

Table 2. ADME screening of active phytoconstituents.

PHYTOCHEMICAL NAME	PUBCHEM ID	SMILES	BIOAVAILABILITY	BOILED EGG	LEPINSKI	GIT AB
Palmatic acid	10889	<chem>CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCCC</chem>	0.55	no	Yes; 1 violation: MLOGP>4.15	Low
Ricinine	10666	<chem>CN1C=CC(=C(C1=O)C#N)OC</chem>	0.55	no	Yes; 0 violation	High
Stearic acid	5281	<chem>CCCCCCCCCCCCCCCCC(=O)O</chem>	0.85	no	Yes; 1 violation: MLOGP>4.15	high
Ricinoleic acid	643684	<chem>CCCCC[C@H](C/C=C\CCCCCCC(=O)O)O</chem>	0.85	yes	Yes; 0 violation	high
Corilagin	73568	<chem>C1[C@@H]2[C@H]([C@@H]([C@H]([C@@H](O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)OC(=O)C4=CC(=C(C(=C4C5=C(C(=C(C5C(=O)O1)O)O)O)O)O)O)O</chem>	0.17	no	No; 3 violations: MW>500, NorO>10, NHorOH>5	no
Dihydroxyoctadecanoic acid	20391236	<chem>CCCCCCCCCCCCCCCC(C(=O)O)(O)O</chem>	0.56	no	Yes; 0 violation	high
Oleic acid	445639	<chem>CCCCCCC/C=C\CCCCCCC(=O)O</chem>	0.85	no	Yes; 1 violation: MLOGP>4.15	high
Lupeol	259846	<chem>CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]3CC[C@@H]4[C@]5(CC[C@@H](C([C@@H]5CC[C@]4([C@@]3(CC2)C)C)(C)O)C)C</chem>	0.55	no	Yes; 1 violation: MLOGP>4.15	low
Linoleic acid	5280450	<chem>CCCC/C=C\C/C=C\CCCCCCC(=O)O</chem>	Data not available		Data not available	