Supporting Information

$AgNO_2$ as the NO Source for the Synthesis of Substituted Pyrazole *N*-oxides from *N*-Propargylamines

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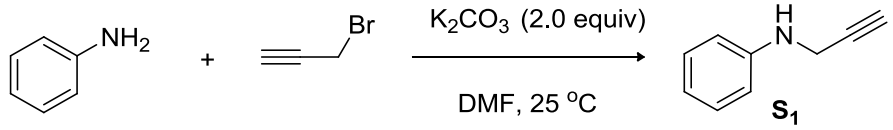
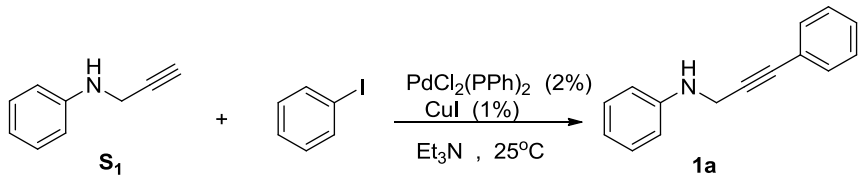
General remark

^{1}H NMR and ^{13}C NMR spectra were recorded on 400MHz and 100MHz in $CDCl_3$. All chemical shifts are given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. All compounds were further characterized by HRMS; copies of ^{1}H NMR and ^{13}C NMR spectra are provided. Products were purified by flash chromatography on 200-300 mesh silica gels. Unless otherwise noted, commercially available reagents and solvents were used without further purification.

General procedure for the synthesis of propargylamine 1a-1ab[1-2]:



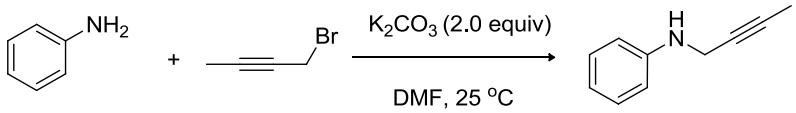
N-(2-Propynyl)aniline (**S_1**). An oven-dried 500 mL, three-necked, round-bottomed flask equipped with magnetic stirring bar, a thermometer, a pressure qualizing dropping funnel, and a rubber septum is charged with aniline (22.35 g, 240.0 mmol, 4.0 equiv), potassium carbonate (16.58 g, 120.0 mmol, 2.0 equiv), and 300 ml DMF. The mixture is stirred for 5 min at room temperature. A solution of propargyl bromide (7.14 g, 1.0 equiv) in 25 ml DMF is added to the flask dropwise. The reaction mixture is stirred at room temperature for 6 h. The reaction mixture is filtered under reduced pressure. The combined filtrate is transferred to separatory funnel and washed with brine (300 mL). The aqueous phase is extracted twice with diethyl ether (2×150 mL). The combined organic phases are washed with water (100 mL) and dried over anhydrous $MgSO_4$, filtered and concentrated by rotary evaporation to give a dark brown oil. The residue is purified by flash column chromatography on silica gel to afford the *N*-(2-propynyl)aniline in 75% yield (5.90 g) as a light yellow oil.



N-(3-Phenyl-2-propynyl)aniline (**1a**). An oven-dried, three-necked round-bottomed

flask equipped with magnetic stirring bar, a thermometer, and two rubber septa is flushed with argon and charged with *N*-(2-propynyl)aniline **S1** (4.76 g, 36.28 mmol, 1.0 equiv), triethylamine (225 mL), iodobenzene (8.15g, 40.0 mmol, 1.1 equiv) and bis(triphenylphosphine) palladium dichloride (0.73 mmol, 0.02 equiv). Copper iodide (0.36 mmol, 0.01 equiv) is then added in a single portion to the flask. The reaction mixture is stirred at room temperature for 6 h. The reaction mixture is filtered under reduced pressure. The combined organic phases are transferred to separatory funnel and washed with brine (300 mL). The aqueous phase is extracted twice with diethyl ether (2×100 mL). The combined organic phases are dried with $MgSO_4$, filtered and concentrated by rotary evaporation to give a dark brown oil. The residue is purified by flashcolumn chromatography on silica gel to give **1a** in 96% yield (7.21 g).

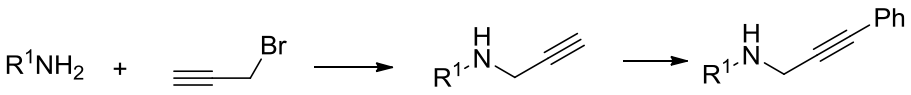
1ac were prepared following this method [3]



1ac

To aniline (0.93 g, 10 mmol) in CH_3CN (5 mL) was added 1-bromo-2-butyne (0.399 g, 3 mmol). The mixture was stirred overnight at room temperature. Saturated aqueous NH_4Cl (5 mL) was added, and mixture was separated. The aqueous layer was extracted with Et_2O (3×10 mL). The combined organic layers were washed with brine (10 mL), dried over $MgSO_4$, filtered and concentrated. Column chromatography (10% EtOAc/Hex) afforded a light yellow oil in 68% yield (0.296 g).

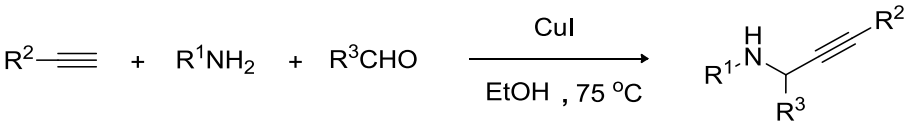
1ad-1af were prepared following this method [2, 4]



Propargyl bromide (3 mL, 10 mmol) was added to amine (60 mmol) over 0.5 h via addition funnel, and allowed to stir overnight. The resulting mixture was diluted in EtOAc, and washed with saturated aq. $NaHCO_3$ and dried over $MgSO_4$. The reaction mixture was concentrated and chromatographed, eluting with 9:1 hexanes/EtOAc, to afford the corresponding pale yellow liquid.

An oven-dried 50-mL, three-necked round-bottomed flask equipped with a magnetic stirring bar, a thermometer, and two rubber septa is flushed with argon and charged with propargylamine (5 mmol), triethylamine (20 mL), iodobenzene (5.5 mmol,) and bis(triphenylphosphine) palladium dichloride (0.1 mmol). Copper iodide (0.05 mmol) is then added in a single portion to the flask. The reaction mixture is stirred at room temperature for 6 h. The reaction mixture is filtered under reduced pressure. The combined organic phases are transferred to separatory funnel and washed with brine (30 mL). The aqueous phase is extracted twice with diethyl ether (3×10 mL). The combined organic phases are dried over anhydrous $MgSO_4$, filtered and concentrated by rotary evaporation. The residue is purified by flashcolumn chromatography on silica gel to give **1ad-1af**.

1ag and 1ah were prepared following this method [5]



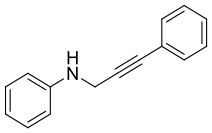
In a typical experiment, CuI (0.6 mmol) was charged in a test tube with a magnetic stirrer. The test tube was sealed and flushed with N_2 and then was charged with alkyne (2 mmol), aldehyde (2 mmol), and amine (2 mmol). The test tube was then placed in an oil bath of 75 ^oC and was allowed to stir overnight. The crude reaction mixture was purified by silica gel column chromatography to provide the desired product.

General procedure for synthesis of substituted pyrazole *N*-oxides from *N*-propargylamines and silver nitrite:

The *N*-propargylamines (**1**, 0.5mmol), silver nitrite (**2**, 0.6 mmol) were mixed in THF (2 mL) and this mixture was carried out under argon at 100 ^oC in sealed tube and the reaction time was monitored by TLC. Then the reaction mixture was cooled to room temperature and the solvent was evaporated in vacuo and the crude product was

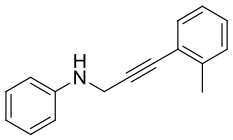
purified by column chromatography, eluting with petroleum ether/EtOAc (1:1) to afford the desired *N*-oxide pyrazole (**3**).

The data of products:



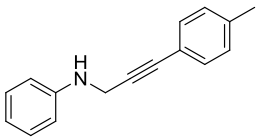
***N*-(3-phenylprop-2-yn-1-yl)aniline (1a)**

Yellow solid (72% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.40-7.38 (m, 2 H), 7.28-7.25 (m, 3 H), 7.24-7.19 (m, 2 H), 6.80-6.76 (m, 1 H), 6.73-6.71 (m, 2 H), 4.13 (s, 2 H), 3.93 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.12, 131.66, 129.18, 128.21, 128.17, 122.85, 118.43, 113.54, 86.36, 83.25, 34.53.



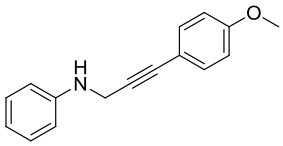
***N*-(3-(o-tolyl)prop-2-yn-1-yl)aniline (1b)**

Yellow oil (75% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.36-7.34 (d, *J* = 8.0 Hz, 2 H), 7.22-7.18 (m, 2 H), 7.16-7.12 (m, 2 H), 7.09-7.06 (m, 1 H), 6.79-6.75 (m, 1 H), 6.73-6.70 (d, *J* = 12.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.01, 140.21, 131.85, 129.29, 129.09, 128.11, 125.37, 122.54, 118.37, 113.63, 90.27, 82.04, 34.52, 20.56.



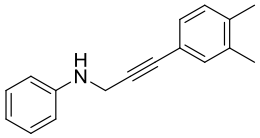
***N*-(3-(p-tolyl)prop-2-yn-1-yl)aniline (1c)**

Yellow solid (75% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.29-7.27 (d, *J* = 8.0 Hz, 2 H), 7.21-7.17 (m, 2 H), 7.05-7.03 (d, *J* = 8.0 Hz, 2 H), 6.77-6.74 (m, 1 H), 7.09-7.07 (m, 2 H), 6.68-6.66 (d, *J* = 8.0 Hz, 2 H), 4.06 (s, 2 H), 3.88 (s, 1 H), 2.28 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.10, 138.17, 131.48, 129.09, 128.91, 119.72, 118.24, 113.43, 85.65, 83.27, 34.42, 21.30.



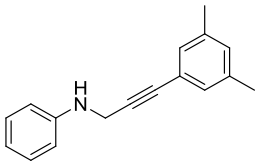
***N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)aniline (1d)**

Yellow solid (68% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.33-7.31 (m, 2 H), 7.22-7.18 (m, 2 H), 6.79-6.68 (m, 5 H), 4.07 (s, 2 H), 3.92 (s, 1 H), 3.72 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 140.92, 134.75, 131.87, 131.74, 130.60, 130.42, 128.32, 126.38, 125.37, 125.42, 86.40, 83.06, 69.25, 29.51, 19.32.



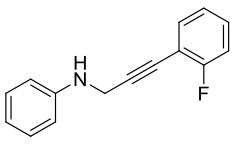
***N*-(3-(3,4-dimethylphenyl)prop-2-yn-1-yl)aniline (1e)**

Yellow solid (71% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.22-7.17 (m, 2 H), 7.14-7.12 (d, *J* = 8.0 Hz, 1 H), 7.02-7.01 (d, *J* = 4.0 Hz, 1 H), 6.78-6.74 (m, 1 H), 6.71-6.69 (d, *J* = 8.0 Hz, 2 H), 4.09 (s, 2 H), 3.91 (s, 1 H), 2.21 (s, 3 H), 2.18 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.18, 137.02, 136.48, 132.68, 129.49, 129.14, 129.07, 120.04, 118.29, 113.47, 85.32, 83.45, 34.53, 19.62, 19.44.



***N*-(3-(3,5-dimethylphenyl)prop-2-yn-1-yl)aniline (1f)**

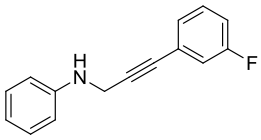
Yellow oil (70% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.19-7.17 (m, 2 H), 7.01 (s, 2 H), 6.90 (s, 1 H), 6.77-6.74 (m, 1 H), 6.70-6.68 (d, *J* = 8.0 Hz, 2 H), 4.09 (s, 2 H), 3.90 (s, 1 H), 2.23 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.15, 137.75, 130.07, 129.33, 129.16, 122.43, 118.33, 113.48, 85.57, 83.51, 34.50, 20.99.



***N*-(3-(2-fluorophenyl)prop-2-yn-1-yl)aniline (1g)**

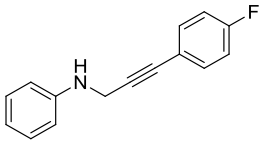
Yellow solid (83% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.35-7.31 (m, 1 H), 7.22-7.15 (m, 3 H), 7.00-6.96 (m, 2 H), 6.79-6.75 (m, 1 H), 6.70-6.68 (d, *J* = 8.0 Hz, 2 H), 4.09 (s, 2 H), 3.94 (s, 1 H), 4.91-4.95 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$,

ppm): δ = 164.31-161.81 (d, *J* = 250.0 Hz, 1 C), 147.26, 133.90, 130.24-130.17 (d, *J* = 7.0 Hz, 1 C), 129.48, 124.16-124.13 (d, *J* = 3.0 Hz, 1 C), 121.17, 118.69, 115.77-115.56 (d, *J* = 21.0 Hz, 1 C), 113.81, 111.69-111.53 (d, *J* = 16.0 Hz, 1 C), 92.16, 34.72.



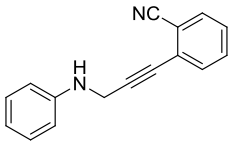
***N*-(3-(3-fluorophenyl)prop-2-yn-1-yl)aniline (1h)**

Yellow oil (69% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.21-7.14 (m, 3 H), 7.09-7.08 (d, *J* = 4.0 Hz, 1 H), 7.06 (d, *J* = 1.2 Hz, 1 H), 6.99-6.94 (m, 1 H), 6.80-6.77 (m, 1 H), 6.71-6.69 (d, *J* = 8.0 Hz, 2 H), 4.098 (s, 2 H), 3.915 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 163.44-160.99 (d, *J* = 245.0 Hz, 1 C), 146.94, 129.79-129.71 (d, *J* = 8.0 Hz, 1 C), 129.18, 127.52, 127.49, 124.70-124.61 (d, *J* = 9.0 Hz, 1 C), 118.54, 118.50-118.31 (d, *J* = 19.0 Hz, 1 C), 115.60-115.39 (d, *J* = 21.0 Hz, 1 C), 113.50, 87.47, 82.00-81.97 (d, *J* = 3.0 Hz, 1 C), 34.33.



***N*-(3-(4-fluorophenyl)prop-2-yn-1-yl)aniline (1i)**

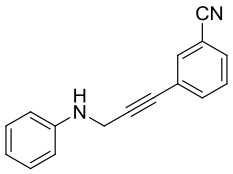
Yellow solid (80% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.40-7.37 (m, 2 H), 7.27-7.23 (m, 2 H), 7.01-6.97 (m, 2 H), 6.83-6.80 (m, 1 H), 6.76-6.74 (d, *J* = 8.0 Hz, 2 H), 4.14 (s, 2 H), 3.97 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 163.77-161.29 (d, *J* = 248.0 Hz, 1 C), 147.18, 133.75-133.67 (d, *J* = 8.0 Hz, 1 C), 129.38, 119.01, 118.63, 115.76-115.54 (d, *J* = 22.0 Hz, 1 C), 113.66, 86.21, 82.31, 34.57.



2-(3-(phenylamino)prop-1-yn-1-yl)benzonitrile (1j)

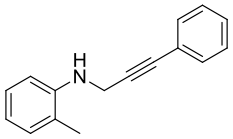
Yellow solid (77% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.58-7.56 (d, *J* = 8.0 Hz, 1 H), 7.46-7.44 (m, 2 H), 7.35-7.31 (m, 1 H), 7.25-7.21 (m, 2 H), 6.81-6.74 (m, 3 H), 4.21 (s, 2 H), 4.04 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 146.73, 132.43, 132.22, 129.18, 128.22, 126.69, 118.55, 117.46, 115.27, 113.59, 93.40, 79.39,

34.37.



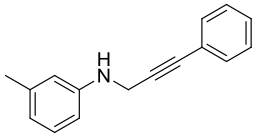
3-(3-(phenylamino)prop-1-yn-1-yl)benzonitrile (1k)

Yellow solid (70% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.62 (s, 1 H), 7.57-7.51 (m, 2 H), 7.37-7.33 (m, 1 H), 7.25-7.21 (m, 2 H), 4.15 (s, 2 H), 3.98 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 146.77, 135.69, 134.91, 131.31, 129.20, 129.08, 124.41, 118.61, 117.94, 113.50, 112.63, 89.19, 80.82, 34.26.



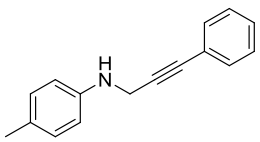
2-methyl-*N*-(3-phenylprop-2-yn-1-yl)aniline (1l)

Yellow oil (73% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.42-7.39 (m, 2 H), 7.27-7.25 (m, 3 H), 7.18-7.15 (m, 1 H), 7.08-7.06 (d, *J* = 8.0 Hz, 1 H), 6.76-6.71 (m, 2 H), 4.16 (s, 2 H), 3.78 (s, 1 H), 2.14(s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 145.33, 131.93, 130.35, 128.46, 127.31, 123.06, 122.95, 118.23, 110.74, 86.76, 83.44, 34.68, 17.72.



***N*-(3-(4-fluorophenyl)prop-2-yn-1-yl)-3-methylaniline (1m)**

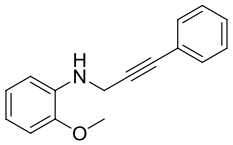
Yellow oil (68% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.41-7.39 (m, 2 H), 7.29-7.25 (m, 3 H), 7.14-7.10 (m, 1 H), 6.62-6.60 (d, *J* = 8.0 Hz, 1 H), 6.54-6.56 (d, *J* = 8.0 Hz, 2 H), 4.14 (s, 2 H), 3.90 (s, 1 H)，2.31 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.27, 139.14, 131.81, 129.21, 128.35, 128.32, 122.98, 119.50, 114.46, 110.76, 86.56, 83.31, 34.69, 21.37.



4-methyl-*N*-(3-phenylprop-2-yn-1-yl)aniline (1n)

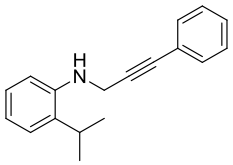
Yellow oil (79% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.40-7.38 (m, 3 H),

7.27-7.26 (m, 2 H), 7.04-7.02 (d, *J* = 8.0 Hz, 2 H), 6.66-6.64 (m, 2 H), 4.10 (s, 2 H), 3.82 (s, 1 H), 2.25 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 144.98, 131.84, 129.87, 128.38, 128.32, 127.87, 123.05, 113.92, 86.77, 83.32, 35.00, 20.61.



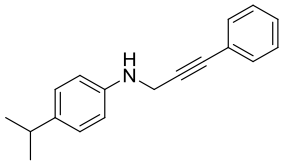
2-methoxy-*N*-(3-phenylprop-1-yn-1-yl)aniline (1o)

Colourless oil (69% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.39-7.37 (m, 2 H), 7.23-7.21 (m, 3 H), 6.92-6.87 (m, 1 H), 6.75-6.69 (m, 3 H), 4.50 (s, 1 H), 4.11 (d, *J* = 0.8 Hz, 2 H), 3.76 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.11, 136.96, 131.55, 128.06, 127.96, 122.88, 121.06, 117.43, 110.61, 109.43, 86.54, 82.92, 55.20, 34.01.



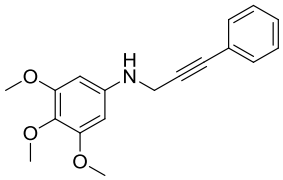
2-isopropyl-*N*-(3-phenylprop-1-yn-1-yl)aniline (1p)

Yellow oil (66% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.42-7.39 (m, 2 H), 7.29-7.27 (m, 3 H), 7.19-7.14 (m, 2 H), 6.83-6.79 (m, 2 H), 4.19 (s, 2 H), 3.96 (s, 1 H), 2.97-2.87 (m, 1 H), 1.28 (s, 3 H), 1.28 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 143.90, 133.18, 131.72, 128.21, 128.18, 126.67, 125.00, 122.93, 118.47, 111.48, 86.65, 83.25, 34.88, 27.12, 22.45.



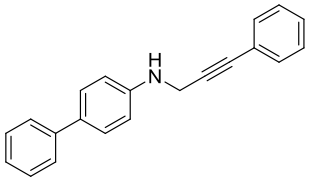
4-isopropyl-*N*-(3-phenylprop-1-yn-1-yl)aniline (1q)

Yellow oil (69% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.38-7.37 (d, *J* = 4.0 Hz, 2 H), 7.20 (d, *J* = 2.4 Hz, 3 H), 7.06-7.04 (m, 2 H), 6.63-6.60 (m, 2 H), 4.02 (s, 2 H), 3.77 (s, 1 H), 2.83-2.76 (m, 1 H), 1.21-1.18 (m, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 145.02, 138.61, 131.51, 128.06, 127.95, 125.55, 126.87, 122.83, 113.46, 86.76, 83.02, 34.56, 33.02, 24.07.



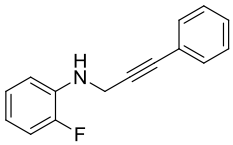
3,4,5-trimethoxy-*N*-(3-phenylprop-2-yn-1-yl)aniline (1r)

Yellow oil (63% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.40-7.37 (m, 2 H), 7.29-7.25 (m, 3 H), 4.13 (s, 2 H), 3.91 (s, 1 H), 3.84 (s, 3 H), 3.78 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 153.97, 143.96, 131.75, 130.78, 128.41, 122.85, 91.23, 86.30, 83.59, 61.21, 56.06, 35.06.



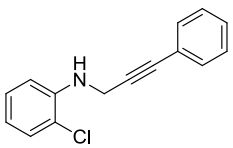
***N*-(3-(4-fluorophenyl)prop-2-yn-1-yl)-[1,1'-biphenyl]-4-amine (1s)**

Yellow solid (68% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.56-7.53 (m, 2 H), 7.49-7.46 (m, 2 H), 7.41-7.36 (m, 4 H), 7.29-7.23 (m, 4 H), 6.80-6.76 (m, 2 H), 4.15 (s, 2 H), 4.02 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 146.45, 141.04, 131.66, 131.23, 128.62, 128.22, 127.85, 126.33, 126.17, 122.73, 113.74, 86.21, 83.30, 34.46.



2-fluoro-*N*-(3-phenylprop-2-yn-1-yl)aniline (1t)

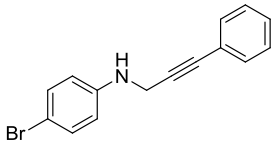
Yellow oil (70% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.39-7.37 (m, 2 H), 7.26-7.24 (m, 3 H), 7.04-6.95 (m, 2 H), 6.87-6.82 (m, 1 H), 6.71-6.66 (s, 1 H), 4.21 (s, 1 H), 4.13-4.15 (d, *J* = 7.2 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 153.06-150.69 (*J* = 237.0 Hz, 1 C), 135.58, 135.46, 131.66, 128.20, 124.50-124.47 (*J* = 3.0 Hz,1 C), 122.71, 117.82-117.76 (*J* = 6.0 Hz, 1 C), 114.57-114.39 (*J* = 18.0 Hz, 1 C), 113.01-112.98 (*J* = 3.0 Hz, 1 C), 85.86, 83.44, 34.09.



2-chloro-*N*-(3-phenylprop-1-yn-1-yl)aniline (1u)

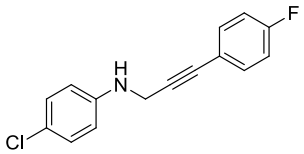
Colourless oil (68% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.39-7.37 (m, 2 H),

7.26-7.22 (m, 4 H), 7.17-7.13 (m, 1 H), 6.81-6.79 (m, 1 H), 6.69-6.65 (m, 1 H), 4.59 (s, 1 H), 4.14 (d, *J* = 3.2 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.96, 131.63, 129.08, 128.20, 128.16, 127.67, 122.65, 119.65, 118.18, 111.91, 85.67, 83.39, 34.05.



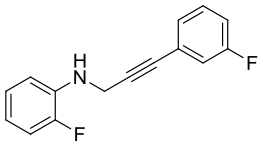
4-bromo-*N*-(3-phenylprop-1-yn-1-yl)aniline (1v)

Yellow solid (63% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.39-7.37 (m, 2 H), 7.30-7.26 (m, 5 H), 6.60-6.58 (m, 2 H), 4.09 (s, 2 H), 3.99 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 146.16, 131.67, 131.53, 128.32, 128.15, 127.59, 123.07, 121.75, 85.41, 83.57, 71.97, 30.56.



4-chloro-*N*-(3-(4-fluorophenyl)prop-2-yn-1-yl)aniline (1w)

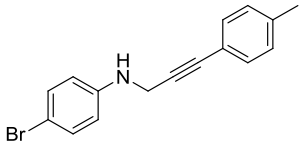
Yellow solid (71% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.38-7.34 (m, 2 H), 7.19-7.16 (m, 2 H), 7.00-6.96 (m, 2 H), 6.66-6.64 (m, 2 H), 4.09 (s, 2 H), 3.98 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 163.82-161.34 (d, *J* = 248.0 Hz, 1 C), 145.67, 133.74-133.66 (d, *J* = 8.0 Hz, 1 C), 129.19, 123.25, 118.84, 115.79-115.57 (d, *J* = 22.0 Hz, 1 C), 114.77, 85.67, 82.52, 34.58.



2-fluoro-*N*-(3-(3-fluorophenyl)prop-2-yn-1-yl)aniline (1x)

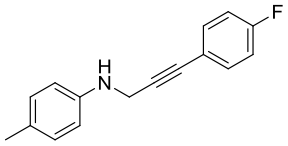
Yellow oil (66% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.24-7.18 (m, 1 H), 7.16-7.14 (d, *J* = 8.0 Hz, 1 H), 7.09-6.95 (m, 4 H), 6.86-6.82 (m, 1 H), 6.73-6.67 (m, 1 H), 4.21 (s, 1 H), 4.15 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 163.49-161.04 (d, *J* = 245.0 Hz, 1 C), 153.10-150.72 (d, *J* = 238.0 Hz, 1 C), 135.46, 135.34, 129.83-129.74 (d, *J* =9.0 Hz, 1 C), 127.57-127.54 (d, *J* = 3.0 Hz, 1 C), 124.60-124.53 (d, *J* = 7.0 Hz, 1 C), 124.50, 118.60-118.37 (d, *J* = 23.0 Hz, 1 C), 117.99-117.93 (d, *J* = 6.0 Hz, 1 C), 115.71-115.50 (d, *J* = 21.0 Hz, 1 C), 114.64-114.46 (d, *J* = 18.0 Hz, 1

C), 113.00, 112.97, 86.93, 82.26-82.22 (d, *J* = 4.0 Hz, 1 C), 34.01.



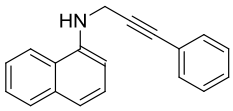
4-bromo-*N*-(3-phenylprop-2-yn-1-yl)aniline (1y)

Yellow solid (64% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.32-7.29 (m, 4 H), 7.11-7.09 (d, *J* = 8.0 Hz, 2 H), 6.61-6.59 (d, *J* = 8.0 Hz, 2 H), 4.10 (s, 2 H), 4.00 (s, 1 H), 2.34 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 146.22, 137.96, 138.61, 132.04, 131.70, 129.19, 119.65, 115.25, 110.24, 85.17, 83.73, 34.60, 21.62.



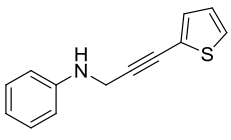
***N*-(3-(4-fluorophenyl)prop-2-yn-1-yl)-4-methylaniline (1z)**

Yellow oil (67% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.38-7.35 (m, 2 H), 7.05-6.97 (m, 4 H), 6.67-6.65 (d, *J* = 8.0 Hz, 2 H), 4.11(s, 2 H), 3.82 (s, 1 H), 2.26 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 144.86-142.48 (d, *J* = 238.0 Hz, 1 C), 133.71-133.63 (d, *J* = 8.0 Hz, 1 C), 129.84, 127.936, 119.04, 115.71-115.49 (d, *J* = 22.0 Hz, 2 C), 113.87, 86.38, 82.22, 34.90, 20.57.



***N*-(3-phenylprop-2-yn-1-yl)naphthalen-1-amine (1aa)**

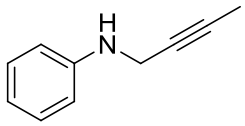
Yellow oil (69% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.81-7.79 (m, 2 H), 7.29-7.45 (m, 9 H), 6.77-6.76 (d, *J* = 4.0 Hz, 1 H), 4.59 (s, 1 H), 4.28 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.50, 134.39, 131.95, 128.85, 128.50, 126.65, 126.03, 125.16, 123.99, 123.01, 120.23, 118.76, 105.71, 86.45, 83.75, 34.95.



***N*-(3-(thiophen-2-yl)prop-2-yn-1-yl)aniline (1ab)**

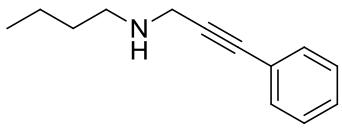
Yellow oil (79% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.23-7.18 (m, 3 H), 7.15-7.14 (m, 1 H) 6.93-6.90 (m, 1 H), 6.80-6.69 (m, 3 H), 4.13 (s, 2 H), 3.91 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 146.96, 131.99, 129.20, 126.88, 126.82,

122.79, 118.48, 113.49, 90.38, 34.63.



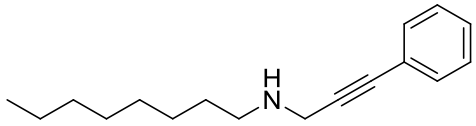
***N*-(but-2-yn-1-yl)aniline (1ac)**

Yellow oil (68% yield). ^{1}H NMR (400 MHz, CDCl3, ppm): δ = 7.22-7.18 (m, 2 H), 6.78-6.74 (m, 1 H), 6.68-6.65 (m, 2 H), 3.87-3.86 (d, *J* = 4.0 Hz, 2 H), 3.83 (s, 1 H), 1.81-1.80 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.33, 129.17, 118.24, 113.40, 79.04, 76.08, 34.05, 3.50.



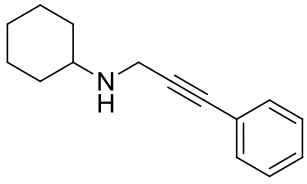
***N*-(3-phenylprop-2-yn-1-yl)butan-1-amine (1ad)**

Yellow solid (62% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.43-7.41 (m, 2 H), 7.30-7.28 (m, 3 H), 3.64 (m, 2 H), 2.77-2.74 (m, 2 H), 1.55-1.48 (m, 2 H), 1.43-1.34 (m, 3 H), 1.96-1.92 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 131.63, 128.23, 127.95, 87.90, 83.27, 48.59, 39.07, 32.04, 20.46, 13.97.



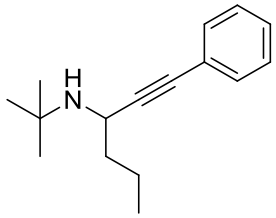
***N*-(3-phenylprop-2-yn-1-yl)octan-1-amine (1ae)**

Yellow solid (57% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.42-7.39 (m, 2 H), 7.27-7.25 (m, 3 H), 3.64 (m, 2 H), 2.71-2.64 (m, 1 H), 1.88-1.85 (m, 2 H), 1.75-1.71 (m, 2 H), 1.62-1.58 (m, 1 H)，1.39 (s, 1 H), 1.32-1.03 (m, 5 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 131.53, 128.14, 127.87, 123.19, 87.78, 83.17, 48.83, 38.97, 31.76, 29.83, 29.44, 29.19, 27.27, 22.59, 14.04.



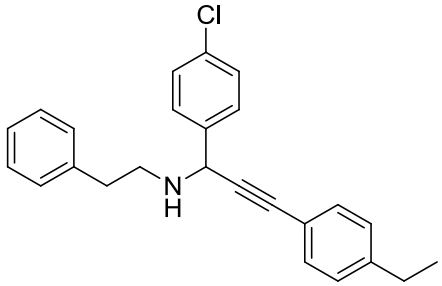
***N*-(3-phenylprop-2-yn-1-yl)cyclohexanamine (1af)**

Yellow solid (68% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.41-7.39 (m, 2 H), 7.28-7.25 (m, 3 H), 3.62 (m, 2 H), 2.74-2.70 (m, 2 H), 1.88-1.85 (m, 2 H), 1.52-1.48 (m, 2 H), 1.36-1.26 (m, 11 H), 0.88-0.84 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 131.50, 128.10, 127.81, 123.20, 87.93, 82.93, 55.11, 35.91, 33.00, 25.99, 24.75.



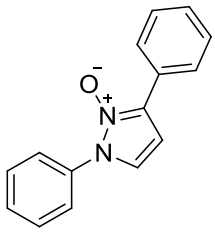
***N*-(tert-butyl)-1-phenylhex-1-yn-3-amine (1ag)**

Yellow oil (53% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.37-7.36 (m, 2 H), 7.26-7.24 (m, 3 H), 3.60-3.57 (m, 1 H), 1.64-1.51 (m, 4 H), 1.19 (s, 9 H), 0.98-0.94 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 131.36, 128.14, 127.60, 94.45, 82.55, 51.25, 44.33, 40.86, 29.90, 19.40, 13.85.



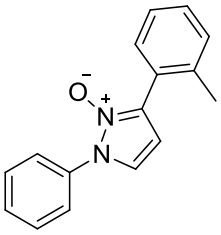
1-(4-chlorophenyl)-3-(4-ethylphenyl)-*N*-phenethylprop-2-yn-1-amine (1ah)

Yellow solid (50% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.48-7.46 (m, 2 H), 7.37-7.35 (m, 3 H), 7.30-7.25 (m, 4 H), 7.21-7.19 (m, 3 H), 7.13-7.11 (m, 2 H), 4.77 (s, 2 H), 3.10-3.04 (m, 1 H), 3.00-2.94 (m, 1 H), 2.89-2.79 (m, 2 H), 2.64-2.59 (m, 2 H), 1.54 (s, 1 H), 1.22-1.18 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 144.88, 139.96, 139.136, 133.56, 131.85, 129.18, 128.91, 128.73, 128.65, 128.05, 126.39, 120.17, 88.13, 86.08, 54.07, 48.37, 36.40, 28.98, 15.61.



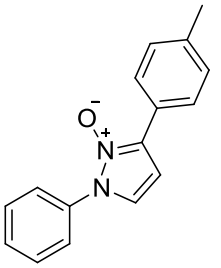
1,3-diphenyl-1H-pyrazole *N*-oxide (3a)

Yellow solid (100 mg, 85% yield). melting point: 147-149 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.24-8.22 (m, 2 H), 7.65-7.62 (m, 2 H), 7.55-7.45(m, 5 H), 7.39-7.37(m, 1 H), 7.20-7.19 (d, *J* = 4.0 Hz, 1 H), 6.61-6.60 (d, *J* = 4.0 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 134.11, 129.62, 129.21, 128.65, 128.59, 128.30, 126.41, 125.91, 118.90, 100.65; HRMS calcd for $C_{15}H_{13}N_2O$ $[M+H]^+$ 237.1023; found: 237.1028.



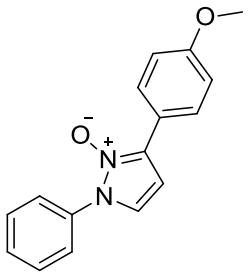
1-phenyl-3-(o-tolyl)-1H-pyrazole *N*-oxide (3b)

Yellow oil (105 mg, 84% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.68-7.65 (m, 2 H), 7.58-7.57 (d, *J* = 4.0 Hz, 1 H), 7.54-7.50 (m, 2 H), 7.47-7.42 (m, 1 H), 7.35-7.25 (m, 4 H), 7.22-7.21 (d, *J* = 4.0 Hz, 1 H), 6.37 -6.36 (d, *J* = 4.0 Hz, 1 H), 2.43 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 137.97, 134.30, 130.86, 130.44, 129.16, 129.13, 128.93, 127.94, 125.60, 125.44, 118.10, 103.54, 20.29; HRMS calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$ 251.1179; found: 251.1172.



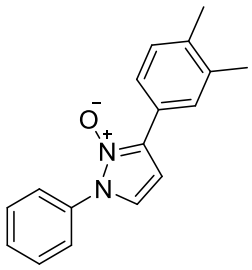
1-phenyl-3-(p-tolyl)-1H-pyrazole *N*-oxide (3c)

Yellow oil (104 mg, 83% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.28-7.26 (d, *J* = 8.0 Hz, 2 H), 7.20-7.16 (m, 2 H), 7.05-7.03 (d, *J* = 8.0 Hz, 2 H), 6.77-6.73 (m, 1 H), 6.68-6.66 (d, *J* = 8.0 Hz, 2 H), 4.05 (s, 2 H), 3.87 (s, 1 H), 2.27 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.10, 138.17, 131.48, 129.09, 128.91, 119.72, 118.24, 113.43, 85.65, 83.27, 34.42, 21.30; HRMS calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$ 251.1179; found: 251.1174.



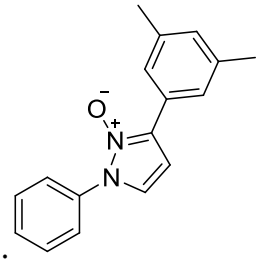
3-(4-methoxyphenyl)-1-phenyl-1H-pyrazole *N*-oxide (3d)

Yellow solid (105 mg, 79% yield). melting point: 192-194 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.21-8.17 (m, 2 H), 7.61-7.64 (m, 2 H), 7.54-7.50 (m, 2 H), 7.48-7.44 (m, 1 H), 7.18-7.17 (d, *J* = 4.0 Hz, 1 H), 7.01-6.97 (m, 2 H), 6.55-6.54 (d, *J* = 4.0 Hz, 1 H), 3.85 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 163.89，161.41， 134.02， 129.31， 129.24, 128.79, 128.43, 128.35, 125.90, 124.57, 124.53, 118.95, 115.71, 115.49, 100.41; HRMS calcd for $C_{16}H_{15}N_2O_2$ $[M+H]^+$ 267.1128; found: 267.1134.



3-(3,4-dimethylphenyl)-1-phenyl-1H-pyrazole *N*-oxide (3e)

Yellow solid (106 mg, 80% yield). melting point: 158-160 ^{o}C. ^{1}H NMR (400 MHz, CDCl3, ppm): δ = 8.08 (s, 1 H), 7.91-7.89 (m, 1 H), 7.63-7.60 (m, 2 H), 7.53-7.48 (m, 2 H), 7.47-7.42 (m, 1 H), 7.22-7.20 (d, *J* = 8.0 Hz, 1 H), 7.17-7.16 (d, *J* = 4.0 Hz, 1 H), 6.56-6.55 (d, *J* = 4.0 Hz, 1 H), 2.31 (s, 3 H), 2.29 (s, 3 H); ^{13}C NMR (100 MHz, CDCl3, ppm): δ = 137.31, 136.68，134.10, 129.72, 129.70, 129.05, 128.98, 127.36, 125.76, 125.72, 123.82, 118.74, 100.45, 19.82, 19.64; HRMS calcd for $C_{17}H_{17}N_2O$ $[M+H]^+$ 265.1336; found: 265.1331.



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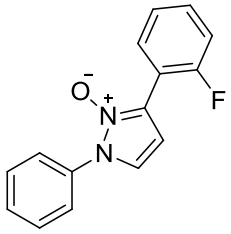
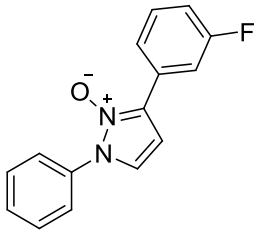
3-(3,5-dimethylphenyl)-1-phenyl-1H-pyrazole *N*-oxide (3f)

Yellow oil (108 mg, 82% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.86 (s, 2 H), 7.63-7.61 (m, 2 H), 7.47-7.44 (m, 3 H), 7.18-7.17 (d, *J* = 4.0 Hz, 1 H), 7.01 (s, 1 H), 6.58-6.57 (d, *J* = 4.0 Hz, 1 H), 2.37 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 138.00, 134.08, 130.34, 129.72, 129.07, 129.05, 127.98, 125.81, 124.08, 118.72, 100.68, 21.38; HRMS calcd for $C_{17}H_{17}N_2O$ $[M+H]^+$ 265.1336; found: 265.1339.



3-(2-fluorophenyl)-1-phenyl-1H-pyrazole *N*-oxide (3g)

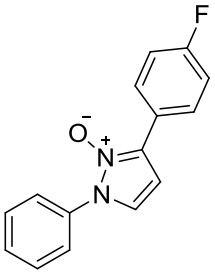
Yellow solid (98 mg, 77% yield). melting point: 125-127 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.82-8.78 (m, 1 H), 7.64-7.61 (m, 2 H), 7.55-7.45 (m, 3 H), 7.38-7.32 (m, 1 H), 7.28-7.24 (m, 1 H), 7.22-7.21 (d, *J* = 4.0 Hz, 1 H),7.19-7.14 (m, 1 H), 6.77-6.75 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 160.90-158.41 (d, *J* = 249.0 Hz, 1 C), 133.97, 130.15-130.07 (d, *J* = 8.0 Hz, 1 C), 129.24-129.18 (d, *J* = 6.0 Hz, 1 C), 129.04, 129.02, 125.84, 124.50, 124.22-124.18 (d, *J* = 4.0 Hz, 1 C), 118.31, 118.29, 116.59, 116.48, 115.72-115.50 (d, *J* = 22.0 Hz, 1 C), 103.80, 103.68; HRMS calcd for $C_{15}H_{12}FN_2O$ $[M+H]^+$ 255.0928; found: 255.0924.



3-(3-fluorophenyl)-1-phenyl-1H-pyrazole *N*-oxide (3h)

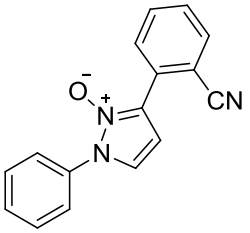
Yellow solid (102 mg, 80% yield). melting point: 127-129 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.15-8.12 (m, 1 H), 7.92-7.90 (m, 1 H), 7.62-7.59 (m, 2 H), 7.54-7.45 (m, 3 H), 7.43-7.38 (m, 1 H), 7.19-7.18 (d, *J* = 4.0 Hz, 1 H), 7.08-7.03 (m, 2 H), 6.59-6.58 (d, *J* = 4.0 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 164.02-161.59 (d, *J* = 243.0 Hz, 1 C), 133.79, 130.26-130.17 (d, *J* = 9.0 Hz, 1 C), 129.99-129.90 (d, *J* = 9.0 Hz, 1 C), 129.27, 129.15, 128.35, 128.32, 125.76,

121.81-121.78 (d, *J* = 3.0 Hz, 1 C), 118.88, 115.45-115.22 (d, *J* = 23.0 Hz, 1 C), 113.27-113.03 (d, *J* = 24.0 Hz, 1 C), 100.50; HRMS calcd for $C_{15}H_{12}FN_2O$ $[M+H]^+$ 255.0928; found: 255.0922.



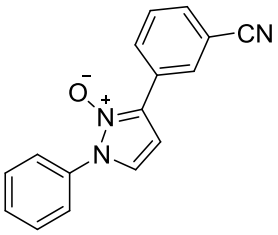
3-(4-fluorophenyl)-1-phenyl-1H-pyrazole *N*-oxide (3i)

Yellow solid (119 mg, 94% yield). melting point: 163-165 ^oC. ^1H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.26-8.22 (m, 2 H), 7.63-7.60 (m, 2 H), 7.55-7.46 (m, 3 H), 7.57-7.56 (d, *J* = 4.0 Hz, 1 H),; ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 163.89-161.41 (d, *J* = 248.0 Hz, 1 C), 134.02, 129.31, 129.24, 128.79, 128.43-128.35 (d, *J* = 8.0 Hz, 1 C), 125.90, 124.57-124.53 (d, *J* = 4.0 Hz, 1 C), 118.95, 115.71-115.49 (d, *J* = 22.0 Hz, 1 C), 100.41; HRMS calcd for $C_{15}H_{12}FN_2O$ $[M+H]^+$ 255.0928; found: 255.0933.



3-(2-cyanophenyl)-1-phenyl-1H-pyrazole *N*-oxide (3j)

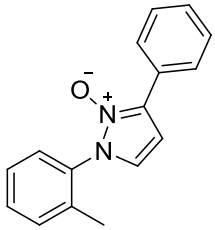
Yellow solid (106 mg, 81% yield). melting point: 167-169 ^oC. ^1H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.59 (d, *J* = 0.8 Hz, 1 H), 7.80-7.77 (m, 1 H), 6.98-6.97 (d, *J* = 4.0 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 133.89, 133.79, 132.90, 131.44, 129.59, 129.55, 129.34, 128.79, 126.38, 125.87, 118.50, 110.62, 102.99; $C_{16}H_{12}N_3O$ $[M+H]^+$ 262.0975; found: 262.0979.



3-(3-cyanophenyl)-1-phenyl-1H-pyrazole *N*-oxide (3k)

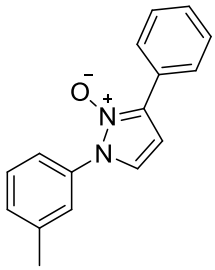
Yellow solid (115 mg, 88% yield). melting point: 189-191 ^oC. ^1H NMR (400 MHz,

$CDCl_3$, ppm): δ = 8.62 (s, 1 H), 8.47-8.45 (d, *J* = 8.0 Hz, 1 H), 7.65-7.61 (m, 3 H), 7.59-7.49(m, 4 H), 7.25-7.24 (d, *J* = 8.0 Hz, 1 H), 7.65-7.64 (d, *J* = 4.0 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 133.63, 131.66, 130.11, 129.64, 129.62, 129.59, 129.39, 129.30, 127.41, 125.85, 119.15, 118.48, 112.92, 100.31; HRMS calcd for $C_{16}H_{12}N_3O$ $[M+H]^+$ 262.0975; found: 262.0978.



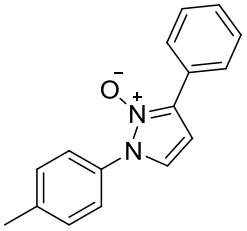
3-phenyl-1-(o-tolyl)-1H-pyrazole *N*-oxide (3l)

Yellow oil (90 mg, 72% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.26-8.23 (m, 2 H), 7.47-7.42 (m, 3 H), 7.39-7.34 (m, 1 H), 7.06-7.05 (d, *J* = 4.0 Hz, 1 H), 6.62-6.61 (d, *J* = 4.0 Hz, 1 H), 2.23 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 139.96, 133.17. 131.03, 130.67, 128.83, 128.78, 128.65, 128.52, 128.46, 128.37, 126.74, 126.16, 119.48, 100.27, 17.83; HRMS calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$251.1179; found: 251.1175.



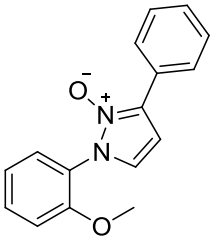
3-phenyl-1-(m-tolyl)-1H-pyrazole *N*-oxide (3m)

Yellow oil (96 mg, 77% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.24-8.22 (m, 2 H), 7.48-7.44 (m, 3 H), 7.40-7.34 (m, 3 H), 7.29-7.27 (m, 1 H), 7.17-7.16 (d, *J* = 4.0 Hz, 1 H), 6.59-6.58 (d, *J* = 4.0 Hz, 1 H), 2.43 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 139.91, 133.94, 130.02, 129.52, 128.95, 128.55, 128.51, 128.33, 126.58, 126.33, 122.90, 118.96, 100.43, 21.27; HRMS calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$ 251.1179; found: 251.1182.



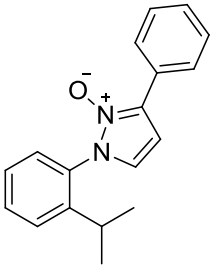
3-phenyl-1-(p-tolyl)-1H-pyrazole *N*-oxide (3n)

Yellow oil (95 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.24-8.22 (m, 1 H), 7.51-7.44 (m, 4 H), 7.39-7.32 (m, 3 H), 7.17-7.16 (d, *J* = 4.0 Hz, 1 H), 6.59-6.58 (d, *J* = 4.0 Hz, 1 H), 2.43 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 139.55, 131.56, 129.78, 129.78, 129.49, 128.55, 128.37, 126.36, 125.93, 118.97, 100.38, 21.25; HRMS calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$ 251.1179; found: 251.1176.



1-(2-methoxyphenyl)-3-phenyl-1H-pyrazole *N*-oxide (3o)

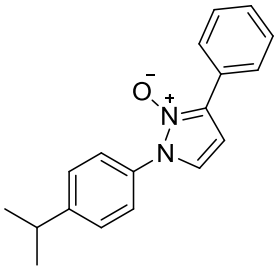
Yellow solid (116 mg, 87% yield). melting point: 200-202 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.26-8.24 (m, 2 H), 7.51-7.46 (m, 2 H), 7.44-7.41 (m, 2 H), 7.36-7.32 (m, 1 H), 7.11-7.05 (m, 3 H), 6.58-6.57 (d, *J* = 4.0 Hz, 1 H), 3.81 (s, 3 H), 2.23 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 155.51, 131.70, 130.12, 128.58, 128.50, 128.42, 128.30, 126.18, 122.42, 120.65, 120.58, 112.23, 99.71, 55.96; HRMS calcd for $C_{16}H_{15}N_2O_2$ $[M+H]^+$ 267.1128; found: 267.1124.



1-(2-isopropylphenyl)-3-phenyl-1H-pyrazole *N*-oxide (3p)

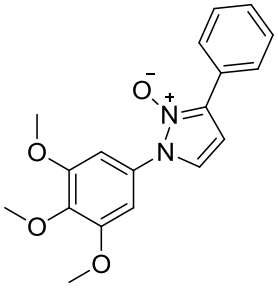
Yellow oil (110 mg, 79% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.25-8.22 (m, 2 H), 7.53-7.43 (m, 4 H), 7.37-7.29 (m, 2 H), 7.23-7.20 (m, 4 H), 7.18-7.08 (m, 2 H), 7.05-7.04 (d, *J* = 4.0 Hz, 1 H), 6.62-6.61 (d, *J* = 4.0 Hz, 1 H), 2.87-2.77 (m, 1 H), 1.30-1.28 (d, *J* = 8.0 Hz, 3 H), 1.15-1.13 (d, *J* = 8.0 Hz, 3 H); ^{13}C NMR (100 MHz,

$CDCl_3$, ppm): δ =148.30, 131.90, 131.14, 129.28, 128.65, 128.61, 128.52, 128.47, 128.39, 126.70, 126.62, 126.22, 126.17, 119.89, 100.18, 28.50; HRMS calcd for $C_{18}H_{19}N_2O$ $[M+H]^+$ 279.1492; found: 279.1496.



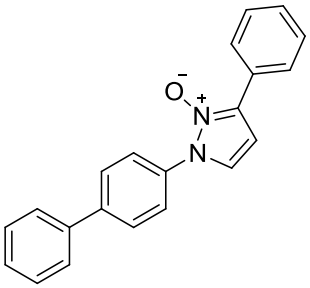
1-(4-isopropylphenyl)-3-phenyl-1H-pyrazole 2-oxide (3q)

Yellow solid (117 mg, 84% yield). melting point: 183-185 ^oC. ^1H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.24-8.22 (m, 2 H), 7.54-7.51 (m, 2 H), 7.48-7.44 (m, 2 H), 7.39-7.34 (m, 3 H), 7.17-7.16 (d, *J* = 4.0 Hz, 1 H), 6.59-6.58 (d, *J* = 4.0 Hz, 1 H), 3.02-2.95 (m, 1 H), 1.29 (s, 3H), 1.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 150.32, 131.71, 129.45, 128.53, 128.37, 127.21, 126.35, 125.99, 118.97, 100.36, 33.97, 23.84; HRMS calcd for $C_{18}H_{19}N_2O$ $[M+H]^+$ 279.1492; found: 279.1489.



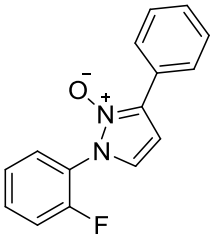
3-phenyl-1-(3,4,5-trimethoxyphenyl)-1H-pyrazole *N*-oxide (3r)

Yellow solid (137 mg, 84% yield). melting point: 136-138 ^oC. ^1H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.22-8.20 (m, 2 H), 7.49-7.46 (m, 2 H), 7.40-7.36 (m, 1 H), 7.18-7.17 (d, *J* = 4.0 Hz, 1 H), 6.84 (s, 2 H), 6.60-6.59 (d, *J* = 4.0 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 153.44, 138.98, 129.55, 129.54, 129.45, 128.68, 128.60, 128.21, 126.41, 119.20, 104.25, 100.51, 60.92, 56.40; HRMS calcd for $C_{18}H_{19}N_2O_4$ $[M+H]^+$ 327.1340; found: 327.1346.



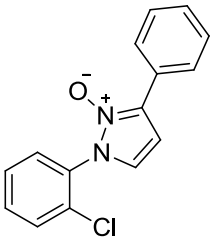
1-([1,1'-biphenyl]-4-yl)-3-phenyl-1H-pyrazole *N*-oxide (3s)

Yellow oil (120 mg, 77% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.26-8.23 (m, 2 H), 7.74-7.72 (d, *J* = 8.0 Hz, 4 H), 7.63-7.61 (d, *J* = 8.0 Hz, 2 H), 7.50-7.46 (m, 4 H), 7.42-7.36 (m, 2 H), 7.25-7.24 (d, *J* = 4.0 Hz, 1 H), 6.64-6.63 (d, *J* = 4.0 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.34, 139.96, 133.14, 129.05, 128.82, 128.72, 128.04, 128.01, 127.35, 126.51, 126.28, 119.08, 100.85; HRMS calcd for $C_{21}H_{17}N_2O$ $[M+H]^+$ 313.1336; found: 313.1345.



1-(2-fluorophenyl)-3-phenyl-1H-pyrazole *N*-oxide (3t)

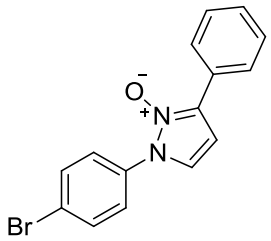
Yellow oil (104 mg, 82% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.24-8.22 (m, 2 H), 7.66-7.16 (m, 1 H), 7.52-7.44 (m, 3 H), 7.38-7.35 (m, 1 H), 7.73-7.26 (m, 2 H), 7.16-7.14 (m, 1 H), 6.63-6.62 (d, *J* = 4.0 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 158.60-156.08 (d, *J* = 252.0 Hz, 1 C), 131.77-131.69 (d, *J* = 8.0 Hz, 2 C), 129.74, 129.05, 128.66-128.50 (d, *J* = 16.0 Hz, 1 C), 126.24, 124.53-124.49 (d, *J* = 4.0 Hz, 1 C), 121.68-121.56 (d, *J* = 12.0 Hz, 1 C), 120.20, 120.19, 116.86-116.67 (d, *J* = 19.0 Hz, 1 C), 100.75; HRMS calcd for $C_{15}H_{12}FN_2O$ $[M+H]^+$ 255.0928; found: 255.0924.



1-(2-chlorophenyl)-3-phenyl-1H-pyrazole *N*-oxide (3u)

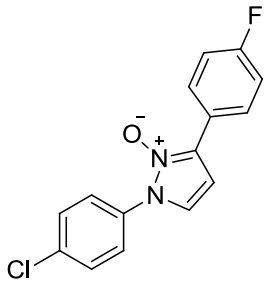
Yellow oil (124 mg, 92% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.26-8.23 (d, 2 H), 7.59-7.55 (m, 2 H), 7.50-7.41 (m, 4 H), 7.38-7.34 (m, 1 H), 7.11-7.10 (d, *J* = 4.0

Hz, 1 H), 6.64-6.63 (d, *J* = 4.0 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 133.43, 131.66, 131.61, 130.80, 130.49, 128.80, 128.60, 128.50, 128.05, 127.53, 126.18, 119.97, 100.54; HRMS calcd for $C_{15}H_{12}ClN_2O$ $[M+H]^+$271.0633; found: 271.0637.



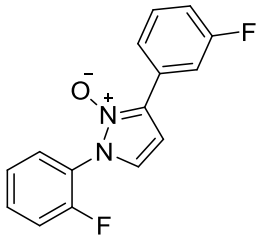
1-(4-bromophenyl)-3-phenyl-1H-pyrazole *N*-oxide (3v)

Yellow solid (138 mg, 88% yield). melting point: 175-177 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.21-8.19 (d, *J* = 8.0 Hz, 2 H), 7.64-7.37 (m, 2 H), 7.54-7.51 (m, 2 H), 7.48-7.45 (m, 2 H), 7.40-7.36 (m, 1 H), 7.18-7.17 (m, 1 H), 6.62-6.60 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 133.00, 132.38, 129.76, 128.80, 128.60, 28.02, 127.16, 126.37, 123.71, 118.63, 101.04; HRMS calcd for $C_{15}H_{12}BrN_2O$ $[M+H]^+$ 315.0128; found: 315.0121.



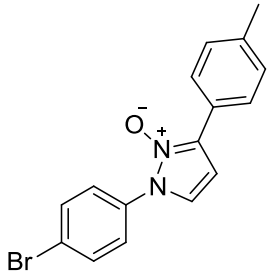
1-(4-chlorophenyl)-3-(4-fluorophenyl)-1H-pyrazole *N*-oxide (3w)

Yellow oil (121 mg, 84% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.24-8.19 (m, 2 H), 7.59-7.57 (d, *J* = 8.0 Hz, 2 H), 7.51-7.49 (d, *J* = 8.0 Hz, 2 H), 7.18-7.13 (m, 3 H), 6.58-6.57 (d, *J* = 4.0 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 163.93-161.45 (d, *J* = 248.0 Hz, 1 C), 135.27, 132.38, 129.43, 128.92, 128.41-128.33 (d, *J* = 7.0 Hz, 1 C), 126.98, 124.28-124.25 (d, *J* = 3.0 Hz, 1 C), 118.75, 115.74-115.52 (d, *J* = 22.0 Hz, 1 C), 100.74; HRMS calcd for $C_{15}H_{11}ClFN_2O$ $[M+H]^+$ 289.0539; found: 289.0535.



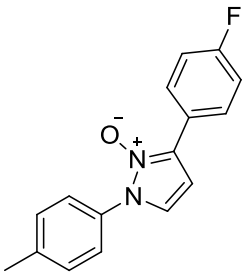
1-(2-fluorophenyl)-3-(3-fluorophenyl)-1H-pyrazole *N*-oxide (3x)

Yellow solid (113 mg, 83% yield). melting point: 105-107 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.14-8.10 (m, 1 H), 7.94-7.91 (m, 1 H), 7.66-7.62 (m, 1 H), 7.55-7.50 (m, 1 H), 7.45-7.39 (m, 1 H), 7.35-7.28 (m, 2 H), 7.18-7.17 (m, 1 H), 7.10-7.05 (m, 1 H), 7.64-7.63 (d, *J* = 4.0 Hz, 1 H) ; ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 164.12-161.68 (d, *J* = 244.0 Hz,), 158.67-156.14 (d, *J* = 253.0 Hz,), 132.03-131.95 (d, *J* = 8.0 Hz, 1 C), 130.08-130.00 (d, *J* = 8.0 Hz, 1 C), 129.74, 128.01, 124.65-124.61, (d, *J* = 4.0 Hz, 1 C), 121.82-121.79, (d, *J* = 3.0 Hz, 1 C), 121.54, 121.42, 120.23-120.21 (d, *J* = 2.0 Hz, 1 C), 116.98-116.79, (d, *J* = 19.0 Hz, 1 C), 115.67-115.46, (d, *J* = 21.0 Hz, 1 C), 113.34, 113.09, 100.76; HRMS calcd for $C_{15}H_{11}F_2N_2O$ $[M+H]^+$ 273.0834; found: 273.0839.



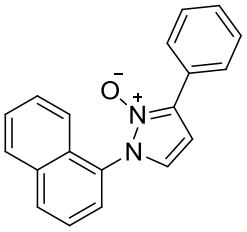
1-(4-bromophenyl)-3-(p-tolyl)-1H-pyrazole *N*-oxide (3y)

Yellow solid (131 mg, 80% yield). melting point: 215-217 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.11-8.09 (d, *J* = 8.0 Hz, 2 H), 7.67-7.64 (m, 2 H), 7.55-7.52 (m, 2 H), 7.29-7.26 (m, 2 H), 7.17-7.16 (d, *J* = 4.0 Hz, 1 H), 6.59-6.58 (d, *J* = 4.0 Hz, 1 H), 2.39 (s, 3 H) ; ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 138.89, 133.09, 132.38, 129.91, 129.31, 27.16, 126.30, 125.20, 123.10, 118.55, 100.91, 21.40; HRMS calcd for $C_{16}H_{14}BrN_2O$ $[M+H]^+$ 329.0284; found: 329.0276.



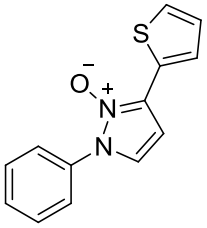
3-(4-fluorophenyl)-1-(p-tolyl)-1H-pyrazole *N*-oxide (3z)

Yellow oil (102 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.26-8.21 (m, 2 H), 7.49-7.47 (d, *J* = 8.0 Hz, 2 H), 7.33-7.31 (d, *J* = 8.0 Hz, 2 H), 7.16-7.12 (m, 3 H), 6.55-6.54 (d, *J* = 8.0 Hz, 1 H), 2.43 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 163.81-161.34 (d, *J* = 247.0 Hz, 1 C), 139.63, 131.44, 129.79, 128.63, 128.35-128.27 (d, *J* = 8.0 Hz, 1 C), 125.89, 124.62-124.59 (d, *J* = 3.0 Hz, 1 C), 119.00, 115.64-115.42 (d, *J* = 3.0 Hz, 1 C), 100.11, 21.22; HRMS calcd for $C_{16}H_{14}FN_2O$ $[M+H]^+$ 269.1085; found: 269.1088.



1-(naphthalen-1-yl)-3-phenyl-1H-pyrazole *N*-oxide (3aa)

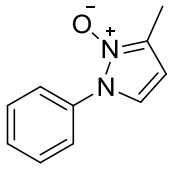
Yellow oil (122 mg, 85% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.31-8.25 (m, 2 H), 8.06-8.04 (m, 1 H), 7.97-7.93 (m, 1 H), 7.65-7.57 (m, 2 H), 7.56-7.45 (m, 5 H), 7.40-7.35 (m, 1 H), 7.21-7.20 (d, *J* = 4.0 Hz, 1 H), 6.73-6.72 (d, *J* = 4.0 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 134.21, 131.17, 130.80, 130.54, 019.03, 128.59, 128.57, 128.32, 128.29, 127.90, 127.33, 126.89, 126.27, 125.07, 122.74, 120.76, 100.47; HRMS calcd for $C_{19}H_{15}N_2O$ $[M+H]^+$ 287.1179; found: 287.1173.



1-phenyl-3-(thiophen-2-yl)-1H-pyrazole *N*-oxide (3ab)

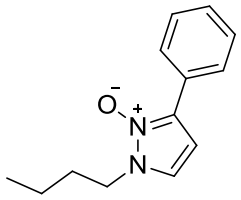
Yellow oil (115 mg, 95% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.65-7.61 (M,

3 H), 7.54-7.51 (m, 2 H), 7.48-7.46 (m, 1 H), 7.44-7.42 (m, 1 H), 7.20-7.19 (d, *J* = 4.0 Hz, 1 H), 7.16-7.13 (m, 1 H), 6.59-6.58 (d, *J* = 4.0 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 133.91, 129.50, 129.22, 129.15, 127.01, 126.76, 126.63, 125.41, 124.91, 118.99, 99.11; HRMS calcd for $C_{13}H_{11}N_2OS$ $[M+H]^+$ 243.0587; found: 243.0592.



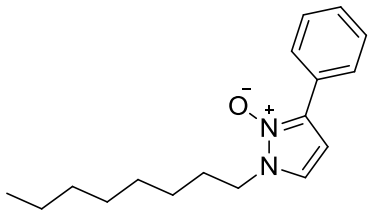
3-methyl-1-phenyl-1H-pyrazole *N*-oxide (3ac)

Yellow oil (70 mg, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.59-7.56 (m, 2 H), 7.51-7.41 (m, 3 H), 7.08-7.07 (d, *J* = 4.0 Hz, 1 H), 6.15-6.13 (d, *J* = 4.0 Hz, 1 H), 2.33(s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 134.38, 129.14, 128.94, 125.50, 118.26, 102.76, 10.79; HRMS calcd for $C_{10}H_{11}N_2O$ $[M+H]^+$ 175.0866; found: 175.0863.



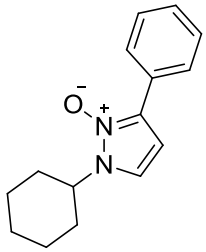
1-butyl-3-phenyl-1H-pyrazole *N*-oxide (3ad)

Yellow oil (92 mg, 85% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.19-8.17 (d, *J* = 8.0 Hz, 2 H), 7.46-7.42 (m, 2 H), 7.35-7.31 (m, 1 H), 6.97-6.96 (d, *J* = 4.0 Hz, 1 H), 6.44 (d, *J* = 3.6 Hz, 2 H), 4.21-4.17 (m, 2 H), 1.87-1.80 (m, 2 H), 1.46-1.36 (m, 2 H), 0.99-0.95 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 129.40, 128.60, 128.49, 128.28, 126.12, 117.91, 99.23, 45.24, 30.59, 19.73, 13.53; HRMS calcd for $C_{13}H_{17}N_2O$ $[M+H]^+$ 217.1336; found: 217.1340.



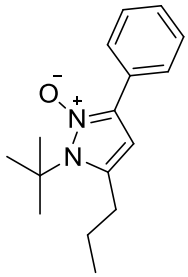
1-octyl-3-phenyl-1H-pyrazole *N*-oxide (3ae)

Yellow oil (117 mg, 86% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.19-8.17 (m, 2 H), 7.46-7.42 (m, 2 H), 7.35-7.31 (m, 1 H), 6.97-6.96 (d, *J* = 4.0 Hz, 1 H), 6.45-6.44 (m, 1 H), 4.20-4.16 (m, 2 H), 1.88-1.81 (m, 2 H), 1.37-1.27 (m, 10 H), 0.89-0.86 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 129.39, 128.61, 128.49, 128.27, 126.12, 117.87, 99.22, 45.54, 31.72, 29.08, 29.03, 28.57, 26.52, 22.58, 14.04; HRMS calcd for $C_{17}H_{25}N_2O$ $[M+H]^+$ 273.1962; found: 273.1969.



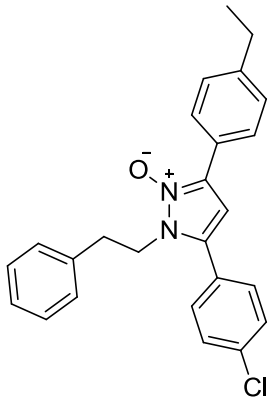
1-cyclohexyl-3-phenyl-1H-pyrazole *N*-oxide (3af)

Yellow oil (103 mg, 85% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.20-8.18 (m, 2 H), 7.45-7.42 (m, 2 H), 7.35-7.31 (m, 1 H), 6.98-6.97 (d, *J* = 4.0 Hz, 1 H), 6.45-6.44 (m, 1 H), 4.83-4.75 (m, 1 H), 2.21-2.19 (d, *J* = 8.0 Hz, 2 H), 1.92-1.89 (d, *J* = 12.0 Hz, 2 H), 1.79-1.75 (m, 1 H), 1.59-1.40 (m, 4 H), 1.28-1.21 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 129.47, 128.67, 128.47, 128.23, 126.20, 115.14, 99.34, 54.04, 32.27, 25.37, 25.30; HRMS calcd for $C_{15}H_{19}N_2O$ $[M+H]^+$ 243.1492; found: 243.1496.



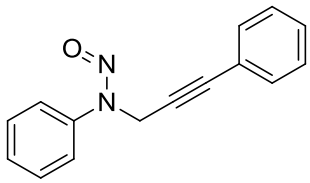
1-(tert-butyl)-3-phenyl-5-propyl-1H-pyrazole *N*-oxide (3ad) (3ag)

Yellow oil (111 mg, 86% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.14-8.12 (m, 2 H), 7.42-7.39 (m, 2 H), 7.32-7.30 (d, *J* = 8.0 Hz, 1 H), 6.16 (s, 1 H), 2.75-2.72 (m, 2 H), 1.87 (s, 9 H), 1.75-1.69 (m, 2 H), 1.06-1.02 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 133.15, 129.61, 128.86, 128.35, 128.07, 126.59, 99.69, 64.04, 32.03, 29.32, 22.79, 13.88; HRMS calcd for $C_{16}H_{23}N_2O$ $[M+H]^+$ 259.1805; found: 259.1811.



5-(4-chlorophenyl)-3-(4-ethylphenyl)-1-phenethyl-1H-pyrazole *N*-oxide (3ah)

Yellow oil (185 mg, 92% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.16-8.14 (d, *J* = 8.0 Hz, 2 H), 7.34-7.31 (m, 4 H), 7.19-7.18 (m, 3 H), 7.01-6.97 (m, 4 H), 76.36 (s, 2 H), 4.46-4.43 (m, 2 H), 3.15-3.11 (m, 2 H), 2.73-2.67 (m, 2 H), 1.28-1.25 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 144.97, 137.27, 134.88, 132.11, 130.06, 129.51, 128.99, 128.56, 128.08, 127.66, 126.72, 126.30, 125.48, 99.21, 45.79, 34.28, 28.73, 15.46; HRMS calcd for $C_{25}H_{24}ClN_2O$ $[M+H]^+$ 403.1572; found:403.1563.



***N*-phenyl-N-(3-phenylprop-2-yn-1-yl)nitrous amide (4a)** [6]

Yellow oil (95% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.70-7.68 (m, 2 H), 7.53-7.49 (m, 2 H), 7.42-7.28 (m, 3 H), 7.27-7.26 (m, 3 H), 4.95 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 141.01, 131.80, 129.48, 128.69, 128.27, 127.62, 122.04, 119.86, 83.73, 81.02, 33.49.

Reference:

[1] L.-C. Hong, Y.-L. Shao, L.-X. Zhang and X.-G. Zhou.*Chem, Eur. J.*, **2014**, *20*, 8551.

[2] L.-L.Zhang, S. Chen, Y.-Z. Gao, P.-B. Zhang, Y.-L. Wu, G. Tang, and Y.-F. Zhao, *Org. Lett.*, **2016**, *18*, 1286.

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[4] O. P. Pereshivko, V. A. Peshkov and E. V. Van der Eycken, *Org. Lett.*, **2010**, *12*, 2638.

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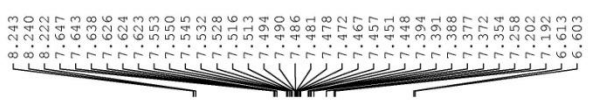
[6] P. Chaudhary, S. Gupta, N. Muniyappan, S. Sabiah, J. Kandasamy, *Green. Chem.*, **2016**, *18*, 2323.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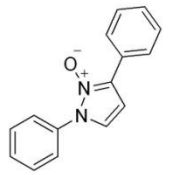
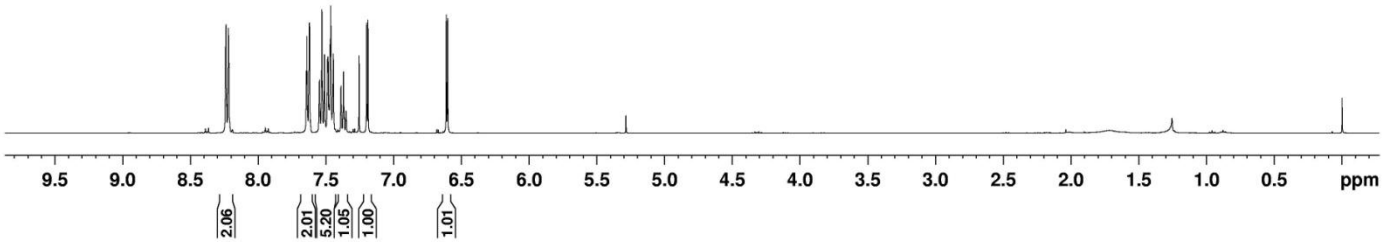


3a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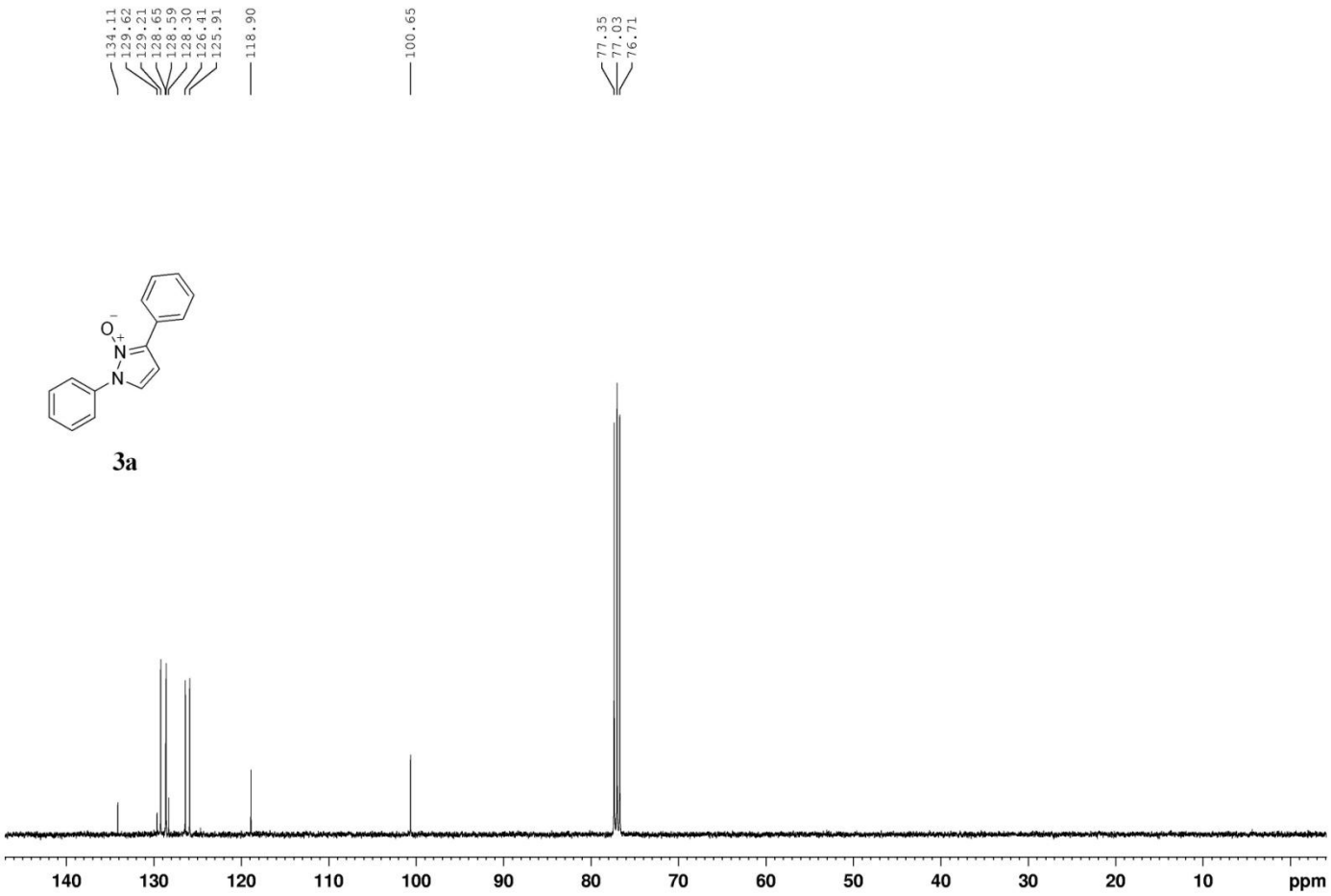
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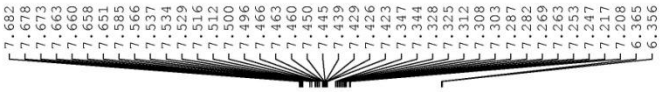
3a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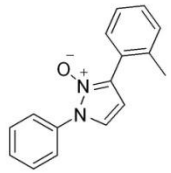
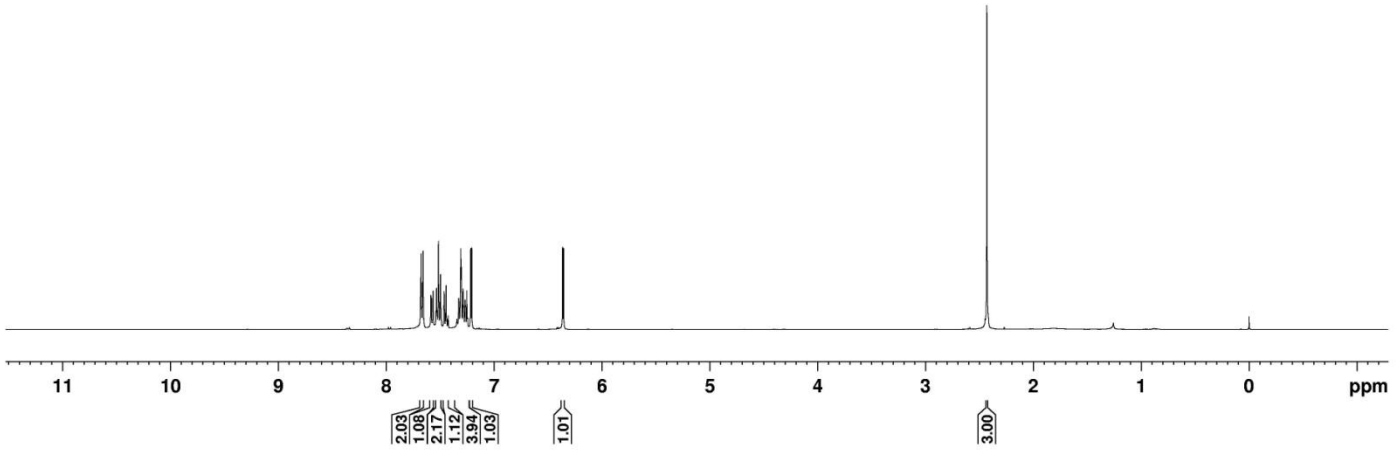


3b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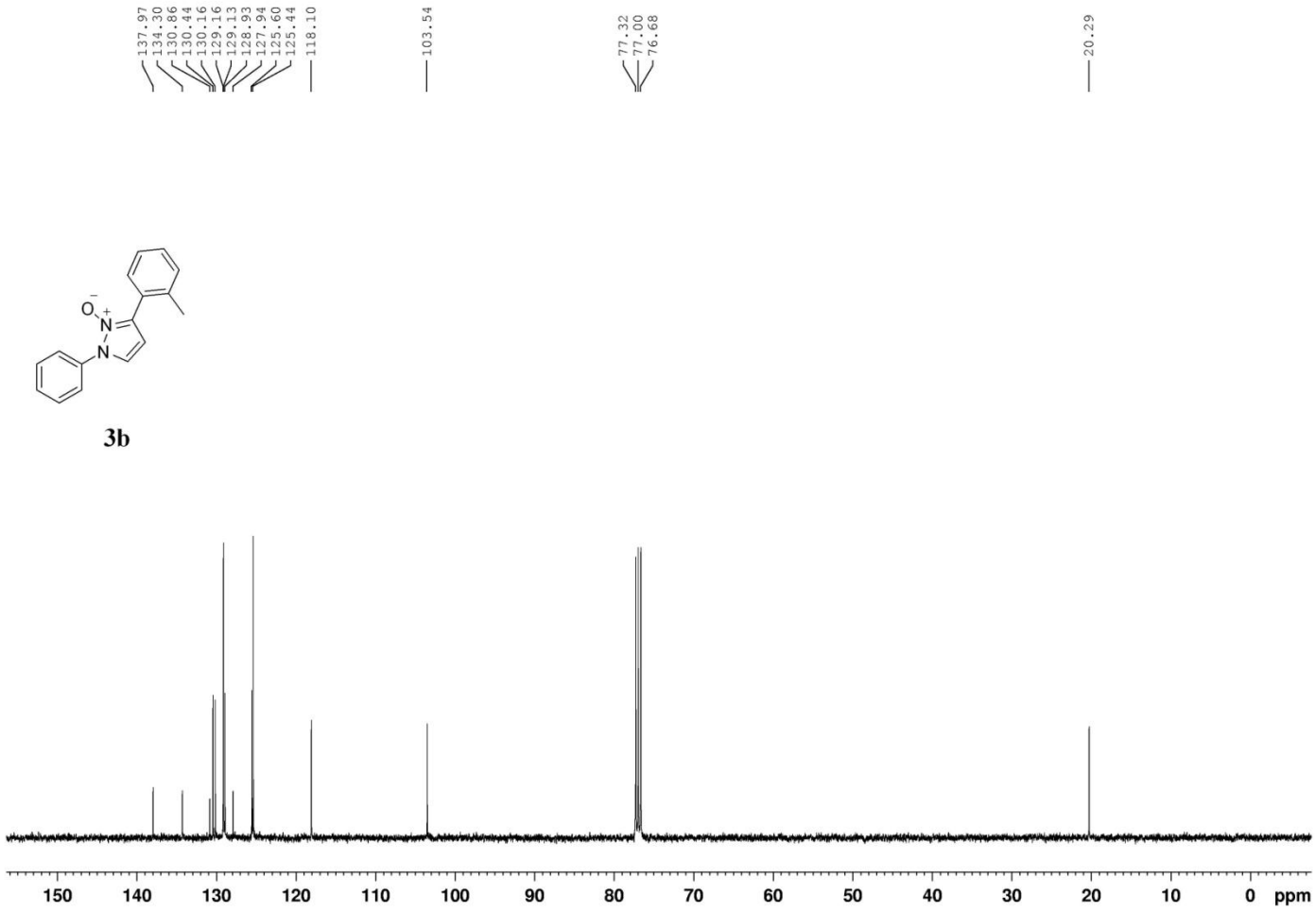
1.03
1.01
3.00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129.16
129.13
128.93
127.94
125.60
125.44
118.10
103.54
77.32
77.00
76.68
20.29
O
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120
110
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50
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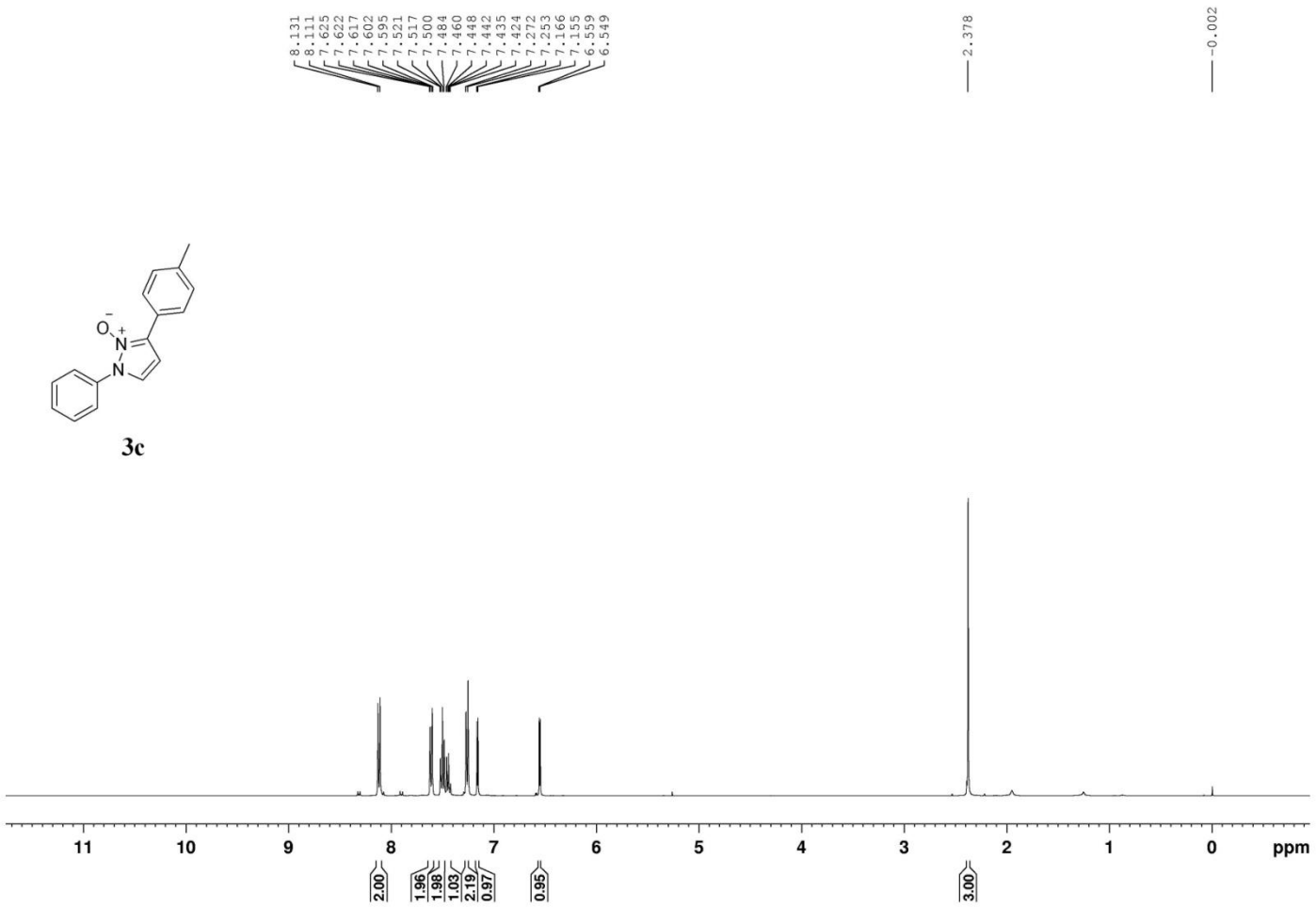
ppm

3b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8.111
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7.521
7.517
7.500
7.484
7.460
7.448
7.442
7.435
7.424
7.272
7.253
7.166
7.155
6.559
6.549
2.378
-0.002
3c
11
10
9
8
7
6
5
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3
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ppm
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1.03
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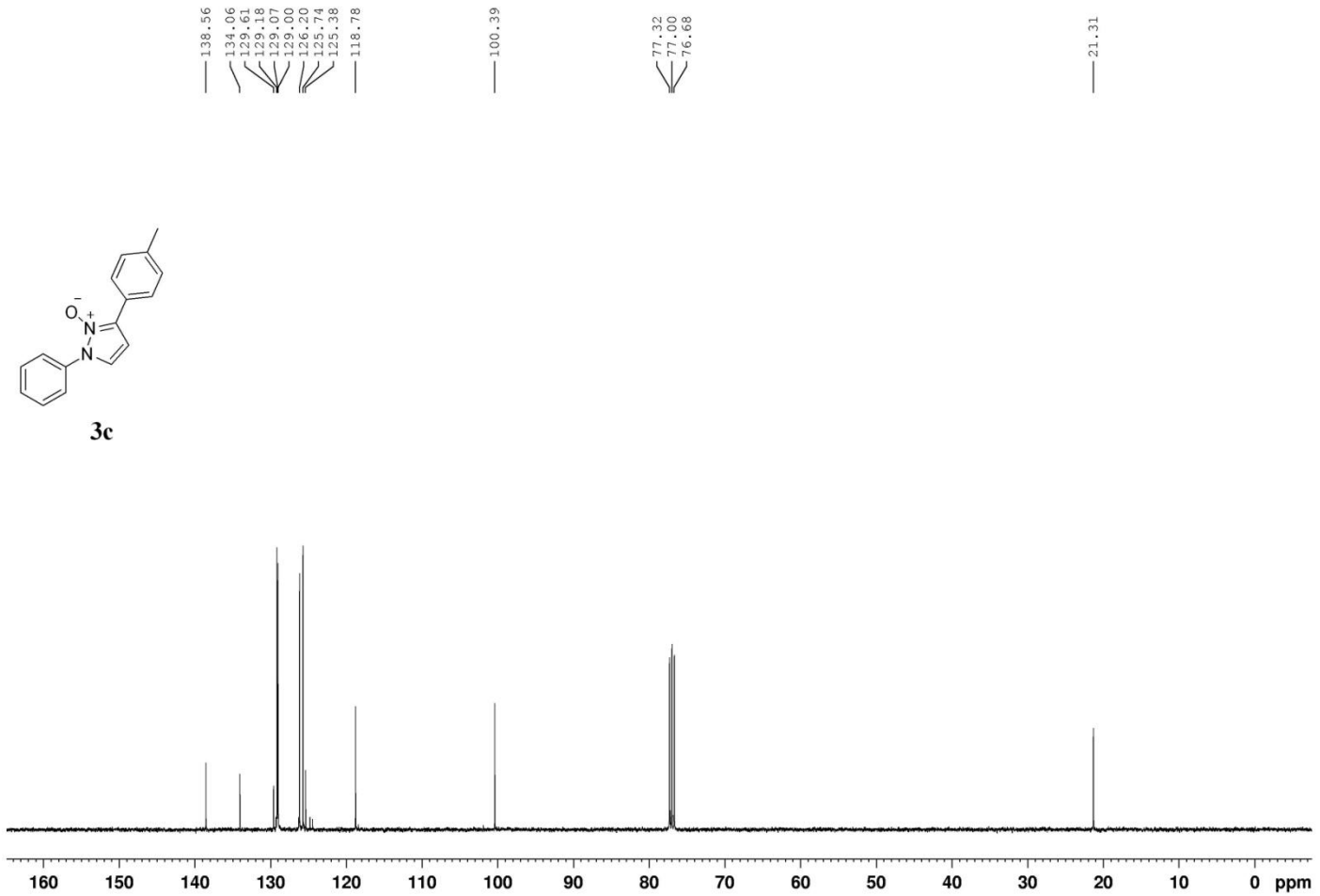
0.97
0.95
3.00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129.00
126.20
125.74
125.38
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100.39
77.32
77.00
76.68
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130
120
110
100
90
80
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60
50
40
30
20
10
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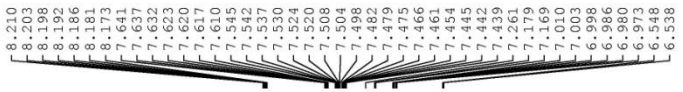
3c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8.203
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8.181
8.173
7.641
7.637
7.632
7.623
7.620
7.617
7.610
7.545
7.542
7.537
7.530
7.524
7.520
7.508
7.504
7.498
7.482
7.479
7.475
7.466
7.461
7.454
7.445
7.442
7.439
7.261
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7.003
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6.986
6.980
6.973
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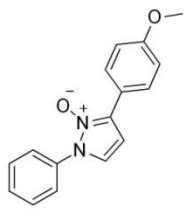
6.538
3.851
0.000



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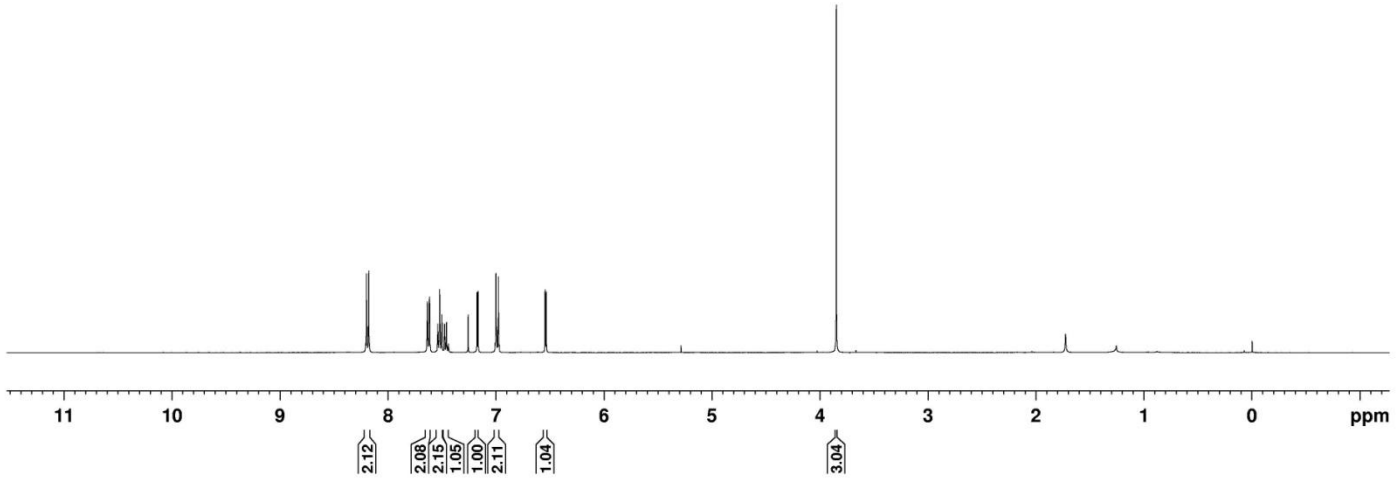
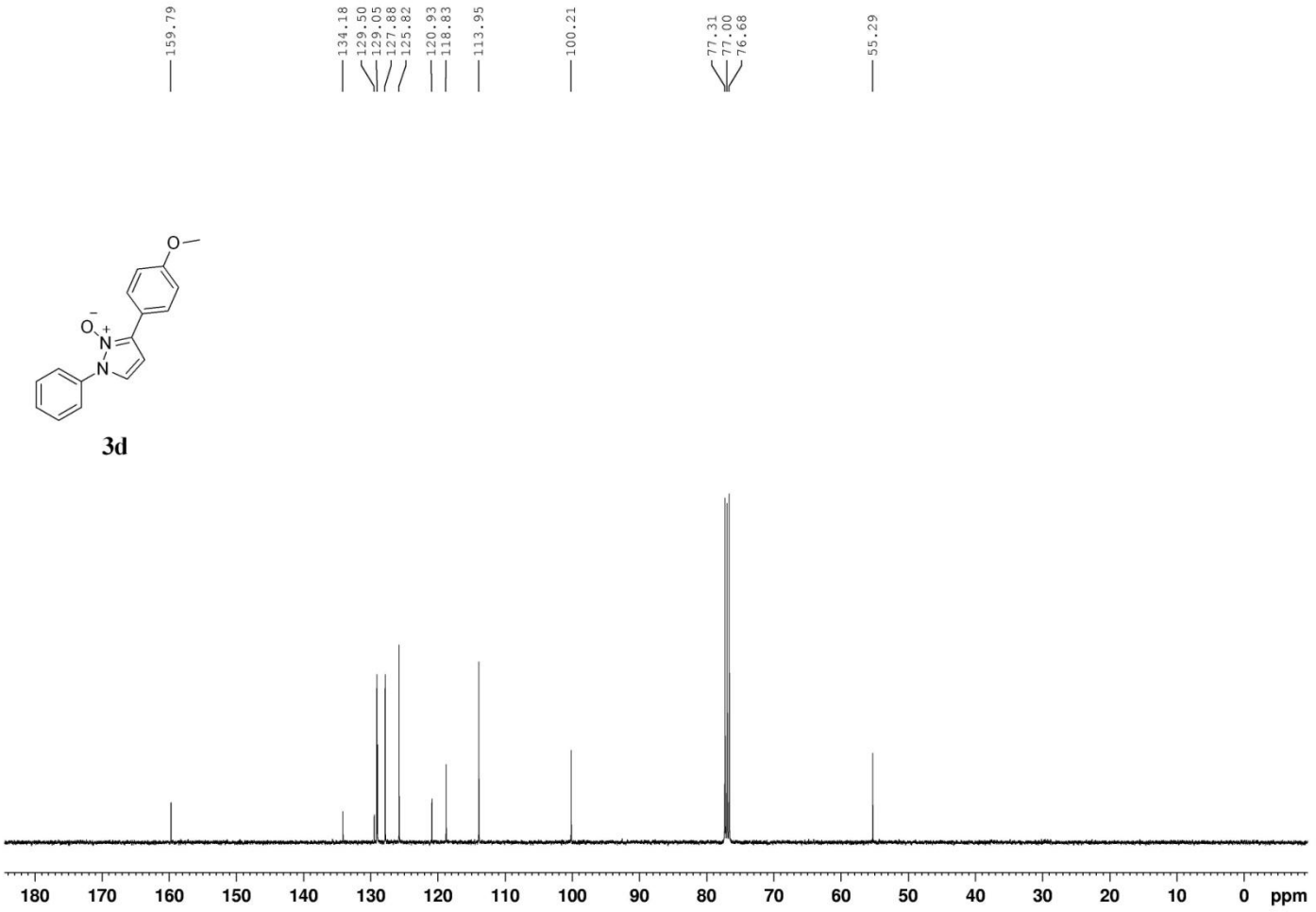

11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.12
2.08
2.15
1.05
1.00
2.11
1.04
3.04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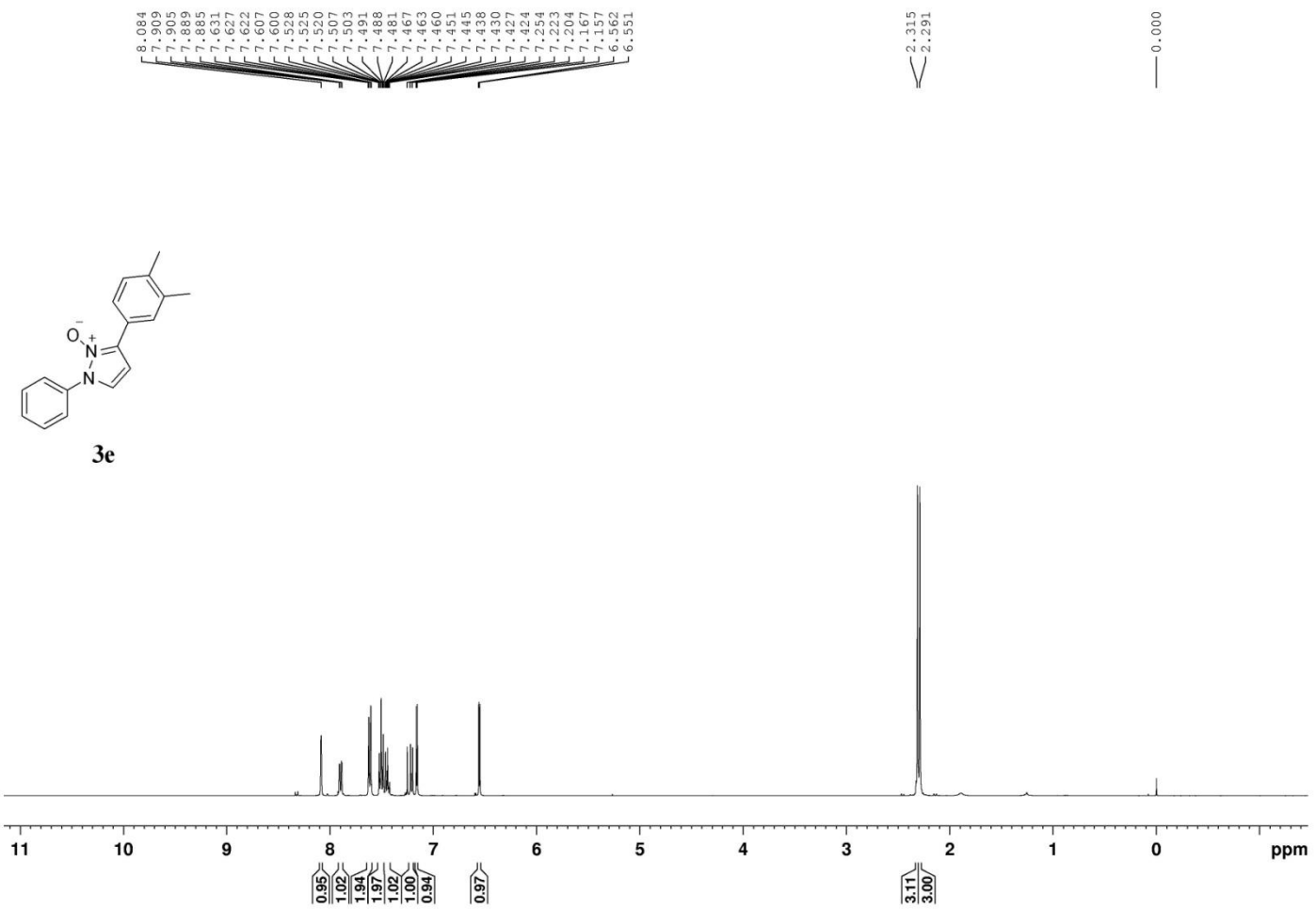
134.18
129.50
129.05
127.88
125.82
120.93
118.83
113.95
100.21
77.31
77.00
76.68
55.29
O
O
N
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3d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7.905
7.889
7.885
7.631
7.627
7.622
7.607
7.600
7.528
7.525
7.520
7.507
7.503
7.491
7.488
7.481
7.467
7.463
7.460
7.451
7.445
7.438
7.430
7.427
7.424
7.254
7.223
7.204
7.167
7.157
6.562
6.551
2.315
2.291
0.000
3e
11
10
9
8
7
6
5
4
3
2
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0
ppm
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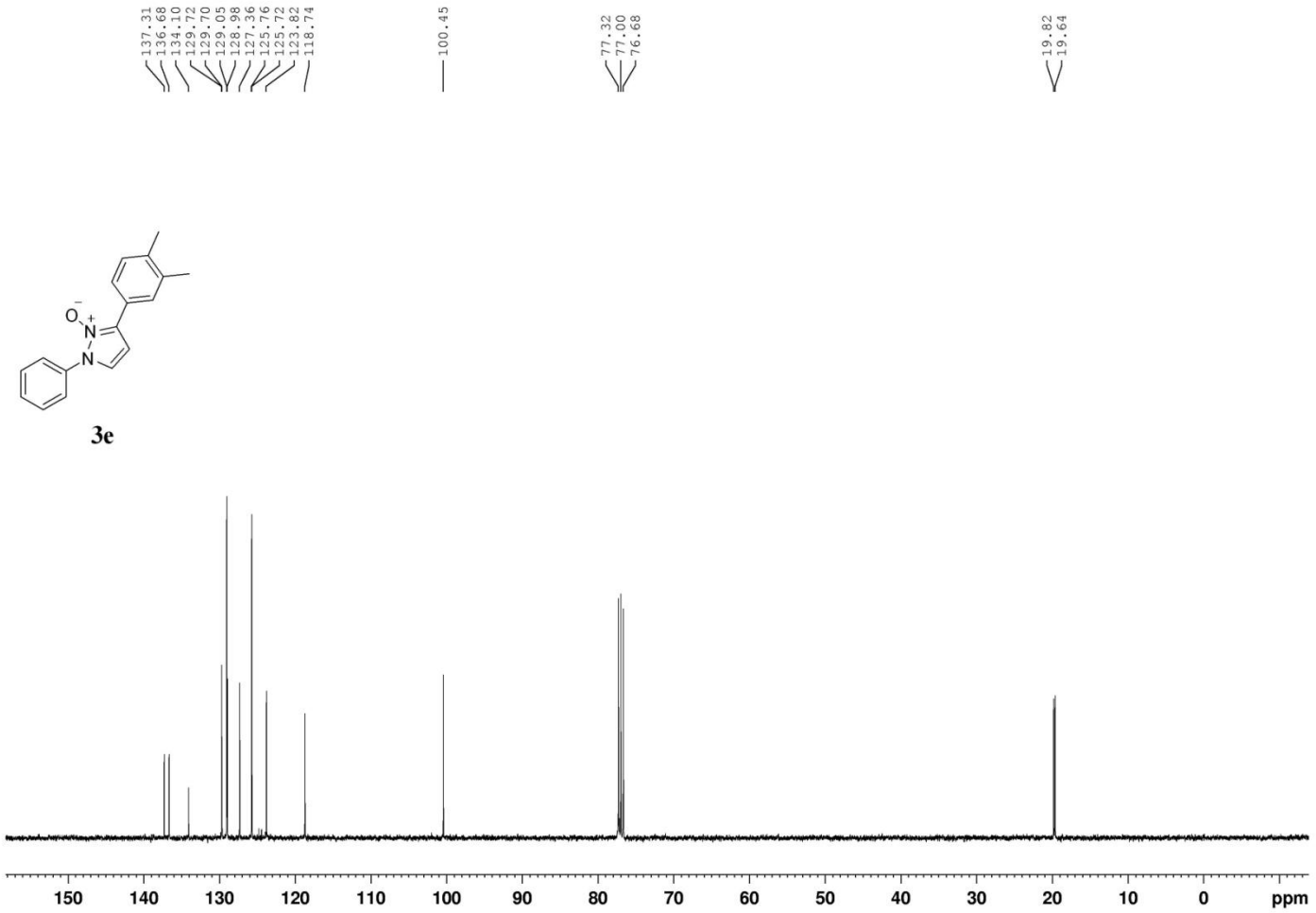
1.02
1.94
1.97
1.02
1.00
0.94
0.97
3.11
3.00


137.31
136.68
134.10
129.72
129.70
129.05
128.98
127.36
125.76
125.72
123.82
118.74
100.45
77.32
77.00
76.68
19.82
19.64
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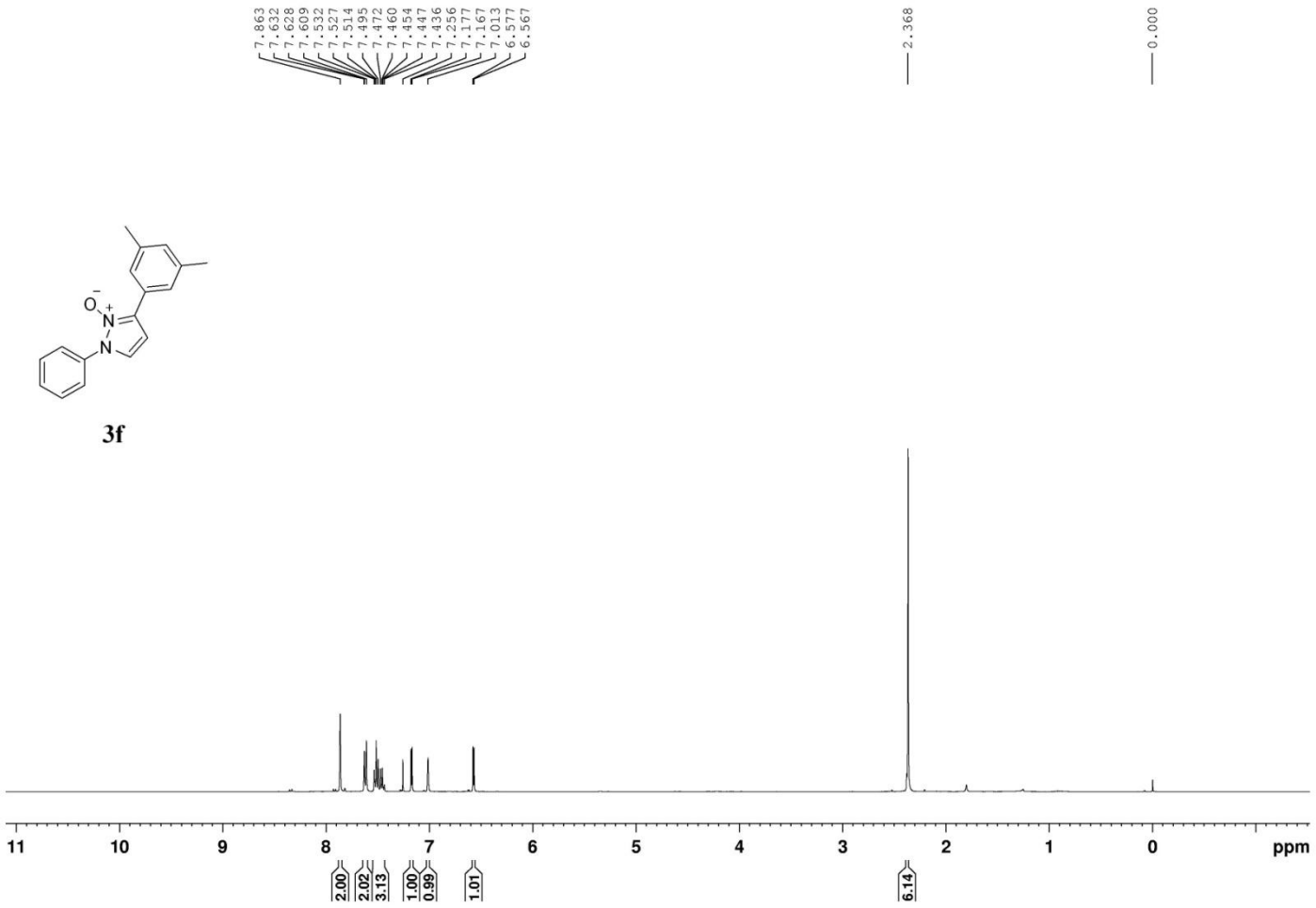
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3e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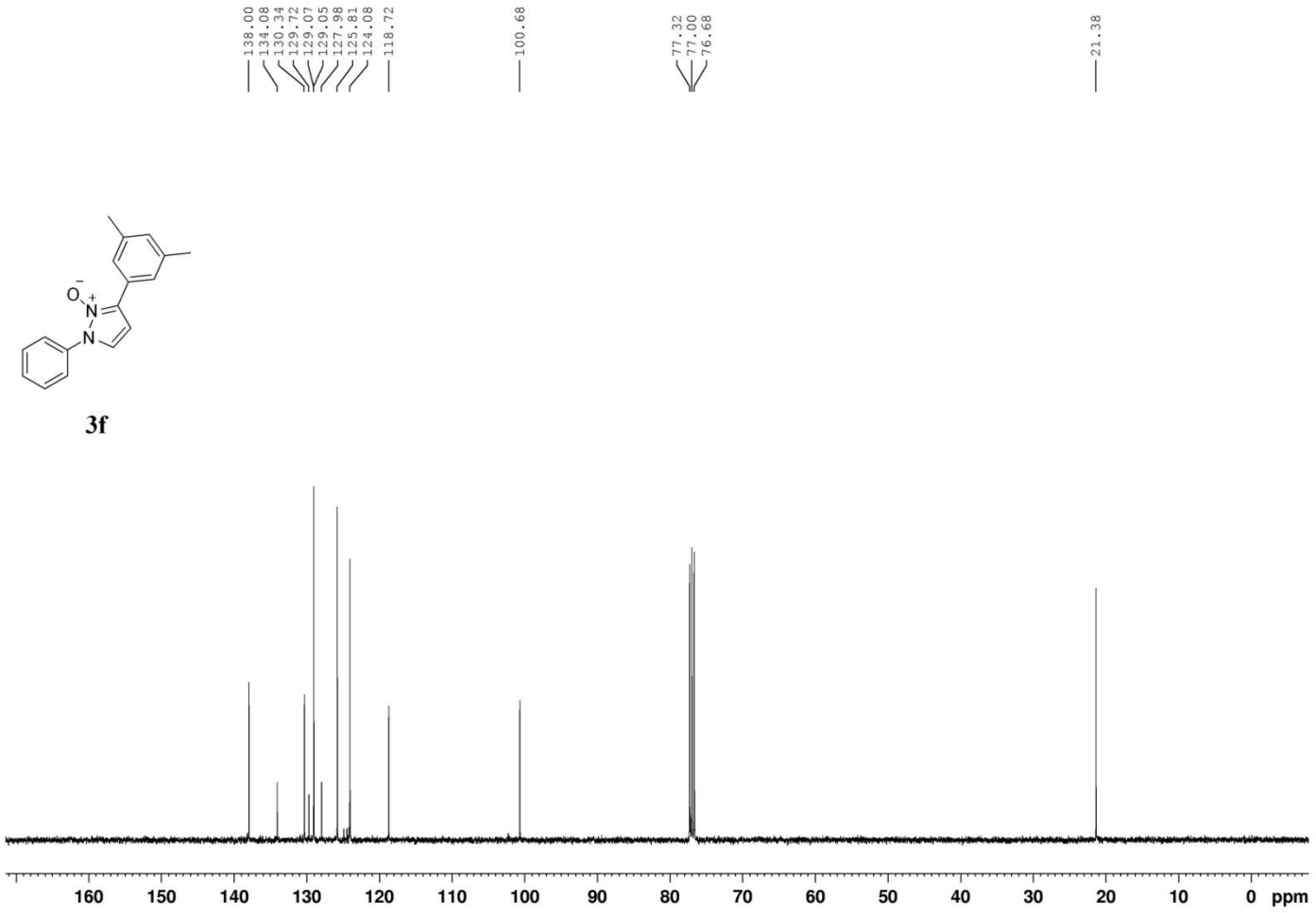
7.632
7.628
7.609
7.532
7.527
7.514
7.495
7.472
7.460
7.454
7.447
7.436
7.256
7.177
7.167
7.013
6.577
6.567
2.368
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.02
3.13
1.00
0.99
1.01
6.14

3f


138.00
134.08
130.34
129.72
129.07
129.05
127.98
125.81
124.08
118.72
100.68
77.32
77.00
76.68
21.38
O
N
N
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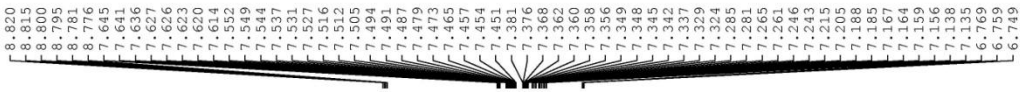
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3f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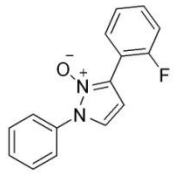
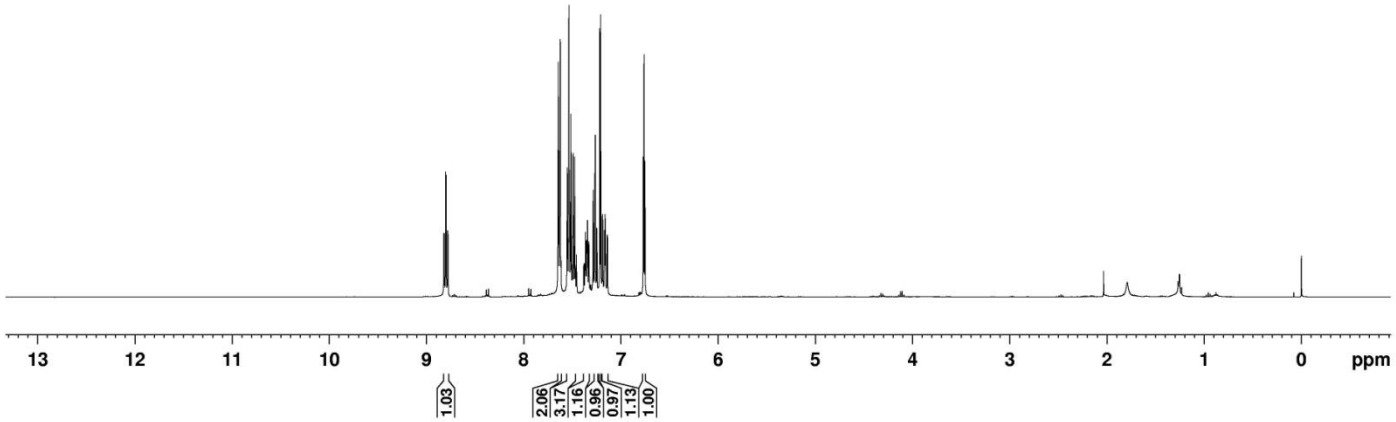
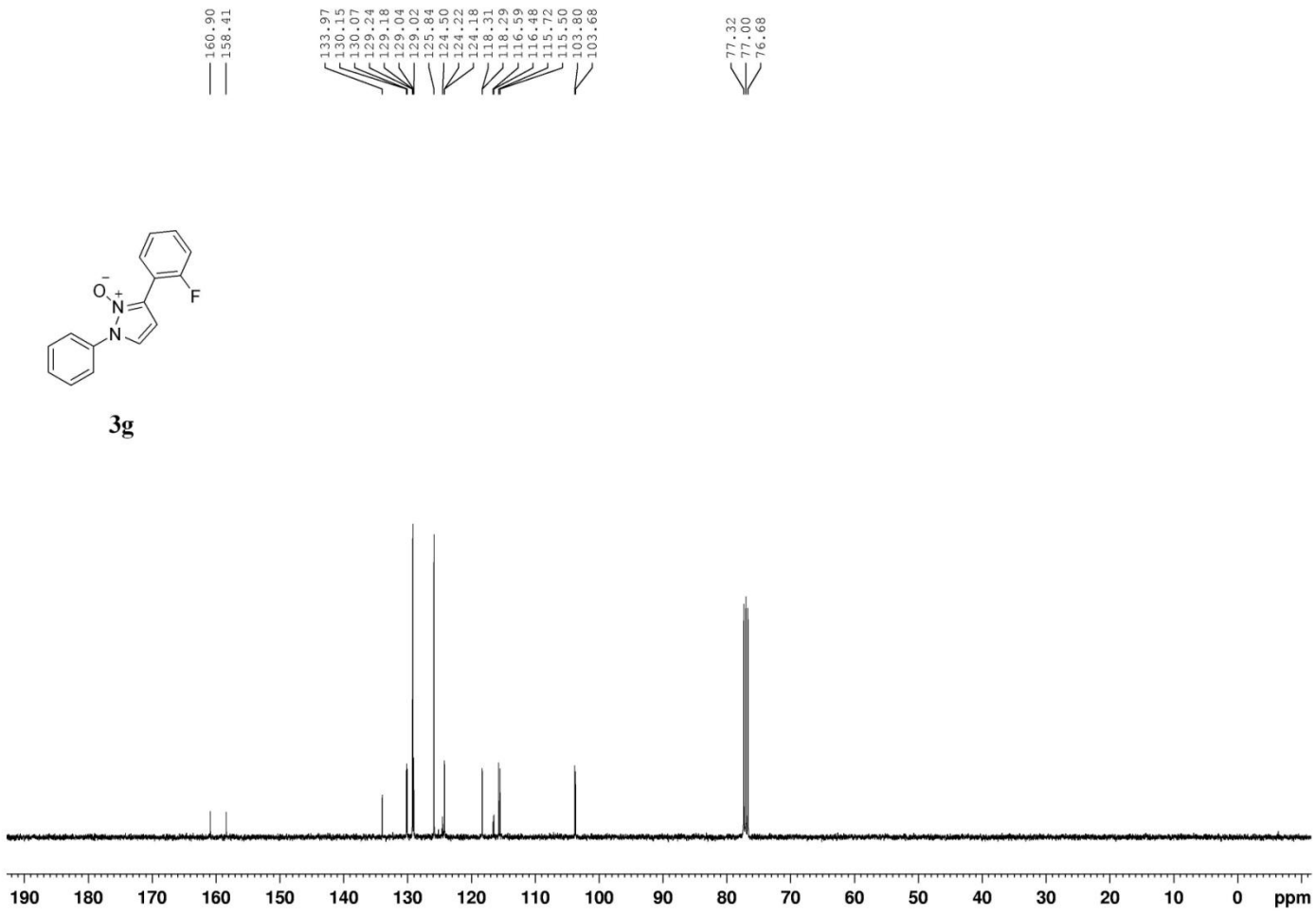
8.815
8.800
8.795
8.781
8.776
7.645
7.641
7.636
7.627
7.626
7.623
7.620
7.614
7.552
7.549
7.544
7.537
7.531
7.527
7.516
7.512
7.505
7.494
7.491
7.487
7.479
7.473
7.465
7.457
7.454
7.451
7.381
7.376
7.368
7.362
7.360
7.358
7.356
7.349
7.348
7.345
7.342
7.337
7.329
7.324
7.285
7.281
7.265
7.261
7.246
7.243
7.215
7.205
7.188
7.185
7.167
7.164
7.159
7.156
7.138
7.135
6.769
6.759
6.749
0.000


O
N
N
F

3g


13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.03
2.06
3.17
1.16
0.96
0.97
1.13
1.00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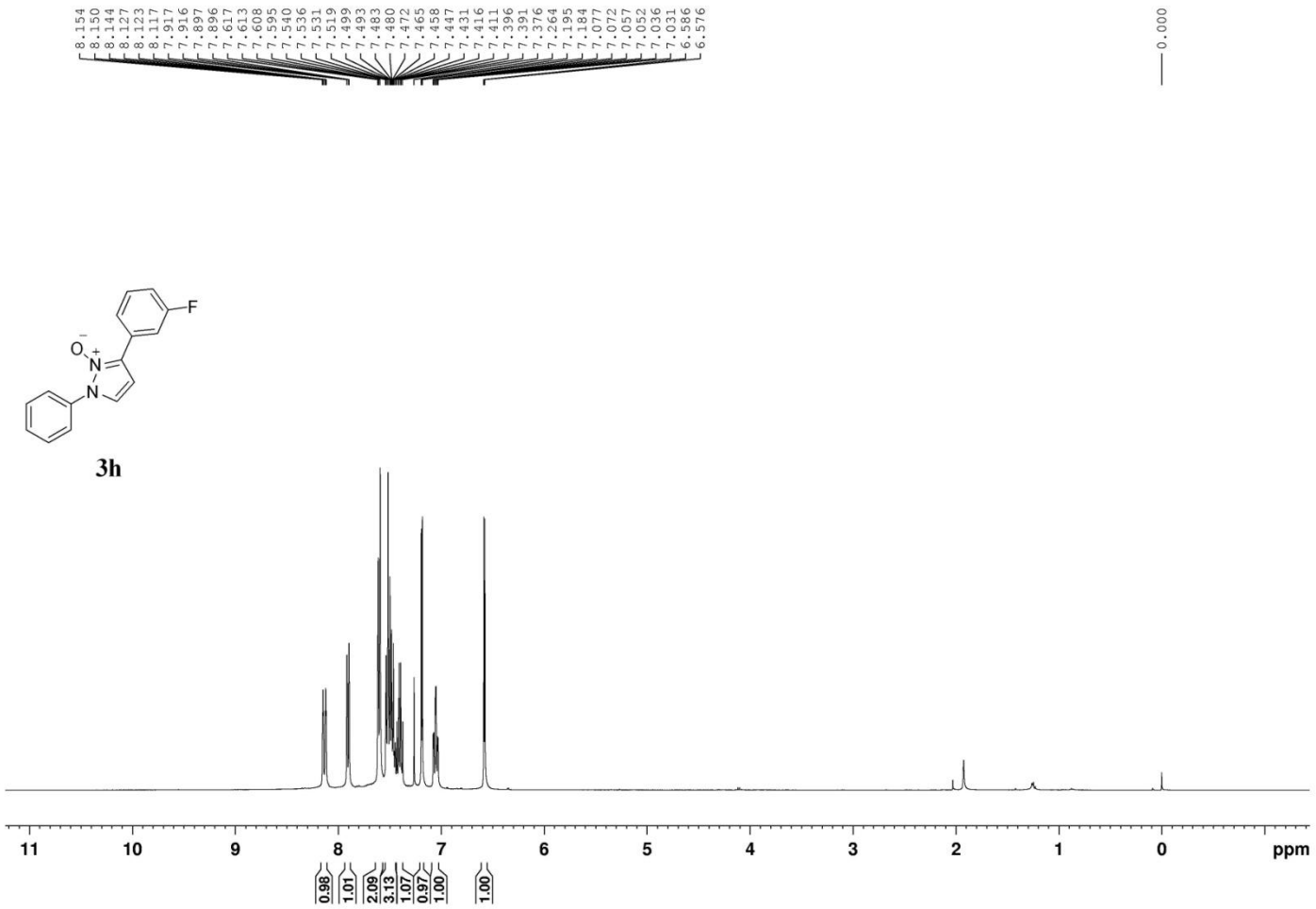
130.07
129.24
129.18
129.04
129.02
125.84
124.50
124.22
124.18
118.31
118.29
116.59
116.48
115.72
115.50
103.80
103.68
77.32
77.00
76.68
O
N
N
F
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3g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8.150
8.144
8.127
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7.896
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7.613
7.608
7.595
7.540
7.536
7.531
7.519
7.499
7.493
7.483
7.480
7.472
7.465
7.458
7.447
7.431
7.416
7.411
7.396
7.391
7.376
7.264
7.195
7.184
7.077
7.072
7.057
7.052
7.036
7.031
6.586
6.576
0.000
F
O
N
N
3h
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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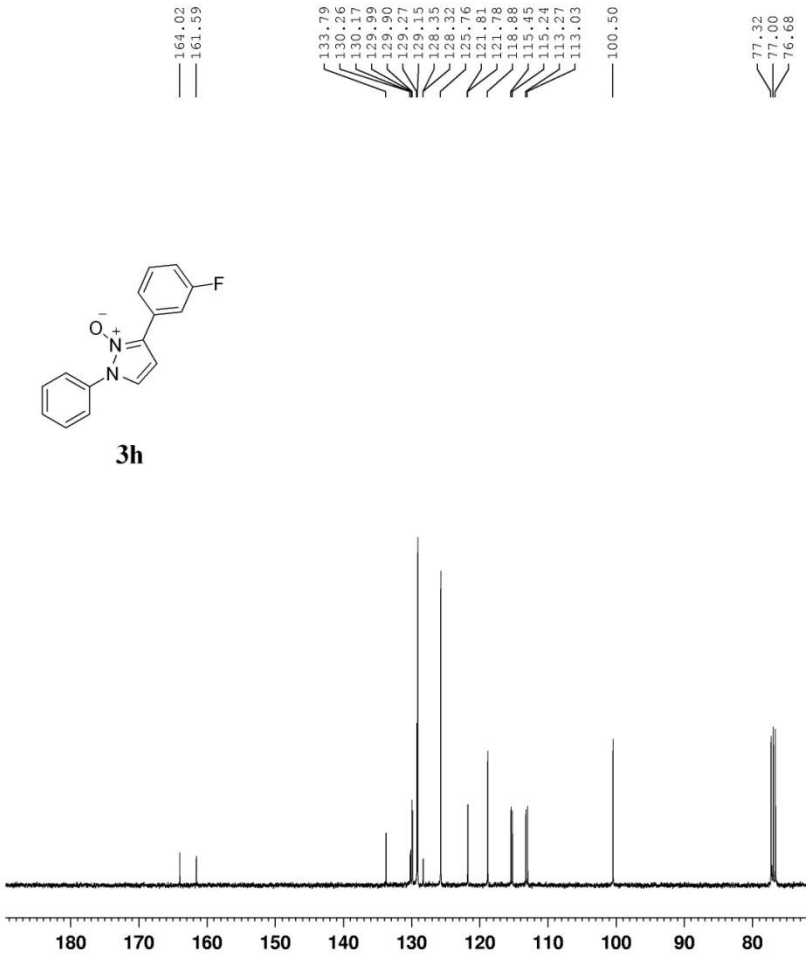
1.01
2.09
3.13
1.07
0.97
1.00
1.00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130.17
129.99
129.90
129.27
129.15
128.35
128.32
125.76
121.81
121.78
118.88
115.45
115.24
113.27
113.03
100.50
77.32
77.00
76.68
F
O
N
N
180
170
160
150
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130
120
110
100
90
80
70
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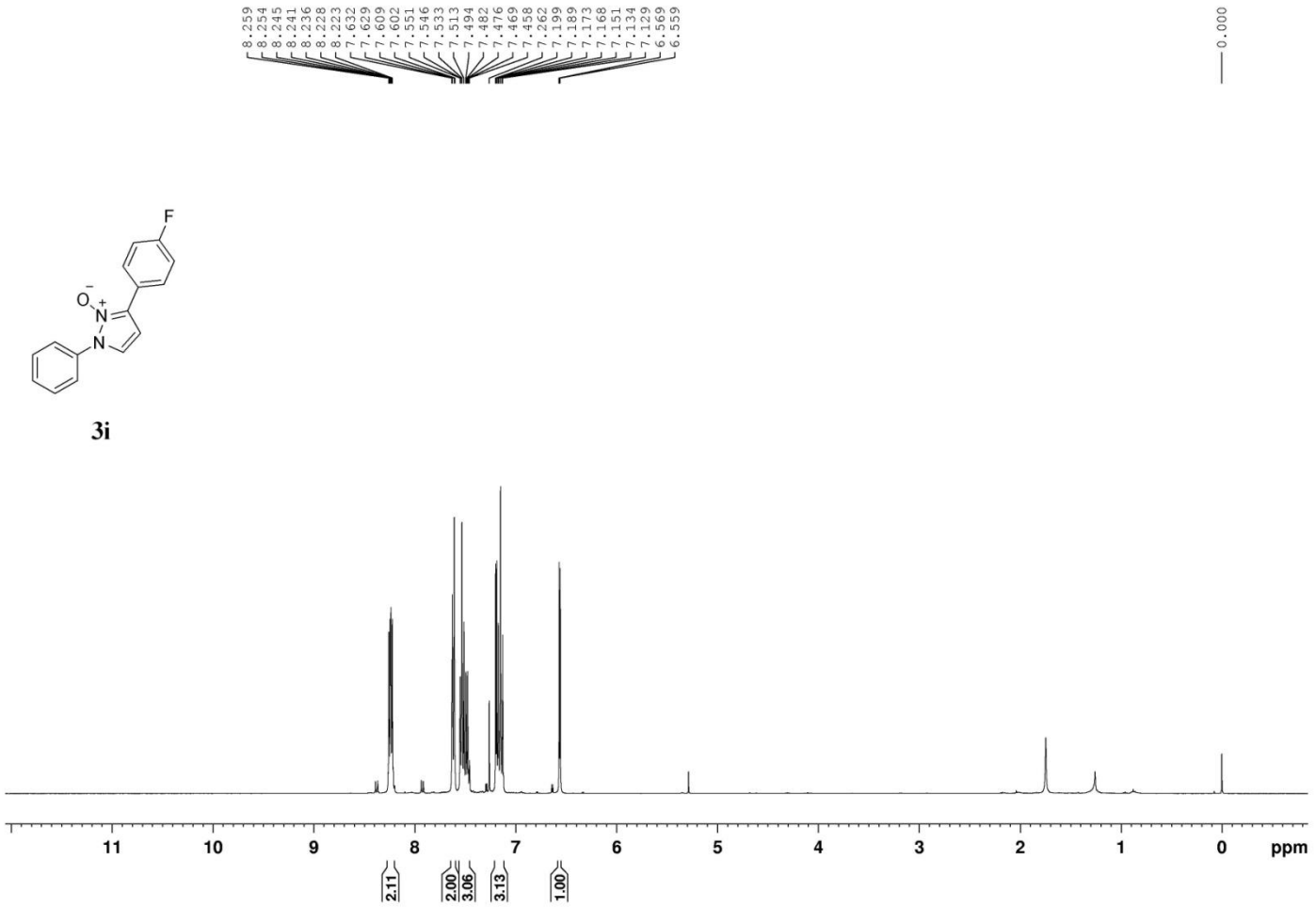
50
40
30
20
10
0
ppm

3h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8.245
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8.228
8.223
7.632
7.629
7.609
7.602
7.551
7.546
7.533
7.513
7.494
7.482
7.476
7.469
7.458
7.262
7.199
7.189
7.173
7.168
7.151
7.134
7.129
6.569
6.559
0.000
F
O
N
N
3i
11
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4
3
2
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0
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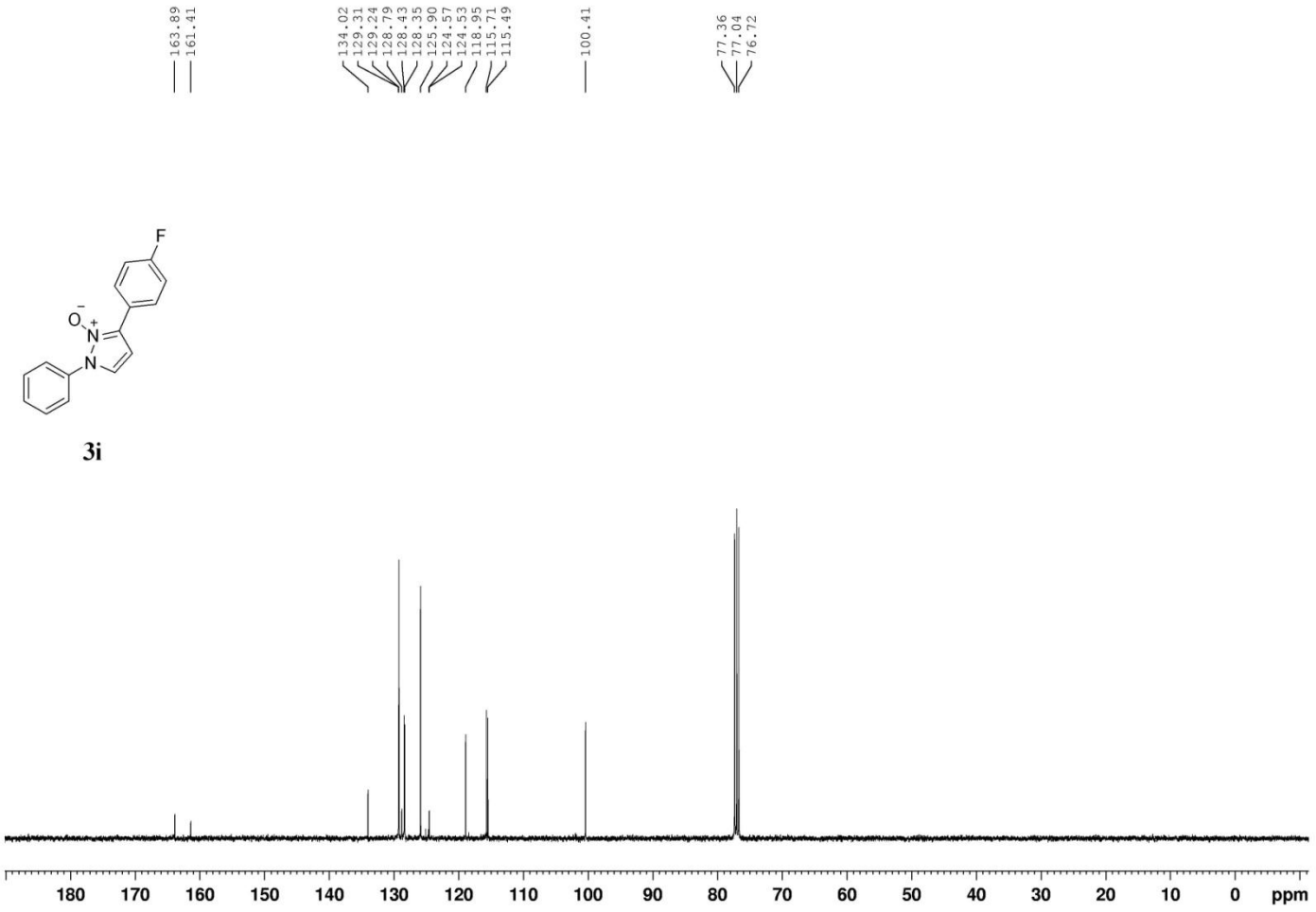
3.06
3.13
1.00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128.43
128.35
125.90
124.57
124.53
118.95
115.71
115.49
100.41
77.36
77.04
76.72
F
O
N
N
180
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150
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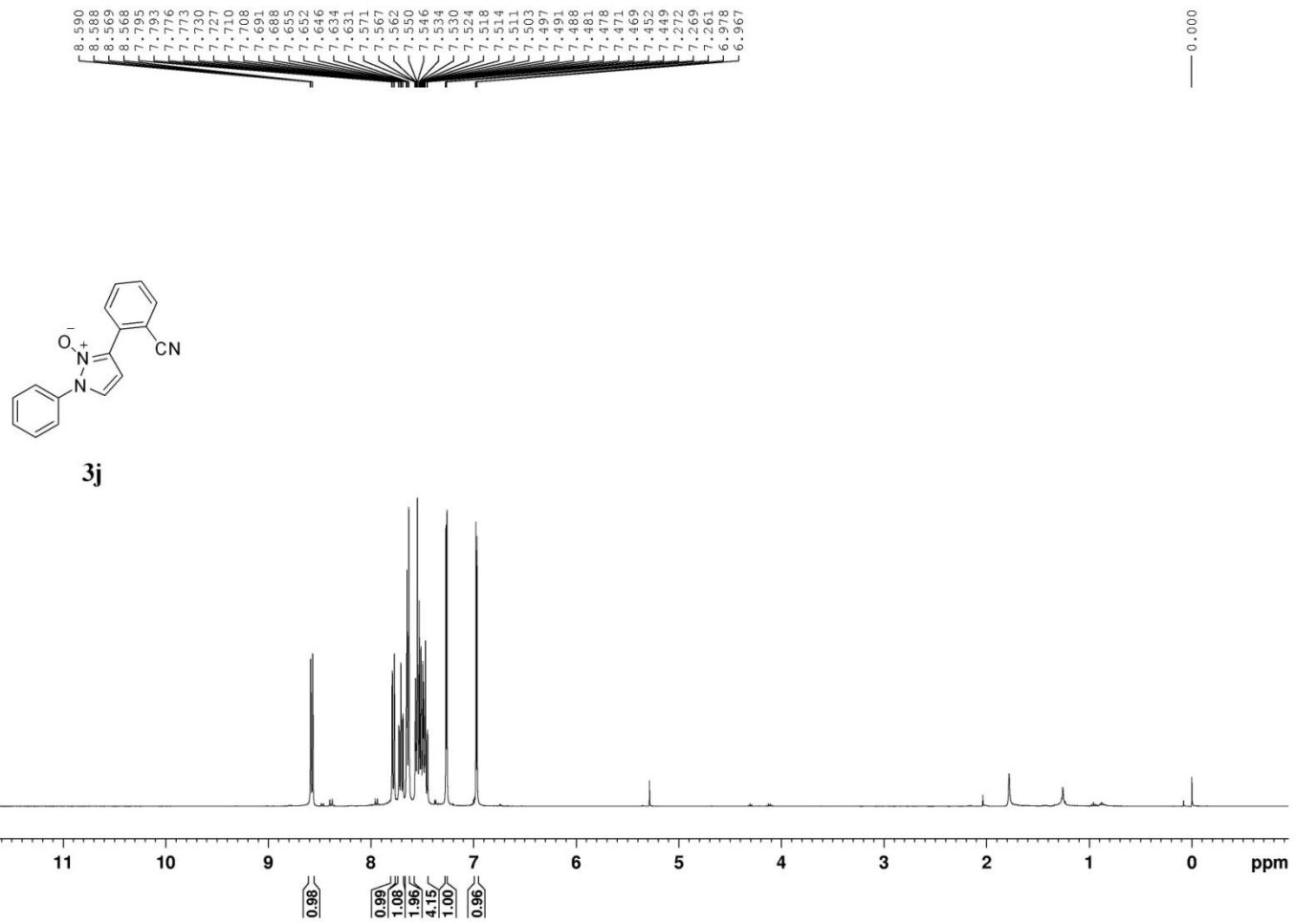
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3i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8.588
8.569
8.568
7.795
7.793
7.776
7.773
7.730
7.727
7.710
7.708
7.691
7.688
7.655
7.652
7.646
7.634
7.631
7.571
7.567
7.562
7.550
7.546
7.534
7.530
7.524
7.518
7.514
7.511
7.503
7.497
7.491
7.488
7.481
7.478
7.471
7.469
7.452
7.449
7.272
7.269
7.261
6.978
6.967
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O
N
N
CN
11
10
9
8
7
6
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1
0
ppm
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1.96
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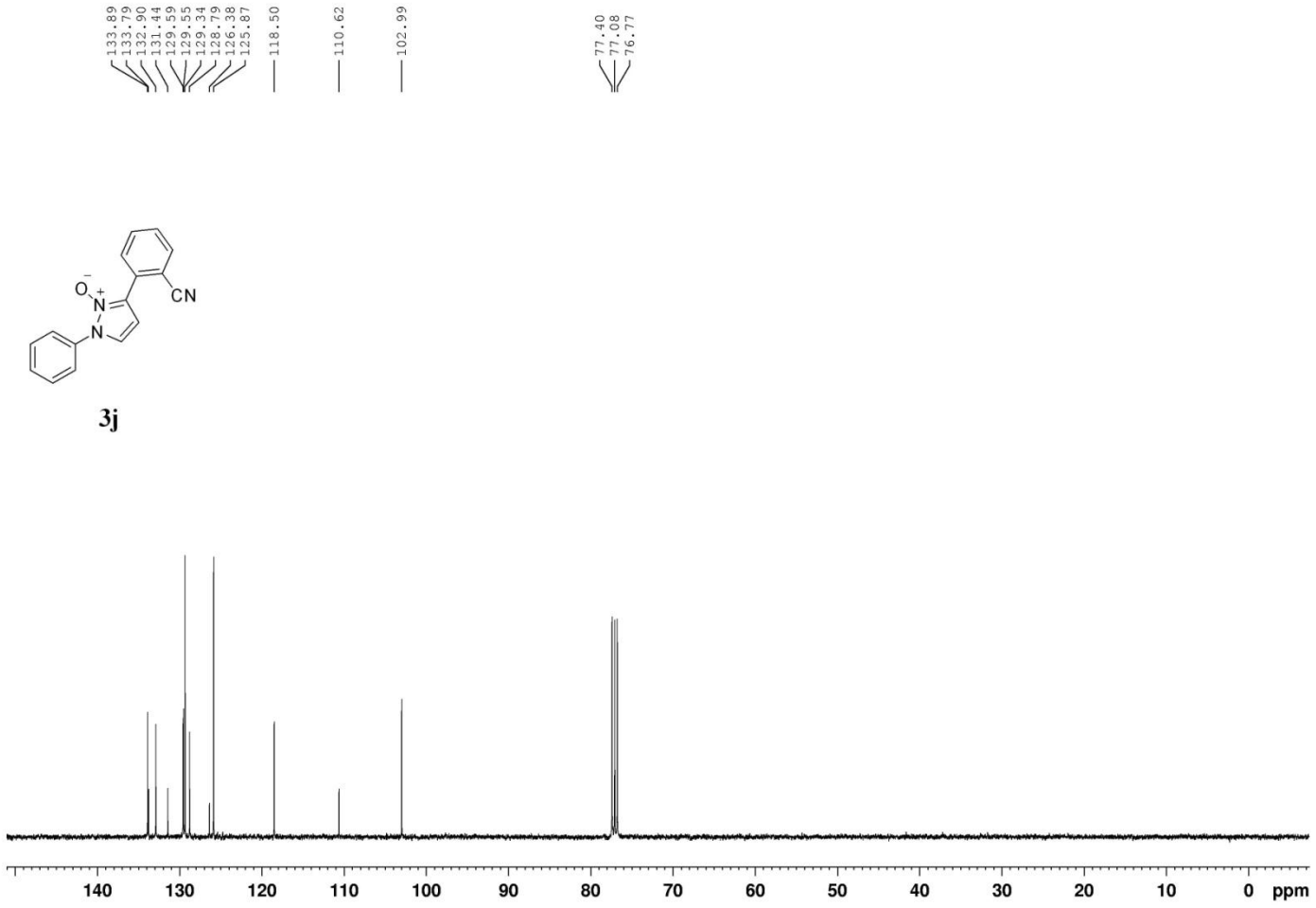
1.00
0.96

3j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129.55
129.34
128.79
126.38
125.87
118.50
110.62
102.99
77.40
77.08
76.77
O
N
N
CN
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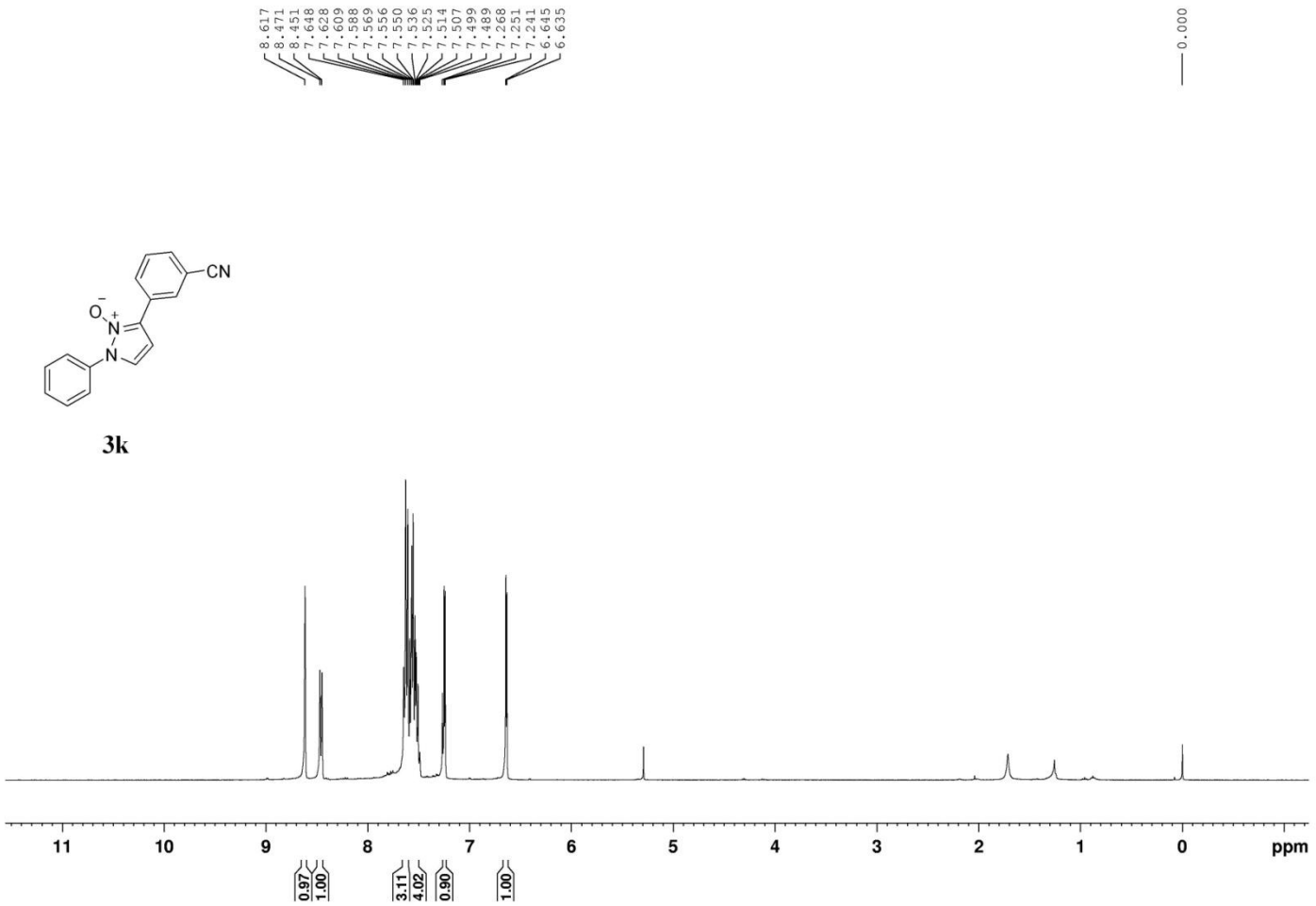
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3j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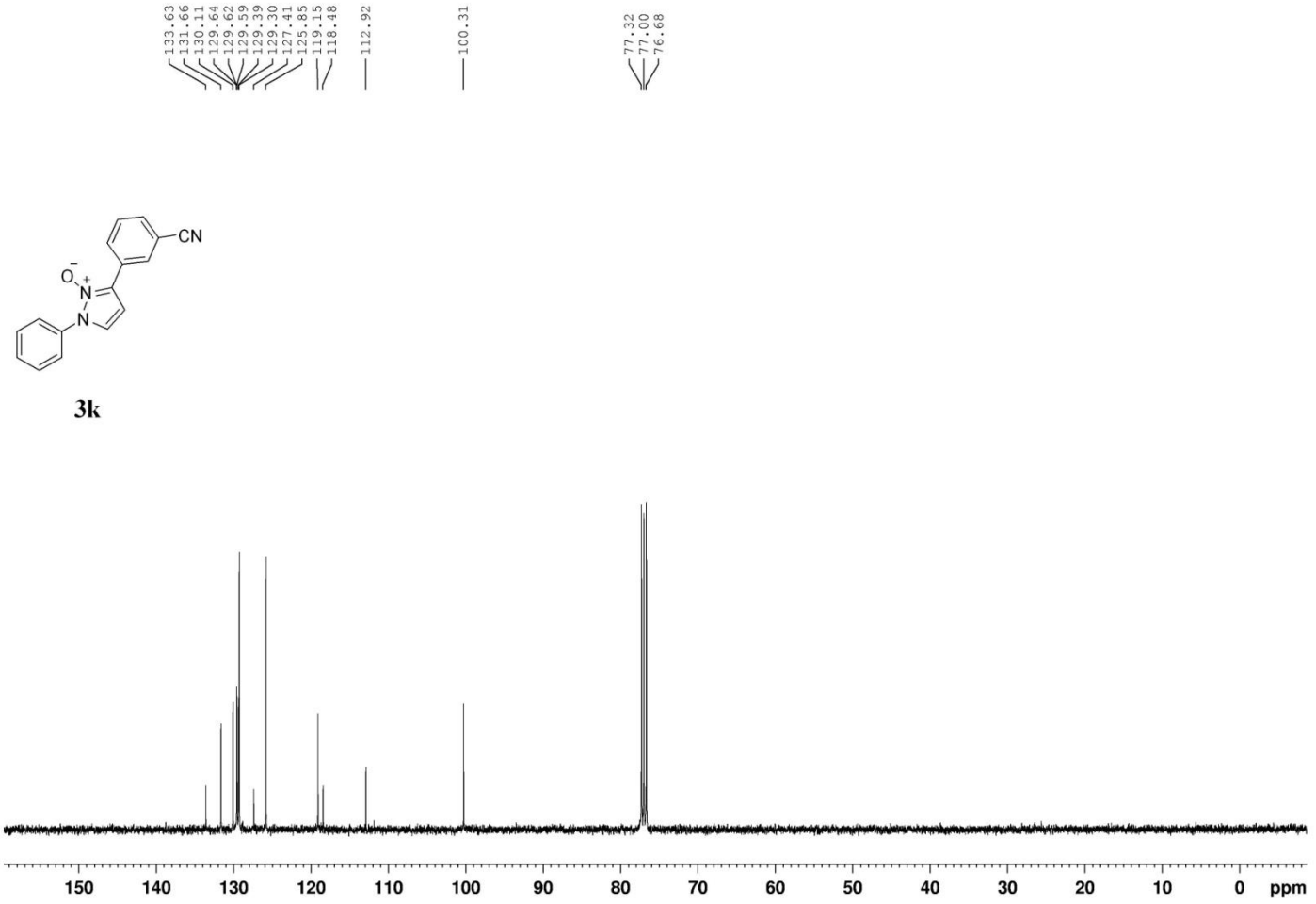
7.609
7.588
7.569
7.556
7.550
7.536
7.525
7.514
7.507
7.499
7.489
7.268
7.251
7.241
6.645
6.635
0.000
CN
O
N
N
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.97
1.00
3.11
4.02
0.90
1.00

3k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131.66
130.11
129.64
129.62
129.59
129.39
129.30
127.41
125.85
119.15
118.48
112.92
100.31
77.32
77.00
76.68
CN
O
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N
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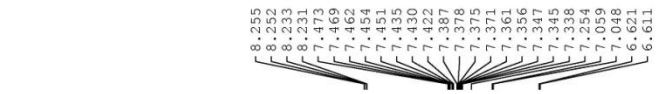
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3k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8.233
8.231
7.473
7.469
7.462
7.454
7.451
7.435
7.430
7.422
7.387
7.378
7.375
7.371
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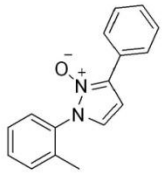
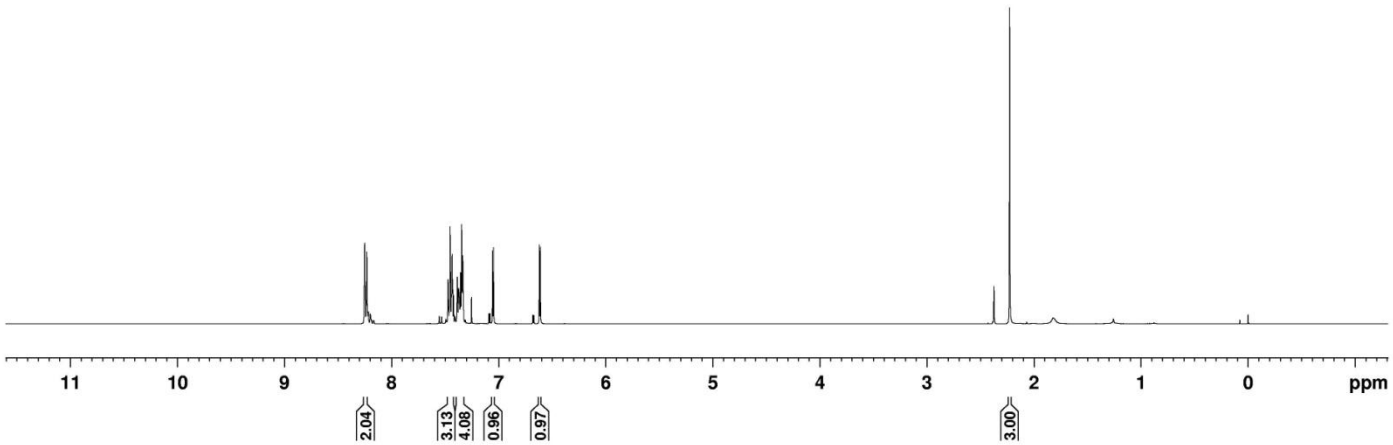
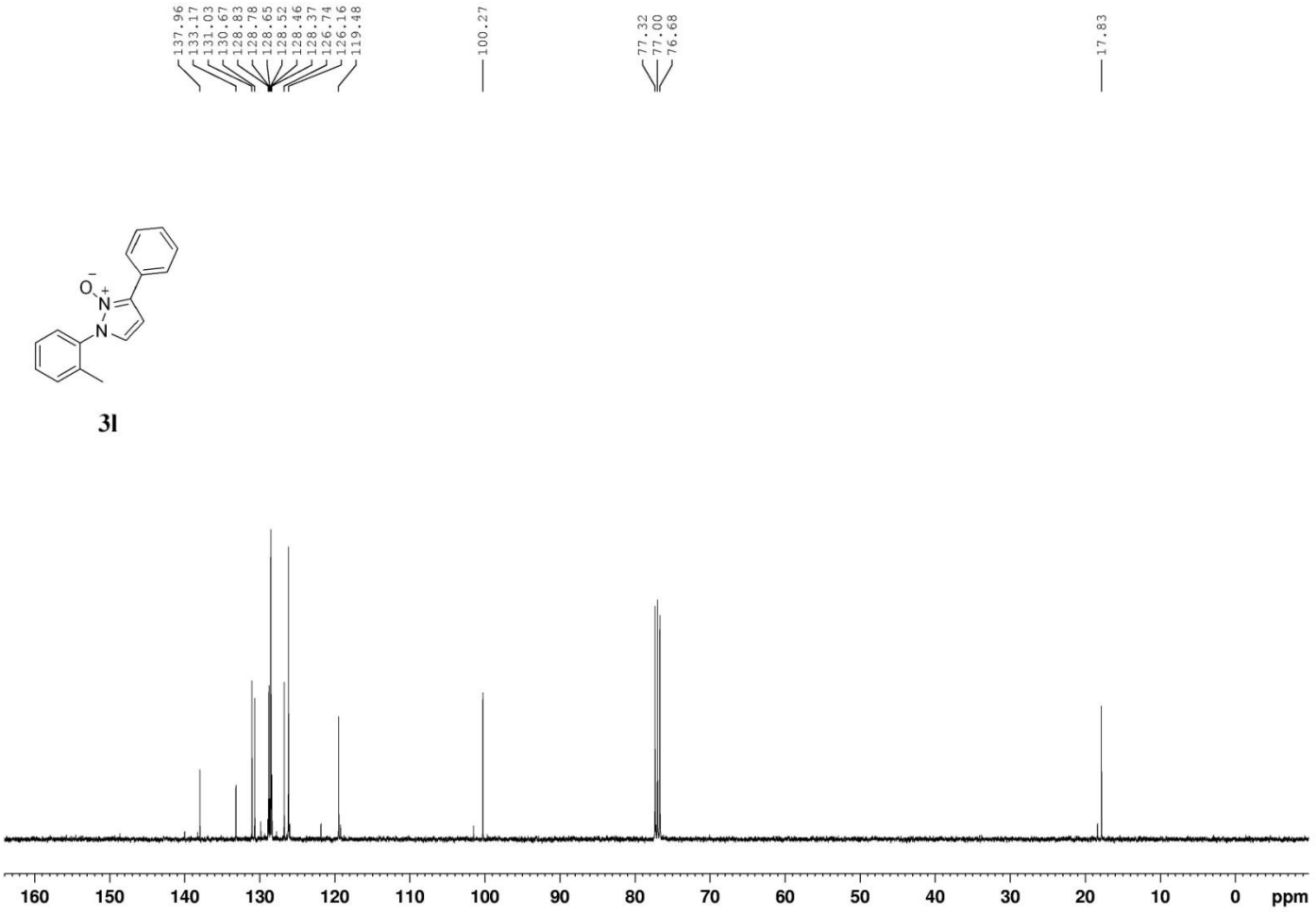
7.048
6.621
6.611
2.229
0.000



3l


11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.04
3.13
4.08
0.96
0.97
3.00


137.96
133.17
131.03
130.67
128.83
128.78
128.65
128.52
128.46
128.37
126.74
126.16
119.48
100.27
77.32
77.00
76.68
17.83
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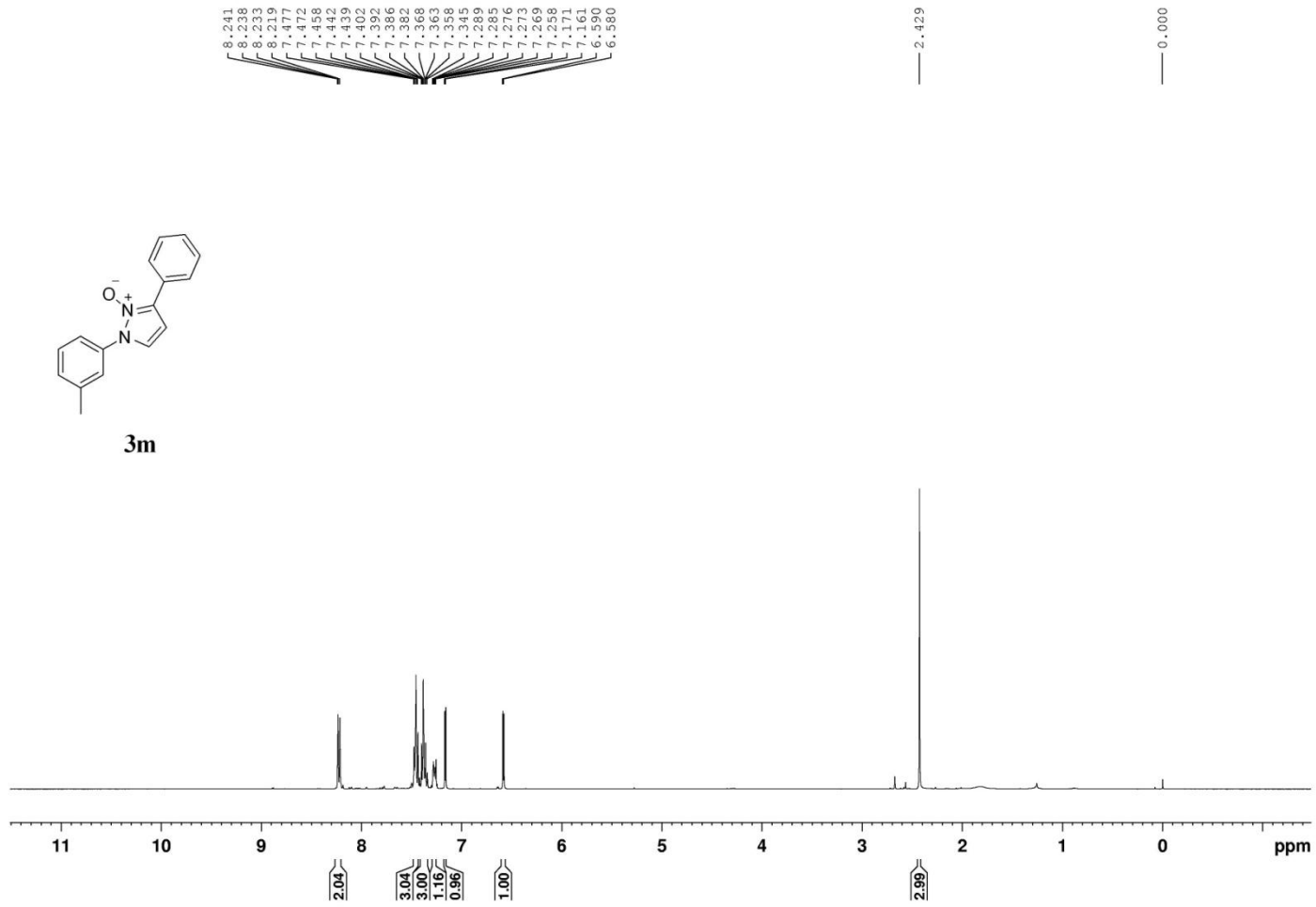
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3l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8.238
8.233
8.219
7.477
7.472
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7.439
7.402
7.392
7.386
7.382
7.368
7.363
7.358
7.345
7.289
7.285
7.276
7.273
7.269
7.258
7.171
7.161
6.590
6.580
2.429
0.000
3m
11
10
9
8
7
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2
1
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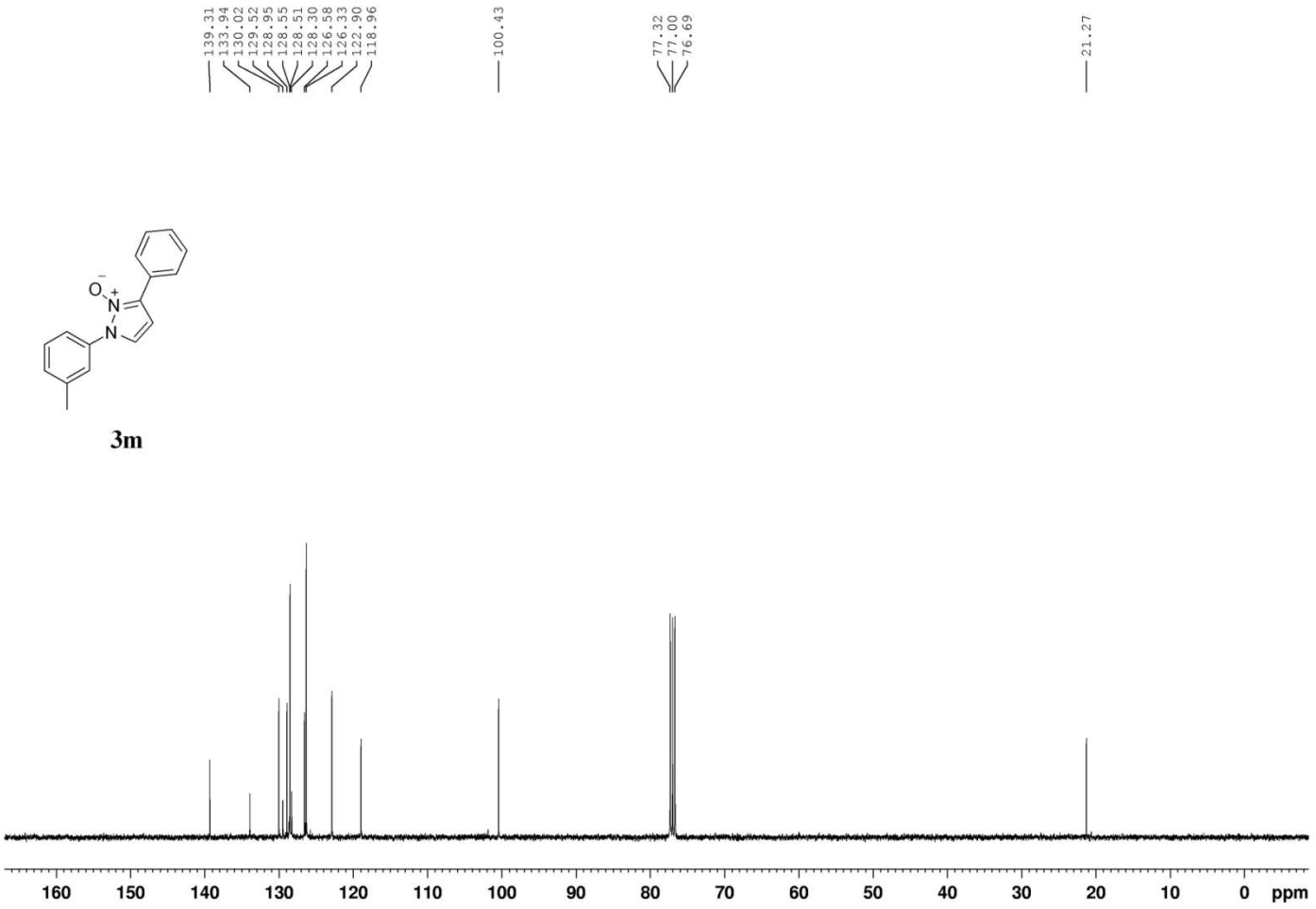
ppm
2.04
3.04
3.00
1.16
0.96
1.00
2.99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133.94
130.02
129.52
128.95
128.55
128.51
128.30
126.58
126.33
122.90
118.96
100.43
77.32
77.00
76.69
21.27
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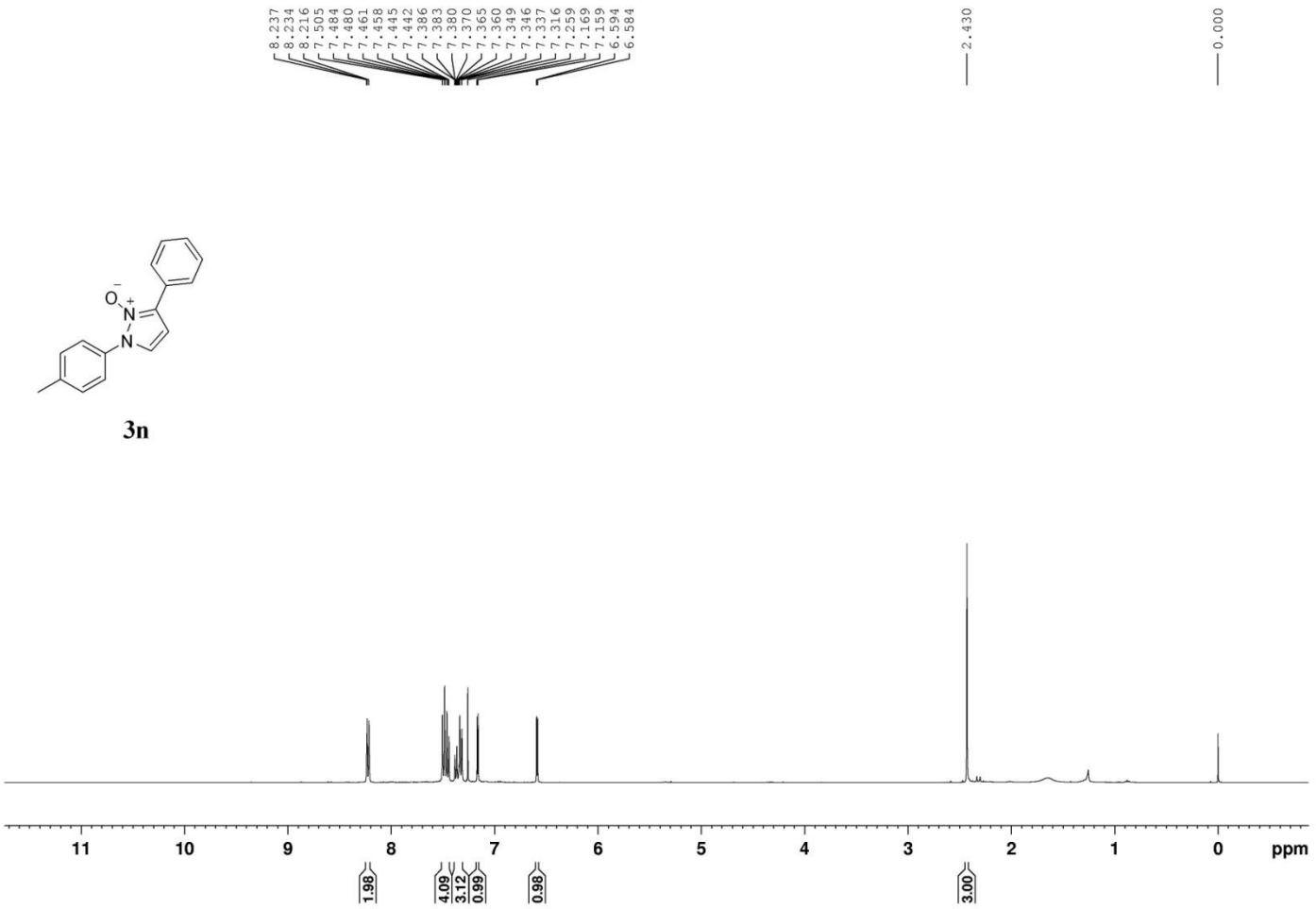
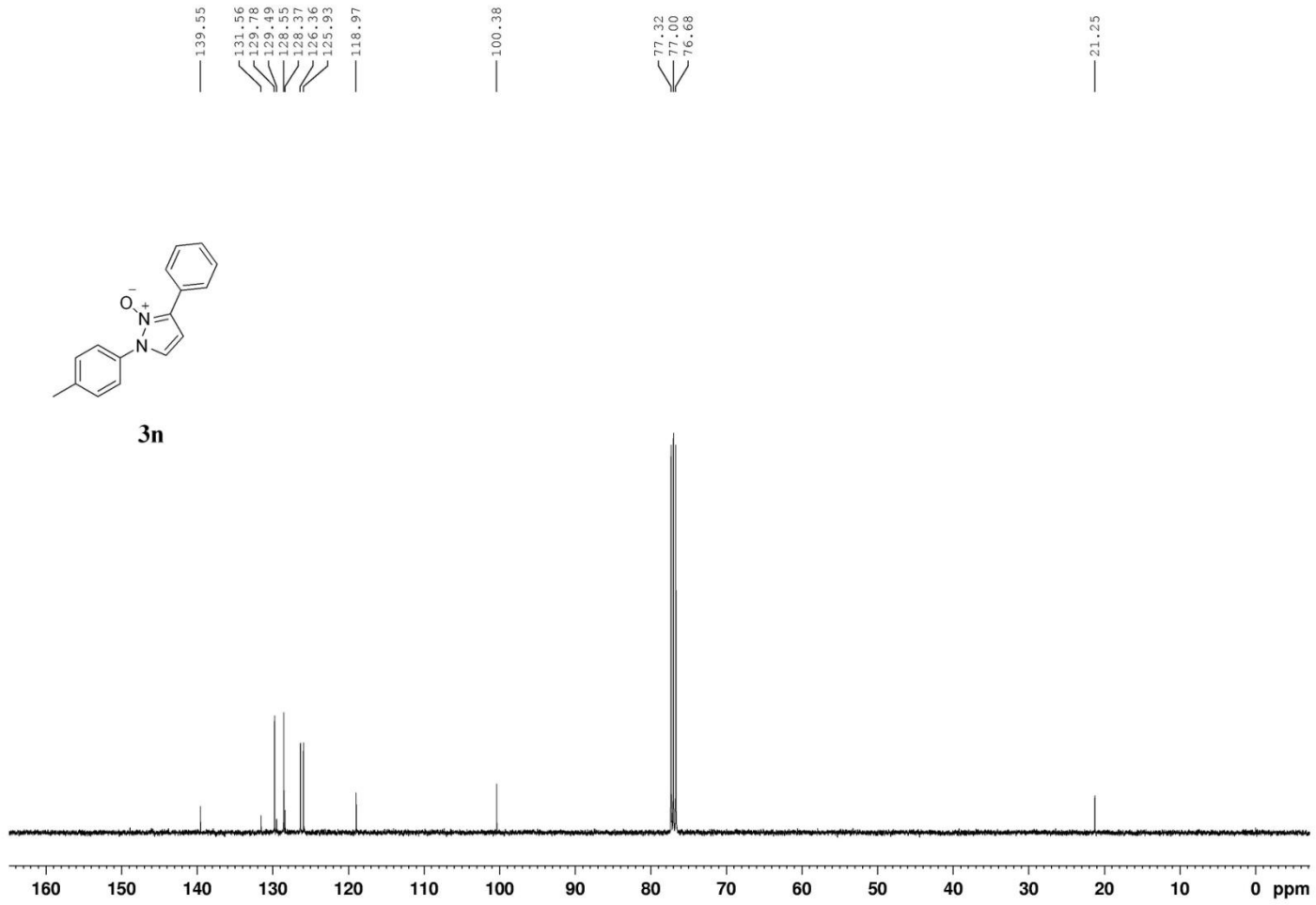
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3m


8.237
8.234
8.216
7.505
7.484
7.480
7.461
7.458
7.445
7.442
7.386
7.383
7.380
7.370
7.365
7.360
7.349
7.346
7.337
7.316
7.259
7.169
7.159
6.594
6.584
2.430
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.98
4.09
3.12
0.99
0.98
3.00

3n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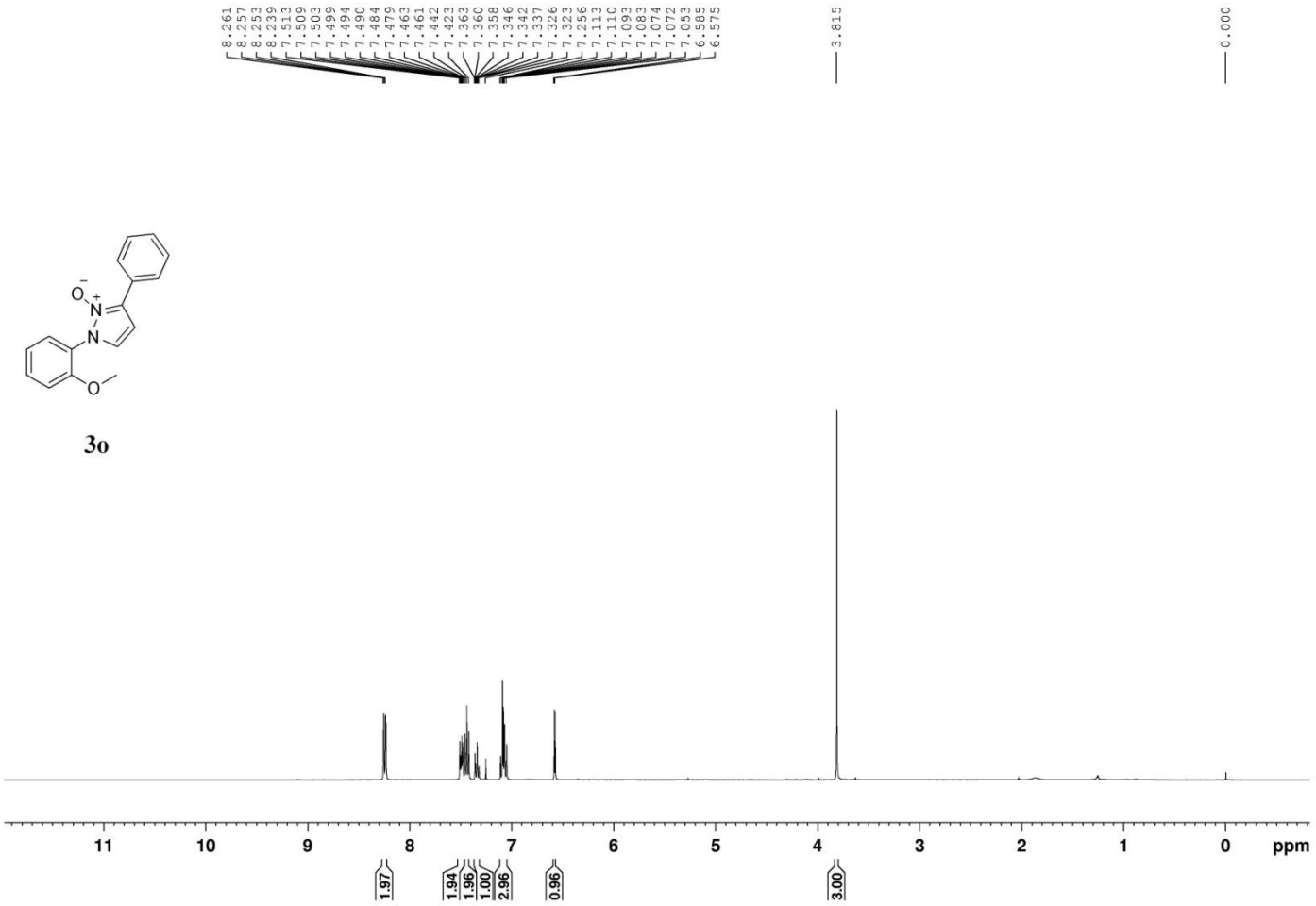
131.56
129.78
129.49
128.55
128.37
126.36
125.93
118.97
100.38
77.32
77.00
76.68
21.25
3n
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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8.257
8.253
8.239
7.513
7.509
7.503
7.499
7.494
7.490
7.484
7.479
7.463
7.461
7.442
7.423
7.363
7.360
7.358
7.346
7.342
7.337
7.326
7.323
7.256
7.113
7.110
7.093
7.083
7.074
7.072
7.053
6.585
6.575
3.815
0.000
11
10
9
8
7
6
5
4
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1
0
ppm
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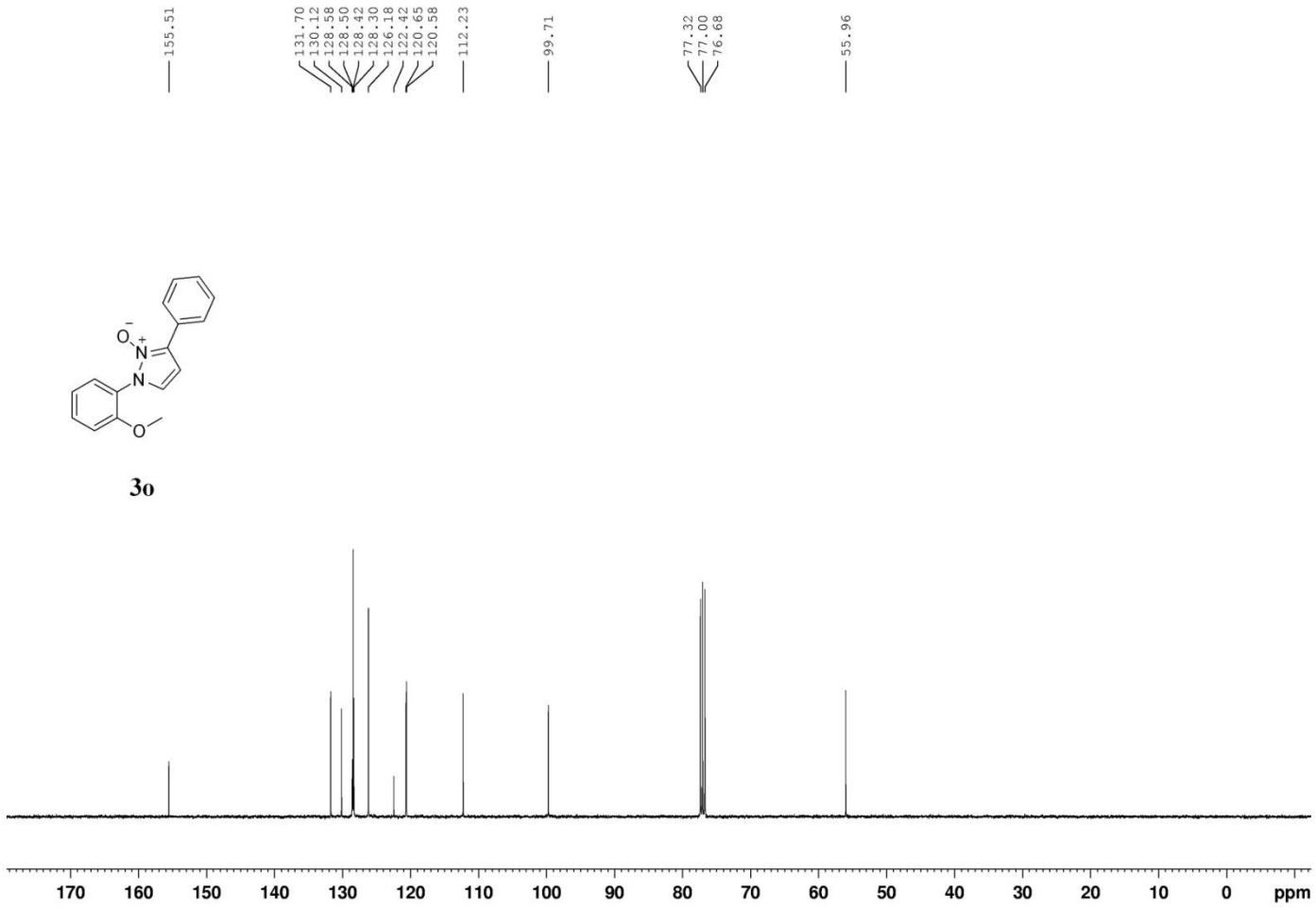
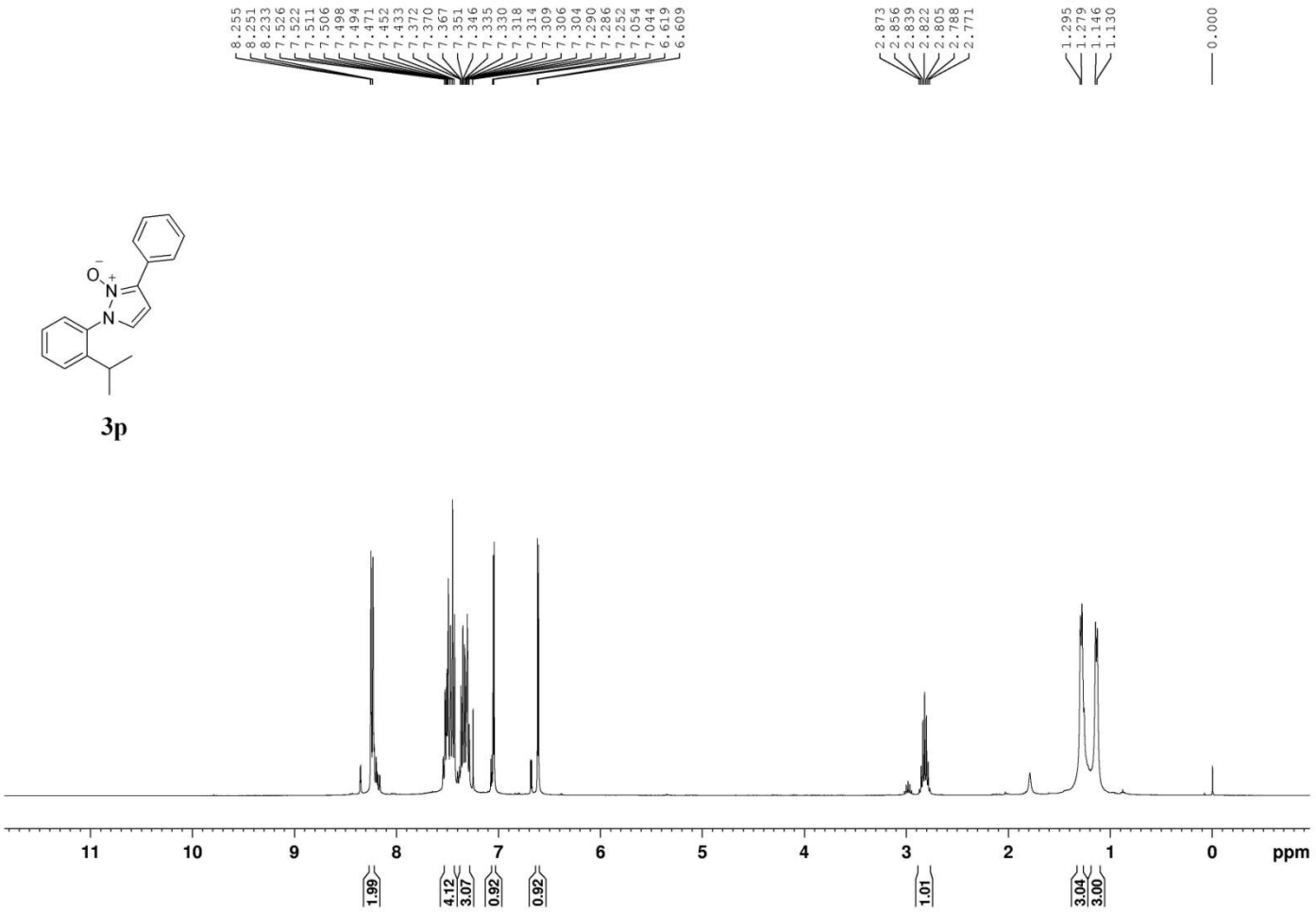
1.94
1.96
1.00
2.96
0.96
3.00

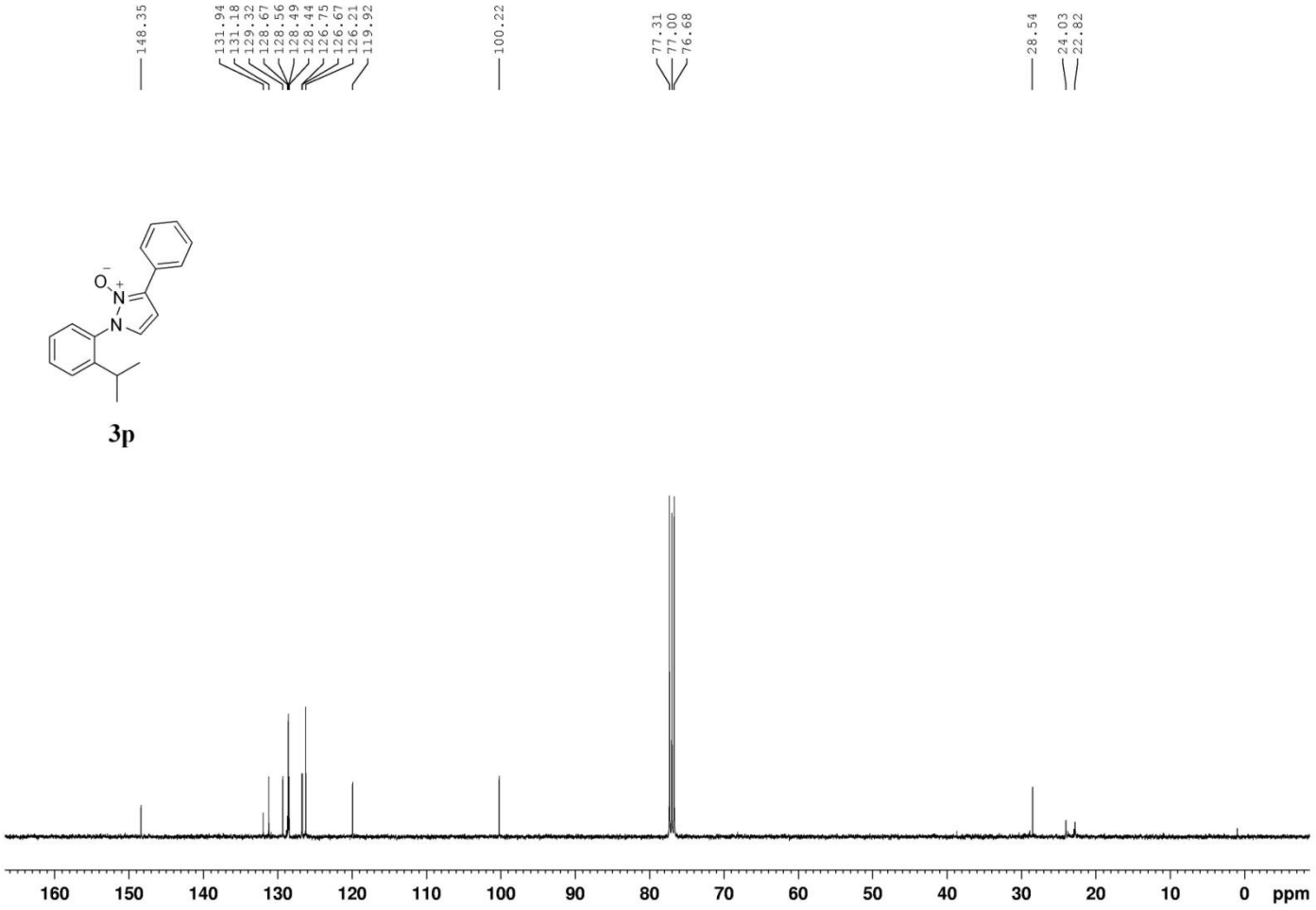
3o


155.51
131.70
130.12
128.58
128.50
128.42
128.30
126.18
122.42
120.65
120.58
112.23
99.71
77.32
77.00
76.68
55.96
O
N
N
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3o


8.255
8.251
8.233
7.526
7.522
7.511
7.506
7.498
7.494
7.471
7.452
7.433
7.372
7.370
7.367
7.351
7.346
7.335
7.330
7.318
7.314
7.309
7.306
7.304
7.290
7.286
7.252
7.054
7.044
6.619
6.609
2.873
2.856
2.839
2.822
2.805
2.788
2.771
1.295
1.279
1.146
1.130
0.000
O
N
N
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.99
4.12
3.07
0.92
0.92
1.01
3.04
3.00

3p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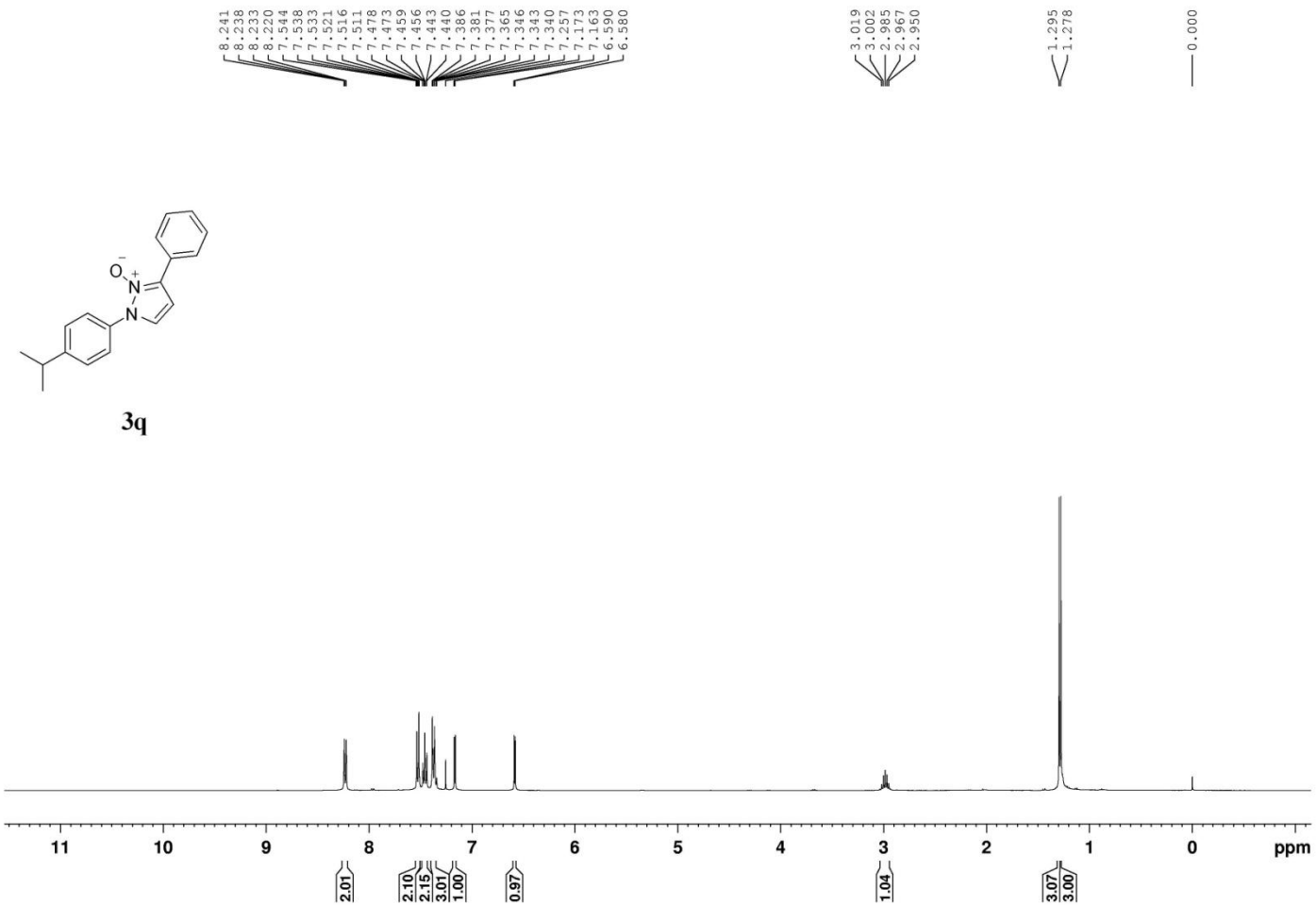
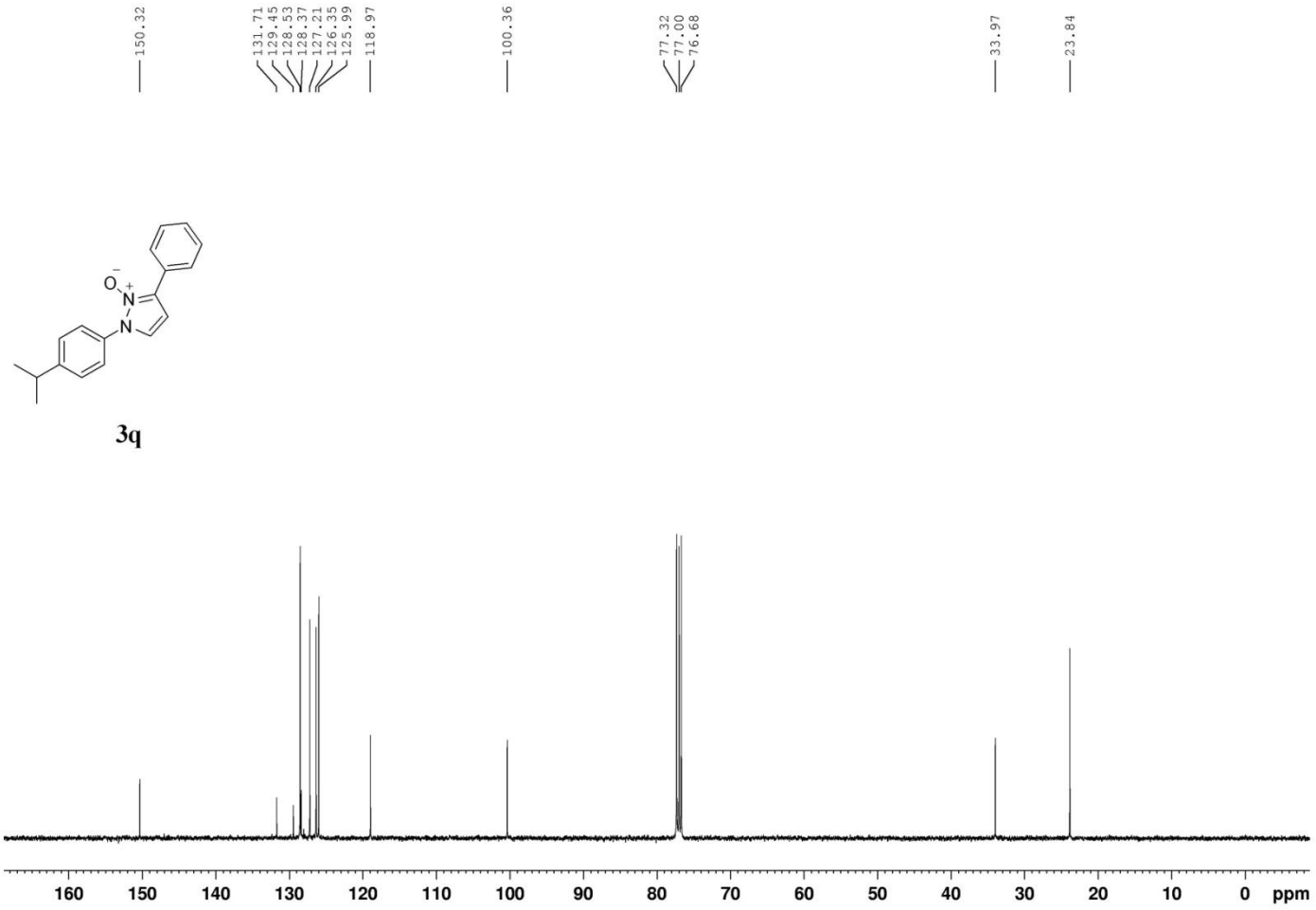
131.94
131.18
129.32
128.67
128.56
128.49
128.44
126.75
126.67
126.21
119.92
100.22
77.31
77.00
76.68
28.54
24.03
22.82
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

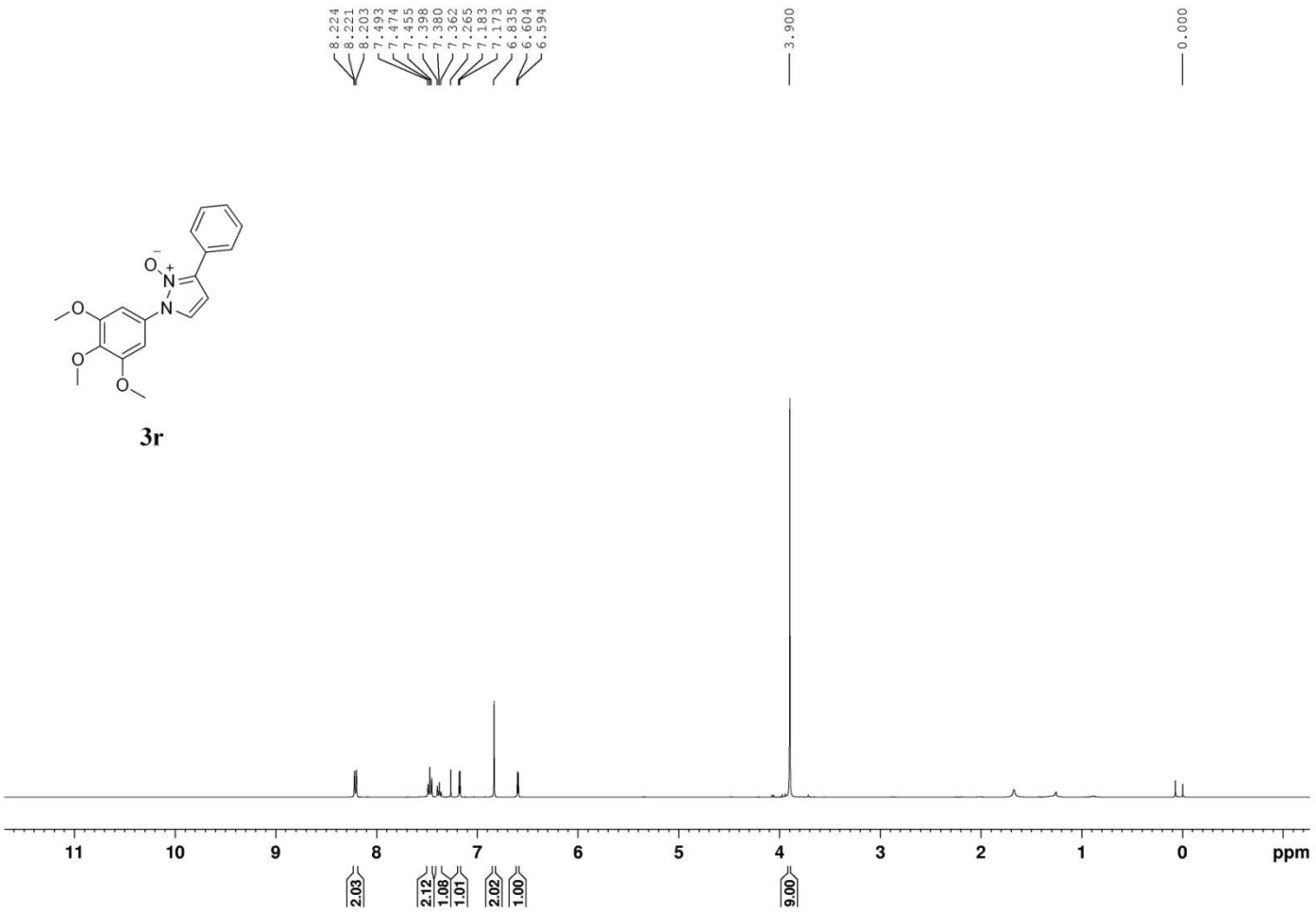
3p


8.241
8.238
8.233
8.220
7.544
7.538
7.533
7.521
7.516
7.511
7.478
7.473
7.459
7.456
7.443
7.440
7.386
7.381
7.377
7.365
7.346
7.343
7.340
7.257
7.173
7.163
6.590
6.580
3.019
3.002
2.985
2.967
2.950
1.295
1.278
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.10
2.15
3.01
1.00
0.97
1.04
3.07
3.00

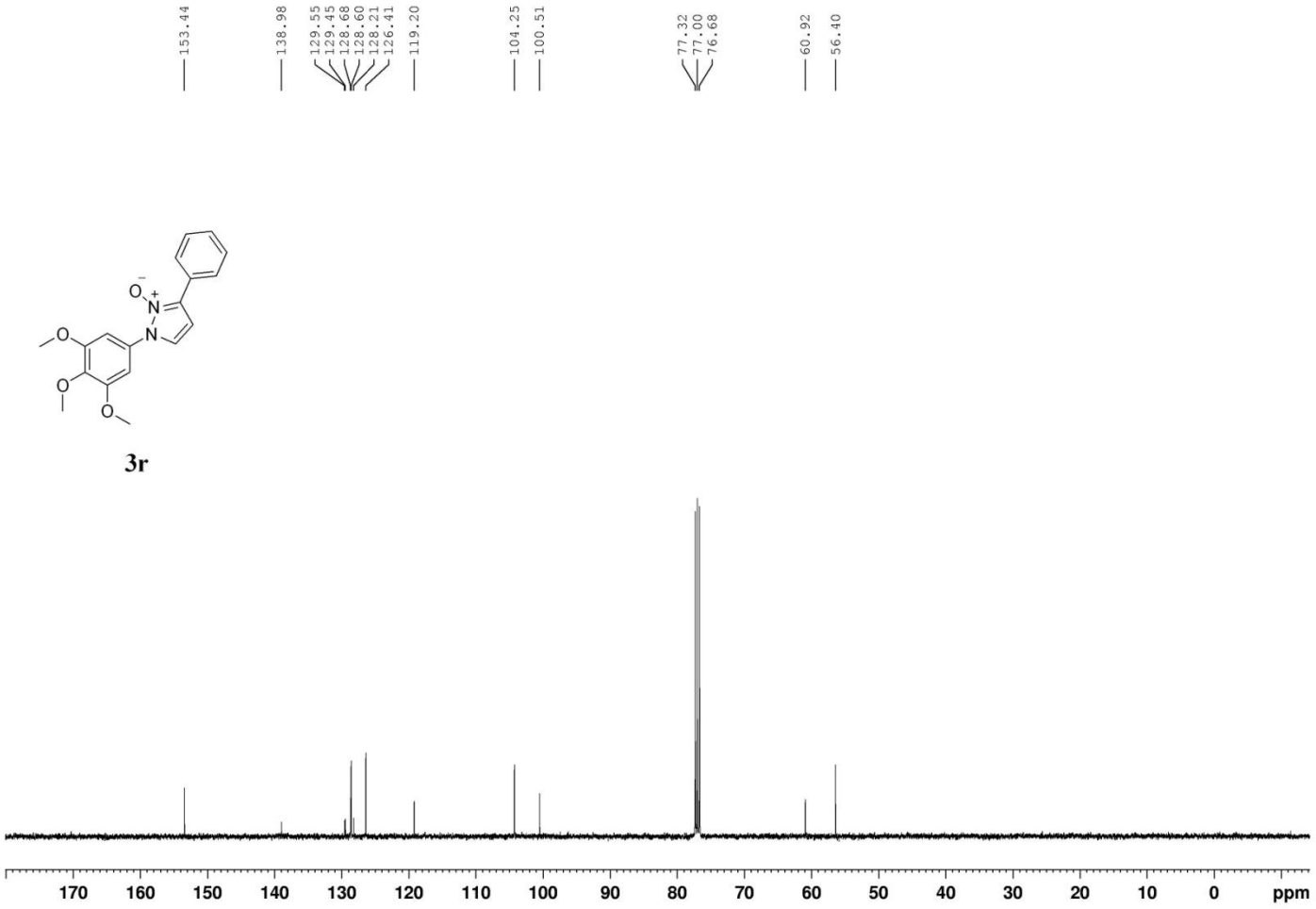
3q


150.32
131.71
129.45
128.53
128.37
127.21
126.35
125.99
118.97
100.36
77.32
77.00
76.68
33.97
23.84
O
N
N
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3q


8.224
8.221
8.203
7.493
7.474
7.455
7.398
7.380
7.362
7.265
7.183
7.173
6.835
6.604
6.594
3.900
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.03
2.12
1.08
1.01
2.02
1.00
9.00

3r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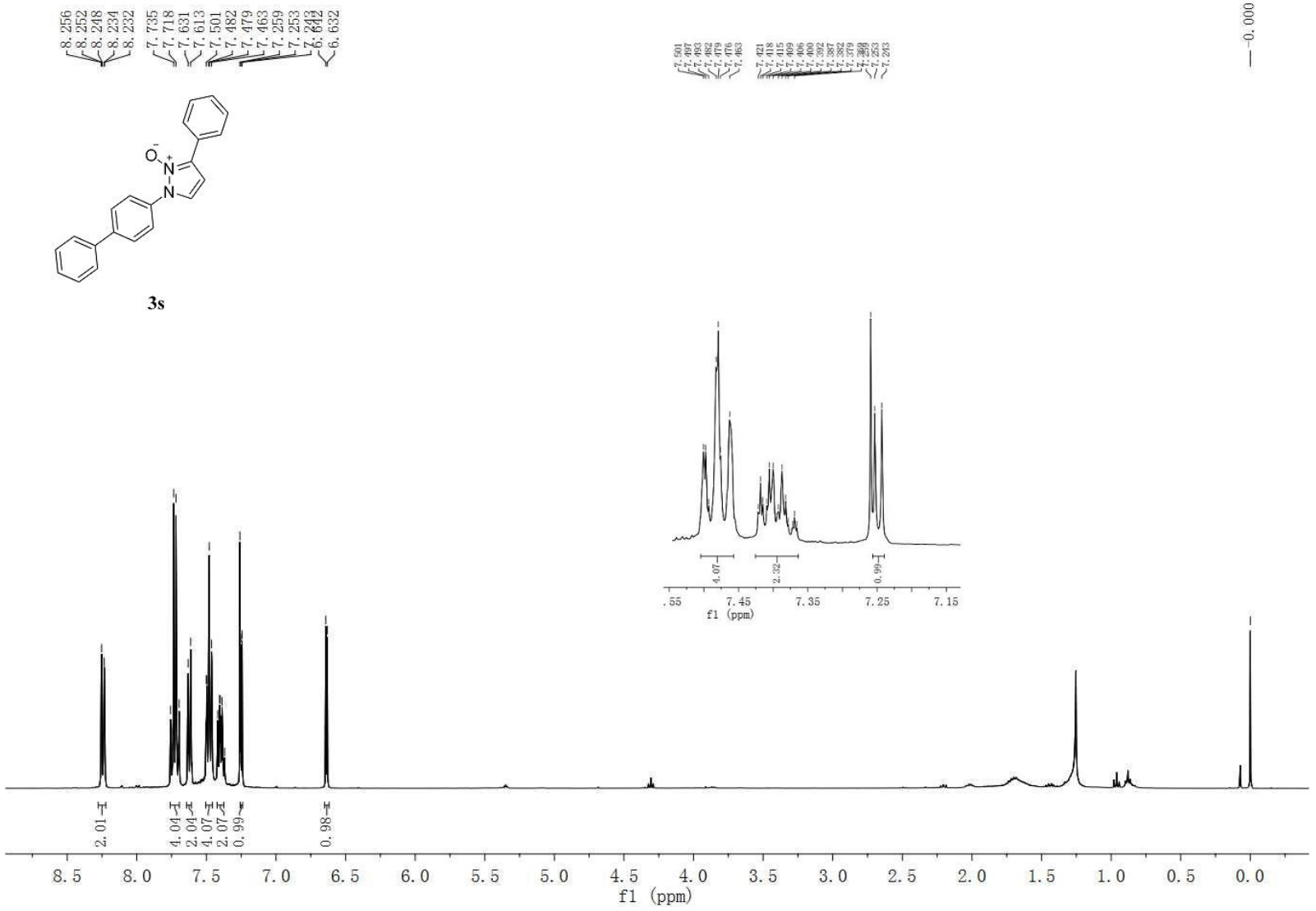
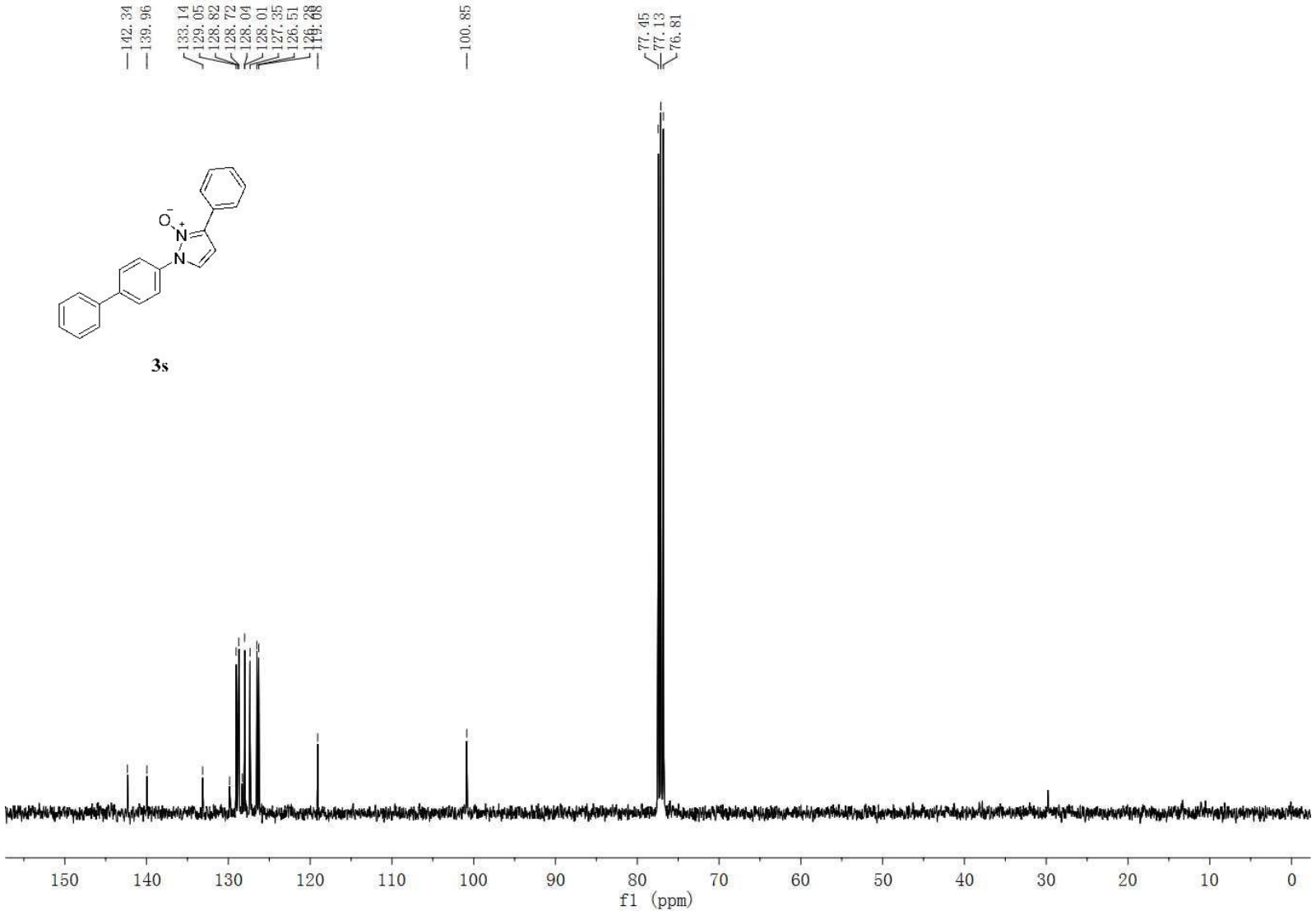
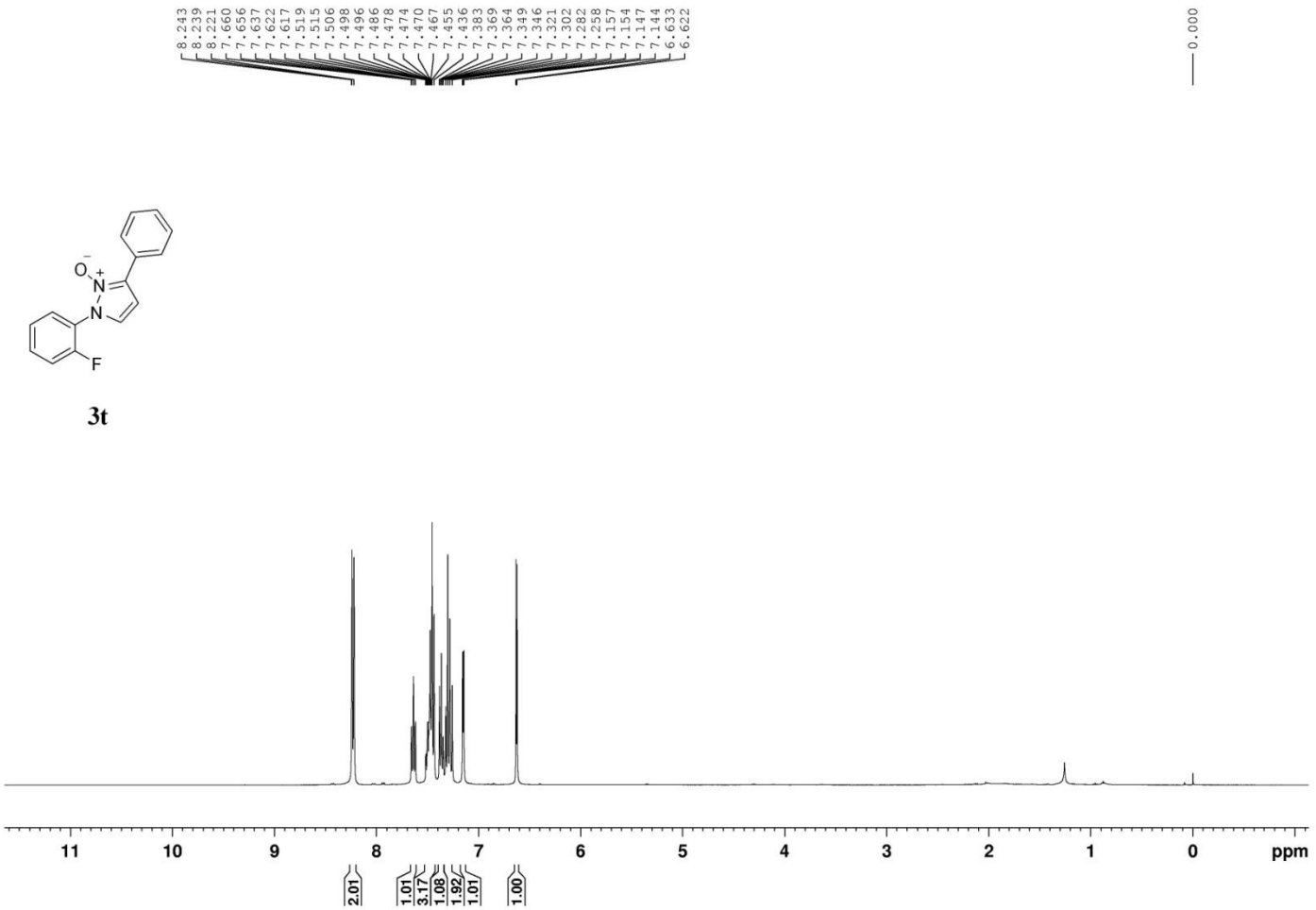
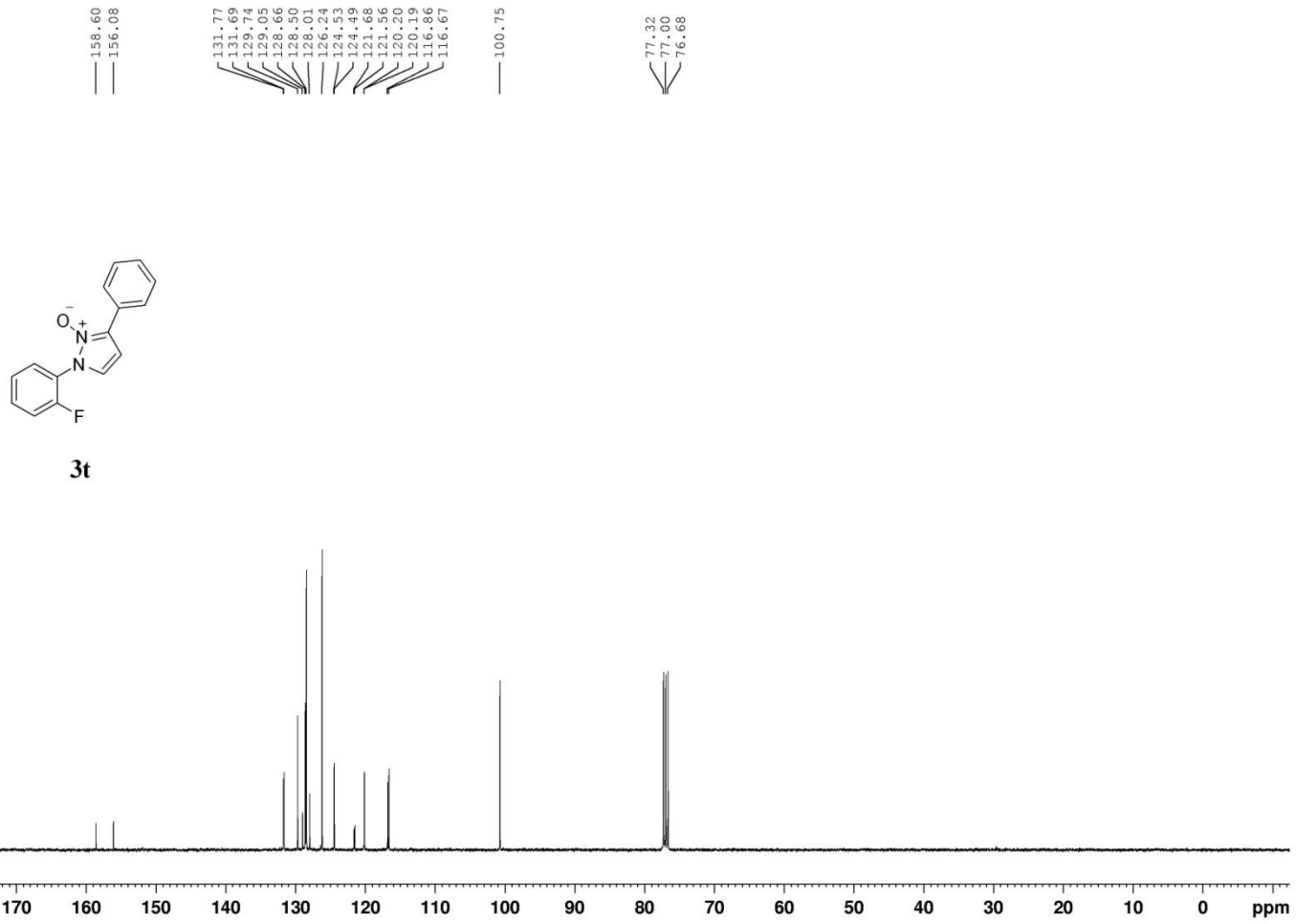
138.98
129.55
129.45
128.68
128.60
128.21
126.41
119.20
104.25
100.51
77.32
77.00
76.68
60.92
56.40
O
N
N
O
O
O
3r
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.256
8.252
8.248
8.234
8.232
7.735
7.718
7.631
7.613
7.501
7.482
7.479
7.463
7.259
7.253
6.642
6.632
7.501
7.497
7.495
7.482
7.479
7.476
7.463
7.421
7.418
7.415
7.409
7.406
7.400
7.392
7.387
7.382
7.379
7.253
7.243
0.000
3s
4.07
2.32
0.99
7.55
7.45
7.35
7.25
7.15
f1 (ppm)
2.01
4.04
2.04
4.07
2.07
0.99
0.98
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
f1 (ppm)

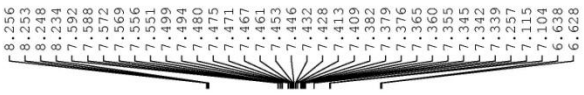

142.34
139.96
133.14
129.05
128.82
128.72
128.04
128.01
127.35
126.51
100.85
77.45
77.13
76.81
O
N
N
3s
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.243
8.239
8.221
7.660
7.656
7.637
7.622
7.617
7.519
7.515
7.506
7.498
7.496
7.486
7.478
7.474
7.470
7.467
7.455
7.436
7.383
7.369
7.364
7.349
7.346
7.321
7.302
7.282
7.258
7.157
7.154
7.147
7.144
6.633
6.622
0.000
O
N
N
F
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
1.01
3.17
1.08
1.92
1.01
1.00

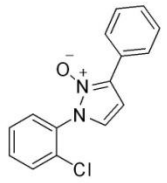
3t


158.60
156.08
131.77
131.69
129.74
129.05
128.66
128.50
128.01
126.24
124.53
124.49
121.68
121.56
120.20
120.19
116.86
116.67
100.75
77.32
77.00
76.68
O
N
N
F
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

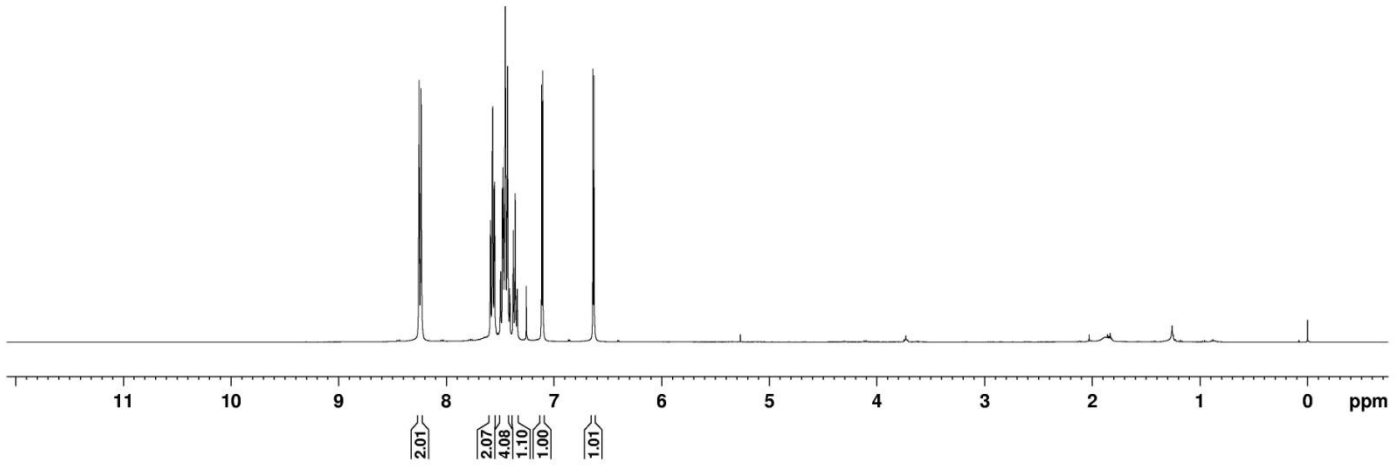
3t

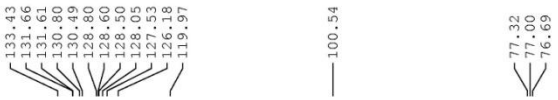

8.256
8.253
8.248
8.234
7.592
7.588
7.572
7.569
7.556
7.551
7.499
7.494
7.480
7.475
7.471
7.467
7.461
7.453
7.446
7.432
7.428
7.413
7.409
7.382
7.379
7.376
7.365
7.360
7.355
7.345
7.342
7.339
7.257
7.115
7.104
6.638
6.628

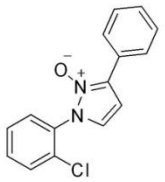
0.000


O
N
N
Cl

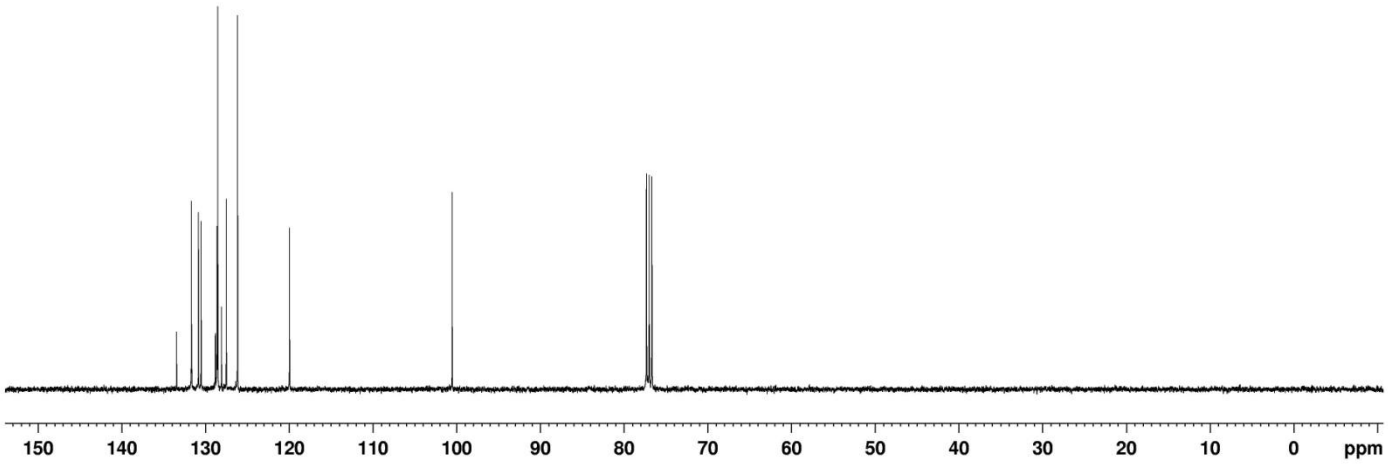
3u

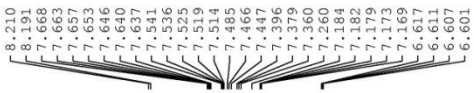

11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.07
4.08
1.10
1.00
1.01


133.43
131.66
131.61
130.80
130.49
128.80
128.60
128.50
128.05
127.53
126.18
119.97
100.54
77.32
77.00
76.69

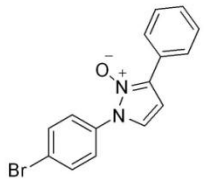

O
N
N
Cl

3u

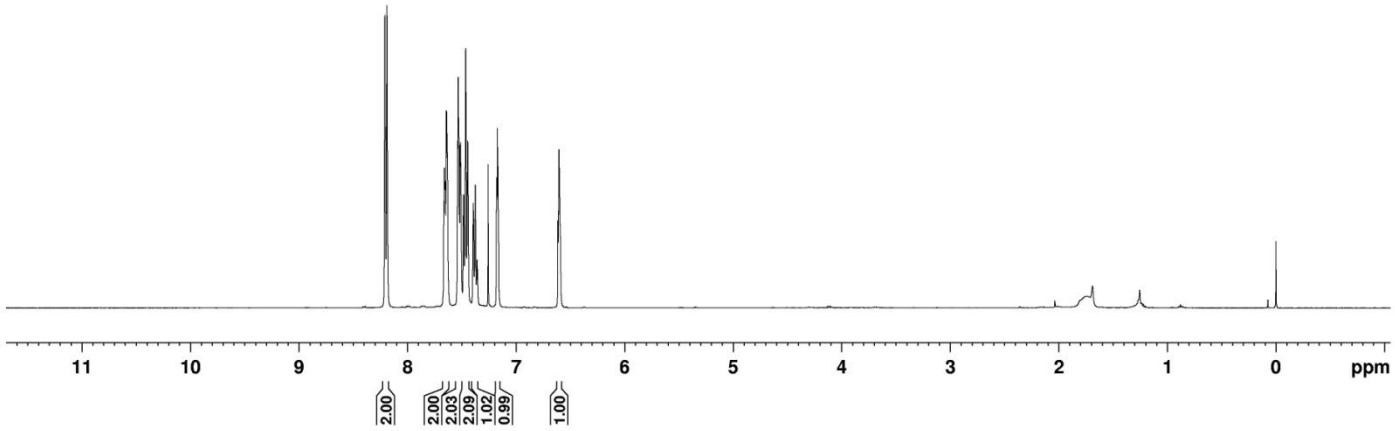

150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

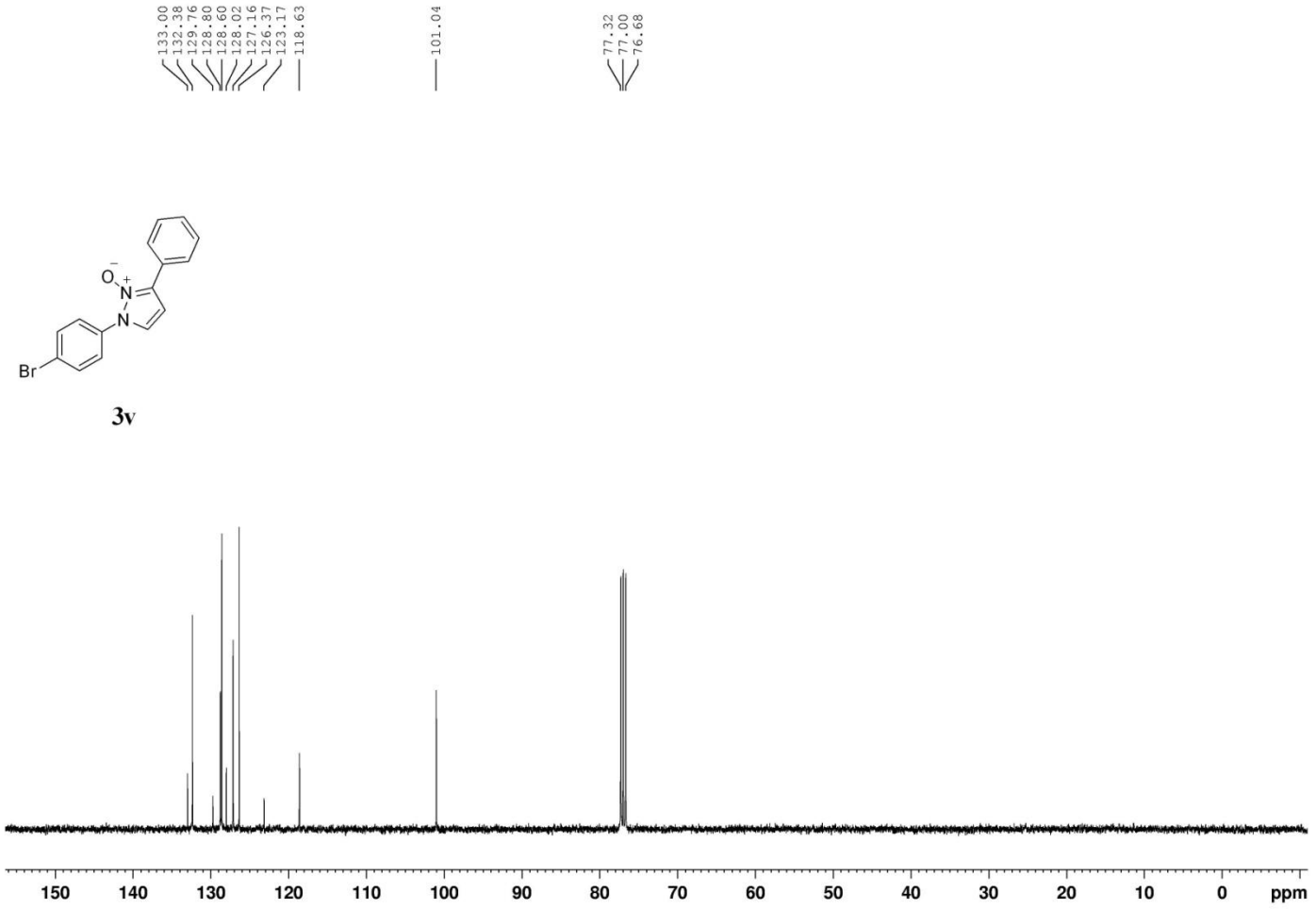

8.210
8.191
7.668
7.663
7.657
7.653
7.646
7.640
7.637
7.541
7.536
7.525
7.519
7.514
7.485
7.466
7.447
7.396
7.379
7.360
7.260
7.184
7.182
7.179
7.173
7.169
6.617
6.611
6.607
6.601

0.000

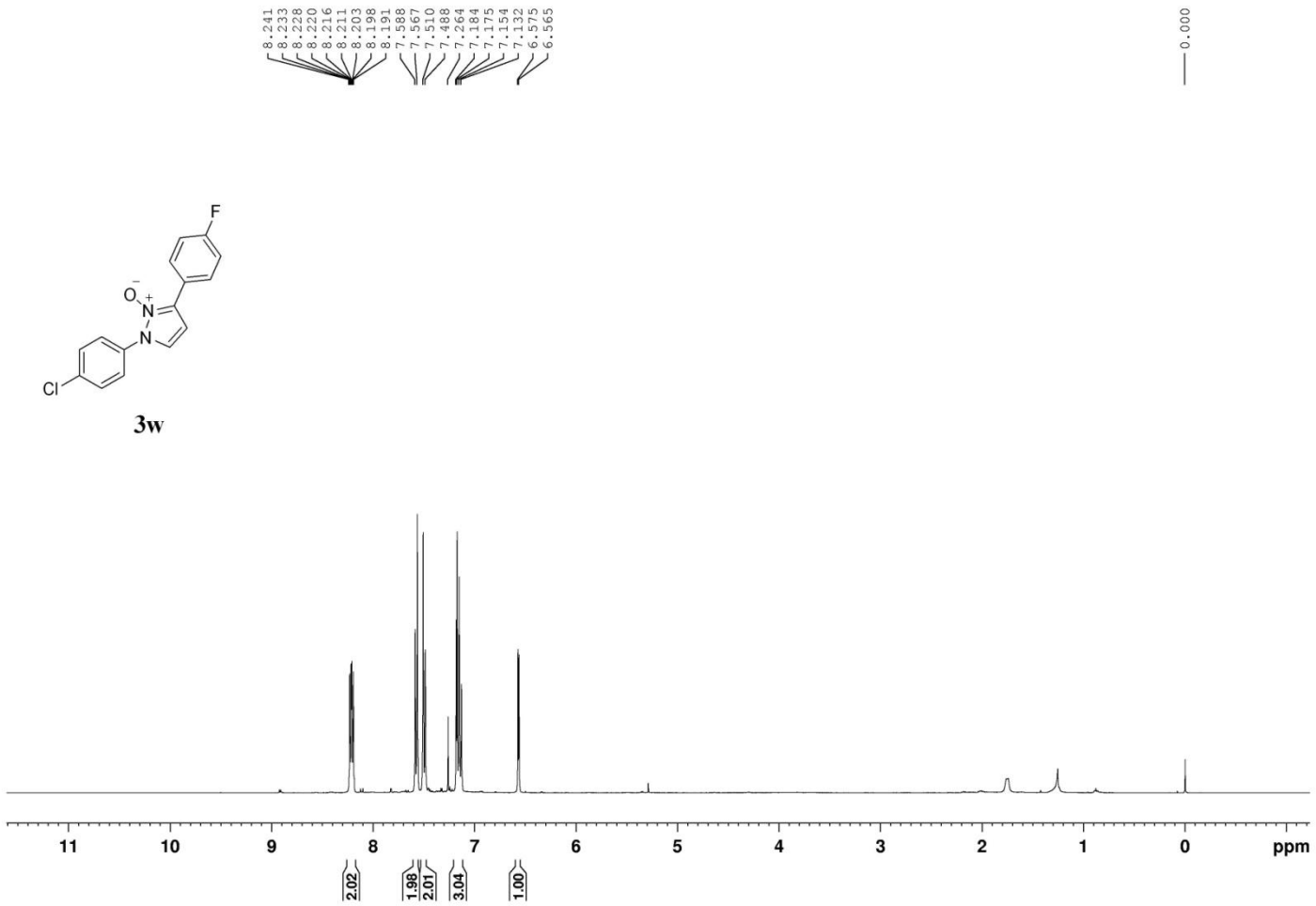

O
N
N
Br

3v

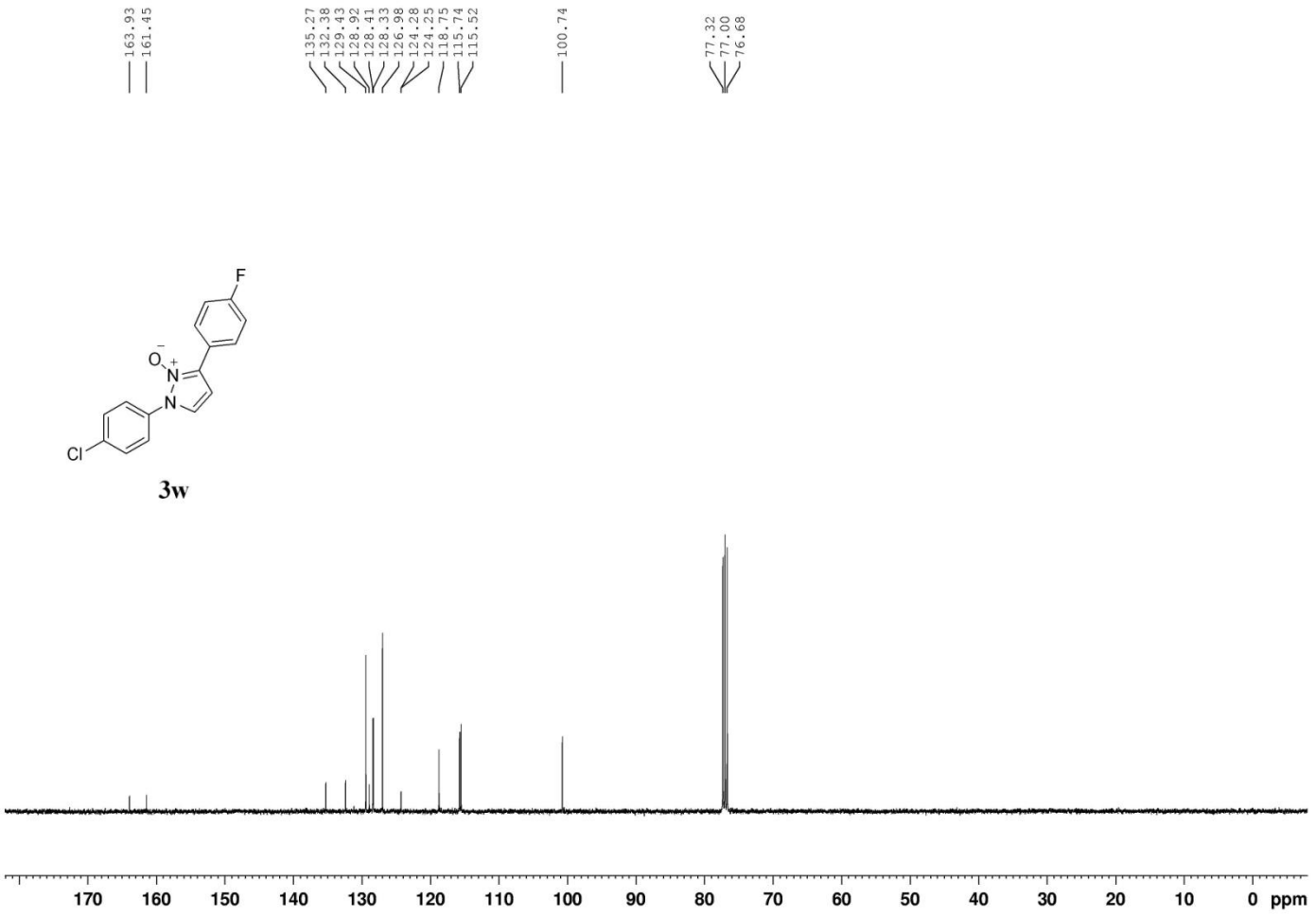

11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.00
2.03
2.09
1.02
0.99
1.00


133.00
132.38
129.76
128.80
128.60
128.02
127.16
126.37
123.17
118.63
101.04
77.32
77.00
76.68
O
N
N
Br
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

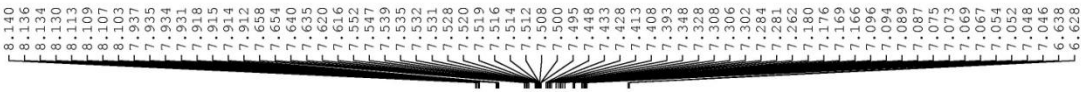
3v


8.241
8.233
8.228
8.220
8.216
8.211
8.203
8.198
8.191
7.588
7.567
7.510
7.488
7.264
7.184
7.175
7.154
7.132
6.575
6.565
0.000
F
Cl
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.02
1.98
2.01
3.04
1.00

3w


163.93
161.45
135.27
132.38
129.43
128.92
128.41
128.33
126.98
124.28
124.25
118.75
115.74
115.52
100.74
77.32
77.00
76.68
F
O
N
N
Cl
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

3w


8.140
8.136
8.134
8.130
8.113
8.109
8.107
8.103
7.937
7.935
7.934
7.931
7.918
7.915
7.914
7.912
7.658
7.654
7.640
7.635
7.620
7.616
7.552
7.547
7.539
7.535
7.532
7.531
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7.520
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7.516
7.514
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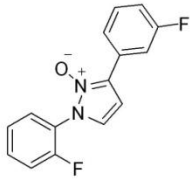
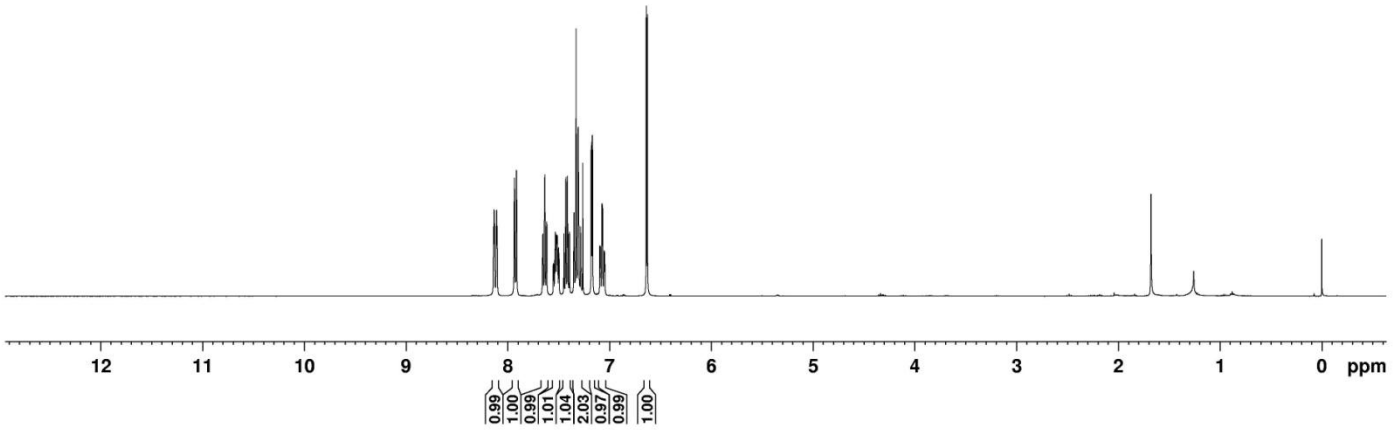
7.428
7.413
7.408
7.393
7.348
7.328
7.308
7.306
7.302
7.284
7.281
7.262
7.180
7.176
7.169
7.166
7.096
7.094
7.089
7.087
7.075
7.073
7.069
7.067
7.054
7.052
7.048
7.046
6.638
6.628
0.000


F
O
N
N
F

3x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11
10
9
8
7
6
5
4
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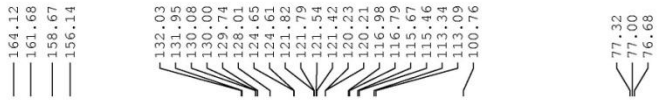
2
1
0
ppm
0.99
1.00
0.99
1.01
1.04
2.03
0.97
0.99
1.00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161.68
158.67
156.14
132.03
131.95
130.08
130.00
129.74
128.01
124.65
124.61
121.82
121.79
121.54
121.42
120.23
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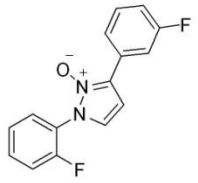
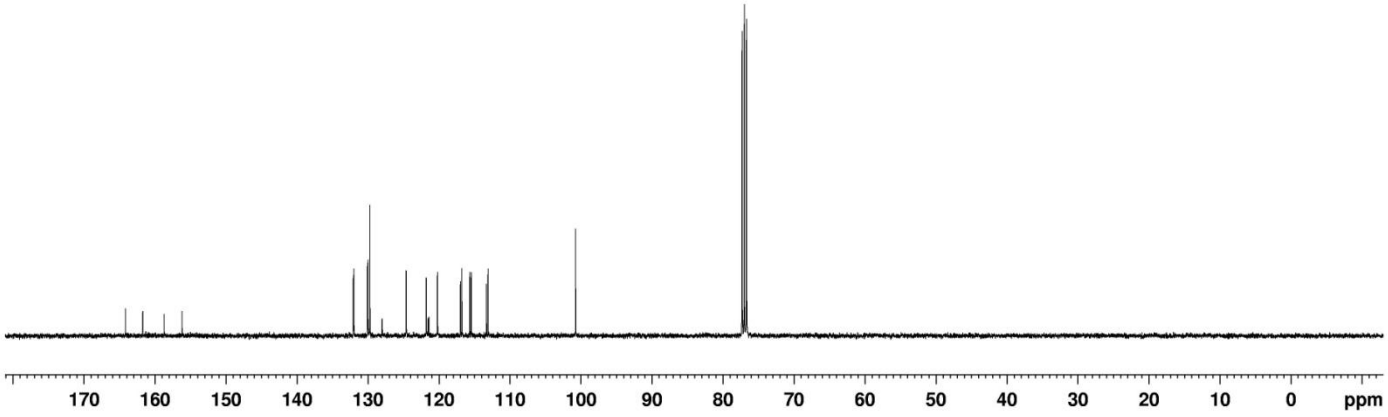
116.98
116.79
115.67
115.46
113.34
113.09
100.76
77.32
77.00
76.68


F
O
N
N
F

3x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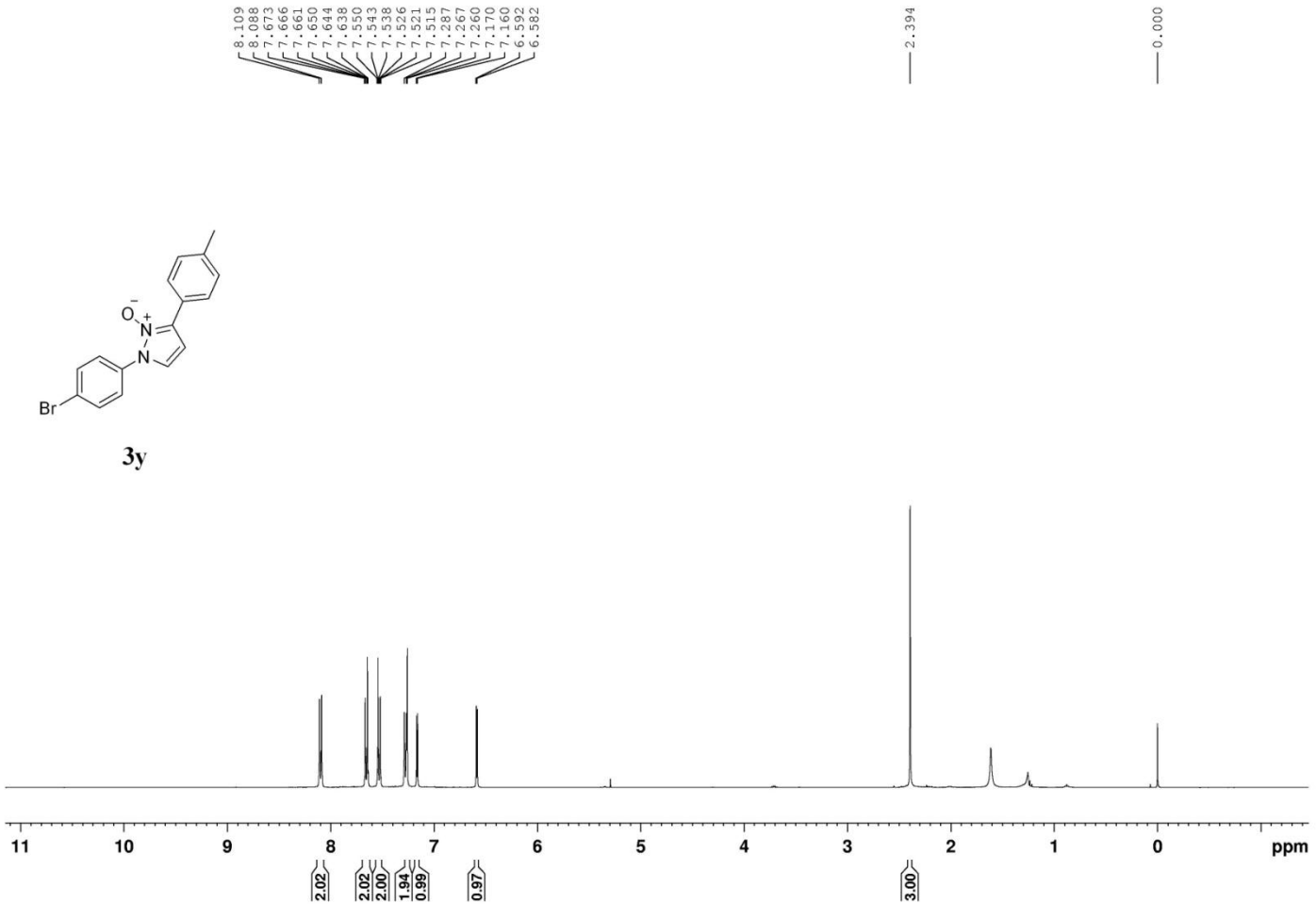
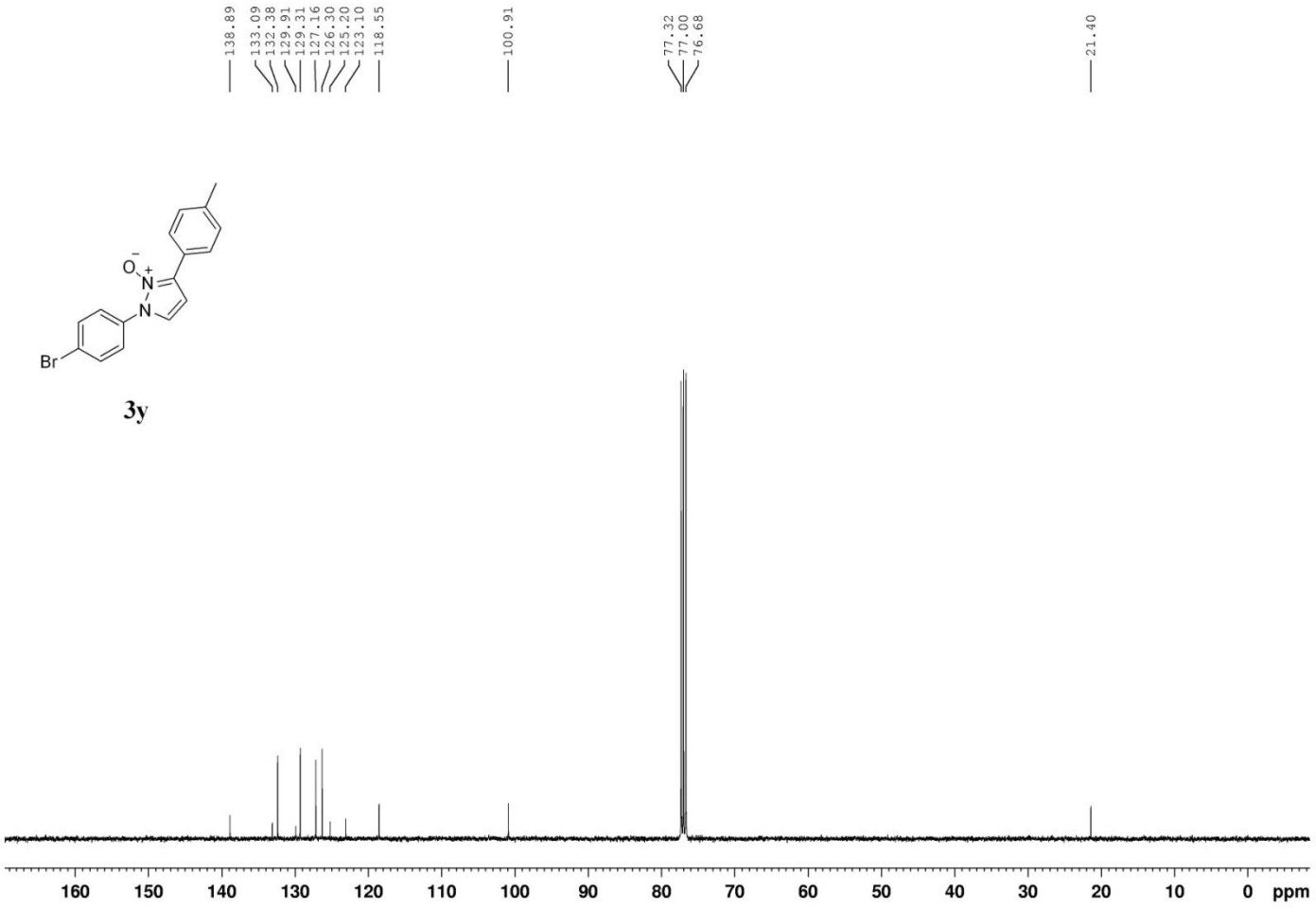
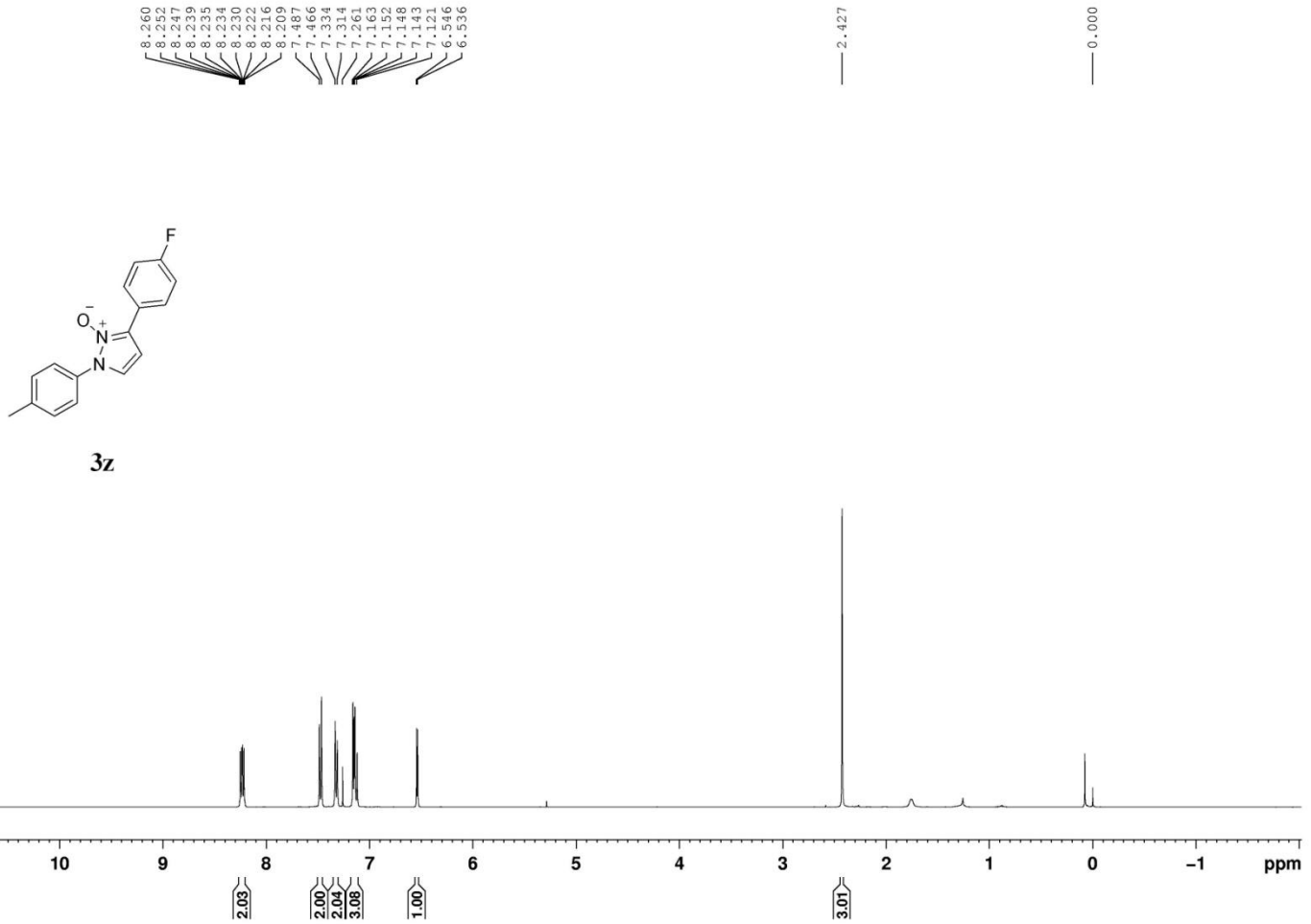
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.109
8.088
7.673
7.666
7.661
7.650
7.644
7.638
7.550
7.543
7.538
7.526
7.521
7.515
7.287
7.267
7.260
7.170
7.160
6.592
6.582
2.394
0.000
Br
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.02
2.02
2.00
1.94
0.99
0.97
3.00

3y


138.89
133.09
132.38
129.91
129.31
127.16
126.30
125.20
123.10
118.55
100.91
77.32
77.00
76.68
21.40
O
N
N
Br
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3y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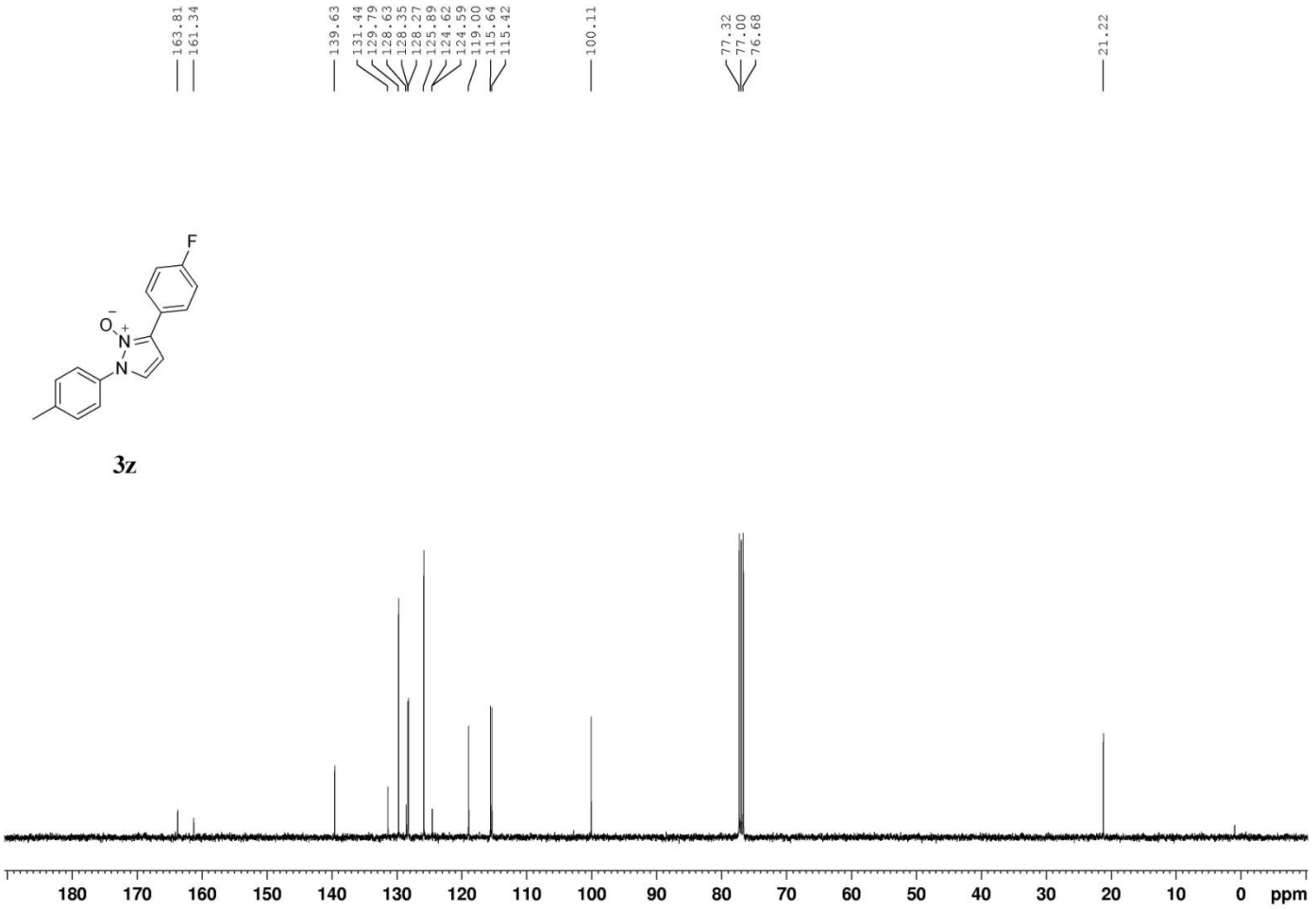
8.252
8.247
8.239
8.235
8.234
8.230
8.222
8.216
8.209
7.487
7.466
7.334
7.314
7.261
7.163
7.152
7.148
7.143
7.121
6.546
6.536
2.427
0.000
F
O
N
N
3z
10
9
8
7
6
5
4
3
2
1
0
−1
ppm
2.03
2.00
2.04
3.08
1.00
3.01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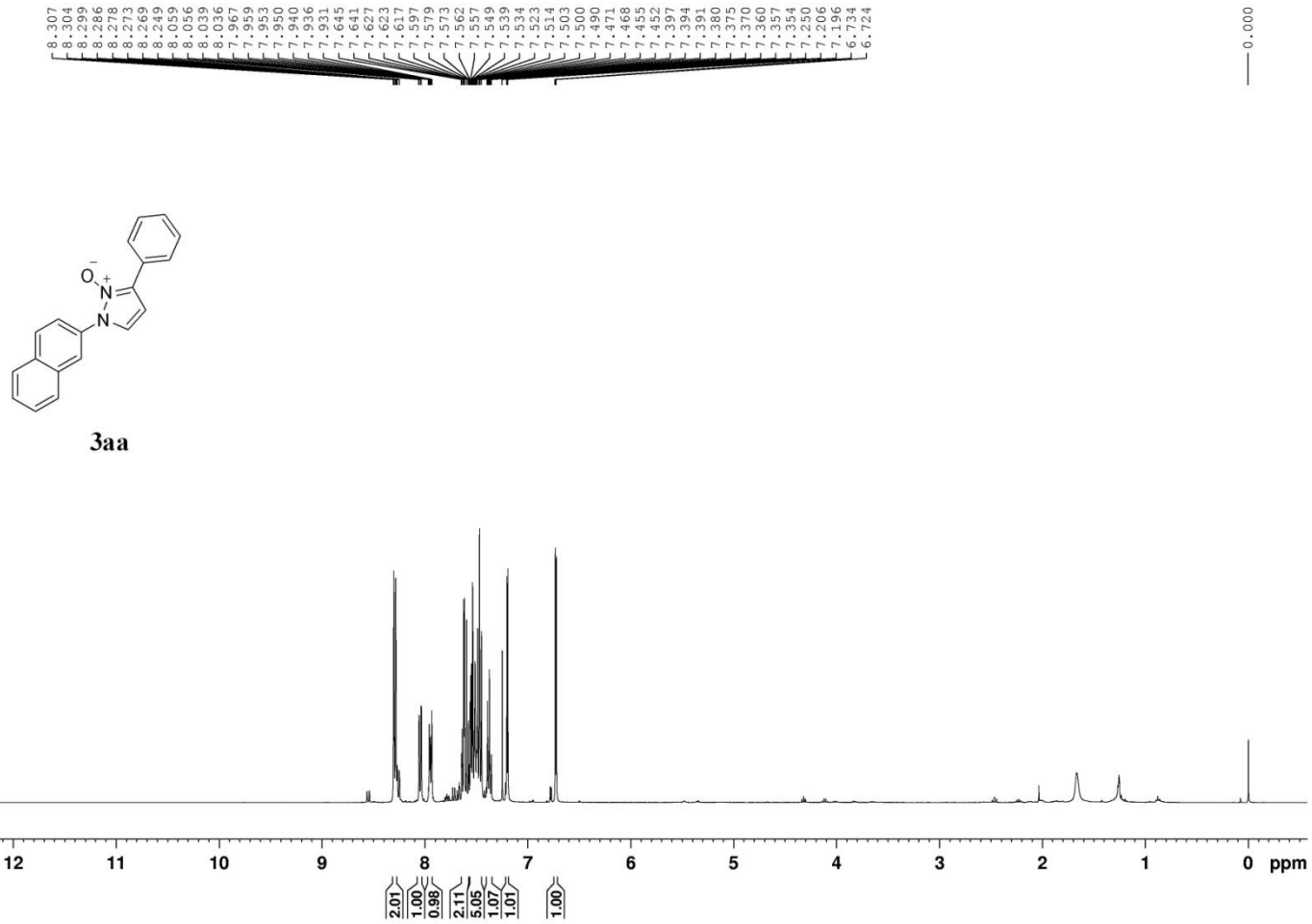
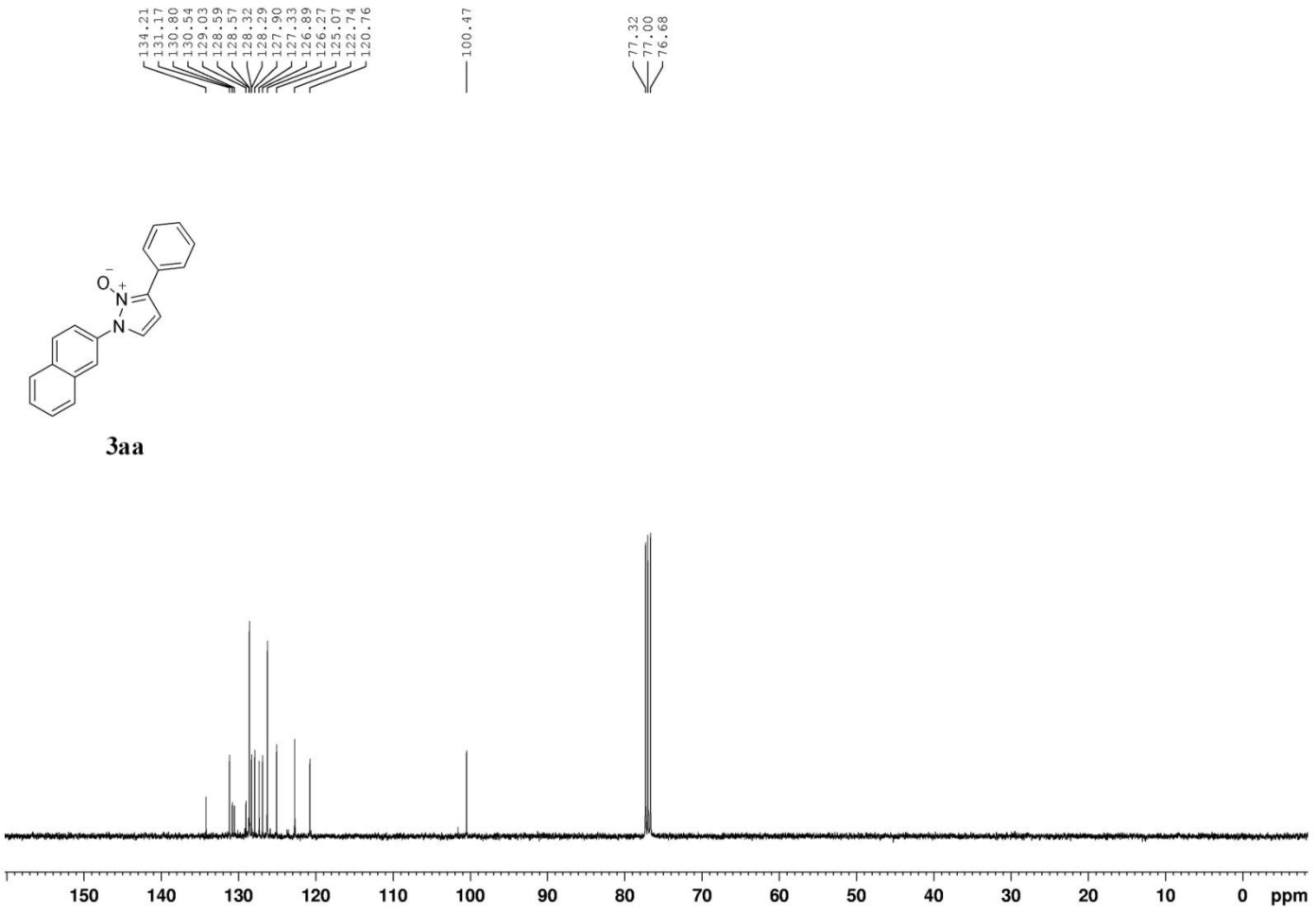
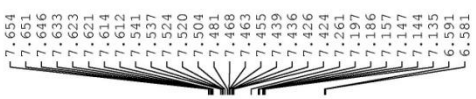
129.79
128.63
128.35
128.27
125.89
124.62
124.59
119.00
115.64
115.42
100.11
77.32
77.00
76.68
21.22
F
O
N
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3z

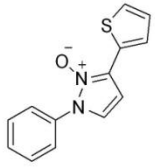

8.307
8.304
8.299
8.286
8.278
8.273
8.269
8.249
8.059
8.056
8.039
8.036
7.967
7.959
7.953
7.950
7.940
7.936
7.931
7.645
7.641
7.627
7.623
7.617
7.597
7.579
7.573
7.562
7.557
7.549
7.539
7.534
7.523
7.514
7.503
7.500
7.490
7.471
7.468
7.455
7.452
7.397
7.394
7.391
7.380
7.375
7.370
7.360
7.357
7.354
7.250
7.206
7.196
6.734
6.724
0.000
3aa
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
1.00
0.98
2.11
5.05
1.07
1.01
1.00


134.21
131.17
130.80
130.54
129.03
128.59
128.57
128.32
128.29
127.90
127.33
126.89
126.27
125.07
122.74
120.76
100.47
77.32
77.00
76.68
O
N
N
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

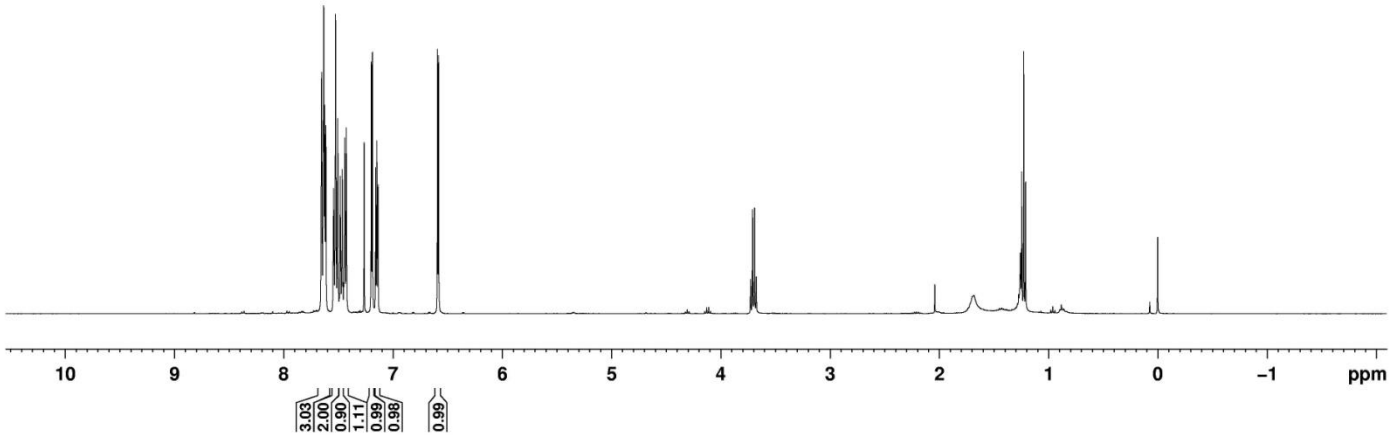
3aa


7.654
7.651
7.646
7.633
7.623
7.621
7.614
7.612
7.541
7.537
7.524
7.520
7.504
7.481
7.468
7.463
7.455
7.439
7.436
7.426
7.424
7.261
7.197
7.186
7.157
7.147
7.144
7.135
6.591
6.581

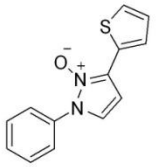
0.000


S
O
N
N

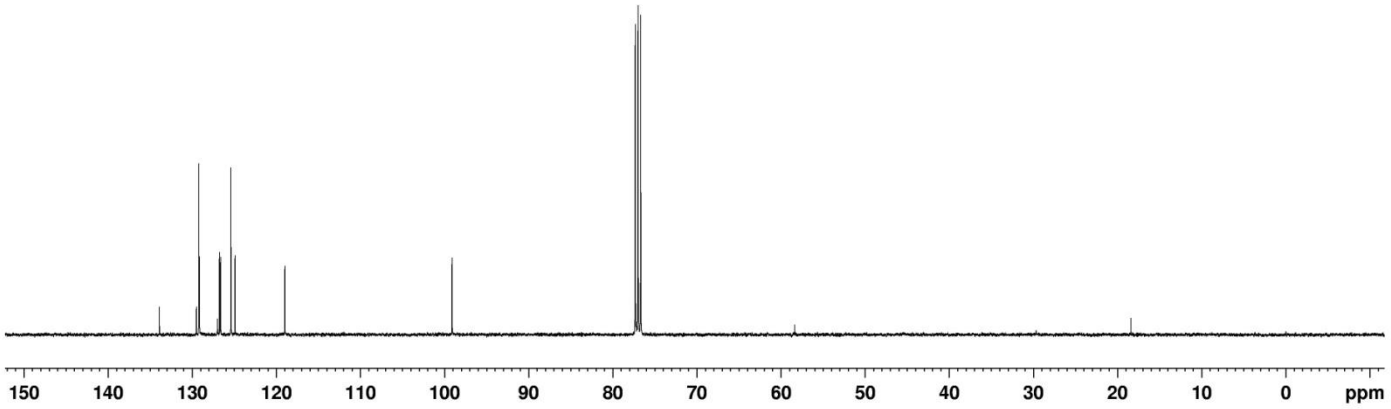
3ab

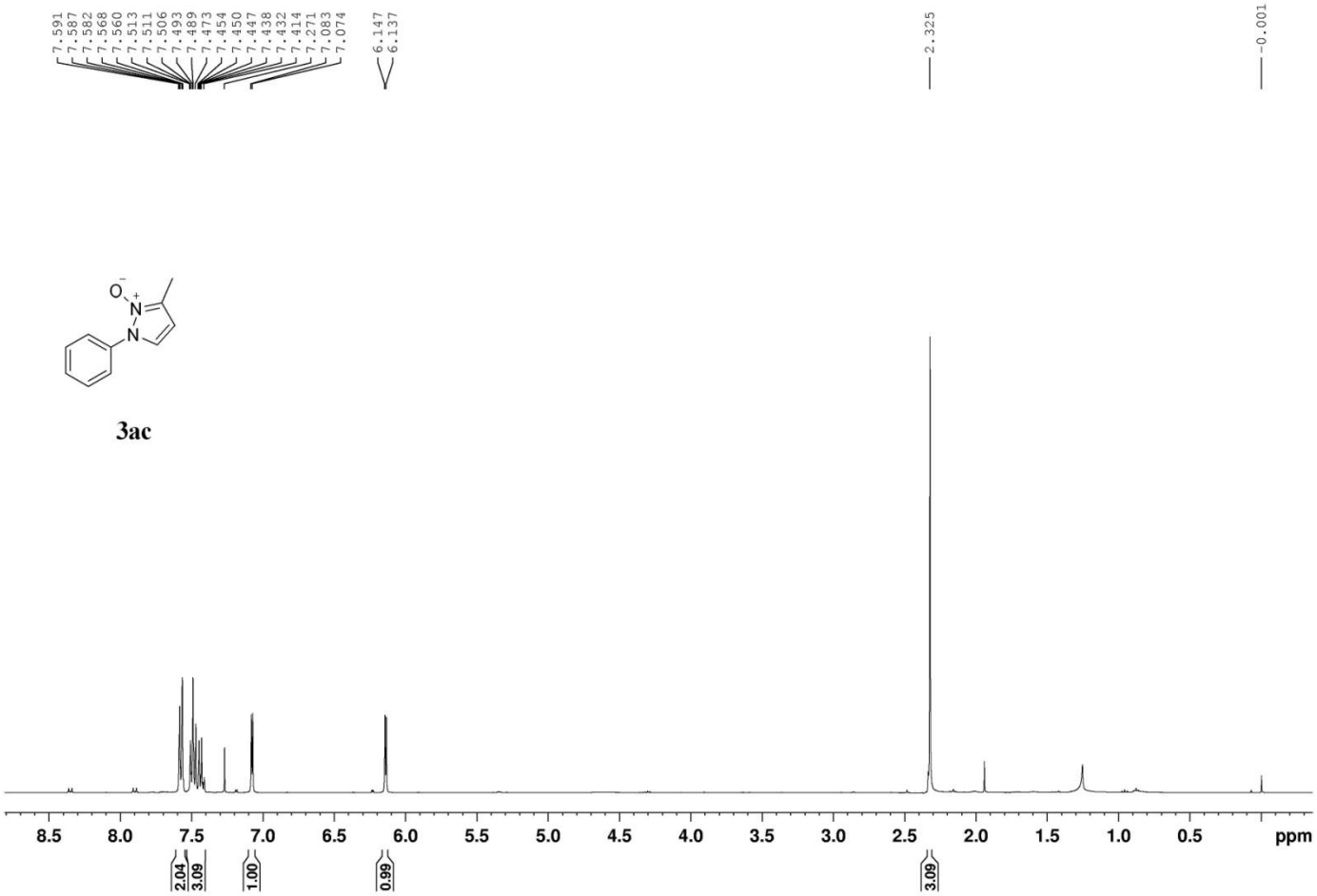

10
9
8
7
6
5
4
3
2
1
0
−1
ppm
3.03
2.00
0.90
1.11
0.99
0.98
0.99

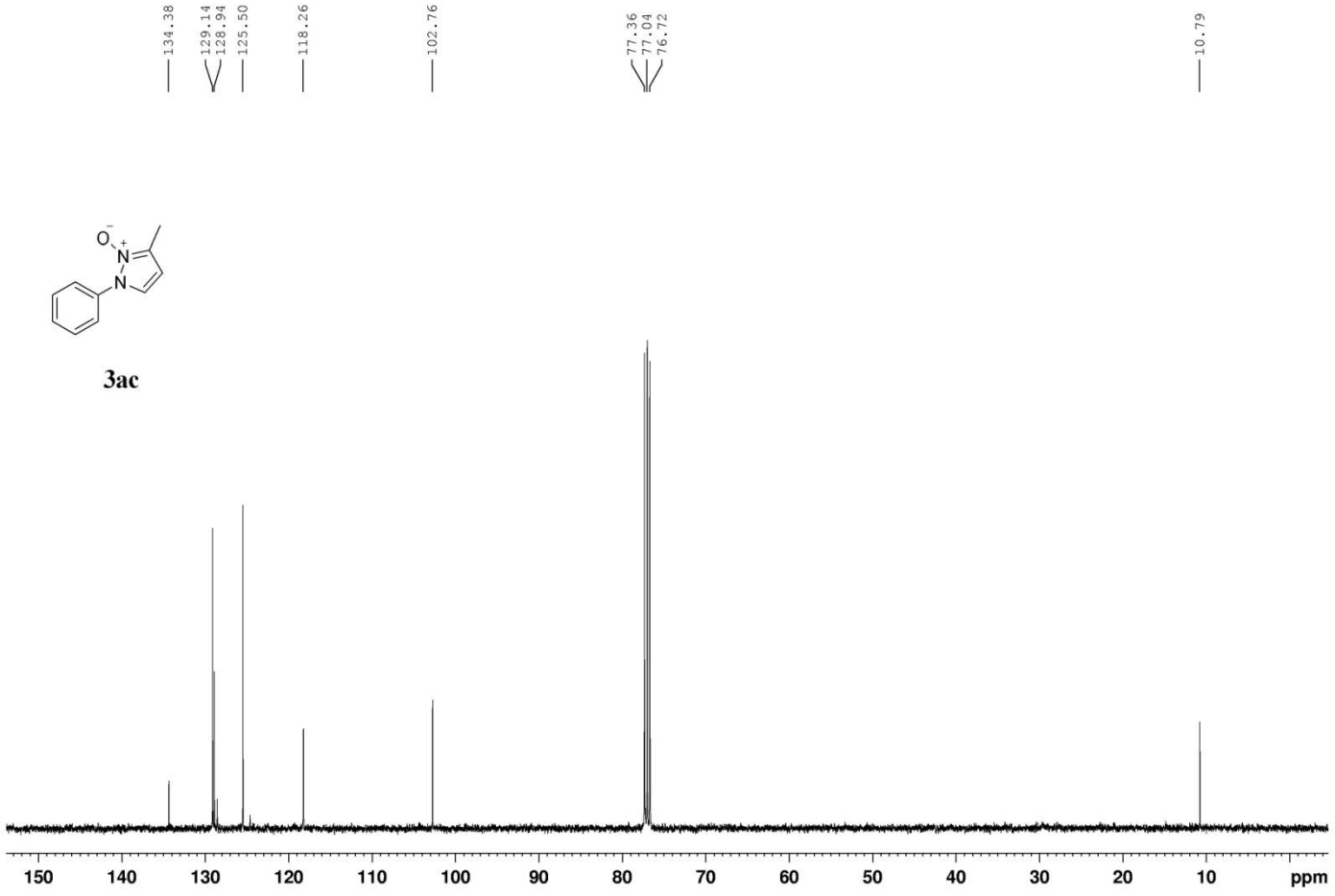

133.91
129.50
129.22
129.15
127.01
126.76
126.63
125.41
124.91
118.99
99.11
77.32
77.00
76.68


S
O
N
N

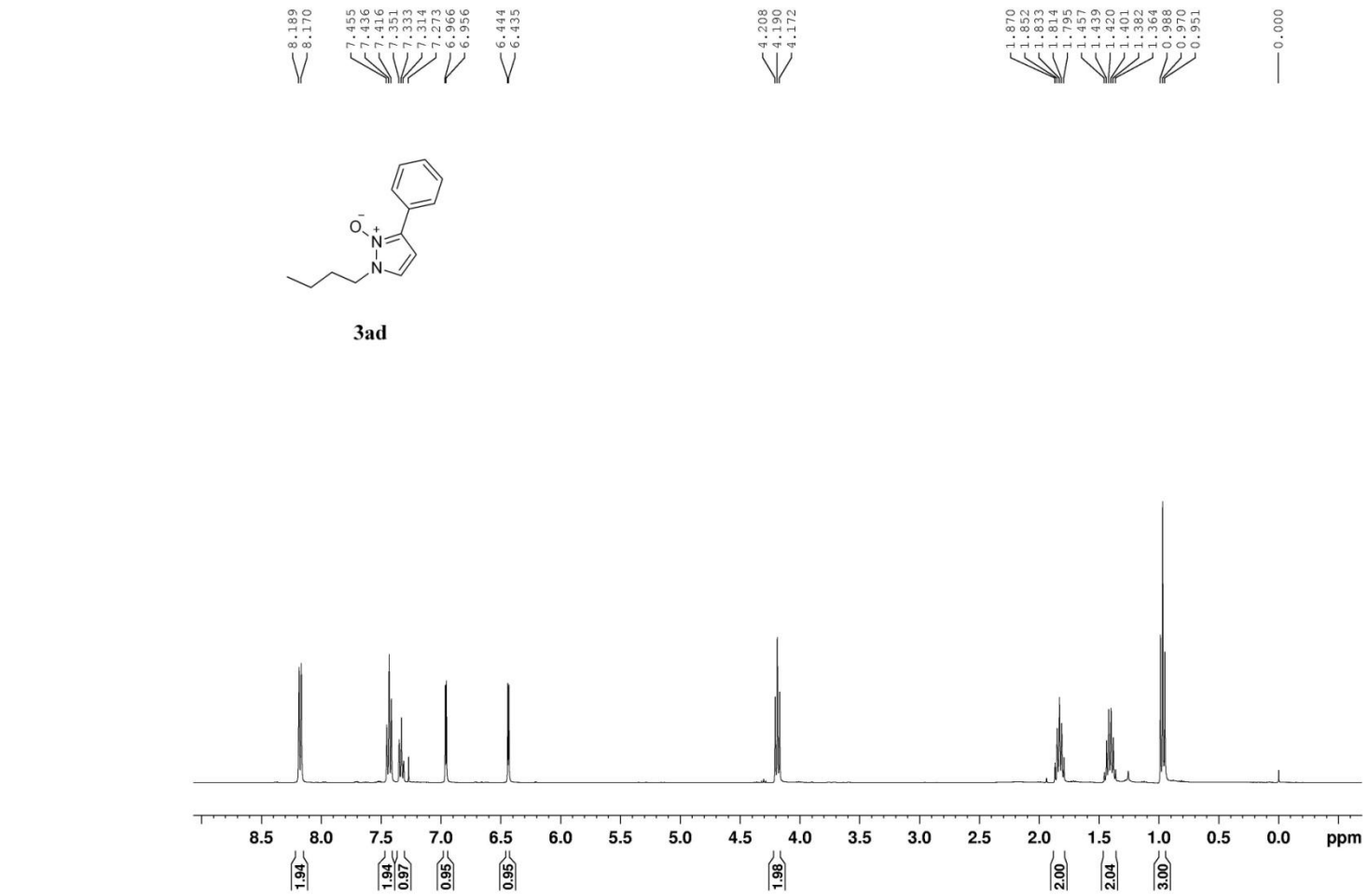
3ab


150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.591
7.587
7.582
7.568
7.560
7.513
7.511
7.506
7.493
7.489
7.473
7.454
7.450
7.447
7.438
7.432
7.414
7.271
7.083
7.074
6.147
6.137
2.325
-0.001
3ac
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
ppm
2.04
3.09
1.00
0.99
3.09


134.38
129.14
128.94
125.50
118.26
102.76
77.36
77.04
76.72
10.79
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

3ac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8.170
7.455
7.436
7.416
7.351
7.333
7.314
7.273
6.966
6.956
6.444
6.435
4.208
4.190
4.172
1.870
1.852
1.833
1.814
1.795
1.457
1.439
1.420
1.401
1.382
1.364
0.988
0.970
0.951
0.000
O
N
N
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
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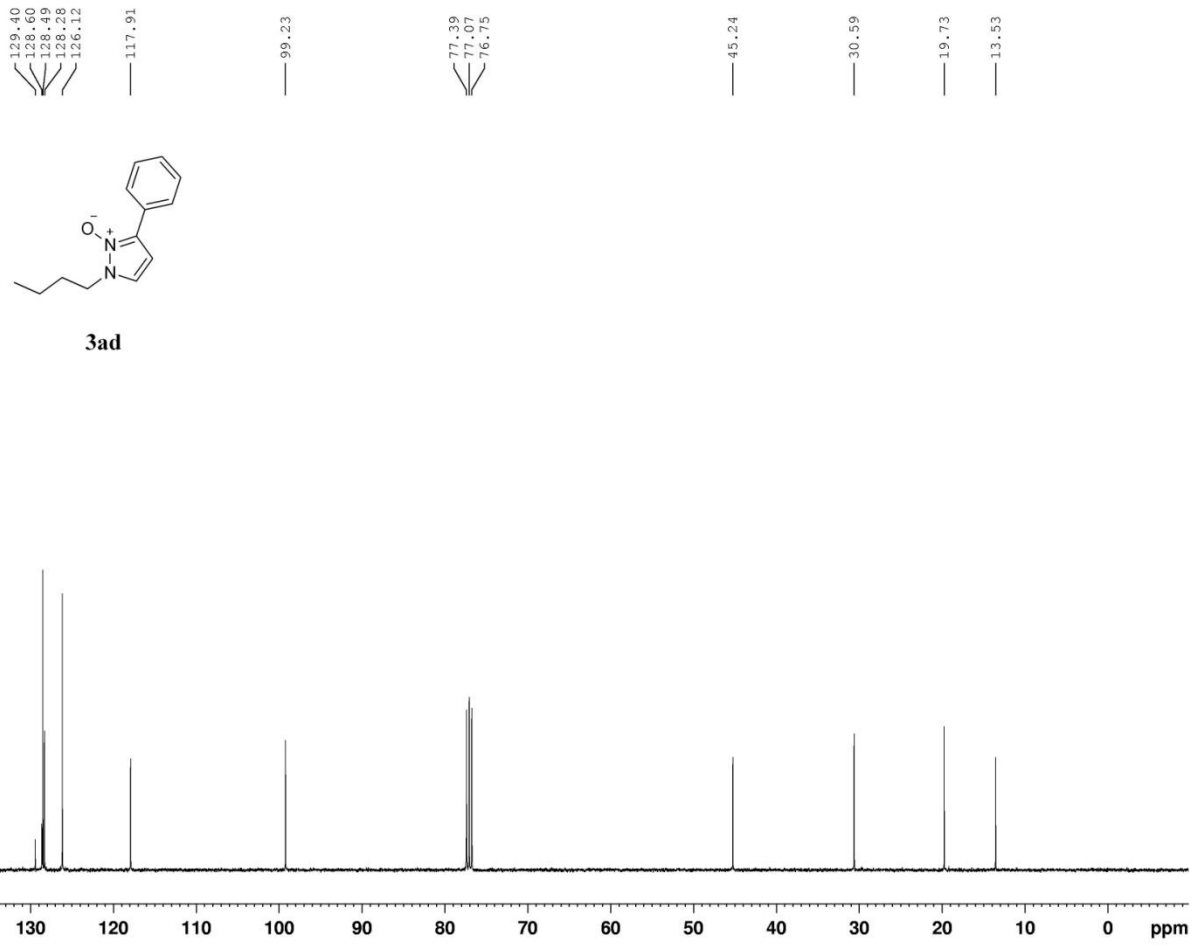
1.94
1.94
0.97
0.95
0.95
1.98
2.00
2.04
3.00

3ad


129.40
128.60
128.49
128.28
126.12
117.91
99.23
77.39
77.07
76.75
45.24
30.59
19.73
13.53
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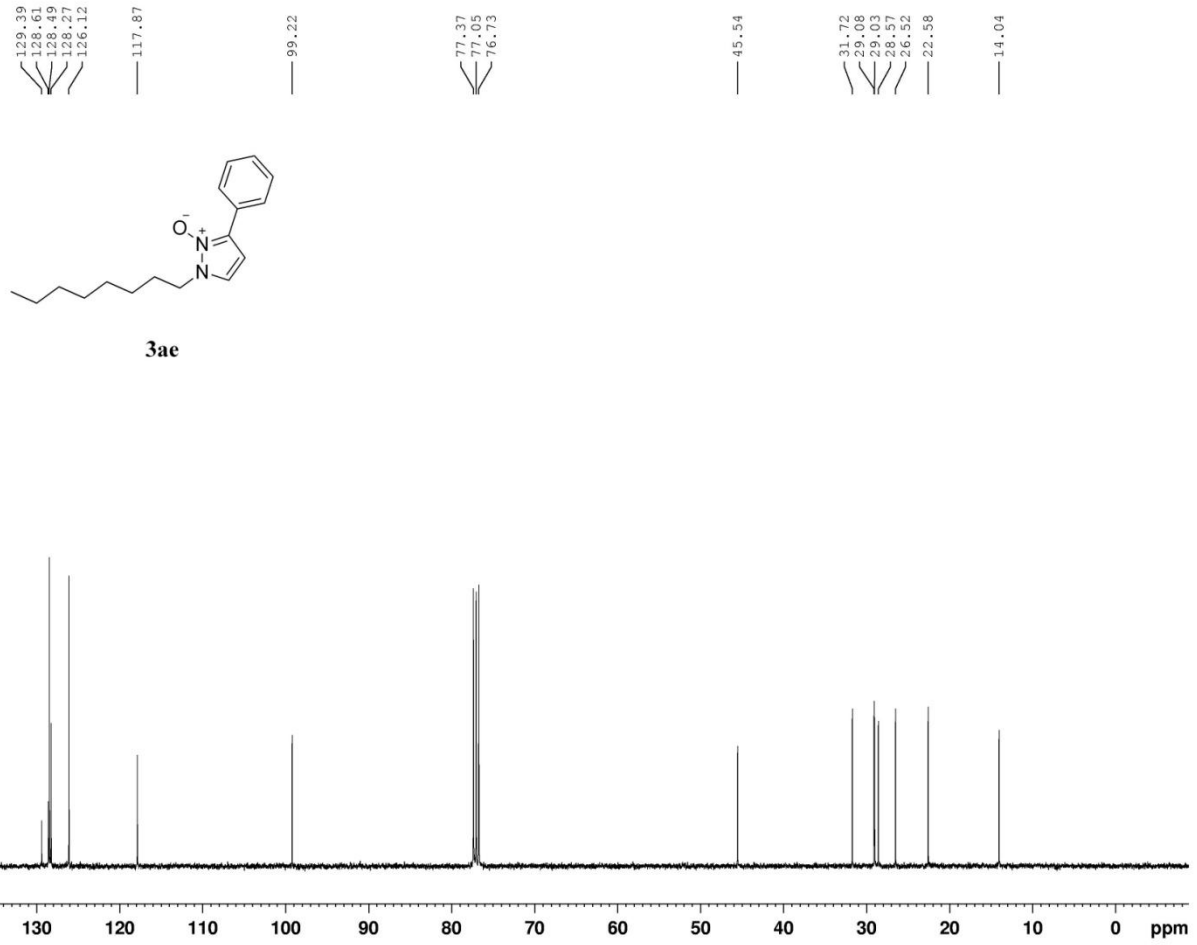
N
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3ad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128.61
128.49
128.27
126.12
117.87
99.22
77.37
77.05
76.73
45.54
31.72
29.08
29.03
28.57
26.52
22.58
14.04
O
N
N
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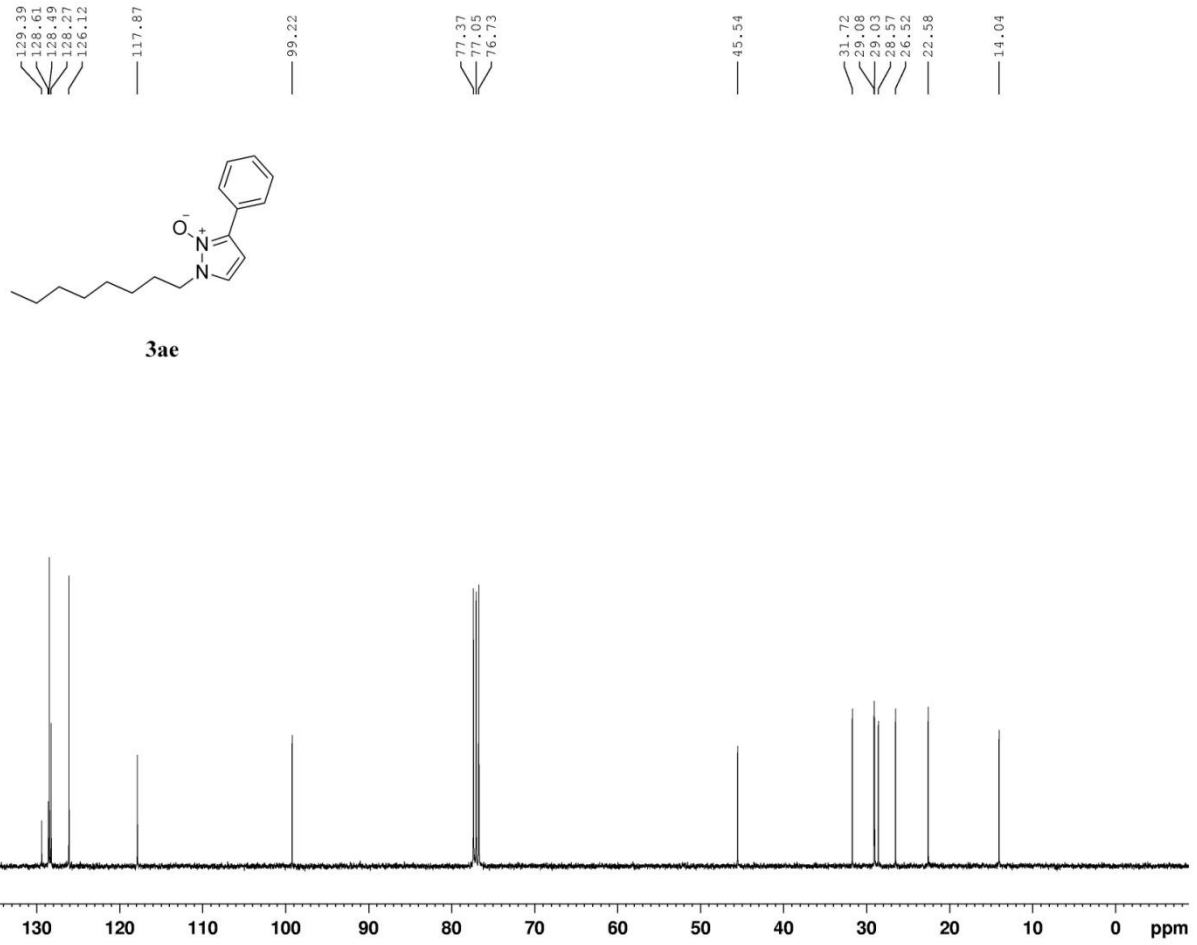
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3ae


129.39
128.61
128.49
128.27
126.12
117.87
99.22
77.37
77.05
76.73
45.54
31.72
29.08
29.03
28.57
26.52
22.58
14.04
O
N
N
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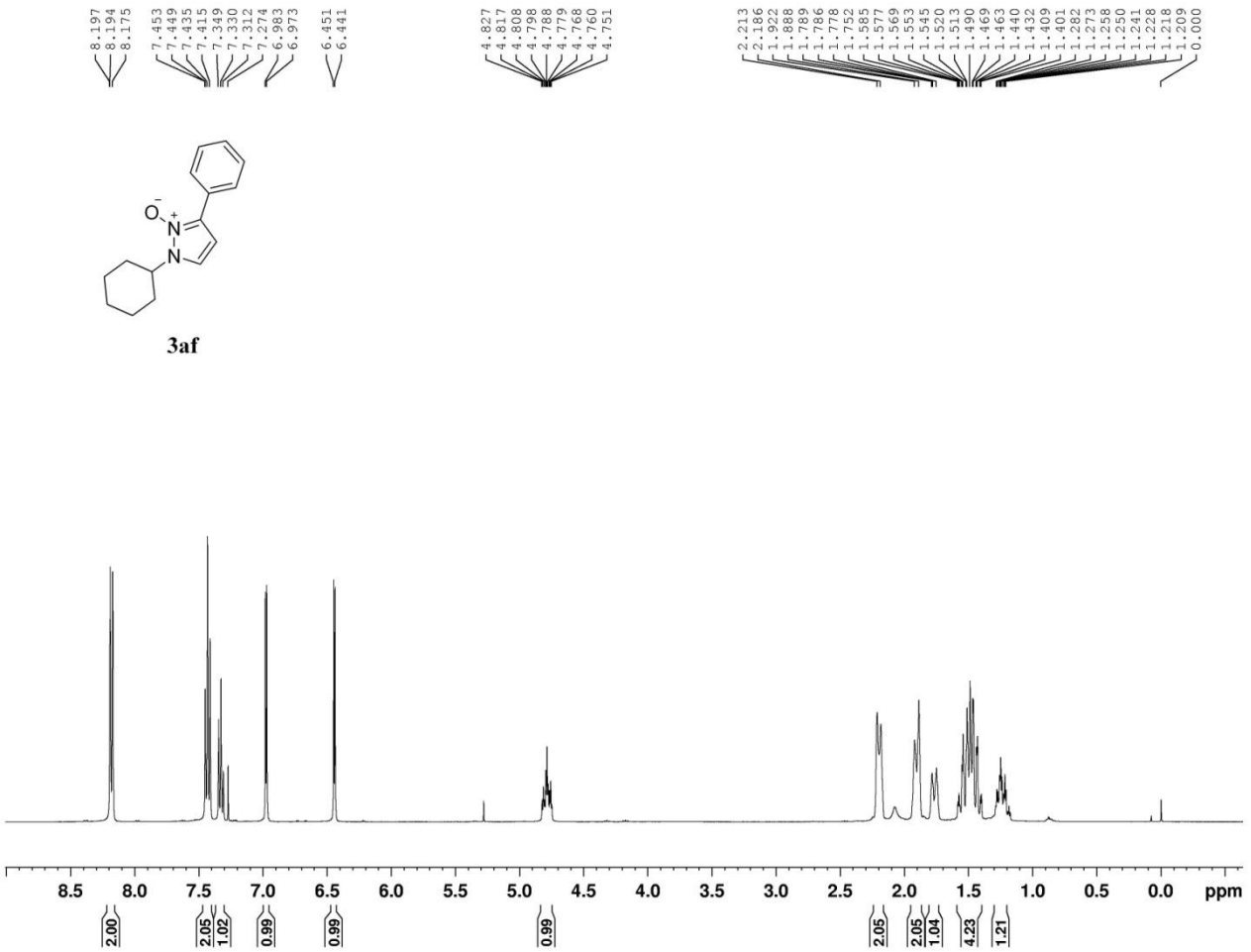
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3ae


8.197
8.194
8.175
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7.449
7.435
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7.349
7.330
7.312
7.274
6.983
6.973
6.451
6.441
4.827
4.817
4.808
4.798
4.788
4.779
4.768
4.760
4.751
2.213
2.186
1.922
1.888
1.789
1.786
1.778
1.752
1.585
1.577
1.569
1.553
1.545
1.520
1.513
1.490
1.469
1.463
1.440
1.432
1.409
1.401
1.282
1.273
1.258
1.250
1.241
1.228
1.218
1.209
0.000
O
N
N
3af
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
ppm
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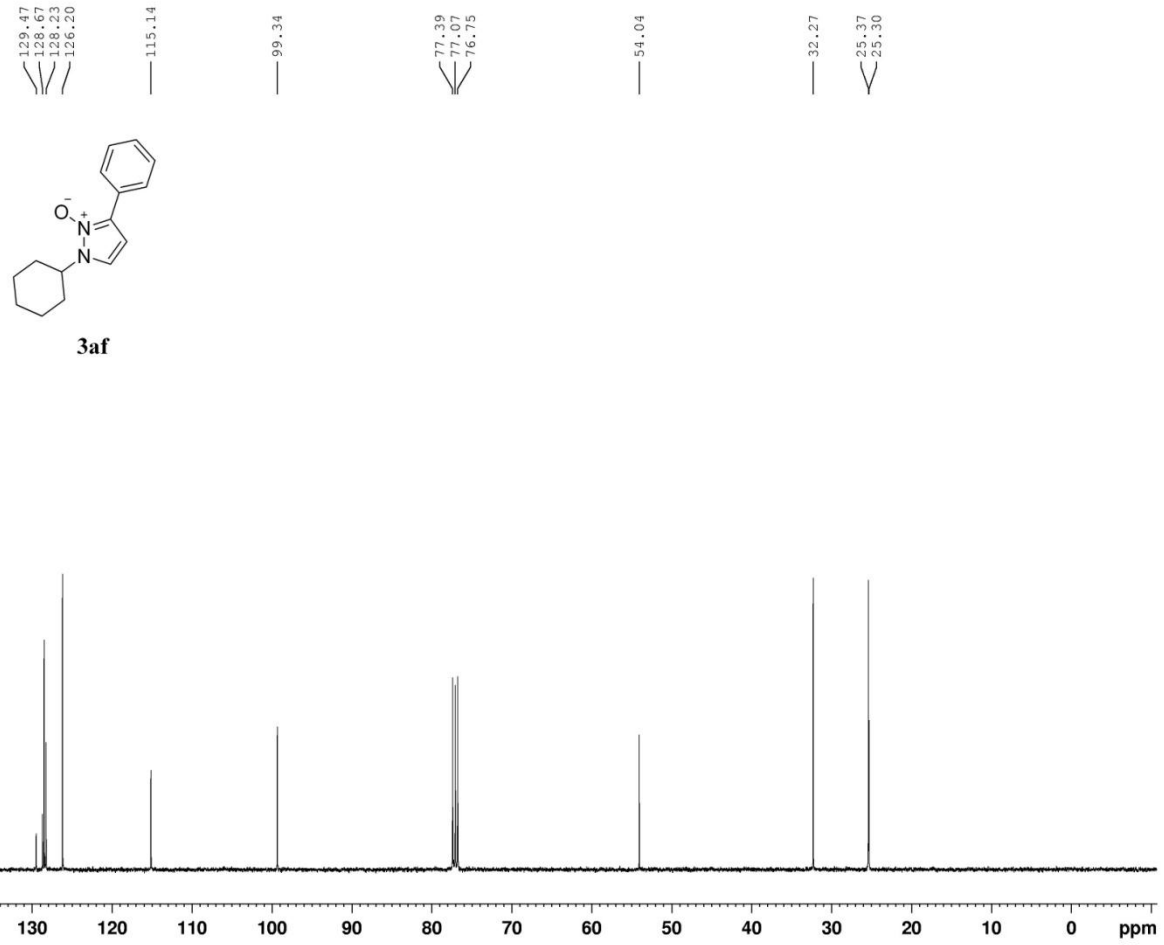
2.05
1.02
0.99
0.99
0.99
2.05
2.05
1.04
4.23
1.21


129.47
128.67
128.23
126.20
115.14
99.34
77.39
77.07
76.75
54.04
32.27
25.37
25.30
O
N
N
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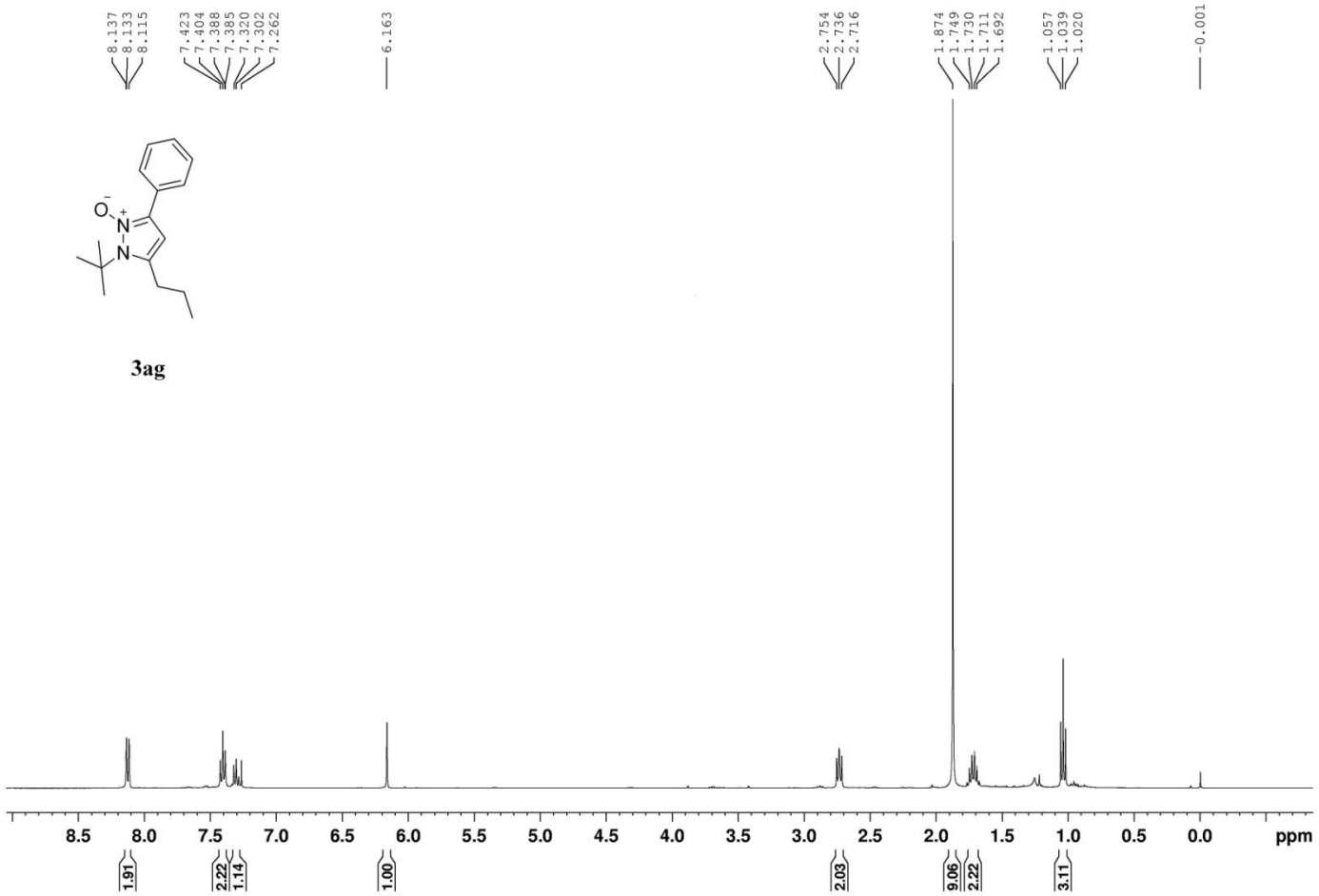
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3af


8.137
8.133
8.115
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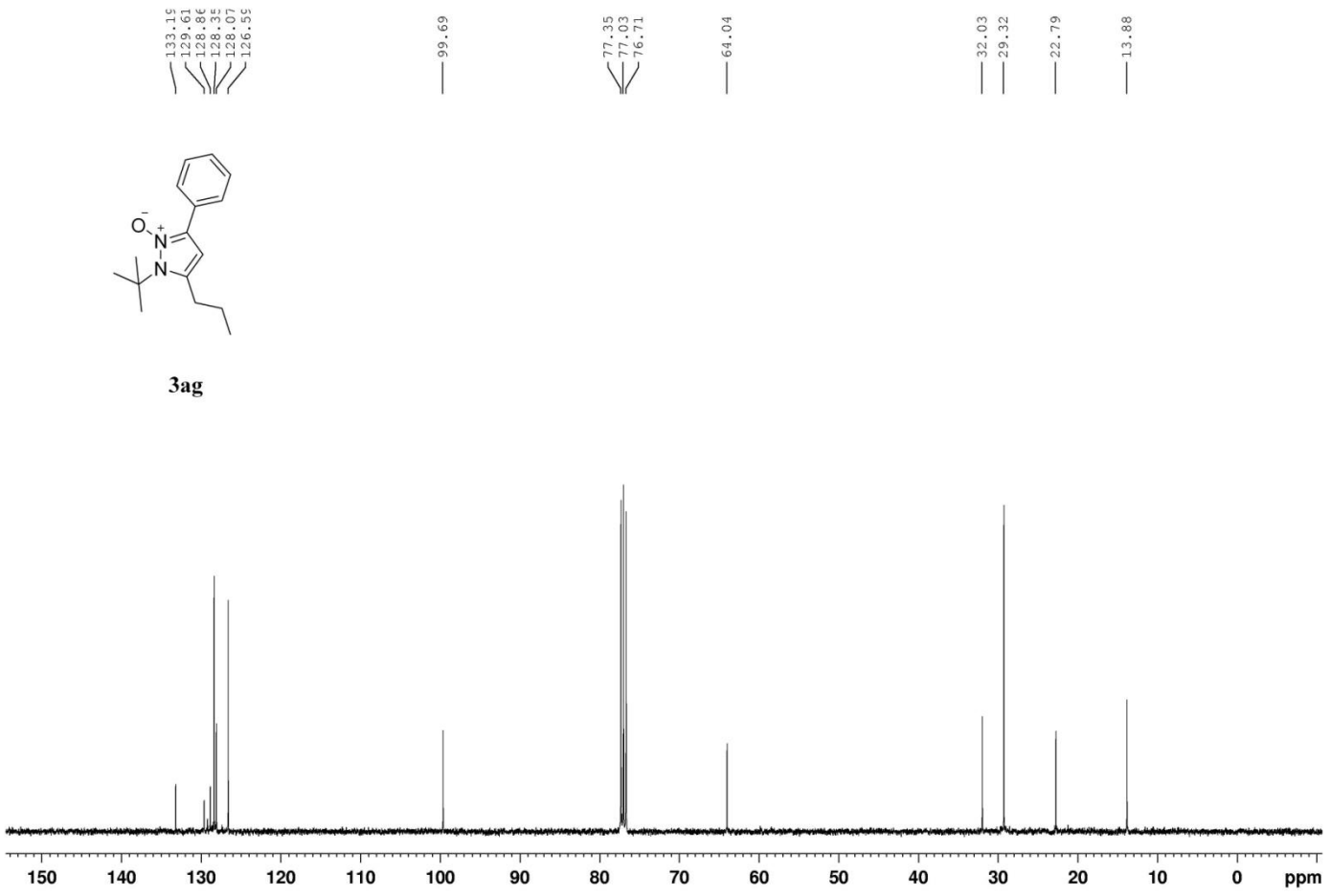
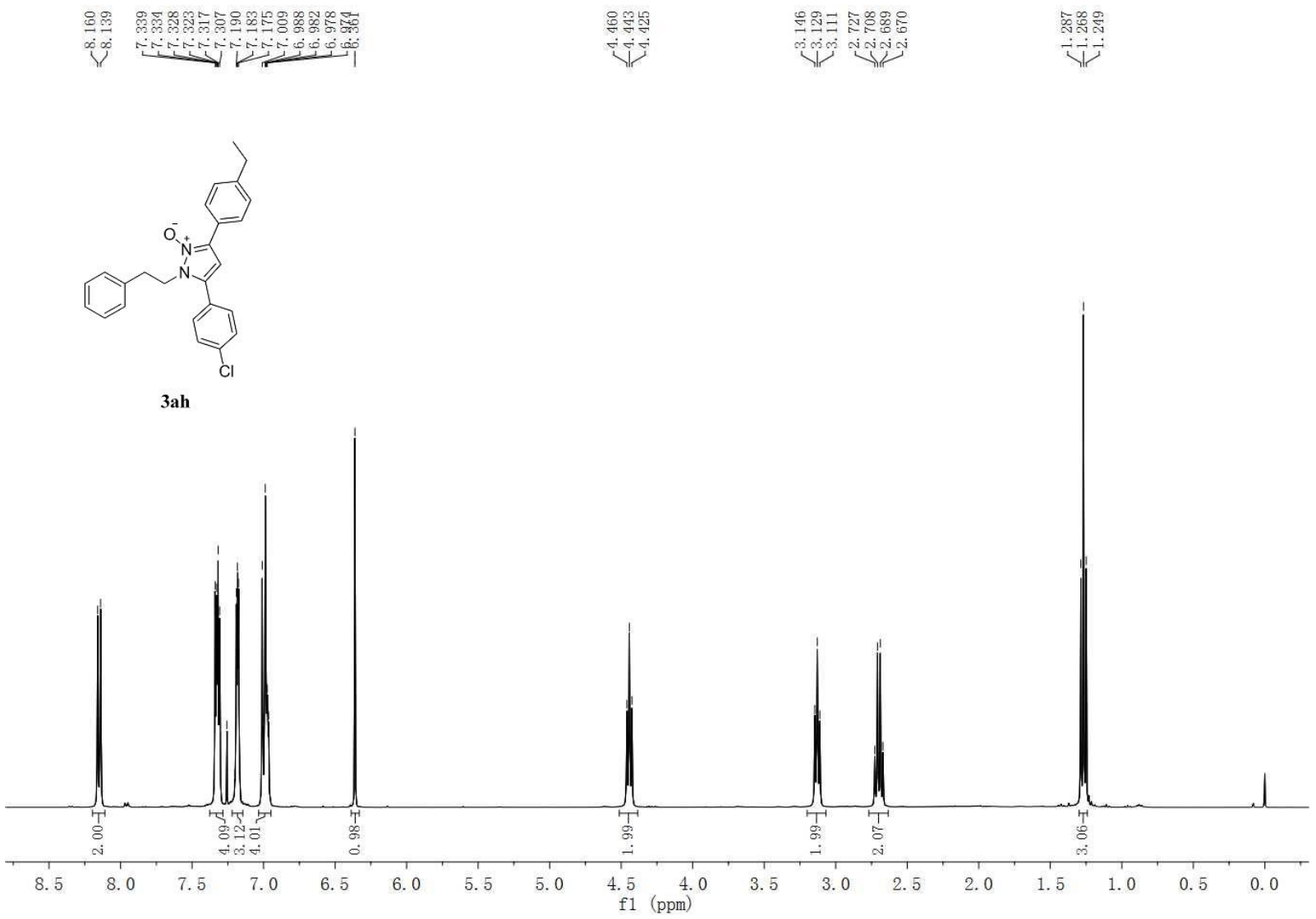
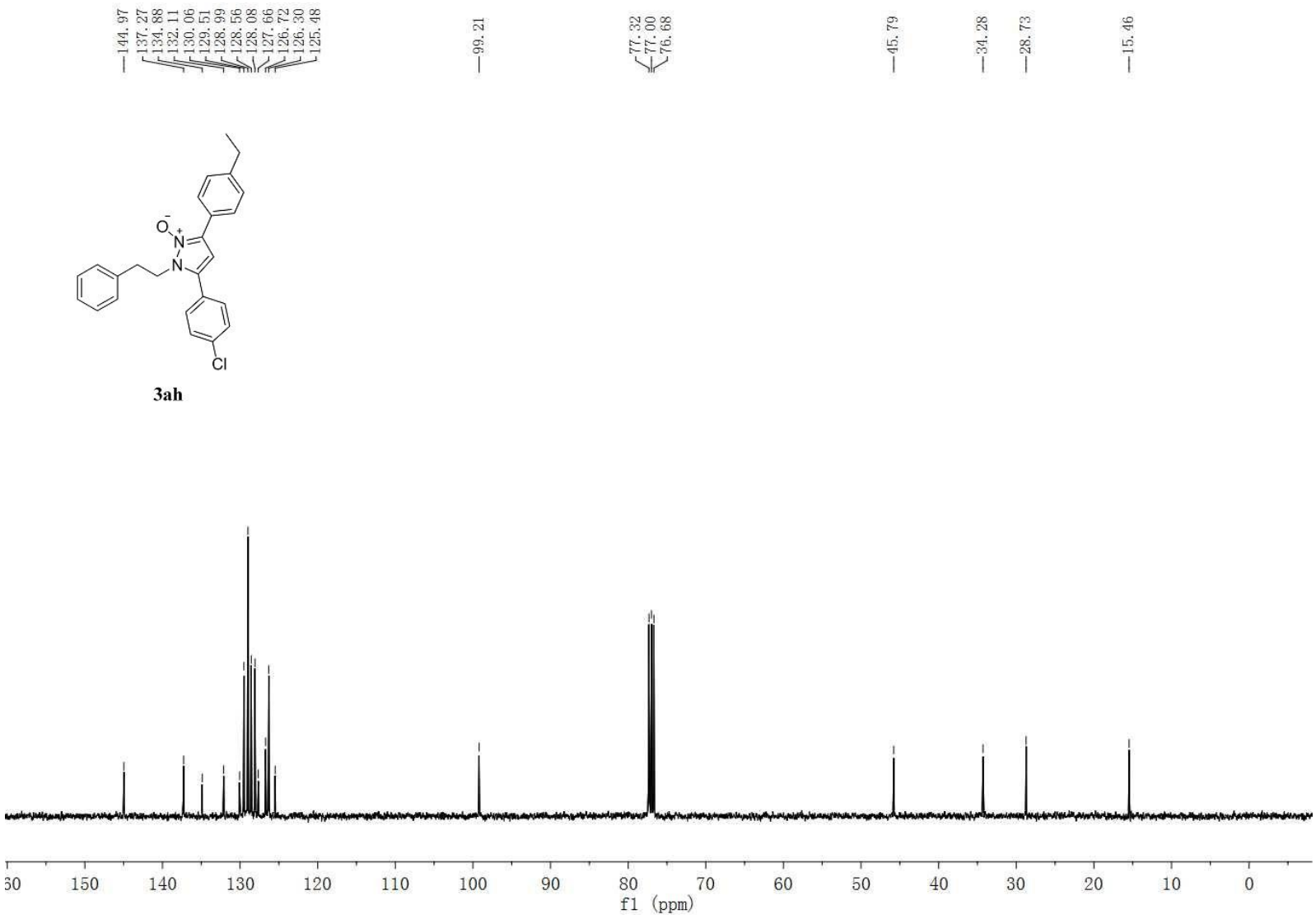
7.404
7.388
7.385
7.320
7.302
7.262
6.163
2.754
2.736
2.716
1.874
1.749
1.730
1.711
1.692
1.057
1.039
1.020
-0.001
3ag
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.91
2.22
1.14
1.00
2.03
9.06
2.22
3.11


133.19
129.61
128.86
128.35
128.07
126.59
99.69
77.35
77.03
76.71
64.04
32.03
29.32
22.79
13.88
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

3ag


8.160
8.139
7.339
7.334
7.328
7.323
7.317
7.307
7.190
7.183
7.175
7.009
6.988
6.982
6.978
6.974
6.961
4.460
4.443
4.425
3.146
3.129
3.111
2.727
2.708
2.689
2.670
1.287
1.268
1.249
O
N
N
Cl
3ah
2.00
4.09
3.12
4.01
0.98
1.99
1.99
2.07
3.06
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
f1 (ppm)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137.27
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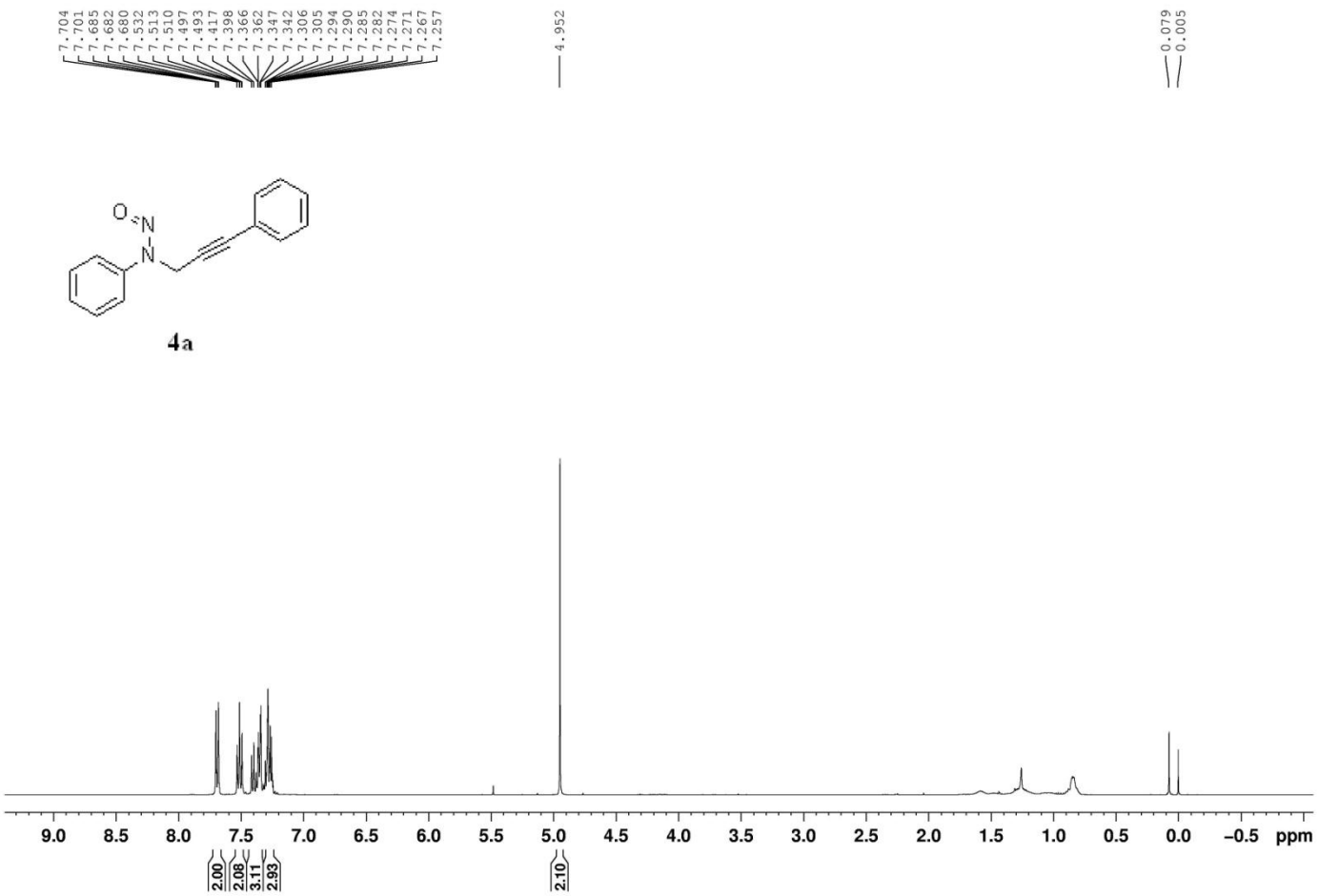
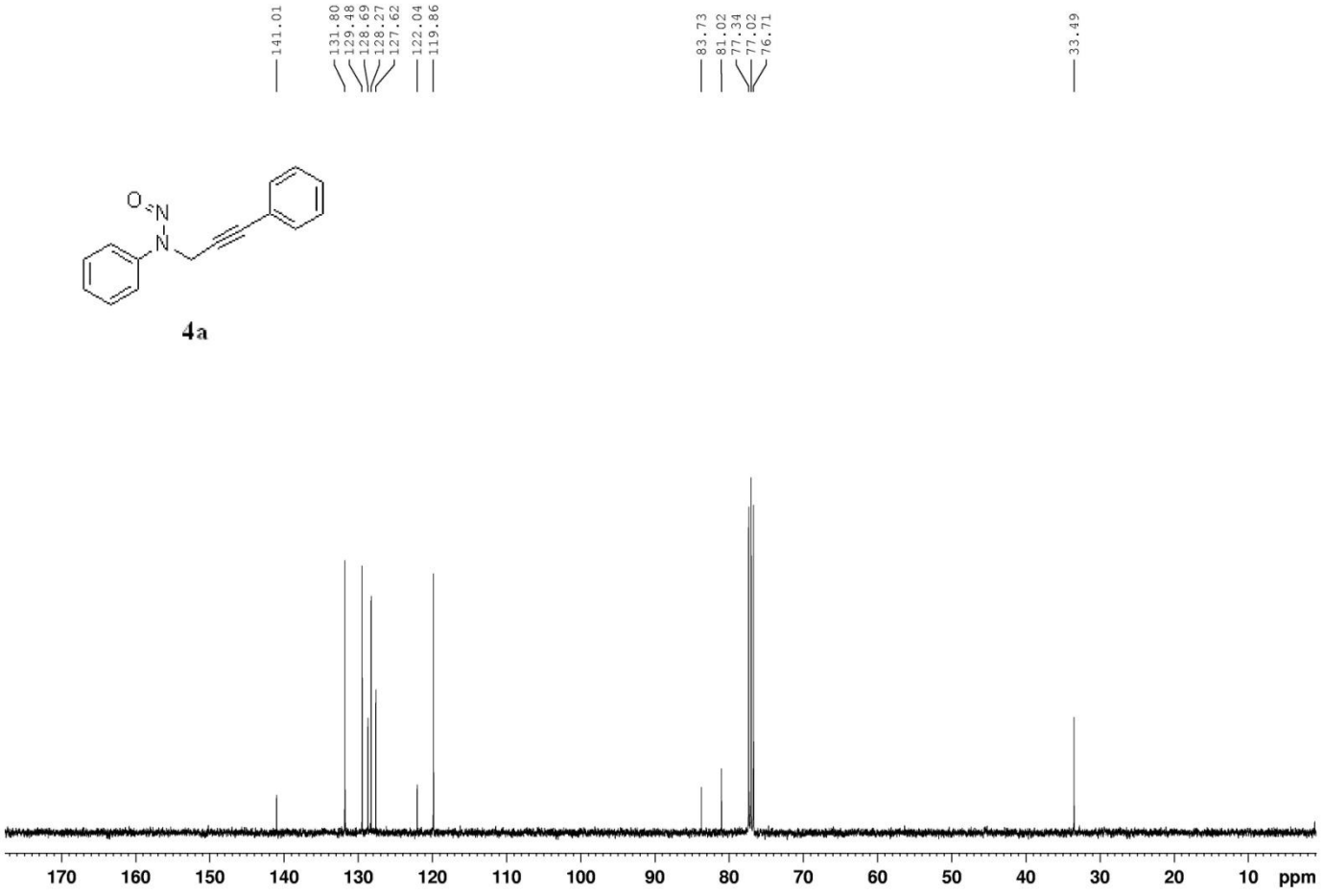
132.11
130.06
129.51
128.99
128.56
128.08
127.66
126.72
126.30
125.48
99.21
77.32
77.00
76.68
45.79
34.28
28.73
15.46
O
N
N
Cl
3ah
f1 (ppm)


7.704
7.701
7.685
7.682
7.680
7.532
7.513
7.510
7.497
7.493
7.417
7.398
7.366
7.362
7.347
7.342
7.306
7.305
7.294
7.290
7.285
7.282
7.274
7.271
7.267
7.257
4.952
0.079
0.005
O
N
N
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
ppm
2.00
2.08
3.11
2.93
2.10

4a


141.01
131.80
129.48
128.69
128.27
127.62
122.04
119.86
83.73
81.02
77.34
77.02
76.71
33.49
O
N
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

4a