Table S-I. Molecular properties predictors calculated by the MolSoft platform [52, 91].

Comp.	TPSA (Å²)[a]	Volume (Å³)[b]	LogP	LogS (in mg/L)	Number of HBA	Number of HBD	%ABS =109-(0.345 x TPSA)[c]	Drug-Likeness Model Score (DLS)	BBB Score
1a	24.31	403.94	5.80 (> 5)	0.07	2	1	100.61	-1.36	4.64
1b	26.89	302.71	2.68	238.66	4	1	99.72	-0.72	5.54
1c	44.60	382.88	3.87	17.56	2	3	93.1	-1.64	4.11
1d	44.42	379.48	3.48	61.76	2	3	93.8	-1.42	4.07
1e	39.31	559.95	7.80 (> 5)	0.42	4	1	95.44	-1.22	3.93
1f	68.44	271.94	0.06	6010.37	4	3	85.39	-0.69	3.53
1g	24.86	306.30	3.48	53.22	2	1	100.42	-1.28	5.57
1h	26.89	336.64	3.94	19.86	4	1	99.72	-1.05	5.53
1i	26.89	350.95	4.07	23.47	4	1	99.72	-0.74	5.55
1j	24.86	318.13	3.61	36.11	2	1	100.42	-1.34	5.57
2a	28.62	151.60	2.22	522.96	2	1	99.13	-1.17	4.26
2b	28.35	200.43	3.19	68.87	2	1	99.22	-1.34	4.86
2c	61.72	174.88	1.27	3541.88	4	3	87.7	-0.35	2.80
3a	28.29	550.36	7.93 (> 5)	0.13	2	0	99.24	-0.75	3.43
3b	28.56	501.54	6.57 (> 5)	0.12	2	0	99.15	-0.75	3.81
3c	28.01	599.18	8.89 (> 5)	0.10	2	0	99.34	-0.79	3.27
3d	28.83	464.54	5.74 (> 5)	0.60	2	0	99.05	-0.56	4.40
3e	30.59	497.95	5.77 (> 5)	0.23	4	0	98.45	-0.55	3.87
3f	28.56	513.37	6.70 (> 5)	0.12	2	0	99.15	-0.35	3.72
3g	28.83	452.72	5.61 (> 5)	0.62	2	0	99.05	-0.76	4.49
3h	61.38	573.63	6.97 (> 5)	0.18	4	2	87.82	0.08	2.45
1k	12.86	394.39	6.86 (> 5)	0.03	1	0	104.56	-0.90	3.98
1l	21.94	299.34	3.91	14.25	2	0	101.43	-1.31	5.17
1m	21.40	396.98	6.23 (> 5)	0.05	2	0	101.62	-1.39	4.10
1n	12.49	413.39	7.22 (> 5)	0.04	2	0	104.69	-1.36	4.22

1o	11.71	313.93	4.18	11.10	2	1	104.96	-1.38	5.74
1p	11.17	411.57	6.50 (>5)	0.03	2	1	105.15	-1.47	4.81
1q	39.78	372.71	5.24 (> 5)	0.22	4	1	95.8	-1.23	4.12
Curcumin (Keto)	73.83	393.60	2.83	428.21	6	2	83.53	-0.82	2.83
Curcumin (Enol)	77.11	401.76	3.29	380.63	6	3	82.4	-0.61	2.78

[a]Topological polar surface area, [b]Molecular volume, [c]Percentage absorption

Number of HBA: Number of hydrogen bond acceptors (n-ON)

Number of HBD: Number of hydrogen bond donors (n-OHNH)

Data were calculated by the **MolSoftplatform** (http://molsoft.com/mprop/). The percentage of absorption (%ABS) was calculated by using %ABS =109-(0,345 x TPSA) and is referred to the degree of absorption.

All molecular property predictors are calculated using fragment-based contributions.
LogP (octanol/water partition coefficient)
LogS (water solubility)
Molecular Polar Surface Area (PSA) and Volume
PSA is defined as sum of surfaces of oxygens, nitrogens and attached hydrogens.