Table S2. Molecular docking details of ligands interaction with Mprotease (6LU7).

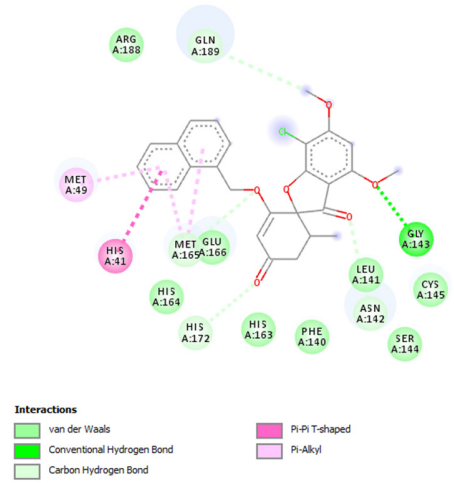
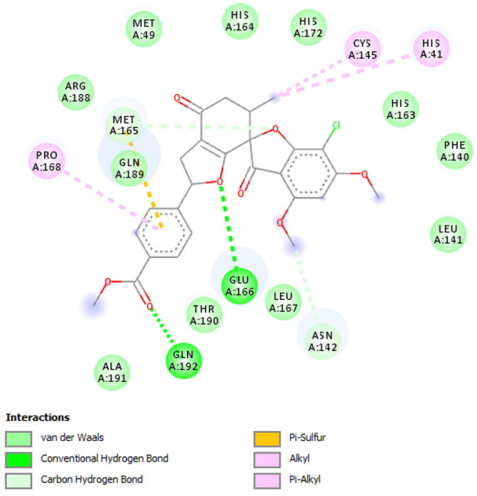
PubChem ID	Binding Energy (kcal/mol)	H-bonds	Hydrophobic interactions	Ligand interaction diagram	Lipinski Analysis	
CID_25171849 (M2)	-8.86	GLY 143	HIS 41 MET 49 LEU 141 MET 165 GLU 166 HIS 172 GLN 189		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	478.9 3.29 0 6 0 Yes No
CID_73330910 (M3)	-8.65	GLU 166 GLN 192	HIS 41 ASN 142 CYS 145 MET 165 PRO 168 GLN 189		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	498.9 4.08 0 8 0 Yes No

Table S2. Molecular docking details of ligands interaction with Mprotease (6LU7).

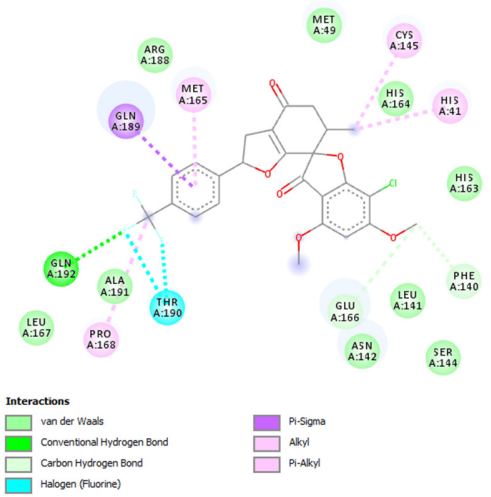
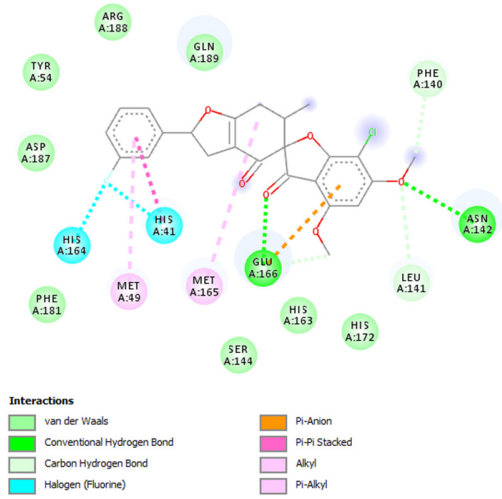
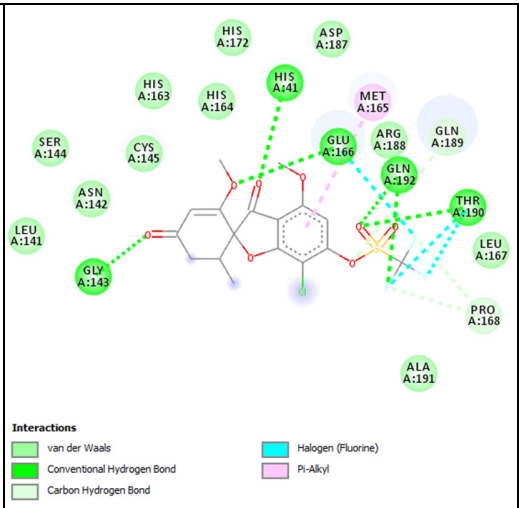
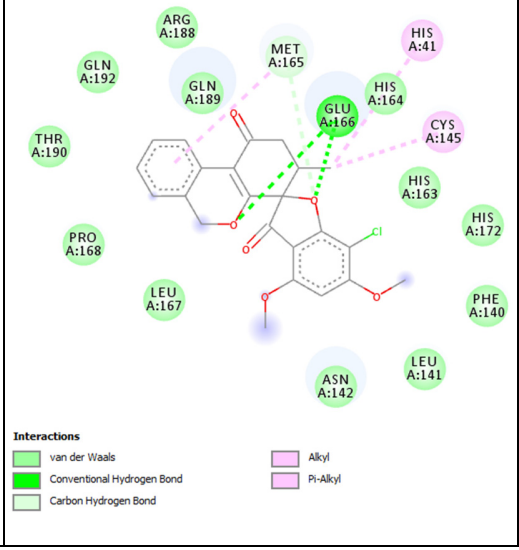
CID_73331488 (M4)	-8.08	GLN 192	HIS 41 PHE 140 CYS 145 MET 165 GLU 166 PRO 168 GLN 189 THR 190 ALA 191		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	508.8 4.00 0 9 1 Yes No
CID_118254214 (M5)	-8.09	ASN 142 GLU 166	HIS 41 MET 49 PHE 140 LEU 141 HIS 164 MET 165 GLU 166		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

Table S2. Molecular docking details of ligands interaction with Mprotease (6LU7).

CID_138490235 (M6)	-7.76	HIS 41 GLY 143 GLU 166 THR 190 GLN 192	MET 165 GLU 166 PRO 168 GLN 189 THR 190		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	470.8 2.84 0 11 1 Yes No
CID_118254145 (M8)	-8.28	GLU 166	HIS 41 CYS 145 MET 165		Molecular weight (<500 Da) Lipophilicity (LogP<5) H bond donor (<5) H bond acceptor (<10) Violations Lipinski Hepatotoxicity	426.85 3.45 0 6 0 Yes No