

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

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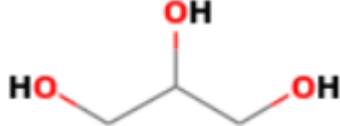
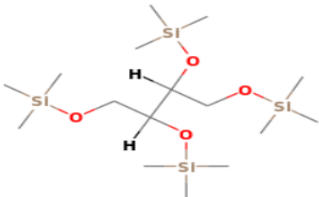
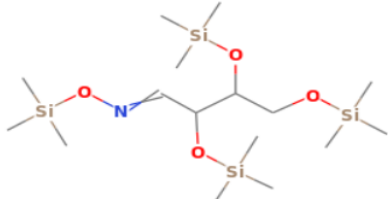
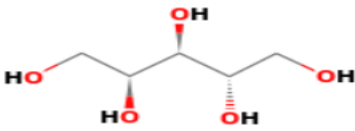
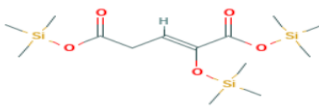
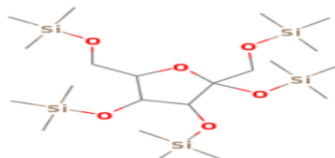
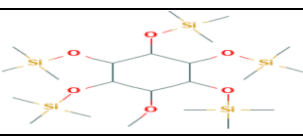
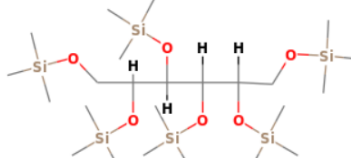
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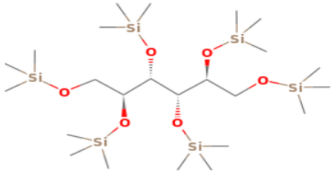
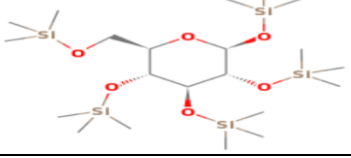
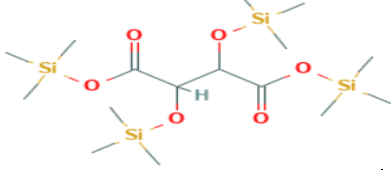

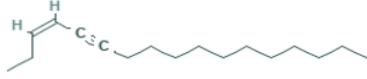


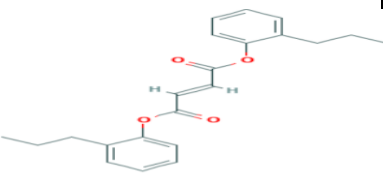
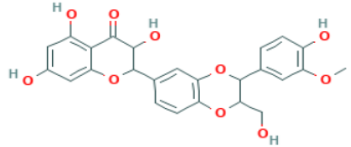
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Supplementary Table 2. 2D structures of identified compounds in DPF, and their binding energies with proteins.

S/No	Name	ID	2D structure	1ilg	1n3u	4nz2
1	Glycerol	PC-CID: 753		-4.2	-4	-4.5
2	L-Threitol, 4TMS derivative	CAS-RN: 32381-52-5		-8.7	-5.6	-6.2
3	L-(+)-Threose [tris(trimethylsilyl) ether], trimethylsilyloxime	PC-CID: 9169 6654		-9.3	-7.8	-9.1
4	D-(+)-Arabitol	PC-CID: 94154		-5.3	-4.4	-5.1
5	2-Pentenedioic acid 2-[(trimethylsilyloxy)-, bis(trimethylsilyloxy) ester	PC-CID: 5366622		-9.1		
6	D-(-)-Tagatofuranose [pentakis(trimethylsilyl) ether] (isomer 1)	PC-CID: 523972		-3	-6.2	
7	D-Pinitol [pentakis(trimethylsilyl) ether]	CID: 1453497 3		-7.6	-5.3	-5.3
8	D-Sorbitol (6TMS derivative)	CAS-RN:		-4.3	-6.5	-5.5

9	D-Mannitol (6TMS derivative)	CAS-RN:1431 7-07-8			-6.7	-6.1
10	Beta-D-Glucopyranose (5TMS derivative)	CAS-RN:2775 -90-8		-8.6	-5.8	
11	L-(+)-Tartaric acid (4TMS derivative)	PC CID: 519591		-9.2	-7.7	-7
12	Palmitic acid (TMS derivative)	CAS-RN: 55520-89-3		-9.1	-7.3	-8.2
13	3-Heptadecen-5-yne, (Z)-	PC-CID: 5367448		-7.7	-6.7	-6.8
14	Stearic acid	PC-CID: 5281		-8	-7	-8.4
15	9-Octadecenoic acid [(E)-TMS derivative]	CAS-RN: 96851-47-7		-9.7	-6.7	-8.4
16	Fumaric acid [di (2-propylphenyl) ester]	PC-CID: 91735211		-8.1	-6.6	-7.8
17	Silymarin (Standard)	PC-CID: 5213		-8.3	-6.5	-8.9