Supplementary Information For

Design, Synthesis and Biological Exploration of Novel *N*-(9-Ethyl-9*H*-Carbazol-3-yl)Acetamide Linked Benzofuran-1,2,4-Triazoles as Anti-SARS-CoV-2 Agents: Combined Wet/Dry Approach Targeting Main Protease (M^{pro}), Spike Glycoprotein and RNA Dependent RNA Polymerase (RdRp)

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1- NMR Spectra of compounds 9a-j

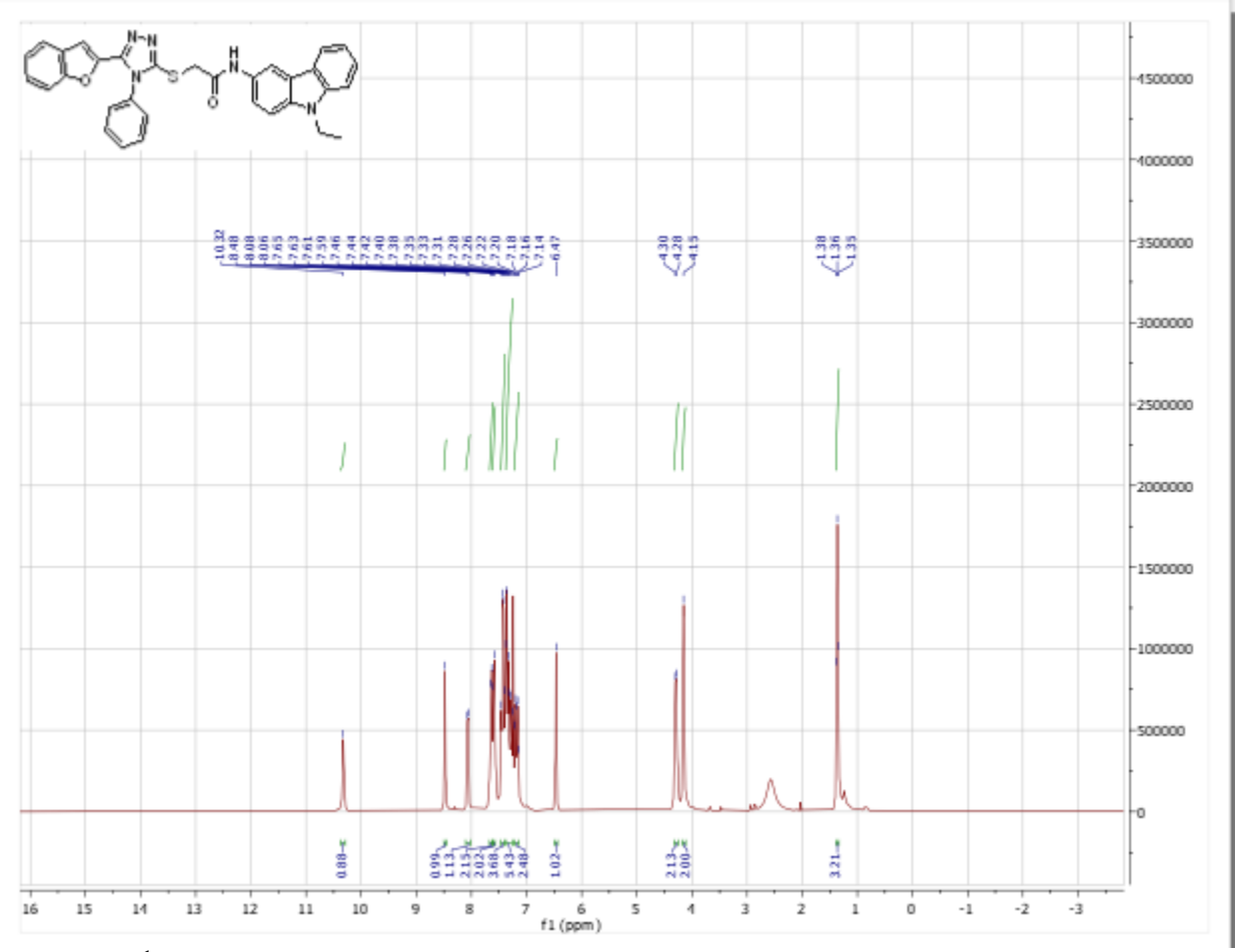


Figure S1: ^{1}H NMR of compound **9a**.

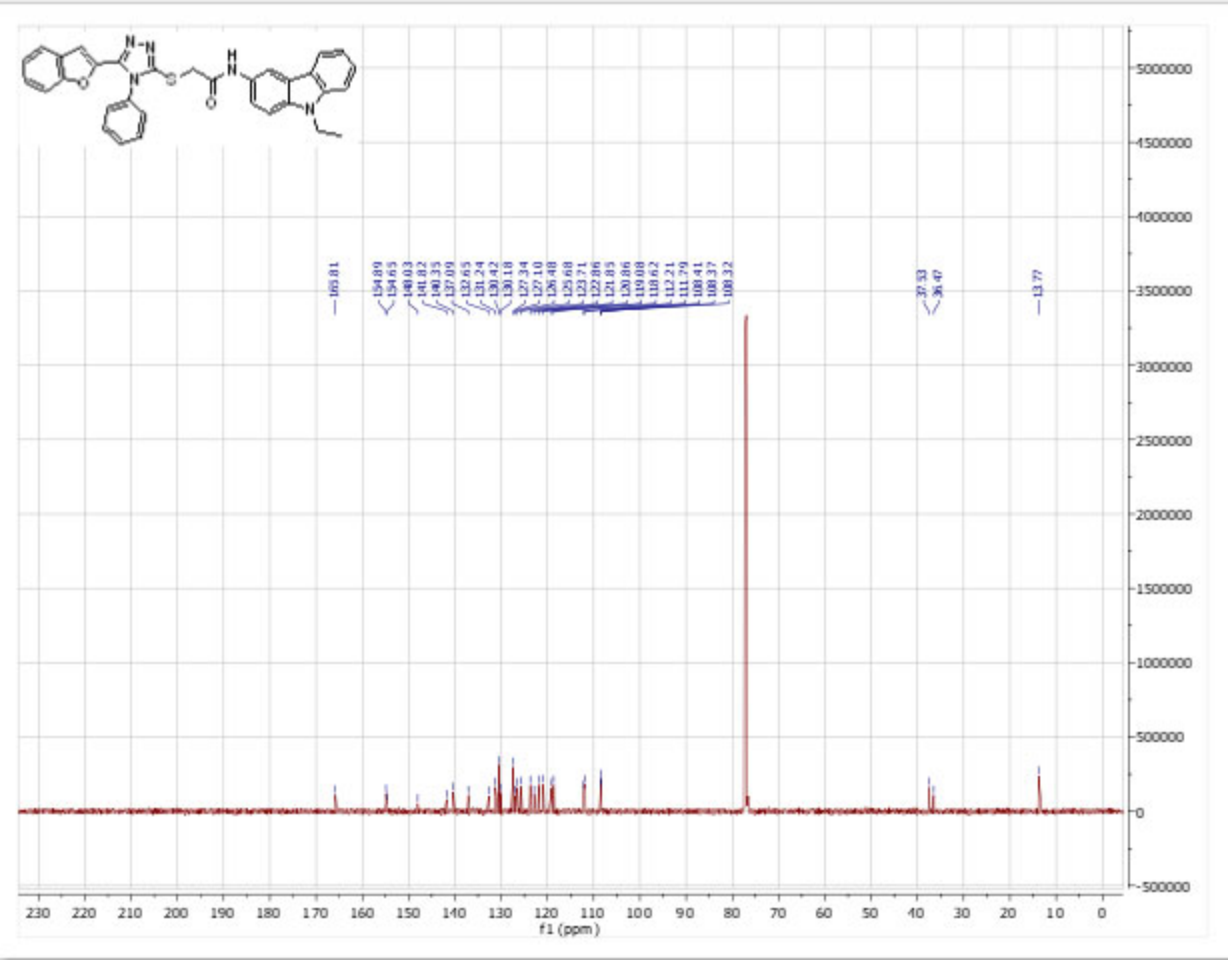


Figure S2: ^{13}C NMR of compound **9a**.

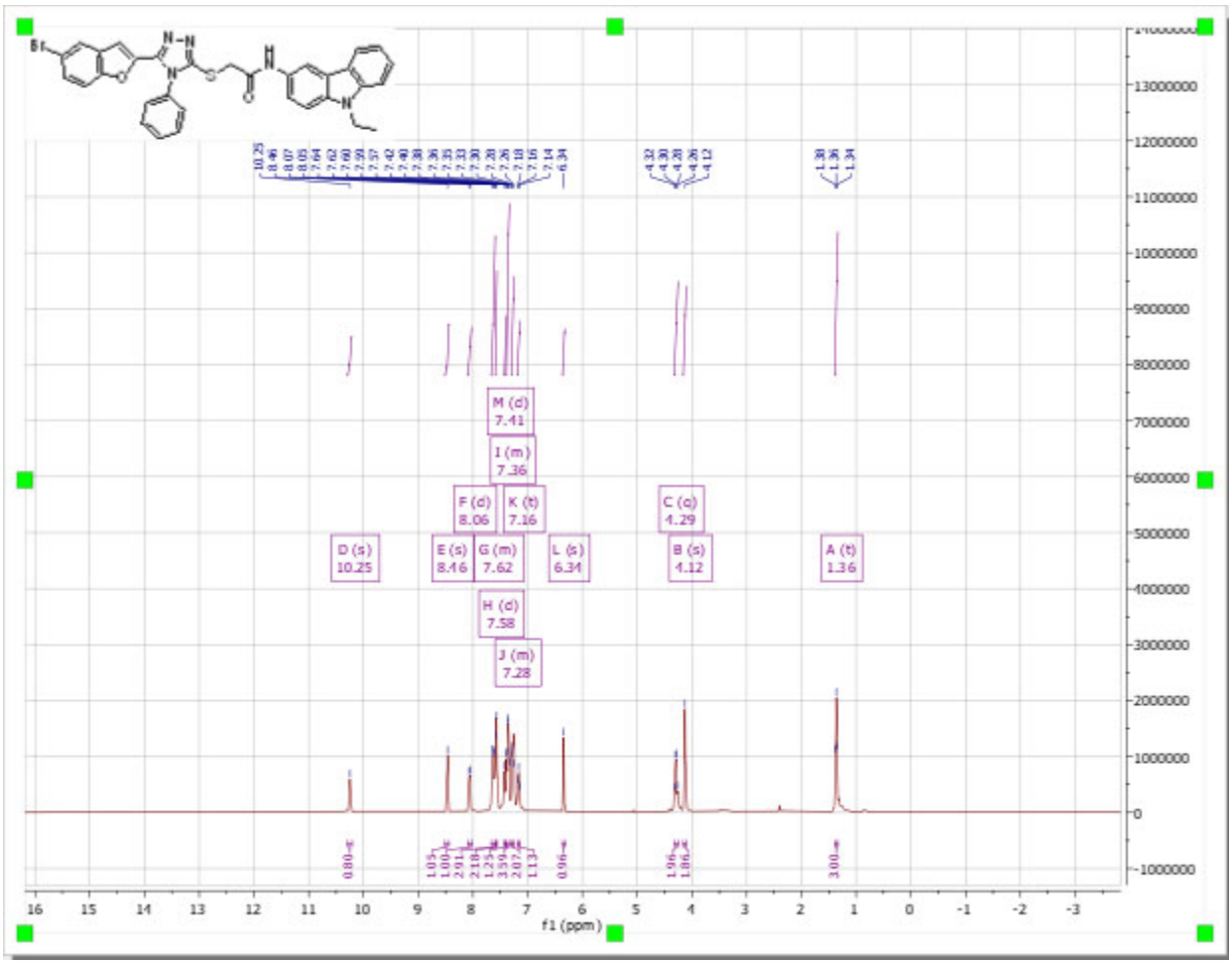


Figure S3: ^{1}H NMR of compound **9b**.

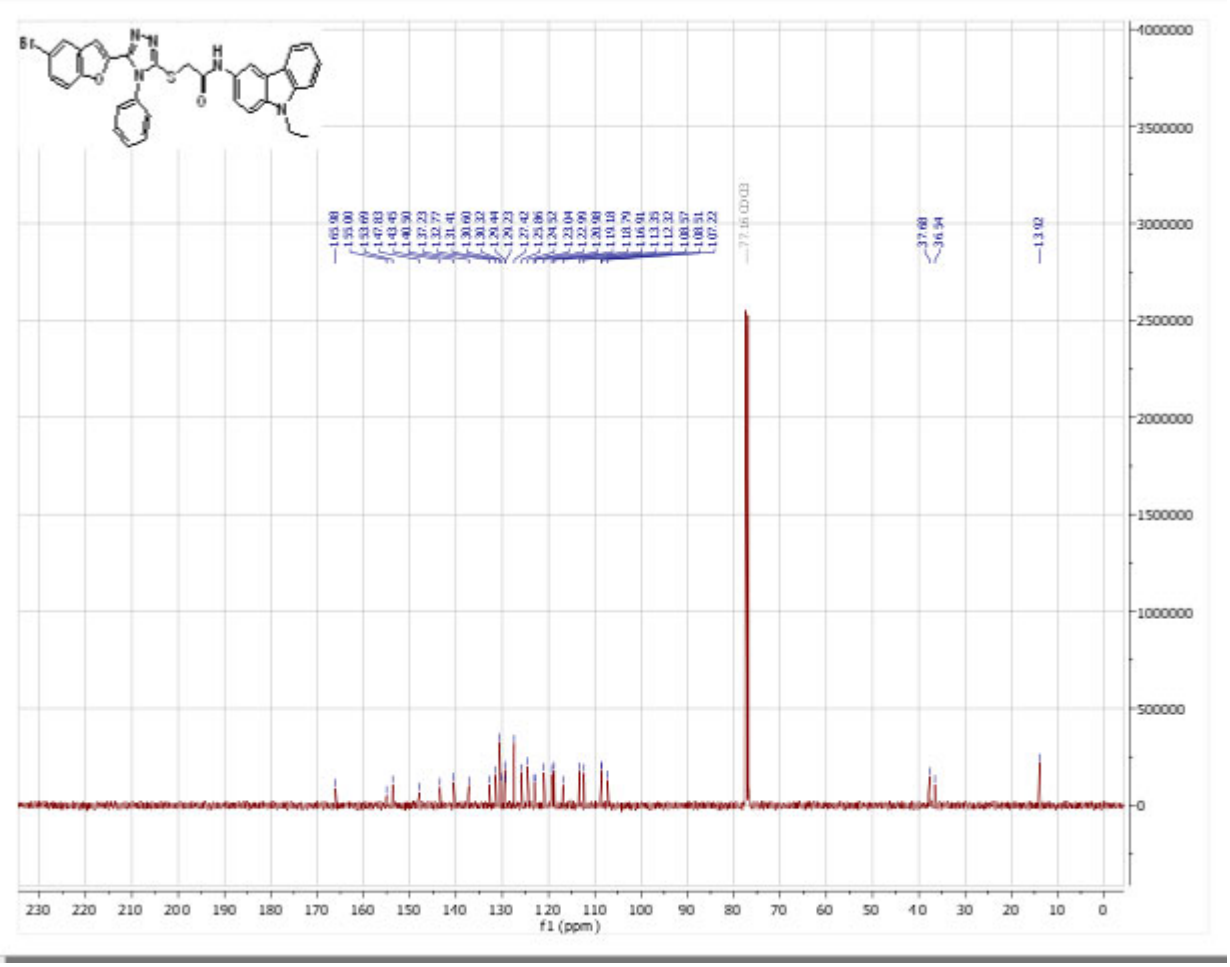


Figure S4: ^{13}C NMR of compound **9b**.

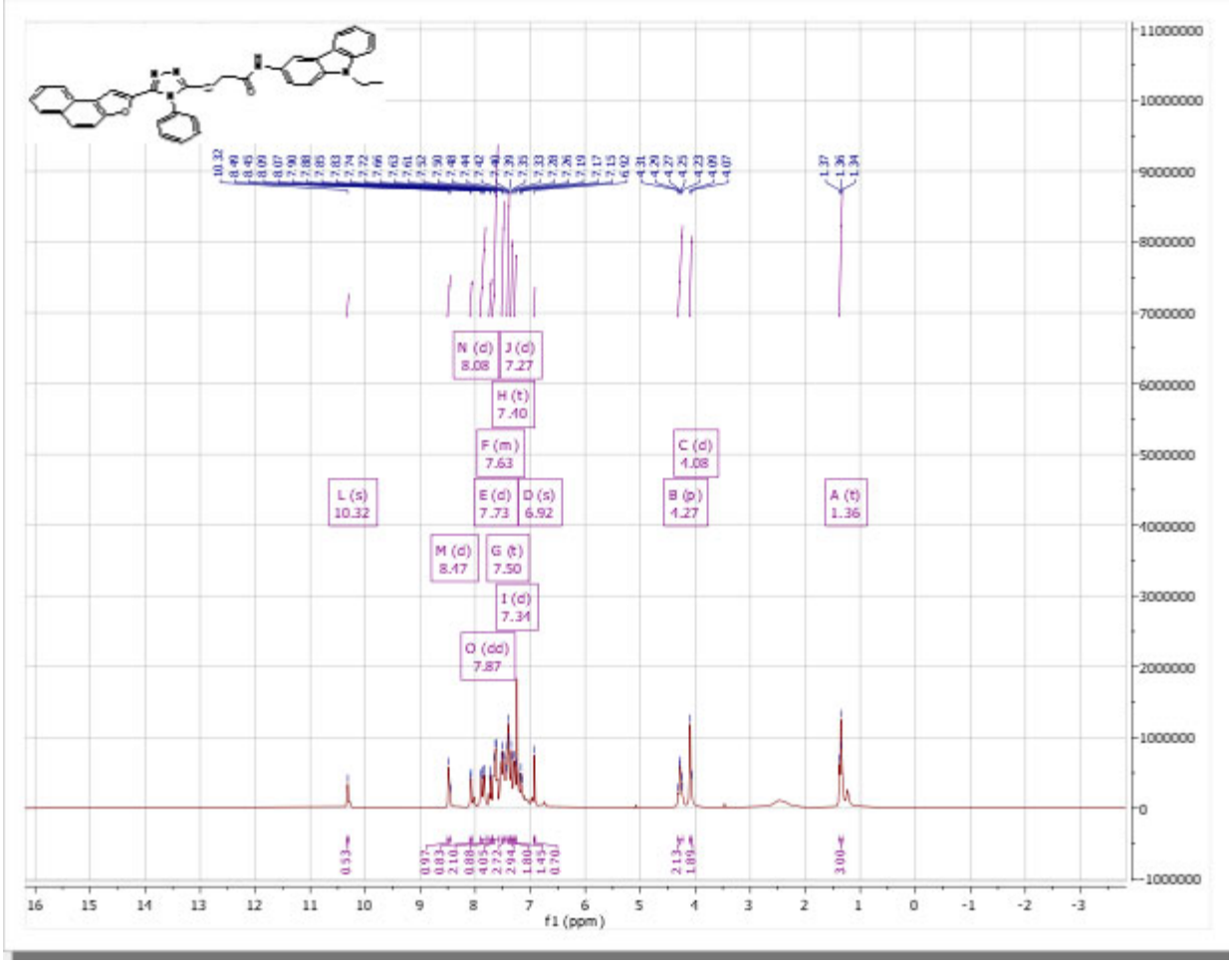


Figure S5: ^{1}H NMR of compound **9c**.

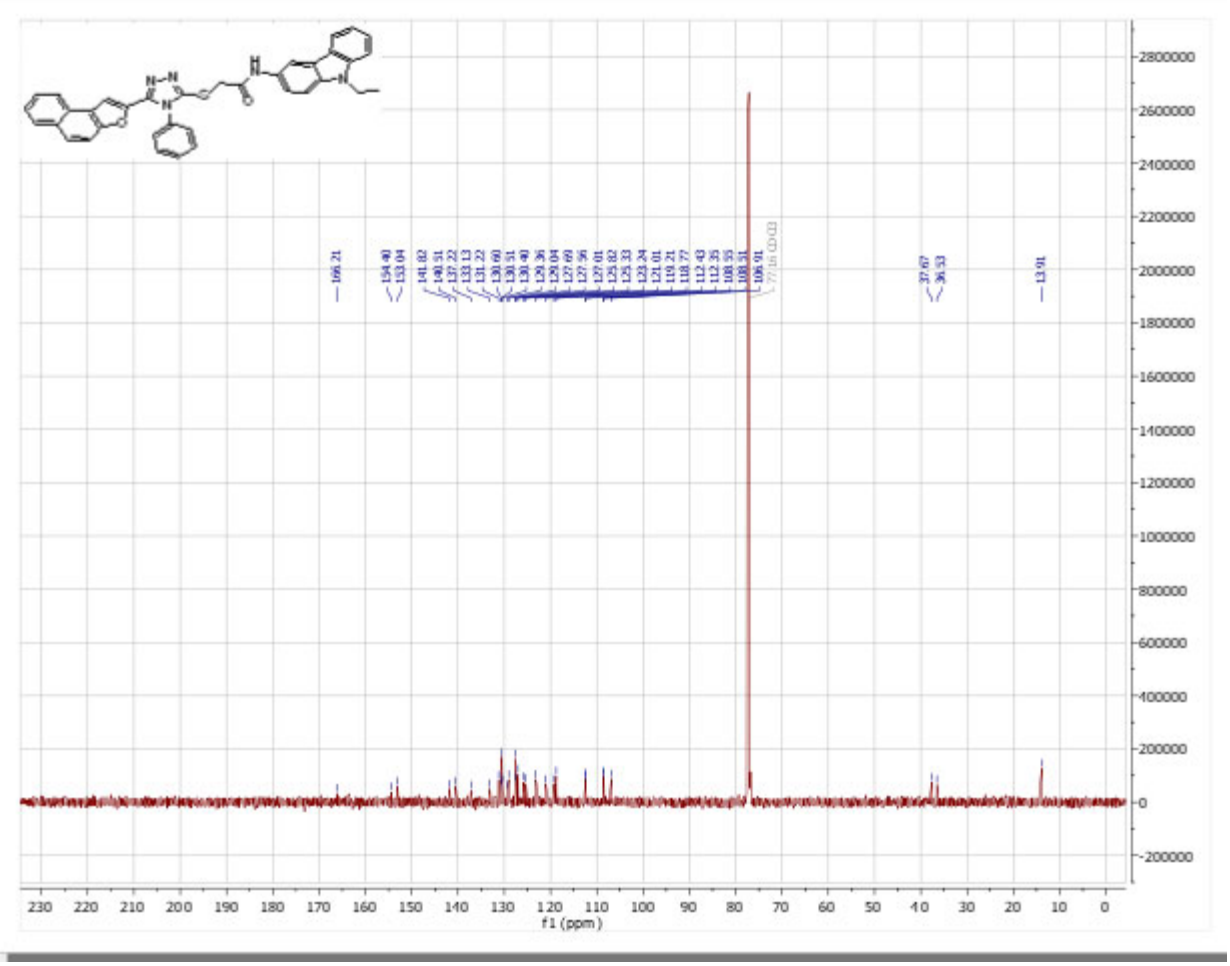


Figure S6: ^{13}C NMR of compound **9c**.

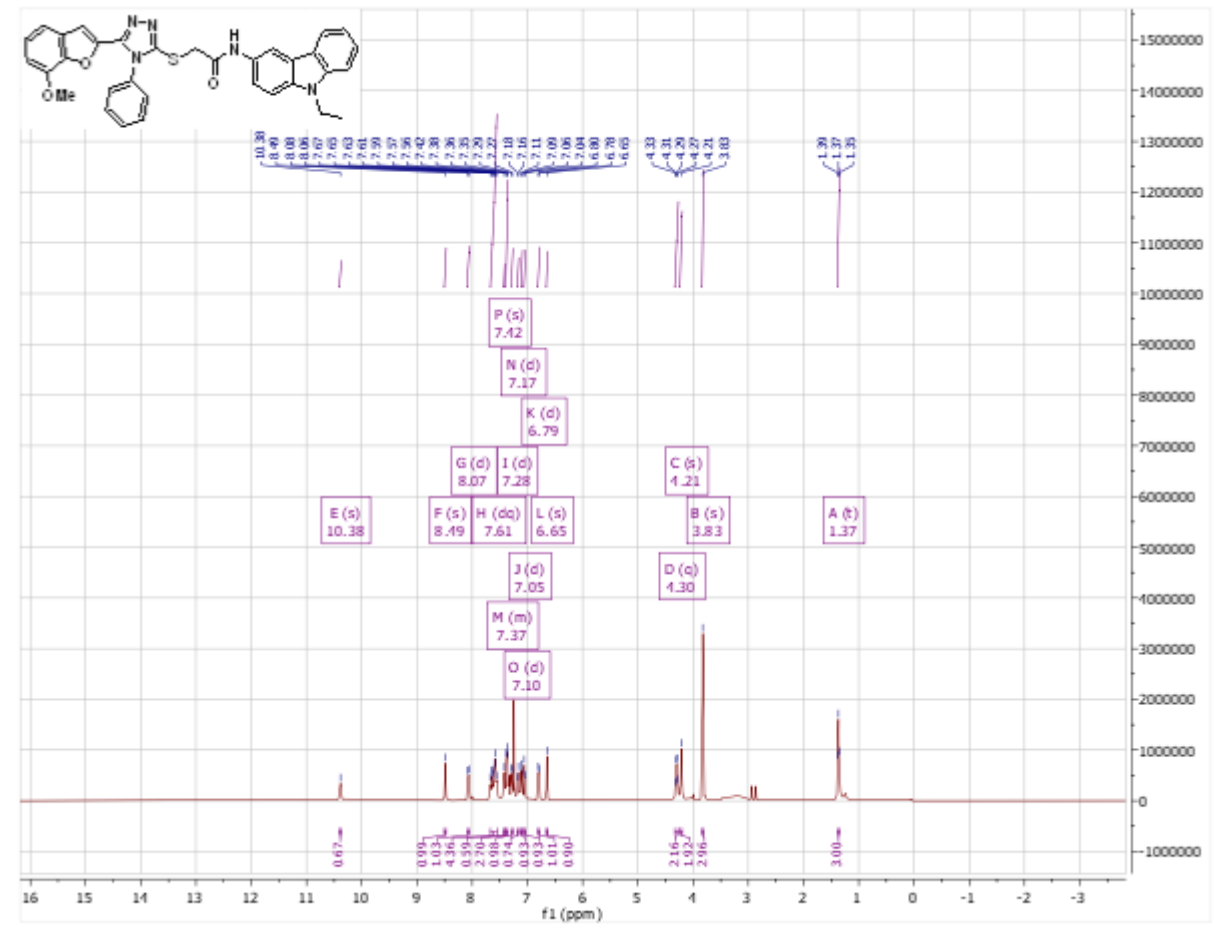


Figure S7: ^{1}H NMR of compound **9d**.

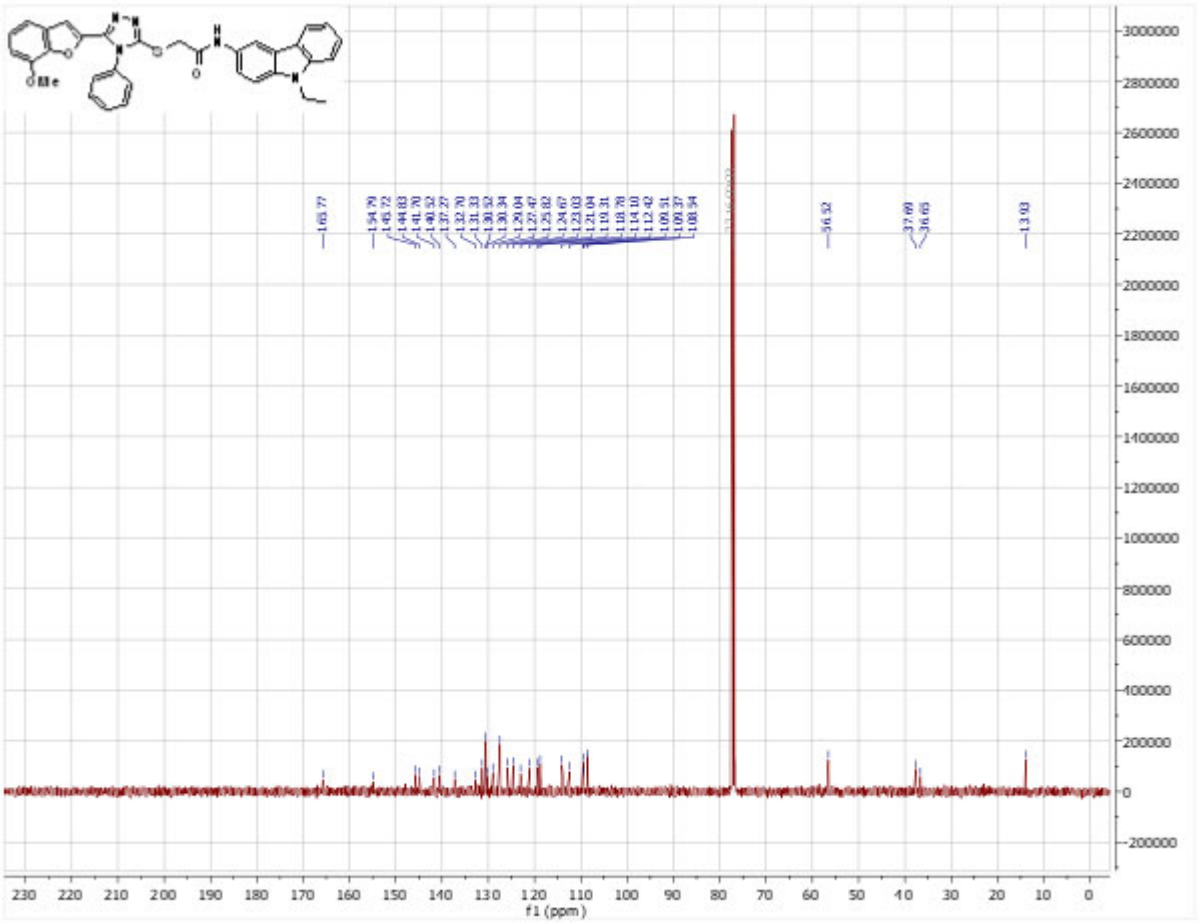


Figure S8: ^{13}C NMR of compound **9d**.

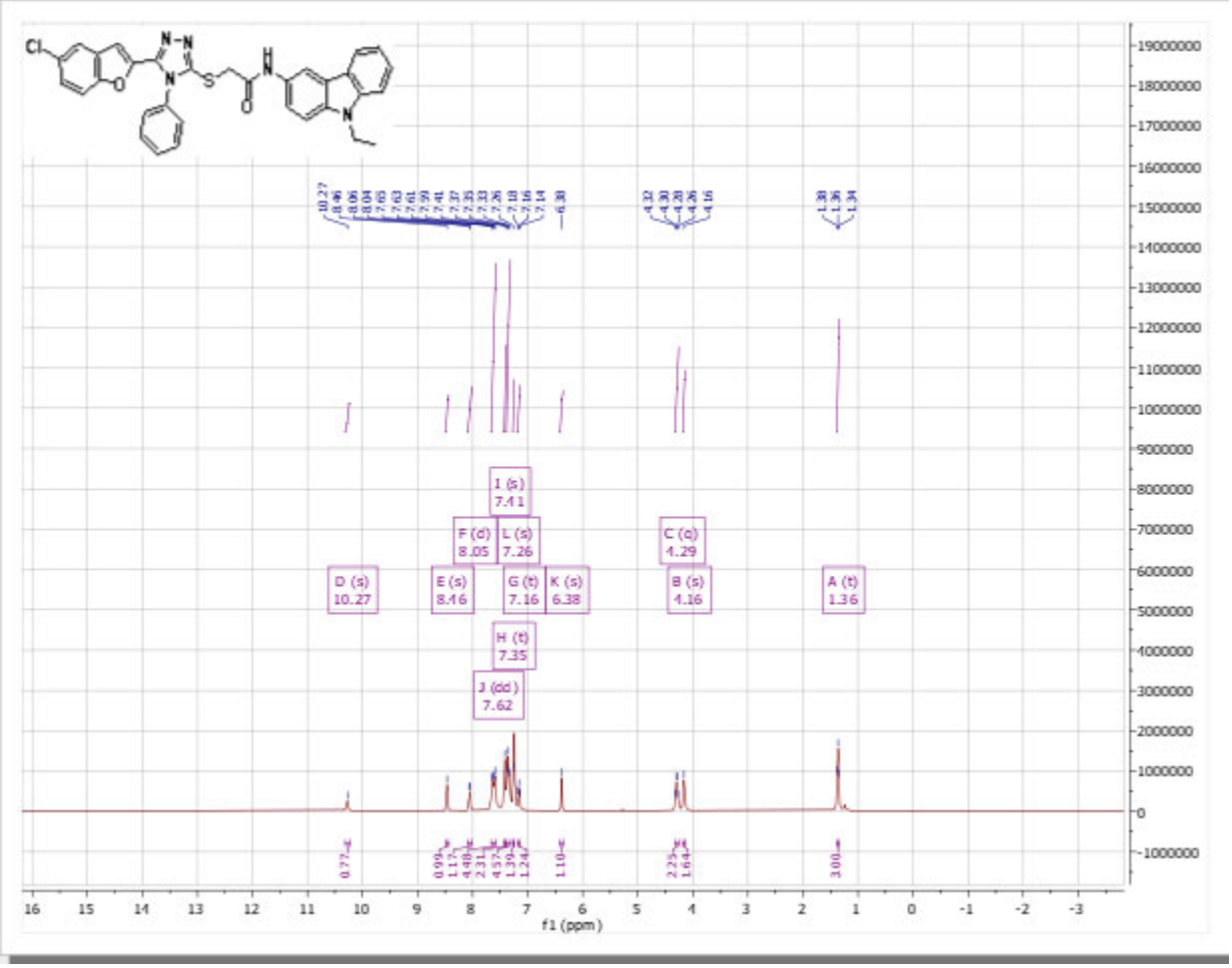


Figure S9: ^{1}H NMR of compound **9e**.

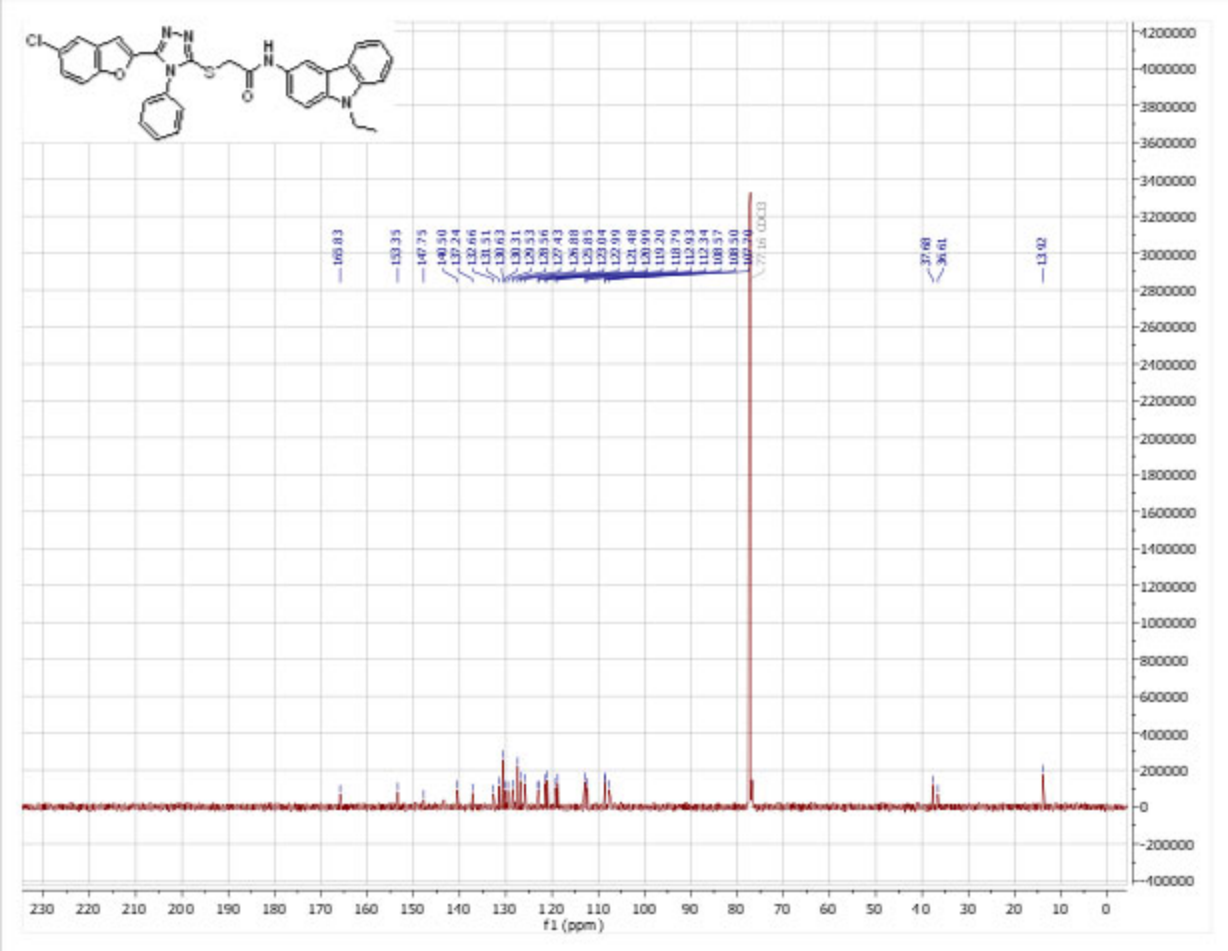


Figure S10: ^{13}C NMR of compound **9e**.

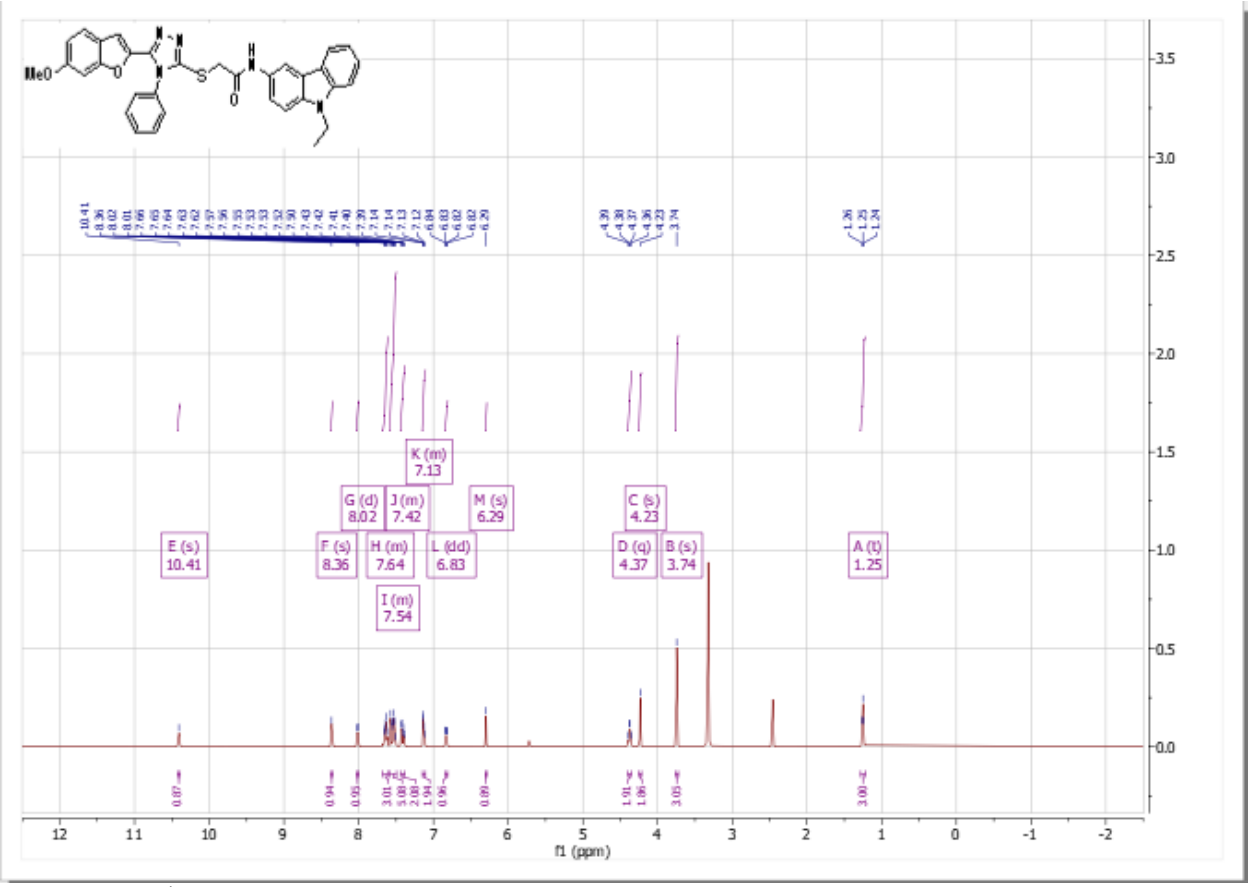


Figure S11: ^{1}H NMR of compound **9f**.

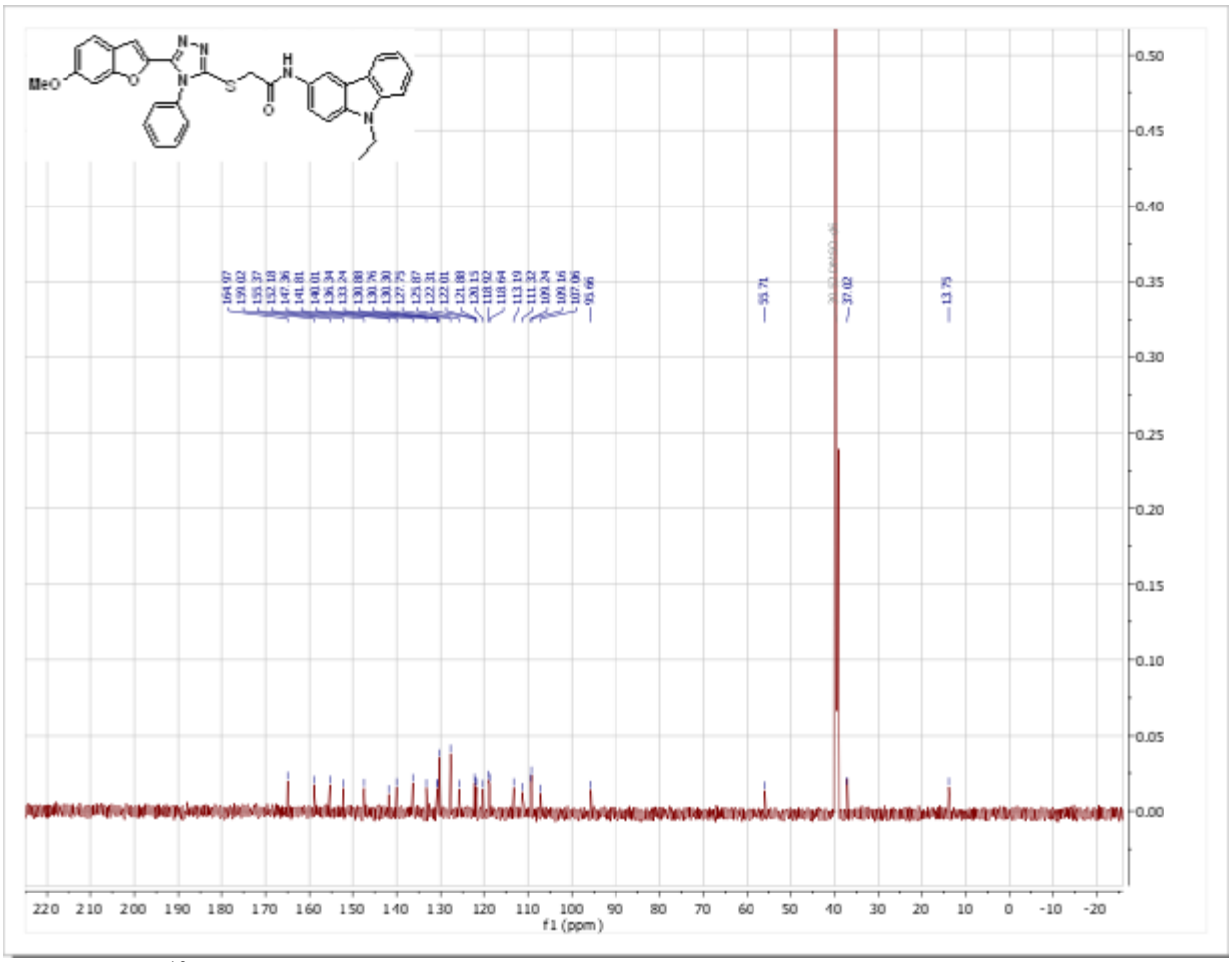


Figure S12: ^{13}C NMR of compound **9f**.

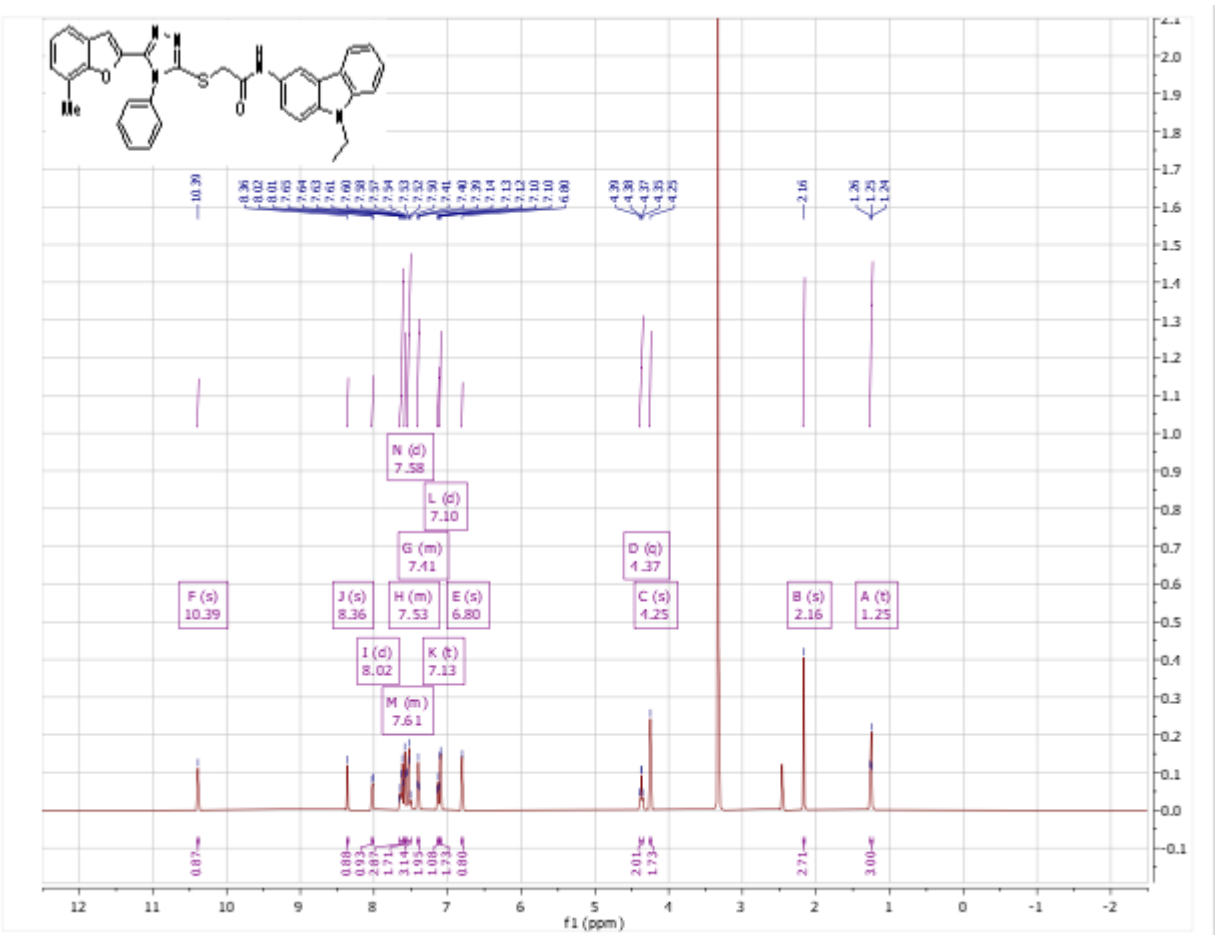


Figure S13: ^{1}H NMR of compound **9g**.

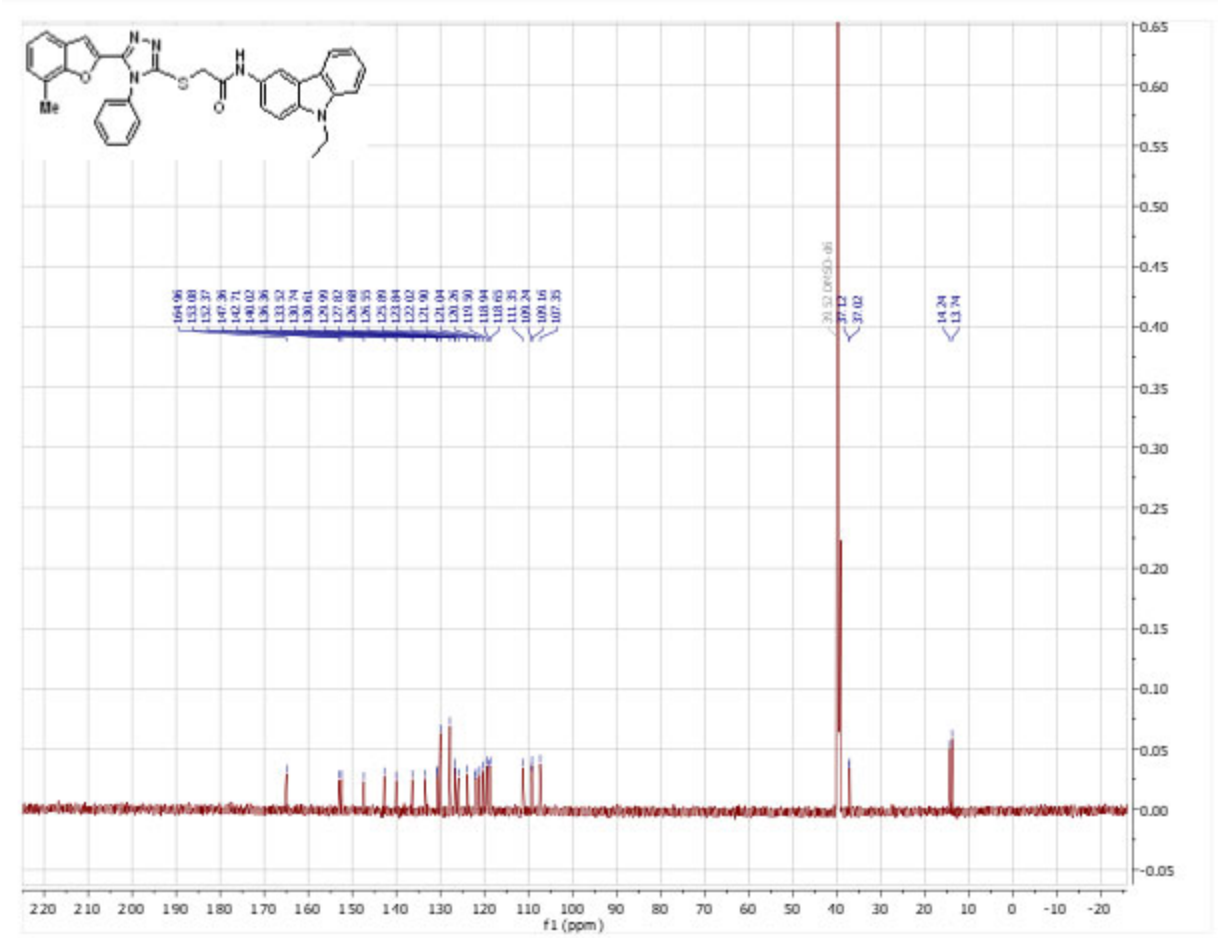


Figure S14: ^{13}C NMR of compound **9g**.

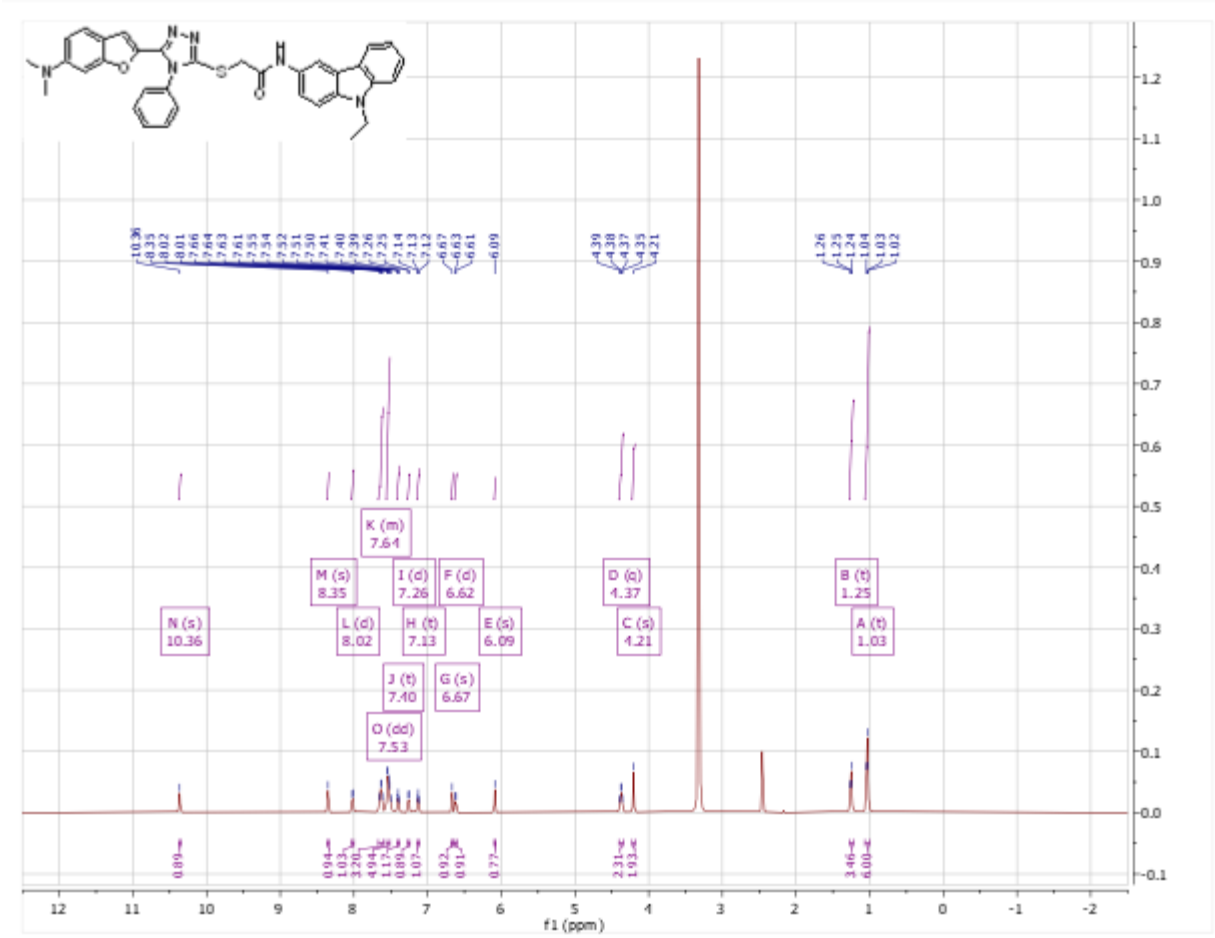


Figure S15: ^{1}H NMR of compound **9h**.

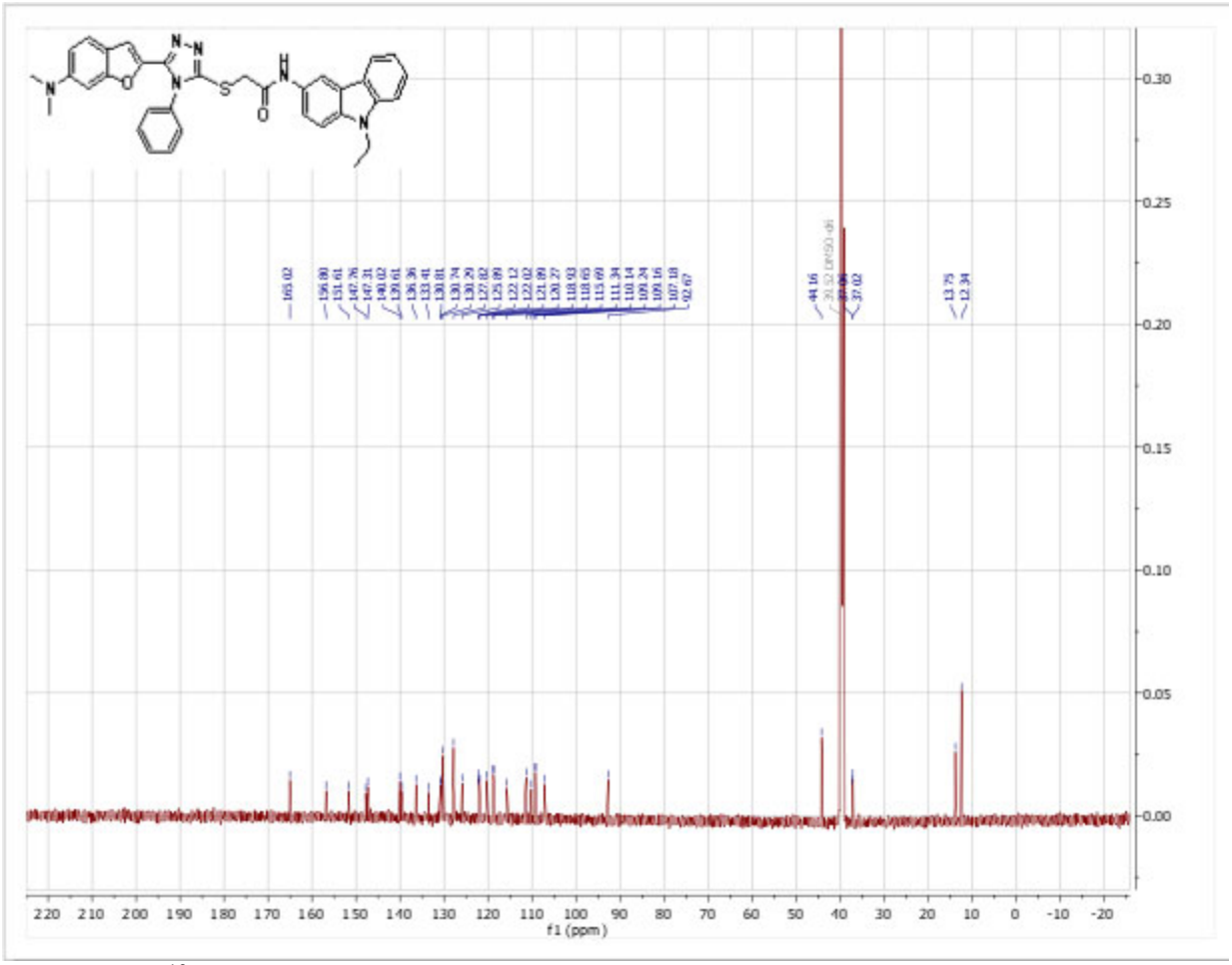


Figure S16: ^{13}C NMR of compound **9h**.

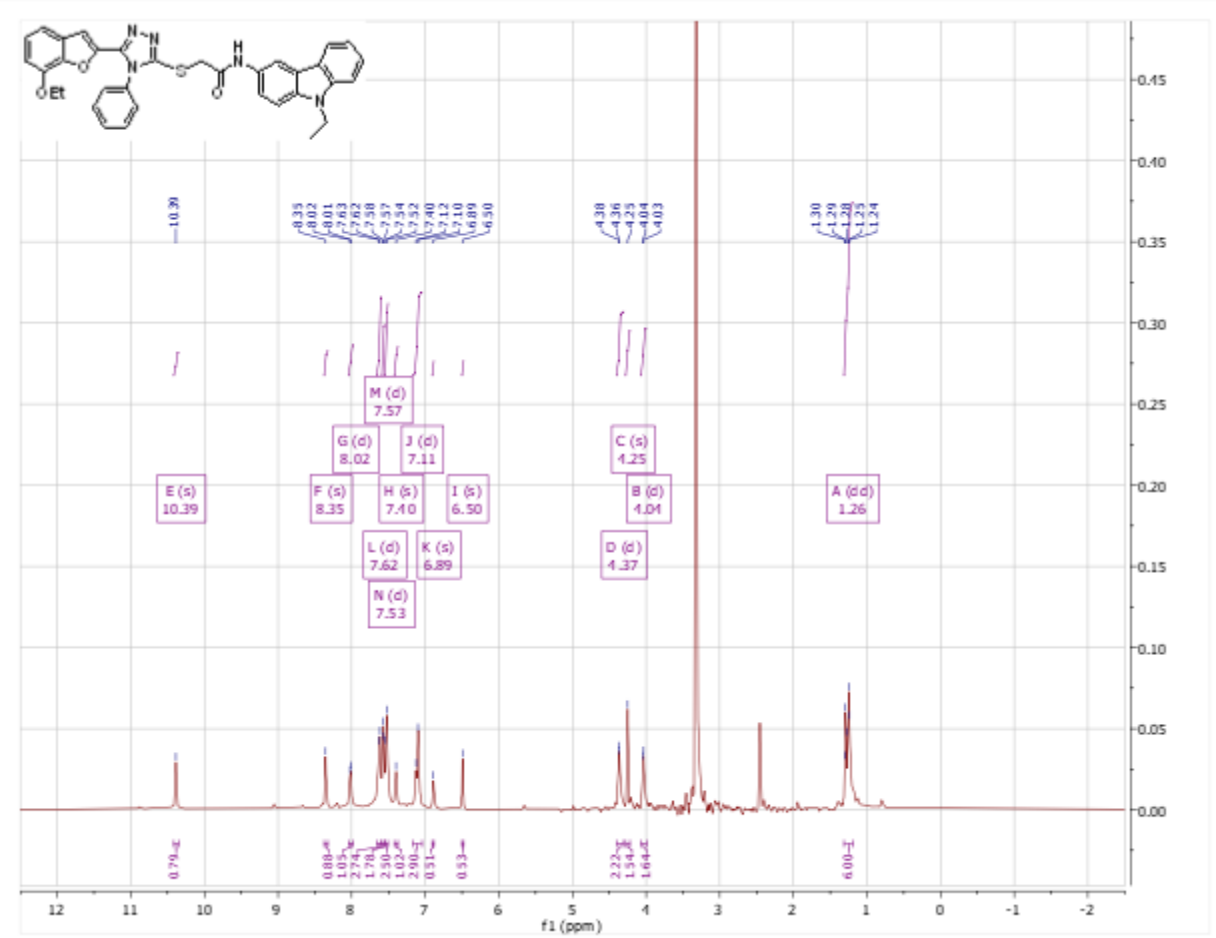


Figure S17: ^{1}H NMR of compound **9i**.

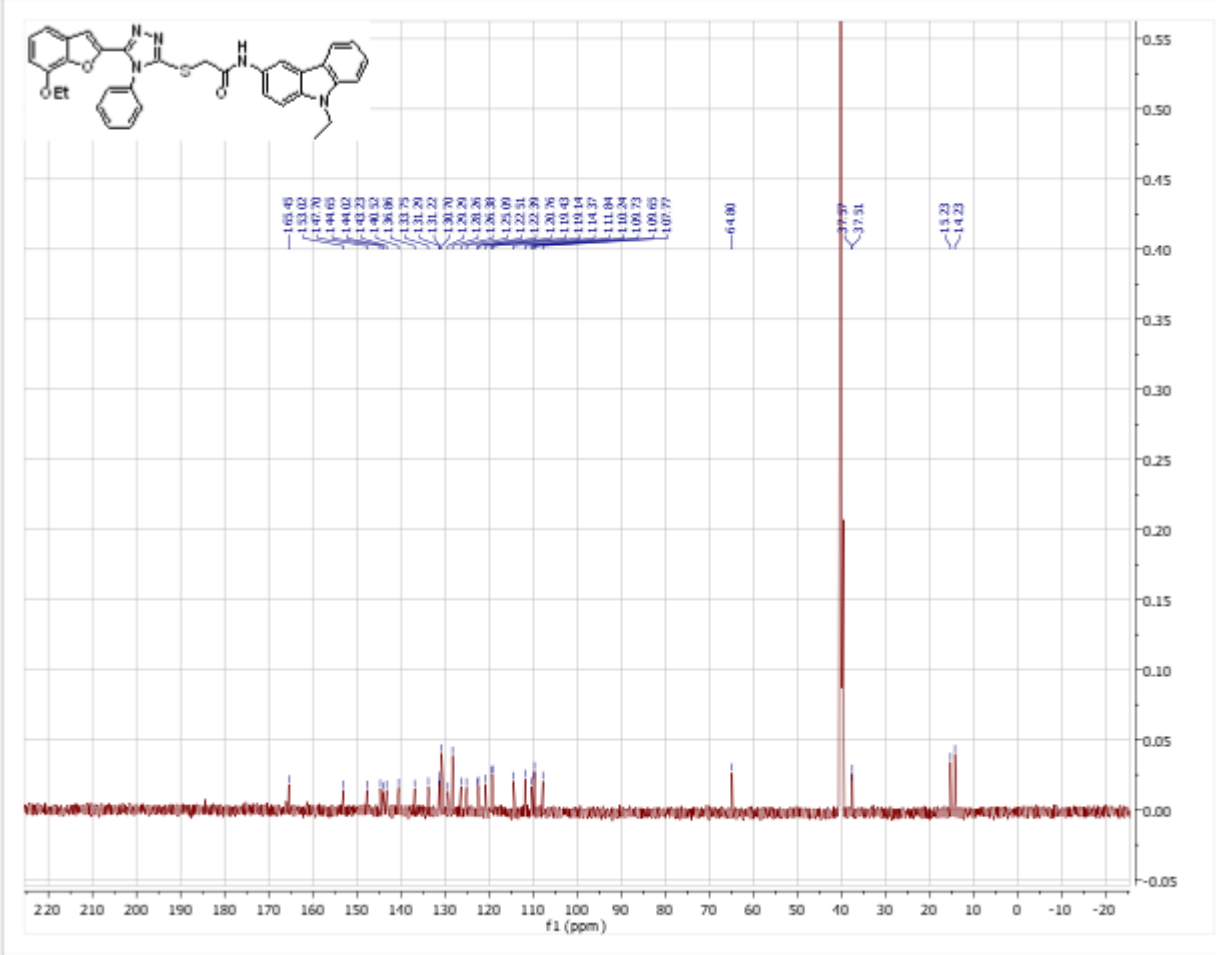


Figure S18: ^{13}C NMR of compound **9i**.

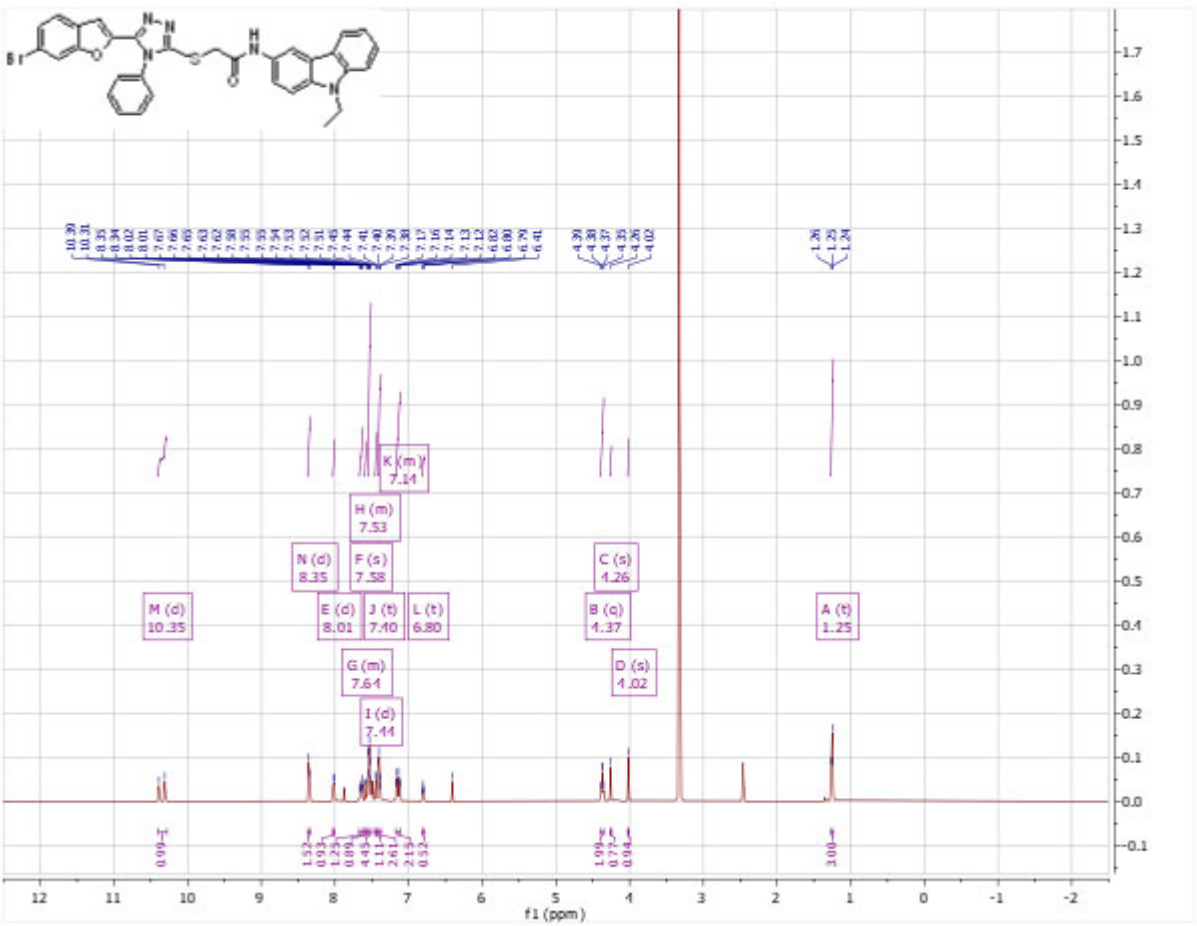


Figure S19: ^{1}H NMR of compound **9j**.

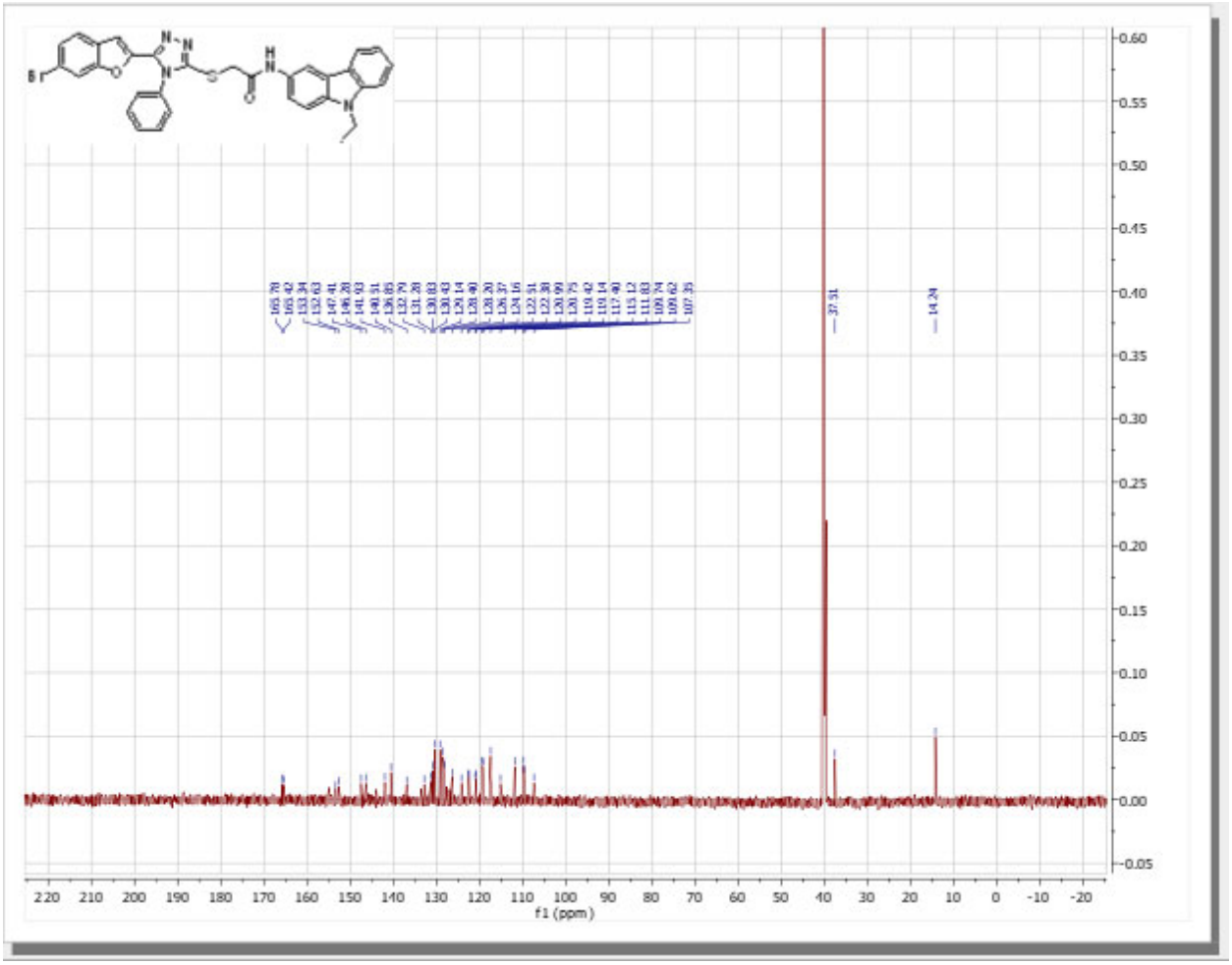
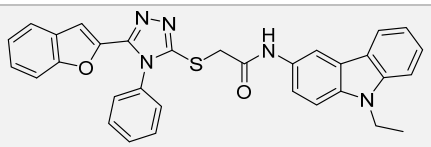
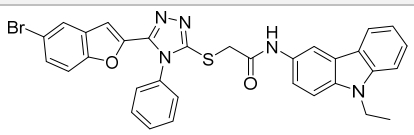
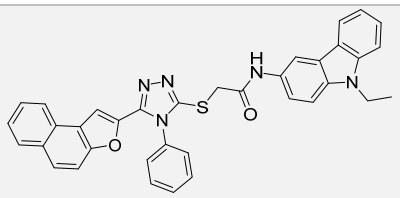
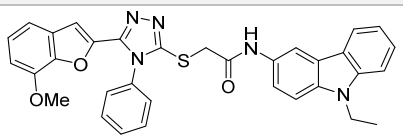
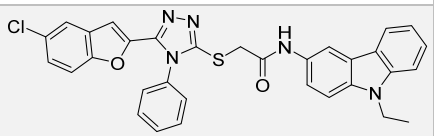
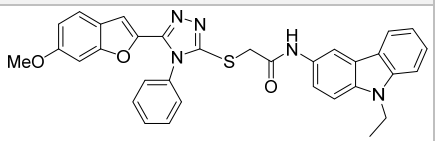
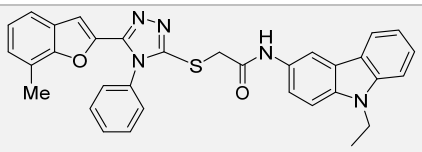
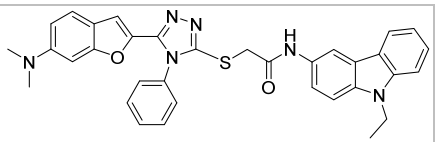
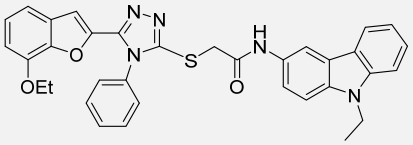
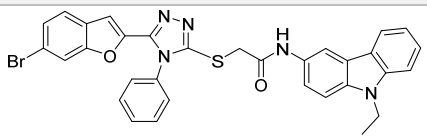
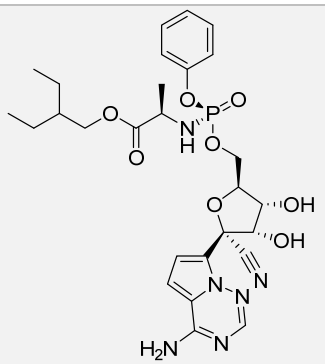
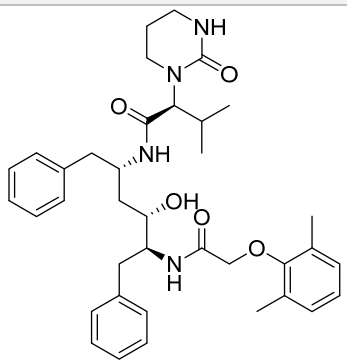
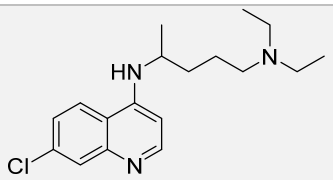
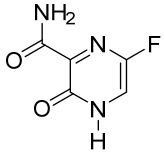
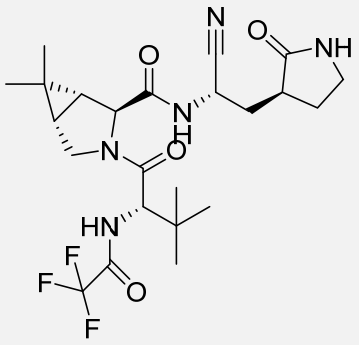


Figure S20: ^{13}C NMR of compound **9j**.

Table 1: Calculated binding energies of the synthesized compounds and FDA-approved drugs against selected proteins.

Sr. No.	Compound Code	Structure	6lu7	6wpt	6m71
1-	9a		-8.5249	-6.146	-6.5752
2-	9b		-8.8316	-6.4390	-6.6509
3-	9c		-8.9203	-5.9347	-6.9193
4-	9d		-8.4681	-6.3866	-6.5356
5-	9e		-8.7770	-6.6934	-7.6139
6-	9f		-8.5097	-6.4124	-7.2549
7-	9g		-8.4871	-5.6443	-7.6298

8-	**9h**		-8.7630	-6.5387	-8.1019
9-	**9i**		-8.8703	-6.4397	-8.0065
10-	**9j**		-8.8492	-6.5619	-7.5397
11-	**Remdesivir**		-8.5523	-6.2612	-6.8211
12-	**Lopinavir**		-8.7372	-6.099	-7.4823
13-	**Chloroquine**		-6.4026	-5.1362	-5.7037
14-	**Favipiravir**		-4.4833	-3.9224	-4.2102

15-	**Nirmatrelvir**		-8.3860	-4.8757	-6.4117

Molecular docking interactions of synthesized compounds with SARS-CoV-2 proteins:

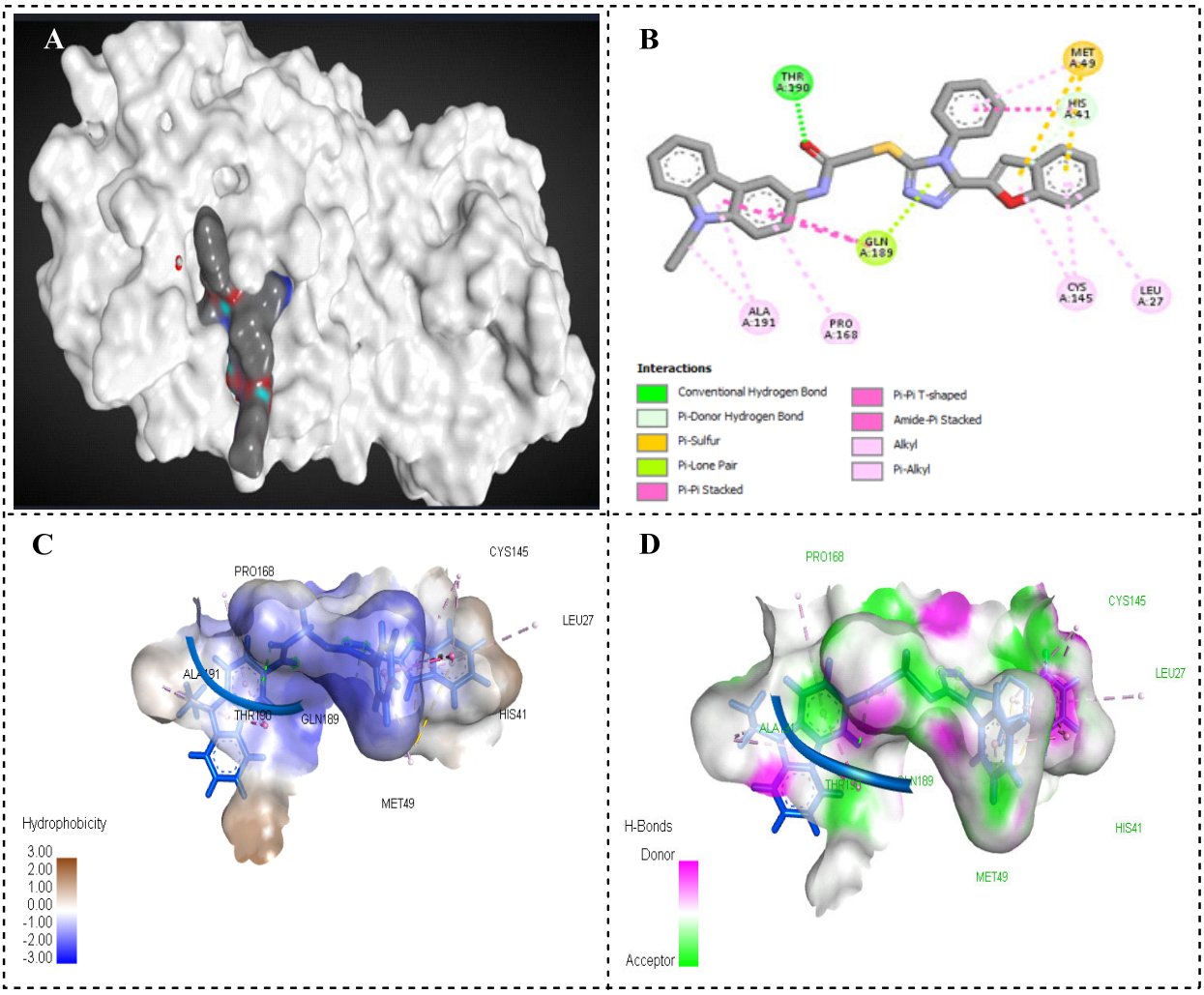


Figure S21: Interaction modes of compound **9a**; **A**: Calculated surface of docked **9a** with main protease, **B**: 2D interactions, **C**: Hydrophobic interactions, **D**: Hydrogen bonding interactions.

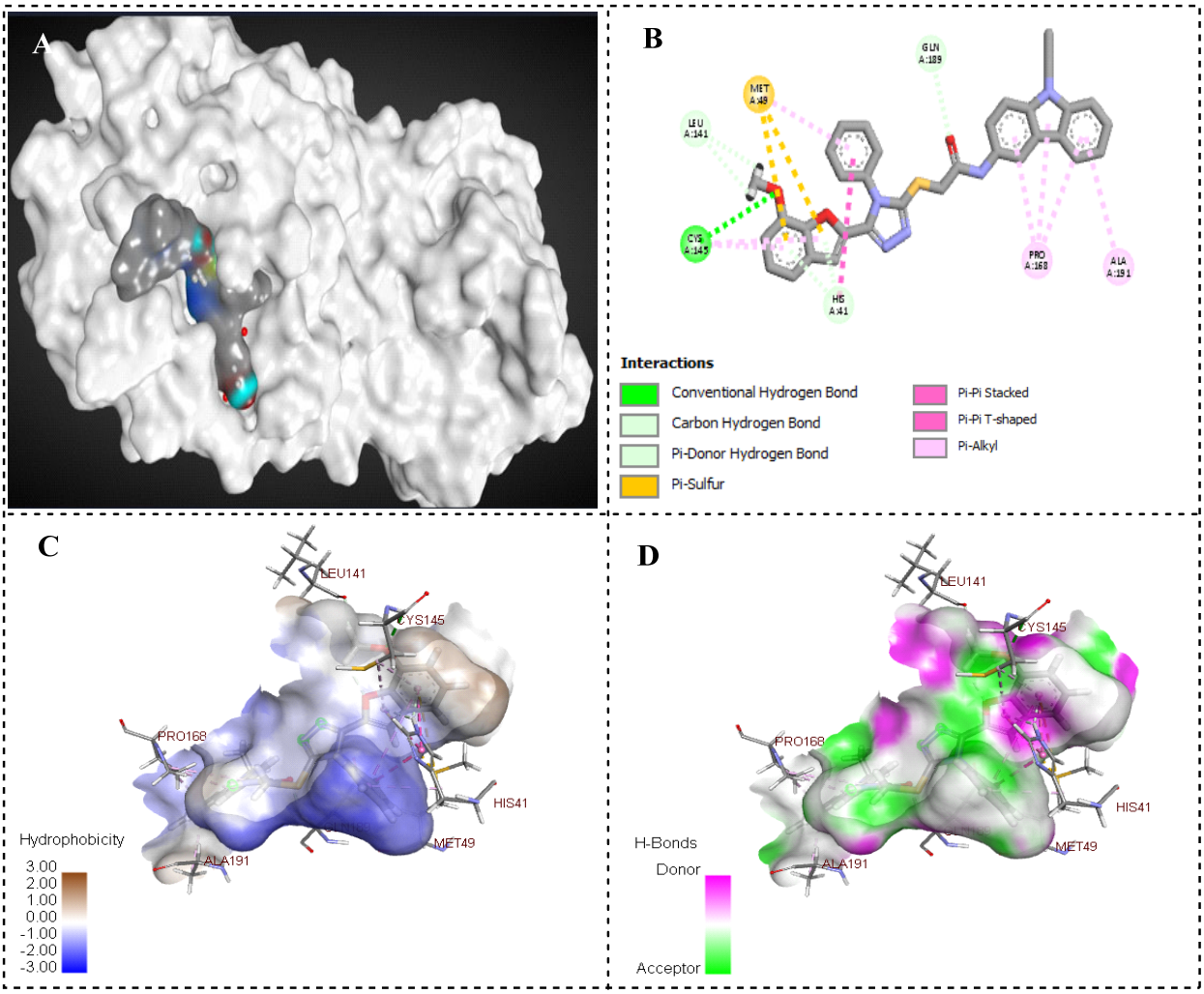


Figure S22: Interaction modes of compound **9d**; **A**: Calculated surface of docked **9d** with main protease, **B**: 2D interactions, **C**: Hydrophobic interactions, **D**: Hydrogen bonding interactions.

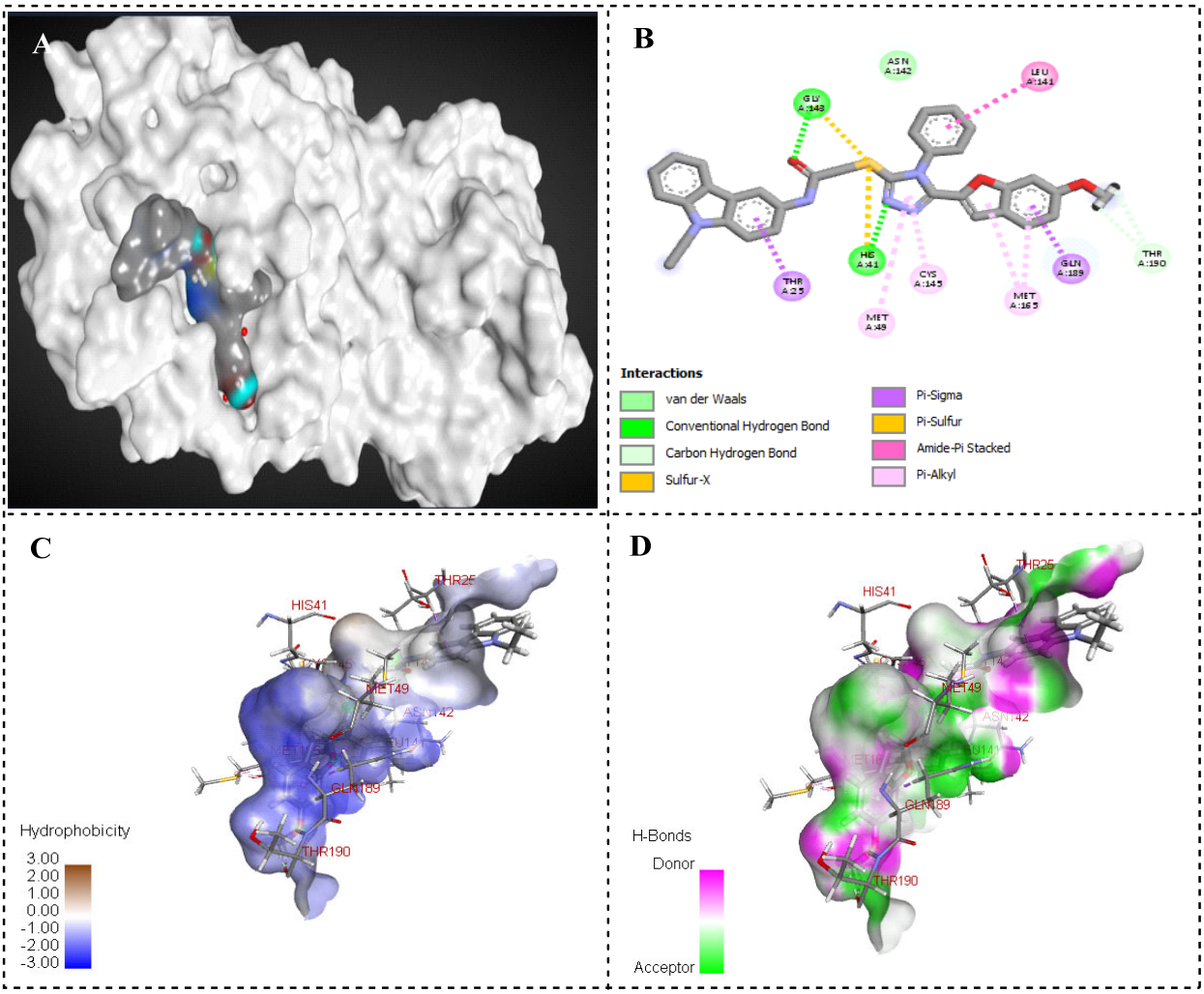


Figure S23: Interaction modes of compound **9f**; **A**: Calculated surface of docked **9f** with main protease, **B**: 2D interactions, **C**: Hydrophobic interactions, **D**: Hydrogen bonding interactions.

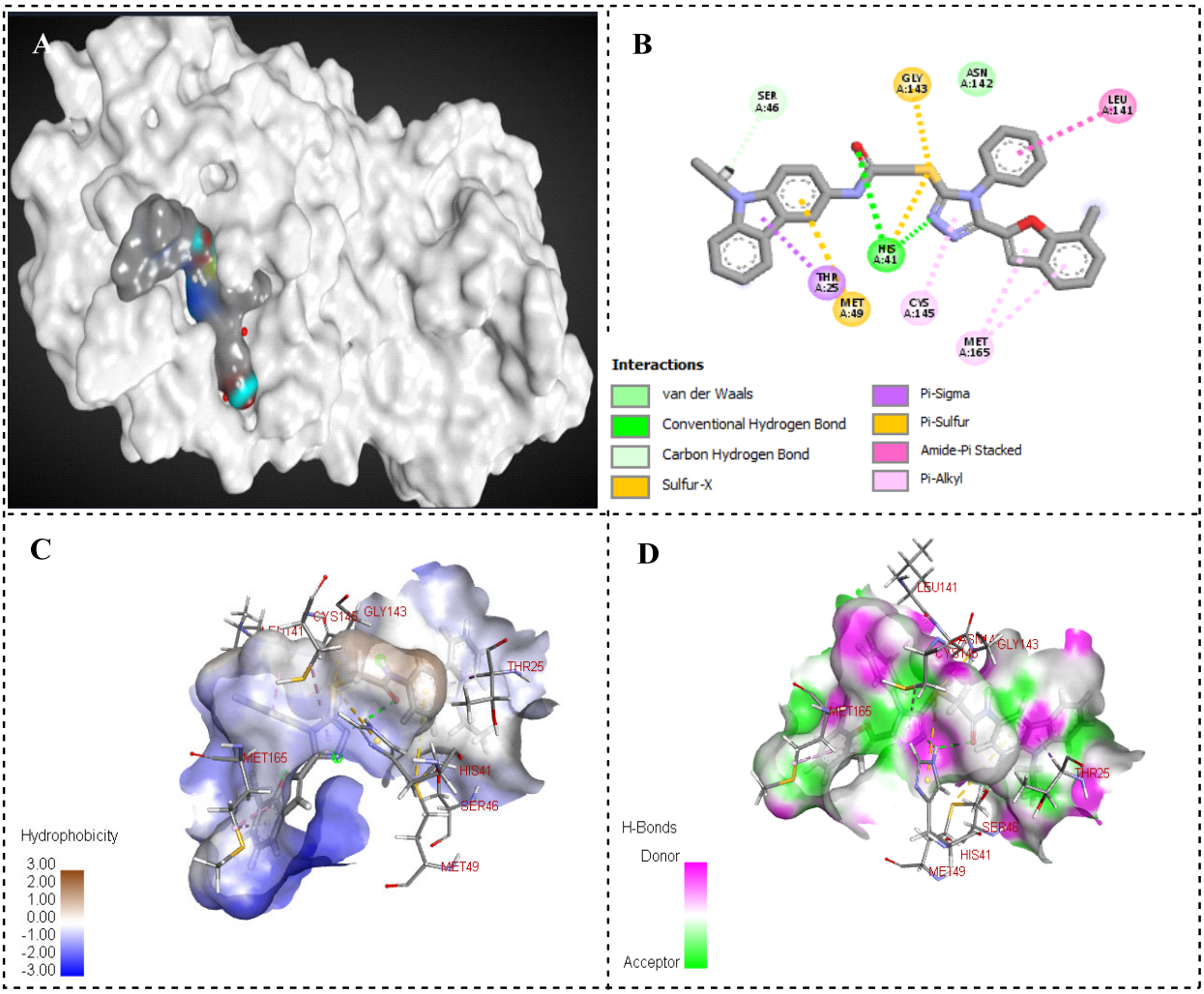


Figure S24: Interaction modes of compound **9g**; **A**: Calculated surface of docked **9g** with main protease, **B**: 2D interactions, **C**: Hydrophobic interactions, **D**: Hydrogen bonding interactions.

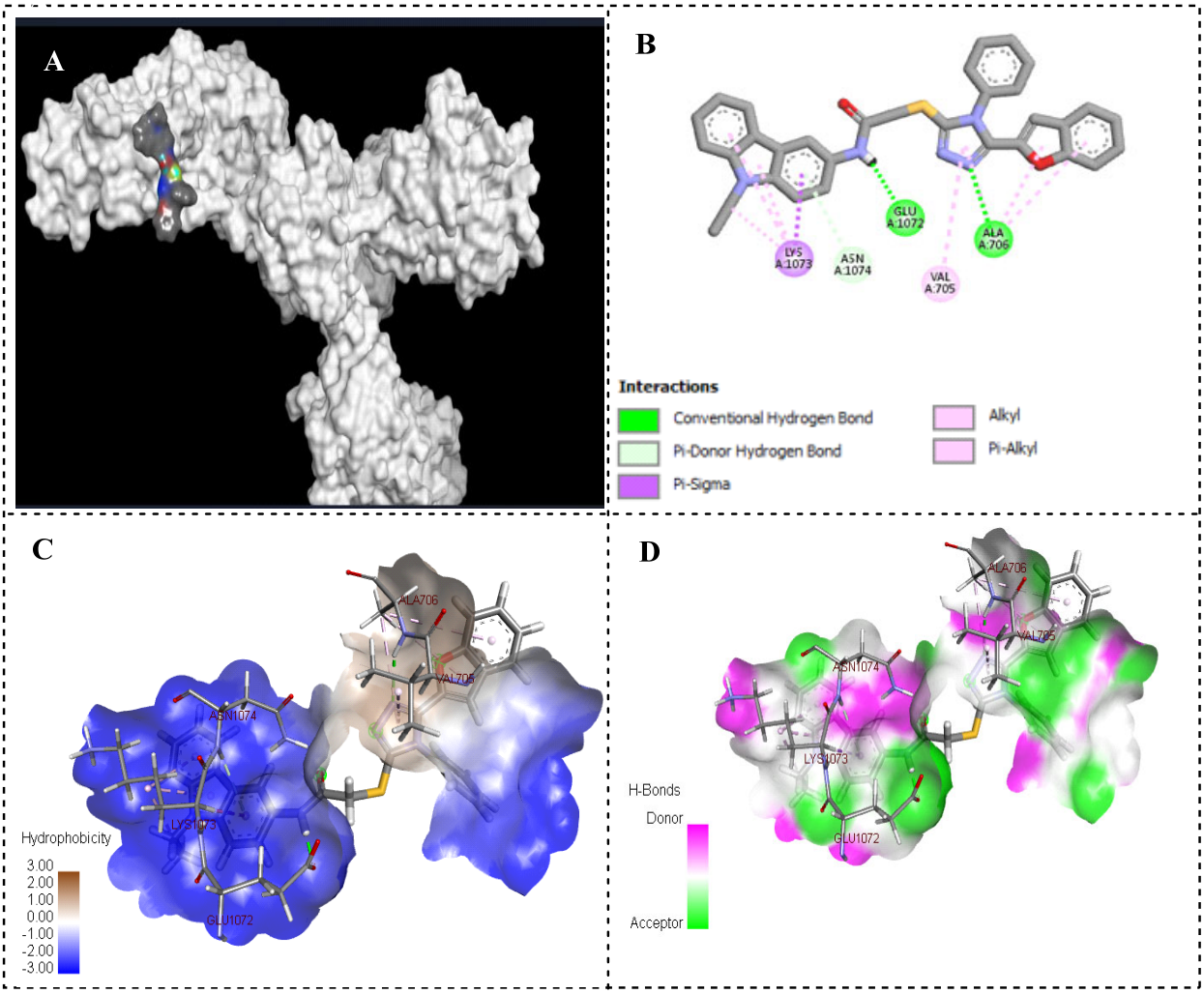


Figure S25: Interaction modes of compound **9a**; **A**: Calculated surface of docked **9a** with spike glycoprotein, **B**: 2D interactions, **C**: Hydrophobic interactions, **D**: Hydrogen bonding interactions.

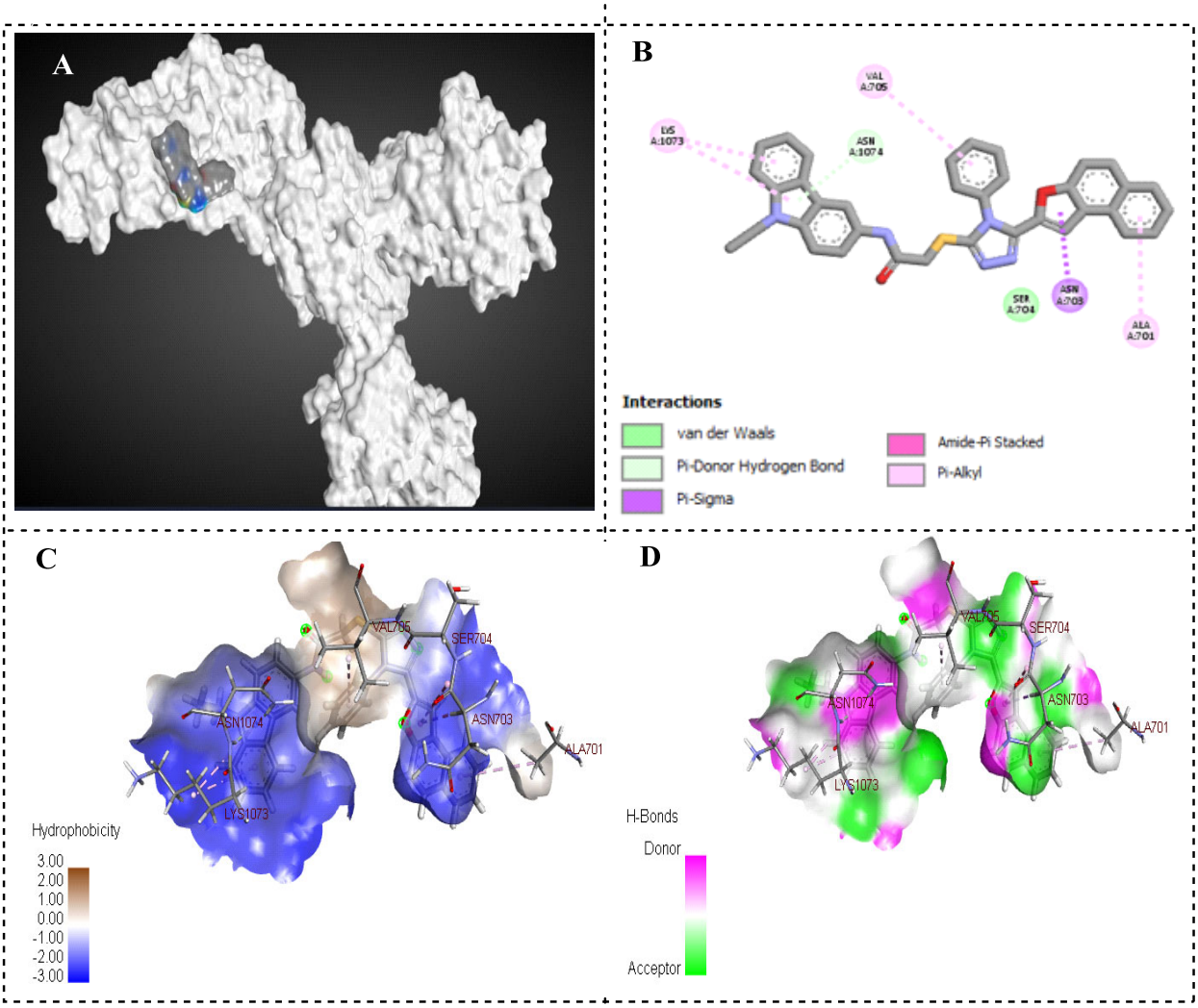


Figure S26: Interaction modes of compound **9c**; **A**: Calculated surface of docked **9c** with spike glycoprotein, **B**: 2D interactions, **C**: Hydrophobic interactions, **D**: Hydrogen bonding interactions.

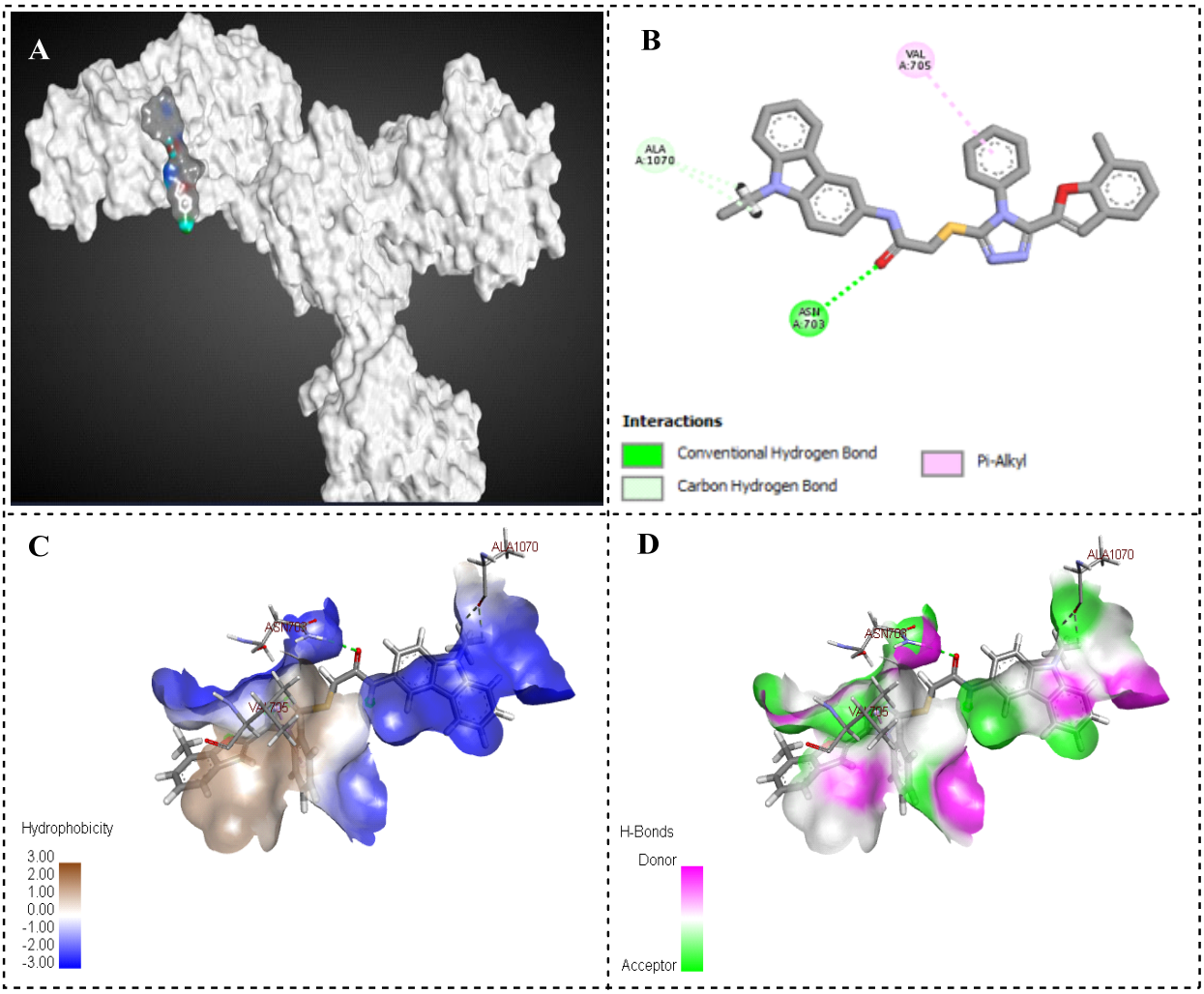


Figure S27: Interaction modes of compound **9g**; **A**: Calculated surface of docked **9g** with spike glycoprotein, **B**: 2D interactions, **C**: Hydrophobic interactions, **D**: Hydrogen bonding interactions.

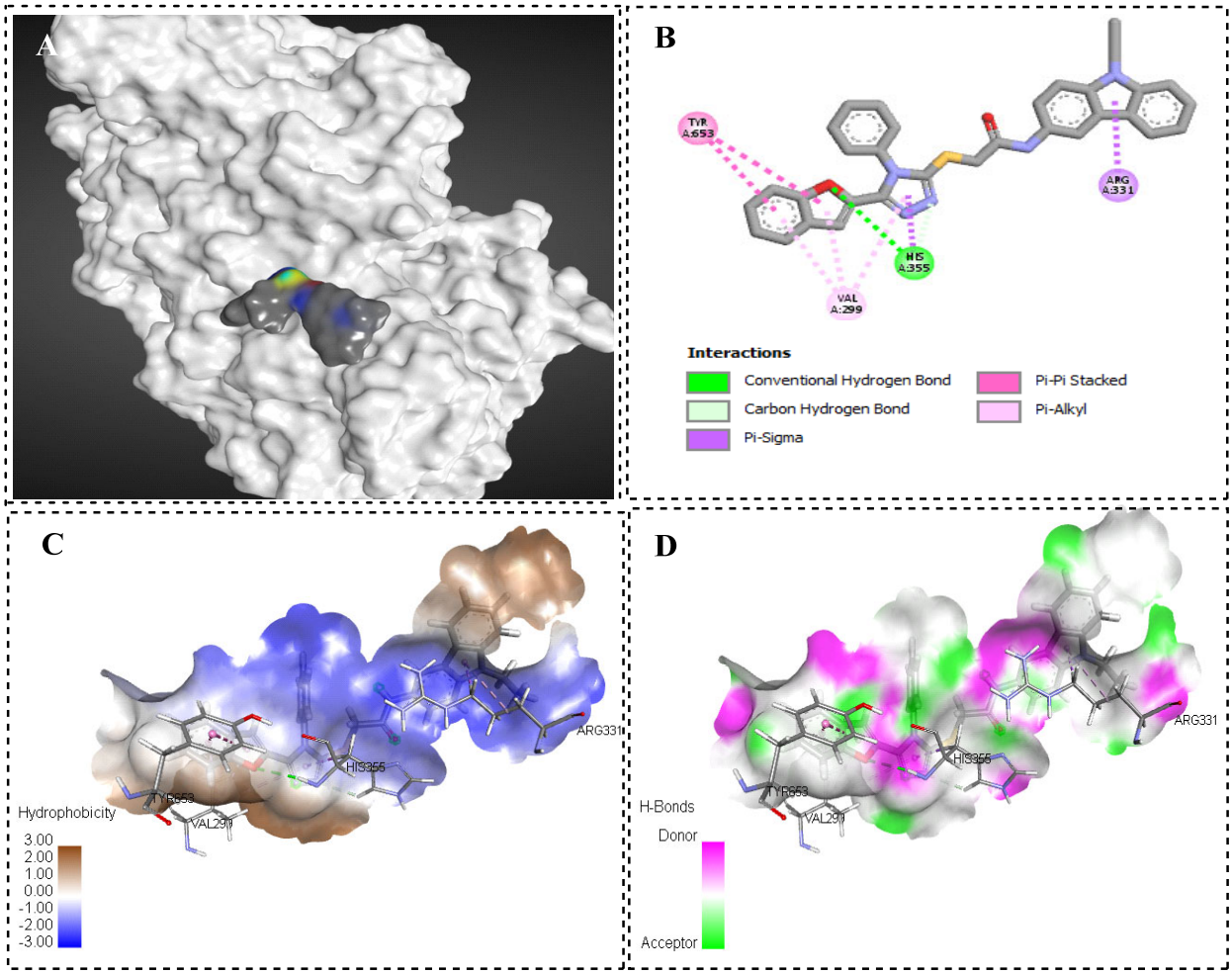


Figure S28: Interaction modes of compound **9a**; **A**: Calculated surface of docked **9a** with RdRp, **B**: 2D interactions, **C**: Hydrophobic interactions, **D**: Hydrogen bonding interactions.

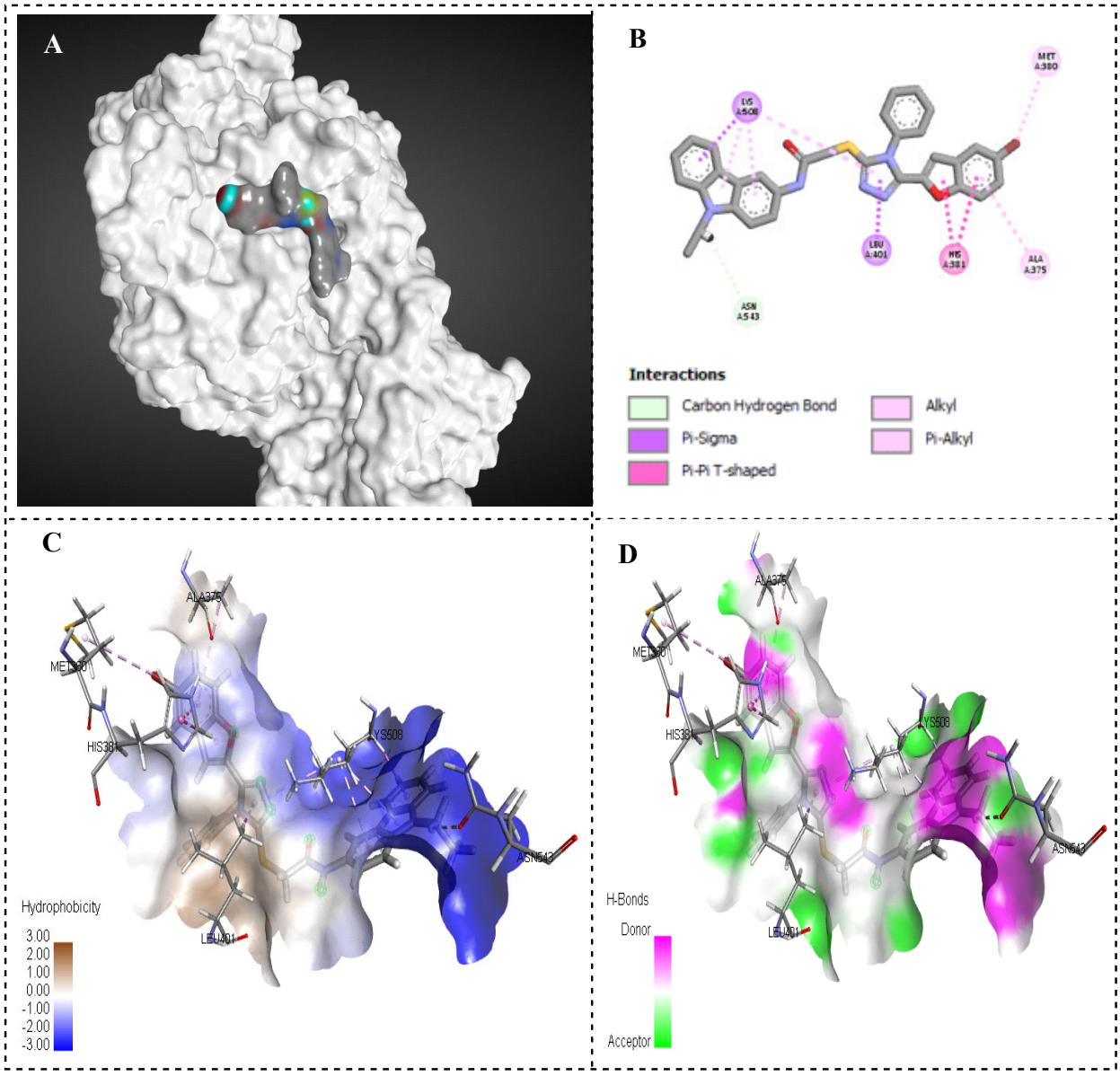


Figure S29: Interaction modes of compound **9b**; **A**: Calculated surface of docked **9b** with RdRp, **B**: 2D interactions, **C**: Hydrophobic interactions, **D**: Hydrogen bonding interactions.

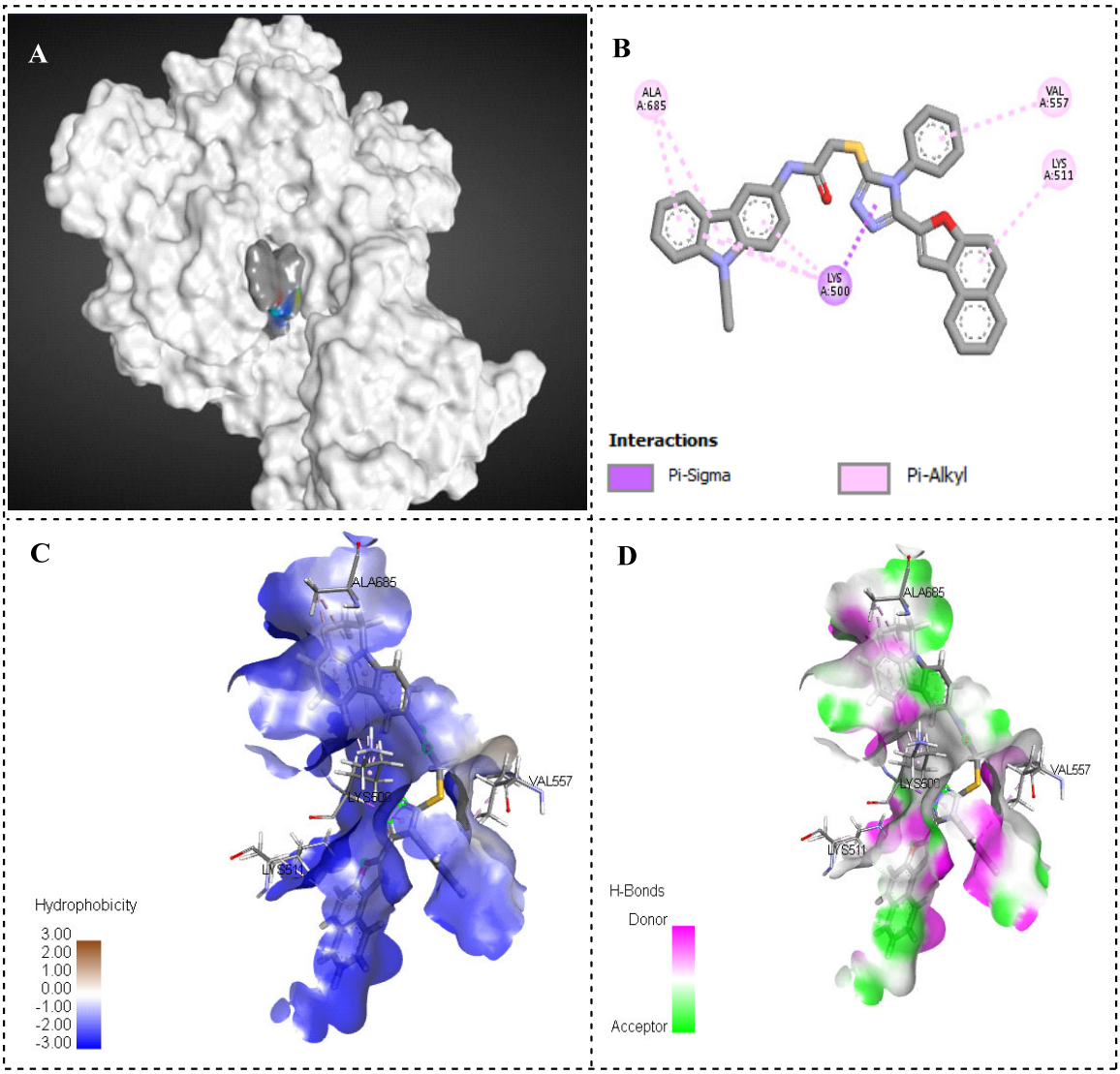


Figure S30: Interaction modes of compound **9c**; **A**: Calculated surface of docked **9c** with RdRp, **B**: 2D interactions, **C**: Hydrophobic interactions, **D**: Hydrogen bonding interactions.

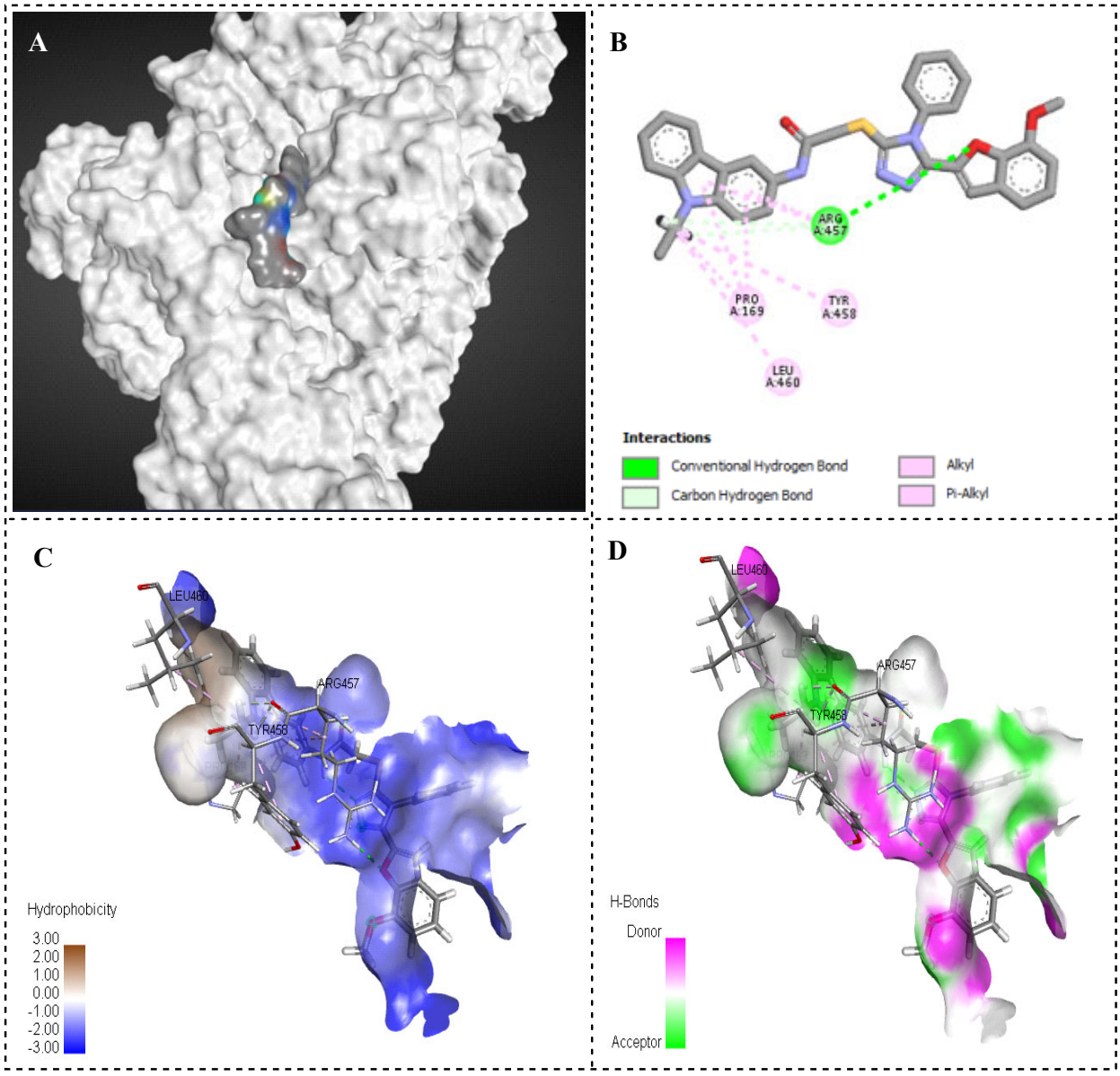


Figure S31: Interaction modes of compound **9d**; **A**: The calculated surface of docked **9d** with RdRp, **B**: 2D interactions, **C**: Hydrophobic interactions, **D**: Hydrogen bonding interactions.

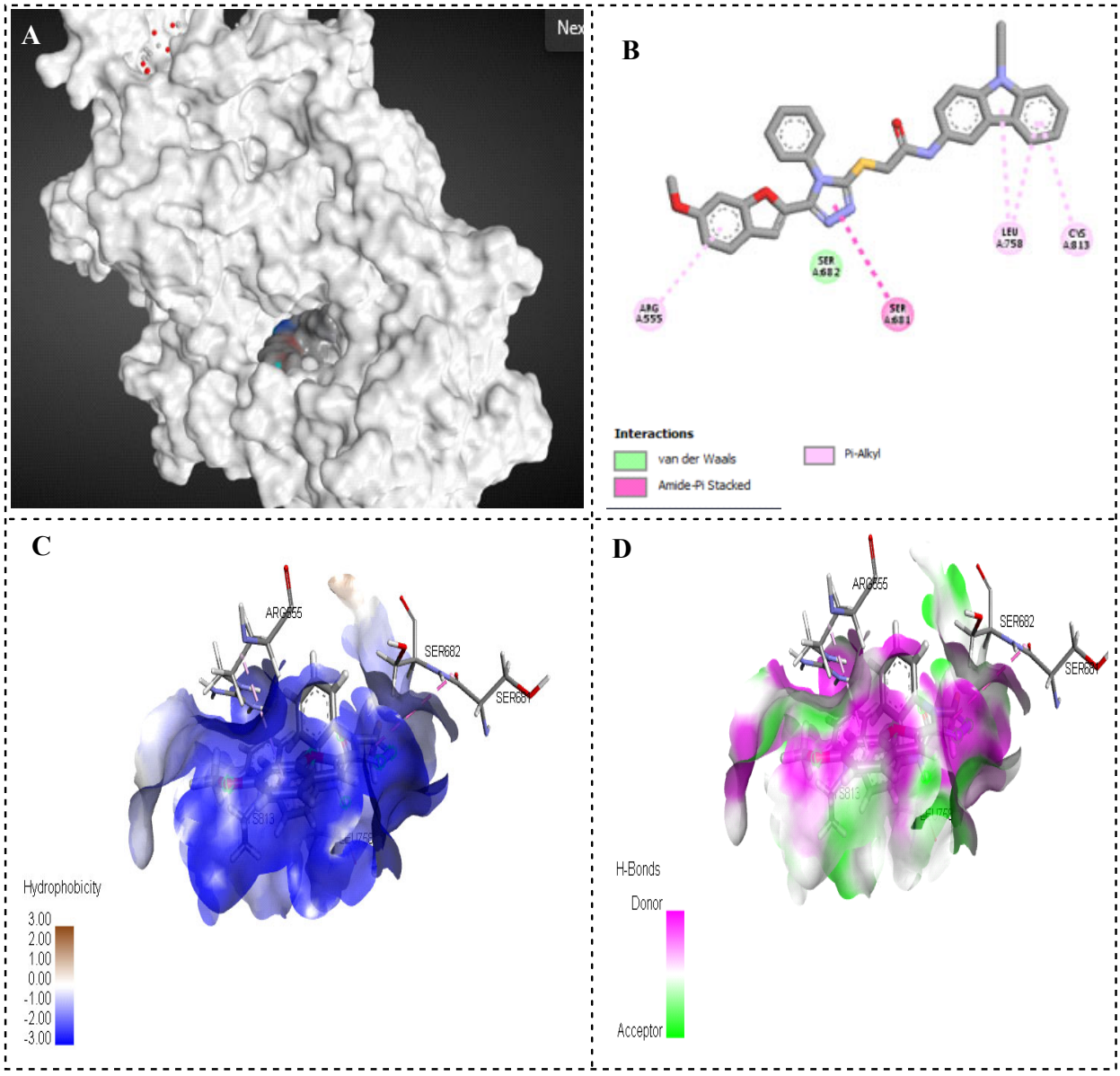


Figure S32: Interaction modes of compound **9f**; **A**: The calculated surface of docked **9f** with RdRp, **B**: 2D interactions, **C**: Hydrophobic interactions, **D**: Hydrogen bonding interactions.

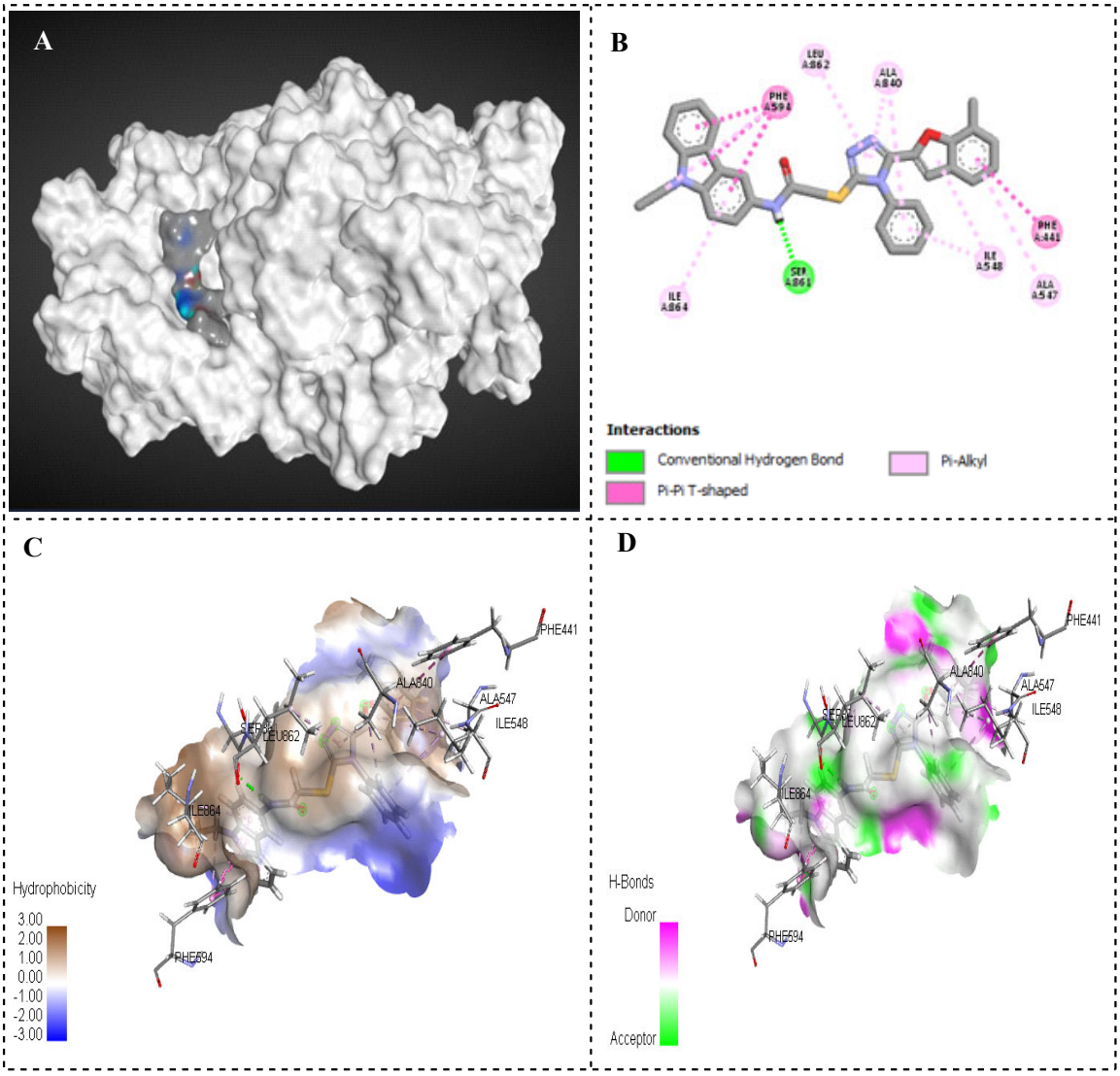


Figure S33: Interaction modes of compound **9g**; **A**: Calculated surface of docked **9g** with RdRp, **B**: 2D interactions, **C**: Hydrophobic interactions, **D**: Hydrogen bonding interactions.

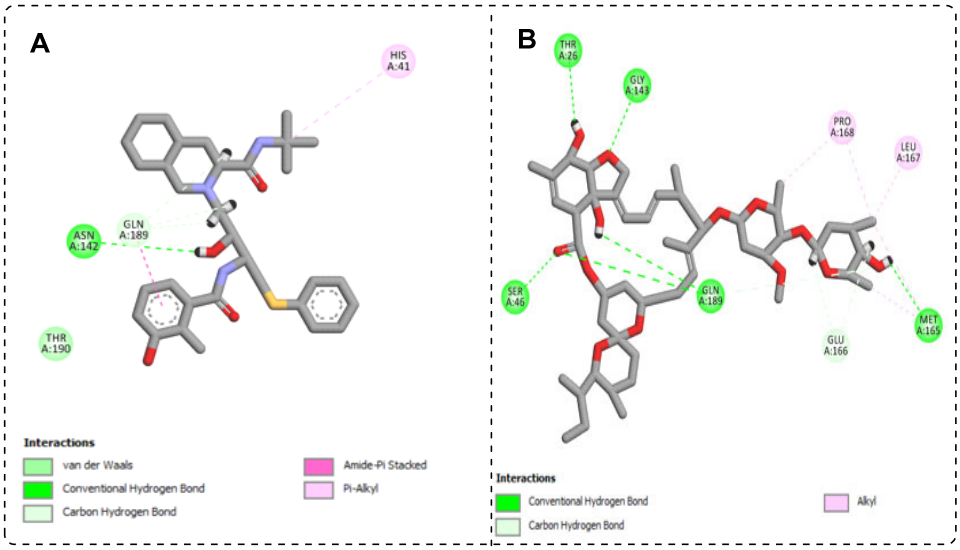


Figure S34. Binding interaction of **A**:Nelfinavir and **B**: Ivermectin with Mpro**.**

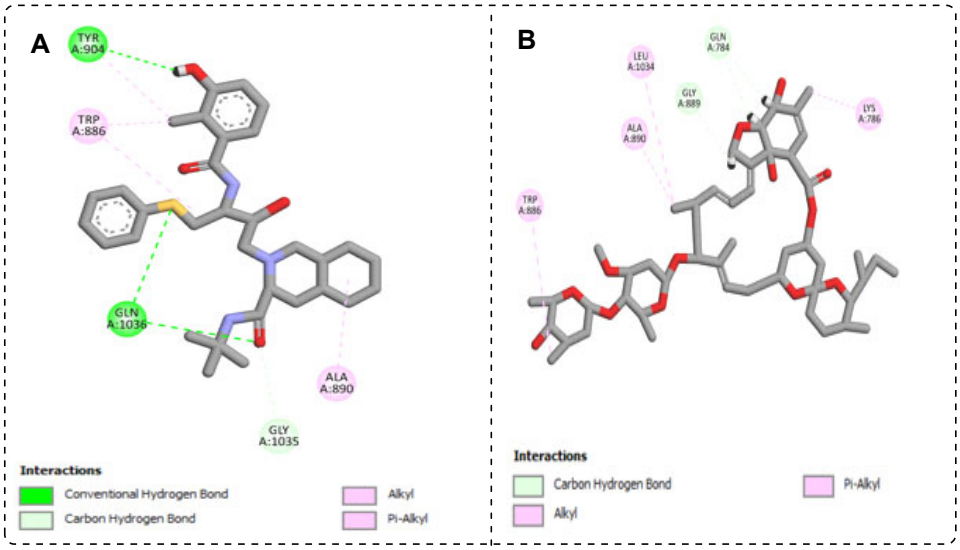


Figure S35. Binding interaction of **A**:Nelfinavir and **B**: Ivermectin with spike glycoprotein**.**

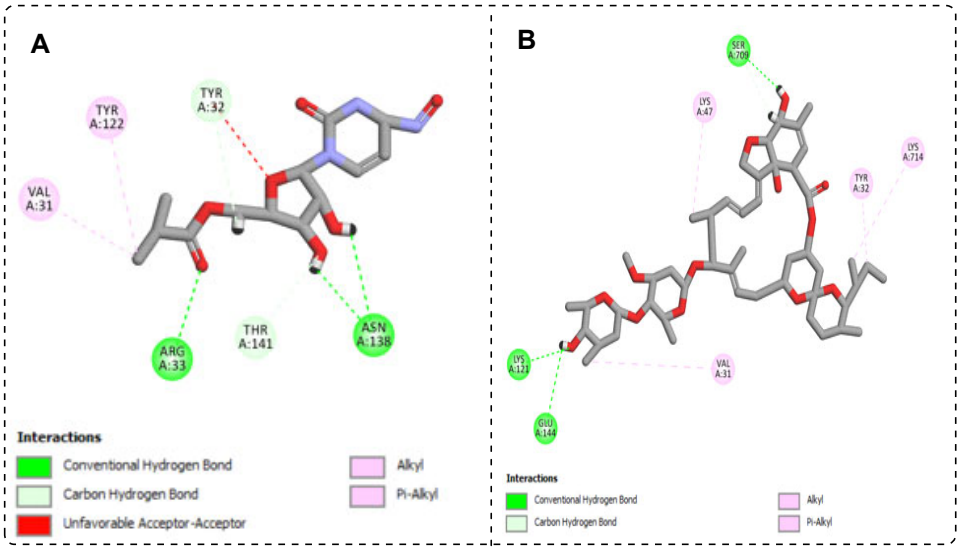


Figure S36. Binding interaction of **A**: Molnupiravir and **B**: Ivermectin with RdRp**.**