N-(4-bromophenyl)furan-2-carboxamides via Suzuki-miyaura Cross-Coupling: Anti-bacterial activities against clinically isolated drug resistant *A. baumannii, K. pneumoniae, E. cloacae and* MRSA and its validation via computational approach.

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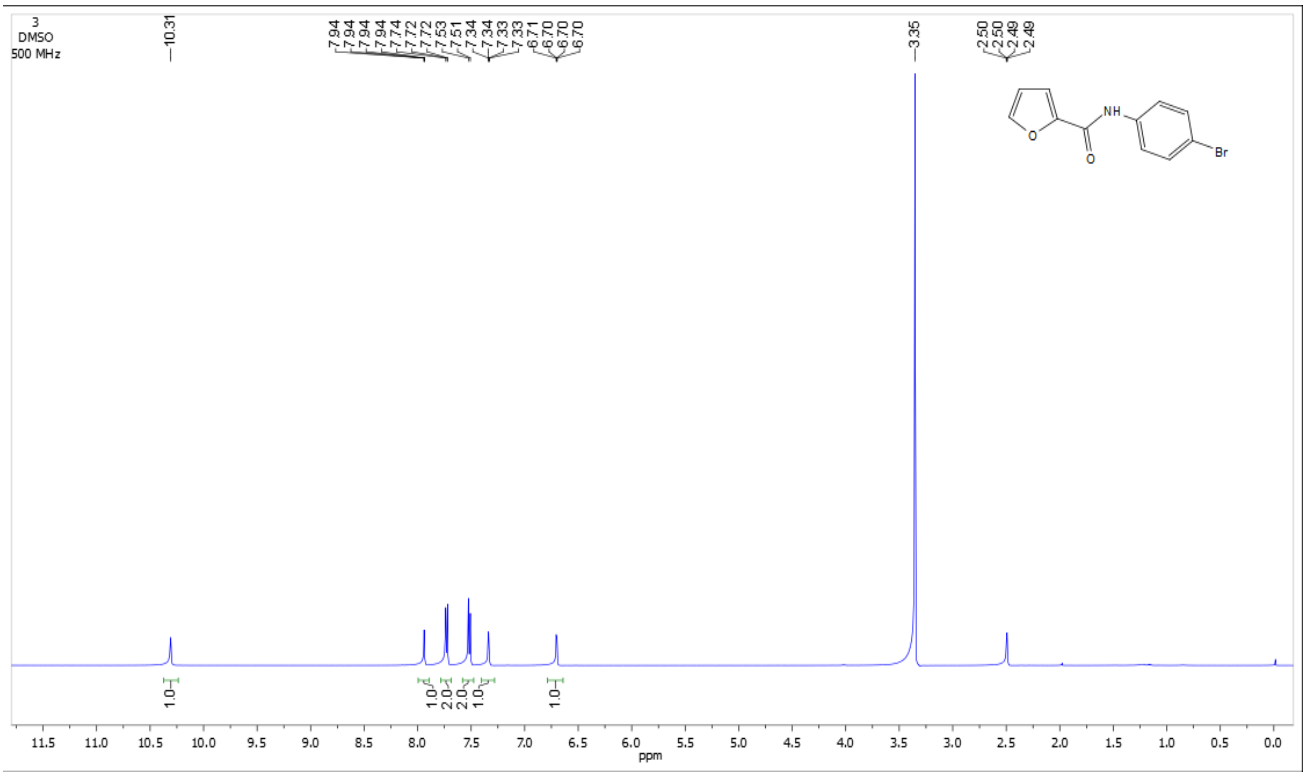


Figure S1: [1]HNMR (500 MHz, DMSO) of compound **3**.

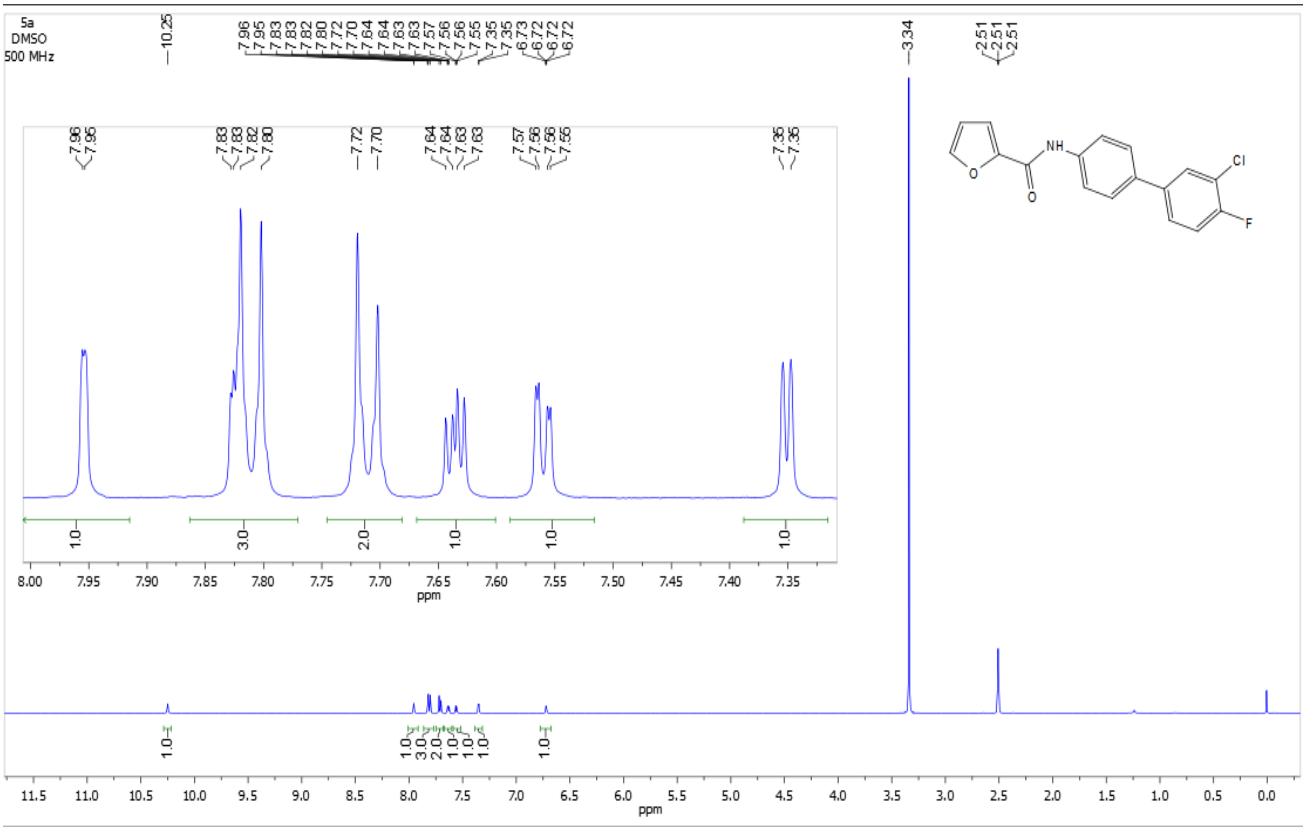


Figure S2: ^{1}HNMR (500 MHz, DMSO) of compound **5a.**

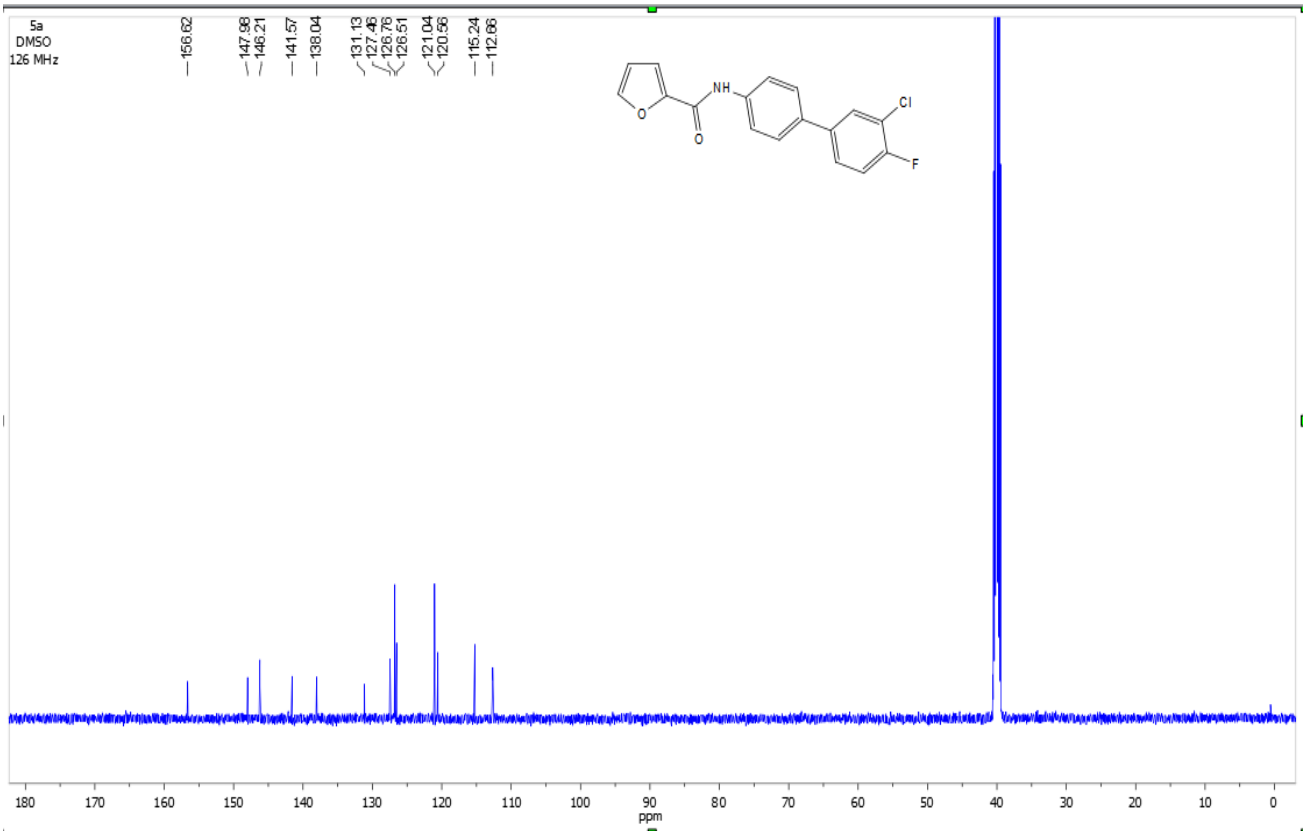


Figure S3: ^{13}CNMR (126 MHz, DMSO) of compound **5a.**

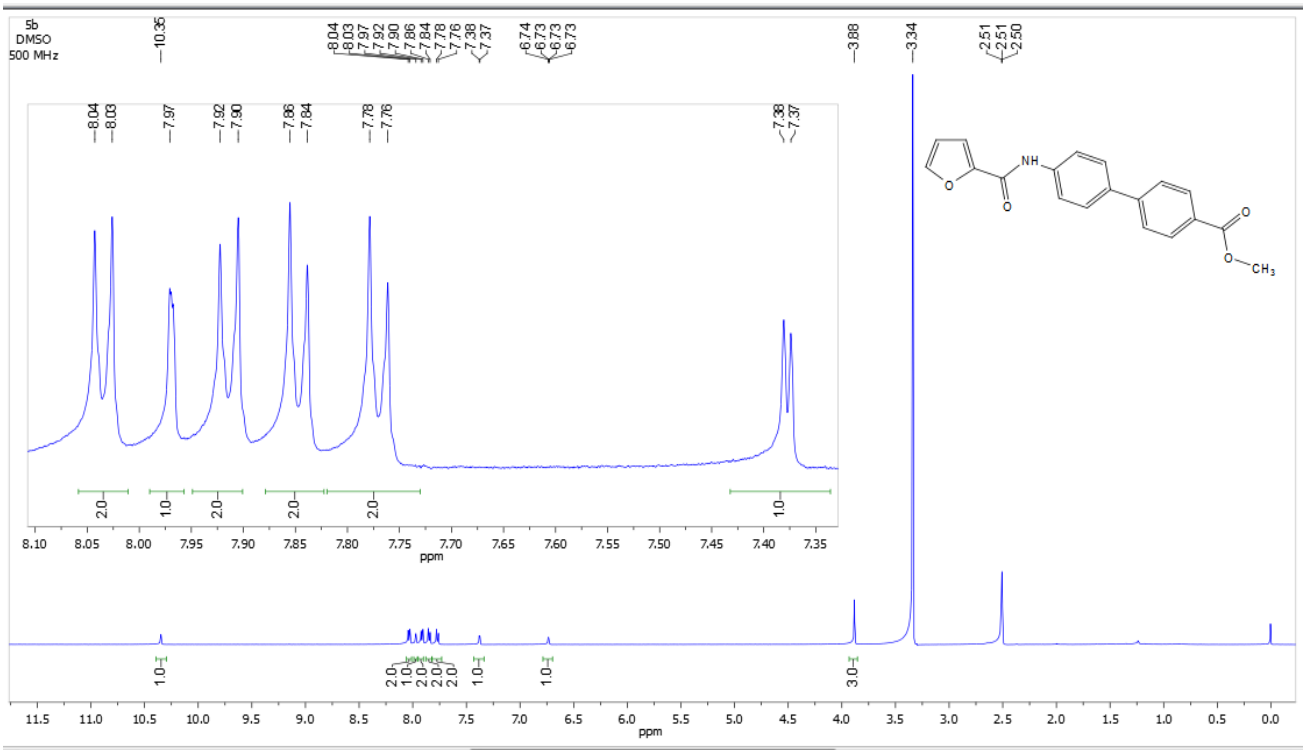


Figure S4: [1]HNMR (500 MHz, DMSO) of compound **5b.**

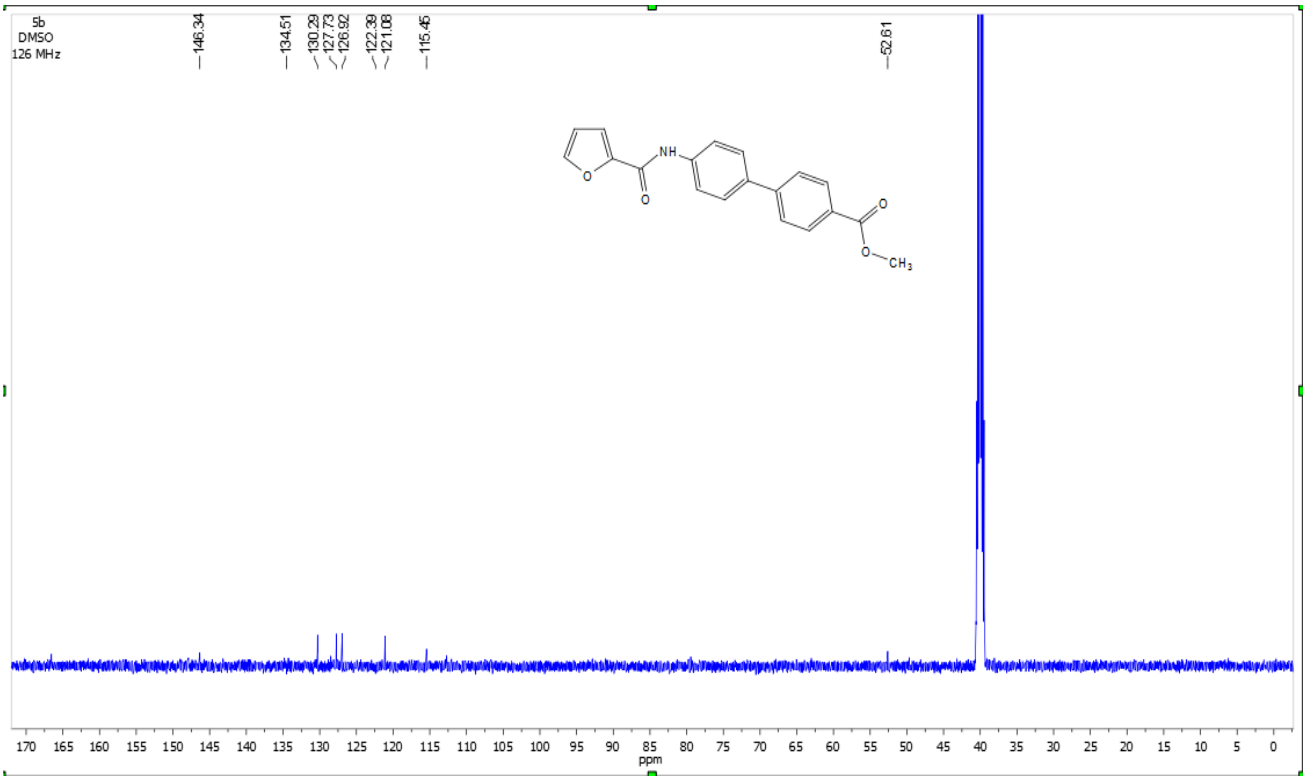


Figure S5: [13]CNMR (126 MHz, DMSO) of compound **5b.**

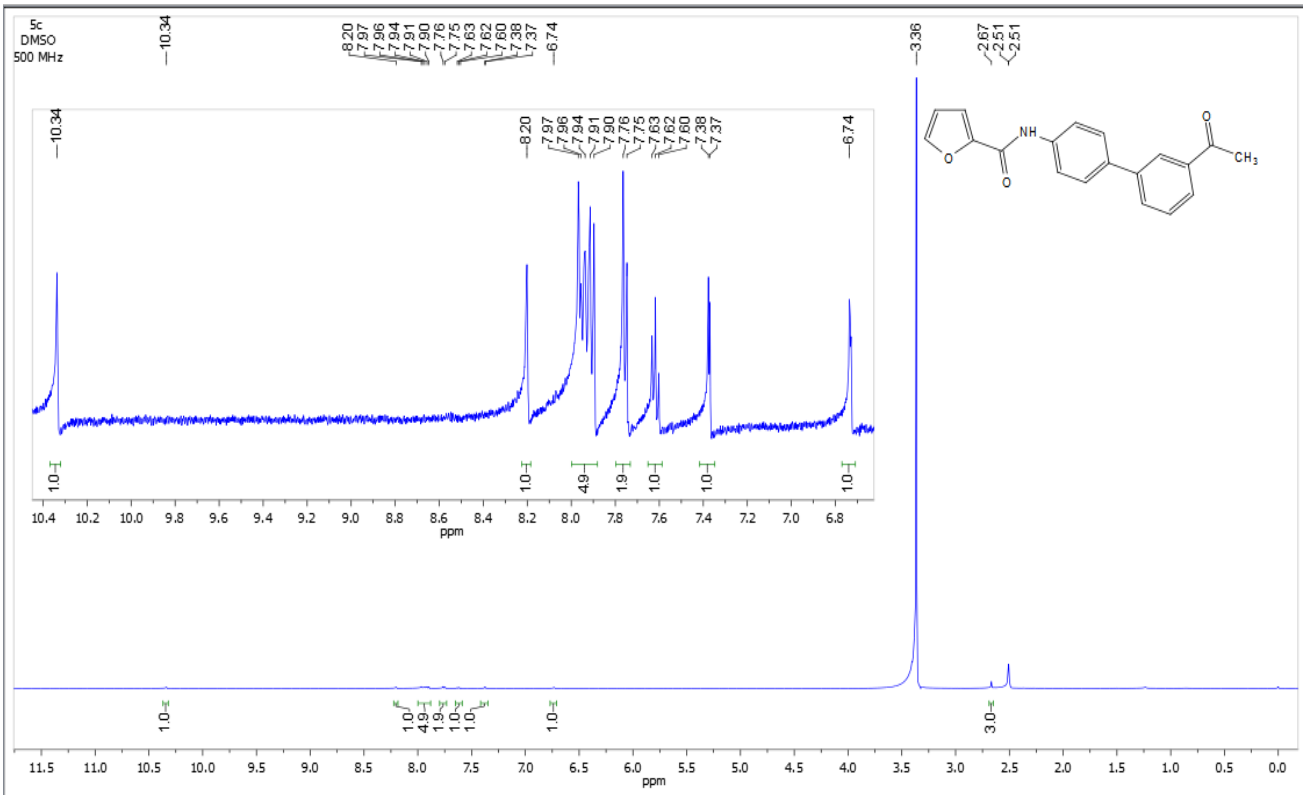


Figure S6: [1]HNMR (500 MHz, DMSO) of compound **5c.**

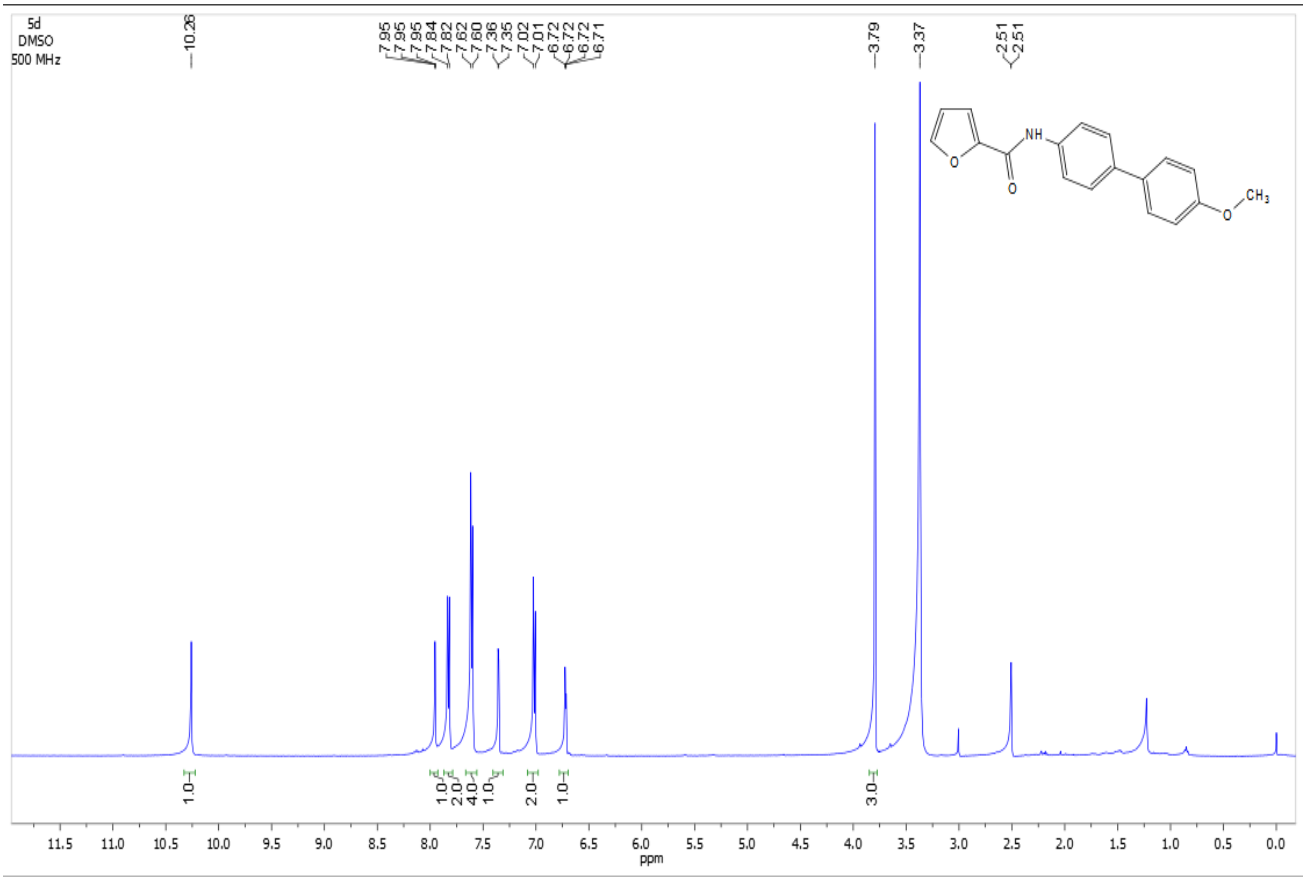


Figure S7: [1]HNMR (500 MHz, DMSO) of compound **5d.**

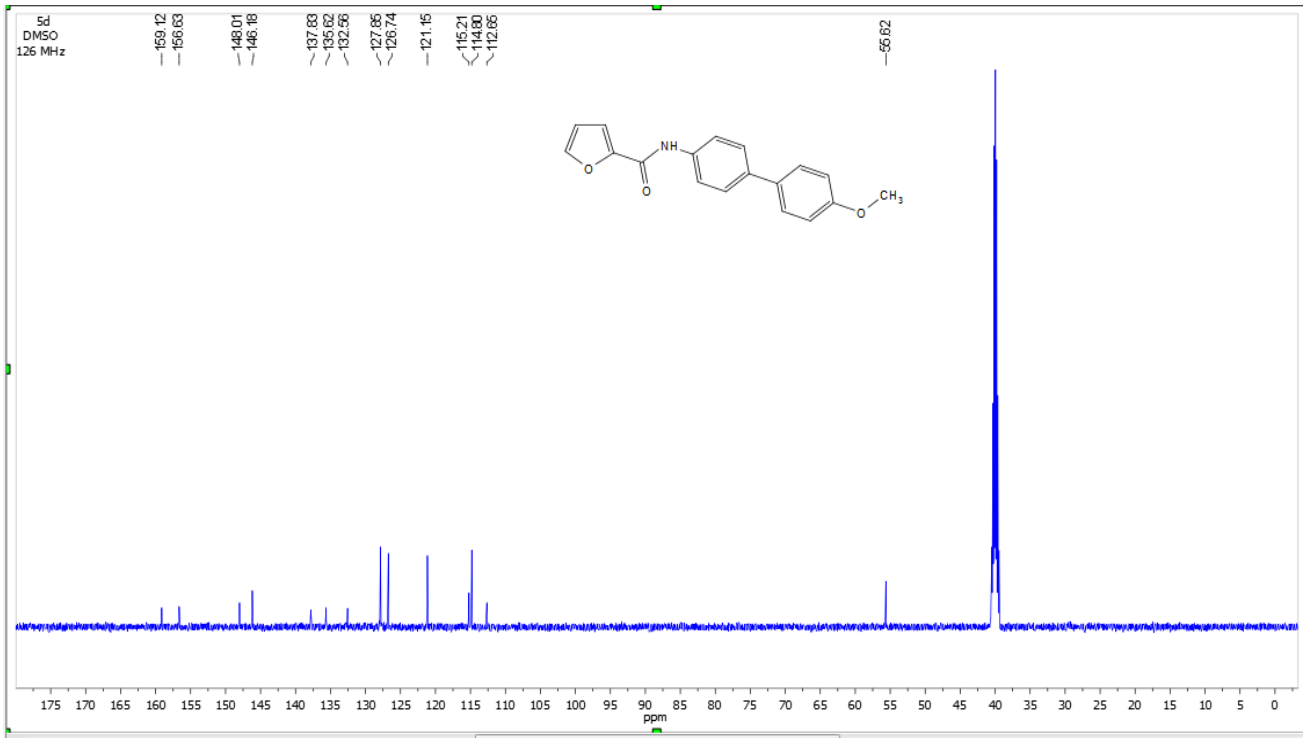


Figure S8: [13]CNMR (126 MHz, DMSO) of compound **5d.**

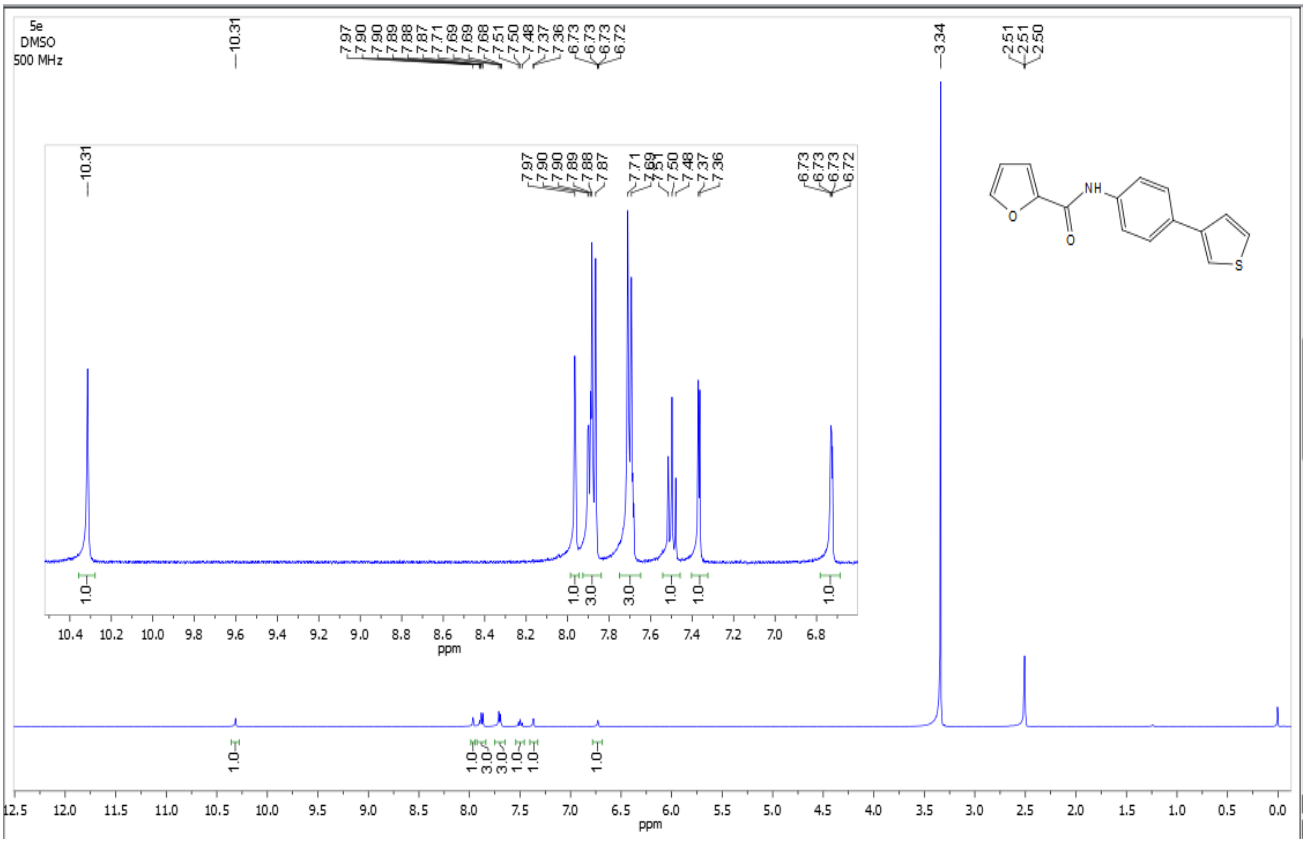


Figure S9: [1]HNMR (500 MHz, DMSO) of compound **5e.**

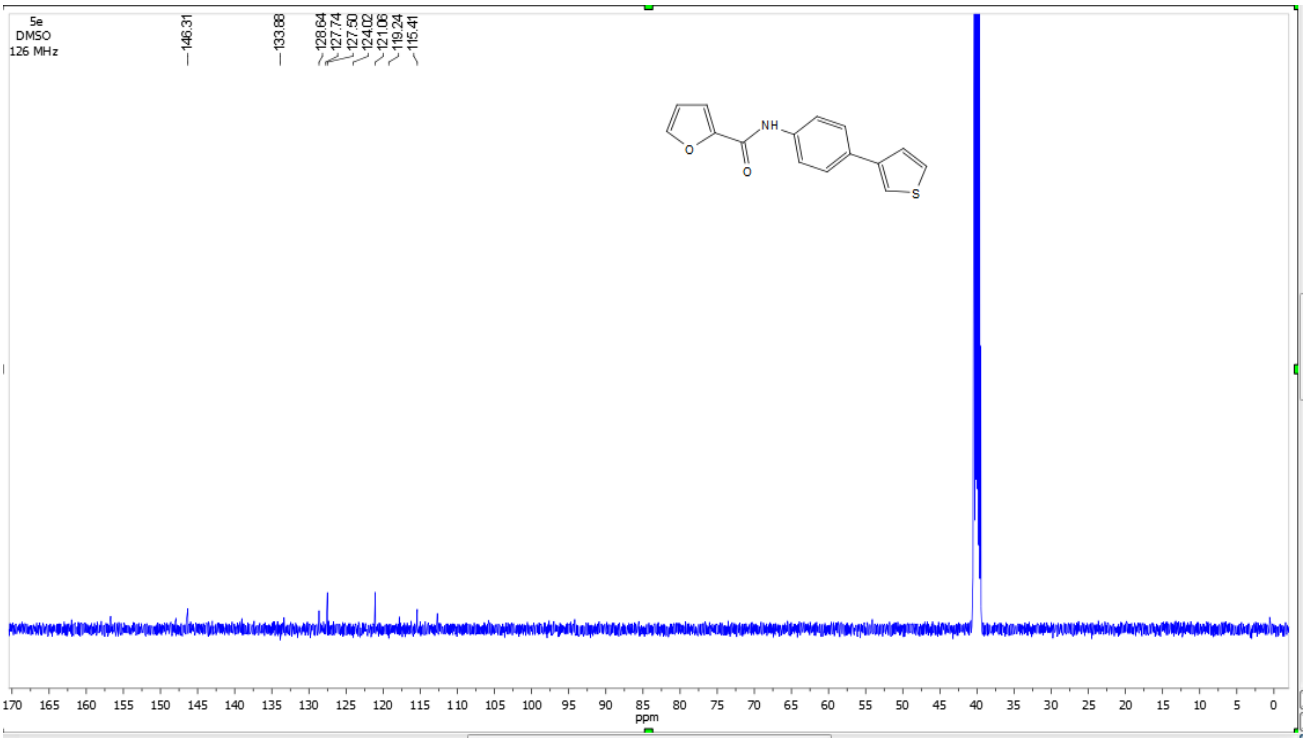


Figure S10: [13]CNMR (126 MHz, DMSO) of compound **5e.**

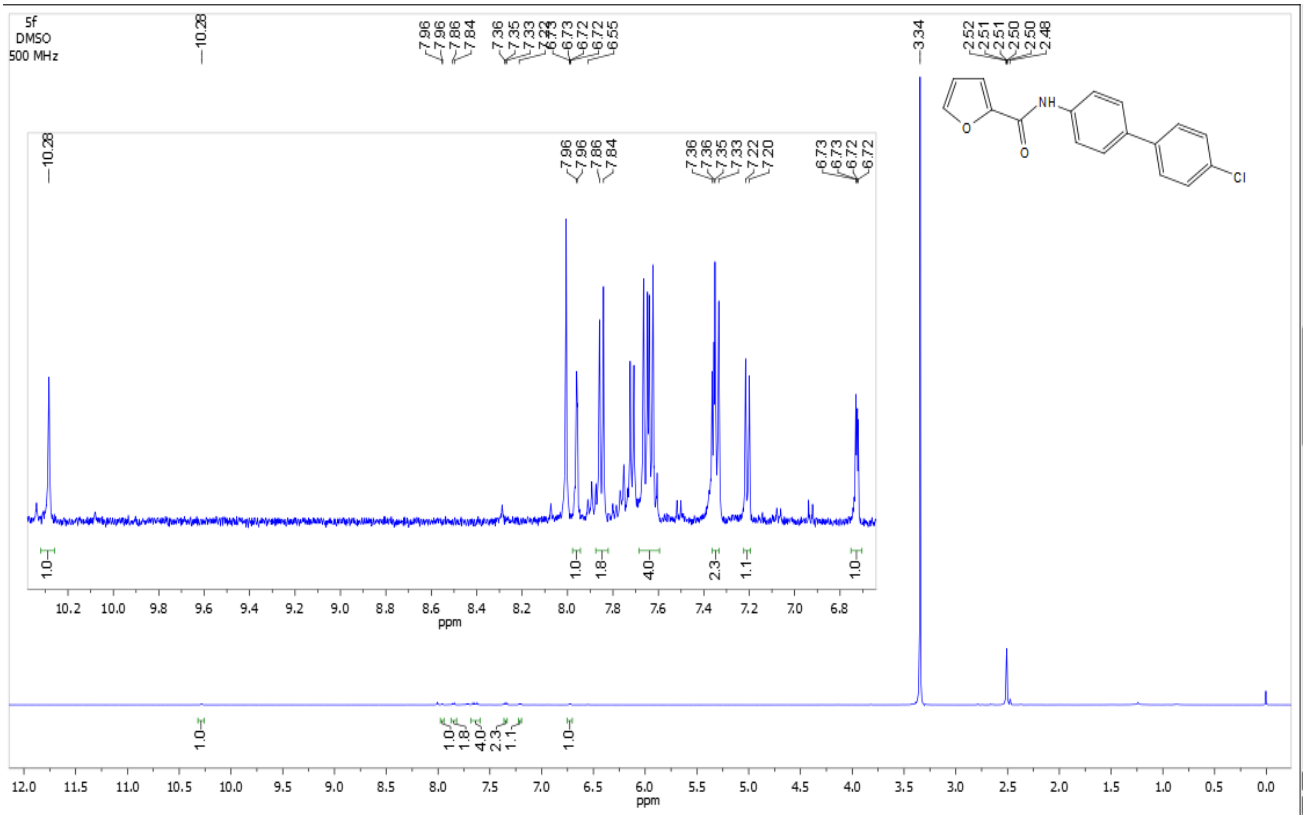


Figure S11: [1]HNMR (500 MHz, DMSO) of compound **5f.**

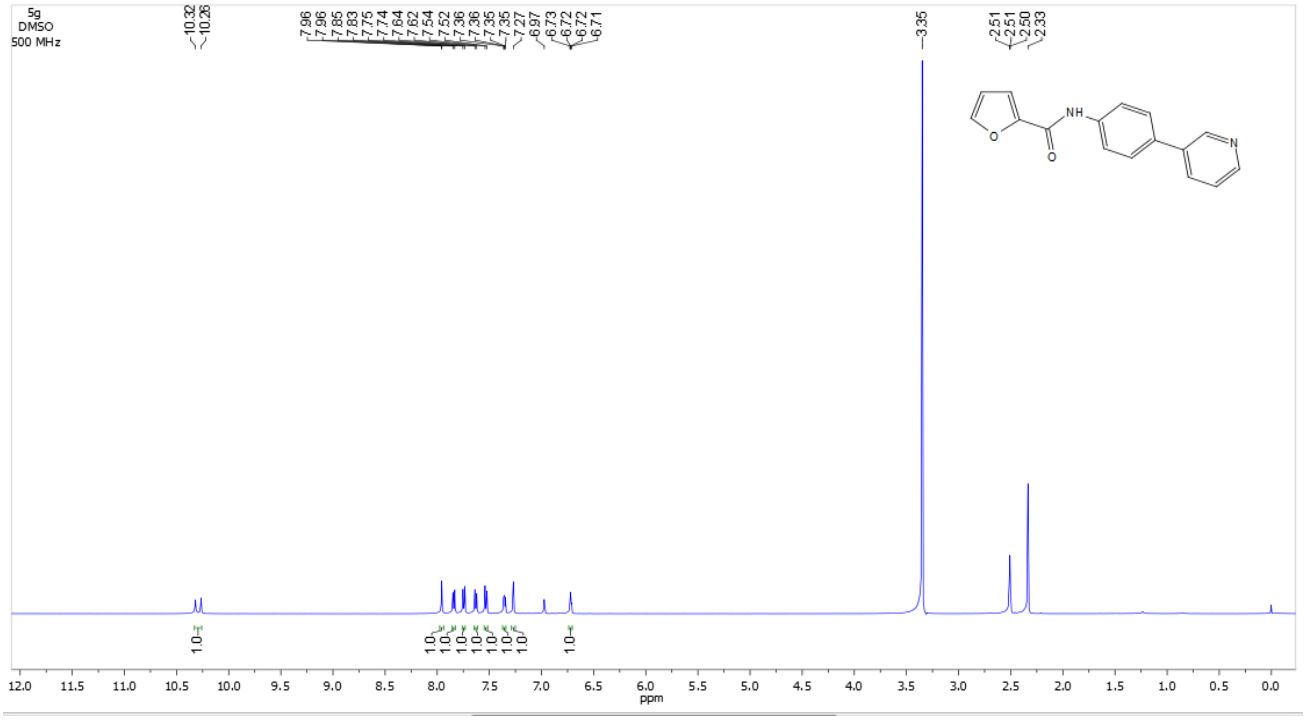


Figure S12: [1]HNMR (500 MHz, DMSO) of compound **5g.**

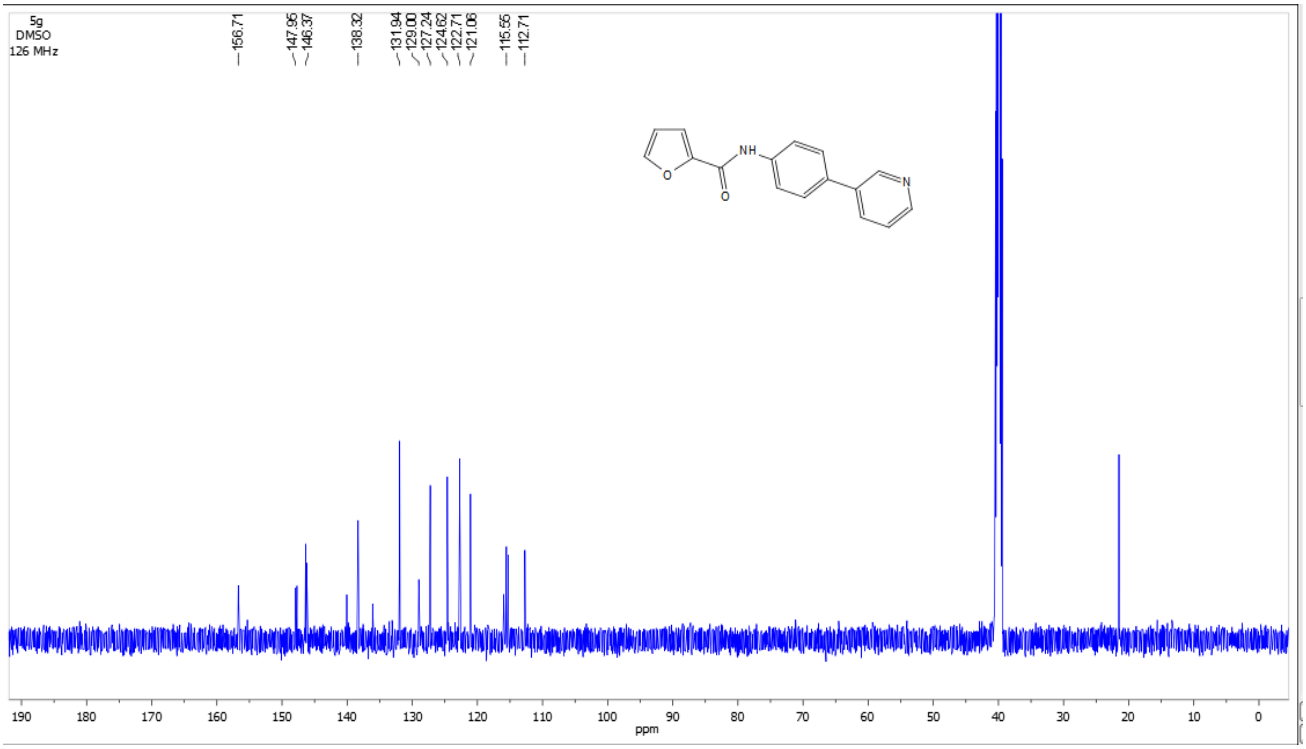


Figure S13: ^{13}CNMR (126 MHz, DMSO) of compound **5g.**

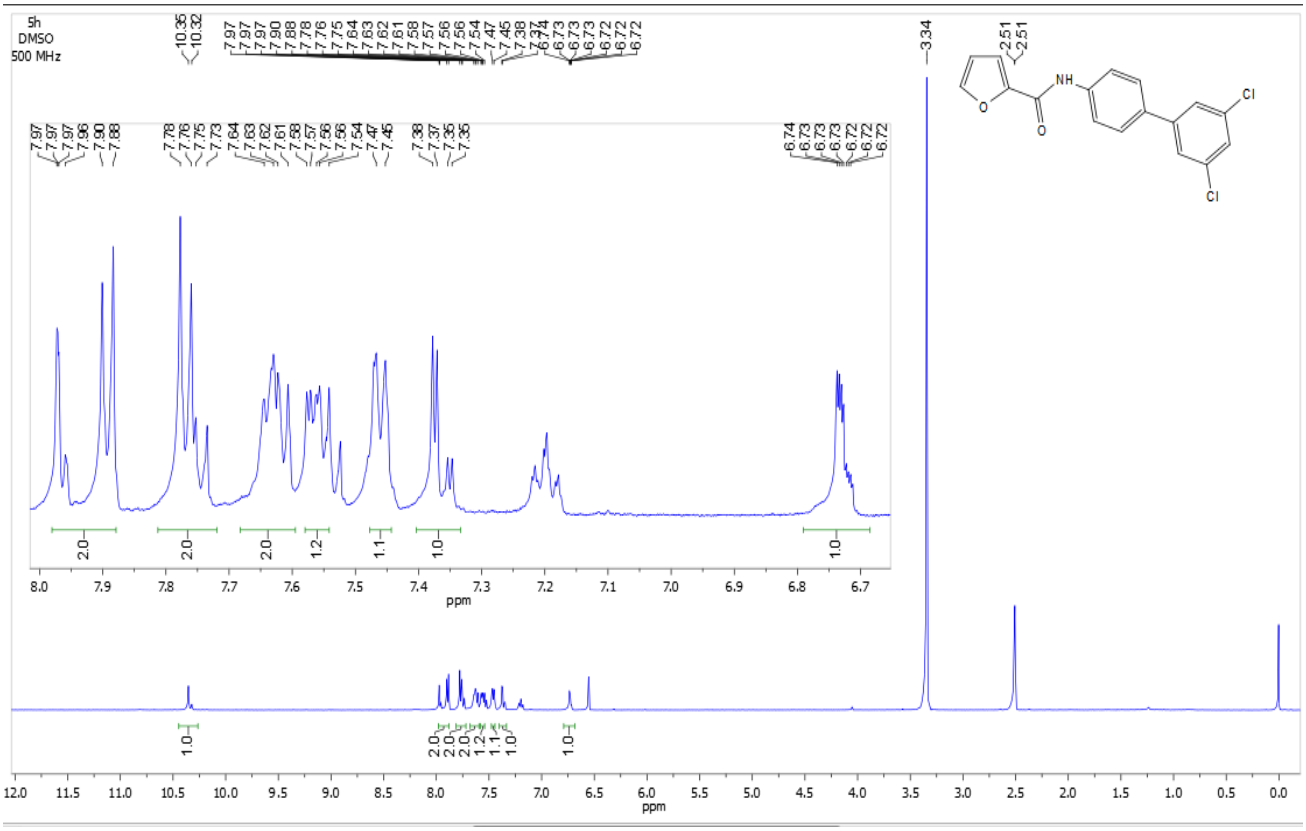


Figure S14: ^{1}HNMR (500 MHz, DMSO) of compound **5h.**

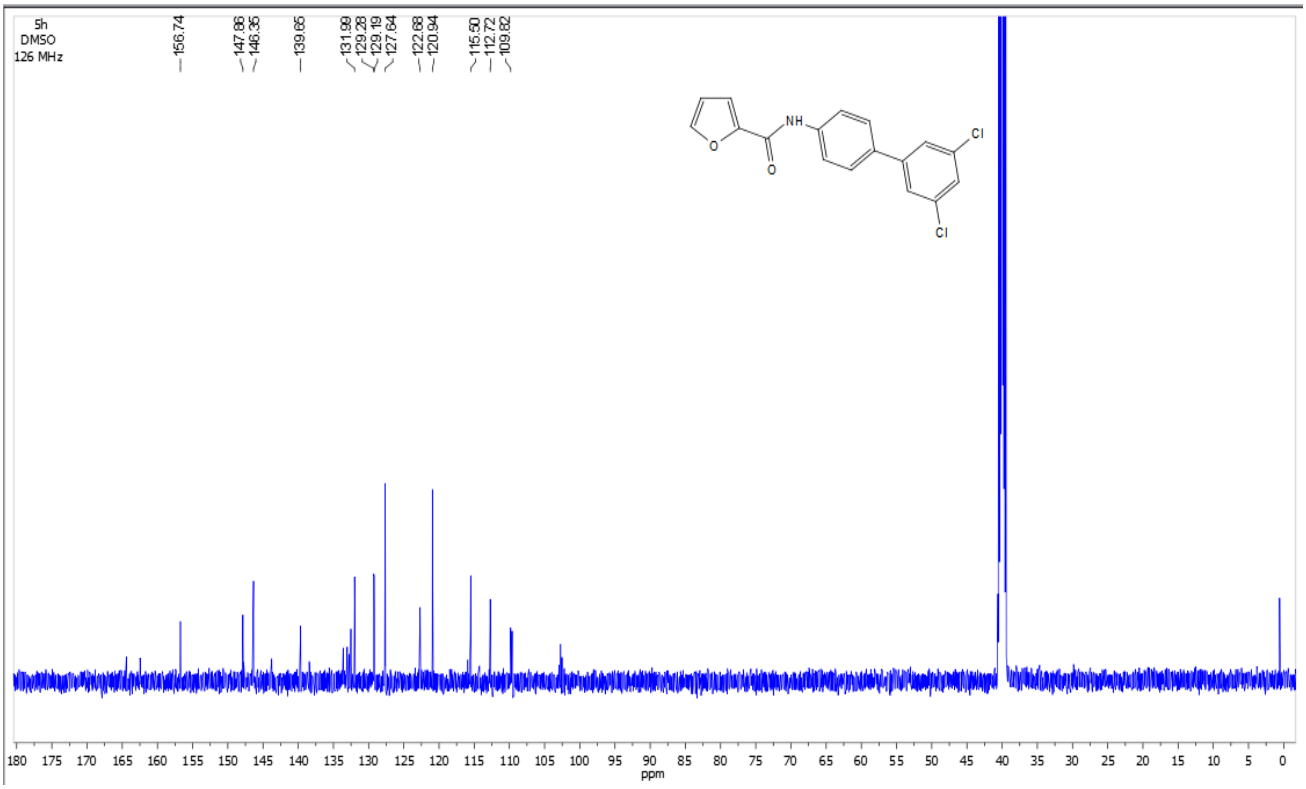


Figure S15: ^{13}CNMR (126 MHz, DMSO) of compound **5h.**

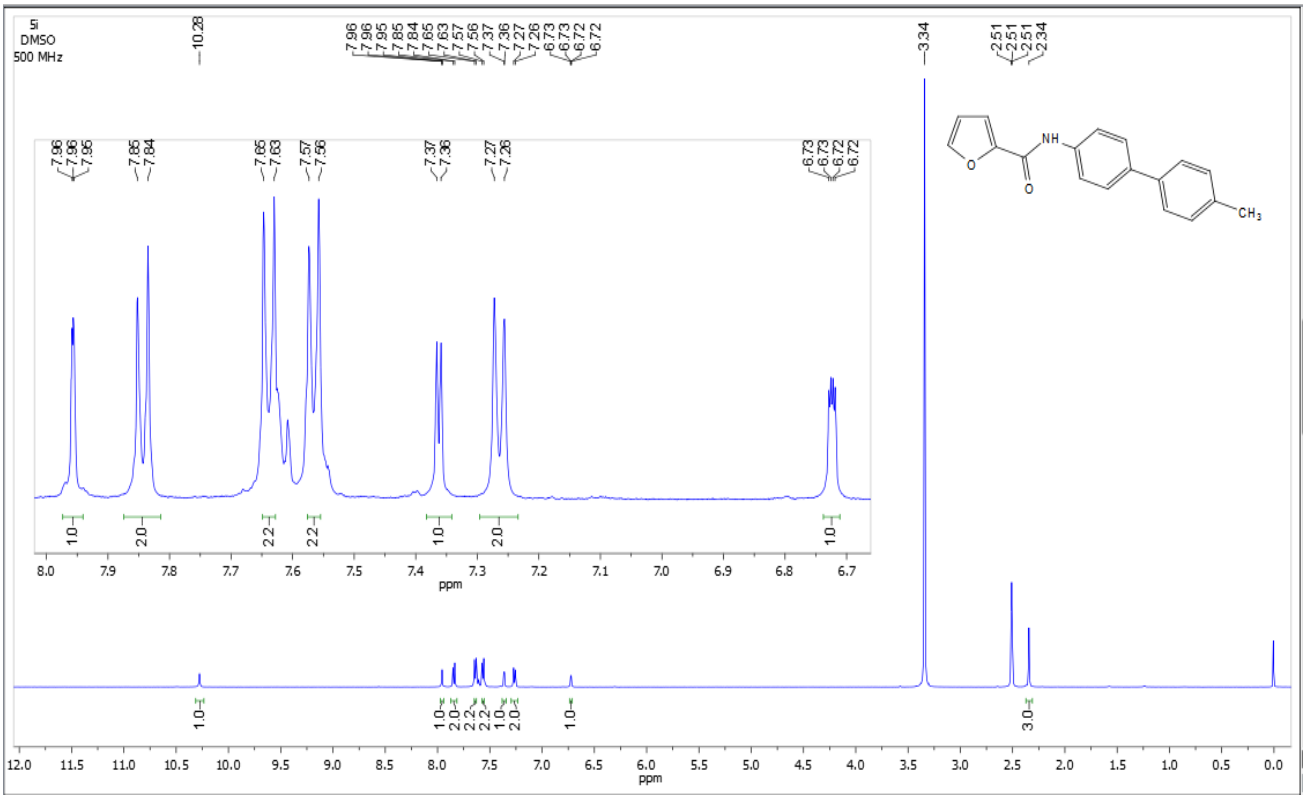
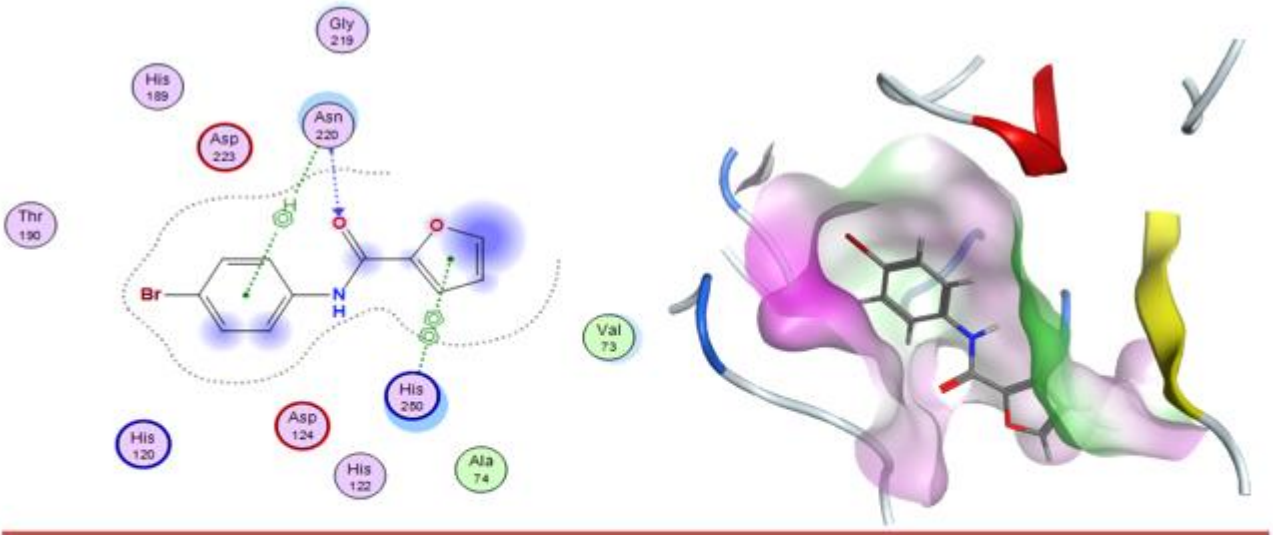
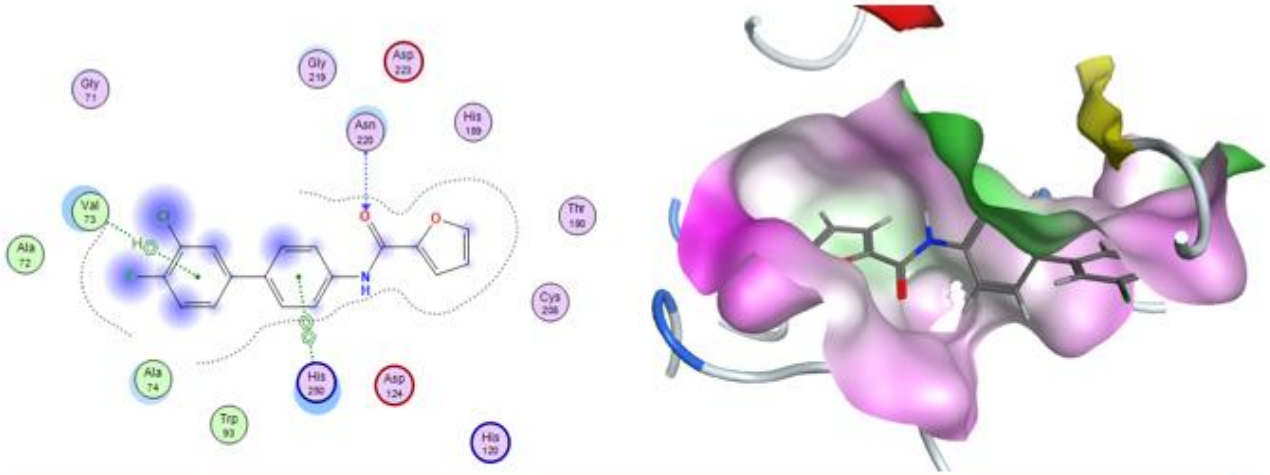


Figure S16: ^{1}HNMR (500 MHz, DMSO) of compound **5i.**



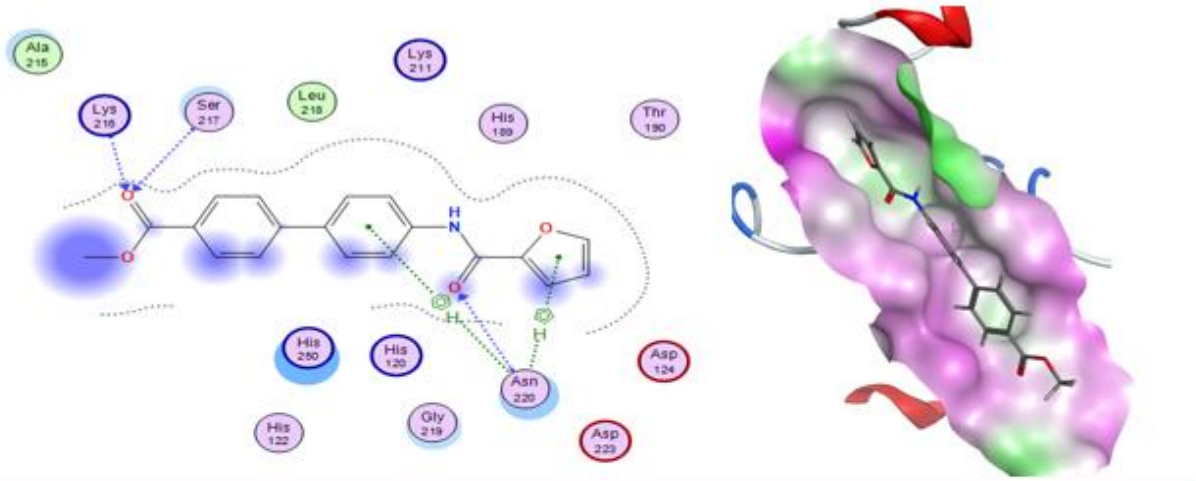
Ligand	Receptor	Interaction	Distance	Energy
O	N ASN 220	H-acceptor	3.17	-0.28
6-ring	CB ASN 220	pi-H	4.53	
5-ring	5-ring HIS 250	pi-pi	3.87	

Figure S17: Molecular docking and interaction pattern of compound **3**.



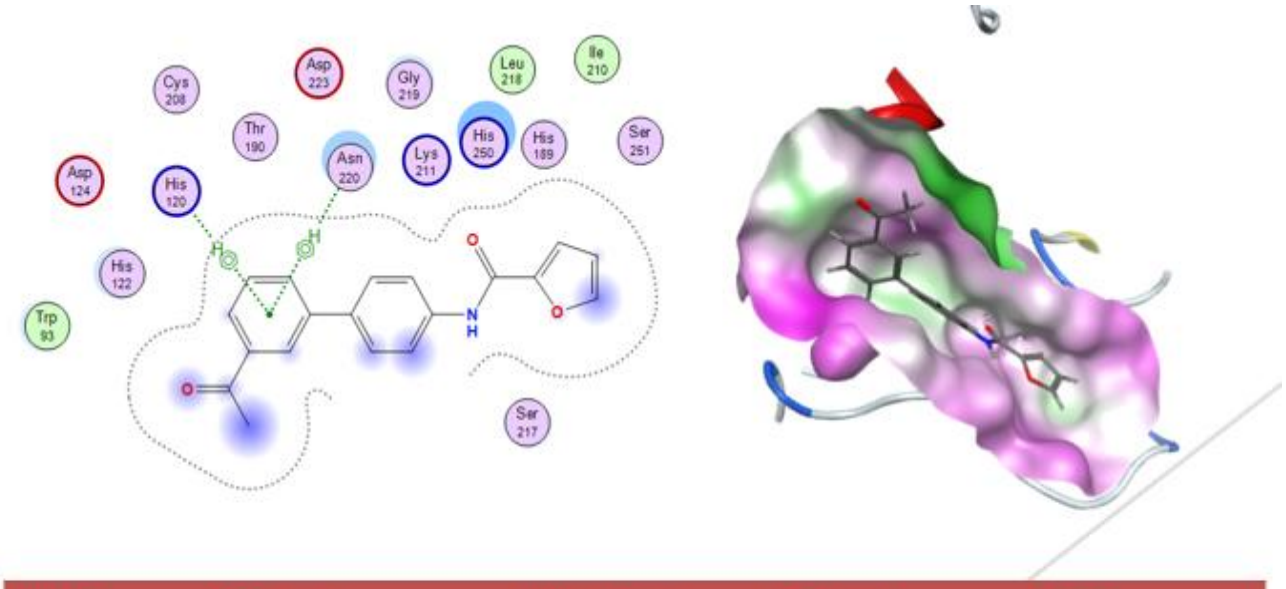
Ligand	Receptor	Interaction	Distance	Energy
O	N ASN 220	H-acceptor	2.66	0.695
6-ring	CA VAL 73	pi-H	4.22	
5-ring	5-ring HIS 250	pi-pi	3.47	

Figure S18: Molecular docking and interaction pattern of compound **5a**.



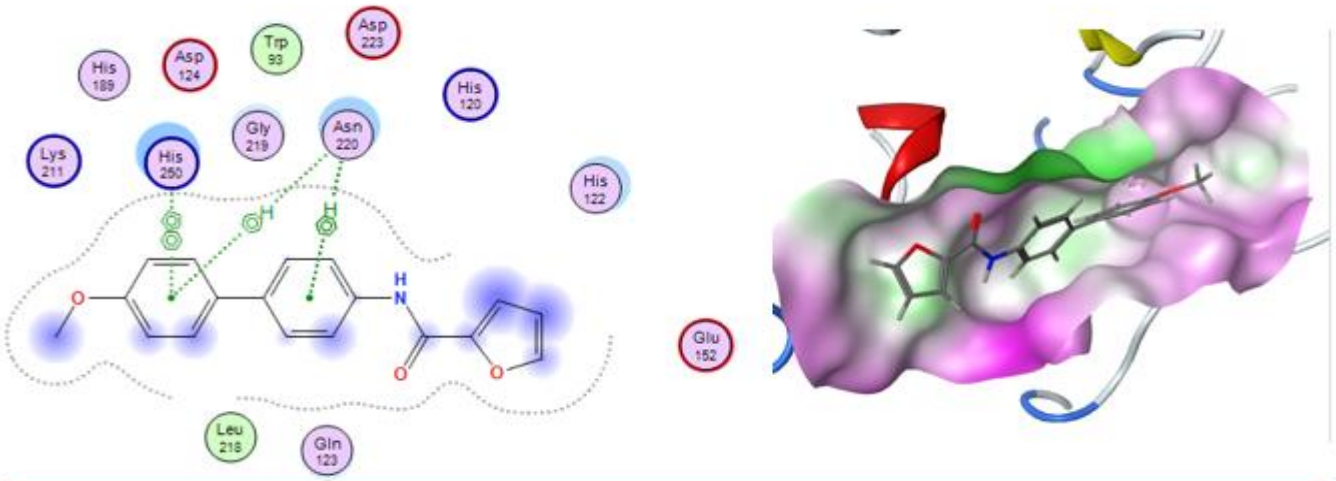
Ligand	Receptor		Interaction	Distance	Energy
O	N	ASN 220	H-acceptor	3.21	-0.25
O	N	LYS 216	H-acceptor	2.55	
O	N	SER 217	H-acceptor	3.40	
6-ring	N	ASN 220	pi-H	4.43	
5-ring	ND2	ASN 220	pi-H	3.64	

Figure S19: Molecular docking and interaction pattern of compound **5b**.



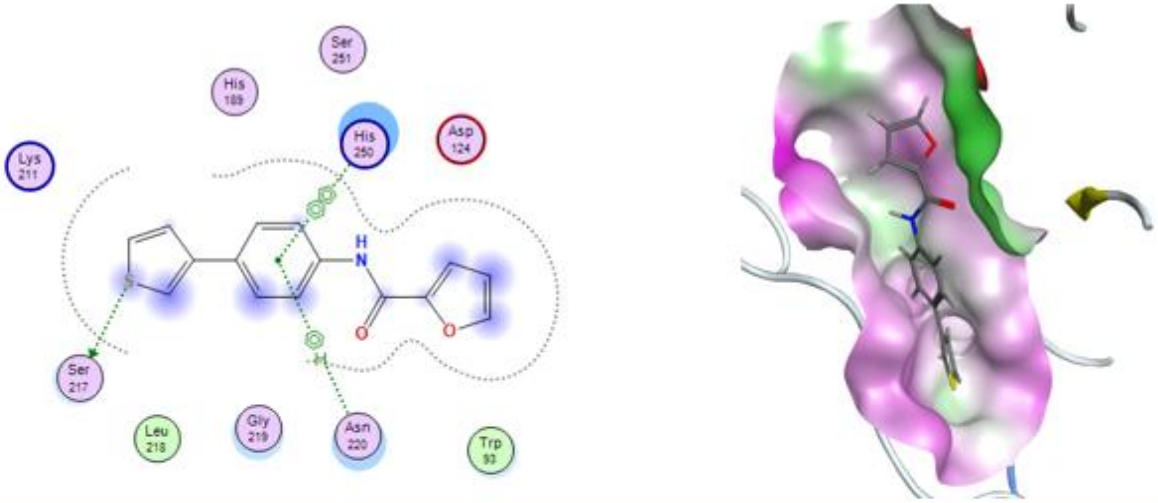
Ligand	Receptor		Interaction	Distance	Energy
O	CE1	HIS 120	pi-H	3.52	-4.5
6-ring	ND2	ASN 220	pi-H	3.67	

Figure S20: Molecular docking and interaction pattern of compound **5c**.



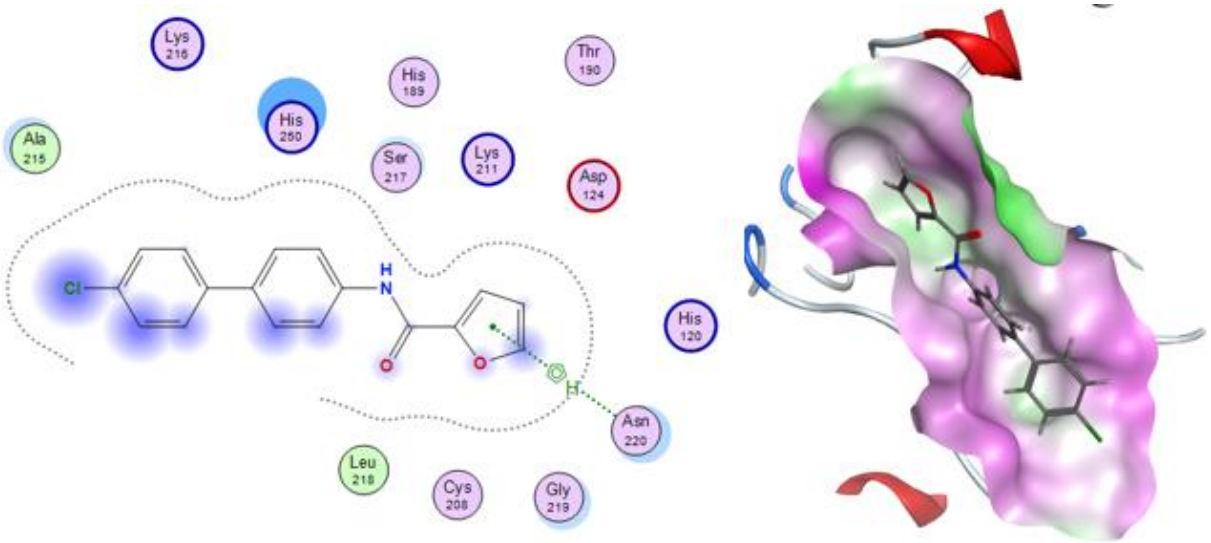
Ligand	Receptor	Interaction	Distance	Energy
6-ring	N ASN 220	pi-H	4.48	-2.1
6-ring	CB ASN 220	pi-H	4.37	
6-ring	ND2 ASN 220	pi-H	4.04	
6-ring	5-ring HIS 250	pi-pi	3.69	

Figure S21: Molecular docking and interaction pattern of compound **5d**



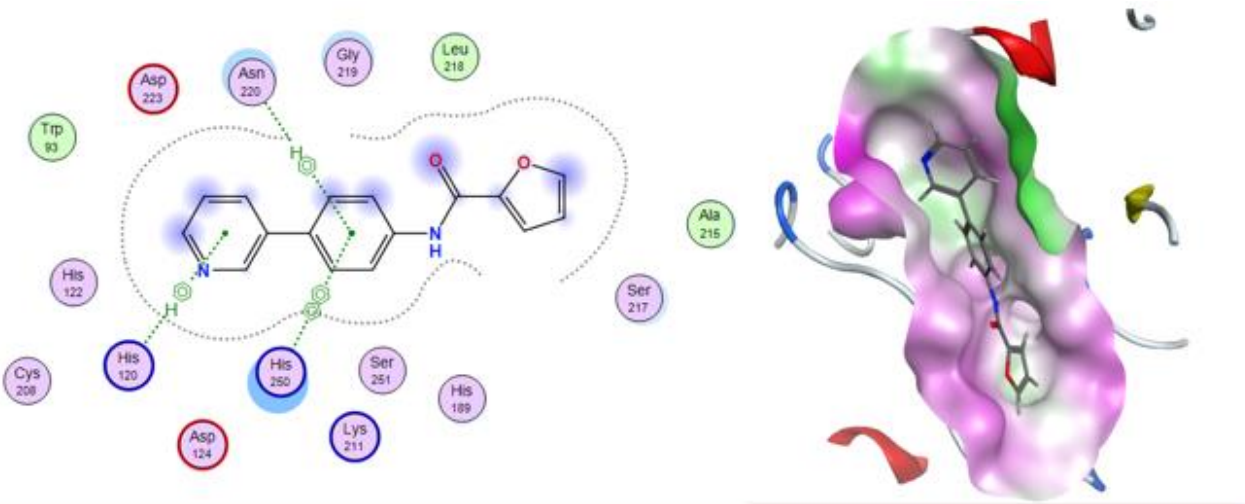
Ligand	Receptor	Interaction	Distance	Energy
S 26	OG SER 217	H-donor	3.48	-1.07
6-ring	N ASN 220	pi-H	4.32	
6-ring	5-ring HIS 250	pi-pi	3.78	
6-ring				

Figure S22: Molecular docking and interaction pattern of compound **5e**.



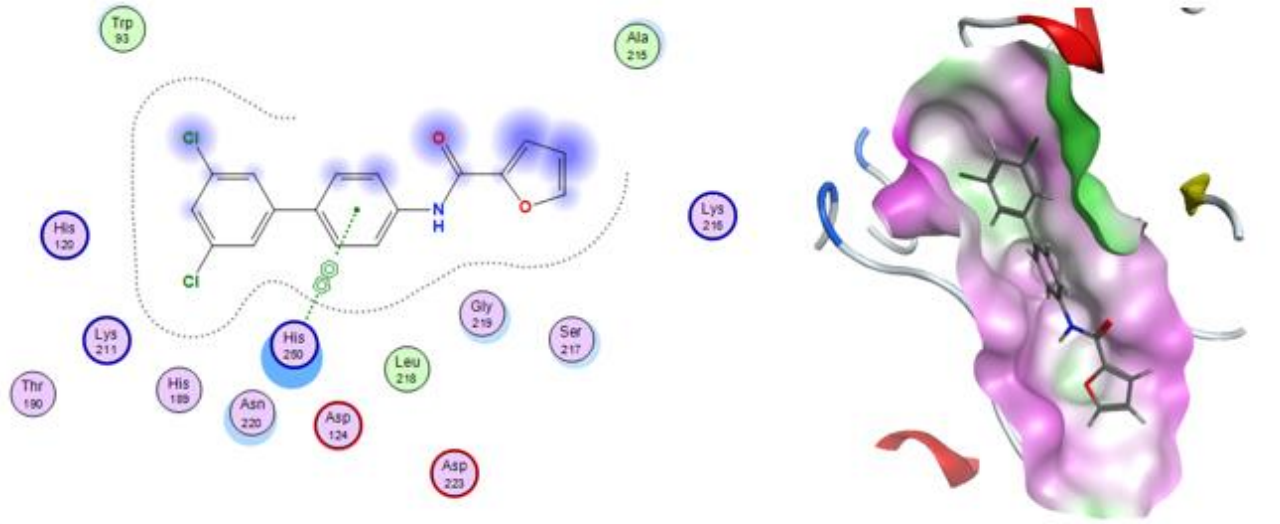
Ligand	Receptor	Interaction	Distance	Energy
6-ring	ND2 ASN 220	pi-H	4.19	

Figure S23: Molecular docking and interaction pattern of compound **5f**.



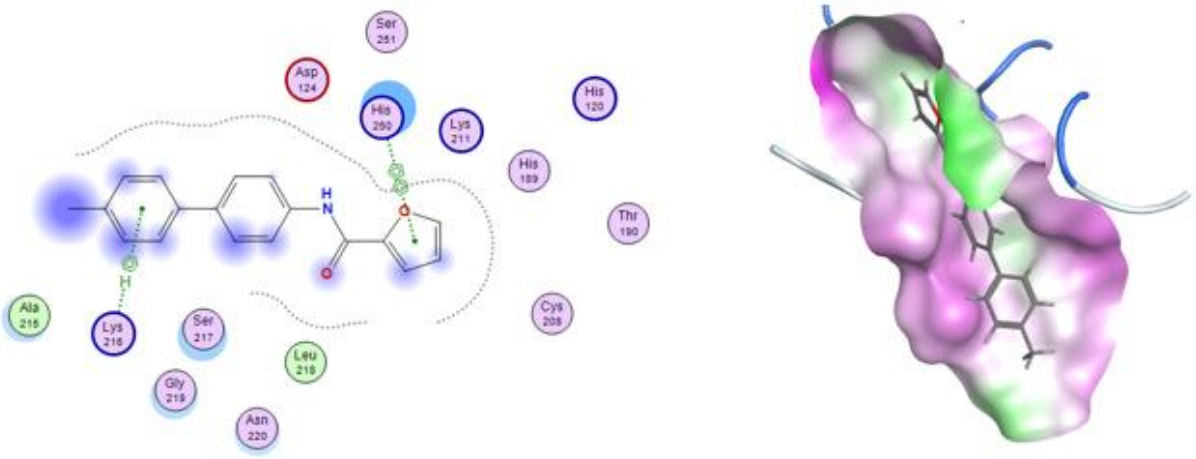
Ligand	Receptor	Interaction	Distance	Energy
6-ring	CE1 HIS 120	pi-H	4.07	-1.3
6-ring	N ASN 220	pi-H	4.29	
6-ring	5-ring HIS 250	pi-pi	3.58	

Figure S24: Molecular docking and interaction pattern of compound **5g**.



Ligand	Receptor	Interaction	Distance	Energy
6-ring	5-ring HIS 250	pi-pi	3.92	-2.17

Figure S25: Molecular docking and interaction pattern of compound **5h**.



Ligand	Receptor	Interaction	Distance	Energy
6-ring 5-ring	N LYS 216 5-ring HIS 250	pi-H pi-pi	4.58 3.99	-3.78

Figure S26: Molecular docking and interaction pattern of compound **5i**.

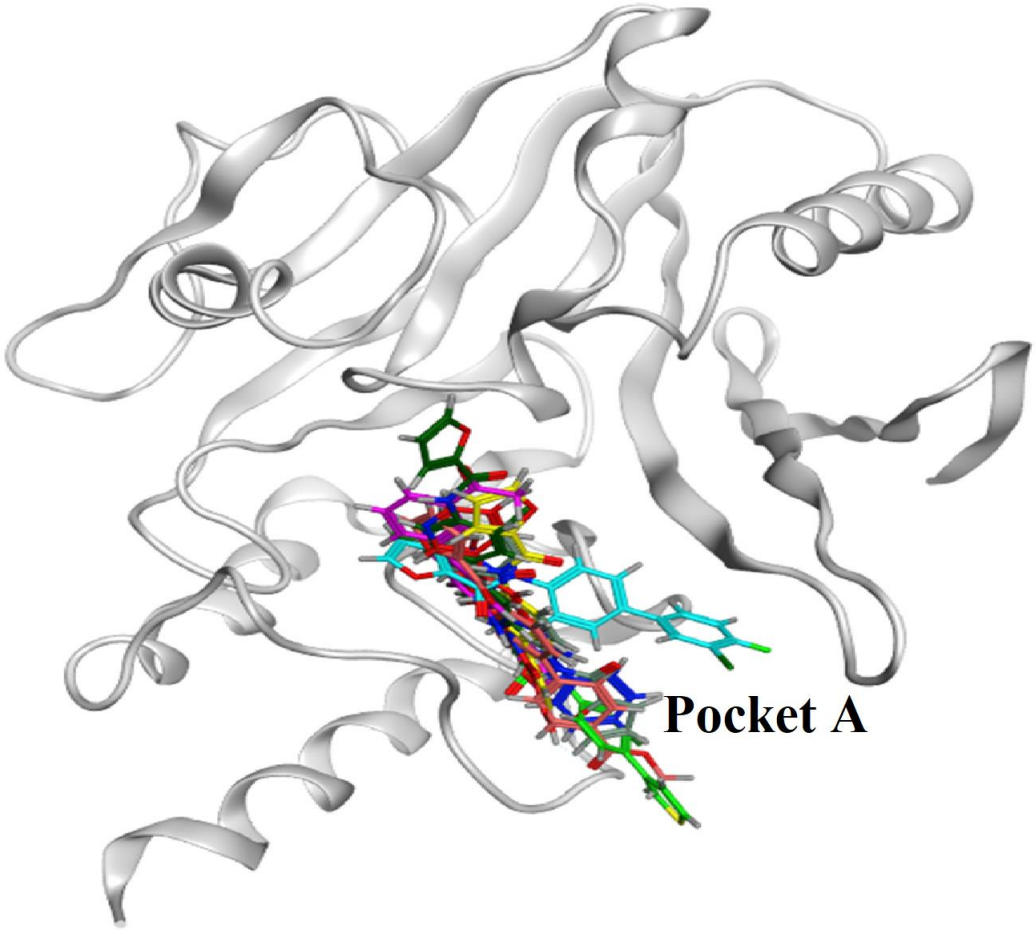


Figure S27: The selected conformation of each Ligand (3, 5a-5i) demonstrate binding in the pocket A of NDM-1 protein.

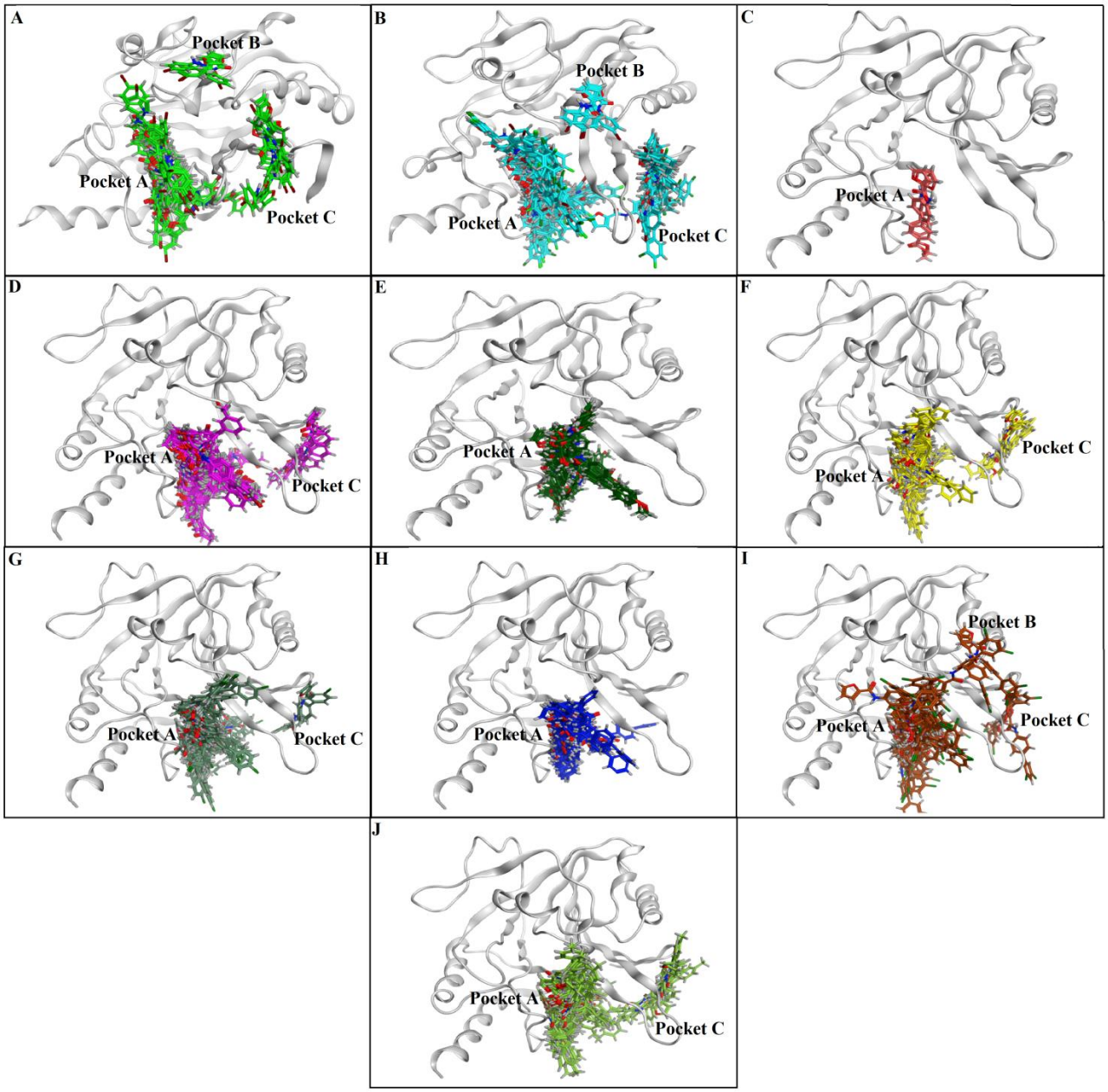


Figure S28: Ligand binding to the NDM-1 protein displaying three major binding cavities (Pocket A, Pocket B and Pocket C). It has been clearly observed that for each ligand maximum conformations are occupied in the pocket A of NDM-1 protein. (A)(C) (I) compound 3 , 5b and 5h occupies pocket A, B and C. (C)(H) compound 5b and 5g conformations only occupies pocket A. (D) (E)(F) (G)(J) Compound 5c, 5d, 5e, 5f and 5i occupies pocket A and C .

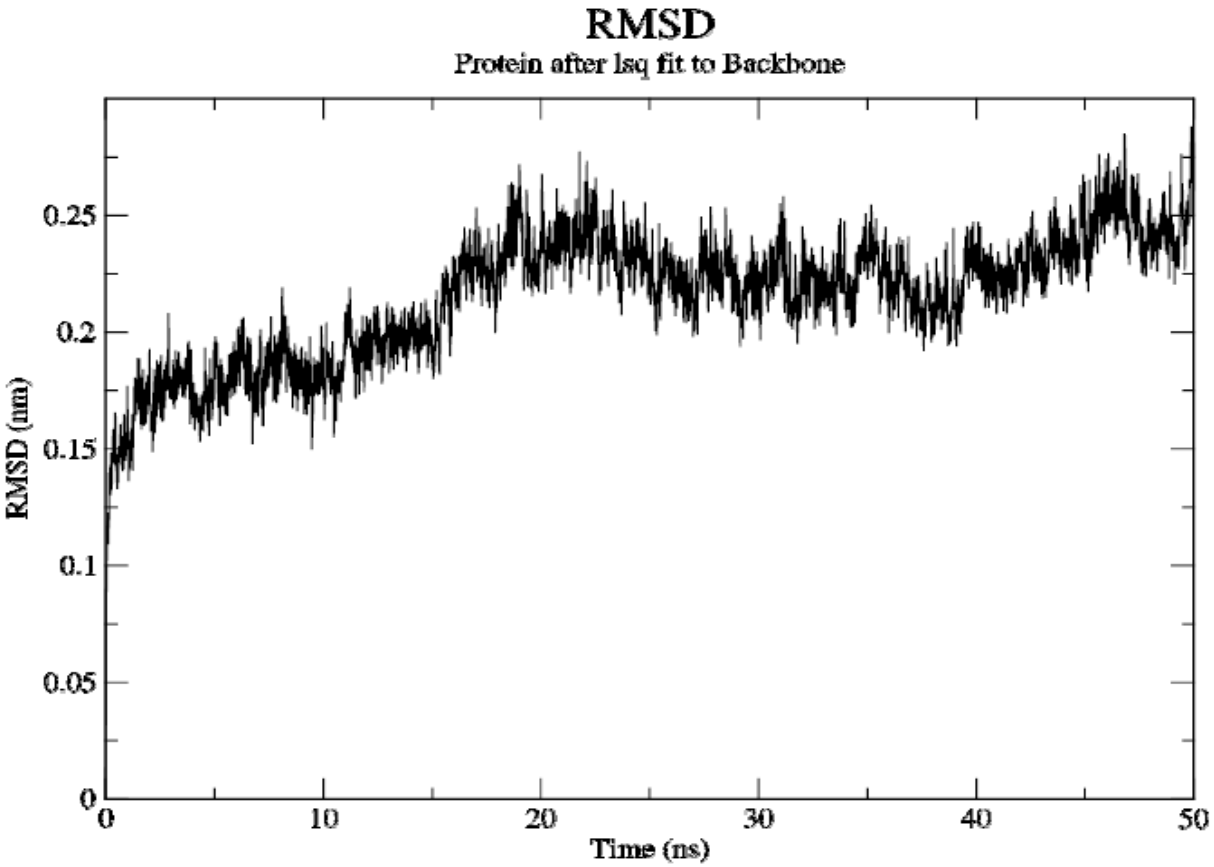


Figure S29: RMSD graph of compound **3**.

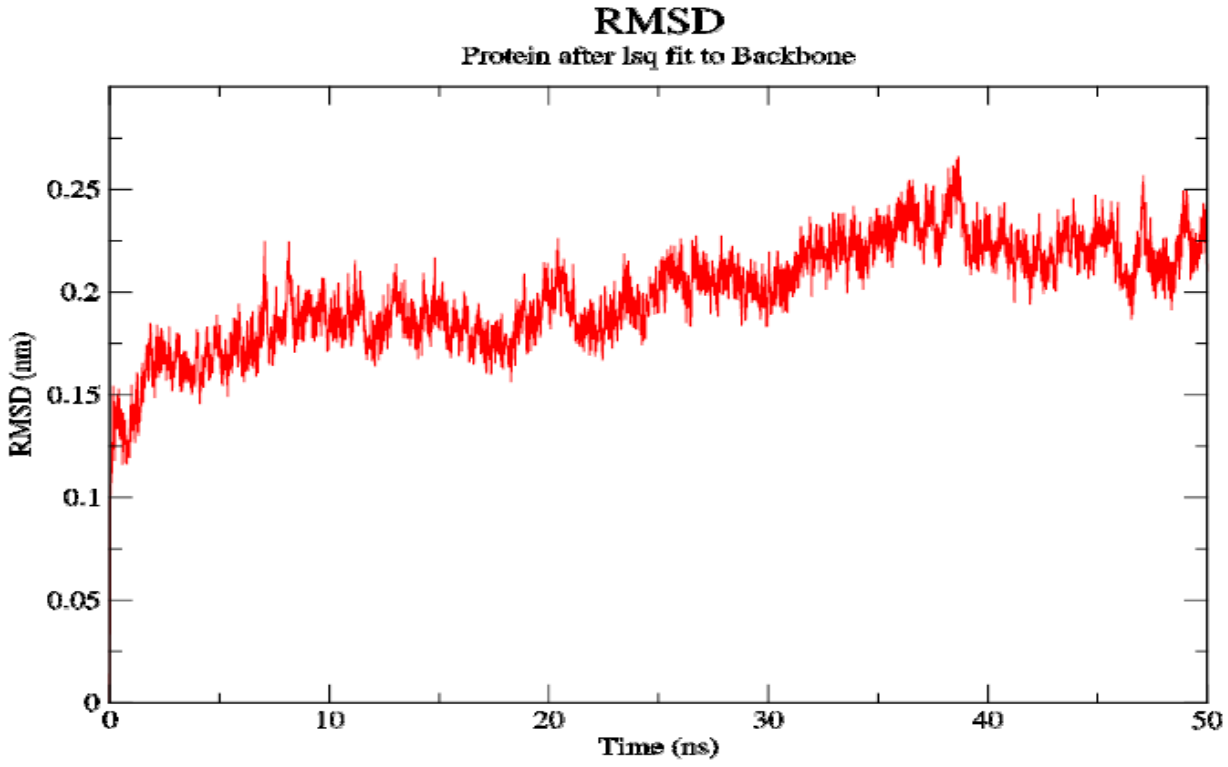


Figure S30: RMSD graph of compound **5c**.

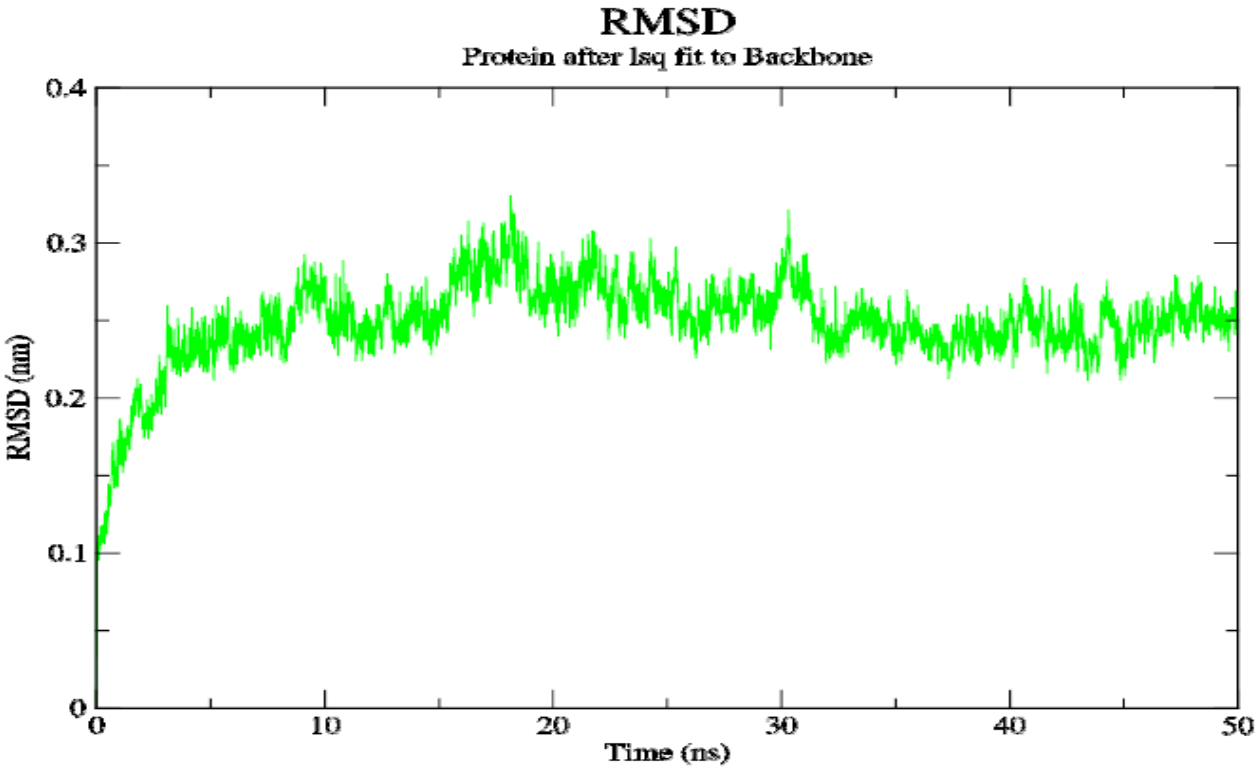


Figure S31: RMSD graph of compound **5g**.

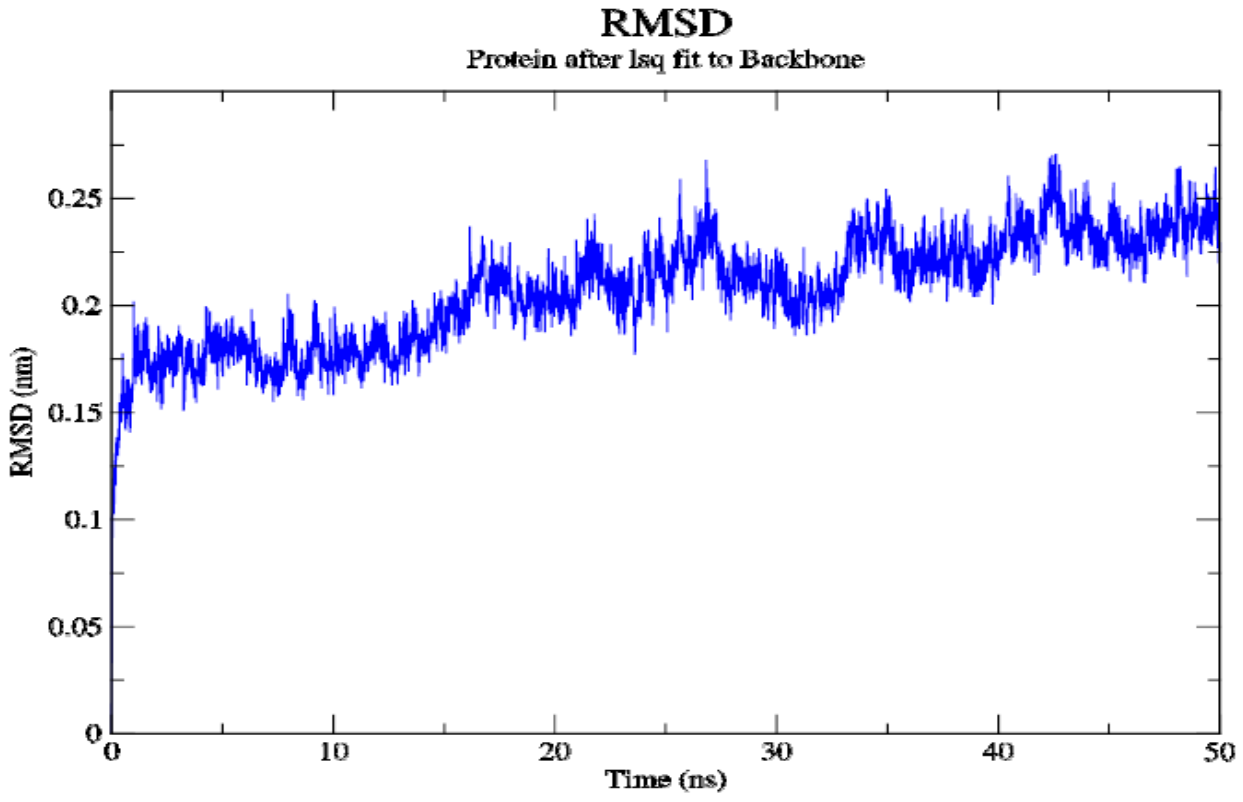


Figure S32: RMSD graph of compound **5h**.

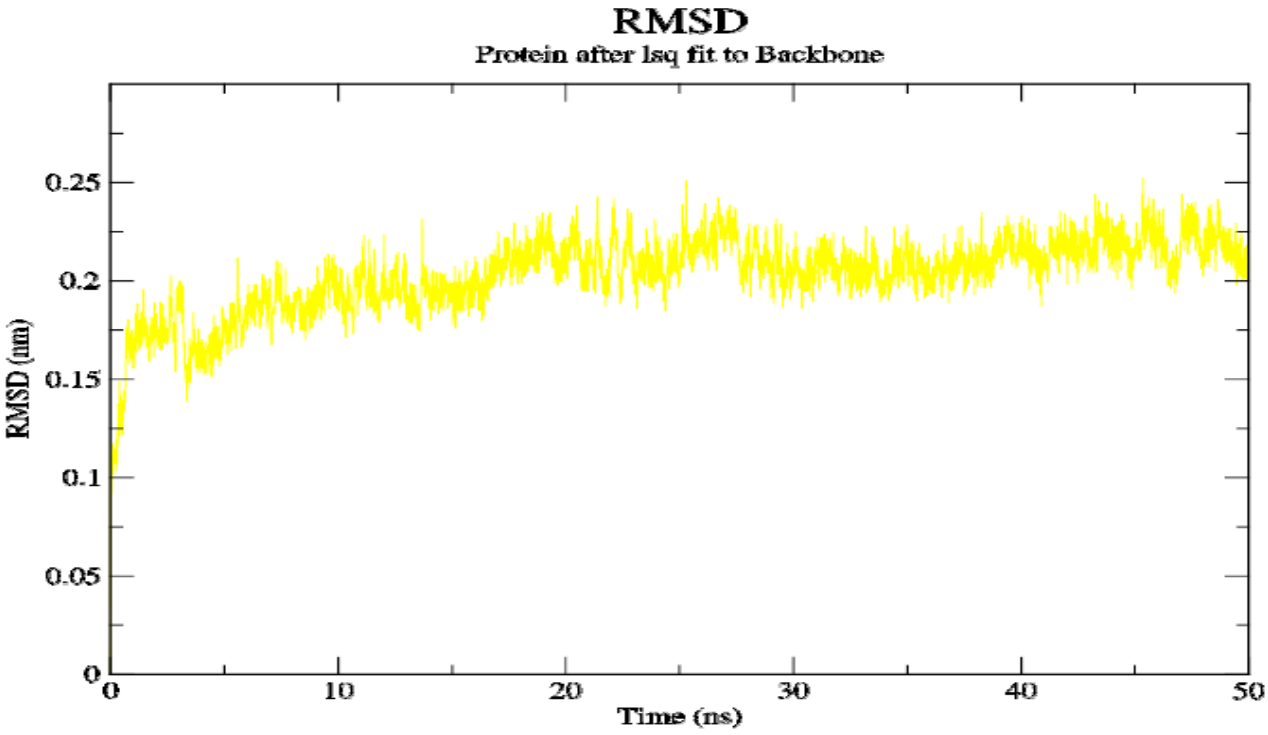
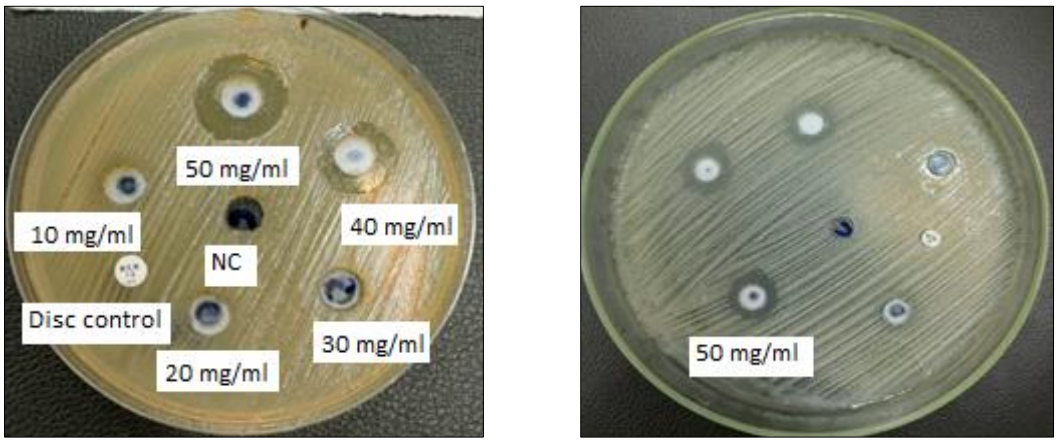
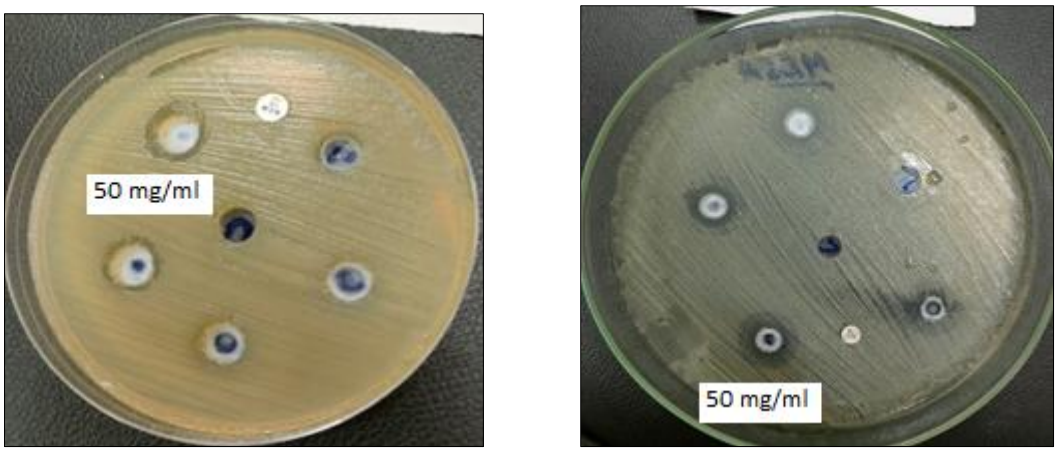


Figure S33: RMSD graph of compound **5i**.



CRAB **CREC**



CRKP **MRSA**

Figure S34. Antibacterial activity of (**3**) against XDR pathogens.

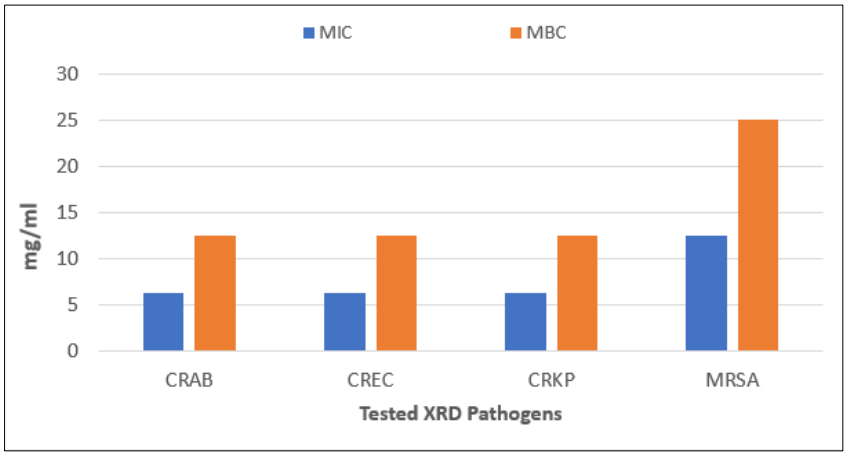
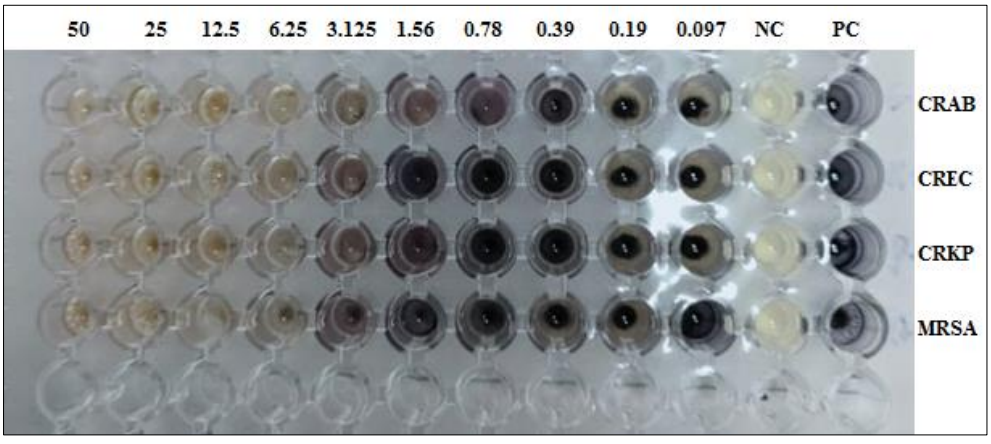


Figure S35. MIC (mg/ml) and MBC of compound **(3)** against XDR pathogens.



NC: Negative control; PC: Positive control

Figure S36. MIC of **3** compound against XDR pathogens