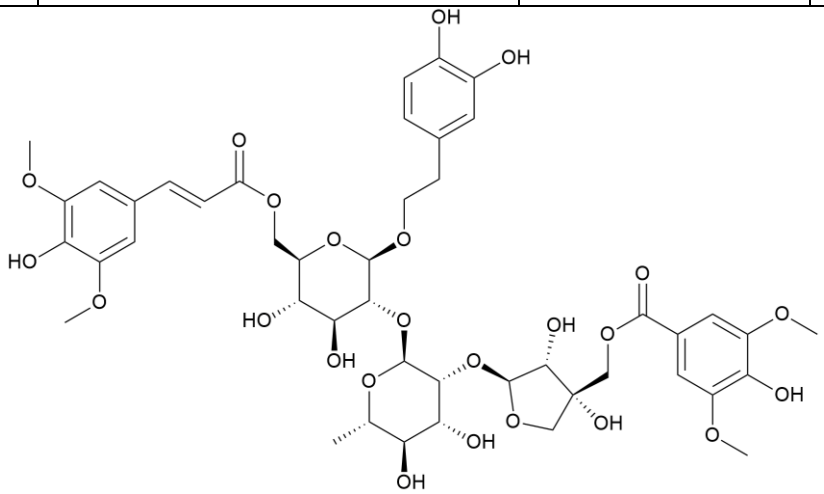
PG_264	Ternstrosides D	(compound 109) – (28)	466.437
			
Code	Compound	Reference	Molecular Weight (Da)
PG_265	Ternstrosides E	(compound 110) – (28)	450.438
			
Code	Compound	Reference	Molecular Weight (Da)
PG_266	Parviflorosides A	(compound 111) – (28)	624.59
			
Code	Compound	Reference	Molecular Weight (Da)
PG_267	Parviflorosides B	(compound 112) – (28)	462.446



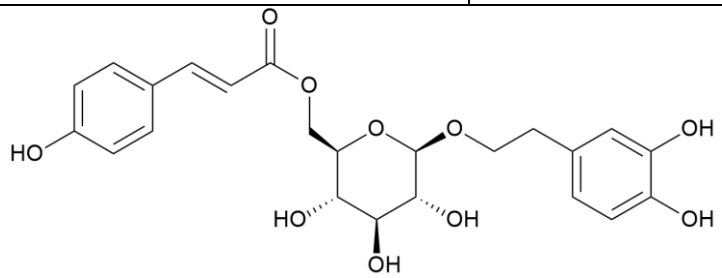
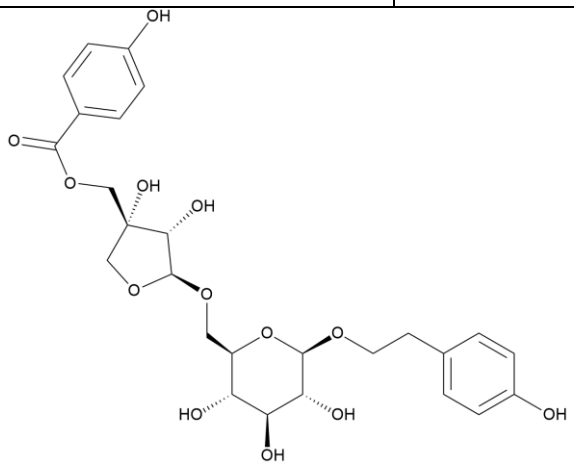
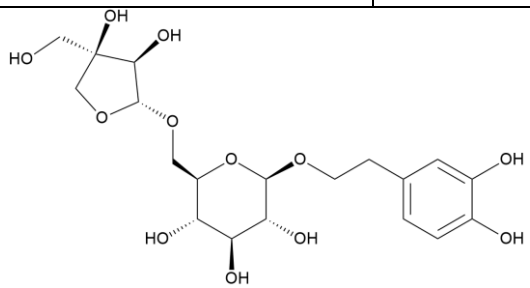
Code	Compound	Reference	Molecular Weight (Da)
PG_268	Heterodontoside	(compound 113) – (28)	446.447

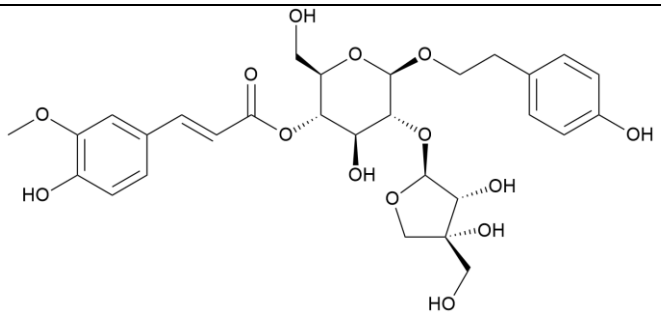


Code	Compound	Reference	Molecular Weight (Da)
PG_269	Newbouldioside C	(compound 114) – (28)	982.932

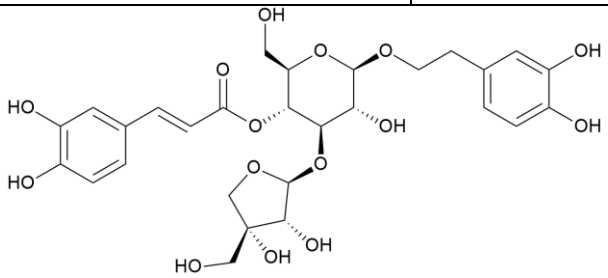


Code	Compound	Reference	Molecular Weight (Da)
PG_270	6'-O-Coumaroyl-1'-O-[2-(3,4-dihydroxy phenyl)ethyl]-β-D-	(compound 115) –	462.449

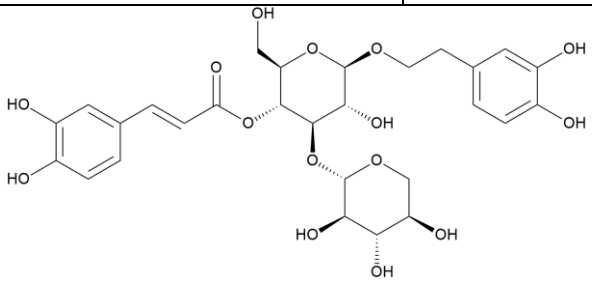
	glucopyranoside	(28)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_271	2-(4-Hydroxyphenyl)ethyl-O-β-D-[5-O-(4- hydroxybenzoyl)]-apiofuranosyl-(1-6)-β-D-glucopyranoside	(compound 116) – (28)	552.527
			
Code	Compound	Reference	Molecular Weight (Da)
PG_273	Cuneatasides C	(compound 118) – (28)	448.419
			
Code	Compound	Reference	Molecular Weight (Da)
PG_274	Clerodendronoside	(compound 119) – (28)	608.591



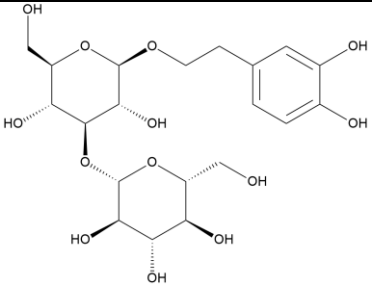
Code	Compound	Reference	Molecular Weight (Da)
PG_275	Cusianoside A	(compound 120) – (28)	610.563

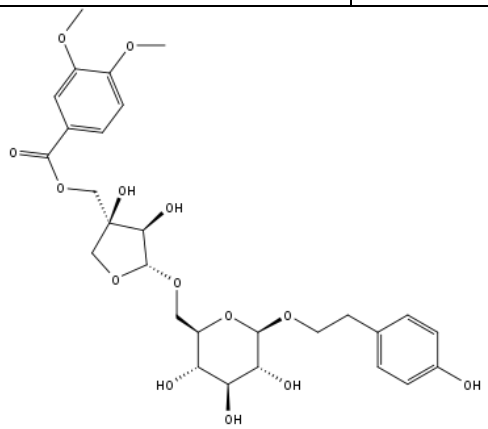
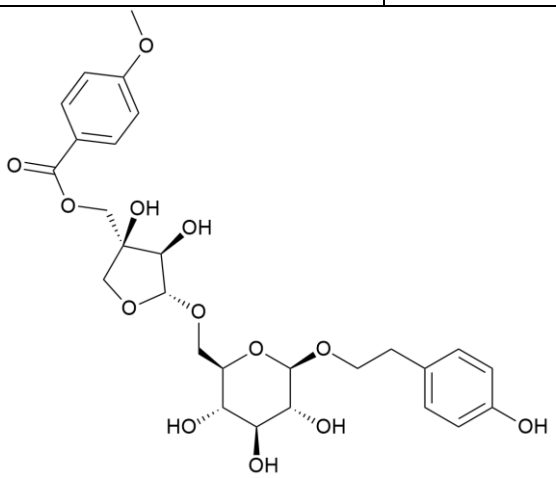


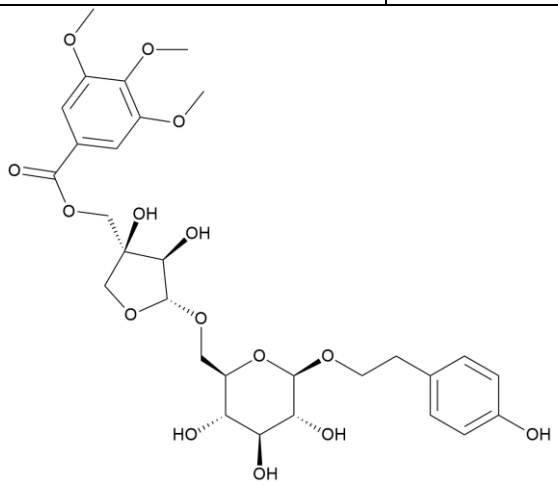
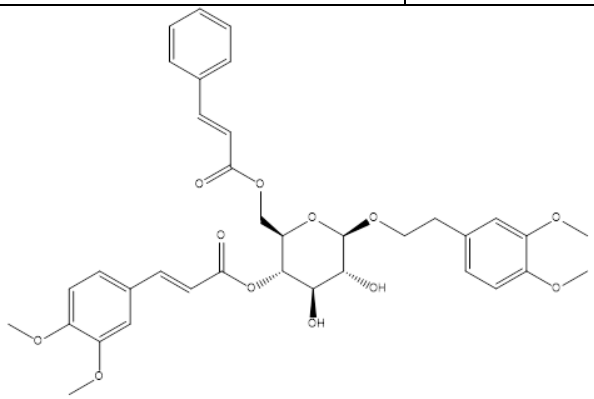
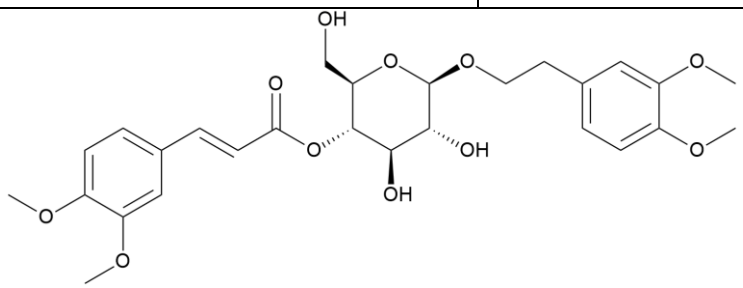
Code	Compound	Reference	Molecular Weight (Da)
PG_276	Cusianoside B	(compound 121) – (28)	610.563

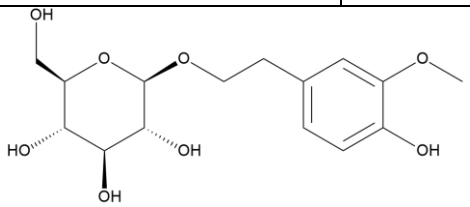
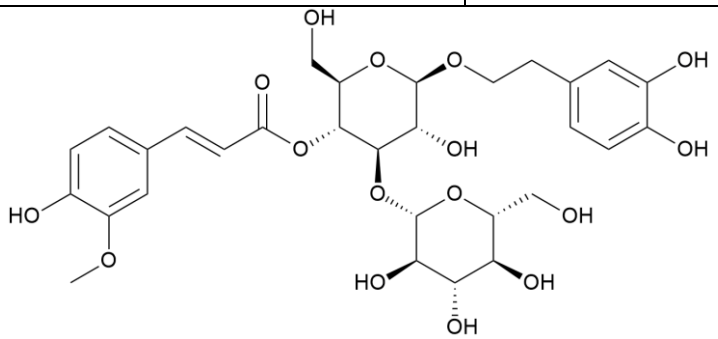
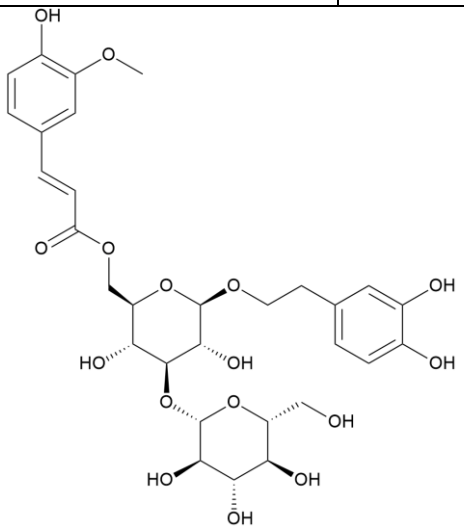


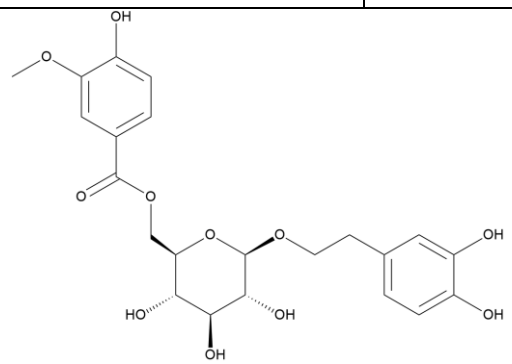
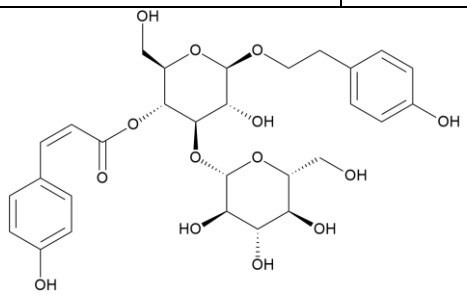
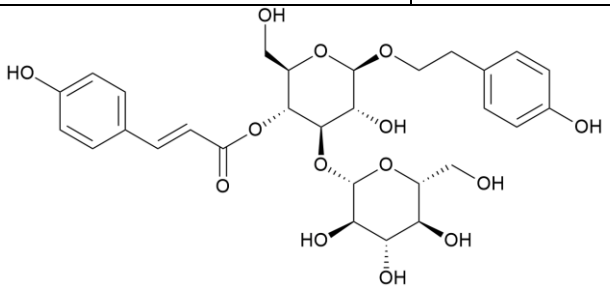
Code	Compound	Reference	Molecular Weight (Da)
PG_277	Scroside D	(compound 122) – (28)	478.445

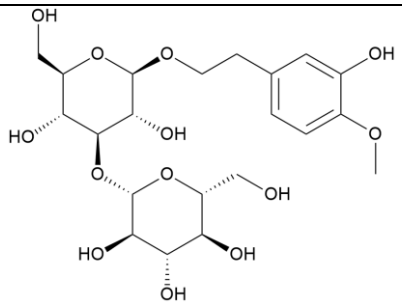


Code	Compound	Reference	Molecular Weight (Da)
PG_278	2-(4-Hydroxyphenyl)ethyl1- O- β -D-[5- O-(3,4-dimethoxybenzoyl)]-apiofuranosyl- (1□6)-β-D-glucopyranoside	(compound 123) – (28)	596.58
			
Code	Compound	Reference	Molecular Weight (Da)
PG_279	2-(4-Hydroxyphenyl)ethyl1- O- β -D-[5-O-(4- methoxybenzoyl)]-apiofuranosyl-(1□6)-β-D-glucopyranoside	(compound 124) – (28)	566.554
			
Code	Compound	Reference	Molecular Weight (Da)
PG_280	2-(4-Hydroxyphenyl)ethyl-1- O-D-[5-O- (3,4,5-trimethoxybenzoyl)]-apiofuranosyl- (1□6)-β-D-	(compound 125) – (28)	626.606

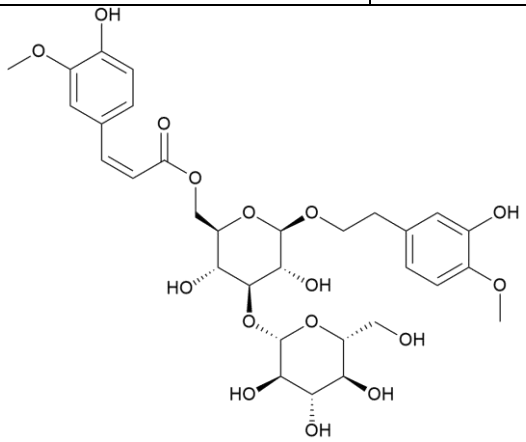
	glucopyranoside		
			
Code	Compound	Reference	Molecular Weight (Da)
PG_281	1- O-3,4-Dimethoxyphenylethyl-4- O-3,4- dimethoxy cinnamoyl-6-O- cinnamoyl-β-D-glucopyranose	(compound 126) – (28)	666.717
			
Code	Compound	Reference	Molecular Weight (Da)
PG_282	1- O-3, 4-Dimethoxyphenylethyl-4- O-3,4- dimethoxy cinnamoyl-β-D-glucopyranose	(compound 127) – (28)	534.556
			
Code	Compound	Reference	Molecular

			Weight (Da)
PG_283	2-(4-Hydroxy-3-methoxyphenyl)-ethyl-O-β-D-glucopyranoside	(compound 128) – (28)	330.332
			
Code	Compound	Reference	Molecular Weight (Da)
PG_284	Scroside D	(compound 129) – (28)	654.616
			
Code	Compound	Reference	Molecular Weight (Da)
PG_285	Scroside E	(compound 130) – (28)	654.616
			
Code	Compound	Reference	Molecular Weight (Da)

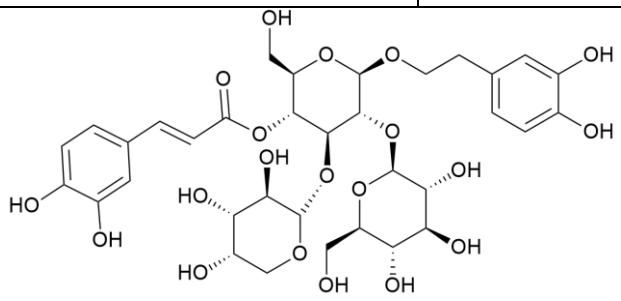
PG_286	1'- O-β-D-(3,4-Dihydroxyphenyl)-ethyl-6'- O-vanilloyl-glucopyranoside	(compound 131) – (28)	466.437
			
Code	Compound	Reference	Molecular Weight (Da)
PG_287-1	Lancetoside (cis)	(compound 132) – (28)	608.591
			
Code	Compound	Reference	Molecular Weight (Da)
PG_287-2	Lancetoside (trans)	(compound 132) – (28)	608.591
			
Code	Compound	Reference	Molecular Weight (Da)
PG_288	2-(3-Hydroxy-4-methoxyphenyl)-ethyl-O-β-D-glucopyranosyl (1-->3) β-D-glucopyranoside	(compound 133) – (28)	492.472



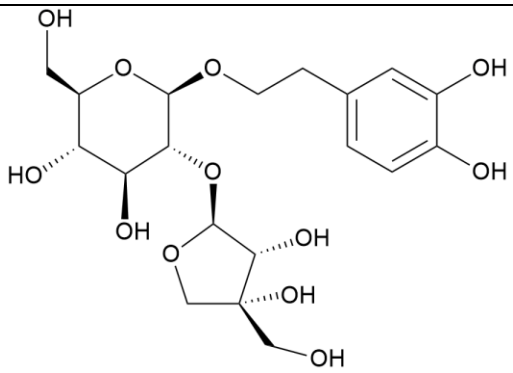
Code	Compound	Reference	Molecular Weight (Da)
PG_289	Hemiphroside C	(compound 134) – (28)	668.643



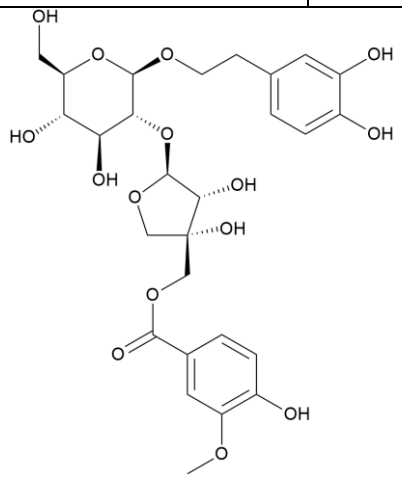
Code	Compound	Reference	Molecular Weight (Da)
PG_290	Aragoside	(compound 135) – (28)	772.703



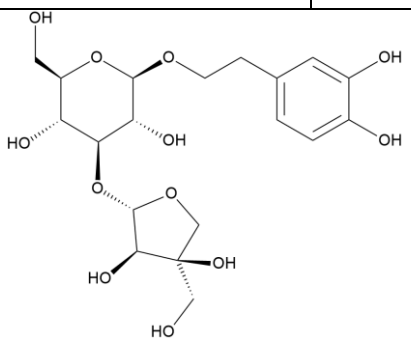
Code	Compound	Reference	Molecular Weight (Da)
PG_291	3,4-Dihydroxyphenylethanol-[8-O-β-D-apiofuranosyl(1 □2)]-β-D-glucopyranoside	(compound 136) – (28)	448.419



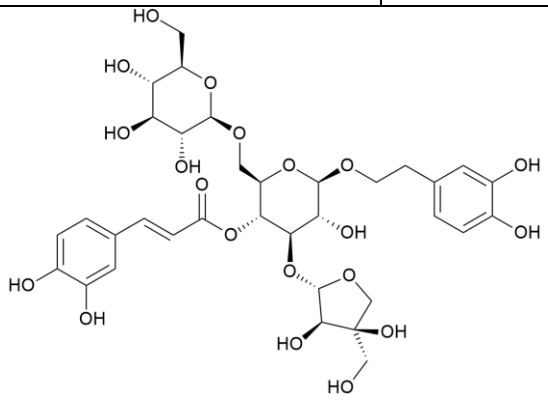
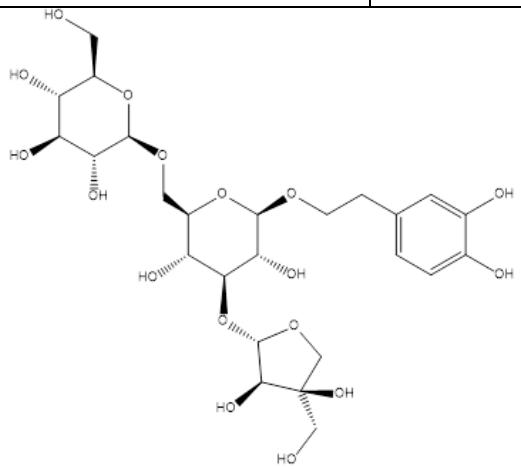
Code	Compound	Reference	Molecular Weight (Da)
PG_292	3,4-Dihydroxyphenylethanol-8-O-[(5-O-vanilloyl)-β-D-apiofuranosyl (1→2)]-β-D-glucopyranoside	(compound 137) – (28)	598.552

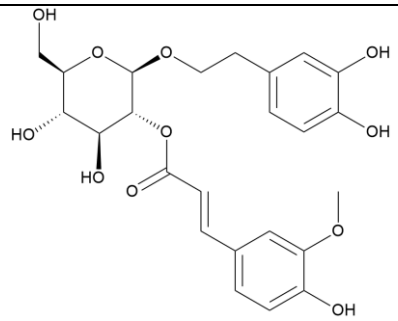
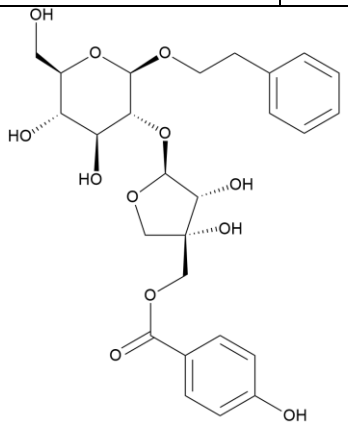
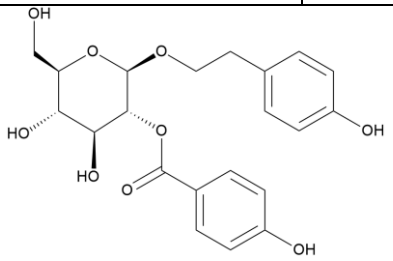


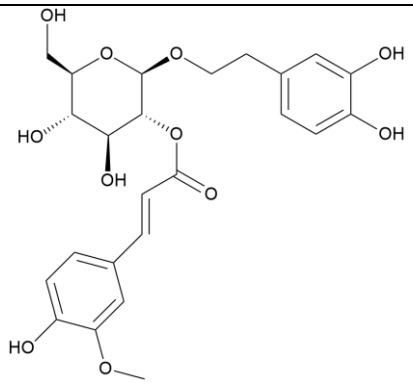
Code	Compound	Reference	Molecular Weight (Da)
PG_293	3,4-Dihydroxyphenylethanol-8- O-[β-D-apiofuranosyl(1□3)]- β-D-glucopyranoside	(compound 138) – (28)	448.419



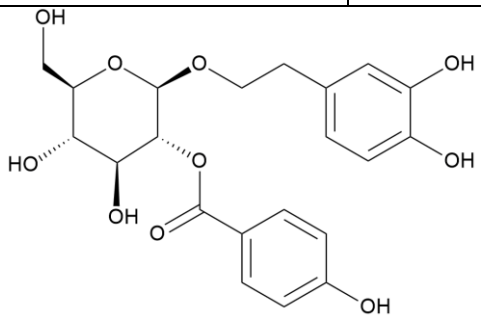
Code	Compound	Reference	Molecular

			Weight (Da)
PG_294	3,4-Dihydroxyphenylethanol-8-O-[4-O-transcaffeoyl-β-D-apiofuranosyl (1→3)-β-D-glucopyranosyl-(1→6)]-β-D-glucopyranoside	(compound 139) – (28)	774.719
			
Code	Compound	Reference	Molecular Weight (Da)
PG_295	3,4-Dihydroxyphenylethanol-8- O-[β-D-apiofuranosyl(1→3)-β-D-glucopyranosyl- (1→6)]-β-D-glucopyranoside	(compound 140) – (28)	774.719
			
Code	Compound	Reference	Molecular Weight (Da)
PG_296	Bacopaside B	(compound 141) – (28)	492.475

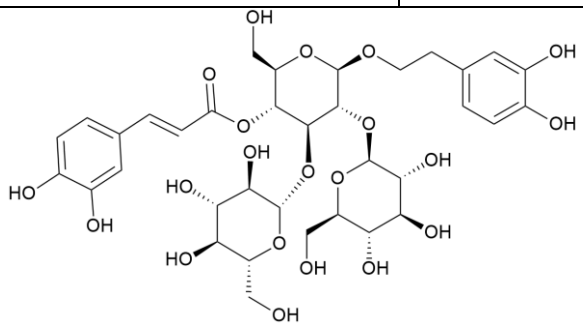
			
Code	Compound	Reference	Molecular Weight (Da)
PG_297	Bacopaside C	(compound 142) – (28)	536.528
			
Code	Compound	Reference	Molecular Weight (Da)
PG_298	Monnierasides I	(compound 143) – (28)	420.413
			
Code	Compound	Reference	Molecular Weight (Da)
PG_299	Monnierasides II	(compound 144) – (28)	492.475



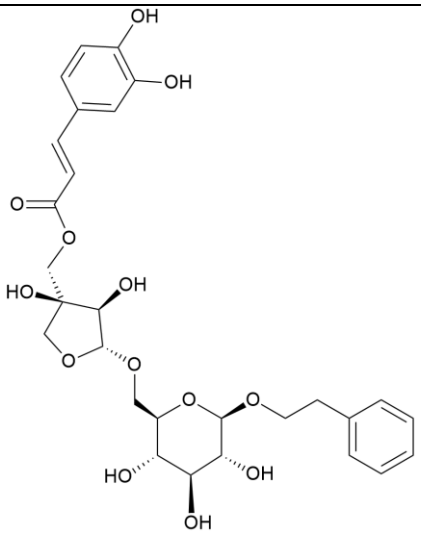
Code	Compound	Reference	Molecular Weight (Da)
PG_300	Monnierasides III	(compound 145) – (28)	436.412



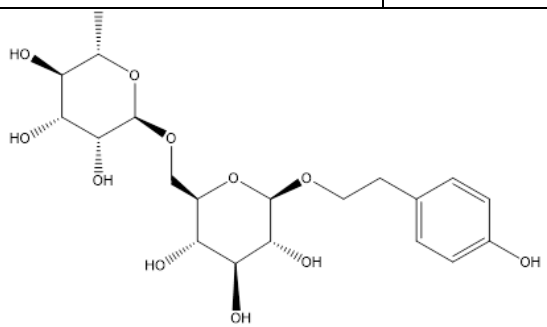
Code	Compound	Reference	Molecular Weight (Da)
PG_301	Persicoside	(compound 146) – (28)	802.729



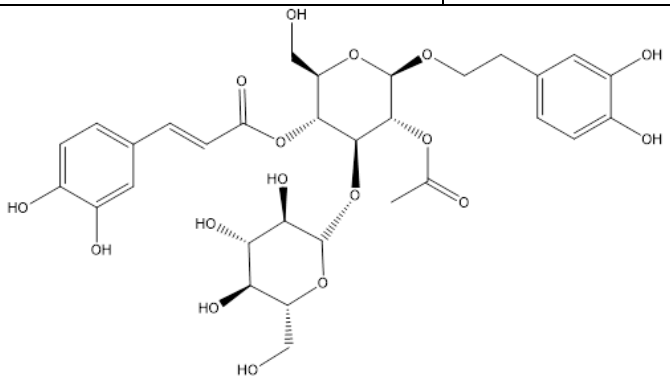
Code	Compound	Reference	Molecular Weight (Da)
PG_302	Dracunculifosides O	(compound 147) – (28)	578.565



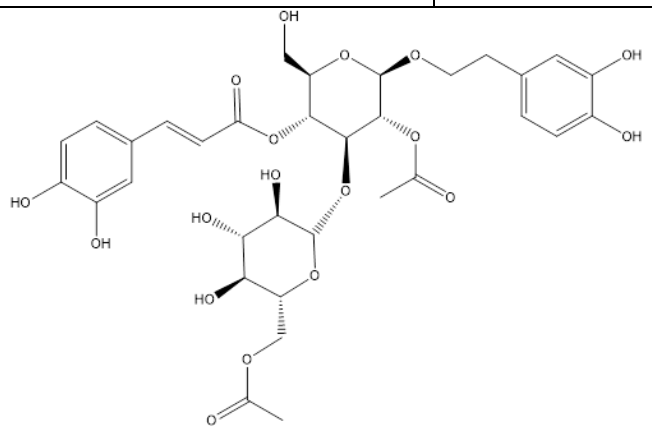
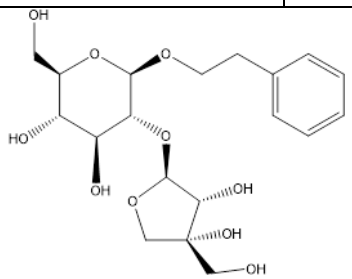
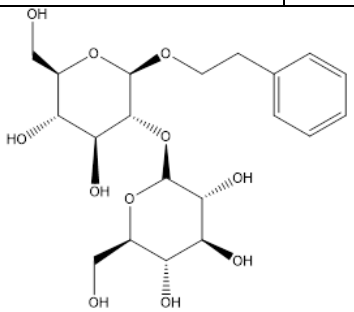
Code	Compound	Reference	Molecular Weight (Da)
PG_303	Echipuroside A	(compound 148) – (28)	446.447

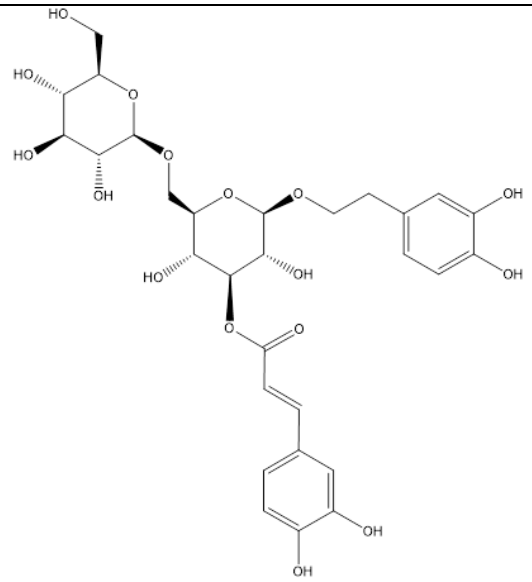


Code	Compound	Reference	Molecular Weight (Da)
PG_304	2'-O-Acetylplantamajoside	(compound 149) – (28)	682.626

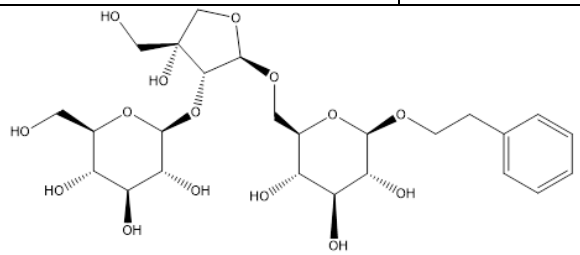


Code	Compound	Reference	Molecular Weight (Da)

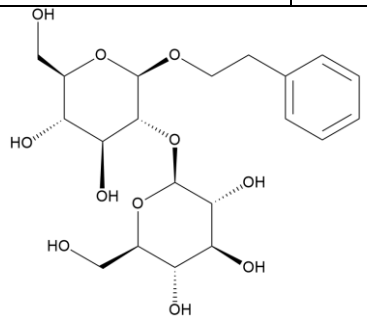
PG_305	2'- O, 6''- O-Diacetylplantamajoside	(compound 150) – (28)	724.663
			
Code	Compound	Reference	Molecular Weight (Da)
PG_306	Sayaendoside	(compound 151) – (28)	416.421
			
Code	Compound	Reference	Molecular Weight (Da)
PG_307	Phenethyl alcohol-D-(2'-O-β-D-glucopyranosyl) glucopyranoside	(compound 152) – (28)	446.447
			
Code	Compound	Reference	Molecular Weight (Da)
PG_308	Isolugrandoside	(compound 153) – (28)	640.589



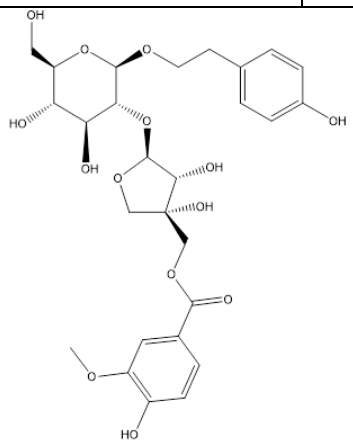
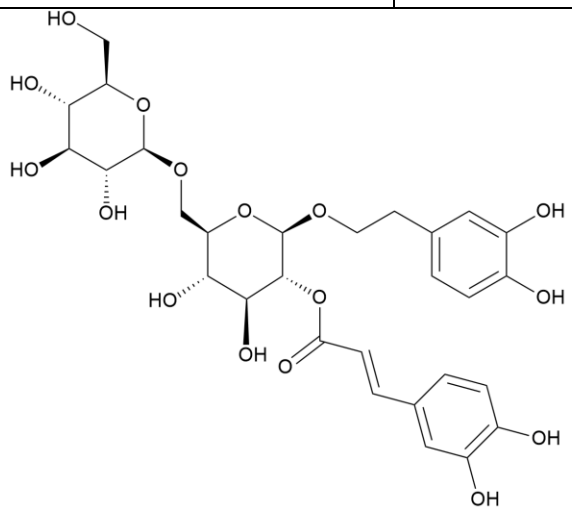
Code	Compound	Reference	Molecular Weight (Da)
PG_309	Phenethyl alcohol 8- O-β-D-gluco-pyranosyl- (1→2)- O-β-D-apiofuranosyl-(1→6)-β-D-glucopyranoside	(compound 154) – (28)	578.562

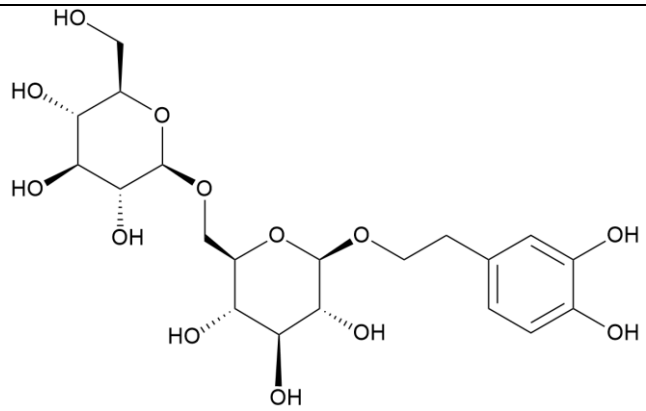


Code	Compound	Reference	Molecular Weight (Da)
PG_310	Phenethyl alcohol 8-O-β-D-glucopyranosyl- (1→2)-β-D-glucopyranoside	(compound 155) – (28)	446.447

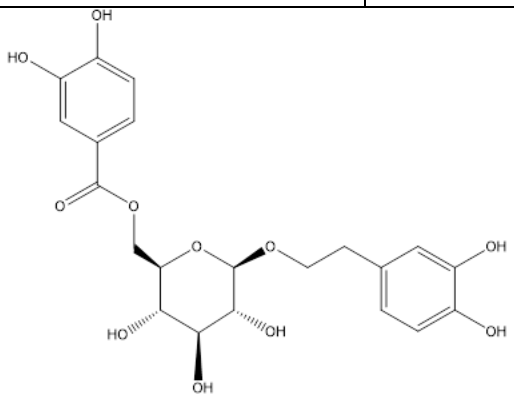


Code	Compound	Reference	Molecular Weight (Da)

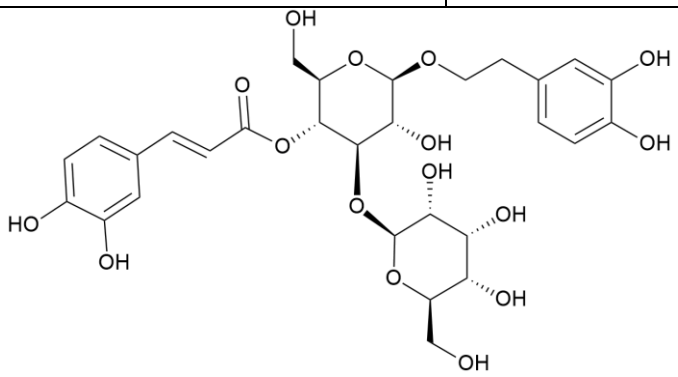
PG_311	Phlomisethanoside	(compound 156) – (28)	582.553
			
Code	Compound	Reference	Molecular Weight (Da)
PG_312	Ferruginoside A	(compound 157) – (28)	640.589
			
Code	Compound	Reference	Molecular Weight (Da)
PG_313	Ferruginoside B	(compound 158) – (28)	478.445



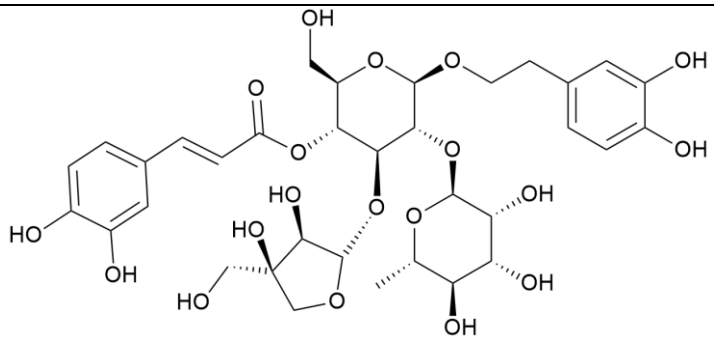
Code	Compound	Reference	Molecular Weight (Da)
PG_314	Fuhsioside	(compound 159) – (28)	452.411



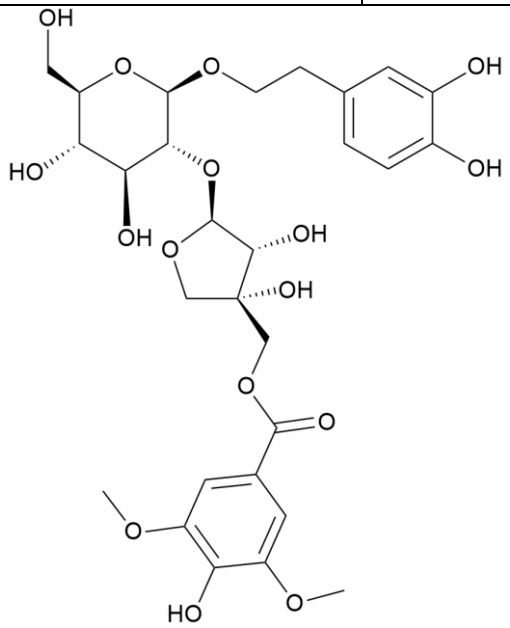
Code	Compound	Reference	Molecular Weight (Da)
PG_315	Plantalloside	(compound 160) – (28)	640.589



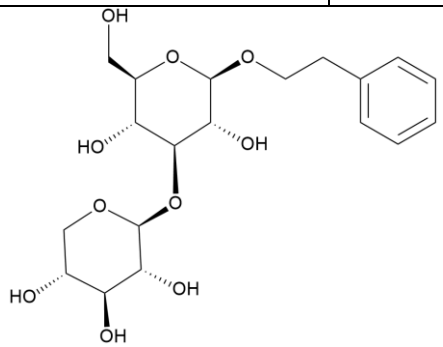
Code	Compound	Reference	Molecular Weight (Da)
PG_316	Lysionotoside	(compound 161) – (28)	758.72



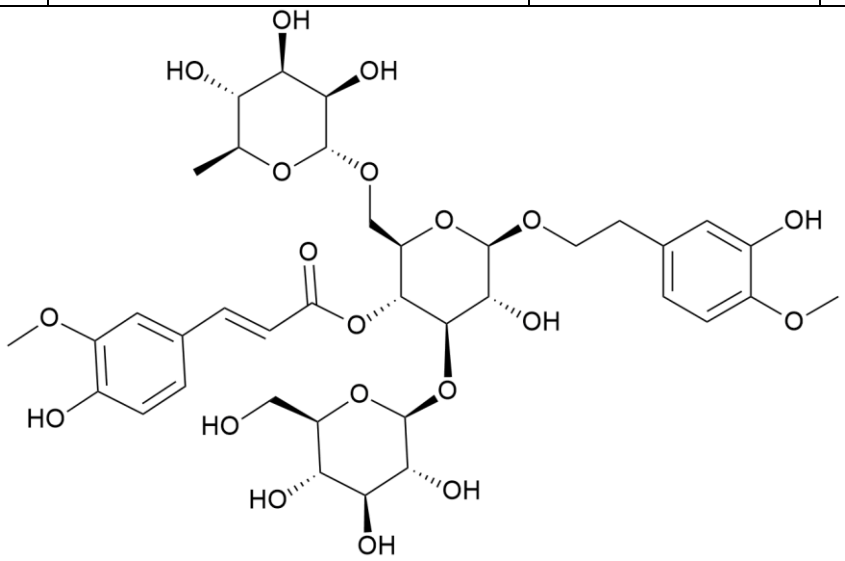
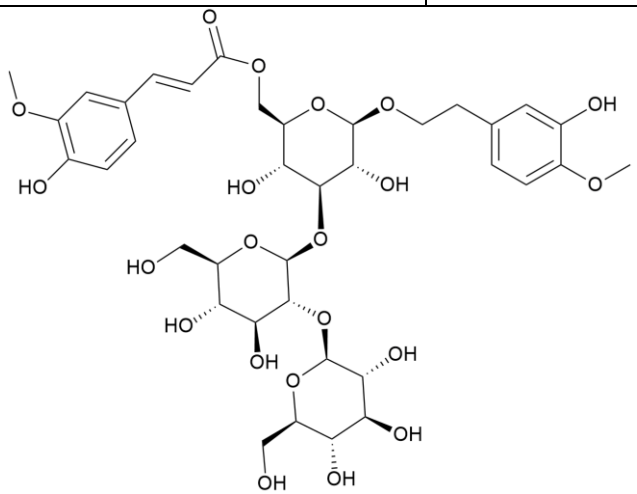
Code	Compound	Reference	Molecular Weight (Da)
PG_317	Hattushoside	(compound 162) – (28)	628.578

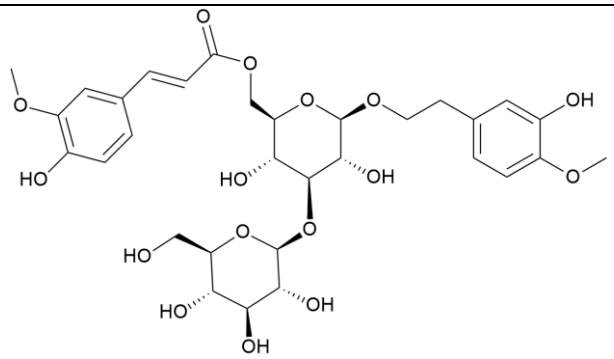


Code	Compound	Reference	Molecular Weight (Da)
PG_318	Artselaeroside A	(compound 163) – (28)	416.421

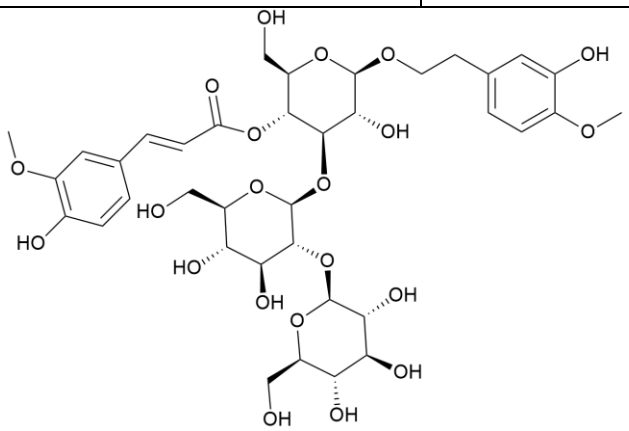


Code	Compound	Reference	Molecular

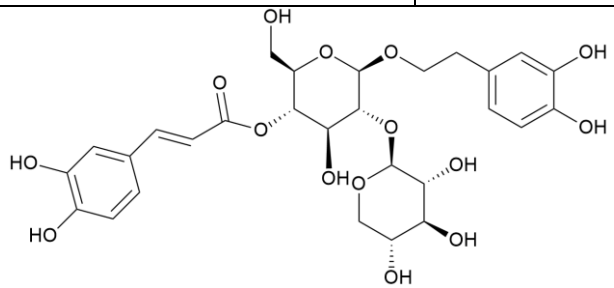
			Weight (Da)
PG_319	Artselaeroside B	(compound 164) – (28)	814.784
			
Code	Compound	Reference	Molecular Weight (Da)
PG_320	Scroside A	(compound 165) – (28)	830.783
			
Code	Compound	Reference	Molecular Weight (Da)
PG_321	Scroside B	(compound 166) – (28)	668.643



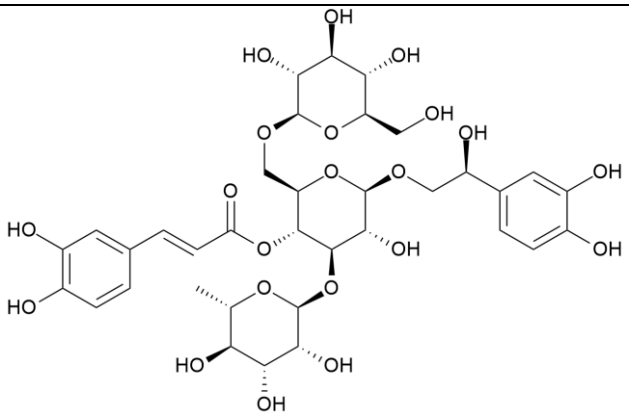
Code	Compound	Reference	Molecular Weight (Da)
PG_322	Scroside C	(compound 167) – (28)	830.783



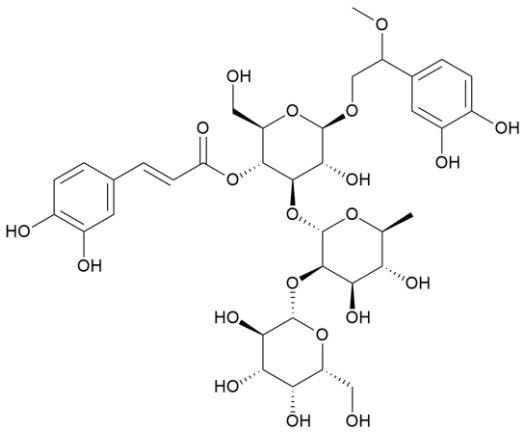
Code	Compound	Reference	Molecular Weight (Da)
PG_323-1	Nyctoside A	(compound 168) – (28)	610.563



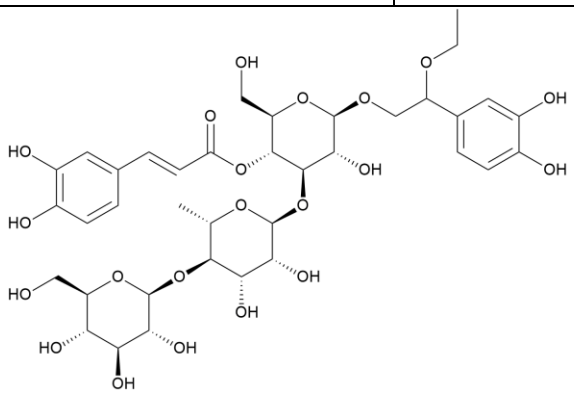
Code	Compound	Reference	Molecular Weight (Da)
PG_323	Cistantubulosides C1/C2	(compound 169) – (28)	802.729



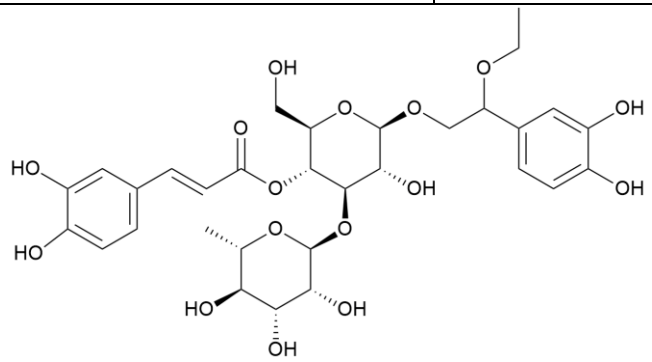
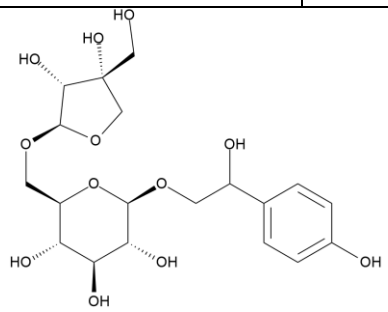
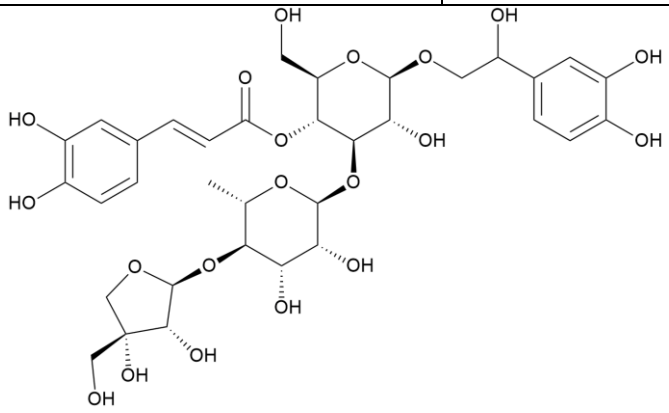
Code	Compound	Reference	Molecular Weight (Da)
PG_324	Lamiusides D	(compound 170) – (28)	818.772

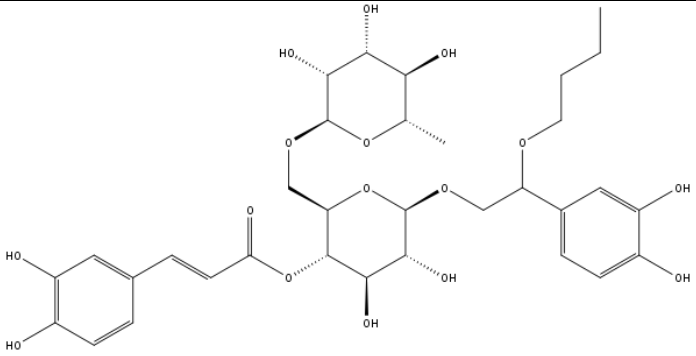
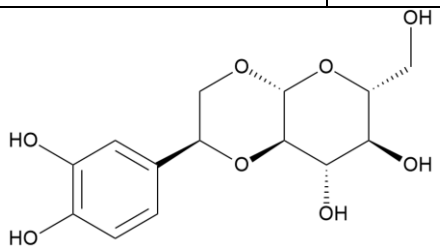
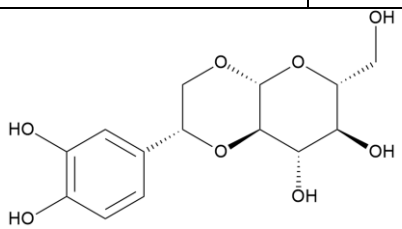


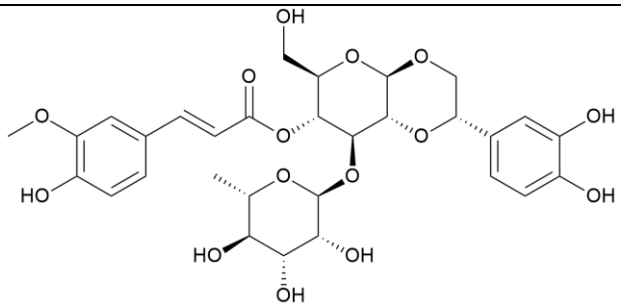
Code	Compound	Reference	Molecular Weight (Da)
PG_325	Rossicaside F	(compound 171) – (28)	830.783



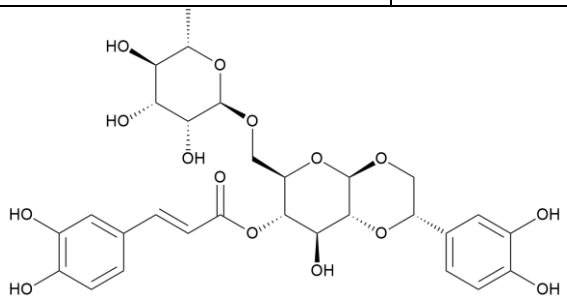
Code	Compound	Reference	Molecular

			Weight (Da)
PG_326	Ilicifolioside A	(compound 172) – (28)	668.643
			
Code	Compound	Reference	Molecular Weight (Da)
PG_327	1'-(4-Hydroxyphenyl)ethane-1',2'-diol 2'-O-β-D-apiofuranosyl -(1→6)-β-D-glucopyranoside	(compound 173) – (28)	448.419
			
Code	Compound	Reference	Molecular Weight (Da)
PG_328	Wedelosin	(compound 174) – (28)	772.703
			

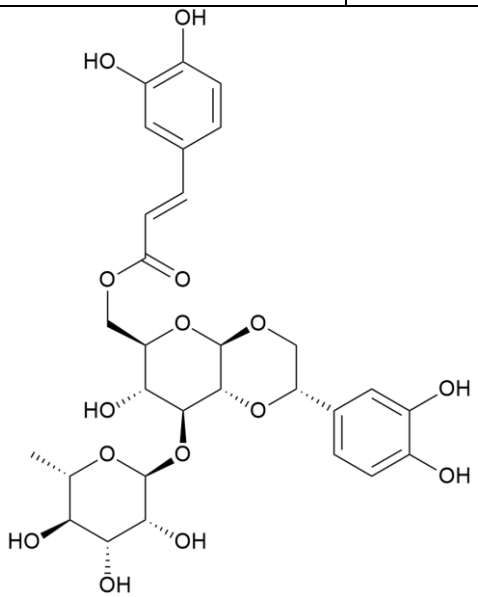
Code	Compound	Reference	Molecular Weight (Da)
PG_329	Suspensaside B	(compound 175) – (28)	696.696
			
Code	Compound	Reference	Molecular Weight (Da)
PG_330	Cuneataside A	(compound 176) – (28)	314.289
			
Code	Compound	Reference	Molecular Weight (Da)
PG_331	Cuneataside B	(compound 177) – (28)	314.289
			
Code	Compound	Reference	Molecular Weight (Da)
PG_332	3'''-O-Methyl crenatoside	(compound 178) – (28)	636.601



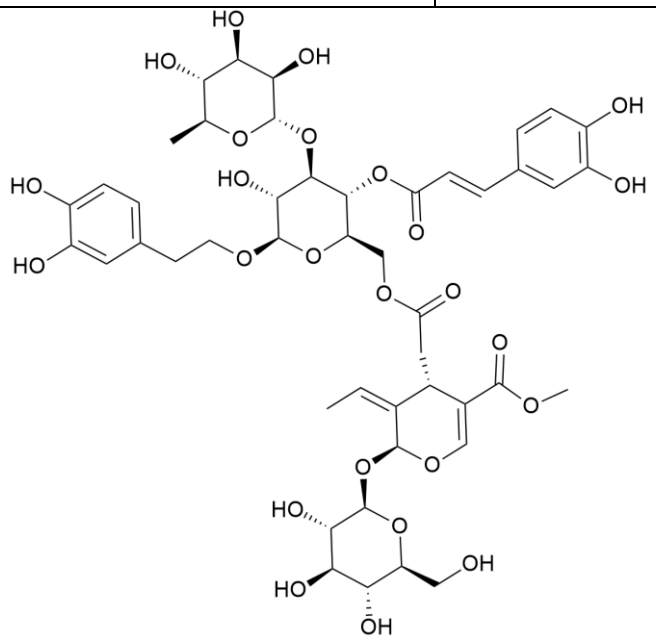
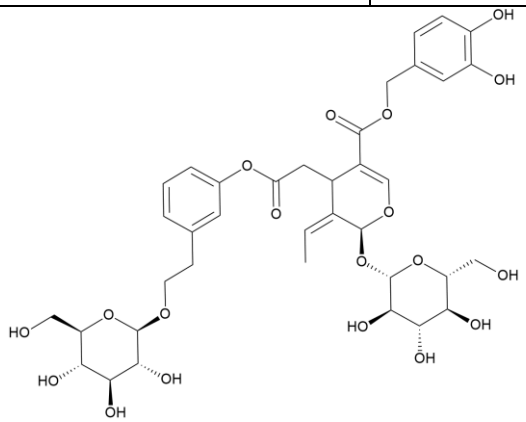
Code	Compound	Reference	Molecular Weight (Da)
PG_333	Suspensaside A	(compound 179) – (28)	622.574

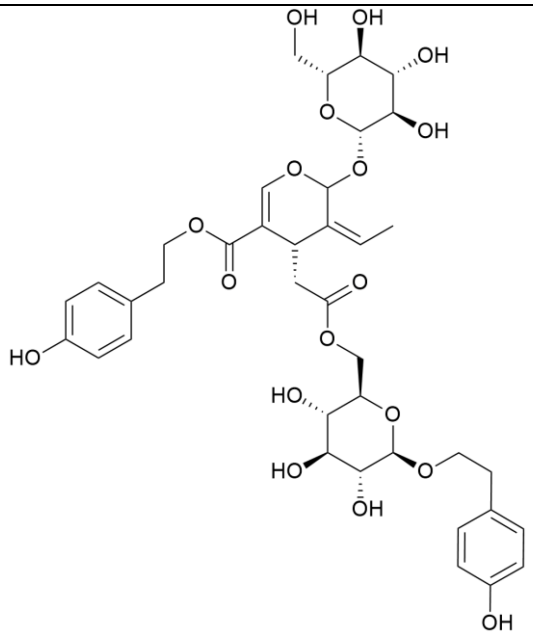


Code	Compound	Reference	Molecular Weight (Da)
PG_334	Isocrenatoside	(compound 180) – (28)	622.574

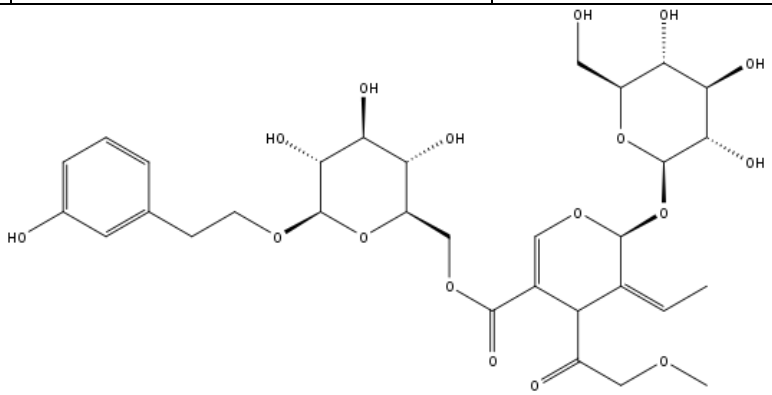


Code	Compound	Reference	Molecular Weight (Da)
PG_335	Isooleoacteoside	(compound 181) –	1012.96

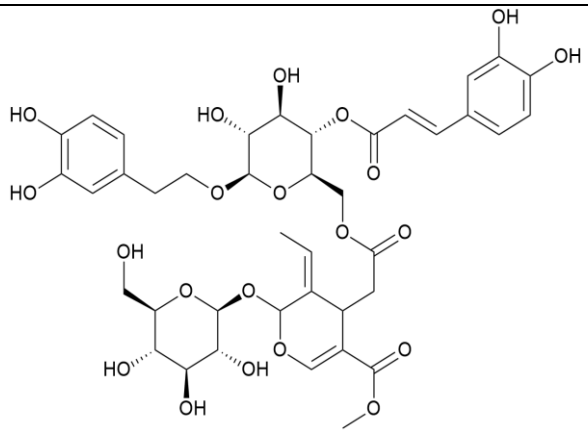
		(28)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_336	Safghanoside E	(compound 182) – (28)	796.769
			
Code	Compound	Reference	Molecular Weight (Da)
PG_337	Safghanoside F	(compound 183) – (28)	796.813



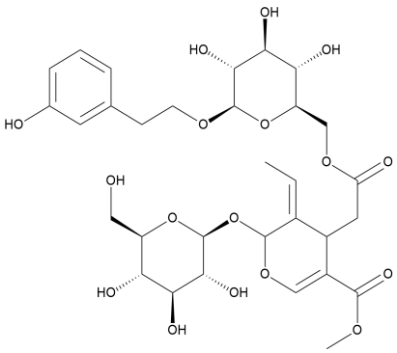
Code	Compound	Reference	Molecular Weight (Da)
PG_338	(8Z)-Nuzhenide	(compound 184) – (28)	688.673



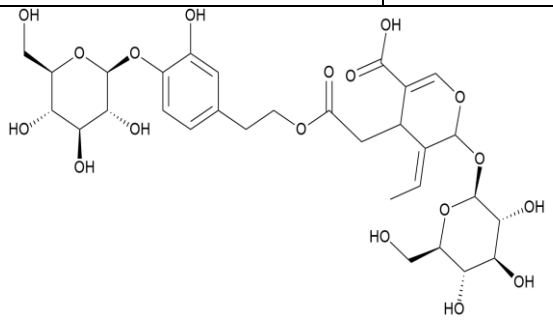
Code	Compound	Reference	Molecular Weight (Da)
PG_339	Desrhamnosyloleoacteoside	(compound 185) – (28)	868.832



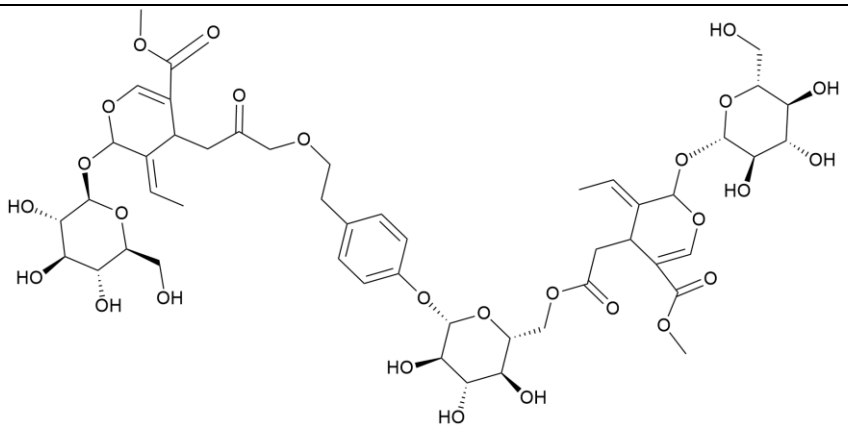
Code	Compound	Reference	Molecular Weight (Da)
PG_340	Specneuzhenide	(compound 186) – (28)	690.689



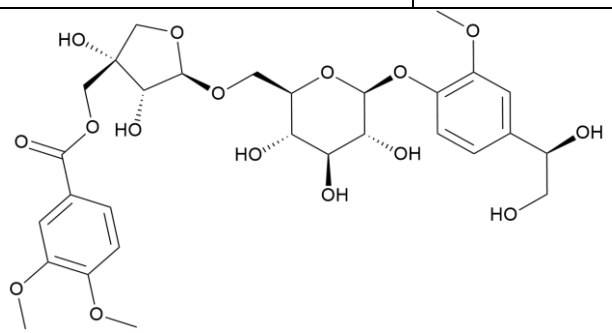
Code	Compound	Reference	Molecular Weight (Da)
PG_341	6"-O-β-D-Glucopyranosyloleuropein	(compound 187) – (28)	690.645



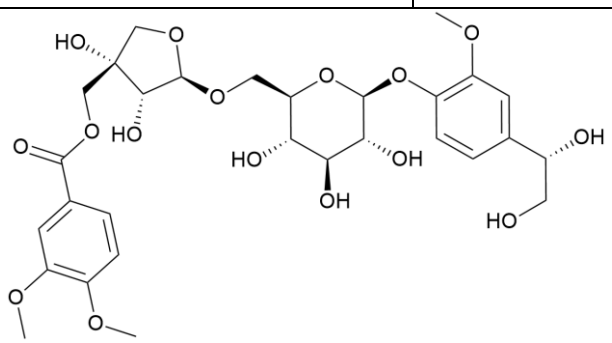
Code	Compound	Reference	Molecular Weight (Da)
PG_342	Neopolyanoside	(compound 188) – (28)	1091.07

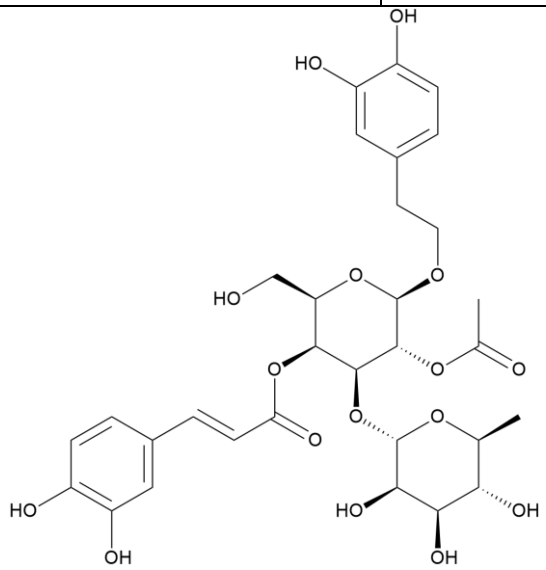
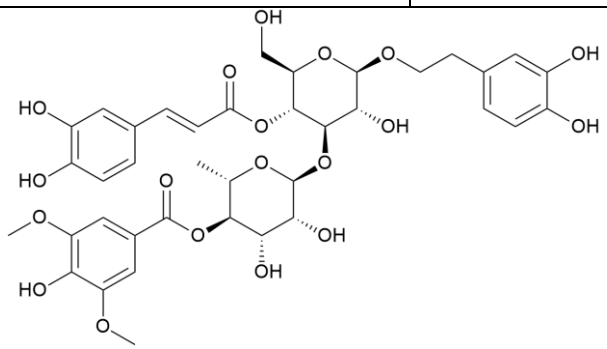


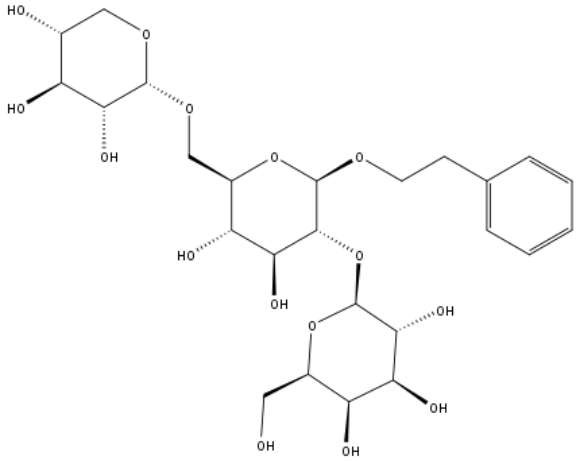
Code	Compound	Reference	Molecular Weight (Da)
PG_343-1	(1,2-Dihydroxyethyl)-2-methoxyphenyl1-O-β-D-[5-O-(3,4-dimethoxybenzoyl)]-apiofuranosyl-(1 → 6)-β-D-glucopyranoside (trans)	(compound 189) – (28)	642.605



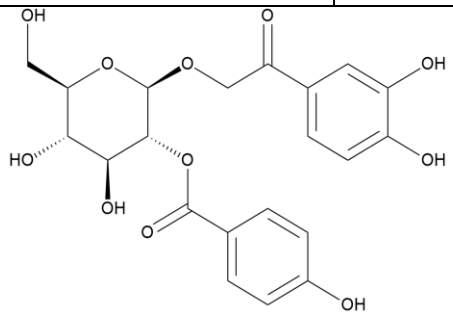
Code	Compound	Reference	Molecular Weight (Da)
PG_343-2	(1,2-Dihydroxyethyl)-2-methoxyphenyl1-O-β-D-[5-O-(3,4-dimethoxybenzoyl)]-apiofuranosyl-(1 → 6)-β-D-glucopyranoside (cis)	(compound 189) – (28)	642.605



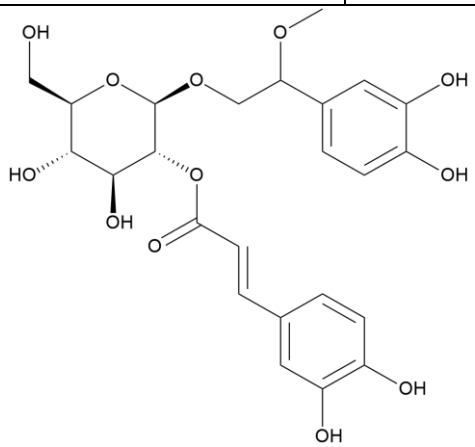
Code	Compound	Reference	Molecular Weight (Da)
PG_344	3,4-Dihydroxyphenethoxy-O-β -L-rhamnopyranosyl-(1→ 3)-β -D-(2-O-acetyl-4-O-caffeoyl)-galactopyranoside	(compound 190) – (28)	682.669
			
Code	Compound	Reference	Molecular Weight (Da)
PG_345	Acanmontanoside	(compound 1) – (31)	804.748
			
Code	Compound	Reference	Molecular Weight (Da)
PG_346	Kansanoside A	(compound 2) – (31)	578.562



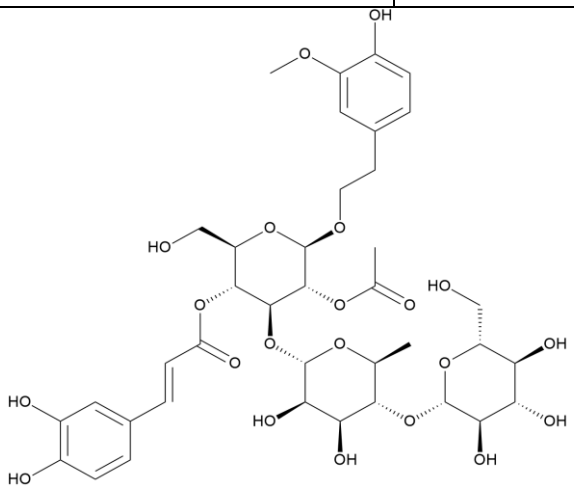
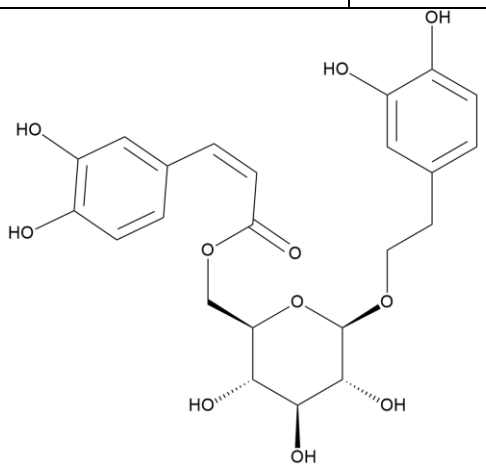
Code	Compound	Reference	Molecular Weight (Da)
PG_347	Bacomoside A	(compound 3) – (31)	450.395

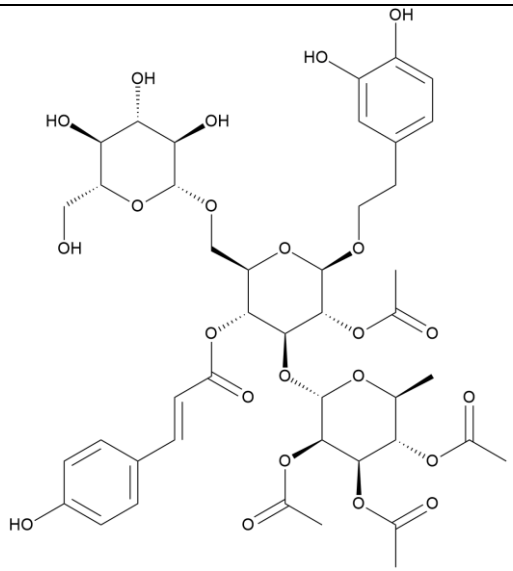


Code	Compound	Reference	Molecular Weight (Da)
PG_348	Bacomoside B1/B2	(compound 4) – (31)	508.474

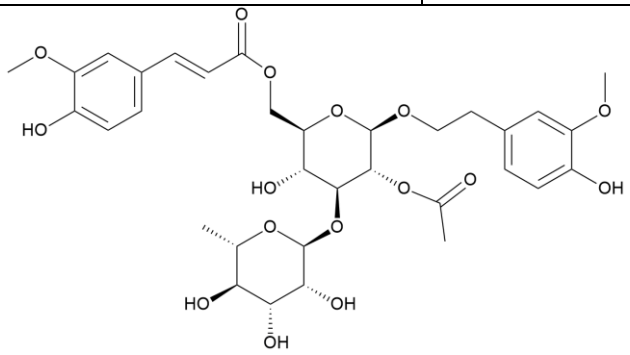


Code	Compound	Reference	Molecular Weight (Da)
PG_349	Himaloside A	(compound 5) –	844.81

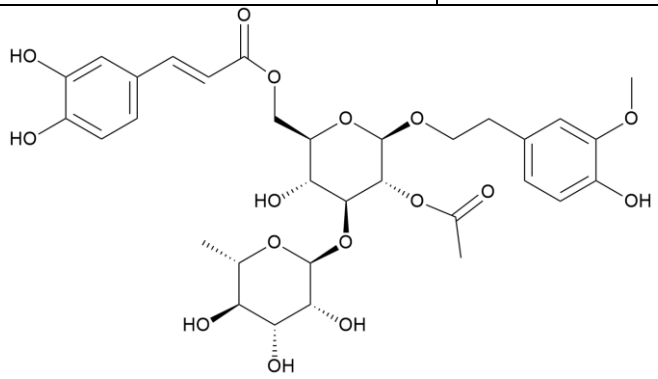
		(31)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_350	Himaloside B	(compound 6) – (31)	478.448
			
Code	Compound	Reference	Molecular Weight (Da)
PG_351	Z-Tubuloside D	(compound 7) – (31)	938.879



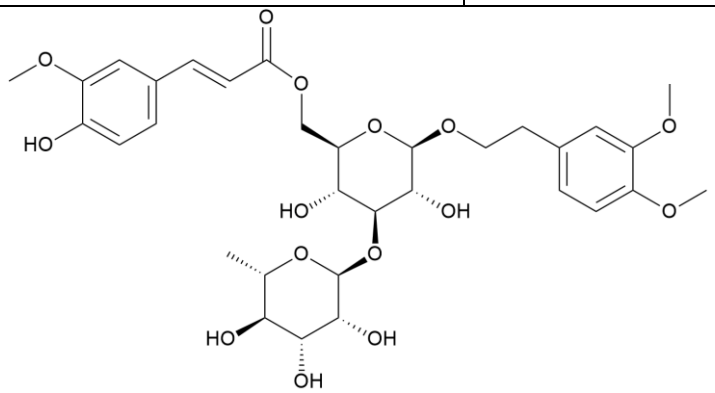
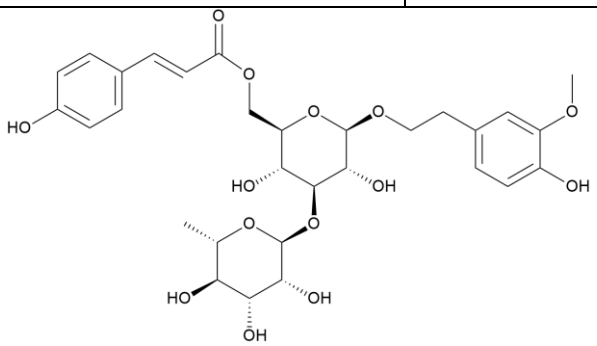
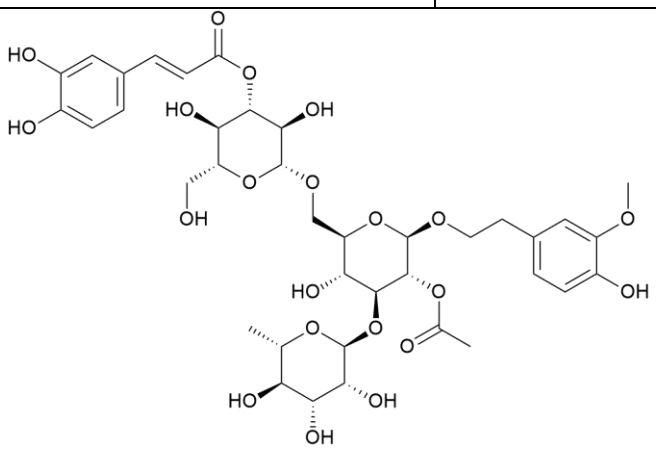
Code	Compound	Reference	Molecular Weight (Da)
PG_352	Cistanoside J	(compound 8) – (31)	694.68

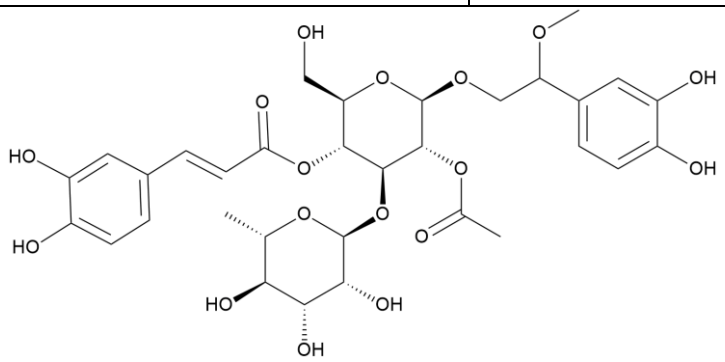
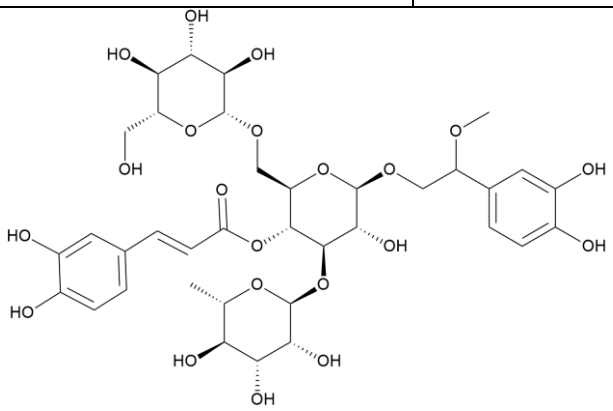
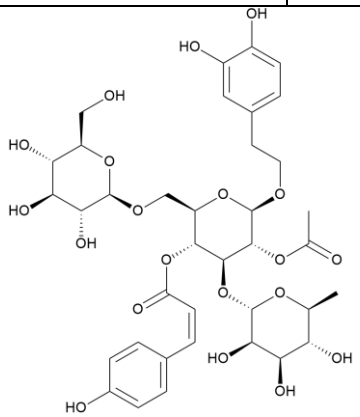


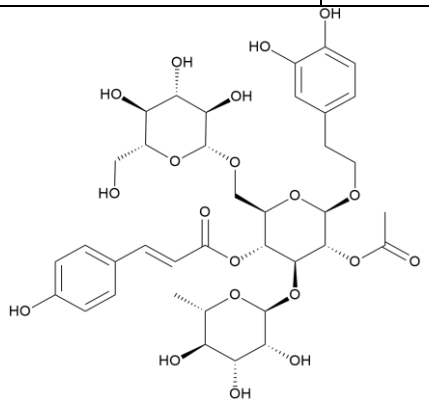
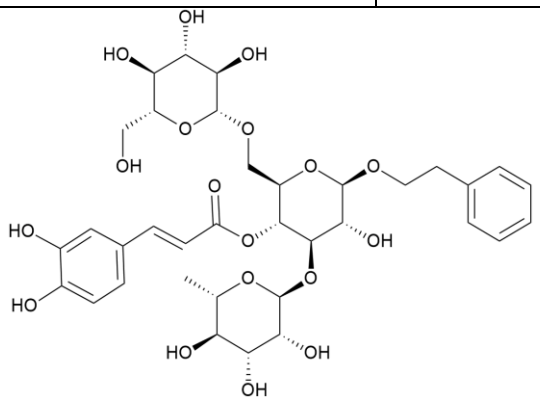
Code	Compound	Reference	Molecular Weight (Da)
PG_353	Cistanoside K	(compound 9) – (31)	680.654

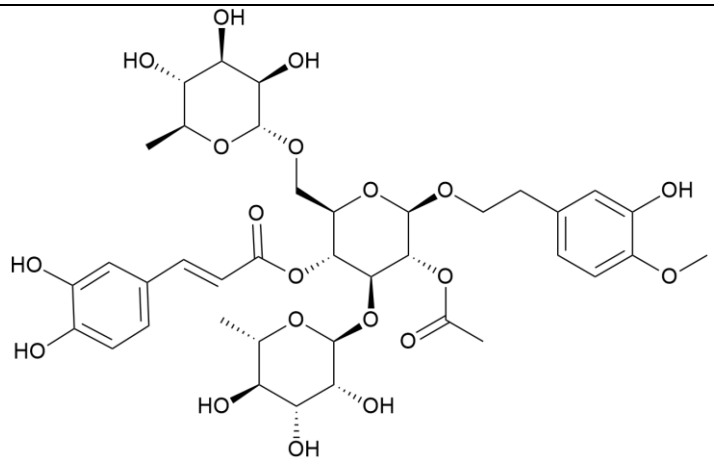


Code	Compound	Reference	Molecular

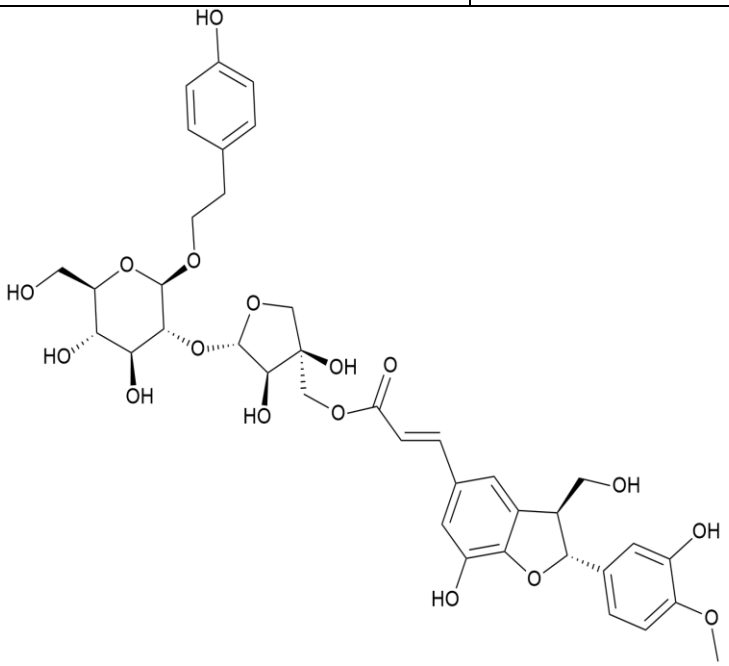
			Weight (Da)
PG_354	Cistanoside L	(compound 10) – (31)	666.67
			
Code	Compound	Reference	Molecular Weight (Da)
PG_355	Cistanoside M	(compound 11) – (31)	622.618
			
Code	Compound	Reference	Molecular Weight (Da)
PG_356	Cistanoside N	(compound 12) – (31)	842.794
			

Code	Compound	Reference	Molecular Weight (Da)
PG_357	Kankanoside J1/J2	(compound 13) – (31)	696.653
			
Code	Compound	Reference	Molecular Weight (Da)
PG_358	Kankanoside K1/K2	(compound 14) – (31)	816.756
			
Code	Compound	Reference	Molecular Weight (Da)
PG_359-1	Kankanoside H1/H2 (cis)	(compound 15) – (31)	812.768
			

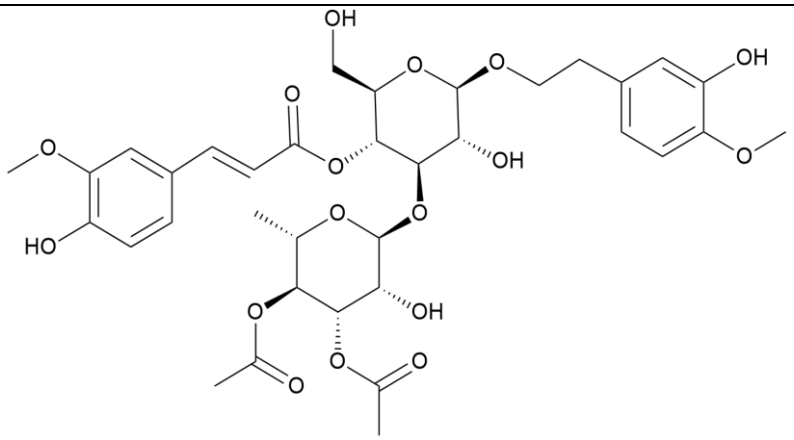
Code	Compound	Reference	Molecular Weight (Da)
PG_359-2	Kankanoside H1/H2 (trans)	(compound 15) – (31)	814.784
			
Code	Compound	Reference	Molecular Weight (Da)
PG_360	Kankanoside I	(compound 16) – (31)	754.732
			
Code	Compound	Reference	Molecular Weight (Da)
PG_361	Cistansinenside B	(compound 17) – (31)	826.795



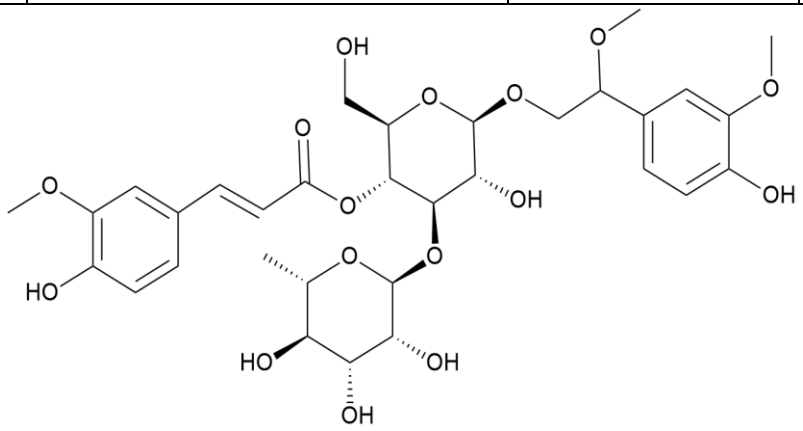
Code	Compound	Reference	Molecular Weight (Da)
PG_362	Bunginoside A	(compound 18) – (31)	772.75



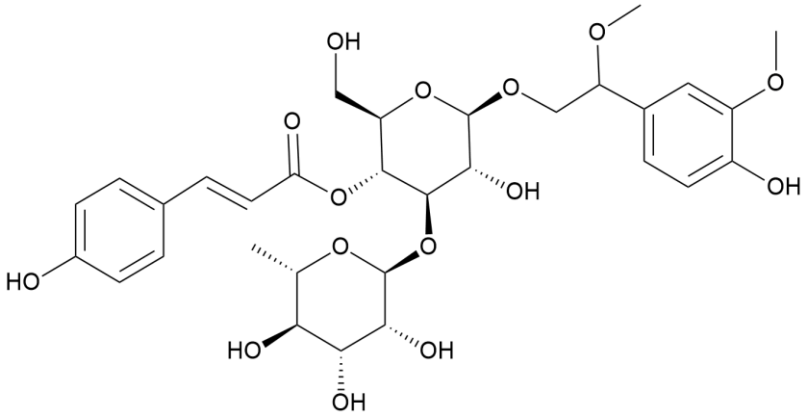
Code	Compound	Reference	Molecular Weight (Da)
PG_363	3”,4”-di-O-acetylmartynoside	(compound 19) – (31)	736.717



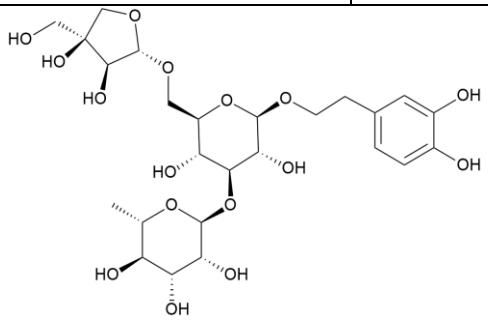
Code	Compound	Reference	Molecular Weight (Da)
PG_364	β-D-Glucopyranoside,1”-O-(7S)-7-(3-methoxyl-4-hydroxy-phenyl-7-methoxyethyl-3”-α-L-rhamnopyranosyl-4”-[(8E)-7-(3-hydroxy-phenyl)-8-propenoate]	(compound 20) – (31)	684.685



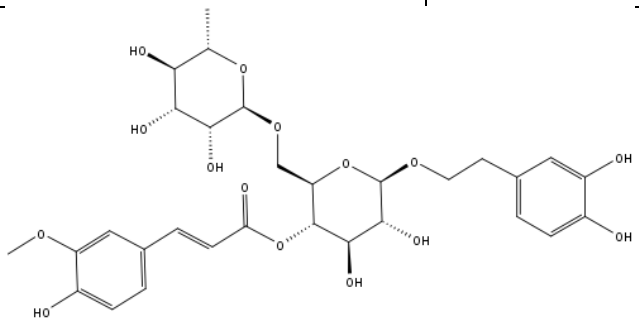
Code	Compound	Reference	Molecular Weight (Da)
PG_365	β-D-Glucopyranoside,1”-O-(7S)-7-(3-methoxyl-4-hydroxy-phenyl-7-methoxyethyl-3”-α-L-rhamnopyranosyl-4”-[(8E)-7-(4-hydroxy-phenyl)-8-propenoate]	(compound 21) – (31)	654.659



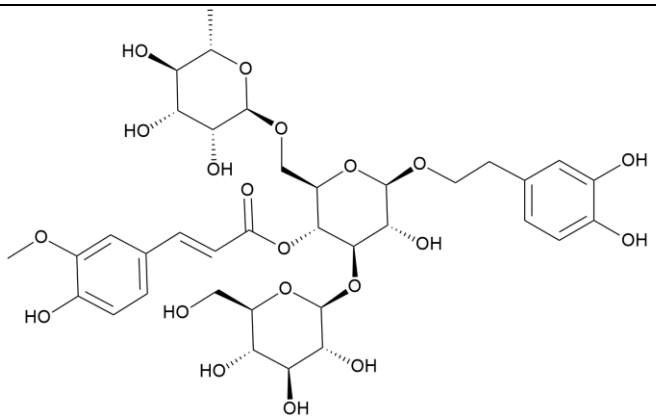
Code	Compound	Reference	Molecular Weight (Da)
PG_366	Peiioside B	(compound 22) – (31)	594.561



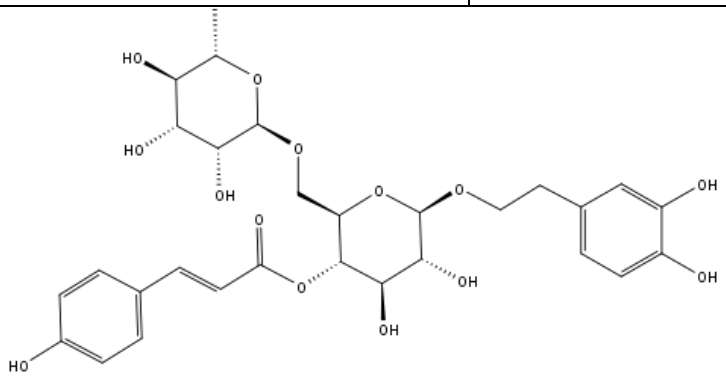
Code	Compound	Reference	Molecular Weight (Da)
PG_367	Purpureaside D	(compound 23) – (31)	638.617



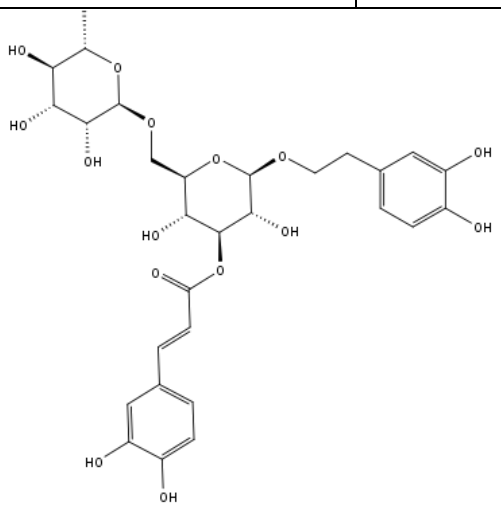
Code	Compound	Reference	Molecular Weight (Da)
PG_368	Purpureaside E	(compound 24) – (31)	800.757

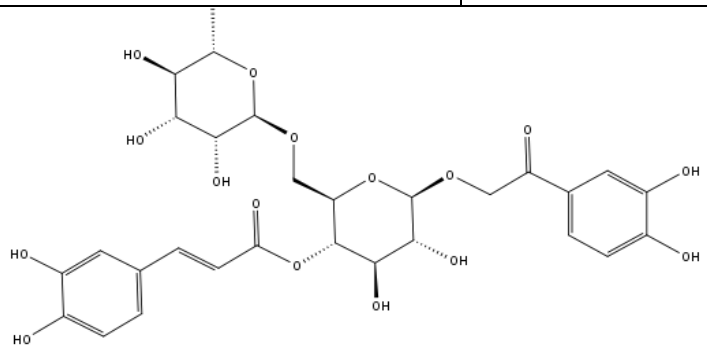
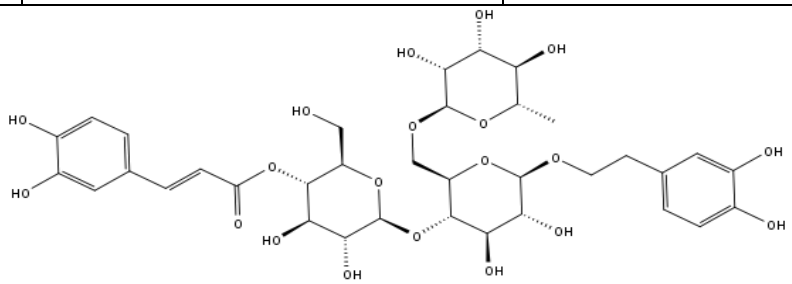


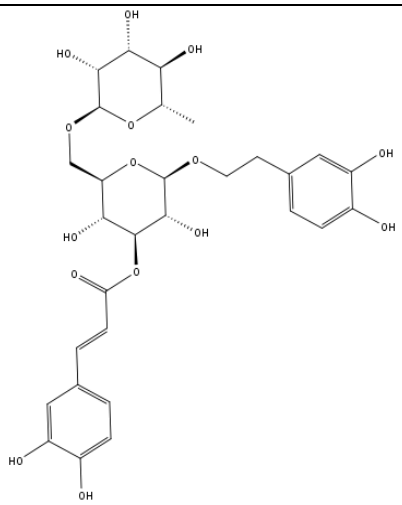
Code	Compound	Reference	Molecular Weight (Da)
PG_369	Forsythenside K	(compound 25) – (31)	608.591



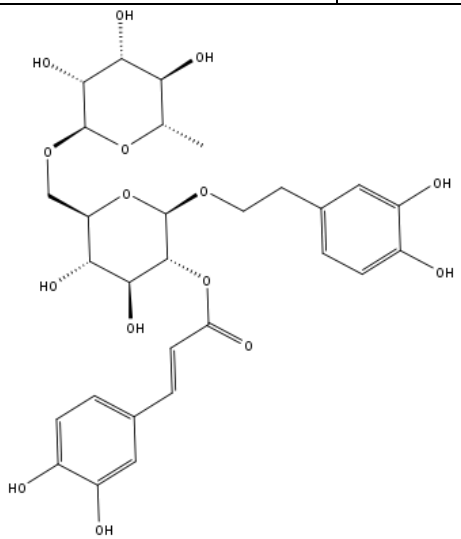
Code	Compound	Reference	Molecular Weight (Da)
PG_370	Lianqiaoxinside A	(compound 26) – (31)	624.59



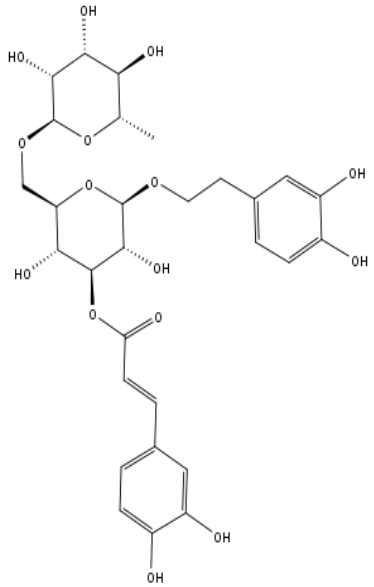
Code	Compound	Reference	Molecular Weight (Da)
PG_371	2-(3,4-Dihydroxyphenyl)-2-oxoethyl- O-α -L-rhamnopyranosyl- (1□6)-(4-O-caffeoyl)- β -D-glucopyranoside	(compound 27) – (31)	624.589
			
Code	Compound	Reference	Molecular Weight (Da)
PG_372	Forsythoside A 4'-O-β -D-glucopyranoside	(compound 28) – (31)	786.73
			
Code	Compound	Reference	Molecular Weight (Da)
PG_373	Isoforsythoside	(compound 29) – (31)	624.59



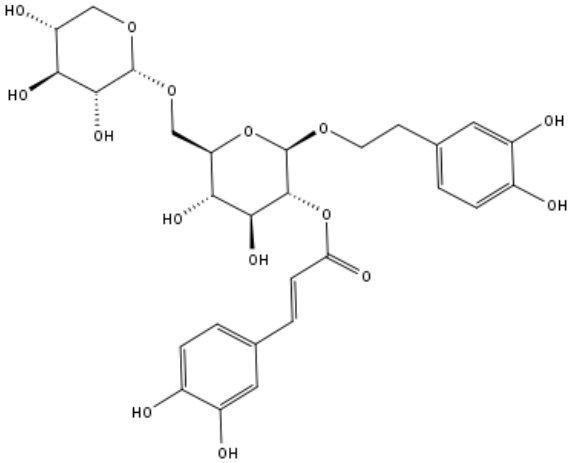
Code	Compound	Reference	Molecular Weight (Da)
PG_374	Forsythoside H	(compound 30) – (31)	624.59



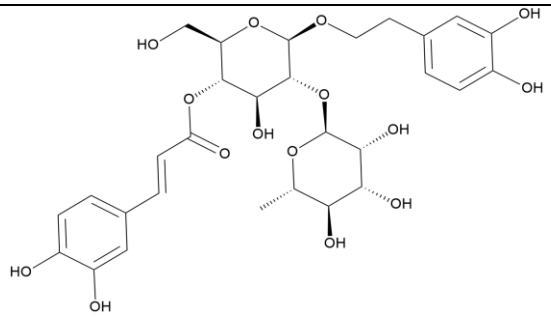
Code	Compound	Reference	Molecular Weight (Da)
PG_375	Forsythoside I	(compound 31) – (31)	624.59



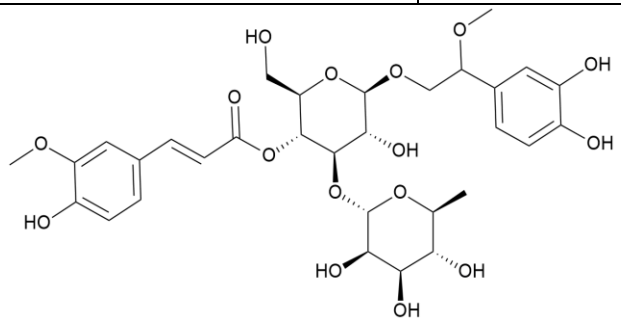
Code	Compound	Reference	Molecular Weight (Da)
PG_376	Forsythoside J	(compound 32) – (31)	610.563



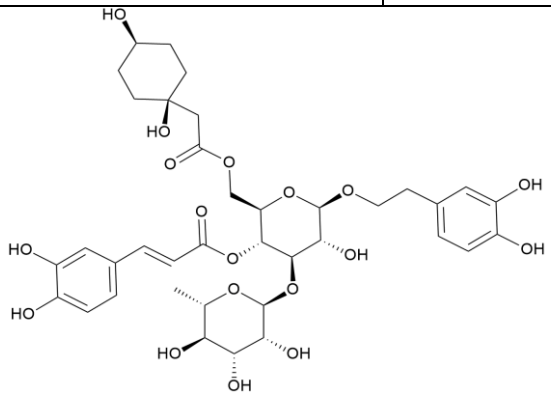
Code	Compound	Reference	Molecular Weight (Da)
PG_377	Calceolarioside A 2'-α-L-rhamnopyranoside	(compound 33) – (31)	624.59



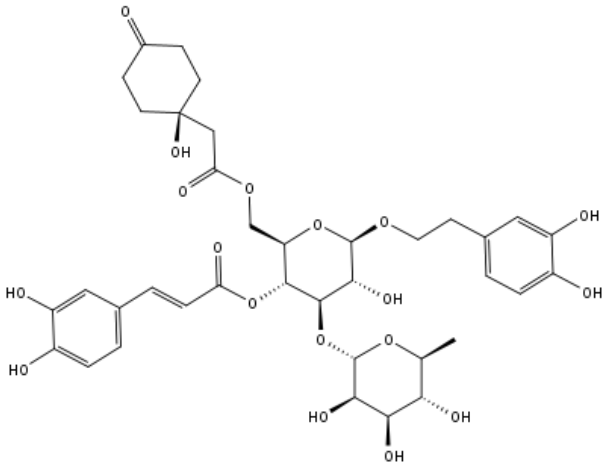
Code	Compound	Reference	Molecular Weight (Da)
PG_378	3'''-O-methylcampneoside I	(compound 34) – (31)	668.643



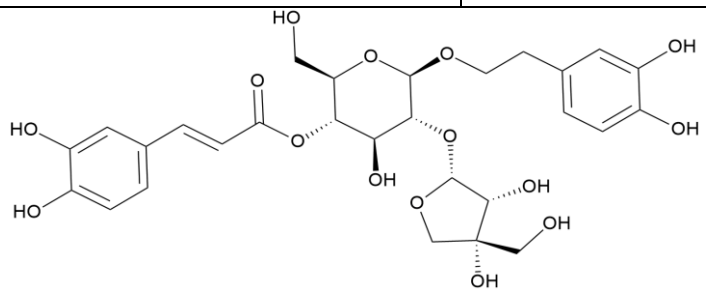
Code	Compound	Reference	Molecular Weight (Da)
PG_379	6'-O-(cis-1,4-Dihydroxycyclohexnacetyl) acteoside	(compound 35) – (31)	780.77



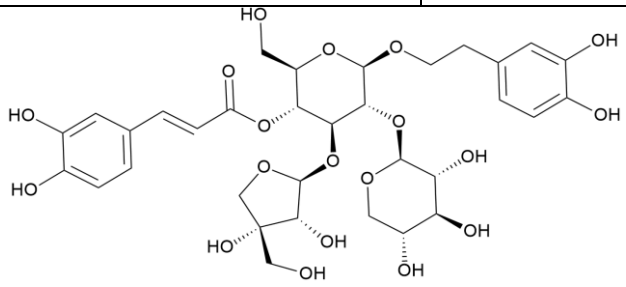
Code	Compound	Reference	Molecular Weight (Da)
PG_380	6'-O-(1-Hydroxy-4-oxocyclohexanacetyl) acteoside	(compound 36) – (31)	778.754



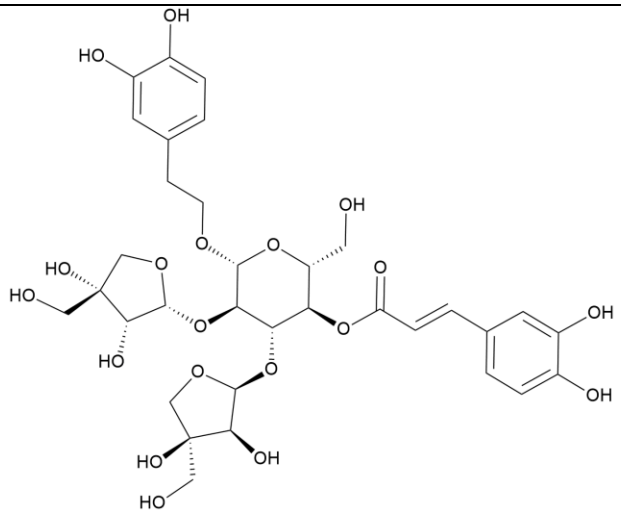
Code	Compound	Reference	Molecular Weight (Da)
PG_381	Fucatoside A	(compound 37) – (31)	610.563



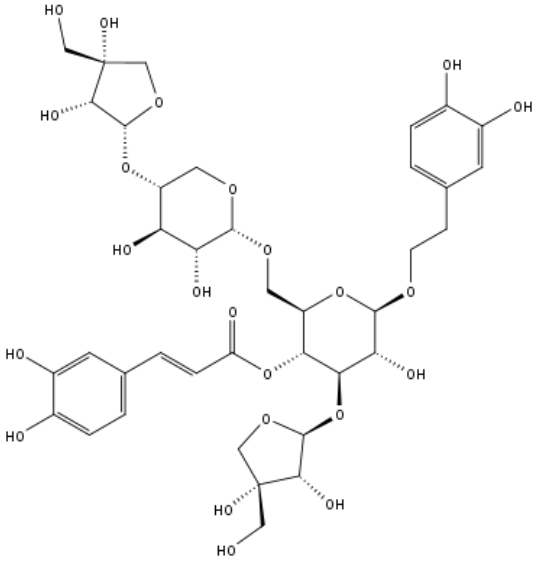
Code	Compound	Reference	Molecular Weight (Da)
PG_382	Fucatoside B	(compound 38) – (31)	742.667



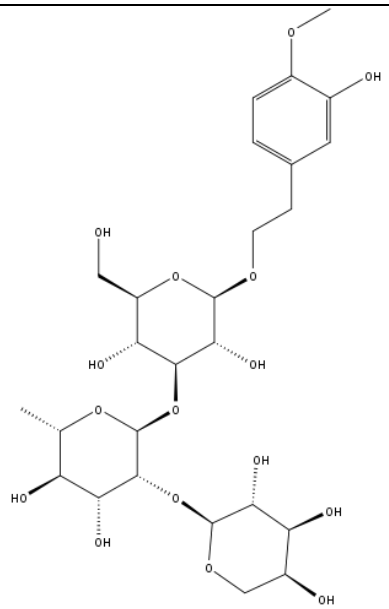
Code	Compound	Reference	Molecular Weight (Da)
PG_383	Fucatoside C	(compound 39) – (31)	744.693



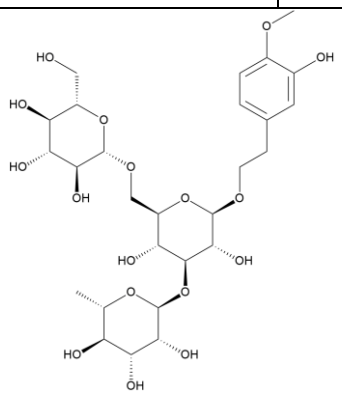
Code	Compound	Reference	Molecular Weight (Da)
PG_384	Raduloside	(compound 40) – (31)	874.792



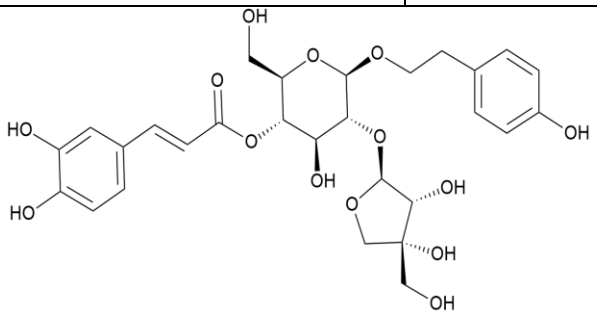
Code	Compound	Reference	Molecular Weight (Da)
PG_385	Leonoside E	(compound 41) – (31)	608.588

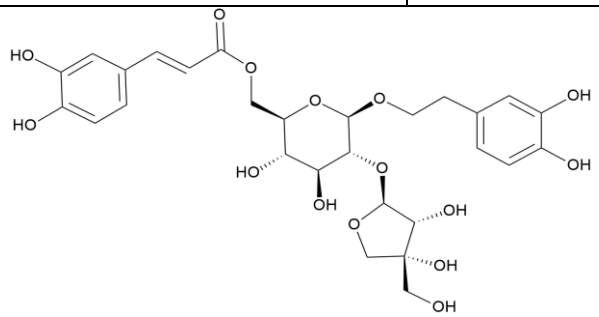
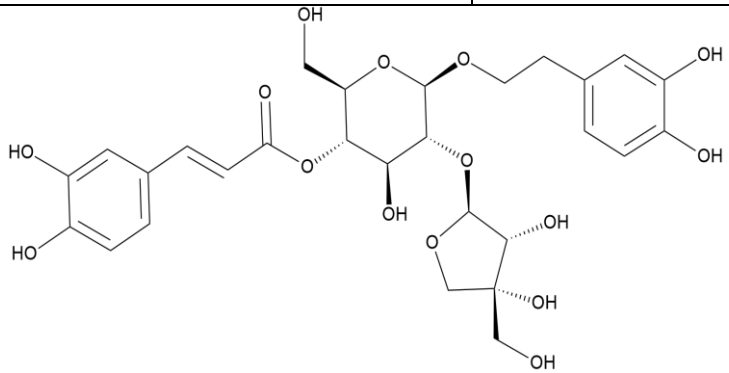


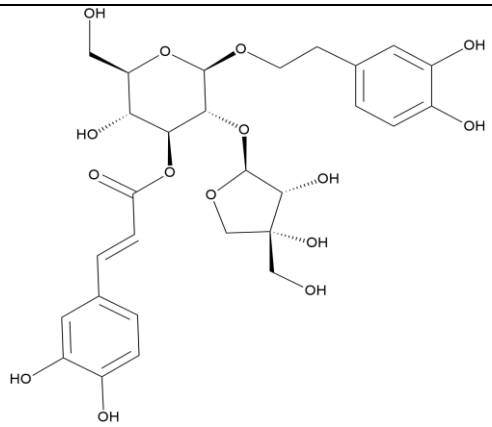
Code	Compound	Reference	Molecular Weight (Da)
PG_386	Leonoside F	(compound 42) – (31)	638.613



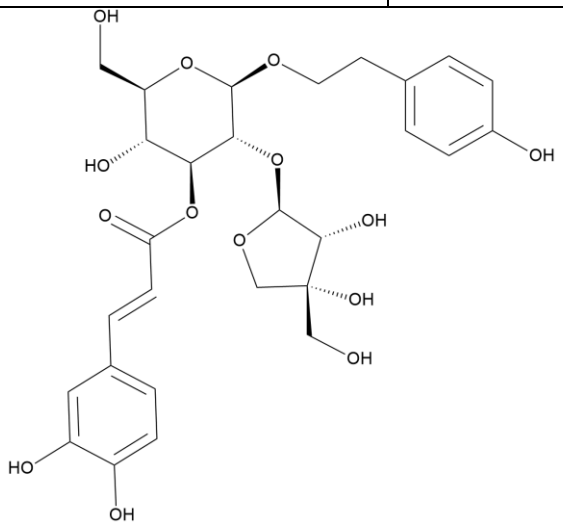
Code	Compound	Reference	Molecular Weight (Da)
PG_387	β -(4-Hydroxyphenyl) ethyl-4-O-E-caffeoyl-O-[β -D-apiofuranosyl-(1→2)]-β - D-glucopyranoside	(compound 43) – (31)	594.564



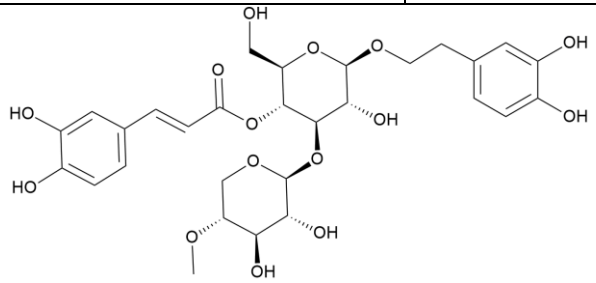
Code	Compound	Reference	Molecular Weight (Da)
PG_388	β-(3,4-Dihydroxyphenyl) ethyl-6-O-E-caffeoyl-O-[β -D-apiofuranosyl-(1→2)]-β- D-glucopyranoside	(compound 44) – (31)	610.563
			
Code	Compound	Reference	Molecular Weight (Da)
PG_389	β -(3,4-Dihydroxyphenyl) ethyl-4-O-E-caffeoyl-O-[β -D-apiofuranosyl-(1→2)]-β - D-glucopyranoside	(compound 45) – (31)	610.563
			
Code	Compound	Reference	Molecular Weight (Da)
PG_390	β-(3,4-Dihydroxyphenyl) ethyl-3-O-E-caffeoyl-O-[β -D-apiofuranosyl-(1→2)]-β - D-glucopyranoside	(compound 46) – (31)	610.563



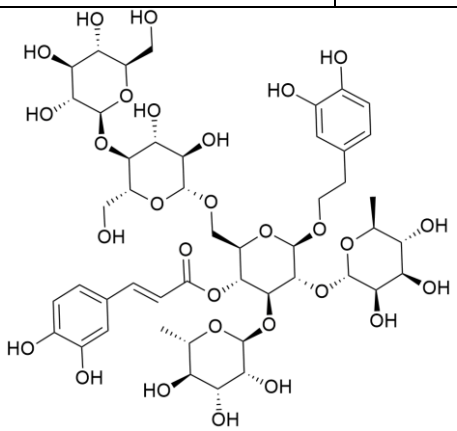
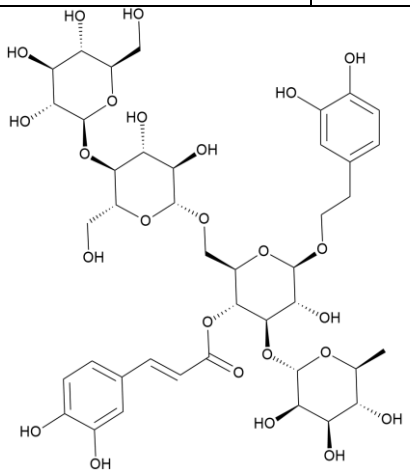
Code	Compound	Reference	Molecular Weight (Da)
PG_391	β-(4-Hydroxyphenyl) ethyl-3-O-E-caffeoyl-O-[β -D-apiofuranosyl-(1→2)]- β -D-glucopyranoside	(compound 47) – (31)	596.58

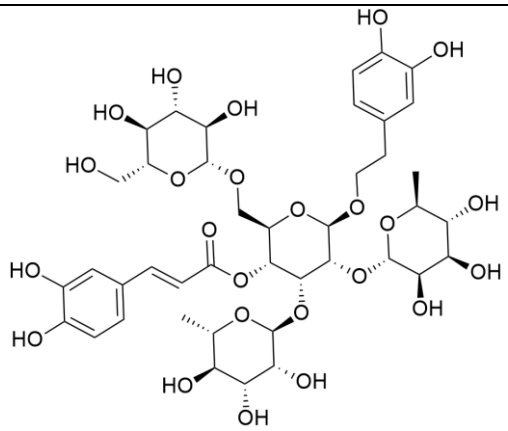


Code	Compound	Reference	Molecular Weight (Da)
PG_392	Lagotiside A	(compound 48) – (31)	624.59

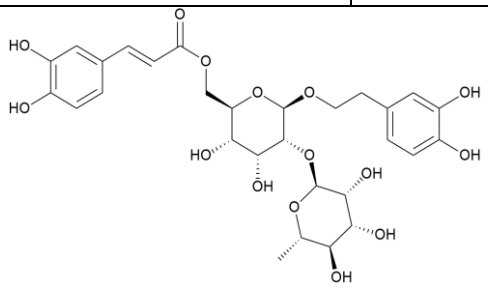


Code	Compound	Reference	Molecular Weight (Da)

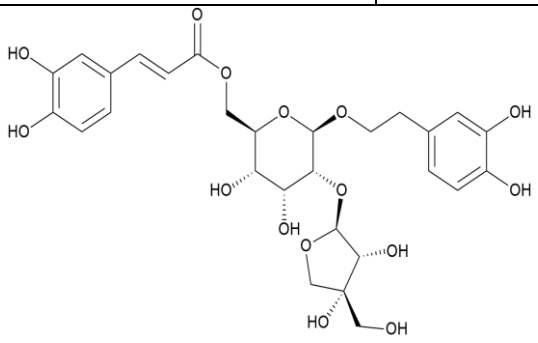
PG_393	Yulanoside A	(compound 49) – (31)	1097.03
			
Code	Compound	Reference	Molecular Weight (Da)
PG_394	Yulanoside B	(compound 50) – (31)	948.871
			
Code	Compound	Reference	Molecular Weight (Da)
PG_395	2'-Rhamnoechinacoside	(compound 51) – (31)	934.888



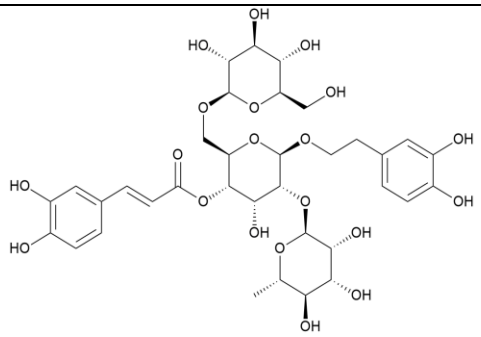
Code	Compound	Reference	Molecular Weight (Da)
PG_396	Magnoloside D	(compound 52) – (31)	624.596



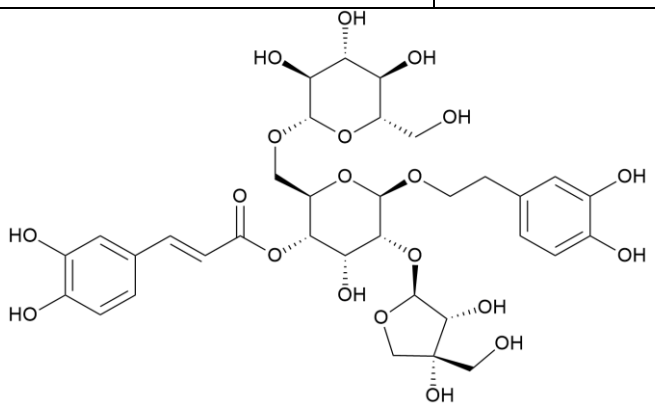
Code	Compound	Reference	Molecular Weight (Da)
PG_397	Magnoloside E	(compound 53) – (31)	610.563



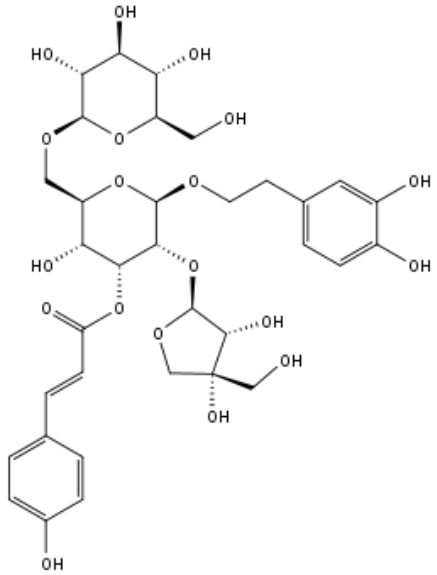
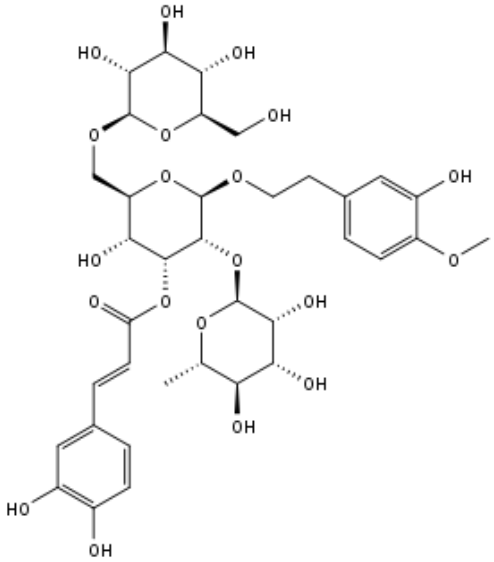
Code	Compound	Reference	Molecular Weight (Da)
PG_398	Magnoloside F	(compound 54) – (31)	786.73

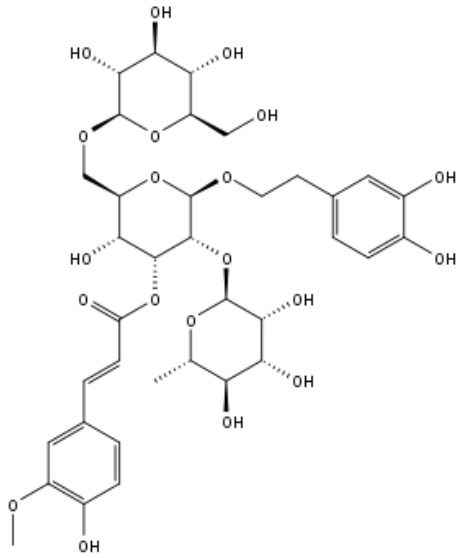


Code	Compound	Reference	Molecular Weight (Da)
PG_399	Magnoloside G	(compound 55) – (31)	772.703

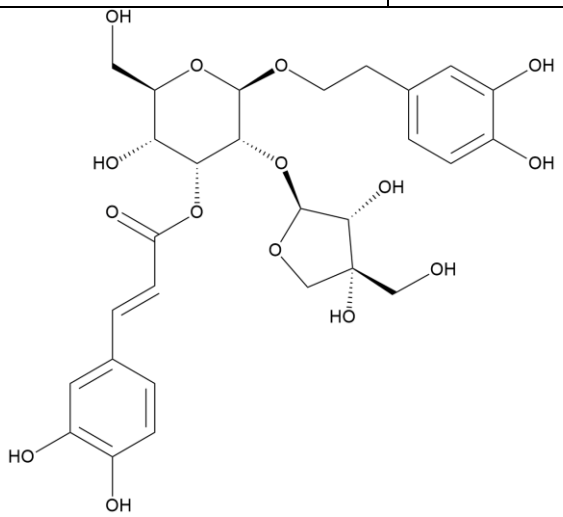


Code	Compound	Reference	Molecular Weight (Da)
PG_400	Magnoloside H	(compound 56) – (31)	774.719

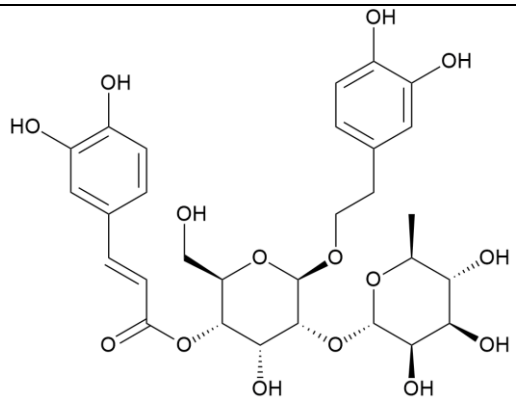
Code	Compound	Reference	Molecular Weight (Da)
PG_401	Magnoloside I	(compound 57) – (31)	756.704
			
Code	Compound	Reference	Molecular Weight (Da)
PG_402	Magnoloside J	(compound 58) – (31)	800.757
			
Code	Compound	Reference	Molecular Weight (Da)
PG_403	Magnoloside K	(compound 59) – (31)	800.757



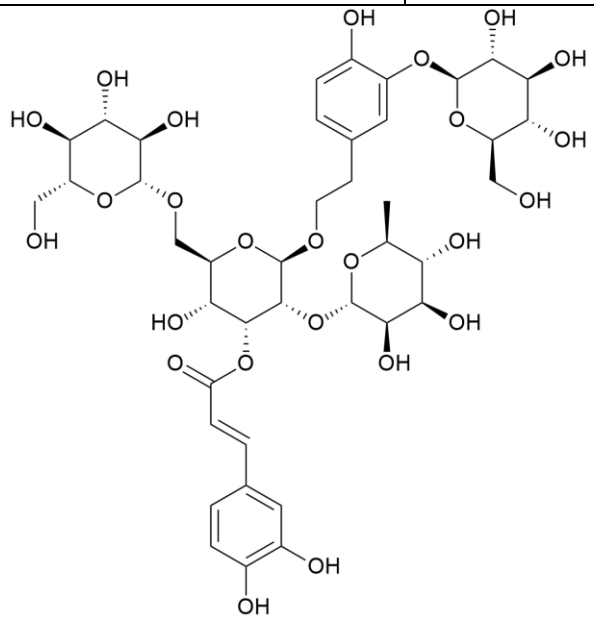
Code	Compound	Reference	Molecular Weight (Da)
PG_404	Magnoloside L	(compound 60) – (31)	610.563



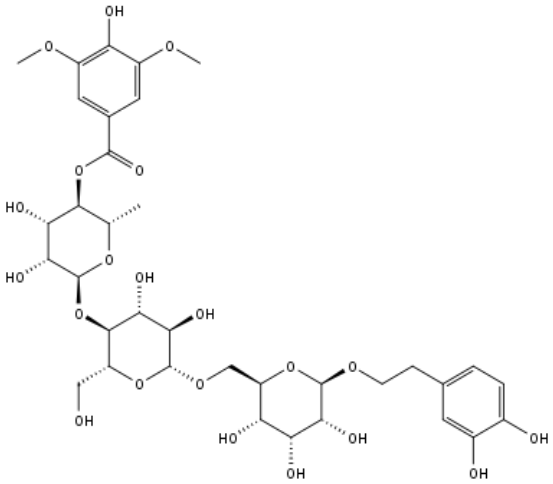
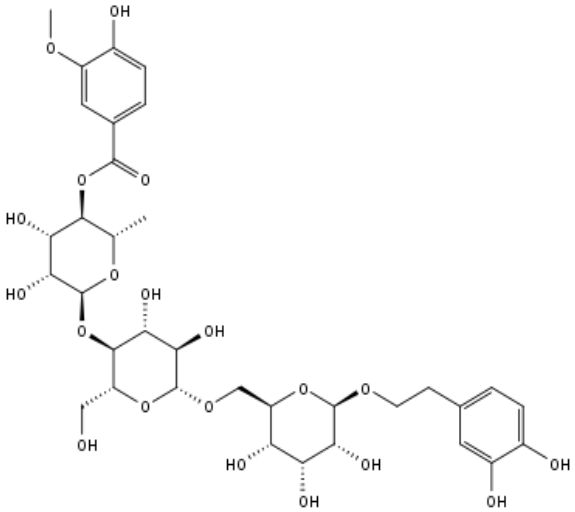
Code	Compound	Reference	Molecular Weight (Da)
PG_405	Magnoloside M	(compound 61) – (31)	626.606

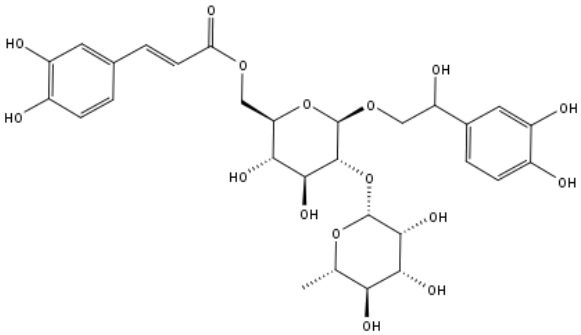


Code	Compound	Reference	Molecular Weight (Da)
PG_406	Magnoloside N	(compound 62) – (31)	948.871

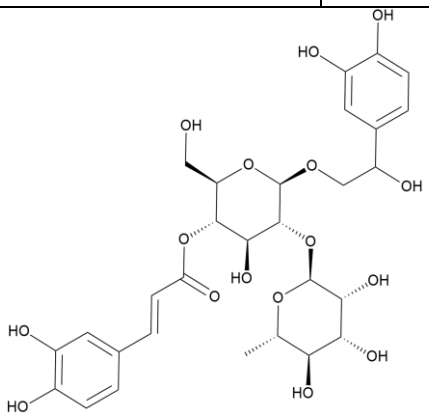


Code	Compound	Reference	Molecular Weight (Da)
PG_407	Magnoloside O	(compound 63) – (31)	804.745

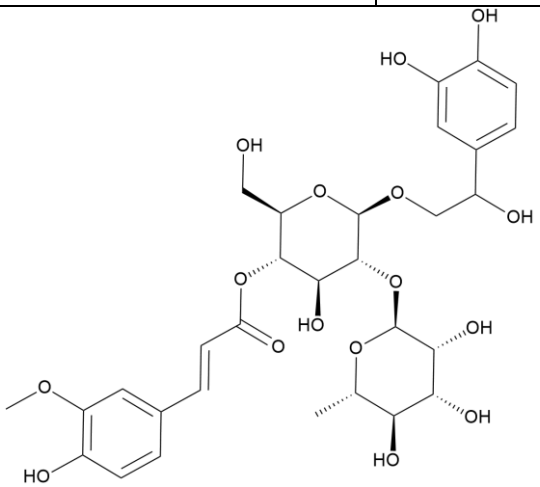
			
Code	Compound	Reference	Molecular Weight (Da)
PG_408	Magnoloside P	(compound 64) – (31)	774.719
			
Code	Compound	Reference	Molecular Weight (Da)
PG_409	Savaside A	(compound 65) – (31)	640.589



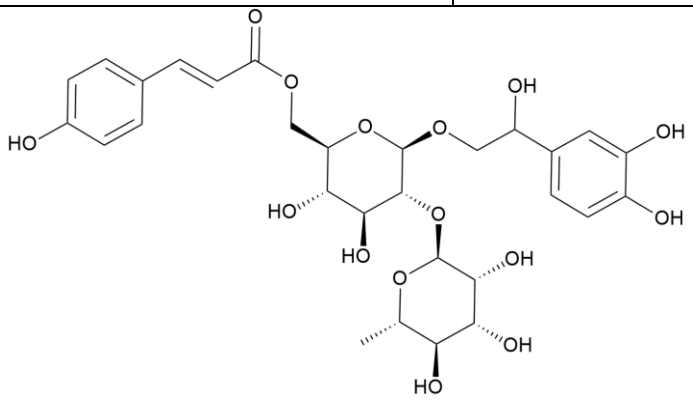
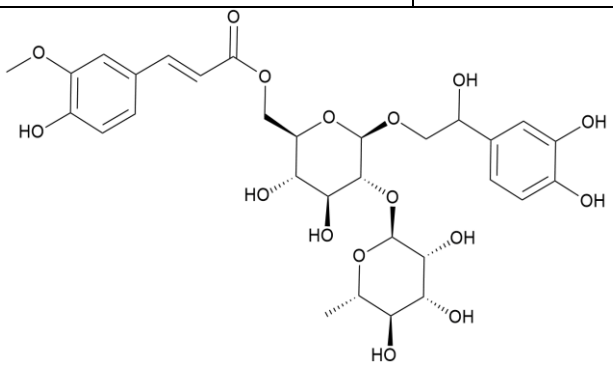
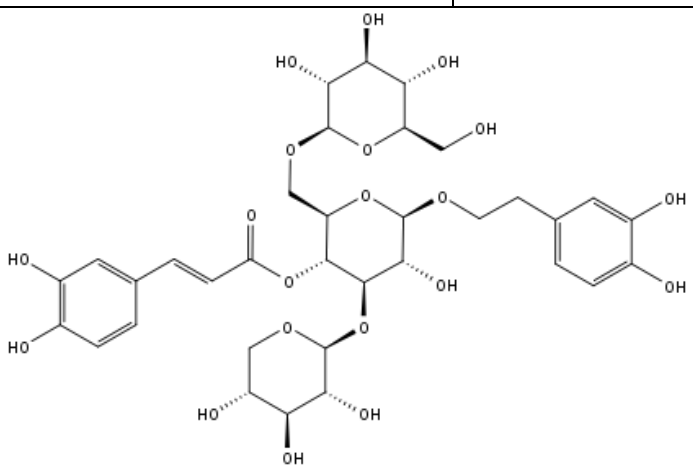
Code	Compound	Reference	Molecular Weight (Da)
PG_410	Savaside B	(compound 66) – (31)	640.589

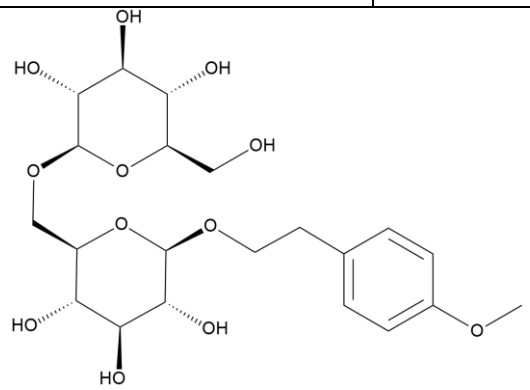
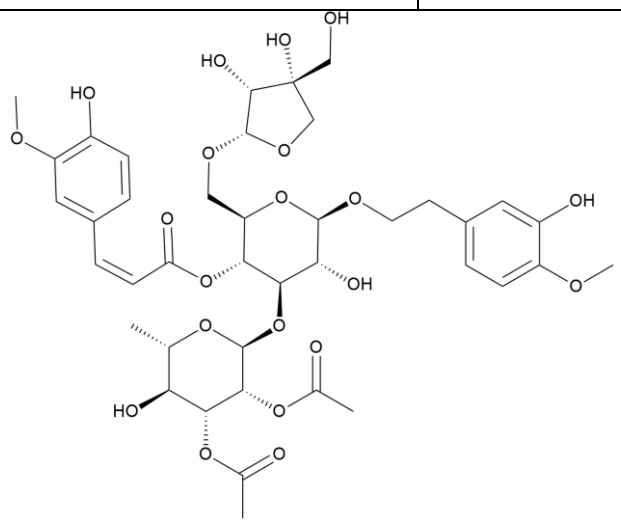


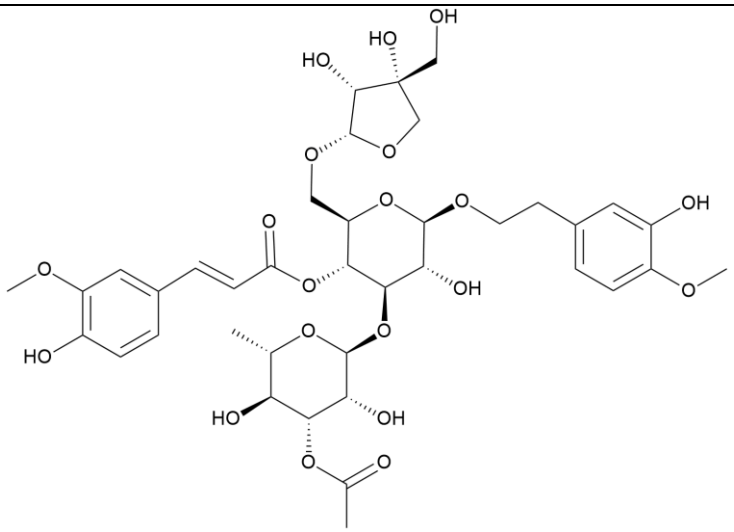
Code	Compound	Reference	Molecular Weight (Da)
PG_411	Savaside C	(compound 67) – (31)	654.616



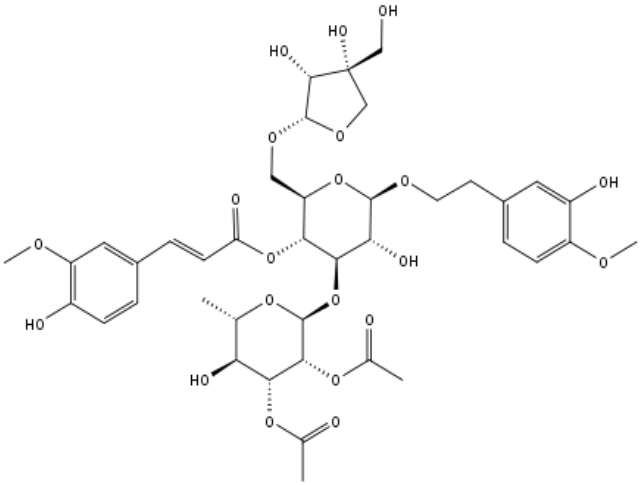
Code	Compound	Reference	Molecular

			Weight (Da)
PG_412	Savaside D	(compound 68) – (31)	624.59
			
Code	Compound	Reference	Molecular Weight (Da)
PG_413	Savaside E	(compound 69) – (31)	656.632
			
Code	Compound	Reference	Molecular Weight (Da)
PG_414	Rashomoside A	(compound 71) – (31)	772.703
			

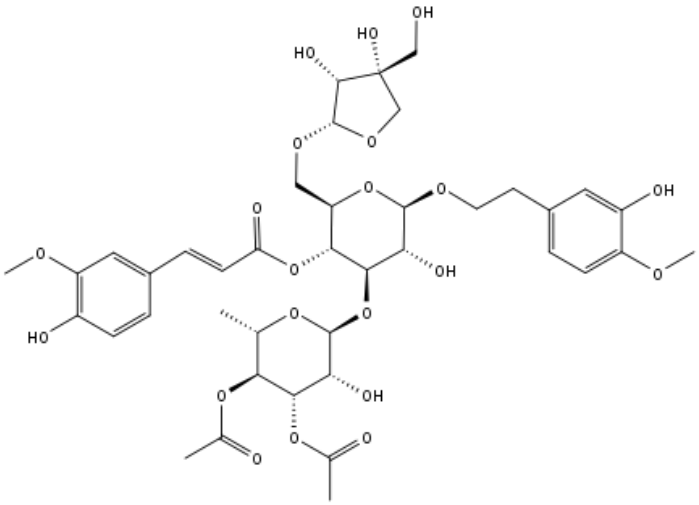
Code	Compound	Reference	Molecular Weight (Da)
PG_415	Tazettoside D (or tazettosides d)	(compound 71) – (31) (compound 22) –(26)	476.473
			
Code	Compound	Reference	Molecular Weight (Da)
PG_416	3-Hydroxy-4-methoxy- β-phenylethoxy-O-[2,3-di-acetyl-α-L-rhamnopyranosyl-(1→3)]-4-O-cisferuloyl-[β -D-apiofuranosyl-(1->6)]-β -D-glucopyranoside	(compound 72) – (31)	868.832
			
Code	Compound	Reference	Molecular Weight (Da)
PG_417	3'''-Acetyl-O-betonyoside D	(compound 73) – (31)	656.632



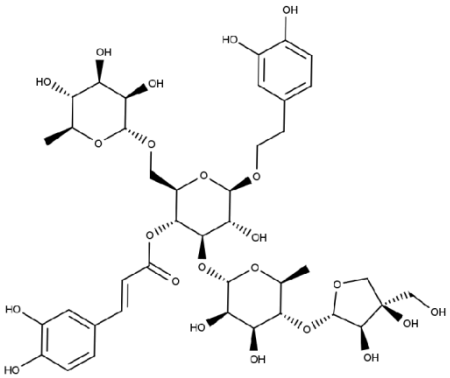
Code	Compound	Reference	Molecular Weight (Da)
PG_418	2‴,3‴-Diacetyl-O-betonyoside D	(compound 74) – (31) (compound 72) – (26)	772.703



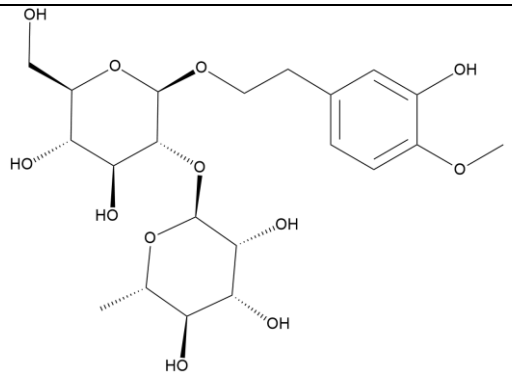
Code	Compound	Reference	Molecular Weight (Da)
PG_419	3‴,4‴-diacety-O-betonyoside D	(compound 75) – (31) (compound 73) – (26)	868.832



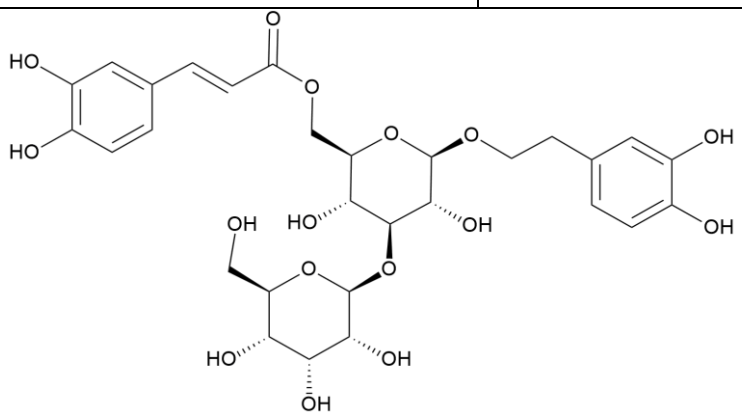
Code	Compound	Reference	Molecular Weight (Da)
PG_420	Stewartiiside	(compound 76) – (31)	904.862



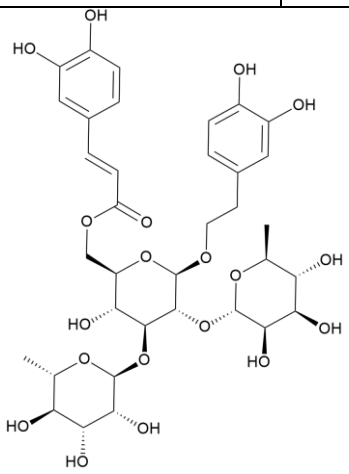
Code	Compound	Reference	Molecular Weight (Da)
PG_421	2-(3-Hydroxy-4-methoxyphenyl) ethanol 1-O-[α-L-rhamnopyranosyl-(1□2)- β -D-glucopyranoside]	(compound 77) – (31)	476.473



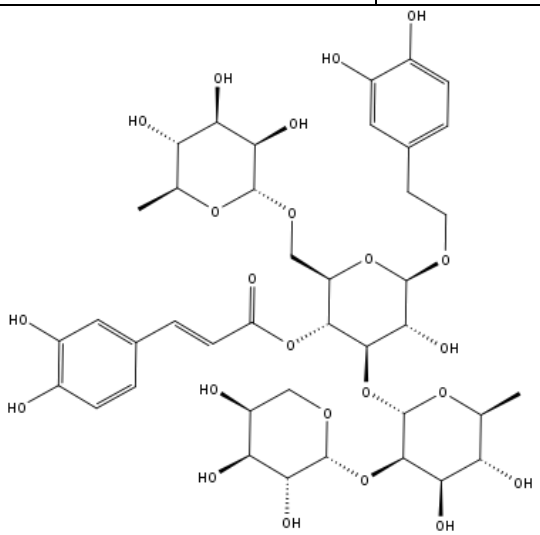
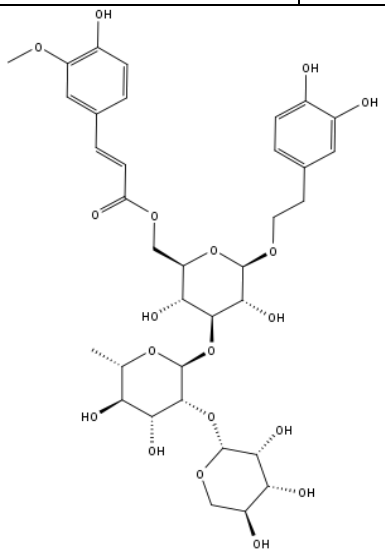
Code	Compound	Reference	Molecular Weight (Da)
PG_422	2-(3,4-Dihydroxyphenyl) ethyl 3-O-β-D-allopyranosyl-6-O-caffeoyl- β- D-glucopyranoside	(compound 78) – (31)	640.589

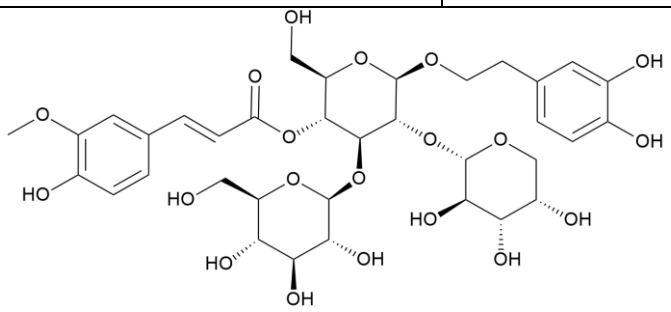
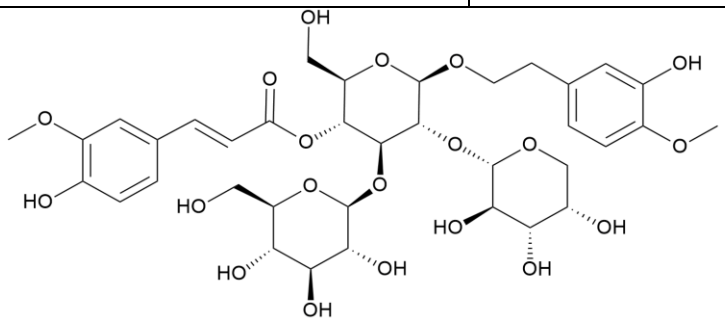
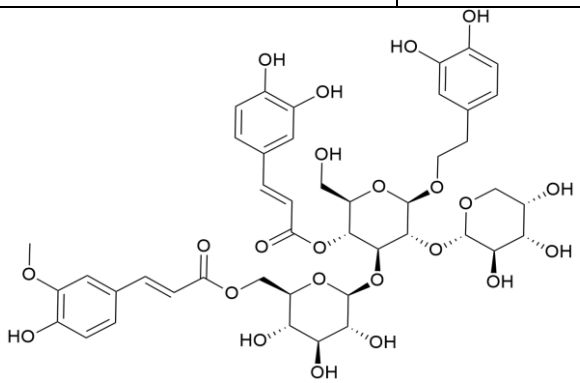


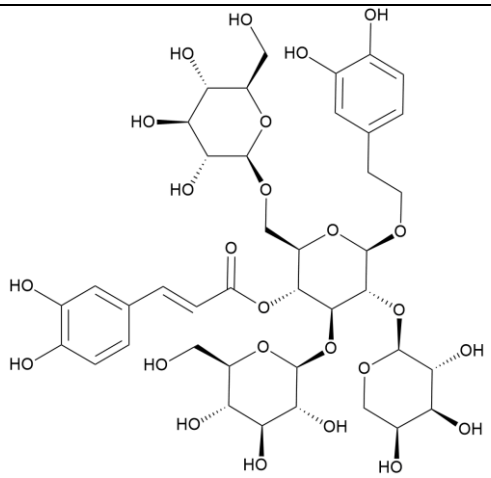
Code	Compound	Reference	Molecular Weight (Da)
PG_423	Isocassifolioside	(compound 79) – (31)	770.731



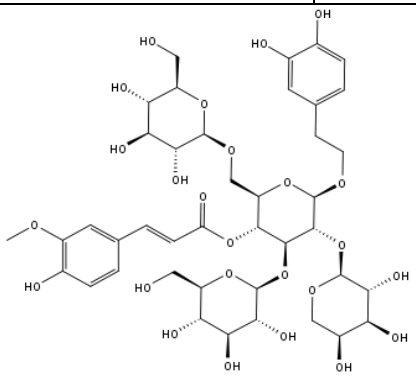
Code	Compound	Reference	Molecular Weight (Da)

PG_424	Poliumoside B	(compound 81) – (31)	902.846
			
Code	Compound	Reference	Molecular Weight (Da)
PG_425	1-(3,4-Dihydroxyphenylethyl)-O-α-L-lyxopyranosyl-(1→2)-α-L-hamnopyranosyl-(1→3)-6-Otransferuloyl- β -D-glucopyranoside	(compound 82) – (31)	770.731
			
Code	Compound	Reference	Molecular Weight (Da)
PG_426	Chionoside A	(compound 83) – (31)	786.73

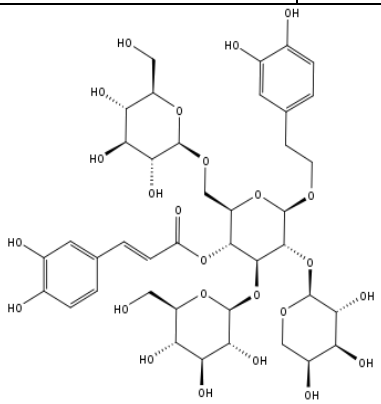
			
Code	Compound	Reference	Molecular Weight (Da)
PG_427	Chionoside B	(compound 84) – (31)	800.757
			
Code	Compound	Reference	Molecular Weight (Da)
PG_428	Chionoside C	(compound 85) – (31)	948.874
			
Code	Compound	Reference	Molecular Weight (Da)
PG_429	Chionoside D	(compound 86) – (31)	936.86



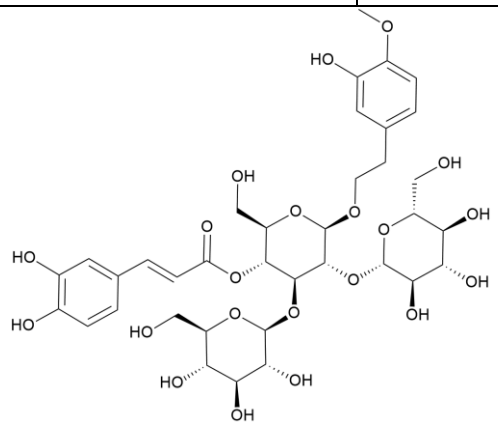
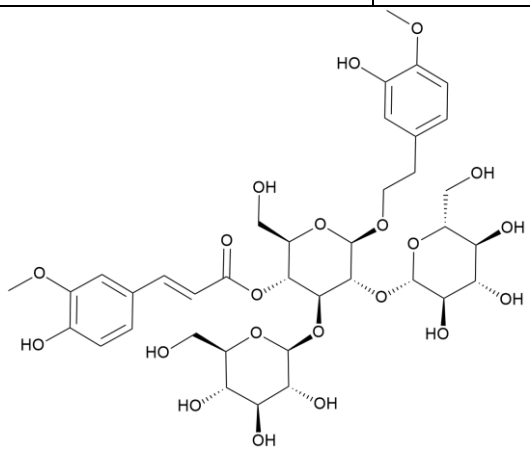
Code	Compound	Reference	Molecular Weight (Da)
PG_430	Chionoside E	(compound 87) – (31)	950.887

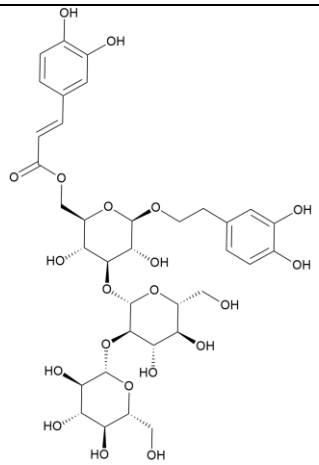


Code	Compound	Reference	Molecular Weight (Da)
PG_431	Chionoside F	(compound 88) – (31)	936.86

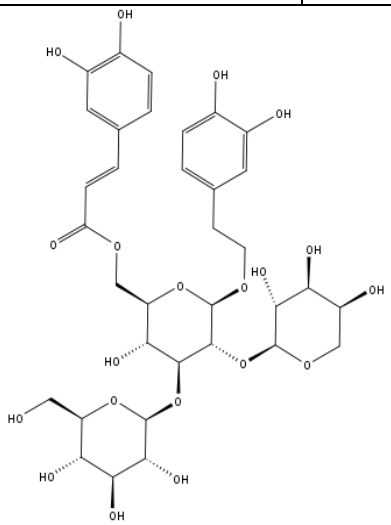


Code	Compound	Reference	Molecular

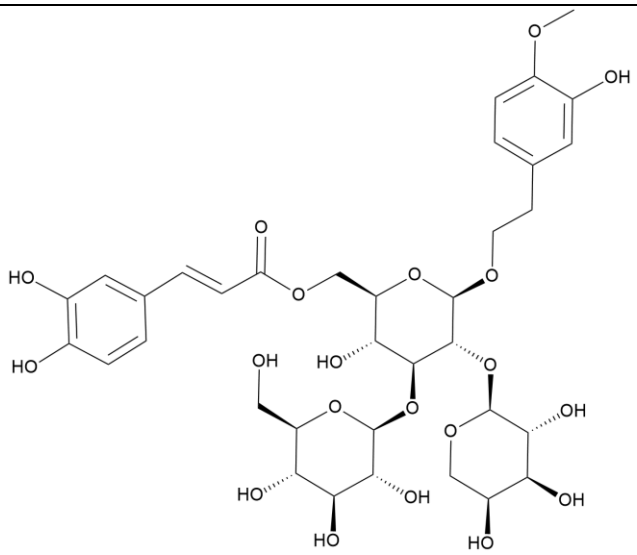
			Weight (Da)
PG_432	Chionoside G	(compound 89) – (31)	818.772
			
Code	Compound	Reference	Molecular Weight (Da)
PG_433	Chionoside I	(compound 90) – (31)	830.783
			
Code	Compound	Reference	Molecular Weight (Da)
PG_434	Isochionoside J	(compound 91) – (31)	802.729



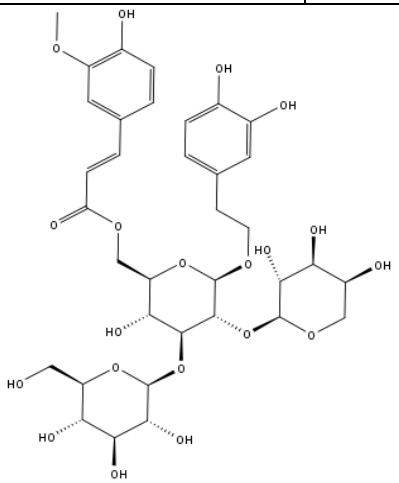
Code	Compound	Reference	Molecular Weight (Da)
PG_435	Isoaragoside	(compound 92) – (31)	774.719



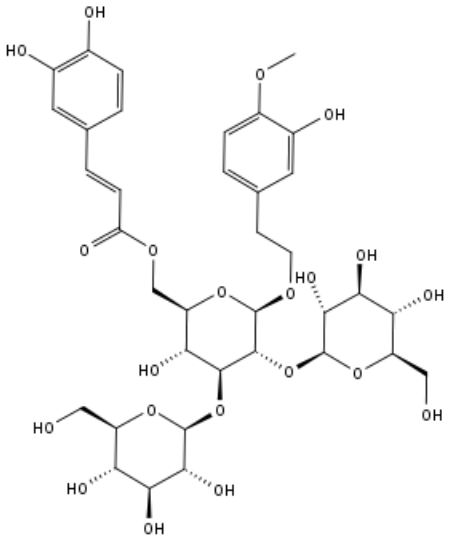
Code	Compound	Reference	Molecular Weight (Da)
PG_436	Isochionoside K	(compound 93) – (31)	788.746



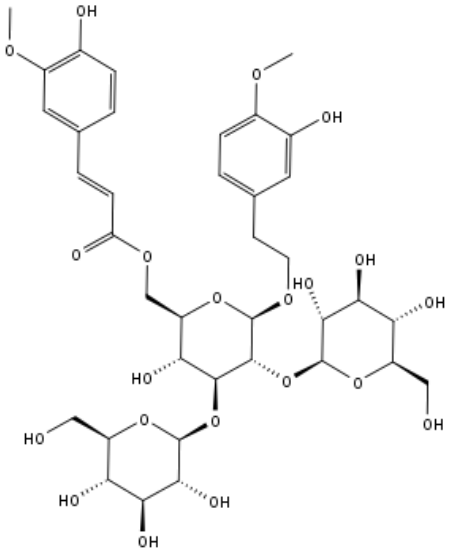
Code	Compound	Reference	Molecular Weight (Da)
PG_437	Isochionoside A	(compound 94) – (31)	786.73



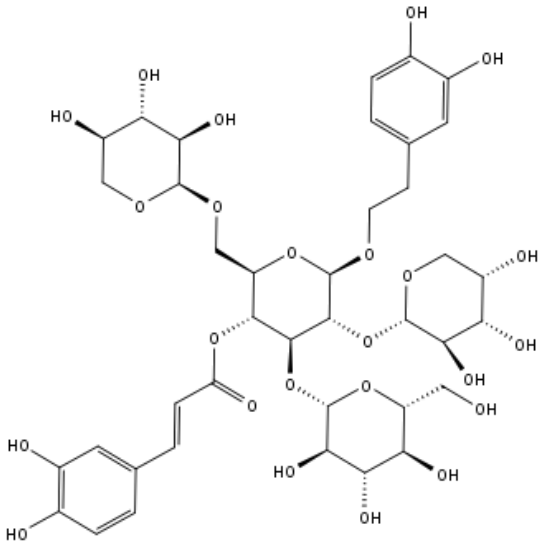
Code	Compound	Reference	Molecular Weight (Da)
PG_438	Isochionoside G	(compound 95) – (31)	816.756



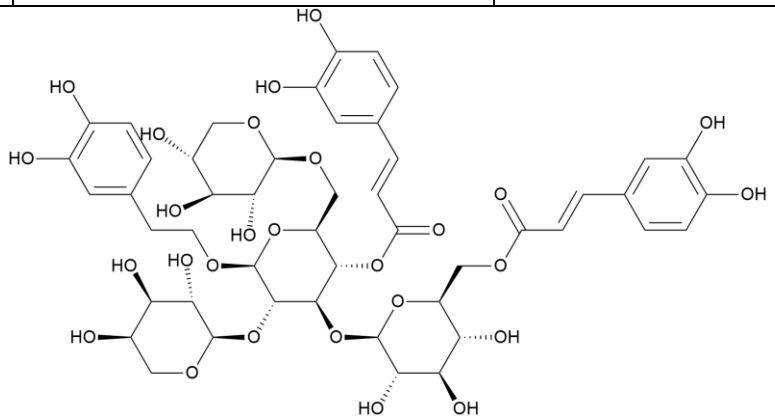
Code	Compound	Reference	Molecular Weight (Da)
PG_439	Isochionoside I	(compound 96) – (31)	830.783



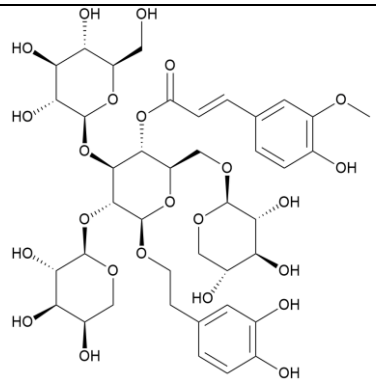
Code	Compound	Reference	Molecular Weight (Da)
PG_440	Helioside A	(compound 97) – (31)	904.818



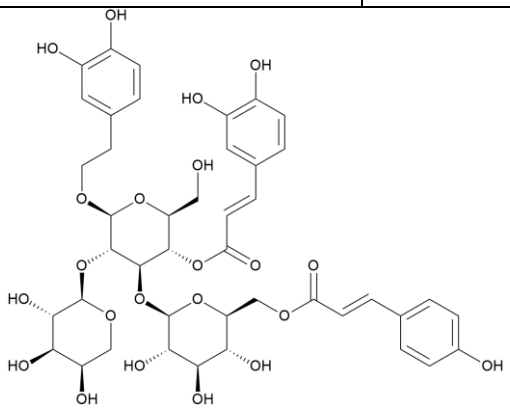
Code	Compound	Reference	Molecular Weight (Da)
PG_441	Helioside B	(compound 98) – (31)	1068.98



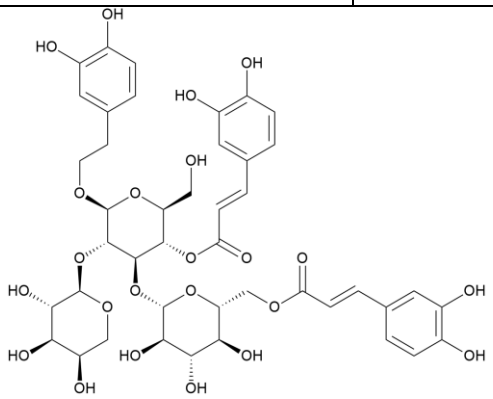
Code	Compound	Reference	Molecular Weight (Da)
PG_442	Helioside C	(compound 99) – (31)	978.845



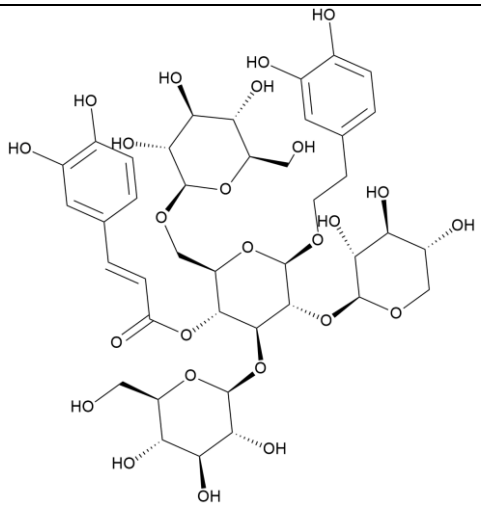
Code	Compound	Reference	Molecular Weight (Da)
PG_443	Helioside D	(compound 100) – (31)	920.864



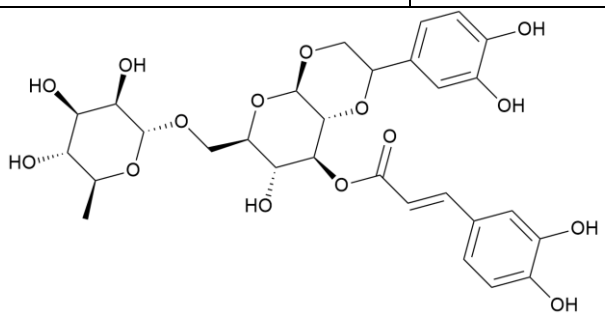
Code	Compound	Reference	Molecular Weight (Da)
PG_444	Helioside E	(compound 101) – (31)	934.847



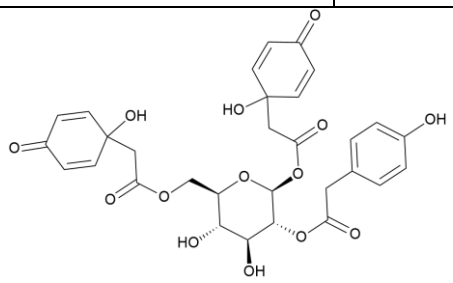
Code	Compound	Reference	Molecular Weight (Da)
PG_445	Helioside F	(compound 102) – (31)	934.844



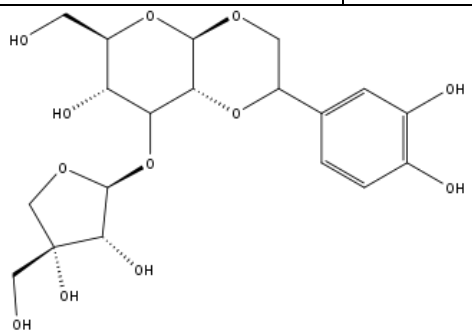
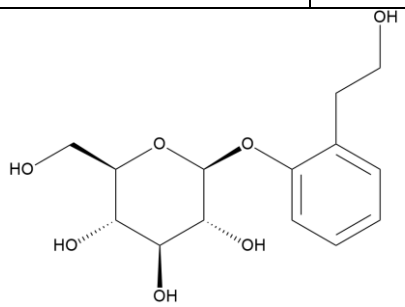
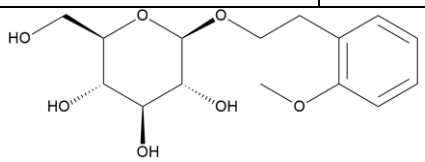
Code	Compound	Reference	Molecular Weight (Da)
PG_446	Lianqiaoxinoside B	(compound 103) – (31)	622.574

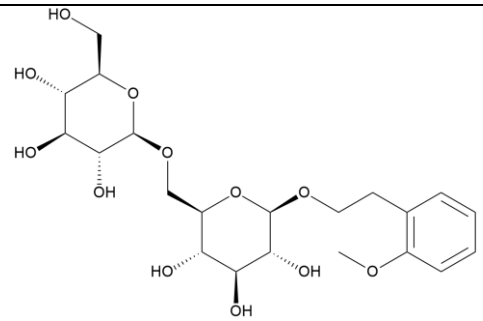


Code	Compound	Reference	Molecular Weight (Da)
PG_447	1,6-bis (1-hydroxy-4-oxo-2,5-cyclohexadiene-1-acetyl)-3- (para-hydroxybenzeneacetyl)-β-glucopyraoside	(compound 105) – (31)	614.554

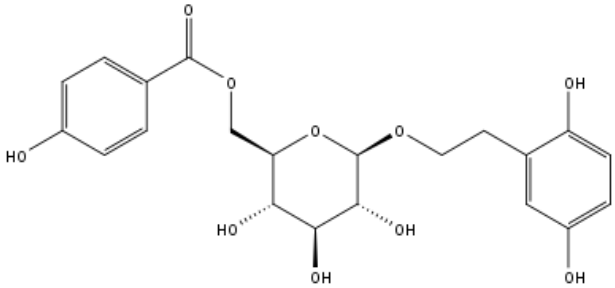


Code	Compound	Reference	Molecular Weight (Da)

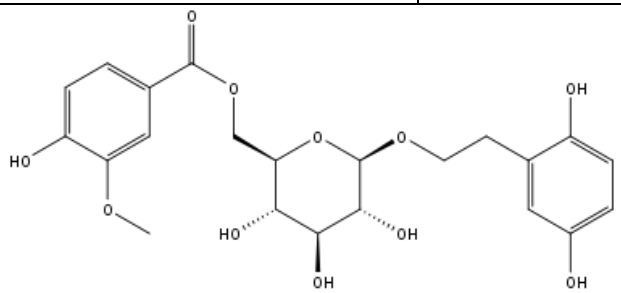
PG_448	Taraffinisoside A	(compound 104) – (31)	446.403
			
Code	Compound	Reference	Molecular Weight (Da)
PG_449	Tazettoside A (or Tazettosides A)	(compound 106) – (31)	300.306
			
Code	Compound	Reference	Molecular Weight (Da)
PG_450	Tazettoside B (or Tazettosides B)	(compound 107) – (31) (compound 86) – (26)	314.333
			
Code	Compound	Reference	Molecular Weight (Da)
PG_451	Tazettoside C (or Tazettosides C)	(compound 108) – (31) (compound 87) – (26)	476.473



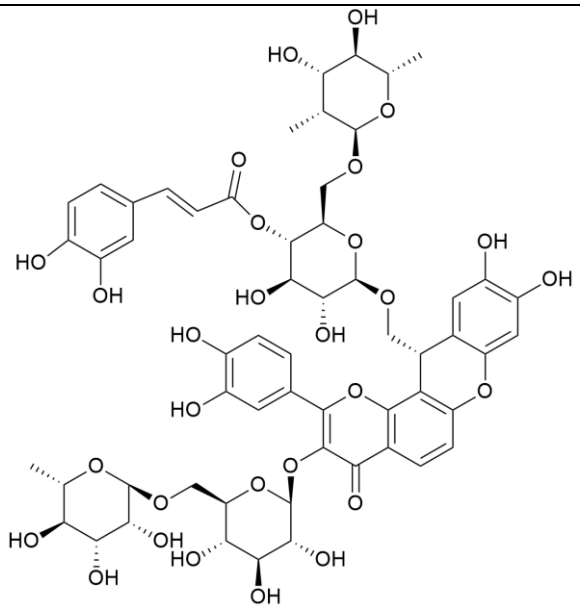
Code	Compound	Reference	Molecular Weight (Da)
PG_452	2-(2,5-dihydroxyphenyl)-ethyl-O-(6-O-p-hydroxybenzoyl)-β-D-glucopyranose	(compound 109) – (31) (compound 88) – (26)	436.412



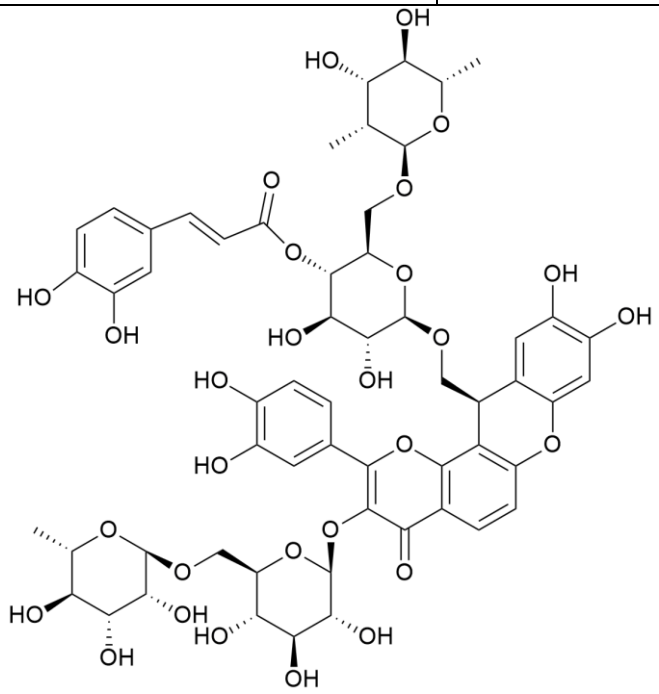
Code	Compound	Reference	Molecular Weight (Da)
PG_453	2-(2,5-dihydroxyphenyl)-ethyl-O-(6-O-vanilloyl)-β-D-glucopyranose	(compound 110) – (31)	466.437



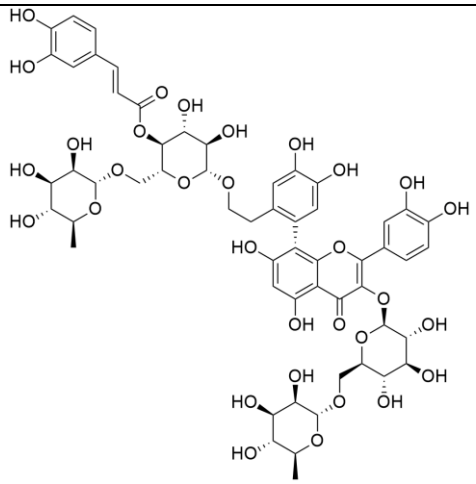
Code	Compound	Reference	Molecular Weight (Da)
PG_454	Forsythoneosides A 7'R	(compound 111) – (31)	1216.13



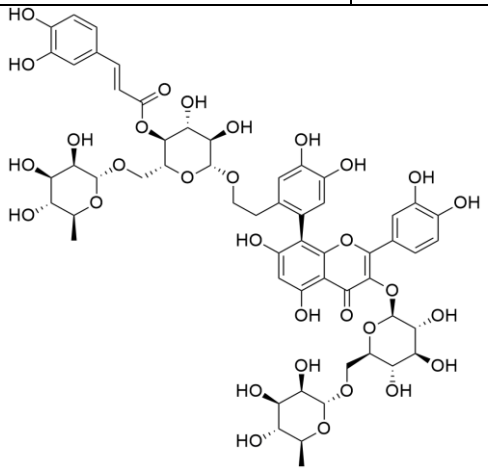
Code	Compound	Reference	Molecular Weight (Da)
PG_455	Forsythoneosides B 7'S	(compound 112) – (31)	1214.11



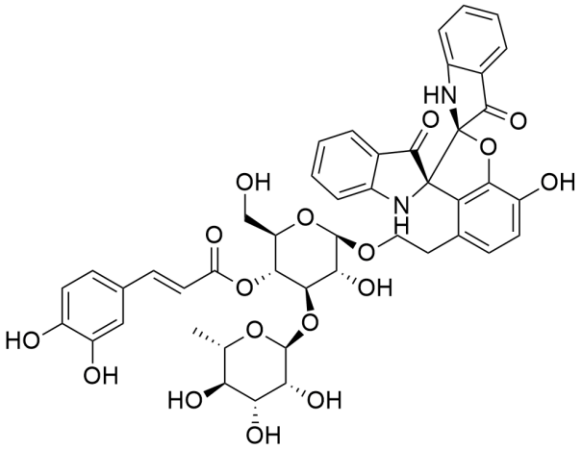
Code	Compound	Reference	Molecular Weight (Da)
PG_456	Forsythoneosides C (*M* CONFIGURATION)	(compound 113) – (31)	1235.11



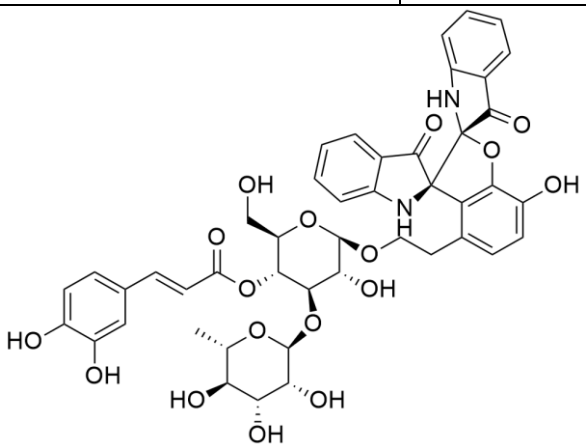
Code	Compound	Reference	Molecular Weight (Da)
PG_457	Forsythoneosides D (*P* CONFIGURATION)	(compound 114) – (31)	1235.11



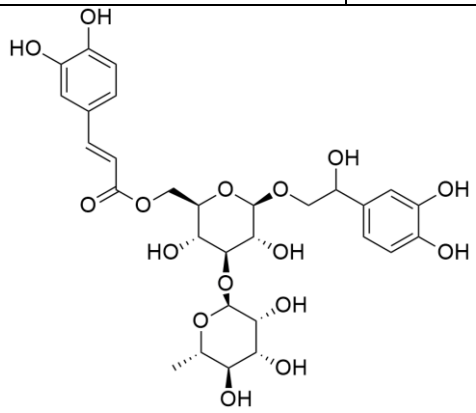
Code	Compound	Reference	Molecular Weight (Da)
PG_458	NO TRIVIAL NAME	(compound 115) – (31)	884.841

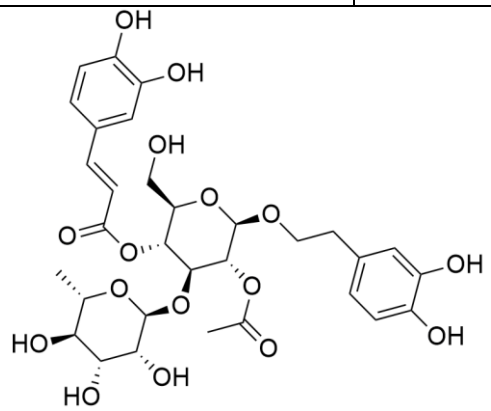
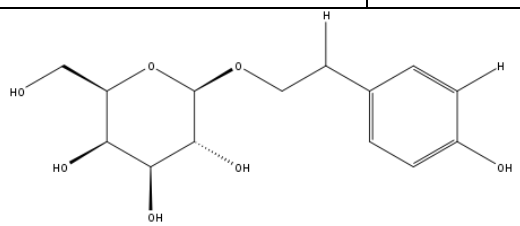
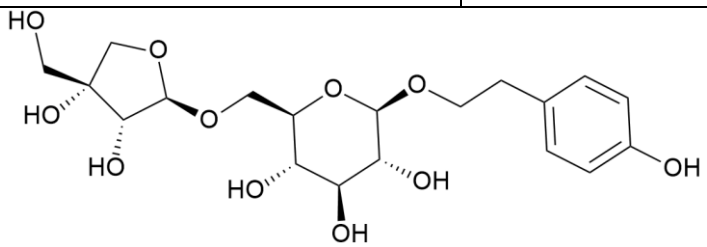


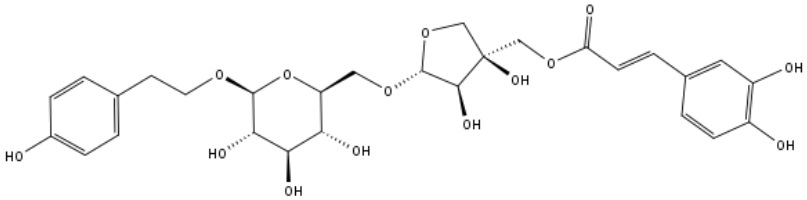
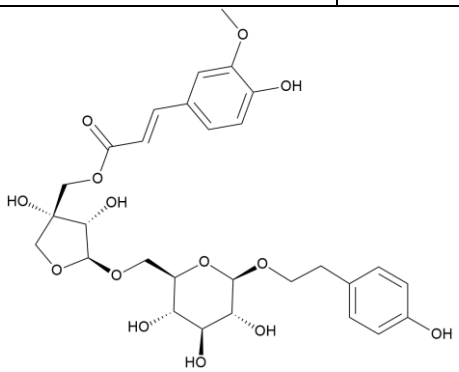
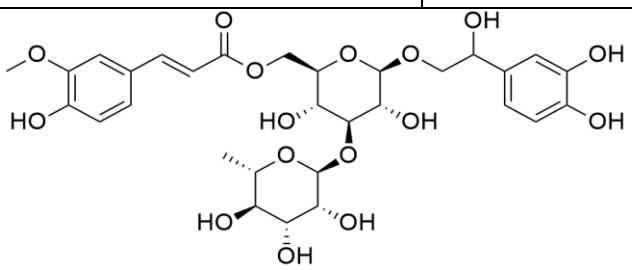
Code	Compound	Reference	Molecular Weight (Da)
PG_459	NO TRIVIAL NAME	(compound 116) – (31)	884.841

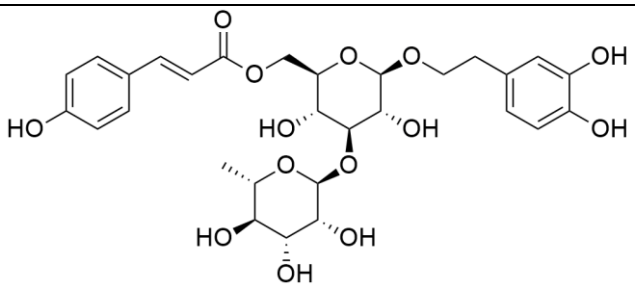


Code	Compound	Reference	Molecular Weight (Da)
PG_460	Isocampneoside II	(compound 131) – (31)	640.589

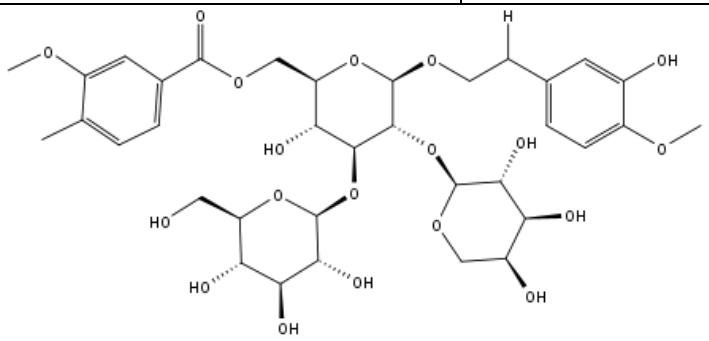


Code	Compound	Reference	Molecular Weight (Da)
PG_462	2'-acetylacteoside	(compound 137) – (31)	666.627
			
Code	Compound	Reference	Molecular Weight (Da)
PG_463	Tyrosol galactoside	(compound 140) – (31)	300.306
			
Code	Compound	Reference	Molecular Weight (Da)
PG_464	Osmanthuside H	(compound 1) – (26)	432.42
			
Code	Compound	Reference	Molecular Weight (Da)
PG_465	Osmanthuside I	(compound 2) –	594.564

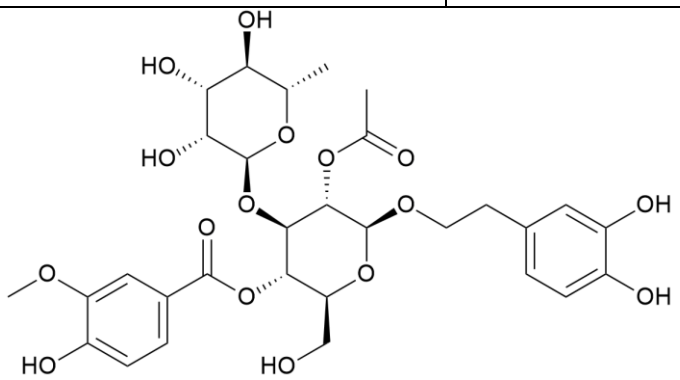
		(26)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_466	Osmanthuside J	(compound 3) – (26)	608.591
			
Code	Compound	Reference	Molecular Weight (Da)
PG_467	NO TRIVIAL NAME (4)	(compound 4) – (26)	654.616
			
Code	Compound	Reference	Molecular Weight (Da)
PG_469	Lipedosides A-II	(compound 6) – (26)	608.591



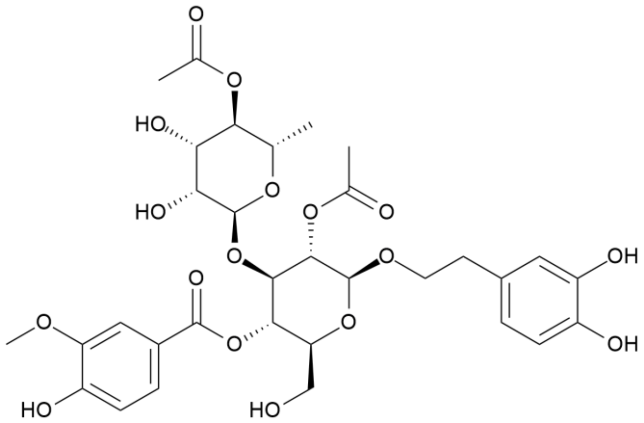
Code	Compound	Reference	Molecular Weight (Da)
PG_470	NO TRIVIAL NAME	(compound 7) – (26)	772.747



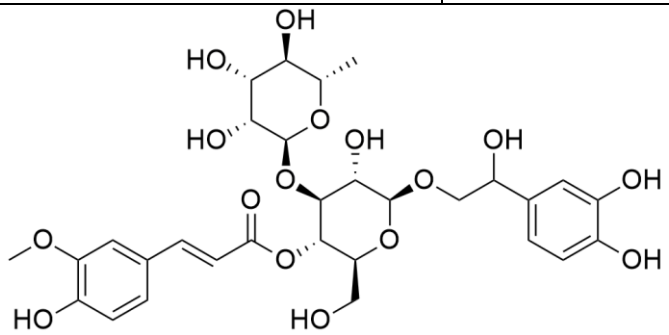
Code	Compound	Reference	Molecular Weight (Da)
PG_471	2-O-Acetyl-3‴-O-methylverbascoside	(compound 8) – (26)	654.616



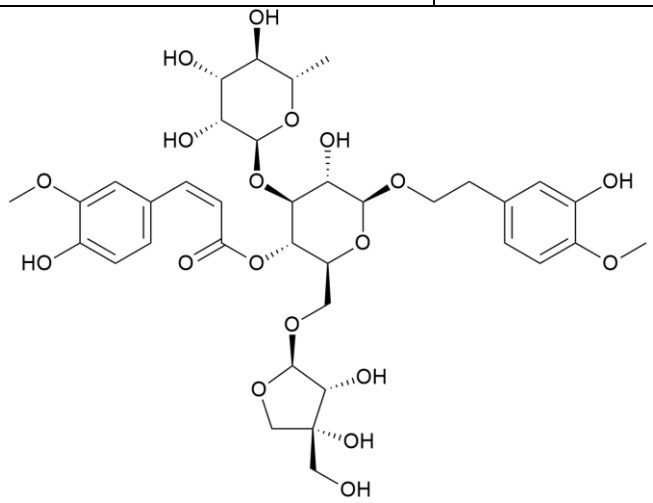
Code	Compound	Reference	Molecular Weight (Da)
PG_472	2,4″-Di-O-acetyl-3‴-O-methylverbascoside	(compound 9) – (26)	696.653



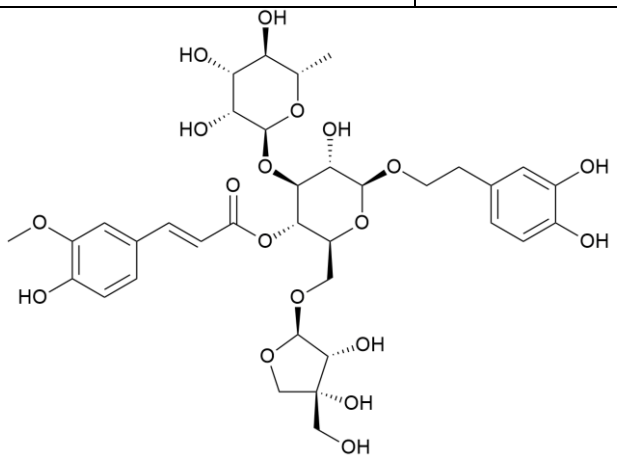
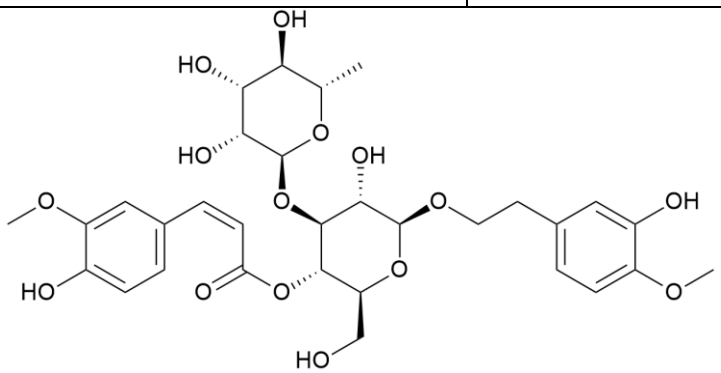
Code	Compound	Reference	Molecular Weight (Da)
PG_473	Betonyosides A	(compound 10) – (26)	654.616

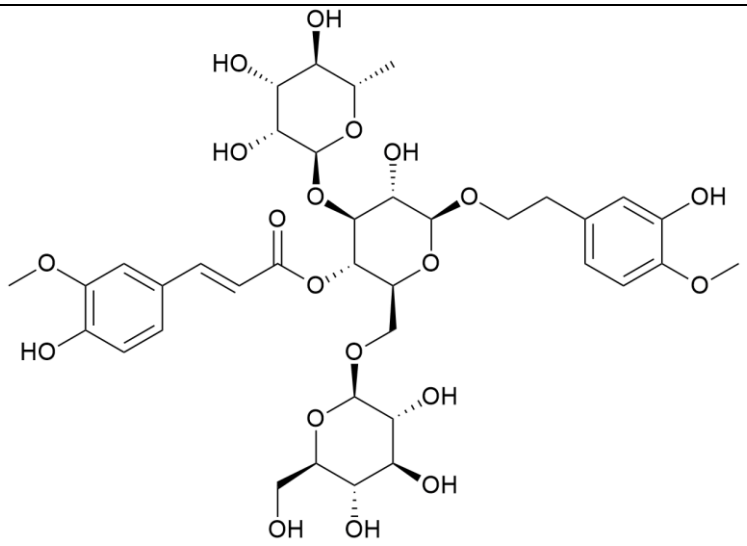


Code	Compound	Reference	Molecular Weight (Da)
PG_474	Betonyosides D	(compound 11) – (26)	784.758

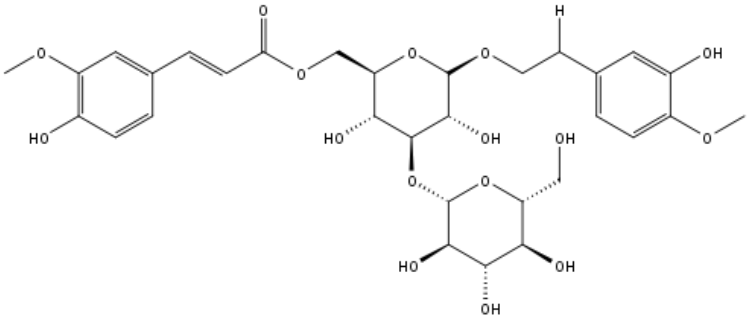


Code	Compound	Reference	Molecular Weight (Da)

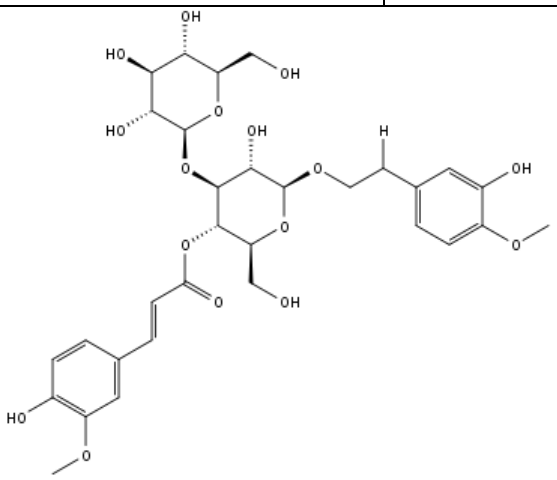
PG_475	Betonyosides E	(compound 12) – (26)	770.731
			
Code	Compound	Reference	Molecular Weight (Da)
PG_476	Betonyosides F	(compound 13) – (26)	652.644
			
Code	Compound	Reference	Molecular Weight (Da)
PG_477	2-(3-Hydroxy-4-methoxy-phenyl)-ethyl-O-(α-Lrhamnosyl)-(1→3)-O-(α-L-rhamnosyl)-(1→6)-4-O-E-feruloyl-β-D-glucopyranoside	(compound 14) – (26)	814.828

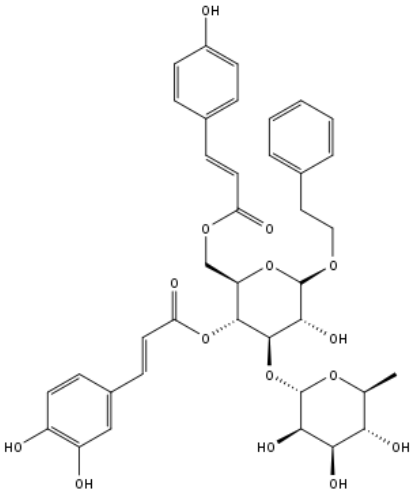
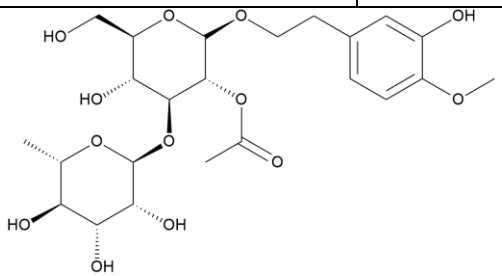


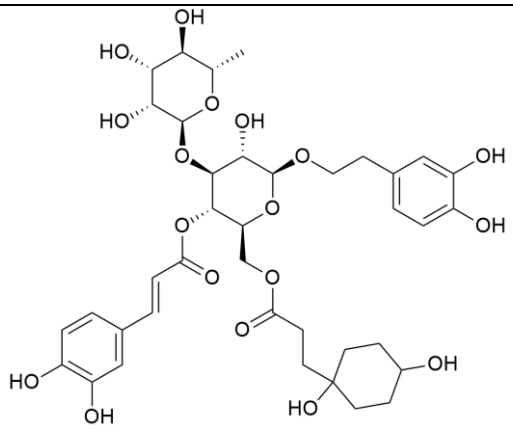
Code	Compound	Reference	Molecular Weight (Da)
PG_478	Scrosides B	(compound 15) – (26)	668.643



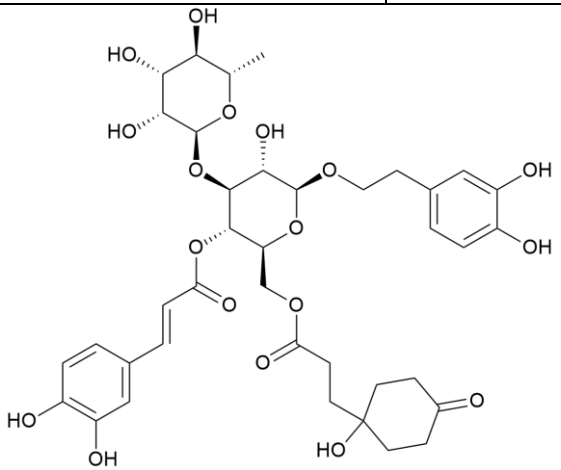
Code	Compound	Reference	Molecular Weight (Da)
PG_479	Scrosides C	(compound 16) – (26)	668.643



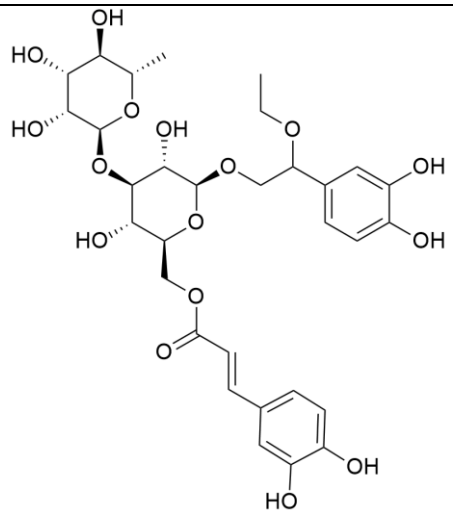
Code	Compound	Reference	Molecular Weight (Da)
PG_480	NO TRIVIAL NAME	(compound 17) – (26)	738.736
			
Code	Compound	Reference	Molecular Weight (Da)
PG_481	Lophanthoside A	(compound 18) – (26)	518.51
			
Code	Compound	Reference	Molecular Weight (Da)
PG_482	NO TRIVIAL NAME	(compound 19) – (26)	794.797



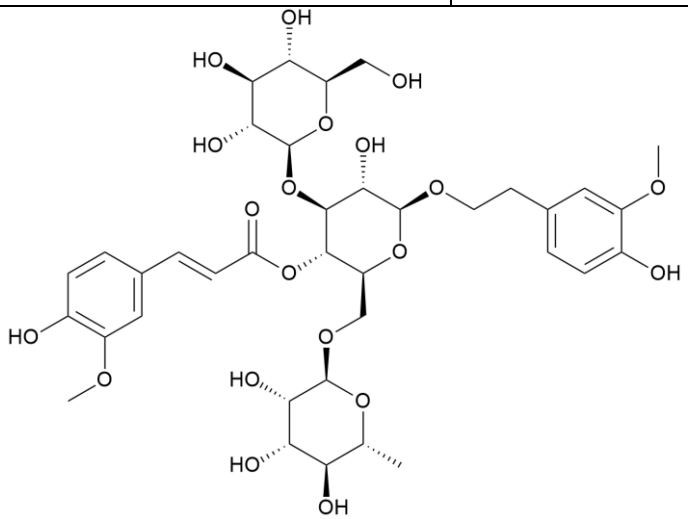
Code	Compound	Reference	Molecular Weight (Da)
PG_483	NO TRIVIAL NAME	(compound 20) – (26)	792.781



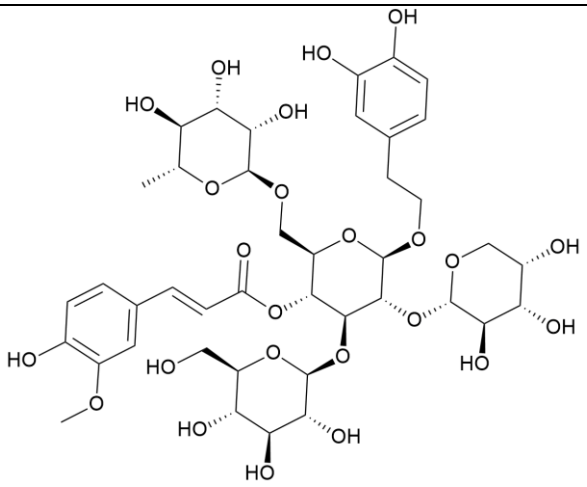
Code	Compound	Reference	Molecular Weight (Da)
PG_484	Isoilicifolioside A	(compound 21) – (26)	668.643



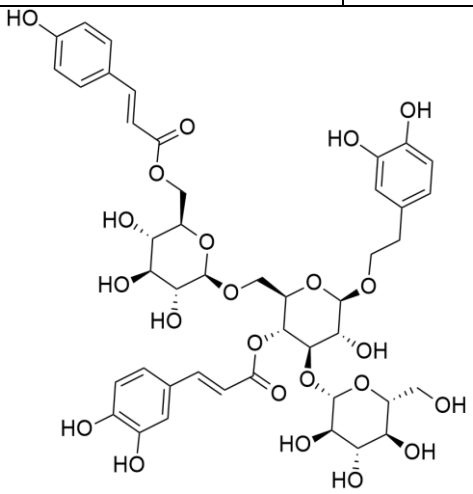
Code	Compound	Reference	Molecular Weight (Da)
PG_485	Digicilisides A	(compound 23) – (26)	814.784



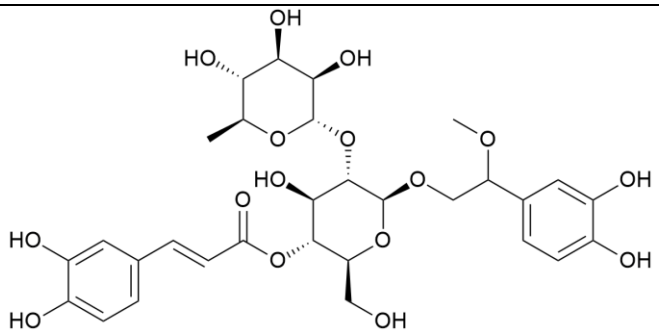
Code	Compound	Reference	Molecular Weight (Da)
PG_486	Digicilisides B	(compound 24) – (26)	932.872



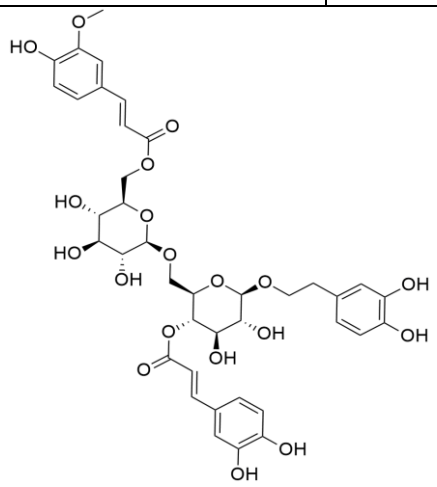
Code	Compound	Reference	Molecular Weight (Da)
PG_487	Digicilisides C	(compound 25) – (26)	950.89



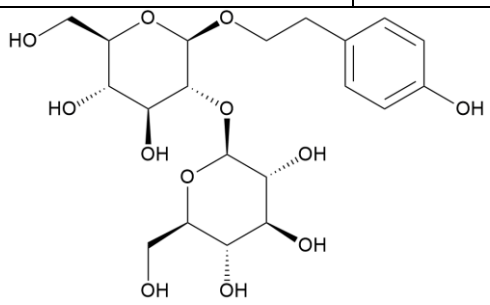
Code	Compound	Reference	Molecular Weight (Da)
PG_488	α-L-Rhamnopyranosyl-(1→2)-β-D-[4”-(8E)-7-(3,4-dihydroxyphenyl)-8-propenoate,1”-O-(7S)-7-(3,4-dihydroxyphenyl)-7-methoxyethyl]-glucopyranoside	(compound 26) – (26)	654.616



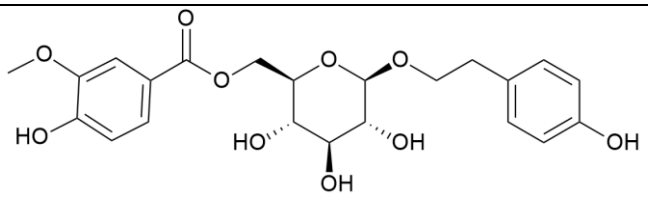
Code	Compound	Reference	Molecular Weight (Da)
PG_489	Digiviridifloroside	(compound 27) – (26)	816.759



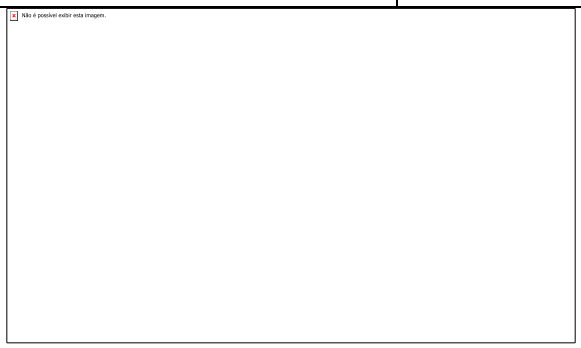
Code	Compound	Reference	Molecular Weight (Da)
PG_490	2-(4-Hydroxyphenyl)ethanol-O-β-Dglucopyranosyl-(1→2)-O-β-Dglucopyranoside	(compound 28) – 29]	462.446



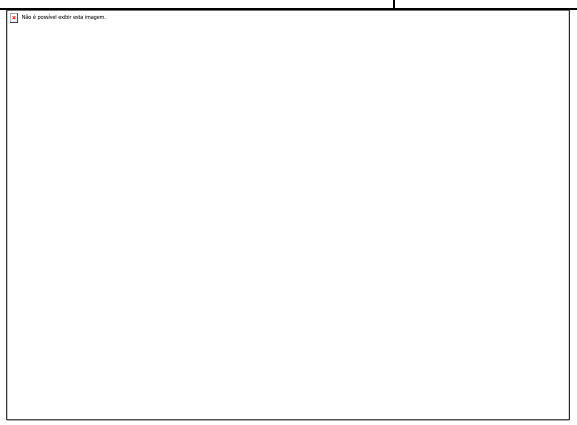
Code	Compound	Reference	Molecular Weight (Da)
PG_491	Forsythoside M	(compound 29) – (26)	450.438



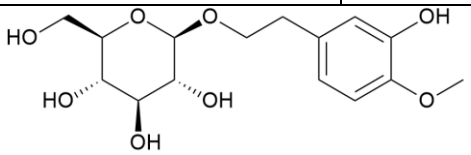
Code	Compound	Reference	Molecular Weight (Da)
PG_492	Forsythoside N	(compound 30) – (26)	450.438



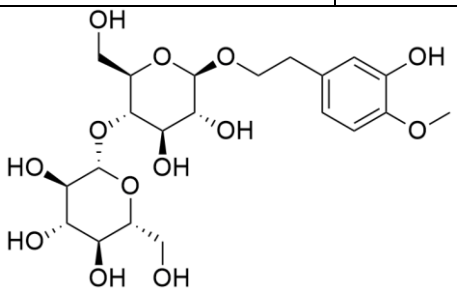
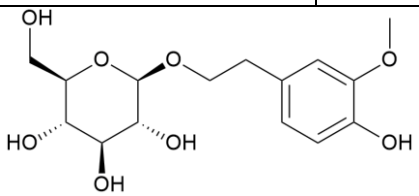
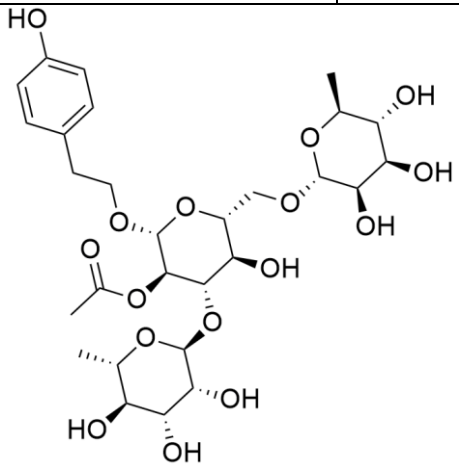
Code	Compound	Reference	Molecular Weight (Da)
PG_493	Forsythoside P	(compound 31) – (26)	608.591

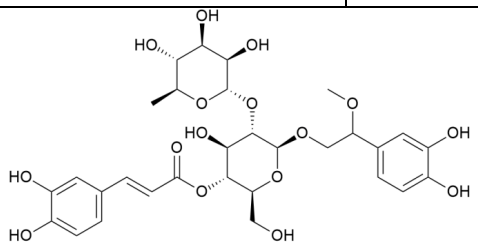
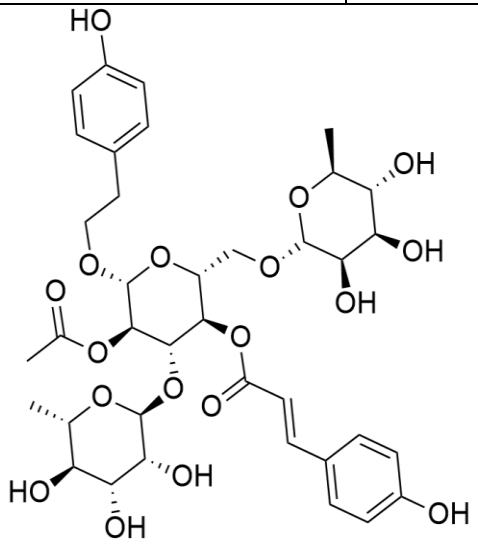


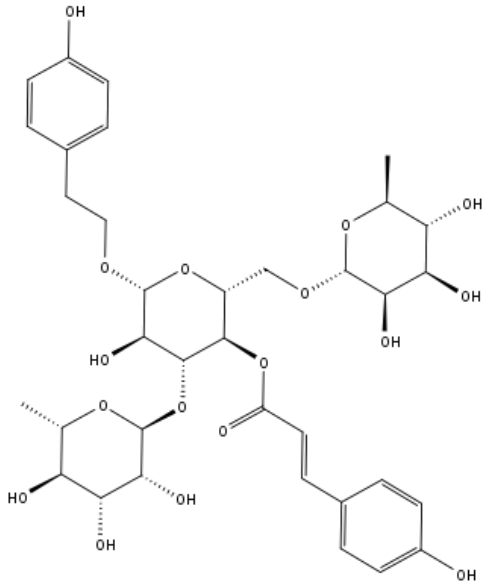
Code	Compound	Reference	Molecular Weight (Da)
PG_494	Hodgsonialloside A	(compound 32) – (26)	330.332



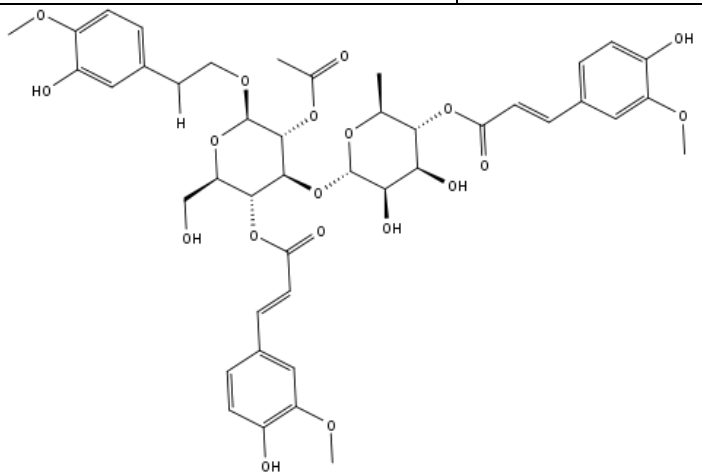
Code	Compound	Reference	Molecular

			Weight (Da)
PG_495	Hodgsonialloside B	(compound 33) – (26)	492.472
			
Code	Compound	Reference	Molecular Weight (Da)
PG_496	Hodgsonialloside C	(compound 34) – (26)	330.332
			
Code	Compound	Reference	Molecular Weight (Da)
PG_497	1-β-p-Hydroxyphenyl-ethyl-2-O-acetyl-3,6-di-α-L-rhamnopyranosyl-β-D-glucopyranoside	(compound 35) – (26)	634.625
			
Code	Compound	Reference	Molecular Weight (Da)
PG_498	1-β-p-Hydroxyphenyl-ethyl-3,6-O-di-α-L-rhamnopyranosyl-β-D-	(compound 36) –	592.589

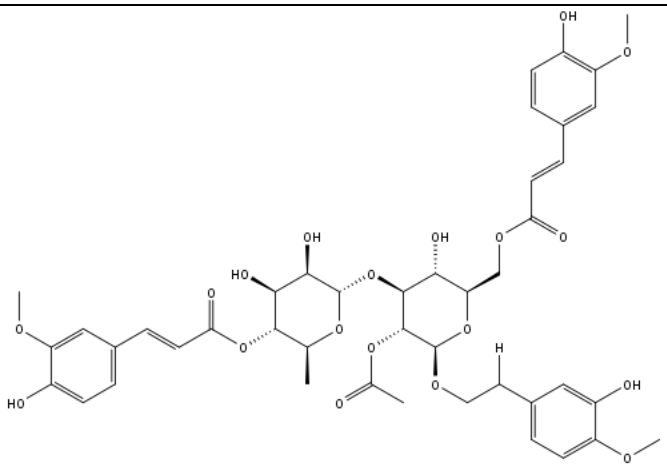
	glucopyranoside	(26)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_499	1-β-p-Hydroxyphenyl-ethyl-2-O-acetyl-3,6-di-α-L-rhamnopyranosyl-4-p-coumaroyl-β-D-glucopyranoside	(compound 37) – (26)	782.786
			
Code	Compound	Reference	Molecular Weight (Da)
PG_500	1-β-p-hydroxyphenyl-ethyl-3,6-di-α-Lrhamnopyranosyl-4-p-coumaroyl-β-Dglucopyranoside	(compound 38) – (26)	738.733



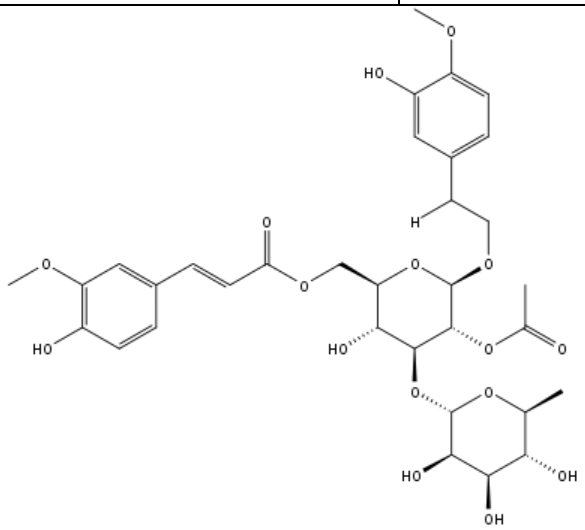
Code	Compound	Reference	Molecular Weight (Da)
PG_501	Ternifoliusoside F	(compound 39) – (26)	872.867



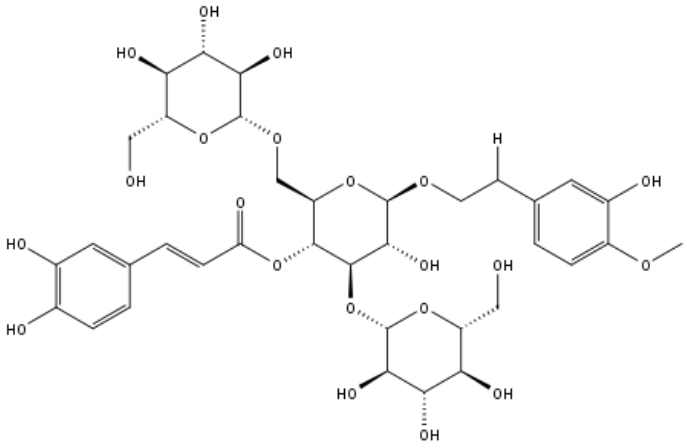
Code	Compound	Reference	Molecular Weight (Da)
PG_502	Ternifoliusoside G	(compound 40) – (26)	874.883



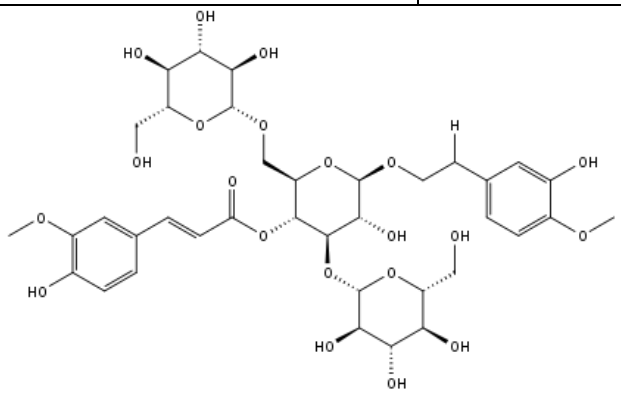
Code	Compound	Reference	Molecular Weight (Da)
PG_503	Ternifoliusoside H	(compound 41) – (26)	694.68



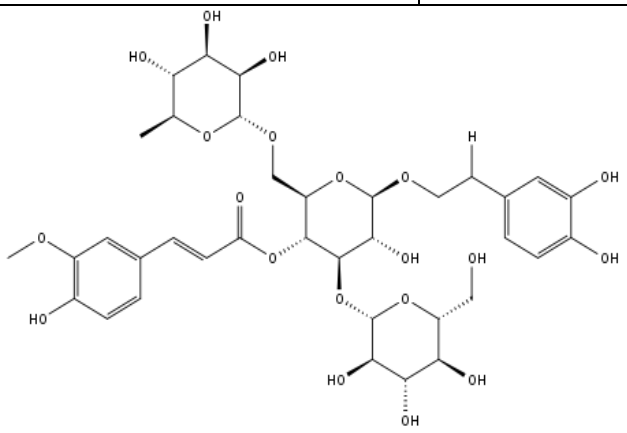
Code	Compound	Reference	Molecular Weight (Da)
PG_504	Digidavisoside A	(compound 44) – (26)	816.756

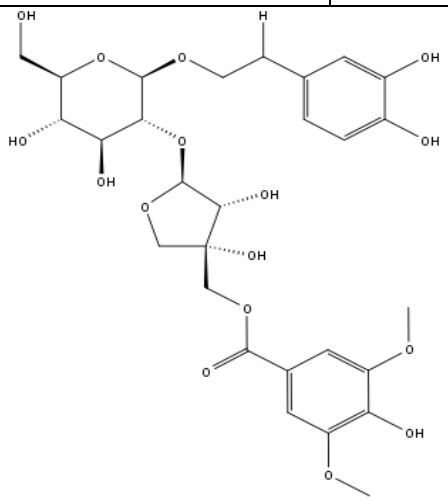
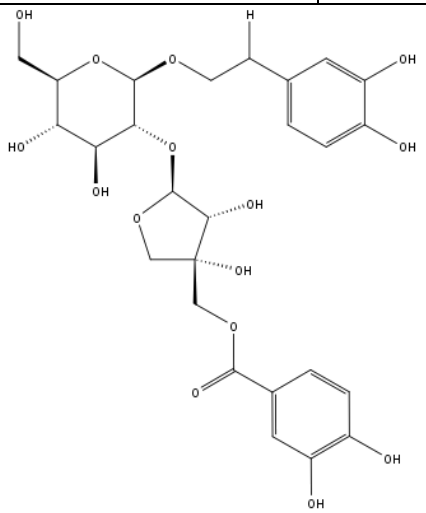


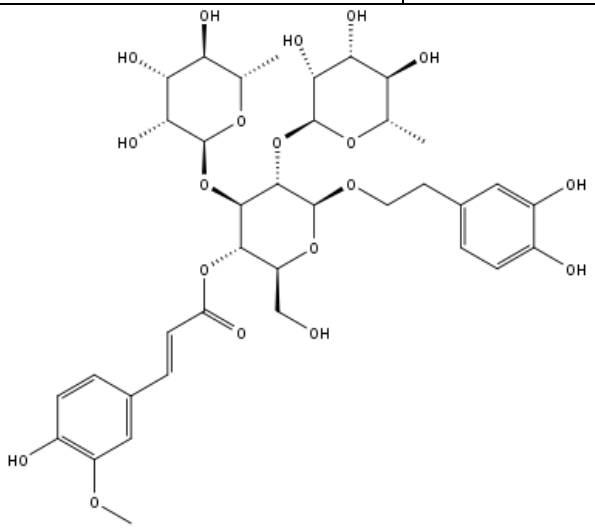
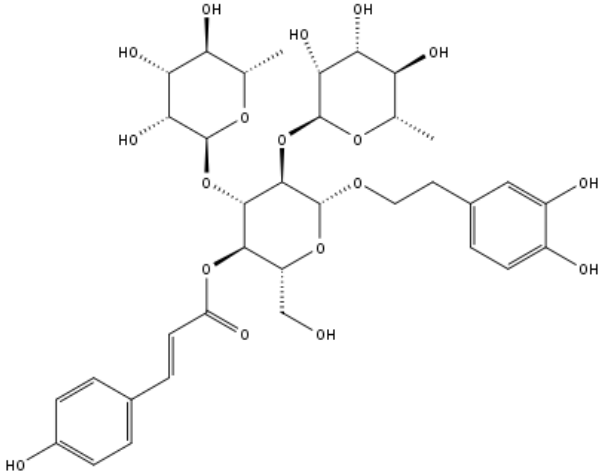
Code	Compound	Reference	Molecular Weight (Da)
PG_505	Digidavisoside B	(compound 45) – (26)	830.783

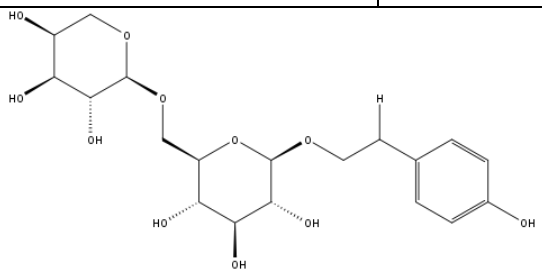
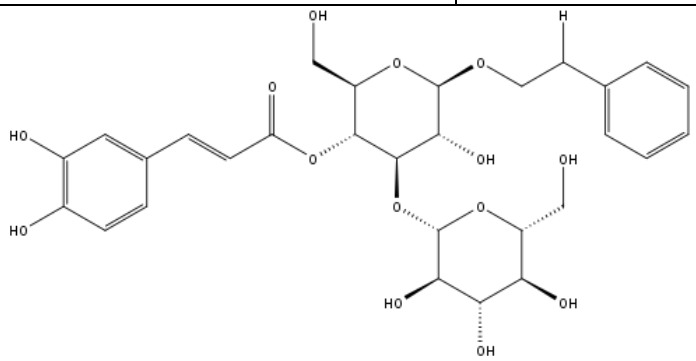
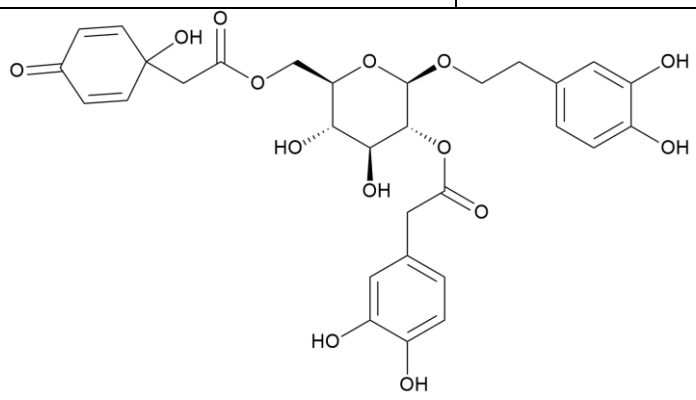


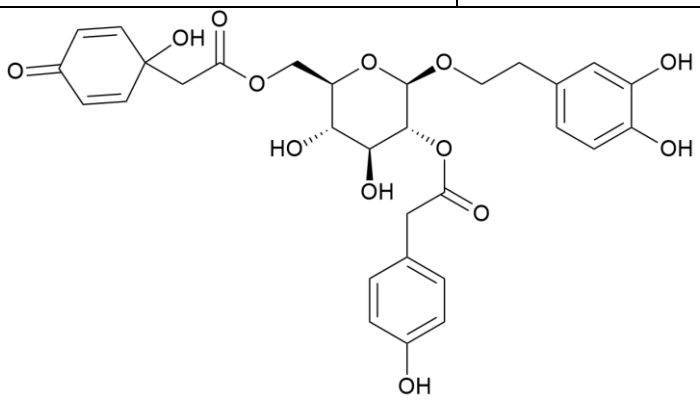
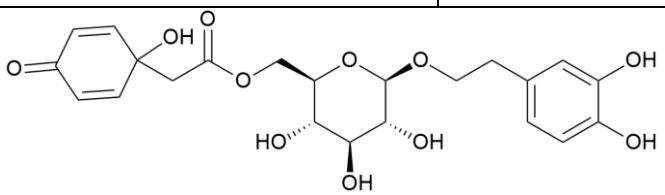
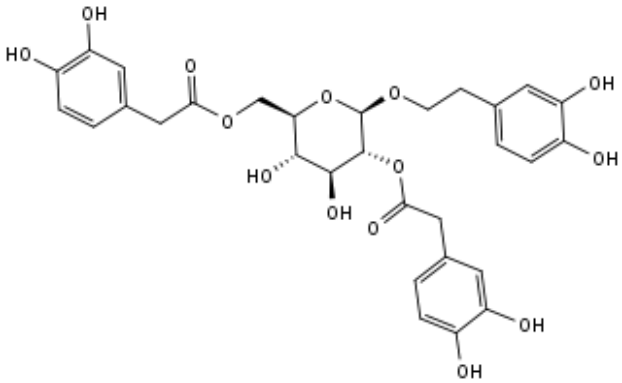
Code	Compound	Reference	Molecular Weight (Da)
PG_506	Davisoside	(compound 46) – (26)	800.757

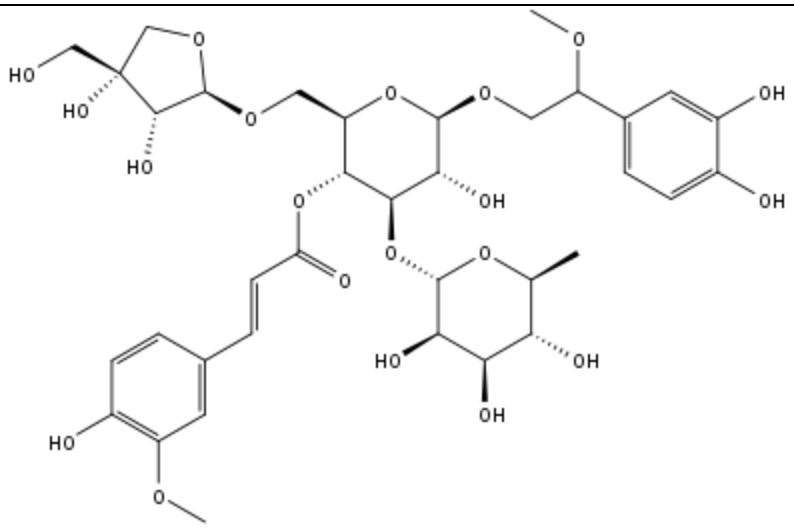


Code	Compound	Reference	Molecular Weight (Da)
PG_507	3,4-Dihydroxyphenyl)ethyl2-O-[5-O-(4-hydroxy-3,5-dimethoxybenzoyl)-β-D-apiofuranosyl]-β-D-glucopyranoside	(compound 47) – (26)	626.578
			
Code	Compound	Reference	Molecular Weight (Da)
PG_508	3,4-Dihydroxyphenyl)ethyl 2-O-[5-O-(3,4-Dihydroxybenzoyl)-β-D-apiofuranosyl]-β-D-glucopyranoside	(compound 48) – (26)	584.525
			
Code	Compound	Reference	Molecular

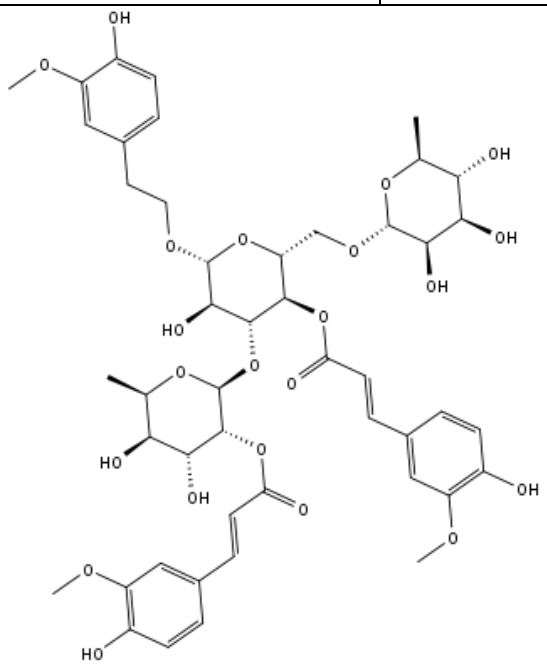
			Weight (Da)
PG_509	2-(3,4-Dihydroxyphenyl)-ethyl 1-O-[4-O-feruloyl-2-O-α-L-rhamnopyranosyl-3-O-α-L-rhamnopyranosyl]-β-D-glucopyranoside	(compound 49) – (26)	786.774
			
Code	Compound	Reference	Molecular Weight (Da)
PG_510	2-(3,4-Dihydroxyphenyl)-ethyl1-O-[4-O-coumaroyl-2-O-α -L-rhamnopyranosyl-3-O- α-L-rhamnopyranosyl]-β-D-glucopyranoside	(compound 50) – (26)	754.732
			
Code	Compound	Reference	Molecular Weight (Da)

PG_511	Steviophethanoside	(compound 51) – (26)	432.42
			
Code	Compound	Reference	Molecular Weight (Da)
PG_512	NO TRIVIAL NAME	(compound 52) – (26)	608.591
			
Code	Compound	Reference	Molecular Weight (Da)
PG_513	Terngymnosides A	(compound 53) – (26)	616.57
			
Code	Compound	Reference	Molecular Weight (Da)

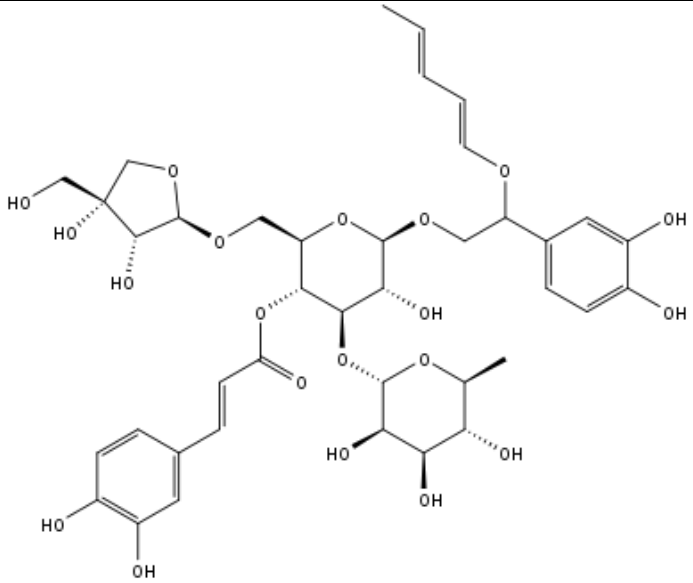
PG_514	Terngymnosides B	(compound 54) – (26)	600.571
			
Code	Compound	Reference	Molecular Weight (Da)
PG_515	Terngymnosides C	(compound 55) – (26)	466.437
			
Code	Compound	Reference	Molecular Weight (Da)
PG_516	Terngymnosides D	(compound 56) – (26)	602.587
			
Code	Compound	Reference	Molecular Weight (Da)
PG_517	Nepetifosides D	(compound 57) – (26)	800.757



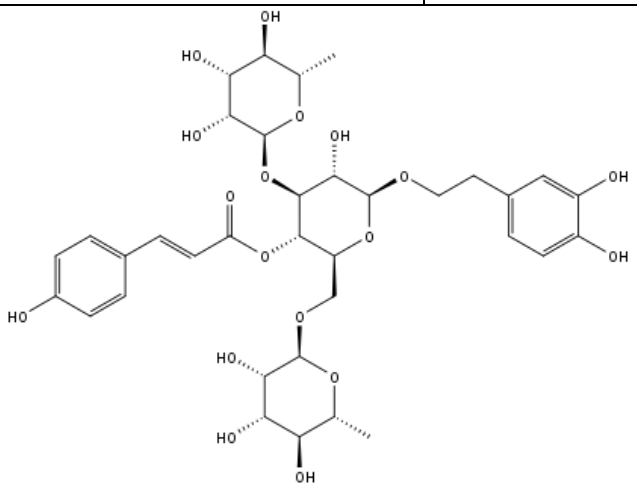
Code	Compound	Reference	Code
PG_518	Flavaioside	(compound 59) – (26)	974.956



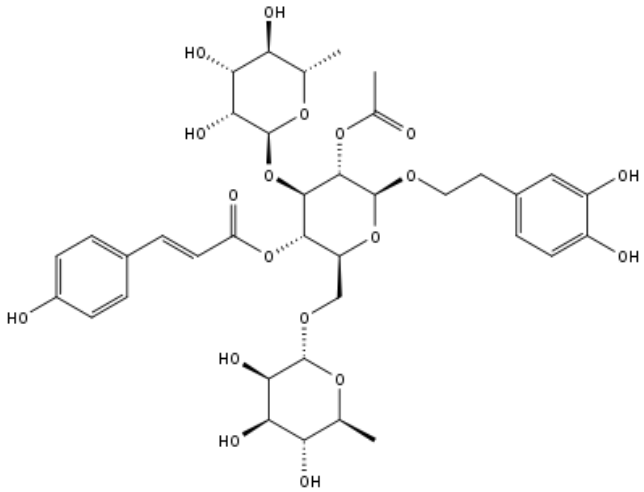
Code	Compound	Reference	Molecular Weight (Da)
PG_519	Nepetifosides F	(compound 58) – (26)	840.822



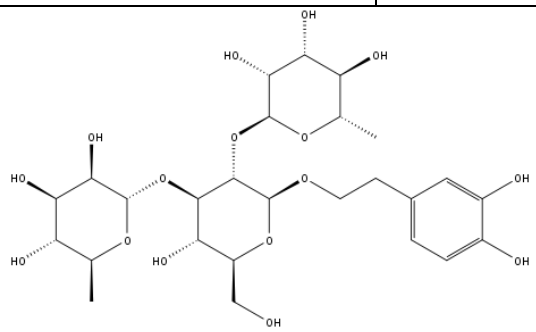
Code	Compound	Reference	Molecular Weight (Da)
PG_520	Ramoside A	(compound 60) – (26)	754.732



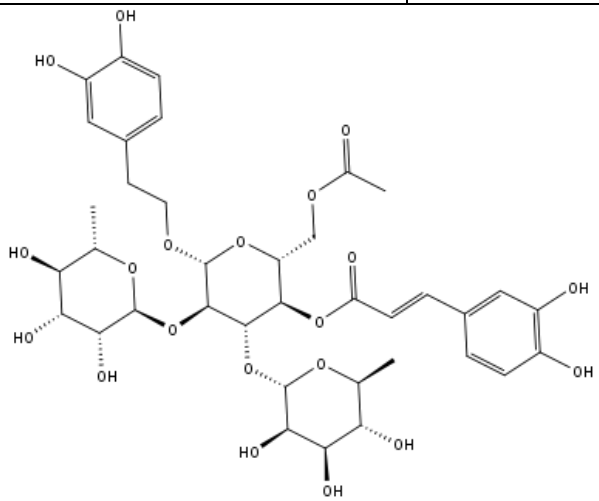
Code	Compound	Reference	Molecular Weight (Da)
PG_521	2′-Acetylramoside A	(compound 61) – (26)	796.769



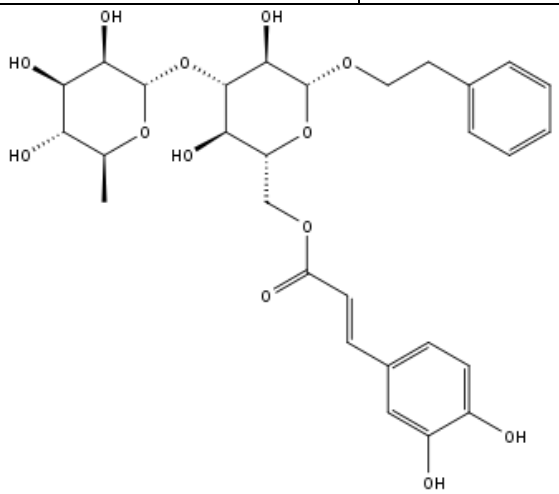
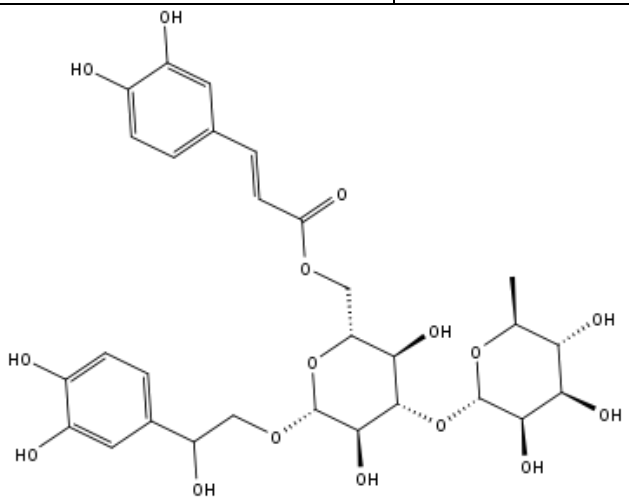
Code	Compound	Reference	Molecular Weight (Da)
PG_522	Rostkovianoside	(compound 62) – (26)	608.588

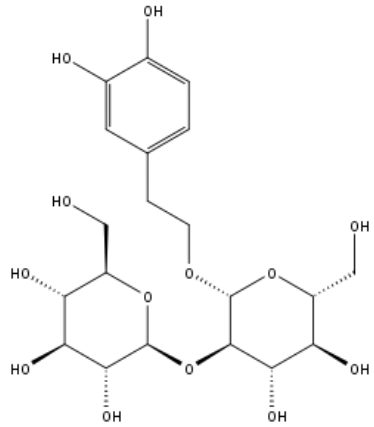


Code	Compound	Reference	Molecular Weight (Da)
PG_523	6′-O-Acetylcrassifolioside	(compound 63) – (26)	814.784

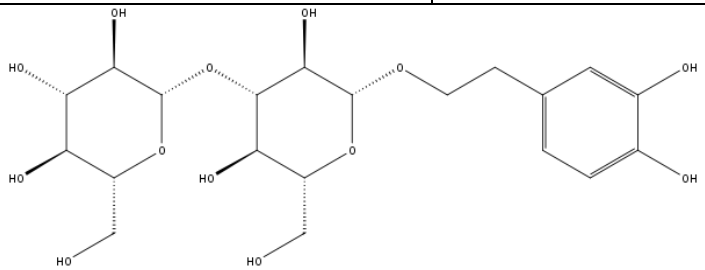


Code	Compound	Reference	Molecular Weight

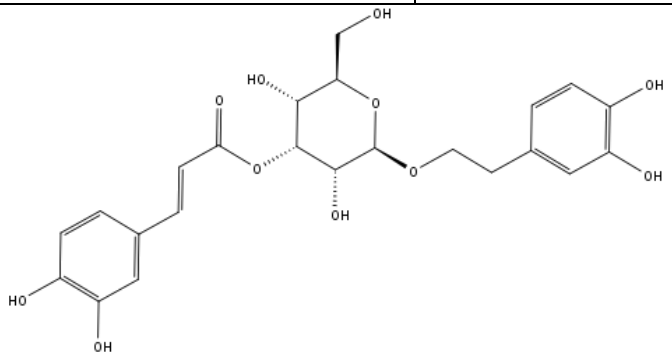
			(Da)
PG_524	Macrophylloside E	(compound 64) – (26)	592.592
			
Code	Compound	Reference	Molecular Weight (Da)
PG_525	Macrophylloside F	(compound 65) – (26)	640.589
			
Code	Compound	Reference	Molecular Weight (Da)
PG_526	Ginkgoside C	(compound 66) – (26)	478.445



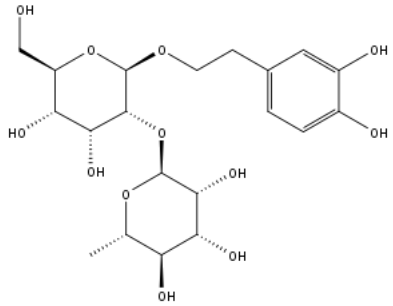
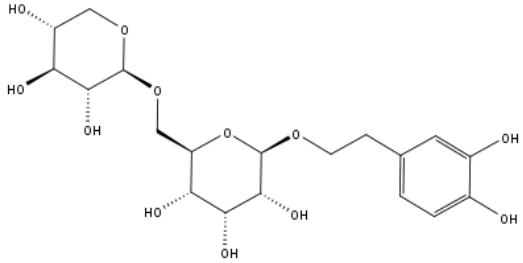
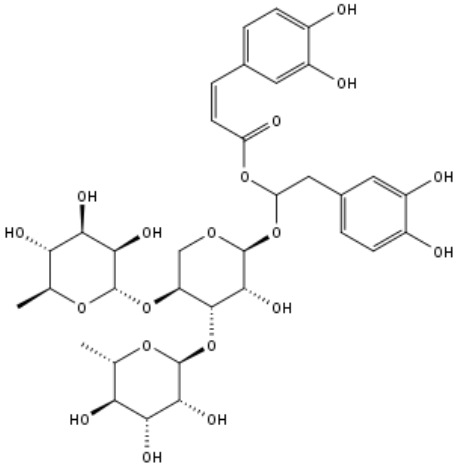
Code	Compound	Reference	Molecular Weight (Da)
PG_527	Ginkgoside D	(compound 67) – (26)	478.445

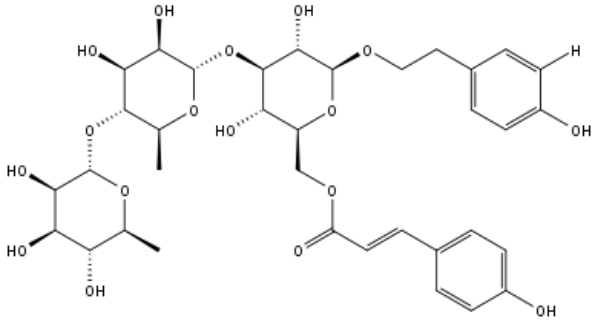
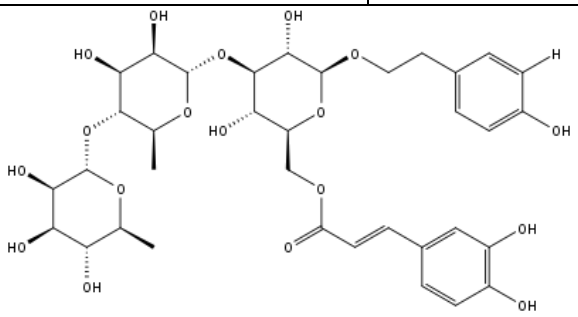
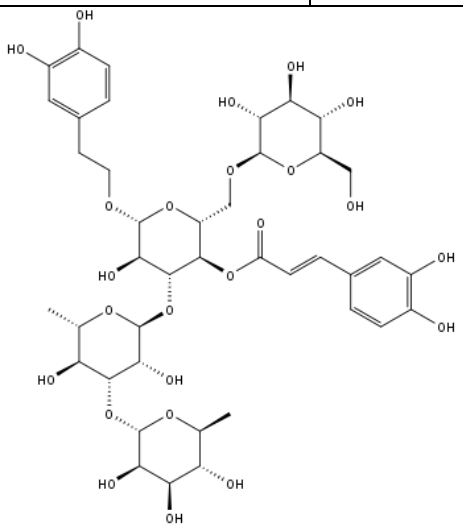


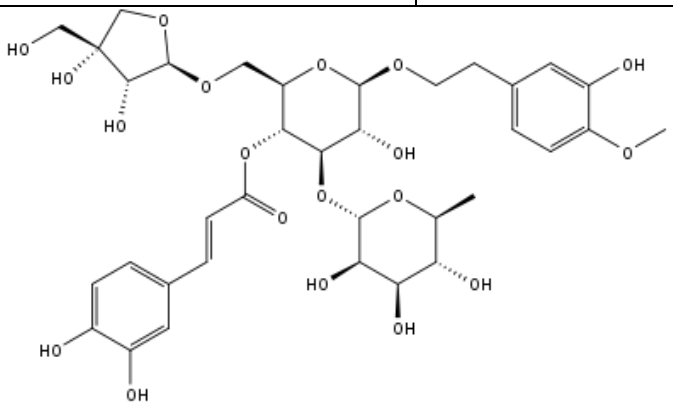
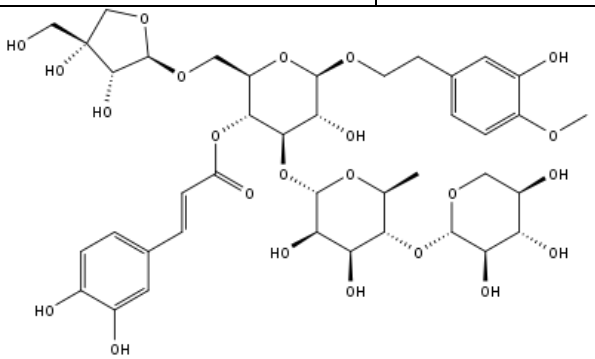
Code	Compound	Reference	Molecular Weight (Da)
PG_528	Sanangoside	(compound 68) – (26)	478.448

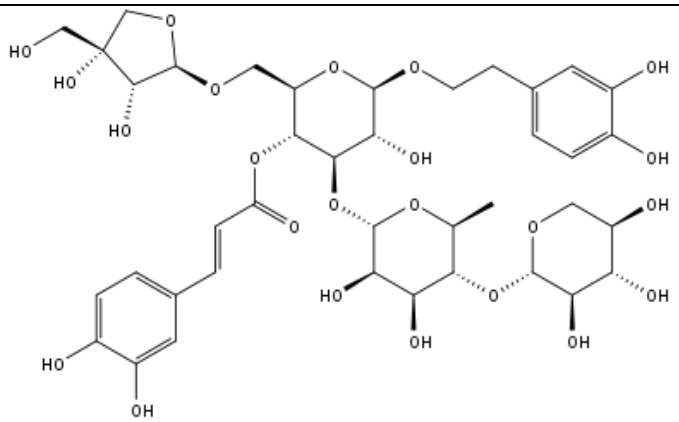


Code	Compound	Reference	Molecular Weight (Da)
PG_529	2-(3,4-Dihydroxyphenyl)ethyl- O-α-L-rhamnopyranosyl-(1→2)-β-D-allopyranoside	(compound 69) – (26)	462.446

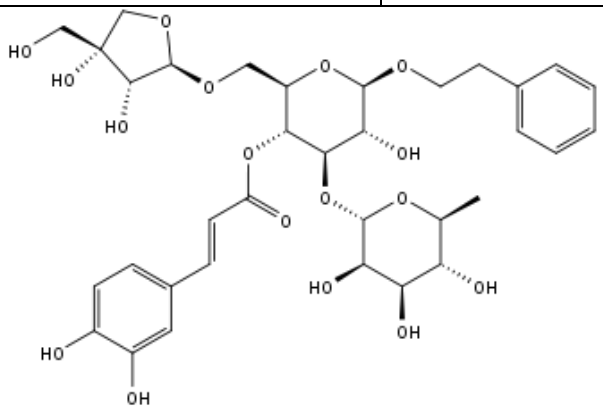
			
Code	Compound	Reference	Molecular Weight (Da)
PG_530	2-(3,4-Dihydroxyphenyl)ethyl-O-β-Dxylopyranosyl-(1→6)-β-D-allopyranoside	(compound 70) – (26)	448.419
			
Code	Compound	Reference	Molecular Weight (Da)
PG_531	8′-(3,4-Dihydroxyphenyl)ethyl-O-α-L-rhamnopyranosyl-(1-4)-2-O-(E)-caffeoyl-α-L-arabinopyranoside	(compound 71) – (26)	756.704
			
Code	Compound	Reference	Molecular Weight (Da)
PG_532	Ligupurpurosides C	(compound 74) –	738.733

		(26)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_533	Ligupurpurosides D	(compound 75) – (26)	754.732
			
Code	Compound	Reference	Molecular Weight (Da)
PG_534	Barlerinoside	(compound 76) – (26)	932.872
			

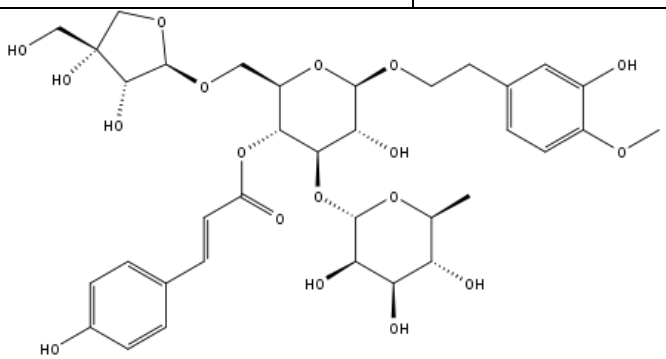
Code	Compound	Reference	Molecular Weight (Da)
PG_535	Nepetifosides B	(compound 77) – (26)	770.731
			
Code	Compound	Reference	Molecular Weight (Da)
PG_536	Nepetifosides C	(compound 78) – (26)	902.846
			
Code	Compound	Reference	Molecular Weight (Da)
PG_537	Nepetifosides E	(compound 79) – (26)	890.835



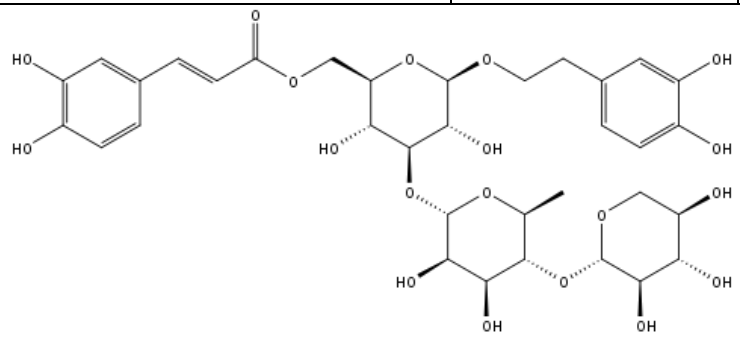
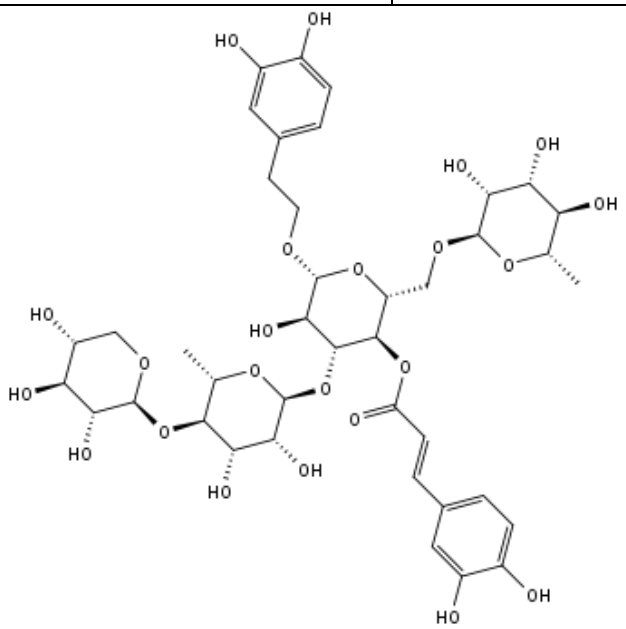
Code	Compound	Reference	Molecular Weight (Da)
PG_538	Nepetifosides G	(compound 80) – (26)	724.706

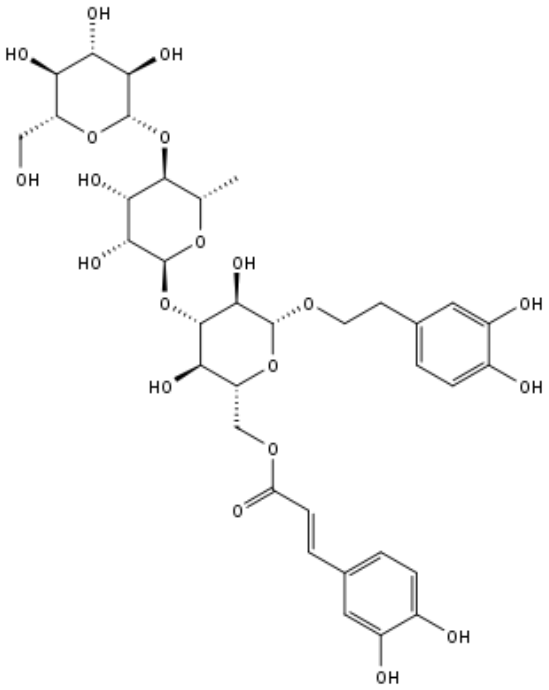


Code	Compound	Reference	Molecular Weight (Da)
PG_539	Nepetifosides H	(compound 81) – (26)	754.732

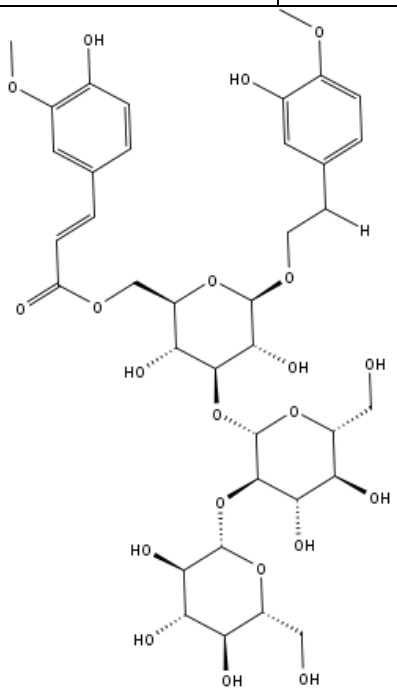


Code	Compound	Reference	Molecular Weight

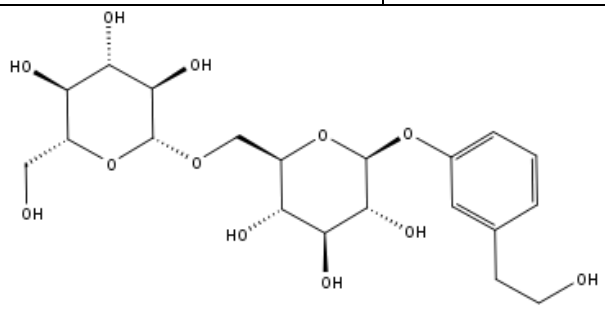
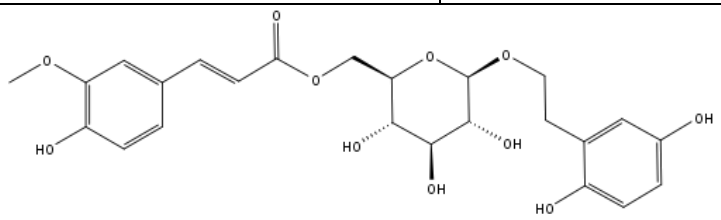
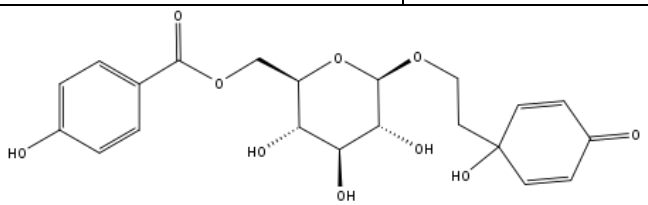
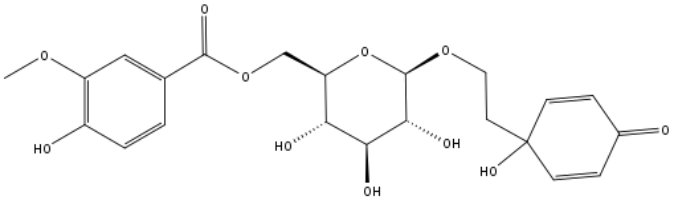
			(Da)
PG_540	Nepetifosides K	(compound 82) – (26)	758.72
			
Code	Compound	Reference	Molecular Weight (Da)
PG_541	Nepetifosides L	(compound 83) – (26)	902.846
			
Code	Compound	Reference	Molecular Weight (Da)
PG_542	Lagotiside C	(compound 84) – (26)	786.73

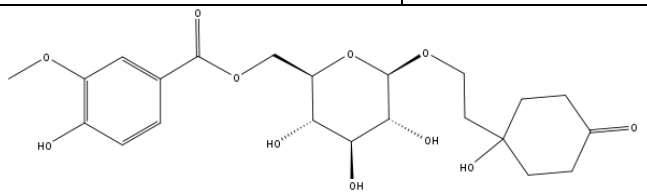
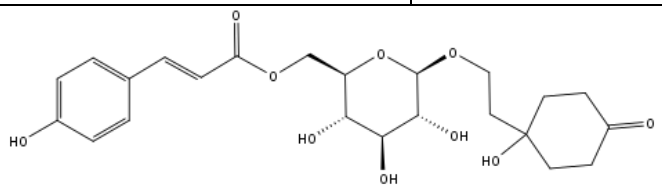
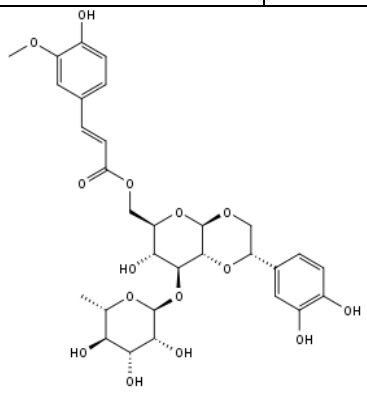


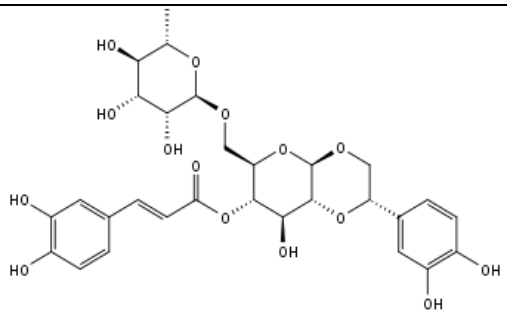
Code	Compound	Reference	Molecular Weight (Da)
PG_543	Scrosides A	(compound 85) – (26)	830.783



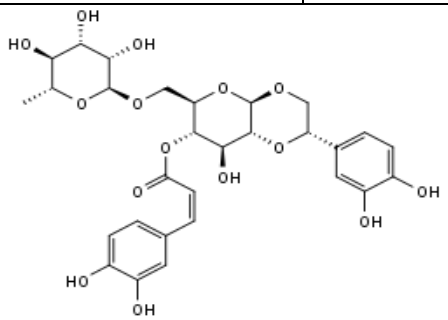
Code	Compound	Reference	Molecular Weight (Da)
PG_544	2-(4-Hydroxyphenyl)ethanol-3-O-β-	(compound 89) –	462.446

	Dglucopyranosyl-(1→6)-O-β-D-glucopyranoside	(26)	
			
Code	Compound	Reference	Molecular Weight (Da)
PG_545	Forsythoside O	(compound 90) – (26)	492.475
			
Code	Compound	Reference	Molecular Weight (Da)
PG_546	Forsythenside M	(compound 91) – (26)	436.412
			
Code	Compound	Reference	Molecular Weight (Da)
PG_547	Forsythenside N	(compound 92) – (26)	466.437
			

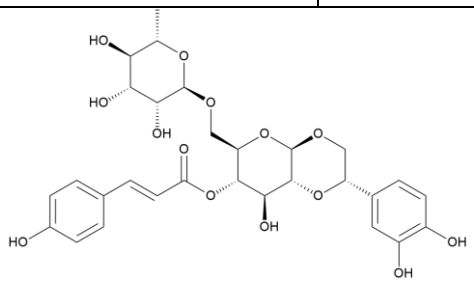
Code	Compound	Reference	Molecular Weight (Da)
PG_548	Rengyoside D	(compound 93) – (26)	470.469
			
Code	Compound	Reference	Molecular Weight (Da)
PG_549	Rengyoside E	(compound 94) – (26)	466.481
			
Code	Compound	Reference	Molecular Weight (Da)
PG_550	3′-O-Methyl isocrenatoside	(compound 95) – (26)	636.601
			
Code	Compound	Reference	Molecular Weight (Da)
PG_551	Forsyoxasides A	(compound 96) – (26)	622.574



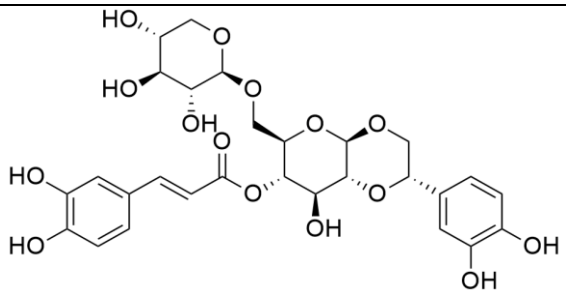
Code	Compound	Reference	Molecular Weight (Da)
PG_552	Forsyoxasides B	(compound 97) – (26)	622.574



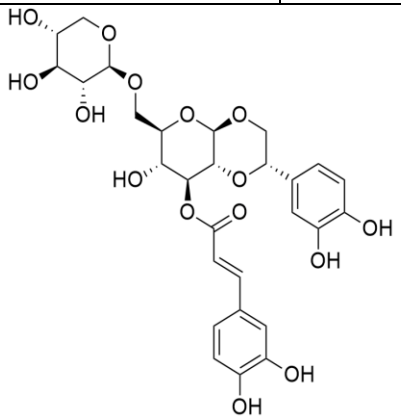
Code	Compound	Reference	Molecular Weight (Da)
PG_553	Forsyoxasides C	(compound 98) – (26)	606.575



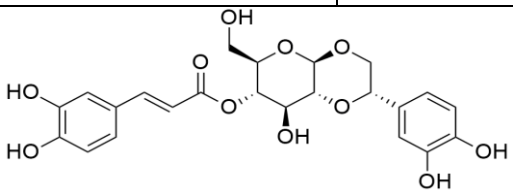
Code	Compound	Reference	Molecular Weight (Da)
PG_554	Forsyoxasides D	(compound 99) – 29]	608.547



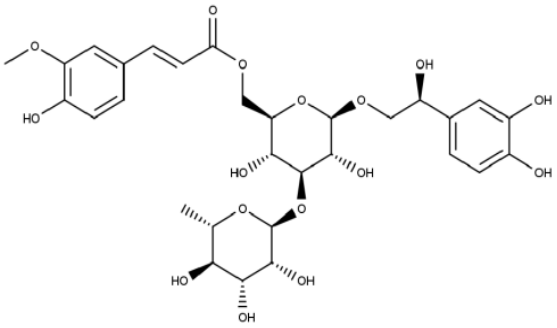
Code	Compound	Reference	Molecular Weight (Da)
PG_555	Forsyoxasides E	(compound 100) – (26)	608.547



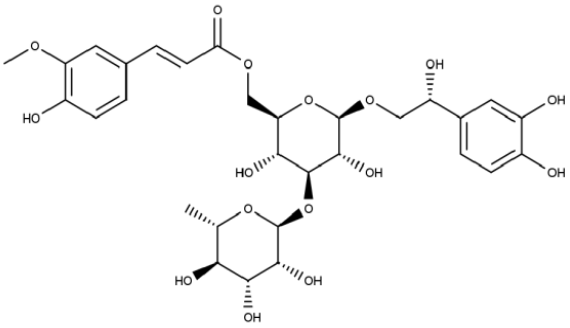
Code	Compound	Reference	Molecular Weight (Da)
PG_556	Forsyoxasides F	(compound 101) - (26)	476.433



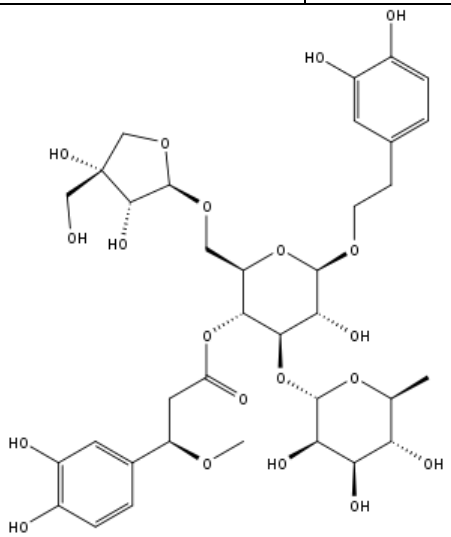
Code	Compound	Reference	Molecular Weight (Da)
PG_557	Betonyosides B	(compound 102) – (26)	654.616



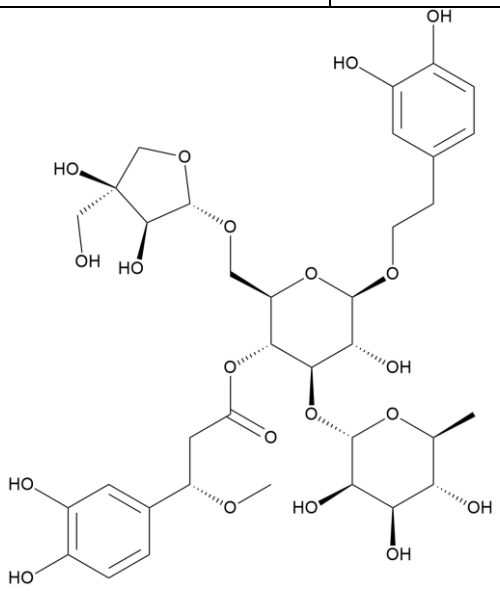
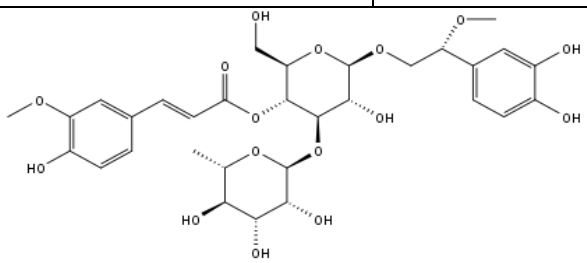
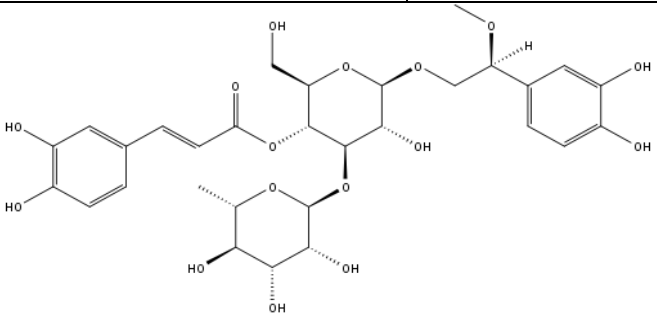
Code	Compound	Reference	Molecular Weight (Da)
PG_558	Betonyosides C	(compound 103) - (26)	654.616

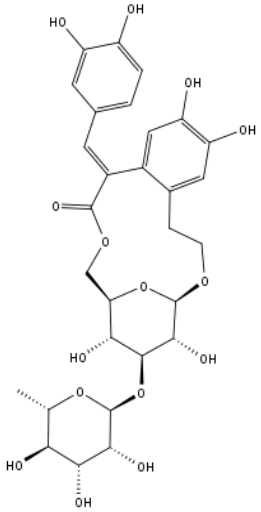
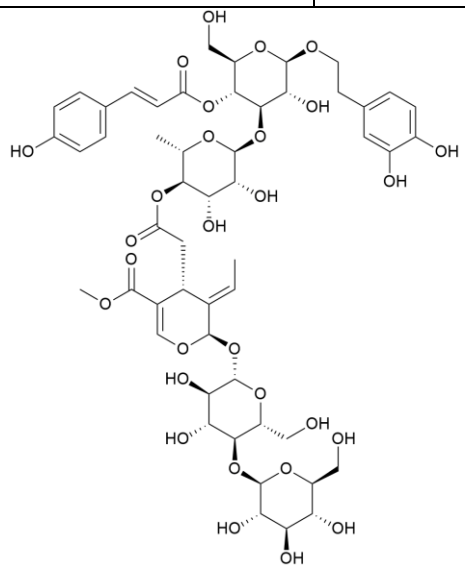


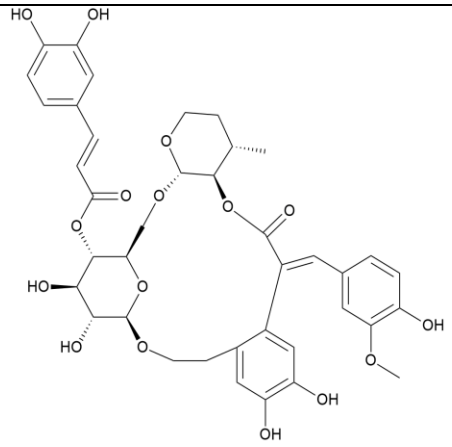
Code	Compound	Reference	Molecular Weight (Da)
PG_559	Nepetifosides I	(compound 104) – (26)	788.746



Code	Compound	Reference	Molecular Weight (Da)

PG_560	Nepetifosides J	(compound 105) – (26)	788.746
			
Code	Compound	Reference	Molecular Weight (Da)
PG_561	(7R)-Campneoside I	(compound 106) – (26)	668.643
			
Code	Compound	Reference	Molecular Weight (Da)
PG_562	(7S)-Campneoside I	(compound 107) – (26)	682.669
			

Code	Compound	Reference	Molecular Weight (Da)
PG_563	Nepetifosides A	(compound 108) – (26)	650.628
			
Code	Compound	Reference	Molecular Weight (Da)
PG_564	Glucooleoacteoside	(compound 109) – (26)	1161.11
			
Code	Compound	Reference	Molecular Weight (Da)
PG_565	Forsythenethosides A	(compound 110) – (26)	766.746



Code	Compound	Reference	Molecular Weight (Da)
PG_566	Forsythenethosides B	(compound 111) – (26)	796.772

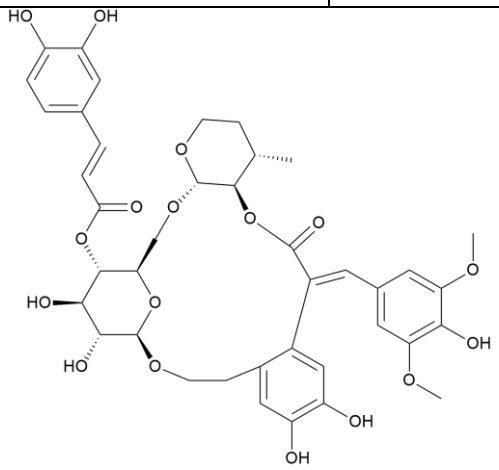


Table S2: The top 80 phenylethanoid glycosides (PG) filtered by the penalty score below 0.3 against $3Cl^{pro}$ of SARS-CoV-2.

Classification				Individual Consensus Score			Penalty Score
PG	**AutoDock Vina**	**GOLD/ GoldScore**	**GOLD/ ChemPLP**	**AutoDock Vina**	**GOLD/ GoldScore**	**GOLD/ ChemPLP**	
PG_441	18	1	10	0,031578947	0,001754386	0,01754386	0,016959064
PG_183	36	8	1	0,063157895	0,014035088	0,001754386	0,026315789
PG_100	9	6	44	0,015789474	0,010526316	0,077192982	0,034502924
PG_414	6	43	26	0,010526316	0,075438596	0,045614035	0,043859649
PG_214	72	23	27	0,126315789	0,040350877	0,047368421	0,071345029
PG_127	55	64	43	0,096491228	0,112280702	0,075438596	0,094736842
PG_442	139	18	8	0,243859649	0,031578947	0,014035088	0,096491228
PG_6	51	72	87	0,089473684	0,126315789	0,152631579	0,122807018
PG_224	12	139	70	0,021052632	0,243859649	0,122807018	0,129239766
PG_251	60	16	146	0,105263158	0,028070175	0,256140351	0,129824561
PG_266	77	51	98	0,135087719	0,089473684	0,171929825	0,132163743
PG_523	32	65	131	0,056140351	0,114035088	0,229824561	0,133333333
PG_98	91	21	126	0,159649123	0,036842105	0,221052632	0,139181287
PG_382	5	49	187	0,00877193	0,085964912	0,328070175	0,140935673
PG_436	41	190	15	0,071929825	0,333333333	0,026315789	0,143859649
PG_369	26	7	217	0,045614035	0,012280702	0,380701754	0,14619883
PG_96	53	47	154	0,092982456	0,08245614	0,270175439	0,148538012
PG_215	73	89	100	0,128070175	0,156140351	0,175438596	0,153216374
PG_445	176	40	55	0,30877193	0,070175439	0,096491228	0,158479532
PG_304	97	20	161	0,170175439	0,035087719	0,28245614	0,162573099
PG_254	39	171	74	0,068421053	0,3	0,129824561	0,166081871
PG_435	138	141	6	0,242105263	0,247368421	0,010526316	0,166666667
PG_48	116	81	92	0,203508772	0,142105263	0,161403509	0,169005848
PG_150	22	125	144	0,038596491	0,219298246	0,252631579	0,170175439
PG_199	37	61	202	0,064912281	0,107017544	0,354385965	0,175438596
PG_103	54	215	31	0,094736842	0,377192982	0,054385965	0,175438596
PG_216	38	236	34	0,066666667	0,414035088	0,059649123	0,180116959
PG_26	153	96	59	0,268421053	0,168421053	0,103508772	0,180116959
PG_205	58	67	190	0,101754386	0,11754386	0,333333333	0,184210526
PG_434	137	197	5	0,240350877	0,345614035	0,00877193	0,198245614
PG_244	47	207	86	0,08245614	0,363157895	0,150877193	0,198830409
PG_377	131	26	184	0,229824561	0,045614035	0,322807018	0,199415205
PG_209	245	79	18	0,429824561	0,138596491	0,031578947	0,2
PG_160	146	126	75	0,256140351	0,221052632	0,131578947	0,202923977
PG_141	289	36	22	0,507017544	0,063157895	0,038596491	0,202923977
PG_429	263	3	84	0,461403509	0,005263158	0,147368421	0,204678363
PG_430	48	90	226	0,084210526	0,157894737	0,396491228	0,212865497
PG_121	111	107	152	0,194736842	0,187719298	0,266666667	0,216374269
PG_426	213	55	103	0,373684211	0,096491228	0,180701754	0,216959064
PG_446	140	158	76	0,245614035	0,277192982	0,133333333	0,21871345
PG_219	74	291	9	0,129824561	0,510526316	0,015789474	0,21871345
PG_483	20	230	125	0,035087719	0,403508772	0,219298246	0,219298246
PG_145	196	35	147	0,343859649	0,061403509	0,257894737	0,221052632
PG_107	223	29	129	0,39122807	0,050877193	0,226315789	0,222807018
PG_389	62	320	3	0,10877193	0,561403509	0,005263158	0,225146199
PG_99	236	95	54	0,414035088	0,166666667	0,094736842	0,225146199
PG_188	293	37	60	0,514035088	0,064912281	0,105263158	0,228070175
PG_359	17	92	289	0,029824561	0,161403509	0,507017544	0,232748538
PG_437	314	75	12	0,550877193	0,131578947	0,021052632	0,234502924
PG_342	305	76	23	0,535087719	0,133333333	0,040350877	0,23625731
PG_184	244	144	17	0,428070175	0,252631579	0,029824561	0,236842105
PG_462	82	106	218	0,143859649	0,185964912	0,38245614	0,237426901
PG_137	160	30	220	0,280701754	0,052631579	0,385964912	0,239766082
PG_324	98	118	198	0,171929825	0,207017544	0,347368421	0,242105263
PG_185	95	183	141	0,166666667	0,321052632	0,247368421	0,24502924
PG_567	28	216	180	0,049122807	0,378947368	0,315789474	0,247953216
PG_1	43	109	274	0,075438596	0,19122807	0,480701754	0,249122807

PG_359-cis	112	82	237	0,196491228	0,143859649	0,415789474	0,252046784
PG_119	8	213	212	0,014035088	0,373684211	0,371929825	0,253216374
PG_189	378	2	53	0,663157895	0,003508772	0,092982456	0,253216374
PG_232	166	10	260	0,29122807	0,01754386	0,456140351	0,25497076
PG_109	276	33	130	0,484210526	0,057894737	0,228070175	0,256725146
PG_486	101	48	291	0,177192982	0,084210526	0,510526316	0,257309942
PG_407	175	180	88	0,307017544	0,315789474	0,154385965	0,259064327
PG_166	163	173	110	0,285964912	0,303508772	0,192982456	0,260818713
PG_424	30	133	287	0,052631579	0,233333333	0,503508772	0,263157895
PG_106	237	136	89	0,415789474	0,238596491	0,156140351	0,270175439
PG_97	287	108	69	0,503508772	0,189473684	0,121052632	0,271345029
PG_120	341	103	21	0,598245614	0,180701754	0,036842105	0,271929825
PG_398	210	24	233	0,368421053	0,042105263	0,40877193	0,273099415
PG_155	162	66	239	0,284210526	0,115789474	0,419298246	0,273099415
PG_231	75	257	138	0,131578947	0,450877193	0,242105263	0,274853801
PG_101	145	132	193	0,254385965	0,231578947	0,338596491	0,274853801
PG_228	24	237	215	0,042105263	0,415789474	0,377192982	0,278362573
PG_113	193	233	50	0,338596491	0,40877193	0,087719298	0,278362573
PG_92	118	223	139	0,207017544	0,39122807	0,243859649	0,280701754
PG_164	291	127	72	0,510526316	0,222807018	0,126315789	0,286549708
PG_158	419	25	52	0,735087719	0,043859649	0,09122807	0,29005848
PG_493	150	268	81	0,263157895	0,470175439	0,142105263	0,291812865
PG_147	93	329	83	0,163157895	0,577192982	0,145614035	0,295321637

Table S3: The top 98 phenylethanoid glycosides (PG) filtered by the penalty score below 0.3 against PL^{pro} of SARS-CoV-2.

Classification				Individual Consensus Score			Penalty Score
PG	AutoDock Vina	GOLD/ GoldScore	GOLD/ ChemPLP	AutoDock Vina	GOLD/ GoldScore	GOLD/ ChemPLP	
PG_78	31	8	3	0,05	0,01	0,01	0,025
PG_514	14	74	16	0,02	0,13	0,03	0,061
PG_21	37	43	46	0,06	0,08	0,08	0,074
PG_348	62	38	36	0,11	0,07	0,06	0,08
PG_513	129	6	2	0,23	0,01	0	0,08
PG_447	70	94	1	0,12	0,16	0	0,096
PG_262	29	77	61	0,05	0,14	0,11	0,098
PG_444	84	50	38	0,15	0,09	0,07	0,101
PG_44	66	62	51	0,12	0,11	0,09	0,105
PG_454	11	5	167	0,02	0,01	0,29	0,107
PG_328	80	24	84	0,140350877	0,042105263	0,147368421	0,11
PG_27	85	67	39	0,149122807	0,11754386	0,068421053	0,112
PG_94	79	44	74	0,138596491	0,077192982	0,129824561	0,115
PG_86	128	53	17	0,224561404	0,092982456	0,029824561	0,116
PG_337	135	51	12	0,236842105	0,089473684	0,021052632	0,116
PG_265	77	101	32	0,135087719	0,177192982	0,056140351	0,123
PG_408	58	116	41	0,101754386	0,203508772	0,071929825	0,126
PG_299	36	29	157	0,063157895	0,050877193	0,275438596	0,13
PG_345	43	175	5	0,075438596	0,307017544	0,00877193	0,13
PG_148	54	152	25	0,094736842	0,266666667	0,043859649	0,135
PG_312	81	15	138	0,142105263	0,026315789	0,242105263	0,137
PG_329	110	96	37	0,192982456	0,168421053	0,064912281	0,142
PG_296	97	78	72	0,170175439	0,136842105	0,126315789	0,144
PG_61	98	135	23	0,171929825	0,236842105	0,040350877	0,15
PG_281	162	25	70	0,284210526	0,043859649	0,122807018	0,15
PG_15	13	141	112	0,022807018	0,247368421	0,196491228	0,156
PG_3	23	154	92	0,040350877	0,270175439	0,161403509	0,157
PG_298	59	188	22	0,103508772	0,329824561	0,038596491	0,157
PG_350	94	134	48	0,164912281	0,235087719	0,084210526	0,161
PG_406	116	158	4	0,203508772	0,277192982	0,007017544	0,163
PG_455	1	27	257	0,001754386	0,047368421	0,450877193	0,167
PG_362	115	65	109	0,201754386	0,114035088	0,19122807	0,169
PG_300	51	186	53	0,089473684	0,326315789	0,092982456	0,17
PG_508	118	70	102	0,207017544	0,122807018	0,178947368	0,17
PG_170	6	106	180	0,010526316	0,185964912	0,315789474	0,171
PG_42	67	155	79	0,11754386	0,271929825	0,138596491	0,176
PG_503	144	57	118	0,252631579	0,1	0,207017544	0,187
PG_31	210	92	18	0,368421053	0,161403509	0,031578947	0,187
PG_35	71	184	65	0,124561404	0,322807018	0,114035088	0,187
PG_465	134	126	63	0,235087719	0,221052632	0,110526316	0,189
PG_136	187	22	115	0,328070175	0,038596491	0,201754386	0,189
PG_261	61	191	76	0,107017544	0,335087719	0,133333333	0,192
PG_399	49	118	162	0,085964912	0,207017544	0,284210526	0,192
PG_11	73	144	116	0,128070175	0,252631579	0,203508772	0,195
PG_139	18	168	150	0,031578947	0,294736842	0,263157895	0,196
PG_201	142	99	107	0,249122807	0,173684211	0,187719298	0,204
PG_197	234	16	100	0,410526316	0,028070175	0,175438596	0,205
PG_534	311	10	34	0,545614035	0,01754386	0,059649123	0,208
PG_457	33	148	175	0,057894737	0,259649123	0,307017544	0,208
PG_129	356	1	9	0,624561404	0,001754386	0,015789474	0,214
PG_308	17	200	152	0,029824561	0,350877193	0,266666667	0,216
PG_354	86	149	134	0,150877193	0,261403509	0,235087719	0,216
PG_314	24	244	104	0,042105263	0,428070175	0,18245614	0,218
PG_17	19	227	127	0,033333333	0,398245614	0,222807018	0,218
PG_222	151	56	170	0,264912281	0,098245614	0,298245614	0,22
PG_343 -1	149	102	130	0,261403509	0,178947368	0,228070175	0,223
PG_363	295	34	57	0,51754386	0,059649123	0,1	0,226

PG_364	171	37	182	0,3	0,064912281	0,319298246	0,228
PG_38	106	231	56	0,185964912	0,405263158	0,098245614	0,23
PG_413	229	97	68	0,401754386	0,170175439	0,119298246	0,23
PG_37	104	239	54	0,18245614	0,419298246	0,094736842	0,232
PG_516	4	114	279	0,007017544	0,2	0,489473684	0,232
PG_528	335	42	26	0,587719298	0,073684211	0,045614035	0,236
PG_138	341	35	28	0,598245614	0,061403509	0,049122807	0,236
PG_271	9	241	154	0,015789474	0,422807018	0,270175439	0,236
PG_518	99	110	195	0,173684211	0,192982456	0,342105263	0,236
PG_380	28	111	268	0,049122807	0,194736842	0,470175439	0,238
PG_234	69	182	158	0,121052632	0,319298246	0,277192982	0,239
PG_245	350	11	62	0,614035088	0,019298246	0,10877193	0,247
PG_71	39	160	228	0,068421053	0,280701754	0,4	0,25
PG_460	22	376	29	0,038596491	0,659649123	0,050877193	0,25
PG_467	91	162	178	0,159649123	0,284210526	0,312280702	0,252
PG_456	26	7	399	0,045614035	0,012280702	0,7	0,253
PG_25	20	209	204	0,035087719	0,366666667	0,357894737	0,253
PG_374	113	40	284	0,198245614	0,070175439	0,498245614	0,256
PG_14	63	247	129	0,110526316	0,433333333	0,226315789	0,257
PG_263	159	180	108	0,278947368	0,315789474	0,189473684	0,261
PG_566	27	23	398	0,047368421	0,040350877	0,698245614	0,262
PG_131	296	73	83	0,519298246	0,128070175	0,145614035	0,264
PG_375	170	120	169	0,298245614	0,210526316	0,296491228	0,268
PG_128	179	86	198	0,314035088	0,150877193	0,347368421	0,271
PG_87	340	93	33	0,596491228	0,163157895	0,057894737	0,273
PG_541	30	417	21	0,052631579	0,731578947	0,036842105	0,274
PG_502	140	107	224	0,245614035	0,187719298	0,392982456	0,275
PG_397	328	72	77	0,575438596	0,126315789	0,135087719	0,279
PG_192	7	323	147	0,012280702	0,566666667	0,257894737	0,279
PG_422	147	198	136	0,257894737	0,347368421	0,238596491	0,281
PG_132	302	33	148	0,529824561	0,057894737	0,259649123	0,282
PG_114	417	28	40	0,731578947	0,049122807	0,070175439	0,284
PG_372	245	26	217	0,429824561	0,045614035	0,380701754	0,285
PG_550	48	177	263	0,084210526	0,310526316	0,461403509	0,285
PG_207	231	171	89	0,405263158	0,3	0,156140351	0,287
PG_60	455	4	35	0,798245614	0,007017544	0,061403509	0,289
PG_340	251	226	31	0,440350877	0,396491228	0,054385965	0,297
PG_20	87	240	183	0,152631579	0,421052632	0,321052632	0,298
PG_67	220	179	111	0,385964912	0,314035088	0,194736842	0,298
PG_565	35	55	420	0,061403509	0,096491228	0,736842105	0,298
PG_512	122	131	259	0,214035088	0,229824561	0,454385965	0,299

Table S4: ADMETox parameters evaluated for the seven phenylethanoid glycosides (PG) that showed interaction with SARS-CoV-2 proteases predicted by SwissADME, pkCSM and DataWarrior.

PG	Consensus Log P			Rotatable bonds		PAINS	AMES	Mutagenic	Tumorigenic
	Swiss.	pkCSM	DW	Swiss.	pkCSM	Swiss.	pkCSM	DW	DW
PG_78	-0,71	-1,40	-0,71	11	10	1	No	No	No
PG_348	0,06	0,28	-0,11	10	9	1	No	No	No
PG_447	-0,01	-0,99	-0,64	13	10	0	No	No	No
PG_514	0,70	0,32	0,75	13	11	1	No	No	No
PG_493	-0,79	-0,72	-0,03	11	10	1	No	No	No
PG_254	-0,54	-10,16	-0,38	11	10	1	No	No	No
PG_266	-0,40	-10,16	-0,38	11	10	1	No	Low	No

*DW = DataWarrior

*Swiss. = SwissADME

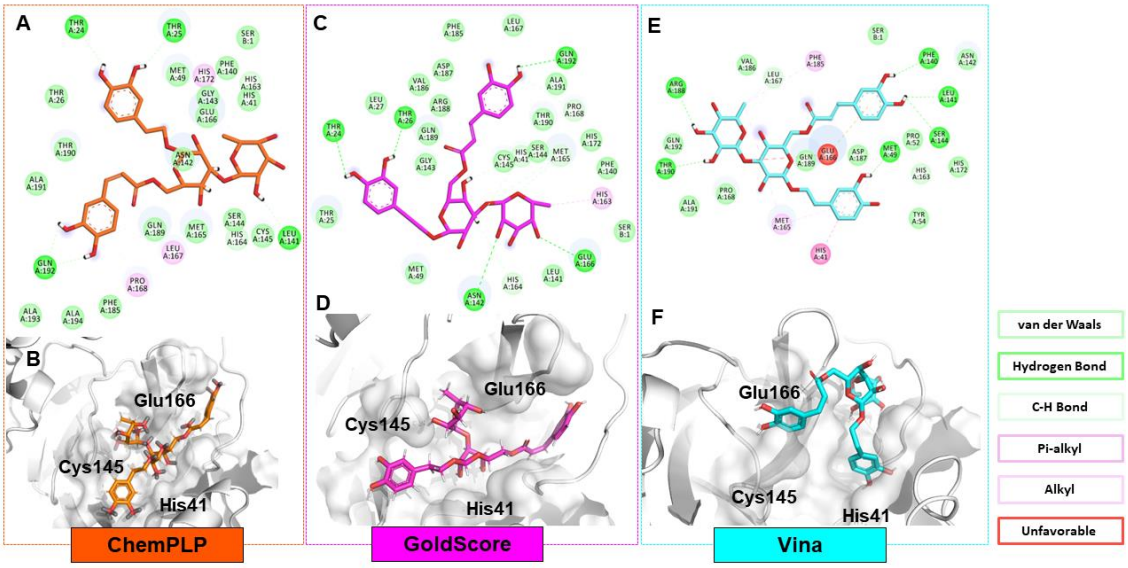


Figure S 1: Interactions between the 3CL^{pro} complex and PG_254 A & B: In orange, the results referring to the ChemPLP algorithm. C&D: In magenta, results referring to GoldScore. E & F: In cyan, results referring to Autodock Vina.

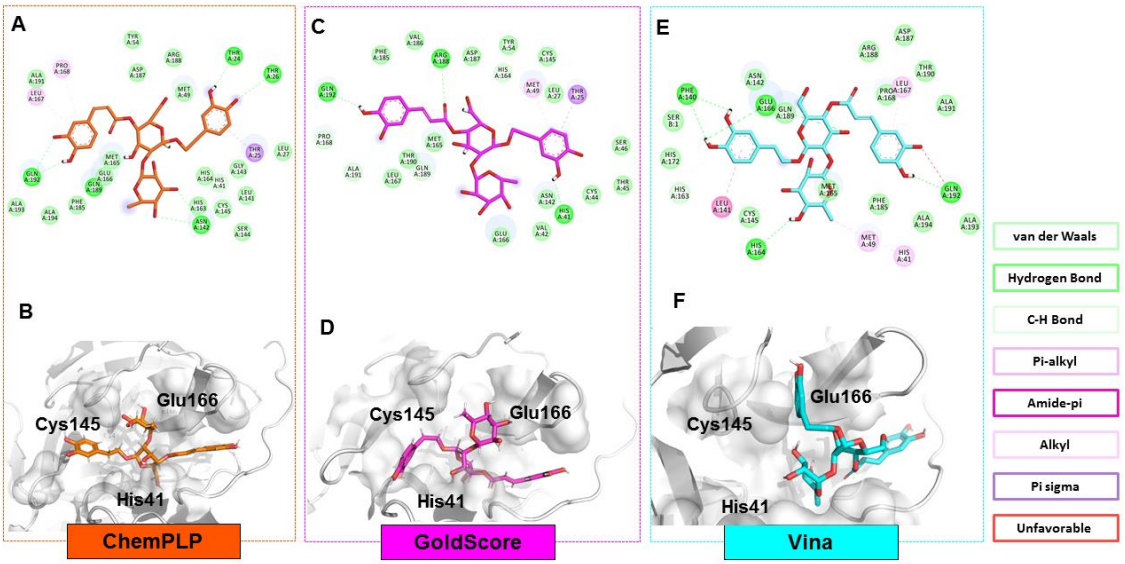


Figure S 2: Interactions between the 3CL^{pro} complex and PG_266 A & B: In orange, the results referring to the ChemPLP algorithm. C&D: In magenta, results referring to GoldScore. E & F: In cyan, results referring to Autodock Vina.

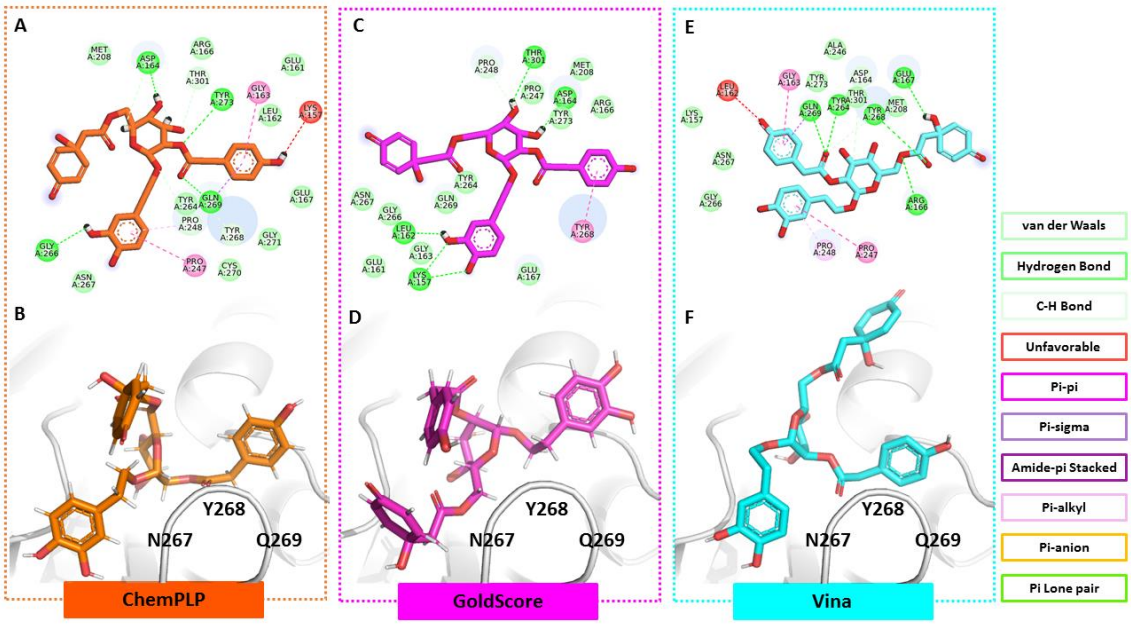


Figure S 3: Interactions between the Pl^{pro} complex and PG_514 A & B: In orange, the results referring to the ChemPLP algorithm. C&D: In magenta, results referring to GoldScore. E & F: In cyan, results referring to Autodock Vina.

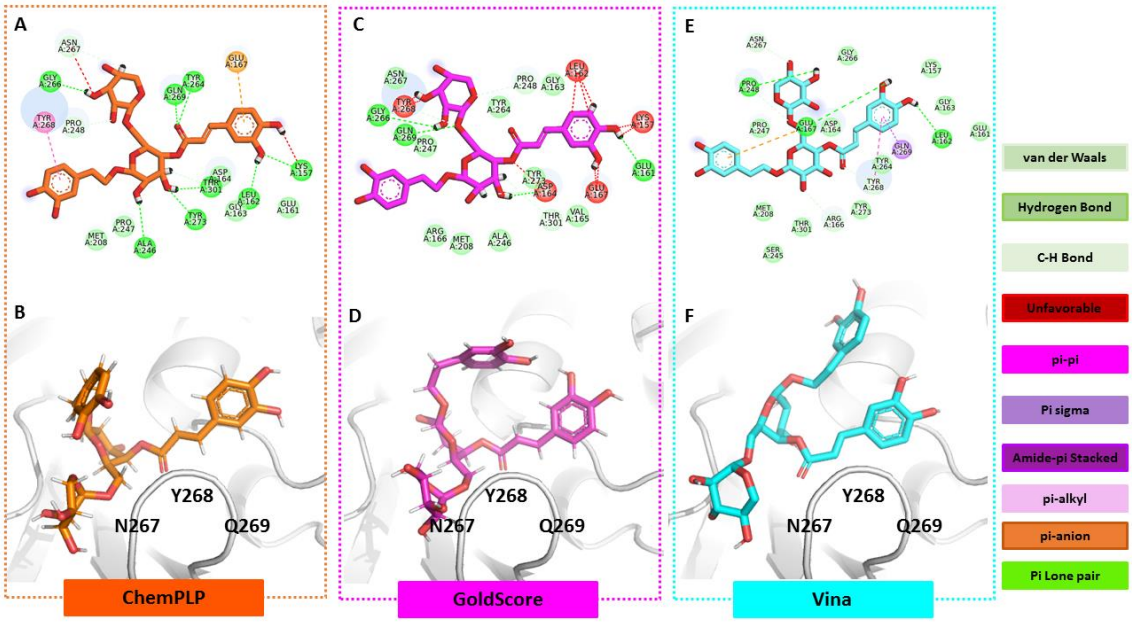


Figure S 4: Interactions between the Pl^{pro} complex and PG_78 A & B: In orange, the results referring to the ChemPLP algorithm. C&D: In magenta, results referring to GoldScore. E & F: In cyan, results referring to Autodock Vina.

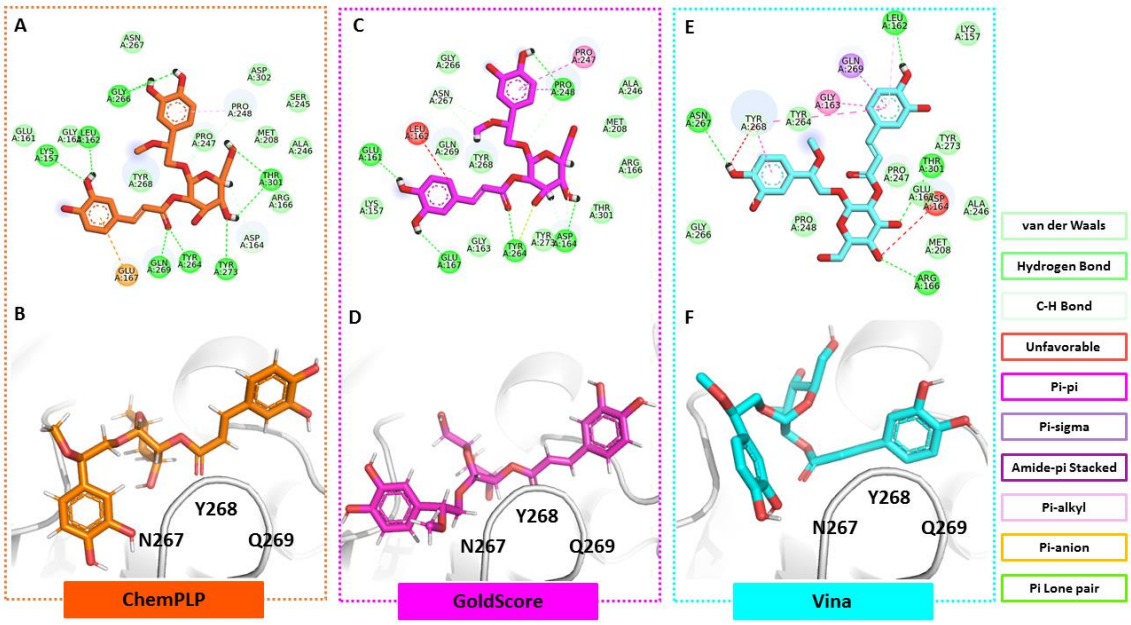


Figure S 5: Interactions between the Pl^{pro} complex and PG_348 A & B: In orange, the results referring to the ChemPLP algorithm. C&D: In magenta, results referring to GoldScore. E & F: In cyan, results referring to Autodock Vina.

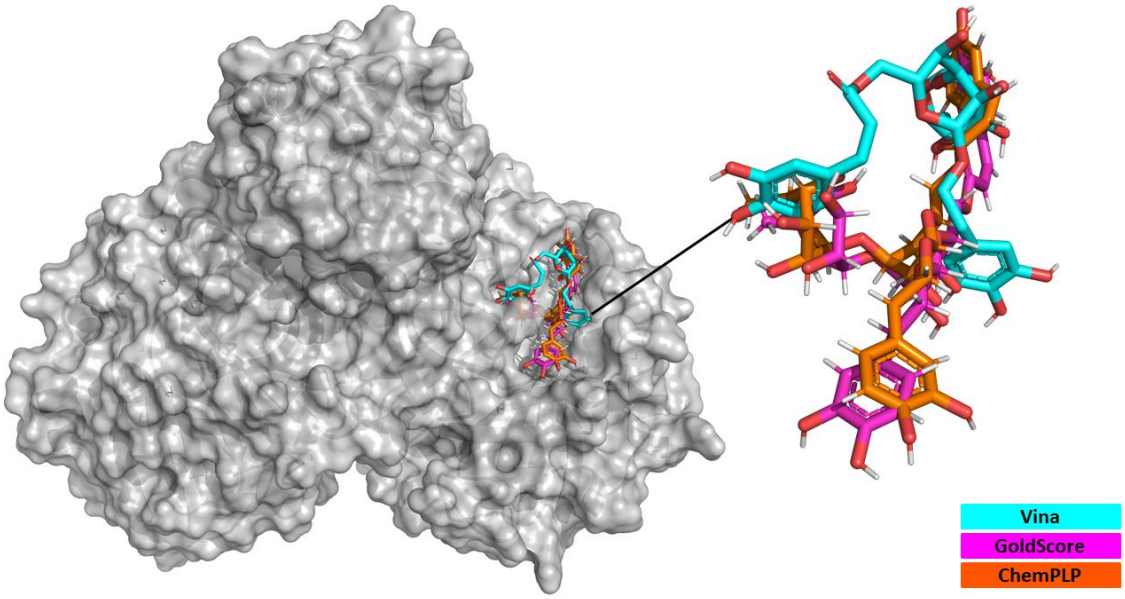


Figure S 6: PG_254 modes overlay. The three-dimensional structure of 3CLpro (PDBid:6XQT) is colored in gray surface. The best modes of the PG resulted from AutoDock Vina (cyan), GOLD/GoldScore (magenta), GOLD/ChemPLP (orange) simulations are in the protease active site region. On the right is the highlight structure overlay.

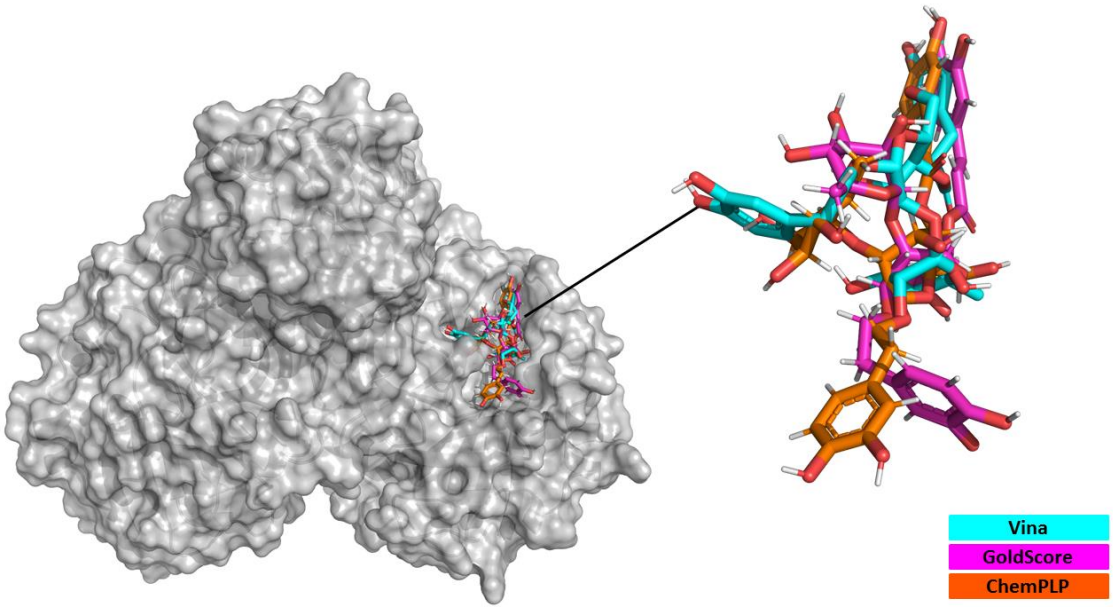


Figure S 7: PG_266 modes overlay. The three-dimensional structure of 3CLpro (PDBid:6XQT) is colored in gray surface. The best modes of the PG resulted from AutoDock Vina (cyan), GOLD/GoldScore (magenta), GOLD/ChemPLP (orange) simulations are in the protease active site region. On the right is the highlight structure overlay.

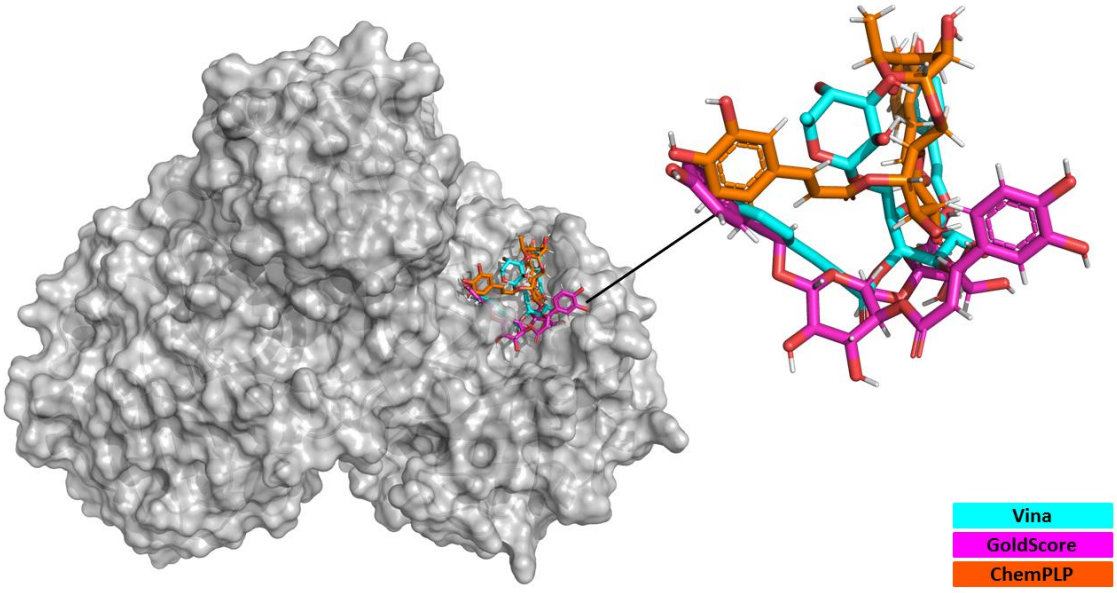


Figure S 8: PG_493 modes overlay. The three-dimensional structure of 3CLpro (PDBid:6XQT) is colored in gray surface. The best modes of the PG resulted from AutoDock Vina (cyan), GOLD/GoldScore (magenta), GOLD/ChemPLP (orange) simulations are in the protease active site region. On the right is the highlight structure overlay.

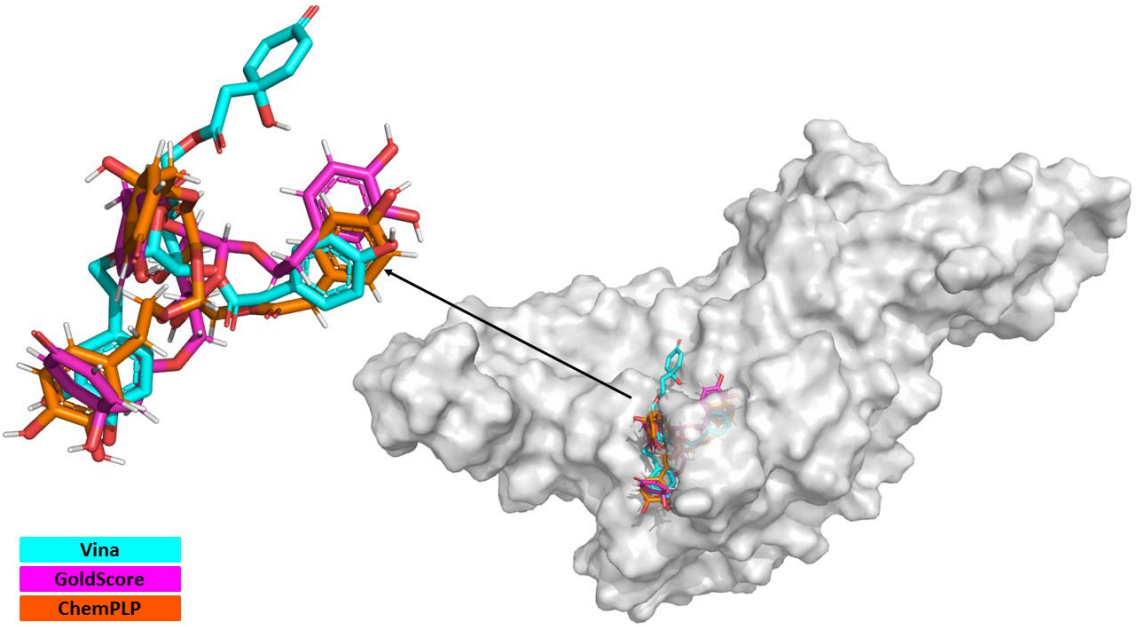


Figure S 9: PG_514 modes overlay. The three-dimensional structure of PLpro (PDBid: 7JRN) is colored in gray surface. The best modes of the PG resulted from AutoDock Vina (cyan), GOLD/GoldScore (magenta), GOLD/ChemPLP (orange) simulations are in the BL2Loop region. On the left is the highlight structure overlay.

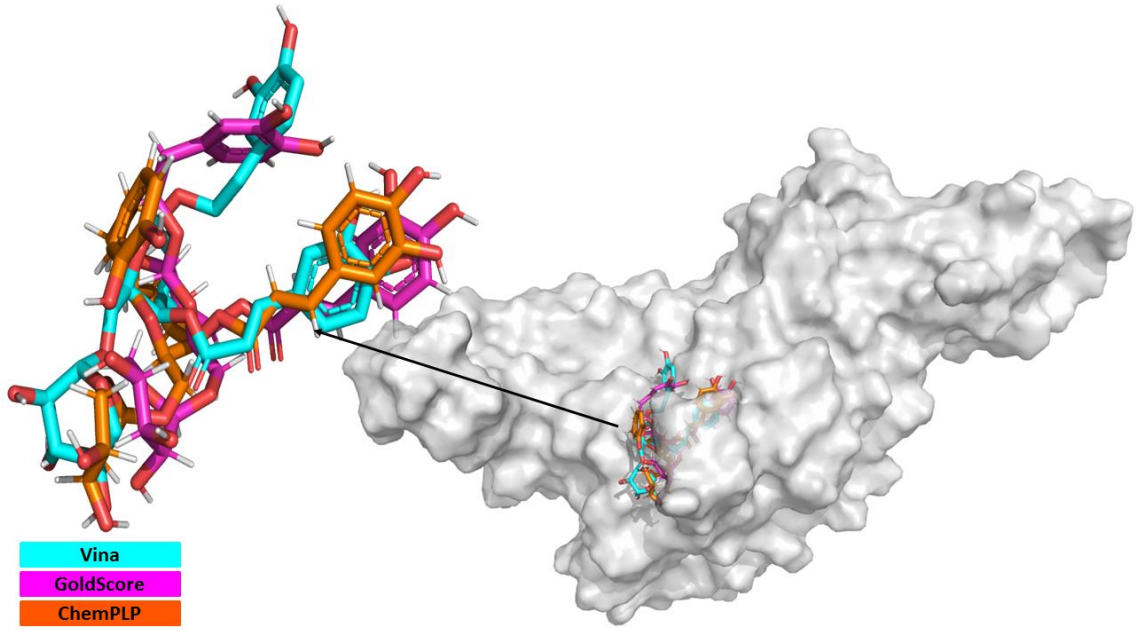


Figure S 10: PG_78 modes overlay. The three-dimensional structure of PLpro (PDBid: 7JRN) is colored in gray surface. The best modes of the PG resulted from AutoDock Vina (cyan), GOLD/GoldScore (magenta), GOLD/ChemPLP (orange) simulations are in the BL2Loop region. On the left is the highlight structure overlay.

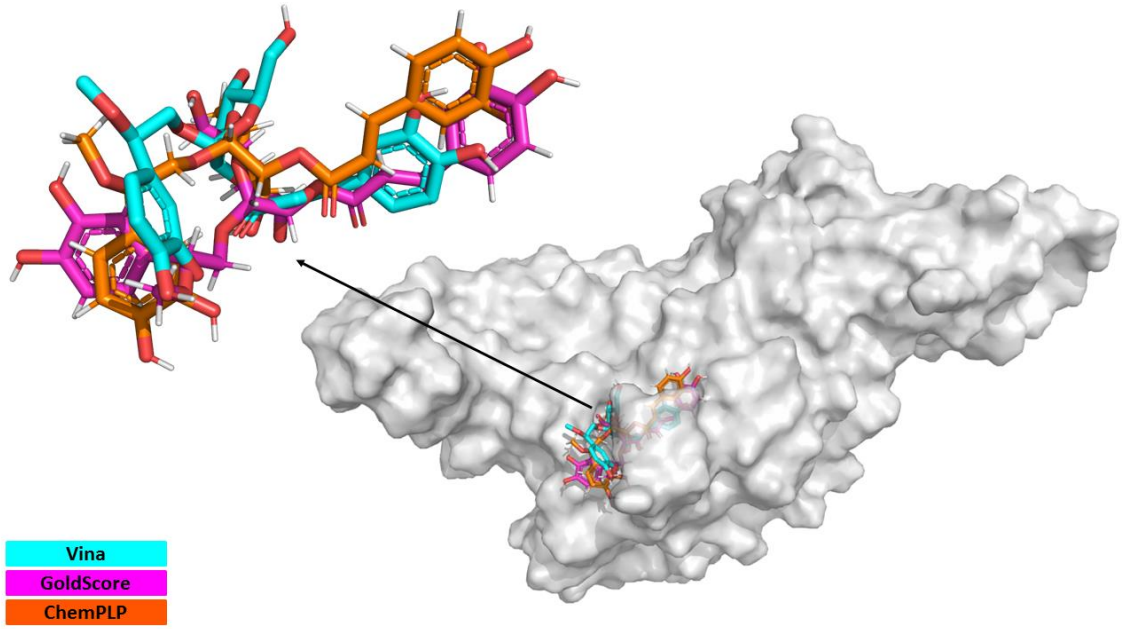


Figure S 11: PG_348 modes overlay. The three-dimensional structure of PLpro (PDBid: 7JRN) is colored in gray surface. The best modes of the PG resulted from AutoDock Vina (cyan), GOLD/GoldScore (magenta), GOLD/ChemPLP (orange) simulations are in the BL2Loop region. On the left is the highlight structure overlay.

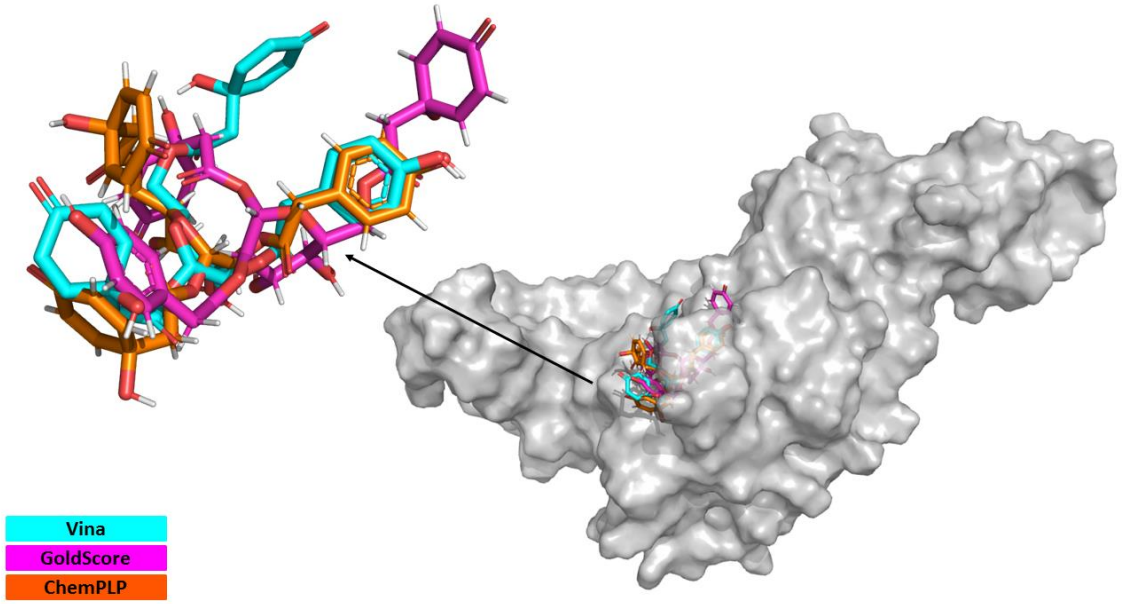


Figure S 12: PG_447 modes overlay. The three-dimensional structure of PLpro (PDBid: 7JRN) is colored in gray surface. The best modes of the PG resulted from AutoDock Vina (cyan), GOLD/GoldScore (magenta), GOLD/ChemPLP (orange) simulations are in the BL2Loop region. On the left is the highlight structure overlay.