Table S1: Pharmacokinetic preperties ADMET of selected *Inula britannica* phytocompounds.

Compound name	Formula	MW < 500	#Heavy atoms 15–50	#Aromatic heavy atoms	Fraction Csp3	#Rotatable bonds	#H-bond acceptors	#H-bond donors	MR	TPSA	iLOGP	XLOGP3	WLOGP	MLOGP	Silicos-IT Log P
1,6-O,O-Diacetylbritannilactone	C19H26O6	350.41	25	0	0.63	8	6	0	92.13	78.9	3.48	1.88	2.72	2.38	3.47
O-acetylbritaanilactone	C17H24O5	308.37	22	0	0.65	6	5	1	82.39	72.83	2.55	1.31	2.14	2	2.95
Neobritannilactone A	C17H26O5	310.39	22	0	0.76	6	5	1	82.9	72.83	2.51	1.59	2.22	2.09	2.67
Neobritannilactone	C15H20O3	248.32	18	0	0.53	0	3	1	71.02	46.53	2.5	1.11	2.52	2.38	2.34
Acetyl neobritannilactone B	C17H22O4	290.35	21	0	0.53	2	4	0	80.75	52.6	2.91	2.44	3.09	2.75	2.77
6β-O-(2-methylbutyryl)britannilactone	C20H30O5	350.45	25	0	0.7	8	5	1	96.81	72.83	2.93	2.71	3.17	2.7	4
Britannilactone	C15H22O4	266.33	19	0	0.67	4	4	2	72.65	66.76	2.4	0.74	1.57	1.62	2.45
Taraxasteryl acetate	C32H52O2	468.75	34	0	0.91	2	2	0	144.88	26.3	4.85	9.7	8.6	7.08	7.31
β-Amyrin	C30H50O	426.72	31	0	0.93	0	1	1	134.88	20.23	4.76	9.15	8.17	6.92	6.92
Lupeol	C30H50O	426.72	31	0	0.93	1	1	1	135.14	20.23	4.76	9.87	8.02	6.92	6.82
Stigmasterol	C29H48O	412.69	30	0	0.86	5	1	1	132.75	20.23	5.08	8.56	7.8	6.62	6.86
ψ-Taraxasterol	C30H50O	426.72	31	0	0.93	0	1	1	135.14	20.23	4.66	8.89	8.02	6.92	6.52
Patuletin	C16H12O8	332.26	24	16	0.06	2	8	5	84.53	140.59	2.02	2.14	2	-0.83	1.59
Luteolin	C15H10O6	286.24	21	16	0	1	6	4	76.01	111.13	1.86	2.53	2.28	-0.03	2.03
Patulitrin	C22H22O13	494.4	35	16	0.32	5	13	8	116.65	219.74	1.44	0.33	-0.53	-2.85	-0.52
Patuletin 7-O-[6"-(2-methylbutyryl)] glucoside	C27H30O14	578.52	41	16	0.41	9	14	7	140.81	225.81	2.35	1.75	1.07	-1.82	1.04
Nepetin	C16H12O7	316.26	23	16	0.06	2	7	4	82.5	120.36	2.13	2.5	2.29	-0.31	2.06
Nepitrin	C22H22O12	478.4	34	16	0.32	5	12	7	114.63	199.51	2.59	1.43	-0.24	-2.37	-0.05
Axillarin	C17H14O8	346.29	25	16	0.12	3	8	4	89	129.59	2.37	2.46	2.3	-0.59	2.12
Hispidulin-7-glucoside	C22H22O11	462.4	33	16	0.32	5	11	6	112.6	179.28	2.45	0.83	0.06	-1.89	0.42
Isorhamnetin 3-glucoside	C22H22O12	478.4	34	16	0.32	5	12	7	114.63	199.51	2.58	0.69	-0.24	-2.37	-0.05
Rhamnetin-3-O-β-D-glucopyranoside	C22H22O12	478.4	34	16	0.32	5	12	7	114.63	199.51	2.23	0.69	-0.24	-2.37	-0.05
Kaemferol-3-O-β-D-glucopyranoside	C21H20O11	448.38	32	16	0.29	4	11	7	108.13	190.28	1.29	0.72	-0.24	-2.1	-0.12
Diosmetin	C16H12O6	300.26	22	16	0.06	2	6	3	80.48	100.13	2.47	3.1	2.59	0.22	2.55
Chrysoeriol	C16H12O6	300.26	22	16	0.06	2	6	3	80.48	100.13	2.44	3.1	2.59	0.22	2.55

Kaempferol	C15H10O6	286.24	21	16	0	1	6	4	76.01	111.13	1.7	1.9	2.28	-0.03	2.03
Quercetin	C15H10O7	302.24	22	16	0	1	7	5	78.04	131.36	1.63	1.54	1.99	-0.56	1.54
Spinacetin	C17H14O8	346.29	25	16	0.12	3	8	4	89	129.59	2.71	2.46	2.3	-0.59	2.12
Eupatin	C18H16O8	360.31	26	16	0.17	4	8	3	93.47	118.59	2.89	2.79	2.6	-0.35	2.65
Compound name	Consensus Log P	ESOL Log S	ESOL Class	Ali Log S	Ali Class	Silicos-IT LogSw	Silicos-IT class	GI absorption	BBB permeant	Pgp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor
1,6-O,O-Diacetylbritannilactone	2.79	-2.67	Soluble	-3.16	Soluble	-3.54	Soluble	High	No	No	No	No	No	No	No
O-acetylbritaanilactone	2.19	-2.18	Soluble	-2.44	Soluble	-2.92	Soluble	High	Yes	No	No	No	No	No	No
Neobritannilactone A	2.22	-2.37	Soluble	-2.73	Soluble	-2.69	Soluble	High	Yes	No	No	No	No	No	No
Neobritannilactone	2.17	-2.08	Soluble	-1.68	Very soluble	-2.25	Soluble	High	Yes	No	No	No	No	No	No
Acetyl neobritannilactone B	2.79	-3.05	Soluble	-3.19	Soluble	-2.88	Soluble	High	Yes	No	No	No	Yes	No	No
6β-O-(2-methylbutyryl)britannilactone	3.1	-3.19	Soluble	-3.89	Soluble	-3.73	Soluble	High	Yes	No	No	No	No	No	Yes
Britannilactone	1.76	-1.69	Very soluble	-1.72	Very soluble	-2.28	Soluble	High	Yes	No	No	No	No	No	No
Taraxasteryl acetate	7.51	-8.73	Poorly soluble	-10.17	Insoluble	-7.57	Poorly soluble	Low	No	No	No	No	No	No	No
β-Amyrin	7.18	-8.25	Poorly soluble	-9.47	Poorly soluble	-7.16	Poorly soluble	Low	No	No	No	No	No	No	No
Lupeol	7.28	-8.64	Poorly soluble	-10.22	Insoluble	-6.74	Poorly soluble	Low	No	No	No	No	No	No	No
Stigmasterol	6.98	-7.46	Poorly soluble	-8.86	Poorly soluble	-5.47	Moderately soluble	Low	No	No	No	No	Yes	No	No
ψ-Taraxasterol	7.01	-8.09	Poorly soluble	-9.2	Poorly soluble	-6.71	Poorly soluble	Low	No	No	No	No	No	No	No
Patuletin	1.38	-3.61	Soluble	-4.72	Moderately soluble	-3.35	Soluble	Low	No	No	Yes	No	No	Yes	Yes
Luteolin	1.73	-3.71	Soluble	-4.51	Moderately soluble	-3.82	Soluble	High	No	No	Yes	No	No	Yes	Yes
Patulitrin	-0.43	-3.12	Soluble	-4.51	Moderately soluble	-1.61	Soluble	Low	No	No	No	No	No	No	No
Patuletin 7-O-[6"-(2-methylbutyryl)] glucoside	0.88	-4.22	Moderately soluble	-6.11	Poorly soluble	-3	Soluble	Low	No	Yes	No	No	No	No	No
Nepetin	1.74	-3.76	Soluble	-4.67	Moderately soluble	-3.94	Soluble	High	No	No	Yes	No	No	Yes	Yes
Nepitrin	0.27	-3.73	Soluble	-5.22	Moderately soluble	-2.2	Soluble	Low	No	Yes	No	No	No	No	No
Axillarin	1.73	-3.81	Soluble	-4.83	Moderately soluble	-4.05	Moderately soluble	High	No	No	Yes	No	Yes	Yes	Yes
Hispidulin-7-glucoside	0.37	-3.26	Soluble	-4.18	Moderately soluble	-2.79	Soluble	Low	No	Yes	No	No	No	No	Yes
Isorhamnetin 3-glucoside	0.12	-3.26	Soluble	-4.46	Moderately soluble	-2.2	Soluble	Low	No	Yes	No	No	No	No	No

Rhamnetin-3-O-β-D-glucopyranoside	0.05	-3.26	Soluble	-4.46	Moderately soluble	-2.2	Soluble	Low	No	Yes	No	No	No	No	No
Kaemferol-3-O-β-D-glucopyranoside	-0.09	-3.18	Soluble	-4.29	Moderately soluble	-2.1	Soluble	Low	No	No	No	No	No	No	No
Diosmetin	2.19	-4.06	Moderately soluble	-4.87	Moderately soluble	-4.52	Moderately soluble	High	No	No	Yes	No	Yes	Yes	Yes
Chrysoeriol	2.18	-4.06	Moderately soluble	-4.87	Moderately soluble	-4.52	Moderately soluble	High	No	No	Yes	No	Yes	Yes	Yes
Kaempferol	1.58	-3.31	Soluble	-3.86	Soluble	-3.82	Soluble	High	No	No	Yes	No	No	Yes	Yes
Quercetin	1.23	-3.16	Soluble	-3.91	Soluble	-3.24	Soluble	High	No	No	Yes	No	No	Yes	Yes
Spinacetin	1.8	-3.81	Soluble	-4.83	Moderately soluble	-4.05	Moderately soluble	High	No	No	Yes	No	Yes	Yes	Yes
Eupatin	2.12	-4.02	Moderately soluble	-4.94	Moderately soluble	-4.74	Moderately soluble	High	No	No	Yes	No	Yes	Yes	Yes
Compound name	log Kp (cm/s)	Lipinski #violations	Ghose #violations	Veber #violations	Egan #violations	Muegge #violations	Bioavailability Score	PAINS #alerts	Brenk #alerts	Leadlikeness #violations	Synthetic Accessibility	AMES mutagenicity	log Kp (cm/s) Lipinski #violations Ghose #violations		
1,6-O,O-Diacetylbritannilactone	-7.1	0	0	0	0	0	0.55	0	3	2	4.89	Carcinogen	Non-Mutagen		
O-acetylbritaanilactone	-7.25	0	0	0	0	0	0.55	0	3	0	4.64	Non-Carcinogen	Non-Mutagen		
Neobritannilactone A	-7.06	0	0	0	0	0	0.55	0	2	0	4.74	Carcinogen	Non-Mutagen		
Neobritannilactone	-7.03	0	0	0	0	0	0.55	0	2	1	4.66	Carcinogen	Non-Mutagen		
Acetyl neobritannilactone B	-6.34	0	0	0	0	0	0.55	0	3	0	4.84	Carcinogen	Non-Mutagen		
6β-O-(2-methylbutyryl)britannilactone	-6.51	0	0	0	0	0	0.55	0	3	2	5.16	Carcinogen	Non-Mutagen		
Britannilactone	-7.4	0	0	0	0	0	0.55	0	2	0	4.46	Carcinogen	Non-Mutagen		
Taraxasteryl acetate	-2.27	1	3	0	1	1	0.55	0	1	2	5.61	Carcinogen	Non-Mutagen		
β-Amyrin	-2.41	1	3	0	1	2	0.55	0	1	2	6.04	Non-Carcinogen	Non-Mutagen		
Lupeol	-1.9	1	3	0	1	2	0.55	0	1	2	5.49	Non-Carcinogen	Non-Mutagen		
Stigmasterol	-2.74	1	3	0	1	2	0.55	0	1	2	6.21	Carcinogen	Non-Mutagen		
ψ-Taraxasterol	-2.59	1	3	0	1	2	0.55	0	1	2	6.17	Non-Carcinogen	Non-Mutagen		
Patuletin	-6.81	0	0	1	1	0	0.55	1	1	0	3.35	Non-Carcinogen	Non-Mutagen		
Luteolin	-6.25	0	0	0	0	0	0.55	1	1	0	3.02	Non-Carcinogen	Mutagen		
Patulitrin	-9.08	2	2	1	1	3	0.17	1	1	1	5.47	Non-Carcinogen	Non-Mutagen		

Patuletin 7-O-[6"-(2-methylbutyryl)] glucoside	-8.59	3	3	1	1	3	0.17	1	1	2	6.09	Non-Carcinogen	Mutagen
Nepetin	-6.45	0	0	0	0	0	0.55	1	1	0	3.18	Non-Carcinogen	Mutagen
Nepitrin	-8.2	2	0	1	1	3	0.17	1	1	1	5.36	Non-Carcinogen	Non-Mutagen
Axillarin	-6.67	0	0	0	0	0	0.55	1	1	0	3.46	Non-Carcinogen	Non-Mutagen
Hispidulin-7-glucoside	-8.53	2	0	1	1	3	0.17	0	0	1	5.31	Non-Carcinogen	Non-Mutagen
Isorhamnetin 3-glucoside	-8.73	2	0	1	1	3	0.17	0	0	1	5.44	Non-Carcinogen	Non-Mutagen
Rhamnetin-3-O-β-D-glucopyranoside	-8.73	2	0	1	1	3	0.17	1	1	1	5.46	Non-Carcinogen	Non-Mutagen
Kaemferol-3-O-β-D-glucopyranoside	-8.52	2	0	1	1	3	0.17	0	0	1	5.29	Non-Carcinogen	Non-Mutagen
Diosmetin	-5.93	0	0	0	0	0	0.55	0	0	0	3.05	Non-Carcinogen	Non-Mutagen
Chrysoeriol	-5.93	0	0	0	0	0	0.55	0	0	0	3.06	Non-Carcinogen	Non-Mutagen
Kaempferol	-6.7	0	0	0	0	0	0.55	0	0	0	3.14	Carcinogen	Mutagen
Quercetin	-7.05	0	0	0	0	0	0.55	1	1	0	3.23	Non-Carcinogen	Mutagen
Spinacetin	-6.67	0	0	0	0	0	0.55	0	0	0	3.45	Non-Carcinogen	Non-Mutagen
Eupatin	-6.52	0	0	0	0	0	0.55	0	0	1	3.59	Non-Carcinogen	Non-Mutagen