

Supplementary materials

2-(2-(Dimethylamino)vinyl)-4*H*-pyran-4-ones as Novel and Convenient Building-Blocks for the Synthesis of Conjugated 4-Pyrone Derivatives

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1. Quantum mechanical calculations details

The ground state molecular geometry of two compounds under investigation was fully optimized at density functional theory (DFT) level, both in vacuo and in the solvated phase (DMSO, MeOH, EtOH). 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 analyzed both in vacuo and in the solvated phase.

The first singlet excited state $S(\pi, \pi^*)$ 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 an expected value and $\sigma = 0.4$ eV.

The integration grid for the calculations was set to 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]

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2. Cartesian coordinates of the GS optimized structure for compounds 4a and 5a

Cartesian coordinates (Å) of the optimized structure for compound **4a** in vacuo

C	6.0	2.0032833288	-1.1754132562	-0.0040824306
C	6.0	0.6575621755	-1.0821830893	0.0350349529
C	6.0	2.1062277022	1.2704216221	-0.0309512678
O	8.0	0.0168863500	0.1289207861	0.0433940306
C	6.0	0.7416680288	1.2977591084	0.0093136134
C	6.0	2.8529514135	0.0222863109	-0.0405000439
H	1.0	2.6599580495	2.2024372589	-0.0574581214
O	8.0	4.0902171232	-0.0390633889	-0.0758866366
C	6.0	-0.0692269393	2.4937861373	0.0150671641
H	1.0	0.4862987396	3.4241871992	-0.0119766366
C	6.0	-1.4314764846	2.4779968539	0.0521031326
N	7.0	-2.2663283378	3.5577275181	0.1311807531
C	6.0	-3.6647951694	3.4003583439	-0.2471491451
H	1.0	-1.9451296486	1.5212124397	0.0452908605
H	1.0	-3.9876786021	2.3787849543	-0.0316380652
H	1.0	-3.8316758487	3.5990545863	-1.3174646067
H	1.0	-4.2881131161	4.0873986809	0.3339870250
C	6.0	-1.7176205991	4.9026236076	0.0759191708
H	1.0	-2.5022906453	5.6212495613	0.3238531549
H	1.0	-1.3174852599	5.1479118448	-0.9207243095
H	1.0	-0.9116260114	5.0086360028	0.8086828472
C	6.0	-0.3205339271	-2.2136110511	0.0743123771
H	1.0	2.4813090524	-2.1485749338	-0.0084167555
H	1.0	0.2042219812	-3.1708946683	0.0679242709
H	1.0	-0.9916287347	-2.1732339612	-0.7916197086
H	1.0	-0.9404386907	-2.1565135877	0.9766418945

Cartesian coordinates (Å) of the optimized structure for compound **5a** in vacuo

C	6.0	1.9801166574	-1.3464803409	-0.0358224973
C	6.0	0.6220811735	-1.2340851112	-0.0349368384
C	6.0	2.1310009547	1.0894226063	0.0418038021
O	8.0	0.0123979074	-0.0019252045	-0.0057379157
C	6.0	0.7692818899	1.1453099952	0.0358294033
C	6.0	2.8506818898	-0.1777509128	0.0005904281
H	1.0	2.7061149964	2.0082715354	0.0728222962
O	8.0	4.0902616966	-0.2554122370	-0.0016032085
C	6.0	-0.0044937784	2.3681357717	0.0646612500
H	1.0	0.5860445931	3.2740467701	0.1419329518
C	6.0	-1.3622164183	2.4153383681	-0.0032946459
N	7.0	-2.1546198094	3.5308772701	0.1016725185
C	6.0	-3.4924368069	3.4936936321	-0.4729072334
H	1.0	-1.9182051616	1.4903609359	-0.1255798151
H	1.0	-3.9042585296	2.4846198002	-0.3839746143
H	1.0	-3.4992371849	3.7752080600	-1.5384817708
H	1.0	-4.1493935790	4.1808017725	0.0699479362
C	6.0	-1.5341002602	4.8411192031	0.2055406816
H	1.0	-2.3000600438	5.5826612978	0.4451828556
H	1.0	-1.0331306078	5.1427614834	-0.7287887755
H	1.0	-0.7934761138	4.8404567961	1.0110514954
H	1.0	2.4364403283	-2.3299191292	-0.0579334383
C	6.0	-0.2966760420	-2.3521028411	-0.0504167991
H	1.0	0.1758668883	-3.3271063550	-0.0809579883
C	6.0	-1.6511926089	-2.2275614424	-0.0237206075
N	7.0	-2.5743067159	-3.2392434725	-0.1079062493
H	1.0	-2.0889494992	-1.2359306339	0.0418115743

C	6.0	-2.1224723204	-4.6206157652	-0.1173851442
C	6.0	-3.9190002927	-2.9998582933	0.3990423980
H	1.0	-4.1937396056	-1.9558833806	0.2262271075
H	1.0	-4.0043484594	-3.2061791884	1.4781882590
H	1.0	-4.6345907173	-3.6351756233	-0.1324026818
H	1.0	-1.3581077075	-4.7583929596	-0.8880317008
H	1.0	-2.9664531006	-5.2739253435	-0.3519655552
H	1.0	-1.6986120535	-4.9282010801	0.8526096805

Cartesian coordinates (Å) of the optimized structure for compound **4a** in DMSO

C	6.0	2.0031902580	-1.1722161931	0.0009063016
C	6.0	0.6541268227	-1.0806273306	0.0241617403
C	6.0	2.1142853094	1.2667484707	-0.0164895426
O	8.0	0.0219258834	0.1316088129	0.0299326128
C	6.0	0.7391355202	1.3027754276	0.0066534212
C	6.0	2.8453178978	0.0241382304	-0.0206366100
H	1.0	2.6646591770	2.2021148037	-0.0345108952
O	8.0	4.0970653122	-0.0455151315	-0.0418728446
C	6.0	-0.0605167010	2.4938950662	0.0062718923
H	1.0	0.4940355918	3.4253621626	-0.0106223254
C	6.0	-1.4347231566	2.4794708853	0.0177049086
N	7.0	-2.2528185554	3.5512491005	0.0625382785
C	6.0	-3.6919800666	3.3973475114	-0.1283876141
H	1.0	-1.9492015530	1.5231383083	0.0053247959
H	1.0	-3.9804719316	2.3561762597	0.0349356577
H	1.0	-3.9957191036	3.6917338342	-1.1424884367
H	1.0	-4.2355574521	4.0188549057	0.5912278955
C	6.0	-1.7117907925	4.9042370172	0.0324157048
H	1.0	-2.5118867866	5.6177149146	0.2389462086
H	1.0	-1.2763635463	5.1440480931	-0.9479150764
H	1.0	-0.9390200892	5.0259814394	0.7993610575
C	6.0	-0.3216106357	-2.2105681266	0.0465291899
H	1.0	2.4746578358	-2.1493877564	-0.0034949777
H	1.0	0.2008459312	-3.1695865238	0.0446438328
H	1.0	-0.9815507656	-2.1691745716	-0.8283867407
H	1.0	-0.9559276277	-2.1586493651	0.9396806611

Cartesian coordinates (Å) of the optimized structure for compound **5a** in DMSO

C	6.0	1.9898183327	-1.3444727799	0.0543058463
C	6.0	0.6233819448	-1.2352286252	0.0289082391
C	6.0	2.1474179748	1.0847303301	-0.0188019552
O	8.0	0.0251562302	0.0012567256	-0.0045391144
C	6.0	0.7770087074	1.1519996362	-0.0291958651
C	6.0	2.8500851244	-0.1798910967	0.0252151794
H	1.0	2.7211252666	2.0059232939	-0.0372046827
O	8.0	4.1056598374	-0.2629544494	0.0358311723
C	6.0	0.0140401788	2.3701710376	-0.0613201861
H	1.0	0.6028723709	3.2781491618	-0.1309983206
C	6.0	-1.3539858796	2.4175599187	0.0290616677
N	7.0	-2.1232224535	3.5282716742	0.0738908895
C	6.0	-3.5755236447	3.4356552058	-0.0381765007
H	1.0	-1.9102671933	1.4877100709	0.0911229421
H	1.0	-3.9002210207	2.4103641339	0.1557276123
H	1.0	-3.9192519447	3.7276472827	-1.0402143666
H	1.0	-4.0533744210	4.0913718040	0.6979462361
C	6.0	-1.5245273363	4.8508118350	-0.0492114479
H	1.0	-2.2819616808	5.6102327071	0.1550245256
H	1.0	-1.1232915484	5.0223107000	-1.0584685559
H	1.0	-0.7125226205	4.9747269605	0.6759685029
H	1.0	2.4392041283	-2.3320826102	0.0790612340

C	6.0	-0.2887514036	-2.3476192049	0.0306859755
H	1.0	0.1801306806	-3.3246365410	0.0663209987
C	6.0	-1.6526910853	-2.2224047457	-0.0328091444
N	7.0	-2.5547692208	-3.2289981527	-0.1125084213
H	1.0	-2.0924141597	-1.2297130967	-0.0383771839
C	6.0	-2.1202169339	-4.6185548696	-0.0595514994
C	6.0	-3.9717485398	-2.9667218122	0.1212311619
H	1.0	-4.1905628509	-1.9095256992	-0.0509752520
H	1.0	-4.2636571794	-3.2177558520	1.1510406340
H	1.0	-4.5825444576	-3.5596605319	-0.5671324862
H	1.0	-1.3298315734	-4.7999511227	-0.7955864939
H	1.0	-2.9635069425	-5.2699339475	-0.2990287250
H	1.0	-1.7426335230	-4.8911526588	0.9371539408

Cartesian coordinates (Å) of the optimized structure for compound **4a** in ethanol

C	6.0	1.9998423545	-1.1704607774	-0.0081791002
C	6.0	0.6506027232	-1.0761958446	0.0300309698
C	6.0	2.1210513744	1.2668028631	0.0103354849
O	8.0	0.0248866481	0.1386705678	0.0548533393
C	6.0	0.7434724401	1.3086268335	0.0394925159
C	6.0	2.8358210844	0.0236050816	-0.0294115767
H	1.0	2.6771473284	2.1985116854	-0.0021133430
O	8.0	4.0961373489	-0.0524691247	-0.0918139796
C	6.0	-0.0533358234	2.4986321121	0.0430686465
H	1.0	0.4997285932	3.4310042984	0.0360392161
C	6.0	-1.4286784193	2.4782766187	0.0277384575
N	7.0	-2.2524586080	3.5452276780	0.0587460076
C	6.0	-3.6855989095	3.3820423075	-0.1747653225
H	1.0	-1.9376178667	1.5188646662	0.0025258955
H	1.0	-3.9735532770	2.3406000357	-0.0126135162
H	1.0	-3.9597077993	3.6674919835	-1.1998464093
H	1.0	-4.2535990279	4.0055555687	0.5235911959
C	6.0	-1.7198396805	4.9027455642	0.0317110511
H	1.0	-2.5257970049	5.6107304030	0.2349082580
H	1.0	-1.2817736259	5.1462629702	-0.9464077634
H	1.0	-0.9530966586	5.0298098414	0.8033867569
C	6.0	-0.3300405742	-2.2006414193	0.0473472485
H	1.0	2.4699043254	-2.1475193776	-0.0320665782
H	1.0	0.1867298387	-3.1623543148	0.0194584991
H	1.0	-1.0026355732	-2.1368599443	-0.8164899176
H	1.0	-0.9490373895	-2.1598393867	0.9517391041

Cartesian coordinates (Å) of the optimized structure for compound **5a** in ethanol

C	6.0	1.9842724216	-1.3426787115	-0.0063520238
C	6.0	0.6160429605	-1.2315086898	0.0097008679
C	6.0	2.1491444453	1.0841700620	0.0428948971
O	8.0	0.0228581152	0.0074240249	0.0328852546
C	6.0	0.7773108356	1.1566590030	0.0490719814
C	6.0	2.8365638995	-0.1813534069	-0.0074533414
H	1.0	2.7279644250	2.0019132293	0.0538112706
O	8.0	4.1018557051	-0.2692758249	-0.0626901018
C	6.0	0.0197176262	2.3770333706	0.0616114288
H	1.0	0.6120652168	3.2848166822	0.0903220590
C	6.0	-1.3503886341	2.4229278857	0.0151109490
N	7.0	-2.1312340745	3.5270898688	0.0705832396
C	6.0	-3.5450397770	3.4373080042	-0.2901727491
H	1.0	-1.9046703516	1.4924723546	-0.0542562000
H	1.0	-3.9069196531	2.4176629095	-0.1349549603
H	1.0	-3.7105318734	3.7123428699	-1.3415034665

H	1.0	-4.1353600124	4.1080814609	0.3420177472
C	6.0	-1.5342511728	4.8570713372	0.0765327300
H	1.0	-2.3062850074	5.5974002195	0.2967283145
H	1.0	-1.0821533541	5.1052246250	-0.8948816591
H	1.0	-0.7651179774	4.9282123743	0.8524417823
H	1.0	2.4309490097	-2.3307856461	-0.0347963093
C	6.0	-0.2922521250	-2.3437139447	0.0052458998
H	1.0	0.1805960280	-3.3193145695	0.0052363981
C	6.0	-1.6584071481	-2.2237085914	-0.0168265451
N	7.0	-2.5566163940	-3.2339691619	-0.0924244666
H	1.0	-2.1042004164	-1.2343111271	0.0134671845
C	6.0	-2.1136603968	-4.6228932133	-0.0613917849
C	6.0	-3.9661403279	-2.9834000971	0.1985790216
H	1.0	-4.2009724696	-1.9284237741	0.0337144675
H	1.0	-4.2156192349	-3.2360076414	1.2391023124
H	1.0	-4.5983567005	-3.5814917217	-0.4652860380
H	1.0	-1.3354529673	-4.7935748484	-0.8123306212
H	1.0	-2.9575387792	-5.2758140740	-0.2948127482
H	1.0	-1.7197362374	-4.9040624135	0.9264994253

Cartesian coordinates (Å) of the optimized structure for compound **4a** in methanol

C	6.0	2.0000929414	-1.1705113088	-0.0026779247
C	6.0	0.6503498696	-1.0757679552	0.0243738104
C	6.0	2.1217179167	1.2665822187	-0.0057836954
O	8.0	0.0250087754	0.1392290303	0.0362603519
C	6.0	0.7433262150	1.3092879128	0.0181337403
C	6.0	2.8346036164	0.0234023724	-0.0228864163
H	1.0	2.6789602840	2.1977046949	-0.0172387401
O	8.0	4.0973843869	-0.0524974480	-0.0567497553
C	6.0	-0.0528631861	2.4986997244	0.0200248515
H	1.0	0.4997567729	3.4312247752	0.0044667322
C	6.0	-1.4286775721	2.4774957191	0.0249245071
N	7.0	-2.2511505612	3.5444117826	0.0634287738
C	6.0	-3.6890131210	3.3821783470	-0.1399192977
H	1.0	-1.9373744986	1.5177448323	0.0118499189
H	1.0	-3.9729391407	2.3391280509	0.0186133583
H	1.0	-3.9849065056	3.6769441957	-1.1560779969
H	1.0	-4.2423864396	3.9988479391	0.5762565572
C	6.0	-1.7183274910	4.9018771531	0.0243071519
H	1.0	-2.5228290991	5.6113327971	0.2278149457
H	1.0	-1.2866030600	5.1386272443	-0.9581401951
H	1.0	-0.9465141221	5.0340021579	0.7901717021
C	6.0	-0.3305514390	-2.1996344445	0.0436895900
H	1.0	2.4699969386	-2.1478673278	-0.0121931923
H	1.0	0.1857777683	-3.1617663331	0.0227844127
H	1.0	-0.9997571853	-2.1395135432	-0.8230004736
H	1.0	-0.9529739714	-2.1533287715	0.9454230681

Cartesian coordinates (Å) of the optimized structure for compound **5a** in methanol

C	6.0	1.9814883262	-1.3420839671	0.0400373673
C	6.0	0.6132189491	-1.2307886054	0.0108577525
C	6.0	2.1483723441	1.0836581617	-0.0138388485
O	8.0	0.0205446854	0.0079614174	-0.0223700777
C	6.0	0.7751907222	1.1577139628	-0.0322536389
C	6.0	2.8330591021	-0.1814305312	0.0280350996
H	1.0	2.7275306830	2.0012382643	-0.0160243064
O	8.0	4.1006086148	-0.2713291965	0.0600092628
C	6.0	0.0196669931	2.3771111332	-0.0550299587
H	1.0	0.6122209090	3.2836885217	-0.1083826926
C	6.0	-1.3502937874	2.4269552794	0.0216784161

N	7.0	-2.1169944066	3.5375764220	0.0745694219
C	6.0	-3.5698239759	3.4476294687	-0.0489561355
H	1.0	-1.9089777318	1.4978411555	0.0659720017
H	1.0	-3.8983489873	2.4223482534	0.1380976941
H	1.0	-3.9054843861	3.7454640454	-1.0518589979
H	1.0	-4.0516470468	4.1000770994	0.6873346062
C	6.0	-1.5167018074	4.8618761928	-0.0372647906
H	1.0	-2.2751012268	5.6201654263	0.1675457413
H	1.0	-1.1109978335	5.0394441350	-1.0433682503
H	1.0	-0.7094746731	4.9819823282	0.6936705401
H	1.0	2.4263822734	-2.3310332859	0.0664651329
C	6.0	-0.2932146819	-2.3440227910	0.0128450441
H	1.0	0.1811377843	-3.3184685335	0.0434402973
C	6.0	-1.6590654319	-2.2279299638	-0.0380427829
N	7.0	-2.5523234990	-3.2422397015	-0.1135976940
H	1.0	-2.1076335761	-1.2392479136	-0.0356066024
C	6.0	-2.1052997286	-4.6292125355	-0.0564398331
C	6.0	-3.9675083763	-2.9933330767	0.1510806225
H	1.0	-4.2028015076	-1.9405004890	-0.0258944478
H	1.0	-4.2331307115	-3.2385872187	1.1893027802
H	1.0	-4.5869149880	-3.5987550244	-0.5182022299
H	1.0	-1.3165041042	-4.8074905536	-0.7945431539
H	1.0	-2.9439616357	-5.2880242109	-0.2920684706
H	1.0	-1.7240239029	-4.8952667054	0.9404293872

3. Cartesian coordinates of the S₁ relaxed geometry for compounds 4a and 5a

Cartesian coordinates (Å) of the S₁ relaxed geometry for compound **4a** in vacuo

C	6.0	2.0017347376	-1.1633371813	-0.0083451048
C	6.0	0.6576075560	-1.0832466531	0.0353167234
C	6.0	2.0951593376	1.2717697196	-0.0339121942
O	8.0	-0.0005409512	0.1235959111	0.0448529186
C	6.0	0.7288854235	1.3036312245	0.0121018727
C	6.0	2.7840224206	0.0411559671	-0.0465719771
H	1.0	2.6459203455	2.2029266602	-0.0598946466
O	8.0	4.1010218243	-0.0279396513	-0.0931852806
C	6.0	-0.0748442153	2.4898601430	0.0260891241
H	1.0	0.4744018750	3.4231191950	-0.0101415006
C	6.0	-1.4301367426	2.4699311587	0.0888145250
N	7.0	-2.2651926775	3.5576615407	0.1829336935
C	6.0	-3.6233421443	3.4030914651	-0.3012920493
H	1.0	-1.9417975773	1.5136081108	0.1005853086
H	1.0	-3.9917285475	2.4078809923	-0.0437986836
H	1.0	-3.6976640288	3.5272382967	-1.3930134985
H	1.0	-4.2734429525	4.1409544109	0.1758431743
C	6.0	-1.6994600369	4.8823410916	0.0698689217
H	1.0	-2.4698392107	5.6230483625	0.2922230283
H	1.0	-1.2992440242	5.0829260786	-0.9370818810
H	1.0	-0.8896772184	5.0067944357	0.7933710741
C	6.0	-0.2973117413	-2.2224159128	0.0783083458
H	1.0	2.4879935290	-2.1294193150	-0.0145095839
H	1.0	0.2358340149	-3.1739597653	0.0701606735
H	1.0	-0.9732058552	-2.1887640849	-0.7833454508
H	1.0	-0.9152687919	-2.1710065058	0.9815296298

Cartesian coordinates (Å) of the S₁ relaxed geometry for compound **5a** in vacuo

C	6.0	2.0011917151	-1.3228726909	0.0103892830
C	6.0	0.6206863997	-1.2268137467	-0.0053472271
C	6.0	2.1516042229	1.0627645714	0.0027047089
O	8.0	-0.0100955141	0.0011456267	-0.0147248991
C	6.0	0.7697273780	1.1405117302	0.0018907812
C	6.0	2.8786429311	-0.1806123236	0.0064367843
H	1.0	2.7174572698	1.9883013100	0.0110706938
O	8.0	4.1307255904	-0.2604174425	0.0092855840
C	6.0	0.0206451203	2.3334857139	0.0187429347
H	1.0	0.5888597450	3.2551126530	0.0061555183
C	6.0	-1.3636642877	2.3456078804	0.0481468604
N	7.0	-2.1435347792	3.4563514953	0.1192680405
C	6.0	-3.5566131405	3.3374135235	-0.1728719712
H	1.0	-1.8987004915	1.4035630706	0.0524143774
H	1.0	-3.9201015476	2.3643228561	0.1642130942
H	1.0	-3.7615277325	3.4299326066	-1.2511147728
H	1.0	-4.1127433629	4.1145045255	0.3562190234
C	6.0	-1.5558414175	4.7751784884	0.0227651421
H	1.0	-2.3129367508	5.5233760430	0.2601144988
H	1.0	-1.1665182855	4.9758258703	-0.9872672536
H	1.0	-0.7359806804	4.8790040547	0.7375628426
H	1.0	2.4457787748	-2.3123572156	0.0180220823
C	6.0	-0.2716790931	-2.3165839348	-0.0149151344
H	1.0	0.1753229341	-3.3021570699	0.0187748384
C	6.0	-1.6462755597	-2.1563876179	-0.0657497931
N	7.0	-2.5578337206	-3.1626849777	-0.1251657043
H	1.0	-2.0601285556	-1.1555882268	-0.0991010489

C	6.0	-2.1436121566	-4.5407673636	0.0270474404
C	6.0	-3.9503250029	-2.8560264391	0.1282135457
H	1.0	-4.1825894688	-1.8618631730	-0.2596431788
H	1.0	-4.1851481651	-2.8732839817	1.2041884808
H	1.0	-4.5895074808	-3.5808273453	-0.3806410220
H	1.0	-1.3335840707	-4.7739614021	-0.6681920458
H	1.0	-2.9859021335	-5.1957005853	-0.1982260158
H	1.0	-1.7967063719	-4.7512366765	1.0504826713

Cartesian coordinates (Å) of the S₁ relaxed geometry for compound **4a** in DMSO

C	6.0	2.0019152971	-1.1403326272	0.0728316384
C	6.0	0.6541725469	-1.0733456972	0.0314668449
C	6.0	2.1211947139	1.2648600540	-0.0707593358
O	8.0	-0.0157771157	0.1136163757	-0.0616966221
C	6.0	0.7112137596	1.2986938803	-0.0664866428
C	6.0	2.8516675975	0.0458773281	0.0064964252
H	1.0	2.6560240423	2.2093376505	-0.1040487863
O	8.0	4.1172872644	-0.0334629350	0.0213987212
C	6.0	-0.0705863570	2.4528841257	-0.0748410141
H	1.0	0.4643288249	3.3951498174	-0.0686215160
C	6.0	-1.4888210528	2.4456501433	-0.0869743108
N	7.0	-2.2443960150	3.5496517252	0.0632216576
C	6.0	-3.6867256291	3.4537832987	-0.0436364497
H	1.0	-2.0197981028	1.5036395117	-0.1321389741
H	1.0	-4.0103280607	2.4274080543	0.1371385457
H	1.0	-4.0280829098	3.7627425544	-1.0428501699
H	1.0	-4.1584462408	4.1036496029	0.6985471159
C	6.0	-1.6698715105	4.8799450443	0.1099346139
H	1.0	-2.4473854614	5.5965073179	0.3731545002
H	1.0	-1.2529830314	5.1671646381	-0.8666084543
H	1.0	-0.8768506558	4.9409336384	0.8611879208
C	6.0	-0.2891593184	-2.2210103875	0.0789615589
H	1.0	2.4740021704	-2.1142915426	0.1453142846
H	1.0	0.2500434510	-3.1667398560	0.1481548354
H	1.0	-0.9171166600	-2.2391831629	-0.8192292107
H	1.0	-0.9593241247	-2.1330036742	0.9417651695

Cartesian coordinates (Å) of the S₁ relaxed geometry for compound **5a** in DMSO

C	6.0	1.9860997167	-1.3172429468	0.0399264266
C	6.0	0.5992446833	-1.2263807349	-0.0008975574
C	6.0	2.1414828996	1.0591849829	0.0040996566
O	8.0	-0.0263699028	0.0051219603	-0.0882482572
C	6.0	0.7536466045	1.1477010743	-0.0242336034
C	6.0	2.8536827911	-0.1809703861	0.0121982756
H	1.0	2.7027417898	1.9883789260	0.0351205313
O	8.0	4.1313742115	-0.2648106773	0.0159522943
C	6.0	0.0227543076	2.3474182238	0.0014432443
H	1.0	0.6027181108	3.2622357523	0.0272988184
C	6.0	-1.3691040881	2.3893292793	-0.0142067704
N	7.0	-2.1161131869	3.5033330668	0.0453602853
C	6.0	-3.5607635109	3.4294984306	-0.0772347885
H	1.0	-1.9226171467	1.4591676379	-0.0461409698
H	1.0	-3.8993580382	2.4062373099	0.0932797376
H	1.0	-3.8911394201	3.7489462613	-1.0743849791
H	1.0	-4.0328846417	4.0754837979	0.6687812523
C	6.0	-1.5095384376	4.8210465805	0.0472622441
H	1.0	-2.2780338638	5.5696915132	0.2400573516
H	1.0	-1.0414983525	5.0461080872	-0.9204289886
H	1.0	-0.7506866706	4.8996896304	0.8320113786
H	1.0	2.4206278779	-2.3110111565	0.0944837579

C	6.0	-0.2789708428	-2.3233745048	0.0273613145
H	1.0	0.1796005489	-3.3028411512	0.0933295528
C	6.0	-1.6630348122	-2.1947088528	-0.0355437191
N	7.0	-2.5394304803	-3.2124123674	-0.0558081724
H	1.0	-2.1009663769	-1.2047926688	-0.0752576052
C	6.0	-2.0984105925	-4.5911780957	0.0355814615
C	6.0	-3.9648876327	-2.9585785728	0.0564934067
H	1.0	-4.1753013747	-1.9058513126	-0.1391796758
H	1.0	-4.3286590410	-3.2066051142	1.0622131515
H	1.0	-4.5152151371	-3.5621527458	-0.6710643177
H	1.0	-1.3477644295	-4.8092246728	-0.7303724992
H	1.0	-2.9505675012	-5.2519710727	-0.1251301119
H	1.0	-1.6708741651	-4.8112761528	1.0231843098

Cartesian coordinates (Å) of the S₁ relaxed geometry for compound **4a** in ethanol

C	6.0	1.9970528836	-1.1429634672	0.0335107084
C	6.0	0.6475438697	-1.0682570814	0.0373600221
C	6.0	2.1283354537	1.2626715075	-0.0033163859
O	8.0	-0.0161337986	0.1276529022	0.0086789453
C	6.0	0.7221566184	1.3082961502	0.0279281044
C	6.0	2.8410887644	0.0379488930	-0.0204049211
H	1.0	2.6717121192	2.2022484635	-0.0167013270
O	8.0	4.1194425945	-0.0434773003	-0.0951883755
C	6.0	-0.0563977740	2.4667276113	0.0305108370
H	1.0	0.4773595555	3.4094436412	0.0486901714
C	6.0	-1.4712036658	2.4486437989	-0.0108989517
N	7.0	-2.2455523612	3.5454953406	0.0479872892
C	6.0	-3.6767577534	3.4207835731	-0.1574113001
H	1.0	-1.9902220845	1.4992850230	-0.0546014818
H	1.0	-4.0002044004	2.4000209565	0.0536563239
H	1.0	-3.9418138183	3.6654687686	-1.1971980861
H	1.0	-4.2137137265	4.1040447734	0.5053748507
C	6.0	-1.6907312483	4.8860260323	0.0724741449
H	1.0	-2.4838507626	5.5974563351	0.3014321758
H	1.0	-1.2578936126	5.1541360701	-0.9023070548
H	1.0	-0.9161766241	4.9758693435	0.8392126852
C	6.0	-0.3034999740	-2.2084223496	0.0634372328
H	1.0	2.4621192164	-2.1223315163	0.0481060777
H	1.0	0.2281105309	-3.1608113028	0.0788591975
H	1.0	-0.9546925183	-2.1810629455	-0.8180481034
H	1.0	-0.9499342676	-2.1495169160	0.9468438992

Cartesian coordinates (Å) of the S₁ relaxed geometry for compound **5a** in ethanol

C	6.0	1.9777500591	-1.3164903752	0.0334019871
C	6.0	0.5896566101	-1.2235967048	0.0306925050
C	6.0	2.1390472775	1.0588825871	0.0293749135
O	8.0	-0.0362461028	0.0114228383	-0.0007961109
C	6.0	0.7503728720	1.1528382227	0.0266784065
C	6.0	2.8349679812	-0.1823450875	0.0017767739
H	1.0	2.7044001208	1.9854043934	0.0417006989
O	8.0	4.1276910648	-0.2721293435	-0.0650248116
C	6.0	0.0264664413	2.3561639115	0.0308545348
H	1.0	0.6109135060	3.2683865763	0.0381911307
C	6.0	-1.3648687286	2.4027267420	0.0067219774
N	7.0	-2.1084479459	3.5185875914	0.0284069506
C	6.0	-3.5534409038	3.4466985031	-0.1042062192
H	1.0	-1.9213320104	1.4741467035	-0.0138843071
H	1.0	-3.8955410436	2.4244966601	0.0649043740
H	1.0	-3.8753365985	3.7654244469	-1.1040311315
H	1.0	-4.0305192659	4.0942269759	0.6376136978

C	6.0	-1.4985670919	4.8359026410	0.0050023677
H	1.0	-2.2672806517	5.5903386092	0.1736315462
H	1.0	-1.0219088733	5.0380267610	-0.9632377415
H	1.0	-0.7480170844	4.9317621053	0.7956889515
H	1.0	2.4082735104	-2.3126510977	0.0390276103
C	6.0	-0.2827424140	-2.3238465104	0.0366307547
H	1.0	0.1823410825	-3.3016617990	0.0728433999
C	6.0	-1.6677194171	-2.2039115601	-0.0201392638
N	7.0	-2.5338964278	-3.2282892740	-0.0663391499
H	1.0	-2.1142340351	-1.2170464979	-0.0401286824
C	6.0	-2.0810971257	-4.6056017757	0.0111645343
C	6.0	-3.9635481996	-2.9898987017	0.0388602417
H	1.0	-4.1840607994	-1.9375565365	-0.1476201434
H	1.0	-4.3324897490	-3.2525239833	1.0387273312
H	1.0	-4.5021098824	-3.5903367734	-0.6999395382
H	1.0	-1.3316211125	-4.8121400697	-0.7590406275
H	1.0	-2.9286833432	-5.2713632554	-0.1531192926
H	1.0	-1.6503377617	-4.8307104124	0.9959031227

Cartesian coordinates (Å) of the S₁ relaxed geometry for compound **4a** in methanol

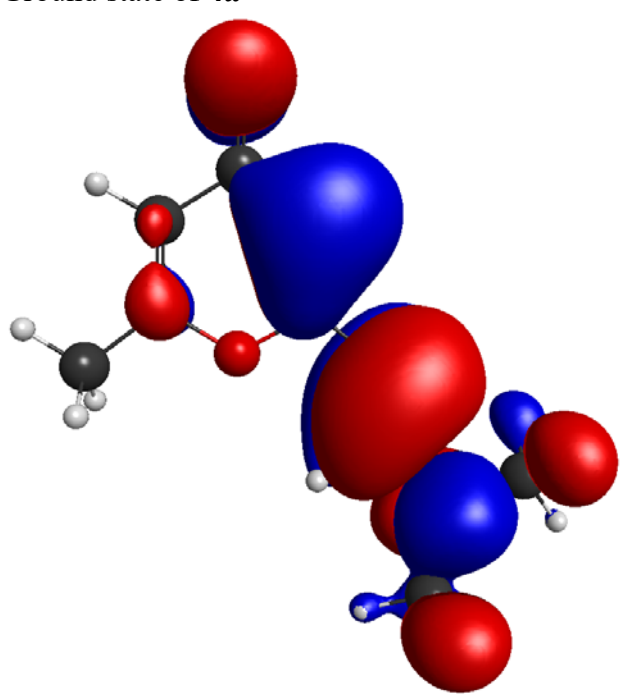
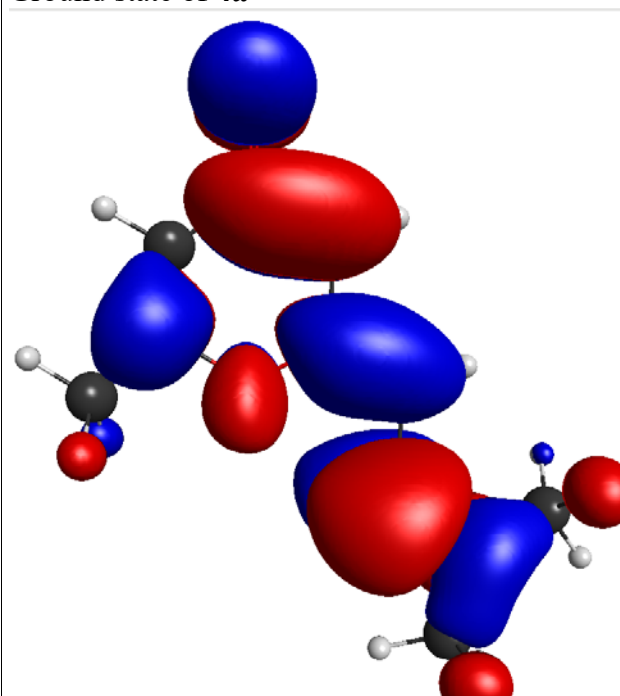
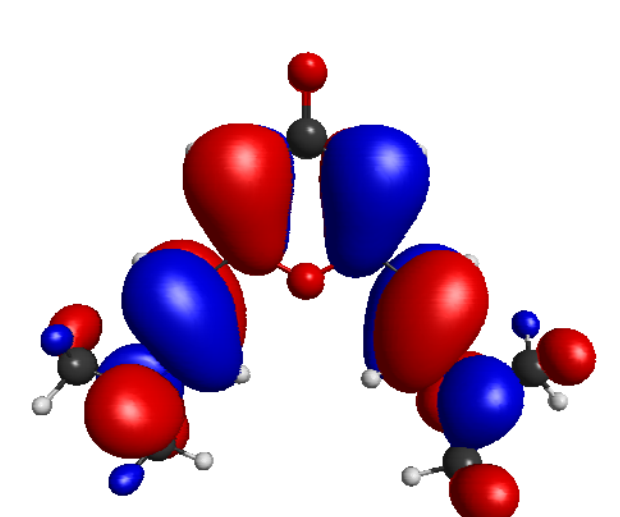
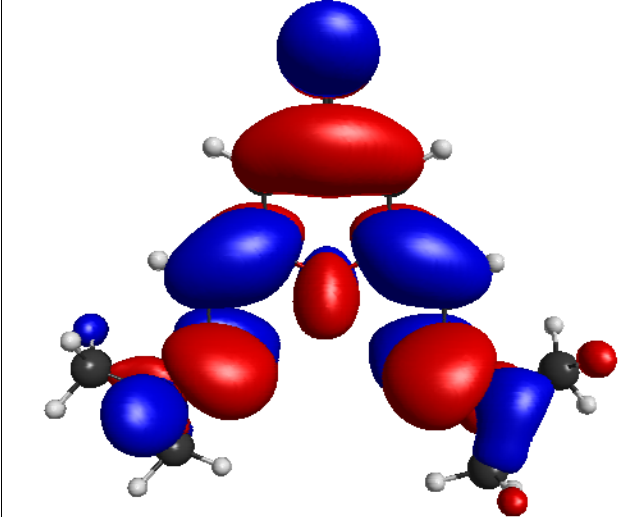
C	6.0	1.9967642032	-1.1371144005	0.0804123092
C	6.0	0.6475802114	-1.0681319875	0.0259255524
C	6.0	2.1252408842	1.2623757072	-0.0828865835
O	8.0	-0.0171652517	0.1213429590	-0.0881420867
C	6.0	0.7188634790	1.3040163303	-0.1015980752
C	6.0	2.8396540242	0.0428792571	0.0105176420
H	1.0	2.6663279569	2.2030031272	-0.1119000055
O	8.0	4.1207865256	-0.0340856812	0.0526732157
C	6.0	-0.0625868717	2.4607445926	-0.0931608907
H	1.0	0.4702784046	3.4042069332	-0.0921621363
C	6.0	-1.4782109608	2.4433063798	-0.0736383498
N	7.0	-2.2401057290	3.5410296435	0.0683478377
C	6.0	-3.6844917509	3.4355940650	-0.0222383824
H	1.0	-2.0021486553	1.4964278291	-0.1105318097
H	1.0	-3.9990577561	2.4056370725	0.1531285889
H	1.0	-4.0386461061	3.7512488512	-1.0141304906
H	1.0	-4.1515590546	4.0746235543	0.7323277056
C	6.0	-1.6736168807	4.8766708456	0.1102360555
H	1.0	-2.4572632989	5.5899802191	0.3638841462
H	1.0	-1.2527058884	5.1608711337	-0.8645624810
H	1.0	-0.8868210566	4.9462617178	0.8675552720
C	6.0	-0.2996893571	-2.2100202127	0.0817506215
H	1.0	2.4598914822	-2.1131009762	0.1732275281
H	1.0	0.2345066726	-3.1576860997	0.1633131652
H	1.0	-0.9237213500	-2.2328361633	-0.8192001586
H	1.0	-0.9727089086	-2.1077435502	0.9410126409

Cartesian coordinates (Å) of the S₁ relaxed geometry for compound **5a** in methanol

C	6.0	1.9704765034	-1.3140971993	0.0337488623
C	6.0	0.5833853593	-1.2185035259	-0.0050952844
C	6.0	2.1407734713	1.0592861052	-0.0208024938
O	8.0	-0.0387127411	0.0165090718	-0.0660990367
C	6.0	0.7515778178	1.1566324169	-0.0464017583
C	6.0	2.8312143687	-0.1837075880	0.0154943252
H	1.0	2.7084374055	1.9845041381	-0.0080051055
O	8.0	4.1263953402	-0.2799589520	0.0574706567
C	6.0	0.0290198202	2.3605366956	-0.0358805115
H	1.0	0.6136575331	3.2727081164	-0.0331717371
C	6.0	-1.3628466950	2.4070910271	-0.0220698437
N	7.0	-2.1046302272	3.5216710667	0.0492177823

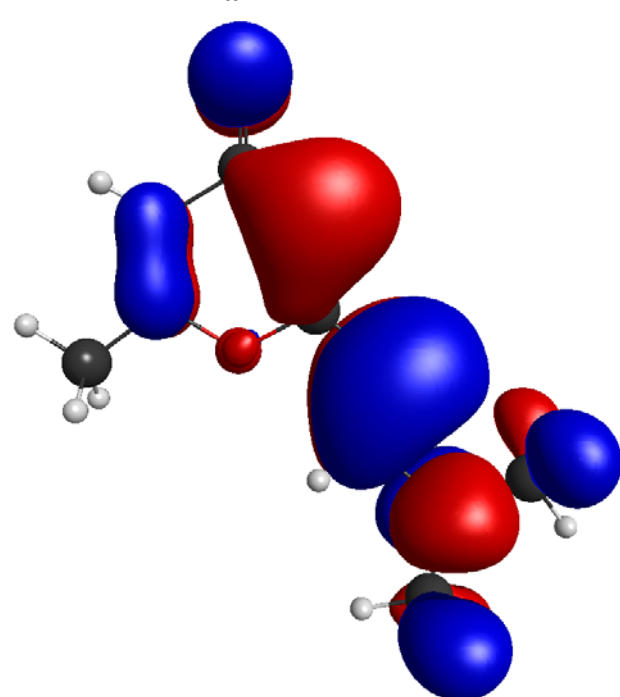
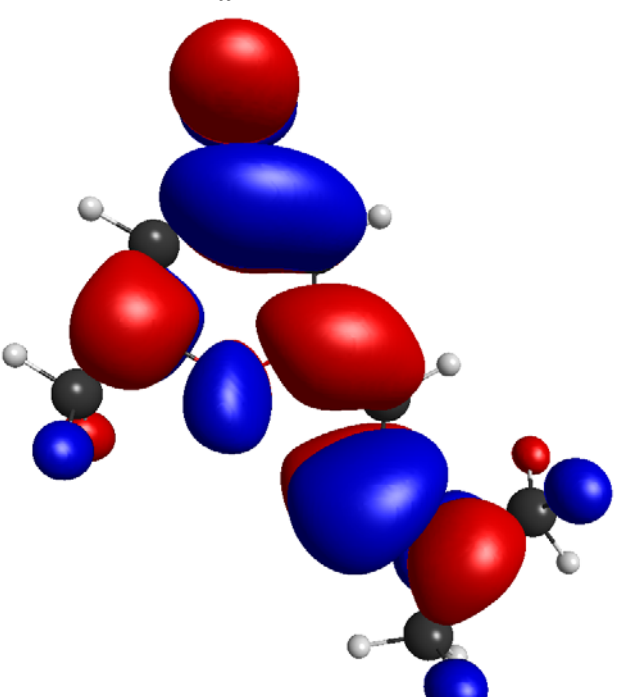
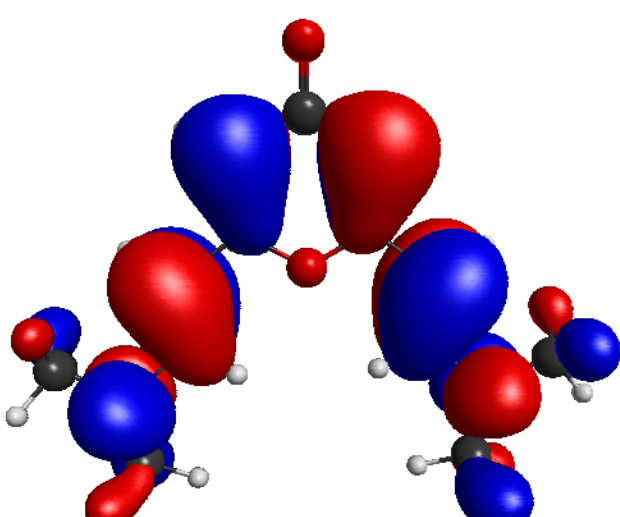
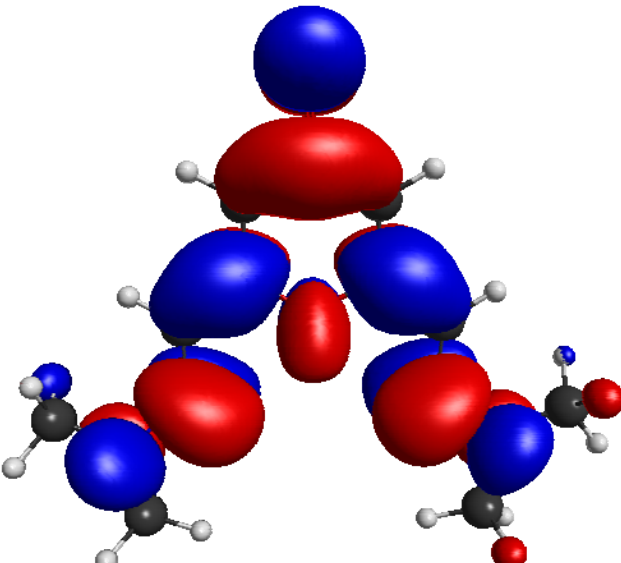
C	6.0	-3.5530487123	3.4537473149	-0.0464235788
H	1.0	-1.9194137129	1.4786517281	-0.0410820073
H	1.0	-3.8928172244	2.4306591111	0.1223343822
H	1.0	-3.8995750032	3.7820644184	-1.0347682921
H	1.0	-4.0081790323	4.0952262255	0.7137568416
C	6.0	-1.4943404905	4.8392484744	0.0417799930
H	1.0	-2.2593642430	5.5901302223	0.2396663247
H	1.0	-1.0358744063	5.0612859541	-0.9307090729
H	1.0	-0.7287468222	4.9180696268	0.8199591785
H	1.0	2.3932590243	-2.3123466234	0.0817787865
C	6.0	-0.2873529655	-2.3196900118	0.0148485201
H	1.0	0.1805840180	-3.2953225713	0.0687363916
C	6.0	-1.6727019235	-2.2063529209	-0.0375394395
N	7.0	-2.5328593290	-3.2361500439	-0.0577350406
H	1.0	-2.1246264422	-1.2221767155	-0.0683961522
C	6.0	-2.0706269374	-4.6096887875	0.0342757318
C	6.0	-3.9628636255	-3.0059267548	0.0612140176
H	1.0	-4.1926114591	-1.9569520068	-0.1327013563
H	1.0	-4.3184687266	-3.2611268494	1.0677732919
H	1.0	-4.5058762363	-3.6171579811	-0.6654170868
H	1.0	-1.3263591556	-4.8215605894	-0.7394023164
H	1.0	-2.9153782530	-5.2824975904	-0.1149178973
H	1.0	-1.6309343992	-4.8196294761	1.0183748821

4. Table S1. Ground state frontier orbitals for compounds 4a and 5a in vacuo

HOMO	LUMO
<p>Ground state of 4a</p>  <p>-5.50 eV</p>	<p>Ground state of 4a</p>  <p>-1.22 eV</p>
<p>Ground state of 5a</p>  <p>-5.20 eV</p>	<p>Ground state of 5a</p>  <p>-1.20 eV</p>

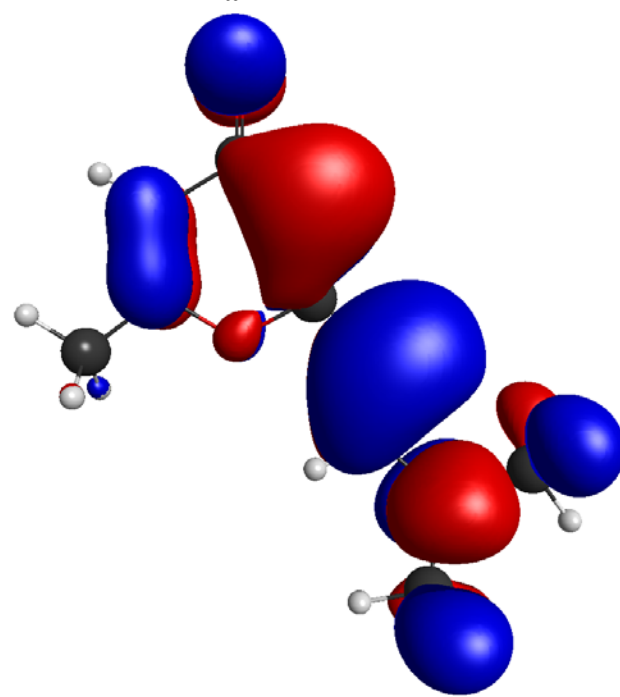
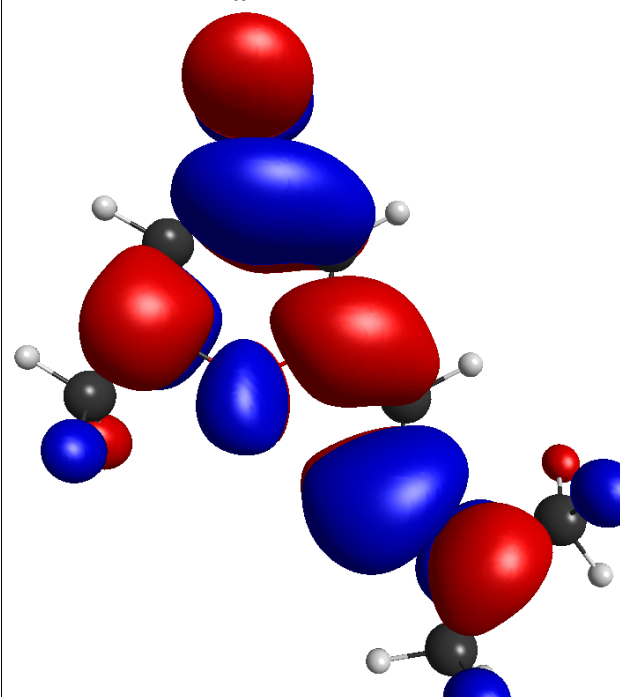
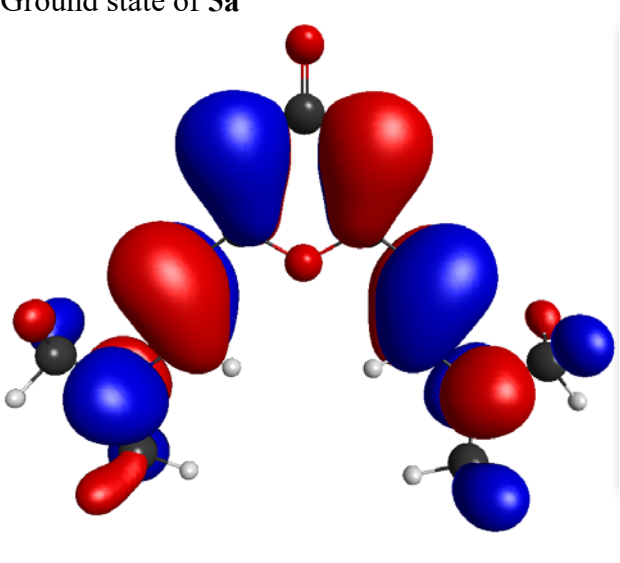
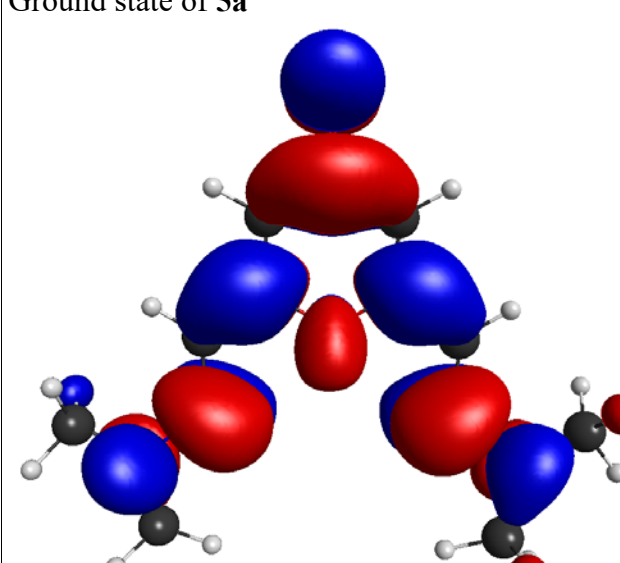
(isosurfaces correspond to 0.02psi/ 0.0004 rho)

5. Table S2. Ground state frontier orbitals for compounds 4a and 5a in DMSO

HOMO	LUMO
<p>Ground state of 4a</p>  <p>-5.28 eV</p>	<p>Ground state of 4a</p>  <p>-1.20 eV</p>
<p>Ground state of 5a</p>  <p>-5.01 eV</p>	<p>Ground state of 5a</p>  <p>-1.25 eV</p>

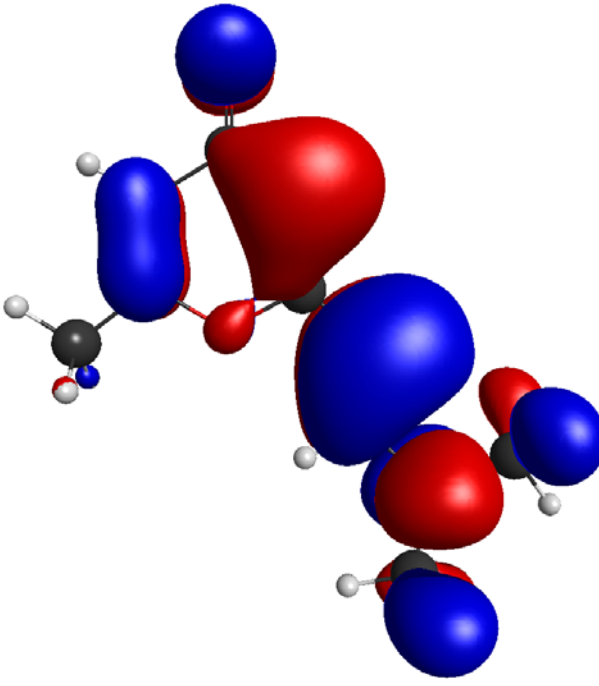
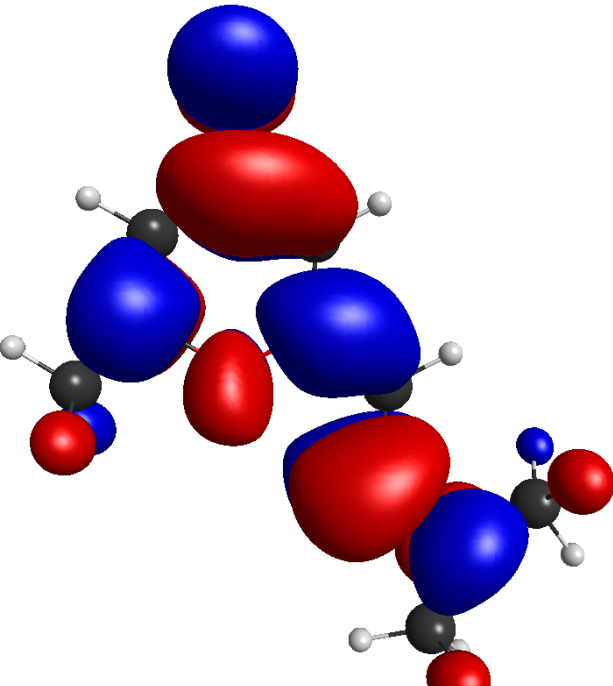
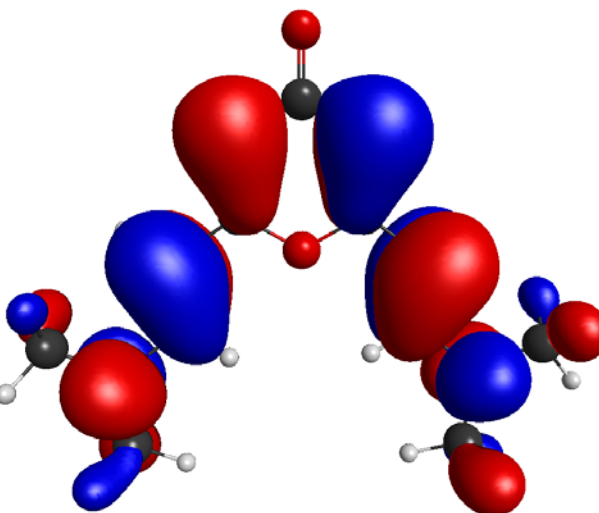
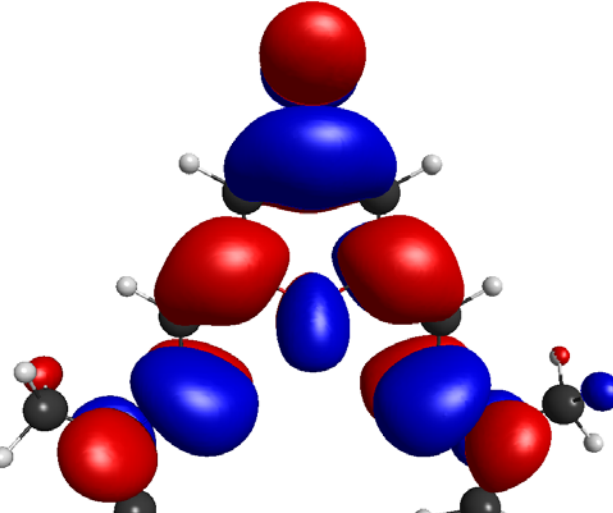
(isosurfaces correspond to 0.02psi/ 0.0004 rho)

6. Table S3. Ground state frontier orbitals for compounds 4a and 5a in ethanol

HOMO	LUMO
<p>Ground state of 4a</p>  <p>-5.36 eV</p>	<p>Ground state of 4a</p>  <p>-1.36 eV</p>
<p>Ground state of 5a</p>  <p>-5.09 eV</p>	<p>Ground state of 5a</p>  <p>-1.41 eV</p>

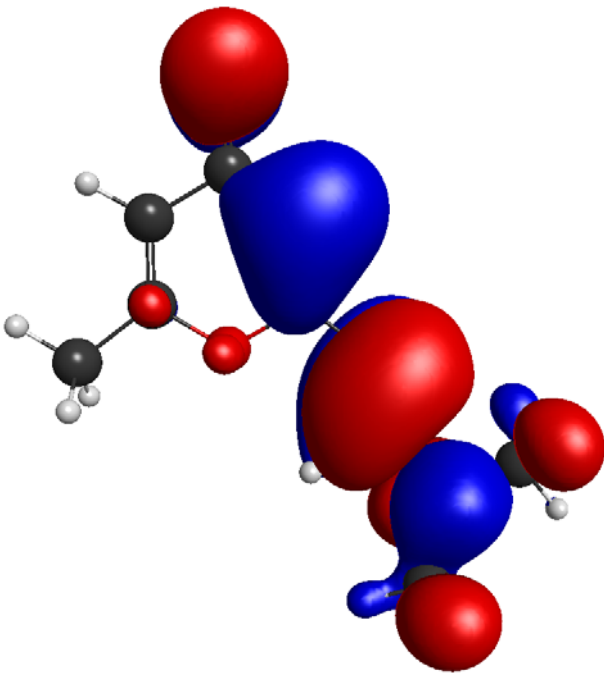
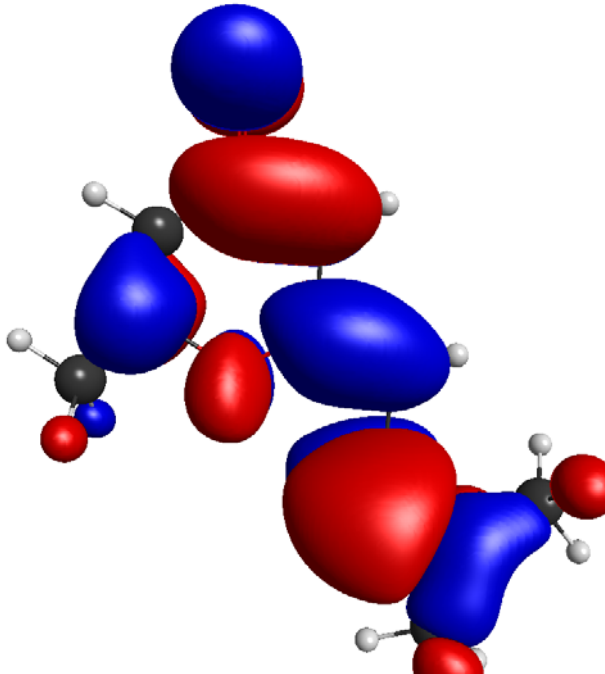
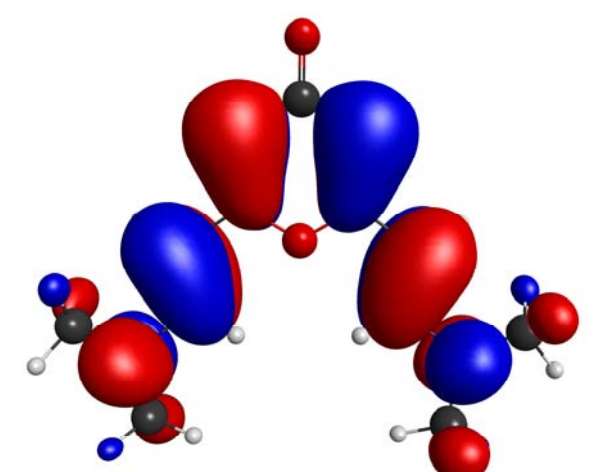
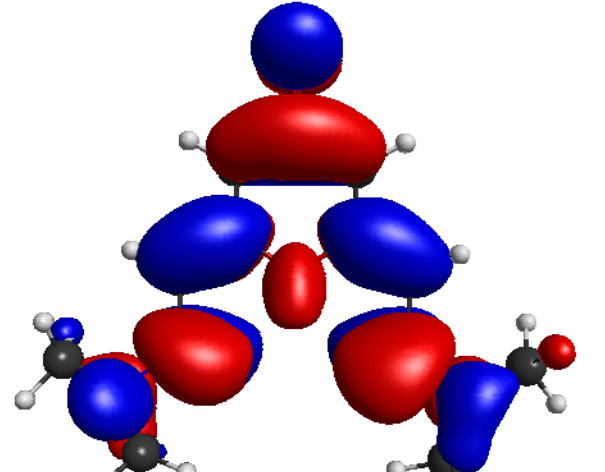
(isosurfaces correspond to 0.02psi/ 0.0004 rho)

7. Table S4. Ground state frontier orbitals for compounds 4a and 5a in methanol

HOMO	LUMO
<p data-bbox="151 306 399 340">Ground state of 4a</p>  <p data-bbox="151 1064 279 1097">-5.36 eV</p>	<p data-bbox="801 306 1048 340">Ground state of 4a</p>  <p data-bbox="801 1064 928 1097">-1.36 eV</p>
<p data-bbox="151 1117 399 1151">Ground state of 5a</p>  <p data-bbox="151 1736 279 1769">-5.06 eV</p>	<p data-bbox="801 1117 1048 1151">Ground state of 5a</p>  <p data-bbox="801 1736 928 1769">-1.41 eV</p>

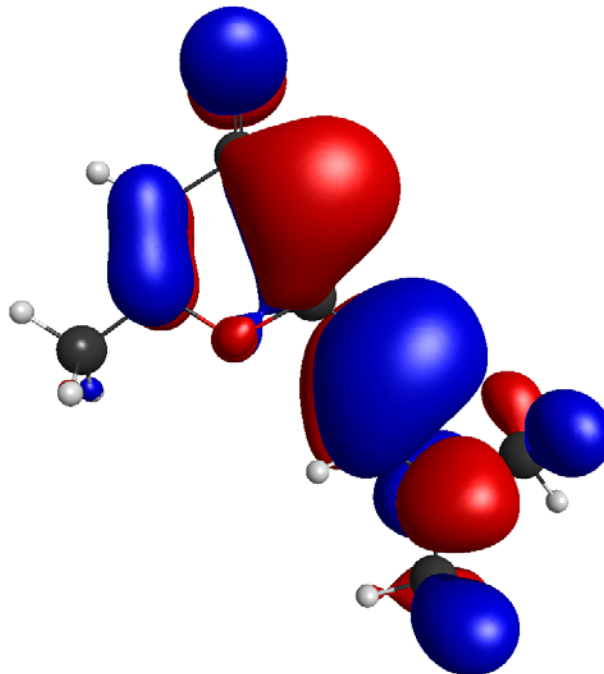
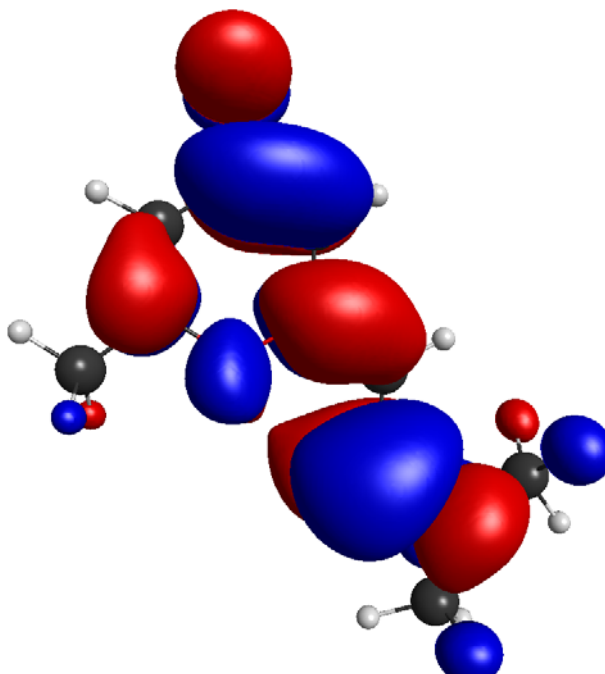
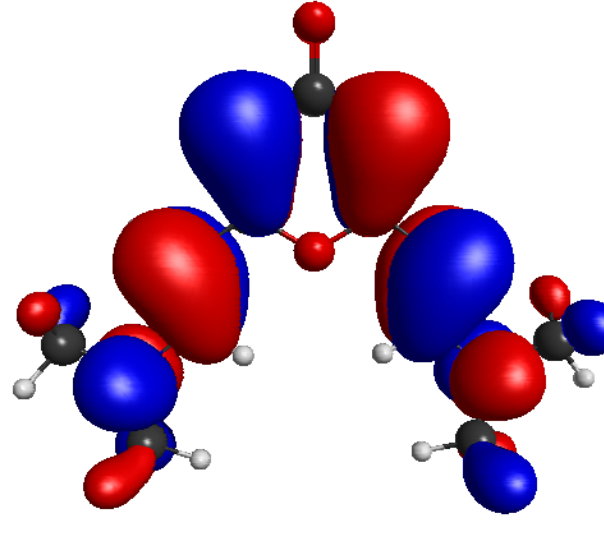
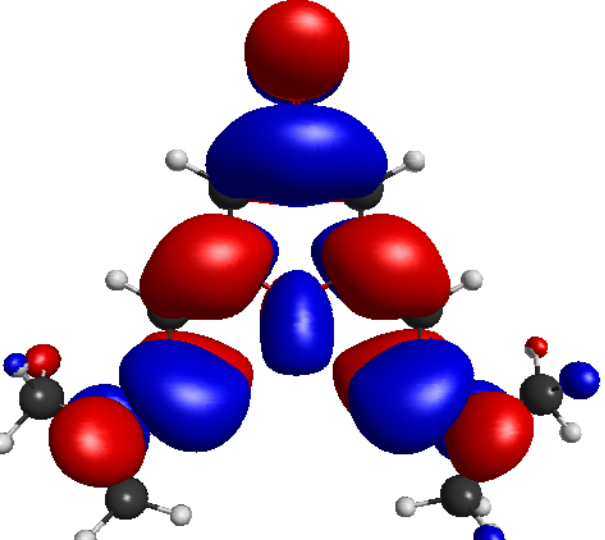
(isosurfaces correspond to 0.02psi/ 0.0004 rho)

8. Table S5. Frontier orbitals of the first singlet excited state for the relaxed geometry of compounds 4a and 5a in vacuo

HOMO	LUMO
<p>S₁ excited state of 4a</p>  <p>-7.05 eV</p>	<p>S₁ excited state of 4a</p>  <p>-0.46 eV</p>
<p>S₁ excited state of 5a</p>  <p>-6.37 eV</p>	<p>S₁ excited state of 5a</p>  <p>-0.33 eV</p>

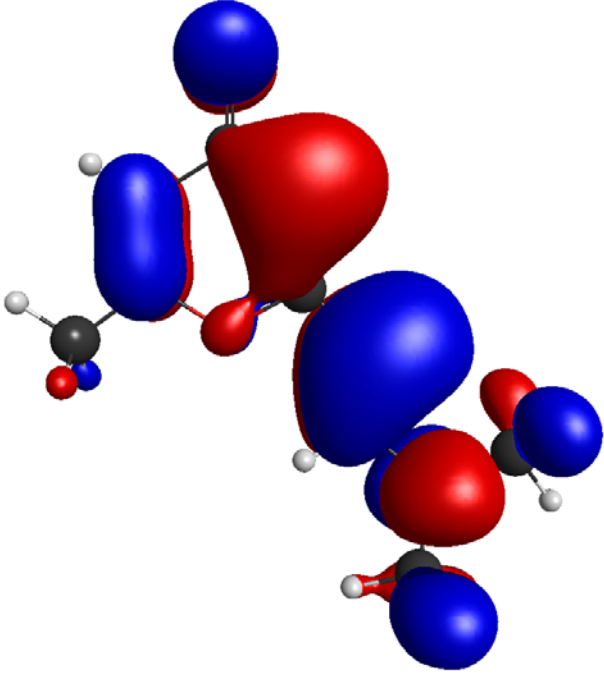
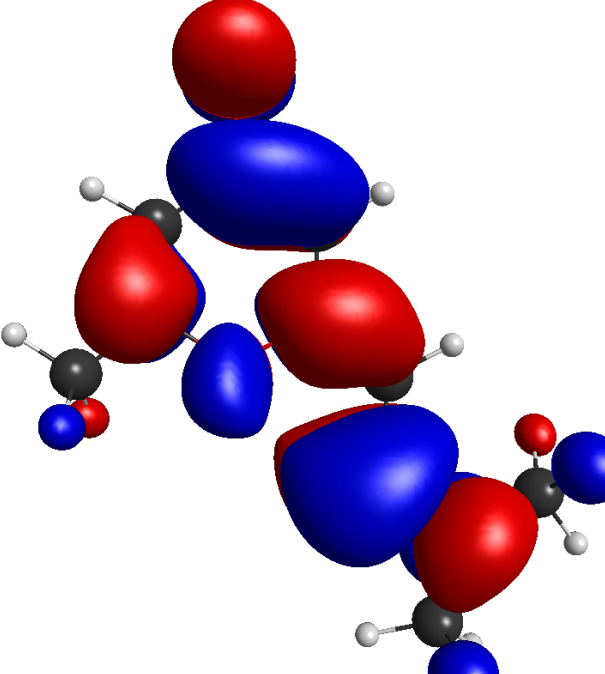
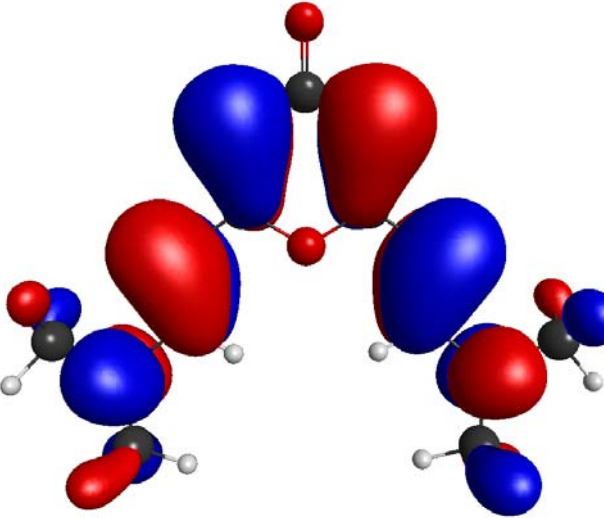
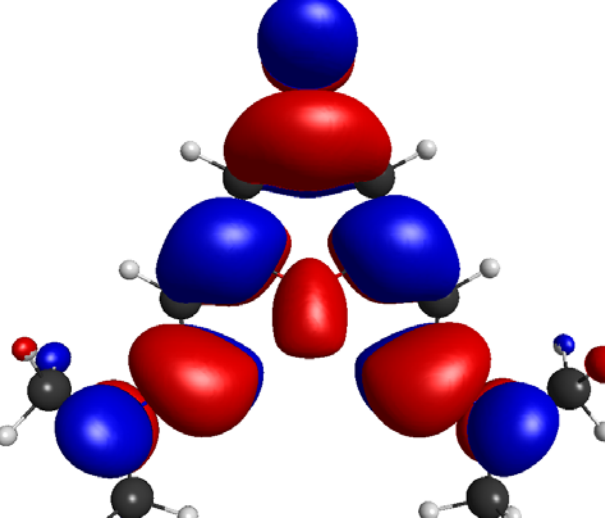
(isosurfaces correspond to 0.02psi/ 0.0004 rho)

9. Table S6. Frontier orbitals of the first singlet excited state for the relaxed geometry of compounds 4a and 5a in DMSO

HOMO	LUMO
<p>S₁ excited state of 4a</p>  <p>-6.59 eV</p>	<p>S₁ excited state of 4a</p>  <p>-0.38 eV</p>
<p>S₁ excited state of 5a</p>  <p>-6.23 eV</p>	<p>S₁ excited state of 5a</p>  <p>-0.38 eV</p>

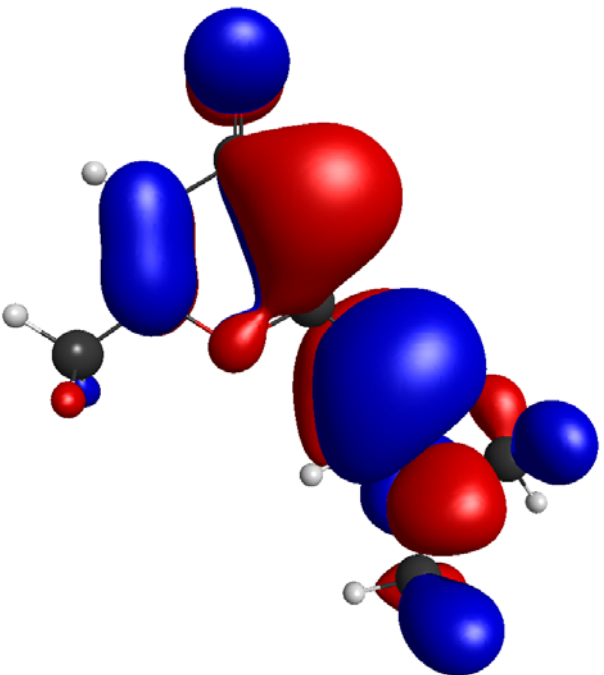
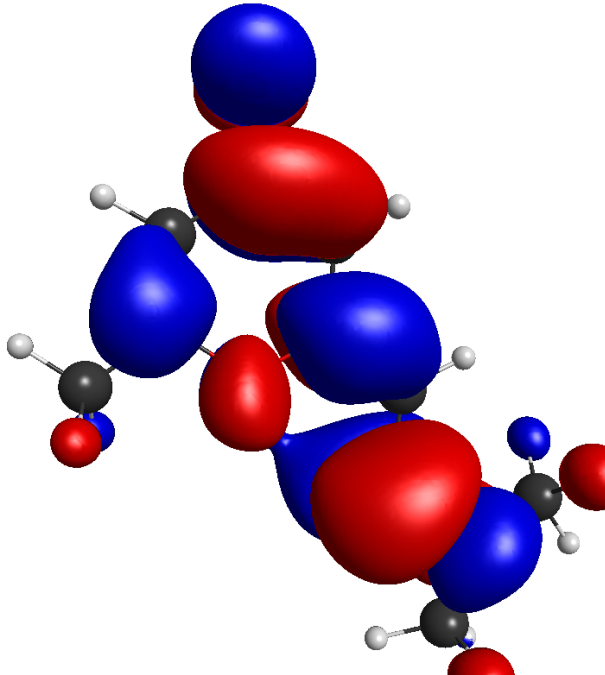
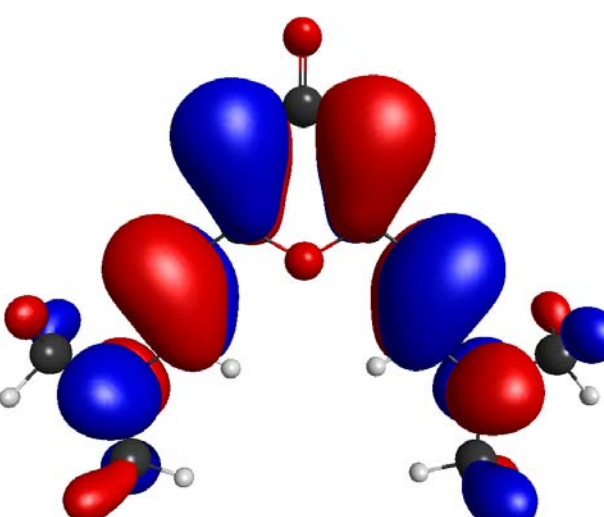
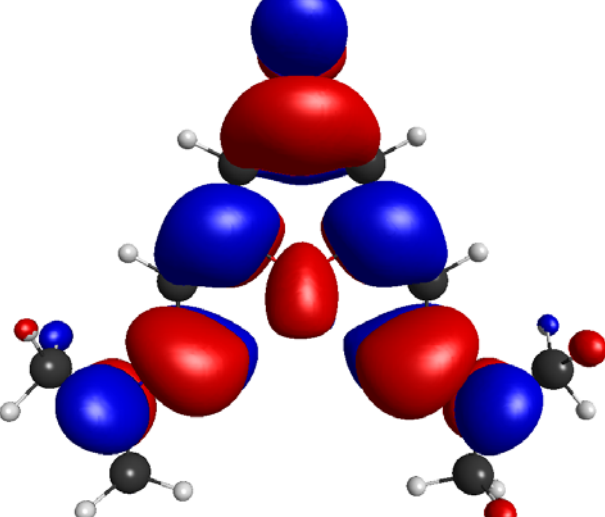
(isosurfaces correspond to 0.02psi/ 0.0004 rho)

10. Table S7. Frontier orbitals of the first singlet excited state for the relaxed geometry of compounds 4a and 5a in ethanol

HOMO	LUMO
<p>S₁ excited state of 4a</p>  <p>-6.69 eV</p>	<p>S₁ excited state of 4a</p>  <p>-0.52 eV</p>
<p>S₁ excited state of 5a</p>  <p>-6.25 eV</p>	<p>S₁ excited state of 5a</p>  <p>-0.52 eV</p>

(isosurfaces correspond to 0.02psi/ 0.0004 rho)

11. Table S8. Frontier orbitals of the first singlet excited state for the relaxed geometry of compounds 4a and 5a in methanol

HOMO	LUMO
<p>S₁ excited state of 4a</p>  <p>-6.69 eV</p>	<p>S₁ excited state of 4a</p>  <p>-0.52 eV</p>
<p>S₁ excited state of 5a</p>  <p>-6.29 eV</p>	<p>S₁ excited state of 5a</p>  <p>-0.54 eV</p>

(isosurfaces correspond to 0.02psi/ 0.0004 rho)

12. Calculated normalized UV-vis spectra for compounds 4a and 5a in DMSO, methanol, and ethanol

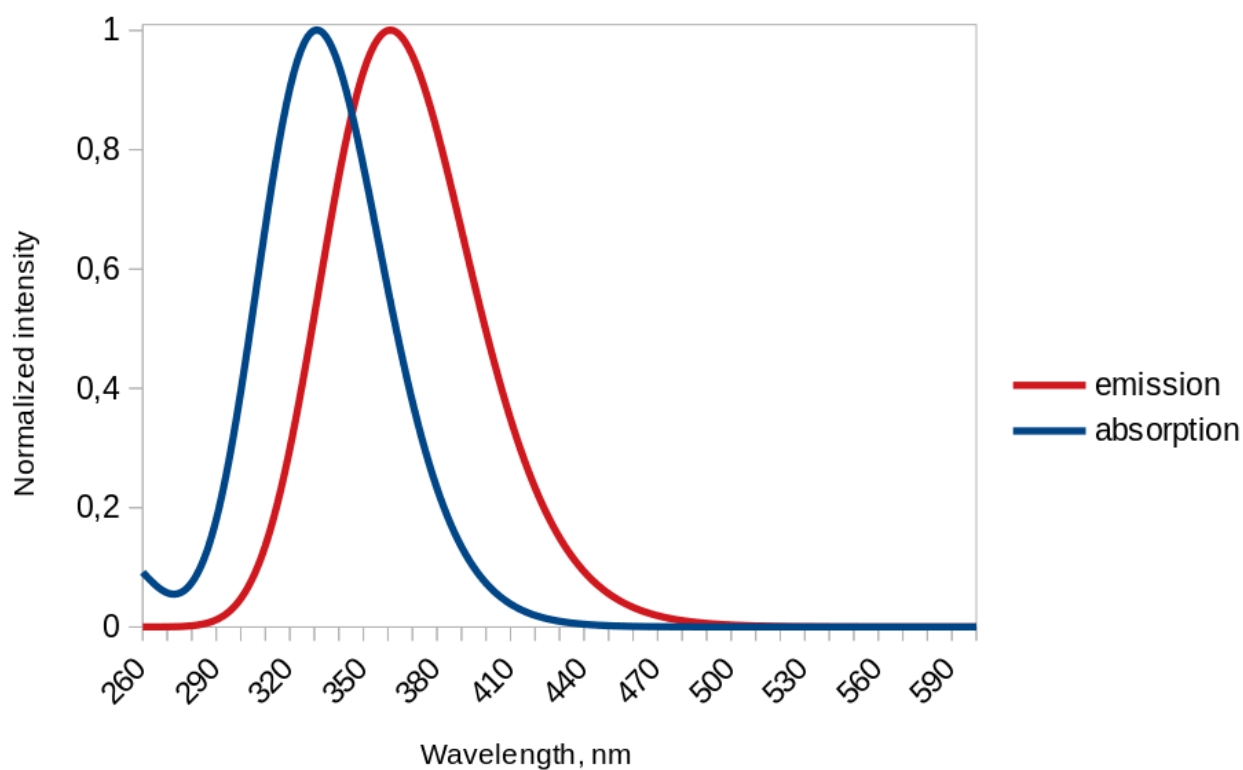


Figure S1. Normalized absorption and emission spectra of **4a** in DMSO at a CAM-B3LYP level.

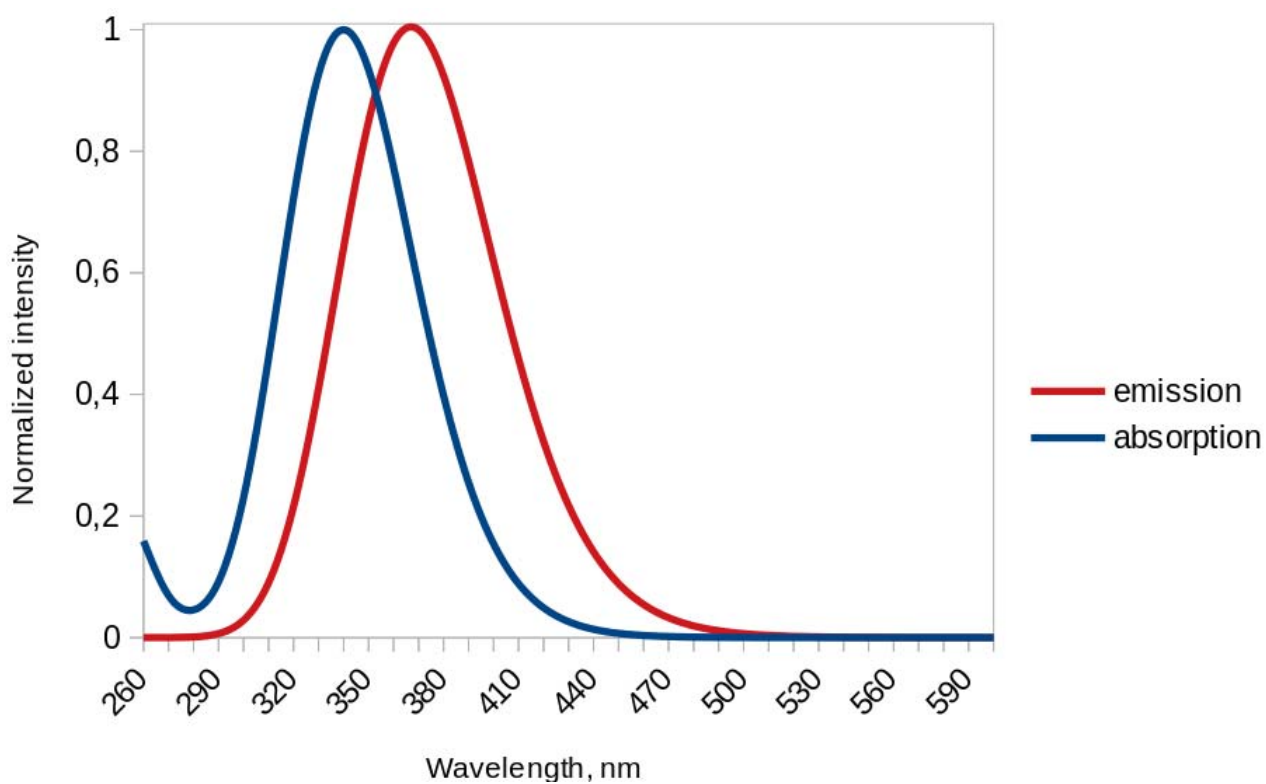


Figure S2. Normalized absorption and emission spectra of **4a** in ethanol at a CAM-B3LYP level.

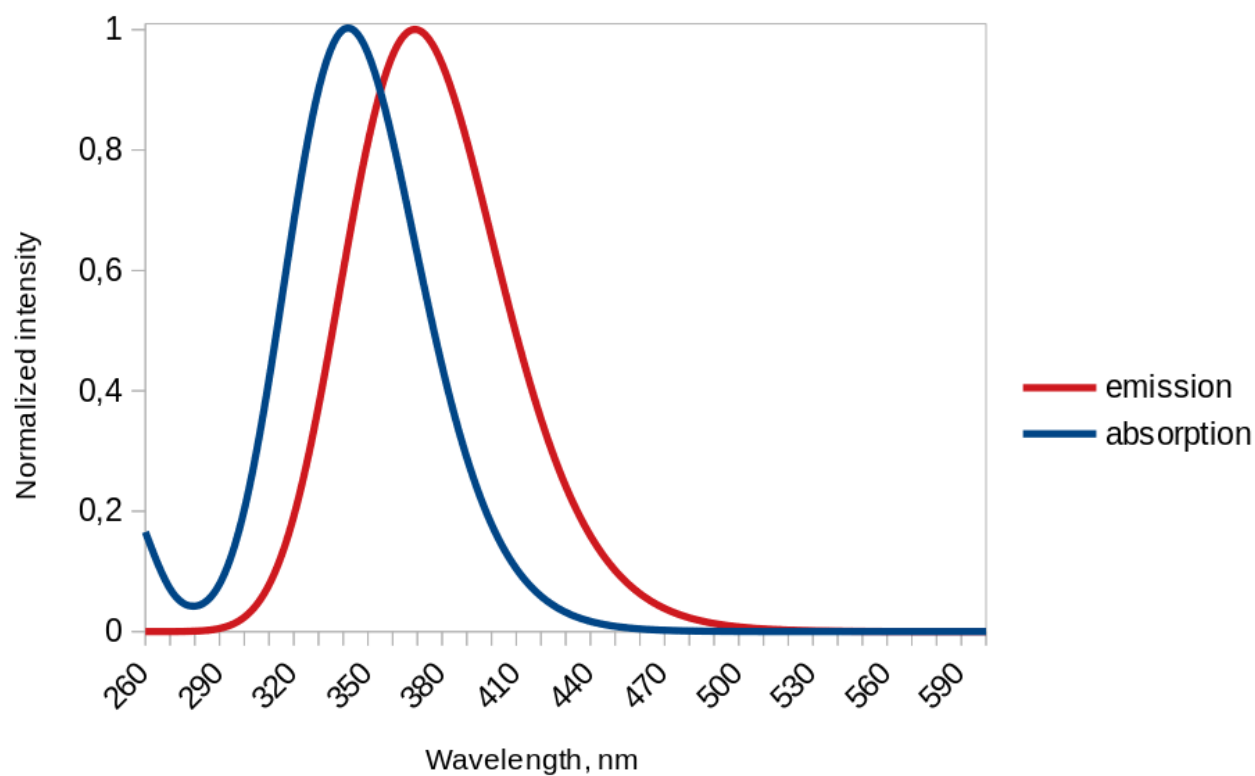


Figure S3. Normalized absorption and emission spectra of **4a** in methanol at a CAM-B3LYP level.

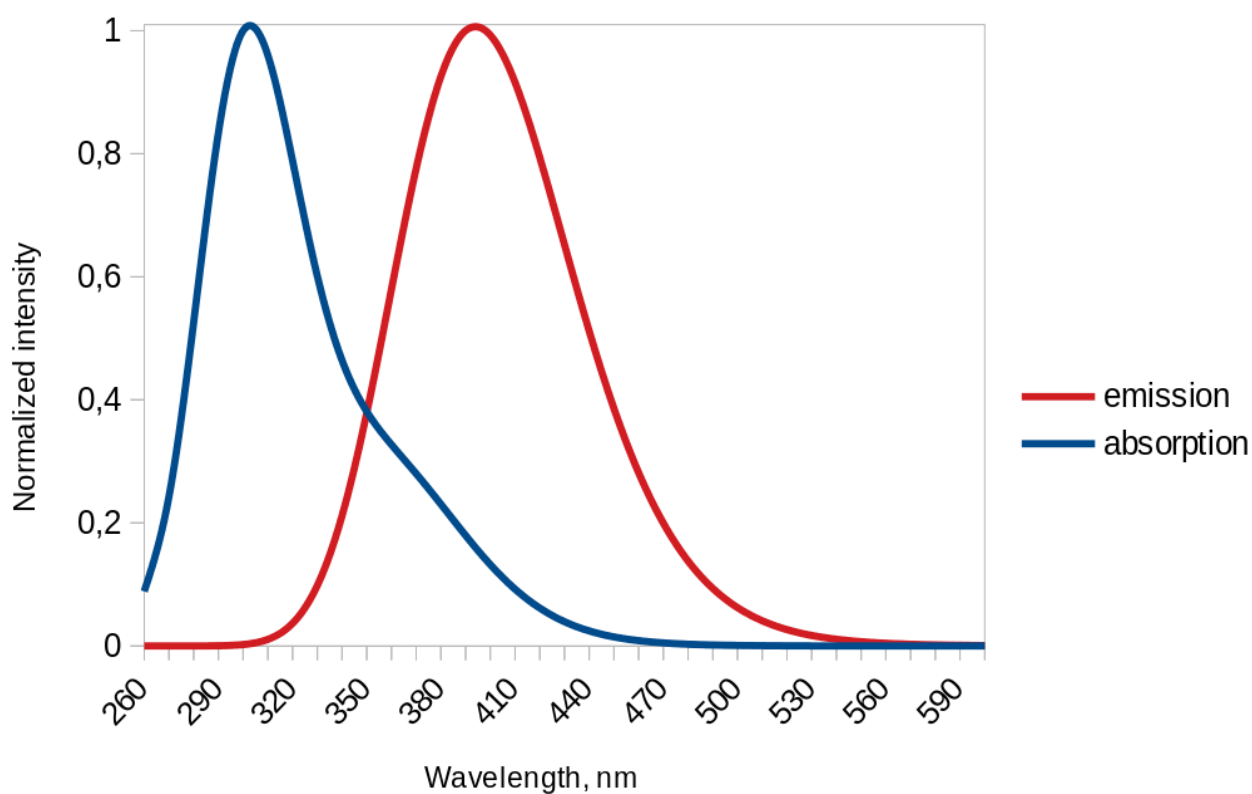


Figure S4. Normalized absorption and emission spectra of **5a** in DMSO at a CAM-B3LYP level.

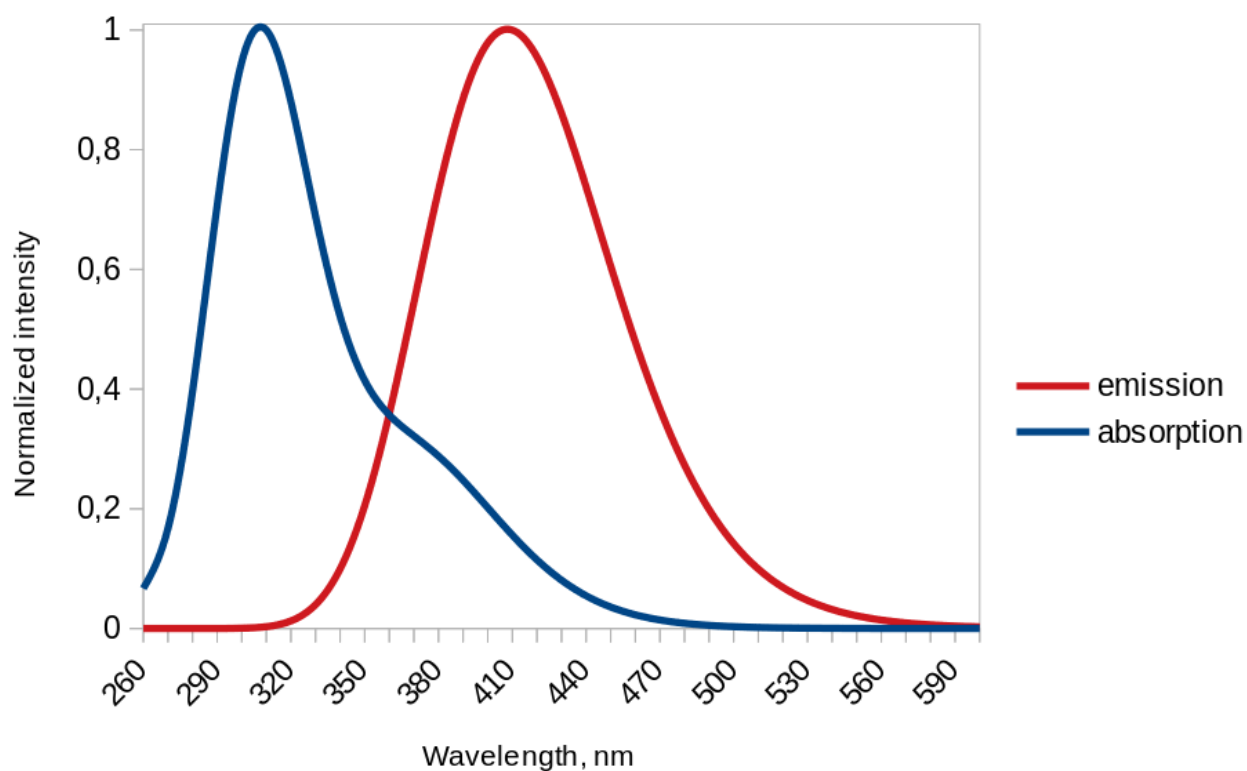


Figure S5. Normalized absorption and emission spectra of **5a** in ethanol at a CAM-B3LYP level.

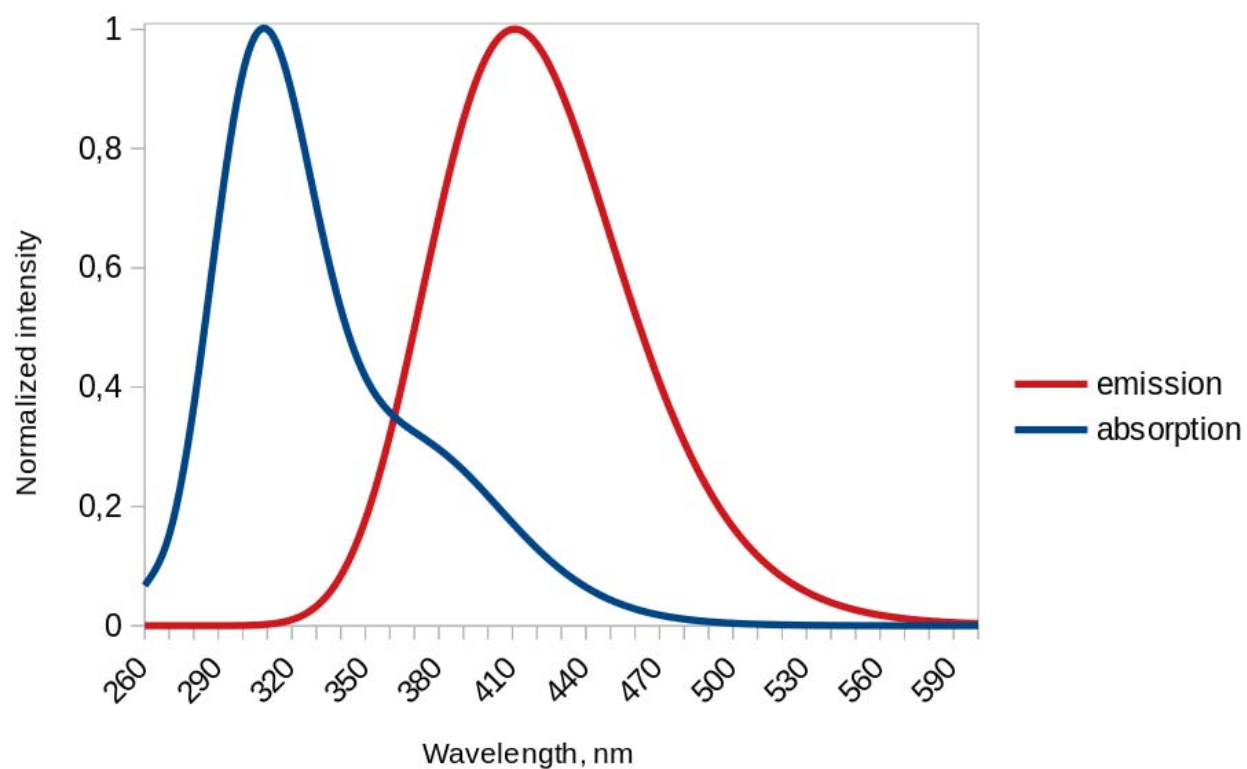


Figure S6. Normalized absorption and emission spectra of **5a** in methanol at a CAM-B3LYP level.

13. Electron density difference maps for compounds 4a and 5a

Blue and green regions correspond to the increase and decrease in electronic density respectively.

Electron density difference maps were calculated with the use of Multiwfn v3.8 [7].

7. Lu, T.; Chen, F. Multiwfn: A multifunctional wavefunction analyzer. *J. Comput. Chem.* **2012**, *33*, 580–592. doi: 10.1002/jcc.22885.

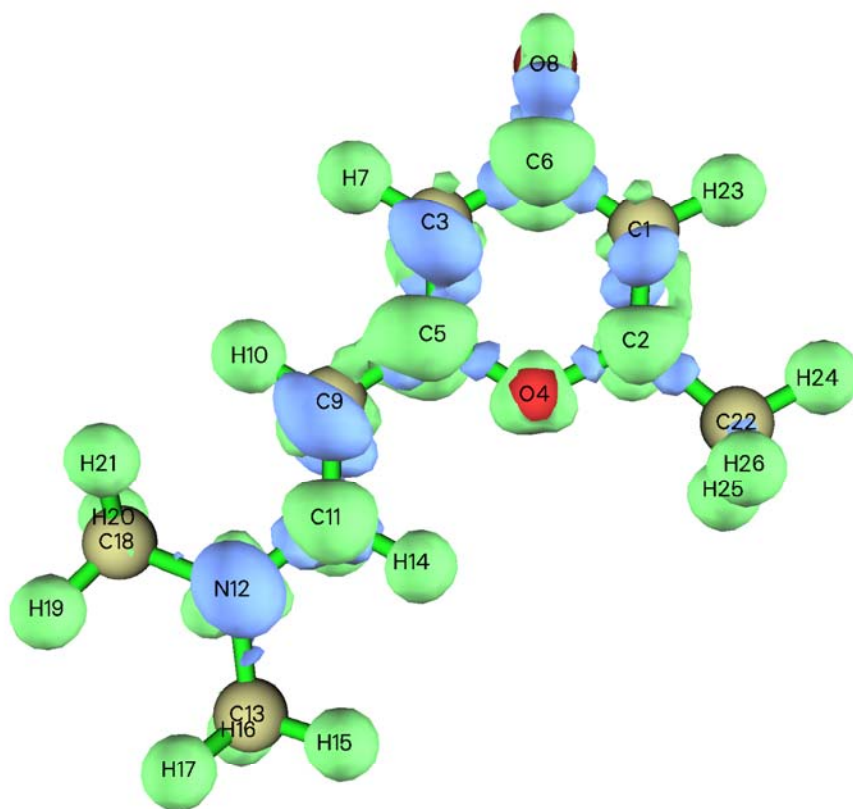


Figure S7. An electron density difference map for the S₀→S₁ transition of compound **4a** in vacuo.

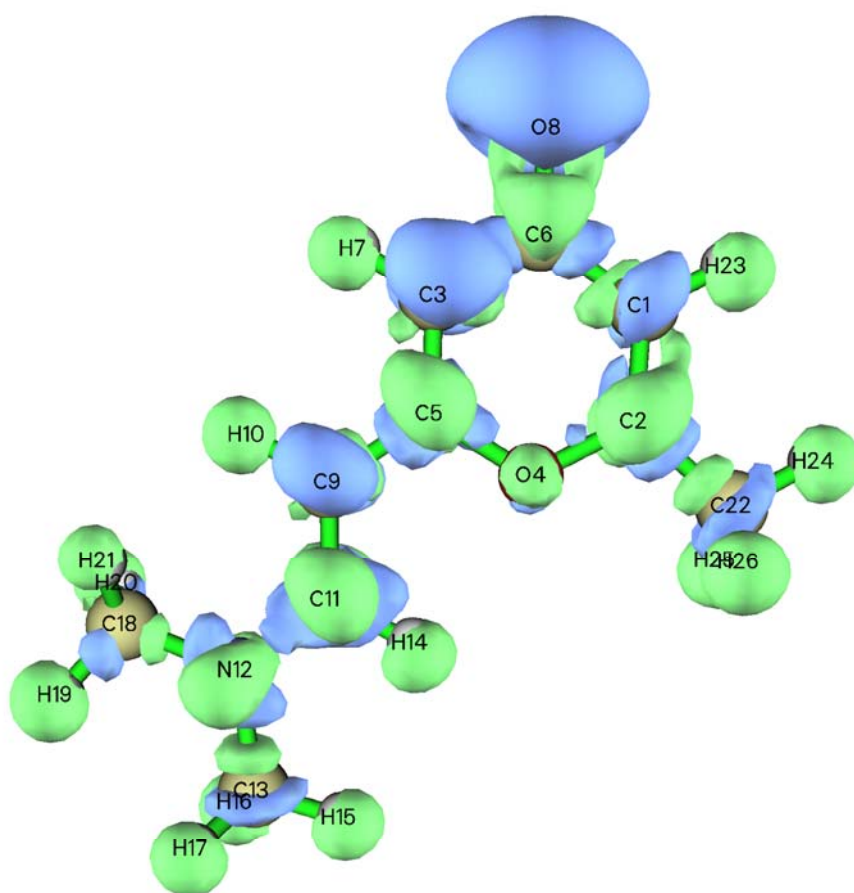


Figure S8. An electron density difference map for the $S_0 \rightarrow S_1$ transition of compound **4a** in methanol.

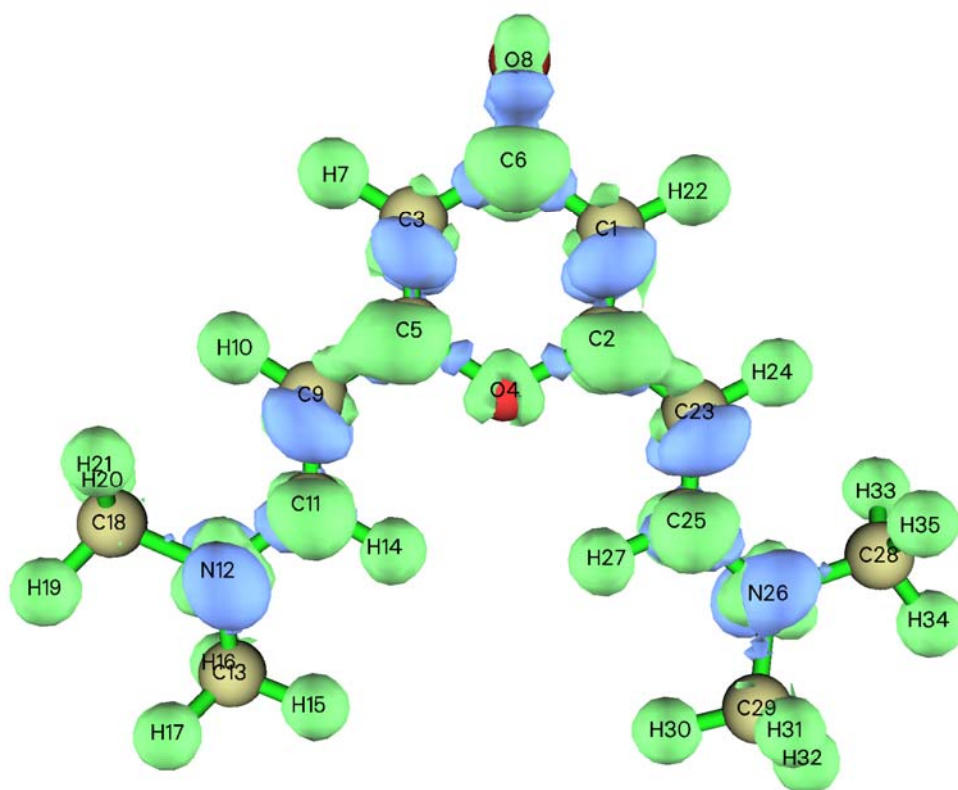


Figure S9. An electron density difference map for the $S_0 \rightarrow S_1$ transition of compound **5a** in vacuo.

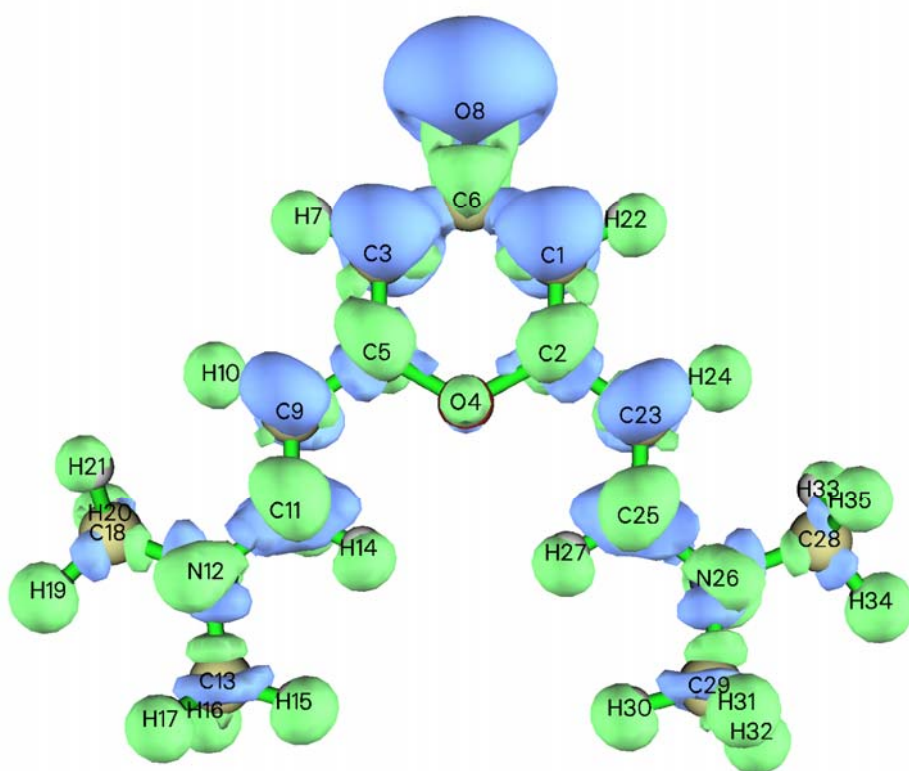
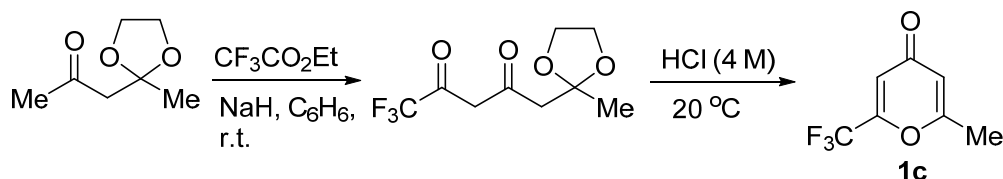


Figure S10. An electron density difference map for the $S_0 \rightarrow S_1$ transition of compound **5a** in methanol.

The method of preparation of 2-methyl-6-trifluoromethyl-4-pyrone (1c)

2-Methyl-6-(trifluoromethyl)-4*H*-pyran-4-one (1c).



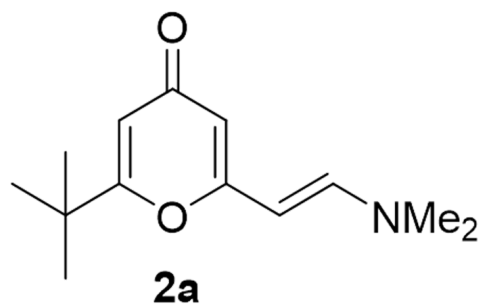
NaH (60% dispersion in mineral oil) (1.67 g, 0.0416 mol) was added to the solution of 1-(2-methyl-1,3-dioxolan-2-yl)propan-2-one [8] (5.0 g, 0.0347 mol) and ethyl 2,2,2-trifluoroacetate (5.92 g, 0.0416 mol) in benzene (20 mL), and the reaction mixture was stirred at room temperature overnight. The obtained precipitate of the salt was filtered. The solid was stirred in HCl (40 mL, 4 M) at $0\text{ }^\circ\text{C}$ for 1 h and then at room temperature overnight. The product was extracted with CHCl_3 ($3 \times 15\text{ mL}$), dried on Na_2SO_4 , evaporated. *n*-Hexane was added to the residue. The *n*-hexane solution was cooled at $-20\text{ }^\circ\text{C}$ overnight. The white crystals were obtained and filtered. Yield 1.85 g (30 %), mp $49\text{--}50\text{ }^\circ\text{C}$, white crystals.

^1H NMR (400 MHz, CDCl_3) δ 2.37 (3H, d, $J = 0.8\text{ Hz}$, Me), 6.26 (1H, d, q, $J = 2.2\text{ Hz}$, $J = 0.8\text{ Hz}$, H-3), 6.67 (1H, d, $J = 2.2\text{ Hz}$, H-5). ^{19}F NMR (376 MHz, CDCl_3) δ 90.1 (s, CF_3).

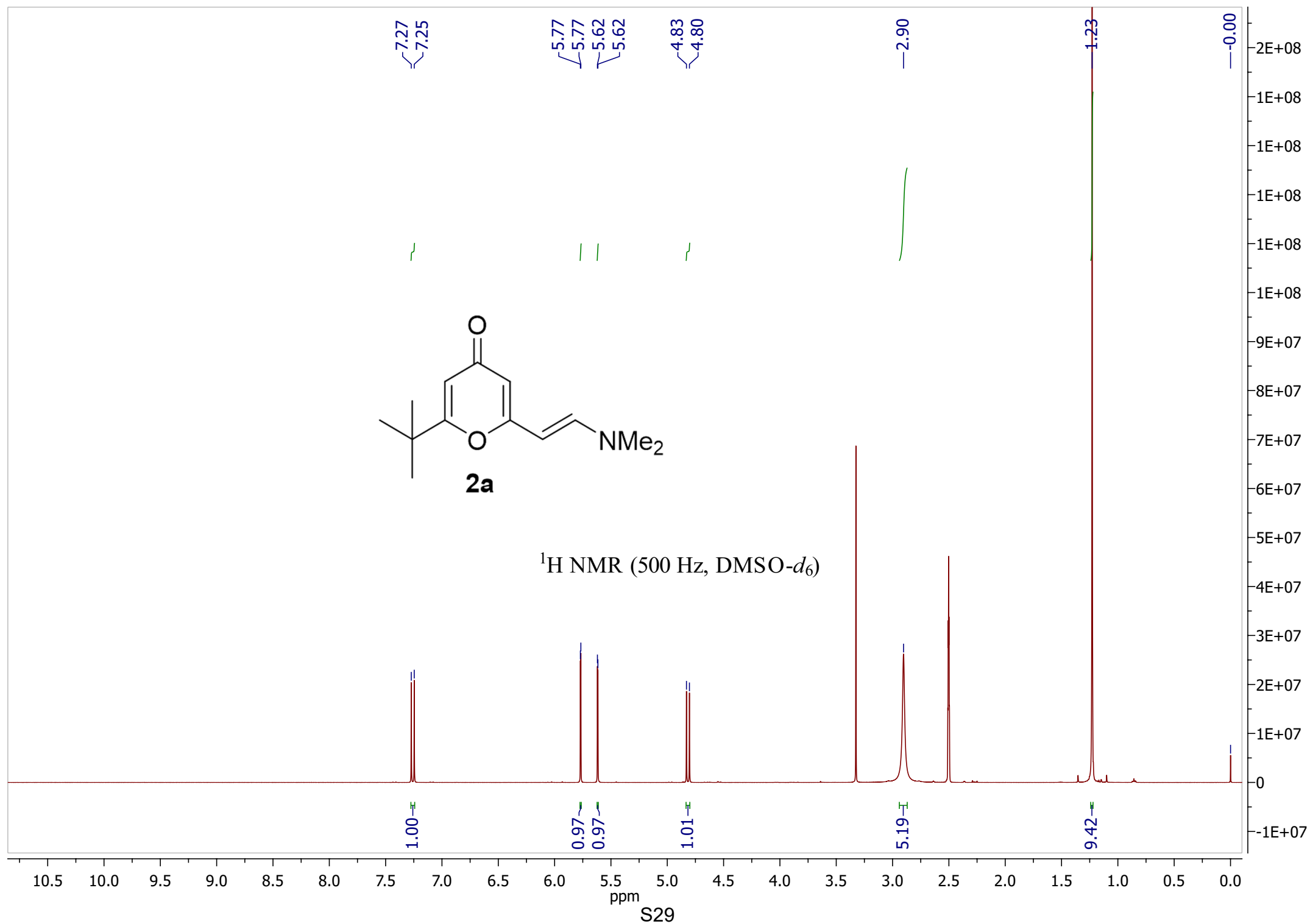
The NMR spectra are in accordance with the literature data [9].

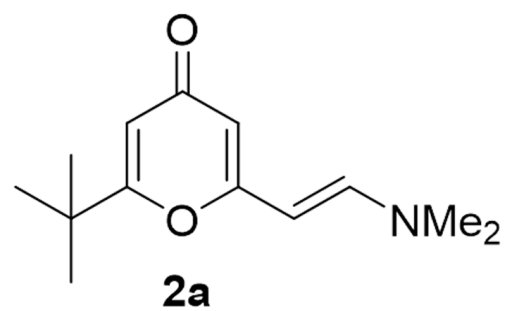
8. Dorman, L. C. Synthesis of 2-methyl-4*H*-pyran-4-one. *J. Org. Chem.* **1967**, 32, 4105–4107. doi: 10.1021/jo01287a101.

9. Tyvorskii, V.I.; Bobrov, D.N.; Kulinkovich, O.G.; De Kimpe, N.; Tehrani, K.A. New synthetic approaches to 2-perfluoroalkyl-4*H*-pyran-4-ones. *Tetrahedron* **1998**, 54, 2819–2826. doi: 10.1016/S0040-4020(98)83018-4.

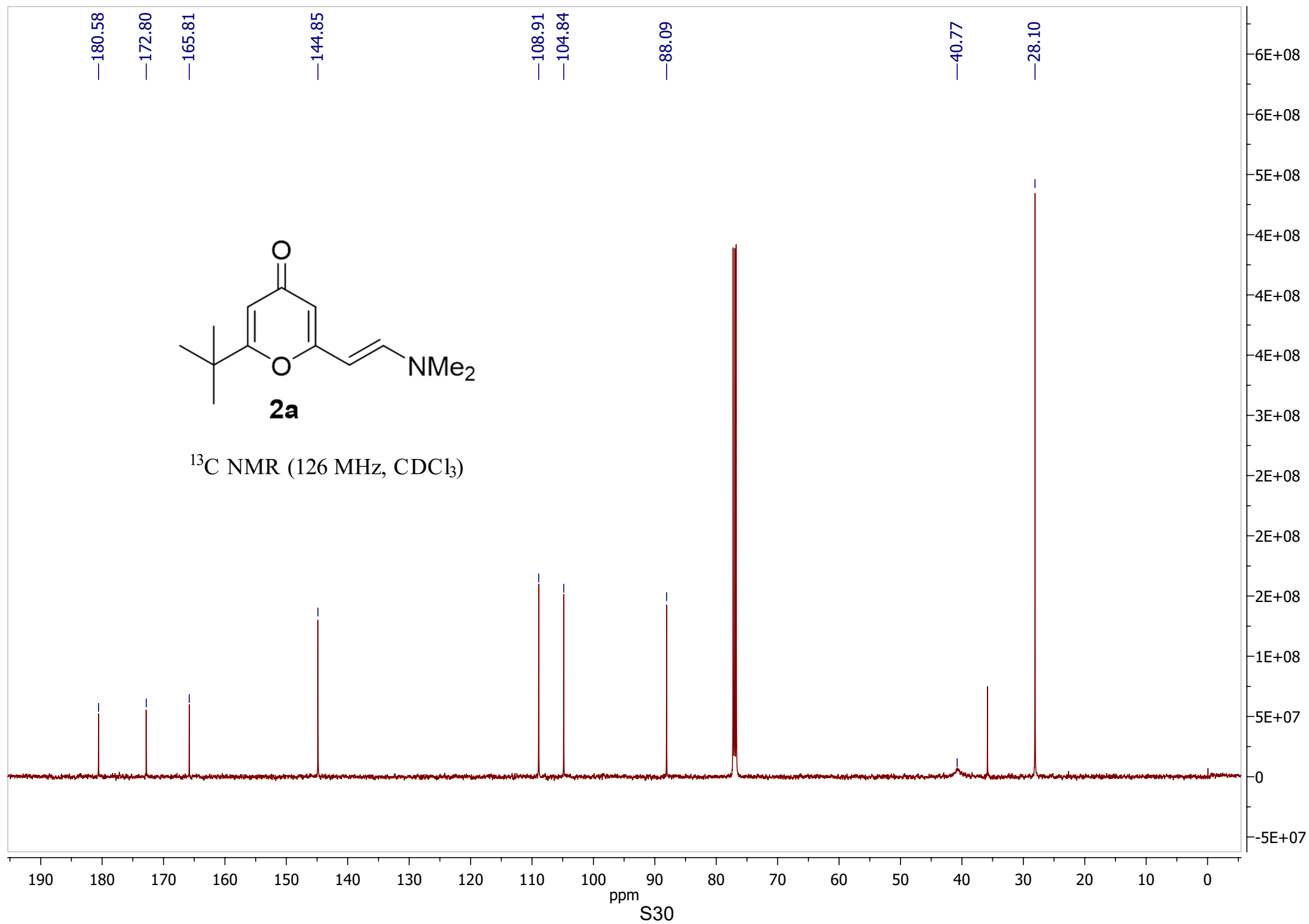


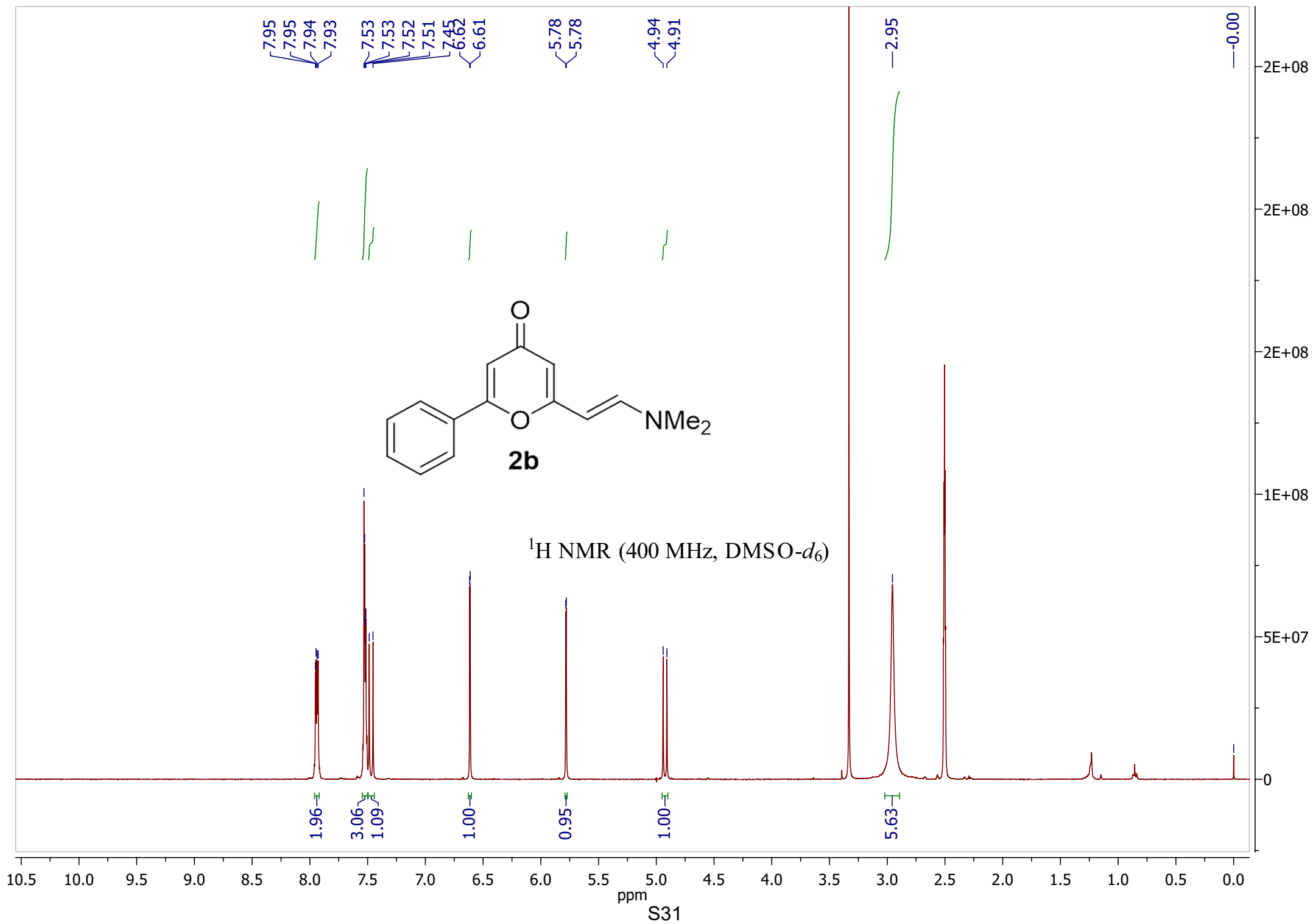
^1H NMR (500 Hz, DMSO- d_6)

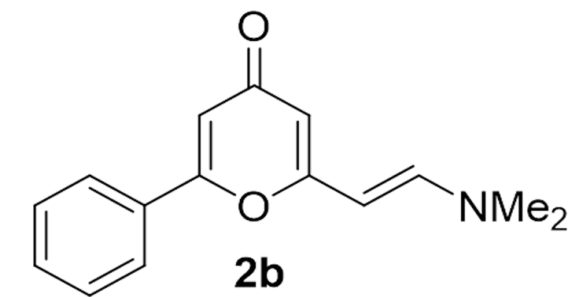




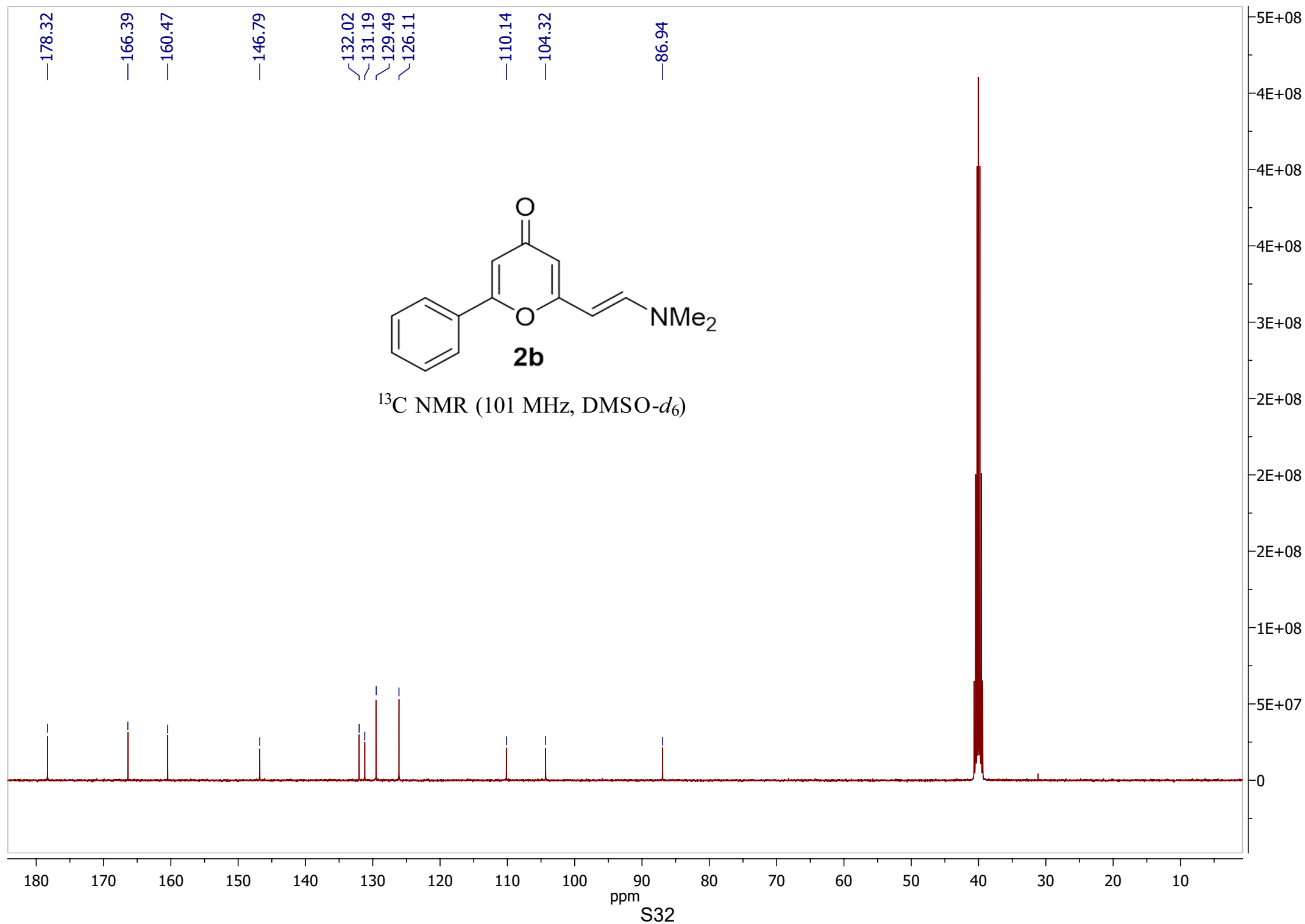
^{13}C NMR (126 MHz, CDCl_3)

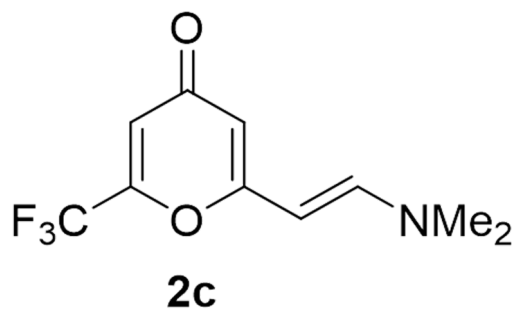




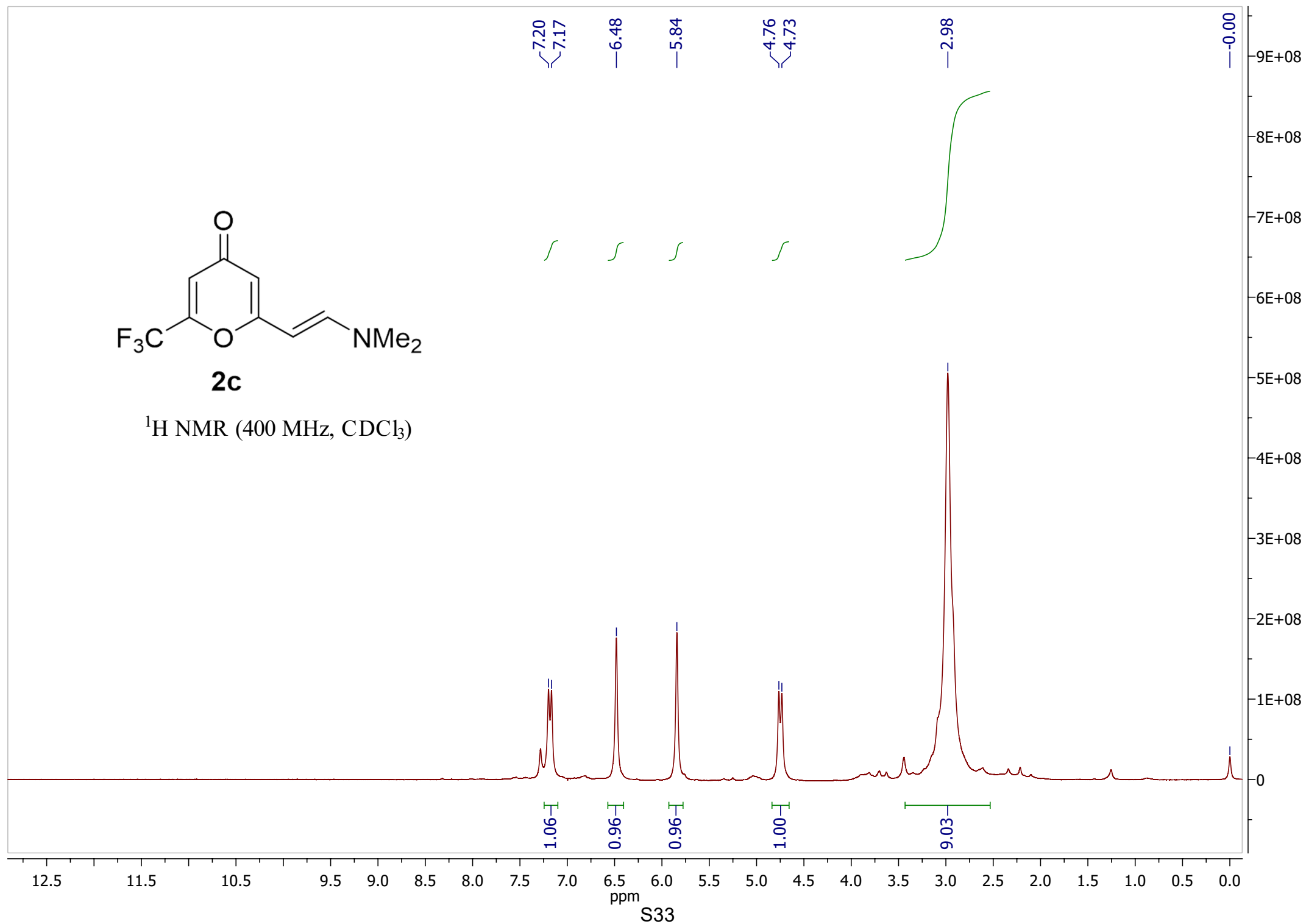


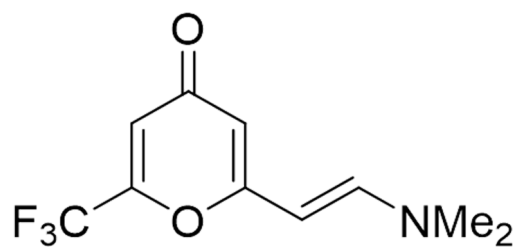
^{13}C NMR (101 MHz, DMSO- d_6)





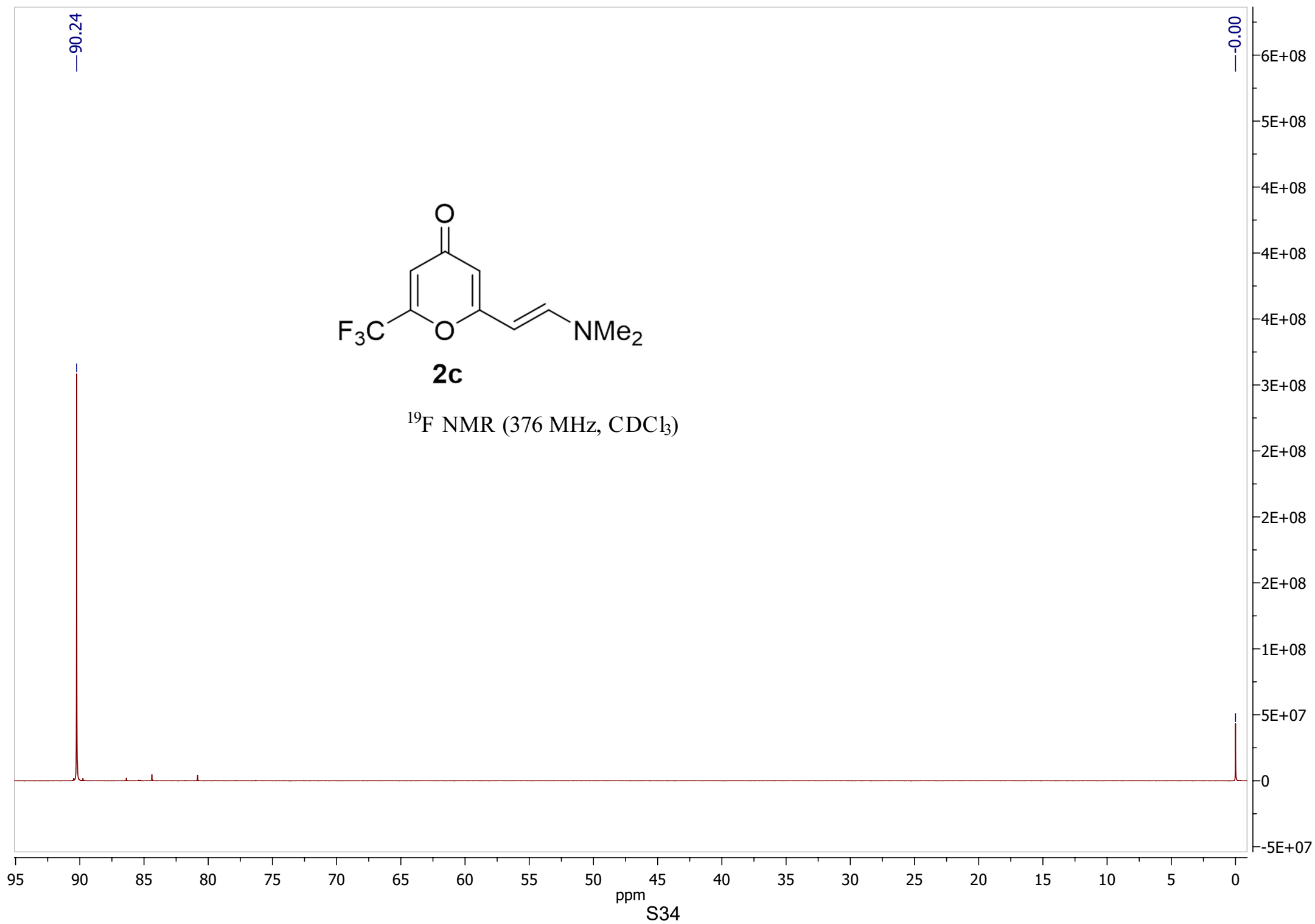
^1H NMR (400 MHz, CDCl_3)

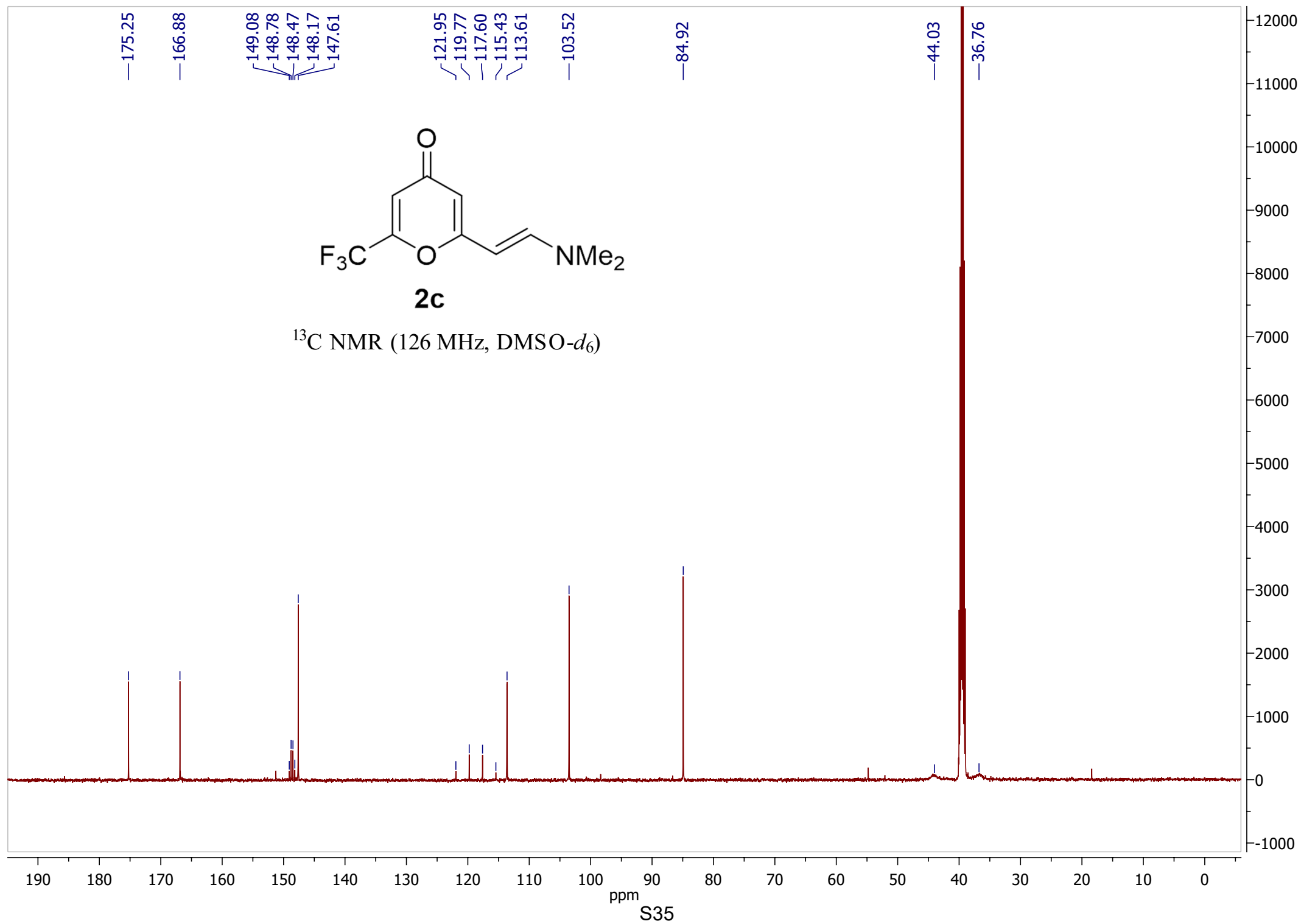


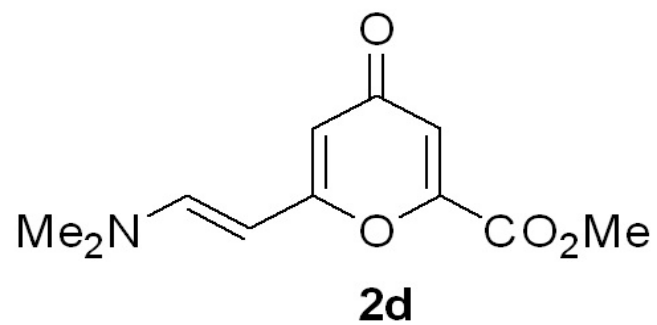


2c

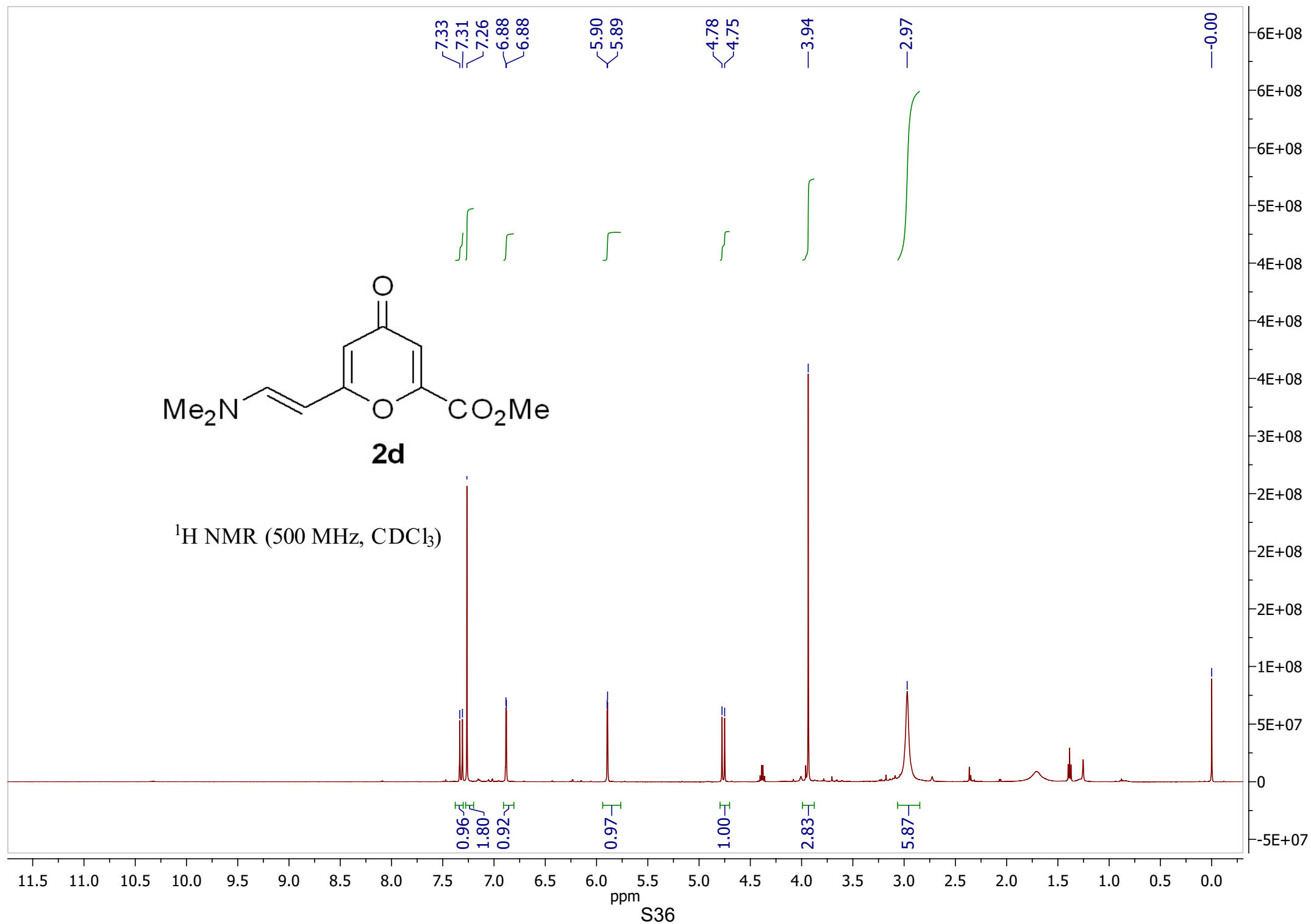
^{19}F NMR (376 MHz, CDCl_3)

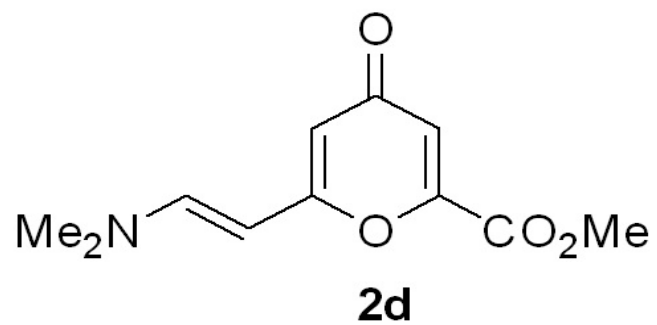




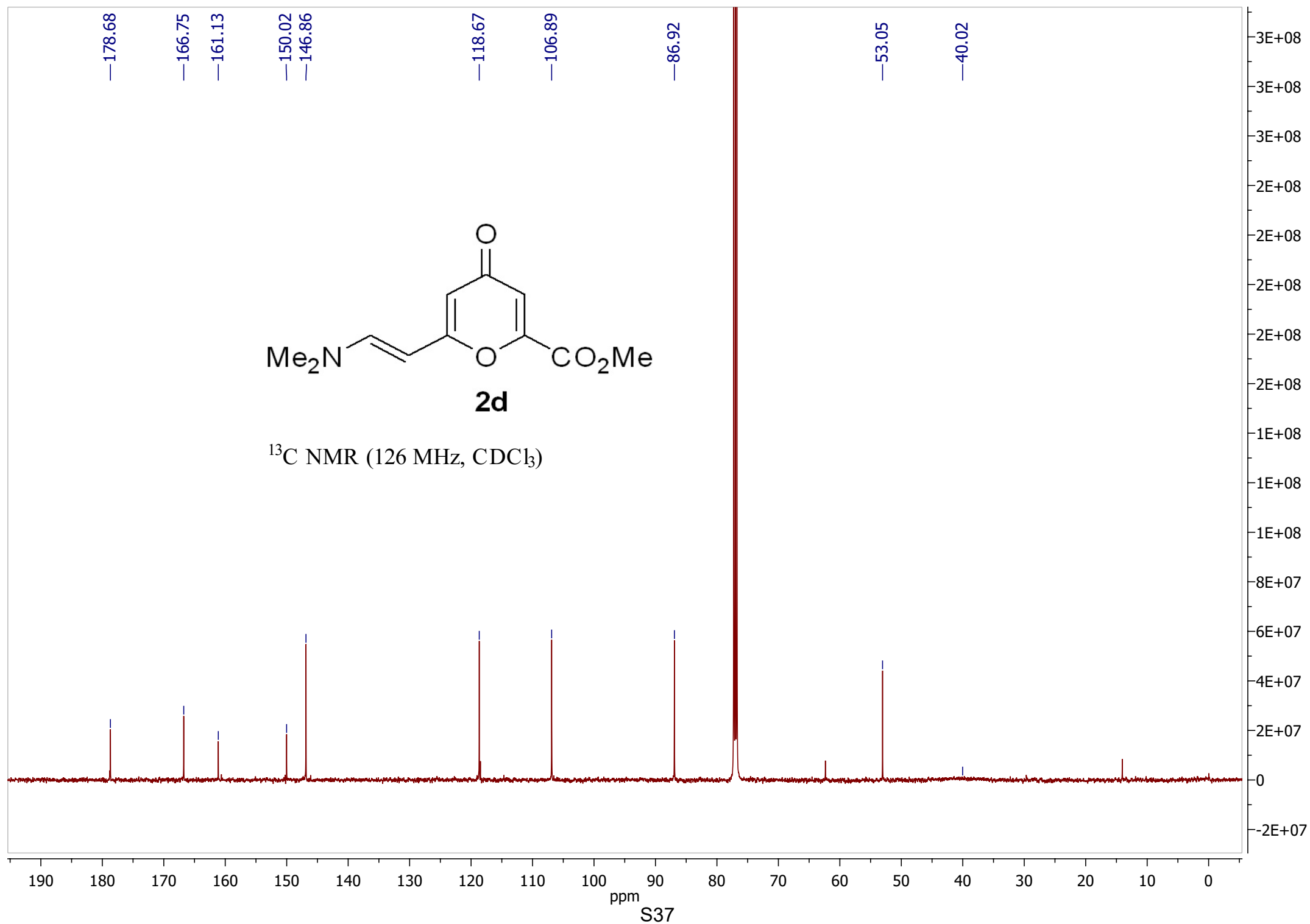


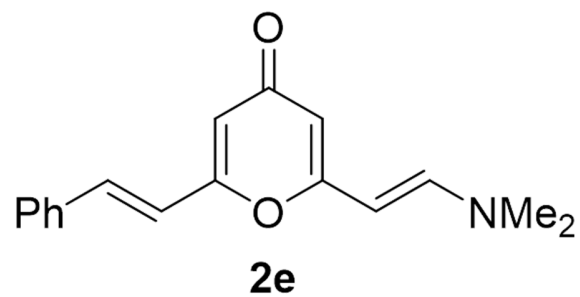
^1H NMR (500 MHz, CDCl_3)



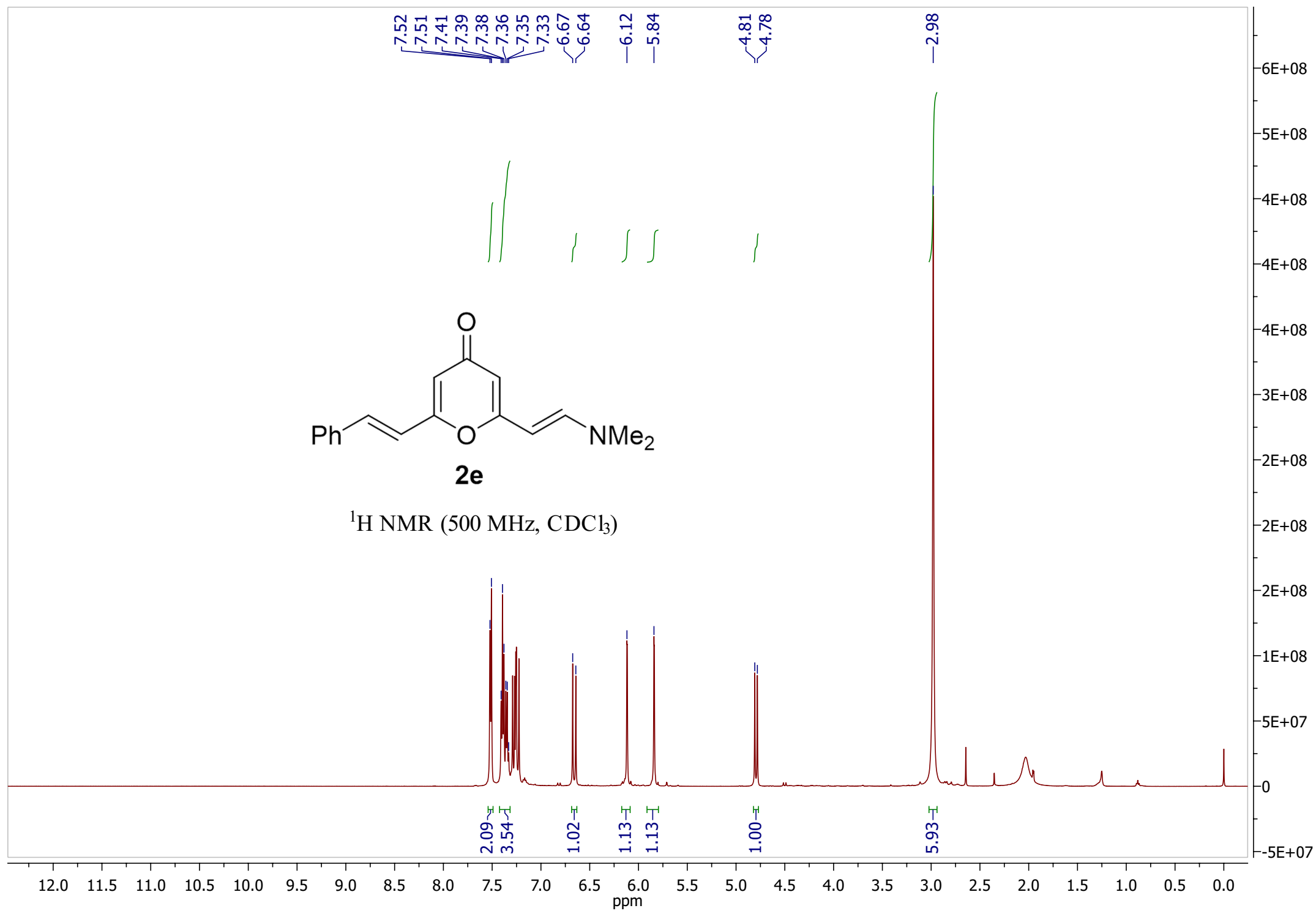


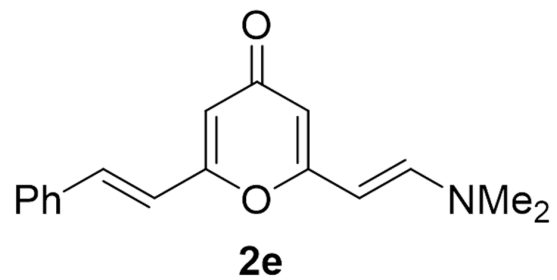
^{13}C NMR (126 MHz, CDCl_3)



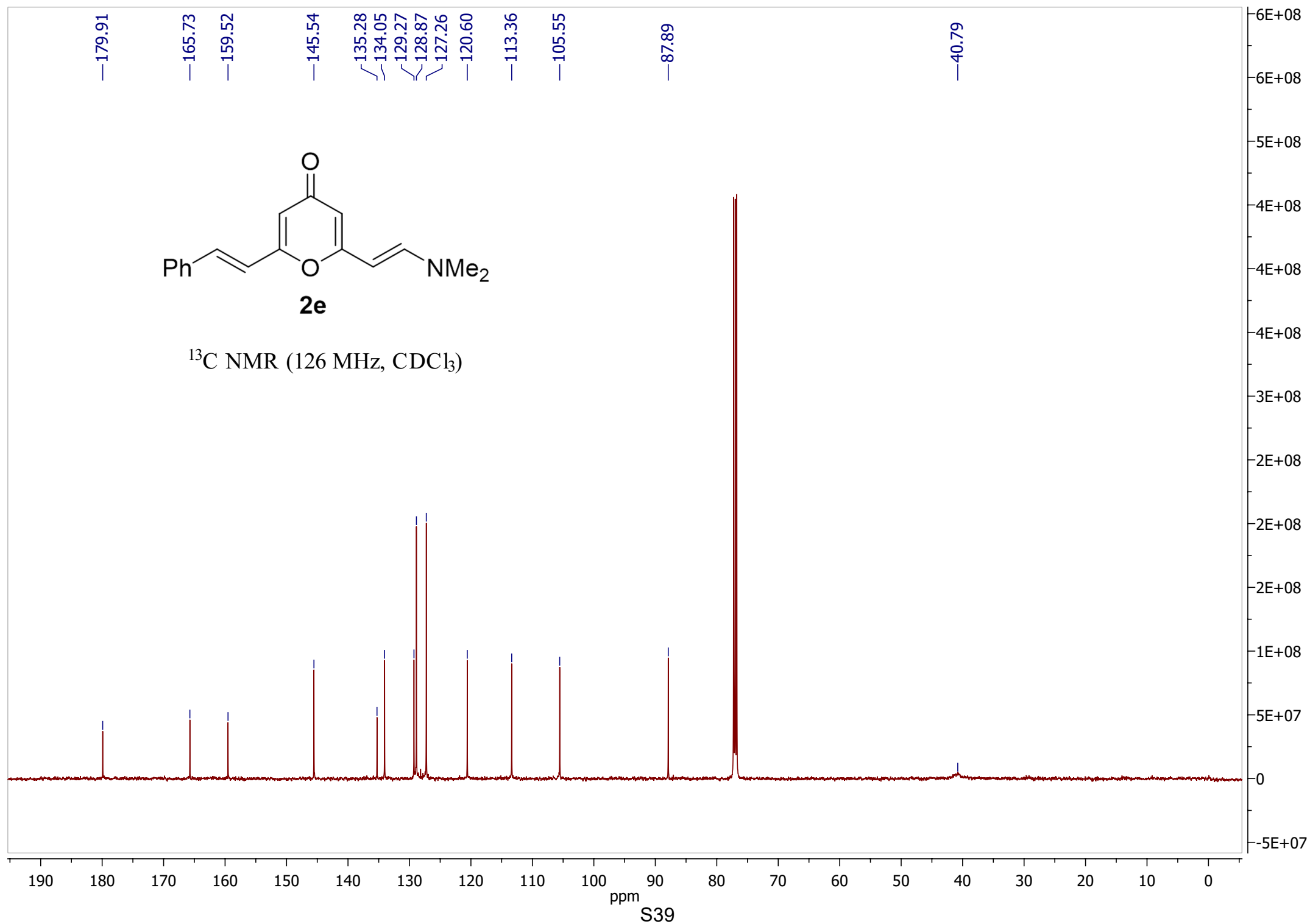


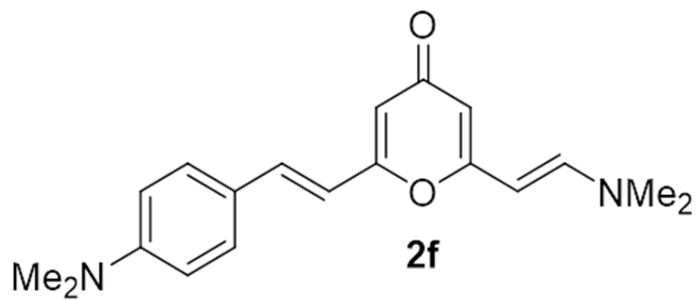
^1H NMR (500 MHz, CDCl_3)



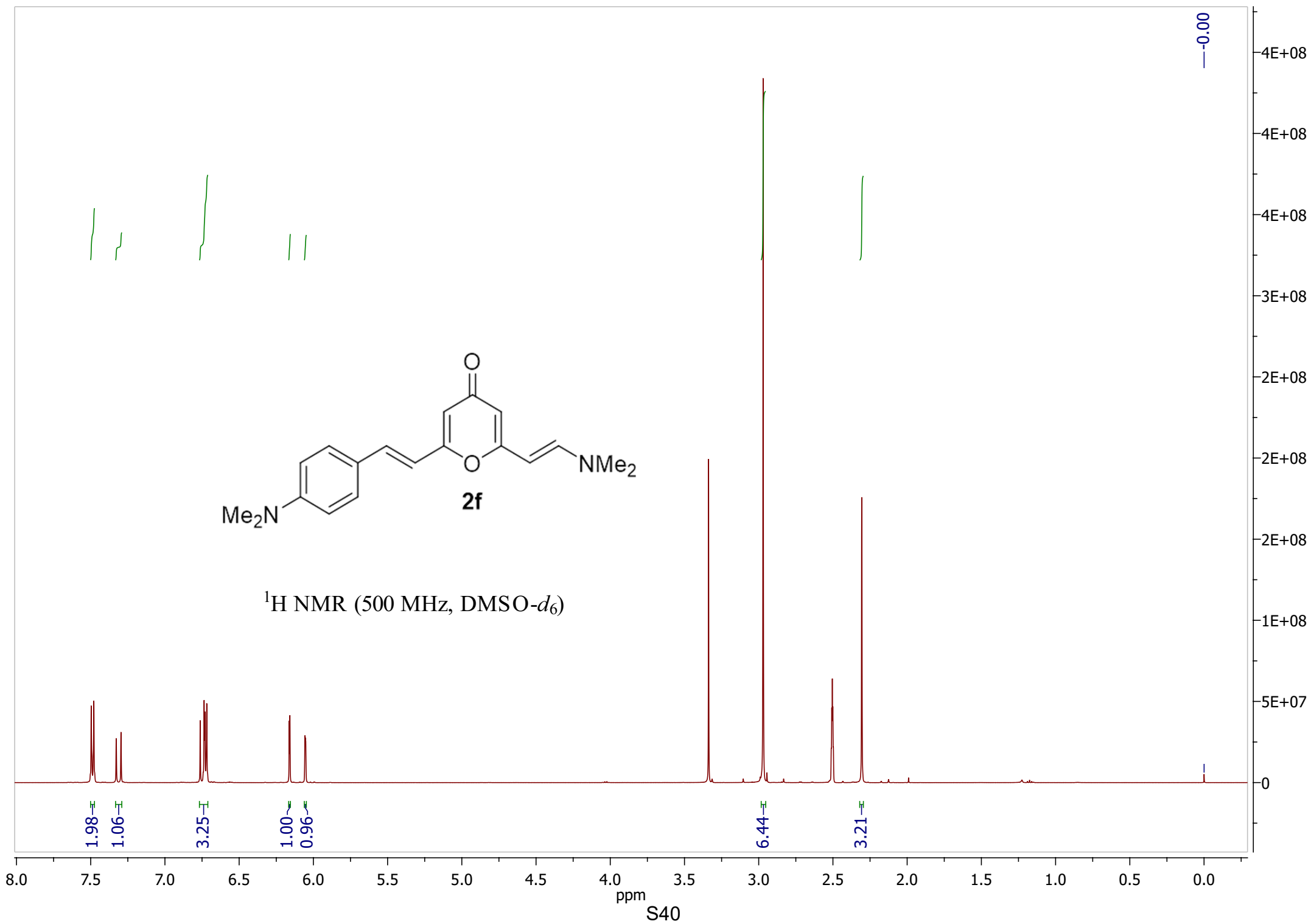


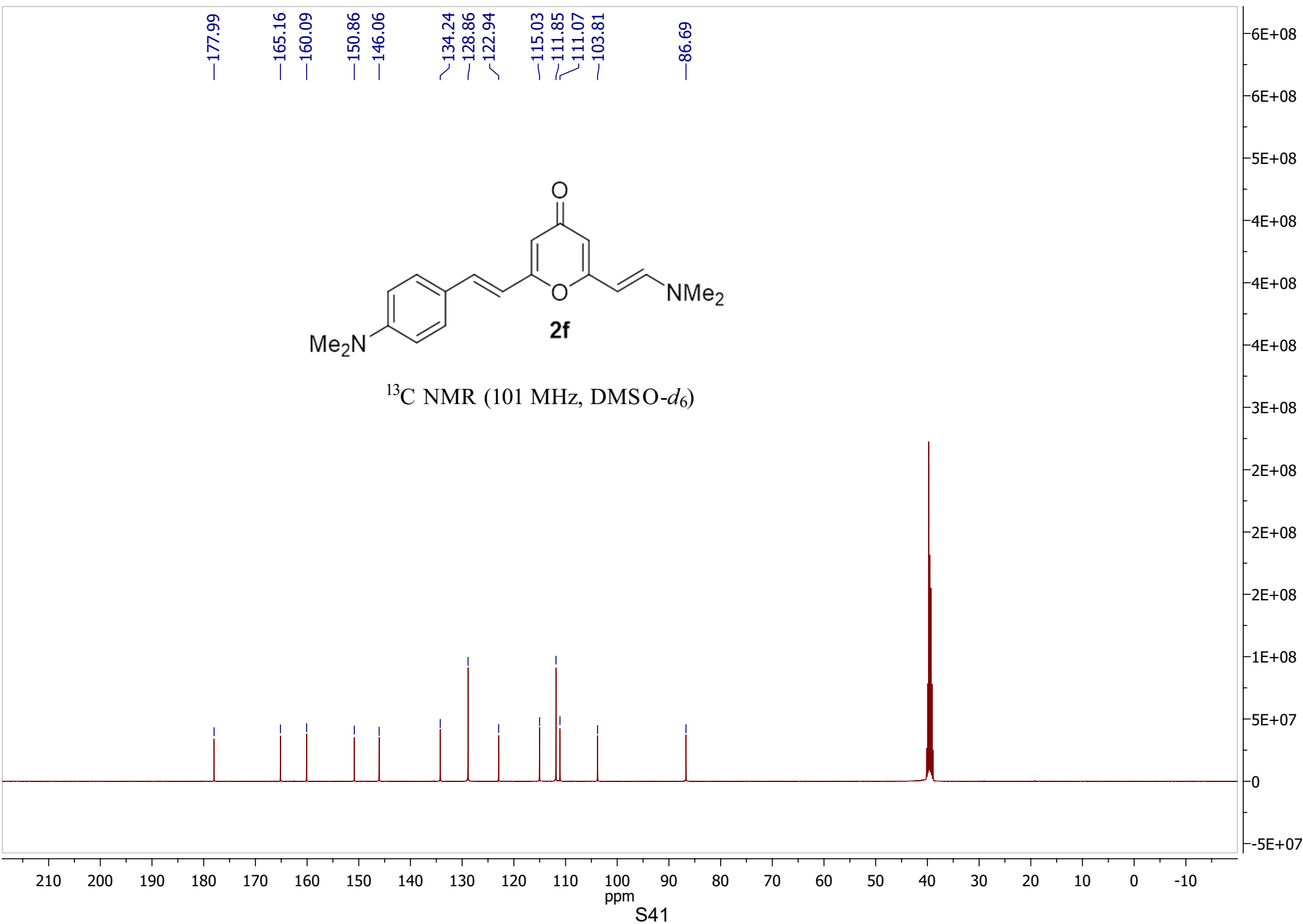
^{13}C NMR (126 MHz, CDCl_3)

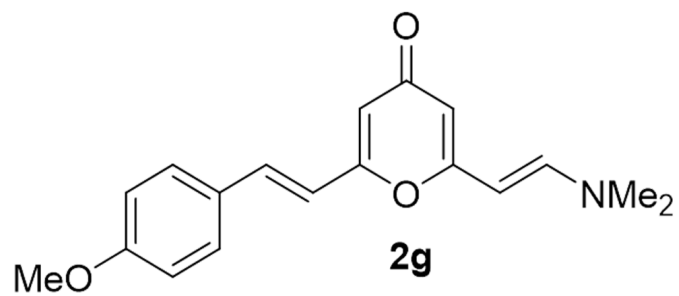




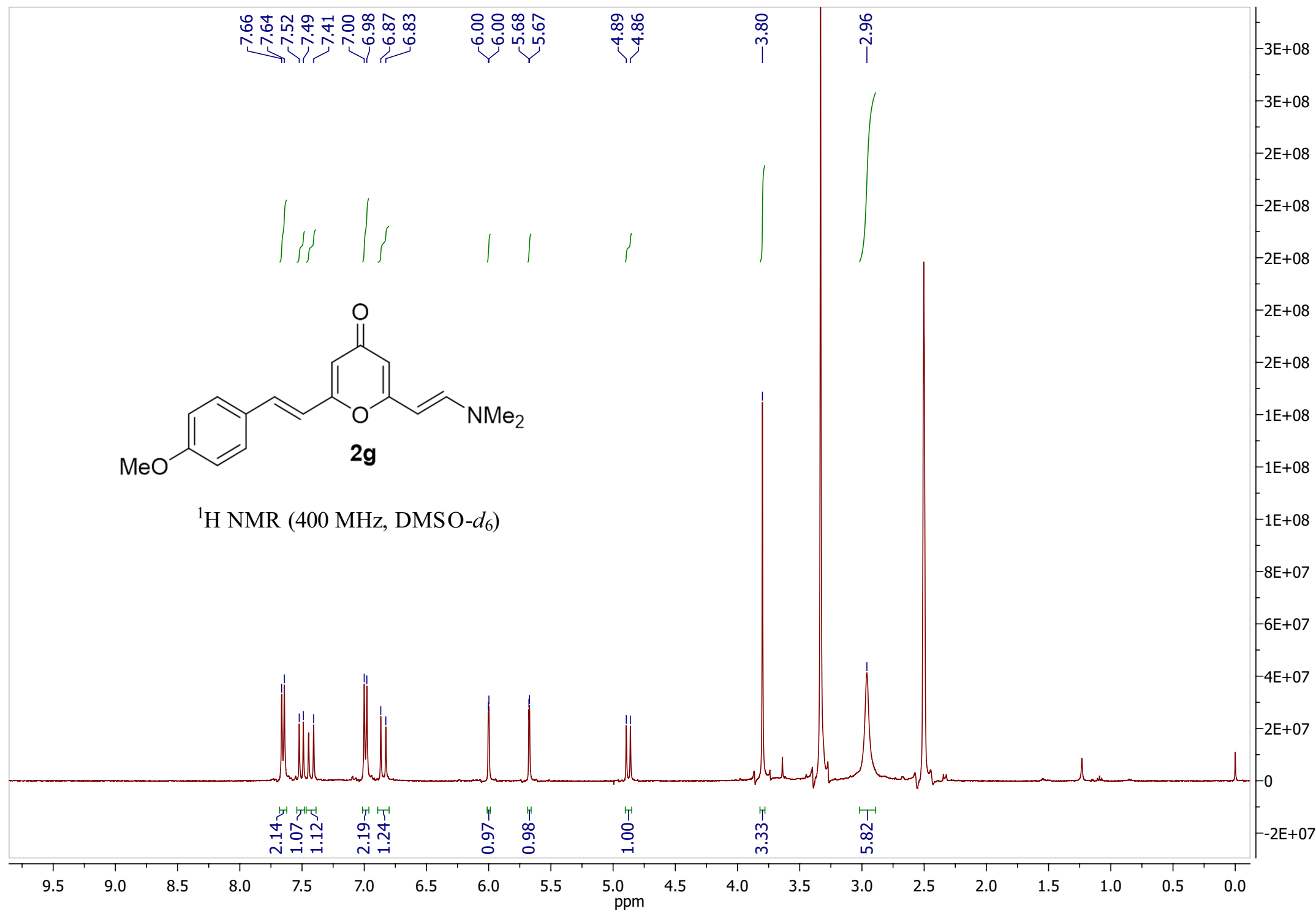
^1H NMR (500 MHz, $\text{DMSO}-d_6$)

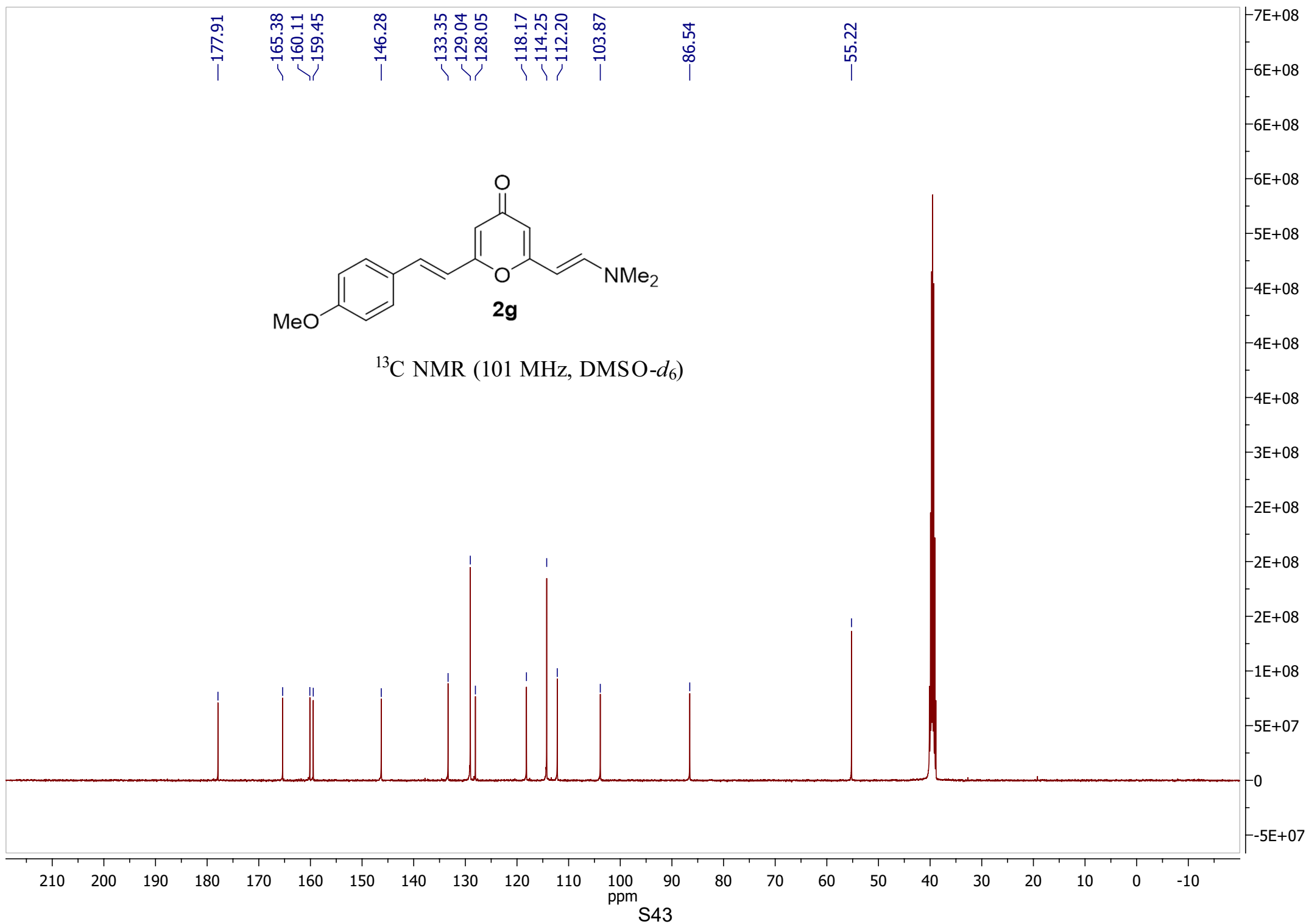


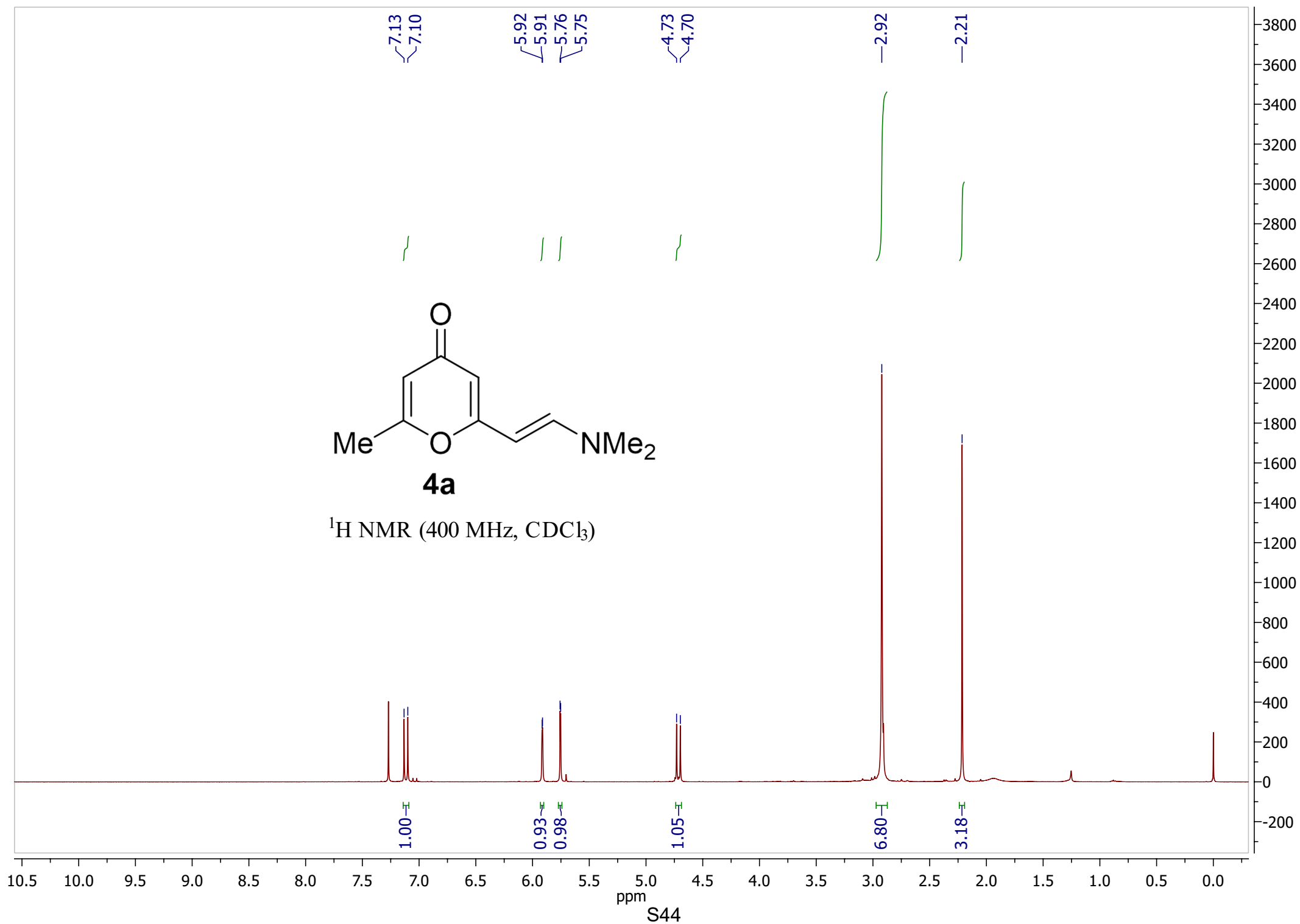


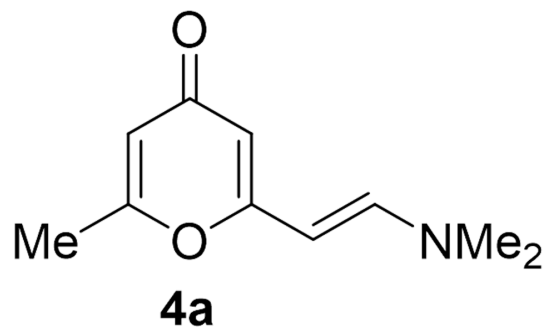


¹H NMR (400 MHz, DMSO-*d*₆)

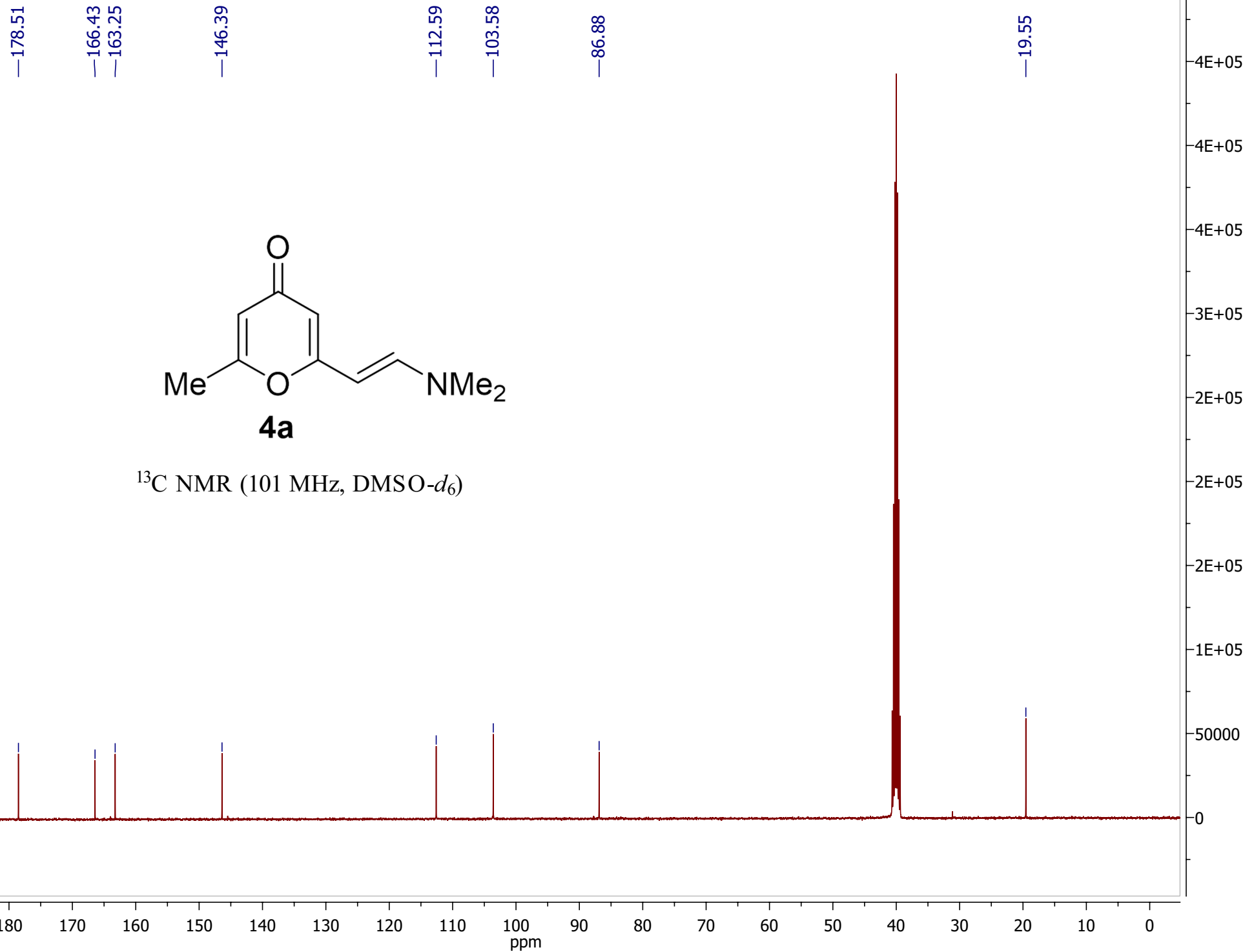


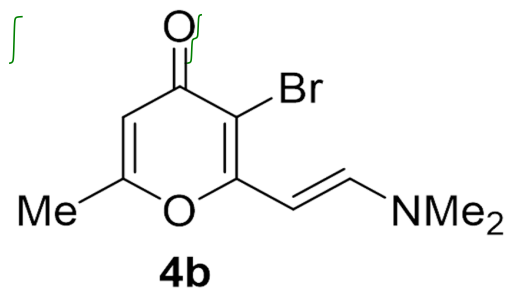




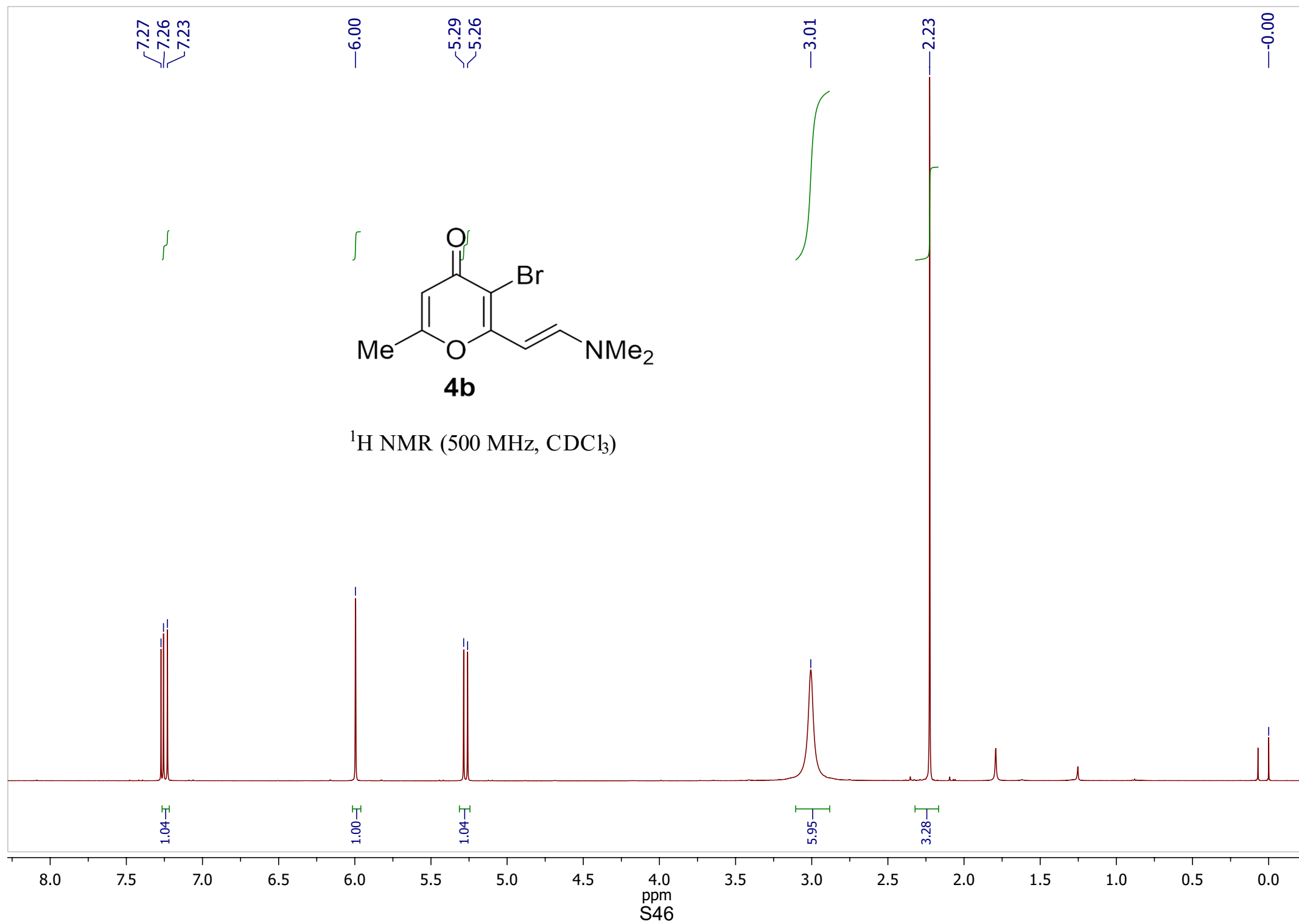


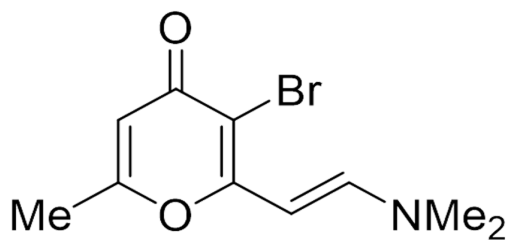
^{13}C NMR (101 MHz, DMSO- d_6)





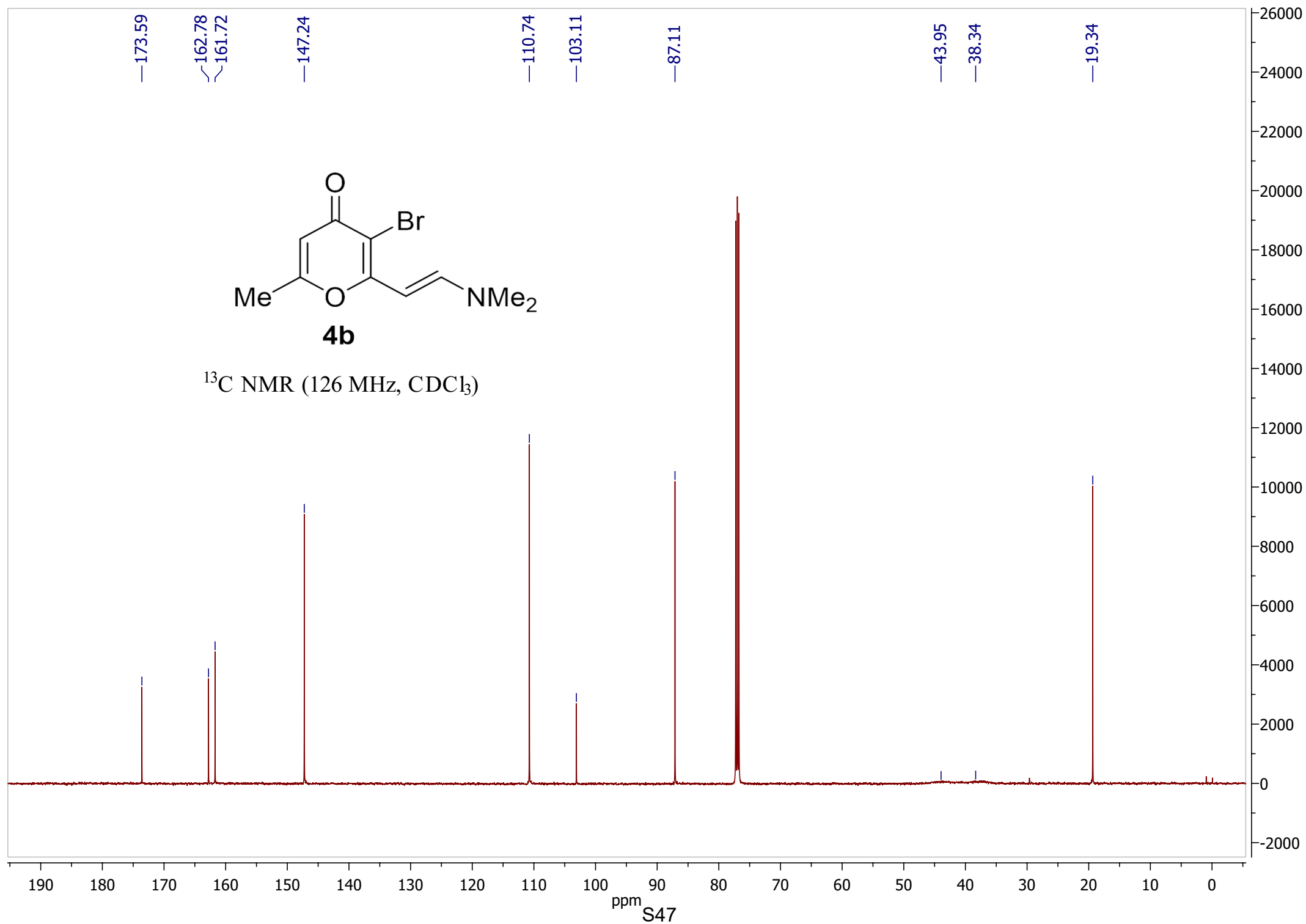
^1H NMR (500 MHz, CDCl_3)

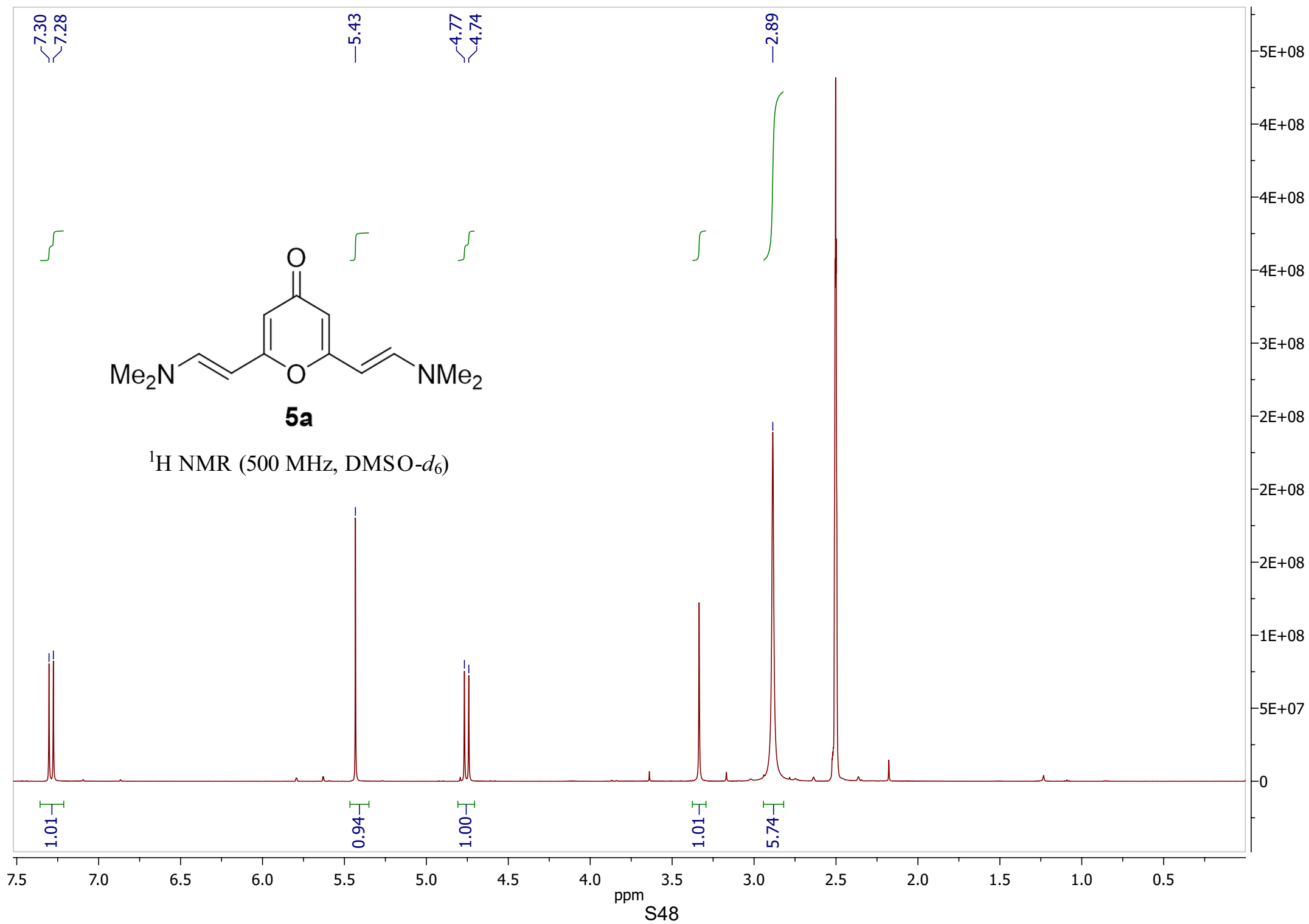


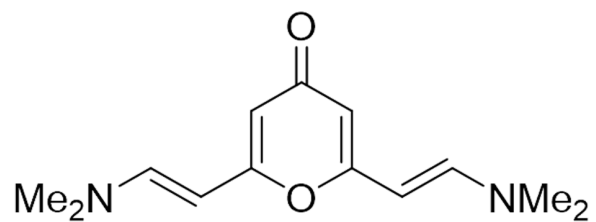


4b

^{13}C NMR (126 MHz, CDCl_3)

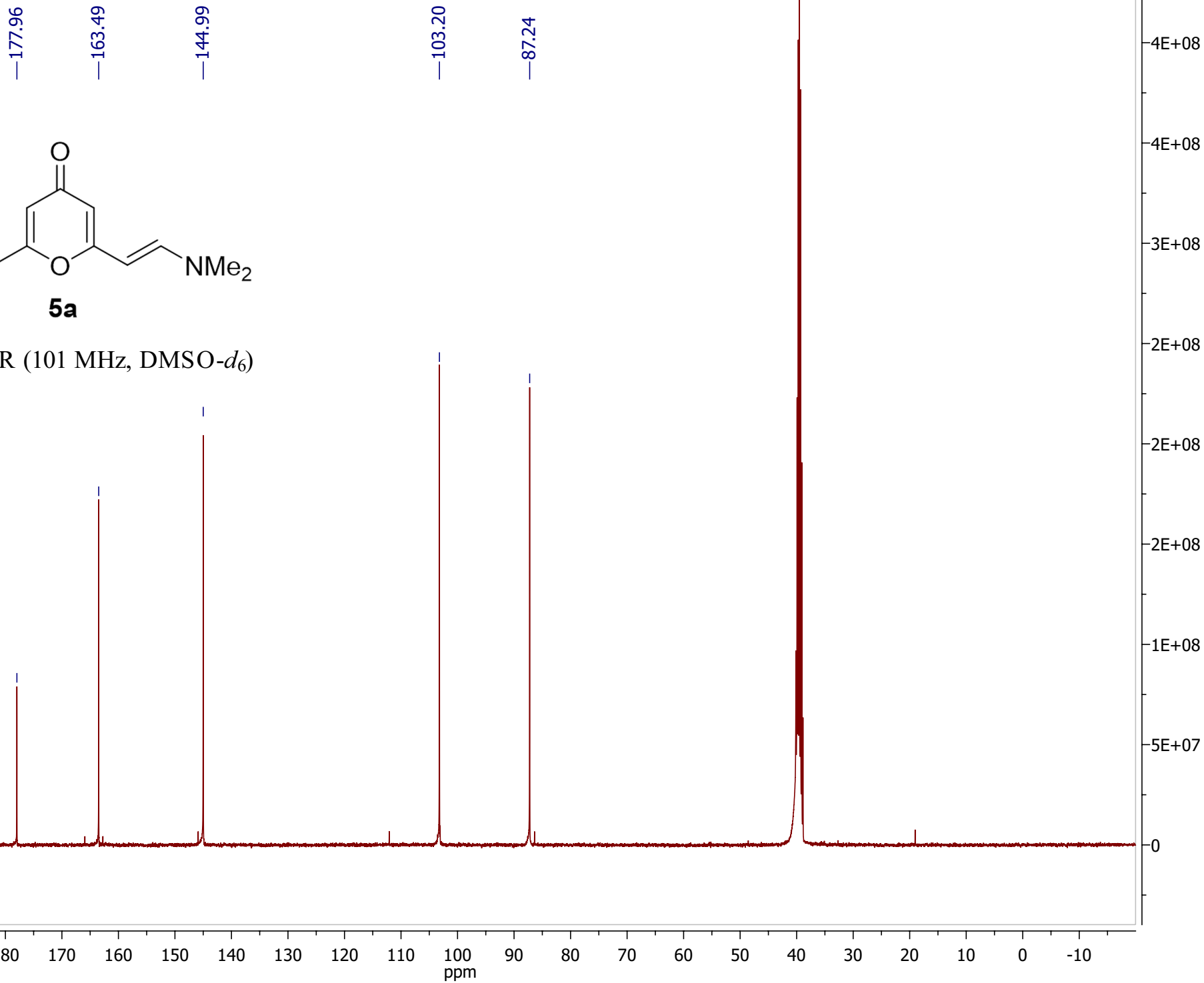




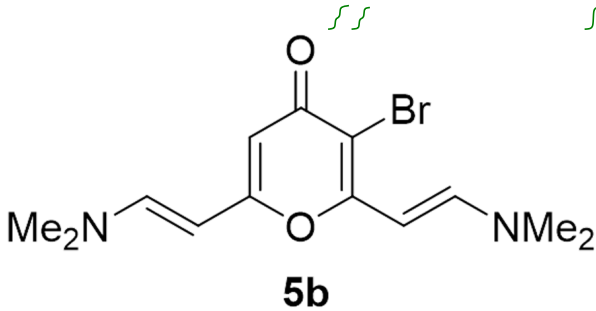


5a

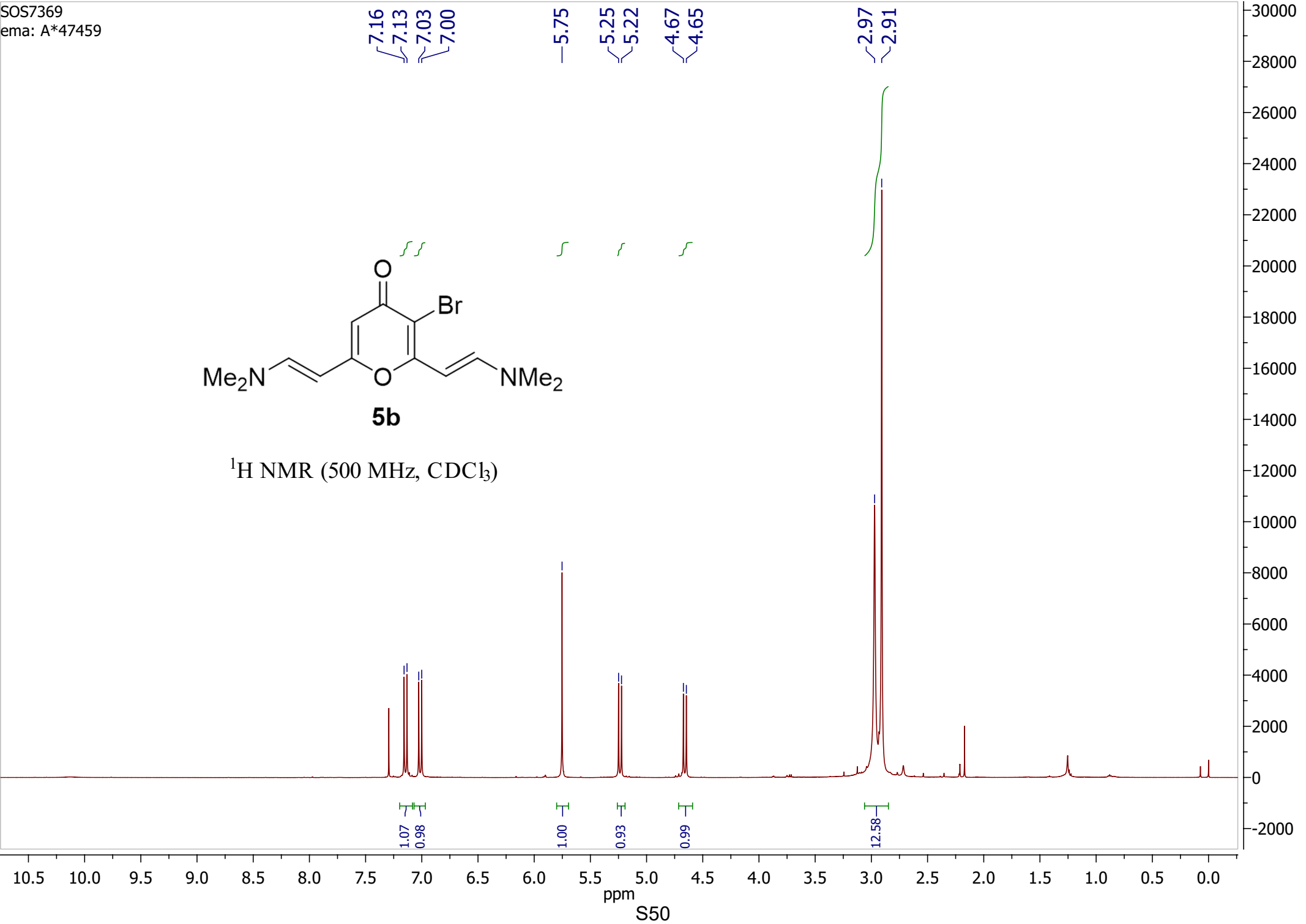
^{13}C NMR (101 MHz, DMSO- d_6)

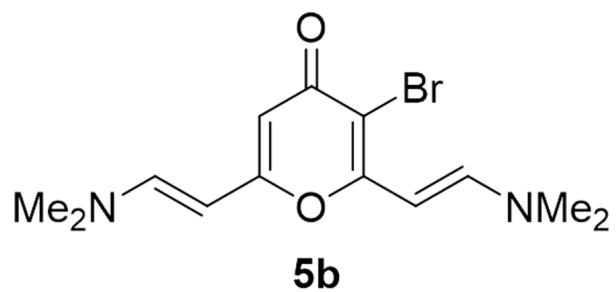


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ema: A*47459

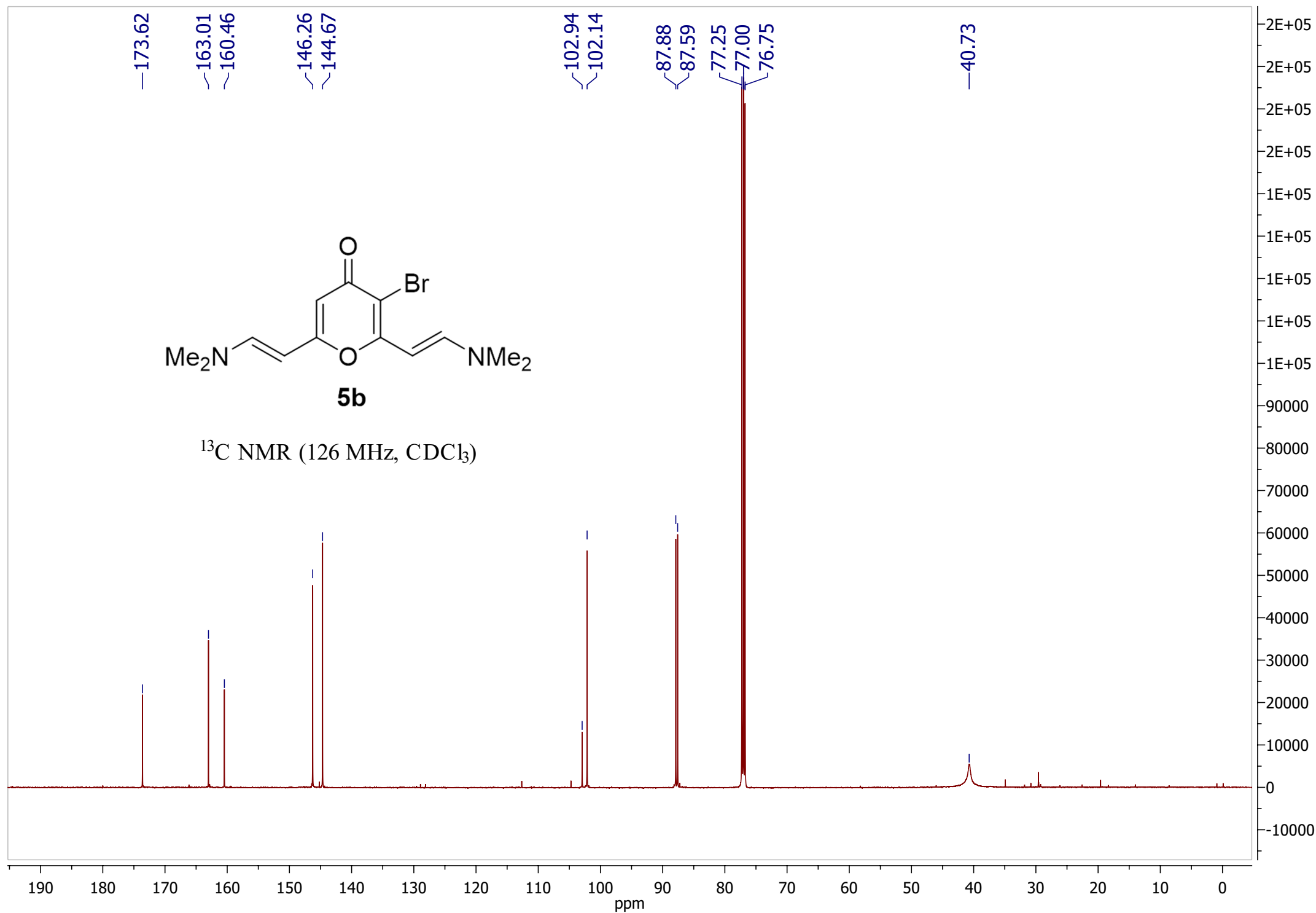


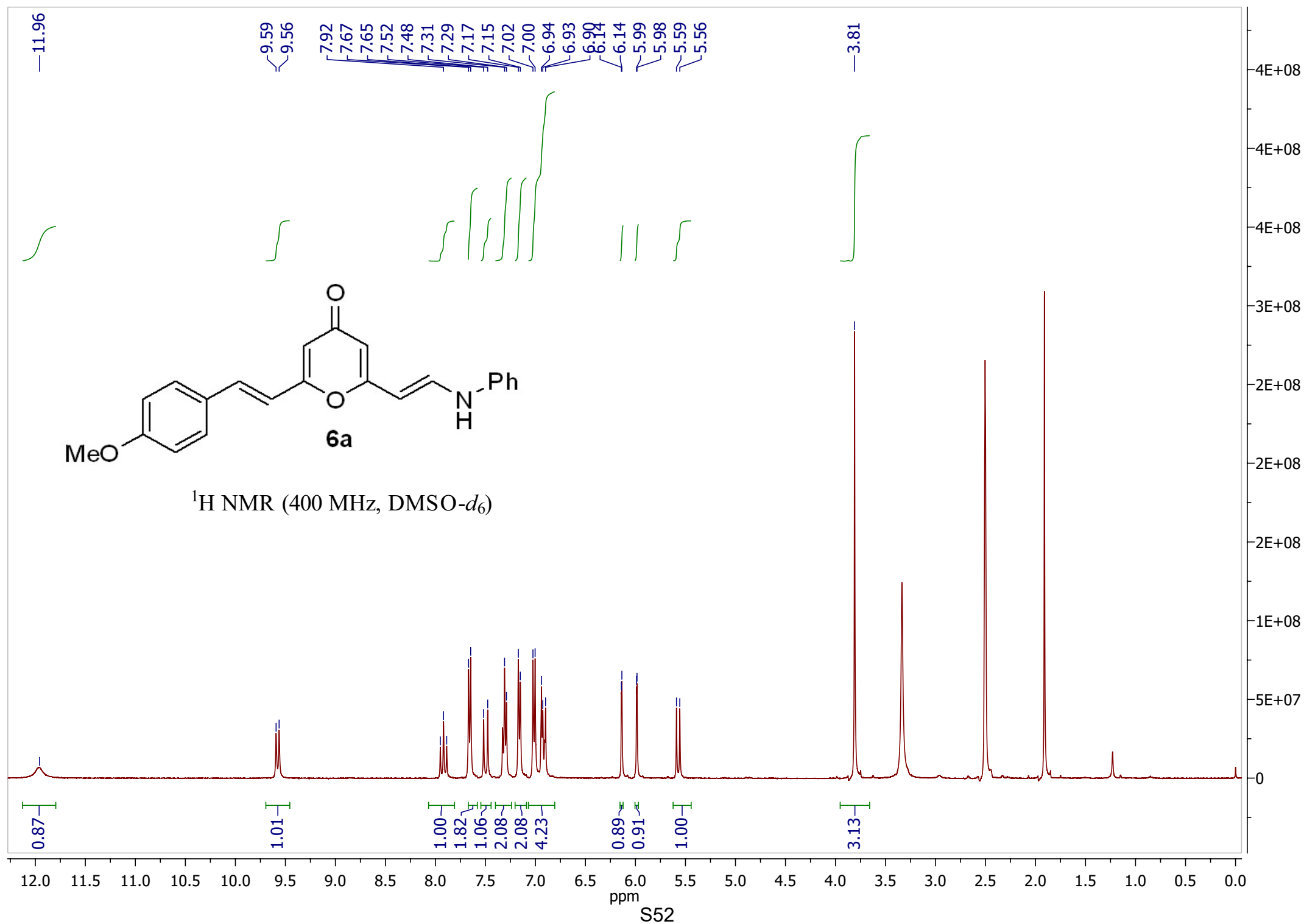
¹H NMR (500 MHz, CDCl₃)

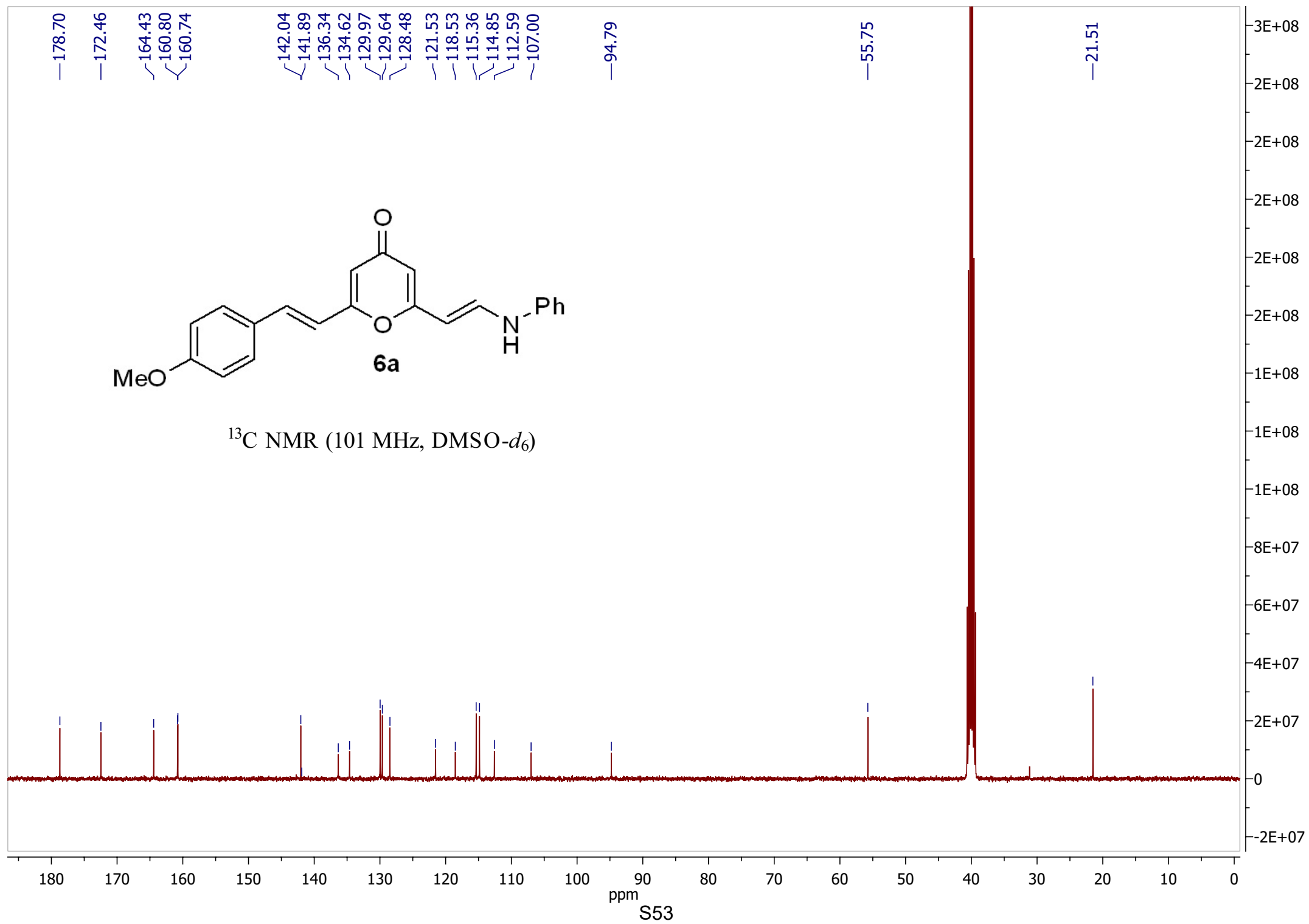


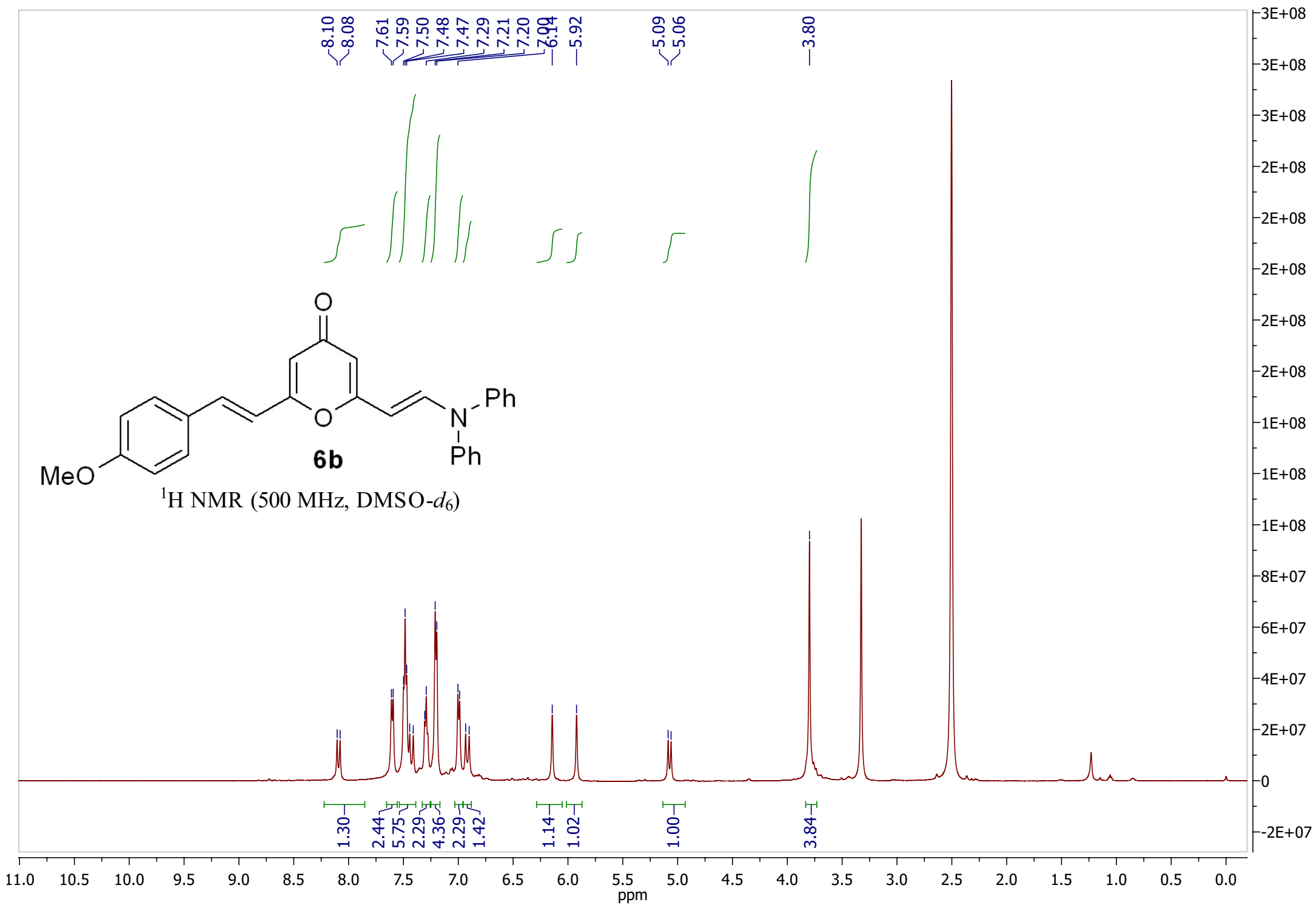


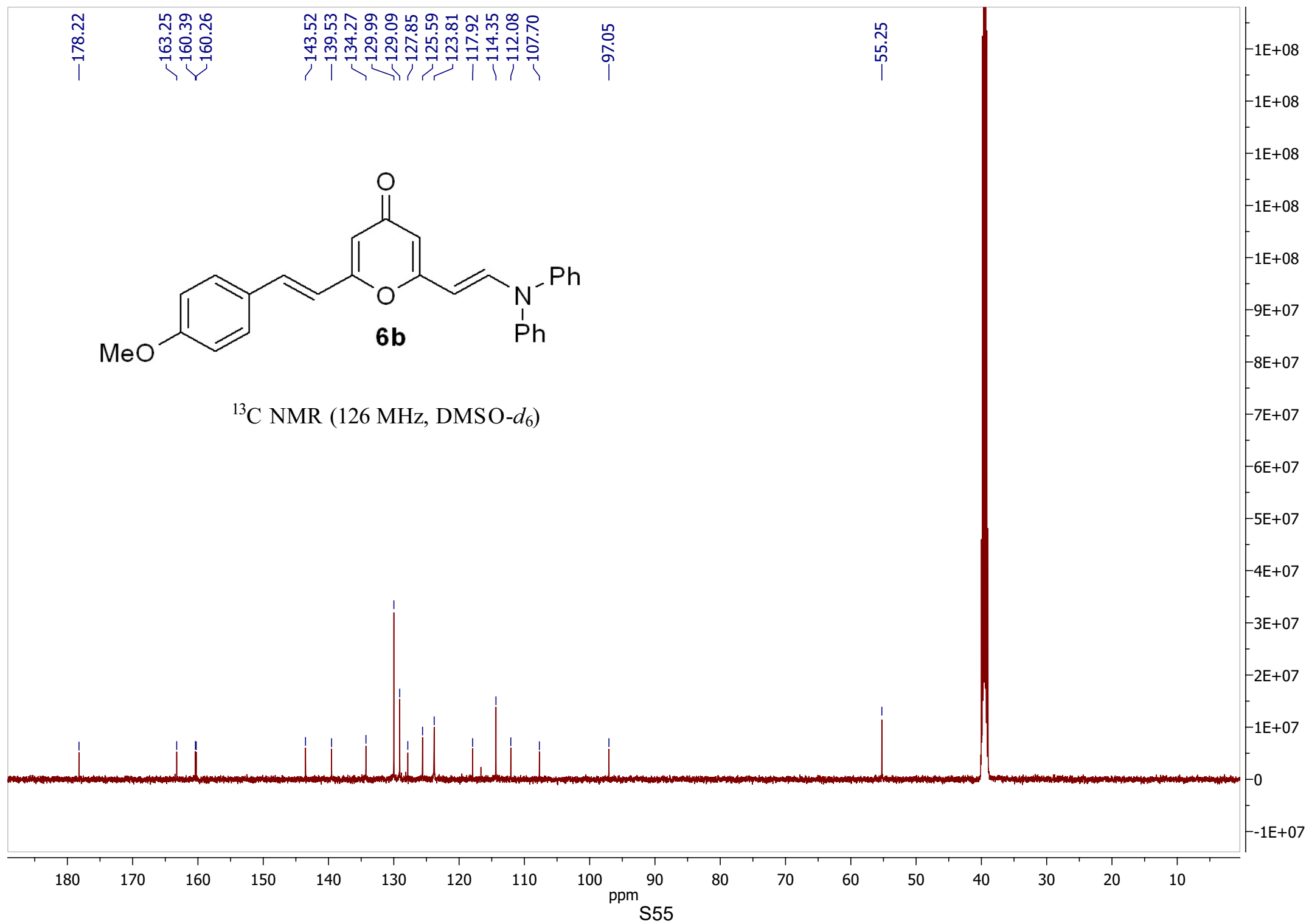
^{13}C NMR (126 MHz, CDCl_3)

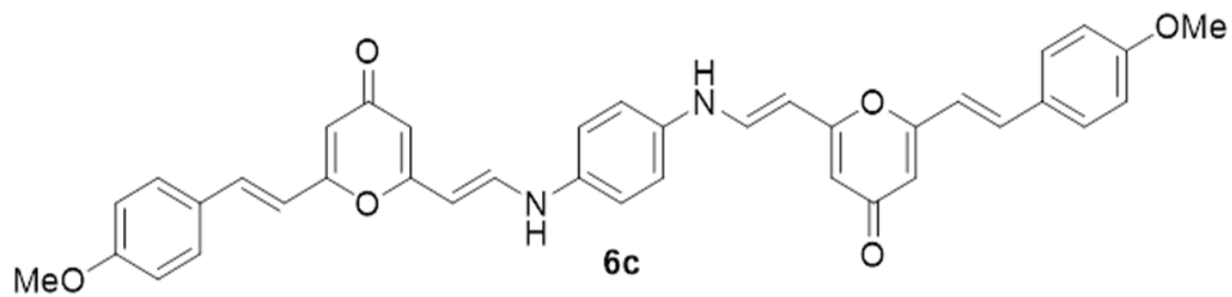




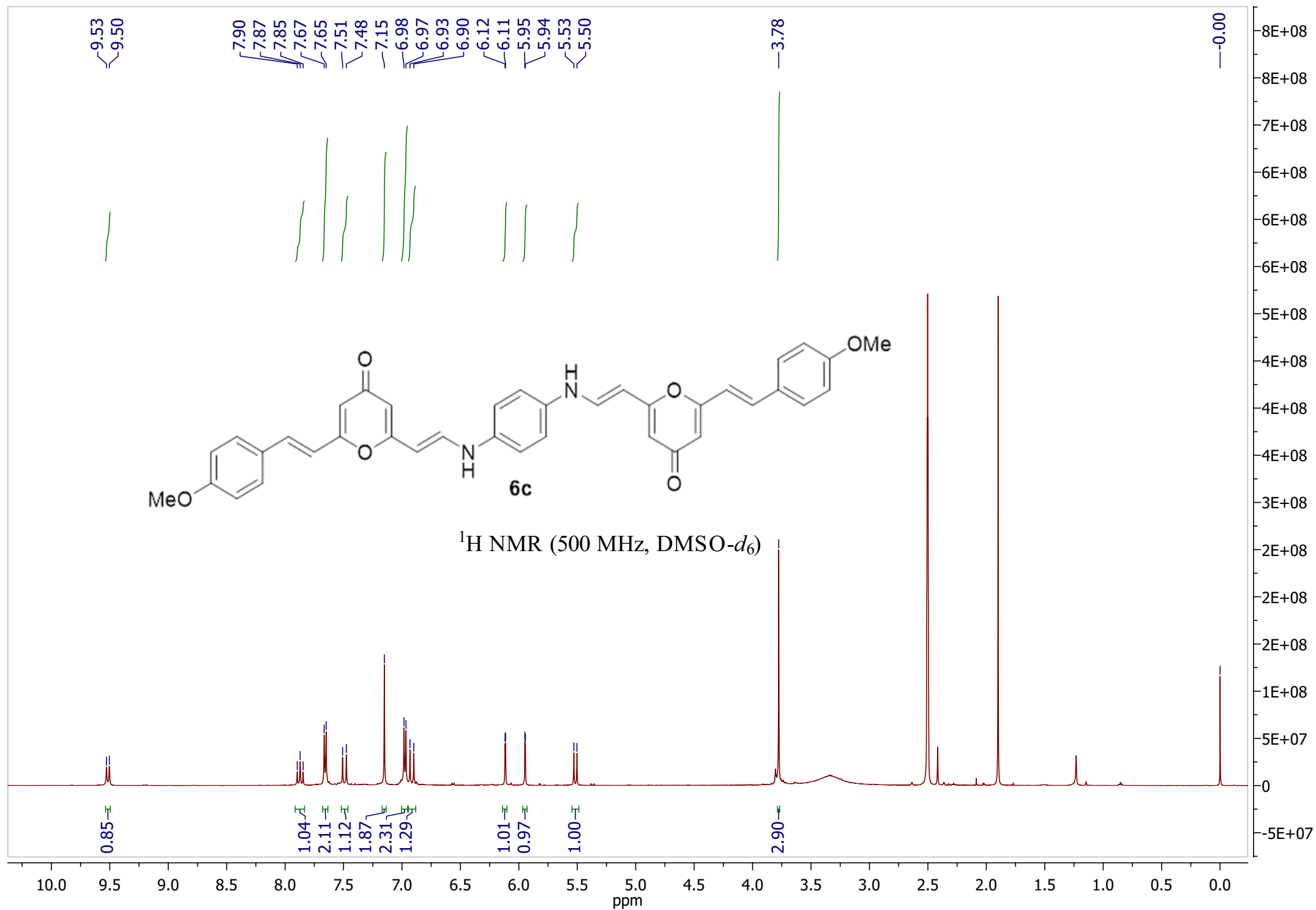


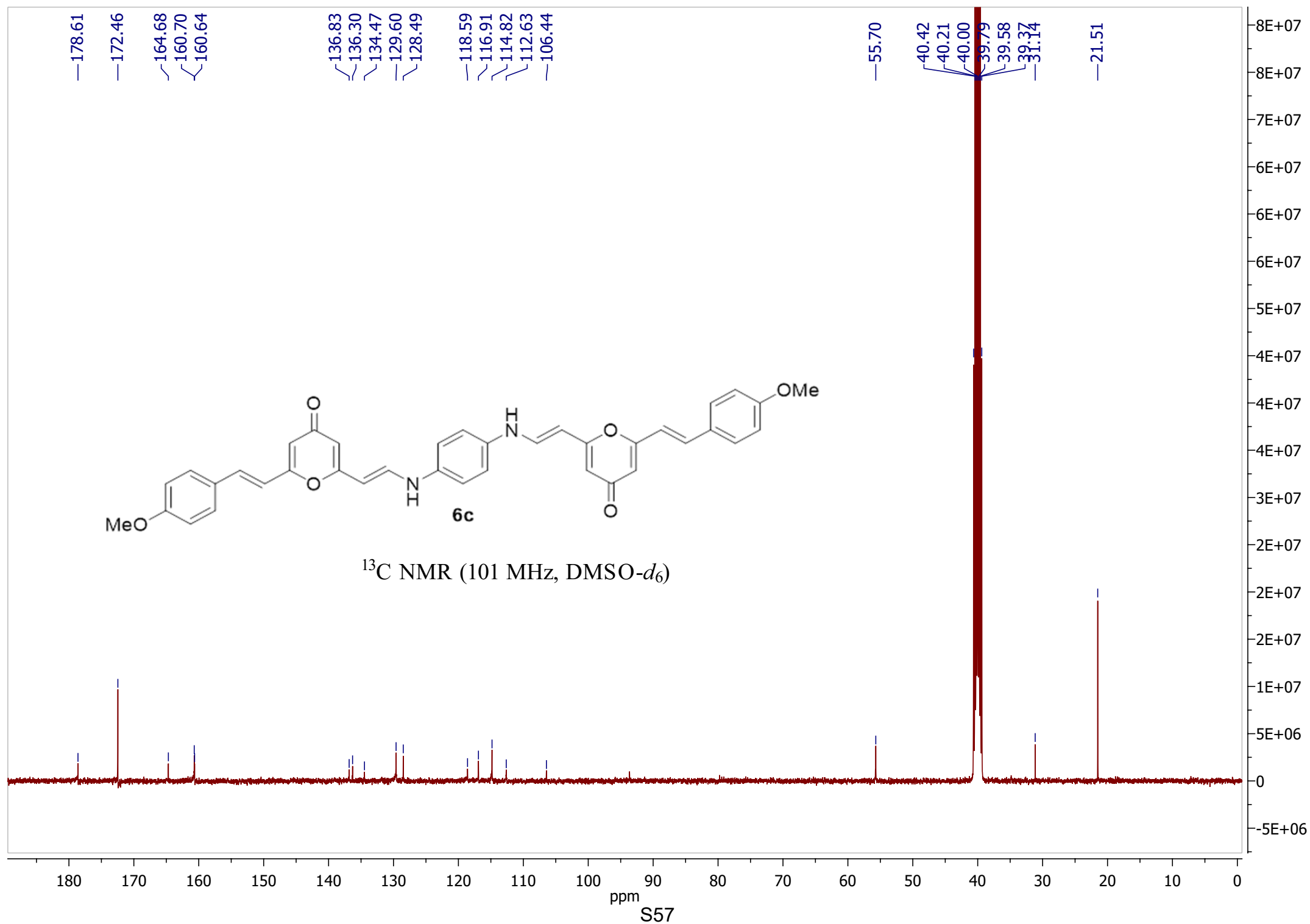


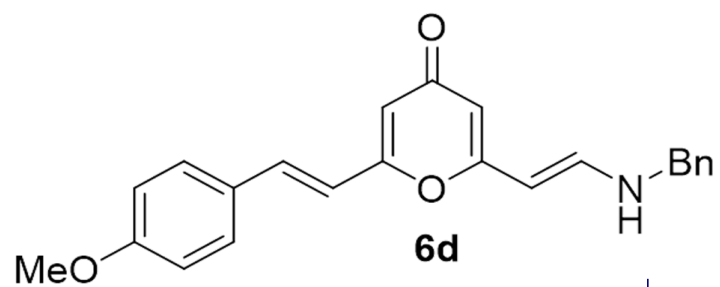




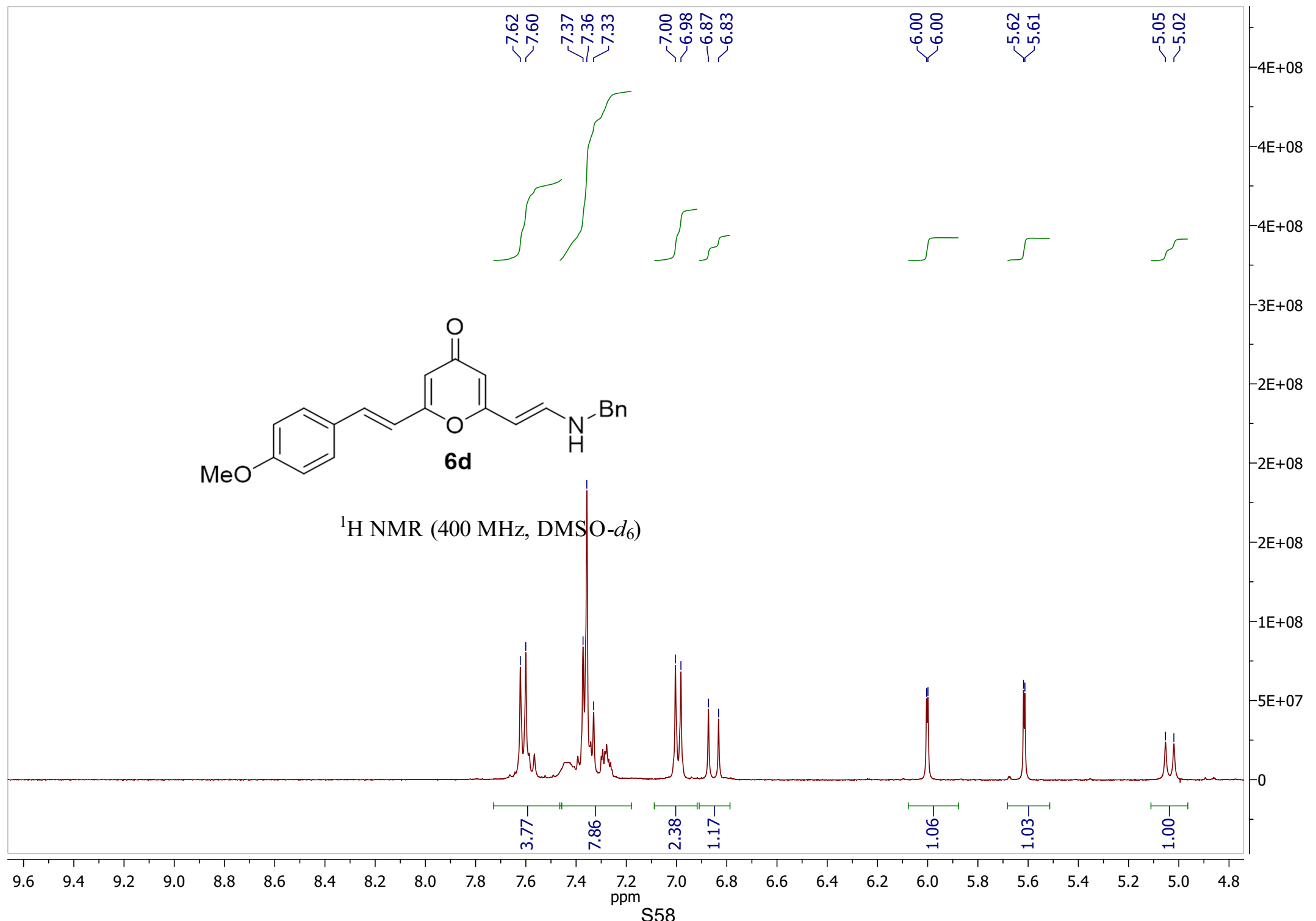
¹H NMR (500 MHz, DMSO-*d*₆)

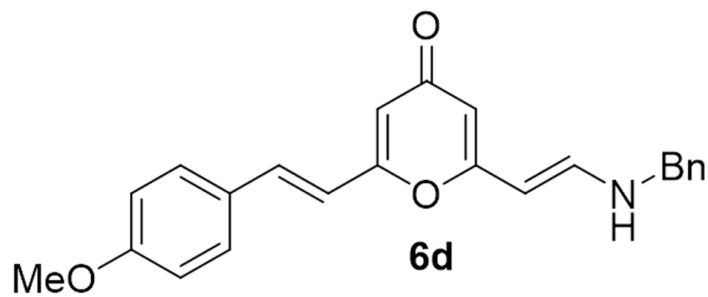




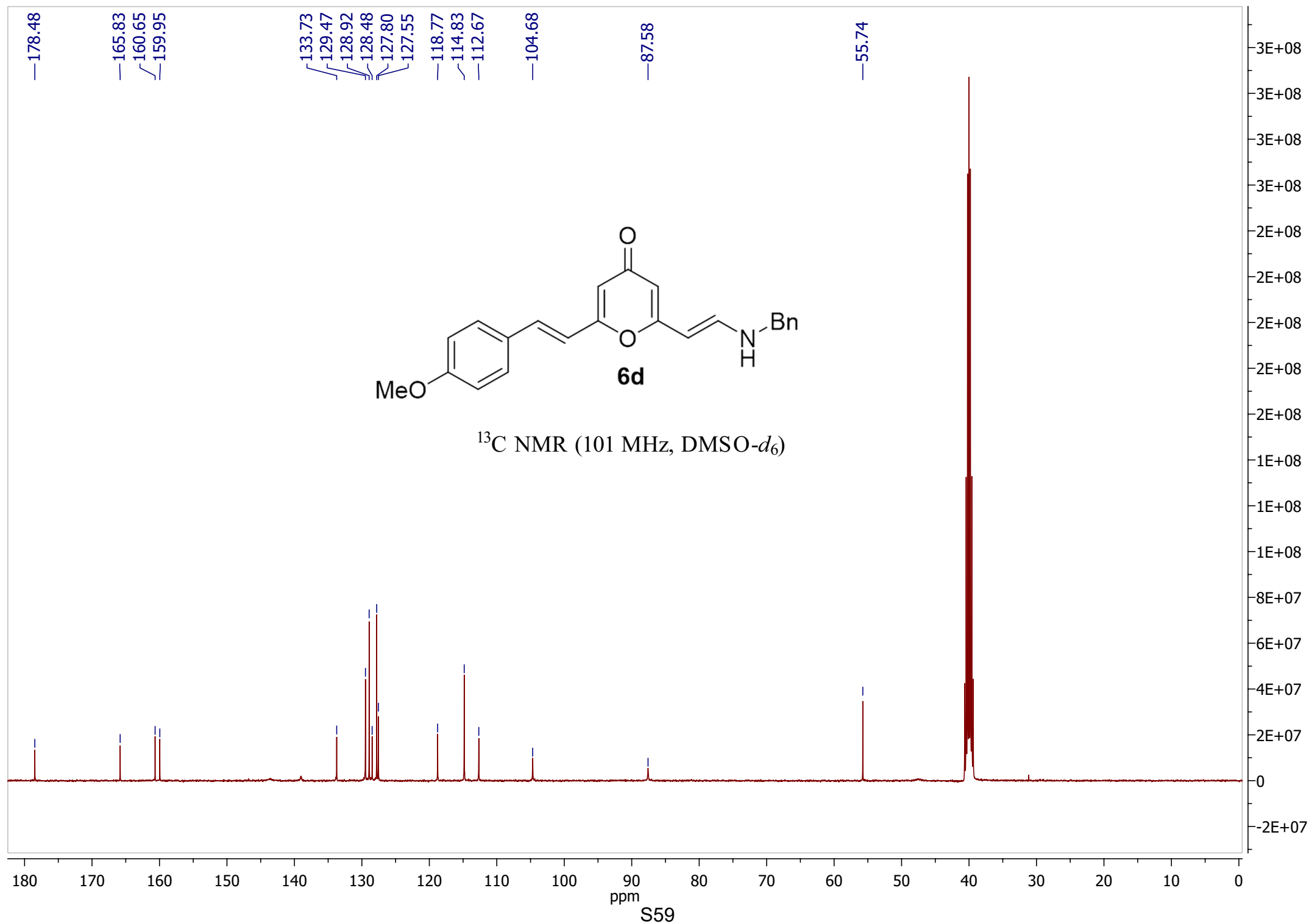


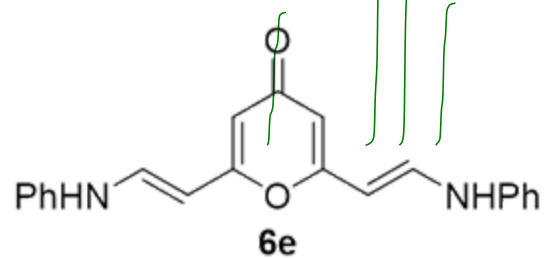
¹H NMR (400 MHz, DMSO-*d*₆)



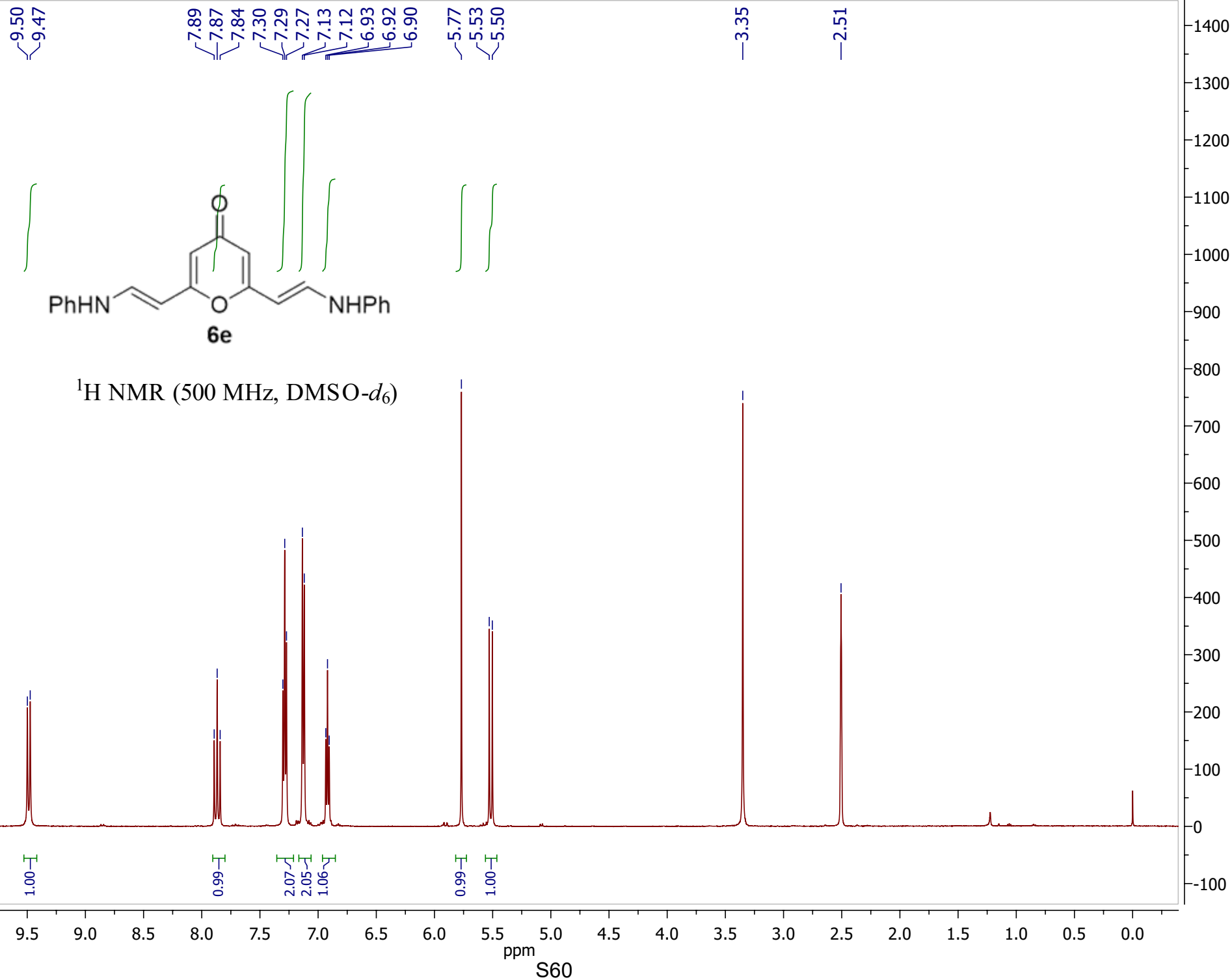


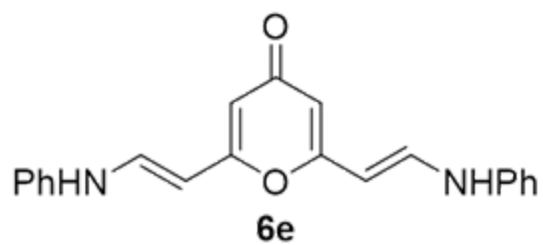
^{13}C NMR (101 MHz, DMSO- d_6)



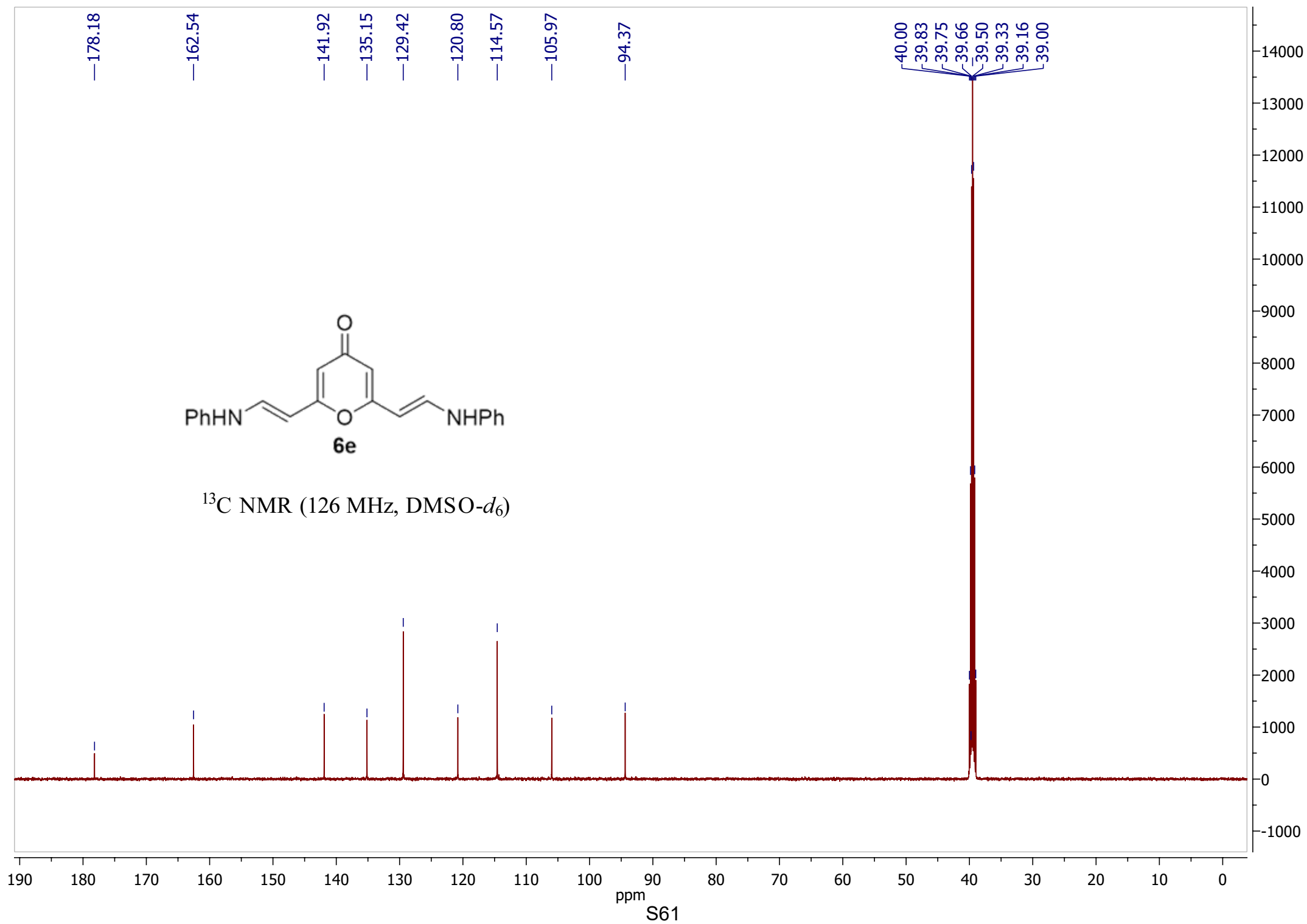


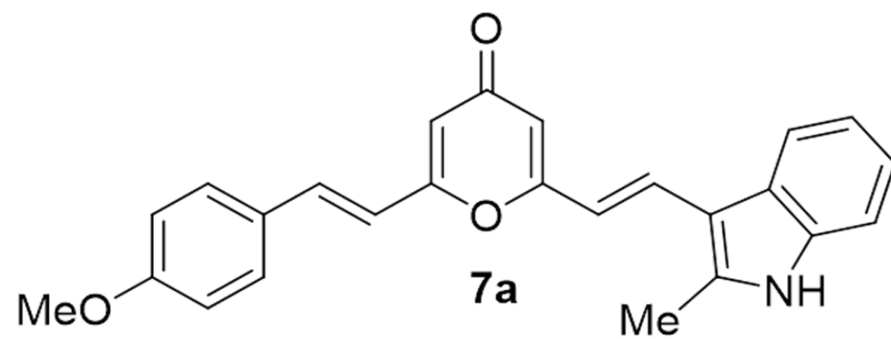
^1H NMR (500 MHz, DMSO- d_6)



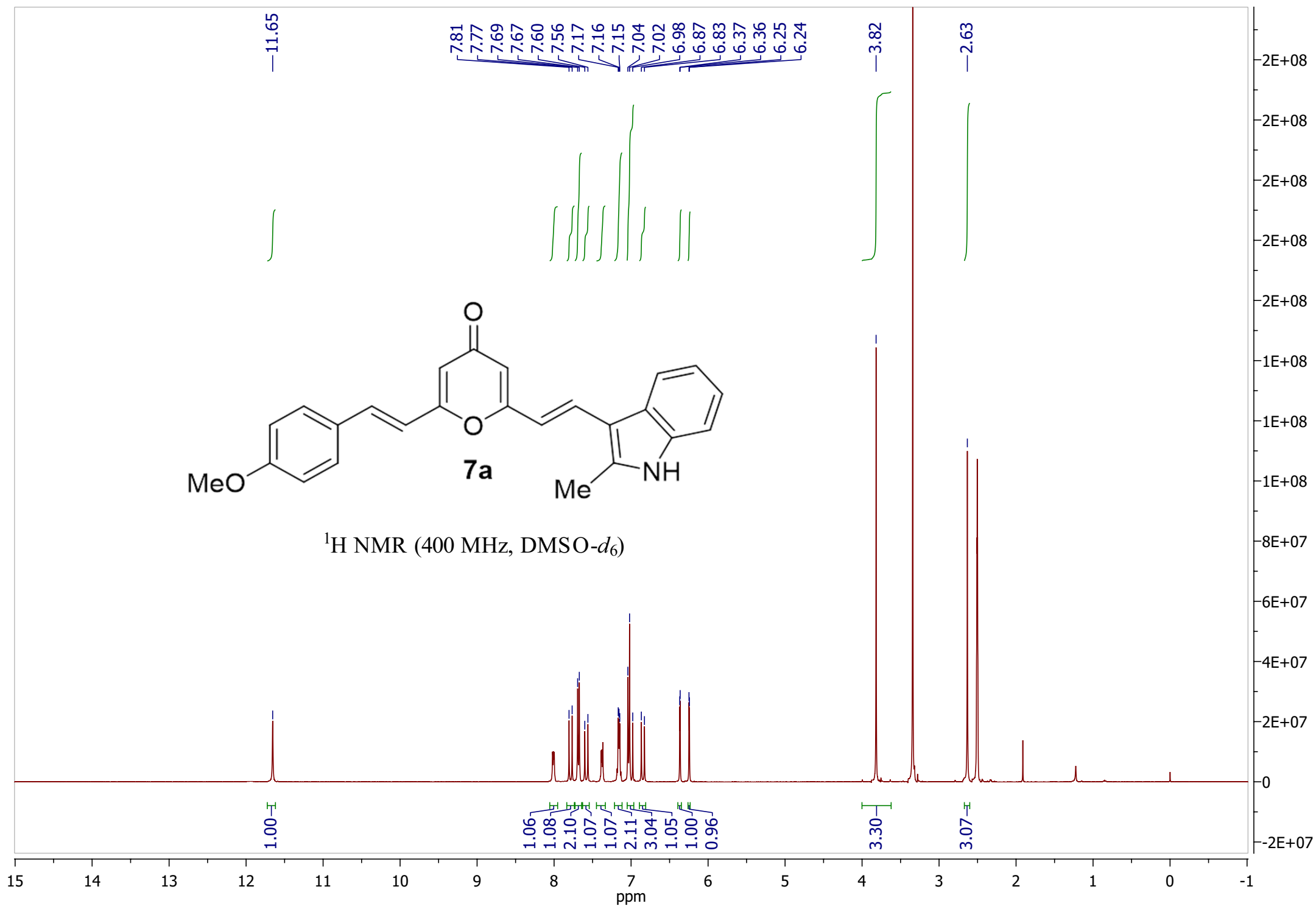


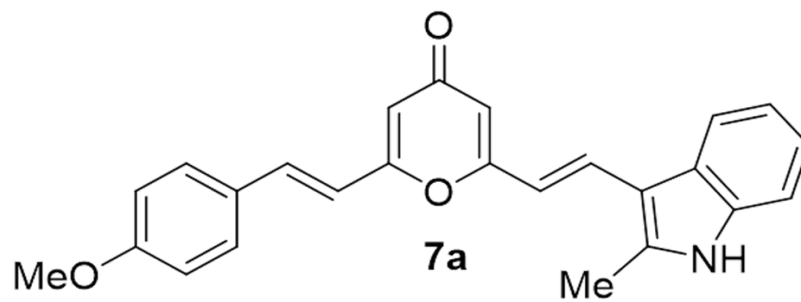
^{13}C NMR (126 MHz, DMSO- d_6)



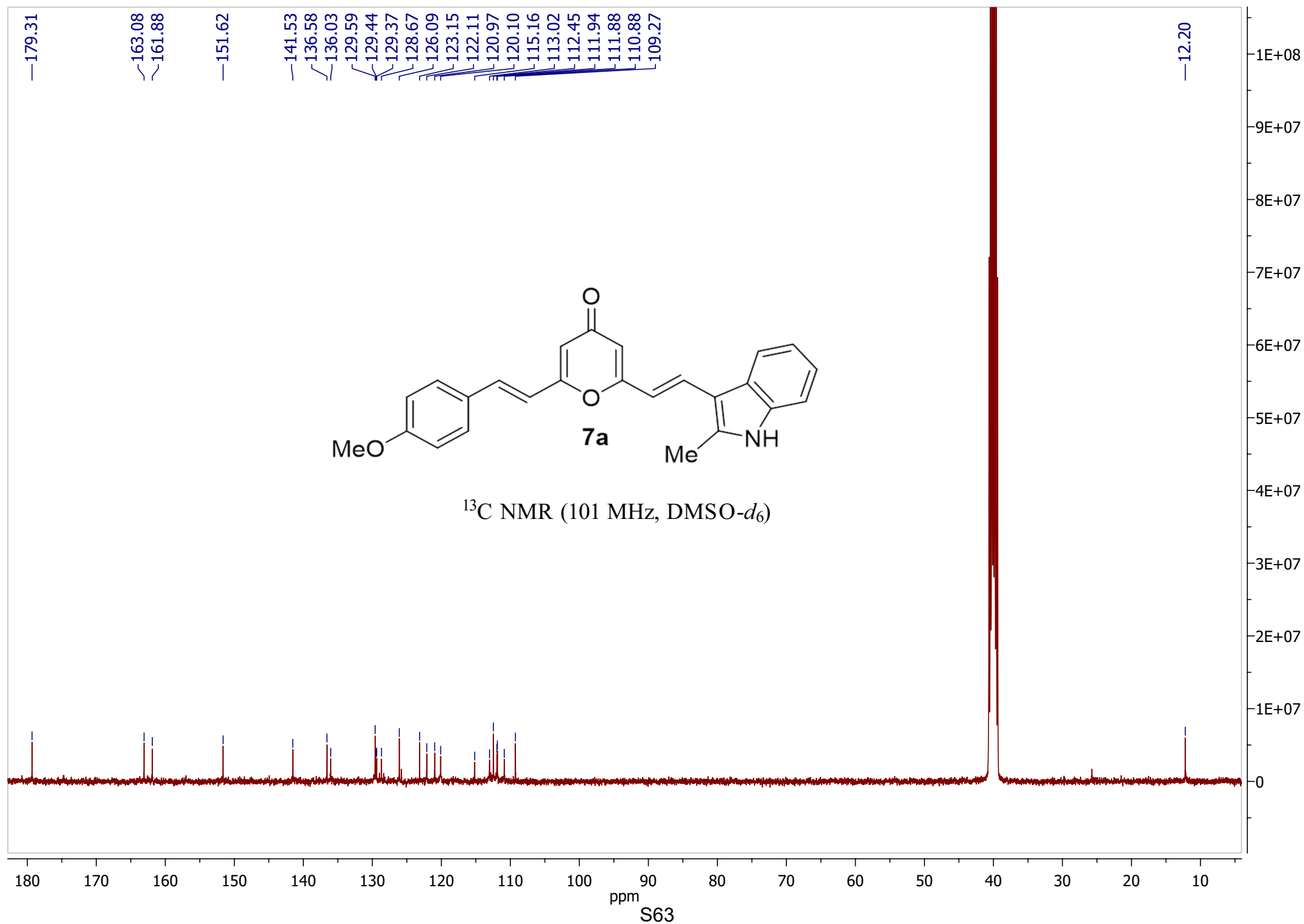


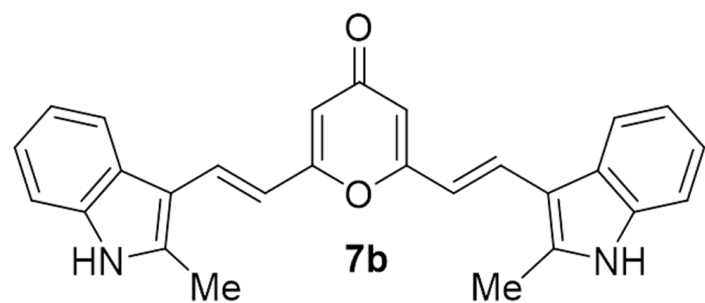
^1H NMR (400 MHz, DMSO- d_6)



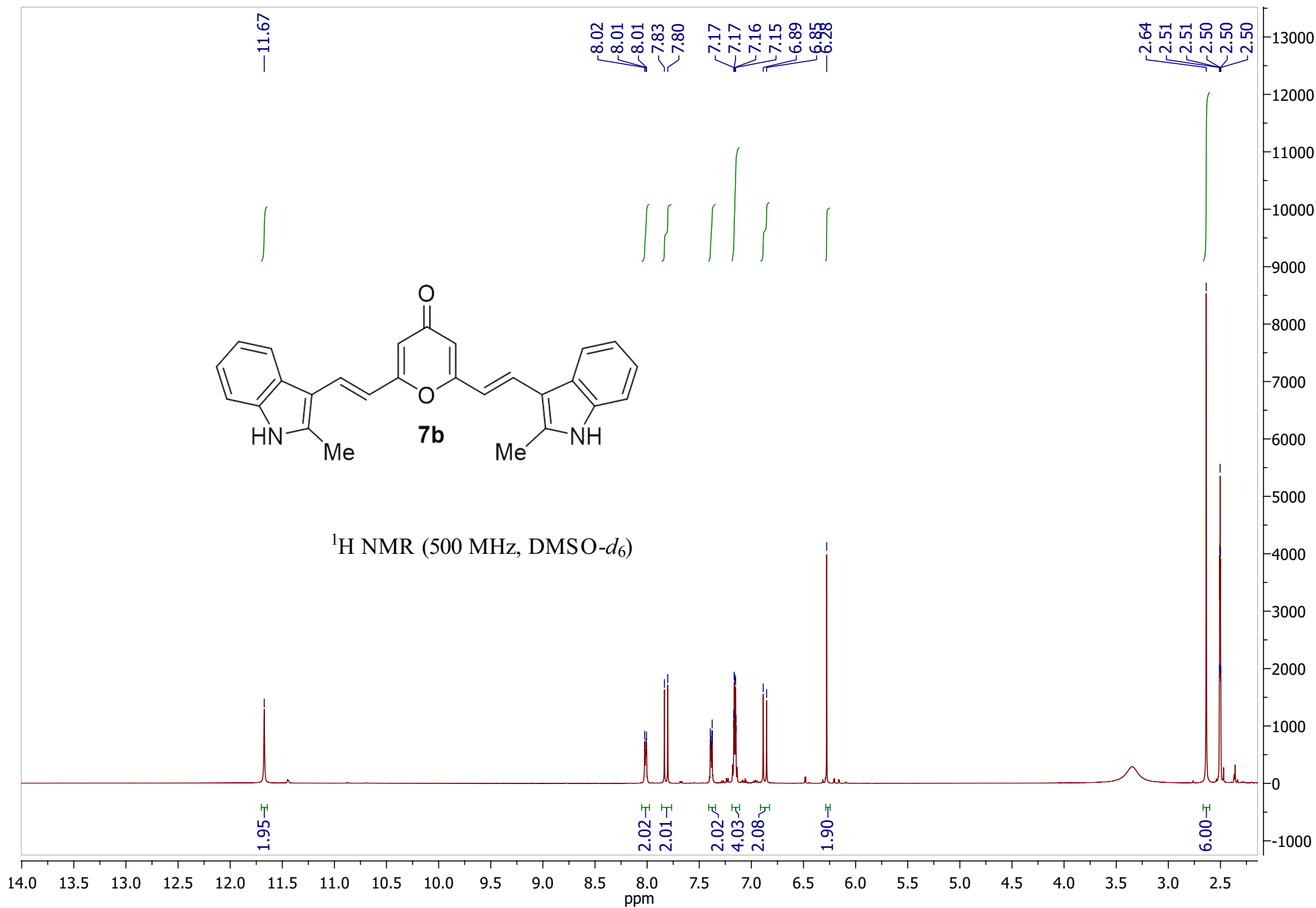


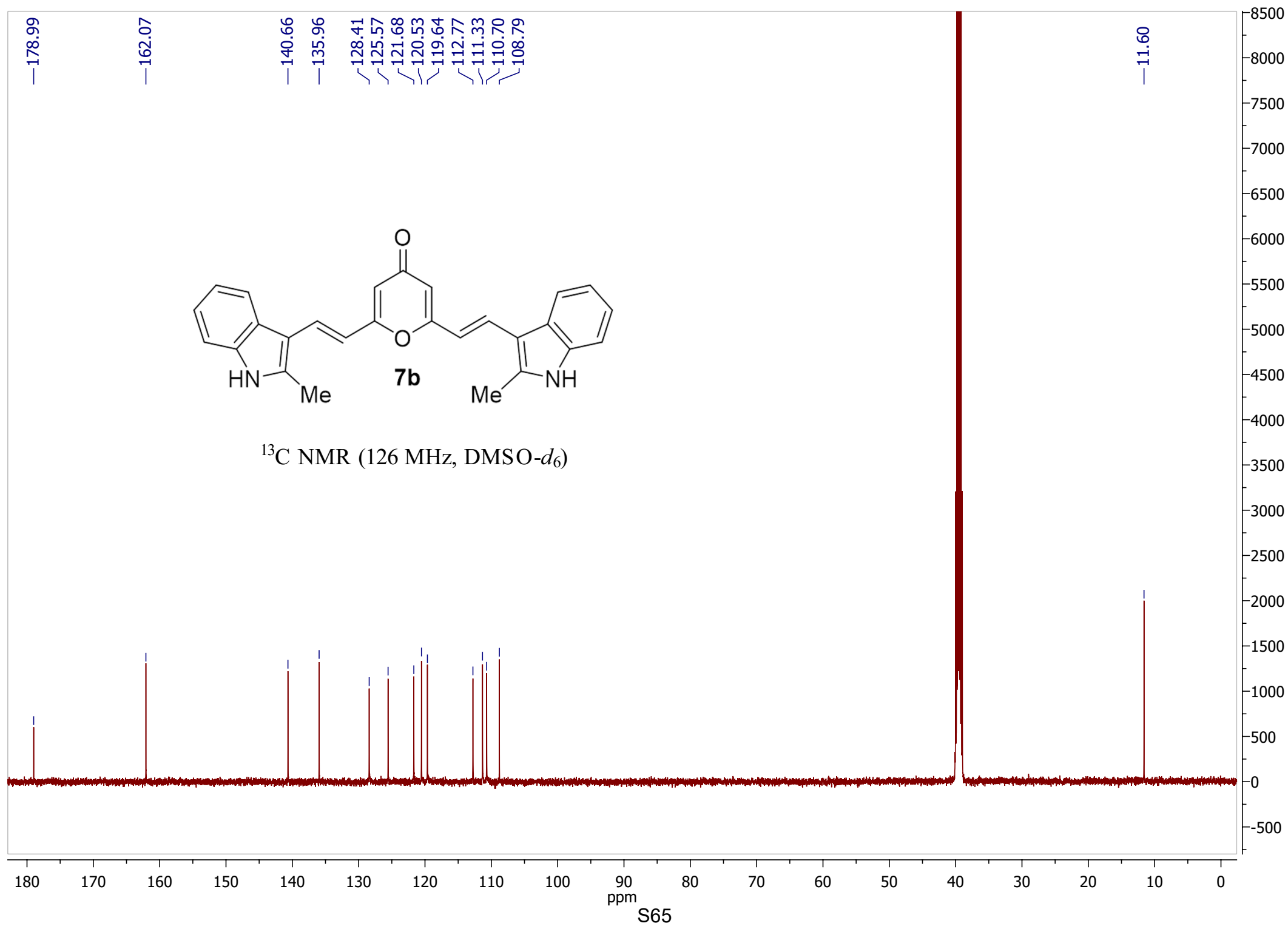
^{13}C NMR (101 MHz, DMSO- d_6)

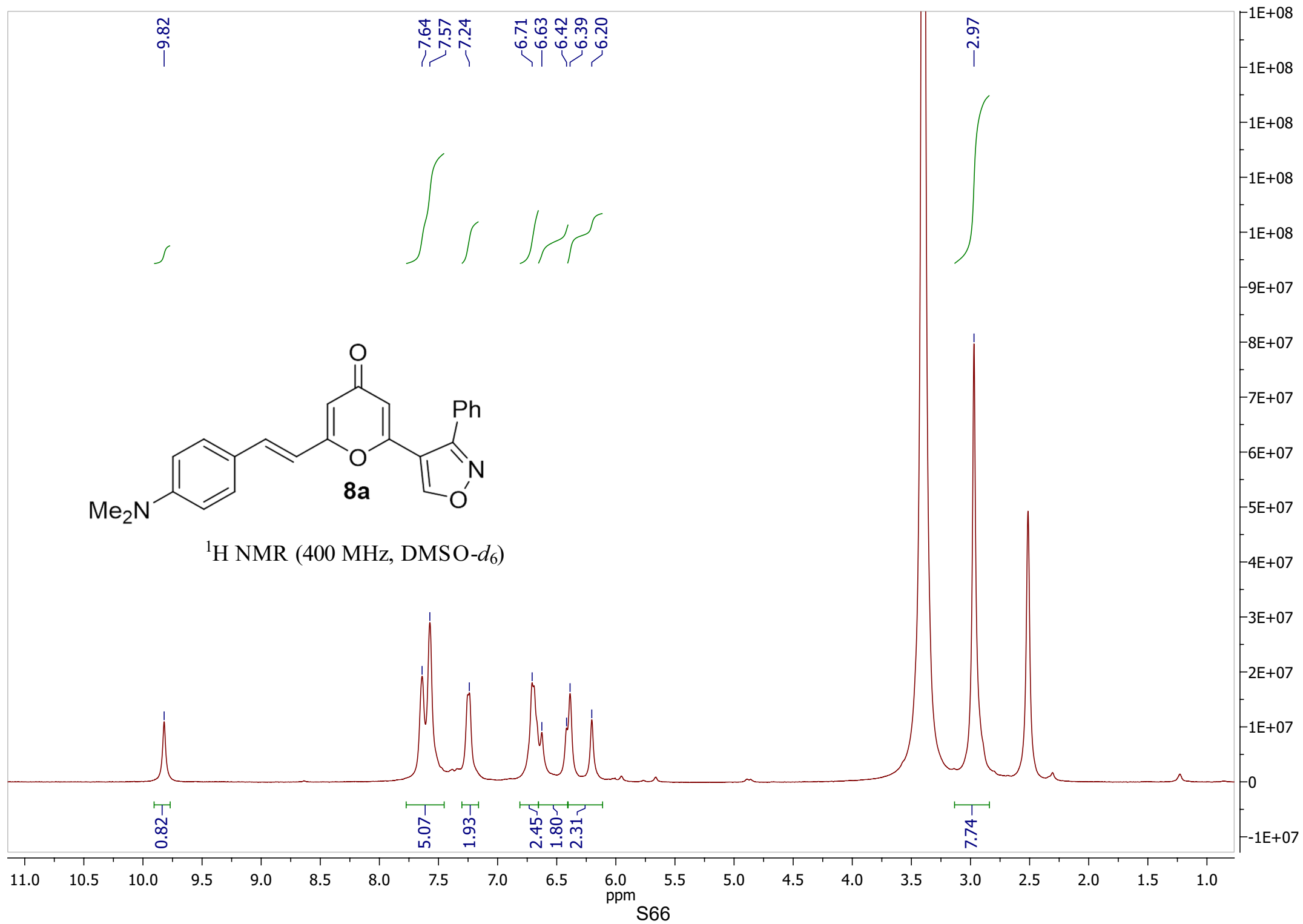


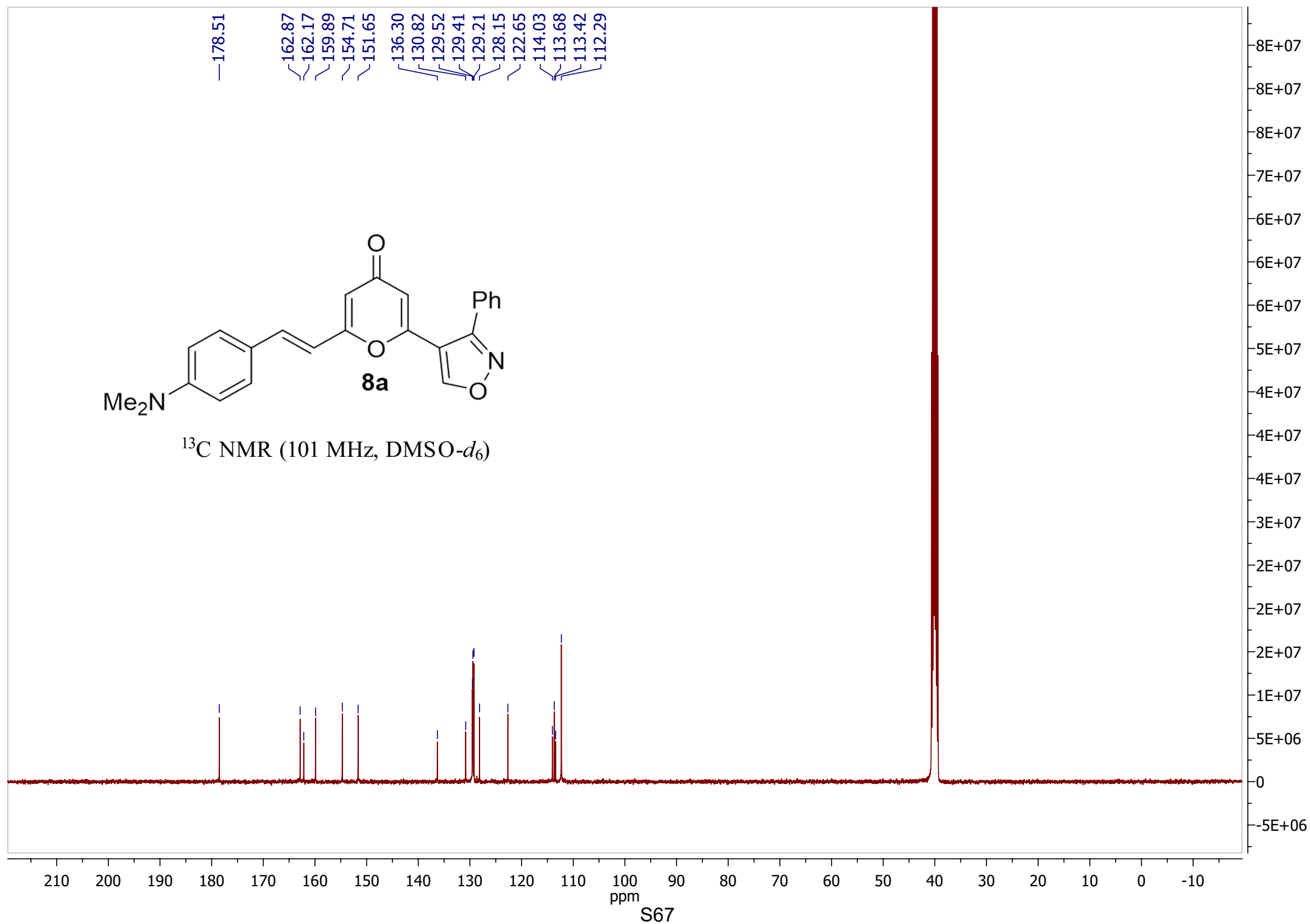


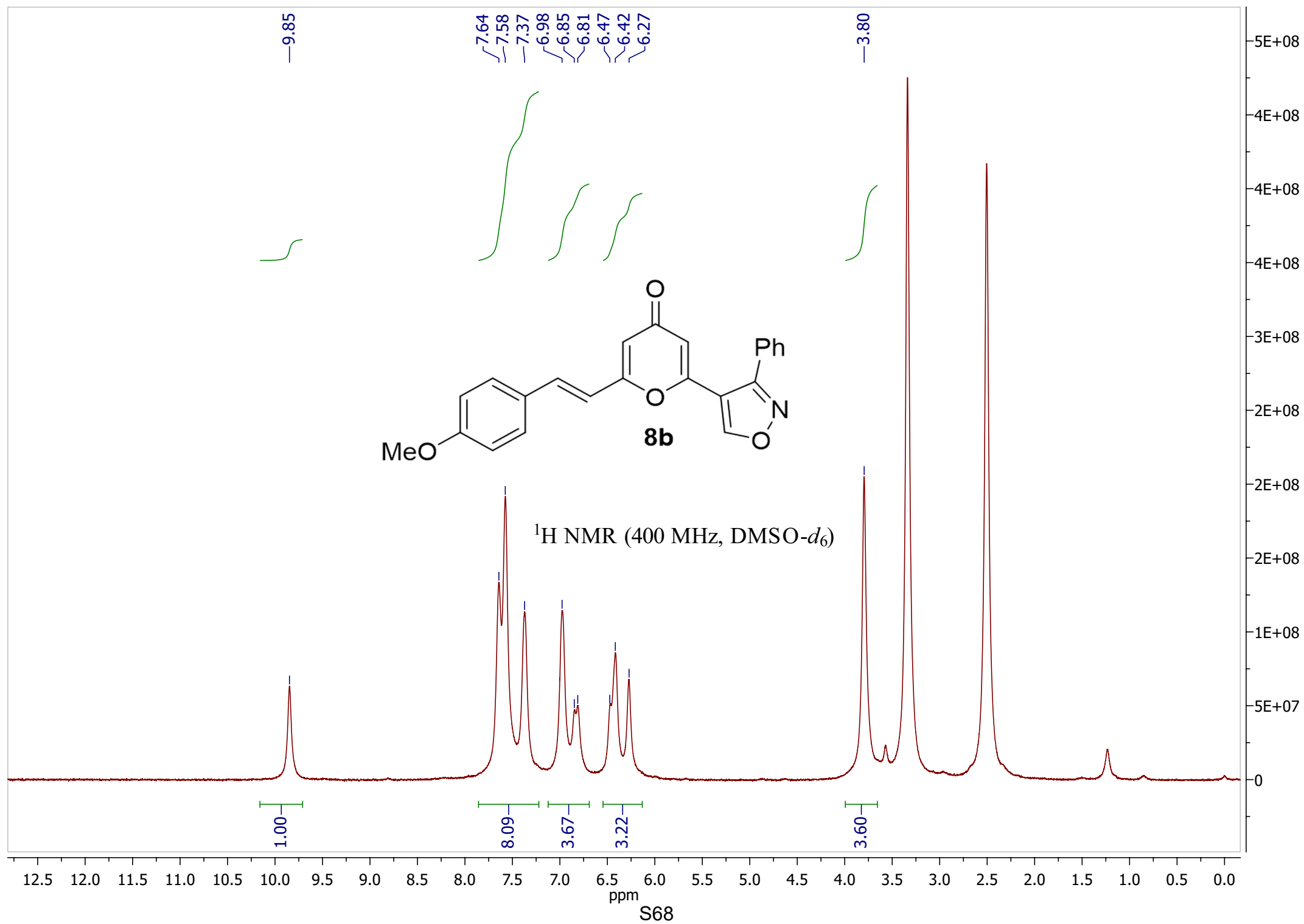
^1H NMR (500 MHz, $\text{DMSO}-d_6$)

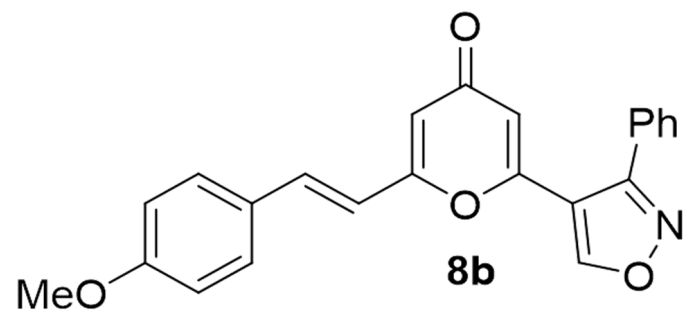












^{13}C NMR (126 MHz, DMSO- d_6)

