Synthesis, Characterization, Antimicrobial and Antibiofilm Activity, Molecular Docking Analysis of NHC Precursors and Their Ag-NHC Complexes

Elvan Üstün,[a] Neslihan Şahin,*[b,c,d] Cem Çelik,[e] Uğur Tutar,[f] Namık Özdemir,[g] Nevin Gürbüz[c,d,h] and İsmail Özdemir[c,d,h]

[a] Department of Chemistry, Faculty of Art and Science, Ordu University, 52200 Ordu, Turkey.

[b] Department of Basic Education, Faculty of Education, Cumhuriyet University, 58040, Sivas, Turkey;

[c] Department of Chemistry, Faculty of Science and Art, İnönü University, 44280 Malatya, Turkey

[d] Catalysis Research and Application Center, İnönü University, 44280, Malatya, Turkey

[e] Department of Medical Microbiology, Faculty of Medicine, Cumhuriyet University, Sivas, Turkey

[f] Department of Botanica, Faculty of Pharmacy, Sivas Cumhuriyet University, Sivas, 58140, Turkey

[g] Department of Mathematics and Science Education, Faculty of Education, Ondokuz Mayıs University, 55139, Samsun, Turkey

[h] Drug Application and Research Center, İnönü University, 44280, Malatya, Turkey

[*]Corresponding Author:

Assoc. Prof. Neslihan Şahin

Cumhuriyet University

Faculty of Education

Department of Basic Education

58040, Sivas, Turkey

E-mail: neslihan4458@gmail.com

Phone: +903464874656

Supplementary Files

Supplementary Files

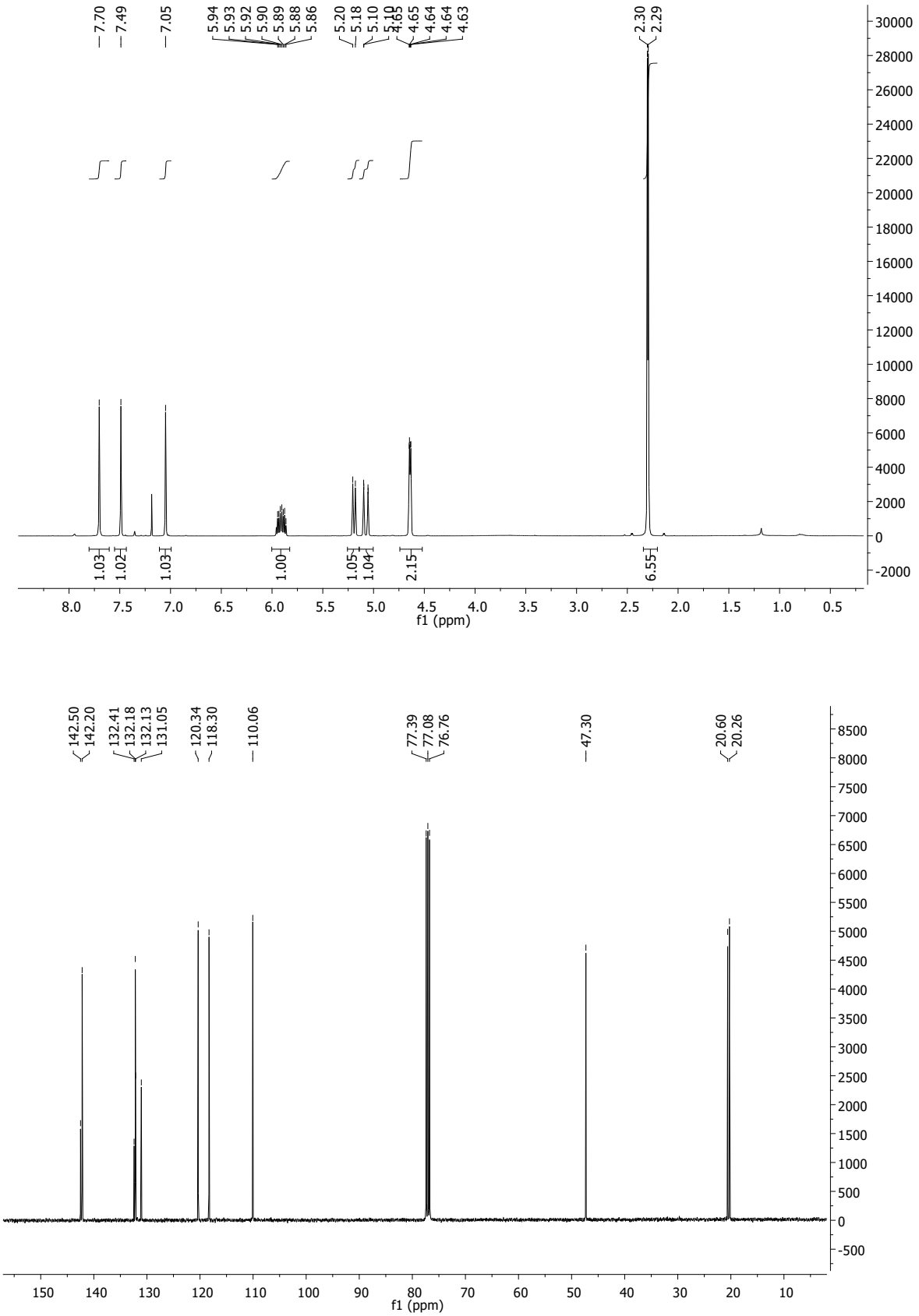


Figure S1. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectrums of **1**

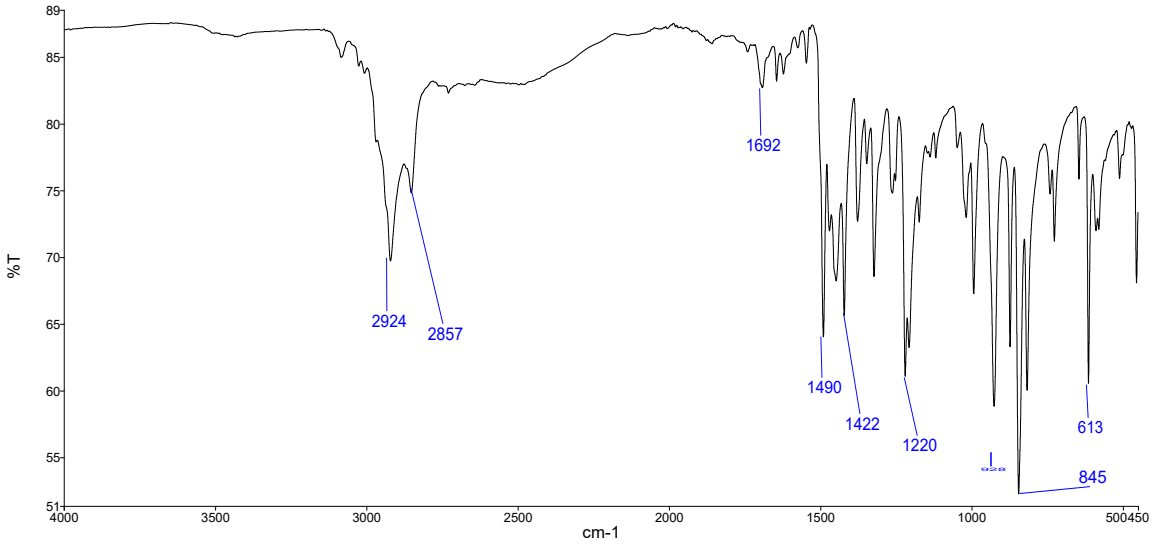


Figure S2. FT-IR spectrum of **1**

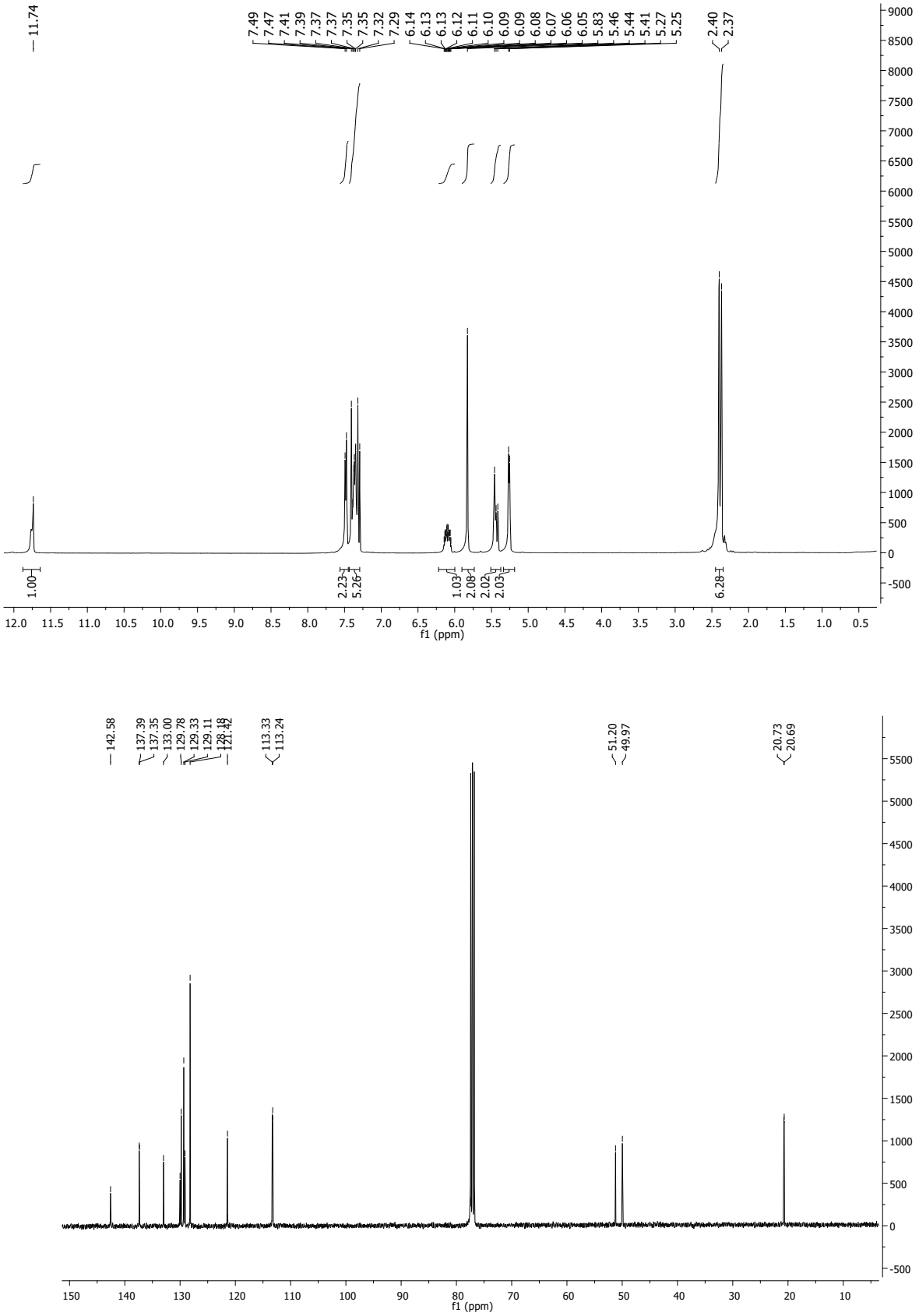


Figure S3. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectrums of **1a**

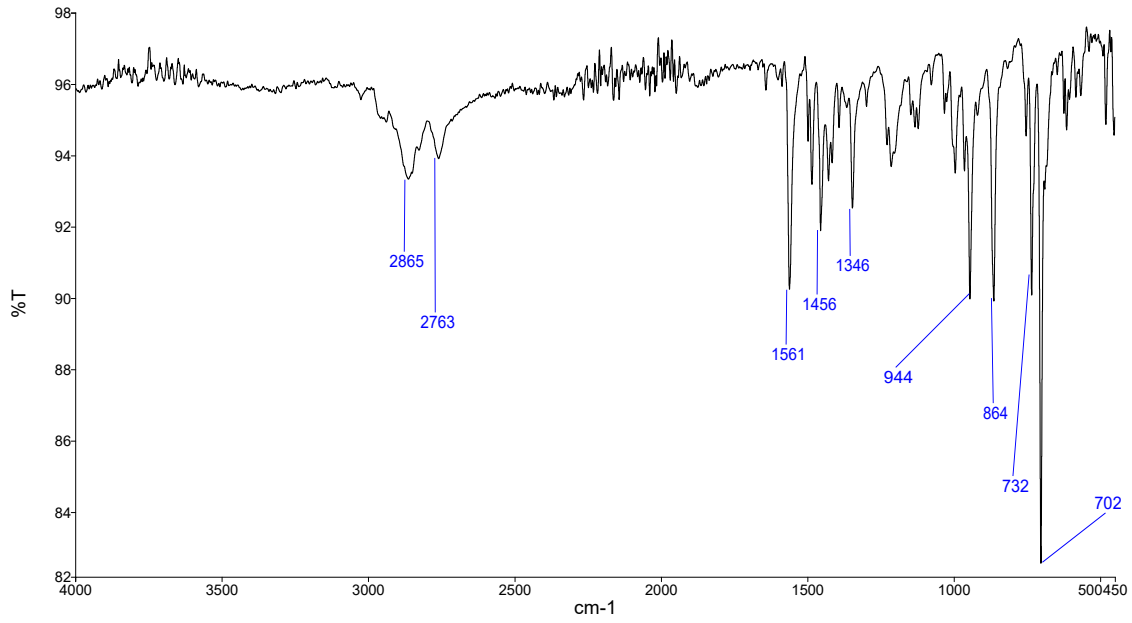


Figure S4. FT-IR spectrum of **1a**

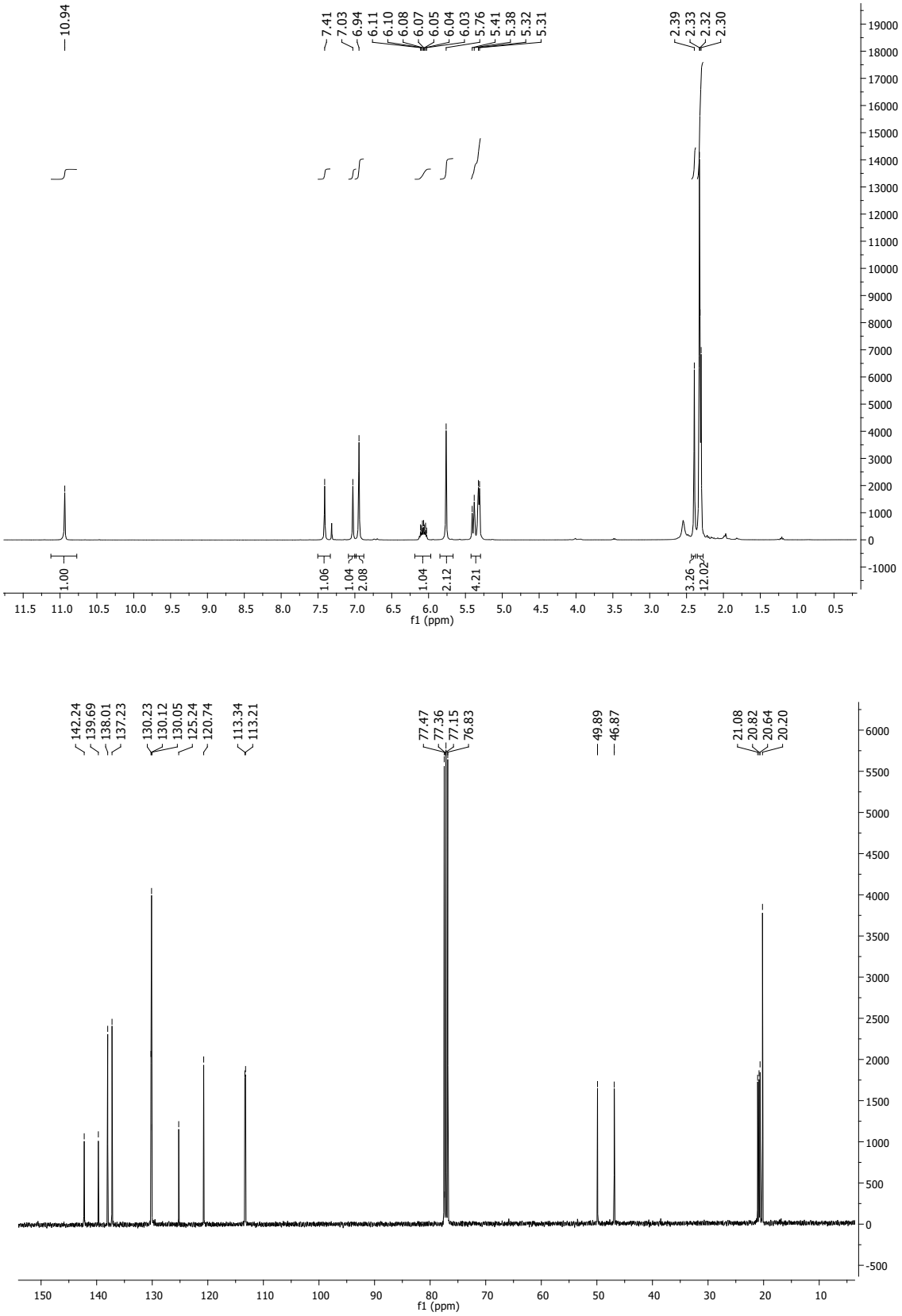


Figure S5. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectrums of **1b**

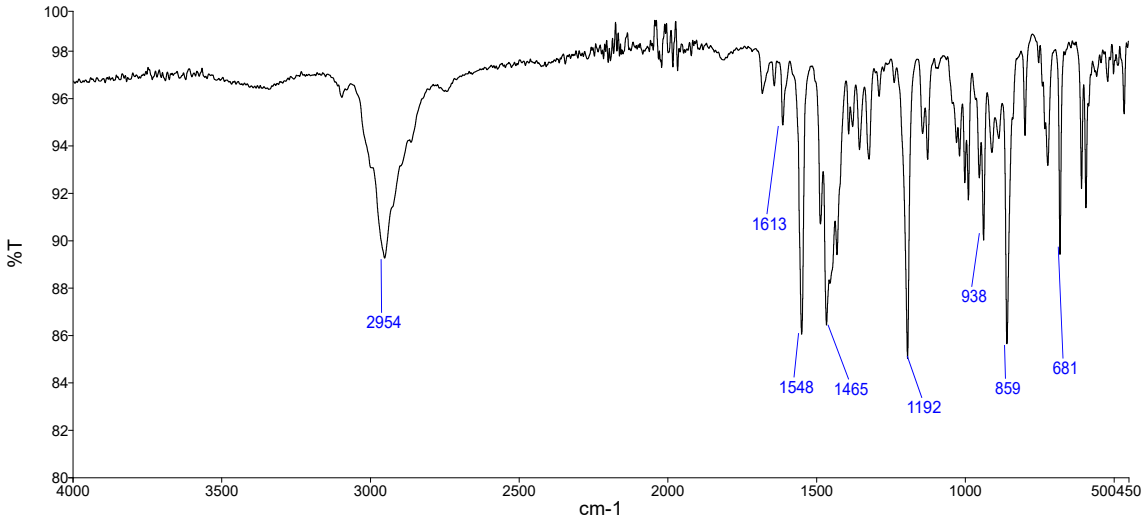


Figure S6. FT-IR spectrum of **1b**

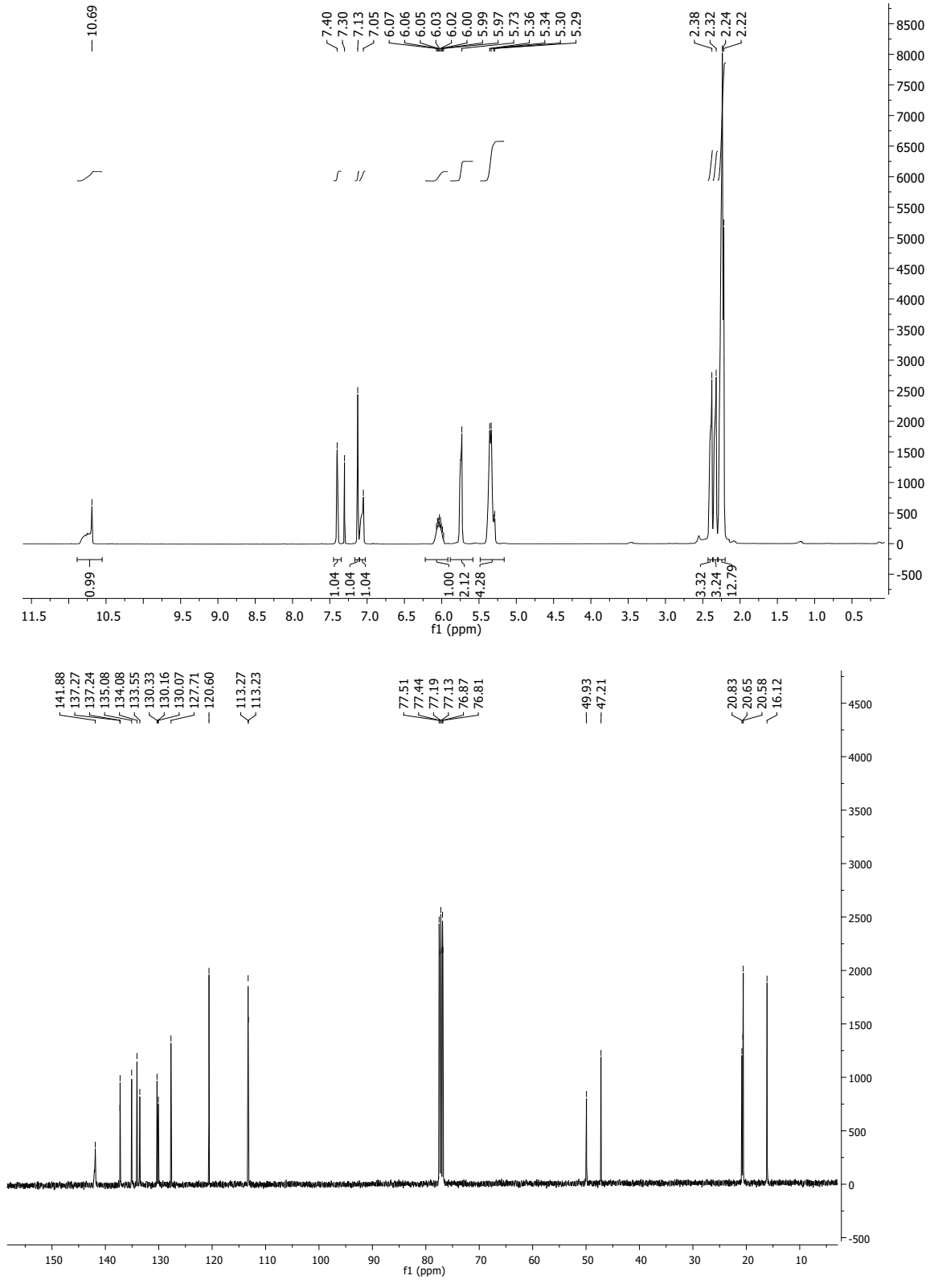


Figure S7. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectrums of **1c**

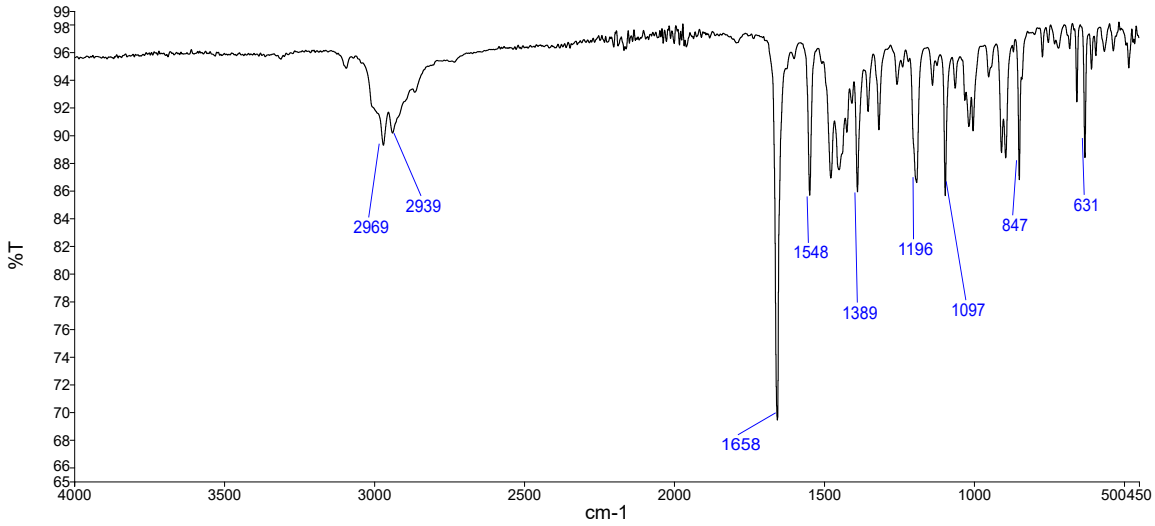


Figure S8. FT-IR spectrum of **1c**

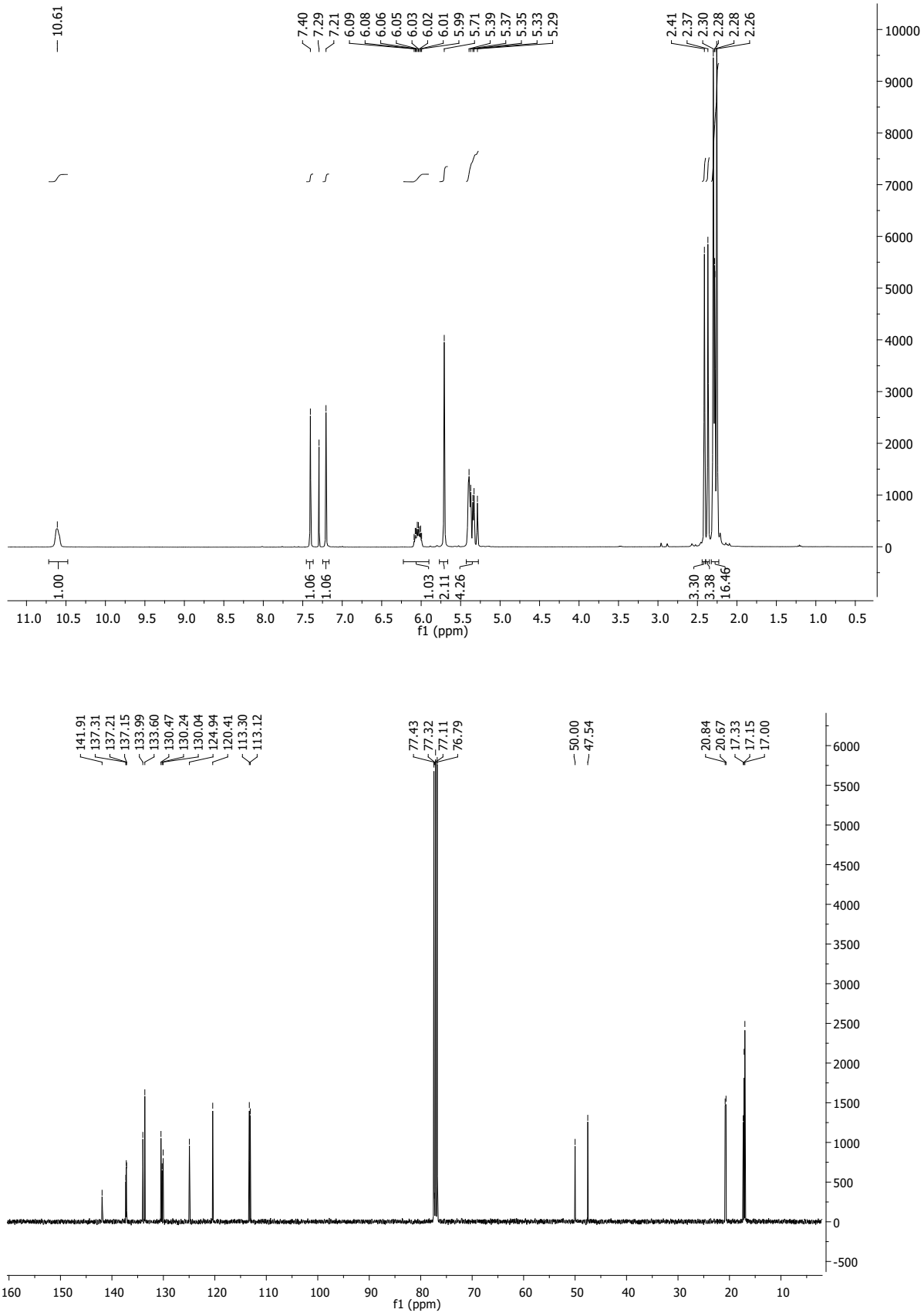


Figure S9. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectrums of **1d**

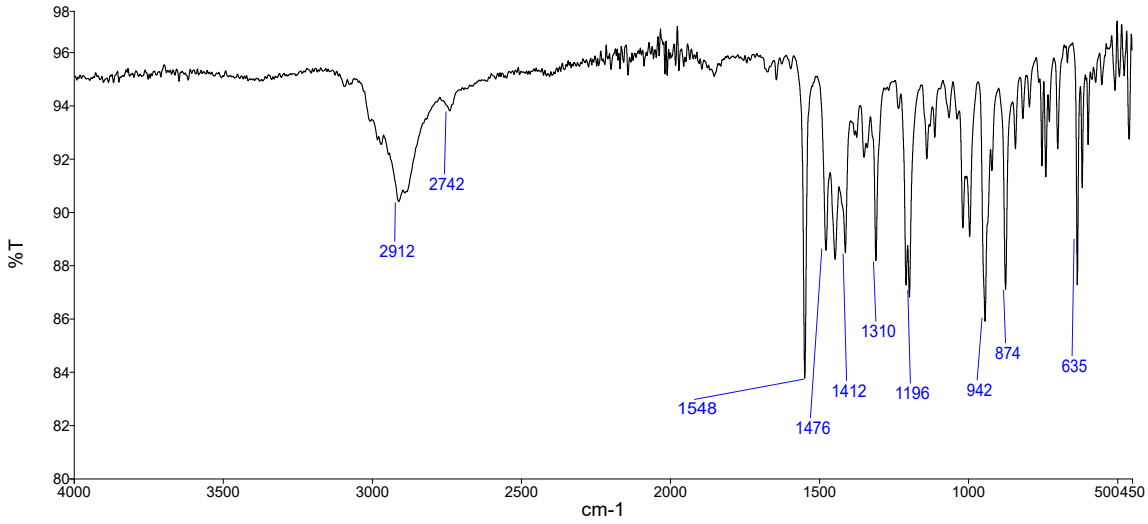


Figure S10. FT-IR spectrum of **1d**

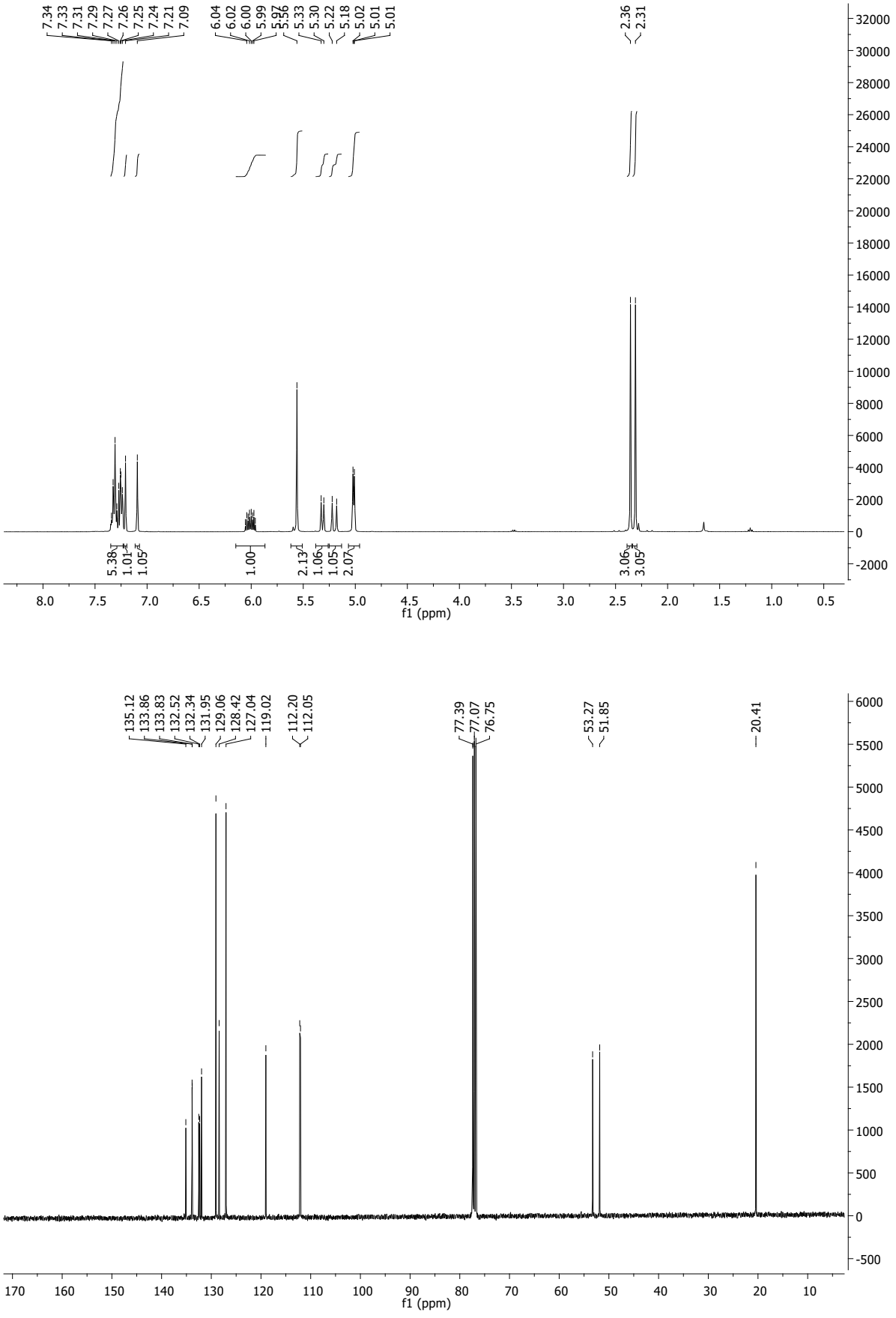


Figure S11. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectrums of **2a**

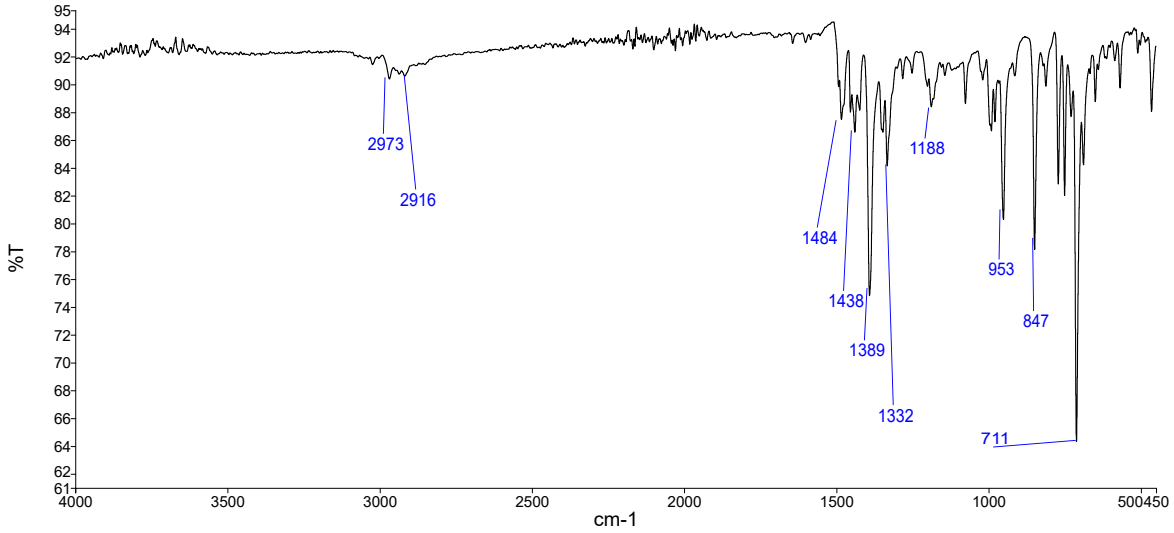


Figure S12. FT-IR spectrum of **2a**

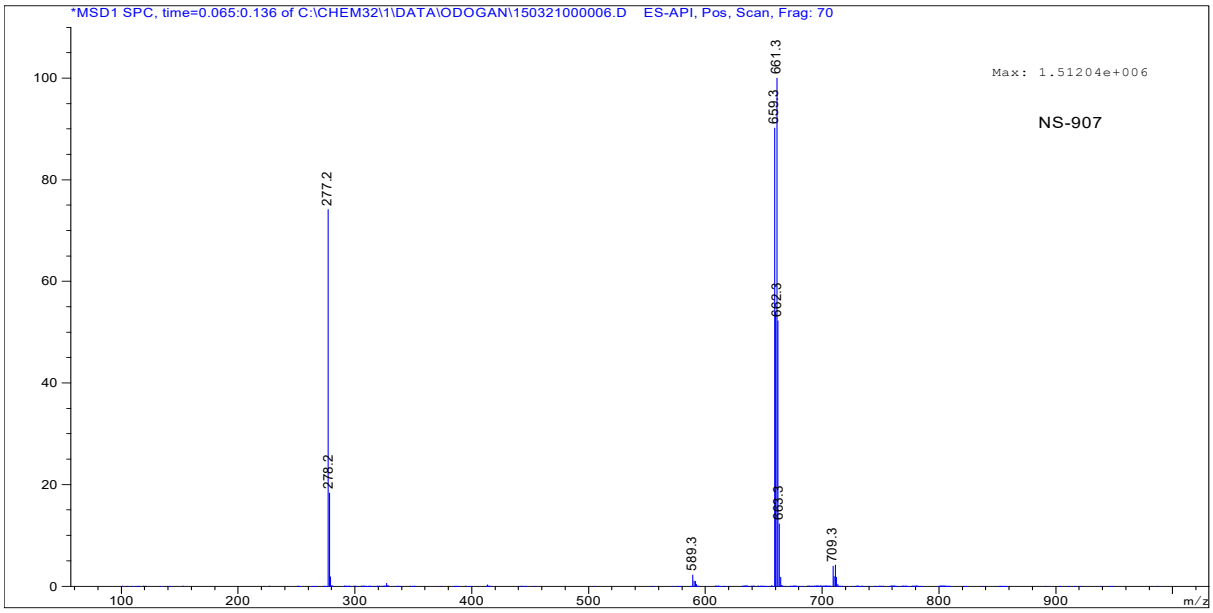


Figure S13. LC-MS spectrum of **2a**

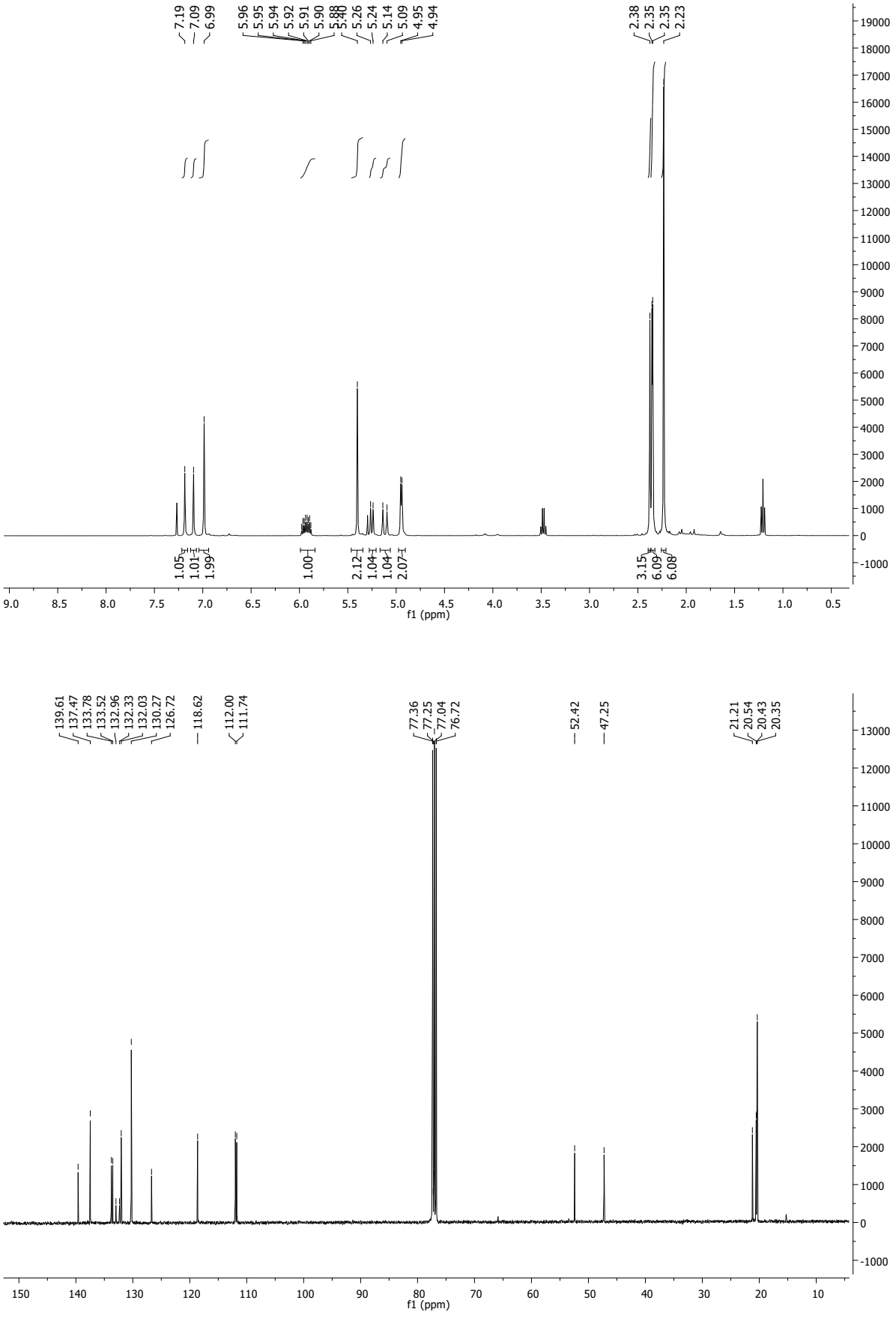


Figure S14. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectrums of **2b**

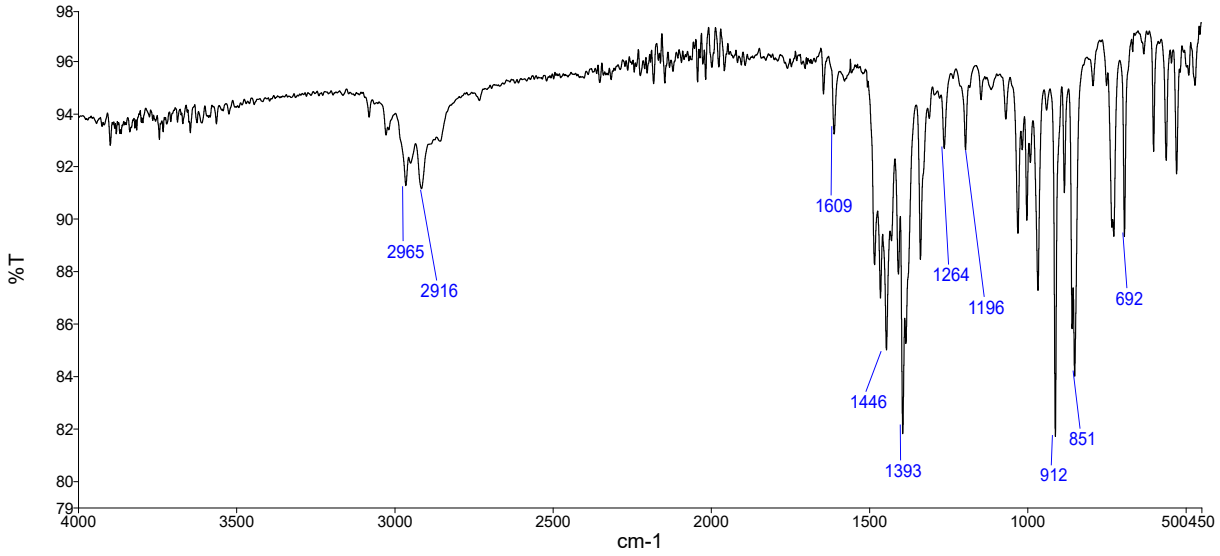


Figure S15. FT-IR spectrum of **2b**

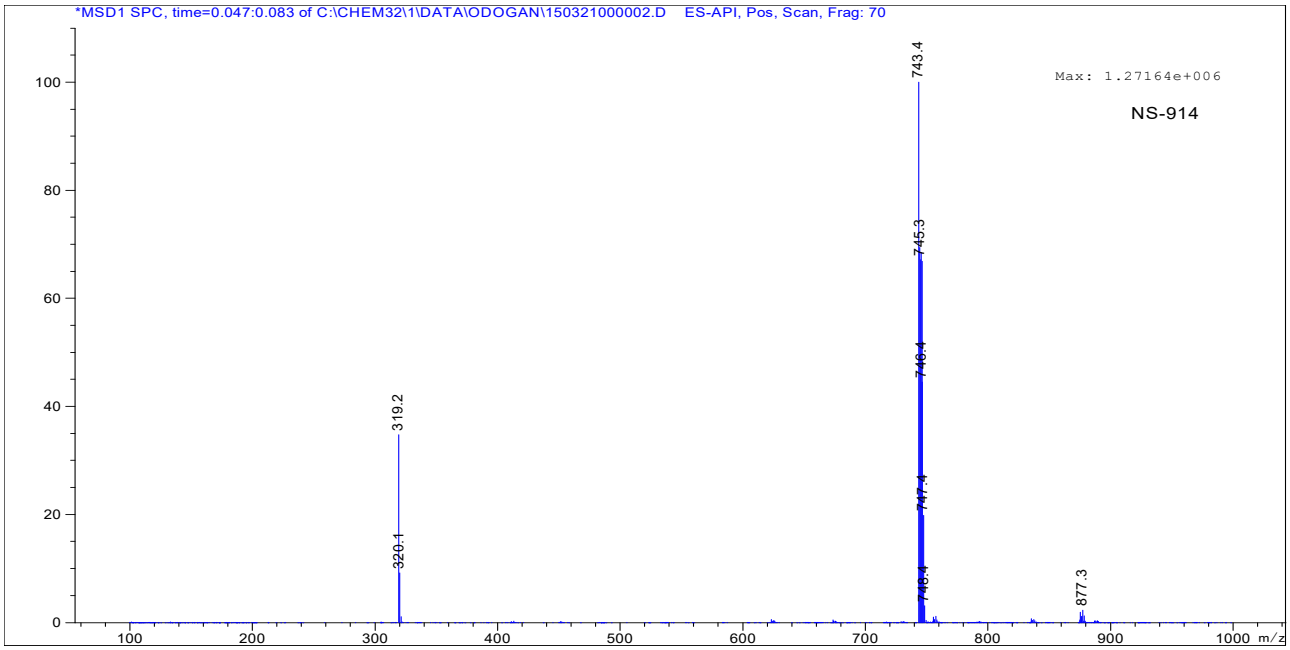


Figure S16. LC-MS spectrum of **2b**

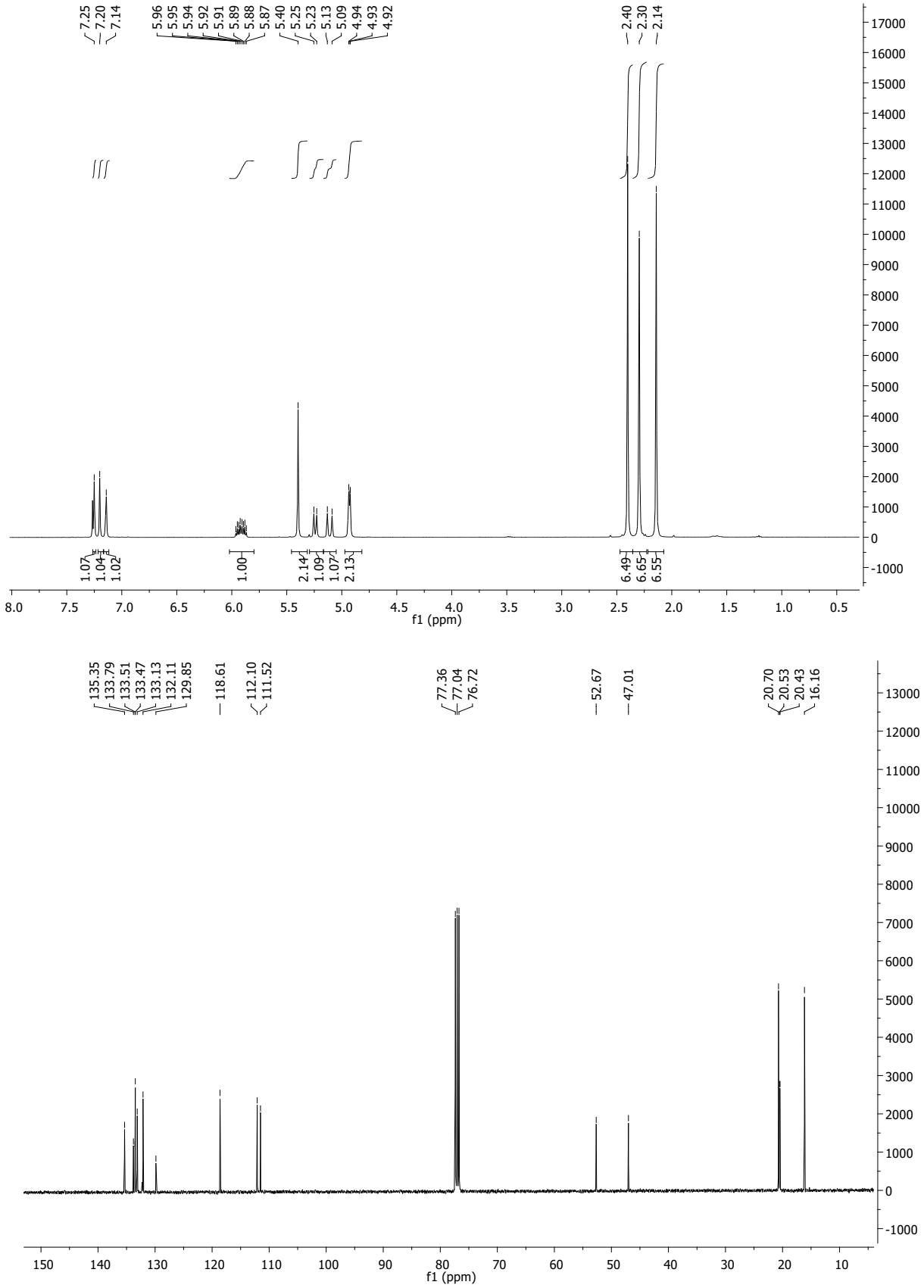


Figure S17. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectrums of **2c**

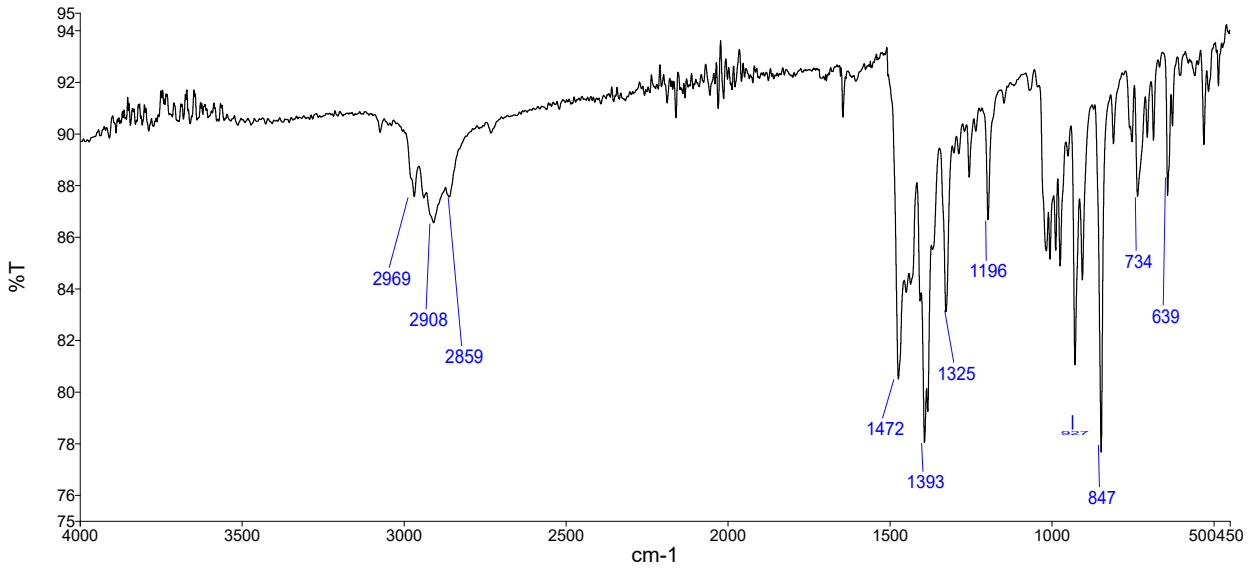


Figure S18. FT-IR spectrum of **2c**

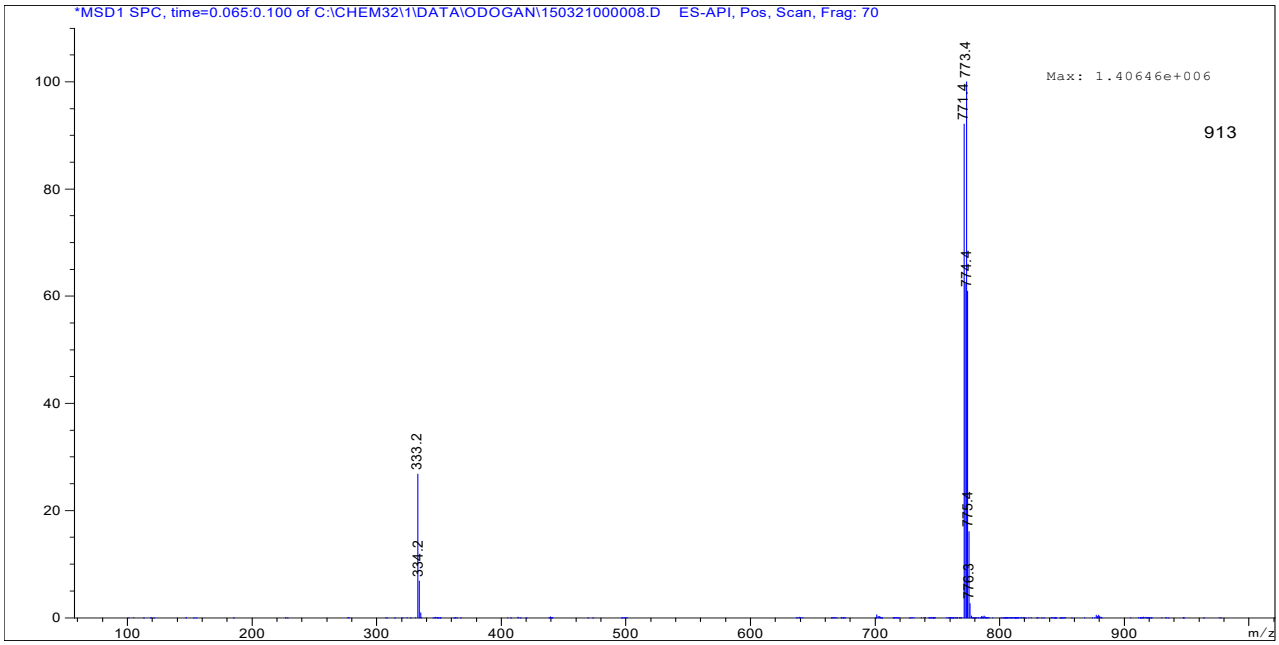


Figure S19. LC-MS spectrum of **2c**

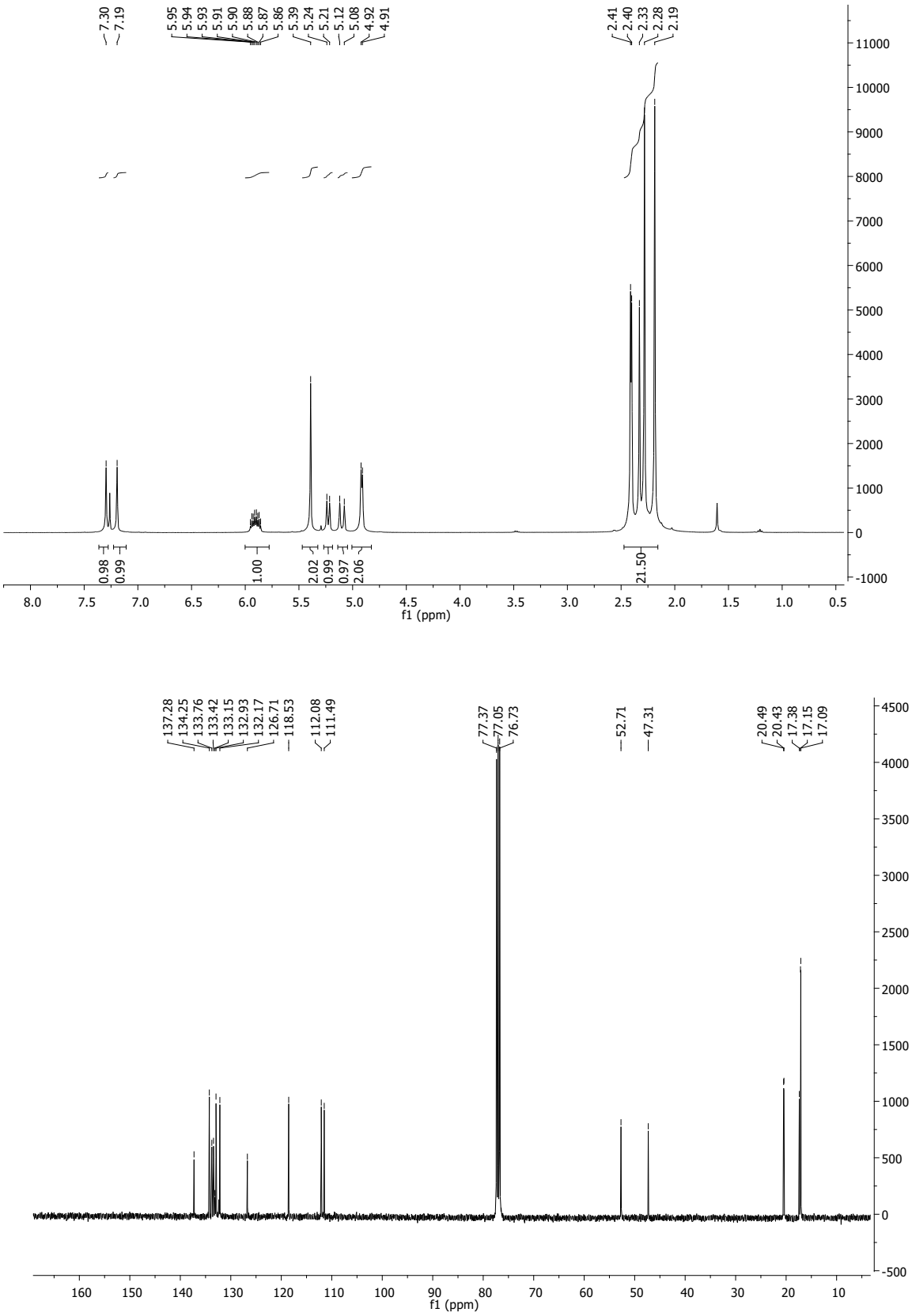


Figure S20. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectrums of **2d**

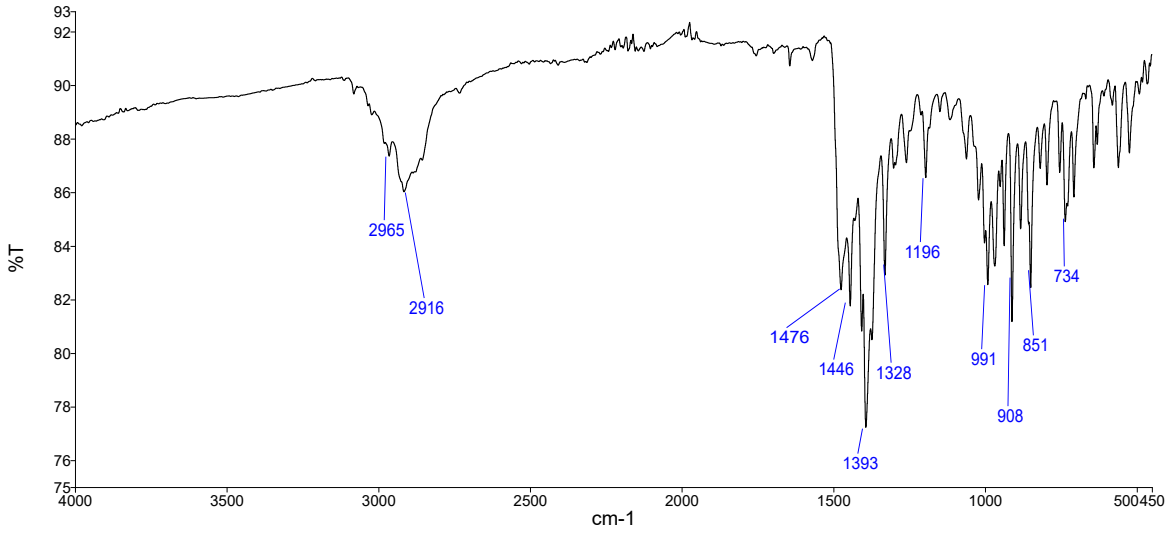


Figure S21. FT-IR spectrum of **2d**

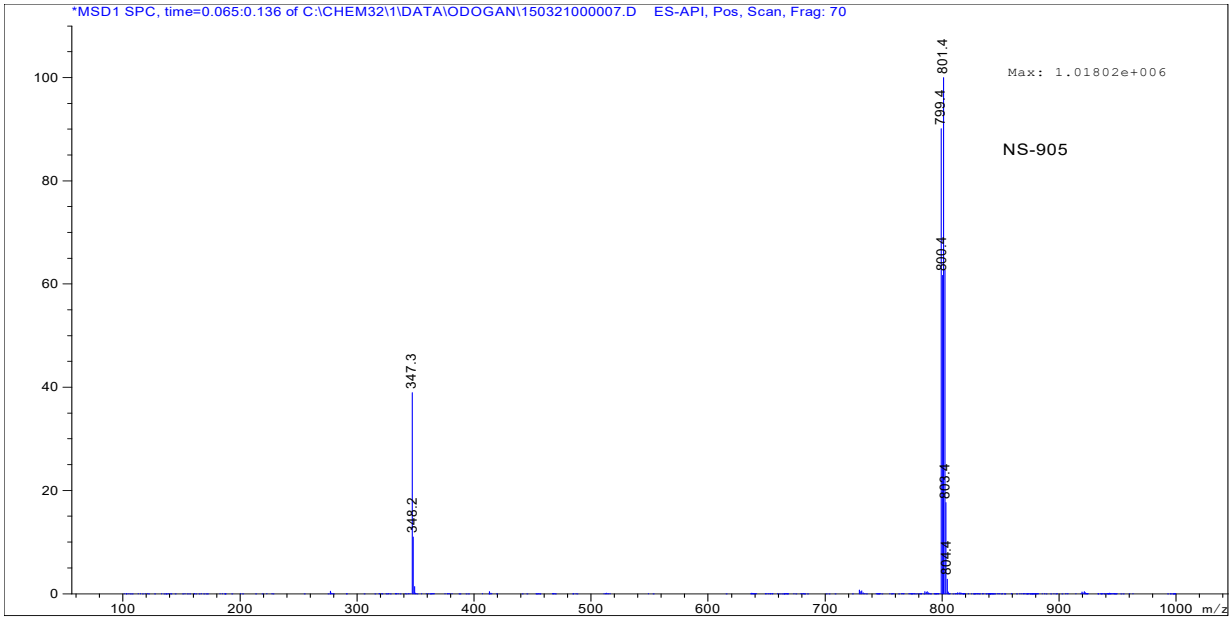
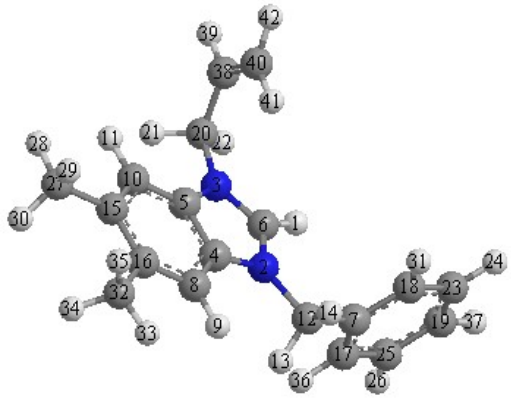


Figure S22. LC-MS spectrum of **2d**

Table S1. Selected optimization results for **2b**, **2c** and **2d.**

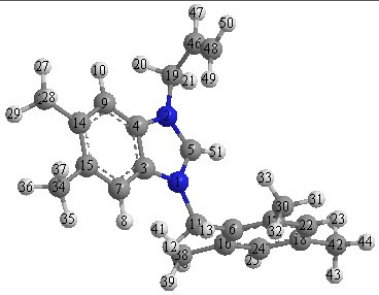
Parameters	2b	2c	2d
Bond lengths (Å)			
Ag1–Cl1	2.382	2.367	2.371
Ag1–C1	2.144	2.138	2.138
N1–C1	1.366	1.361	1.362
N1–C2	1.402	1.402	1.402
N1–C10	1.478	1.472	1.464
N2–C1	1.361	1.365	1.364
N2–C9	1.402	1.402	1.403
N2–C13	1.464	1.474	1.475
Bond angles (°)			
Cl1–Ag1–C1	170.5	169.5	169.6
Ag1–C1–N1	125.3	124.3	128.3
Ag1–C1–N2	127.7	128.7	124.8
N1–C1–N2	107.0	106.9	106.9
C1–N1–C2	110.3	110.4	110.5
C1–N1–C10	125.8	124.2	124.2
C2–N1–C10	123.8	125.4	125.3
C1–N2–C9	110.5	110.4	110.4
C1–N2–C13	124.4	125.7	125.8
C9–N2–C13	125.2	123.9	123.8

Table S2. Calculated Cartesian Coordinates of **1a**



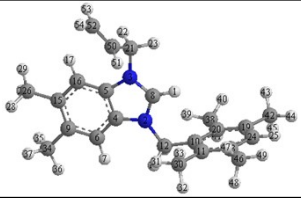
Atom(label)	x	y	z
H(1)	-0.5369	-0.8091	-1.8930
N(2)	-0.6675	0.4587	-0.1464
N(3)	1.1842	-0.6792	-0.5704
C(4)	0.2332	0.7596	0.8846
C(5)	1.4141	0.0287	0.6180
C(6)	-0.0679	-0.4019	-0.9907
C(7)	-2.7616	0.5215	-1.5097
C(8)	0.1315	1.5959	2.0080
H(9)	-0.7842	2.1668	2.2191
C(10)	2.5274	0.1076	1.4689
H(11)	3.4407	-0.4717	1.2719
C(12)	-2.0435	1.0092	-0.2733
H(13)	-1.9451	2.1143	-0.2749
H(14)	-2.5889	0.7205	0.6489
C(15)	2.4421	0.9404	2.5972
C(16)	1.2391	1.6892	2.8675
C(17)	-2.6675	1.2423	-2.7205
C(18)	-3.5209	-0.6685	-1.4711
C(19)	-4.0665	-0.4126	-3.8294
C(20)	2.1222	-1.5943	-1.2324
H(21)	3.1198	-1.1038	-1.2332
H(22)	1.8232	-1.6649	-2.2999
C(23)	-4.1692	-1.1338	-2.6268
H(24)	-4.7652	-2.0579	-2.5857
C(25)	-3.3178	0.7766	-3.8747
H(26)	-3.2489	1.3502	-4.8113
C(27)	3.6170	1.0480	3.5366
H(28)	4.4682	0.4270	3.2006
H(29)	3.3445	0.7250	4.5636
H(30)	3.9730	2.0961	3.6232
H(31)	-3.6184	-1.2283	-0.5267
C(32)	1.1705	2.5811	4.0814
H(33)	0.1900	3.0859	4.1651
H(34)	1.9561	3.3654	4.0513
H(35)	1.3381	2.0070	5.0168
H(36)	-2.0947	2.1829	-2.7567
H(37)	-4.5804	-0.7734	-4.7331
C(38)	2.2055	-2.9695	-0.6125
H(39)	2.9687	-3.6158	-1.0805
C(40)	1.4584	-3.4367	0.4001
H(41)	0.6894	-2.8259	0.9010
H(42)	1.5954	-4.4623	0.7736

Table S3. Calculated Cartesian Coordinates of **1b**



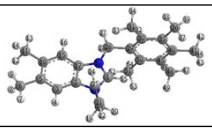
Atom(label)	x	y	z
N(1)	-0.0652	0.4421	0.2988
N(2)	1.7475	-0.7746	-0.0746
C(3)	0.8572	0.7788	1.2985
C(4)	2.0137	-0.0010	1.0643
C(5)	0.4974	-0.4862	-0.4960
C(6)	-2.1765	0.4664	-1.0468
C(7)	0.7935	1.6835	2.3704
H(8)	-0.1045	2.2906	2.5558
C(9)	3.1398	0.0982	1.8962
H(10)	4.0338	-0.5184	1.7251
C(11)	-1.4315	1.0198	0.1449
H(12)	-1.2979	2.1173	0.0742
H(13)	-1.9643	0.8120	1.0940
C(14)	3.0921	1.0000	2.9725
C(15)	1.9136	1.7966	3.2110
C(16)	-2.0725	1.1144	-2.3113
C(17)	-2.9814	-0.6973	-0.8999
C(18)	-3.5776	-0.5761	-3.2896
C(19)	2.6476	-1.7574	-0.6896
H(20)	3.6605	-1.3010	-0.7314
H(21)	2.3328	-1.8826	-1.7474
C(22)	-3.6637	-1.1948	-2.0274
H(23)	-4.2913	-2.0934	-1.9133
C(24)	-2.7759	0.5786	-3.4055
H(25)	-2.7025	1.0852	-4.3816
C(26)	4.2817	1.1305	3.8908
H(27)	5.1123	0.4688	3.5817
H(28)	4.0142	0.8746	4.9381
H(29)	4.6659	2.1721	3.9126
C(30)	-3.1412	-1.3950	0.4348
H(31)	-3.7549	-2.3095	0.3314
H(32)	-3.6498	-0.7463	1.1805
H(33)	-2.1712	-1.7025	0.8800
C(34)	1.8823	2.7577	4.3723
H(35)	0.9157	3.2916	4.4374
H(36)	2.6867	3.5190	4.2903
H(37)	2.0463	2.2338	5.3375
C(38)	-1.2496	2.3728	-2.4970
H(39)	-1.6617	3.2236	-1.9122
H(40)	-1.2397	2.6874	-3.5577
H(41)	-0.1914	2.2475	-2.1835
C(42)	-4.3127	-1.1298	-4.4861
H(43)	-4.8602	-0.3314	-5.0272
H(44)	-5.0403	-1.9119	-4.1961
H(45)	-3.6052	-1.5821	-5.2141
C(46)	2.6951	-3.0953	0.0105
H(47)	3.4135	-3.8017	-0.4414
C(48)	1.9663	-3.4673	1.0744
H(49)	1.2432	-2.7928	1.5621
H(50)	2.0728	-4.4736	1.5060
H(51)	-0.0002	-0.9307	-1.3656

Table S4. Calculated Cartesian Coordinates of **1c**



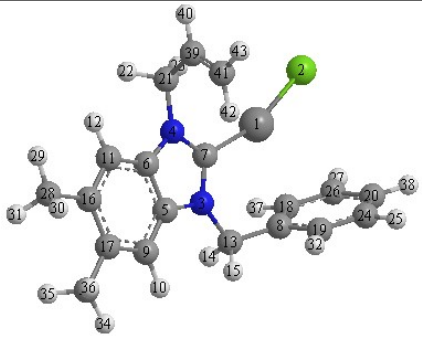
Atom(label)	x	y	z
H(1)	-0.7279	1.3572	0.1074
N(2)	0.1404	-0.6137	-0.0301
N(3)	-0.0263	0.3986	1.9333
C(4)	0.6754	-1.4921	0.9211
C(5)	0.5735	-0.8458	2.1756
C(6)	1.2258	-2.7786	0.8056
H(7)	1.3048	-3.2836	-0.1679
C(8)	-0.2652	0.4990	0.6084
C(9)	1.6769	-3.4155	1.9740
C(10)	-0.5823	0.2796	-2.2618
C(11)	0.2628	1.3010	-2.7835
C(12)	0.0319	-0.8715	-1.4919
H(13)	-0.5621	-1.7991	-1.6041
H(14)	1.0544	-1.0993	-1.8501
C(15)	1.5735	-2.7569	3.2528
C(16)	1.0215	-1.4682	3.3517
H(17)	0.9560	-0.9633	4.3249
C(18)	-0.3164	2.3384	-3.5620
C(19)	-2.5573	1.3387	-3.2542
C(20)	-1.9925	0.2984	-2.4697
C(21)	-0.3344	1.4380	2.9369
H(22)	-0.9629	0.9791	3.7280
H(23)	-0.9609	2.1936	2.4168
C(24)	-1.7055	2.3279	-3.7780
H(25)	-2.1474	3.1327	-4.3887
C(26)	2.0654	-3.4543	4.4965
H(27)	1.5300	-4.4122	4.6637
H(28)	3.1431	-3.7094	4.4193
H(29)	1.9285	-2.8276	5.3977
C(30)	1.7609	1.3218	-2.5623
H(31)	2.1213	0.5909	-1.8146
H(32)	2.3116	1.1226	-3.5074
H(33)	2.1002	2.3221	-2.2220
C(34)	2.2743	-4.7979	1.8884
H(35)	1.7008	-5.5257	2.4999
H(36)	2.2951	-5.1716	0.8474
H(37)	3.3142	-4.8134	2.2758
C(38)	-2.9069	-0.7718	-1.9093
H(39)	-2.4779	-1.3198	-1.0492
H(40)	-3.8652	-0.3384	-1.5626
H(41)	-3.1713	-1.5274	-2.6817
C(42)	-4.0392	1.3893	-3.5459
H(43)	-4.6445	1.4884	-2.6190
H(44)	-4.2892	2.2476	-4.1985
H(45)	-4.3927	0.4673	-4.0540
C(46)	0.5357	3.4283	-4.1673
H(47)	1.0986	3.9954	-3.3946
H(48)	1.2959	3.0187	-4.8663
H(49)	-0.0807	4.1542	-4.7313
C(50)	0.9000	2.0783	3.5228
H(51)	1.6209	2.4936	2.7963
C(52)	1.1200	2.2059	4.8423
H(53)	0.4123	1.8138	5.5925
H(54)	2.0124	2.7253	5.2242

Table S5. Calculated Cartesian Coordinates of **1d**



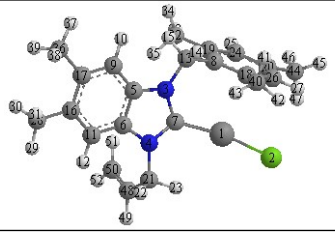
Atom(label)	x	y	z
C(1)	0.9347	-0.0302	-0.3728
C(2)	2.2588	1.6414	0.2768
C(3)	3.2890	2.5719	0.4853
H(4)	4.2263	2.5284	-0.0880
C(5)	3.0890	3.5804	1.4430
C(6)	4.1743	4.5979	1.6913
H(7)	5.0605	4.4161	1.0547
H(8)	4.5090	4.5846	2.7500
H(9)	3.8168	5.6297	1.4890
C(10)	1.8550	3.6532	2.1856
C(11)	1.6593	4.7438	3.2089
H(12)	2.4320	4.6962	4.0050
H(13)	0.6681	4.6758	3.6949
H(14)	1.7456	5.7514	2.7506
C(15)	0.8319	2.7158	1.9631
H(16)	-0.1096	2.7747	2.5281
C(17)	1.0478	1.7126	1.0046
C(18)	3.1499	0.0683	-1.5381
H(19)	4.1419	0.1122	-1.0380
H(20)	2.9600	-1.0097	-1.7283
C(21)	3.1742	0.8378	-2.8379
H(22)	3.9643	0.5012	-3.5321
C(23)	2.3504	1.8365	-3.1921
H(24)	1.5528	2.2102	-2.5290
H(25)	2.4491	2.3274	-4.1716
C(26)	-1.1185	0.3184	1.0570
H(27)	-1.7431	1.2123	0.8680
H(28)	-1.0373	0.2108	2.1557
C(29)	-1.7047	-0.9203	0.4134
C(30)	-2.4934	-0.7918	-0.7658
C(31)	-2.7034	0.5544	-1.4363
H(32)	-2.5827	0.4814	-2.5353
H(33)	-1.9927	1.3306	-1.0958
H(34)	-3.7269	0.9511	-1.2569
C(35)	-3.0971	-1.9489	-1.3185
C(36)	-3.9973	-1.8514	-2.5329
H(37)	-3.5127	-2.2712	-3.4421
H(38)	-4.2941	-0.8151	-2.7684
H(39)	-4.9315	-2.4297	-2.3877
C(40)	-2.8736	-3.2286	-0.7328
C(41)	-3.5029	-4.4309	-1.4036
H(42)	-4.6063	-4.4442	-1.2625
H(43)	-3.1149	-5.3920	-1.0270
H(44)	-3.3303	-4.4147	-2.4986
C(45)	-2.0839	-3.3495	0.4417
C(46)	-1.8679	-4.6759	1.1398
H(47)	-2.4517	-5.5000	0.6973
H(48)	-2.1585	-4.6163	2.2093
H(49)	-0.7995	-4.9829	1.1263
C(50)	-1.4852	-2.1910	1.0103
C(51)	-0.6344	-2.3607	2.2530
H(52)	-0.0680	-1.4560	2.5390
H(53)	0.1076	-3.1748	2.1255
H(54)	-1.2525	-2.6486	3.1308
H(55)	0.5481	-0.9158	-0.8901
N(56)	2.1478	0.5295	-0.5704
N(57)	0.2497	0.6478	0.5650

Table S6. Calculated Cartesian Coordinates of **2a**



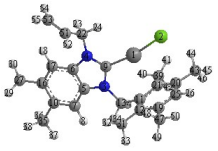
Atom(label)	x	y	z
Ag(1)	0.0235	-0.5481	-2.9358
Cl(2)	-0.2187	-1.5172	-5.0916
N(3)	0.1272	0.8660	-0.1310
N(4)	1.9552	-0.3021	-0.4515
C(5)	0.9031	1.0376	1.0215
C(6)	2.0782	0.2721	0.8189
C(7)	0.7841	0.0791	-1.0322
C(8)	-2.0717	0.7524	-1.3094
C(9)	0.7229	1.7965	2.1882
H(10)	-0.1778	2.4072	2.3467
C(11)	3.0972	0.2345	1.7817
H(12)	4.0048	-0.3672	1.6301
C(13)	-1.1691	1.5318	-0.3745
H(14)	-0.9759	2.5499	-0.7739
H(15)	-1.6609	1.6504	0.6102
C(16)	2.9249	0.9738	2.9653
C(17)	1.7298	1.7621	3.1690
C(18)	-2.0005	0.9650	-2.7201
C(19)	-2.9943	-0.1849	-0.8143
C(20)	-3.7610	-0.6881	-3.0842
C(21)	2.9269	-1.2086	-1.0685
H(22)	3.9454	-0.8204	-0.8497
H(23)	2.8029	-1.1198	-2.1699
C(24)	-3.8349	-0.8956	-1.6941
H(25)	-4.5601	-1.6163	-1.2858
C(26)	-2.8485	0.2423	-3.6014
H(27)	-2.7999	0.4377	-4.6830
C(28)	3.9901	0.9423	4.0296
H(29)	4.8437	0.3024	3.7385
H(30)	3.5904	0.5602	4.9928
H(31)	4.3835	1.9596	4.2397
H(32)	-3.0696	-0.3600	0.2706
C(33)	1.5628	2.5531	4.4399
H(34)	0.5985	3.0946	4.4628
H(35)	2.3760	3.2998	4.5629
H(36)	1.6077	1.8982	5.3356
H(37)	-1.3847	1.7908	-3.1181
H(38)	-4.4248	-1.2442	-3.7627
C(39)	2.8051	-2.6516	-0.6398
H(40)	3.5779	-3.3095	-1.0752
C(41)	1.8705	-3.1650	0.1770
H(42)	1.0846	-2.5449	0.6378
H(43)	1.8633	-4.2377	0.4224

Table S7. Calculated Cartesian Coordinates of **2b**



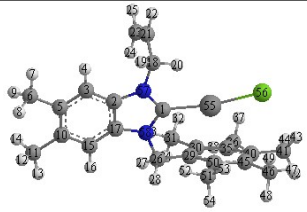
Atom(label)	x	y	z
Ag(1)	7.9629	4.3776	4.4876
Cl(2)	7.4223	3.5366	2.3255
N(3)	8.1463	5.8208	7.2673
N(4)	9.9749	4.6665	6.9138
C(5)	8.9631	6.0331	8.3872
C(6)	10.1368	5.2798	8.1641
C(7)	8.7749	5.0070	6.3689
C(8)	5.9693	5.7840	6.0306
C(9)	8.8075	6.8108	9.5461
H(10)	7.9022	7.4103	9.7211
C(11)	11.1844	5.2736	9.0966
H(12)	12.0930	4.6772	8.9298
C(13)	6.8280	6.4630	7.0781
H(14)	6.9940	7.5315	6.8304
H(15)	6.3194	6.4421	8.0602
C(16)	11.0416	6.0398	10.2678
C(17)	9.8468	6.8134	10.4931
C(18)	6.0978	6.1543	4.6443
C(19)	5.0327	4.7915	6.4033
C(20)	4.3597	4.4857	4.0289
C(21)	10.9504	3.7801	6.2762
H(22)	11.9539	4.2527	6.3610
H(23)	10.7151	3.7700	5.1889
C(24)	4.2382	4.1799	5.3973
H(25)	3.5058	3.4163	5.7061
C(26)	5.2939	5.4758	3.6694
H(27)	5.3844	5.7828	2.6161
C(28)	12.1455	6.0484	11.2951
H(29)	12.9980	5.4152	10.9857
H(30)	11.7881	5.6792	12.2797
H(31)	12.5311	7.0752	11.4692
C(32)	4.8616	4.3562	7.8396
H(33)	4.1236	3.5364	7.9241
H(34)	4.5019	5.1884	8.4828
H(35)	5.8151	3.9942	8.2780
C(36)	9.7114	7.6346	11.7510
H(37)	8.7391	8.1608	11.7944
H(38)	10.5142	8.3985	11.8263
H(39)	9.7968	7.0038	12.6607
C(40)	6.8945	7.3591	4.1983
H(41)	6.2856	8.2797	4.3471
H(42)	7.1324	7.3033	3.1189
H(43)	7.8425	7.5023	4.7510
C(44)	3.5603	3.7647	2.9774
H(45)	3.1293	4.4700	2.2388
H(46)	2.7362	3.1708	3.4156
H(47)	4.2268	3.0759	2.4151
C(48)	10.9837	2.3710	6.8181
H(49)	11.7848	1.7478	6.3826
C(50)	10.1493	1.8473	7.7309
H(51)	9.3409	2.4361	8.1938
H(52)	10.2520	0.8011	8.0553

Table S8. Calculated Cartesian Coordinates of **2c**



Atom(label)	x	y	z
Ag(1)	1.1503	7.6964	3.1859
Cl(2)	-0.1518	9.5720	2.5625
N(3)	2.8124	5.0704	3.4488
N(4)	2.5753	5.9679	5.4328
C(5)	3.4617	4.2094	4.3443
C(6)	3.3166	4.7934	5.6229
C(7)	4.1539	3.0009	4.1693
H(8)	4.2618	2.5359	3.1784
C(9)	2.2802	6.1365	4.1146
C(10)	4.7065	2.3773	5.3030
C(11)	2.2099	6.0002	1.1867
C(12)	3.1372	6.8236	0.5083
C(13)	2.6913	4.8121	2.0028
H(14)	2.0099	3.9475	1.8612
H(15)	3.6830	4.4798	1.6432
C(16)	4.5639	2.9751	6.6056
C(17)	3.8698	4.1885	6.7621
H(18)	3.7738	4.6498	7.7547
C(19)	2.6481	7.8548	-0.3655
C(20)	0.3139	7.2811	0.1864
C(21)	0.7880	6.2294	1.0668
C(22)	2.1805	6.9077	6.4948
H(23)	1.6257	6.3483	7.2772
H(24)	1.4603	7.6090	6.0171
C(25)	1.2630	8.0512	-0.5012
H(26)	0.9049	8.8442	-1.1759
C(27)	5.1622	2.2958	7.8128
H(28)	4.7516	1.2735	7.9506
H(29)	6.2619	2.1788	7.7110
H(30)	4.9665	2.8663	8.7401
C(31)	4.6309	6.6743	0.6658
H(32)	4.9265	5.9920	1.4823
H(33)	5.1041	6.3080	-0.2711
H(34)	5.1007	7.6560	0.8811
C(35)	5.4498	1.0729	5.1514
H(36)	4.9837	0.2662	5.7557
H(37)	5.4740	0.7354	4.0979
H(38)	6.4992	1.1597	5.5039
C(39)	-0.2247	5.2631	1.6370
H(40)	0.1405	4.7006	2.5146
H(41)	-1.1597	5.7760	1.9317
H(42)	-0.5119	4.5200	0.8584
C(43)	-1.1545	7.4723	-0.0744
H(44)	-1.7195	7.6488	0.8625
H(45)	-1.3286	8.3387	-0.7386
H(46)	-1.5921	6.5736	-0.5615
C(47)	3.6030	8.7342	-1.1222
H(48)	4.2372	9.3301	-0.4297
H(49)	4.3045	8.1404	-1.7459
H(50)	3.0686	9.4424	-1.7822
C(51)	3.3421	7.6653	7.0874
H(52)	4.0075	8.1674	6.3622
C(53)	3.5621	7.7932	8.4072
H(54)	2.9082	7.3144	9.1558

Table S9. Calculated Cartesian Coordinates of **2d**



Atom(label)	x	y	z
C(1)	8.1841	6.9123	4.5136
C(2)	9.3756	8.7673	5.0591
C(3)	10.3305	9.7862	5.2008
H(4)	11.2999	9.7375	4.6844
C(5)	10.0171	10.8888	6.0156
C(6)	11.0249	11.9981	6.1915
H(7)	11.9497	11.8053	5.6162
H(8)	11.3097	12.1250	7.2570
H(9)	10.6162	12.9750	5.8577
C(10)	8.7417	10.9672	6.6792
C(11)	8.4196	12.1558	7.5509
H(12)	9.1427	12.2559	8.3875
H(13)	7.4061	12.0801	7.9877
H(14)	8.4729	13.1061	6.9789
C(15)	7.7914	9.9417	6.5189
H(16)	6.8192	10.0067	7.0290
C(17)	8.1226	8.8471	5.7047
C(18)	10.4716	7.0603	3.5218
H(19)	11.4172	7.1797	4.0955
H(20)	10.3209	5.9633	3.4119
C(21)	10.5942	7.7084	2.1638
H(22)	11.4791	7.3766	1.5920
C(23)	9.7447	8.5986	1.6262
H(24)	8.8515	8.9565	2.1635
H(25)	9.9166	9.0075	0.6196
C(26)	6.0710	7.3572	5.8268
H(27)	5.4579	8.2731	5.7424
H(28)	6.1429	7.1326	6.9114
C(29)	5.3991	6.2078	5.0950
C(30)	4.4450	6.4578	4.0875
C(31)	4.1837	7.8577	3.5775
H(32)	4.0989	7.8672	2.4729
H(33)	4.9897	8.5662	3.8392
H(34)	3.2302	8.2717	3.9712
C(35)	3.7142	5.3595	3.5125
C(36)	2.6143	5.6456	2.5217
H(37)	2.9881	5.5712	1.4748
H(38)	2.1869	6.6573	2.6405
H(39)	1.7848	4.9198	2.6119
C(40)	4.0331	4.0145	3.8509
C(41)	3.3655	2.8569	3.1425
H(42)	2.6433	2.3267	3.7994
H(43)	4.1305	2.1216	2.8239
H(44)	2.8201	3.1714	2.2369
C(45)	4.9957	3.7523	4.8577
C(46)	5.2331	2.3566	5.3738
H(47)	4.6746	1.5948	4.8072
H(48)	4.9202	2.2767	6.4378
H(49)	6.3049	2.0804	5.3237
C(50)	5.6948	4.8534	5.4922
C(51)	6.5522	4.5590	6.7012
H(52)	7.2552	5.3714	6.9542
H(53)	7.1394	3.6303	6.5769
H(54)	5.8990	4.3912	7.5882

Ag(55)	7.5736	5.0337	3.6963
Cl(56)	7.2700	2.9662	2.5759
N(57)	9.3718	7.5581	4.3495
N(58)	7.4218	7.6888	5.3365

Table S10. Analysis of the docking of all molecules, Ciprofloxacin, and Fluconazole in the active site of receptors.

Compounds	Bind. Aff.*	Amino Acids Residue
		2br6
1a	-6.55	Asp108, His169, Met138, Glu136, His106, Leu16, Tyr194, Ala206, His235, Ile73, Leu105, Phe107, Tyr137, Gly207
1b	-6.56	Met138, His106, Ile73, Phe107, His109, His169, Tyr194, Ala206, His235, Asp108, Glu136, Tyr137, Asp191, Gly207
1c	-6.75	Asp108, His169, Met138, Leu16, Ile73, His106, Phe107, Tyr137, Tyr194, Ala206, His235, Leu105, Glu136, Gly207, Phe208
1d	-6.37	Met138, His106, Ile73, Phe107, His109, His169, Tyr194, Ala206, His235, Asp108, Glu136, Tyr137, Asp191, Gly207, Phe208
2a	-6.27	Met138, Glu136, Cys14, Ile73, His106, Phe107, Tyr194, His235, Leu16, Asp108, Arg134, Tyr137, His169, Ser170, Asp191, Gly207, Phe208
2b	-6.33	Asp108, His106, Phe107, Glu136, Cys14, Leu16, Ile73, Tyr137, Met138, Cys141, His169, Tyr194, His235
2c	-6.55	Met138, Cys14, Ile73, His106, Phe107, Tyr137, His169, Tyr194, His235, Leu16, Leu105, Asp108, Arg134, Glu136, Asp191, Gly207, Phe208
2d	-6.64	His106, Phe107, Met138, Cys14, Leu16, Ile73, Tyr137, Tyr194, His235, Leu105, Asp108, Arg134, His169, Asp191, Ala206, Gly207, Phe208
Cipro	-4.93	His19, His106, Tyr194, Asp108, Asp191, Leu16, Ala206, Cys14, Ser20, Leu33, Val35, Ile73, Phe107, His109, Gly207, Phe208, His235
Flu	-5.81	His106, Phe107, Asp108, Tyr194, Glu136, His169, Asp191, Hs235, Cys14, Leu16, Ile73, Cys14, Ala206, Leu33, Ser20, His109
		2fnp
1a	-5.09	Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, His159, Asn161
1b	-5.34	Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215
1c	-5.46	Phe137, Leu122, Lys123, Ile126, Phe134, Ala138, Val211, Ile215, Thr141, Tyr142, Glu145, Leu160, Tyr162, Leu208, Asn212
1d	-5.44	Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212
2a	-4.55	Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162
2b	-4.87	Phe134, Lys123, Phe137, Ala138, Tyr142, Tyr162, Thr141, His159, Asn161
2c	-4.64	Leu160, Phe137, Tyr162, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn161, His159
2d	-4.84	Tyr162, Leu160, Phe1Leu160, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159
Cipro	-5.34	Glu145, Leu160, Tyr162, Lys123, Phe134, Phe137, Ala138, Thr141, Tyr142, Asn161
Flu	-3.94	Tyr162, Thr141, Ala138, Glu145, Leu160, Phe134, Lys123, Phe137, Tyr142, Asn161
		3cuz
1a	-8.07	Trp277, Cys274, Arg276, Met303, Met332, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Trp365, Leu444
1b	-8.77	Trp277, Leu248, Arg276, Met303, Met303, Ala332, Trp365, Ala449, Glu250, Cys274, Gly275, Asp278, Gly329, Leu444, Glu446
1c	-8.64	Trp365, Trp277, Leu248, Arg276, Met330, Ala332, Phe333, Ala449, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Ala331, Leu444, Met445, Glu446, Asp447, Thr450
1d	-9.00	Trp365, Trp277, Leu248, Cys274, Arg276, Met303, Met330, Ala332, Ala449, Glu250, Asn273, Gly275, Asp278, Tyr279, Gly329, Glu356, Leu444
2a	-8.48	Asp447, Arg276, Trp277, Met330, Trp365, Met303, Ala332, Glu119, Asp120, Arg166, Lys215, Leu248, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Met445, Glu446, Ala449, Thr450
2b	-9.07	Trp365, Leu248, Arg276, Trp277, Met330, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Ala367, Leu444, Met445
2c	-8.75	Met330, Trp365, Leu248, Arg276, Trp277, Met303, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Gly328, Ala331, Glu356, Met445, Glu446, Asp447
2d	-8.78	Trp277, Met330, Leu248, Arg276, Met303, Ala332, Trp365, Leu444, Arg166, Glu250, Gly275, Asp278, Gly329, Asp352, Glu356, Met445, Glu446, Asp447
Cipro	-8.80	Asp120, Arg276, Asp278, Met330, Glu250, Gly275, Trp277, Asp447, Ala332, Glu119, Lys215, Leu248, Gly329, Trp365, Ala331, Met445, Glu446, Ala449
Flu	-6.82	Arg166, Arg276, Met330, Glu250, Cys274, Asp447, Trp365, Ala449, Leu248, Asn273, Gly275, Trp277, Asp278, Gly329

* Binding Affinity in kcal/mol.

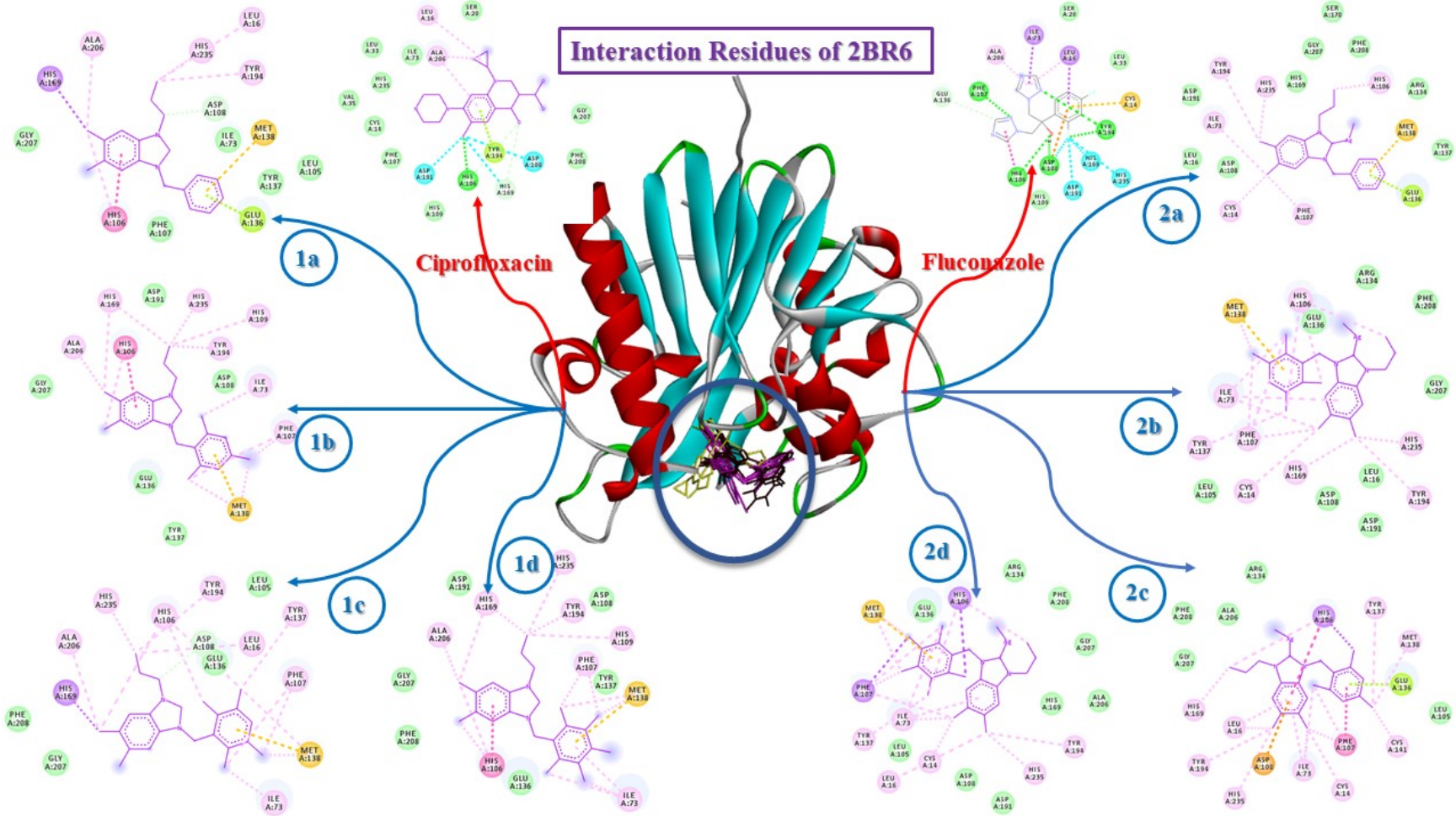


Figure S23. Interaction residues of all molecules, Ciprofloxacin, and Fluconazole with Quorum-Quenching N-Acyl Homoserine Lactone Lactonase (dark green and turquoise: H-bonds; green: van der Waals; orange: pi-anion/cation; pink: alkyl and pi-alkyl; yellow: pi-sulfur; fuchsia: pi-pi stacked and pi-pi T shaped)

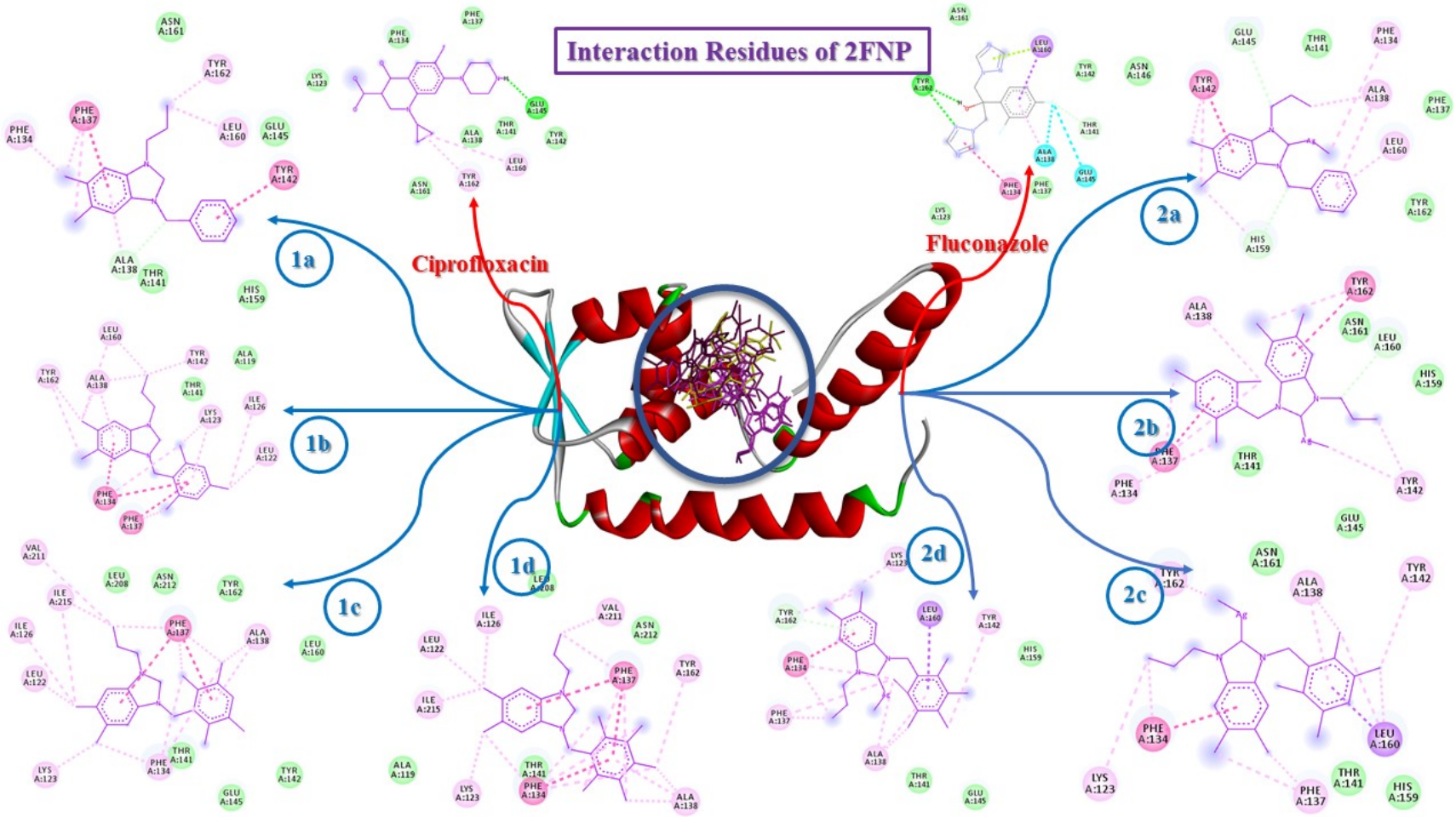


Figure S24. Interaction residues of all molecules, Ciprofloxacin, and Fluconazole with Crystal structure of SarA (dark green and turquoise: H-bonds; green: van der Waals; orange: pi-anion/cation; pink: alkyl and pi-alkyl; yellow: pi-sulfur; fuchsia: pi-pi stacked and pi-pi T shaped)

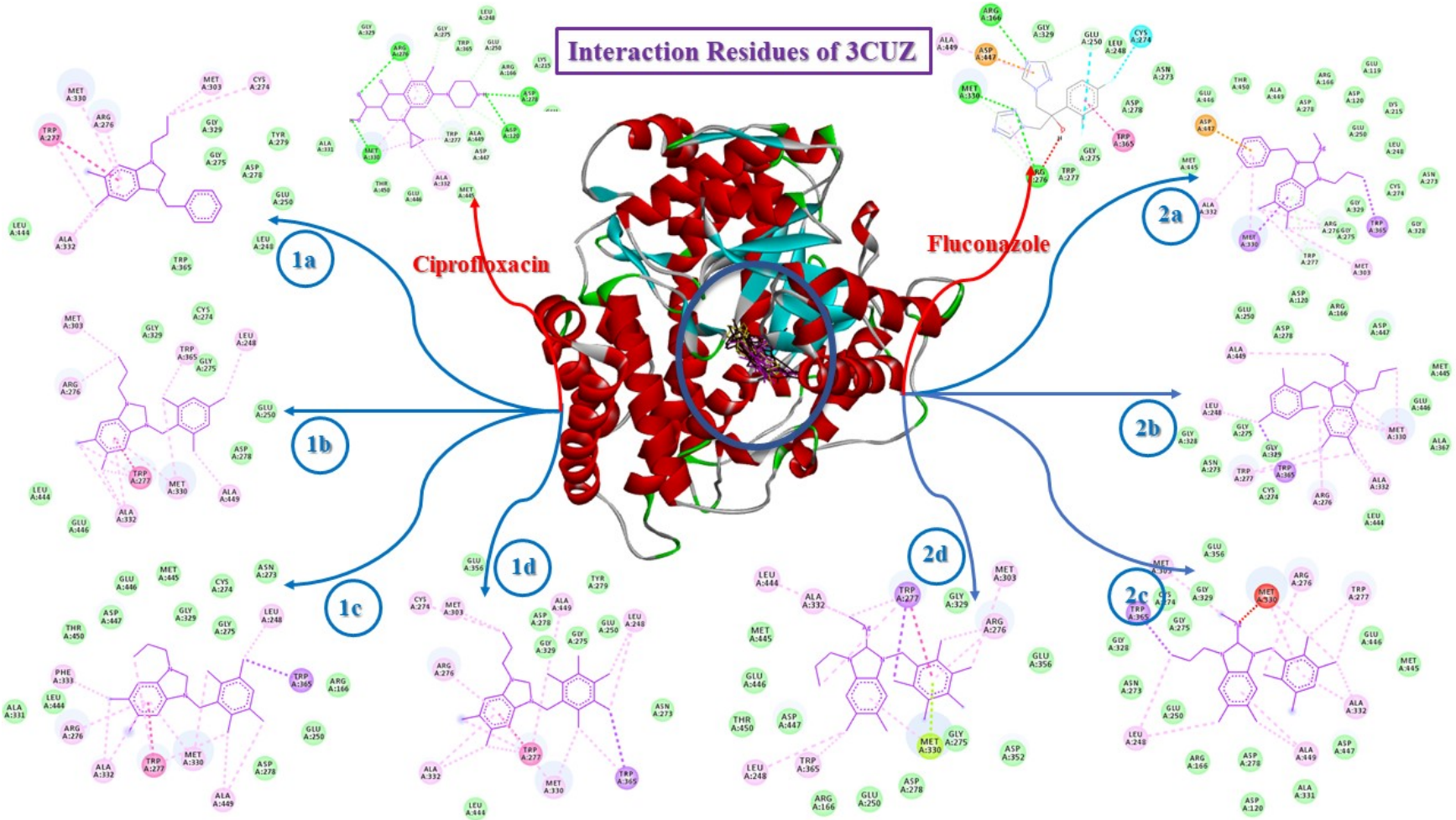


Figure S25. Interaction residues of all molecules, Ciprofloxacin, and Fluconazole with Atomic Resolution Structures of Escherichia coli and Bacillis anthracis Malate Synthase A (dark green and turquoise: H-bonds; green: van der Waals; orange: pi-anion/cation; pink: alkyl and pi-alkyl; yellow: pi-sulfur; fuchsia: pi-pi stacked and pi-pi T shaped).