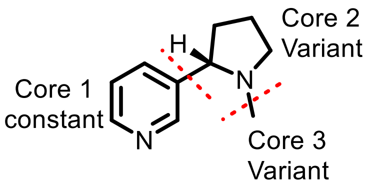
Supplementary Information

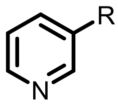
Tables

Table S1: Details of the receptors and its co-crystal used in the present study. Stereological aspect of the receptors was studied using Schrödinger 2020-3 suite, and the % residues of the receptors in the allowed and disallowed regions of the Ramachandran plot are shown.

Name of the Receptor (PDB ID)	**No. of residues**	**Co-crystal ligand**	**Resolution; R-factor; R-free**	**% of residues in different regions**		**References**
				Allowed region	Disallowed region	
MMP-9 (4XCT)	157	(2~{R})-3-methyl-~{N}-oxidanylidene-2-[(4-phenylphenyl)sulfonyl-propan-2-yloxy-amino]butanamide	1.30; 0.167; 0.231	98.5%	1.5%	Nuti et al., **2015**
GSK-3β (5F95)	683	2-[(cyclopropylcarbonyl)amino]-N-(4-phenylpyridin-3-yl)pyridine-4-carboxamide	2.52; 0.202; 0.242	97.5%	2.5%	Luo et al., 2016
TNF-α (2AZ5)	148	6,7-dimethyl-3-[(methyl{2-[methyl({1-[3-(trifluoromethyl)phenyl]-1h-indol-3-yl}methyl)amino]ethyl}amino)methyl]-4h-chromen-4-one	2.1; 0.220; 0.278	95.59%	4.41%	He MM et al., **2005**
MURC (4C13)	490	Uridine 5'Diphospho N-acetyl muramoyl-L-Alanyl-D-Glutamyl-L-Lysine	1.90; 0.196; 0.241	97%	3%	Wang et al., **2013**
ParE (4MOT)	226	AZ13072886	1.75; 0.190; 0.228	95.5%	4.42%	Kale et al., **2014**

Table S2: Different hops obtained during Scaffold hopping





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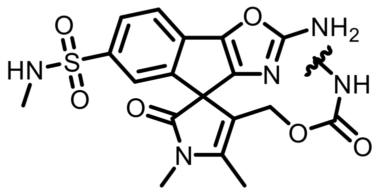	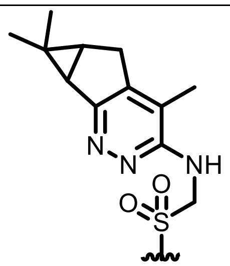	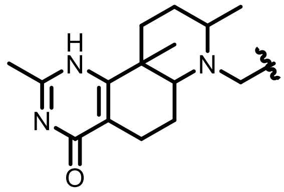
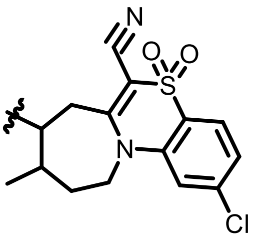	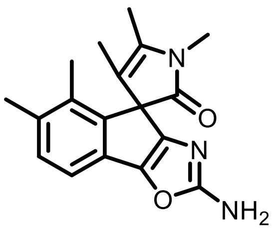	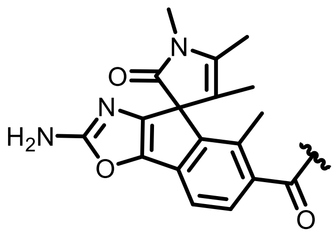
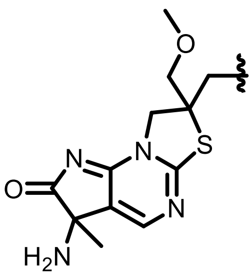	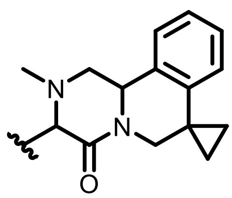	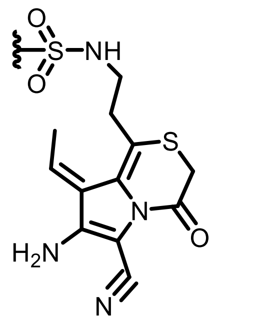
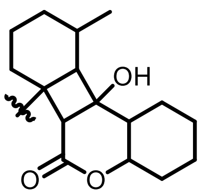	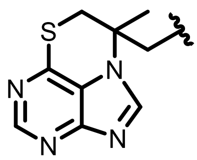	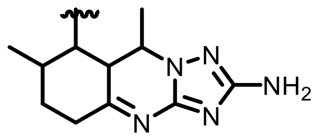
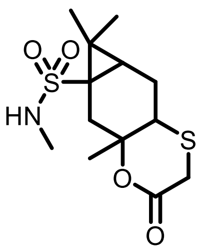	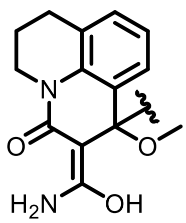	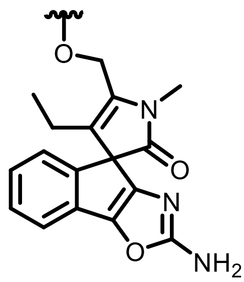

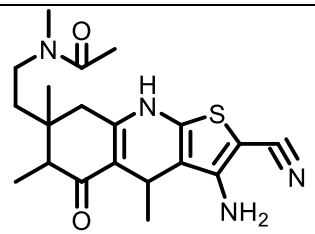
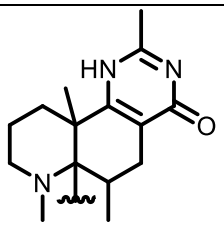
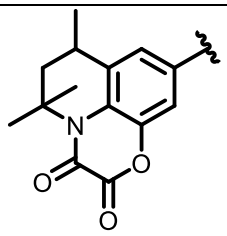
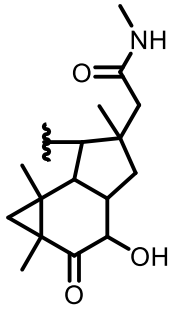
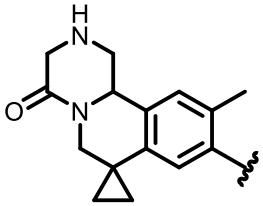
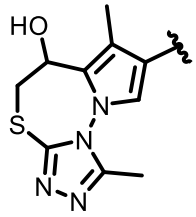
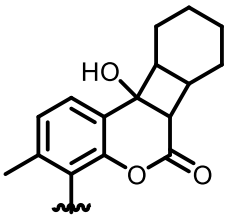
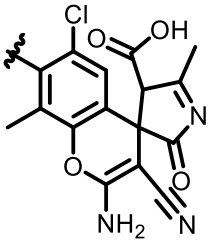
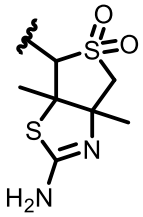
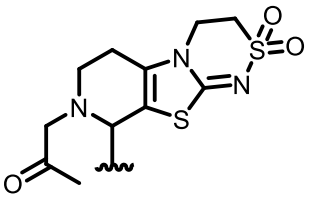
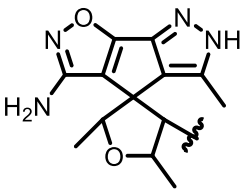
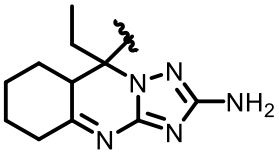
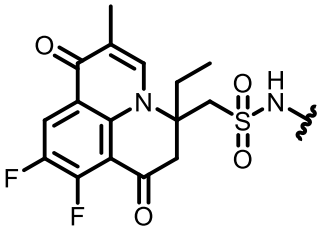
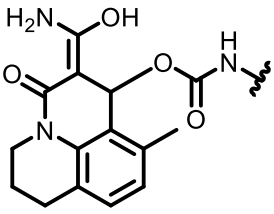
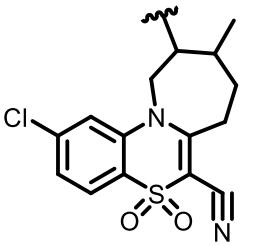
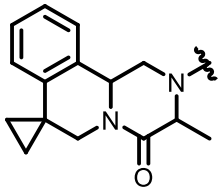
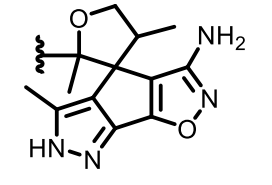
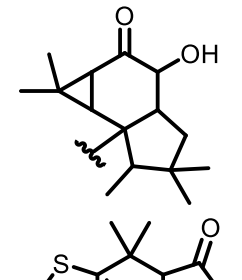
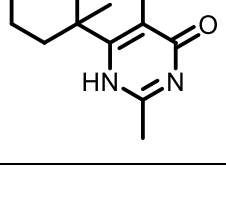
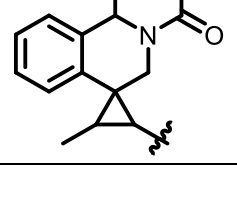
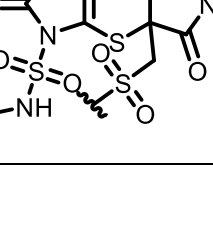

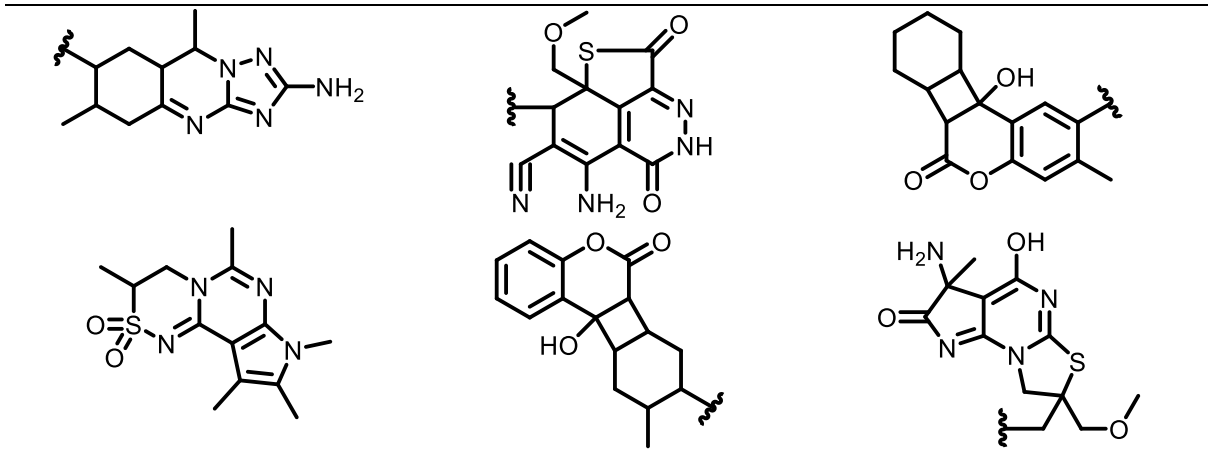

Table S3: MMGBSA calculations for the different trajectory frames obtained during MD simulation.

Protein-ligand complex	Average ΔGbind (kcal/mol)
H1/4XCT	-59.235
H1/5F95	-49.369
H1/2AZ5	-42.321
H1/4C13	-62.689
H1/4MOT	-69.519

Figures

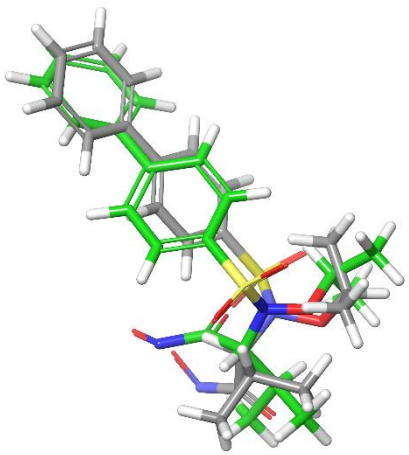

Figure S1a. Overlay of co-crystallized ligand (green) of 4XCT with its XP-docked pose (grey) [RMSD: 1.26 Å]

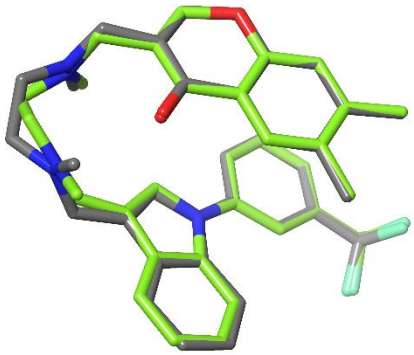

Figure S1b. Overlay of co-crystallized ligand (green) of 2AZ5 with its XP-docked pose (grey) [RMSD: 0.299 Å]

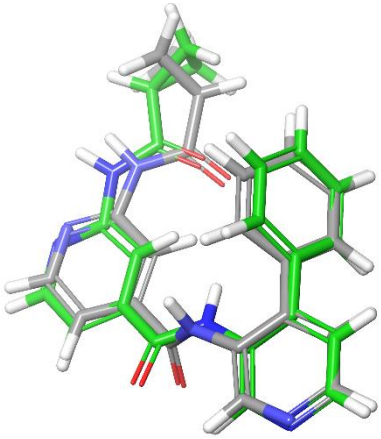

Figure S1c. Overlay of co-crystallized ligand (green) of 5F95 with its XP-docked pose (grey) [RMSD: 0.989 Å]

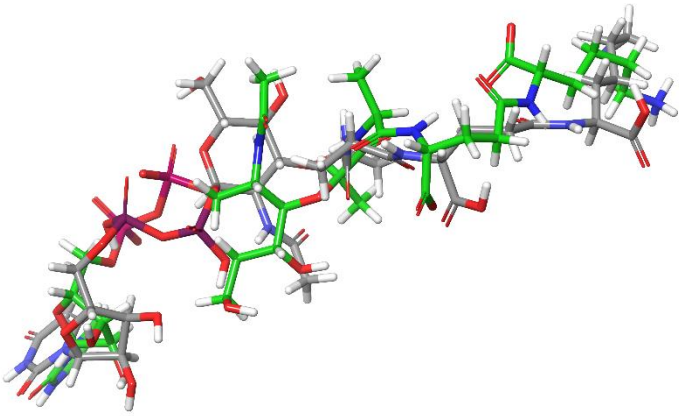

Figure S1d. Overlay of co-crystallized ligand (green) of 4C13 with its XP-docked pose (grey) [RMSD: 1.898 Å]

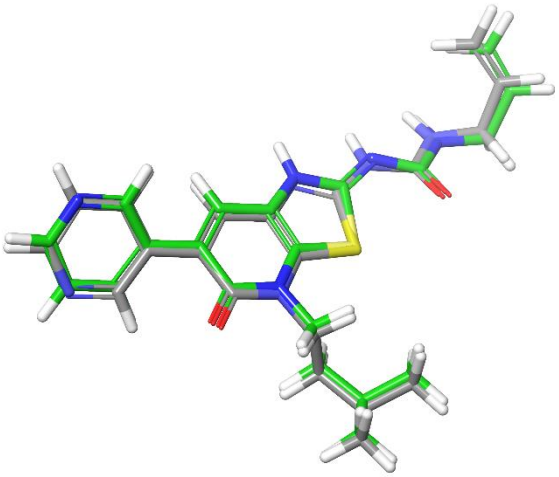

Figure S1e. Overlay of co-crystallized ligand (green) of 4MOT with its XP-docked pose (grey) [RMSD: 0.728 Å]

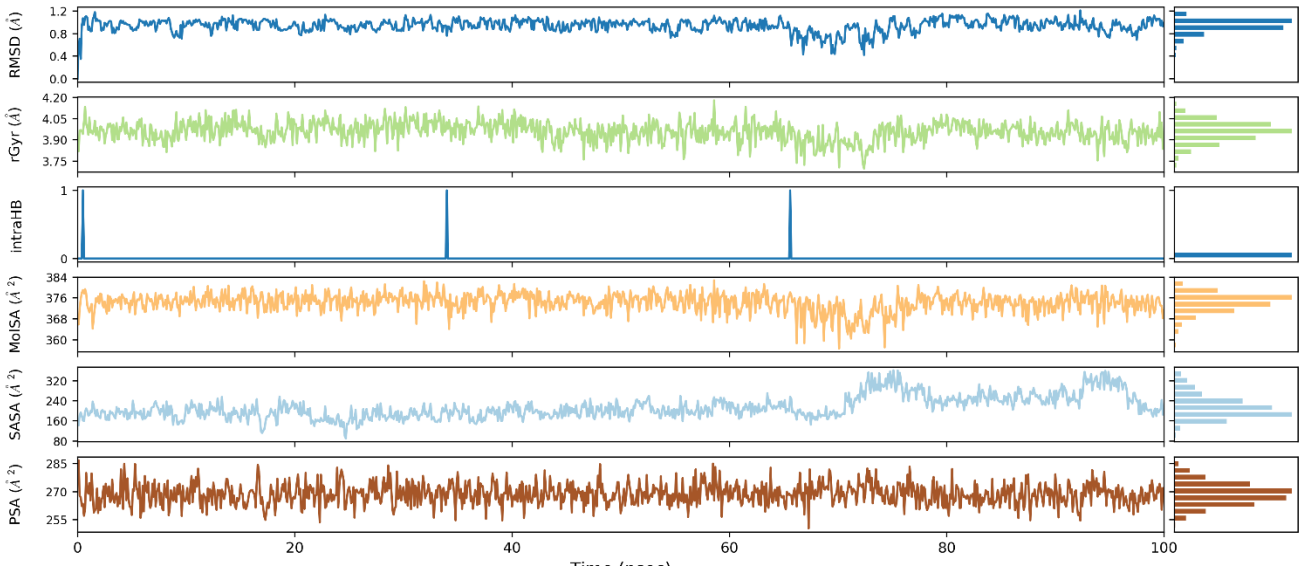

Figure S2a: Ligand H1 property during MD simulation against 4XCT. RMSD: Root mean square deviation of a ligand with respect to the reference conformation; rGyr: Radius of Gyration which measures the 'extendedness' of a ligand; intraHB: Intramolecular Hydrogen Bonds; MolSA: Molecular Surface Area; SASA: Solvent Accessible Surface Area; PSA: Polar Surface Area.

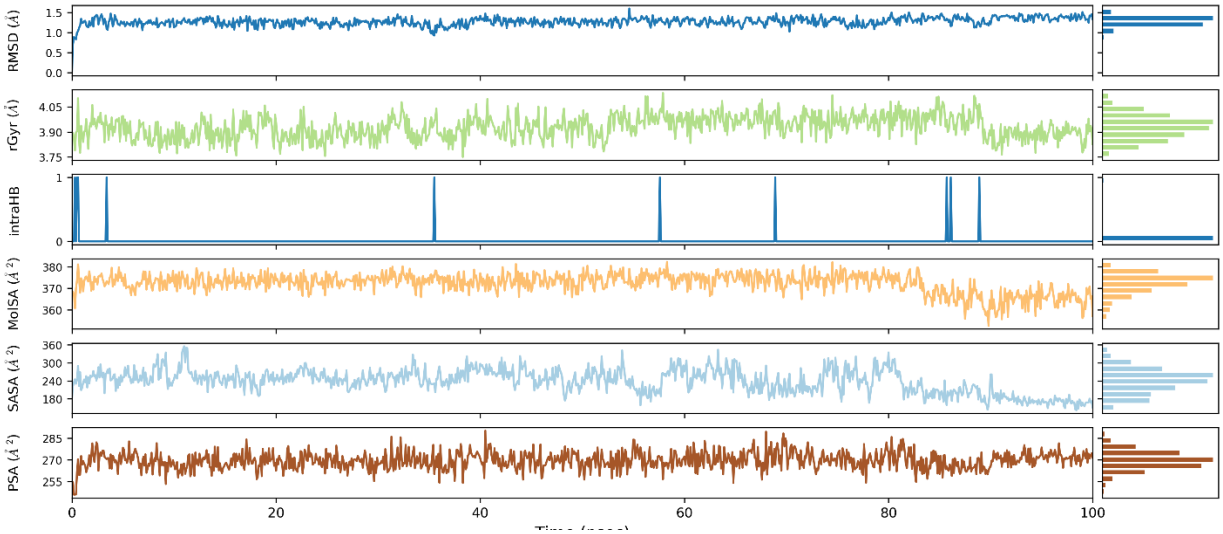

Figure S2b: Ligand H1 property during MD simulation against 5F95. RMSD: Root mean square deviation of a ligand with respect to the reference conformation; rGyr: Radius of Gyration which measures the 'extendedness' of a ligand; intraHB: Intramolecular Hydrogen Bonds; MolSA: Molecular Surface Area; SASA: Solvent Accessible Surface Area; PSA: Polar Surface Area.

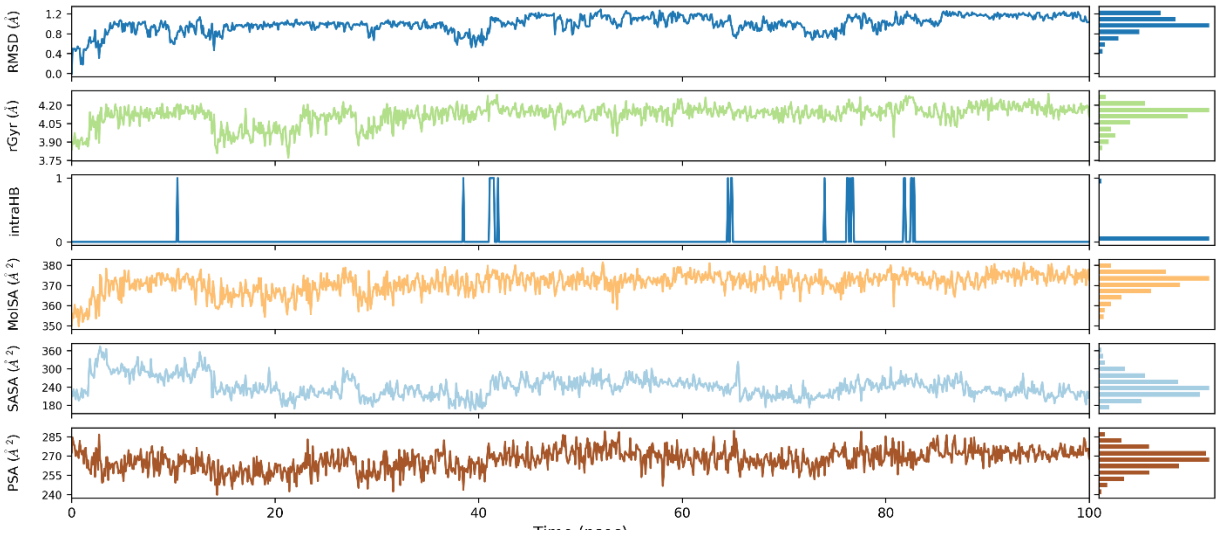

Figure S2c: Ligand H1 property during MD simulation against 2AZ5. RMSD: Root mean square deviation of a ligand with respect to the reference conformation; rGyr: Radius of Gyration which measures the 'extendedness' of a ligand; intraHB: Intramolecular Hydrogen Bonds; MolSA: Molecular Surface Area; SASA: Solvent Accessible Surface Area; PSA: Polar Surface Area.

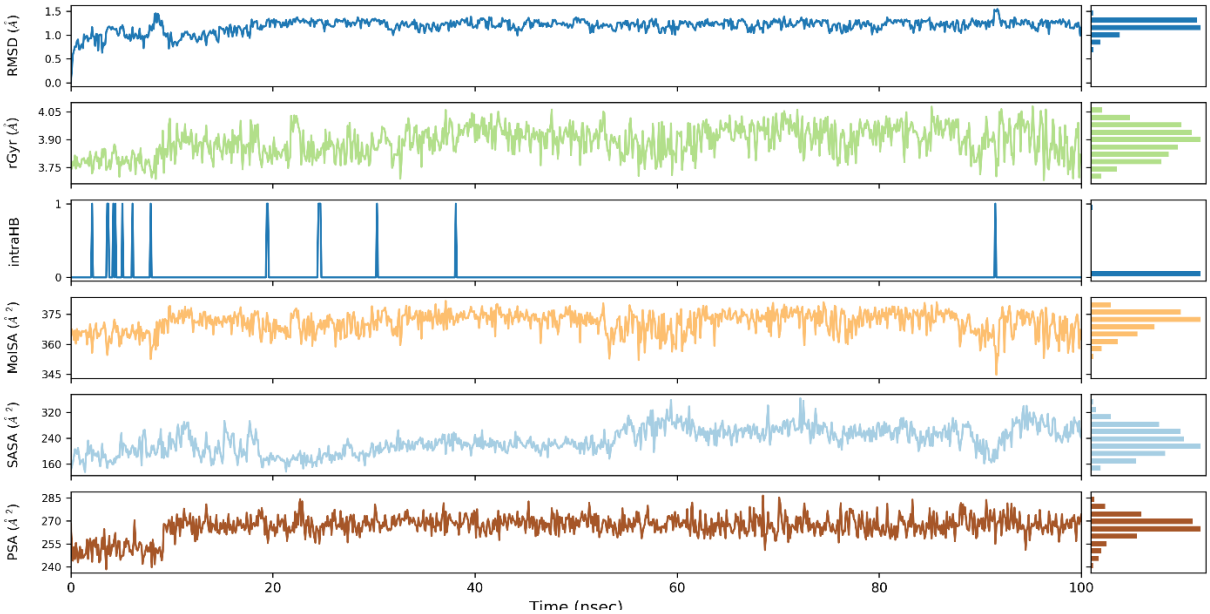

Figure S2d: Ligand H1 property during MD simulation against 4C13. RMSD: Root mean square deviation of a ligand with respect to the reference conformation; rGyr: Radius of Gyration which measures the 'extendedness' of a ligand; intraHB: Intramolecular Hydrogen Bonds; MolSA: Molecular Surface Area; SASA: Solvent Accessible Surface Area; PSA: Polar Surface Area.

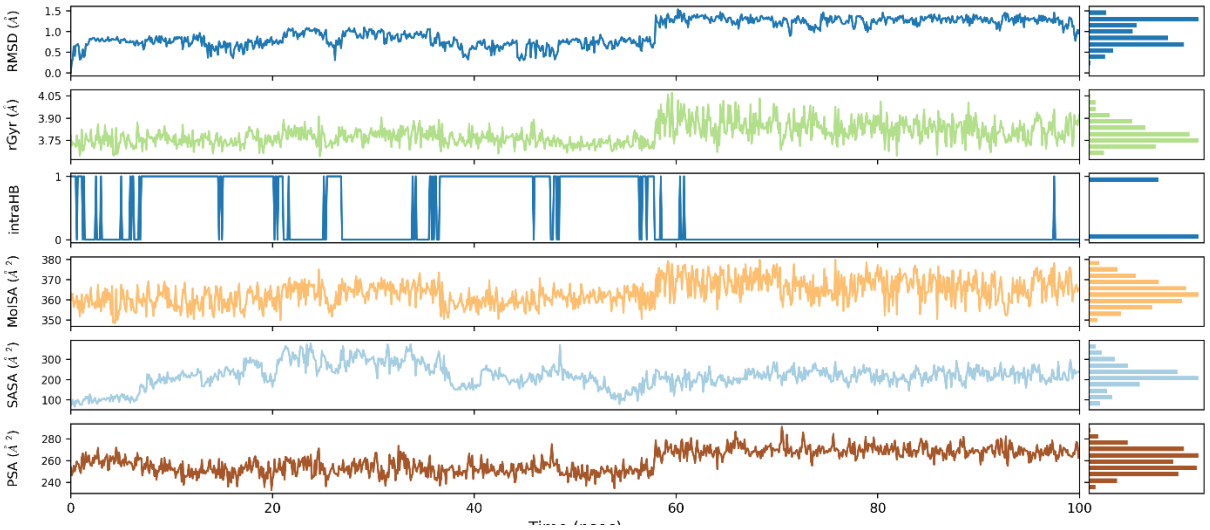

Figure S2e: Ligand H1 property during MD simulation against 4MOT. RMSD: Root mean square deviation of a ligand with respect to the reference conformation; rGyr: Radius of Gyration which measures the 'extendedness' of a ligand; intraHB: Intramolecular Hydrogen Bonds; MolSA: Molecular Surface Area; SASA: Solvent Accessible Surface Area; PSA: Polar Surface Area.

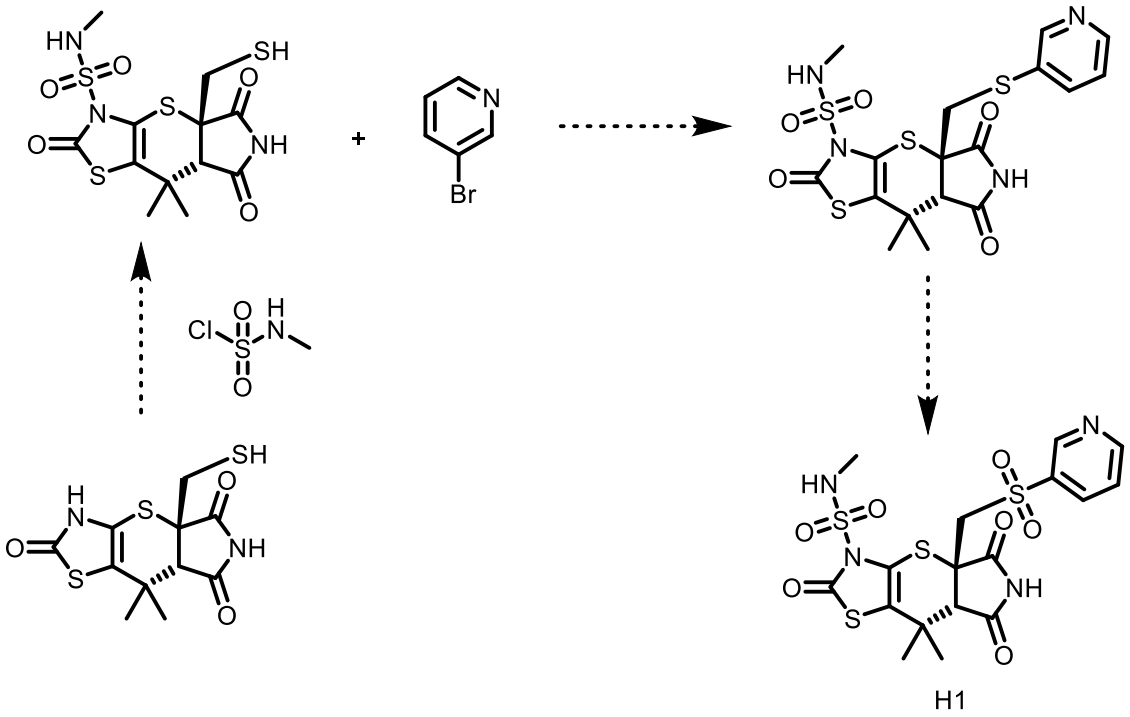

Figure S3: Plausible synthetic scheme of H1