Article

Efficacy and Tolerability of a Chemically Characterized *Scutellaria lateriflora* L. Extract-Based Food Supplement for Sleep Management: A Single-Center, Controlled, Randomized, Crossover, Double-Blind Clinical Trial

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Table S1. Identified compounds in *S. lateriflora* extract according to molecular formula, *m/z*, and the retention time (RT)

Name	Formula	Δ [ppm]	*m/z*	RT [min]	Reference Ion
Gallic acid	C7 H6 O5	-4,59	169,0135	1,588	[M-H]-1
Chlorogenic acid	C16 H18 O9	0,76	353,0881	4,76	[M-H]-1
Chlorogenic acid dimer	C32 H36 O18	2,06	707,1844	5,597	[M-H]-1
Chlorogenic acid isomer	C16 H18 O9	0,41	353,0880	5,609	[M-H]-1
Chlorogenic acid isomer	C16 H18 O9	0,6	353,0880	6,059	[M-H]-1
Kaempferol-3-O-hexo rhamnoside isomer	C27 H30 O15	0,96	593,1518	6,312	[M-H]-1
Carthamidin 7-O-glucoronide	C21 H20 O12	1,18	463,0887	6,676	[M-H]-1
Ferulic acid	C10 H10 O4	-3,16	193,0500	6,733	[M-H]-1
Pentahydroxyflavanone	C21 H22 O11	0,64	449,1092	6,846	[M-H]-1
Schaftoside	C26 H28 O14	0,48	563,1409	6,865	[M-H]-1
Quercetin-dihexoside	C27 H30 O17	0,74	625,1415	6,965	[M-H]-1
Myricetin-hexoside	C21 H20 O13	0,12	479,0832	6,966	[M-H]-1
Luteolin 7,3'-diglucuronide	C27 H26 O18	0,87	637,1052	7,011	[M-H]-1
Quercetin-hexoside	C21 H20 O12	0,56	463,0885	7,129	[M-H]-1
6-C-Glucopyranosyldihydrokaempferol	C21 H22 O11	0,95	449,1094	7,222	[M-H]-1
Taxifolin	C15 H12 O7	0,32	303,0512	7,272	[M-H]-1
Quercetin 3-glucuronide	C21 H18 O13	0,79	477,0678	7,353	[M-H]-1
Schaftoside isomer	C26 H28 O14	0,53	563,1409	7,39	[M-H]-1
Luteolin 7-glucuronide	C21 H18 O12	0,98	461,0730	7,532	[M-H]-1
Ellagic acid	C14 H6 O8	0,38	300,9991	7,592	[M-H]-1
Rutin	C27 H30 O16	0,21	609,1462	7,595	[M-H]-1
6-C-beta-D-Hexosyl apigenin	C21 H20 O10	-0,27	431,0983	7,619	[M-H]-1
Kaempferol-3-O-hexo rhamnoside	C27 H30 O15	0,5	593,1515	7,642	[M-H]-1
Verbascoside	C29 H36 O15	0,65	623,1986	7,669	[M-H]-1
Quercetin-3-O-glucopyranoside (isoquercitrin)	C21 H20 O12	0,82	463,0886	7,686	[M-H]-1
Persicogenin-hexoside	C23 H26 O11	0,66	477,1406	7,754	[M-H]-1
Ferulic acid isomer	C10 H10 O4	-3,44	193,0500	7,762	[M-H]-1
Quercetin-hexoside isomer	C21 H20 O12	0,72	463,0885	7,789	[M-H]-1

Kaempferol 3-hexoside-7-glucuronide	C27 H28 O17	0,38	623,1256	7,849	[M-H]-1
Chrysin 8-C-β-d-hexoside	C21 H20 O9	0,29	415,1036	7,945	[M-H]-1
Ferulic acid isomer	C10 H10 O4	-3,63	193,0499	7,951	[M-H]-1
Quercetin 4'-methyl ether 3-hexoside	C22 H22 O12	0	477,1039	8,092	[M-H]-1
Kaempferol-3-O-hexo rhamnoside isomer	C27 H30 O15	0,7	593,1516	8,25	[M-H]-1
Isoorientin 3'-O-glucuronide	C27 H28 O17	0,48	623,1257	8,337	[M-H]-1
Dihydrokaempferol	C15 H12 O6	0,46	287,0562	8,382	[M-H]-1
Hesperetin 7-O-hexoside	C22 H24 O11	1,35	463,1252	8,384	[M-H]-1
Scutellarein 7,4'-dimethyl ether 6-sophoroside	C29 H34 O16	0,43	637,1777	8,442	[M-H]-1
Luteolin 3',4'-diglucuronide	C27 H26 O18	0,37	318,0487	8,471	[M-2H]-2