Table S4 - Prediction Tools and Parameter Classification Used for ADMET and Drug-Likeness Profiling of Monoterpenoids

ADMET Category	Parameter	References	Prediction Tools
Physicochemical	Molecular Weight	100–600 Da	SwissADME, ADMETlab 2.0, Molinspiration
	Molecular Volume	MW/Vol	SwissADME, ADMETlab 2.0
	Density	–	SwissADME
	Rotatable Bonds (Flexibility)	Rot/RTB	Molinspiration, SwissADME
	H-Bond Acceptors (nHA)	0–12	SwissADME, Molinspiration, ADMETlab 2.0
	H-Bond Donors (nHD)	0–7	SwissADME, Molinspiration
	Topological Polar Surface Area (TPSA)	0–140 Å²	SwissADME, Molinspiration, ADMETlab 2.0
	LogP (octanol/water partition)	0–3	SwissADME, Molinspiration, ADMETlab 2.0
	LogD (at pH 7.4)	0–3	ADMETlab 2.0
Absorption	Human Intestinal Absorption (%)	>90%	pKCSM, ADMETlab 2.0, VNN-ADMET
	Caco-2 Permeability	>30.90	pKCSM, ADMETlab 2.0, SwissADME
	Water Solubility (log S)	–	SwissADME, ADMETlab 2.0, AI Drug Lab
	Skin Permeability (log Kp)	-2.5 to -4.0	ADMETlab 2.0, SwissADME
	P-glycoprotein Substrate/Inhibitor	No	pKCSM, ADMETlab 2.0, SwissADME
Distribution	Plasma Protein Binding (%)	<90%	ADMETlab 2.0, pKCSM, ProTox-III
	Volume of Distribution (VDss) (log VDss)	low < –0.15	pKCSM, ADMETlab 2.0, SwissADME
	Blood-Brain Barrier (log BB)	< –1	pKCSM, ADMETlab 2.0, SwissADME
	CNS Permeability (log PS)	< 3	pKCSM, ADMETlab 2.0, VNN-ADMET
Metabolism	CYP1A2, 2C19, 2C9, 2D6, 3A4 Inhibition/Substrate	No	ADMETlab 2.0, SwissADME, AI Drug Lab, XenoSite
Excretion	Total Clearance (mL/min/kg)	high > 1.17 / low < 0.66	pKCSM, ADMETlab 2.0
	OCT & OAT Transporter Substrate/Inhibitor	No	ADMETlab 2.0, AI Drug Lab
Toxicity	Ames Mutagenicity	0–0.3 (excellent)	ProTox-III, ToxinPRED, ADMETlab 2.0, pKCSM
	Hepatotoxicity	0–0.3 (excellent)	ProTox-III, ADMETlab 2.0, VNN-ADMET
	Skin Sensitization	No	ToxinPRED, VNN-ADMET
	Carcinogenicity	No	ProTox-III, ToxinPRED, ADMETlab 2.0
	hERG I & II Inhibition	No / 0.1	PRED-hERGG, ADMETlab 2.0, ProTox-III
	LD50 (oral toxicity, log mg/kg)	> 0.5 / < 0.4	ProTox-III, ADMETlab 2.0, ToxinPRED
	ORC (oral rat chronic)	Acceptable	ProTox-III, VNN-ADMET
Medicinal Chemistry	Quantitative Estimate of Drug-likeness (QED)	> 0.5 good / < 0.3 poor	SwissADME, ADMETopt, Molinspiration
	Synthetic Accessibility	> 0.42 (good) / < 0.42 (poor)	SwissADME, AI Drug Lab, ADMETopt
	Fraction of sp^3 Carbon (Fsp^3)	< or > 0.42	Molinspiration, SwissADME, ADMETlab 2.0
	Natural Product-likeness	>5 = good	SwissADME
	Lipinski's Rule Violations	0 (Accepted)	SwissADME, ADMETlab 2.0
	PAINS, Brenk, Chelator Alerts	0 (Accepted)	SwissADME, ADMETlab 2.0
	Pfizer, GSK, Golden Triangle Filters	Accepted	SwissADME, ADMETopt