

Supplementary Table 1: Physio-chemical properties of anti-inflammatory chromenols and chromanols.^a Thresholds proposed by “Lipinski's Rule of Five” are given in brackets.

Compound	Molecular weight [<500 Da]	Octanol-water partition coefficient [<5 log <i>P</i>]	Number of atoms [20-70]	Number of hydrogen bond acceptors (O and N atoms) [<10]	Number of hydrogen bond donors (N-H and O-H bonds) [<5]	Polar surface area [≤140 Å ²]	Number of rotatable bonds [<10]	Number of violations	Lipinski's Rule ^b
δ-Sargachromenol (51)	424.58	7.44	31	4	2	66.76	10	1	Y
Epitaondiol (79)	412.61	6.36	30	3	2	49.69	0	1	Y
δ-Garcionic acid (30)	426.6	7.59	31	4	2	66.76	10	1	Y
13'-α-COOH (205)	460.7	8.37	33	4	2	66.76	13	2	Y
13'-α-OH (204)	446.7	8.45	32	3	2	49.69	13	2	Y
13'-δ-OH (231)	418.66	7.56	30	3	2	49.69	13	2	Y
13'-δ-COOH (229)	432.64	7.43	31	4	2	66.76	13	2	Y

Sargachromanol D/E (57/58)	428.6	6.89	31	4	3	69.92	9	1	Y
Sargachromanol G (60)	426.6	6.7	31	4	2	66.76	9	1	Y
α -CMBHC (207)	320.4	4.86	23	4	2	66.76	5	0	Y

^a Values were calculated by Molinspiration WebME editor version 1.16 (<http://www.molinspiration.com>).

^b Y = passed the rule (max. 1 violation)

