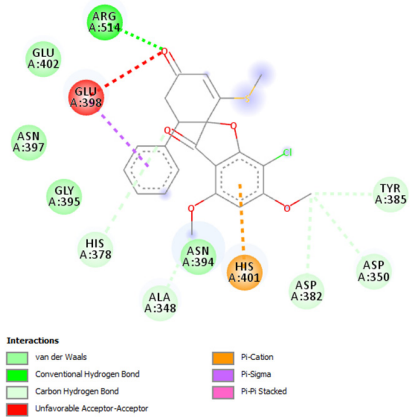
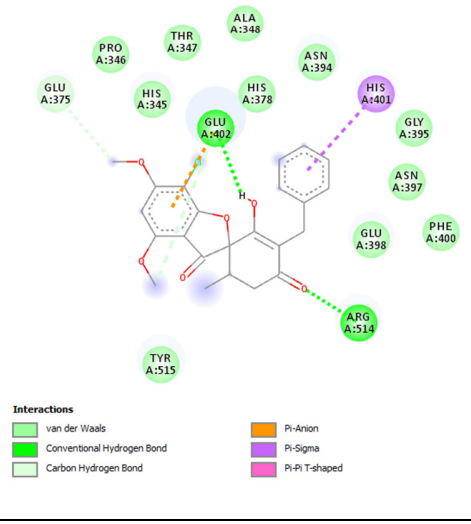
Table S3. Molecular docking details of ligands interaction with ACE2.

PubChem ID	Binding Energy (kcal/mol)	H- bonds	Hydrophobic interactions	Ligand interaction diagram	Lipinski Analysis	
CID_10574693 (A1)	-6.66	ARG 514	ALA 348 ASP 350 HIS 378 ASP 382 TYR 385 ASN 394 GLU 398 HIS 401		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	430.9 3.39 0 5 0 Yes No
CID_44566075 (A2)	-5.85	GLU 402 ARG 514	GLU 375 HIS 401 GLU 402		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	428.8 3.25 1 6 0 Yes No

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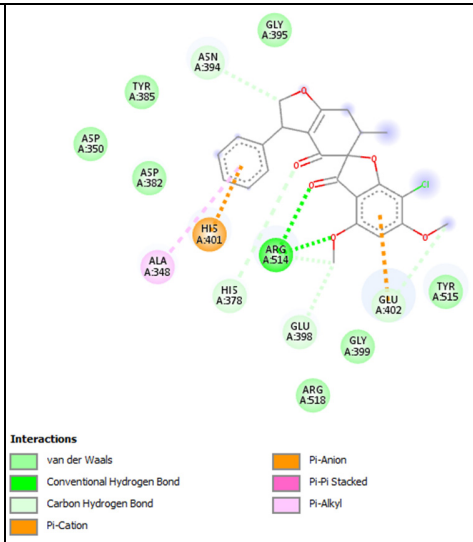
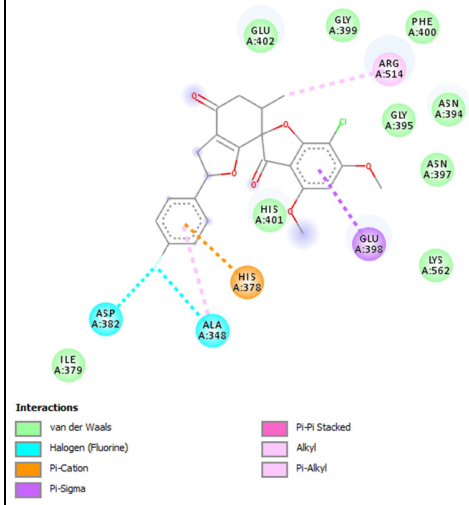
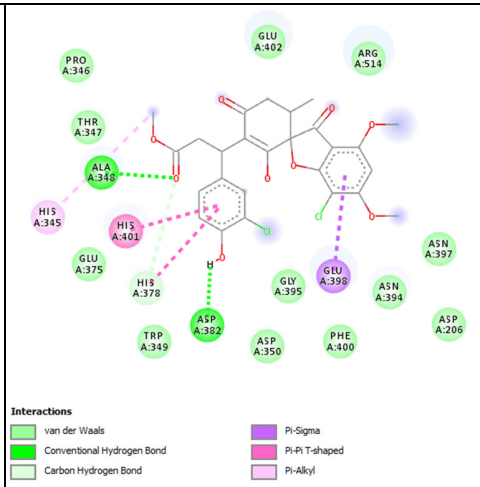
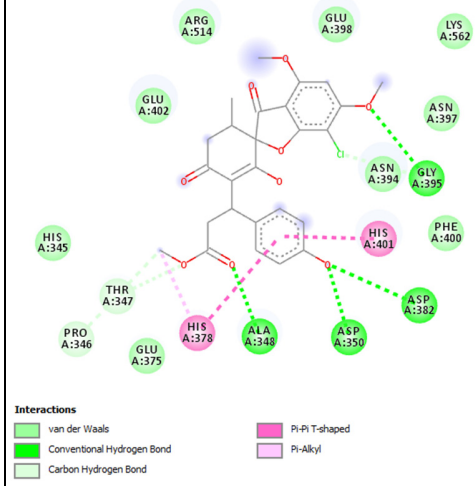
CID_118254131 (A4)	-5.74	ARG 514	ALA 348 HIS 378 ASN 394 GLU 398 HIS 401 GLU 402 ARG 514		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	440.8 3.58 0 6 0 Yes No
CID_118254232 (A5)	-6.30	-	ALA 348 HIS 378 ASP 382 GLU 398 ARG 514		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	458.8 3.76 0 7 0 Yes No

Table S3. Molecular docking details of ligands interaction with ACE2.

CID_129895222 (A6)	-6.55	ALA 348 ASP 382	HIS 345 HIS 378 GLU 398 HIS 401		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	551.37 3.61 2 9 1 Yes No
CID_132286067 (A8)	-6.57	ALA 348 ASP 350 ASP 382 GLY 395	PRO 346 THR 347 HIS 378 HIS 401		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	516.9 3.52 2 9 1 Yes No