

Table S2. Metabolites detected by HPLC-MS² in the soluble (SE) and the insoluble extracts (IE) of *Brittonodoxa subpinnata*. The mark (X) in each column indicates in which extract the compound is present; the presence of double mark (XX) indicates the compound is present in the respective extract in more than ¾ of the total in both extracts.

N°	Rt (min)	Annotation	[M-H] ⁻	MS ²	SE	IE	Reference for annotation
1	4.25	Asparagine	131	113; 101; 95	XX	X	(Ragheb et al., 2021)
2	4.37	Maltooctaose	1313	1133; 1031; 869; 707; 545; 502; 485; 443; 382	X	X	Frag. Pattern
3	4.41	Maltononaose	1475	1295; 1193; 1133; 1031; 869; 707; 545	X	X	Frag. Pattern
4	4.46	Isomaltononaose	1476	1295; 1193; 1133; 1031; 869; 707; 545	X	X	Frag. Pattern
5	4.47	Maltoheptaose	1151	971; 869; 809; 707; 545; 383	X	X	Frag. Pattern
6	4.58	Verbascose	827	759; 647; 545; 383	XX	X	Frag. Pattern
7	4.59	Stachyose	665	485; 383; 341; 220	XX	X	(Sawada et al., 2009)
8	4.60	Maltohexaose	989	809; 707; 647; 545; 383	XX	X	Frag. Pattern
9	4.63	D-Gluconic acid	195	177; 159; 129; 99; 75	X	X	(Allamberganova et al., 2022)
10	4.72	Ribonic acid	165	147; 129; 97; 75	XX	X	Massbank
11	4.73	3,4,5-Trihydroxycinnamic acid-3'-hexoside	357	329; 219; 195; 167; 149; 125	X	X	(Zhang et al., 2015)
12	4.75	Sucrose	341	179; 161; 143; 113	XX	X	(Ragheb et al., 2021)
13	4.76	Citric acid	191	173; 111	XX	X	(Ragheb et al., 2021)
14	4.92	Protochatechuic acid	153	125; 109; 107	XX	X	(Zhang et al., 2015)
15	5.36	Raffinose	503	341; 322; 221; 179; 161; 143	XX	X	GNPS
16	5.82	3,4,5-Trihydroxycinnamic acid-3'-hexoside	357	329; 219; 195; 167; 149; 125	X	X	(Zhang et al., 2015)
17	5.88	Catechin 7-O-glucopyranoside	451	423; 331; 289; 151	X	XX	(Kang et al., 2016)
18	5.91	Quinic acid	191	171; 111	XX	X	(Zhang et al., 2015)
19	5.96	Homogentisate	167	151; 149; 139; 125; 123	X	XX	GNPS
20	5.98	Luteolin-6,8-di-C-hexopyranoside	609	591; 519; 489; 399; 369; 285	X	X	(Zhang et al., 2015)
21	6.00	Rhamnetin 3-O-hexopyranoside	477	445; 357; 339; 325; 315; 297; 283	XX	X	Frag. Pattern
22	6.18	Gentisic acid	153	137; 123; 109	XX	X	GNPS
23	6.25	Sinapic acid	223	193; 179; 163; 151	XX	X	(Díaz-Rivas et al., 2018)
24	6.26	Possible flavonoid	275	257; 231; 151	X	XX	GNPS
25	6.53	Tricetin	301	273; 257; 193; 179; 151	X	X	(Kang et al., 2016)
26	7.56	Octadecatetraenoic acid	275	257; 231; 151	X	XX	GNPS

Table 2. – continue

N°	Rt (min)	Annotation	[M-H] ⁻	MS ²	SE	IE	Reference for annotation
27	7.91	Prunin	433	373; 369; 313; 295; 271	XX	X	(Kang et al., 2016)
28	7.98	Taxifolin 3- <i>O</i> -hexopyranoside	465	303; 270	XX	X	(Kang et al., 2016)
29	7.99	5,7,3',4',5'-Pentahydroxyflavanone	303	271; 227; 179; 151	X		GNPS
30	8.16	Orobol-4'- <i>O</i> -hexopyranoside	447	327; 285	XX	X	Frag. Pattern
31	8.29	Isorhamnetin-3- <i>O</i> -hexopyranoside	477	445; 357; 315; 283	XX	X	(Kang et al., 2016)
32	9.23	Selgin	315	300; 283; 271; 256; 229	X		Frag. Pattern
33	9.24	Hovenodulinol-3- <i>O</i> -hexopyranoside	509	347; 315	XX	X	Frag. Pattern
34	9.42	Epicatechin-5- <i>O</i> -hexopyranosyl-3-benzoate	555	537; 435; 417; 393; 361	XX	X	(Hwang et al., 2001)
35	9.47	<i>p</i> -Hydroxymandelic acid	167	151; 139; 125; 123	X	XX	GNPS
36	10.06	Rhamnetin 3- <i>O</i> -hexopyranoside	477	445; 357; 328. 325; 315; 283	XX	X	Frag. Pattern
37	10.15	Isorhamnetin	315	300; 287; 284; 283; 271; 256; 229	X		(Kang et al., 2016)
38	10.57	Orobol-7- <i>O</i> -hexopyranoside	447	327; 285	XX	X	Frag. Pattern
39	10.83	Fisetin	285	267; 257; 241; 229; 217; 175; 151; 137; 125; 109	X	X	Massbank and (Fabre et al., 2001)
40	10.87	3-Hydroxyphenyl acetic acid	151	123; 107; 83; 65	X	X	GNPS
41	11.12	Dihydroxyringtonin-3- <i>O</i> -hexoside	509	341; 315; 283	X		Frag. Pattern
42	11.98	Orobol	285	267; 257; 241; 229; 217; 175; 151	X	X	Frag. Pattern
43	12.62	Diosmetin	299	284; 231; 147	X	X	(Zou et al., 2015)
44	12.65	Isorhamnetin-3- <i>O</i> -hexopyranoside	477	445; 357; 325; 315; 283	XX	X	Frag. Pattern
45	12.99	Rhamnetin	315	300; 284; 271; 256; 229	X		Frag. Pattern
46	14.18	Biochanin A	283	265; 255; 239; 227; 211; 151	XX	X	(Hossain et al., 2010)
47	20.23	Luteolin	285	267; 257; 241; 229; 213; 177; 151; 121	X	X	(Kang et al., 2016)
48	20.86	Tetrahydroxyheptadecenoic acid	331	313; 295; 171; 157; 127		X	GNPS
49	21.74	Tetrahydroxyoctadecenoic acid	345	327; 309; 265; 247		X	(Kang et al., 2016)
50	22.18	Ferulic acid	193	178; 149; 133		X	(Díaz-Rivas et al., 2018)
51	22.59	Trihydroxyoctadecenoic acid	329	311; 293; 229; 211; 171	X	XX	(Ragheb et al., 2021)

Table 2. – continue

N°	Rt (sec)	Annotation	[M-H] ⁻	MS ²	SE	IE	Reference for annotation
52	23.19	5'-Hydroxyamentoflavone	555	537; 429; 403; 385; 377		X	Frag. Pattern
53	23.98	Dihydrosinapic acid	225	207; 197; 181; 119; 93		X	Frag. Pattern
54	24.08	Dihydroxy benzoic acid- <i>O</i> -hexoside	315	297; 271; 189; 163; 151; 107		X	(Ragheb et al., 2021)
55	24.38	2,3-Dihydrobiapigenin (isomer A)	539	495; 413; 387; 361; 177		X	(Caldas et al., 2019)
56	24.44	<i>p</i> -Coumaric acid	163	135; 119		X	(Ragheb et al., 2021)
57	24.53	Trihydroxyoctadecenoic acid	329	311; 293; 229; 211; 171	X	X	(Ragheb et al., 2021)
58	24.55	Fukugetin	555	513; 429; 403; 385; 377		X	GNPS
59	25.24	Dihydrokaempferol	287	269; 241; 155; 127		X	(Kang et al., 2016)
60	25.97	2,3-Dihydrobiapigenin (isomer B)	539	521; 495; 413; 387; 361		X	(Caldas et al., 2019)
61	26.69	Octadecadienoic acid (isomer A)	279	261; 246; 237; 233		X	GNPS
62	27.00	Octadecadienoic acid (isomer B)	279	261; 246; 237; 217		X	GNPS
63	27.10	3a-Hydroxy-3,5a,9-trimethyl-3,4,5,6,7,9b-hexahydrobenzo[g][1]benzofuran-2,8-dione	263	263; 245; 235; 219		X	GNPS
64	28.65	2,3-Dihydrobiapigenin (isomer C)	539	495; 413; 387; 361; 177		X	(Caldas et al., 2019)
65	30.26	3a-Hydroxy-3,5a,9-trimethyl-3,4,5,6,7,9b-hexahydrobenzo[g][1]benzofuran-2,8-dione	263	263; 245; 219; 217		X	GNPS
66	30.58	Binaringenin (isomer A)	541	415; 389; 363; 177		X	(Yao et al., 2017)
67	30.91	Binaringenin (isomer B)	541	415; 389; 363; 177		X	(Yao et al., 2017)
68	33.08	Dihydroxyoctadecadienoic acid	311	293; 275; 201; 171		X	Frag. Pattern
69	37.19	Dihydroxyoctadecenoic acid	313	295; 277; 201; 171		X	GNPS
70	37.41	Caffeic acid	179	151; 135; 111; 93		X	(Díaz-Rivas et al., 2018)
71	37.67	LPC 18:2	504	279; 243; 224		X	GNPS
72	44.31	Canrenone	339	275; 268; 239; 225; 197; 183; 170	XX	X	GNPS
73	45.97	Nonadecanoic acid	297	268; 239; 233; 197; 183; 169	X	X	Frag. Pattern
74	47.97	Eicosanoic acid	311	268; 247; 239; 225; 211; 183; 169		X	(Perret et al., 2004)
75	50.64	Behenic acid	339	275; 253; 239; 225; 212; 197; 169	X	X	(Perret et al., 2004)
76	55.24	Possible steroid	339	295; 275; 239; 183	X	XX	GNPS