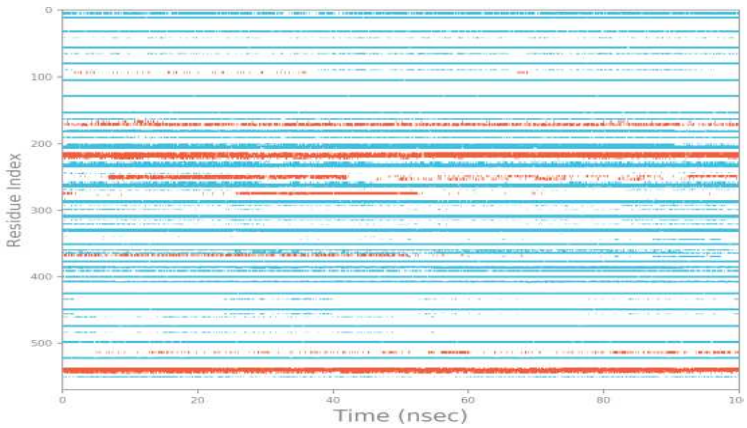
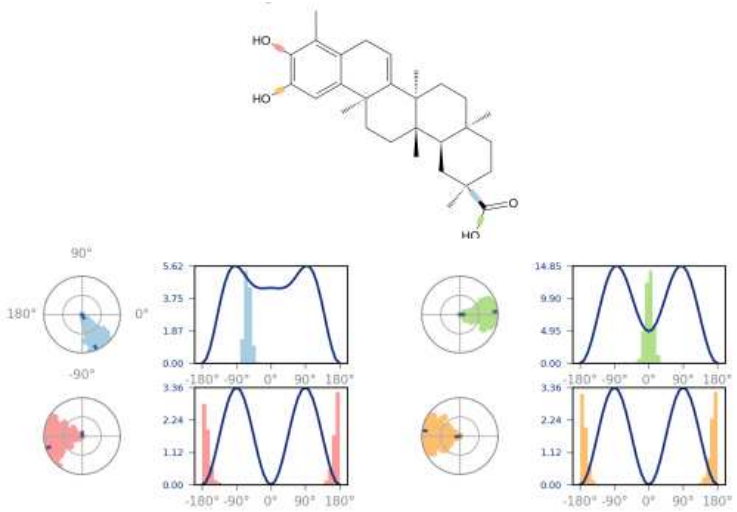
Supplementary documents

Supplementary Table 1: Docking score of compounds in the binding pocket of human TLR4 and hagfish" (PDB ID: 2Z63.pdb).

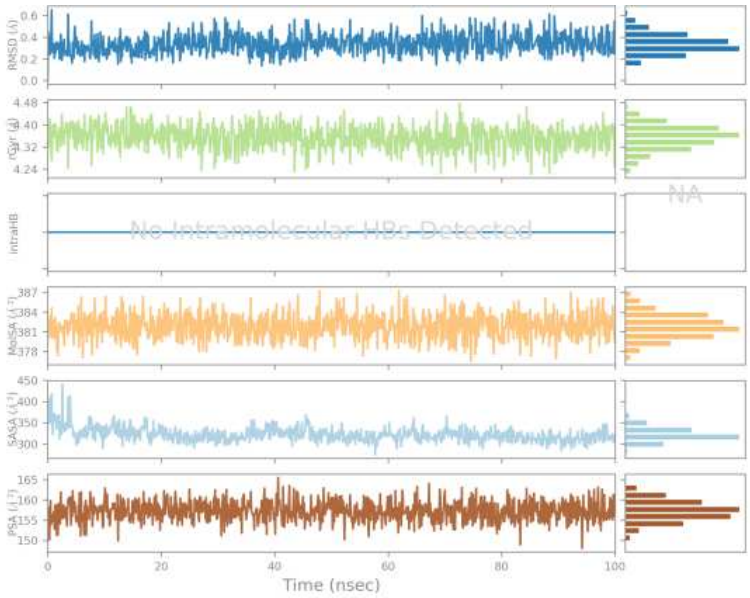
Compounds	Pubchem ID	Docking Score
Adapalene	60164	-7.7
Antrafenine	68723	-7.9
Atractylenolide	155948	-6.5
Cabozantinib	25102847	-7.8
Celastrol	122724	-8.0
Cyclosporin	5284373	-6.4
Difenoxin	34328	-6.7
Epigallocatechin	72277	-7.2
Ergocalciferol	5280793	-7.5
Ferulic_acid	445858	-5.1
Hispidulin	5281628	-6.5
Irinotecan	60838	-7.9
Kaempferol	5280863	-6.4
Lifitegrast	11965427	-8.7
Loteprednol	9865442	-5.7
Lumacaftor	16678941	-8.3
Meclizine	4034	-6.9
Nandrolone	9904	-7.9
Nilotinib	644241	-8.5
Pranlukast	4887	-6.7
Quercetin	5280343	-7.0
Resatorvid	11703255	-5.9
Resveratrol	445154	-5.9
Sparstolonin	135659042	-6.8
Varenicline	170361	-6.0
Vorapaxar	10077130	-7.9
Xanthohumol	639665	-6.3



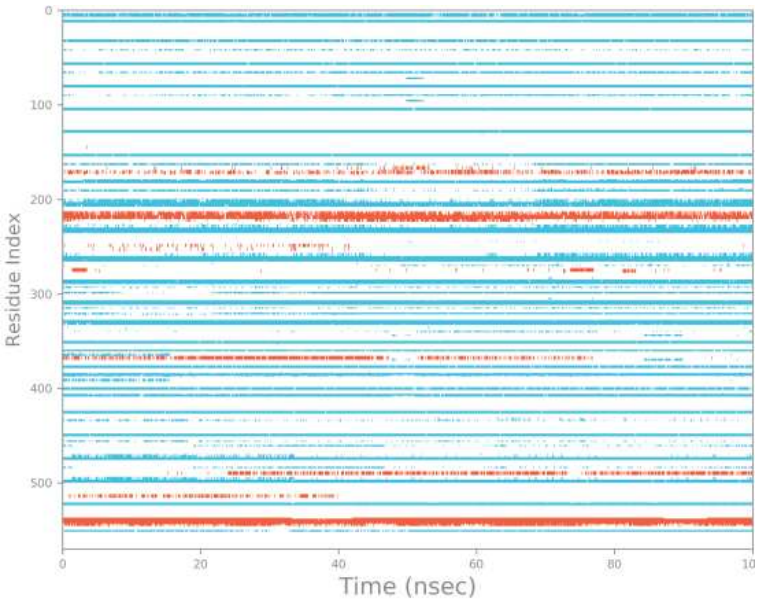
Supplementary Figure1-SSE of 2Z63 in complex with Celastrol.



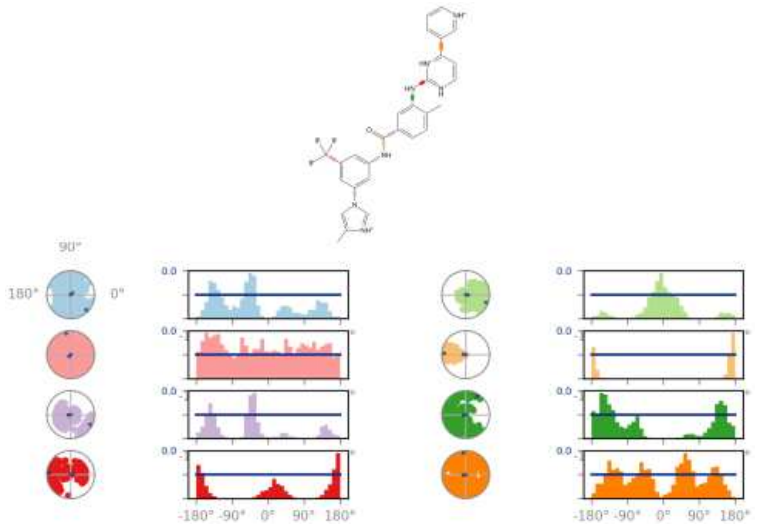
Supplementary Figure2- Ligand Torsion profile of Celastrol



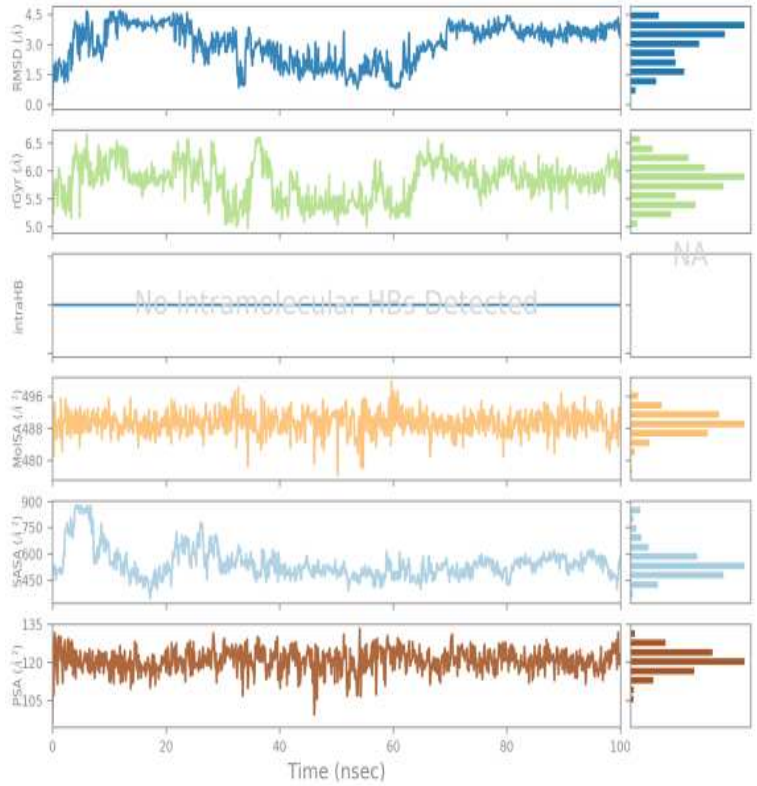
Supplementary Figure3- Ligand properties of Celastrol when complexed with 2Z63.



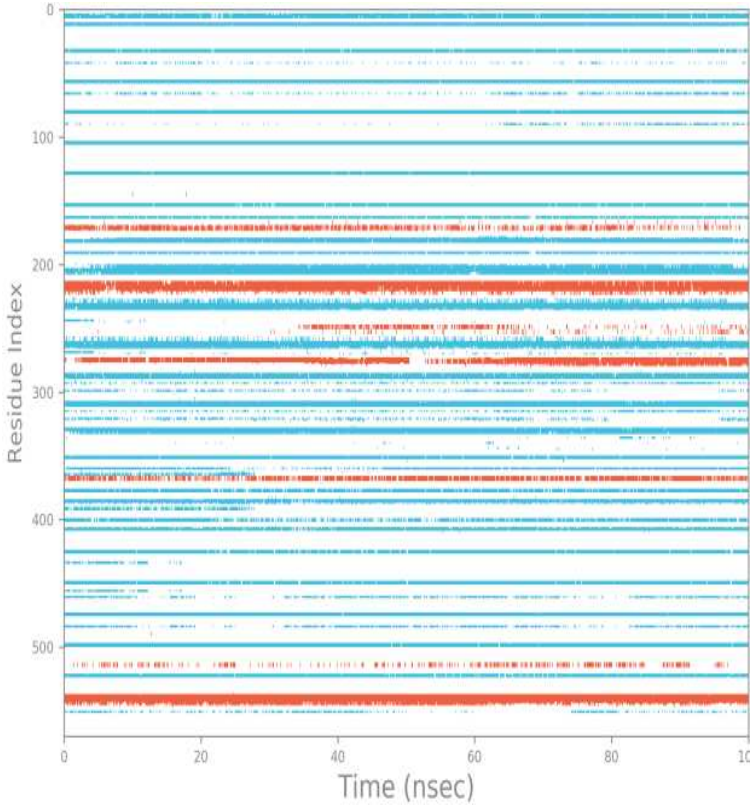
Supplementary Figure4-SSE of 2Z63 in complex with Nilotinib.



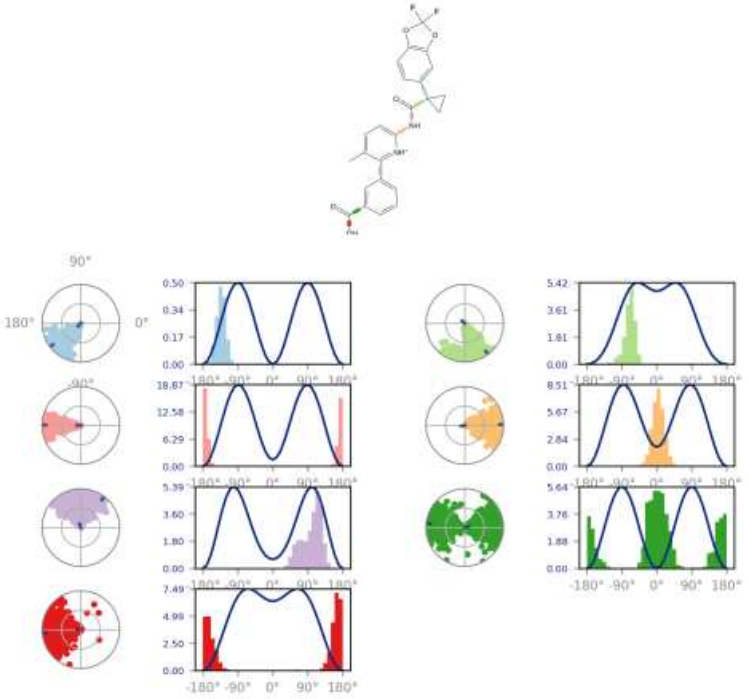
Supplementary Figure5- Ligand Torsion profile of Nilotinib



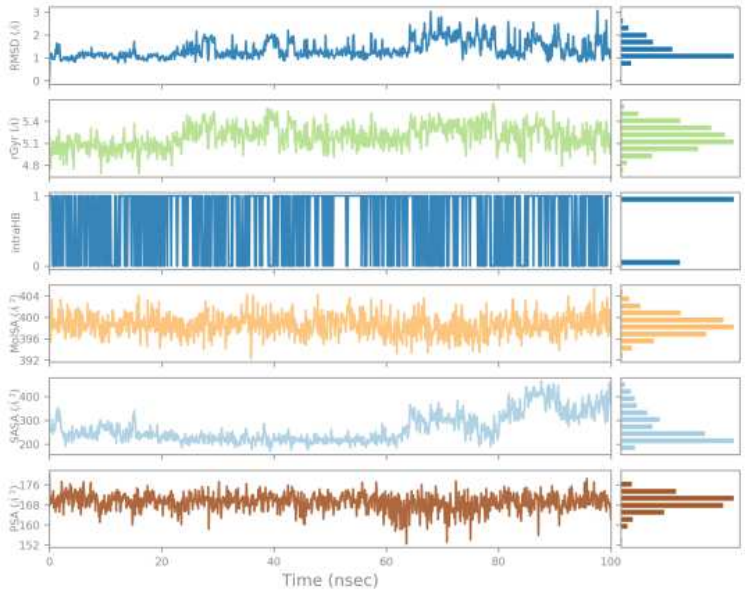
Supplementary Figure6- Ligand properties of Nilotinib when complexed with 2Z63.



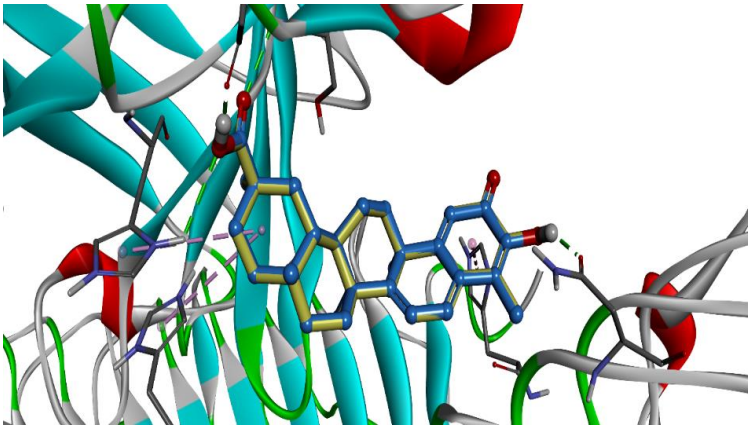
Supplementary Figure7-SSE of 2Z63 in complex with Lumacaftor.



Supplementary Figure8- Ligand Torsion profile of Lumacaftor



Supplementary Figure9- Ligand properties of Lumacaftor when complexed with 2Z63.



Supplementary Figure10- Plot of interaction of celastrol with target protein receptor tlr4 ([DB ID = **2Z63**) the blue color show docking and yellow color show redocking