

Table S1. Chemical and physical properties of Cucurbitacin B, E and I.

	Cucurbitacin B	Cucurbitacin E	Cucurbitacin I
Molecular Weight	558.7	556.7	514.6
Molecular Formula	C ₃₂ H ₄₆ O ₈	C ₃₂ H ₄₄ O ₈	C ₃₀ H ₄₂ O ₇
XLogP3-AA	2.6	3.2	2.7
Hydrogen Bond Donor Count	3	3	4
Hydrogen Bond Acceptor Count	8	8	7
Rotatable Bond Count	6	6	4
Exact Mass	558.31926842	556.30361836	514.29305367
Monoisotopic Mass	558.31926842	556.30361836	514.29305367
Topological Polar Surface Area	138	138	132
Heavy Atom Count	40	40	37
Formal Charge	0	0	0
Complexity	1210	1270	1160
Isotope Atom Count	0	0	0
Defined Atom Stereocenter Count	9	8	8
Undefined Atom Stereocenter Count	0	0	0
Defined Bond Stereocenter Count	1	1	1
Undefined Bond Stereocenter Count	0	0	0
Covalently-Bonded Unit Count	1	1	1
Compound Is Canonicalized	Yes	Yes	Yes