Pharmacognostic assessment of pods of *Acacia nilotica* (L.) Willd. ex Delile *with in vitro* anti-microbial and *in-vivo* hepatoprotective potential of its n-hexane and methanol extracts

Supplementary Docking Data

Table S1: Molecular docking data of ligands (constituents) isolated from *A. nilotica* methanolic extract, showing antibacterial activity with the target protein (PDB ID: 3WD1)

Ligand	docking score (kcal/mol)	glide gscore (kcal/mol)	glide emodel (kcal/mol)
co-crystallized ligand (Antibacterial-3WD1)	-10.030	-12.233	-156.222
ciprofloxacin 2764	-6.299	-6.399	-56.826
Ergost-5-en-3-ol 18660356	-6.223	-6.223	-46.164
Pyrogallol 1057	-5.955	-5.960	-35.451
4-O methylmannose 345716	-5.525	-5.525	-44.395
Ergosta-5,22-dien-3-ol, (3-beta.22E)- 5281327	-5.496	-5.496	-42.928
Phthalic acid, bis(2-ethylhexyl) ester 8343	-5.478	-5.478	-54.307
4-methylbenzenethiol 7811	-5.043	-5.225	-20.796
N,N-Dimethylglycine 673	-4.973	-4.973	-32.677
Oxiranyl methyl ester 9-octadecenoic acid 5354568	-4.670	-4.670	-47.787
Glycedyl palmitate (Methyl ricinoleate) 5354133	-3.955	-3.955	-54.034
15-Hydroxypentadecanoic Acid 78360	-1.583	-1.586	-33.770
Methyl 9-cis,11-trans-octadecadienoate 11748436	-0.830	-0.830	-37.037
Methyl oleate 5364509	-0.829	-0.829	-35.966
Methyl linoleate 5284421	-0.761	-0.761	-40.585
14,17-Octadecadienoic acid, methyl ester 5365751	-0.752	-0.752	-38.355
9-Octadecenamide 1930	-0.601	-0.601	-36.789
hexadecanoic acid, methyl ester 8181	-0.068	-0.068	-33.277
9,12-Octadecadienoic acid (Z,Z)- 5280450	-0.039	-0.043	-27.857
1,8,11-Heptadecatriene, (Z,Z)- 5352709	0.119	0.119	-27.641

Methyl stearate 8201	0.273	0.273	-33.279

Table S2: Molecular docking data of ligands (constituents) isolated from *A. nilotica* methanolic extract, showing hepatoprotective activity with the target protein (PDB ID: 5HYK)

Ligand	docking score (kcal/mol)	glide gscore (kcal/mol)	glide emodel (kcal/mol)
co-crystallized ligand (Hepatoprotective-5HYK)	-9.023	-9.023	-59.095
Oxiranyl methyl ester 9-octadecenoic acid 5354568	-6.882	-6.882	-51.783
Glycedyl palmitate (Methyl ricinoleate) 5354133	-6.874	-6.874	-46.628
Phthalic acid, bis(2-ethylhexyl) ester 8343	-6.108	-6.108	-20.247
4-O methylmannose 345716	-6.069	-6.069	-37.856
N,N-Dimethylglycine 673	-5.926	-5.926	-31.603
4-methylbenzenethiol 7811	-5.842	-6.632	-32.340
Pyrogallol 1057	-5.685	-5.690	-30.454
9,12-Octadecadienoic acid (Z,Z)- 5280450	-3.806	-3.810	-49.930
9-Octadecenamide 1930	-3.784	-3.784	-51.397
15-Hydroxypentadecanoic Acid 78360	-3.647	-3.651	-56.487
Methyl linoleate 5284421	-3.422	-3.422	-44.004
Silymarin 5213	-3.097	-5.682	-42.161
Methyl 9-cis,11-trans- octadecadienoate 11748436	-2.444	-2.444	-35.475
Methyl stearate 8201	-2.432	-2.432	-40.650
Methyl oleate 5364509	-2.141	-2.141	-38.522
hexadecanoic acid, methyl ester 8181	-1.937	-1.937	-38.283
14,17-Octadecadienoic acid, methyl ester 5365751	-1.937	-1.937	-34.827