Supplementary materials

A novel strategy for the functionalization and design of 4-methylene-4*H*-pyran merocyanines *via* enamination and 1,8-conjugate addition

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Table of Contents

1. Quantum mechanical calculations details

The ground state molecular geometry of the 5 compounds under investigation was fully optimized at the density functional theory (DFT) level, both in vacuo and in the solvated phase (DMSO). For all geometry optimizations, the B3LYP hybrid functional[1], coupled with the 6-31G(d,p)++ basis set was chosen. Solvent effects were taken into account via the implicit conductor-like polarizable continuum model (C-PCM). For the evaluation of energetics, Solvation Model Density (SMD) parametrization was employed.[2] The vibrational frequencies and thermochemicals were computed in harmonic approximation at T = 298.15 K and p = 1 atm, and no imaginary frequencies were found.

The UV-vis absorption spectra for the equilibrium geometries were calculated at time dependent density functional theory (TD-DFT) level, accounting for $S_0 \rightarrow S_n$ (n = 1 to 7). The nature of the vertical excited electronic state was analysed both in vacuo and in the solvated phase.

The first singlet excited state S(π,π*) state geometry was optimized using analytical gradients and the first transitions $S_1 \rightarrow S_0$ of the emission. Properties of the excited states were calculated using the long-range corrected functional CAM-B3LYP[3] coupled with the 6−31G(d,p)++ basis set. The non-equilibrium solvation regime was set for vertical excited states calculations in the solvent phase, whereas the equilibrium solvation was used for adiabatic ones. All calculated UV-vis spectra were plotted as gaussian curves with wavelengths of absorption/emission maxima as expected value and $\sigma = 0.4$ eV.

The integration grid for the calculations was set as 96 radial shells and 302 angular points.
The RMS gradient convergence tolerance was set to 10^{-7} Hartree/Bohr for GS optimizations, and to 10^{-5} Hartree/Bohr for S_1 optimizations. The density matrix convergence threshold for the self-consistent field was set to 10^{-5} a.u. for all DFT and to 10^{-6} a.u. for all TD-DFT optimizations.

All calculations were performed using the US GAMESS (ver. 30 sep 2021, R2 Patch 1) software package for Linux x64.[4] Frontier MOs were plotted with MacMolPlt software (ver. 7.7).[5]

References

[1] A. D. Becke, *J. Chem. Phys.,* 1993, **98**, 5648–5652.
[2] A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B,* 2009, **113**, 6378–6396.
[3] T. Yanai, D. P. Tew and N. C. Handy, *Chem. Phys. Lett.* 2004, **393**, 51–57.
[4] G. M. J. Barca, C. Bertoni, L. Carrington, D. Datta, N. De Silva, J. E. Deustua, D. G. Fedorov, J. R. Gour, A. O. Gunina, E. Guidez, T. Harville, S. Irle, J. Ivanic, K. Kowalski, S. S. Leang, H. Li, W. Li, J. J. Lutz, I. Magoulas, J. Mato, V. Mironov, H. Nakata, B. Q. Pham, P. Piecuch, D. Poole, S. R. Pruitt, A. P. Rendell, L. B. Roskop, K. Ruedenberg, T. Sattasathuchana, M. W. Schmidt, J. Shen, L. Slipchenko, M. Sosonkina, V. Sundriyal, A. Tiwari, J. L. Galvez Vallejo, B. Westheimer, M. Włoch, P. Xu, F. Zahariev and M. S. Gordon, *J. Chem. Phys.*, 2020, **152**, 154102.
[5] B.M. Bode and M.S.Gordon, *J. Mol. Graphics and Modeling*, 1998, **16**, 133–138.

2. Cartesian coordinates of the GS optimized structure for compounds 2a,d, 3a,d, 11e

Cartesian coordinates (Å) of the optimized structure for compound **2a** in vacuo

C	6.0	0.7492009613	1.6266125869	0.0377781925
C	6.0	0.1390505696	0.3990313814	0.1098108243
O	8.0	0.8538686196	-0.7474693457	-0.1405455284
C	6.0	2.1800110808	-0.6718455426	-0.4720539548
C	6.0	2.8250438025	0.5133213465	-0.5552824414
C	6.0	2.1298218121	1.7536686921	-0.2959533155
C	6.0	2.7810729516	2.9914547697	-0.3719974884
C	6.0	-1.2416805253	0.1926094110	0.4403149564
C	6.0	-1.8211709627	-1.0429016579	0.5404447757
C	6.0	2.7692812615	-2.0220354669	-0.7172013249
N	7.0	-3.1312917840	-1.3030017238	0.7850214340
C	6.0	-4.0670622086	-0.2126418466	1.0183063661
C	6.0	-3.5632877116	-2.6470490492	1.1470335695
C	6.0	4.1604986148	3.0760958999	-0.7097993579
N	7.0	5.2936079718	3.1087678887	-0.9900591697
C	6.0	2.0786739361	4.2011682940	-0.1120204763
N	7.0	1.4680985151	5.1715935704	0.1086480813
H	1.0	0.1557475701	2.5101219957	0.2421649915
H	1.0	3.8757041984	0.5242241292	-0.8205080845
H	1.0	-1.8114948224	1.0976254131	0.6144175399
H	1.0	-1.2074143340	-1.9277278669	0.3997566773
H	1.0	2.2344189980	-2.5344688147	-1.5251866208
H	1.0	3.8213313190	-1.9318620253	-0.9938205316
H	1.0	2.6931362831	-2.6473727334	0.1800491414
H	1.0	-3.8835824711	0.2863115723	1.9813501592
H	1.0	-3.9832391628	0.5306196281	0.2192021605
H	1.0	-5.0853555037	-0.6066623078	1.0174613148
H	1.0	-2.8099446605	-3.3724238512	0.8316359918
H	1.0	-3.7102900071	-2.7486995888	2.2320895702
H	1.0	-4.5062041112	-2.8869134286	0.6445034843

Cartesian coordinates (Å) of the optimized structure for compound **3a** in vacuo

C	6.0	-0.2906717599	-1.1769955718	2.2300764794
C	6.0	0.2906717599	1.1769955718	2.2300764794
C	6.0	-0.2830879297	-1.1575047382	0.8618314837
C	6.0	0.2830879297	1.1575047382	0.8618314837
O	8.0	-0.0000000000	-0.0000000000	0.1780691935
C	6.0	-0.0000000000	-0.0000000000	2.9911956046
C	6.0	-0.0000000000	-0.0000000000	4.3965383989
C	6.0	-0.5517919381	-2.3015510157	0.0312612970
C	6.0	0.5517919381	2.3015510157	0.0312612970
C	6.0	-0.4949250308	-2.2841076598	-1.3319782436
C	6.0	0.4949250308	2.2841076598	-1.3319782436
N	7.0	-0.8058903417	-3.3088822419	-2.1772107139
N	7.0	0.8058903417	3.3088822419	-2.1772107139
C	6.0	-0.3375500577	-3.2705641519	-3.5559572289
C	6.0	0.3375500577	3.2705641519	-3.5559572289
C	6.0	-1.1710807600	-4.6119054777	-1.6430855605
C	6.0	1.1710807600	4.6119054777	-1.6430855605
C	6.0	-0.2923801183	-1.1838156826	5.1270026760
C	6.0	0.2923801183	1.1838156826	5.1270026760
N	7.0	-0.5371191132	-2.1756214439	5.6938079325
N	7.0	0.5371191132	2.1756214439	5.6938079325
H	1.0	-0.5180409738	-2.1092094909	2.7336740813
H	1.0	0.5180409738	2.1092094909	2.7336740813
H	1.0	-0.8012486554	-3.2076667576	0.5710780186
H	1.0	0.8012486554	3.2076667576	0.5710780186

H	1.0	-0.1965791389	-1.3696842357	-1.8359624434
H	1.0	0.1965791389	1.3696842357	-1.8359624434
H	1.0	0.6313686097	-3.7785984270	-3.6798182130
H	1.0	-0.6313686097	3.7785984270	-3.6798182130
H	1.0	-1.0681546284	-3.7547269934	-4.2119143886
H	1.0	1.0681546284	3.7547269934	-4.2119143886
H	1.0	-0.2235238853	-2.2319192234	-3.8766029329
H	1.0	0.2235238853	2.2319192234	-3.8766029329
H	1.0	-1.9398151210	-4.4986835596	-0.8730936728
H	1.0	1.9398151210	4.4986835596	-0.8730936728
H	1.0	-1.5800417606	-5.2266107072	-2.4483903997
H	1.0	1.5800417606	5.2266107072	-2.4483903997
H	1.0	-0.3089088192	-5.1361004532	-1.2028487394
H	1.0	0.3089088192	5.1361004532	-1.2028487394

Cartesian coordinates (Å) of the optimized structure for compound **11e** in vacuo

O	8.0	0.0000118858	0.0000036213	0.0631501531
C	6.0	-0.2802858319	1.1804451888	2.1143262755
C	6.0	0.2801328320	-1.1805556757	2.1142682042
C	6.0	-0.2819545766	1.1572566870	0.7464804240
C	6.0	0.2819501006	-1.1572857792	0.7464320787
C	6.0	-0.0001341151	-0.0000870128	2.8761196885
H	1.0	-0.5095554915	2.1128239038	2.6168694022
H	1.0	0.5093450861	-2.1129671315	2.6167772292
C	6.0	-0.0001853268	-0.0001627686	4.2802982781
C	6.0	-0.5832098382	2.2917964290	-0.0863830172
C	6.0	0.5833737142	-2.2917566099	-0.0864575312
H	1.0	-0.7502292704	3.2254594452	0.4388411635
H	1.0	0.7505043018	-3.2254101246	0.4387495111
C	6.0	-0.6734062561	2.2264546284	-1.4419782423
C	6.0	0.6734594999	-2.2264032401	-1.4420567114
H	1.0	-0.5406885363	1.2738069524	-1.9420596674
H	1.0	0.5406109510	-1.2737784308	-1.9421489541
N	7.0	-0.9151350583	3.2773496723	-2.3006678220
N	7.0	0.9152403442	-3.2772977101	-2.3007470849
C	6.0	-0.8460210604	4.6347519268	-1.8297937609
C	6.0	0.8460513010	-4.6347072453	-1.8299159093
C	6.0	0.3739451740	5.1555343244	-1.3810645267
C	6.0	-0.3739303819	-5.1554059586	-1.3811237695
H	1.0	1.2601349250	4.5283320350	-1.3940067062
H	1.0	-1.2600752935	-4.5281396115	-1.3939986088
C	6.0	0.4387261788	6.4707353623	-0.9173135874
C	6.0	-0.4387869738	-6.4706096197	-0.9173948058
H	1.0	1.3863533168	6.8709315849	-0.5686493245
H	1.0	-1.3864280908	-6.8707408808	-0.5686939244
C	6.0	-0.7083602179	7.2712388358	-0.9080461563
C	6.0	0.7082392258	-7.2712027242	-0.9082016618
H	1.0	-0.6551896509	8.2940914244	-0.5472043791
H	1.0	0.6550072909	-8.2940602954	-0.5473835929
C	6.0	-1.9232156340	6.7498924426	-1.3628603707
C	6.0	1.9231131854	-6.7499360601	-1.3630573060
H	1.0	-2.8182043939	7.3653238266	-1.3535818639
H	1.0	2.8180571463	-7.3654338792	-1.3538345847
C	6.0	-1.9967319364	5.4317760019	-1.8194798181
C	6.0	1.9967112153	-5.4318098883	-1.8196426422
H	1.0	-2.9380158329	5.0179147428	-2.1683952306
H	1.0	2.9380160424	-5.0180049725	-2.1685645702
C	6.0	-1.3196907819	3.0238220600	-3.6427909554
C	6.0	1.3198537190	-3.0237373525	-3.6428420202
C	6.0	-2.0917052920	1.8929903157	-3.9574065723
C	6.0	2.0919924533	-1.8929609296	-3.9573539523
H	1.0	-2.4352697173	1.2320476323	-3.1682287163
H	1.0	2.4355915124	-1.2321095898	-3.1681141374

C	6.0	-2.4494851945	1.6348876139	-5.2826992547
C	6.0	2.4498037504	-1.6347884637	-5.2826265739
H	1.0	-3.0469735995	0.7564073331	-5.5094623509
H	1.0	3.0473961355	-0.7563616316	-5.5093201189
C	6.0	-2.0684668322	2.5071293857	-6.3044544172
C	6.0	2.0687414714	-2.5069359740	-6.3044472509
H	1.0	-2.3565118284	2.3081799722	-7.3322074649
H	1.0	2.3568297835	-2.3079367855	-7.3321784924
C	6.0	-1.3196794183	3.6458107519	-5.9872145621
C	6.0	1.3198306971	-3.6455656665	-5.9873096700
H	1.0	-1.0175785037	4.3341484603	-6.7714771967
H	1.0	1.0176903610	-4.3338248358	-6.7716258462
C	6.0	-0.9411120920	3.9043589392	-4.6704741539
C	6.0	0.9412249801	-3.9041717966	-4.6705919648
H	1.0	-0.3482268014	4.7820764631	-4.4355222593
H	1.0	0.3482294880	-4.7818348334	-4.4357103031
C	6.0	-0.2775212413	1.1870215199	5.0119366363
C	6.0	0.2770854162	-1.1874274562	5.0118313709
N	7.0	-0.5088859922	2.1803609655	5.5811879330
N	7.0	0.5084065876	-2.1808208635	5.5810063052

Cartesian coordinates (Å) of the optimized structure for compound **2d** in vacuo

C	6.0	0.9731323602	-0.8350629516	-0.4706946159
C	6.0	0.8892272848	-2.2100555558	-0.4940910645
C	6.0	-1.3305985940	-0.7521012365	0.2291419864
O	8.0	-0.2734610756	-2.8459428132	-0.1671233008
C	6.0	-1.3624811498	-2.1059884092	0.1919697917
C	6.0	-0.1329501412	-0.0089077023	-0.1100069775
H	1.0	-2.2223857871	-0.2180588298	0.5174690387
C	6.0	-2.5386322969	-2.9697015812	0.5139934527
H	1.0	1.9145588785	-0.3790365291	-0.7337884436
H	1.0	-2.8513441593	-3.5430676883	-0.3669213222
H	1.0	-3.3771515921	-2.3568498020	0.8490672800
H	1.0	-2.2866121971	-3.6878618485	1.3030248311
C	6.0	-0.0743502813	1.4185313975	-0.0818742901
C	6.0	1.1573082411	2.1195591312	-0.4221825264
N	7.0	1.1299767452	3.5399079165	-0.4240466728
C	6.0	0.0498264413	4.3114665654	-0.0438070923
N	7.0	-1.0881489564	3.6242032147	0.3302242085
C	6.0	-1.2390901580	2.2123474010	0.2904111723
O	8.0	2.2284891368	1.5781153845	-0.7208618744
S	16.0	0.1173609593	5.9967063456	-0.0353945611
O	8.0	-2.3506906657	1.7586285686	0.5877450905
C	6.0	-2.2859383823	4.3744472047	0.7828928562
C	6.0	2.3947455964	4.1972224144	-0.8384878490
C	6.0	1.9808487714	-3.0738763292	-0.8460753998
H	1.0	2.8967741080	-2.5642585684	-1.1200608210
C	6.0	1.8990943654	-4.4391134622	-0.8339391445
H	1.0	0.9741200905	-4.9091871823	-0.5125210610
N	7.0	2.8679071849	-5.3147067294	-1.2113264127
C	6.0	4.1769765762	-4.8313087815	-1.6247193997
C	6.0	2.7630160134	-6.7220010809	-0.8476263435
H	1.0	4.7542258004	-4.4320902727	-0.7771271723
H	1.0	4.0666900359	-4.0408968042	-2.3731786327
H	1.0	4.7380307635	-5.6543656913	-2.0724017153
H	1.0	1.7167169142	-6.9781520859	-0.6655409711
H	1.0	3.3398645348	-6.9534897331	0.0601660254
H	1.0	3.1349380009	-7.3494511985	-1.6642268154
C	6.0	3.3393712015	4.4507990877	0.3367692524
H	1.0	2.1200946288	5.1334101273	-1.3218732309
H	1.0	2.8621346389	3.5309435838	-1.5623421206
H	1.0	-2.7874533761	3.7397628070	1.5127512796
C	6.0	-3.2362090981	4.7177622811	-0.3648252069

H	1.0	-1.9251026677	5.2798144340	1.2680875489
H	1.0	2.8745559857	5.1104967861	1.0749039987
H	1.0	4.2509616850	4.9380057462	-0.0280982787
H	1.0	3.6245199387	3.5106637750	0.8179312004
H	1.0	-3.6007532344	3.8097565950	-0.8537718542
H	1.0	-2.7399008193	5.3539765581	-1.1031360759
H	1.0	-4.1009787714	5.2639529156	0.0291293439

Cartesian coordinates (Å) of the optimized structure for compound **3d** in vacuo

C	6.0	1.2609280994	1.9705031668	-0.4937369314
C	6.0	1.1955598860	0.6264804731	-0.2237356202
C	6.0	-1.1306318090	2.0903819930	-0.2873764971
O	8.0	-0.0005088136	0.0104048678	0.0199456660
C	6.0	-1.1528609154	0.7461941758	-0.0113527669
C	6.0	0.0906565961	2.7963711607	-0.5411132803
H	1.0	-2.0680332184	2.6237019376	-0.3086785181
H	1.0	2.2294436039	2.4081205199	-0.6775814145
C	6.0	0.1385592510	4.2058045677	-0.8021487748
C	6.0	1.4112920487	4.8905228373	-0.9674973603
N	7.0	1.3856150997	6.3077698206	-1.0944509003
C	6.0	0.2412074952	7.0718250478	-1.1927865158
N	7.0	-0.9541350415	6.3847802912	-1.1444614559
C	6.0	-1.0832116632	4.9885784492	-0.9015446828
O	8.0	2.5237817132	4.3484053075	-0.9845446525
S	16.0	0.2989311163	8.7507225427	-1.3692042844
O	8.0	-2.2340216159	4.5424977564	-0.8082695473
C	6.0	-2.2328650488	7.1185602369	-1.3114234650
C	6.0	2.7157477048	6.9623043790	-1.1465720578
C	6.0	2.3500766523	-0.2319130132	-0.1738477358
H	1.0	3.2896655690	0.2653127792	-0.3838137022
C	6.0	2.3048821363	-1.5652937307	0.1108137998
H	1.0	1.3514502545	-2.0239572677	0.3565758338
N	7.0	3.3537192497	-2.4399014743	0.0945952332
C	6.0	4.7010864514	-1.9558498242	-0.1635694429
C	6.0	3.2375321588	-3.7087841152	0.8008639020
H	1.0	5.0953253153	-1.3598787529	0.6741119389
H	1.0	4.7101999731	-1.3369027558	-1.0654657702
H	1.0	5.3629194560	-2.8097377578	-0.3272705544
H	1.0	2.1923469809	-4.0287298472	0.8119934677
H	1.0	3.5896675294	-3.6376173339	1.8417447302
H	1.0	3.8258943216	-4.4761226410	0.2879225273
C	6.0	3.2645768281	7.0780862771	-2.5688564730
H	1.0	2.5989448649	7.9478601706	-0.6985575559
H	1.0	3.3798213313	6.3541936242	-0.5335620568
H	1.0	-2.0276617617	7.9579780233	-1.9738584775
C	6.0	-2.8176897610	7.6060056697	0.0143224391
H	1.0	-2.9202636910	6.4254903066	-1.7953116624
H	1.0	2.5964605348	7.6738049294	-3.1975016727
H	1.0	4.2396376878	7.5783785143	-2.5407834635
H	1.0	3.4002084488	6.0896728735	-3.0172624789
H	1.0	-2.1270806695	8.2894520854	0.5164185980
H	1.0	-3.0416752766	6.7637490883	0.6752733175
H	1.0	-3.7512464783	8.1472867979	-0.1791123717
C	6.0	-2.3580887556	0.0104850934	0.2687450275
H	1.0	-3.2668857143	0.5978817780	0.2113260203
C	6.0	-2.3931283034	-1.3143729901	0.5917058591
N	7.0	-3.5094559160	-2.0746894346	0.7945661015
C	6.0	-3.3972594243	-3.3303898003	1.5243026622
H	1.0	-3.5525761224	-3.1965185384	2.6062968487
H	1.0	-2.4034739518	-3.7592512207	1.3706700199
H	1.0	-4.1397278183	-4.0443947758	1.1540650322
H	1.0	-1.4607527442	-1.8640535516	0.6837981958
C	6.0	-4.8255562844	-1.4558523543	0.7569830968

H	1.0	-5.5888195891	-2.2373391794	0.7604161116
H	1.0	-4.9380843039	-0.8695840613	-0.1598347419
H	1.0	-4.9971025428	-0.7928206627	1.6192893576

Cartesian coordinates (Å) of the optimized structure for compound **2a** in DMSO

C	6.0	0.7454890544	1.6328618673	0.0381125953
C	6.0	0.1230775423	0.3943391740	0.1294522466
O	8.0	0.8480076503	-0.7407827667	-0.1139886266
C	6.0	2.1718525587	-0.6805081932	-0.4370228721
C	6.0	2.8169539700	0.5078617832	-0.5283871717
C	6.0	2.1110348406	1.7413218221	-0.2918909399
C	6.0	2.7792737136	2.9938832471	-0.3922791250
C	6.0	-1.2410972346	0.1954251210	0.4674602466
C	6.0	-1.8277826396	-1.0548178868	0.5392076982
C	6.0	2.7556907300	-2.0319179713	-0.6649027811
N	7.0	-3.0980537538	-1.3123712864	0.8694605241
C	6.0	-4.0285469289	-0.2342717394	1.1951370979
C	6.0	-3.6210994210	-2.6774681143	0.8749697361
C	6.0	4.1513353138	3.0803103841	-0.7207539718
N	7.0	5.2880915416	3.1476028069	-0.9927973682
C	6.0	2.1007088169	4.2126640668	-0.1637959094
N	7.0	1.5324211831	5.2176233408	0.0294494414
H	1.0	0.1477087864	2.5165225955	0.2316045716
H	1.0	3.8712018298	0.5116099119	-0.7792389375
H	1.0	-1.8108054251	1.0951001113	0.6697166525
H	1.0	-1.2308818387	-1.9323999035	0.3100493026
H	1.0	2.2589737028	-2.5265780100	-1.5085299344
H	1.0	3.8231788357	-1.9588100020	-0.8827674172
H	1.0	2.6191070250	-2.6683777546	0.2174448732
H	1.0	-3.6537016183	0.3657406800	2.0325168157
H	1.0	-4.1880666040	0.4213942821	0.3300625538
H	1.0	-4.9889574279	-0.6635416041	1.4835290549
H	1.0	-2.8313348961	-3.3824822003	0.6079418441
H	1.0	-3.9976168929	-2.9371999878	1.8708568139
H	1.0	-4.4388026608	-2.7768683806	0.1512557152

Cartesian coordinates (Å) of the optimized structure for compound **3a** in DMSO

C	6.0	-0.2581105335	-1.1820800972	2.0508132074
C	6.0	0.2719674202	1.1791491134	2.0508325058
C	6.0	-0.2400248963	-1.1726373505	0.6695821752
C	6.0	0.2667707040	1.1664829836	0.6695271044
O	8.0	0.0186626996	-0.0042004828	0.0001415704
C	6.0	0.0024696202	-0.0004927256	2.7921513632
C	6.0	-0.0082646443	0.0016341770	4.2240689423
C	6.0	-0.4732224049	-2.3149000015	-0.1503436506
C	6.0	0.4982157217	2.3081206278	-0.1514841476
C	6.0	-0.4404972160	-2.2880197260	-1.5283892504
C	6.0	0.4506068590	2.2838895335	-1.5291095735
N	7.0	-0.6559364257	-3.3282589391	-2.3485326004
N	7.0	0.6620333142	3.3261819562	-2.3480715342
C	6.0	-0.5649021172	-3.1855395698	-3.7994006131
C	6.0	0.5062093004	3.2008283795	-3.7950473283
C	6.0	-0.9574604278	-4.6536474087	-1.8168829591
C	6.0	0.9735835977	4.6486435560	-1.8154108064
C	6.0	-0.3065945247	-1.1633593334	4.9625510379
C	6.0	0.2837952880	1.1684653403	4.9619177299
N	7.0	-0.5586631391	-2.1345837039	5.5679615921
N	7.0	0.5364909701	2.1421598569	5.5632076665
H	1.0	-0.4675163192	-2.1198085396	2.5524088218
H	1.0	0.4773506361	2.1182140523	2.5518412914
H	1.0	-0.6752932792	-3.2357639222	0.3848821102
H	1.0	0.7036275300	3.2286374616	0.3828735134

H	1.0	-0.2245531546	-1.3525596993	-2.0337654676
H	1.0	0.2233651650	1.3510646048	-2.0349246667
H	1.0	0.2056864764	-3.8523217978	-4.2044638686
H	1.0	-0.3174531954	3.8319154683	-4.1506494087
H	1.0	-1.5239911741	-3.4302316499	-4.2713807756
H	1.0	1.4268903668	3.5045582686	-4.3064936923
H	1.0	-0.3030062504	-2.1576885572	-4.0594631792
H	1.0	0.2891969611	2.1637717740	-4.0601024470
H	1.0	-1.8370520296	-4.6215715064	-1.1627201689
H	1.0	1.8566934147	4.6076430146	-1.1667972571
H	1.0	-1.1714087453	-5.3336629878	-2.6429528118
H	1.0	1.1875918457	5.3285498434	-2.6414779307
H	1.0	-0.1078232969	-5.0539963232	-1.2490036675
H	1.0	0.1307822593	5.0547352283	-1.2408121828

Cartesian coordinates (Å) of the optimized structure for compound **11e** in DMSO

O	8.0	-0.0121045027	-0.0093924471	0.1033699887
C	6.0	-0.3132395915	1.1742235090	2.1441860305
C	6.0	0.2827226776	-1.1738913463	2.1562738722
C	6.0	-0.3046378201	1.1511942319	0.7675115969
C	6.0	0.2858917958	-1.1613874407	0.7796342171
C	6.0	-0.0217604464	0.0025757187	2.8961839054
H	1.0	-0.5529416990	2.1080967842	2.6393317039
H	1.0	0.5272864668	-2.1015947583	2.6608363858
C	6.0	-0.0328489595	0.0074778416	4.3213318072
C	6.0	-0.5919985514	2.2793284768	-0.0655674401
C	6.0	0.5960014380	-2.2896805148	-0.0449273738
H	1.0	-0.7426859699	3.2207329239	0.4509221221
H	1.0	0.7759686727	-3.2217758843	0.4786337125
C	6.0	-0.6838594141	2.1995172796	-1.4271497530
C	6.0	0.6759649001	-2.2151502565	-1.4069865514
H	1.0	-0.5792071321	1.2354840645	-1.9103717580
H	1.0	0.5282571052	-1.2593038653	-1.8958897456
N	7.0	-0.9002665411	3.2341080770	-2.2924380335
N	7.0	0.9227942500	-3.2444902768	-2.2717018704
C	6.0	-0.8373282673	4.6011106289	-1.8361526864
C	6.0	0.8967909511	-4.6137442104	-1.8208601682
C	6.0	0.3890284103	5.1411973992	-1.4323463207
C	6.0	-0.3029179122	-5.1690124950	-1.3605603637
H	1.0	1.2861650449	4.5295958701	-1.4652640660
H	1.0	-1.2054246893	-4.5647604121	-1.3396991299
C	6.0	0.4460906027	6.4664505050	-0.9942114007
C	6.0	-0.3305172066	-6.5009279530	-0.9400124318
H	1.0	1.3980440221	6.8886156598	-0.6833478928
H	1.0	-1.2629359113	-6.9318892193	-0.5855506965
C	6.0	-0.7134662570	7.2495988126	-0.9636766486
C	6.0	0.8321761167	-7.2782997839	-0.9876767297
H	1.0	-0.6620874764	8.2803575912	-0.6238746929
H	1.0	0.8071366398	-8.3159096160	-0.6651802027
C	6.0	-1.9349277690	6.7041393026	-1.3733320149
C	6.0	2.0268704223	-6.7175764141	-1.4518259900
H	1.0	-2.8382541311	7.3078613590	-1.3497978275
H	1.0	2.9335213888	-7.3159430127	-1.4868068614
C	6.0	-2.0009885575	5.3777573345	-1.8088273677
C	6.0	2.0650362013	-5.3829366849	-1.8650401164
H	1.0	-2.9472747024	4.9454171542	-2.1218447880
H	1.0	2.9912480089	-4.9428305926	-2.2232787476
C	6.0	-1.2368545429	2.9720316590	-3.6566344995
C	6.0	1.2270992772	-2.9686505885	-3.6405958939
C	6.0	-2.0315847582	1.8645647696	-3.9934205340
C	6.0	1.9533628755	-1.8185440584	-3.9904325748
H	1.0	-2.4449244032	1.2276943571	-3.2170489497
H	1.0	2.3466437060	-1.1609430143	-3.2209137917

C	6.0	-2.3245315440	1.5972780113	-5.3334986981
C	6.0	2.2055510191	-1.5332219884	-5.3350280534
H	1.0	-2.9414342677	0.7374623505	-5.5811799608
H	1.0	2.7667031663	-0.6386485172	-5.5919336170
C	6.0	-1.8533541765	2.4394883409	-6.3440407926
C	6.0	1.7647845077	-2.3993305300	-6.3394152514
H	1.0	-2.0893532445	2.2351996371	-7.3846311215
H	1.0	1.9696959001	-2.1795821651	-7.3833595996
C	6.0	-1.0799705075	3.5555026105	-6.0032782450
C	6.0	1.0661213618	-3.5596721229	-5.9857591730
H	1.0	-0.7066556267	4.2184349180	-6.7794173093
H	1.0	0.7190654315	-4.2437986877	-6.7557483315
C	6.0	-0.7686431497	3.8240358433	-4.6698667716
C	6.0	0.7928063779	-3.8460094300	-4.6474669364
H	1.0	-0.1563355951	4.6839050319	-4.4174832486
H	1.0	0.2342158987	-4.7392746492	-4.3873548426
C	6.0	-0.3566198672	1.1707908522	5.0555473432
C	6.0	0.2822896374	-1.1509790212	5.0666052687
N	7.0	-0.6295750018	2.1367312743	5.6583303883
N	7.0	0.5510234408	-2.1151637978	5.6741579998

Cartesian coordinates (Å) of the optimized structure for compound **2d** in DMSO

C	6.0	0.9690610550	-0.8259234256	-0.4998751630
C	6.0	0.9129009926	-2.2169903756	-0.4519243778
C	6.0	-1.2078215971	-0.7414325753	0.5190852831
O	8.0	-0.1749846151	-2.8329086280	0.0898959946
C	6.0	-1.2147181567	-2.0967201956	0.5748730982
C	6.0	-0.0857412632	-0.0145538886	-0.0329775853
H	1.0	-2.0625173118	-0.2084675942	0.9023308126
C	6.0	-2.2948173397	-2.9564182392	1.1388305443
H	1.0	1.8542175268	-0.3757250815	-0.9195273190
H	1.0	-2.7021420998	-3.6230221913	0.3686801343
H	1.0	-3.1072776343	-2.3418630579	1.5323134105
H	1.0	-1.9085733694	-3.5866231038	1.9491415359
C	6.0	-0.0545578252	1.4320215377	-0.0755352593
C	6.0	1.1834627736	2.1331702253	-0.3229316665
N	7.0	1.1505493148	3.5621359014	-0.3090122764
C	6.0	0.0292196765	4.3137382369	-0.0591862012
N	7.0	-1.1421943569	3.6257704875	0.1424417634
C	6.0	-1.2615097573	2.2028165549	0.1180910121
O	8.0	2.2846006827	1.6022955536	-0.5313116863
S	16.0	0.0873900032	6.0174691462	-0.0070912495
O	8.0	-2.4018185163	1.7344142809	0.2531019529
C	6.0	-2.4080372136	4.3595659839	0.3916775425
C	6.0	2.4518731357	4.2248892723	-0.5748799251
C	6.0	1.9343587478	-3.0721161743	-0.9445033034
H	1.0	2.7937398669	-2.5721765235	-1.3761169337
C	6.0	1.8626327209	-4.4519196832	-0.8906262062
H	1.0	0.9897107802	-4.9194207582	-0.4449052245
N	7.0	2.7841450128	-5.3077703661	-1.3477762010
C	6.0	4.0079027865	-4.8305952154	-1.9876749500
C	6.0	2.6163154180	-6.7533360829	-1.2121627608
H	1.0	4.6306259013	-4.2713306049	-1.2783570606
H	1.0	3.7745347779	-4.1855691089	-2.8424772791
H	1.0	4.5806127874	-5.6860009506	-2.3491157259
H	1.0	1.6737905385	-6.9774419272	-0.7091232659
H	1.0	3.4353576318	-7.1773087409	-0.6192893649
H	1.0	2.6120457522	-7.2312130484	-2.1986776576
C	6.0	3.2868291201	4.4234483485	0.6883811628
H	1.0	2.2315799026	5.1803601313	-1.0464008161
H	1.0	2.9825526949	3.5900384471	-1.2831898482
H	1.0	-2.9978709420	3.7390132126	1.0649879837
C	6.0	-3.1905609316	4.6457515036	-0.8880373404

H	1.0	-2.1434817440	5.2853472329	0.8983757658
H	1.0	2.7709672886	5.0648624022	1.4097996503
H	1.0	4.2351843770	4.9061419097	0.4238293225
H	1.0	3.5160675934	3.4663308441	1.1667239643
H	1.0	-3.4622668787	3.7191503115	-1.4024250588
H	1.0	-2.6180359354	5.2763512814	-1.5757338242
H	1.0	-4.1159807194	5.1767378808	-0.6346466034

Cartesian coordinates (Å) of the optimized structure for compound **3d** in DMSO

C	6.0	1.2667075113	1.9977886376	-0.4529183323
C	6.0	1.2105797388	0.6383877505	-0.2024052502
C	6.0	-1.1047785581	2.1369251375	-0.1061019780
O	8.0	0.0180905012	0.0448657917	0.1061278408
C	6.0	-1.1340515769	0.7794040663	0.1552216178
C	6.0	0.1040520410	2.8171667250	-0.4233084070
H	1.0	-2.0385871401	2.6740413627	-0.0736030847
H	1.0	2.2290796582	2.4279939868	-0.6779191475
C	6.0	0.1470244566	4.2461460969	-0.7035978130
C	6.0	1.4004608263	4.9580220276	-0.6963392903
N	7.0	1.3670393444	6.3644617696	-0.9682041288
C	6.0	0.2301390066	7.0753868926	-1.2570790930
N	7.0	-0.9466324362	6.3713988125	-1.2826379453
C	6.0	-1.0621399789	4.9712319400	-1.0053701063
O	8.0	2.5140849011	4.4663468233	-0.4544932026
S	16.0	0.2770611409	8.7543781179	-1.5677599244
O	8.0	-2.2019585207	4.4836777154	-1.0701152334
C	6.0	-2.2216220806	7.0540091782	-1.6114072083
C	6.0	2.6848719740	7.0446799659	-0.9314794791
C	6.0	2.3408981979	-0.2318418443	-0.2461657851
H	1.0	3.2831826824	0.2447735048	-0.4916429243
C	6.0	2.2730216849	-1.5853072766	0.0049854554
H	1.0	1.3166522444	-2.0260673694	0.2675637197
N	7.0	3.2932851757	-2.4579507141	-0.0422601743
C	6.0	4.6440803912	-2.0206170191	-0.3792055137
C	6.0	3.1071750980	-3.8634183796	0.3091199373
H	1.0	5.0542707576	-1.3609541702	0.3968689251
H	1.0	4.6528841587	-1.4886729679	-1.3375954951
H	1.0	5.2917675564	-2.8942232599	-0.4673817019
H	1.0	2.0590835298	-4.0516739469	0.5517108507
H	1.0	3.7172628497	-4.1284465218	1.1812639136
H	1.0	3.3928367859	-4.5104505180	-0.5284647229
C	6.0	3.3997670559	7.0159602901	-2.2810916892
H	1.0	2.5091898432	8.0695586946	-0.6107234976
H	1.0	3.2780607768	6.5284849407	-0.1784267690
H	1.0	-1.9844426144	7.8721593030	-2.2885437514
C	6.0	-2.9514307662	7.5712979192	-0.3732821881
H	1.0	-2.8361435333	6.3224438280	-2.1338640994
H	1.0	2.8145434603	7.5263888521	-3.0524945878
H	1.0	4.3643297540	7.5297167919	-2.1920728481
H	1.0	3.5915360503	5.9887114652	-2.6065825955
H	1.0	-2.3497913937	8.3137356659	0.1604269608
H	1.0	-3.1944306957	6.7539281738	0.3125017273
H	1.0	-3.8894620680	8.0509572714	-0.6771407130
C	6.0	-2.3207556419	0.0558591123	0.4811524563
H	1.0	-3.2251081456	0.6522778229	0.5215108529
C	6.0	-2.3537994676	-1.2982742742	0.7306543078
N	7.0	-3.4465291270	-2.0358416686	0.9958969766
C	6.0	-3.3349418884	-3.4378649202	1.3908015251
H	1.0	-3.6422271385	-3.5721268567	2.4357888168
H	1.0	-2.3009468031	-3.7737970865	1.2890357871
H	1.0	-3.9713066008	-4.0646865973	0.7560243886
H	1.0	-1.4267740189	-1.8620069744	0.7108630860
C	6.0	-4.7701301946	-1.4263178037	1.0617058345

H	1.0	-5.5257653735	-2.2133870477	1.0981078147
H	1.0	-4.9562322432	-0.8152365085	0.1720607688
H	1.0	-4.8805717288	-0.7965391517	1.9548649064

3. Cartesian coordinates of the S_1 relaxed geometry for compounds 2a,d, 3a,d, 11e

Cartesian coordinates (Å) of the S_1 relaxed geometry for compound **2a** in vacuo

C	6.0	0.7747824593	1.6196400044	0.0324203794
C	6.0	0.1428612991	0.3737624763	0.1121100433
O	8.0	0.8566105898	-0.7726022892	-0.1269696882
C	6.0	2.1945951242	-0.6850400808	-0.4690144889
C	6.0	2.8253342632	0.5014583245	-0.5555246180
C	6.0	2.1298522234	1.7313163959	-0.2979024493
C	6.0	2.7823936049	3.0193921934	-0.3755410347
C	6.0	-1.2126731632	0.1949736630	0.4374161661
C	6.0	-1.8115579279	-1.0525331873	0.5339354800
C	6.0	2.7744081173	-2.0317456387	-0.7062037206
N	7.0	-3.1175020106	-1.2723012037	0.7916876523
C	6.0	-4.0244491650	-0.1712834202	1.0450971667
C	6.0	-3.5845461984	-2.6102332073	1.1002715137
C	6.0	4.1455195615	3.1047094742	-0.7115483013
N	7.0	5.2768120919	3.1088724237	-0.9952349024
C	6.0	2.0581492773	4.1957334655	-0.1127207585
N	7.0	1.3948696697	5.1273661142	0.1183917992
H	1.0	0.1809370542	2.5043227466	0.2342038537
H	1.0	3.8747033120	0.5167562128	-0.8251844442
H	1.0	-1.7785555082	1.0995703732	0.6222270870
H	1.0	-1.2094623697	-1.9407364325	0.3792280230
H	1.0	2.2391255710	-2.5458792911	-1.5121669698
H	1.0	3.8266209529	-1.9491211758	-0.9801377800
H	1.0	2.6919234810	-2.6530042706	0.1926253318
H	1.0	-3.8078502249	0.3183373655	2.0053580974
H	1.0	-3.9489041877	0.5746235558	0.2490118361
H	1.0	-5.0470334601	-0.5481720052	1.0694894610
H	1.0	-2.8733181043	-3.3447925698	0.7205043854
H	1.0	-3.6906398778	-2.7553467821	2.1845141304
H	1.0	-4.5545983207	-2.7873087808	0.6284349068

Cartesian coordinates (Å) of the S_1 relaxed geometry for compound **3a** in vacuo

C	6.0	-0.2525300400	-1.1644603816	2.2399137638
C	6.0	0.2525109857	1.1644225581	2.2399076391
C	6.0	-0.2553251467	-1.1553165710	0.8590612185
C	6.0	0.2552109322	1.1553074082	0.8590598754
O	8.0	-0.0001246296	0.0000123143	0.1437104327
C	6.0	-0.0000213437	-0.0000144586	3.0132791147
C	6.0	0.0000158148	0.0000022836	4.4352734980
C	6.0	-0.5124970321	-2.2827764432	0.0501847563
C	6.0	0.5125181131	2.2827440118	0.0502001520
C	6.0	-0.5322174792	-2.2222887293	-1.3297545441
C	6.0	0.5321246777	2.2222908768	-1.3297431951
N	7.0	-0.8127267688	-3.2524996036	-2.1597868958
N	7.0	0.8127436003	3.2524787202	-2.1597642061
C	6.0	-0.5640437058	-3.1214034957	-3.5815897227
C	6.0	0.5639476504	3.1214848800	-3.5815564908
C	6.0	-1.0377207884	-4.5856043797	-1.6382107272
C	6.0	1.0380552603	4.5855233697	-1.6381704414
C	6.0	-0.2596742545	-1.1934895580	5.1416690402
C	6.0	0.2596975039	1.1935230637	5.1416231556
N	7.0	-0.4818899177	-2.2146351988	5.6565009362
N	7.0	0.4819130832	2.2146929244	5.6564066353
H	1.0	-0.4591830835	-2.1073817388	2.7343427136
H	1.0	0.4592623175	2.1073191311	2.7343452595
H	1.0	-0.6979883818	-3.2133744321	0.5718012846

H	1.0	0.6981645909	3.2133018749	0.5718331675
H	1.0	-0.3299398668	-1.2757534984	-1.8173201886
H	1.0	0.3296262812	1.2758079148	-1.8173192705
H	1.0	0.4202735596	-3.5246896532	-3.8599300067
H	1.0	-0.4202542258	3.5250955436	-3.8598293981
H	1.0	-1.3316510447	-3.6556949688	-4.1469753962
H	1.0	1.3316949361	3.6555441532	-4.1469737896
H	1.0	-0.5988622742	-2.0678601338	-3.8635397236
H	1.0	0.5984096351	2.0679363600	-3.8635279198
H	1.0	-1.8016727152	-4.5653219432	-0.8565073628
H	1.0	1.8020022822	4.5650432138	-0.8564688945
H	1.0	-1.3884244316	-5.2306572755	-2.4440579879
H	1.0	1.3889158879	5.2305027376	-2.4440097129
H	1.0	-0.1177844871	-5.0158323686	-1.2181940250
H	1.0	0.1182242417	5.0159693562	-1.2181473360

Cartesian coordinates (Å) of the S_1 relaxed geometry for compound **11e** in vacuo

O	8.0	0.0001538568	0.0000299985	0.0390894166
C	6.0	-0.3631268837	1.1385592572	2.1216408912
C	6.0	0.3643871310	-1.1384147820	2.1215010516
C	6.0	-0.3504528071	1.1325180716	0.7436671620
C	6.0	0.3512157846	-1.1324001038	0.7435621858
C	6.0	0.0006758599	0.0000484373	2.8889146042
H	1.0	-0.6525329402	2.0574189343	2.6194161625
H	1.0	0.6540457631	-2.0572454867	2.6191831009
C	6.0	0.0008328213	0.0000136985	4.3080058921
C	6.0	-0.6677438349	2.2432300587	-0.0688310102
C	6.0	0.6682823253	-2.2431045700	-0.0690669091
H	1.0	-0.9820905422	3.1441967219	0.4434833979
H	1.0	0.9831849574	-3.1439477286	0.4431208787
C	6.0	-0.5763492420	2.2054730463	-1.4406478792
C	6.0	0.5759555615	-2.2054863487	-1.4407935435
H	1.0	-0.2722050392	1.2904020006	-1.9304802981
H	1.0	0.2710817907	-1.2905836601	-1.9304833654
N	7.0	-0.8281095927	3.2564780014	-2.2865581707
N	7.0	0.8274679555	-3.2564576136	-2.2868196135
C	6.0	-0.8800823919	4.5967113926	-1.7963817476
C	6.0	0.8809071975	-4.5965706792	-1.7964106676
C	6.0	0.1880427996	5.1165348512	-1.0632127434
C	6.0	-0.1863887723	-5.1172655339	-1.0626735393
H	1.0	1.0607242886	4.5004954032	-0.8757779159
H	1.0	-1.0595892834	-4.5020346854	-0.8749953075
C	6.0	0.1243013442	6.4197399845	-0.5844732814
C	6.0	-0.1211553026	-6.4202964732	-0.5836432913
H	1.0	0.9562493696	6.8216541067	-0.0158352779
H	1.0	-0.9524702820	-6.8229021121	-0.0145689185
C	6.0	-0.9962968603	7.2073694098	-0.8363989565
C	6.0	1.0001139262	-7.2068738866	-0.8358541117
H	1.0	-1.0430709016	8.2233657657	-0.4591386499
H	1.0	1.0480520248	-8.2227341666	-0.4583725157
C	6.0	-2.0584286691	6.6851459287	-1.5710559503
C	6.0	2.0613944466	-6.6837999087	-1.5711299685
H	1.0	-2.9373619896	7.2910613234	-1.7645937810
H	1.0	2.9408227323	-7.2889059041	-1.7649468601
C	6.0	-2.0060225092	5.3817507032	-2.0489841701
C	6.0	2.0074999820	-5.3805581905	-2.0493212943
H	1.0	-2.8330585664	4.9651402086	-2.6137276320
H	1.0	2.8338680721	-4.9632773913	-2.6145505100
C	6.0	-1.0450014303	3.0105230731	-3.6625752208
C	6.0	1.0429564455	-3.0106494669	-3.6630745682
C	6.0	-1.6348166216	1.8119404111	-4.0831347379
C	6.0	1.6313585824	-1.8116693283	-4.0844972515
H	1.0	-1.9917467068	1.0968124613	-3.3507084177

H	1.0	1.9883098023	-1.0960133239	-3.3525991164
C	6.0	-1.8003793992	1.5560215819	-5.4387325733
C	6.0	1.7955526664	-1.5560056254	-5.4403071597
H	1.0	-2.2639456426	0.6252995090	-5.7494294730
H	1.0	2.2580634123	-0.6249788229	-5.7516654750
C	6.0	-1.3956014560	2.4876880031	-6.3897235221
C	6.0	1.3908092077	-2.4883079299	-6.3906943347
H	1.0	-1.5308631701	2.2859890352	-7.4468446530
H	1.0	1.5250172200	-2.2867870122	-7.4479834395
C	6.0	-0.8209179794	3.6866512755	-5.9697319694
C	6.0	0.8175424278	-3.6876463192	-5.9698617423
H	1.0	-0.4987437449	4.4206631163	-6.7011518740
H	1.0	0.4954034841	-4.4221856540	-6.7007681030
C	6.0	-0.6403927360	3.9506515499	-4.6200329443
C	6.0	0.6383984678	-3.9514104196	-4.6199285874
H	1.0	-0.1767025576	4.8775030000	-4.3032605822
H	1.0	0.1757933478	-4.8785831040	-4.3025094810
C	6.0	-0.3641663633	1.1648656359	5.0181180728
C	6.0	0.3659441218	-1.1648946337	5.0179677455
N	7.0	-0.6742538196	2.1578762990	5.5410549055
N	7.0	0.6759780451	-2.1579885961	5.5407722802

Cartesian coordinates (Å) of the S_1 relaxed geometry for compound **2d** in vacuo

C	6.0	0.7874659466	-0.8177665615	-0.6813527239
C	6.0	0.8755256195	-2.1692793544	-0.5107701218
C	6.0	-0.2402736687	-0.6355217775	1.4977694217
O	8.0	0.4093674517	-2.7564866278	0.6474812033
C	6.0	-0.1403807981	-1.9724399918	1.6353937031
C	6.0	0.2256070906	0.0121952386	0.3120032575
H	1.0	-0.6807212905	-0.0671020356	2.3070302516
C	6.0	-0.5773324385	-2.7918699790	2.7969959824
H	1.0	1.1652976245	-0.4022105111	-1.6072372463
H	1.0	-1.3308088707	-3.5254023421	2.4903933060
H	1.0	-1.0028341399	-2.1572845018	3.5752513761
H	1.0	0.2680643891	-3.3462936208	3.2183653558
C	6.0	0.1309966741	1.4579486065	0.1417594469
C	6.0	1.2185975379	2.3185771321	0.5716468889
N	7.0	1.0866844679	3.6936626974	0.3188567835
C	6.0	-0.0451556933	4.2874816493	-0.2062514014
N	7.0	-1.0914540740	3.4512322263	-0.5465723678
C	6.0	-1.0536447228	2.0507189151	-0.4523330751
O	8.0	2.2199667373	1.8797276116	1.1202812228
S	16.0	-0.1451984457	5.9376534587	-0.4165583638
O	8.0	-1.9938818895	1.3753941140	-0.8479111338
C	6.0	-2.3453749454	4.0068102908	-1.0951349615
C	6.0	2.2539590937	4.5145043979	0.7006170273
C	6.0	1.4270668598	-3.0948131904	-1.4618093860
H	1.0	1.7938813300	-2.6537370834	-2.3805230604
C	6.0	1.5004357516	-4.4296207684	-1.2406409305
H	1.0	1.0982587791	-4.8309136593	-0.3163611066
N	7.0	2.0767582689	-5.3675675416	-2.0578240056
C	6.0	2.5583594114	-4.9638917647	-3.3591576692
C	6.0	1.6347012165	-6.7428954706	-1.9355555523
H	1.0	3.2434779091	-4.1181905746	-3.2590281392
H	1.0	1.7410541541	-4.6705570922	-4.0363244540
H	1.0	3.1063908303	-5.7918304998	-3.8126934224
H	1.0	1.4229733414	-6.9680733675	-0.8882906682
H	1.0	2.4242069336	-7.4178813077	-2.2759550896
H	1.0	0.7260151785	-6.9464876690	-2.5223560293
C	6.0	2.1841216039	4.9862655706	2.1454623436
H	1.0	2.2910097044	5.3571707563	0.0148185840
H	1.0	3.1277076294	3.8821678410	0.5498361827
H	1.0	-3.1416034471	3.3434818903	-0.7599972254

C	6.0	-2.3266818225	4.0895907795	-2.6142873112
H	1.0	-2.4796205571	4.9899145208	-0.6513755746
H	1.0	1.3046276785	5.6132134251	2.3086736713
H	1.0	3.0722673669	5.5811109609	2.3767710053
H	1.0	2.1573144298	4.1370202907	2.8321450660
H	1.0	-2.2115871595	3.0977488530	-3.0575979471
H	1.0	-1.5178886764	4.7379022866	-2.9591277174
H	1.0	-3.2724740666	4.5105397016	-2.9670590500

Cartesian coordinates (Å) of the S_1 relaxed geometry for compound **3d** in vacuo

C	6.0	1.2448467596	1.9985933737	-0.4250655923
C	6.0	1.1883995825	0.6426781151	-0.1638094123
C	6.0	-1.1149305961	2.1121596132	-0.2294772359
O	8.0	0.0002572629	-0.0100140622	0.0822288932
C	6.0	-1.1452996638	0.7548201915	0.0301911676
C	6.0	0.0903183567	2.8330143981	-0.4710043130
H	1.0	-2.0557529591	2.6438567329	-0.2510489708
H	1.0	2.2159930559	2.4384622929	-0.6023974156
C	6.0	0.1380154586	4.2493682200	-0.7345589730
C	6.0	1.3939607741	4.9149158312	-0.9257644874
N	7.0	1.3724661233	6.3169489761	-1.1331614705
C	6.0	0.2355810944	7.0727977428	-1.2427392138
N	7.0	-0.9507465487	6.4034149371	-1.0993546049
C	6.0	-1.0687497436	5.0211548697	-0.8077335460
O	8.0	2.5066910623	4.3693134911	-0.9133177226
S	16.0	0.2939205963	8.7321660530	-1.5376670066
O	8.0	-2.2155706504	4.5792947195	-0.6483201966
C	6.0	-2.2258981912	7.1319745097	-1.2221160947
C	6.0	2.6955577494	6.9534418821	-1.2600174161
C	6.0	2.3253333044	-0.1952386708	-0.1172004803
H	1.0	3.2772374357	0.2874664617	-0.2987113051
C	6.0	2.2484273983	-1.5462218874	0.1499150764
H	1.0	1.2796625842	-1.9879863388	0.3546339495
N	7.0	3.2896291235	-2.4079691610	0.1641724417
C	6.0	4.6445077088	-1.9393085106	-0.0483866484
C	6.0	3.1218340179	-3.7422139947	0.7042397859
H	1.0	5.0012012589	-1.3350192014	0.7970338222
H	1.0	4.6994953021	-1.3342686674	-0.9569965535
H	1.0	5.3050001868	-2.7988237238	-0.1669426180
H	1.0	2.0677541742	-4.0222859750	0.6708549445
H	1.0	3.4641950941	-3.8021538454	1.7470865689
H	1.0	3.6903119020	-4.4627252856	0.1101864396
C	6.0	3.2051982698	6.9444329804	-2.6942803758
H	1.0	2.5945062217	7.9714771216	-0.8922232914
H	1.0	3.3690450199	6.3912534599	-0.6160934232
H	1.0	-2.0566622784	7.9502351943	-1.9178079576
C	6.0	-2.7256519813	7.6558346427	0.1166995372
H	1.0	-2.9417578781	6.4292548501	-1.6441523497
H	1.0	2.5287771266	7.4997086187	-3.3484532628
H	1.0	4.1895181394	7.4212973498	-2.7392786653
H	1.0	3.3047055827	5.9193384224	-3.0590802009
H	1.0	-2.0015678769	8.3453569856	0.5570630920
H	1.0	-2.9092239698	6.8301094296	0.8083956199
H	1.0	-3.6660595411	8.1970722776	-0.0281407134
C	6.0	-2.3321225528	0.0264855521	0.2714844275
H	1.0	-3.2511503712	0.5985527645	0.2531311423
C	6.0	-2.3378405977	-1.3298378467	0.5210341404
N	7.0	-3.4366277658	-2.0924068914	0.7178016025
C	6.0	-3.2971820126	-3.4468943492	1.2146241281
H	1.0	-3.4088266368	-3.4921031724	2.3073353931
H	1.0	-2.3114844459	-3.8341126513	0.9509902745
H	1.0	-4.0537206362	-4.0920939656	0.7609035063
H	1.0	-1.3941070514	-1.8627805466	0.5506655182

C	6.0	-4.7554359163	-1.4934131945	0.7631333785
H	1.0	-5.5071076024	-2.2830273908	0.7716720545
H	1.0	-4.9208965936	-0.8700140985	-0.1194840183
H	1.0	-4.8869912586	-0.8720976771	1.6598087279

Cartesian coordinates (Å) of the S_1 relaxed geometry for compound **2a** in DMSO

C	6.0	0.7602837061	1.6161073768	0.0436457128
C	6.0	0.1322760594	0.3759072028	0.1308669067
O	8.0	0.8377206933	-0.7851374635	-0.1261718936
C	6.0	2.1751479561	-0.6949230919	-0.4406451613
C	6.0	2.8112582557	0.4916717734	-0.5275274366
C	6.0	2.1225605365	1.7312307129	-0.2938328845
C	6.0	2.7733501169	3.0090306951	-0.3939997913
C	6.0	-1.2171590924	0.1914205935	0.4725671013
C	6.0	-1.8217329462	-1.0727390008	0.5334403625
C	6.0	2.7674150635	-2.0377528122	-0.6609191092
N	7.0	-3.0914133134	-1.2929239067	0.8736724124
C	6.0	-3.9932996239	-0.2092687286	1.2266783885
C	6.0	-3.6460010205	-2.6365121727	0.8457501998
C	6.0	4.1388925292	3.1111144519	-0.7132261796
N	7.0	5.2738102344	3.1700260899	-0.9787447974
C	6.0	2.0849406171	4.2149055214	-0.1729319811
N	7.0	1.5023309115	5.2080153104	0.0187134479
H	1.0	0.1600347536	2.4959494788	0.2504851975
H	1.0	3.8658173509	0.4867279761	-0.7780574188
H	1.0	-1.7879321827	1.0863467125	0.6920871613
H	1.0	-1.2391436671	-1.9501490733	0.2783036165
H	1.0	2.2607293175	-2.5522685505	-1.4855783768
H	1.0	3.8292837387	-1.9589435126	-0.8985181292
H	1.0	2.6532336948	-2.6630643096	0.2320117332
H	1.0	-3.5926797095	0.3764927149	2.0607029579
H	1.0	-4.1609651954	0.4537576967	0.3692463063
H	1.0	-4.9518970817	-0.6282586216	1.5302063760
H	1.0	-2.8772499803	-3.3560123902	0.5633538311
H	1.0	-4.0333529875	-2.9048409902	1.8341065991
H	1.0	-4.4661107513	-2.6910829551	0.1205596380

Cartesian coordinates (Å) of the S_1 relaxed geometry for compound **3a** in DMSO

C	6.0	-0.2443313901	-1.1667257591	2.2147712119
C	6.0	0.3000444084	1.1501264596	2.2166166566
C	6.0	-0.2280663286	-1.1673650917	0.8257104987
C	6.0	0.3043810719	1.1482995228	0.8276414594
O	8.0	0.0377994450	-0.0087147900	0.1211040363
C	6.0	0.0164471944	-0.0064473268	2.9733479704
C	6.0	-0.0095963365	0.0000081865	4.4262487118
C	6.0	-0.4793415616	-2.2995314978	0.0329768615
C	6.0	0.5471295386	2.2824271750	0.0355645043
C	6.0	-0.4584880535	-2.2734365682	-1.3579182773
C	6.0	0.5022228701	2.2610403292	-1.3549425482
N	7.0	-0.7125774839	-3.3146031464	-2.1523411372
N	7.0	0.6918836899	3.3181970541	-2.1461832560
C	6.0	-0.6564223798	-3.1854802106	-3.5992359555
C	6.0	0.5809070259	3.2051287526	-3.5911655297
C	6.0	-1.0460271503	-4.6206638394	-1.6086164274
C	6.0	0.9925379713	4.6306699538	-1.5995081578
C	6.0	-0.3513900466	-1.1448929410	5.1558669891
C	6.0	0.3034416314	1.1565287387	5.1502434348
N	7.0	-0.6410813495	-2.1091001475	5.7510935873
N	7.0	0.5758841024	2.1372021129	5.7266578232
H	1.0	-0.4655801945	-2.1097311054	2.7031894871
H	1.0	0.5191456432	2.0929171641	2.7067072760

H	1.0	-0.6974918230	-3.2183105673	0.5638696293
H	1.0	0.7570628221	3.2030315265	0.5664900005
H	1.0	-0.2270671951	-1.3450401175	-1.8655540151
H	1.0	0.2858930733	1.3291915865	-1.8634423416
H	1.0	0.0770043511	-3.8834415027	-4.0168303955
H	1.0	-0.2333766887	3.8379649616	-3.9606307405
H	1.0	-1.6357060059	-3.4025006260	-4.0396971310
H	1.0	1.5138014184	3.5193812061	-4.0705012897
H	1.0	-0.3670194840	-2.1707317379	-3.8742067621
H	1.0	0.3751158786	2.1715752145	-3.8721983356
H	1.0	-1.9237317899	-4.5606104903	-0.9559693603
H	1.0	1.9130567149	4.6038544341	-1.0057625013
H	1.0	-1.2742227973	-5.3023497877	-2.4276050065
H	1.0	1.1353513032	5.3351249179	-2.4185586767
H	1.0	-0.2056182865	-5.0338841589	-1.0390160861
H	1.0	0.1723401780	4.9924206435	-0.9690851955

Cartesian coordinates (Å) of the S_1 relaxed geometry for compound **11e** in DMSO

O	8.0	0.0504751716	0.0097555176	0.0087440296
C	6.0	-0.3054528585	1.1404648705	2.0972826729
C	6.0	0.3676467259	-1.1464877595	2.0891882251
C	6.0	-0.2964899068	1.1442948210	0.7107397009
C	6.0	0.3676295140	-1.1371780974	0.7031358838
C	6.0	0.0327236773	-0.0050226278	2.8467615881
H	1.0	-0.5842455395	2.0643644481	2.5921967159
H	1.0	0.6327883197	-2.0778896146	2.5776523585
C	6.0	0.0306595662	-0.0124658977	4.2948956298
C	6.0	-0.6301691650	2.2597576903	-0.0777115121
C	6.0	0.6801322485	-2.2500297430	-0.0965780145
H	1.0	-0.9050869815	3.1625597289	0.4546562995
H	1.0	0.9288331435	-3.1668323114	0.4244107880
C	6.0	-0.6257843038	2.2316797631	-1.4586999517
C	6.0	0.6835007914	-2.2033088850	-1.4765146776
H	1.0	-0.3894343661	1.3110177396	-1.9738336472
H	1.0	0.4763050996	-1.2700334026	-1.9829288465
N	7.0	-0.9034903827	3.2837510510	-2.2743858955
N	7.0	0.9234149958	-3.2608736265	-2.2965918396
C	6.0	-0.9149749644	4.6278272479	-1.7841312688
C	6.0	0.8668894707	-4.6025332669	-1.7945156816
C	6.0	0.2076676924	5.1413421341	-1.1336113508
C	6.0	-0.3207569053	-5.0761907663	-1.2376651817
H	1.0	1.0903793340	4.5238195962	-1.0027696211
H	1.0	-1.1928149604	-4.4313717712	-1.1940872133
C	6.0	0.1905681325	6.4534333995	-0.6741448893
C	6.0	-0.3805010064	-6.3802083099	-0.7597693723
H	1.0	1.0668924231	6.8557471665	-0.1752182003
H	1.0	-1.3062711316	-6.7531860877	-0.3331772193
C	6.0	-0.9360991051	7.2509170324	-0.8646791464
C	6.0	0.7393885630	-7.2060844184	-0.8375259467
H	1.0	-0.9427975723	8.2758959042	-0.5068321431
H	1.0	0.6894865471	-8.2245788165	-0.4643888870
C	6.0	-2.0523359825	6.7318520076	-1.5181431618
C	6.0	1.9215269497	-6.7255538543	-1.3975627801
H	1.0	-2.9337662426	7.3476953113	-1.6678475547
H	1.0	2.7974455714	-7.3646063125	-1.4548142209
C	6.0	-2.0466490465	5.4202608095	-1.9784028706
C	6.0	1.9916566190	-5.4218764564	-1.8772438312
H	1.0	-2.9152093599	5.0089166740	-2.4825898663
H	1.0	2.9116382430	-5.0387563857	-2.3069589165
C	6.0	-1.1859407543	3.0470392028	-3.6462862850
C	6.0	1.2125439319	-3.0467563397	-3.6678913940
C	6.0	-1.8787331879	1.8937347351	-4.0293088658
C	6.0	1.8835190600	-1.8874426809	-4.0751428046

H	1.0	-2.2638677535	1.2120324056	-3.2784192660
H	1.0	2.2440998559	-1.1724013103	-3.3436673643
C	6.0	-2.1082445579	1.6395714497	-5.3767132566
C	6.0	2.1249474079	-1.6649506314	-5.4258246364
H	1.0	-2.6516220036	0.7446857895	-5.6640439639
H	1.0	2.6493543068	-0.7639443750	-5.7294007727
C	6.0	-1.6662459397	2.5338875807	-6.3477069740
C	6.0	1.7212268270	-2.5952844903	-6.3799776933
H	1.0	-1.8491129767	2.3356071448	-7.3989126877
H	1.0	1.9165176913	-2.4200865236	-7.4330914889
C	6.0	-0.9928044772	3.6922129163	-5.9606421626
C	6.0	1.0681547383	-3.7569103643	-5.9694548698
H	1.0	-0.6419448555	4.3944905510	-6.7106108973
H	1.0	0.7463961131	-4.4892754646	-6.7034992280
C	6.0	-0.7498277525	3.9541226120	-4.6190679328
C	6.0	0.8111447008	-3.9874608710	-4.6245787933
H	1.0	-0.2082143636	4.8473648429	-4.3281423394
H	1.0	0.2861958822	-4.8858202737	-4.3200864289
C	6.0	-0.3250694063	1.1257172430	5.0312674470
C	6.0	0.3840436733	-1.1624086378	5.0139330834
N	7.0	-0.6252583244	2.0819913508	5.6319775123
N	7.0	0.6845693110	-2.1349471193	5.5879450484

Cartesian coordinates (Å) of the S_1 relaxed geometry for compound **2d** in DMSO

C	6.0	0.8929978211	-0.8050776683	-0.5416219777
C	6.0	0.8564523358	-2.1917778679	-0.5033230308
C	6.0	-1.1345343398	-0.7547031245	0.7464913544
O	8.0	-0.1535397772	-2.8505003849	0.1596377579
C	6.0	-1.1337719129	-2.1035885918	0.7746203032
C	6.0	-0.0912832151	-0.0058875474	0.0922337531
H	1.0	-1.9437551646	-0.2396757293	1.2414590752
C	6.0	-2.1308849147	-2.9778008465	1.4442667304
H	1.0	1.7026092276	-0.3407241509	-1.0855979215
H	1.0	-2.5861293579	-3.6680065159	0.7246908496
H	1.0	-2.9215664942	-2.3821772556	1.9032651335
H	1.0	-1.6566903833	-3.5867724626	2.2227279102
C	6.0	-0.0475140890	1.4313363411	0.0296389647
C	6.0	1.2109494635	2.1196097803	-0.0914170037
N	7.0	1.1752757948	3.5262988168	-0.2201104791
C	6.0	0.0403635207	4.2839345648	-0.1243099470
N	7.0	-1.1376759577	3.6125174435	0.0578809311
C	6.0	-1.2581832678	2.2053634360	0.0932292112
O	8.0	2.3157123131	1.5609358857	-0.0896185484
S	16.0	0.0902659882	5.9769051555	-0.2266320483
O	8.0	-2.3911264003	1.7157615187	0.1746283940
C	6.0	-2.4104382923	4.3506694825	0.1766179198
C	6.0	2.4901545598	4.1692496404	-0.4137658279
C	6.0	1.8350958761	-3.0205722025	-1.0865252558
H	1.0	2.6285423675	-2.5184648592	-1.6279845390
C	6.0	1.8166674351	-4.4115022865	-0.9754326892
H	1.0	1.0070234014	-4.8880569720	-0.4340741493
N	7.0	2.7268131938	-5.2323590772	-1.4985473362
C	6.0	3.8698394390	-4.7317039760	-2.2434594105
C	6.0	2.5895038807	-6.6751811094	-1.3767891780
H	1.0	4.4505142470	-4.0261725744	-1.6404944420
H	1.0	3.5481794550	-4.2336452283	-3.1658505831
H	1.0	4.5156806314	-5.5665778189	-2.5134033634
H	1.0	1.6746340801	-6.9212126445	-0.8373726456
H	1.0	3.4442722219	-7.0911294896	-0.8326388628
H	1.0	2.5478851330	-7.1343326876	-2.3704006588
C	6.0	3.1803709246	4.4913397425	0.9020169821
H	1.0	2.3251310858	5.0697447534	-0.9991886294
H	1.0	3.0896482232	3.4714494091	-0.9946674665

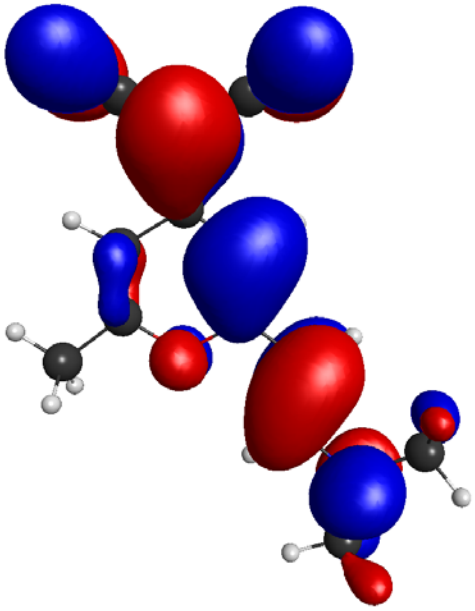
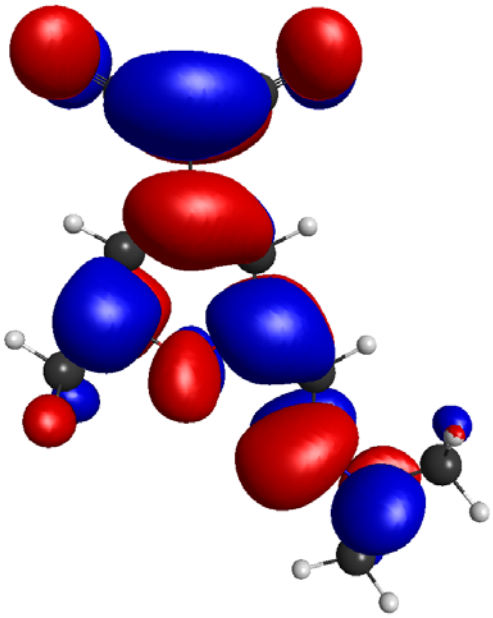
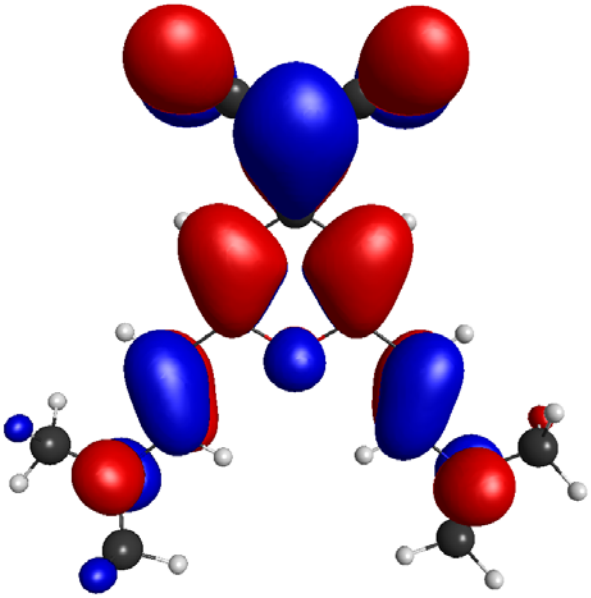
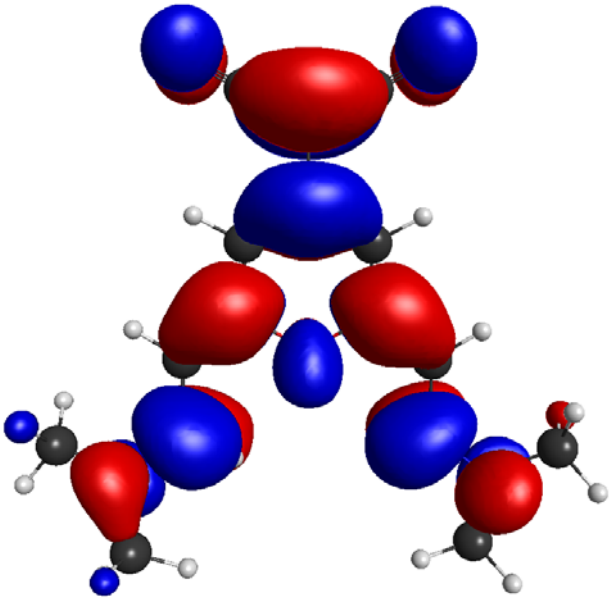
H	1.0	-3.0448629707	3.7630583434	0.8370269536
C	6.0	-3.0906087067	4.5553605303	-1.1677156028
H	1.0	-2.1880210971	5.3029896234	0.6504560055
H	1.0	2.5935499517	5.1972617614	1.4953609039
H	1.0	4.1562929380	4.9456114168	0.7030952708
H	1.0	3.3427620708	3.5849866078	1.4905397692
H	1.0	-3.3004293049	3.5972647907	-1.6498958965
H	1.0	-2.4709358421	5.1581593992	-1.8365767711
H	1.0	-4.0417010962	5.0776054843	-1.0232922627

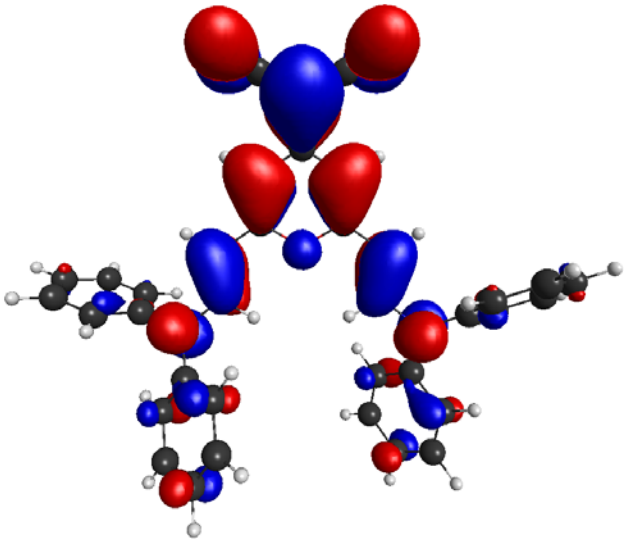
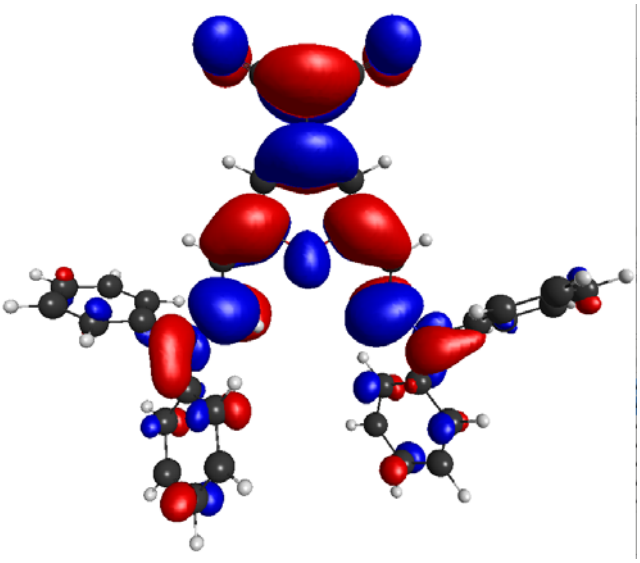
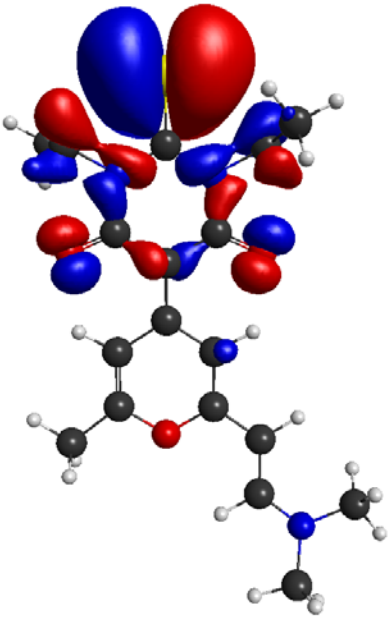
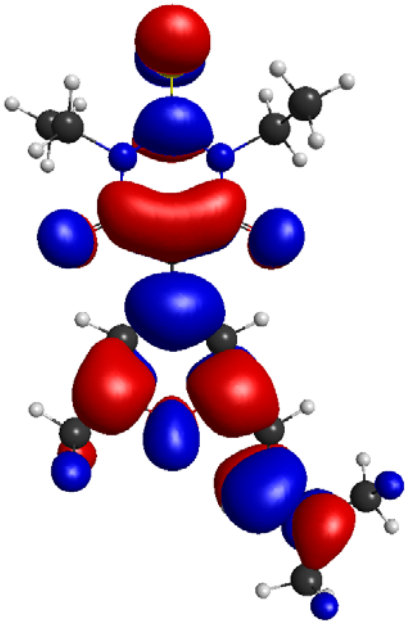
Cartesian coordinates (Å) of the S_1 relaxed geometry for compound **3d** in DMSO

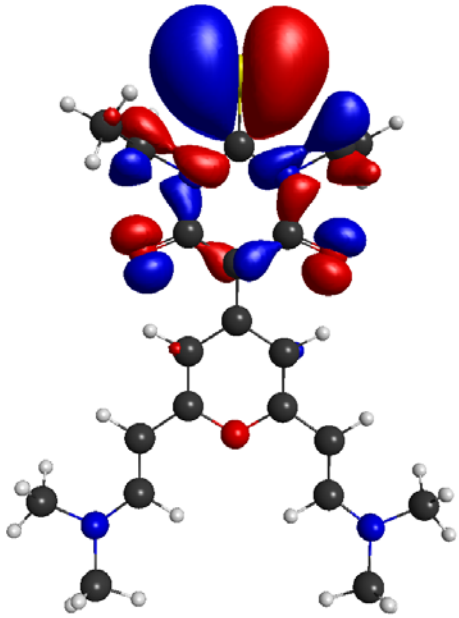
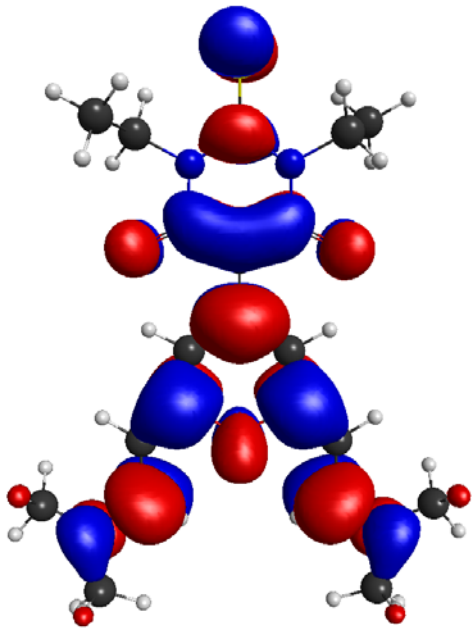
C	6.0	1.2366050656	1.9929678513	-0.5067521501
C	6.0	1.1985380933	0.6321183136	-0.2311675324
C	6.0	-1.0798837145	2.1493120803	-0.0238175224
O	8.0	0.0326397031	0.0200078636	0.1802463334
C	6.0	-1.1122384165	0.7863353291	0.2419280181
C	6.0	0.0996513511	2.8297571575	-0.4065606690
H	1.0	-2.0133477784	2.6880602439	0.0468335269
H	1.0	2.1866169721	2.4062860511	-0.8125886042
C	6.0	0.1384246160	4.2622725345	-0.6961306479
C	6.0	1.3575734044	4.9803053386	-0.5663359811
N	7.0	1.3355059461	6.3755545043	-0.8663771828
C	6.0	0.2285385430	7.0535971992	-1.2778689296
N	7.0	-0.9269779820	6.3408137355	-1.3839238060
C	6.0	-1.0396746581	4.9459646643	-1.1006972596
O	8.0	2.4420708884	4.4982013579	-0.2001595599
S	16.0	0.2881064137	8.7198964151	-1.6449112218
O	8.0	-2.1609311171	4.4298591727	-1.2446481677
C	6.0	-2.1739067749	6.9964262376	-1.8159267348
C	6.0	2.6217231528	7.0737477115	-0.6947638081
C	6.0	2.3073329391	-0.2253361334	-0.3441278841
H	1.0	3.2428177511	0.2333903089	-0.6410438272
C	6.0	2.2324955408	-1.5915929281	-0.0963215723
H	1.0	1.2822557880	-2.0209510969	0.1983972198
N	7.0	3.2443193098	-2.4542773191	-0.1969100319
C	6.0	4.5789136978	-2.0223051268	-0.5775384664
C	6.0	3.0632420514	-3.8621507613	0.1181175354
H	1.0	5.0133002211	-1.3657436980	0.1859405075
H	1.0	4.5598464434	-1.4931584425	-1.5358287058
H	1.0	5.2189654514	-2.8976763484	-0.6832595045
H	1.0	2.0285745041	-4.0505548657	0.4071779547
H	1.0	3.7155977082	-4.1545093828	0.9482817884
H	1.0	3.3032025674	-4.4824039453	-0.7519422895
C	6.0	3.4679817446	7.0547037059	-1.9579969883
H	1.0	2.4004496434	8.0935083598	-0.3905519361
H	1.0	3.1402504623	6.5615920250	0.1125473057
H	1.0	-1.9026874808	7.7912949735	-2.5057182938
C	6.0	-2.9753852419	7.5450027471	-0.6454826219
H	1.0	-2.7500175719	6.2408253120	-2.3448471320
H	1.0	2.9655275764	7.5732948667	-2.7785422674
H	1.0	4.4218855608	7.5590456208	-1.7721447051
H	1.0	3.6829069627	6.0288186358	-2.2689471291
H	1.0	-2.4083232320	8.3043981179	-0.1009098055
H	1.0	-3.2510183962	6.7458045592	0.0475419923
H	1.0	-3.8967326804	8.0082227799	-1.0130972771
C	6.0	-2.2819792677	0.0846359219	0.5852716196
H	1.0	-3.1904871708	0.6718564758	0.6409862995
C	6.0	-2.3054761063	-1.2806382212	0.8425405182
N	7.0	-3.3953113318	-1.9984040463	1.1234729228
C	6.0	-3.2940139303	-3.4019321944	1.4899894362
H	1.0	-3.6193122452	-3.5502214596	2.5260549395
H	1.0	-2.2609816762	-3.7387960960	1.3993299629
H	1.0	-3.9238740417	-4.0116239221	0.8345117228

H	1.0	-1.3769412521	-1.8381049854	0.8152780122
C	6.0	-4.7133916409	-1.3908007442	1.1865183006
H	1.0	-5.4669323023	-2.1780970887	1.2212620732
H	1.0	-4.8982048652	-0.7807535536	0.2979526957
H	1.0	-4.8255268632	-0.7648863006	2.0804882970

4. Table S1. Ground state frontier orbitals for compounds 2a,d, 3a,d, 11e in vacuo

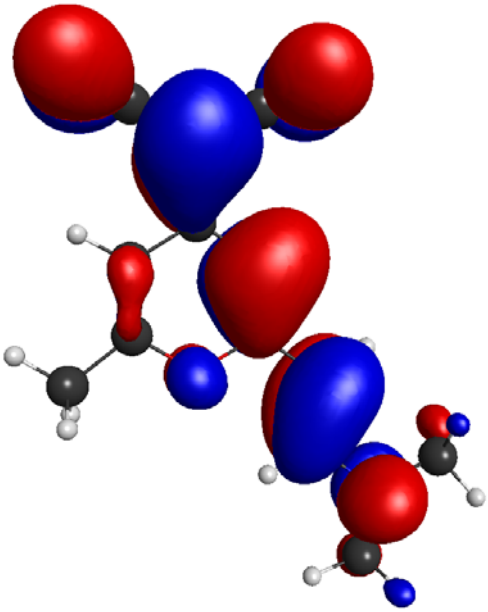
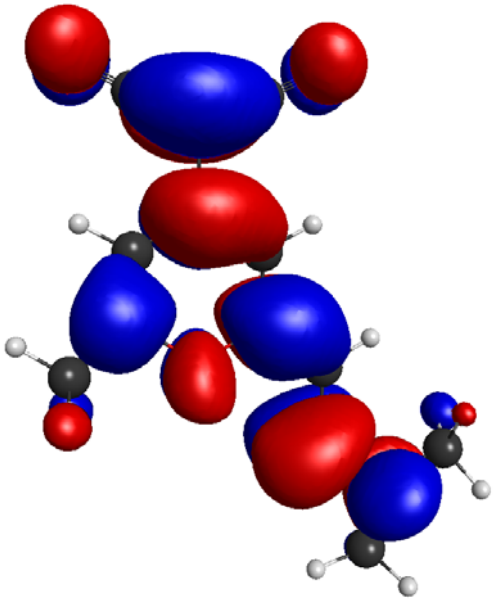
HOMO	LUMO
Ground state of **2a** 	Ground state of **2a** 
Ground state of **3a** 	Ground state of **3a** 

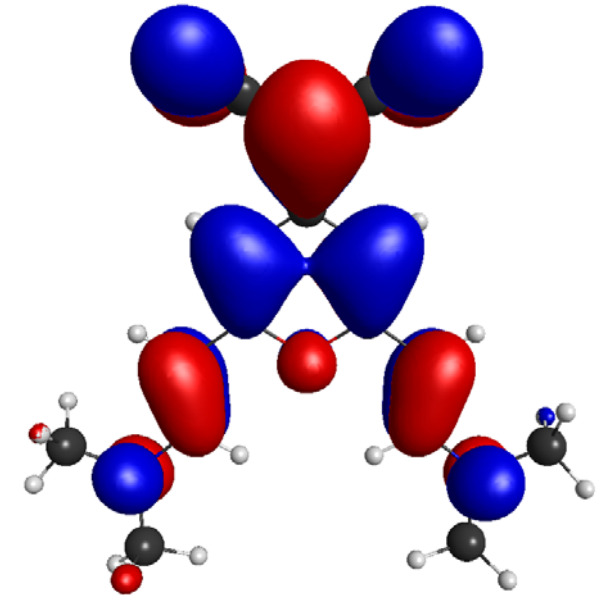
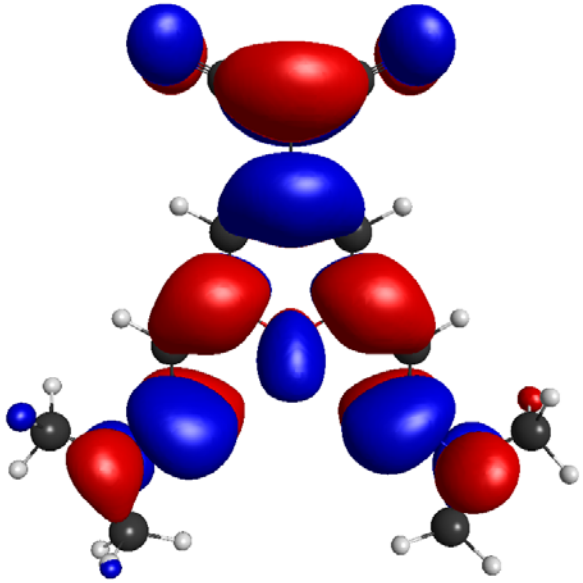
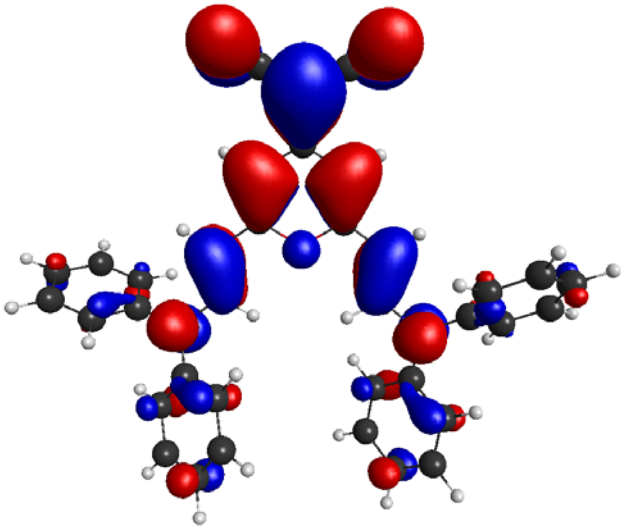
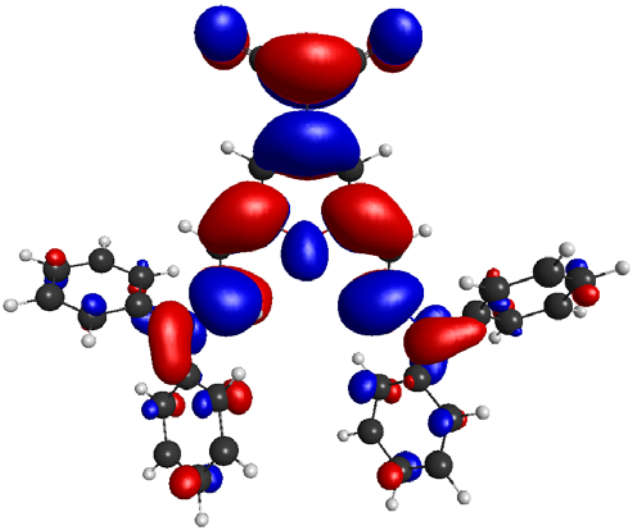
Ground state of **11e** 	Ground state of **11e** 
Ground state of **2d** 	Ground state of **3d** 

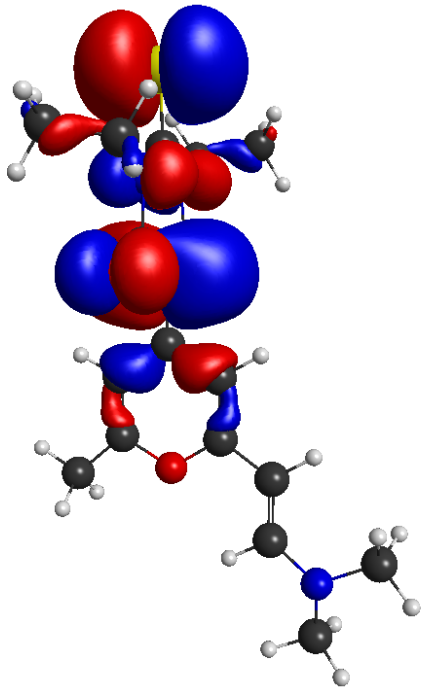
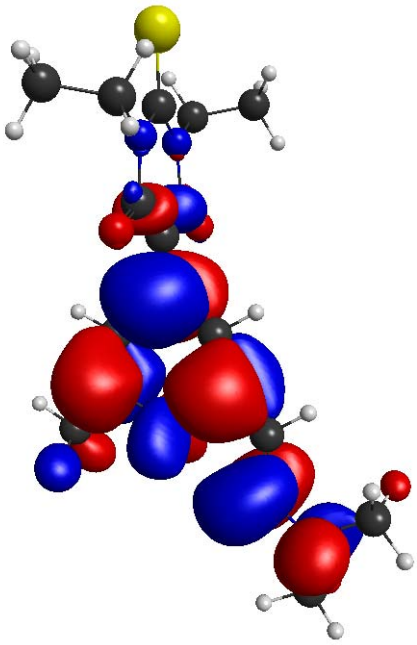
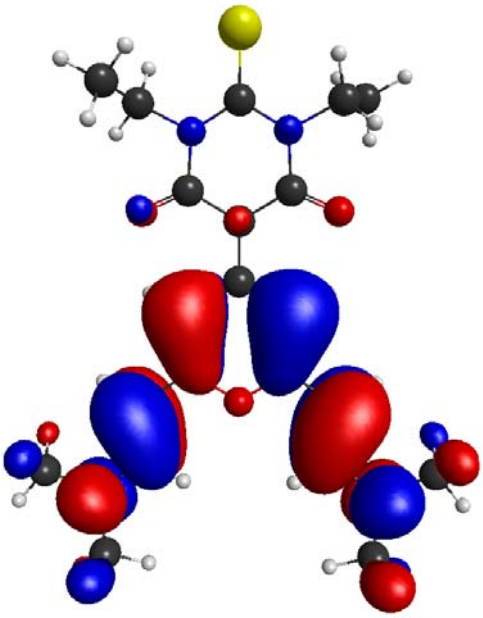
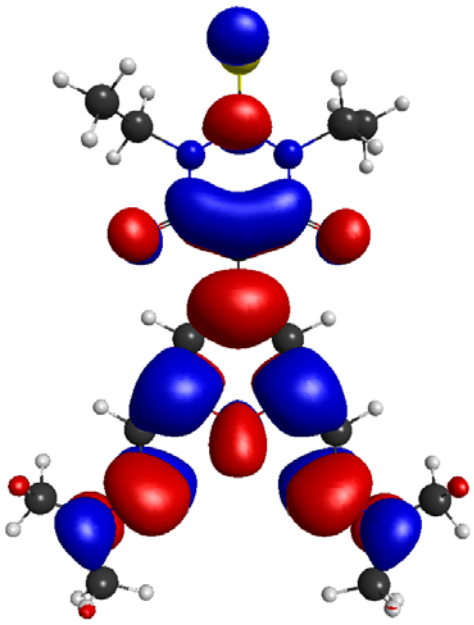
Ground state of **3d**	Ground state of **3d**
	

(isosurfaces correspond to 0.02 psi/ 0.0004 rho)

5. Table S2. Frontier orbitals of the first singlet excited states for the relaxed geometry of compounds 2a,d, 3a,d, 11e in vacuo

HOMO	LUMO
S_1 excited state of **2a**	S_1 excited state of **2a**
	

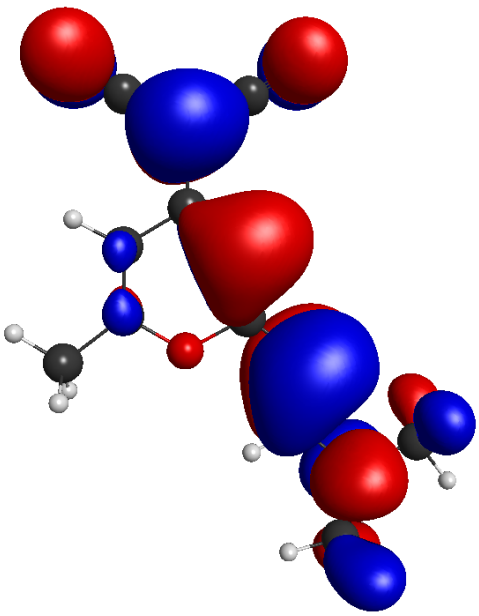
S_1 excited state of **3a**	S_1 excited state of **3a**
	
S_1 excited state of **11e**	S_1 excited state of **11e**
	

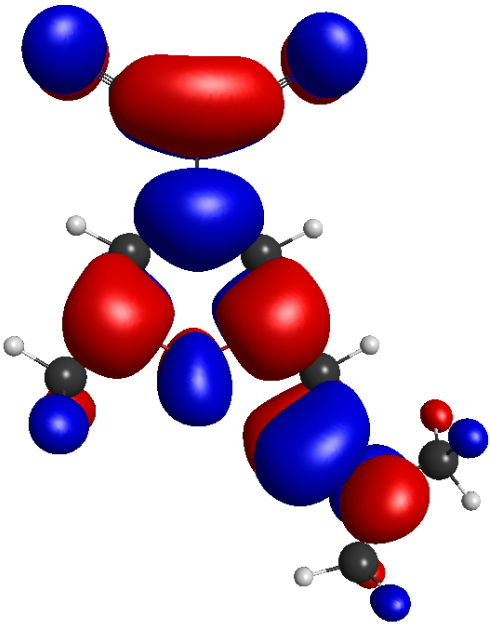
S_1 excited state of **2d** 	S_1 excited state of **2d** 
S_1 excited state of **3d** 	S_1 excited state of **3d** 

(isosurfaces correspond to 0.02 psi/ 0.0004 rho)

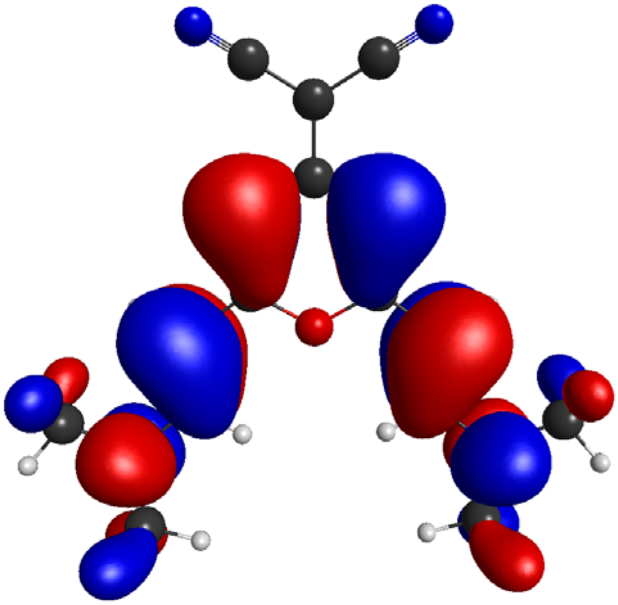
6. Table S3. Ground state frontier orbitals for compounds 2a,d, 3a,d, 11e in DMSO

HOMO	LUMO
Ground state of **2a**	Ground state of **2a**

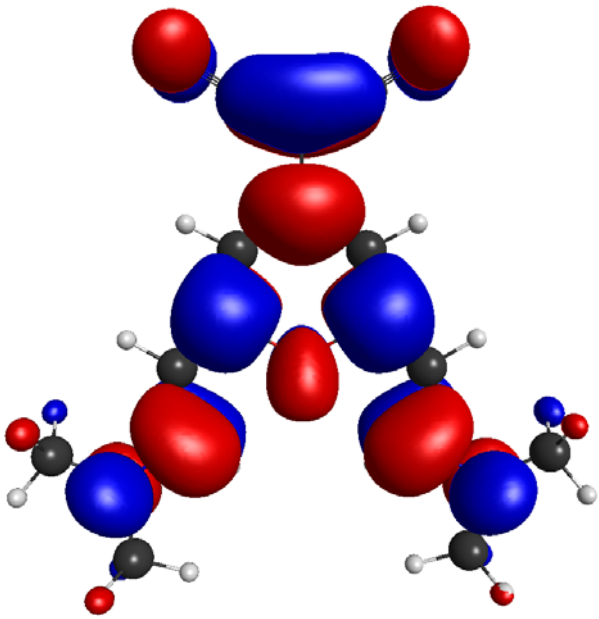




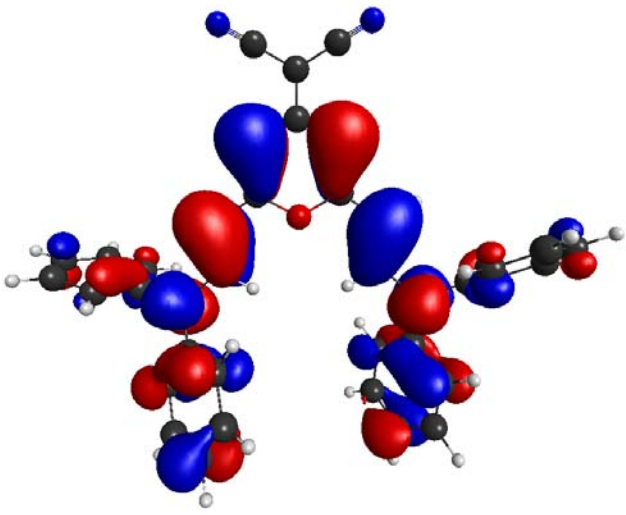
Ground state of **3a**



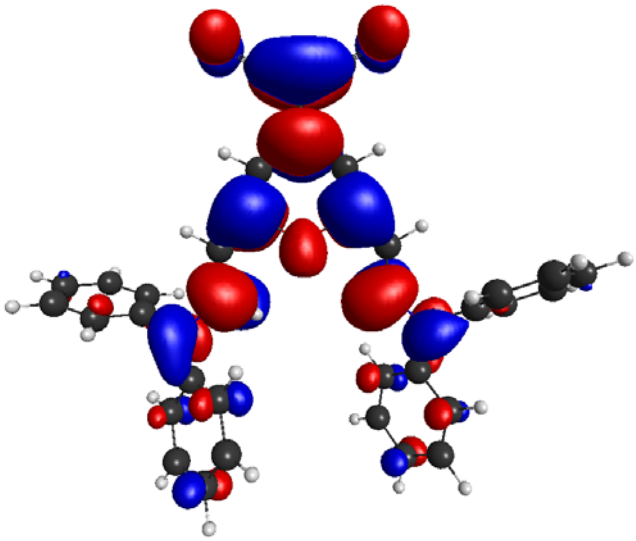
Ground state of **3a**

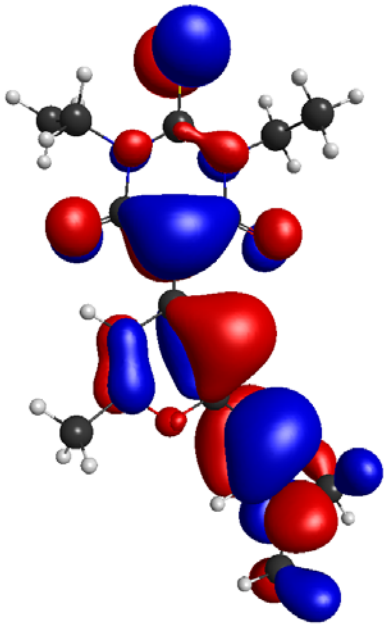
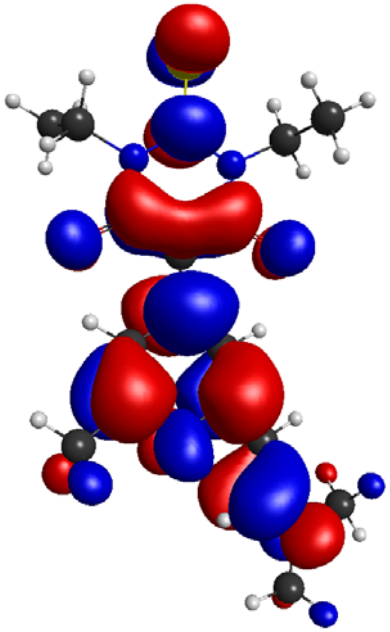
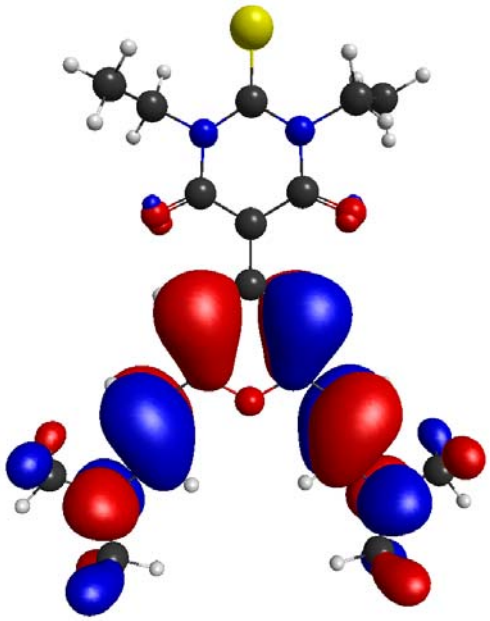
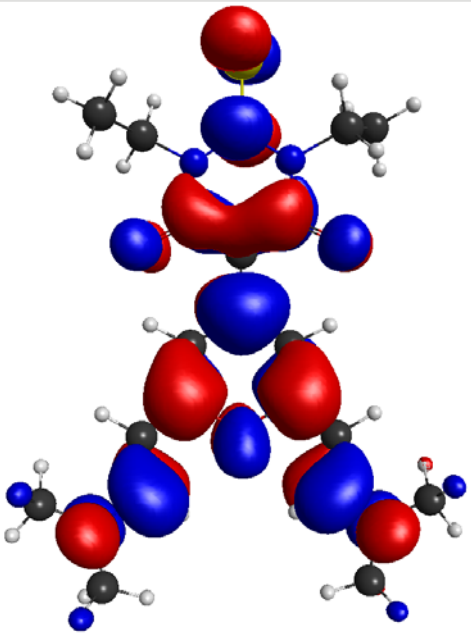


Ground state of **11e**



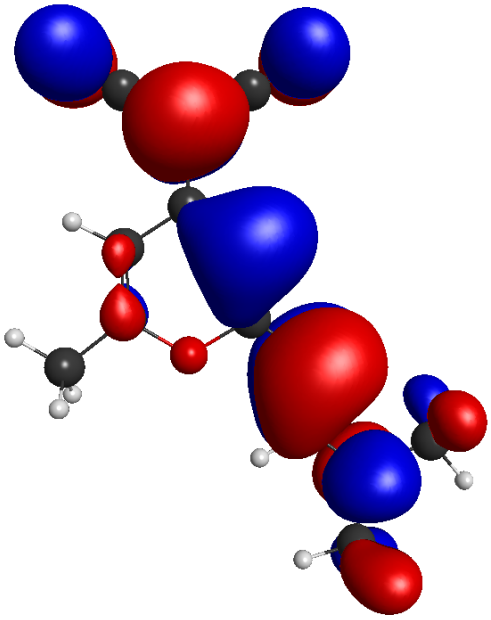
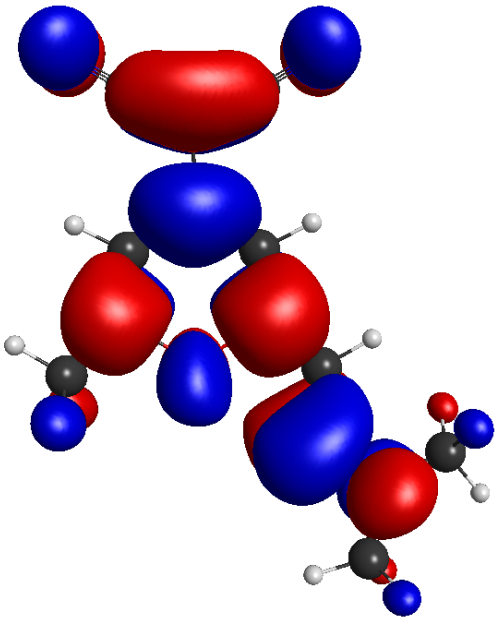
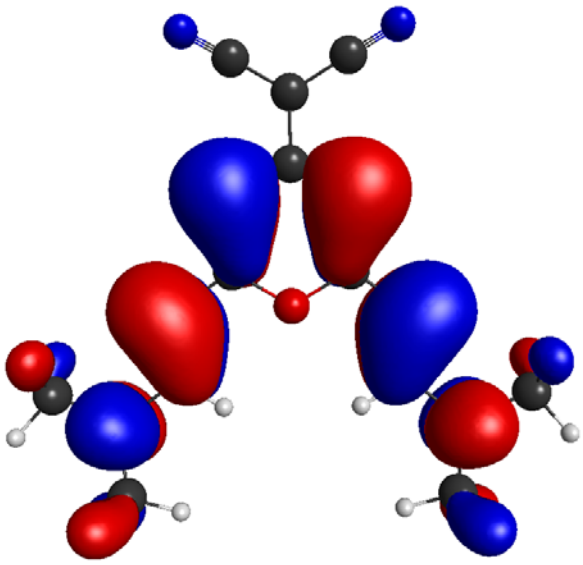
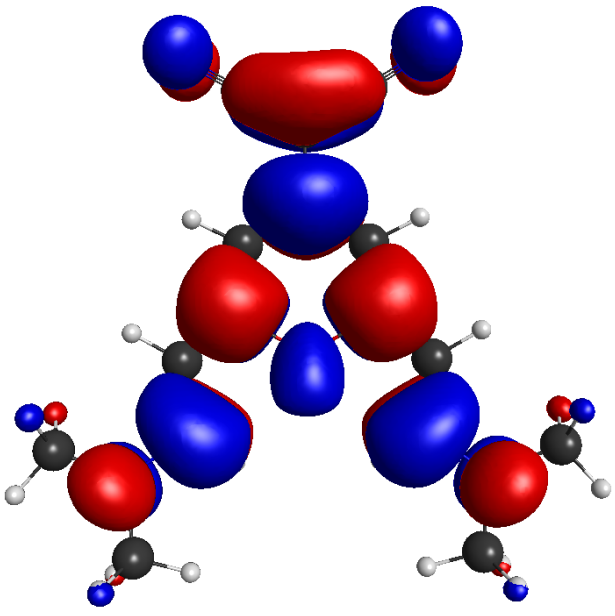
Ground state of **11e**

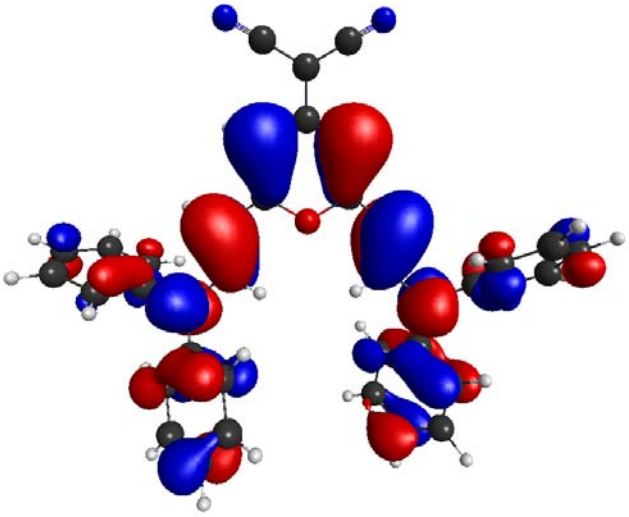
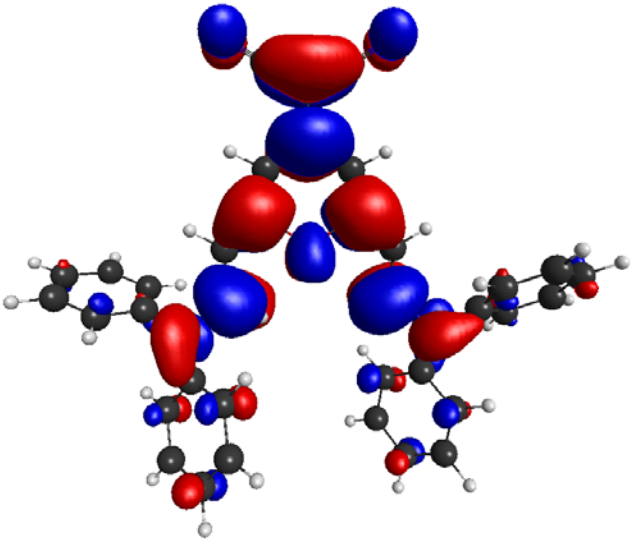
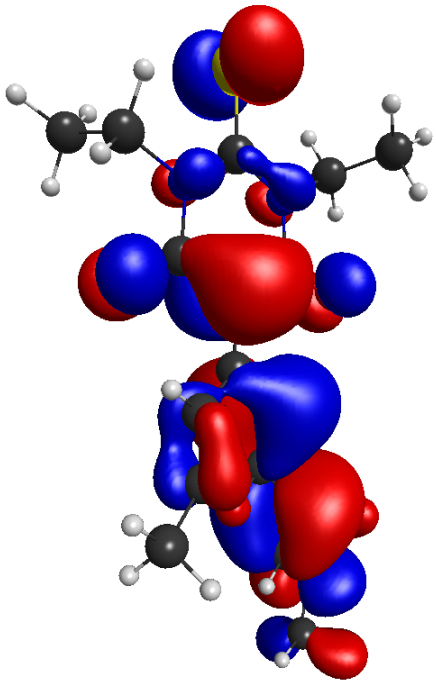
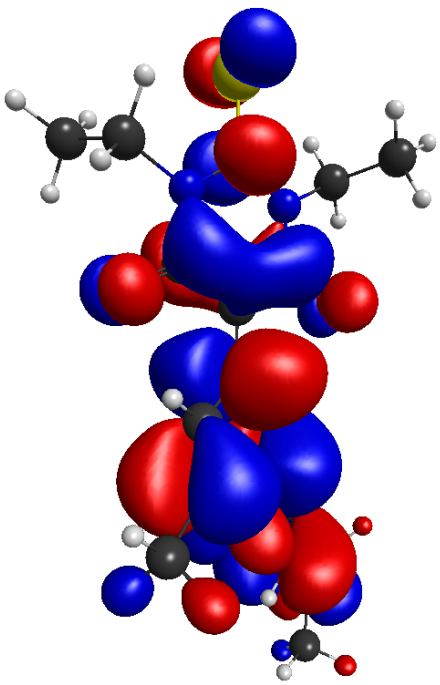


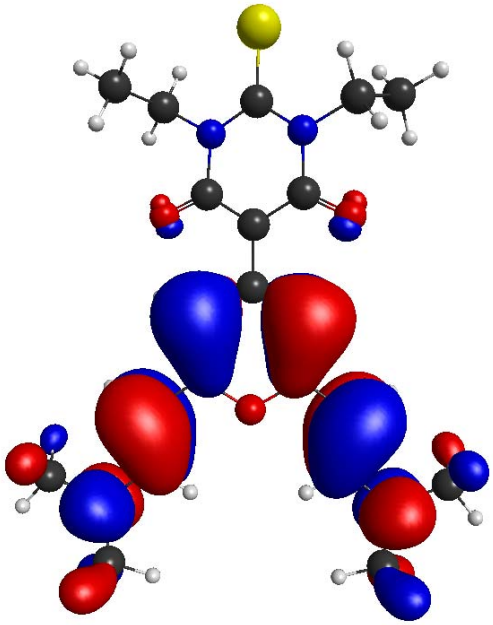
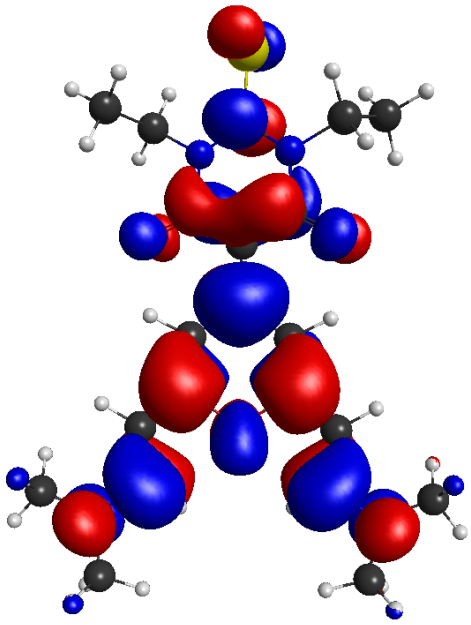
Ground state of **2d** 	Ground state of **2d** 
Ground state of **3d** 	Ground state of **3d** 

(isosurfaces correspond to 0.02 psi/ 0.0004 rho)

7. Table S4. Frontier orbitals of first singlet excited states for relaxed geometry of compounds 2a,d, 3a,d, 11e in DMSO

HOMO	LUMO
S_1 excited state of **2a** 	S_1 excited state of **2a** 
S_1 excited state of **3a** 	S_1 excited state of **3a** 

S_1 excited state of **11e**	S_1 excited state of **11e**
	
S_1 excited state of **2d**	S_1 excited state of **2d**
	

S_1 excited state of **3d**	S_1 excited state of **3d**
	

(isosurfaces correspond to 0.02 psi/ 0.0004 rho)

8. Calculated normalized UV-vis spectra for compounds 2a,d, 3a,d, 11e in DMSO

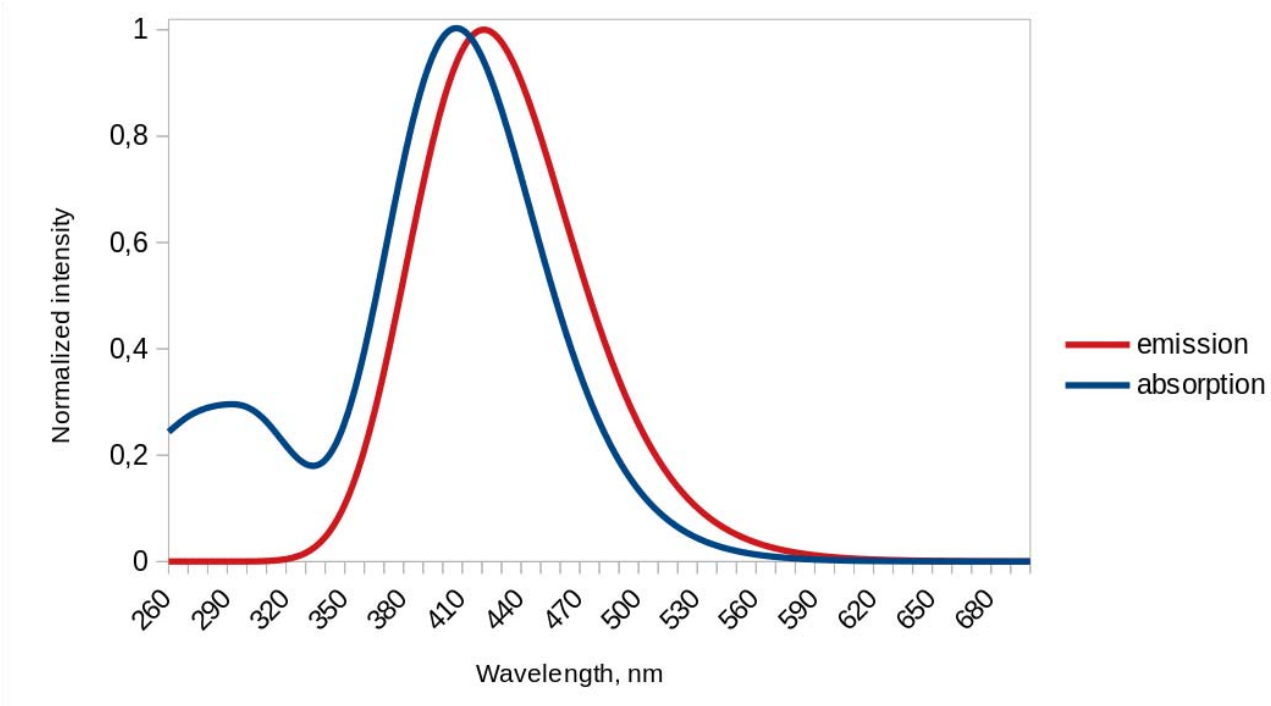


Fig. S1. Normalized absorption and emission spectra of **2a** in DMSO at the CAM-B3LYP level.

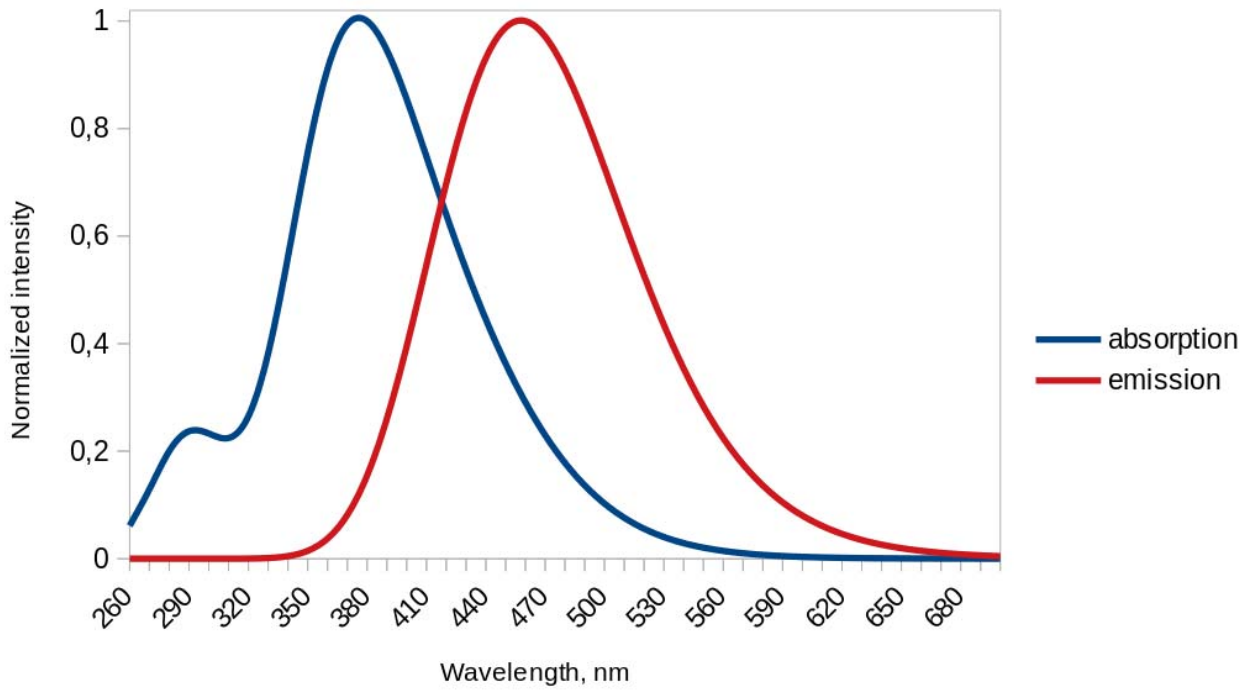


Fig. S2. Normalized absorption and emission spectra of **3a** in DMSO at the CAM-B3LYP level.

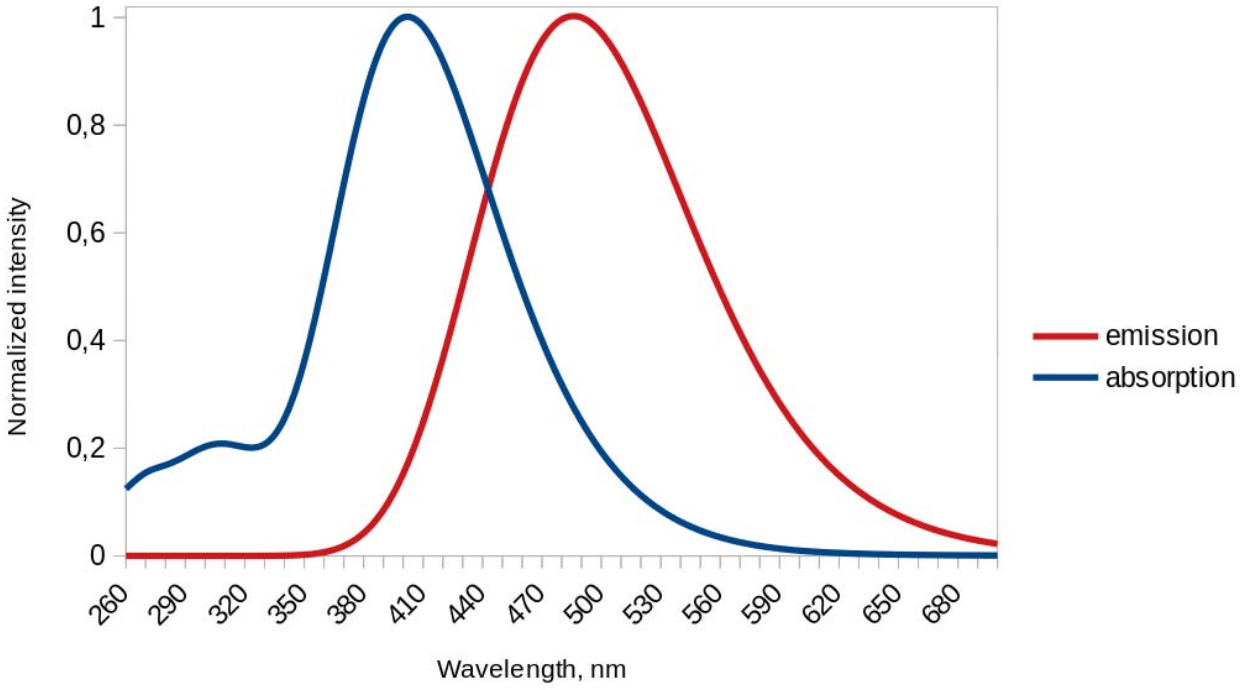


Fig. S3. Normalized absorption and emission spectra of **11e** in DMSO at the CAM-B3LYP level.

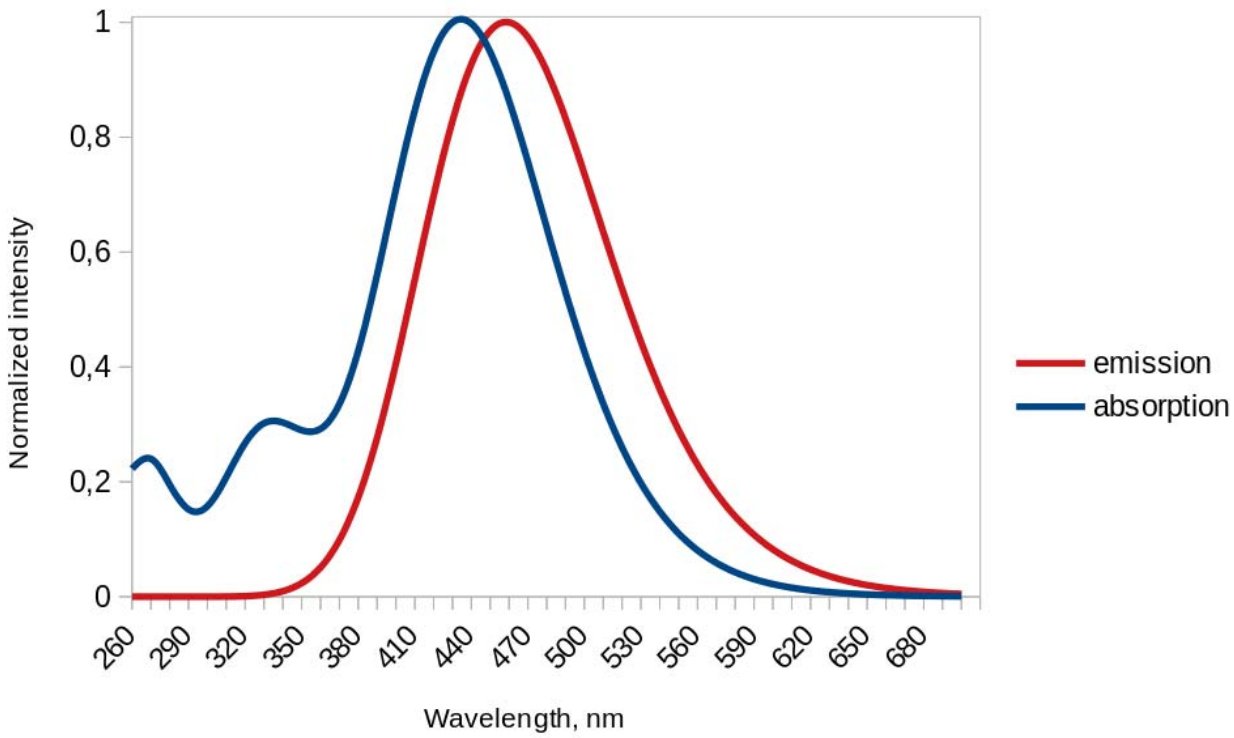


Fig. S4. Normalized absorption and emission spectra of **2d** in DMSO at the CAM-B3LYP level.

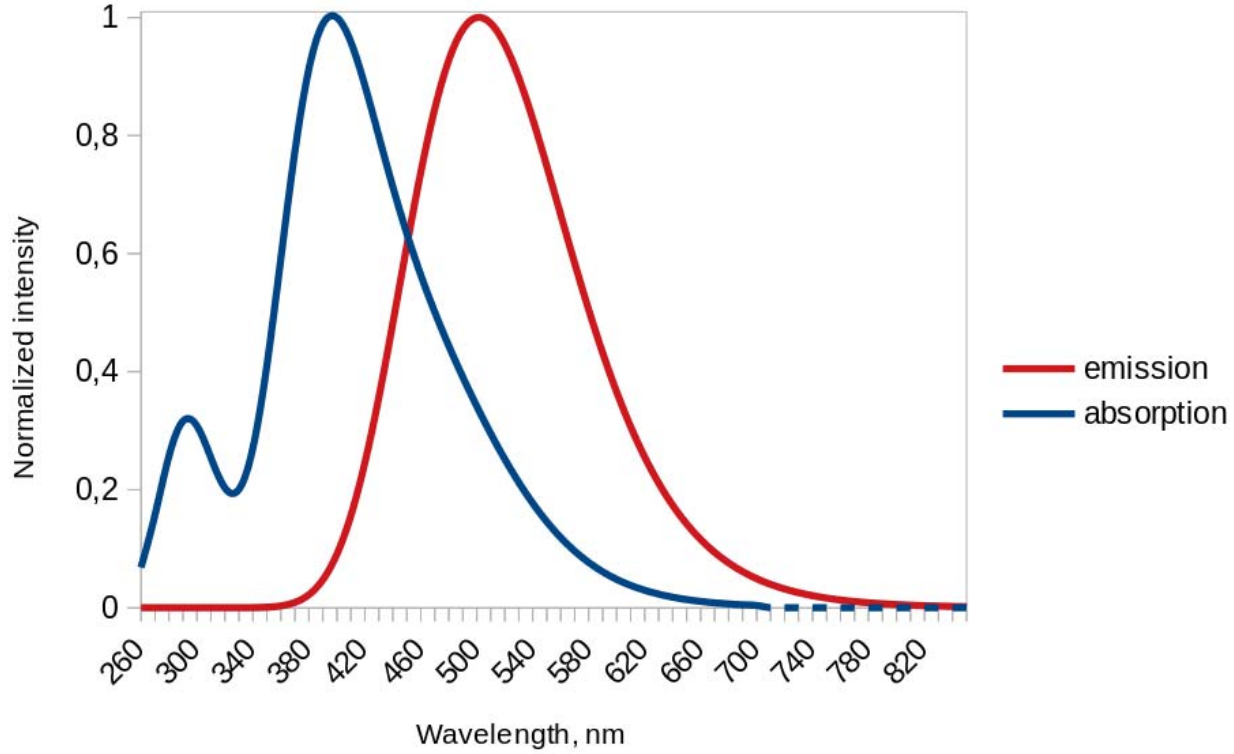


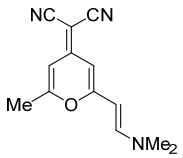
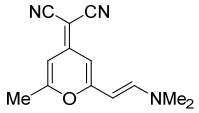
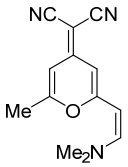
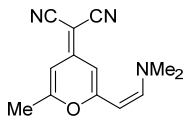
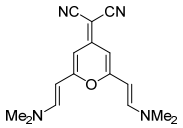
Fig. S5. Normalized absorption and emission spectra of **3d** in DMSO at the CAM-B3LYP level.

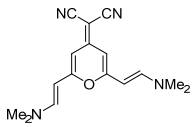
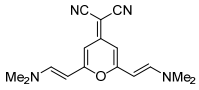
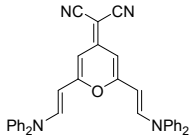
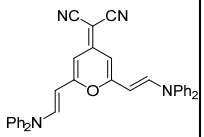
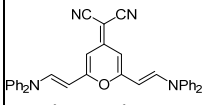
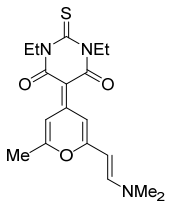
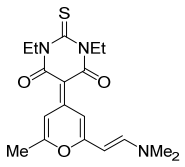
9. Table S5. Calculated absorption and emission properties for 2a,d, 3a,d, 11e in vacuo and in DMSO

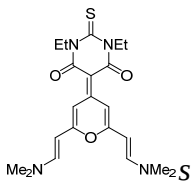
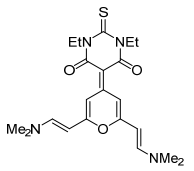
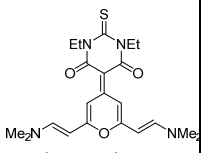
Entry	Cmpd	Solvent	λ_{abs}, nm	f_{GS}	λ_{em}, nm	f_{S1}	μ_{GS}, D	μ_{S1}, D	$\mu_{\|GS->S1\|}$, D
1 2	**2a**	Vacuum DMSO	345 407	1,059 1,350	368 421	1,041 1,305	14,508 0,769	15,777 3,794	1,269 3,025
3 4	**3a**	Vacuum DMSO	344 370	1,057 1,793	357 462	0,997 0,582	17,338 0,927	21,043 4,820	3,705 3,893
5 6	**11e**	Vacuum DMSO	358 396	1,323 2,794	417 486	0,440 0,650	15,153 0,305	19,780 24,209	4,627 23,904
7 8	**2d**	Vacuum DMSO	379 435	1,193 1,375	360* 460	0,441* 1,250	13,223 0,775	4,425 3,149	8,808 2,374
9 10	**3d**	Vacuum DMSO	393 476	0,372 0,559	421 507	0,353 0,556	16,273 0,770	21,669 5,275	5,396 4,505

* Oscillator strengths turned out to be negligible for S_1-S_4, S_5 wavelength and oscillator strength provided

10. Table S6. Calculated energies of the ground state, frontier orbitals, conformer populations in DMSO, and important angles for the S_1 excited state for compounds 2a,d, 3a,d, 11e

Compound	Energy of GS, Hartrees	HOMO energy, eV	LUMO energy, eV	S_1 MDN-Pyran ring angle, degrees	S_1 TB-Pyran ring dihedral angle, degrees	S_1 Enamine double bond-Pyran ring angle, degrees	Relative energy, kcal/mol	DMSO populations *, %
 *s-trans-E*-**2a**	–742.2538560703	–5.44	–2.04	0.6–0.8	-	0.9	0	96.90
 *s-cis-E*-**2a**	–742.2506015618	–5.50	–1.99	4.3–5.2	-	8.6	+2.04	3.10
 *s-trans-Z*-**2a**	–742.2408961328	–5.47	–2.07	n/d	-	n/d	+8.13	~0
 *s-cis-Z*-**2a**	–742.2393898005	–5.55	–2.07	n/d	-	n/d	+9.09	~0
 *s-trans-s-trans-E*-**3a**	–914.2249613805	–5.17	–1.96	2.6–2.7	-	2.2; 0.1	0	80.90

Compound	Energy of GS, Hartrees	HOMO energy, eV	LUMO energy, eV	S_1 MDN-Pyran ring angle, degrees	S_1 TB-Pyran ring dihedral angle, degrees	S_1 Enamine double bond-Pyran ring angle, degrees	Relative energy, kcal/mol	DMSO populations *, %
 *s-cis-s-trans-E*-**3a**	–914.2229249549	–5.19	–1.85	0.5–0.7	-	0.4; 1.9	+1.28	18.70
 *s-cis-s-cis-E*-**3a**	–914.2199711401	–5.19	–1.77	0.4–0.8	-	3.1; 3.6	+3.13	0.40
 *s-trans-s-trans-E*-**11e**	–1680.7552654405	–5.36	–2.29	0.6–1.0	-	0.7; 0.7	0	89.47
 *s-trans-s-cis-E*-**11e**	–1680.7525737227	–5.39	–2.20	0.1–0.8	-	4.8 (trans); 16.6 (cis)	+1.69	10.32
 *s-cis-s-cis-E*-**11e**	–1680.7495365241	–5.42	–2.12	0.2–1.5	-	11.7; 2.6	+3.60	0.21
 *s-trans-E*-**2d**	–1487.2881759075	–5.42	–2.23	-	26.9–29.3	3.5	0	91.53
 *s-cis-E*-**2d**	–1487.2859282924	–5.44	–2.15	-	84.9–86.9	25.3	+1.41	8.47

Compound	Energy of GS, Hartrees	HOMO energy, eV	LUMO energy, eV	S_1 MDN-Pyran ring angle, degrees	S_1 TB-Pyran ring dihedral angle, degrees	S_1 Enamine double bond-Pyran ring angle, degrees	Relative energy, kcal/mol	DMSO populations *, %
 *-trans-s-trans-E-* **3d**	–1659.2587790345	–5.06	–2.12	-	24.0–25.5	0.3; 1.8	0	77.15
 *s-trans-s-cis-E-* **3d**	–1659.2569222035	–5.06	–2.04	-	26.3–27.2	1.1; 3.8	+1.16	21.74
 *s-cis-s-cis-E-* **3d**	–1659.2541133737	–5.06	–1.96	-	15.4–16.7	3.8; 4.8	+2.51	1.11

* Boltzmann populations were calculated assuming that only the considered conformers contribute to the total population.

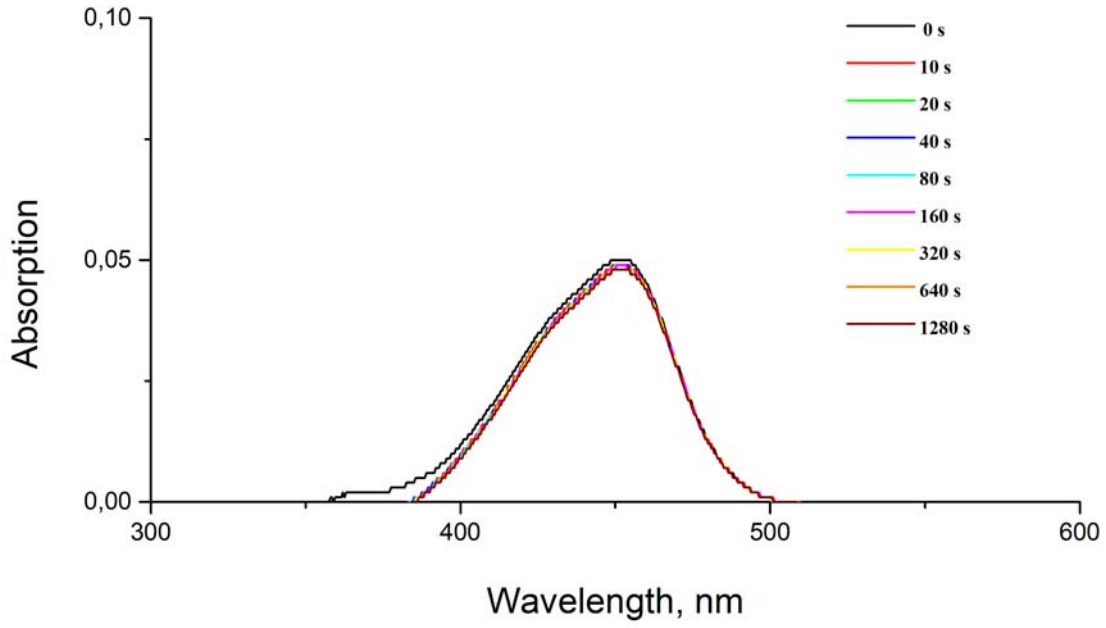
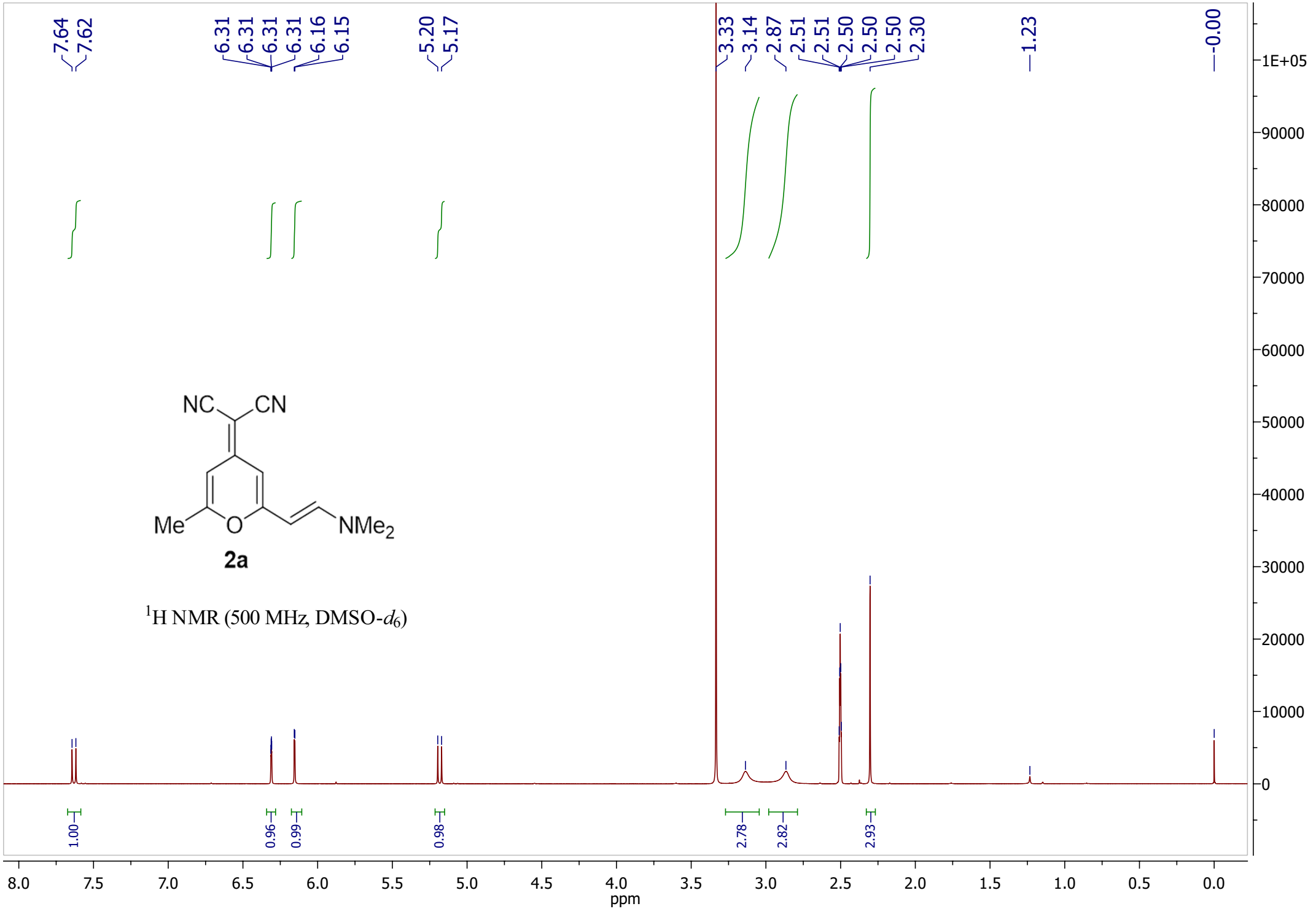
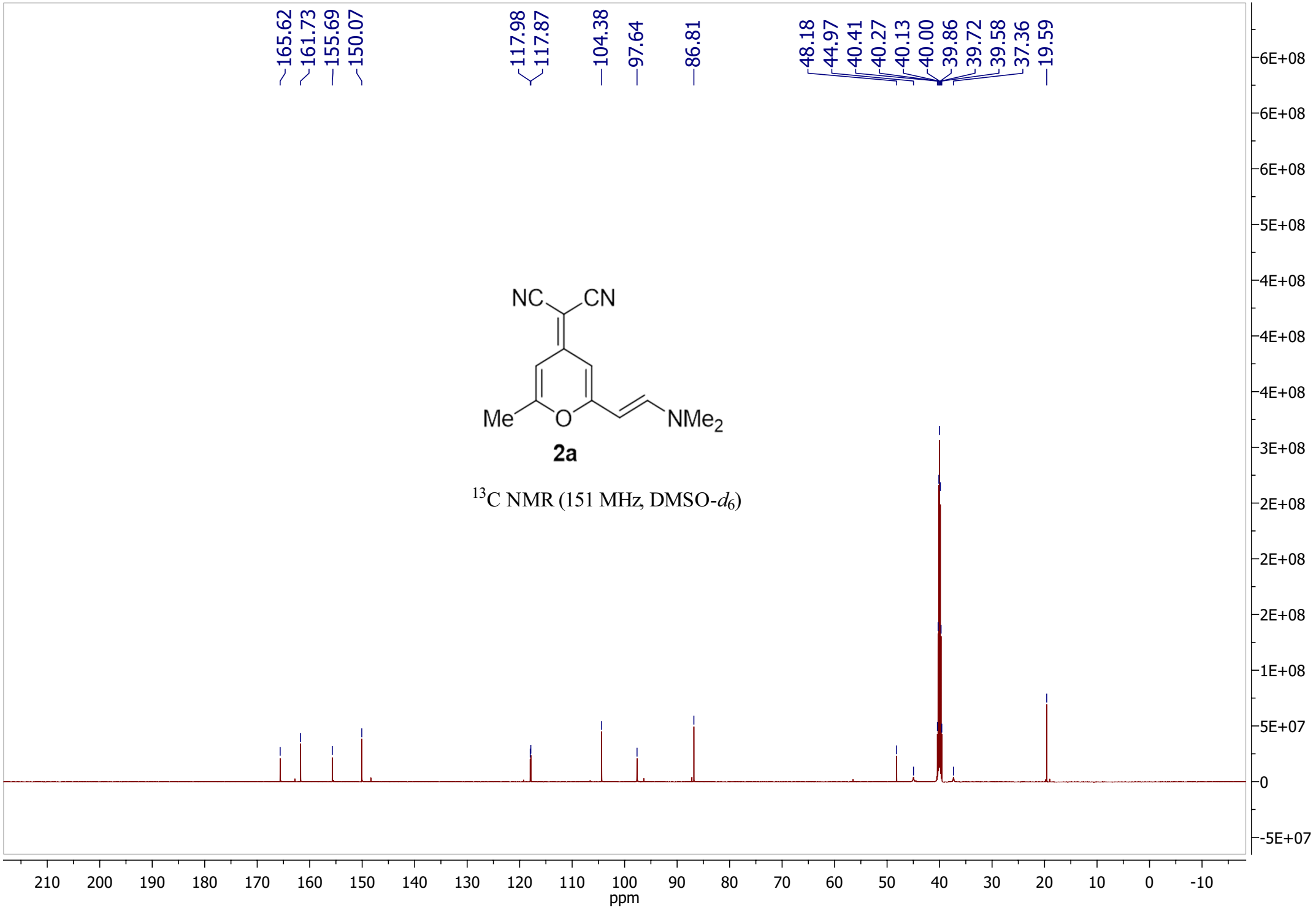
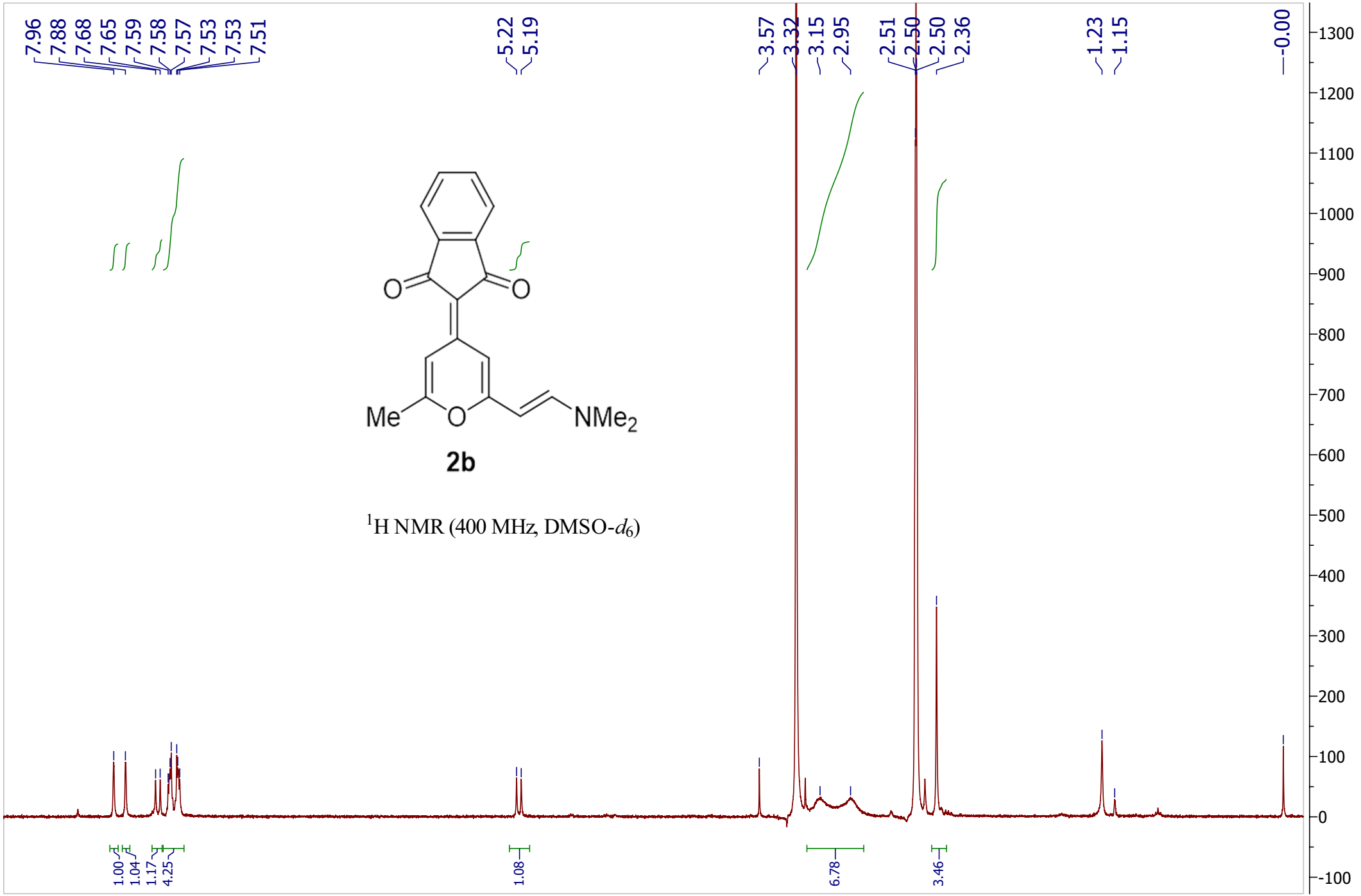


Fig. S6. The absorbance spectra of **8f** upon prolonged photoexcitation at 400 nm.

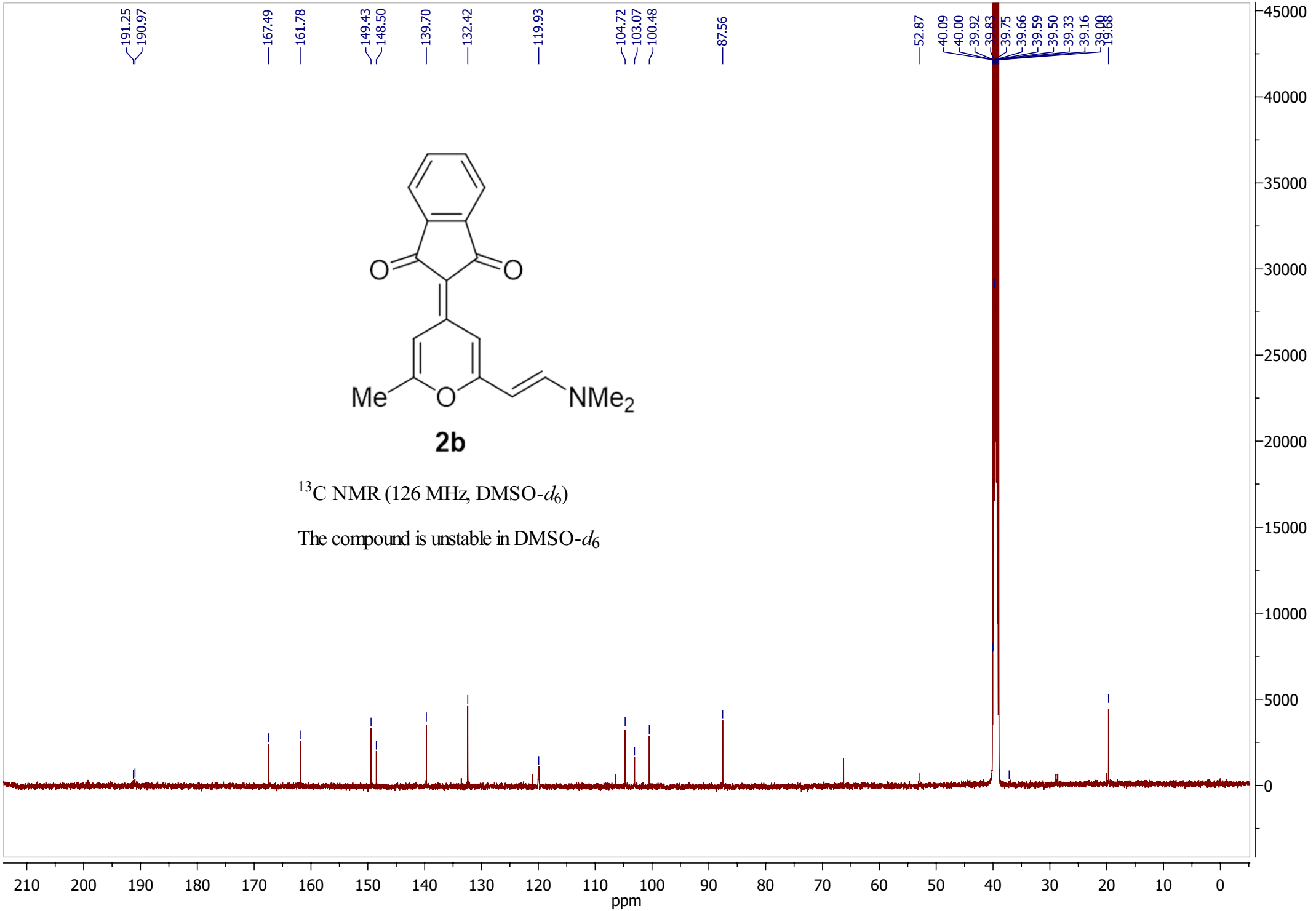

7.64
7.62
6.31
6.31
6.31
6.31
6.16
6.15
5.20
5.17
3.33
3.14
2.87
2.51
2.51
2.50
2.50
2.50
2.30
1.23
-0.00
NC
CN
Me
O
NMe2
2a
1H NMR (500 MHz, DMSO-d6)
1.00
0.96
0.99
0.98
2.78
2.82
2.93
ppm



^{13}C NMR (151 MHz, DMSO-d_6)



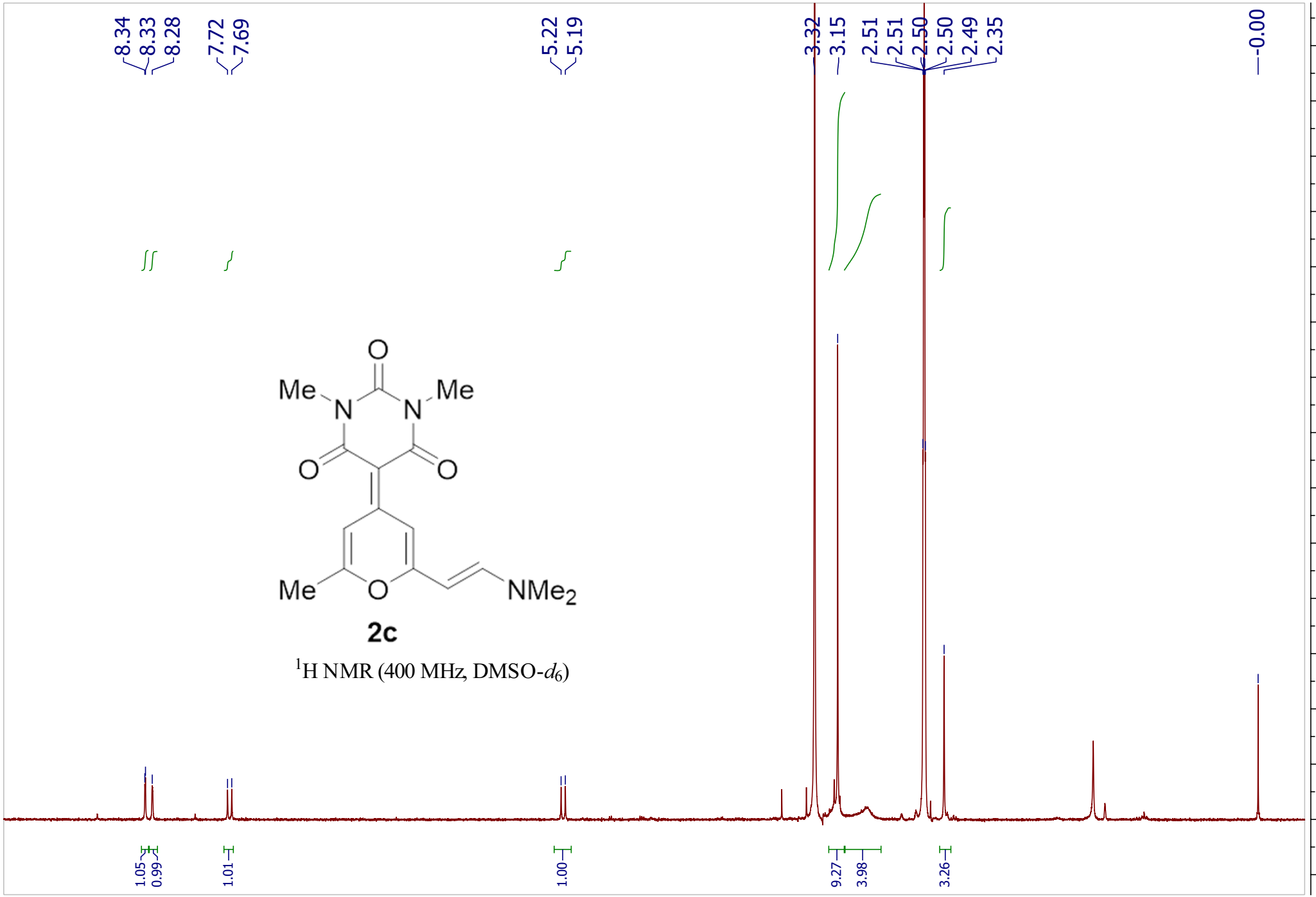
^{1}H NMR (400 MHz, DMSO-d_6)



2b

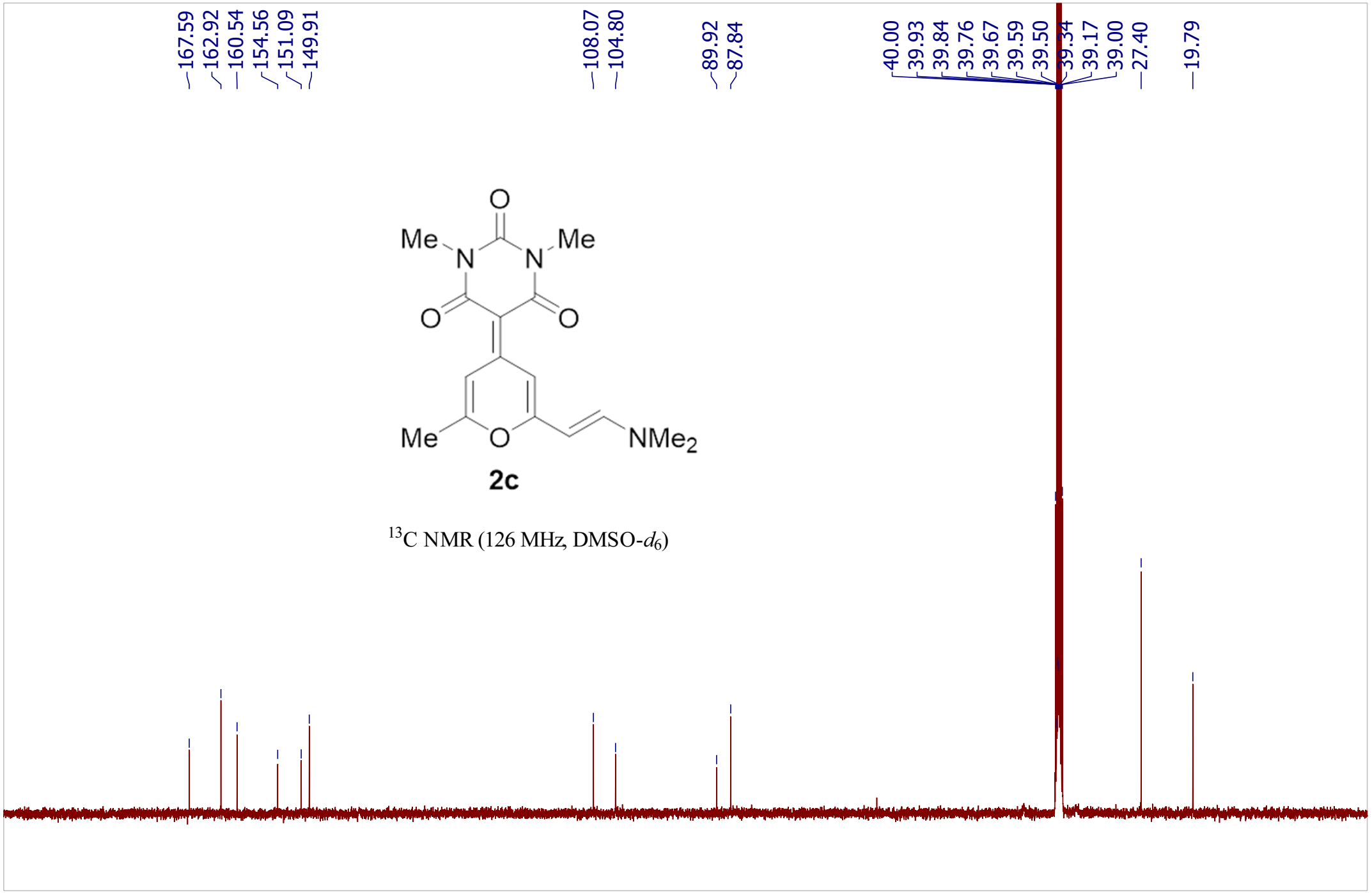
^{13}C NMR (126 MHz, DMSO-d_6)

The compound is unstable in DMSO-d_6

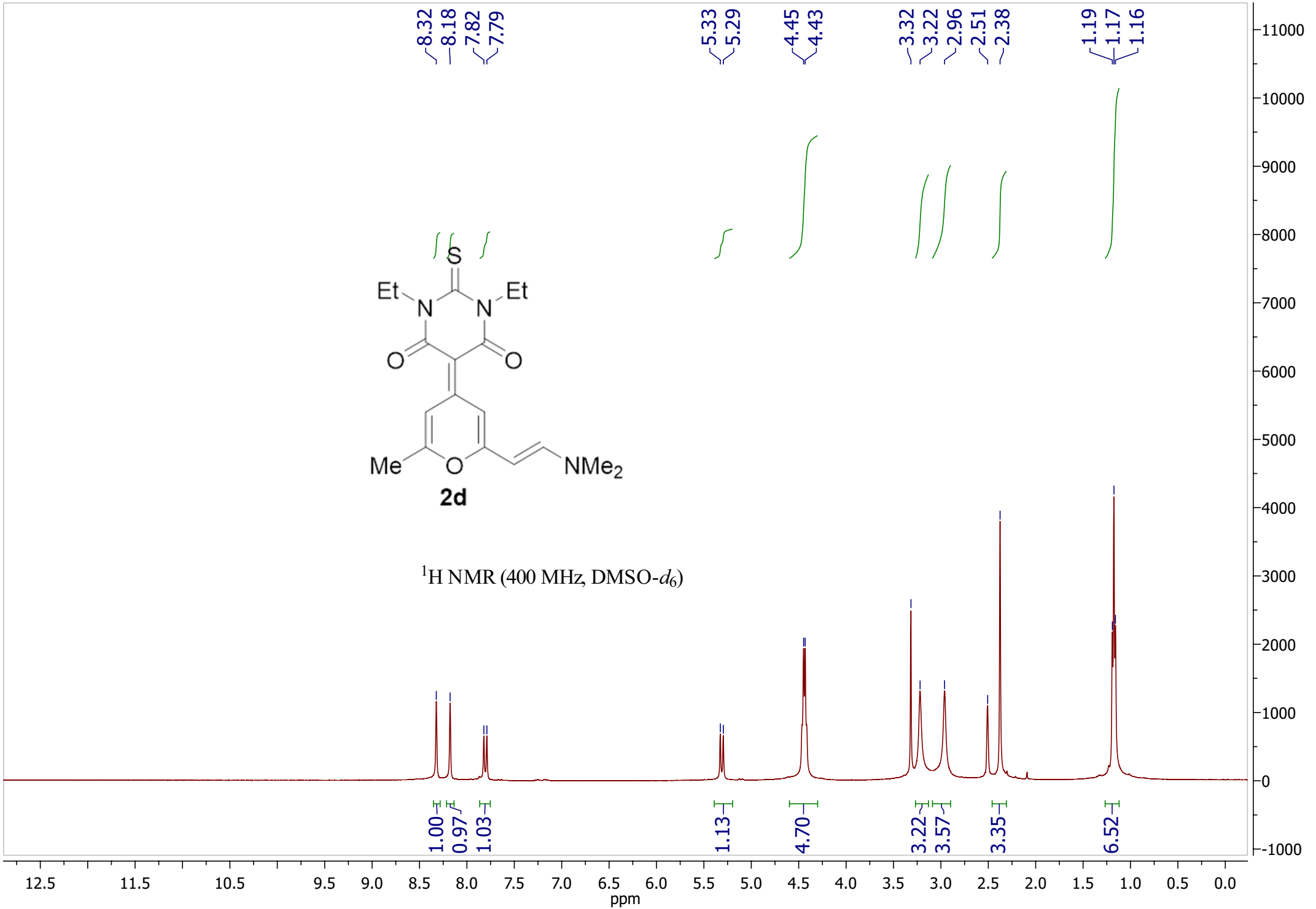


2c

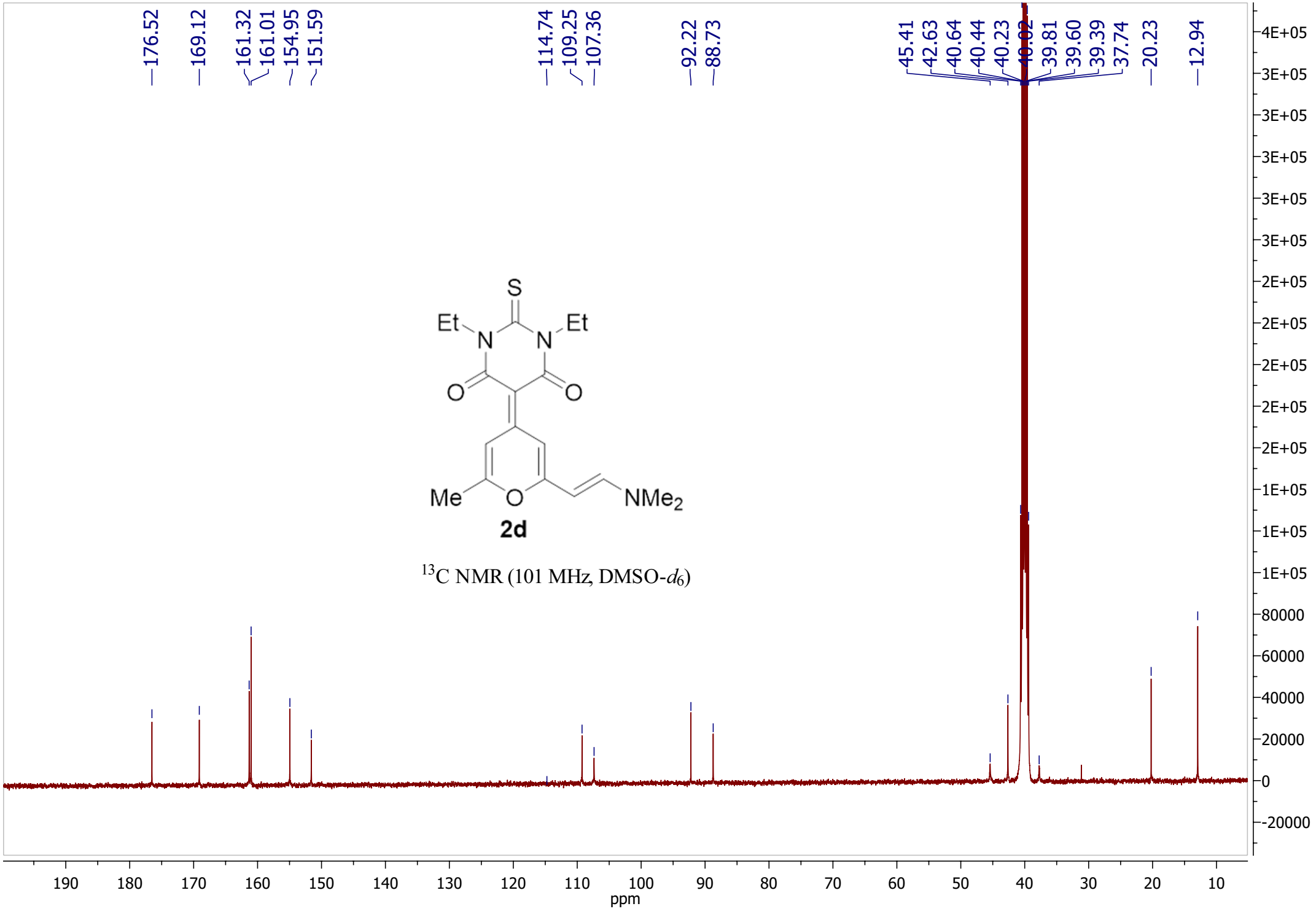
^{1}H NMR (400 MHz, DMSO-d_6)



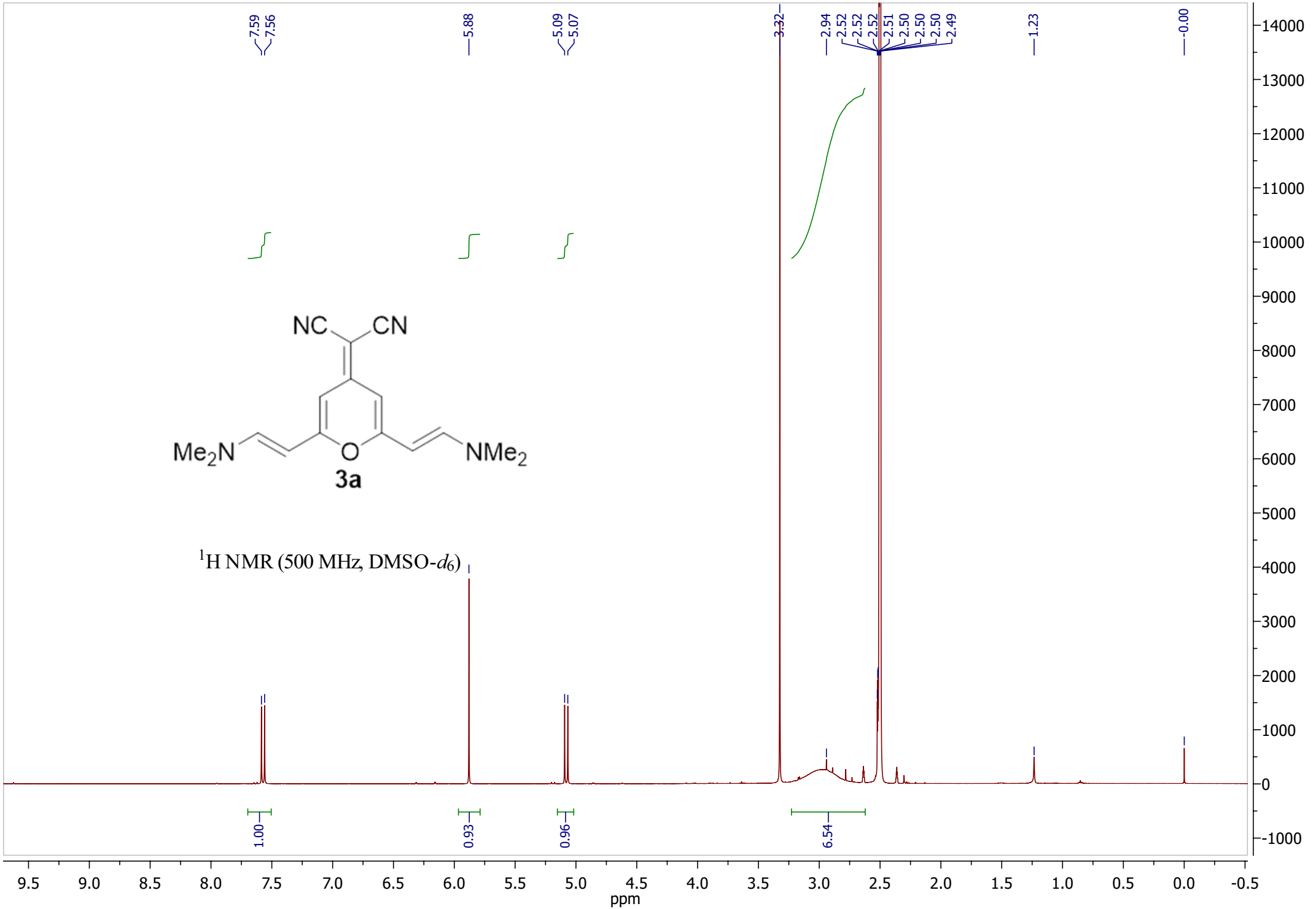
^{13}C NMR (126 MHz, DMSO-d_6)

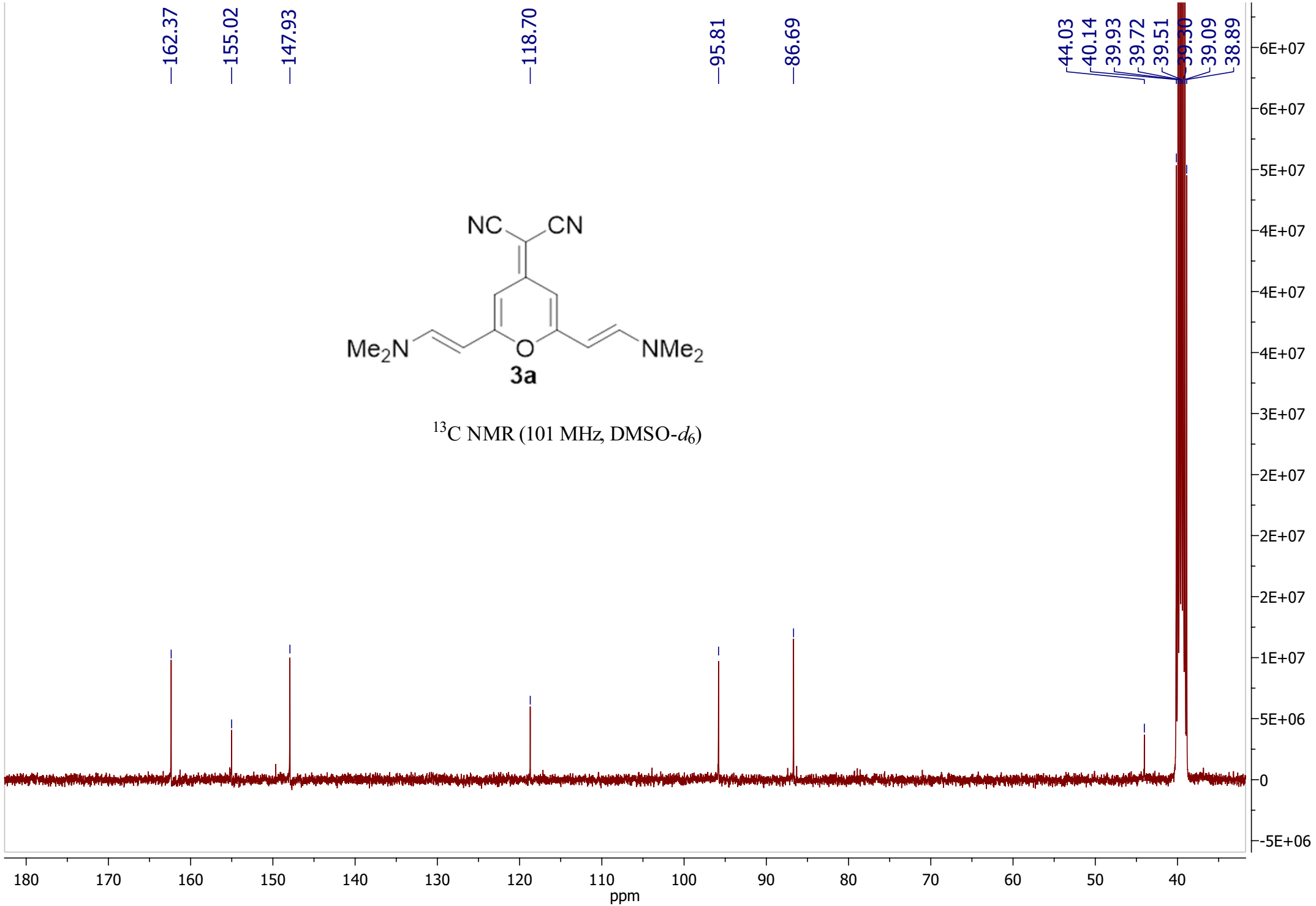


^{1}H NMR (400 MHz, DMSO-d_6)

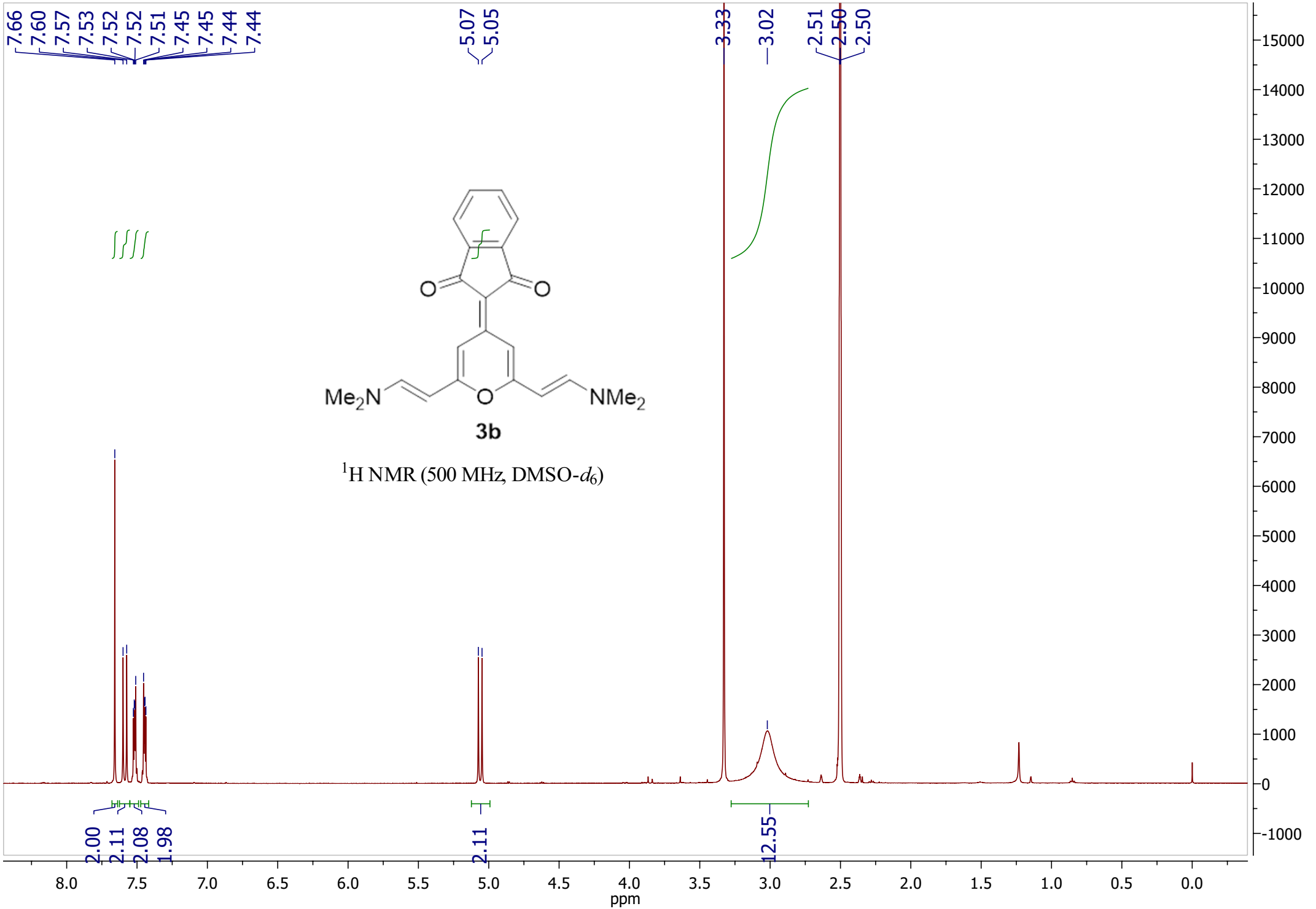


^{13}C NMR (101 MHz, DMSO-d_6)

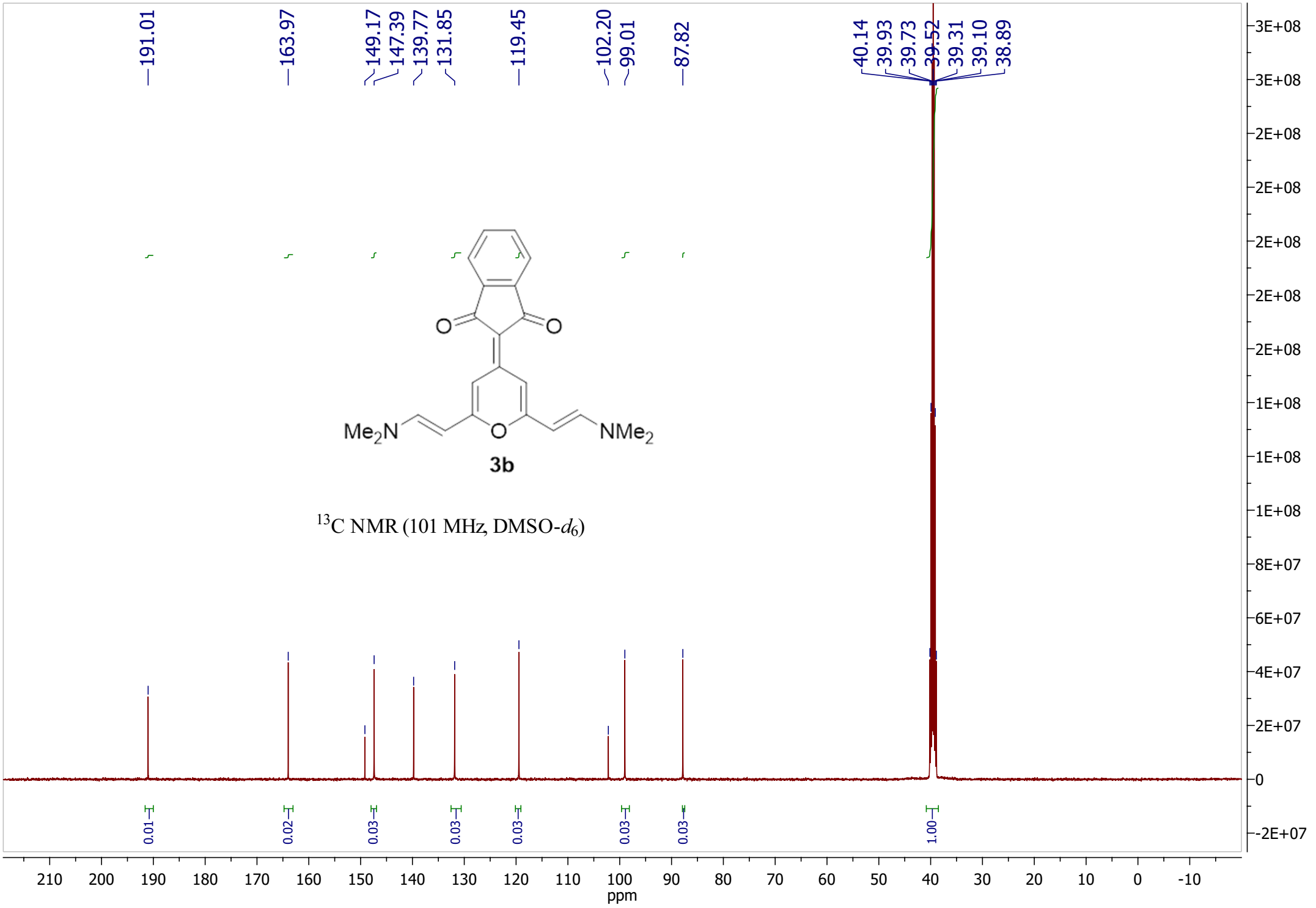

7.59
7.56
5.88
5.09
5.07
3.32
2.94
2.52
2.52
2.52
2.51
2.50
2.50
2.50
2.49
1.23
-0.00
NC
CN
Me2N
O
NMe2
3a
1H NMR (500 MHz, DMSO-d6)
1.00
0.93
0.96
6.54
ppm



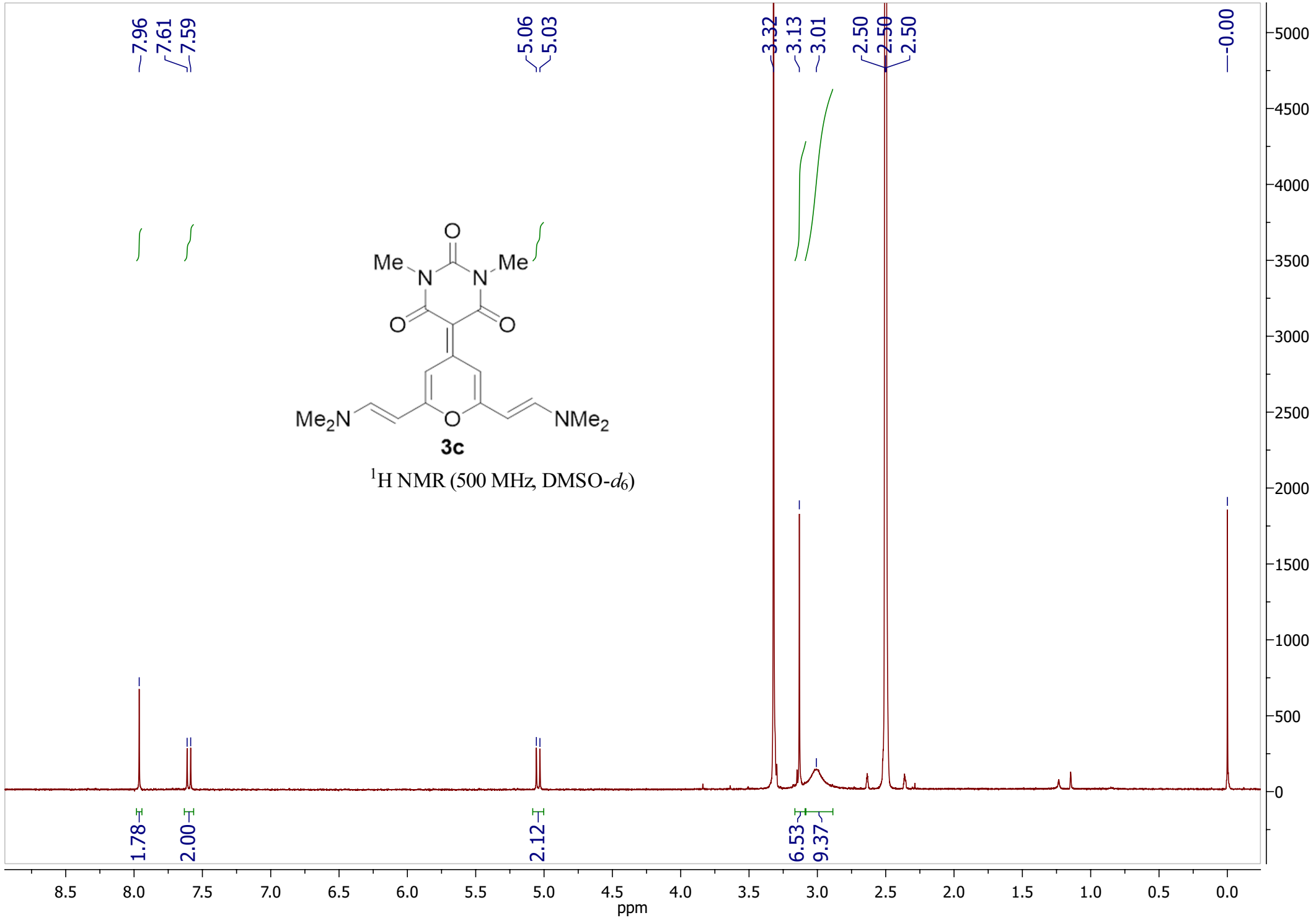
^{13}C NMR (101 MHz, DMSO-d_6)



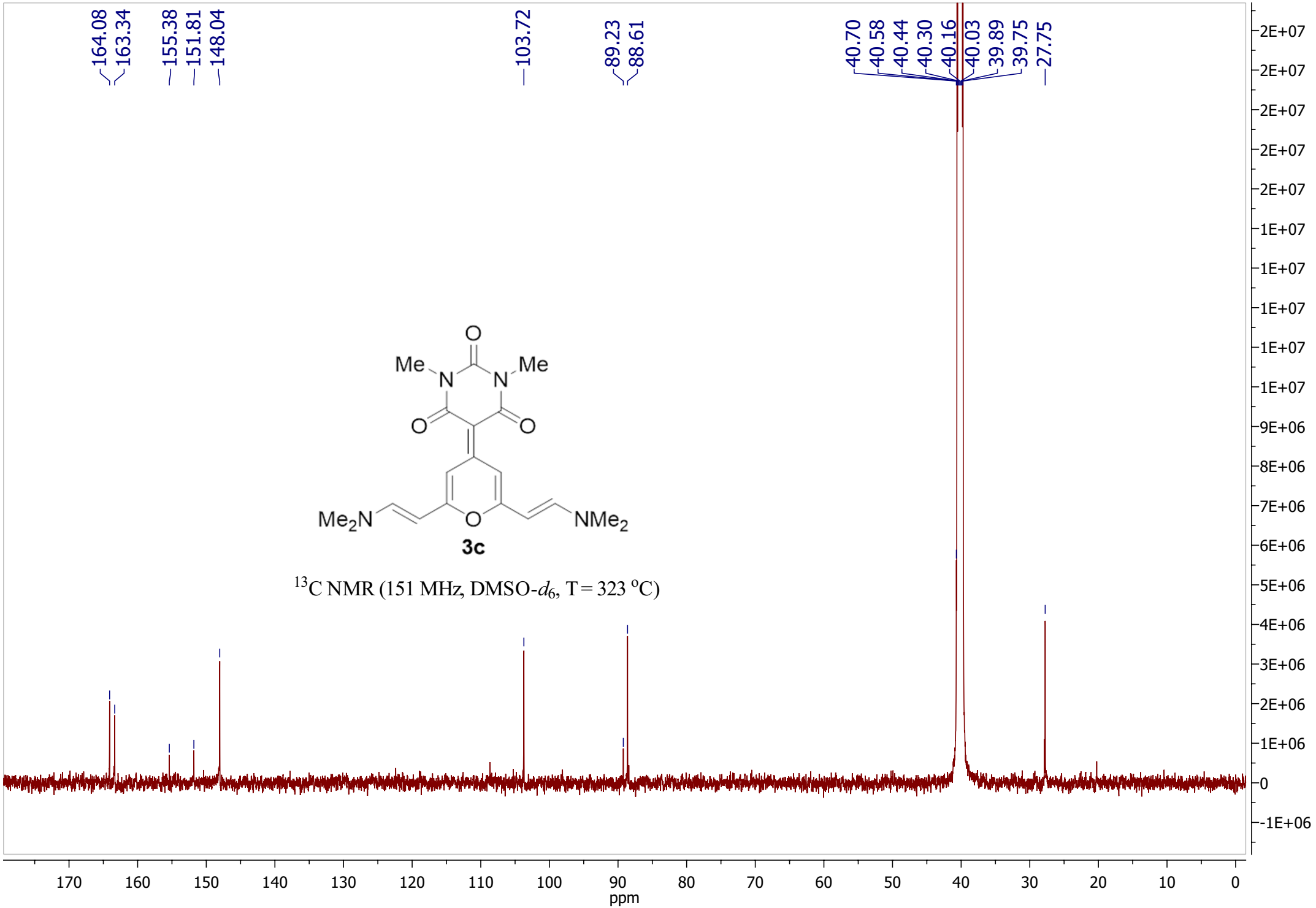
^{1}H NMR (500 MHz, DMSO-d_6)



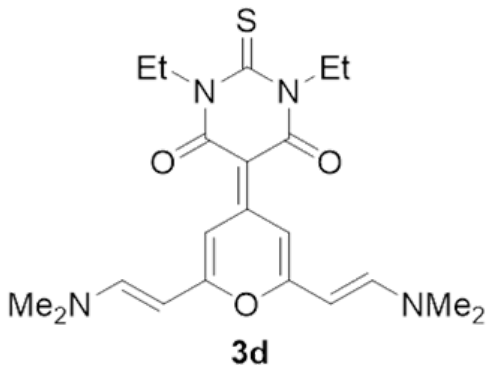
^{13}C NMR (101 MHz, DMSO-d_6)



^{1}H NMR (500 MHz, DMSO-d_6)

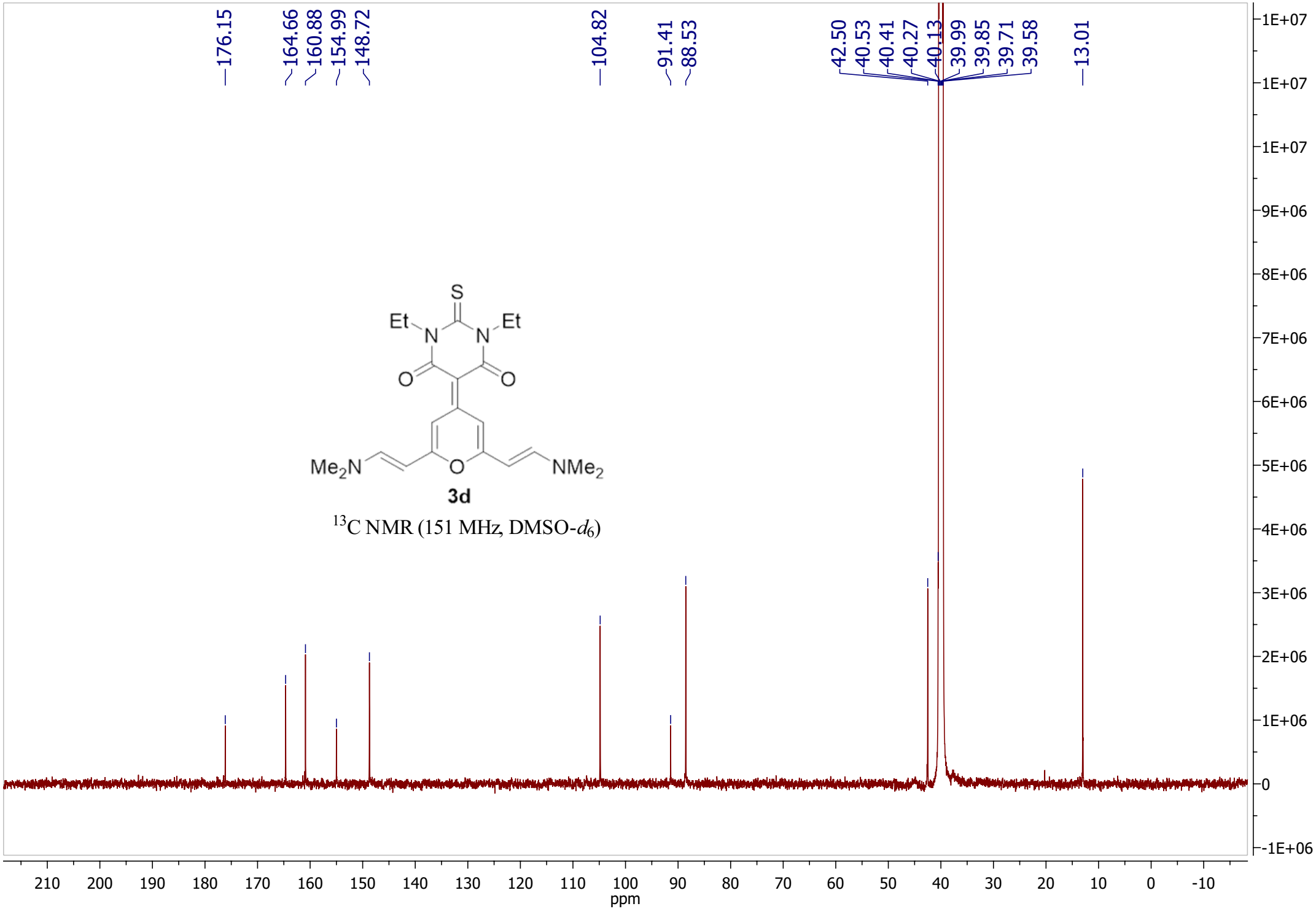


^{13}C NMR (151 MHz, DMSO-d_6, T = 323 ^{o}C)



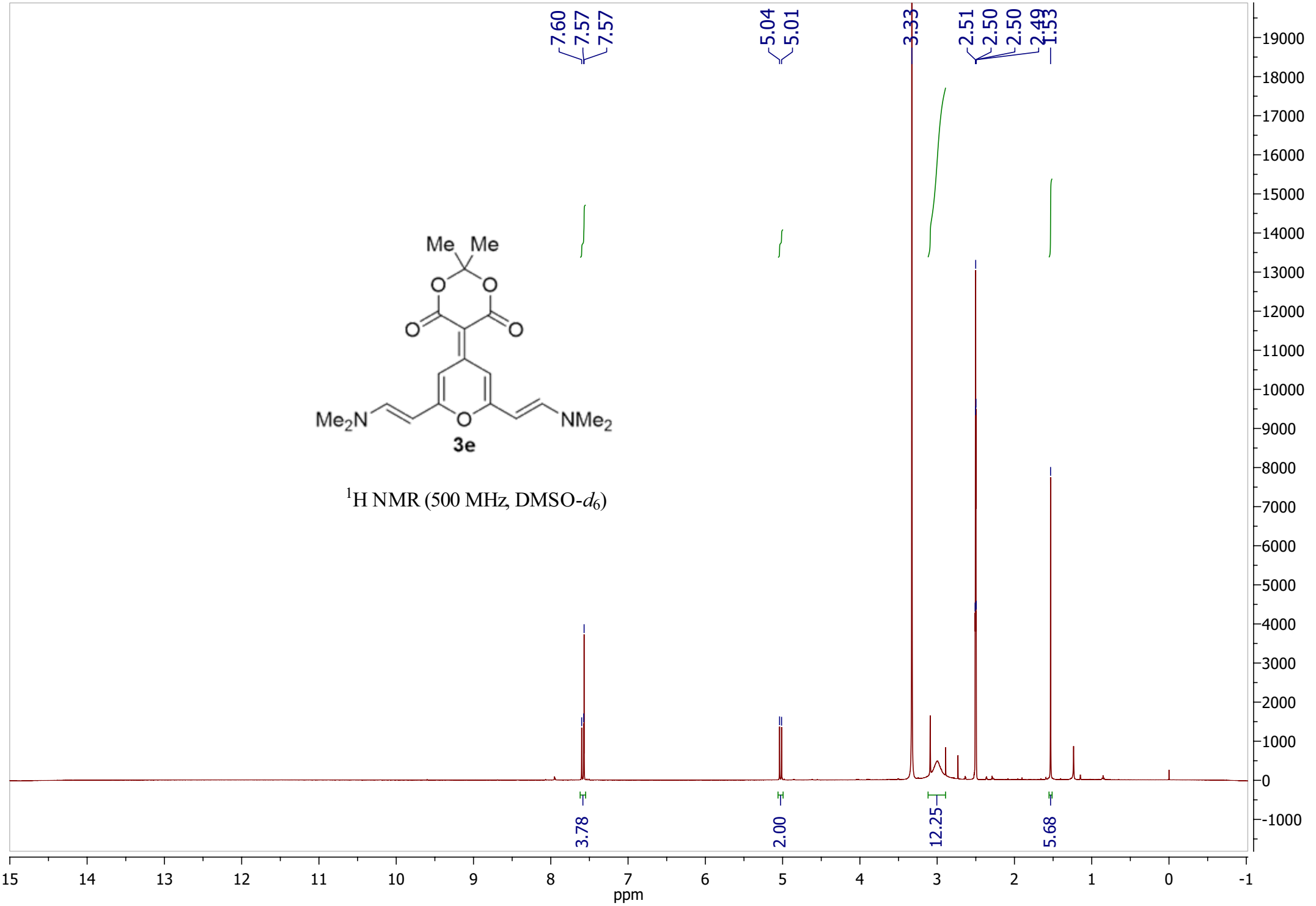
3d

^{1}H NMR (500 MHz, DMSO-d_6)

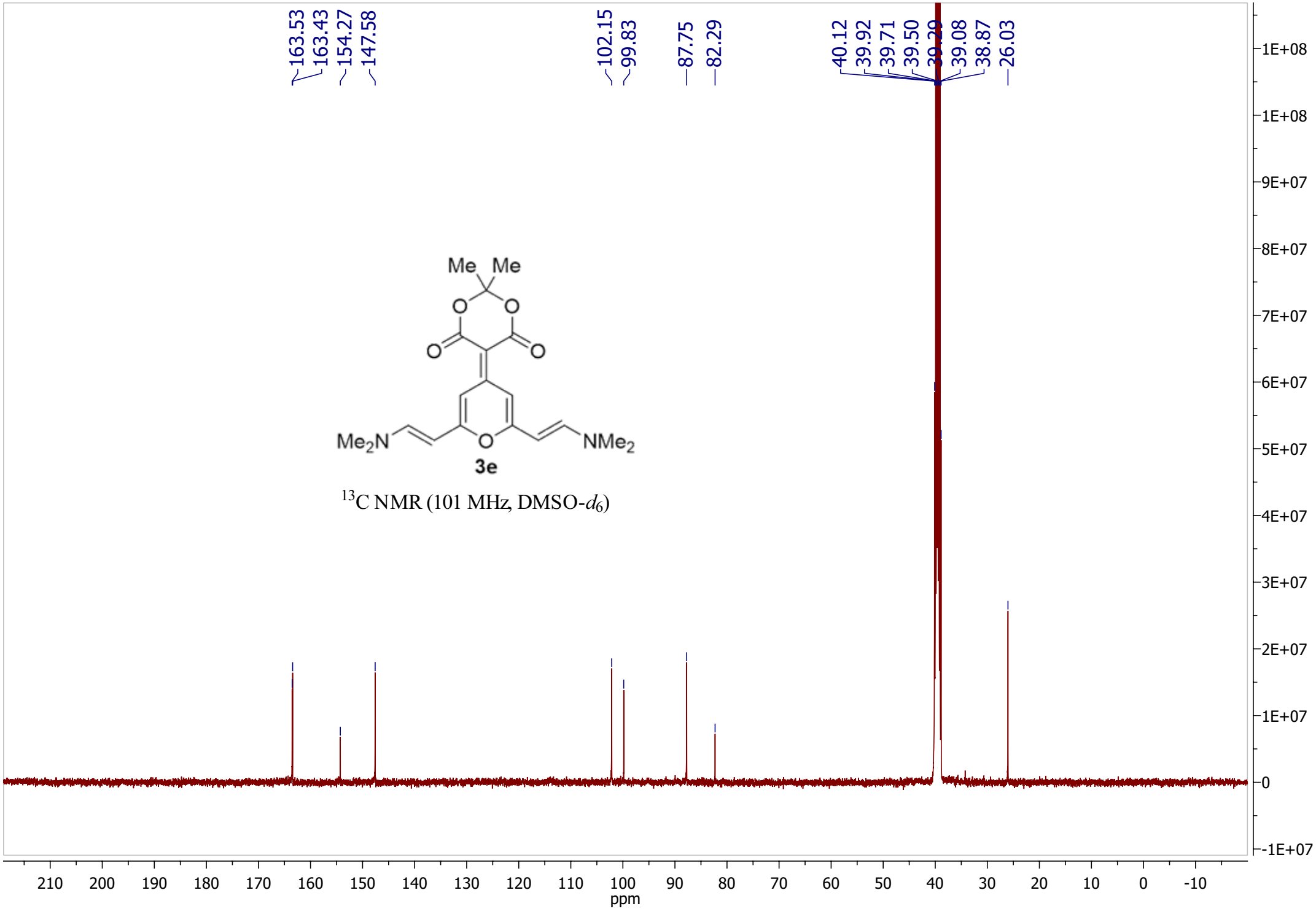


3d

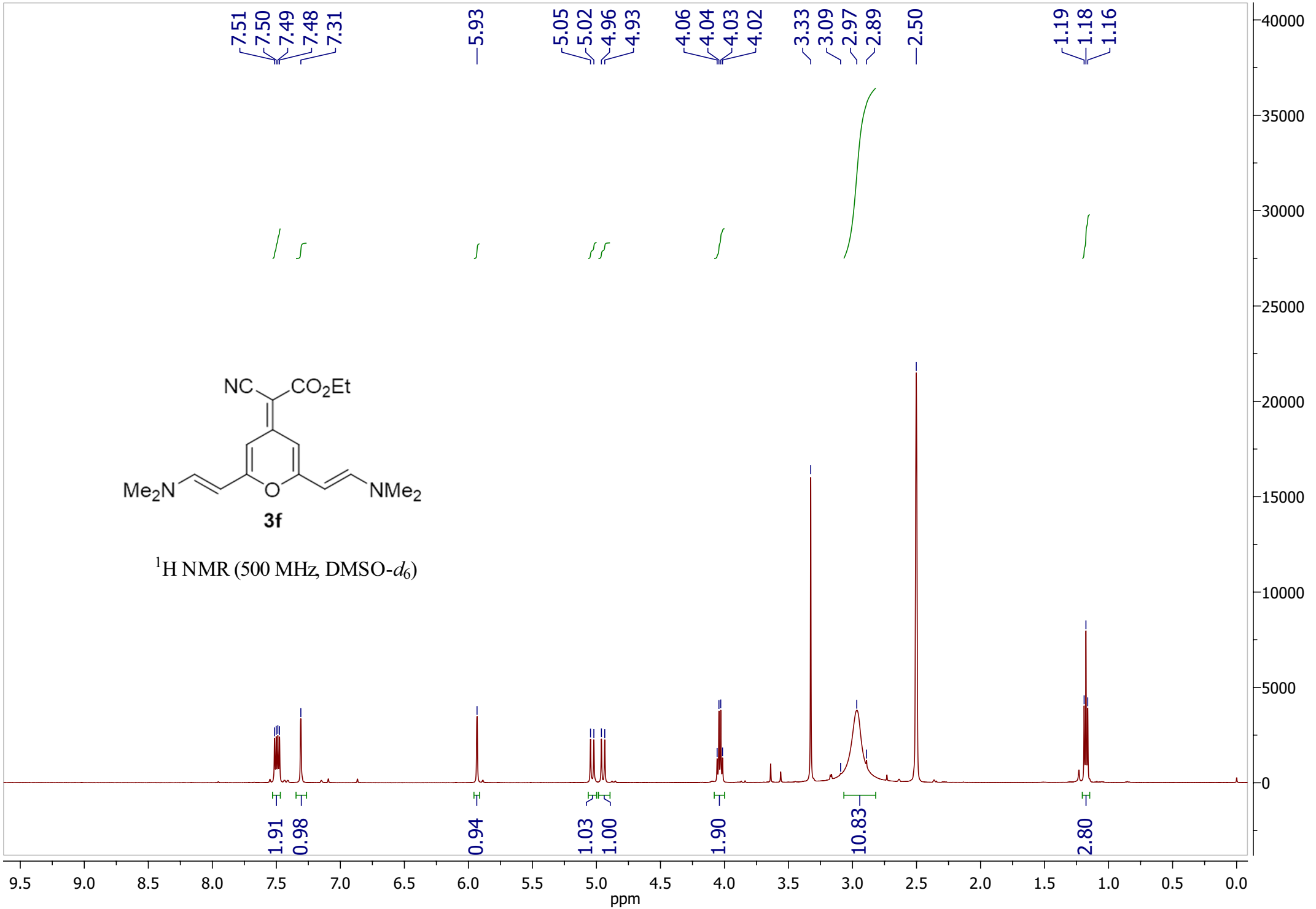
^{13}C NMR (151 MHz, DMSO-d_6)

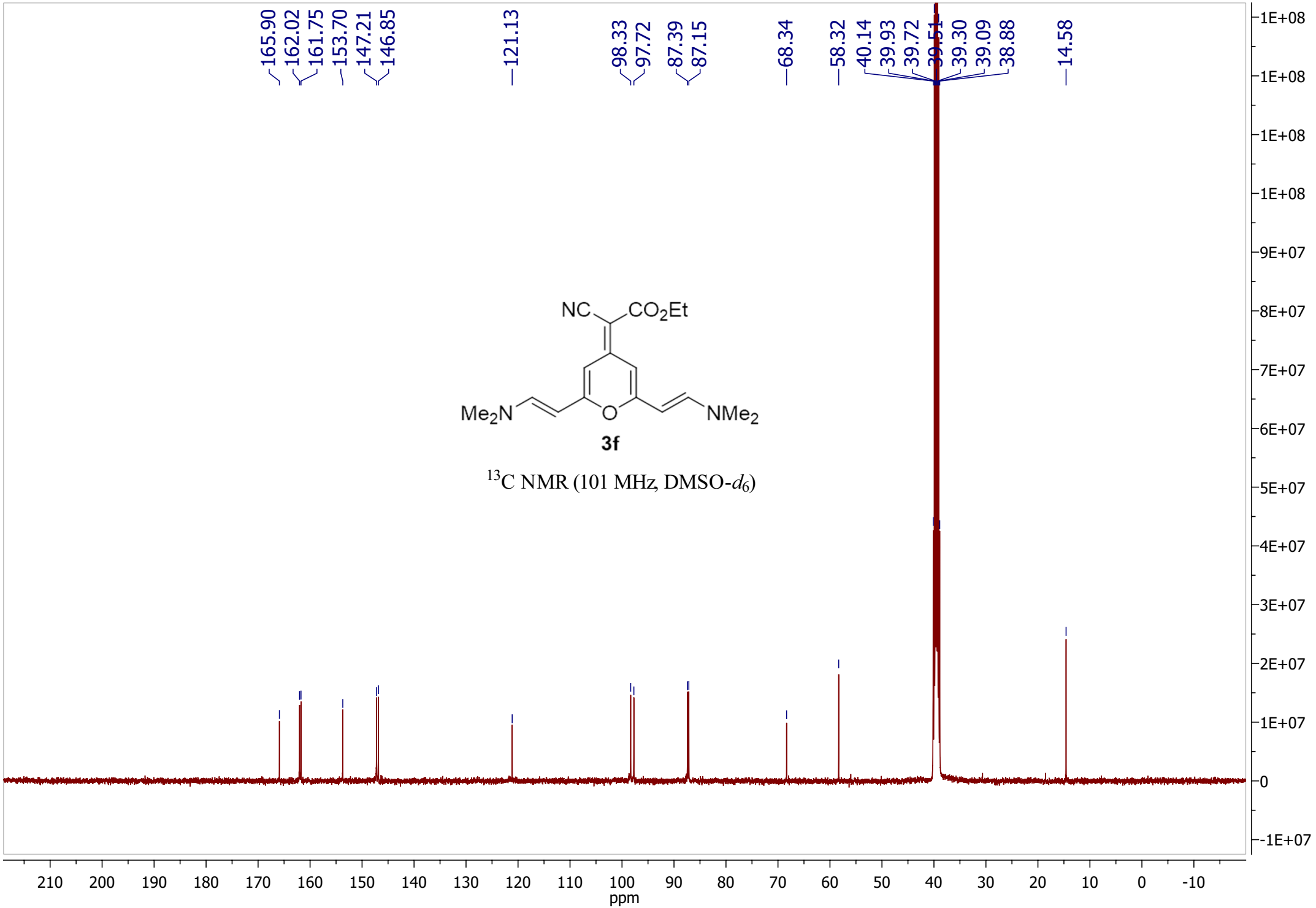


^{1}H NMR (500 MHz, DMSO-d_6)

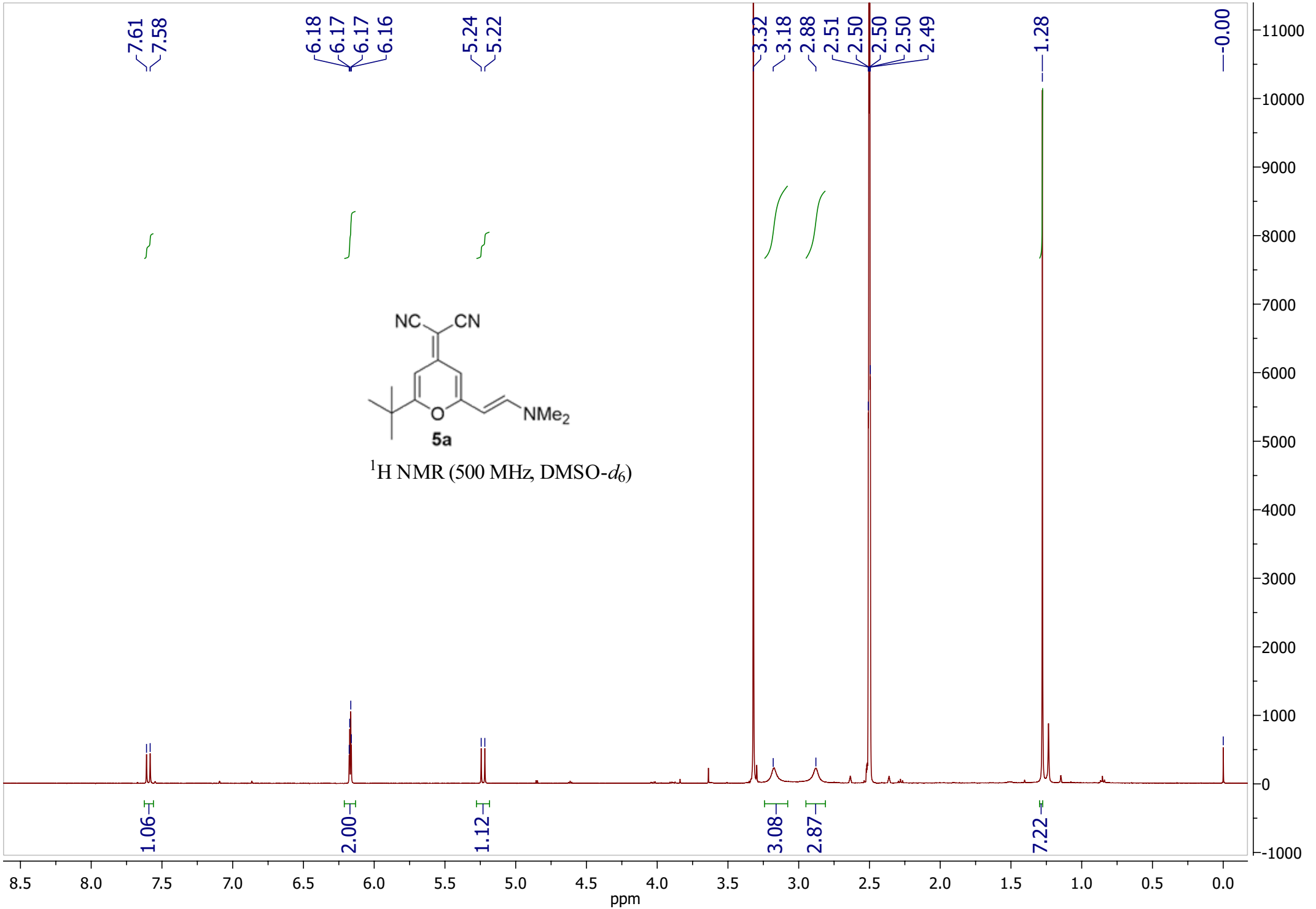


^{13}C NMR (101 MHz, DMSO-d_6)

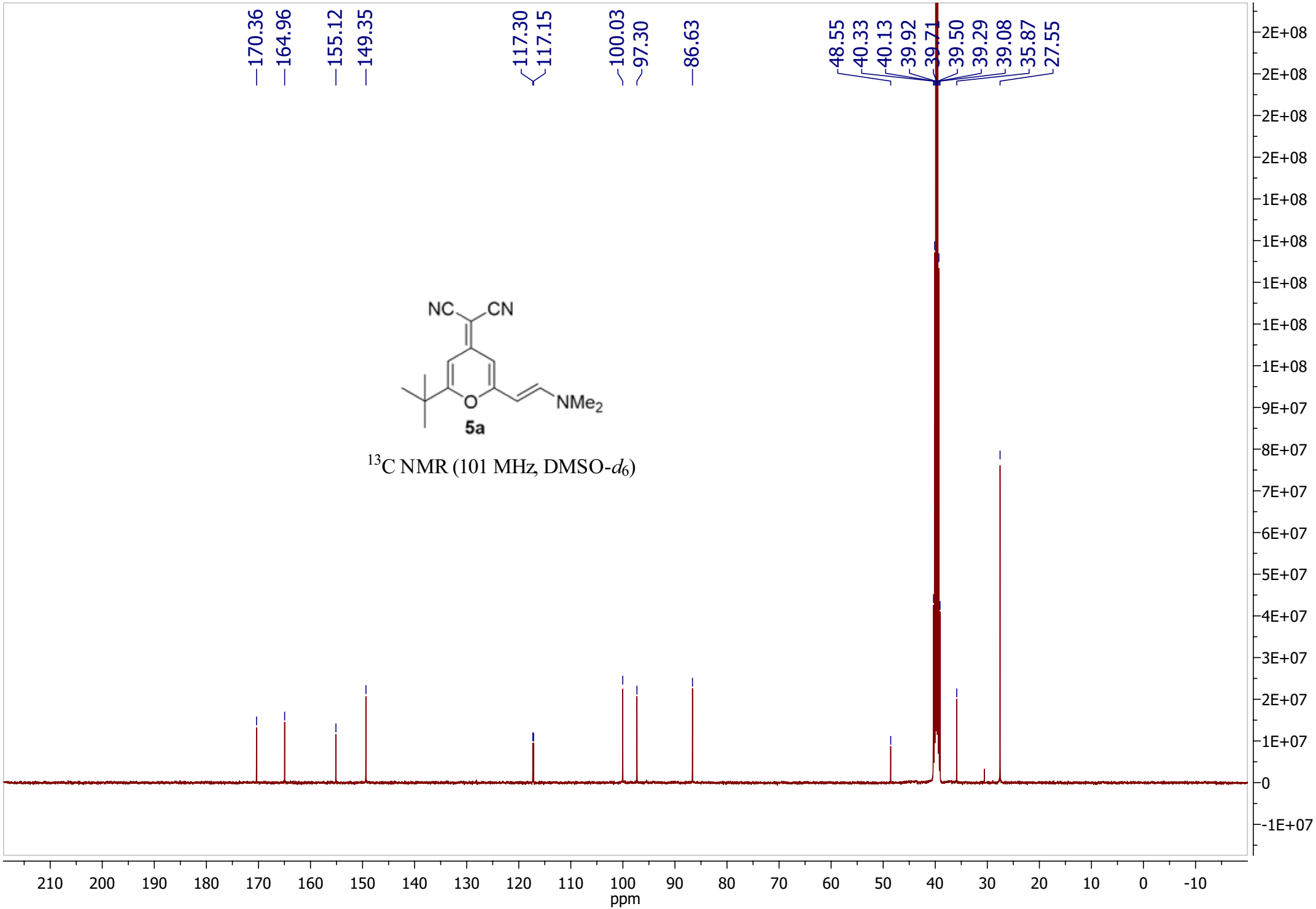

7.51
7.50
7.49
7.48
7.31
5.93
5.05
5.02
4.96
4.93
4.06
4.04
4.03
4.02
3.33
3.09
2.97
2.89
2.50
1.19
1.18
1.16
NC
CO2Et
Me2N
NMe2
O
3f
1H NMR (500 MHz, DMSO-d6)
1.91
0.98
0.94
1.03
1.00
1.90
10.83
2.80
ppm



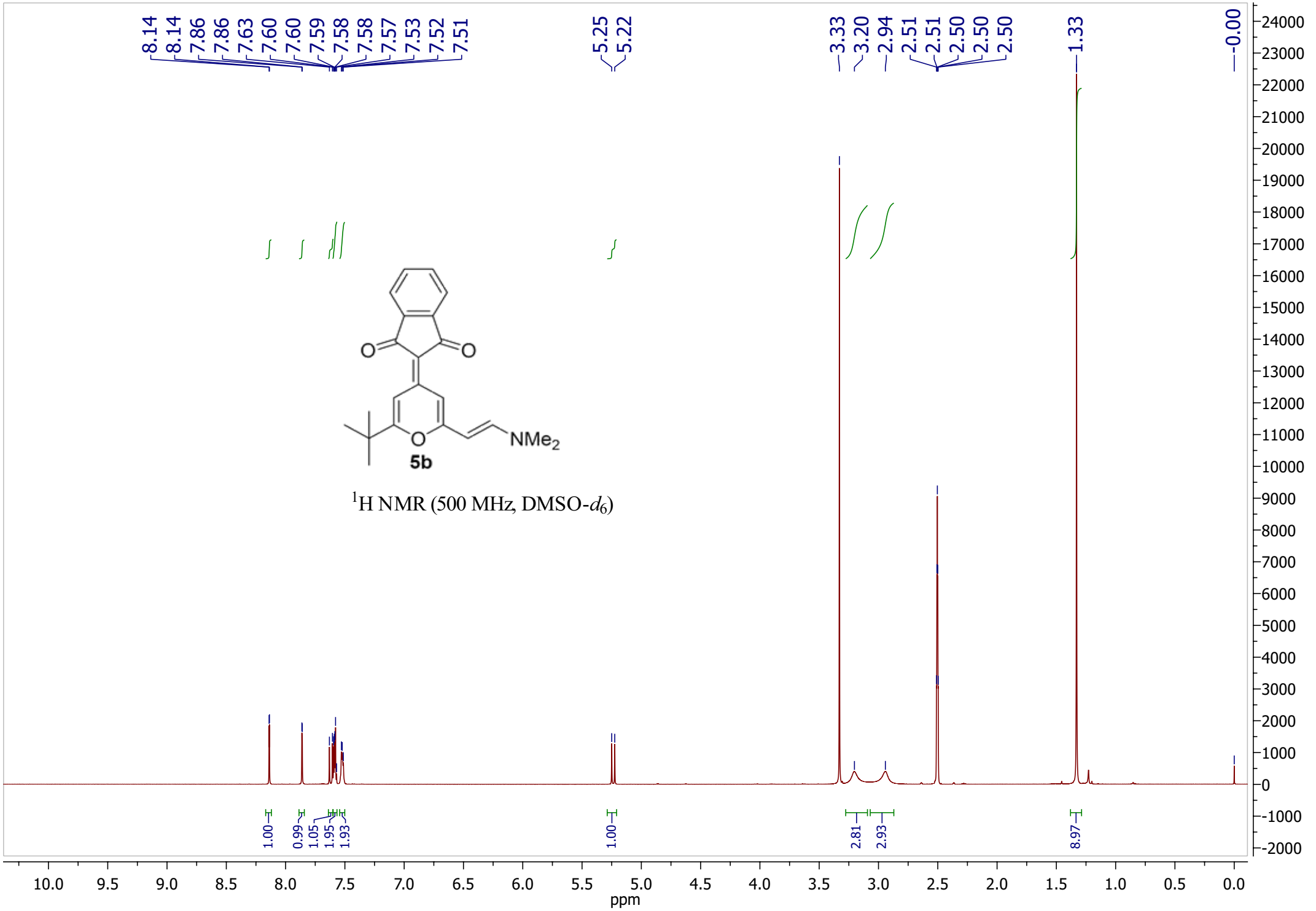
^{13}C NMR (101 MHz, DMSO-d_6)



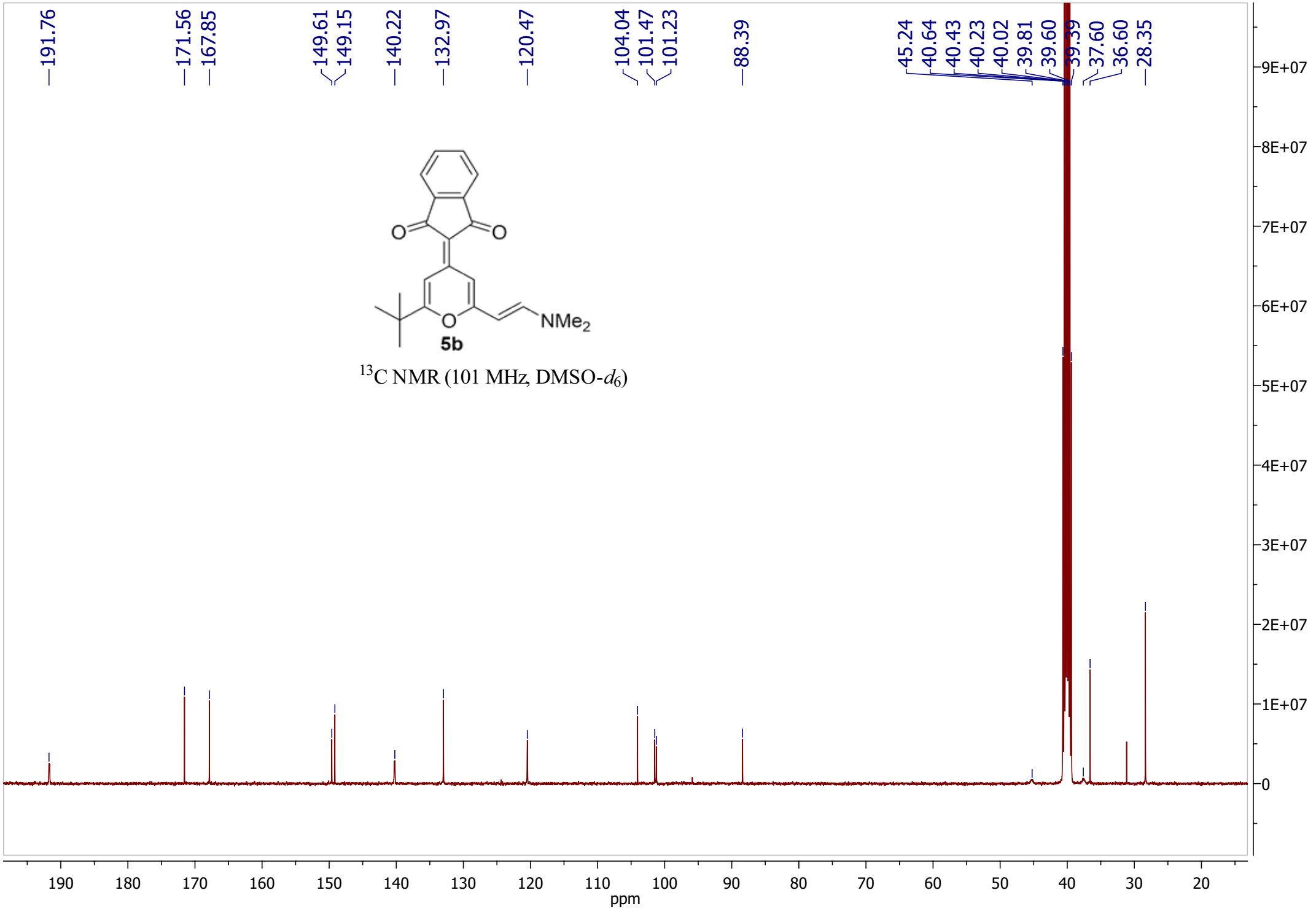
^{1}H NMR (500 MHz, DMSO-d_6)



^{13}C NMR (101 MHz, DMSO-d_6)

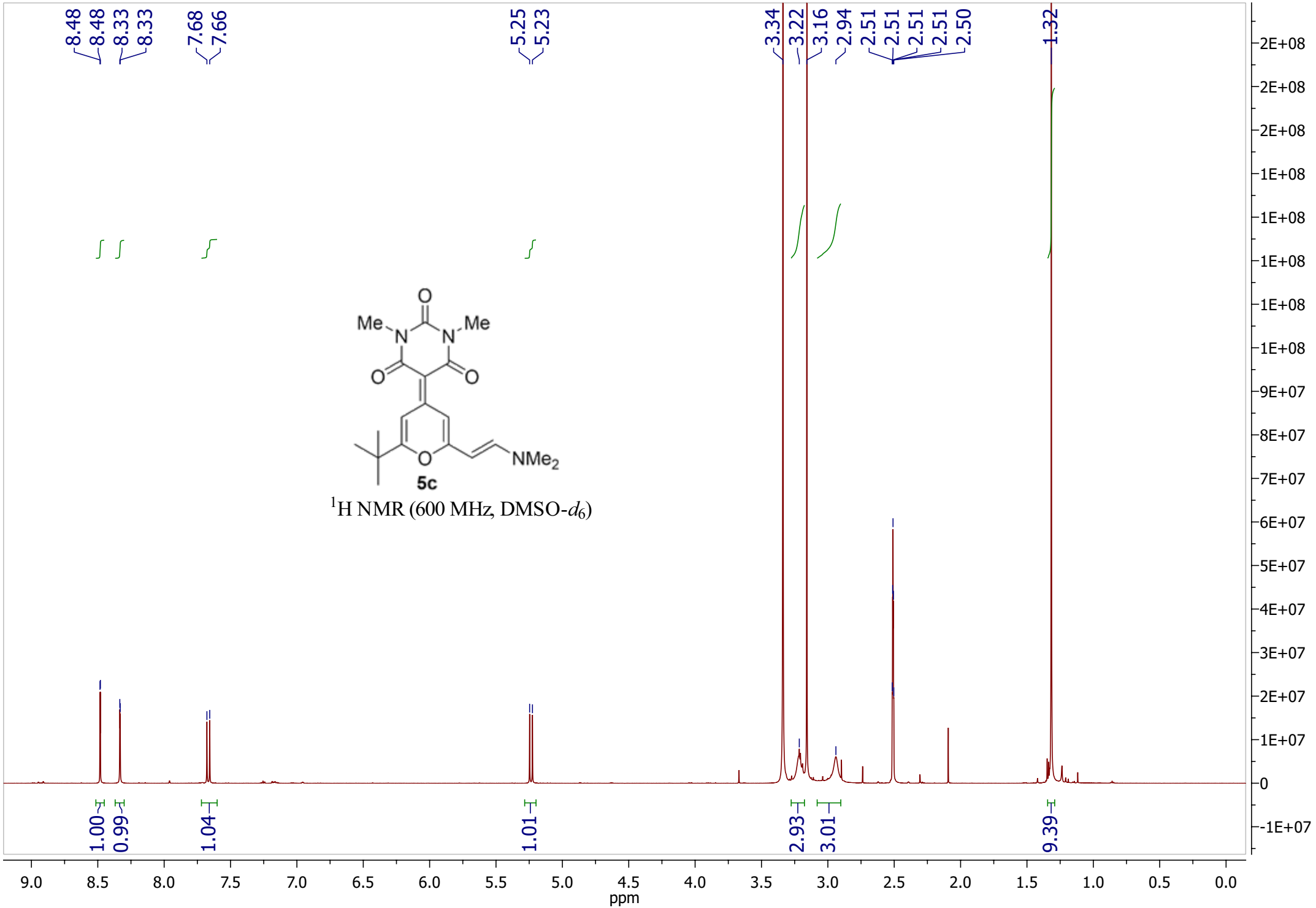


^{1}H NMR (500 MHz, DMSO-d_6)

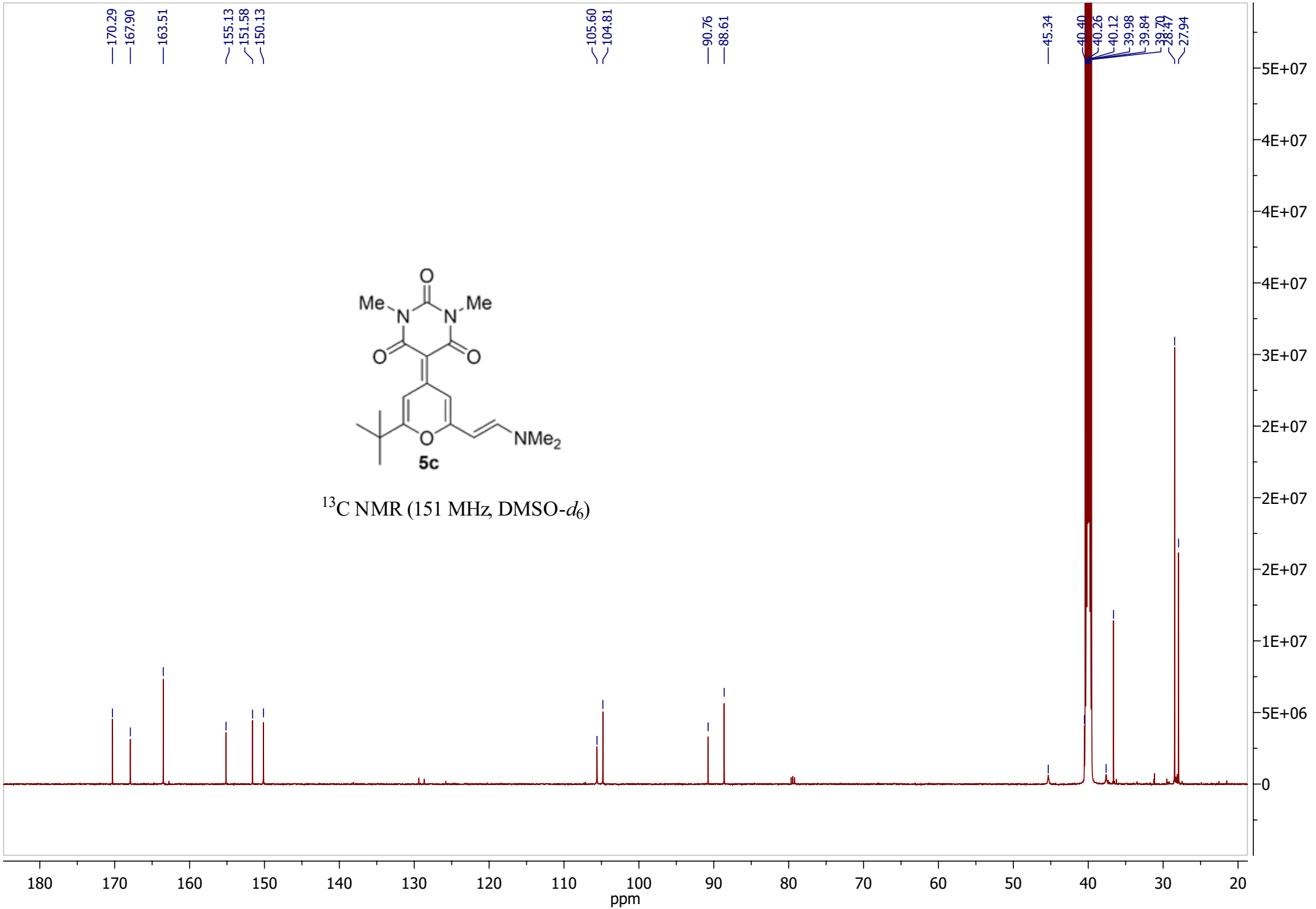


5b

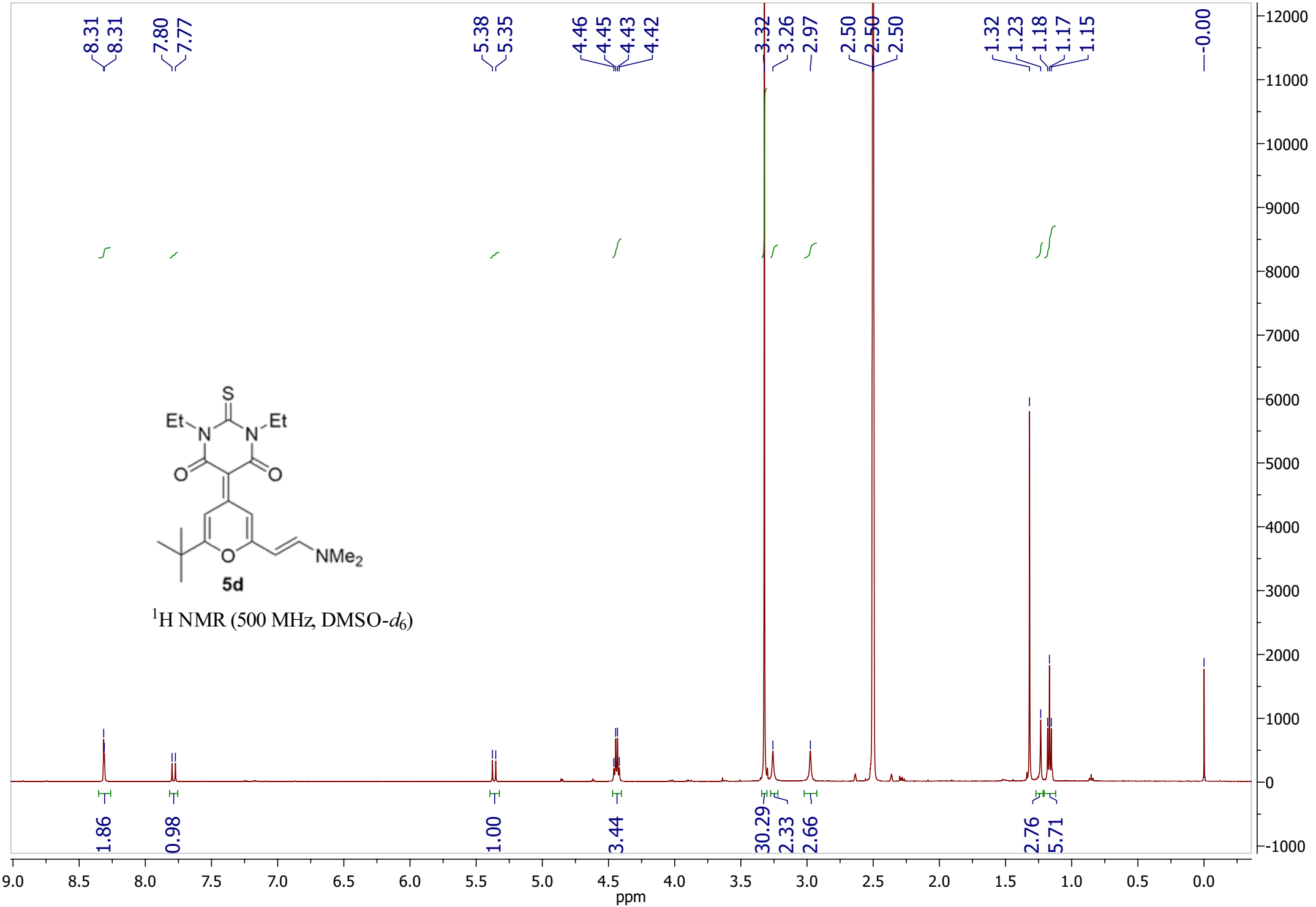
^{13}C NMR (101 MHz, DMSO-d_6)



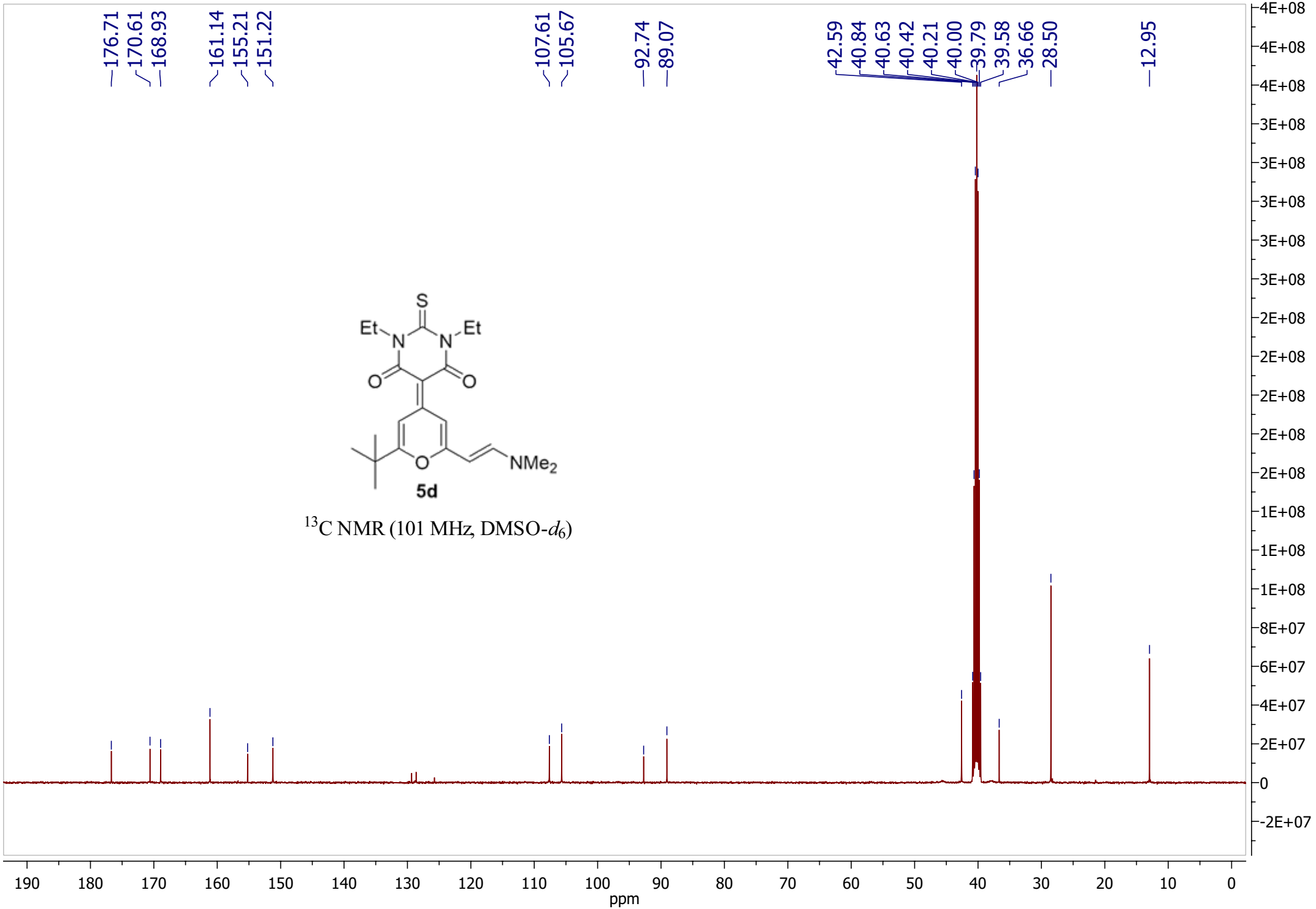
^{1}H NMR (600 MHz, DMSO-d_6)



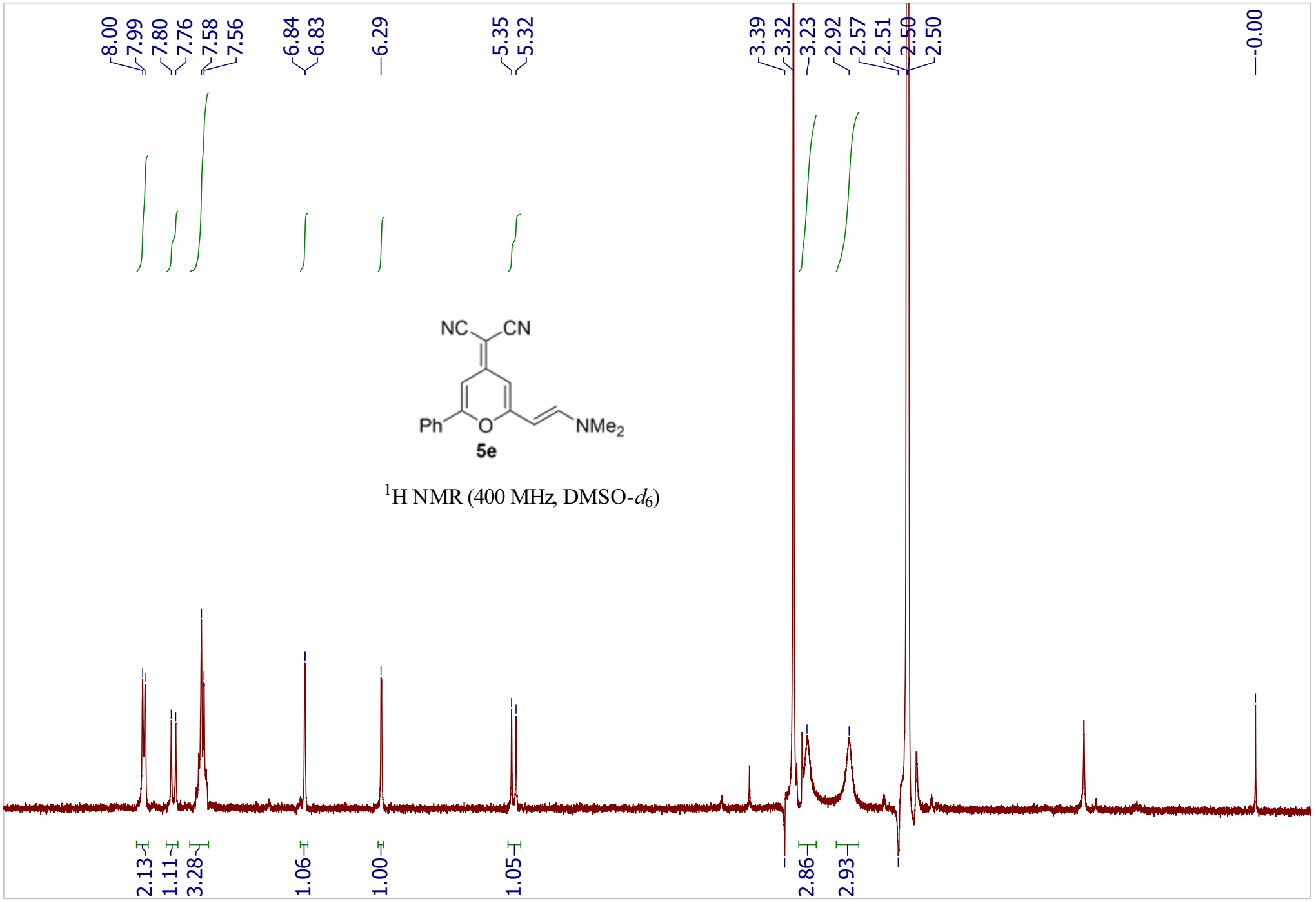
^{13}C NMR (151 MHz, DMSO-d_6)



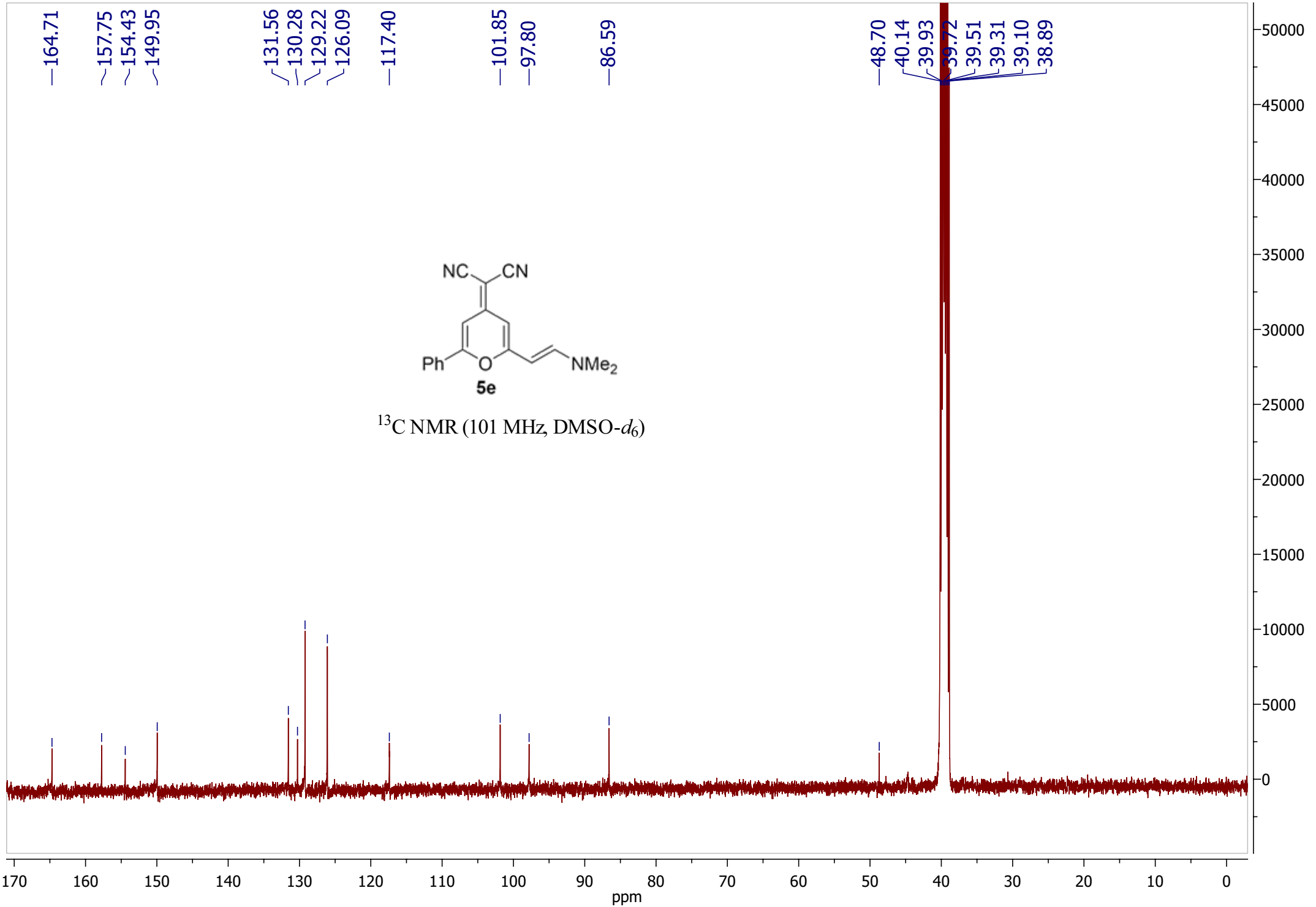
^{1}H NMR (500 MHz, DMSO-d_6)



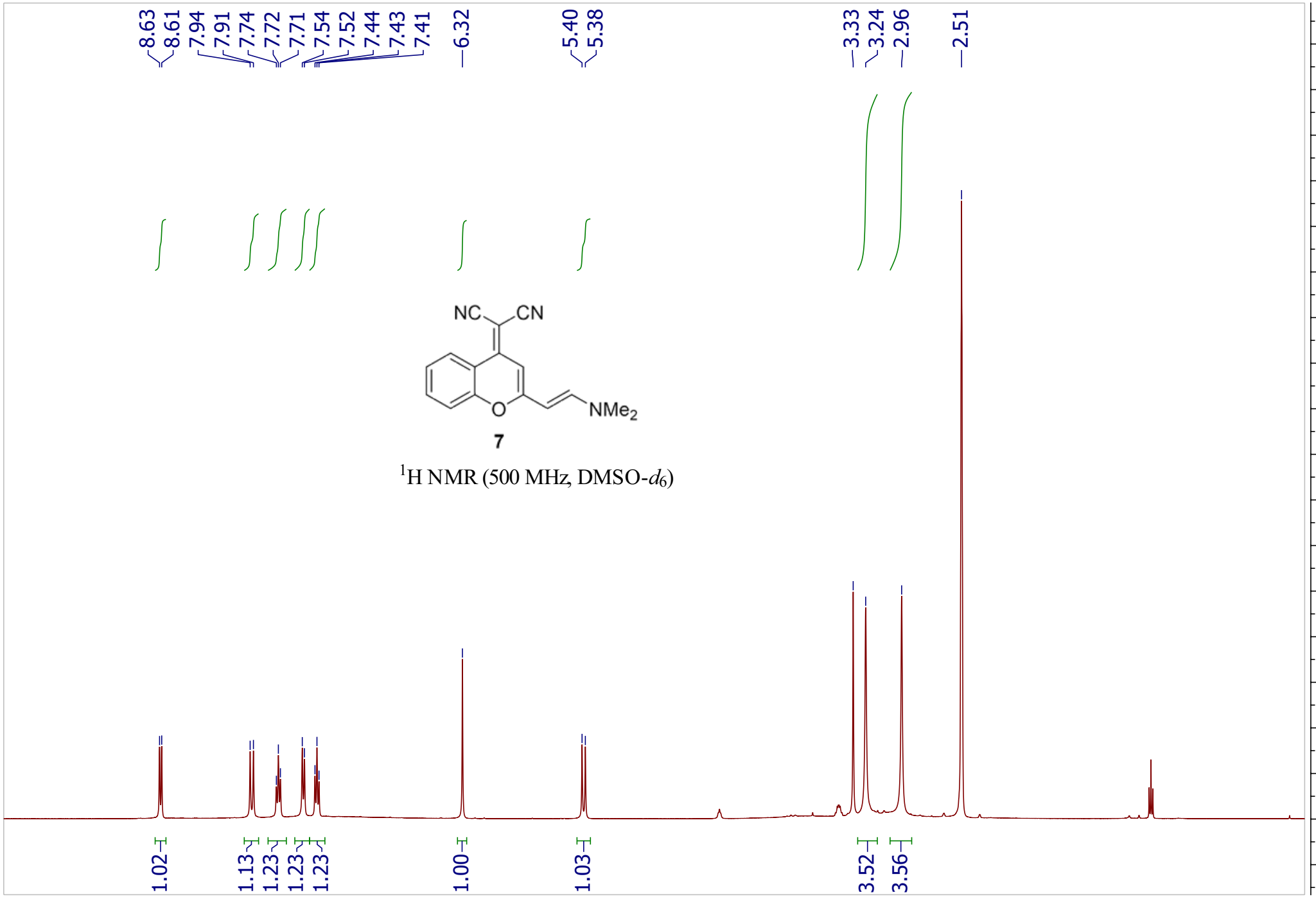
^{13}C NMR (101 MHz, DMSO-d_6)



^{1}H NMR (400 MHz, DMSO-d_6)

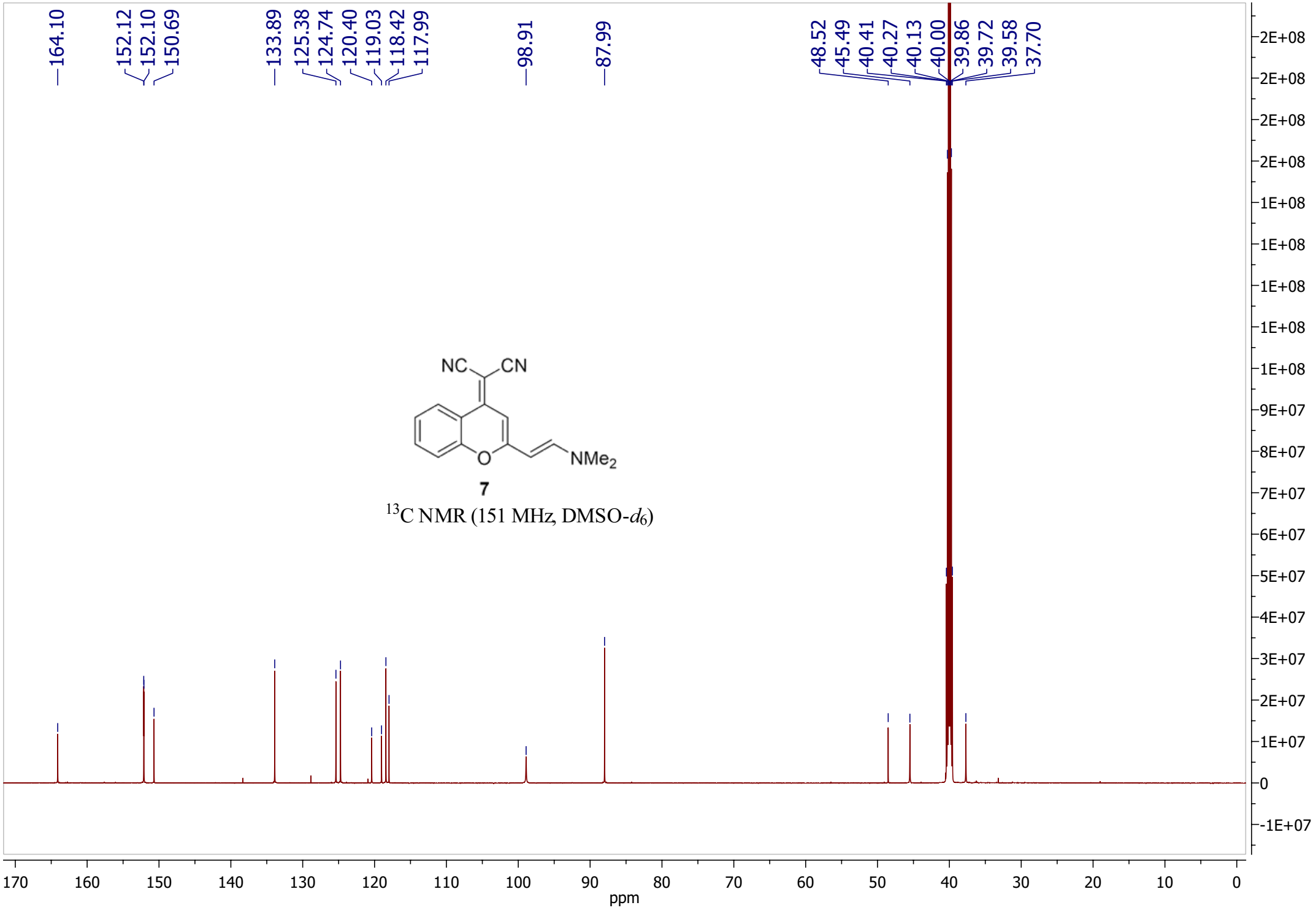


^{13}C NMR (101 MHz, DMSO-d_6)



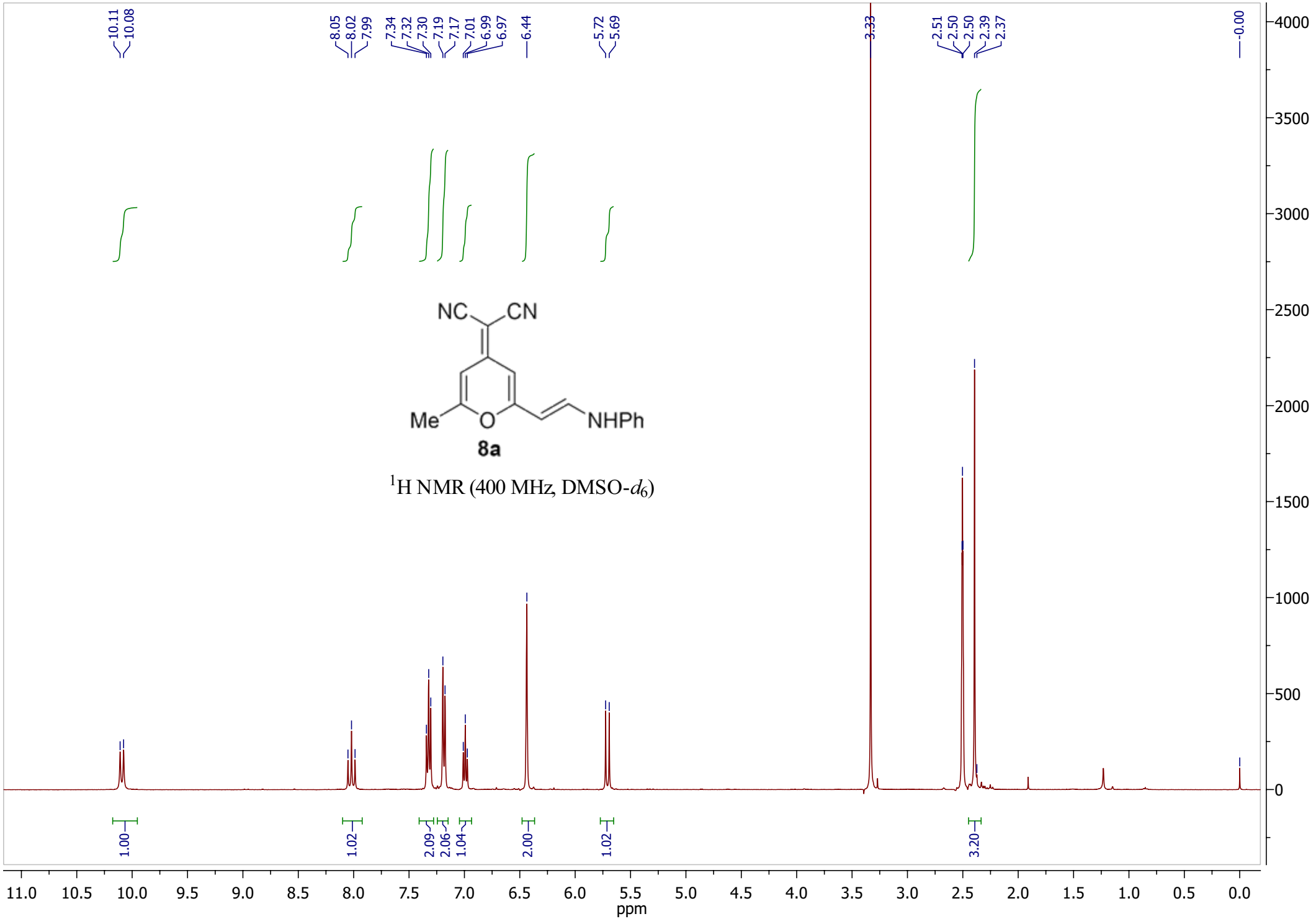
7

^{1}H NMR (500 MHz, DMSO-d_6)

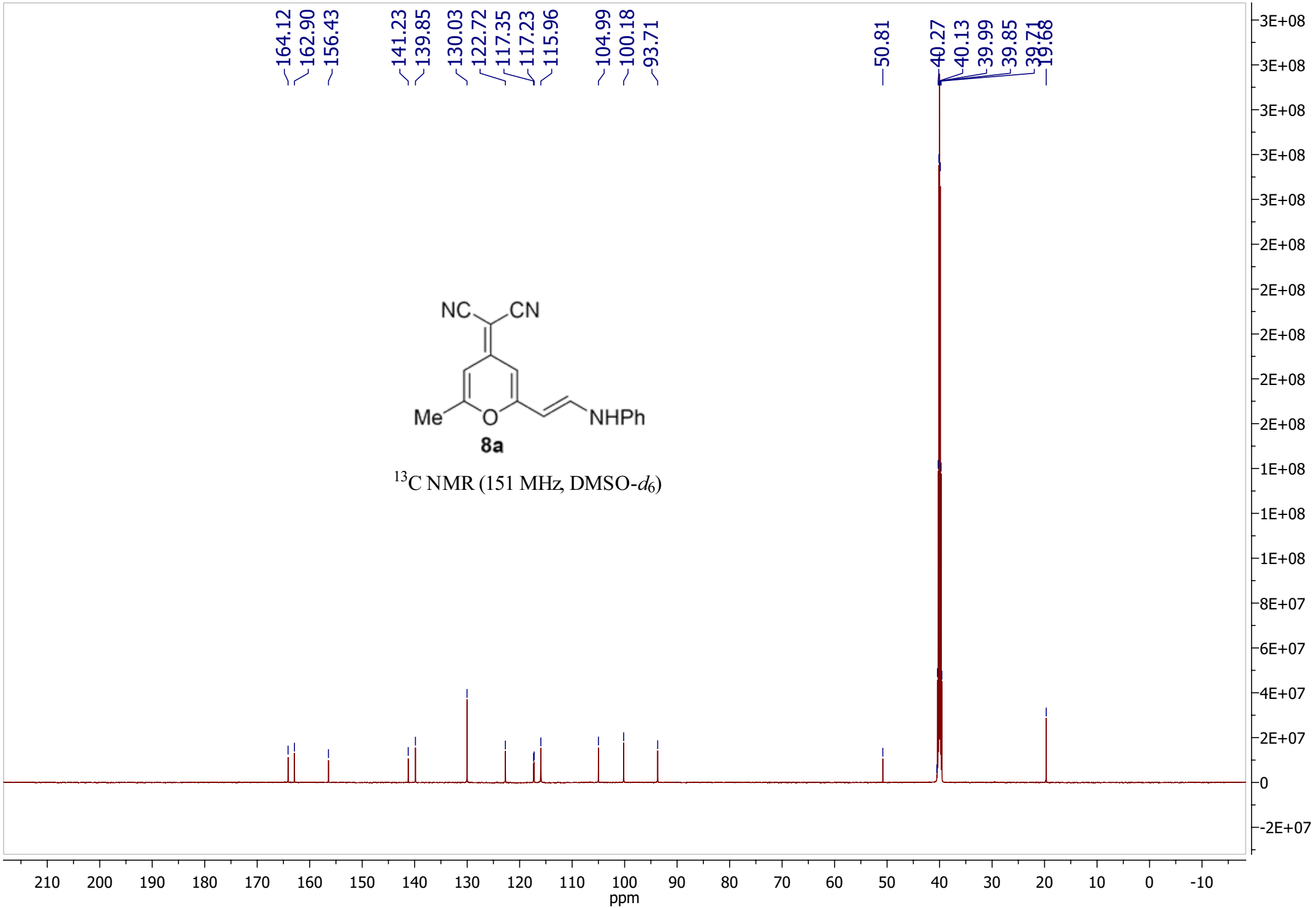


7

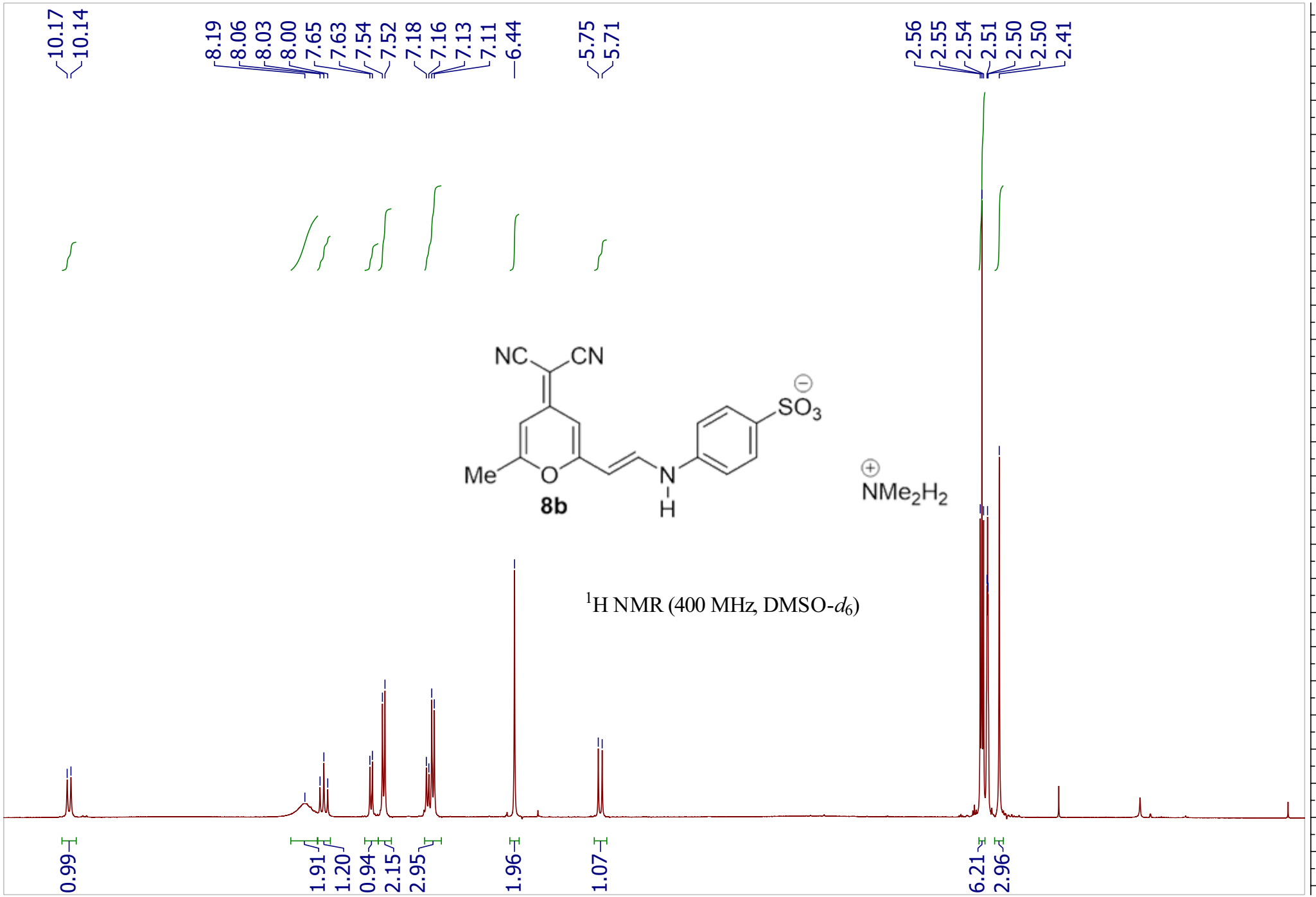
^{13}C NMR (151 MHz, DMSO-d_6)



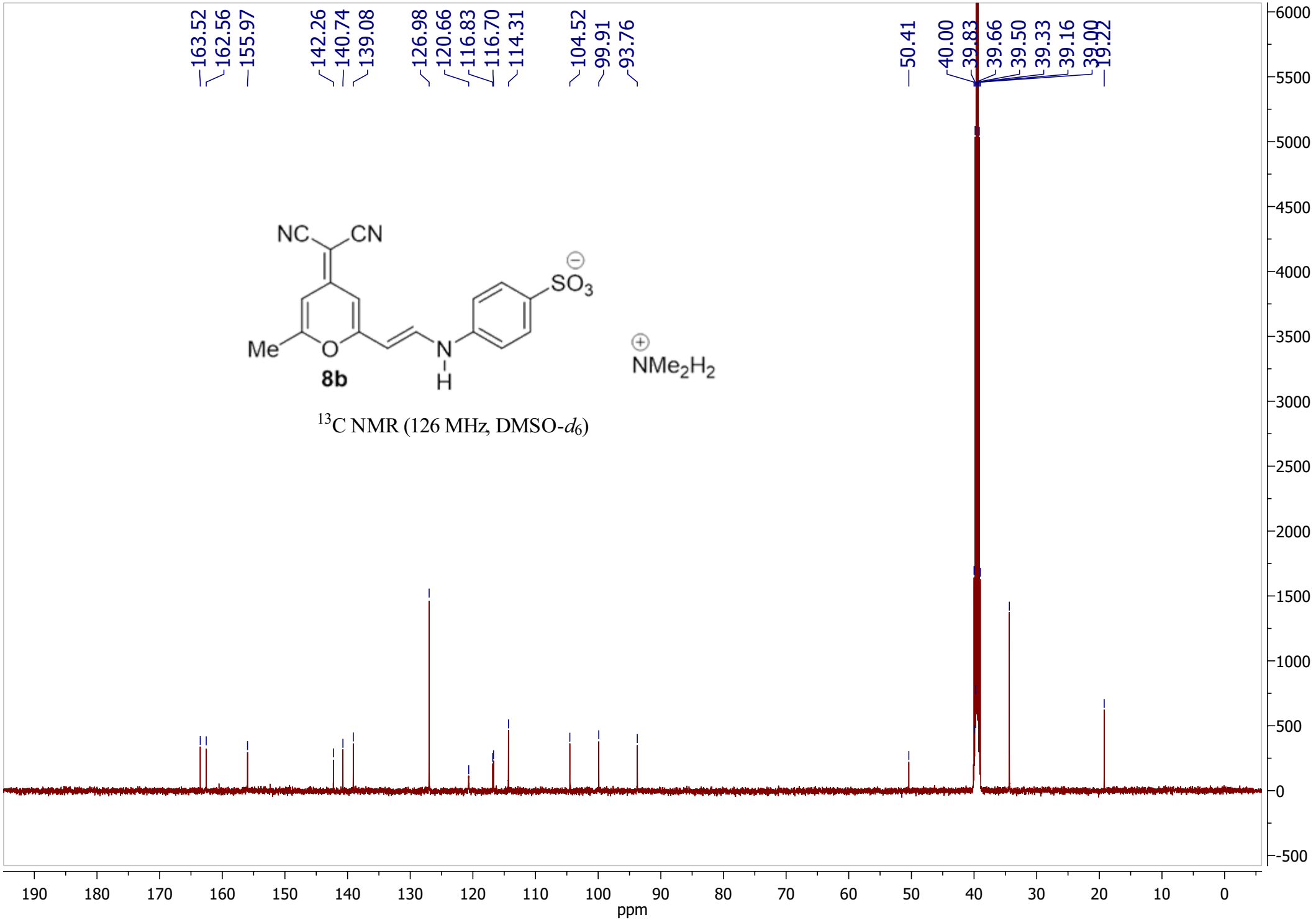
^{1}H NMR (400 MHz, DMSO-d_6)



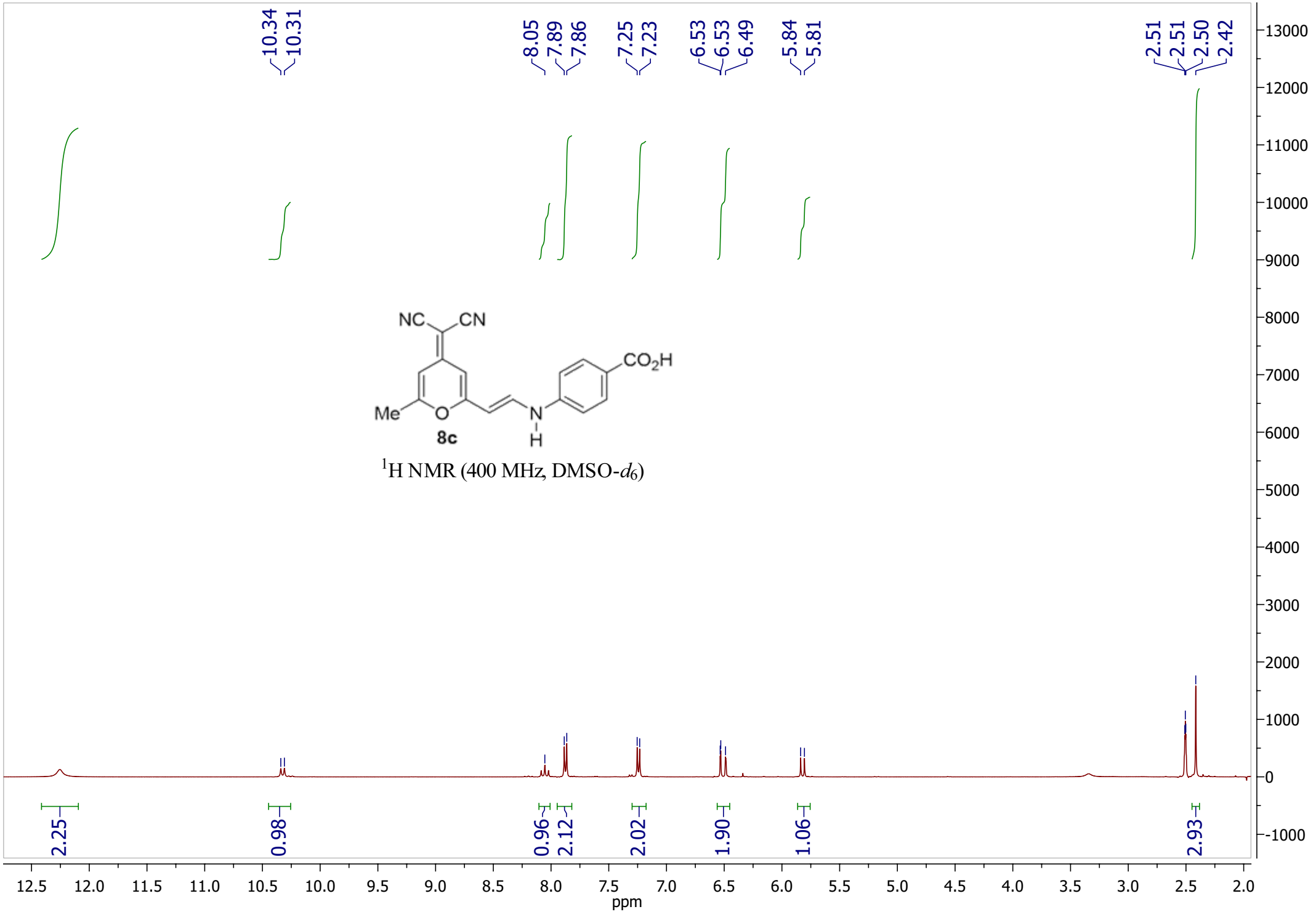
^{13}C NMR (151 MHz, DMSO-d_6)



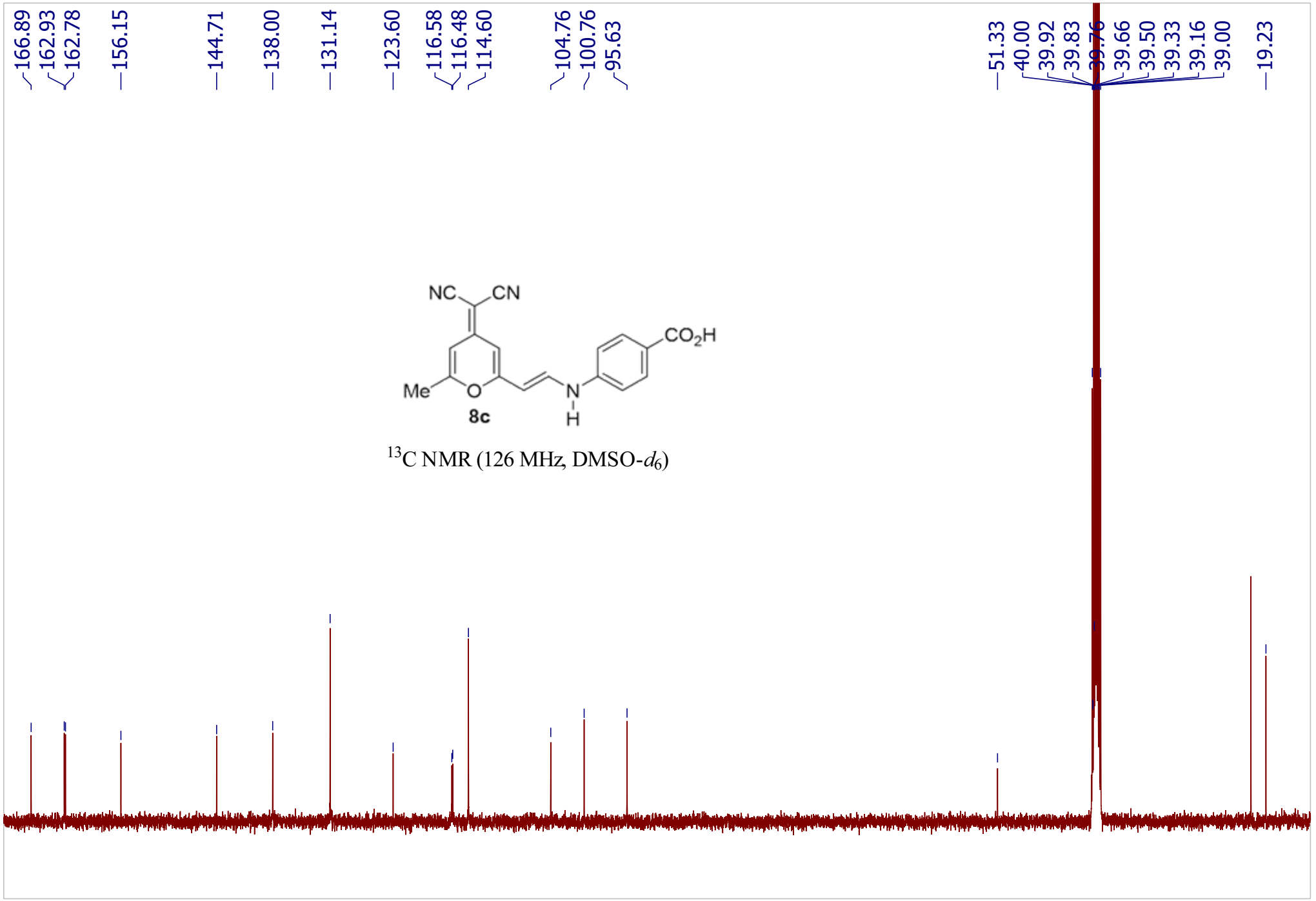
^{1}H NMR (400 MHz, DMSO-d_6)



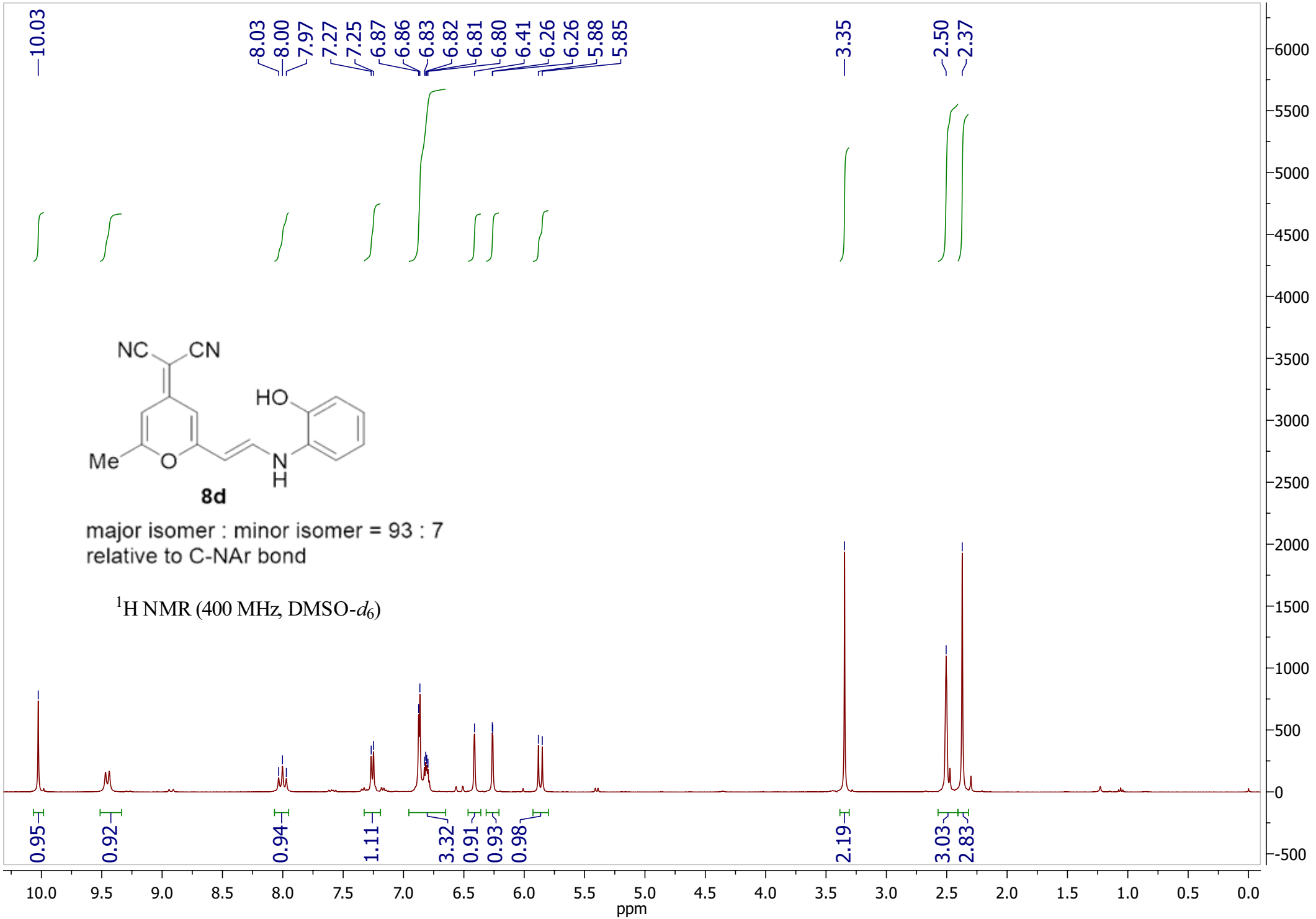
^{13}C NMR (126 MHz, DMSO-d_6)

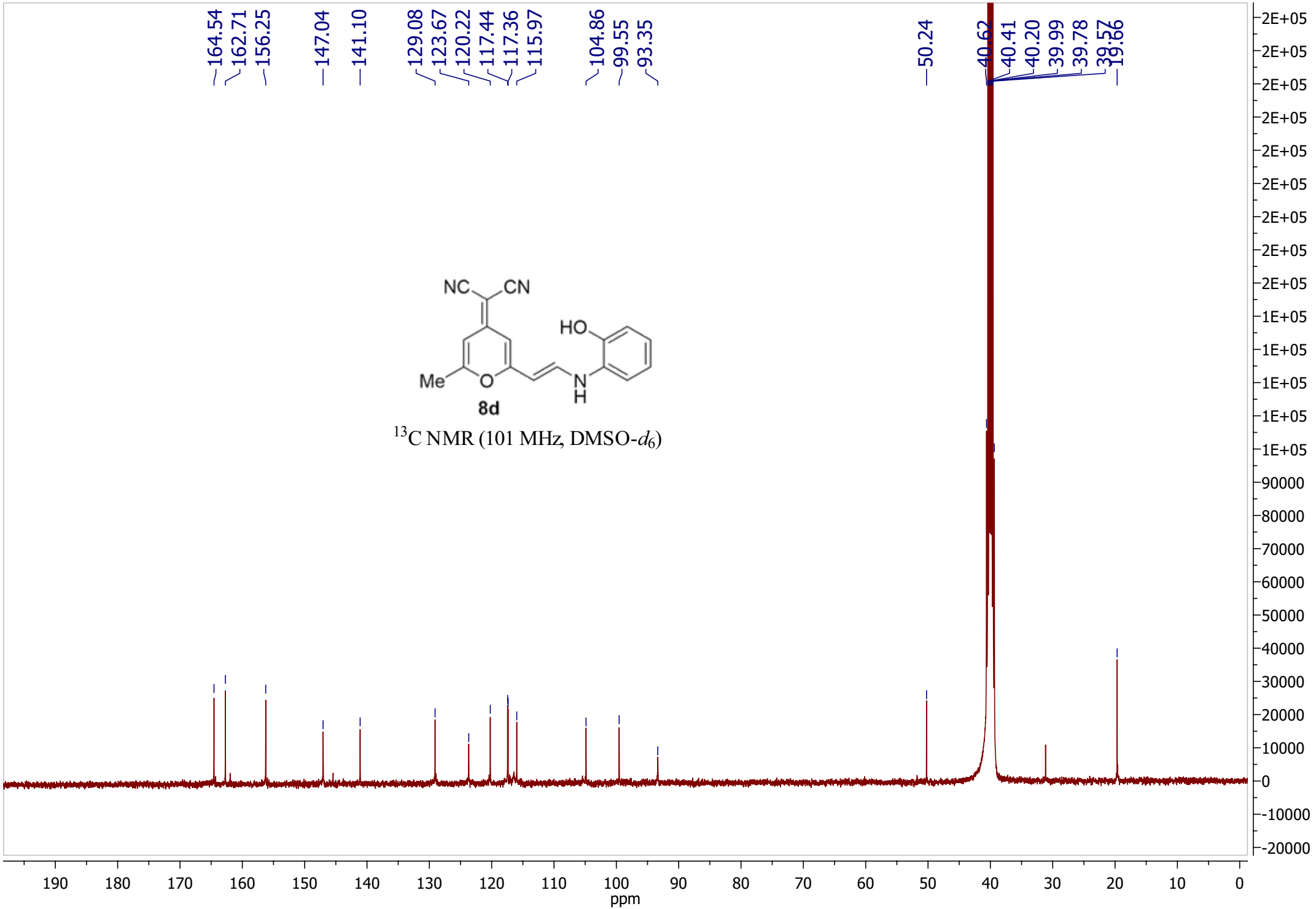


^{1}H NMR (400 MHz, DMSO-d_6)

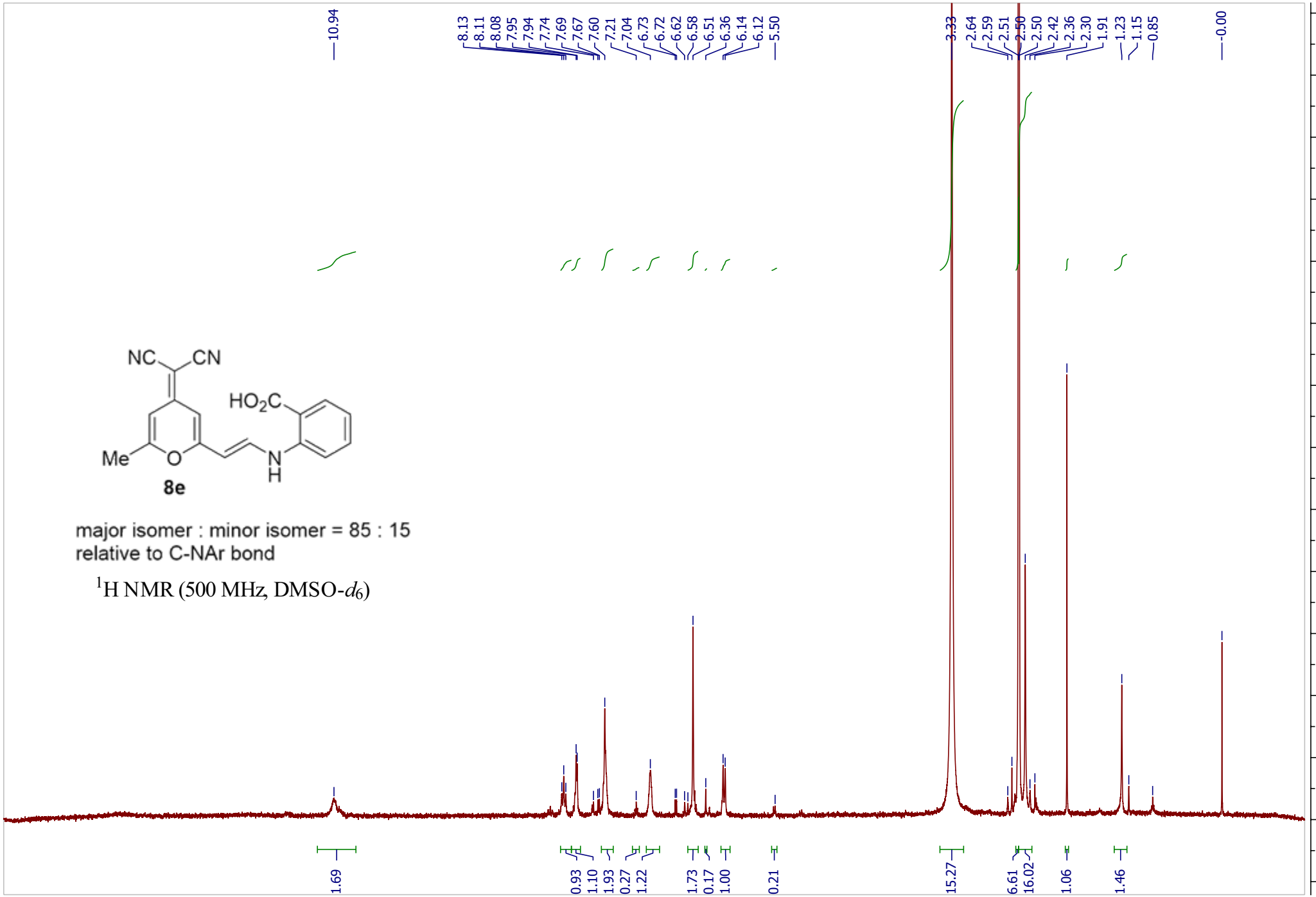


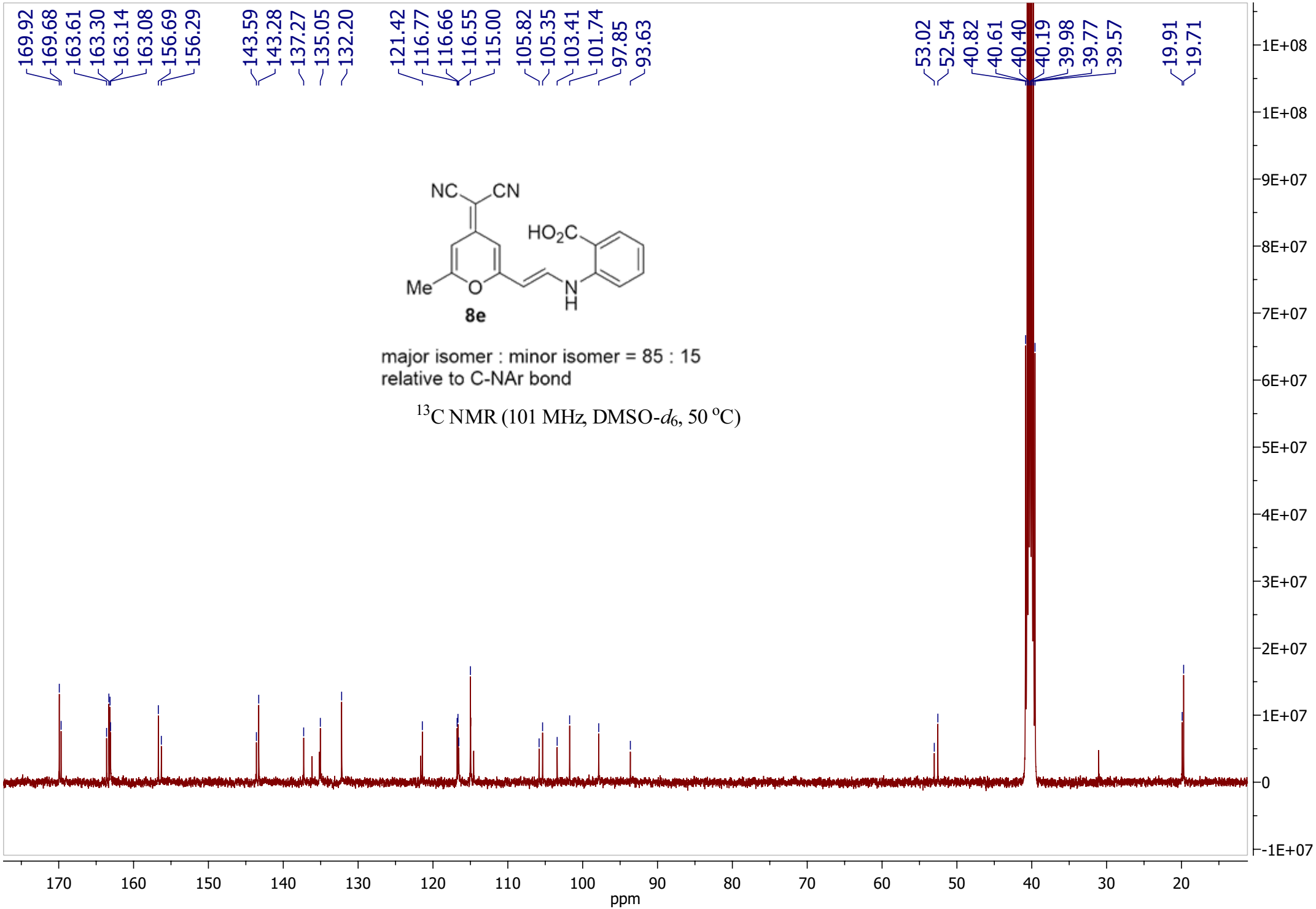
^{13}C NMR (126 MHz, DMSO-d_6)

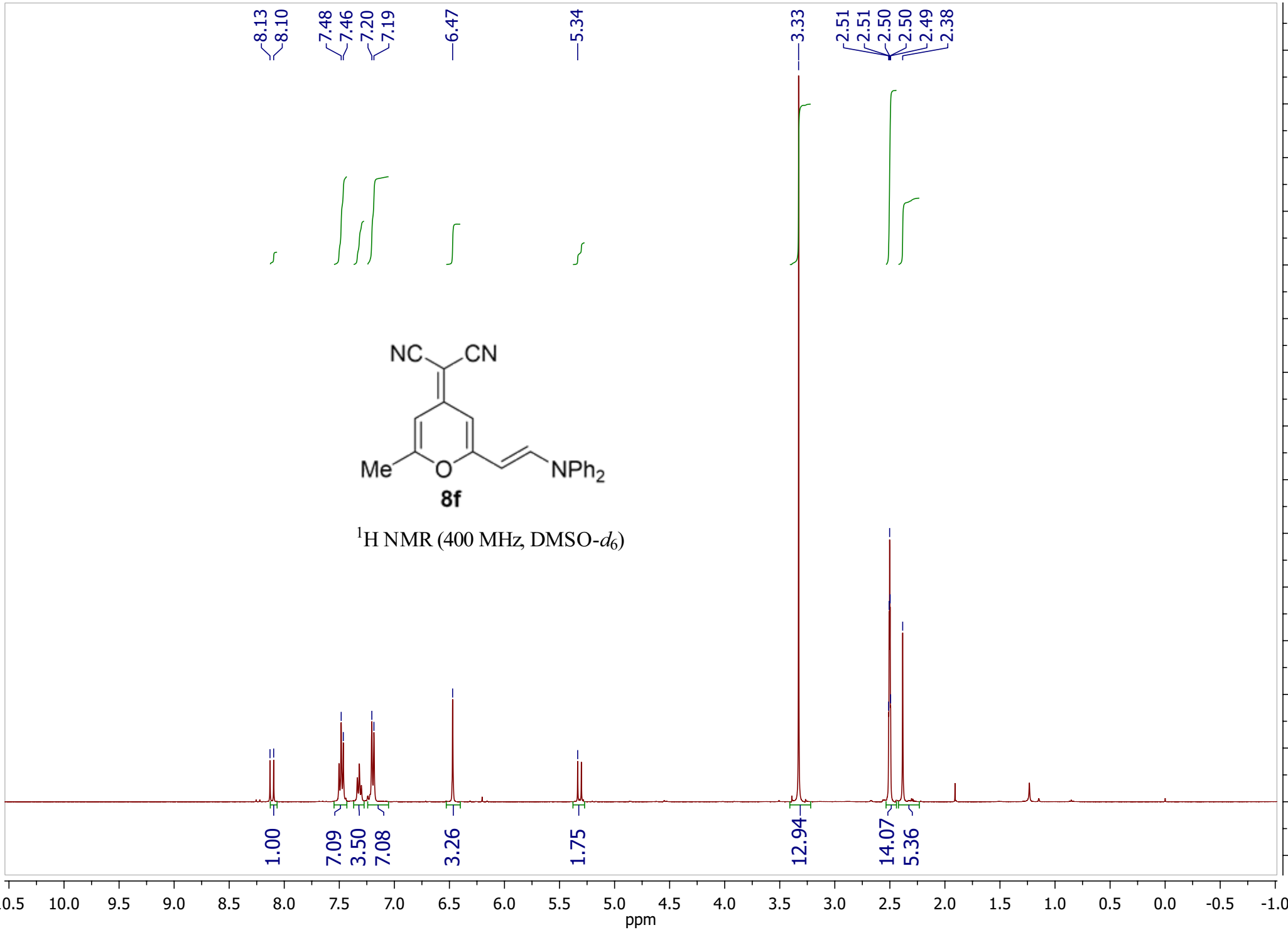

10.03
8.03
8.00
7.97
7.27
7.25
6.87
6.86
6.83
6.82
6.81
6.80
6.41
6.26
6.26
5.88
5.85
3.35
2.50
2.37
NC
CN
HO
Me
O
N
H
8d
major isomer : minor isomer = 93 : 7
relative to C-NAr bond
^{1}H NMR (400 MHz, DMSO-d_6)
0.95
0.92
0.94
1.11
3.32
0.91
0.93
0.98
2.19
3.03
2.83
ppm



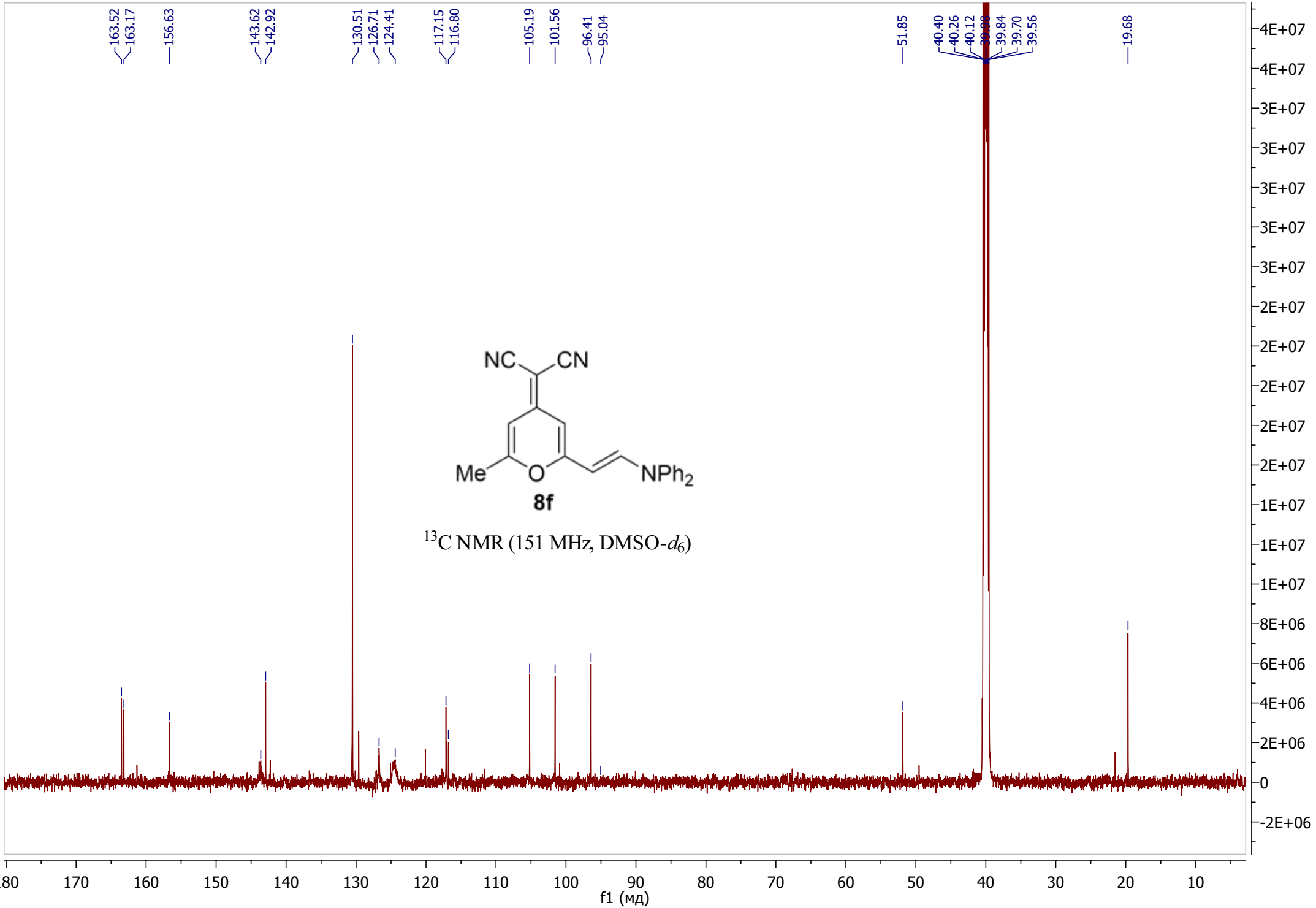
^{13}C NMR (101 MHz, DMSO-d_6)


10.94
8.13
8.11
8.08
7.95
7.94
7.74
7.69
7.67
7.60
7.21
7.04
6.73
6.72
6.62
6.58
6.51
6.36
6.14
6.12
5.50
3.33
2.64
2.59
2.51
2.50
2.50
2.42
2.36
2.30
1.91
1.23
1.15
0.85
-0.00
NC
CN
HO2C
Me
O
N
H
8e
major isomer : minor isomer = 85 : 15
relative to C-NAr bond
1H NMR (500 MHz, DMSO-d6)
1.69
0.93
1.10
1.93
0.27
1.22
1.73
0.17
1.00
0.21
15.27
6.61
16.02
1.06
1.46
ppm

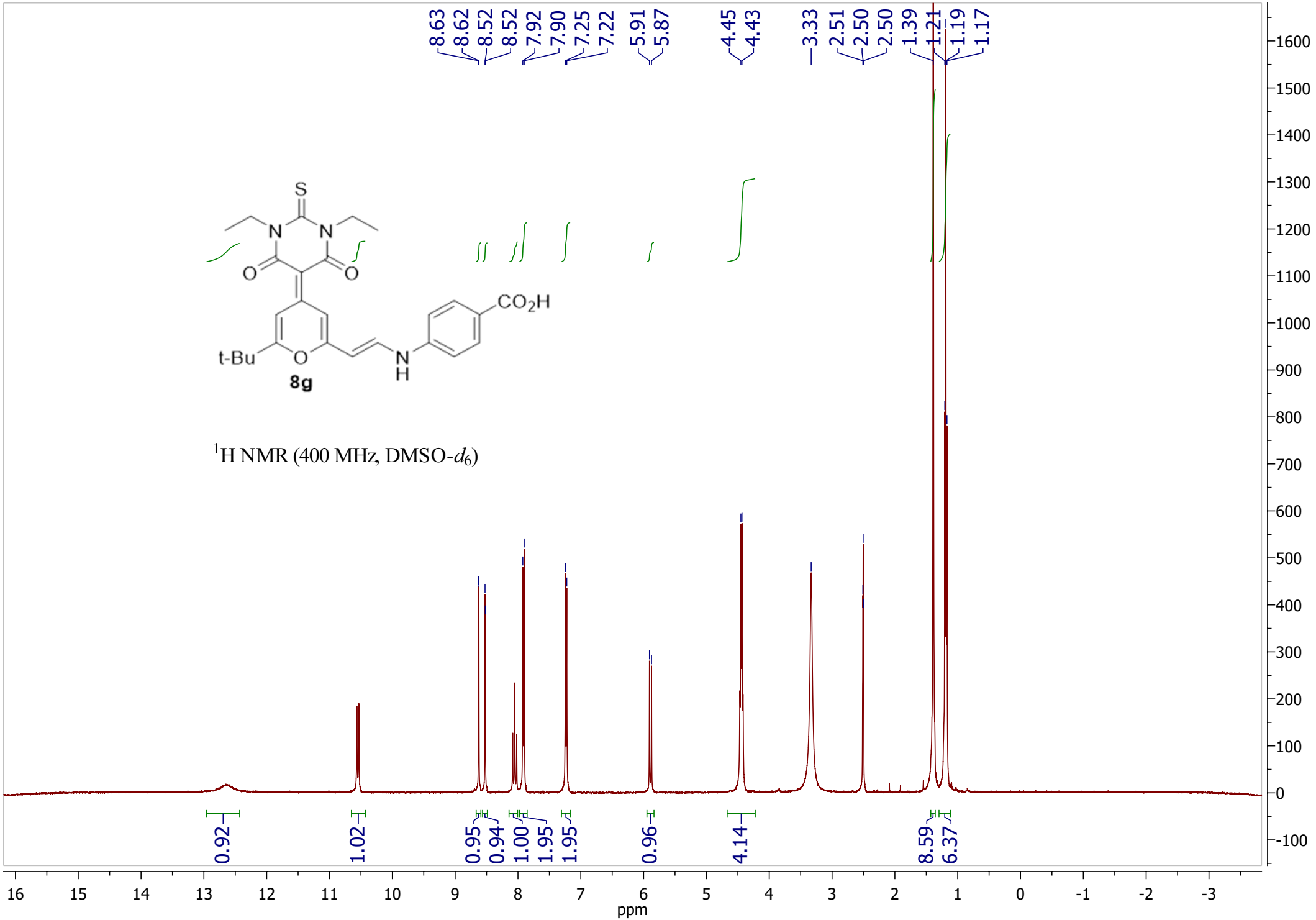

169.92
169.68
163.61
163.30
163.14
163.08
156.69
156.29
143.59
143.28
137.27
135.05
132.20
121.42
116.77
116.66
116.55
115.00
105.82
105.35
103.41
101.74
97.85
93.63
53.02
52.54
40.82
40.61
40.40
40.19
39.98
39.77
39.57
19.91
19.71
NC
CN
HO2C
Me
O
N
H
8e
major isomer : minor isomer = 85 : 15
relative to C-NAr bond
13C NMR (101 MHz, DMSO-d6, 50 °C)
1E+08
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
-1E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm



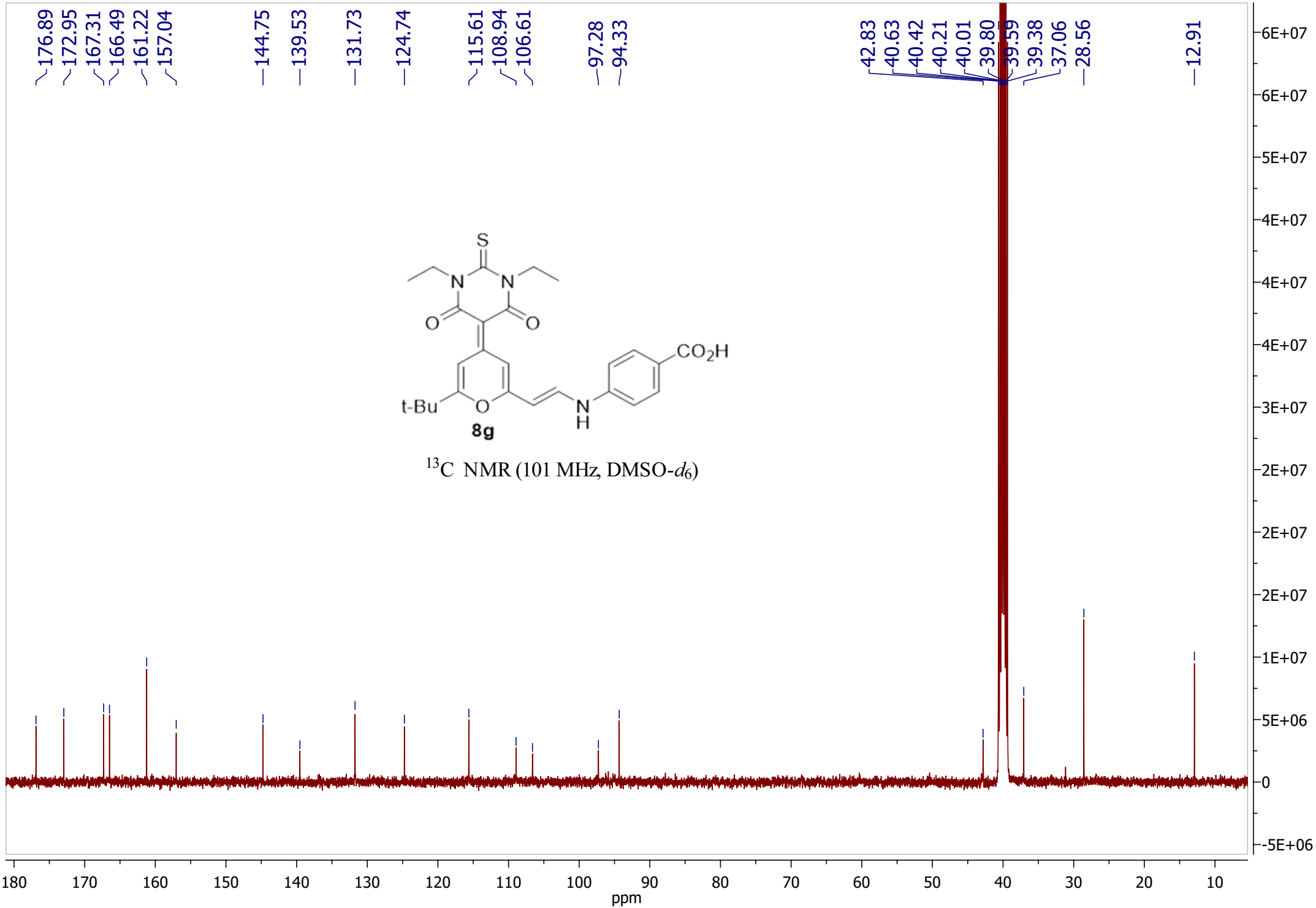
^{1}H NMR (400 MHz, DMSO-d_6)



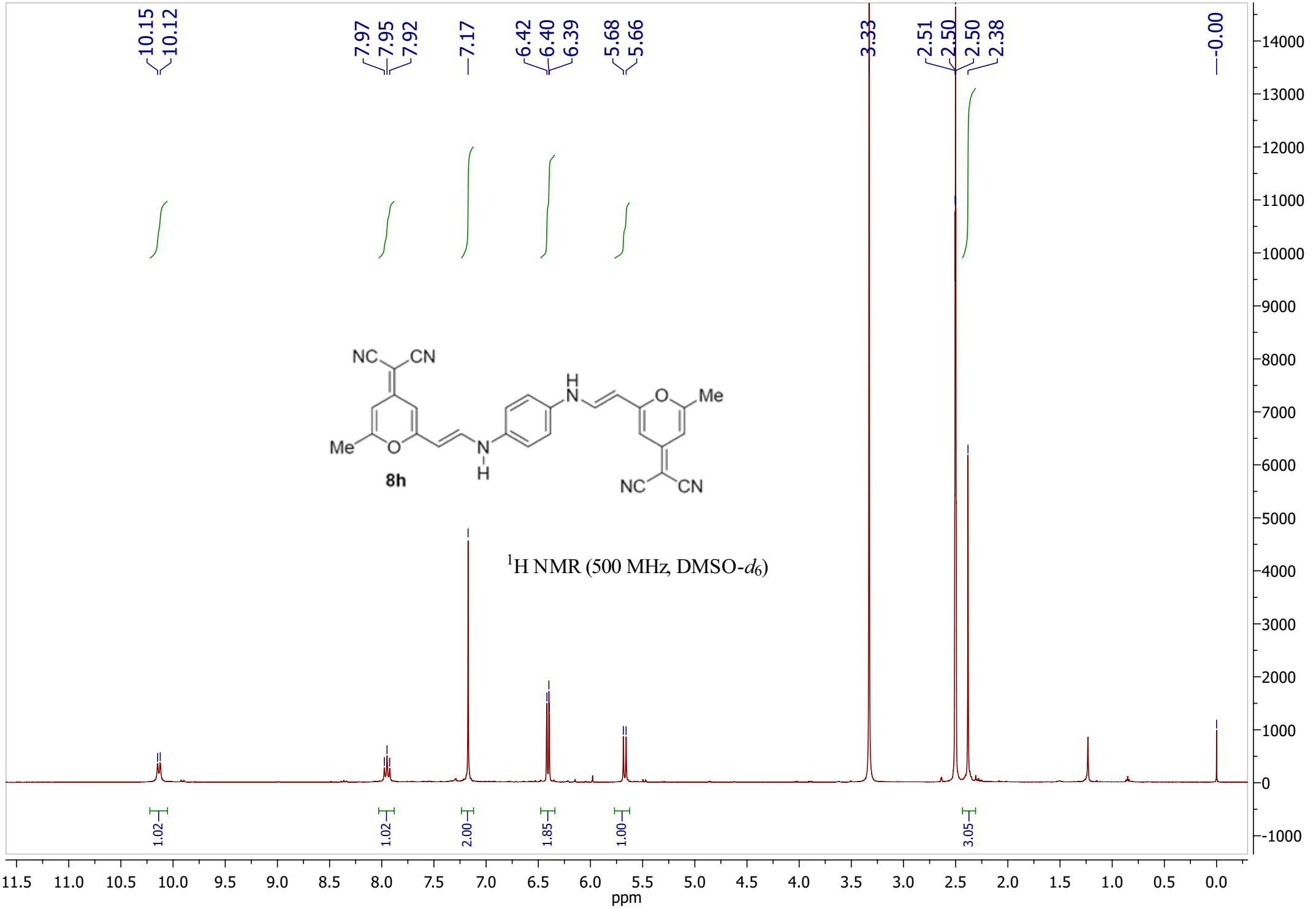
^{13}C NMR (151 MHz, DMSO-d_6)

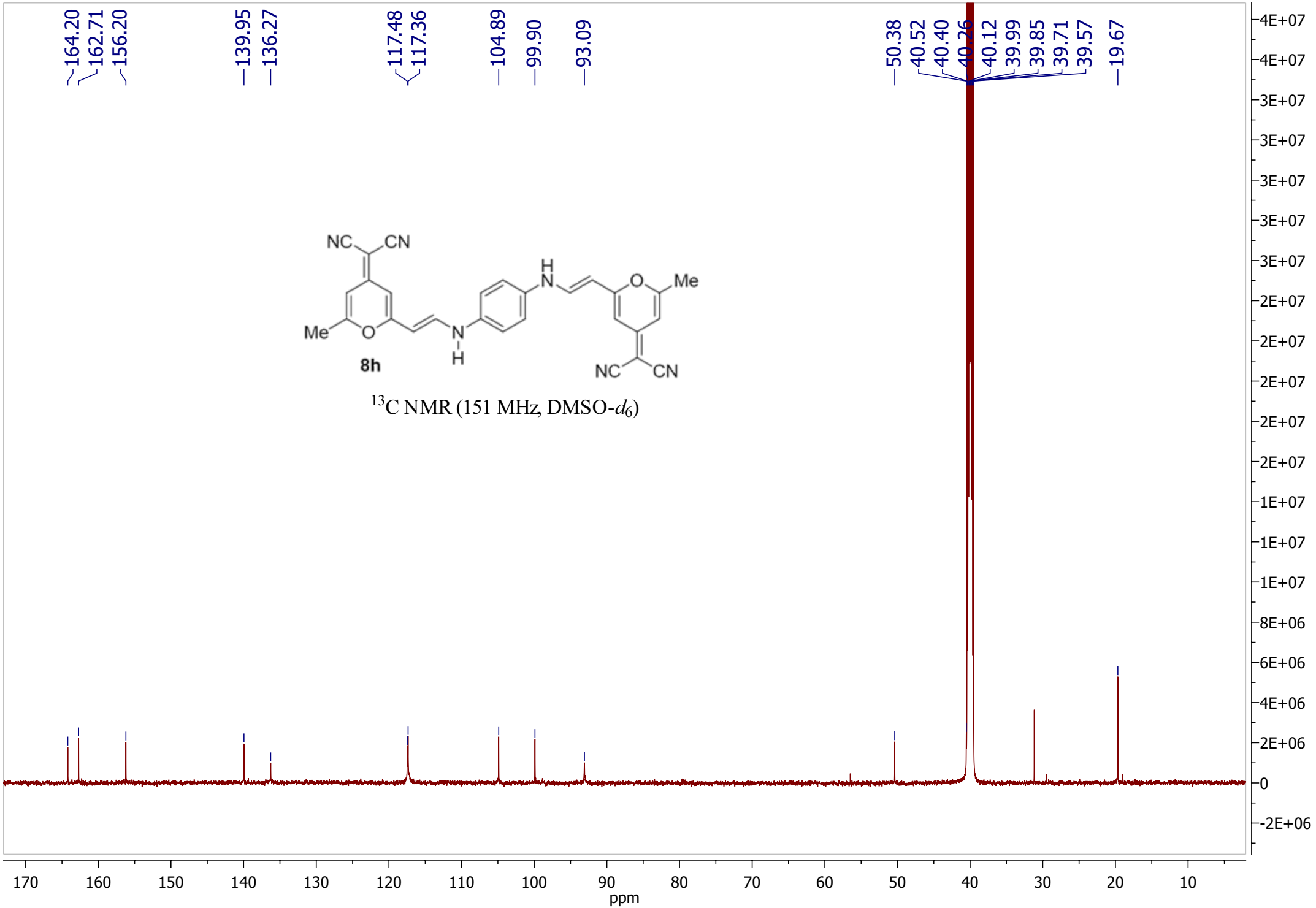


^{1}H NMR (400 MHz, DMSO-d_6)

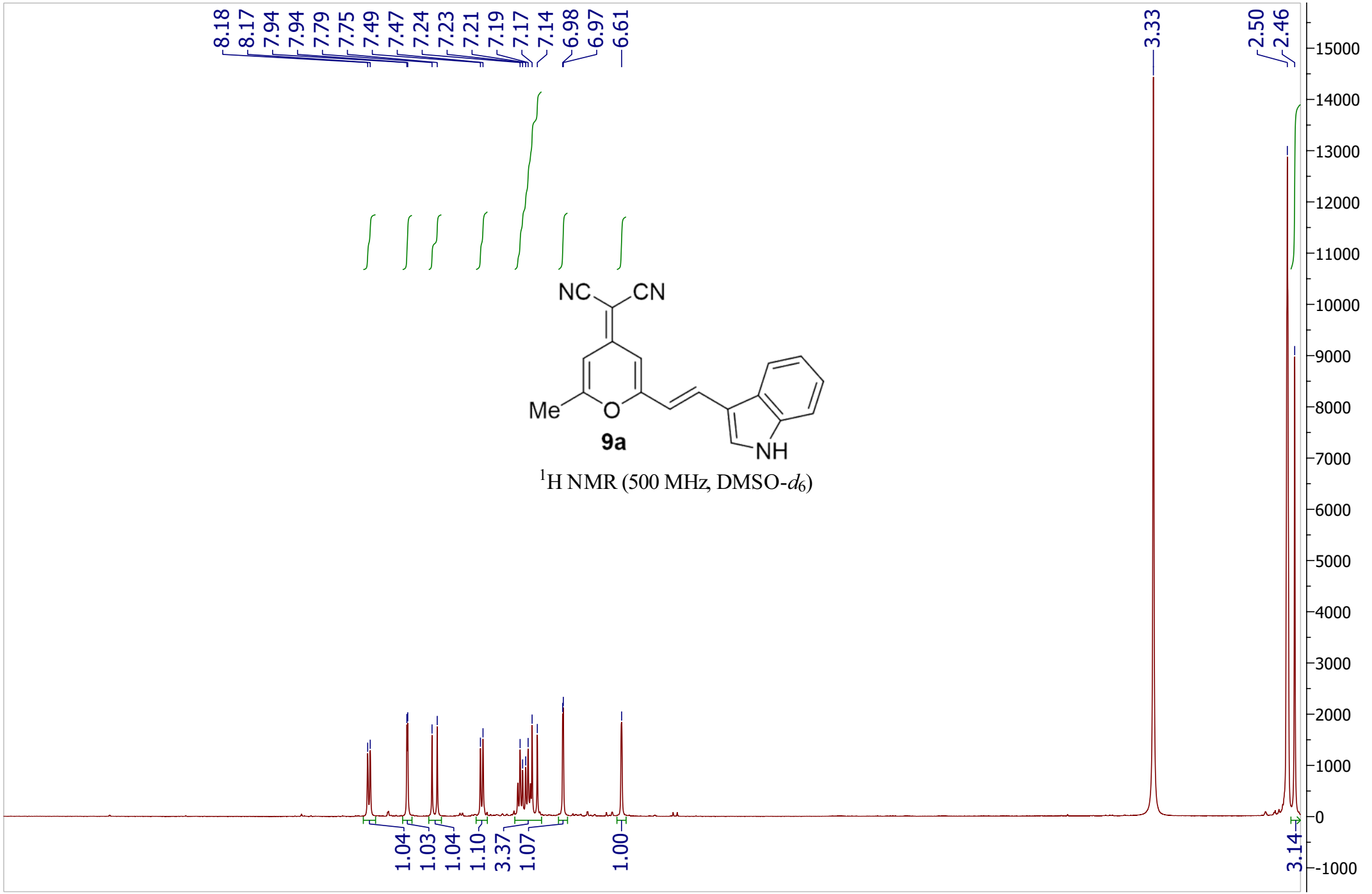


^{13}C NMR (101 MHz, DMSO-d_6)

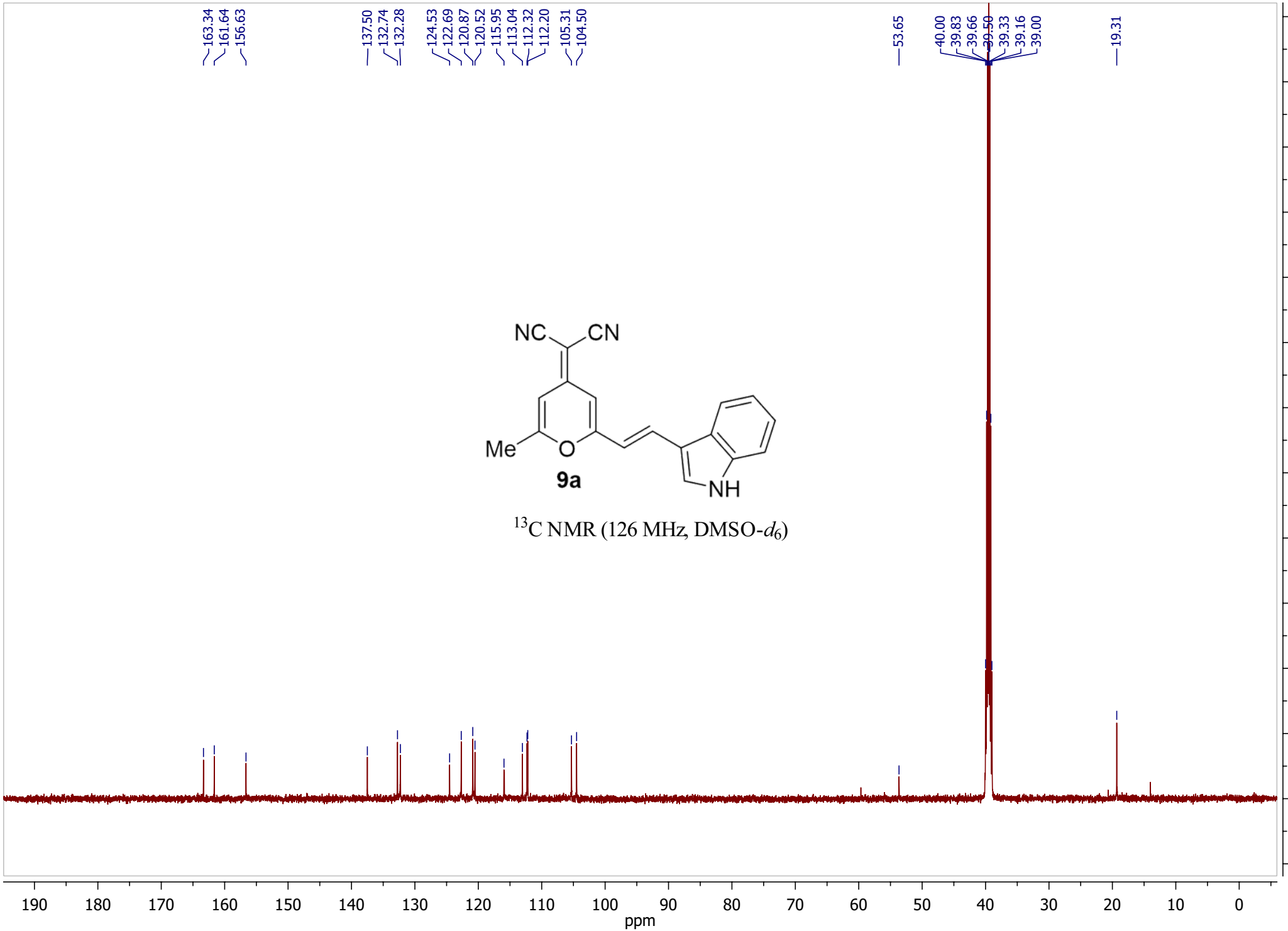

10.15
10.12
7.97
7.95
7.92
7.17
6.42
6.40
6.39
5.68
5.66
3.33
2.51
2.50
2.50
2.38
-0.00
NC
CN
Me
O
N
H
O
Me
NC
CN
8h
1H NMR (500 MHz, DMSO-d6)
1.02
1.02
2.00
1.85
1.00
3.05
ppm



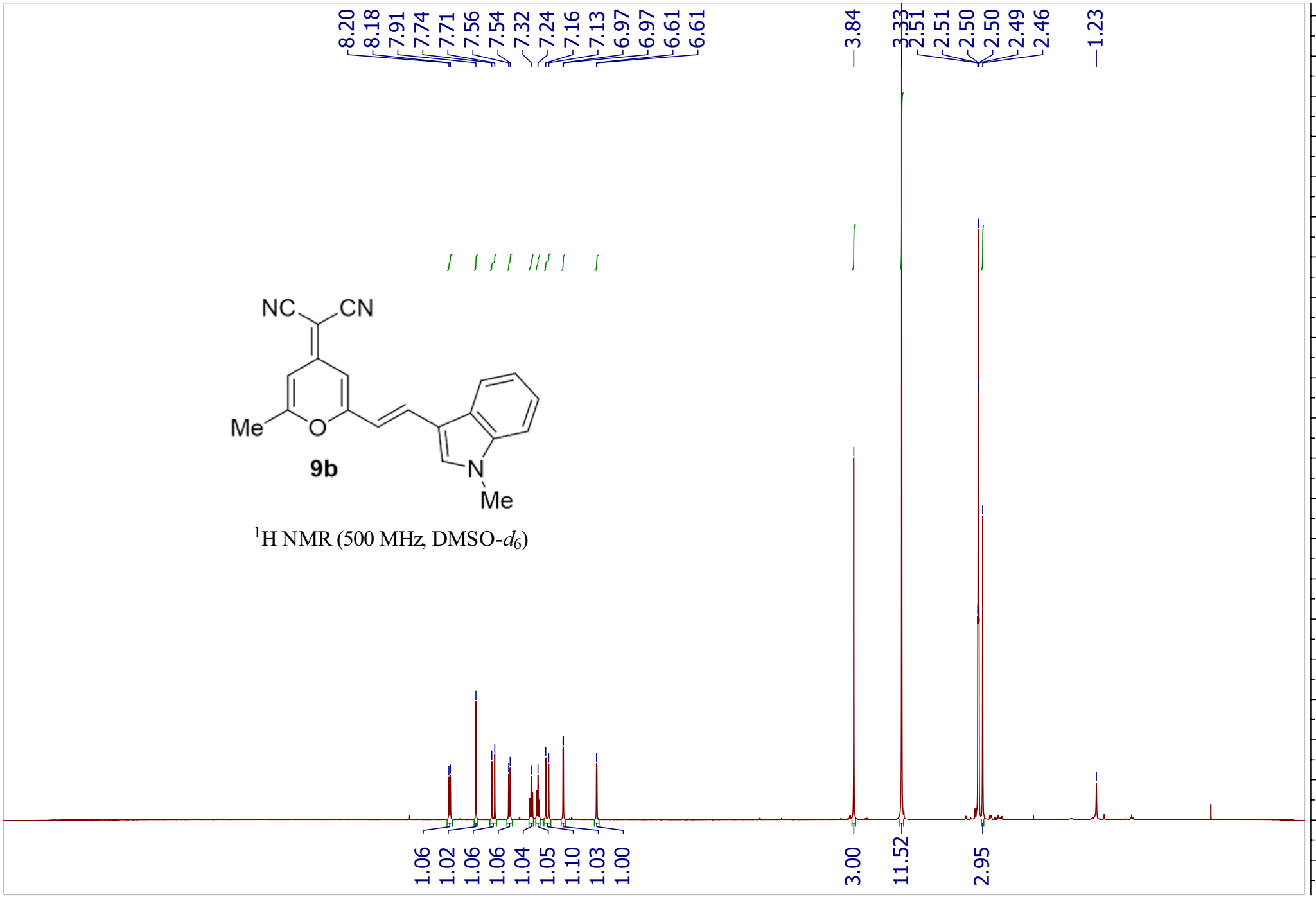
^{13}C NMR (151 MHz, DMSO-d_6)



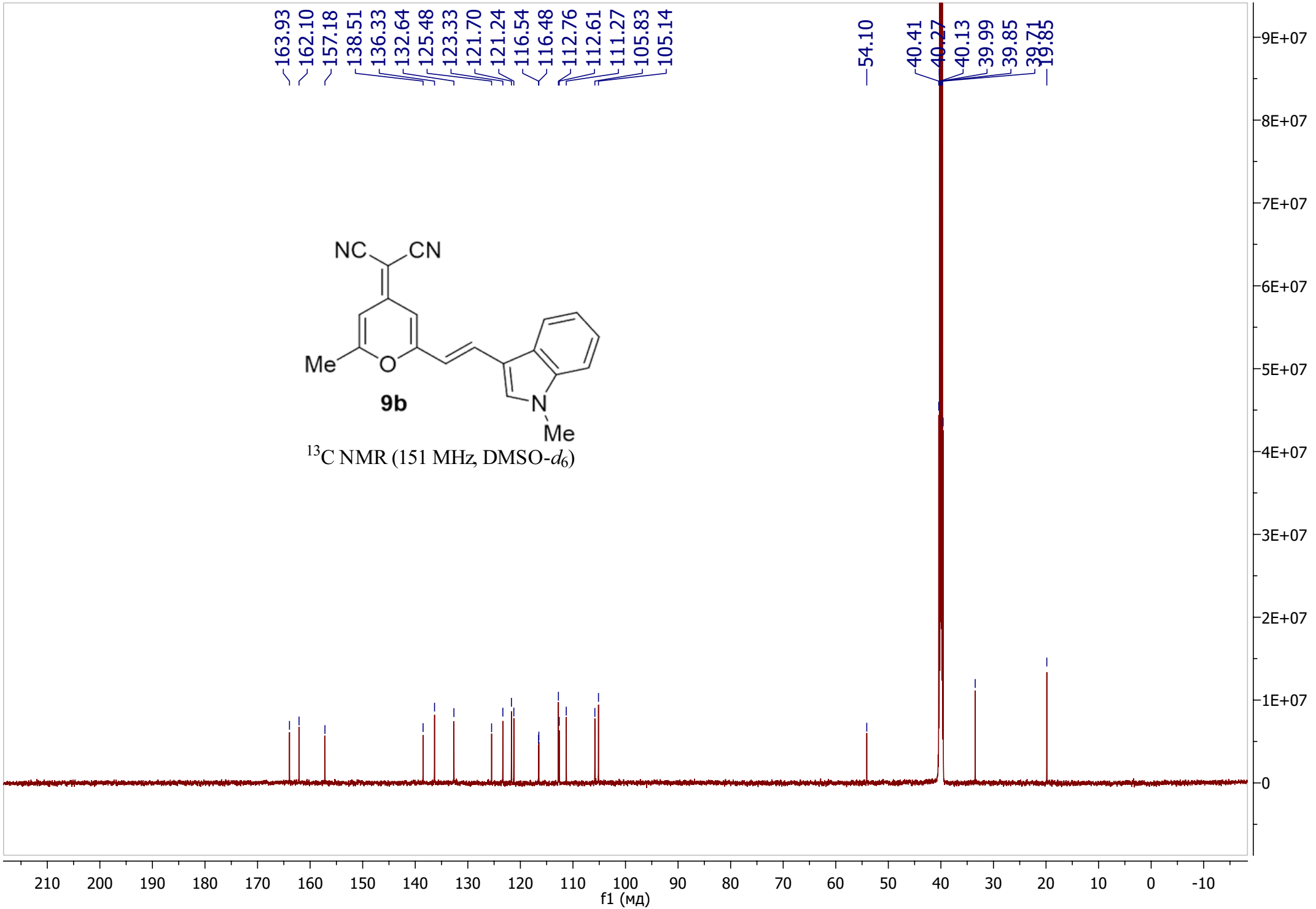
^{1}H NMR (500 MHz, DMSO-d_6)



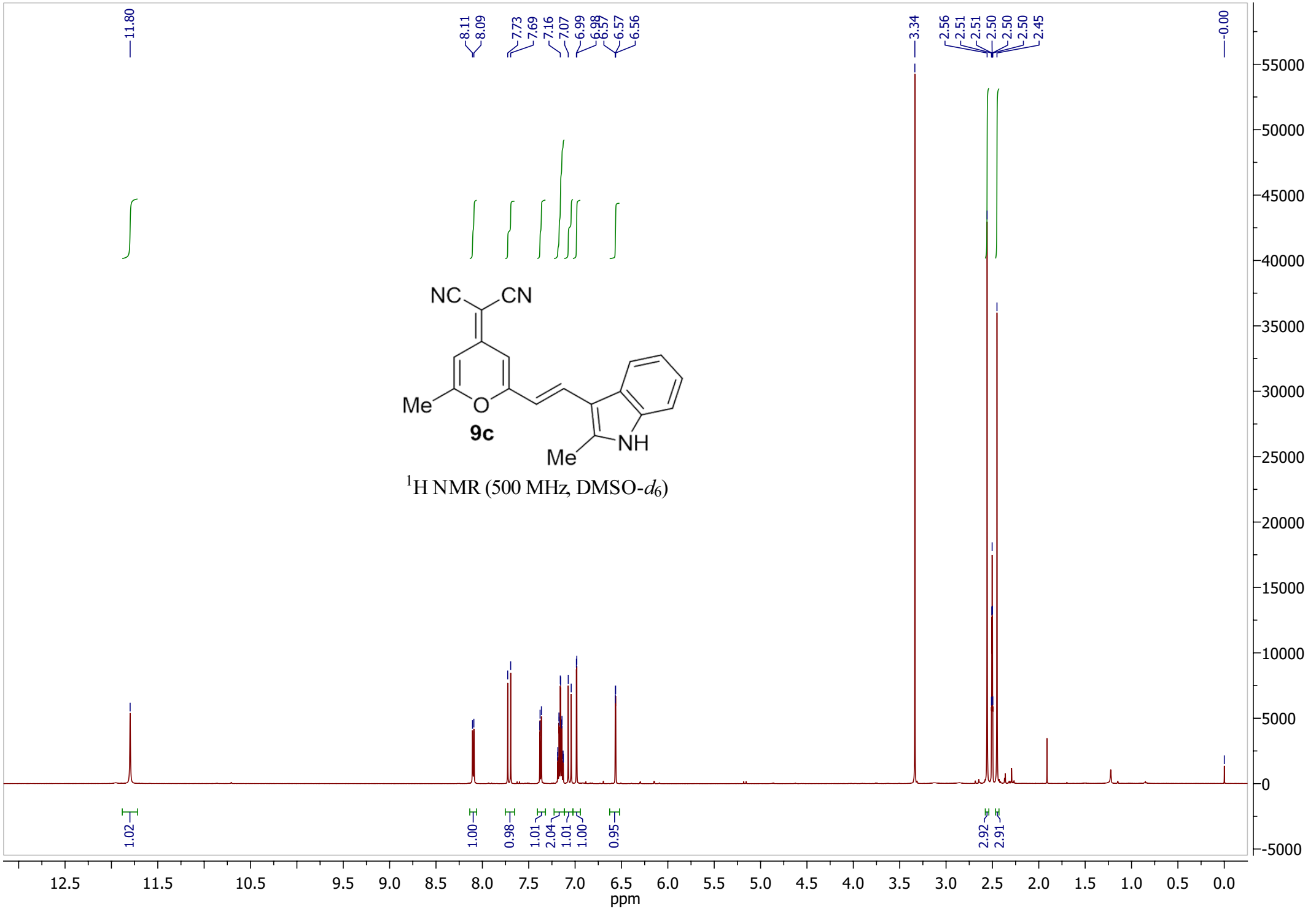
^{13}C NMR (126 MHz, DMSO-d_6)



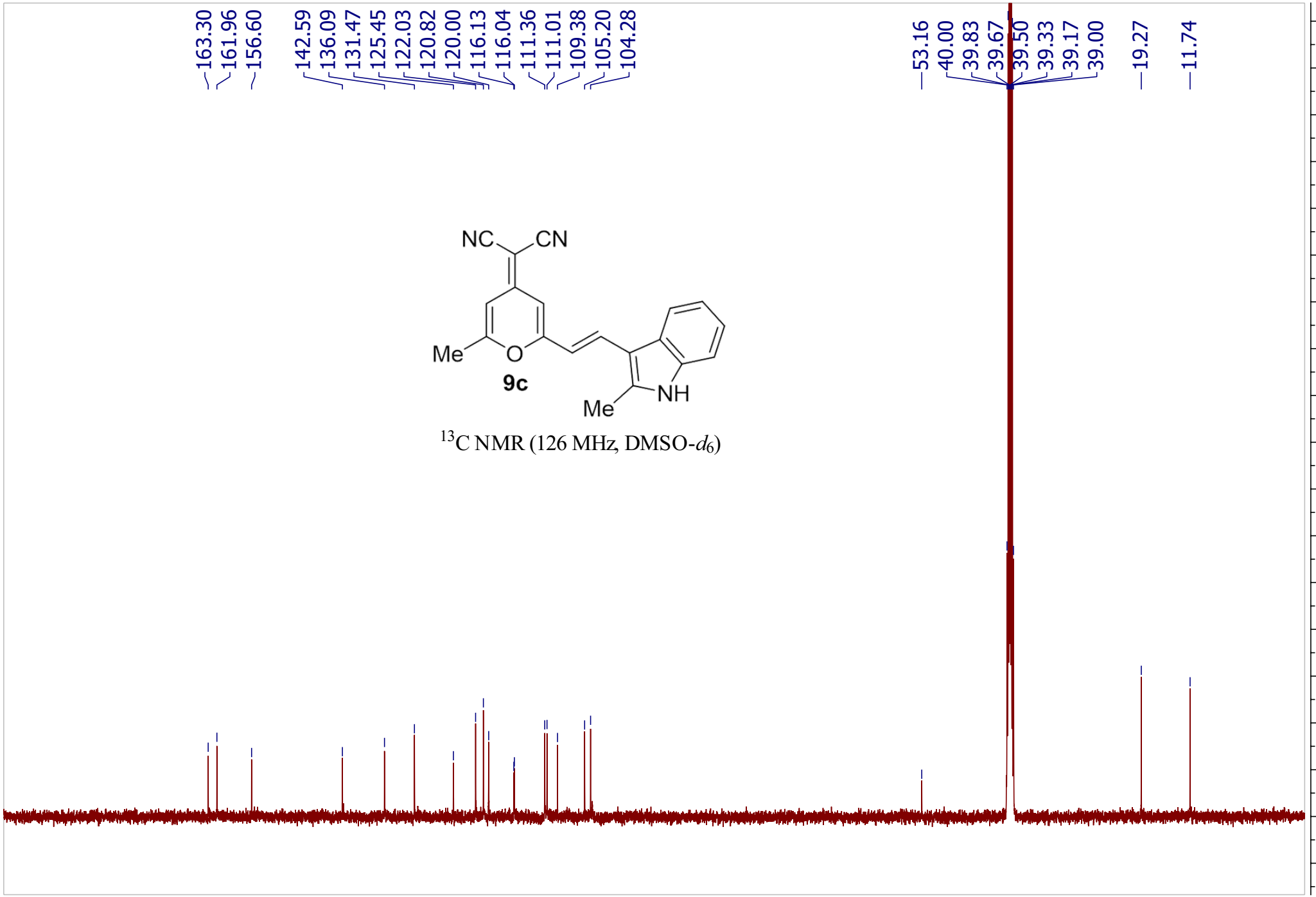
^{1}H NMR (500 MHz, DMSO-d_6)



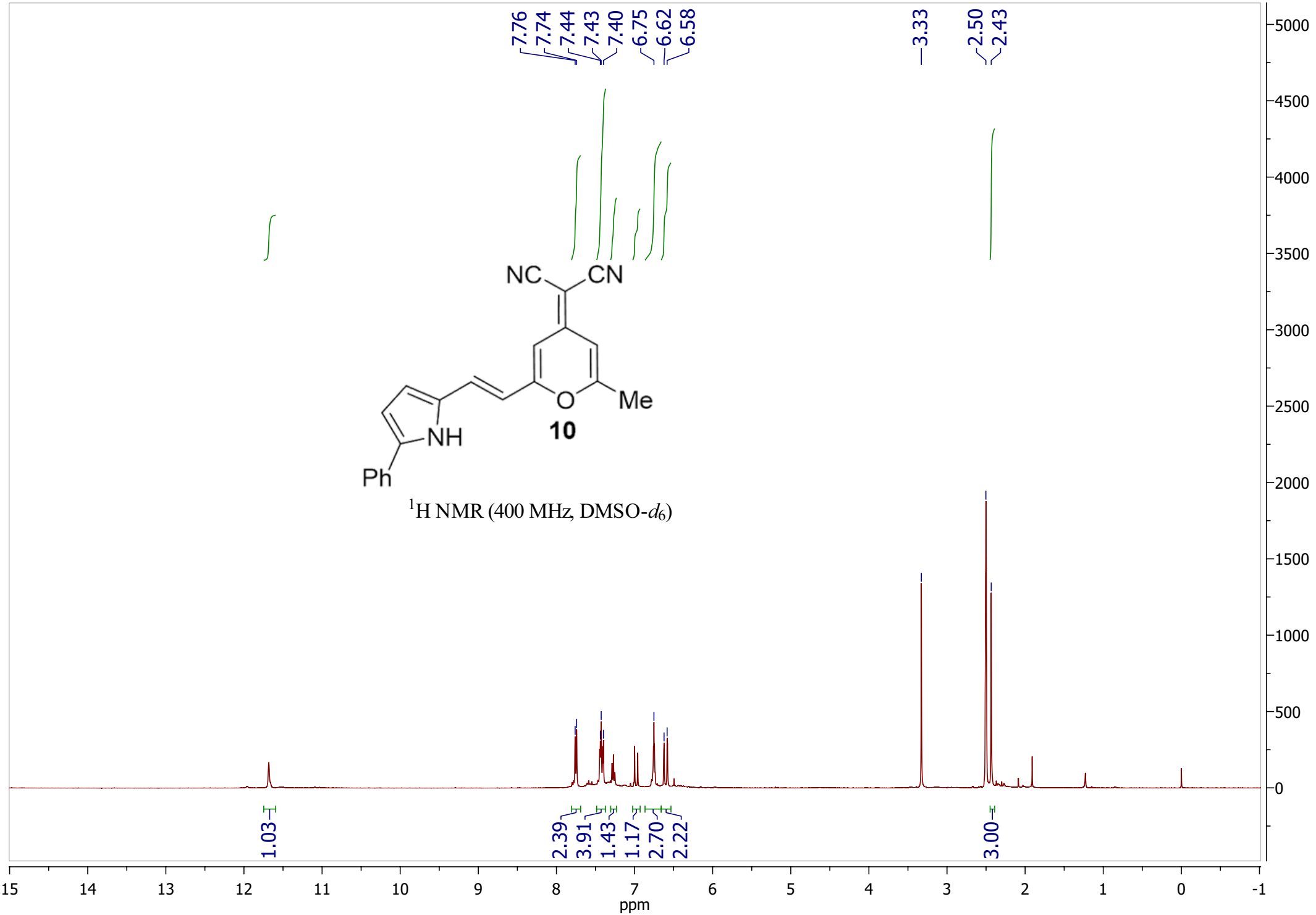
^{13}C NMR (151 MHz, DMSO-d_6)



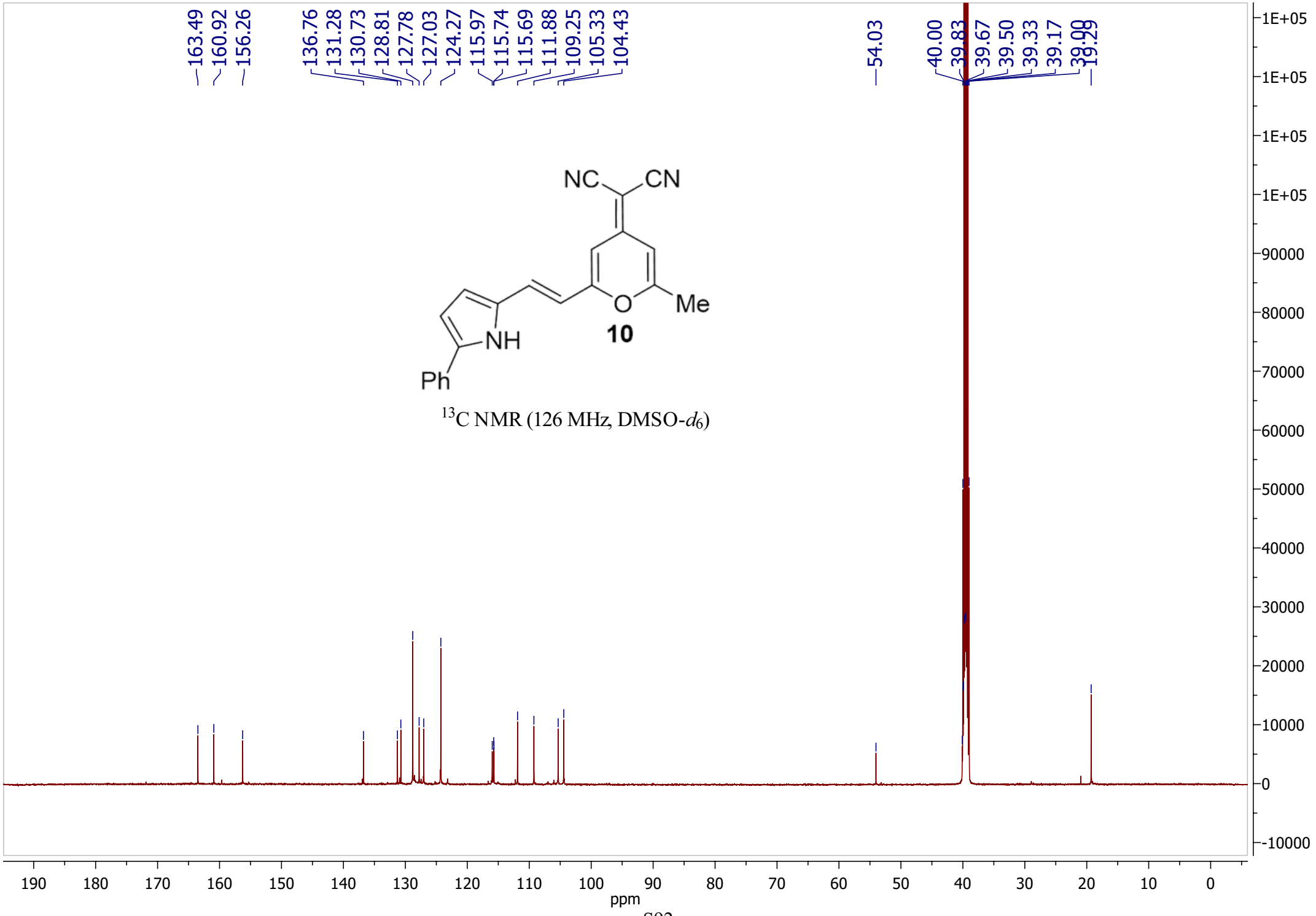
^{1}H NMR (500 MHz, DMSO-d_6)



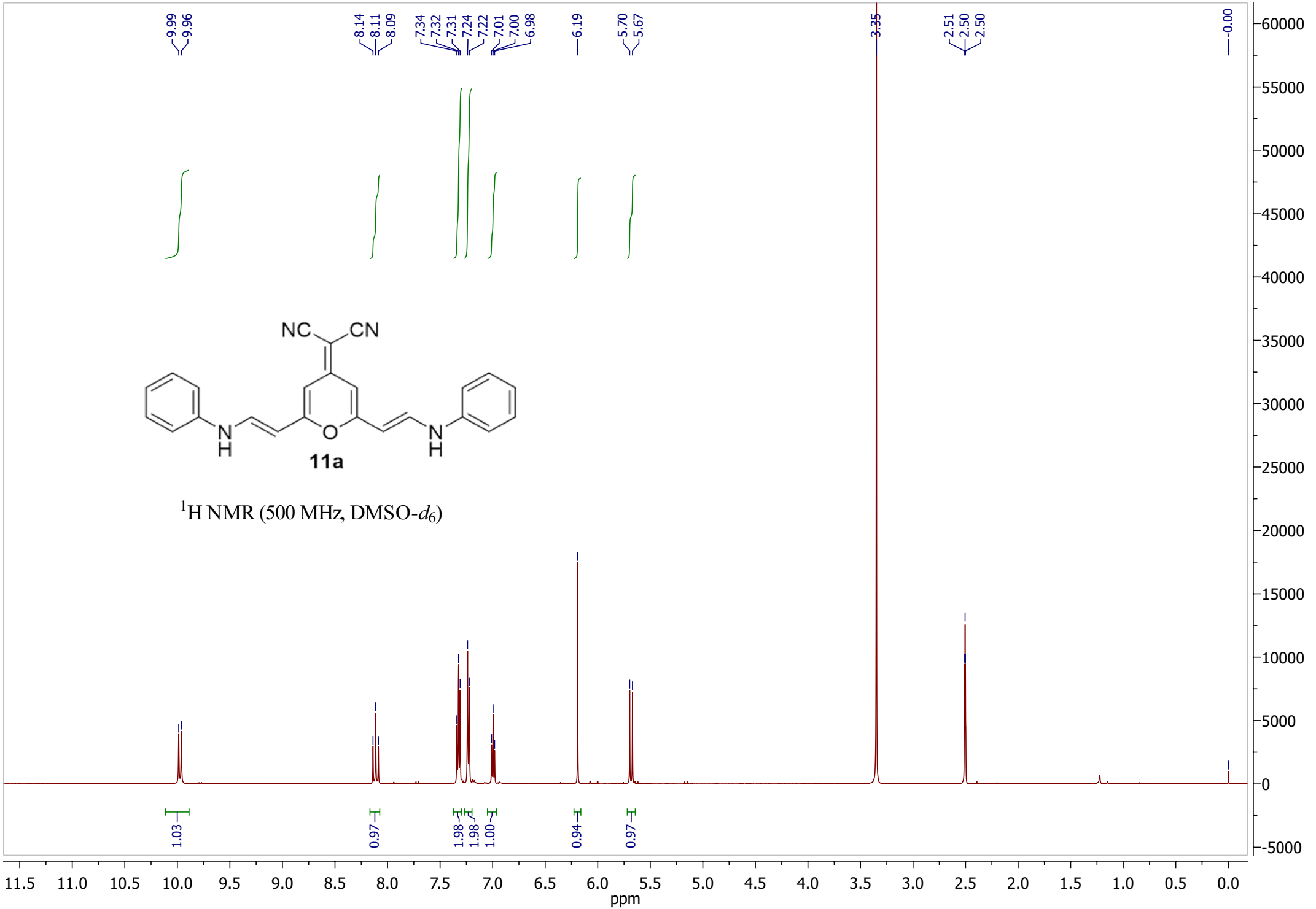
^{13}C NMR (126 MHz, DMSO-d_6)



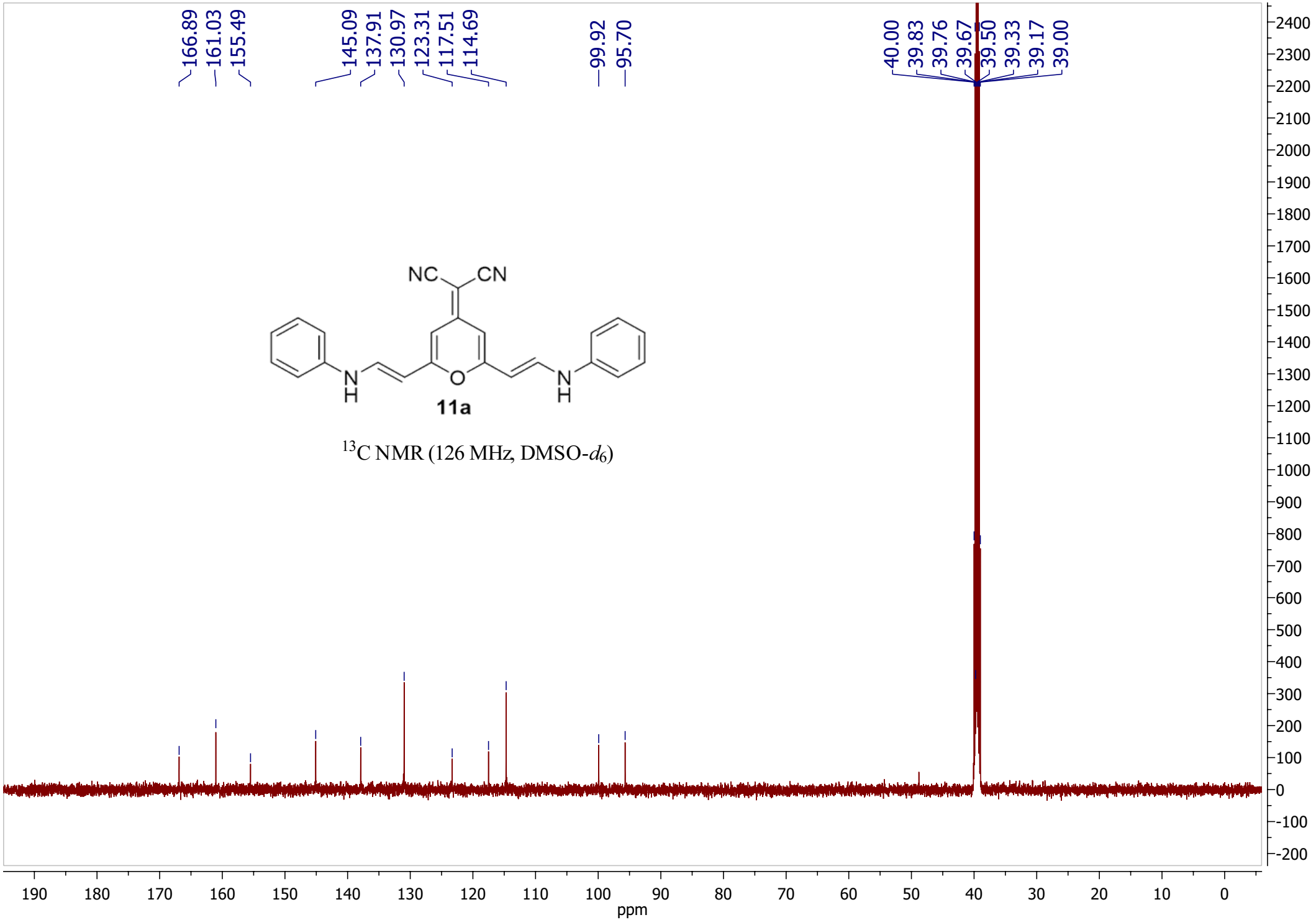
^{1}H NMR (400 MHz, DMSO-d_6)



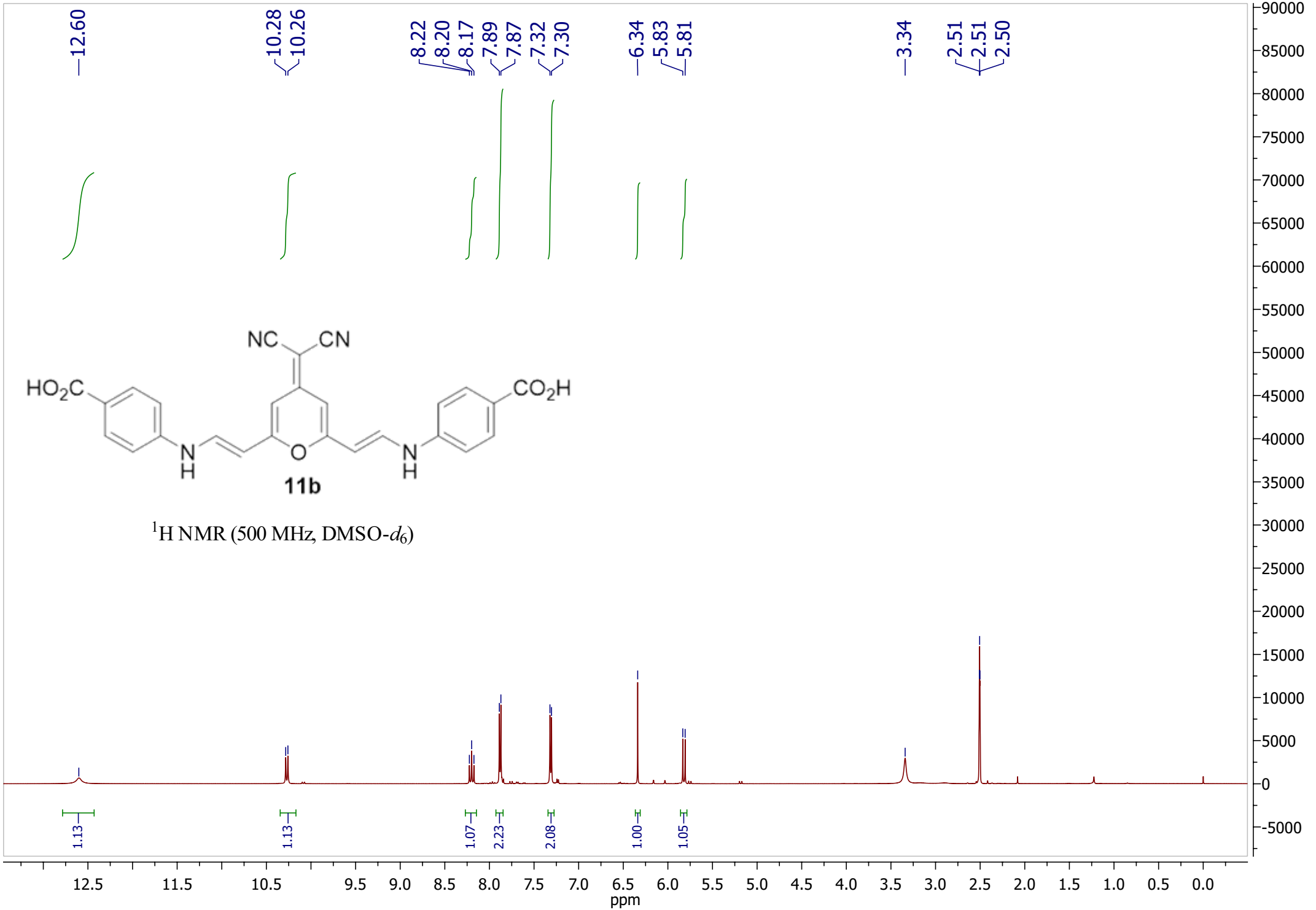
^{13}C NMR (126 MHz, DMSO-d_6)



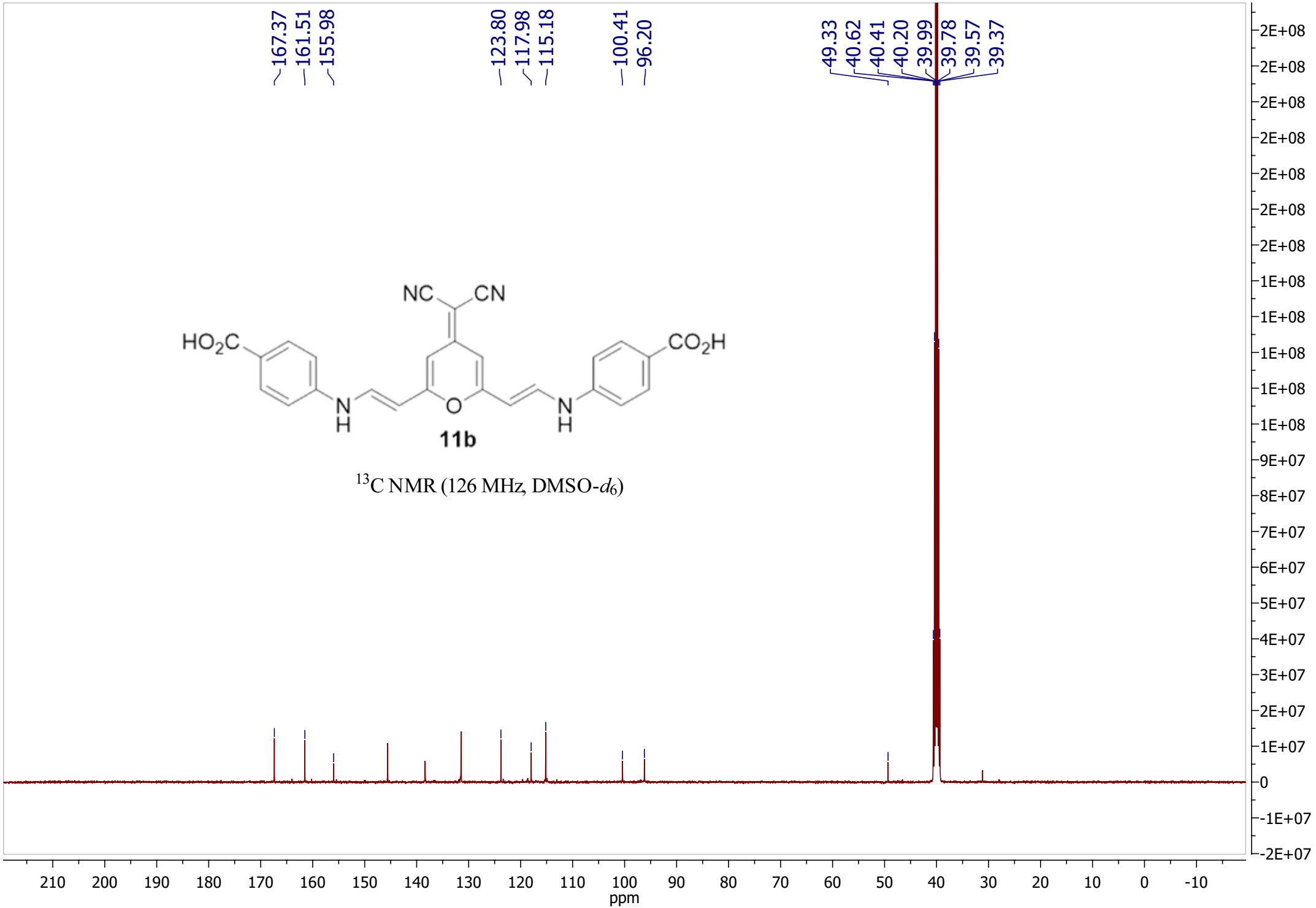
^{1}H NMR (500 MHz, DMSO-d_6)



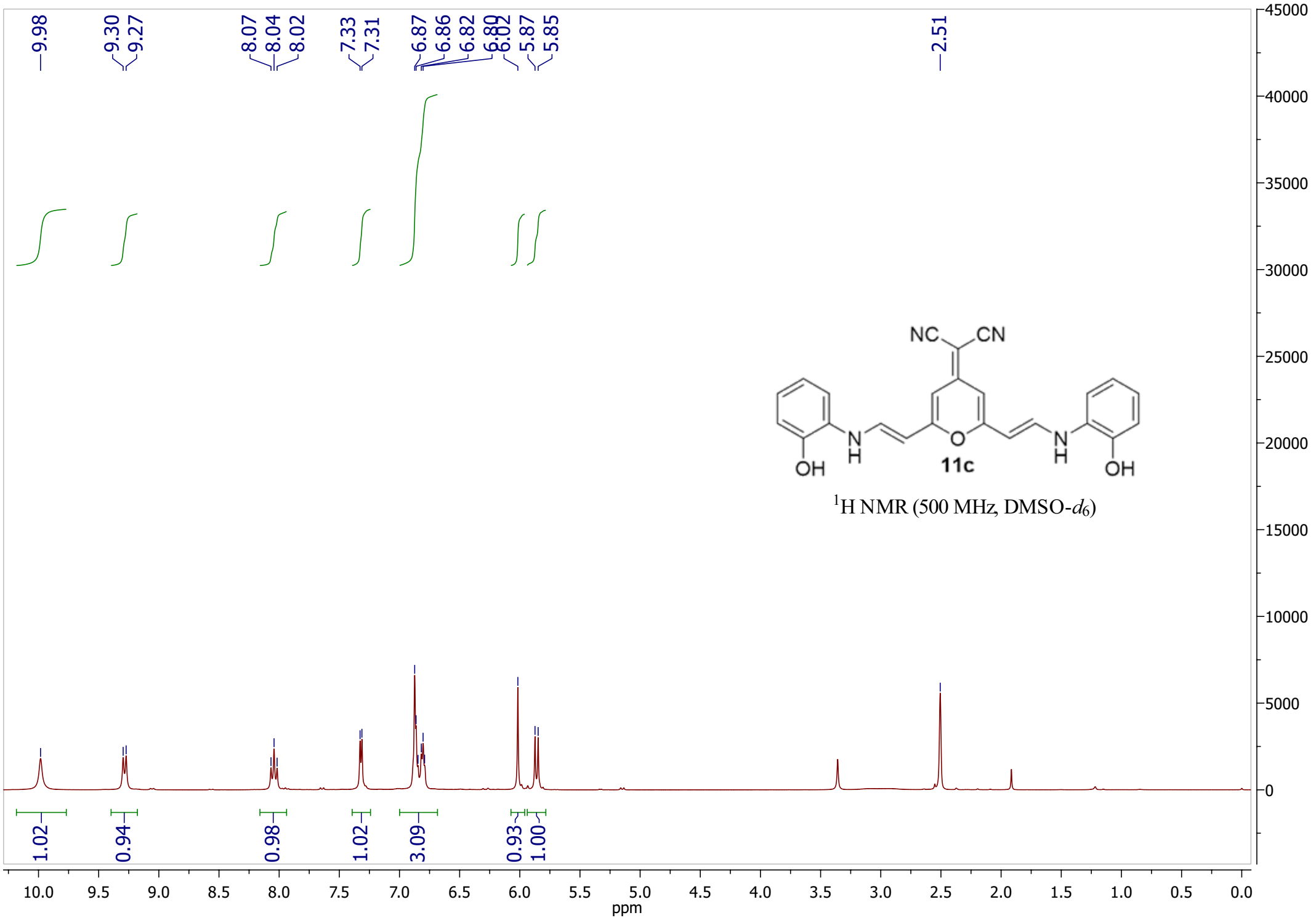
^{13}C NMR (126 MHz, DMSO-d_6)



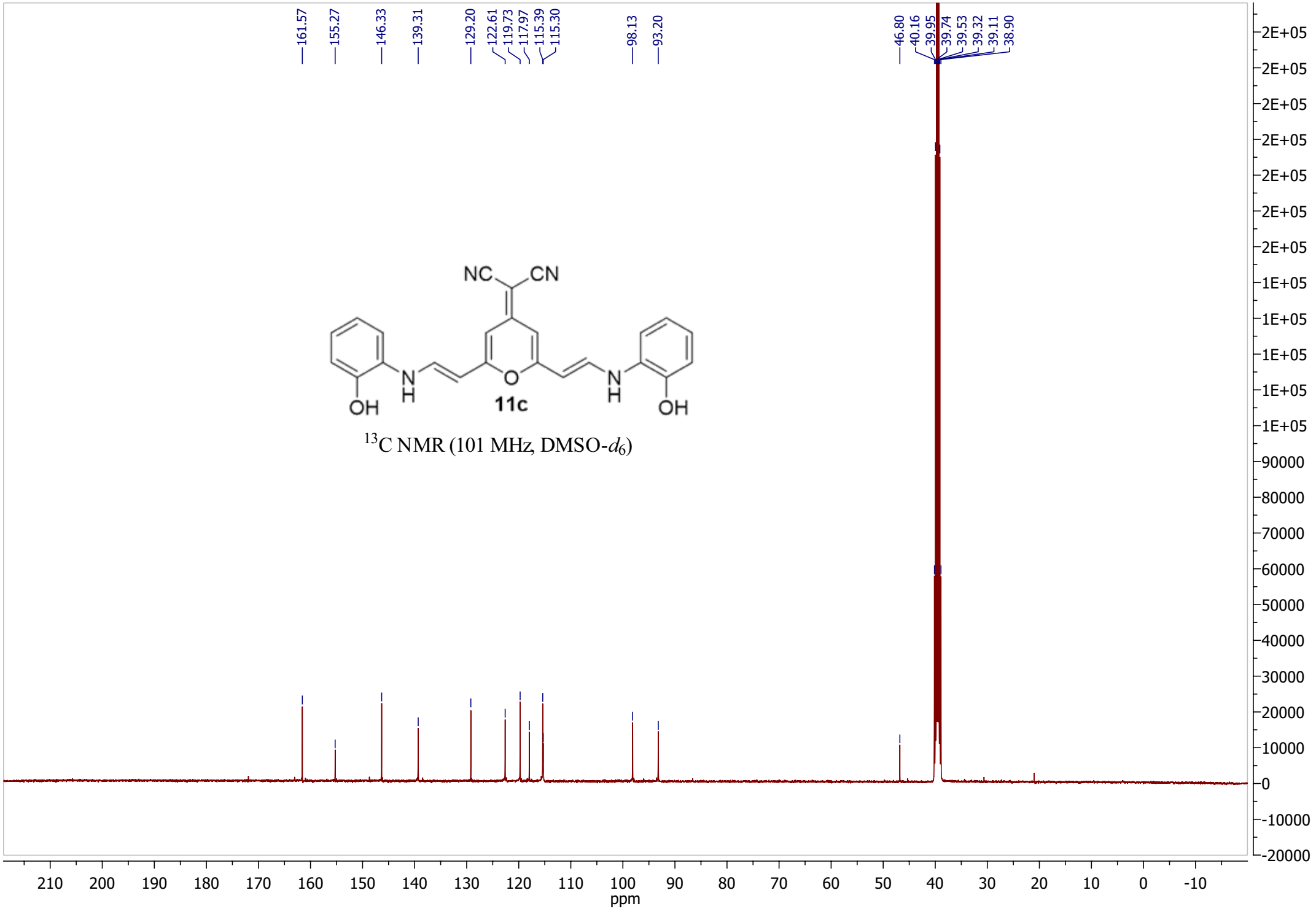
^{1}H NMR (500 MHz, DMSO-d_6)



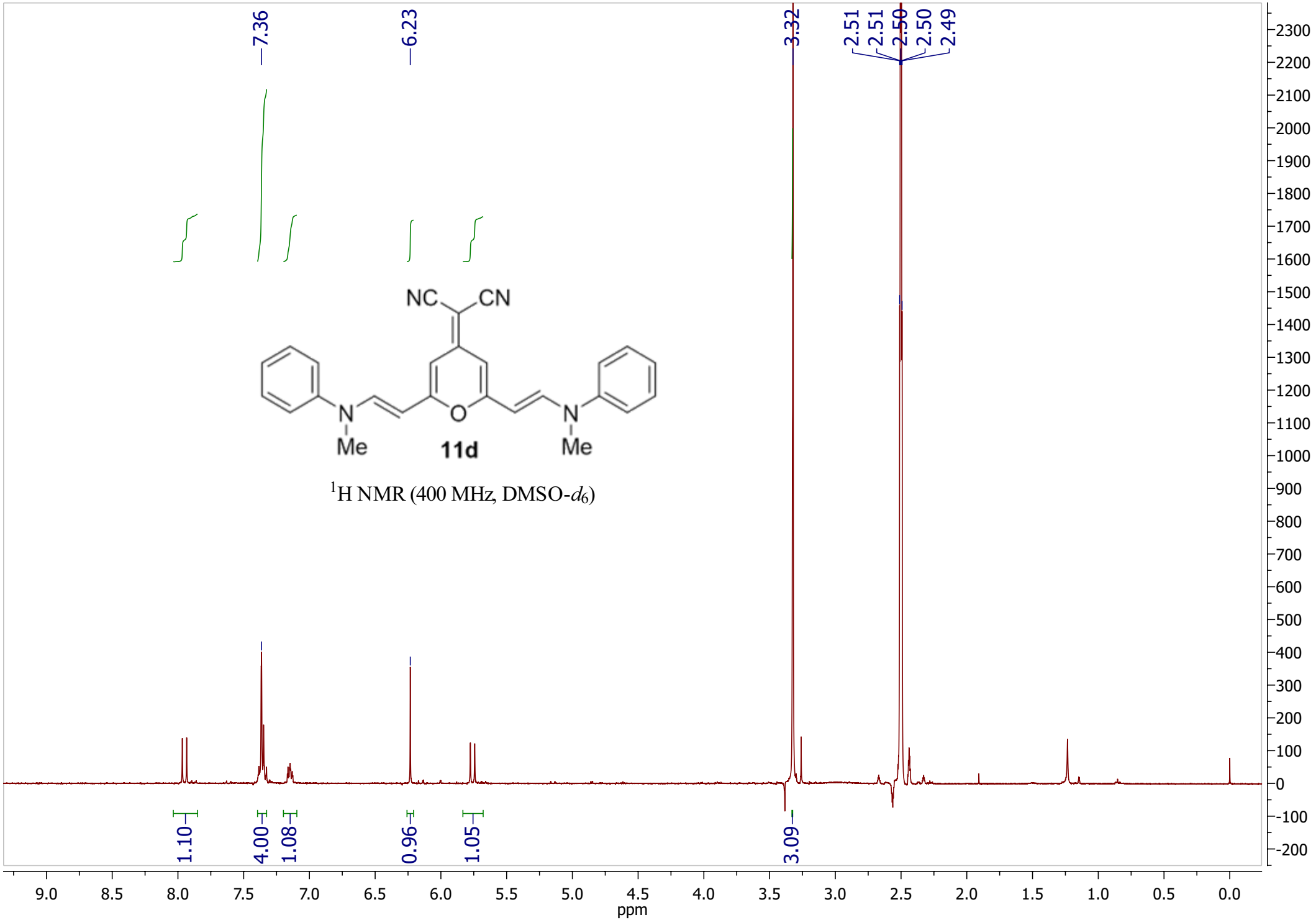
^{13}C NMR (126 MHz, DMSO-d_6)



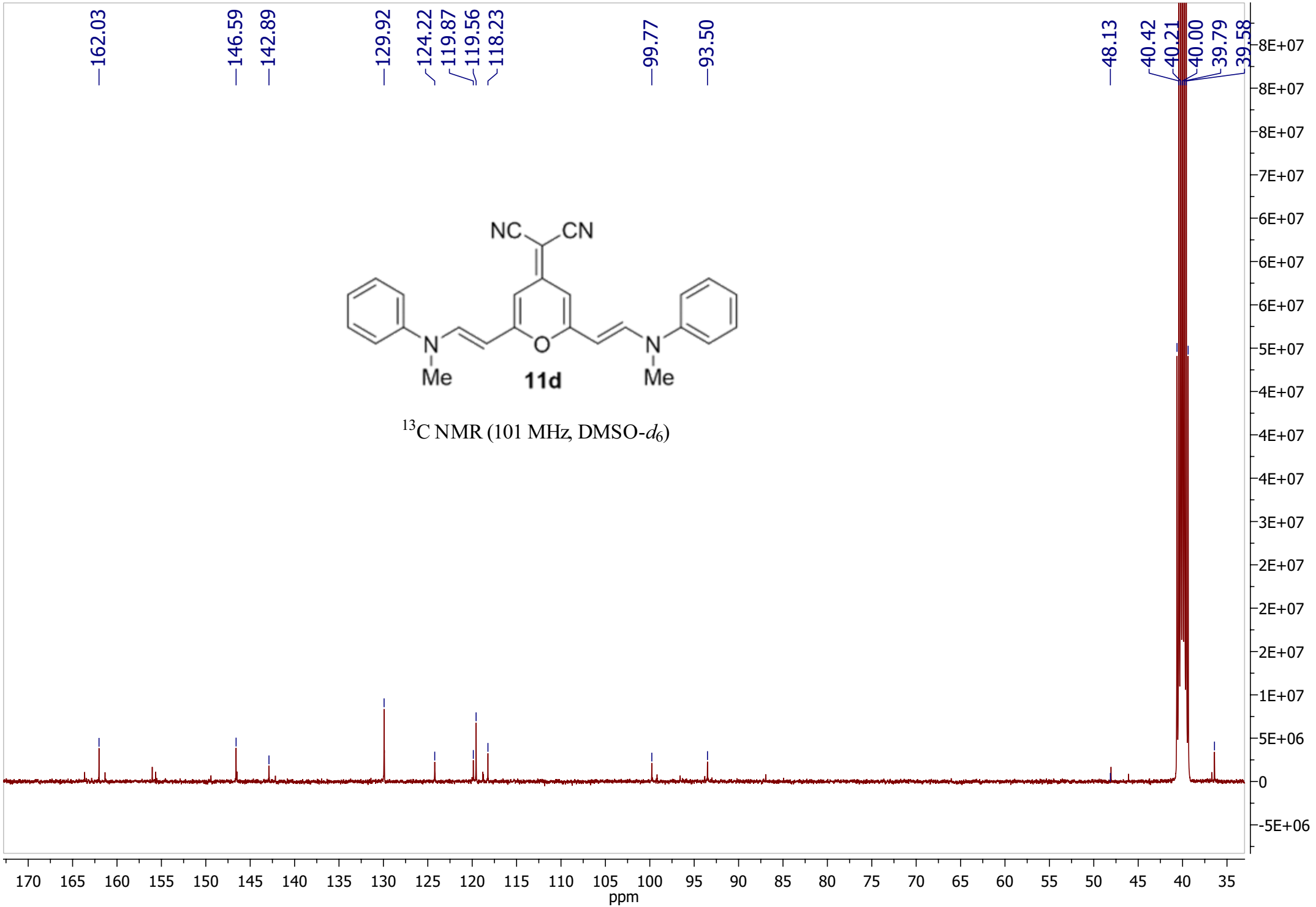
^{1}H NMR (500 MHz, DMSO-d_6)



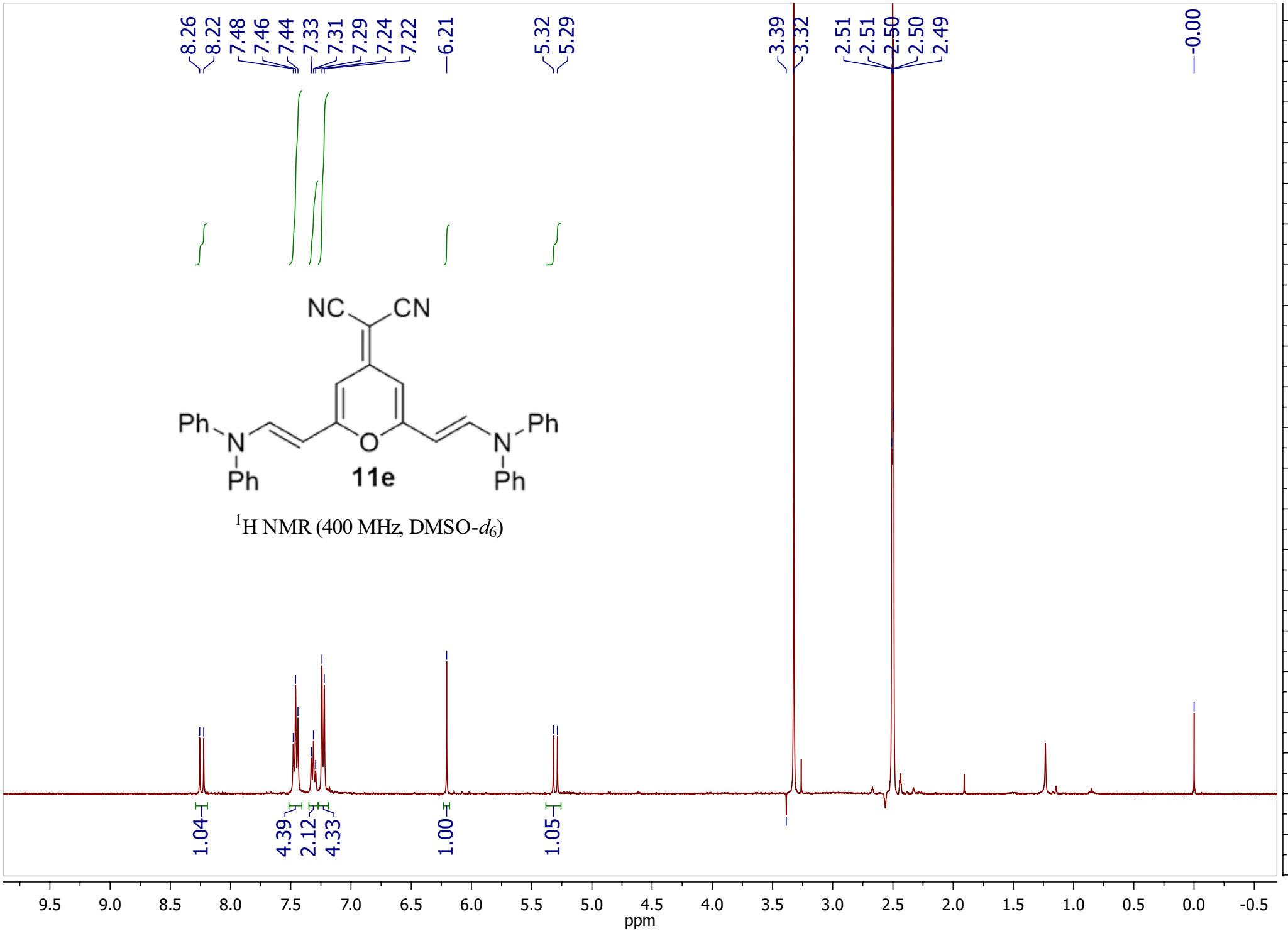
^{13}C NMR (101 MHz, DMSO-d_6)



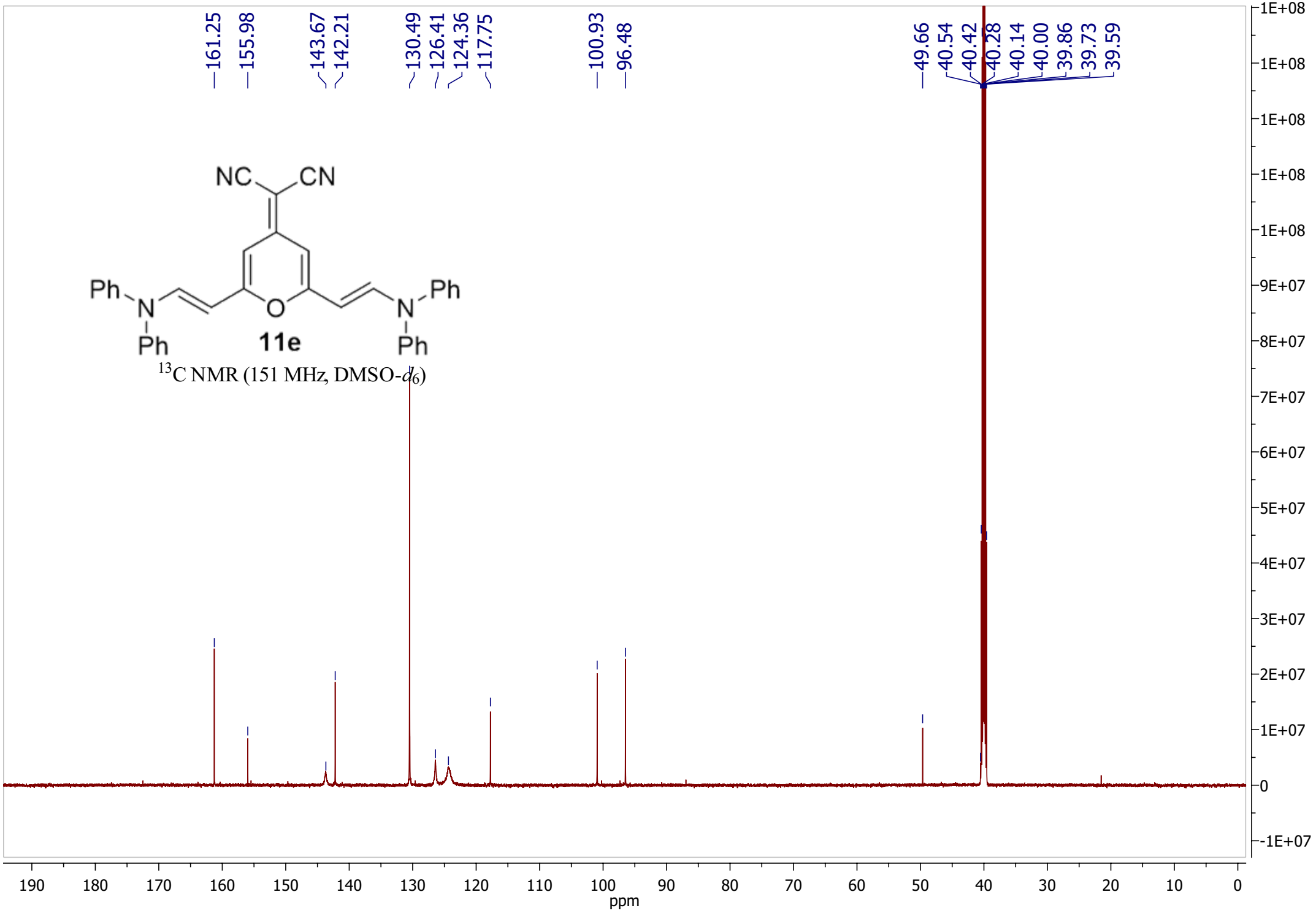
^{1}H NMR (400 MHz, DMSO-d_6)



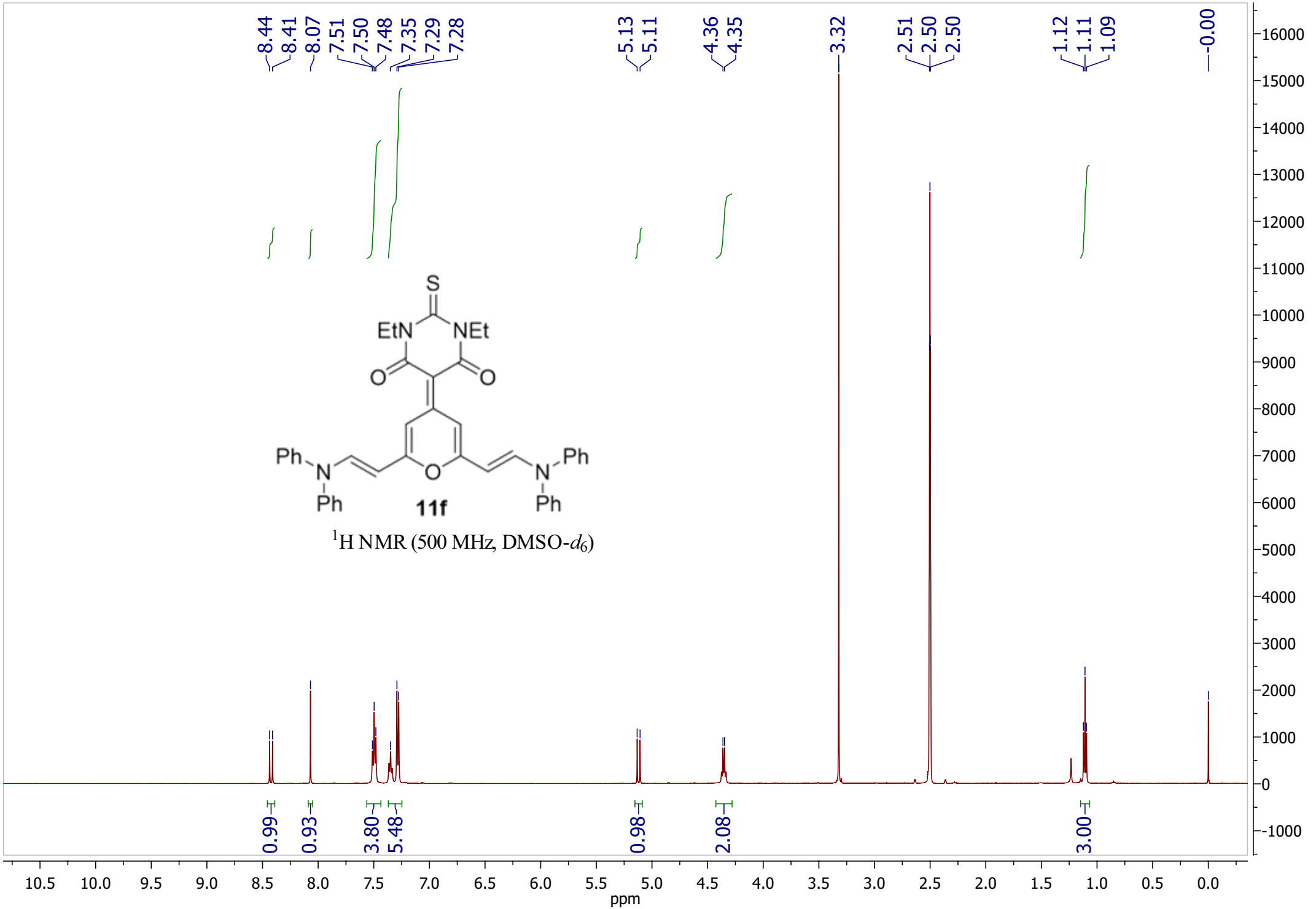
^{13}C NMR (101 MHz, DMSO-d_6)



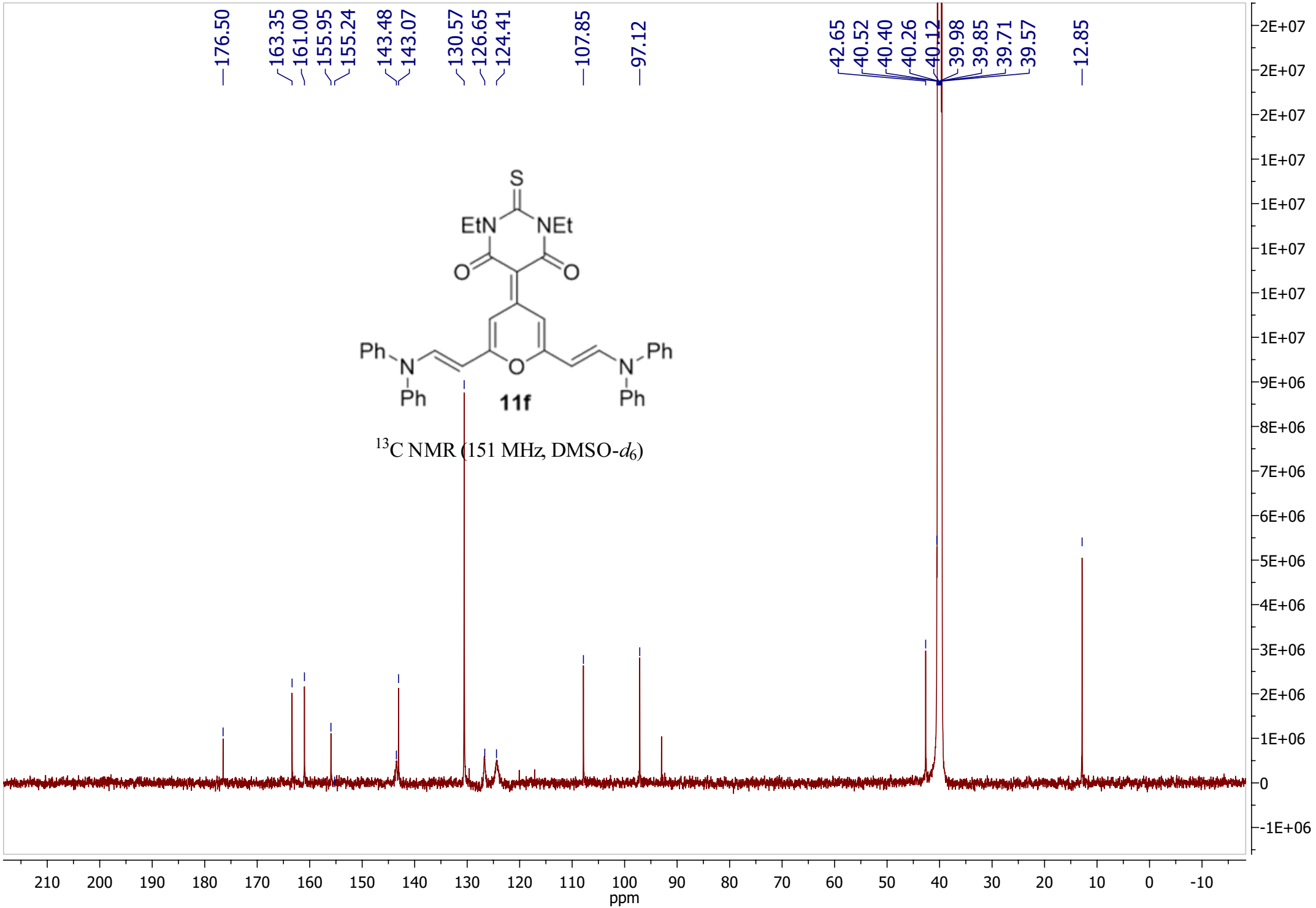
^{1}H NMR (400 MHz, DMSO-d_6)



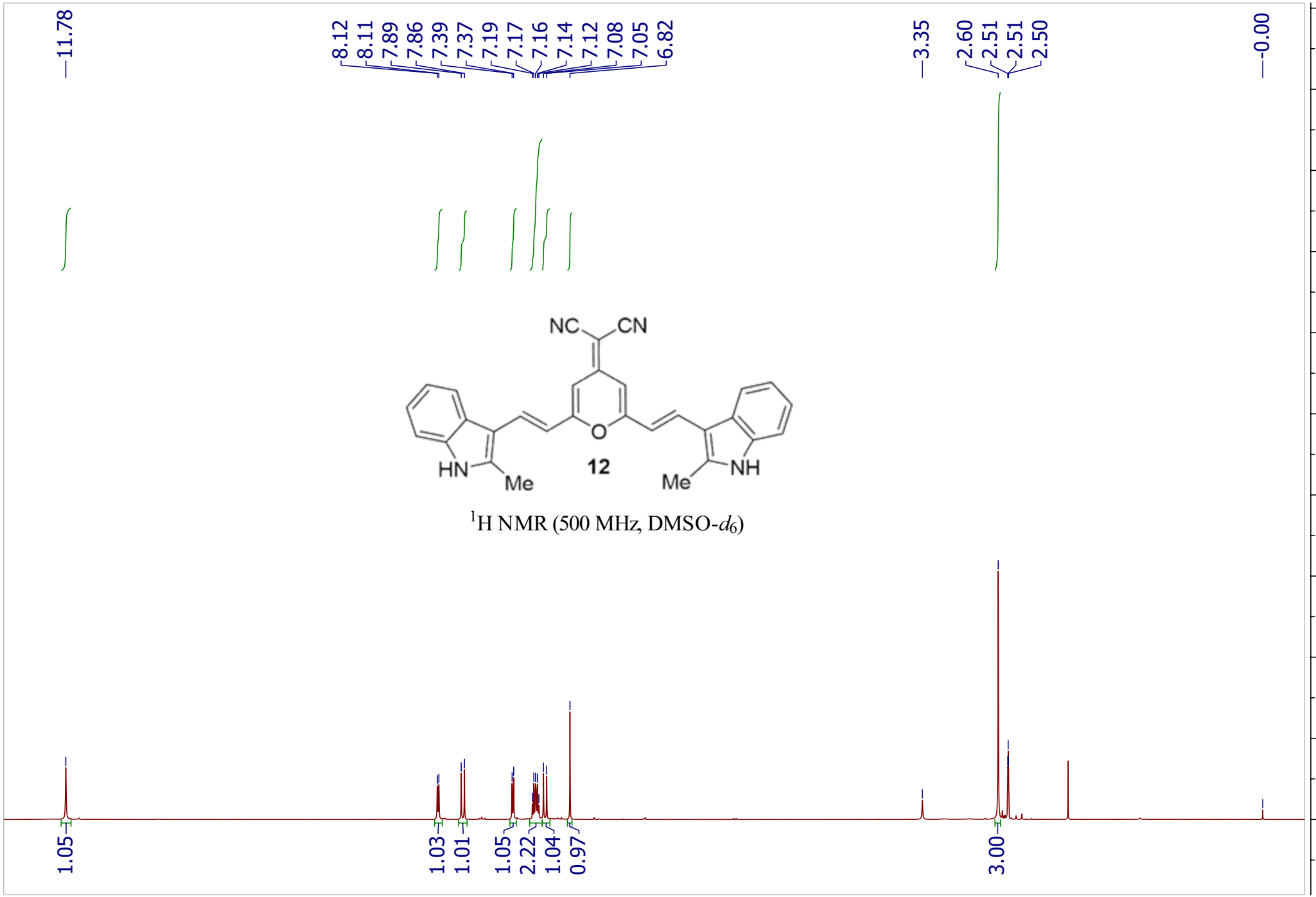
^{13}C NMR (151 MHz, DMSO-d_6)



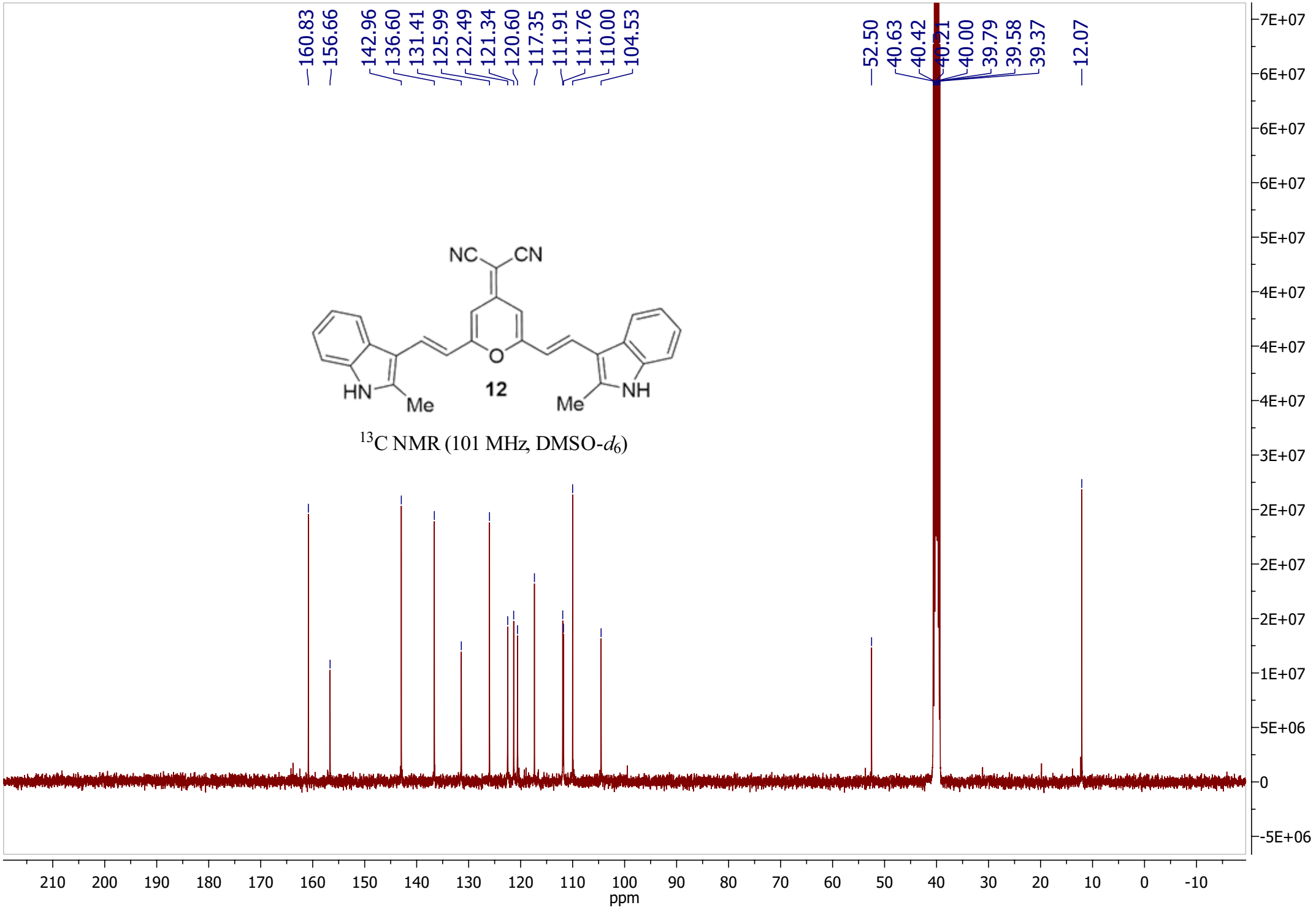
^{1}H NMR (500 MHz, DMSO-d_6)



^{13}C NMR (151 MHz, DMSO-d_6)



^{1}H NMR (500 MHz, DMSO-d_6)



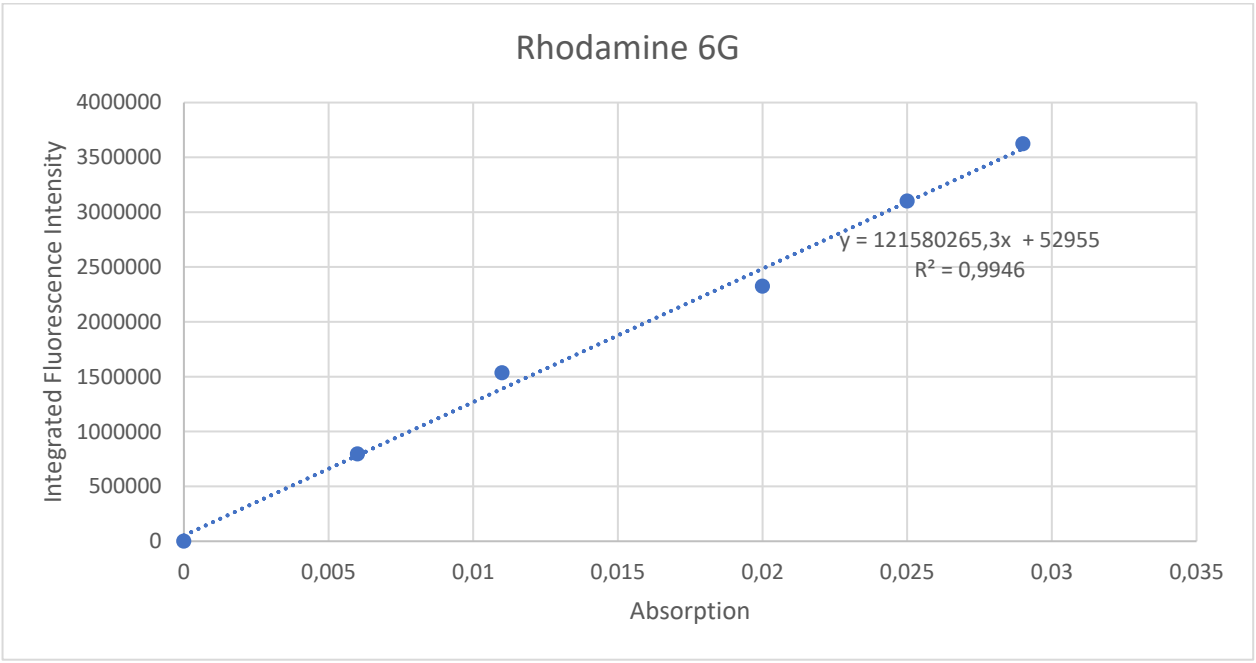
^{13}C NMR (101 MHz, DMSO-d_6)

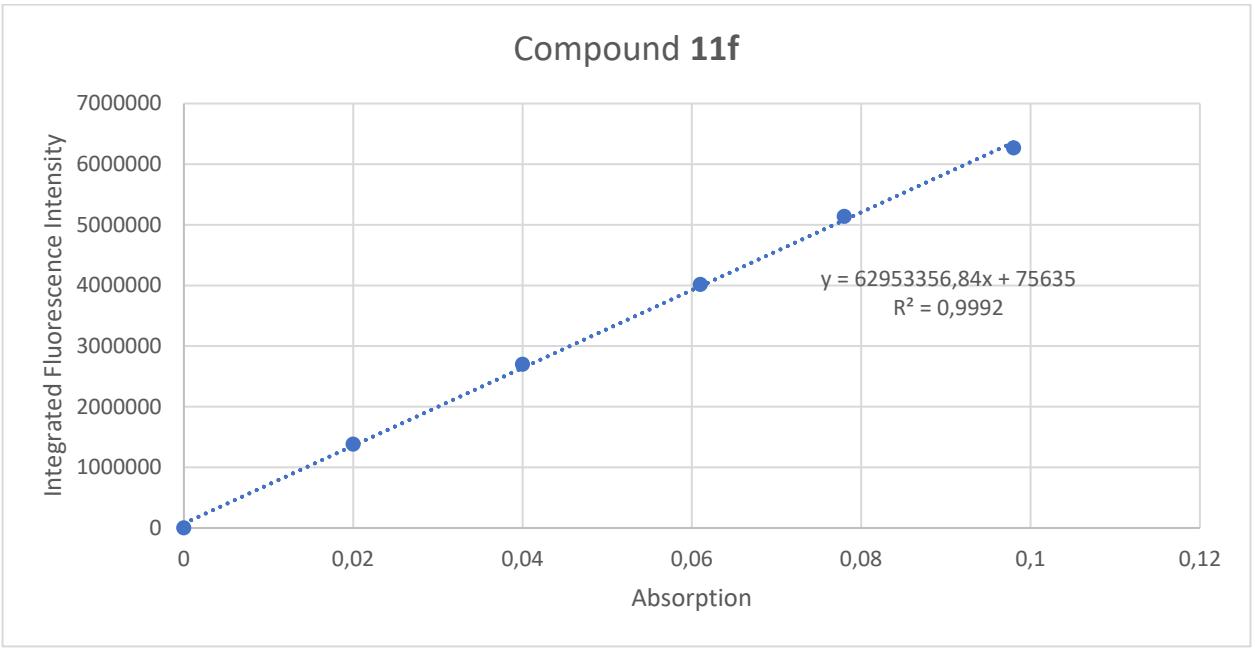
Determination of relative fluorescence quantum yields

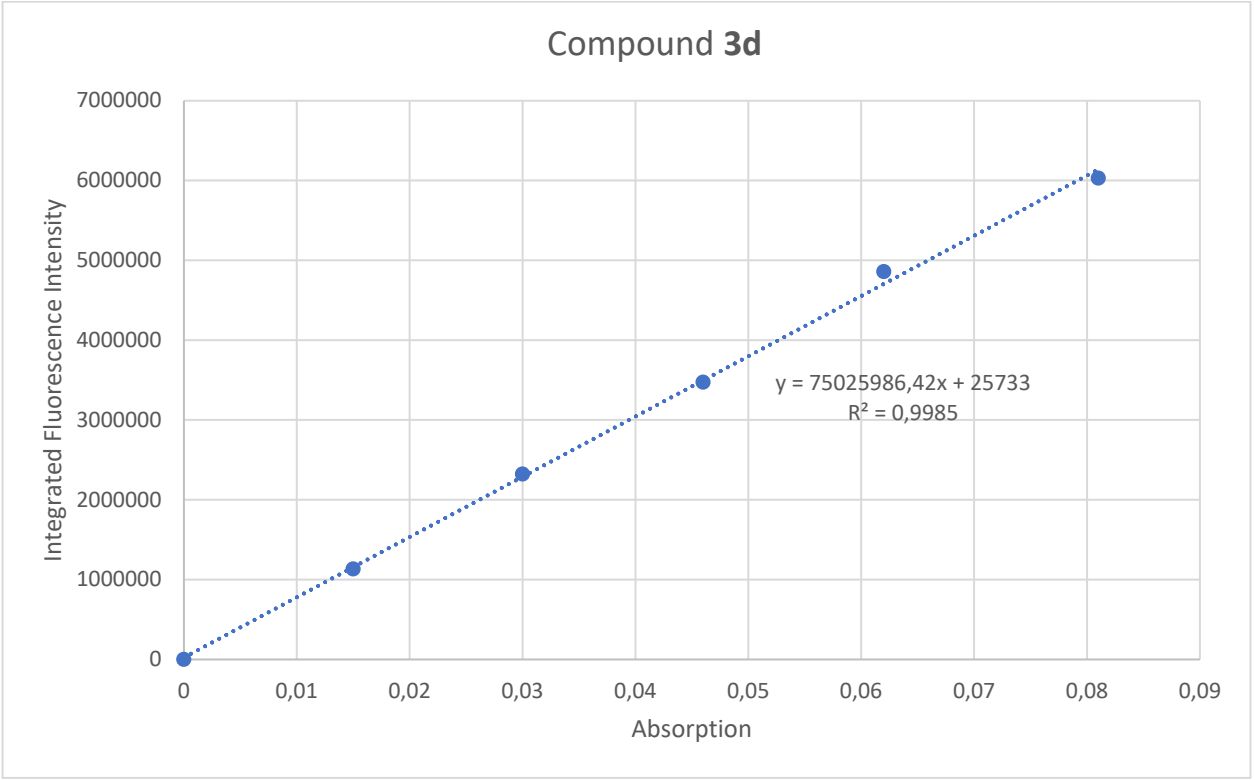
The quantum yield for synthesized fluorescent derivatives was calculated according to the procedure described in the literature with the use of Rhodamine 6G as a standard. All measurements were proceeded in 3-4 various concentrations ($2 \times 10^{-7} - 10^{-6}$ M). The quantum yield was calculated by the formula:

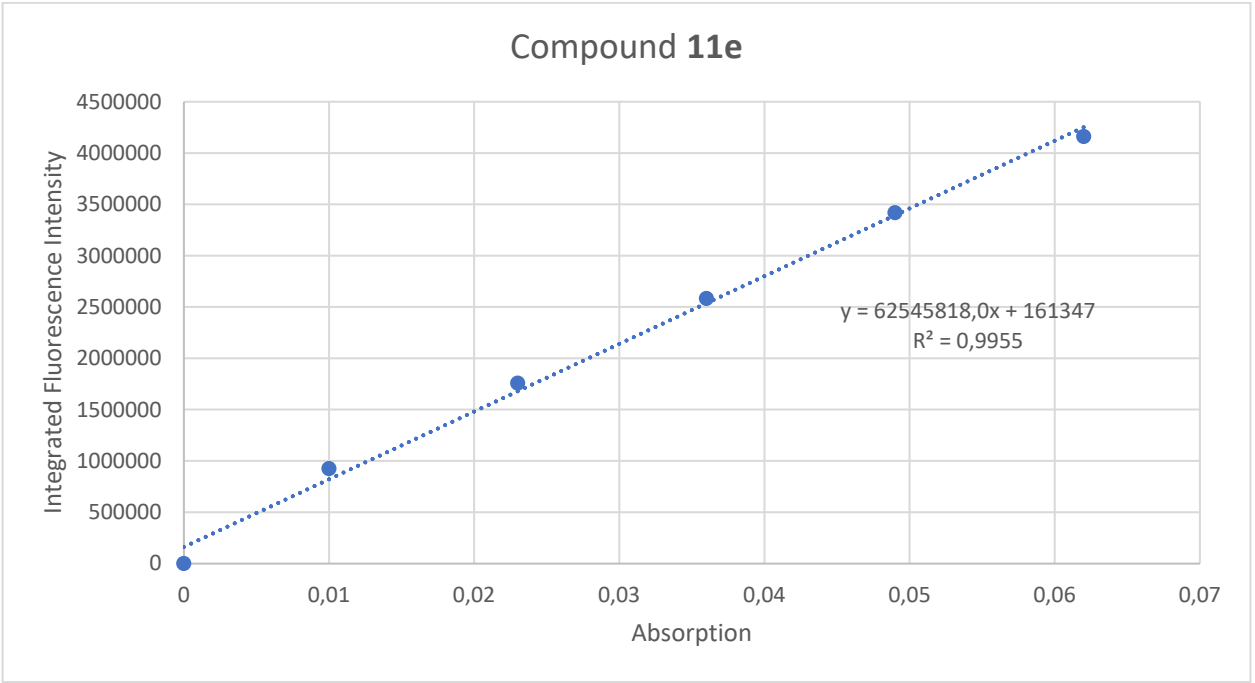
$$\Phi_x = \Phi_{st} \times \left(\frac{Grad_x}{Grad_{st}}\right) \times \left(\frac{n_x^2}{n_{st}^2}\right)$$

where *Grad* is the gradient from the plot of integrated fluorescence intensity, *n* is the refractive index of the solvent, *Φ* is the quantum yield, the subscript *x* corresponds to the novel compounds, the subscript *st* – for the standard.






Compound 3d
Integrated Fluorescence Intensity
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
0
0,01
0,02
0,03
0,04
0,05
0,06
0,07
0,08
0,09
Absorption
y = 75025986,42x + 25733
R² = 0,9985


Compound 11e
Integrated Fluorescence Intensity
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
0
0,01
0,02
0,03
0,04
0,05
0,06
0,07
Absorption
y = 62545818,0x + 161347
R² = 0,9955