

Table S6 The ADMET profiling enlisting absorption, metabolism, and toxicity-related parameters of best selected molecules.

Molecule	Formula	MW	Log s	Abs	BBB	Pgp-s	CYP1A2	CYP2C19	CYP2C9	CYP2D6	CYP3A4	Bio	AOT	CL	T1/2	hERG blocker	Oral acute toxicity	Bioconcentration factors
Luteolin	C15H10O6	286.2	-3.71	High	No	No	Yes	No	No	Yes	Yes	0.55	-	8.146	0.898	NO	NO	1.016
CBNA	C22H26O4	354.4	-5.95	High	No	No	Yes	Yes	Yes	No	No	0.85	-	1.072	0.164	NO	NO	0.426
Stigamasterol	C29H48O	412.6	-7.46	Low	No	No	No	No	Yes	No	No	0.55	-	4.515	0.036	NO	NO	3.047