

Fig. (5). Binding mode of Octadecanoic acid in the active site region of receptor 1JIK (a-3D interaction, b-2D interaction).

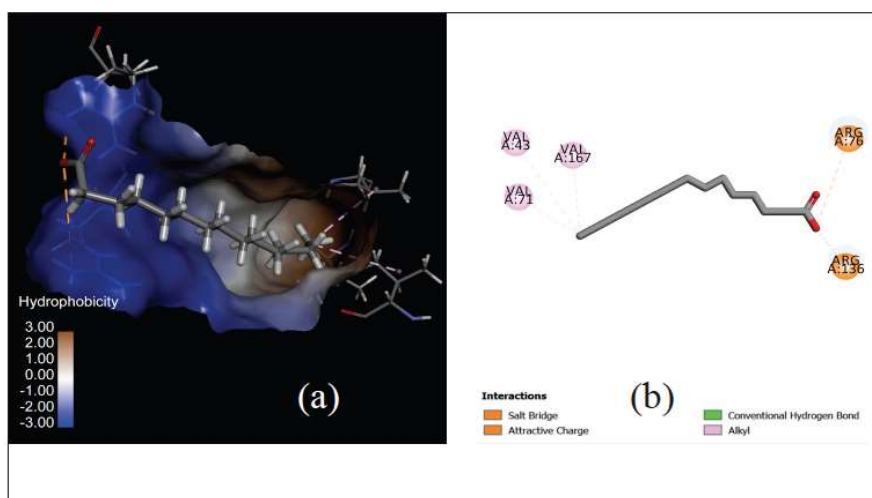


Fig. (6). Binding mode of Tetradecanoic acid in the active site region of receptor 1KZN (a-3D interaction, b-2D interaction).

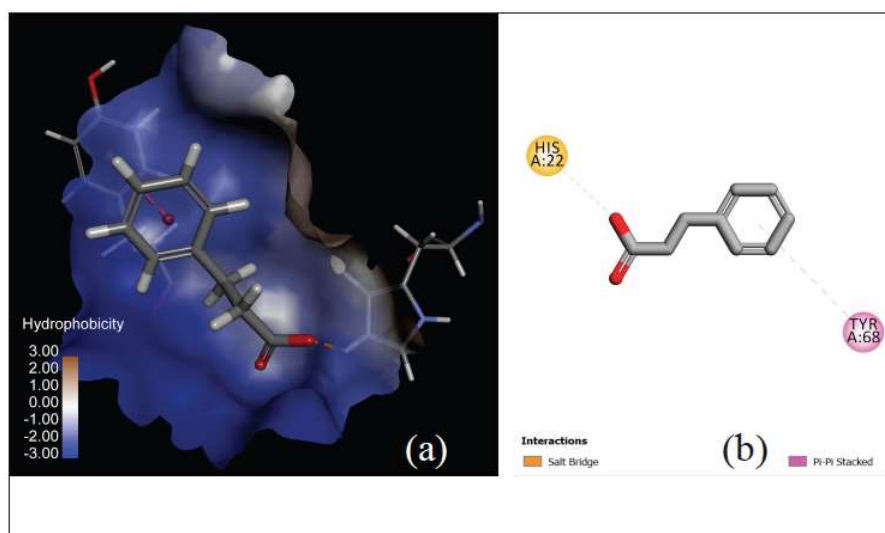


Fig. (7). Binding mode of Hydrocinnamic acid in the active site region of receptor 4JX9 (a-3D interaction, b-2D interaction).

**Table 5. Dock score and interaction types of best fit ligands with the particular bacterial proteins.**

Bacterial Protein ID	Best Fit Ligand	-CDOCKER Energy*	-CDOCKER Interaction Energy*	Ligand Interactions: Color Notations in 2D Diagram, Interaction type with Respective Amino Acid Residue with Bond Distance
1JIK	Octadecanoic acid	50.9251	53.94	Short dashed Orange, Salt Bridge with LYS A: 84 with bond distance 1.87; Green, Conventional Hydrogen bond LYS A: 84 with bond distance 1.99; Pea green, Carbon Hydrogen bond ARG A: 88 with bond distance 2.54
1KZN	Tetradecanoic acid	48.472	46.96	Long dashed Orange, Salt Bridge with ARG A: 76 with bond distance 5.09; Short dashed Orange, Attractive charges with ARG A: 136 with bond distance 2.46; Light Pink, Alkyl Interaction with VAL A: 43, VAL A: 71, VAL A: 167 with bond distance 4.77, 4.44, 4.77 respectively
4JX9	Hydrocinamic acid	31.3638	31.137	Short Dashed Orange, Salt Bridge with HIS A: 22 with bond distance 2.26; Pink, Pi-Pi Stacked Interaction with TYR A: 68 with bond distance 4.70
6C3U	Benzene acetic acid	52.3382	53.4671	Yellow, Pi-Sulfur Interaction with CYS D: 48 with bond distance 5.35; Long Dashed Orange, Pi-Cation interaction with LYC C: 93 with bond distance 4.75; Pea Green, Pi-Donor Hydrogen bond with TYR C: 65 with bond distance 2.65; Short Dashed Orange, Attractive charges HIS C: 67 with bond distance 4.19; Short Dashed Orange, Attractive charges ARG C: 122 with bond distance 4.75; Green, Conventional Hydrogen bond with THR D: 9 and HIS C: 67 with bond distance 2.32 and 2.64 respectively; Grey, Metal acceptor with MN C: 201 with bond distance 2.67 and 2.73 respectively
5KID	n-Hexadecanoic acid	40.733	47.904	Pink, Pi-Alkyl interaction with TYR A:223 with bond distance 5.00; Pink, Alkyl-Alkyl interaction with VAL A:213 with bond distance 5.10; Short Dashed Orange, Salt Bridge with ARG A: 149 with bond distance 2.68; Long Dashed Orange, Attractive charges with LYS A: 312 with bond distance 4.97; Long Dashed Orange, Pi-Anion Interaction with TYR A: 151 with bond distance 3.16; Green, Conventional Hydrogen bond with ARG A: 149 with bond distance 2.90
1JIK	Hexadecanoic acid ethyl ester	47.2219	44.902	Pink, Alkyl Interaction with CYS A: 37 with bond distance 3.93 and 4.66; Green, Conventional Hydrogen bond TYR A: 36 and GLN A: 174 with bond distance 2.69 and 3.08 respectively; Pea green, Carbon Hydrogen bond GLN A: 190 with bond distance 2.37
5KID	Hexadecanoic acid ethyl ester	46.6395	47.904	Green, Conventional Hydrogen bond TYR A: 151 and LYS A: 312 with bond distance 2.32 and 2.26 respectively; Pea green, Carbon Hydrogen bond ASN A: 287 with bond distance 2.51; Pink, Alkyl Interaction with ILE A: 292 and VAL A: 291 with bond distance 4.18 and 5.10 respectively

\*Energy released due to ligand-protein interactions is expressed as positive value of -CDOCKER energy.

**Table 6. Drug Likeness Prediction of compounds from hexane and methanol extract of *O. smargnida*.**

Sl. No.	Name of the Compound	ADMET Absorption Level	ADMET BBB Level	ADMET_EXT_Hepatotoxicity Prediction	ADMET_EXT_PPB_Prediction	ADMET_Solubility Level	TOPKAT_Ames_Prediction
1	Tetradecanoic acid	0	1	FALSE	TRUE	3	Non-Mutagen
2	Hexadecanoic acid methyl ester	1	0	FALSE	TRUE	2	Non-Mutagen
3	n-Hexadecanoic acid	0	0	FALSE	TRUE	2	Non-Mutagen
4	Oleic acid	3	4	FALSE	TRUE	2	Non-Mutagen
5	cis-13-Octadecenoic acid	3	4	FALSE	TRUE	2	Non-Mutagen
6	Hexadecanamide	0	0	FALSE	FALSE	2	Non-Mutagen
7	Pentacosane	3	4	FALSE	TRUE	0	Non-Mutagen
8	3-Methylpentacosane	3	4	FALSE	TRUE	0	Non-Mutagen

\*Four identified compounds namely [Cyclo(L-Propyl-L-Valine), Cyclo(L-Propyl-L-Valine), 3-(2-Methylpropyl)hexahydrophyrollo [1,2-a]pyrazine-1,4-dione] are not presented in the table because of their True ADMET\_EXT\_Hepatotoxicity Prediction.