Supporting Information

Discovery of Novel Inhibitors for Human Farnesyltransferase (*h*FTase) *via* Structure-based Virtual Screening

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Figure S1. Multiple sequence alignment between the proteins 3E33 (*r*FTase) and 1S63 (*h*FTase). The amino acid residues of protein sequences were colored by Clustal x2. Residues within 5 Å of ligands were highlighted by red rectangles.

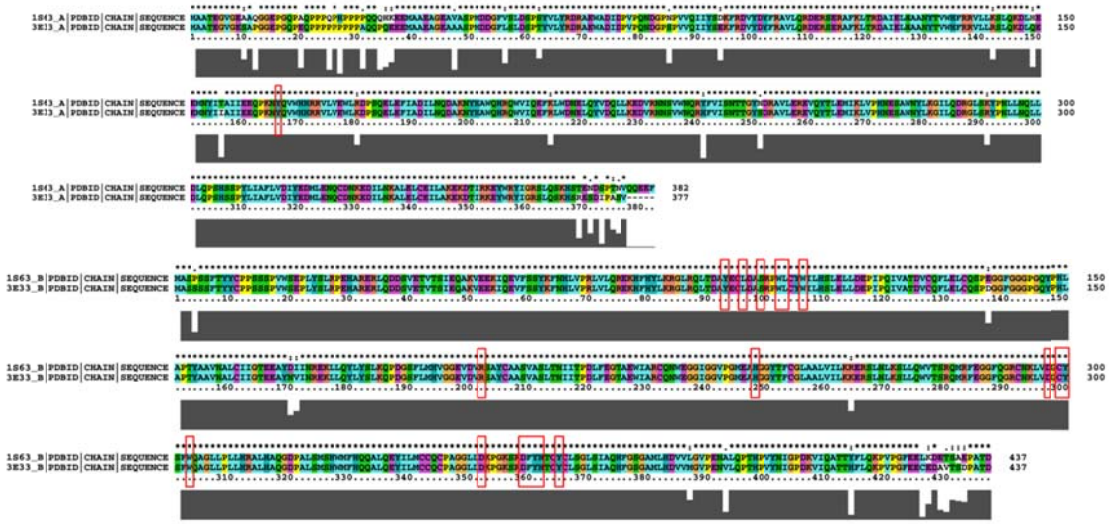

Figure S2. The crystal structure superposition for the human and rat Ftase with the residues within 5 Å of ligands. The protein 3E33 was colored cyans, 1S63 was colored pink, the ligands and residues were shown as sticks and lines, respectively.

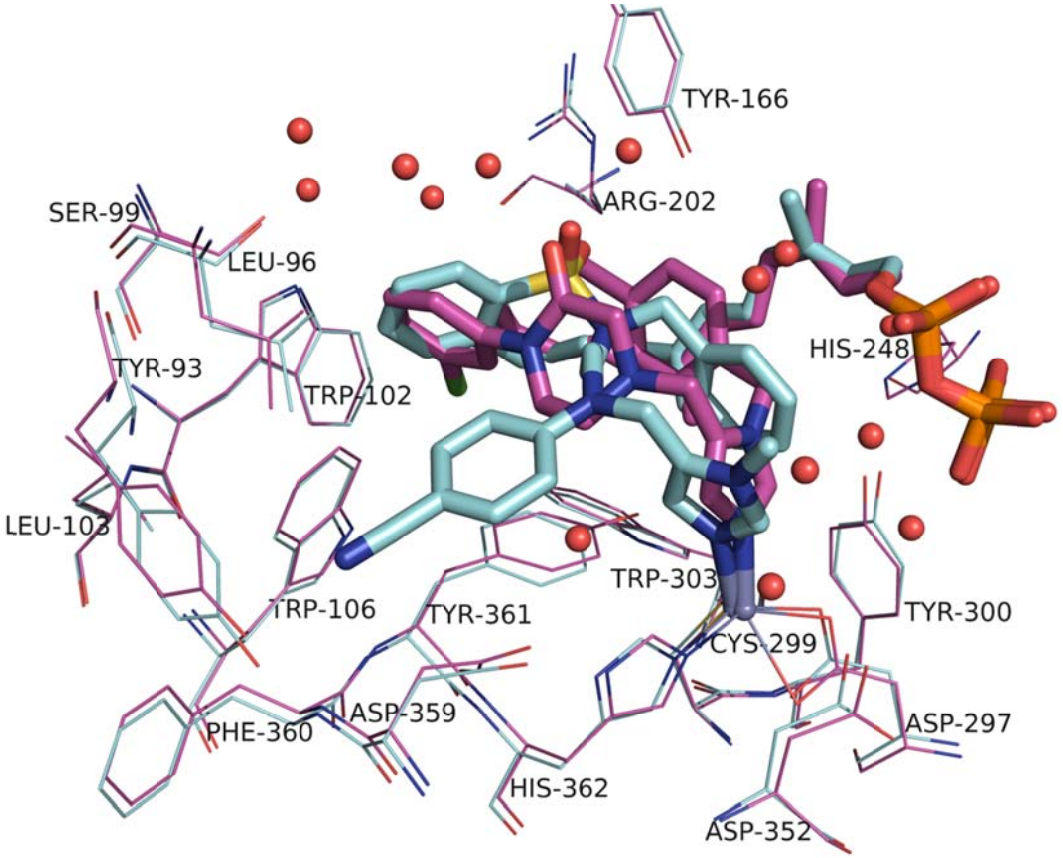

Figure S3. (A) The top 20 docked conformations. (B) The best docked pose that ranked 3th obtained the minimum RMSD as 0.96Å against the original binding pose in the cystal structure. The conformation of the bound ligandr was colored green and the docked poses were colored cyan.