**Supplementary Material**

*Article*

# Investigation of the Biological Activities and Characterization of Bioactive Constituents of *Ophiorrhiza rugosa* var. *prostrata* (D.Don) & Mondal Leaves through In Vivo, In Vitro, and In Silico Approaches

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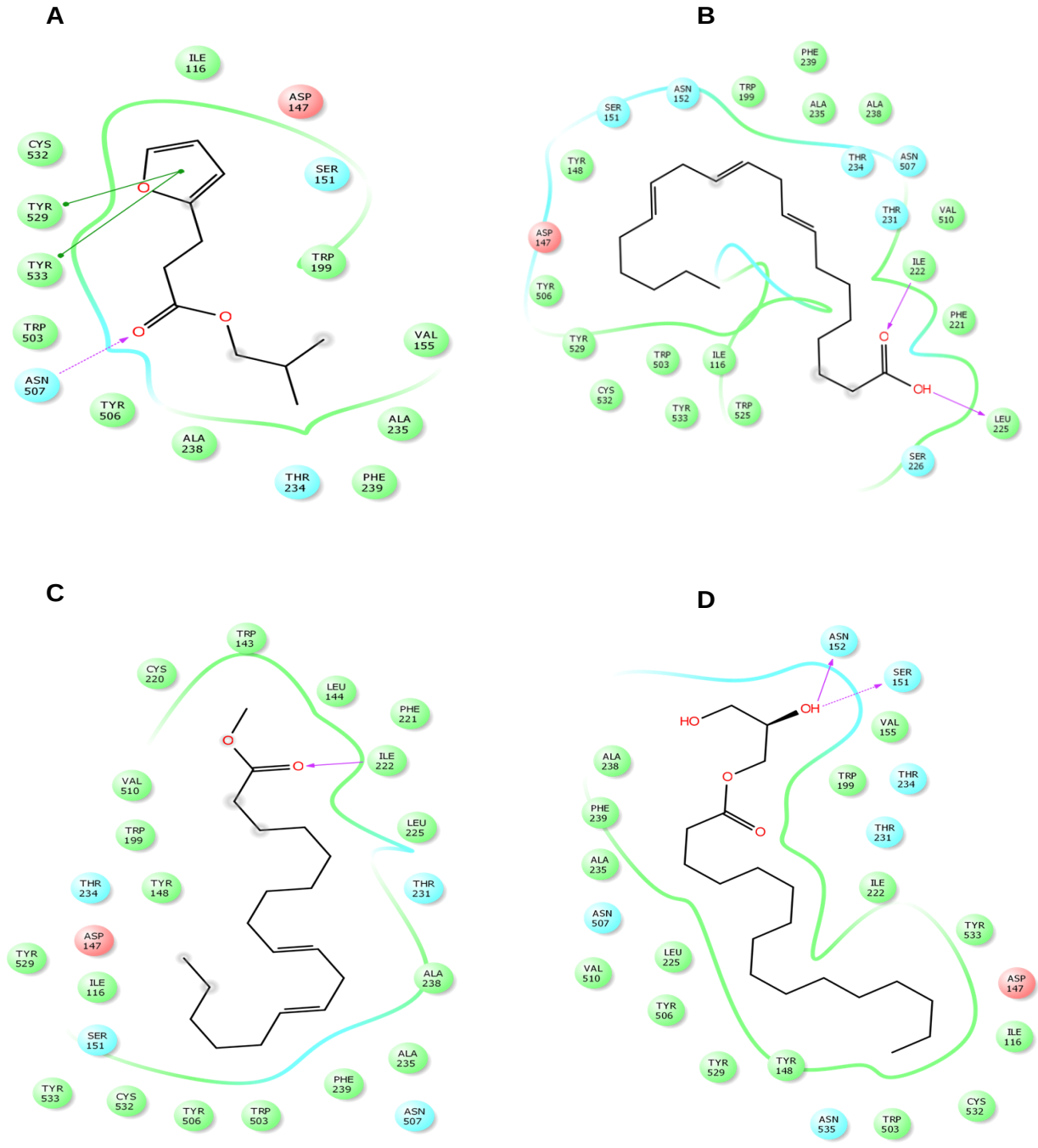
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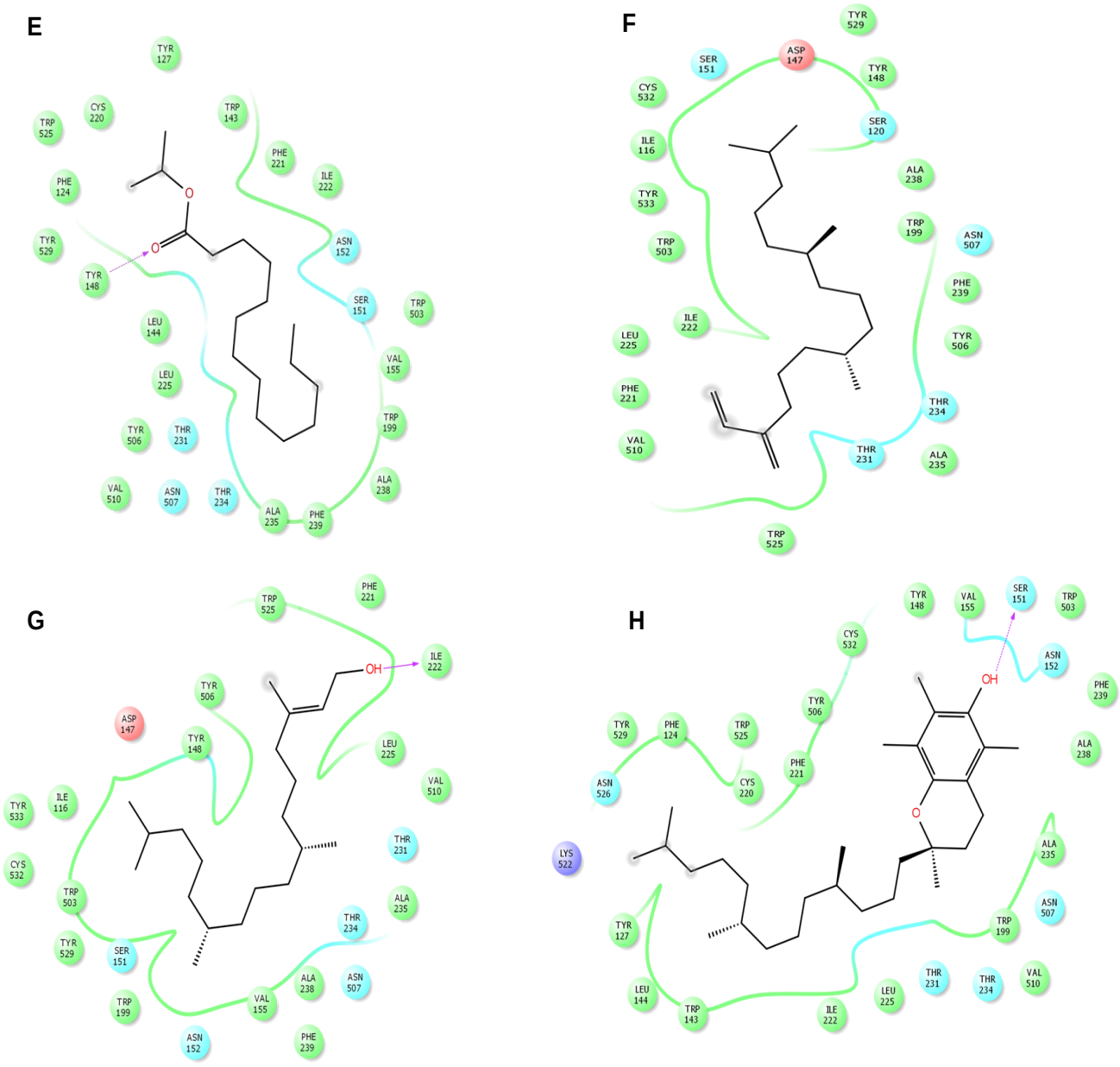



**Figure S1.** 2D interactions of the best fit found for (A) Loliolide, (B) Ethyl linolenate, (C) Methyl linoleate, (D) 2-Palmitoylglycerol, (E) Methyl palmitate, (F) Neophytadiene, (G) Phytol, and (H) Vitamin E docked to the M3 muscarinic acetylcholine receptor (PDB ID: 4U14). Colors indicate the residue (or species) type: Red-acidic (Asp, Glu), Green-hydrophobic (Ala, Val,Ile, Leu, Tyr, Phe, Trp, Met, Cys, Pro), Purple-basic (Hip, Lys, Arg), Blue-polar (Ser, Thr, Gln, Asn, His, Hie, Hid), Light gray-other (Gly, water) and Darker gray-metal atoms. Interactions with the protein are marked with lines between ligand atoms and protein residues: Solid pink: H-bonds to the protein backbone, Dotted pink: H-bonds to protein side chains, Green: pi-pi stacking interactions, Orange: pi-cation interactions. Ligand atoms exposed to solvent are marked with gray spheres. The protein "pocket" is displayed with a line around the ligand, colored with the color of the nearest protein residue. The gap in the line shows the opening of the pocket.

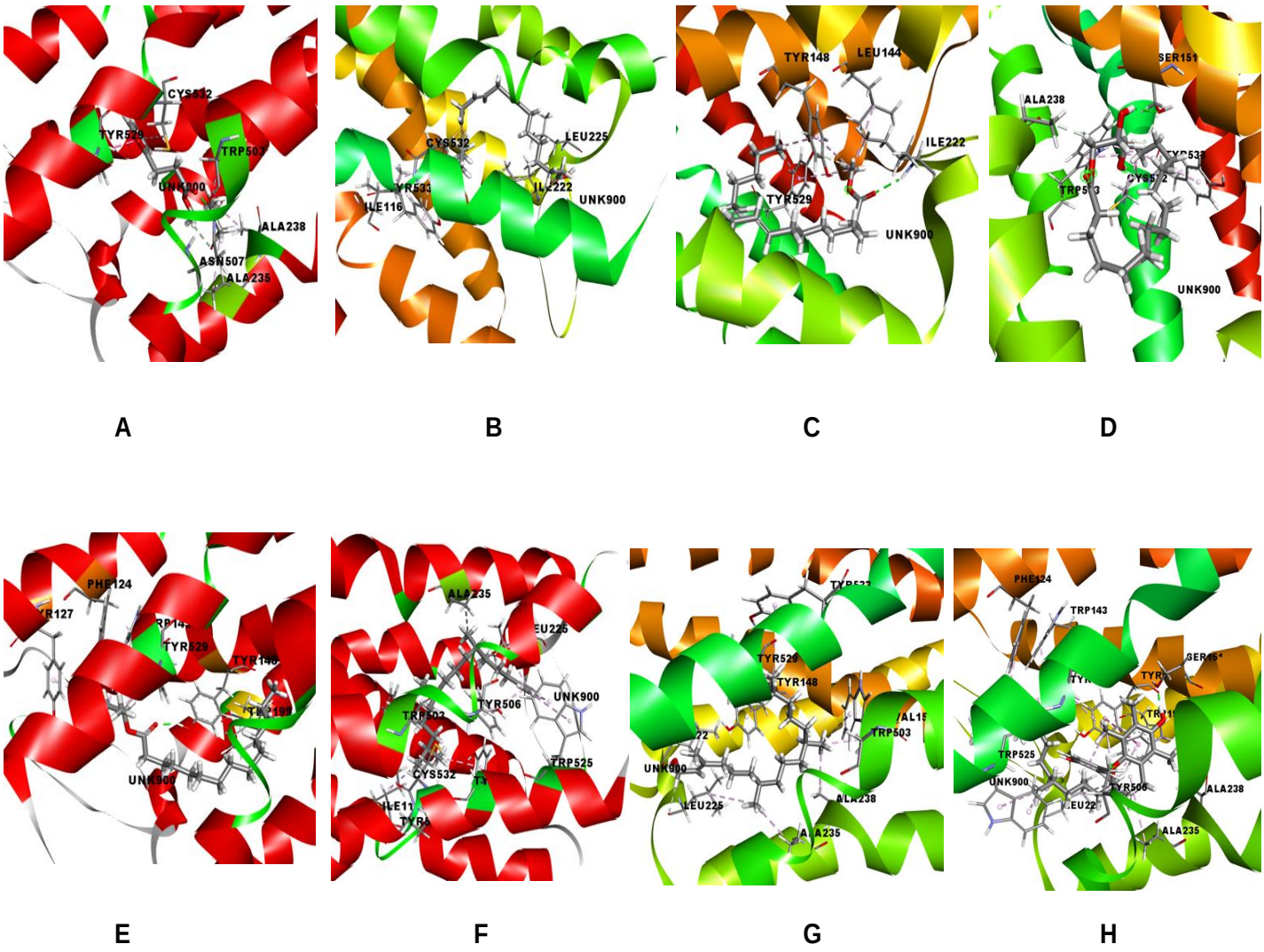



**Figure S2.** Best ranked fit of (A) Loliolide, (B) Ethyl linolenate, (C) Methyl linoleate, (D) 2-Palmitoylglycerol, (E) Methyl palmitate, (F) Neophytadiene, (G) Phytol and (H) Vitamin E in the binding pocket of the M3 muscarinic acetylcholine receptor (PDB ID: 4U14).

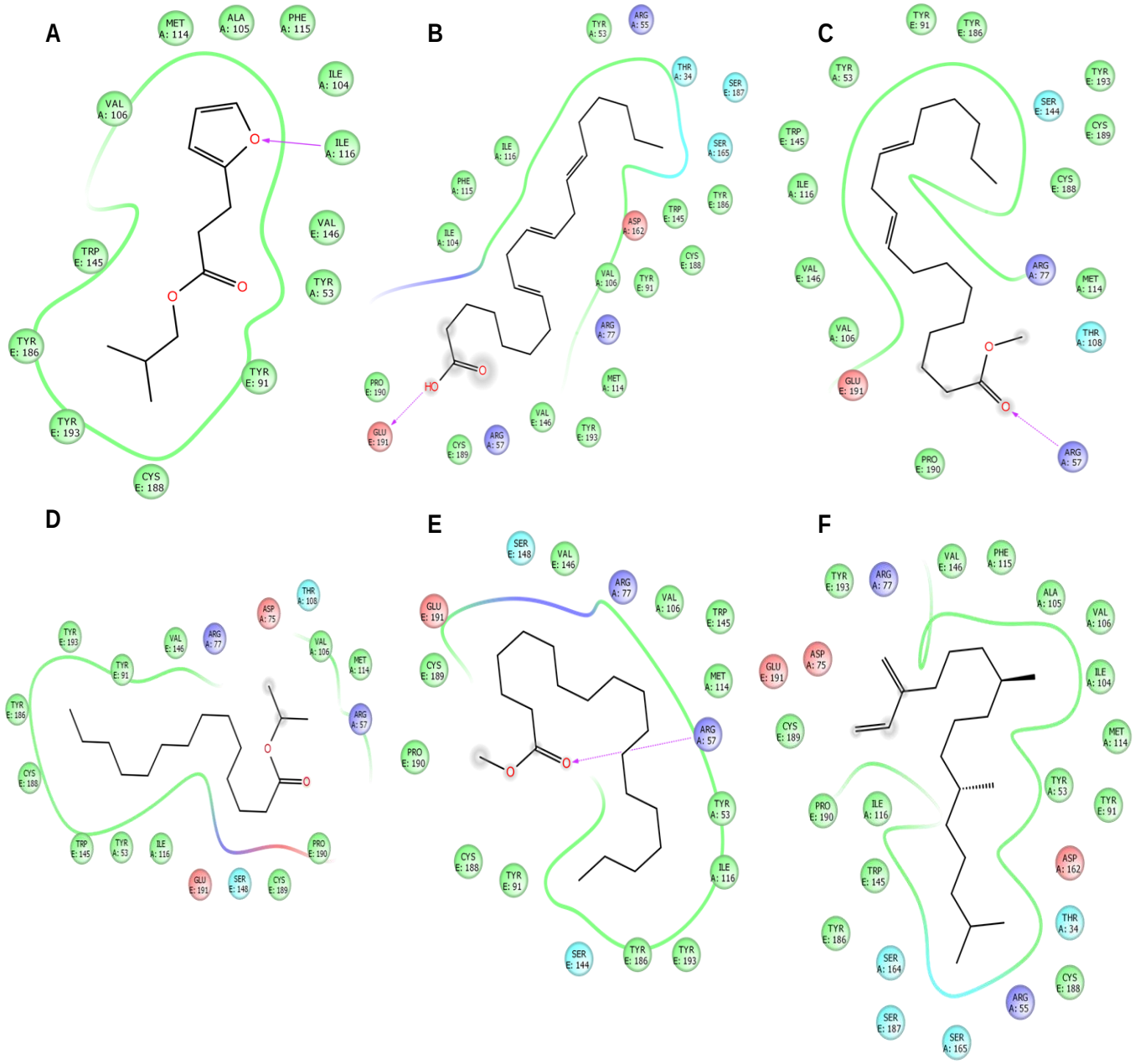



**Figure S3.** 2D interactions of the best fit found for (A) Loliolide, (B) Ethyl linolenate, (C) Methyl linoleate, (D) Methyl palmitate, (E) Methyl stearate and (F) Neophytadiene docked to the 5-HT3 receptor (PDB ID: 5AIN).

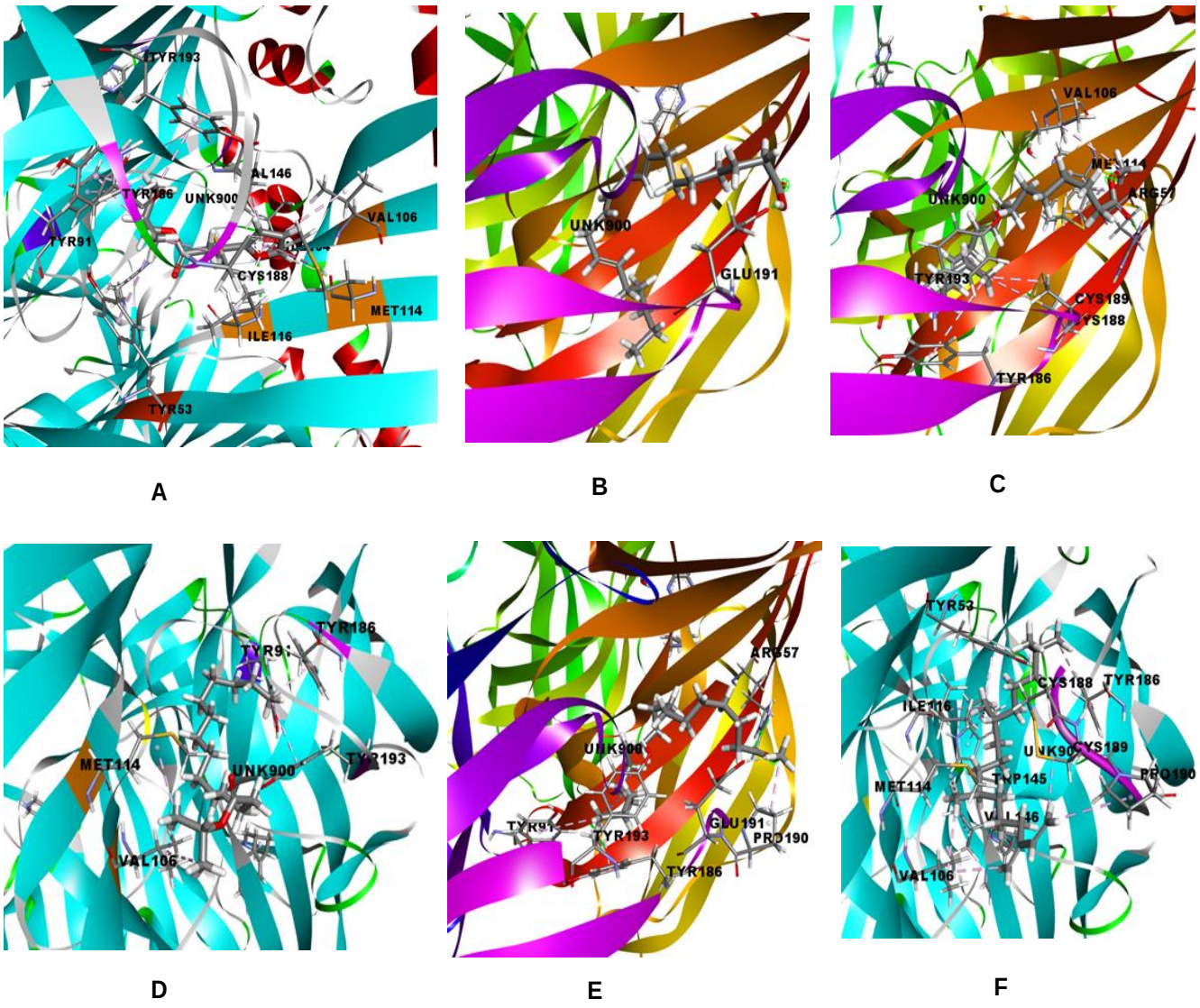



**Figure S4.** Best ranked fit of (A) Loliolide, (B) Ethyl linolenate, (C) Methyl linoleate, (D) Methyl palmitate, (E) Methyl stearate and (F) Neophytadiene in the binding pocket of the 5-HT3 receptor (PDB ID: 5AIN).

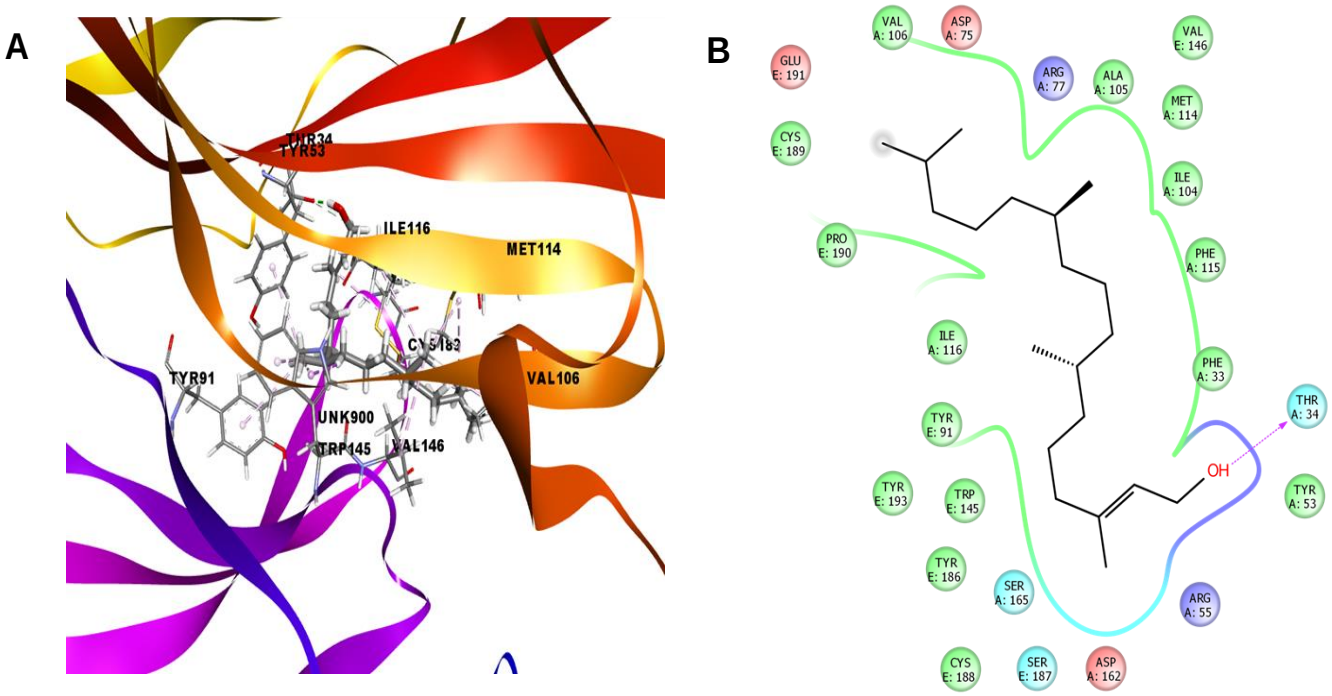
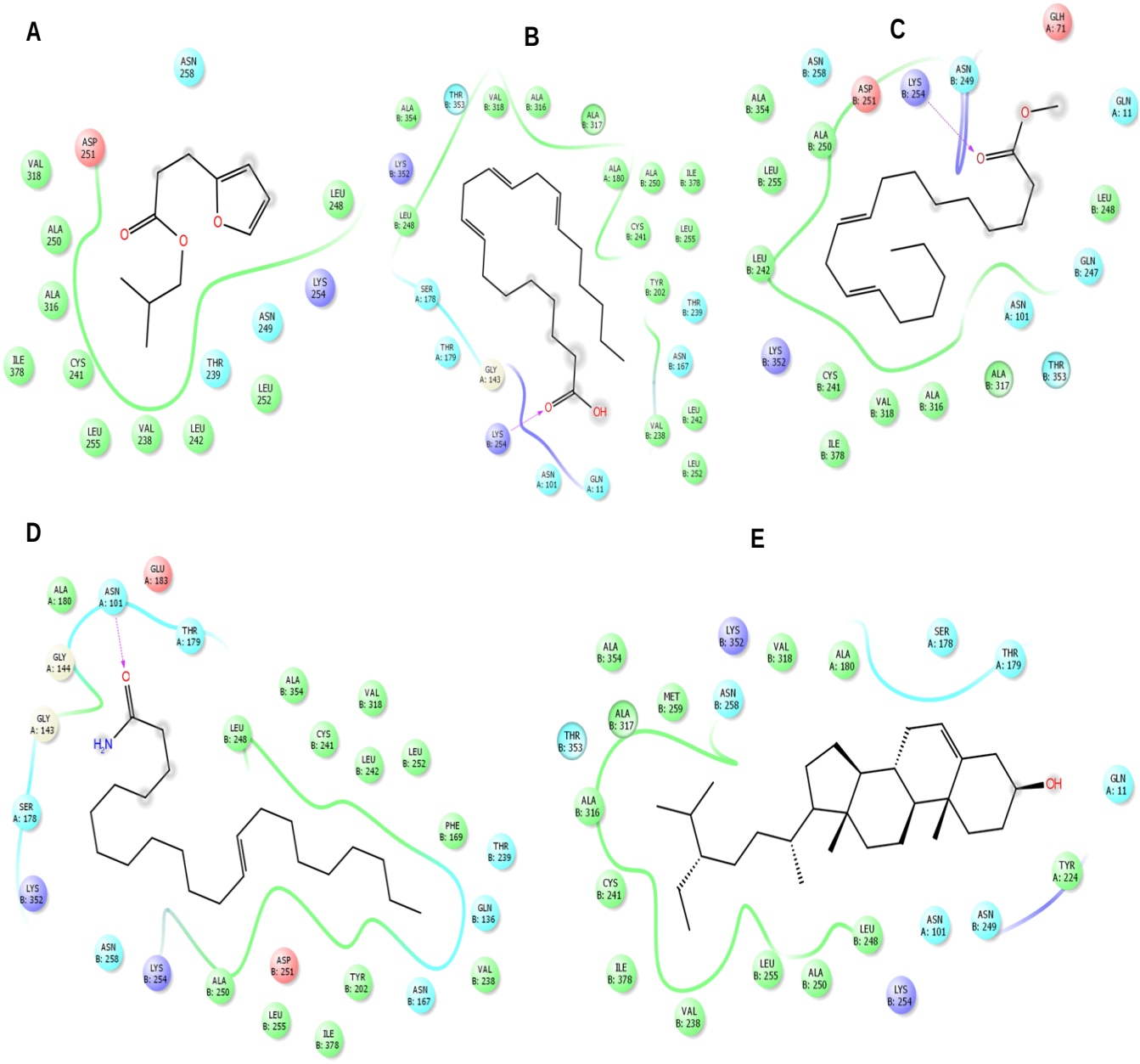



**Figure S5.** Best ranked fit of Phytol (A) in the binding pocket of 5-HT3 (PDB ID: 5AIN) and 2D representation of key interactions in the binding pocket for Phytol (B).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ALA B: 316
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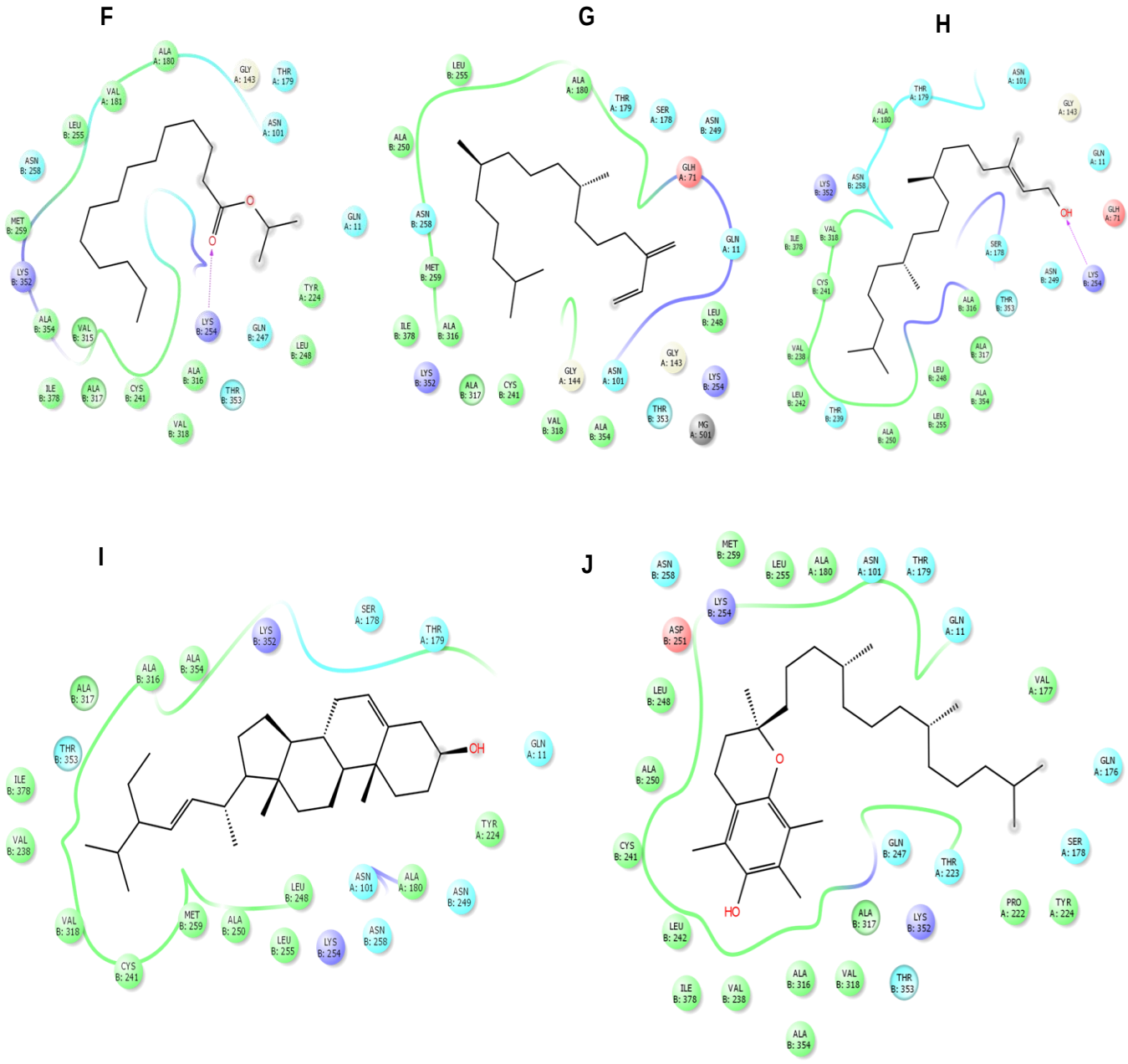


**Figure S6.** 2D interactions of the best fit found for (A) Loliolide, (B) Ethyl linolenate, (C) Methyl linoleate, (D) Erucamide, (E) gamma-Sitosterol, (F) Methyl palmitate, (G) Neophytadiene, (H) Phytol, (I) Stigmasterol and (J) Vitamin E docked to tubulin (PDB ID: 1SA0).

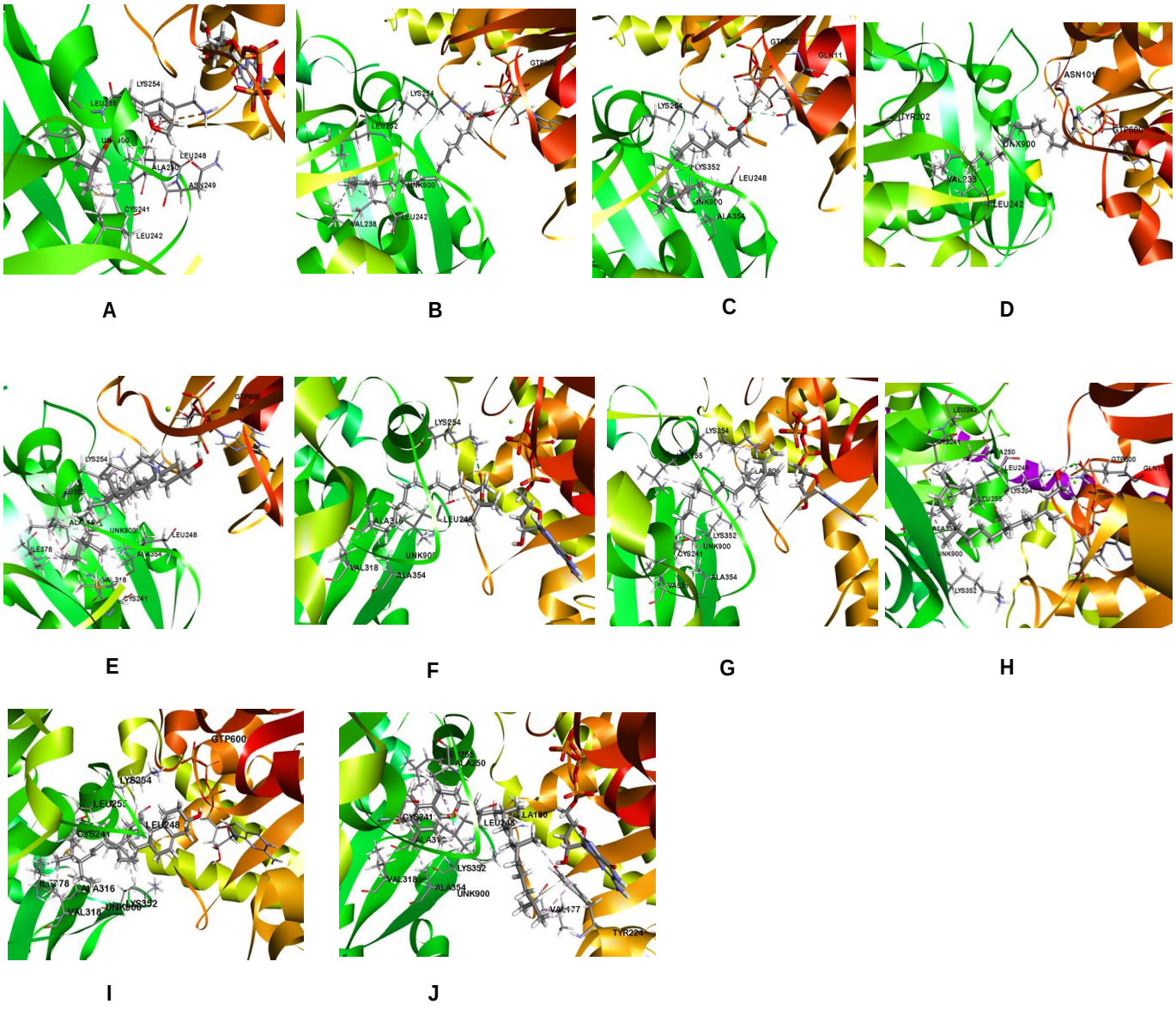


**Figure S7.** Best ranked fit of (A) Loliolide, (B) Ethyl linolenate, (C) Methyl linoleate, (D) Erucamide, (E) gamma-Sitosterol, (F) Methyl palmitate, (G) Neophytadiene, (H) Phytol, (I) Stigmasterol and (J) Vitamin E in the binding pocket of tubulin (PDB ID: 1SA0).

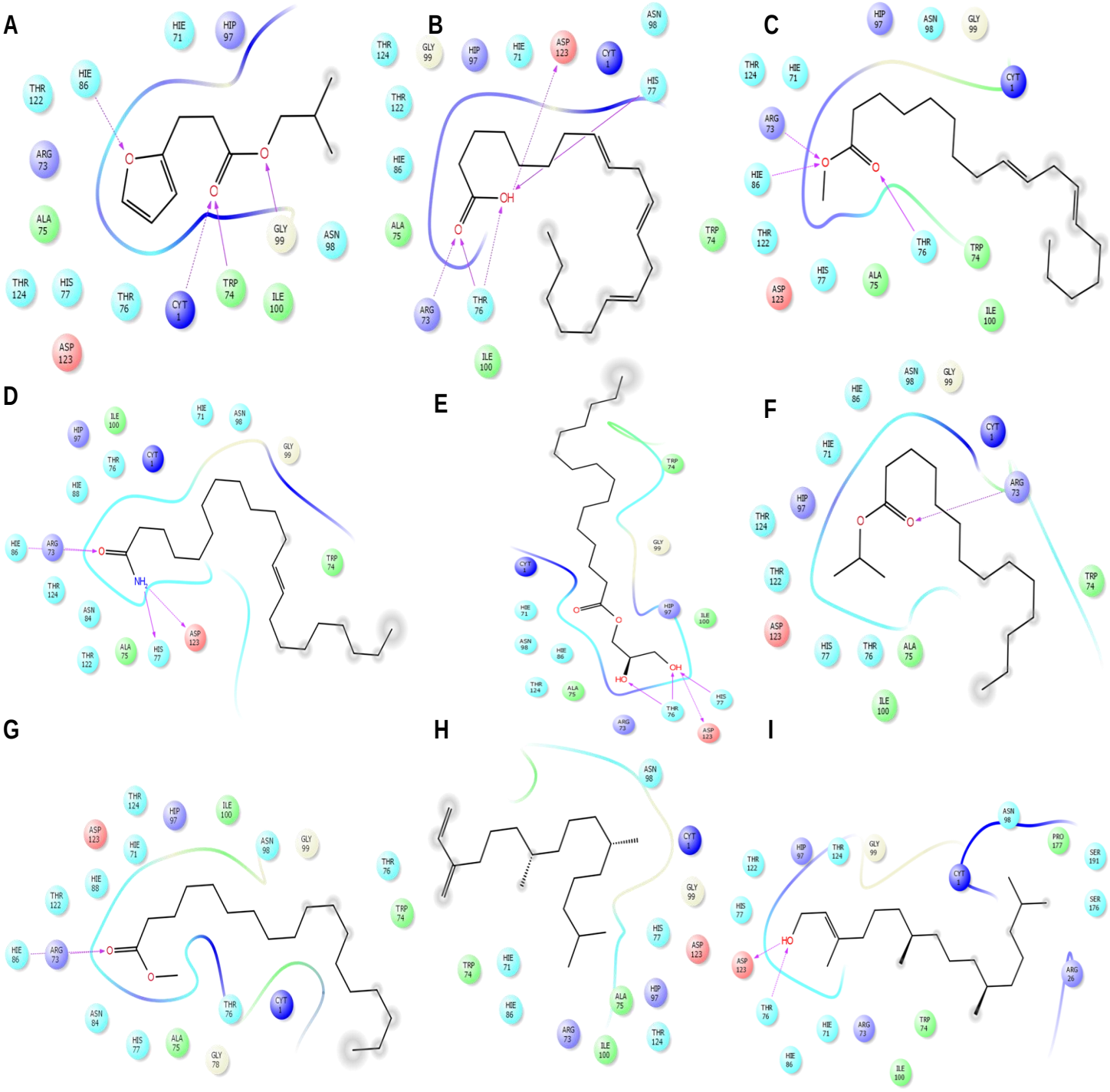


**Figure S8.** 2D interactions of the best fit found for (A) Loliolide, (B) Ethyl linolenate, (C) Methyl linoleate, (D) Erucamide, (E) 2-Palmitoylglycerol, (F) Methyl palmitate, (G) Methyl stearate, (H) Neophytadiene and (I) Phytol docked to GlcN-6-P synthase (PDB ID: 1XFF).

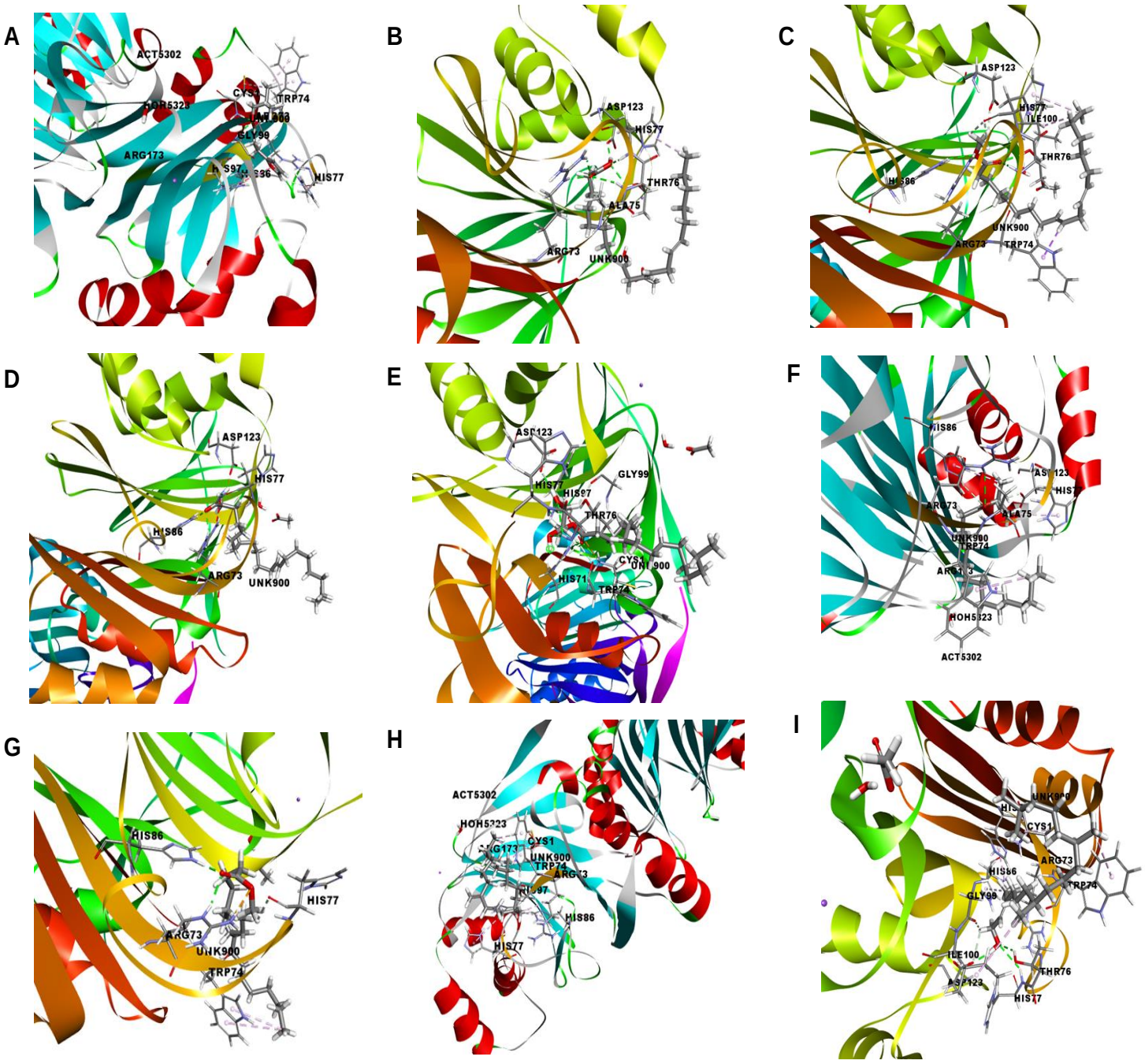


**Figure S9.** Best ranked fit of (A) Loliolide, (B) Ethyl linolenate, (C) Methyl linoleate, (D) Erucamide, (E) 2-Palmitoylglycerol, (F) Methyl palmitate, (G) Methyl stearate, (H) Neophytadiene and (I) Phytol in the binding pocket of GlcN-6-P synthase (PDB ID: 1XFF).

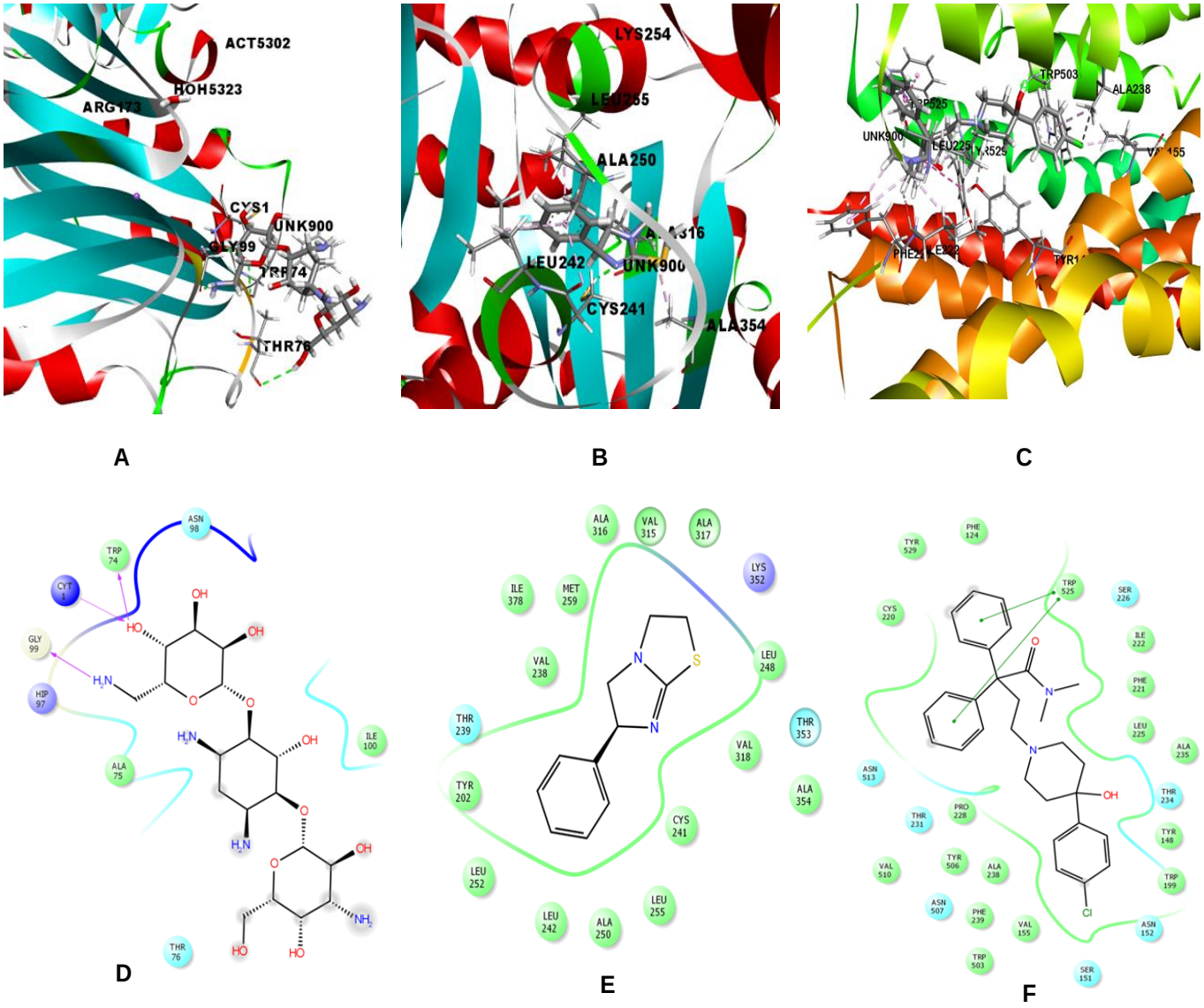


**Figure S10.** (A) Best fit and (D) 2D interaction diagram of Kanamycin docked at the binding pocket of GlcN-6-P synthase (PDB ID: 1XFF). (B) Best fit and (E) 2D interaction diagram of Levamisole docked at the binding pocket of tubulin (PDB ID: 1SA0). (C) Best fit and (F) 2D interaction diagram of Loperamide docked at the binding pocket of M3 muscarinic acetylcholine receptor (PDB ID: 4U14).