Supplementary Table S2: Assigned compounds detected in the 70% methanol extract of *Scutellaria barbata* leaves and the aqueous BZL decoction by LC-PDA-MSn analysis.

Assigned compound (or isomer)	Retent-ion time (min)	Molecular formula	*m/z*	Ion	*S. barbata* 70% methanol extract ppm*	*S. barbata* aqueous decoction ppm*
Sucrose or isomer	1.6	$C_{12}H_{22}O_{11}$	387.1141	$[M + HCOO]^-$	2.358	2.901
Pentahydroxyflavone	11.5	$C_{15}H_{10}O_7$	303.0505	$[M + H]^+$	1.719	Nd
Pentahydroxyflavanone	11.5	$C_{15}H_{12}O_7$	305.0662	$[M + H]^+$	Nd	1.904
Pentahydroxyflavanone	14.2	$C_{15}H_{12}O_7$	305.0661	$[M + H]^+$	1.707	1.806
Pentahydroxyflavanone	14.4	$C_{15}H_{12}O_7$	305.0661	$[M + H]^+$	1.806	1.609
Pentahydroxyflavanone	14.9	$C_{15}H_{12}O_7$	305.0660	$[M + H]^+$	Nd	1.511
Tetrahydroxyflavone	15.4	$C_{15}H_{10}O_6$	287.0556	$[M + H]^+$	1.517	2.353
Pentahydroxyflavanone	16.2	$C_{15}H_{12}O_7$	305.0661	$[M + H]^+$	Nd	1.707
Pentahydroxyflavanone	16.4	$C_{15}H_{12}O_7$	305.0661	$[M + H]^+$	Nd	1.806
6-Hydroxyluteolin 7-hexuronide	16.7	$C_{21}H_{18}O_{13}$	479.0827	$[M + H]^+$	2.574	1.363
Tetrahydroxyflavanone	17.2	$C_{15}H_{12}O_6$	289.0711	$[M + H]^+$	1.541	2.267
Tetrahydroxyflavone	17.5	$C_{15}H_{10}O_6$	287.0555	$[M + H]^+$	Nd	1.726
Tetrahydroxyflavanone	18.1	$C_{15}H_{12}O_6$	289.0710	$[M + H]^+$	0.780	1.541
Tetrahydroxyflavanone hexuronide	18.2	$C_{21}H_{20}O_{12}$	465.1030	$[M + H]^+$	0.403	1.973
Trihydroxyflavone hexoside	18.9	$C_{21}H_{20}O_{10}$	433.1140	$[M + H]^+$	Nd	2.094
6-Hydroxyluteolin 4'-hexuronide	19.2	$C_{21}H_{18}O_{13}$	479.0832	$[M + H]^+$	Nd	2.386
Scutellarein 7-hexoside	19.5	$C_{21}H_{20}O_{11}$	449.1083	$[M + H]^+$	1.051	1.319
Tetrahydroxyflavanone	19.9	$C_{15}H_{12}O_6$	289.0709	$[M + H]^+$	0.572	0.884
Tetrahydroxyflavanone	20.1	$C_{15}H_{12}O_6$	289.0710	$[M + H]^+$	1.195	1.299
Scutellarein 7-hexuronide	20.4	$C_{21}H_{18}O_{12}$	463.0874	$[M + H]^+$	0.707	0.837
2',5,7-Trihydroxyflavone	21.4	$C_{15}H_{10}O_5$	271.0605	$[M + H]^+$	1.328	1.328
Tetrahydroxyflavanone	22.5	$C_{16}H_{14}O_6$	303.0867	$[M + H]^+$	0.875	1.370
Tetrahydroxyflavone	22.5	$C_{15}H_{10}O_6$	287.0555	$[M + H]^+$	1.517	Nd
Trihydroxyflavanone hexuronide	22.7	$C_{21}H_{20}O_{11}$	449.1082	$[M + H]^+$	0.762	1.385
Hydroxyapigenin	22.9	$C_{15}H_{10}O_6$	287.0553	$[M + H]^+$	0.994	1.831
Isoscutellarein 7-hexuronide	23.0	$C_{21}H_{18}O_{12}$	463.0876	$[M + H]^+$	1.571	2.219
Scutellarein 6-hexuronide	23.6	$C_{21}H_{18}O_{12}$	463.0874	$[M + H]^+$	0.578	1.377
Apigenin hexuronide	24.1	$C_{21}H_{18}O_{11}$	447.0928	$[M + H]^+$	0.301	0.900
Tetrahydroxyflavone	24.4	$C_{15}H_{10}O_6$	287.0555	$[M + H]^+$	1.622	Nd
Trihydroxyflavone hexuronide	24.8	$C_{21}H_{18}O_{11}$	447.0929	$[M + H]^+$	Nd	1.660
Tetrahydroxyflavone methyl ether hexuronide	25.1	$C_{22}H_{20}O_{12}$	477.1030	$[M + H]^+$	0.456	0.770
1-Octen-3-ol pentosyl dihexoside	25.5	$C_{24}H_{22}O_{13}$	602.3024	$[M + NH_4]^+$	Nd	0.970
6-Methoxyapigenin (hispidulin) 7-hexuronide	25.8	$C_{22}H_{20}O_{12}$	477.1033	$[M + H]^+$	1.336	1.672
Trihydroxyflavone malonyl-hexoside	25.9	$C_{24}H_{22}O_{13}$	519.1141	$[M + H]^+$	1.585	Nd
Pentahydroxyflavone 7-hexuronide	26.0	$C_{21}H_{18}O_{13}$	479.0831	$[M + H]^+$	Nd	2.261
Tetrahydroxyflavanone methyl ether	26.0	$C_{16}H_{14}O_6$	303.0867	$[M + H]^+$	1.271	Nd
Scutellarein	27.0	$C_{15}H_{10}O_6$	287.0554	$[M + H]^+$	1.308	1.935

Hydroxyapigenin	27.5	$C_{15}H_{10}O_6$	287.0553	$[M + H]^+$	1.099	1.308
Tetrahydroxyflavone	28.0	$C_{15}H_{10}O_6$	287.0555	$[M + H]^+$	1.517	Nd
Isoscutellarein 8-hexuronide	28.3	$C_{21}H_{18}O_{12}$	463.0877	$[M + H]^+$	0.049	0.448
Dihydroxy-methoxyflavone rhamnosyl hexoside	30.0	$C_{28}H_{32}O_{14}$	593.1867	$[M + H]^+$	0.384	0.384
Scutalbin A (= 19-Deacetyljodrellin A)	30.0	$C_{22}H_{30}O_7$	407.2072	$[M + H]^+$	1.990	Nd
Tetrahydroxyflavone	30.4	$C_{15}H_{10}O_6$	287.0555	$[M + H]^+$	1.517	1.203
6α,19-Di-O-acetyl-2,19:4,18:11,16:15,16-tetraepoxyneoclerodane-6,15,19-triol	30.6	$C_{24}H_{34}O_9$	484.2548	$[M + NH_4]^+$	Nd	1.470
11-Episcutecolumnin C or Scutecolumnin C	31.6	$C_{22}H_{32}O_7$	426.2493	$[M + NH_4]^+$	1.504	1.504
Scupolin H or isomer	31.9	$C_{23}H_{32}O_7$	421.2229	$[M + H]^+$	1.520	Nd
Wogonoside	32.1	$C_{22}H_{20}O_{11}$	461.1083	$[M + H]^+$	-3.002	1.024
Scutebata I (= 6-Acetoxybarbatin C)	32.3	$C_{22}H_{30}O_6$	391.2121	$[M + H]^+$	Nd	1.418
Scutebata C or Barbatin G	32.5	$C_{28}H_{35}NO_9$	530.2394	$[M + H]^+$	Nd	1.739
Scutellarein Me ether	32.7	$C_{16}H_{12}O_6$	301.0711	$[M + H]^+$	1.247	1.679
Scutebata A1 or Scutebata Z	33.4	$C_{28}H_{33}NO_8$	512.2289	$[M + H]^+$	Nd	1.926
Scutellarein Me ether	33.7	$C_{16}H_{12}O_6$	301.0712	$[M + H]^+$	1.778	1.479
2',5,7-Trihydroxyflavone	34.0	$C_{15}H_{10}O_5$	271.0604	$[M + H]^+$	1.070	1.550
Jodrellin A	34.2	$C_{24}H_{32}O_8$	466.2441	$[M + NH_4]^+$	Nd	1.344
8-Hydroxyflavone methyl ether	34.3	$C_{16}H_{12}O_6$	301.0710	$[M + H]^+$	1.247	1.380
Cirsiliol	34.4	$C_{17}H_{14}O_7$	331.0816	$[M + H]^+$	1.120	1.694
Scutellone J	34.5	$C_{24}H_{34}O_8$	468.2598	$[M + H]^+$	Nd	1.359
Tetrahydroxyflavone	35.1	$C_{15}H_{10}O_6$	287.0555	$[M + H]^+$	Nd	1.517
Tetrahydroxyflavone Me ether	35.5	$C_{16}H_{12}O_6$	301.0712	$[M + H]^+$	Nd	1.778
Deacetyl scuterulein C or Scutorientalin D	35.7	$C_{28}H_{40}O_{10}$	554.2970	$[M + H]^+$	1.402	2.069
Tetrahydroxyflavone Me ether	35.8	$C_{16}H_{12}O_6$	301.0711	$[M + H]^+$	Nd	1.579
Scutebarbatine G or Scutelinquanine D	36.3	$C_{26}H_{33}NO_7$	472.2335	$[M + H]^+$	1.019	1.337
Barbatin C or isomer	36.6	$C_{20}H_{28}O_5$	366.2281	$[M + NH_4]^+$	Nd	1.612
11-Episcutecolumnin C or Scutecolumnin C	37.3	$C_{22}H_{32}O_7$	426.2496	$[M + NH_4]^+$	2.654	1.926
2α-Hydroxydeacetylajugarin V	37.4	$C_{20}H_{30}O_5$	351.2149	$[M + H]^+$	Nd	-4.927
Dihydroxy-tetramethoxyflavone	37.7	$C_{19}H_{18}O_8$	375.1079	$[M + H]^+$	1.162	1.722
Barbatin C or isomer	37.8	$C_{20}H_{28}O_5$	349.2015	$[M + H]^+$	Nd	1.516
Dihydroxy-trimethoxyflavone	37.9	$C_{18}H_{16}O_7$	345.0974	$[M + H]^+$	1.538	1.886
Barbatellarine C or Barbatellarine D	38.3	$C_{30}H_{37}NO_{10}$	572.2501	$[M + H]^+$	1.498	1.393
Dihydroxy-dimethoxyflavone	38.5	$C_{17}H_{14}O_6$	315.0871	$[M + H]^+$	Nd	2.112
Scutebata C or Barbatin G	38.7	$C_{28}H_{35}NO_9$	530.2394	$[M + H]^+$	1.852	Nd
Dihydroxy-dimethoxyflavone	39.1	$C_{17}H_{14}O_6$	315.0867	$[M + H]^+$	1.794	1.318
6-*O*-Nicotinoylscutebarbatine G or isomer	39.3	$C_{32}H_{36}N_2O_8$	577.2551	$[M + H]^+$	0.966	1.503
11-Episcutecolumnin C or Scutecolumnin C	39.4	$C_{22}H_{32}O_7$	426.2494	$[M + NH_4]^+$	1.129	1.856
6-*O*-Nicotinoylscutebarbatine G or isomer	39.5	$C_{32}H_{36}N_2O_8$	577.2548	$[M + H]^+$	0.654	Nd
Scutolide I or isomer	39.6	$C_{26}H_{36}O_9$	510.2703	$[M + NH_4]^+$	1.297	1.101

Scutolide I or isomer	39.8	$C_{26}H_{36}O_9$	510.2706	$[M + NH_4]^+$	0.572	0.565
6-*O*-Nicotinoylscutebarbatine G or isomer	40.3	$C_{32}H_{36}N_2O_8$	577.2551	$[M + H]^+$	1.087	1.919
5-Hydroxy-2',6',7,8-tetramethoxyflavone	40.8	$C_{19}H_{18}O_7$	359.1130	$[M + H]^+$	2.007	1.255
Scutelinquanine A	40.8	$C_{28}H_{35}NO_8$	514.2443	$[M + H]^+$	1.627	1.393
6-*O*-Nicotinoylscutebarbatine G or isomer	41.1	$C_{32}H_{36}N_2O_8$	577.2552	$[M + H]^+$	1.295	1.191
Deacetyl scuterulein C or Scutorientalin D	41.3	$C_{28}H_{40}O_{10}$	554.2969	$[M + NH_4]^+$	1.745	0.752
Scutebata F isomer	41.6	$C_{30}H_{37}NO_9$	556.2549	$[M + H]^+$	Nd	1.388
Scutebata C or Barbatin G	41.8	$C_{28}H_{35}NO_9$	530.2392	$[M + H]^+$	1.399	1.286
Scutebarbatine Z	41.9	$C_{26}H_{33}NO_5$	440.2439	$[M + H]^+$	1.773	-0.993
Scutehenanine A or isomer	41.9	$C_{26}H_{31}NO_6$	454.2231	$[M + H]^+$	Nd	1.598
Barbatin H or isomer	42.0	$C_{34}H_{38}N_2O_9$	619.2654	$[M + H]^+$	1.200	0.602
Scutebata F	42.3	$C_{30}H_{37}NO_9$	556.2547	$[M + H]^+$	1.064	0.291
6-*O*-Nicotinoylscutebarbatine G or isomer	42.3	$C_{32}H_{36}N_2O_8$	577.2554	$[M + H]^+$	1.607	1.607
Scubartine E	42.6	$C_{31}H_{39}NO_9$	570.2705	$[M + H]^+$	-1.132	Nd
6,7-Di-*O*-acetoxybarbatin A	42.6	$C_{24}H_{32}O_7$	450.2495	$[M + H]^+$	Nd	1.957
Scutebarbatine A isomer	42.8	$C_{32}H_{34}N_2O_7$	559.2444	$[M + H]^+$	0.898	Nd
Scutehenanine A or isomer	43.0	$C_{26}H_{31}NO_6$	454.2230	$[M + H]^+$	1.400	1.334
6,7-Di-*O*-nicotinoylscutebarbatine G	43.2	$C_{38}H_{39}N_3O_9$	682.2770	$[M + H]^+$	-0.306	1.838
Scutellone J	44.5	$C_{24}H_{34}O_8$	468.2599	$[M + NH_4]^+$	1.872	1.551
Scutelinquanine A	43.5	$C_{28}H_{35}NO_8$	514.2441	$[M + H]^+$	1.160	1.627
Salvigenin	43.7	$C_{18}H_{16}O_6$	329.1025	$[M + H]^+$	1.475	0.988
Scutebarbatine K or 6-*O*-Acetylscutehenanine A	44.0	$C_{28}H_{33}NO_7$	496.2340	$[M + H]^+$	1.030	1.957
Scutebarbatine X	44.2	$C_{34}H_{38}N_2O_{10}$	635.2598	$[M + H]^+$	0.422	Nd
Scutolide I or isomer	44.3	$C_{26}H_{36}O_9$	510.2695	$[M + NH_4]^+$	Nd	0.513
Barbatin H or isomer	44.4	$C_{34}H_{38}N_2O_9$	619.2660	$[M + H]^+$	1.587	2.088
Barbatellarine C or D	44.6	$C_{30}H_{37}NO_{10}$	572.2497	$[M + H]^+$	Nd	1.166
Scutebata O	44.7	$C_{28}H_{35}NO_7$	498.2494	$[M + H]^+$	Nd	1.588
Clerodin	44.8	$C_{24}H_{34}O_7$	452.2648	$[M + NH_4]^+$	Nd	1.152
Scutebarbatine A	44.9	$C_{32}H_{34}N_2O_7$	559.2437	$[M + H]^+$	0.898	1.023
Scutebata E or R or Scutolide G	45.4	$C_{28}H_{40}O_9$	538.3010	$[M + NH_4]^+$	0.393	1.304
Scutebata E or R or Scutolide G	45.6	$C_{28}H_{40}O_9$	538.3016	$[M + NH_4]^+$	0.951	1.749
Scutebata F isomer	46.0	$C_{30}H_{37}NO_9$	556.2552	$[M + H]^+$	1.701	1.729
Scutebartine A or isomer	46.0	$C_{33}H_{37}NO_8$	576.2510	$[M + H]^+$	0.046	1.729
Scutebarbatine K or 6-*O*-Acetylscutehenanine A	46.1	$C_{28}H_{33}NO_7$	496.2333	$[M + H]^+$	1.574	1.897
Scutolide B	46.5	$C_{30}H_{37}NO_7$	524.2650	$[M + H]^+$	Nd	-1.157
Scutebatin A or Scutebatin B	46.5	$C_{39}H_{40}N_2O_9$	681.2817	$[M + H]^+$	0.837	Nd
Scutolide H	46.6	$C_{32}H_{41}NO_9$	584.2864	$[M + H]^+$	1.441	1.766
Scuetbata O	46.8	$C_{28}H_{35}NO_7$	498.2491	$[M + H]^+$	0.905	1.166
Scutebata B	47.0	$C_{35}H_{39}NO_{10}$	634.2651	$[M + H]^+$	1.020	Nd
Scutebarbatine B or Y or Scutebartine F	47.4	$C_{33}H_{35}NO_7$	558.2493	$[M + H]^+$	1.148	1.363
Scutebartine A or isomer	47.6	$C_{33}H_{37}NO_8$	576.2597	$[M + H]^+$	0.671	2.059
Methylwogonin	47.7	$C_{17}H_{14}O_5$	299.0919	$[M + H]^+$	Nd	1.538
Scutebata T (= Scutolide A)	47.9	$C_{26}H_{36}O_7$	461.2540	$[M + H]^+$	Nd	1.409
Barbatellarine B	47.9	$C_{35}H_{39}NO_9$	618.2705	$[M + H]^+$	1.216	Nd
Scutebarbatolide C or isomer	48.1	$C_{31}H_{38}O_9$	572.2861	$[M + NH_4]^+$	1.261	1.471
Scutebata M	48.2	$C_{33}H_{43}NO_9$	598.3023	$[M + H]^+$	-0.244	Nd

6-*O*-(2-oxo-3-methylbutanoyl)scutehenanine A or isomer	49.5	$C_{31}H_{37}NO_8$	552.2606	$[M + H]^+$	2.474	2.148
Scutellone G or isomer	49.6	$C_{29}H_{36}O_8$	530.2756	$[M + NH_4]^+$	Nd	1.483
Barbatellarine B	49.7	$C_{35}H_{39}NO_9$	618.2709	$[M + H]^+$	1.911	1.119
6-*O*-(2-oxo-3-methylbutanoyl)scutehenanine A or isomer	50.0	$C_{31}H_{37}NO_8$	552.2602	$[M + H]^+$	Nd	1.804
Scutebata B	50.2	$C_{35}H_{39}NO_{10}$	634.2661	$[M + H]^+$	1.399	2.077
Scutebarbatine B or Y or Scutebartine F	50.6	$C_{33}H_{35}NO_7$	558.2492	$[M + H]^+$	0.933	1.686
Scutebata S	51.0	$C_{33}H_{42}O_9$	600.3177	$[M + NH_4]^+$	1.635	1.435

All compounds assigned by comparison of accurate mass data (ppm*), and by interpretation of available
MSn and/or UV spectra.
Nd: Not detected / below level of detection.