Table S4. Molecular docking details of ligands interaction with Rbd.

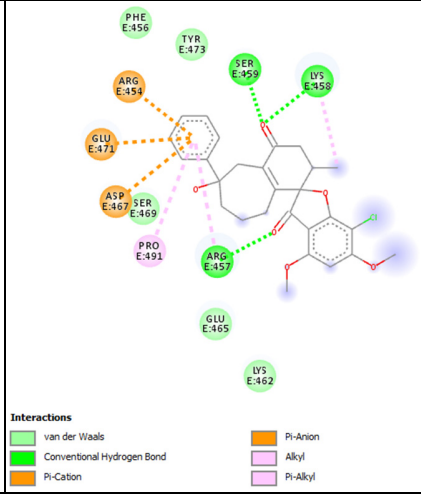
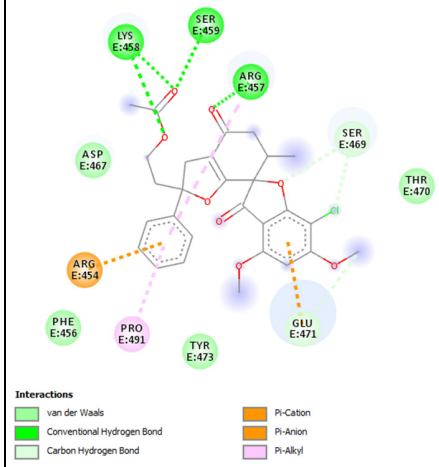
PubChem ID	Binding Energy (kcal/mol)	H-bonds	Hydrophobic interactions	Ligand interaction diagram	Lipinski Analysis	
CID_7331772 (Rb2)	-5.92	ARG 457 LYS 458 SER 459	ARG 454 ARG 457 LYS 458 ASP 467 GLU 471 PRO 491		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	417.5 3.47 0 5 0 Yes No
CID_73330911 (Rb4)	-7.07	ARG 457 LYS 458 SER 459	ARG 454 ARG 457 SER 469 GLU 471 PRO 491		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	526.9 4.27 0 8 1 Yes No

Table S4. Molecular docking details of ligands interaction with Rbd.

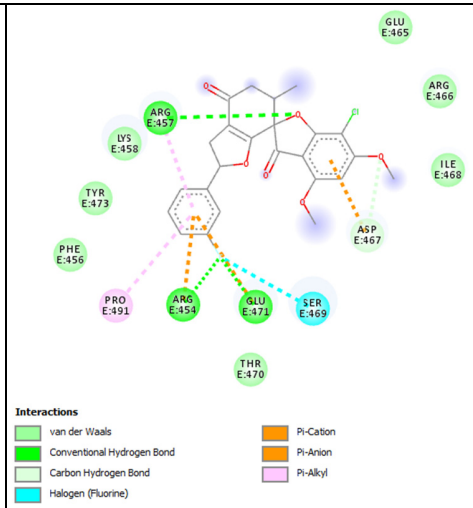
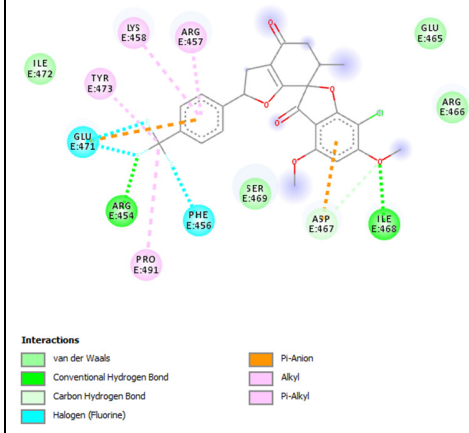
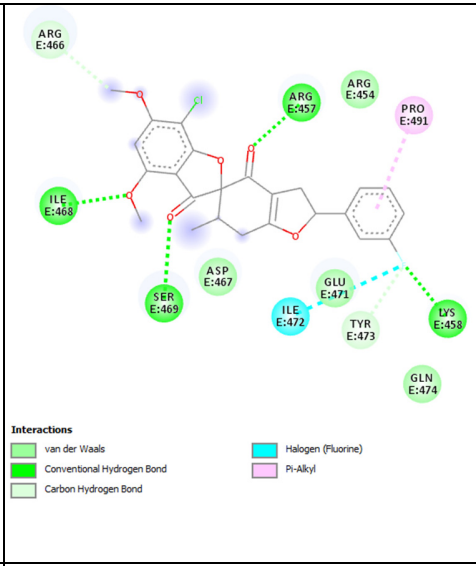
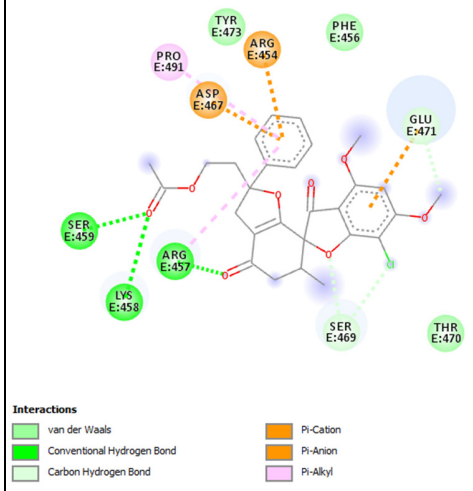
CID_73331346 (Rb5)	-6.08	ARG 454 ARG 457 GLU 471	ARG 454 ARG 457 ASP 467 SER 469 GLU 471 PRO 491		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	458.8 3.73 0 7 0 Yes No
CID_73331488 (Rb6)	-5.49	ILE 468 ARG 454	PHE 456 ARG 457 LYS 458 ASP 467 GLU 471 TYR 473 PRO 491		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	508.8 4.00 0 9 1 Yes No

Table S4. Molecular docking details of ligands interaction with Rbd.

CID_118254214 (Rb7)	-6.68	ARG 457 LYS 458 ILE 468 SER 469	ARG 466 ILE 472 TYR 473 PRO 491		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	458.8 3.83 0 7 0 Yes No
CID_118263246 (Rb8)	-7.02	ARG 457 LYS 458 SER 459	ARG 454 ARG 457 ASP 467 SER 469 GLU 471 PRO 491		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	526.9 4.27 0 8 1 Yes No