

Table S5. Molecular docking details of ligands interaction with RdRp.

PubChem ID	Binding Energy (kcal/mol)	H- bonds	Hydrophobic interactions	Ligand interaction diagram	Lipinski Analysis	
CID_56924747 (Rd1)	-6.48	CYS 622	ASP 761 Glu 811 CYS 813	<p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Sulfur 	Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	478.9 3.68 0 6 0 Yes No
CID_46844082 (Rd3)	-6.58	LYS 551 TYR 619 LYS 621	ASP 618 CYS 622 LYS 798	<p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Pi-Sigma Alkyl Pi-Alkyl 	Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	641.1 5.51 0 8 2 Yes No

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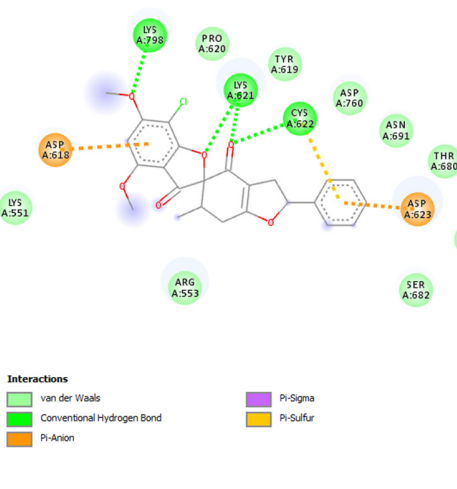
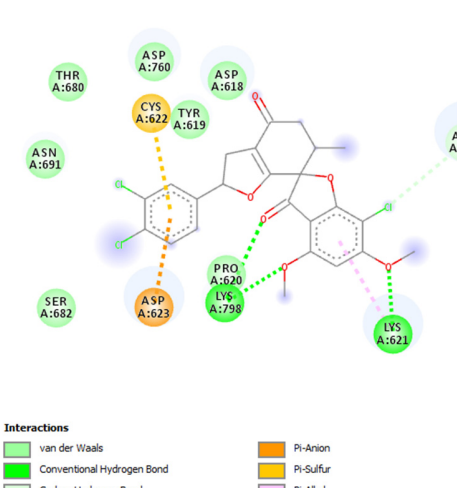
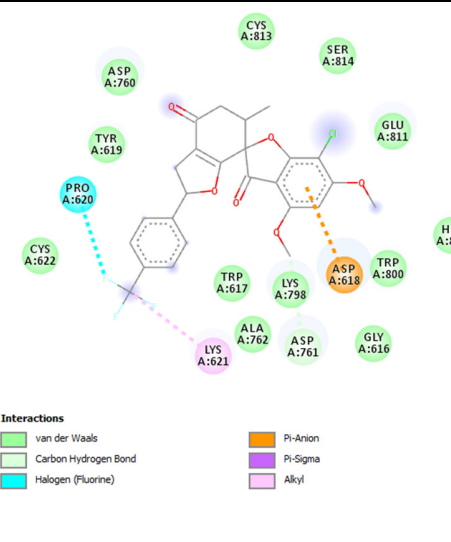
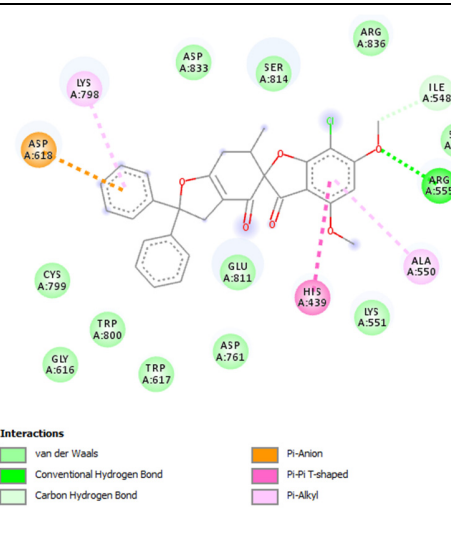
CID_118254216 (Rd4)	-6.62	LYS 621 CYS 622 LYS 798	ASP 618 CYS 622 ASP 623	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Pi-Anion Pi-Sigma Pi-Sulfur 	Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	440.8 3.65 0 6 0 Yes No
CID_73331060 (Rd5)	-6.87	LYS 621 LYS 798	LYS 621 CYS 622 ASP 623	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Anion Pi-Sulfur Pi-Alkyl 	Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	509.7 4.09 0 6 1 Yes No

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CID_73331487 (Rd8)	-6.01	-	ASP 618 PRO 620 LYS 621 ASP 761	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Carbon Hydrogen Bond Halogen (Fluorine) Pi-Anion Pi-Sigma Alkyl 	Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	508.8 4.01 0 9 1 Yes No
CID_73330763 (Rd9)	-6.84	ARG 555	HIS 439 ILE 548 ALA 550 ASP 618 LYS 798	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Anion Pi-Pi T-shaped Pi-Alkyl 	Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	516.9 4.22 0 6 1 Yes No