Facile synthesis of 4-aryl-*N*-(5-methyl-1*H*-pyrazol-3-yl)benzamides *via* Suzuki Miyaura reaction: antibacterial activity against clinically isolated NDM-1-positive bacteria and their Docking Studies

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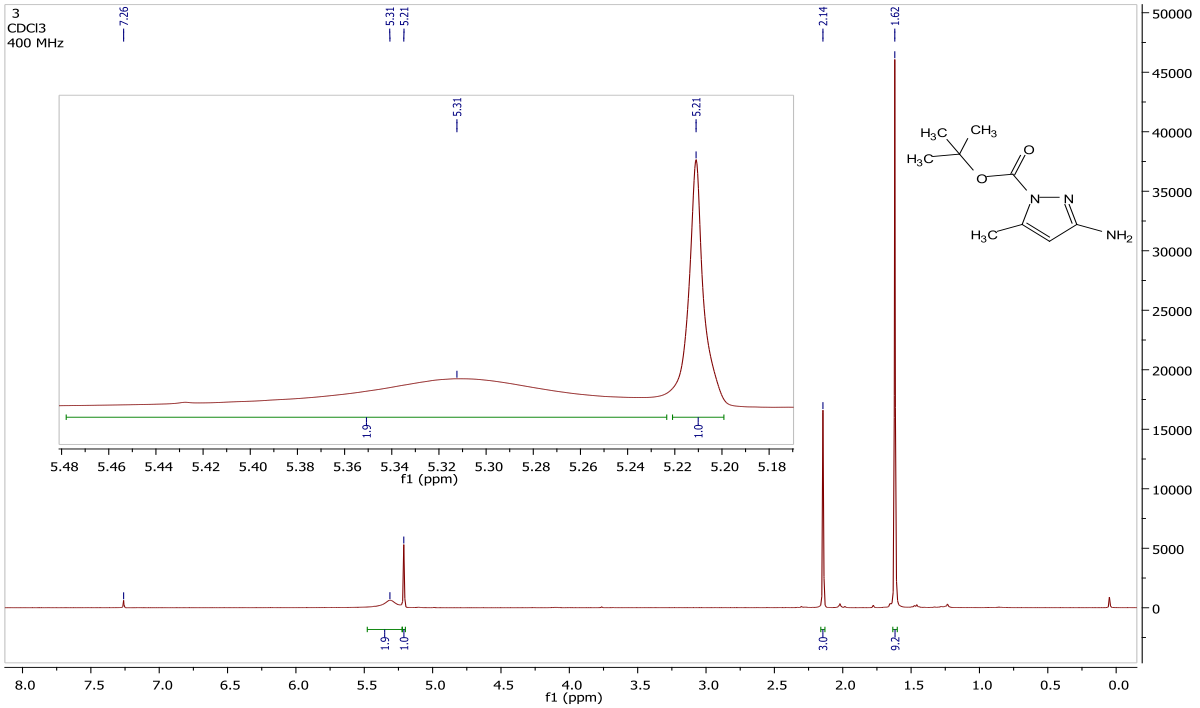

Figure S1: ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3**.

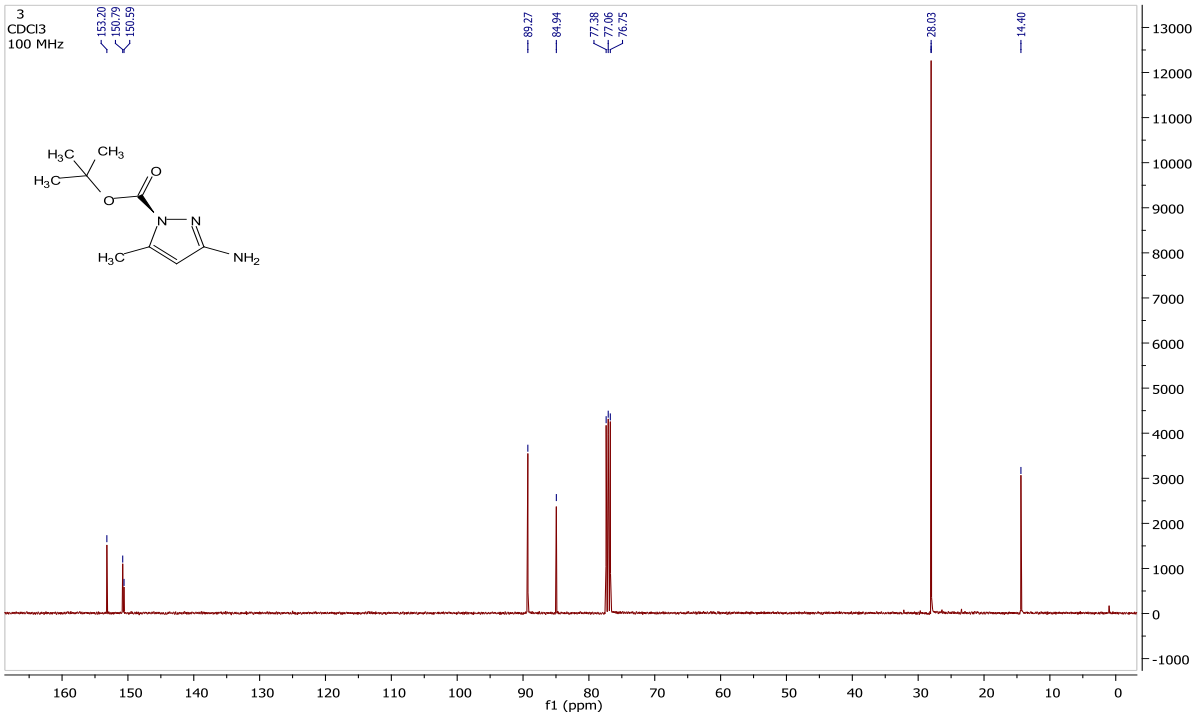

Figure S2: ^{13}C NMR (100 MHz, $CDCl_3$) of compound **3**.

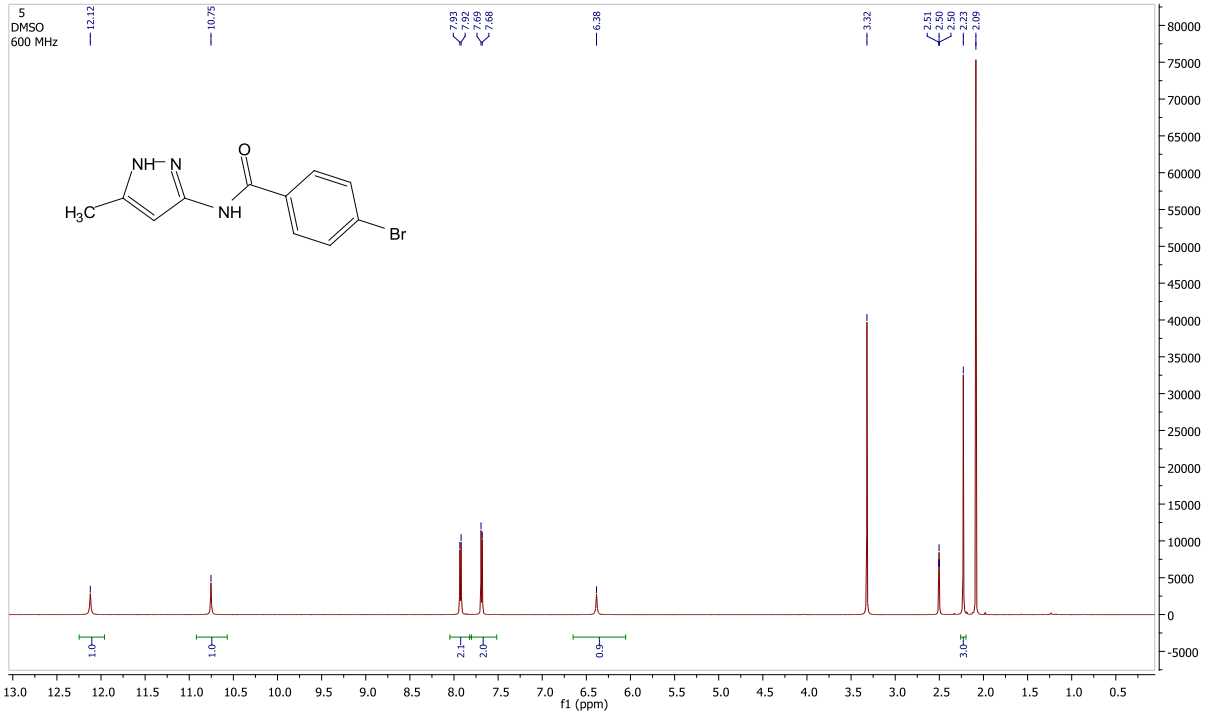

Figure S3: ^{1}H NMR (600 MHz, DMSO-d_6) of compound **5**.

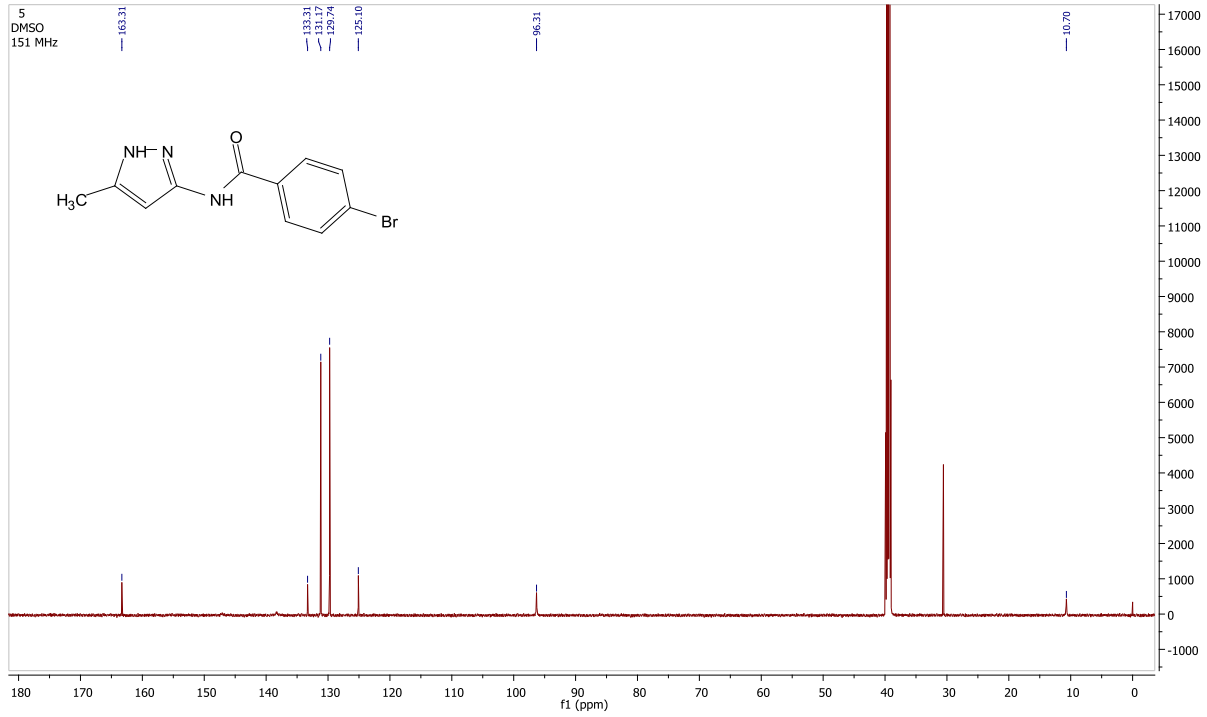

Figure S4: ^{13}C NMR (151 MHz, DMSO-d_6) of compound **5**.

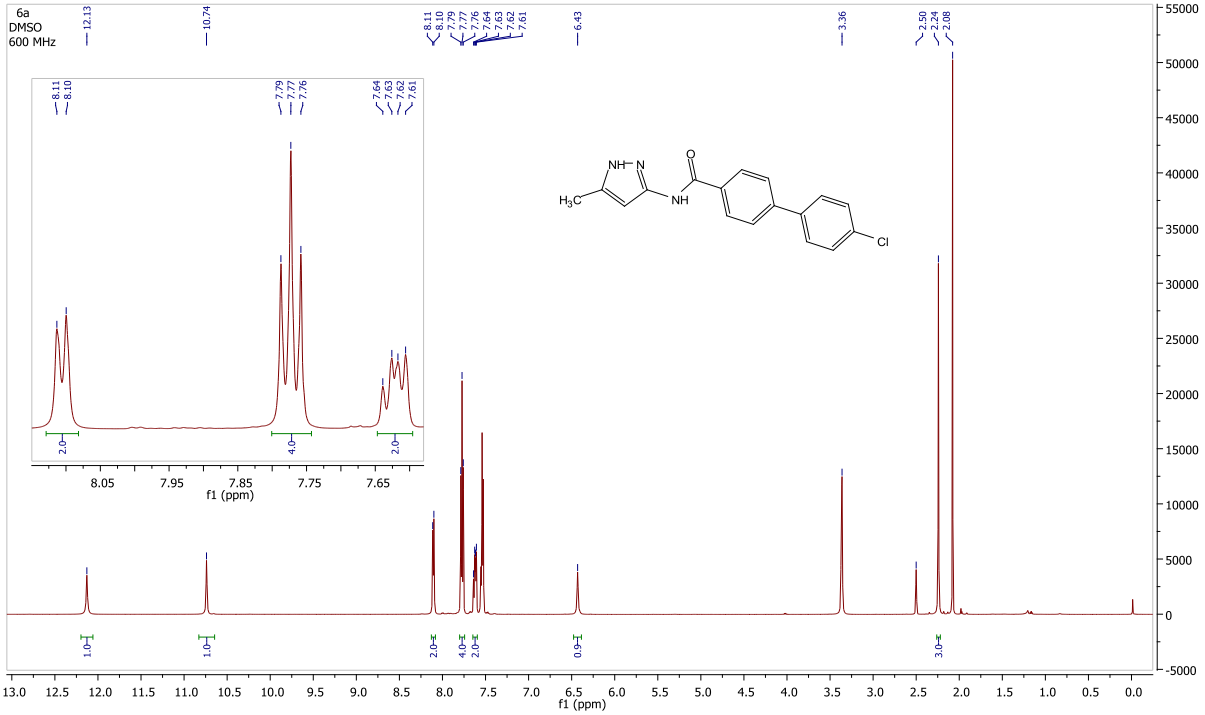

Figure S5: ^{1}H NMR (600 MHz, DMSO-d_6) of compound **6a**.

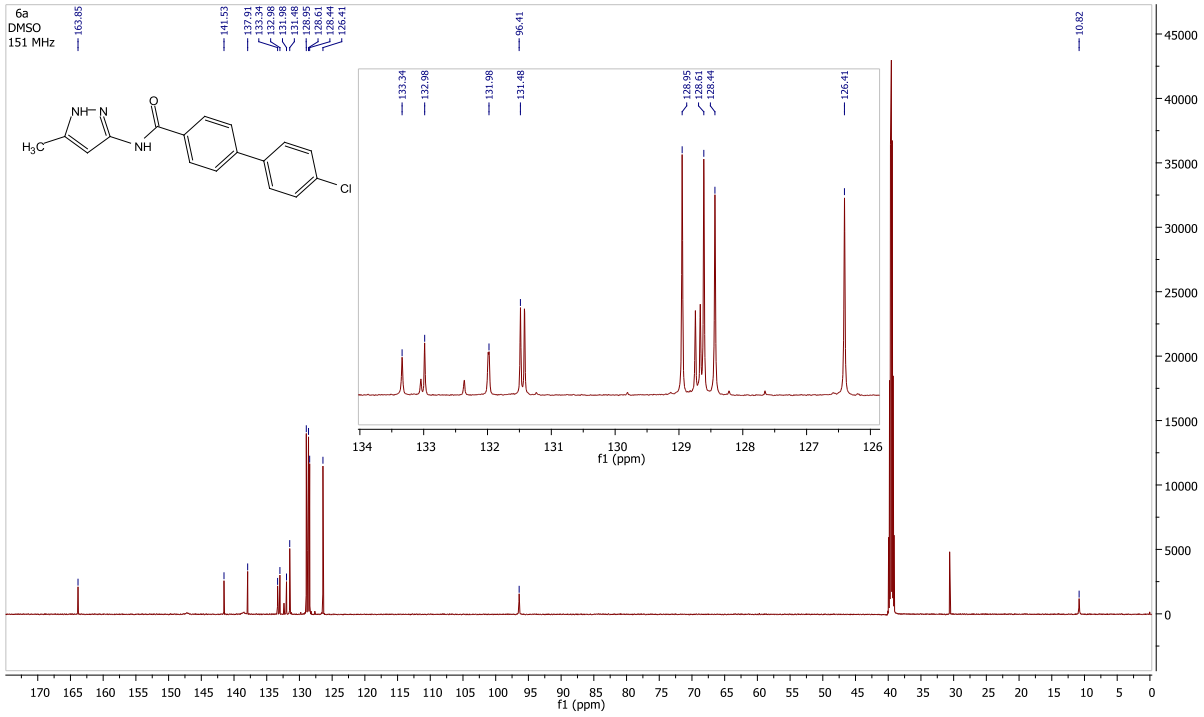

Figure S6: ^{13}C NMR (151 MHz, DMSO-d_6) of compound **6a**.

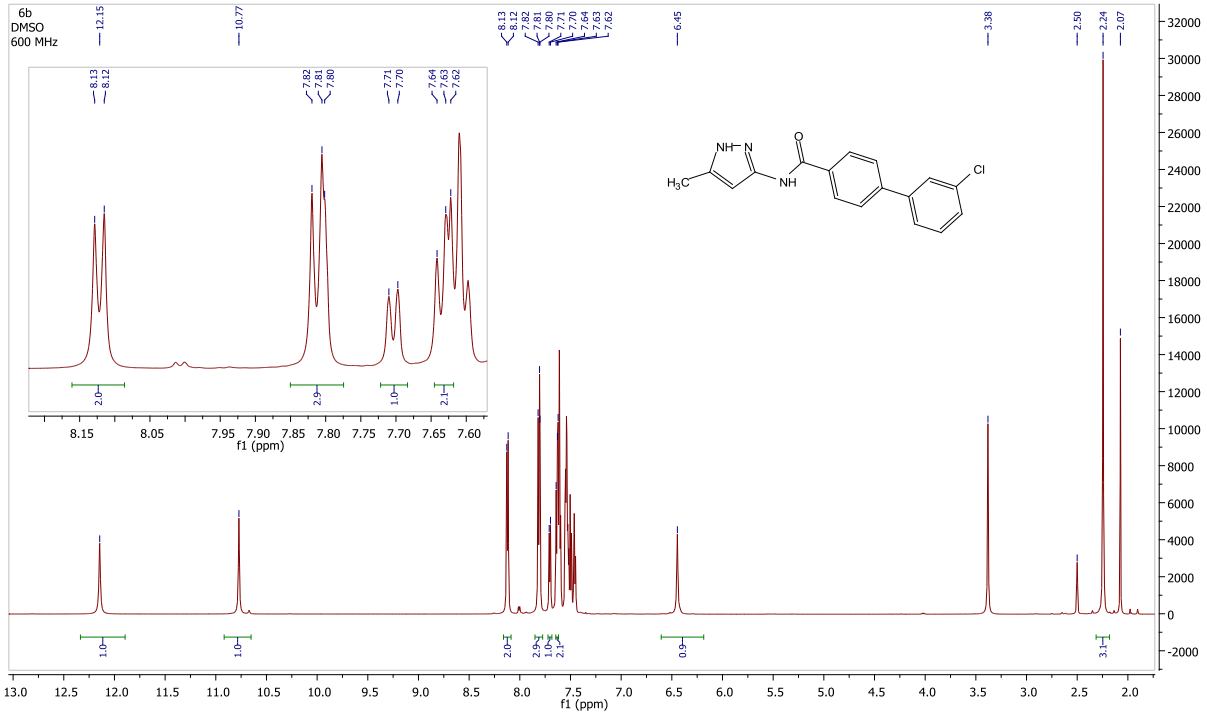

Figure S7: ^{1}H NMR (600 MHz, DMSO-d_6) of compound **6b**.

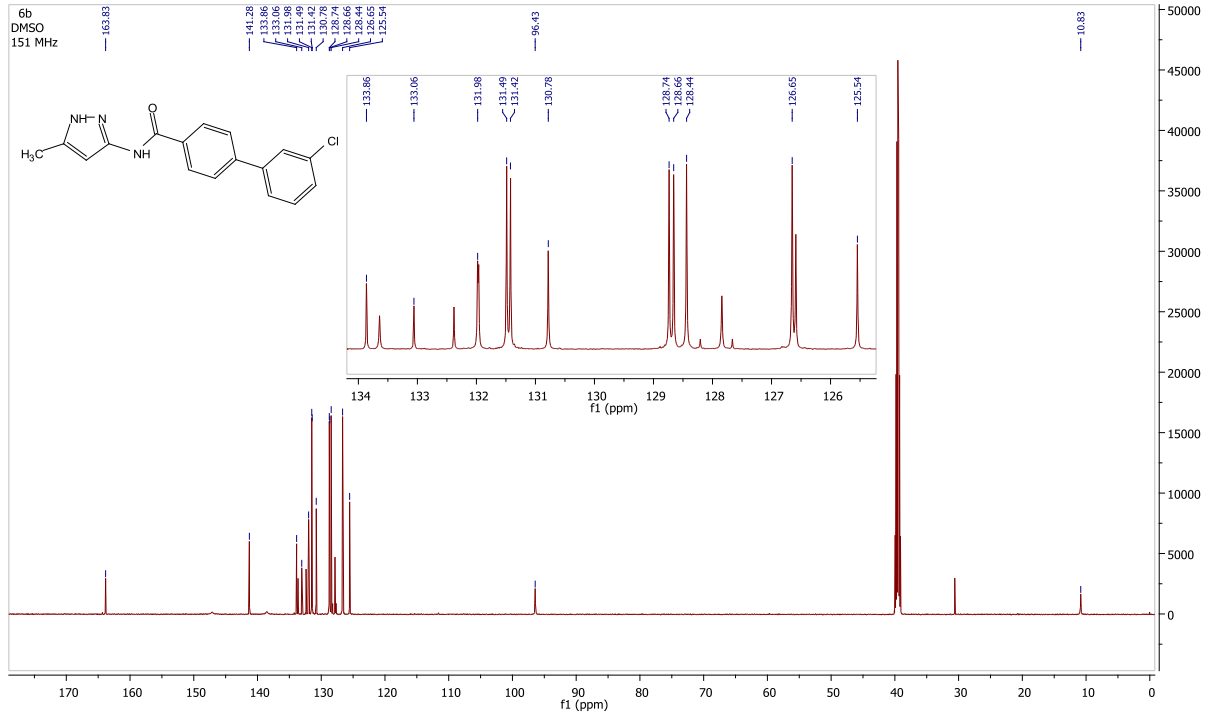

Figure S8: ^{13}C NMR (151 MHz, DMSO-d_6) of compound **6b**.

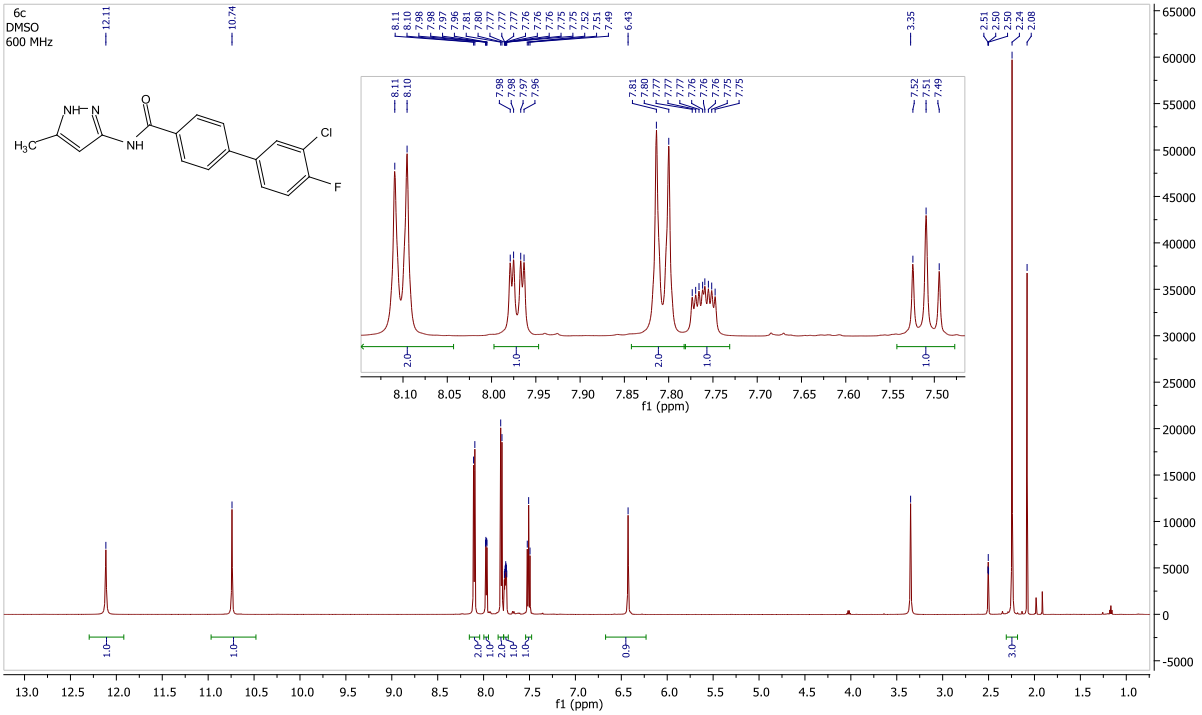

Figure S9: ^{1}H NMR (600 MHz, DMSO-d_6) of compound **6c**.

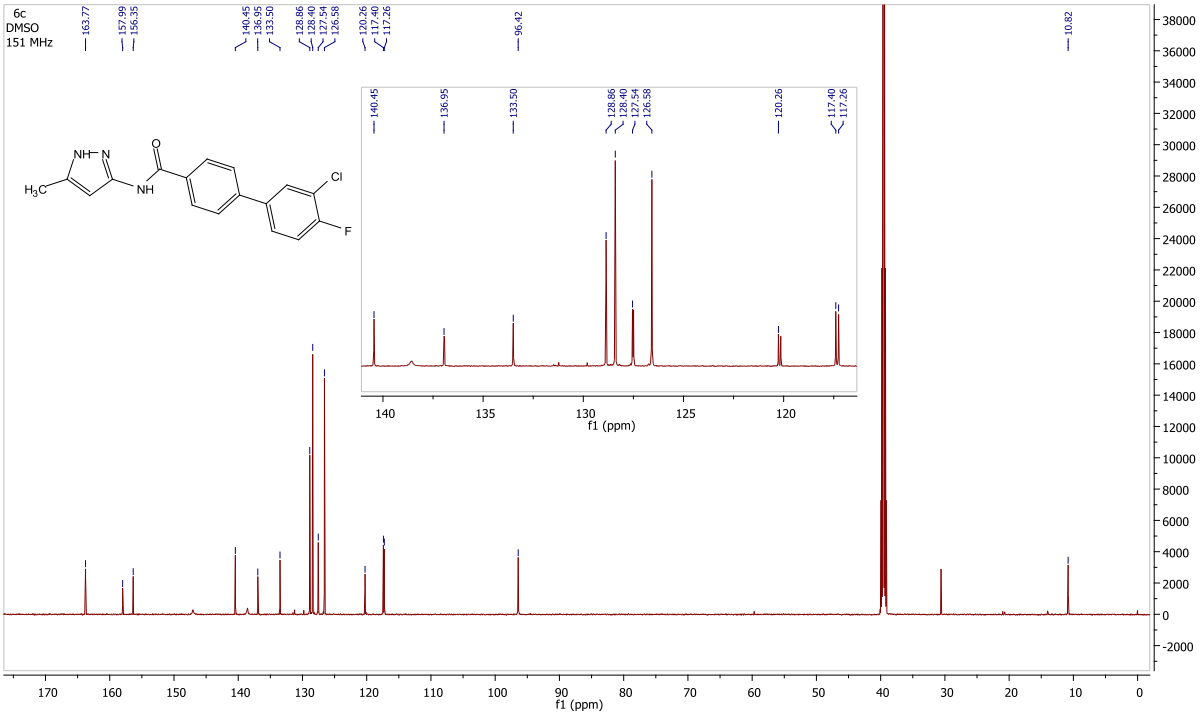

Figure S10: ^{13}C NMR (151 MHz, DMSO-d_6) of compound **6c**.

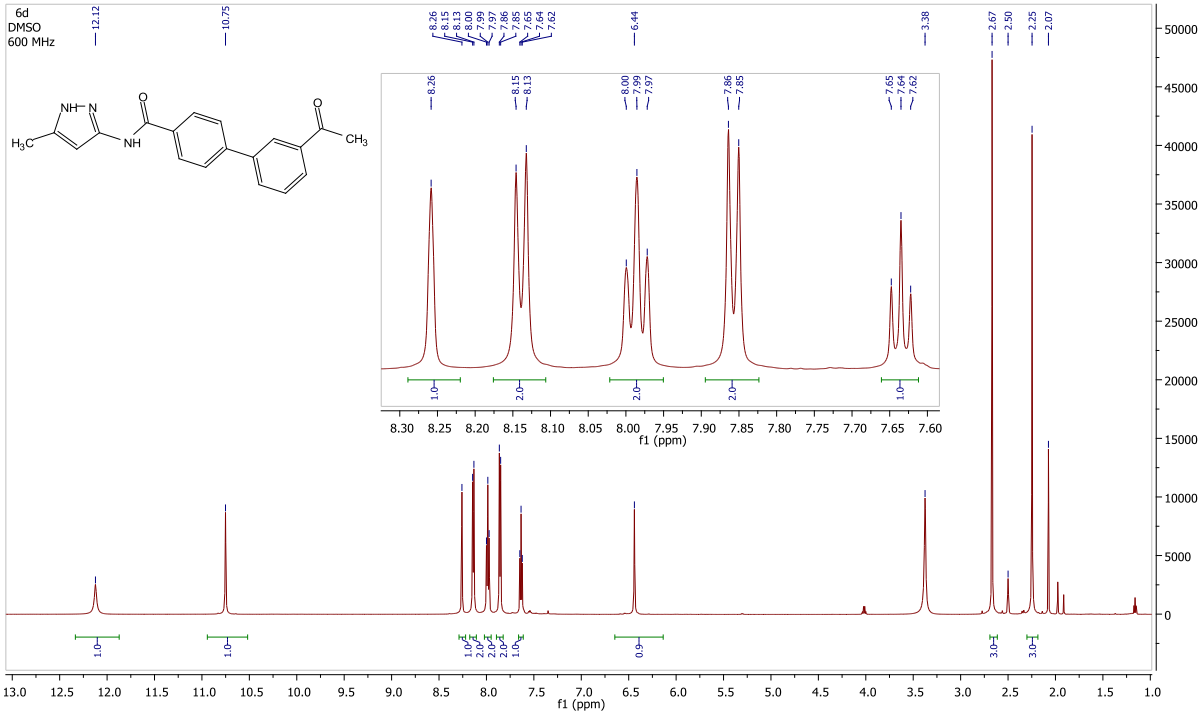

Figure S11: ^{1}H NMR (600 MHz, DMSO-d_6) of compound **6d**.

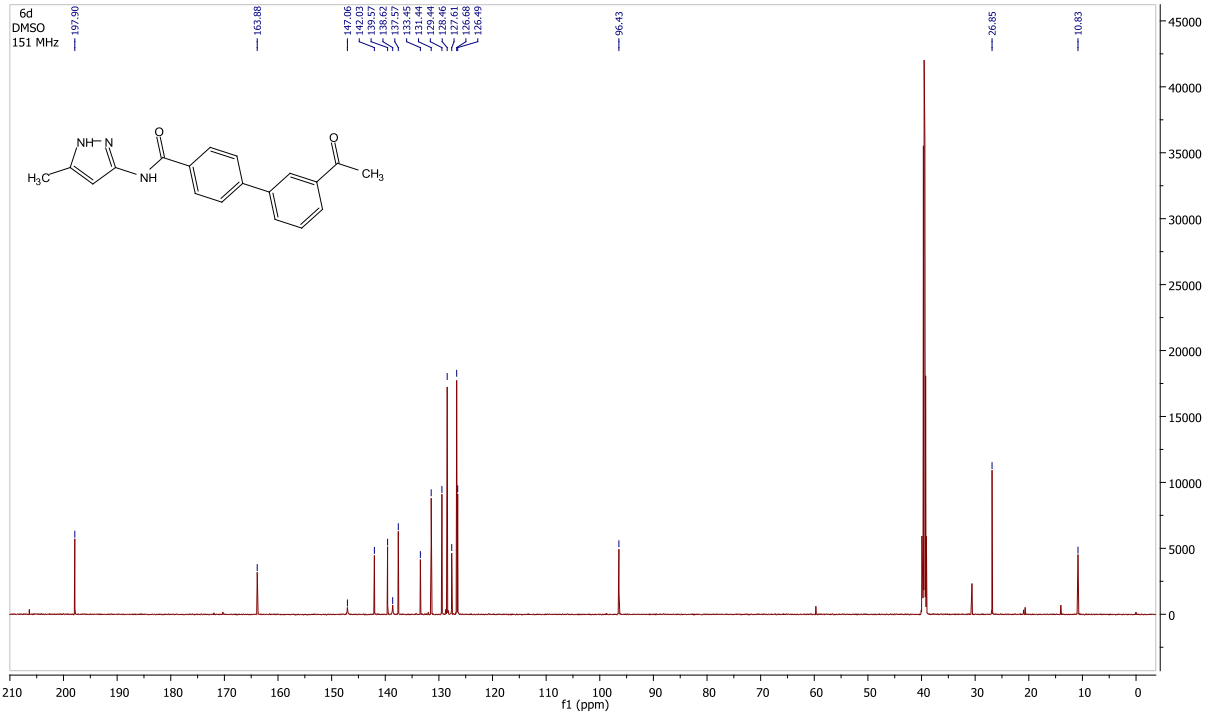

Figure S12: ^{13}C NMR (151 MHz, DMSO-d_6) of compound **6d**.

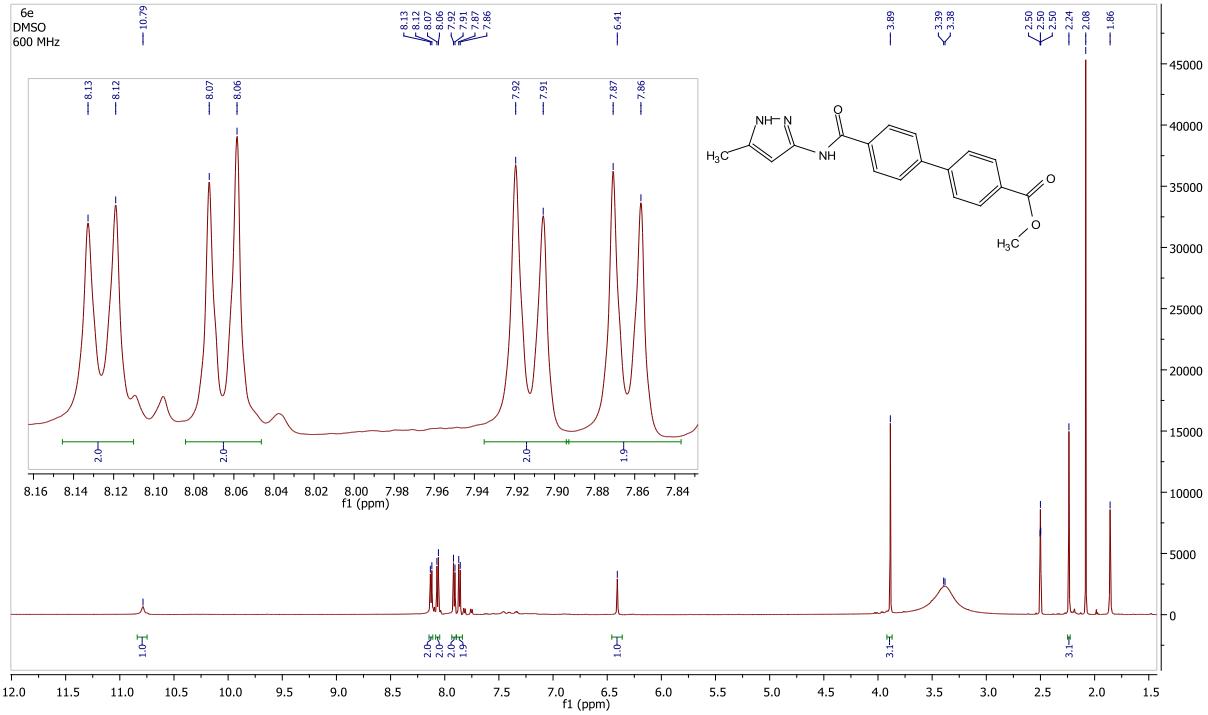

Figure S13: ^{1}H NMR (600 MHz, DMSO-d_6) of compound **6e**.

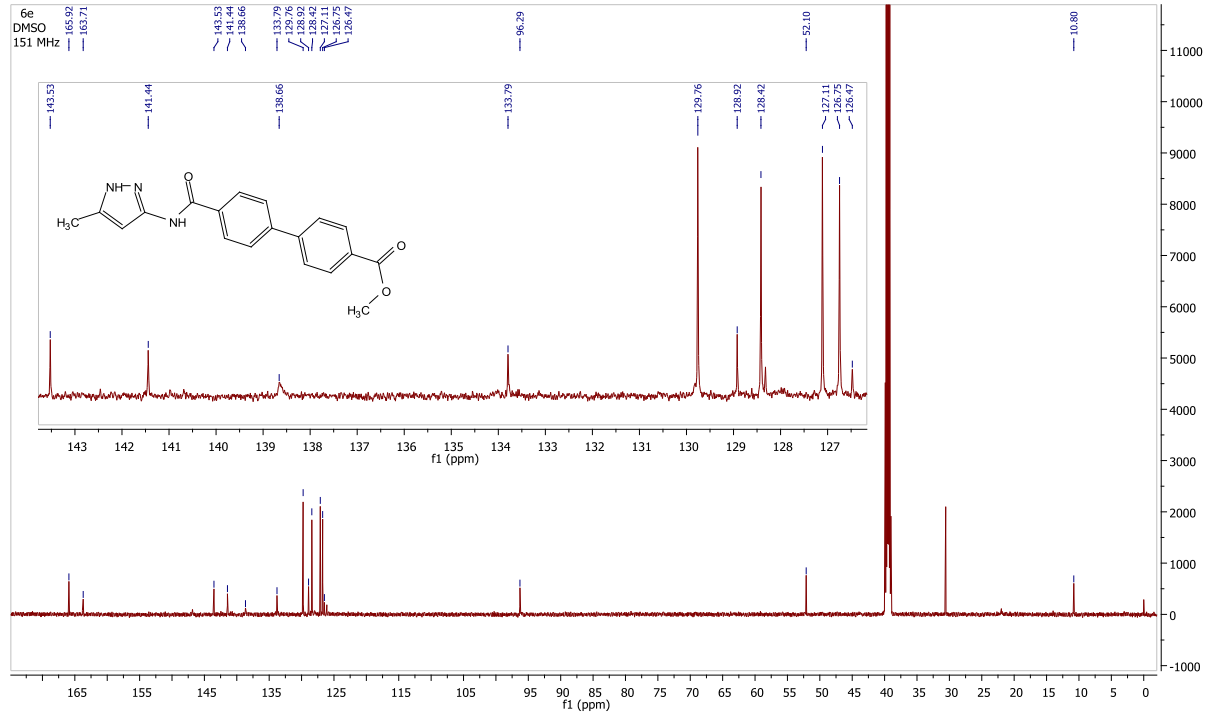

Figure S14: ^{13}C NMR (151 MHz, DMSO-d_6) of compound **6e**.

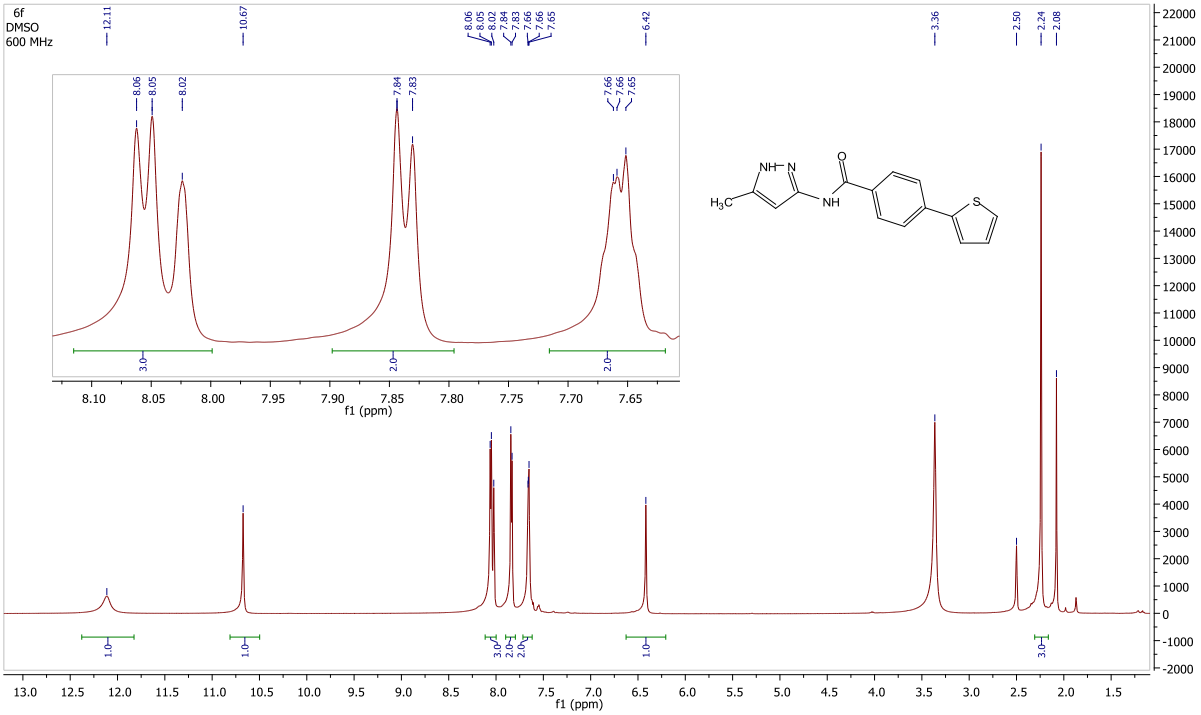

Figure S15: ^{1}H NMR (600 MHz, DMSO-d$_6$) of compound **6f**.

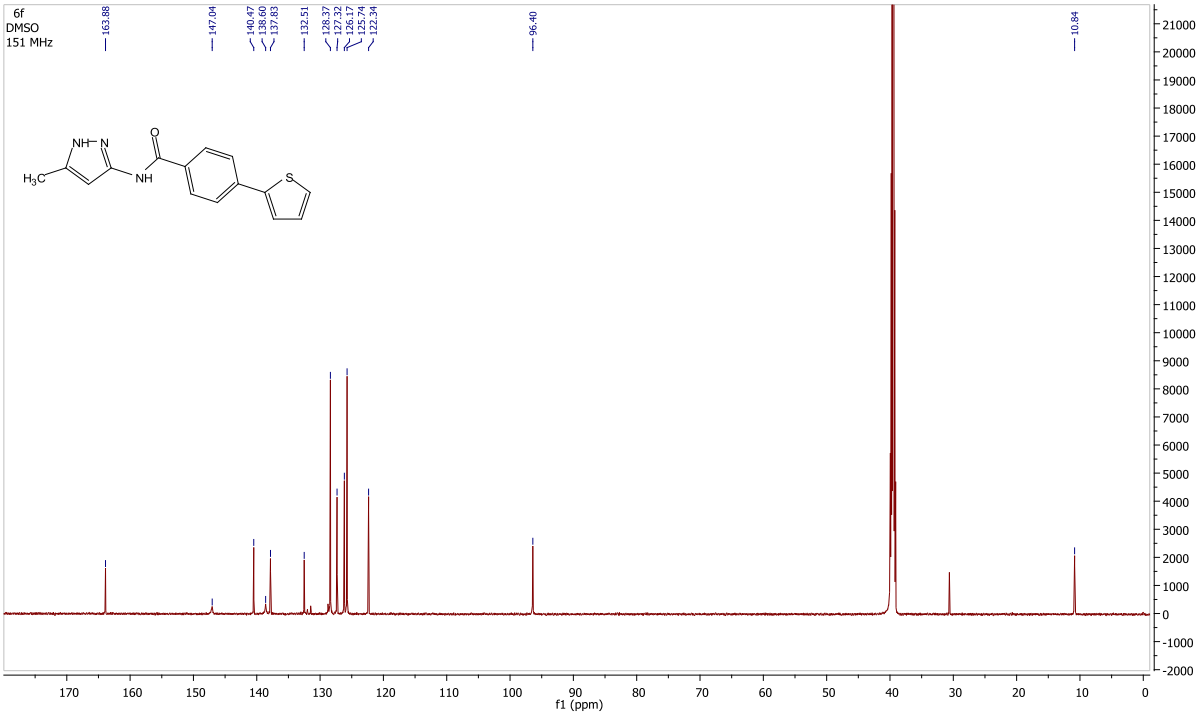

Figure S16: ^{13}C NMR (151 MHz, DMSO-d$_6$) of compound **6f**.

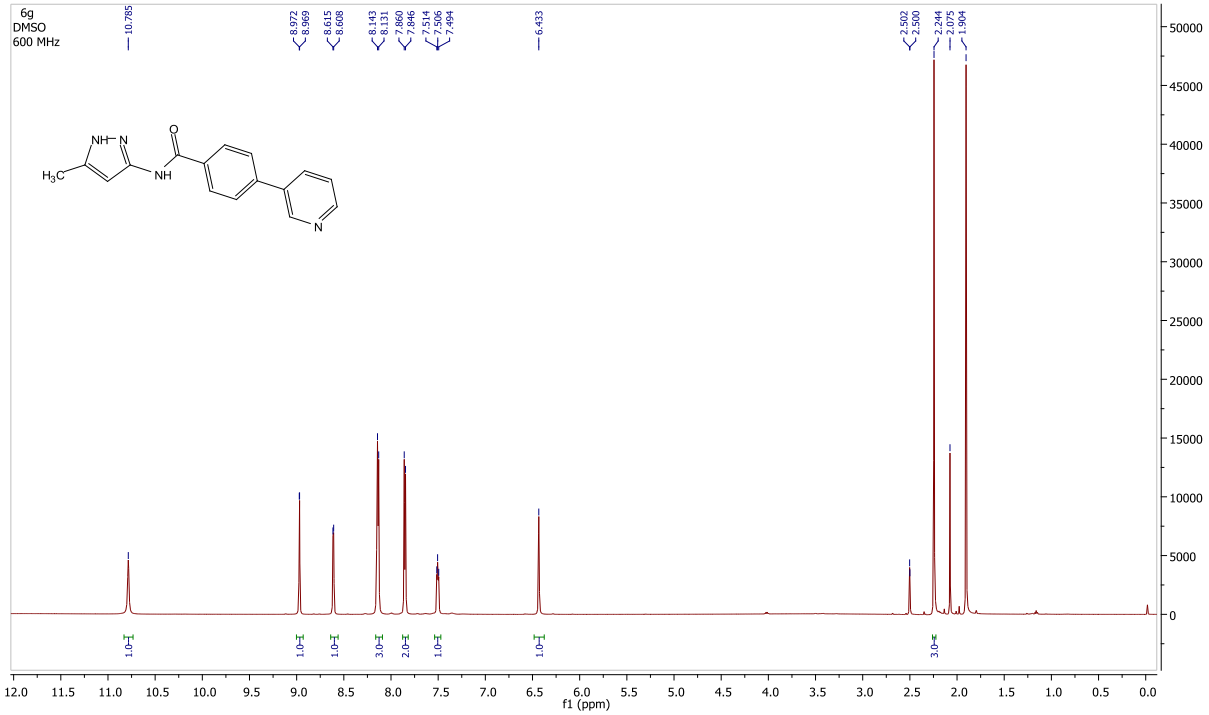

Figure S17: ^{1}H NMR (600 MHz, DMSO-d_6) of compound **6g**.

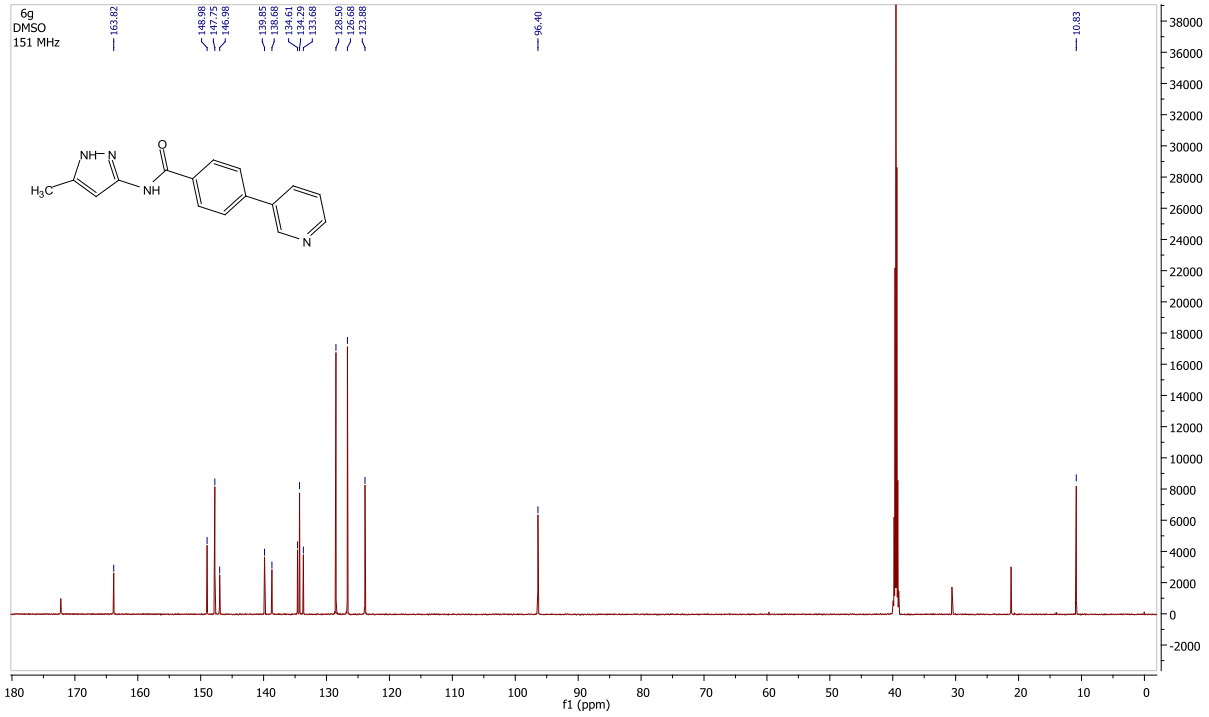

Figure S18: ^{13}C NMR (151 MHz, DMSO-d_6) of compound **6g**.

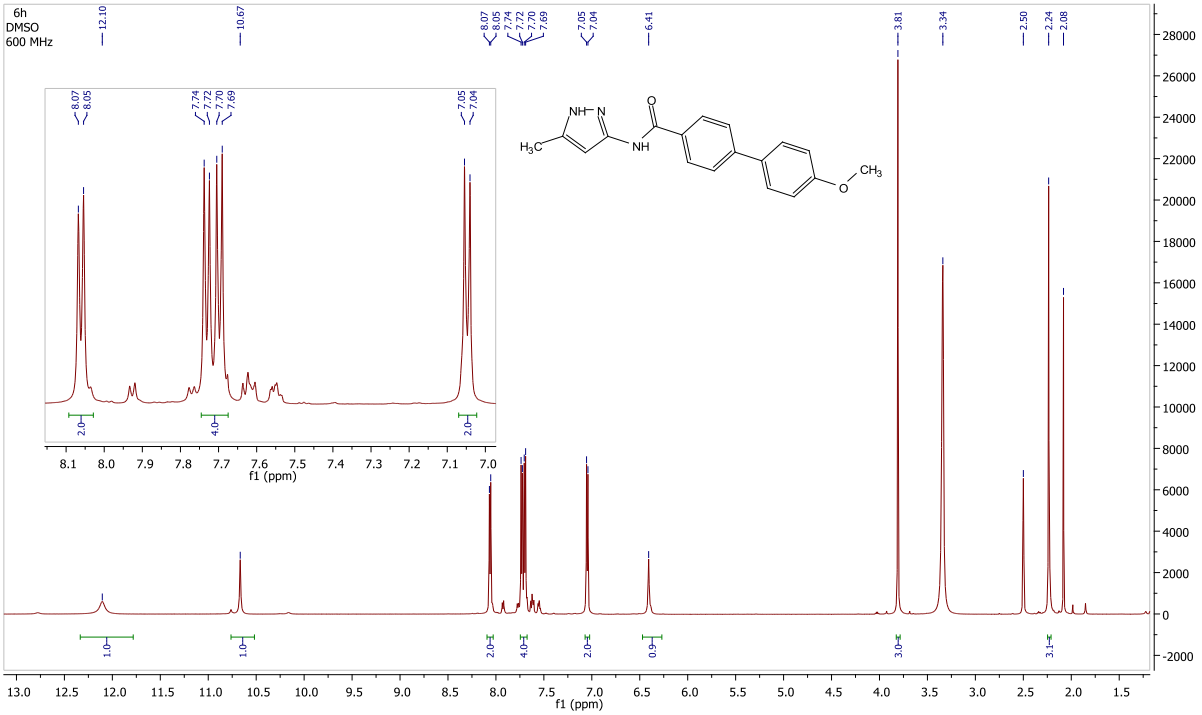

Figure S19: ^{1}H NMR (600 MHz, DMSO-d$_6$) of compound **6h**.

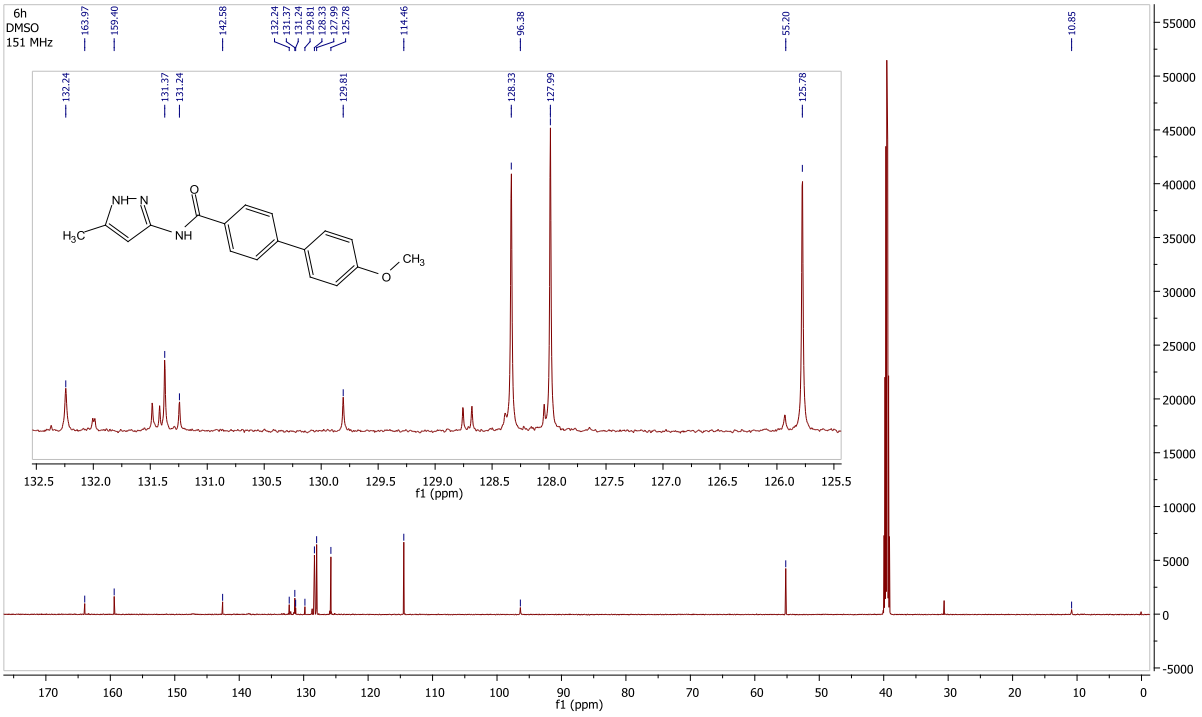

Figure S20: ^{13}C NMR (151 MHz, DMSO-d$_6$) of compound **6h**.

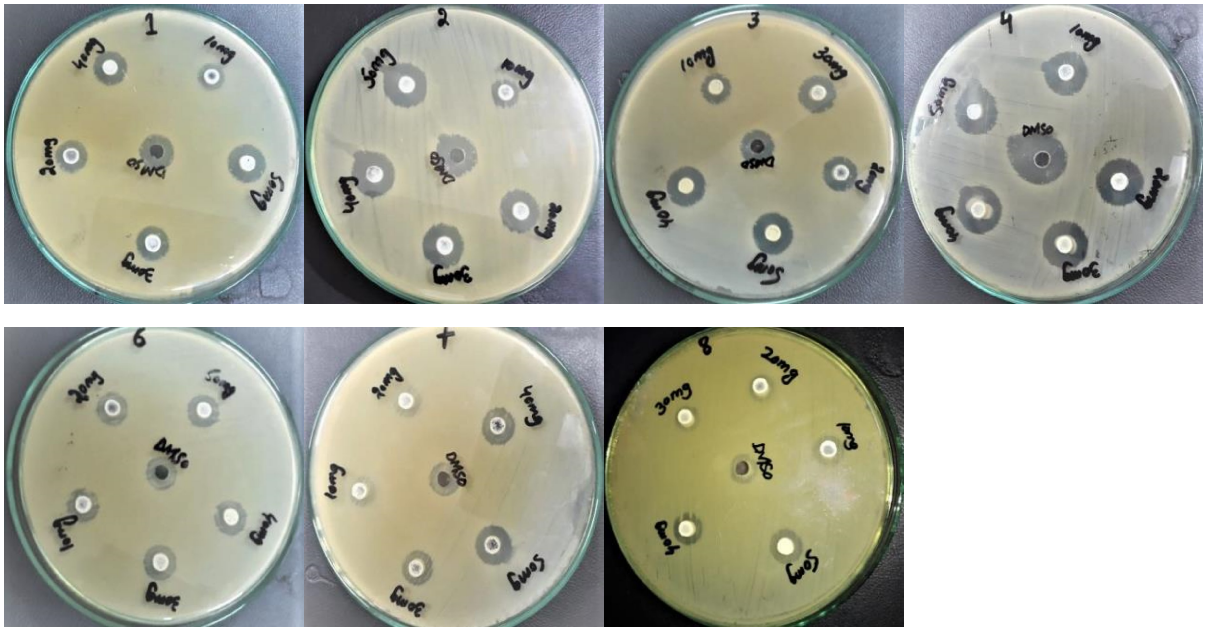

Figure S21: Antibacterial activity of compounds (1=6a, 2=6b, 3=6c, 4=6d, 6=6f, 7=6g and 8=6h) at different concentration against *A. baumannii*

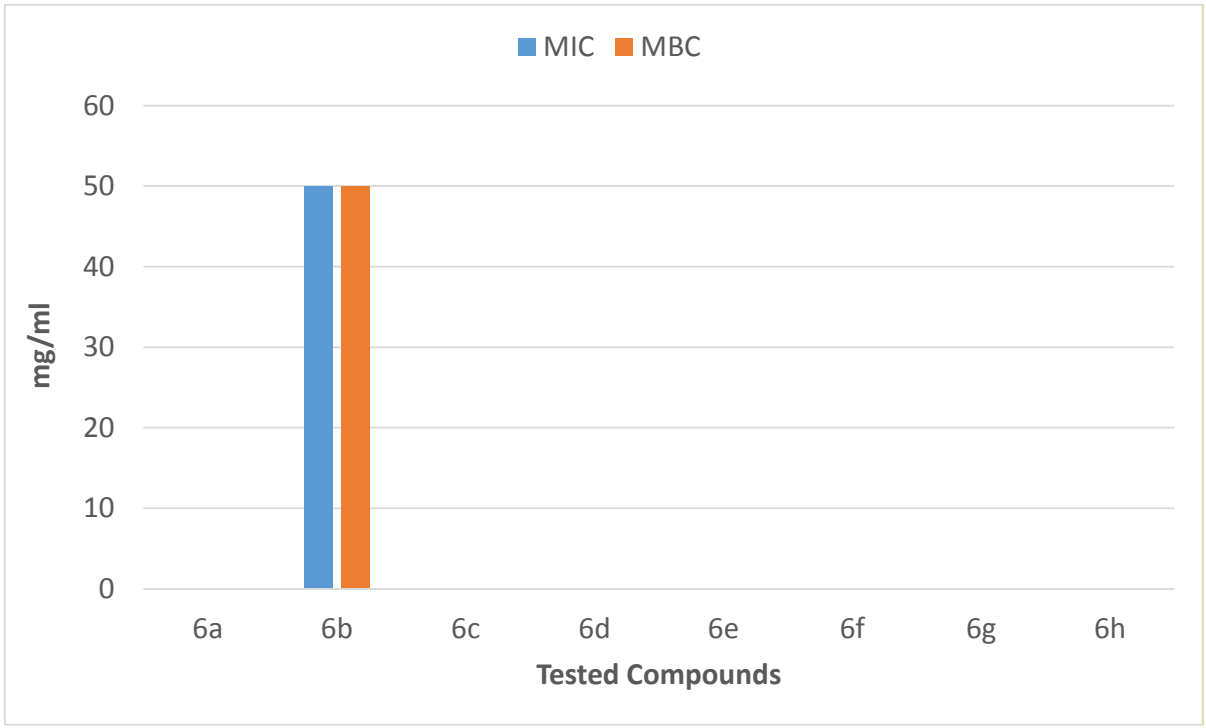

Figure S22: Graphical representation of MIC and MBC values of compounds (6a-6h) against *A. baumannii.*

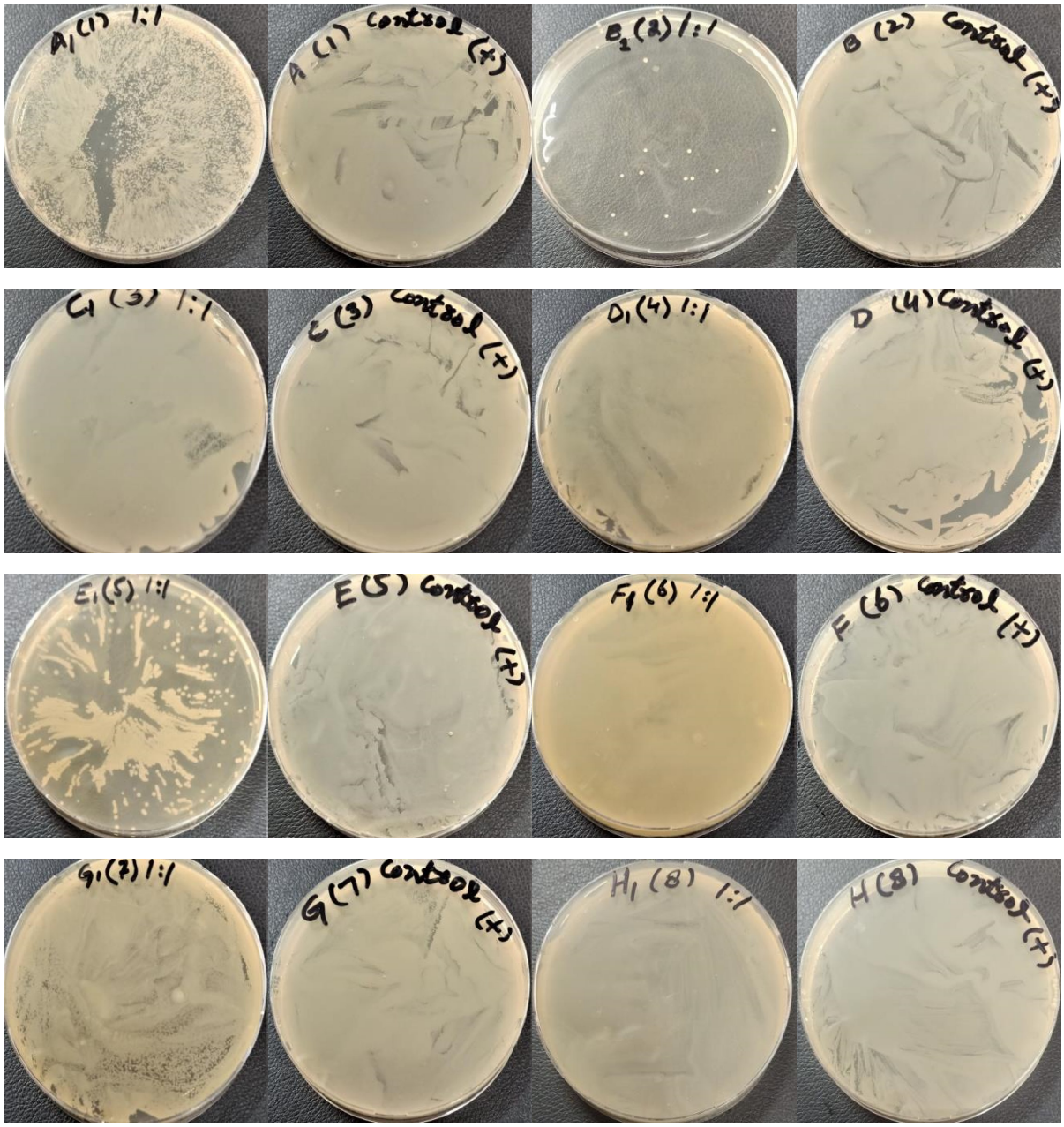

Figure S23: MBC of different compounds (1=6a, 2=6b, 3=6c, 4=6d, 5=6e, 6=6f, 7=6g and 8=6h) against *A. baumannii***.**

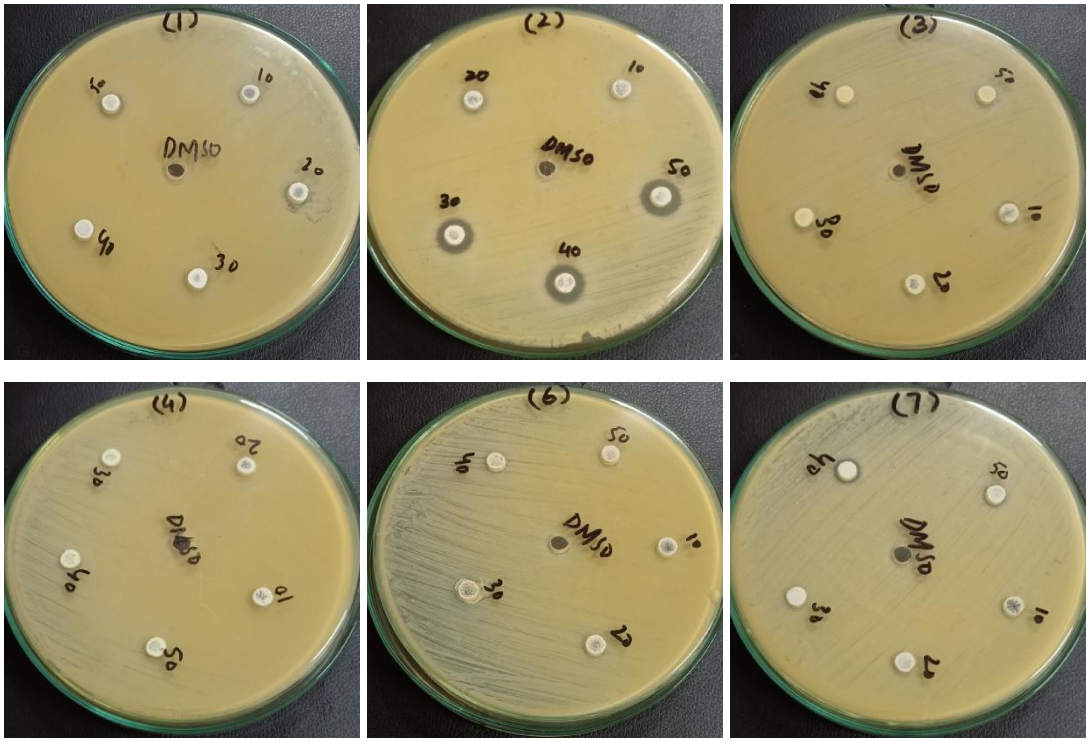

Figure S24: Antibacterial activity of compounds (1=6a, 2=6b, 3=6c, 4=6d, 6=6f and 7=6g) at different concentration against *K. pneumoniae.*

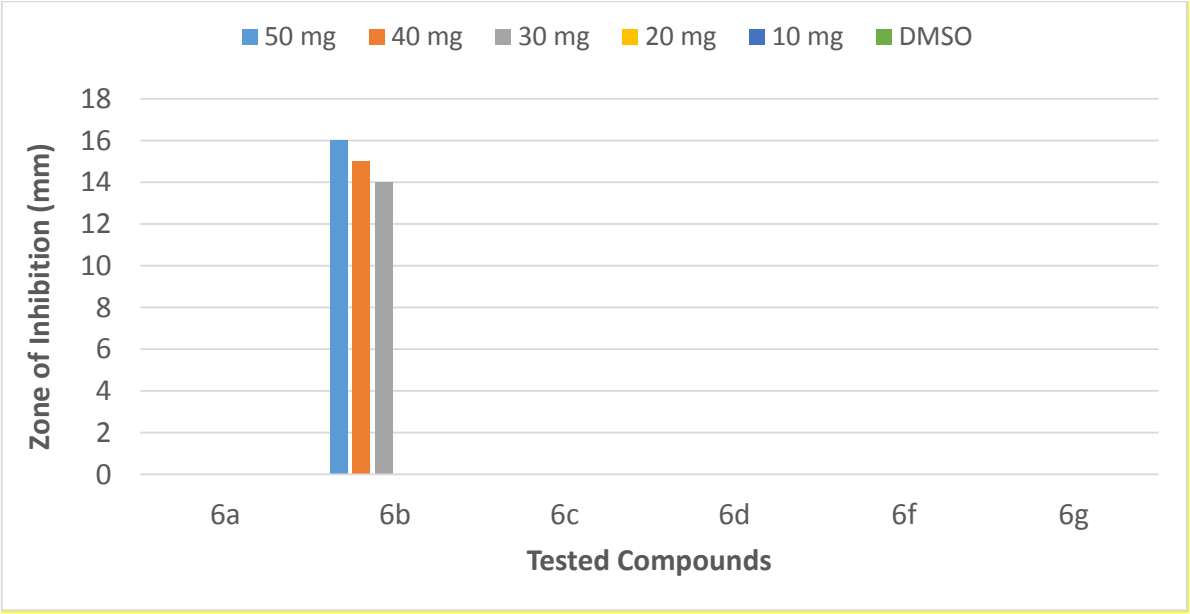

Figure S25: Graphical representation of inhibition zone of each fraction of compounds (6a-6h) against *K. pneumoniae.*

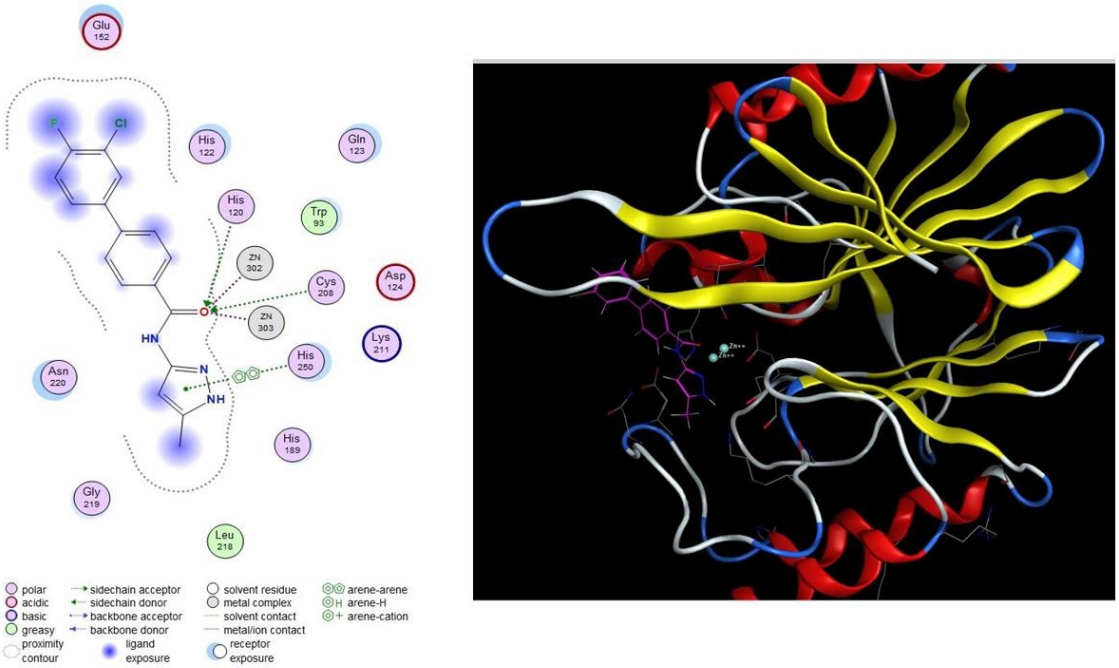

Figure S26: Two-dimensional (2D, left side) and three-dimensional (3D, right side) diagram of the **6d** compound with NDM1 protein.

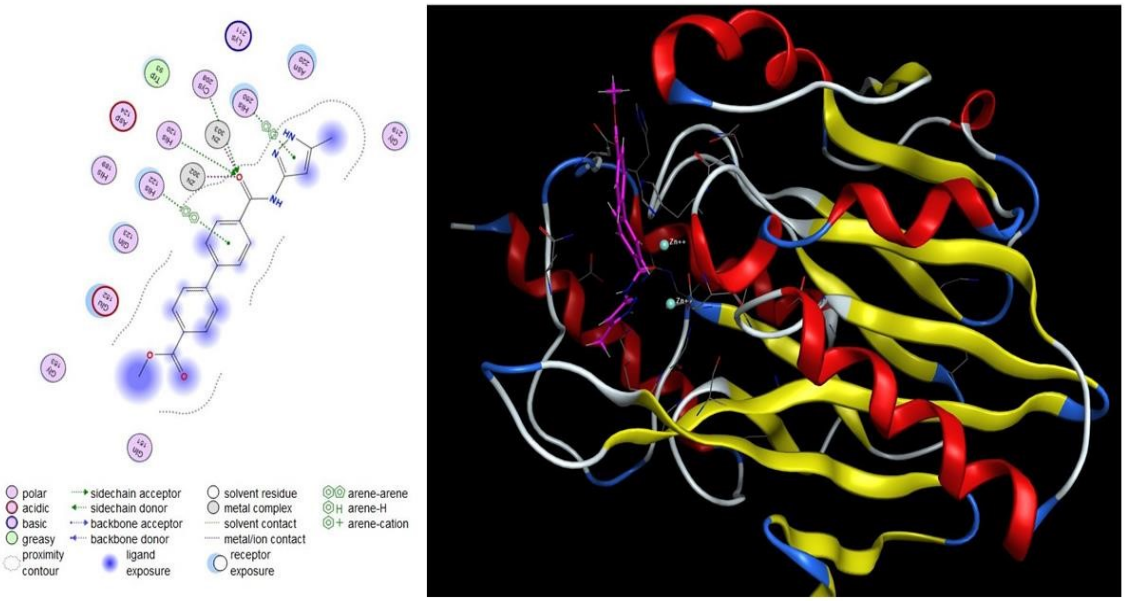

Figure S27: Two-dimensional (2D, left side) and three-dimensional (3D, right side) diagram of the **6e** compound with NDM1 protein.

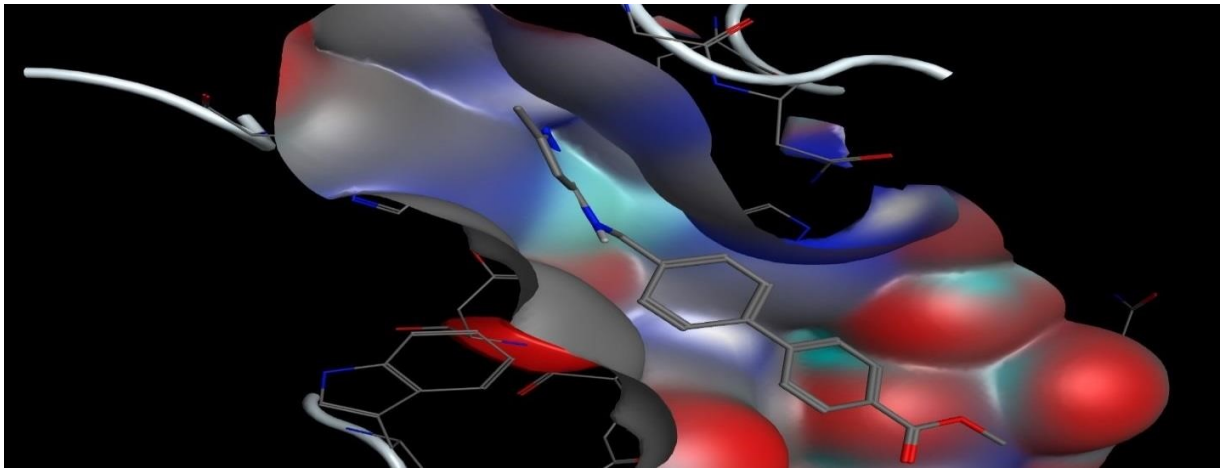

Figure S28: Three-dimensional (3D) diagram of the **6e** compound (from above surface) with NDM1 protein.

Table S1: Docking data of experimentally synthesized compounds (**6a-6h)**

	mol	rseq	mseq	S	rmsd_refine	E_conf	E_place	E_score1	E_refine	E_score2
1		1	1	-8.3146	2.5386	0.3353	-73.9350	-9.8894	-70.1938	-8.3146
2		1	1	-6.8485	2.2179	-3.6971	-110.2271	-10.3160	-51.0652	-6.8485
3		1	1	-6.8148	1.8764	-3.3301	-82.6581	-9.7868	-50.7804	-6.8148
4		1	1	-6.4344	1.4021	-2.4504	-79.9837	-10.7905	-44.4694	-6.4344
5		1	1	-6.3081	0.9582	-1.8509	-110.0710	-9.7474	-44.9361	-6.3081
6		1	1	-5.0115	1.2054	-2.1723	-117.8862	-9.8790	-23.3753	-5.0115
7		1	1	-4.8699	1.0643	-7.8777	-77.8386	-9.6368	-11.7204	-4.8699
8		1	2	-8.2875	2.3382	-4.2828	-73.8056	-10.1097	-71.1200	-8.2875
9		1	2	-7.1453	0.9713	-4.2849	-130.9264	-10.2157	-54.6752	-7.1453
10		1	2	-6.3854	1.3943	-6.7751	-76.7086	-9.1716	-45.1601	-6.3854
11		1	2	-6.2861	1.3535	-5.8823	-107.0672	-9.1620	-41.2404	-6.2861
12		1	2	-6.1744	1.2742	-6.1734	-77.7197	-10.5605	-43.7992	-6.1744
13		1	2	-6.0731	2.1078	-6.4365	-91.0935	-9.4351	-39.0530	-6.0731
14		1	2	-5.6283	1.5936	-7.2045	-78.6436	-9.4512	-33.6642	-5.6283
15		1	2	-4.9222	0.8624	-5.8403	-84.1240	-9.2796	-19.3735	-4.9222
16		1	3	-8.3324	4.5879	7.3722	-77.5584	-9.7750	-71.9231	-8.3324
17		1	3	-6.3253	1.9798	5.0179	-110.3713	-9.4524	-43.1903	-6.3253
18		1	3	-6.1097	1.6061	5.0842	-74.8789	-9.8765	-39.9813	-6.1097
19		1	3	-5.6135	1.3703	4.3597	-84.5985	-9.5225	-33.4436	-5.6135
20		1	3	-4.8657	0.5388	-0.8244	-76.1094	-9.5815	-9.8560	-4.8657
21		1	3	-4.6466	1.4525	2.1793	-77.1723	-9.5008	-9.1189	-4.6466
22		1	4	-8.4231	5.5308	-4.3207	-78.2275	-9.6635	-73.2905	-8.4231
23		1	4	-8.2856	4.4290	-3.8575	-73.7636	-9.7831	-70.5829	-8.2856
24		1	4	-6.4193	1.6674	-4.3911	-102.2714	-9.6711	-41.8419	-6.4193
25		1	4	-6.3223	0.7849	-6.7651	-123.6475	-9.9000	-43.6144	-6.3223

26		1	4	-4.3689	1.7130	-11.3261	-81.6318	-9.6106	-6.2071	-4.3689
27		1	4	-4.3292	1.7610	-11.3609	-71.7602	-9.7033	-5.3382	-4.3292
28		1	4	-4.1926	1.9898	-10.1392	-79.9701	-9.8338	-4.6878	-4.1926
29		1	5	-8.7300	4.7493	19.4164	-73.6489	-9.8603	-74.5501	-8.7300
30		1	5	-8.5699	4.9349	25.1984	-89.9571	-10.7830	-72.6184	-8.5699
31		1	5	-7.4681	1.7640	18.4842	-73.0413	-10.1730	-58.0132	-7.4681
32		1	5	-6.8519	2.7484	21.9259	-79.3519	-9.9526	-47.3507	-6.8519
33		1	5	-5.2190	0.7615	13.5929	-74.7296	-10.2671	-13.6666	-5.2190
34		1	5	-5.0154	1.0026	17.1512	-73.8127	-10.3184	-15.0259	-5.0154
35		1	5	-4.6744	1.0238	16.2820	-93.7541	-9.8364	-10.5122	-4.6744
36		1	5	-4.6200	1.3163	11.2283	-83.4865	-10.3598	-5.4264	-4.6200
37		1	5	-4.3170	1.5575	21.9536	-75.2271	-10.1599	-3.4608	-4.3170
38		1	6	-8.2313	3.6655	19.8998	-85.2839	-9.7011	-70.2826	-8.2313
39		1	6	-8.1812	2.0259	20.2981	-89.9530	-9.6784	-69.6141	-8.1812
40		1	6	-6.7103	1.4159	20.3023	-84.1198	-9.5025	-49.2639	-6.7103
41		1	6	-6.6345	2.0109	20.2172	-80.0693	-9.5409	-47.7233	-6.6345
42		1	6	-5.3793	1.2422	16.5740	-103.1550	-9.2277	-30.6818	-5.3793
43		1	7	-8.2043	1.2172	4.9598	-100.8668	-9.6021	-69.5656	-8.2043
44		1	7	-6.8678	1.8332	5.8038	-92.2635	-9.4439	-46.8649	-6.8678
45		1	7	-6.8508	1.8186	3.9397	-79.5941	-9.2706	-51.8221	-6.8508
46		1	7	-6.7786	1.4730	3.9518	-107.7256	-9.3733	-50.7954	-6.7786
47		1	7	-6.0289	1.3175	1.8531	-82.9173	-9.3433	-39.4399	-6.0289
48		1	7	-4.5635	1.9733	3.8116	-97.7002	-9.6193	-9.6968	-4.5635
49		1	8	-8.3118	1.8892	-3.5642	-100.8533	-10.2074	-70.3263	-8.3118
50		1	8	-8.3057	1.8993	-3.2842	-98.7659	-11.2048	-69.6480	-8.3057
51		1	8	-7.2406	2.1472	-4.2244	-87.2566	-9.8492	-54.1136	-7.2406
52		1	8	-5.3222	1.1146	-11.8806	-82.8279	-9.8160	-16.8344	-5.3222
53		1	8	-5.2476	1.0490	-7.0970	-83.1890	-9.8078	-18.8549	-5.2476
54		1	8	-4.5561	1.9568	-4.5933	-79.5113	-9.7579	-10.5914	-4.5561