

Oldenlandia umbellata as a promising agent for obesity management: Enzyme inhibition and antiadipogenic effects

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Supplementary data

Suppl. Table 1 — Predicted Pharmacokinetic Properties of *O. Umbellata* Compounds

Phytocompounds	Molecular weight	Rotatable bonds	H-bond acceptors	H-bond donors	TPSA	Log P	Bioavailability score
Ursolic acid	456.7	1	3	2	57.53	5.88	0.85
Nicotiflorin	594.52	6	15	9	249.2	-0.73	0.17
Anthraquinone	208.21	0	2	0	34.14	2.64	0.55
Purpurin	256.21	0	5	3	94.83	1.88	0.55
Ruberythric acid	534.47	5	13	7	212.67	-1.21	0.17
Alizarin	240.21	0	4	2	74.6	2.02	0.55
1,3-Dimethoxy-2-hydroxy-9,10-anthraquinone	284.26	2	5	1	72.83	2.09	0.55
Alizarin 1-methyl ether	254.24	1	4	1	63.6	2.11	0.55
Beta-Sitosterol	414.71	6	1	1	20.23	7.19	0.55
Cedrelopsin	260.29	3	4	1	59.67	2.98	0.55
Pheophorbide A methyl ester	606.71	8	8	2	121.94	4.14	0.55
Deacetylasperuloside	372.32	4	10	5	155.14	-1.78	0.11
scandoside methyl ester	404.37	6	11	6	175.37	-2.05	0.11
Asperulosidic acid	432.38	7	12	6	192.44	-1.99	0.11
Scan-doside	390.34	5	11	7	186.37	-2.34	0.11
Nicotinic acid	123.11	1	3	1	50.19	0.32	0.85
Hexadecanamide	255.44	14	1	1	43.09	4.83	0.55
3-Methylisoxazolo[4,5-b]pyridine	134.14	0	3	0	38.92	1.37	0.55
3-Cyclohexen-1-ol,4-methyl-1-(1-methylethyl)-	154.25	1	1	1	20.23	2.6	0.55
Flavone	222.24	1	2	0	30.21	3.18	0.55
Cyclopentanetridecanoic acid, methyl ester	296.49	14	2	0	26.3	5.93	0.55
Octadec-9-enoic acid	282.46	15	2	1	37.3	5.71	0.85
Butanoic acid, 3-methyl-,hexadecyl ester	326.56	18	2	0	26.3	6.84	0.55
Pyrimidine, 5-ethyl-2-[4-(4-ethylcyclohexyl)phenyl]-	294.43	4	2	0	25.78	4.99	0.55
Coumarine, 3-[2-(1-methyl-2-imidazolylthio)-1-oxoethyl]-	300.33	4	4	0	90.4	2.14	0.55
Z-13-octadecen-1-yl acetate	310.51	17	2	0	26.3	6.33	0.55
Glucose	180.16	1	6	5	110.38	-2.26	0.55
1,5-Naphthalenediol, decahydro-	170.25	0	2	2	40.46	1.46	0.55

Suppl. Table 2 — Toxicity profiling of <i>O. Umbellata</i> compounds					
Phytocompounds	OSIRIS		ProTox-3.0		
	Drug score	Predicted adverse effects	Drug likeness	Predicted LD ₅₀ (mg/kg)	Predicted toxicity class
IMPPAT Compounds					
Ursolic acid	0.17	Nil	-3.66	2000	IV
Nicotiflorin	0.58	Nil	2.81	5000	V
Anthraquinone	0.08	Mutagenic, Tumorigenic, and Irritant properties	-3.88	5000	V
Purpurin	0.09	Mutagenic, Tumorigenic, and Irritant properties	-3.88	500	V
Ruberythric acid	0.15	Mutagenic and Irritant properties	-6.58	300	V
Alizarin	0.15	Mutagenic and Irritant properties	-3.59	700	V
1,3-Dimethoxy-2-hydroxy-9,10-anthraquinone	0.23	Irritant properties	-3.58	700	V
Alizarin 1-methyl ether	0.19	Mutagenic and Irritant properties	-3.08	700	V
Beta-Sitosterol	0.13	Nil	-4.48	89	IV
Literature Compounds					
Cedrelopsin	0.27	Irritant properties	-3.21	150	IV
Pheophorbide A methyl ester	0.15	Nil	-8.64	4	II
Deacetylasperuloside	0.47	Nil	-3.27	200	IV
Scandoside methyl ester	0.44	Nil	-5.28	200	IV
Asperulosidic acid	0.27	Irritant properties	-2.34	200	IV
Scan-doside	0.46	Nil	-3.17	200	IV
Nicotinic acid	0.78	Nil	0.37	372	V
GC-MS Compounds					
Hexadecanamide	0.27	Nil	-23.8	100	IV
3-Methylisoxazolo[4,5-b]pyridine	0.79	Nil	0.56	140	IV
3-Cyclohexen-1-ol,4-methyl-1-(1-methylethyl)-	0.28	Irritant properties	-7.41	1016	IV
Flavone	0.45	Mutagenic properties	1.85	250	V
Cyclopentanetridecanoic acid, methyl ester	0.21	Nil	-21.32	500	V
Octadec-9-enoic acid	0.22	Nil	-28.92	48	V
Butanoic acid, 3-methyl-, hexadecyl ester	0.10	Irritant properties	-23.75	500	V
Pyrimidine, 5-ethyl-2-[4-(4-ethylcyclohexyl)phenyl]-	0.35	Nil	-0.07	56	IV
Coumarine, 3-[2-(1-methyl-2-imidazolylthio)-1-oxoethyl]-	0.66	Reproductive effects	1.41	500	V
Z-13-octadecen-1-yl acetate	0.15	Irritant properties	-18.8	346	V
Glucose	0.50	Nil	-3.78	2300	VI
1,5-Naphthalenediol, decahydro-	0.50	Nil	-2.94	500	V