

Mol ID	MoleculeName	CAS ID	OB (%)	DL
M001	Chrysarobin	491-59-8	30.24	0.18
M002	Chrysophanic acid	481-74-3	18.64	0.21
M003	2-hydroxyemodin-1-methyl ether	346434-45-5	20.40	0.30
M004	Chrysoobtusin	70588-06-6	72.84	0.44
M005	Chryso-obtusin glucoside	96820-54-1	32.48	0.87
M006	Chrysophanol-1- β -gentiobioside	54944-38-6	30.40	0.70
M007	Luteolin	491-70-3	36.16	0.25
M008	Cassiaside B2	218155-40-9	3.01	0.11
M009	Cassiaside B2_qt	218155-40-9	39.40	0.24
M010	Cassiaside C	119170-52-4	6.36	0.74
M011	Cassiaside C_qt	119170-52-4	35.29	0.19
M012	Alaternin	641-90-7	6.17	0.33
M013	1-hydroxy-8-methoxy-3-methylanthracene-9,10-dione	3300-25-2	33.73	0.23
M014	1-O-Methylemodin	3775-08-4	20.67	0.27
M015	Linolenic acid	463-40-1	45.01	0.15
M016	Oleic acid	112-80-1	33.13	0.14
M017	Stearic acid	57-11-4	17.83	0.14
M018	Arachidic acid	506-30-9	16.66	0.19
M019	Docosanoic acid	112-85-6	15.69	0.26
M020	Lignoceric acid	557-59-5	14.90	0.33
M021	Methyl stearate	112-61-8	16.80	0.16
M022	Ethyl oleate	111-62-6	32.40	0.19
M023	Methyl heneicosanoate	6064-90-0	15.36	0.26
M024	Methyl docosanoate	929-77-1	14.96	0.29
M025	Daidzin	552-66-9	14.32	0.73
M026	7-methoxy-obtusifolin	—	20.61	0.33
M027	Cassitoroside	170384-73-3	45.33	0.83
M028	Physcion 8-gentiobioside	84268-38-2	41.65	0.63
M029	Glucoaurantio-obtusin	129025-96-3	18.17	0.86
M030	Cassitoroside qt	170384-73-3	38.44	0.15
M031	1-desmethyaurantio-obtusin	—	18.64	0.34
M032	1-desmethylobtusin	90985-57-2	83.10	0.37
M033	1-desmethylchryso-obtusin	90985-58-3	18.82	0.40
M034	Chrysophanol-10,10'-bianthrone	17062-54-3	20.68	0.72
M035	Alizarin	72-48-0	18.10	0.19
M036	1,3-dihydroxy-6-methoxy-7-methyl anthraquinone	—	69.14	0.27
M037	1-hydroxy-3,7-diformyl anthraquinone	—	6.91	0.28
M038	8-hydroxy-1,2-dimethoxy-3-methylanthracene-9,10-dione	82868-99-3	37.45	0.29
M039	1,3-dihydroxy-2,7,8-trimethoxy-6-methylanthracene-9,10-dione	—	18.84	0.40
M040	Emodin-1-O- β -gentiobioside	849789-95-3	30.40	0.70
M041	Alaternin-1-O- β -D-glucopyranoside	—	10.55	0.78
M042	Alaternin-2-O- β -D-glucopyranoside	—	10.14	0.79
M043	Obtusifolin-2-O- β -D-(6'-O-acetyl) glucopyranoside	—	40.37	0.87
M044	2-methoxyl-chrysophanol-8-O- β -D-glucopyranoside	—	28.95	0.84
M045	2-methoxyl-chrysophanol-8-O- β -D-glucopyranoside qt	—	19.95	0.27

Mol ID	MoleculeName	CAS ID	OB (%)	DL
M046	1-demethylaurantio-obtusin-2-O-β-D-glucopyranoside	—	3.60	0.86
M047	1,7,8-trimethoxyl-2-hydroxyl-3-methylanthraquinone-2-O-β-D-glucopyranoside	—	27.15	0.87
M048	1,7-dimethoxyl-2,8-dihydroxyl-3-methylanthraquinone-2-O-β-D-glucopyranoside	—	53.03	0.86
M049	1,7-dimethoxyl-2,8-dihydroxyl-3-methylanthraquinone-2-O-β-D-glucopyranoside qt	—	18.85	0.33
M050	1,2,7-trimethoxyl-6,8-dihydroxy-3-methylanthraquinone-6-O-β-D-glucopyranoside	—	19.60	0.87
M051	2,8-dimethoxyl-1,6-dihydroxy-3-methylanthraquinone-6-O-β-D-glucopyranoside	—	43.52	0.87
M052	2,8-dimethoxyl-1,6-dihydroxy-3-methylanthraquinone-6-O-β-D-glucopyranoside qt	—	18.63	0.33
M053	4,6,7-trimethoxyl-aloe-emodin-8-O-β-D-glucopyranoside	—	27.00	0.86
M054	Nor-rubrofusarin gentiobioside	—	9.99	0.70
M055	Cassiaside B	119170-51-3	31.98	0.77
M056	Cassiaside B qt	119170-51-3	38.45	0.24
M057	Isorubrofusarin 10-gentiobioside	200127-93-1	40.12	0.67
M058	Isorubrofusarin 10-gentiobioside qt	200127-93-1	18.47	0.24
M059	Cassialactone gentiobioside	—	14.93	0.64
M060	Torosachryson	93798-36-8	65.56	0.27
M061	Cassialactone	80489-64-1	75.42	0.30
M062	Cassiaside C2	—	3.01	0.11
M063	Cassiaside C2 qt	—	20.40	0.24
M064	Nor-rubrofusarin-6-O-β-D(6'-O-acetyl)glucopyranoside	—	7.87	0.87
M065	Mandelic acid	90-64-2	42.78	0.03
M066	Chrysin-7-O-β-D-glucoside	—	8.93	0.69
M067	Galangin	548-83-4	45.49	0.21
M068	Palmitic acid	57-10-3	19.30	0.10
M069	Linoleic acid	60-33-3	41.90	0.14
M070	Benzoic acid	65-85-0	31.55	0.02
M071	Stigmasterol	83-48-7	43.83	0.76
M072	Aloe emodin	481-72-1	83.38	0.24
M073	Emodin	518-82-1	24.40	0.24
M074	Physcion	521-61-9	22.29	0.27
M075	Raffinose	512-69-6	11.79	0.66
M076	Paeonol	552-41-0	28.79	0.04
M077	Methyl palmitate	112-39-0	18.09	0.12
M078	Cholesterol	57-88-5	37.87	0.68
M079	m-Cresol	108-39-4	53.95	0.01
M080	(+)-Dihydroactinidiolide	81800-41-1	36.84	0.07
M081	Chrysophanic acid	481-74-3	18.64	0.21
M082	Torachryson	22649-04-3	51.06	0.13
M083	Methyl oleate	112-62-9	31.90	0.16
M084	Glucosmodin	34298-85-6	16.09	0.80
M085	Rhein	478-43-3	47.07	0.28
M086	Toralactone	41743-74-2	46.46	0.24
M087	Physcion 8-glucoside	26296-54-8	18.31	0.82

Mol ID	MoleculeName	CAS ID	OB (%)	DL
M088	Chrysin	480-40-0	22.61	0.18
M089	Aspidinol	519-40-4	4.88	0.08
M090	Emodin anthrone	491-60-1	24.72	0.21
M091	Campesterol	474-62-4	37.58	0.71
M092	Malvalic acid	503-05-9	30.99	0.15
M093	5,7-Dihydroxychromone	31721-94-5	26.04	0.07
M094	1,2,4-Trihydroxyanthraquinone	81-54-9	18.41	0.21
M095	Naphthoresorcinol	132-86-5	55.32	0.05
M096	1,5-Dihydroxy-3-methylanthraquinone	21891-63-4	18.92	0.21
M097	1,6,7-Trihydroxy-3-methoxy-anthraquinone	—	24.50	0.27
M098	1-Hydroxy-7-methoxy-3-methyl-anthraquinone	—	18.44	0.24
M099	1-[(beta-D-glucopyranosyl-(1-3)-O-beta-D-glucopyranosyl-(1-6)-O-beta-D-glucopyranosyl)oxy]-8-hydroxy-3-methyl-9,10-anthraquinone	—	7.25	0.29
M100	1-[(beta-D-glucopyranosyl-(1-6)-O-beta-D-glucopyranosyl-(1-3)-O-beta-D-glucopyranosyl (1-6)-O-beta-D-glucopyranosyl)oxy]-8-hydroxy-3-methyl-9,10-anthraquinone	—	3.01	0.11
M101	1-hydroxy-2-hydroxymethyl-3-methoxyanthraquinone	—	8.01	0.30
M102	2,5-dihydroxy-1-methoxyanthracene-9,10-dione	34425-63-3	21.12	0.24
M103	Obtusifolin	477-85-0	25.49	0.27
M104	2-benzyl-4,6-dihydroxy benzoic acid-6-O-β-D-glucopyranoside	—	14.55	0.49
M105	2-benzyl-4,6-dihydroxy benzoic acid-6-O-β-D-glucopyranoside qt	—	33.68	0.12
M106	6-hydroxymusizin,8-o-beta-d-glucoside	—	10.81	0.50
M107	9-[(beta-D-glucopyranosyl-(1-6)-O-D-glucopyranosyl)oxy]-10-hydroxy-7-methoxy-3-methyl-1H-naphthol[2,3-c]pyran-1-one	—	8.33	0.67
M108	Rubrofusarin gentiobioside	24577-90-0	40.12	0.67
M109	Rubrofusarin	3567-00-8	45.55	0.24
M110	Anthraglycoside A	23451-01-6	28.92	0.83
M111	Anthraquinone	84-65-1	56.10	0.14
M112	Aurantio-obtusin,6-o-beta-d-glucoside	129025-96-3	22.83	0.87
M113	Aurantio-obtusin,6-o-beta-d-glucoside qt	129025-96-3	24.17	0.37
M114	Aurantio-obtusin	67979-25-3	31.55	0.37
M115	Cassiaside A	123914-49-8	17.78	0.74
M116	Cassiaside A qt	123914-49-8	27.23	0.19
M117	Obtusin	70588-05-5	81.43	0.40
M118	Chrysophanol, triglucoside	120181-07-9	3.16	0.31
M119	Chrysophanol-8-beta-d-glucoside	13241-28-6	16.55	0.72
M120	Dantron	117-10-2	28.74	0.19
M121	Emodin-8-glucoside	23313-21-5	8.50	0.75
M122	Galactomannan	11078-30-1	10.92	0.70
M123	Isotoralactone	80503-54-4	63.25	0.24
M124	Norrubrofusarin	3566-98-1	22.08	0.21
M125	Nor-toralactone	—	21.92	0.21
M126	Obtusifolin 2-glucoside	120163-18-0	42.41	0.81
M127	Ononitol monohydrate	—	14.08	0.06

Mol ID	MoleculeName	CAS ID	OB (%)	DL
M128	Questin	3774-64-9	20.44	0.27
M129	Quinizarin	81-64-1	47.34	0.19
M130	Rubrofusarin triglucoside	245724-07-6	3.03	0.29
M131	Sterculic acid	738-87-4	29.77	0.18
M132	Torachryson,8-o-[beta-d-glucopyranosyl(1-3)-o-beta-d-glucopyranosyl(1-6)-o-beta-d-glucopyranoside]	—	7.52	0.42
M133	Torachryson,8-o-beta-d-gentiobioside	—	21.56	0.84
M134	Torachryson,tetraglucoside	—	3.01	0.18
M135	Toralactone,9-o-[beta-d-glucopyranosyl(1-3)-o-beta-d-glucopyranosyl(1-6)-o-beta-dglucopyranoside]	—	4.35	0.28
M136	Toralactone,9-o-beta-d-gentiobioside	—	27.78	0.71
M137	(2S,4S)-4-hydroxy-L-arginine	—	18.86	0.04