

Hepatoprotective effect of date palm fruit extract against doxorubicin intoxication in Wistar rats: *In vivo* and *in silico* studies

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Supplementary Table 3: PreADMET profiling of the top *in silico* bioactive compounds and the control.

	L-(+)-Threose, tris(trimethylsilyl) ether, trimethylsilyloxime	L-(+)-Tartaric acid (4TMS derivative)	Palmitic acid (TMS derivative)	Stearic acid
ID	Value	Value	Value	Value
Buffer_Solubility (mg/L)	2.18297e+012**	2.26496e+014**	4174.07**	36.4798
CaCO ₂	43.164	31.4203	54.0241	29.76664
CYP 2C19 inhibition	Inhibitor	Inhibitor	Inhibitor	Inhibitor
CYP 2C9 inhibition	Inhibitor	Inhibitor	Inhibitor	Inhibitor
CYP_2D6_inhibition	Nil	Nil	Nil	Nil
CYP_2D6_substrate	Nil	Nil	Nil	Nil
CYP 3A4 Inhibition	Inhibitor	Inhibitor	Inhibitor	Inhibitor
CYP 3A4 substrate	Substrate	Substrate	Substrate	Weak
HIA	98.2737	98.08026	100	98.44944
MDCK	68.0166*	68.0163*	60.2384*	71.1033*
Pgp_inhibition	Inhibitor	Inhibitor	Inhibitor	Inhibitor
Plasma_Protein_binding	100	100	99.16693	100
Pure_water_solubility_(mg)	0.081309	0.224771	0.033728	0.31

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Skin_ permeability	-1.68655*	-2.28015*	-0.563483*	-0.574 65
SKlogD_value	4.68831	5.24154	8.04197	6.1771 3
SKlogP_value	4.68831	5.24154	8.04197	6.1771 3
SKlogS_buffer	6.711840**	8.712780**	1.896120**	-3.890 46
SKlogS_pure	-6.71707	-6.29054	-6.98869	-5.953 19