Supplementary Table S1. The LC-MS library of 53 flavonoids from soybean (*Glycine max* L.) leaves based on the literature sources.

No.	Class	Compound names	Molecular weight	Fragmentations (*m/z*)		Literatures[3)]
				Positive[1)]	Negative[2)]	
1	Flavonol	3, 4',5,7-tetrahydroxyflavonol (kaempferol)	286	325, 309, 287		3, 4, 10
2		3,3',4',5,7-pentahydroxyflavonol (quercetin)	302	341, 325, 303		3
3		kaempferol 3-*O*-glucoside (astragalin)	448	487, 471, **449**, **287**	447	2, 11
4		quercetin 3-O-galactosdie (hyperoside)	464	503, 487, 465, **303**		18
5		quercetin 3-O-glucoside (isoquercitrin)	464	503, 487, 465, **303**		18
6		kaempferol 3-*O*-(2"-*O*-rhamnosyl)galactoside	594	633, 617, **595**, 449, 287		3, 6
7		kaempferol 3-*O*-(6"-*O*-rhamnosyl)galactoside (kaempferol 3-*O*-robinobioside, biorobin)	594	633, 617, **595**, 449, 287	593	1, 3, 7, 11, 15, 18
8		kaempferol 3-*O*-(6"-*O*-rhamnosyl)glucoside (kaempferol 3-O-rutinoside, nicotiflorin)-	594	633, 617, **595**, 449, 287		1, 3, 7, 18
9		kaempferol 3-*O*-(2"-*O*-glucosyl)galactoside	610	649, 633, 611, 449, 287	609, 285	3, 5, 13
10		kaempferol 3-*O*-(6"-*O*-galactosyl)galactoside	610	649, 633, **611**, **449**, **287**	609	1, 3, 11, 15
11		kaempferol 3-*O*-(2"-*O*-glucosyl)glucoside (kaempferol 3-*O*-sophoroside)	610	649, 633, 611, 449, 287		2, 3, 5
12		kaempferol 3-*O*-(6"-*O*-glucosyl)glucoside (kaemperol 3-*O*-gentiobioside)	610	649, 633, **611**, **449**, **287**	609	1, 3, 11, 15
13		quercetin 3-*O*-(6"-*O*-rhamnosyl)galactoside (quercetin 3-*O*-robinobioside)	610	649, 633, 611, 465, 303		7, 18
14		quercetin 3-*O*-(6"-*O*-rhamnosyl)glucoside (quercetin 3-*O*-rutinoside, rutin)	610	649, 633, 611, 465, 303		7, 18
15		isorhamnetin 3-*O*-(2"-*O*-rhamnosyl)galactoside	624	663, 647, 625, 479, 317		3, 6
16		isorhamnetin 3-*O*-(6"-*O*-rhamnosyl)galactoside (isorhamnetin 3-*O*-robinobioside)	624	663, 647, 625, 479, 317		7, 18
17		isorhamnetin 3-*O*-(6"-*O*-rhamnosyl)glucoside (isorhamnetin 3-*O*-rutinoside, narcissin)	624	663, 647, 625, 479, 317		3, 7, 18
18		quercetin 3-*O*-(2"-*O*-rhamnosyl)galactoside	626	665, 649, 627, 465, 303		3, 6
19		quercetin 3-*O*-(2"-*O*-glucosyl)galactoside	626	665, 649, 627, 465, 303		3, 6
20		quercetin 3-*O*-(2"-*O*-glucosyl)glucoside (quercetin 3-*O*-sophorosde)	626	665, 649, 627, 465, 303		3, 6
21		isorhamnetin 3-*O*-(2"-*O*-glucosyl)galactoside	640	679, 663, 641, 479, 317		3, 6
22		kaempferol 3-*O*-(2",6"-di-*O*-rhamnosyl)galactoside	740	779, 763, **741**, **595**, **449**, **287**	739, 285	1, 3, 5, 6, 11, 13, 15
23		kaempferol 3-*O*-(4",6"-di-*O*-rhamnosyl)galactoside	740	779, **763**, 741, **595**, **449**, **287**	739	3, 7, 8, 18
24		kaempferol 3-*O*-(2"-*O*-rhamnosyl-6"-*O*-glucosyl)galactoside	756	795, 779, **757**, **611**, 595, **449**, **287**		1, 3
25		kaempferol 3-*O*-(4"-*O*-rhamnosyl-6"-*O*-glucosyl)galactoside	756	795, **779**, 757, 611, 595, **449**, **287**	755	3, 8
26		kaempferol 3-*O*-(2"-*O*-glucosyl-6"-*O*-rhamnosyl)galactoside	756	795, **779**, 757, 611, 595, **449**, **287**	755, 285	3, 5, 8, 11, 13, 15
27		kaempferol 3-*O*-(2"-*O*-glucosyl-6"-*O*-rhamnosyl)glucoside	756	795, **779**, 757, 611, 595, **449**, **287**	755, 285	3, 5, 8, 11, 13, 15
28		quercetin 3-*O*-(4",6"-di-*O*-rhamnosyl)galactoside	756	795, 779, **757**, **611**, **465**, **303**	755	7, 18
29		quercetin 3-*O*-(2"-*O*-glucosyl-6"-*O*-rhamnosyl)galactoside	772	811, **795**, 773, 627, 611, **465**, **303**	771	3, 6, 8
30		quercetin 3-*O*-(2"-*O*-glucosyl-6"-*O*-rhamnosyl)glucoside	772	811, **795**, **773**, 627, 611, **465**, **303**		3, 6, 8
31	Flavone	4',7 -dihydroxyflavone	254	287, 271, **255**		9
32		5,7-dihydroxyflavone (chrysin)	254	287, 271, 255	253	11
33		4',5,7 -trihydroxyflavone (apigenin)	270	309, 293, 271		2, 3, 4
34		3',4',5,7-tetrahydroxyflavone (luteolin)	286	325, 309, 287		3, 4
35		apigenin 7-*O*-glucoside (cosmosiin)	432	471, 455, 433, 271	431	11
36		luteolin 7-*O*-glucoside (cynaroside)	448	487, 471, 449, 287		3, 4, 18

37		chrysoeriol 7-*O*-glucoside (thermopsoside)	462	485, 463, 301, 286		18
38	Isoflavone	4',7-dihydroxyisoflavone (daidzein)	254	293, 277, **255**	253	3, 4, 9, 10, 11, 16, 17
39		4'-methoxy-7-hydroxyisoflavone (formononetin)	268	307, 291, **269**		3, 9, 12
40		4'-hydroxy-7-methoxyisoflavone (isoformononetin)	268	307, 291, **269**		3, 12, 14
41		4',5,7-trihydroxyisoflavone (genistein)	270	309, 293, 271	269	3, 4, 10, 11, 16, 17
42		4',7-dihydroxy-6-methoxyisoflavone (glycitein)	284	323, 307, 285	283	3, 4, 11, 17
43		4',6-dimethoxy-7-hydroxyisoflavone (afromosin)	298	337, 321, **299**		3, 12, 16
44		daidzein 7-*O*-glucoside (daidzin)	416	461, 455, 439, **417**, 255	415,253	3, 4, 9, 10, 11, 15, 16, 17, 18
45		formononetin 7-*O*-glucoside (ononin)	430	468, 452, **431**, 269		9
46		genistein 7-*O*-glucoside (genistin)	432	477, 471, 455, **433**, 271	431, 269	1, 2, 3, 4, 10, 11, 15, 16, 17, 18
47		glyctein 7-*O*-glucoside (glycitin)	446	491, 469, 447, 285	445	15, 16, 17
48		afromosin 7-*O*-glucoside	460	505, 461, 299		16
49		daidzein 7-*O*-(6"-*O*-malonyl)glucoside (6"-*O*-malonyldaidzin)	502	541, 525, **503**, 255	253	3, 6, 9, 10, 15, 16, 17
50		formononetin 7-*O*-(6"-*O*-malonyl)glucoside (6"-*O*-malonylononin)	516	555, 539, **517**, 269		9
51		afromosin 7-*O*-malonyl glucoside	546	547, 299		16
52		glyctein 7-*O*-(6"-*O*-malonyl)glucoside (6"-*O*-malonylglycitin)	532	555, 533, 285	283	16
53		genistein 7-*O*-(6"-*O*-malonyl)glucoside (6"-*O*-malonylgenistin)	518	557, 541, **519**, 271	517, 269	1, 3, 6, 10, 11, 15, 16

[1)] Positive fragmentations under (+) ESI-ionization mode, bold font indicates fragment ions reported from literature; the remaining's are fragment ions proposed in this study (*m/z,* $[M+H]^+$, including adduct ions of $[M+Na]^+$ and $[M+K]^+$).

[2)] Negative fragmentations under (-) ESI-ionization mode from literature (*m/z*, $[M-H]^-$).

[3)] **1**, Ho et al., 2002; **2**, Hur et al., 2001; **3**, Jeong et al., 2019; **4**, Lee et al., 2008; **5**, Li et al, 2015; **6**, Li et al., 2019; **7**, Murai et al., 2019; **8**, Murai et al., 2013; **9**, Murakami et al., 2014; **10**, Romani et al., 2003; **11**, Song et al., 2014; **12**, Yuk et al., 2011; **13**, Zang et al., 2011; **14**, Ingham et al., 1981; **15**, Yuk et al., 2016; **16**, Veremeichik et al., 2021; **17**, Veremeichik et al., 2019; **18**, Iwashina et al., 2018.

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