Table S1. Compounds detected by GC-MS in the polar phase of *Brittonodoxa subpinnata*, and their respective Cosine and Linear Retention Index (LRI) calculated by GNPS and from the databases used in their annotation, Golm metabolome database (GMD), NIST and European Mass bank.

Peak	Rt (s)	Compound	Cosine (GNPS)	LRI	LRI (GMD)	LRI (Mass bank)	LRI (NIST)
Polar extract							
1	679	Hydroxylamine	0.80	1116	1105	1112	-
2	716	Oxalic acid	0.75	1133	1118	1125	-
3	747	Dihydrouracil	0.88	1145	-	1134	-
4	778	Hydroxybutyric acid	0.83	1162	-	1152	-
5	825	3-Methyl-2-oxovaleric acid	0.72	1188	-	1191	-
6	857	Malonic acid	0.95	1206	1197	1193	-
7	872	L-Norvaline	0.96	1215	1229	1232	-
8	917	Methylmalonic acid	0.89	1242	-	1207	-
9	927	Urea	0.87	1248	1234	1238	-
10	932	Benzoic acid	0.83	1251	-	1251	-
11	964	3-aminopropionitrile	0.89	1270	1261	1271	-
12	977	L-Proline	0.72	1283	1295	1294	-
13	1002	L-Isoleucine	0.90	1292	1286	1287	-
14	1013	Nicotinic acid	0.83	1299	1301	1295	-
15	1042	Succinic acid	0.92	1317	1311	1303	-
16	1078	Uracil	0.67	1339	1335	1332	-
17	1106	L-Serine	0.80	1357	1351	1348	-
18	1112	L-Alanine	0.88	1360	1360	-	-
19	1151	L-Threonine	0.87	1384	1377	1375	-
20	1216	DL-2.3-Diaminopropionic acid	0.80	1425	1403	1399	-
21	1310	Malic acid	0.82	1486	1479	1476	-
22	1360	L-5-Oxoproline	0.96	1519	1521	1519	-
23	1367	GABA	0.92	1524	1527	1527	-
24	1498	L-Glutamic acid	0.86	1616	1614	1607	-
25	1505	L-Phenylalanine	0.96	1622	1629	1625	-
26	1567	L-Asparagine	0.72	1668	1666	1661	-
27	1672	Aconitic acid	0.87	1748	1741	1737	-
28	1746	Shikimic acid	0.88	1805	1795	1792	-
29	1756	Citric acid	0.97	1811	1804	1804	-
30	1774	L-Iditol	0.90	1826	-	1829	-
31	1800	Mannitol	0.70	1857	1913	1908	-
32	1807	D-Fructose[1]	0.97	1862	1853	1854	-
33	1819	D-Fructose[1]	0.99	1871	1863	1864	-
34	1828	D-Glucose[2]	0.89	1878	1880	1882	-
35	1837	D-Mannose	0.90	1886	1885	1888	-
36	1858	D-Glucose[2]	0.93	1904	1900	1902	-
37	1866	D-Galactose	0.83	1910	1902	1899	-
38	1876	L-Iditol	0.90	1903	-	1900	-
39	1914	L-Ascorbic acid	0.83	1939	1937	-	-
40	1962	Chiro-Inositol	0.83	1983	1951	1973	-
41	1998	Scyllo-Inositol	0.91	2016	2027	-	-
42	2067	Myo-Inositol	0.95	2077	2080	2075	-
43	2013	Uric acid	0.50	2093	2094	2088	-
44	2168	Phytol	0.92	2172	2171	2168	-
45	2245	Stearic acid	0.88	2245	-	2236	-
46	2603	Sucrose[3]	0.95	2613	2623	2614	-
47	2609	Sucrose[3]	0.97	2621	2623	2614	-
48	2670	α-Lactose	0.89	2682	2670	2670	-

Rt: retention time. LRI: linear retention index. GMD: Golm Metabolome Database.
-: linear retention index not found in the database.
NI: not identified. GABA: gamma-aminobutyric acid.
[1] Fructose stereoisomers produced by methoximation reaction.

[2] Glucose stereoisomers produced by methoximation reaction.
[3] Sucrose stereoisomers produced by methoximation reaction.

Table 1. - Continue

Peak	Rt (sec)	Compound	Cosine	LRI	LRI (GMD)	LRI (Mass bank)	LRI (NIST)
49	2681	Maltose	0.84	2706	2719	2718	-
50	2696	D-Trehalose	0.94	2723	2727	2726	-
51	2806	Melibiose[4]	0.90	-	2837	2839	-
52	2932	Melibiose[4]	0.89	-	2868	2872	-
53	2955	Galactinol	0.82	-	2966	-	-
		Non-polar extract					
54	570	*o*-Toluic acid	0.80	1354	1359	1326	-
55	723.6	Capric acid (C10:0)	0.82	1452	-	1456	-
56	768.6	3,4-Dimethylbenzoic acid	0.75	1482	-	-	1493
57	816.6	2,4-Di-tert-butylphenol	0.74	1515	-	-	1525
58	928.2	Hexadecane (C_{16})	0.75	1591	-	-	1600
59	1004.4	Lauric acid (C12:0)	0.84	1647	1654	-	-
60	1062	Heptadecane (C_{17})	0.83	1689	-	-	1700
61	1134.6	Tridecanoic acid (Internal Standard)					
62	1159.2	Tetradecanol (C_{14})	0.86	1764	1760	-	1754
63	1167	Octadecene (C_{18})	0.90	1770	-	-	1795
64	1186.2	Glycerol 1-phosphate	0.83	1785	-	1740	-
65	1198.8	Azelaic acid	0.79	1794	1790	-	1788
66	1216.8	Octadecane (C_{18})	0.78	1808	-	-	1800
67	1237.8	11-Tetradecen-1-ol, acetate	0.84	1824	-	-	1810
68	1246.8	Pentadecanol (C_{15})	0.81	1831	1860	-	-
69	1249.2	Glucose	0.88	1833	-	1851	1844
70	1255.8	Myristic acid (C14:0)	0.76	1838	1845	-	1850
71	1318.2	Nonadecene (C_{19})	0.86	1886	-	-	1894
72	1356.6	Nonadecane (C_{19})	0.82	1918	-	-	1900
73	1372.8	Pentadecanoic acid (C15:0)	0.79	1934	1945	-	-
74	1407	Eicosene (C_{20})	0.82	1966	-	-	1997
75	1414.2	Hexadecanol (C_{16})	0.84	1973	1958	-	-
76	1432.8	Eicosane (C_{20})	0.87	1990	-	-	2000
77	1453.8	Palmitoleic acid (C16:1)	0.77	2010	-	2024	2030
78	1483.8	Palmitic acid (C16:0)	0.93	2036	2045	2038	-
79	1554	Heneicosane (C_{21})	0.80	2098	-	-	2100
80	1569	Isophytol	0.77	2112	2170	2168	2122
81	1626.6	Phytol	0.94	2167	2170	2168	2122
82	1646.4	Octadecanol (C_{18})	0.83	2185	2152	-	-
83	1657.8	Linoleic acid ethyl ester	0.76	2196	-	-	2173
84	1664.4	Oleic acid (C18:1)	0.92	2202	2217	2225	-
85	1672.2	Elaidic acid (C18:1)	0.77	2210	-	2223	-
86	1687.2	Nonadecanol (C_{19})	0.84	2224	2252	-	-
87	1693.8	Stearic acid (C18:0)	0.93	2231	2243	2236	-
88	1731	Pimaric acid	0.71	2266	-	-	2287
89	1753.2	Linoleic acid (C18:2)	0.82	2288	-	2267	2218

Rt: retention time. LRI: linear retention index. GMD: Golm Metabolome Database.
-: linear retention index not found in the database.
NI: not identified.

[4] Melibiose stereoisomers produced by methoximation reaction.

Table 1. – Continue

Peak	Rt (sec)	Compound	Cosine	LRI	LRI (GMD)	LRI (Mass bank)	LRI (NIST)
90	1812.6	Arachidonic acid (C20:4)	0.84	2348	2383	-	2372
91	1827	Juniperic acid	0.78	2363	2386	2382	-
92	1908	*Myo*-Inositol 1-phosphate	0.78	2449	2414	-	-
93	1913.4	Retinol	0.73	2455	-	-	2454
94	1969.8	Pentacosane (C_{25})	0.76	2516	-	-	2500
95	1989	Docosanol (C_{22})	0.77	2537	-	-	2549
96	2035.8	1-monopalmitin	0.76	2589	-	-	2606
97	2106	Heptacosene (C_{27})	0.82	2670	-	-	2670
98	2129.4	Alpha lactose	0.85	2697	2670	2670	-
99	2136.6	Maltose	0.83	2705	2718	2719	-
100	2214	Nervonic acid (C24:1)	0.85	2795	2815	-	2745
101	2220.6	Squalene	0.90	2803	-	-	2823
102	2235.6	Lignoceric acid (C24:0)	0.74	2821	2834	-	2838
103	2243.4	Maltitol	0.73	2831	2811	2807	-
104	2273.4	Octacosene (C_{28})	0.83	2868	-	-	2873
105	2358	Guanosine	0.71	2971	2761	2929	-
106	2392.8	Cerotic acid (C26:0)	0.77	3014	3036	-	-
107	2473.2	Alpha-tocopherol	0.88	3121	3160	3152	3149
108	2541	Montanic acid (C28:0)	0.78	3210	3232	-	3232
109	2551.8	Epicampesterol	0.90	3224	3188	-	3145
110	2559	β-sitosterol	0.73	3233	-	-	3203
111	2615.4	Stigmasterol	0.78	3304	3319	-	3286
112	2641.8	12-Oleanen-3-yl acetate	0.82	3337	-	-	3339
113	2656.8	Lanosterol	0.75	3356	3390	-	3375
114	2697.6	Alpha-spinasterol acetate	0.72	3407	-	-	3353

Rt: retention time. LRI: linear retention index. GMD: Golm Metabolome Database.
-: linear retention index not found in the database.
NI: not identified.