Electronic supplementary materials *Mendeleev Commun.*, 2021, **31**, 265–267

Transamination of 2-piperidinochromanes with (het)arylamines as a convenient route to 2-(het)arylaminochromanes

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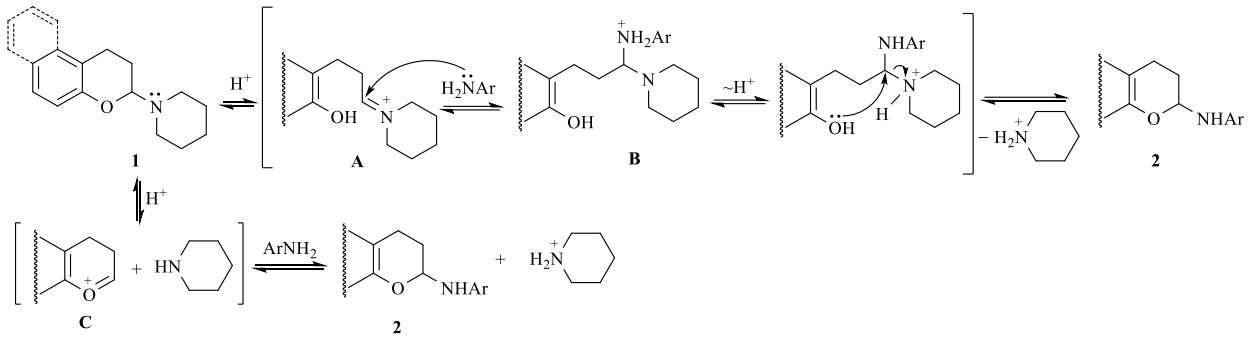
Solvents were purified and dried by standard procedures before use. Reagents were generally the best quality commercial grade and used without further purification. All reactions were carried out in oven-dried glassware. IR spectra were registered on a Shimadzu IR Affinity-1 spectrometer with a Specac Diamond ATR GS10800-B attachment and were reported in reciprocal centimeters (cm^{-1}). ^{1}H, ^{13}C, and ^{19}F NMR spectra (400, 100, and 376 MHz, respectively), as well as DEPT-135 spectra were acquired on a JEOL JNM-ECX400 spectrometer in $CDCl_3$ or DMSO-d_6 using residual solvent signals (DMSO-d_6: 2.50 ppm for ^{1}H nuclei, 39.5 ppm for ^{13}C nuclei; $CDCl_3$: 7.26 ppm for ^{1}H nuclei, 77.2 ppm for ^{13}C nuclei) or $CFCl_3$ – 0.0 ppm for ^{19}F nuclei as internal standards. Chemical shifts are reported in δ unit-parts per million (ppm). Splitting patterns are designated as s = singlet; br. s = broad singlet; d = doublet, t = triplet; q = quartet; m = multiplet. Elemental analysis was performed on a Euro Vector EA-3000 CHNS-analyzer. Melting points were determined by the capillary method on an SRS OptiMelt MPA100 apparatus. The starting compounds **1a**–**d** were as previously published [V. A. Osyanin, D. V. Osipov, I. V. Melnikova, K. S. Korzhenko, I. A. Semenova and Yu. N. Klimochkin, *Synthesis*, 2020, **52**, 3604].

Mechanism for the formation of 2-aminochromanes:

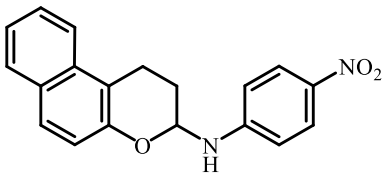
As for the reaction mechanism (Scheme S1), we assume that the aminochromane **1** undergoes the acid-catalyzed ring-opening reaction to give iminium salt **A** to which an aromatic amine is added to form intermediate **B**. The subsequent migration of the proton to piperidine moiety due to its higher basicity compared to arylamine fragment and the direct displacement of the piperidine or substitution *via* iminium salt and 6-*exo*-*trig* cyclization (this path is not shown on Scheme S1) lead to the final product **2**. On the other hand, nucleophilic substitution *via* the step of the formation of oxocarbenium ion **C** is also highly possible. At the current time, we have no evidence that enables distinction between these possibilities.



Scheme S1

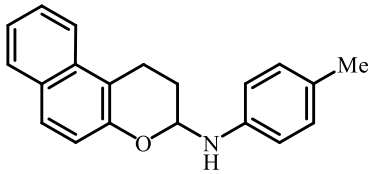
General procedure: A mixture of 1-(chroman-2-yl)piperidine **1a–d** (0.5 mmol), aromatic amine (0.5 mmol) and PPTS (0.5 mmol) in DCE (for products **2a,j,l−n**), MeOH−DCE (2:1) (for **2v**) or MeOH (4 ml) was stirred under reflux for 1.5 h. When the reaction was completed, the mixture was stored at −30 °C for 1 h, the solid was filtered off, washed by ice-cold MeOH (2×3 ml) and purified by recrystallization from a suitable solvent.

***N*-(4-Nitrophenyl)-2,3-dihydro-1*H*-benzo[*f*]chromen-3-amine (2a).**



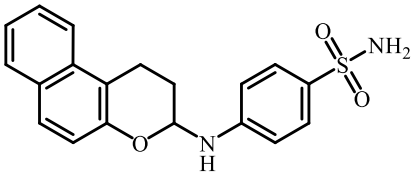
Yield 154 mg (96%), mp: 233-234 °C (DCE). ^{1}H NMR (DMSO-d_6): δ 2.12-2.21 (m, 1H, CH_2), 2.31-2.34 (m, 1H, CH_2), 3.09-3.27 (m, 2H, CH_2), 5.66 (dt, *J*=6.6 Hz, *J*=2.3 Hz, 1H, CH−O), 6.93-6.97 (m, 3H, NH, $H_{o\text{-NH}}$), 7.32-7.35 (m, 1H, Ar), 7.47-7.51 (m, 1H, Ar), 7.64 (d, *J*=8.7 Hz, 1H, Ar), 7.79 (d, *J*=8.0 Hz, 1H, Ar), 7.83 (d, *J*=8.5 Hz, 1H, Ar), 8.02 (d, *J*=7.8 Hz, 1H, Ar), 8.06 (d, *J*=8.9 Hz, 2H, $H_{m\text{-NH}}$). ^{13}C NMR (DMSO-d_6): δ 20.0 (CH_2), 26.4 (CH_2), 79.6 (CH−O), 113.3 ($2CH_{o\text{-NH}}$), 114.0 (C), 119.5 (CH), 122.6 (CH), 123.9 (CH), 126.5 ($2CH_{m\text{-NH}}$), 127.1 (CH), 128.2 (CH), 128.8 (CH), 129.1 (C), 133.0 (C), 138.4 (C), 150.9 (C), 153.2 (C). IR: 3358 (NH), 1628, 1603, 1587, 1551, 1537, 1483, 1450, 1317, 1298, 1273, 1225, 1177, 1148, 1111, 1092, 1072, 978, 870, 833, 797. Found (%): C, 71.32; H, 5.10; N, 8.81. Calc. for $C_{19}H_{16}N_2O_3$ (%): C, 71.24; H, 5.03; N, 8.74.

***N*-(*p*-Tolyl)-2,3-dihydro-1*H*-benzo[*f*]chromen-3-amine (2b).**



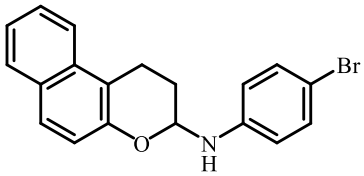
Yield 125 mg (88%), mp: 195-196 °C (MeOH). ^{1}H NMR (DMSO-d_6): δ 2.08-2.16 (m, 4H, CH_2, CH_3), 2.23-2.30 (m, 1H, CH_2), 3.06-3.24 (m, 2H, CH_2), 5.47-5.51 (m, 1H, CH−O), 6.55 (d, *J*=8.9 Hz, 1H, Ar), 6.72 (d, *J*=8.2 Hz, 2H, $H_{p\text{-tolyl}}$), 6.91-6.94 (m, 3H, NH, $H_{p\text{-tolyl}}$), 7.29-7.33 (m, 1H, Ar), 7.45-7.49 (m, 1H, Ar), 7.61 (d, *J*=8.7 Hz, 1H, Ar), 7.77 (d, *J*=8.0 Hz, 1H, Ar), 7.81 (d, *J*=8.5 Hz, 1H, Ar). ^{13}C NMR (DMSO-d_6): *δ* 20.4 (CH_2), 20.7 (CH_3), 27.0 (CH_2), 81.1 (CH−O), 113.9 (C), 114.1 ($2CH_{o\text{-NH}}$), 119.7 (CH), 122.5 (CH), 123.6 (CH), 126.5 (C), 126.9 (CH), 128.0 (CH), 128.7 (CH), 128.9 (C), 129.9 ($2CH_{m\text{-NH}}$), 133.1 (C), 144.4 (C), 151.6 (C-4a). IR: 3395 (NH), 1618, 1595, 1585, 1522, 1466, 1433, 1389, 1377, 1300, 1260, 1221, 1207, 1184, 1179, 1155, 1142, 1067, 1042, 1028, 964, 858, 824, 804, 746. Found (%): C, 83.11; H, 6.67; N, 4.96. Calc. for $C_{20}H_{19}NO$ (%): C, 83.01; H, 6.62; N, 4.84.

4-[(2,3-Dihydro-1*H*-benzo[*f*]chromen-3-yl)amino]benzenesulfonamide (2c).



Yield 155 mg (74%), mp: 208-210 °C (MeOH). ^{1}H NMR (DMSO-d_6): δ 2.12-2.19 (m, 1H, CH_2), 2.28-2.31 (m, 1H, CH_2), 3.08-3.26 (m, 2H, CH_2), 5.59-5.62 (m, 1H, CH−O), 6.91 (d, *J*=8.5 Hz, 2H, $H_{o\text{-NH}}$), 6.95 (d, *J*=8.9 Hz, 1H, Ar), 7.00 (s, 2H, NH_2), 7.31-7.38 (m, 2H, NH, Ar), 7.47-7.51 (m, 1H, Ar), 7.58 (d, *J*=8.5 Hz, 2H, $H_{m\text{-NH}}$), 7.63 (d, *J*=8.9 Hz, 1H, Ar), 7.78 (d, *J*=8.0 Hz, 1H, Ar), 7.83 (d, *J*=8.5 Hz, 1H, Ar). ^{13}C NMR (DMSO-d_6): δ 20.2 (CH_2), 26.7 (CH_2), 80.0 (CH−O), 113.2 ($2CH_{o\text{-NH}}$), 113.9 (C), 119.6 (CH), 122.5 (CH), 123.8 (CH), 127.0 (CH), 127.8 ($2CH_{m\text{-NH}}$), 128.2 (CH), 128.8 (CH), 129.1 (C), 133.0 (C), 133.1 (C), 149.7 (C), 151.2 (C). Found (%): C, 64.64; H, 5.10; N, 7.80; S, 8.91. Calc. for $C_{19}H_{18}N_2O_3S$ (%): C, 64.39; H, 5.12; N, 7.90; S, 9.05.

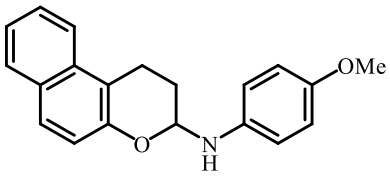
***N*-(4-Bromophenyl)-2,3-dihydro-1*H*-benzo[*f*]chromen-3-amine (2d).**



Yield 120 mg (68%), mp: 208-209 °C (MeOH). ^{1}H NMR ($CDCl_3$): *δ* 2.15-2.24 (m, 1H, CH_2), 2.41-2.46 (m, 1H, CH_2), 3.21-3.25 (m, 2H, CH_2), 4.61 (d, *J*=9.4 Hz, 1H, NH), 5.46-5.51 (m, 1H, CH−O), 6.74 (d, *J*=8.5 Hz, 2H, $H_{o\text{-NH}}$), 7.03 (d, *J*=8.9 Hz, 1H, Ar), 7.31 (d, *J*=8.5 Hz, 2H, $H_{m\text{-NH}}$), 7.35-7.38 (m, 1H, Ar), 7.49-7.53 (m, 1H, Ar), 7.63 (d, *J*=8.7 Hz, 1H, Ar), 7.77 (d, *J*=8.2 Hz, 1H, Ar), 7.81 (d, *J*=8.5 Hz, 1H, Ar). ^{13}C NMR ($CDCl_3$): δ 20.6 (CH_2), 27.3 (CH_2), 80.4 (CH−O), 111.4 (C), 112.8 (C), 116.1 ($2CH_{o\text{-NH}}$), 119.4 (CH), 121.9 (CH), 123.6 (CH), 126.6 (CH), 128.3

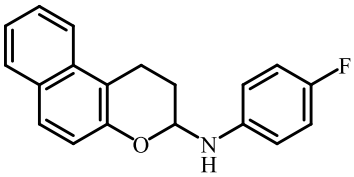
(CH), 128.6 (CH), 129.2 (C), 132.2 (2CH$_{m\text{-NH}}$), 132.8 (C), 144.2 (C), 151.0 (C-4a). IR: 3389 (NH), 1618, 1589, 1506, 1485, 1466, 1393, 1306, 1221, 1209, 1175, 1152, 1140, 1069, 1045, 976, 968, 858, 818, 810, 743. Found (%): C, 64.53; H, 4.61; N, 3.98. Calc. for $C_{19}H_{16}BrNO$ (%): C, 64.42; H, 4.55; N, 3.95.

***N*-(4-Methoxyphenyl)-2,3-dihydro-1*H*-benzo[*f*]chromen-3-amine (2e).**



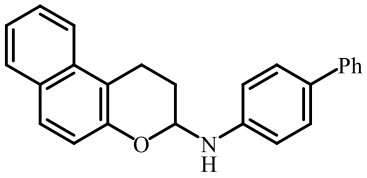
Yield 120 mg (79%), mp: 166-167 °C (MeOH). ^{1}H NMR ($CDCl_3$): δ 2.14-2.24 (m, 1H, CH_2), 2.40-2.47 (m, 1H, CH_2), 3.20-3.28 (m, 2H, CH_2), 3.77 (s, 3H, OMe), 4.39 (br. s, 1H, NH), 5.46-5.48 (m, 1H, CH−O), 6.80-6.87 (m, 4H, H$_{o\text{-NH}}$, H$_{m\text{-NH}}$), 7.05 (d, *J*=8.9 Hz, 1H, Ar), 7.34-7.38 (m, 1H, Ar), 7.49-7.53 (m, 1H, Ar), 7.63 (d, *J*=8.9 Hz, 1H, Ar), 7.77 (d, *J*=8.0 Hz, 1H, Ar), 7.82 (d, *J*=8.5 Hz, 1H, Ar). ^{13}C NMR ($CDCl_3$): δ 20.8 (CH_2), 27.6 (CH_2), 55.8 (OMe), 81.8 (CH−O), 112.9 (C), 114.9 (2CH), 116.1 (2CH), 119.6 (CH), 121.9 (CH), 123.4 (CH), 126.5 (CH), 128.1 (CH), 128.6 (CH), 129.1 (C), 132.9 (C), 139.0 (C), 151.3 (C), 153.5 (C). IR: 3400, 3375 (NH), 1620, 1595, 1512, 1466, 1433, 1391, 1258, 1244, 1231, 1221, 1207, 1182, 1173, 1155, 1140, 1028, 970, 858, 818, 741. Found (%): C, 78.78; H, 6.24; N, 4.48 Calc. for $C_{20}H_{19}NO_2$ (%): C, 78.66; H, 6.27; N, 4.59.

***N*-(4-Fluorophenyl)-2,3-dihydro-1*H*-benzo[*f*]chromen-3-amine (2f).**



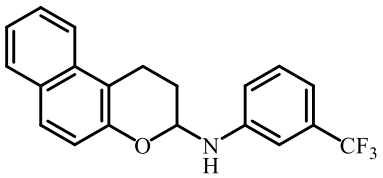
Yield 139 mg (78%), mp: 168-169 ºC (MeOH). ^{1}H NMR (DMSO-d_6): δ 2.07-2.16 (m, 1H, CH_2), 2.25-2.28 (m, 1H, CH_2), 3.06-3.23 (m, 2H, CH_2), 5.46-5.49 (m, 1H, CH−O), 6.72 (d, *J*=8.7 Hz, 1H, Ar), 6.78-6.83 (m, 2H, Ar), 6.91-6.99 (m, 3H, NH, Ar), 7.29-7.33 (m, 1H, Ar), 7.46-7.49 (m, 1H, Ar), 7.62 (d, *J*=8.9 Hz, 1H, Ar), 7.77 (d, *J*=8.0 Hz, 1H, Ar), 7.81 (d, *J*=8.5 Hz, 1H, Ar). ^{13}C NMR (DMSO-d_6): δ 20.4 (CH_2), 27.0 (CH_2), 81.2 (CH−O), 113.9 (C), 115.0 (d, $^3J_{CF}$=7.6 Hz, 2CH$_{o\text{-NH}}$), 115.9 (d, $^2J_{CF}$=21.9 Hz, 2CH$_{m\text{-NH}}$), 119.7 (CH), 122.5 (CH), 123.7 (CH), 126.9 (CH), 128.1 (CH), 128.7 (CH), 129.0 (C), 133.0 (C), 143.4 (C), 151.4 (C-4a), 155.8 (d, $^1J_{CF}$=231.7 Hz, C–F). ^{19}F NMR (DMSO-d_6): δ −127.4 (s, F). IR: 3387 (NH), 1620, 1595, 1520, 1504, 1466, 1391, 1306, 1260, 1225, 1207, 1177, 1151, 1094, 1067, 1043, 976, 966, 860, 851, 822, 768, 741. Found (%): C, 77.80; H, 5.50; N, 4.67. Calc. for $C_{19}H_{16}FNO$ (%): C, 77.91; H, 5.48; N, 4.79.

***N*-([1,1'-Biphenyl]-4-yl)-2,3-dihydro-1*H*-benzo[*f*]chromen-3-amine (2g).**



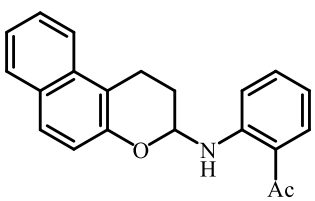
Yield 158 mg (90%), mp: 169-170 ºC (DMF-MeOH). ^{1}H NMR (DMSO-d_6): δ 1.52-1.60 (m, 1H, CH_2), 2.17-2.21 (m, 1H, CH_2), 3.05-3.16 (m, 2H, CH_2), 6.04 (d, *J*=10.3 Hz, 1H, CH−O), 7.02-7.09 (m, 7H, Ar, NH), 7.27-7.34 (m, 5H, Ar), 7.43-7.47 (m, 1H, Ar), 7.66 (d, *J*=8.9 Hz, 1H, Ar), 7.75 (d, *J*=8.9 Hz, Ar), 7.78 (d, *J*=8.2 Hz, Ar). ^{13}C NMR (DMSO-d_6): δ 22.6 (CH_2), 27.5 (CH_2), 85.1 (CH−O), 114.0 (C), 119.5 (CH), 122.6 (CH), 123.79 (CH), 123.82 (CH), 123.9 (3CH), 127.0 (CH), 128.2 (CH), 128.8 (CH), 129.0 (C), 129.8 (5CH, C), 132.9 (C), 145.8 (2C), 152.5 (C-4a). IR: 1620, 1597, 1585, 1494, 1466, 1400, 1290, 1259, 1227, 1213, 1204, 1130, 1070, 1034, 1026, 974, 897, 856, 818, 750. Found (%): C, 85.39; H, 5.95; N, 4.06. Calc. for $C_{25}H_{21}NO$ (%): C, 85.44; H, 6.02; N, 3.99.

***N*-[3-(Trifluoromethyl)phenyl]-2,3-dihydro-1*H*-benzo[*f*]chromen-3-amine (2h).**



Yield 106 mg (86%), mp: 161-162 ºC (MeOH). ^{1}H NMR (DMSO-d_6): δ 2.10-2.18 (m, 1H, CH_2), 2.29-2.31 (m, 1H, CH_2), 3.08-3.26 (m, 2H, CH_2), 5.60-5.64 (m, 1H, CH−O), 6.92-6.97 (m, 2H, Ar, NH), 7.09-7.13 (m, 2H, Ar), 7.21 (d, *J*=8.5 Hz, 1H, Ar), 7.30-7.36 (m, 2H, Ar), 7.49 (t, *J*=7.6 Hz, 1H, Ar), 7.63 (d, *J*=8.7 Hz, 1H, Ar), 7.78 (d, *J*=8.0 Hz, 1H, Ar), 7.83 (d, *J*=8.2 Hz, 1H, Ar). ^{13}C NMR (DMSO-d_6): *δ* 20.1 (CH_2), 26.7 (CH_2), 80.2 (CH−O), 110.1 (q, $^{3}J_{CF}$=3.8 Hz, $CH_{o\text{-}CF_3}$), 114.0 (C), 114.2 (q, $^{3}J_{CF}$=3.8 Hz, $CH_{o\text{-}CF_3}$), 117.5 (CH), 119.6 (CH), 122.5 (CH), 123.8 (CH), 125.0 (q, $^{1}J_{CF}$=272.2 Hz, CF_3), 127.0 (CH), 128.2 (CH), 128.8 (CH), 129.0 (C), 130.3 (q, $^{2}J_{CF}$=30.7 Hz, C−CF_3), 130.5 (CH), 133.0 (C), 147.5 (C), 151.2 (C-4a). ^{19}F NMR (DMSO-d_6): δ −61.2 (s, CF_3). IR: 3408 (NH), 1597, 1504, 1465, 1340, 1259, 1225, 1209, 1192, 1156, 1123, 1067, 1015, 966, 860, 854, 812, 745, 896. Found (%): C, 69.88; H, 4.77; N, 3.95. Calc. for $C_{20}H_{16}F_3NO$ (%): C, 69.96; H, 4.70; N, 4.08.

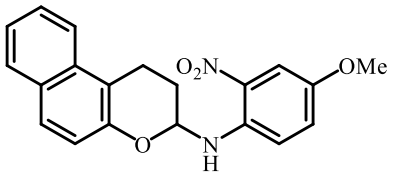
1-[2-((2,3-Dihydro-1*H*-benzo[*f*]chromen-3-yl)amino)phenyl]ethan-1-one (2i).



Yield 95 mg (60%), mp: 136-137 °C (MeOH). ^{1}H NMR (DMSO-d_6): δ 2.18-2.25 (m, 1H, CH_2), 2.30-2.35 (m, 1H, CH_2), 2.49 (s, 3H, CH_3), 3.08-3.24 (m, 2H, CH_2), 5.76-5.80 (m, 1H, CH−O), 6.73-6.77 (m, 1H, Ar), 6.93 (d, *J*=8.9 Hz, 1H, Ar), 7.21 (d, *J*=8.7 Hz, 1H, Ar), 7.31-7.35 (m, 1H,

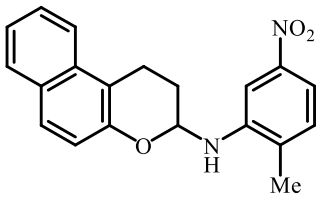
Ar), 7.44-7.52 (m, 2H, Ar), 7.63 (d, *J*=8.9 Hz, 1H, Ar), 7.78 (d, *J*=8.0 Hz, 1H, Ar), 7.85 (d, *J*=8.2 Hz, 2H, Ar), 9.54 (d, *J*=8.7 Hz, 1H, NH). ^{13}C NMR (DMSO-d_6): δ 19.4 (CH_2), 26.6 (CH_2), 29.7 (CH_3), 78.5 (CH−O), 113.7 (C), 114.1 (CH), 117.1 (CH), 118.6 (C), 119.6 (CH), 122.5 (CH), 123.9 (CH), 127.1 (CH), 128.3 (CH), 128.8 (CH), 129.1 (C), 133.0 (C), 133.4 (CH), 135.6 (CH), 148.6 (C), 150.6 (C), 202.3 (C=O). IR: 3269 (NH), 1740 (C=O), 1636, 1578, 1520, 1456, 1431, 1400, 1360, 1325, 1229, 1219, 1196, 1165, 1105, 1055, 1040, 982, 943, 858, 844, 804, 740. Found (%): C, 79.57; H, 5.96; N, 4.30. Calc. for $C_{21}H_{19}NO_2$ (%): C, 79.47; H, 6.03; N, 4.41.

_N_-(4-Methoxy-2-nitrophenyl)-2,3-dihydro-1_H_-benzo[_f_]chromen-3-amine (2j).



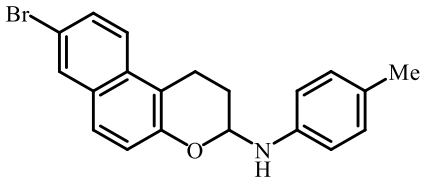
Yield 121 mg (69%), mp: 159-160 °C (MeOH). ^{1}H NMR (DMSO-d_6): δ 2.29-2.40 (m, 2H, CH_2), 3.09-3.24 (m, 2H, CH_2), 3.74 (s, 3H, OCH_3), 5.79-5.85 (m, 1H, CH−O), 6.96 (d, *J*=8.9 Hz, 1H), 7.32-7.37 (m, 2H), 7.41-7.43 (m, 1H), 7.48-7.51 (m, 2H), 7.65 (d, *J*=8.9 Hz, 1H, Ar), 7.79 (d, *J*=8.2 Hz, 1H, Ar), 7.85 (d, *J*=8.5 Hz, 1H, Ar), 8.21 (d, *J*=7.8 Hz, 1H, Ar). ^{13}C NMR (DMSO-d_6): δ 19.8 (CH_2), 26.5 (CH_2), 56.2 (CH_3), 79.3 (CH−O), 107.6 (CH), 113.7 (C), 118.4 (CH), 119.4 (CH), 122.6 (CH), 124.0 (CH), 126.9 (CH), 127.2 (CH), 128.4 (CH), 128.8 (CH), 129.2 (C), 132.6 (C), 132.9 (C), 138.4 (C), 150.6 (C), 151.3 (C). IR: 3361 (NH), 1622, 1597, 1573, 1514, 1504, 1416, 1391, 1342, 1317, 1296, 1236, 1211, 1175, 1146, 1057, 1042, 1030, 982, 966, 870, 853, 816, 793, 768, 762, 746. Found (%): C, 68.49; H, 5.20; N, 8.17. Calc. for $C_{20}H_{18}N_2O_4$ (%): C, 68.56; H, 5.18; N, 8.00.

_N_-(2-Methyl-5-nitrophenyl)-2,3-dihydro-1_H_-benzo[_f_]chromen-3-amine (2k).



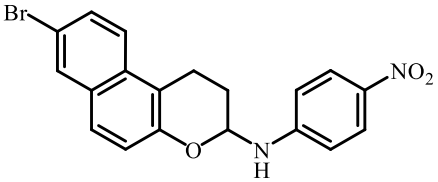
Yield 147 mg (88%), mp: 173-174 ºC (DMF-MeOH). ^{1}H NMR (DMSO-d_6): δ 2.26 (s, 3H, CH_3), 2.31-2.35 (m, 2H, CH_2), 3.12-3.25 (m, 2H, CH_2), 5.60-5.65 (m, 1H, CH−O), 6.44 (d, *J*=8.5 Hz, 1H, NH), 6.98 (d, *J*=8.7 Hz,1H, Ar), 7.29 (d, *J*=8.2 Hz, 1H, Ar), 7.32-7.36 (m, 1H, Ar), 7.47-7.54 (m, 2H, Ar), 7.66 (d, *J*=8.9 Hz, 1H, Ar), 7.72 (s, 1H, Ar), 7.80 (d, *J*=8.2 Hz, 1H, Ar), 7.83 (d, *J*=8.5 Hz, 1H, Ar). ^{13}C NMR (DMSO-d_6): δ 18.6 (CH_3), 21.3 (CH_2), 26.9 (CH_2), 81.4 (CH−O), 106.6 (CH), 113.3 (CH), 114.1 (C), 119.3 (CH), 122.6 (CH), 123.8 (CH), 127.1 (CH), 128.3 (CH), 128.8 (CH), 129.1 (C), 131.3 (CH), 132.1 (C), 133.0 (C), 145.6 (C), 147.4 (C), 151.6 (C). IR: 3387 (NH), 1616, 1593, 1514, 1464, 1433, 1396, 1260, 1223, 1175, 1146, 1070, 1043, 980, 947, 858, 810, 744. Found (%): C, 78.76; H, 5.50; N, 8.27. Calc. for $C_{20}H_{18}N_2O_3$ (%): C, 71.84; H, 5.43; N, 8.38.

8-Bromo-*N*-(*p*-tolyl)-2,3-dihydro-1*H*-benzo[*f*]chromen-3-amine (2l).



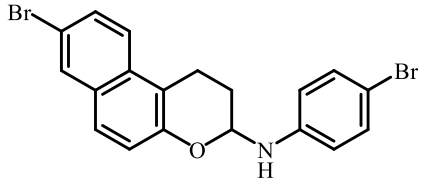
Yield 140 mg (73%), mp: 193-194 ºC (EtOH). ^{1}H NMR (DMSO-d_6): δ 2.08-2.14 (m, 4H, CH_3, CH_2), 2.23-2.26 (m, 1H, CH_2), 3.06-3.20 (m, 2H, CH_2), 5.48-5.53 (m, 1H, CH−O), 6.56 (d, *J*=8.9 Hz, 1H, Ar), 6.72 (d, *J*=8.2 Hz, 2H, $H_{p\text{-tolyl}}$), 6.92 (d, *J*=8.2 Hz, 2H, $H_{p\text{-tolyl}}$), 6.97 (d, *J*=8.9 Hz, 1H, Ar), 7.57 (dd, *J*=8.9 Hz, *J*=2.0 Hz, 1H, Ar), 7.62 (d, *J*=8.9 Hz, 1H, Ar), 7.76 (d, *J*=8.9 Hz, 1H, Ar), 8.04 (d, *J*=2.0 Hz, 1H, H-7). ^{13}C NMR (DMSO-d_6): δ 20.4 (CH_2), 20.7 (CH_3), 26.8 (CH_2), 81.3 (CH−O), 114.2 ($2CH_{o\text{-NH}}$), 114.3 (C), 116.5 (C), 121.0 (CH), 125.0 (CH), 126.6 (C), 127.4 (CH), 129.6 (CH), 129.9 ($2CH_{m\text{-NH}}$), 130.3 (C), 130.5 (CH), 131.7 (C), 144.3 (C), 152.1 (C−O). IR: 3395 (NH), 1612, 1587, 1522, 1497, 1387, 1302, 1223, 1188, 1175, 1155, 1043, 1069, 1043, 970, 962, 808. Found (%): C, 65.29; H, 4.85; N, 3.68. Calc. for $C_{20}H_{18}BrNO$ (%): C, 65.23; H, 4.93; N, 3.80.

8-Bromo-N-(4-nitrophenyl)-2,3-dihydro-1*H*-benzo[*f*]chromen-3-amine (2m).



Yield 174 mg (87%), mp: 214-215 ºC (DMF-*i*-PrOH). ^{1}H NMR (DMSO-d_6): δ 2.11-2.19 (m, 1H, CH_2), 2.30-2.33 (m, 1H, CH_2), 3.08-3.26 (m, 2H, CH_2), 5.66-5.69 (m, 1H, CH−O), 6.94 (d, *J*=8.9 Hz, 2H, $H_{o\text{-NH}}$), 7.01 (d, *J*=8.9 Hz, 1H, Ar), 7.59 (d, *J*=8.7 Hz, 1H, Ar), 7.65 (d, *J*=8.9 Hz, 1H, Ar), 7.79 (d, *J*=8.9 Hz, 1H, Ar), 8.00-8.09 (m, 4H, NH, H-7, $H_{m\text{-NH}}$). ^{13}C NMR (DMSO-d_6): δ 19.9 (CH_2), 26.3 (CH_2), 79.7 (CH−O), 113.3 ($2CH_{o\text{-NH}}$), 114.4 (C), 116.8 (C), 120.8 (CH), 125.0 (CH), 126.5 ($2CH_{m\text{-NH}}$), 127.5 (CH), 129.8 (CH), 130.49 (C), 130.54 (CH), 131.6 (C), 138.4 (C), 151.4 (C), 153.1 (C). IR: 3340 (NH), 1599, 1587, 1503, 1485, 1314, 1300, 1277, 1225, 1192, 1155, 1146, 1109, 1067, 1034, 972, 868, 856, 835, 800. Found (%): C, 57.02; H, 3.84; N, 6.91. Calc. for $C_{19}H_{15}BrN_2O_3$ (%): C, 57.16; H, 3.79; N, 7.02.

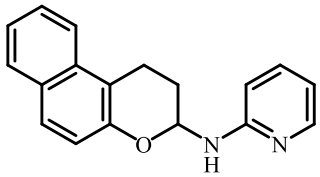
8-Bromo-*N*-(4-bromophenyl)-2,3-dihydro-1*H*-benzo[*f*]chromen-3-amine (2n).



Yield 152 mg (70%), mp: 192-193 ºC (MeOH). ^{1}H NMR (DMSO-d_6): δ 2.06-2.15 (m, 1H, CH_2), 2.24-2.27 (m, 1H, CH_2), 3.05-3.22 (m, 2H, CH_2), 5.50-5.53 (m, 1H, CH−O), 6.78 (d, *J*=8.2 Hz, 2H, $H_{o\text{-NH}}$), 6.95-6.99 (m, 2H, Ar, NH), 7.26 (d, *J*=8.2 Hz, 2H, $H_{m\text{-NH}}$), 7.57 (d, *J*=8.9 Hz, 1H, Ar), 7.63 (d, *J*=8.9 Hz, 1H, Ar), 7.76 (d, *J*=8.7 Hz, 1H, Ar), 8.05 (s, 1H, H-7). ^{13}C NMR

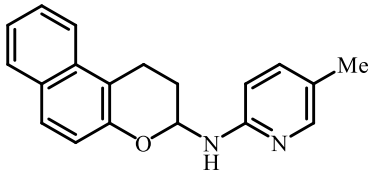
(DMSO-d_6): δ 20.2 (CH_2), 26.6 (CH_2), 80.7 (CH−O), 109.2 (C), 114.3 (C), 116.1 ($2CH_{o\text{-}NH}$), 116.6 (C), 120.9 (CH), 125.0 (CH), 127.4 (CH), 129.7 (CH), 130.3 (C), 130.5 (CH), 131.7 (C), 132.1 ($2CH_{m\text{-}NH}$), 146.1 (C), 151.8 (C−O). IR: 3387 (NH), 1614, 1587, 1514, 1487, 1387, 1312, 1304, 1258, 1221, 1188, 1173, 1148, 1069, 1045, 858, 806, 775. Found (%): C, 52.57; H, 3.56; N, 3.15. Calc. for $C_{19}H_{15}Br_2NO$ (%): C, 52.69; H, 3.49; N, 3.23.

_N_-(2,3-Dihydro-1_H_-benzo[_f_]chromen-3-yl)pyridin-2-amine (2o).



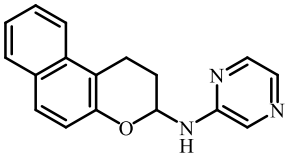
Yield 87 mg (63%), mp: 146-148 °C (MeOH). ^{1}H NMR (DMSO-d_6): δ 2.11-2.14 (m, 1H, CH_2), 2.24-2.27 (m, 1H, CH_2), 3.07-3.24 (m, 2H, CH_2), 6.00-6.04 (m, 1H, CH−O), 6.60-6.66 (m, 2H, NH, Ar), 6.93 (d, *J*=8.7 Hz, 1H, Ar), 7.29-7.34 (m, 1H, Ar), 7.44-7.53 (m, 3H, Ar), 7.62 (d, *J*=8.9 Hz, 1H, Ar), 7.77 (d, *J*=8.0 Hz, 1H, Ar), 7.81 (d, *J*=8.2 Hz, 1H, Ar), 8.03 (d, *J*=3.7 Hz, 1H, Ar). ^{13}C NMR (DMSO-d_6): δ 20.7 (CH_2), 26.9 (CH_2), 78.4 (CH−O), 109.3 (CH), 113.7 (C), 114.3 (CH), 119.6 (CH), 122.5 (CH), 123.7 (CH), 126.9 (CH), 128.1 (CH), 128.7 (CH), 128.9 (C), 133.1 (C), 137.9 (CH), 148.1 (CH), 151.8 (C), 157.7 (C). IR: 3209 (NH), 1622, 1589, 1558, 1514, 1506, 1465, 1421, 1377, 1332, 1261, 1231, 1261, 1230, 1207, 1766, 1140, 1095, 1063, 1045, 1005, 988, 966, 868, 833, 810, 769, 748, 741. Found (%): C, 78.31; H, 5.79; N, 10.02. Calc. for $C_{18}H_{16}N_2O$ (%): C, 78.24; H, 5.84; N, 10.14.

_N_-(2,3-Dihydro-1_H_-benzo[_f_]chromen-3-yl)-5-methylpyridin-2-amine (2p).



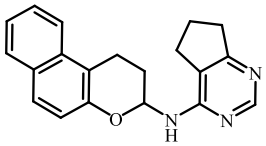
Yield 126 mg (87%), mp: 167-168 ºC (MeOH). ^{1}H NMR (DMSO-d_6): δ 2.05-2.15 (m, 4H, CH_3, CH_2), 2.22-2.26 (m, 1H, CH_2), 3.06-3.23 (m, 2H, CH_2), 5.96-5.99 (m, 1H, CH−O), 6.58 (d, *J*=8.5 Hz, 1H, NH), 6.91 (d, *J*=8.9 Hz, 1H, Ar), 7.29-7.33 (m, 3H, Ar), 7.45-7.49 (m, 1H, Ar), 7.61 (d, *J*=8.9 Hz, 1H, Ar), 7.77 (d, *J*=8.2 Hz, 1H, Ar), 7.81 (d, *J*=8.5 Hz, 1H, Ar), 7.86 (s, 1H, Ar). ^{13}C NMR (DMSO-d_6): δ 17.6 (CH_3), 20.7 (CH_2), 26.9 (CH_2), 78.7 (CH−O), 108.9 (CH), 113.7 (C), 119.6 (CH), 122.5 (CH), 122.6 (C), 123.6 (CH), 126.9 (CH), 128.1 (CH), 128.7 (CH), 128.9 (C), 133.1 (C), 138.7 (CH), 147.6 (CH), 151.9 (C), 155.8 (C). IR: 3408 (NH), 1607, 1595, 1580, 1499, 1466, 1433, 1389, 1369, 1304, 1281, 1260, 1221, 1209, 1175, 1151, 1130, 1043, 1020, 974, 962, 862, 823, 741. Found (%): C, 78.49; H, 6.27; N, 9.55. Calc. for $C_{19}H_{18}N_2O$ (%): C, 78.59; H, 6.25; N, 9.65.

***N*-(2,3-Dihydro-1*H*-benzo[*f*]chromen-3-yl)pyrazin-2-amine (2q).**



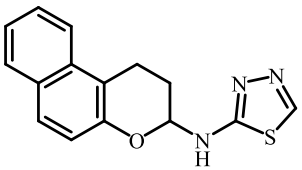
Yield 122 mg (88%), mp: 145-146 °C (MeOH). ^{1}H NMR (DMSO-d_6): δ 2.10-2.19 (m, 1H, CH_2), 2.27-2.30 (m, 1H, CH_2), 3.09-3.24 (m, 2H, CH_2), 5.98-6.03 (m, 1H, CH−O), 6.94 (d, *J*=8.9 Hz, 1H, Ar), 7.30-7.35 (m, 1H, Ar), 7.46-7.51 (m, 1H, Ar), 7.63 (d, *J*=8.9 Hz, 1H, Ar), 7.78 (d, *J*=8.0 Hz, 1H, Ar), 7.83 (d, *J*=8.7 Hz, 1H, Ar), 7.85 (d, *J*=2.8 Hz, 1H, $H_{pyrazine}$), 8.00-8.08 (m, 3H, NH, $H_{pyrazine}$). ^{13}C NMR (DMSO-d_6): δ 20.3 (CH_2), 26.6 (CH_2), 77.7 (CH−O), 113.8 (C), 119.5 (CH), 122.6 (CH), 123.8 (CH), 127.0 (CH), 128.2 (CH), 128.8 (CH), 129.0 (C), 133.0 (C), 133.7 (CH), 134.2 (CH), 142.2 (CH), 151.4 (C), 154.0 (C). IR: 3210 (NH), 1558, 1465, 1422, 1377, 1333, 1231, 1200, 1140, 1045, 868, 810, 741. Found (%): C, 73.54; H, 5.43; N, 15.21. Calc. for $C_{17}H_{15}N_3O$ (%): C, 73.63; H, 5.45; N, 15.15.

***N*-(2,3-Dihydro-1*H*-benzo[*f*]chromen-3-yl)-6,7-dihydro-5*H*-cyclopenta[*d*]pyrimidin-4-amine (2r).**



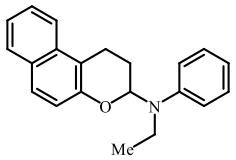
Yield 92 mg (58%), mp: 195-196 ºC (*i*-PrOH). ^{1}H NMR ($CDCl_3$): δ 2.07-2.15 (m, 2H, CH_2), 2.21-2.30 (m, 1H, CH_2), 2.40-2.47 (m, 1H, CH_2), 2.77 (t, *J*=7.3 Hz, 2H, CH_2), 2.97 (t, *J*=7.8 Hz, 2H, CH_2), 3.22-3.26 (m, 2H, CH_2), 5.79 (br. s, 1H, NH), 6.23-6.34 (m, 1H, CH−O), 7.02 (d, *J*=8.7 Hz, 1H, Ar), 7.34-7.38 (m, 1H, Ar), 7.48-7.52 (m, 1H, Ar), 7.61 (d, *J*=8.9 Hz, 1H, Ar), 7.75 (d, *J*=8.0 Hz, 1H, Ar), 7.80 (d, *J*=8.5 Hz, 1H, Ar), 8.53 (s, 1H, $H_{pyrimidine}$). ^{13}C NMR ($CDCl_3$): δ 20.4 (CH_2), 21.6 (CH_2), 27.1 (CH_2), 27.2 (CH_2), 33.7 (CH_2), 77.0 (CH−O), 112.7 (C), 117.3 (C), 119.2 (CH), 122.0 (CH), 123.7 (CH), 126.7 (CH), 128.3 (CH), 128.6 (CH), 129.2 (C), 132.7 (C), 151.0 (C−O), 155.5 ($CH_{pyrimidine}$), 158.2 ($C_{pyrimidine}$), 170.4 ($C_{pyrimidine}$). Found (%): C, 75.56; H, 6.05; N, 13.18. Calc. for $C_{20}H_{19}N_3O$ (%): C, 75.69; H, 6.03; N, 13.24.

***N*-(2,3-Dihydro-1*H*-benzo[*f*]chromen-3-yl)-1,3,4-thiadiazol-2-amine (2s).**



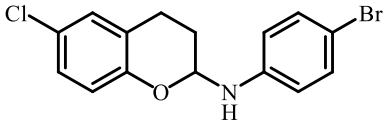
Yield 71 mg (50%), mp: 221-222 ºC (DMF-MeOH). ^{1}H NMR (DMSO-d_6): δ 2.12-2.20 (m, 1H, CH_2), 2.26-2.32 (m, 1H, CH_2), 3.07-3.22 (m, 2H, CH_2), 5.72-5.77 (m, 1H, CH−O), 6.98 (d, *J*=8.7 Hz, 1H, Ar), 7.32-7.36 (m, 1H, Ar), 7.47-7.51 (m, 1H, Ar), 7.65 (d, *J*=8.9 Hz, 1H, Ar), 7.78 (d, *J*=8.3 Hz, Ar), 7.82 (d, *J*=8.5 Hz, Ar), 8.78 (s, 1H, $H_{thiadiazole}$), 8.86 (d, *J*=8.3 Hz, 1H, NH). ^{13}C NMR (DMSO-d_6): δ 19.5 (CH_2), 26.4 (CH_2), 81.4 (CH−O), 114.0 (C), 119.4 (CH), 122.6 (CH), 124.0 (CH), 127.1 (CH), 128.3 (CH), 128.8 (CH), 129.2 (C), 132.9 (C), 144.7 (CH), 150.7 (C), 168.0 (C). Found (%): C, 63.62; H, 4.69; N, 14.77; S, 11.25. Calc. for $C_{15}H_{13}N_3OS$ (%): C, 63.58; H, 4.62; N, 14.83; S, 11.31.

***N*-Ethyl-*N*-phenyl-2,3-dihydro-1*H*-benzo[*f*]chromen-3-amine (2t).**



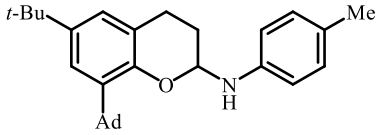
Yield 94 mg (62%), mp: 102-103 °C (MeOH). ^{1}H NMR (DMSO-d_6): δ 1.17 (t, J=7.1 Hz, 3H, CH_3), 2.24-2.32 (m, 2H, CH_2), 3.16-3.21 (m, 2H, CH_2), 3.34-3.43 (m, 1H, C$\underline{H}_2$CH$_3$), 3.57-3.66 (m, 1H, C$\underline{H}_2$CH$_3$), 5.62 (dd, J=9.4 Hz, J=2.5 Hz, 1H, CH−O), 6.77 (t, J=7.3 Hz, 1H, Ar), 6.97-7.02 (m, 3H, Ar), 7.17-7.23 (m, 2H, Ar), 7.30-7.34 (m, 1H, Ar), 7.45-7.50 (m, 1H, Ar), 7.65 (d, J=8.9 Hz, 1H, Ar), 7.77-7.81 (m, 2H, Ar). ^{13}C NMR (DMSO-d_6): δ 15.6 (CH_3), 23.0 (CH_2), 26.5 (CH_2), 40.5 (CH_2N), 87.2 (CH−O), 114.0 (C), 116.4 (2CH), 119.5 (2CH), 122.6 (CH), 123.7 (CH), 127.0 (CH), 128.2 (CH), 128.8 (CH), 129.0 (C), 129.6 (2CH), 133.0 (C), 148.2 (C), 153.0 (C). IR: 1620, 1597, 1504, 1466, 1259, 1223, 1209, 1192, 1123, 1067, 1030, 1015, 966, 910, 860, 852, 812, 744, 694. Found (%): C, 83.19; H, 6.95; N, 4.51. Calc. for $C_{21}H_{21}NO$ (%): C, 83.13; H, 6.98; N, 4.62.

***N*-(4-Bromophenyl)-6-chlorochroman-2-amine (2u).**

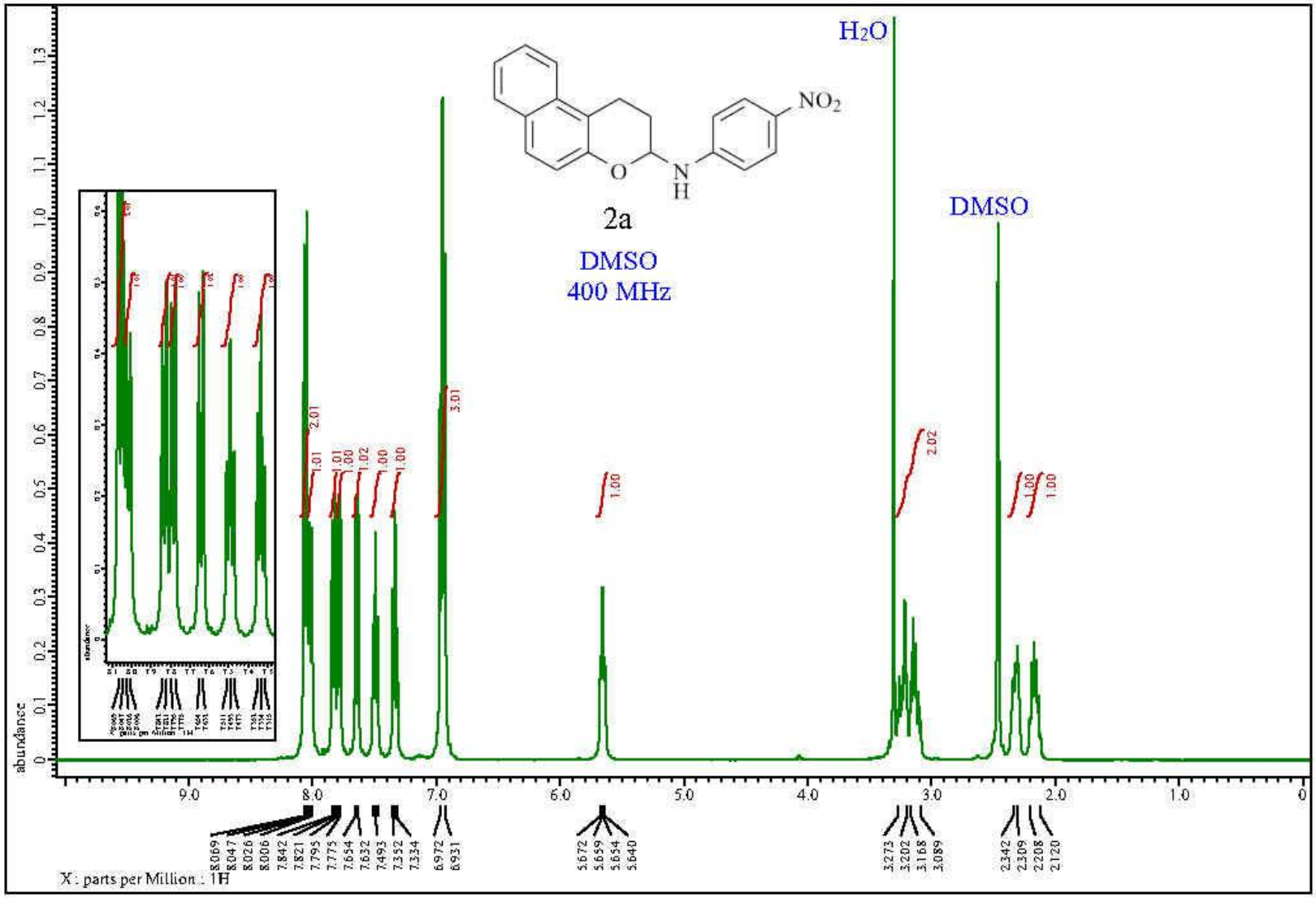


Yield 86 mg (51%), mp: 132-133 ºC (MeOH). ^{1}H NMR ($CDCl_3$): δ 1.95-2.06 (m, 1H, CH_2), 2.23-2.29 (m, 1H, CH_2), 2.82-3.03 (m, 2H, CH_2), 4.55 (br. s, 1H, NH), 5.39 (d, J=6.4 Hz, 1H, CH−O), 6.69-6.75 (m, 3H, Ar), 7.02-7.08 (m, 2H, Ar), 7.30 (d, J=8.5 Hz, 2H, Ar). ^{13}C NMR ($CDCl_3$): δ 23.7 (CH_2), 27.2 (CH_2), 80.9 (CH−O), 111.5 (C), 116.1 (2CH$_{o\text{-NH}}$), 118.7 (CH), 122.6 (C), 125.4 (C), 127.7 (CH), 128.9 (CH), 132.2 (2CH$_{m\text{-NH}}$), 144.0 (C), 152.2 (C). Found (%):C, 53.12; H, 3.80; N, 4.03. Calc. for $C_{15}H_{13}BrClNO$ (%): C, 53.20; H, 3.87; N, 4.14.

8-(Adamantan-1-yl)-6-(*tert*-butyl)-*N*-(*p*-tolyl)chroman-2-amine (2v).



Yield 110 mg (51%), mp: 151-152 ºC (*i*-PrOH). ^{1}H NMR ($CDCl_3$): δ 1.29 (s, 9H, *t*-Bu), 1.42-1.47 (m, 3H, Ad), 1.54-1.58 (m, 3H, Ad), 1.83 (br. s, 3H, Ad), 1.90-2.02 (m, 7H, Ad, CH_2), 2.24-2.32 (m, 4H, CH_3, CH_2), 2.84-2.91 (m, 1H, CH_2), 2.99-3.08 (m, 1H, CH_2), 4.33 (d, J=10.8 Hz, 1H, NH), 5.51 (t, J=8.7 Hz, 1H, CH−O), 6.76 (d, J=8.0 Hz, 2H$_{p\text{-tolyl}}$), 6.93 (s, 1H, Ar), 6.99 (d, J=8.0 Hz, 2H$_{p\text{-tolyl}}$), 7.07 (s, 1H, Ar). ^{13}C NMR ($CDCl_3$): δ 20.6 (CH_3), 25.3 (CH_2), 28.0 (CH_2), 29.1 (3CH$_{Ad}$), 31.7 (3CH$_3$ $_{t\text{-Bu}}$), 34.3 (C$_{t\text{-Bu}}$), 36.9 (3CH$_2$ $_{Ad}$), 37.2 (C$_{Ad}$), 40.5 (3CH$_2$ $_{Ad}$), 81.1 (CH−O), 115.2 (2CH$_{o\text{-NH}}$), 120.5 (C), 122.0 (CH), 123.6 (CH), 128.7 (C), 129.6 (2CH$_{m\text{-NH}}$), 137.9 (C), 142.1 (C), 143.0 (C), 150.6 (C-8a). IR: 3395 (NH), 2959, 2899, 2849, 1616, 1518, 1464, 1298, 1198, 1184, 1177, 1167, 1123, 1036, 997, 976, 928, 891, 862, 812. Found (%): C, 88.79; H, 9.18; N, 3.18. Calc. for $C_{30}H_{39}NO$ (%): C, 88.87; H, 9.15; N, 3.26.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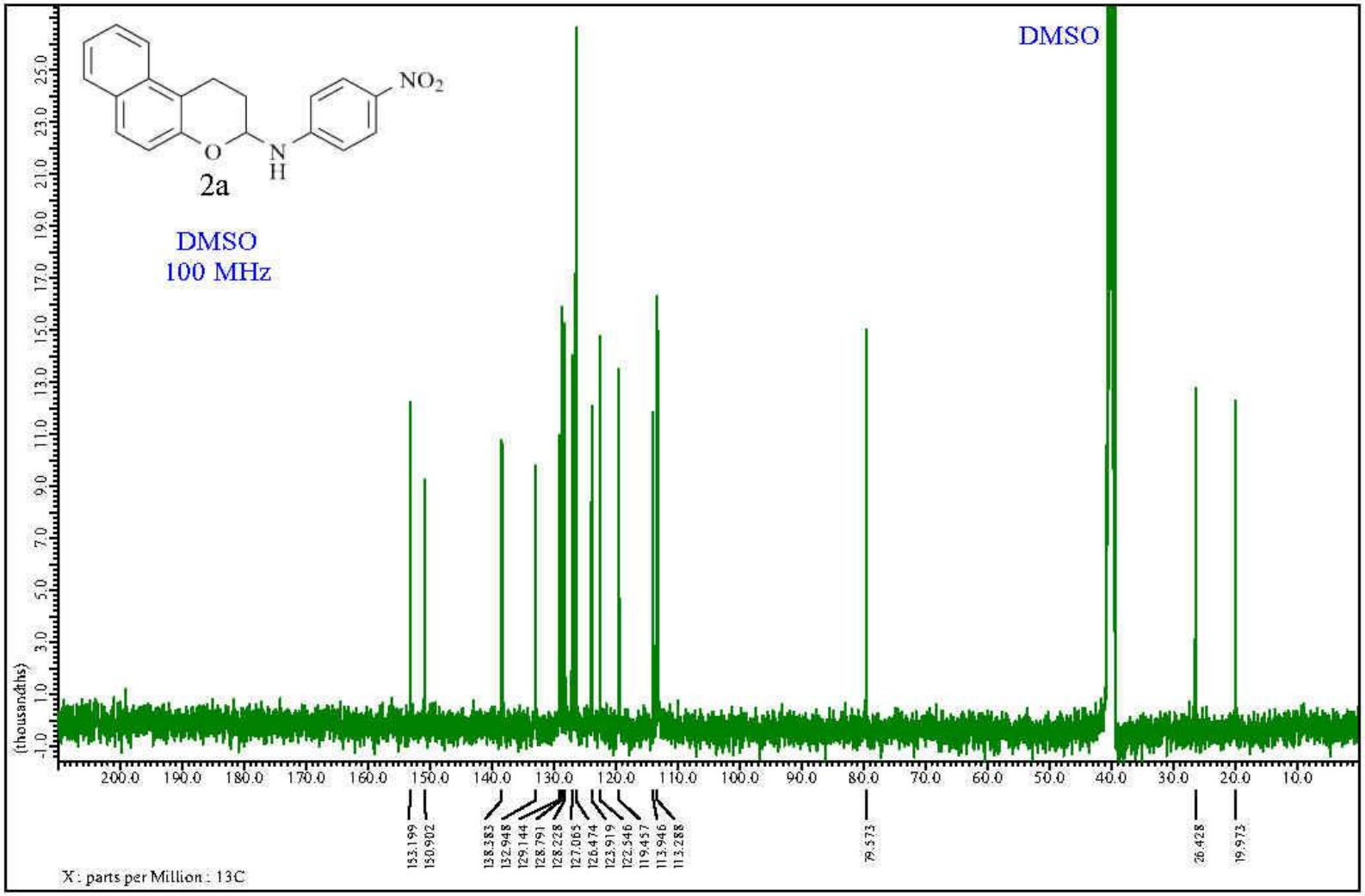
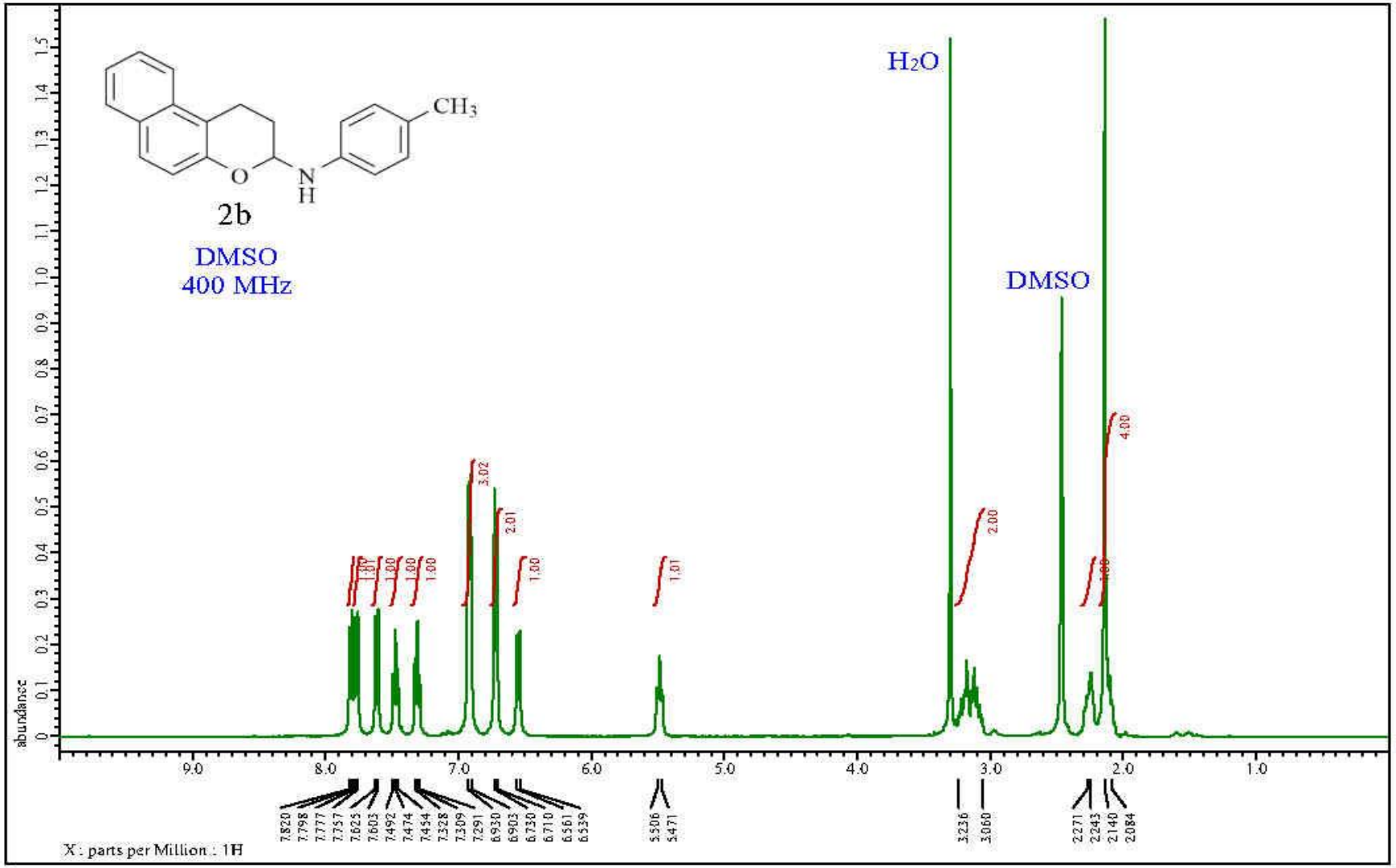
DMSO
NO2
O
N
H
2a
DMSO
400 MHz
abundance
X : parts per Million : 1H


DMSO
2a
DMSO
100 MHz
(thousandths)
X: parts per Million : 13C
153.199
150.902
138.383
132.948
129.144
128.791
128.228
127.065
126.474
123.919
122.546
119.457
113.946
113.288
79.573
26.428
19.973


2b
DMSO
400 MHz
H2O
DMSO
CH3
O
N
H
abundance
X : parts per Million : 1H
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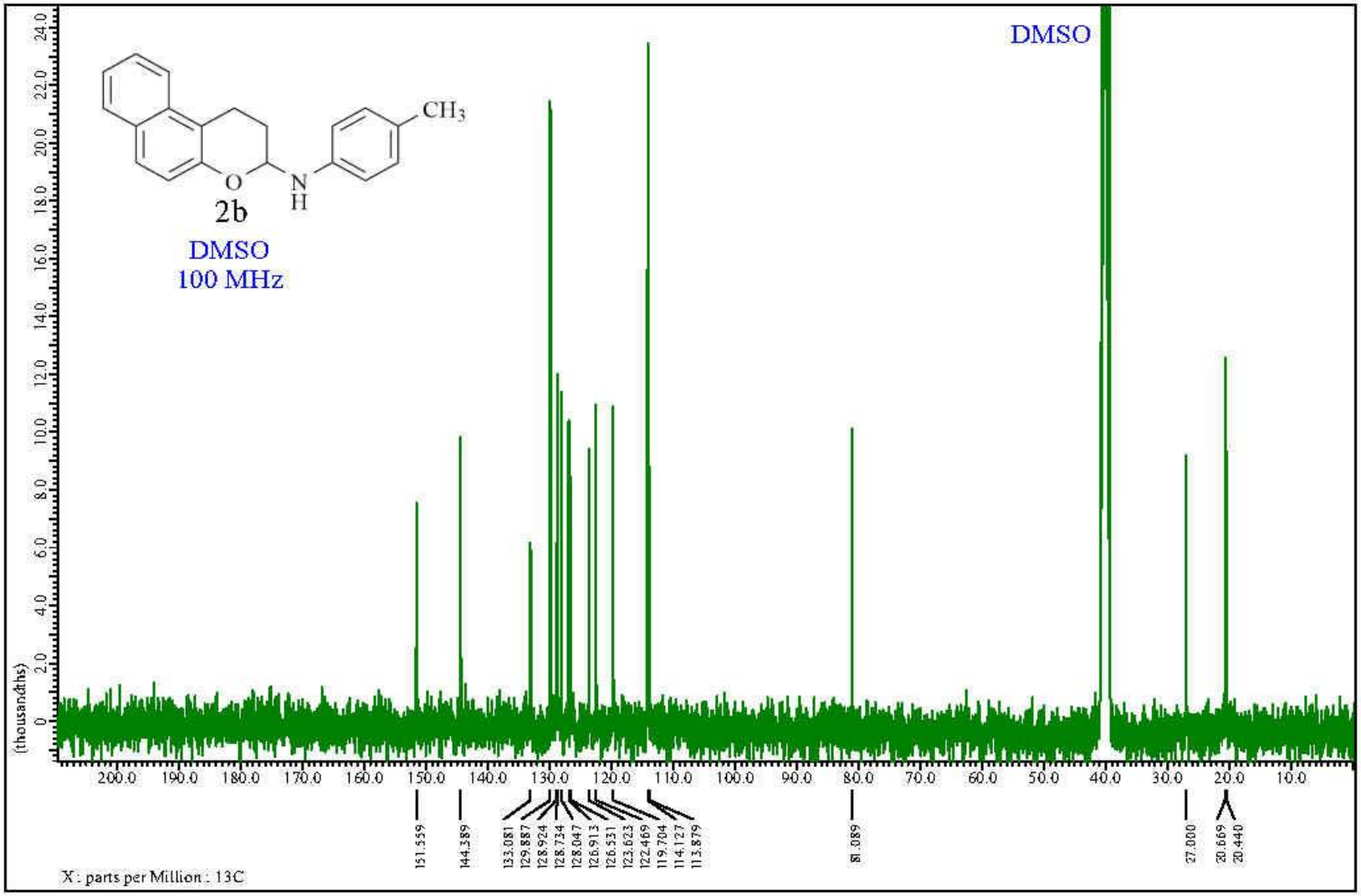
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
3.02
2.01
1.00
1.01
2.00
4.00
7.820
7.798
7.777
7.757
7.625
7.603
7.492
7.474
7.454
7.328
7.309
7.291
6.930
6.903
6.730
6.710
6.561
6.539
5.506
5.471
3.236
3.060
2.271
2.243
2.140
2.084


DMSO
2b
DMSO
100 MHz
(thousandths)
X : parts per Million : 13C
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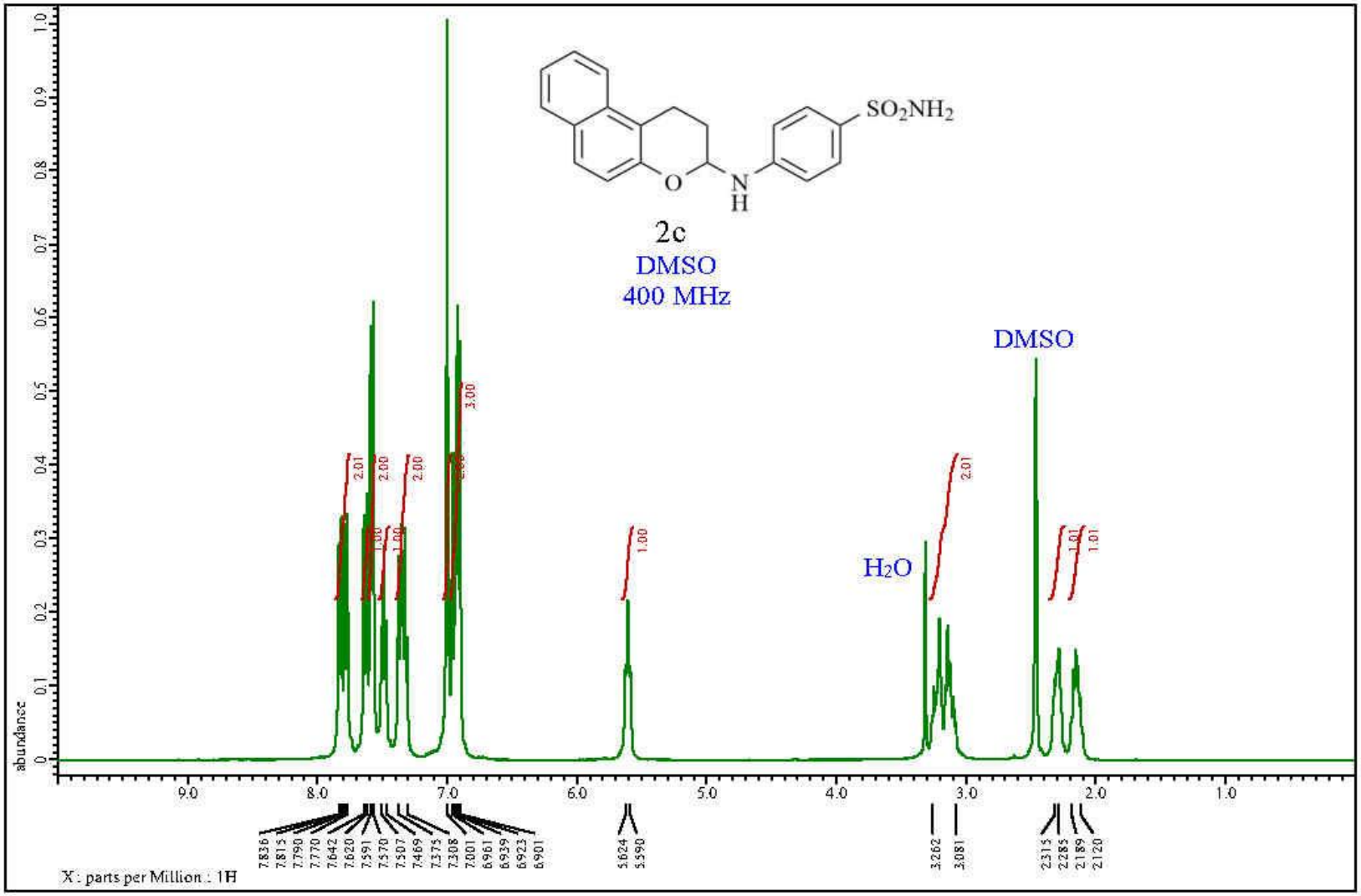
144.389
133.081
129.887
128.924
128.734
128.047
126.913
126.531
123.623
122.469
119.704
114.127
113.879
81.089
27.000
20.669
20.440


SO2NH2
O
N
H
2c
DMSO
400 MHz
DMSO
H2O
abundance
X : parts per Million : 1H
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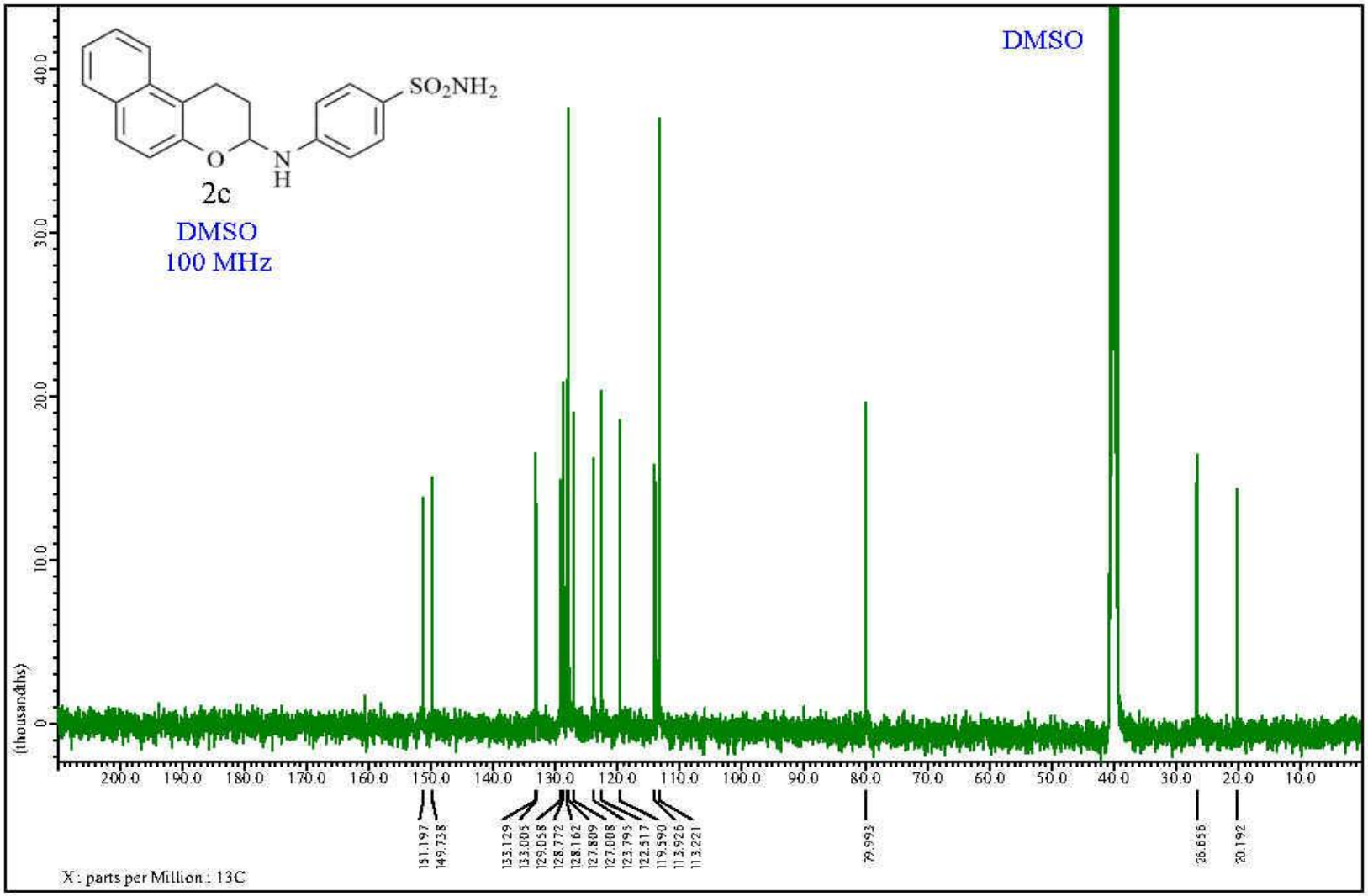
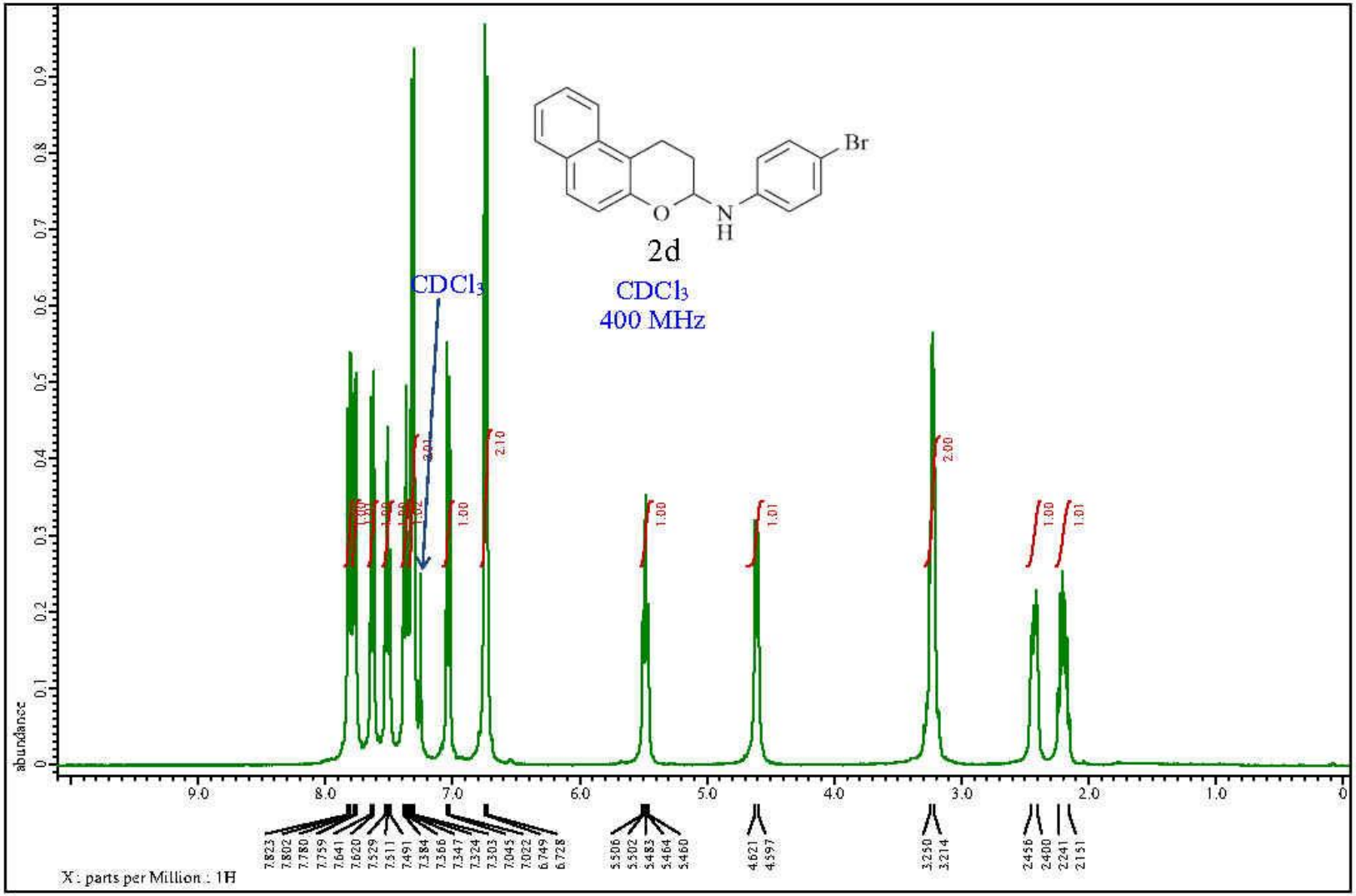
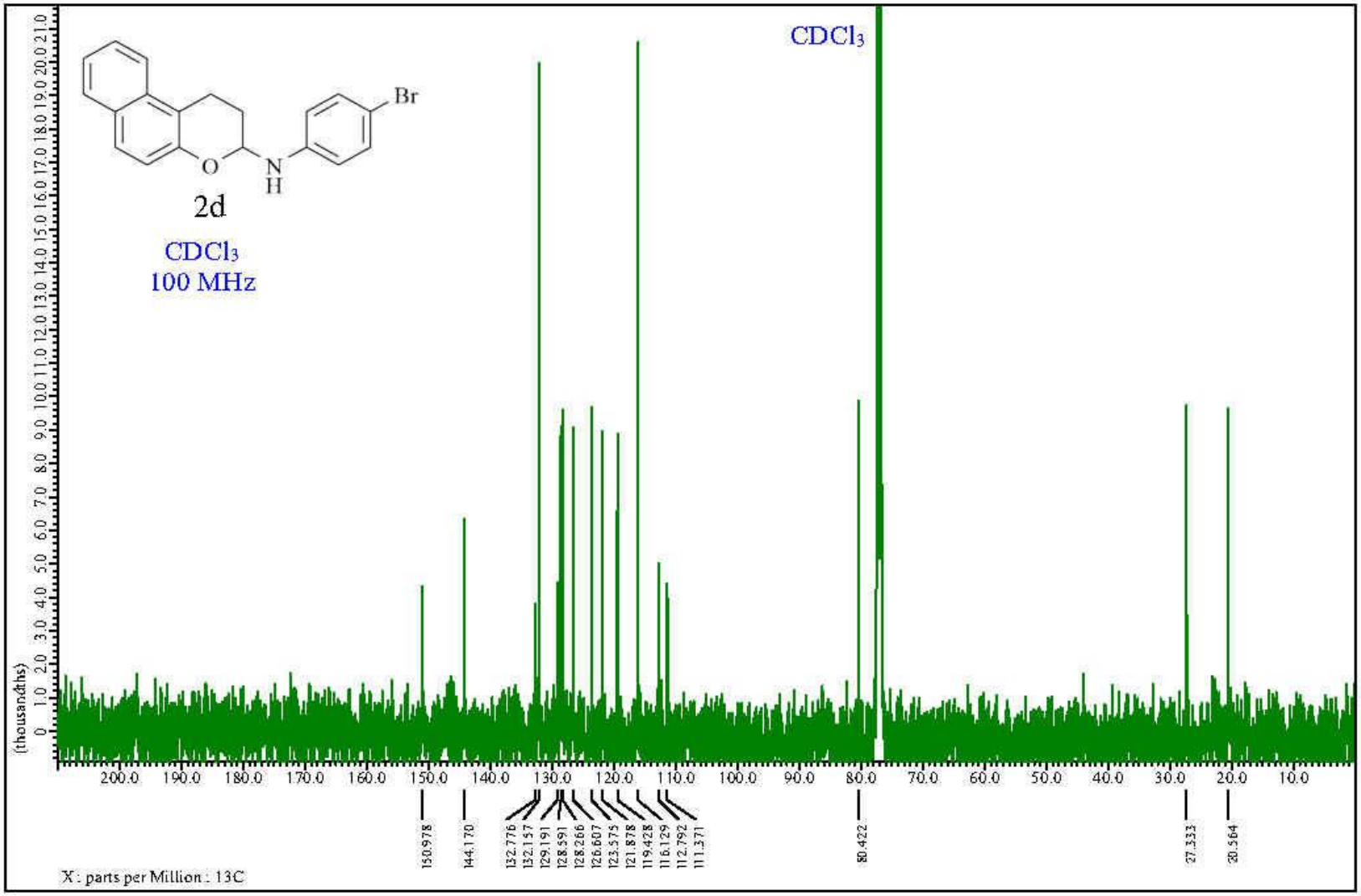
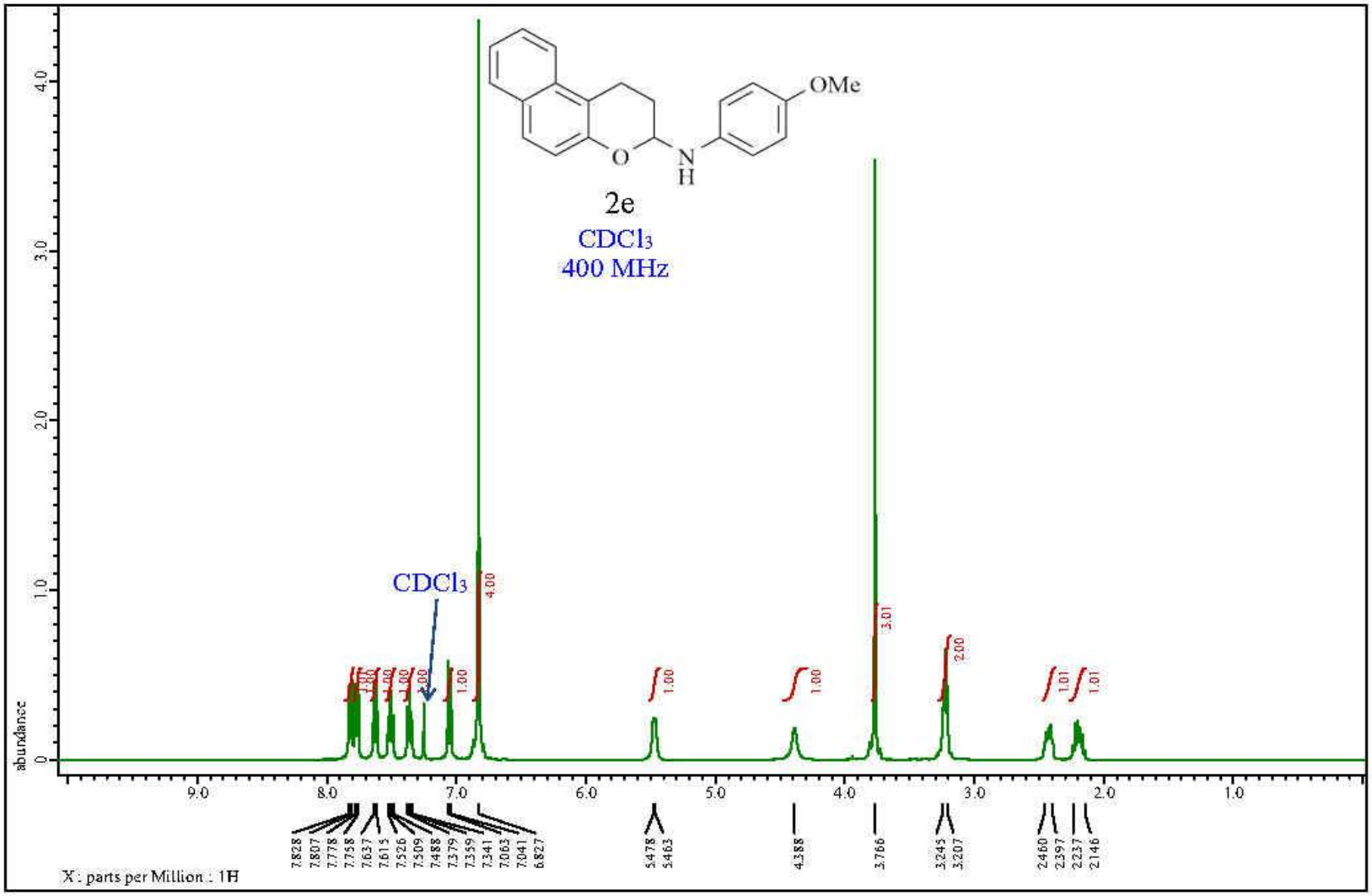
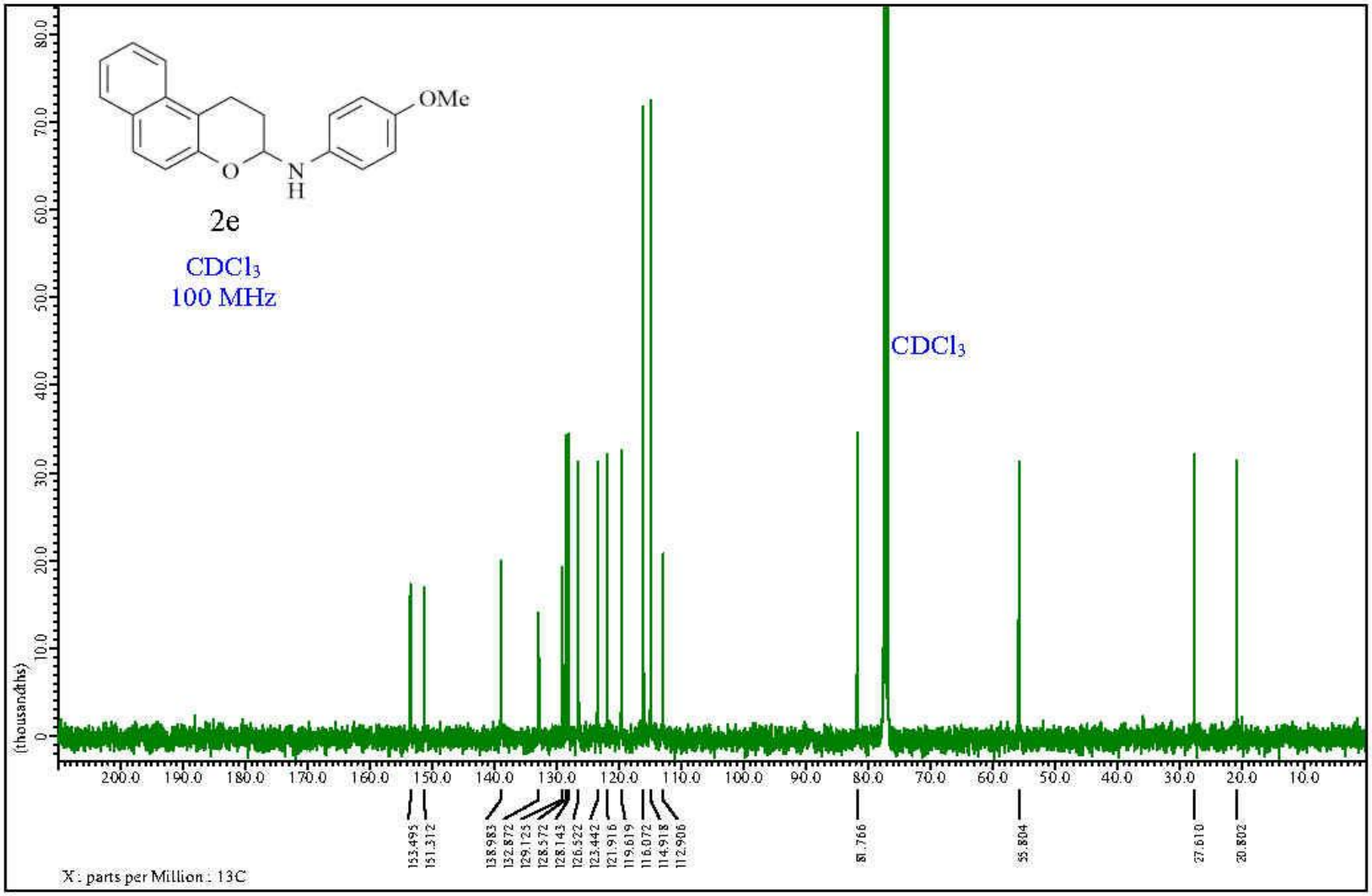
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
2.01
2.00
3.00
1.00
2.01
1.01
1.01
7.836
7.815
7.790
7.770
7.642
7.620
7.591
7.570
7.507
7.469
7.375
7.308
7.001
6.961
6.939
6.923
6.901
5.624
5.590
3.262
3.081
2.315
2.285
2.189
2.120

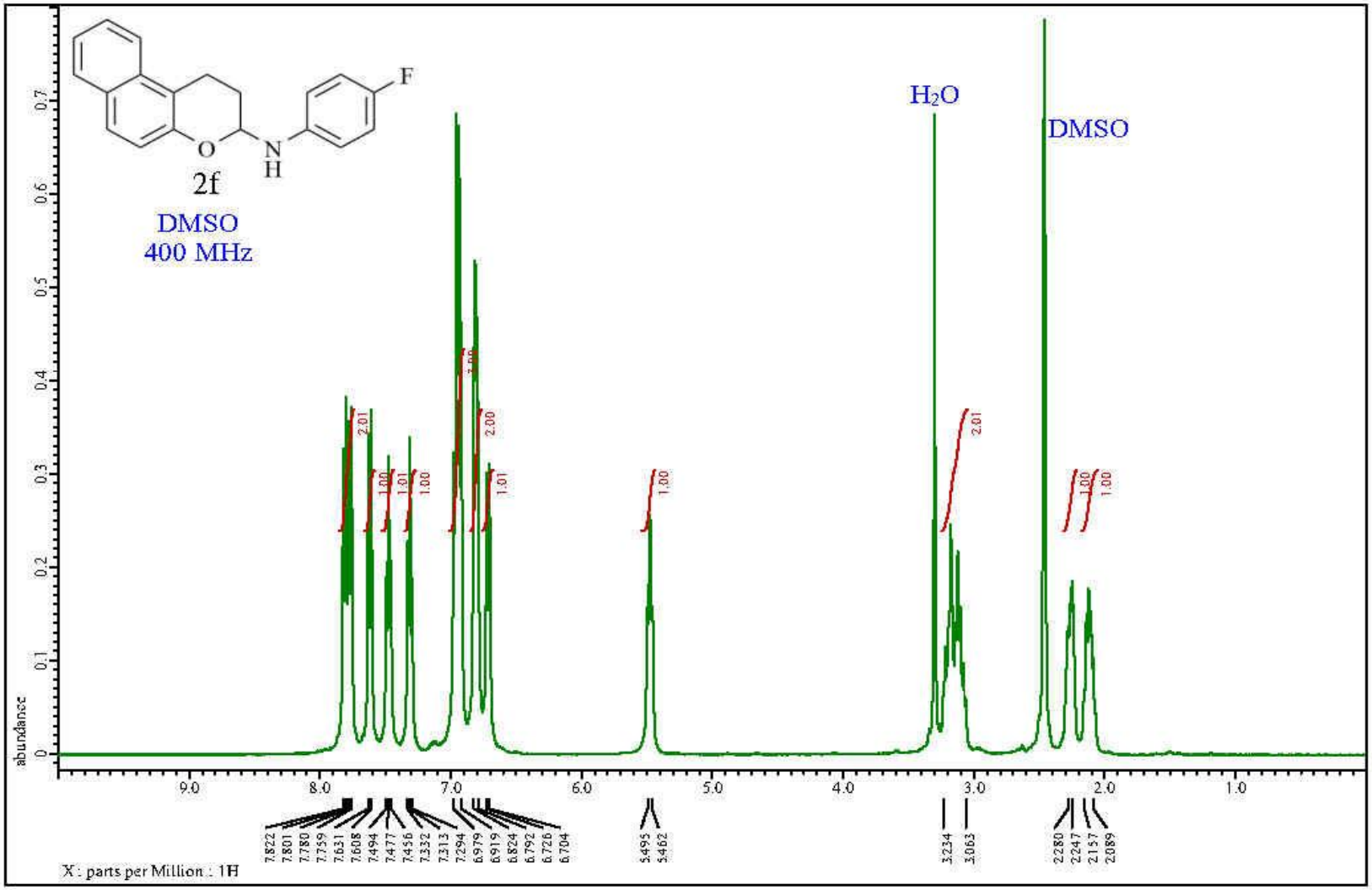

DMSO
SO_2NH_2
O
N
H
2c
DMSO
100 MHz
(thousandths)
40.0
30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
151.197
149.738
133.129
133.005
129.058
128.772
128.162
127.809
127.008
123.795
122.517
119.590
113.926
113.221
79.993
26.656
20.192
X : parts per Million : 13C

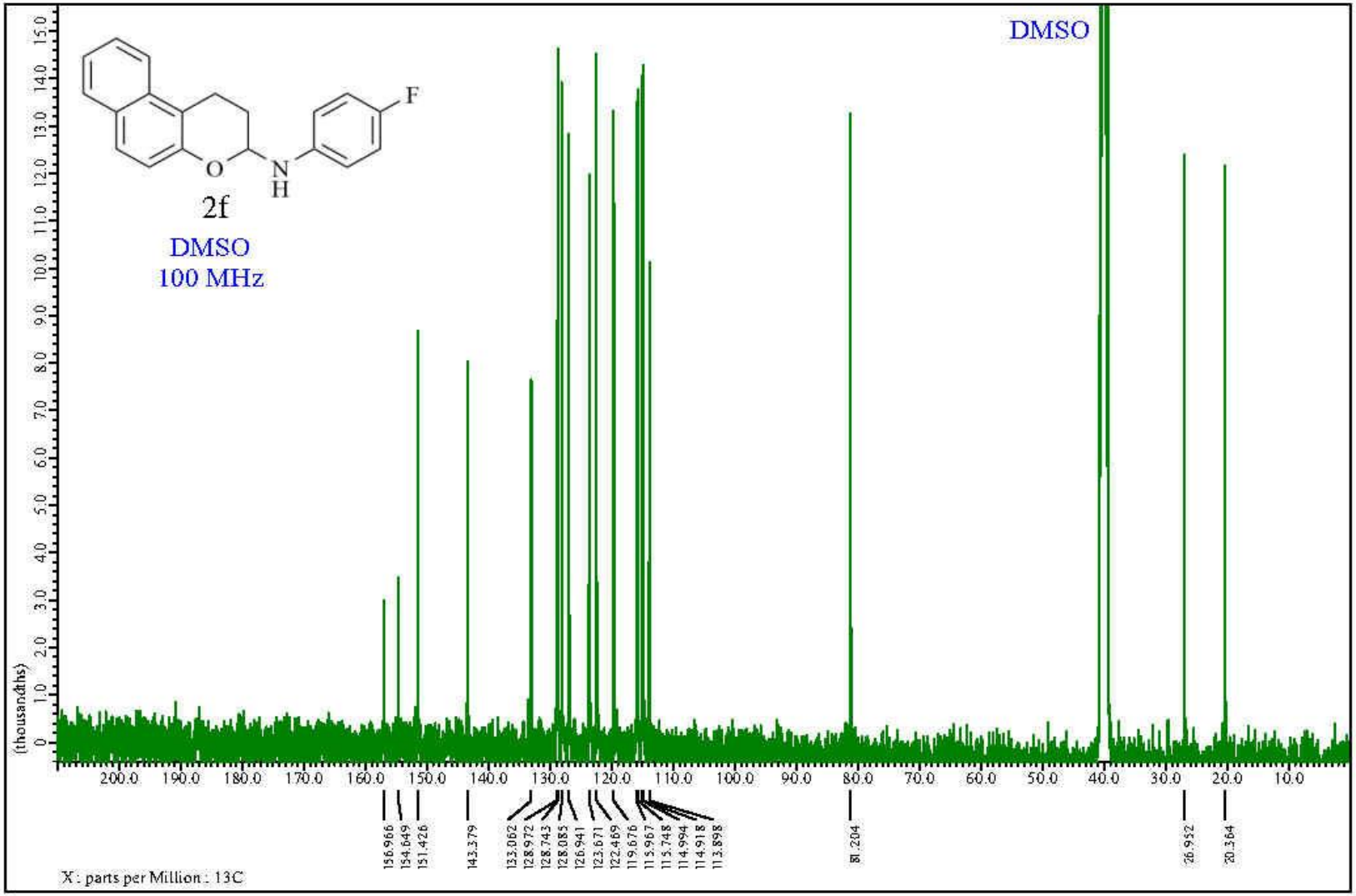

Br
O
N
H
2d
CDCl3
CDCl3
400 MHz
abundance
X : parts per Million : 1H

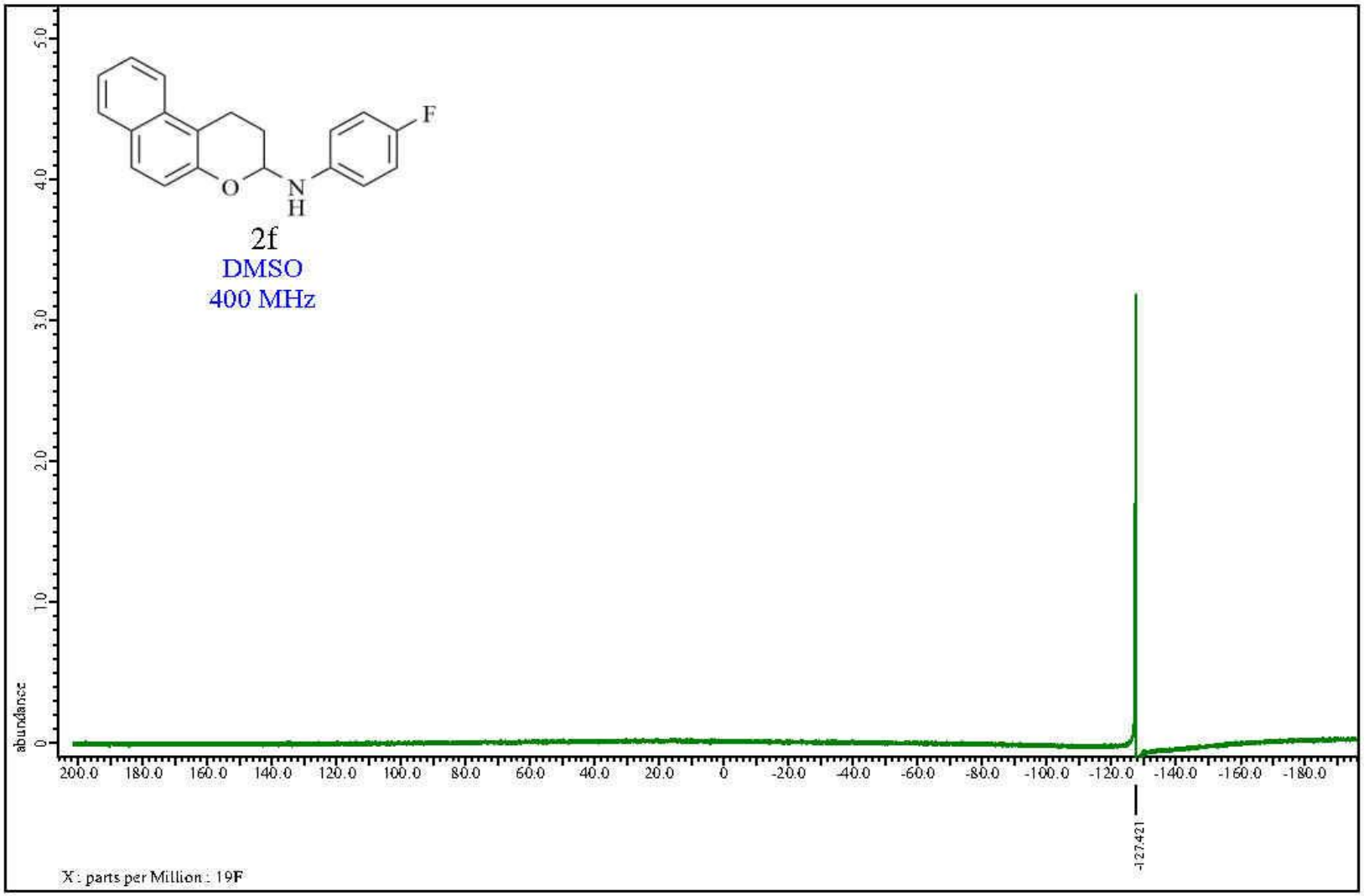

Br
O
N
H
2d
CDCl3
100 MHz
CDCl3
(thousandths)
X : parts per Million : 13C
150.978
144.170
132.776
132.157
129.191
128.591
128.266
126.607
123.575
121.878
119.428
116.129
112.792
111.371
80.422
27.333
20.364


OMe
O
N
H
2e
CDCl3
400 MHz
CDCl3
abundance
4.00
1.00
1.00
3.01
2.00
1.01
1.01
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.828
7.807
7.778
7.758
7.637
7.615
7.526
7.509
7.488
7.379
7.359
7.341
7.063
7.041
6.827
5.478
5.463
4.388
3.766
3.245
3.207
2.460
2.397
2.237
2.146
X : parts per Million : 1H


OMe
O
N
H
2e
CDCl3
100 MHz
CDCl3
(thousandths)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
153.495
151.312
138.983
132.872
129.125
128.572
128.143
126.522
123.442
121.916
119.619
116.072
114.918
112.906
81.766
55.804
27.610
20.802
X : parts per Million : 13C


2f
DMSO
400 MHz
H2O
DMSO
abundance
X : parts per Million : 1H


2f
DMSO
100 MHz
DMSO
(thousandths)
X : parts per Million : 13C
156.966
154.649
151.426
143.379
133.062
128.972
128.743
128.083
126.941
123.671
122.469
119.676
115.967
115.748
114.994
114.918
113.898
81.204
26.952
20.364


F
O
N
H
2f
DMSO
400 MHz
abundance
5.0
4.0
3.0
2.0
1.0
0
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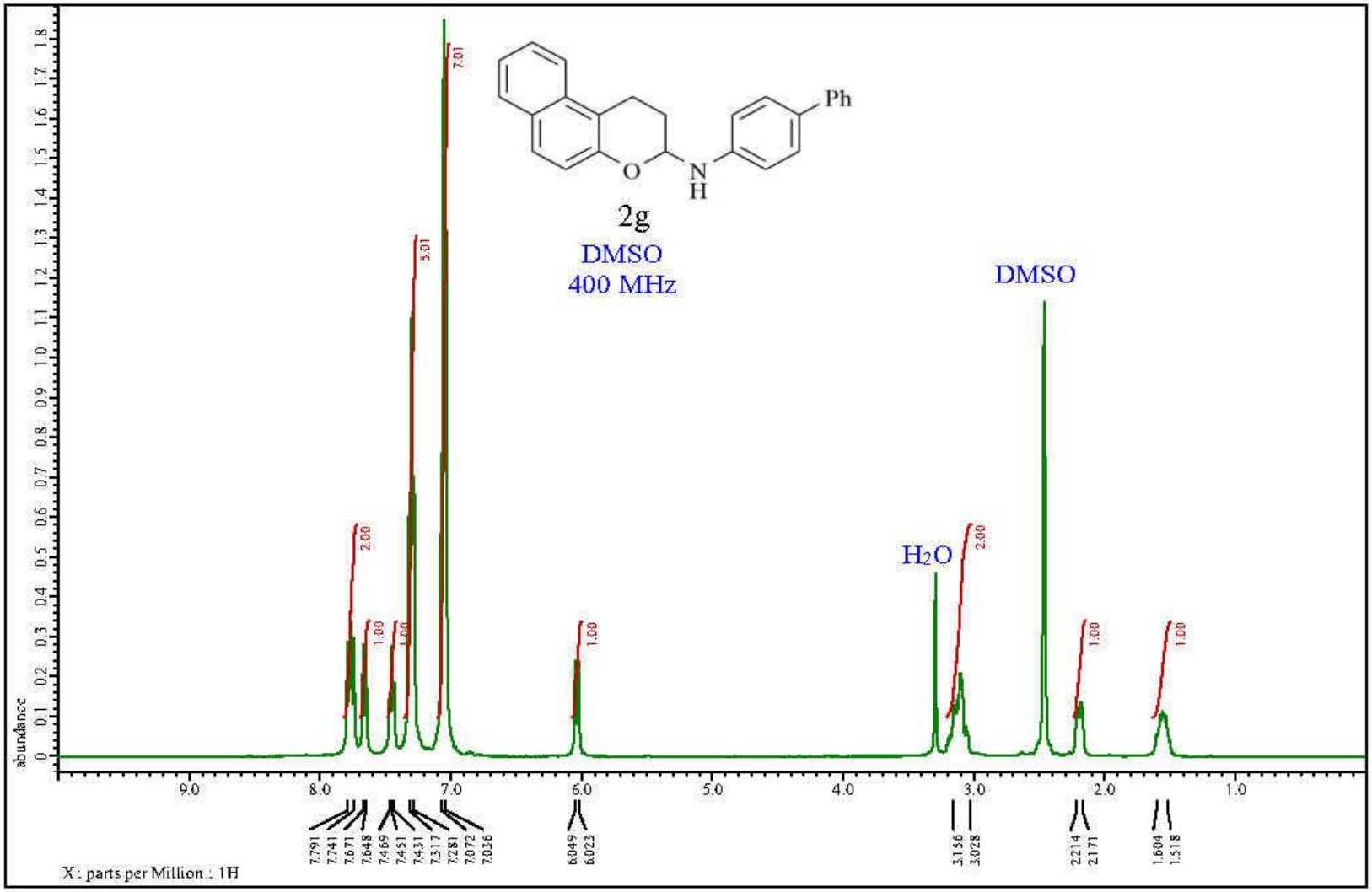
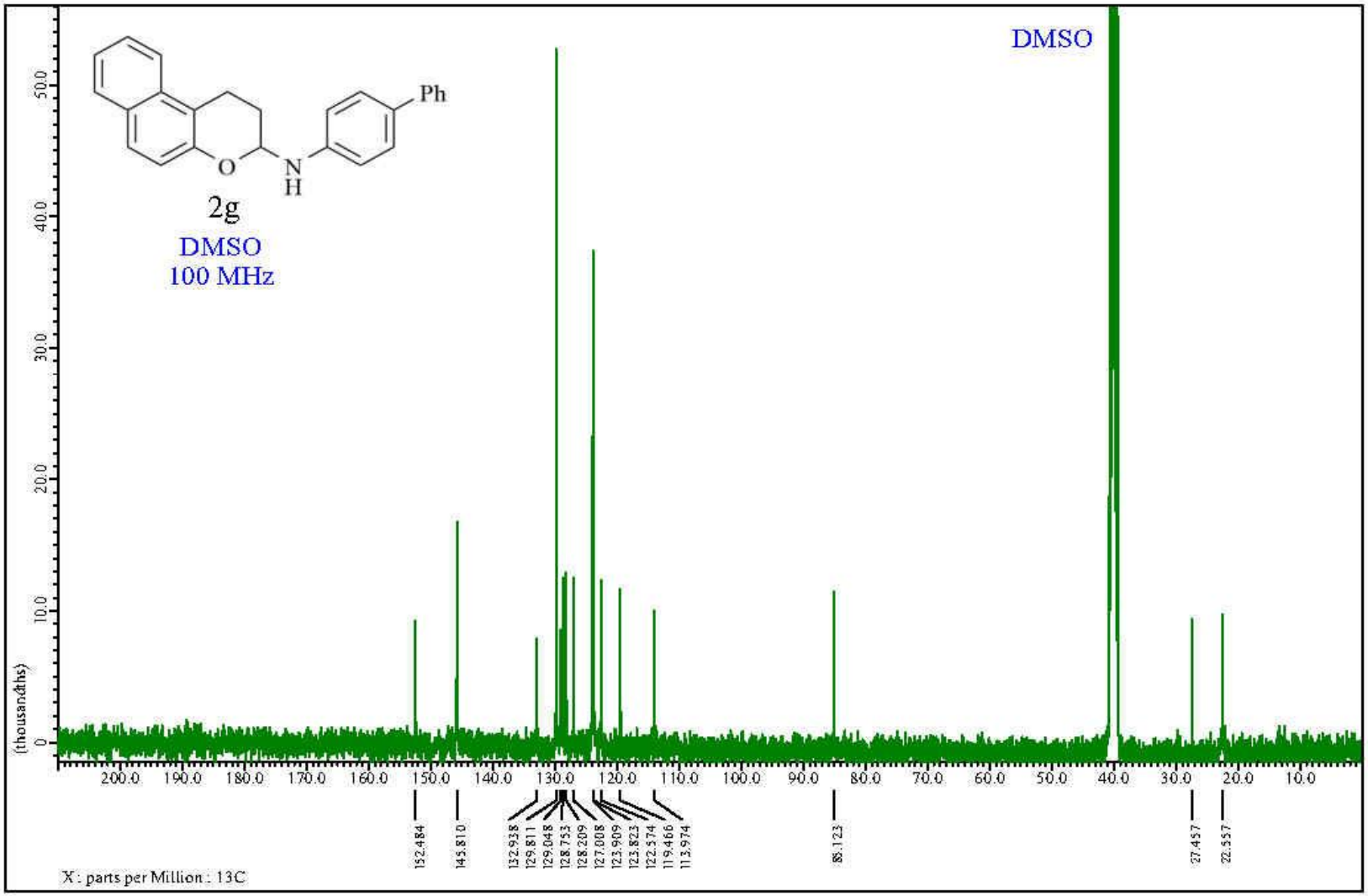
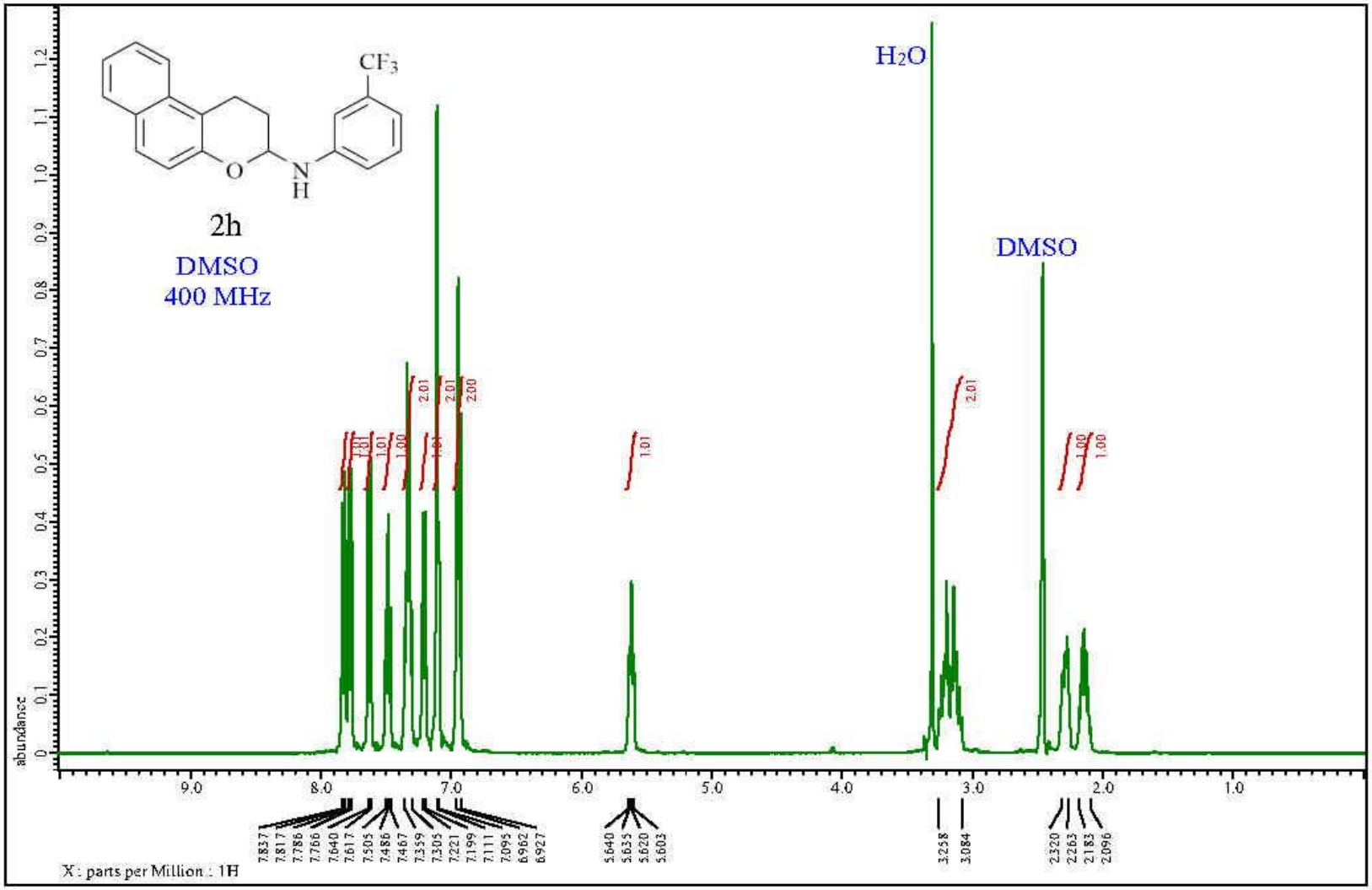
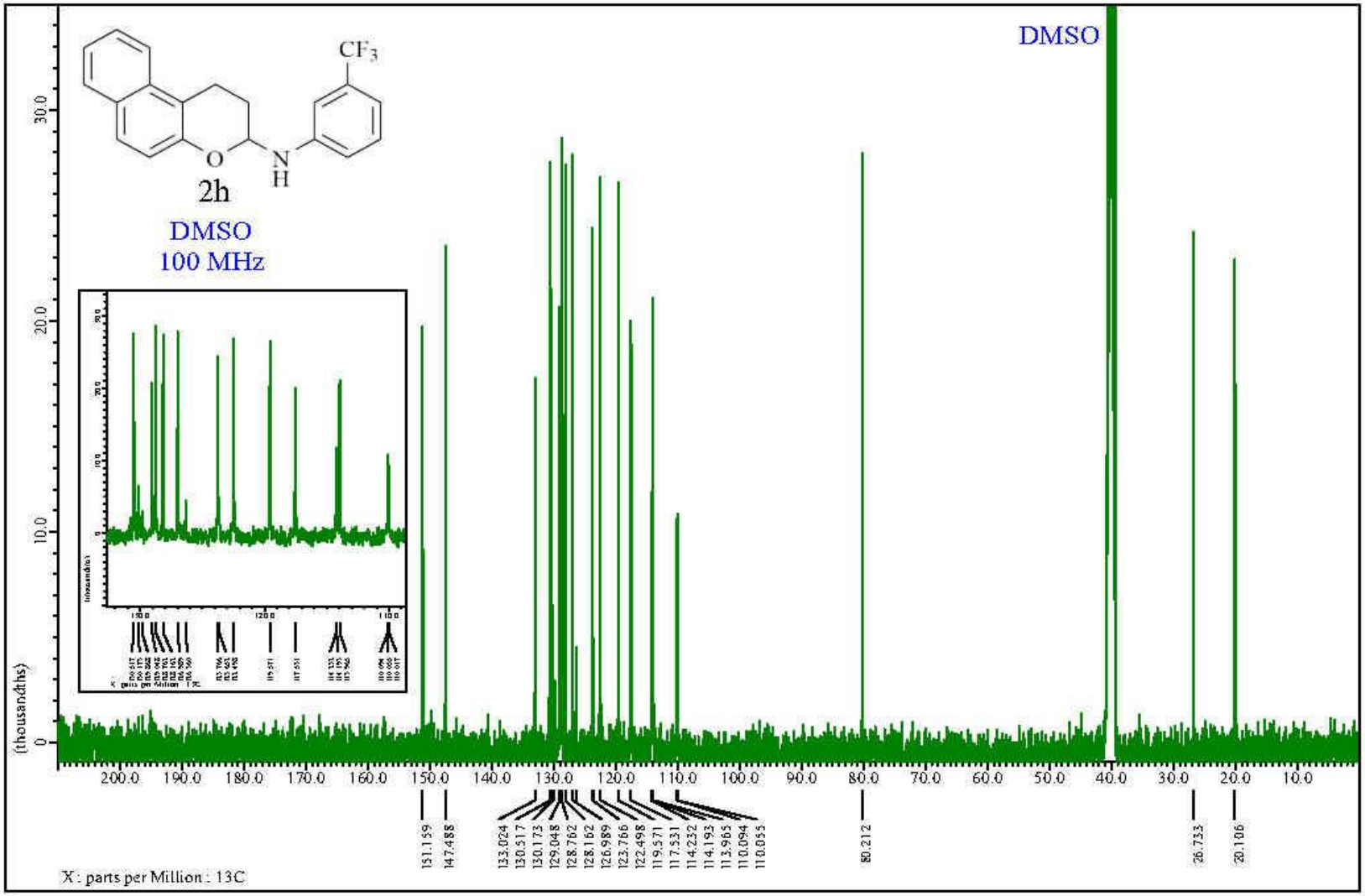
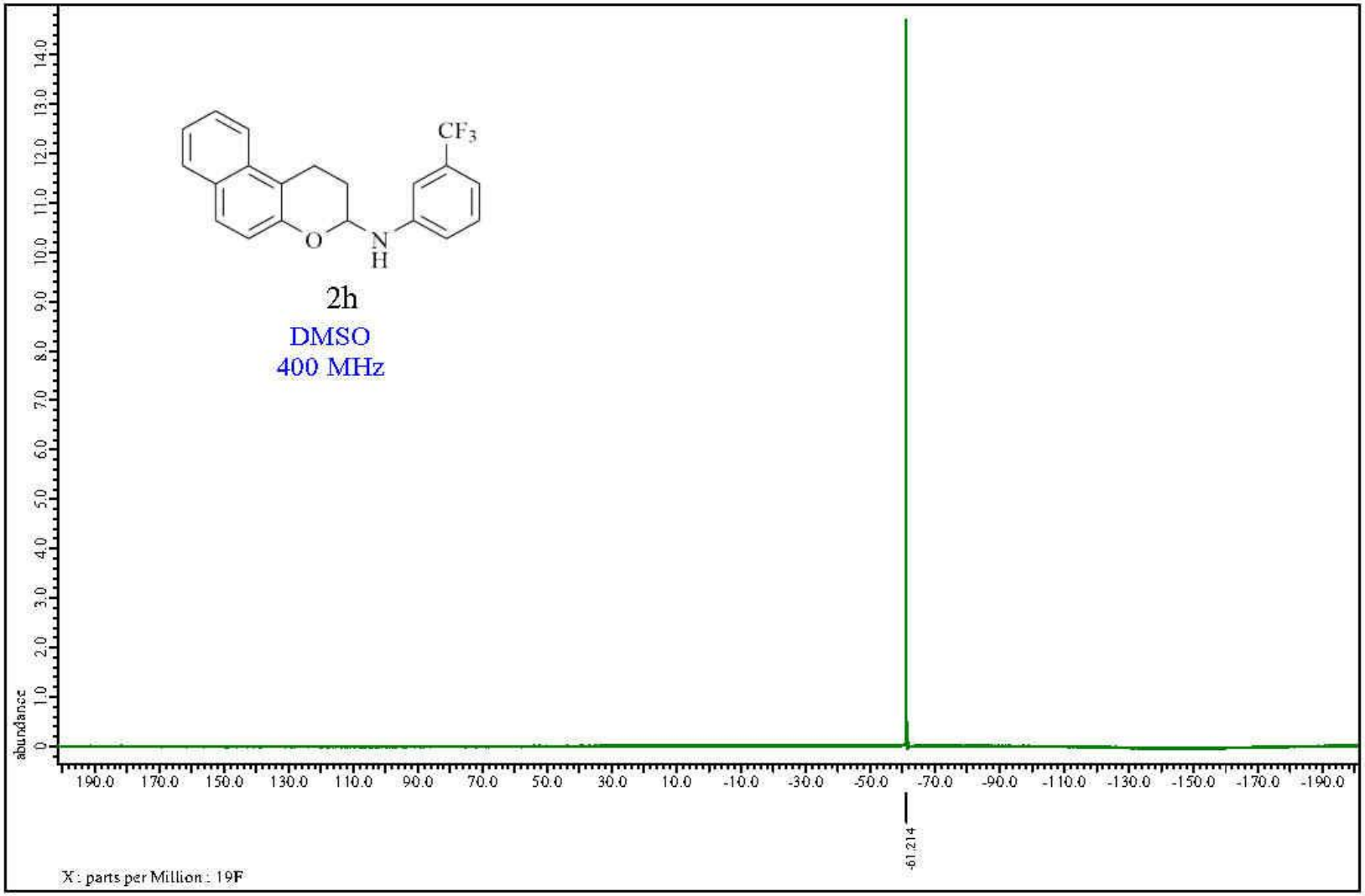
-127.421
X : parts per Million : 19F


Ph
O
N
H
2g
DMSO
400 MHz
DMSO
H2O
abundance
X : parts per Million : 1H


DMSO
Ph
O
N
H
2g
DMSO
100 MHz
(thousandths)
50.0
40.0
30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
152.484
145.810
132.938
129.811
129.048
128.753
128.209
127.008
123.909
123.823
122.574
119.466
113.974
85.123
27.457
22.557
X : parts per Million : 13C


2h
DMSO
400 MHz
H2O
DMSO
abundance
X : parts per Million : 1H


CF3
O
N
H
2h
DMSO
100 MHz
DMSO
(thousandths)
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
151.159
147.488
133.024
130.517
130.173
129.048
128.762
128.162
126.989
123.766
122.498
119.571
117.531
114.232
114.193
113.965
110.094
110.055
80.212
26.733
20.106
X : parts per Million : 13C


CF3
O
N
H
2h
DMSO
400 MHz
abundance
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
190.0
170.0
150.0
130.0
110.0
90.0
70.0
50.0
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-190.0
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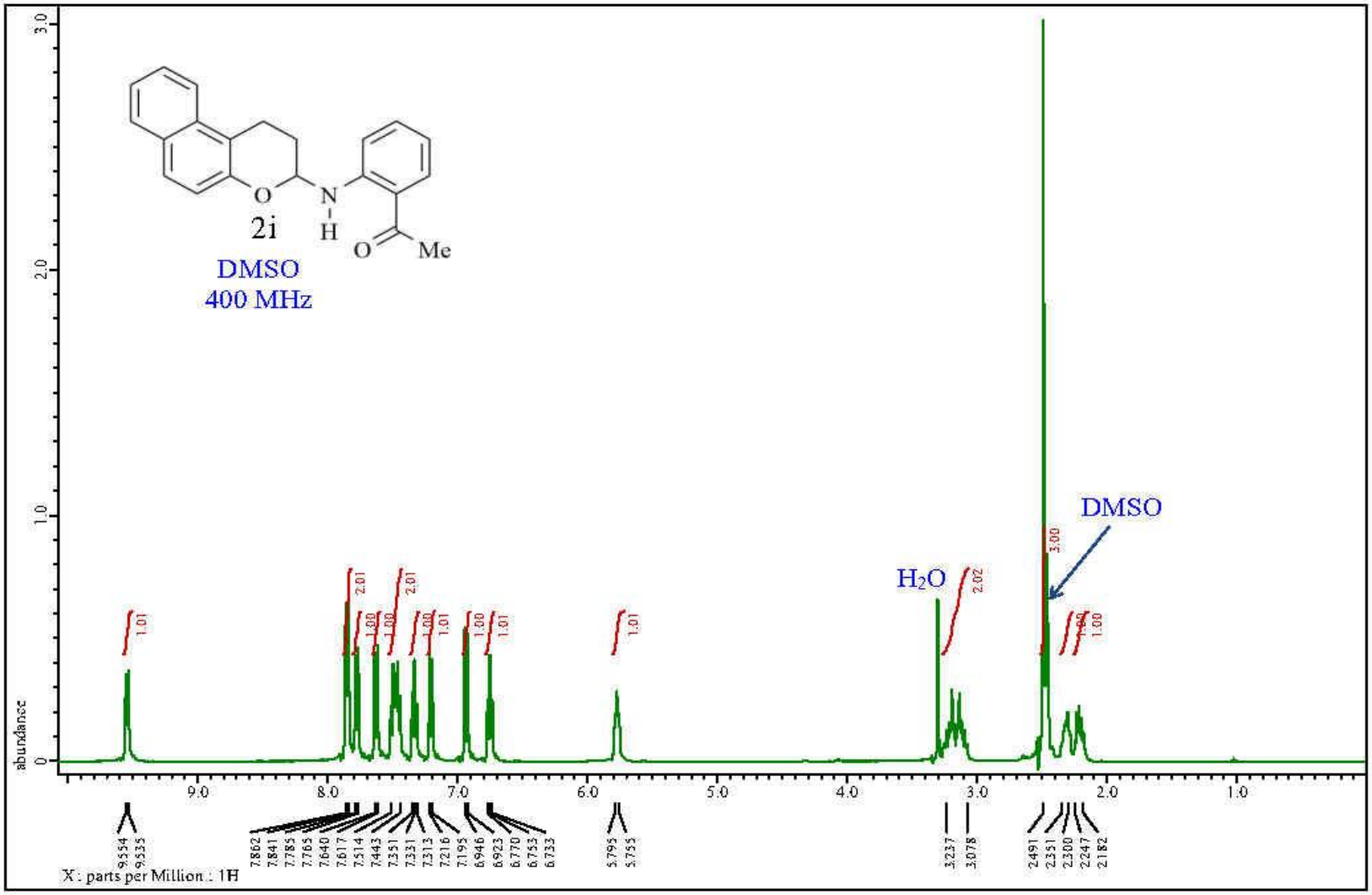
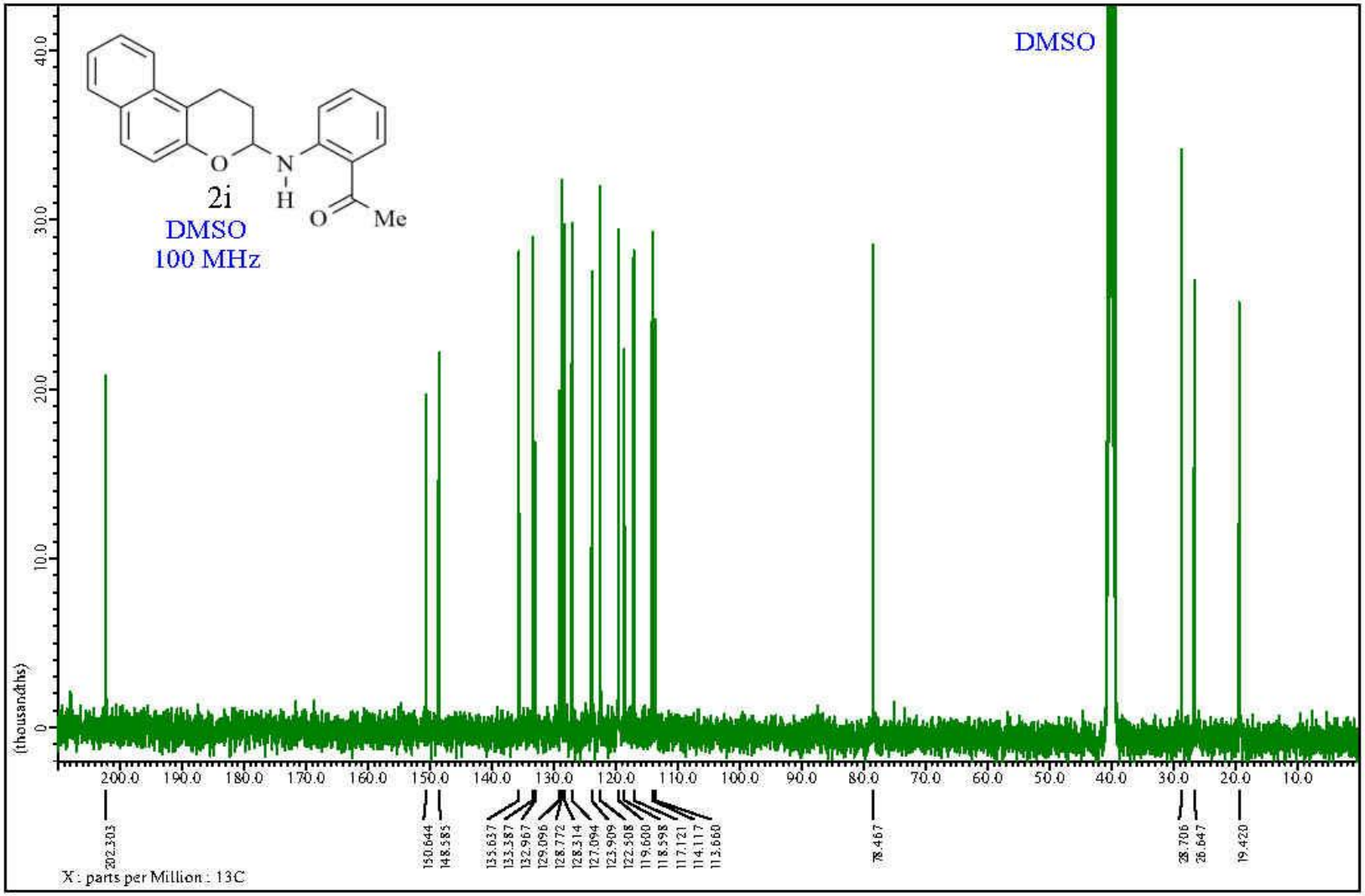

2i
DMSO
400 MHz
DMSO
H2O
abundance
X : parts per Million : 1H


2i
DMSO
100 MHz
DMSO
(thousandths)
X : parts per Million : 13C
202.303
150.644
148.585
135.637
133.387
132.967
129.096
128.772
128.314
127.094
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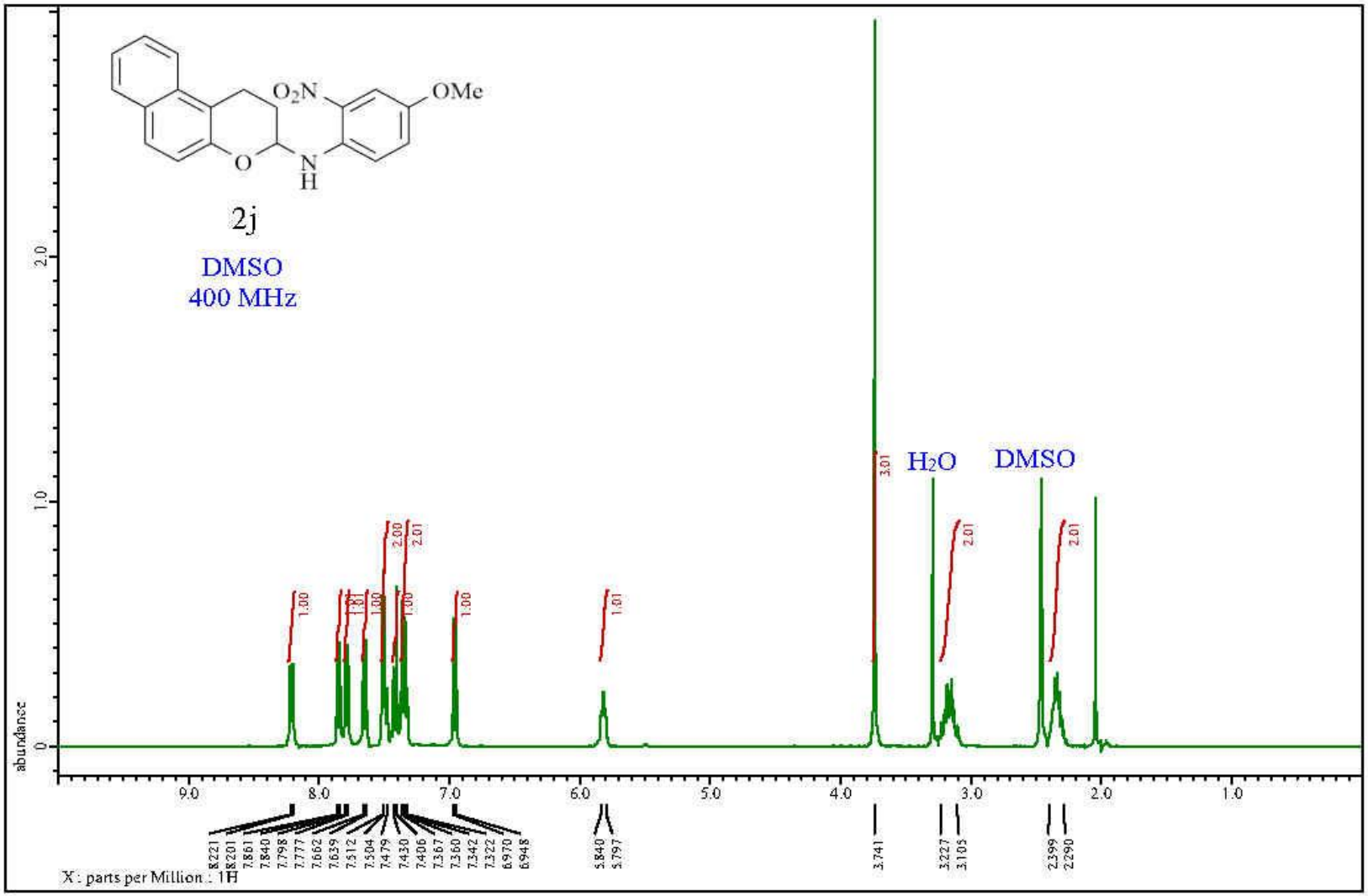
119.600
118.598
117.121
114.117
113.660
78.467
28.706
26.647
19.420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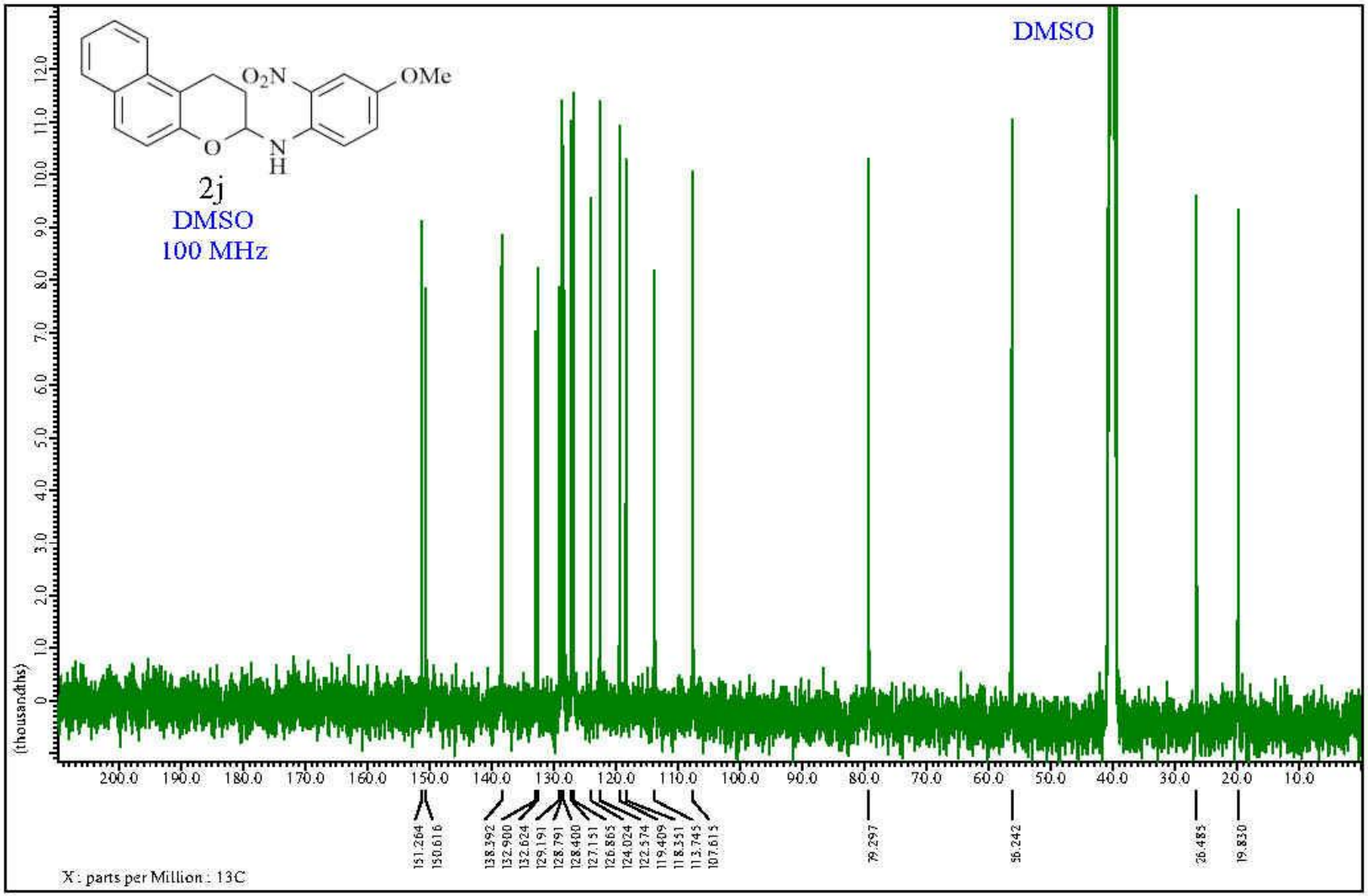
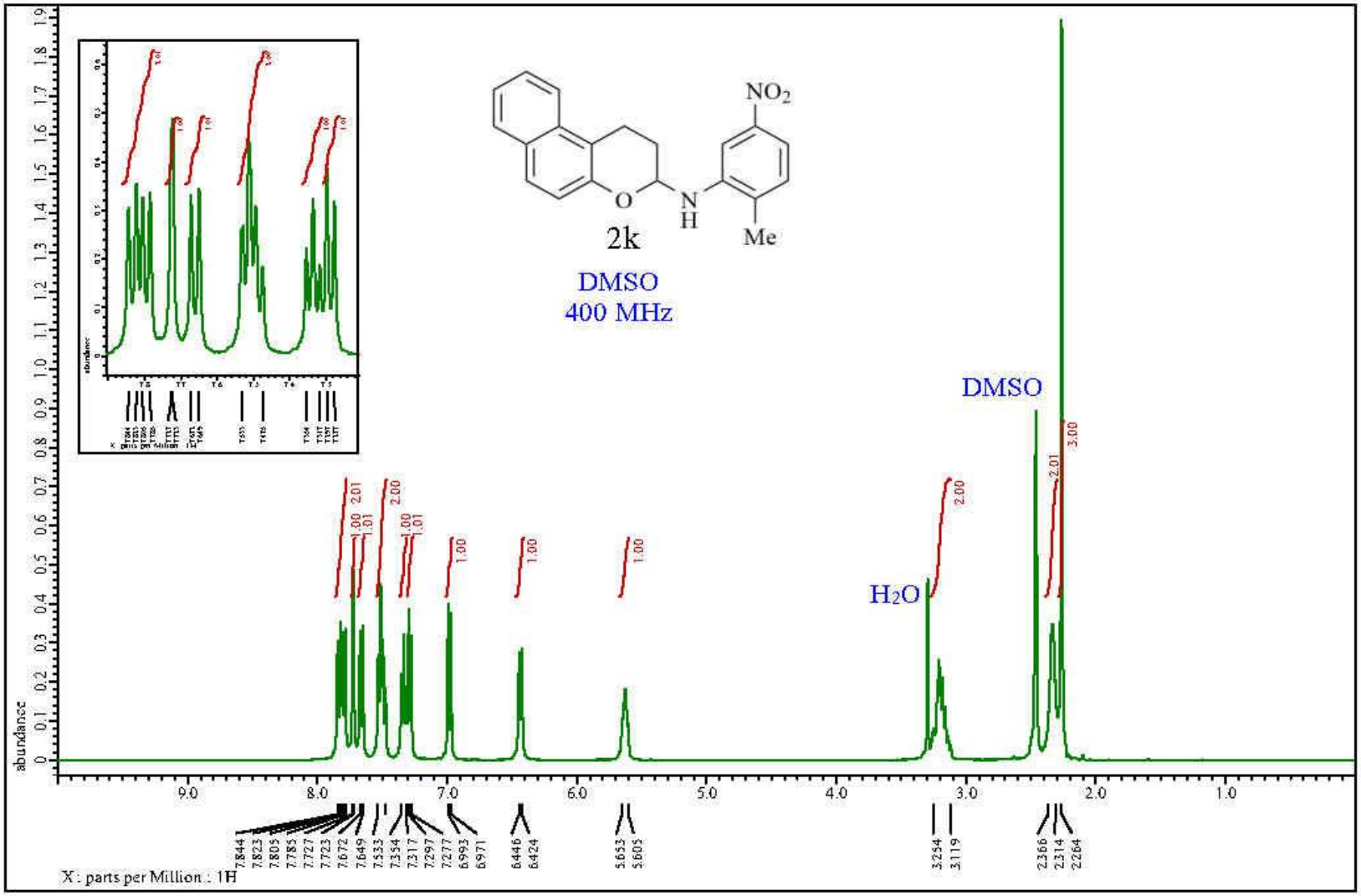
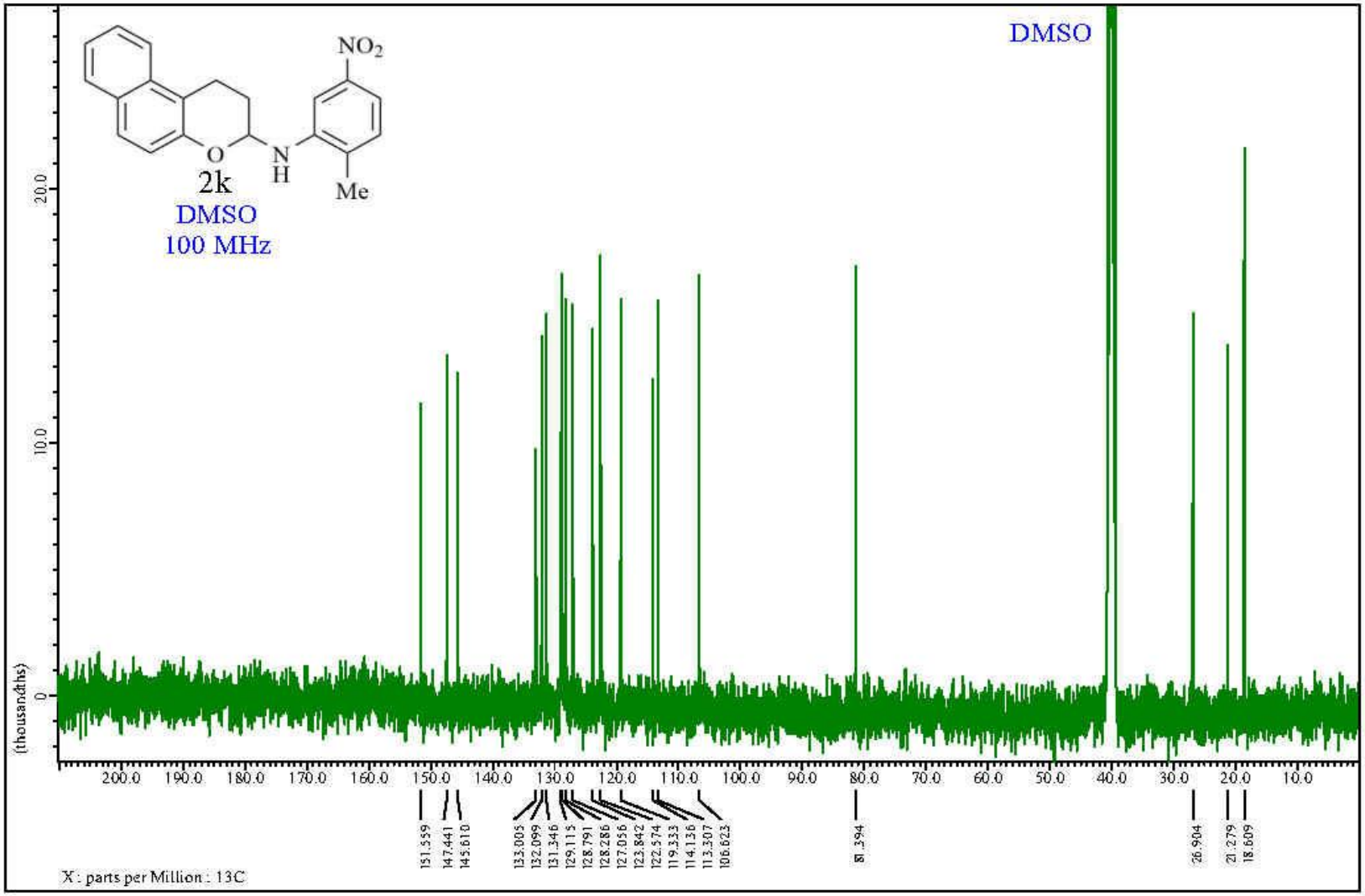
DMSO
400 MHz
O_2N
OMe
O
N
H
H_2O
DMSO
abundance
X : parts per Million : 1H


DMSO
O2N
OMe
O
N
H
2j
DMSO
100 MHz
(thousandths)
X : parts per Million : 13C
151.264
150.616
138.392
132.900
132.624
129.191
128.791
128.400
127.151
126.865
124.024
122.574
119.409
118.351
113.745
107.615
79.297
56.242
26.485
19.830


NO2
O
N
H
Me
2k
DMSO
400 MHz
DMSO
H2O
abundance
X : parts per Million : 1H


DMSO
NO2
O
N
H
Me
2k
DMSO
100 MHz
20.0
10.0
0
(thousandths)
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
151.559
147.441
145.610
133.005
132.099
131.346
129.115
128.791
128.286
127.056
123.842
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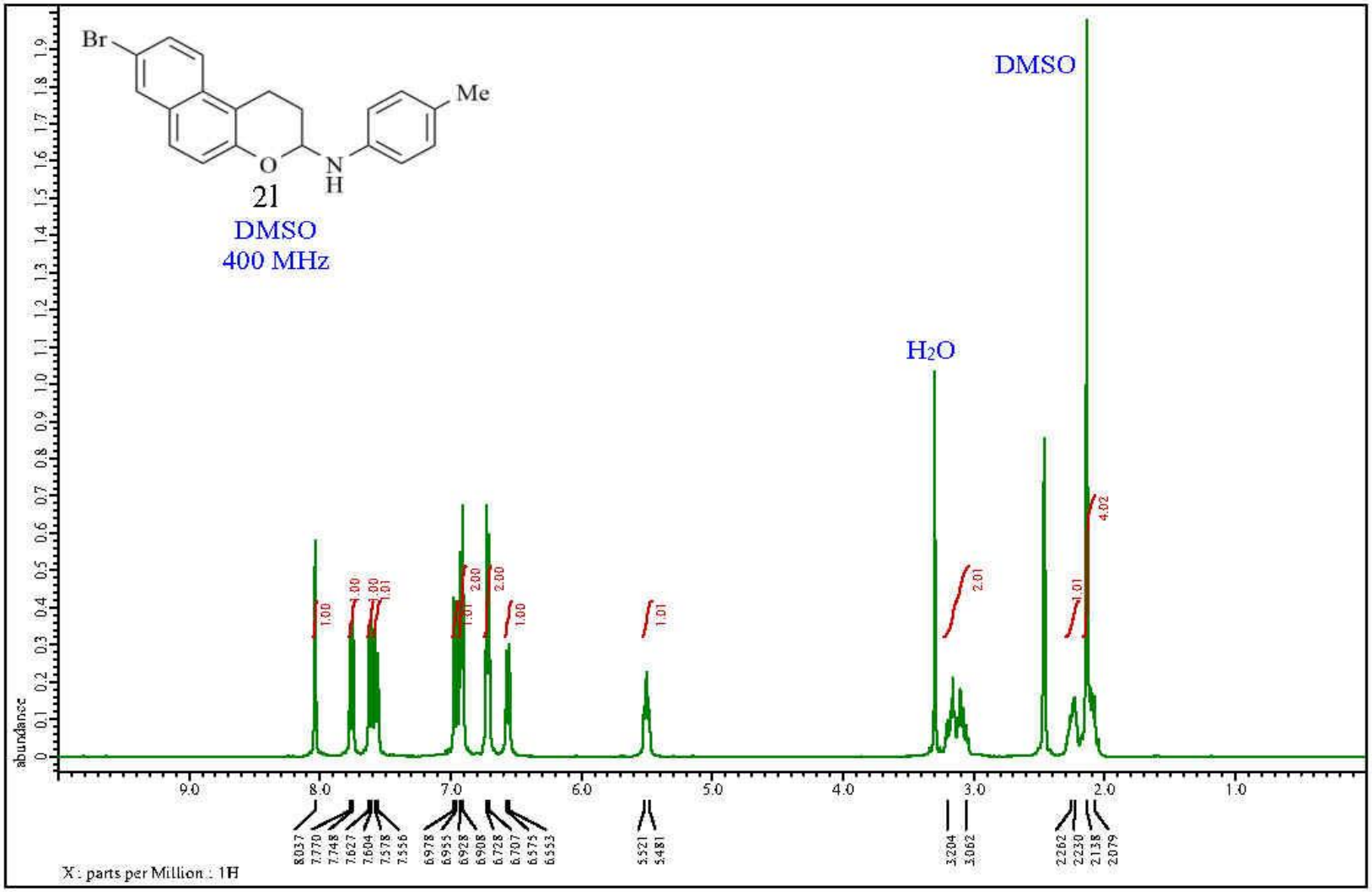
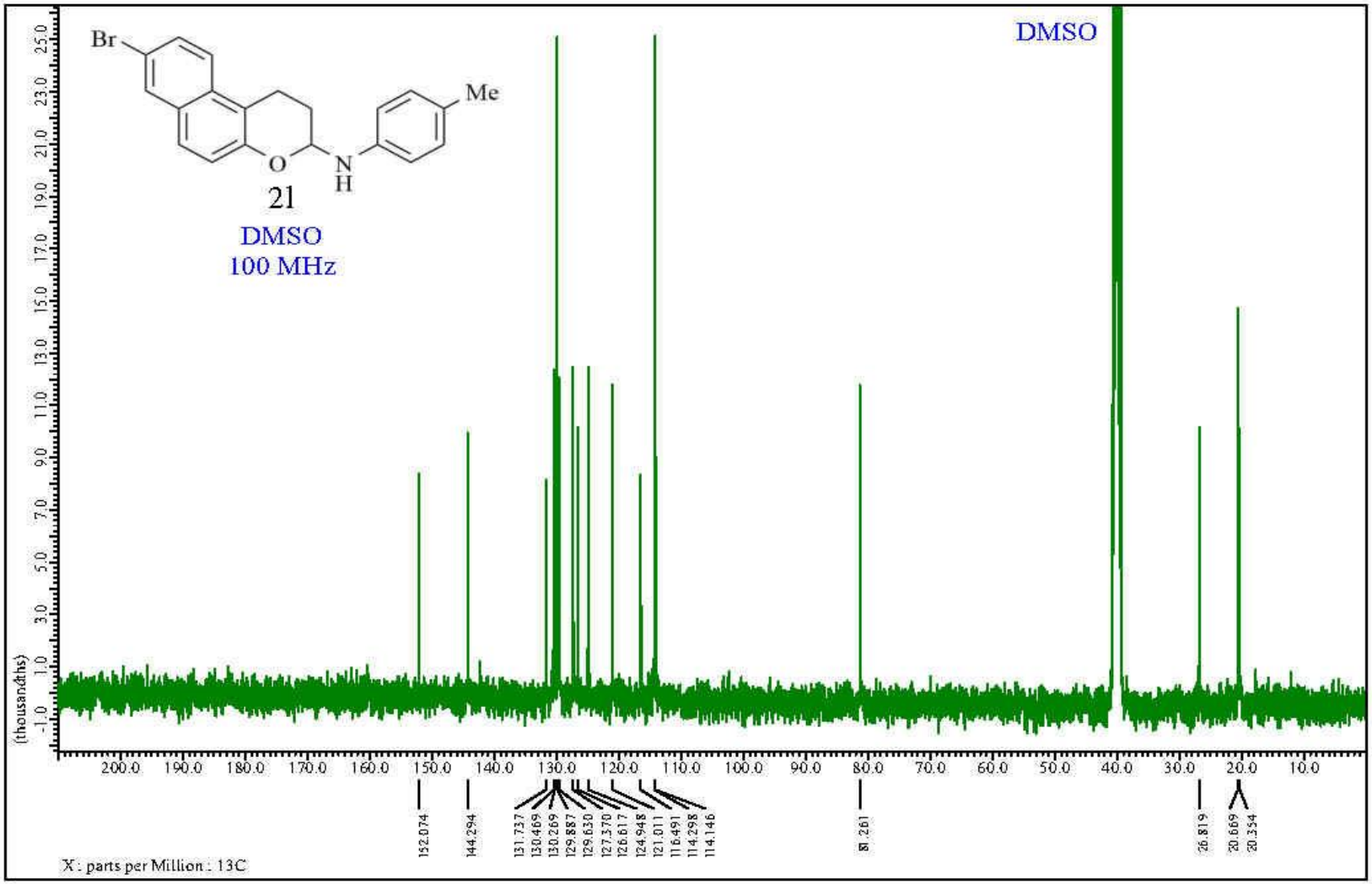
119.333
114.136
113.307
106.623
81.394
26.904
21.279
18.609
X : parts per Million : 13C


Br
Me
O
N
H
21
DMSO
400 MHz
DMSO
H2O
abundance
X : parts per Million : 1H


Br
Me
O
N
H
21
DMSO
100 MHz
DMSO
(thousandths)
X : parts per Million : 13C
152.074
144.294
131.737
130.469
130.269
129.887
129.630
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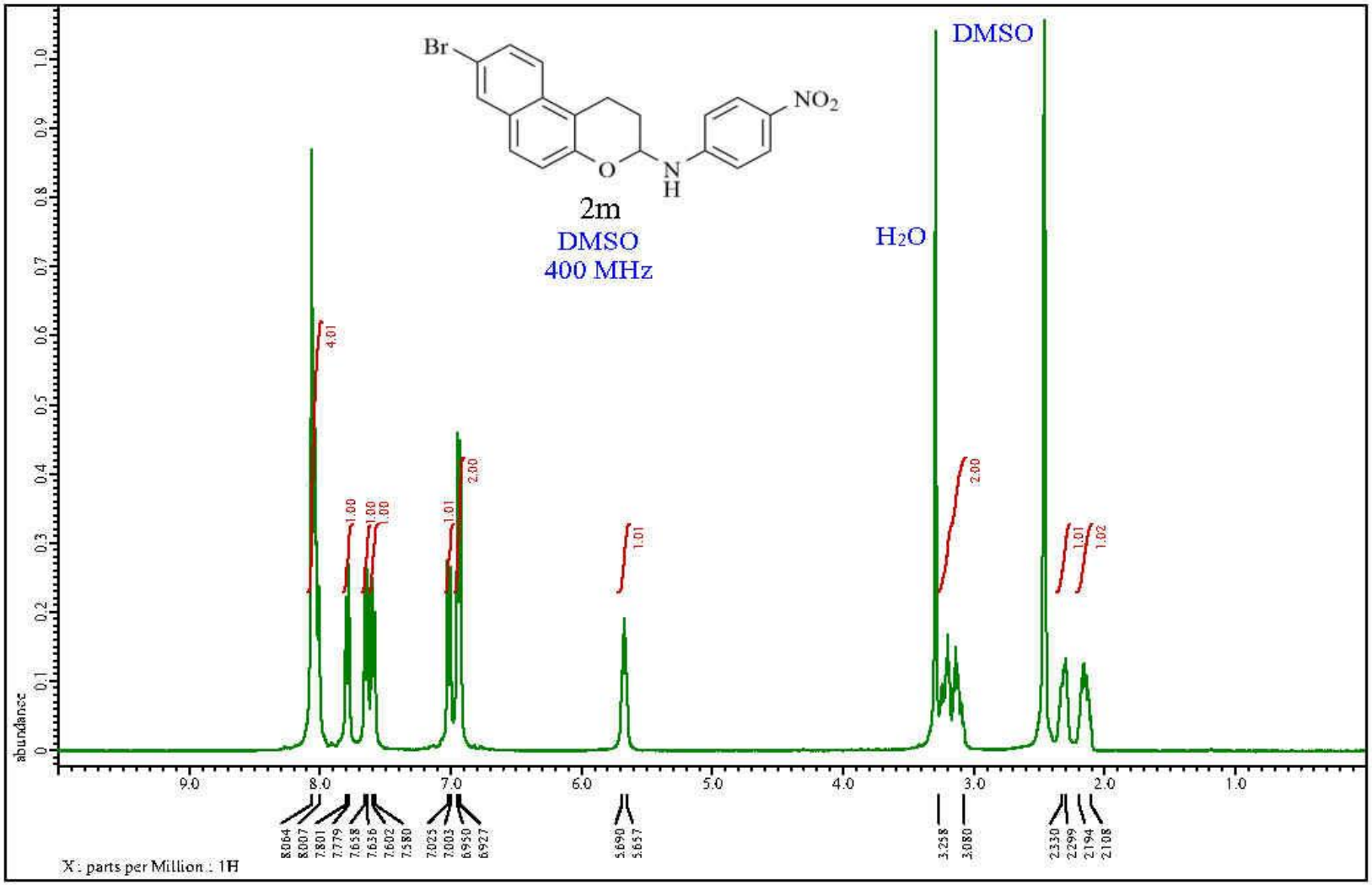
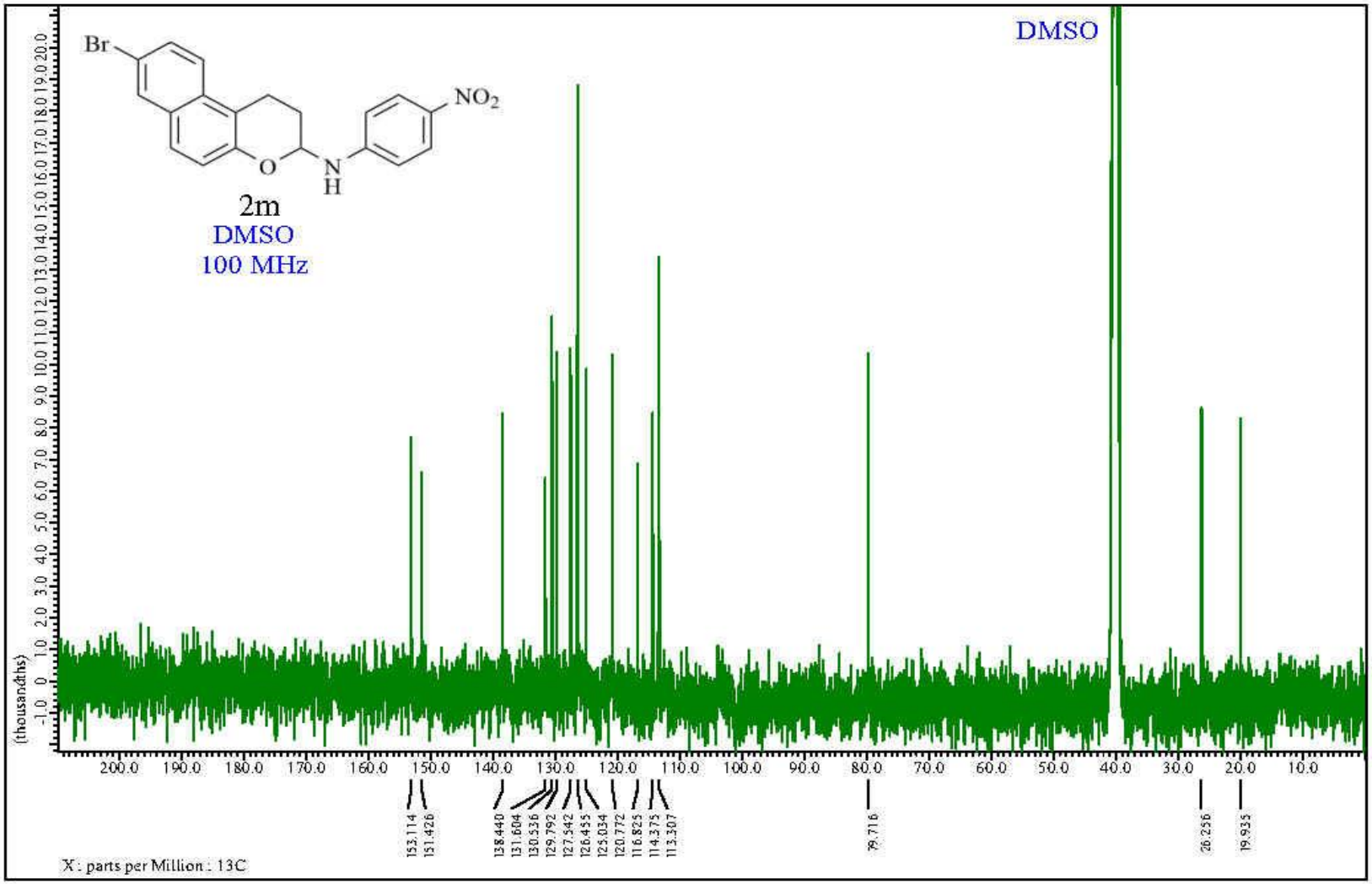
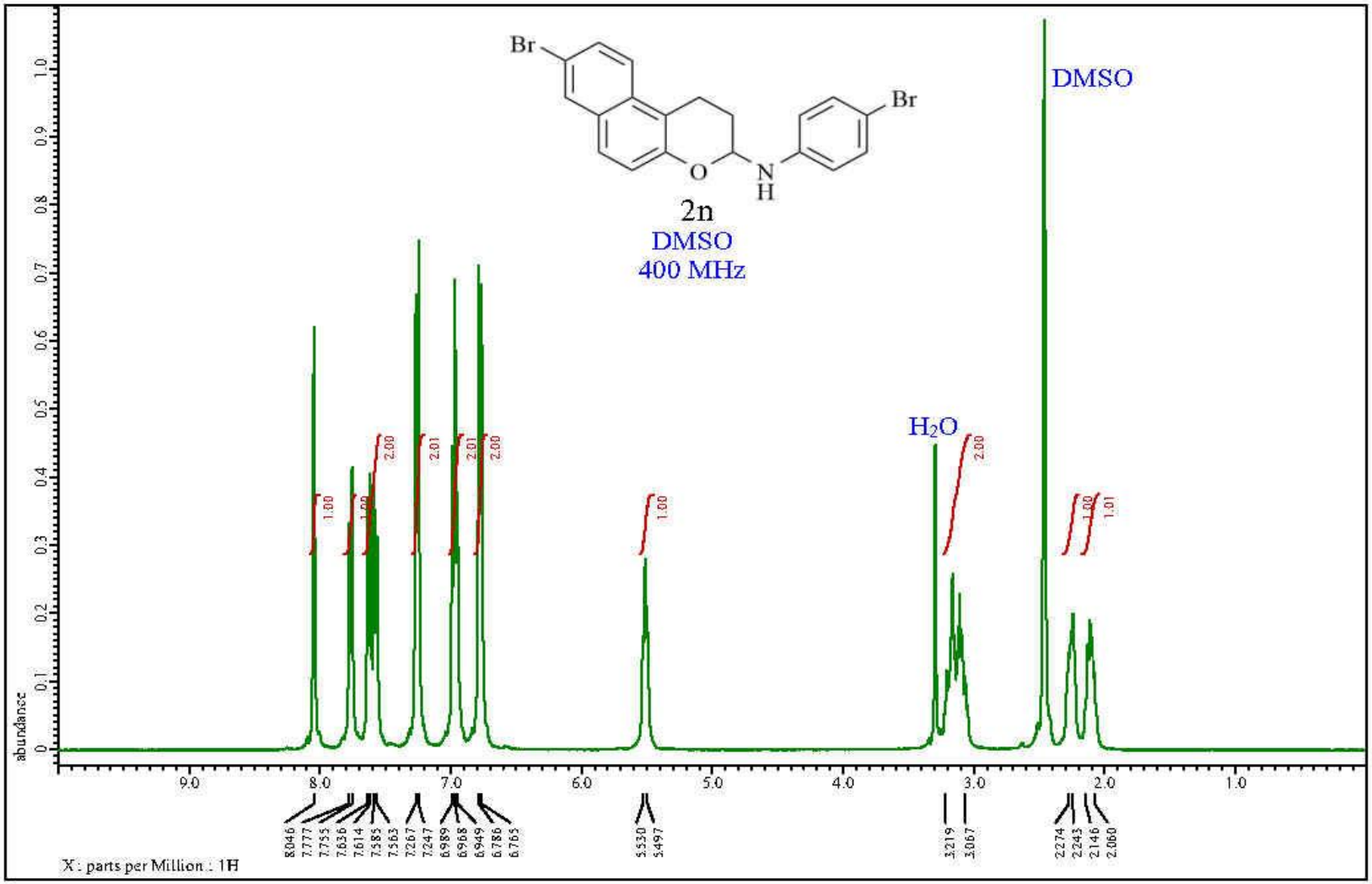
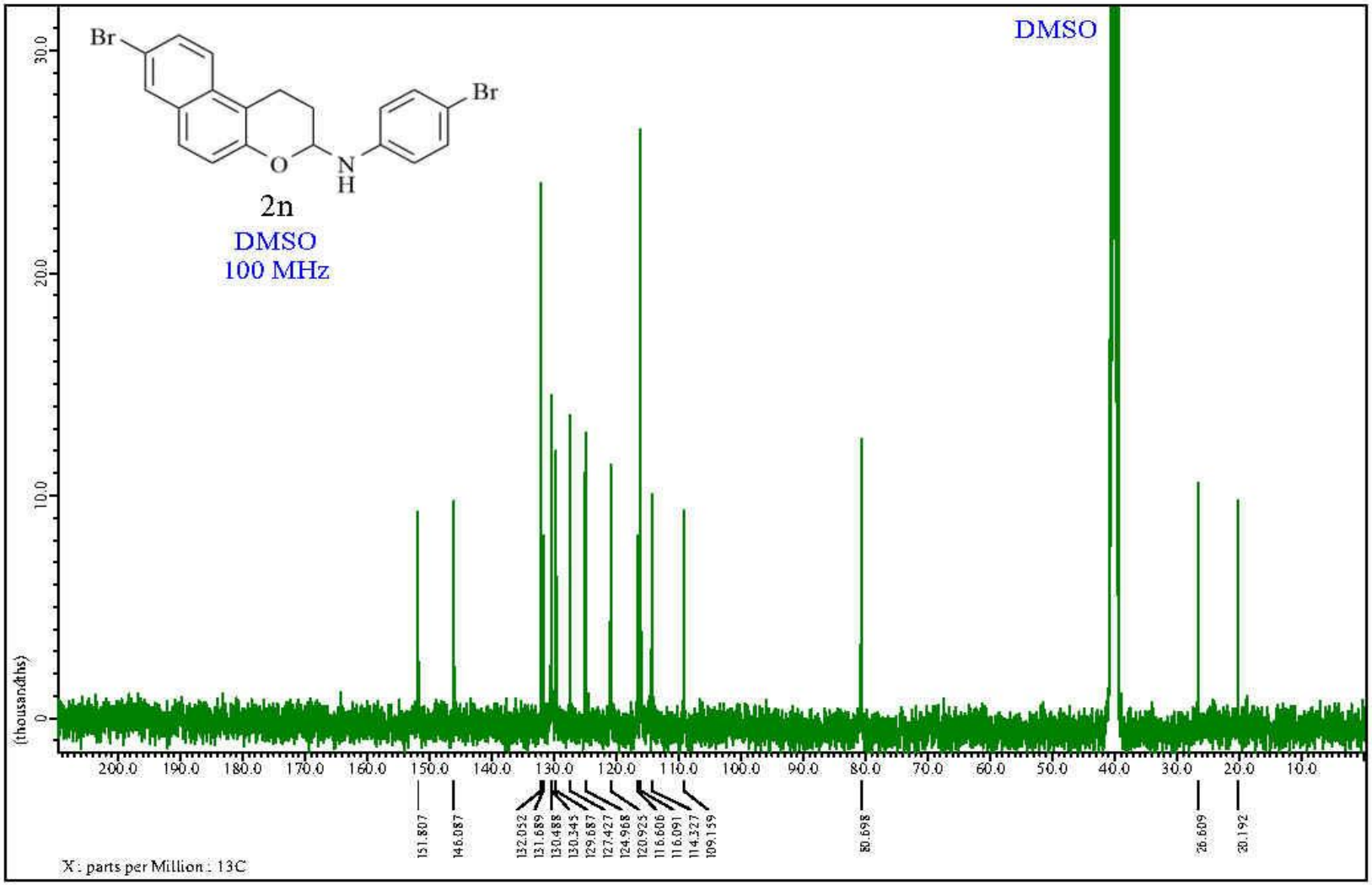
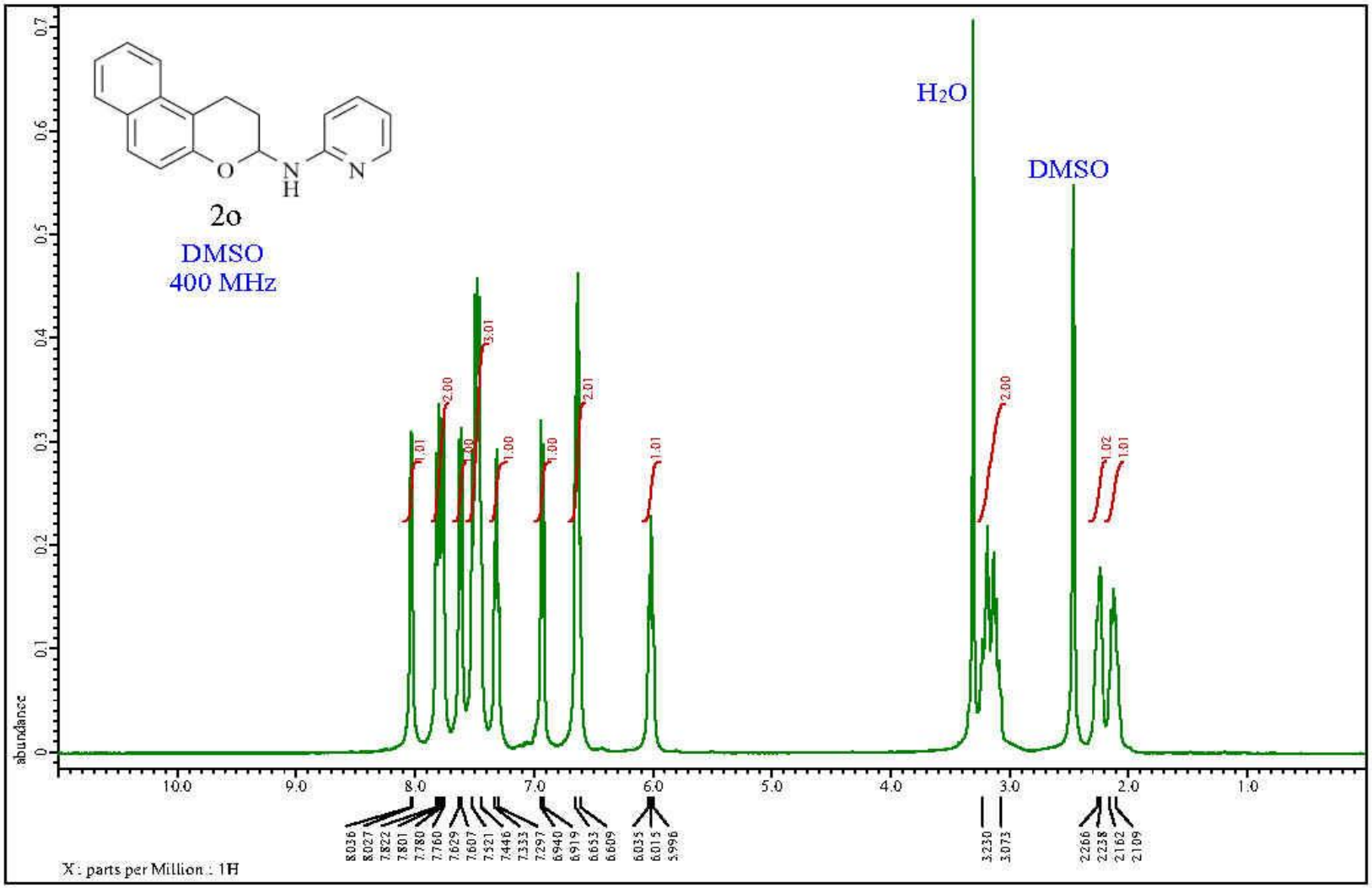
124.948
121.011
116.491
114.298
114.146
81.261
26.819
20.669
20.354

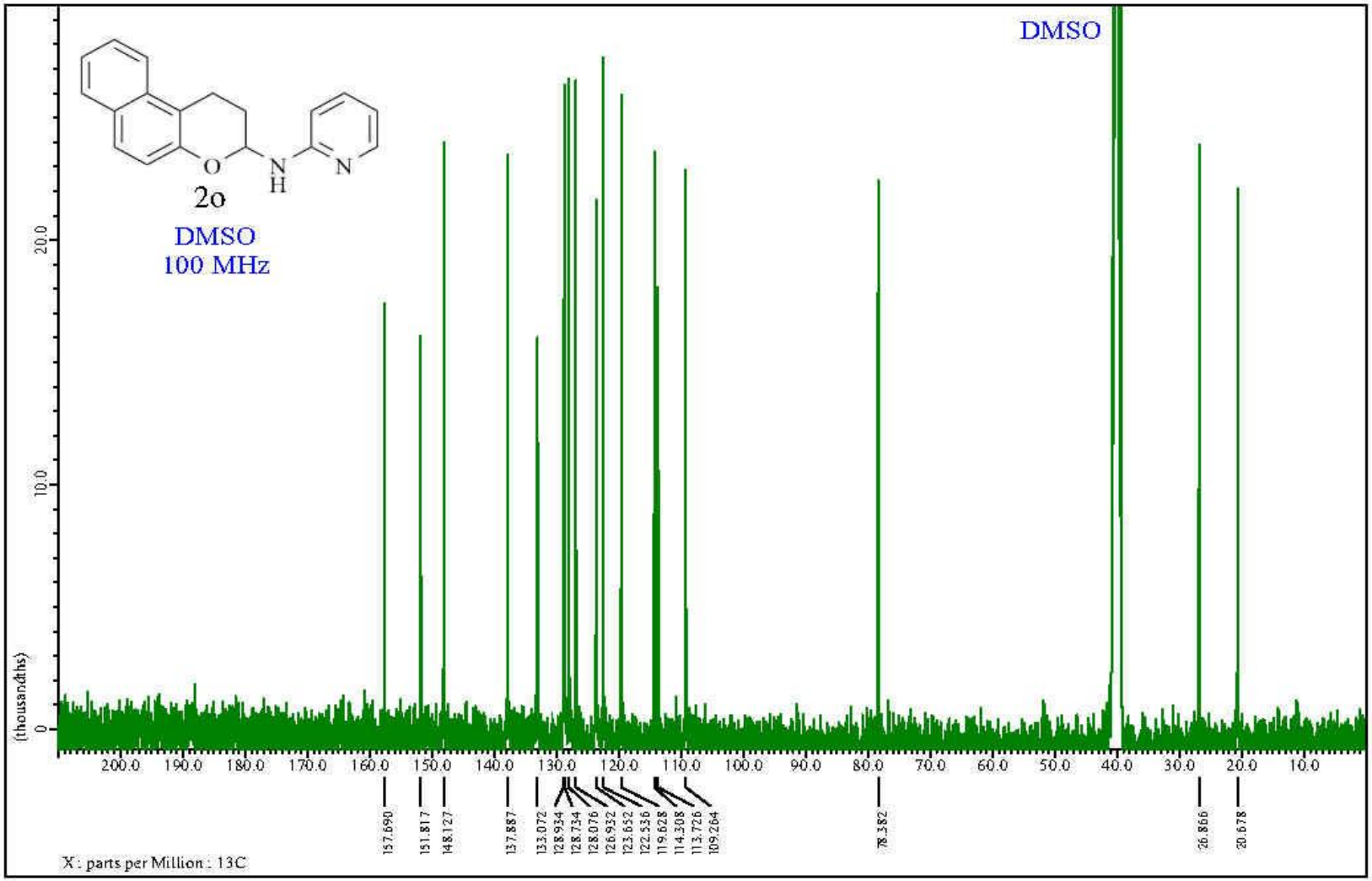

Br
NO2
O
N
H
2m
DMSO
400 MHz
DMSO
H2O
abundance
X : parts per Million : 1H
8.064
8.007
7.801
7.779
7.658
7.636
7.602
7.580
7.025
7.003
6.950
6.927
5.690
5.657
3.258
3.080
2.330
2.299
2.194
2.108

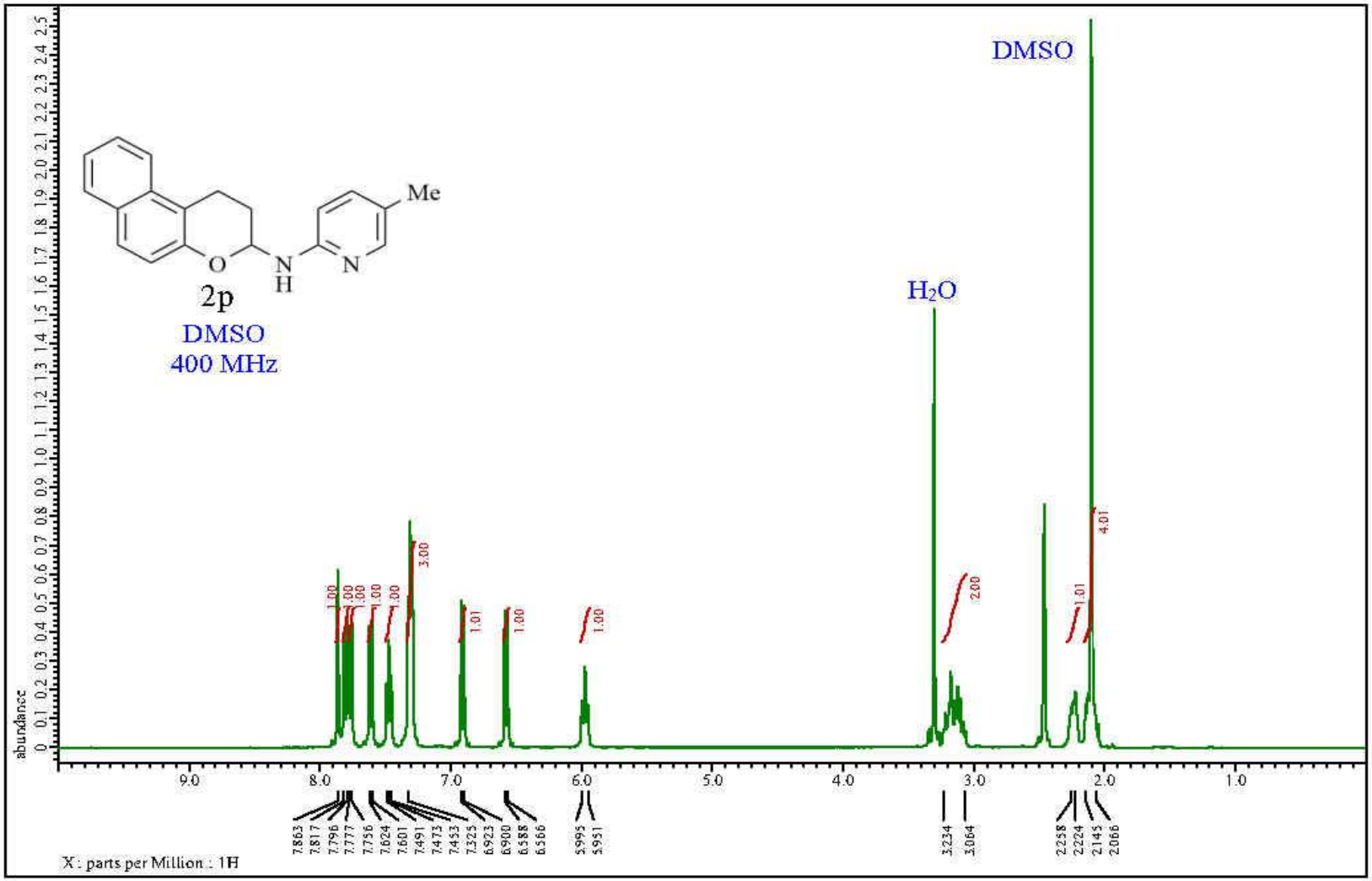

Br
NO2
O
N
H
2m
DMSO
100 MHz
DMSO
(thousandths)
X : parts per Million : 13C
153.114
151.426
138.440
131.604
130.536
129.792
127.542
126.455
125.034
120.772
116.825
114.375
113.307
79.716
26.256
19.935

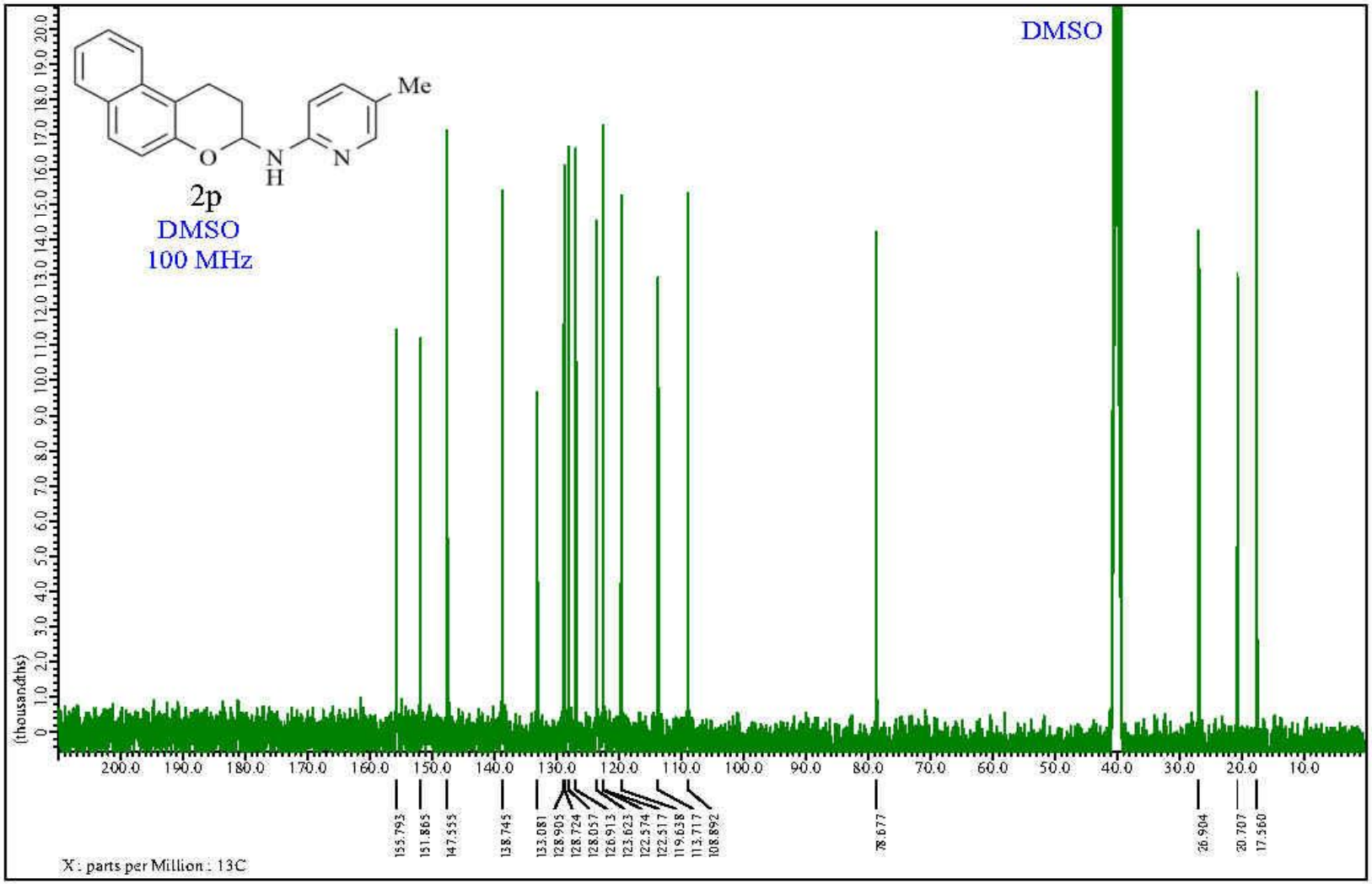

Br
Br
O
N
H
2n
DMSO
400 MHz
DMSO
H2O
abundance
X : parts per Million : 1H

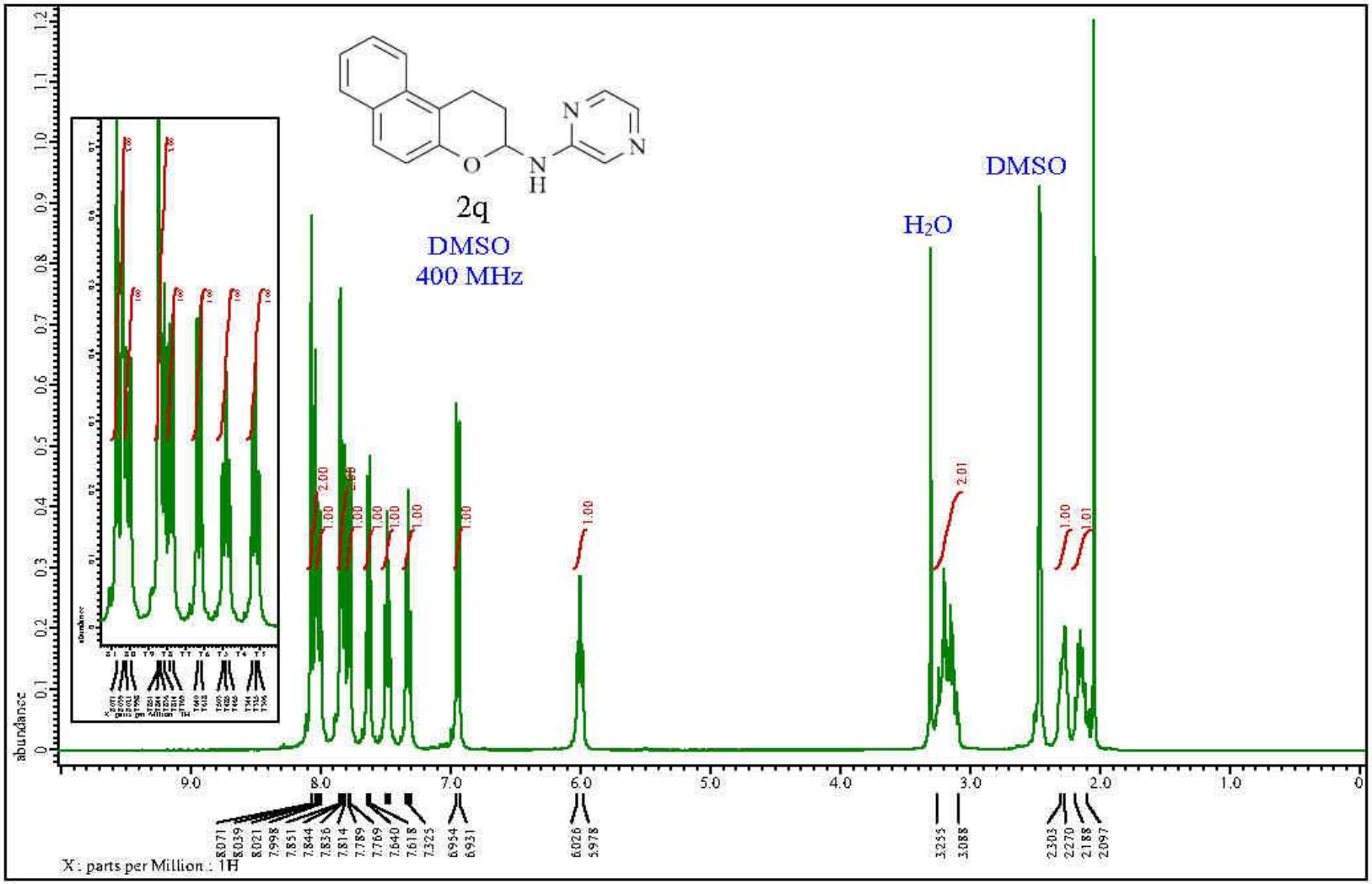

Br
Br
O
N
H
2n
DMSO
100 MHz
DMSO
(thousandths)
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
151.807
146.087
132.052
131.689
130.488
130.345
129.687
127.427
124.968
120.925
116.606
116.091
114.327
109.159
80.698
26.609
20.192
X : parts per Million : 13C

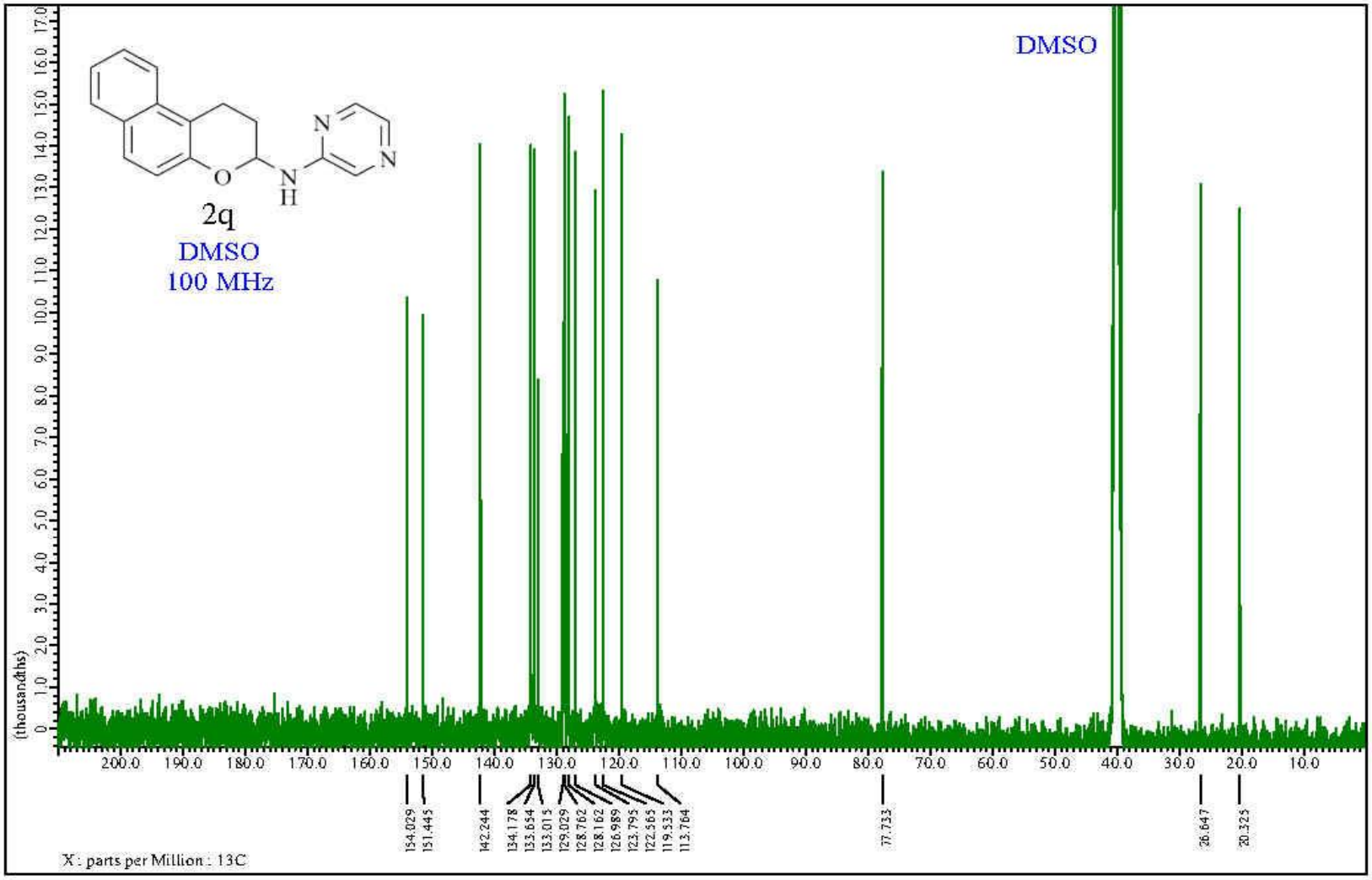

2o
DMSO
400 MHz
H2O
DMSO
abundance
X : parts per Million : 1H

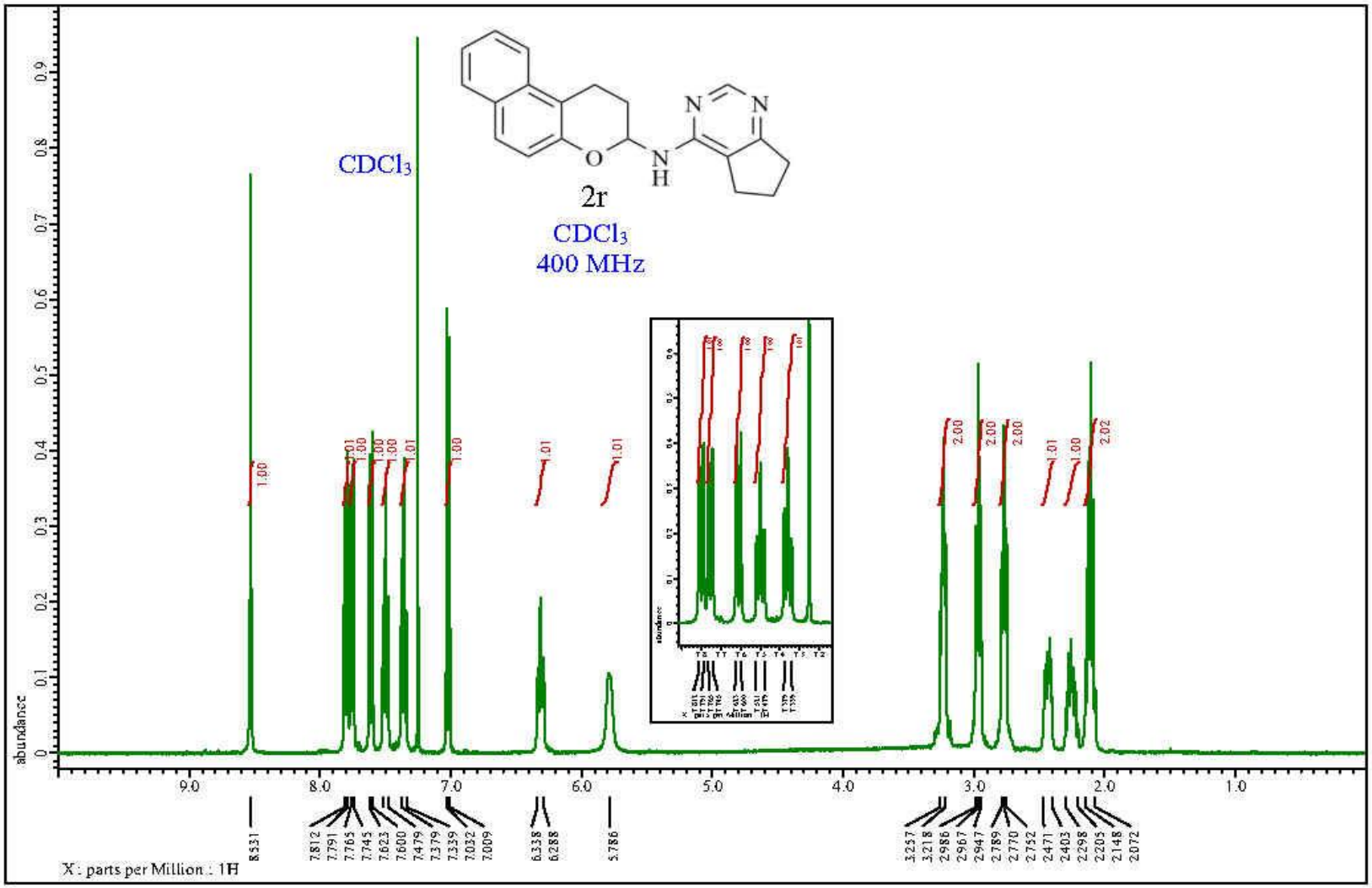

DMSO
2o
DMSO
100 MHz
(thousandths)
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
157.690
151.817
148.127
137.887
133.072
128.934
128.734
128.076
126.932
125.652
122.536
119.628
114.308
113.726
109.264
78.382
26.866
20.678
X : parts per Million : 13C

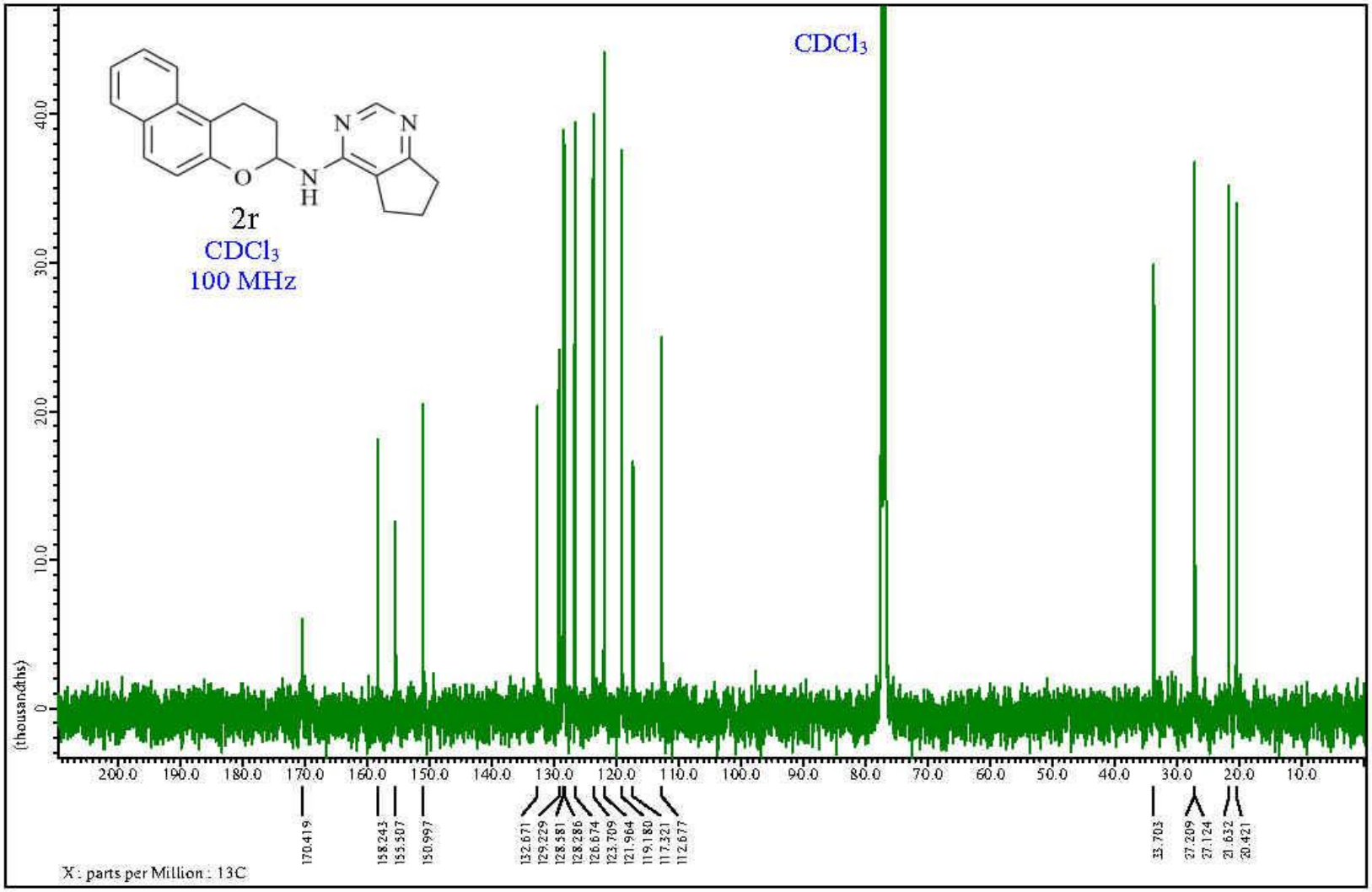

DMSO
Me
O
N
H
N
2p
DMSO
400 MHz
H2O
abundance
X : parts per Million : 1H

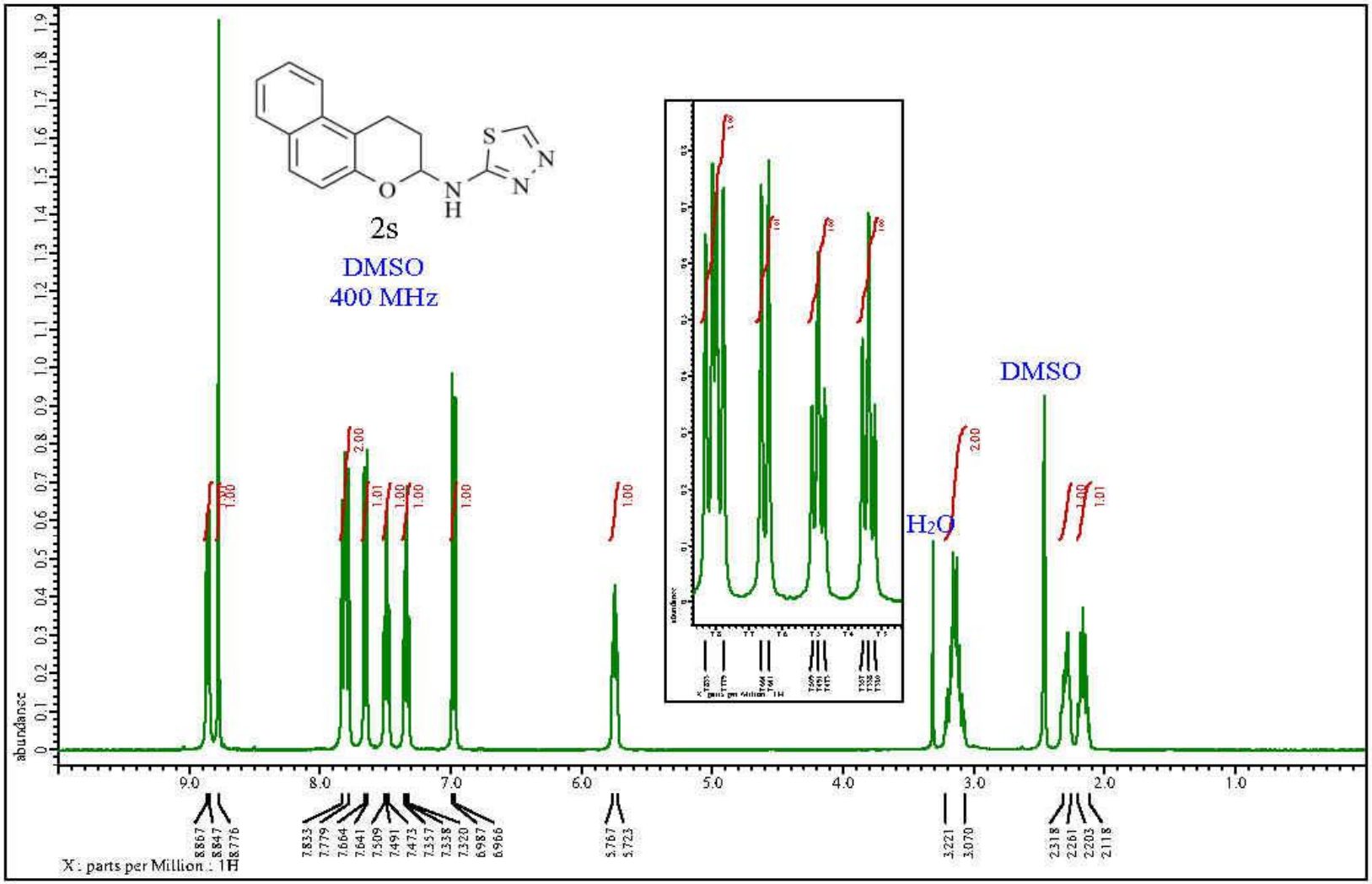

DMSO
Me
O
N
H
N
2p
DMSO
100 MHz
(thousandths)
X : parts per Million : 13C
155.793
151.865
147.555
138.745
133.081
128.905
128.724
128.057
126.913
123.623
122.574
122.517
119.638
113.717
108.892
78.677
26.904
20.707
17.560

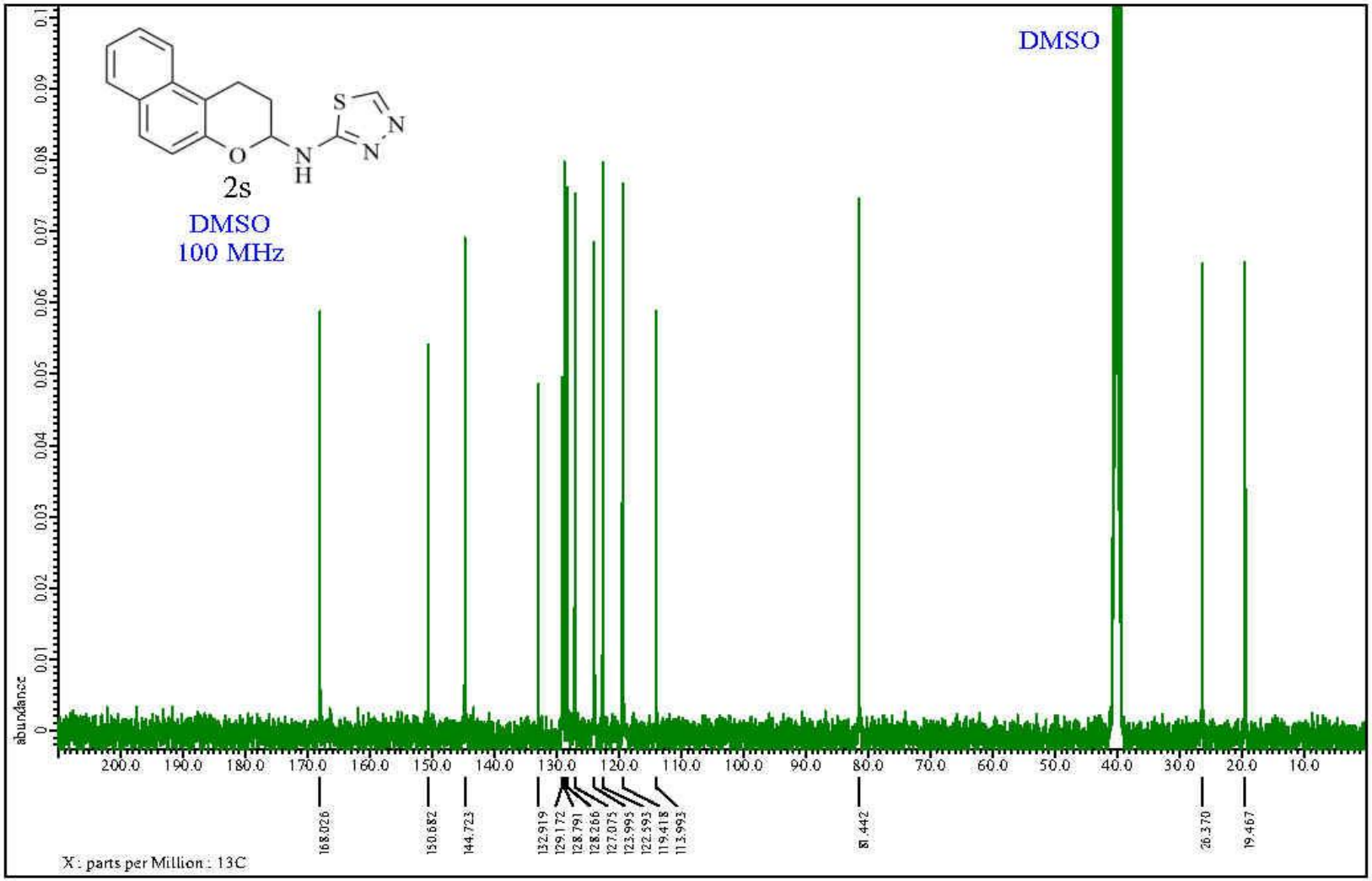

2q
DMSO
400 MHz
H2O
DMSO
abundance
X : parts per Million : 1H

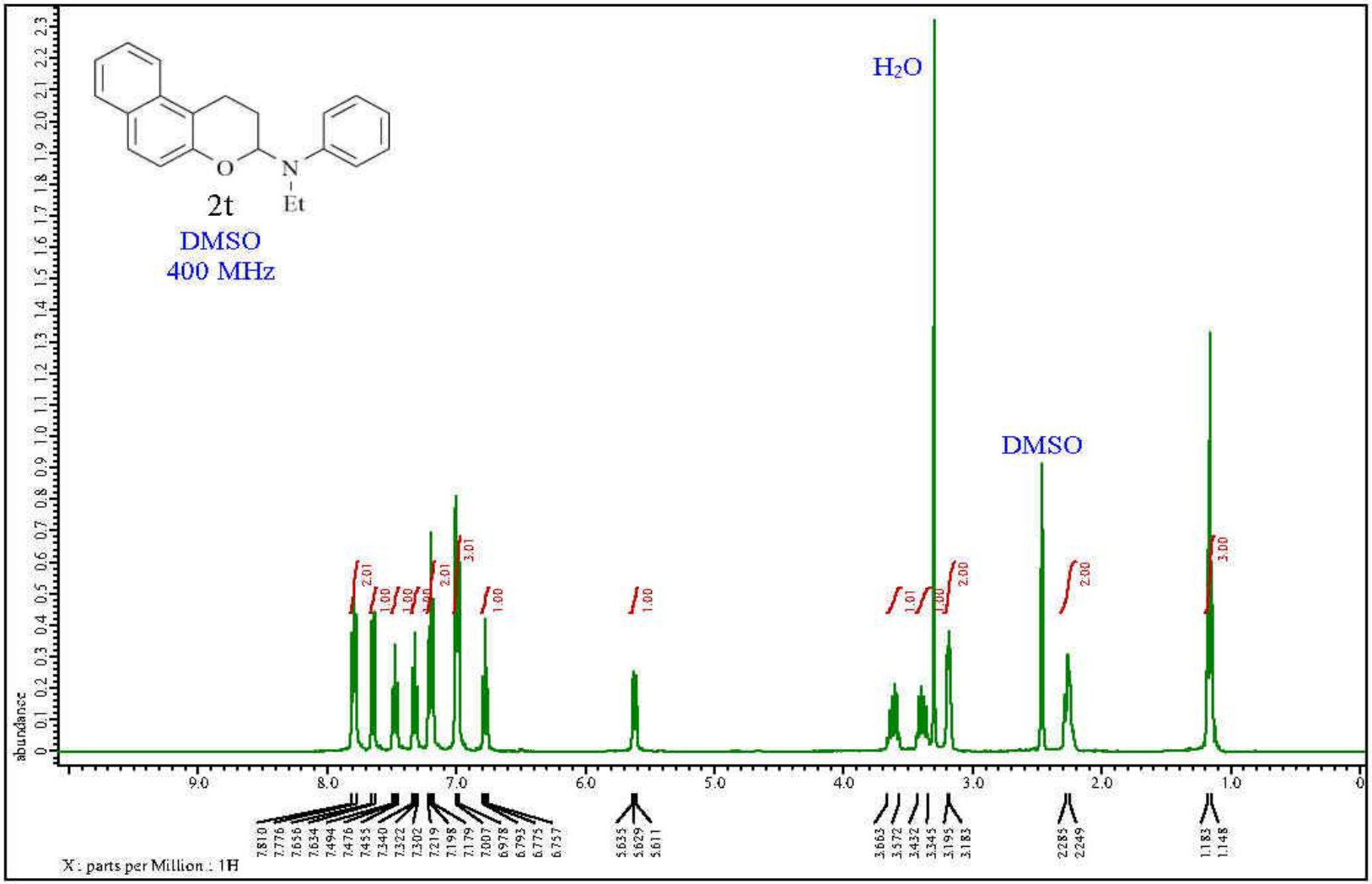

2q
DMSO
100 MHz
DMSO
(thousandths)
X : parts per Million : 13C
154.029
151.445
142.244
134.178
133.654
133.015
129.029
128.762
128.162
126.989
123.795
122.565
119.533
113.764
77.733
26.647
20.325

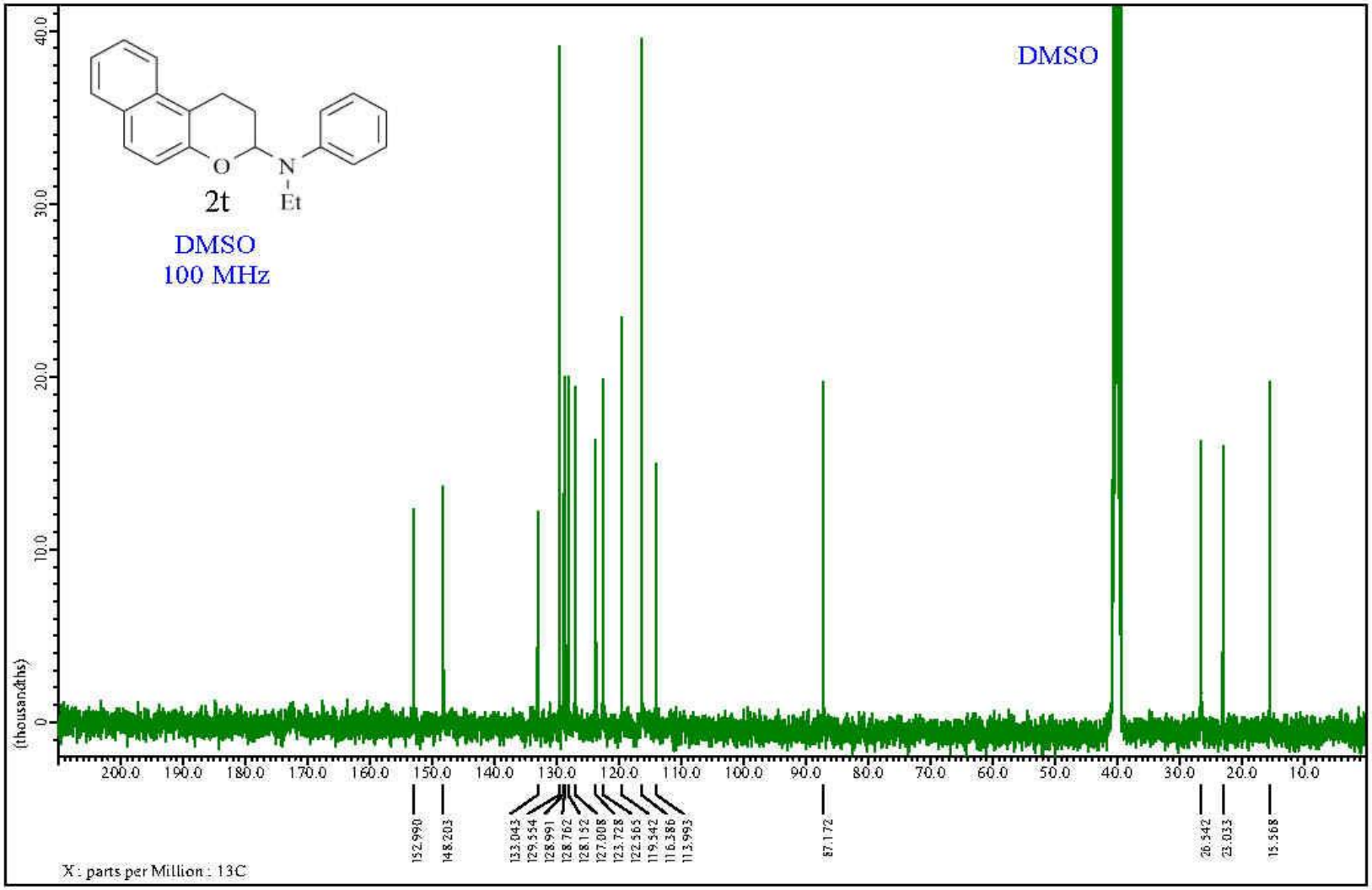

CDCl3
2r
CDCl3
400 MHz
abundance
X : parts per Million : 1H

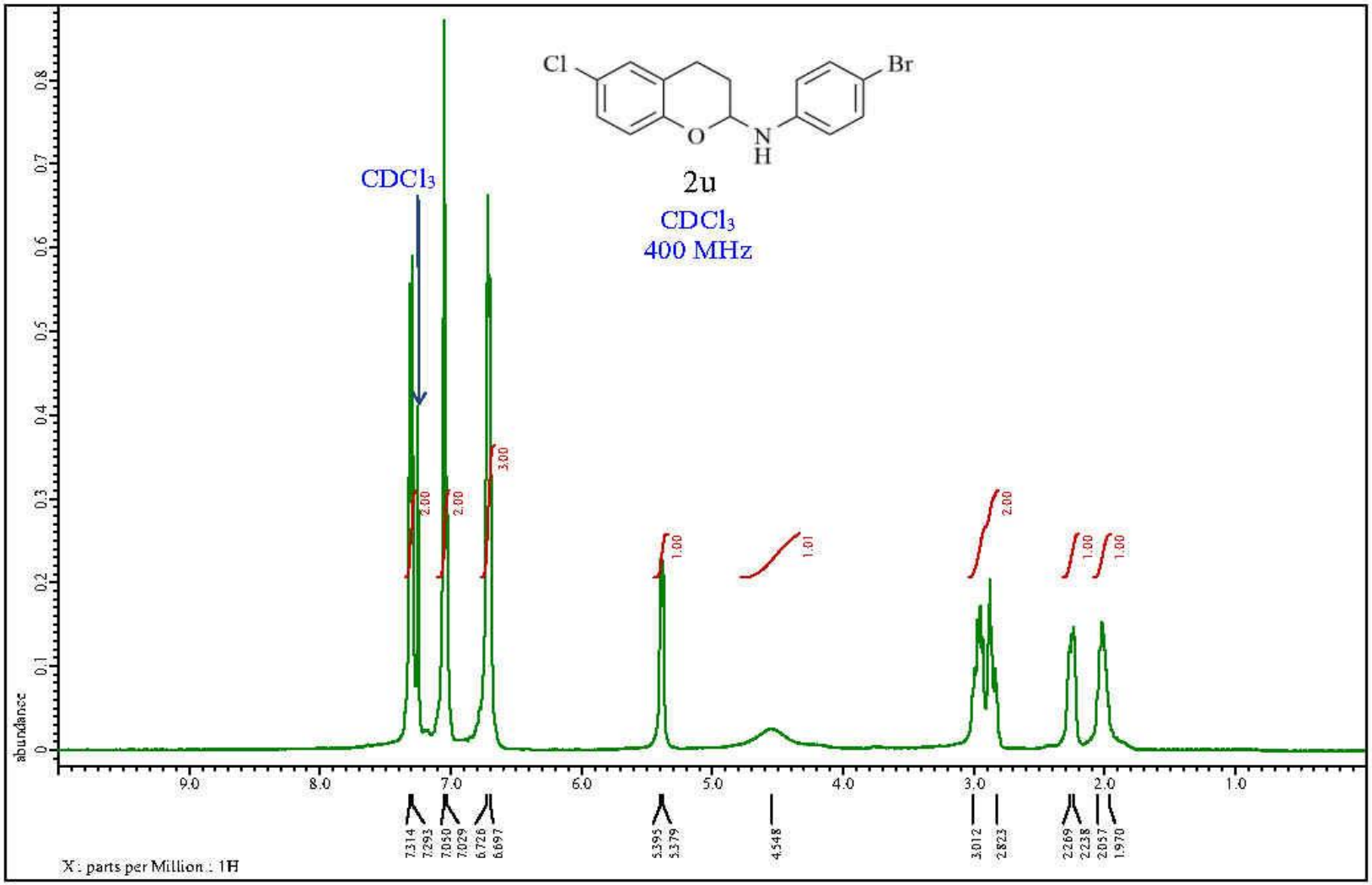

2r
CDCl3
100 MHz
CDCl3
(thousandths)
X : parts per Million : 13C
170.419
158.243
155.507
150.997
132.671
129.229
128.581
128.286
126.674
123.709
121.964
119.180
117.321
112.677
33.703
27.209
27.124
21.632
20.421

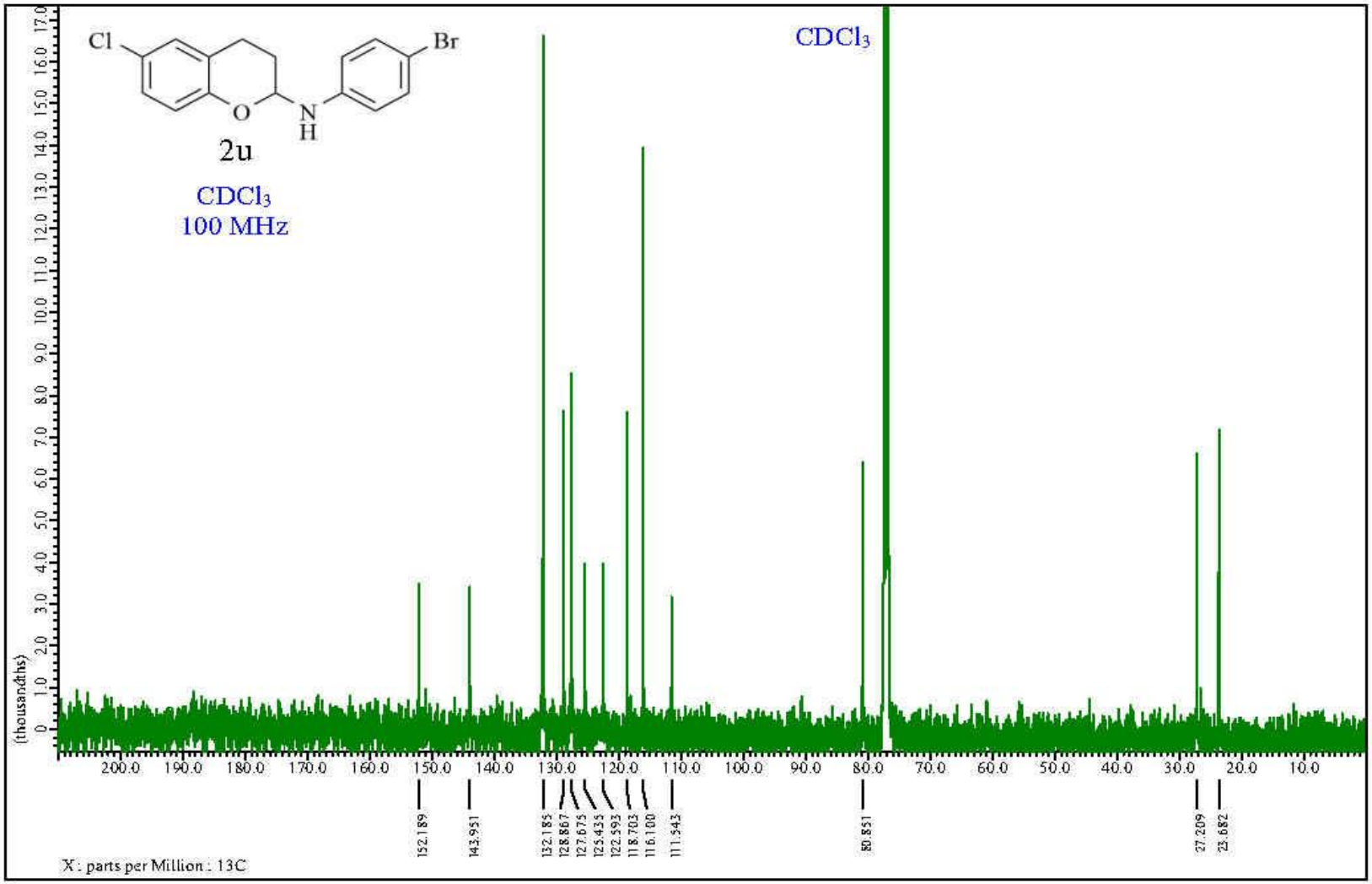

2s
DMSO
400 MHz
DMSO
H2O
abundance
X : parts per Million : 1H

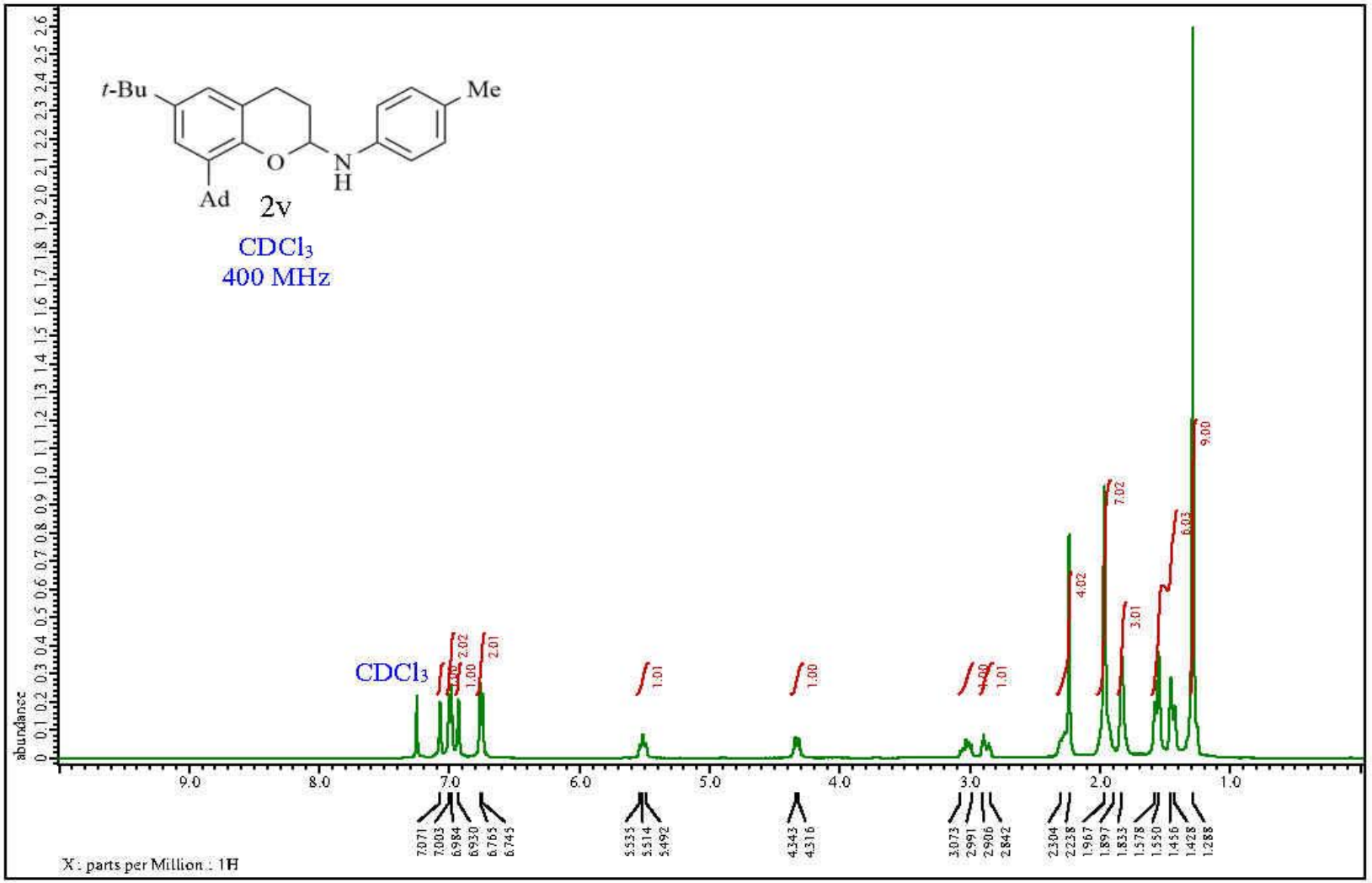

2s
DMSO
100 MHz
DMSO
abundance
X : parts per Million : 13C
168.026
150.682
144.723
132.919
129.172
128.791
128.266
127.075
125.995
122.593
119.418
113.993
81.442
26.370
19.467

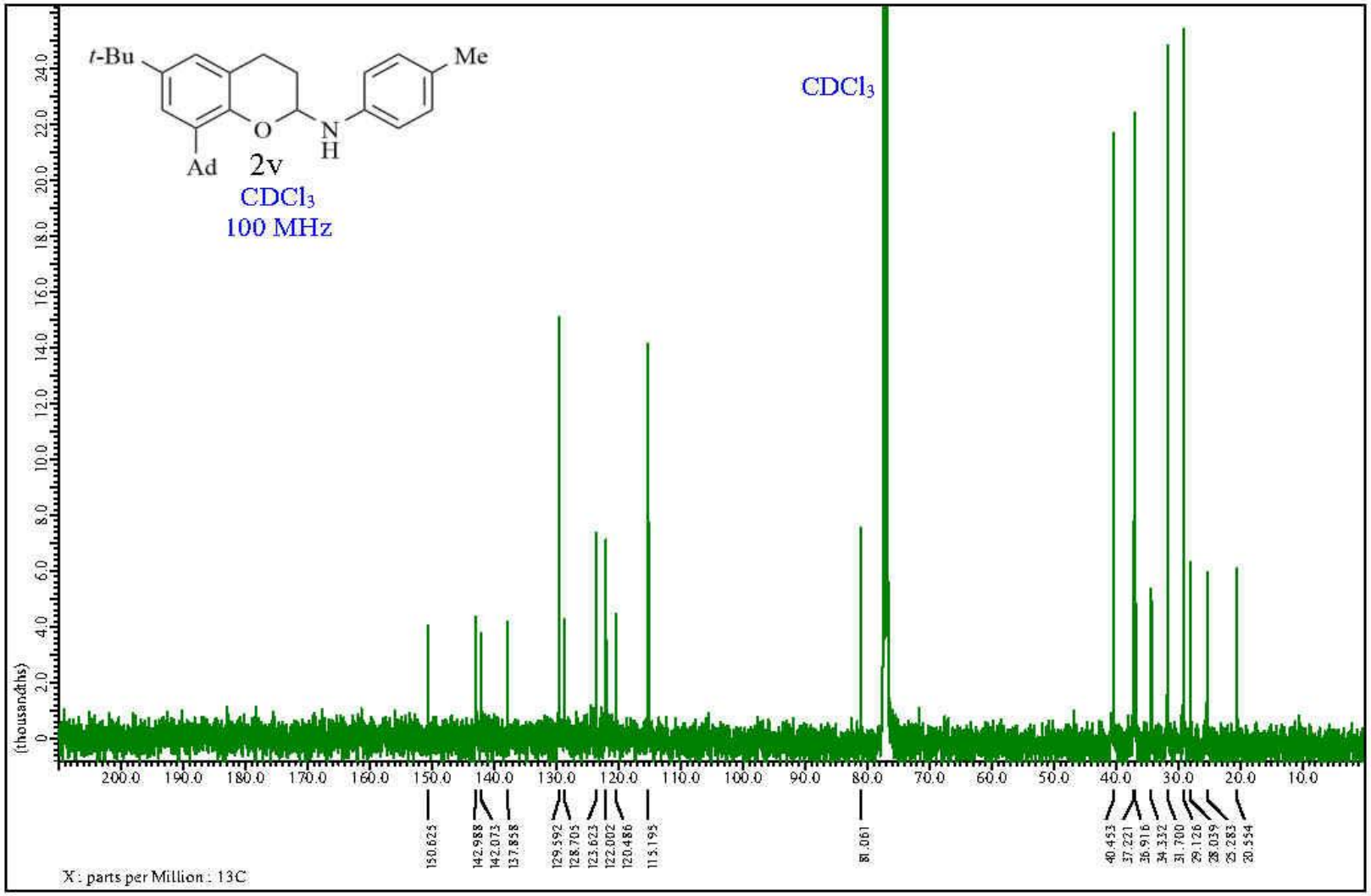

2t
DMSO
400 MHz
H2O
DMSO
abundance
X : parts per Million : 1H


2t
DMSO
100 MHz
DMSO
(thousandths)
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
152.990
148.203
133.043
129.554
128.991
128.762
128.152
127.008
123.728
122.565
119.342
116.386
113.993
87.172
26.342
23.033
15.568
X : parts per Million : 13C


Cl
Br
O
N
H
2u
CDCl3
400 MHz
CDCl3
abundance
X : parts per Million : 1H
7.314
7.293
7.050
7.029
6.726
6.697
5.395
5.379
4.548
3.012
2.823
2.269
2.238
2.057
1.970
2.00
2.00
3.00
1.00
1.01
2.00
1.00
1.00


Cl
Br
O
N
H
2u
CDCl3
100 MHz
CDCl3
(thousandths)
X : parts per Million : 13C
152.189
143.951
132.185
128.867
127.675
125.435
122.593
118.703
116.100
111.543
80.851
27.209
23.682


t-Bu
Me
O
N
H
Ad
2v
CDCl3
400 MHz
CDCl3
abundance
X : parts per Million : 1H


t-Bu
Me
O
N
H
Ad
2v
CDCl3
100 MHz
CDCl3
(thousandths)
X : parts per Million : 13C
150.625
142.988
142.073
137.858
129.592
128.705
123.623
122.002
120.486
115.195
81.061
40.453
37.221
36.916
34.332
31.700
29.126
28.039
25.283
20.554