

Supporting Information for

**Catalyst-free formal [3 + 2] cycloaddition of stabilized N,N-cyclic azomethine imines to 3-nitrobenzofurans and 3-nitro-4H-chromenes.
Access to heteroannulated pyrazolo[1,2-a]pyrazoles**

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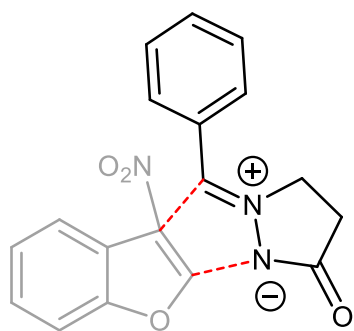
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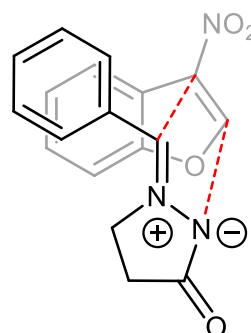
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I. Structures disclosure

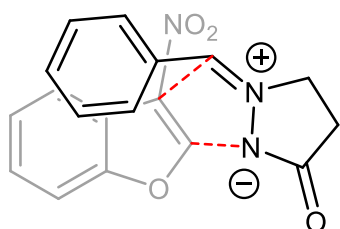
3-nitrobenzofuran:



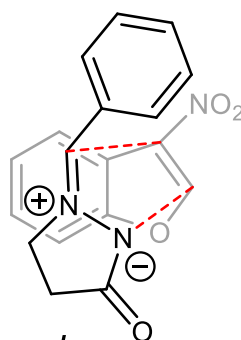
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anti endo

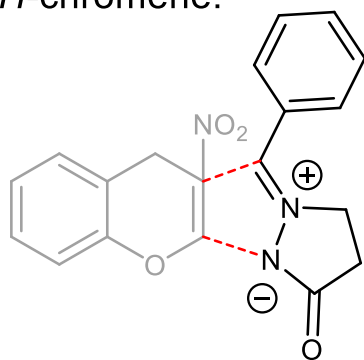


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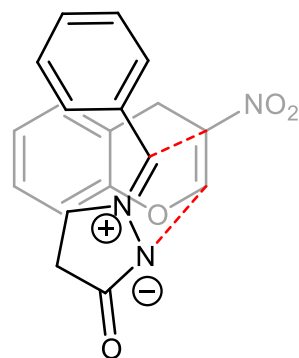


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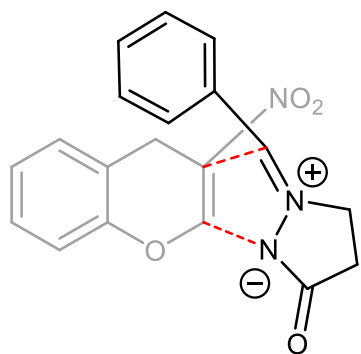
3-nitro-4*H*-chromene:



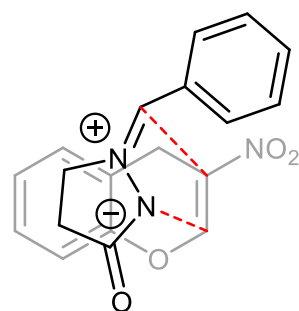
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anti endo



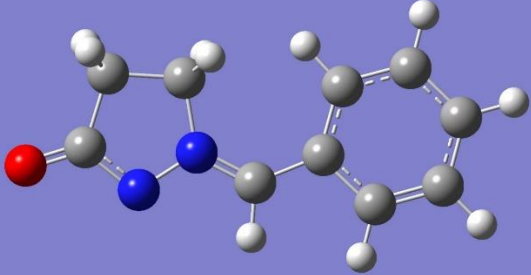
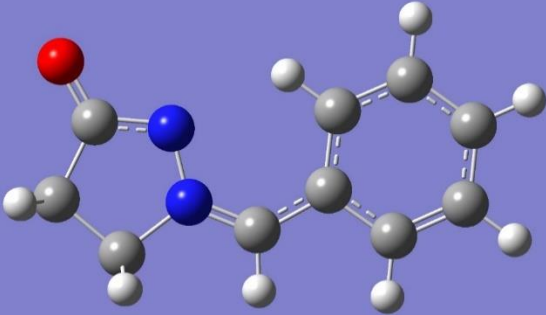
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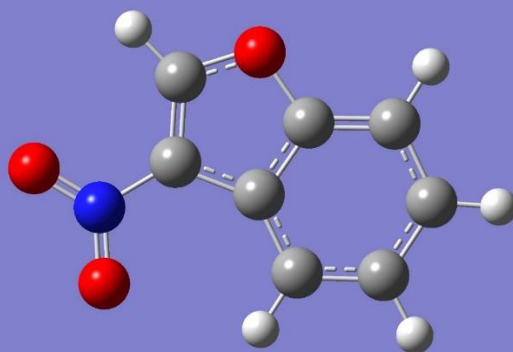
II. Cartesian coordinates of the geometries optimized in DMSO

at the level of the DFT theory with mPW1PW91 functional in the 6-311 ++ (d, p)

3-Nitrobenzofuran + azomethine imine 2a				
<i>anti-2a</i>				
		X	Y	Z
1	O	-4.5080000	-0.5634000	-0.0072000
2	N	-1.1380000	-0.3068000	-0.0298000
3	N	-2.2778000	-1.0408000	-0.0609000
4	C	1.3564000	-0.3552000	-0.0241000
5	C	0.0157000	-0.9008000	-0.0443000
6	C	2.3778000	-1.3230000	0.0404000
7	H	2.1078000	-2.3728000	0.0708000
8	C	-3.3352000	-0.2006000	0.0037000
9	C	1.7322000	0.9993000	-0.0717000
10	H	0.9990000	1.7879000	-0.1374000
11	C	-1.3810000	1.1612000	0.0227000
12	H	-0.9677000	1.6060000	-0.8812000
13	H	-0.8709000	1.5626000	0.8966000
14	C	-2.8870000	1.2492000	0.0974000
15	H	-3.2392000	1.6756000	1.0375000
16	H	-3.3202000	1.8234000	-0.7216000
17	C	3.0727000	1.3557000	-0.0469000
18	H	3.3406000	2.4052000	-0.0863000
19	C	3.7134000	-0.9584000	0.0674000
20	H	4.4782000	-1.7246000	0.1199000
21	C	4.0680000	0.3862000	0.0251000
22	H	5.1118000	0.6774000	0.0447000
23	H	-0.0626000	-1.9815000	-0.0687000
<i>syn-2a</i>				
		X	Y	Z
1	O	-3.4061000	1.8561000	0.0002000
2	N	-1.1384000	-0.6313000	-0.0001000
3	N	-1.4537000	0.6745000	-0.0001000
4	C	1.3270000	-0.4160000	0.0000000

5	C	0.0645000	-1.1186000	0.0000000
6	C	1.4844000	0.9807000	-0.0001000
7	H	0.6084000	1.6121000	-0.0001000
8	C	-2.8082000	0.7879000	-0.0001000
9	C	2.4785000	-1.2251000	0.0000000
10	H	2.3676000	-2.3042000	0.0001000
11	C	-2.3270000	-1.5445000	-0.0001000
12	H	-2.2691000	-2.1698000	0.8887000
13	H	-2.2693000	-2.1694000	-0.8892000
14	C	-3.4840000	-0.5766000	0.0002000
15	H	-4.1165000	-0.6656000	-0.8834000
16	H	-4.1159000	-0.6655000	0.8843000
17	C	3.7429000	-0.6606000	0.0000000
18	H	4.6183000	-1.2998000	0.0001000
19	C	2.7567000	1.5362000	-0.0001000
20	H	2.8653000	2.6149000	-0.0001000
21	C	3.8868000	0.7248000	0.0000000
22	H	4.8757000	1.1689000	0.0000000
23	H	0.0994000	-2.2014000	0.0000000

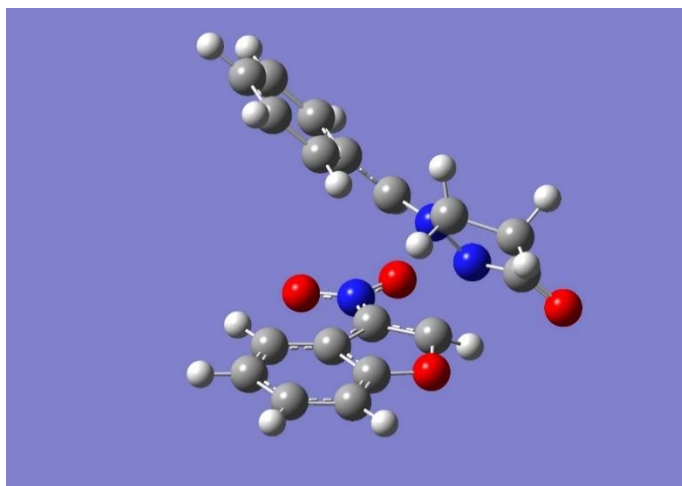
3-nitro-
benzofuran



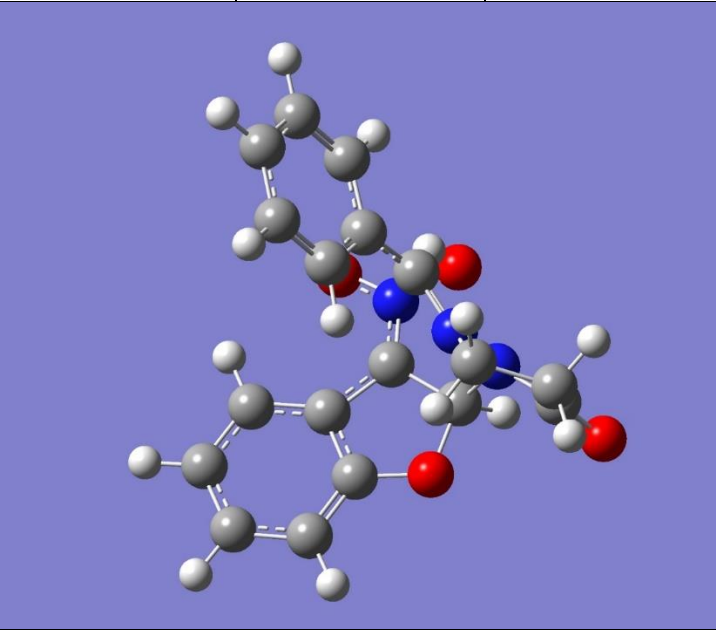
		X	Y	Z
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4	O	-2.1891000	-1.6747000	0.0000000
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6	C	0.2965000	-0.2474000	0.0000000
7	C	-0.9636000	1.6308000	0.0000000
8	C	1.0939000	0.9011000	0.0000000
9	C	0.9101000	-1.5017000	0.0000000
10	H	0.3217000	-2.4089000	0.0000000
11	C	2.2962000	-1.5419000	0.0000000
12	C	3.0675000	-0.3717000	0.0000000
13	H	4.1483000	-0.4465000	0.0000000
14	C	2.4752000	0.8840000	0.0000000
15	H	3.0562000	1.7974000	0.0000000
16	H	2.7973000	-2.5028000	0.0000000
17	H	-1.7210000	2.3986000	0.0000000

anti-endo cycloaddition

TS1

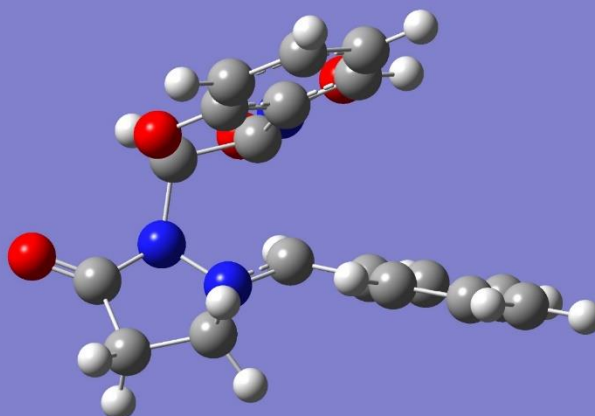


		X	Y	Z
1	O	-2.7157000	-0.1534000	-0.1791000
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3	O	-3.0349000	3.0278000	0.0382000
4	N	0.0315000	1.6078000	-0.1560000
5	N	-1.1481000	1.8222000	0.4980000
6	N	-0.4852000	-0.8770000	2.4974000
7	O	0.2301000	-1.8637000	2.7300000
8	C	-1.1339000	-0.7980000	1.2906000
9	C	2.3116000	0.6725000	0.0052000
10	C	-1.1022000	-1.7309000	0.1984000
11	C	1.0262000	1.0989000	0.5061000
12	H	0.8607000	1.0513000	1.5766000
13	C	-2.0718000	0.2204000	0.9644000
14	H	-2.6924000	0.7396000	1.6782000
15	C	-2.0759000	-1.2618000	-0.6899000
16	C	-0.3793000	-2.8748000	-0.1373000
17	H	0.3737000	-3.2656000	0.5336000
18	C	-0.6597000	-3.4982000	-1.3511000
19	C	3.3248000	0.5407000	0.9705000
20	H	3.1011000	0.7666000	2.0071000
21	C	-1.6323000	-3.0002000	-2.2192000
22	H	-1.8276000	-3.5079000	-3.1564000
23	C	-2.3660000	-1.8571000	-1.8966000
24	H	-3.1296000	-1.4616000	-2.5550000
25	C	-1.9207000	2.6679000	-0.2778000
26	C	2.5988000	0.3490000	-1.3311000
27	H	1.8324000	0.3880000	-2.0921000
28	C	-0.0133000	2.0628000	-1.5657000
29	H	-0.2218000	1.2056000	-2.2067000
30	H	0.9490000	2.4971000	-1.8251000
31	C	-1.1647000	3.0490000	-1.5328000
32	H	-0.8175000	4.0805000	-1.4376000
33	H	-1.8176000	2.9803000	-2.4012000

34	C	3.8730000	-0.0662000	-1.6841000
35	H	4.0834000	-0.3212000	-2.7160000
36	C	4.5984000	0.1369000	0.6061000
37	H	5.3724000	0.0496000	1.3594000
38	C	4.8761000	-0.1648000	-0.7235000
39	H	5.8702000	-0.4874000	-1.0106000
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		X	Y	Z
1	O	-2.4579000	0.5402000	-0.5665000
2	O	-0.5380000	0.3698000	3.0718000
3	O	-2.1143000	3.6658000	0.1317000
4	N	0.4717000	1.4588000	-0.2105000
5	N	-0.7223000	1.8566000	0.3682000
6	N	-0.7961000	-0.6599000	2.3779000
7	O	-0.5448000	-1.8148000	2.8034000
8	C	-1.2941000	-0.4839000	1.1455000
9	C	2.4687000	0.0596000	0.0050000
10	C	-1.6672000	-1.4827000	0.1886000
11	C	1.2603000	0.6845000	0.4724000
12	H	0.9803000	0.5621000	1.5162000
13	C	-1.7708000	0.8409000	0.6547000
14	H	-2.4540000	1.3642000	1.3240000
15	C	-2.3373000	-0.7959000	-0.8329000
16	C	-1.4959000	-2.8616000	0.0787000
17	H	-0.9906000	-3.4082000	0.8634000
18	C	-1.9938000	-3.5080000	-1.0540000
19	C	3.3627000	-0.3755000	0.9977000
20	H	3.1135000	-0.2230000	2.0416000
21	C	-2.6489000	-2.7997000	-2.0579000
22	H	-3.0294000	-3.3225000	-2.9279000
23	C	-2.8323000	-1.4157000	-1.9583000
24	H	-3.3491000	-0.8538000	-2.7270000
25	C	-1.0977000	3.0946000	-0.1660000

26	C	2.7723000	-0.1682000	-1.3473000
27	H	2.0729000	0.1037000	-2.1264000
28	C	0.7111000	2.2229000	-1.4486000
29	H	0.2694000	1.6893000	-2.2913000
30	H	1.7804000	2.3448000	-1.5950000
31	C	-0.0272000	3.5180000	-1.1398000
32	H	0.6260000	4.2474000	-0.6537000
33	H	-0.4798000	3.9767000	-2.0162000
34	C	3.9595000	-0.7922000	-1.6892000
35	H	4.1863000	-0.9777000	-2.7321000
36	C	4.5553000	-0.9834000	0.6443000
37	H	5.2458000	-1.3063000	1.4139000
38	C	4.8555000	-1.1898000	-0.6988000
39	H	5.7840000	-1.6755000	-0.9762000
40	H	-1.8692000	-4.5807000	-1.1510000

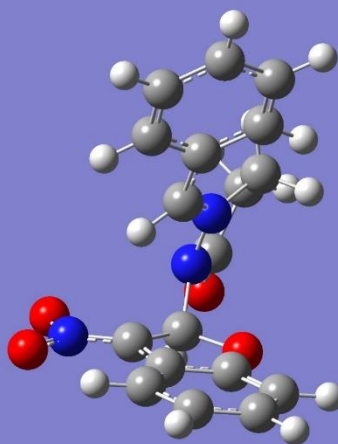
TS2



		X	Y	Z
1	O	2.2767000	1.0972000	-0.1098000
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3	O	4.1345000	-1.4586000	-0.1591000
4	N	0.7271000	-1.5385000	-0.3565000
5	N	1.8952000	-1.2213000	0.3219000
6	N	-0.0388000	0.3857000	2.5028000
7	O	-1.0523000	0.9969000	2.8609000
8	C	0.4262000	0.5389000	1.2024000
9	C	-1.7052000	-1.2402000	-0.1284000
10	C	0.1005000	1.6741000	0.3627000
11	C	-0.3556000	-1.3422000	0.3979000
12	H	-0.2490000	-1.7096000	1.4175000
13	C	1.8518000	0.1596000	0.8852000
14	H	2.5445000	0.1914000	1.7222000
15	C	1.2290000	1.9122000	-0.4253000
16	C	-1.0378000	2.4558000	0.1827000
17	H	-1.9179000	2.2886000	0.7887000
18	C	-1.0093000	3.4613000	-0.7813000
19	C	-2.7561000	-1.6627000	0.6982000
20	H	-2.5317000	-2.0722000	1.6767000
21	C	0.1280000	3.6753000	-1.5588000
22	H	0.1290000	4.4629000	-2.3037000
23	C	1.2741000	2.8974000	-1.3916000
24	H	2.1670000	3.0641000	-1.9816000

25	C	2.9832000	-1.6463000	-0.4553000
26	C	-1.9986000	-0.6961000	-1.3866000
27	H	-1.2068000	-0.3298000	-2.0265000
28	C	0.9948000	-1.7853000	-1.7740000
29	H	0.9609000	-0.8623000	-2.3587000
30	H	0.2701000	-2.4968000	-2.1627000
31	C	2.4182000	-2.3319000	-1.6815000
32	H	2.4224000	-3.4124000	-1.5126000
33	H	3.0328000	-2.1087000	-2.5512000
34	C	-3.3154000	-0.6042000	-1.8123000
35	H	-3.5357000	-0.1815000	-2.7856000
36	C	-4.0697000	-1.5705000	0.2648000
37	H	-4.8747000	-1.9075000	0.9072000
38	C	-4.3510000	-1.0437000	-0.9924000
39	H	-5.3780000	-0.9696000	-1.3314000
40	H	-1.8841000	4.0837000	-0.9291000

IM-TS

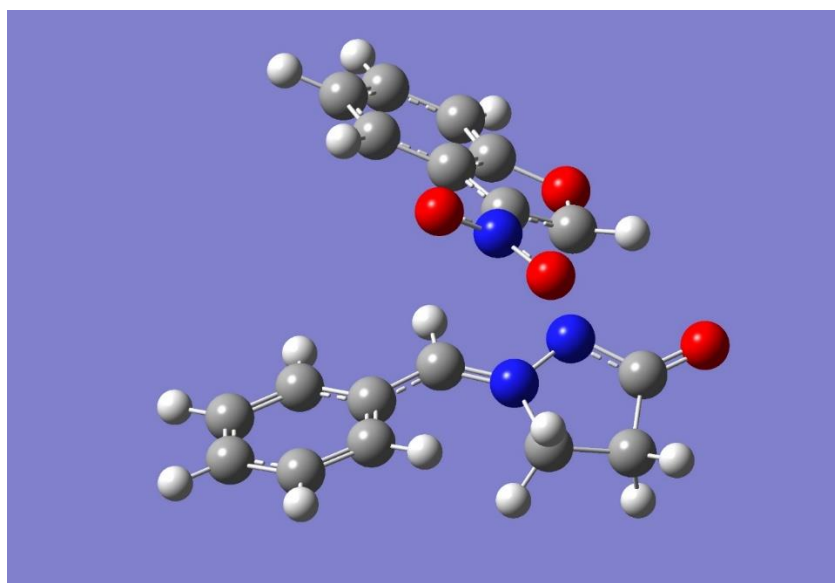


		X	Y	Z
1	O	-1.6944000	0.2879000	-1.5016000
2	O	-2.2780000	1.0657000	2.4925000
3	O	-1.8914000	3.7455000	-0.4702000
4	N	0.6366000	1.4518000	-0.1798000
5	N	-0.6877000	1.8409000	-0.0517000
6	N	-2.1618000	-0.1070000	2.0343000
7	O	-2.2932000	-1.1167000	2.7776000
8	C	-1.8775000	-0.2671000	0.7352000
9	C	2.4349000	-0.1290000	0.3529000
10	C	-1.7916000	-1.4773000	-0.0233000
11	C	1.1094000	0.4271000	0.4524000
12	H	0.4119000	-0.0564000	1.1274000
13	C	-1.8013000	0.8869000	-0.2065000
14	H	-2.6692000	1.5500000	-0.1731000
15	C	-1.6695000	-1.0766000	-1.3632000
16	C	-1.7984000	-2.8393000	0.2733000
17	H	-1.8960000	-3.1670000	1.2996000
18	C	-1.6849000	-3.7550000	-0.7763000
19	C	2.8304000	-0.9352000	1.4337000
20	H	2.1439000	-1.0943000	2.2572000
21	C	-1.5638000	-3.3286000	-2.0949000
22	H	-1.4782000	-4.0559000	-2.8940000
23	C	-1.5562000	-1.9624000	-2.4087000
24	H	-1.4704000	-1.6151000	-3.4315000
25	C	-0.8302000	3.1770000	-0.4208000
26	C	3.3068000	0.0459000	-0.7342000
27	H	3.0051000	0.6063000	-1.6082000

28	C	1.3699000	2.4696000	-0.9617000
29	H	1.3612000	2.1672000	-2.0095000
30	H	2.3887000	2.5336000	-0.5913000
31	C	0.5393000	3.7168000	-0.7255000
32	H	0.8938000	4.2840000	0.1388000
33	H	0.5004000	4.3746000	-1.5905000
34	C	4.5557000	-0.5512000	-0.7143000
35	H	5.2216000	-0.4257000	-1.5594000
36	C	4.0895000	-1.5102000	1.4525000
37	H	4.3927000	-2.1182000	2.2961000
38	C	4.9539000	-1.3163000	0.3796000
39	H	5.9360000	-1.7747000	0.3872000
40	H	-1.6934000	-4.8169000	-0.5568000

anti-exo cycloaddition

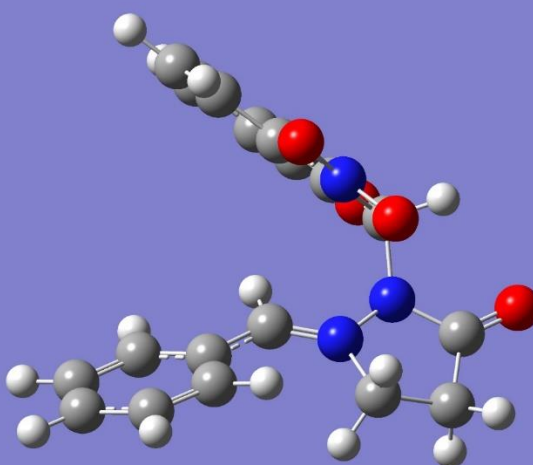
TS1



		X	Y	Z
1	O	-2.8488000	0.5478000	-0.4816000
2	O	-0.0979000	1.3758000	2.3808000
3	O	-1.6374000	3.8889000	-0.7718000
4	N	0.6755000	1.4251000	-0.6264000
5	N	-0.6089000	1.8525000	-0.8020000
6	N	-0.4443000	0.2080000	2.1183000
7	O	-0.0258000	-0.7714000	2.7525000
8	C	-1.3187000	0.0079000	1.0800000
9	C	2.2029000	-0.5194000	-0.5802000
10	C	-1.8164000	-1.2245000	0.5355000
11	C	0.9545000	0.1707000	-0.8087000
12	H	0.1448000	-0.4082000	-1.2367000
13	C	-1.9139000	1.0718000	0.3535000
14	H	-2.1800000	2.0344000	0.7668000
15	C	-2.7321000	-0.8241000	-0.4452000
16	C	-1.5966000	-2.5859000	0.7383000
17	H	-0.8977000	-2.9235000	1.4918000
18	C	-2.3049000	-3.4914000	-0.0487000
19	C	2.3247000	-1.7653000	-1.2195000
20	H	1.5070000	-2.1266000	-1.8328000
21	C	-3.2094000	-3.0610000	-1.0203000
22	H	-3.7454000	-3.7900000	-1.6167000
23	C	-3.4398000	-1.7010000	-1.2360000
24	H	-4.1424000	-1.3500000	-1.9817000

25	C	-0.6164000	3.2312000	-0.7462000
26	C	3.2512000	-0.0715000	0.2400000
27	H	3.1754000	0.8563000	0.7877000
28	C	1.5940000	2.5266000	-0.2463000
29	H	2.5303000	2.3997000	-0.7847000
30	H	1.7649000	2.4804000	0.8282000
31	C	0.7982000	3.7527000	-0.6424000
32	H	0.8530000	4.5568000	0.0891000
33	H	1.1027000	4.1442000	-1.6159000
34	C	4.3947000	-0.8413000	0.3840000
35	H	5.1956000	-0.4903000	1.0239000
36	C	3.4763000	-2.5216000	-1.0802000
37	H	3.5606000	-3.4743000	-1.5892000
38	C	4.5162000	-2.0591000	-0.2797000
39	H	5.4168000	-2.6510000	-0.1638000
40	H	-2.1495000	-4.5543000	0.0979000

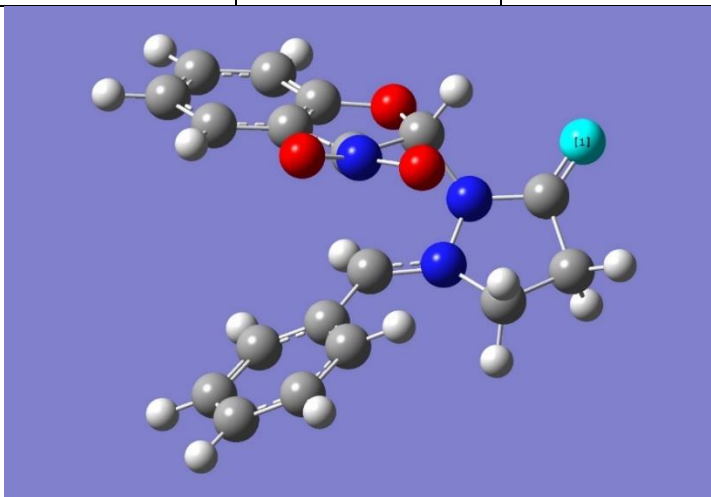
IM



		X	Y	Z
1	O	-2.3380000	0.6482000	-1.0963000
2	O	-0.1991000	1.5868000	2.2727000
3	O	-1.1520000	4.0391000	-0.7241000
4	N	0.8714000	1.2932000	-0.5014000
5	N	-0.3624000	1.8940000	-0.6304000
6	N	-0.7091000	0.4412000	2.0975000
7	O	-0.6142000	-0.4602000	2.9674000
8	C	-1.3427000	0.2010000	0.9405000
9	C	2.1714000	-0.7903000	-0.4758000
10	C	-2.0122000	-0.9838000	0.4989000
11	C	0.9994000	0.0196000	-0.7018000
12	H	0.1406000	-0.4748000	-1.1392000
13	C	-1.5761000	1.2770000	-0.0627000
14	H	-2.1353000	2.1394000	0.3095000
15	C	-2.5800000	-0.6528000	-0.7415000
16	C	-2.1824000	-2.2736000	0.9985000
17	H	-1.7533000	-2.5442000	1.9541000
18	C	-2.9175000	-3.1912000	0.2445000
19	C	2.2074000	-2.0126000	-1.1681000
20	H	1.3835000	-2.2797000	-1.8200000
21	C	-3.4692000	-2.8370000	-0.9830000
22	H	-4.0370000	-3.5649000	-1.5511000
23	C	-3.3054000	-1.5447000	-1.4979000
24	H	-3.7341000	-1.2533000	-2.4493000
25	C	-0.2186000	3.2782000	-0.6932000
26	C	3.2221000	-0.4623000	0.3961000

27	H	3.1969000	0.4426000	0.9863000
28	C	1.8963000	2.3128000	-0.1953000
29	H	2.8207000	2.0399000	-0.6967000
30	H	2.0360000	2.3481000	0.8840000
31	C	1.2526000	3.5848000	-0.7186000
32	H	1.4661000	4.4562000	-0.1038000
33	H	1.5462000	3.7975000	-1.7495000
34	C	4.2919000	-1.3298000	0.5407000
35	H	5.0954000	-1.0775000	1.2221000
36	C	3.2899000	-2.8644000	-1.0298000
37	H	3.3150000	-3.7983000	-1.5782000
38	C	4.3347000	-2.5228000	-0.1768000
39	H	5.1787000	-3.1927000	-0.0598000
40	H	-3.0611000	-4.1964000	0.6249000

TS2

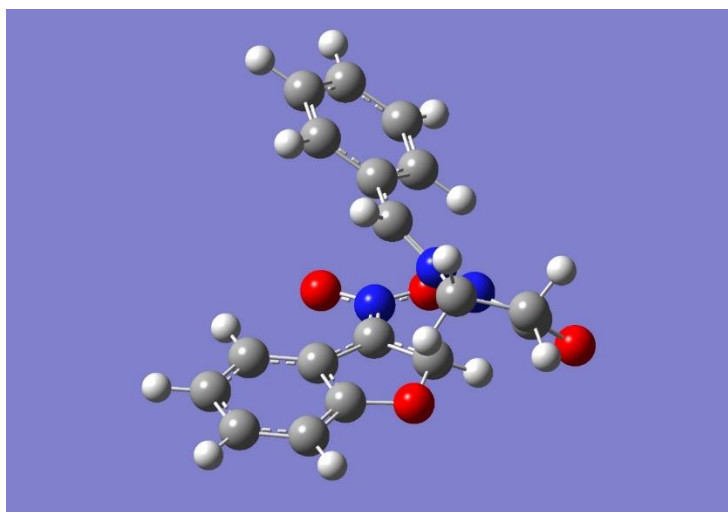


		X	Y	Z
1	O	-2.5709000	0.7909000	-0.4762000
2	O	0.4942000	1.1099000	2.2022000
3	O	-1.3787000	4.1299000	-0.0919000
4	N	0.7173000	1.4970000	-0.7074000
5	N	-0.5465000	2.0372000	-0.5144000
6	N	0.0161000	0.0035000	1.8896000
7	O	0.2962000	-1.0422000	2.4877000
8	C	-0.7912000	-0.0425000	0.7692000
9	C	1.8861000	-0.6770000	-0.6390000
10	C	-1.6694000	-1.1352000	0.4118000
11	C	0.7141000	0.1672000	-0.8063000
12	H	-0.0624000	-0.2348000	-1.4506000
13	C	-1.4542000	1.2256000	0.3048000
14	H	-1.8171000	1.8710000	1.1068000
15	C	-2.6830000	-0.5648000	-0.3653000
16	C	-1.6549000	-2.5104000	0.6213000
17	H	-0.8768000	-2.9638000	1.2204000
18	C	-2.6699000	-3.2802000	0.0542000
19	C	2.9596000	-0.3654000	0.2076000
20	H	2.9674000	0.5506000	0.7815000
21	C	-3.6707000	-2.6898000	-0.7144000
22	H	-4.4500000	-3.3064000	-1.1474000
23	C	-3.6939000	-1.3113000	-0.9358000
24	H	-4.4729000	-0.8424000	-1.5245000
25	C	-0.4558000	3.4186000	-0.4059000
26	C	1.8951000	-1.8972000	-1.3315000
27	H	1.0605000	-2.1487000	-1.9760000
28	C	1.7432000	2.5119000	-0.4312000
29	H	2.5977000	2.3434000	-1.0820000

30	H	2.0495000	2.4893000	0.6144000
31	C	0.9700000	3.7909000	-0.7352000
32	H	1.2877000	4.6421000	-0.1374000
33	H	1.0255000	4.0585000	-1.7940000
34	C	2.9630000	-2.7714000	-1.2038000
35	H	2.9624000	-3.7066000	-1.7512000
36	C	4.0233000	-1.2471000	0.3329000
37	H	4.8489000	-0.9979000	0.9891000
38	C	4.0314000	-2.4461000	-0.3735000
39	H	4.8675000	-3.1286000	-0.2725000
40	H	-2.6791000	-4.3520000	0.2147000

syn-endo cycloaddition

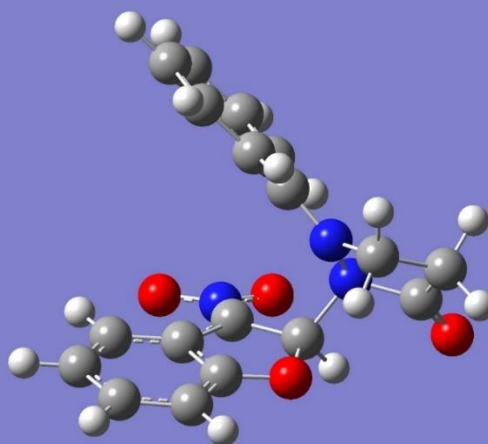
TS1



		X	Y	Z
1	O	-2.3351000	0.2079000	0.6616000
2	O	1.1327000	-0.0322000	2.7631000
3	O	-1.4480000	3.4262000	1.4907000
4	N	-0.3271000	1.4955000	-1.0466000
5	N	-0.3846000	1.7933000	0.2926000
6	N	0.7157000	-0.9646000	2.0493000
7	O	1.2763000	-2.0752000	2.0118000
8	C	-0.3932000	-0.7607000	1.2793000
9	C	1.8963000	0.3878000	-1.1109000
10	C	-1.0862000	-1.6991000	0.4430000
11	C	0.6207000	0.8234000	-1.6220000
12	H	0.4213000	0.6216000	-2.6690000
13	C	-1.1406000	0.4546000	1.2938000
14	H	-1.2249000	1.0863000	2.1686000
15	C	-2.2662000	-1.0403000	0.0766000
16	C	-0.8649000	-2.9910000	-0.0310000
17	H	0.0333000	-3.5281000	0.2424000
18	C	-1.8299000	-3.5663000	-0.8575000
19	C	2.6329000	-0.4597000	-1.9577000
20	H	2.1873000	-0.8033000	-2.8847000
21	C	-2.9916000	-2.8800000	-1.2087000
22	H	-3.7243000	-3.3535000	-1.8517000
23	C	-3.2310000	-1.5857000	-0.7370000
24	H	-4.1322000	-1.0413000	-0.9918000
25	C	-1.1940000	2.9229000	0.4191000
26	C	2.4831000	0.8514000	0.0783000
27	H	1.9268000	1.4986000	0.7401000
28	C	-1.4309000	2.1401000	-1.8027000

29	H	-2.2801000	1.4567000	-1.8246000
30	H	-1.0949000	2.3534000	-2.8132000
31	C	-1.6981000	3.3575000	-0.9397000
32	H	-1.1238000	4.2261000	-1.2724000
33	H	-2.7496000	3.6320000	-0.8819000
34	C	3.7787000	0.4779000	0.3941000
35	H	4.2321000	0.8465000	1.3065000
36	C	3.9177000	-0.8479000	-1.6178000
37	H	4.4739000	-1.5079000	-2.2728000
38	C	4.4951000	-0.3737000	-0.4435000
39	H	5.5052000	-0.6664000	-0.1803000
40	H	-1.6729000	-4.5710000	-1.2336000

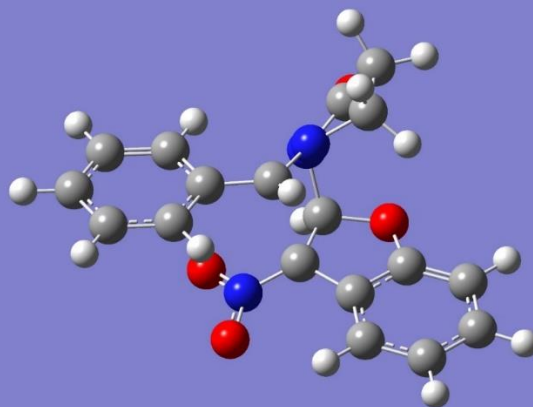
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		X	Y	Z
1	O	-2.3253000	0.2471000	0.3636000
2	O	0.9270000	0.0713000	2.8056000
3	O	-1.3923000	3.4075000	1.5776000
4	N	-0.3156000	1.5314000	-1.0547000
5	N	-0.4741000	1.7144000	0.3198000
6	N	0.5635000	-0.9026000	2.0874000
7	O	1.0768000	-2.0425000	2.2253000
8	C	-0.3799000	-0.7024000	1.1543000
9	C	1.8808000	0.3564000	-1.1019000
10	C	-1.0760000	-1.6857000	0.3787000
11	C	0.6638000	0.9071000	-1.6294000
12	H	0.5362000	0.8480000	-2.7059000
13	C	-1.1248000	0.5759000	1.0651000
14	H	-1.3578000	1.0336000	2.0271000
15	C	-2.2356000	-1.0469000	-0.0864000
16	C	-0.8629000	-3.0204000	0.0390000
17	H	0.0171000	-3.5362000	0.3992000
18	C	-1.8084000	-3.6682000	-0.7604000
19	C	2.6285000	-0.4231000	-2.0027000
20	H	2.2244000	-0.6381000	-2.9848000
21	C	-2.9461000	-3.0066000	-1.2120000
22	H	-3.6675000	-3.5293000	-1.8294000
23	C	-3.1793000	-1.6673000	-0.8709000
24	H	-4.0681000	-1.1432000	-1.2014000
25	C	-1.0936000	2.9776000	0.4965000
26	C	2.4128000	0.6631000	0.1616000
27	H	1.8511000	1.2577000	0.8680000
28	C	-1.2701000	2.3922000	-1.7857000
29	H	-2.2318000	1.8809000	-1.8332000
30	H	-0.8883000	2.5929000	-2.7819000
31	C	-1.3152000	3.5968000	-0.8599000

32	H	-0.5039000	4.2982000	-1.0731000
33	H	-2.2632000	4.1298000	-0.8778000
34	C	3.6703000	0.1981000	0.5007000
35	H	4.0871000	0.4437000	1.4699000
36	C	3.8724000	-0.9087000	-1.6392000
37	H	4.4396000	-1.5184000	-2.3320000
38	C	4.3963000	-0.5920000	-0.3896000
39	H	5.3764000	-0.9588000	-0.1068000
40	H	-1.6526000	-4.7070000	-1.0298000

TS2

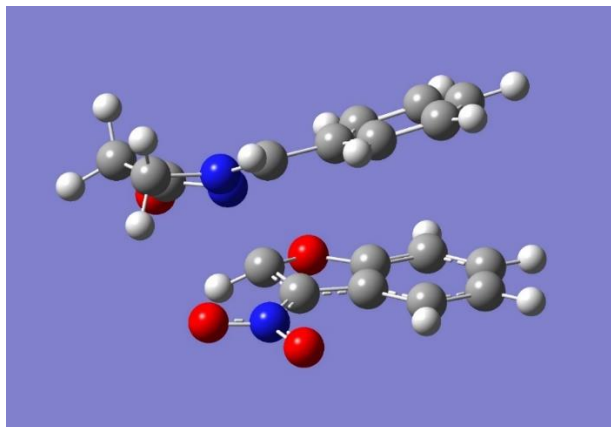


		X	Y	Z
1	O	-2.1461000	0.7620000	0.9594000
2	O	1.3736000	-0.8348000	2.0802000
3	O	-0.8997000	3.5997000	1.3690000
4	N	0.0907000	1.3261000	-0.9575000
5	N	-0.0265000	1.7126000	0.3684000
6	N	0.6046000	-1.4464000	1.3231000
7	O	0.7270000	-2.6558000	1.0812000
8	C	-0.3845000	-0.7299000	0.6722000
9	C	2.1196000	-0.0821000	-0.7634000
10	C	-1.6040000	-1.3260000	0.1653000
11	C	0.7637000	0.2081000	-1.2014000
12	H	0.4356000	-0.3157000	-2.0954000
13	C	-0.7349000	0.6367000	1.1684000
14	H	-0.5056000	0.8355000	2.2116000
15	C	-2.6026000	-0.3636000	0.3346000
16	C	-1.9279000	-2.5477000	-0.4187000
17	H	-1.1698000	-3.3079000	-0.5507000
18	C	-3.2437000	-2.7662000	-0.8219000
19	C	2.6978000	-1.2719000	-1.2304000
20	H	2.1044000	-1.9509000	-1.8324000
21	C	-4.2192000	-1.7845000	-0.6517000
22	H	-5.2366000	-1.9750000	-0.9735000
23	C	-3.9099000	-0.5573000	-0.0630000
24	H	-4.6618000	0.2075000	0.0885000
25	C	-0.6552000	2.9862000	0.3665000
26	C	2.8972000	0.8030000	-0.0028000
27	H	2.4654000	1.7242000	0.3651000
28	C	-0.8840000	2.0206000	-1.8063000
29	H	-1.8434000	1.4981000	-1.8234000
30	H	-0.4880000	2.0999000	-2.8153000
31	C	-0.9660000	3.3535000	-1.0678000
32	H	-0.2068000	4.0550000	-1.4249000
33	H	-1.9406000	3.8350000	-1.1224000
34	C	4.2263000	0.5097000	0.2567000
35	H	4.8257000	1.2082000	0.8293000

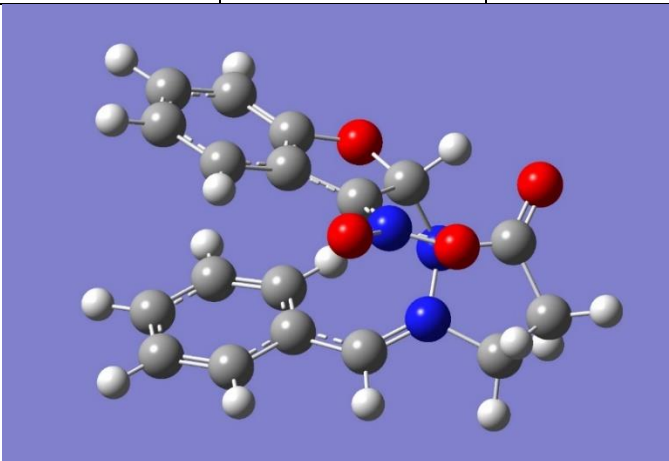
36	C	4.0226000	-1.5680000	-0.9484000
37	H	4.4596000	-2.4879000	-1.3190000
38	C	4.7915000	-0.6754000	-0.2081000
39	H	5.8310000	-0.8996000	0.0031000
40	H	-3.5114000	-3.7132000	-1.2762000

syn-exo cycloaddition

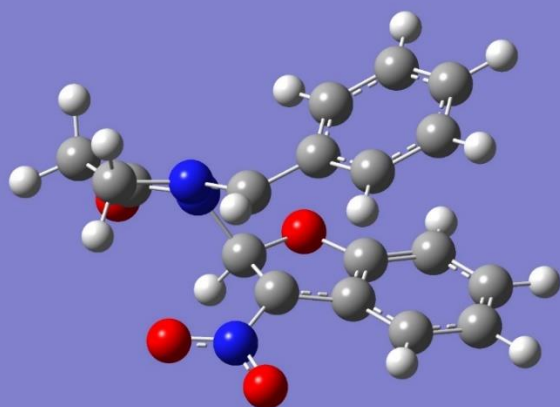
TS1



		X	Y	Z
1	O	-0.1637000	-1.7300000	-1.4260000
2	O	-2.0620000	-1.2583000	2.1335000
3	O	-3.3134000	-0.8336000	-2.2349000
4	N	-1.8946000	1.0939000	0.1450000
5	N	-1.7881000	0.1843000	-0.8664000
6	N	-0.8163000	-1.2782000	2.0394000
7	O	-0.0763000	-1.2672000	3.0374000
8	C	-0.2553000	-1.3198000	0.7936000
9	C	0.4508000	1.9056000	0.2022000
10	C	1.1306000	-1.3991000	0.4336000
11	C	-0.9046000	1.7511000	0.6677000
12	H	-1.1871000	2.3187000	1.5478000
13	C	-1.0226000	-1.4305000	-0.4079000
14	H	-1.9528000	-1.9806000	-0.4629000
15	C	1.1221000	-1.6367000	-0.9467000
16	C	2.3555000	-1.3015000	1.0923000
17	H	2.3922000	-1.1202000	2.1580000
18	C	3.5208000	-1.4559000	0.3444000
19	C	1.3381000	2.5327000	1.0937000
20	H	0.9905000	2.8060000	2.0839000
21	C	3.4782000	-1.7027000	-1.0286000
22	H	4.4022000	-1.8231000	-1.5821000
23	C	2.2601000	-1.8001000	-1.7034000
24	H	2.2087000	-1.9927000	-2.7681000
25	C	-3.0704000	-0.0168000	-1.3753000
26	C	0.8954000	1.5753000	-1.0881000
27	H	0.2197000	1.1072000	-1.7903000
28	C	-3.3014000	1.2755000	0.5883000
29	H	-3.4382000	2.3038000	0.9101000
30	H	-3.4878000	0.5844000	1.4096000
31	C	-4.0534000	0.8882000	-0.6680000
32	H	-4.9836000	0.3568000	-0.4774000
33	H	-4.2630000	1.7538000	-1.3019000
34	C	2.1934000	1.8785000	-1.4676000
35	H	2.5263000	1.6367000	-2.4699000
36	C	2.6417000	2.8040000	0.7147000
37	H	3.3199000	3.2782000	1.4142000

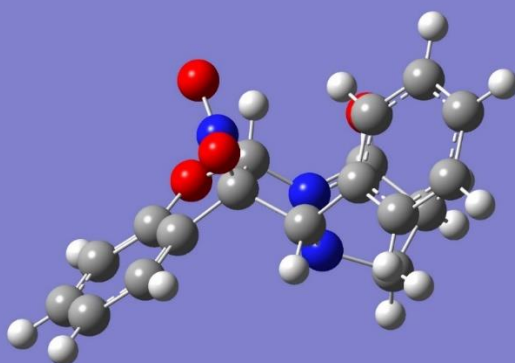
38	C	3.0710000	2.4802000	-0.5694000
39	H	4.0879000	2.7017000	-0.8728000
40	H	4.4818000	-1.3867000	0.8416000
IM				
		X	Y	Z
1	O	-0.0391000	0.9011000	-1.7723000
2	O	2.1160000	1.7424000	1.5910000
3	O	3.3056000	0.5203000	-2.2957000
4	N	1.9146000	-0.9361000	0.4472000
5	N	1.8115000	-0.2032000	-0.7180000
6	N	0.8508000	1.7820000	1.5794000
7	O	0.1984000	2.1853000	2.5731000
8	C	0.2142000	1.3698000	0.4718000
9	C	-0.3973000	-1.8278000	0.6114000
10	C	-1.1778000	1.4533000	0.1510000
11	C	0.9402000	-1.5276000	1.0605000
12	H	1.2306000	-1.9150000	2.0322000
13	C	0.9579000	1.0369000	-0.7685000
14	H	1.6671000	1.8035000	-1.0901000
15	C	-1.2640000	1.1600000	-1.2184000
16	C	-2.3435000	1.7540000	0.8532000
17	H	-2.2952000	1.9874000	1.9084000
18	C	-3.5569000	1.7606000	0.1620000
19	C	-1.3321000	-2.1606000	1.6047000
20	H	-1.0474000	-2.0919000	2.6486000
21	C	-3.6123000	1.4733000	-1.1991000
22	H	-4.5648000	1.4881000	-1.7164000
23	C	-2.4494000	1.1689000	-1.9169000
24	H	-2.4770000	0.9490000	-2.9774000
25	C	3.0813000	-0.1395000	-1.3148000
26	C	-0.7481000	-1.9530000	-0.7409000
27	H	-0.0294000	-1.7275000	-1.5171000
28	C	3.3359000	-1.0441000	0.8501000
29	H	3.4789000	-1.9738000	1.3917000
30	H	3.5728000	-0.1818000	1.4710000
31	C	4.0278000	-0.9788000	-0.5000000
32	H	5.0088000	-0.5106000	-0.4651000
33	H	4.1172000	-1.9665000	-0.9601000
34	C	-2.0131000	-2.4025000	-1.0813000
35	H	-2.2755000	-2.5188000	-2.1261000
36	C	-2.6060000	-2.5733000	1.2529000
37	H	-3.3276000	-2.8143000	2.0241000
38	C	-2.9463000	-2.6994000	-0.0910000
39	H	-3.9376000	-3.0391000	-0.3684000
40	H	-4.4705000	1.9981000	0.6956000

TS2



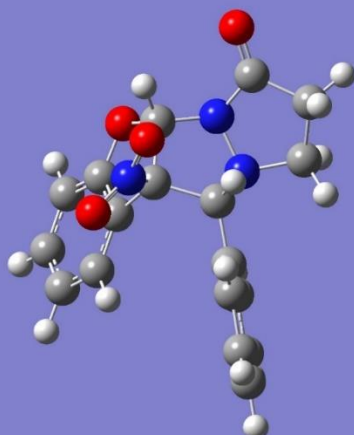
		X	Y	Z
1	O	-0.0327000	-0.4896000	1.8845000
2	O	2.1785000	-2.0026000	-1.1740000
3	O	3.4623000	-0.0358000	2.2528000
4	N	1.8408000	0.8917000	-0.5998000
5	N	1.8335000	0.4254000	0.7058000
6	N	0.9343000	-2.0078000	-1.2155000
7	O	0.2963000	-2.6547000	-2.0555000
8	C	0.2607000	-1.2150000	-0.3032000
9	C	-0.5470000	1.4920000	-0.8634000
10	C	-1.1259000	-1.3777000	0.0631000
11	C	0.7007000	0.8601000	-1.2793000
12	H	0.8387000	0.7493000	-2.3521000
13	C	0.9876000	-0.7715000	0.9303000
14	H	1.6567000	-1.5266000	1.3483000
15	C	-1.2306000	-0.8919000	1.3717000
16	C	-2.2633000	-1.8522000	-0.5840000
17	H	-2.1979000	-2.2329000	-1.5942000
18	C	-3.4762000	-1.8358000	0.1027000
19	C	-1.6407000	1.4020000	-1.7341000
20	H	-1.5444000	0.8325000	-2.6520000
21	C	-3.5555000	-1.3441000	1.4041000
22	H	-4.5091000	-1.3384000	1.9197000
23	C	-2.4231000	-0.8635000	2.0648000
24	H	-2.4720000	-0.4915000	3.0809000
25	C	3.1437000	0.4484000	1.1963000
26	C	-0.6655000	2.2472000	0.3101000
27	H	0.1753000	2.3401000	0.9859000
28	C	3.2138000	0.9540000	-1.1265000
29	H	3.2889000	1.8010000	-1.8036000
30	H	3.4724000	0.0298000	-1.6420000
31	C	4.0068000	1.1285000	0.1630000
32	H	4.9925000	0.6692000	0.1397000
33	H	4.1139000	2.1830000	0.4322000
34	C	-1.8556000	2.8980000	0.5979000
35	H	-1.9350000	3.4917000	1.5013000
36	C	-2.8314000	2.0466000	-1.4344000
37	H	-3.6706000	1.9720000	-2.1162000
38	C	-2.9424000	2.7953000	-0.2668000
39	H	-3.8704000	3.3052000	-0.0344000
40	H	-4.3697000	-2.2093000	-0.3842000

cis-product



		X	Y	Z
1	O	-2.0787000	1.3950000	1.0250000
2	O	-0.5578000	-1.3655000	2.4547000
3	O	1.2683000	3.1573000	1.3715000
4	N	0.1510000	1.0493000	-1.2016000
5	N	0.0557000	1.7341000	0.0437000
6	N	-0.4562000	-1.5832000	1.2667000
7	O	-0.2267000	-2.6632000	0.7692000
8	C	-0.7066000	-0.4448000	0.2958000
9	C	1.7760000	-0.7576000	-0.4334000
10	C	-2.1265000	-0.5636000	-0.1785000
11	C	0.3646000	-0.3704000	-0.8203000
12	H	0.0551000	-0.9822000	-1.6666000
13	C	-0.7152000	0.9667000	0.9617000
14	H	-0.3002000	1.0258000	1.9649000
15	C	-2.8331000	0.5331000	0.2963000
16	C	-2.7531000	-1.5368000	-0.9408000
17	H	-2.2035000	-2.3934000	-1.3132000
18	C	-4.1093000	-1.3860000	-1.2139000
19	C	2.5450000	-1.4280000	-1.3882000
20	H	2.0975000	-1.6888000	-2.3416000
21	C	-4.8083000	-0.2808000	-0.7271000
22	H	-5.8643000	-0.1784000	-0.9498000
23	C	-4.1830000	0.7006000	0.0365000
24	H	-4.7229000	1.5618000	0.4098000
25	C	1.1137000	2.5639000	0.3240000
26	C	2.3627000	-0.4481000	0.7969000
27	H	1.8065000	0.0537000	1.5800000
28	C	1.1983000	1.7763000	-1.9473000
29	H	0.6993000	2.4369000	-2.6573000
30	H	1.8121000	1.0714000	-2.5045000
31	C	1.9819000	2.5871000	-0.9135000
32	H	2.9455000	2.1457000	-0.6489000
33	H	2.1584000	3.6145000	-1.2311000
34	C	3.6854000	-0.7906000	1.0566000
35	H	4.1214000	-0.5442000	2.0181000
36	C	3.8667000	-1.7690000	-1.1307000
37	H	4.4448000	-2.2903000	-1.8854000
38	C	4.4423000	-1.4479000	0.0939000
39	H	5.4724000	-1.7156000	0.3001000
40	H	-4.6246000	-2.1310000	-1.8078000

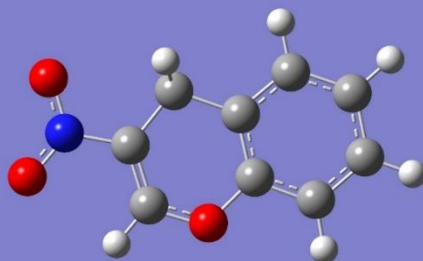
trans-product



		X	Y	Z
1	O	1.4983290	2.2053600	-0.5248960
2	O	1.3366610	-0.0765380	2.7580680
3	O	4.3235860	-0.3948880	0.0585330
4	N	1.0452840	-0.8290990	-1.0790400
5	N	2.1739620	-0.0567470	-0.6750040
6	N	0.3580700	0.4211260	2.2387050
7	O	-0.6149740	0.8234870	2.8328400
8	C	0.3572400	0.4915310	0.7154100
9	C	-1.1090310	-1.5205170	-0.0513240
10	C	-0.5851250	1.5088760	0.1709110
11	C	0.2721280	-0.9735500	0.1675120
12	H	0.8057920	-1.6106170	0.8867600
13	C	1.7425160	0.9919850	0.1839400
14	H	2.4932520	1.1793190	0.9485200
15	C	0.1614150	2.4437980	-0.5363800
16	C	-1.9662770	1.6361250	0.2482770
17	H	-2.5592970	0.9191880	0.8003300
18	C	-2.5721480	2.7148000	-0.3870760
19	C	-1.7220750	-2.2423490	0.9736490
20	H	-1.1863690	-2.4185880	1.9009770
21	C	-1.8041080	3.6429950	-1.0910640
22	H	-2.2921970	4.4774370	-1.5818510
23	C	-0.4210580	3.5248020	-1.1777210
24	H	0.1799210	4.2430340	-1.7212820
25	C	3.3064670	-0.8202260	-0.4426120
26	C	-1.7955650	-1.3193420	-1.2493110
27	H	-1.3226320	-0.7680490	-2.0527080
28	C	1.6411880	-2.0688610	-1.6186280
29	H	1.7554010	-1.9400720	-2.6955820
30	H	0.9681100	-2.9045130	-1.4382860
31	C	3.0034340	-2.2112230	-0.9431660
32	H	2.9946470	-2.8757930	-0.0751690
33	H	3.7830670	-2.5562570	-1.6212790
34	C	-3.0773400	-1.8311440	-1.4148150
35	H	-3.6004310	-1.6751040	-2.3516400
36	C	-3.0087410	-2.7424540	0.8113400
37	H	-3.4752940	-3.2997860	1.6156950
38	C	-3.6890910	-2.5381320	-0.3846400
39	H	-4.6896330	-2.9346920	-0.5159190
40	H	-3.6473290	2.8354870	-0.3333740

3-Nitro-4*H*-chromene + azomethine imine 2a

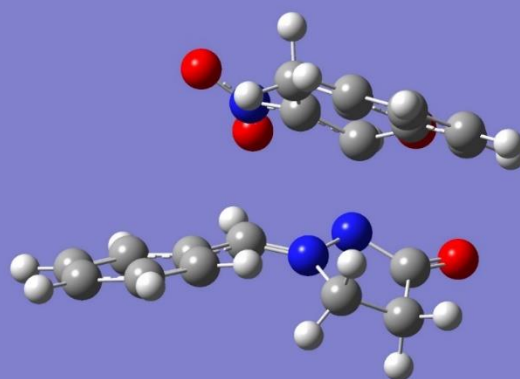
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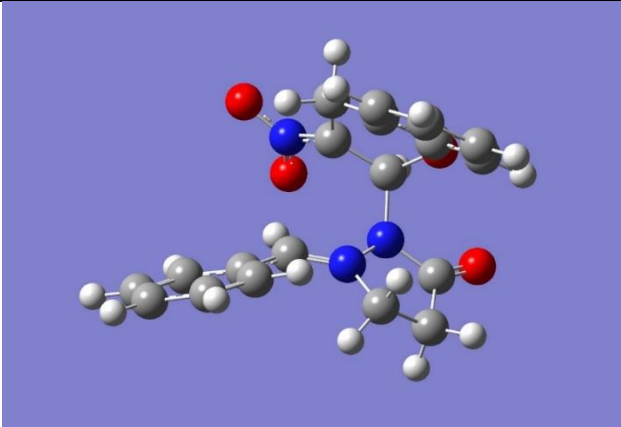
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1	O	0.2240000	-1.7104000	0.0001000
2	O	-3.6453000	-0.7217000	-0.0005000
3	O	-3.1914000	1.3887000	-0.0005000
4	N	-2.8510000	0.2120000	0.0004000
5	C	1.2121000	-0.7368000	0.0001000
6	C	-0.5136000	1.1153000	0.0002000
7	H	-0.6920000	1.7469000	-0.8756000
8	H	-0.6918000	1.7468000	0.8761000
9	C	0.9101000	0.6194000	0.0001000
10	C	-1.4445000	-0.0471000	0.0002000
11	C	1.9809000	1.5127000	0.0001000
12	C	-1.0487000	-1.3297000	0.0002000
13	C	2.5162000	-1.2106000	0.0000000
14	H	2.6937000	-2.2793000	-0.0001000
15	C	3.2947000	1.0644000	0.0000000
16	C	3.5632000	-0.3017000	-0.0001000
17	H	4.5855000	-0.6607000	-0.0002000
18	H	1.7704000	2.5769000	0.0001000
19	H	4.1087000	1.7797000	-0.0001000
20	H	-1.7383000	-2.1627000	0.0002000

anti-endo cycloaddition

TS1

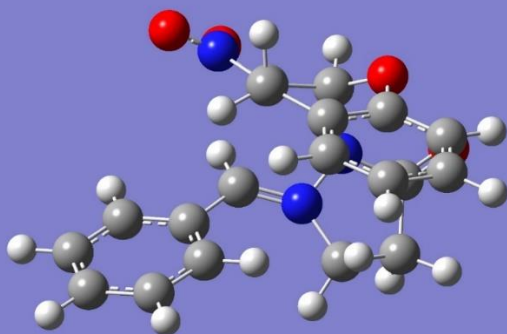


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1	O	2.5780000	0.8993000	0.3317000
2	O	-0.5234000	3.3475000	0.9177000
3	O	2.5869000	1.6370000	-2.6162000
4	O	-1.1533000	2.1786000	2.6517000

5	N	-0.3010000	0.3743000	-1.3761000
6	N	0.7014000	1.3022000	-1.3612000
7	N	-0.4248000	2.3318000	1.6495000
8	C	-4.9049000	-0.3196000	-0.0089000
9	H	-5.8364000	0.1884000	0.2108000
10	C	2.4904000	-0.4261000	0.7065000
11	C	-4.8568000	-1.7095000	-0.0514000
12	H	-5.7534000	-2.2894000	0.1350000
13	C	-1.4091000	0.6477000	-0.7583000
14	H	-1.4940000	1.6818000	-0.4404000
15	C	1.5985000	0.9827000	-2.3652000
16	C	0.5248000	0.1158000	2.1672000
17	H	0.8185000	0.3605000	3.1972000
18	H	-0.4638000	-0.3463000	2.2440000
19	C	1.5072000	-0.8631000	1.5879000
20	C	0.4744000	1.3539000	1.3344000
21	C	-2.5010000	-1.6262000	-0.5616000
22	H	-1.5736000	-2.1534000	-0.7361000
23	C	-2.5419000	-0.2231000	-0.5384000
24	C	1.4942000	-2.2160000	1.9243000
25	C	1.4342000	1.6366000	0.3321000
26	H	1.6466000	2.6732000	0.1138000
27	C	1.1357000	-0.2709000	-3.0802000
28	H	1.9717000	-0.9525000	-3.2249000
29	H	0.7380000	0.0071000	-4.0591000
30	C	-3.7553000	0.4182000	-0.2384000
31	C	-3.6533000	-2.3568000	-0.3183000
32	H	-3.6107000	-3.4395000	-0.3303000
33	C	0.0590000	-0.8238000	-2.1668000
34	H	-0.8271000	-1.1906000	-2.6789000
35	H	0.4451000	-1.5881000	-1.4909000
36	C	3.4486000	-1.2845000	0.1836000
37	H	4.1962000	-0.8957000	-0.4974000
38	C	2.4430000	-3.0932000	1.4138000
39	C	3.4252000	-2.6245000	0.5454000
40	H	4.1695000	-3.3018000	0.1429000
41	H	0.7303000	-2.5779000	2.6047000
42	H	2.4162000	-4.1403000	1.6924000
43	H	-3.7858000	1.5011000	-0.1956000
IM				
		X	Y	Z
1	O	2.6440000	0.6573000	0.3119000
2	O	-0.3716000	3.1984000	1.0919000
3	O	2.5452000	1.9564000	-2.4262000
4	O	-0.7873000	2.1127000	2.9668000
5	N	-0.2734000	0.4567000	-1.2147000
6	N	0.8186000	1.2884000	-1.0706000

7	N	-0.1868000	2.1944000	1.8591000
8	C	-4.8817000	-0.2026000	0.0582000
9	H	-5.7973000	0.2992000	0.3469000
10	C	2.4442000	-0.6797000	0.5604000
11	C	-4.8822000	-1.5702000	-0.1989000
12	H	-5.8022000	-2.1365000	-0.1105000
13	C	-1.3420000	0.7121000	-0.5223000
14	H	-1.3498000	1.6880000	-0.0383000
15	C	1.5485000	1.3009000	-2.2558000
16	C	0.7818000	-0.0142000	2.2861000
17	H	1.3366000	0.2330000	3.2046000
18	H	-0.1876000	-0.3929000	2.6205000
19	C	1.5283000	-1.0759000	1.5321000
20	C	0.5989000	1.2014000	1.4389000
21	C	-2.5206000	-1.5052000	-0.6728000
22	H	-1.6063000	-2.0312000	-0.9137000
23	C	-2.5148000	-0.1214000	-0.4342000
24	C	1.3773000	-2.4386000	1.7759000
25	C	1.4836000	1.4654000	0.2790000
26	H	1.8358000	2.4945000	0.2634000
27	C	0.8618000	0.3688000	-3.2267000
28	H	1.6015000	-0.2241000	-3.7606000
29	H	0.2952000	0.9620000	-3.9489000
30	C	-3.7028000	0.5171000	-0.0433000
31	C	-3.7010000	-2.2189000	-0.5519000
32	H	-3.7007000	-3.2882000	-0.7264000
33	C	-0.0546000	-0.4659000	-2.3425000
34	H	-1.0113000	-0.7137000	-2.7930000
35	H	0.4400000	-1.3669000	-1.9770000
36	C	3.2131000	-1.6005000	-0.1399000
37	H	3.9194000	-1.2501000	-0.8834000
38	C	2.1391000	-3.3761000	1.0861000
39	C	3.0617000	-2.9550000	0.1328000
40	H	3.6596000	-3.6807000	-0.4068000
41	H	0.6615000	-2.7636000	2.5239000
42	H	2.0130000	-4.4327000	1.2928000
43	H	-3.6904000	1.5801000	0.1682000

TS2

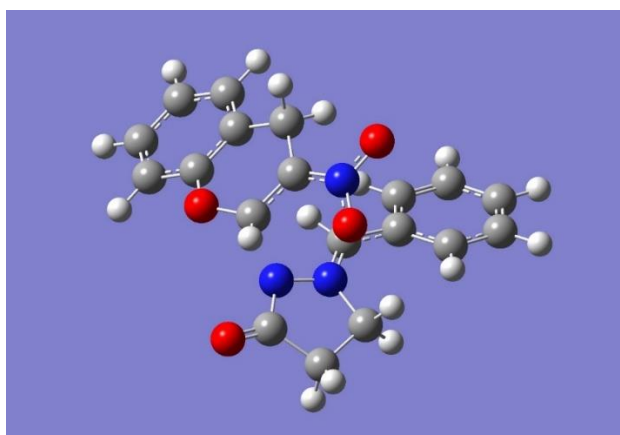


		X	Y	Z
1	O	2.3797000	-0.7463000	-0.9270000
2	O	-0.7575000	-3.1864000	-1.2014000
3	O	3.1208000	-1.9668000	1.7664000
4	O	-1.6226000	-1.8090000	-2.6649000
5	N	0.0152000	-0.6142000	1.3356000
6	N	1.0410000	-1.4456000	0.9317000
7	N	-0.7997000	-2.0619000	-1.7613000

8	C	-4.6541000	0.3084000	0.5065000
9	H	-5.6353000	-0.1346000	0.3827000
10	C	2.2104000	0.6178000	-0.9160000
11	C	-4.5195000	1.6875000	0.6344000
12	H	-5.3981000	2.3220000	0.6103000
13	C	-1.1255000	-0.8469000	0.7112000
14	H	-1.3163000	-1.8975000	0.4931000
15	C	2.0782000	-1.3690000	1.8587000
16	C	0.0155000	0.2384000	-2.0156000
17	H	0.2442000	0.0614000	-3.0768000
18	H	-0.9744000	0.7005000	-1.9952000
19	C	1.0429000	1.1678000	-1.4389000
20	C	0.0065000	-1.0668000	-1.2813000
21	C	-2.1278000	1.4523000	0.8173000
22	H	-1.1517000	1.9108000	0.9078000
23	C	-2.2558000	0.0602000	0.7058000
24	C	0.9100000	2.5536000	-1.4378000
25	C	1.2473000	-1.5105000	-0.5666000
26	H	1.4987000	-2.5417000	-0.7966000
27	C	1.6309000	-0.4175000	2.9518000
28	H	2.4661000	0.2018000	3.2725000
29	H	1.2783000	-1.0038000	3.8047000
30	C	-3.5293000	-0.5013000	0.5334000
31	C	-3.2569000	2.2559000	0.7832000
32	H	-3.1523000	3.3313000	0.8665000
33	C	0.4957000	0.3721000	2.3044000
34	H	-0.3116000	0.6370000	2.9826000
35	H	0.8694000	1.2642000	1.7951000
36	C	3.2387000	1.4109000	-0.4253000
37	H	4.1340000	0.9434000	-0.0328000
38	C	1.9303000	3.3661000	-0.9534000
39	C	3.0965000	2.7937000	-0.4540000
40	H	3.8952000	3.4223000	-0.0771000
41	H	0.0027000	2.9968000	-1.8348000
42	H	1.8149000	4.4438000	-0.9665000
43	H	-3.6270000	-1.5762000	0.4316000

anti-exo cycloaddition

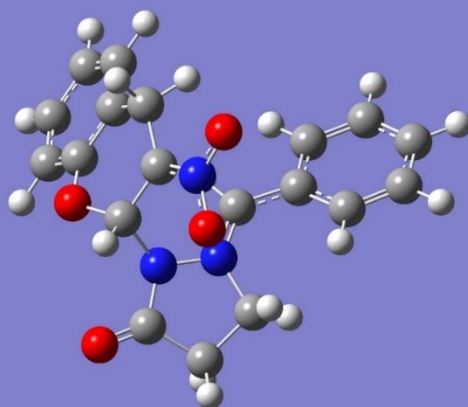
TS1



		X	Y	Z
1	O	2.6671000	0.8918000	0.1536000
2	O	-0.6301000	2.0187000	2.0666000
3	O	1.3142000	3.7494000	-1.0433000
4	O	-0.7774000	0.1062000	3.1114000
5	N	-0.8401000	1.1536000	-0.8054000

6	N	0.4293000	1.6540000	-0.8214000
7	N	-0.2385000	0.8420000	2.2609000
8	C	-3.2847000	-3.0484000	-0.8591000
9	H	-3.2116000	-4.0929000	-1.1377000
10	C	2.8796000	-0.4463000	-0.1001000
11	C	-4.4927000	-2.5249000	-0.4092000
12	H	-5.3672000	-3.1611000	-0.3370000
13	C	-1.0104000	-0.1313000	-0.7363000
14	H	-0.1049000	-0.7099000	-0.8688000
15	C	0.3517000	3.0110000	-1.0744000
16	C	1.2231000	-1.0704000	1.6837000
17	H	1.6734000	-1.2221000	2.6743000
18	H	0.3633000	-1.7455000	1.6413000
19	C	2.2171000	-1.4383000	0.6161000
20	C	0.7951000	0.3492000	1.5145000
21	C	-3.4655000	-0.3592000	-0.1325000
22	H	-3.5563000	0.6694000	0.1840000
23	C	-2.2449000	-0.8718000	-0.6011000
24	C	2.5167000	-2.7663000	0.3134000
25	C	1.4791000	1.2655000	0.6873000
26	H	1.5121000	2.3045000	0.9896000
27	C	-1.0773000	3.4002000	-1.3738000
28	H	-1.1846000	3.5484000	-2.4509000
29	H	-1.3280000	4.3306000	-0.8677000
30	C	-2.1683000	-2.2332000	-0.9432000
31	C	-4.5746000	-1.1853000	-0.0398000
32	H	-5.5098000	-0.7806000	0.3288000
33	C	-1.8753000	2.2136000	-0.8772000
34	H	-2.2702000	2.3801000	0.1231000
35	H	-2.6630000	1.8833000	-1.5502000
36	C	3.8229000	-0.7477000	-1.0744000
37	H	4.3155000	0.0594000	-1.6035000
38	C	3.4575000	-3.0899000	-0.6556000
39	C	4.1141000	-2.0763000	-1.3489000
40	H	4.8490000	-2.3183000	-2.1078000
41	H	2.0031000	-3.5534000	0.8560000
42	H	3.6769000	-4.1292000	-0.8708000
43	H	-1.2234000	-2.6406000	-1.2844000

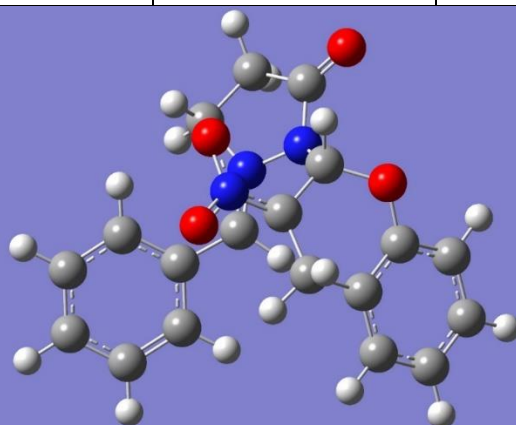
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		X	Y	Z
1	O	2.6727000	0.7127000	0.1662000
2	O	-0.6253000	2.0722000	1.9868000
3	O	1.6601000	3.6517000	-0.9190000
4	O	-0.7706000	0.2564000	3.2240000
5	N	-0.6654000	1.1694000	-0.7453000
6	N	0.6231000	1.6353000	-0.6044000
7	N	-0.2390000	0.8969000	2.2779000

8	C	-3.3865000	-2.8342000	-0.8140000
9	H	-3.3868000	-3.8896000	-1.0587000
10	C	2.7228000	-0.6292000	-0.1181000
11	C	-4.5713000	-2.1960000	-0.4597000
12	H	-5.4993000	-2.7552000	-0.4293000
13	C	-0.8986000	-0.1009000	-0.6070000
14	H	-0.0279000	-0.7433000	-0.6315000
15	C	0.6886000	2.9515000	-1.0580000
16	C	1.2277000	-1.0353000	1.8364000
17	H	1.8404000	-1.0450000	2.7512000
18	H	0.3878000	-1.7061000	2.0324000
19	C	2.0453000	-1.5463000	0.6833000
20	C	0.7311000	0.3398000	1.5400000
21	C	-3.3862000	-0.1165000	-0.1695000
22	H	-3.4018000	0.9255000	0.1178000
23	C	-2.1888000	-0.7472000	-0.5429000
24	C	2.1688000	-2.9009000	0.3803000
25	C	1.4457000	1.2340000	0.6094000
26	H	1.6817000	2.1950000	1.0677000
27	C	-0.6291000	3.2880000	-1.7023000
28	H	-0.5324000	3.1658000	-2.7843000
29	H	-0.9041000	4.3177000	-1.4855000
30	C	-2.2008000	-2.1193000	-0.8432000
31	C	-4.5650000	-0.8433000	-0.1295000
32	H	-5.4845000	-0.3527000	0.1670000
33	C	-1.5826000	2.2712000	-1.0996000
34	H	-2.0477000	2.6487000	-0.1910000
35	H	-2.3316000	1.8943000	-1.7909000
36	C	3.5185000	-1.0381000	-1.1818000
37	H	4.0327000	-0.2935000	-1.7781000
38	C	2.9634000	-3.3285000	-0.6771000
39	C	3.6417000	-2.3943000	-1.4555000
40	H	4.2622000	-2.7195000	-2.2828000
41	H	1.6386000	-3.6253000	0.9900000
42	H	3.0516000	-4.3867000	-0.8947000
43	H	-1.2723000	-2.6134000	-1.1064000

TS2

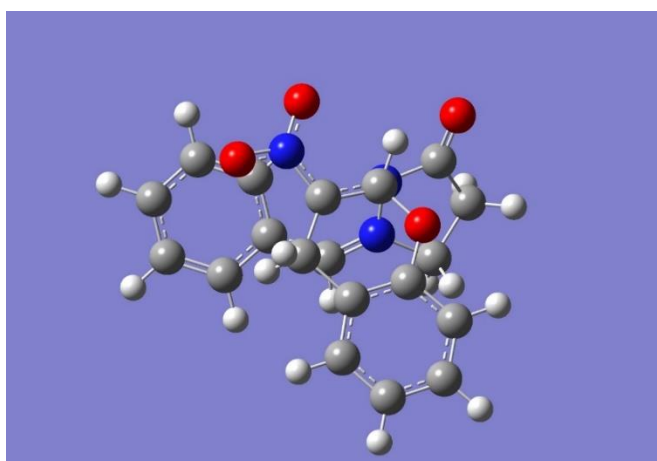


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1	O	2.5752000	0.7328000	0.5793000
2	O	-1.0642000	1.7219000	1.9342000
3	O	1.6860000	3.7662000	-0.4251000
4	O	-1.2865000	-0.2463000	2.8679000
5	N	-0.5711000	1.2472000	-0.8245000
6	N	0.6831000	1.7043000	-0.4775000
7	N	-0.6822000	0.5354000	2.1046000
8	C	-3.2702000	-2.7631000	-1.0357000
9	H	-3.2873000	-3.8004000	-1.3489000

10	C	2.7562000	-0.5427000	0.1053000
11	C	-4.4416000	-2.1385000	-0.6170000
12	H	-5.3747000	-2.6900000	-0.6042000
13	C	-0.7559000	-0.0500000	-0.6815000
14	H	0.1084000	-0.6708000	-0.8846000
15	C	0.7722000	3.0617000	-0.7760000
16	C	0.9312000	-1.2720000	1.6297000
17	H	1.3651000	-1.3347000	2.6386000
18	H	0.1295000	-2.0128000	1.5958000
19	C	1.9835000	-1.5887000	0.6054000
20	C	0.3832000	0.0951000	1.3792000
21	C	-3.2262000	-0.0946000	-0.2200000
22	H	-3.2192000	0.9284000	0.1294000
23	C	-2.0446000	-0.7104000	-0.6577000
24	C	2.2335000	-2.8763000	0.1368000
25	C	1.2546000	1.1566000	0.8089000
26	H	1.3329000	2.0171000	1.4731000
27	C	-0.4595000	3.4326000	-1.5661000
28	H	-0.2202000	3.3830000	-2.6319000
29	H	-0.7766000	4.4438000	-1.3213000
30	C	-2.0776000	-2.0578000	-1.0481000
31	C	-4.4143000	-0.8095000	-0.2038000
32	H	-5.3231000	-0.3288000	0.1387000
33	C	-1.4670000	2.3648000	-1.1607000
34	H	-2.0355000	2.6764000	-0.2858000
35	H	-2.1358000	2.0535000	-1.9595000
36	C	3.7670000	-0.7613000	-0.8220000
37	H	4.3493000	0.0779000	-1.1837000
38	C	3.2444000	-3.1149000	-0.7877000
39	C	4.0130000	-2.0559000	-1.2628000
40	H	4.8017000	-2.2344000	-1.9849000
41	H	1.6315000	-3.6981000	0.5104000
42	H	3.4302000	-4.1236000	-1.1379000
43	H	-1.1610000	-2.5408000	-1.3675000

syn-endo cycloaddition

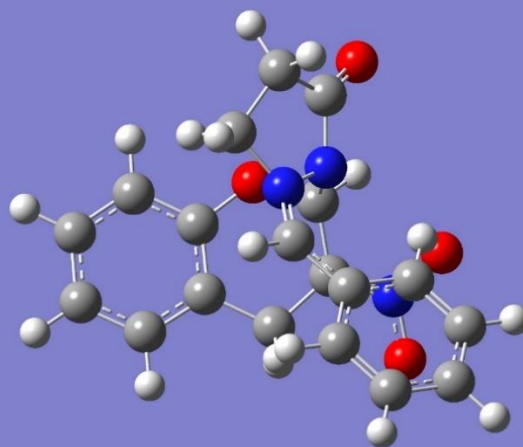
TS1



		X	Y	Z
1	O	1.9753000	0.5561000	0.9987000
2	O	-1.5641000	0.8267000	2.7938000
3	O	0.7715000	3.6844000	0.9801000
4	O	-1.8560000	-1.3359000	2.6891000
5	N	0.1813000	1.2163000	-1.2595000
6	N	0.0357000	1.7481000	0.0022000
7	N	-1.2062000	-0.3079000	2.3861000

8	C	-3.7531000	-1.5959000	-1.9229000
9	H	-4.1777000	-2.3765000	-2.5427000
10	C	2.3867000	-0.6258000	0.4205000
11	C	-4.4922000	-1.0469000	-0.8803000
12	H	-5.4974000	-1.4020000	-0.6837000
13	C	-0.6250000	0.3655000	-1.8111000
14	H	-0.2822000	0.0250000	-2.7818000
15	C	0.7064000	2.9721000	0.0043000
16	C	0.2518000	-1.7904000	1.0820000
17	H	0.2632000	-2.5131000	1.9057000
18	H	-0.5032000	-2.1647000	0.3779000
19	C	1.6011000	-1.7733000	0.4207000
20	C	-0.1059000	-0.4408000	1.6002000
21	C	-2.6578000	0.4153000	-0.3159000
22	H	-2.2329000	1.1823000	0.3167000
23	C	-1.9098000	-0.1219000	-1.3767000
24	C	2.1238000	-2.9145000	-0.1890000
25	C	0.6554000	0.7296000	1.3388000
26	H	0.5574000	1.5278000	2.0647000
27	C	1.3268000	3.2251000	-1.3523000
28	H	2.3275000	3.6366000	-1.2364000
29	H	0.7094000	3.9431000	-1.8981000
30	C	-2.4745000	-1.1285000	-2.1788000
31	C	-3.9441000	-0.0410000	-0.0860000
32	H	-4.5233000	0.3834000	0.7253000
33	C	1.3013000	1.8538000	-1.9969000
34	H	1.0786000	1.8464000	-3.0599000
35	H	2.2120000	1.2878000	-1.7991000
36	C	3.6600000	-0.6088000	-0.1403000
37	H	4.2419000	0.3047000	-0.1044000
38	C	3.3877000	-2.9169000	-0.7632000
39	C	4.1607000	-1.7588000	-0.7320000
40	H	5.1523000	-1.7484000	-1.1697000
41	H	1.5217000	-3.8174000	-0.2011000
42	H	3.7706000	-3.8179000	-1.2280000
43	H	-1.9025000	-1.5311000	-3.0076000

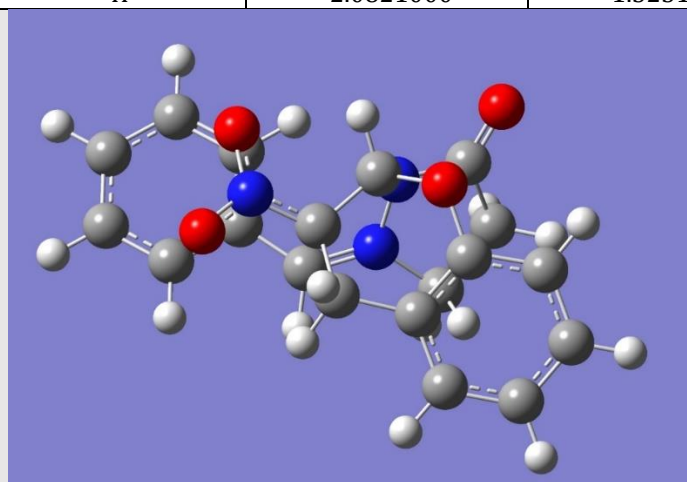
IM



		X	Y	Z
1	O	1.9801000	0.5201000	1.1275000
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3	O	0.8106000	3.5851000	1.1060000
4	O	-1.7815000	-1.6017000	2.5883000
5	N	0.2085000	1.1346000	-1.1852000
6	N	0.1394000	1.6184000	0.1210000
7	N	-1.1878000	-0.5208000	2.3013000

8	C	-3.8967000	-1.4024000	-1.9305000
9	H	-4.3773000	-2.1102000	-2.5949000
10	C	2.4362000	-0.5761000	0.4408000
11	C	-4.5722000	-0.9113000	-0.8178000
12	H	-5.5846000	-1.2405000	-0.6127000
13	C	-0.6854000	0.3974000	-1.7675000
14	H	-0.4018000	0.1312000	-2.7805000
15	C	0.7109000	2.9113000	0.1158000
16	C	0.2921000	-1.8326000	0.8653000
17	H	0.2966000	-2.5960000	1.6526000
18	H	-0.4053000	-2.2121000	0.1048000
19	C	1.6692000	-1.7270000	0.2722000
20	C	-0.1644000	-0.5384000	1.4422000
21	C	-2.6602000	0.4237000	-0.2019000
22	H	-2.1917000	1.1200000	0.4793000
23	C	-1.9739000	-0.0591000	-1.3292000
24	C	2.2355000	-2.7884000	-0.4356000
25	C	0.5804000	0.7148000	1.2568000
26	H	0.4337000	1.3666000	2.1146000
27	C	1.1605000	3.2312000	-1.2879000
28	H	2.1014000	3.7766000	-1.2648000
29	H	0.4005000	3.8465000	-1.7772000
30	C	-2.6094000	-0.9682000	-2.1947000
31	C	-3.9569000	0.0043000	0.0351000
32	H	-4.4913000	0.3846000	0.8970000
33	C	1.2644000	1.8571000	-1.9282000
34	H	1.0442000	1.8276000	-2.9909000
35	H	2.2240000	1.3821000	-1.7217000
36	C	3.7381000	-0.4939000	-0.0503000
37	H	4.3058000	0.4148000	0.1135000
38	C	3.5280000	-2.7212000	-0.9376000
39	C	4.2841000	-1.5686000	-0.7358000
40	H	5.2971000	-1.5030000	-1.1164000
41	H	1.6450000	-3.6878000	-0.5807000
42	H	3.9454000	-3.5626000	-1.4785000
43	H	-2.0821000	-1.3231000	-3.0733000

TS2

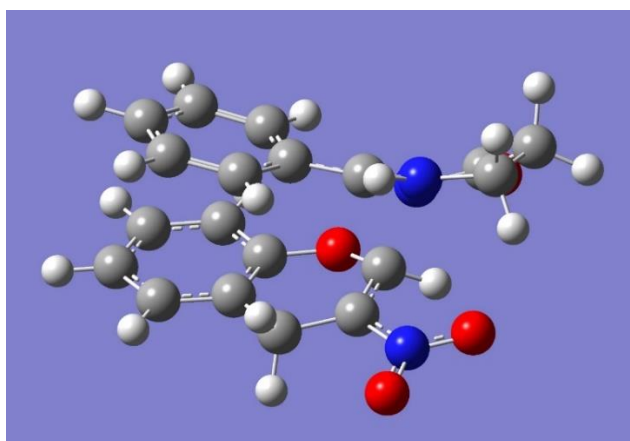


		X	Y	Z
1	O	1.7369000	0.0026000	1.6477000
2	O	-2.0332000	-0.9192000	1.9366000
3	O	1.3272000	2.9705000	1.5597000
4	O	-1.6528000	-2.7981000	0.8986000
5	N	-0.0027000	1.0390000	-0.9025000
6	N	0.1431000	1.3456000	0.4330000
7	N	-1.3188000	-1.6327000	1.1999000

8	C	-4.5532000	-0.7178000	-1.1877000
9	H	-5.1949000	-1.4592000	-1.6496000
10	C	2.5642000	-0.4614000	0.6538000
11	C	-5.0978000	0.2742000	-0.3780000
12	H	-6.1675000	0.3065000	-0.2040000
13	C	-0.9492000	0.1847000	-1.2450000
14	H	-0.7466000	-0.3310000	-2.1803000
15	C	1.0052000	2.4524000	0.5228000
16	C	0.7911000	-2.1046000	0.0527000
17	H	0.9085000	-2.9516000	0.7442000
18	H	0.4007000	-2.5326000	-0.8726000
19	C	2.1378000	-1.4882000	-0.1849000
20	C	-0.1669000	-1.1175000	0.6594000
21	C	-2.8986000	1.1903000	-0.0026000
22	H	-2.2626000	1.9324000	0.4611000
23	C	-2.3438000	0.2096000	-0.8368000
24	C	3.0077000	-1.9275000	-1.1798000
25	C	0.3660000	0.1043000	1.3205000
26	H	-0.1490000	0.3147000	2.2513000
27	C	1.4290000	2.8238000	-0.8855000
28	H	2.4824000	3.0966000	-0.8957000
29	H	0.8398000	3.6841000	-1.2149000
30	C	-3.1871000	-0.7462000	-1.4224000
31	C	-4.2681000	1.2276000	0.2062000
32	H	-4.6913000	2.0020000	0.8356000
33	C	1.1023000	1.5769000	-1.7027000
34	H	0.7479000	1.7849000	-2.7085000
35	H	1.9399000	0.8752000	-1.7345000
36	C	3.8305000	0.0983000	0.5401000
37	H	4.1263000	0.8909000	1.2172000
38	C	4.2788000	-1.3786000	-1.3112000
39	C	4.6924000	-0.3716000	-0.4436000
40	H	5.6830000	0.0583000	-0.5381000
41	H	2.6848000	-2.7185000	-1.8491000
42	H	4.9450000	-1.7365000	-2.0877000
43	H	-2.7630000	-1.4962000	-2.0808000

syn-exo cycloaddition

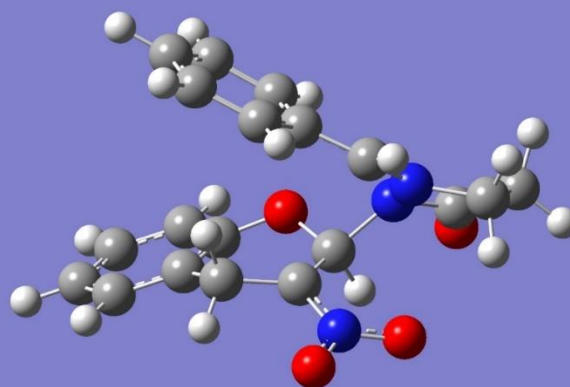
TS1



		X	Y	Z
1	O	-0.0208000	-1.8797000	-0.8420000
2	O	2.9153000	-0.9456000	1.6530000
3	O	2.8901000	-1.3895000	-2.3287000
4	O	1.5367000	-0.6352000	3.3239000
5	N	1.9144000	1.1428000	-0.3179000

6	N	1.6340000	-0.0004000	-1.0114000
7	N	1.7424000	-0.8586000	2.1093000
8	C	-2.4932000	2.9887000	0.6624000
9	H	-3.0650000	3.5749000	1.3728000
10	C	-1.3347000	-1.6800000	-0.4921000
11	C	-3.1032000	2.4828000	-0.4822000
12	H	-4.1547000	2.6746000	-0.6654000
13	C	1.0275000	1.9246000	0.2124000
14	H	1.4575000	2.6916000	0.8477000
15	C	2.7948000	-0.3638000	-1.6948000
16	C	-0.6968000	-0.8895000	1.8151000
17	H	-0.8163000	-1.5696000	2.6676000
18	H	-0.8913000	0.1118000	2.2179000
19	C	-1.7175000	-1.2193000	0.7633000
20	C	0.6845000	-1.0022000	1.2708000
21	C	-1.0234000	1.4712000	-1.1652000
22	H	-0.4558000	0.8900000	-1.8795000
23	C	-0.3959000	1.9914000	-0.0222000
24	C	-3.0832000	-1.0848000	1.0155000
25	C	0.9842000	-1.3705000	-0.0735000
26	H	1.8681000	-1.9836000	-0.2045000
27	C	3.8660000	0.6799000	-1.4804000
28	H	3.9223000	1.3230000	-2.3626000
29	H	4.8327000	0.2008000	-1.3383000
30	C	-1.1441000	2.7630000	0.8817000
31	C	-2.3634000	1.7381000	-1.3975000
32	H	-2.8367000	1.3559000	-2.2944000
33	C	3.3727000	1.4306000	-0.2622000
34	H	3.7651000	1.0187000	0.6649000
35	H	3.5138000	2.5068000	-0.2992000
36	C	-2.2713000	-2.0146000	-1.4654000
37	H	-1.9274000	-2.3746000	-2.4286000
38	C	-4.0335000	-1.4080000	0.0568000
39	C	-3.6229000	-1.8779000	-1.1892000
40	H	-4.3544000	-2.1355000	-1.9473000
41	H	-3.3983000	-0.7216000	1.9892000
42	H	-5.0889000	-1.2958000	0.2790000
43	H	-0.6551000	3.1882000	1.7516000

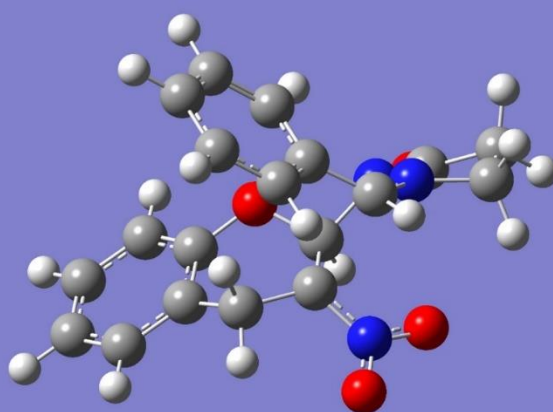
IM



		X	Y	Z
1	O	-0.5947000	-1.0601000	-1.0459000
2	O	2.1120000	-1.4564000	1.8847000
3	O	2.2971000	-2.4822000	-1.8456000
4	O	0.7789000	-0.5739000	3.3950000
5	N	2.3321000	0.5025000	-0.2175000
6	N	1.6570000	-0.5469000	-0.7985000

7	N	1.0155000	-0.8863000	2.1951000
8	C	-1.0506000	3.9741000	0.3173000
9	H	-1.3819000	4.7838000	0.9566000
10	C	-1.8709000	-1.2387000	-0.5858000
11	C	-1.7813000	3.6303000	-0.8156000
12	H	-2.6878000	4.1722000	-1.0602000
13	C	1.8157000	1.6331000	0.1411000
14	H	2.5046000	2.2426000	0.7173000
15	C	2.5972000	-1.4190000	-1.3686000
16	C	-1.2237000	-0.0979000	1.5331000
17	H	-1.2977000	0.9908000	1.3953000
18	H	-1.4281000	-0.2852000	2.5884000
19	C	-2.2529000	-0.7731000	0.6709000
20	C	0.1401000	-0.6136000	1.2183000
21	C	-0.1943000	1.8914000	-1.3374000
22	H	0.1381000	1.0949000	-1.9876000
23	C	0.5433000	2.2283000	-0.1934000
24	C	-3.5801000	-0.9386000	1.0601000
25	C	0.4662000	-1.1678000	-0.1102000
26	H	0.7630000	-2.2197000	-0.0408000
27	C	3.9607000	-0.7960000	-1.2422000
28	H	4.2117000	-0.2970000	-2.1820000
29	H	4.7040000	-1.5629000	-1.0369000
30	C	0.1162000	3.2900000	0.6186000
31	C	-1.3441000	2.5993000	-1.6448000
32	H	-1.9038000	2.3478000	-2.5380000
33	C	3.7783000	0.1925000	-0.1067000
34	H	3.9475000	-0.2677000	0.8647000
35	H	4.3399000	1.1155000	-0.2129000
36	C	-2.7855000	-1.8379000	-1.4461000
37	H	-2.4522000	-2.1845000	-2.4174000
38	C	-4.5082000	-1.5329000	0.2119000
39	C	-4.1083000	-1.9773000	-1.0453000
40	H	-4.8238000	-2.4425000	-1.7140000
41	H	-3.8868000	-0.5868000	2.0400000
42	H	-5.5373000	-1.6507000	0.5314000
43	H	0.7050000	3.5678000	1.4857000

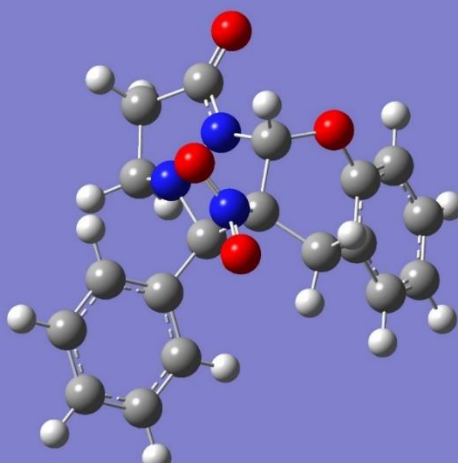
TS2



		X	Y	Z
1	O	-0.6938000	-0.7911000	-1.1550000
2	O	1.8278000	-1.7322000	1.8077000
3	O	2.1236000	-2.5363000	-1.9779000
4	O	0.5241000	-0.8688000	3.3260000
5	N	2.3236000	0.2979000	-0.1052000
6	N	1.5995000	-0.6056000	-0.8537000
7	N	0.8203000	-1.0586000	2.1312000

8	C	-0.7547000	4.0531000	0.4825000
9	H	-1.1432000	4.7902000	1.1756000
10	C	-1.9644000	-1.0463000	-0.7086000
11	C	-1.1576000	4.0615000	-0.8486000
12	H	-1.8647000	4.8050000	-1.1983000
13	C	1.6904000	1.2446000	0.5576000
14	H	2.2494000	1.6116000	1.4147000
15	C	2.4842000	-1.5386000	-1.4076000
16	C	-1.2901000	0.0200000	1.4284000
17	H	-1.4908000	-0.1355000	2.4880000
18	H	-1.3540000	1.1023000	1.2528000
19	C	-2.3269000	-0.6653000	0.5815000
20	C	0.0817000	-0.4927000	1.1167000
21	C	0.2585000	2.1600000	-1.2994000
22	H	0.6539000	1.4359000	-1.9992000
23	C	0.6678000	2.1439000	0.0406000
24	C	-3.6328000	-0.9025000	1.0002000
25	C	0.3368000	-1.0889000	-0.2261000
26	H	0.4556000	-2.1756000	-0.1603000
27	C	3.8891000	-1.0689000	-1.1274000
28	H	4.2683000	-0.5484000	-2.0109000
29	H	4.5299000	-1.9238000	-0.9229000
30	C	0.1570000	3.1049000	0.9240000
31	C	-0.6426000	3.1184000	-1.7356000
32	H	-0.9434000	3.1335000	-2.7769000
33	C	3.7261000	-0.1274000	0.0576000
34	H	3.8593000	-0.6368000	1.0098000
35	H	4.3611000	0.7531000	0.0042000
36	C	-2.8759000	-1.6282000	-1.5802000
37	H	-2.5584000	-1.9070000	-2.5782000
38	C	-4.5599000	-1.4842000	0.1407000
39	C	-4.1815000	-1.8390000	-1.1509000
40	H	-4.9000000	-2.2912000	-1.8251000
41	H	-3.9258000	-0.6172000	2.0055000
42	H	-5.5747000	-1.6600000	0.4786000
43	H	0.4894000	3.1073000	1.9564000

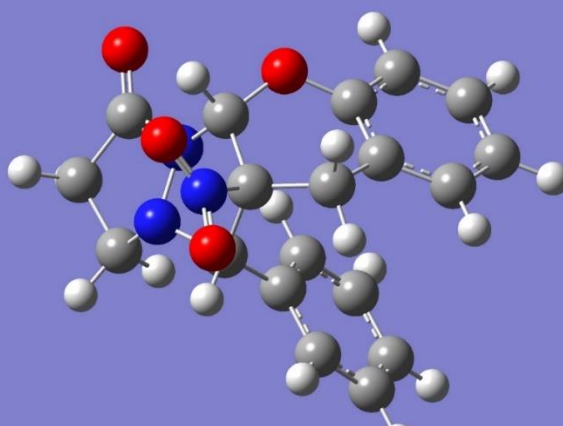
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2	O	-1.3039000	1.2594000	2.4214000
3	O	2.4956000	3.3102000	-0.0468000
4	O	-1.7581000	-0.8387000	2.5216000
5	N	-0.4432000	1.5058000	-0.5314000
6	N	0.8596000	1.6941000	0.0231000
7	N	-1.1192000	0.1024000	2.1030000

8	C	-3.7265000	-1.9643000	-1.2859000
9	H	-3.9403000	-2.9463000	-1.6927000
10	C	2.6056000	-0.7618000	0.3798000
11	C	-4.7669000	-1.0971000	-0.9690000
12	H	-5.7958000	-1.4016000	-1.1244000
13	C	-0.6792000	0.0840000	-0.3604000
14	H	-0.0466000	-0.4988000	-1.0468000
15	C	1.4792000	2.7950000	-0.4746000
16	C	0.4482000	-1.6127000	1.2127000
17	H	0.7013000	-1.7801000	2.2648000
18	H	-0.3305000	-2.3243000	0.9415000
19	C	1.6690000	-1.7908000	0.3607000
20	C	-0.0617000	-0.1873000	1.0547000
21	C	-3.1634000	0.5604000	-0.2618000
22	H	-2.9445000	1.5486000	0.1245000
23	C	-2.1159000	-0.3085000	-0.5713000
24	C	1.9252000	-2.9123000	-0.4207000
25	C	1.0796000	0.8674000	1.1799000
26	H	1.0043000	1.4338000	2.1068000
27	C	0.6254000	3.2323000	-1.6525000
28	H	1.2423000	3.4952000	-2.5101000
29	H	0.0614000	4.1188000	-1.3454000
30	C	-2.4081000	-1.5690000	-1.0939000
31	C	-4.4817000	0.1663000	-0.4619000
32	H	-5.2881000	0.8505000	-0.2231000
33	C	-0.2882000	2.0337000	-1.8912000
34	H	-1.2593000	2.2913000	-2.3094000
35	H	0.2082000	1.2948000	-2.5356000
36	C	3.7885000	-0.8354000	-0.3394000
37	H	4.4968000	-0.0166000	-0.2955000
38	C	3.1096000	-3.0082000	-1.1448000
39	C	4.0389000	-1.9729000	-1.0998000
40	H	4.9613000	-2.0451000	-1.6645000
41	H	1.1981000	-3.7170000	-0.4500000
42	H	3.3065000	-3.8893000	-1.7443000
43	H	-1.5974000	-2.2396000	-1.3580000

trans-
product

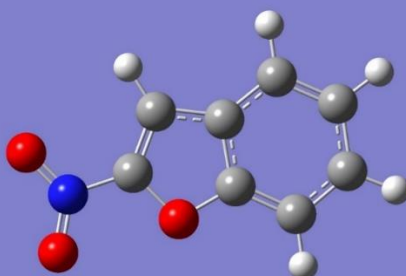


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2	O	-2.8130000	1.3583000	2.1795000
3	O	-2.8228000	0.9163000	-2.7274000
4	O	-1.6037000	0.0302000	3.3499000
5	N	-1.8850000	-1.0682000	-0.0429000
6	N	-1.7300000	0.0864000	-0.8812000
7	N	-1.8472000	0.6442000	2.3335000
8	C	2.6018000	-2.7834000	0.9427000

9	H	3.1914000	-3.3213000	1.6766000
10	C	0.9259000	1.8710000	-0.5755000
11	C	3.0671000	-2.6369000	-0.3589000
12	H	4.0242000	-3.0568000	-0.6473000
13	C	-0.7432000	-1.0129000	0.8603000
14	H	-0.9972000	-1.5724000	1.7595000
15	C	-2.5363000	0.0041000	-1.9762000
16	C	0.4782000	1.1447000	1.7539000
17	H	0.2116000	2.0823000	2.2552000
18	H	0.9280000	0.4892000	2.4996000
19	C	1.4387000	1.4350000	0.6410000
20	C	-0.7978000	0.5108000	1.2091000
21	C	1.0688000	-1.4071000	-0.9261000
22	H	0.4906000	-0.8684000	-1.6652000
23	C	0.5931000	-1.5457000	0.3810000
24	C	2.8184000	1.3157000	0.7792000
25	C	-1.3320000	1.2137000	-0.0690000
26	H	-2.1850000	1.8488000	0.1624000
27	C	-2.9982000	-1.4415000	-2.0359000
28	H	-2.8962000	-1.8496000	-3.0402000
29	H	-4.0591000	-1.4501000	-1.7669000
30	C	1.3696000	-2.2496000	1.3036000
31	C	2.2934000	-1.9534000	-1.2917000
32	H	2.6457000	-1.8396000	-2.3108000
33	C	-2.1416000	-2.1536000	-0.9885000
34	H	-2.6565000	-2.9684000	-0.4821000
35	H	-1.2195000	-2.5336000	-1.4407000
36	C	1.7574000	2.2029000	-1.6370000
37	H	1.3225000	2.5427000	-2.5694000
38	C	3.6665000	1.6449000	-0.2715000
39	C	3.1327000	2.0911000	-1.4778000
40	H	3.7882000	2.3480000	-2.3021000
41	H	3.2249000	0.9661000	1.7222000
42	H	4.7394000	1.5521000	-0.1505000
43	H	1.0027000	-2.3831000	2.3162000

2-Nitrobenzofuran + azomethine imine 2a

2-nitro-
benzofuran

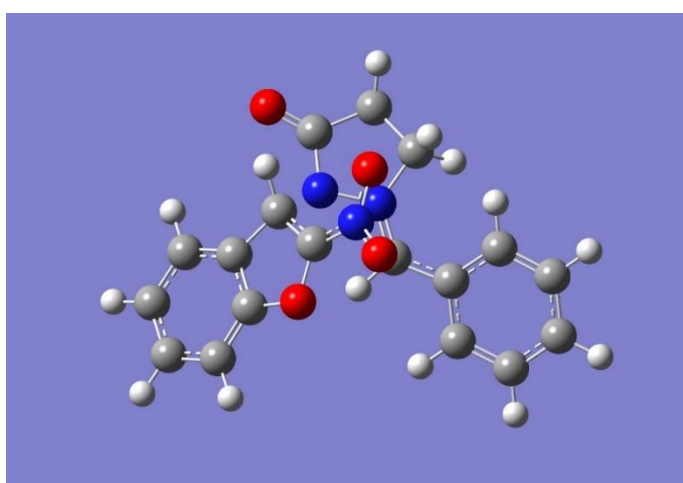


		X	Y	Z
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2	C	1.2775000	2.9745000	0.0000000
3	C	0.0206000	2.3899000	0.0000000

4	C	0.000000	1.005800	0.000000
5	C	1.155900	0.208200	0.000000
6	C	2.414600	0.824700	0.000000
7	C	0.695800	-1.142600	0.000000
8	C	-0.656500	-1.042700	0.000000
9	O	-1.115700	0.226800	0.000000
10	N	-1.635200	-2.071500	0.000000
11	H	3.321700	0.232900	0.000000
12	H	3.412900	2.713100	0.000000
13	H	1.354100	4.055500	0.000000
14	H	-0.889000	2.976500	0.000000
15	H	1.275100	-2.051600	0.000000
16	O	-1.224000	-3.223100	0.000000
17	O	-2.811600	-1.749500	0.000000

anti-exo cycloaddition

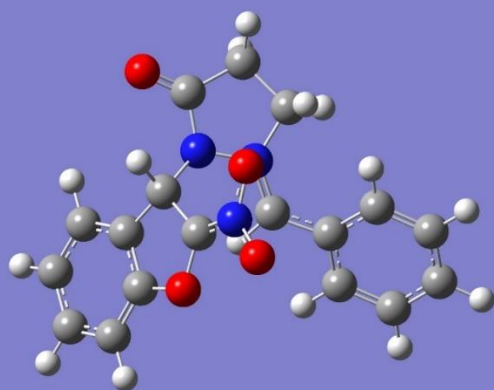
TS1



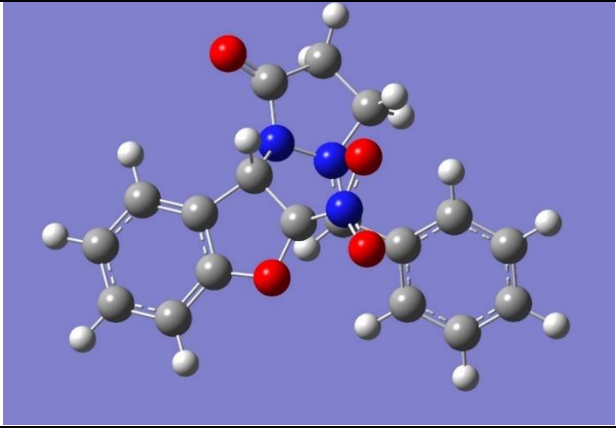
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1	O	-1.071700	-1.666200	1.075700
2	O	0.424000	1.173000	2.433600
3	O	-2.039900	3.366300	-0.471100
4	N	0.601700	1.260000	-0.648600
5	N	-0.742100	1.492200	-0.626800
6	N	0.172100	-0.043000	2.249400
7	O	0.761300	-0.951100	2.861900
8	C	-0.774000	-0.339900	1.325400
9	C	2.366100	-0.470700	-0.714200
10	C	-2.607100	-0.327100	0.035500
11	C	1.016500	0.037000	-0.802300
12	C	-1.634300	0.579500	0.663400
13	C	-2.187800	-1.632100	0.299500
14	C	-3.754200	-0.109700	-0.721700
15	C	-4.449400	-1.213800	-1.197900
16	C	2.578700	-1.728700	-1.304300
17	H	1.749800	-2.234200	-1.787000
18	C	-4.002600	-2.512500	-0.927800
19	C	-2.859700	-2.747700	-0.172400
20	C	-0.946700	2.862700	-0.610400
21	C	3.437100	0.164000	-0.064300
22	H	3.302800	1.108000	0.443200
23	C	1.392400	2.497800	-0.449500
24	H	2.255600	2.468700	-1.110000
25	H	1.708800	2.547800	0.591100
26	C	0.375900	3.571700	-0.782000

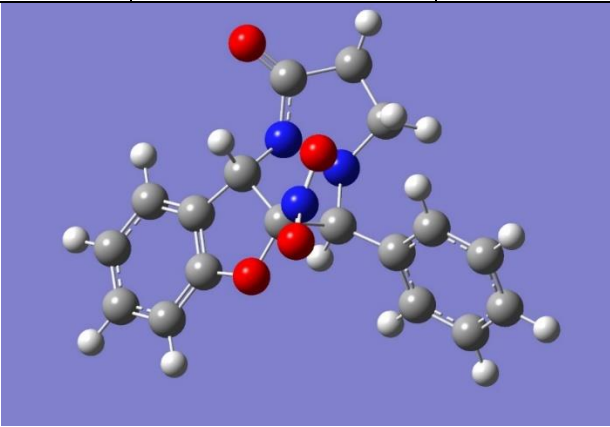
27	H	0.4292000	4.4360000	-0.1228000
28	H	0.4621000	3.9131000	-1.8165000
29	C	4.6856000	-0.4372000	-0.0378000
30	H	5.5040000	0.0579000	0.4712000
31	C	3.8323000	-2.3165000	-1.2829000
32	H	3.9834000	-3.2813000	-1.7522000
33	C	4.8903000	-1.6697000	-0.6516000
34	H	5.8717000	-2.1294000	-0.6285000
35	H	-1.9674000	1.4727000	1.1788000
36	H	-4.5618000	-3.3579000	-1.3123000
37	H	-2.5137000	-3.7508000	0.0440000
38	H	-4.0933000	0.8962000	-0.9386000
39	H	-5.3468000	-1.0710000	-1.7883000
40	H	0.2485000	-0.6596000	-1.1171000

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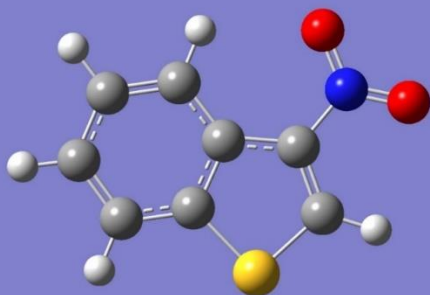
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3	O	-2.0107000	3.3818000	-0.4544000
4	N	0.5859000	1.1806000	-0.6410000
5	N	-0.7498000	1.4739000	-0.5023000
6	N	0.0581000	0.2762000	2.3112000
7	O	0.5678000	-0.4943000	3.1678000
8	C	-0.7836000	-0.1700000	1.3889000
9	C	2.3075000	-0.5743000	-0.6408000
10	C	-2.4683000	-0.3698000	-0.1378000
11	C	0.9580000	-0.0642000	-0.6925000
12	C	-1.5813000	0.6791000	0.4736000
13	C	-2.1687000	-1.5898000	0.4609000
14	C	-3.4606000	-0.2967000	-1.1035000
15	C	-4.1372000	-1.4630000	-1.4520000
16	C	2.4907000	-1.8729000	-1.1447000
17	H	1.6386000	-2.4120000	-1.5433000
18	C	-3.8215000	-2.6764000	-0.8376000
19	C	-2.8275000	-2.7630000	0.1325000
20	C	-0.9534000	2.8384000	-0.6616000
21	C	3.4050000	0.1092000	-0.0937000
22	H	3.2880000	1.0878000	0.3497000
23	C	1.3843000	2.4216000	-0.7068000
24	H	2.1890000	2.2806000	-1.4237000
25	H	1.7815000	2.6362000	0.2834000
26	C	0.3436000	3.4466000	-1.1225000
27	H	0.4893000	4.4177000	-0.6549000
28	H	0.3050000	3.5775000	-2.2068000
29	C	4.6546000	-0.4890000	-0.0833000
30	H	5.4959000	0.0404000	0.3479000
31	C	3.7461000	-2.4569000	-1.1424000

32	H	3.8779000	-3.4546000	-1.5439000
33	C	4.8312000	-1.7641000	-0.6141000
34	H	5.8138000	-2.2216000	-0.6049000
35	H	-2.1422000	1.4676000	0.9859000
36	H	-4.3606000	-3.5737000	-1.1198000
37	H	-2.5781000	-3.7019000	0.6113000
38	H	-3.7037000	0.6457000	-1.5809000
39	H	-4.9158000	-1.4291000	-2.2048000
40	H	0.1712000	-0.7798000	-0.8943000
TS2				
		X	Y	Z
1	O	-0.8386000	-1.7827000	0.7699000
2	O	0.7785000	0.8967000	2.2439000
3	O	-2.1812000	3.3260000	0.1059000
4	N	0.4794000	1.3444000	-0.7131000
5	N	-0.8589000	1.5228000	-0.3909000
6	N	0.4838000	-0.2896000	2.0004000
7	O	0.9907000	-1.2509000	2.5871000
8	C	-0.3759000	-0.4932000	0.9374000
9	C	2.2316000	-0.3976000	-0.7137000
10	C	-2.4921000	-0.3631000	0.0430000
11	C	0.8494000	0.0587000	-0.7768000
12	C	-1.4170000	0.5323000	0.5879000
13	C	-2.0753000	-1.6792000	0.1930000
14	C	-3.7286000	-0.0890000	-0.5198000
15	C	-4.5242000	-1.1577000	-0.9267000
16	C	2.5525000	-1.5689000	-1.4147000
17	H	1.7834000	-2.0687000	-1.9932000
18	C	-4.0833000	-2.4720000	-0.7677000
19	C	-2.8431000	-2.7593000	-0.2035000
20	C	-1.1387000	2.8751000	-0.3095000
21	C	3.2248000	0.2349000	0.0469000
22	H	2.9973000	1.1181000	0.6272000
23	C	1.2063000	2.6094000	-0.5519000
24	H	2.0170000	2.6543000	-1.2753000
25	H	1.5956000	2.7174000	0.4613000
26	C	0.0853000	3.6116000	-0.8043000
27	H	0.2084000	4.5472000	-0.2633000
28	H	-0.0366000	3.8283000	-1.8692000
29	C	4.5107000	-0.2861000	0.0814000
30	H	5.2719000	0.2089000	0.6730000
31	C	3.8400000	-2.0813000	-1.3793000
32	H	4.0770000	-2.9825000	-1.9328000
33	C	4.8235000	-1.4383000	-0.6334000
34	H	5.8310000	-1.8372000	-0.6046000
35	H	-1.7448000	1.1201000	1.4489000
36	H	-4.7168000	-3.2907000	-1.0896000

37	H	-2.4941000	-3.7769000	-0.0796000
38	H	-4.0685000	0.9324000	-0.6449000
39	H	-5.4938000	-0.9674000	-1.3714000
40	H	0.1737000	-0.5780000	-1.3437000
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		X	Y	Z
1	O	-0.7552000	-1.6515000	0.7578000
2	O	0.7510000	1.1079000	2.1694000
3	O	-1.8290000	3.5500000	0.2638000
4	N	0.3636000	1.1938000	-1.0702000
5	N	-0.8743000	1.6002000	-0.4644000
6	N	0.4563000	-0.0614000	1.9967000
7	O	0.7200000	-0.9698000	2.7455000
8	C	-0.2509000	-0.3530000	0.7053000
9	C	2.0922000	-0.5762000	-0.5277000
10	C	-2.4691000	-0.3263000	-0.0271000
11	C	0.6451000	-0.1491000	-0.5645000
12	C	-1.4189000	0.6355000	0.4591000
13	C	-2.0190000	-1.6148000	0.2131000
14	C	-3.7266000	-0.1208000	-0.5693000
15	C	-4.5073000	-1.2351000	-0.8705000
16	C	2.4796000	-1.5836000	-1.4157000
17	H	1.7441000	-2.0089000	-2.0901000
18	C	-4.0332000	-2.5222000	-0.6203000
19	C	-2.7705000	-2.7384000	-0.0717000
20	C	-0.9371000	2.9566000	-0.3112000
21	C	3.0547000	-0.0390000	0.3328000
22	H	2.8047000	0.7436000	1.0364000
23	C	1.2685000	2.3410000	-0.8708000
24	H	2.0436000	2.3329000	-1.6346000
25	H	1.7280000	2.3507000	0.1208000
26	C	0.2976000	3.5090000	-0.9887000
27	H	0.6376000	4.4166000	-0.4948000
28	H	0.0594000	3.7372000	-2.0322000
29	C	4.3645000	-0.5032000	0.3018000
30	H	5.0958000	-0.0760000	0.9784000
31	C	3.7895000	-2.0454000	-1.4479000
32	H	4.0666000	-2.8274000	-2.1454000
33	C	4.7370000	-1.5055000	-0.5866000
34	H	5.7602000	-1.8632000	-0.6065000
35	H	-1.7461000	1.1631000	1.3583000
36	H	-4.6551000	-3.3771000	-0.8597000
37	H	-2.3934000	-3.7352000	0.1197000
38	H	-4.0909000	0.8823000	-0.7588000
39	H	-5.4916000	-1.1006000	-1.3030000
40	H	0.1472000	-0.8362000	-1.2564000

3-Nitrobenzothiophene + azomethine imine 2a

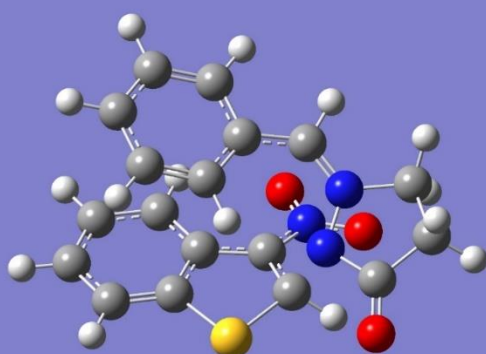
3-nitrobenzothiophene



		X	Y	Z
1	C	-0.7036000	2.7696000	0.0000000
2	C	-2.0478000	2.3779000	0.0000000
3	C	-2.3907000	1.0377000	0.0000000
4	C	-1.3608000	0.1007000	0.0000000
5	C	0.0000000	0.4724000	0.0000000
6	C	0.3190000	1.8382000	0.0000000
7	C	0.8235000	-0.7117000	0.0000000
8	C	0.1288000	-1.8832000	0.0000000
9	S	-1.5594000	-1.6360000	0.0000000
10	H	1.3514000	2.1551000	0.0000000
11	H	-0.4572000	3.8249000	0.0000000
12	H	-2.8287000	3.1292000	0.0000000
13	H	-3.4282000	0.7261000	0.0000000
14	H	0.5376000	-2.8828000	0.0000000
15	N	2.2585000	-0.7268000	0.0000000
16	O	2.8267000	-1.8089000	0.0000000
17	O	2.8428000	0.3466000	0.0000000

anti-exo Cycloaddition

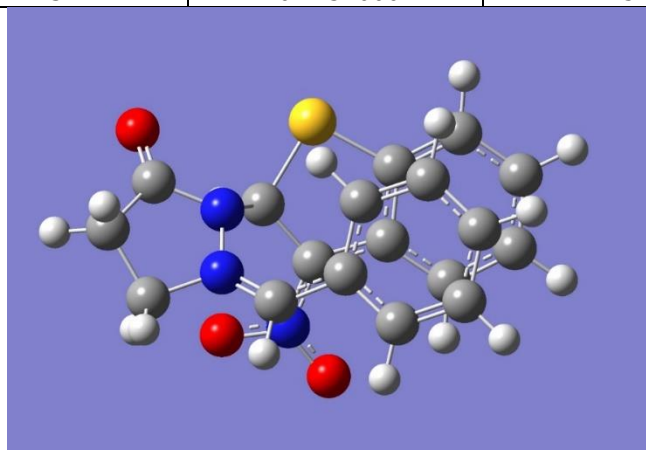
TS1



		X	Y	Z
1	O	-1.9664000	-0.7702000	2.3776000
2	O	-3.4295000	-1.1736000	-1.8774000
3	N	-1.9598000	1.1653000	0.0628000
4	N	-1.8757000	0.0940000	-0.7778000
5	N	-0.7245000	-0.7892000	2.2452000
6	O	0.0364000	-0.5721000	3.2025000
7	C	-0.1961000	-1.0709000	1.0037000

8	C	0.3674000	2.0128000	-0.1429000
9	C	1.2071000	-1.1828000	0.6882000
10	C	-0.9635000	1.9252000	0.4032000
11	H	-1.2219000	2.6451000	1.1719000
12	C	-1.0797000	-1.3957000	-0.0717000
13	H	-2.0080000	-1.9034000	0.1560000
14	C	1.3894000	-1.7536000	-0.5876000
15	C	2.3456000	-0.8190000	1.4170000
16	H	2.2332000	-0.3811000	2.3985000
17	C	3.6072000	-1.0338000	0.8741000
18	C	1.2573000	2.8518000	0.5503000
19	H	0.9306000	3.3314000	1.4665000
20	C	3.7624000	-1.6053000	-0.3881000
21	H	4.7539000	-1.7685000	-0.7944000
22	C	2.6447000	-1.9694000	-1.1331000
23	H	2.7551000	-2.4123000	-2.1163000
24	C	-3.1725000	-0.2122000	-1.1888000
25	C	0.7855000	1.4121000	-1.3411000
26	H	0.1106000	0.7699000	-1.8897000
27	C	-3.3522000	1.4034000	0.5258000
28	H	-3.4968000	2.4705000	0.6695000
29	H	-3.4936000	0.8640000	1.4614000
30	C	-4.1437000	0.7933000	-0.6133000
31	H	-5.0569000	0.2939000	-0.2960000
32	H	-4.3912000	1.5316000	-1.3805000
33	C	2.0582000	1.6600000	-1.8285000
34	H	2.3705000	1.2049000	-2.7610000
35	C	2.5372000	3.0703000	0.0693000
36	H	3.2179000	3.7110000	0.6174000
37	C	2.9393000	2.4768000	-1.1237000
38	H	3.9376000	2.6534000	-1.5075000
39	H	4.4842000	-0.7516000	1.4459000
40	S	-0.1432000	-2.1751000	-1.3532000

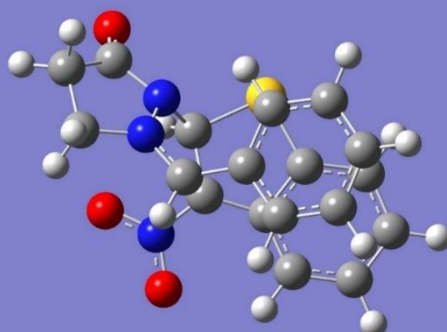
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		X	Y	Z
1	O	-1.9280000	-0.8758000	2.3000000
2	O	-3.4054000	-1.2906000	-1.7941000
3	N	-1.9950000	1.0582000	0.2163000
4	N	-1.9007000	-0.0443000	-0.6085000
5	N	-0.6697000	-0.8870000	2.1843000
6	O	0.0709000	-0.7682000	3.1884000
7	C	-0.1404000	-1.0250000	0.9455000
8	C	0.2942000	1.9940000	-0.0377000
9	C	1.2567000	-1.1596000	0.6278000
10	C	-1.0260000	1.8607000	0.5246000
11	H	-1.3083000	2.5813000	1.2854000

12	C	-1.0750000	-1.2583000	-0.1779000
13	H	-1.8339000	-2.0025000	0.0616000
14	C	1.4539000	-1.5977000	-0.6979000
15	C	2.3891000	-0.9260000	1.4180000
16	H	2.2603000	-0.5960000	2.4389000
17	C	3.6597000	-1.1316000	0.8870000
18	C	1.2128000	2.7531000	0.7055000
19	H	0.9258000	3.1307000	1.6806000
20	C	3.8287000	-1.5673000	-0.4240000
21	H	4.8234000	-1.7262000	-0.8244000
22	C	2.7145000	-1.8063000	-1.2286000
23	H	2.8358000	-2.1501000	-2.2497000
24	C	-3.1732000	-0.3150000	-1.1261000
25	C	0.6490000	1.5367000	-1.3154000
26	H	-0.0560000	0.9726000	-1.9110000
27	C	-3.4109000	1.2902000	0.5814000
28	H	-3.5593000	2.3481000	0.7765000
29	H	-3.6308000	0.6910000	1.4639000
30	C	-4.1160000	0.7612000	-0.6562000
31	H	-5.0969000	0.3379000	-0.4526000
32	H	-4.2077000	1.5274000	-1.4309000
33	C	1.8998000	1.8349000	-1.8281000
34	H	2.1646000	1.4954000	-2.8224000
35	C	2.4737000	3.0163000	0.1974000
36	H	3.1829000	3.5896000	0.7825000
37	C	2.8178000	2.5601000	-1.0715000
38	H	3.7994000	2.7770000	-1.4769000
39	H	4.5290000	-0.9488000	1.5090000
40	S	-0.0638000	-1.8976000	-1.5545000

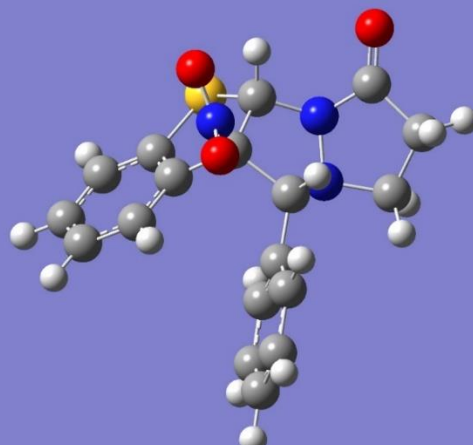
TS2



		X	Y	Z
1	O	2.1314000	-2.0165000	-1.1831000
2	O	3.6143000	-0.1045000	2.0555000
3	N	1.8868000	0.8279000	-0.7281000
4	N	1.9314000	0.3995000	0.5876000
5	N	0.8897000	-1.9933000	-1.2283000
6	O	0.2490000	-2.6162000	-2.0808000
7	C	0.2293000	-1.1820000	-0.2997000
8	C	-0.4798000	1.5371000	-0.8881000
9	C	-1.1905000	-1.3181000	-0.0162000
10	C	0.7057000	0.8103000	-1.3399000
11	H	0.7781000	0.6568000	-2.4143000
12	C	1.0554000	-0.7784000	0.8837000
13	H	1.7397000	-1.5672000	1.1952000
14	C	-1.5133000	-0.9135000	1.2907000
15	C	-2.2255000	-1.7382000	-0.8564000
16	H	-2.0013000	-2.0491000	-1.8663000

17	C	-3.5346000	-1.7608000	-0.3867000
18	C	-1.6245000	1.4812000	-1.6930000
19	H	-1.6164000	0.8707000	-2.5890000
20	C	-3.8323000	-1.3563000	0.9111000
21	H	-4.8558000	-1.3756000	1.2676000
22	C	-2.8173000	-0.9286000	1.7625000
23	H	-3.0426000	-0.6226000	2.7776000
24	C	3.2599000	0.3803000	1.0086000
25	C	-0.4816000	2.3540000	0.2488000
26	H	0.4032000	2.4264000	0.8684000
27	C	3.2329000	0.8528000	-1.3241000
28	H	3.2943000	1.6969000	-2.0066000
29	H	3.4451000	-0.0766000	-1.8510000
30	C	4.0950000	1.0144000	-0.0768000
31	H	5.0599000	0.5162000	-0.1419000
32	H	4.2567000	2.0673000	0.1699000
33	C	-1.6097000	3.0939000	0.5699000
34	H	-1.5982000	3.7345000	1.4443000
35	C	-2.7540000	2.2143000	-1.3597000
36	H	-3.6340000	2.1647000	-1.9905000
37	C	-2.7501000	3.0210000	-0.2261000
38	H	-3.6295000	3.6002000	0.0319000
39	H	-4.3292000	-2.0945000	-1.0442000
40	S	-0.1107000	-0.4619000	2.2591000

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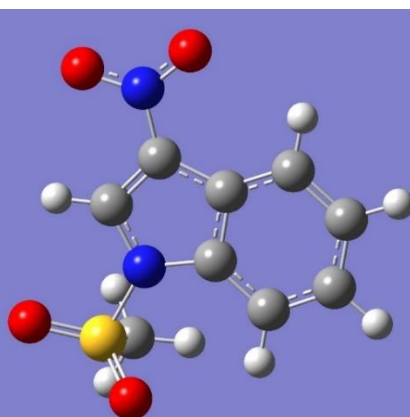
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1	O	1.1631000	1.4292000	2.6617000
2	O	4.3099000	-0.5494000	0.2335000
3	N	1.0841000	-1.0502000	-1.0046000
4	N	2.2121000	-0.2628000	-0.6563000
5	N	0.4681000	0.5612000	2.1801000
6	O	-0.2343000	-0.1981000	2.8110000
7	C	0.3989000	0.4608000	0.6545000
8	C	-1.1039000	-1.5996000	-0.0215000
9	C	-0.6824000	1.4130000	0.2214000
10	C	0.2707000	-1.0444000	0.2291000
11	H	0.7583000	-1.6336000	1.0169000
12	C	1.7586000	0.9009000	0.0295000
13	H	2.4950000	1.1984000	0.7721000
14	C	-0.2600000	2.3971000	-0.6727000
15	C	-2.0057000	1.3840000	0.6486000
16	H	-2.3379000	0.6300000	1.3522000
17	C	-2.9011000	2.3330000	0.1711000
18	C	-1.6881000	-2.4504000	0.9160000
19	H	-1.1498000	-2.6958000	1.8244000

20	C	-2.4745000	3.3016000	-0.7343000
21	H	-3.1763000	4.0386000	-1.1075000
22	C	-1.1535000	3.3450000	-1.1622000
23	H	-0.8254000	4.1083000	-1.8574000
24	C	3.3102000	-1.0108000	-0.2736000
25	C	-1.7973000	-1.3050000	-1.1970000
26	H	-1.3452000	-0.6576000	-1.9386000
27	C	1.6690000	-2.3539000	-1.3779000
28	H	1.8283000	-2.3503000	-2.4568000
29	H	0.9693000	-3.1503000	-1.1326000
30	C	3.0015000	-2.4444000	-0.6343000
31	H	2.9461000	-3.0126000	0.2977000
32	H	3.8007000	-2.8711000	-1.2395000
33	C	-3.0580000	-1.8445000	-1.4224000
34	H	-3.5864000	-1.6101000	-2.3398000
35	C	-2.9522000	-2.9854000	0.6932000
36	H	-3.3948000	-3.6454000	1.4307000
37	C	-3.6407000	-2.6823000	-0.4765000
38	H	-4.6245000	-3.1024000	-0.6536000
39	H	-3.9314000	2.3160000	0.5048000
40	S	1.4479000	2.3350000	-1.0815000

1-Mesyl-3-nitroindole + azomethine imine 2a

anti-exo cycloaddition

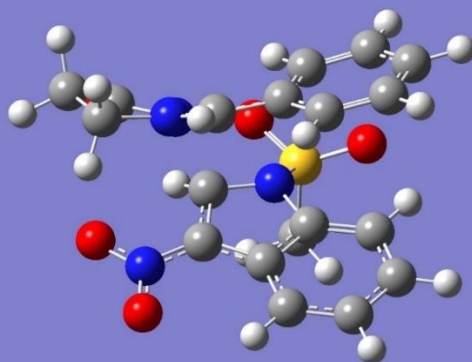
1-mesyl-3-nitroindole



		X	Y	Z
1	O	2.4497000	-2.8709000	0.0022000
2	N	2.5879000	-1.6544000	0.0252000
3	O	3.6738000	-1.0923000	0.0877000
4	C	1.4299000	-0.8394000	-0.0208000
5	C	1.3683000	0.5964000	-0.0127000

6	C	0.1601000	-1.3450000	-0.0841000
7	C	-0.0043000	0.9137000	-0.0806000
8	C	2.3098000	1.6273000	0.0431000
9	H	3.3661000	1.4028000	0.0929000
10	C	1.8537000	2.9347000	0.0354000
11	C	0.4859000	3.2289000	-0.0301000
12	H	0.1615000	4.2626000	-0.0369000
13	C	-0.4670000	2.2242000	-0.0918000
14	H	-1.5210000	2.4585000	-0.1537000
15	H	2.5691000	3.7475000	0.0796000
16	H	-0.1808000	-2.3669000	-0.1077000
17	N	-0.7115000	-0.2981000	-0.1279000
18	S	-2.4237000	-0.5024000	-0.1244000
19	O	-2.9528000	0.5059000	-1.0177000
20	O	-2.6287000	-1.9097000	-0.3963000
21	C	-2.8474000	-0.1238000	1.5487000
22	H	-3.9315000	-0.2265000	1.6216000
23	H	-2.3443000	-0.8379000	2.1993000
24	H	-2.5431000	0.9003000	1.7633000

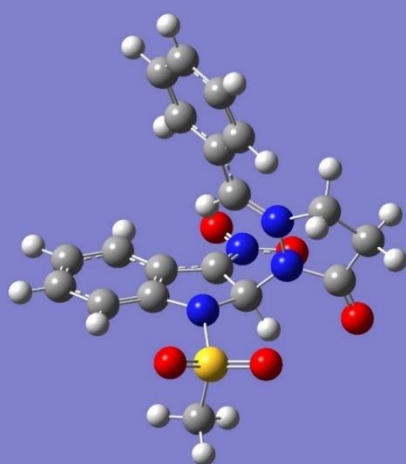
TS1



		X	Y	Z
1	O	-3.2221000	-0.3144000	1.5207000
2	O	-3.2588000	-1.0875000	-1.7651000
3	N	-1.6588000	1.6529000	-0.5952000
4	N	-1.6341000	0.3524000	-1.0284000
5	N	-2.1423000	-0.1241000	2.1262000
6	O	-2.1075000	0.3003000	3.2970000
7	C	-0.9787000	-0.3824000	1.4677000
8	C	0.7407000	2.2258000	-0.8639000
9	C	0.3657000	-0.2078000	1.9397000
10	C	-0.6267000	2.4191000	-0.4423000
11	H	-0.8647000	3.3706000	0.0215000
12	C	-0.9650000	-0.9015000	0.1313000
13	H	-1.6843000	-1.6371000	-0.2118000
14	C	1.2077000	-0.7063000	0.9276000
15	C	0.9288000	0.3243000	3.0986000
16	H	0.2909000	0.7072000	3.8834000
17	C	2.3160000	0.3418000	3.2195000
18	C	1.6905000	3.0982000	-0.3097000
19	H	1.3827000	3.8044000	0.4534000
20	C	3.1334000	-0.1479000	2.2037000
21	H	4.2110000	-0.1197000	2.3157000
22	C	2.5857000	-0.6721000	1.0310000
23	H	3.2186000	-1.0448000	0.2381000
24	C	-2.9405000	0.0169000	-1.3879000

25	C	1.1292000	1.3358000	-1.8761000
26	H	0.4018000	0.6683000	-2.3163000
27	C	-3.0429000	2.1519000	-0.3653000
28	H	-3.0818000	3.1997000	-0.6485000
29	H	-3.2827000	2.0325000	0.6899000
30	C	-3.8459000	1.2194000	-1.2427000
31	H	-4.7969000	0.9208000	-0.8081000
32	H	-4.0261000	1.6447000	-2.2332000
33	C	2.4397000	1.3331000	-2.3220000
34	H	2.7327000	0.6596000	-3.1184000
35	C	3.0082000	3.0623000	-0.7362000
36	H	3.7380000	3.7299000	-0.2940000
37	C	3.3825000	2.1836000	-1.7476000
38	H	4.4094000	2.1635000	-2.0946000
39	H	2.7656000	0.7473000	4.1190000
40	N	0.3933000	-1.1774000	-0.1436000
41	S	0.8155000	-2.5489000	-1.0508000
42	C	0.7376000	-3.8854000	0.1125000
43	H	1.0260000	-4.7876000	-0.4288000
44	H	1.4385000	-3.6849000	0.9218000
45	H	-0.2844000	-3.9685000	0.4802000
46	O	-0.2242000	-2.7100000	-2.0484000
47	O	2.1944000	-2.3635000	-1.4662000

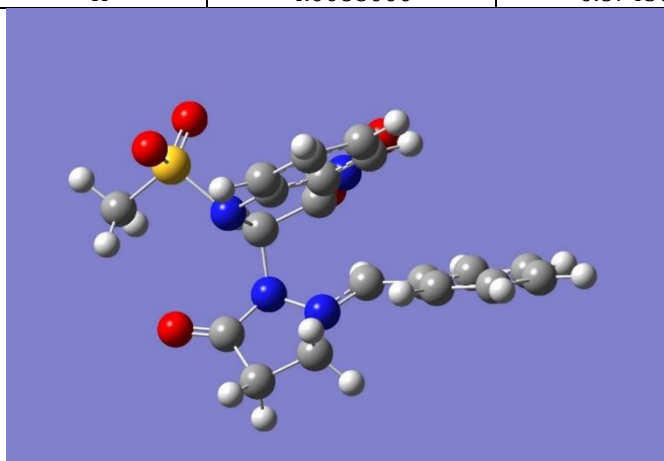
IM



		X	Y	Z
1	O	1.1343000	-0.9292000	3.2925000
2	O	1.5870000	-3.4191000	1.0656000
3	N	-1.0725000	-1.4191000	0.2291000
4	N	0.2424000	-1.6336000	0.5602000
5	N	1.0908000	0.2662000	2.8896000
6	O	1.0052000	1.2259000	3.7024000
7	C	1.1254000	0.5108000	1.5714000
8	C	-2.9634000	0.1003000	-0.1891000
9	C	1.1586000	1.7789000	0.9125000
10	C	-1.6181000	-0.2477000	0.2065000
11	H	-0.9971000	0.5635000	0.5660000
12	C	1.2781000	-0.5967000	0.5731000
13	H	2.1781000	-1.1984000	0.7402000
14	C	1.2826000	1.5423000	-0.4720000
15	C	1.0772000	3.0957000	1.3709000
16	H	0.9800000	3.2827000	2.4312000
17	C	1.1361000	4.1391000	0.4484000
18	C	-3.4262000	1.3278000	0.3152000
19	H	-2.7761000	1.9204000	0.9488000
20	C	1.2567000	3.8848000	-0.9129000

21	H	1.2948000	4.7059000	-1.6192000
22	C	1.3210000	2.5716000	-1.3921000
23	H	1.4003000	2.3732000	-2.4517000
24	C	0.5012000	-2.9781000	0.7923000
25	C	-3.7927000	-0.6465000	-1.0413000
26	H	-3.4480000	-1.5631000	-1.4974000
27	C	-1.7119000	-2.7268000	-0.0447000
28	H	-1.7152000	-2.8762000	-1.1242000
29	H	-2.7271000	-2.7025000	0.3407000
30	C	-0.8005000	-3.7144000	0.6533000
31	H	-1.1581000	-3.9652000	1.6547000
32	H	-0.6595000	-4.6329000	0.0883000
33	C	-5.0607000	-0.1814000	-1.3491000
34	H	-5.6910000	-0.7563000	-2.0170000
35	C	-4.7030000	1.7732000	0.0182000
36	H	-5.0540000	2.7139000	0.4248000
37	C	-5.5232000	1.0176000	-0.8135000
38	H	-6.5194000	1.3689000	-1.0566000
39	H	1.0833000	5.1633000	0.8010000
40	N	1.3052000	0.1332000	-0.7083000
41	S	2.1591000	-0.5429000	-1.9922000
42	O	1.9241000	-1.9744000	-1.9051000
43	O	1.7591000	0.1755000	-3.1907000
44	C	3.8684000	-0.2051000	-1.6568000
45	H	4.1405000	-0.6807000	-0.7150000
46	H	4.4416000	-0.6327000	-2.4802000
47	H	4.0088000	0.8745000	-1.6127000

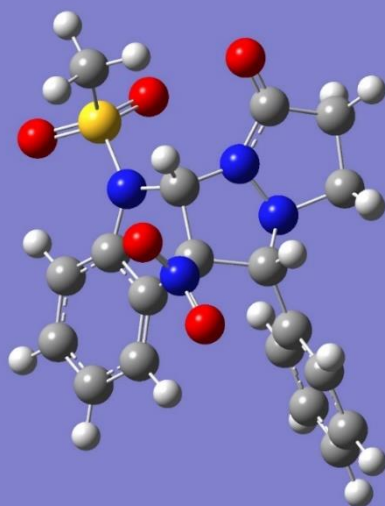
TS2



		X	Y	Z
1	O	-0.2540000	-0.3147000	3.1610000
2	O	2.3995000	-3.0240000	-0.4812000
3	N	-0.7766000	-1.7928000	-0.3064000
4	N	0.5077000	-1.9051000	0.1968000
5	N	-0.4894000	0.5705000	2.3187000
6	O	-1.1499000	1.5828000	2.5828000
7	C	-0.0848000	0.3405000	1.0118000
8	C	-2.8980000	-0.6425000	0.1554000
9	C	-0.0511000	1.3627000	-0.0163000
10	C	-1.6048000	-1.1828000	0.5336000
11	H	-1.4736000	-1.4712000	1.5757000
12	C	1.0575000	-0.6076000	0.7434000
13	H	1.6349000	-0.8505000	1.6309000
14	C	1.0676000	1.1234000	-0.8254000
15	C	-0.9348000	2.3881000	-0.3485000
16	H	-1.7933000	2.5942000	0.2758000
17	C	-0.6844000	3.1392000	-1.4921000

18	C	-3.8867000	-0.5819000	1.1483000
19	H	-3.6655000	-0.9541000	2.1422000
20	C	0.4111000	2.8608000	-2.3085000
21	H	0.5762000	3.4452000	-3.2063000
22	C	1.3030000	1.8405000	-1.9860000
23	H	2.1613000	1.6285000	-2.6080000
24	C	1.2343000	-2.7577000	-0.6347000
25	C	-3.1808000	-0.1449000	-1.1247000
26	H	-2.4234000	-0.1446000	-1.8970000
27	C	-0.8314000	-2.2169000	-1.7062000
28	H	-0.6171000	-1.3857000	-2.3819000
29	H	-1.8141000	-2.6296000	-1.9213000
30	C	0.2947000	-3.2462000	-1.7163000
31	H	-0.0661000	-4.2422000	-1.4455000
32	H	0.8224000	-3.3097000	-2.6658000
33	C	-4.4360000	0.3737000	-1.4051000
34	H	-4.6481000	0.7567000	-2.3964000
35	C	-5.1396000	-0.0638000	0.8600000
36	H	-5.8996000	-0.0288000	1.6318000
37	C	-5.4171000	0.4115000	-0.4182000
38	H	-6.3964000	0.8177000	-0.6445000
39	H	-1.3612000	3.9423000	-1.7607000
40	N	1.8758000	0.0638000	-0.2894000
41	S	3.4060000	0.6279000	0.2813000
42	O	3.9822000	1.3909000	-0.8151000
43	O	3.2424000	1.2895000	1.5729000
44	C	4.3320000	-0.8599000	0.5107000
45	H	4.3972000	-1.3849000	-0.4381000
46	H	5.3159000	-0.5233000	0.8422000
47	H	3.8679000	-1.4753000	1.2777000

trans-
product

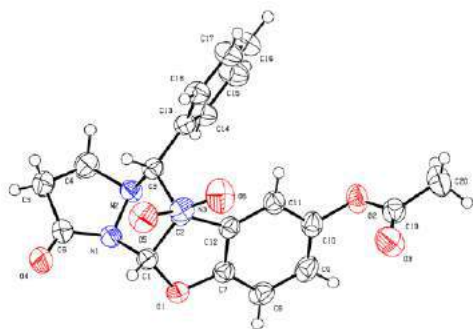


		X	Y	Z
1	O	0.2615000	0.3036000	3.2568000
2	O	2.6346000	-2.9961000	0.4304000
3	N	-0.3858000	-1.5889000	-0.6788000
4	N	0.8864000	-1.5969000	-0.0451000
5	N	-0.6681000	0.1749000	2.4904000
6	O	-1.8381000	0.1895000	2.8034000
7	C	-0.3740000	0.0586000	1.0008000
8	C	-2.6093000	-0.6583000	-0.2037000
9	C	-0.4259000	1.4359000	0.4140000
10	C	-1.2740000	-1.0538000	0.3657000
11	H	-1.4266000	-1.8139000	1.1452000
12	C	1.0818000	-0.4271000	0.7407000

13	H	1.6278000	-0.6760000	1.6484000
14	C	0.8050000	1.7559000	-0.1622000
15	C	-1.4835000	2.3308000	0.4031000
16	H	-2.4254000	2.0759000	0.8730000
17	C	-1.3117000	3.5622000	-0.2192000
18	C	-3.7739000	-0.9378000	0.5104000
19	H	-3.7050000	-1.4260000	1.4758000
20	C	-0.0943000	3.8657000	-0.8211000
21	H	0.0347000	4.8220000	-1.3154000
22	C	0.9780000	2.9783000	-0.8049000
23	H	1.9162000	3.2424000	-1.2668000
24	C	1.5641000	-2.7674000	-0.1068000
25	C	-2.7088000	-0.0493000	-1.4558000
26	H	-1.8109000	0.1538000	-2.0266000
27	C	-0.6348000	-3.0128000	-1.0150000
28	H	-1.1463000	-3.0817000	-1.9726000
29	H	-1.2621000	-3.4703000	-0.2425000
30	C	0.7492000	-3.6565000	-1.0167000
31	H	0.7499000	-4.6860000	-0.6635000
32	H	1.2140000	-3.6316000	-2.0066000
33	C	-3.9534000	0.2858000	-1.9759000
34	H	-4.0190000	0.7564000	-2.9506000
35	C	-5.0182000	-0.5972000	-0.0074000
36	H	-5.9158000	-0.8202000	0.5584000
37	C	-5.1105000	0.0175000	-1.2517000
38	H	-6.0808000	0.2792000	-1.6591000
39	H	-2.1246000	4.2775000	-0.2391000
40	N	1.7197000	0.7100000	0.0521000
41	S	3.2729000	0.5994000	-0.5914000
42	O	3.2766000	-0.3250000	-1.7146000
43	O	3.7168000	1.9653000	-0.8267000
44	C	4.1904000	-0.1078000	0.7449000
45	H	3.8448000	-1.1279000	0.9174000
46	H	5.2277000	-0.1186000	0.4059000
47	H	4.0805000	0.5268000	1.6229000

III. Single crystal X-ray structure analysis

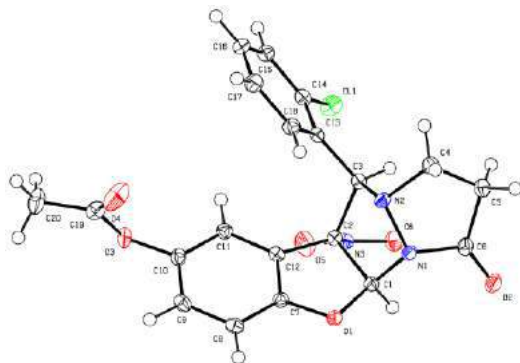
Table S1 Crystal data and structure refinement for 3aa.



CCDC Number	2076737
Empirical formula	C ₂₀ H ₁₇ N ₃ O ₆
Formula weight	395.36
Temperature/K	293(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	17.08060(10)
b/Å	12.64680(10)
c/Å	17.15760(10)
α/°	90
β/°	92.4370(10)
γ/°	90
Volume/Å ³	3702.95(4)
Z	8
ρ _{calc} /cm ³	1.418
μ/mm ⁻¹	0.897
F(000)	1648.0
Crystal size/mm ³	0.602 × 0.348 × 0.26
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	8.702 to 152.746
Index ranges	-21 ≤ h ≤ 21, -10 ≤ k ≤ 15, -21 ≤ l ≤ 21
Reflections collected	19784
Independent reflections	3883 [R _{int} = 0.0124, R _{sigma} = 0.0086]
Data/restraints/parameters	3883/0/264
Goodness-of-fit on F ²	1.044
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0354, wR ₂ = 0.0965
Final R indexes [all data]	R ₁ = 0.0366, wR ₂ = 0.0977
Largest diff. peak/hole / e Å ⁻³	0.25/-0.16

Crystal structure determination of 3aa

Crystal Data for C₂₀H₁₇N₃O₆ (*M* = 395.36 g/mol): monoclinic, space group C2/c (no. 15), *a* = 17.08060(10) Å, *b* = 12.64680(10) Å, *c* = 17.15760(10) Å, β = 92.4370(10)°, *V* = 3702.95(4) Å³, *Z* = 8, *T* = 293(2) K, μ(Cu Kα) = 0.897 mm⁻¹, *D*_{calc} = 1.418 g/cm³, 19784 reflections measured (8.702° ≤ 2θ ≤ 152.746°), 3883 unique (*R*_{int} = 0.0124, *R*_{sigma} = 0.0086) which were used in all calculations. The final *R*₁ was 0.0354 (*I* > 2σ(*I*)) and *wR*₂ was 0.0977 (all data). The crystals were grown from MeCN.

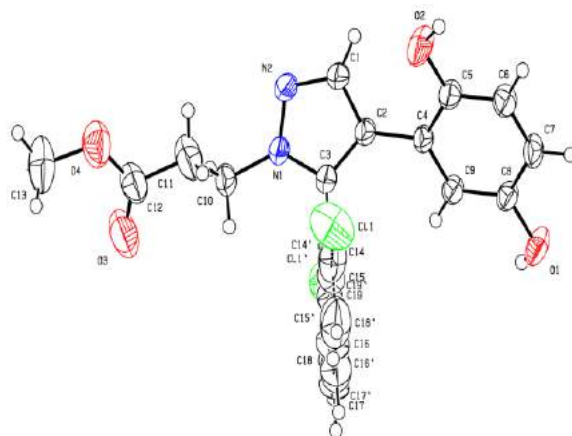
Table S2 Crystal data and structure refinement for 3ac.

CCDC Number	2076749
Empirical formula	$C_{20}H_{16}ClN_3O_6$
Formula weight	429.81
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	I2/a
a/Å	18.28800(10)
b/Å	8.88670(10)
c/Å	24.7898(2)
$\alpha/^\circ$	90
$\beta/^\circ$	110.7630(10)
$\gamma/^\circ$	90
Volume/Å ³	3767.18(6)
Z	8
$\rho_{\text{calc}}/\text{cm}^3$	1.516
μ/mm^{-1}	2.207
F(000)	1776.0
Crystal size/mm ³	0.399 × 0.322 × 0.266
Radiation	Cu K α ($\lambda = 1.54184$)
2 Θ range for data collection/ $^\circ$	7.628 to 152.602
Index ranges	-23 ≤ h ≤ 23, -10 ≤ k ≤ 10, -31 ≤ l ≤ 30
Reflections collected	21644
Independent reflections	3899 [$R_{\text{int}} = 0.0184$, $R_{\text{sigma}} = 0.0108$]
Data/restraints/parameters	3899/0/273
Goodness-of-fit on F ²	1.070
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0288$, $wR_2 = 0.0739$
Final R indexes [all data]	$R_1 = 0.0291$, $wR_2 = 0.0742$
Largest diff. peak/hole / e Å ⁻³	0.34/-0.22

Crystal structure determination of 3ac

Crystal Data for $C_{20}H_{16}ClN_3O_6$ ($M = 429.81$ g/mol): monoclinic, space group I2/a (no. 15), $a = 18.28800(10)$ Å, $b = 8.88670(10)$ Å, $c = 24.7898(2)$ Å, $\beta = 110.7630(10)^\circ$, $V = 3767.18(6)$ Å³, $Z = 8$, $T = 100.00(10)$ K, $\mu(\text{Cu K}\alpha) = 2.207$ mm⁻¹, $D_{\text{calc}} = 1.516$ g/cm³, 21644 reflections measured ($7.628^\circ \leq 2\Theta \leq 152.602^\circ$), 3899 unique ($R_{\text{int}} = 0.0184$, $R_{\text{sigma}} = 0.0108$) which were used in all calculations. The final R_1 was 0.0288 ($I > 2\sigma(I)$) and wR_2 was 0.0742 (all data). The crystals were grown from MeCN.

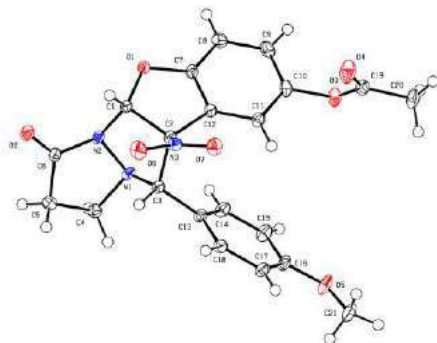
Table S3 Crystal data and structure refinement for 3ac'.



CCDC Number	2083589
Empirical formula	$C_{19}H_{17}ClN_2O_4$
Formula weight	372.79
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
$a/\text{\AA}$	8.63400(10)
$b/\text{\AA}$	13.47330(10)
$c/\text{\AA}$	15.5128(2)
$\alpha/^\circ$	90
$\beta/^\circ$	92.0160(10)
$\gamma/^\circ$	90
Volume/ \AA^3	1803.46(3)
Z	4
$\rho_{\text{calc}}/\text{g/cm}^3$	1.373
μ/mm^{-1}	2.112
F(000)	776.0
Crystal size/ mm^3	$0.33 \times 0.202 \times 0.157$
Radiation	Cu $K\alpha$ ($\lambda = 1.54184$)
2θ range for data collection/ $^\circ$	8.696 to 152.984
Index ranges	$-10 \leq h \leq 10, -12 \leq k \leq 16, -19 \leq l \leq 17$
Reflections collected	20601
Independent reflections	3783 [$R_{\text{int}} = 0.0214, R_{\text{sigma}} = 0.0139$]
Data/restraints/parameters	3783/72/303
Goodness-of-fit on F^2	1.174
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0707, wR_2 = 0.1605$
Final R indexes [all data]	$R_1 = 0.0722, wR_2 = 0.1612$
Largest diff. peak/hole / $e \text{\AA}^{-3}$	0.24/-0.28

Crystal structure determination of 3ac'

Crystal Data for $C_{19}H_{17}ClN_2O_4$ ($M = 372.79$ g/mol): monoclinic, space group $P2_1/n$ (no. 14), $a = 8.63400(10)$ \AA , $b = 13.47330(10)$ \AA , $c = 15.5128(2)$ \AA , $\beta = 92.0160(10)^\circ$, $V = 1803.46(3)$ \AA^3 , $Z = 4$, $T = 293(2)$ K, $\mu(\text{Cu } K\alpha) = 2.112$ mm^{-1} , $D_{\text{calc}} = 1.373$ g/cm^3 , 20601 reflections measured ($8.696^\circ \leq 2\theta \leq 152.984^\circ$), 3783 unique ($R_{\text{int}} = 0.0214, R_{\text{sigma}} = 0.0139$) which were used in all calculations. The final R_1 was 0.0707 ($I > 2\sigma(I)$) and wR_2 was 0.1612 (all data).

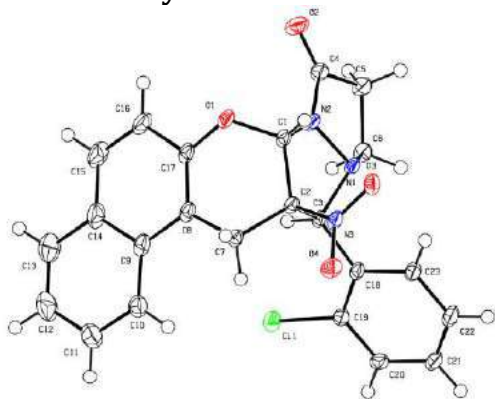
Table S4 Crystal data and structure refinement for 3ah.

CCDC Number	2076734
Empirical formula	C ₂₁ H ₁₉ N ₃ O ₇
Formula weight	425.39
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	14.40077(10)
b/Å	16.91016(12)
c/Å	8.11294(5)
α/°	90
β/°	91.4865(6)
γ/°	90
Volume/Å ³	1974.99(2)
Z	4
ρ _{calc} /cm ³	1.431
μ/mm ⁻¹	0.921
F(000)	888.0
Crystal size/mm ³	0.468 × 0.401 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	6.14 to 152.836
Index ranges	-18 ≤ h ≤ 17, -21 ≤ k ≤ 21, -10 ≤ l ≤ 7
Reflections collected	21205
Independent reflections	4136 [R _{int} = 0.0375, R _{sigma} = 0.0256]
Data/restraints/parameters	4136/0/283
Goodness-of-fit on F ²	1.049
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0358, wR ₂ = 0.0946
Final R indexes [all data]	R ₁ = 0.0375, wR ₂ = 0.0964
Largest diff. peak/hole / e Å ⁻³	0.33/-0.26

Crystal structure determination of 3ah

Crystal Data for C₂₁H₁₉N₃O₇ (*M* = 425.39 g/mol): monoclinic, space group P2₁/c (no. 14), *a* = 14.40077(10) Å, *b* = 16.91016(12) Å, *c* = 8.11294(5) Å, β = 91.4865(6)°, *V* = 1974.99(2) Å³, *Z* = 4, *T* = 100.00(10) K, μ(Cu Kα) = 0.921 mm⁻¹, *D*_{calc} = 1.431 g/cm³, 21205 reflections measured (6.14° ≤ 2θ ≤ 152.836°), 4136 unique (*R*_{int} = 0.0375, *R*_{sigma} = 0.0256) which were used in all calculations. The final *R*₁ was 0.0358 (*I* > 2σ(*I*)) and *wR*₂ was 0.0964 (all data). The crystals were grown from a mixture CCl₄/CHCl₃.

Table S5 Crystal data and structure refinement for 5bc.

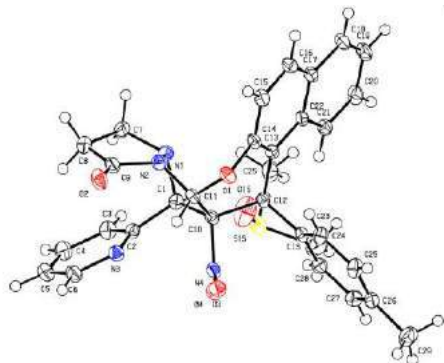


CCDC Number	2077063
Empirical formula	C ₂₃ H ₁₈ ClN ₃ O ₄
Formula weight	435.85
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	7.5805(2)
b/Å	8.9682(3)
c/Å	15.1658(5)
α/°	92.886(3)
β/°	97.851(3)
γ/°	102.333(3)
Volume/Å ³	994.41(6)
Z	2
ρ _{calc} /cm ³	1.456
μ/mm ⁻¹	2.022
F(000)	452.0
Crystal size/mm ³	0.579 × 0.421 × 0.381
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	5.902 to 153.186
Index ranges	-9 ≤ h ≤ 9, -11 ≤ k ≤ 11, -18 ≤ l ≤ 19
Reflections collected	7849
Independent reflections	7849 [R _{sigma} = 0.0090]
Data/restraints/parameters	7849/0/281
Goodness-of-fit on F ²	1.069
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0759, wR ₂ = 0.2129
Final R indexes [all data]	R ₁ = 0.0762, wR ₂ = 0.2134
Largest diff. peak/hole / e Å ⁻³	0.45/-0.80

Crystal structure determination of 5bc

Crystal Data for C₂₃H₁₈ClN₃O₄ (*M* = 435.85 g/mol): triclinic, space group P-1 (no. 2), *a* = 7.5805(2) Å, *b* = 8.9682(3) Å, *c* = 15.1658(5) Å, α = 92.886(3)°, β = 97.851(3)°, γ = 102.333(3)°, *V* = 994.41(6) Å³, *Z* = 2, *T* = 100.00(10) K, μ(Cu Kα) = 2.022 mm⁻¹, *D*_{calc} = 1.456 g/cm³, 7849 reflections measured (5.902° ≤ 2θ ≤ 153.186°), 7849 unique (*R*_{int} = ?, *R*_{sigma} = 0.0090) which were used in all calculations. The final *R*₁ was 0.0759 (*I* > 2σ(*I*)) and *wR*₂ was 0.2134 (all data). Twinned data refinement Scales: 0.3908 0.6092. The crystals were grown from MeCN.

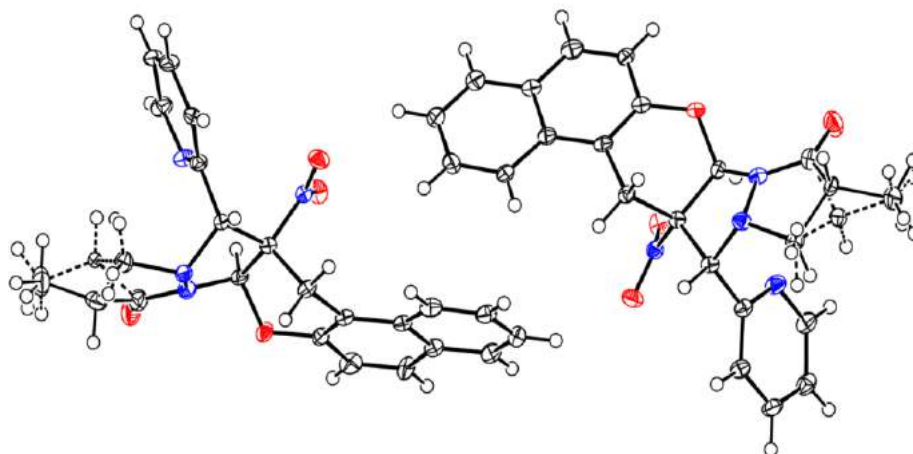
Table S6 Crystal data and structure refinement for 5cf.



CCDC Number	2076671
Empirical formula	C ₃₁ H ₃₀ N ₄ O ₅ S
Formula weight	570.65
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	Cc
a/Å	11.55130(10)
b/Å	17.20680(10)
c/Å	14.50100(10)
α/°	90
β/°	106.9860(10)
γ/°	90
Volume/Å ³	2756.50(4)
Z	4
ρ _{calc} /g/cm ³	1.375
μ/mm ⁻¹	1.449
F(000)	1200.0
Crystal size/mm ³	0.359 × 0.303 × 0.178
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	9.514 to 153.02
Index ranges	-14 ≤ h ≤ 14, -21 ≤ k ≤ 21, -16 ≤ l ≤ 18
Reflections collected	28113
Independent reflections	4672 [R _{int} = 0.0276, R _{sigma} = 0.0196]
Data/restraints/parameters	4672/2/373
Goodness-of-fit on F ²	1.050
Final R indexes [I>=2σ (I)]	R ₁ = 0.0281, wR ₂ = 0.0745
Final R indexes [all data]	R ₁ = 0.0282, wR ₂ = 0.0746
Largest diff. peak/hole / e Å ⁻³	0.35/-0.37
Flack parameter	0.002(8)

Crystal structure determination of 5cf

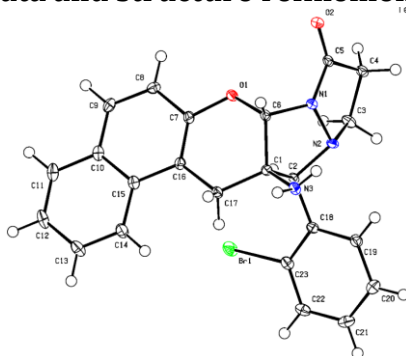
Crystal Data for C₃₁H₃₀N₄O₅S (M = 570.65 g/mol): monoclinic, space group Cc (no. 9), a = 11.55130(10) Å, b = 17.20680(10) Å, c = 14.50100(10) Å, β = 106.9860(10)°, V = 2756.50(4) Å³, Z = 4, T = 100.00(10) K, μ(Cu Kα) = 1.449 mm⁻¹, D_{calc} = 1.375 g/cm³, 28113 reflections measured (9.514° ≤ 2θ ≤ 153.02°), 4672 unique (R_{int} = 0.0276, R_{sigma} = 0.0196) which were used in all calculations. The final R₁ was 0.0281 (I > 2σ(I)) and wR₂ was 0.0746 (all data). The crystals were grown from DMSO.

Table S7 Crystal data and structure refinement for 5bj.

CCDC Number	2083590
Empirical formula	C ₂₃ H ₂₀ N ₄ O ₄
Formula weight	416.43
Temperature/K	99.99(10)
Crystal system	orthorhombic
Space group	Pna2 ₁
a/Å	16.82982(8)
b/Å	5.65071(4)
c/Å	41.3175(2)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	3929.32(4)
Z	8
ρ _{calc} /g/cm ³	1.408
μ/mm ⁻¹	0.812
F(000)	1744.0
Crystal size/mm ³	0.466 × 0.217 × 0.04
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	4.278 to 153.184
Index ranges	-21 ≤ h ≤ 21, -6 ≤ k ≤ 7, -52 ≤ l ≤ 52
Reflections collected	140500
Independent reflections	8234 [R _{int} = 0.0558, R _{sigma} = 0.0166]
Data/restraints/parameters	8234/13/581
Goodness-of-fit on F ²	1.080
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0469, wR ₂ = 0.1234
Final R indexes [all data]	R ₁ = 0.0472, wR ₂ = 0.1236
Largest diff. peak/hole / e Å ⁻³	0.31/-0.27
Flack parameter	0.64(8)

Crystal structure determination of 5bj

Crystal Data for C₂₃H₂₀N₄O₄ (*M* = 416.43 g/mol): orthorhombic, space group Pna2₁ (no. 33), *a* = 16.82982(8) Å, *b* = 5.65071(4) Å, *c* = 41.3175(2) Å, *V* = 3929.32(4) Å³, *Z* = 8, *T* = 99.99(10) K, μ(Cu Kα) = 0.812 mm⁻¹, *D*_{calc} = 1.408 g/cm³, 140500 reflections measured (4.278° ≤ 2θ ≤ 153.184°), 8234 unique (*R*_{int} = 0.0558, *R*_{sigma} = 0.0166) which were used in all calculations. The final *R*₁ was 0.0469 (*I* > 2σ(*I*)) and *wR*₂ was 0.1236 (all data).

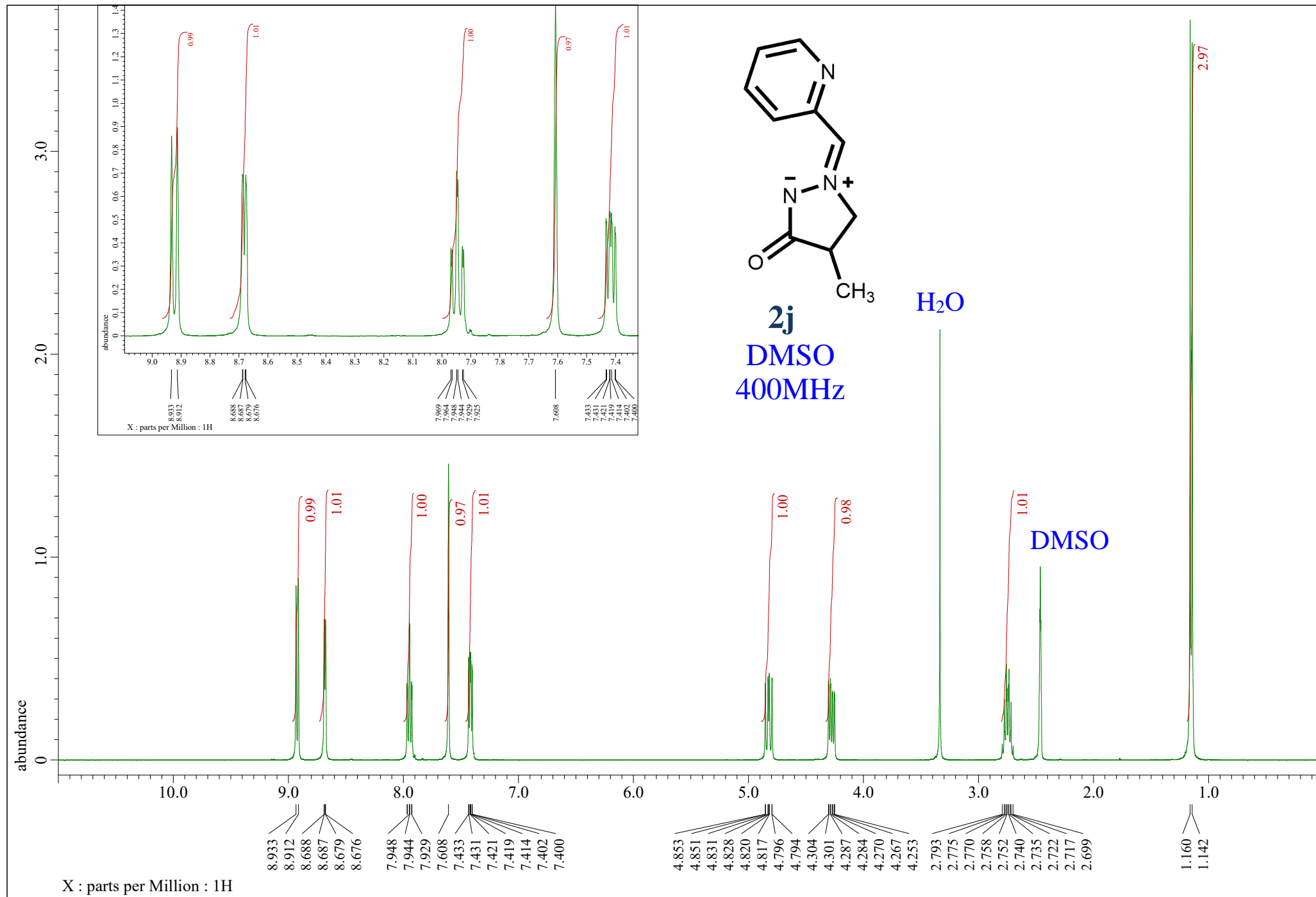
Table S8 Crystal data and structure refinement for 5bd'

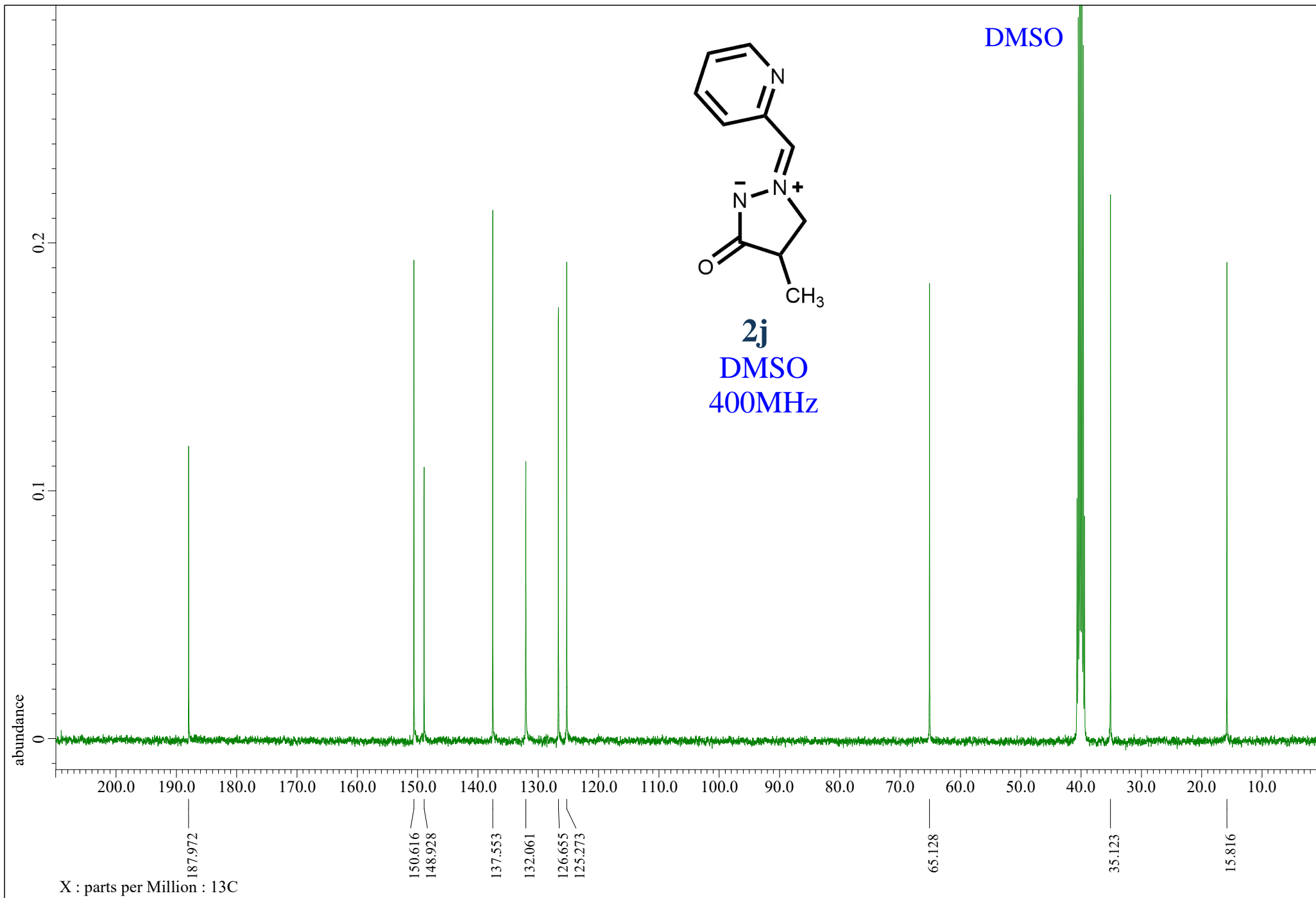
CCDC Number	2117341
Empirical formula	$C_{23}H_{20}BrN_3O_2$
Formula weight	450.34
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$I 1 2/a 1$
$a/\text{\AA}$	22.22011(17)
$b/\text{\AA}$	7.84209(3)
$c/\text{\AA}$	24.48716(18)
$\alpha/^\circ$	90
$\beta/^\circ$	116.6327(9)
$\gamma/^\circ$	90
Volume/ \AA^3	3814.21
Z	8
$\rho_{\text{calc}}/\text{g/cm}^3$	1.568
μ/mm^{-1}	3.148
F(000)	1840.0
Crystal size/ mm^3	$0.483 \times 0.208 \times 0.121$
Radiation	Cu $K\alpha$ ($\lambda = 1.54184$)
2Θ range for data collection/ $^\circ$	4.039 to 76.086
Index ranges	$-27 \leq h \leq 23, -9 \leq k \leq 7, -30 \leq l \leq 30$
Reflections collected	20647
Independent reflections	3971 [$R_{\text{int}} = 0.0226, R_{\text{sigma}} = 0.0157$]
Data/restraints/parameters	3971/0/271
Goodness-of-fit on F^2	1.096
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.093, wR_2 = 0.0655$
Final R indexes [all data]	$R_1 = 0.0254, wR_2 = 0.0657$
Largest diff. peak/hole / $e \text{\AA}^{-3}$	0.41/-0.47

Crystal structure determination of 5bd'

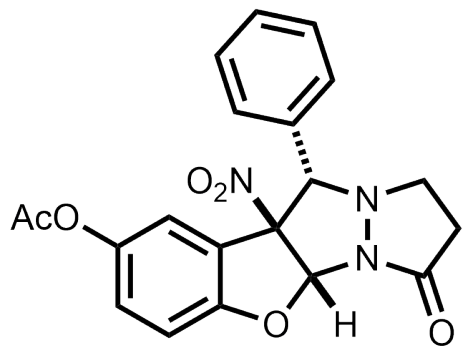
Crystal Data $C_{23}H_{20}BrN_3O_2$ ($M = 450.34$ g/mol): monoclinic, space group $I 1 2/a 1$, $a = 22.22011(17)$ \AA , $b = 7.84209(3)$ \AA , $c = 24.48716(18)$ \AA , $\alpha = 90^\circ$, $\beta = 116.6327(9)^\circ$, $\gamma = 90^\circ$, $V = 3814.21$ \AA^3 , $Z = 8$, $T = 100.00(10)$ K, $\mu(\text{Cu } K\alpha) = 2.022$ mm^{-1} , $D_{\text{calc}} = 1.568$ g/cm^3 , 20647 reflections measured ($4.039^\circ \leq 2\Theta \leq 76.086^\circ$), 3971 unique ($R_{\text{int}} = 0.0226, R_{\text{sigma}} = 0.0157$) which were used in all calculations. The final R_1 was 0.093 ($I > 2\sigma(I)$) and wR_2 was 0.0657 (all data).

IV. Copies of NMR spectra

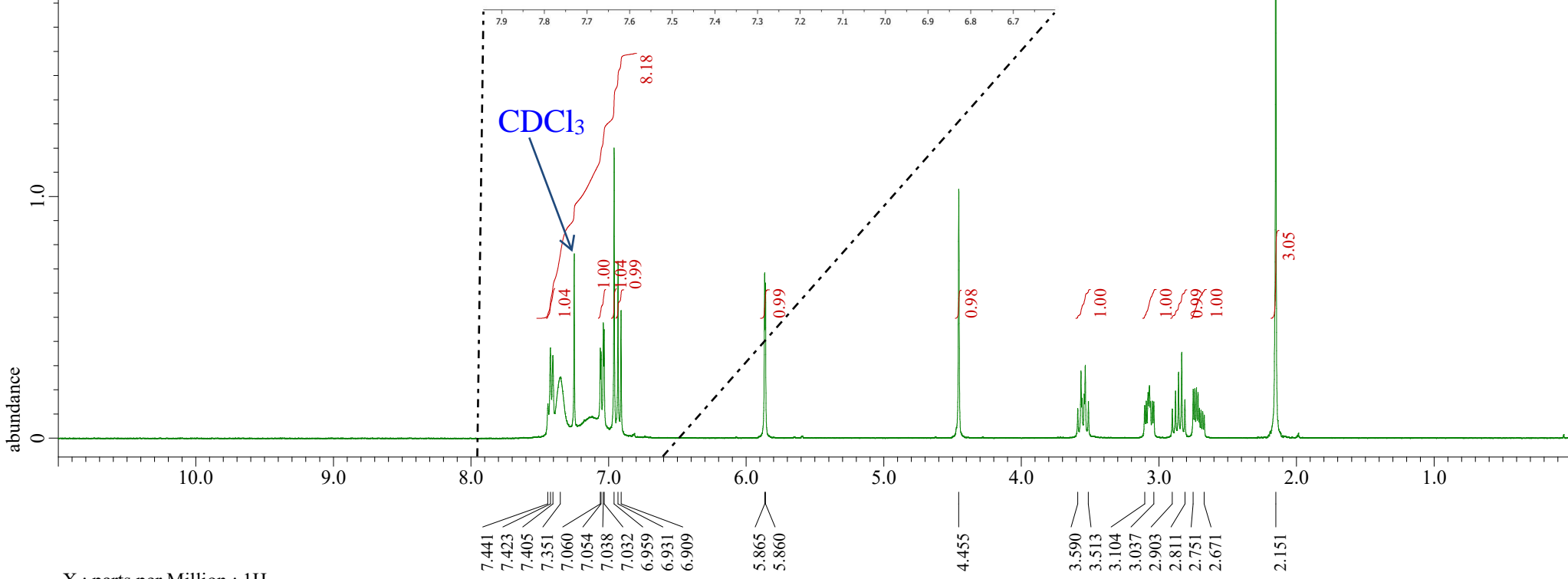
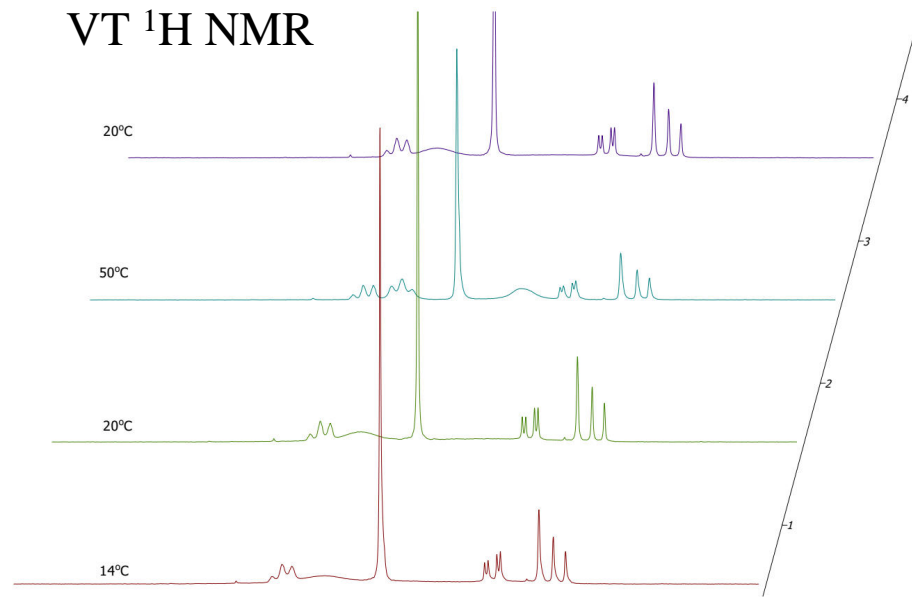




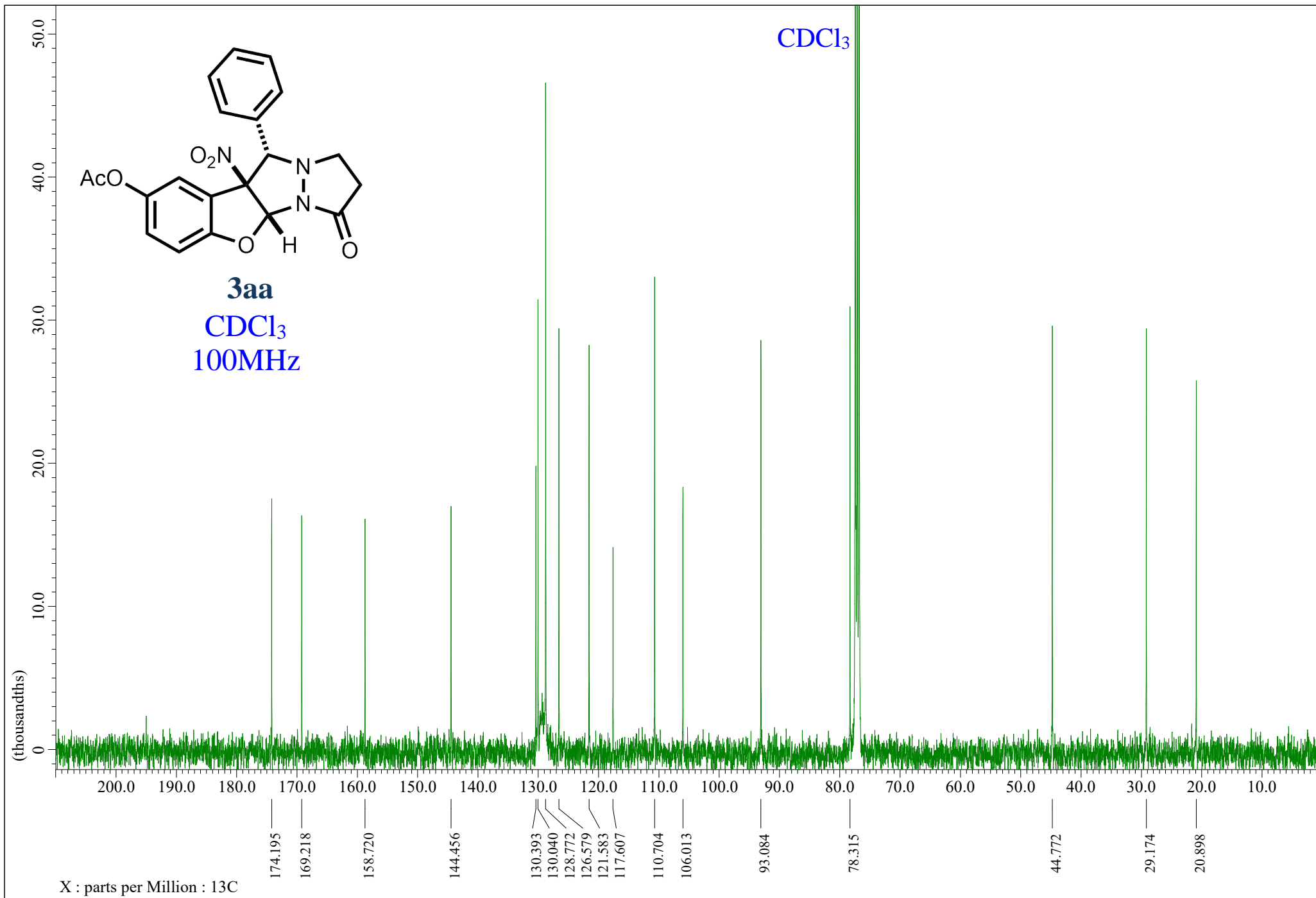
VT ¹H NMR

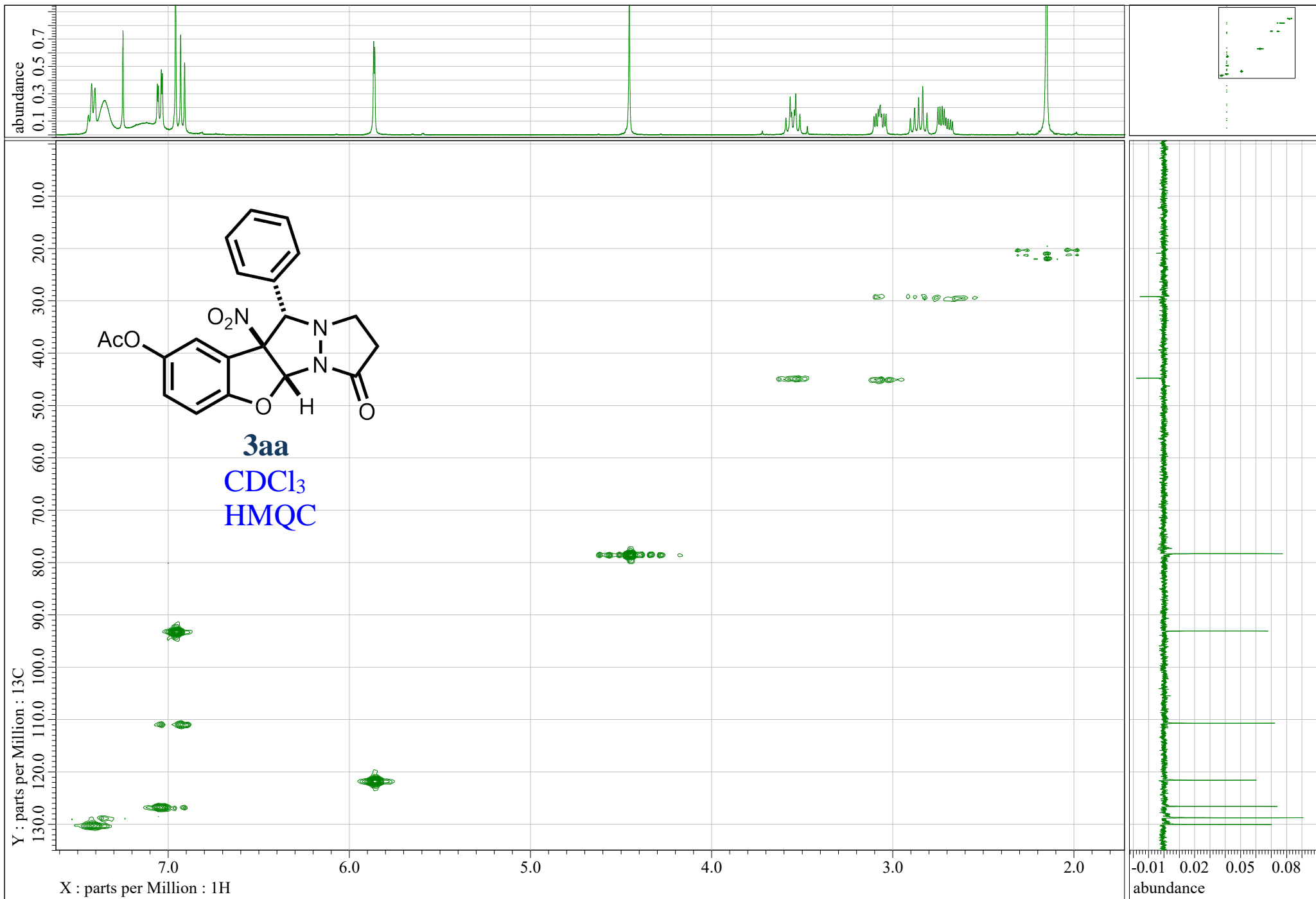


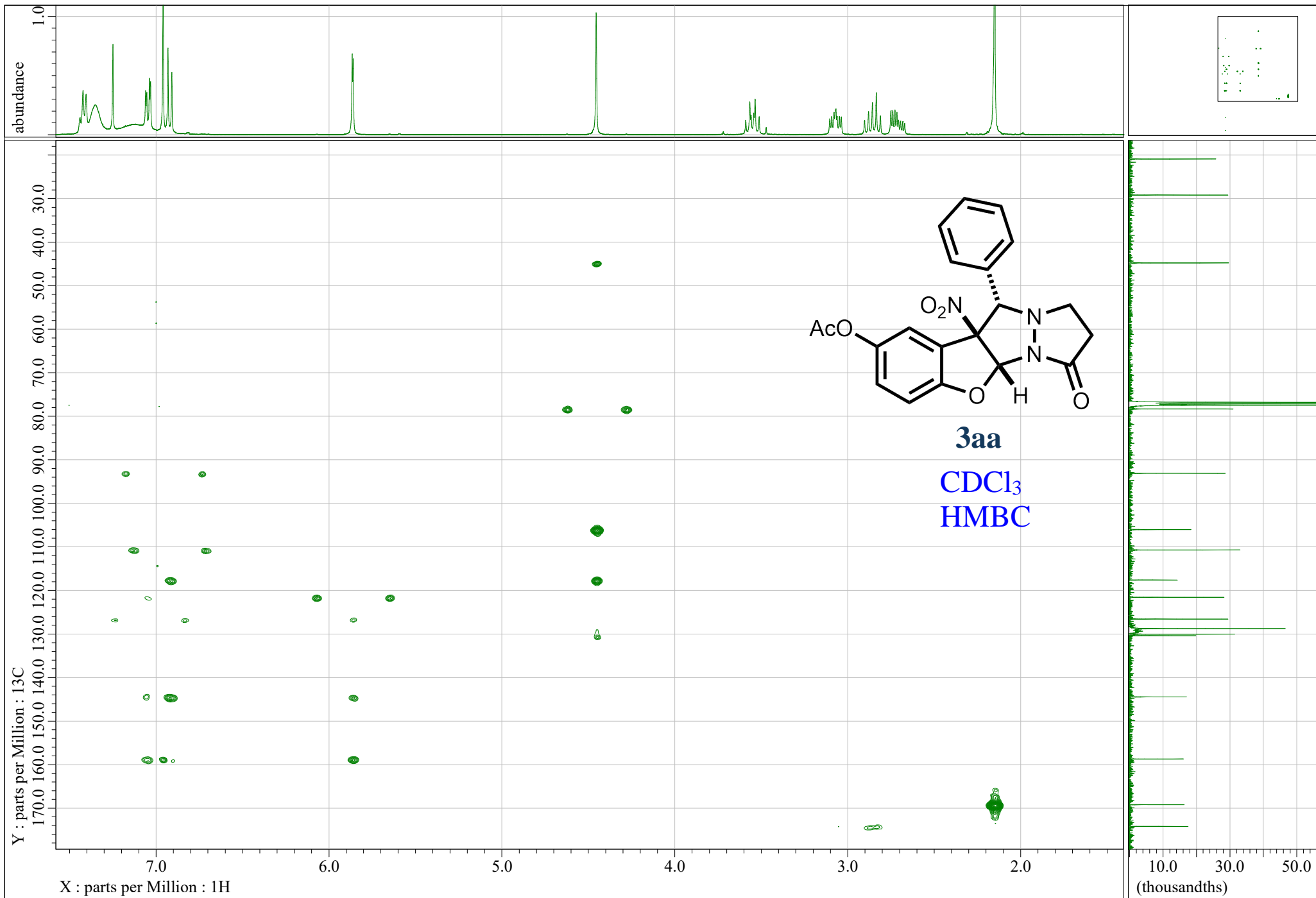
3aa
CDCl₃
400MHz

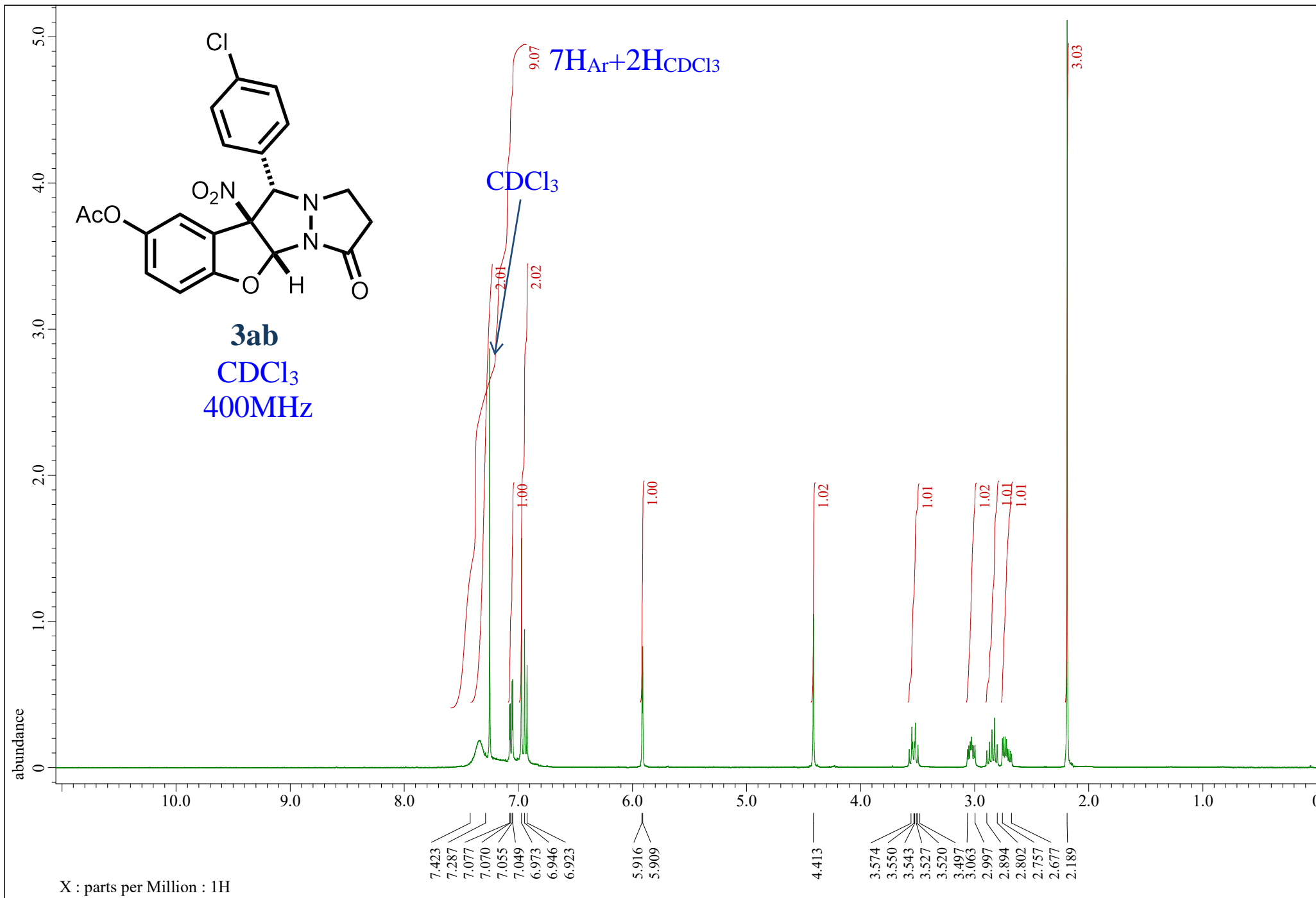


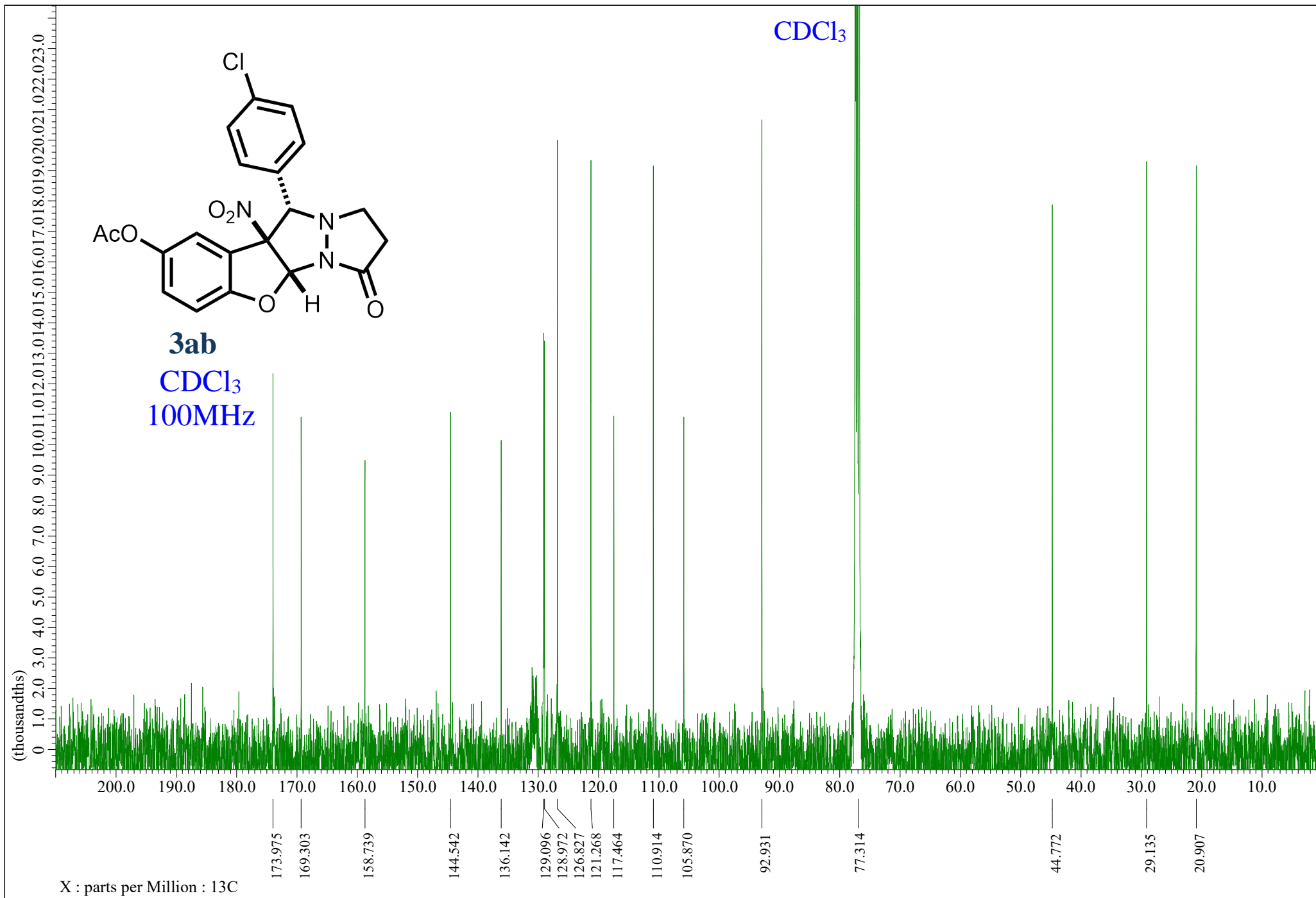
X : parts per Million : ¹H

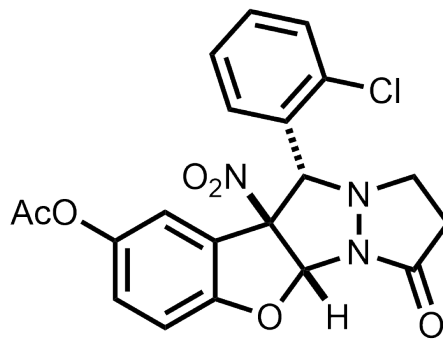




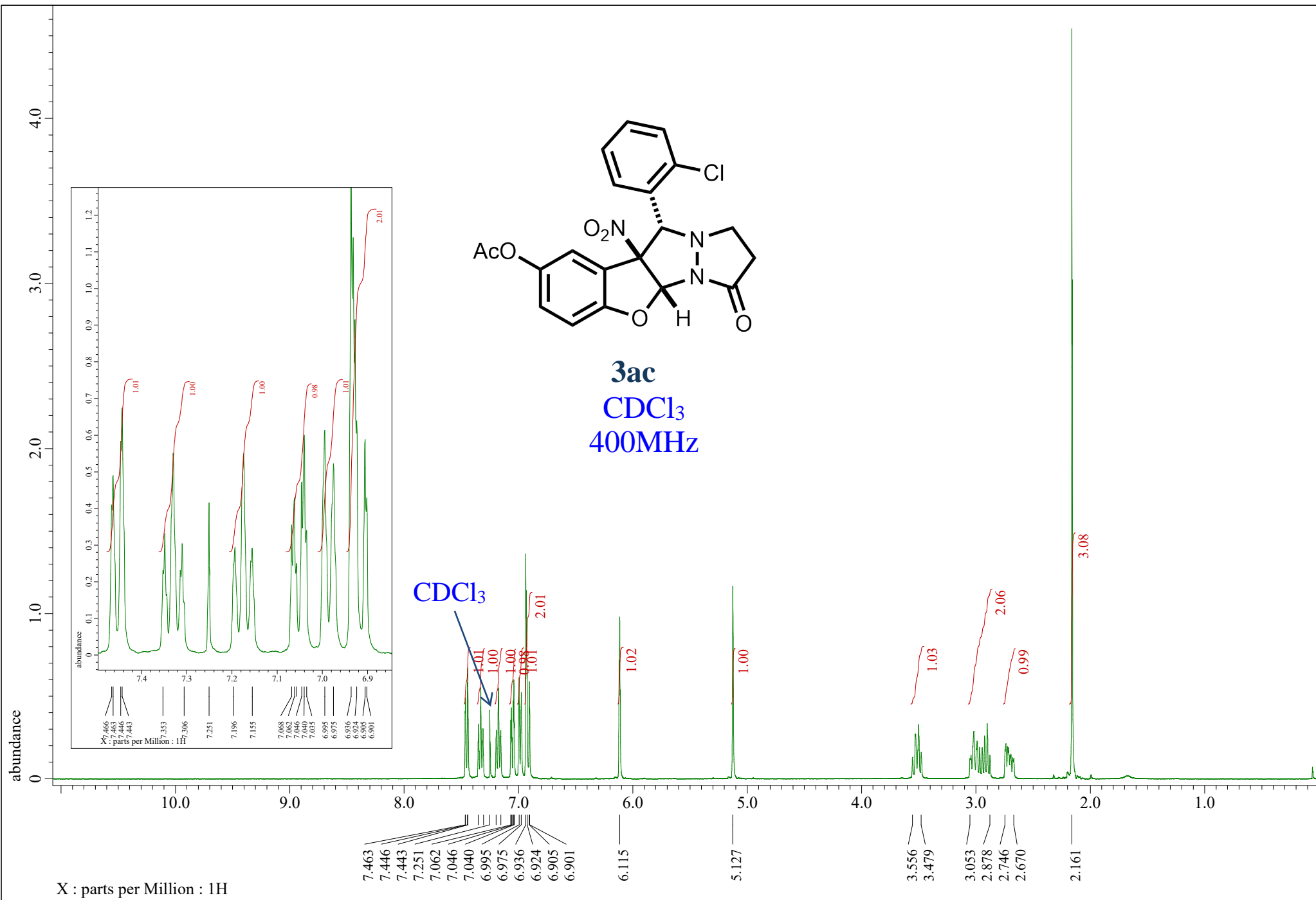


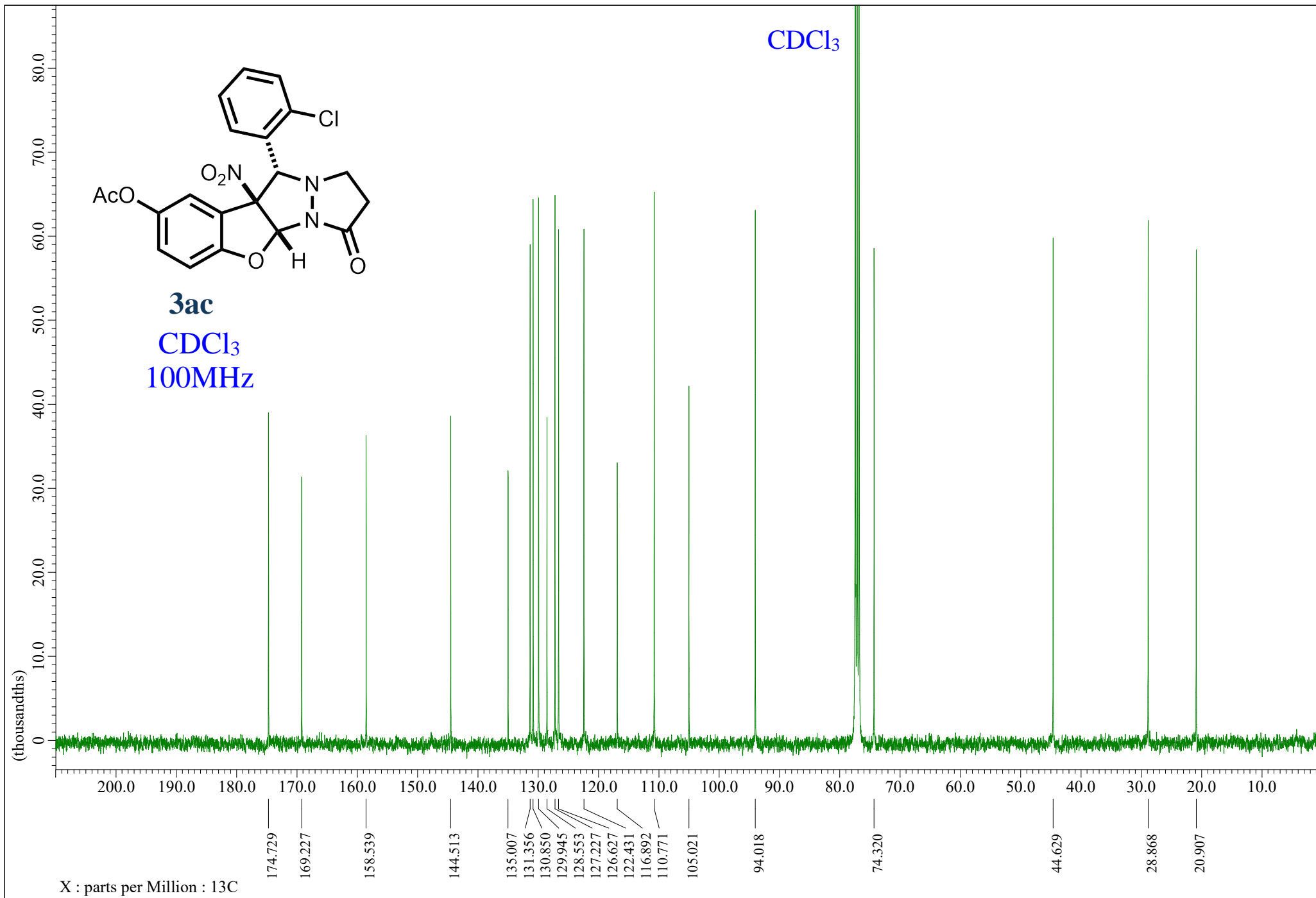


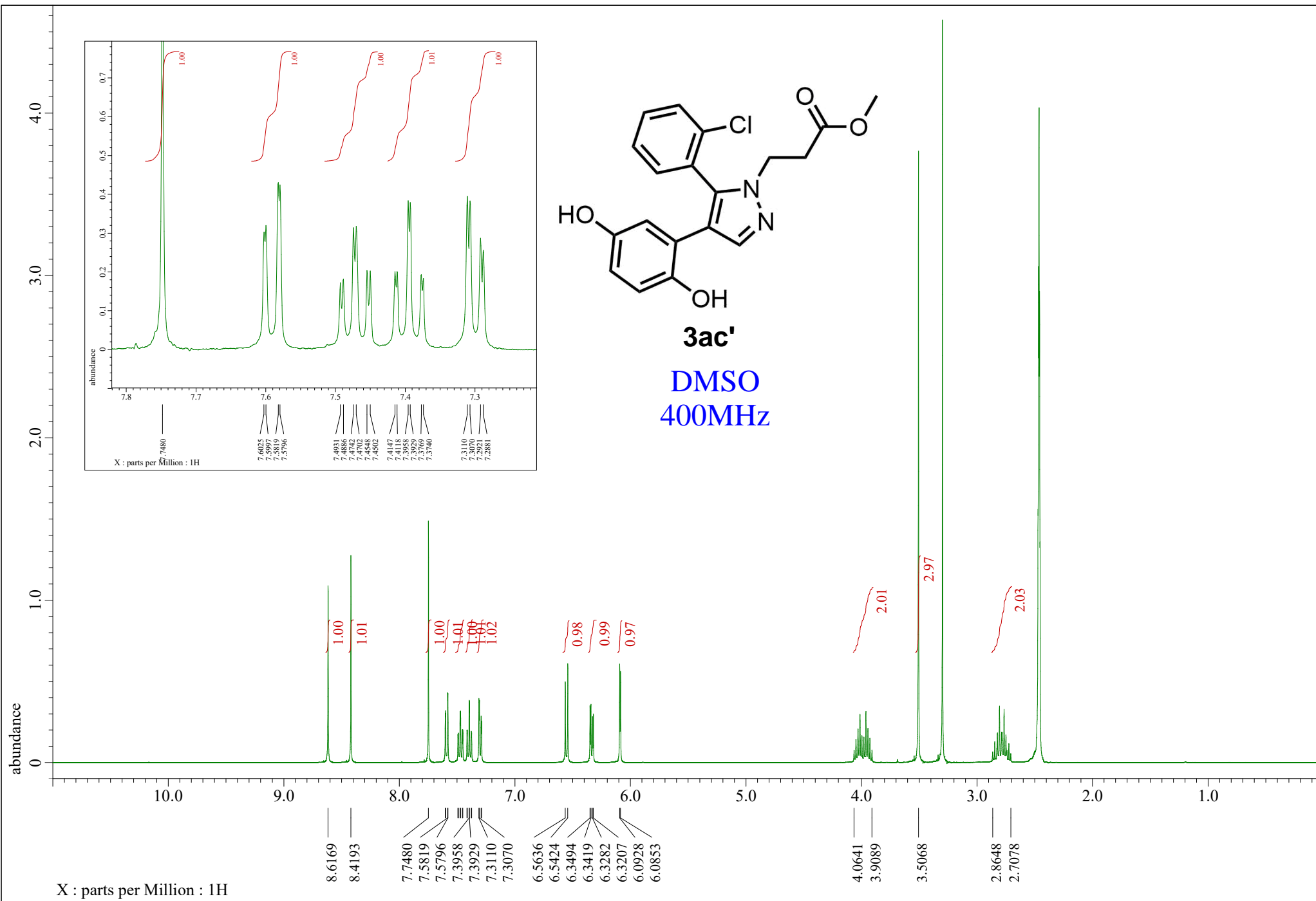


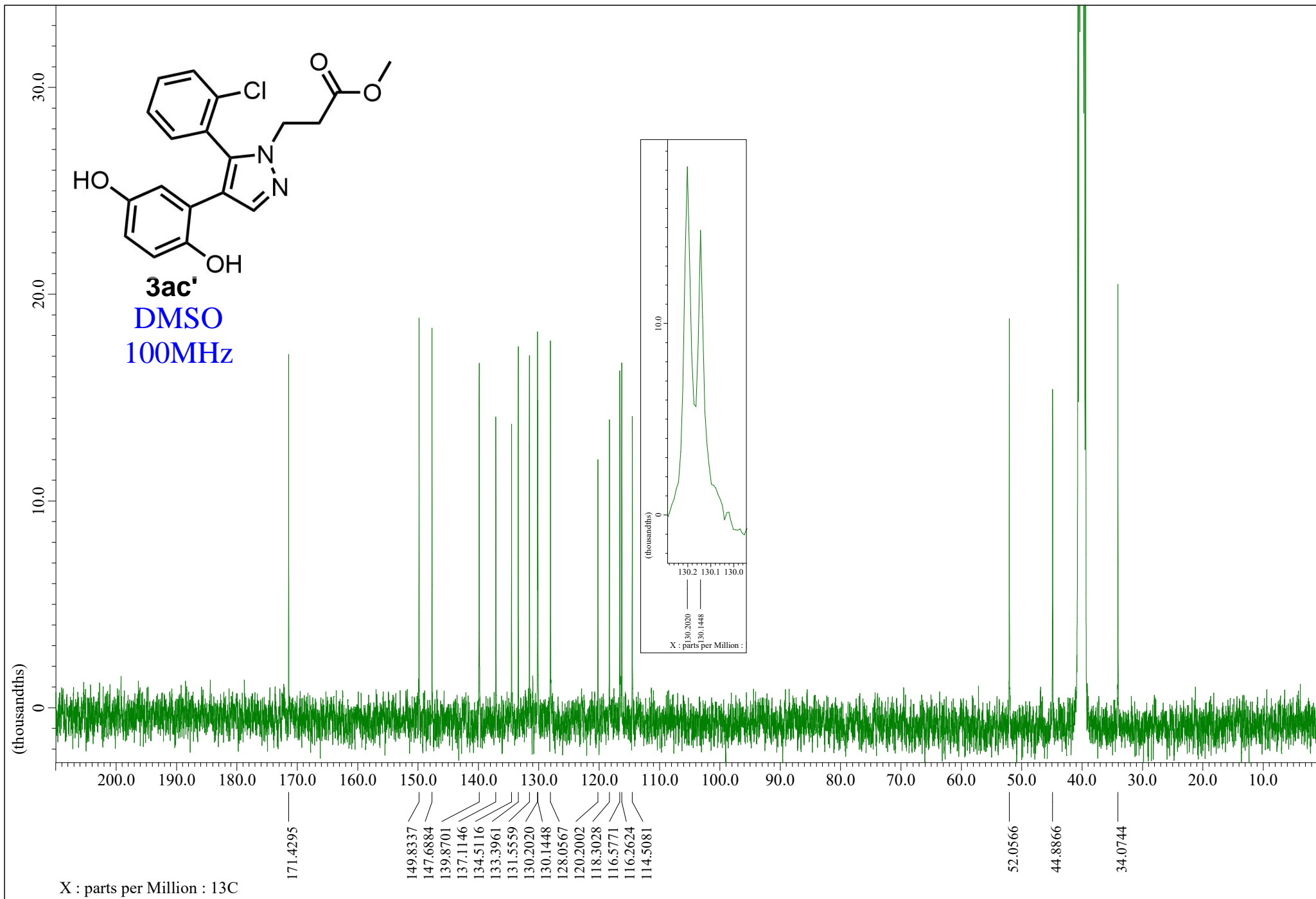


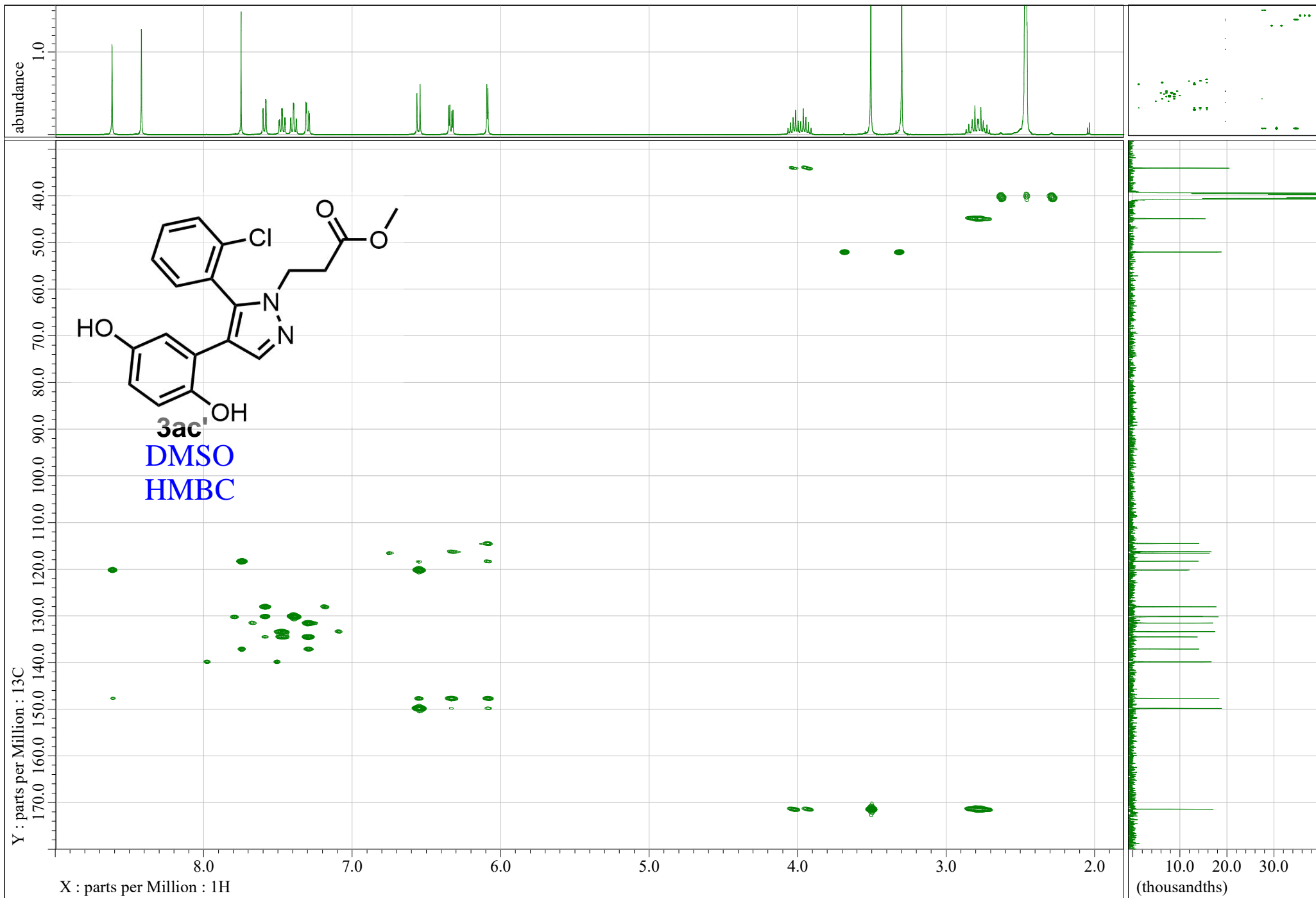
3ac
 CDCl₃
 400MHz

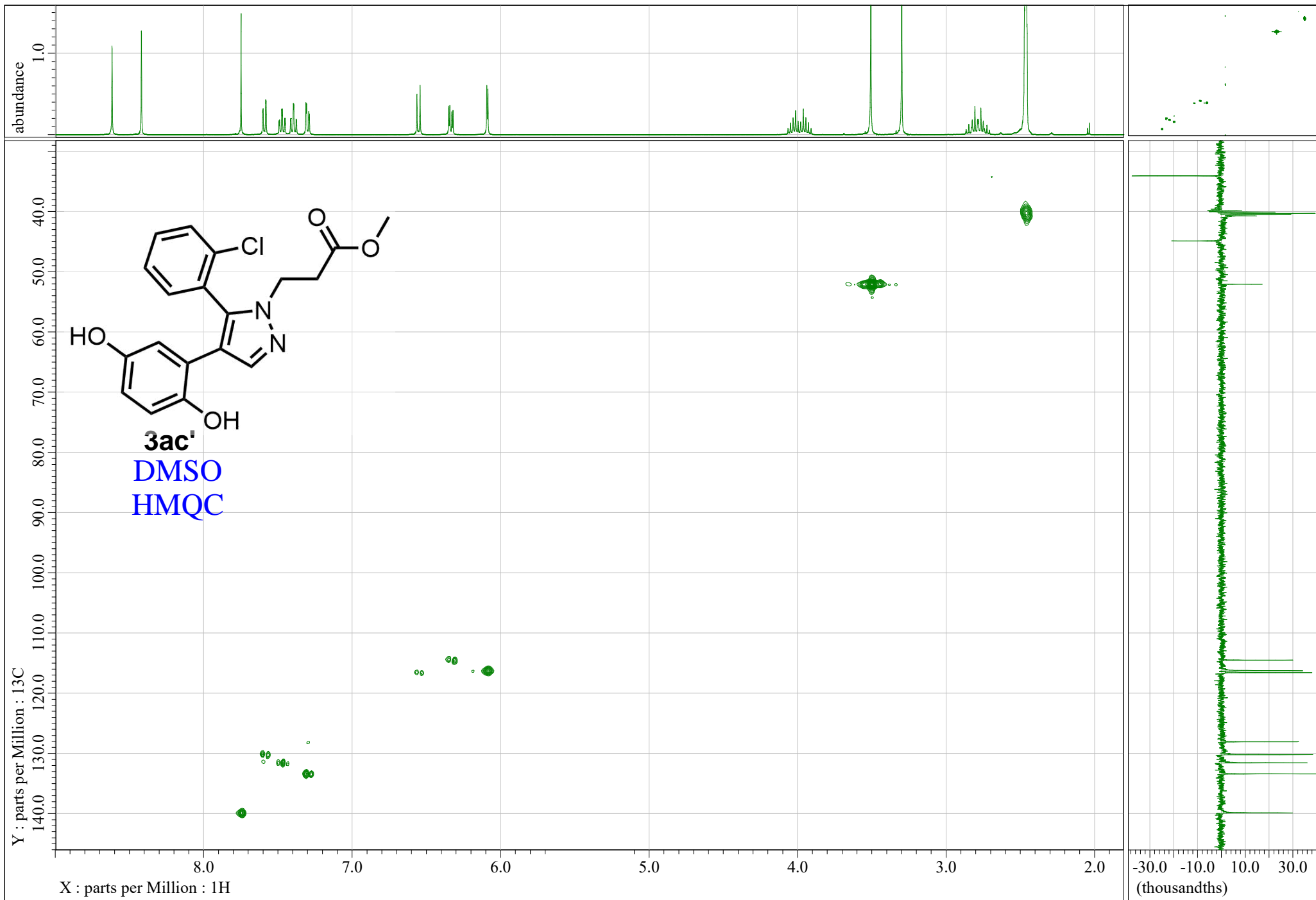


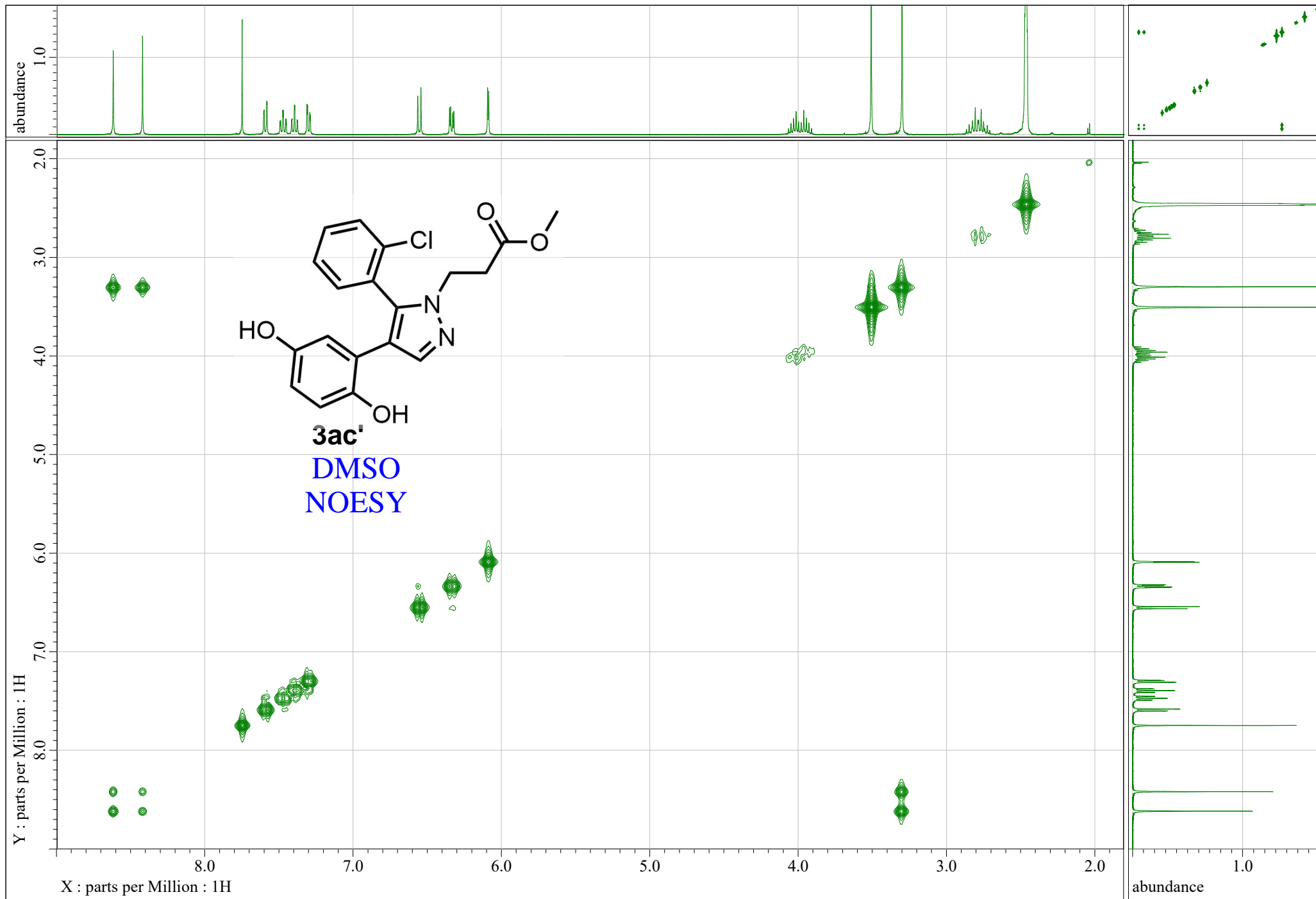


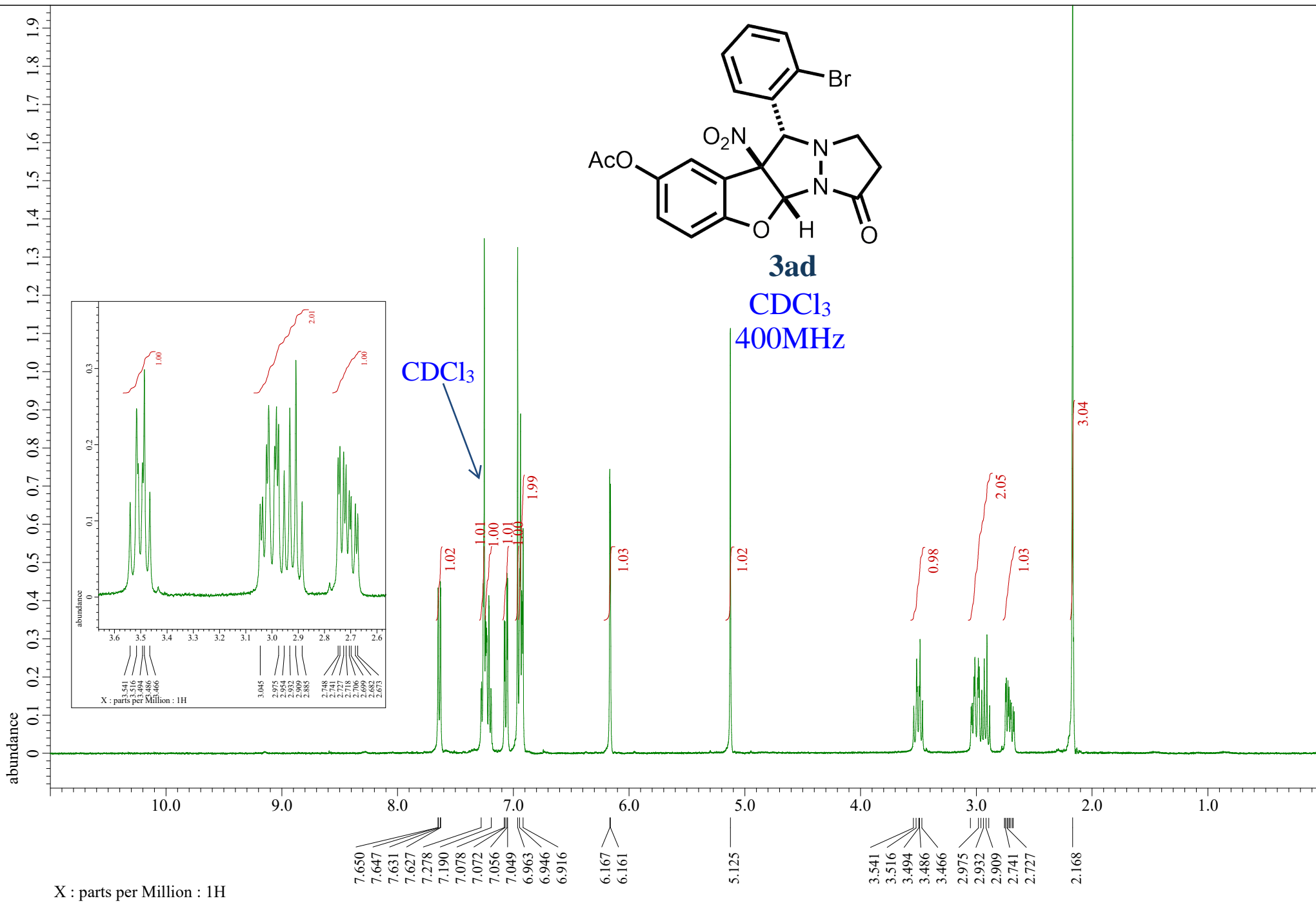


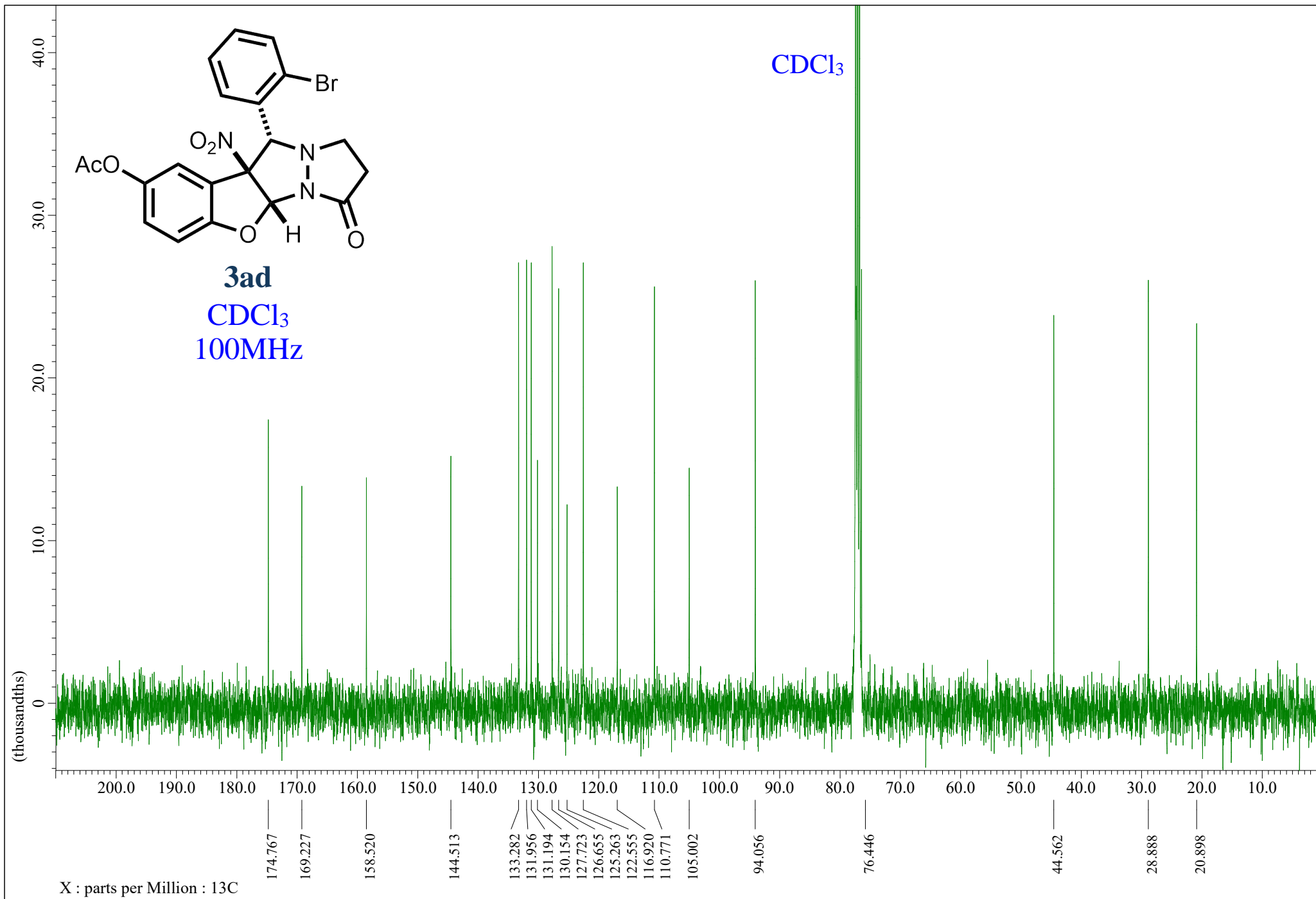


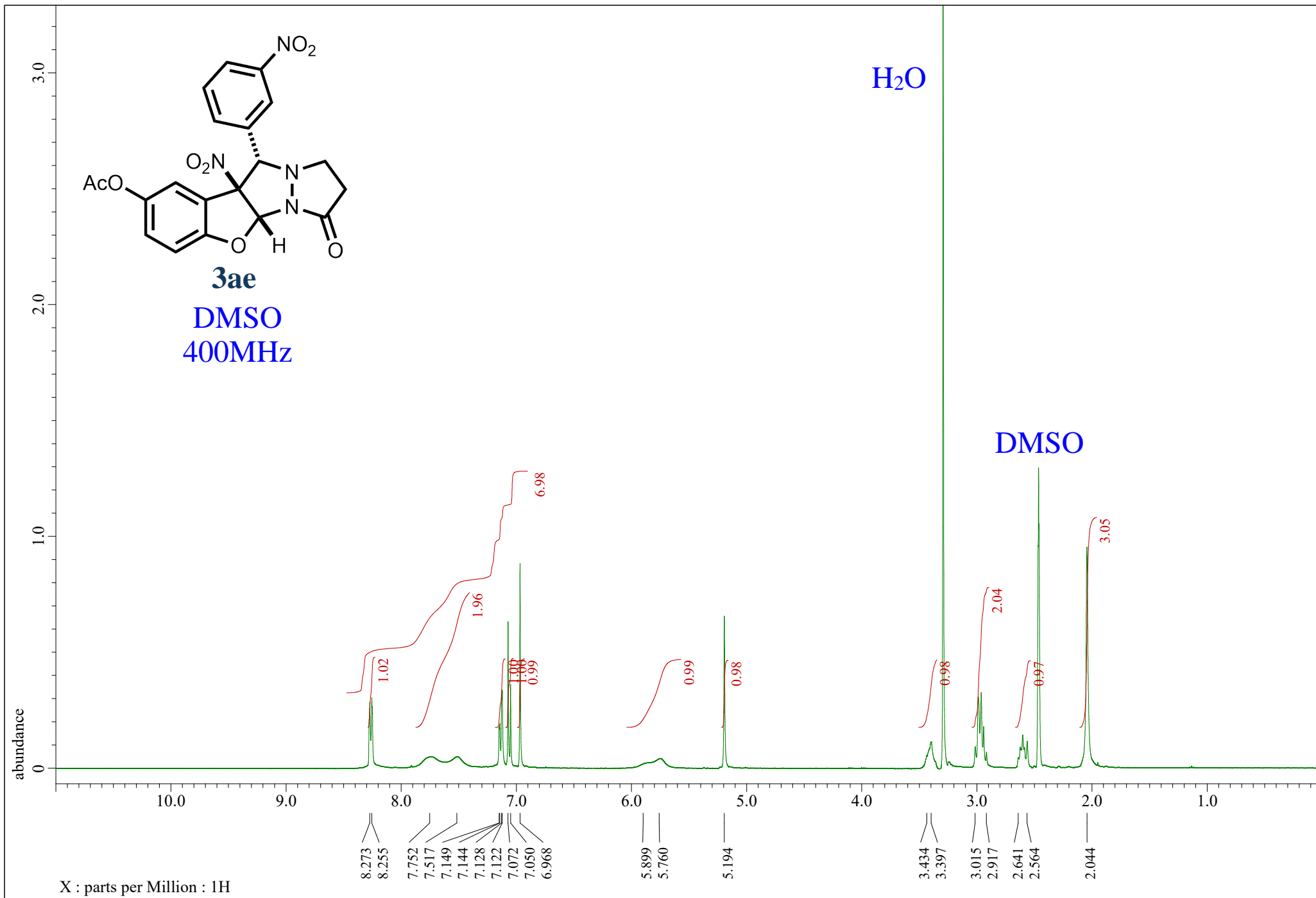


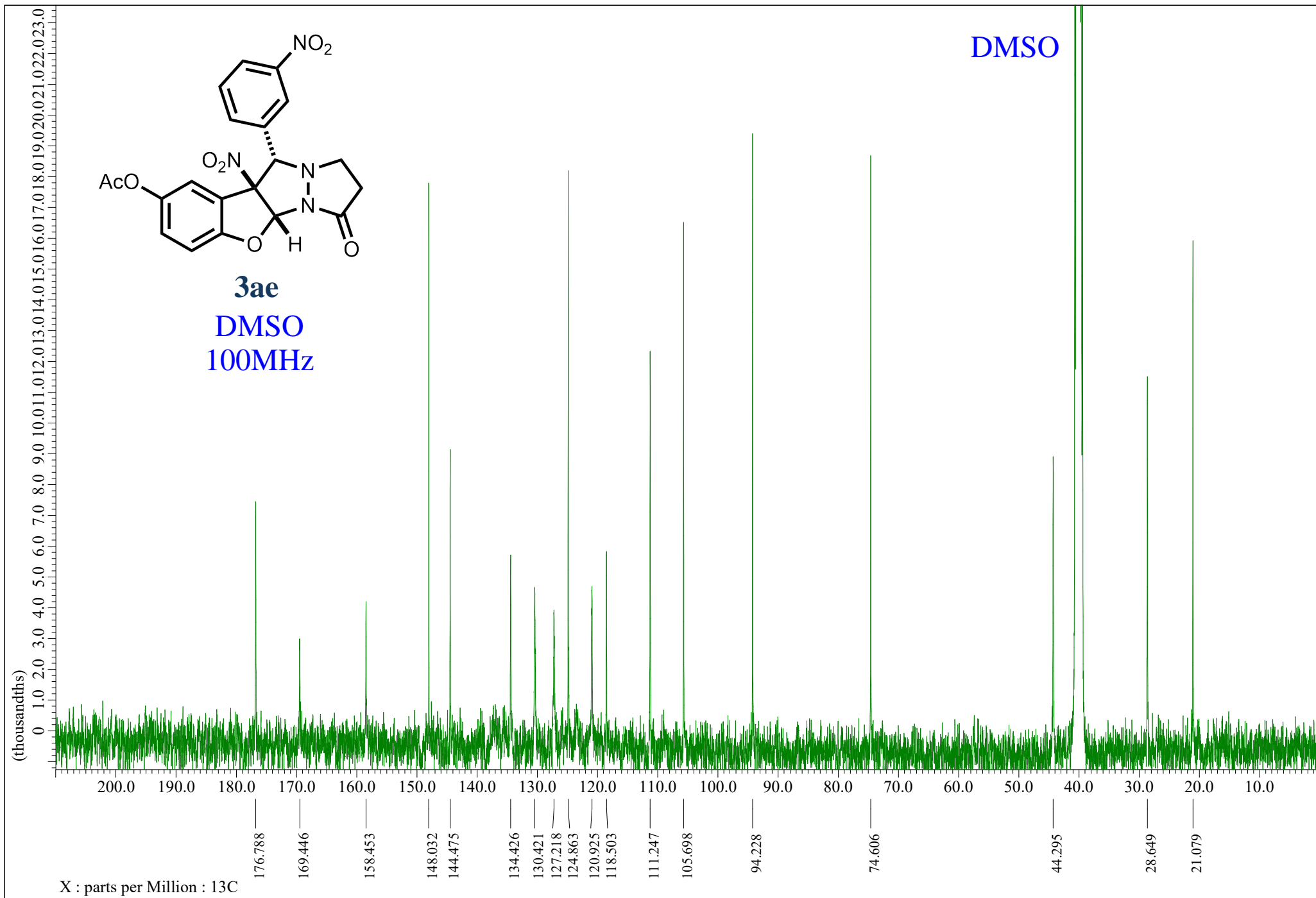


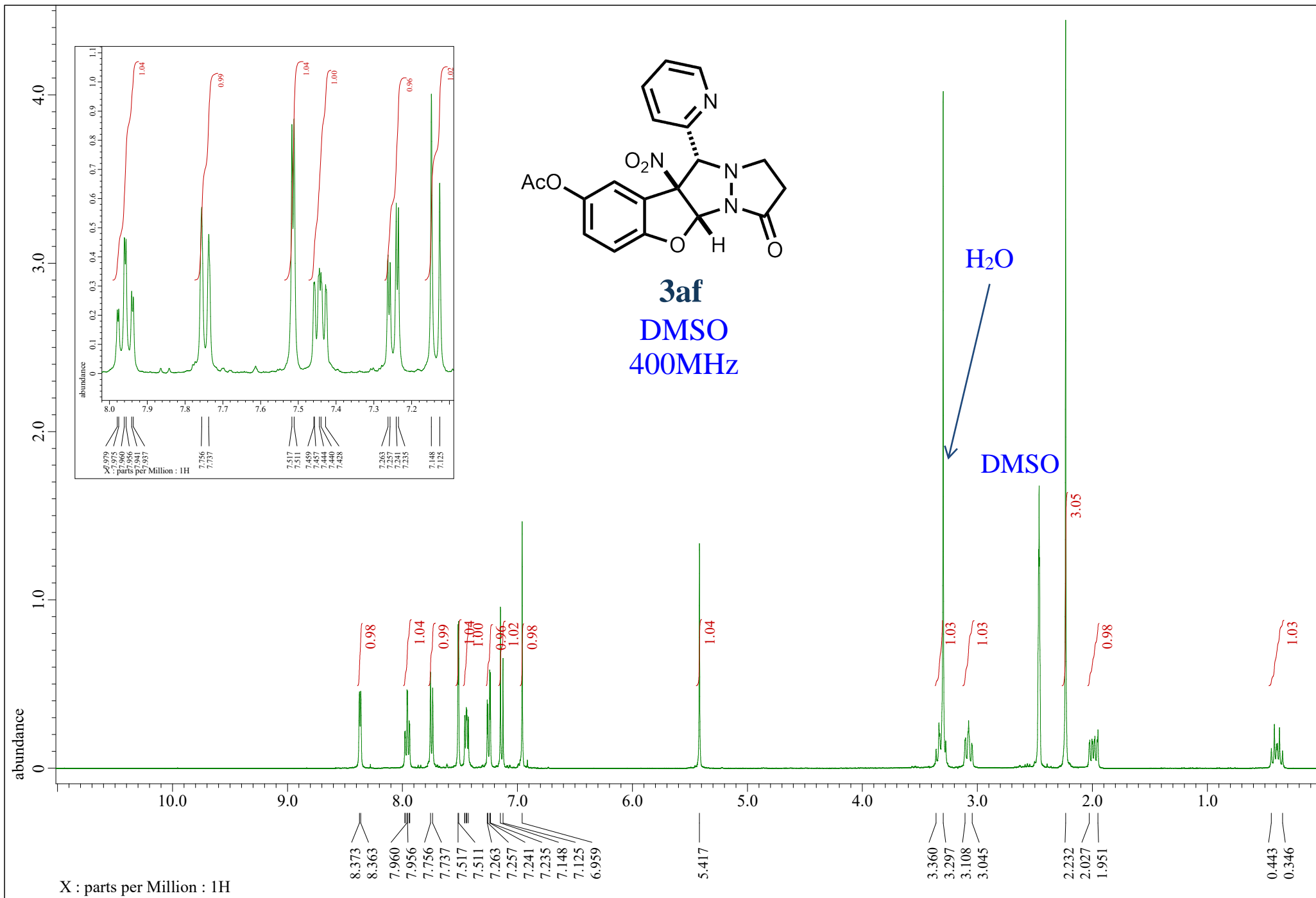


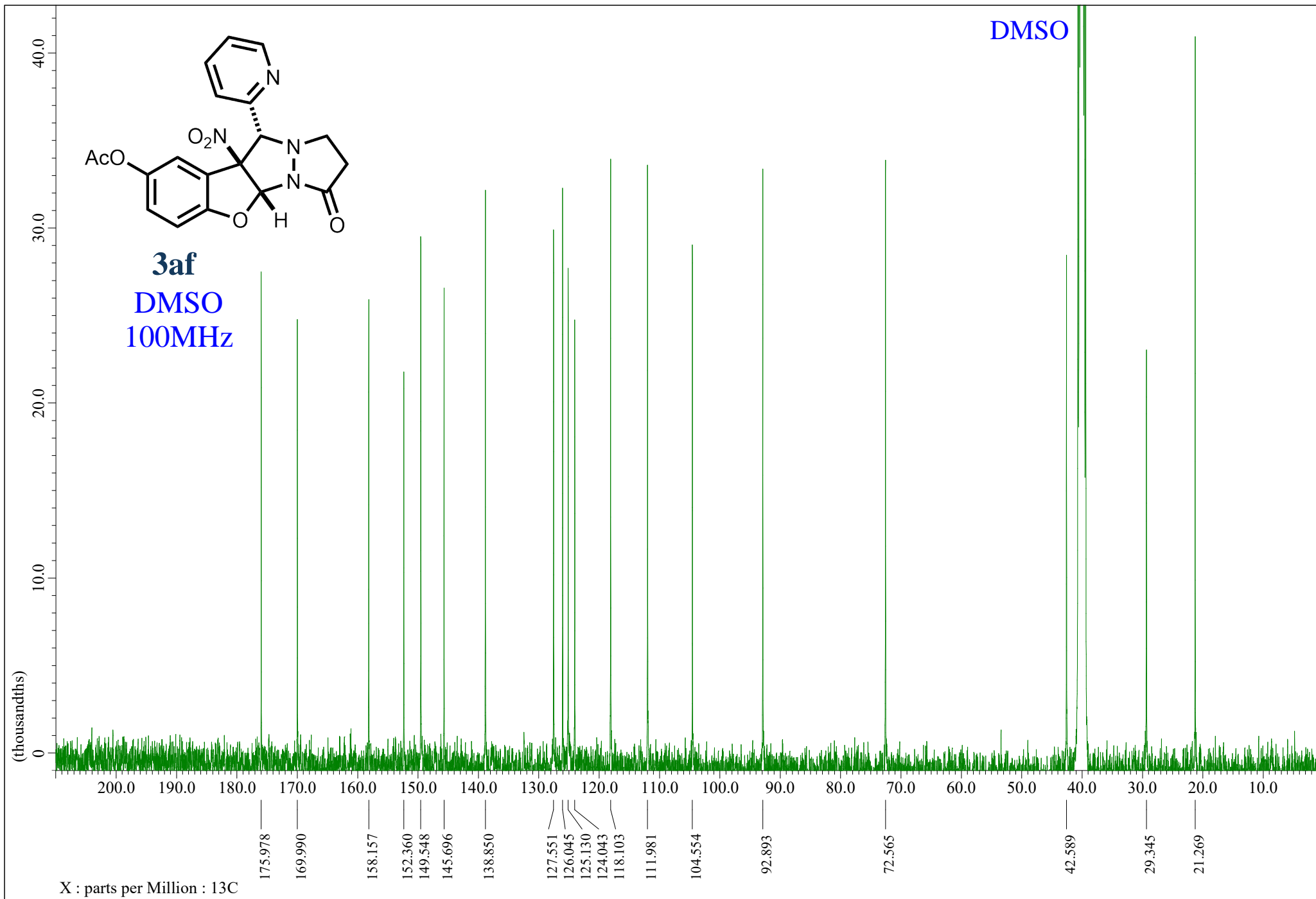


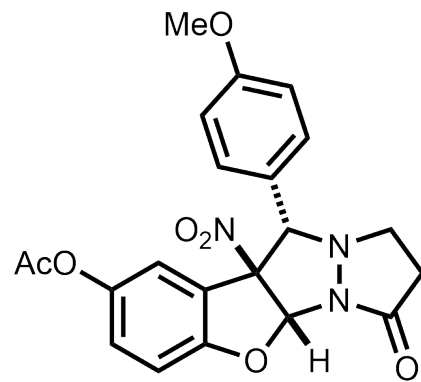








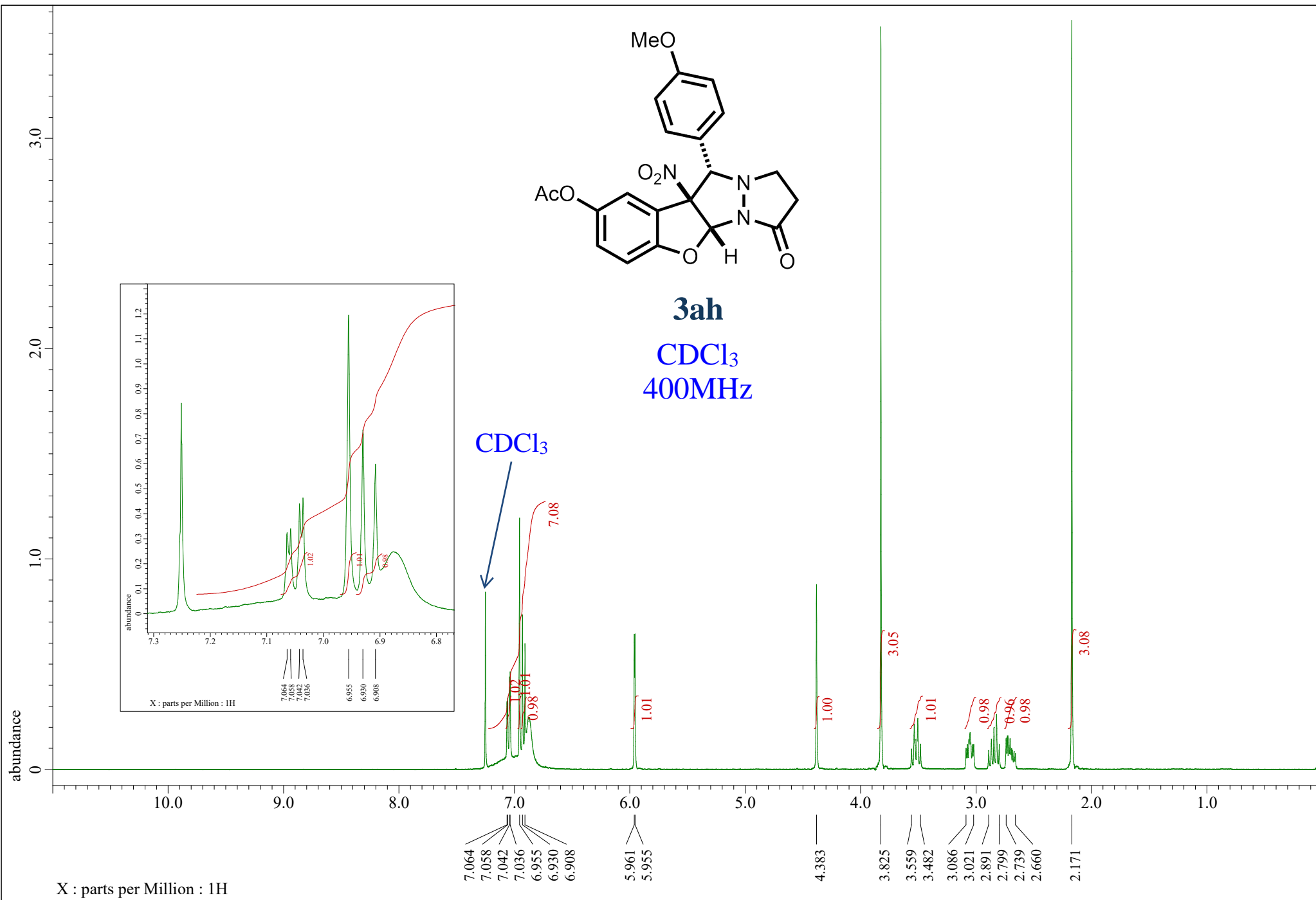


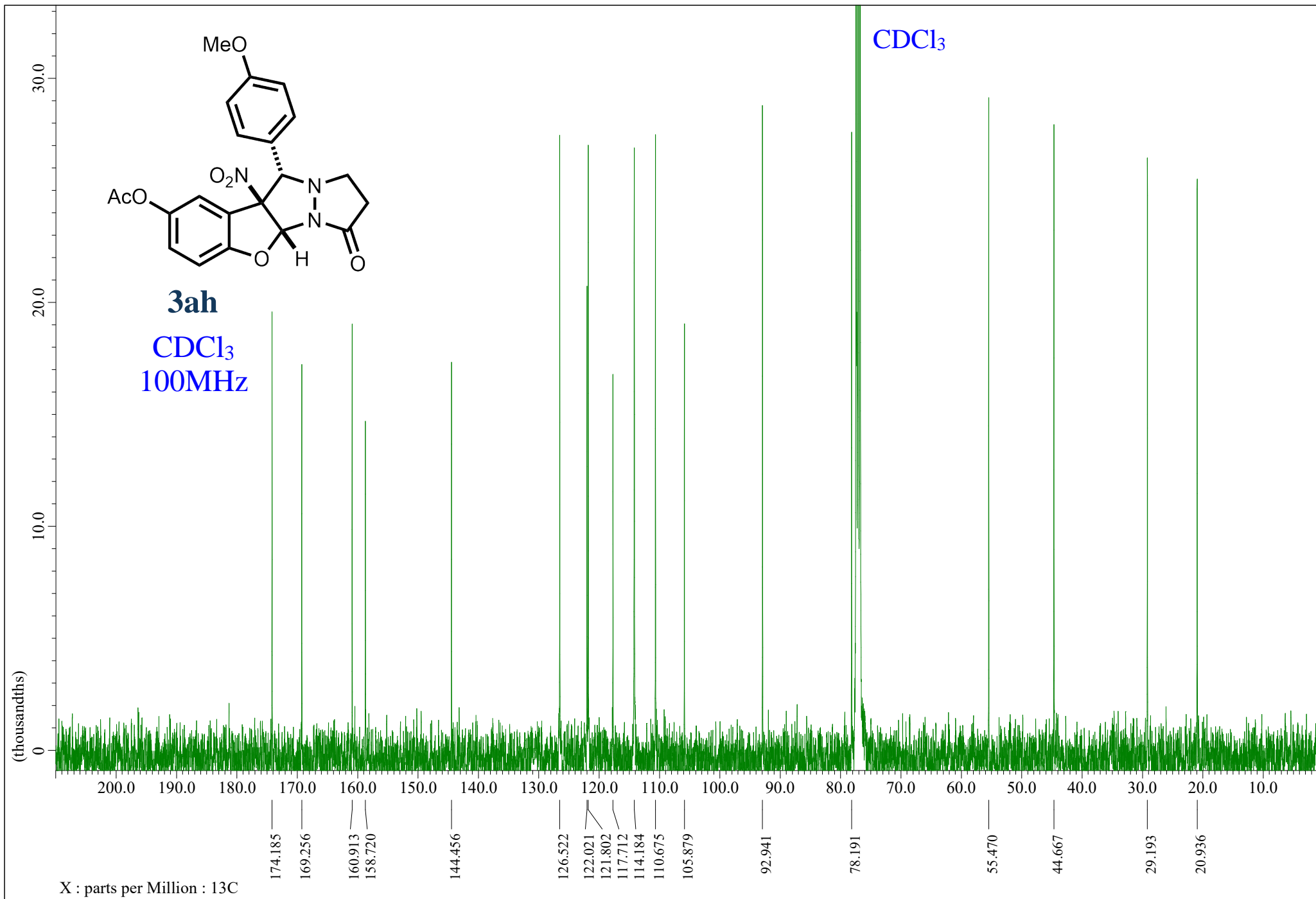


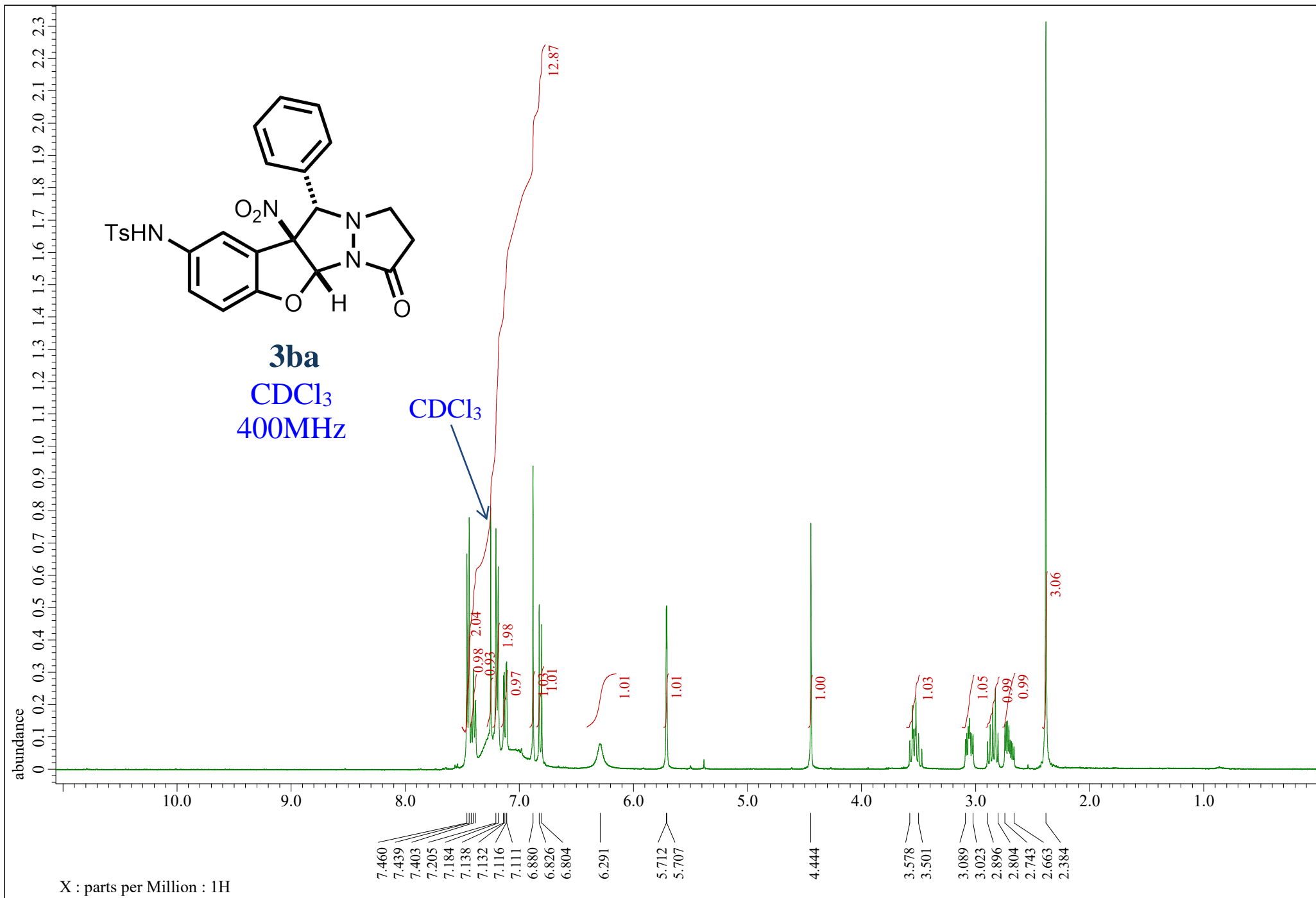
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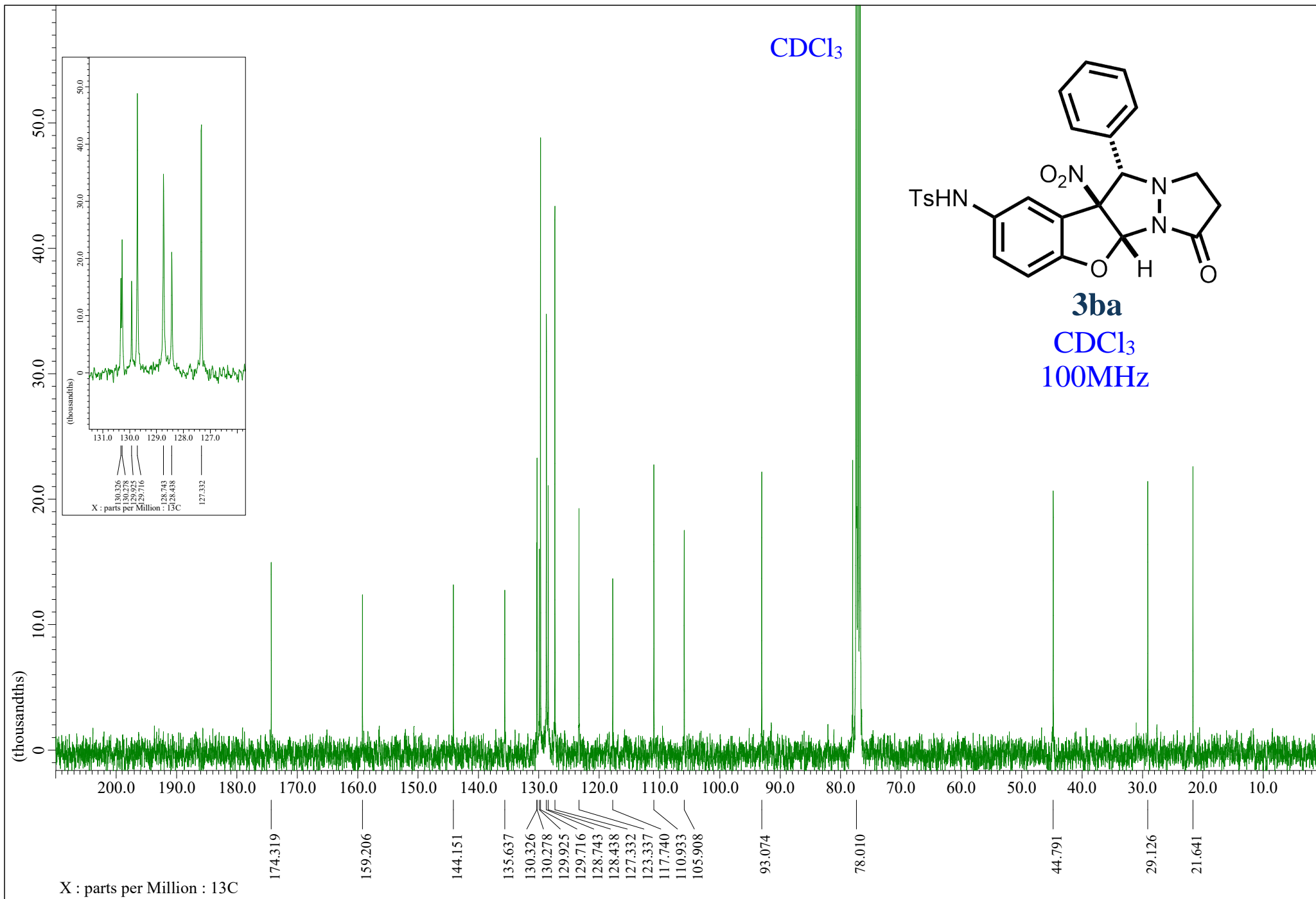
CDCl₃
400MHz

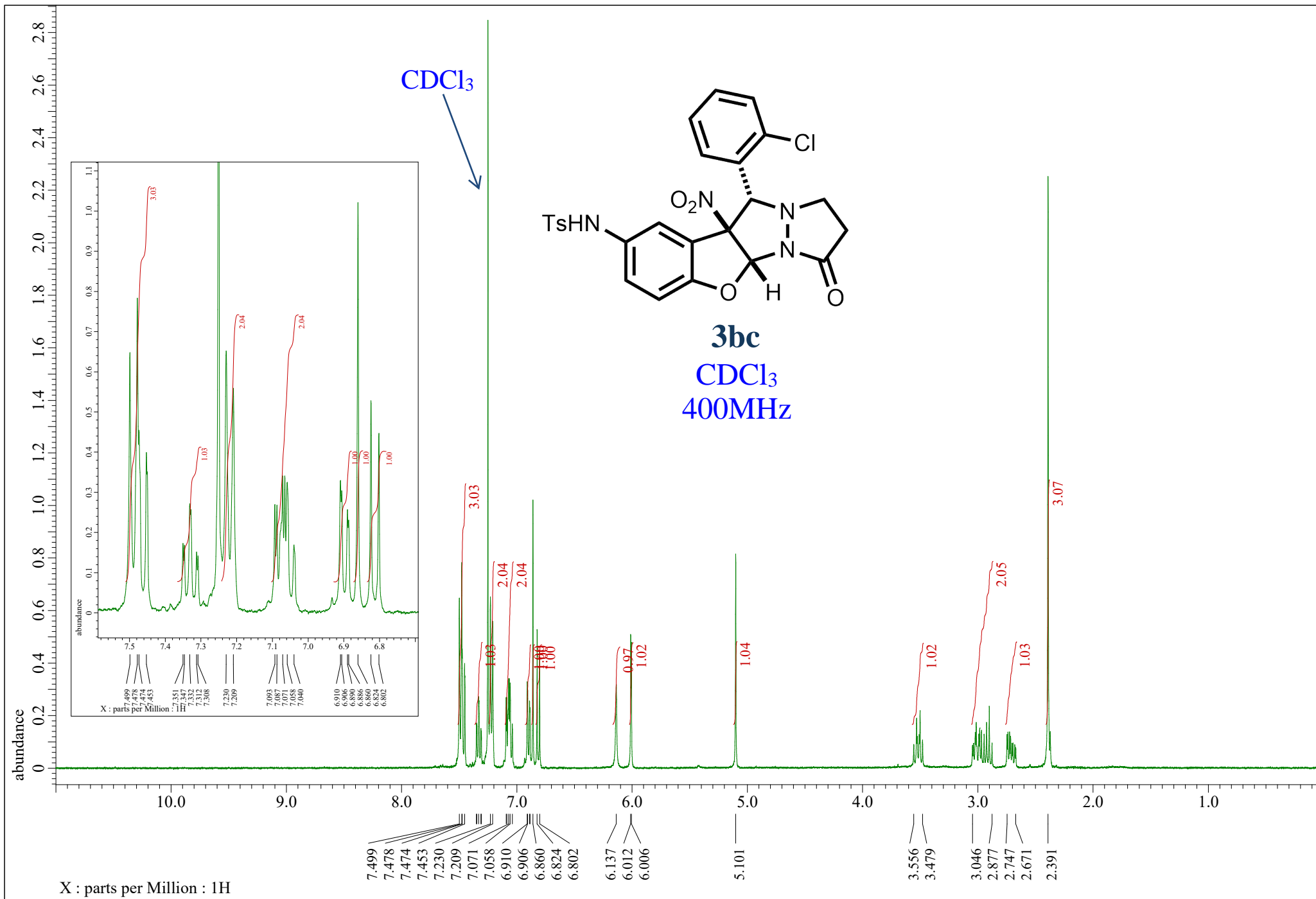
CDCl₃

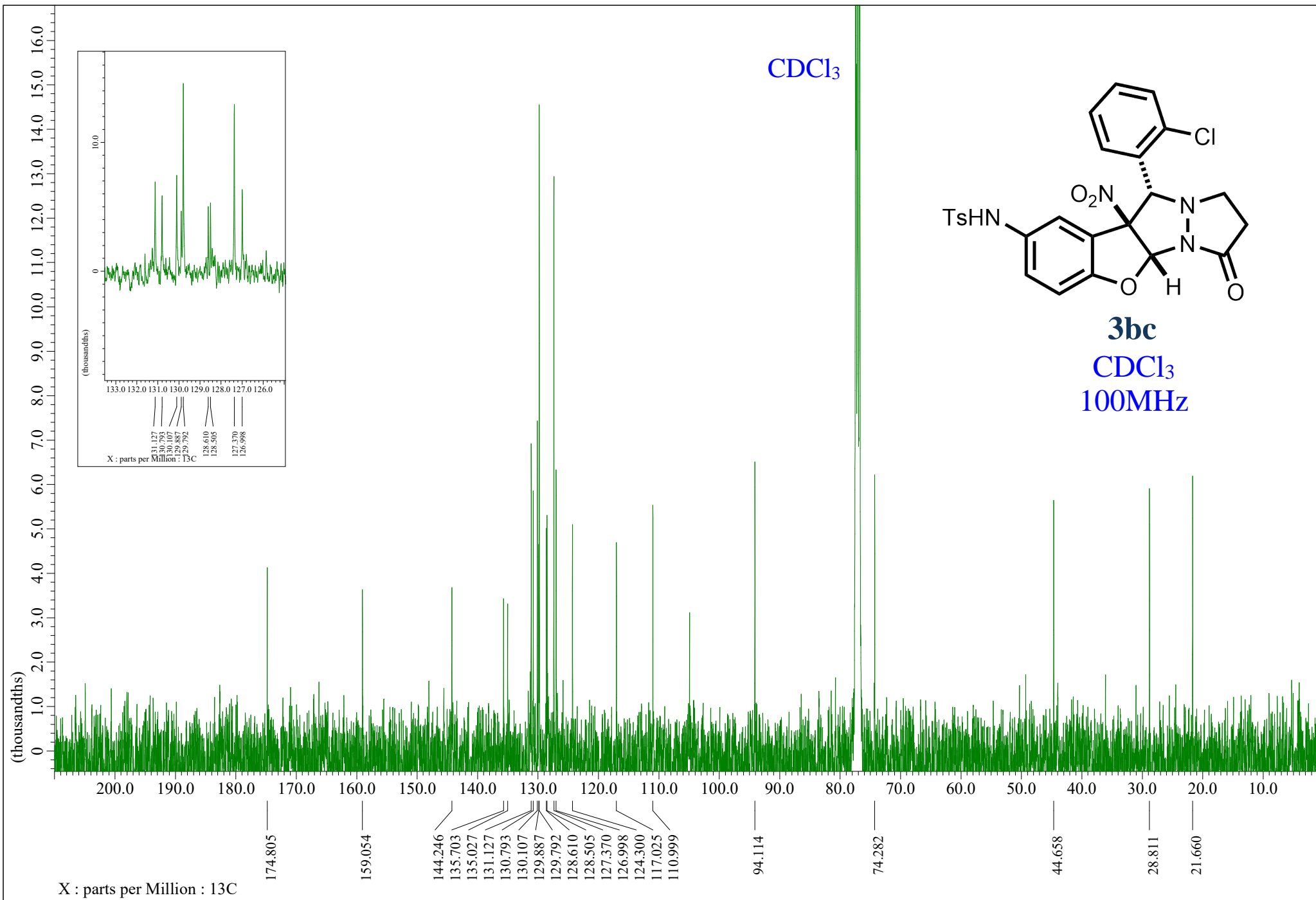


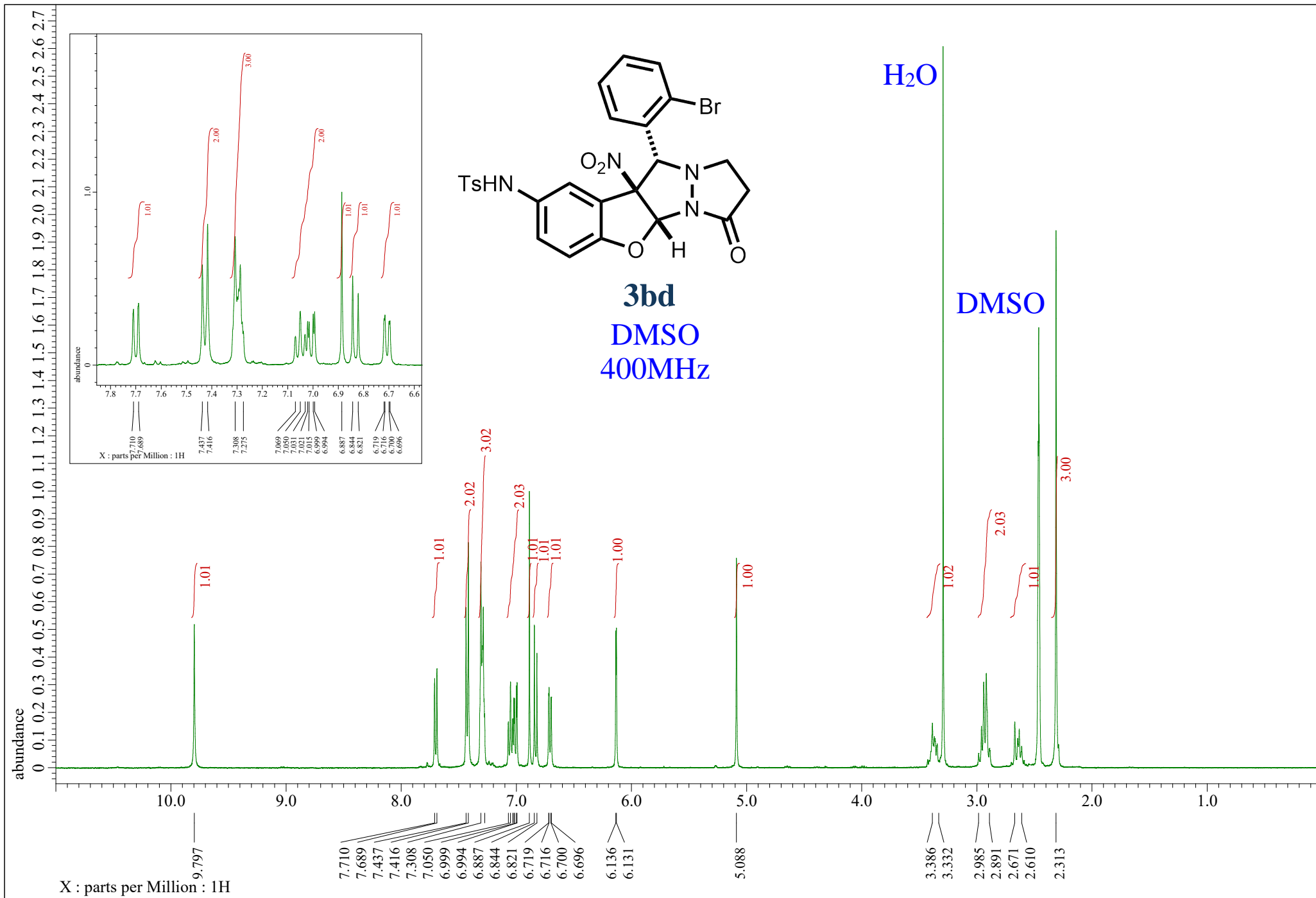


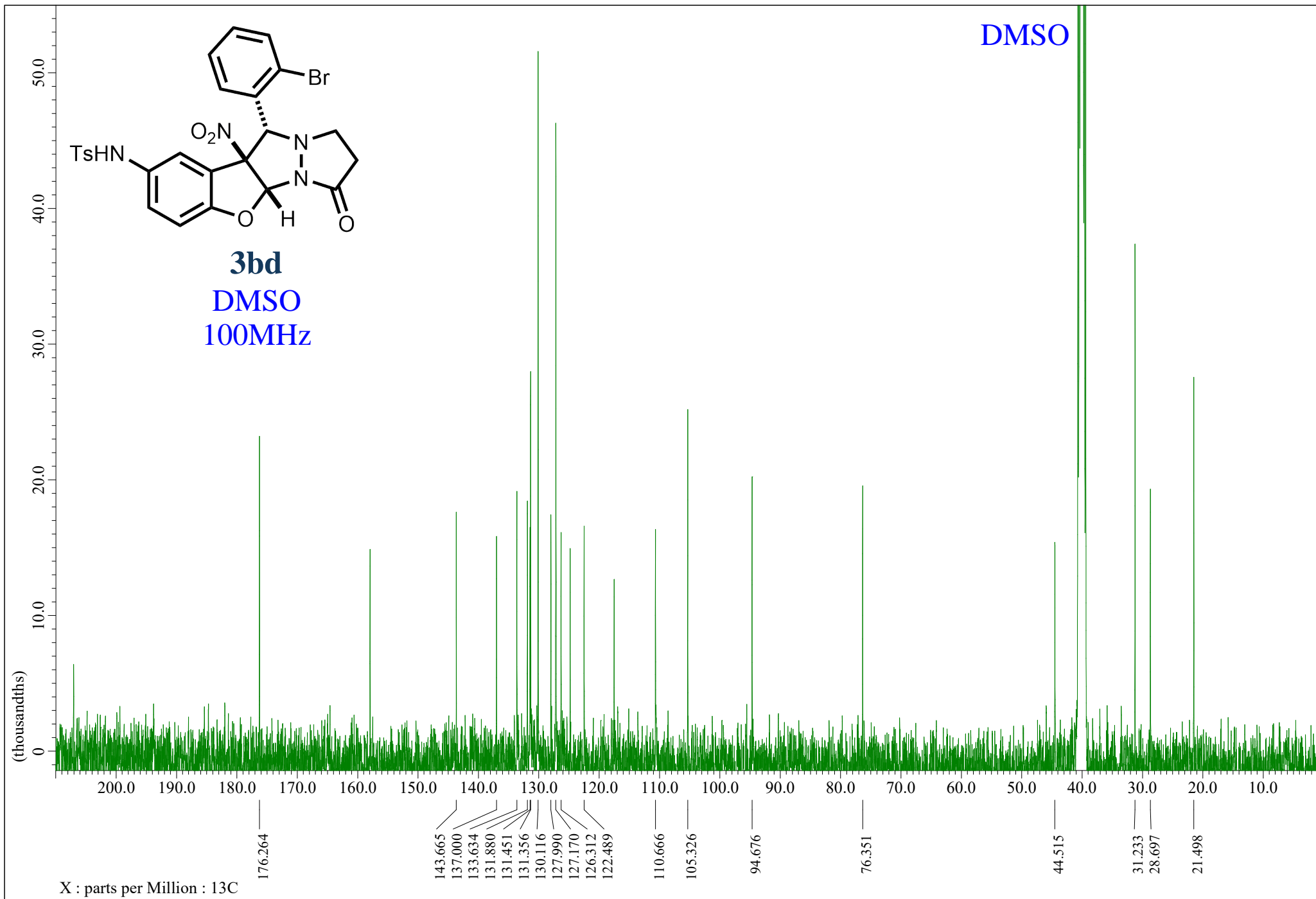


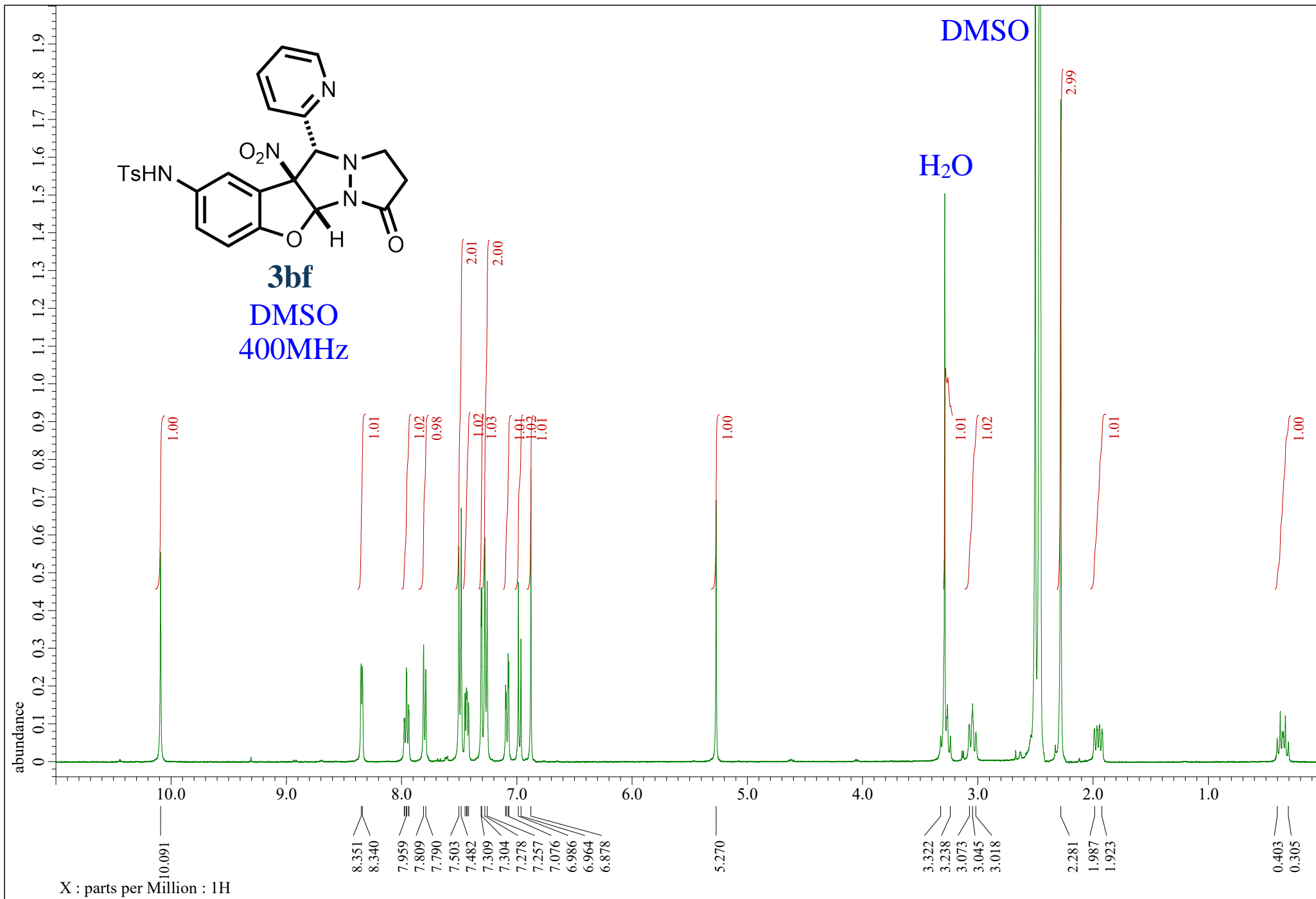


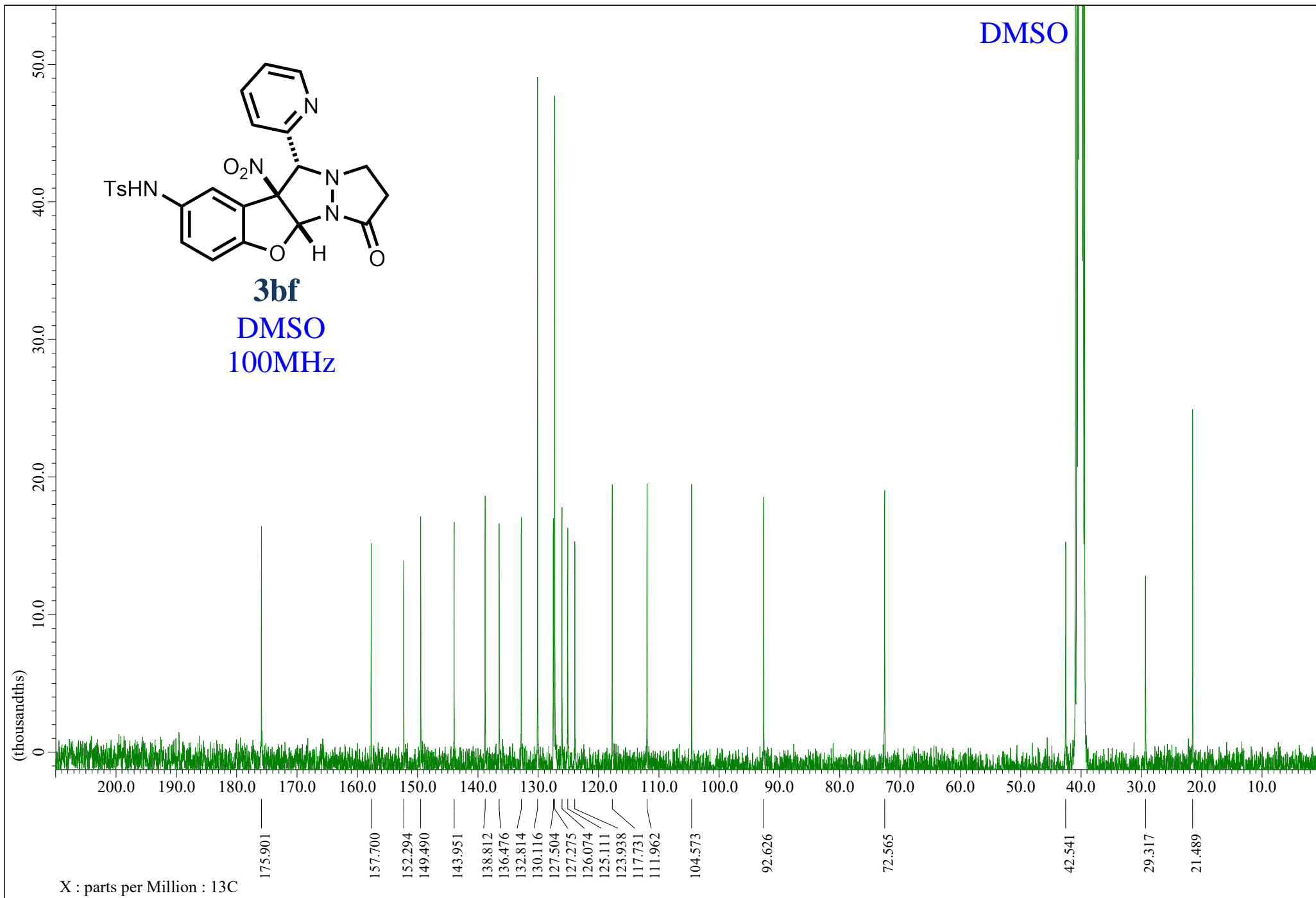


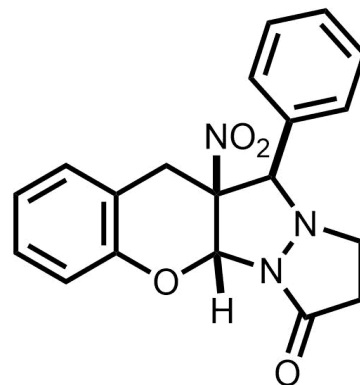




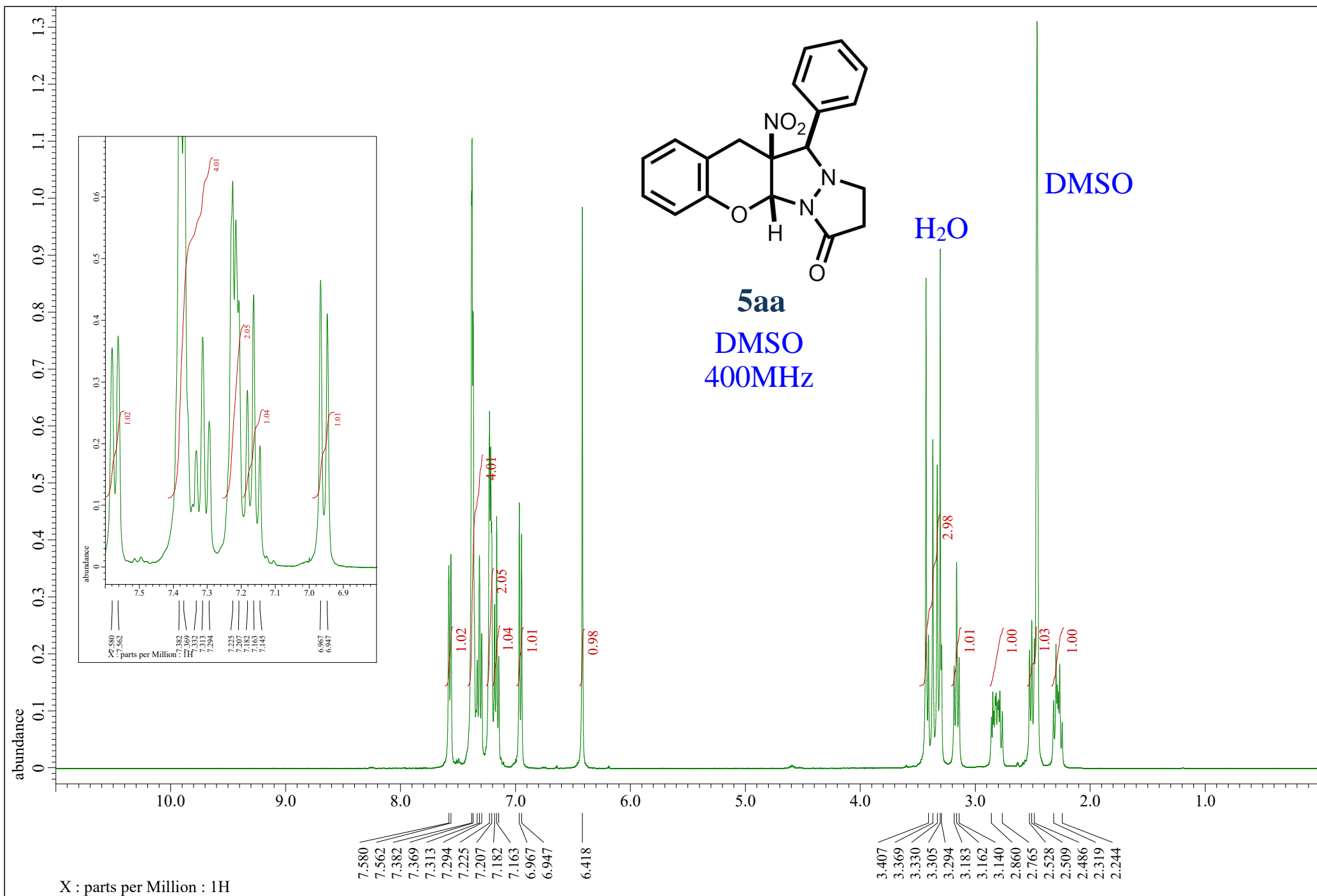




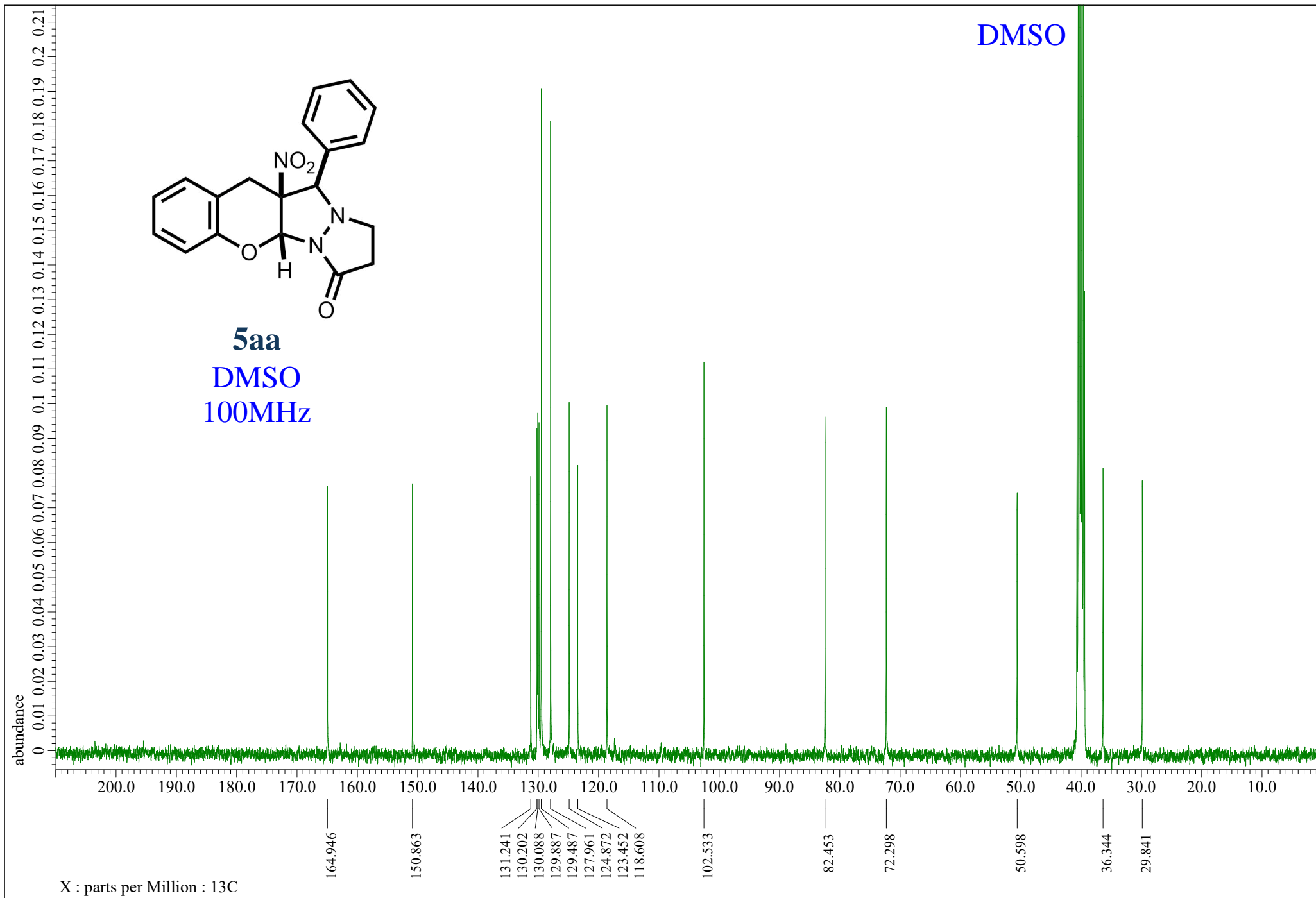


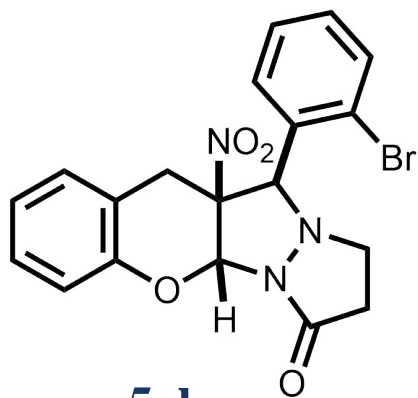


5aa
DMSO
400MHz

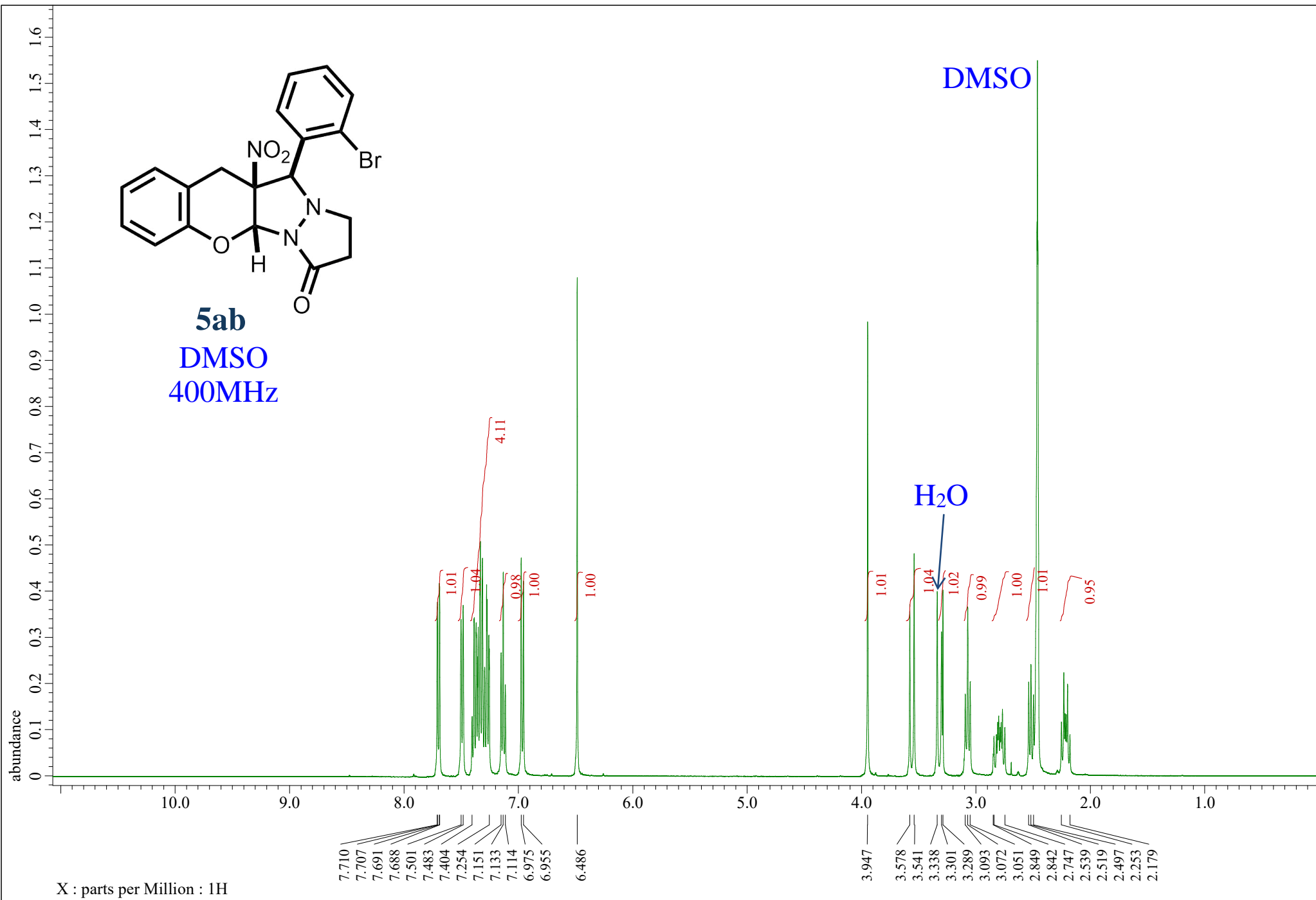


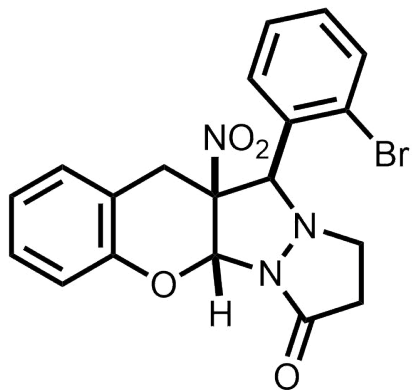
X : parts per Million : 1H



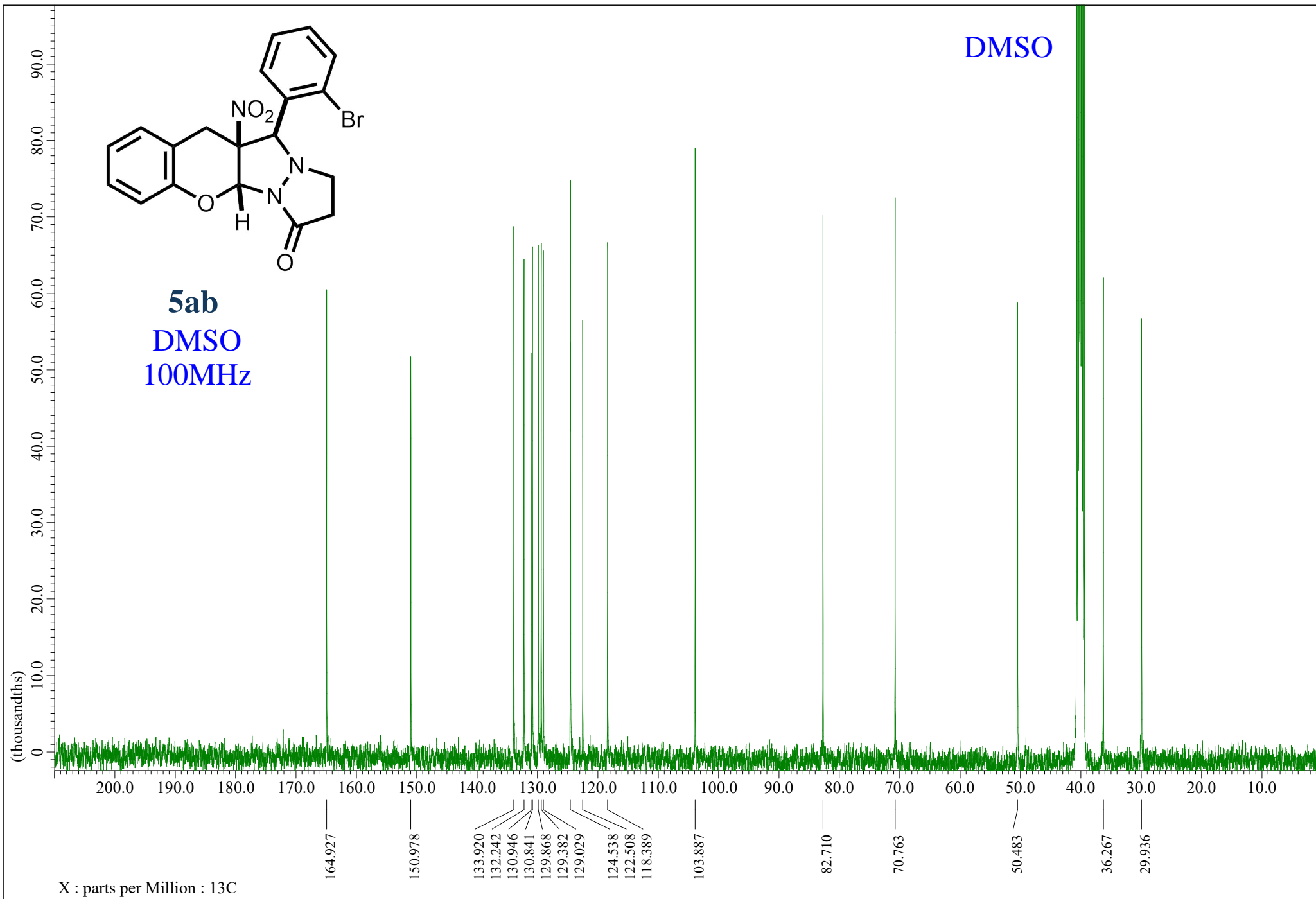


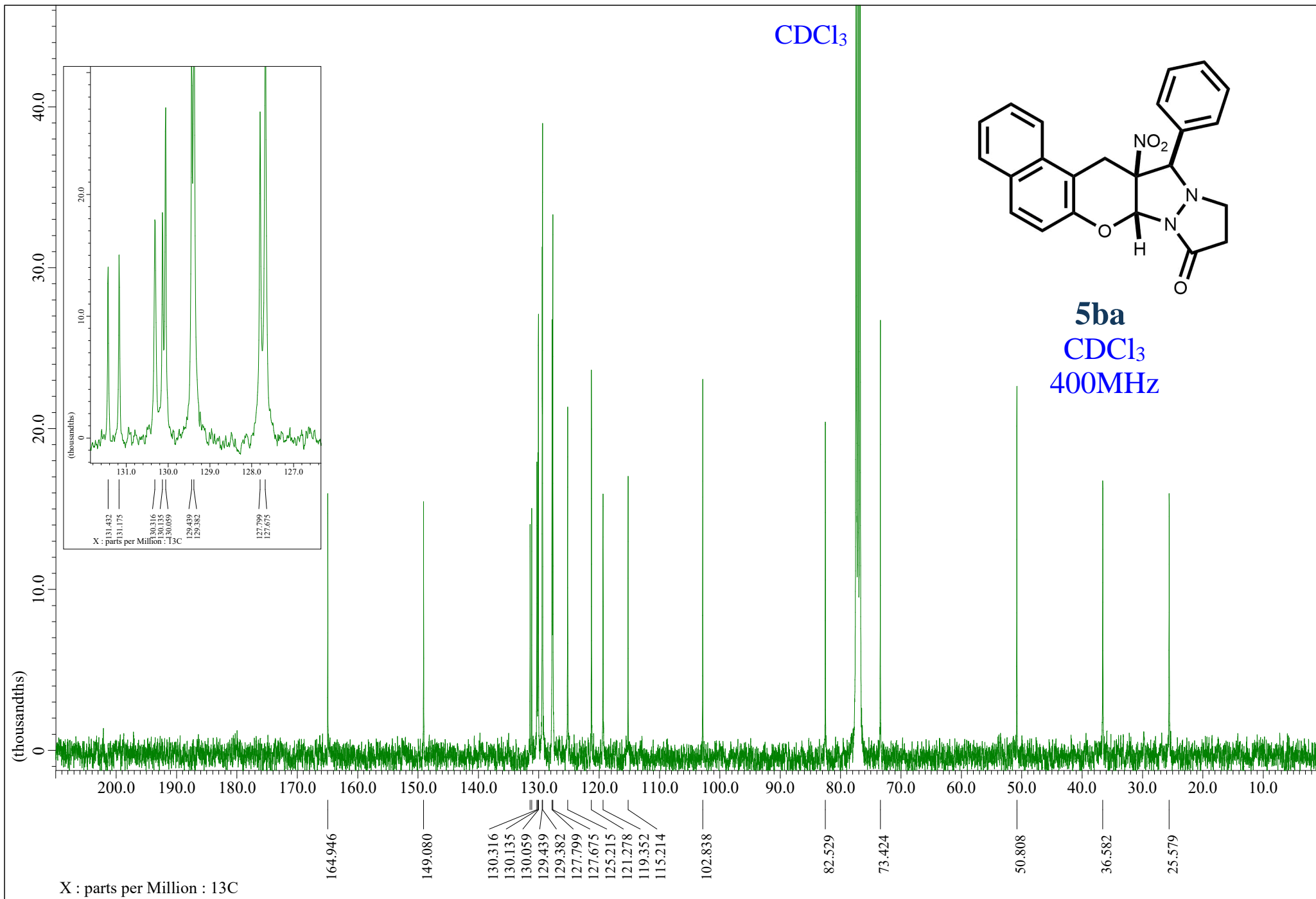
5ab
DMSO
400MHz

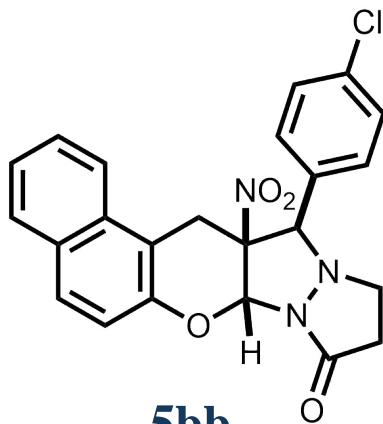




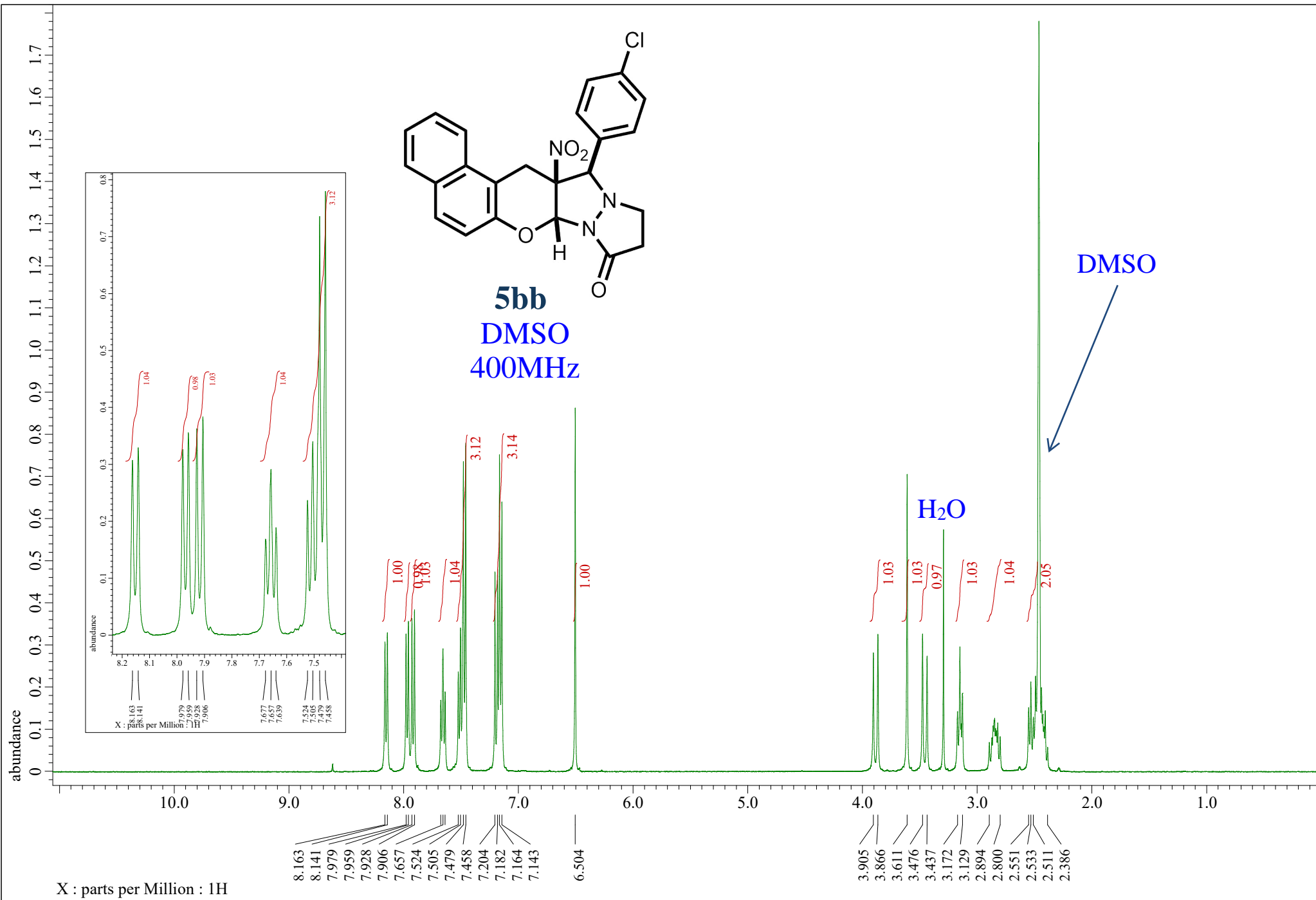
5ab
DMSO
100MHz



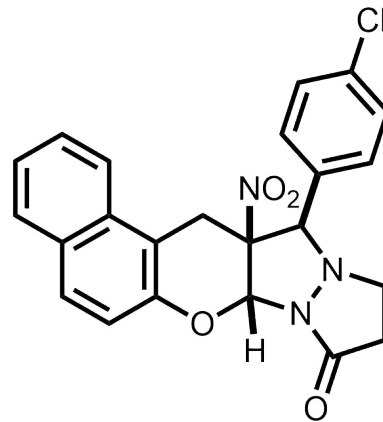




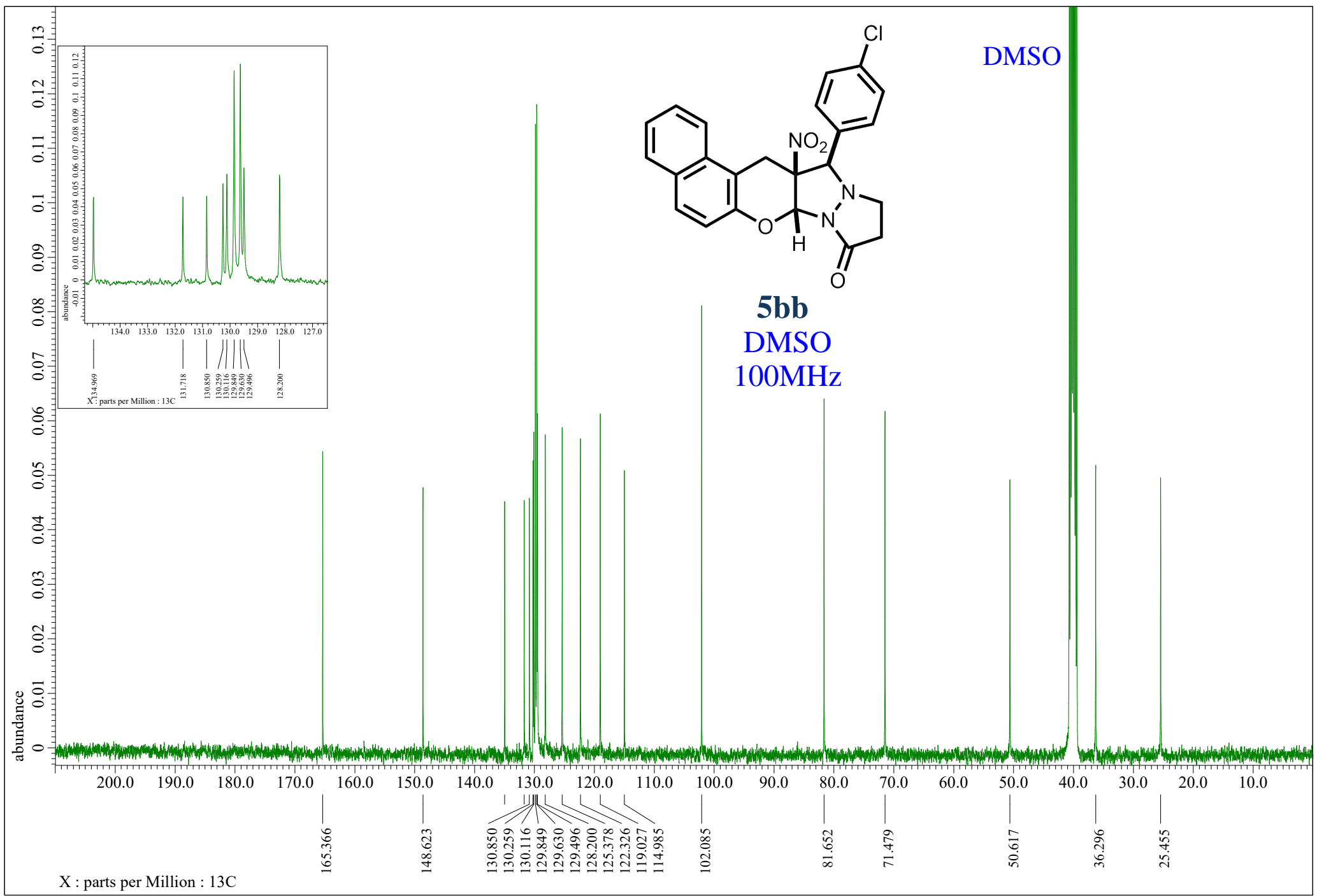
5b
DMSO
400MHz

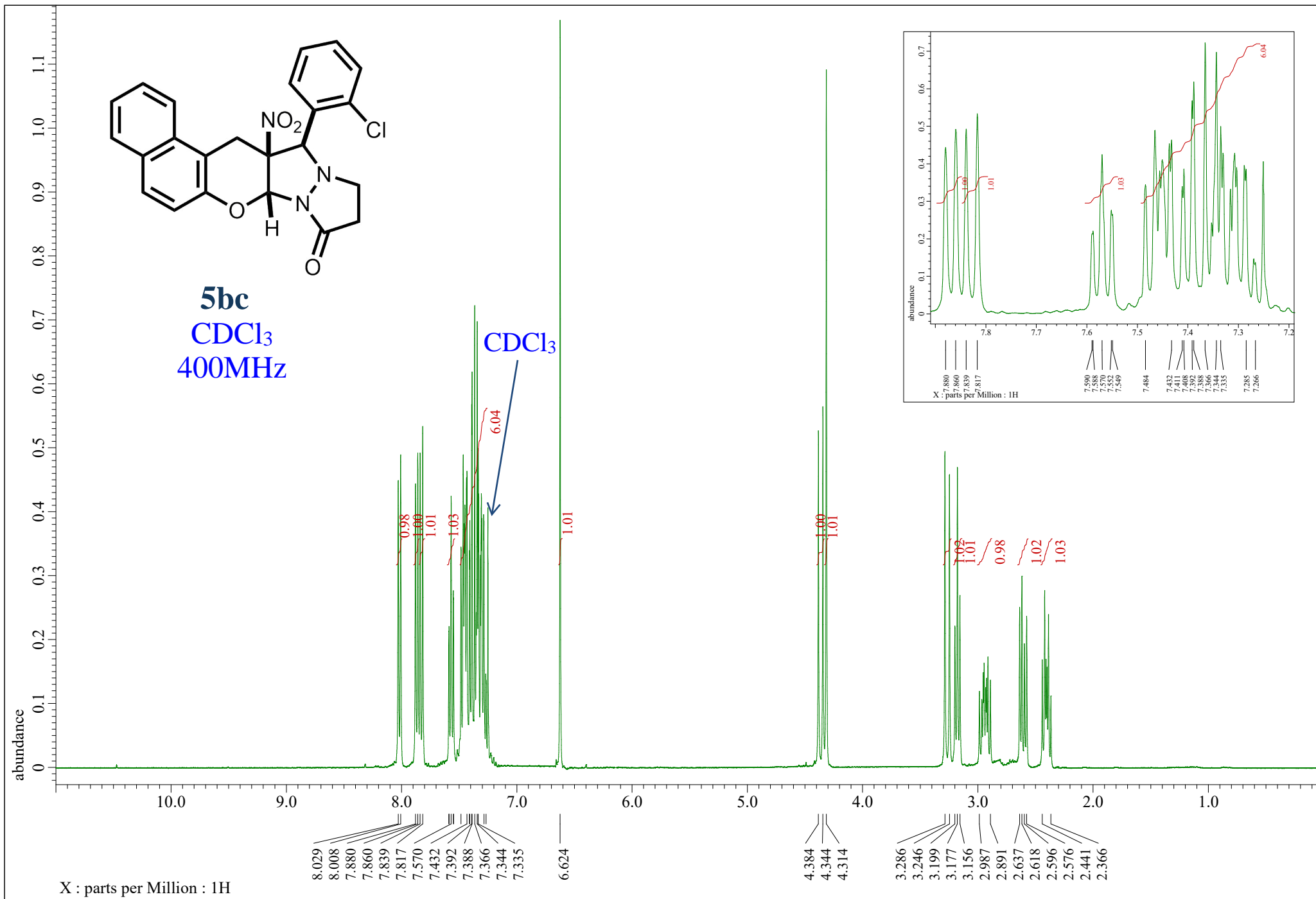


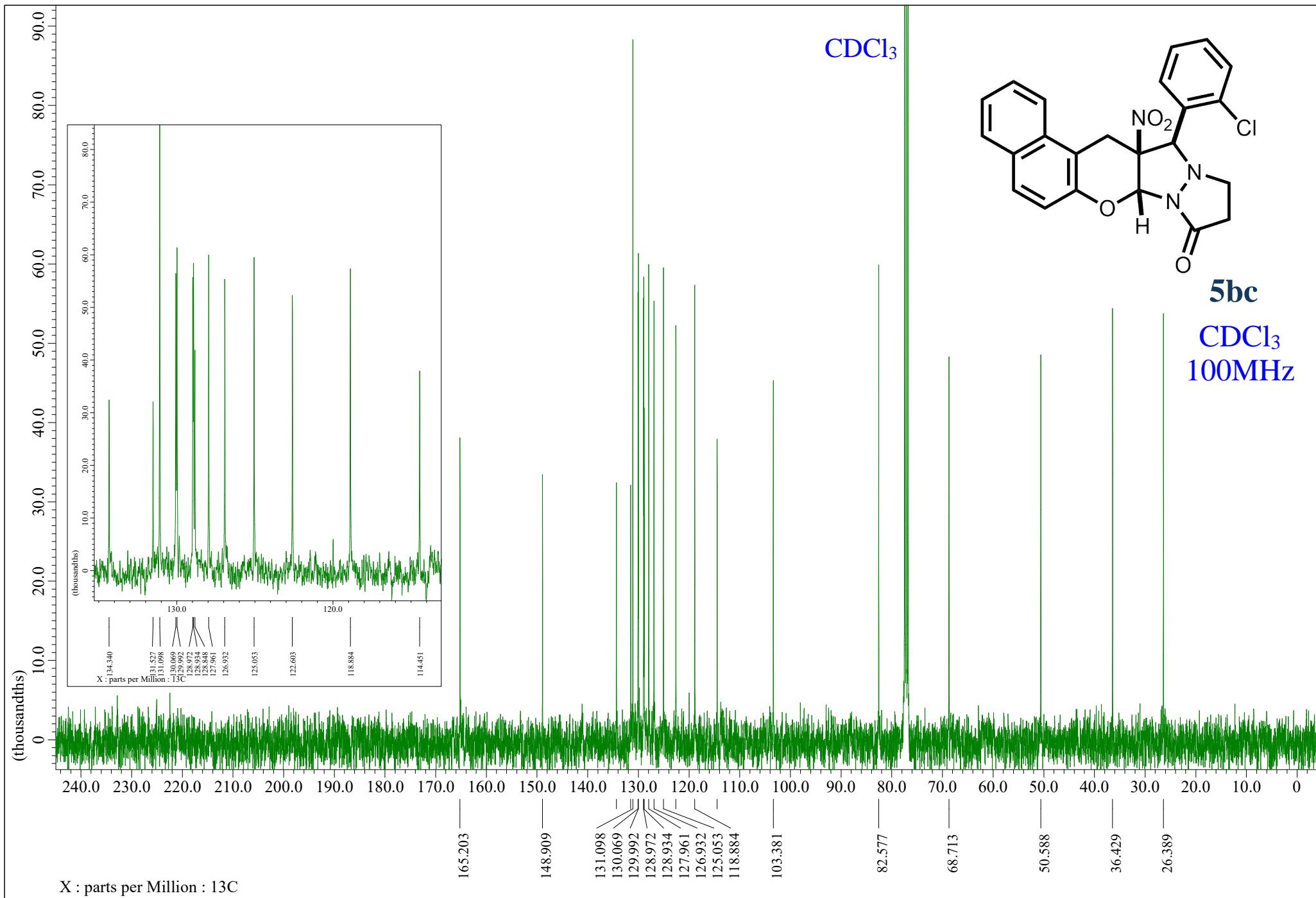
X : parts per Million : ¹H

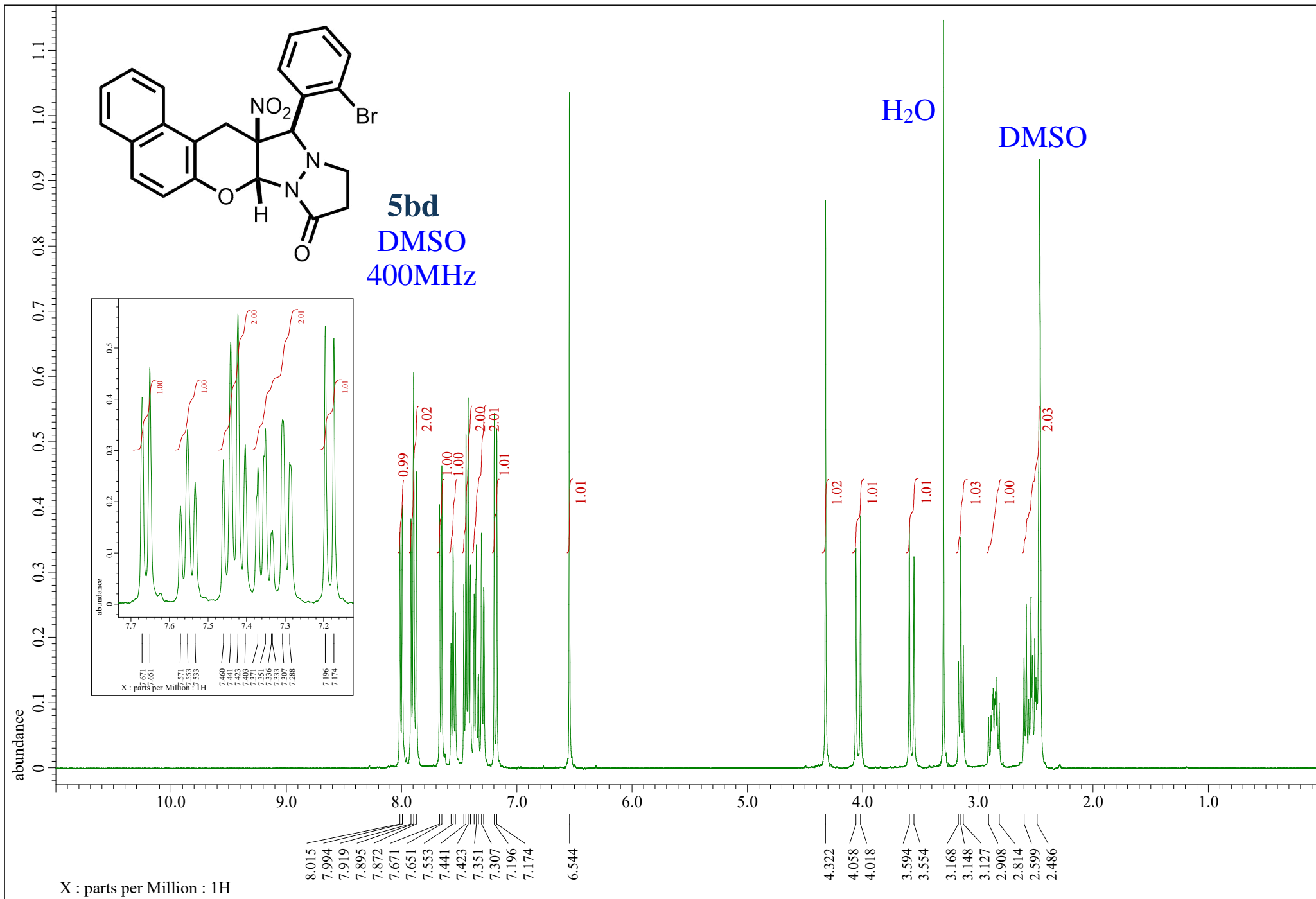


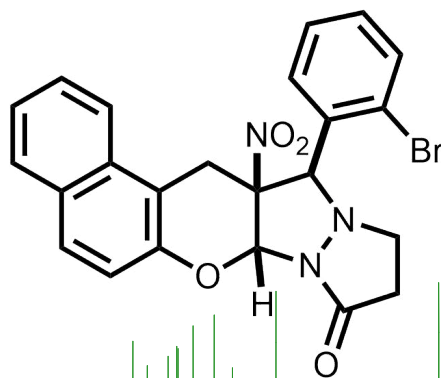
5bb
DMSO
100MHz





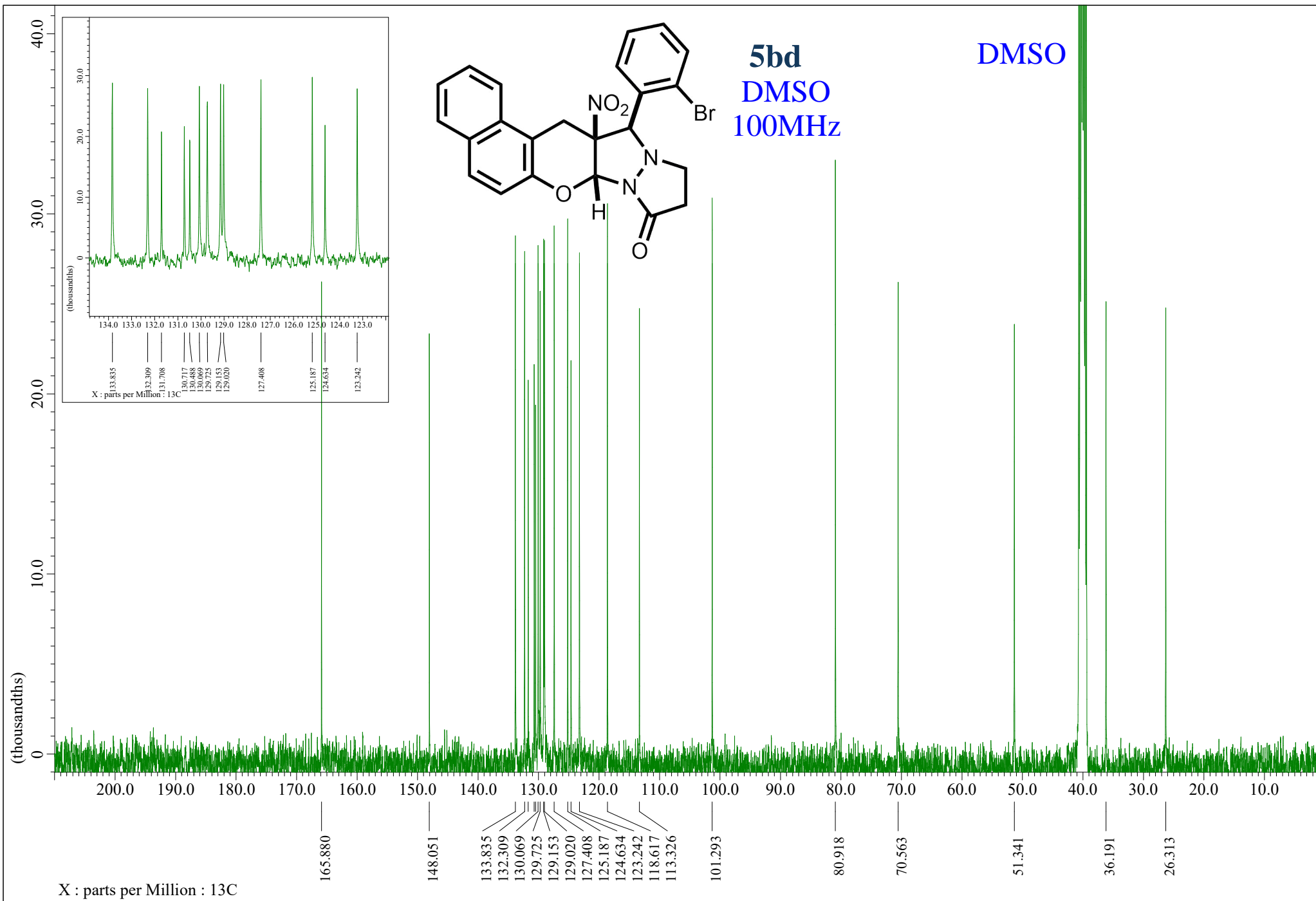


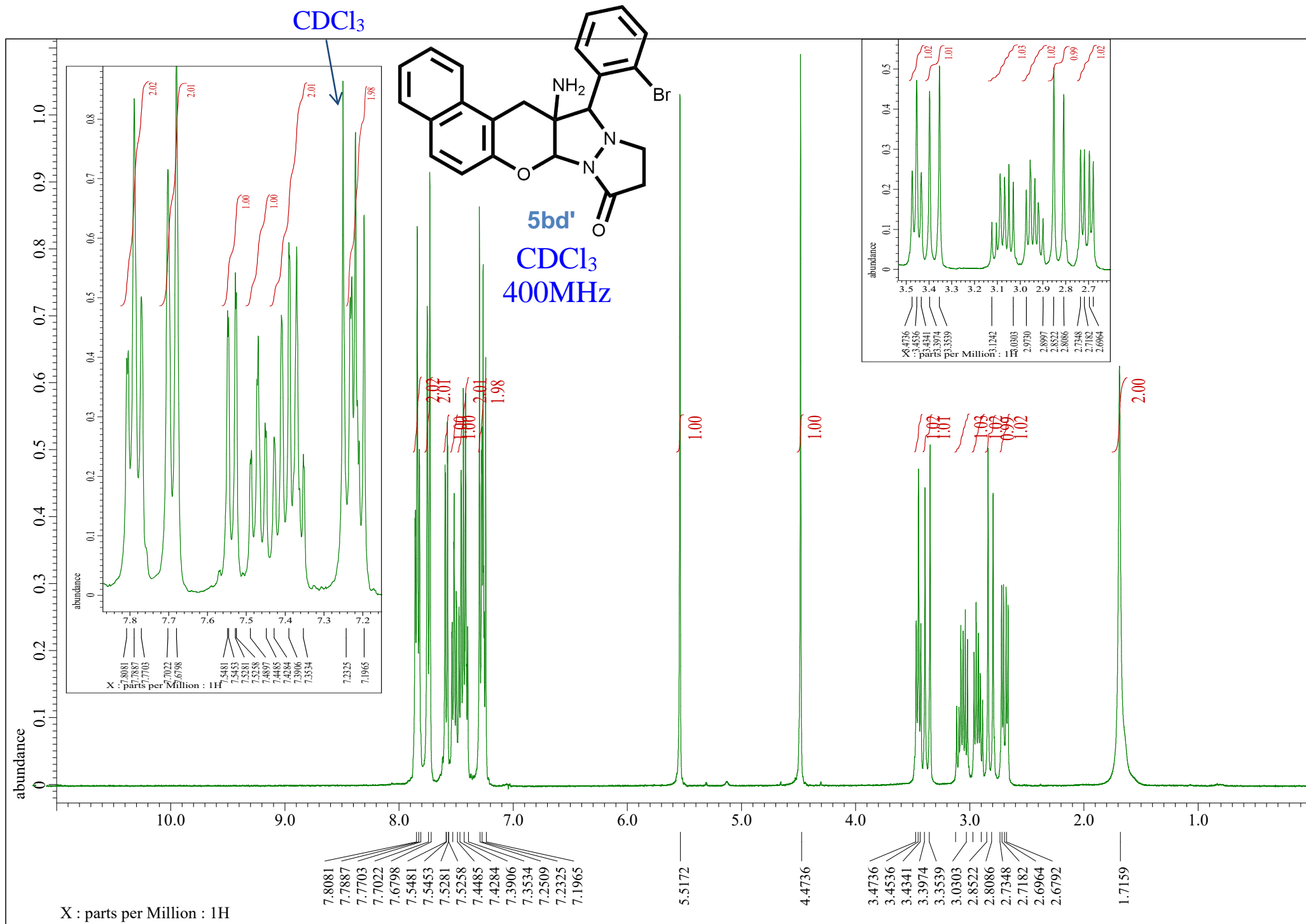


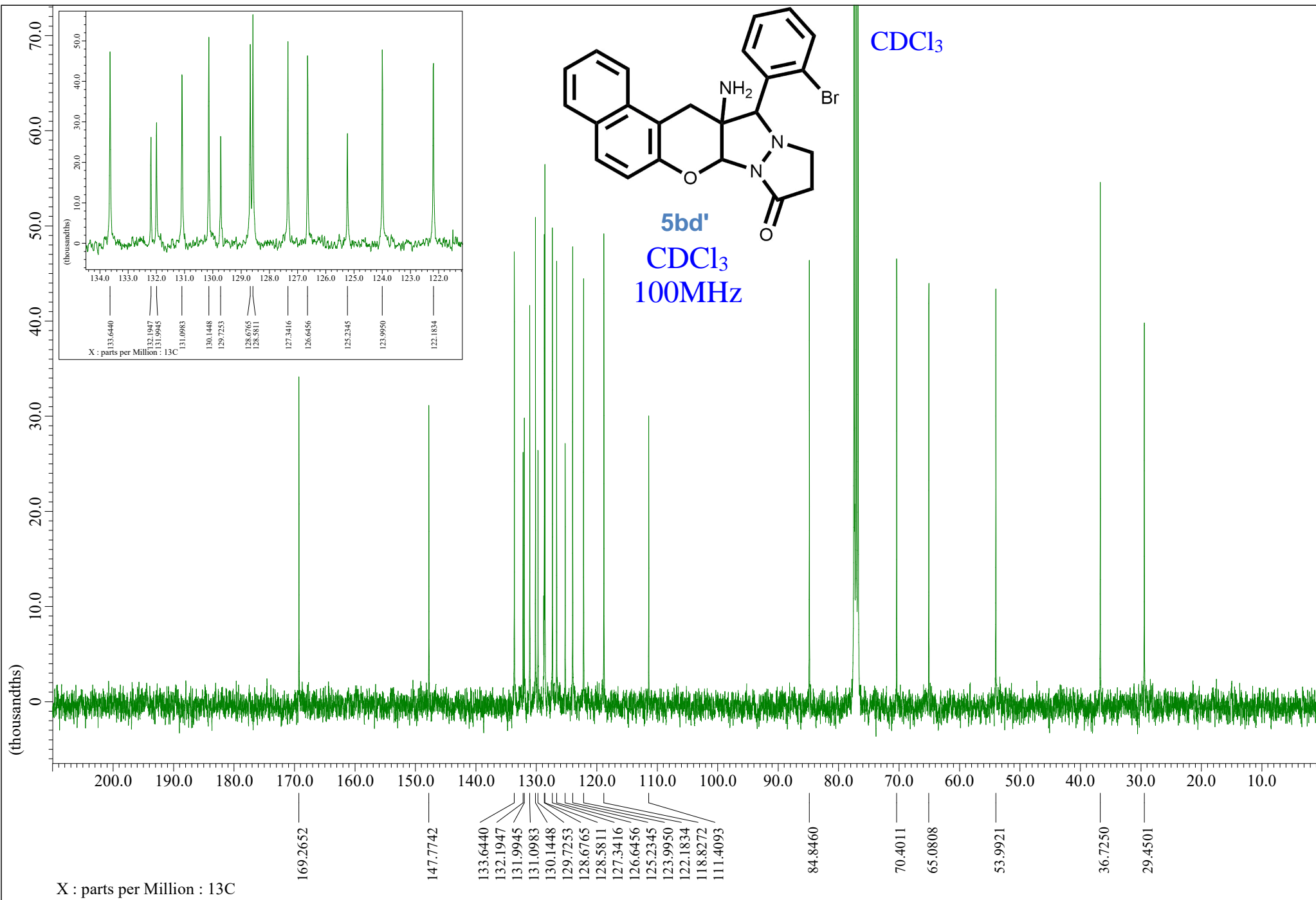


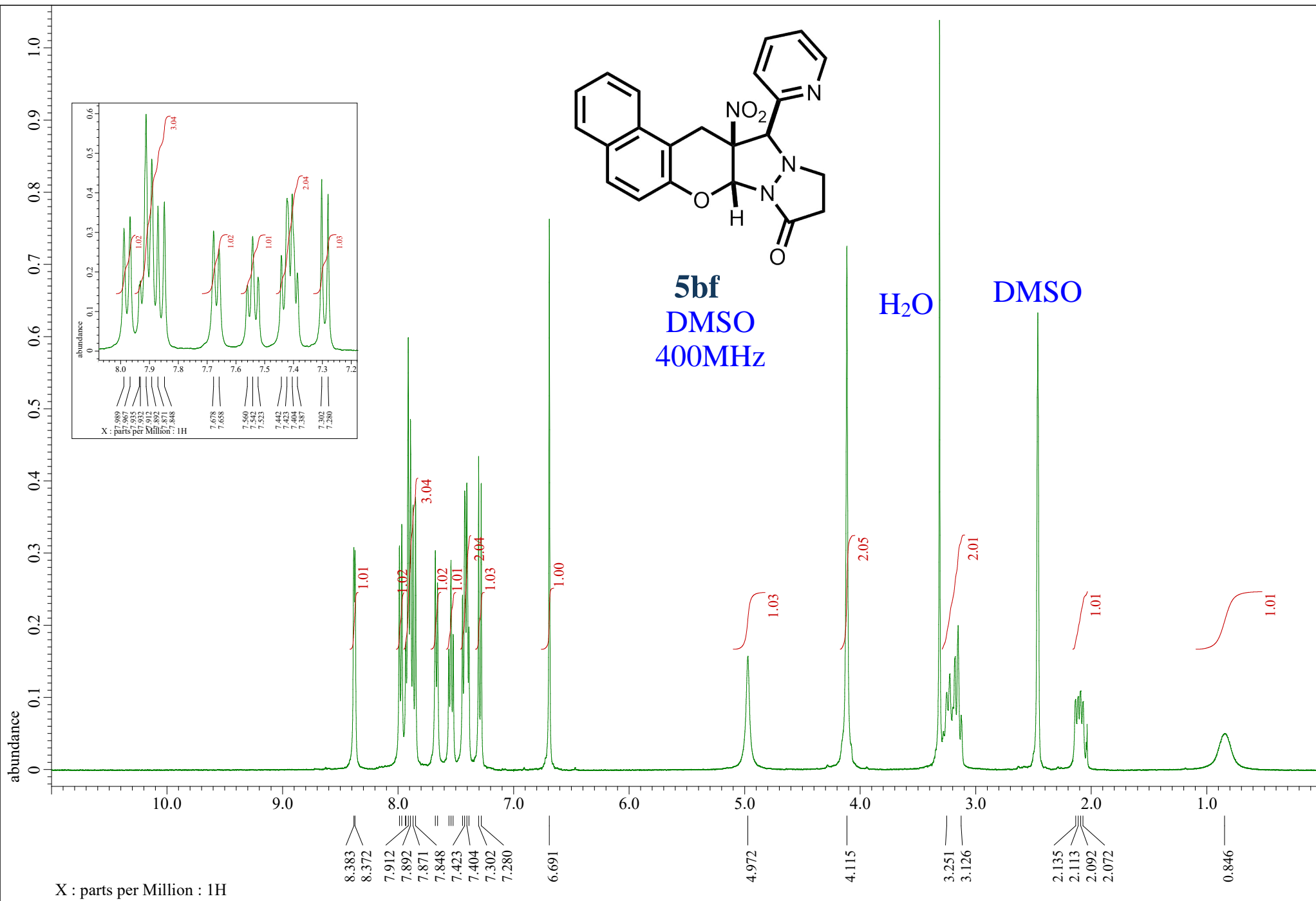
5bd
DMSO
100MHz

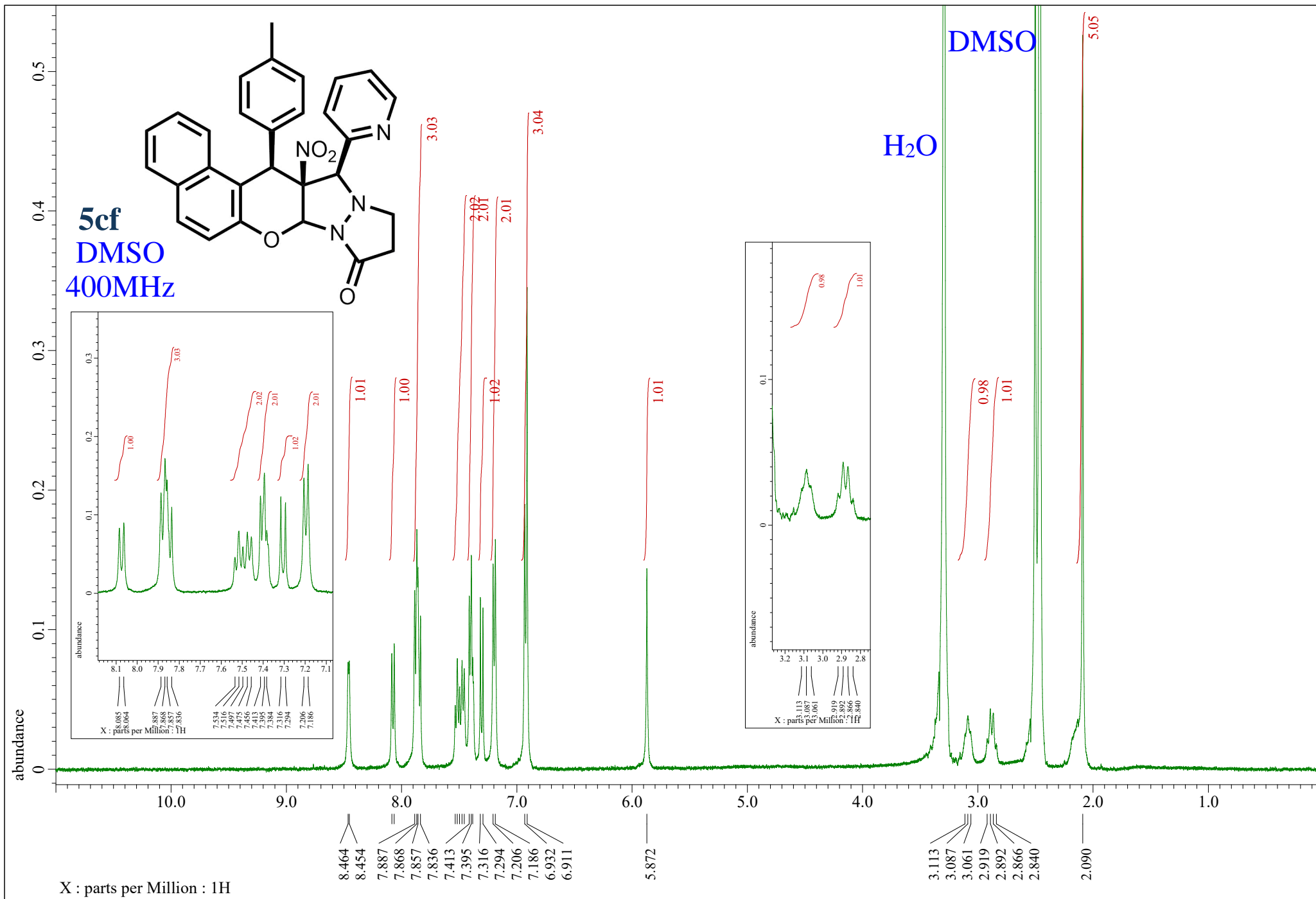
DMSO

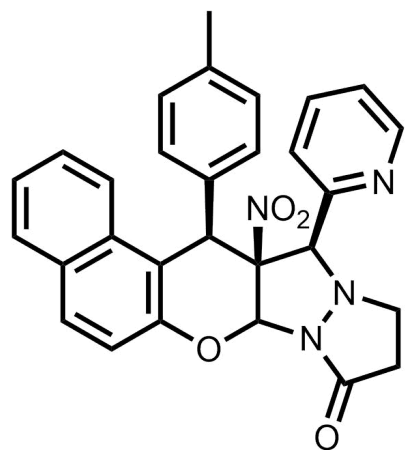












5cf
DMSO
100MHz

DMSO

