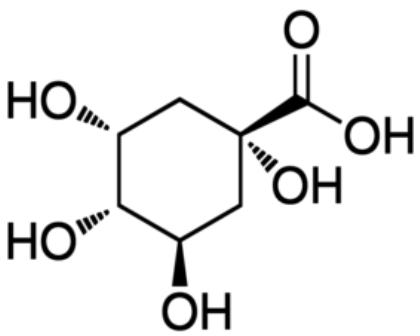
ID table

No.	Rt[a] (min)	Tentative Identification	m/z [M+H]+	m/z [M–H]–	M.W.[b]	MS Fragments pattern (m/z)	Molecular Formula	Δ ppm	REF[c]
Phenolic acid									
1	0.51	Quinic acid	215.0527[e]	191.0553	192	191> 173	C7H12O6	-4.508	STD[d]
2	4.32	*p*-Coumaric acid hexoside	349.1831[e]	325.0930	326	325> 163, 121, 119	C15H18O8	0.490	REF[1]
Flavonoids									
3	3.41	Gallocatechin	307.0811	305.0668	306	305, 289, 219, 181, 167, 137, 125	C15H14O7	0.308	REF[2,3]
4	4.02	Procyanidin B	579.1500	577.1359	578	577> 521, 475, 443, 407, 289, 271	C30H26O12	1.353	REF[1,4]
5	4.27	Catechin	291.0863	289.0719	290	289> 245, 203, 191, 163, 137	C15H14O6	1.310	STD[d]
6	6.34	Quercitrin	449.1079	447.0939	448	447> 299, 179, 150	C21H20O11	0.585	STD[d]
7	6.49	Isorhamnetin O-glucoside	479.1188	477.1045	478	477> 314, 299, 165	C22H22O12	0.731	REF[5,6]
8	8.17	Quercetin (coumaroyl-glucoside)	611.1399	609.1260	610	609> 579, 531, 491, 445, 463, 329, 315, 300, 291	C30H26O14	1.001	REF[7]
9	10.31	Pinocembrin	257.0808	255.0663	256	255> 213, 185, 171, 151, 145, 107	C15H12O4	-0.012	STD[d]
Lignan									
10	5.64	Secoisolariciresinol-diglucoside	709.2681[e]	731.2786[f]	686	731> 475, 359, 345, 327, 313, 179, 167	C32H46O16	1.767	REF[8-10]
11	5.94	Lignan deriv.	985.4066	491.1930	492	491>473, 327, 313, 149	C25H32O10	1.404	REF[8,11]
12	6.07	Secoisolariciresinol-glucoside	547.2153[e]	523.2196	524	523>475, 419, 361, 343, 327, 195, 165	C26H36O11	1.558	REF[8,10]
13	6.35	Secoisolariciresinol-xyloside	989.4346[g]	539.2142[f]	494	539> 493, 477, 361, 343, 300, 165	C25H34O10	1.540	REF[8.10]
14	6.44	Icariside E4	529.2053[e]	551.2145[f]	506	551> 381, 367, 341, 329, 314	C26H34O10	0.744	REF[7,8]
Sesquiterpenoid									
15	4.66	Roseoside	409.1831[e]	431.1925[f]	386	431>385, 367, 223	C19H30O8	0.765	REF[12,13]
Long chain fatty acid									
16	8.91	Pinellic acid	353.2300[e]	329.2337	330	329> 229, 211, 179, 171	C18H34O5	0.293	REF[14,15]

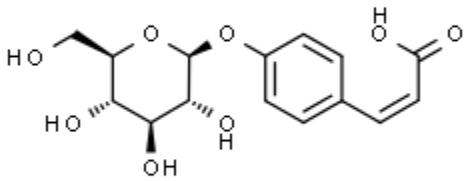
[a] Retention time; [b] Molecular weight; [c] Reference; [d] Standard; [e] [M+Na]; [f] [M+FA-H]; [g] [2M+H]

Compound chemical structure derived from *PTP*

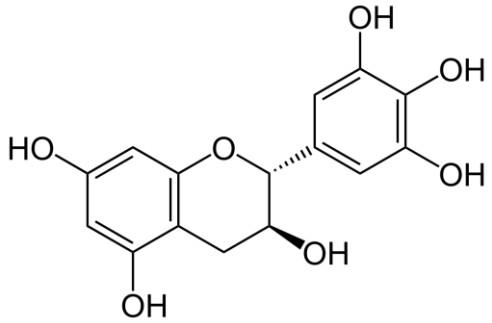
No.1 Quinic acid



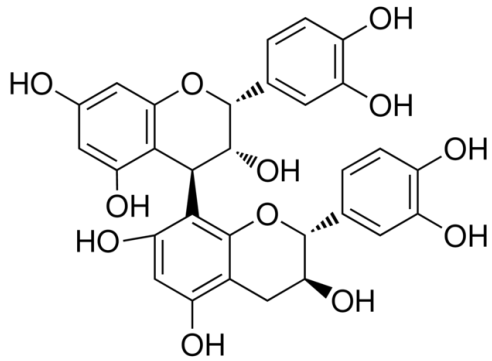
No.2 *p*-Coumaric acid hexoside



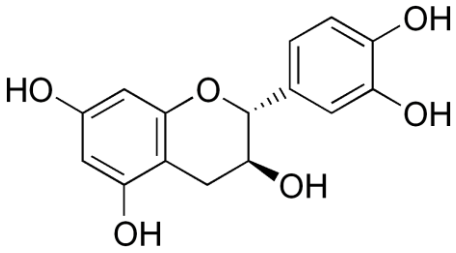
No.3 Gallocatechin



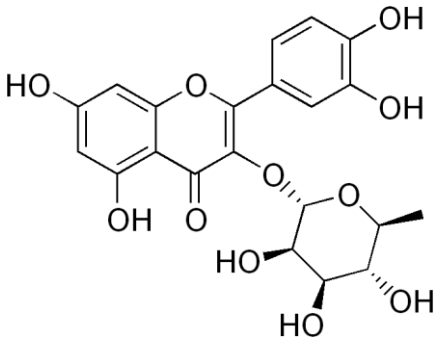
No.4 Procyanidin B



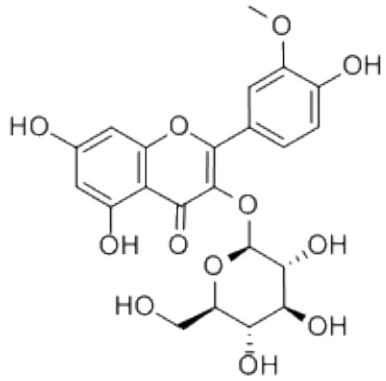
No.5 Catechin



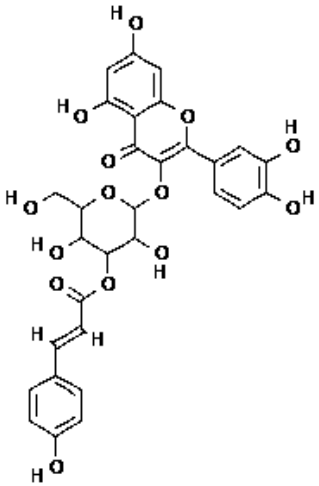
No.6 Quercitrin



No.7 Isorhamnetin O-glucoside

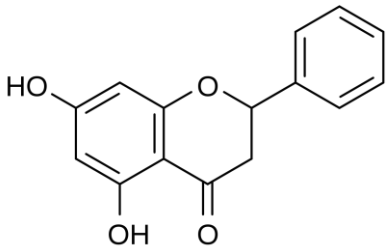


No.8 Quercetin (coumaroyl-glucoside)

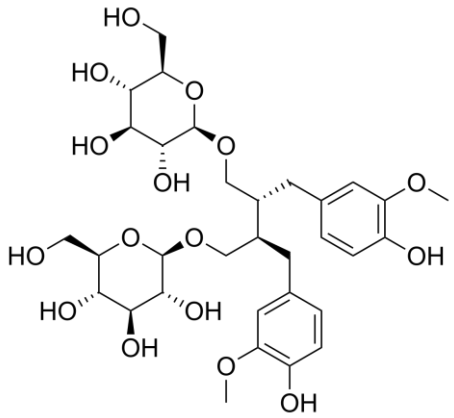


Compound chemical structure derived from *PTP*

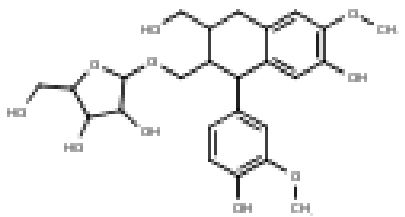
No.9 Pinocembrin



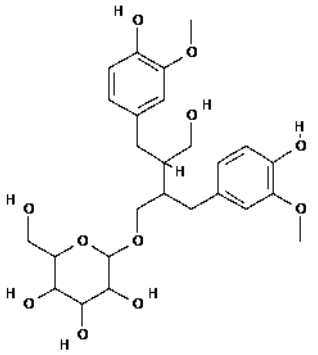
No.10 Secoisolariciresinol-diglucoside



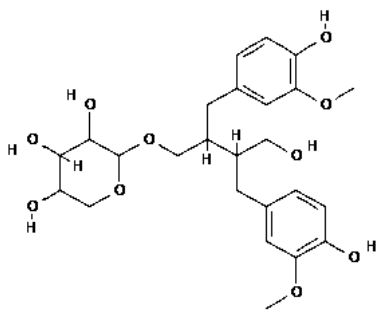
No.11 Lignan deriv.



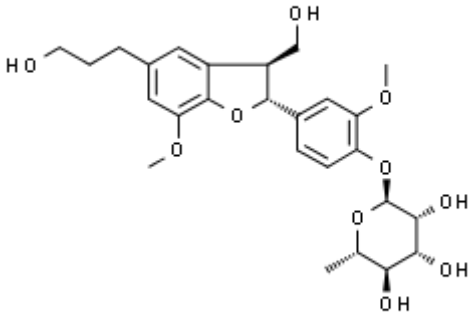
No.12 Secoisolariciresinol-glucoside



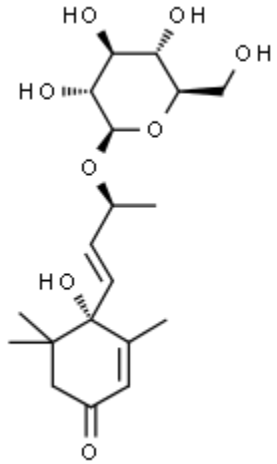
No.13 Secoisolariciresinol-xyloside



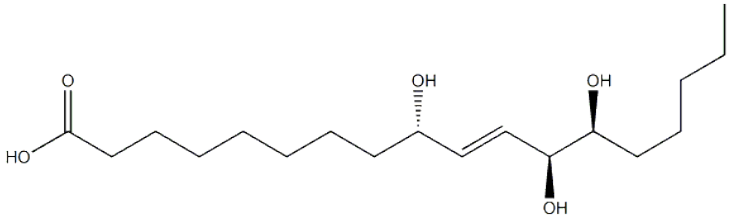
No.14 Icariside E4



No.15 Roseoside



No.16 Pinellic acid



Reference

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