Copper nitrate-enabled ring expansion reaction of cyclopropanes: A direct approach to 3-cyano-isoxazoline *N*-oxides

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Electronic Supplementary Information

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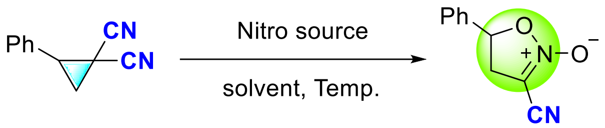
1. General Information

All reagents and metal catalysts were obtained from commercial sources without further purification, and commercially available solvents were purified before use. All new compounds were fully characterized. All melting points were taken on a SGWX-4A Digital Melting Point Apparatus without correction. Infrared spectra were obtained using a Nicolet AVATAR 370 FT-IR spectrometer. ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded with a Bruker AV-500 spectrometer, a Bruker AV-600 spectrometer operating or JNM-ECZ400S spectrometer, respectively, with chemical shift values being reported in ppm relative to chloroform (δ = 7.26 ppm), acetone (δ = 2.05 ppm) or TMS (δ = 0.00 ppm) for ^{1}H NMR; chloroform (δ = 77.16 ppm) or acetone (δ = 29.84 and 206.26 ppm) for ^{13}C NMR; and C_6F_6 (δ = -164.9 ppm) for ^{19}F NMR. Mass spectra (MS) and high resolution mass spectra (HRMS) were recorded with an Agilent 5975C or JEOL AccuTOF-MS using an Electron impact (EI), Electrospray ionization (ESI), direct analysis in real-time (DART) techniques or field ionization (FI). Silica gel plate GF254 were used for thin layer chromatography (TLC) and silica gel H or 300-400 mesh were used for flash column chromatography. The starting materials cyclopropanes **1** and **3** were all prepared according to the literature reported procedures,[1] unless otherwise indicated.

2. Optimization of the Reaction Conditions

Table S1 Optimization of nitrate-mediated ring expansion reaction of cyclopropane.[a]



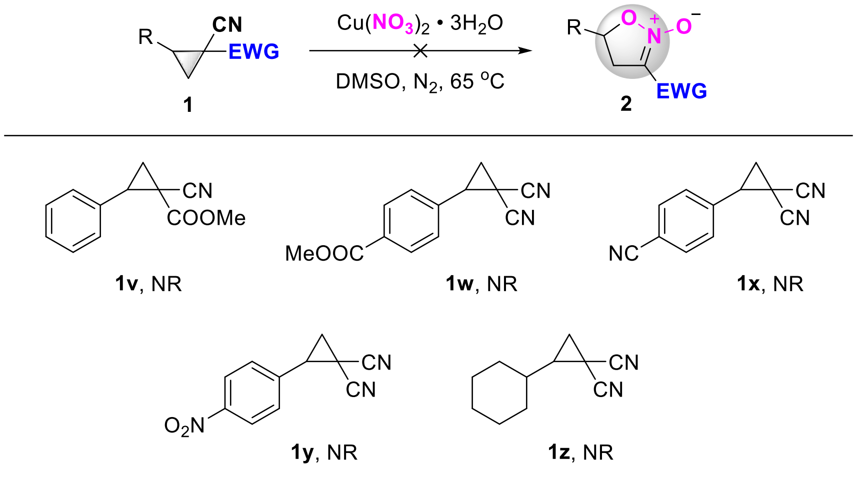
1a **2a**

Entry	Nitro source (equiv)	Solvent (mL)	Temp (°C)	Yield (%)[b]
1	$Cu(NO_3)_2 \cdot 3H_2O$ (2.0)	DMSO (2)	70	75
2	$Cu(NO_3)_2 \cdot 3H_2O$ (2.0)	DMF (2)	70	39
3	$Cu(NO_3)_2 \cdot 3H_2O$ (2.0)	NMP (2)	70	45
4	$Cu(NO_3)_2 \cdot 3H_2O$ (2.0)	PhCl (2)	70	N.P.
5	$Cu(NO_3)_2 \cdot 3H_2O$ (2.0)	toluene (2)	70	N.P.
6	$Cu(NO_3)_2 \cdot 3H_2O$ (2.0)	CH_3CN (2)	70	N.P.
7	$Cu(NO_3)_2 \cdot 3H_2O$ (2.0)	dioxane (2)	70	N.P.
8	$Co(NO_3)_3 \cdot 3H_2O$ (2.0)	DMSO (2)	70	71
9	KNO_3 (3.0)	DMSO (2)	70	23
10	$Fe(NO_3)_3 \cdot 3H_2O$ (1.0)	DMSO (2)	70	trace
11	$Cu(NO_3)_2 \cdot 3H_2O$ (1.5)	DMSO (2)	70	77
12	$Cu(NO_3)_2 \cdot 3H_2O$ (1.2)	DMSO (2)	70	80
13	$Cu(NO_3)_2 \cdot 3H_2O$ (1.0)	DMSO (2)	70	77
14	$Cu(NO_3)_2 \cdot 3H_2O$ (0.5)	DMSO (2)	70	31
15	**$Cu(NO_3)_2 \cdot 3H_2O$ (1.2)**	**DMSO (2)**	**65**	**82**
16	$Cu(NO_3)_2 \cdot 3H_2O$ (1.2)	DMSO (2)	80	70
17	$Cu(NO_3)_2 \cdot 3H_2O$ (1.2)	DMSO (1)	65	75
18[c]	$Cu(NO_3)_2 \cdot 3H_2O$ (1.2)	DMSO (2)	65	75
19	$Cu(NO_3)_2 \cdot 3H_2O$ (0.2) KNO_3 (3.0)	DMSO (2)	65	44

[a]Reaction conditions: **1a** (0.2 mmol, 1.0 equiv), nitro source (x equiv), solvent (y mL), temp, under N_2 for 15 h. [b]Isolated yields. [c]Under air.

3. Unsuccessful Substrate Scope

We attempt to use other alternative cyclopropanes such as methyl 1-cyano-2-phenylcyclopropane-1-carboxylate (**1v**), methyl 4-(2,2-dicyanocyclopropyl)benzoate (**1w**), 2-(4-cyanophenyl)cyclopropane-1,1-dicarbonitrile (**1x**), 2-(4-nitrophenyl)cyclopropane-1,1-dicarbonitrile (**1y**), and 2-cyclohexylcyclopropane-1,1-dicarbonitrile (**1z**) to react with copper nitrate. Unfortunately, the desired products were not observed.



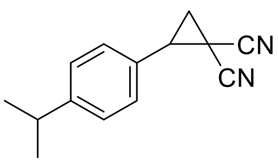
Scheme S1 Substrate scope for the ring expansion reaction of cyclopropanes. Reaction conditions: **1** (0.2 mmol, 1.0 equiv), $Cu(NO_3)_2 \cdot 3H_2O$ (1.2 equiv) in DMSO (2.0 mL) at 65 °C under N_2.

4. Synthesis and Characterization of Substrates and Products

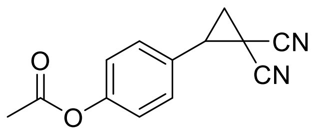
Part 1. Preparation of 1,1-dicyanocyclopropanes

Reported cyclopropanes **1** and **3** were prepared according to the literature procedures.[1] Cyclopropanes were purified by column chromatography on silica gel using petroleum ether/ethyl acetate as an eluent.

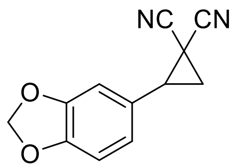
A general procedure for the preparation of 1,1-dicyanocyclopropanes: The cyclopropanes were prepared according to a literature procedure from the corresponding olefins. $PhI(OAc)_2$ (2.2 equiv), K_2CO_3 (2.2 equiv), malononitrile (1.2 equiv) and olefins (1.0 equiv) were dissolved in DCE (2 M) in a 100 mL flask. The mixture was stirred at 50 °C for 4 h as monitored by TLC. Then the reaction mixture was cooled to room temperature, poured into water and extracted with CH_2Cl_2 (3 × 20 mL). The combined organic phase was washed with water and brine. The solvent was removed under reduced pressure, and the residue was purified by flash column chromatography on silica gel to afford the pure product.



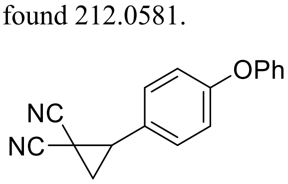
2-(4-isopropylphenyl)cyclopropane-1,1-dicarbonitrile (1f): This compound was prepared according to the general procedure using 1-isopropyl-4-vinylbenzene (800 mg, 5.4 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **1f** as a yellow crystal (816,4 mg, 72%). mp: 108-109 °C; IR (KBr, cm^{-1}): 3848, 3741, 3681, 3098, 3030, 2965, 2874, 2243, 1918, 1687, 1609, 1513, 1456, 1373, 1275, 1196, 1092, 1068, 986, 840, 765, 636, 586, 535; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30-7.26 (m, 2H), 7.23-7.20 (m, 2H), 3.27 (t, *J* = 9.1 Hz, 1H), 2.93 (hept, *J* = 6.9 Hz, 1H), 2.31-2.18 (m, 2H), 1.25 (d, *J* = 6.9 Hz, 6H).; ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.6, 128.4, 127.9, 127.4, 115.6, 113.3, 35.3, 34.0, 23.9, 22.6, 7.3.; HRMS (DART POSITIVE) *m/z* calcd for $C_{14}H_{15}N_2$ $[M+H]^+$ 211.1230, found 211.1229.



4-(2,2-Dicyanocyclopropyl)phenyl acetate (1i): This compound was prepared according to the general procedure using 4-vinylphenyl acetate (1.62 g, 10 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **1i** as a colorless crystal (1.36 g, 60%). mp: 117-118 °C; IR (KBr, cm^{-1}): 3103, 3019, 2248, 1751, 1515, 1373, 1227, 1105, 1019, 914, 845, 630, 514; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35-7.29 (m, 2H), 7.21-7.14 (m, 2H), 3.29 (t, *J* = 9.0 Hz, 1H), 2.31 (s, 3H), 2.30-2.19 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.2, 151.6, 129.6, 128.2, 122.6, 115.3, 113.0, 34.7, 22.7, 21.3, 7.4; HRMS (DART POSITIVE) *m/z* calcd for $C_{13}H_{11}N_2O_2$ $[M+H]^+$ 227.0815, found 227.0813.

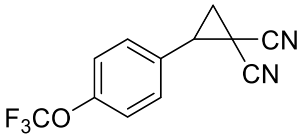


2-(Benzo[*d*][1,3]dioxol-5-yl)cyclopropane-1,1-dicarbonitrile (1j): This compound was prepared according to the general procedure using 5-vinylbenzo[*d*][1,3]dioxole (1.03 g, 7.0 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **1j** as a white solid (601.8 mg, 41%). mp: 95-96 °C; IR (KBr, cm^{-1}): 3101, 3038, 2979, 2896, 2795, 2249, 1612, 1498, 1443, 1395, 1250, 1193, 1126, 1084, 1035, 981, 927, 827, 777, 737, 660, 596, 489; ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.83 (d, *J* = 8.4 Hz, 1H), 6.77 (d, *J* = 7.0 Hz, 2H), 6.00 (s, 2H), 3.24 (t, *J* = 9.0 Hz, 1H), 2.23-2.16 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.8, 148.4, 124.2, 122.4, 115.4, 113.2, 108.8, 108.6, 101.8, 35.4, 22.6, 7.3; HRMS (FI Positive) m/z calcd for $C_{12}H_8N_2O_2$ $[M]^+$ 212.0580, found 212.0581.

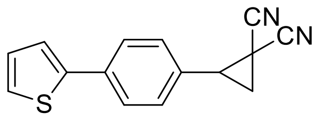


2-(4-Phenoxyphenyl)cyclopropane-1,1-dicarbonitrile (1k): This compound was prepared according to the general procedure using 1-phenoxy-4-vinylbenzene (981.2 mg, 5 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 8:1, v/v) to give **1k** as a white solid (924.9 mg, 71%). mp: 101-102 °C; IR (KBr, cm^{-1}): 3739, 3101, 3029, 2405, 2245, 2038, 1955, 1905, 1784, 1679, 1589, 1483, 1372, 1244, 1167, 1113, 1071, 983, 861, 760, 690, 627, 499; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.34 (m, 2H), 7.27-7.22 (m, 2H), 7.16 (tt, *J* = 7.4, 1.1 Hz, 1H), 7.03 (td, *J* =

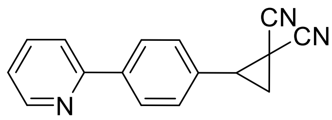
7.3, 6.8, 1.7 Hz, 4H), 3.28 (t, J = 9.0 Hz, 1H), 2.23 (dq, J = 8.8, 6.4 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.0, 156.4, 130.3, 130.2, 125.0, 124.4, 119.9, 119.0, 115.6, 113.4, 35.1, 22.8, 7.5; HRMS (DART POSITIVE) *m/z* calcd for $C_{17}H_{13}N_2O$ $[M+H]^+$ 261.1022, found 261.1022.



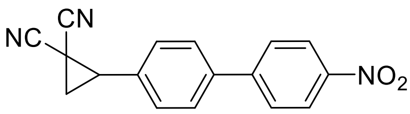
2-(4-(trifluoromethoxy)phenyl)cyclopropane-1,1-dicarbonitrile(1q): This compound was prepared according to the general procedure using 1-phenoxy-4-vinylbenzene(981.2mg,5mmol). The crude residue was purified by silica gel chromatography (PE/EA = 8:1, v/v) to give **1q** as a yellow oil (770mg, 46%). IR (KBr, cm^{-1}): 3879, 3743, 3045, 2254, 1514, 1449, 1268, 1215, 1166, 1019, 987, 925, 854, 822, 674, 633, 513; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37-7.33 (m, 2H), 7.31-7.27 (m, 2H), 3.29 (t, J = 9.0Hz, 1H), 2.29 (dd, J = 9.4, 6.5Hz, 1H), 2.24 (dd, J = 8.7, 6.5Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.0, 130.0, 129.2, 121.5, 121.2, 114.9, 112.7, 34.2, 22.5, 7.3; ^{19}FNMR (565MHz, CDCl3) δ -57.8; HRMS (FI Positive Ion) m/z calcd for $C_{12}H_7N_2OF_3$ $[M]^+$ 252.0505, found 252.0499.



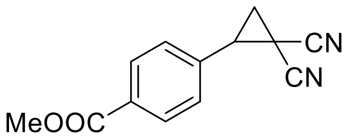
2-(4-(Thiophen-2-yl)phenyl)cyclopropane-1,1-dicarbonitrile (1s): This compound was prepared according to the general procedure using 2-(4-vinylphenyl)thiophene (279.4 mg, 1.5 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **1s** as a white solid (83.5 mg, 23%). mp: 155-156 ºC; IR (KBr, cm^{-1}): 3984, 3859, 3739, 3506, 3434, 3104, 3033, 2921, 2250, 1617, 1506, 1427, 1263, 1208, 1132, 988, 834, 716, 636; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66 (d, J = 8.3 Hz, 2H), 7.37-7.28 (m, 4H), 7.10 (dd, J = 5.1, 3.6 Hz, 1H), 3.31 (t, J = 9.0 Hz, 1H), 2.31-2.24 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.3, 135.9, 129.7, 129.2, 128.5, 126.8, 126.0, 124.2, 115.6, 113.3, 35.3, 22.7, 7.7; HRMS (FI Positive Ion) m/z calcd for $C_{15}H_{10}N_2S$ $[M]^+$ 250.0559, found 250.0558.



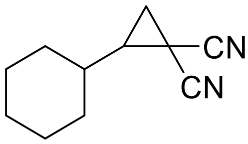
2-(4-(Pyridin-2-yl)phenyl)cyclopropane-1,1-dicarbonitrile (1t): This compound was prepared according to the general procedure using 1-(pyridin-2-yl)-4-vinylbenzene (363.0 mg, 2.0 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **1t** as a white solid (278.5 mg, 57%). mp: 115-116 ºC; IR (KBr, cm^{-1}): 3952, 3743, 3677, 3103, 3044, 2244, 1697, 1584, 1516, 1465, 1433, 1374, 1279, 1095, 984, 852, 788, 738, 632, 596, 454; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (ddd, J = 4.8, 1.8, 1.0 Hz, 1H), 8.10-8.03 (m, 2H), 7.82-7.70 (m, 2H), 7.44-7.37 (m, 2H), 7.30-7.23 (m, 1H), 3.35 (t, J = 9.1 Hz, 1H), 2.30 (dq, J = 9.5, 6.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.3, 149.9, 140.6, 137.0, 131.2, 128.8, 127.7, 122.8, 120.8, 115.4, 113.0, 35.1, 22.5, 7.5; HRMS (ESI Positive) m/z: calcd for $C_{16}H_{11}N_3$ $[M+H]^+$ 246.1026, found 246.1023.



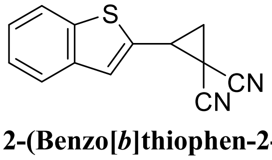
3-(4'-Nitro-[1,1'-biphenyl]-4-yl)cyclopropane-1,1-dicarbonitrile (**1u**): This compound was prepared according to the general procedure using 4-nitro-4'-vinyl-1,1'-biphenyl (360.0 mg, 1.6 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **1u** as a white solid (267.5 mg, 58%). mp: 105-106 °C; IR (KBr, cm^{-1}): 3740, 3106, 2247, 1600, 1564, 1529, 1486, 1346, 1110, 984, 858, 831, 756, 733, 693, 633, 485; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34-8.27 (m, 2H), 7.77-7.70 (m, 2H), 7.69-7.66 (m, 2H), 3.36 (t, *J* = 9.1 Hz, 1H), 2.32 (d, *J* = 9.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.5, 146.4, 140.0, 131.4, 129.3, 128.2, 128.0, 124.3, 115.2, 113.0, 34.8, 22.5, 7.5; HRMS (FI Positive) *m/z* calcd for $C_{17}H_{11}O_2N_3$ $[M]^+$ 289.0846, found 289.0849.



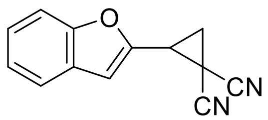
methyl 4-(2,2-dicyanocyclopropyl)benzoate (**1w**): This compound was prepared according to the general procedure using methyl 4-vinylbenzoate (396.0 mg, 6.0 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **1w** as a white solid (897.9 mg, 79%). mp: 67-68 °C; IR (KBr, cm^{-1}): 3103, 3021, 2946, 2251, 1950, 1715, 1611, 1443, 1282, 1186, 1111, 979, 867, 789, 748, 632, 486; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13-8.07 (m, 2H), 7.43-7.34 (m, 2H), 3.93 (s, 3H), 3.34 (t, *J* = 9.0 Hz, 1H), 2.31 (d, *J* = 9.0 Hz, 2H), 1.57 (s, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.3, 135.5, 131.5, 130.5, 128.6, 115.1, 112.8, 52.5, 34.7, 22.6, 7.6; HRMS (DART Positive) *m/z* calcd for $C_{13}H_{11}O_2N_2$ $[M]^+$ 227.0815, found 227.0813.



2-cyclohexylcyclopropane-1,1-dicarbonitrile (**1z**): This compound was prepared according to the general procedure using vinylcyclohexane (1.10 g, 10.0 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **1z** as a yellow oil (636.3 mg, 37%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.04-1.97 (m, 1H), 1.89 (dd, *J* = 9.0, 5.5 Hz, 1H), 1.83-1.74 (m, 4H), 1.72-1.65 (m, 1H), 1.53 (dd, *J* = 8.3, 5.6 Hz, 1H), 1.33 – 1.16 (m, 5H), 1.05 (tt, *J* = 10.4, 3.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 115.8, 114.1, 39.9, 37.2, 31.9, 31.9, 25.9, 25.7, 25.5, 24.1, 3.3. Compound **1z** was consistent with the literature data.[1g]



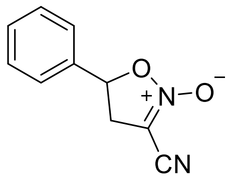
2-(Benzo[*b*]thiophen-2-yl)cyclopropane-1,1-dicarbonitrile (**3b**): This compound was prepared according to the general procedure using 2-vinylbenzo[*b*]thiophene (1.6 g, 10.0 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **3b** as a white solid (794.0 mg, 36%). mp: 125-126 °C; IR (KBr, cm^{-1}); 3745, 3678, 3615, 3096, 3029, 2245, 1689, 1550, 1431, 1379, 1256, 1188, 1128, 1067, 1013, 940, 865, 758, 660, 628, 589, 485; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84-7.74 (m, 2H), 7.42-7.36 (m, 2H), 7.29 (s, 1H), 3.48 (t, *J* = 8.8 Hz, 1H), 2.35 (ddd, *J* = 24.8, 8.9, 6.4 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 140.3, 139.3, 134.3, 125. 9, 125.4, 125.2, 124.5, 122.7, 115.0, 112.9, 31.0, 24.1, 8.7; HRMS (FI Positive) *m/z* calcd for $C_{13}H_8N_2S$ $[M]^+$ 224.0403, found 224.0398.



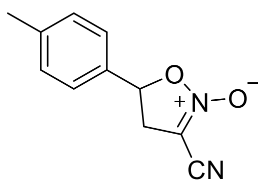
2-(Benzofuran-2-yl)cyclopropane-1,1-dicarbonitrile (**3c**): This compound was prepared according to the general procedure using 2-vinylbenzofuran (1.16 g, 8.0 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **3c** as a white solid (516.0 mg, 31%). mp: 97-98 ºC; IR (KBr, cm^{-1}): 3887, 3735, 3108, 3025, 2245, 1446, 1391, 1308, 1258, 1172, 1097, 989, 926, 870, 811, 749, 703, 629, 594; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57 (dt, *J* = 7.6, 1.1 Hz, 1H), 7.47 (dq, *J* = 8.3, 0.9 Hz, 1H), 7.33 (ddd, *J* = 8.4, 7.2, 1.3 Hz, 1H), 7.28-7.23 (m, 1H), 6.82 (d, *J* = 0.9 Hz, 1H), 3.38 (ddd, *J* = 9.4, 8.4, 0.7 Hz, 1H), 2.44 (dd, *J* = 8.4, 6.4 Hz, 1H), 2.30 (dd, *J* = 9.5, 6.4 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.2, 147.3, 127.5, 125.6, 123.6, 121.5, 114.5, 112.6, 111.5, 107.9, 28.8, 21.8, 7.3; HRMS (FI Positive) *m/z* calcd for $C_{13}H_8ON_2$ $[M]^+$ 208.0631, found 208.0626.

Part 2. Ring Expansion Reactions of Cyclopropanes

General Procedure *(Method A):* To a test tube were added 2-arylcyclopropane-1,1-dicarbonitrile (0.2 mmol), $Cu(NO_3)_2{\cdot}3H_2O$ (0.2-0.24 mmol), DMSO (2.0 mL). The reaction mixture was stirred at 60-70 °C for 15-36 h under N_2 as monitored by TLC. Upon completion, the reaction mixture was cooled down to room temperature, extracted with DCM (3×10 mL). The combined organic phase was washed with water and brine, and dried over anhydrous Na_2SO_4, then evaporated under reduced pressure to give the crude product, which was further purified by column chromatography on silica gel to afford the pure product.

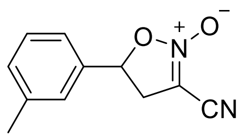


3-Cyano-5-phenyl-4,5-dihydroisoxazole 2-oxide (2a): This compound was prepared according to ***Method A*** using 2-phenylcyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 65 °C for 15 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2a** as a white solid (30.7 mg, 82%). mp: 93-94 ºC; IR (KBr, cm^{-1}): 2222, 1601, 1494, 1459, 1360, 1286, 1261, 1228, 1210, 1156, 941, 878, 818, 763, 699, 626, 538, 483, 433; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38-7.48 (m, 5H), 5.93 (t, *J* = 8.9 Hz, 1H), 3.74 (dd, *J* = 16.3, 9.5 Hz, 1H), 3.43 (dd, *J* = 16.3, 8.3 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.1, 130.1, 129.5, 126.0, 109.8, 92.8, 80.3, 37.4; HRMS (DART Positive) m/z: calcd for $C_{10}H_9N_2O_2$ $[M+H]^+$ 189.0659, found 189.0657. Compound **2a** was consistent with the literature data.[2]

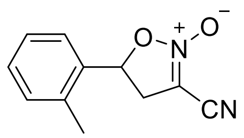


3-Cyano-5-(*p*-tolyl)-4,5-dihydroisoxazole 2-oxide (2b): This compound was prepared according to ***Method A*** using 2-(*p*-tolyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$

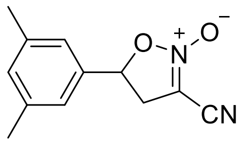
(0.24 mmol) at 65 °C for 15 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2b** as a yellow oil (34.1 mg, 84%). IR (KBr, cm^{-1}): 3440, 2922, 2859, 2220, 1606, 1448, 1367, 1257, 1219, 1154, 1104, 1034, 941, 877, 818, 733, 628, 535; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.27 (q, *J* = 8.0 Hz, 4H), 5.85 (t, *J* = 9.0 Hz, 1H), 3.65 (dd, *J* = 16.3, 9.5 Hz, 1H), 3.38 (dd, *J* = 16.3, 8.6 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.2, 132.8, 130.1, 126.2, 109.9, 93.1, 80.6, 37.2, 21.4; HRMS (DART Positive) m/z: calcd for $C_{11}H_{11}N_2O_2$ $[M+H]^+$ 203.0815, found 203.0813. Compound **2b** was consistent with the literature data.[2]



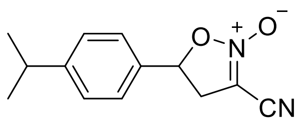
3-Cyano-5-(*m*-tolyl)-4,5-dihydroisoxazole 2-oxide (2c): This compound was prepared according to ***Method A*** using 2-(*m*-tolyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol) at 65 °C for 15 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2c** as a yellow oil (35.1 mg, 87%). IR (KBr, cm^{-1}): 3851, 3739, 2923, 2221, 1618, 1456, 1368, 1260, 1168, 1041, 906, 847, 789, 704, 629; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (t, *J* = 7.6 Hz, 1H), 7.25-7.14 (m, 3H), 5.85 (t, *J* = 8.9 Hz, 1H), 3.68 (dd, *J* = 16.3, 9.5 Hz, 1H), 3.38 (dd, *J* = 16.3, 8.4 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 139.6, 136.2, 131.0, 129.5, 126.8, 123.3, 110.0, 93.2, 80.6, 37.5, 21.7; HRMS (DART Positive) m/z: calcd for $C_{11}H_{11}N_2O_2$ $[M+H]^+$ 203.0815, found 203.0815.



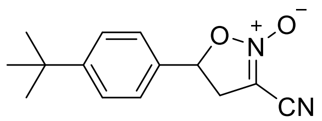
3-Cyano-5-(*o*-tolyl)-4,5-dihydroisoxazole 2-oxide (2d): This compound was prepared according to ***Method A*** using 2-(*o*-tolyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol) at 65 °C for 15 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2d** as a yellow oil (37.6 mg, 93%). IR (KBr, cm^{-1}): 3904, 3738, 2948, 2221, 1618, 1458, 1372, 1257, 1170, 1040, 882, 824, 761, 627; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.40 (m, 1H), 7.37-7.21 (m, 3H), 6.10 (dd, *J* = 9.6, 8.1 Hz, 1H), 3.72 (dd, *J* = 16.2, 9.7 Hz, 1H), 3.30 (dd, *J* = 16.2, 8.1 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 134.9, 134.3, 131.5, 129.7, 127.1, 125.0, 109.8, 92.8, 77.8, 36.5, 19.1; HRMS (DART Positive) m/z: calcd for $C_{11}H_{11}N_2O_2$ $[M+H]^+$ 203.0815, found 203.0815.



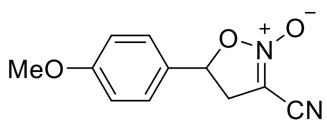
3-Cyano-5-(3,5-dimethylphenyl)-4,5-dihydroisoxazole 2-oxide (2e): This compound was prepared according to ***Method A*** using 2-(3,5-dimethylphenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol) at 65 °C for 15 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2e** as a yellow oil (28.9 mg, 67%). IR (KBr, cm^{-1}): 3853, 3741, 2922, 2220, 1617, 1462, 1368, 1259, 1170, 1036, 909, 845, 700, 631; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.06 (s, 1H), 6.99 (s, 2H), 5.81 (t, *J* = 9.0 Hz, 1H), 3.66 (dd, *J* = 16.3, 9.6 Hz, 1H), 3.37 (dd, *J* = 16.3, 8.3 Hz, 1H), 2.35 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 139.3, 136.0, 131.6, 123.7, 109.9, 93.0, 80.5, 37.3, 21.4; HRMS (FI Positive) m/z: calcd for $C_{12}H_{12}N_2O_2$ $[M]^+$ 216.0893, found 216.0897.



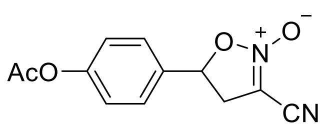
3-Cyano-5-(4-isopropylphenyl)-4,5-dihydroisoxazole 2-oxide (2f): This compound was prepared according to ***Method A*** using 2-(4-isopropylphenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 65 °C for 15 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2f** as a yellow oil (37.4 mg, 81%). IR (KBr, cm^{-1}): 2962, 2876, 2221, 1612, 1512, 1456, 1370, 1264, 1220, 1153, 1053, 879, 829, 730, 631, 561; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (m, 4H), 5.86 (dd, *J* = 9.4, 8.5 Hz, 1H), 3.66 (dd, *J* = 16.3, 9.4 Hz, 1H), 3.40 (dd, *J* = 16.3, 8.5 Hz, 1H), 2.94 (hept, *J* = 6.9 Hz, 1H), 1.26 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) 151.2, 133.2, 127.5, 126.3, 109.9, 93.1, 80.5, 37.2, 34.1, 24.0; HRMS (DART Positive) m/z: calcd for $C_{13}H_{15}N_2O_2$ $[M+H]^+$ 231.1128, found 231.1128.



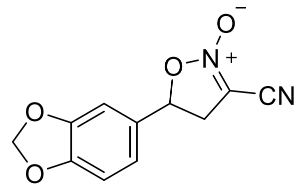
5-(4-(*tert*-Butyl)phenyl)-3-cyano-4,5-dihydroisoxazole 2-oxide (2g): This compound was prepared according to ***Method A*** using 2-(4-(*tert*-butyl)phenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 65 °C for 15 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give product **2g** as a white solid (37.4 mg, 69%). mp: 84-85 °C; IR (KBr, cm^{-1}): 2963, 2221, 1612, 1369, 1265, 1221, 1113, 1026, 881, 834, 762, 628, 569; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 2H), 5.87 (t, *J* = 8.9 Hz, 1H), 3.66 (dd, *J* = 16.2, 9.4 Hz, 1H), 3.40 (dd, *J* = 16.2, 8.4 Hz, 1H), 1.33 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.5, 132.9, 126.4, 126.0, 109.9, 93.0, 80.4, 37.2, 34.9, 31.3; HRMS (DART Positive) m/z: calcd for $C_{14}H_{17}N_2O_2$ $[M+H]^+$ 245.1285, found 245.1282.



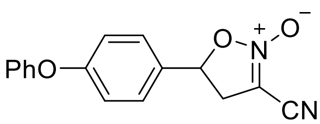
3-Cyano-5-(4-methoxyphenyl)-4,5-dihydroisoxazole 2-oxide (2h): This compound was prepared according to ***Method A*** using 2-(4-methoxyphenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 60 °C for 15 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2h** as a yellow oil (32.6 mg, 75%). IR (KBr, cm^{-1}): 3612, 3538, 2951, 2845, 2221, 1615, 1514, 1456, 1300, 1255, 1179, 1029, 945, 876, 828, 629, 551; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37-7.29 (m, 2H), 7.00-6.89 (m, 2H), 5.83 (t, *J* = 9.1 Hz, 1H), 3.83 (s, 3H), 3.62 (dd, *J* = 16.3, 9.4 Hz, 1H), 3.39 (dd, *J* = 16.3, 8.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.0, 128.1, 127.4, 114.7, 109.9, 93.3, 80.7, 55.5, 37.0; HRMS (DART Positive) m/z: calcd for $C_{11}H_{11}N_2O_3$ $[M+H]^+$ 219.0764, found 219.0764.



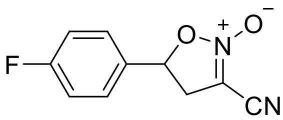
5-(4-Acetoxyphenyl)-3-cyano-4,5-dihydroisoxazole 2-oxide (2i): This compound was prepared according to ***Method A*** using 2-(4-acetoxyphenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol) at 65 °C for 15 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2i** as a yellow oil (34.4 mg, 70%). IR (KBr, cm^{-1}): 3991, 3826, 3745, 3614, 2940, 2222, 1761, 1618, 1509, 1432, 1369, 1203, 1015, 882, 606, 546; ^1H NMR (500 MHz, $CDCl_3$) δ 7.44-7.37 (m, 2H), 7.22-7.13 (m, 2H), 5.88 (t, J = 8.9 Hz, 1H), 3.68 (dd, J = 16.3, 9.5 Hz, 1H), 3.36 (dd, J = 16.3, 8.3 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.6, 152.0, 133.7, 127.6, 123.0, 109.9, 93.0, 79.9, 37.5, 21.4; HRMS (FI Positive) m/z: calcd for $C_{12}H_{10}O_4N_2$ $[M]^+$ 246.0635, found 246.0637.



5-(Benzo[*d*][1,3]dioxol-5-yl)-3-cyano-4,5-dihydroisoxazole 2-oxide (2j): This compound was prepared according to ***Method A*** using 2-(benzo[*d*][1,3]dioxol-5-yl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol) at 65 °C for 30 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2j** as a yellow oil (42.8 mg, 92%). IR (KBr, cm^{-1}): 2906, 2222, 1616, 1500, 1374, 1336, 1252, 1109, 1038, 922, 859, 812; ^1H NMR (400 MHz, $CDCl_3$) δ 6.89-6.80 (m, 3H), 6.02 (s, 2H), 5.79 (t, J = 9.1 Hz, 1H), 3.63 (dd, J = 16.4, 9.4 Hz, 1H), 3.36 (dd, J = 16.4, 8.7 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.4, 148.9, 129.5, 120.9, 110.0, 109.0, 106.6, 102.0, 93.3, 80.8, 37.4; HRMS (FI Positive) m/z: calcd for $C_{11}H_8N_2O_4$ $[M]^+$ 232.0479, found 232.0482.

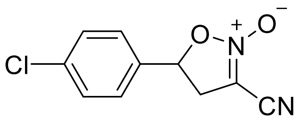


3-Cyano-5-(4-phenoxyphenyl)-4,5-dihydroisoxazole 2-oxide (2k): This compound was prepared according to ***Method A*** using 2-(4-phenoxyphenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol) at 65 °C for 23 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2k** as a white solid (46.1 mg, 82%). mp: 151-152 °C; IR (KBr, cm^{-1}): 3898, 3740, 2859, 2221, 1602, 1500, 1365, 1256, 1160, 1109, 943, 880, 831, 755, 693, 632, 536, 484; ^1H NMR (600 MHz, $CDCl_3$) δ 7.39-7.33 (m, 4H), 7.17 (t, J = 7.4 Hz, 1H), 7.05 (t, J = 8.4 Hz, 4H), 5.87 (t, J = 9.0 Hz, 1H), 3.67 (dd, J = 16.3, 9.4 Hz, 1H), 3.41 (dd, J = 16.3, 8.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.2, 156.3, 130.1, 129.9, 128.0, 124.3, 119.7, 119.0, 109.1 93.0, 80.2, 37.2; HRMS (FI Positive) m/z: calcd for $C_{16}H_{12}N_2O_3$ $[M]^+$ 280.0842, found 280.0847.

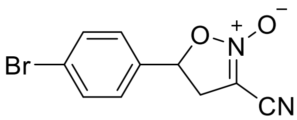


3-Cyano-5-(4-fluorophenyl)-4,5-dihydroisoxazole 2-oxide (2l): This compound was prepared according to ***Method A*** using 2-(4-fluorophenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol) at 65 °C for 23 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2l** as a yellow oil (32.1 mg, 78%). IR (KBr, cm^{-1}):

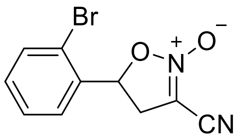
3848, 3744, 2935, 2222, 1617, 1513, 1456, 1368, 1232, 1160, 882, 836, 627, 548; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.36 (m, 2H), 7.18-7.11 (m, 2H), 5.88 (t, J = 9.0 Hz, 1H), 3.69 (dd, J = 16.3, 9.5 Hz, 1H), 3.37 (dd, J = 16.3, 8.5 Hz, 1H); ^{19}F NMR (471 MHz, $CDCl_3$) δ -110.5 (tt, F); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.6 (d, $^{1}J_{C-F}$ = 250.1 Hz), 131.8 (d, $^{4}J_{C-F}$ = 3.5 Hz), 128.2 (d, $^{3}J_{C-F}$ = 8.6 Hz), 116.6 (d, $^{2}J_{C-F}$ = 22.0 Hz), 109.7, 92.9, 79.7, 37.3; HRMS (DART Positive) m/z: calcd for $C_{10}H_8N_2O_2F$ $[M+H]^+$ 207.0564, found 207.0564.



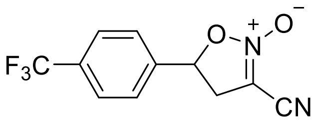
5-(4-Chlorophenyl)-3-cyano-4,5-dihydroisoxazole 2-oxide (2m): This compound was prepared according to ***Method A*** using 2-(4-chlorophenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 65 °C for 23 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2m** as a yellow oil (40.2 mg, 90%). IR (KBr, cm^{-1}): 3744, 2923, 2858, 2224, 1916, 1609, 1490, 1428, 1367, 1254, 1152, 1091, 1011, 938, 880, 828, 611, 535, 443; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.43 (d, J = 8.5 Hz, 2H), 7.34 (d, J = 8.3 Hz, 2H), 5.87 (t, J = 8.9 Hz, 1H), 3.71 (dd, J = 16.3, 9.5 Hz, 1H), 3.35 (dd, J = 16.3, 8.3 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 136.3, 134.7, 129.9, 127.6, 109.8, 92.9, 79.7, 37.5; HRMS (FI Positive) m/z: calcd for $C_{10}H_7ClN_2O_2$ $[M]^+$ 222.0191, found 222.0187.



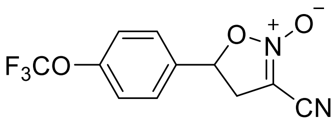
5-(4-Bromophenyl)-3-cyano-4,5-dihydroisoxazole 2-oxide (2n): This compound was prepared according to ***Method A*** using 2-(4-bromophenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 65 °C for 24 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2n** as a yellow oil (34.8 mg, 65%). IR (KBr, cm^{-1}): 2922, 2858, 2222, 1916, 1609, 1484, 1367, 1256, 1150, 1072, 1010, 879, 821, 604, 531, 481; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 8.3 Hz, 2H), 7.28 (d, J = 8.4 Hz, 2H), 5.86 (t, J = 8.9 Hz, 1H), 3.71 (dd, J = 16.3, 9.5 Hz, 1H), 3.34 (dd, J = 16.3, 8.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 135.2, 132.9, 127.9, 124.4, 109.8, 92.9, 79.7, 37.4; HRMS (DART Positive) m/z: calcd for $C_{10}H_8N_2O_2Br$ $[M+H]^+$ 266.9764, found 266.9763.



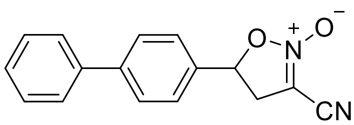
5-(2-Bromophenyl)-3-cyano-4,5-dihydroisoxazole 2-oxide (2o): This compound was prepared according to ***Method A*** using 2-(2-bromophenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 65 °C for 24 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2o** as a yellow oil (27.8 mg, 52%). IR (KBr, cm^{-1}): 3859, 3741, 3677, 3648, 3619, 2924, 2222, 1623, 1469, 1439, 1373, 1237, 1160, 1028, 889, 758, 623, 484, 456; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (dt, J = 7.9, 0.9 Hz, 1H), 7.51 (dd, J = 7.7, 1.7 Hz, 1H), 7.43 (td, J = 7.7, 1.1 Hz, 1H), 7.30 (td, J = 7.7, 1.8 Hz, 1H), 6.15 (dd, J = 9.9, 6.2 Hz, 1H), 3.95 (dd, J = 16.5, 9.9 Hz, 1H), 3.21 (dd, J = 16.5, 6.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.4, 133.7, 131.0, 128.4, 126.2, 120.5, 109.5, 92.5, 78.5, 37.0; HRMS (DART Positive) m/z: calcd for $C_{10}H_8N_2O_2Br$ $[M+H]^+$ 266.9764, found 266.9764.



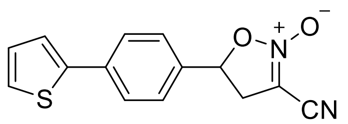
3-Cyano-5-(4-(trifluoromethyl)phenyl)-4,5-dihydroisoxazole 2-oxide (2p): This compound was prepared according to ***Method A*** using 2-(4-(trifluoromethyl)phenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol) at 65 °C for 24 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2p** as a yellow oil (43.9 mg, 86%). IR (KBr, cm^{-1}): 3739, 3677, 2224, 1623, 1424, 1375, 1327, 1261, 1169, 1122, 1068, 1018, 886, 843, 616; ^1H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 8.1 Hz, 2H), 7.53 (d, J = 8.1 Hz, 2H), 5.96 (dd, J = 9.6, 7.9 Hz, 1H), 3.79 (dd, J = 16.3, 9.6 Hz, 1H), 3.35 (dd, J = 16.3, 7.9 Hz, 1H); ^{19}F NMR (375 MHz, $CDCl_3$) δ -62.8 (s, CF_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.2, 132.1 (q, $^2J_{C-F}$ = 32.9 Hz), 126.2 (q, $^3J_{C-F}$ = 3.8 Hz), 126.2, 123.7 (q, $^1J_{C-F}$ = 272.3 Hz), 109.4, 92.3, 78.9, 37.4; HRMS (DART Positive) m/z: calcd for $C_{11}H_8N_2O_2F_3$ $[M+H]^+$ 257.0532, found 257.0533.



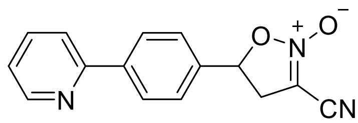
3-Cyano-5-(4-(trifluoromethoxy)phenyl)-4,5-dihydroisoxazole 2-oxide (2q): This compound was prepared according to ***Method A*** using 2-(4-(trifluoromethoxy)phenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol) at 65 °C for 20 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2q** as a yellow oil (30.9 mg, 56%). IR (KBr, cm^{-1}): 3734, 2224, 1621, 1513, 1454, 1374, 1262, 1223, 1167, 1019, 883, 677, 608, 550; ^1H NMR (600 MHz, $CDCl_3$) δ 7.47-7.42 (m, 2H), 7.38-7.25 (m, 2H), 5.91 (t, J = 8.8 Hz, 1H), 3.73 (dd, J = 16.3, 9.5 Hz, 1H), 3.36 (dd, J = 16.3, 8.2 Hz, 1H); ^{19}F NMR (565 MHz, $CDCl_3$) δ -57.9 (s, CF_3); ^{13}C NMR (150 MHz, $CDCl_3$) δ 150.2, 134.6, 127.59, 121.8, 120.4 (q, $^1J_{C-F}$ = 258.2 Hz), 109.5, 92.5, 79.1, 37.2; HRMS (FI Positive) m/z: calcd for $C_{11}H_7O_3N_2F_3$ $[M]^+$ 272.0403, found 272.0402.



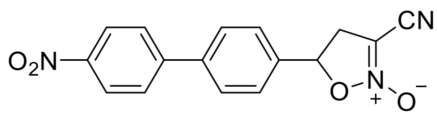
5-([1,1'-Biphenyl]-4-yl)-3-cyano-4,5-dihydroisoxazole 2-oxide (2r): This compound was prepared according to ***Method A*** using 2-([1,1'-biphenyl]-4-yl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol) at 65 °C for 20 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2r** as a yellow solid (28.3 mg, 54%). mp: 176-177 °C. IR (KBr, cm^{-1}): 3847, 3743, 3577, 2923, 2220, 1688, 1603, 1490, 1447, 1408, 1368, 1256, 1156, 1038, 1006, 941, 883, 832, 765, 725, 690, 632, 556, 518; ^1H NMR (400 MHz, Acetone-d_6) δ 7.81-7.72 (m, 2H), 7.72-7.65 (m, 4H), 7.53-7.44 (m, 2H), 7.44-7.35 (m, 1H), 6.18 (t, J = 9.2 Hz, 1H), 3.96 (dd, J = 16.4, 9.5 Hz, 1H), 3.67 (dd, J = 16.4, 9.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.1, 140.0, 134.8, 129.1, 128.1, 128.0, 127.3, 126.6, 109.8, 92.8, 80.2, 37.3; HRMS (DART Positive) m/z: calcd for $C_{16}H_{13}N_2O_2$ $[M+H]^+$ 265.0972, found 265.0969.



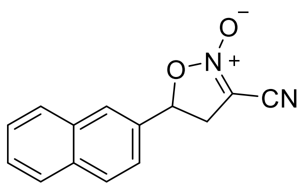
3-Cyano-5-(4-(thiophen-2-yl)phenyl)-4,5-dihydroisoxazole 2-oxide (2s): This compound was prepared according to ***Method A*** using 2-(4-(thiophen-2-yl)phenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol) at 65 °C for 36 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2s** as a yellow solid (44.5 mg, 82%). mp: 161-162 °C. IR (KBr, cm^{-1}): 3847, 3743, 3577, 2923, 2220, 1688, 1603, 1490, 1447, 1408, 1368, 1256, 1156, 1038, 1006, 941, 883, 832, 765, 725, 690, 632, 556, 518; ^1H NMR (600 MHz, $CDCl_3$) δ 7.69 (d, J = 8.0 Hz, 2H), 7.42-7.32 (m, 4H), 7.11 (t, J = 4.4 Hz, 1H), 5.90 (t, J = 8.9 Hz, 1H), 3.71 (dd, J = 16.3, 9.5 Hz, 1H), 3.41 (dd, J = 16.3, 8.4 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.1, 136.3, 134. 8, 128.4, 128.1, 126.8, 126.7, 125.9, 124.2, 120.5, 109.7, 92.8, 80.1, 37.3; HRMS (DART Positive) m/z: calcd for $C_{14}H_{11}O_2N_2S$ $[M+H]^+$ 271.0536, found 271.0536.



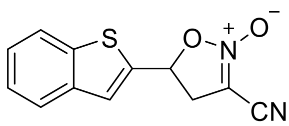
3-Cyano-5-(4-(pyridin-2-yl)phenyl)-4,5-dihydroisoxazole 2-oxide (2t): This compound was prepared according to ***Method A*** using 2-(4-(pyridin-2-yl)phenyl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol) at 65 °C for 36 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2t** as a white solid (29.7 mg, 56%). mp: 150-151 °C. IR (KBr, cm^{-1}): 3851, 3741, 3675, 3617, 2223, 1604, 1560, 1465, 1366, 1259, 1224, 1155, 885, 827, 783, 732, 557, 523; ^1H NMR (400 MHz, $CDCl_3$) δ 8.71 (dt, J = 5.6, 1.2 Hz, 1H), 8.11-8.05 (m, 2H), 7.83-7.71 (m, 2H), 7.53-7.46 (m, 2H), 7.32-7.24 (m, 1H), 5.94 (t, J = 8.9 Hz, 1H), 3.73 (dd, J = 16.3, 9.5 Hz, 1H), 3.42 (dd, J = 16.3, 8.4 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.2, 150.0, 141.1, 137.1, 136.5, 127.9, 126.4, 122.9, 120.8, 109.7, 92.9, 80.0, 37.3; HRMS (DART Positive) m/z: calcd for $C_{15}H_{12}O_2N_3$ $[M+H]^+$ 266.0924, found 266.0924.



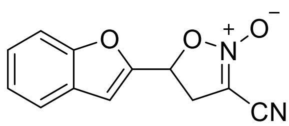
3-Cyano-5-(4'-nitro-[1,1'-biphenyl]-4-yl)-4,5-dihydroisoxazole 2-oxide (2u): This compound was prepared according to ***Method A*** using 2-(4'-nitro-[1,1'-biphenyl]-4-yl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol) at 65 °C for 36 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **2u** as a yellow oil (48.4 mg, 78%). IR (KBr, cm^{-1}): 3739, 3441, 2926, 2222, 1624, 1511, 1447, 1374, 1343, 1241, 1110, 966, 884, 835, 808, 731, 687, 638, 586, 554, 485, 458; ^1H NMR (600 MHz, $CDCl_3$) δ 8.31 (d, J = 8.7 Hz, 2H), 7.73 (dd, J = 16.6, 8.3 Hz, 4H), 7.54 (d, J = 8.1 Hz, 2H), 5.98 (t, J = 8.8 Hz, 1H), 3.79 (dd, J = 16.3, 9.6 Hz, 1H), 3.43 (dd, J = 16.3, 8.1 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 147.6, 146.4, 140.5, 136.8, 128.4, 128.1, 126.8, 124.4, 109.7, 92.8, 79.7, 37.3; HRMS (DART Positive) m/z: calcd for $C_{16}H_{12}O_4N_3$ $[M+H]^+$ 310.0822, found 310.0822.



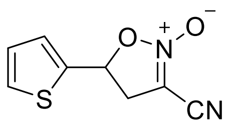
3-Cyano-5-(naphthalen-2-yl)-4,5-dihydroisoxazole 2-oxide (4a): This compound was prepared according to ***Method A*** using 2-(naphthalen-2-yl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 65 °C for 24 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **4a** as a white solid (39.5 mg, 83%). mp: 146-147 °C; IR (KBr, cm^{-1}): 2923, 2219, 1607, 1508, 1445, 1369, 1324, 1258, 1175, 940, 898, 830, 750, 609, 482; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.6 Hz, 1H), 7.87 (ddd, *J* = 9.0, 4.5, 2.2 Hz, 3H), 7.62-7.52 (m, 2H), 7.45 (dd, *J* = 8.5, 1.9 Hz, 1H), 6.04 (t, *J* = 8.9 Hz, 1H), 3.74 (dd, *J* = 16.3, 9.6 Hz, 1H), 3.47 (dd, *J* = 16.3, 8.3 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 133.7, 133.0, 132.9, 129.7, 128.2, 127.9, 127.3, 127.2, 125.9, 122.5, 109.7, 92.8, 80.4, 37.2; HRMS (DART Positive) m/z: calcd for $C_{14}H_{11}N_2O_2$ $[M+H]^+$ 239.0815, found 239.0814.



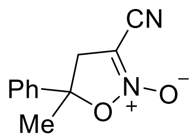
5-(Benzo[*b*]thiophen-2-yl)-3-cyano-4,5-dihydroisoxazole 2-oxide (4b): This compound was prepared according to ***Method A*** using 2-(benzo[*b*]thiophen-2-yl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 65 °C for 24 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **4b** as a white solid (25.3 mg, 52%). mp: 156-157 °C; IR (KBr, cm^{-1}): 3106, 2922, 2858, 2221, 1612, 1438, 1372, 1259, 1159, 1039, 930, 864, 835, 715, 640; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (dt, *J* = 7.5, 3.4 Hz, 1H), 7.83-7.77 (m, 1H), 7.44-7.39 (m, 3H), 6.19 (dd, *J* = 9.3, 7.5 Hz, 1H), 3.77 (dd, *J* = 16.4, 9.3 Hz, 1H), 3.58 (dd, *J* = 16.4, 7.5 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 140.0, 138.7, 138.2, 126.0, 125.3, 124.7, 124.5, 122.8, 109.5, 92.6, 76.7, 37.2; HRMS (DART Positive) m/z: calcd for $C_{12}H_9N_2O_2S$ $[M+H]^+$ 245.0379, found 245.0376.



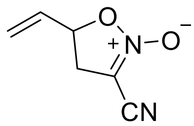
5-(Benzofuran-2-yl)-3-cyano-4,5-dihydroisoxazole 2-oxide (4c): This compound was prepared according to ***Method A*** using 2-(benzofuran-2-yl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 65 °C for 24 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **4c** as a white solid (25.0 mg, 55%). mp: 100-101 °C; IR (KBr, cm^{-1}): 3105, 2922, 2853, 2225, 1706, 1610, 1450, 1370, 1261, 1234, 1169, 1047, 986, 924, 861, 813, 763, 633, 559, 466; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (dt, *J* = 7.8, 1.0 Hz, 1H), 7.53 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.39 (ddd, *J* = 8.4, 7.2, 1.3 Hz, 1H), 7.32-7.27 (m, 1H), 6.93 (s, 1H), 6.01 (dd, *J* = 9.7, 7.0 Hz, 1H), 3.73 (qd, *J* = 16.4, 8.3 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.6, 149.5, 127.1, 126.3, 123.8, 122.0, 111.9, 109.6, 108.3, 92.5, 73.4, 33.5; HRMS (FI Positive) m/z: calcd for $C_{12}H_8N_2O_3$ $[M]^+$ 228.0529, found 228.0536.



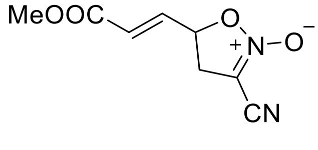
3-Cyano-5-(thiophen-2-yl)-4,5-dihydroisoxazole 2-oxide (4d): This compound was prepared according to ***Method A*** using 2-(thiophen-2-yl)cyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 60 °C for 36 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **4d** as a yellow oil (24.5 mg, 63%). IR (KBr, cm^{-1}): 3106, 2922, 2858, 2221, 1612, 1438, 1372, 1259, 1159, 1039, 930, 864, 835, 715, 640; ^1H NMR (500 MHz, $CDCl_3$) δ 7.46 (dd, J = 5.2, 1.2 Hz, 1H), 7.22 (dt, J = 3.7, 0.9 Hz, 1H), 7.07 (dd, J = 5.1, 3.6 Hz, 1H), 6.13 (dd, J = 9.0, 8.1 Hz, 1H), 3.72 (dd, J = 16.3, 9.2 Hz, 1H), 3.53 (dd, J = 16.3, 8.1 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.7, 128.3, 128.3, 127.7, 109.6, 92.8, 76.4, 37.3; HRMS (DART Positive) m/z: calcd for $C_8H_7N_2O_2S$ $[M+H]^+$ 195.0223, found 195.0221.



3-Cyano-5-methyl-5-phenyl-4,5-dihydroisoxazole 2-oxide (4e): This compound was prepared according to ***Method A*** using 2-methyl-2-phenylcyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 65 °C for 24 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **4e** as a yellow oil (25.0 mg, 62%). IR (KBr, cm^{-1}): 3848, 3739, 2983, 2222, 1616, 1499, 1447, 1377, 1262, 1076, 977, 902, 846, 767, 700, 655, 556; ^1H NMR (400 MHz, $CDCl_3$) δ 7.49-7.32 (m, 5H), 3.57-3.41 (m, 2H), 1.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 129.2, 128.9, 124.0, 109.9, 93.4, 86.8, 43.3, 27.9; HRMS (DART Positive) m/z: calcd for $C_{11}H_{11}N_2O_2$ $[M+H]^+$ 203.0815, found 203.0815.



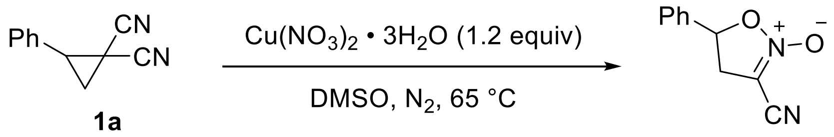
3-Cyano-5-vinyl-4,5-dihydroisoxazole 2-oxide (4f): This compound was prepared according to ***Method A*** using 2-vinylcyclopropane-1,1-dicarbonitrile (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 70 °C for 12 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **4f** as a yellow oil (6.6 mg, 24%). IR (KBr, cm^{-1}): 3833, 3740, 3618, 2923, 2854, 2223, 1617, 1428, 1375, 1259, 991, 948, 903, 838; ^1H NMR (400 MHz, $CDCl_3$) δ 5.94 (ddd, J = 17.2, 10.4, 6.7 Hz, 1H), 5.59-5.43 (m, 2H), 5.34 (dddt, J = 9.6, 7.7, 6.7, 1.0 Hz, 1H), 3.49 (ddd, J = 16.1, 9.4, 0.8 Hz, 1H), 3.15 (ddd, J = 16.1, 7.6, 0.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 132.1, 121.4, 109.7, 92.6, 79.4, 35.1; HRMS (FI Positive) m/z: calcd for $C_6H_6N_2O_2$ $[M]^+$ 138.0424, found 138.0427.



(*E*)-3-Cyano-5-(3-methoxy-3-oxoprop-1-en-1-yl)-4,5-dihydroisoxazole 2-oxide (4g): This compound was prepared according to ***Method A*** using methyl (*E*)-3-(2,2-dicyanocyclopropyl)-

acrylate (0.2 mmol) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.24 mmol) at 65 °C for 24 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **4g** as a yellow oil (11.8 mg, 30%). IR (KBr, cm^{-1}): 3739, 2440, 2956, 2225, 1726, 1622, 1440, 1363, 1314, 1273, 1202, 978, 907, 844, 461; ^1H NMR (400 MHz, $CDCl_3$) δ 6.88 (dd, *J* = 15.7, 5.4 Hz, 1H), 6.22 (dd, *J* = 15.7, 1.5 Hz, 1H), 5.51 (dddd, *J* = 9.8, 6.8, 5.4, 1.5 Hz, 1H), 3.79 (s, 3H), 3.61 (dd, *J* = 16.2, 9.8 Hz, 1H), 3.18 (dd, *J* = 16.2, 6.7 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.3, 139.7, 124.7, 109.2, 91.8, 76.2, 52.2, 34.9; HRMS (FI Positive) m/z: calcd for $C_8H_9N_2O_4$ $[M+H]^+$ 197.0557, found 197.0557.

Part 3: Gram-scale synthesis of product 2a

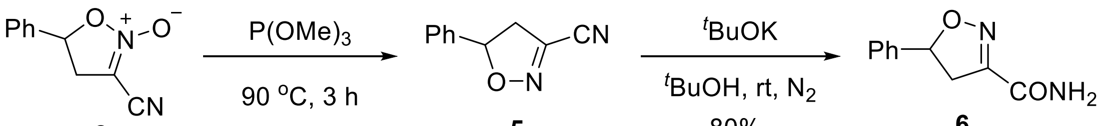


1a
(1.009 g, 6.0 mmol)

2a, 76%

To a flask were added 2-phenylcyclopropane-1,1-dicarbonitrile (1.01 g, 6.0 mmol), $Cu(NO_3)_2{\cdot}3H_2O$ (1.74 g, 7.2 mmol, 1.2 equiv), DMSO (20 mL). The reaction was stirred at 65 ℃ for 24 h under N_2 as monitored by TLC. Upon completion, the reaction mixture was cooled down to room temperature, washed by water triple times, then extracted with DCM (3×10 mL). The combined organic phase was washed with water and brine, and dried over anhydrous Na_2SO_4, then evaporated under reduced pressure to give the crude product, which was further purified by column chromatography (PE/EA = 10:1, v/v) on silica gel to afford product **2a** (852.4 mg, 76%).

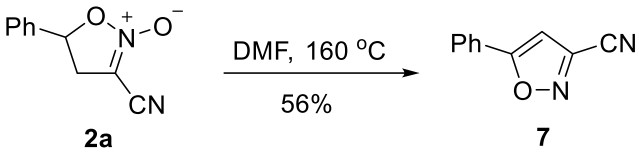
5. Further Transformation of Product 2a



5-Phenyl-4,5-dihydroisoxazole-3-carbonitrile (5): Under a nitrogen atmosphere, isoxazoline *N*-oxide (**2a**, 18.8 mg, 0.1 mmol) was placed in a 10 mL Schlenk tube. Trimethylphosphite (1.5 mL) was then added at room temperature. The mixture was stirred at 90 °C for 3 h. After the mixture was cooled to room temperature, the volatiles were evaporated, the resulting residue was purified by flash chromatography (PE/EA = 10:1, v/v) to provide compound **5** as a colorless oil (18.0 mg, 99%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.48-7.35 (m, 3H), 7.35-7.26 (m, 2H), 5.84 (dd, *J* = 11.7, 9.1 Hz, 1H), 3.61 (dd, *J* = 17.5, 11.7 Hz, 1H), 3.18 (dd, *J* = 17.4, 9.1 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) *δ* 138.0, 134.3, 129.4, 129.3, 126.0, 110.9, 128.1, 85.6, 42.9. Compound **5** was consistent with the literature data.[3]

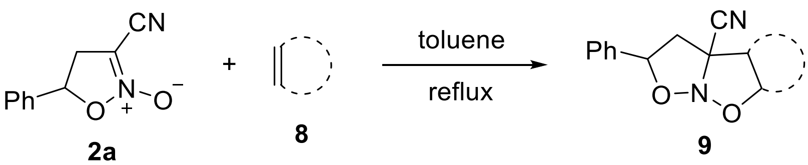
5-Phenyl-4,5-dihydroisoxazole-3-carboxamide (6): To a dry flask were added compound **5** (34.4 mg, 0.2 mmol), potassium *t*-butoxide (67.3 mg, 0.6 mmol) and *t*-butanol (3 mL). The mixture was stirred at room temperature for 2 h. After completion, the volatiles were evaporated, the resulting residue was purified by column chromatography (PE/EA = 1:1, v/v) to afford compound **6** as a white solid (30.3 mg, 80%). mp: 170-171 ºC; ^1H NMR (500 MHz, DMSO-d_6) δ 7.45-7.31 (m, 5H), 5.73

(dd, J = 11.2, 8.8 Hz, 1H), 3.64 (dd, J = 17.8, 11.3 Hz, 1H), 3.10 (dd, J = 17.8, 8.9 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 161.1, 154.0, 140.2, 128.7, 128.4, 126.2, 83.4, 41.2. Compound **6** was consistent with the literature data.[4]

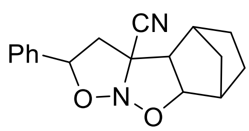


5-Phenylisoxazole-3-carbonitrile (7): Under a nitrogen atmosphere, isoxazoline *N*-oxide (**2a**, 0.2 mmol, 37.6 mg) was placed in a 10 mL Schlenk tube. *N,N*-dimethylformamide (2.0 mL) was then added at room temperature. The mixture was stirred at 160 °C for 2 h. After the mixture was cooled to room temperature, water (10 mL) was added to the mixture. The mixture was extracted with ethyl acetate (10 mL) three times. The combined organic layer was washed with brine (10 mL) and dried over anhydrous sodium sulfate, then evaporated under reduced pressure to give the crude product, which was further purified by column chromatography (PE/EA = 4:1, v/v) on silica gel to afford compound **7** as a white solid (19.2 mg, 56%). mp: 85-87 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83-7.77 (m, 2H), 7.60-7.45 (m, 3H), 6.83 (s, 1H). Compound **7** was consistent with the literature data.[5]

6. Synthesis of Nitrosolacetols 9



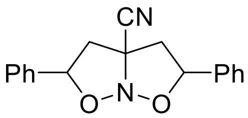
General Procedure *(Method B):* Under a nitrogen atmosphere, isoxazoline *N*-oxide (**2a**, 37.6 mg, 0.2 mmol) and olefins **8** (0.4 mmol) were placed in a 10 mL Schlenk tube. Toluene (2.0 mL) was then added at room temperature. The mixture was heated to reflux for 24 h. After the mixture was cooled to room temperature, the volatiles were evaporated, the resulting residue was purified by column chromatography (PE/EA) to afford the pure products.



2-Phenyloctahydro-3a*H*-4,7-methanobenzo[d]isoxazolo[2,3-*b*]isoxazole-3a-carbonitrile (**9a**): This compound was prepared according to ***Method B*** using norbornene (37.6 mg, 0.4 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **9a** (major isomer) as a white solid (18.5 mg, 33%) and **9a'** (minor isomer) as a white solid (15.7 mg, 28%) with 61% total yield, d.r. = 1.2:1.

9a (major isomer): mp: 129-130 °C; IR (KBr, cm^{-1}): 3037, 2919, 2245, 1495, 1456, 1381, 1324, 1287, 1217, 1018, 953, 895, 851, 798, 757, 696, 631, 568, 508; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46-7.30 (m, 5H), 5.33 (dd, J = 9.2, 7.4 Hz, 1H), 4.73 (d, J = 6.3 Hz, 1H), 3.18 (dd, J = 13.0, 7.4 Hz, 1H), 2.60-2.56 (m, 2H), 2.49 (d, J = 4.1 Hz, 1H), 2.43 (dd, J = 6.4, 1.7 Hz, 1H), 1.96 (dt, J = 11.1, 2.2 Hz, 1H), 1.66-1.50 (m, 2H), 1.28 (d, *J* = 11.1 Hz, 1H), 1.17-1.02 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.9, 128.9, 128.7, 126.4, 116.9, 90.2, 80.8, 76.8, 58.2, 48.2, 40.0, 39.0, 33.5, 27.9, 22.9; HRMS (ESI Positive) m/z: calcd for $C_{17}H_{19}N_2O_2$ $[M+H]^+$ 283.1441, found 283.1441.

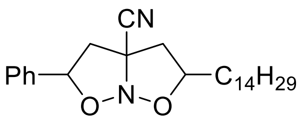
9a' (minor isomer): mp: 137-138 °C; IR (KBr, cm^{-1}): 3306, 2965, 2883, 2247, 1610, 1454, 1370, 1285, 1218, 1121, 1021, 956, 917, 872, 827, 777, 706, 562; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40-7.31 (m, 5H), 5.48 (dd, *J* = 9.1, 6.6 Hz, 1H), 4.61 (dt, *J* = 6.4, 1.4 Hz, 1H), 2.87 (dd, *J* = 12.9, 6.6 Hz, 1H), 2.81 (dd, *J* = 12.9, 9.1 Hz, 1H), 2.62 (d, *J* = 3.6 Hz, 1H), 2.52 (dd, *J* = 6.5, 1.8 Hz, 1H), 2.48 (d, *J* = 4.3 Hz, 1H), 1.91 (dp, *J* = 11.1, 2.0 Hz, 1H), 1.69-1.55 (m, 2H), 1.29 (dp, *J* = 11.1, 1.6 Hz, 1H), 1.23-1.06 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.0, 129.1, 129.0, 126.8, 116.9, 89.8, 82.4, 77.3, 58.3, 48.8, 40.7, 39.4, 33.4, 27.9, 22.8; HRMS (DART Positive) m/z: calcd for $C_{17}H_{19}N_2O_2$ $[M+H]^+$ 283.1441, found 283.1437.



2,5-Diphenyltetrahydro-3a*H*-isoxazolo[2,3-*b*]isoxazole-3a-carbonitrile (9b): This compound was prepared according to ***Method B*** using styrene (41.7 mg, 0.4 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **9b** (major isomer) as a white solid (29.2 mg, 50%) and **9b'** (minor isomer) as a white solid (25.5 mg, 44%) with 94% total yield, d.r. = 1.1:1.

9b (major isomer): mp: 78-79 °C; IR (KBr, cm^{-1}): 2962, 2880, 2245, 1456, 1386, 1305, 1248, 1122, 1008, 922, 879, 804, 765, 699, 626, 556; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52-7.36 (m, 10H), 5.75 (dd, *J* = 9.8, 6.2 Hz, 1H), 5.22 (dd, *J* = 9.9, 6.0 Hz, 1H), 3.24 (dd, *J* = 13.0, 6.0 Hz, 1H), 2.84 (dd, *J* = 12.9, 6.2 Hz, 1H), 2.76 (dd, *J* = 12.9, 9.8 Hz, 1H), 2.56 (dd, *J* = 13.0, 9.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.2, 135.4, 129.4, 129.1, 129.0, 127.2, 126.3, 119.2, 84.7, 77.6, 72.8, 47.8, 47.4; HRMS (DART Positive) m/z: calcd for $C_{18}H_{17}N_2O_2$ $[M+H]^+$ 293.1285, found 293.1280.

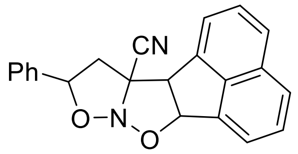
9b' (minor isomer): mp: 81-82 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46-7.37 (m, 10H), 5.61 (dd, *J* = 9.5, 6.3 Hz, 2H), 3.00 (dd, *J* = 13.1, 6.3 Hz, 2H), 2.90 (dd, *J* = 13.2, 9.6 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.6, 129.2, 129.0, 126.7, 118.7, 83.9, 73.5, 47.7. Compound **9b**' (minor isomer) was consistent with the literature data.[4]



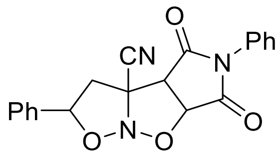
2-Phenyl-5-tetradecyltetrahydro-3a*H*-isoxazolo[2,3-*b*]isoxazole-3a-carbonitrile (9c): This compound was prepared according to ***Method B*** using 1-hexadecene (89.8 mg, 0.4 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **9c** (major isomer) as a white solid (43.9 mg, 53%) and **9c'** (minor isomer) as a white solid (31.0 mg, 38%) with 91% total yield, d.r. = 1.4:1.

9c (major isomer): mp: 73-74 °C; IR (KBr, cm^{-1}): 2919, 2851, 2242, 1462, 1381, 1311, 1053, 996, 917, 844, 804, 767, 707; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.32 (m, 5H), 5.12 (dd, *J* = 10.0, 5.8 Hz, 1H), 4.77 (dq, *J* = 9.7, 6.1 Hz, 1H), 3.15 (dd, *J* = 12.9, 5.8 Hz, 1H), 2.52 (dd, *J* = 12.5, 5.5 Hz, 1H), 2.38 (ddd, *J* = 15.2, 12.7, 9.9 Hz, 2H), 1.83 (dtd, *J* = 16.6, 6.8, 3.4 Hz, 1H), 1.68 (dq, *J* = 13.8, 5.3 Hz, 1H), 1.52-1.14 (m, 24H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.26, 128.97, 128.95, 126.24, 119.51, 82.85, 77.31, 72.22, 47.63, 45.73, 32.35, 32.05, 29.82, 29.80, 29.78, 29.75, 29.63, 29.61, 29.49, 26.19, 22.82, 14.25; HRMS (ESI Positive) m/z: calcd for $C_{26}H_{40}N_2O_2Na$ $[M+Na]^+$ 435.2982, found 435.2983.

9c' (minor isomer): mp: 80-81 °C; IR (KBr, cm^{-1}): 3431, 2921, 2850, 2246, 1460, 1340, 1325, 1022, 905, 803, 758, 697, 624, 560; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44-7.34 (m, 5H), 5.48 (dd, *J* = 9.5, 6.4 Hz, 1H), 4.61 (ddt, *J* = 9.4, 7.1, 5.8 Hz, 1H), 2.94-2.81 (m, 2H), 2.71 (dd, *J* = 12.9, 5.9 Hz, 1H), 2.56 (dd, *J* = 12.9, 9.4 Hz, 1H), 1.81 (dddd, *J* = 13.7, 9.9, 7.0, 5.2 Hz, 1H), 1.70-1.59 (m, 1H), 1.54-1.16 (m, 24H), 0.94-0.88 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.71, 129.11, 128.96, 126.65, 119.07, 83.73, 82.72, 72.90, 48.14, 45.50, 33.75, 32.05, 29.81, 29.80, 29.78, 29.74, 29.63, 29.57, 29.55, 29.48, 26.07, 22.81, 14.24; HRMS (ESI Positive) m/z: calcd for $C_{26}H_{40}N_2O_2Na$ $[M+Na]^+$ 435.2982, found 435.2983.

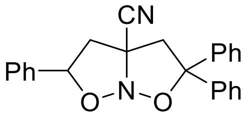


11a-((l2-Azanylidene)-l3-methyl)-10-phenyl-6b,11,11a,11b-tetrahydro-10*H*-acenaphtho[1,2-*d*]isoxazolo[2,3-*b*]isoxazole (9d): This compound was prepared according to ***Method B*** using acenaphthylene (60.9 mg, 0.4 mmol). The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **9d** (mixture of isomers) as a yellow solid (31.6 mg, 46%), d.r. = 1.5:1. mp: 113-114 °C; IR (KBr, cm^{-1}): 3645, 3042, 2915, 2244, 1760, 1610, 1493, 1449, 1366, 1312, 1214, 1014, 902, 831, 775, 701, 572; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94-7.90 (m, 1.46H), 7.87 (dd, *J* = 8.2, 5.5 Hz, 2.61H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.74-7.61 (m, 7.47H), 7.60-7.54 (m, 1.12H), 7.51 (dd, *J* = 10.4, 6.9 Hz, 2.57H), 7.38-7.29 (m, 8.29H), 7.16 (qd, *J* = 8.6, 7.7, 3.6 Hz, 3.04H), 6.98-6.93 (m, 2.06H), 6.22 (d, *J* = 6.9 Hz, 1H), 6.14 (d, *J* = 6.9 Hz, 1.42H), 5.57 (dd, *J* = 10.4, 6.9 Hz, 1.10H), 5.34 (dd, *J* = 9.0, 6.4 Hz, 1.51H), 5.08 (d, *J* = 6.9 Hz, 1.37H), 4.99 (d, *J* = 6.9 Hz, 0.95H), 2.63 (dd, *J* = 13.3, 6.9 Hz, 1.10H), 2.34 (qd, *J* = 13.5, 7.7 Hz, 3.19H), 1.99 (dd, *J* = 13.2, 10.4 Hz, 1.05H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.9, 138.5, 138.4, 138.1, 138.0, 137.6, 137.2, 137.2, 131.8, 131.7, 129.0, 128.92, 128.86, 128.8, 128.62, 128.58, 128.4, 127.1, 127.0, 126.5, 126.3, 125.59, 125.56, 122.9, 122.6, 121.5, 121.4, 119.5, 118.2, 88.0, 86.4, 84.1, 83.0, 75.4, 75.3, 57.8, 56.0, 42.0, 41.5; HRMS (ESI Positive) m/z: calcd for $C_{22}H_{16}N_2O_2Na$ $[M+Na]^+$ 363.1104, found 363.1103.

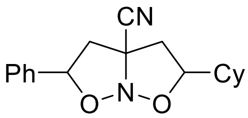


4,6-Dioxo-2,5-diphenylhexahydroisoxazolo[2,3-*b*]pyrrolo[3,4-*d*]isoxazole-3a(3b*H*)-carbonitrile (9e): This compound was prepared according to ***Method B*** using *N*-phenylmaleimide (69.3 mg, 0.4 mmol). The mixture was heated to reflux for 72 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **9e** (mixture of isomers) as a white solid (14.0 mg, 34%) and **2a** (15.3 mg, 59% conv.). mp: 175-176 °C; IR (KBr, cm^{-1}): 3485, 2925, 1720, 1496, 1453, 1392, 1320, 1206, 1005, 952, 829, 752, 696, 622; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55-7.11 (m, 10H), 6.63-6.56 (m, 1.20 H), 5.60 (dd, *J* = 8.2, 7.1 Hz, 0.99 H), 5.37 (t, *J* = 8.3 Hz, 0.62 H), 5.03 (dd, *J* = 9.2, 6.1 Hz, 0.44H), 4.06 (dd, *J* = 8.2, 3.0 Hz, 1.08H), 3.98-3.88 (m, 0.54H), 3.62 (dd,

J = 13.8, 8.6 Hz, 0.65H), 3.09 (dd, J = 13.8, 8.0 Hz, 0.60H), 2.81 (dd, J = 13.7, 6.1 Hz, 0.43 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.1, 173.6, 170.8, 170.3, 146.2, 133.9, 130.4, 129.8, 129.5, 129.3, 129.1, 129.0, 126.9, 126.4, 126.0, 119.9, 116.6, 114.1, 83.6, 76.6, 75.0, 53.3, 51.9, 38.6, 36.4; HRMS (ESI Positive) m/z: calcd for $C_{20}H_{15}N_3O_4Na$ $[M+Na]^+$ 384.0955, found 384.0955.



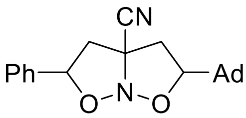
2,2,5-Triphenyltetrahydro-3a*H*-isoxazolo[2,3-*b*]isoxazole-3a-carbonitrile (9f): This compound was prepared according to ***Method B*** using ethene-1,1-diyldibenzene (72.1 mg, 0.4 mmol). The mixture was heated to reflux for 5 days. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **9f** as a white solid (18.4 mg, 34%). mp: 123-124 °C; IR (KBr, cm^{-1}): 3394, 3024, 2933, 2831, 2245, 1604, 1492, 1445, 1366, 1228, 1070, 975, 916, 763, 697; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (dd, J = 7.4, 1.8 Hz, 2H), 7.48-7.27 (m, 13H), 5.59 (dd, J = 10.2, 5.7 Hz, 1H), 3.78 (d, J = 13.1 Hz, 1H), 3.16 (d, J = 13.1 Hz, 1H), 2.78 (dd, J = 12.8, 5.8 Hz, 1H), 2.68 (dd, J = 12.8, 10.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.4, 142.1, 135.1, 129.3, 129.0, 128.8, 128.7, 128.2, 128.1, 127.2, 125.9, 125.6, 118.7, 87.3, 84.0, 72.7, 51.2, 48.2; HRMS (ESI Positive) m/z: calcd for $C_{24}H_{20}N_2O_2Na$ $[M+Na]^+$ 391.1417, found 391.1414.



2-Cyclohexyl-5-phenyltetrahydro-3a*H*-isoxazolo[2,3-*b*]isoxazole-3a-carbonitrile (9g): This compound was prepared according to ***Method B*** using vinylcyclohexane (44.1 mg, 0.4 mmol). The mixture was heated to reflux for 48 h.The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **9g** (major isomer) as a white solid (24.5 mg, 41%) and **9g'** (minor isomer) as a white solid (17.0 mg, 29%) with 70% total yield, d.r. = 1.4:1.

9g (major isomer): mp: 145-146 °C; IR (KBr, cm^{-1}): 3436, 2930, 2858, 2246, 1637, 1453, 1390, 1114, 1060, 977, 846, 760, 699, 628, 569; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42-7.32 (m, 5H), 5.13 (dd, J = 9.9, 5.9 Hz, 1H), 4.51 (q, J = 7.7 Hz, 1H), 3.15 (dd, J = 12.9, 5.9 Hz, 1H), 2.47-2.36 (m, 3H), 1.99 (ddt, J = 13.2, 3.9, 2.0 Hz, 1H), 1.80-1.73 (m, 2H), 1.73-1.59 (m, 3H), 1.26 (dddd, J = 29.4, 16.9, 6.8, 3.4 Hz, 3H), 1.07 (dtd, J = 11.9, 8.2, 4.1 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.3, 130.0, 129.9, 126.3, 119.5, 87.0, 72.1, 47.6, 43.6, 40.6, 29.9, 29.3, 25.9. 25.6; HRMS (DART Positive) m/z: calcd for $C_{18}H_{23}N_2O_2$ $[M+H]^+$ 299.1754, found 299.1753.

9g' (minor isomer): mp: 127-128 °C; IR (KBr, cm^{-1}): 3039, 2928, 2855, 2246, 1453, 1372, 1283, 1066, 1016, 963, 894, 823, 755, 697, 632, 570; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43-7.32 (m, 5H), 5.45 (dd, J = 9.9, 6.4 Hz, 1H), 4.31 (dt, J = 8.5, 7.3 Hz, 1H), 2.91-2.78 (m, 2H), 2.66-2.56 (m, 2H), 2.00 (dtd, J = 13.1, 3.6, 1.8 Hz, 1H), 1.86-1.66 (m, 2H), 1.62-1.58 (m, 2H), 1.29-1.15 (m, 4H), 1.05 (qd, J = 12.2, 3.6 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.8, 129.1, 129.0, 128.7, 119.0, 86.9, 83.7, 72.9, 48.1, 43.4, 41.8, 29.8, 29.0, 26.3, 25.8, 25.6; HRMS (DART Positive) m/z: calcd for $C_{18}H_{23}N_2O_2$ $[M+H]^+$ 299.1754, found 299.1753.

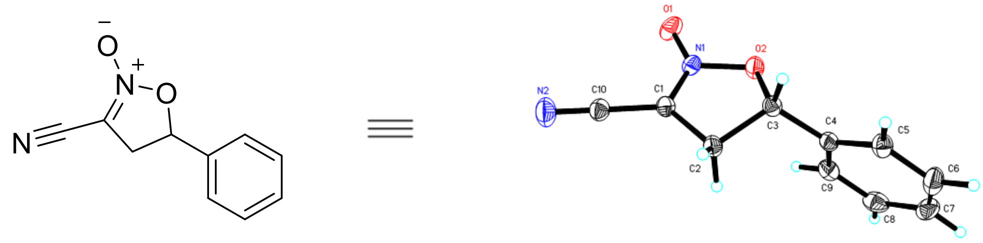


2-((3s)-Adamantan-1-yl)-5-phenyltetrahydro-3a*H*-isoxazolo[2,3-*b*]isoxazole-3a-carbonitrile (9h): This compound was prepared according to ***Method B*** using 1-vinyladamantane (64.9 mg, 0.4 mmol). The mixture was heated to reflux for 48 h. The crude residue was purified by silica gel chromatography (PE/EA = 10:1, v/v) to give **9h** (major isomer) as a white solid (32.2 mg, 46%) and **9h'** (minor isomer) as a white solid (20.1 mg, 29%) with 75% total yield, d.r. = 1.6:1.

9h (major isomer): mp: 146-147 °C; IR (KBr, cm^{-1}): 3037, 2900, 2850, 2669, 2246, 1496, 1452, 1374, 1299, 1049, 976, 911, 843, 808, 759, 693, 626, 565, 507; ^1H NMR (500 MHz, $CDCl_3$) δ 7.40-7.32 (m, 5H), 5.16 (dd, J = 9.5, 6.4 Hz, 1H), 4.37 (dd, J = 9.5, 6.6 Hz, 1H), 3.16 (dd, J = 12.9, 6.4 Hz, 1H), 2.66-2.57 (m, 1H), 2.46 (dd, J = 12.9, 9.5 Hz, 1H), 2.25 (dd, J = 12.7, 6.6 Hz, 1H), 2.03 (p, J = 3.2 Hz, 3H), 1.76-1.67 (m, 9H), 1.57-1.52 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.7, 129.0, 128.9, 126.3, 119.4, 90.7, 72.1, 47.4, 39.2, 38.5, 37.0, 34.4, 28.1; HRMS (DART Positive) m/z: calcd for calcd for $C_{22}H_{27}N_2O_2$ $[M+H]^+$ 351.2067, found 351.2064.

9h' (minor isomer): mp: 146-147 °C; IR (KBr, cm^{-1}): 3437, 3030, 2906, 2850, 2669, 2250, 1641, 1454, 1330, 1099, 1029, 903, 807, 757, 697, 627, 567, 511; ^1H NMR (500 MHz, $CDCl_3$) δ 7.40-7.32 (m, 5H), 5.16 (dd, J = 9.5, 6.4 Hz, 1H), 4.37 (dd, J = 9.5, 6.6 Hz, 1H), 3.16 (dd, J = 12.9, 6.4 Hz, 1H), 2.66-2.57 (m, 1H), 2.46 (dd, J = 12.9, 9.5 Hz, 1H), 2.25 (dd, J = 12.7, 6.6 Hz, 1H), 2.03 (p, J = 3.2 Hz, 3H), 1.76-1.67 (m, 9H), 1.57-1.52 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.2, 129.0, 128.9, 126.6, 118.9, 90.5, 83.3, 72.9, 47.9, 38.7, 38.2, 37.0, 35.1, 28.1; HRMS (DART Positive) m/z: calcd for calcd for $C_{22}H_{27}N_2O_2$ $[M+H]^+$ 351.2067, found 351.2064.

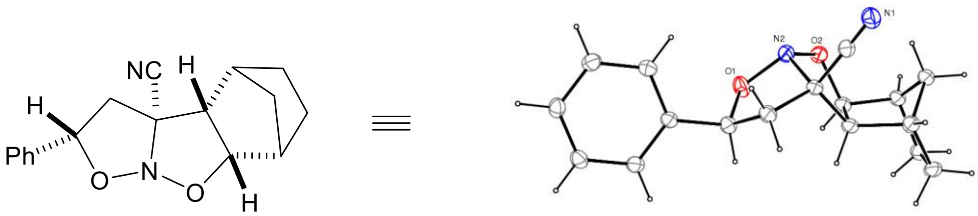
7. X-Ray Crystallographic Analysis for Compounds 2a and 9a



molecular structure of **2a**

The compound **2a** was recrystallized in toluene by a solvent evaporation method, affording a single crystal suitable for X-ray diffraction.

Crystallographic data for **2a**: $C_{10}H_8N_2O_2$, M = 188.18, Crystal system: Orthorhombic, Space group: P 212121 (No. 8), a = 6.1062 (2) Å, b = 7.7462 (4) Å, c = 19.4842 (8) Å, α = 90°, β = 90°, γ = 90°, V = 921.60(7) $Å^3$, Z = 4, Crystal size: 0.16 × 0.13 × 0.10 mm, T = 193(2) K, ρ_{calcd} = 1.356 g·cm^{-3}, Final R indices [I>2sigma(I)]: R_1 = 0.0317, wR_2 = 0.0747, R indices (all data): R_1 = 0.0349, wR_2 = 0.0773, GOF = 1.046, Reflections collected: 4576, Independent reflections: 1799 [R(int) = 0.0203], Data: 1799, restraints: 0, parameters: 127. CCDC 2072311 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

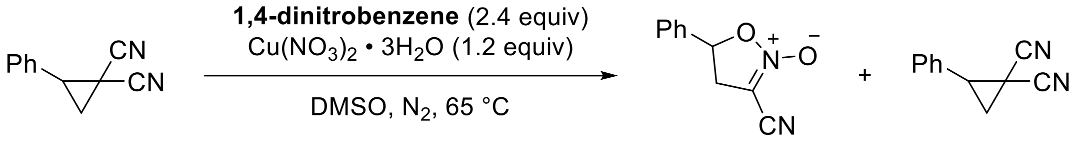


molecular structure of **9a** (minor isomer)

The compound **9a** was recrystallized in toluene by a solvent evaporation method, affording a single crystal suitable for X-ray diffraction.

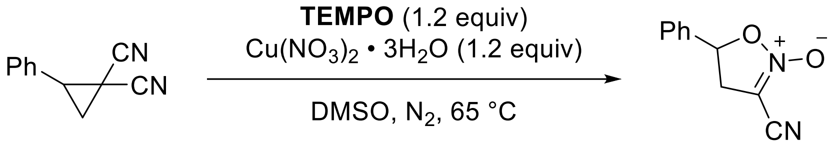
Crystallographic data for **9a** (minor isomer): $C_{17}H_{18}N_2O_2$, M = 282.33, monoclinic, P 21 (No. 10), a = 9.5508 (7) Å, b = 5.7679 (4) Å, c = 13.0789 (10) Å, β = 104.975 (4)º, V = 696.02 (9) $Å^3$, Z = 2, Crystal size: 0.25 × 0.18 × 0.15 mm, T = 150 K, ρ_{calcd} = 1.347 g·cm^{-3}, R_1 = 0.0550 (I>4σ(I)), wR_2 = 0.1457 (all data), GOF = 1.089, reflections collected/unique: 3744 / 2273 (Rint = 0.0374), Data: 2143 restraints: 0, parameters: 190. CCDC 2072312 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

8. Mechanistic Studies



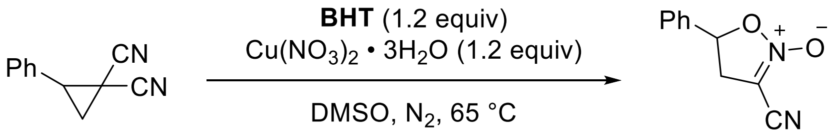
1a **2a**, 46% **1a**, 31%

To a test tube were added **1a** (0.2 mmol), $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol), 1,4-dinitrobenzene (0.48 mmol), DMSO (2.0 mL). The reaction was stirred at 65 °C for 15 h under N_2 as monitored by TLC. Upon completion, the reaction mixture was cooled down to room temperature, extracted with DCM (3×10 mL). The combined organic phase was washed with water and brine, and dried over anhydrous Na_2SO_4, then evaporated under reduced pressure to give the crude product, which was further purified by column chromatography on silica gel to afford **2a** (17.2 mg, 46%), **1a** (10.3 mg, 31%) and 1,4-dinitrobenzene (77.1 mg, 96%).



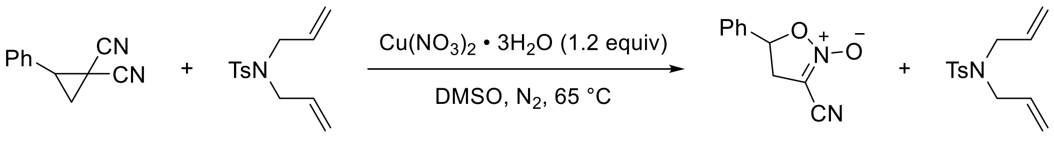
1a **2a**, 40%

To a test tube were added **1a** (0.2 mmol), 2,2,6,6-tetramethylpiperidine-1-oxy (TEMPO) (0.24 mmol), $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol), DMSO (2.0 mL). The reaction was stirred at 65 °C for 15 h under N_2 as monitored by TLC. Upon completion, the reaction mixture was cooled down to room temperature, extracted with DCM (3×10 mL). The combined organic phase was washed with water and brine, and dried over anhydrous Na_2SO_4, then evaporated under reduced pressure to give the crude product, which was further purified by column chromatography on silica gel to afford **2a** (15.1 mg, 40%).



1a **2a**, 58%

To a test tube were added **1a** (0.2 mmol), butylated hydroxytoluene (BHT) (0.24 mmol), $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol), DMSO (2.0 mL). The reaction was stirred at 65 °C for 15 h under N_2 as monitored by TLC. Upon completion, the reaction mixture was cooled down to room temperature, extracted with DCM (3×10 mL). The combined organic phase was washed with water and brine, and dried over anhydrous Na_2SO_4, then evaporated under reduced pressure to give the crude product, which was further purified by column chromatography on silica gel to afford **2a** (21.7 mg, 46%).



1a **10** **2a**, 75% **10**, 99%

To a test tube were added **1a** (33.6 mg, 0.2 mmol), *N*,*N*-diallyl-4-methylbenzenesulfonamide (60.3 mg, 0.24 mmol), $Cu(NO_3)_2 \cdot 3H_2O$ (0.24 mmol), DMSO (2.0 mL). The reaction was stirred at 65 °C for 15 h under N_2 as monitored by TLC. Upon completion, the reaction mixture was cooled down to room temperature, extracted with DCM (3×10 mL). The combined organic phase was washed with water and brine, and dried over anhydrous Na_2SO_4, then evaporated under reduced pressure to give the crude product, which was further purified by column chromatography on silica gel to afford **2a** (28.3 mg, 75%) and *N*,*N*-diallyl-4-methylbenzenesulfonamide (60.5 mg, 99%).

9. Details of Calculation and Discussion

All of the DFT calculations were performed with the Gaussian 09 program package.[6] The geometry optimization of all the minima involved were performed at the M06 level of theory[7] with Grimme's D3 empirical dispersion correction[8] with 6-31G(d) + SDD (for Cu) basis set[9] (keyword 5D) and the SMD model[10] in DMSO as a solvent. The structures of the reactants, intermediates, transition states, and products were fully optimized without any restriction. The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum or a transition state and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K. IRC calculations[11] were used to confirm that the transition states found from the optimization calculations connect the related reactants and products. Single-point calculations were performed with 6-311+G(d,p) + SDD (for Cu) basis set at the optimized geometries with 6-31G(d) + SDD (for Cu) basis set for all the intermediates and transition states. Through the same approach full optimization, without any restriction, was carried out for the model reactions. The reported energies are Gibbs free energies in DMSO solution (ΔG_{DMSO}).

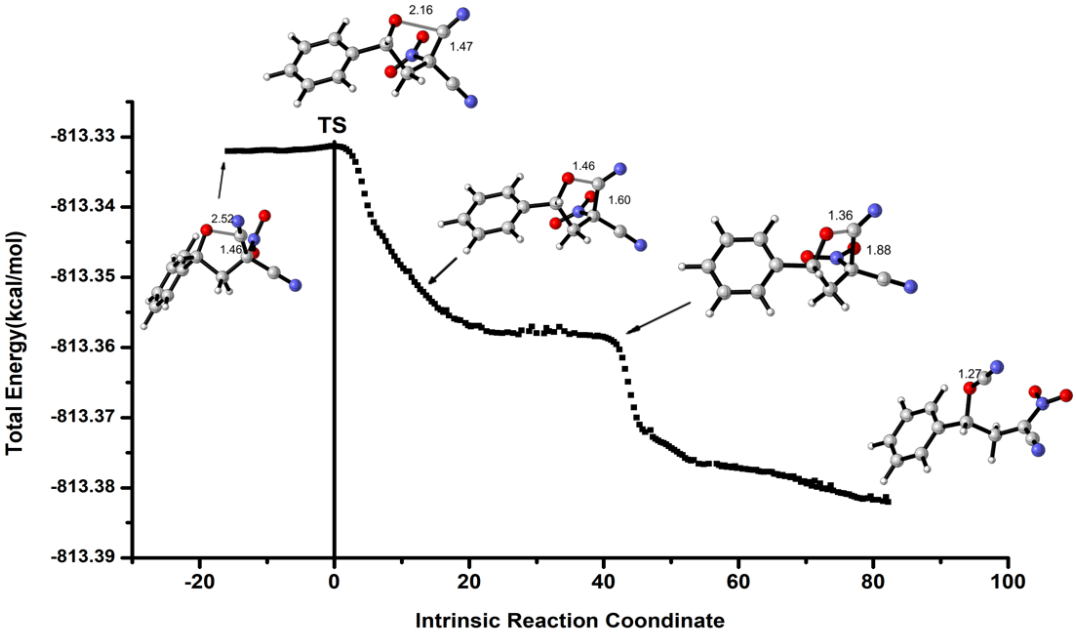


Figure S1 The novel cyano-migration process around IRC of **TS3a**.

DFT-Computed Energies of All Stationary Points

Table S2. Sum of electronic and thermal enthalpies (*H*, in Hartree), sum of electronic and thermal free energies (*G*, in Hartree), thermal Correction to Gibbs free energy (*CGFE*, in Hartree), electronic energy in DMSO (E_{DMSO}, in Hartree), and free energies in DMSO (G_{DMSO}, in Hartree). For transition state structures, one imaginary frequency (IFreq) was observed and given below. For all minimum structures, no imaginary frequency was observed.

Structure	*H*	*G*	*CGFE*	E_{DMSO}	G_{DMSO}	IFreq
1a	-532.866156	-532.913331	0.123409	-533.182542	-533.059133	
TS1a	-813.133882	-813.195836	0.129384	-813.569636	-813.440252	-302.59
INT1a	-813.155194	-813.215833	0.132816	-813.588379	-813.455563	
TS2a	-813.132755	-813.190021	0.133696	-813.564709	-813.431013	-271.83
INT2a	-813.140773	-813.200713	0.131374	-813.575328	-813.443954	
TS3a	-813.141622	-813.197390	0.133959	-813.569861	-813.435021	-61.47
INT3a	-813.190847	-813.250889	0.133714	-813.627664	-813.49395	
TS3a	-813.166434	-813.224861	0.133419	-813.601654	-813.468235	-495.99
2a	-645.095372	-645.147065	0.125959	-645.450727	-645.324768	
OCN^-	-168.103938	-168.128830	-0.010134	-168.190118	-168.200252	
NO_3^-	-280.278827	-280.307714	-0.009980	-280.406777	-280.416757	
INT1b	-1570.917318	-1571.00297	0.151732	-1571.55091	-1571.39918	
TS1b	-1570.890538	-1570.97767	0.149922	-1571.52708	-1571.37716	-376.00
INT2b	-1570.926018	-1571.01159	0.154058	-1571.55564	-1571.40158	
TS2b	-1570.882107	-1570.96471	0.153559	-1571.5137	-1571.36015	-235.35
INT3b	-1570.888751	-1570.97906	0.146441	-1571.52111	-1571.37467	
TS3b	-1570.879868	-1570.96195	0.154266	-1571.51247	-1571.35821	-91.13
TS3c	-1570.88675	-1570.97065	0.152366	-1571.51857	-1571.3662	-57.26
INT4b	-1570.945471	-1571.03073	0.154416	-1571.5766	-1571.42219	
INT4c	-1570.967173	-1571.04895	0.158309	-1571.59426	-1571.43595	
TS4c	-1570.938794	-1571.02127	0.155744	-1571.56773	-1571.41199	-276.82
INT5c	-1570.939349	-1571.02594	0.152444	-1571.57642	-1571.42397	
TS4b	-1570.917318	-1571.00297	0.151732	-1571.550912	-1571.39918	-492.39
TS5c	-1570.938468	-1571.02382	0.152451	-1571.56883	-1571.41638	-455.06
$Cu(NO_3)_2(OCN)^-$	-925.885149	-925.943037	0.001921	-926.160763	-926.158842	
1v	-668.418357	-668.459689	0.163176	-668.807400	-668.644224	
TS1v	-948.683710	-948.732076	0.171782	-949.188078	-949.016296	-335.18
INT1v	-948.699263	-948.746210	0.175476	-949.202617	-949.027141	
TS2v	-948.679270	-948.723662	0.176510	-949.181679	-949.005169	-282.84
INT1w	-1426.146943	-1426.22557	0.186598	-1426.75136	-1426.56476	
TS1w	-1706.420723	-1706.51564	0.188733	-1707.143863	-1706.95513	-352.12
INT2w	-1706.456265	-1706.54630	0.197058	-1707.17206	-1706.97500	
TS2w	-1706.416605	-1706.50568	0.194727	-1707.13473	-1706.94000	-282.00

The coordinates of all stationary points (Å)

1a

C	-1.76612600	-0.16579100	-0.16164000
C	-0.65817800	-0.67798400	0.80525000
C	-1.41989800	-1.64718500	0.00425800
C	-2.98612600	0.31918600	0.42124900
N	-3.96837200	0.69872300	0.91241000
C	-1.33768600	0.49797900	-1.36178600
N	-0.96687000	1.03505800	-2.32295200
H	-2.18399600	-2.24751800	0.49211800
H	-0.95361700	-2.10150900	-0.86840900
H	-0.96947800	-0.56401000	1.84493700
C	0.75546200	-0.31620800	0.51460200
C	1.23097800	0.93690400	0.91531600
C	1.61520800	-1.19563600	-0.14358200
C	2.54654200	1.30271900	0.66036100
H	0.55685500	1.62558900	1.42599700
C	2.93461700	-0.82868500	-0.39696400
H	1.25934900	-2.17852500	-0.45035300
C	3.40150700	0.41938100	0.00244200
H	2.90735400	2.28032500	0.97612900
H	3.59930200	-1.52419000	-0.90674400
H	4.43311700	0.70529000	-0.19692000

TS1a

C	0.38947600	0.13349400	0.01852300
C	0.74971000	1.07745400	-1.03138500
C	0.05725500	2.19407000	-0.26823700
H	1.82929200	1.22820600	-1.11230700
H	0.31014400	0.89650300	-2.01612600
C	0.77733800	2.94952600	0.66882800
N	1.39999200	3.56484300	1.44835300
C	-1.28155600	2.50870000	-0.53260700
N	-2.40678300	2.73372700	-0.77290900
H	0.99717900	0.19006600	0.91927100
N	2.80648000	-1.43743700	-0.19530400
O	3.18932400	-0.39020300	0.35040800
O	3.57696600	-2.37063600	-0.43446700
O	1.57763800	-1.56874700	-0.52391700
C	-0.87374100	-0.57628600	0.11543100
C	-1.76529900	-0.68525400	-0.96121400
C	-1.18127300	-1.21541400	1.32566600
C	-2.94549300	-1.40346300	-0.81929300
H	-1.53668100	-0.21207500	-1.91487300
C	-2.35942600	-1.93443700	1.46360200
H	-0.47975200	-1.13717600	2.15644000
C	-3.24550200	-2.02597400	0.39108400
H	-3.63499100	-1.48055700	-1.65800400
H	-2.59040000	-2.42445600	2.40780400
H	-4.17295800	-2.58625400	0.49822100

INT1a

C	-0.96379100	-0.95187600	0.69076900
C	-0.03593800	-0.46257700	-0.41594500
C	-2.42990700	-0.85820700	0.33872300
H	-0.69016800	-2.00169800	0.87460700
H	-0.76936800	-0.41387400	1.62683400
H	-0.25072800	-1.06456400	-1.31231400
O	-0.44280600	0.84336900	-0.95512300
N	-0.28583100	1.93412800	-0.13407500
C	-3.04074200	-1.86810900	-0.40046400
N	-3.53471100	-2.74480700	-1.01356800
C	-3.12050300	0.32399500	0.59680900
N	-3.66892800	1.33678700	0.84460800
O	-0.60674800	2.96768500	-0.66353300
O	0.14000800	1.76472600	0.98317400
C	1.45046700	-0.49659000	-0.15970700
C	1.99388300	-0.91588300	1.05455200
C	2.31235200	-0.11791900	-1.19331200
C	3.37470100	-0.95377400	1.23198100
H	1.34280200	-1.21165400	1.87529800
C	3.69020900	-0.14627300	-1.01427300
H	1.89337100	0.20762200	-2.14619700
C	4.22572300	-0.56655600	0.20173900
H	3.78475900	-1.28419500	2.18522400
H	4.34829200	0.15501400	-1.82795300
H	5.30497300	-0.59302300	0.34437500

TS2a

C	-0.48570900	-0.84320200	0.79785800
C	0.30653400	-0.72331500	-0.54025200
C	-1.90397200	-0.46958900	0.48458700
H	-0.37311500	-1.85426100	1.20766000
H	-0.10983700	-0.13007700	1.54156700
H	0.28043000	-1.72742000	-1.00809400
O	-0.32400400	0.15751600	-1.39980400
N	-1.44067200	1.08565900	-0.57432000
C	-2.62426700	-1.31578500	-0.41066300

N	-3.19387700	-1.98545600	-1.17575900
C	-2.69219300	0.10554000	1.52169600
N	-3.32288000	0.62502000	2.35367300
O	-2.33144000	1.37857200	-1.35600500
O	-0.87187600	1.86359400	0.19104600
C	1.74900600	-0.37572300	-0.24552800
C	2.62982300	-1.37439400	0.17278300
C	2.20725300	0.93761000	-0.34836900
C	3.94972100	-1.06576300	0.49039300
H	2.27626900	-2.40525000	0.24386000
C	3.52745300	1.24731800	-0.03402500
H	1.50899500	1.70626700	-0.67553300
C	4.40230900	0.24792200	0.38779700
H	4.62886800	-1.85400800	0.81369300
H	3.87730500	2.27587900	-0.11903000
H	5.43589500	0.49112800	0.63116100

INT2a

C	-0.45938600	0.88612300	-0.55252800
C	0.36523600	0.63510800	0.76539800
C	-1.83789000	0.31513800	-0.25935100
H	-0.54478900	1.94429200	-0.83208000
H	-0.06577200	0.33509900	-1.41618600
H	0.38335600	1.63539800	1.28370100
O	-0.23160700	-0.32601200	1.48178900
N	-1.70990100	-1.21458100	0.01249600
C	-2.47056900	0.92996600	0.90853400
N	-3.03364200	1.51481700	1.73843800
C	-2.71480900	0.42835100	-1.43007200
N	-3.39783400	0.50069700	-2.36554100
O	-2.54477300	-1.70536300	0.75517000
O	-1.00185800	-1.82327300	-0.77386100
C	1.80711500	0.35233600	0.35189600
C	2.64816000	1.36919500	-0.10501100
C	2.28995300	-0.95372500	0.39645600
C	3.94886400	1.08497500	-0.51290600
H	2.27868400	2.39753900	-0.13458100
C	3.59046400	-1.24378400	-0.00772000
H	1.61317900	-1.72451500	0.76415400
C	4.42468200	-0.22484000	-0.46487400
H	4.59695800	1.88765600	-0.86480700
H	3.95891000	-2.26895400	0.03577600
H	5.44410700	-0.44892900	-0.77743100

TS3a

C	0.70445400	0.17379800	-1.26516800
C	0.32340800	-0.88101900	-0.74855900
C	1.65559400	0.39698600	-0.09815200
H	0.29437600	1.13681500	-1.59338500
H	1.31314000	-0.21503600	-2.08913900
H	0.46967200	-1.59376200	-1.60536800
O	0.18092600	-1.46728300	0.35834600
N	2.39792400	-0.93283200	0.22202600
C	0.97916700	0.83045500	1.12614600
N	0.50536500	1.35255900	2.05005000
C	2.70881000	1.35503400	-0.45757600
N	3.55533600	2.09452900	-0.74654900
O	2.76415500	-1.08571500	1.37566700
O	2.80186900	-1.55518100	-0.74686100
C	1.71921000	-0.30823500	-0.46858500
C	2.69462600	-1.24105900	-0.09138900
C	2.08390600	1.03810400	-0.49311300
C	3.98605600	-0.85139000	0.23603300
H	2.41369300	-2.29445700	-0.05210200
C	3.37868900	1.44004600	-0.15682000
H	1.36176900	1.80623100	-0.77110400
C	4.33554200	0.49975000	0.20610100
H	4.72589900	-1.60057900	0.51777900
H	3.63541000	2.49905500	-0.18045800
H	5.34657600	0.81255900	0.46436400

INT3a

C	-0.43278300	0.09896200	-1.03309100
C	0.35593000	0.12863500	0.26778500
C	-1.91354000	0.09598600	-0.84800000
H	-0.10709100	0.97904500	-1.60923200
H	-0.13485900	-0.78996300	-1.60751400
H	0.06672200	1.00495300	0.86144000
O	-0.02553900	-1.07491000	1.07108000
N	-2.53969100	1.21297800	-0.34506400
C	-2.69461100	-1.04498600	-1.05182300
N	-3.30180800	-2.03133800	-1.24055900
C	-1.05292200	-0.95198300	1.81115600
N	-1.96871400	-0.88845700	2.53622400
O	-3.77371600	1.20439500	-0.15412500
O	-1.83889600	2.22068500	-0.09330700
C	1.83694300	0.06983900	0.08205800
C	2.61401900	1.18182700	0.40476900
C	2.44841200	-1.06443900	-0.45925000

C	3.98890400	1.16562800	0.18696400
H	2.13547600	2.06497200	0.82874500
C	3.82333000	-1.08541900	-0.66178600
H	1.84767700	-1.93839300	-0.71324500
C	4.59544200	0.03071200	-0.34250500
H	4.58714100	2.03940000	0.44058000
H	4.29511500	-1.97548200	-1.07518800
H	5.67177000	0.01324500	-0.50664100

TS4a

C	0.47964300	0.41844400	-0.65399000
C	0.38975700	1.80014200	-0.05420000
C	1.85827100	-0.12091000	-0.39026500
H	0.35564400	0.53923000	-1.73976300
H	0.96066300	2.61209600	-0.48898200
H	-0.13942700	1.98841400	0.87306200
O	-1.15957600	2.35825500	-1.06994500
N	2.55904900	0.44809700	0.61520400
C	2.37639600	-1.25548300	-1.02420700
N	2.76904600	-2.20432800	-1.58475500
C	-2.22315800	2.16399000	-0.45860300
N	-3.23448100	1.98203600	0.12640900
O	3.66719000	0.04692500	0.99439700
O	2.00497700	1.46623000	1.17410900
C	-0.61611700	-0.49770300	-0.14835300
C	-1.51219400	-1.08034000	-1.04201700
C	-0.74823200	-0.75435000	1.21891200
C	-2.53779600	-1.90118400	-0.57777300
H	-1.41199900	-0.87655900	-2.10911500
C	-1.77406500	-1.56853400	1.68404700
H	-0.04514200	-0.30688800	1.92419700
C	-2.67340000	-2.14212700	0.78573100
H	-3.23677400	-2.34623400	-1.28456500
H	-1.87475600	-1.75597400	2.75215300
H	-3.47885600	-2.77766700	1.15082700

2a

C	0.92452600	-1.15654200	-0.23000200
C	0.01381100	-0.06492300	-0.80769400
C	2.18702500	-0.39353400	-0.04029700
H	0.54970600	-1.55074000	0.72589500
H	1.02982200	-1.99377800	-0.92690200
H	0.04273900	-0.08967900	-1.90547800
O	0.64428900	1.19224900	-0.40758900
N	1.97604900	0.91228000	-0.11650800
C	3.47490700	-0.85596500	0.27870000
N	4.53466500	-1.26483400	0.53827400
O	2.71304200	1.86555300	0.04263700
C	-1.39804100	-0.06829800	-0.31257300
C	-2.44799800	-0.26808300	-1.20625700
C	-1.67016700	0.11830400	1.04546100
C	-3.76248900	-0.29451200	-0.74694300
H	-2.23219300	-0.40629200	-2.26585900
C	-2.98230100	0.10369500	1.50106100
H	-0.85070100	0.28351600	1.74613600
C	-4.03042900	-0.10648600	0.60534700
H	-4.57770700	-0.45529900	-1.45044200
H	-3.19001300	0.25638800	2.55891800
H	-5.05837000	-0.12058400	0.96416000

NO_3^-

N	0.00000000	0.00000000	-0.00028100
O	0.00000000	1.08408800	-0.62545000
O	0.00000000	0.00000000	1.25114700
O	0.00000000	-1.08408800	-0.62545000

OCN^-

O	0.00000000	0.00000000	1.15197100
C	0.00000000	0.00000000	-0.06414400
N	0.00000000	0.00000000	-1.26155800

INT1b

Cu	2.54426600	-0.19935500	0.46383100
O	3.42592500	-1.09635100	-1.10271200
N	4.24866600	-0.12602200	-1.24875000
O	5.07463700	-0.09349400	-2.11481800
O	4.09789700	0.79945400	-0.38352900
C	-2.22445600	-0.42138700	1.13939300
C	-2.36797500	-1.69342900	1.85199700
C	-1.46616300	-1.71316100	0.61466600
H	-1.85358400	-1.81474200	2.80217200
H	-3.27876700	-2.27854500	1.73530500
C	-0.05488400	-1.65454500	0.76879600
N	1.09238700	-1.52943400	0.89937800
C	-1.95070300	-2.33673500	-0.58317600
N	-2.37153900	-2.82256400	-1.55035500
H	-1.51126300	0.27821300	1.58029400
N	0.95644300	1.79903300	0.82484900

O	0.82574300	1.31944000	-0.31452800
O	1.83744300	1.23619100	1.59575100
O	0.31893900	2.73747000	1.25247600
C	-3.23082800	0.21215200	0.25725800
C	-4.48790900	-0.34650600	0.01335800
C	-2.88009300	1.41531300	-0.36461400
C	-5.37892200	0.29145700	-0.84380400
H	-4.78059000	-1.27764200	0.49792500
C	-3.77130400	2.04923500	-1.22067300
H	-1.89866500	1.85028900	-0.17007900
C	-5.02283200	1.48677600	-1.46264200
H	-6.35839600	-0.14798800	-1.02473800
H	-3.48920800	2.98531500	-1.69954600
H	-5.72317400	1.98259700	-2.13276100

INT2b

C	-2.01934100	-0.60255400	-0.33319000
C	-1.75531600	-0.33665100	-1.81039200
C	-0.57047700	0.59191100	-1.97226100
H	-1.54097300	-1.29974000	-2.29365000
H	-2.62395000	0.09476800	-2.31754700
C	0.70154900	0.11444600	-1.90421700
N	1.80228300	-0.34150200	-1.90954300
C	-0.75466600	1.97746600	-2.13500000
N	-0.93612300	3.12497700	-2.27564600
H	-1.08238400	-0.97677600	0.09889700
N	-4.12458000	-1.81709500	-0.52915900
O	-4.54105000	-0.85167100	-1.12306100
O	-4.71282400	-2.82636100	-0.23670500
O	-2.81527000	-1.82348400	-0.11233700
C	-2.50015200	0.53959600	0.52219600
C	-3.26476800	1.59836800	0.02643900
C	-2.15391700	0.52431400	1.87696800
C	-3.67868200	2.62083700	0.87431200
H	-3.54243600	1.63282400	-1.02536200
C	-2.57616400	1.54105100	2.72597000
H	-1.52525200	-0.28423300	2.25518300
C	-3.34112500	2.59150700	2.22486500
H	-4.27073000	3.44344900	0.47640400
H	-2.29777700	1.51948400	3.77844500
H	-3.66831200	3.39289200	2.88576600
Cu	2.91773600	-0.53854900	-0.35588700
O	4.28656700	0.94142300	-0.69893200
N	4.95741900	0.60273800	0.33451000
O	5.95270200	1.18103400	0.68451000
O	4.47813400	-0.39952700	0.96073000
N	1.08643400	-1.26709600	1.34076500
O	1.19387300	-0.02981800	1.32298300
O	1.87083100	-1.94532400	0.56913400
O	0.27676100	-1.86885100	2.02892400

INT3b

C	1.59017200	0.61626200	0.22682600
C	3.01835400	0.68804600	-0.33751500
C	0.85182100	1.96884200	0.28717700
H	0.96769700	-0.05400800	-0.37927700
H	1.61069800	0.22312500	1.25288000
H	2.92809100	0.89611300	-1.44103200
O	3.71458300	1.76254900	0.08461300
N	0.89058600	2.61383100	-1.14961400
C	-0.54945400	1.66670800	0.56439800
N	-1.62873700	1.27018800	0.70597300
C	1.40060600	2.92531000	1.24677900
N	1.78470600	3.66416500	2.05206900
O	1.48785500	3.65544400	-1.27443800
O	0.33667400	1.96564400	-2.00846300
C	3.72005500	-0.65375000	-0.22107800
C	3.05081600	-1.82930700	-0.56973700
C	5.03320300	-0.71787700	0.24256500
C	3.68875300	-3.05838200	-0.43352900
H	2.02021200	-1.80716700	-0.92418100
C	5.66929300	-1.94868400	0.37016300
H	5.55208600	0.20048300	0.51088700
C	4.99807400	-3.12236600	0.03511400
H	3.15296200	-3.96999800	-0.69488000
H	6.69233700	-1.99087600	0.74097800
H	5.49357600	-4.08606000	0.14329200
Cu	-2.91632000	-0.11882300	0.46174100
O	-4.40257900	-0.20575000	-1.11991600
N	-5.31096200	-0.55130500	-0.30827700
O	-6.45415300	-0.77157900	-0.67757600
O	-4.97234500	-0.65654000	0.90840900
N	-0.83940000	-1.94622500	0.07262900
O	-0.78996100	-1.18842900	-0.91923400
O	-1.83775700	-1.86326600	0.86166100
O	0.04919600	-2.76421300	0.31049100

INT4b

C	1.70096600	-0.04858800	0.24464700
C	2.01176700	0.85838600	1.43047100
C	0.78332000	0.60067700	-0.76066300
H	1.10499500	-0.87544300	0.66331000
H	1.10091600	1.26318800	1.88267500
H	2.70378600	1.67074500	1.19507900
O	2.61178300	0.04397000	2.50088200
N	0.98622400	1.88258800	-1.29729500
C	-0.35934300	-0.02838700	-1.16469700
N	-1.35400300	-0.60310500	-1.46149500
C	3.87389500	-0.13048200	2.45104900
N	5.02828400	-0.31222800	2.47182100
O	0.20770800	2.29644500	-2.16311300
O	1.93281000	2.55985200	-0.87039900
C	2.96166600	-0.66331900	-0.33447100
C	3.19874800	-2.02636800	-0.14778300
C	3.93004000	0.10991200	-0.98477000
C	4.38553800	-2.60856200	-0.58482900
H	2.44868300	-2.63345300	0.36116500
C	5.11445100	-0.47161500	-1.42253500
H	3.75799300	1.17474800	-1.13508000
C	5.34932600	-1.82980300	-1.21783000
H	4.55800000	-3.67199800	-0.42559200
H	5.86315500	0.14210200	-1.92159500
H	6.28164600	-2.27946600	-1.55628900
Cu	-2.98819900	-0.22098700	-0.46148900
O	-3.75530800	-2.08620800	-0.24533800
N	-4.82343800	-1.61878700	0.28071400
O	-5.72165700	-2.31690000	0.66598800
O	-4.84485900	-0.34458000	0.36021100
N	-1.95254900	1.70240200	0.91317400
O	-1.82128600	0.61678800	1.50773100
O	-2.64733400	1.69198800	-0.18326000
O	-1.46876800	2.75001600	1.29223800

INT4c

C	2.52895900	1.64704900	0.96213100
C	2.22930500	0.15177200	1.19294200
C	1.26340200	2.20202200	0.33290200
H	2.69732000	2.15326600	1.91838800
H	3.40707600	1.81341100	0.33080300
H	2.48650900	-0.10859800	2.22852900
O	0.81047500	0.01527900	1.08867900
N	1.36671200	2.33489700	-1.18801300
C	0.18283500	1.09452600	0.55421000
N	-1.01588000	1.24784900	0.25765300
C	0.81184300	3.47410200	0.87170100
N	0.45837500	4.46895100	1.35148200
O	0.75211200	3.24112100	-1.71261000
O	2.00887800	1.47593900	-1.75828500
C	2.93839200	-0.79935500	0.26305200
C	4.33445500	-0.84005800	0.29605600
C	2.24780000	-1.65367000	-0.59443300
C	5.03428600	-1.71197000	-0.53031900
H	4.87691300	-0.18317200	0.97870900
C	2.95151200	-2.52657800	-1.42160500
H	1.15831700	-1.64276900	-0.61358900
C	4.34238300	-2.55828400	-1.39486800
H	6.12259600	-1.73344200	-0.49687200
H	2.40330500	-3.18865500	-2.09087100
H	4.88791900	-3.24314200	-2.04251300
Cu	-2.33477300	-0.08057500	0.33415900
O	-3.53427400	0.51573800	-1.31605400
N	-4.42391400	-0.31901200	-0.96703600
O	-5.45035900	-0.48440200	-1.58188000
O	-4.14998500	-0.97943900	0.09286100
N	-1.00199700	-2.18126600	1.03337500
O	-1.10497000	-2.09393900	-0.20776800
O	-1.66364100	-1.32951300	1.73990900
O	-0.31894500	-3.01921800	1.59189200

INT5c

C	-3.59740900	-0.97728500	1.47510100
C	-2.22781300	-0.32654200	1.55445700
C	-4.10435600	-1.27215100	0.10592500
H	-3.57095700	-1.88496000	2.09536700
H	-4.28815300	-0.27362300	1.95834900
H	-1.94774000	-0.15554500	2.60077500
O	-1.26482500	-1.43222500	1.10164300
N	-4.93289400	-0.37482900	-0.53589400
C	-0.09812700	-1.09657000	0.80871000
N	0.99764500	-0.82904200	0.52887900
C	-3.71636900	-2.40499200	-0.61438700
N	-3.35582900	-3.37479400	-1.16855800
O	-5.31570100	-0.62459900	-1.69954000
O	-5.28785000	0.66227900	0.06235700
C	-2.01109000	0.90212400	0.73403500
C	-1.98087500	2.13264300	1.39262100

C	-1.88330600	0.86102200	-0.65905200
C	-1.85240400	3.31333900	0.66881600
H	-2.06707500	2.16136500	2.47890800
C	-1.73720200	2.04248900	-1.37779700
H	-1.89260600	-0.09229200	-1.18771000
C	-1.72871100	3.26945400	-0.71705400
H	-1.83698300	4.26869600	1.19041200
H	-1.63544300	2.00297500	-2.46092100
H	-1.62001600	4.19241700	-1.28432100
Cu	2.64671700	-0.11994700	-0.21728900
O	2.54587400	1.76660400	0.44321100
N	3.57142800	2.10642100	-0.24925400
O	4.02840200	3.21372300	-0.23925700
O	4.05418000	1.15036400	-0.94349700
N	4.14802300	-2.15295000	0.05043400
O	4.19886300	-1.38330000	1.02885700
O	3.36001200	-1.79622600	-0.92145200
O	4.77248600	-3.18479900	-0.04444200

TS1b

C	-1.76833300	-0.23826000	-0.50011500
C	-1.81645000	-0.26965900	-1.94676600
C	-0.64986800	0.70665300	-1.80136500
H	-1.53369500	-1.21828700	-2.40425800
H	-2.68104800	0.18224200	-2.43103700
C	0.66141200	0.26642900	-1.76356000
N	1.77010800	-0.12206200	-1.74518800
C	-0.88556600	2.09960200	-1.85769500
N	-1.12274600	3.24136500	-1.88651400
H	-1.06218000	-0.91781100	-0.02526600
N	-4.29132700	-2.04717600	-0.46047000
O	-4.51647500	-1.29179100	-1.42501200
O	-5.18018700	-2.77543100	0.00517100
O	-3.13640700	-2.08164600	0.05681900
C	-2.46148000	0.68846200	0.37392700
C	-3.53865600	1.47279300	-0.06538800
C	-2.04108800	0.77455400	1.70987300
C	-4.17924700	2.32607400	0.82200100
H	-3.88580600	1.39927600	-1.09380800
C	-2.68289800	1.63292300	2.59036500
H	-1.20391000	0.16009200	2.04597800
C	-3.75293800	2.40858600	2.14684100
H	-5.01911700	2.92872300	0.48122700
H	-2.35158100	1.69755500	3.62504300
H	-4.25893900	3.08104200	2.83770100
Cu	3.07438200	-0.52801200	-0.36088900
O	4.46278000	0.88923800	-0.71639600
N	5.20145600	0.44600300	0.23155000
O	6.24496200	0.94899000	0.53852900
O	4.71676000	-0.58072900	0.81861500
N	1.26398000	-1.10563500	1.38315900
O	1.52340200	0.10774200	1.41164000
O	1.96603500	-1.84401900	0.57871700
O	0.39157900	-1.63446400	2.04738300

TS2b

C	1.89675800	0.69283900	0.99066400
C	1.79931700	-0.12870900	-0.32944300
C	1.06346100	1.92666800	0.75698600
H	1.55026900	0.09183200	1.84075800
H	2.92274900	1.02790600	1.19010900
H	0.89458800	-0.76755200	-0.22655700
O	1.66418200	0.71372300	-1.40004100
N	1.73796800	2.43117200	-0.85708400
C	-0.31234400	1.63063600	0.52149000
N	-1.39430300	1.29879300	0.27065100
C	1.29752200	3.06594600	1.59414500
N	1.52605700	4.00511600	2.24100400
O	0.92654100	3.04216200	-1.53380400
O	2.91684000	2.72789000	-0.70313100
C	2.99799400	-1.05032000	-0.40687800
C	2.92559800	-2.33304600	0.13422600
C	4.19228800	-0.61259200	-0.97895500
C	4.03869100	-3.17030700	0.11433700
H	1.98245700	-2.67606000	0.56678400
C	5.30480400	-1.44771900	-1.00129300
H	4.22738200	0.39016800	-1.40559200
C	5.23141800	-2.72806600	-0.45255300
H	3.97195700	-4.17236300	0.53691900
H	6.23552000	-1.10078000	-1.44949400
H	6.10268500	-3.38162600	-0.47226000
Cu	-2.83067600	-0.04221600	0.27852800
O	-3.93906000	0.50581800	-1.28668300
N	-4.77540300	-0.44563800	-1.07757300
O	-5.73032600	-0.64102000	-1.77186300
O	-4.48372400	-1.15959700	-0.05900500
N	-1.22578000	-1.83169300	1.14391200
O	-1.30070100	-1.83283700	-0.09841400

O	-2.02154500	-1.01467600	1.76970600
O	-0.46856000	-2.52439800	1.78814800

TS3b

C	1.54572000	0.64621200	-1.20578200
C	3.10712300	0.87642500	-1.12186000
C	1.00382100	1.65475100	-0.20968200
H	1.12005500	0.87326000	-2.19212400
H	1.21398400	-0.35793200	-0.91367400
H	3.41602200	1.15071800	-2.16233800
O	3.34096200	1.85534400	-0.22037400
N	1.36486000	1.22724400	1.25471300
C	1.57153400	2.99276900	-0.42759500
N	1.55695900	4.14136900	-0.66093900
C	-0.45559300	1.61992000	-0.21485400
N	-1.60215800	1.48042400	-0.15265400
O	1.43750000	2.11380800	2.07835000
O	1.40928500	0.03273600	1.46401600
C	3.79947200	-0.44535500	-0.81746400
C	3.75816100	-1.49452600	-1.73909900
C	4.48786600	-0.62601800	0.37961300
C	4.38742100	-2.70527800	-1.46715000
H	3.22707300	-1.35455600	-2.68409700
C	5.11993400	-1.83648900	0.65713800
H	4.51519200	0.20552900	1.08286700
C	5.07056100	-2.88029300	-0.26370300
H	4.34692900	-3.51536600	-2.19506600
H	5.65321700	-1.96733500	1.59884800
H	5.56544000	-3.82673000	-0.04820600
Cu	-3.06625000	0.16491400	0.17701300
O	-3.99059100	0.16316400	-1.58234400
N	-4.86330100	-0.68910000	-1.17639900
O	-5.73184900	-1.11564400	-1.88078300
O	-4.70744800	-1.03285500	0.04220400
N	-1.57449000	-1.39229200	1.51684600
O	-1.52576700	-1.60568900	0.28992600
O	-2.34128800	-0.40599600	1.89415200
O	-0.97653800	-2.02690600	2.35136400

TS3c

C	2.24296600	0.48606000	1.31630200
C	2.11432300	-0.54042700	0.12614400
C	1.28305500	1.60519900	0.94197400
H	1.95664500	0.07811600	2.29402600
H	3.23872300	0.93602900	1.41707300
H	1.62224500	-1.44336900	0.57530100
O	1.37727500	0.03135200	-0.84540400
N	1.72965100	2.27508700	-0.38845400
C	-0.07693000	1.10723700	0.71591700
N	-1.14918600	0.71478500	0.53760300
C	1.29907200	2.67490500	1.94869600
N	1.32832900	3.53172800	2.73029000
O	0.85299500	2.79949100	-1.05203000
O	2.92908300	2.43063500	-0.51473800
C	3.51175200	-0.98166700	-0.29181400
C	4.29481800	-1.78211700	0.54298800
C	4.03349600	-0.57022300	-1.51608100
C	5.57930000	-2.16122100	0.16358200
H	3.88809600	-2.11587300	1.50120700
C	5.31715600	-0.94836000	-1.90177800
H	3.40209600	0.05162000	-2.15009300
C	6.09519800	-1.74389500	-1.06301800
H	6.18035400	-2.78691100	0.82328000
H	5.71482000	-0.62014900	-2.86237200
H	7.09920800	-2.04108300	-1.36423900
Cu	-2.90170200	-0.06168200	0.20051500
O	-3.42482600	0.91638500	-1.46193700
N	-4.61493300	0.43725000	-1.41726400
O	-5.44717900	0.68093600	-2.24332800
O	-4.81934600	-0.32078400	-0.41099900
N	-2.43675100	-2.43475800	0.96163700
O	-2.27193500	-2.26973700	-0.26248500
O	-2.82176500	-1.38872800	1.63338200
O	-2.26403100	-3.48095100	1.54338200

TS4b

C	-1.95378600	-0.61960300	0.34785900
C	-3.02324200	-1.64872700	0.64080400
C	-0.99378600	-1.22471600	-0.63994800
H	-1.41772700	-0.44118500	1.29086000
H	-2.82342000	-2.46263600	1.32688000
H	-4.00507300	-1.59120700	0.18331400
O	-3.74550400	-0.64770700	2.21941800
N	-1.37062300	-2.39338600	-1.23947600
C	0.18358800	-0.62925100	-1.02334500
N	1.15753000	-0.04349200	-1.32576200
C	-4.67802800	0.11892400	1.93827900
N	-5.56974700	0.85138000	1.67402500

O	-0.70364900	-2.96470600	-2.09702600
O	-2.49050800	-2.86423700	-0.84537400
C	-2.52017600	0.69581700	-0.14210500
C	-2.22568400	1.87348400	0.54137300
C	-3.34173100	0.74122300	-1.27036300
C	-2.76545700	3.08529300	0.11766500
H	-1.58519100	1.83442400	1.42364700
C	-3.88528800	1.94952500	-1.69078800
H	-3.56576100	-0.17575200	-1.81967900
C	-3.60177400	3.12315600	-0.99381100
H	-2.53644800	3.99986200	0.66262400
H	-4.53342800	1.97561500	-2.56542000
H	-4.03018200	4.06860600	-1.32308700
Cu	2.88609600	0.15934500	-0.44483100
O	2.91403500	2.16378100	-0.24498600
N	4.09346700	2.13415200	0.25297000
O	4.67198000	3.11784200	0.62155400
O	4.59103800	0.95977000	0.32103100
N	2.68165300	-1.90838300	1.05055200
O	2.17200700	-0.90282500	1.57816900
O	3.23096300	-1.73744000	-0.11716600
O	2.69547100	-3.01215000	1.54951600

TS4c

C	-2.98151000	1.95825300	-0.44033300
C	-2.84235400	0.62644900	-1.20379200
C	-1.67012300	2.43443200	0.08363400
H	-3.36968200	2.71143600	-1.13599600
H	-3.71812200	1.84022100	0.36379300
H	-3.53274100	0.61325500	-2.05449600
O	-1.53393700	0.63593800	-1.86753300
N	-1.18410500	1.97437000	1.31396300
C	-0.49776600	0.91068800	-1.16736600
N	0.63838100	0.88751100	-0.85453500
C	-1.07429400	3.61678900	-0.39944400
N	-0.59396200	4.57966000	-0.85724900
O	-0.14705800	2.48183300	1.76503800
O	-1.77381800	1.03451000	1.86509000
C	-3.00418900	-0.63250200	-0.39148800
C	-4.18158500	-0.79622200	0.34419900
C	-2.05315200	-1.65127300	-0.38022700
C	-4.38396400	-1.93955600	1.10595000
H	-4.94893000	-0.02189800	0.32168800
C	-2.25065700	-2.79225700	0.39585200
H	-1.15596900	-1.57706900	-0.99477800
C	-3.41159500	-2.93737000	1.14553300
H	-5.30532900	-2.04964600	1.67584300
H	-1.48211800	-3.56409300	0.40910300
H	-3.56534500	-3.82851000	1.75185000
Cu	2.20912400	-0.15185100	-0.49095300
O	3.28170700	1.11113800	0.67205700
N	4.27254700	0.30320800	0.68864100
O	5.28720900	0.51980500	1.29212200
O	4.07888500	-0.75819500	0.00392000
N	1.20130500	-2.51219000	-0.37977700
O	1.26713000	-1.99292000	0.74617500
O	1.61647600	-1.79630900	-1.38197900
O	0.77110600	-3.62736400	-0.59886000

TS5b

C	2.76956300	-0.90362200	-0.13581400
C	2.49510600	-0.88859400	-1.61768600
C	4.15119600	-0.36830100	0.12852800
H	2.76533300	-1.96209400	0.16645600
H	3.12458200	-1.48051400	-2.27537600
H	1.93076800	-0.08280700	-2.07675600
O	1.11665000	-2.08057200	-1.65965100
N	4.71662600	0.46469800	-0.78275800
C	4.80491000	-0.58006700	1.34696700
N	5.31147100	-0.79274800	2.38061400
C	0.01977400	-1.56119000	-1.47961400
N	-1.04896000	-1.08031400	-1.36452400
O	5.81016500	1.01653500	-0.58698200
O	4.07266900	0.64700200	-1.86809200
C	1.68703900	-0.18656700	0.64845000
C	0.93483800	-0.88097700	1.59512600
C	1.42748900	1.16926000	0.42399500
C	-0.07681100	-0.23526900	2.30395000
H	1.13803600	-1.93837400	1.77109800
C	0.41664800	1.81397100	1.12702300
H	2.01816000	1.71977700	-0.31032600
C	-0.33949100	1.11264900	2.06957700
H	-0.66118900	-0.78606200	3.03952200
H	0.21689100	2.86965300	0.94467500
H	-1.12492300	1.62146800	2.62680400
Cu	-2.19018800	0.02858700	-0.26411800
O	-1.91999400	1.79270500	-1.19717400
N	-2.66278800	2.39811000	-0.34899400

O	-2.86383800	3.58157100	-0.38376000
O	-3.16024000	1.62778300	0.53695900
N	-4.04590900	-1.67424300	0.22784800
O	-4.28182500	-1.02115300	-0.80379000
O	-2.94915200	-1.38447100	0.86307000
O	-4.76529100	-2.54769300	0.66504500

$Cu(NO_3)_2(OCN)^-$

O	2.75296000	-2.91495500	0.13737100
C	1.69633300	-2.37423000	0.06487100
N	0.58929100	-1.90091100	-0.00190400
Cu	0.07108400	-0.09244900	-0.24614900
O	1.71711700	0.90395600	0.40119100
N	1.22318600	2.02734500	0.03953900
O	1.79095600	3.07388900	0.20414500
O	0.07548100	1.93300600	-0.50823500
N	-2.46917500	-0.25387700	0.17297700
O	-1.76139600	-0.41443200	-0.90039000
O	-1.85712500	0.05331000	1.21199600
O	-3.67331300	-0.40746000	0.11327300

1v

C	0.11506200	-0.67420700	0.85346000
C	-0.52514800	0.11900000	1.91419300
C	-1.04113100	0.30602100	0.49601600
H	-0.23123900	-1.70454200	0.76597200
H	0.01098400	0.96523100	2.33958400
H	-1.21749300	-0.38431700	2.58526100
C	-0.69760300	1.51840600	-0.18621000
N	-0.38625300	2.49931600	-0.72737400
C	1.48784000	-0.44400400	0.33896300
C	2.04090300	-1.40746500	-0.51049900
C	2.24408300	0.68853300	0.65727300
C	3.31850400	-1.24529700	-1.03385700
H	1.45625800	-2.29373600	-0.75889700
C	3.52143100	0.85186300	0.13121400
H	1.84158500	1.45169400	1.32351500
C	4.06264100	-0.11208300	-0.71535600
H	3.73355900	-2.00625300	-1.69299000
H	4.09876700	1.73838200	0.38949600
H	5.06352400	0.01852600	-1.12396900
C	-2.34239600	-0.34439700	0.16690200
O	-2.73003800	-1.35920000	0.70018200
O	-3.00236800	0.32254300	-0.77590900
C	-4.26178800	-0.23842600	-1.16489500
H	-4.93948100	-0.28895600	-0.30667800
H	-4.66573800	0.43462100	-1.92319900
H	-4.12209200	-1.24027900	-1.58389200

TS1v

C	0.23738800	0.43080600	-0.37738300
C	-0.61618300	0.47470300	-1.56274000
C	-1.74763200	-0.20731900	-0.82707100
H	-0.87899000	1.49464600	-1.85673200
H	-0.25205300	-0.08841500	-2.42729800
C	-1.90004100	-1.59377400	-0.91848000
N	-1.98545000	-2.76031100	-1.01958000
H	-0.01740500	1.13925500	0.40766400
N	2.26081900	2.41711900	-0.09307600
O	1.72224200	2.48041500	1.01945200
O	3.24652200	3.09271100	-0.39105900
O	1.78813800	1.62470900	-0.98672200
C	1.02783600	-0.72783100	0.02693700
C	1.38066800	-1.74432500	-0.87107300
C	1.48127300	-0.80116200	1.35171800
C	2.16044500	-2.81298000	-0.44840500
H	1.04884000	-1.69927000	-1.90726200
C	2.26380200	-1.86869100	1.77060000
H	1.21622100	-0.00414900	2.04531100
C	2.60319100	-2.87806000	0.87164000
H	2.42710300	-3.59877500	-1.15304800
H	2.60931800	-1.91598500	2.80193700
H	3.21481900	-3.71740200	1.19908200
C	-2.63898500	0.60744700	-0.04865300
O	-2.54535600	1.82069300	0.09012400
O	-3.62719700	-0.11348500	0.54155500
C	-4.52810100	0.63770700	1.33959800
H	-5.06205400	1.38749600	0.74323100
H	-5.24341400	-0.08099600	1.74924100
H	-4.00673700	1.14647600	2.15953400

INT1v

C	-0.62178100	-0.25150400	0.91460300
C	0.31285000	-0.19571900	-0.28961800
C	-2.03472600	0.16667200	0.60733100
H	-0.60741900	-1.29678000	1.25402300
H	-0.21150300	0.34731300	1.73824800
H	-0.11745600	-0.84908200	-1.06358300

O	0.21368800	1.07554500	-1.02028900
N	0.69379400	2.19640200	-0.38750000
C	-2.37431200	1.50979600	0.75805900
N	-2.61117700	2.65439000	0.90942300
O	0.58565800	3.19335600	-1.05648400
O	1.16175700	2.08602700	0.72023800
C	1.75705800	-0.57883000	-0.07778100
C	2.22392800	-1.04600800	1.15074500
C	2.64701200	-0.49757000	-1.15359800
C	3.55577400	-1.42410300	1.30218800
H	1.54793600	-1.11345300	2.00152600
C	3.97873000	-0.86450300	-1.00056700
H	2.29105700	-0.13980300	-2.12023100
C	4.43724000	-1.33128600	0.22968200
H	3.90619200	-1.78735400	2.26729400
H	4.66065000	-0.79161200	-1.84662100
H	5.47950800	-1.62309100	0.34988600
C	-2.99761800	-0.70210500	0.02858800
C	-3.40515800	-2.90583000	-0.69018600
H	-2.86555000	-3.85508500	-0.76929300
H	-4.28022100	-3.03749500	-0.04041400
H	-3.75900700	-2.60462200	-1.68485000
O	-4.15716900	-0.44256600	-0.29042600
O	-2.49099500	-1.97217900	-0.15505500

TS2v

C	0.13347600	0.21925300	1.10686200
C	-0.58757800	0.70806200	-0.19192100
C	1.46946700	-0.32914500	0.72382000
H	0.19116200	1.05038700	1.82146600
H	-0.45102700	-0.58071600	1.57801400
H	-0.40775800	1.79547500	-0.25920100
O	-0.00959600	0.13960700	-1.31496900
N	0.82813500	-1.19376100	-0.93032700
C	1.93336700	-1.47335800	1.42728900
N	2.28280700	-2.43582500	1.98760400
O	1.73349700	-1.32040300	-1.74403800
O	0.07303800	-2.09801700	-0.55916900
C	-2.07885300	0.48128100	-0.07966300
C	-2.83953500	1.32421800	0.73390700
C	-2.71151600	-0.56467100	-0.75121500
C	-4.20883800	1.12285800	0.88166700
H	-2.34920100	2.15082500	1.25314400
C	-4.08186000	-0.76531400	-0.60772200
H	-2.10746000	-1.21765300	-1.37848000
C	-4.83520900	0.07550000	0.20875200
H	-4.79088600	1.78865500	1.51830200
H	-4.56742900	-1.58462200	-1.13766500
H	-5.90763600	-0.08167600	0.31783000
C	2.56074100	0.53807500	0.26315900
O	3.71088800	0.17423800	0.10757200
O	2.14127200	1.78648300	-0.00384200
C	3.13049000	2.65669200	-0.54165000
H	2.63945700	3.62187500	-0.68745700
H	3.97308000	2.76872500	0.14995600
H	3.50339100	2.27985100	-1.50099200

INT1w

Cu	2.79408900	-0.03877900	-0.51039300
O	3.79013600	1.36356200	0.49143200
N	4.62001500	0.50235000	0.95908300
O	5.50442800	0.79081200	1.71180900
O	4.40267100	-0.68568100	0.54394400
C	-1.92571400	-0.20207300	-1.42147900
C	-2.10894500	0.95314400	-2.30810600
C	-1.21923900	1.16624300	-1.09337600
H	-1.60352500	0.94802600	-3.27064400
H	-3.04270400	1.50977100	-2.26933100
C	0.19249800	1.12931900	-1.22203500
N	1.34948400	1.05489900	-1.29833700
H	-1.20656400	-0.94690700	-1.76935600
N	1.19238800	-2.01136600	-0.16772100
O	1.13663500	-1.20736400	0.78149600
O	2.05748900	-1.74517400	-1.10355800
O	0.49870400	-2.99883800	-0.27174100
C	-2.93658300	-0.69821800	-0.45023300
C	-4.30473900	-0.56948600	-0.68883500
C	-2.49506000	-1.29213800	0.73652400
C	-5.22362100	-1.02665100	0.25076100
H	-4.65052000	-0.10685800	-1.61281700
C	-3.41495400	-1.74454300	1.67606600
H	-1.42261700	-1.39074900	0.92280600
C	-4.78113300	-1.61058200	1.43500300
H	-6.29022200	-0.92330900	0.05753700
H	-3.06386000	-2.19994700	2.60062700
H	-5.50144700	-1.96473500	2.17081900
C	-1.67894200	1.87491500	0.14105200
O	-0.95360000	2.08409500	1.08680000

O	-2.96777000	2.17084600	0.07478300
C	-3.58386100	2.56000700	1.30845300
H	-3.18760500	3.52108600	1.65125600
H	-4.65054900	2.64441500	1.09253000
H	-3.40995100	1.79491500	2.07429600

INT2w

C	-1.89387300	-0.79110800	-0.50266200
C	-1.68765200	0.14451800	-1.69301700
C	-0.53454000	1.08168200	-1.43748200
H	-1.47730200	-0.48702600	-2.56802700
H	-2.58473800	0.72538000	-1.92168100
C	0.74353500	0.65903400	-1.62139800
N	1.85810700	0.30667000	-1.86356400
H	-0.93238900	-1.28896700	-0.31681700
N	-3.96304100	-1.86517000	-1.23205700
O	-4.43347800	-0.75487800	-1.30264800
O	-4.50457500	-2.91932900	-1.44944800
O	-2.64881000	-2.00715400	-0.86681700
C	-2.36794000	-0.21354400	0.80686800
C	-3.27227000	0.84845700	0.90517500
C	-1.86913900	-0.78756200	1.98086100
C	-3.65758200	1.32985400	2.15222000
H	-3.67180300	1.31523900	0.00925700
C	-2.26170100	-0.31216500	3.22778100
H	-1.14965300	-1.60470900	1.90860500
C	-3.15580400	0.75097800	3.31547000
H	-4.35675200	2.16308200	2.21321800
H	-1.85991400	-0.76689300	4.13206600
H	-3.46060800	1.13119100	4.28951000
Cu	3.03102600	-0.43011100	-0.53917100
O	4.25460100	1.17643600	-0.19019900
N	5.01421800	0.48135200	0.56591900
O	5.98033200	0.94324300	1.11822500
O	4.66329200	-0.73744900	0.68633400
N	1.35546400	-2.03960200	0.60118400
O	1.39735100	-0.93751000	1.17714600
O	2.16149200	-2.22229600	-0.38901500
O	0.58822800	-2.93661900	0.91610000
C	-0.67849400	2.43184700	-0.91703300
O	0.23045400	3.13490900	-0.50542800
O	-1.96190600	2.84579900	-0.94233600
C	-2.22359800	4.07127300	-0.27065000
H	-1.71003900	4.90787100	-0.75788600
H	-3.30587300	4.21874000	-0.32230000
H	-1.90541000	4.01577100	0.77754400

TS1w

C	-1.89317200	0.76115200	-0.29569100
C	-1.22953800	0.44949400	0.95924400
C	-0.61351600	-0.70333300	0.18213200
H	-0.49838200	1.18820000	1.29387200
H	-1.86598700	0.11123300	1.77561100
C	0.56496900	-0.49557700	-0.49945200
N	1.55415000	-0.26971900	-1.10098900
H	-1.29690800	1.27575600	-1.04685600
N	-3.22287300	3.16058300	1.08695400
O	-3.22707100	2.32953500	2.01221900
O	-3.77296600	4.26271100	1.20596000
O	-2.64162000	2.88667100	-0.00814800
C	-3.16169500	0.20270600	-0.74009500
C	-4.18494700	-0.11549500	0.16449000
C	-3.35168100	-0.02919300	-2.10888600
C	-5.37475400	-0.65833300	-0.29998100
H	-4.05287500	0.10317100	1.22233900
C	-4.53586600	-0.59127400	-2.56680800
H	-2.55147400	0.22141300	-2.80554700
C	-5.54792600	-0.90627300	-1.66193300
H	-6.17295800	-0.89228900	0.40234200
H	-4.67273900	-0.78098900	-3.62987500
H	-6.47997800	-1.34030000	-2.02068000
Cu	3.39656000	-0.21299500	-0.49495700
O	4.04259400	1.40331300	-1.53275100
N	5.22960200	1.25989900	-1.07820700
O	6.12921000	2.00707000	-1.34938500
O	5.36610700	0.25040700	-0.30780900
N	2.94014900	-0.98350300	1.91651200
O	2.83341600	0.25075500	1.80654400
O	3.26988800	-1.63992600	0.84275700
O	2.75578100	-1.59794300	2.94571600
C	-1.17805800	-2.04891500	0.10412100
O	-0.77032900	-2.92707200	-0.63354400
O	-2.21952700	-2.19486900	0.93404000
C	-2.98757300	-3.38186200	0.75052000
H	-2.38857500	-4.27345100	0.96425500
H	-3.82022300	-3.31367400	1.45470000
H	-3.36866200	-3.43682800	-0.27706400

TS2w

C	-1.80480400	0.30550700	-0.68976400
C	-1.57142000	-0.73812800	0.43912400
C	-1.09916100	1.55098300	-0.26009300
H	-1.44427200	-0.10327300	-1.64379000
H	-2.86841300	0.54799300	-0.79704800
H	-0.60078000	-1.23150900	0.21605300
O	-1.49843300	-0.11374000	1.66392500
N	-1.75502600	1.59925000	1.51453000
C	0.29413000	1.38766100	-0.08192000
N	1.41395000	1.14818300	0.11894300
O	-0.97319300	2.15018100	2.27353900
O	-2.96092300	1.81421800	1.45080400
C	-2.64838200	-1.79727800	0.36771800
C	-2.44741300	-2.94589400	-0.39687900
C	-3.86149200	-1.61961300	1.03316500
C	-3.45046900	-3.90704700	-0.50175100
H	-1.48989800	-3.08471200	-0.90610800
C	-4.86372100	-2.57852000	0.93041400
H	-3.99925700	-0.72075200	1.63419500
C	-4.66092500	-3.72541900	0.16277900
H	-3.28293200	-4.80375100	-1.09744100
H	-5.80889800	-2.43465200	1.45343300
H	-5.44472400	-4.47800800	0.08584100
Cu	2.99127700	0.05989900	-0.25016200
O	4.09934900	0.33217600	1.39317200
N	5.07335500	-0.33187800	0.88899400
O	6.09963900	-0.53341900	1.47216100
O	4.83849100	-0.75673900	-0.29358900
N	1.57352600	-1.71227900	-1.42392200
O	1.73427600	-1.96781600	-0.21622000
O	2.22176900	-0.68583600	-1.88989100
O	0.85995500	-2.34717000	-2.17034200
C	-1.46526100	2.90521400	-0.72679800
O	-0.76552900	3.88192400	-0.54420400
O	-2.65657000	2.92937300	-1.32106500
C	-3.12021800	4.22716500	-1.69829500
H	-4.10772100	4.07668400	-2.13913600
H	-3.19230400	4.87950300	-0.82153900
H	-2.44430000	4.67946500	-2.43209900

10. References

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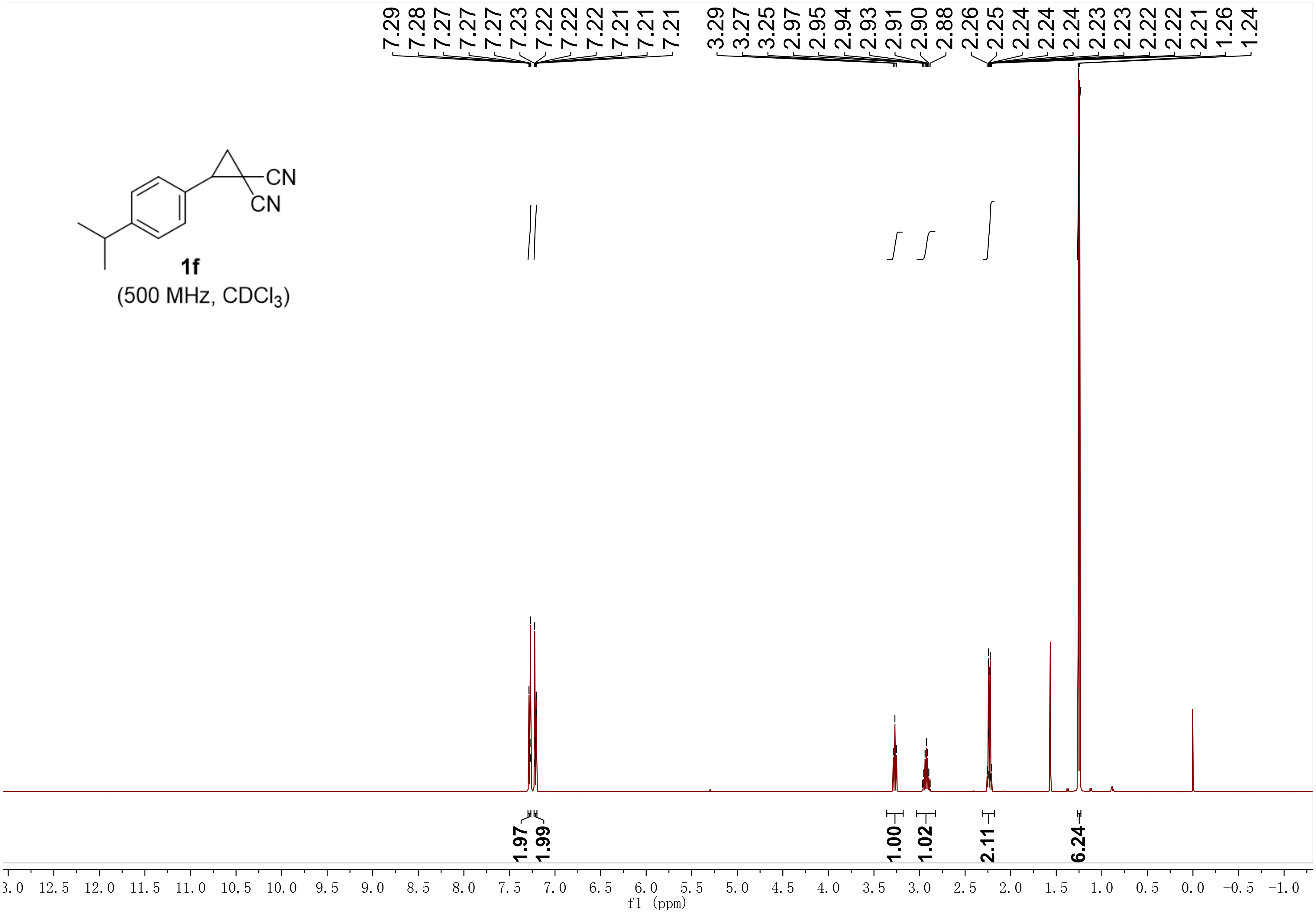
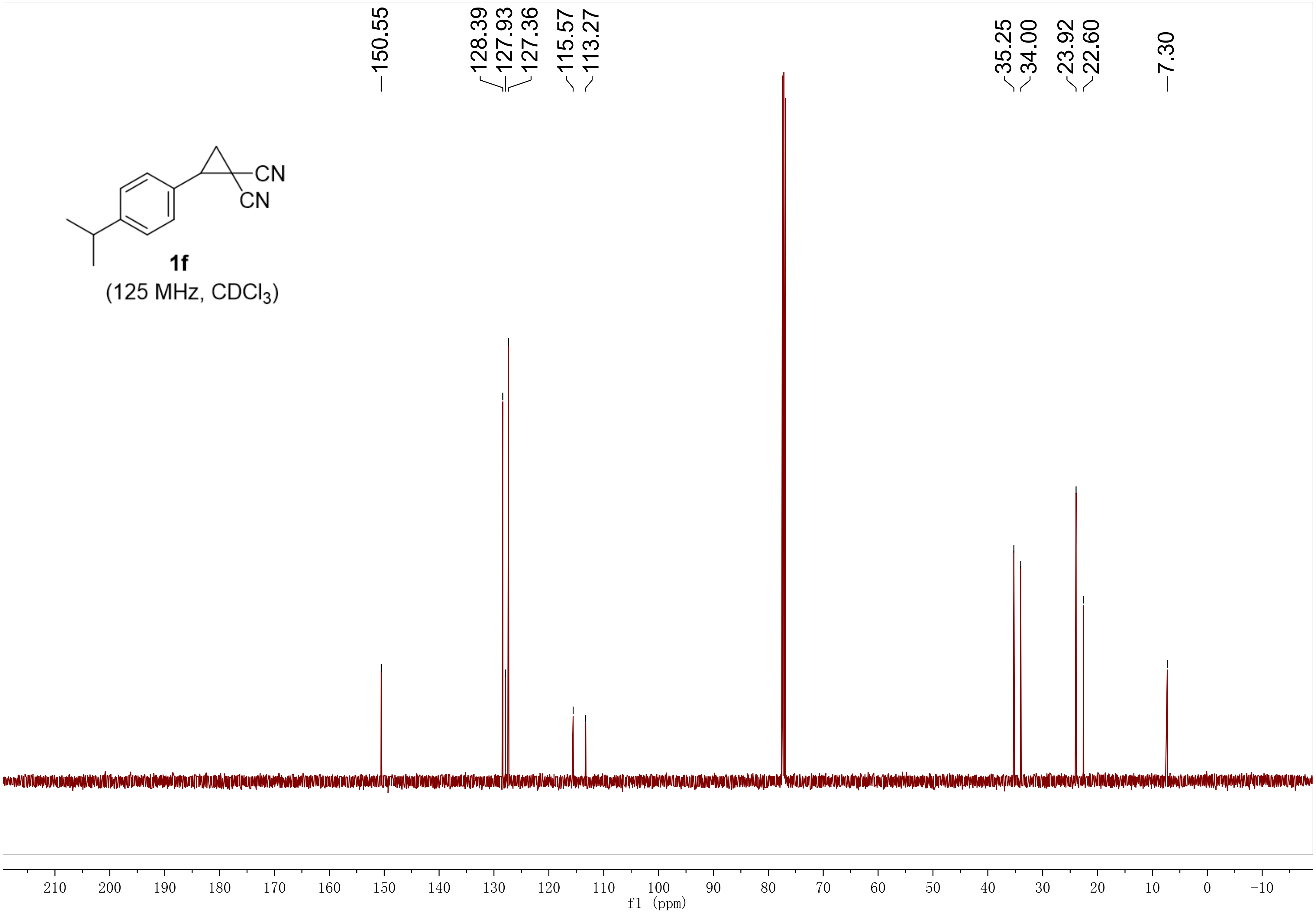
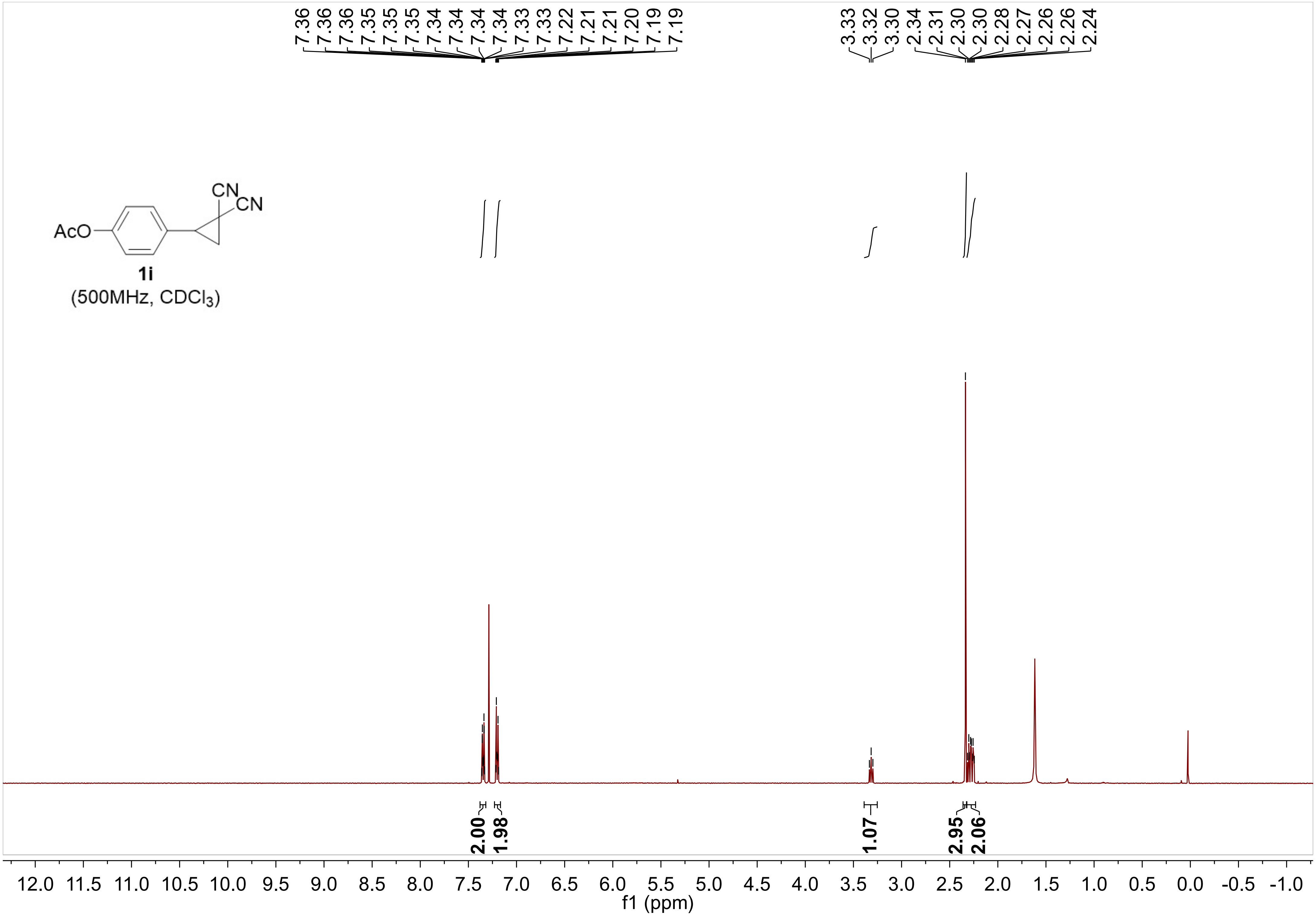
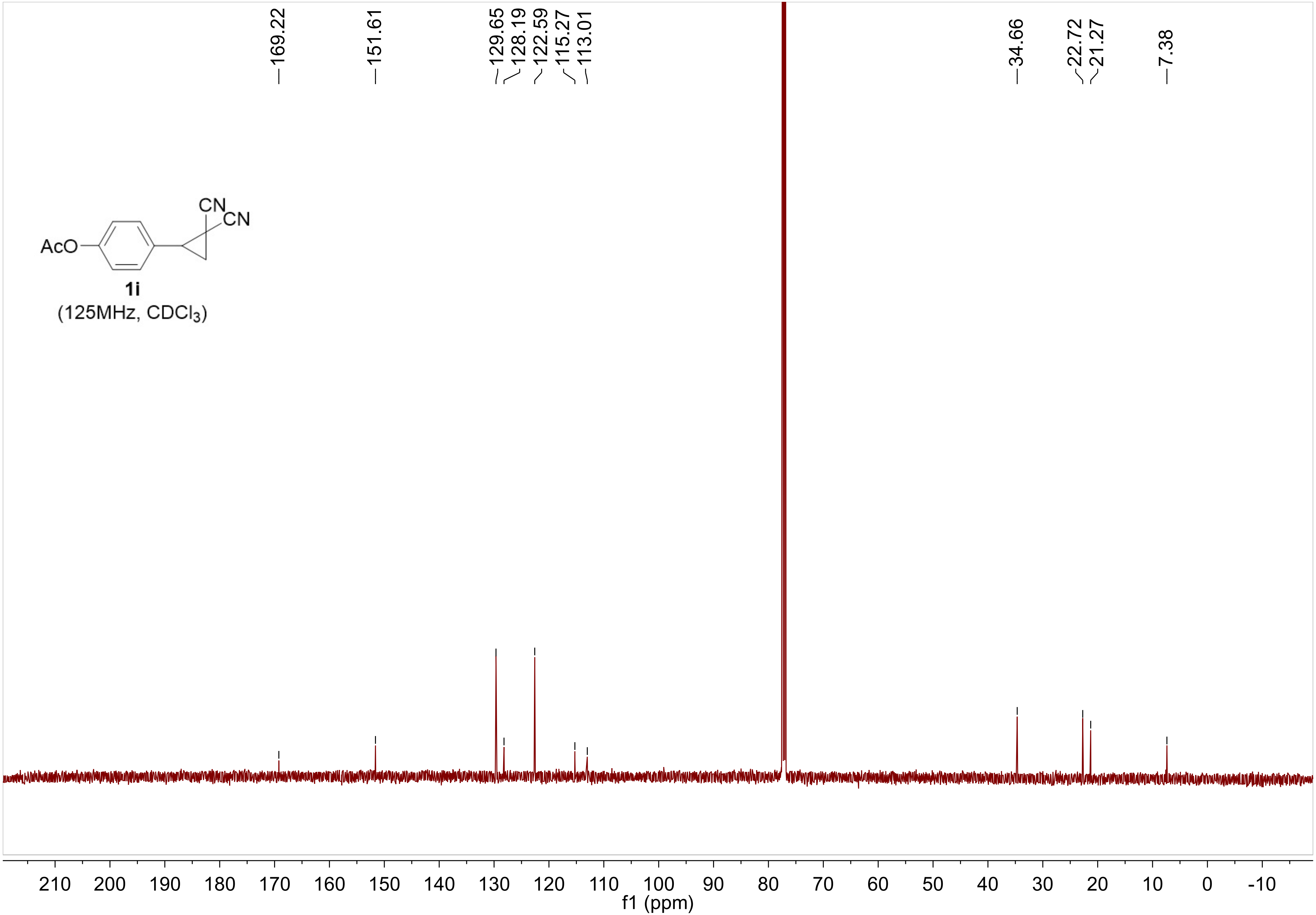
11. Copies of ^{1}H, ^{13}C and ^{19}F NMR Spectra

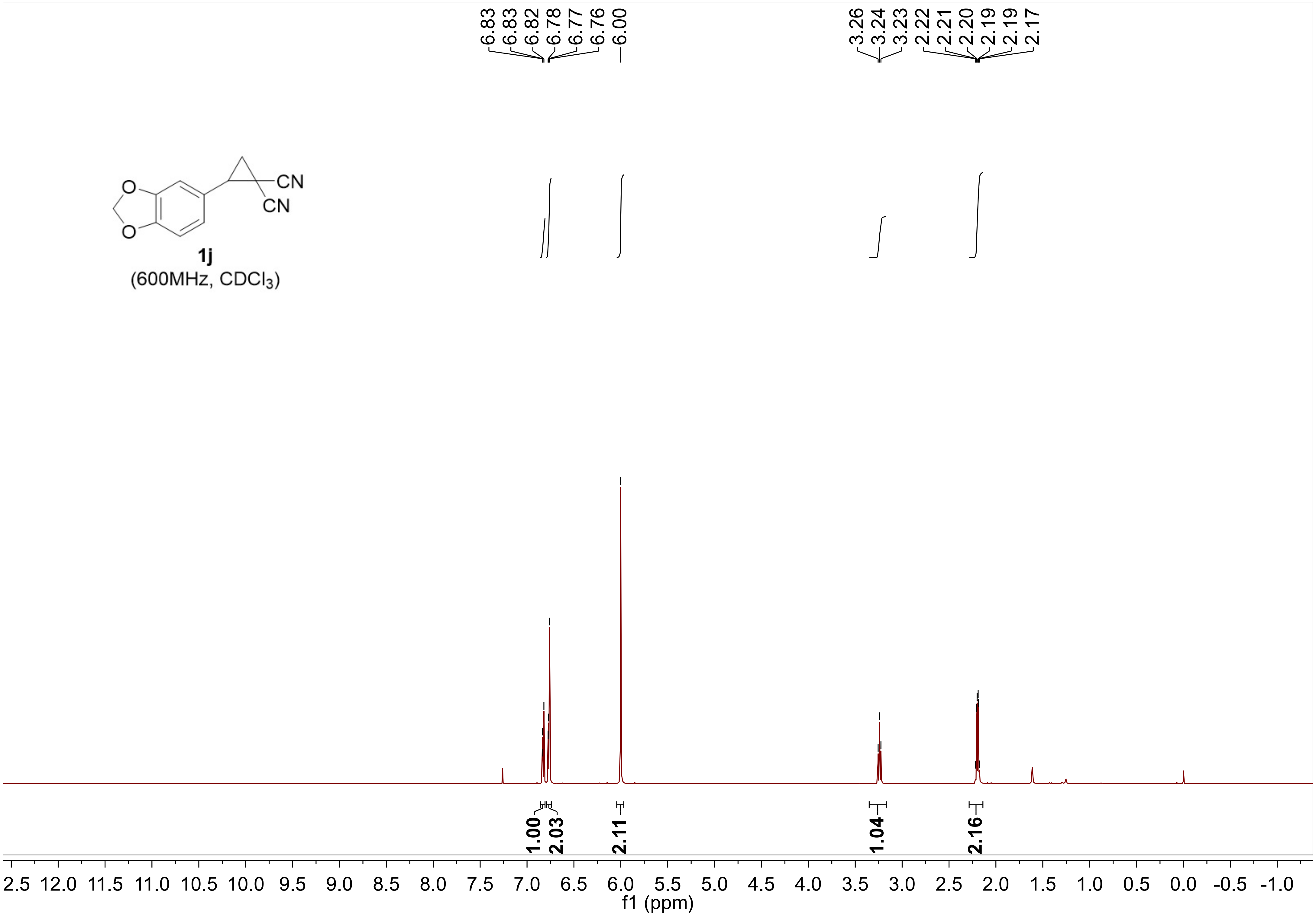

7.29 7.28 7.27 7.27 7.27 7.23 7.22 7.22 7.22 7.21 7.21 7.21
3.29 3.27 3.25 2.97 2.95 2.94 2.93 2.91 2.90 2.88
2.26 2.25 2.24 2.24 2.24 2.23 2.23 2.22 2.22 2.21 1.26 1.24
CN
CN
1f
(500 MHz, CDCl3)
1.97 1.99 1.00 1.02 2.11 6.24
3.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

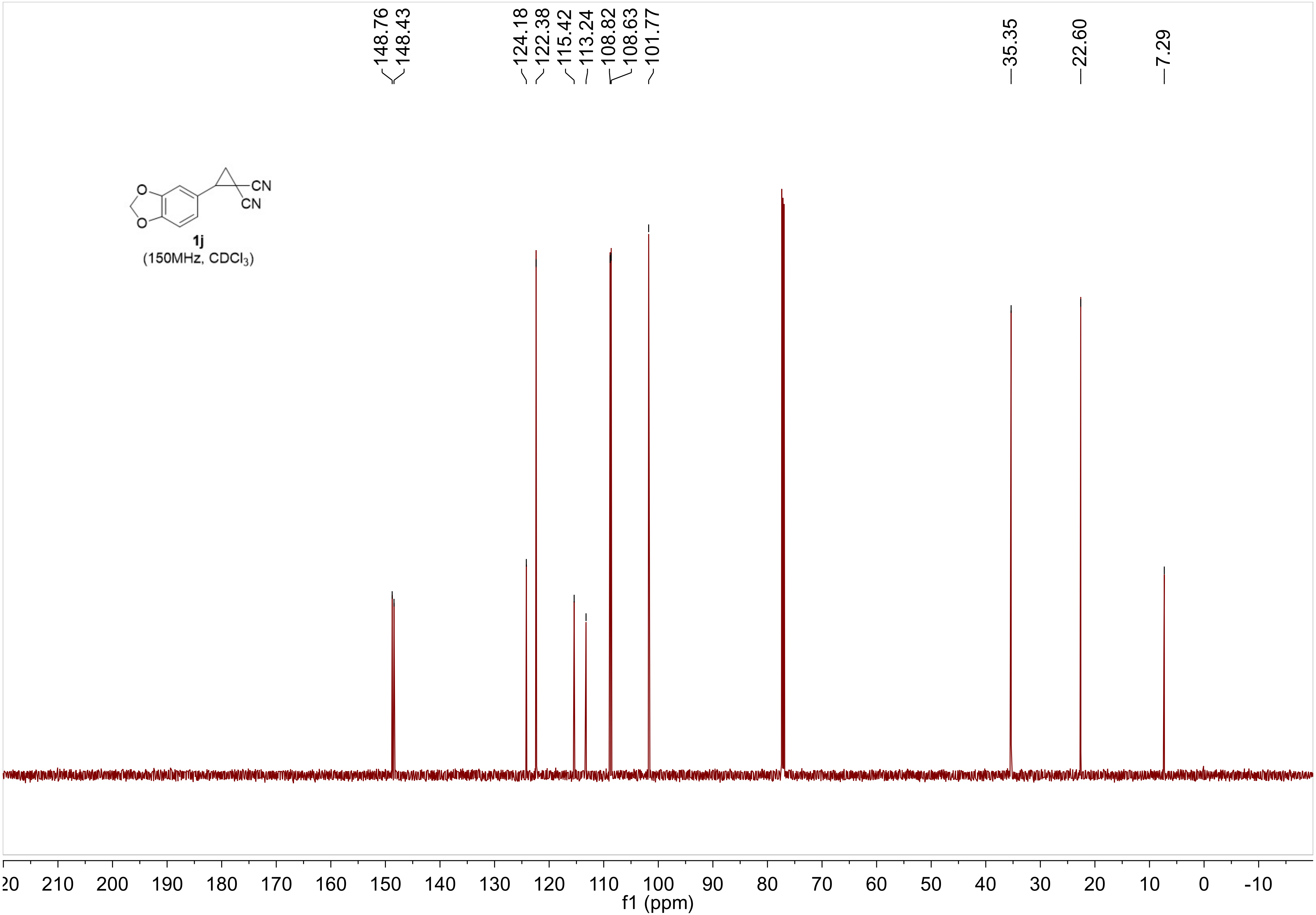

150.55
128.39
127.93
127.36
115.57
113.27
35.25
34.00
23.92
22.60
7.30
CN
CN
1f
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


7.36
7.36
7.36
7.35
7.35
7.35
7.34
7.34
7.34
7.34
7.33
7.33
7.22
7.21
7.21
7.20
7.19
7.19
3.33
3.32
3.30
2.34
2.31
2.30
2.30
2.28
2.27
2.26
2.26
2.24
CN
CN
AcO
1i
(500MHz, CDCl3)
2.00
1.98
1.07
2.95
2.06
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)



1i
(125MHz, $CDCl_3$)


6.83
6.83
6.82
6.78
6.77
6.76
6.00
3.26
3.24
3.23
2.22
2.21
2.20
2.19
2.19
2.17
CN
CN
O
O
1j
(600MHz, CDCl3)
1.00
2.03
2.11
1.04
2.16
2.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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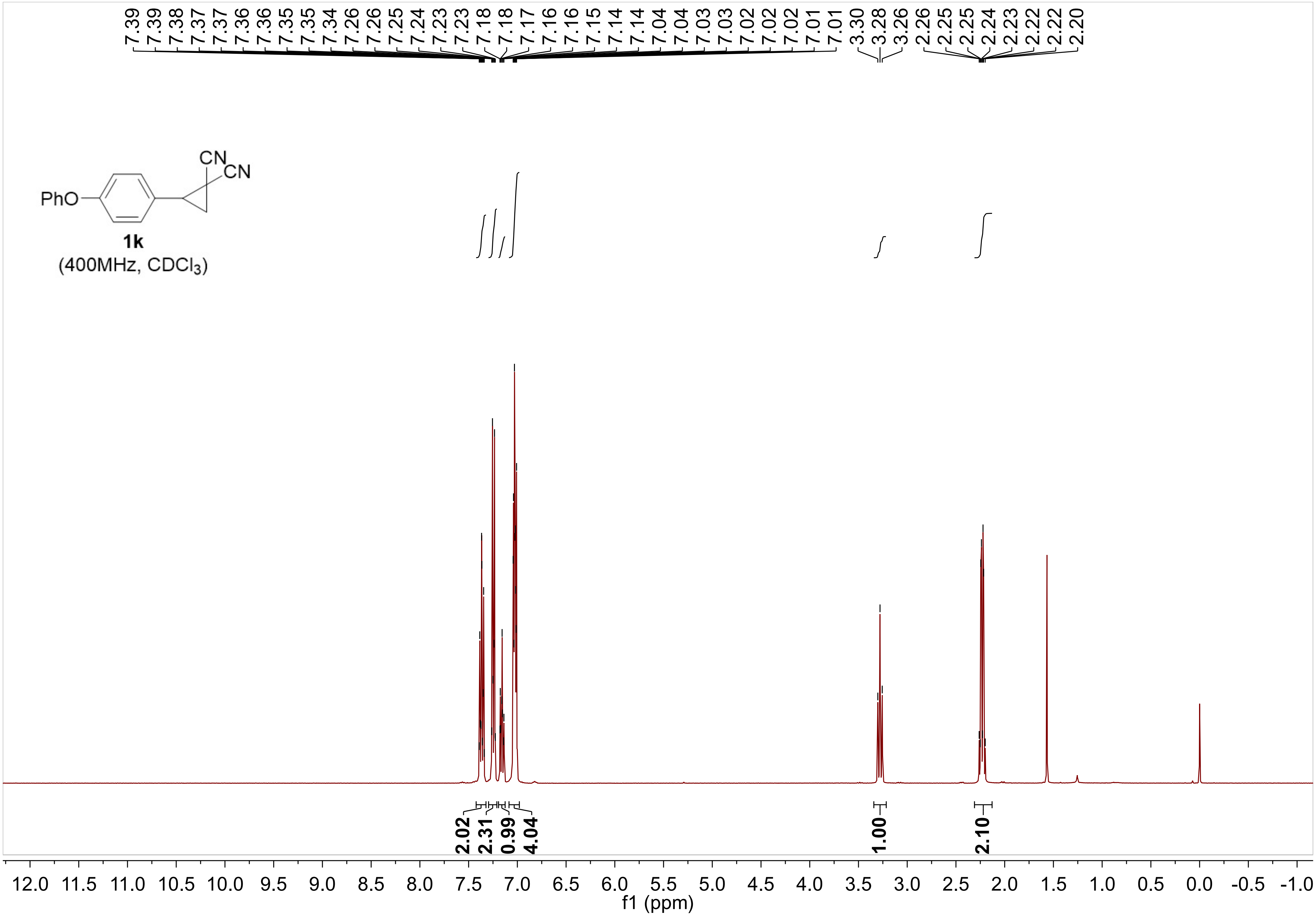
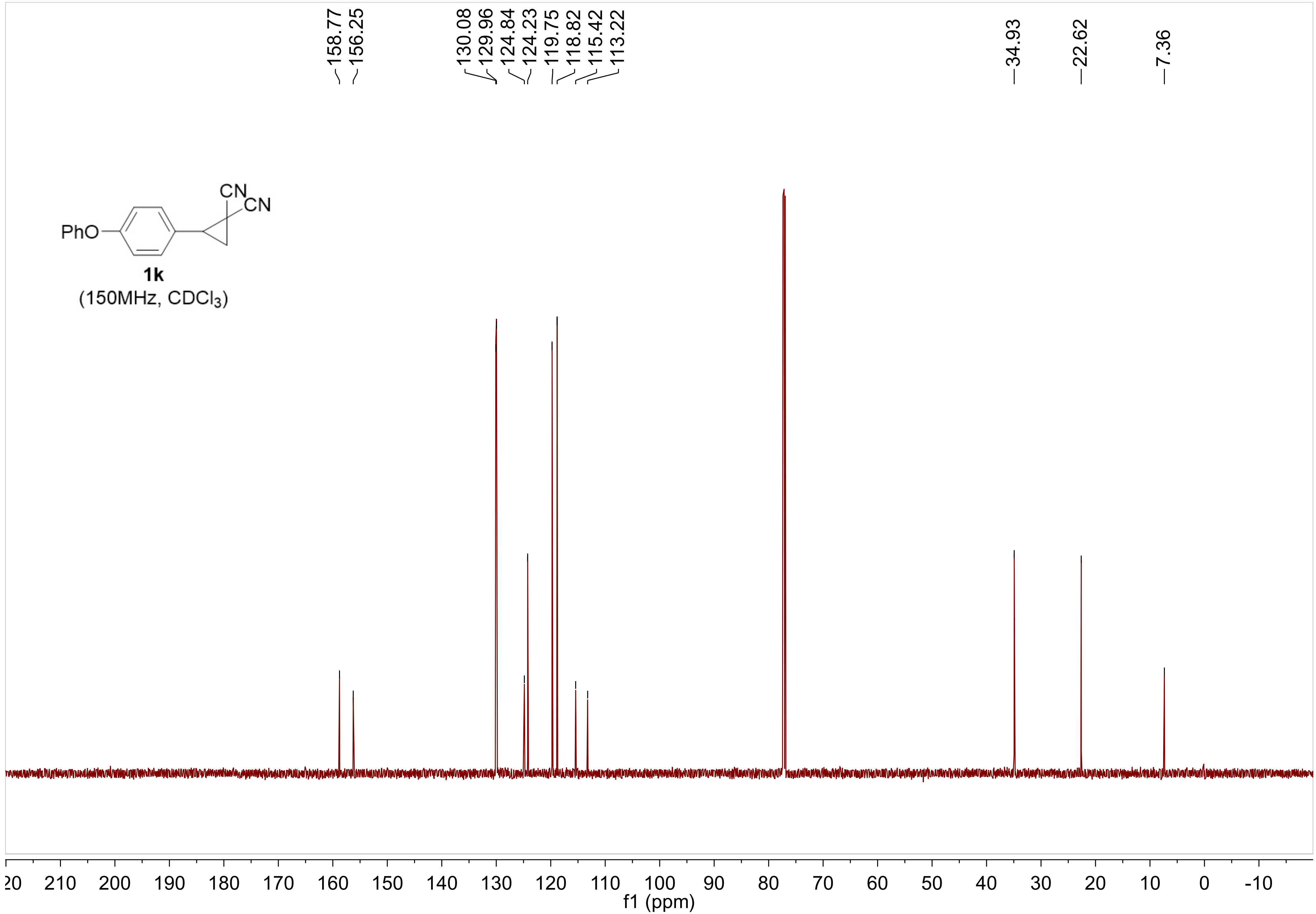
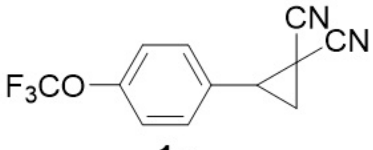
148.43
124.18
122.38
115.42
113.24
108.82
108.63
101.77
35.35
22.60
7.29
CN
CN
O
O
1j
(150MHz, CDCl3)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

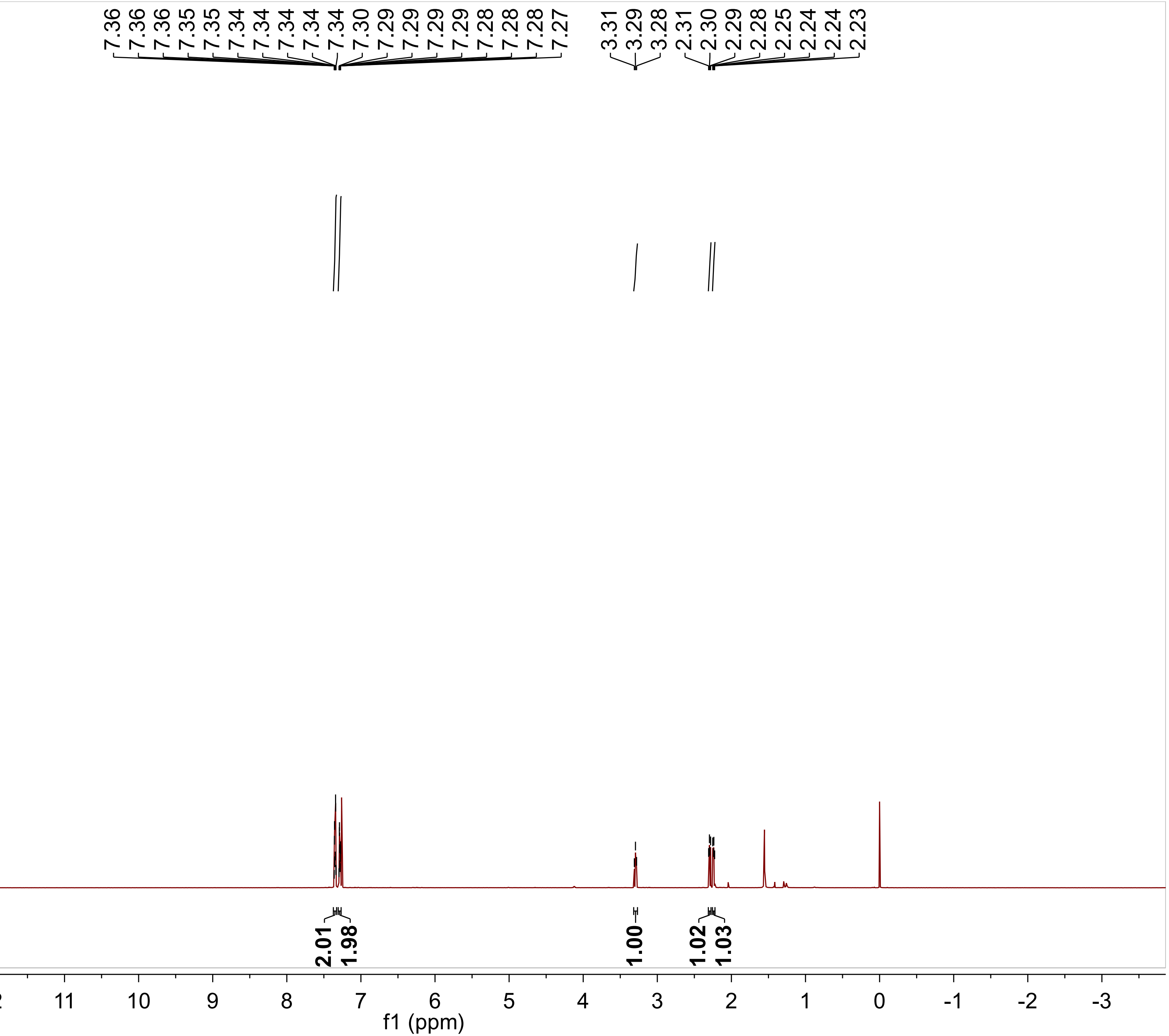

7.39 7.39 7.38 7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.26 7.26 7.25 7.24 7.23 7.23 7.18 7.18 7.17 7.16 7.16 7.15 7.14 7.14 7.04 7.04 7.03 7.03 7.02 7.02 7.02 7.01 7.01 3.30 3.28 3.26 2.26 2.25 2.25 2.24 2.24 2.23 2.22 2.22 2.20
CN
CN
PhO
1k
(400MHz, CDCl$_3$)
2.02
2.31
0.99
4.04
1.00
2.10
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

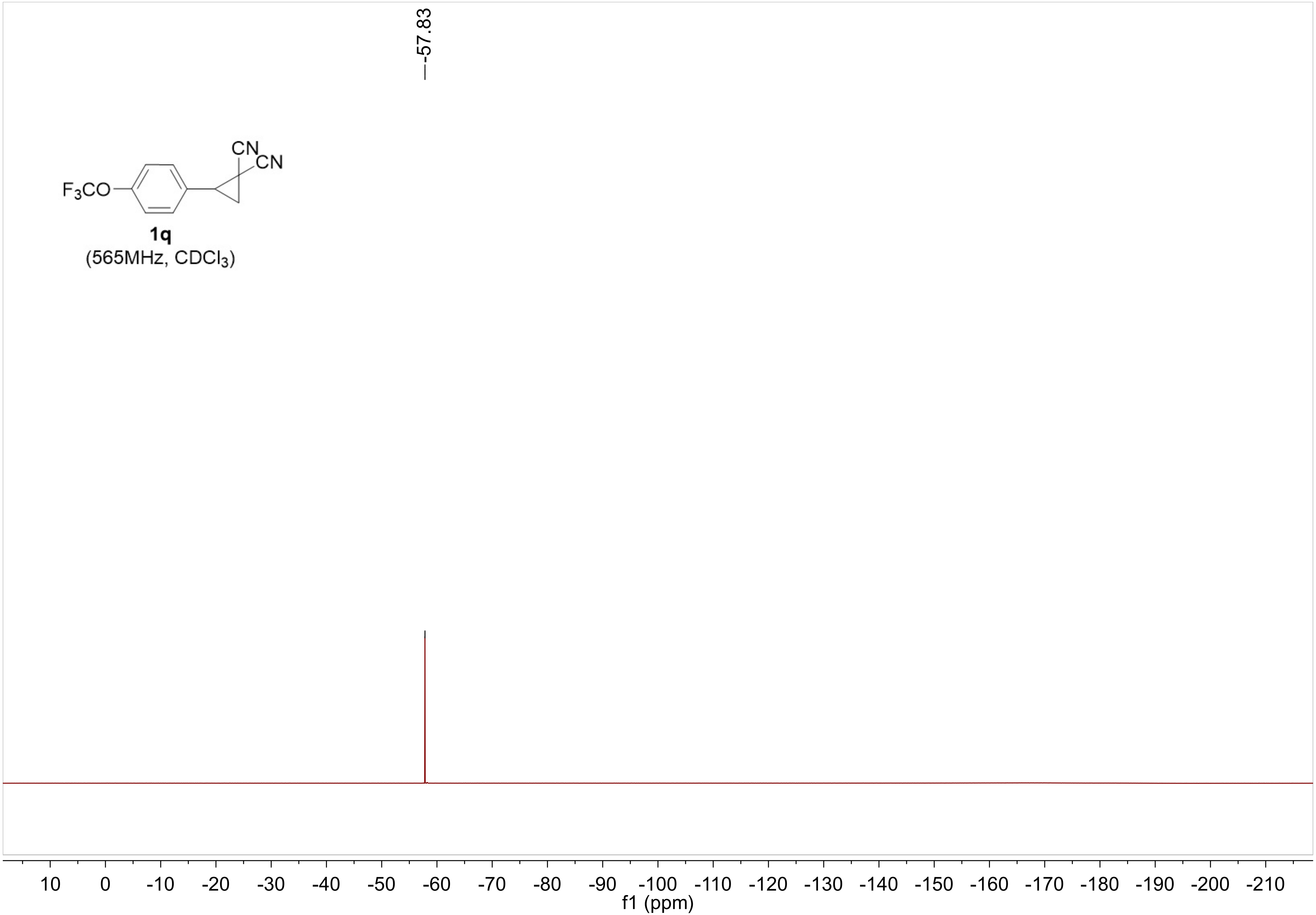

158.77
156.25
130.08
129.96
124.84
124.23
119.75
118.82
115.42
113.22
34.93
22.62
7.36
CN
CN
PhO
1k
(150MHz, CDCl3)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



1q

(600MHz, $CDCl_3$)

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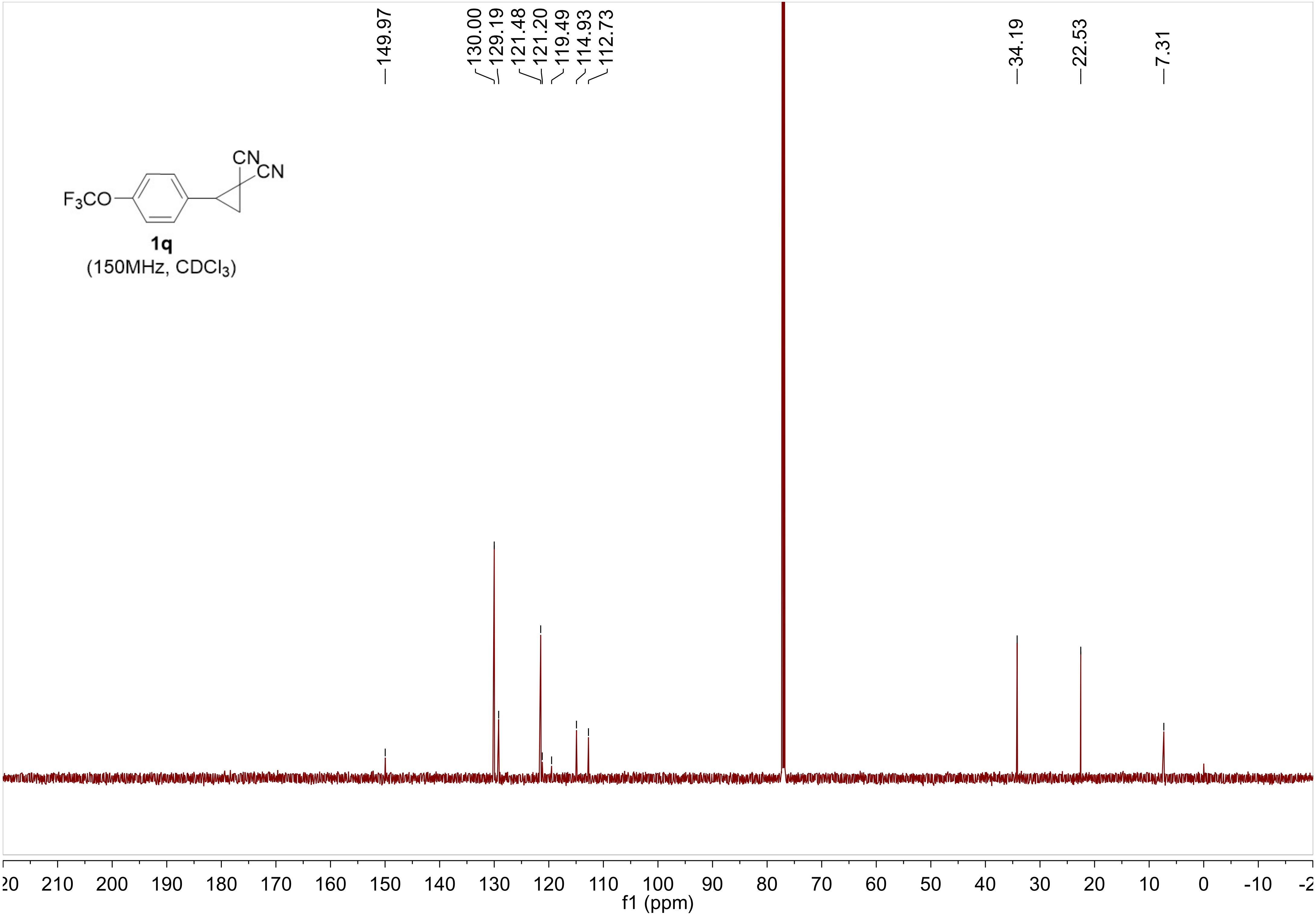
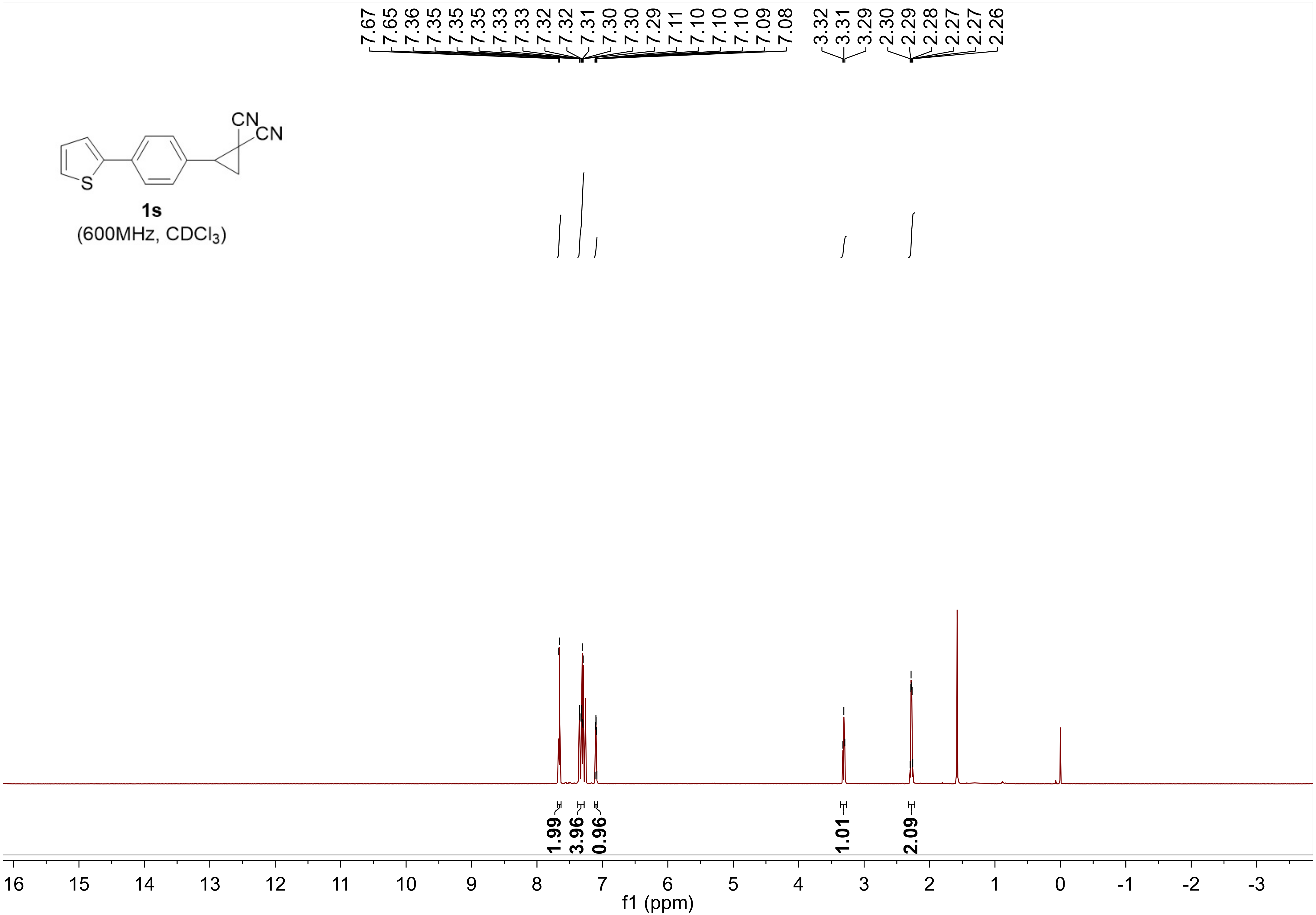
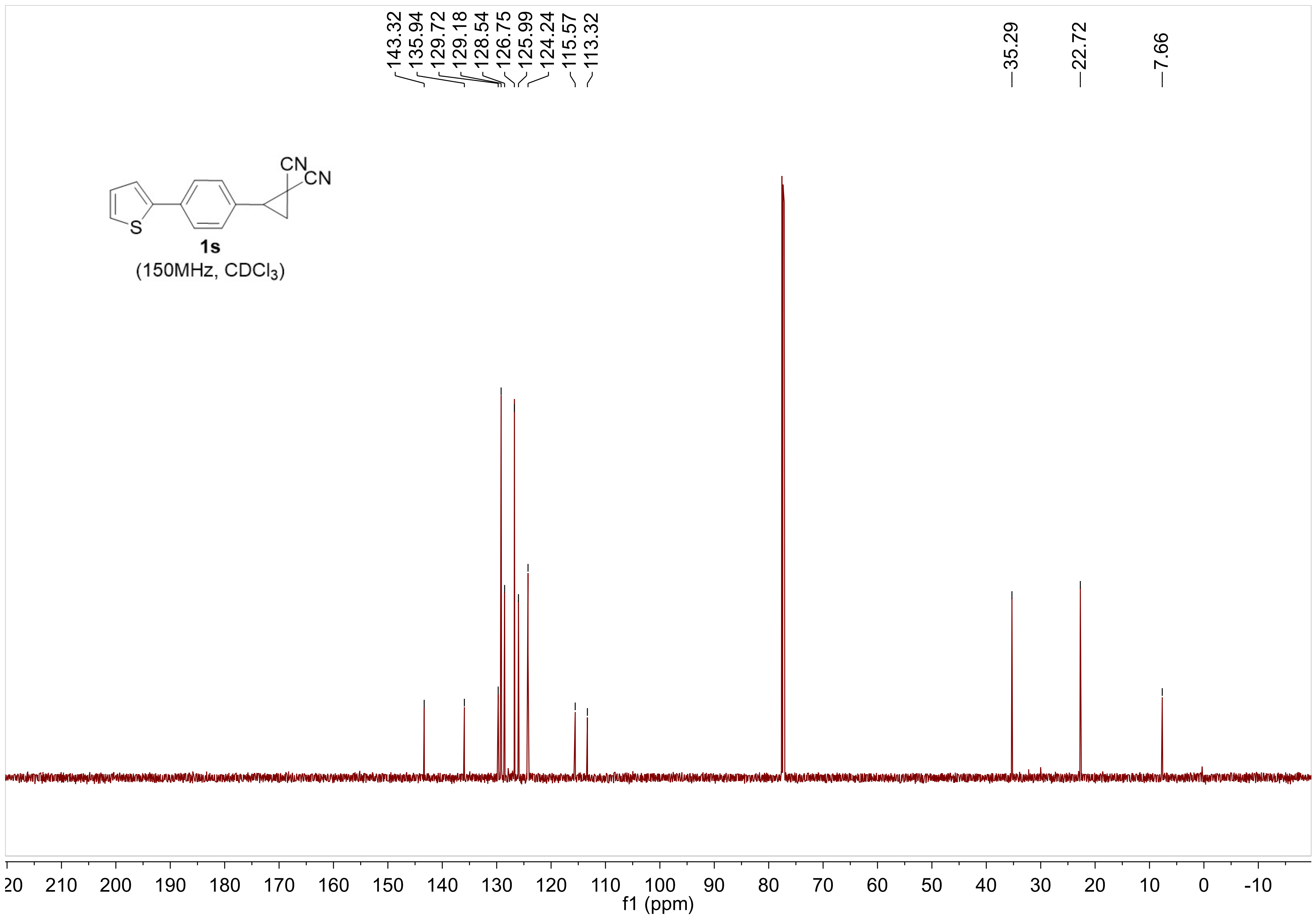
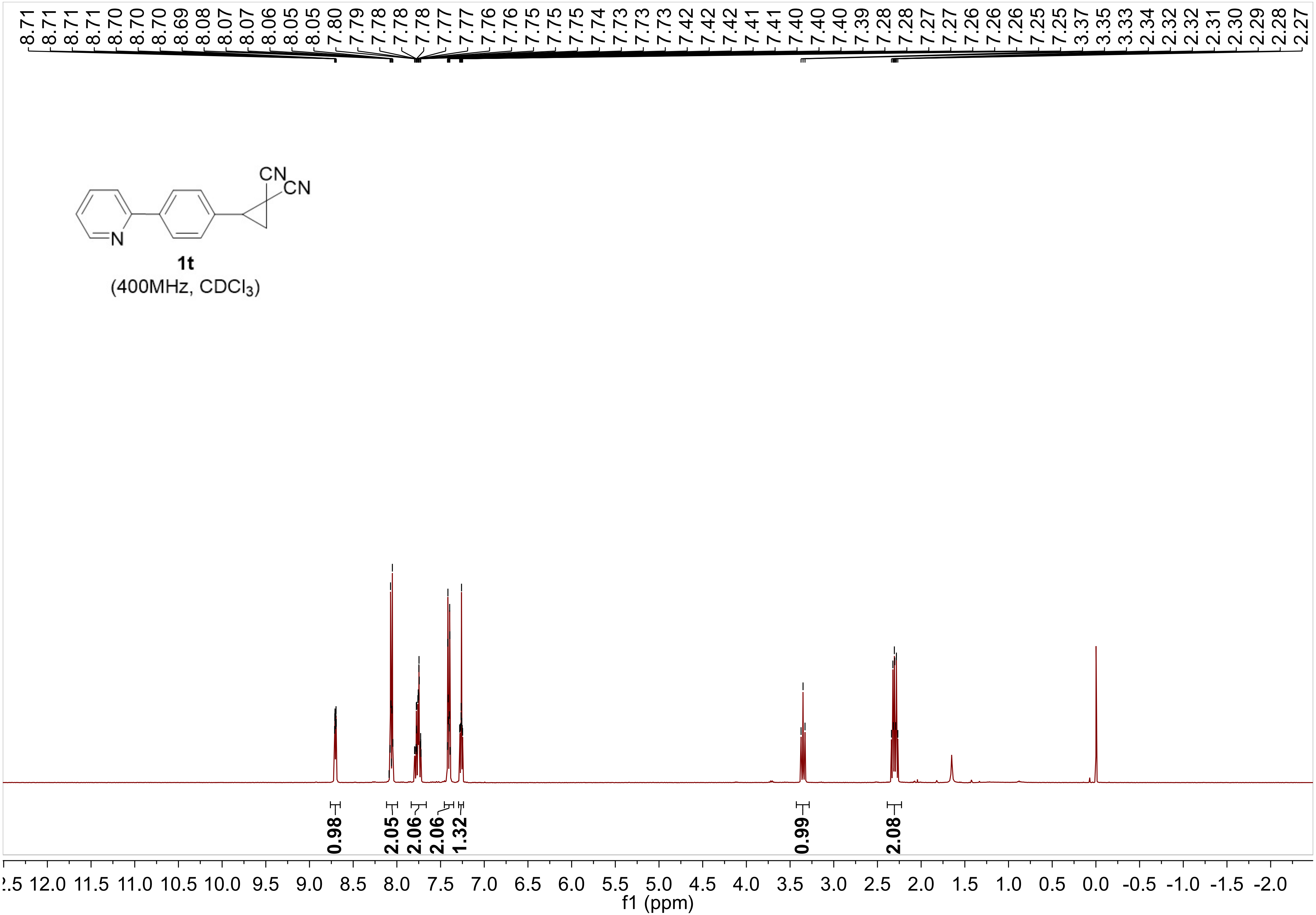
F3CO
CN
CN
1q
(565MHz, CDCl3)
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)



1q
(150MHz, $CDCl_3$)


7.67 7.65 7.36 7.35 7.35 7.35 7.33 7.33 7.32 7.32 7.31 7.30 7.30 7.29 7.11 7.10 7.10 7.10 7.09 7.08
3.32 3.31 3.29 2.30 2.29 2.28 2.27 2.27 2.26
CN
CN
S
1s
(600MHz, CDCl3)
1.99
3.96
0.96
1.01
2.09
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


143.32
135.94
129.72
129.18
128.54
126.75
125.99
124.24
115.57
113.32
35.29
22.72
7.66
CN
CN
S
1s
(150MHz, CDCl3)
f1 (ppm)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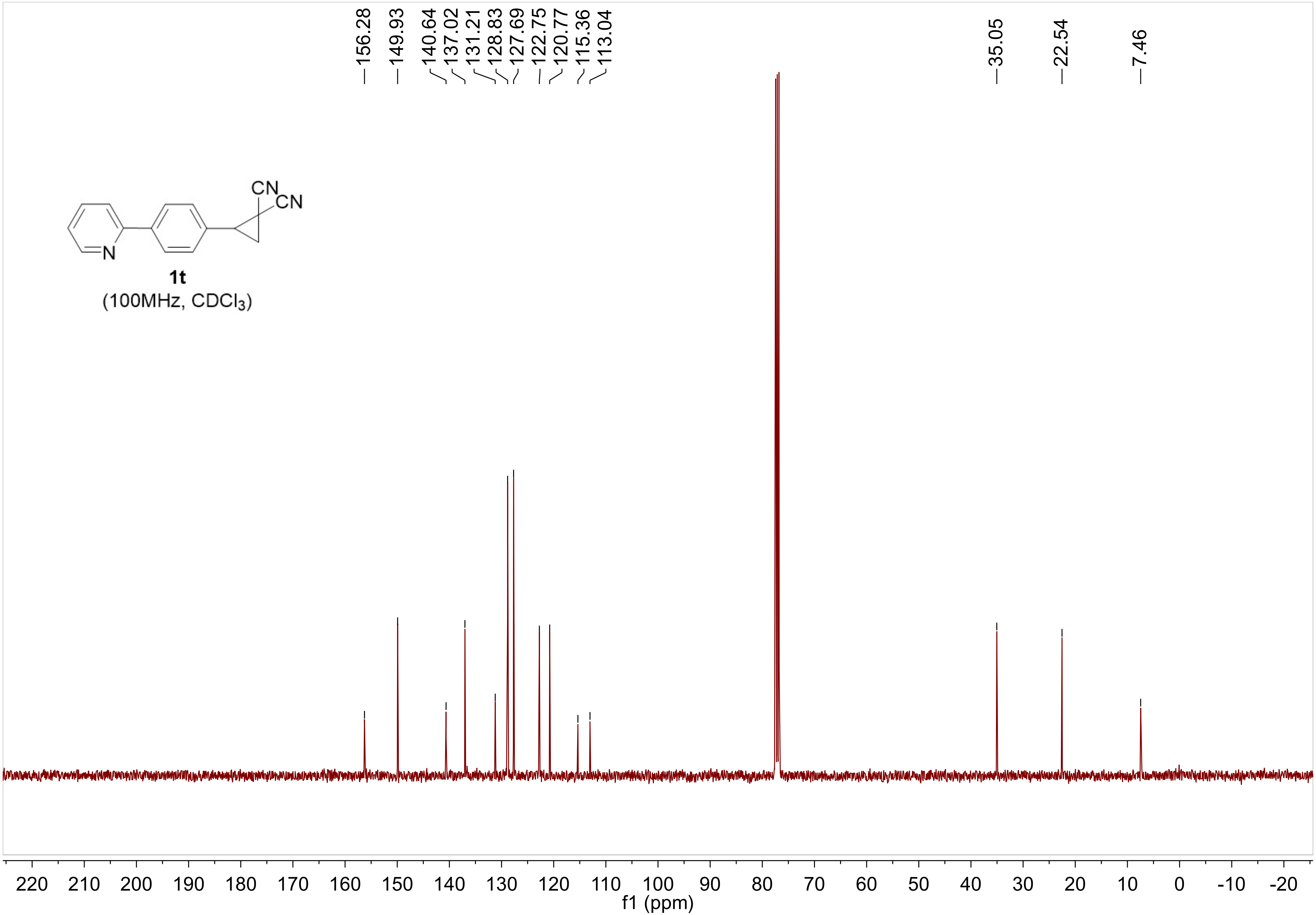
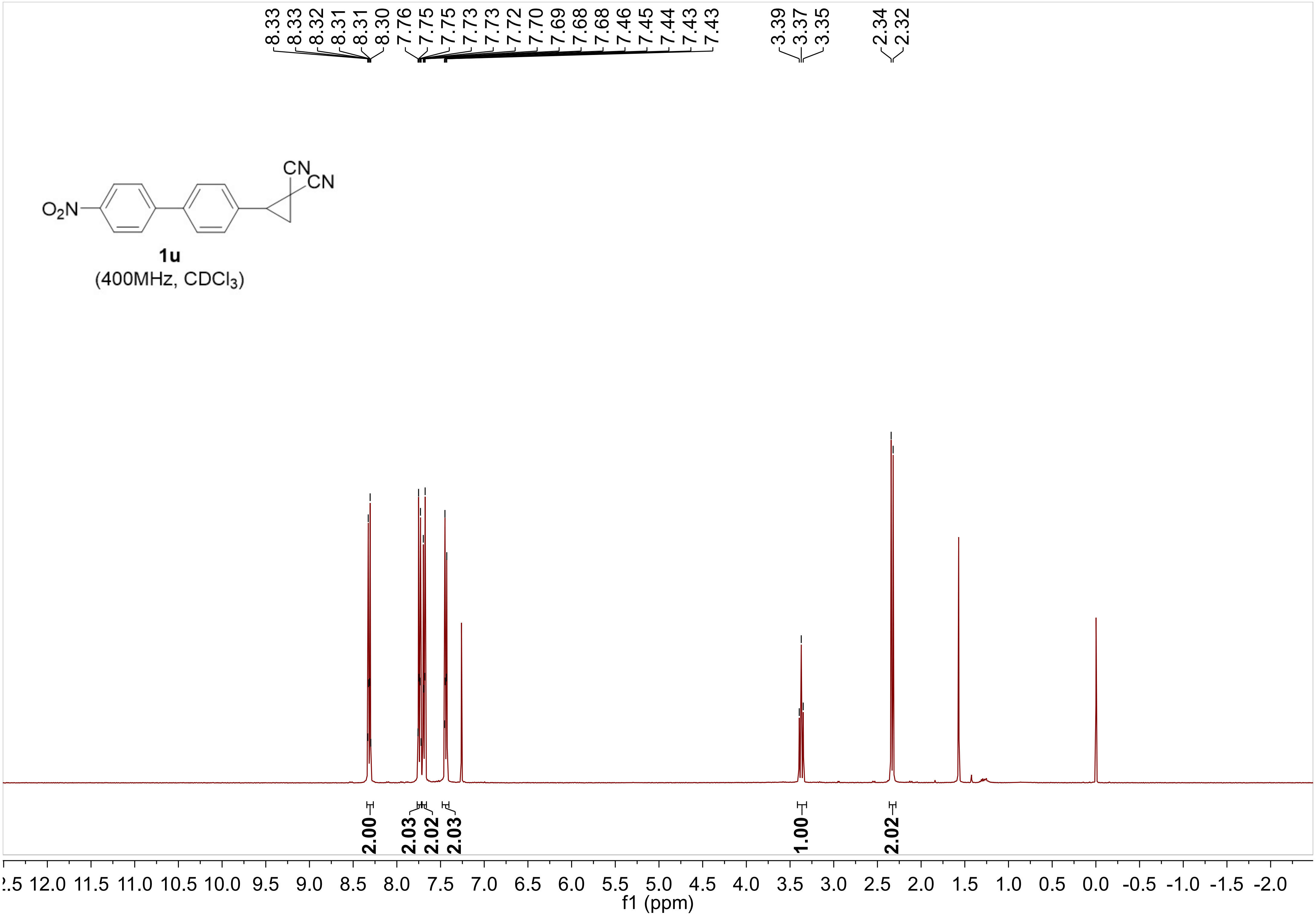
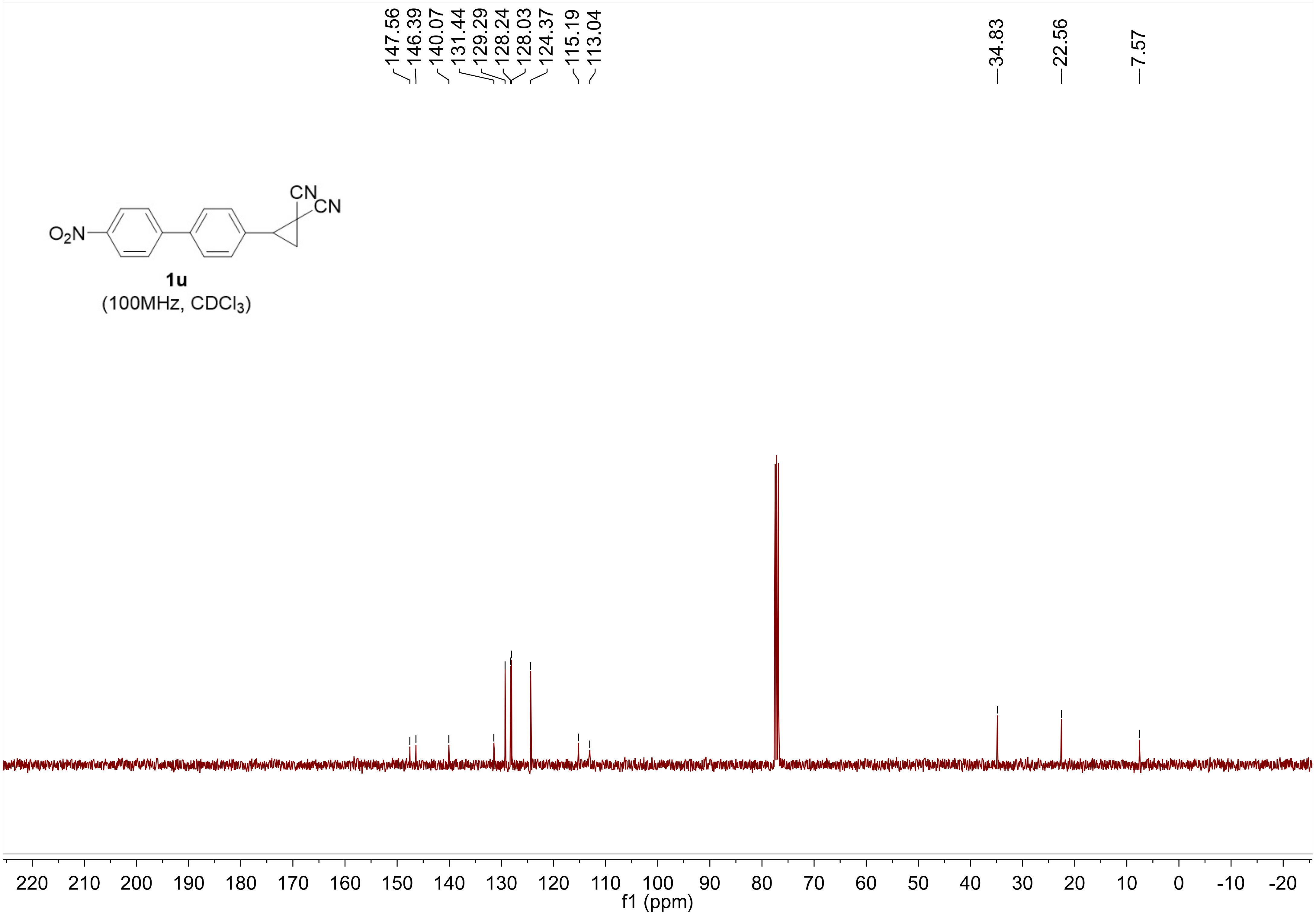
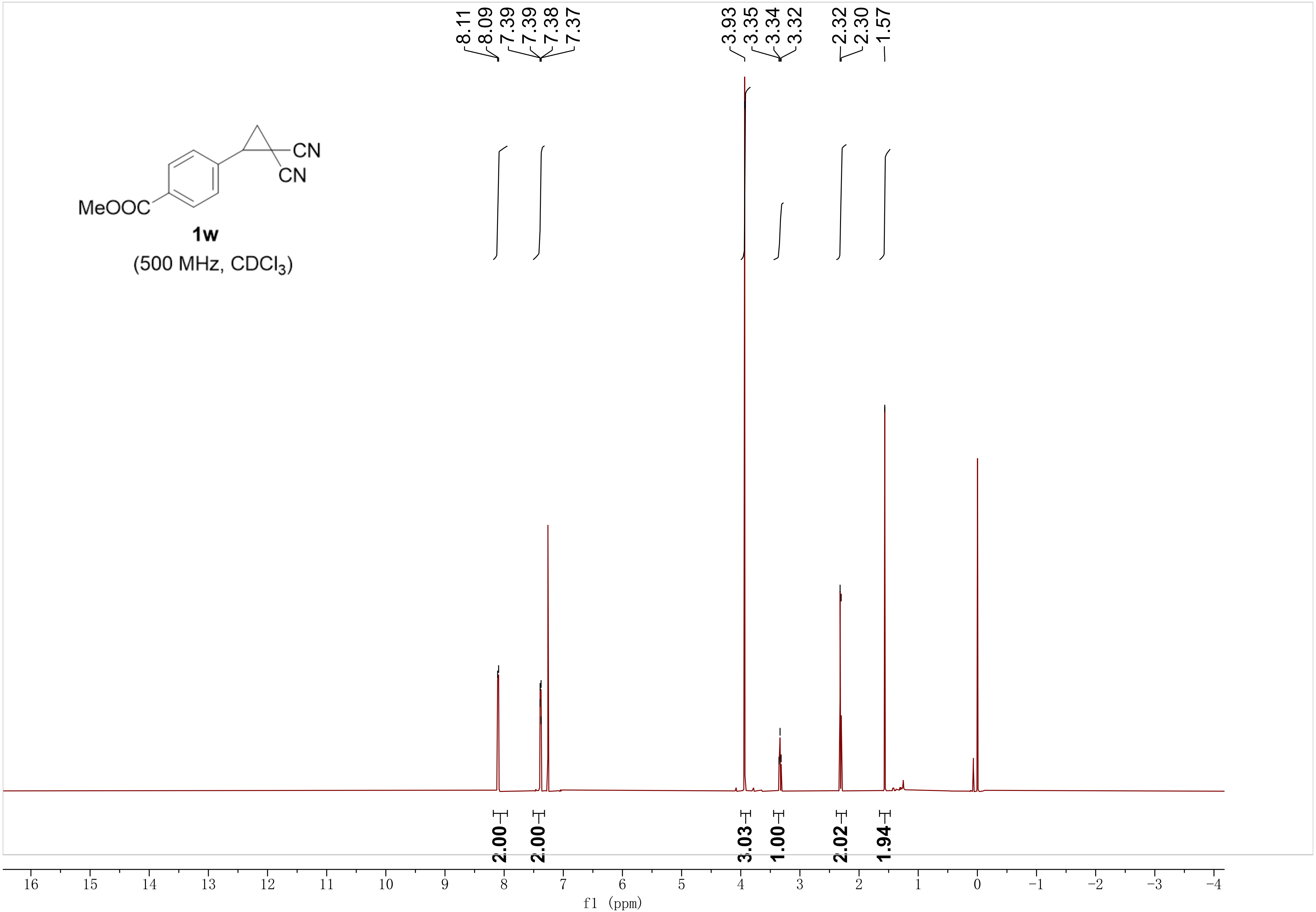
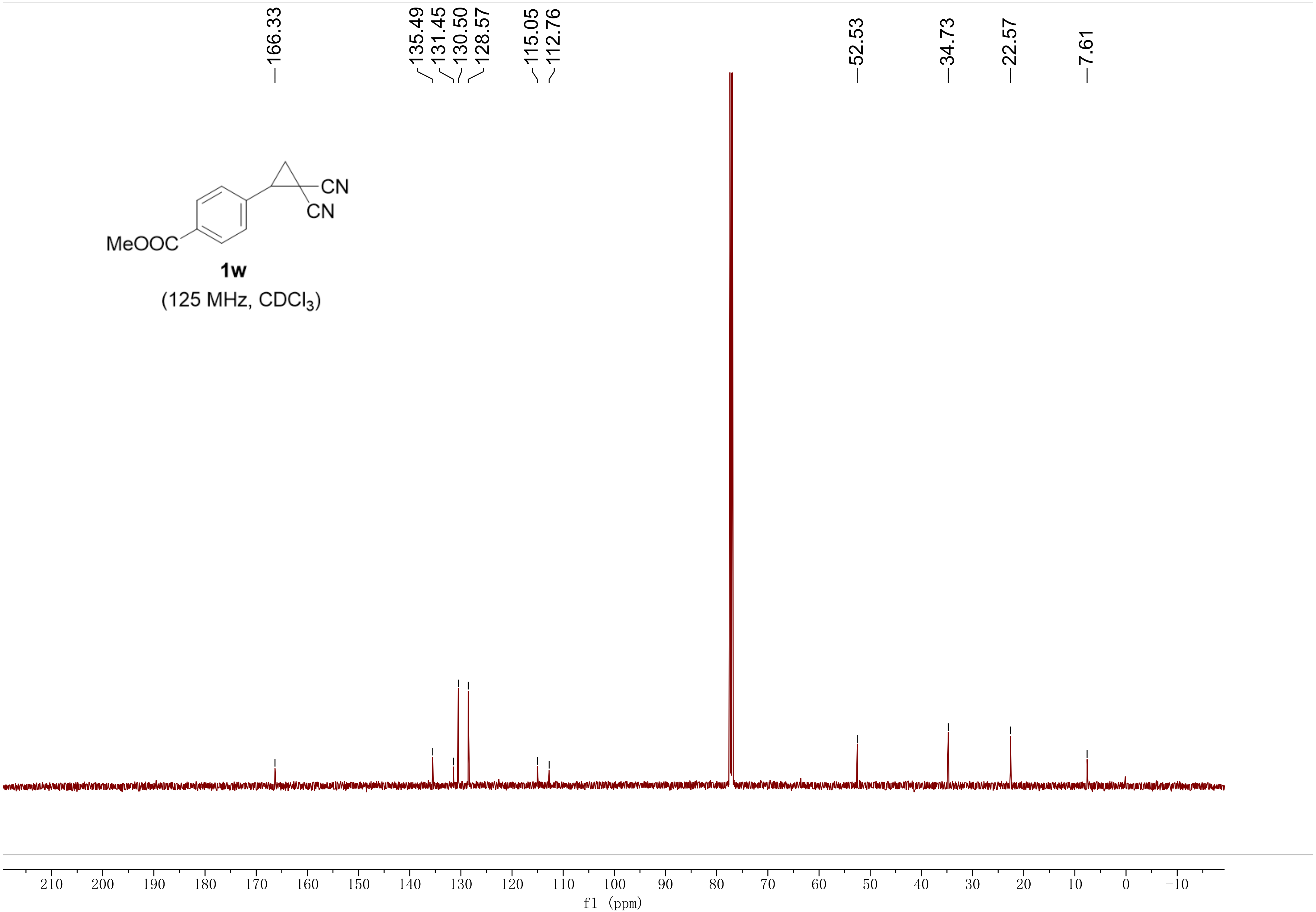
CN
CN
N
1t
(400MHz, CDCl3)
0.98
2.05
2.06
2.06
1.32
0.99
2.08
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

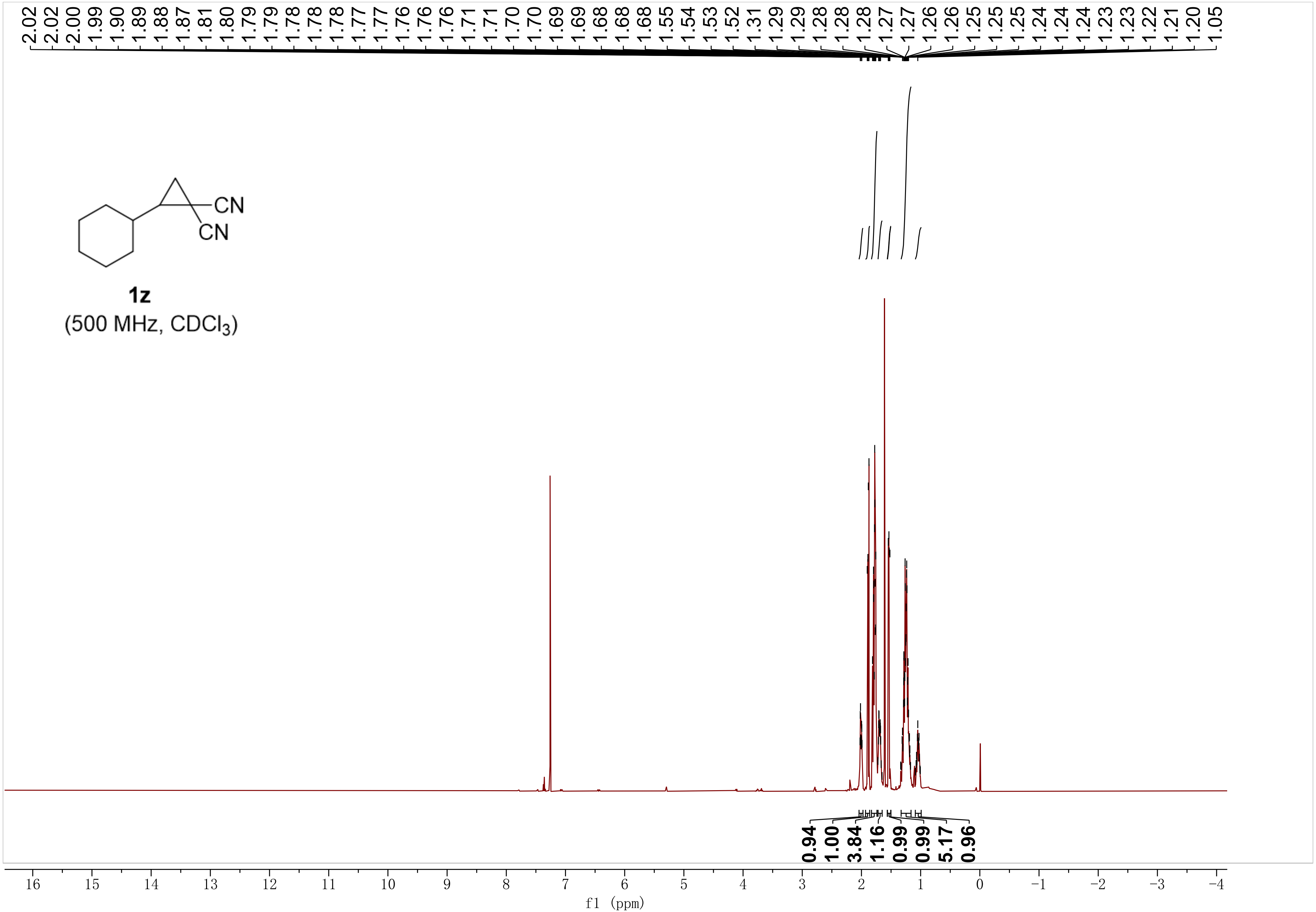

156.28
149.93
140.64
137.02
131.21
128.83
127.69
122.75
120.77
115.36
113.04
35.05
22.54
7.46
CN
CN
N
1t
(100MHz, CDCl3)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

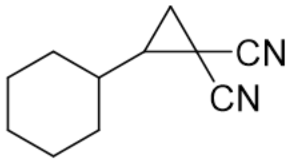

8.33 8.33 8.32 8.31 8.31 8.30 7.76 7.75 7.75 7.73 7.73 7.72 7.70 7.69 7.68 7.68 7.46 7.45 7.44 7.43 7.43
3.39 3.37 3.35
2.34 2.32
CN
CN
O2N
1u
(400MHz, CDCl3)
2.00
2.03
2.02
2.03
1.00
2.02
2.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)


147.56
146.39
140.07
131.44
129.29
128.24
128.03
124.37
115.19
113.04
34.83
22.56
7.57
CN
CN
O2N
1u
(100MHz, CDCl3)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


8.11
8.09
7.39
7.39
7.38
7.37
3.93
3.35
3.34
3.32
2.32
2.30
1.57
MeOOC
CN
CN
1w
(500 MHz, CDCl3)
2.00
2.00
3.03
1.00
2.02
1.94
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3 −4
f1 (ppm)

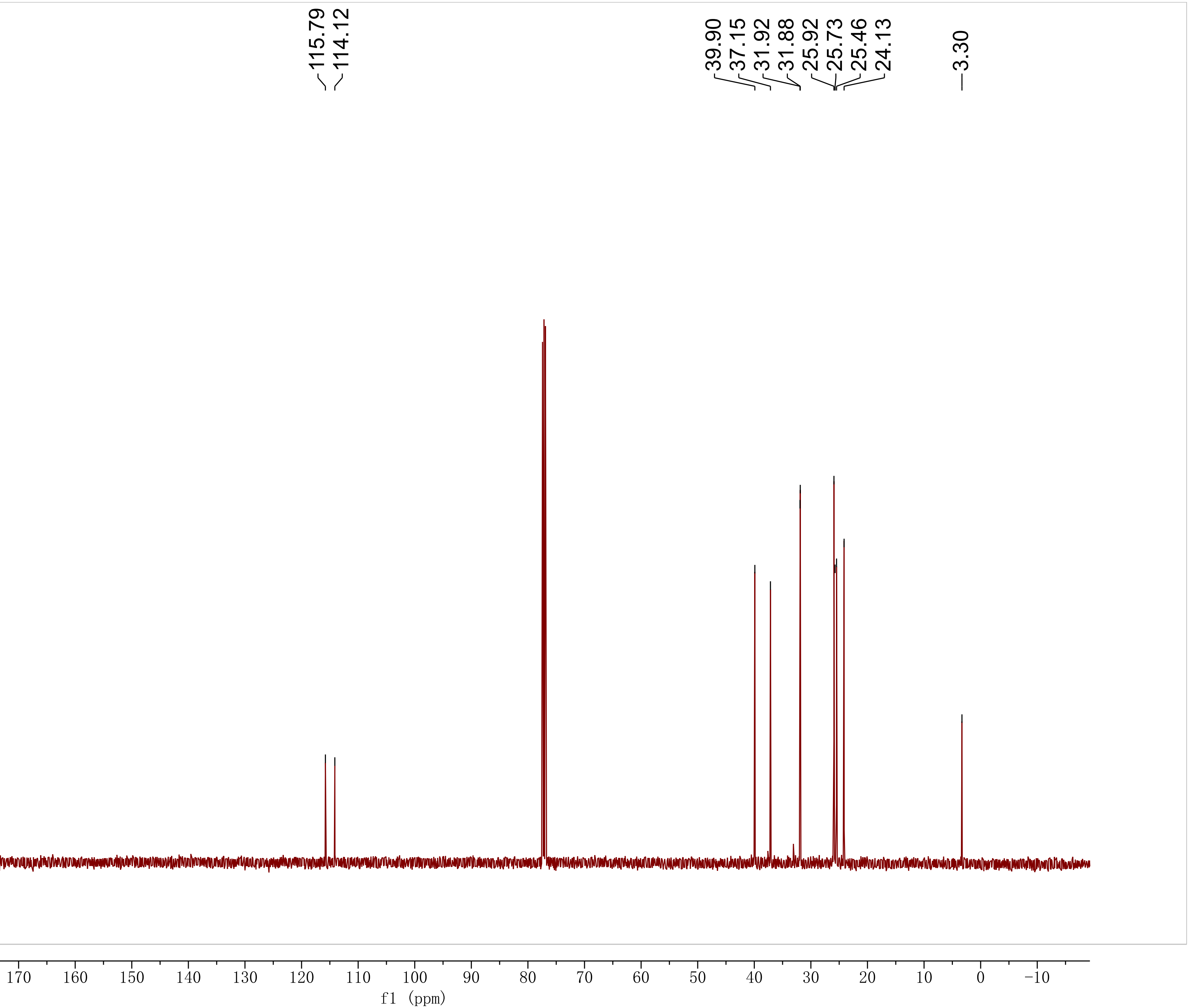

166.33
135.49
131.45
130.50
128.57
115.05
112.76
52.53
34.73
22.57
7.61
CN
CN
MeOOC
1w
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

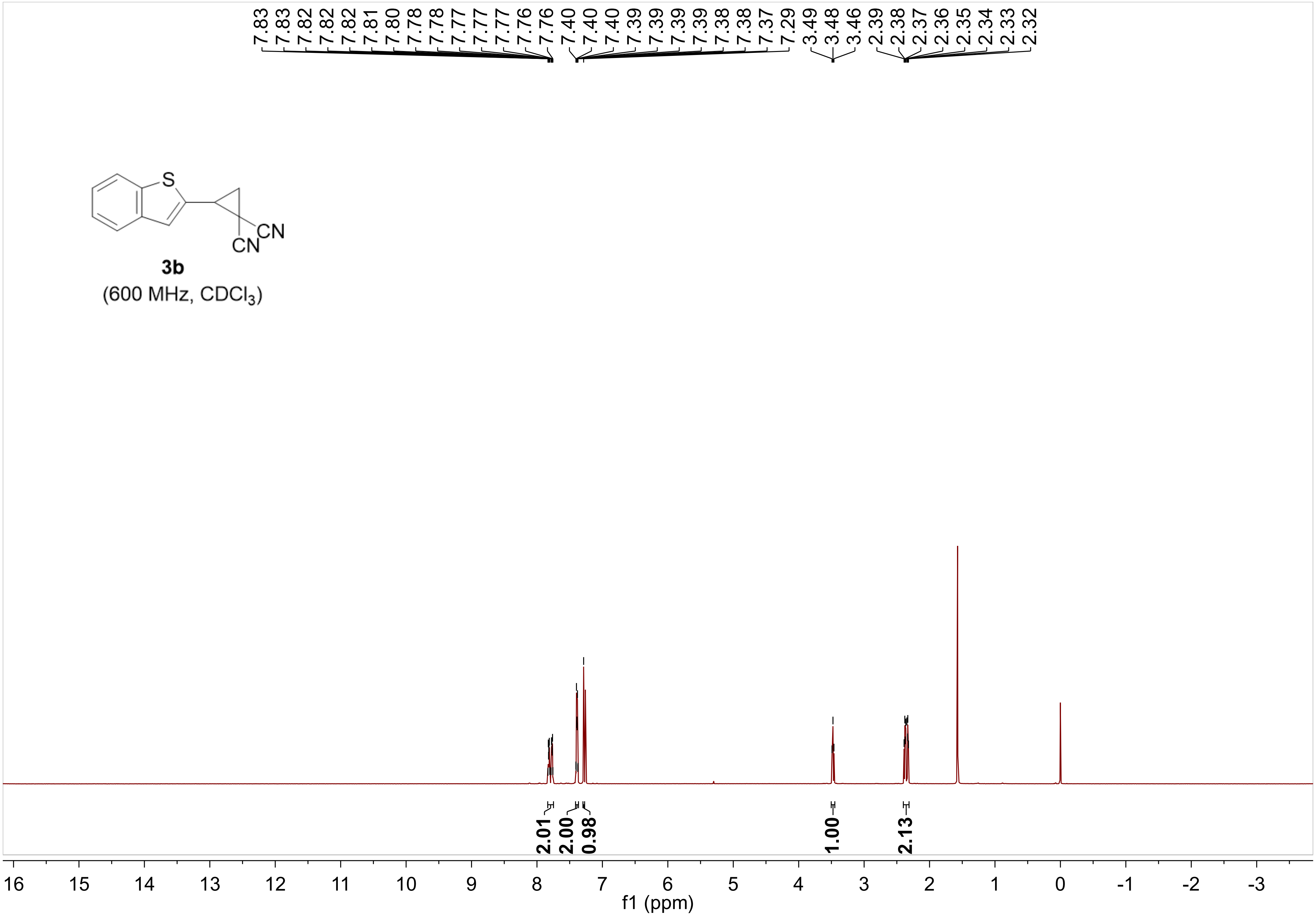

2.02 2.02 2.00 1.99 1.90 1.89 1.88 1.87 1.81 1.80 1.79 1.79 1.78 1.78 1.78 1.77 1.77 1.76 1.76 1.76 1.71 1.71 1.70 1.70 1.69 1.69 1.68 1.68 1.68 1.55 1.54 1.53 1.52 1.31 1.29 1.29 1.28 1.28 1.28 1.27 1.27 1.26 1.26 1.25 1.25 1.25 1.24 1.24 1.24 1.23 1.23 1.22 1.21 1.20 1.05
CN
CN
1z
(500 MHz, CDCl3)
0.94 1.00 3.84 1.16 0.99 0.99 5.17 0.96
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3 −4
f1 (ppm)

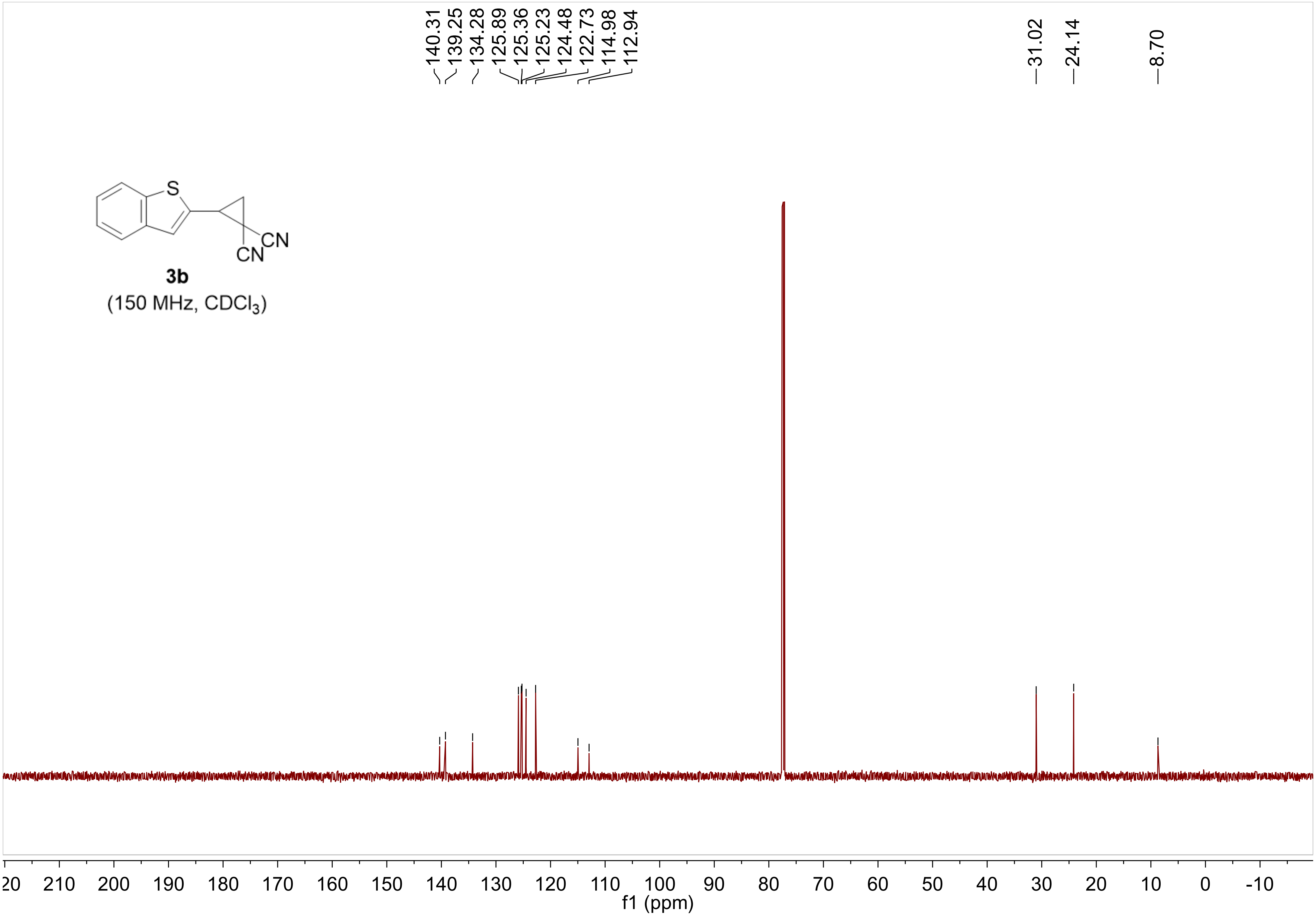


1z

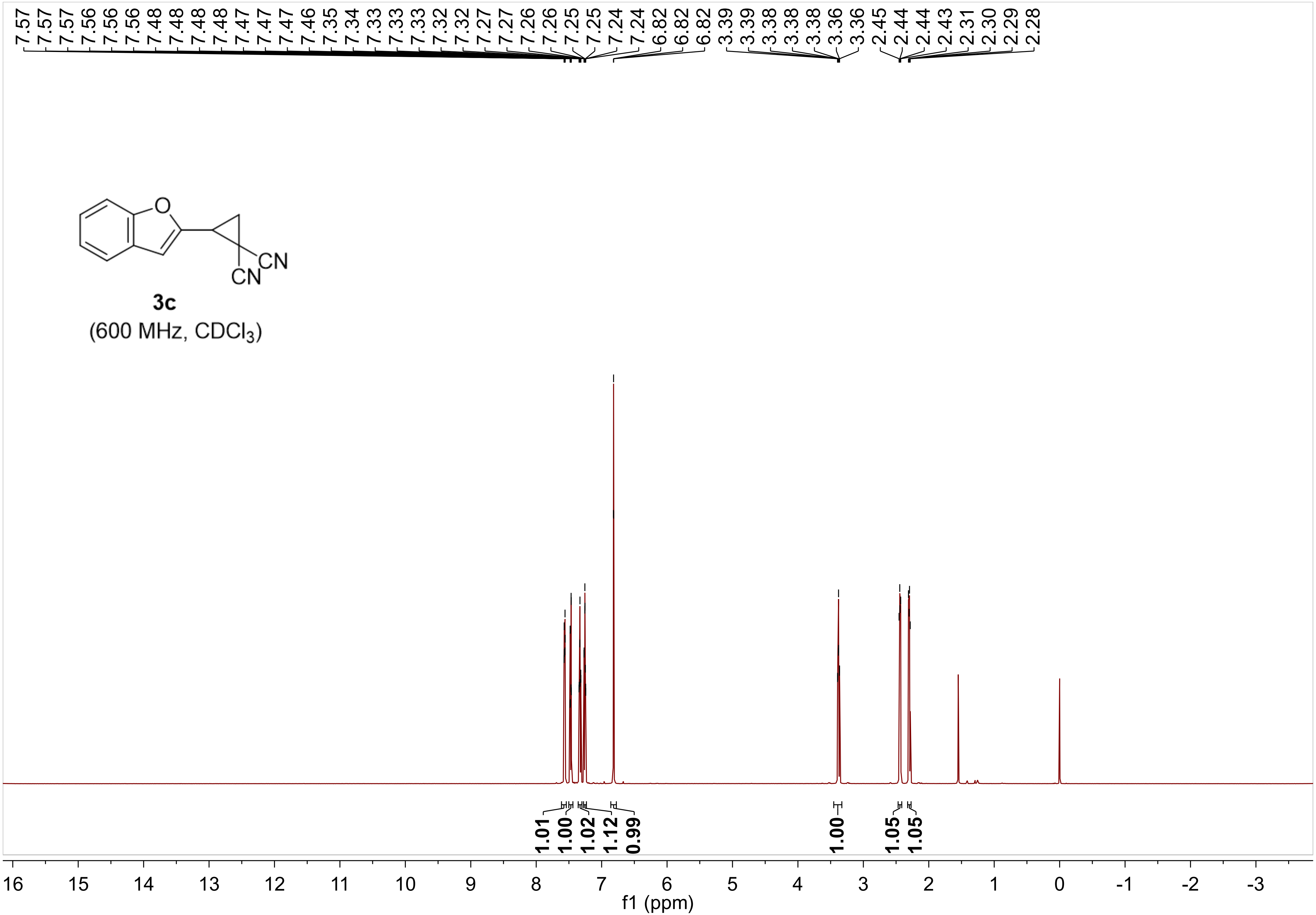
(125 MHz, $CDCl_3$)

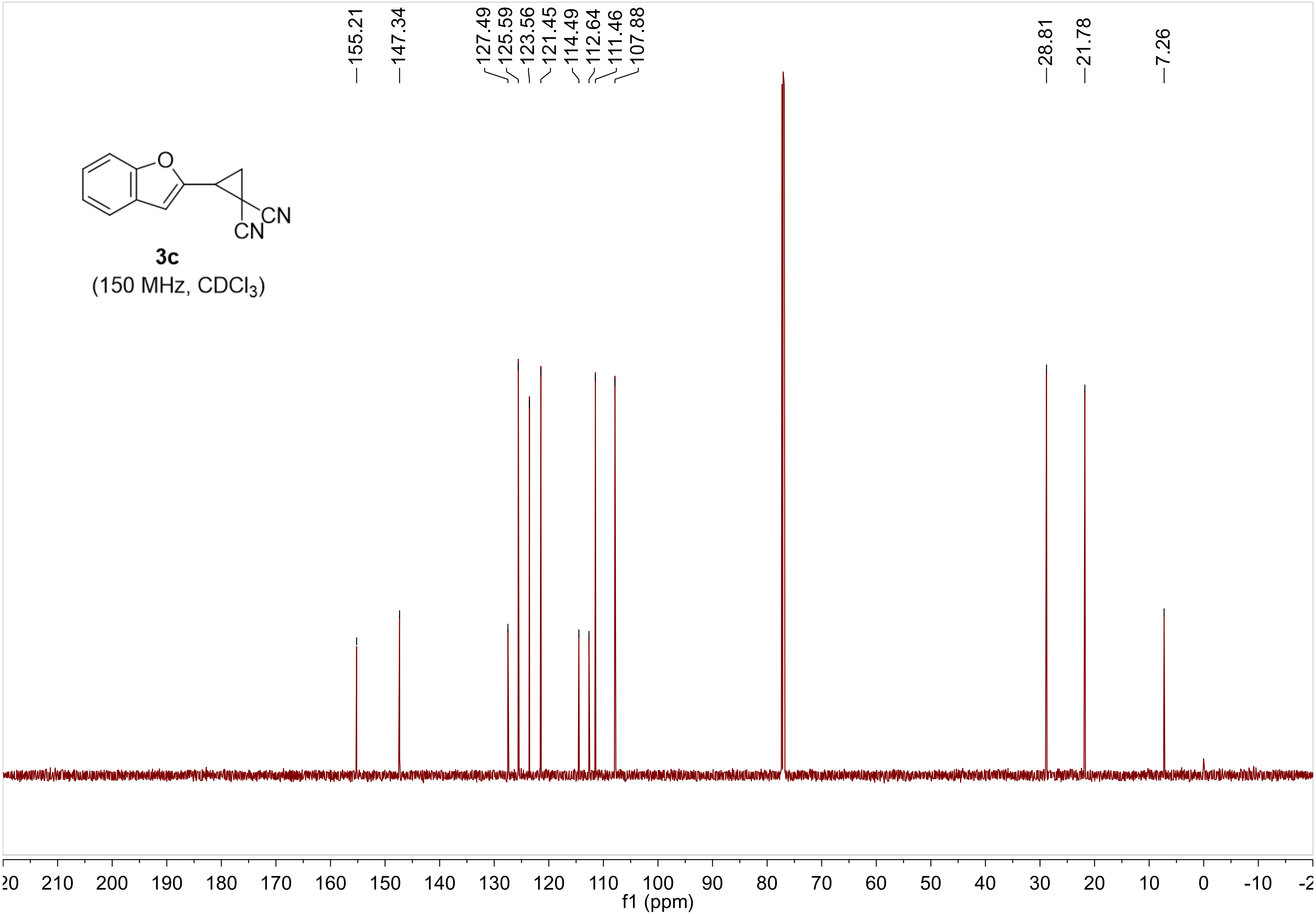


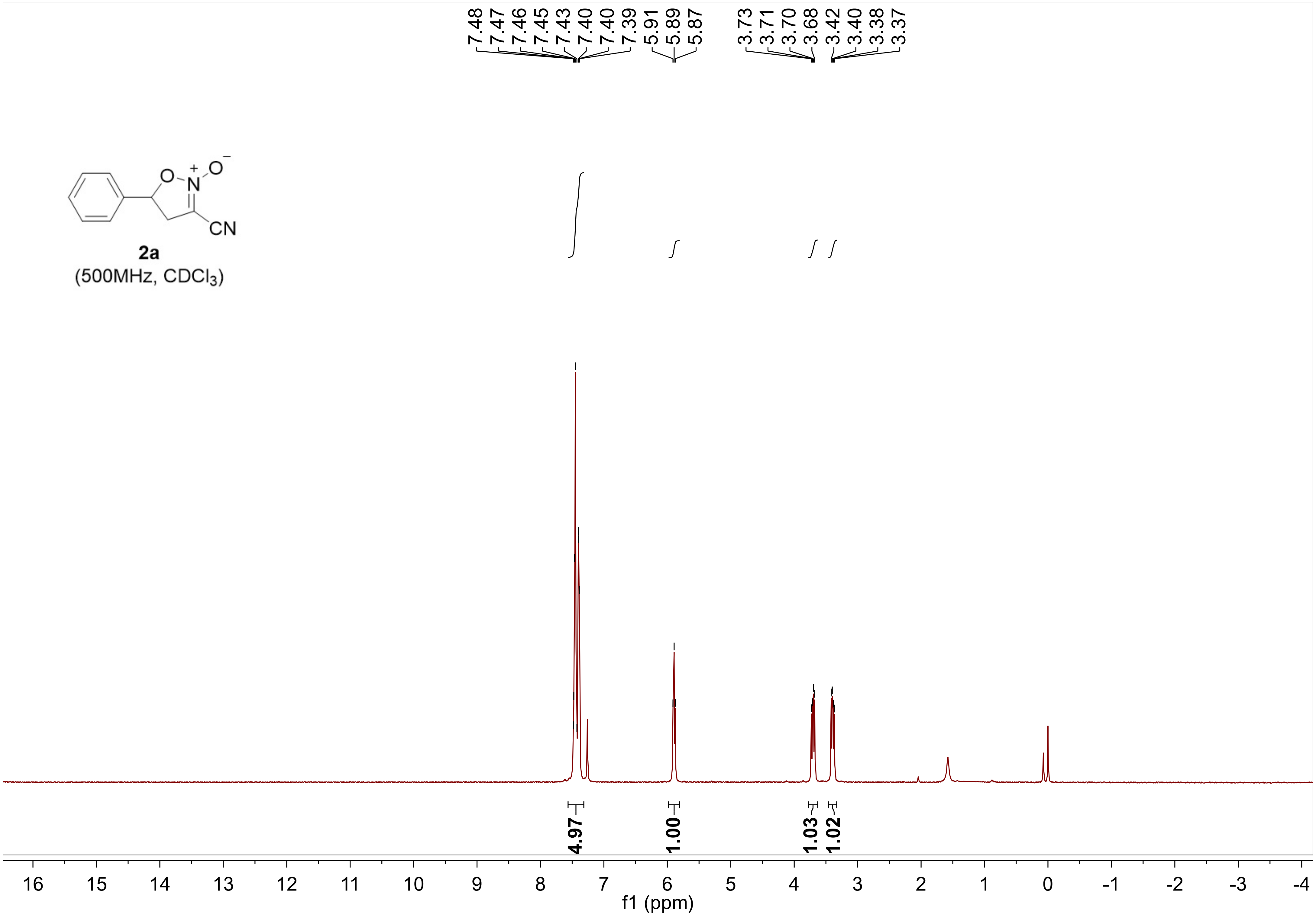

7.83 7.83 7.82 7.82 7.82 7.81 7.80 7.78 7.78 7.77 7.77 7.77 7.76 7.76 7.40 7.40 7.40 7.39 7.39 7.39 7.39 7.38 7.38 7.37 7.29 3.49 3.48 3.46 2.39 2.38 2.37 2.36 2.35 2.34 2.33 2.32
S
CN
CN
3b
(600 MHz, $CDCl_3$)
2.01
2.00
0.98
1.00
2.13
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

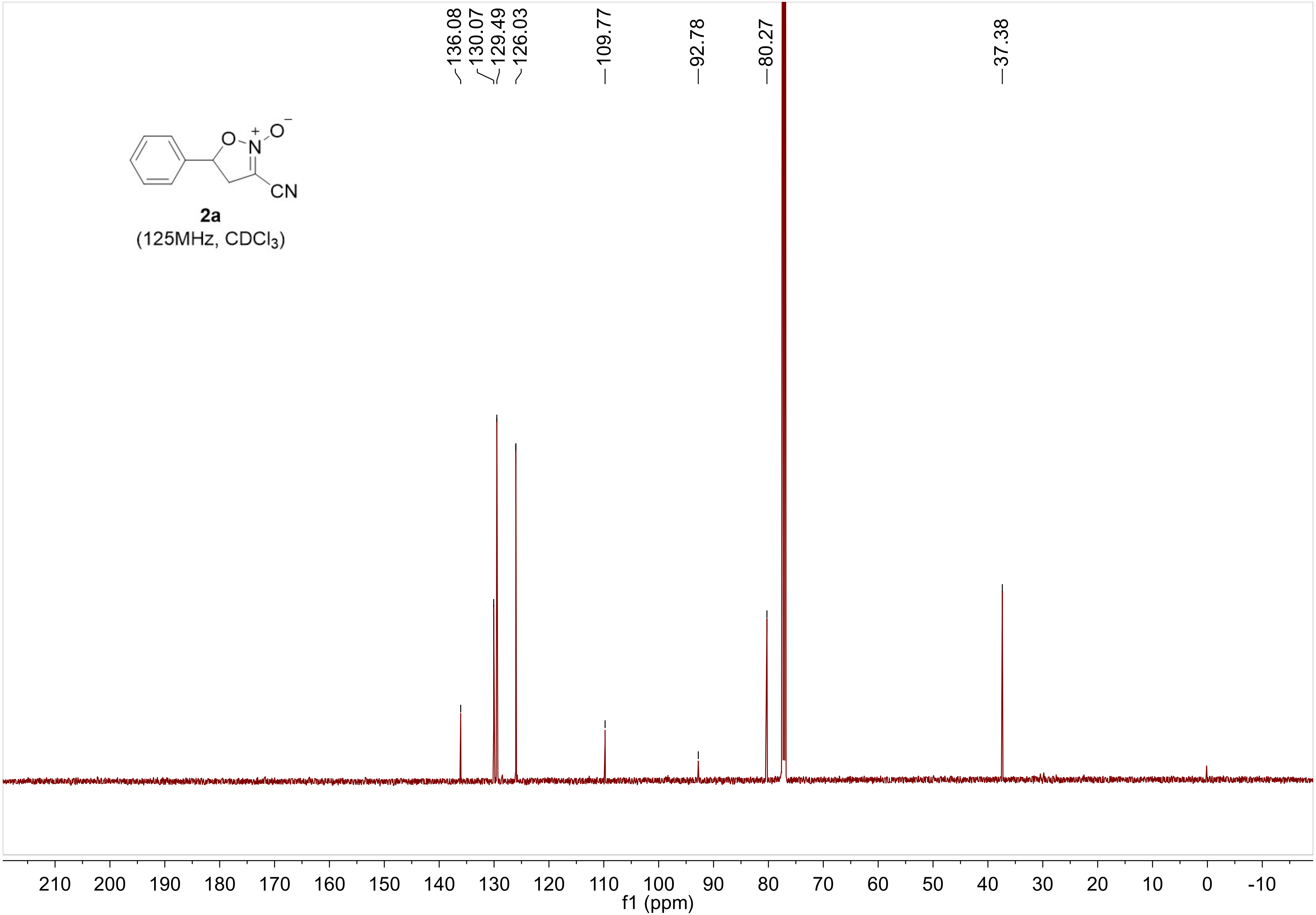


3b
(150 MHz, $CDCl_3$)

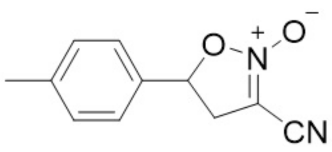

7.57 7.57 7.57 7.56 7.56 7.56 7.48 7.48 7.48 7.48 7.47 7.47 7.47 7.46 7.35 7.34 7.33 7.33 7.33 7.32 7.32 7.27 7.27 7.26 7.26 7.25 7.25 7.24 7.24 6.82 6.82 6.82 3.39 3.39 3.38 3.38 3.38 3.36 3.36 2.45 2.44 2.44 2.43 2.31 2.30 2.29 2.28
O
CN
CN
3c
(600 MHz, $CDCl_3$)
1.01 1.00 1.02 1.12 0.99
1.00
1.05 1.05
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


155.21
147.34
127.49
125.59
123.56
121.45
114.49
112.64
111.46
107.88
28.81
21.78
7.26
O
CN
CN
3c
(150 MHz, CDCl3)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

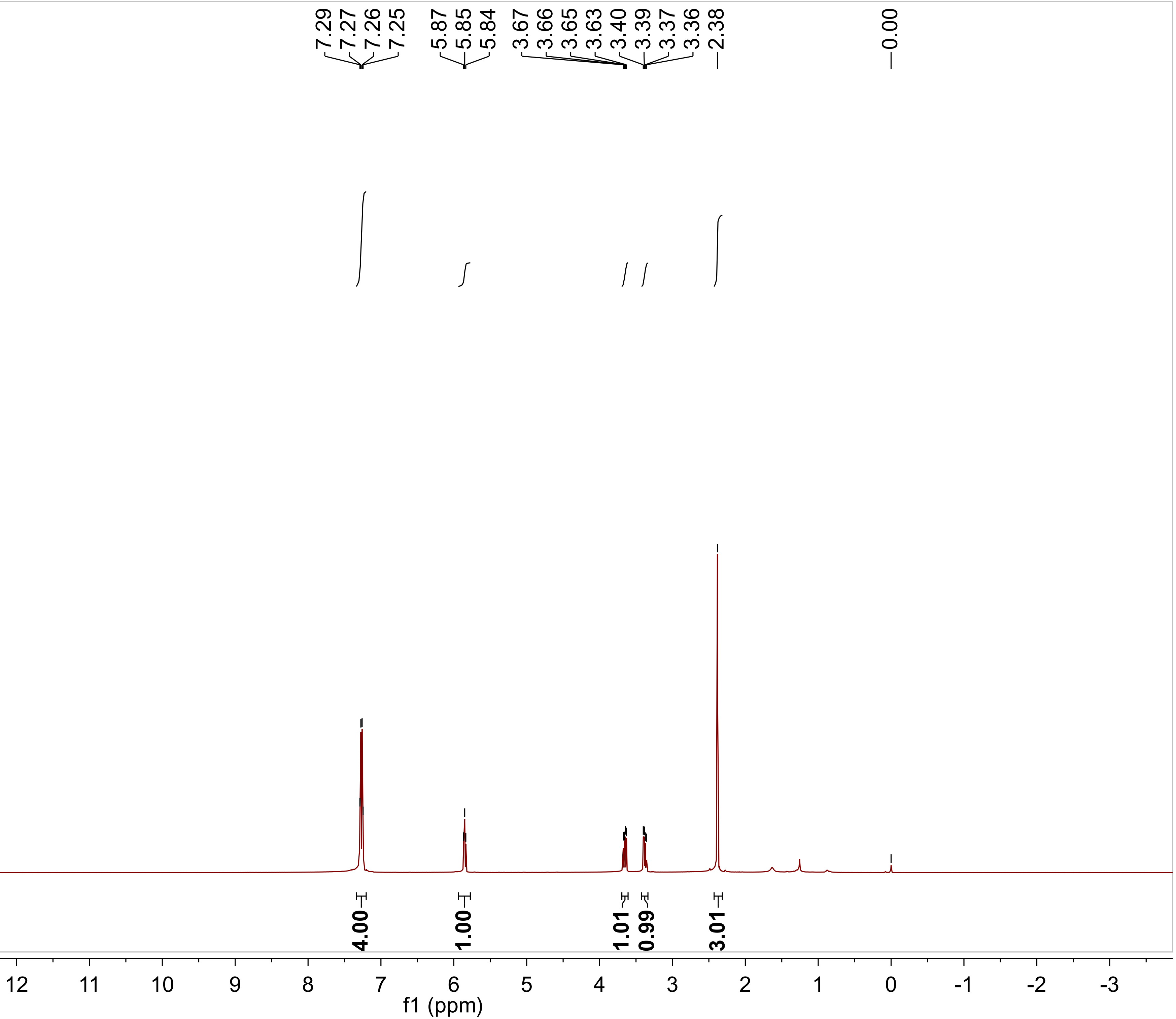

7.48
7.47
7.46
7.45
7.43
7.40
7.40
7.39
5.91
5.89
5.87
3.73
3.71
3.70
3.68
3.42
3.40
3.38
3.37
CN
2a
(500MHz, CDCl3)
4.97
1.00
1.03
1.02
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

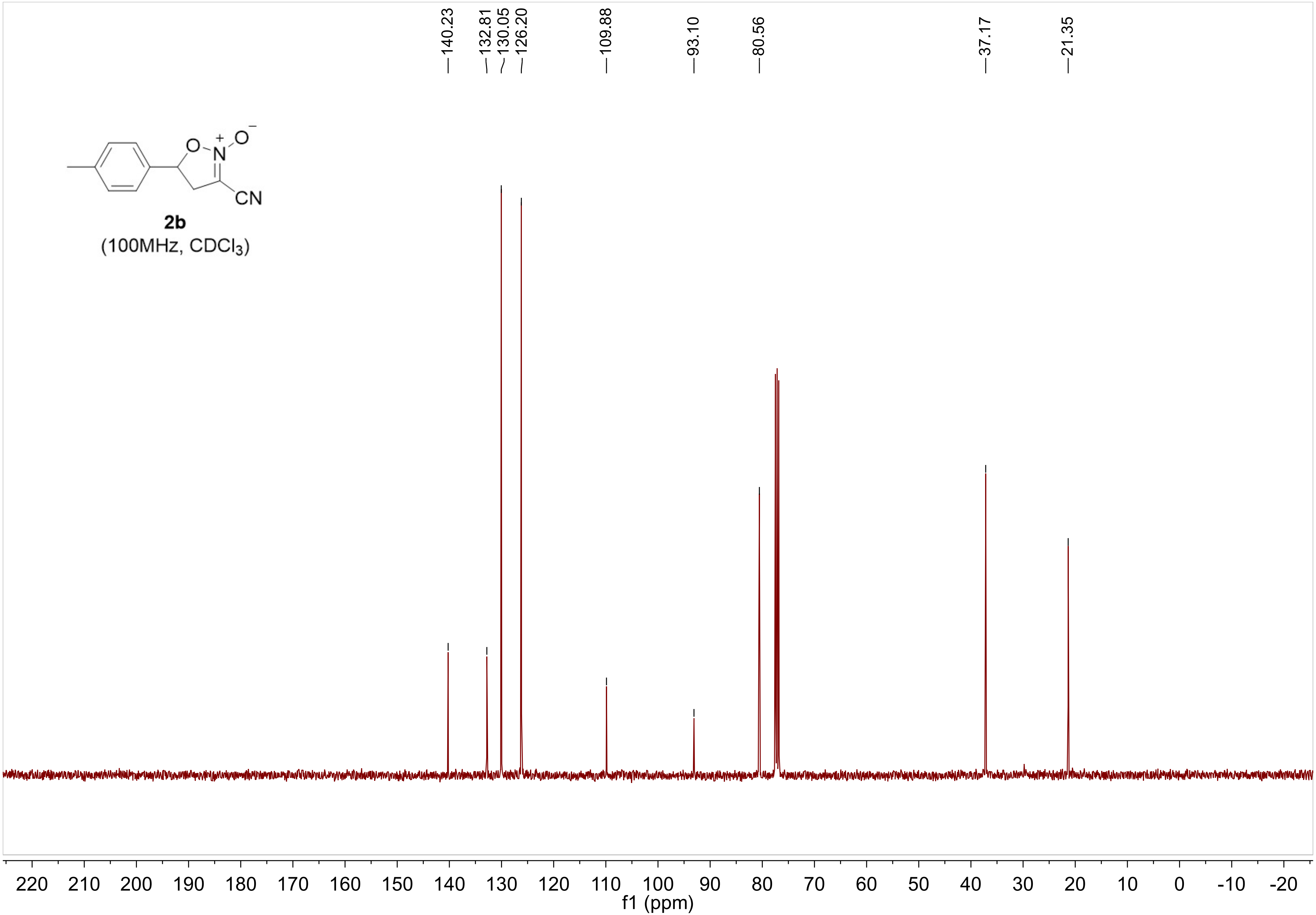


136.08
130.07
129.49
126.03
109.77
92.78
80.27
37.38
2a
(125MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

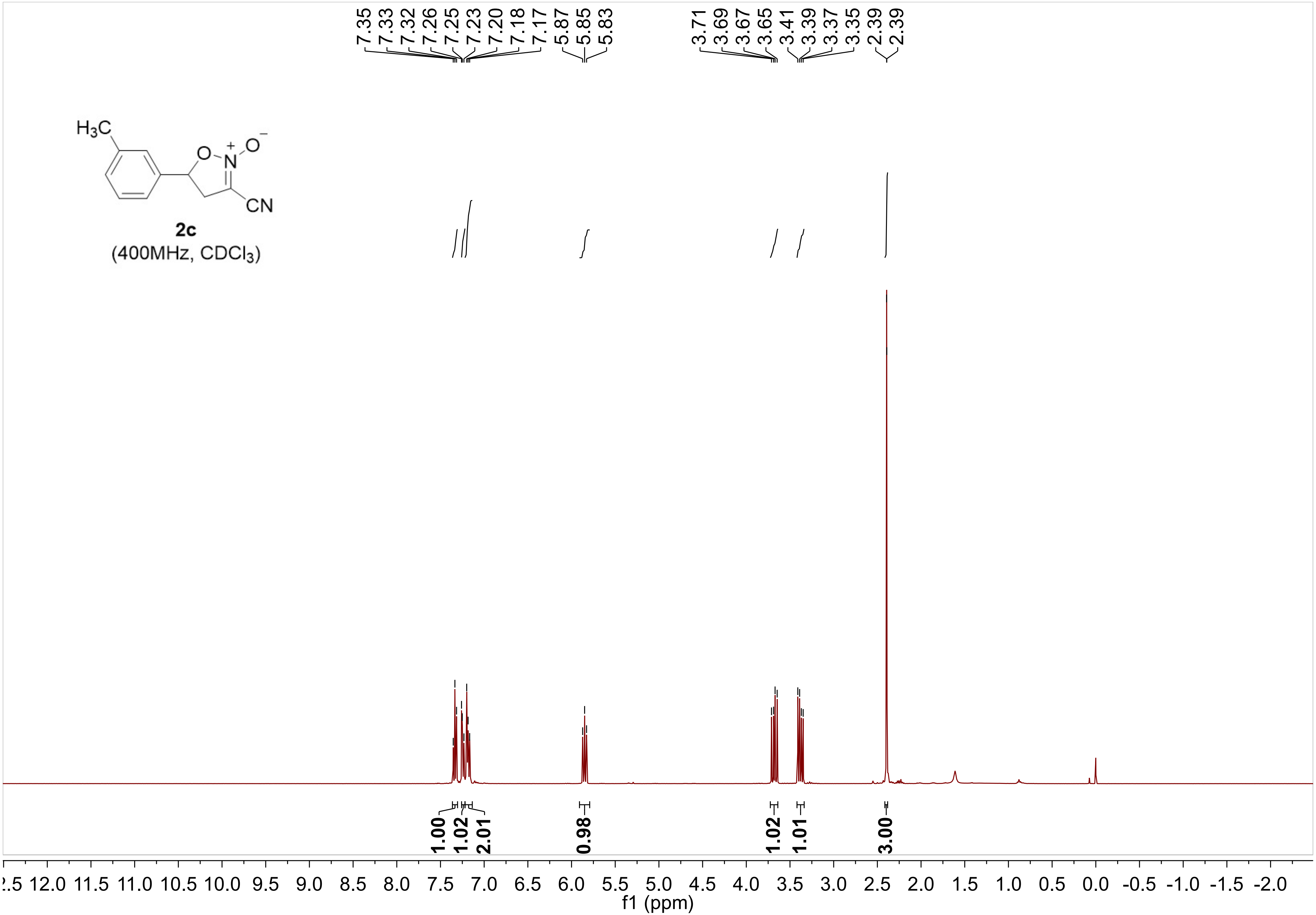


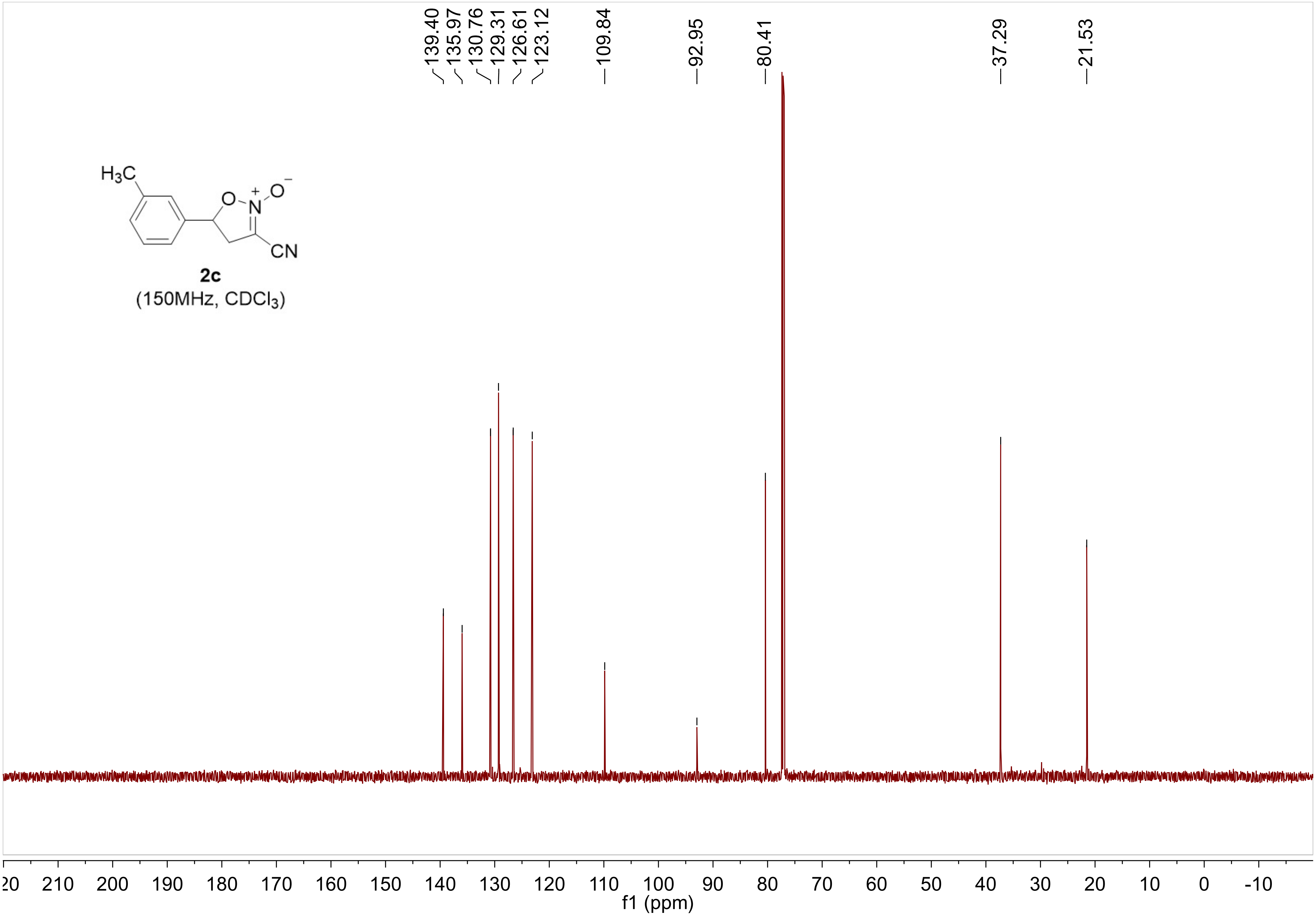
2b
(600MHz, $CDCl_3$)

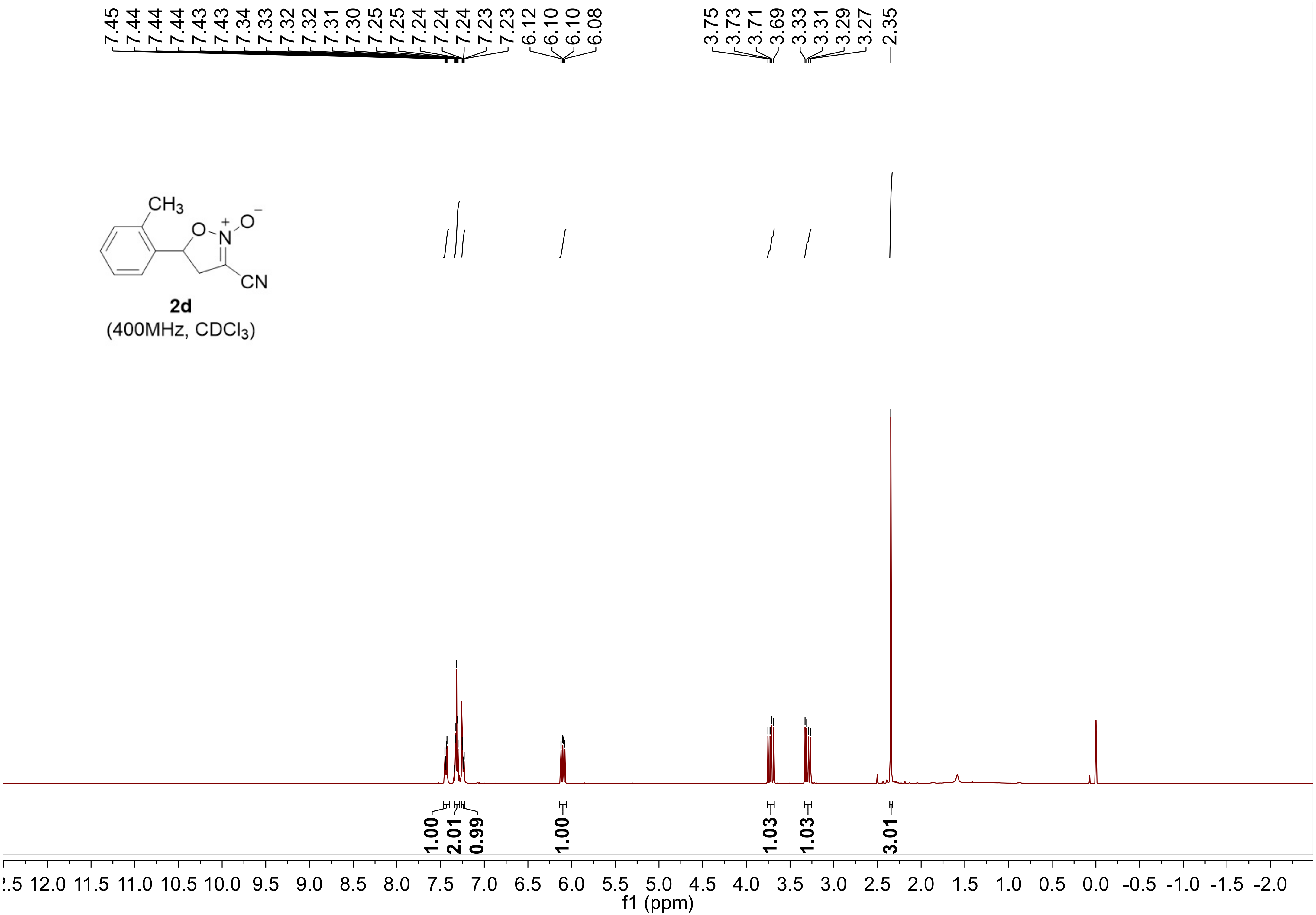


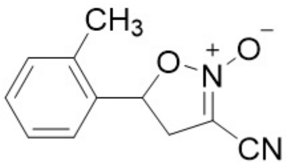


140.23
132.81
130.05
126.20
109.88
93.10
80.56
37.17
21.35
CN
2b
(100MHz, $CDCl_3$)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

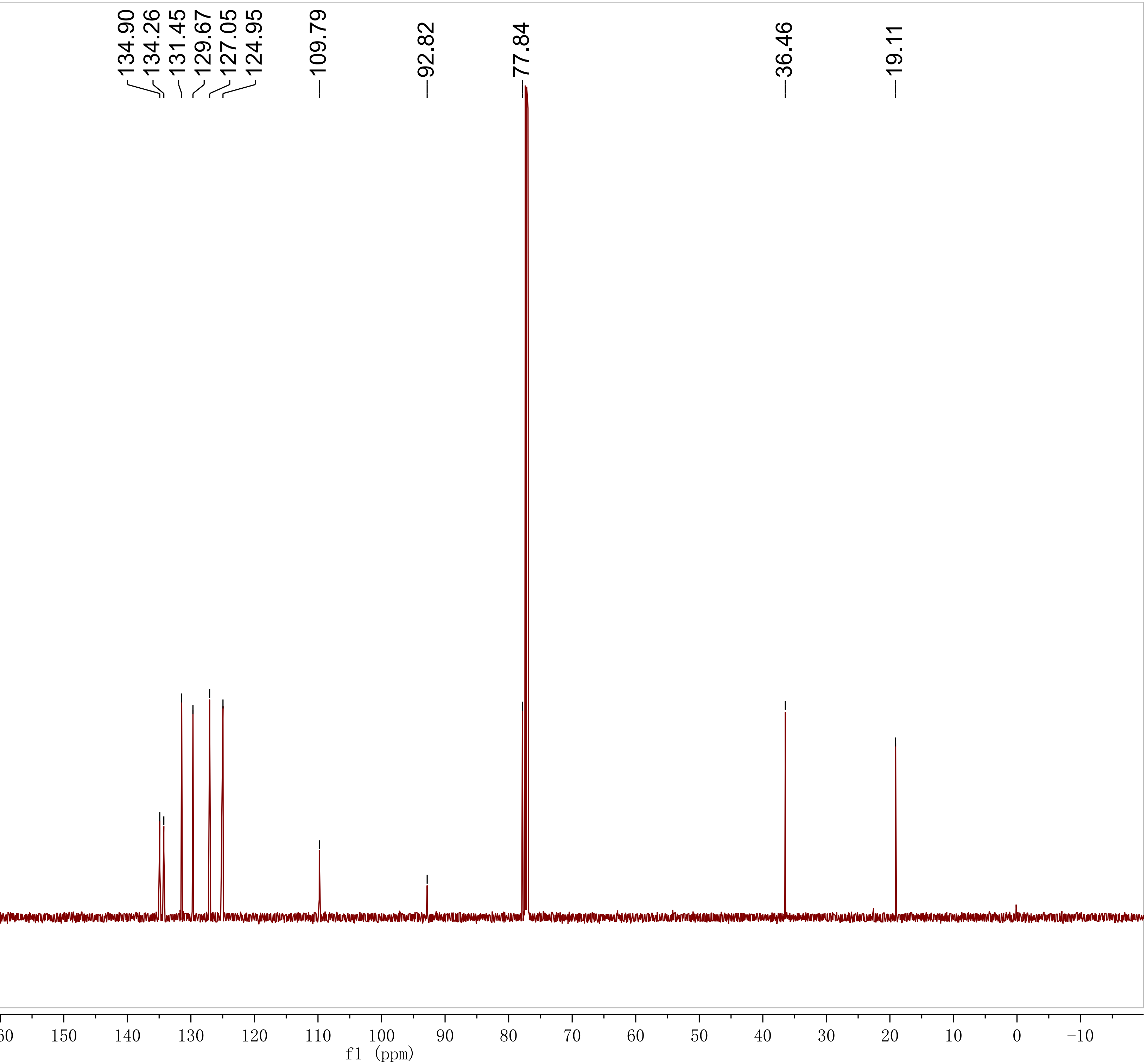

7.35 7.33 7.32 7.26 7.25 7.23 7.20 7.18 7.17 5.87 5.85 5.83 3.71 3.69 3.67 3.65 3.41 3.39 3.37 3.35 2.39 2.39
H_3C
O N + O −
CN
2c
(400MHz, $CDCl_3$)
1.00 1.02 2.01 0.98 1.02 1.01 3.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

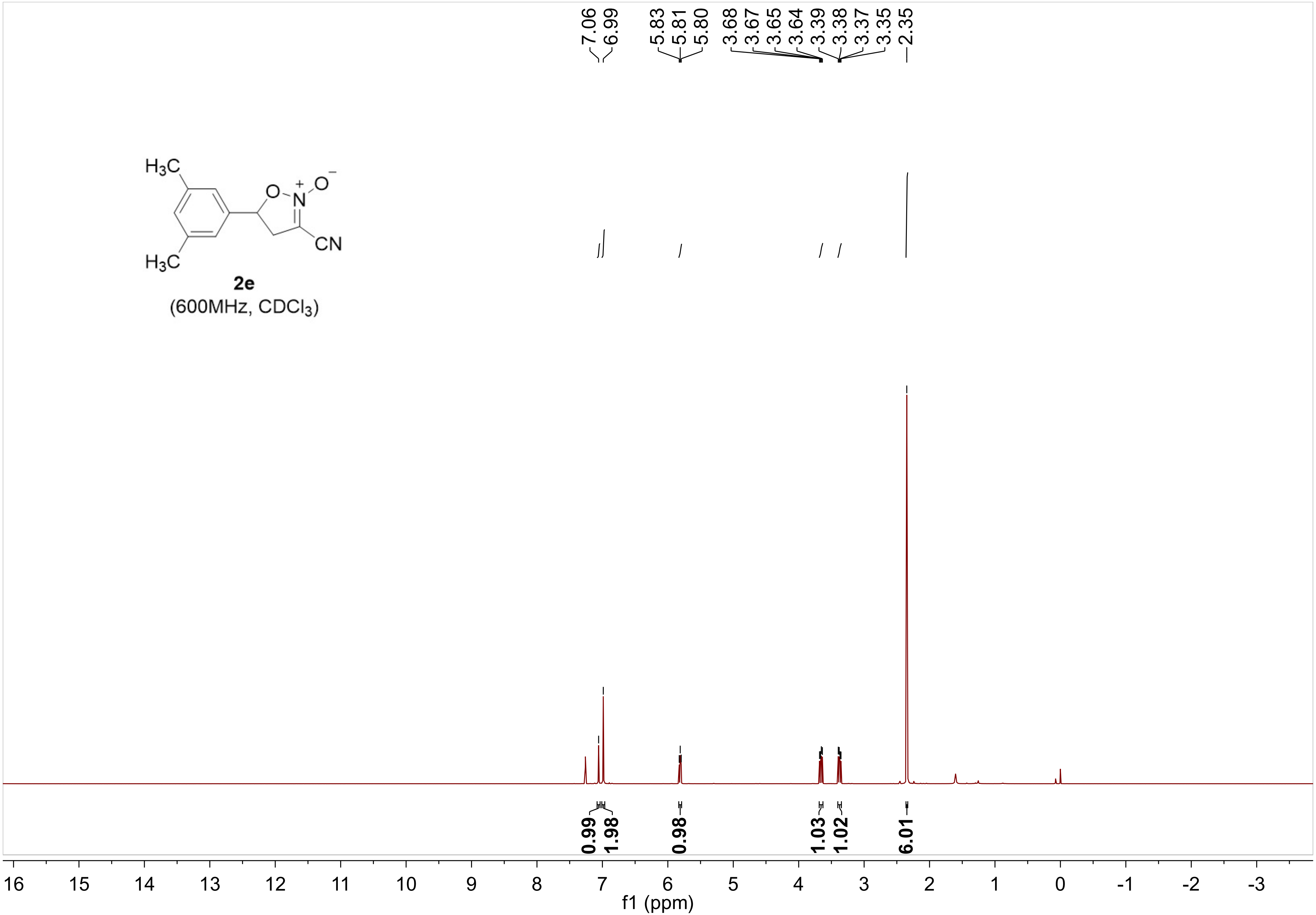

139.40
135.97
130.76
129.31
126.61
123.12
109.84
92.95
80.41
37.29
21.53
H3C
O
N
O
CN
2c
(150MHz, CDCl3)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

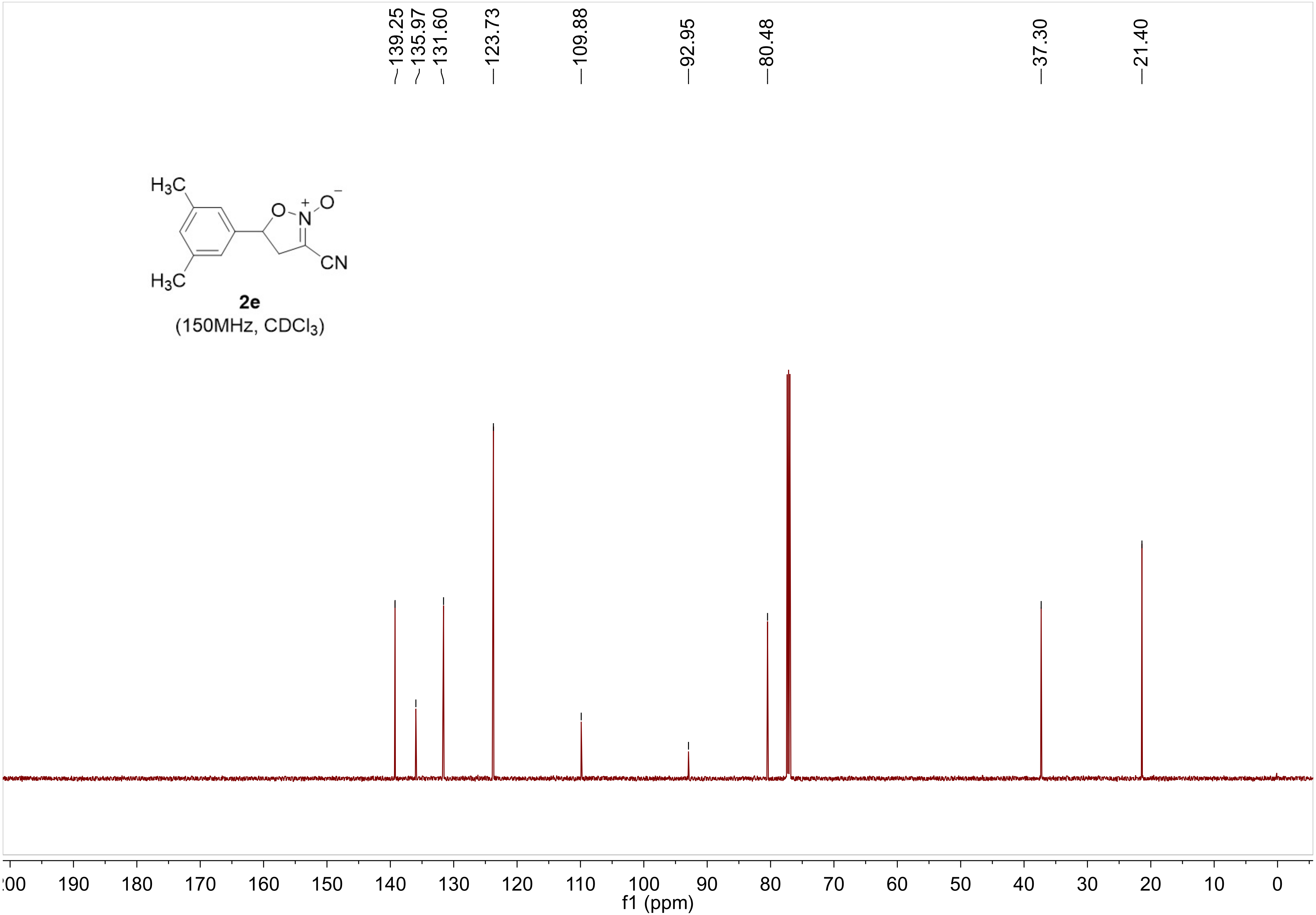

7.45
7.44
7.44
7.44
7.43
7.43
7.34
7.33
7.32
7.32
7.31
7.30
7.25
7.25
7.24
7.24
7.24
7.23
7.23
6.12
6.10
6.10
6.08
3.75
3.73
3.71
3.69
3.33
3.31
3.29
3.27
2.35
CH3
O
N
+
O
−
CN
2d
(400MHz, CDCl3)
1.00
2.01
0.99
1.00
1.03
1.03
3.01
f1 (ppm)

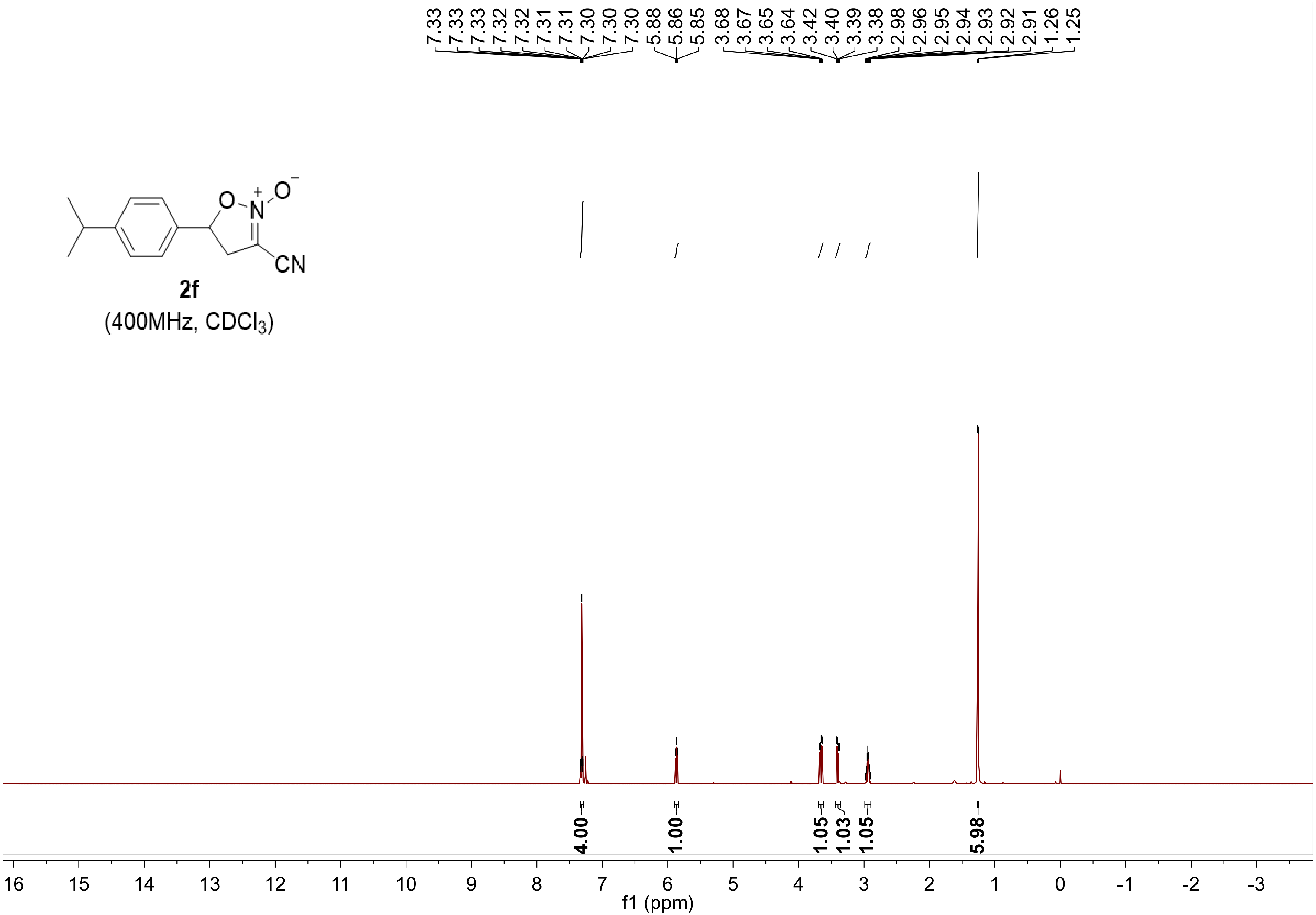


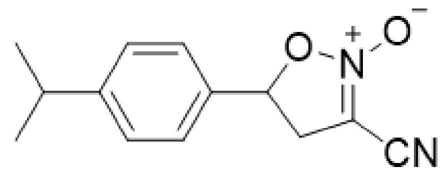
2d
(150MHz, $CDCl_3$)




7.06
6.99
5.83
5.81
5.80
3.68
3.67
3.65
3.64
3.39
3.38
3.37
3.35
2.35
H3C
O
N
O
CN
H3C
2e
(600MHz, CDCl3)
0.99
1.98
0.98
1.03
1.02
6.01
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

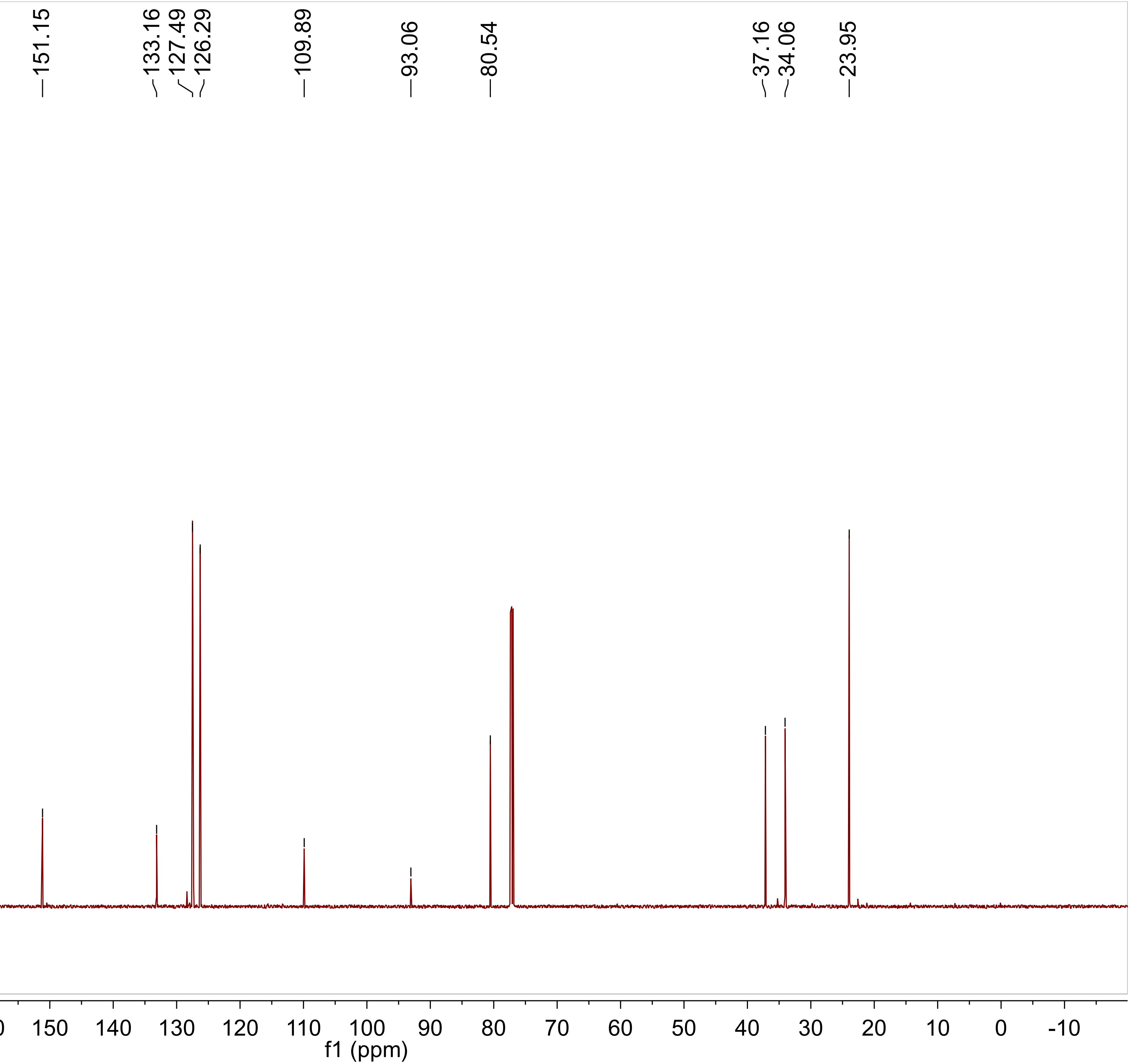

139.25
135.97
131.60
123.73
109.88
92.95
80.48
37.30
21.40
H3C
H3C
O
N
O
CN
2e
(150MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

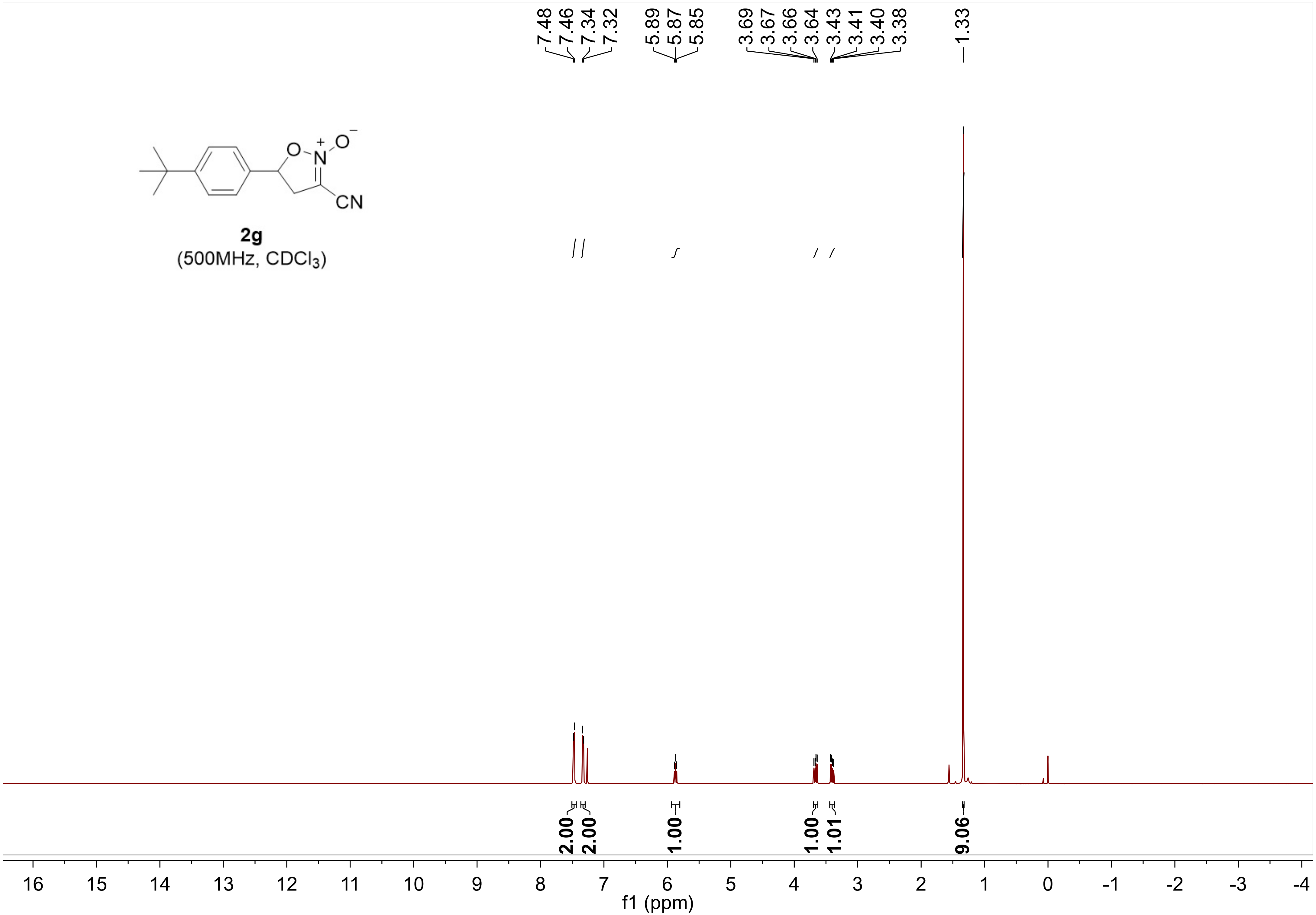

7.33 7.33 7.33 7.32 7.32 7.31 7.31 7.30 7.30 7.30 5.88 5.86 5.85 3.68 3.67 3.65 3.64 3.42 3.40 3.39 3.38 2.98 2.96 2.95 2.94 2.93 2.92 2.91 1.26 1.25
2f
(400MHz, $CDCl_3$)
4.00
1.00
1.05
1.03
1.05
5.98
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

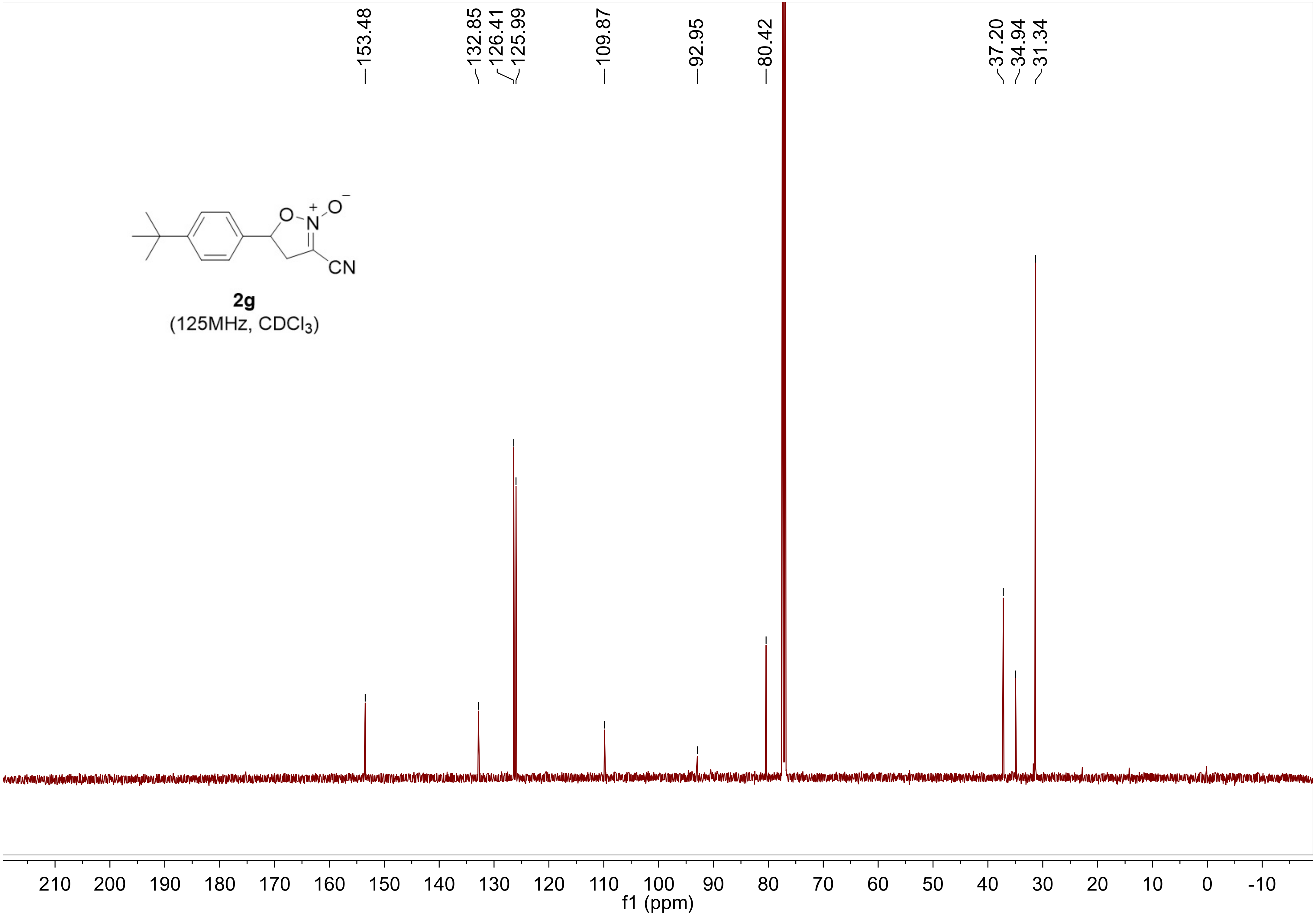


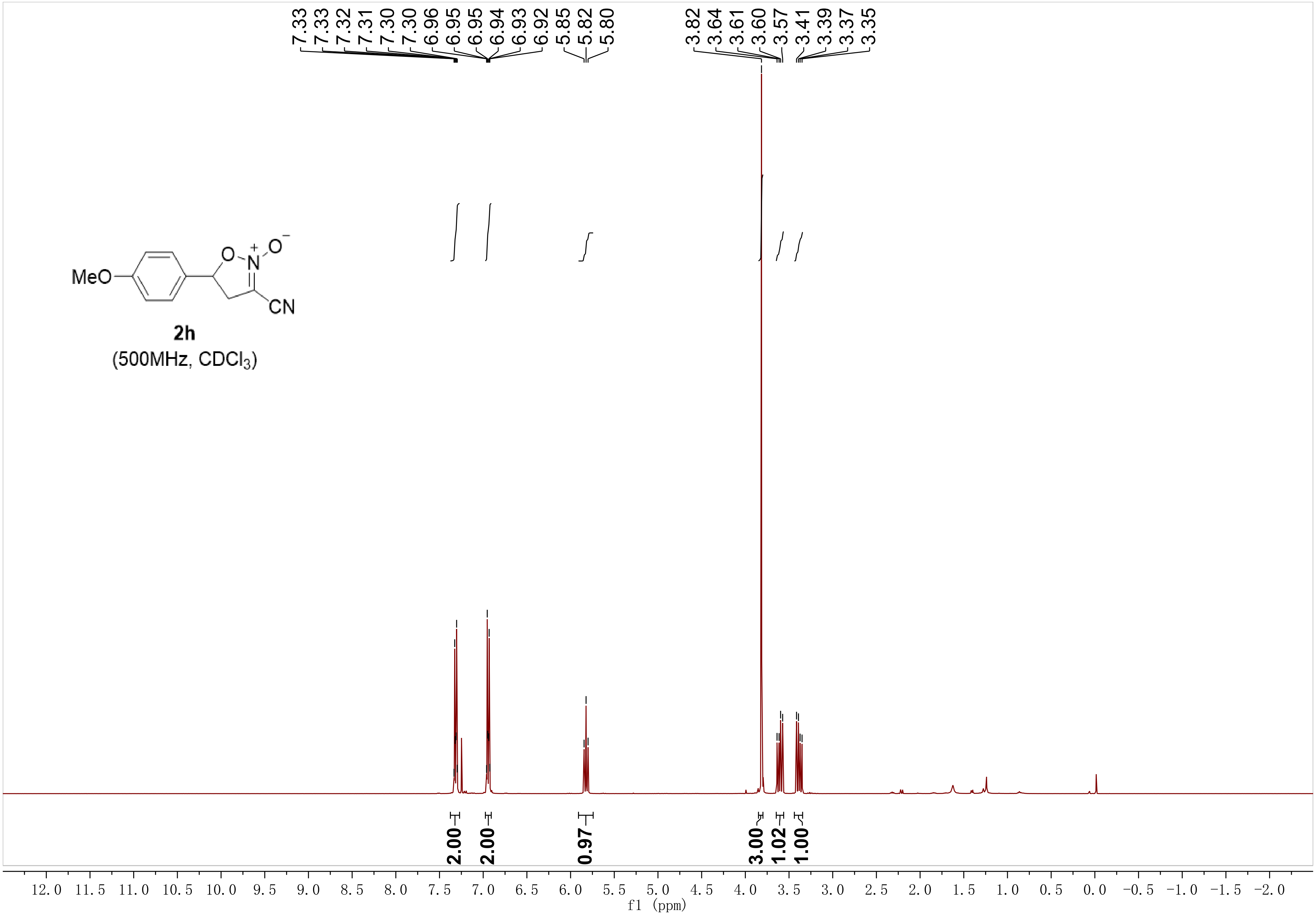
2f

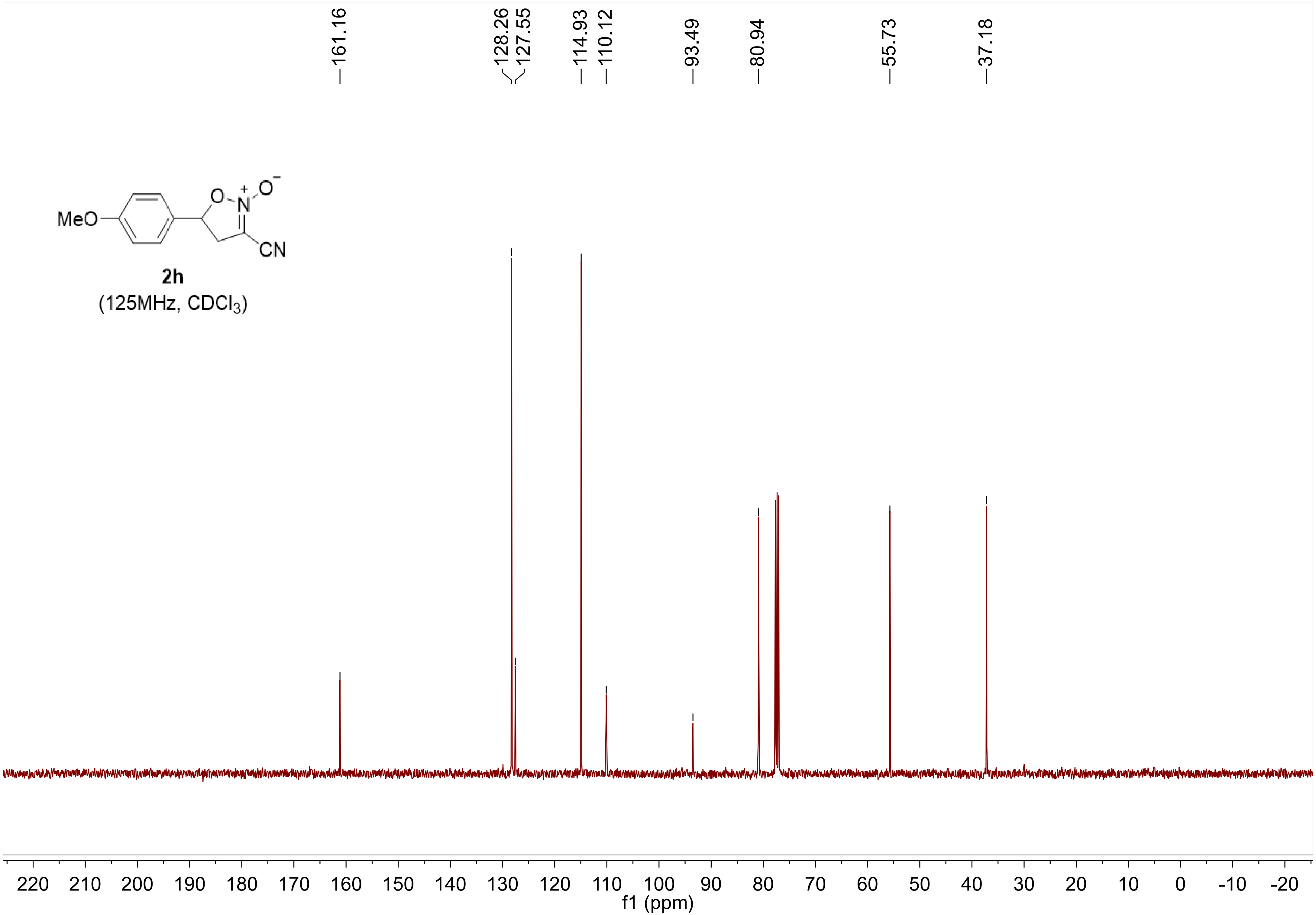
(125MHz, $CDCl_3$)

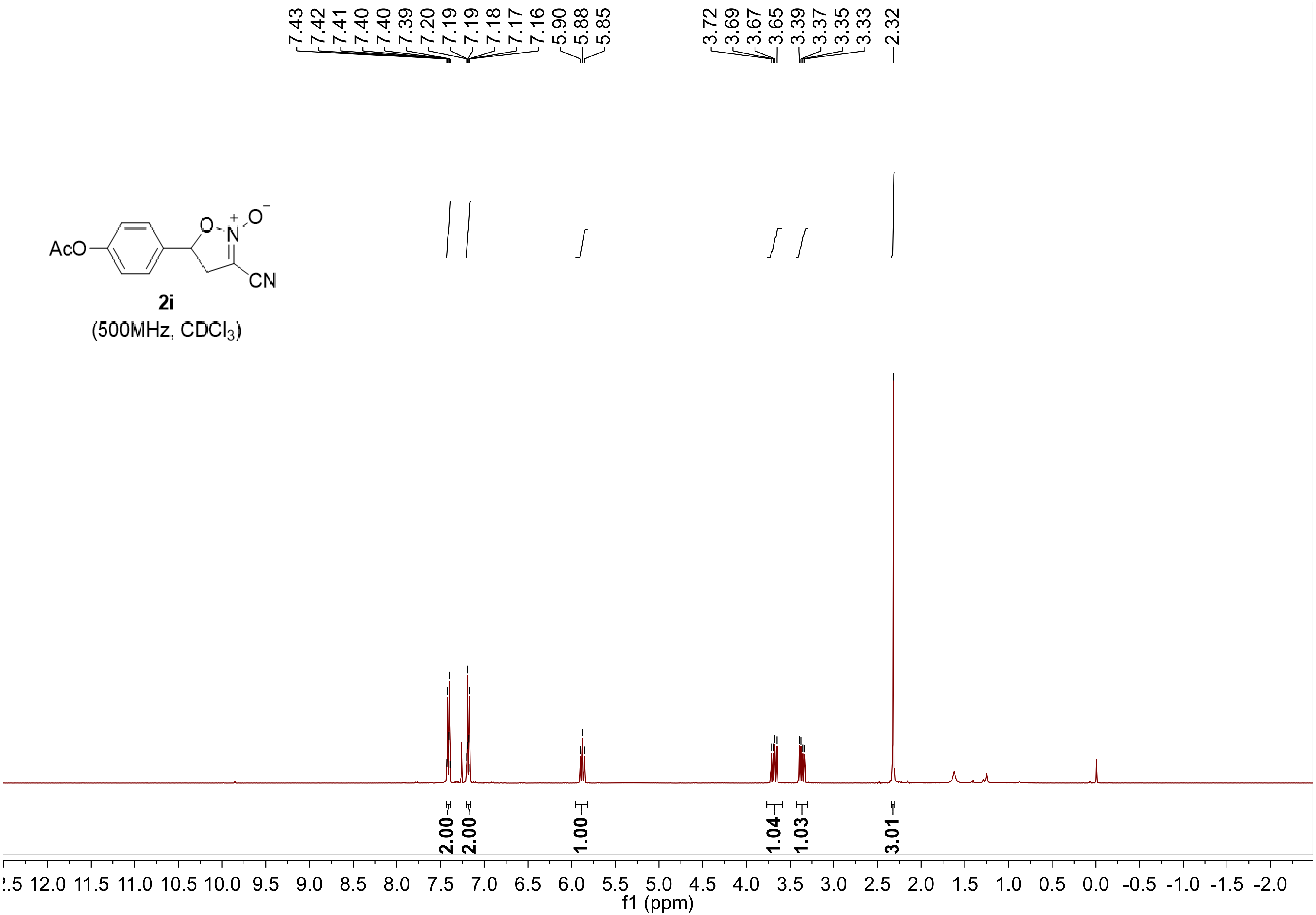


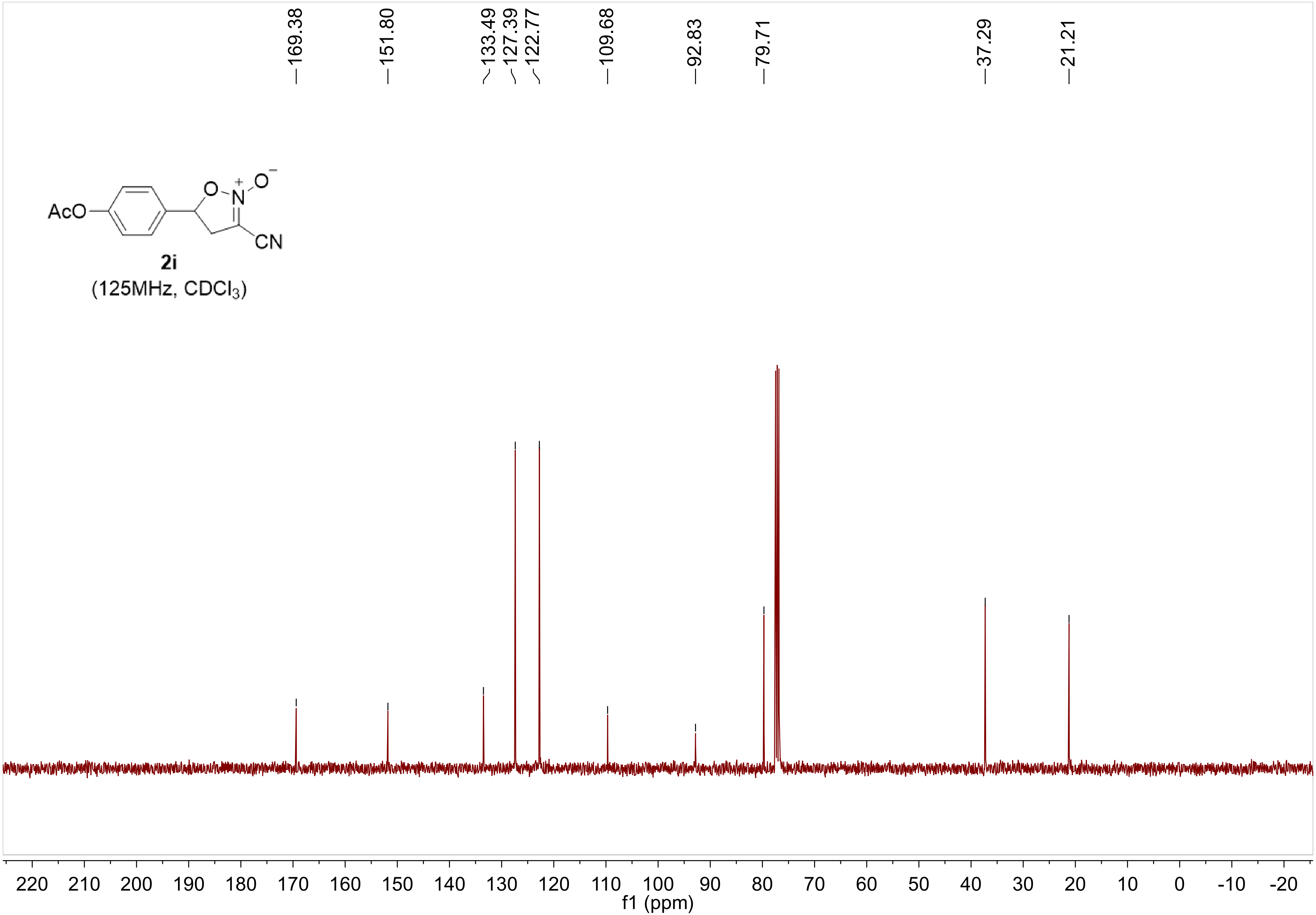

7.48
7.46
7.34
7.32
5.89
5.87
5.85
3.69
3.67
3.66
3.64
3.43
3.41
3.40
3.38
1.33
O
N
+
O
−
CN
2g
(500MHz, CDCl$_3$)
2.00
2.00
1.00
1.00
1.01
9.06
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

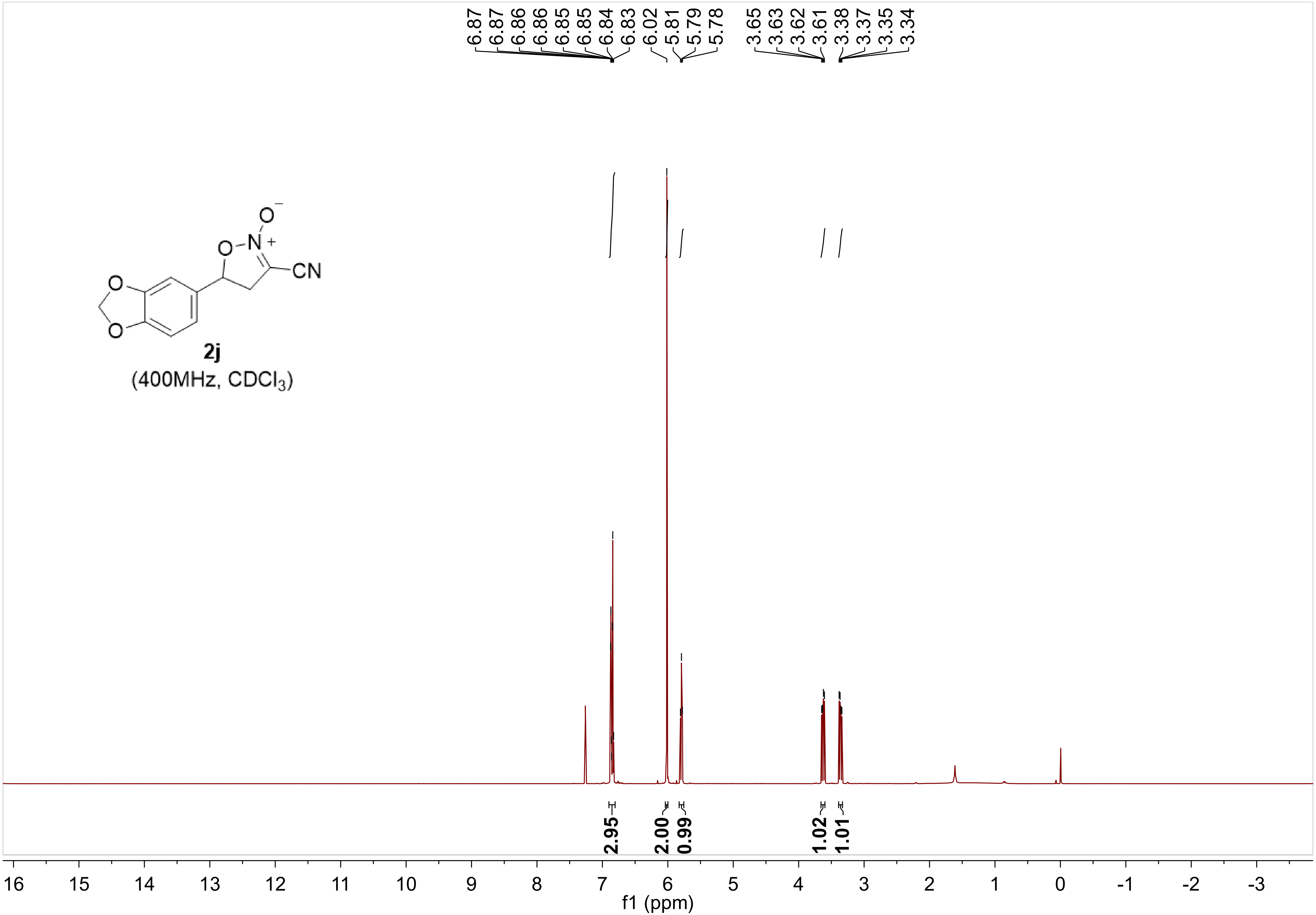

153.48
132.85
126.41
125.99
109.87
92.95
80.42
37.20
34.94
31.34
2g
(125MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

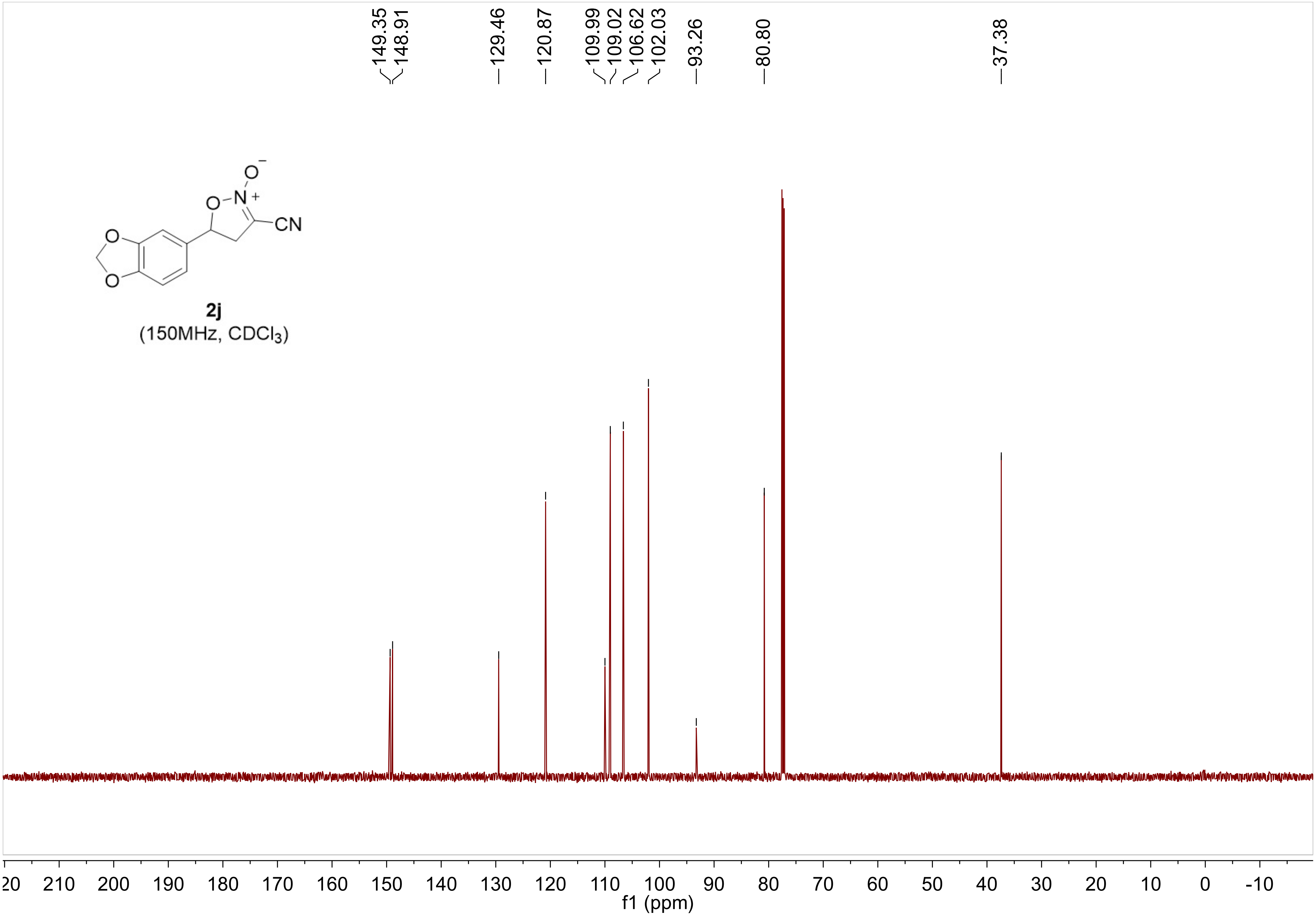

7.33 7.33 7.32 7.31 7.30 7.30 6.96 6.95 6.95 6.94 6.93 6.92 5.85 5.82 5.80
3.82 3.64 3.61 3.60 3.57 3.41 3.39 3.37 3.35
MeO
O
N
+
O
−
CN
2h
(500MHz, CDCl$_3$)
2.00
2.00
0.97
3.00
1.02
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5 −2.0
f1 (ppm)

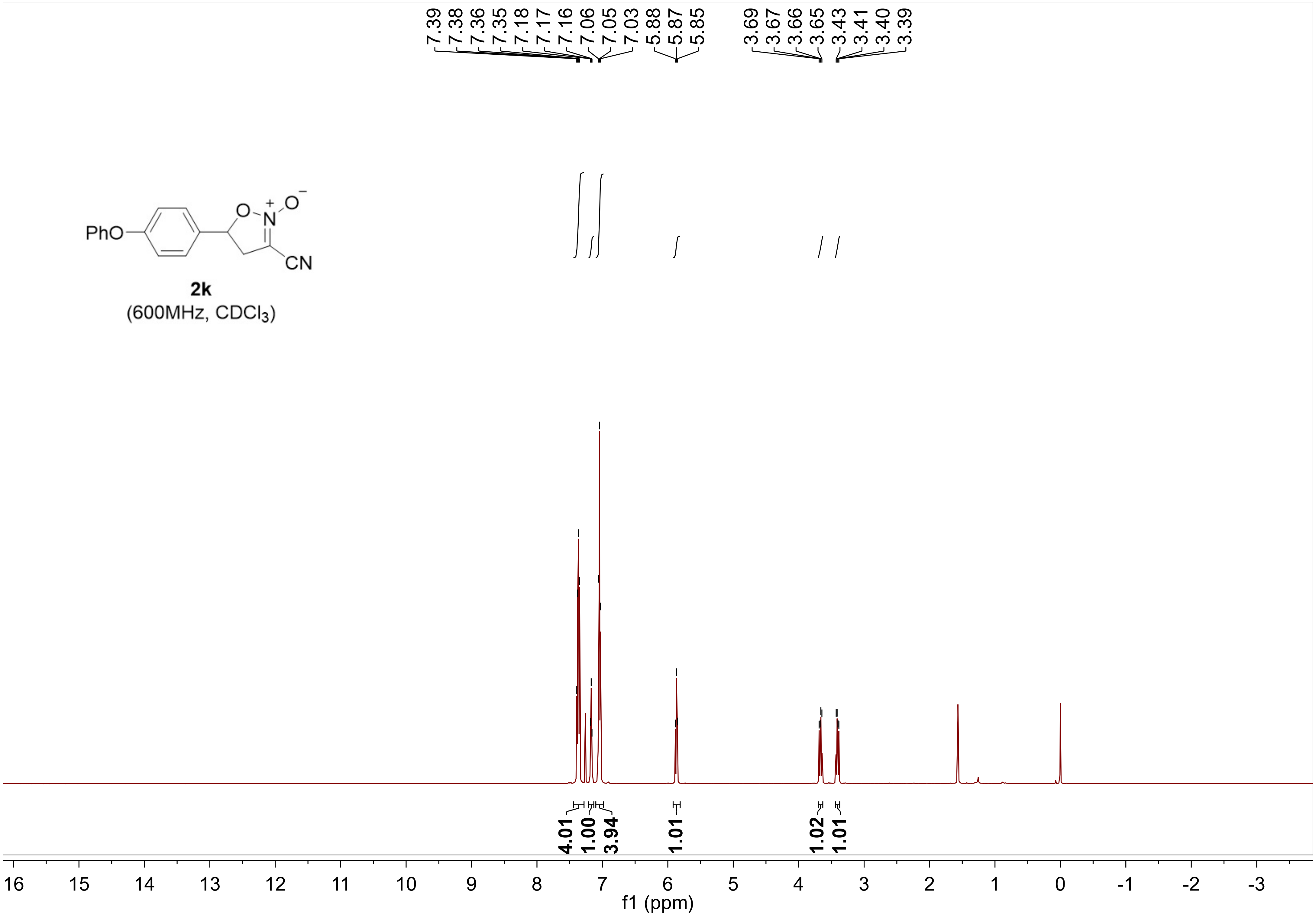

161.16
128.26
127.55
114.93
110.12
93.49
80.94
55.73
37.18
MeO
O
N
O
CN
2h
(125MHz, CDCl3)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.43
7.42
7.41
7.40
7.40
7.39
7.20
7.19
7.19
7.18
7.17
7.16
5.90
5.88
5.85
3.72
3.69
3.67
3.65
3.39
3.37
3.35
3.33
2.32
AcO
O
N
+
O
−
CN
2i
(500MHz, $CDCl_3$)
2.00
2.00
1.00
1.04
1.03
3.01
.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

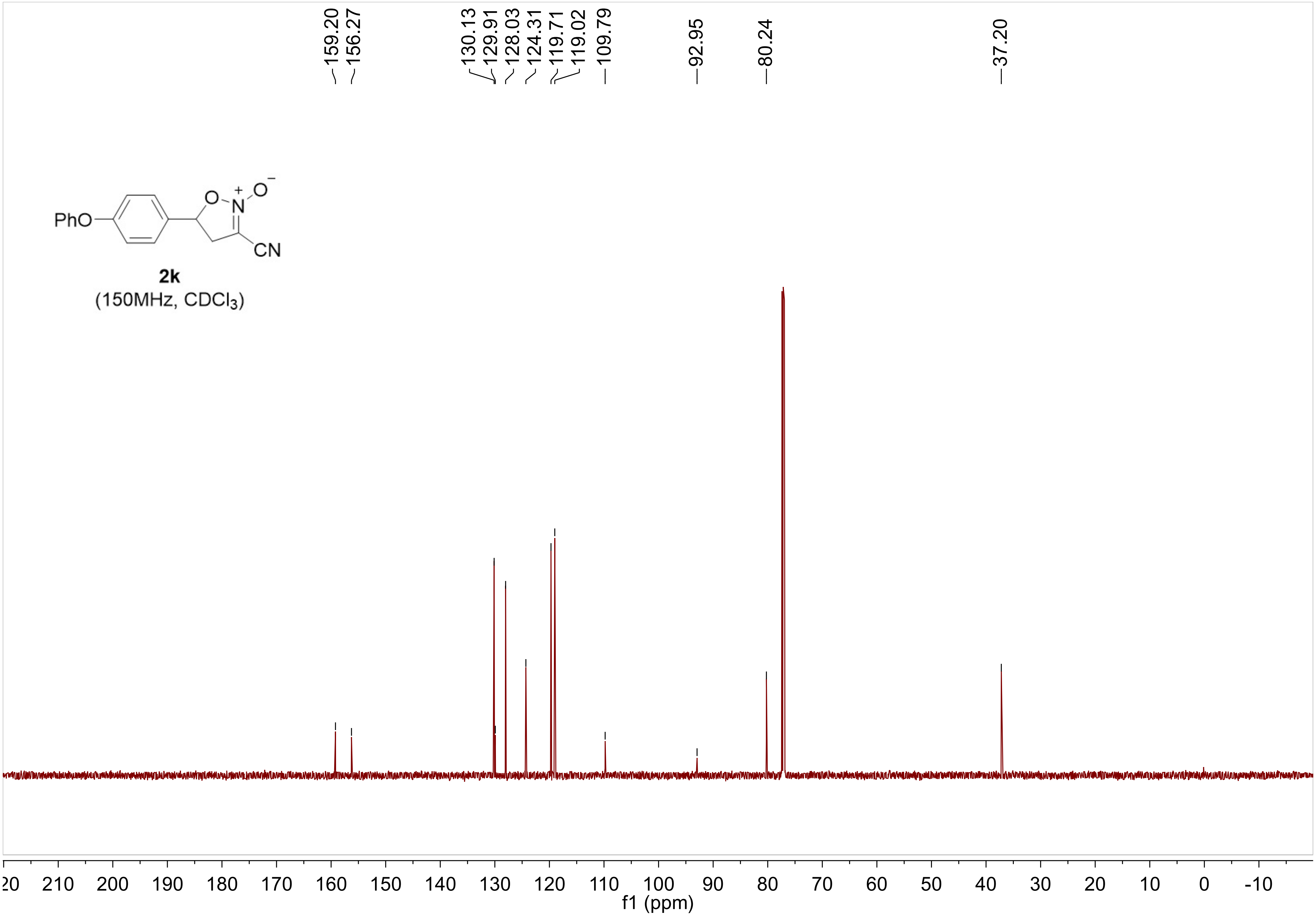

169.38
151.80
133.49
127.39
122.77
109.68
92.83
79.71
37.29
21.21
AcO
O
N
O
CN
2i
(125MHz, $CDCl_3$)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


6.87
6.87
6.86
6.86
6.85
6.85
6.84
6.83
6.02
5.81
5.79
5.78
3.65
3.63
3.62
3.61
3.38
3.37
3.35
3.34
O
N+
O−
CN
O
O
2j
(400MHz, CDCl3)
2.95
2.00
0.99
1.02
1.01
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

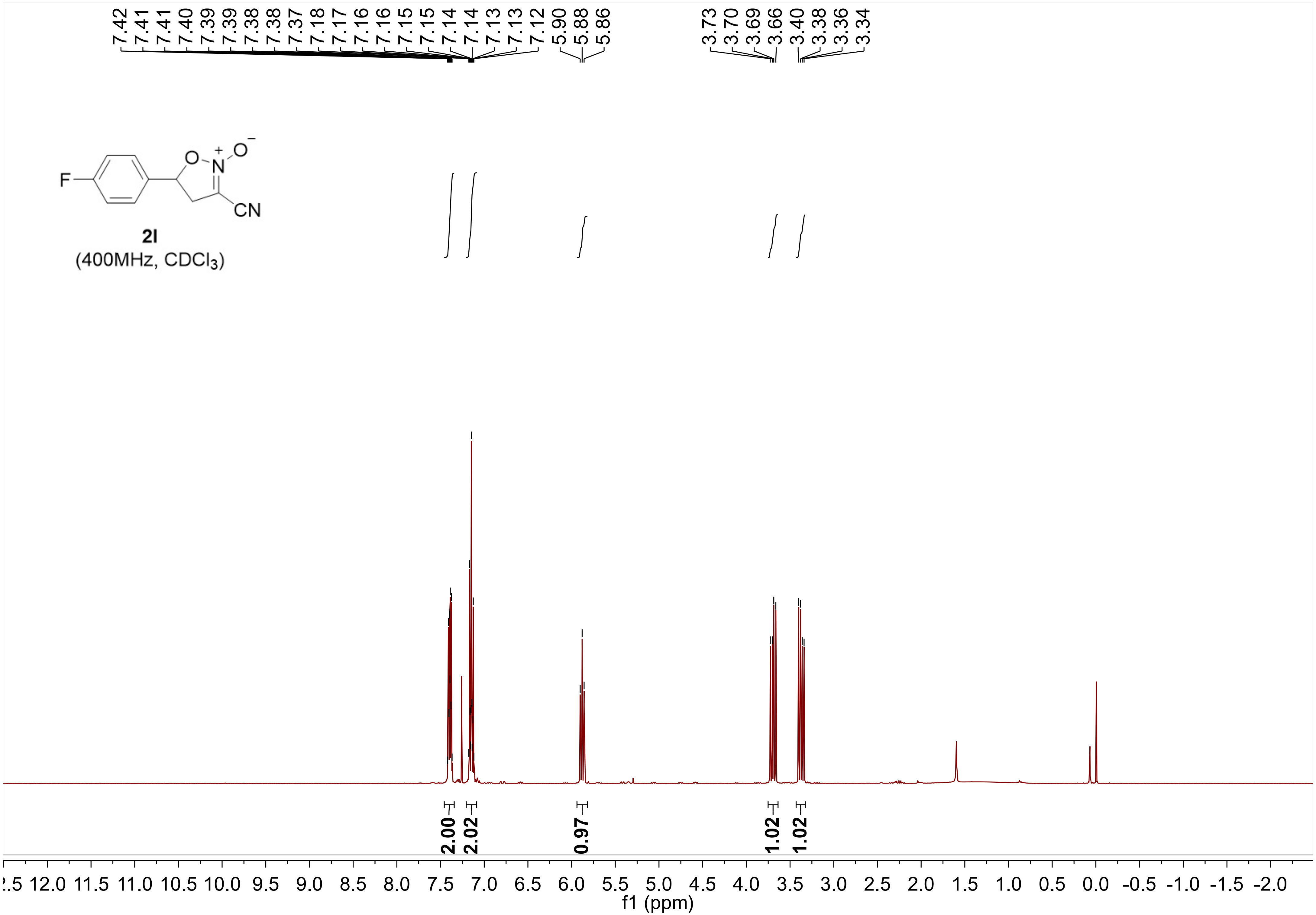

149.35
148.91
129.46
120.87
109.99
109.02
106.62
102.03
93.26
80.80
37.38
O⁻
O
N+
CN
O
O
2j
(150MHz, $CDCl_3$)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

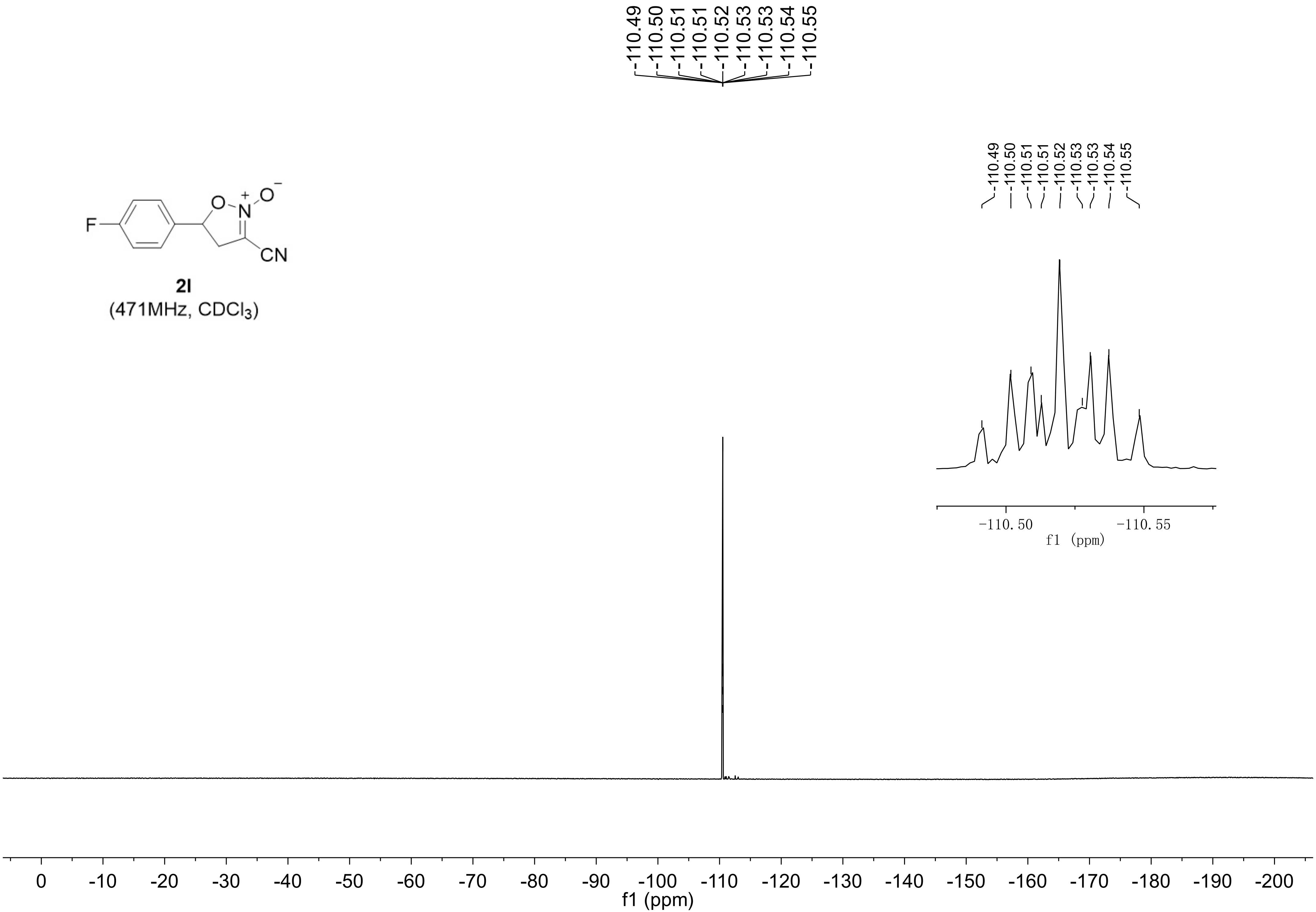


7.39
7.38
7.36
7.35
7.18
7.17
7.16
7.06
7.05
7.03
5.88
5.87
5.85
3.69
3.67
3.66
3.65
3.43
3.41
3.40
3.39
PhO
O
N
O
CN
2k
(600MHz, CDCl3)
4.01
1.00
3.94
1.01
1.02
1.01
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

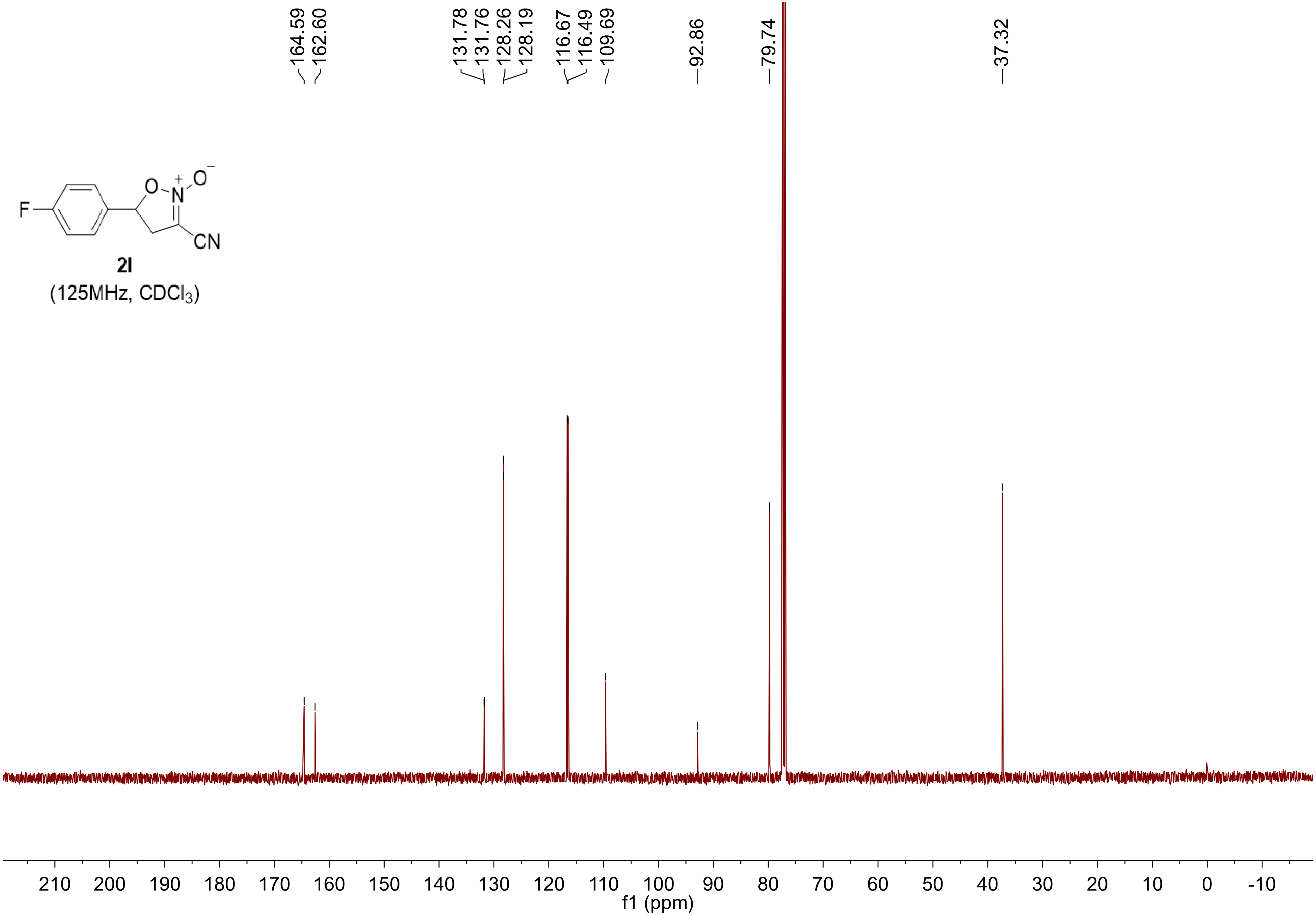


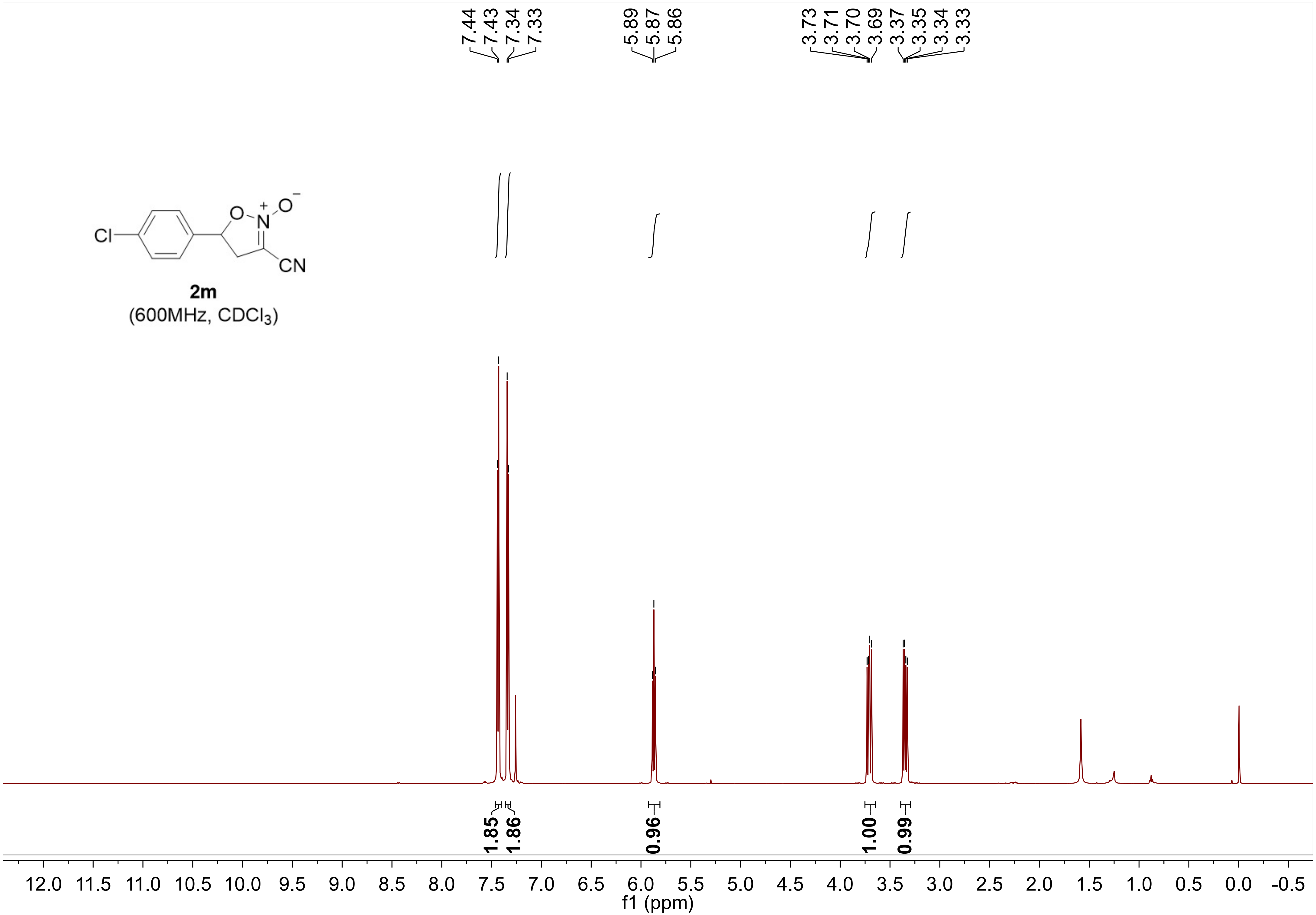
2k
(150MHz, $CDCl_3$)


7.42 7.41 7.41 7.40 7.39 7.39 7.38 7.38 7.37 7.18 7.17 7.16 7.16 7.15 7.15 7.14 7.14 7.13 7.13 7.12 5.90 5.88 5.86
3.73 3.70 3.69 3.66 3.40 3.38 3.36 3.34
F
O
N
O
CN
2l
(400MHz, CDCl3)
2.00
2.02
0.97
1.02
1.02
2.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

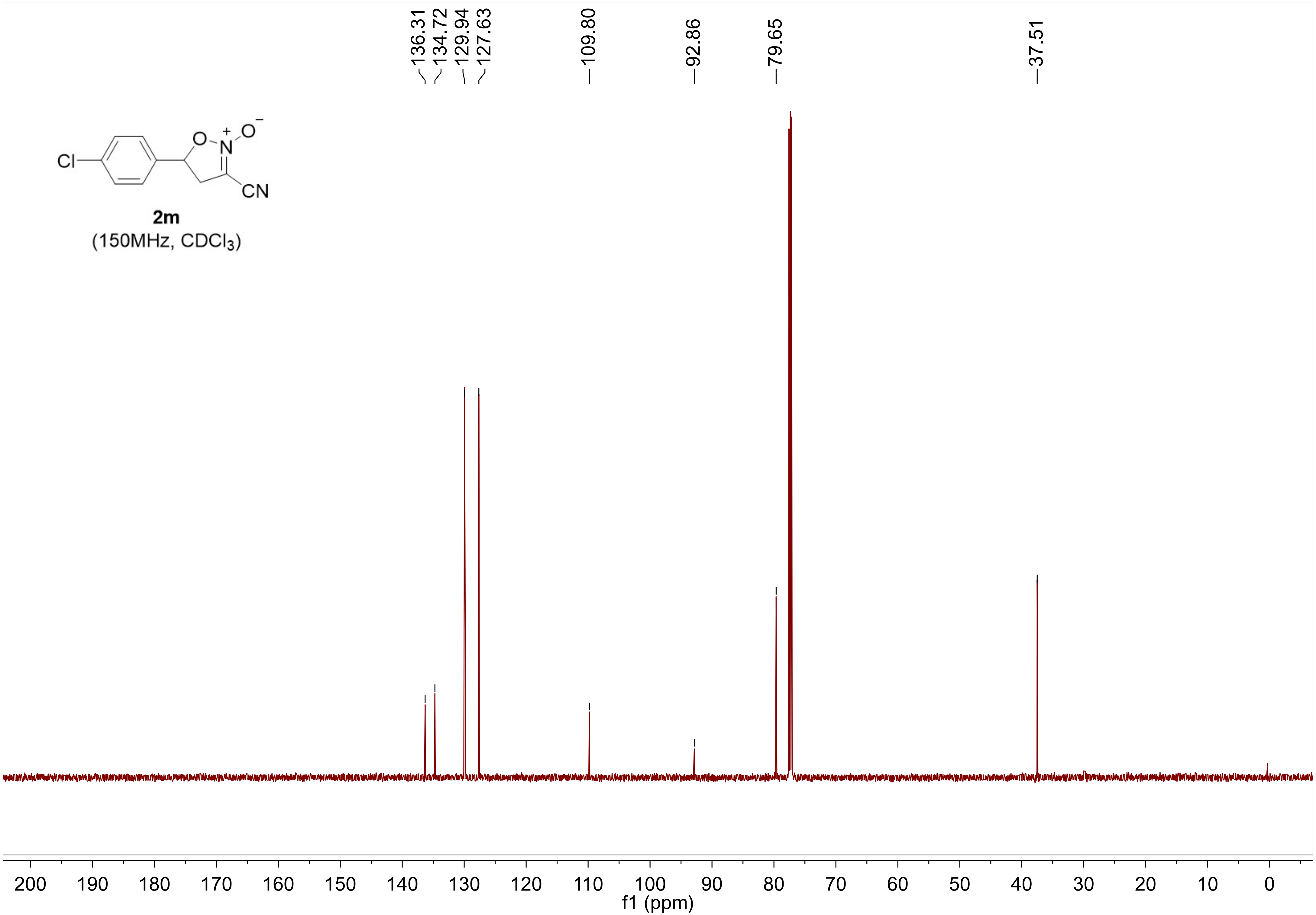


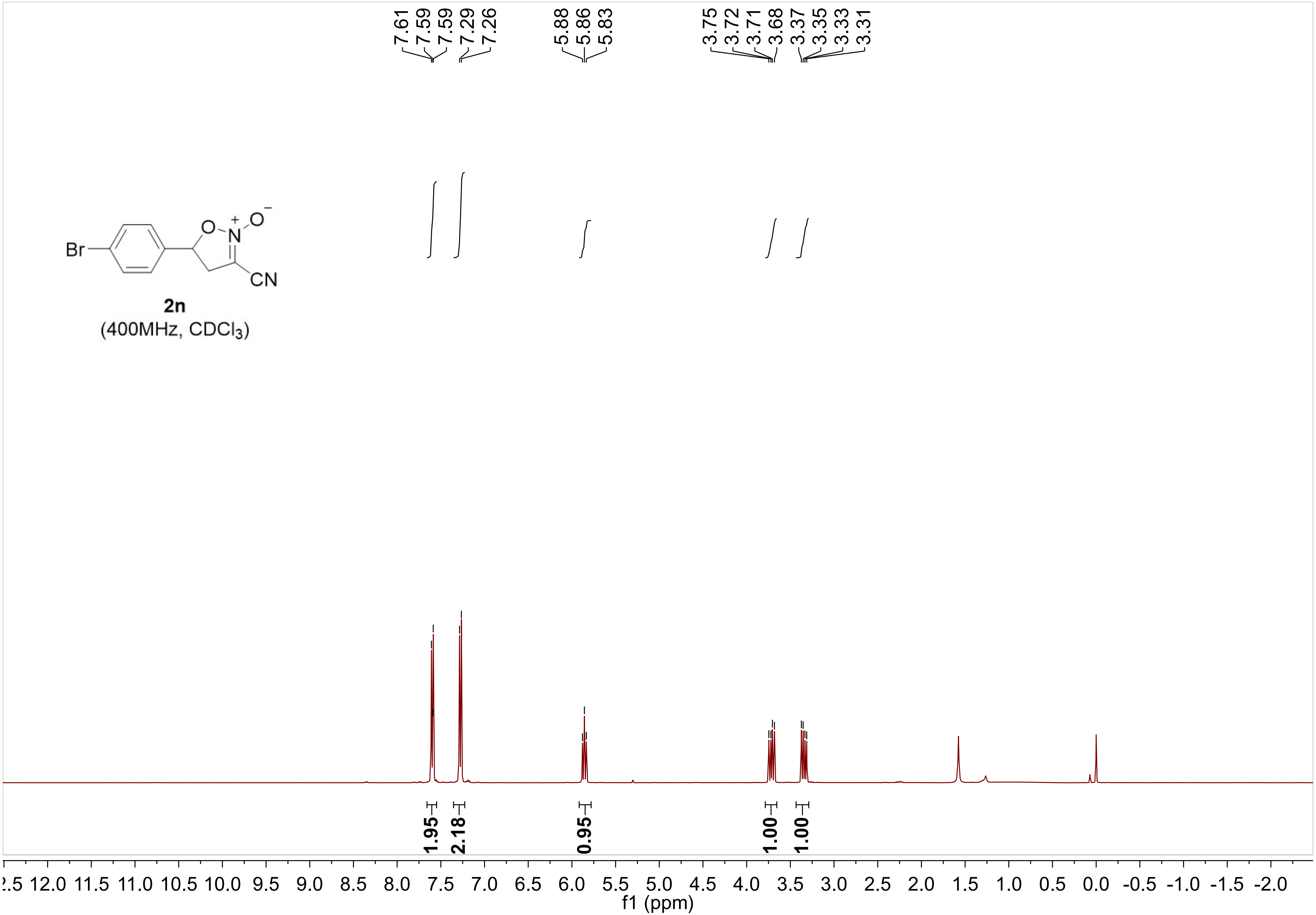
2l
(471MHz, $CDCl_3$)


164.59
162.60
131.78
131.76
128.26
128.19
116.67
116.49
109.69
92.86
79.74
37.32
F
O
N
O
CN
2l
(125MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

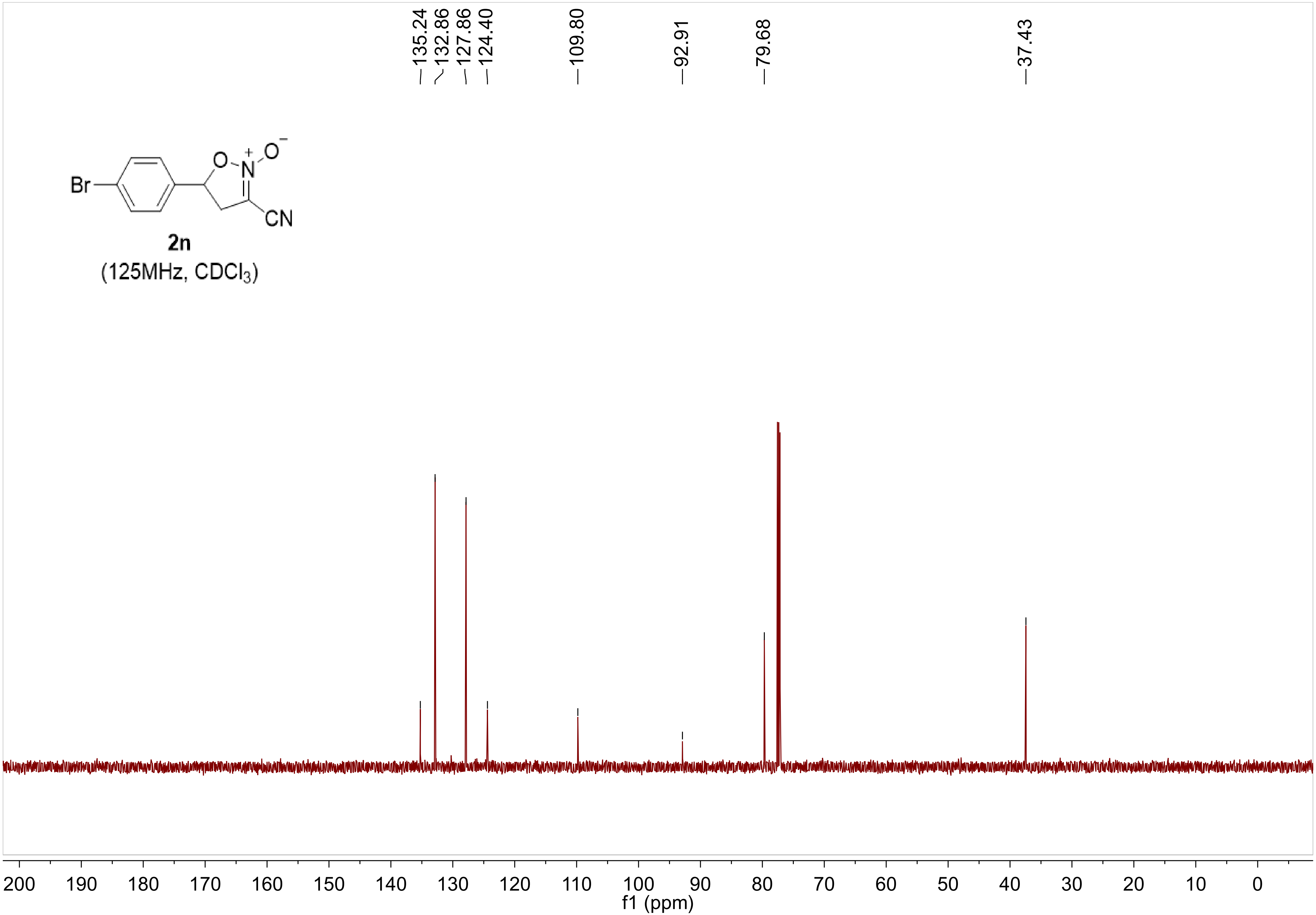


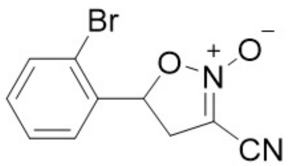
7.44
7.43
7.34
7.33
5.89
5.87
5.86
3.73
3.71
3.70
3.69
3.37
3.35
3.34
3.33
Cl
O
N
O
CN
2m
(600MHz, CDCl3)
1.85
1.86
0.96
1.00
0.99
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


136.31
134.72
129.94
127.63
109.80
92.86
79.65
37.51
Cl
O
N
+
O
−
CN
2m
(150MHz, $CDCl_3$)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

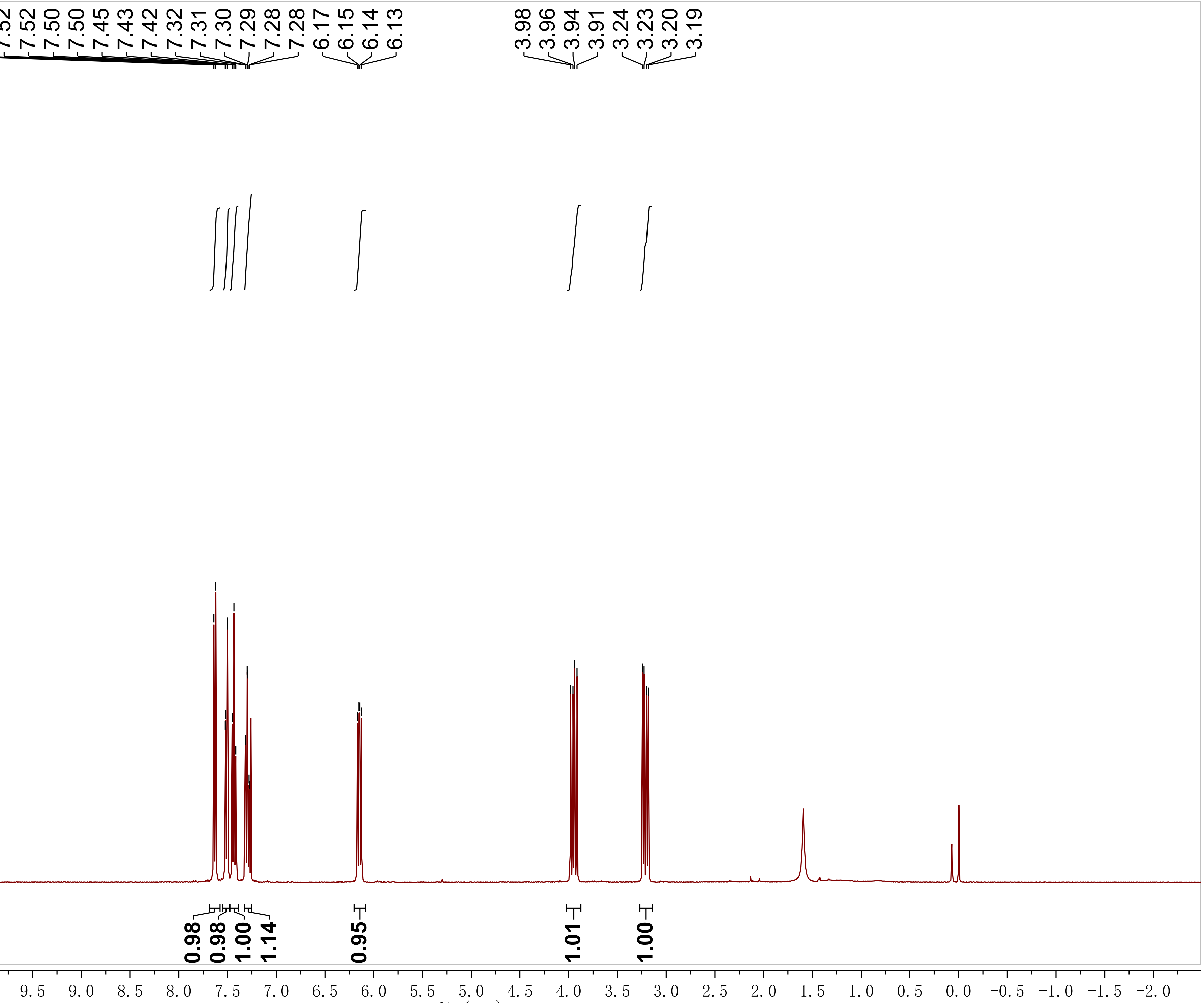


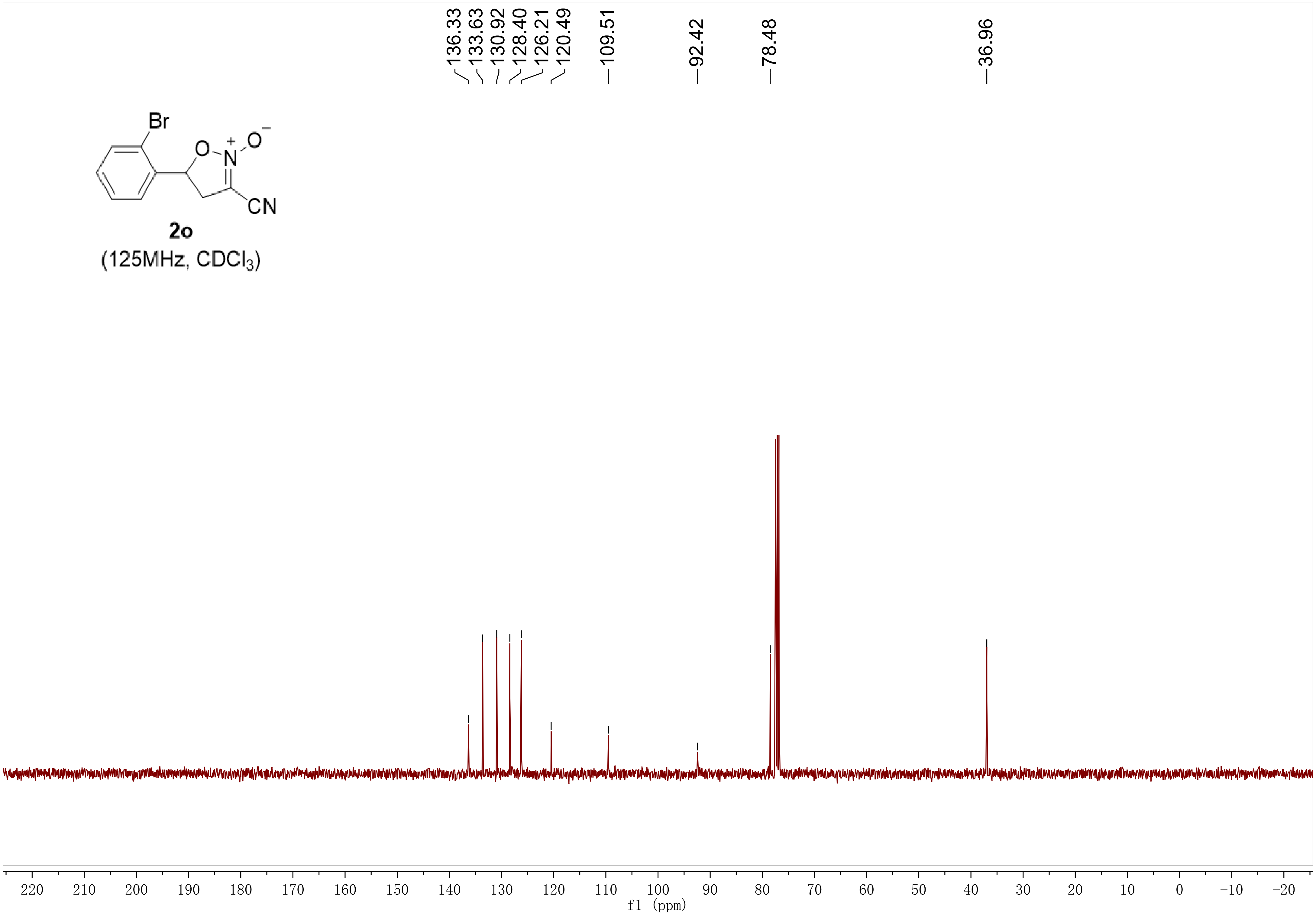
7.61
7.59
7.59
7.29
7.26
5.88
5.86
5.83
3.75
3.72
3.71
3.68
3.37
3.35
3.33
3.31
Br
O
N
O
CN
2n
(400MHz, CDCl3)
1.95
2.18
0.95
1.00
1.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)


135.24
132.86
127.86
124.40
109.80
92.91
79.68
37.43
Br
O
N
O
CN
2n
(125MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

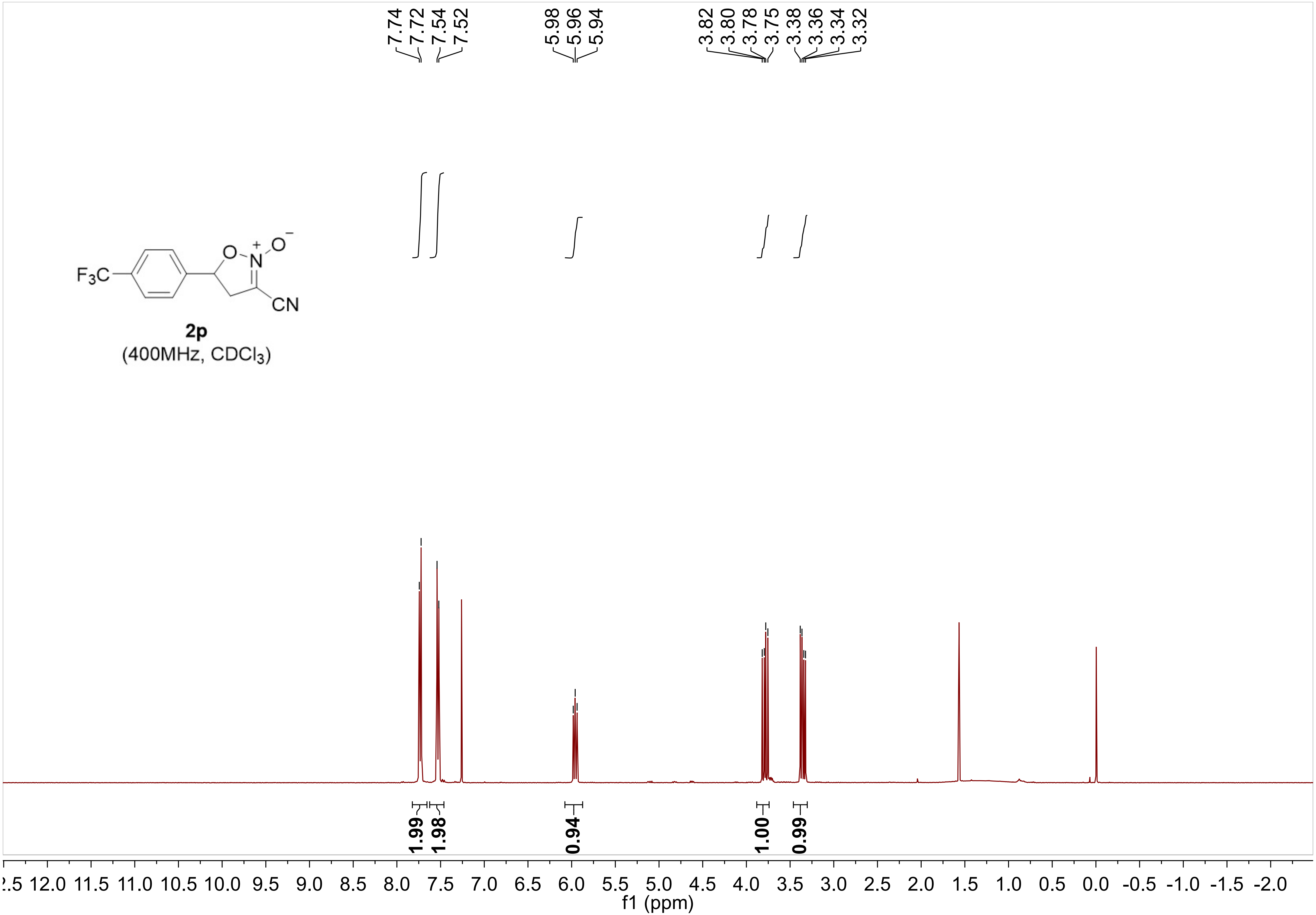


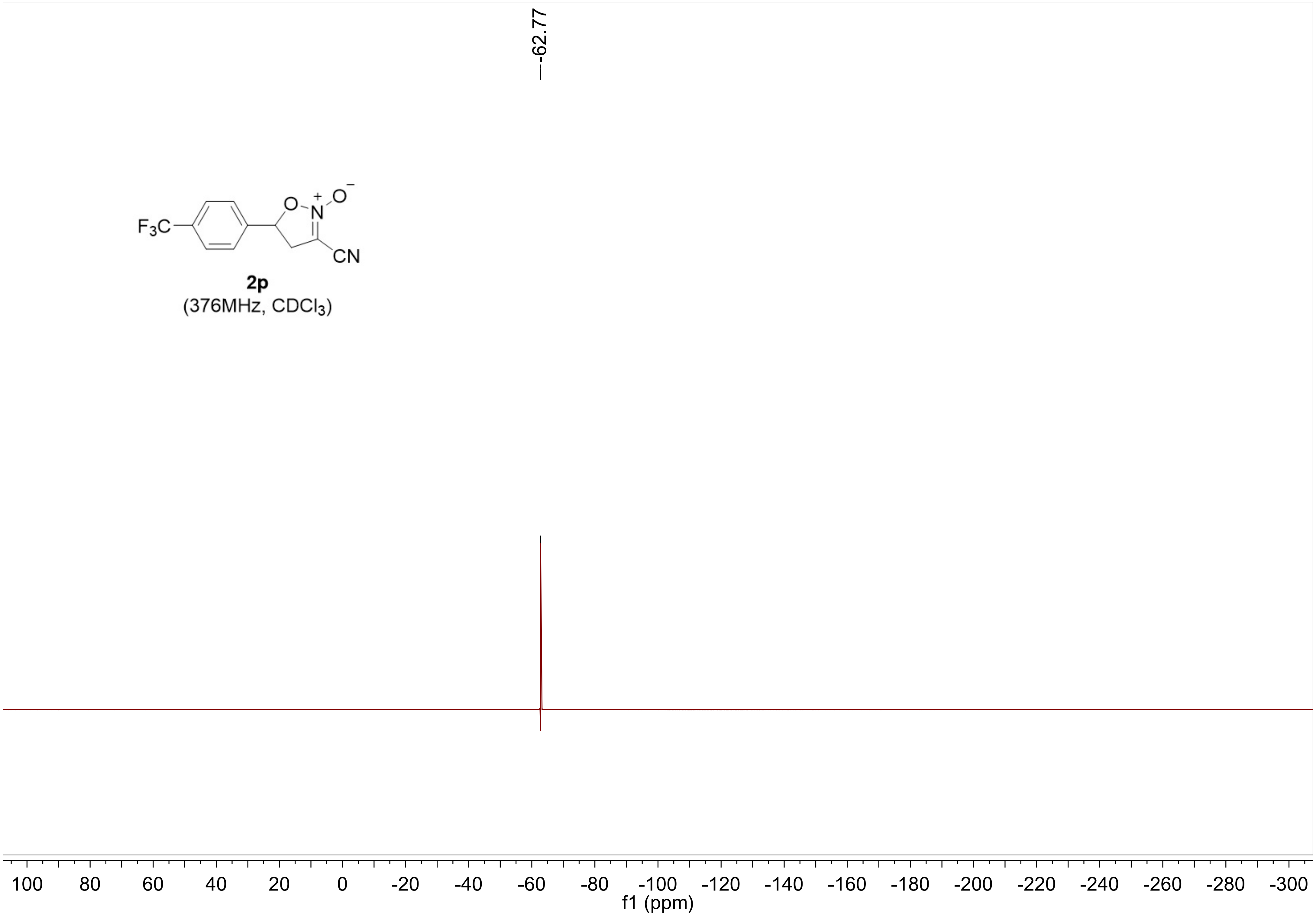
2o
(400MHz, $CDCl_3$)

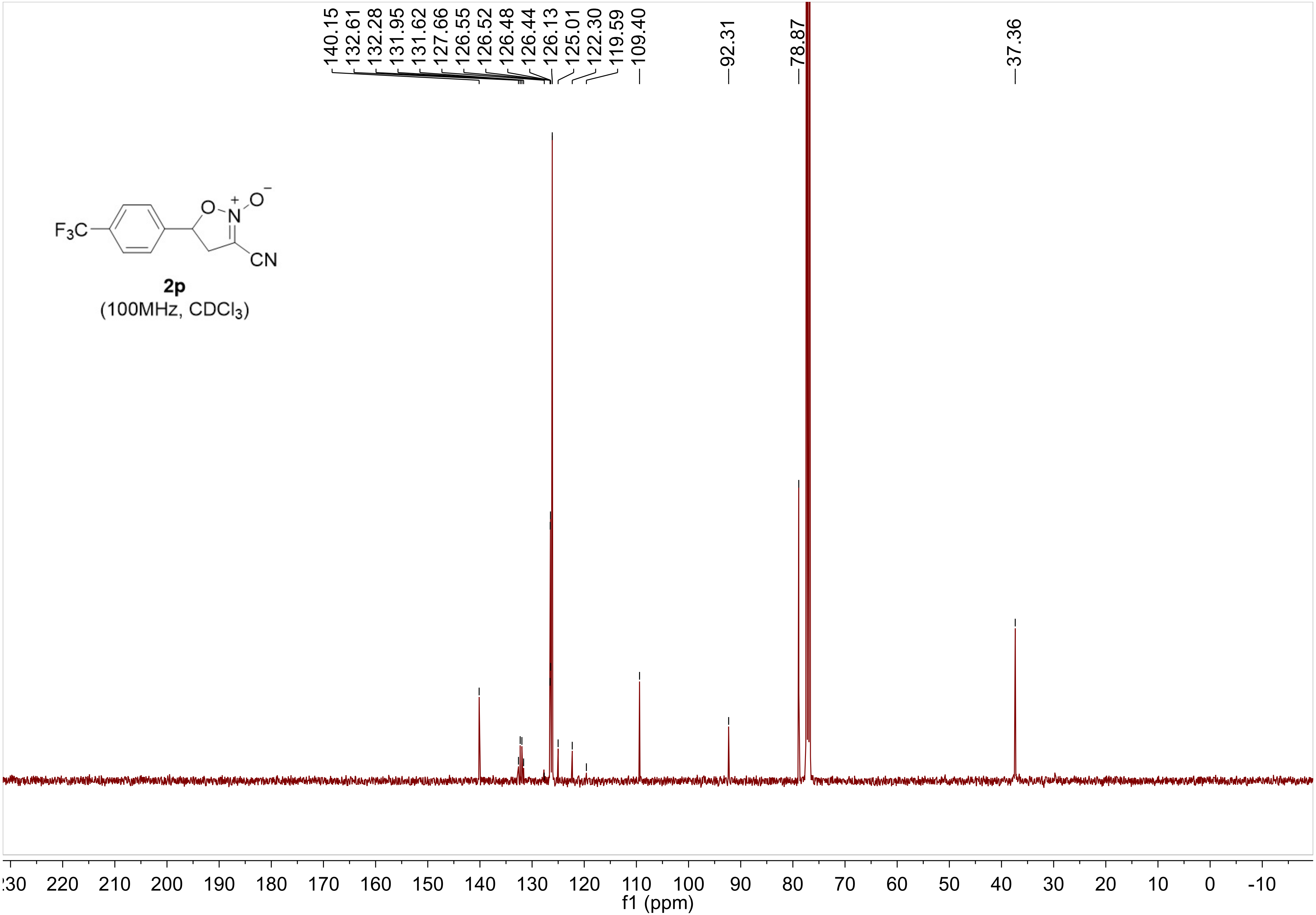


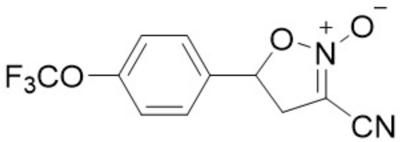


2o
(125MHz, $CDCl_3$)

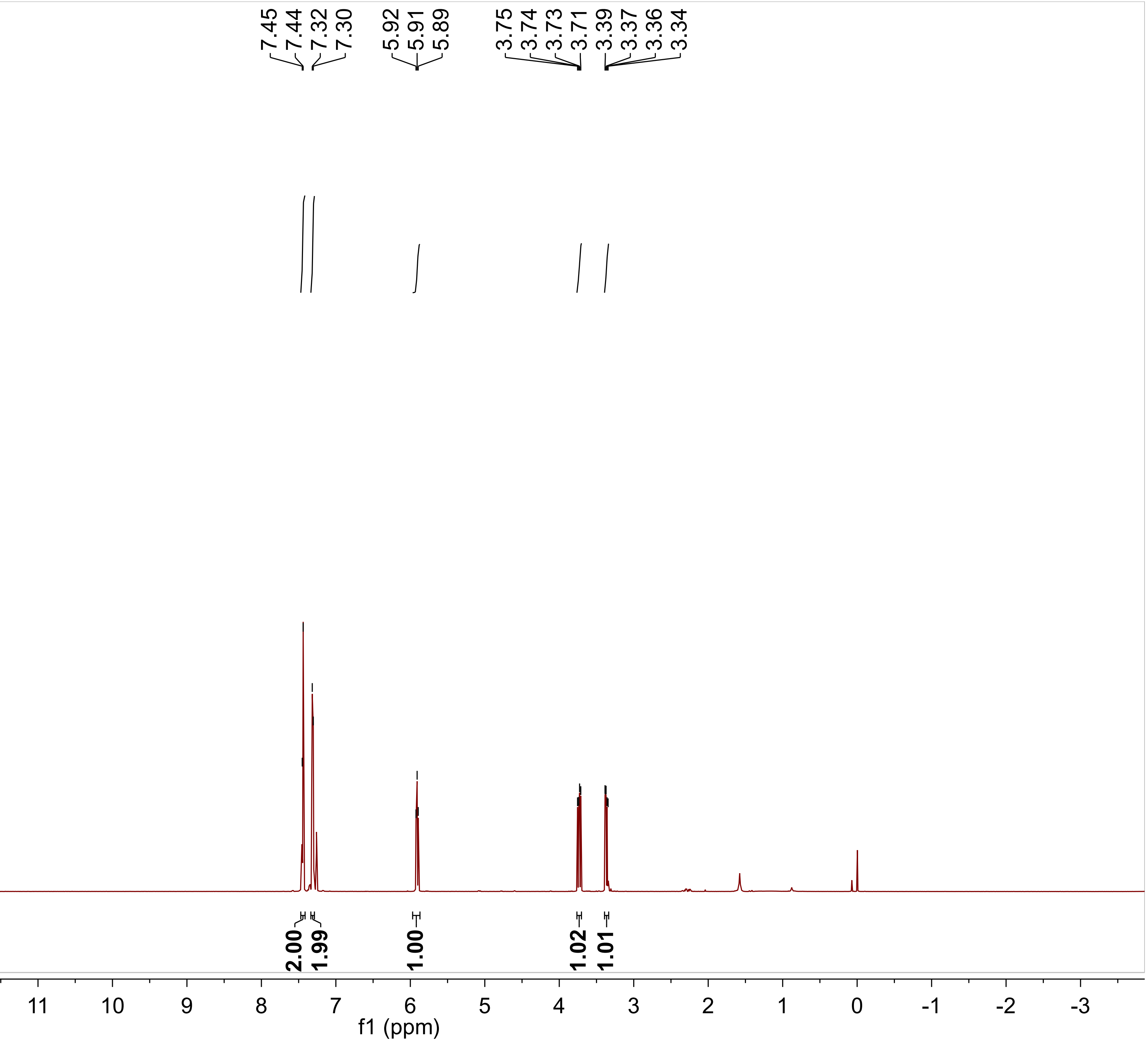

7.74
7.72
7.54
7.52
5.98
5.96
5.94
3.82
3.80
3.78
3.75
3.38
3.36
3.34
3.32
F3C
O
N
O
CN
2p
(400MHz, CDCl3)
1.99
1.98
0.94
1.00
0.99
.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

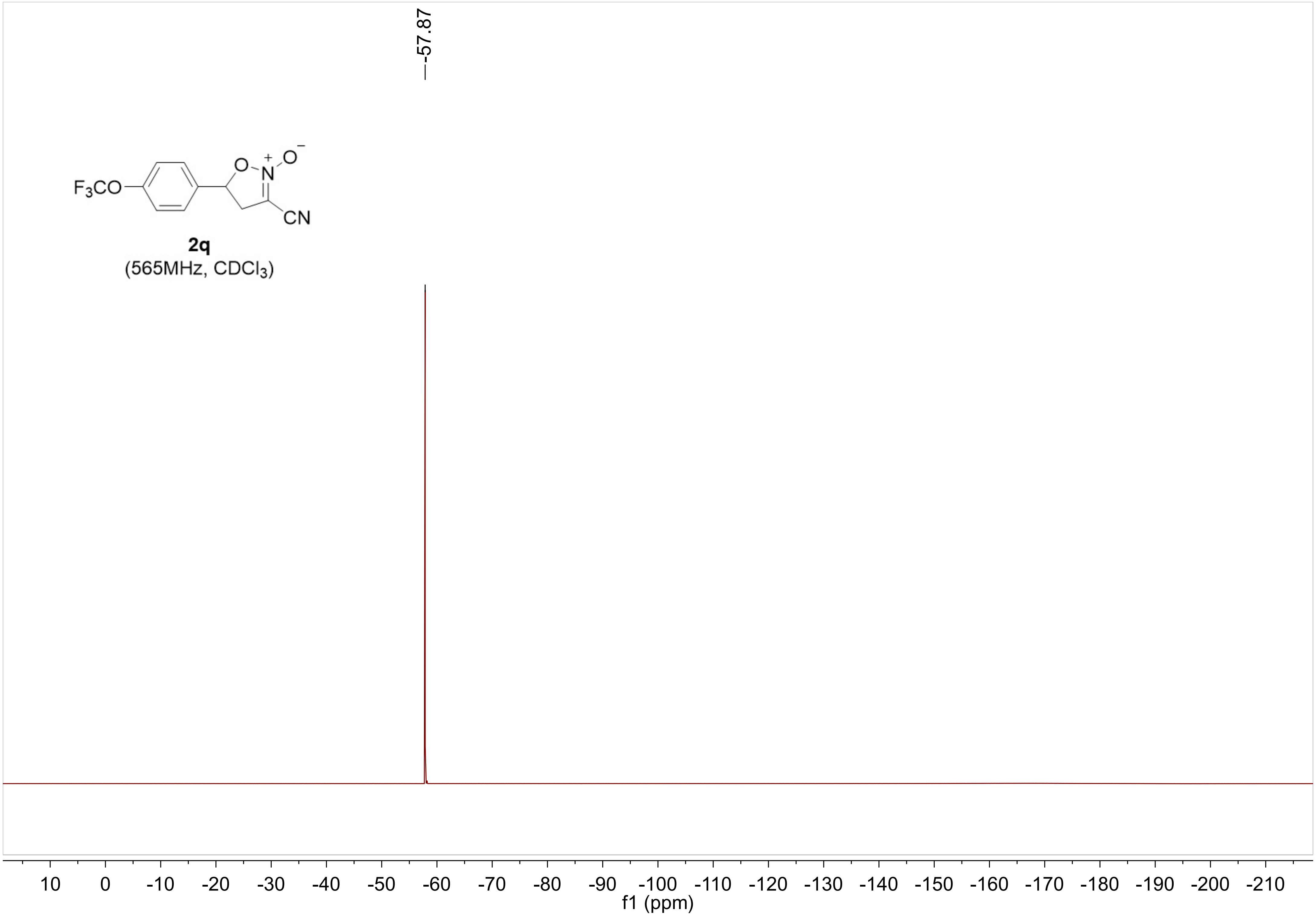

-62.77
F_3C
O
N
+
O
−
CN
2p
(376MHz, $CDCl_3$)
100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300
f1 (ppm)

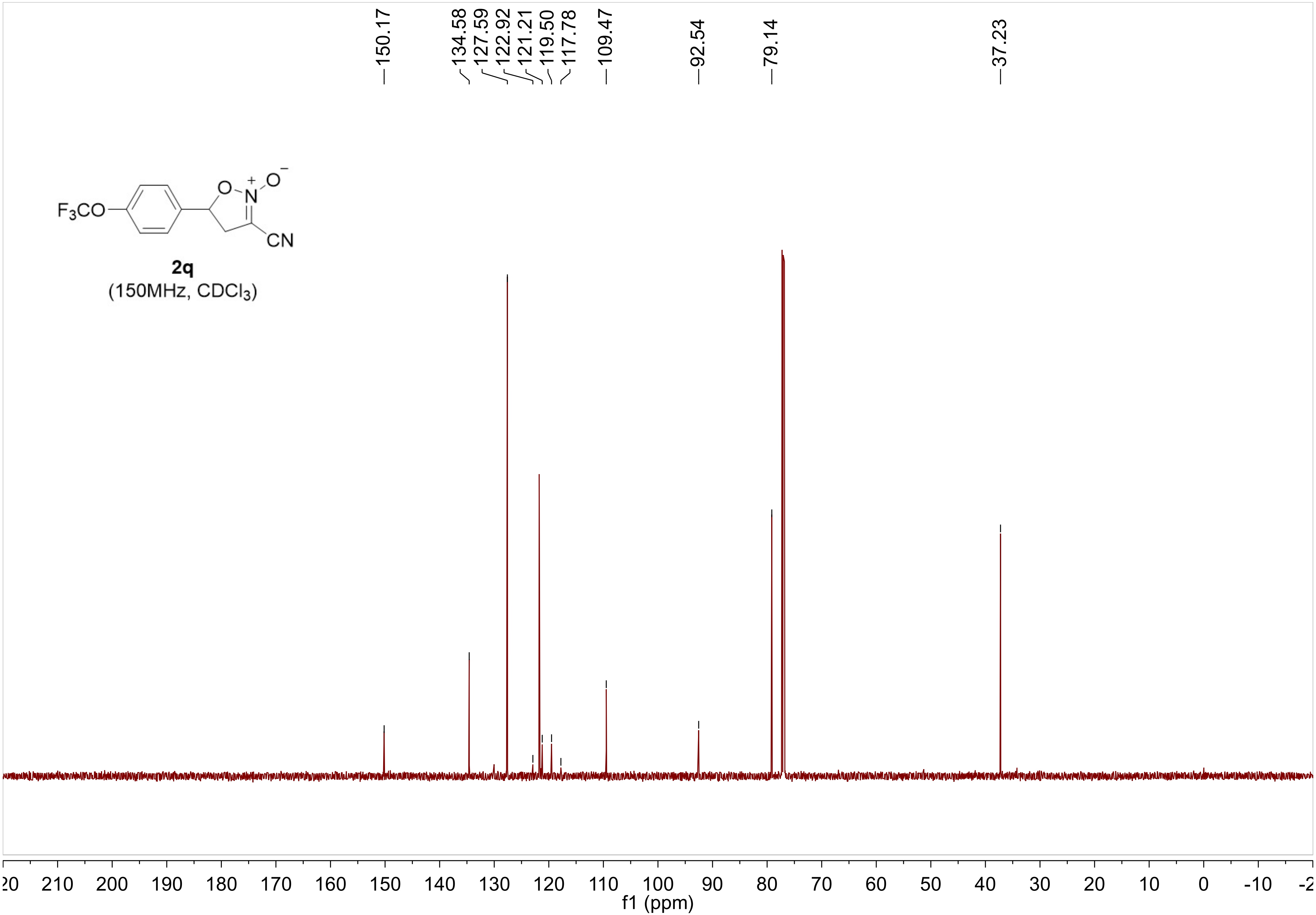

140.15
132.61
132.28
131.95
131.62
127.66
126.55
126.52
126.48
126.44
126.13
125.01
122.30
119.59
109.40
92.31
78.87
37.36
F3C
O
N
O
CN
2p
(100MHz, CDCl3)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



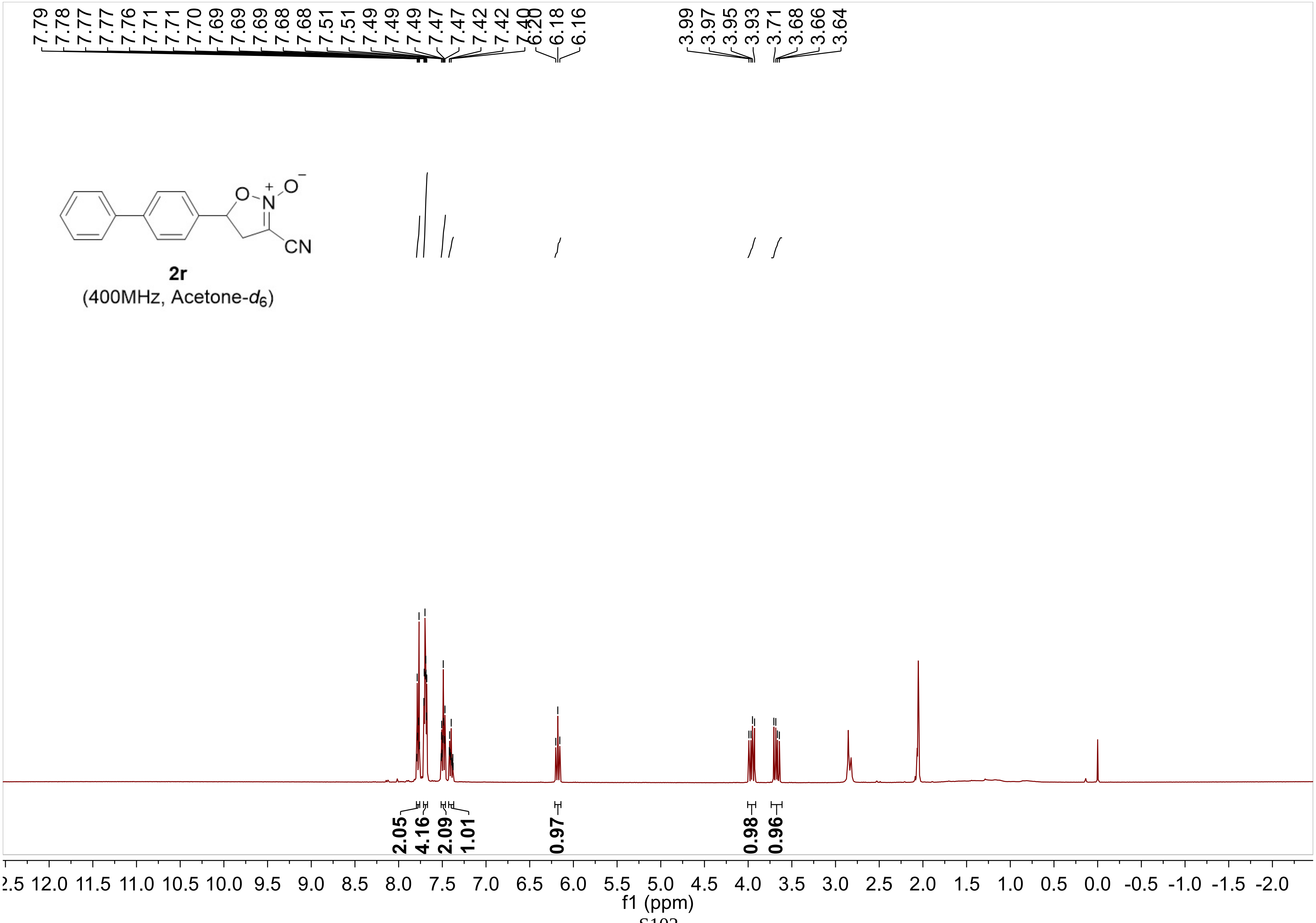
2q
(600MHz, $CDCl_3$)



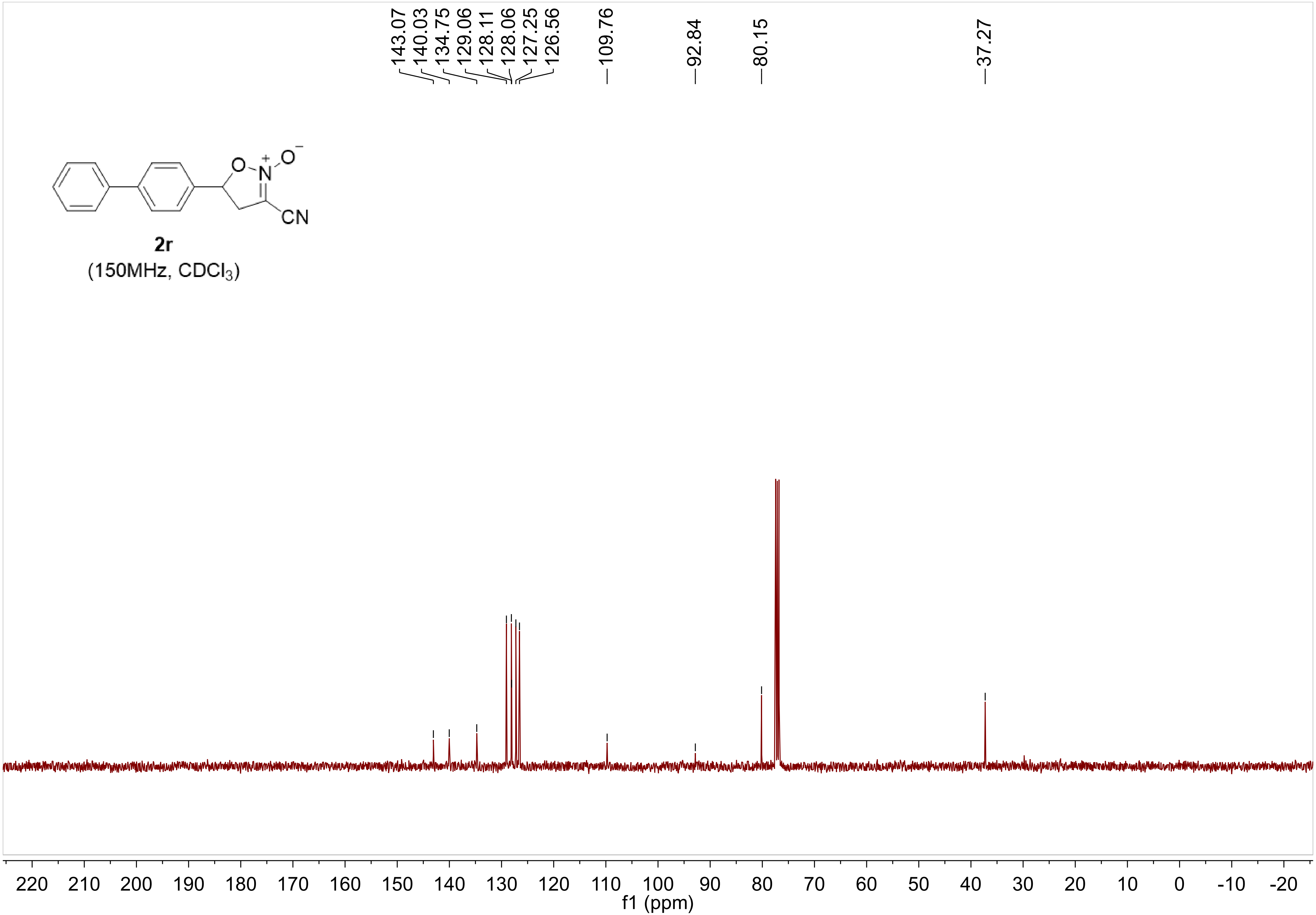

-57.87
F3CO
O
N
O
CN
2q
(565MHz, CDCl3)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

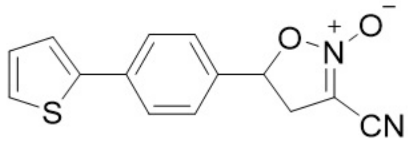


150.17
134.58
127.59
122.92
121.21
119.50
117.78
109.47
92.54
79.14
37.23
F3CO
O
N
O
CN
2q
(150MHz, CDCl3)
f1 (ppm)

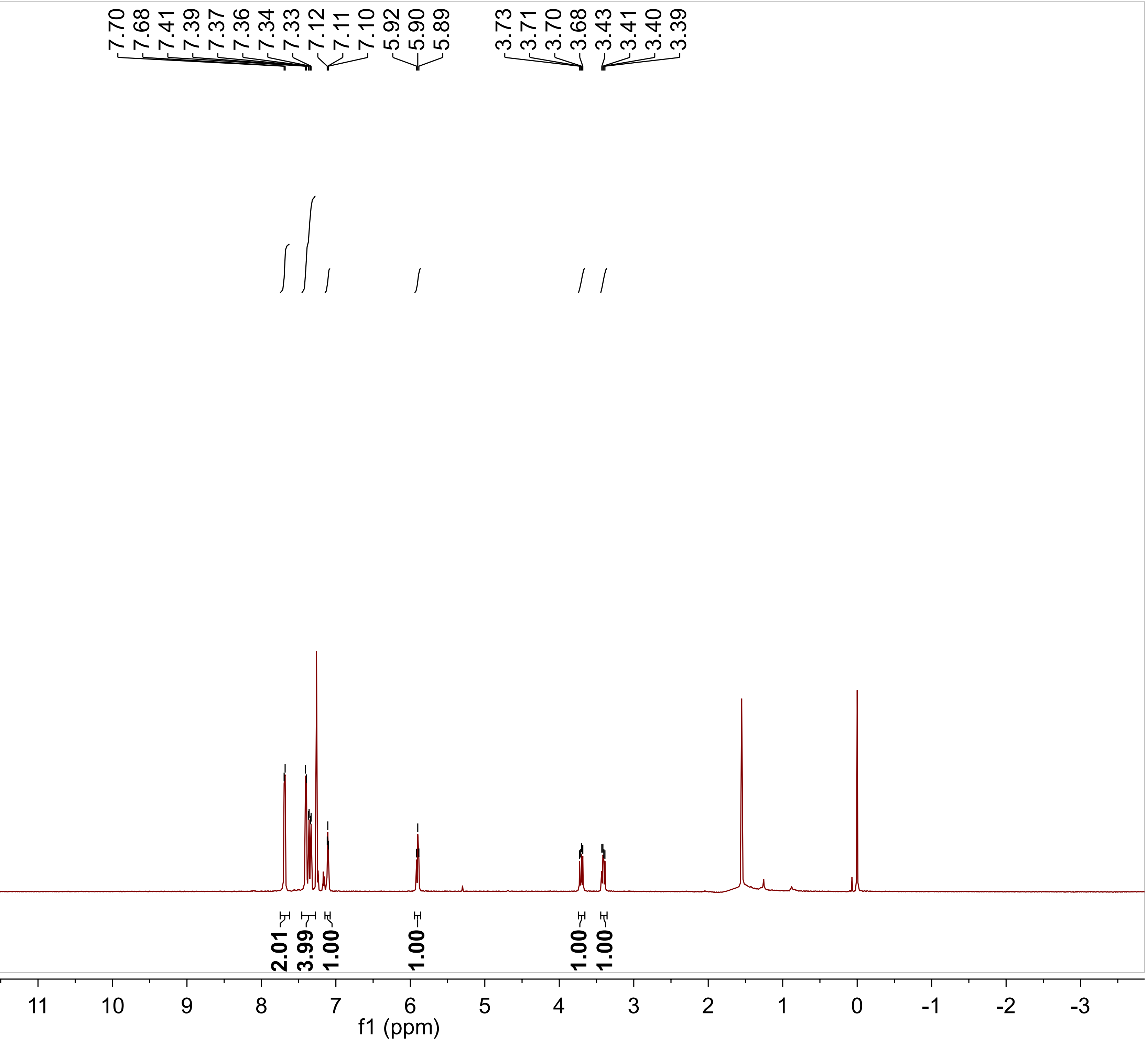


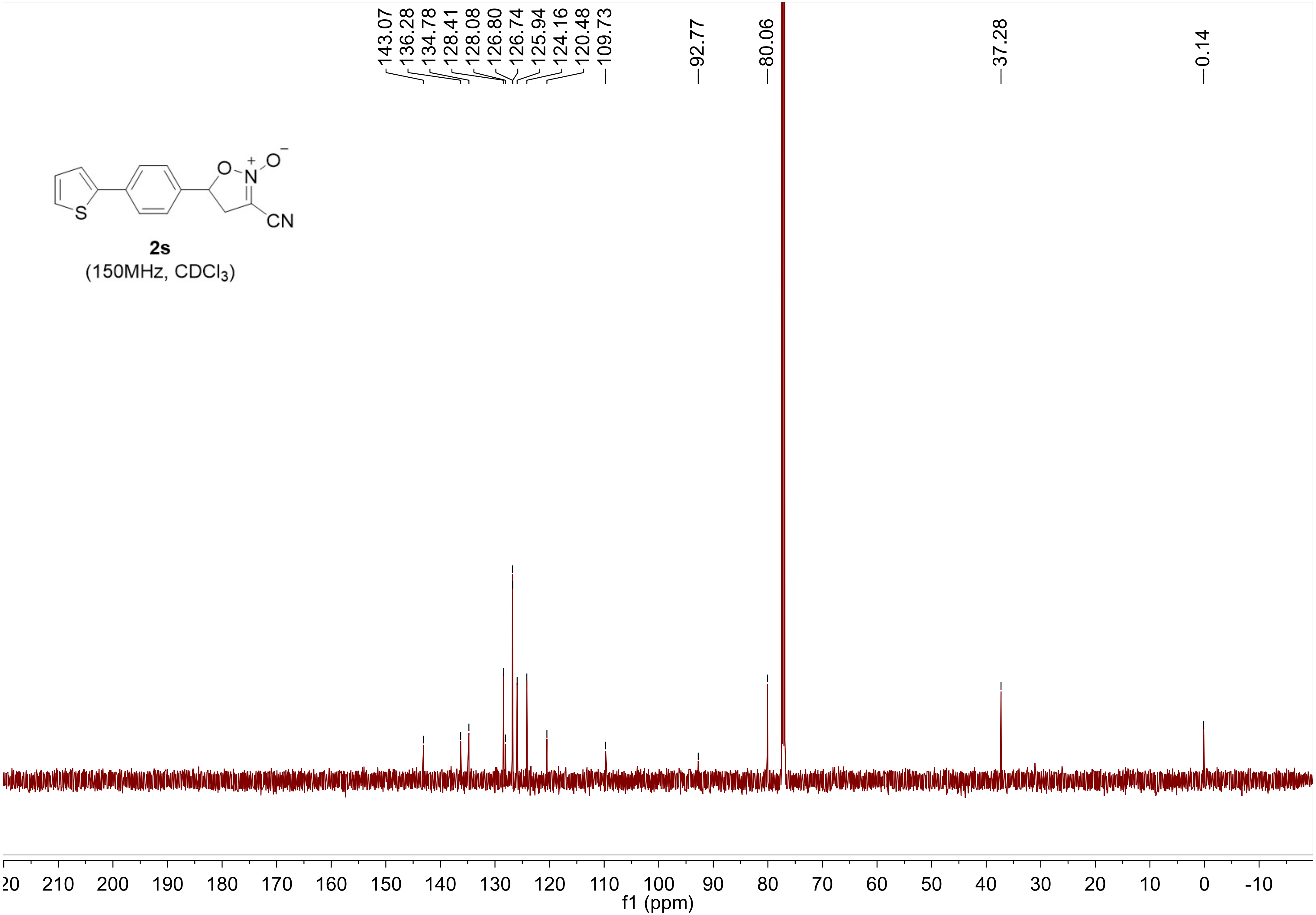
7.79
7.78
7.77
7.77
7.76
7.71
7.71
7.70
7.69
7.69
7.69
7.68
7.68
7.51
7.51
7.49
7.49
7.49
7.47
7.47
7.42
7.42
7.40
6.20
6.18
6.16
3.99
3.97
3.95
3.93
3.71
3.68
3.66
3.64
2r
(400MHz, Acetone-d_6)
2.05
4.16
2.09
1.01
0.97
0.98
0.96
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)


143.07
140.03
134.75
129.06
128.11
128.06
127.25
126.56
109.76
92.84
80.15
37.27
O
N
+
O
−
CN
2r
(150MHz, CDCl3)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)



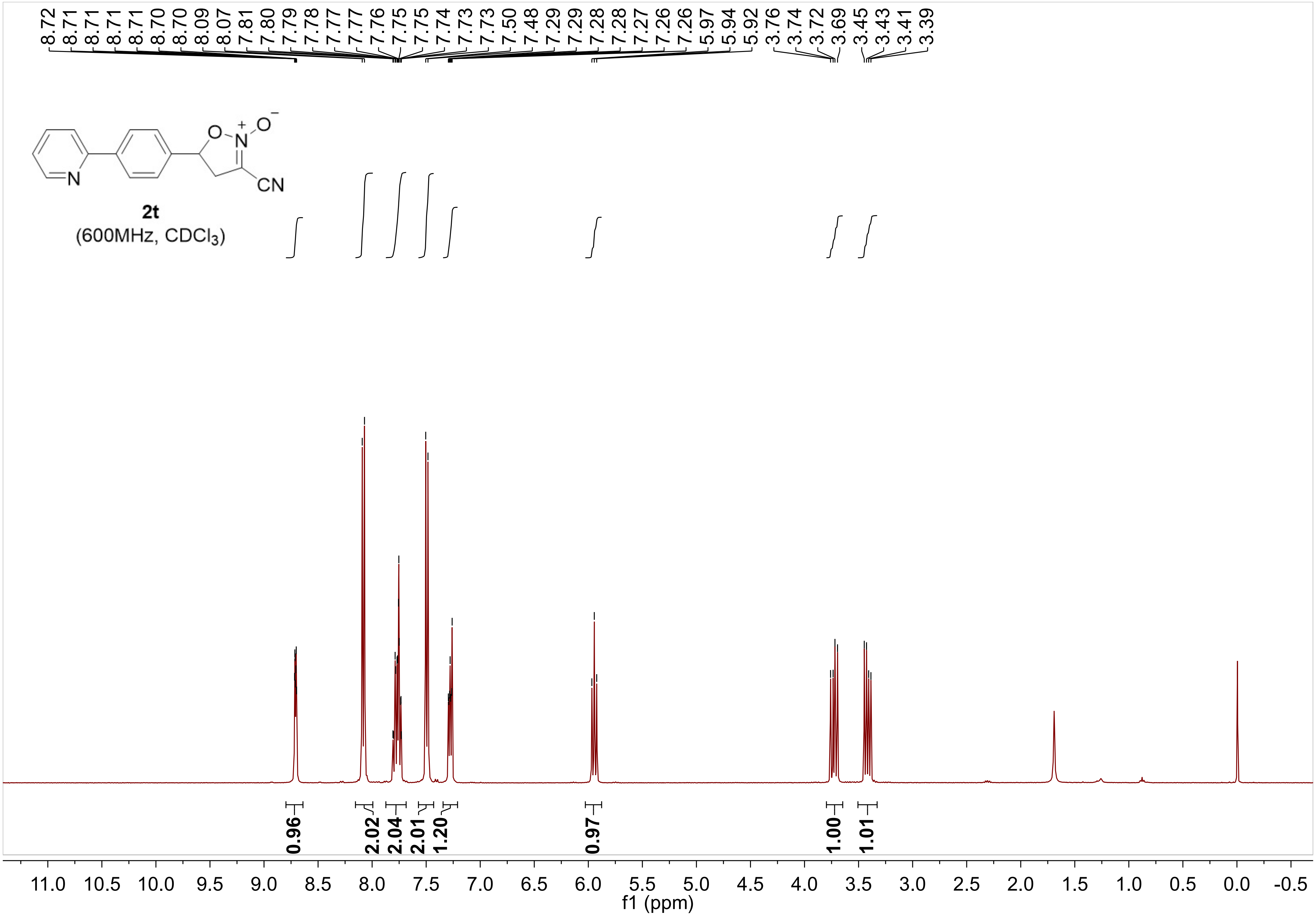
2s
(600MHz, $CDCl_3$)

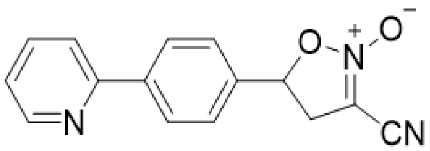




2s

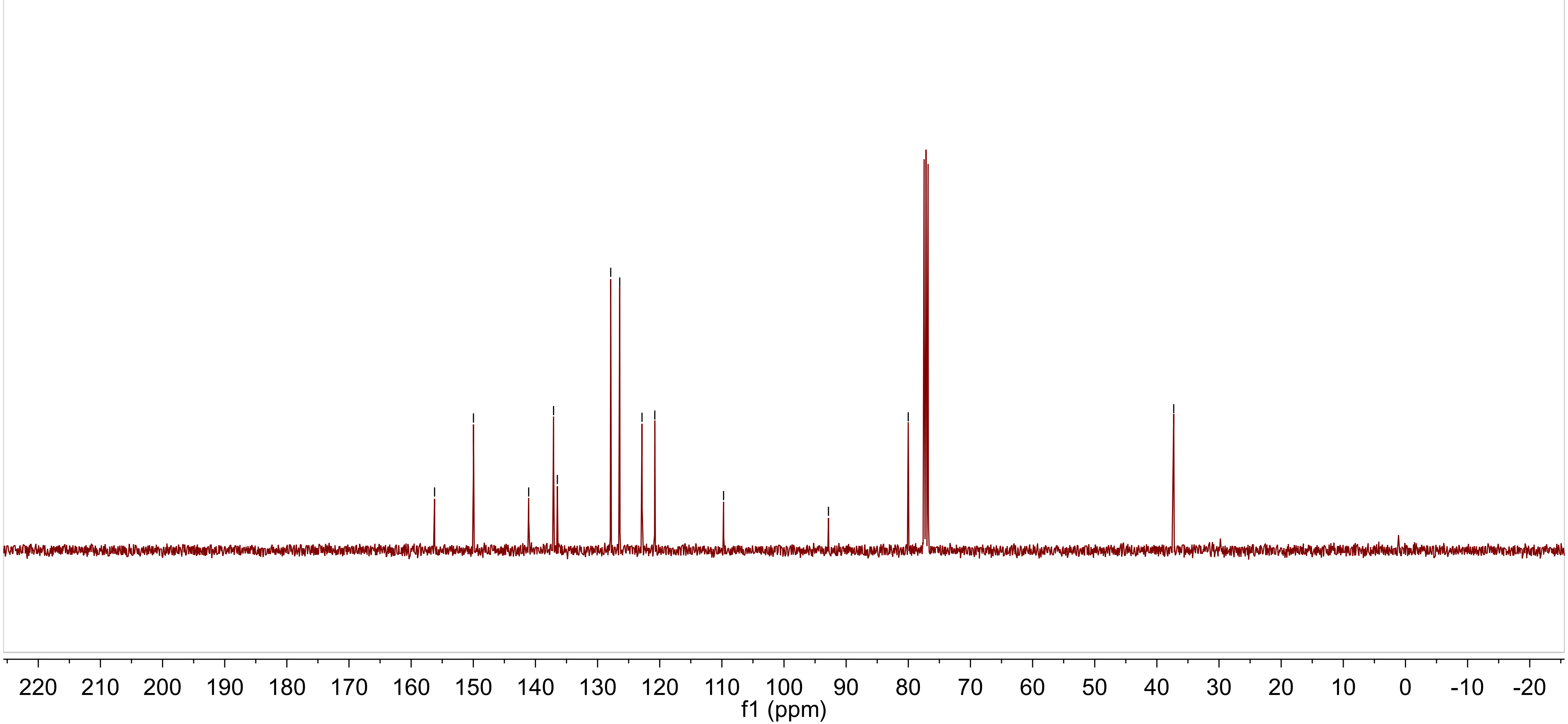
(150MHz, $CDCl_3$)

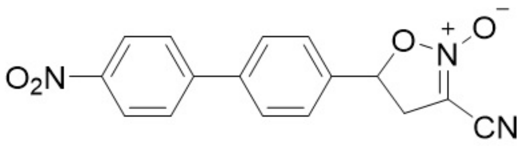

8.72 8.71 8.71 8.71 8.71 8.70 8.70 8.09 8.07 7.81 7.80 7.79 7.78 7.77 7.77 7.76 7.75 7.75 7.74 7.73 7.73 7.50 7.48 7.29 7.29 7.28 7.28 7.27 7.26 7.26 5.97 5.94 5.92 3.76 3.74 3.72 3.69 3.45 3.43 3.41 3.39
2t
(600MHz, $CDCl_3$)
0.96 2.02 2.04 2.01 1.20 0.97 1.00 1.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



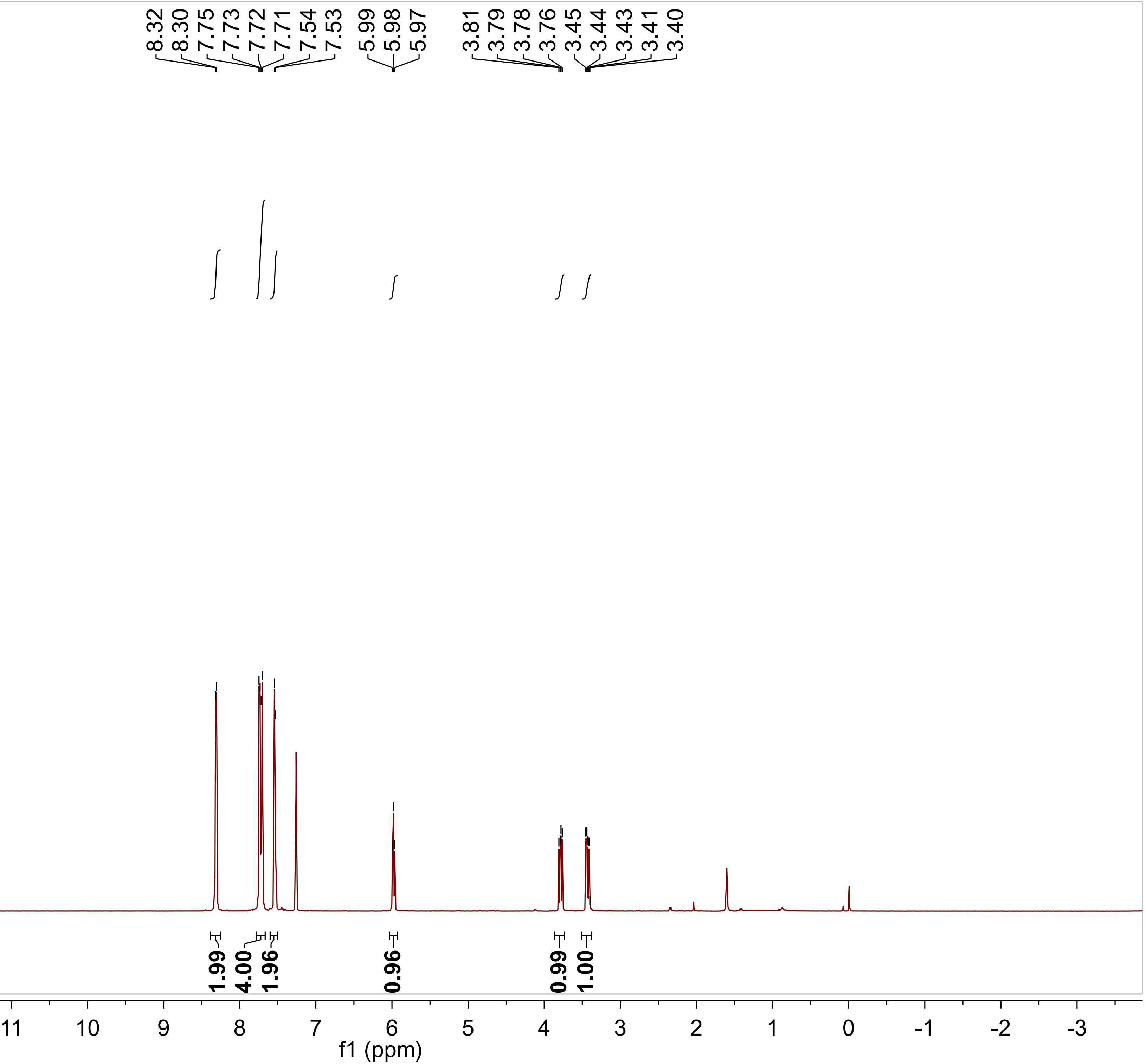
2t

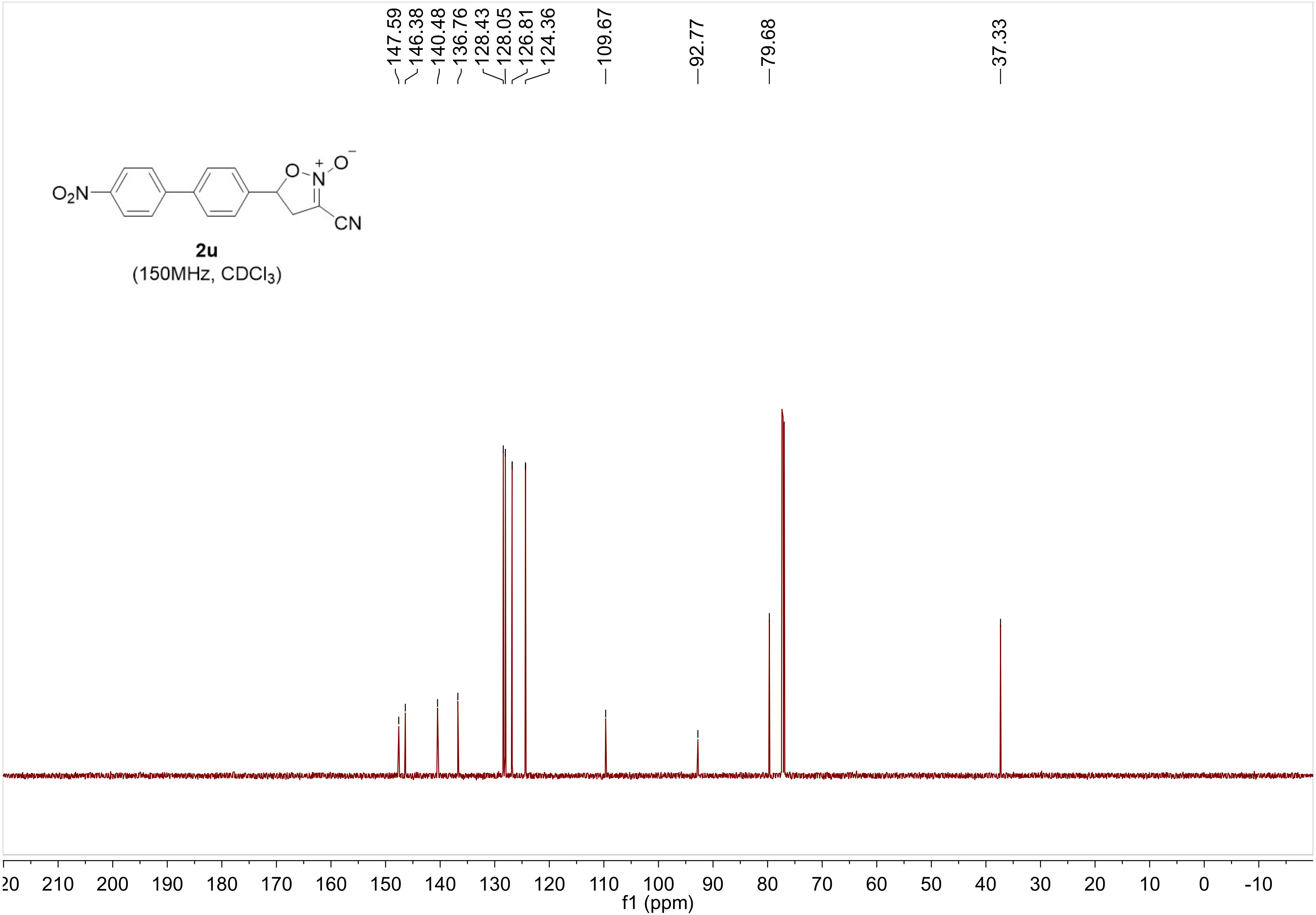
(150MHz, $CDCl_3$)

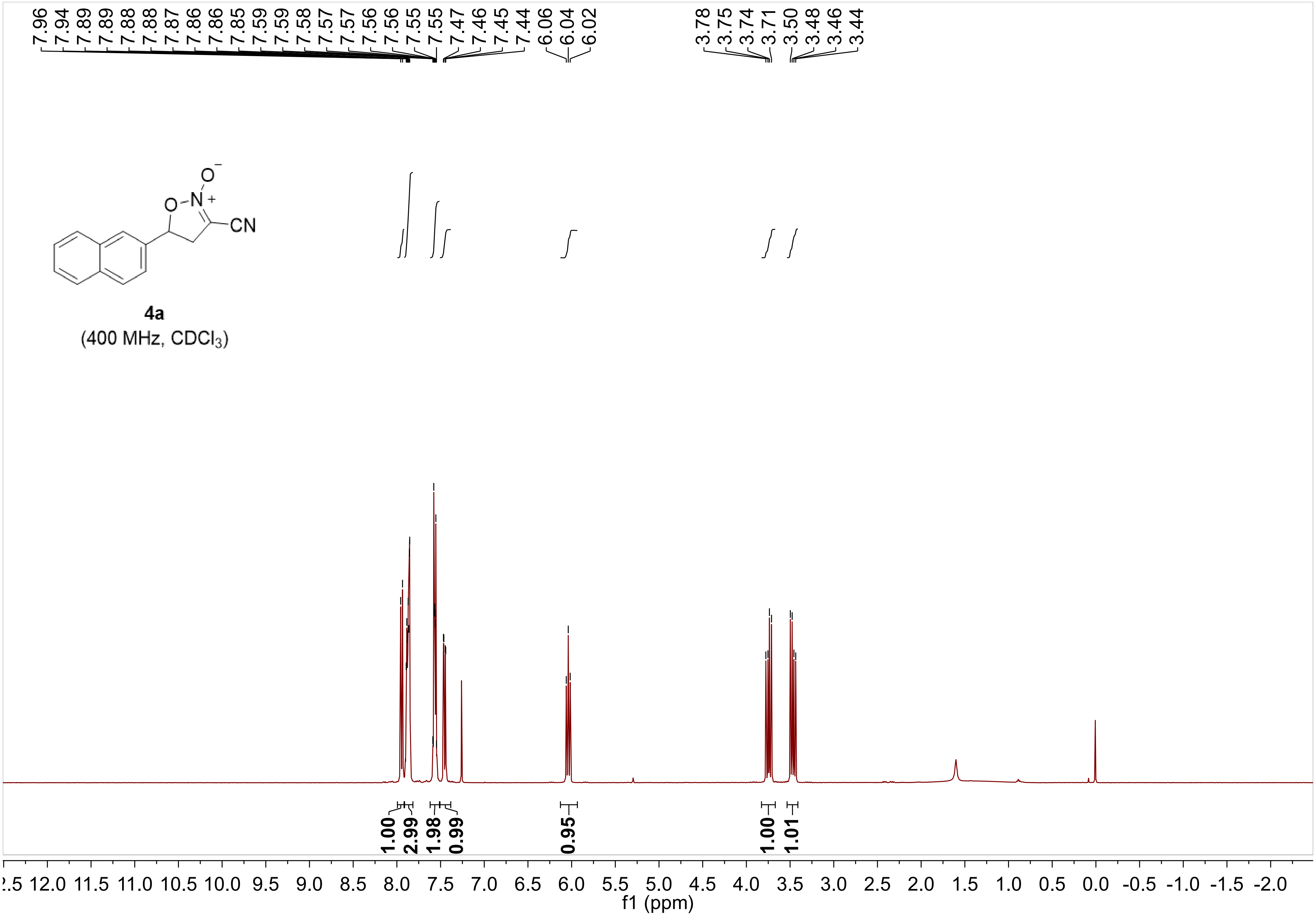


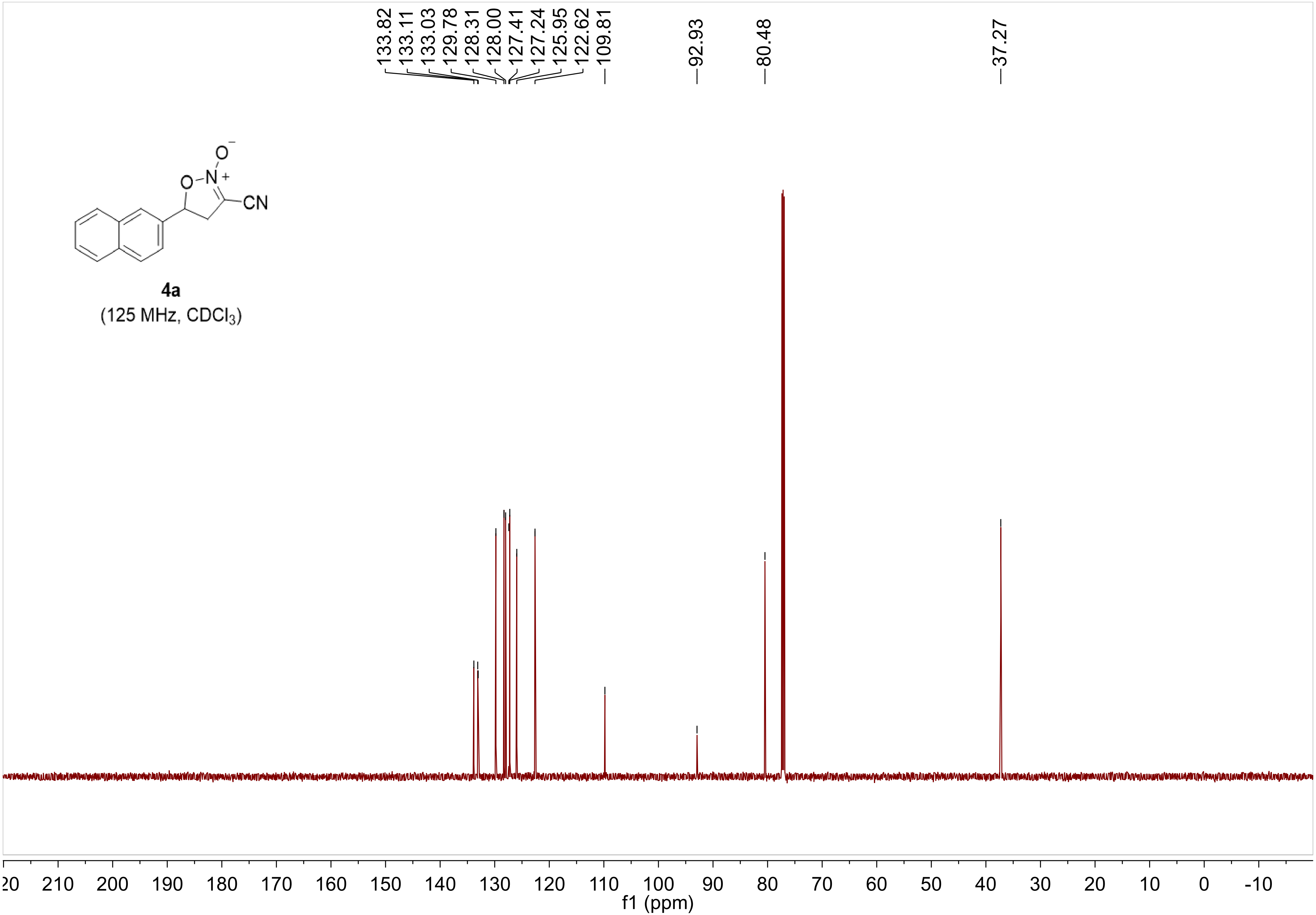


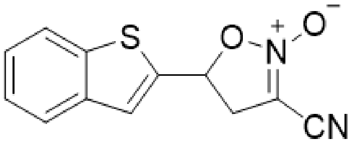
2u
(600MHz, $CDCl_3$)




147.59
146.38
140.48
136.76
128.43
128.05
126.81
124.36
109.67
92.77
79.68
37.33
O_2N
O
N
+
O
−
CN
2u
(150MHz, $CDCl_3$)
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

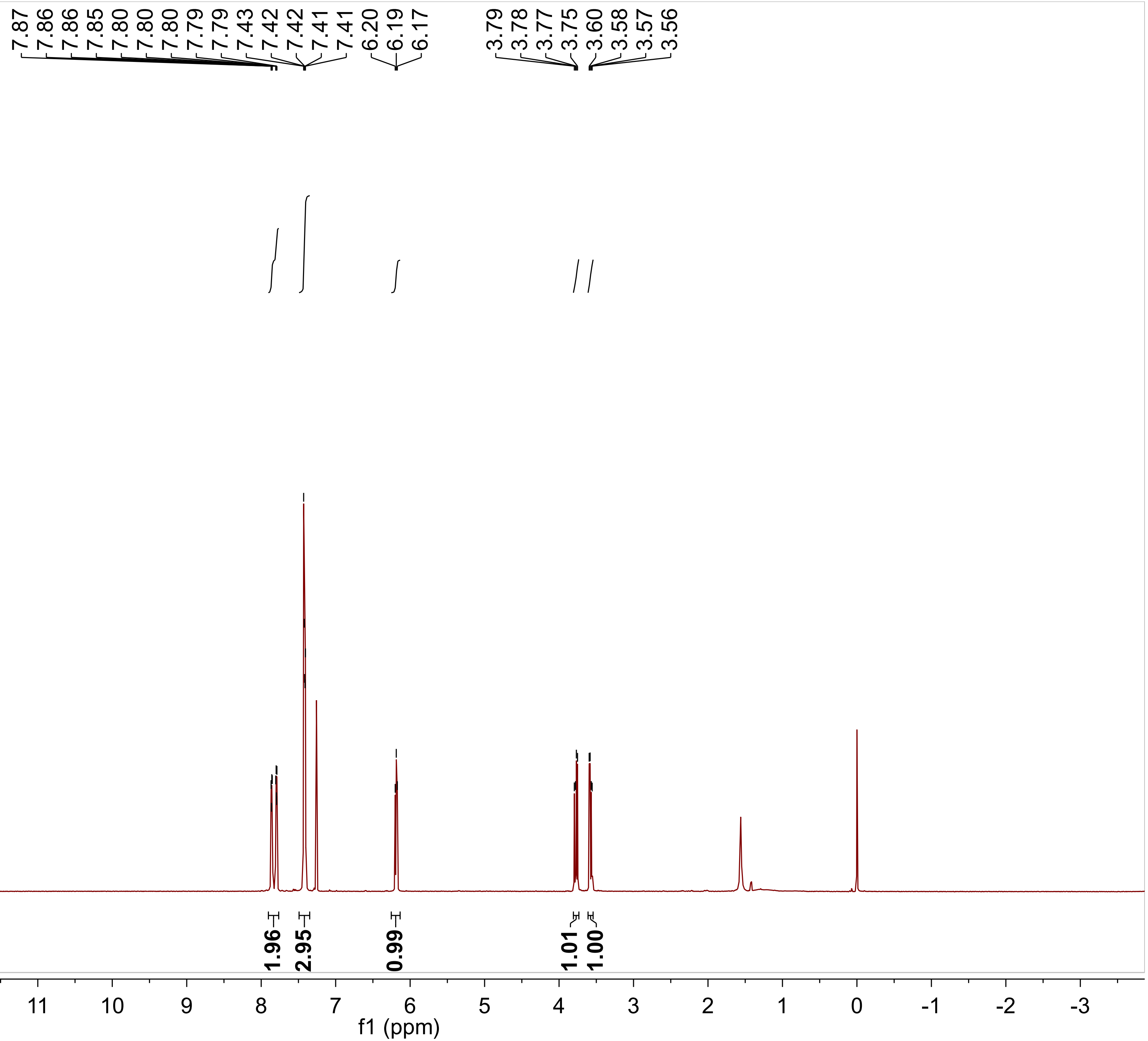

7.96 7.94 7.89 7.89 7.88 7.88 7.87 7.86 7.86 7.85 7.59 7.59 7.58 7.57 7.57 7.56 7.56 7.55 7.55 7.47 7.46 7.45 7.44 6.06 6.04 6.02
3.78 3.75 3.74 3.71 3.50 3.48 3.46 3.44
O
O
N
+
CN
4a
(400 MHz, CDCl3)
1.00 2.99 1.98 0.99
0.95
1.00 1.01
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

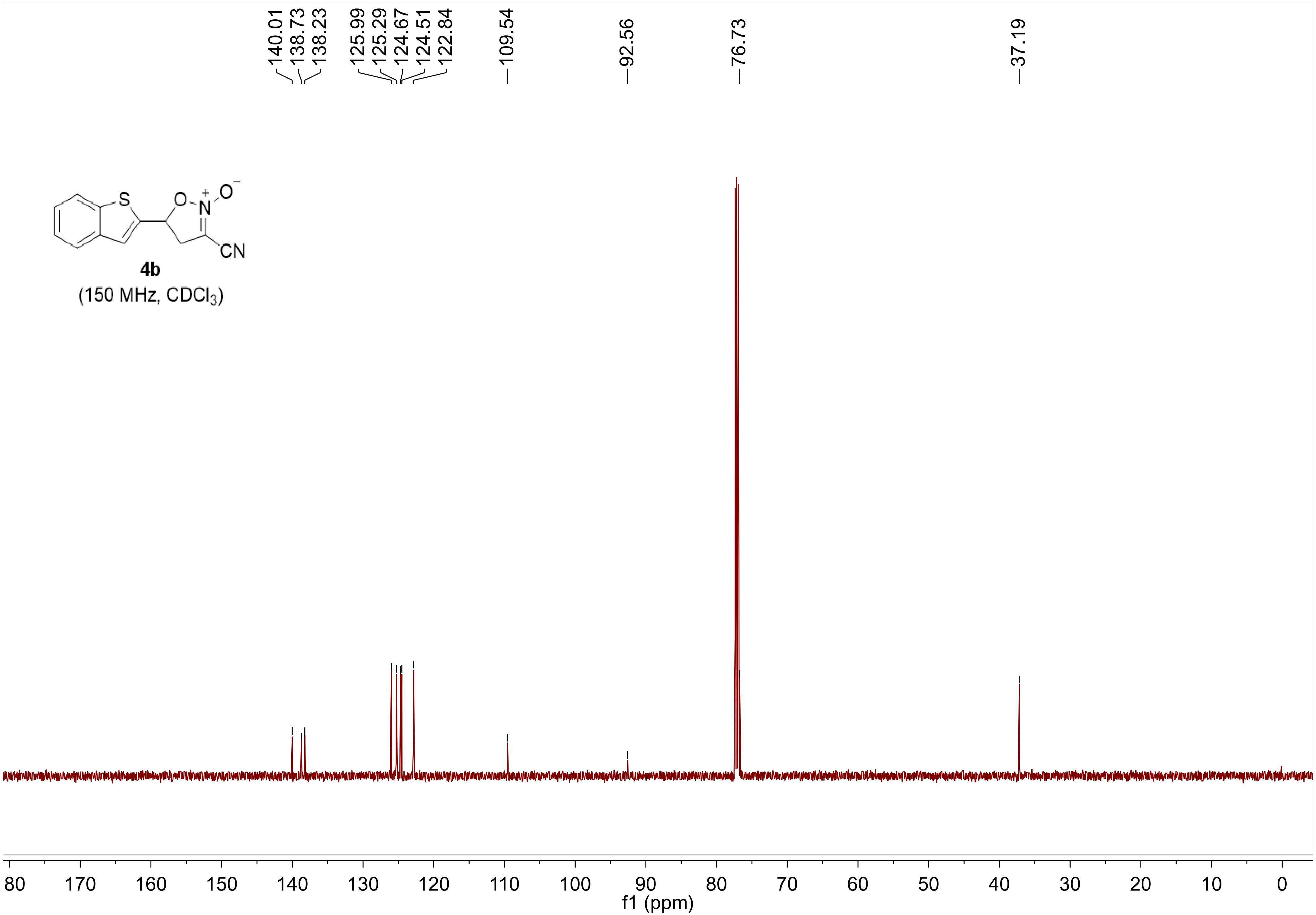

133.82
133.11
133.03
129.78
128.31
128.00
127.41
127.24
125.95
122.62
109.81
92.93
80.48
37.27
CN
4a
(125 MHz, CDCl3)
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

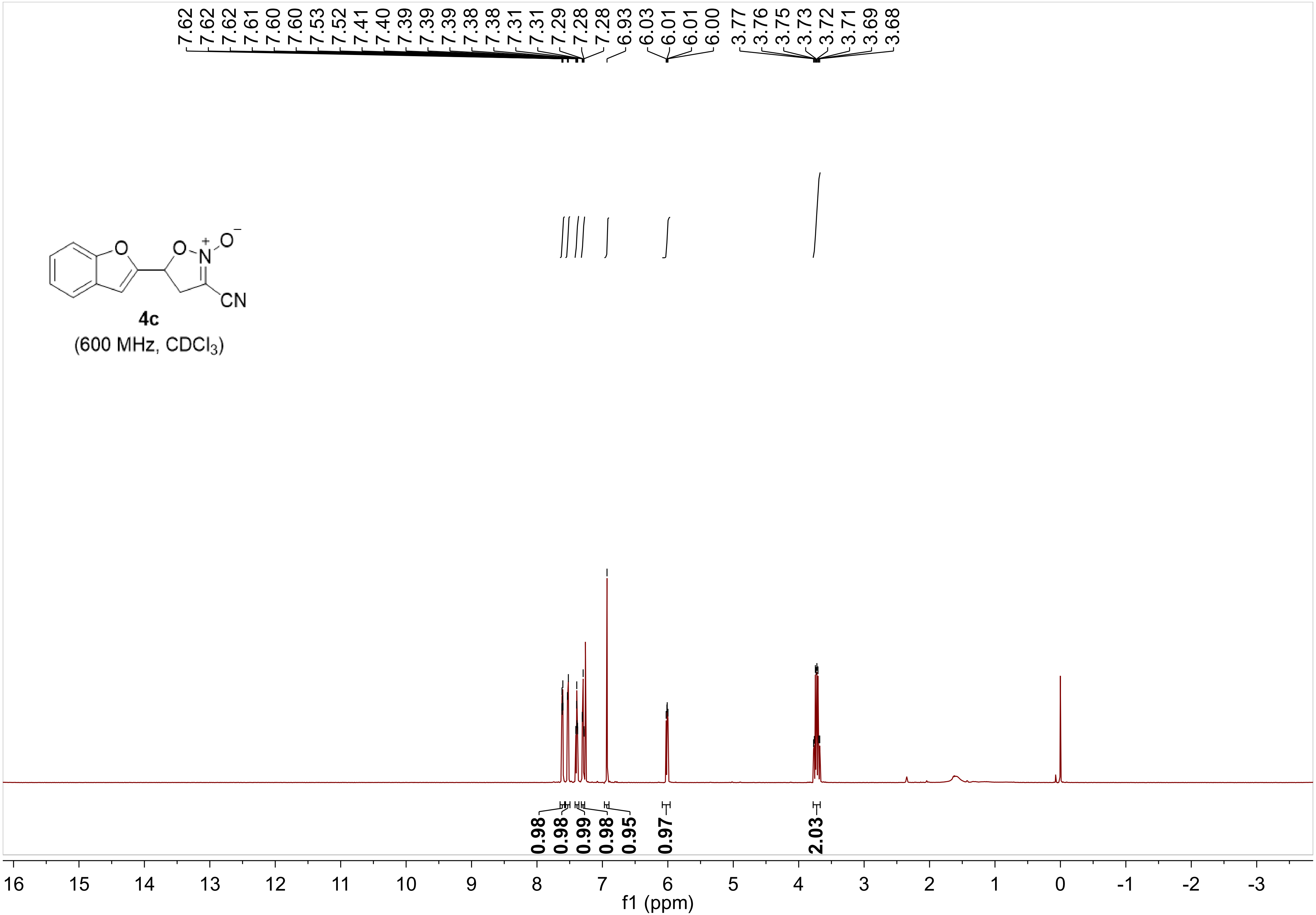


4b

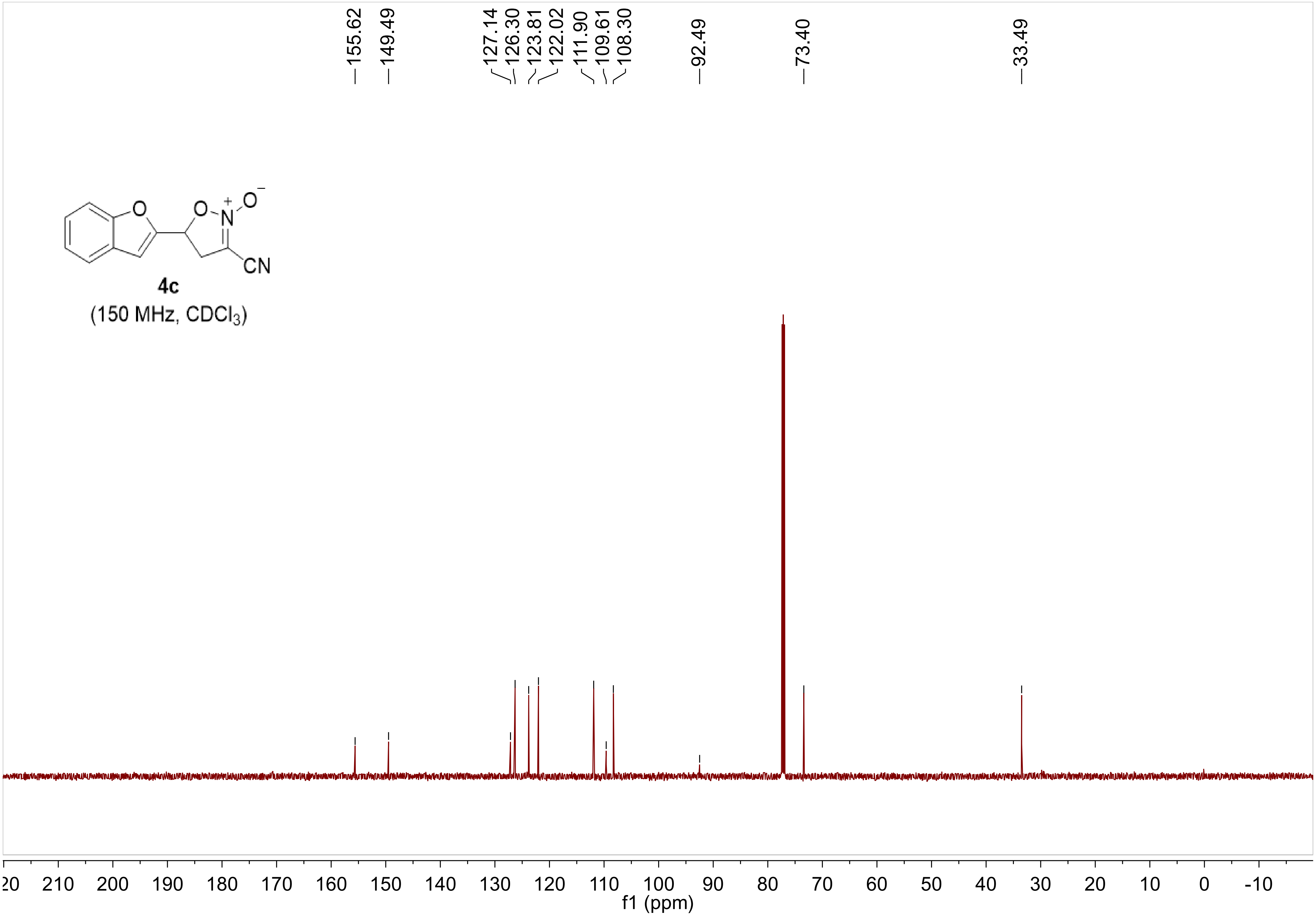
(600 MHz, $CDCl_3$)

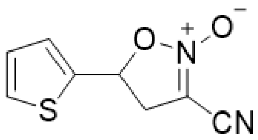



140.01
138.73
138.23
125.99
125.29
124.67
124.51
122.84
109.54
92.56
76.73
37.19
S
O
N
O
CN
4b
(150 MHz, $CDCl_3$)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



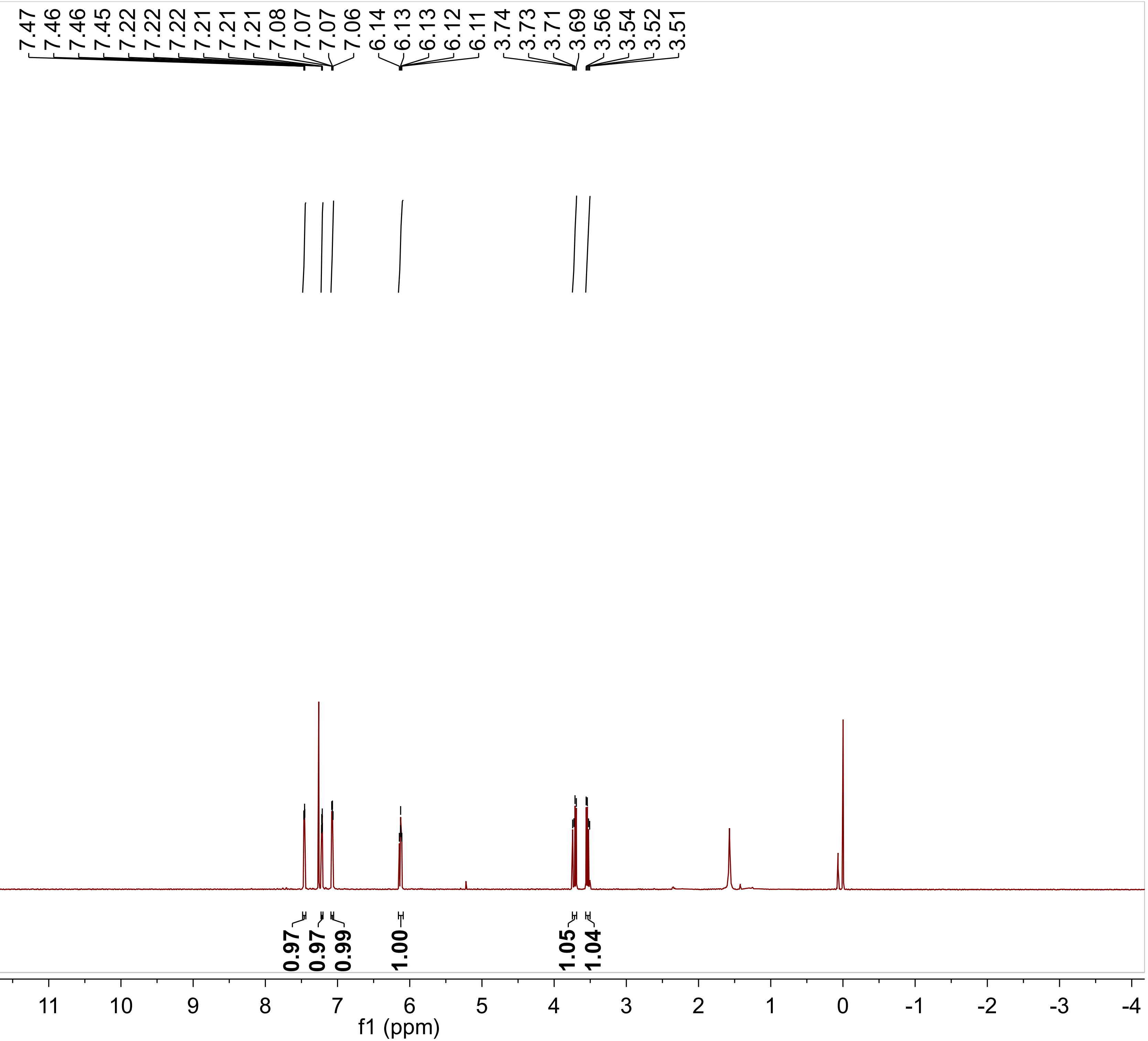
7.62 7.62 7.62 7.61 7.60 7.60 7.53 7.52 7.41 7.40 7.39 7.39 7.39 7.38 7.38 7.31 7.31 7.29 7.28 7.28 6.93 6.03 6.01 6.01 6.00 3.77 3.76 3.75 3.73 3.72 3.71 3.69 3.68
4c
(600 MHz, CDCl3)
0.98 0.98 0.99 0.98 0.95 0.97 2.03
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

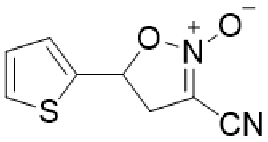

155.62
149.49
127.14
126.30
123.81
122.02
111.90
109.61
108.30
92.49
73.40
33.49
O
O
N
+
O
−
CN
4c
(150 MHz, CDCl3)
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



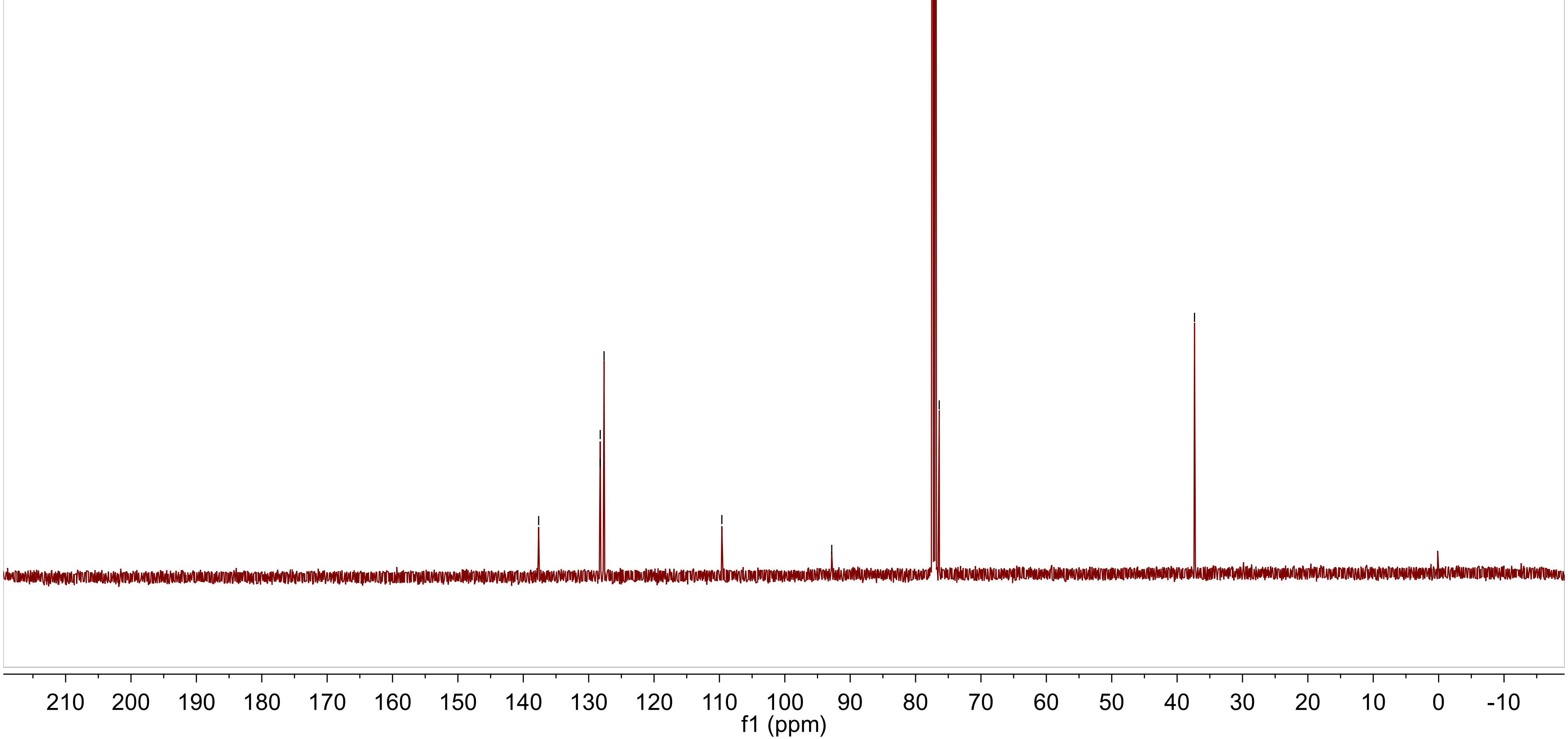
4d

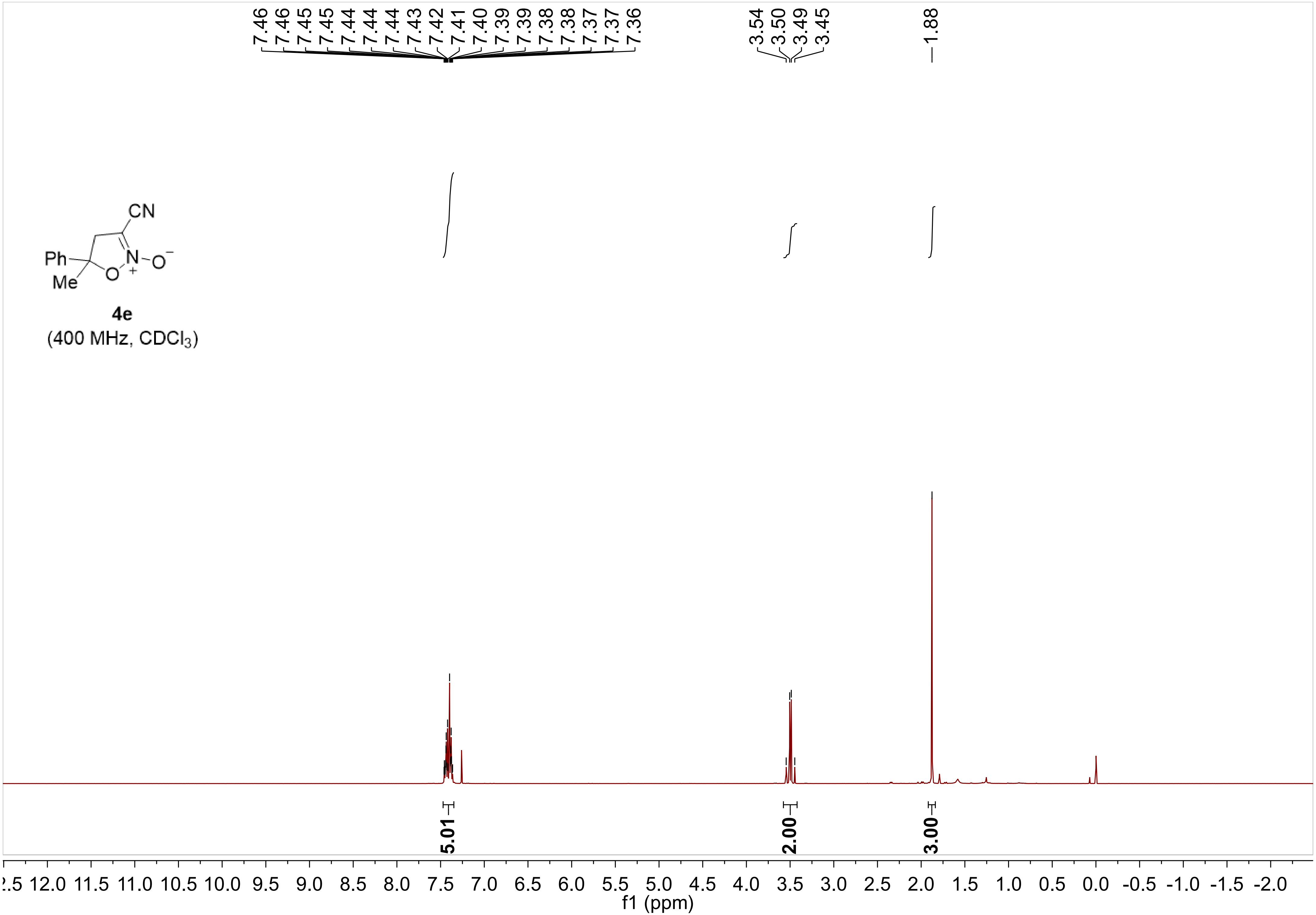
(500 MHz, $CDCl_3$)



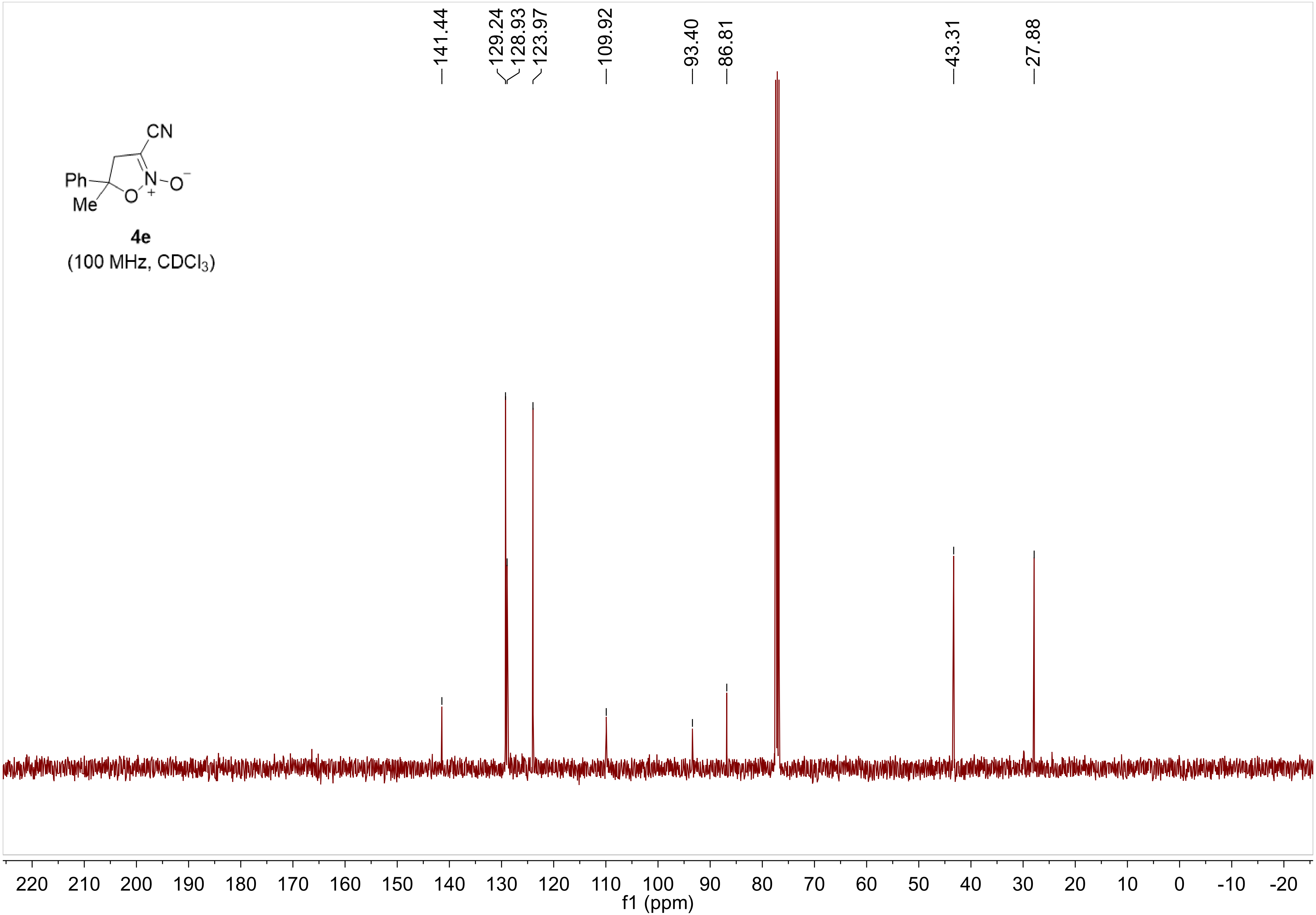


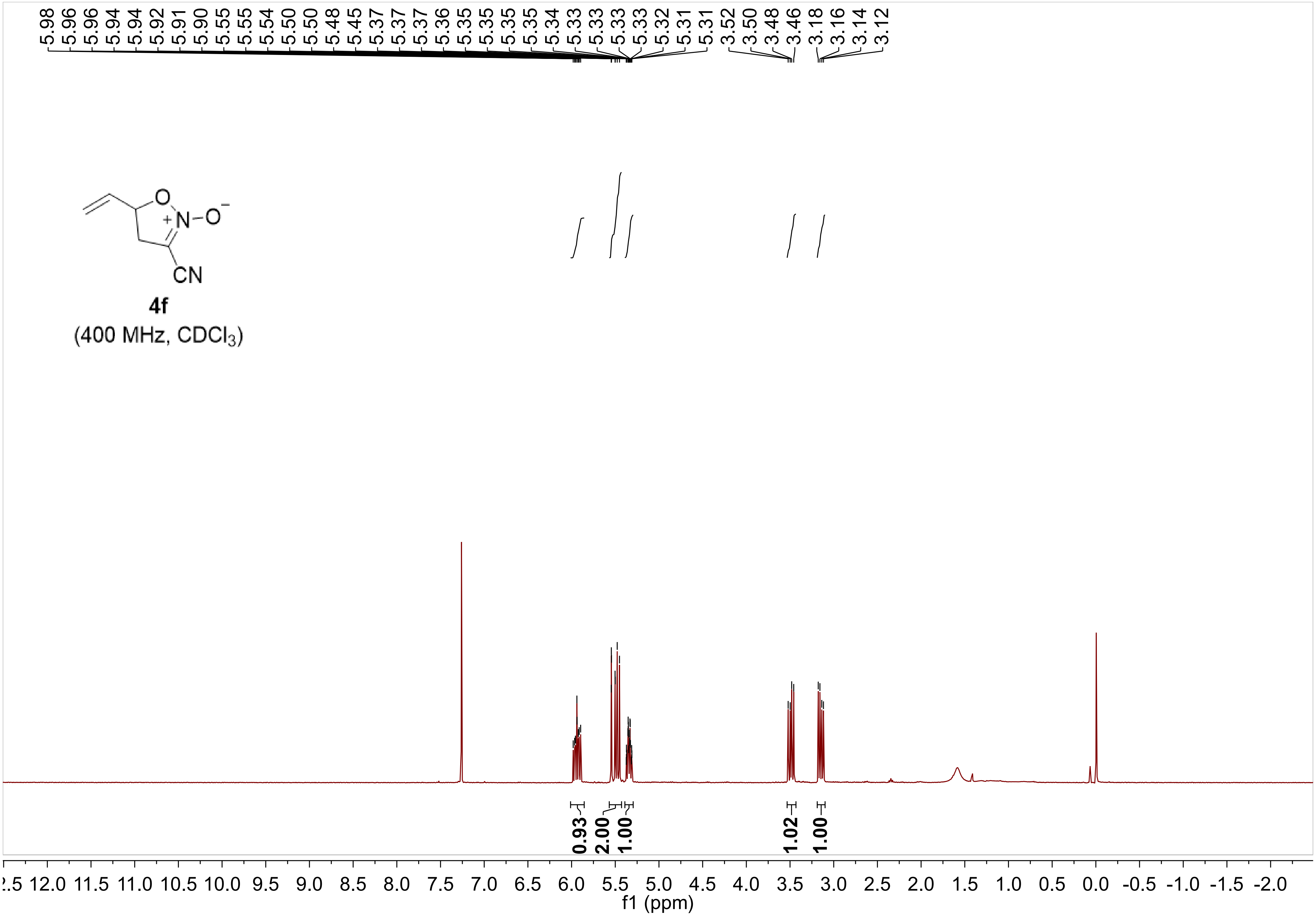
4d
(125 MHz, $CDCl_3$)

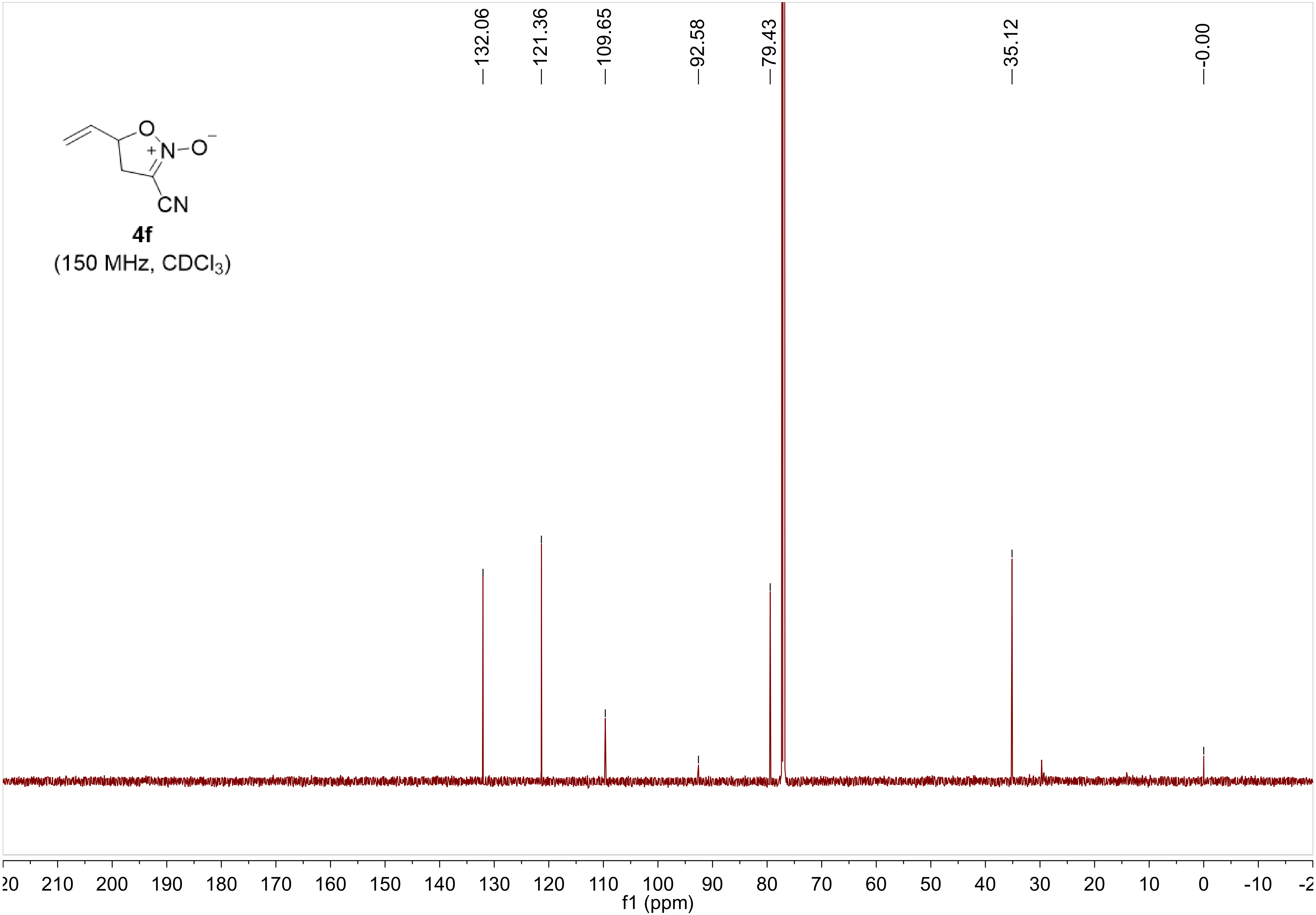




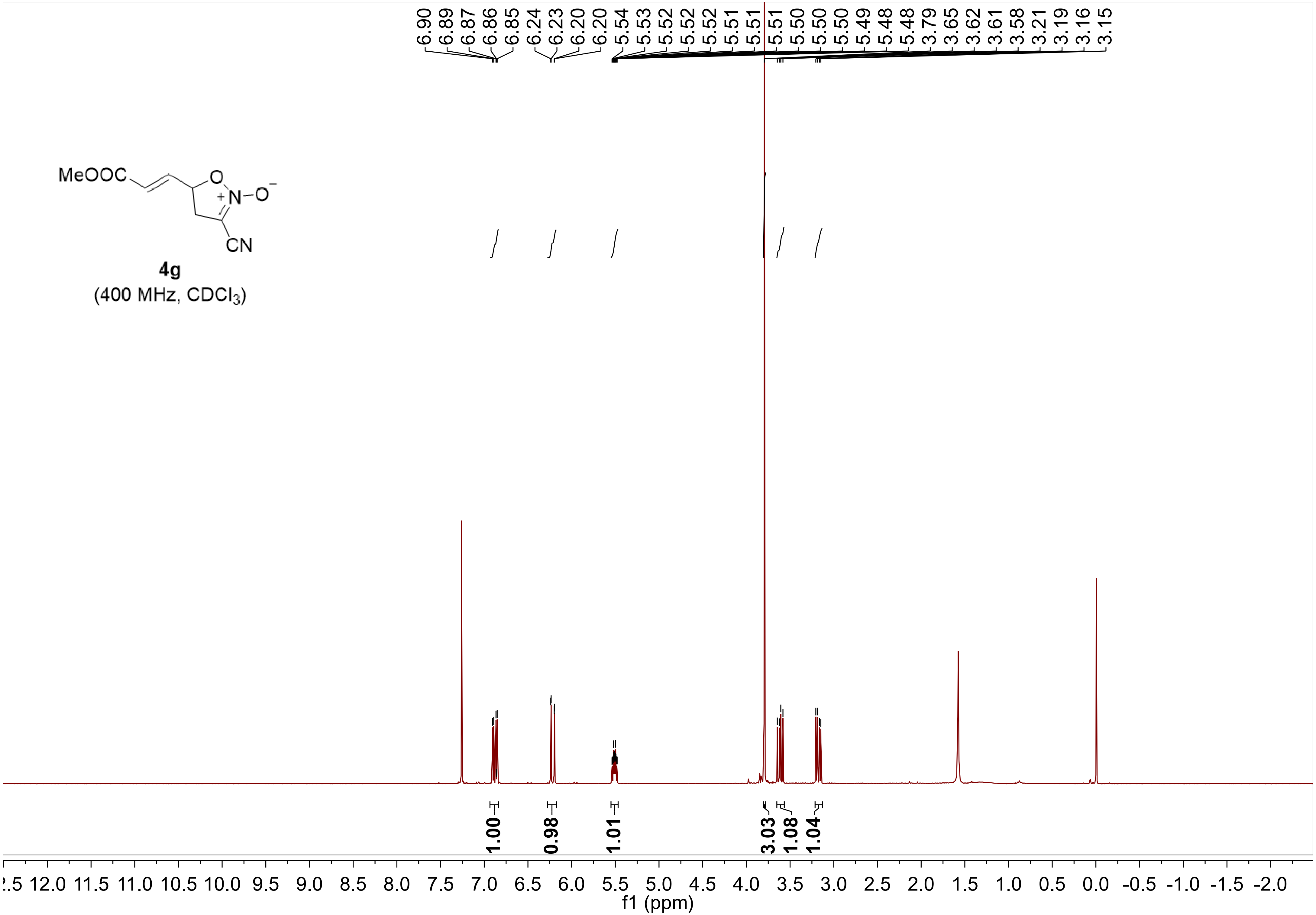
7.46
7.46
7.45
7.45
7.44
7.44
7.44
7.43
7.42
7.41
7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.36
3.54
3.50
3.49
3.45
1.88
CN
Ph
Me
O
N
O
4e
(400 MHz, CDCl3)
5.01
2.00
3.00
f1 (ppm)

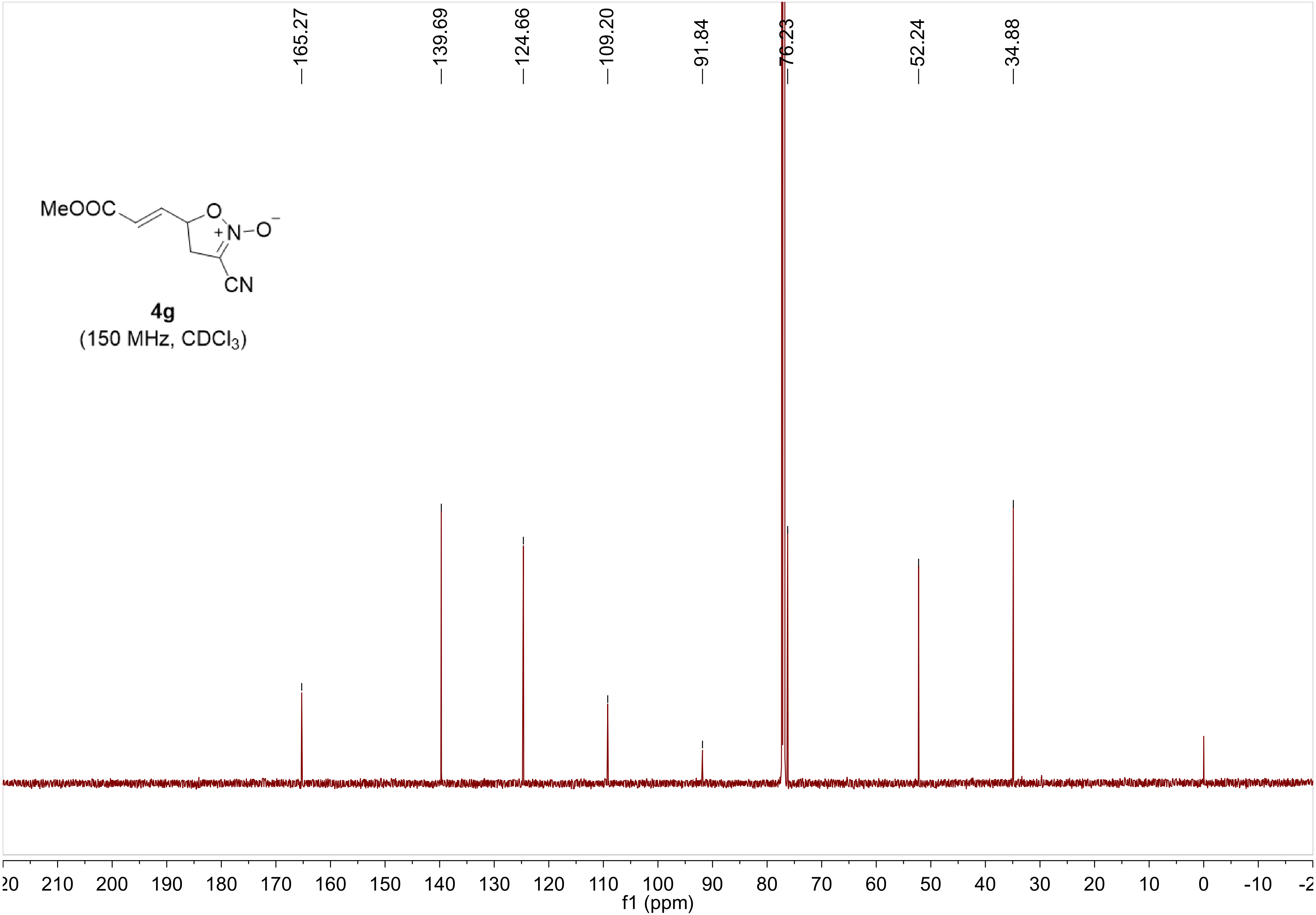

141.44
129.24
128.93
123.97
109.92
93.40
86.81
43.31
27.88
CN
Ph
Me
N
O
O
4e
(100 MHz, CDCl3)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


5.98 5.96 5.96 5.94 5.94 5.92 5.91 5.90 5.55 5.55 5.54 5.50 5.50 5.48 5.45 5.37 5.37 5.37 5.36 5.35 5.35 5.35 5.35 5.34 5.33 5.33 5.33 5.33 5.32 5.31 5.31 3.52 3.50 3.48 3.46 3.18 3.16 3.14 3.12
O
N
O
CN
4f
(400 MHz, $CDCl_3$)
0.93
2.00
1.00
1.02
1.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

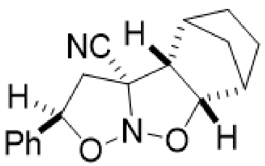


132.06
121.36
109.65
92.58
79.43
35.12
-0.00
O
+N
O−
CN
4f
(150 MHz, CDCl3)
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-2
f1 (ppm)

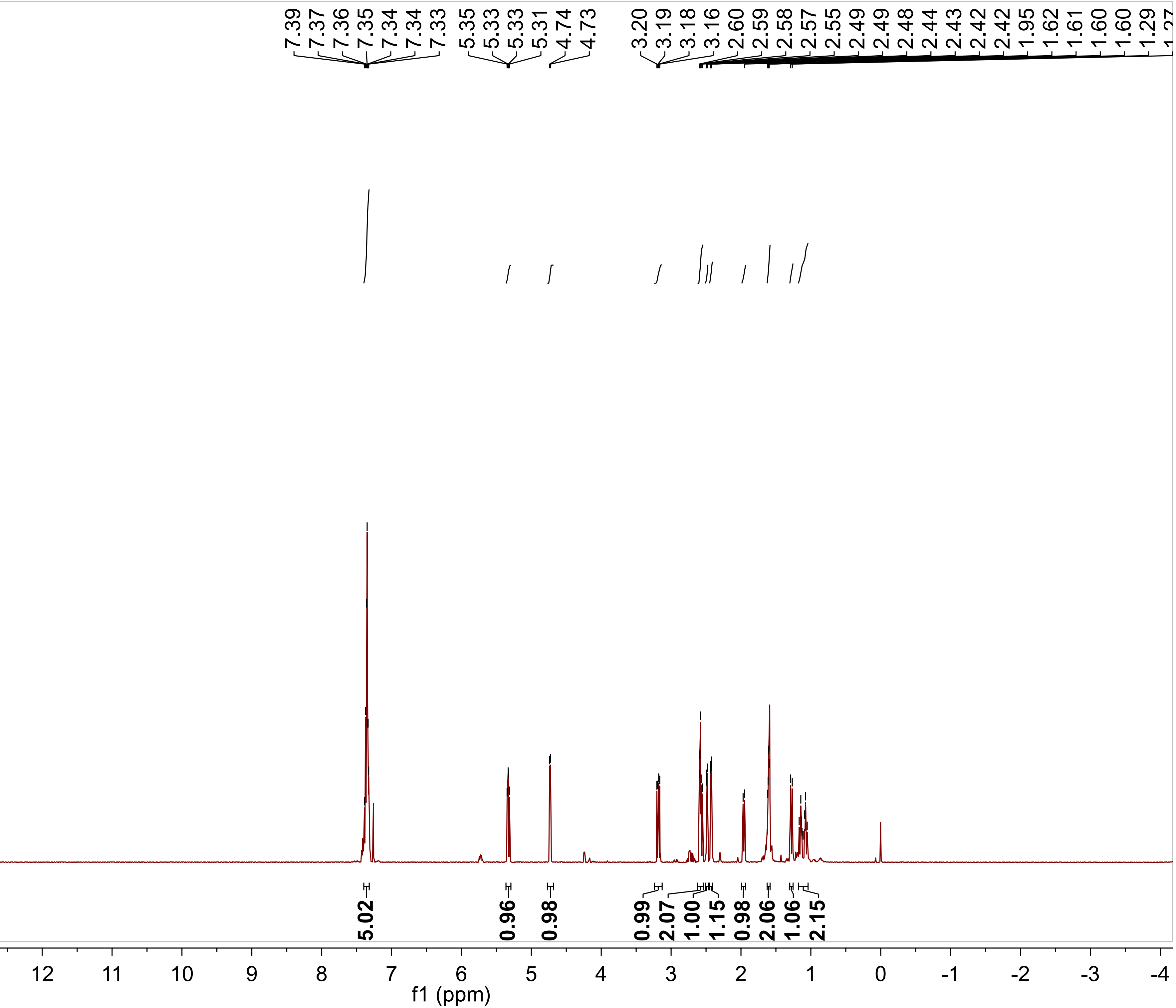

6.90 6.89 6.87 6.86 6.85 6.24 6.23 6.20 6.20 5.54 5.53 5.52 5.52 5.52 5.51 5.51 5.51 5.50 5.50 5.50 5.49 5.48 5.48 3.79 3.65 3.62 3.61 3.58 3.21 3.19 3.16 3.15
MeOOC
O
N
O
CN
4g
(400 MHz, $CDCl_3$)
1.00
0.98
1.01
3.03
1.08
1.04
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

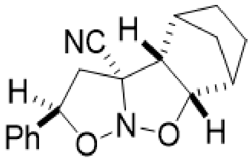


4g
(150 MHz, $CDCl_3$)

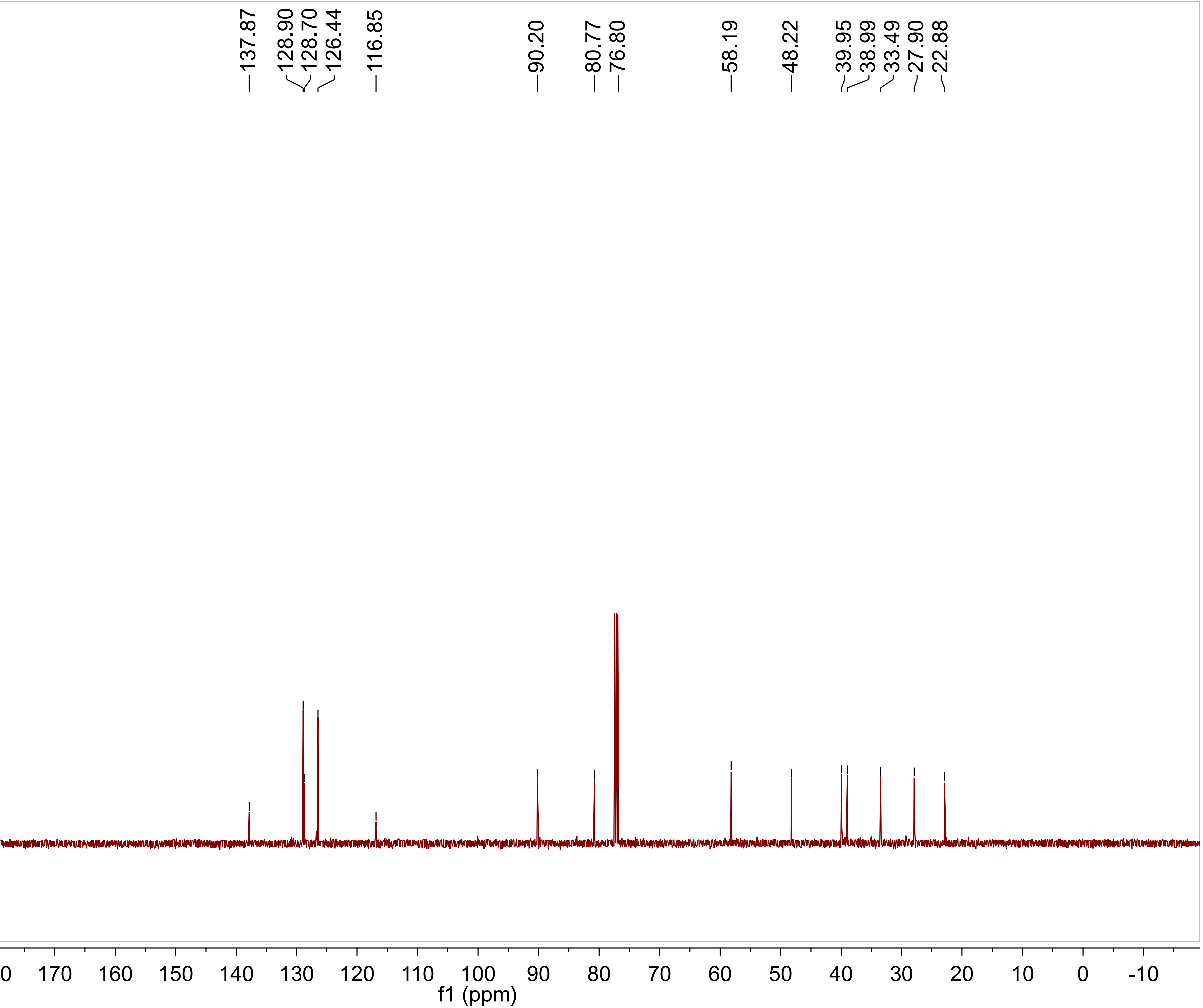


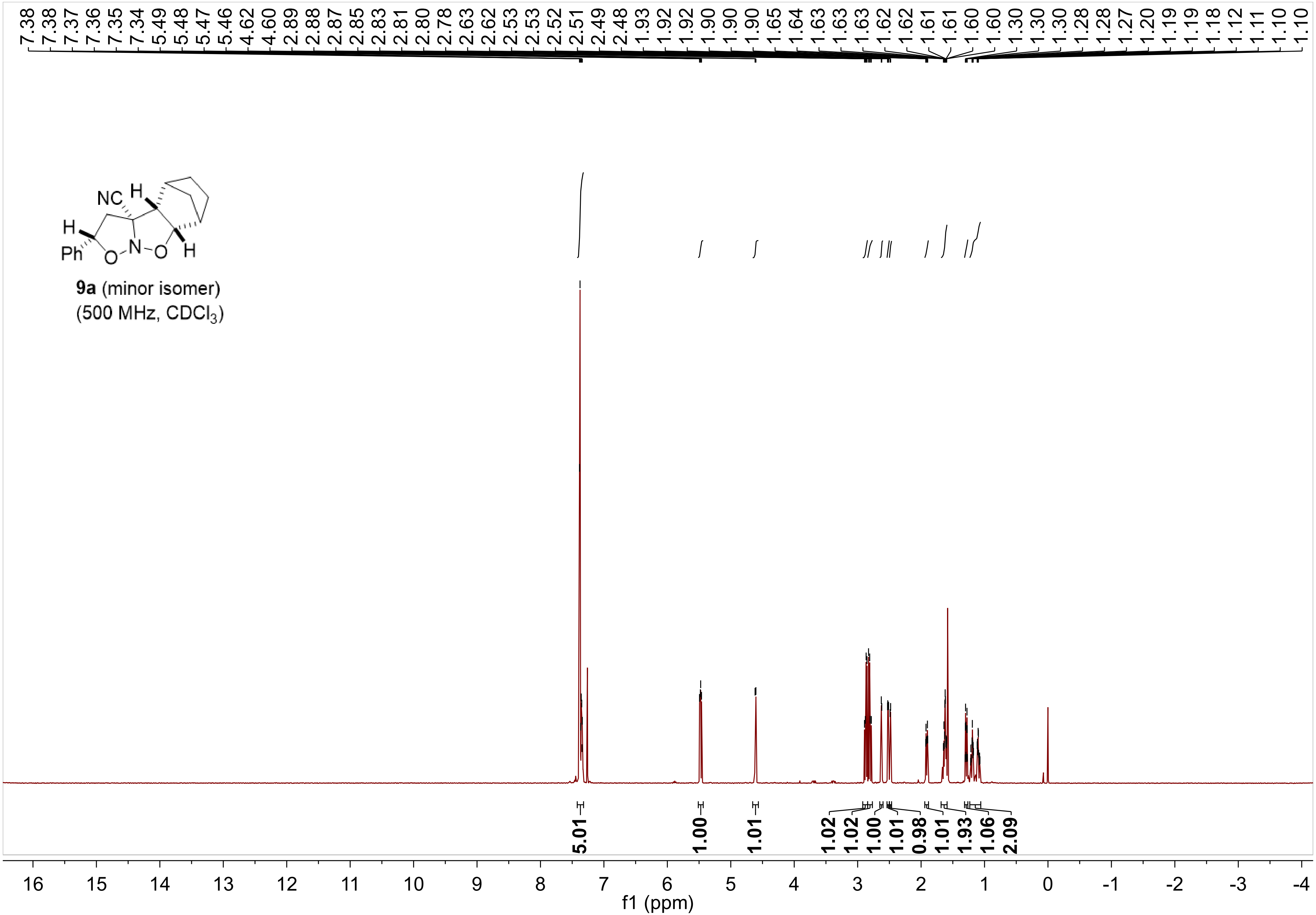
9a (major isomer)
(500 MHz, $CDCl_3$)

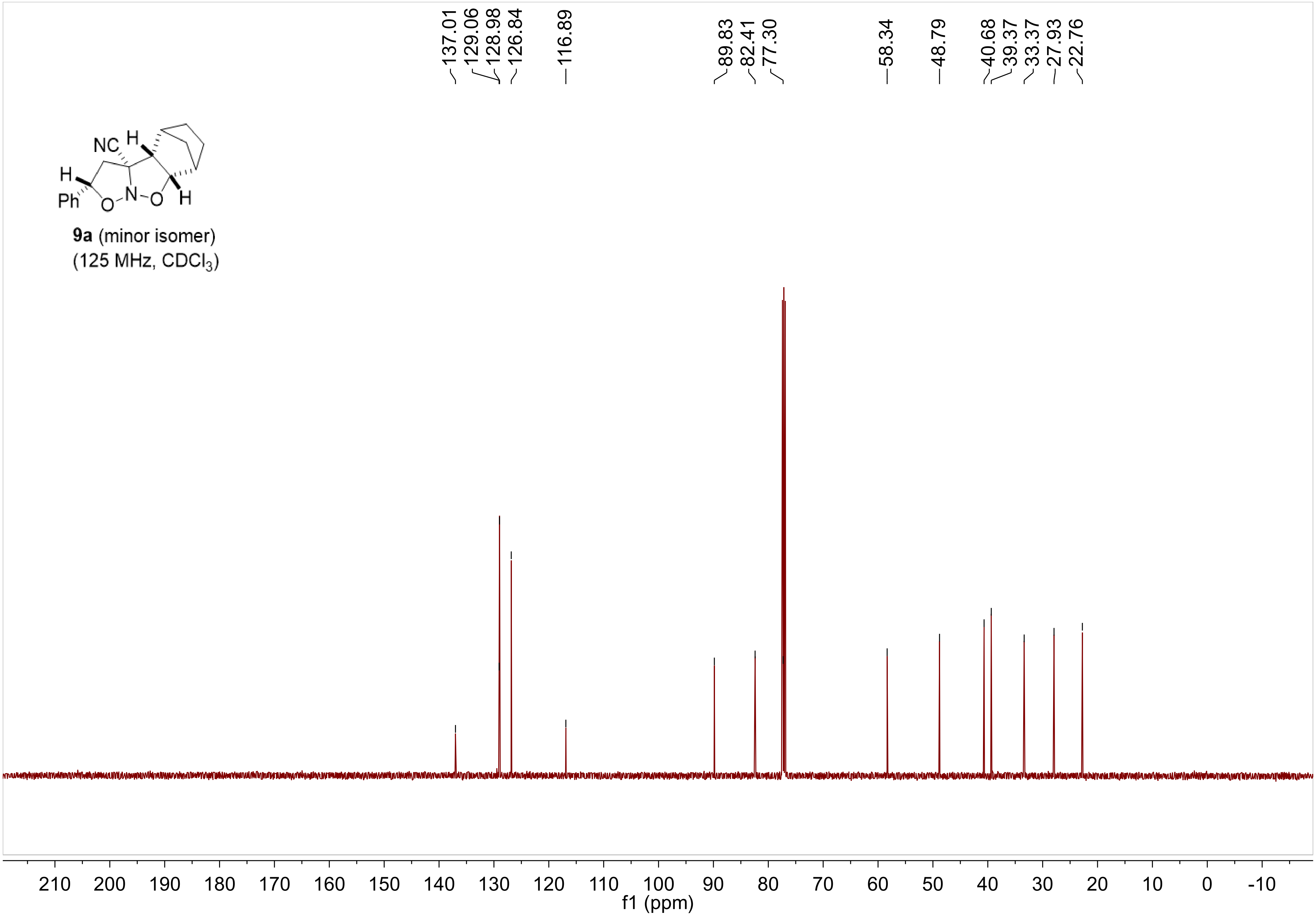


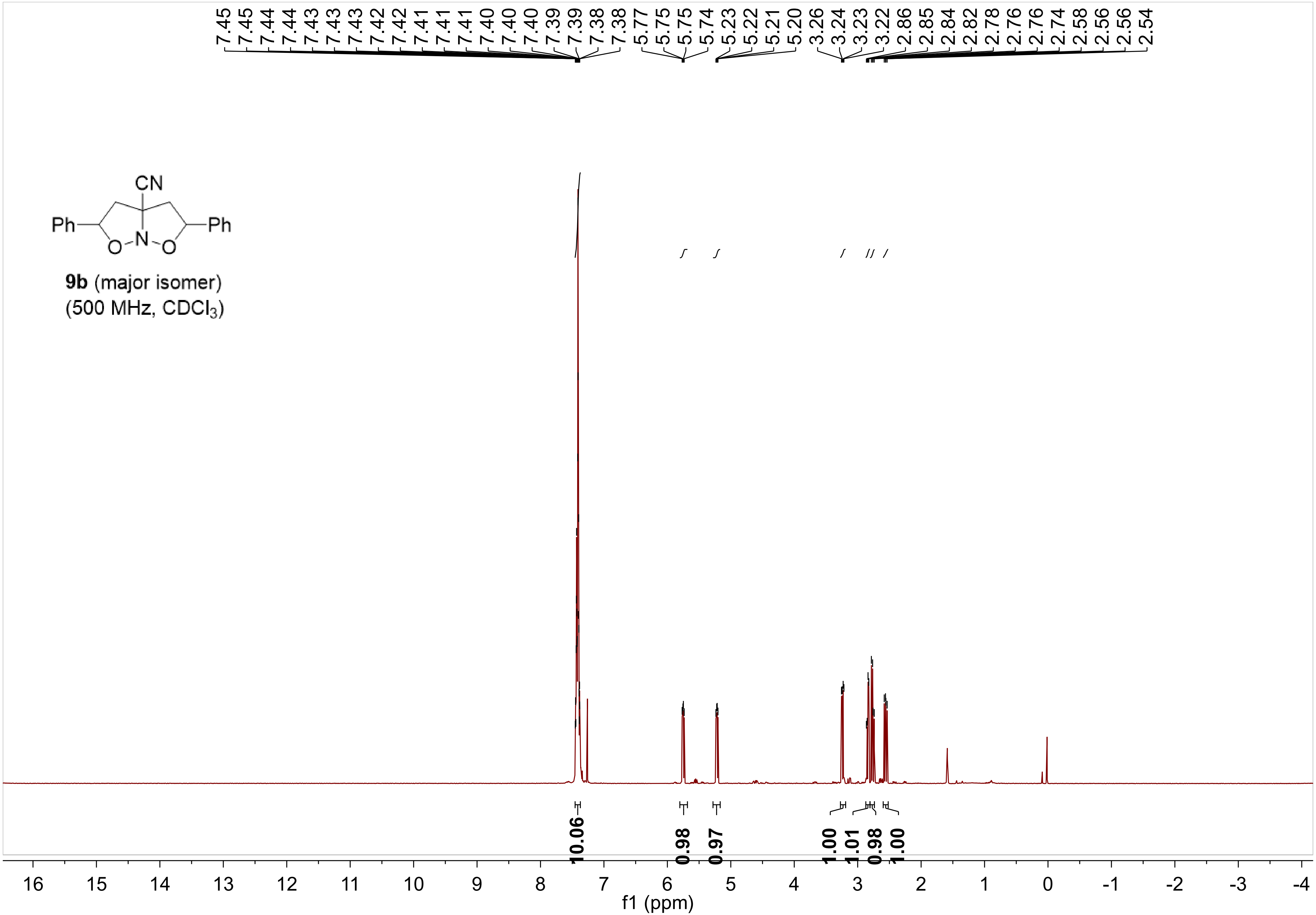


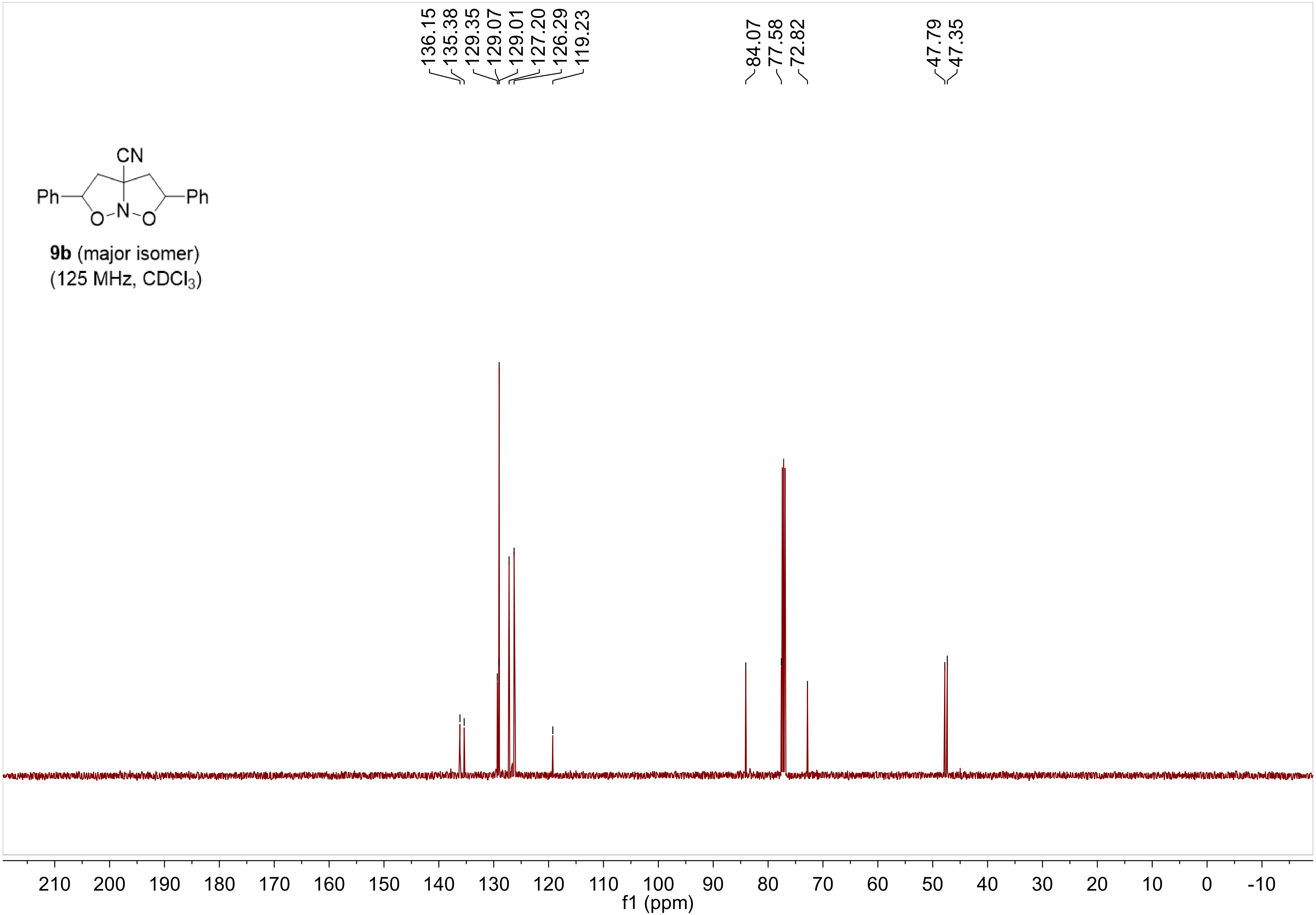
9a (major isomer)
(125 MHz, $CDCl_3$)

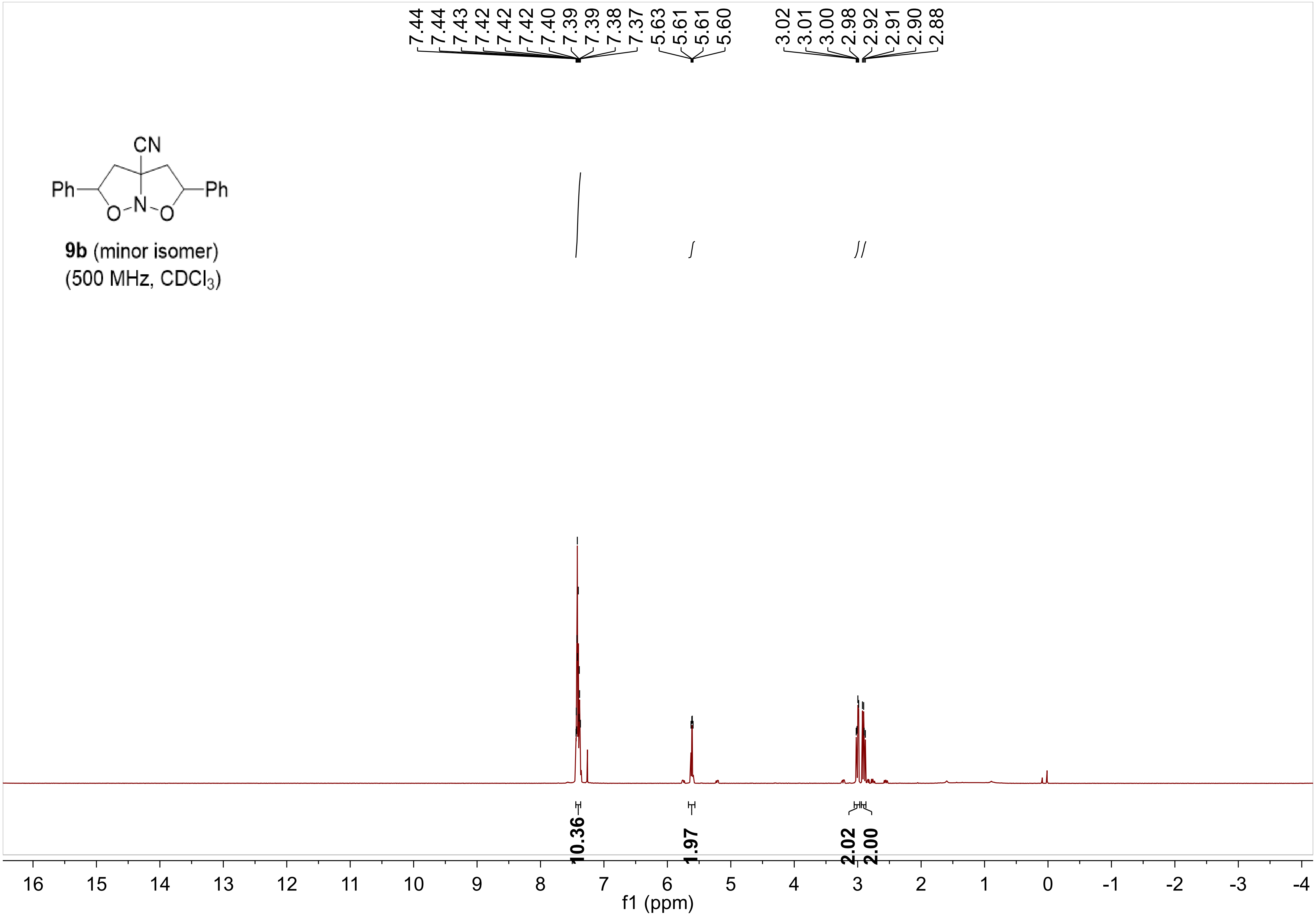



7.38 7.38 7.37 7.36 7.35 7.34 5.49 5.48 5.47 5.46 4.62 4.60 2.89 2.88 2.87 2.85 2.83 2.81 2.80 2.78 2.63 2.62 2.53 2.53 2.52 2.51 2.49 2.48 1.93 1.92 1.92 1.90 1.90 1.90 1.65 1.64 1.63 1.63 1.63 1.62 1.62 1.61 1.61 1.60 1.60 1.30 1.30 1.30 1.28 1.28 1.27 1.20 1.19 1.19 1.18 1.12 1.11 1.10 1.10
NC
H
H
Ph
O
N
O
H
9a (minor isomer)
(500 MHz, CDCl3)
5.01
1.00
1.01
1.02
1.02
1.00
1.01
0.98
1.01
1.93
1.06
2.09
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

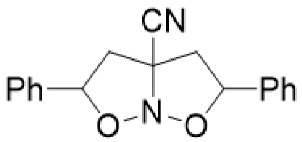

137.01
129.06
128.98
126.84
116.89
89.83
82.41
77.30
58.34
48.79
40.68
39.37
33.37
27.93
22.76
NC
H
Ph
O
N
O
9a (minor isomer)
(125 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.45 7.45 7.44 7.44 7.43 7.43 7.43 7.42 7.42 7.41 7.41 7.41 7.40 7.40 7.39 7.39 7.38 7.38 5.77 5.75 5.75 5.74 5.23 5.22 5.21 5.20 3.26 3.24 3.23 3.22 2.86 2.85 2.84 2.82 2.78 2.76 2.76 2.74 2.58 2.56 2.56 2.54
CN
Ph
Ph
O
N
O
9b (major isomer)
(500 MHz, $CDCl_3$)
10.06
0.98
0.97
1.00
1.01
0.98
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

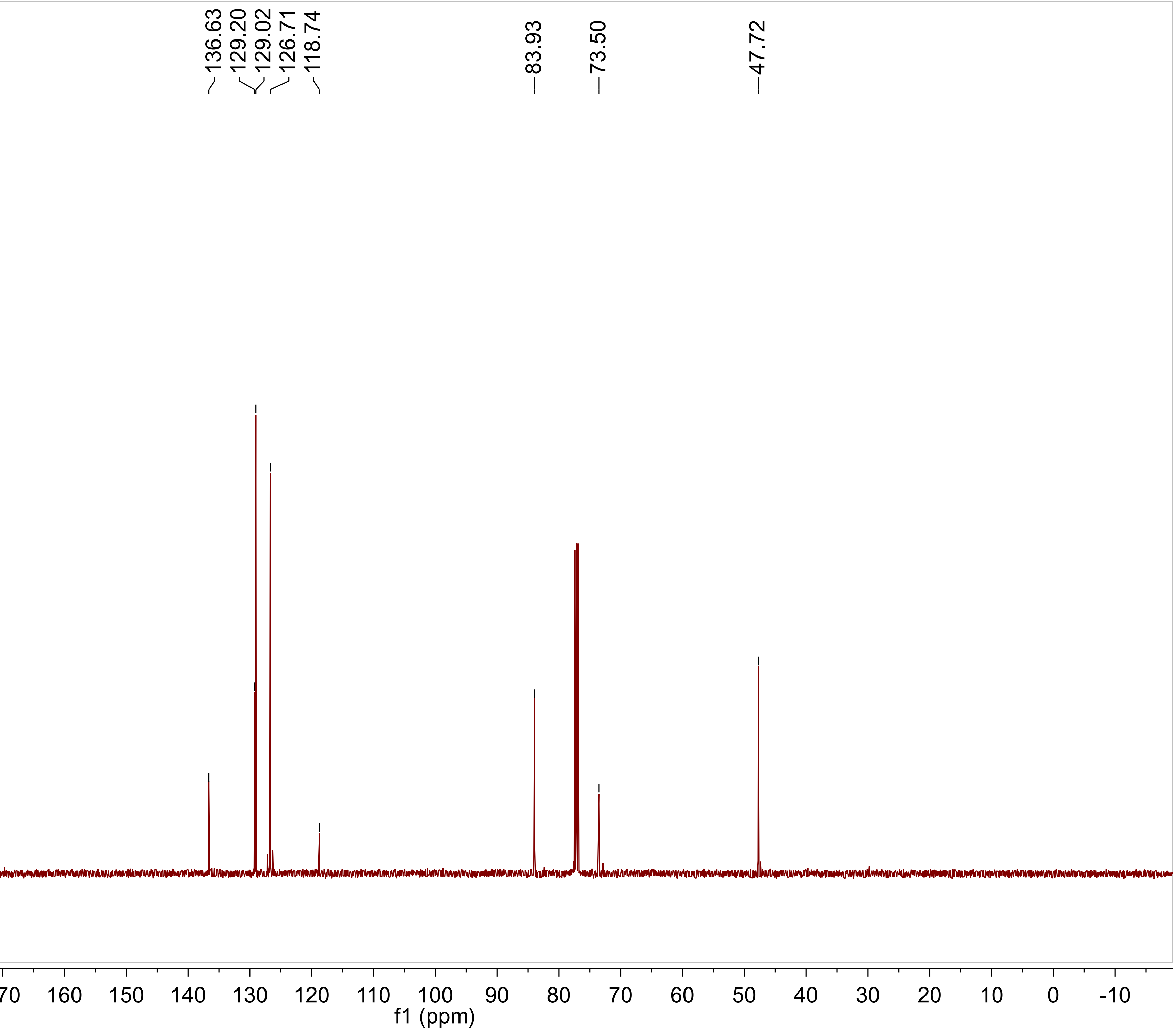

136.15
135.38
129.35
129.07
129.01
127.20
126.29
119.23
84.07
77.58
72.82
47.79
47.35
CN
Ph
Ph
O
N
O
9b (major isomer)
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

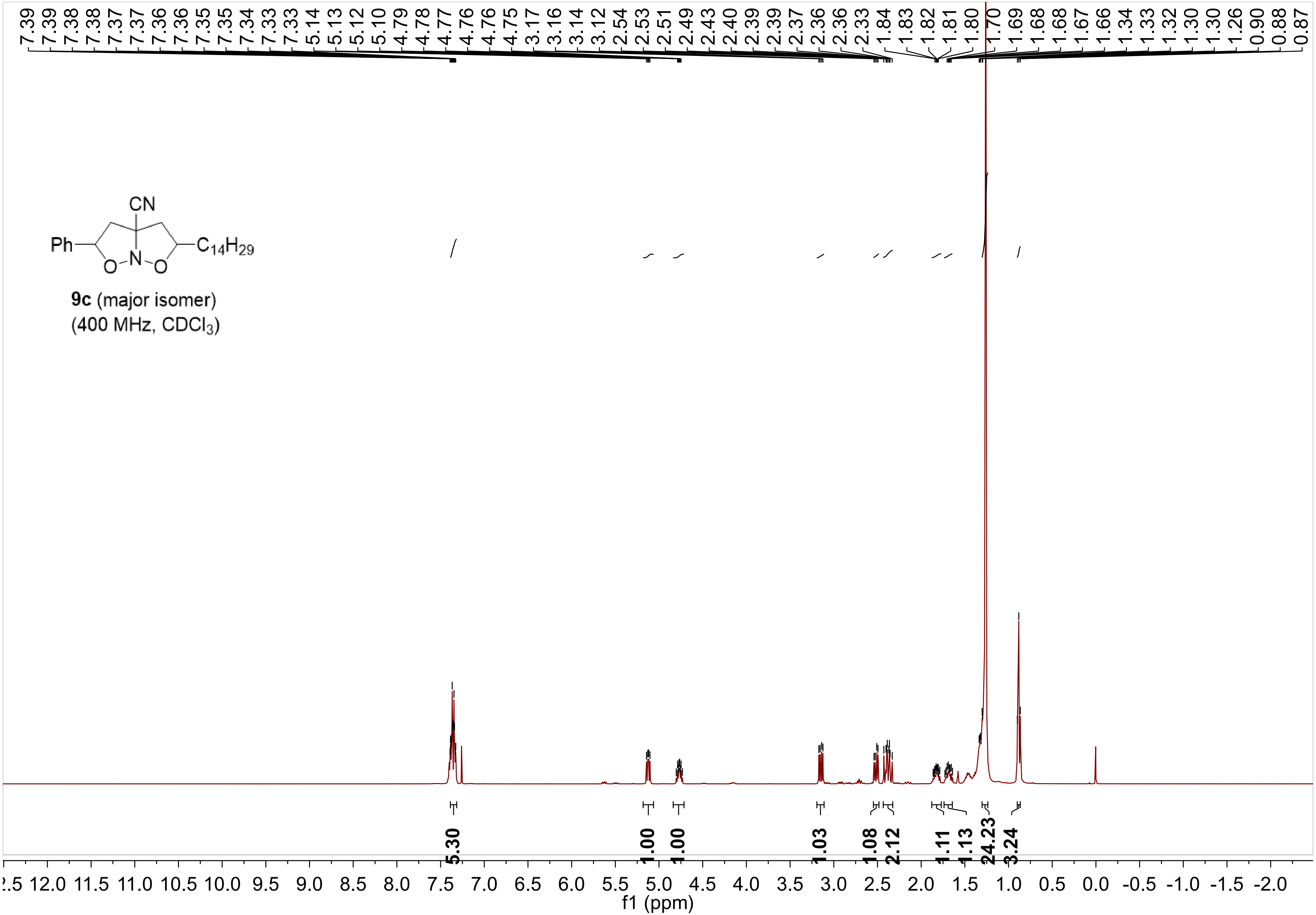


7.44
7.44
7.43
7.42
7.42
7.42
7.40
7.39
7.39
7.38
7.37
5.63
5.61
5.61
5.60
3.02
3.01
3.00
2.98
2.92
2.91
2.90
2.88
CN
Ph
Ph
O
N
O
9b (minor isomer)
(500 MHz, CDCl3)
10.36
1.97
2.02
2.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

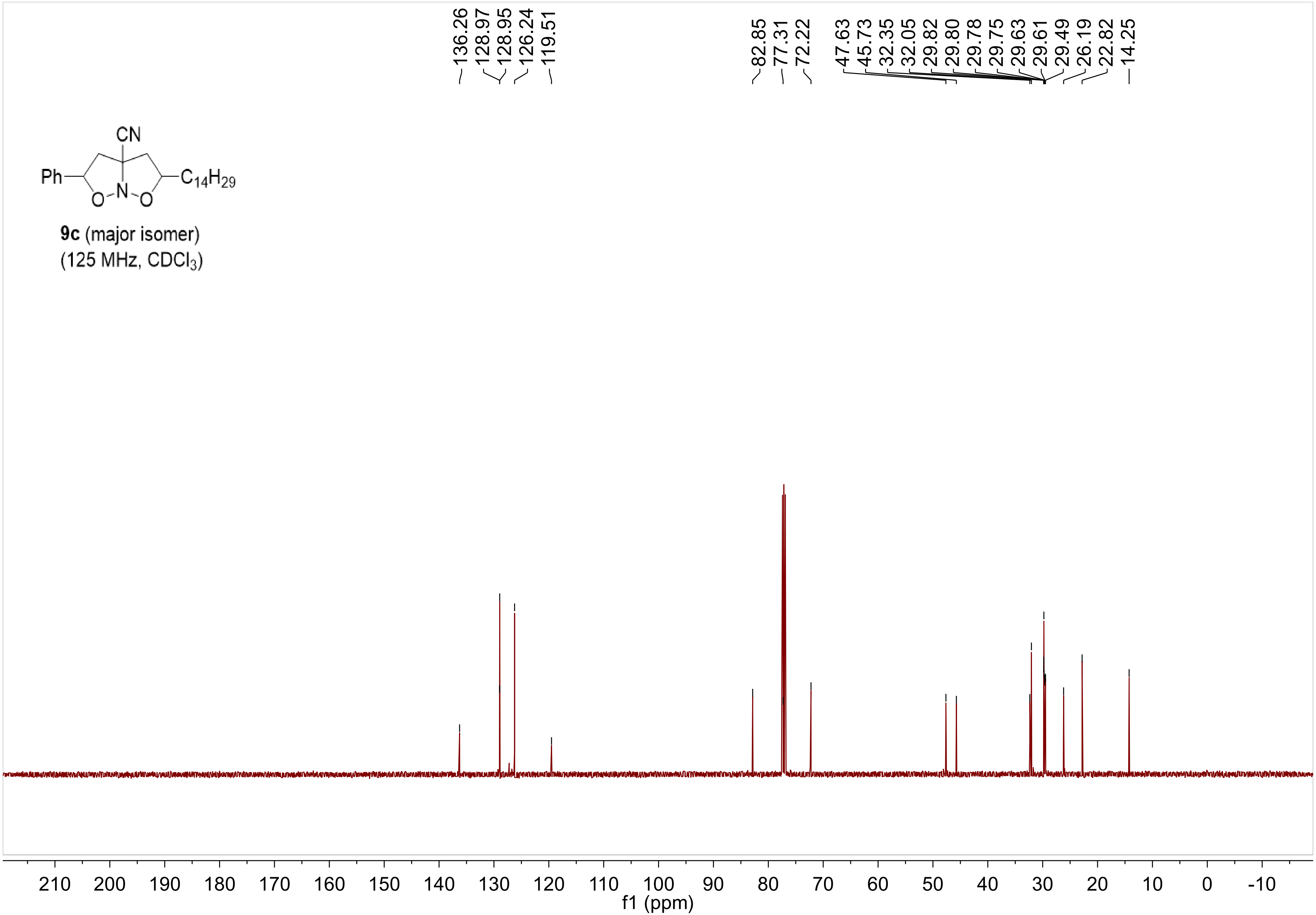


9b (minor isomer)
(125 MHz, $CDCl_3$)

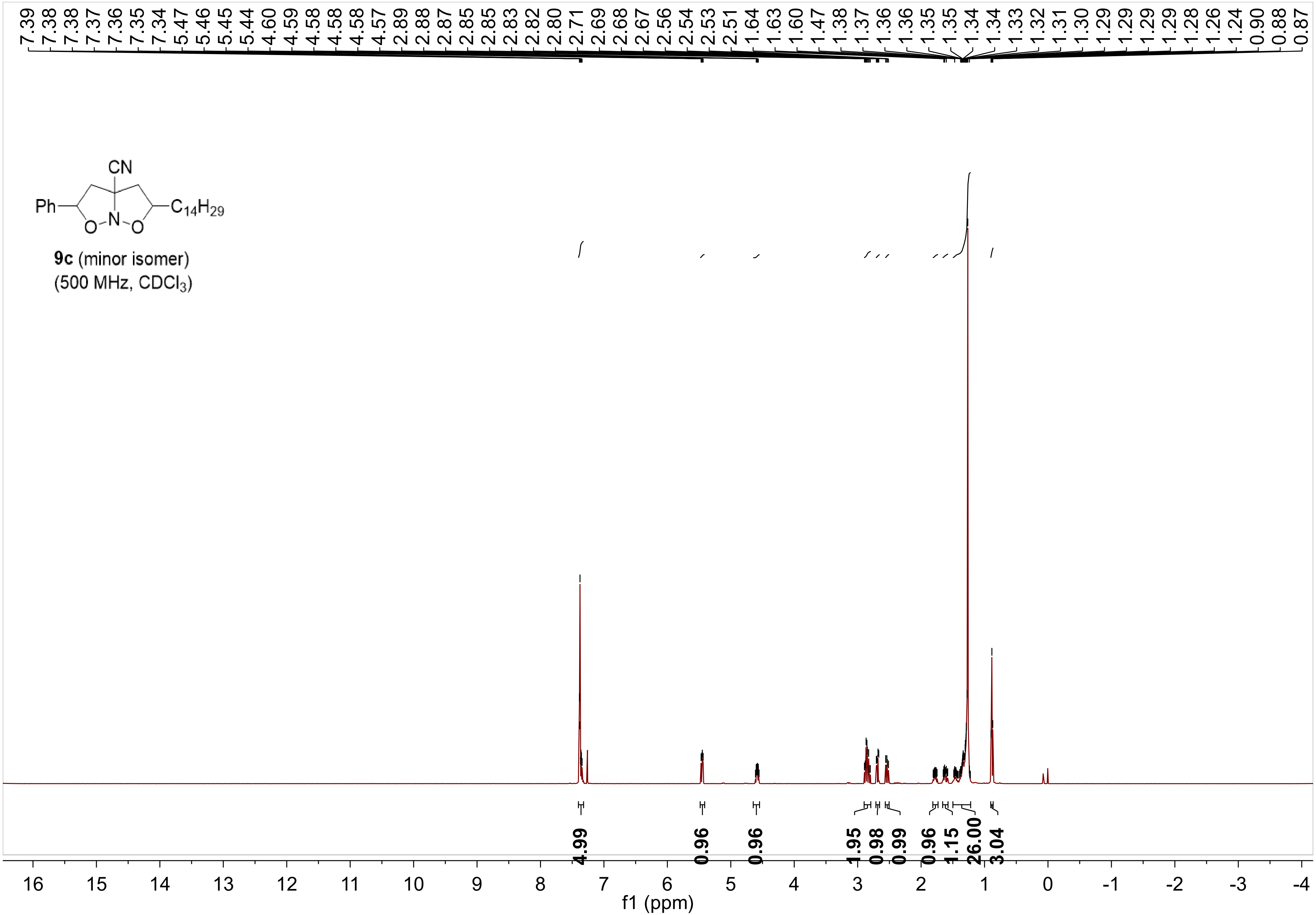


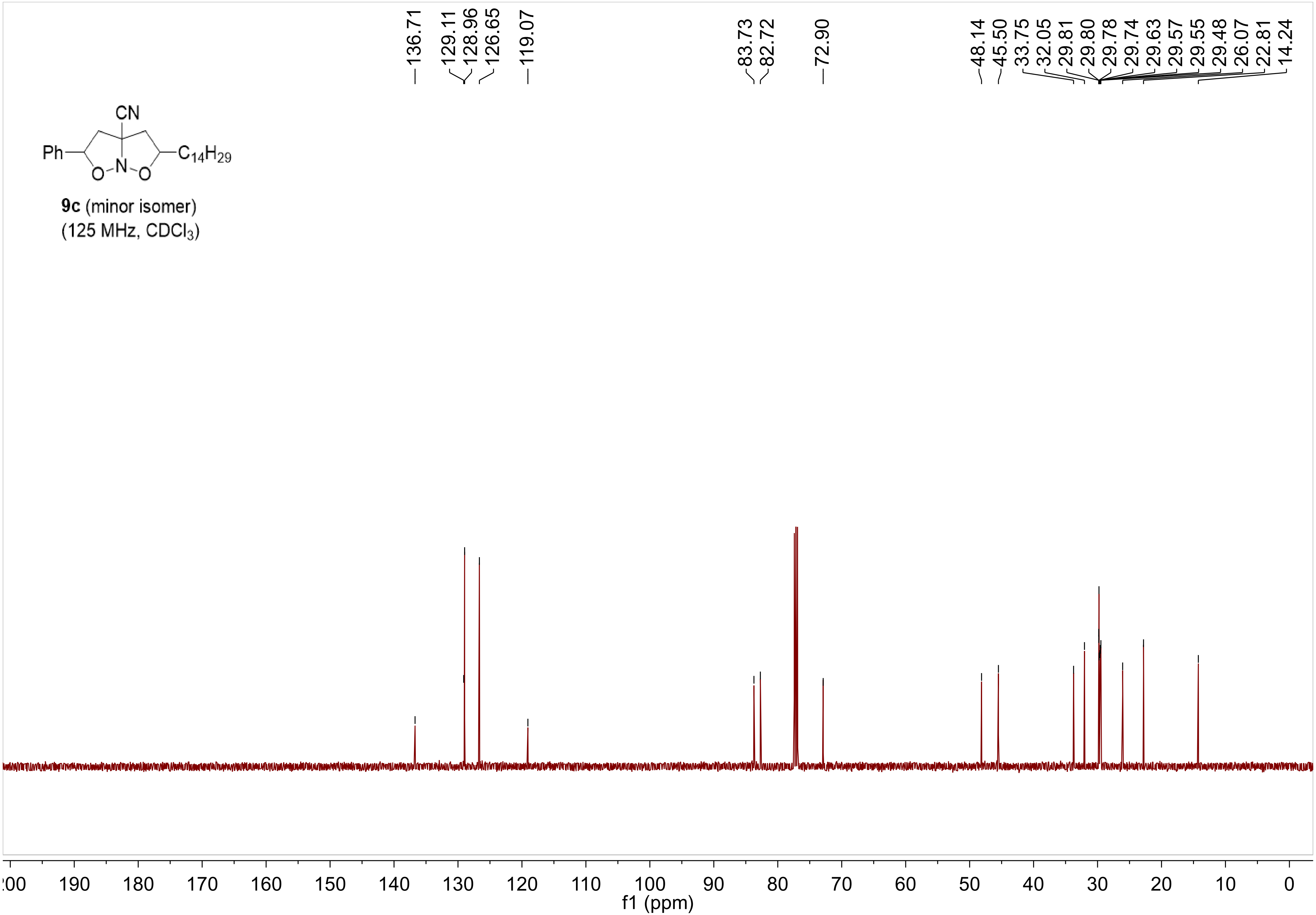


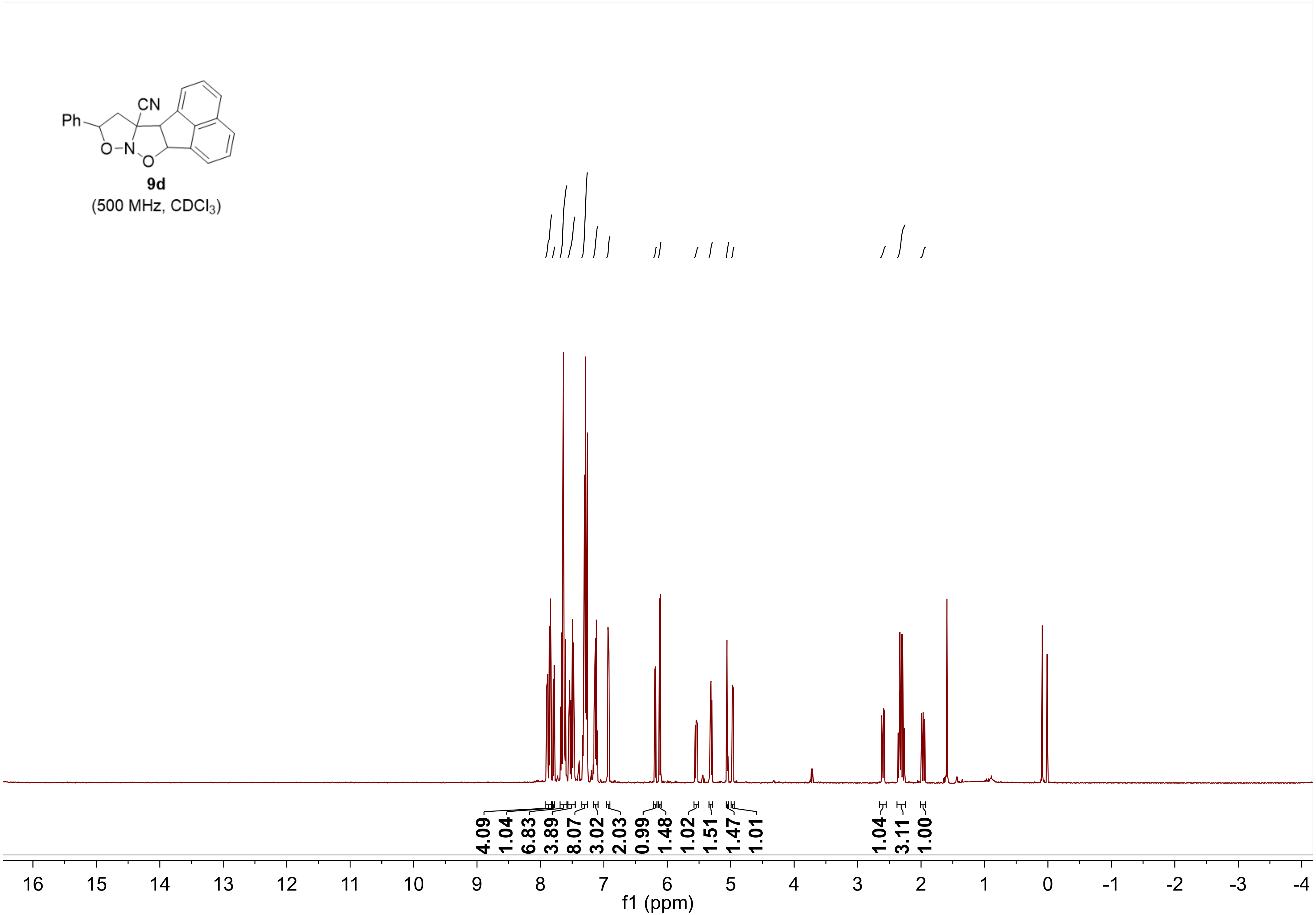
9c (major isomer)
(400 MHz, $CDCl_3$)

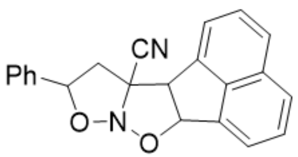


136.26
128.97
128.95
126.24
119.51
82.85
77.31
72.22
47.63
45.73
32.35
32.05
29.82
29.80
29.78
29.75
29.63
29.61
29.49
26.19
22.82
14.25
CN
Ph
$C_{14}H_{29}$
O
N
O
9c (major isomer)
(125 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.39 7.38 7.38 7.37 7.36 7.35 7.34 5.47 5.46 5.45 5.44 4.60 4.59 4.58 4.58 4.58 4.57 2.89 2.88 2.87 2.85 2.85 2.83 2.82 2.80 2.71 2.69 2.68 2.67 2.56 2.54 2.53 2.51 1.64 1.63 1.60 1.47 1.38 1.37 1.36 1.36 1.35 1.35 1.34 1.34 1.33 1.32 1.31 1.30 1.29 1.29 1.29 1.29 1.28 1.26 1.24 0.90 0.88 0.87
CN
Ph
$C_{14}H_{29}$
O
N
O
9c (minor isomer)
(500 MHz, $CDCl_3$)
4.99
0.96
0.96
1.95
0.98
0.99
0.96
1.15
26.00
3.04
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

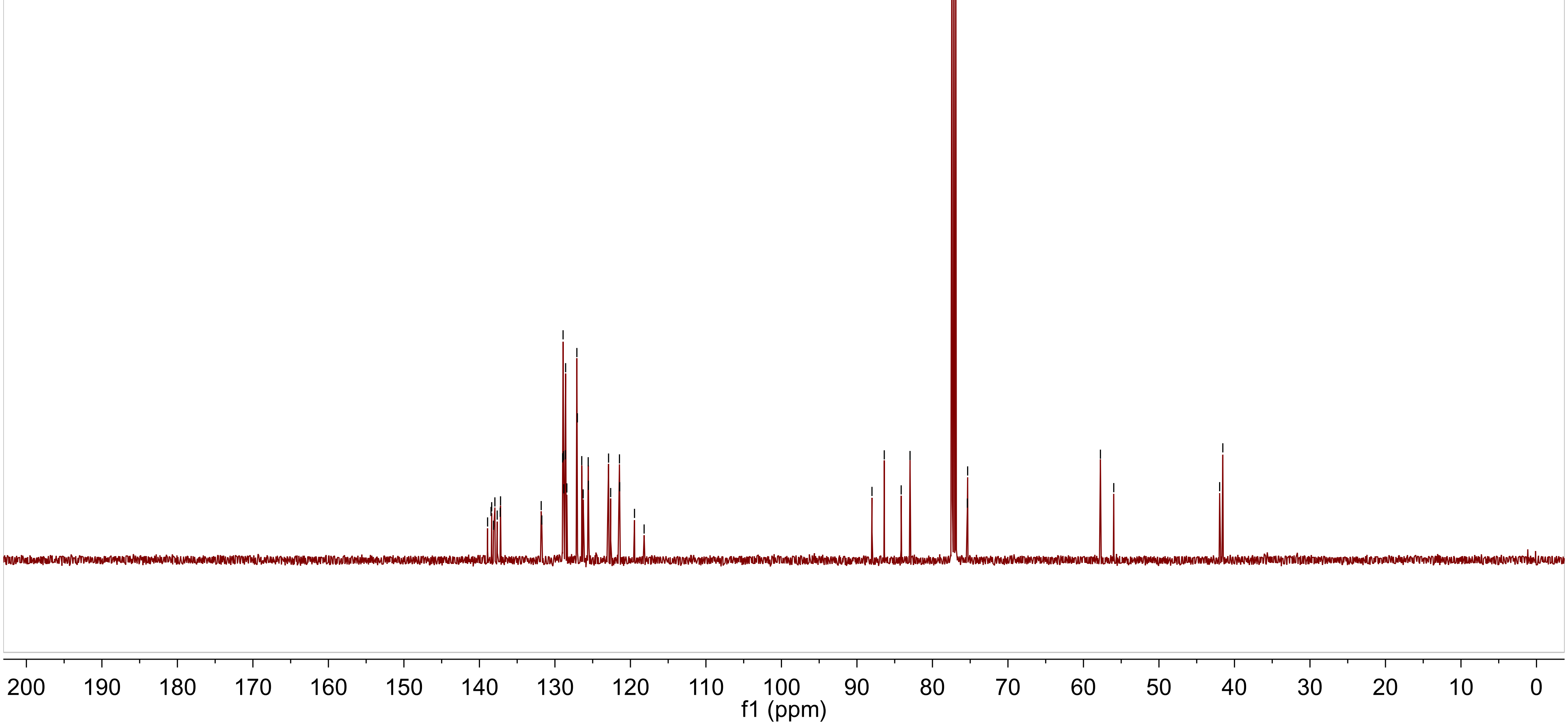

CN
Ph
$C_{14}H_{29}$
O
N
O
9c (minor isomer)
(125 MHz, $CDCl_3$)
136.71
129.11
128.96
126.65
119.07
83.73
82.72
72.90
48.14
45.50
33.75
32.05
29.81
29.80
29.78
29.74
29.63
29.57
29.55
29.48
26.07
22.81
14.24
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

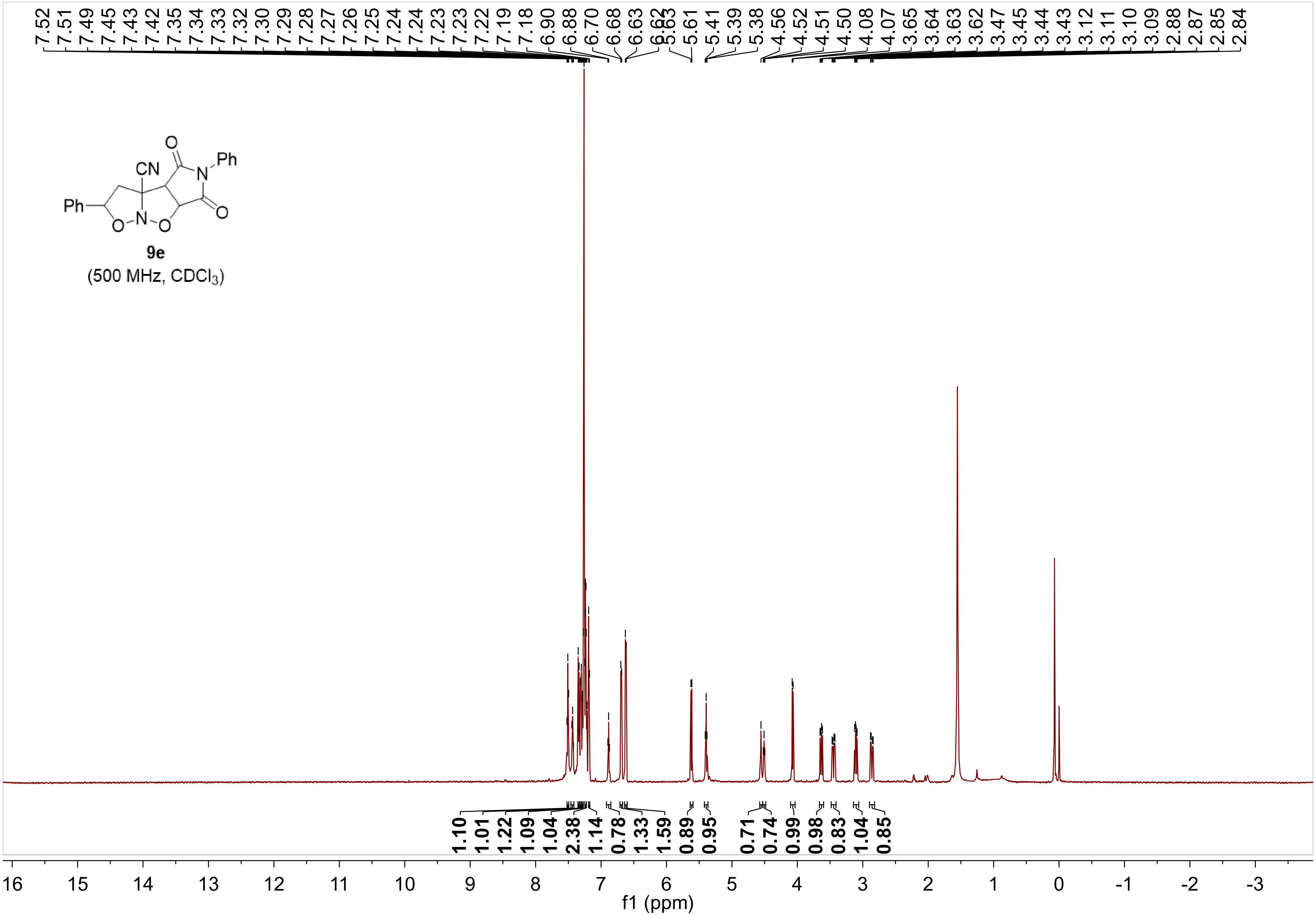

Ph
CN
O
N
O
9d
(500 MHz, CDCl3)
4.09
1.04
6.83
3.89
8.07
3.02
2.03
0.99
1.48
1.02
1.51
1.47
1.01
1.04
3.11
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)



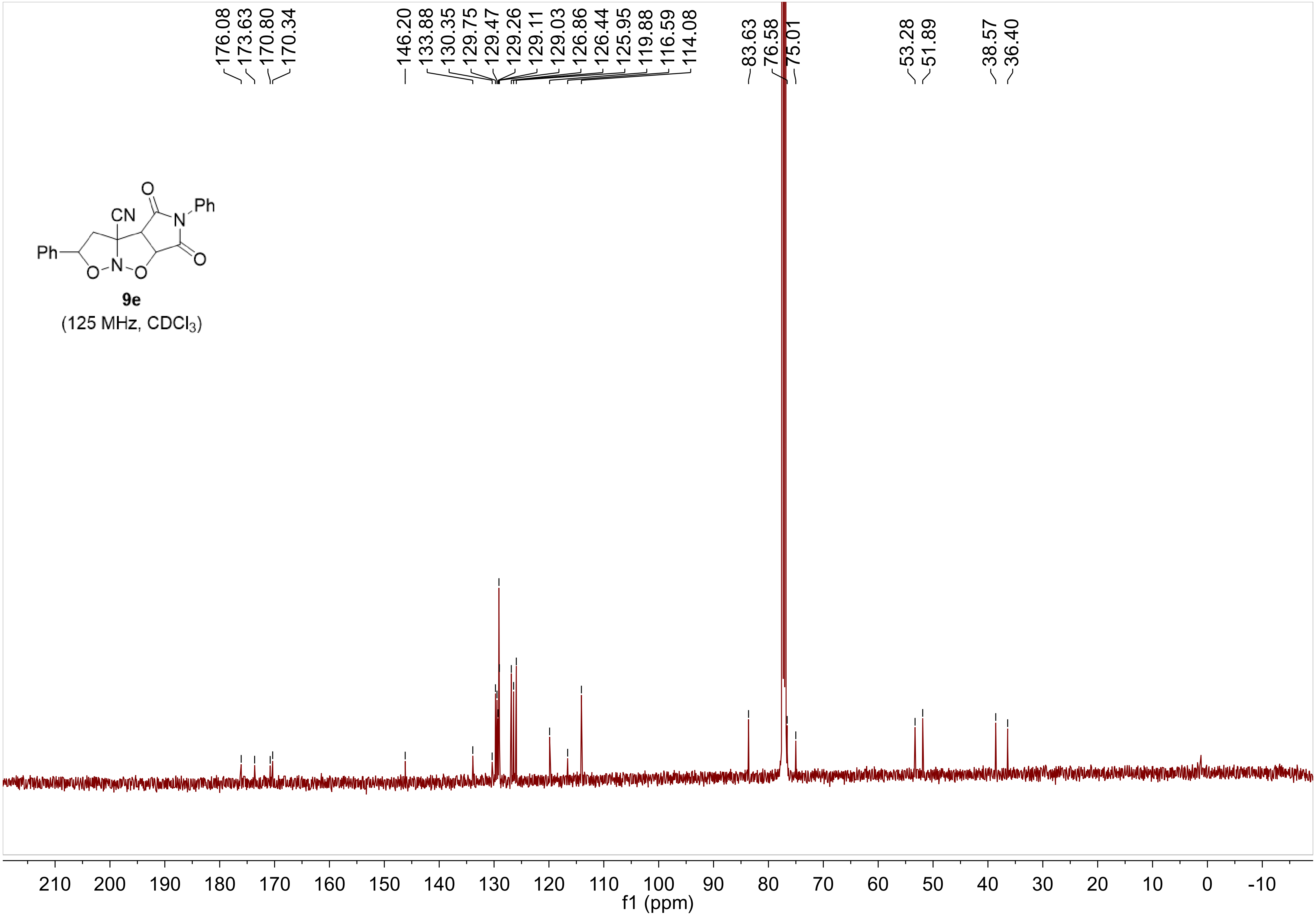
9d

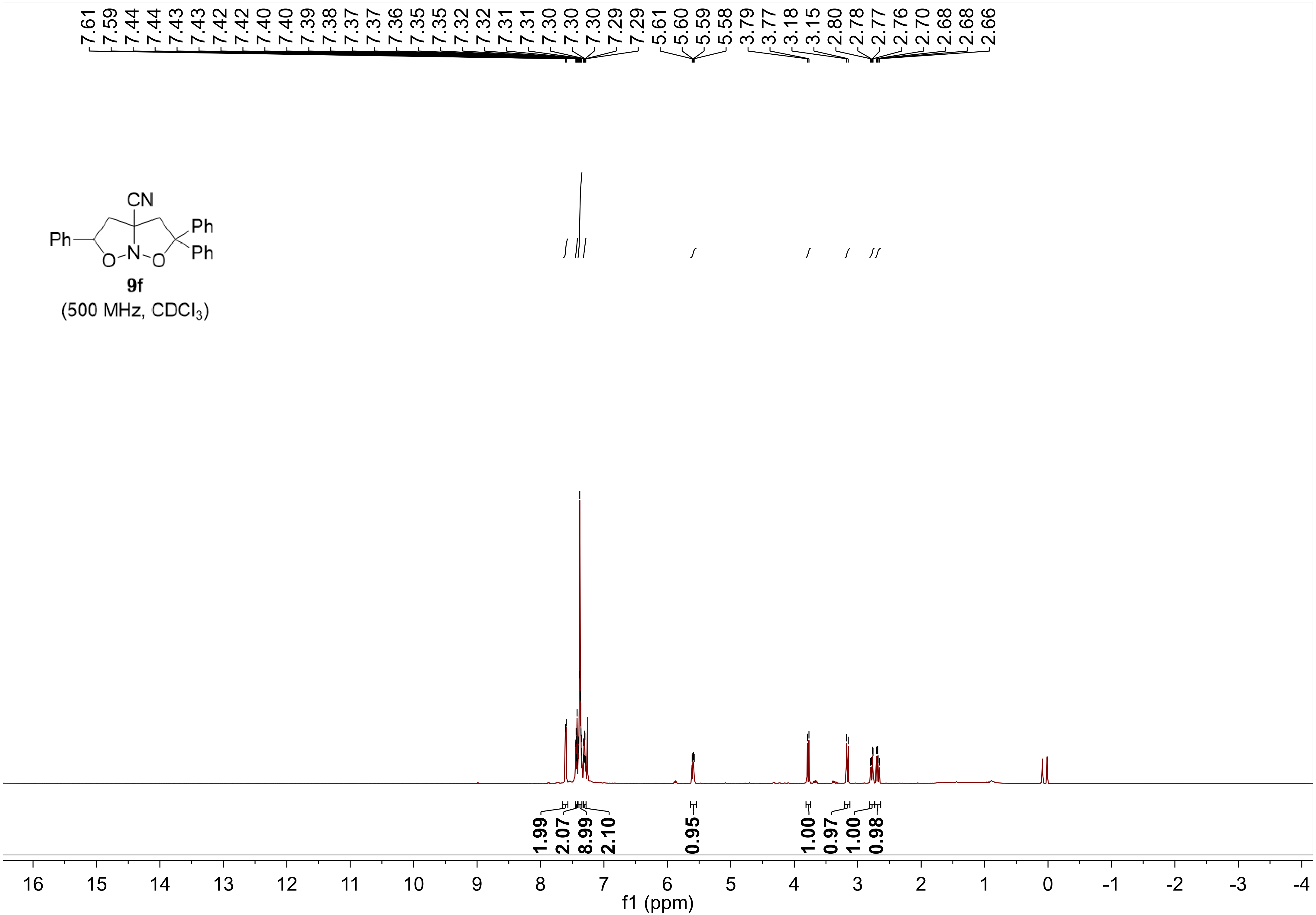
(125 MHz, $CDCl_3$)

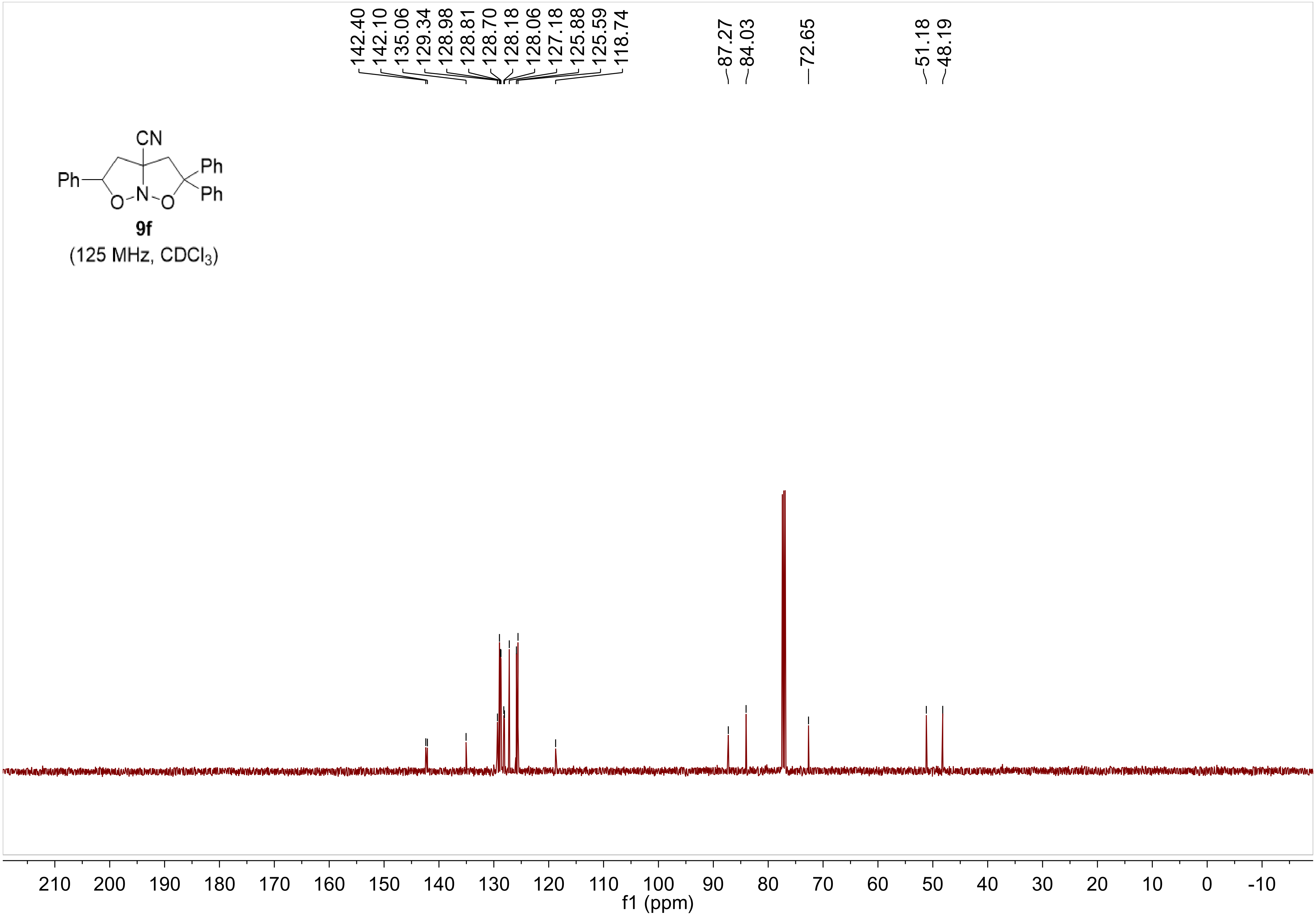




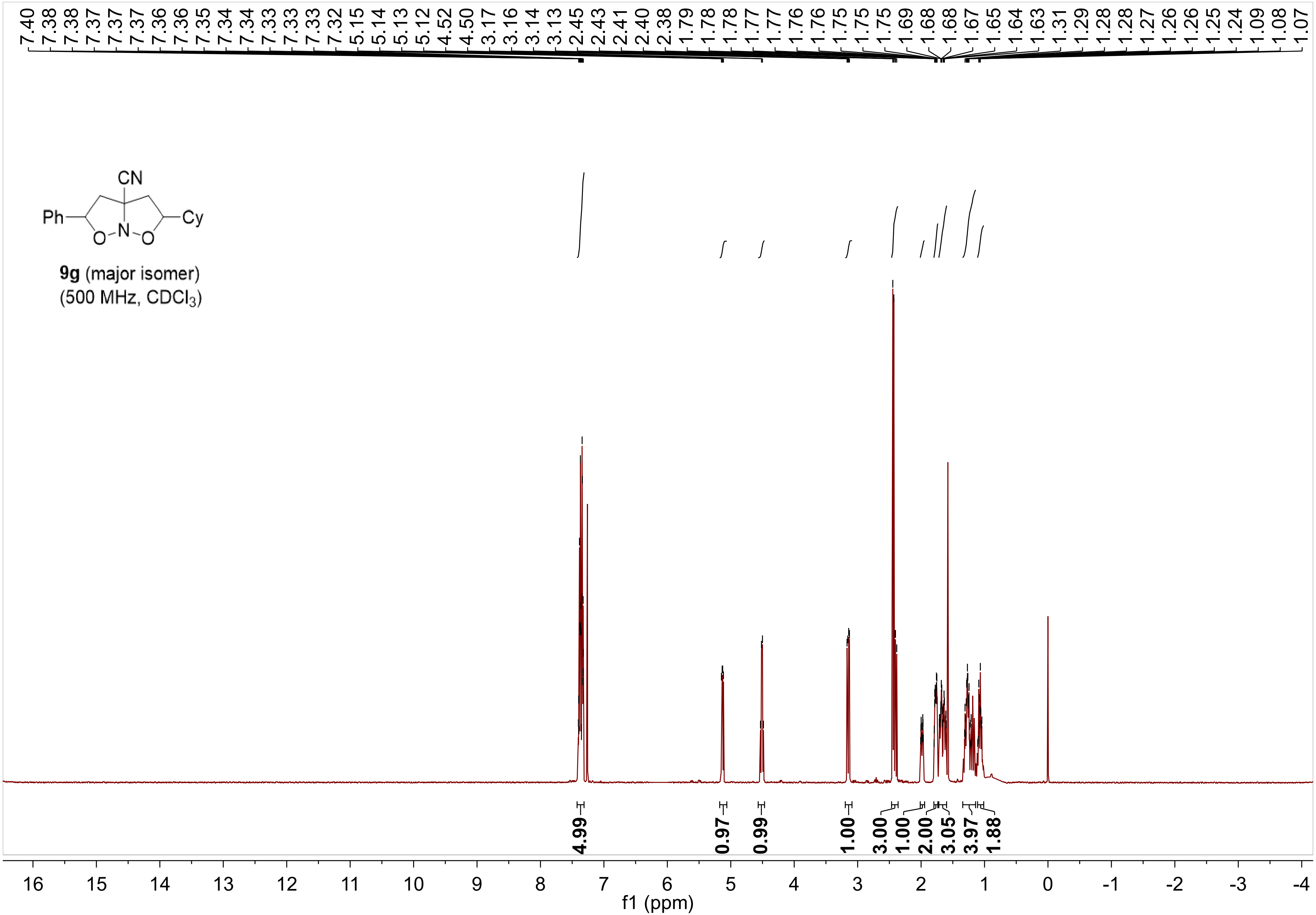
7.52 7.51 7.49 7.45 7.43 7.42 7.35 7.34 7.33 7.32 7.30 7.29 7.28 7.27 7.26 7.25 7.24 7.24 7.23 7.23 7.22 7.19 7.18 6.90 6.88 6.70 6.68 6.63 6.62 5.63 5.61 5.41 5.39 5.38 4.56 4.52 4.51 4.50 4.08 4.07 3.65 3.64 3.63 3.62 3.47 3.45 3.44 3.43 3.12 3.11 3.10 3.09 2.88 2.87 2.85 2.84
CN
Ph
N
O
Ph
O
N
O
O
9e
(500 MHz, CDCl3)
1.10 1.01 1.22 1.09 1.04 2.38 1.14 0.78 1.33 1.59 0.89 0.95 0.71 0.74 0.99 0.98 0.83 1.04 0.85
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

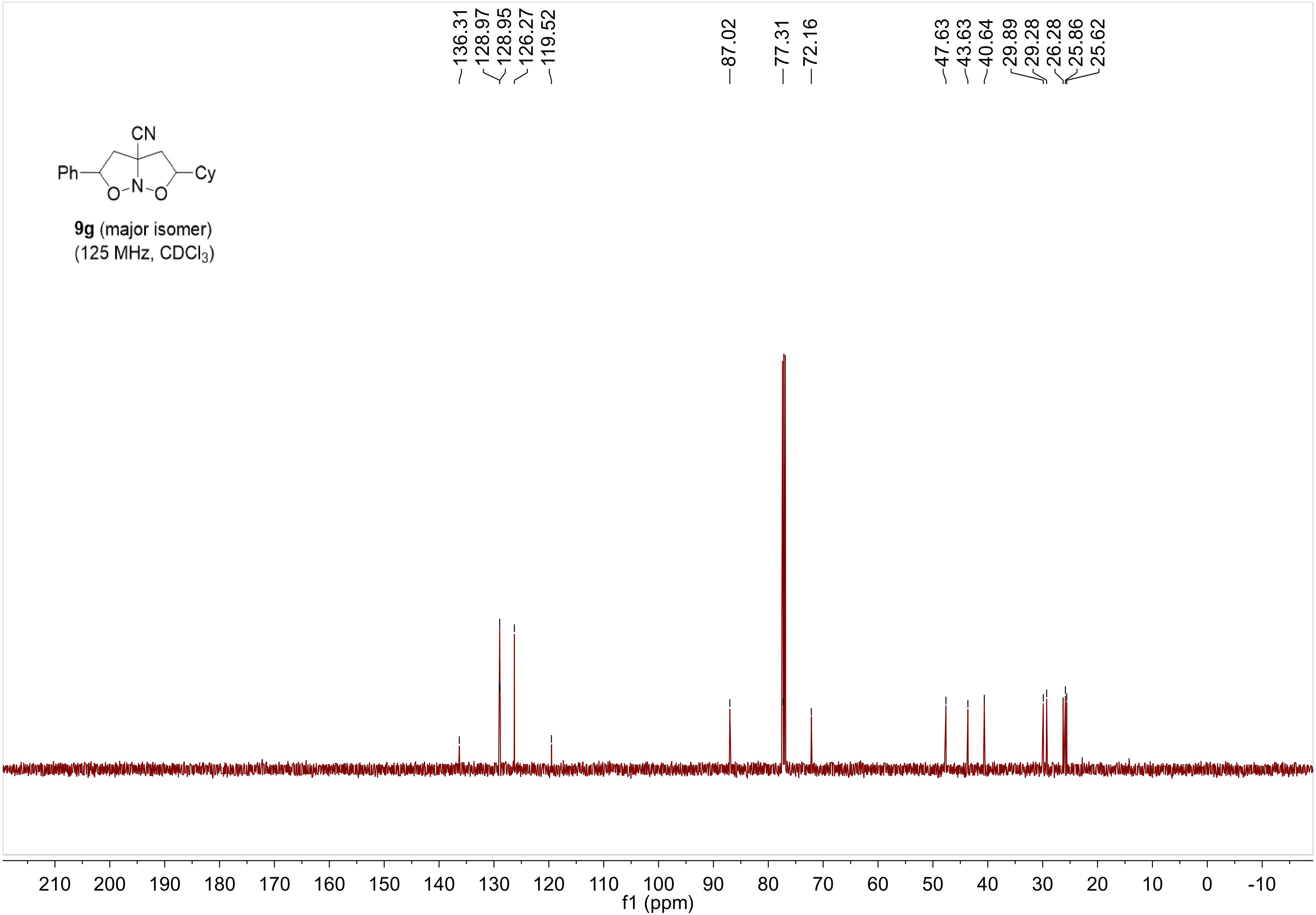

176.08
173.63
170.80
170.34
146.20
133.88
130.35
129.75
129.47
129.26
129.11
129.03
126.86
126.44
125.95
119.88
116.59
114.08
83.63
76.58
75.01
53.28
51.89
38.57
36.40
O
CN
N
Ph
Ph
O
N
O
O
9e
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

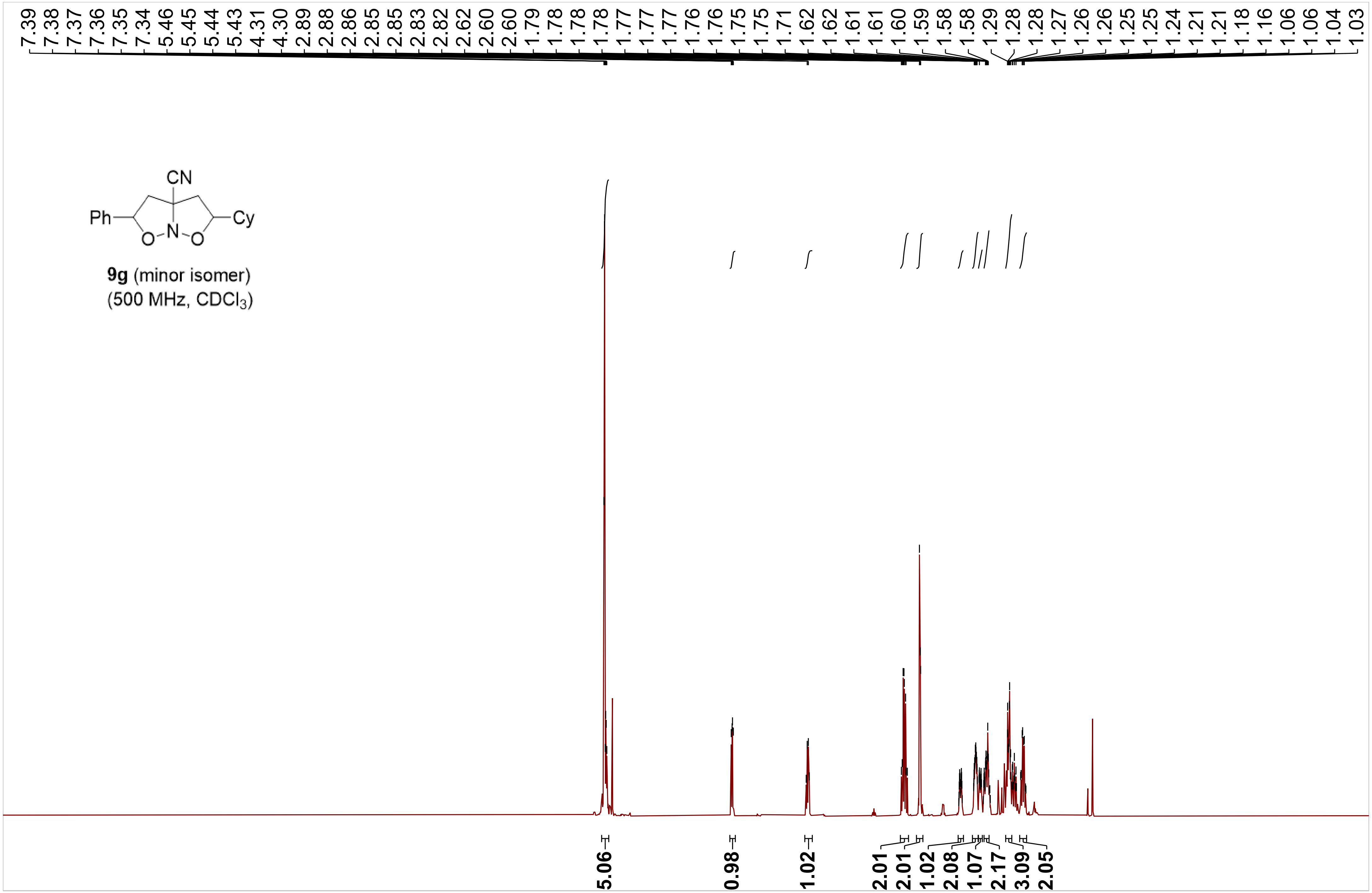

7.61 7.59 7.44 7.44 7.43 7.43 7.42 7.42 7.40 7.40 7.39 7.38 7.37 7.37 7.36 7.35 7.35 7.32 7.32 7.31 7.31 7.30 7.30 7.30 7.29 7.29 5.61 5.60 5.59 5.58 3.79 3.77 3.18 3.15 2.80 2.78 2.77 2.76 2.70 2.68 2.68 2.66
CN
Ph
Ph
Ph
O
N
O
9f
(500 MHz, $CDCl_3$)
1.99 2.07 8.99 2.10 0.95 1.00 0.97 1.00 0.98
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

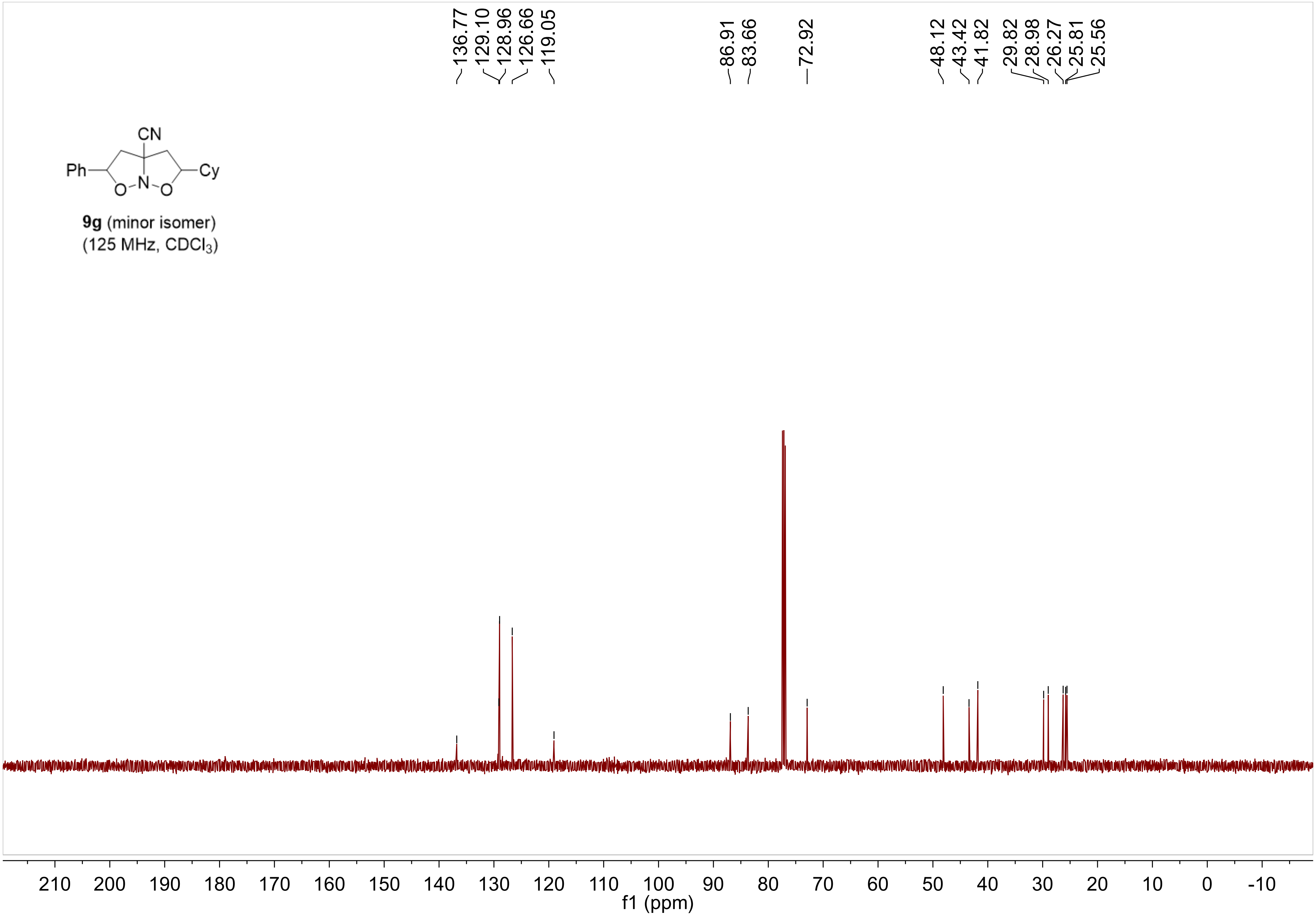


142.40
142.10
135.06
129.34
128.98
128.81
128.70
128.18
128.06
127.18
125.88
125.59
118.74
87.27
84.03
72.65
51.18
48.19
CN
Ph
Ph
Ph
O
N
O
9f
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

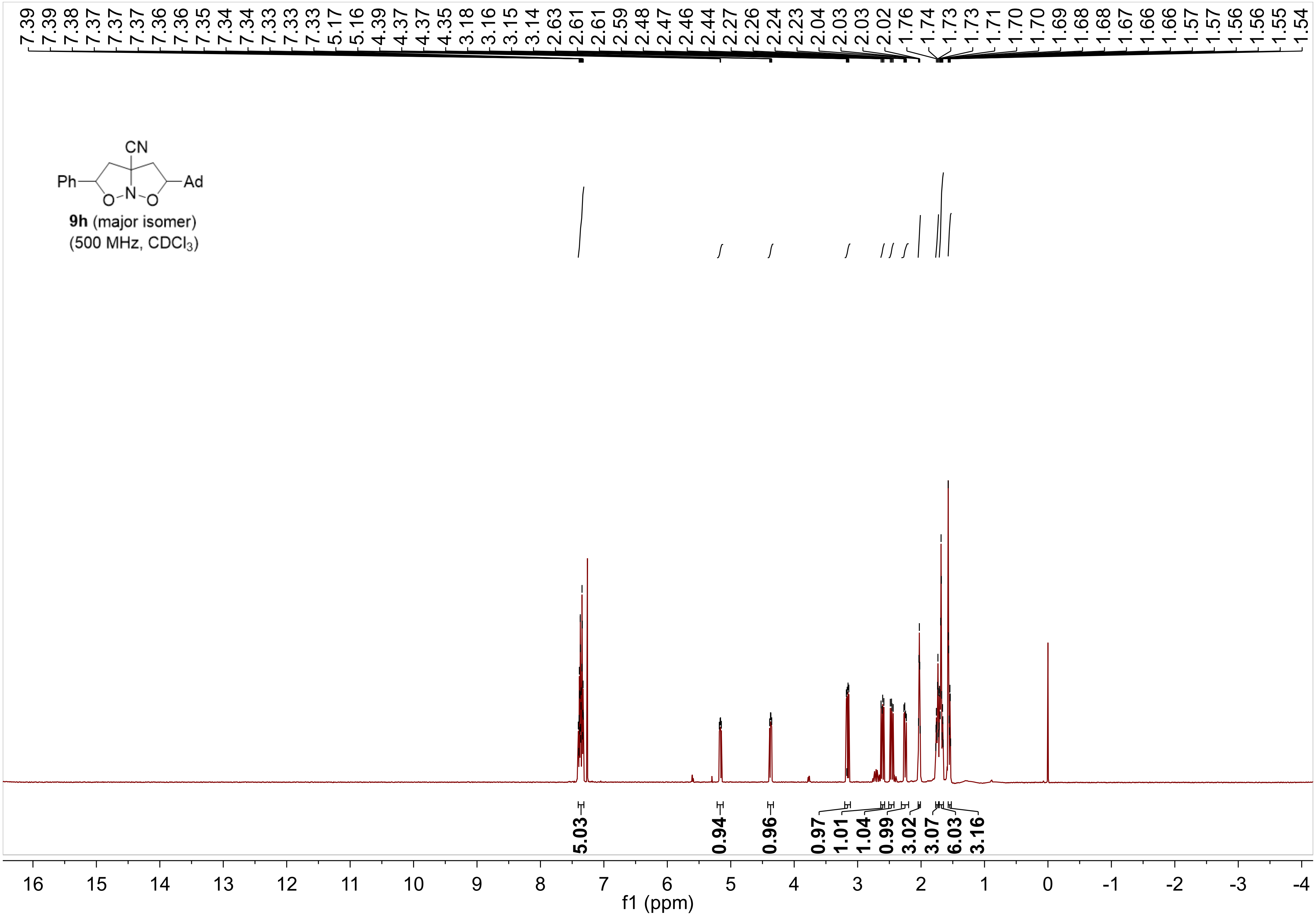

7.40 7.38 7.38 7.37 7.37 7.37 7.36 7.36 7.35 7.34 7.34 7.33 7.33 7.33 7.32 5.15 5.14 5.13 5.12 4.52 4.50 3.17 3.16 3.14 3.13 2.45 2.43 2.41 2.40 2.38 1.79 1.78 1.78 1.77 1.77 1.76 1.76 1.75 1.75 1.75 1.69 1.68 1.68 1.67 1.65 1.64 1.63 1.31 1.29 1.28 1.28 1.27 1.26 1.26 1.25 1.24 1.09 1.08 1.07
CN
Ph
Cy
O
N
O
9g (major isomer)
(500 MHz, $CDCl_3$)
4.99
0.97
0.99
1.00
3.00
1.00
2.00
3.05
3.97
1.88
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

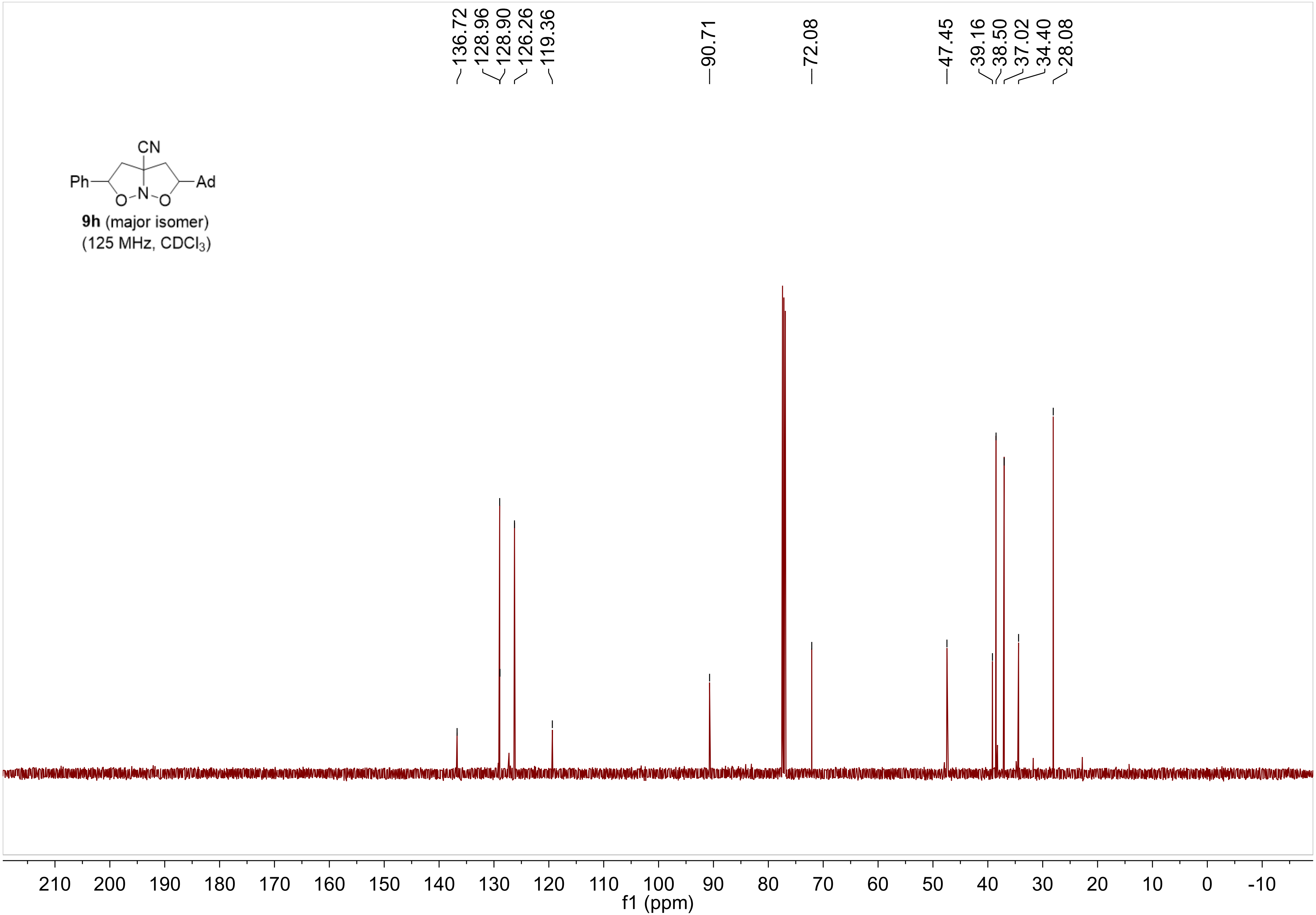

136.31
128.97
128.95
126.27
119.52
87.02
77.31
72.16
47.63
43.63
40.64
29.89
29.28
26.28
25.86
25.62
CN
Ph
Cy
O
N
O
9g (major isomer)
(125 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

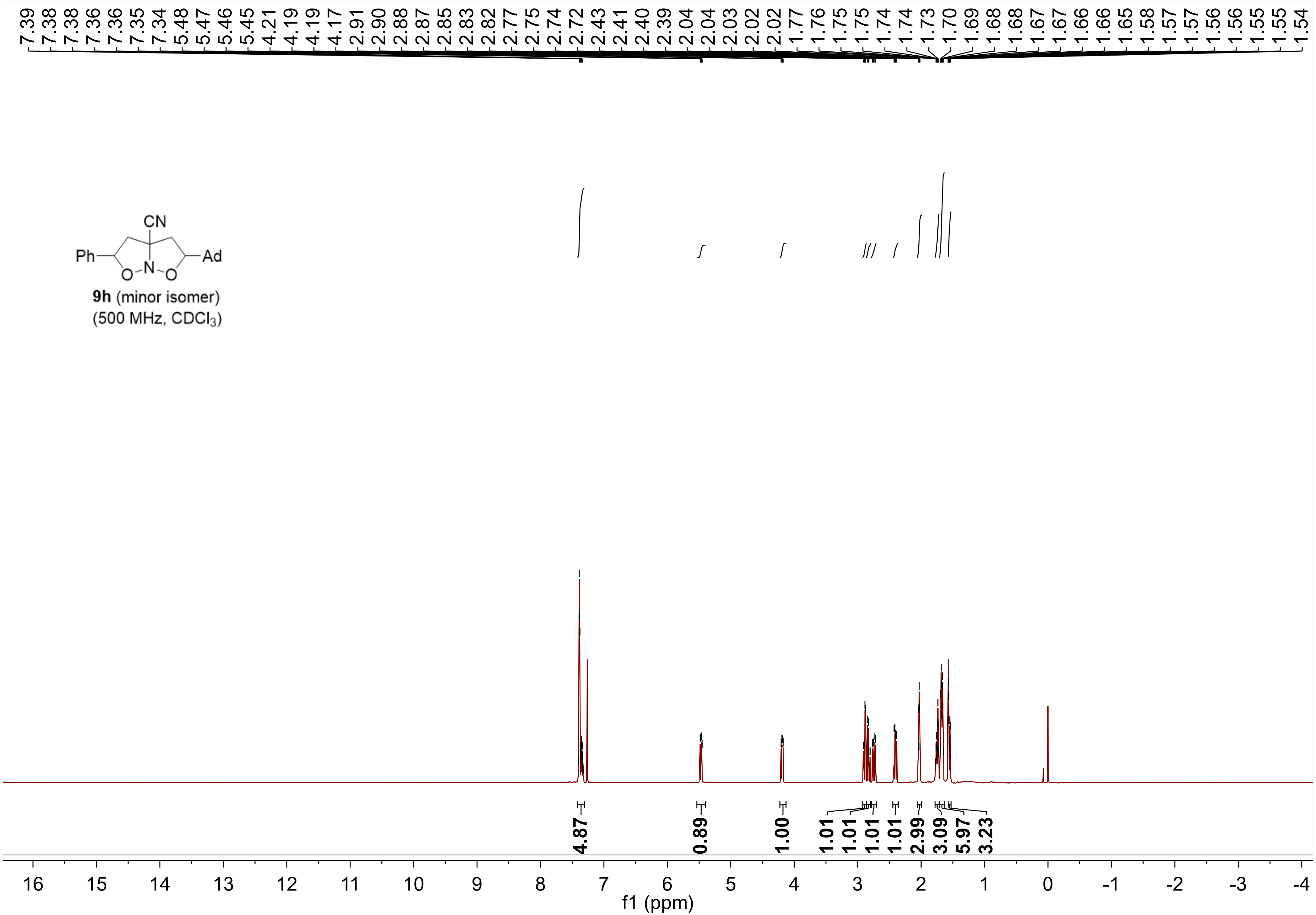

CN
Ph
Cy
O
N
O
9g (minor isomer)
(500 MHz, CDCl3)
7.39 7.38 7.37 7.36 7.35 7.34 5.46 5.45 5.44 5.43 4.31 4.30 2.89 2.88 2.86 2.85 2.85 2.83 2.82 2.62 2.60 2.60 1.79 1.78 1.78 1.78 1.77 1.77 1.77 1.76 1.76 1.75 1.75 1.71 1.62 1.62 1.61 1.61 1.60 1.59 1.58 1.58 1.29 1.28 1.28 1.27 1.26 1.26 1.25 1.25 1.24 1.21 1.21 1.18 1.16 1.06 1.06 1.04 1.03
5.06
0.98
1.02
2.01
2.01
1.02
2.08
1.07
2.17
3.09
2.05
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

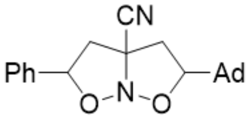


136.77
129.10
128.96
126.66
119.05
86.91
83.66
72.92
48.12
43.42
41.82
29.82
28.98
26.27
25.81
25.56
CN
Ph
Cy
O
N
O
9g (minor isomer)
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

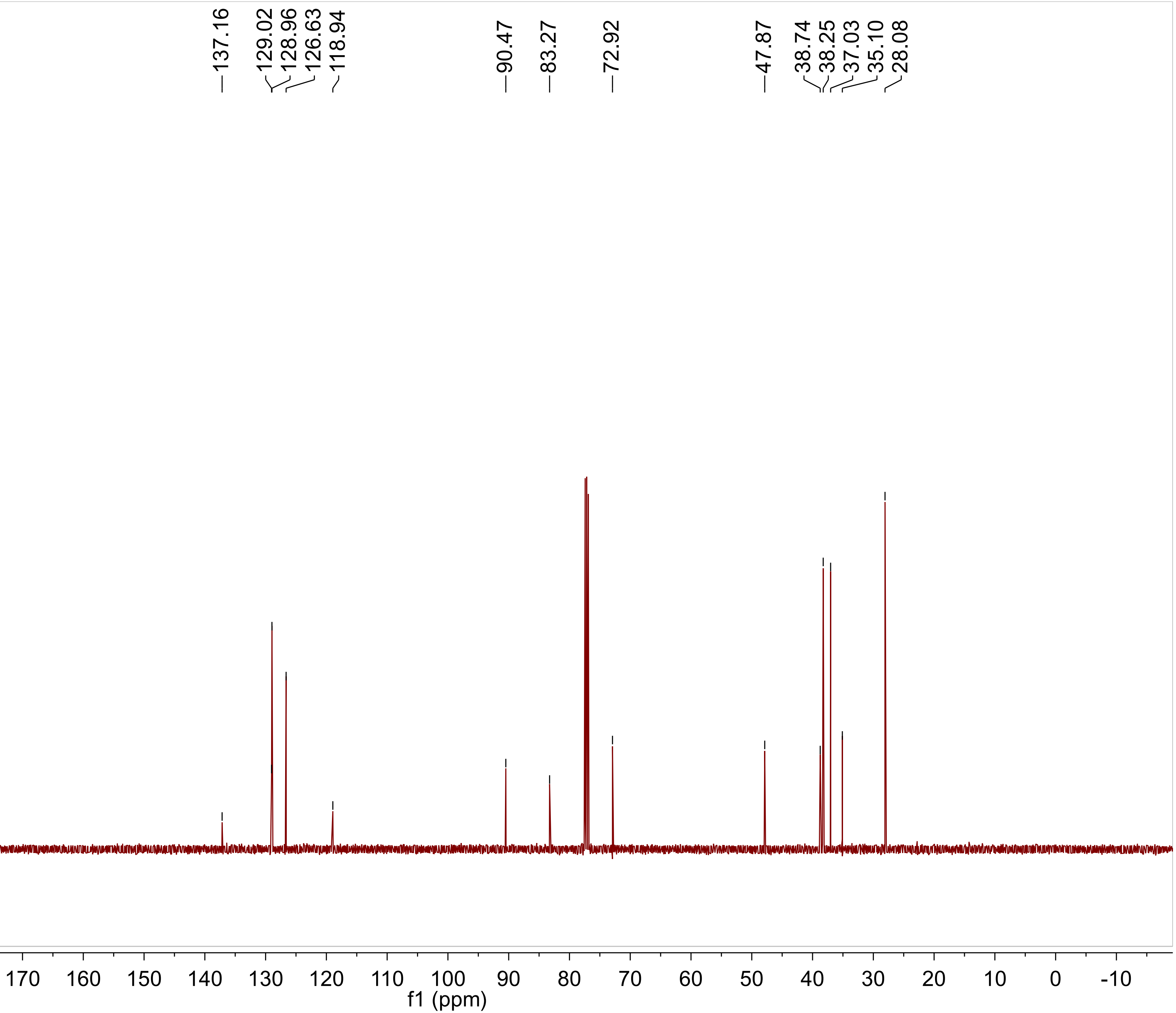

7.39 7.39 7.38 7.37 7.37 7.37 7.36 7.36 7.35 7.34 7.34 7.33 7.33 7.33 5.17 5.16 4.39 4.37 4.37 4.35 3.18 3.16 3.15 3.14 2.63 2.61 2.61 2.59 2.48 2.47 2.46 2.44 2.27 2.26 2.24 2.23 2.04 2.03 2.03 2.02 1.76 1.74 1.73 1.73 1.71 1.70 1.70 1.69 1.68 1.68 1.67 1.66 1.66 1.57 1.57 1.56 1.56 1.55 1.54
CN
Ph
Ad
O
N
O
9h (major isomer)
(500 MHz, CDCl3)
5.03
0.94
0.96
0.97
1.01
1.04
0.99
3.02
3.07
6.03
3.16
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


136.72
128.96
128.90
126.26
119.36
90.71
72.08
47.45
39.16
38.50
37.02
34.40
28.08
CN
Ph
Ad
O
N
O
9h (major isomer)
(125 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.39 7.38 7.38 7.36 7.36 7.35 7.34 5.48 5.47 5.46 5.45 4.21 4.19 4.19 4.17 2.91 2.90 2.88 2.87 2.85 2.83 2.82 2.77 2.75 2.74 2.72 2.43 2.41 2.40 2.39 2.04 2.04 2.03 2.02 2.02 1.77 1.76 1.75 1.75 1.74 1.74 1.73 1.70 1.69 1.68 1.68 1.67 1.67 1.66 1.66 1.65 1.58 1.57 1.57 1.56 1.56 1.55 1.55 1.54
CN
Ph
Ad
O
N
O
9h (minor isomer)
(500 MHz, CDCl3)
4.87
0.89
1.00
1.01
1.01
1.01
1.01
2.99
3.09
5.97
3.23
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

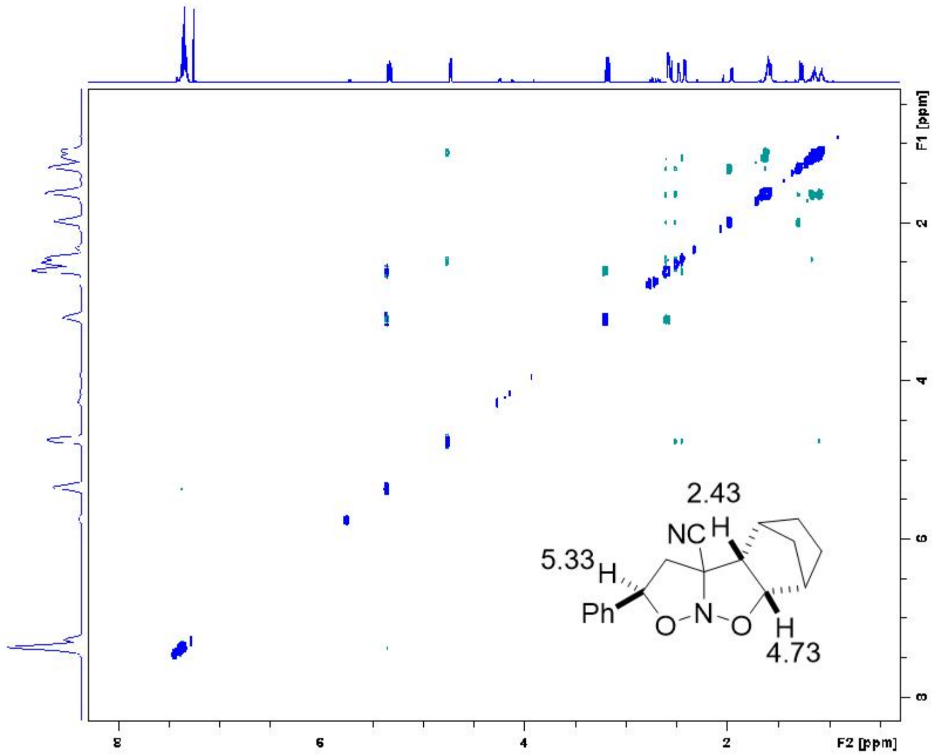


9h (minor isomer)
(125 MHz, $CDCl_3$)



12. Copies of NOESY Spectra

NOESY Spectra of 9a (major isomer):



NOESY Spectra of 9a' (minor isomer):