Supporting Information

Pharmacophore Modeling and Docking Studies on Some Nonpeptide Based Caspase-3 Inhibitors

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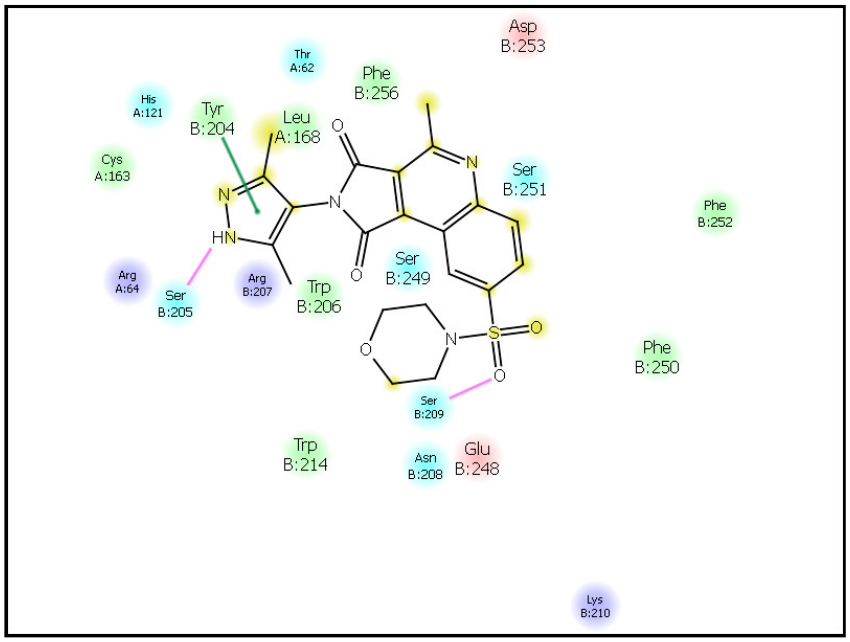

Figure S_1: Ligand interaction diagram of compound 49 with receptor where pink sphere: charged (negative); blue sphere: charged (positive); light sky blue sphere: polar residues; light green sphere: hydrophobic; green line is showing π-π stacking between Tyr 204 and aromatic substituent at position 2 of molecule; pink line is showing H-bond (backbone).

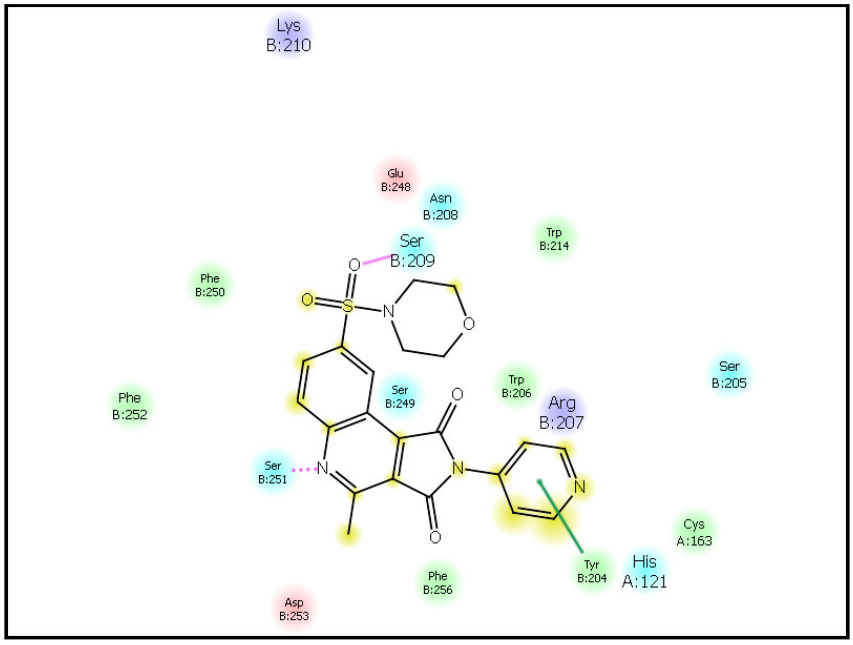

Figure S_2: Ligand interaction diagram of compound 58 with receptor where pink sphere: charged (negative); blue sphere charged (positive); light sky blue sphere: polar residues; light green sphere: hydrophobic; green line is showing π-π stacking between Tyr 204 and aromatic ring of substituent at position 2 of molecule; pink dashed line is showing H-bond (backbone) and pink dotted line is showing H-bond (side chain).

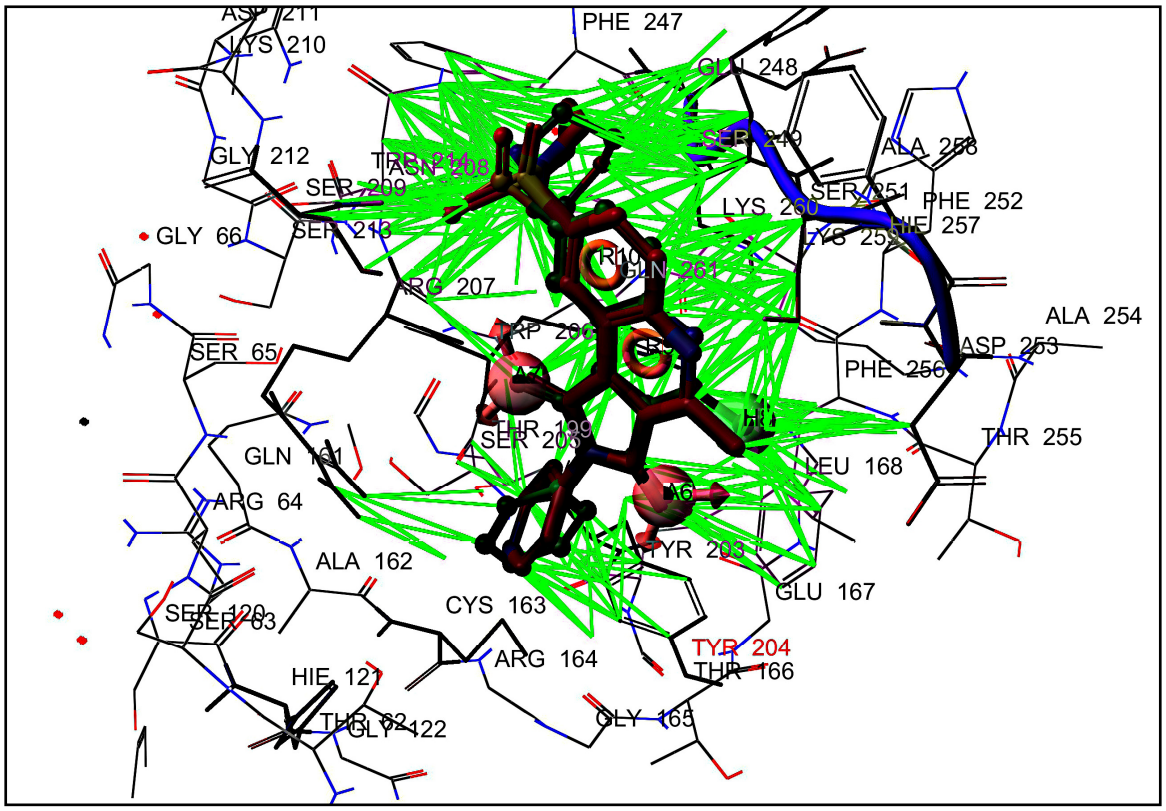

Figure S_3: Overlay study of developed pharmacophore site and docked pose of potent compound (58) and their molecular interactions with active site residues. The figure is showing the consistency of developed pharmacophore features with surrounding residues in binding pocket.