Electronic Supplementary Material (ESI) for ChemComm.

Supporting information

Organophotoredox Assisted Cyanation of Bromoarenes via Silyl-Radical-Mediated Bromine Abstraction

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1. General information:

All reactions were carried out in oven-dried glass vials under N_2 atmosphere. All the chemicals were purchased from Aldrich or Spectrochem, and they were used without further purification. All glassware's were washed properly and dried in an oven prior to use. Commercial solvents were purified according to procedures described in Perrin's handbook. TLC (Thin Layer Chromatography) was performed on silica gel coated aluminium plates (MERCK, 60F254), which were visualized by UV fluorescence. Preparative Thin Layer Chromatography was performed on silica gel coated glass plates (silica gel GF-254). ^{1}H and $^{13}C\{^{1}H\}$ NMR spectroscopy were performed on a Bruker FT-NMR spectrometer (400 MHz, 500 MHz, and 600 MHz). The coupling constants (*J*) are reported in hertz (Hz), corresponding multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, br = broad), chemical shift (δ ppm). Infrared spectra were recorded on a spectrometer as neat using a Perkin-Elmer FT-IR Spectrum RX1 spectrometer and reported in wavenumbers (cm^{-1}).

2. Synthesis of TMS_3SiOH reagent:

The reagent TMS_3SiOH was synthesised by the literature procedure[1].To a 20 mL reaction vial equipped with magnetic stir bar, TMS_3SiH (1.8 mL, 6.25 mmol), 2-bromopropane (1.2 mL, 12.5 mmol, 2 equiv) and Et_2O (2mL) were added and capped under air. Then reaction vial was irradiated with 34 W blue LEDs (with fan cooling) for 12 h. After irradiation, the vial was slowly opened to allow for a slow gas evolution and the solution was poured into a round-bottom flask containing 10% aq. NaOH solution (5.5 mL, 1.1 equiv). Excess Et_2O was added to ensure the complete transfer. This mixture was stirred for 24 h under air at rt. Et_2O was added and organic layer was separated. The organic layer was dried over with anhydrous $NaSO_4$ followed by concentration to yield the crude silanol as a clear solution.

3. Synthesis of 4CzIPN (1,2,3,5-tetrakis(carbazol-9-yl)-4,6-dicyanobenzene), 4CzTPN (2,3,5,6-Tetra(carbazol-9-yl)terephthalonitrile), 4DPAIPN (1,3-Dicyano-2,4,5,6-tetrakis(*N,N*-diphenylamino)-benzene):

4CzIPN, 4CzTPN and 4DPAIPN was synthesized according to the literature procedure.[2] NaH (60% in oil, 0.30 g, 7.5 mmol) was added slowly to a stirred solution of carbazole (0.835 g, 5 mmol), or diphenylamine (0.845 g, 5 mmol) in dry THF (25 mL) at room temperature under a nitrogen atmosphere. After 45 min, tetrafluoroisophthalonitrile (0.20 g, 1.00 mmol), Tetrafluoroterephthalonitrile (0.20 g, 1.00 mmol), or tetrafluoroisophthalonitrile (0.20 g, 1.00 mmol) was added respectively. The reaction mixture was stirred at room temperature for 12 h, then water was added to the reaction mixture to quench the excess NaH. The resulting mixture

was then concentrated using rotavapor. The crude product was washed by water and EtOH, which was further purified by recrystalization from hexane/CH_2Cl_2 to yield 0.755 g (96%, 4CzIPN), 0.765 g (97%, 4CzTPN), or 0.715 g (90%, 4DPAIPN) respectively.

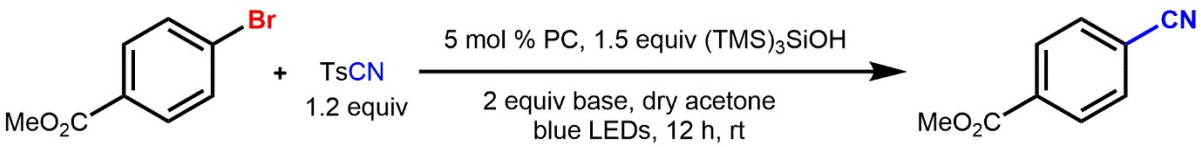
4. Preparation of Aryl Bromides:

The following compounds were prepared according to literature procedures. 3-bromo-indole,[3] 3-Bromo-9-ethyl-9*H*-carbazole, [4] 2-(4-bromophenyl)-1-methyl-1*H*-benzo[*d*]imidazole, [5] 2-(4-bromophenyl)benzo[*d*]thiazole,[6] 2-(4-bromophenyl)thiophene and 2-(4-bromophenyl)furan,[7] 2-(4-bromophenyl)pyridine,[8] 3-bromo-10-ethyl-10*H*-phenothiazine[9].

5. Optimization of reaction conditions:

5a. Base screening

To an oven-dried 15 mL vial equipped with magnatic stir bar was added methyl 4-bromobenzoate (107.5 mg, 0.50 mmol). After that, corresponding base (1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv) and 4CzIPN (20 mg, 5 mol%) were added followed by dry Acetone (6.0 mL). The vials were capped with septum and degassed by sparging with N_2 for 15 min. Then $(TMS)_3SiOH$ (225 μL, 0.75 mmol, 1.5 equiv) was added. Finally, the reaction vial was equipped with N_2 a balloon and was parafilmed to protect from air during the course of the reaction. The yellowish reaction mixture was irradiated with two 15W blue LEDs from 7 cm away with fan cooling for 12 h. Once the reaction is complete, the reaction mixture was quenched by exposure to air. The final reaction mixture was treated with Ammonium fluoride in EtOAc (30 mL) for 45 minutes then filtered over celite. The organic solution was washed by aqueous Na_2CO_3, water, brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduce pressure to yield the crude product. The crude product was purified via silica gel column chromatography (EtOAc/hexane) to yield the pure product.



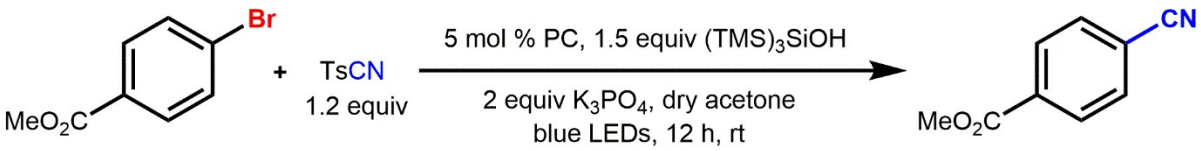
entry	base	yield
1	Na_2CO_3	46%
2	K_2CO_3	53%
3	Cs_2CO_3	37%
4	K_3PO_4	71%
5	Na_2HPO_4	62%
6	NaOAc	32%
7	KOAc	35%
5	DBU	6%
6	2,6-lutidine	13%

Figure S1. Base screening for the cyanation of aryl bromides; yield was reported from isolated product.

5b. Control experiments

To each oven-dried 15 mL vial equipped with magnatic stir bar was added methyl 4-bromobenzoate (107.5 mg, 0.50 mmol). When not omitted, K_3PO_4 (214 mg, 1.0 mmol, 2 equiv) and 4CzIPN (20 mg, 5 mol%) followed by TsCN (109 mg, 0.60 mmol, 1.2 equiv) and dry Acetone (6.0 mL) were added. The vials were capped with septum and degassed by sparging with N_2 for 15 min. When not omitted, $(TMS)_3SiOH$ or $(TMS)_3SiH$ (0.75 mmol, 1.5 equiv) was added. Finally, the reaction vial was equipped with N_2 a balloon and was parafilmed to protect from air during the course of the reaction. The yellowish reaction mixture was irradiated with two 15W blue LEDs from 7 cm away with fan cooling for 12 h. The no-light vial was placed in front of the blue LEDs after being wrapped in aluminum foil. Once the reaction is complete, the reaction mixture was quenched by exposure to air. The final reaction mixture was treated with Ammonium fluoride in EtOAc (30 mL) for 45 minutes then filtered over

celite. The organic solution was washed by aqueous Na_2CO_3, water, brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduce pressure to yield the crude product. The crude product was purified via silica gel column chromatography (EtOAc/hexane) to yield the pure product.



entry	deviation	yield
1	none	78%
2	TMS_3SiH instead of silanol	43%
3	no TMS_3SiOH	0%
4	no photocatalyst	0%
5	no light	0%
6	no base	32%

Figure S2. Control experiments for the cyanation of aryl bromides; yield was reported from isolated product.

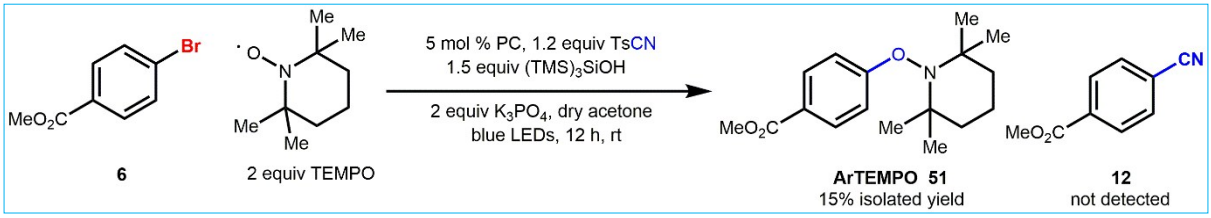
6. General procedure for the cyanation of aryl bromides:

To an oven-dried 15 mL vial equipped with magnatic stir bar was added corresponding aryl bromide (0.5 mmol). After that, K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv) and 4CzIPN (20 mg, 5 mol%) were added followed by dry Acetone (6.0 mL). The vials were capped with septum and degassed by sparging with N_2 for 15 min. Then $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) was added. Finally, the reaction vial was equipped with N_2 a balloon and was parafilmed to protect from air during the course of the reaction. The yellowish reaction mixture was irradiated with two 15W blue LED from 7 cm away with fan cooling for 12 h. Once the reaction is complete, the reaction mixture was quenched by exposure to air. The final reaction mixture was treated with Ammonium fluoride in EtOAc (30 mL) for 45 minutes then filtered over celite. The organic solution was washed by aqueous Na_2CO_3, water, brine, dried over anhydrous Na_2SO_4, filtered, and concentrated

under reduce pressure to yield the crude product. The crude product was purified via silica gel column chromatography (EtOAc/hexane) to yield the pure product. Visualization was performed using Phosphomolybdic acid (PMA) stain.

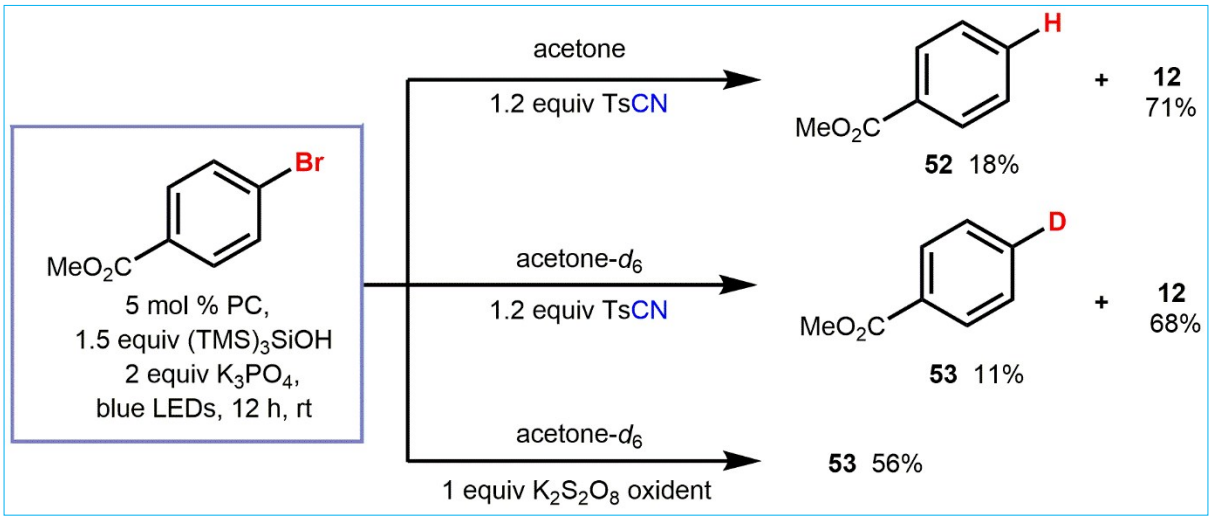
7. Mechanistic Studies:

7.1 TEMPO trapping experiments



General procedure: To an oven-dried 15 mL vial equipped with magnatic stir bar was charged with methyl 4-bromobenzoate (107.5 mg, 0.50 mmol). After that, K_3PO_4 (212 mg, 1.00 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 4CzIPN (20 mg, 5 mol%) and TEMPO (156.3 mg, 1.00 mmol, 2 equiv) were added followed by dry Acetone (5.0 mL). The vials were capped with septum and degassed by sparging with N_2 for 20 min. Then $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) was added. Finally, the reaction vial was equipped with N_2 balloon and was parafilmed to protect from air during the course of the reaction. The reaction mixture was irradiated with two 15W blue LED from 7 cm away with fan cooling for 12 h. The reaction mixture was quenched by exposure to air. ArTEMPO **51** product yield was determined by isolation.

7.2 Deuteration incorporation experiment

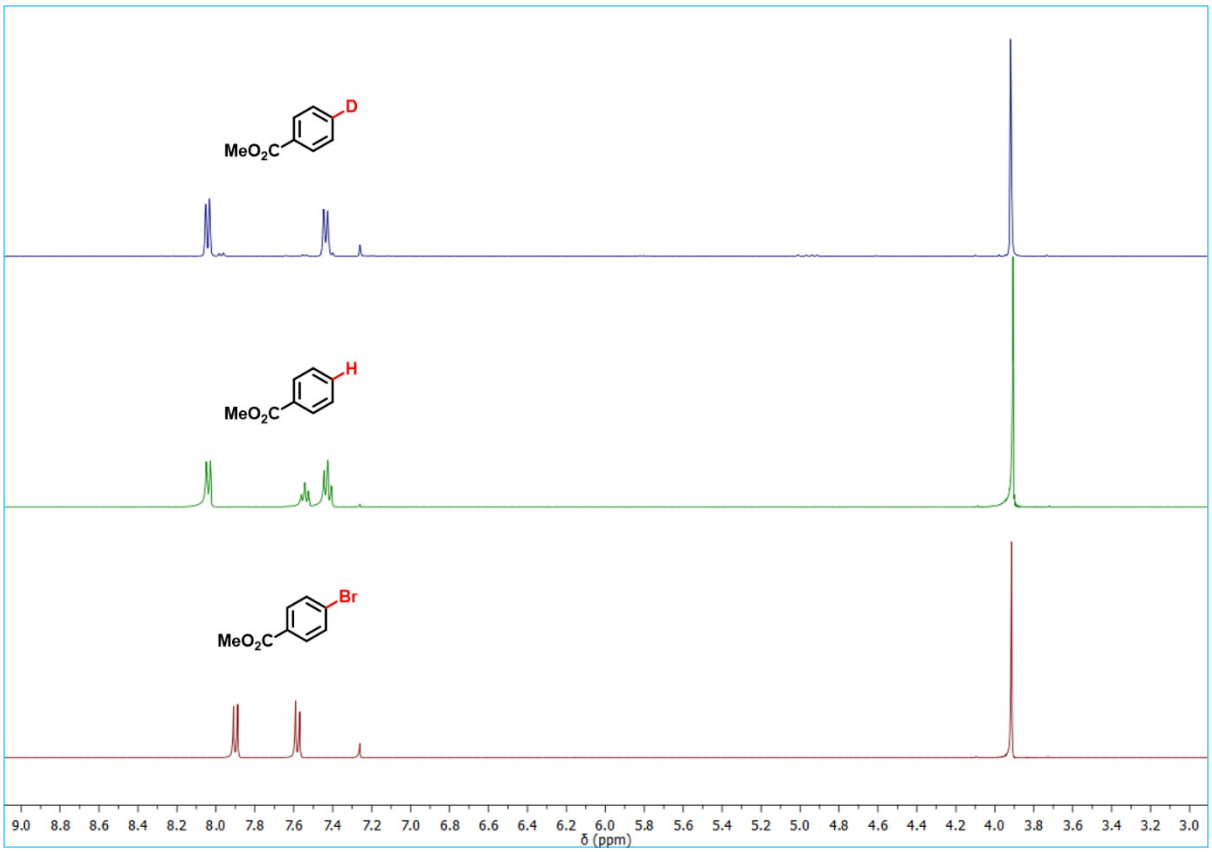


General procedure: To an oven-dried 15 mL vial equipped with magnatic stir bar was charged with methyl 4-bromobenzoate (107.5 mg, 0.50 mmol). After that, K_3PO_4 (212 mg, 1.00 mmol,

2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 4CzIPN (20 mg, 5 mol%) and were added followed by dry Acetone (5.0 mL). The vials were capped with septum and degassed by sparging with N_2 for 20 min. Then $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) was added. Finally, the reaction vial was equipped with N_2 a balloon and was parafilmed to protect from air during the course of the reaction. The reaction mixture was irradiated with two 15W blue LED from 7 cm away with fan cooling for 12 h. The reaction mixture was quenched by exposure to air. Yield of the desired product **12** was 71% along with 18% dehalogenation product **52** observed.

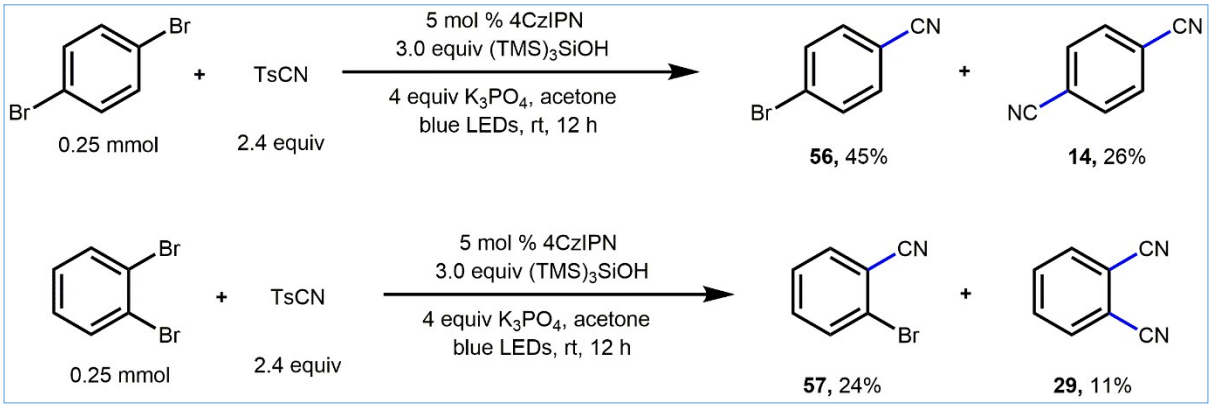
When the reaction was carried out in acetone-d_6 solvent with same condition, 11% deuterium incorporated product (**53**) was observed.

In addition, the standard reaction was carried out using $K_2S_2O_8$ as an oxidant instead of TsCN in acetone-d_6 solvent resulted in high incorporation of deuterium to the arene (56% yield of **53**).



8. Cyanation of dibromoarenes:

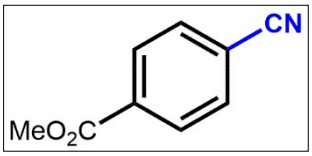
General procedure: To an oven-dried 15 mL vial equipped with magnatic stir bar was charged with dibromobenzene (118 mg, 0.5 mmol). After that, K_3PO_4 (107 mg, 1.0 mmol, 2 equiv), TsCN (218 mg, 1.2 mmol, 2.4 equiv) and 4CzIPN (20 mg, 5 mol%) were added followed by dry Acetone (6.0 mL). The vials were capped with septum and degassed by sparging with N_2 for 15 min. Then $(TMS)_3SiOH$ (450 µL, 1.5 mmol, 3 equiv) was added. Finally, the reaction vial was equipped with N_2 a balloon and was parafilmed to protect from air during the course of the reaction. The reaction mixture was irradiated with two 15W blue LED from 7 cm away with fan cooling for 12 h. Once the reaction is complete, the reaction mixture was quenched by exposure to air. The final reaction mixture was treated with Ammonium fluoride in EtOAc (30 mL) for 45 minutes then filtered over celite. The organic solution was washed by aqueous Na_2CO_3, water, brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduce pressure to yield the crude product. The crude product was purified via silica gel column chromatography (EtOAc/hexane) to yield the pure product.



For 1,4-dibromobenzene substrate mono-cyantion product **56** yield 45% and di-cyanation product **14** yield 26% were observed. Whereas 1,2-dibromobenzene substrate mono-cyantion product **57** yield 24% and di-cyanation product **29** yield 11% were observed.

9. Synthesis and characterization of products:

Methyl 4-cyanobenzoate (12)

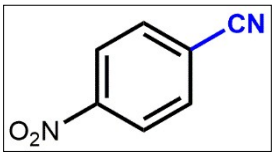


Compound **12** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), methyl 4-bromobenzoate (107.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography

(100% Hexane to 90:10 Hexane/EtOAc) and obtained as a white solid (57.2 mg, 0.355 mmol, 71%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.4 Hz, 2H), 7.72 (d, *J* = 8.4 Hz, 2H), 3.93 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.5, 134.0, 132.3, 130.2, 118.0, 116.5, 52.8. **IR (film)** ν_{max} 2230, 1723, 1439, 1274, 1109, 766 cm^{-1}. Spectral data matched with the literature report.[10]

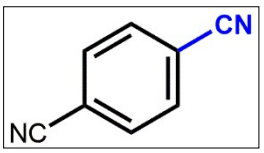
4-Nitrobenzonitrile (13)



Compound **13** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 1-bromo-4-nitrobenzene (101 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a white solid (46.6 mg, 0.315 mmol, 63%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.2 Hz, 2H), 7.89 (d, *J* = 7.2 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 150.2, 133.6, 124.4, 118.5, 116.9. **IR (film)** ν_{max} 2232, 1602, 1520, 1350, 856 cm^{-1}. Spectral data matched with the literature report.[11]

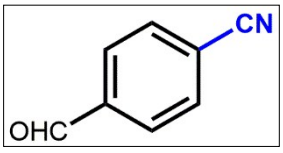
Terephthalonitrile (14)



Compound **14** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 4-bromobenzonitrile (91 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a white solid (42.3 mg, 0.33 mmol, 66%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 4H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 132.9, 117.1, 116.8. **IR (film)** ν_{max} 2232, 1481, 1208, 776 cm^{-1}. Spectral data matched with the literature report.[11]

4-Formylbenzonitrile (15)

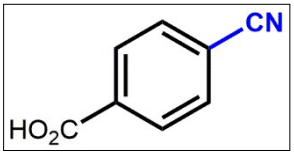


Compound **15** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 4-bromobenzaldehyde (92.5

mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a white solid (47.2 mg, 0.360 mmol, 72%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.09 (s, 1H), 7.99 (d, J = 8.2 Hz, 2H), 7.85 (d, J = 8.2 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.7, 138.6, 132.8, 129.8, 117.7, 117.4. **IR (film)** ν_{max} 2851, 2749, 2228, 1702, 1607, 1382, 1202, 830, 736 cm^{-1}. Spectral data matched with the literature report.[12]

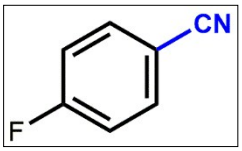
4-Cyanobenzoic acid (16)



Compound **16** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 4-bromobenzoic acid (100.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 60:40 Hexane/EtOAc) and obtained as a white solid (52.2 mg, 0.355 mmol, 71%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, J = 8.3 Hz, 2H), 7.79 (d, J = 8.3 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 169.1, 133.1, 132.5, 130.8, 117.9, 117.5. **IR (film)** ν_{max} 2229, 1683, 1282, 863, 763 cm^{-1}. Spectral data matched with the literature report.[10]

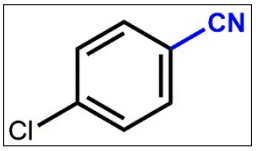
4-Fluorobenzonitrile (17)



Compound **17** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 1-Bromo-4-fluorobenzene (55 µL, 87.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 95:5 Hexane/EtOAc) and obtained as a colorless liquid (45.4 mg, 0.375 mmol, 75%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.63 (m, 2H), 7.18 (t, J = 8.5 Hz, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 165.2 (d, $^1J_{C\text{-}F}$ = 249 Hz), 134.8 (d, $^3J_{C\text{-}F}$ = 10 Hz), 118.2, 117.0 (d, $^2J_{C\text{-}F}$ = 23 Hz), 108.7 (d, $^4J_{C\text{-}F}$ = 3 Hz). **IR (film)** ν_{max} 2232, 1607, 1506, 1239, 828 cm^{-1}. Spectral data matched with the literature report.[11]

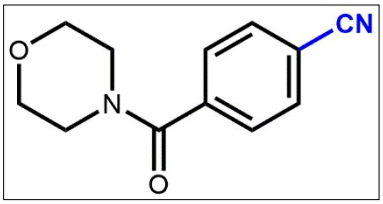
4-Chlorobenzonitrile (18)



Compound **18** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 1-Bromo-4-chlorobenzene (95.7 mg, 0.25 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 95:5 Hexane/EtOAc) and obtained as a white solid (46.8 mg, 0.34 mmol, 68%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.5 Hz, 2H), 7.46 (d, *J* = 8.5 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 139.7, 133.5, 129.8, 118.0, 110.9. **IR (film)** ν_{max} 2226, 1592, 1484, 1089, 828 cm^{-1}. Spectral data matched with the literature report.[10]

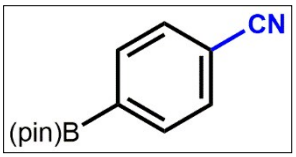
4-(Morpholine-4-carbonyl)benzonitrile (19)



Compound **19** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), (4-bromophenyl)(morpholino)methanone (135 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 80:20 Hexane/EtOAc) and obtained as a white solid (76.6 mg, 0.355 mmol, 71%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.9 Hz, 2H), 7.49 (d, *J* = 7.9 Hz, 2H), 3.95 – 3.21 (m, 8H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 168.3, 139.6, 132.5, 127.8, 118.0, 113.7, 66.76, 48.0, 42.6. **IR (film)** ν_{max} 2231, 1632, 1432, 1272, 1112, 1008, 836 cm^{-1}. Spectral data matched with the literature report.[13]

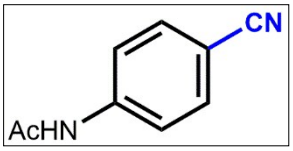
4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)benzonitrile (20)



Compound **20** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 2-(4-bromophenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (148.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 95:5 Hexane/EtOAc) and obtained as a white solid (74.4 mg, 0.325 mmol, 65%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, J = 7.9 Hz, 2H), 7.62 (d, J = 7.9 Hz, 2H), 1.34 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 135.2, 131.2, 118.9, 114.7, 84.6, 24.9. **IR (film)** ν_{max} 2228, 1395, 1352, 1272, 1138, 1090 cm^{-1}. Spectral data matched with the literature report.[12]

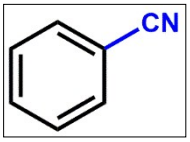
_N_-(4-Cyanophenyl)acetamide (21)



Compound **21** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), N-(4-bromophenyl)acetamide (106.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 70:30 Hexane/EtOAc) and obtained as a white solid (45.6 mg, 0.285 mmol, 57%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.36 (s, 1H), 7.82-7.66 (m, 4H), 2.09 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 169.3, 143.6, 133.3, 119.2, 119.0, 104.8, 24.3. **IR (film)** ν_{max} 2217, 1674, 1595, 1538, 1322, 833 cm^{-1}. Spectral data matched with the literature report.[10]

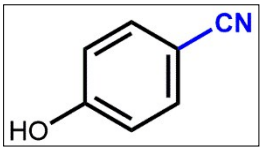
Benzonitrile (22)



Compound **22** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), bromobenzene (52.5 µL, 78.5 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane) and obtained as a colorless liquid (37.6 mg, 0.365 mmol, 73%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 7.7 Hz, 2H), 7.60 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.7 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 132.8, 132.2, 129.2, 118.9, 112.5. **IR (film)** ν_{max} 2229, 1488, 1449 cm^{-1}. Spectral data matched with the literature report.[11]

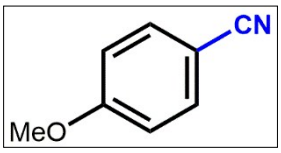
4-Hydroxybenzonitrile (23)



Compound **23** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 4-Bromophenol (86.8 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 85:15 Hexane/EtOAc) and obtained as a brown solid (33.9 mg, 0.285 mmol, 57%).

^{1}H NMR (400 MHz $CDCl_3$) δ 7.55 (d, *J* = 8.7 Hz, 2H), 6.92 (d, *J* = 8.7 Hz, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.9, 134.4, 119.3, 116.5, 103.7. **IR (film)** ν_{max} 3262, 2230, 1587, 1281, 838 cm^{-1}. Spectral data matched with the literature report.[11]

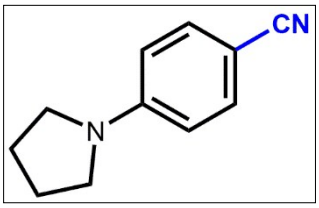
4-Methoxybenzonitrile (24)



Compound **24** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 1-bromo-4-methoxybenzene (62.6 µL, 93.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 95:5 Hexane/EtOAc) and obtained as a white solid (57.2 mg, 0.43 mmol, 86%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 9.0 Hz, 2H), 6.92 (d, *J* = 9.0 Hz, 2H), 3.83 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.9, 133.9, 119.2, 114.8, 103.9, 55.5. **IR (film)** ν_{max} 2215, 1606, 1510, 1455, 1260, 1024, 832 cm^{-1}. Spectral data matched with the literature report.[11]

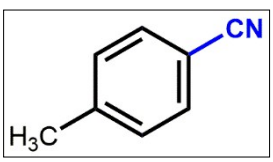
4-(Pyrrolidin-1-yl)benzonitrile (25)



Compound **25** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 1-(4-bromophenyl)pyrrolidine (113 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a pale yellow solid (71.4 mg, 0.415 mmol, 83%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (dd, *J* = 8.8, 2.2 Hz, 2H), 6.45 (dd, *J* = 8.8, 1.8 Hz, 2H), 3.31 – 3.25 (m, 4H), 2.00 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.9, 133.2, 120.9, 111.4, 96.2, 47.4, 25.3. **IR (film)** ν_{max} 2208, 1601, 1518, 1391, 1170, 812 cm^{-1}. Spectral data matched with the literature report.[14]

4-Methylbenzonitrile (26)

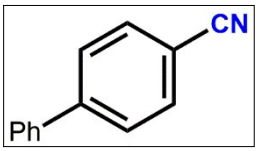


Compound **26** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 1-bromo-4-methylbenzene (86 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used.

The crude product was purified by column chromatography (100% Hexane to 98:2 Hexane/EtOAc) and obtained as a colorless liquid (47.4 mg, 0.405 mmol, 81%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.8 Hz, 2H), 7.22 (d, *J* = 7.8 Hz, 2H), 2.37 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.6, 131.8, 129.7, 119.0, 109.1, 21.6. **IR (film)** ν_{max} 2226, 1610, 1505, 1172, 816 cm^{-1}. Spectral data matched with the literature report.[11]

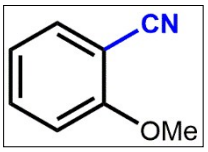
[1,1'-Biphenyl]-4-carbonitrile (27)



Compound **27** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 4-bromo-1,1'-biphenyl (116.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 97:3 Hexane/EtOAc) and obtained as a white solid (68.1 mg, 0.38 mmol, 76%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.66 (d, *J* = 8.1 Hz, 2H), 7.59 (d, *J* = 7.1 Hz, 2H), 7.49 (t, *J* = 7.3 Hz, 2H), 7.43 (t, *J* = 7.2 Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.4, 138.9, 132.4, 129.0, 128.6, 127.5, 127.1, 118.8, 110.7. **IR (film)** ν_{max} 2227, 1606, 1484, 849, 768, 698 cm^{-1}. Spectral data matched with the literature report.[11]

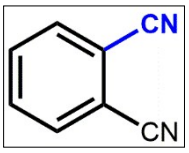
2-Methoxybenzonitrile (28)



Compound **28** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 1-bromo-2-methoxybenzene (62.4 µL, 93.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 95:5 Hexane/EtOAc) and obtained as a colorless oil (26.6 mg, 0.20 mmol, 40%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.51 (m, 2H), 7.03-6.94 (m, 2H), 3.93 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.3, 134.5, 133.9, 120.8, 116.6, 111.4, 101.9, 56.1. **IR (film)** ν_{max} 2213, 1602, 1514, 1260, 835 cm^{-1}. Spectral data matched with the literature report.[11]

Phthalonitrile (29)

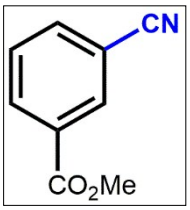


Compound **29** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 2-bromobenzonitrile (91 mg, 0.5 mmol),

$(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a white solid (26.9 mg, 0.21 mmol, 42%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 5.8, 3.4 Hz, 2H), 7.76 (dd, *J* = 5.8, 3.4 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 133.7, 133.2, 116.1, 115.4. **IR (film)** ν_{max} 2233, 1483, 1203, 774 cm^{-1}. Spectral data matched with the literature report.[15]

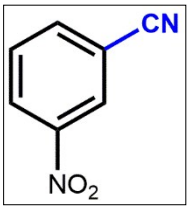
Methyl 3-cyanobenzoate (30)



Compound **30** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), methyl 3-bromobenzoate (107.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a yellow solid (49.1 mg, 0.305 mmol, 61%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 8.28 – 8.22 (m, 1H), 7.82 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 3.94 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 165.1, 136.0, 133.7, 133.3, 131.5, 129.5, 117.9, 113.0, 52.7. **IR (film)** ν_{max} 2230, 1715, 1442, 1290, 1180 cm^{-1}. Spectral data matched with the literature report.[15]

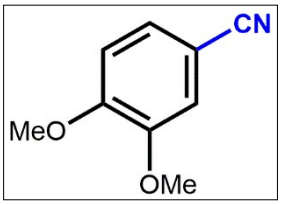
3-Nitrobenzonitrile (31)



Compound **31** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 1-Bromo-3-nitrobenzene (101 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a yellow solid (43.7 mg, 0.295 mmol, 59%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1H), 8.46 (d, *J* = 8.6 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.76 (t, *J* = 8.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 148.2, 137.7, 130.8, 127.6, 127.2, 116.6, 114.0. **IR (film)** ν_{max} 2231, 1605, 1522, 1350, 851 cm^{-1}. Spectral data matched with the literature report.[10]

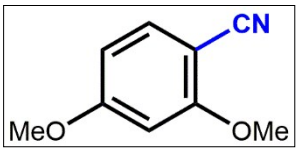
3,4-Dimethoxybenzonitrile (32)



Compound **32** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 4-Bromoveratrole (108.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a white solid (44.1 mg, 0.27 mmol, 54%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.02 (d, *J* = 1.6 Hz, 1H), 6.85 (d, *J* = 8.4 Hz, 1H), 3.87 (s, 3H), 3.84 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.8, 149.1, 126.4, 119.2, 113.8, 111.2, 103.8, 56.1, 56.0. **IR (film)** ν_{max} 2222, 1503, 1282, 1017, 814 cm^{-1}. Spectral data matched with the literature report.[16]

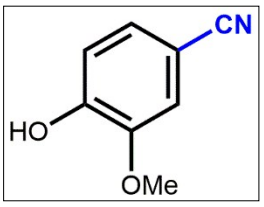
2,4-Dimethoxybenzonitrile (33)



Compound **33** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 1-bromo-2,4-dimethoxybenzene (108.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a white solid (29.4 mg, 0.18 mmol, 36%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.6 Hz, 1H), 6.50 (dd, *J* = 8.6, 2.2 Hz, 1H), 6.44 (d, *J* = 2.1 Hz, 1H), 3.88 (s, 3H), 3.84 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.7, 162.9, 134.95, 117.0, 105.9, 98.5, 94.0, 56.0, 55.8. **IR (film)** ν_{max} 2225, 1507, 1282, 1015, 819 cm^{-1}. Spectral data matched with the literature report.[16]

4-Hydroxy-3-methoxybenzonitrile (34)

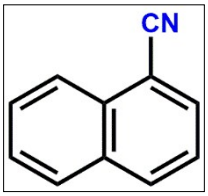


Compound **34** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 4-bromo-2-methoxyphenol (101.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography

(100% Hexane to 90:10 Hexane/EtOAc) and obtained as a brown solid (30.6 mg, 0.205 mmol, 41%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.07 (d, *J* = 1.7 Hz, 1H), 6.95 (d, *J* = 8.3 Hz, 1H), 3.92 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 150.1, 146.8, 127.1, 119.3, 115.3, 113.9, 103.2, 56.3. **IR (film)** ν_{max} 3388, 2226, 1605, 1591, 1028, 819 cm^{-1}. Spectral data matched with the literature report.[17]

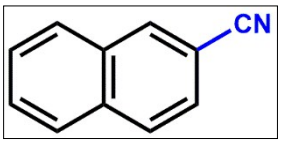
1-Naphthonitrile (35)



Compound **35** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 1-bromonaphthalene (103.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 97:3 Hexane/EtOAc) and obtained as a brown liquid (46.7 mg, 0.305 mmol, 61%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.3 Hz, 1H), 8.07 (d, *J* = 8.3 Hz, 1H), 7.91 (t, *J* = 6.9 Hz, 2H), 7.72 – 7.66 (m, 1H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.52 (t, *J* = 8.0 Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 133.4, 133.0, 132.7, 132.4, 128.8, 128.7, 127.6, 125.2, 125.0, 117.9, 110.3. **IR (film)** ν_{max} 2224, 867, 814, 752 cm^{-1}. Spectral data matched with the literature report.[11]

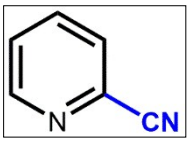
2-Naphthonitrile (36)



Compound **36** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 2-bromonaphthalene (103.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 97:3 Hexane/EtOAc) and obtained as a white solid (52.1 mg, 0.34 mmol, 68%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (s, 1H), 7.93–7.89 (m, 3H), 7.69 – 7.57 (m, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 134.8, 134.2, 132.4, 129.3, 129.1, 128.5, 128.1, 127.7, 126.4, 119.3, 109.5. **IR (film)** ν_{max} 2226, 864, 814, 749 cm^{-1}. Spectral data matched with the literature report.[11]

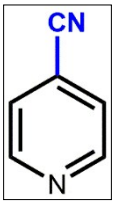
Picolinonitrile (37)



Compound **37** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 2-Bromopyridine (79 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a colorless liquid (27.6 mg, 0.265 mmol, 53%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, *J* = 3.5 Hz, 1H), 7.85 (t, *J* = 7.7 Hz, 1H), 7.71 (d, *J* = 7.7 Hz, 1H), 7.57 – 7.49 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.2, 137.1, 134.1, 128.6, 126.9, 117.2. **IR (film)** ν_{max} 2235, 1579, 1431, 995, 778, 547 cm^{-1}. Spectral data matched with the literature report.[10]

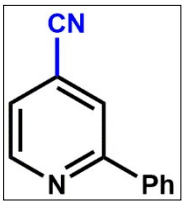
Isonicotinonitrile (38)



Compound **38** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 4-Bromopyridine (79 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a white solid (29.1 mg, 0.28 mmol, 56%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (dd, *J* = 4.5, 1.4 Hz, 2H), 7.54 (dd, *J* = 4.4, 1.4 Hz, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.8, 125.4, 120.6, 116.4. **IR (film)** ν_{max} 2241, 1595, 1417, 828 cm^{-1}. Spectral data matched with the literature report.[18]

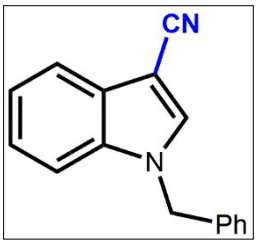
2-Phenylisonicotinonitrile (39)



Compound **39** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 4-bromo-2-phenylpyridine (117 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a yellow solid (41.4 mg, 0.23 mmol, 46%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (d, *J* = 4.9 Hz, 1H), 7.99 (dd, *J* = 7.6, 1.5 Hz, 2H), 7.93 (s, 1H), 7.49 (m, 3H), 7.43 (d, *J* = 4.9 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.8, 150.7, 137.4, 130.3, 129.1, 127.0, 123.2, 122.1, 121.3, 116.8. **IR (film)** ν_{max} 2238, 1598, 1545, 1450, 1387 cm^{-1}. Spectral data matched with the literature report.[19]

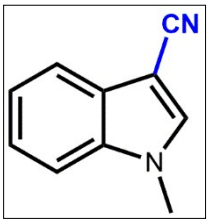
1-Benzyl-1*H*-indole-3-carbonitrile (40)



Compound **40** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 1-benzyl-3-bromo-1*H*-indole (142.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a yellow solid (47.8 mg, 0.21 mmol, 42%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.75 (m, 1H), 7.56 (s, 1H), 7.42 – 7.28 (m, 6H), 7.18 – 7.13 (m, 2H), 5.29 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 135.8, 135.4, 135.1, 129.3, 128.6, 128.2, 127.3, 124.2, 122.5, 120.2, 115.9, 111.1, 86.5, 51.1. **IR (film)** ν_{max} 2216, 1533, 1467, 1392, 1171, 739 cm^{-1}. Spectral data matched with the literature report.[16]

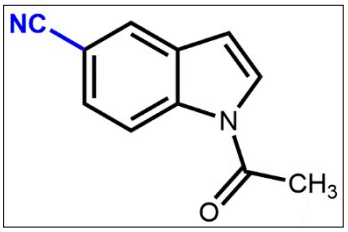
1-Methyl-1*H*-indole-3-carbonitrile (41)



Compound **41** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 3-bromo-1-methyl-1*H*-indole (106.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as yellow liquid (33.6 mg, 0.215 mmol, 43%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.9 Hz, 1H), 7.54 (s, 1H), 7.39 (d, *J* = 7.8 Hz, 1H), 7.37 – 7.32 (m, 1H), 7.32 – 7.26 (m, 1H), 3.84 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 136.1, 135.7, 127.8, 123.9, 122.2, 119.8, 116.1, 110.4, 85.4, 33.7. **IR (film)** ν_{max} 2215, 1528, 1465, 738 cm^{-1}. Spectral data matched with the literature report.[16]

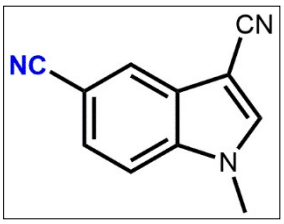
1-Acetyl-1*H*-indole-5-carbonitrile (42)



Compound **42** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 1-(5-bromo-1*H*-indol-1-yl)ethan-1-one (119 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 80:20 Hexane/EtOAc) and obtained as a white solid (42.3 mg, 0.23 mmol, 46%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, J = 8.6 Hz, 1H), 7.82 (s, 1H), 7.52 (t, J = 5.9 Hz, 2H), 6.66 (d, J = 3.7 Hz, 1H), 2.65 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.7, 137.2, 130.3, 128.1, 127.4, 125.5, 119.5, 117.3, 108.6, 106.9, 23.9. **IR (film)** ν_{max} 2225, 1720, 1468, 1337, 1320, 1200, 930 cm^{-1}. Spectral data matched with the literature report.[20]

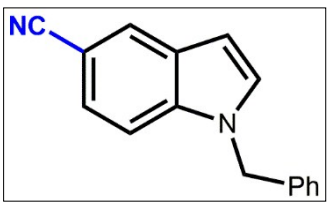
1-Methyl-1*H*-indole-3,5-dicarbonitrile (43)



Compound **43** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 5-bromo-1-methyl-1*H*-indole-3-carbonitrile (117 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a white solid (37.1 mg, 0.205 mmol, 41%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.72 (s, 1H), 7.57 (d, J = 8.6 Hz, 1H), 7.50 (d, J = 8.6 Hz, 1H), 3.92 (s, 3H).**^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.9, 137.6, 127.5, 126.9, 125.2, 119.4, 114.4, 111.7, 105.9, 87.1, 34.1. **IR (film)** ν_{max} 2222, 1532, 1488, 811, 636 cm^{-1}. Spectral data matched with the literature report.[21]

1-Benzyl-1*H*-indole-5-carbonitrile (44)

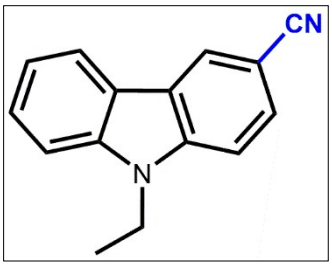


Compound **44** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 1-benzyl-5-bromo-1*H*-indole (143 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by

column chromatography (100% Hexane to 80:20 Hexane/EtOAc) and obtained as a colorless liquid (59.2 mg, 0.255 mmol, 51%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.38 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.35 – 7.28 (m, 4H), 7.26 (d, *J* = 3.1 Hz, 1H), 7.09 (d, *J* = 6.4 Hz, 2H), 6.63 (d, *J* = 3.0 Hz, 1H), 5.34 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 137.8, 136.4, 130.7, 129.0, 128.5, 128.1, 126.8, 126.6, 124.7, 120.8, 110.6, 102.8, 102.7, 50.4. **IR (film)** ν_{max} 2215, 1608, 1477, 1339, 693 cm^{-1}. Spectral data matched with the literature report.[22]

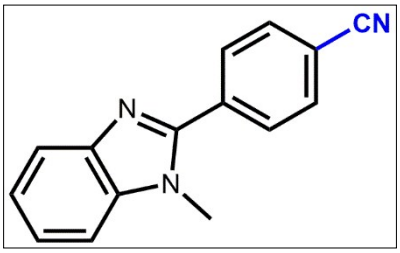
9-Ethyl-9*H*-carbazole-3-carbonitrile (45)



Compound **45** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 3-bromo-9-ethyl-9*H*-carbazole (137 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a yellow solid (49.5 mg, 0.225 mmol, 45%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 8.11 (d, *J* = 7.8 Hz, 1H), 7.71 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 1H), 7.46 (t, *J* = 8.1 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 1H), 4.40 (q, *J* = 7.2 Hz, 2H), 1.46 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.7, 140.6, 129.1, 127.2, 125.4, 123.3, 122.2, 120.9, 120.7, 120.5, 109.2, 109.2, 101.7, 38.0, 13.9. **IR (film)** ν_{max} 2210, 1597, 1228, 744 cm^{-1}. Spectral data matched with the literature report.[23]

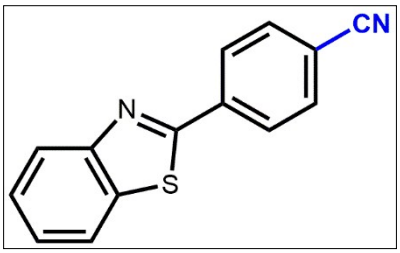
4-(1-Methyl-1H-benzo[d]imidazol-2-yl)benzonitrile (46)



Compound **46** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 2-(4-bromophenyl)-1-methyl-1*H*-benzo[*d*]imidazole (143.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 60:40 Hexane/EtOAc) and obtained as a white solid (71.1 mg, 0.305 mmol, 61%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.3 Hz, 2H), 7.83 (t, *J* = 6.8 Hz, 3H), 7.43 (d, *J* = 7.3 Hz, 1H), 7.36 (m, 2H), 3.90 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 151.5, 143.0, 136.8, 134.7, 132.5, 130.1, 123.8, 123.1, 120.3, 118.3, 113.5, 109.9, 31.9. **IR (film)** ν_{max} 2224, 1612, 1457, 1253, 840 cm^{-1}. Spectral data matched with the literature report.[24]

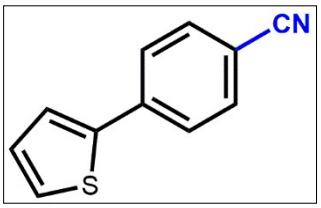
4-(Benzo[d]thiazol-2-yl)benzonitrile (47)



Compound **47** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 2-(4-bromophenyl)benzo[*d*]thiazole (144.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a white solid (66.1 mg, 0.28 mmol, 56%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.4 Hz, 2H), 8.05 (d, *J* = 8.5 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 7.7 Hz, 2H), 7.50 (td, *J* = 7.8, 1.0 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 165.5, 154.2, 137.6, 135.5, 132.9, 128.1, 127.0, 126.2, 124.0, 121.9, 118.4, 114.3. **IR (film)** ν_{max} 2224, 1478, 1255, 968, 764 cm^{-1}. Spectral data matched with the literature report.[25]

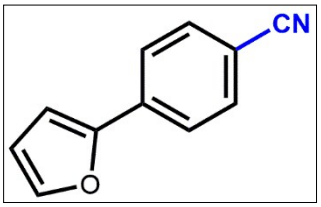
4-(Thiophen-2-yl)benzonitrile (48)



Compound **48** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 2-(4-bromophenyl)thiophene (119.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 95:5 Hexane/EtOAc) and obtained as a white solid (49.0 mg, 0.265 mmol, 53%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (q, *J* = 8.5 Hz, 4H), 7.41 (dd, *J* = 8.2, 4.2 Hz, 2H), 7.16 – 7.11 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 142.2, 138.8, 132.8, 128.6, 127.2, 126.2, 125.2, 118.9, 110.7. **IR (film)** ν_{max} 2223, 1607, 1423, 821 cm^{-1}. Spectral data matched with the literature report.[26]

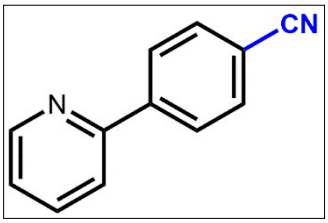
4-(Furan-2-yl)benzonitrile (49)



Compound **49** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 2-(4-bromophenyl)furan (111.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a white solid (39.8 mg, 0.235 mmol, 47%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.4 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.51 (d, J = 1.5 Hz, 1H), 6.78 (d, J = 3.4 Hz, 1H), 6.50 (dd, J = 3.4, 1.8 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 152.0, 143.7, 134.6, 132.5, 123.9, 118.9, 112.3, 110.3, 108.2. **IR (film)** ν_{max} 2226, 1611, 1510, 1011, 846 cm^{-1}. Spectral data matched with the literature report.[26]

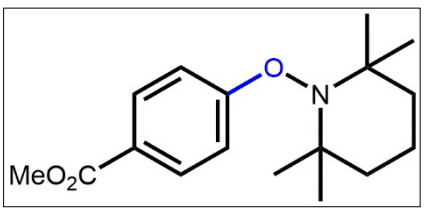
4-(Pyridin-2-yl)benzonitrile (50)



Compound **50** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 2-(4-bromophenyl)pyridine (116.6 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 80:20 Hexane/EtOAc) and obtained as a white solid (49.6 mg, 0.275 mmol, 55%).

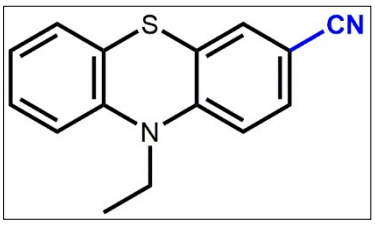
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, J = 4.2 Hz, 1H), 8.11 (d, J = 8.4 Hz, 2H), 7.85 – 7.79 (m, 1H), 7.76 (dd, J = 8.7, 1.6 Hz, 3H), 7.32 (dd, J = 6.5, 5.4 Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 155.3, 150.1, 143.6, 137.2, 132.6, 127.5, 123.4, 121.1, 118.9, 112.5. **IR (film)** ν_{max} 2223, 1588,1465, 776 cm^{-1}. Spectral data matched with the literature report.[10]

Methyl 4-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)benzoate (51)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 8.1 Hz, 2H), 7.37 (brs, 2H), 4.02 (s, 3H), 1.86 – 1.68 (m, 5H), 1.58 (d, J = 8.2 Hz, 1H), 1.39 (s, 6H), 1.15 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.0, 166.5, 130.6, 121.6, 113.3, 60.1, 51.2, 39.3, 31.9, 20.0, 16.5. **IR (film)** 1710, 1600, 1254, 1158, 1096, 777 ν_{max} cm^{-1}.

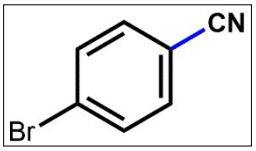
10-Ethyl-10*H*-phenothiazine-3-carbonitrile (55)



Compound **55** was prepared following the general procedure outlined in **6**. 4CzIPN (20 mg, 5 mol%), K_3PO_4 (214 mg, 1.0 mmol, 2 equiv), TsCN (109 mg, 0.60 mmol, 1.2 equiv), 3-bromo-10-ethyl-10*H*-phenothiazine **54** (153.1 mg, 0.5 mmol), $(TMS)_3SiOH$ (225 µL, 0.75 mmol, 1.5 equiv) and dry Acetone (6.0 mL) were used. The crude product was purified by column chromatography (100% Hexane to 90:10 Hexane/EtOAc) and obtained as a yellow solid (47.9 mg, 0.19 mmol, 38%).

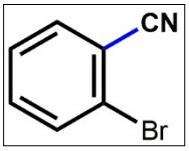
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.22 – 7.10 (m, 2H), 7.05 (dd, *J* = 7.6, 1.2 Hz, 1H), 6.94 (t, *J* = 7.3 Hz, 1H), 6.86 (d, *J* = 8.1 Hz, 1H), 6.77 (d, *J* = 8.5 Hz, 1H), 3.89 (q, *J* = 6.9 Hz, 2H), 1.39 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 148.7, 143.0, 131.6, 130.0, 127.7, 127.4, 124.9, 123.5, 122.6, 118.8, 115.6, 114.6, 104.8, 42.1, 12.7. **IR (film)** ν_{max} 2220, 1601, 1576, 1463, 1237, 742 cm^{-1}. Spectral data matched with the literature report.[27]

4-Bromobenzonitrile (56)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.5 Hz, 2H), 7.52 (d, *J* = 8.5 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 133.5, 132.7, 128.1, 118.1, 111.3. Spectral data matched with the literature report.[11]

2-Bromobenzonitrile (57)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.60 (m, 2H), 7.50 – 7.38 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 134.2, 134.0, 133.1, 127.7, 125.1, 117.1, 115.7. Spectral data matched with the literature report.[10]

10. References

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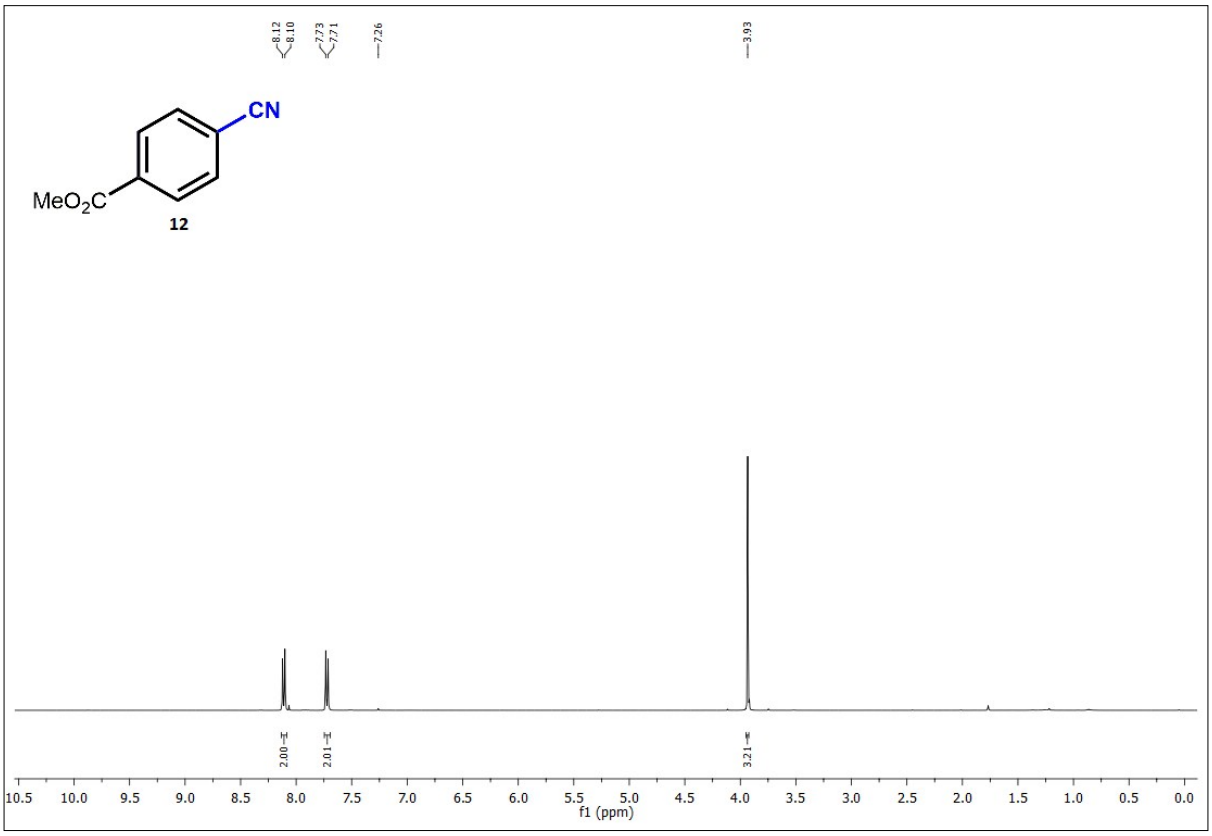
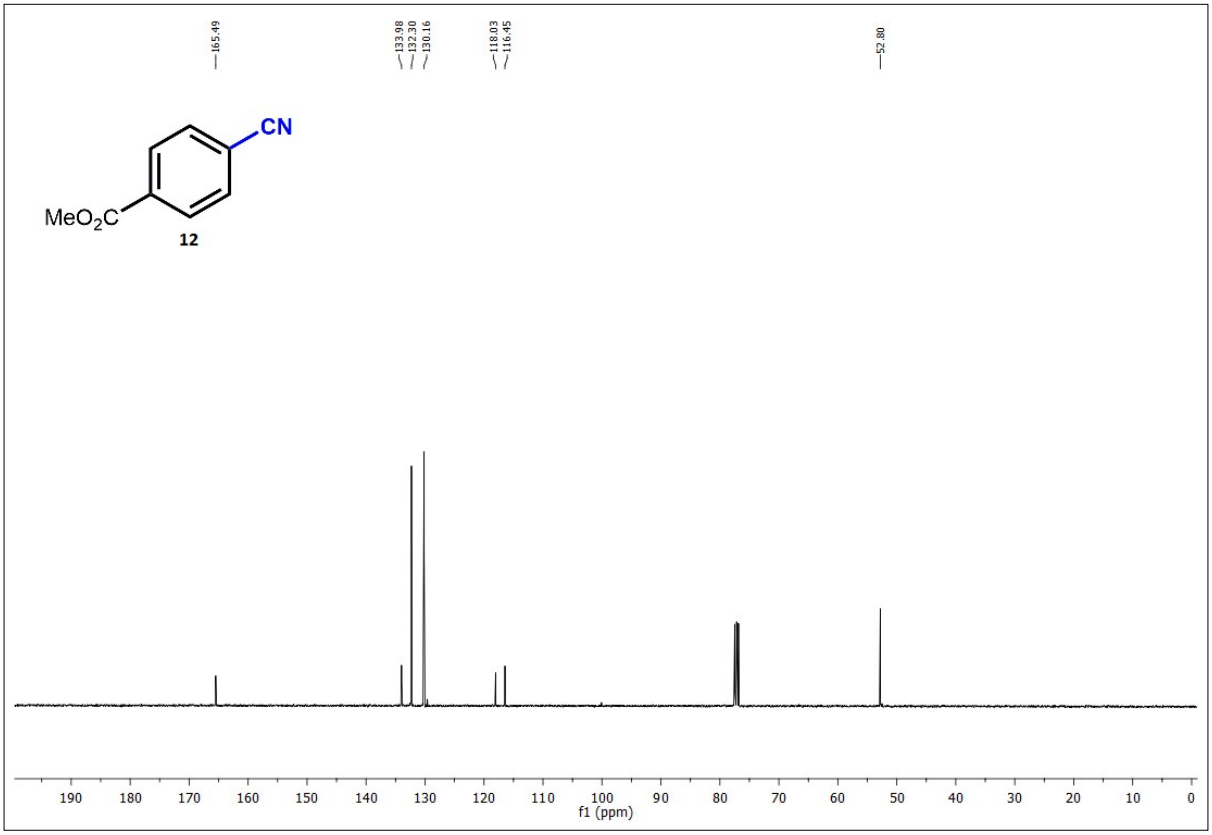
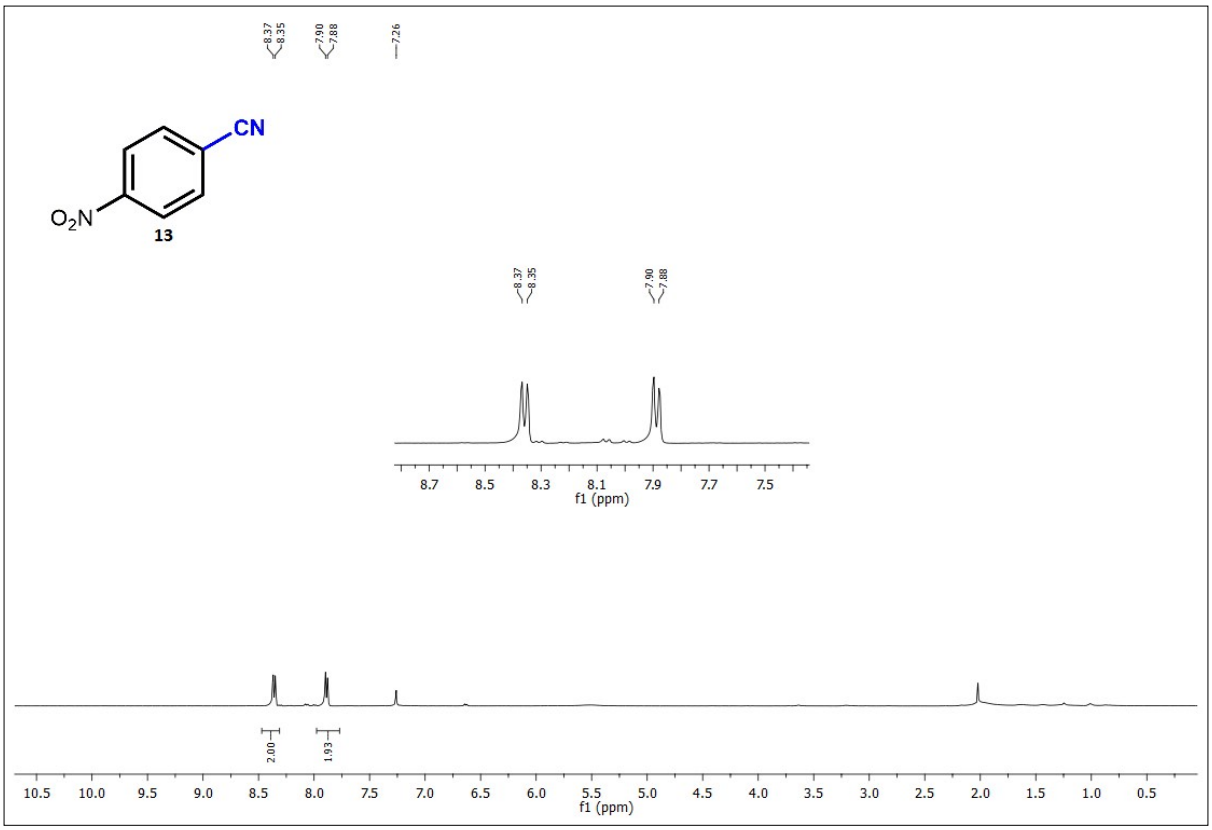
11. Spectral Data



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7.26
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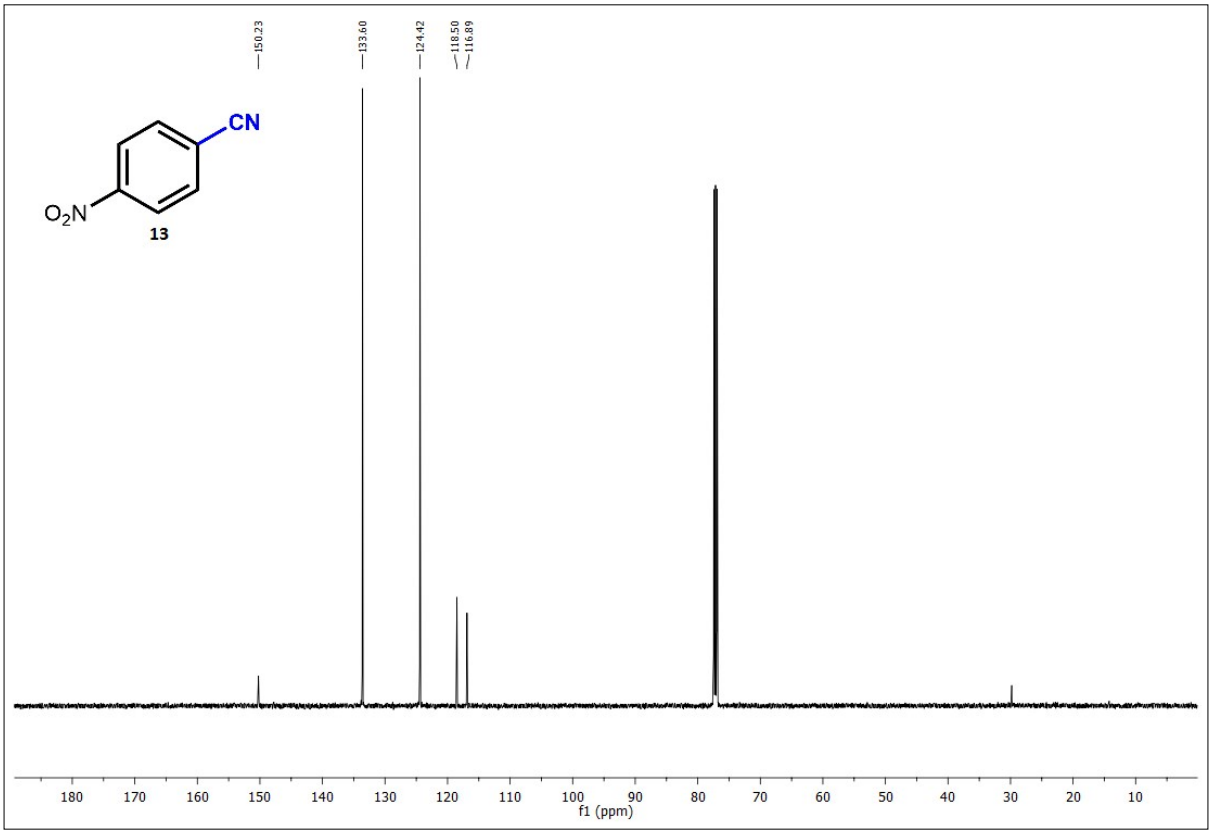
O_2N
13
8.37
8.35
7.90
7.88
8.7
8.5
8.3
8.1
7.9
7.7
7.5
f1 (ppm)
2.00
1.93
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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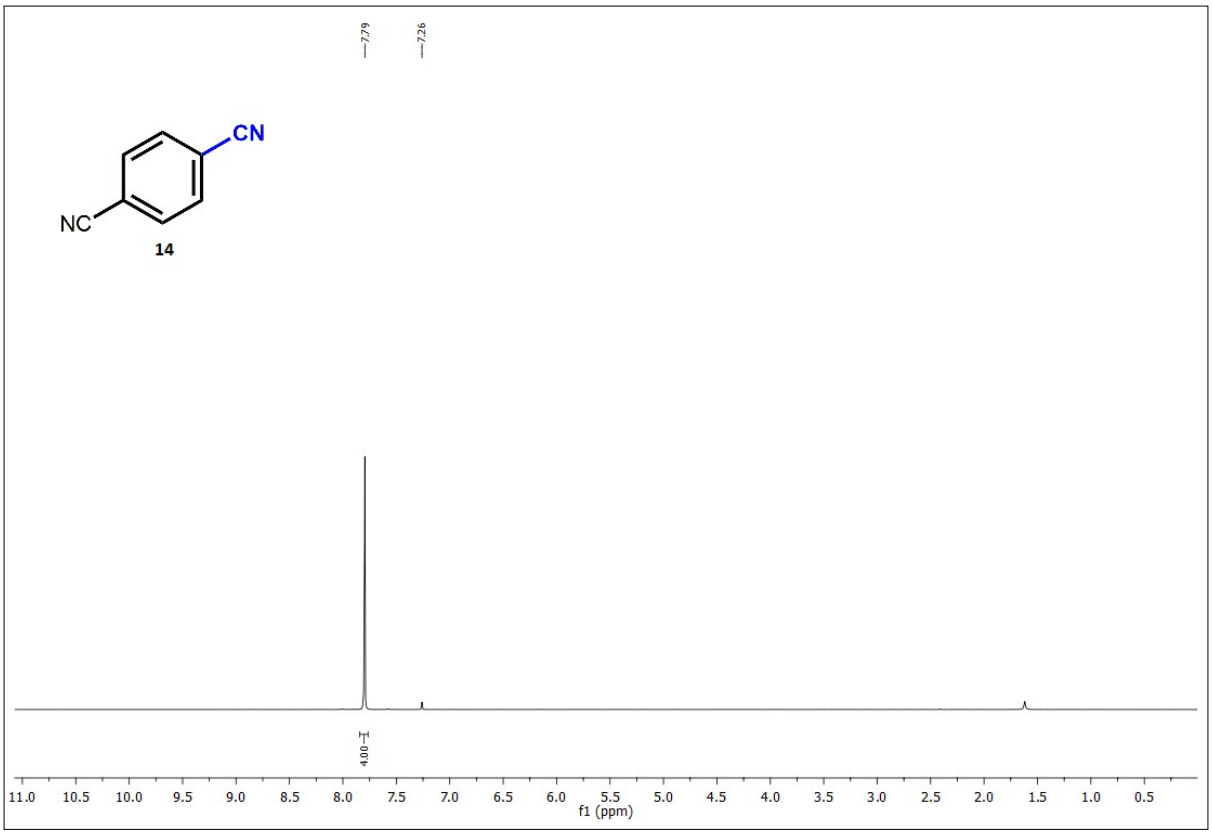
133.60
124.42
118.50
116.89
CN
O_2N
13
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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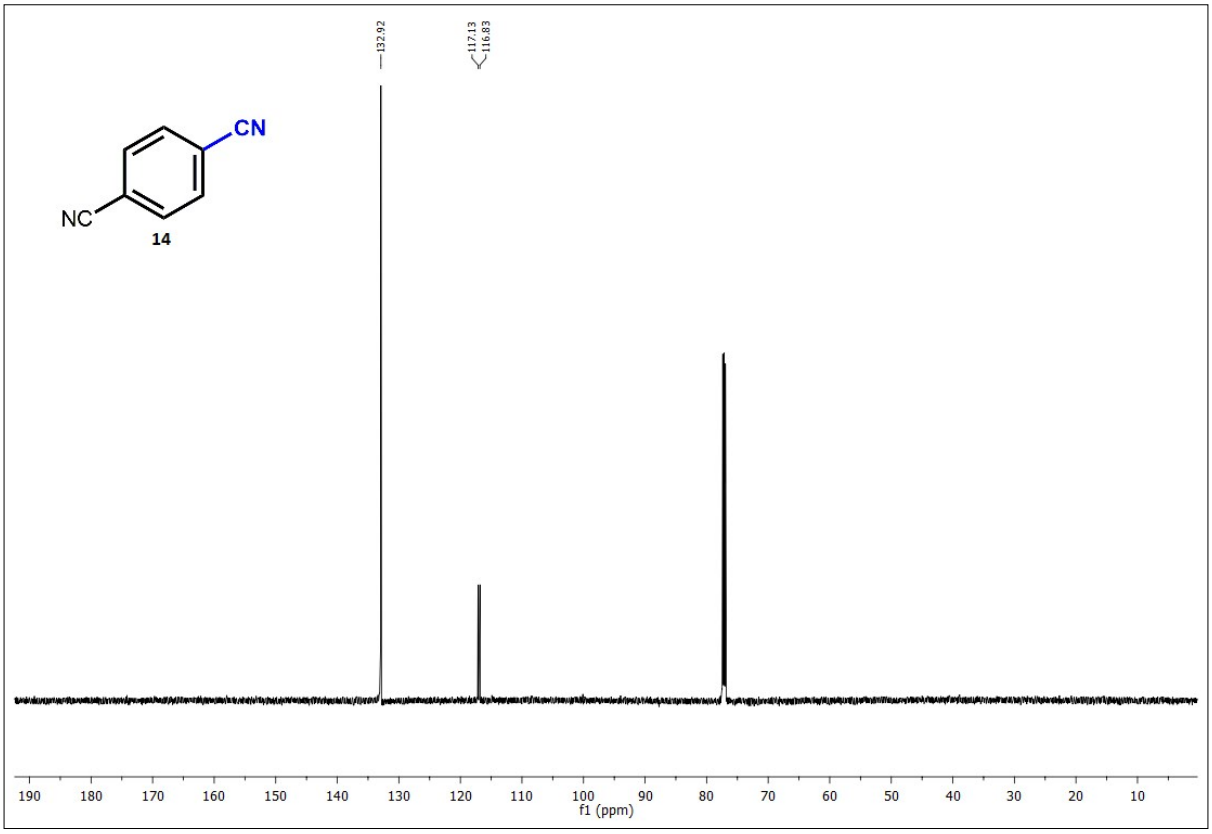
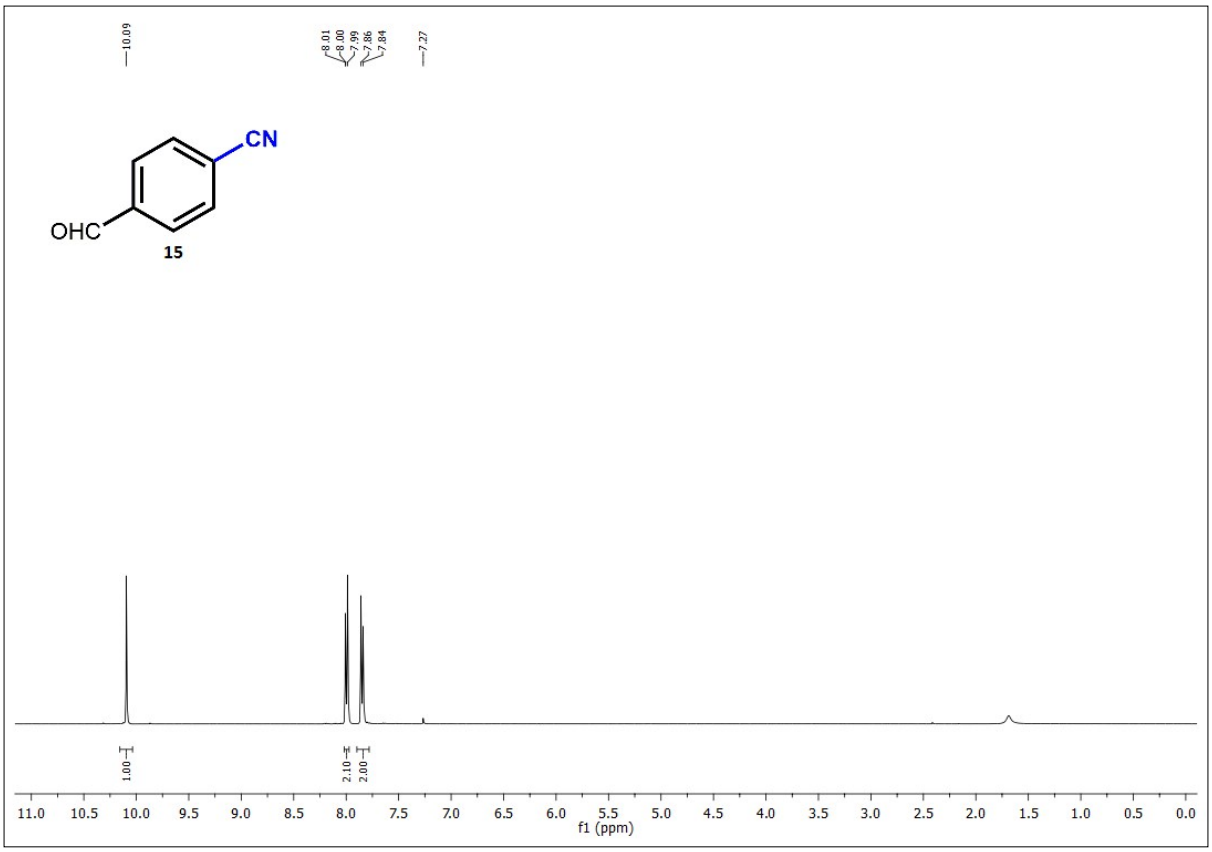
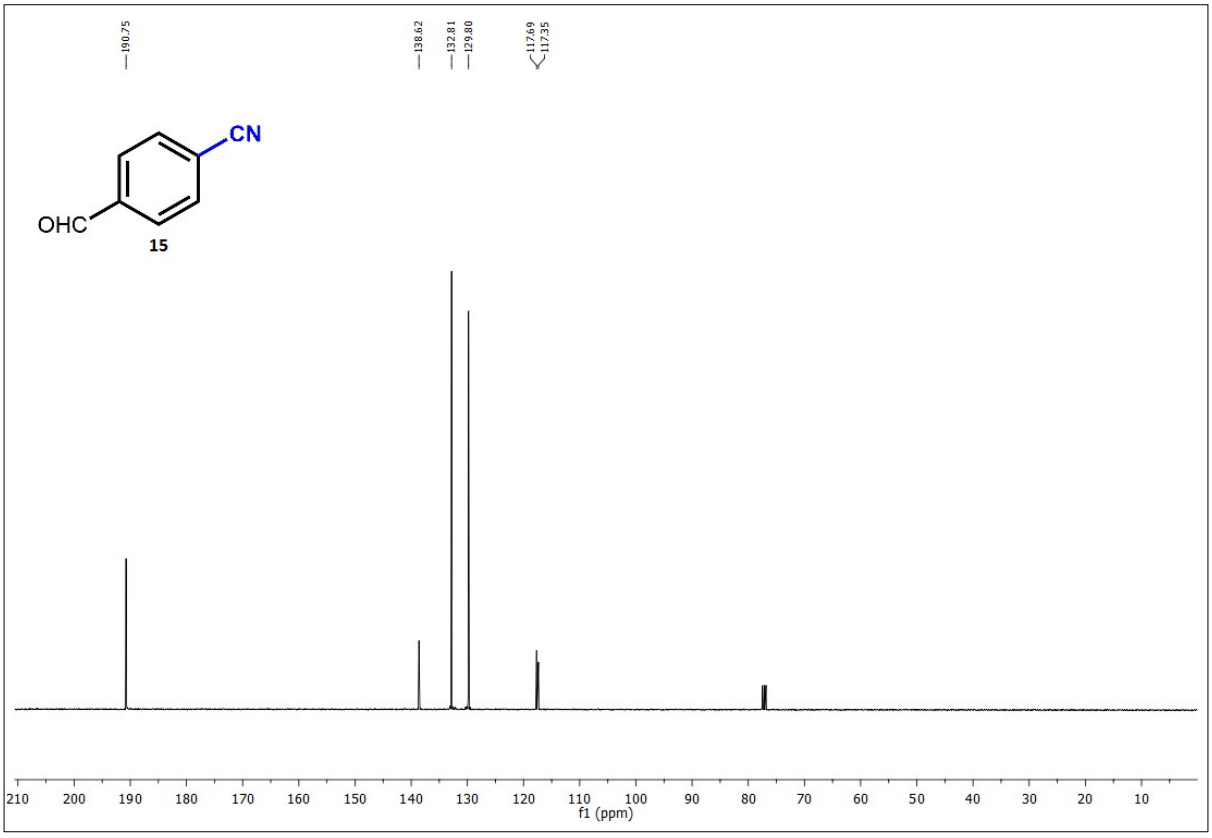
7.26
CN
NC
14
4.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


132.92
117.13
116.83
CN
NC
14
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


10.09
8.01
8.00
7.99
7.86
7.84
7.27
CN
OHC
15
1.00
2.10
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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OHC
15
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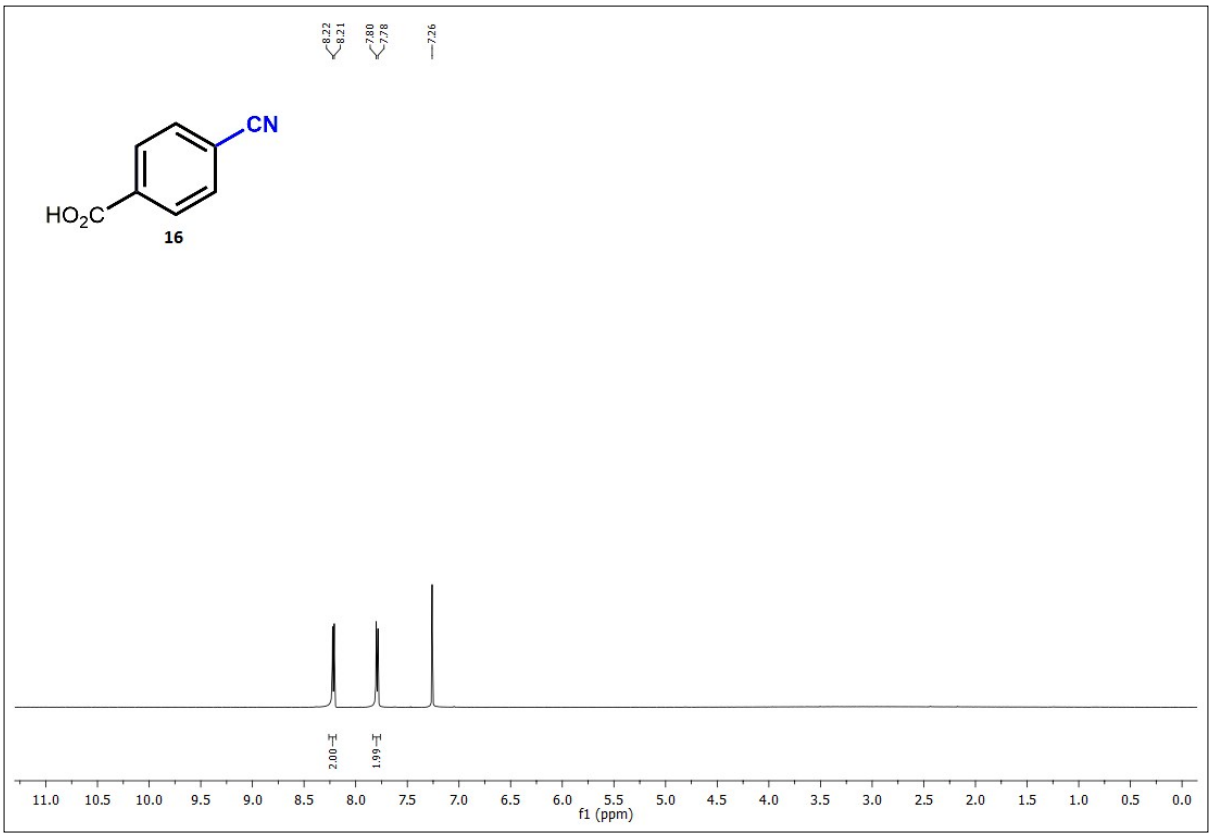
f1 (ppm)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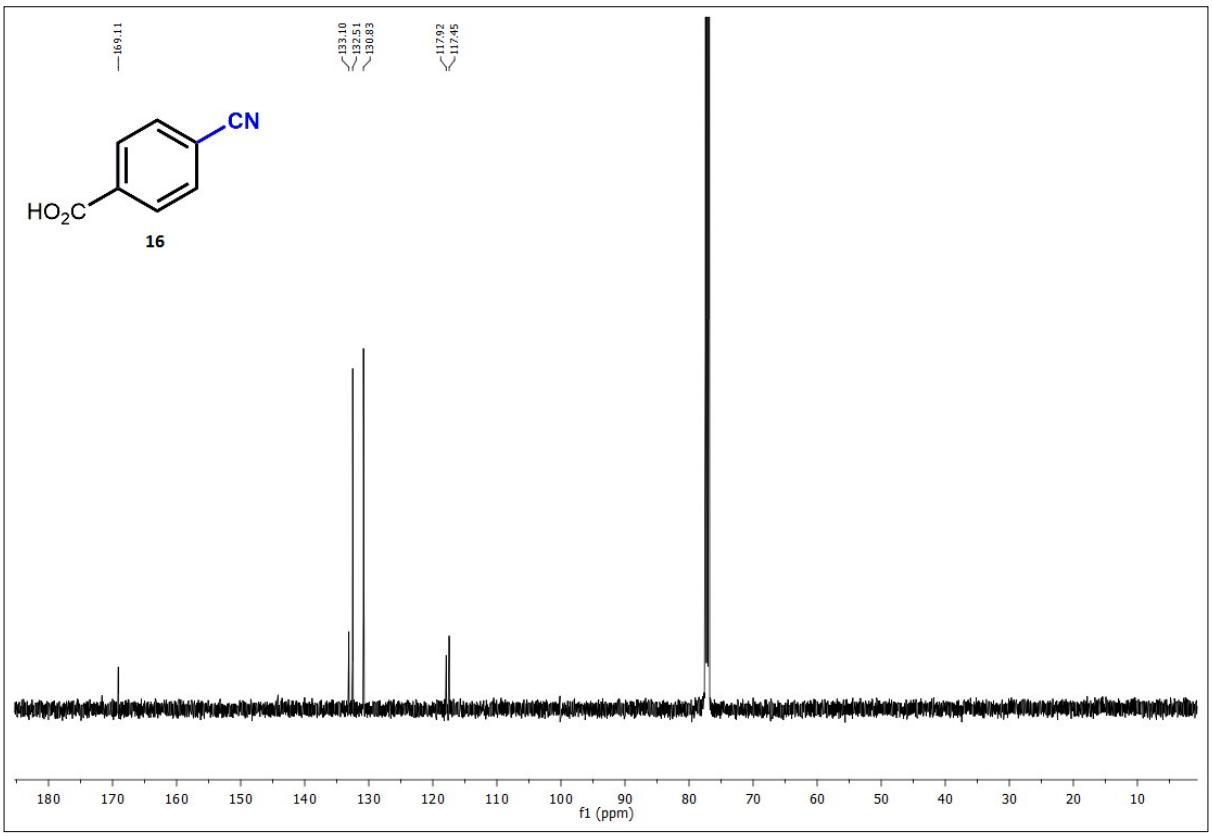
2.00
1.99
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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132.51
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117.92
117.45
CN
HO2C
16
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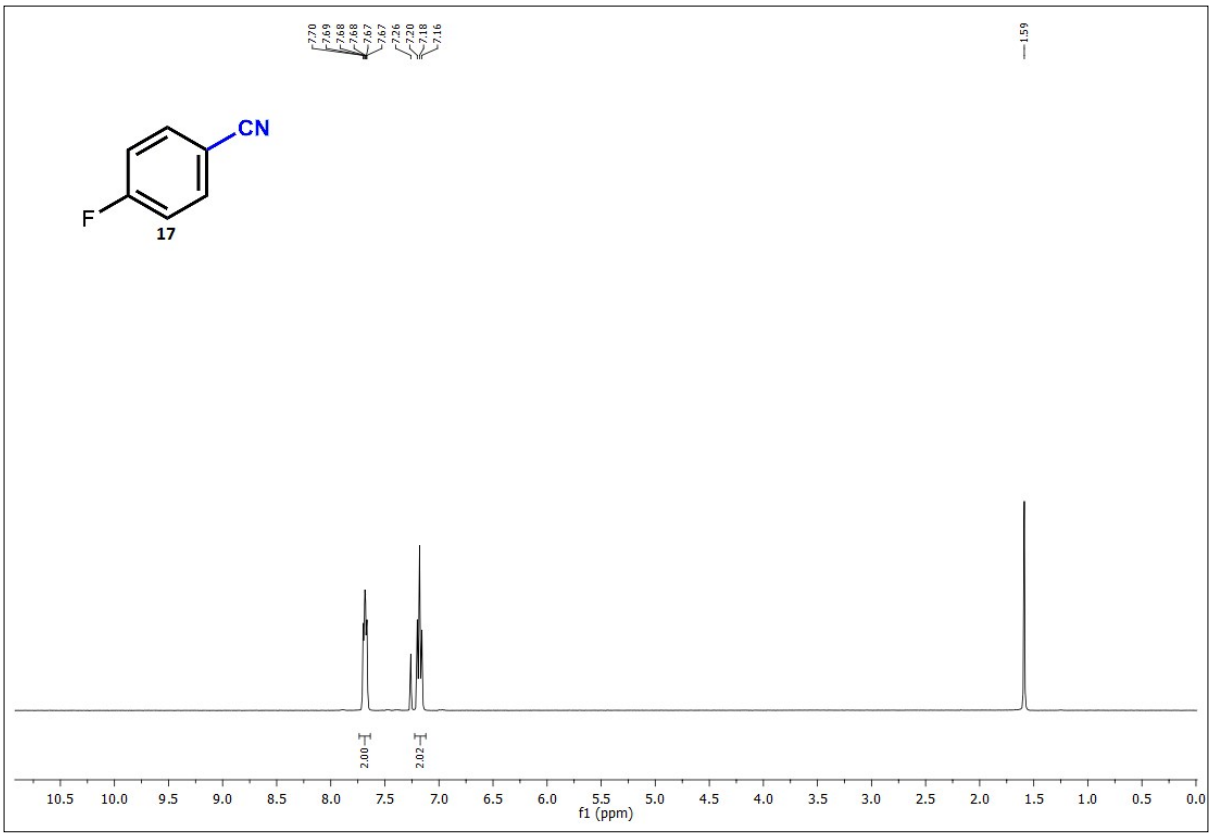
f1 (ppm)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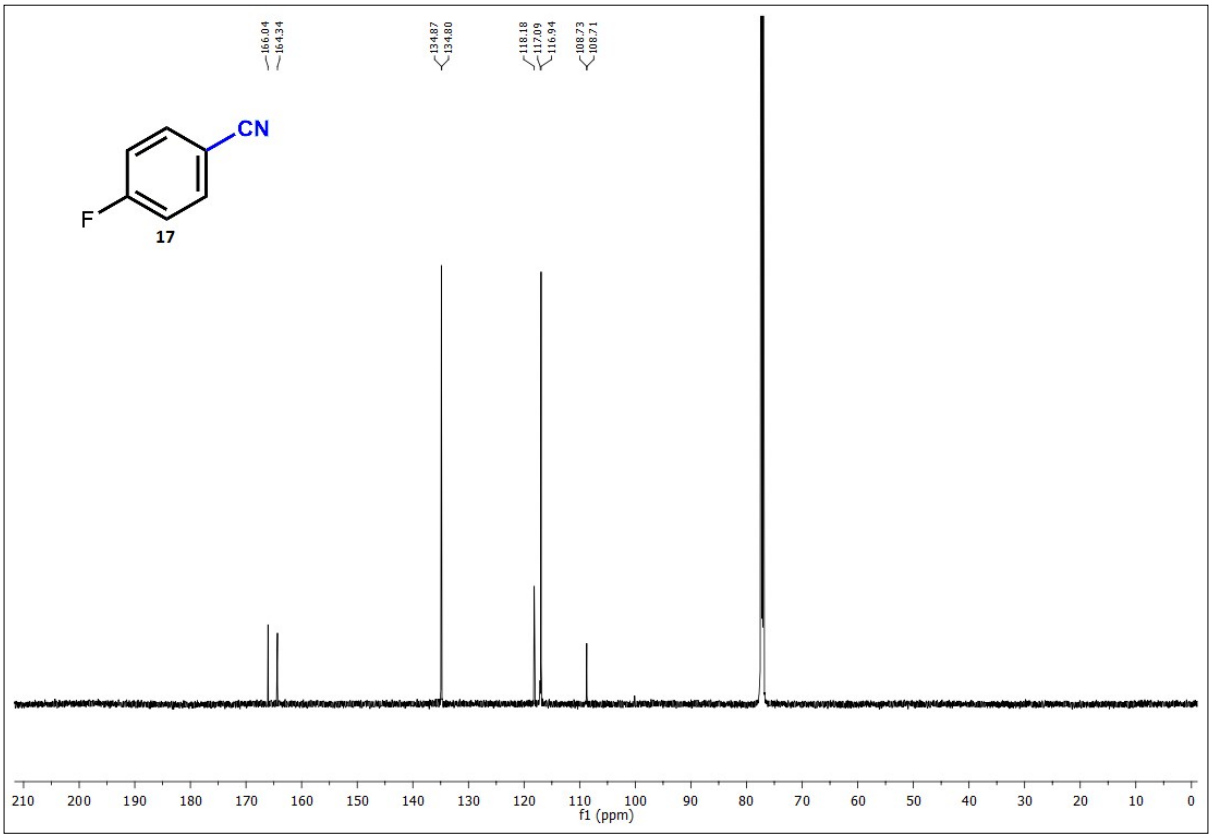
7.69
7.68
7.68
7.67
7.67
7.26
7.20
7.18
7.16
1.59
CN
F
17
2.00
2.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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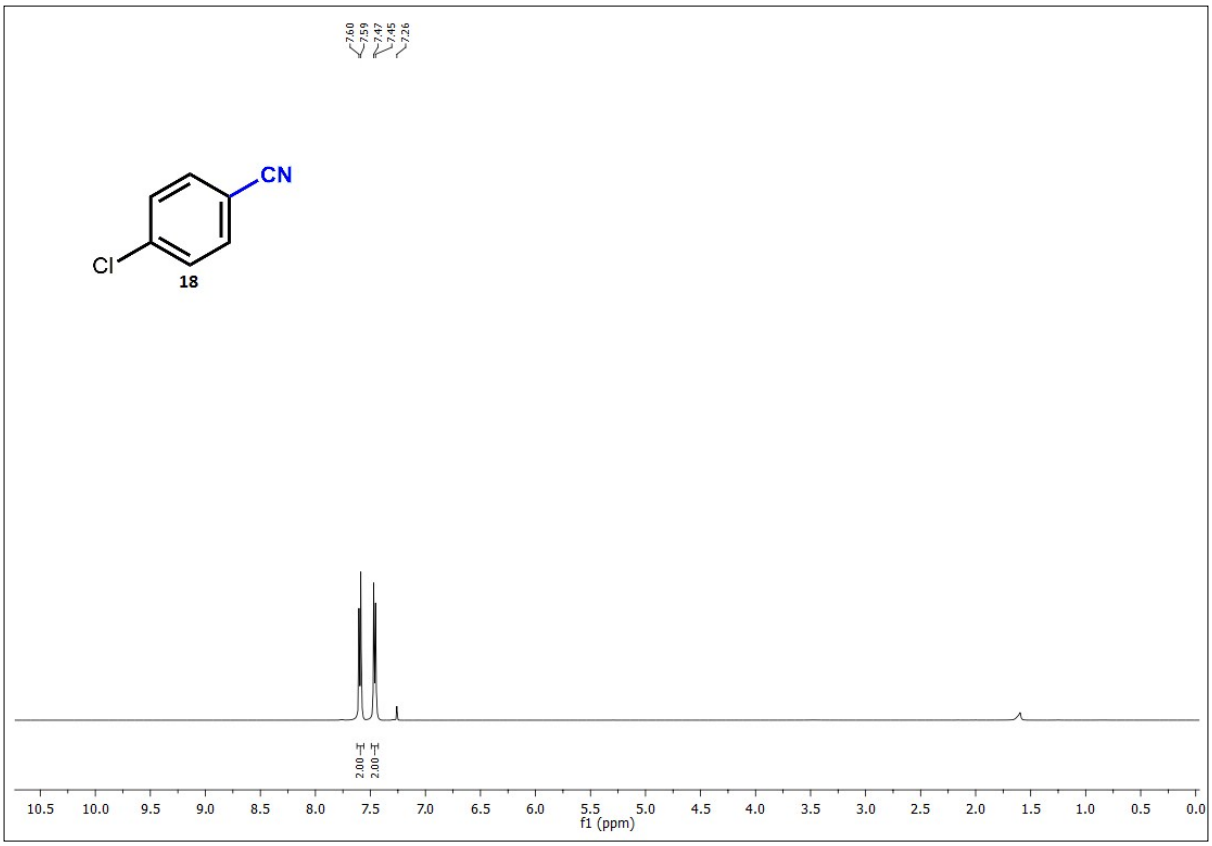
f1 (ppm)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7.59
7.47
7.45
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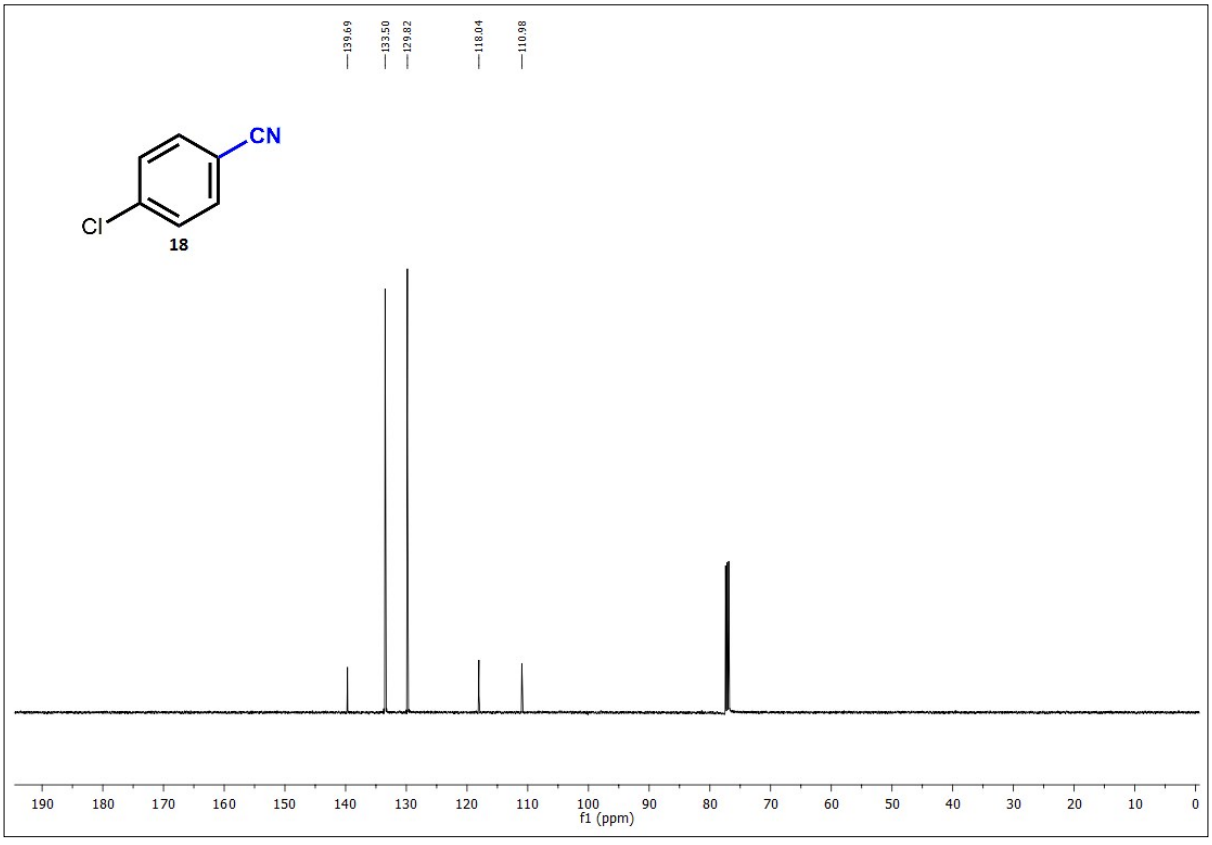
CN
Cl
18
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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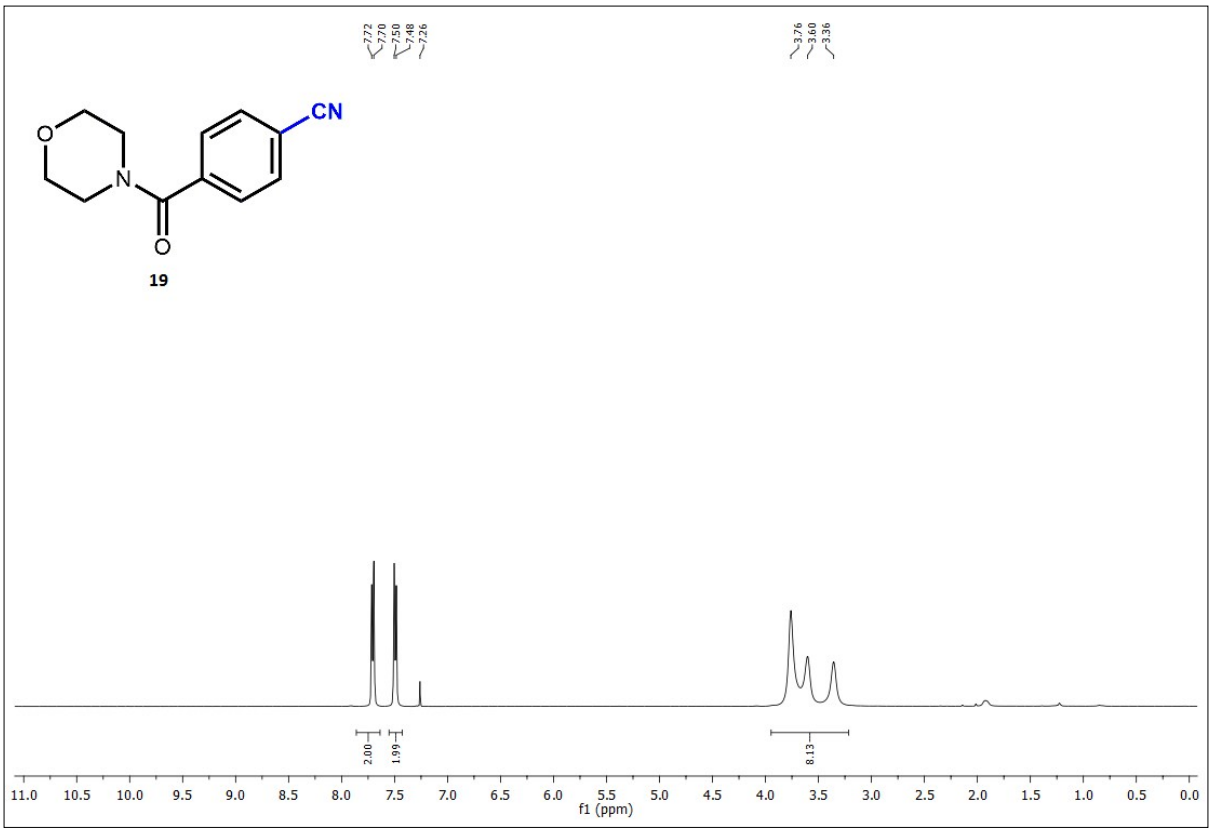
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N
O
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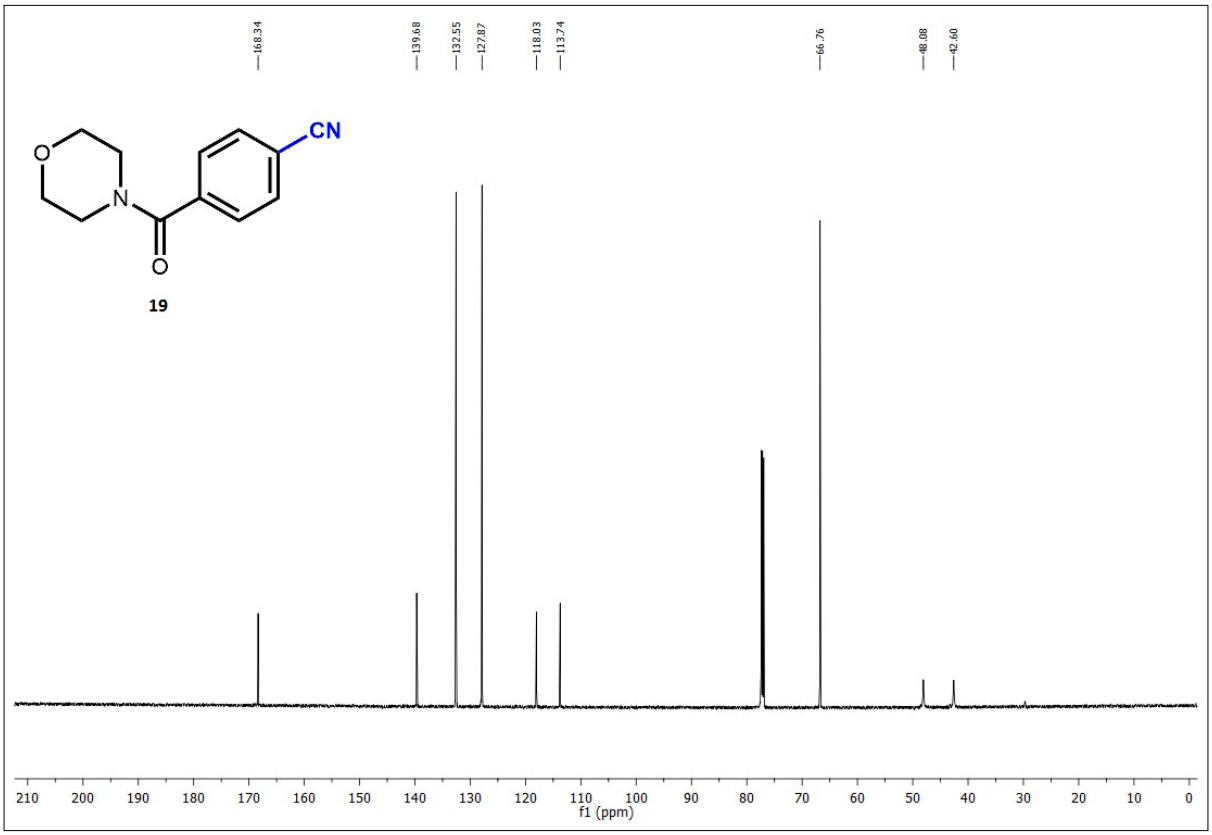
f1 (ppm)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O
N
O
19
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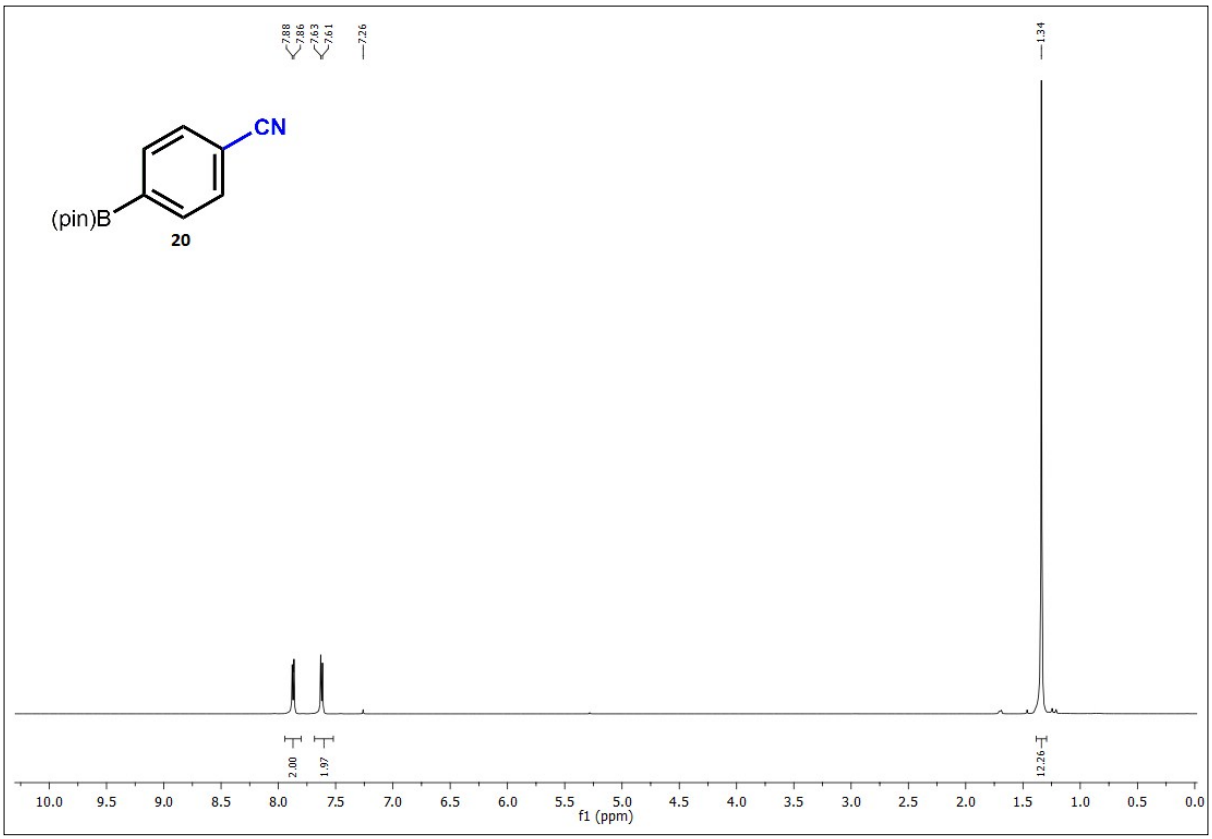
f1 (ppm)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7.61
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1.34
CN
(pin)B
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2.00
1.97
12.26
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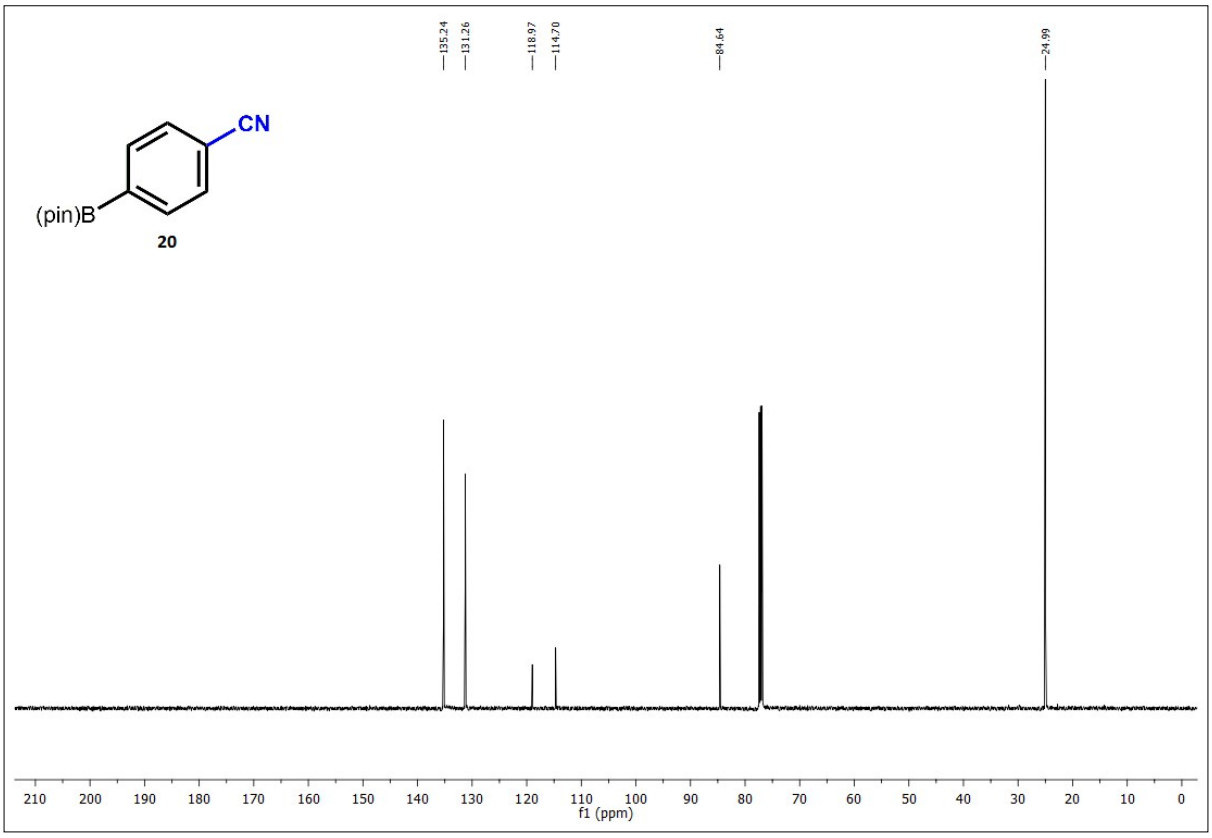
f1 (ppm)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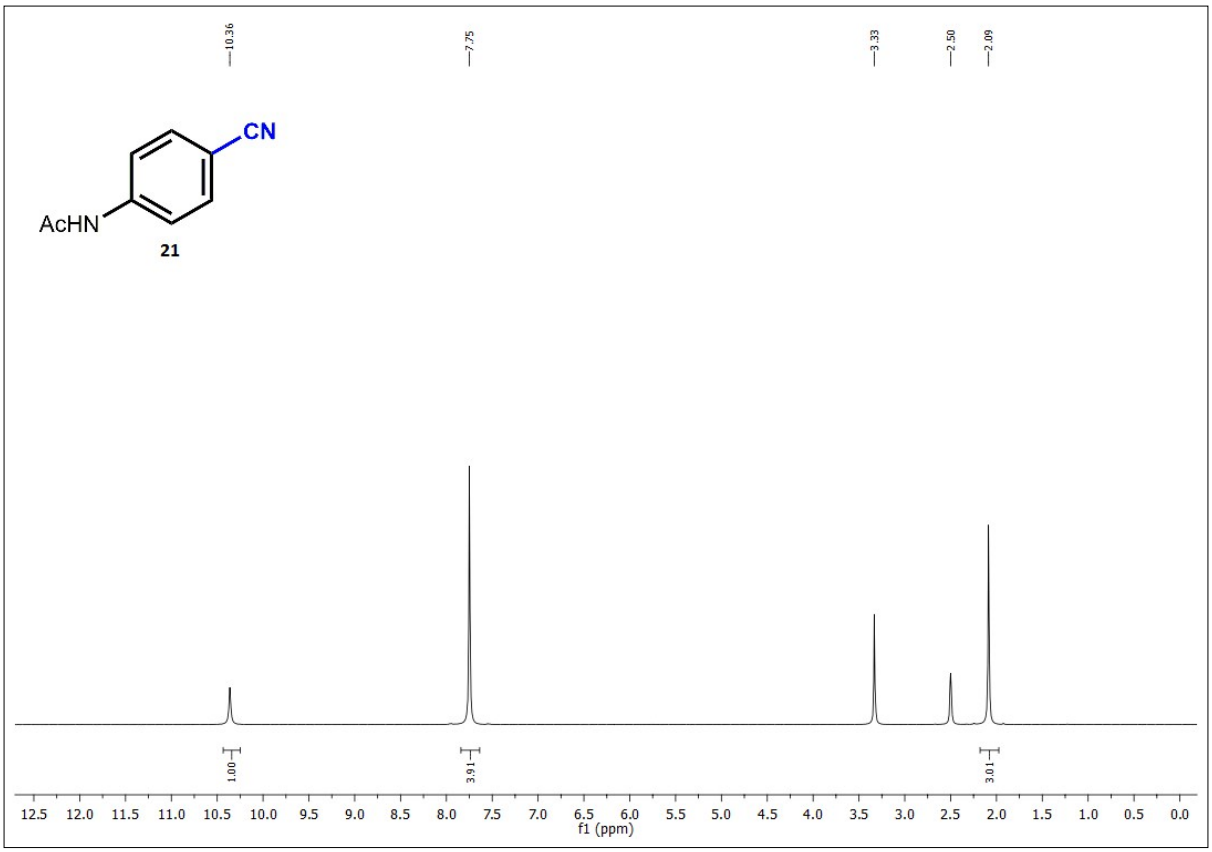
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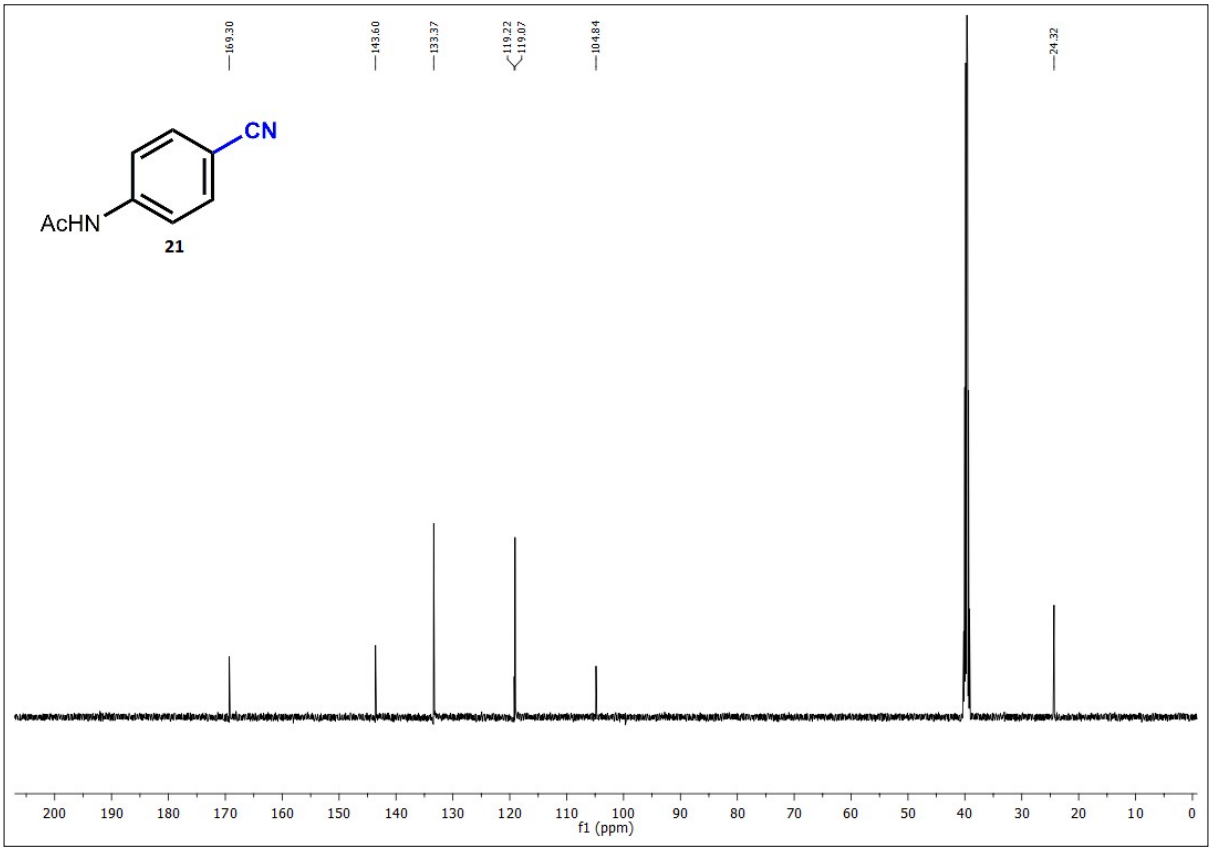
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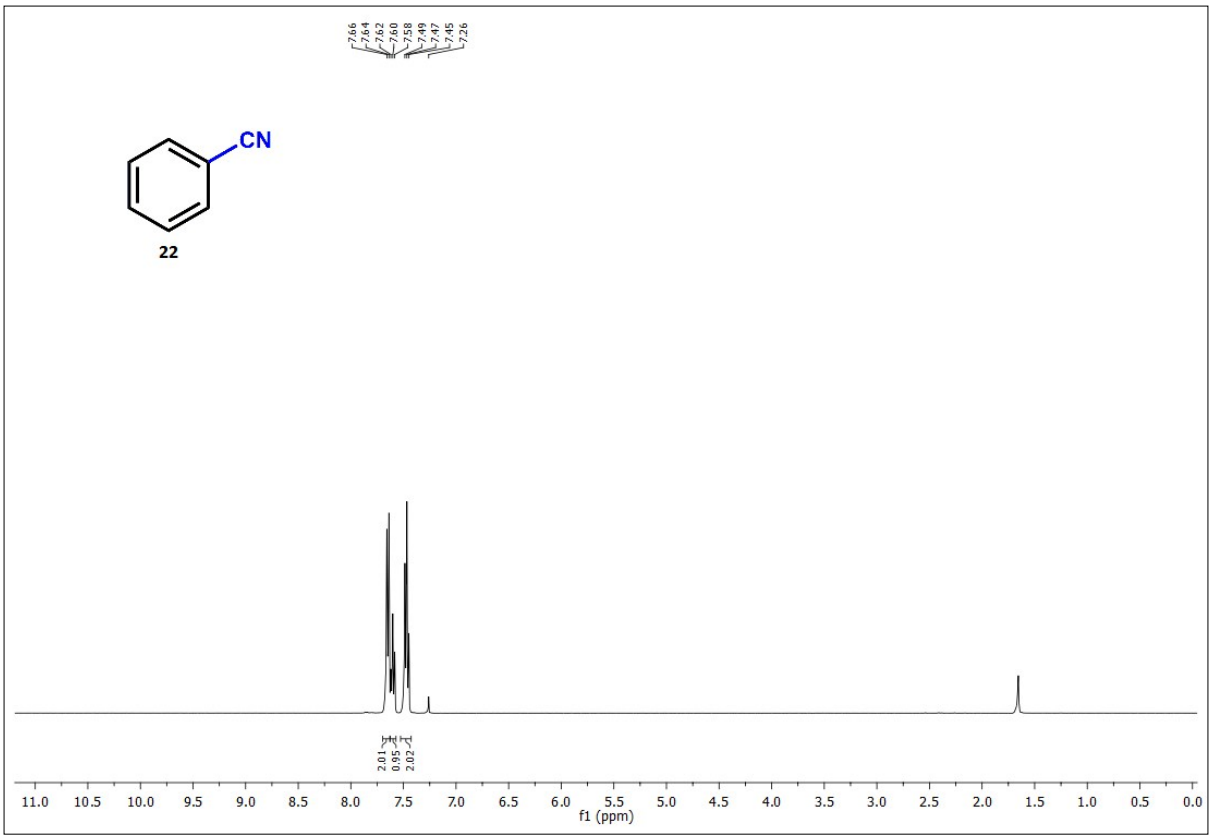
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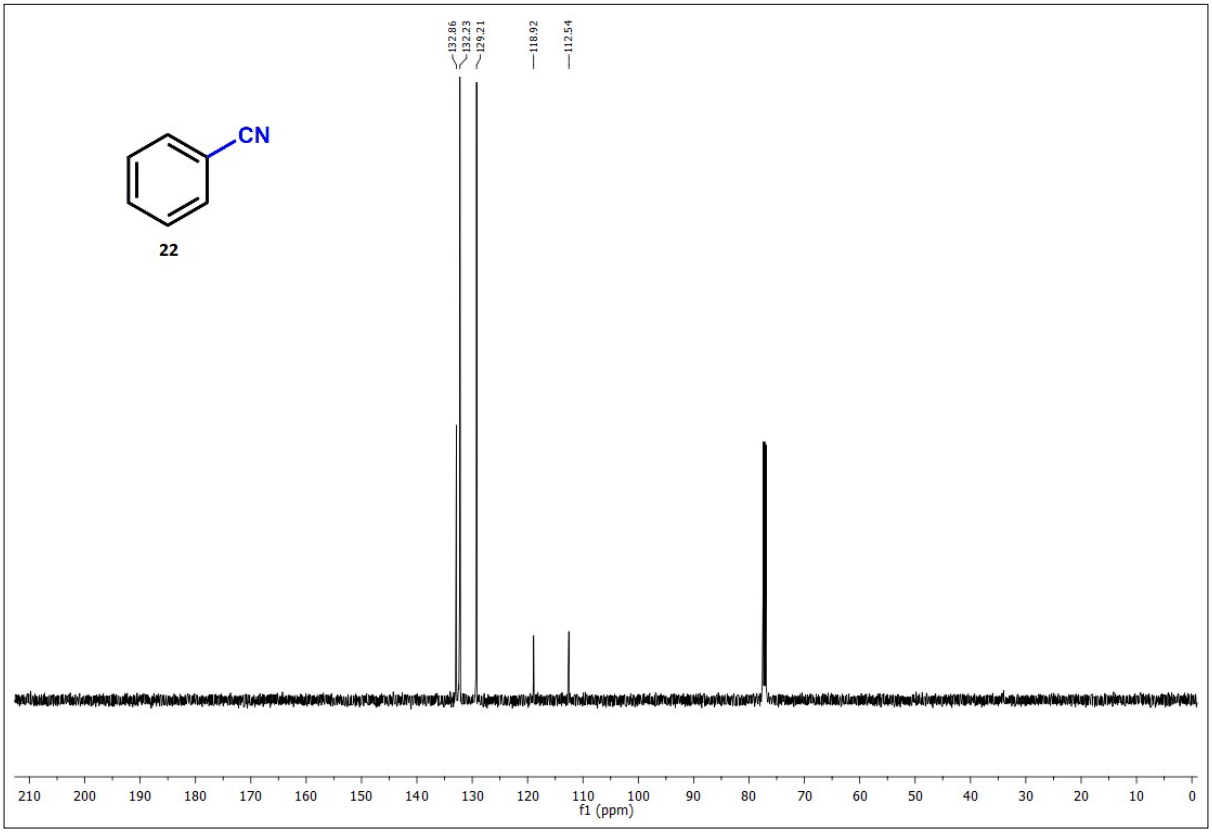
7.62
7.60
7.58
7.49
7.47
7.45
7.26
CN
22
2.01
0.95
2.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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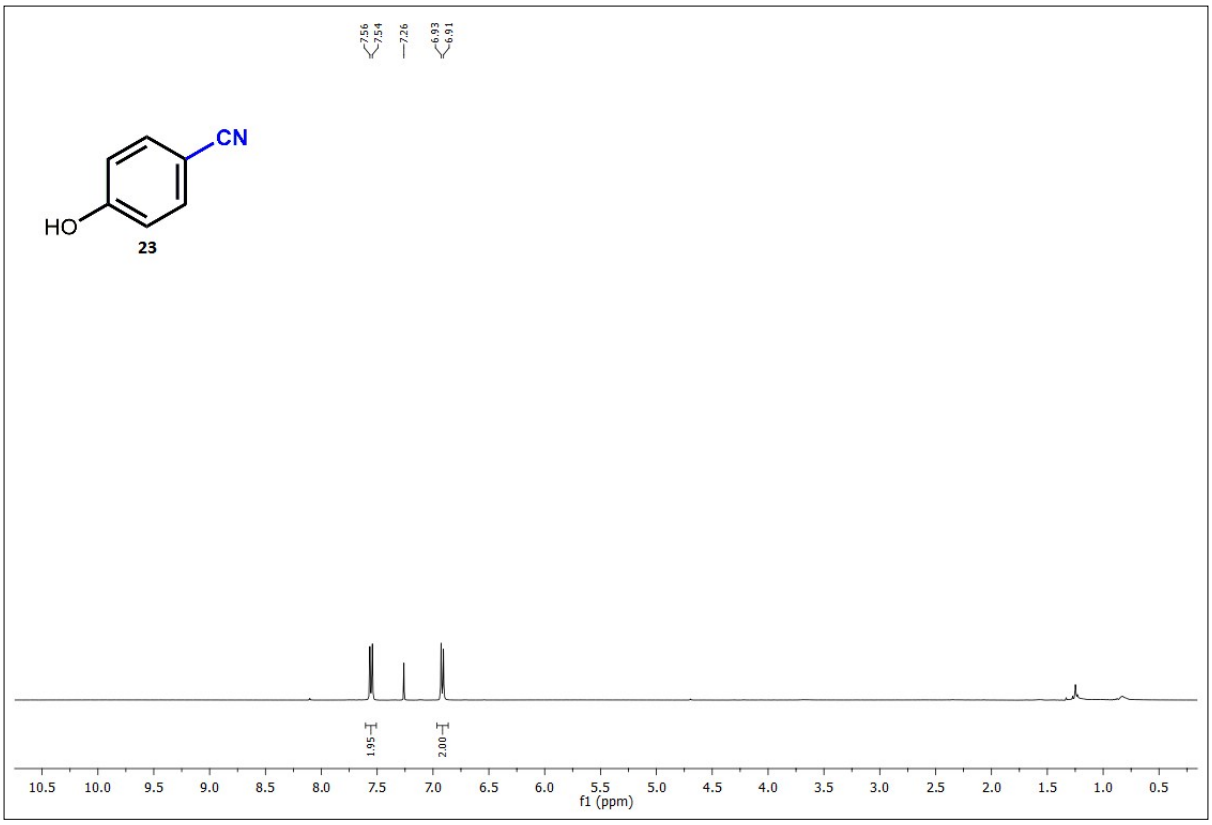
f1 (ppm)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7.54
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6.91
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HO
23
1.95
2.00
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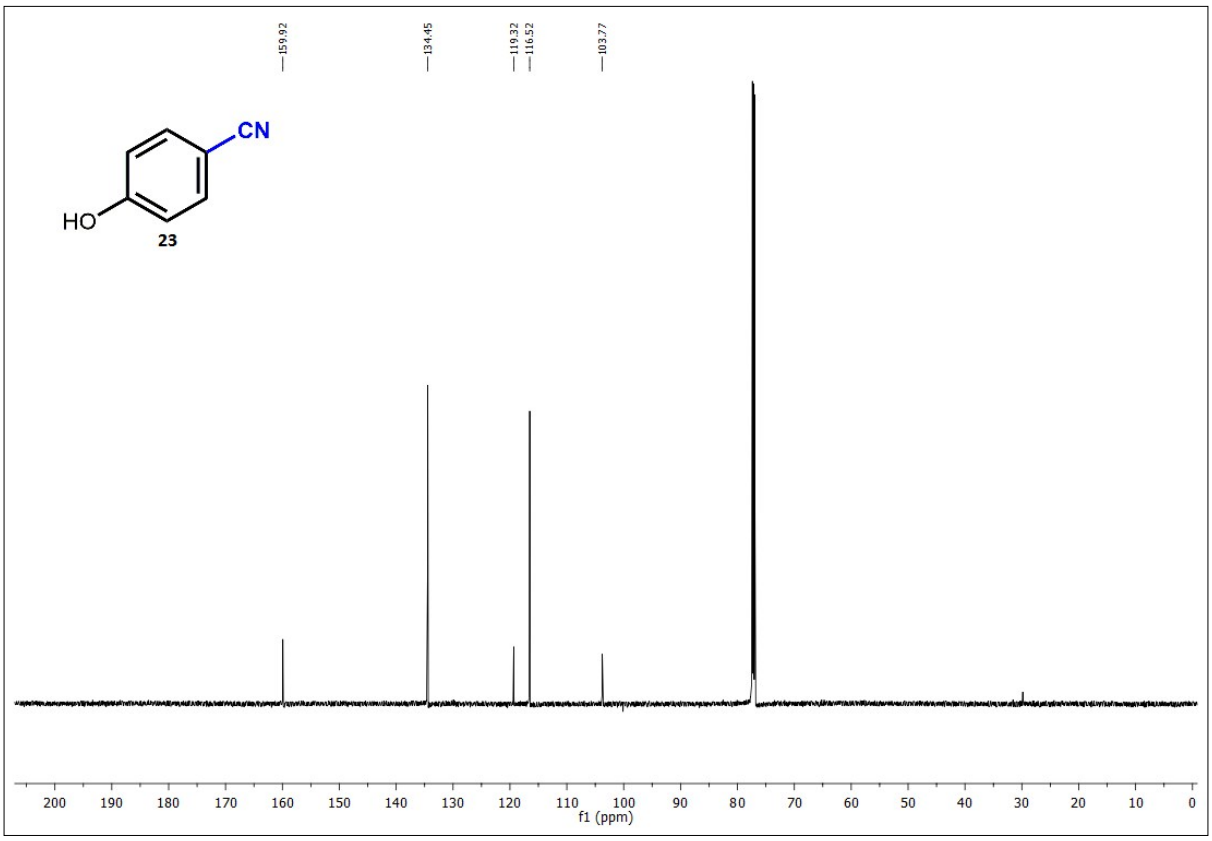
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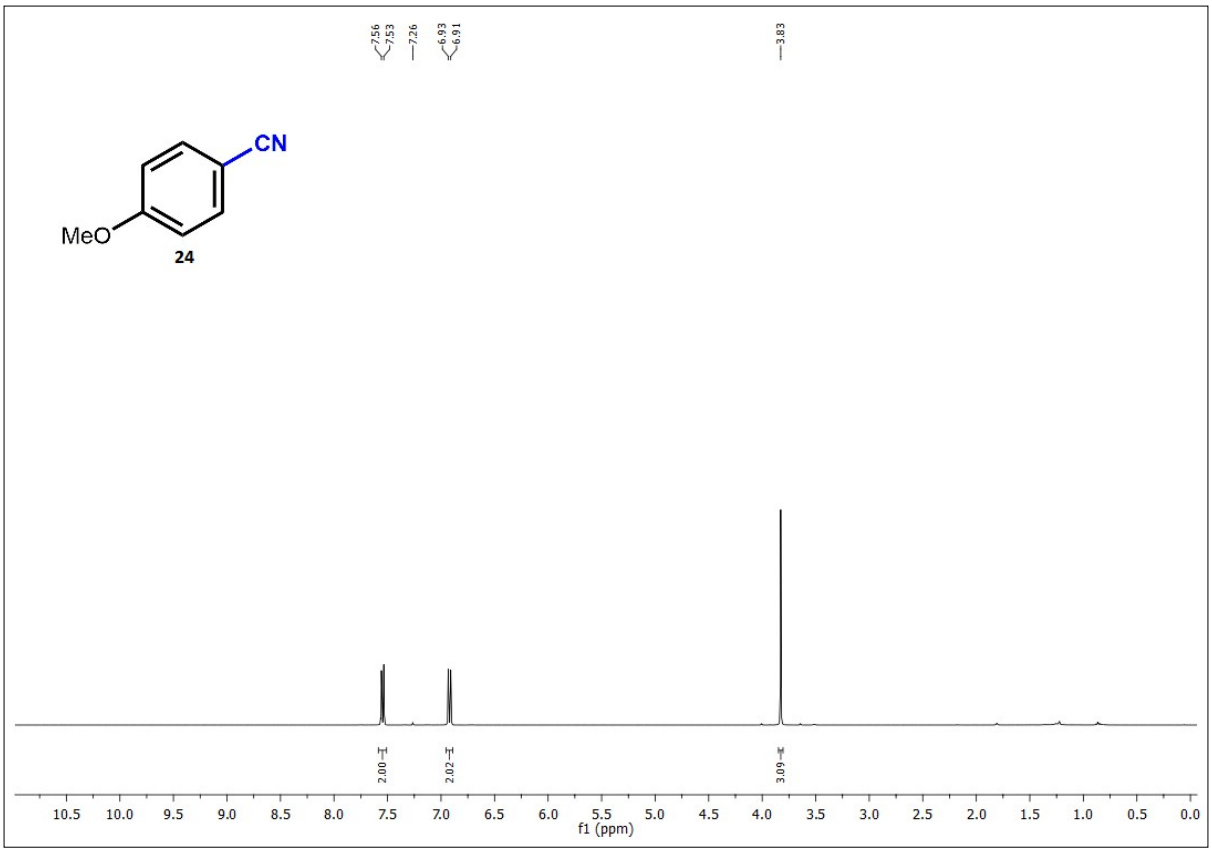
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CN
MeO
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2.02
3.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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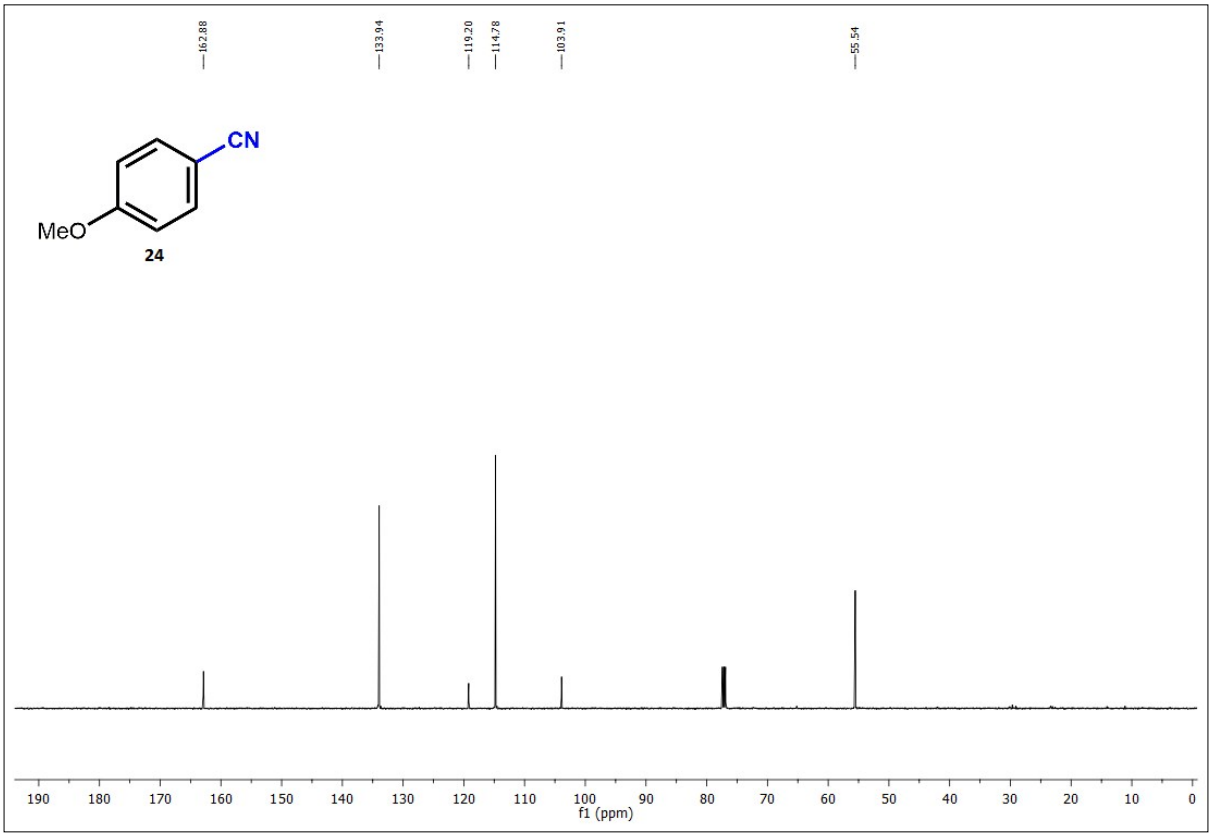
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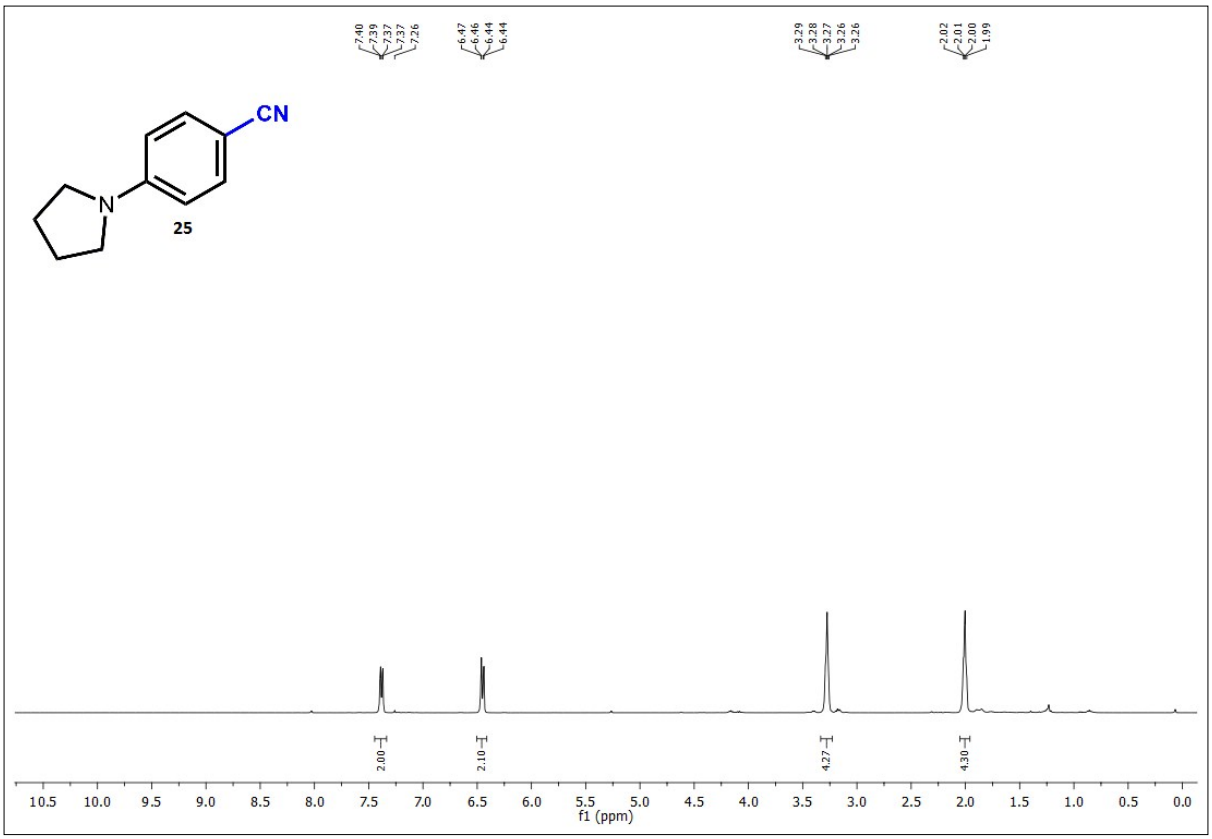
MeO
24
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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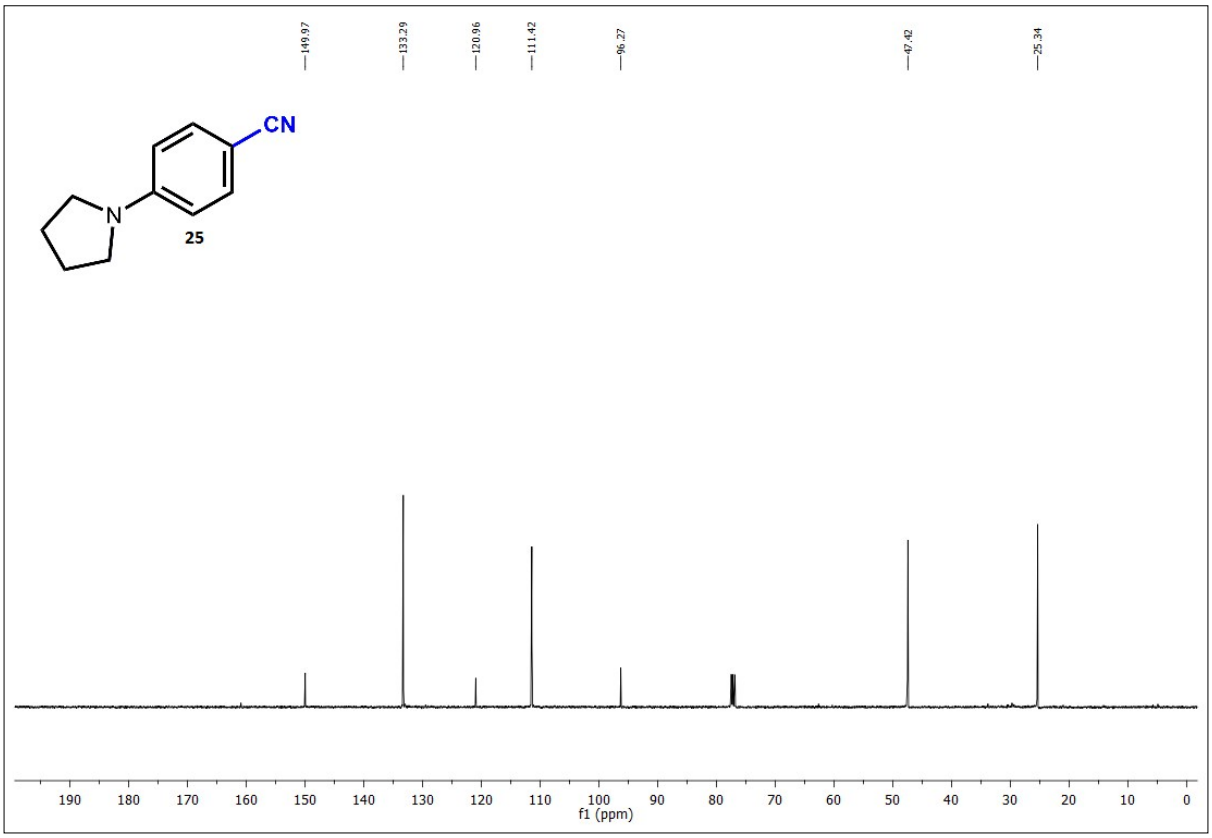
7.39
7.37
7.37
7.26
6.47
6.46
6.44
6.44
3.29
3.28
3.27
3.26
3.26
2.02
2.01
2.00
1.99
CN
N
25
2.00
2.10
4.27
4.30
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.29
120.96
111.42
96.27
47.42
25.34
CN
N
25
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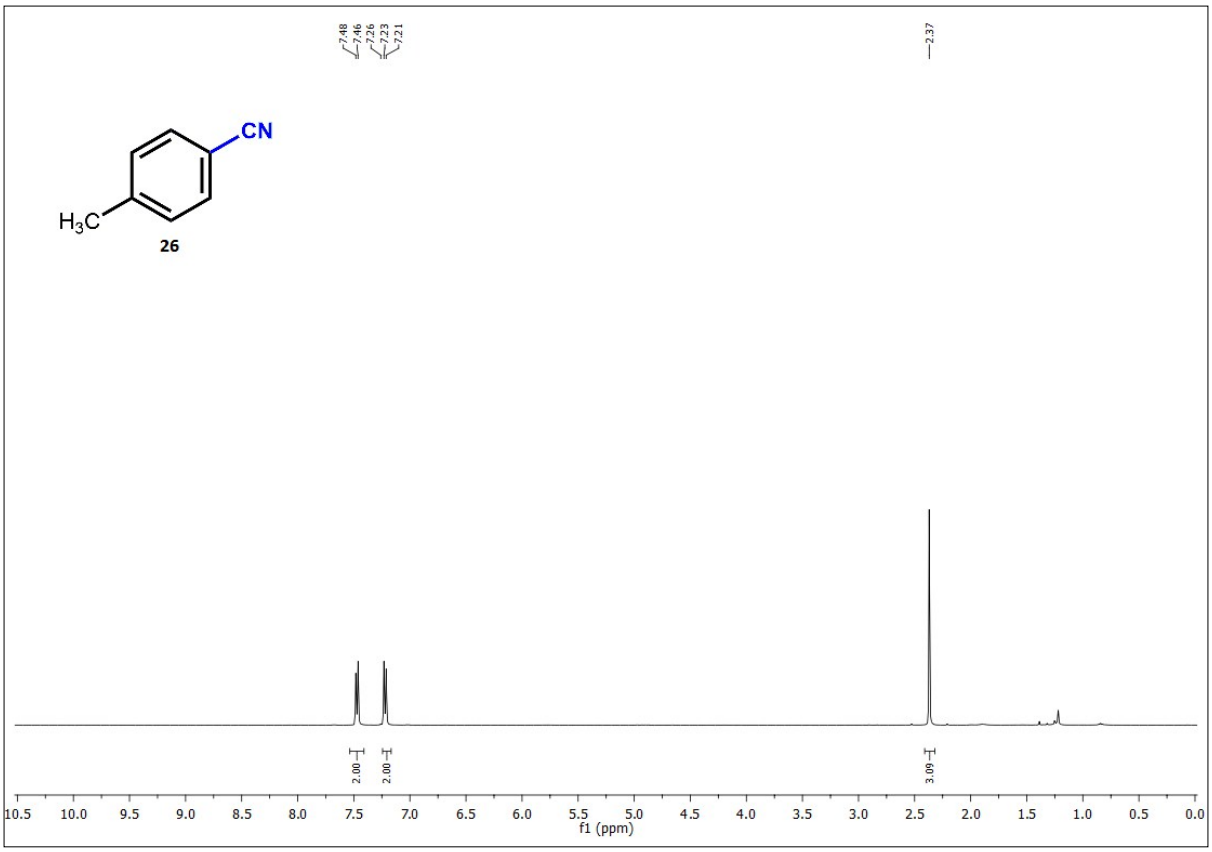
f1 (ppm)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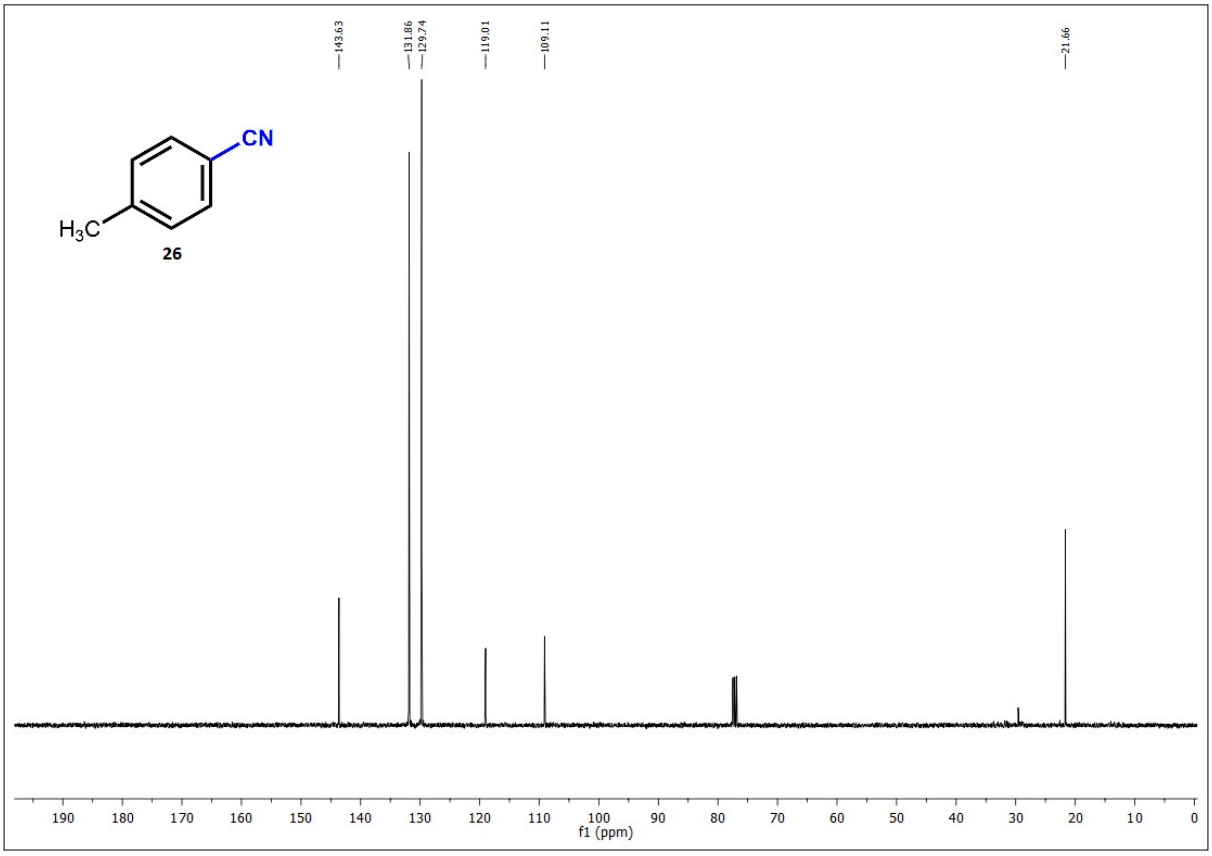
7.46
7.26
7.23
7.21
2.37
CN
H3C
26
2.00
2.00
3.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


143.63
131.86
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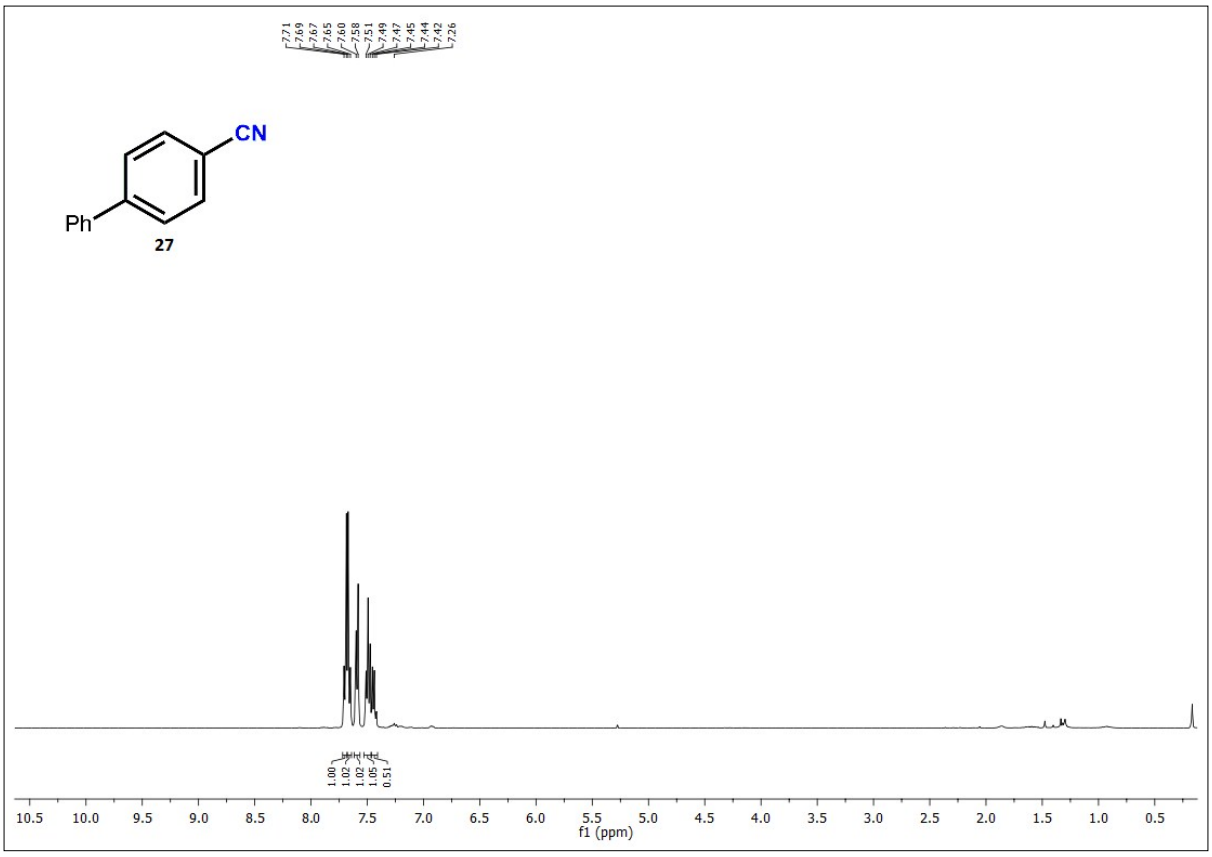
119.01
109.11
21.66
CN
H3C
26
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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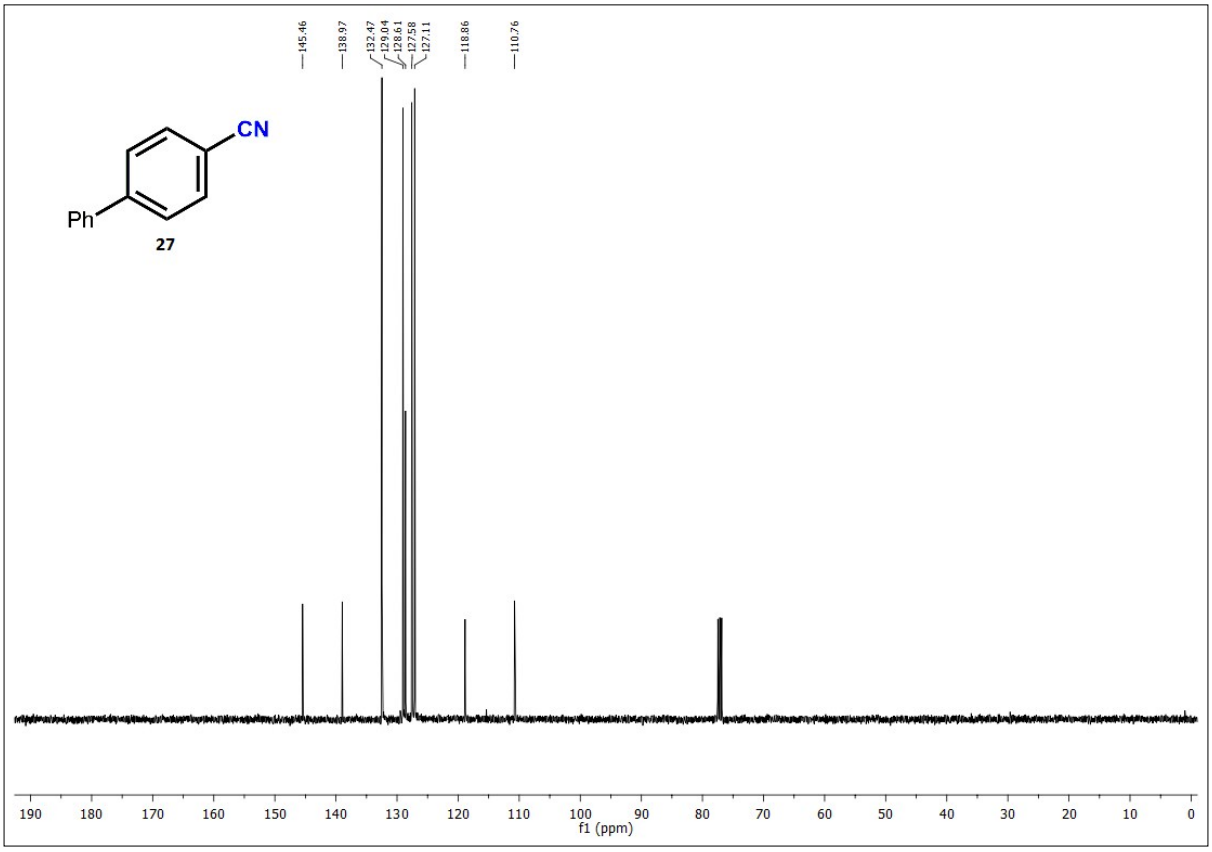
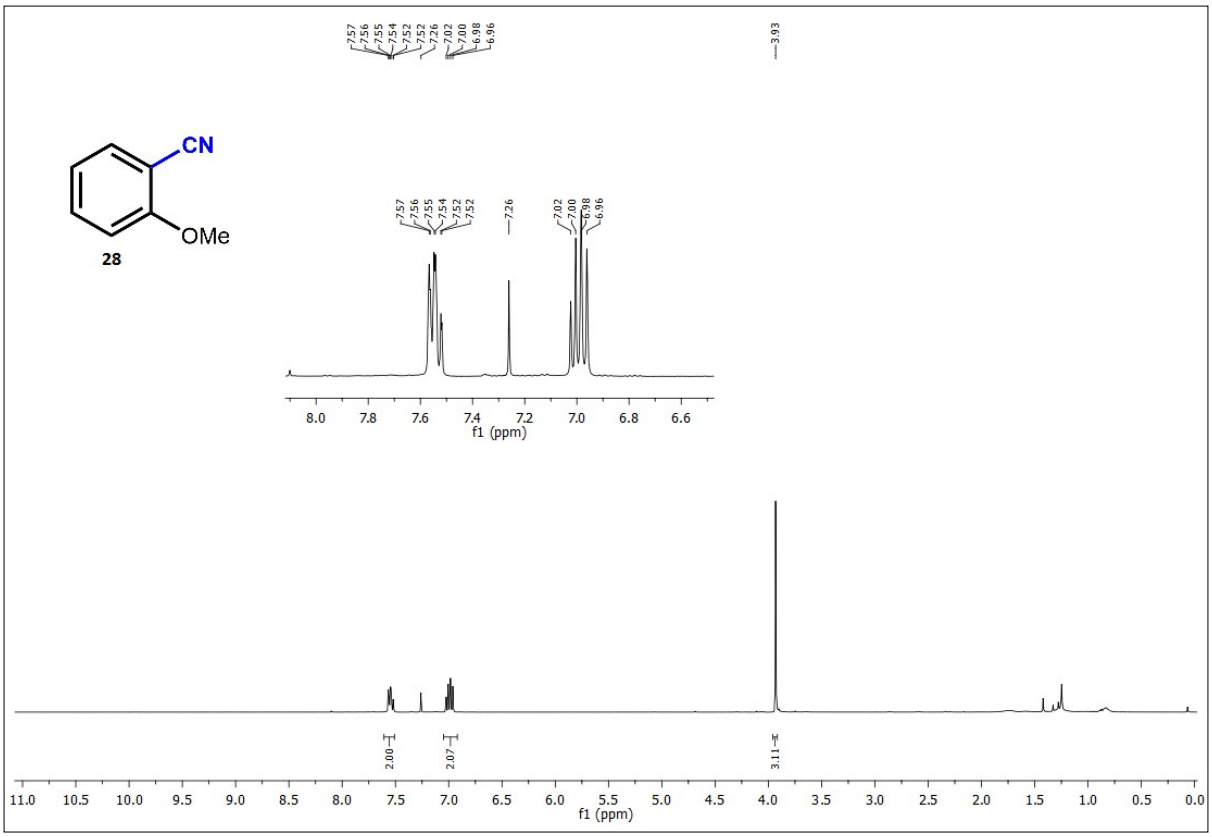
7.51
7.49
7.47
7.45
7.44
7.42
7.26
CN
Ph
27
1.00
1.02
1.02
1.05
0.51
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


145.46
138.97
132.47
129.04
128.61
127.58
127.11
118.86
110.76
CN
Ph
27
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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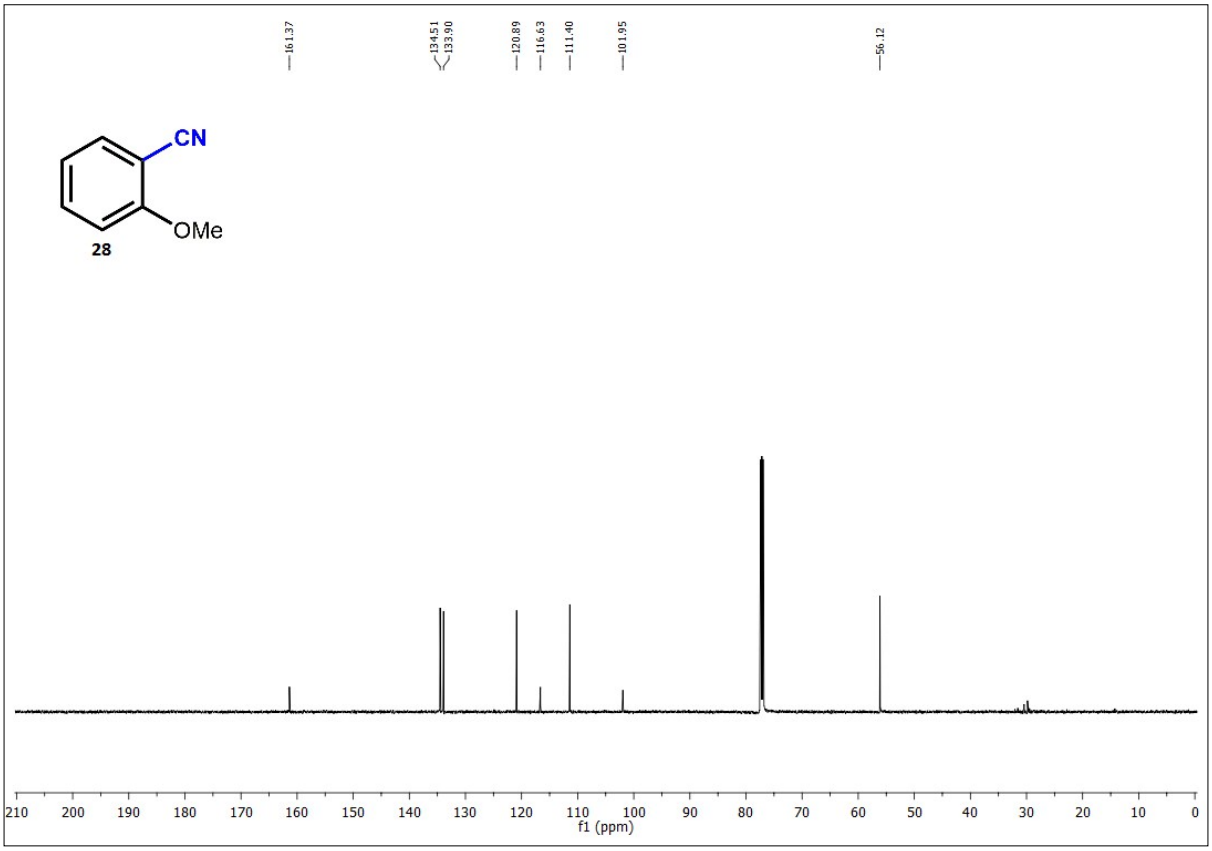
7.56
7.55
7.54
7.52
7.52
7.26
7.02
7.00
6.98
6.96
3.93
CN
OMe
28
f1 (ppm)
2.00
2.07
3.11
f1 (ppm)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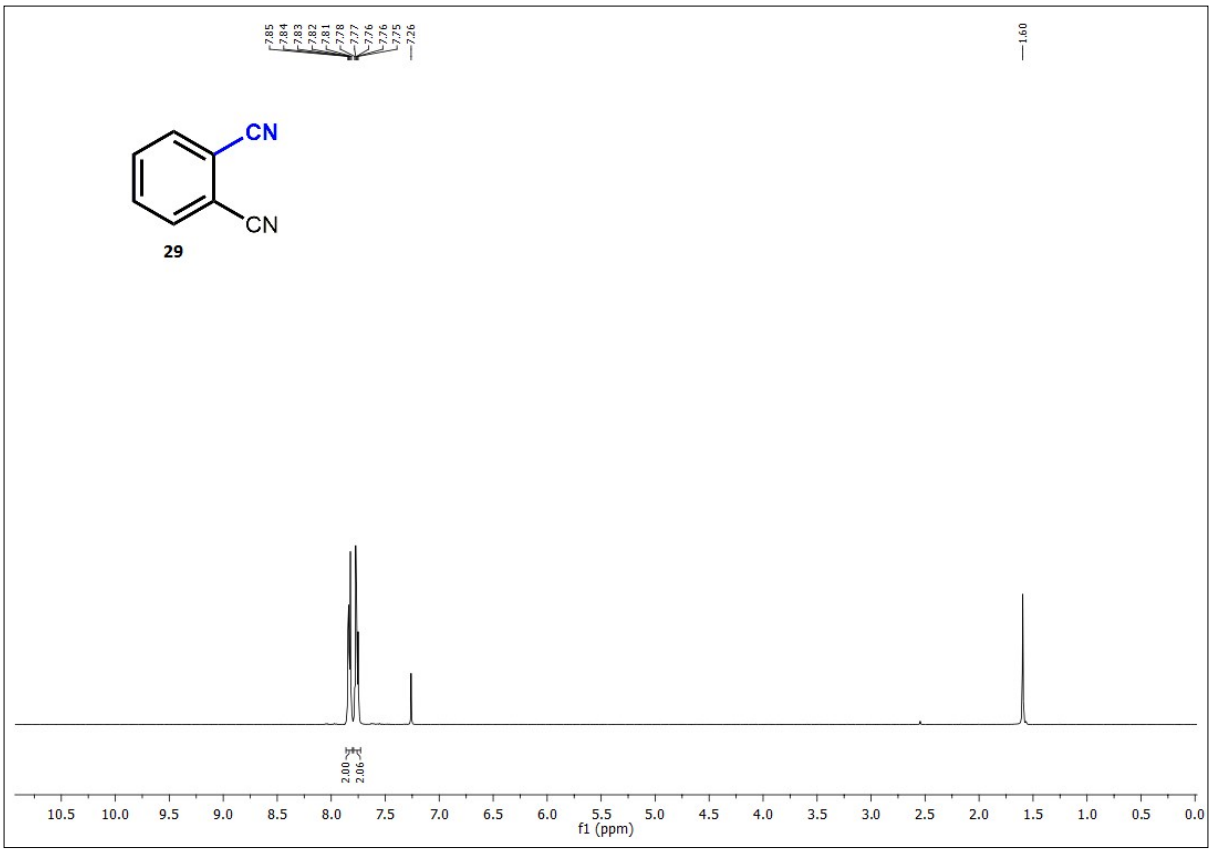
116.63
111.40
101.95
56.12
CN
OMe
28
f1 (ppm)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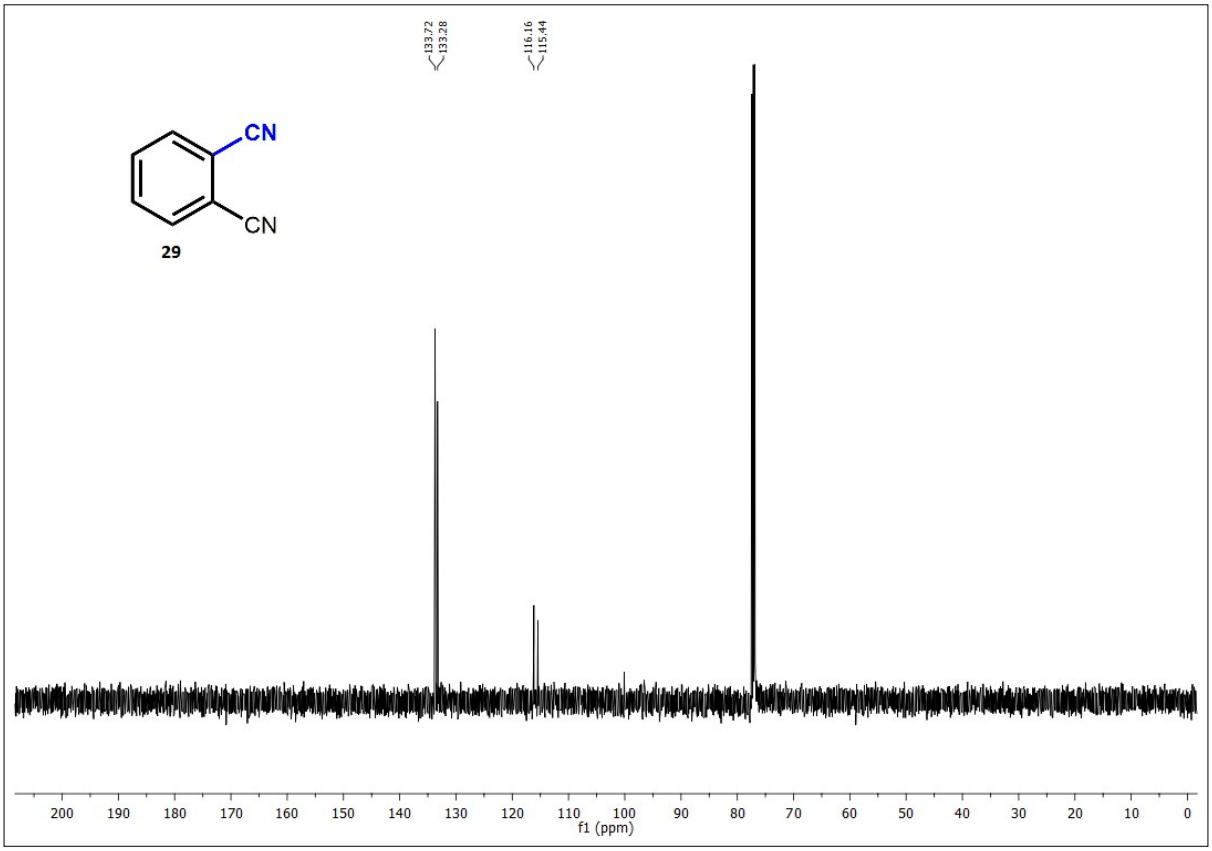
7.84
7.83
7.82
7.81
7.78
7.77
7.76
7.76
7.75
7.26
1.60
CN
CN
29
2.00
2.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.28
116.16
115.44
CN
CN
29
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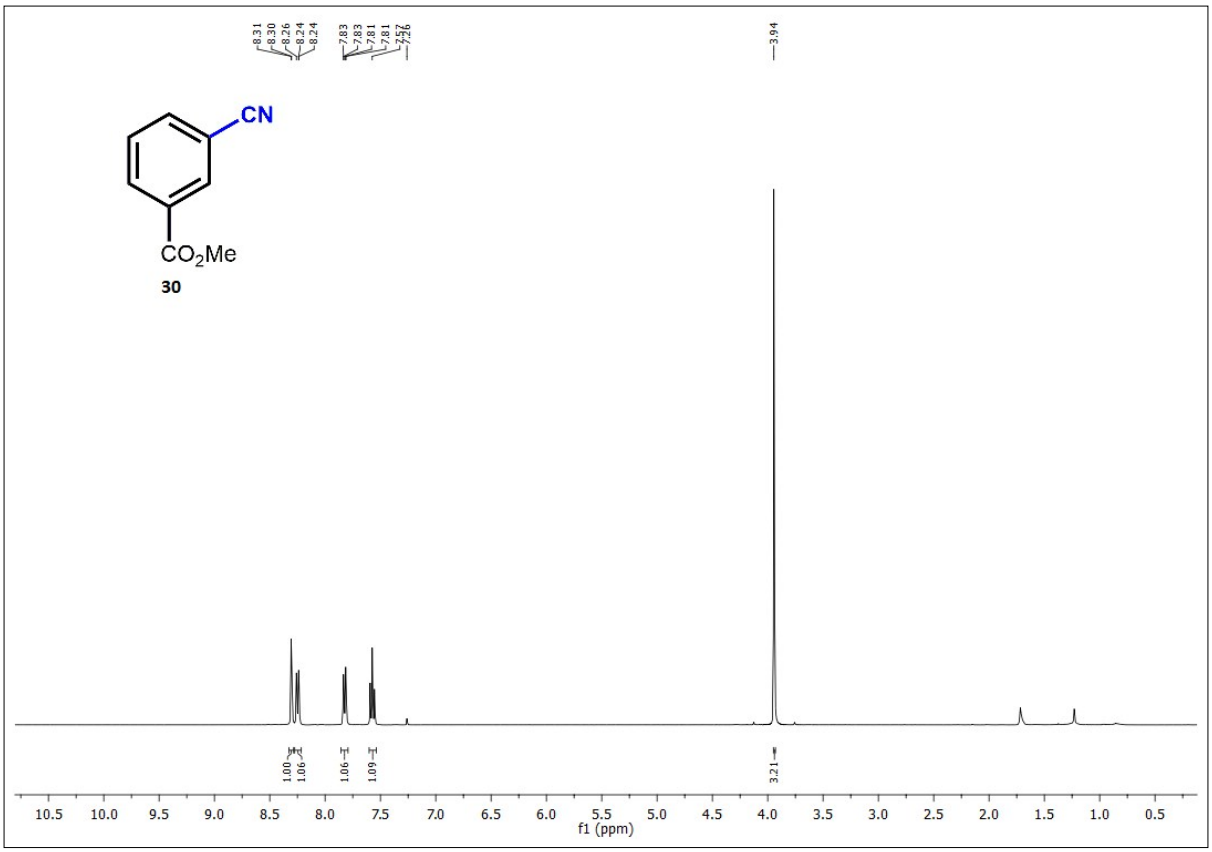
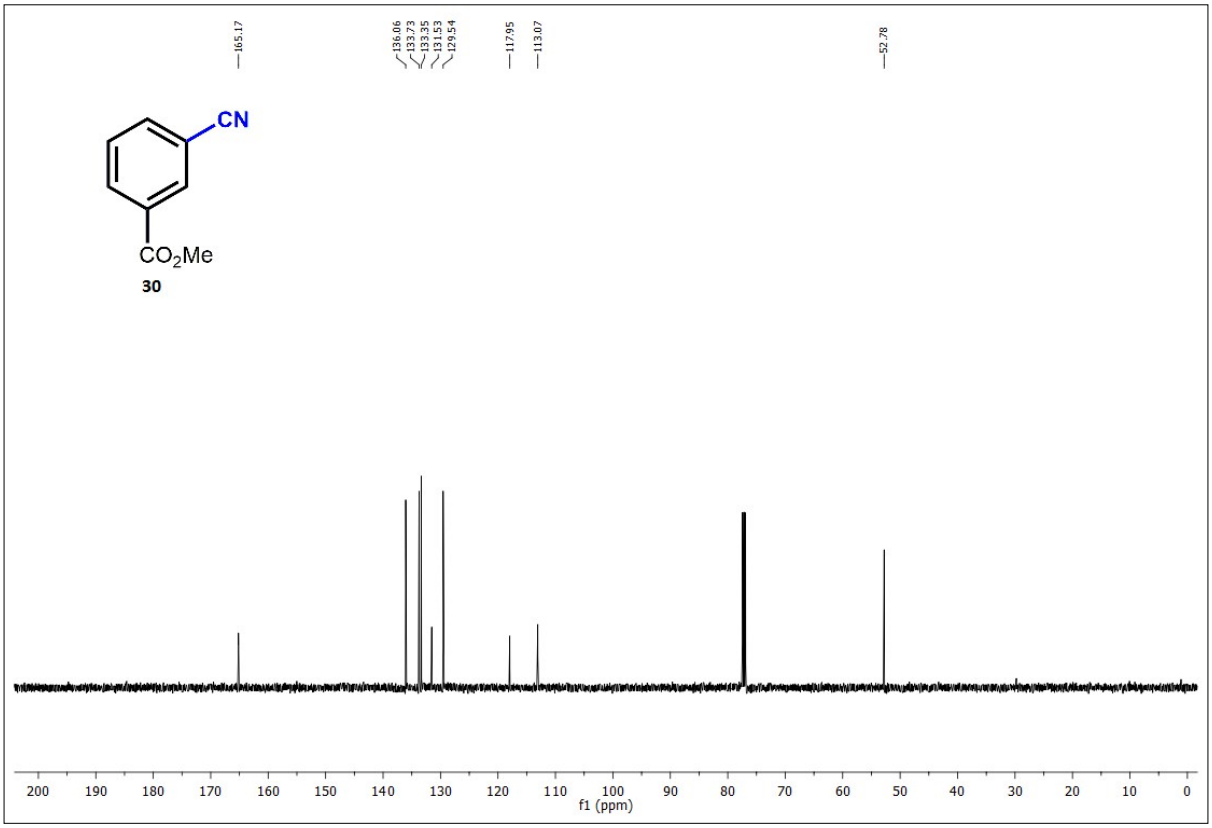
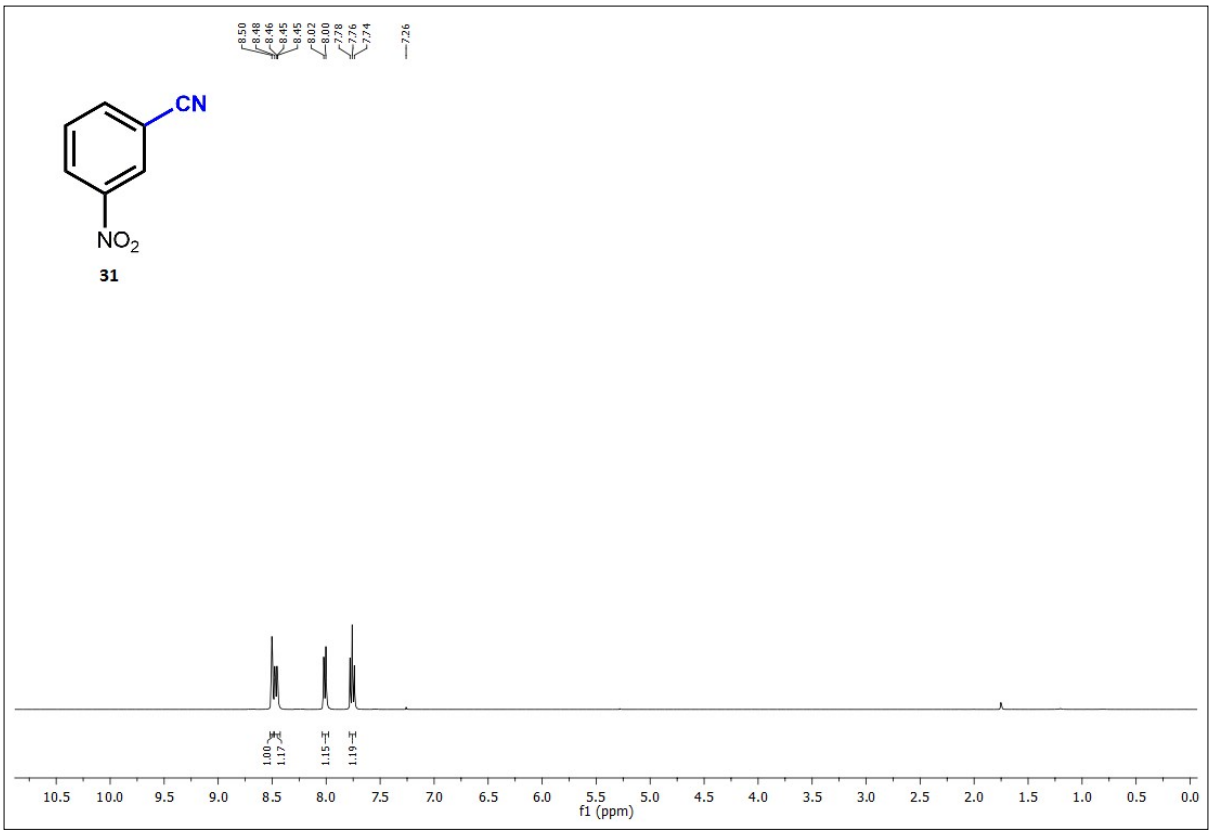
f1 (ppm)


8.31
8.30
8.26
8.24
8.24
7.83
7.83
7.81
7.81
7.58
7.56
3.94
CN
CO2Me
30
1.00
1.06
1.06
1.09
3.21
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


165.17
136.06
133.73
133.55
131.53
129.54
117.95
113.07
52.78
CN
CO2Me
30
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.50
8.48
8.46
8.45
8.45
8.02
8.00
7.78
7.76
7.74
7.26
CN
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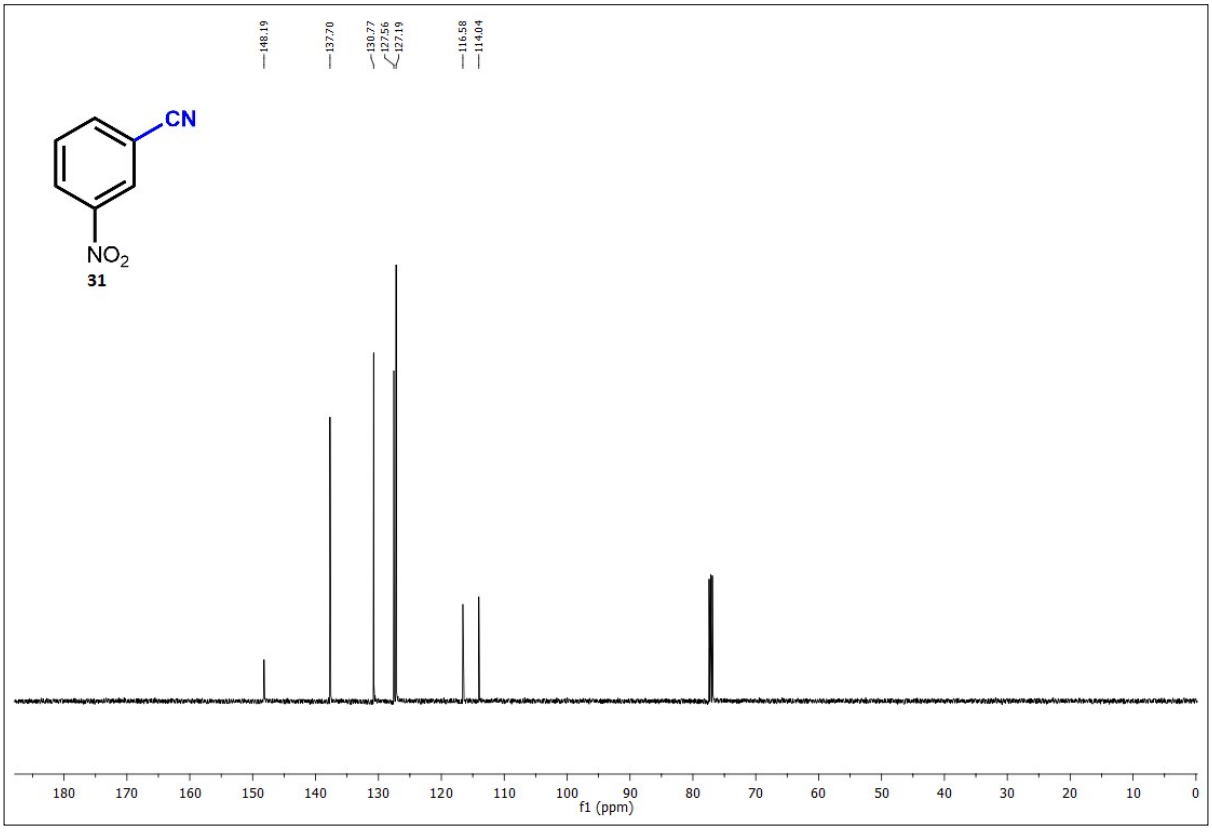
1.00
1.17
1.15
1.19
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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137.70
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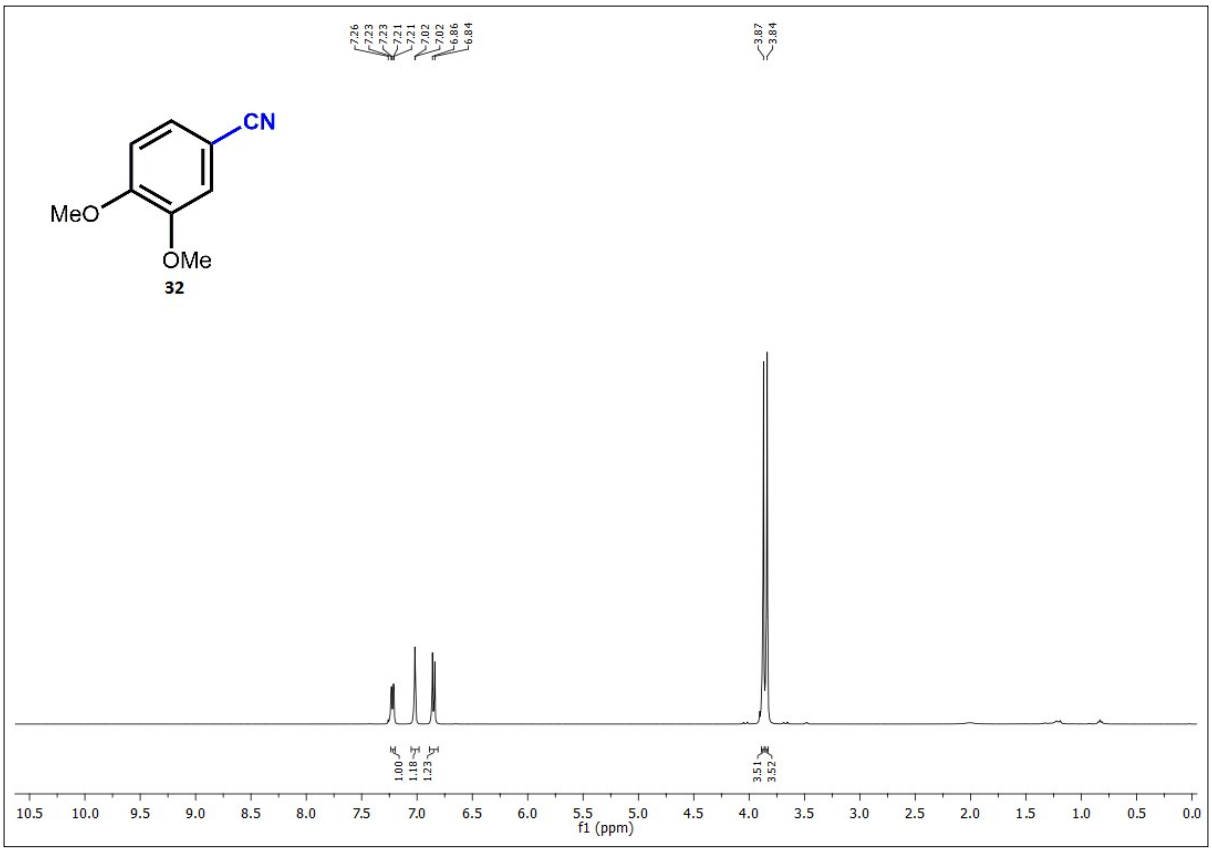
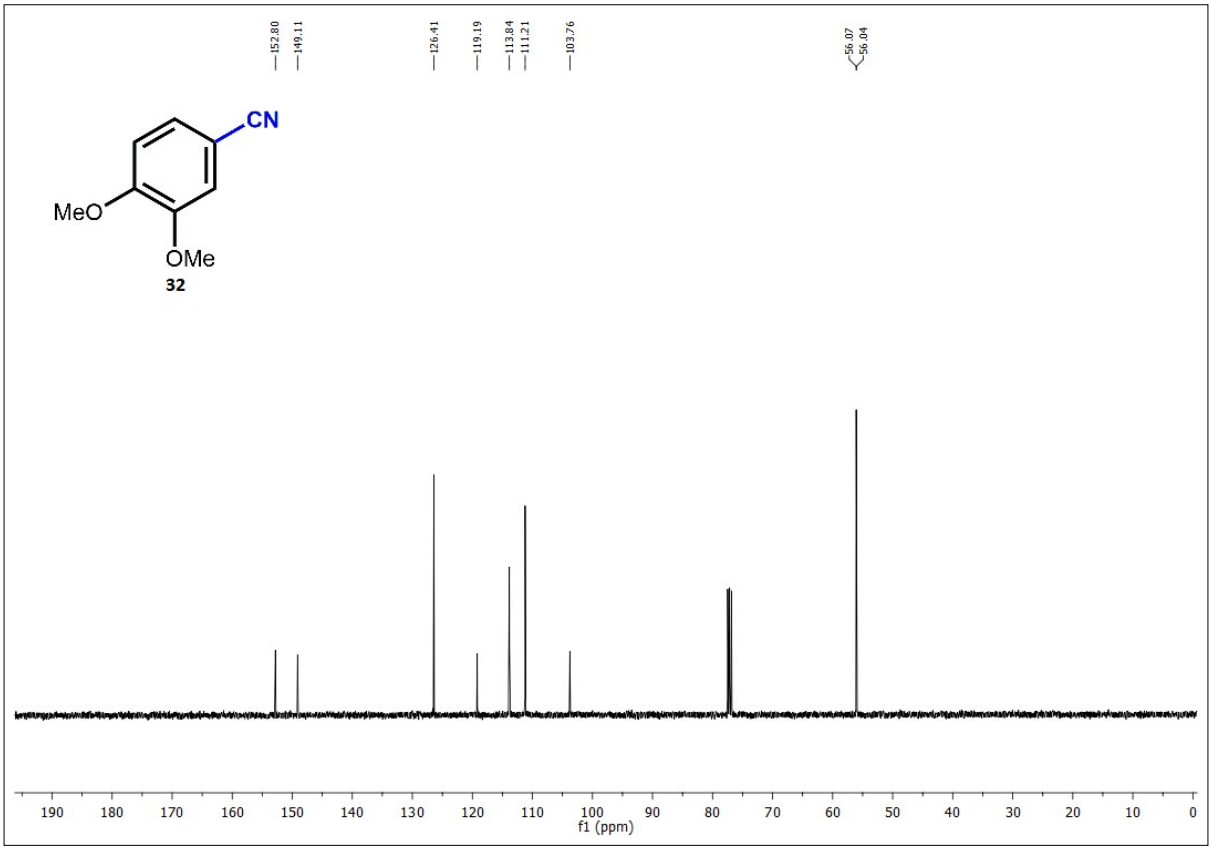
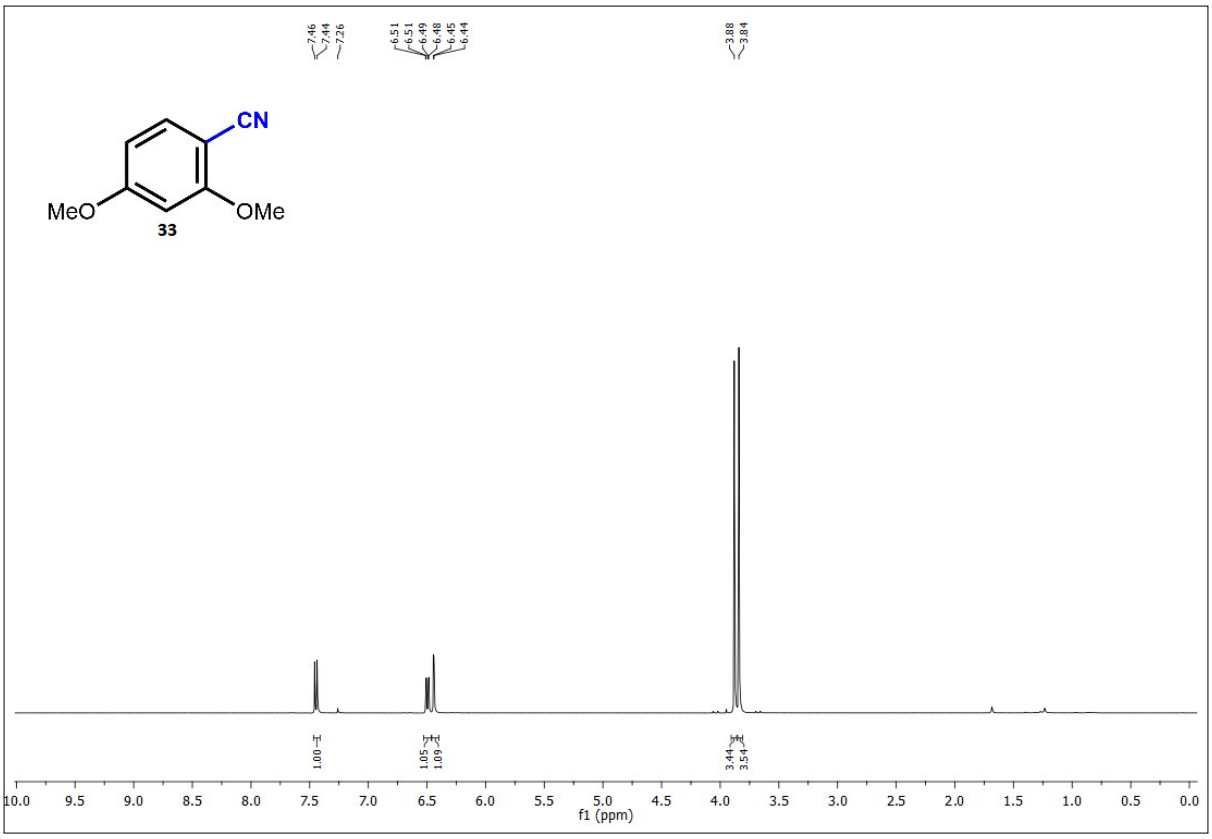
127.56
127.19
116.58
114.04
CN
NO2
31
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.26
7.23
7.23
7.21
7.21
7.02
7.02
6.86
6.84
3.87
3.84
CN
MeO
OMe
32
1.00
1.18
1.23
3.51
3.52
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


152.80
149.11
126.41
119.19
113.84
111.21
103.76
56.07
56.04
CN
MeO
OMe
32
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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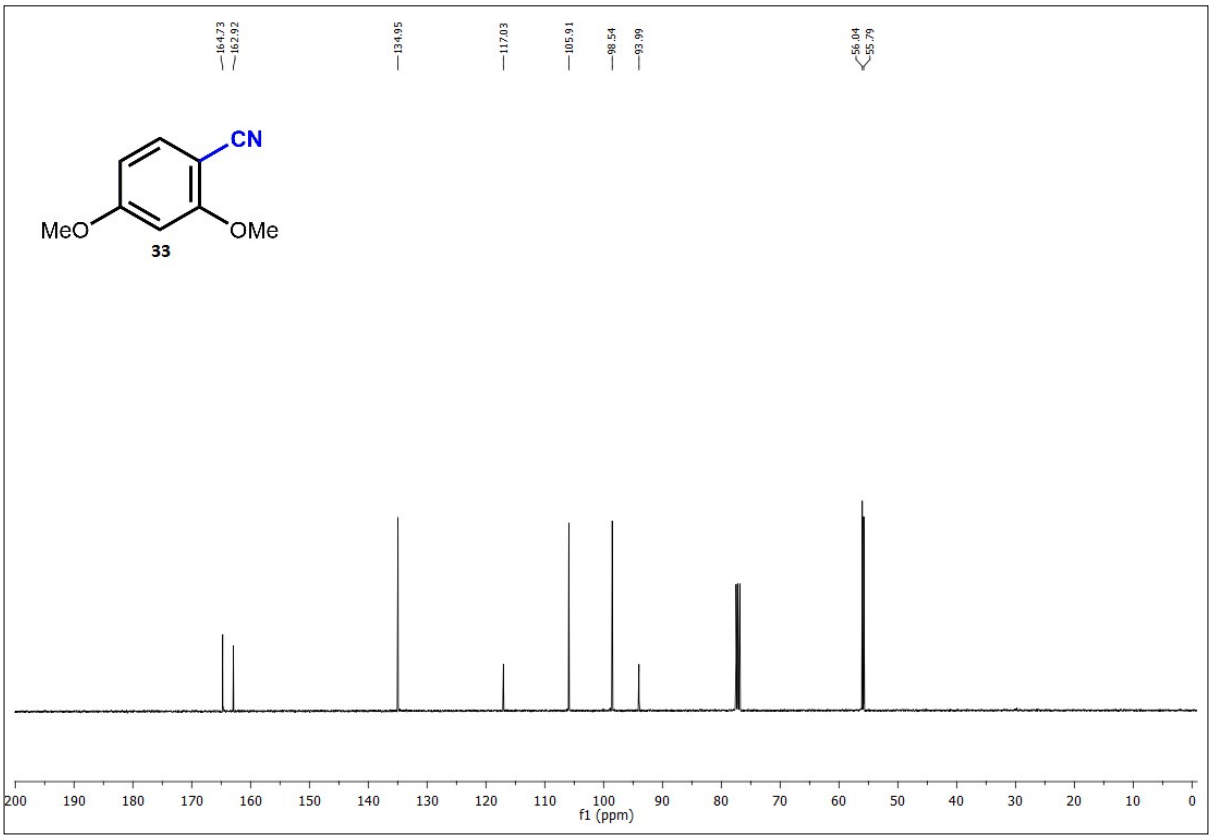
7.44
7.26
6.51
6.51
6.49
6.48
6.45
6.44
3.88
3.84
CN
MeO
OMe
33
1.00
1.05
1.09
3.44
3.54
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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162.92
134.95
117.03
105.91
98.54
93.99
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55.79
CN
MeO
OMe
33
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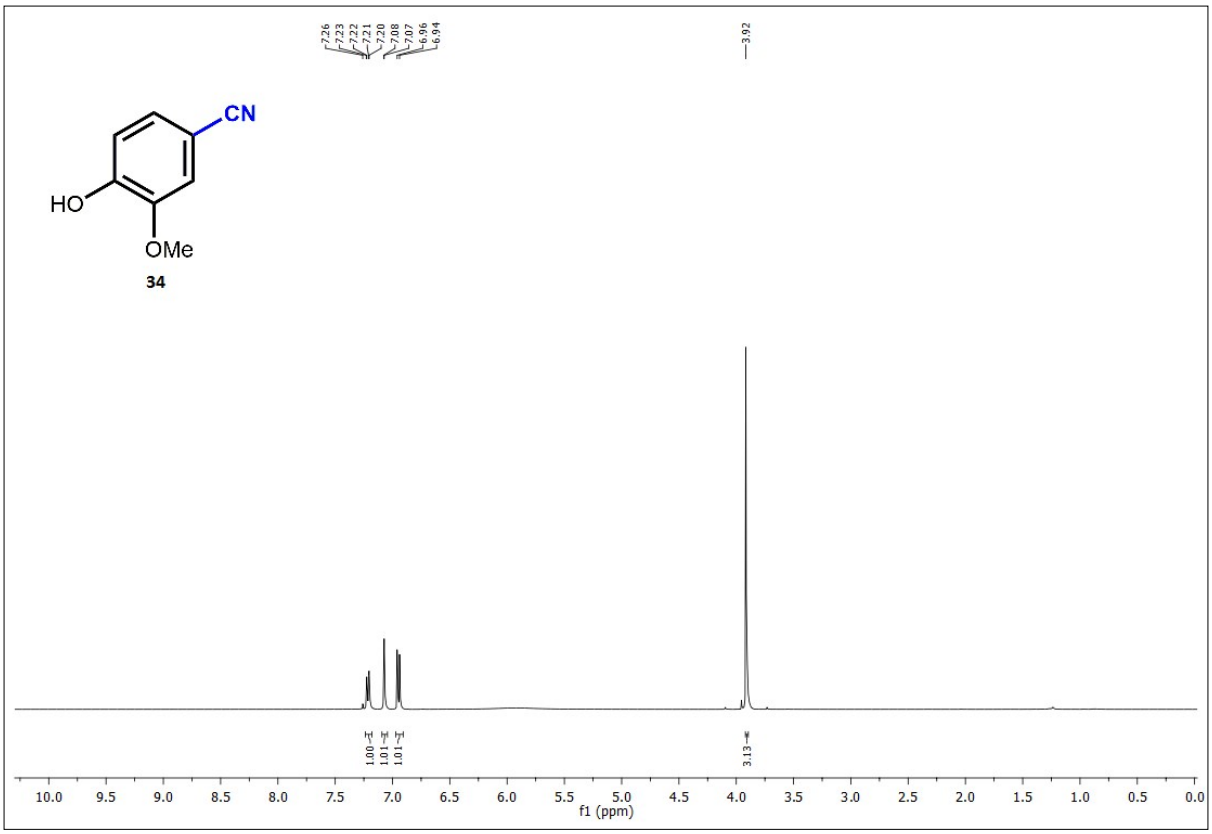
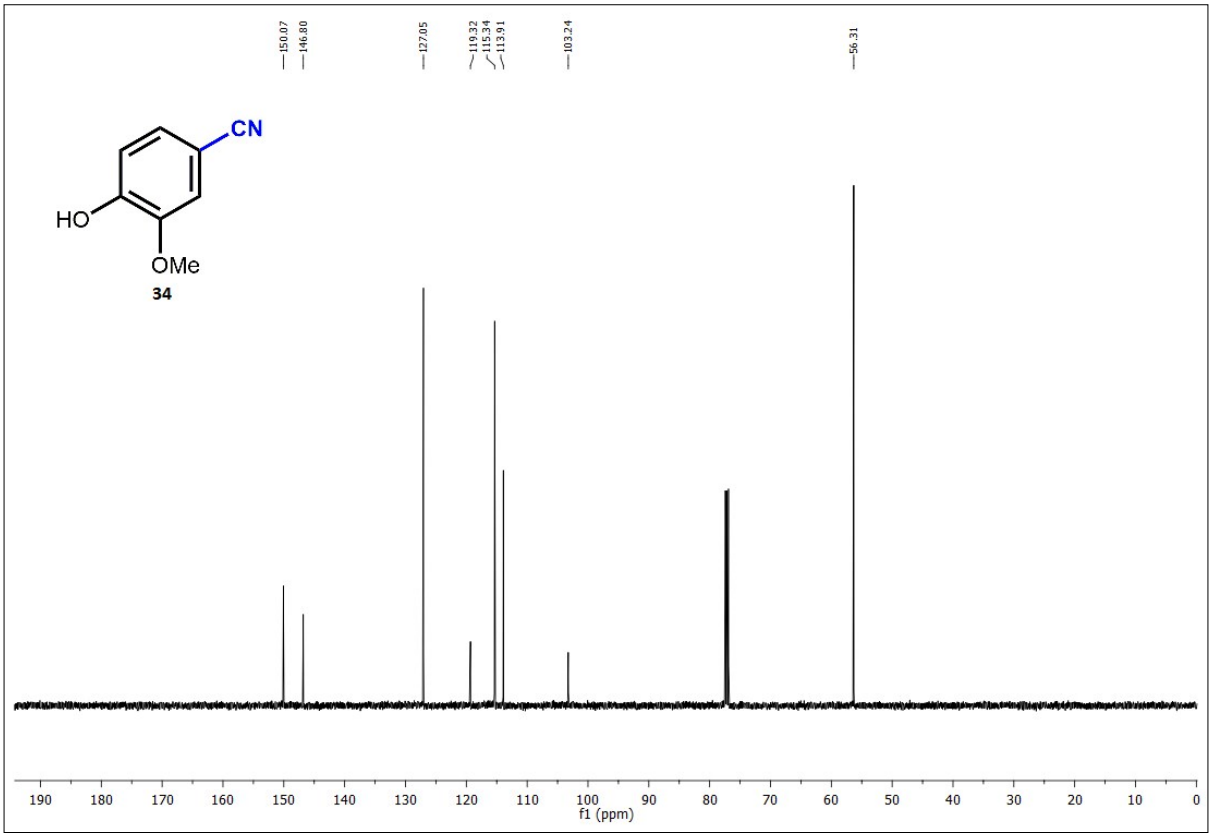
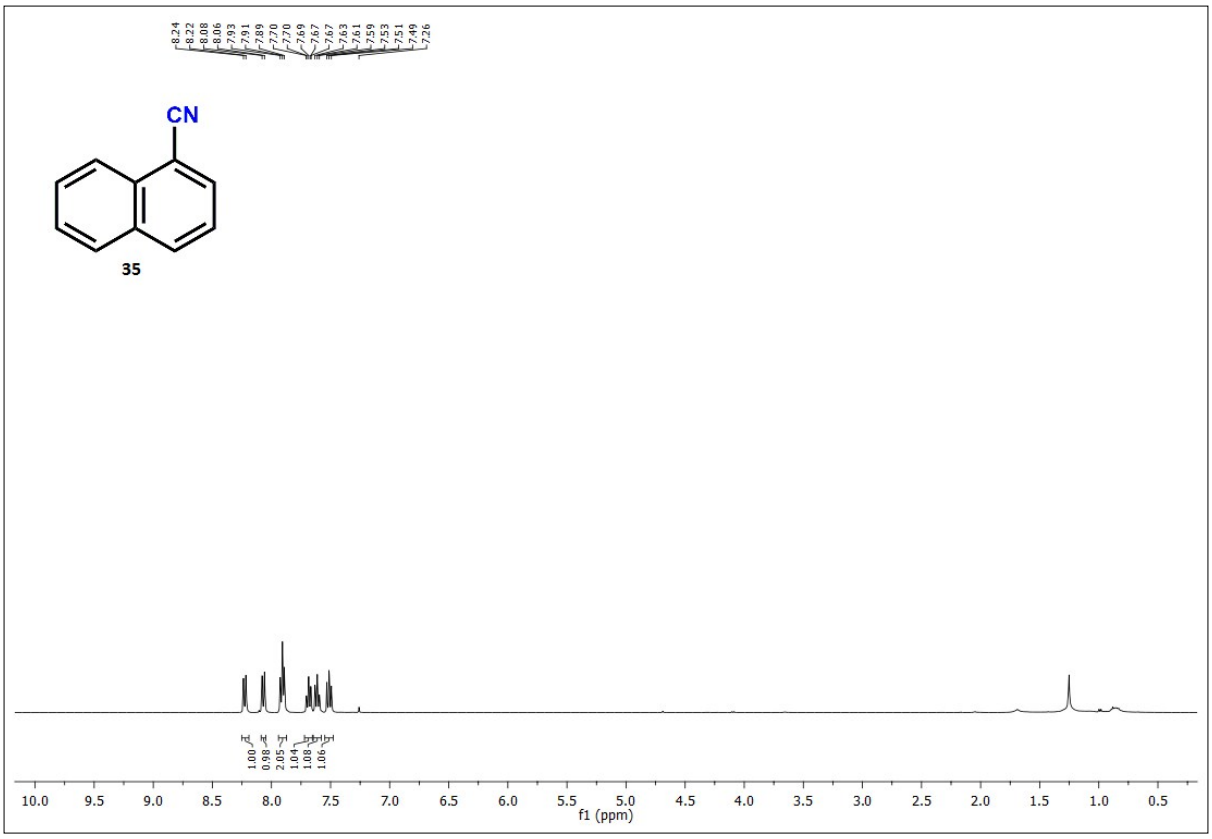
f1 (ppm)


7.26
7.23
7.22
7.21
7.20
7.08
7.07
6.96
6.94
3.92
CN
HO
OMe
34
1.00
1.01
1.01
3.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


150.07
146.80
127.05
119.32
115.34
113.91
103.24
56.31
CN
HO
OMe
34
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.91
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7.70
7.69
7.67
7.67
7.63
7.61
7.59
7.53
7.51
7.49
7.26
CN
35
1.00
0.98
2.05
1.04
1.08
1.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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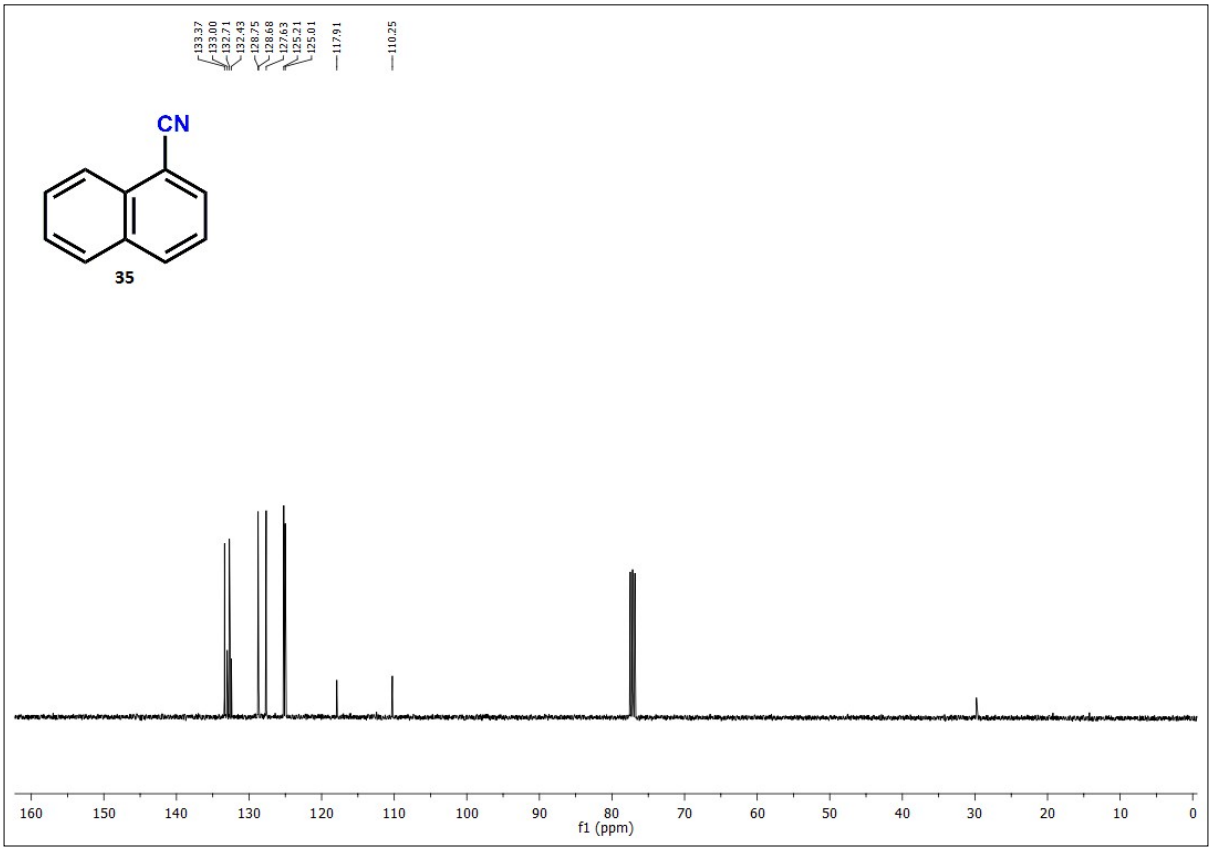
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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127.63
125.21
125.01
117.91
110.25
CN
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130
120
110
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90
80
70
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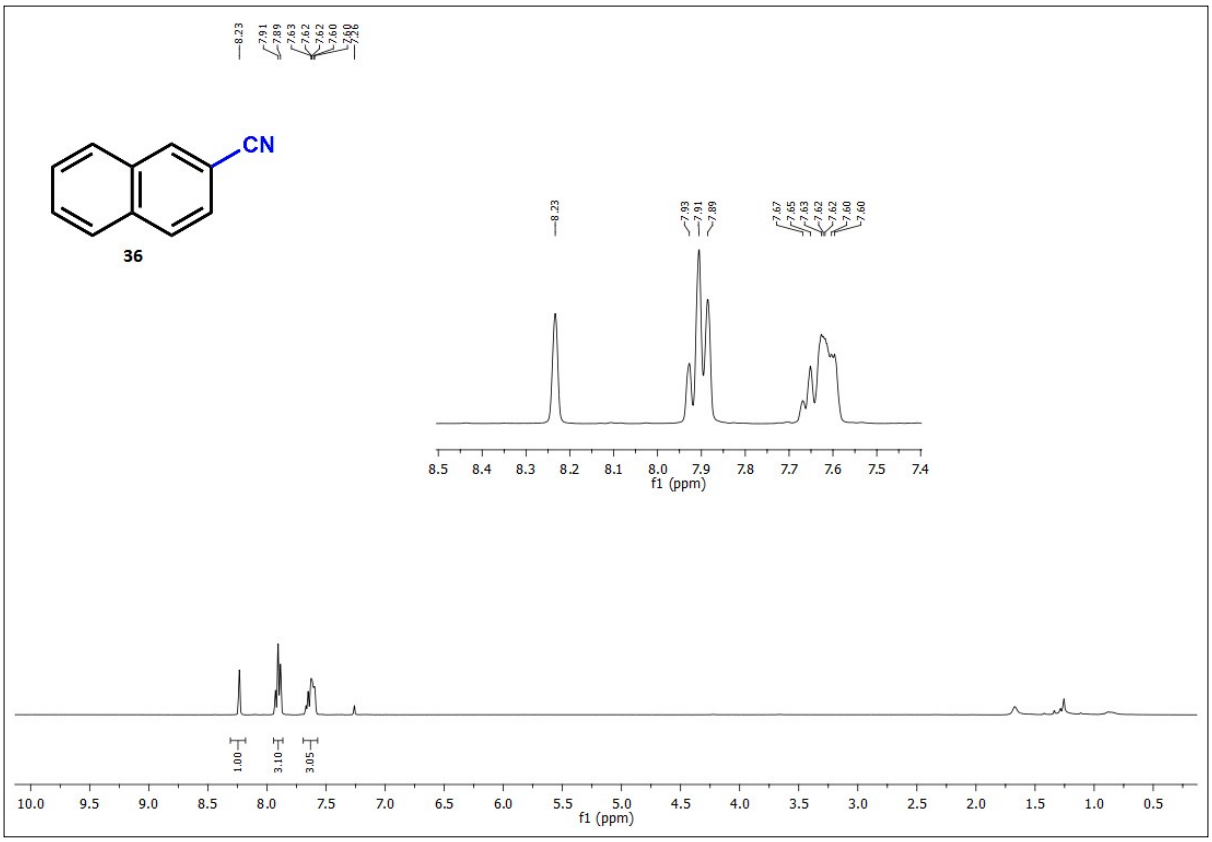
50
40
30
20
10
0
f1 (ppm)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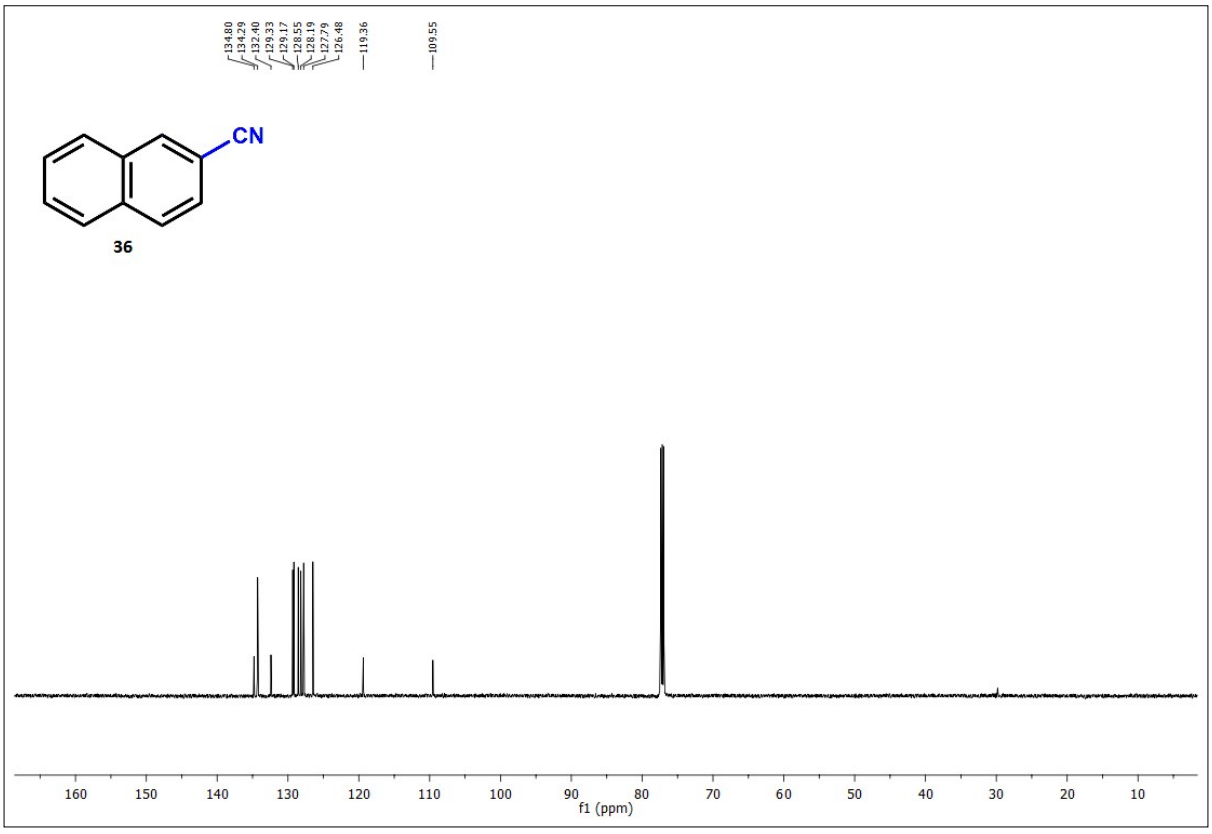
7.62
7.62
7.60
7.60
7.28
CN
36
8.23
7.93
7.91
7.89
7.67
7.65
7.63
7.62
7.62
7.60
7.60
8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4
f1 (ppm)
1.00
3.10
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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134.20
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129.33
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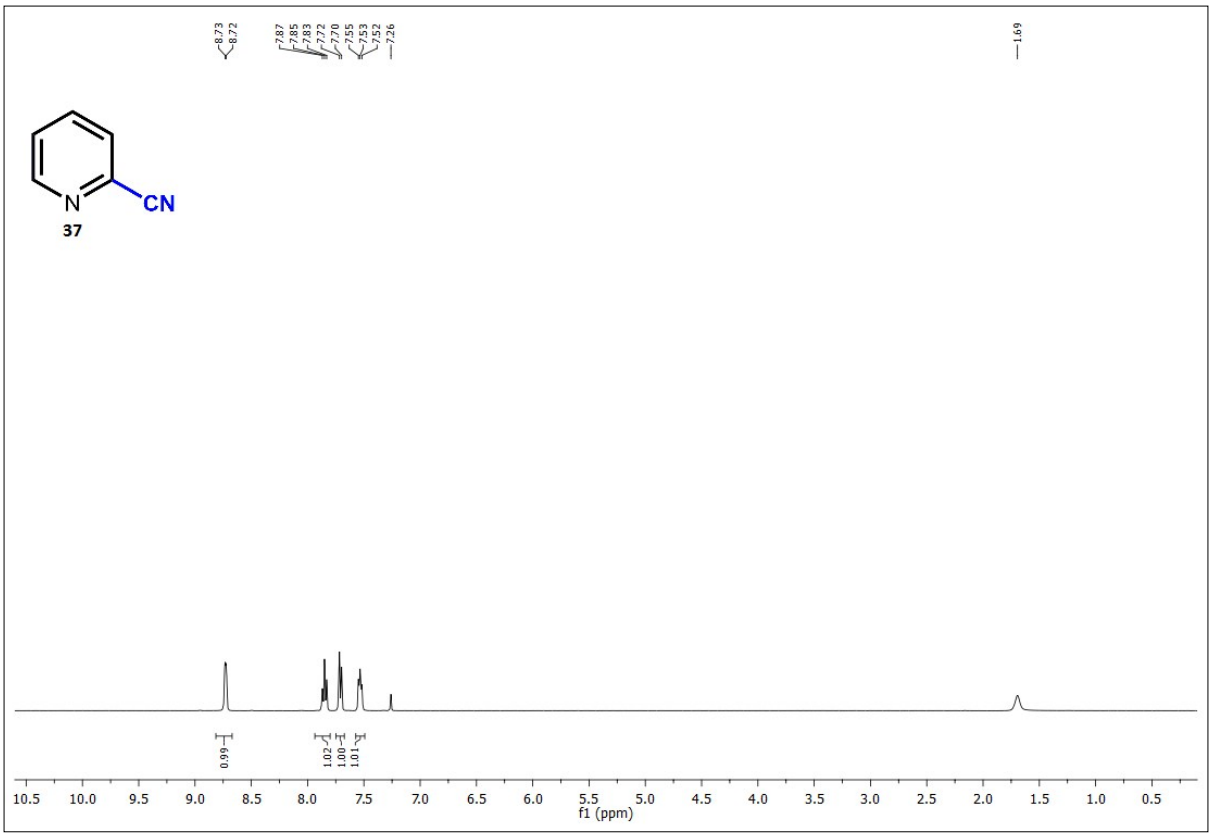
128.19
127.79
126.48
119.36
109.55
CN
36
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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7.72
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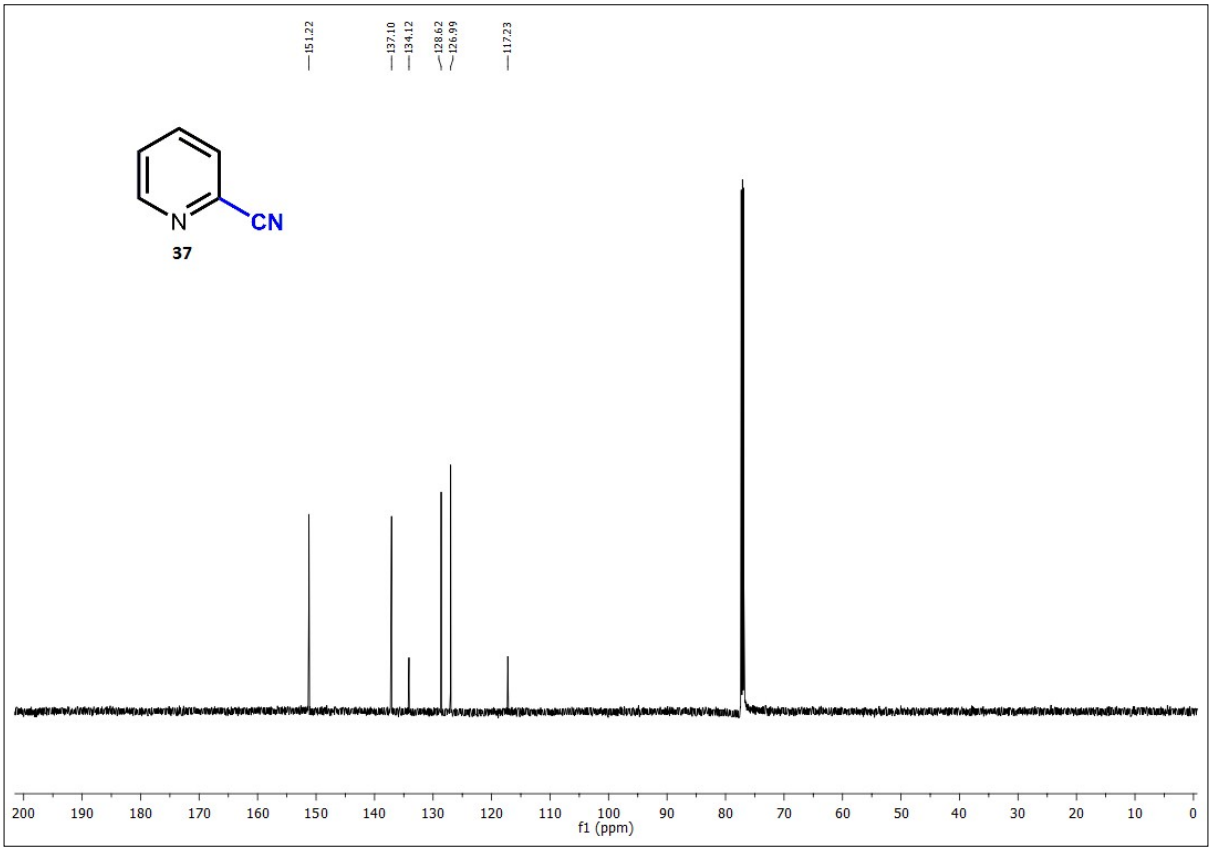
7.55
7.53
7.52
7.26
1.69
N
CN
37
0.99
1.02
1.00
1.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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126.99
117.23
N
CN
37
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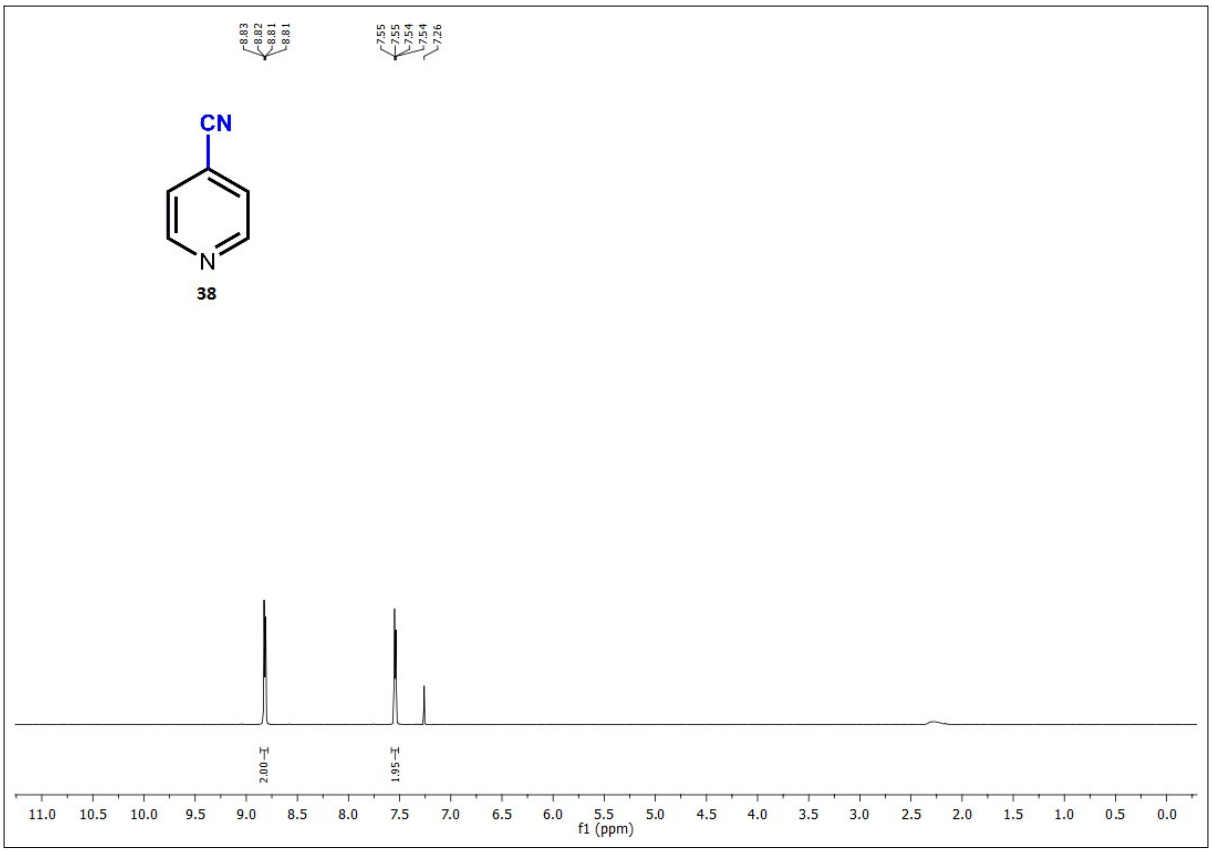
f1 (ppm)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7.54
7.54
7.26
CN
N
38
2.00
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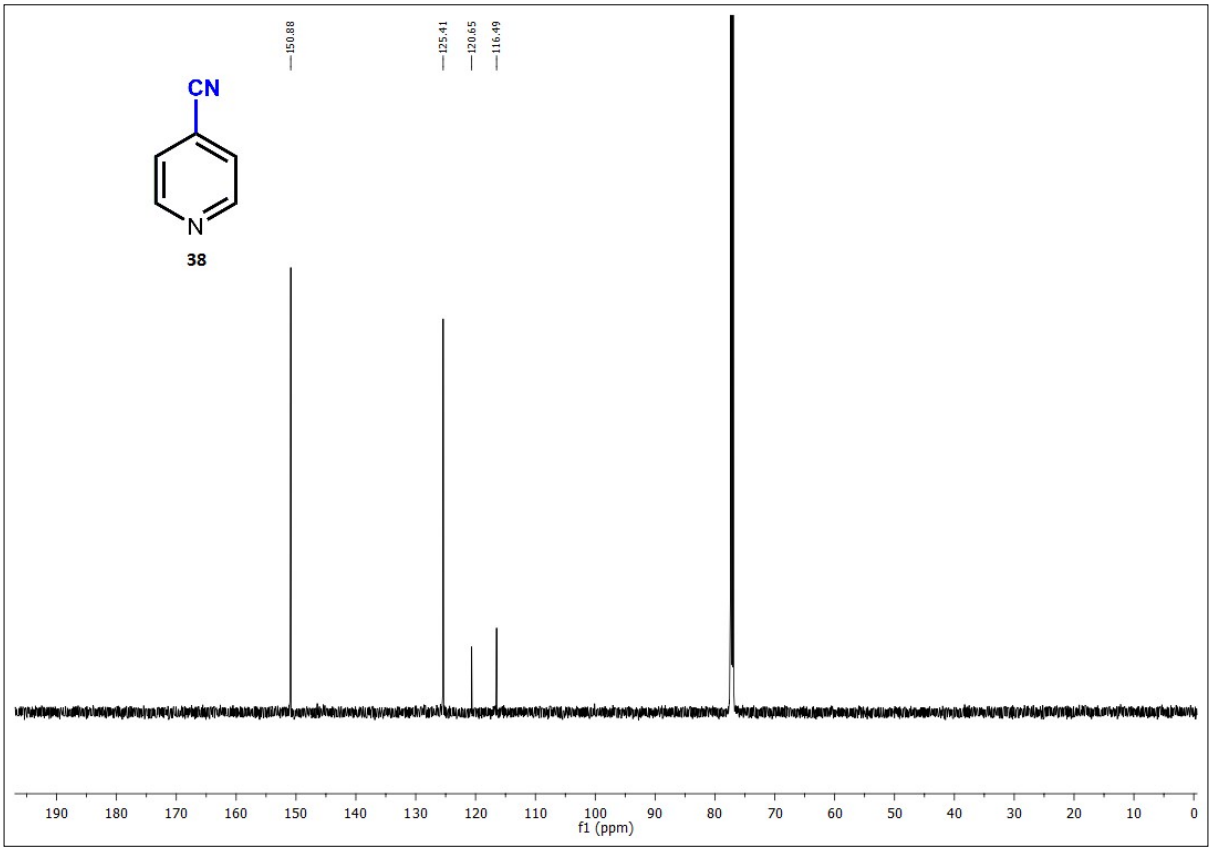
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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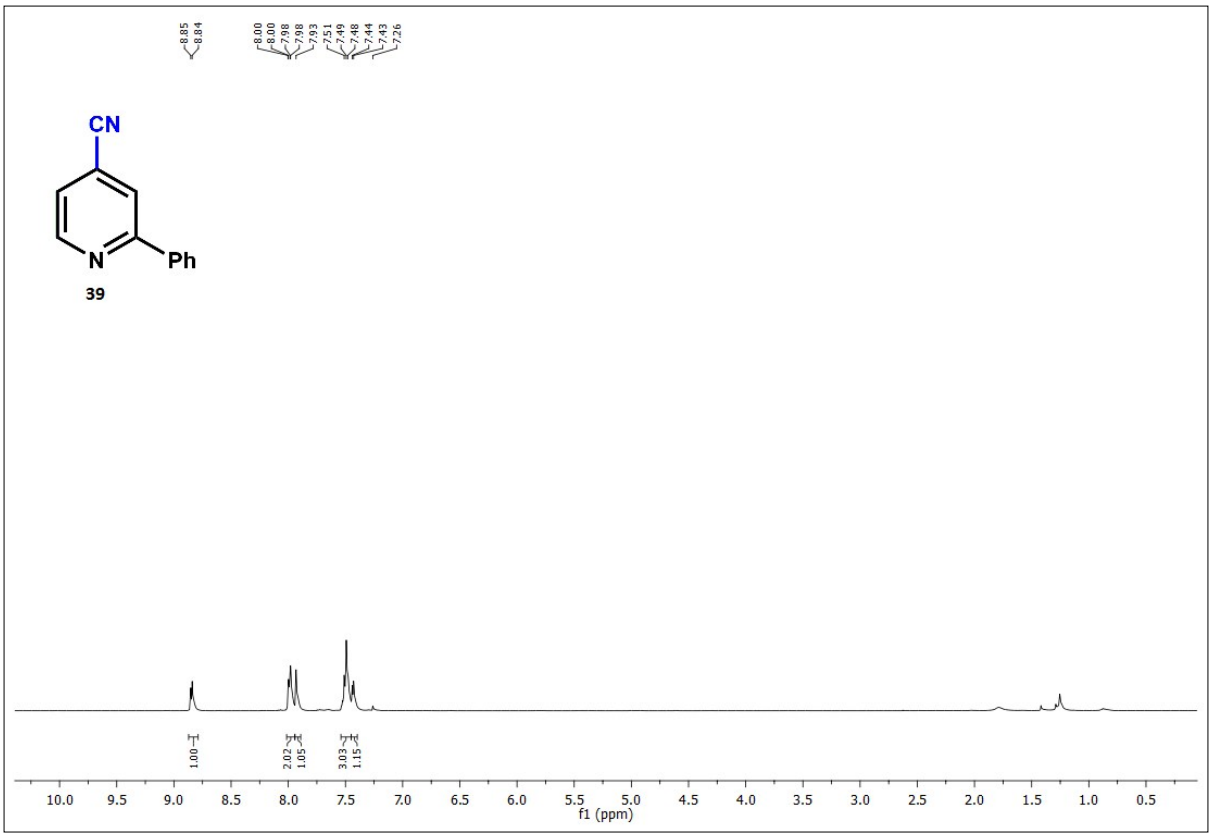
f1 (ppm)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7.49
7.48
7.44
7.43
7.26
CN
N
Ph
39
1.00
2.02
1.05
3.03
1.15
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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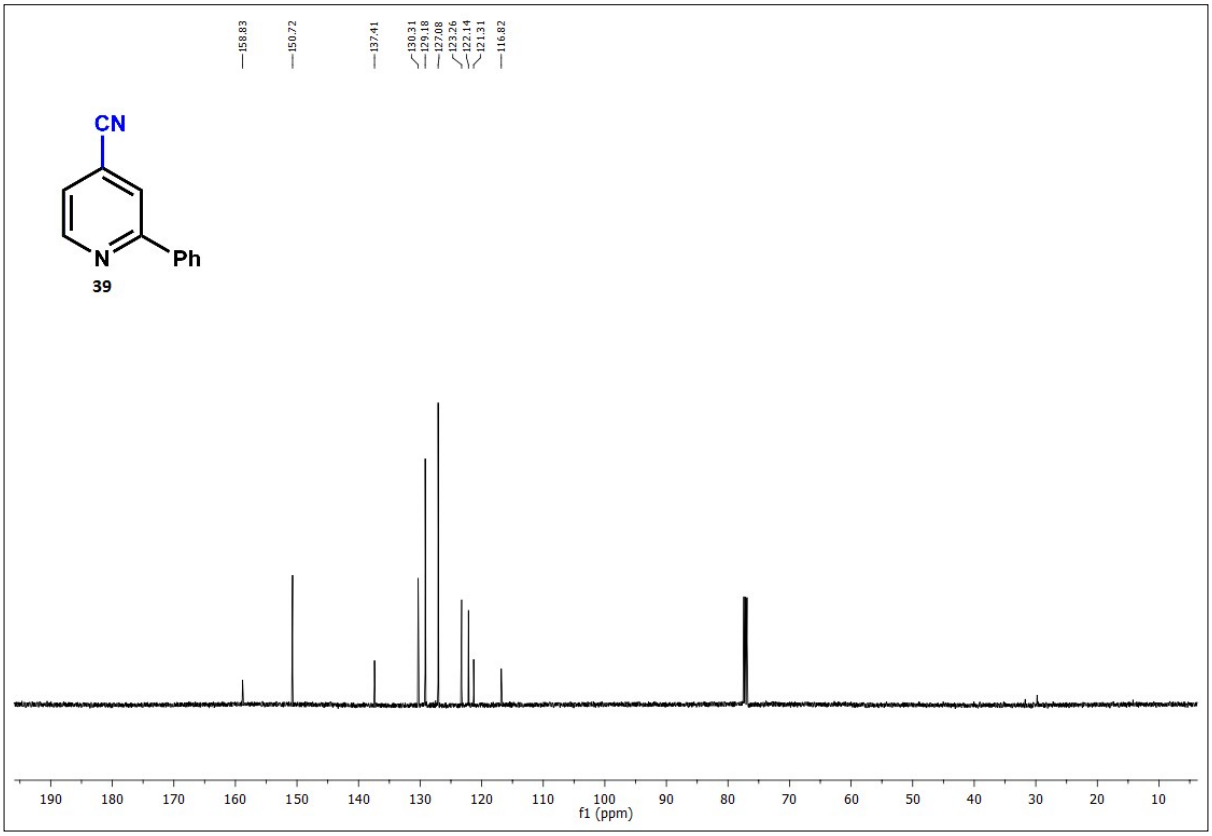
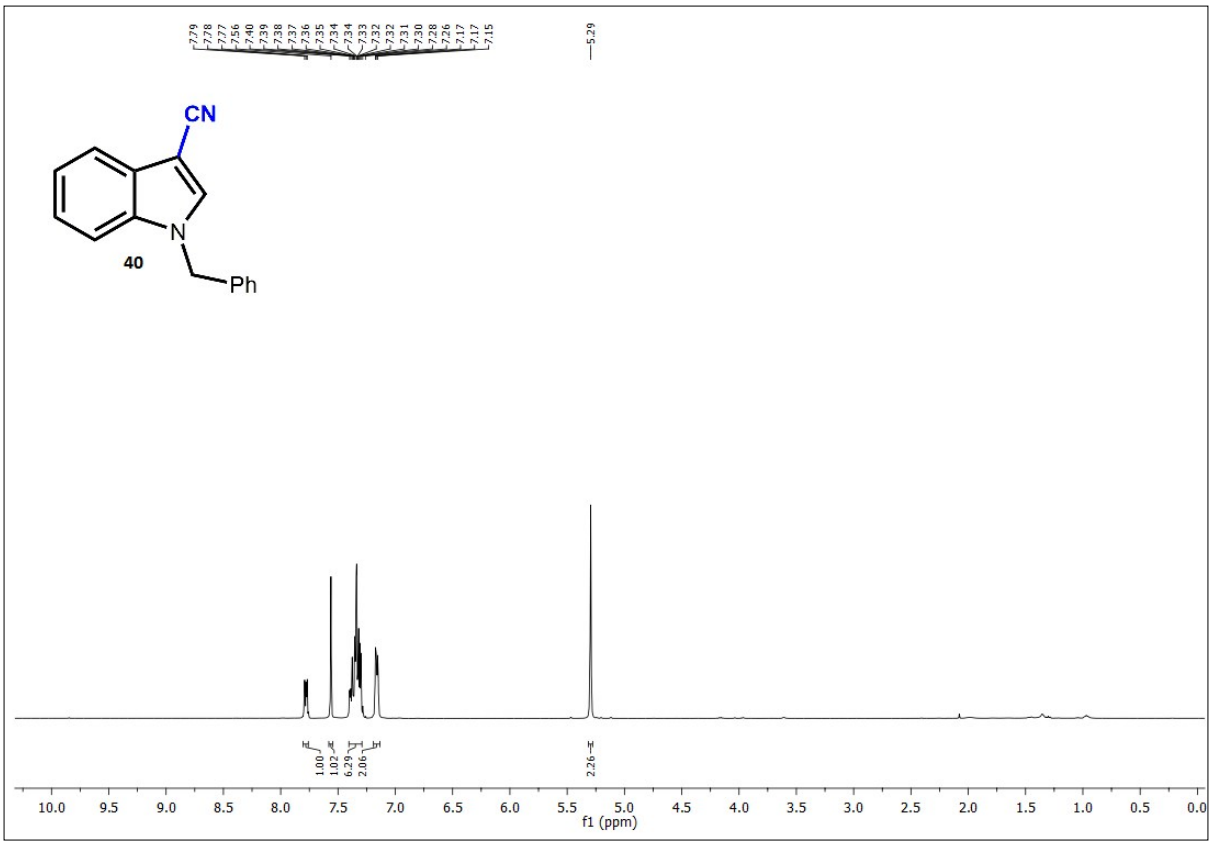
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


158.83
150.72
137.41
130.31
129.18
127.08
123.26
122.14
121.31
116.82
CN
N
Ph
39
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.32
7.32
7.31
7.30
7.28
7.26
7.17
7.17
7.15
5.29
CN
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Ph
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1.00
1.02
6.29
2.06
2.26
10.0
9.5
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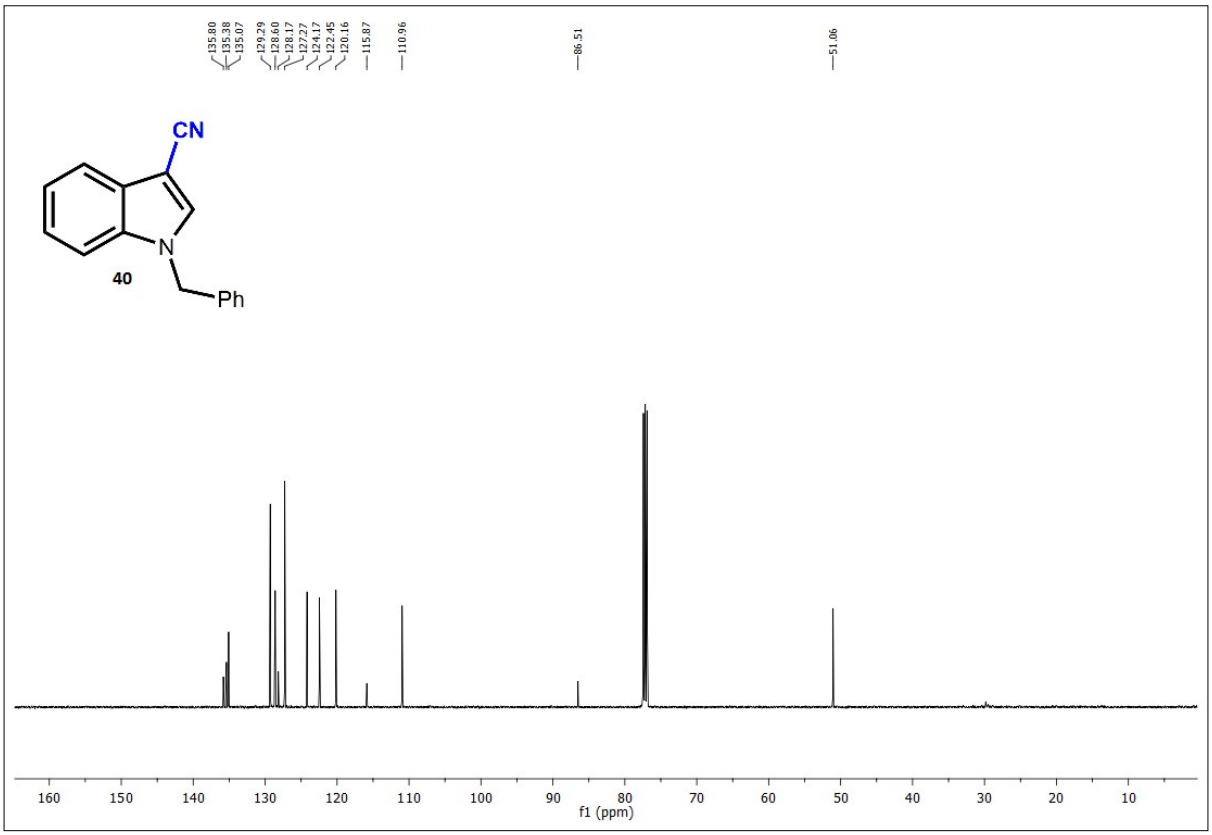
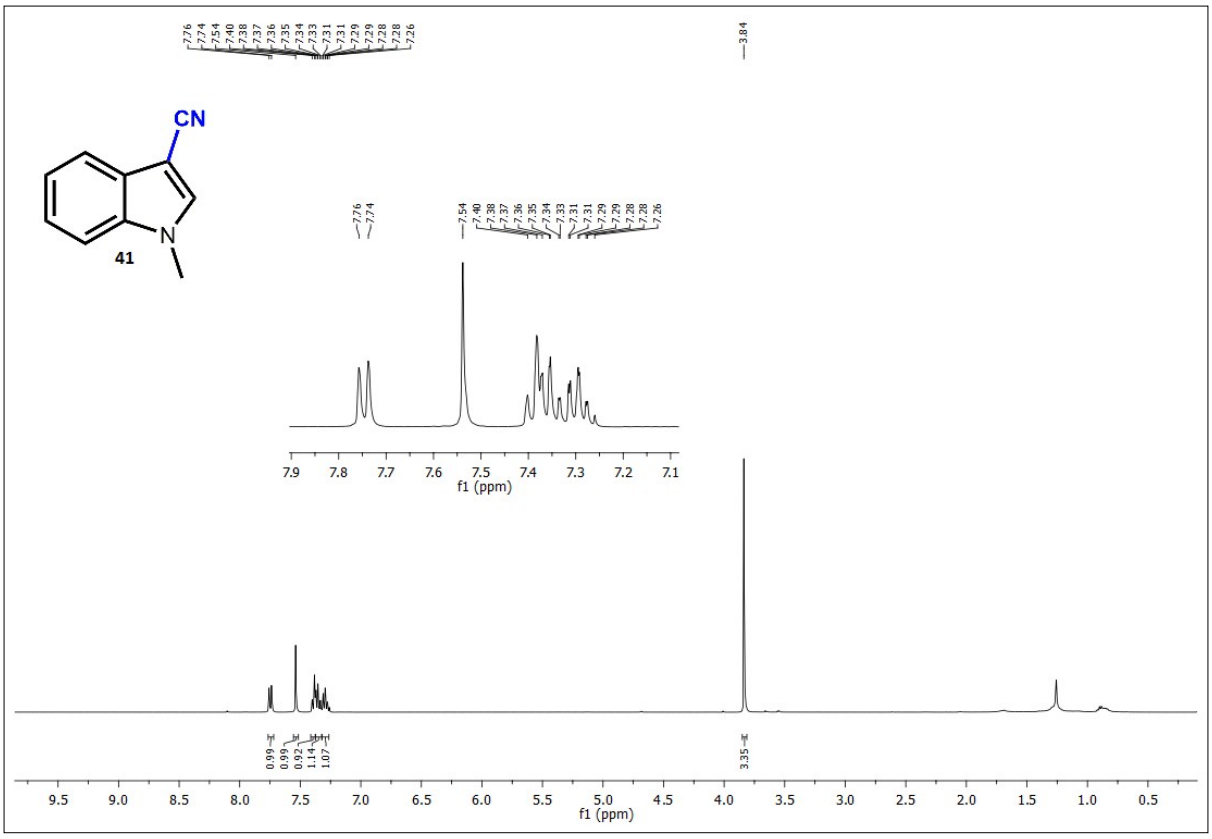
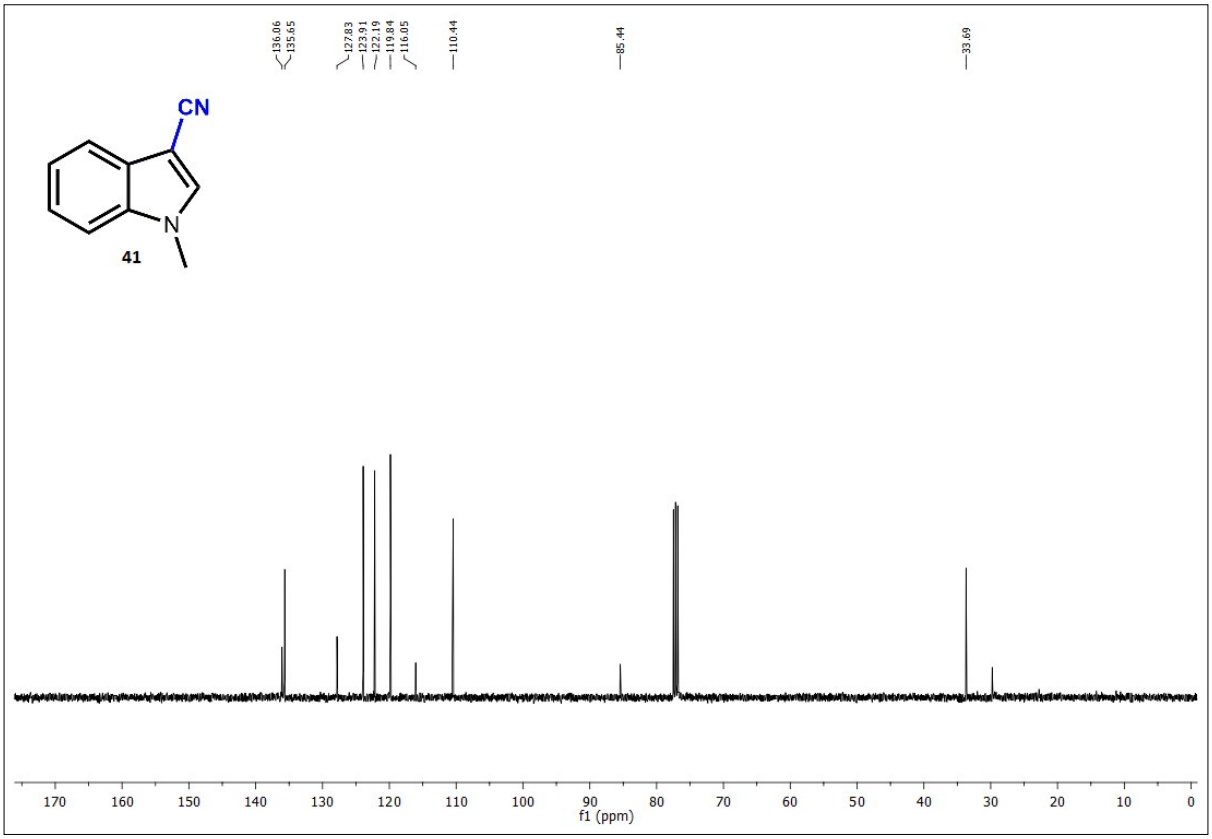
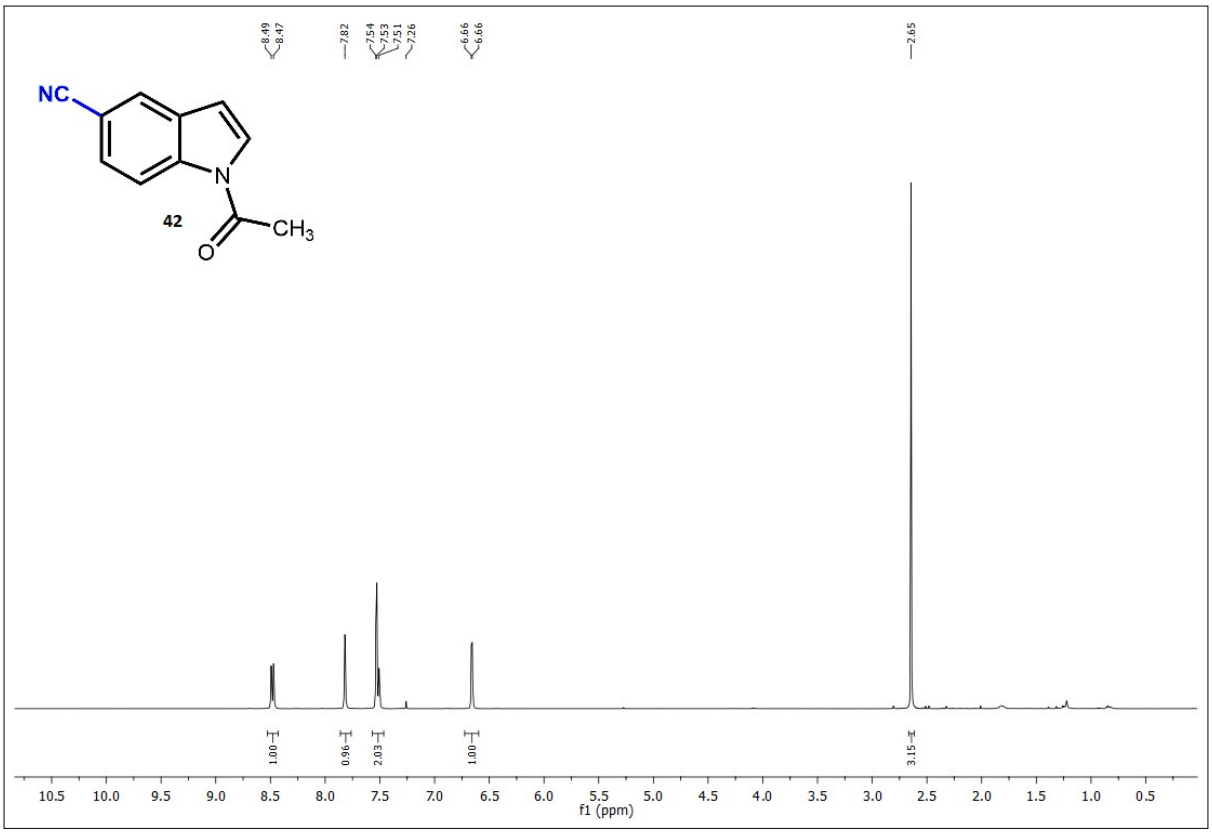
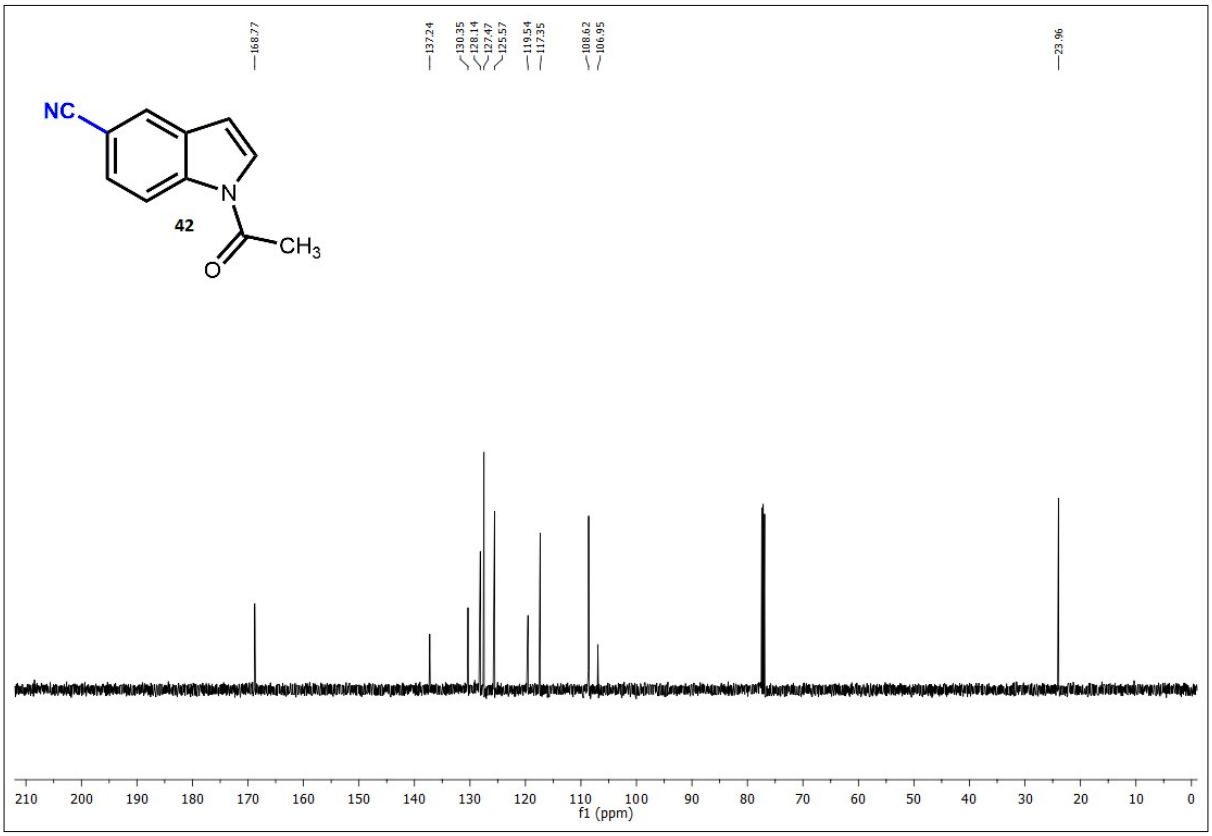
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

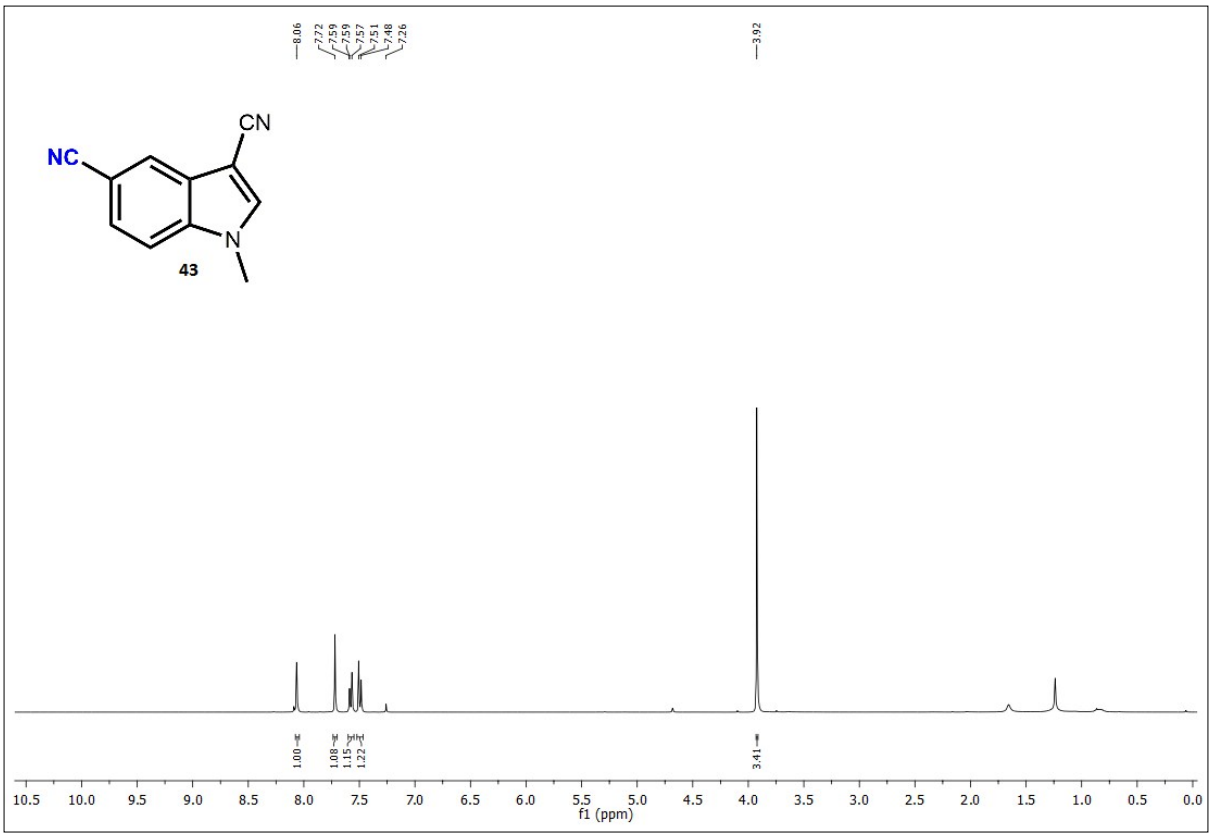

135.80
135.38
135.07
129.29
128.60
128.17
127.27
124.17
122.45
120.16
115.87
110.96
86.51
51.06
CN
N
Ph
40
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

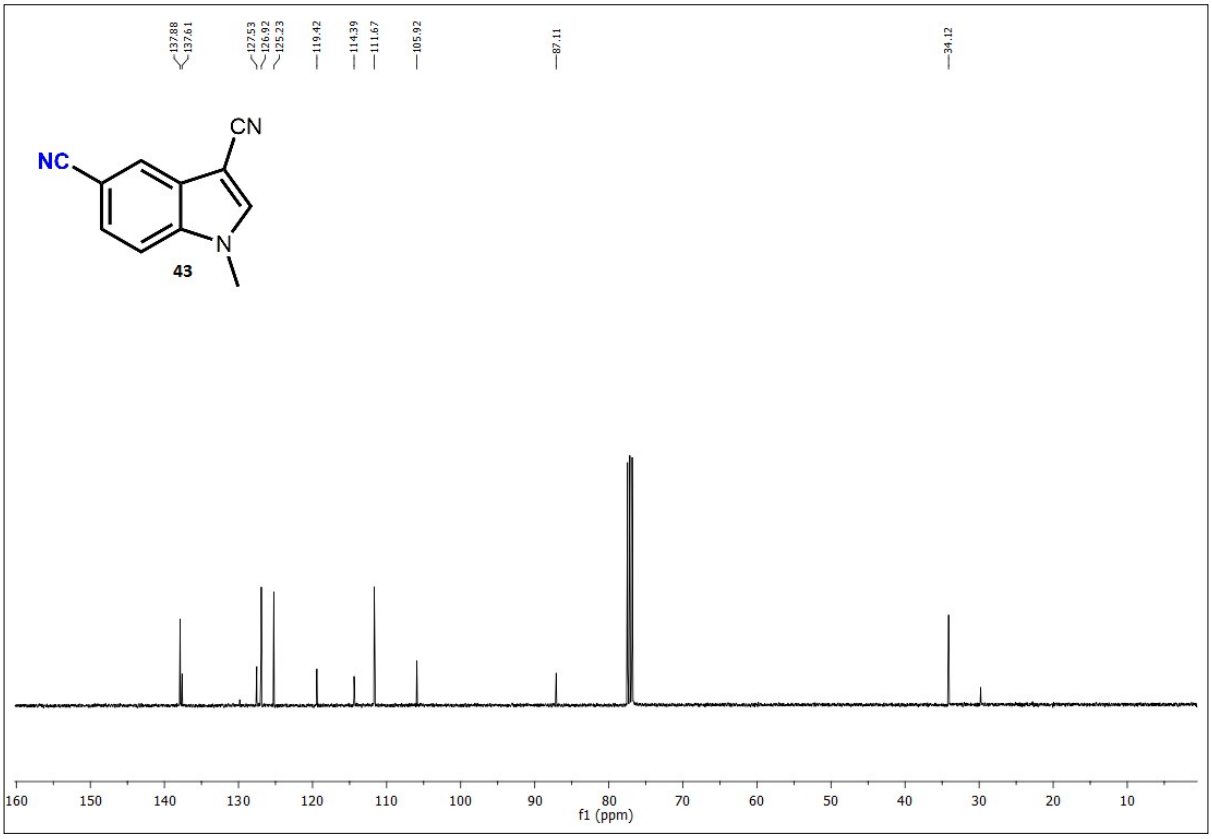

CN
N
41
f1 (ppm)

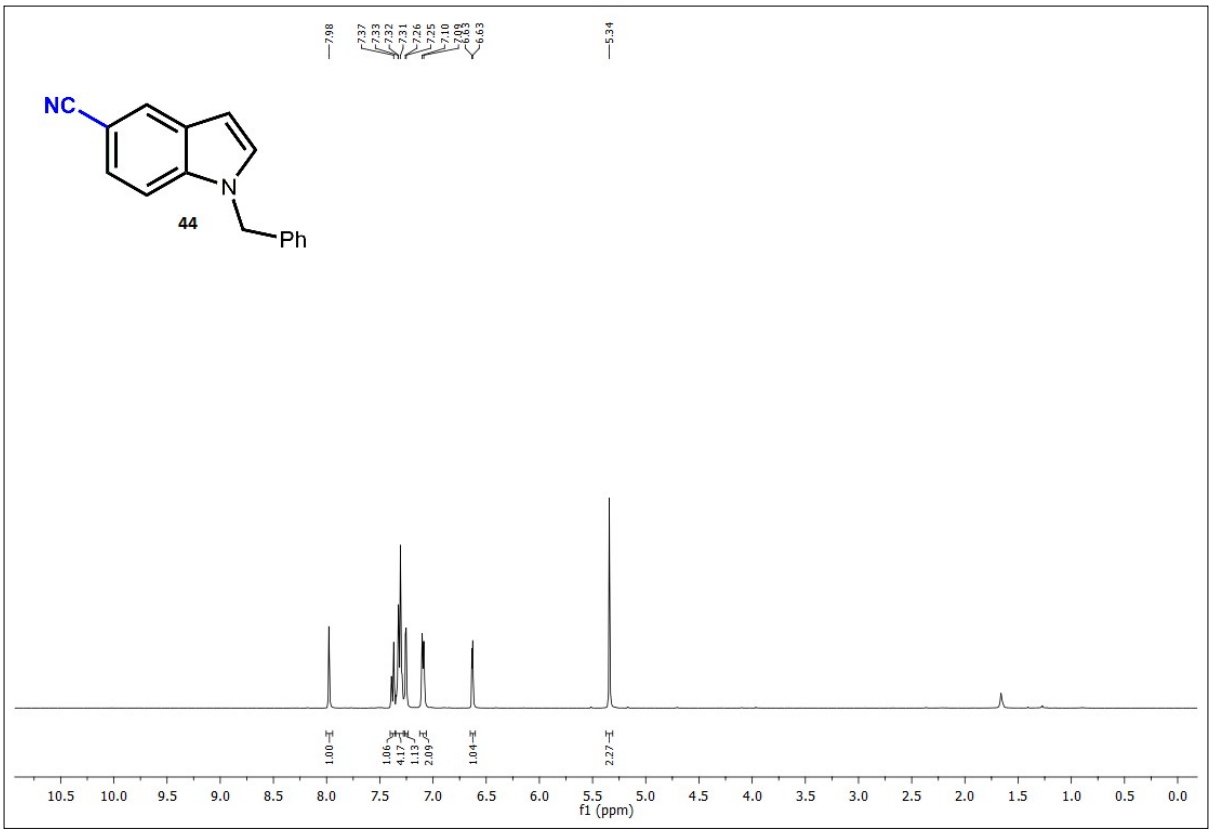

CN
N
41
f1 (ppm)

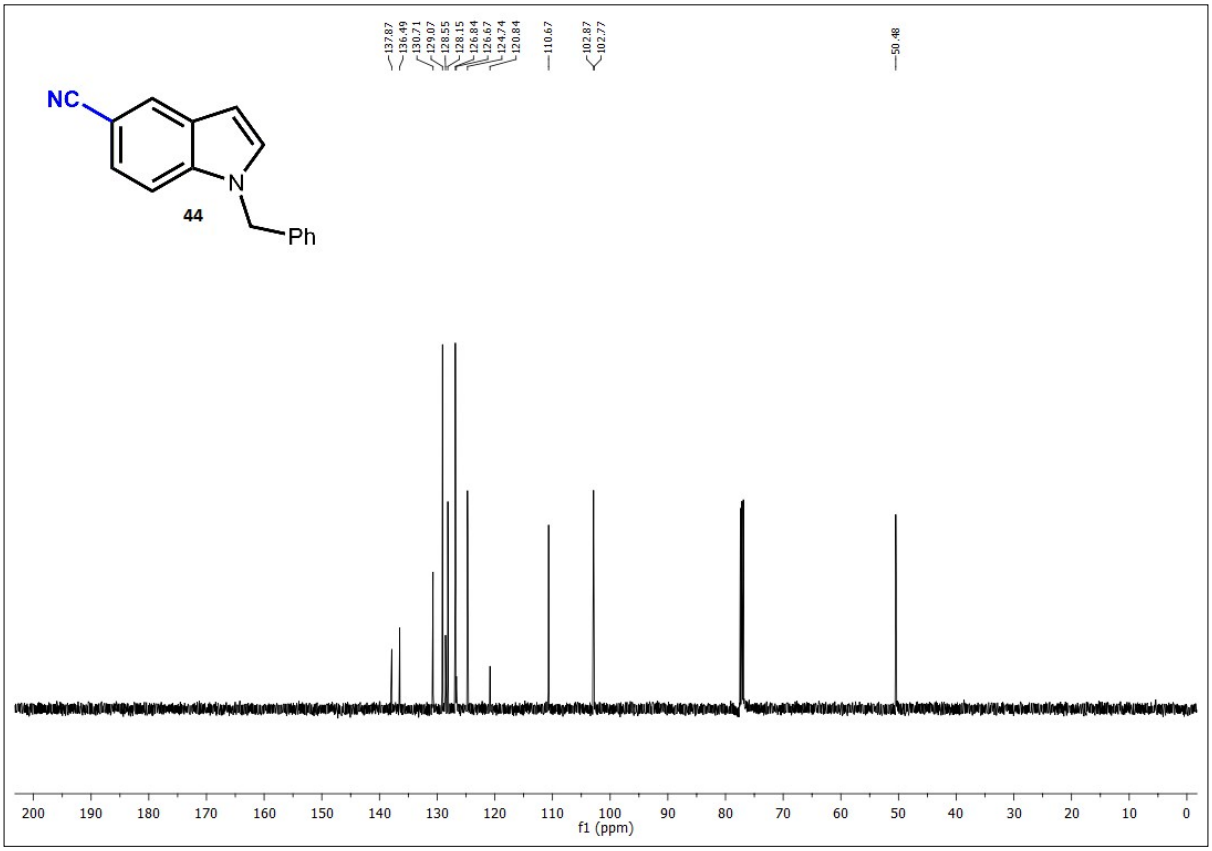

8.49
8.47
7.82
7.54
7.53
7.51
7.26
6.66
6.66
2.65
NC
N
42
CH3
O
1.00
0.96
2.03
1.00
3.15
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

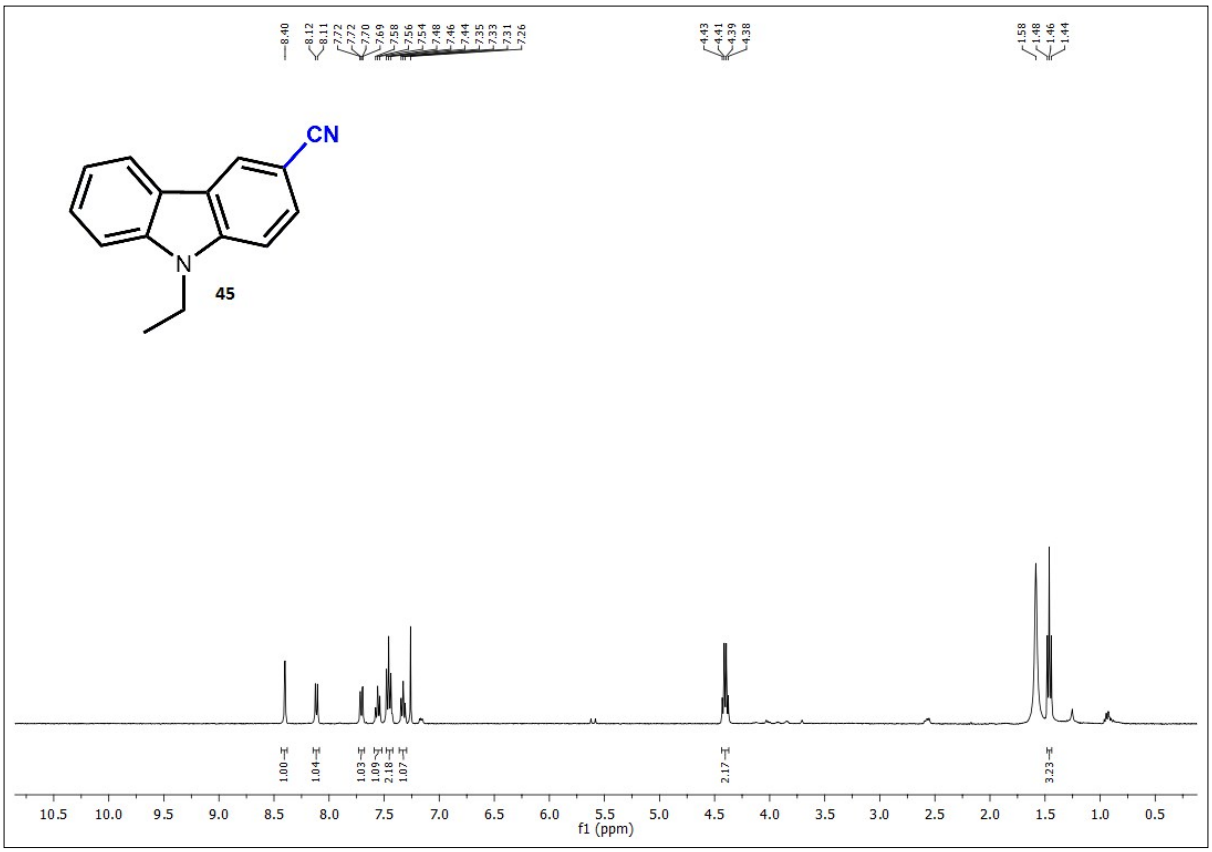

168.77
137.24
130.35
128.14
127.47
125.57
119.54
117.35
108.62
106.95
23.96
NC
N
42
CH3
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

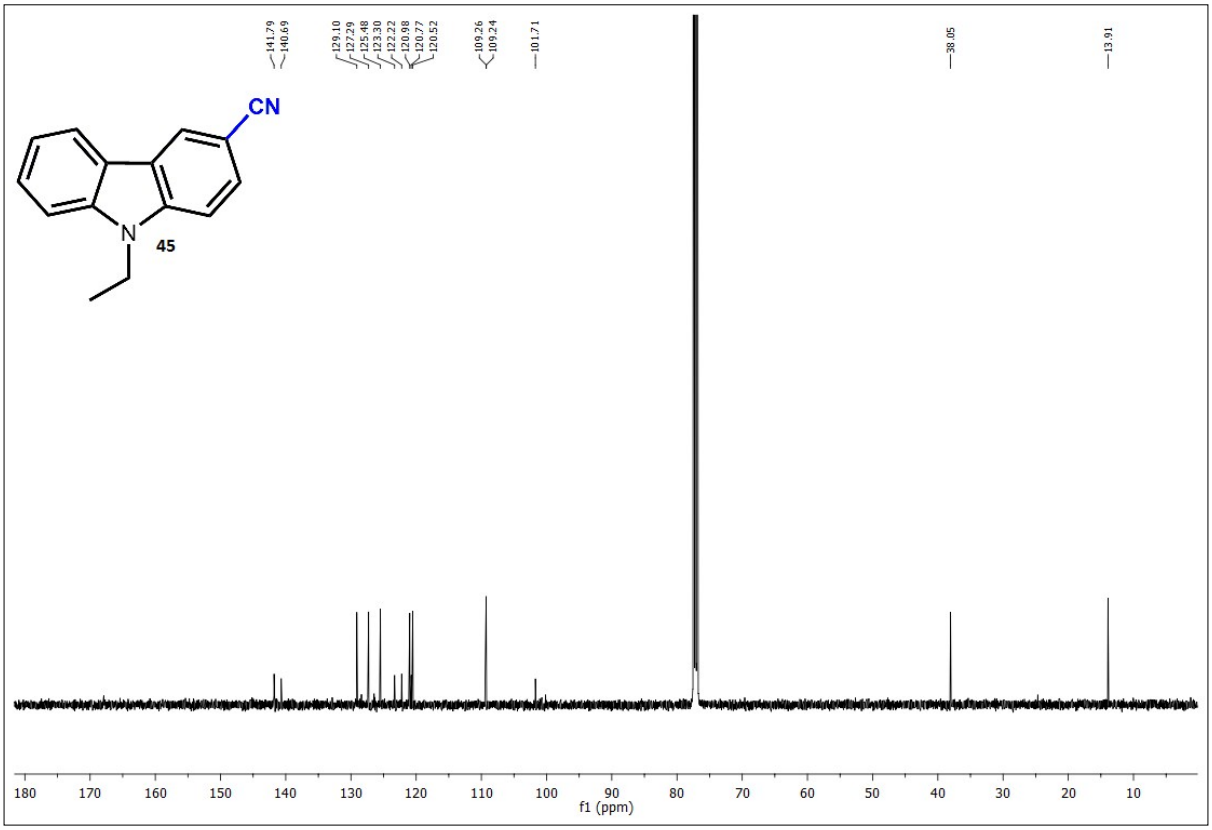

8.06
7.72
7.59
7.59
7.57
7.51
7.48
7.26
3.92
CN
NC
N
43
1.00
1.08
1.15
1.22
3.41
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

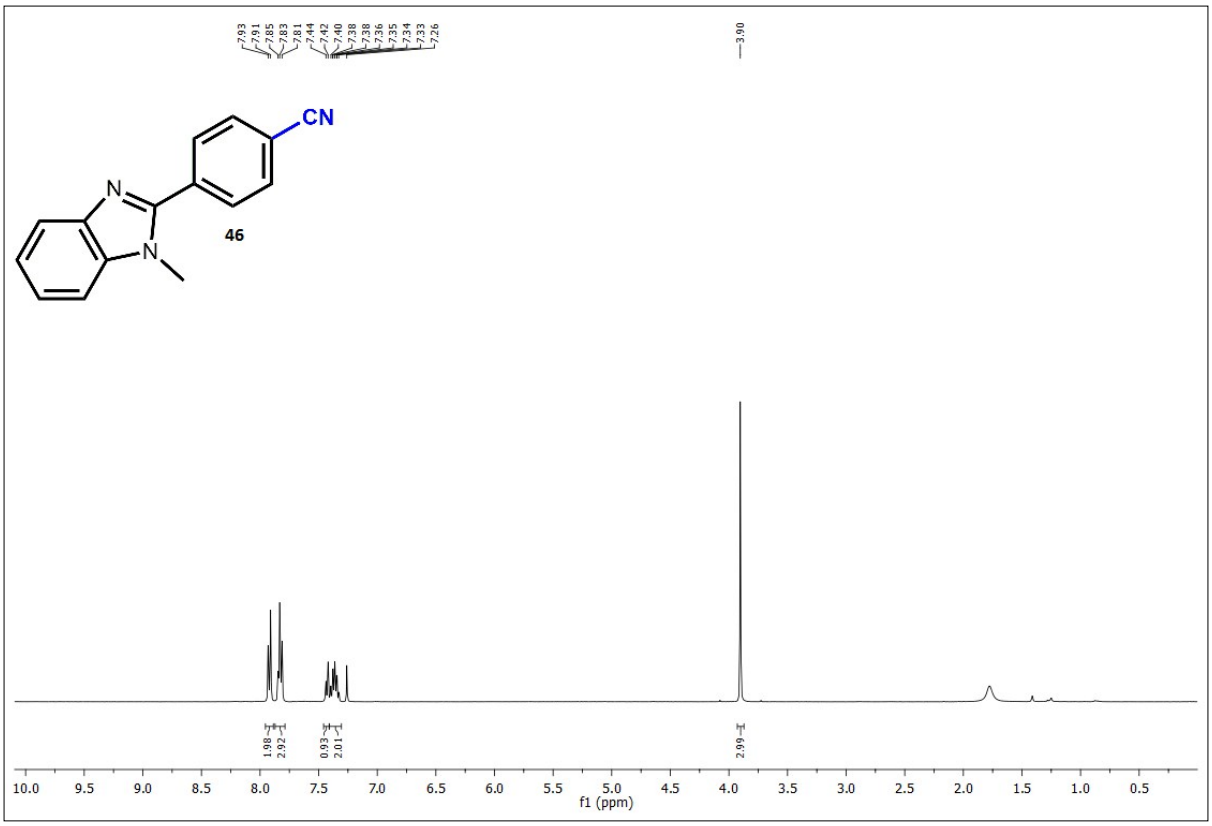

137.88
137.61
127.53
126.92
125.23
119.42
114.39
111.67
105.92
87.11
34.12
CN
NC
N
43
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

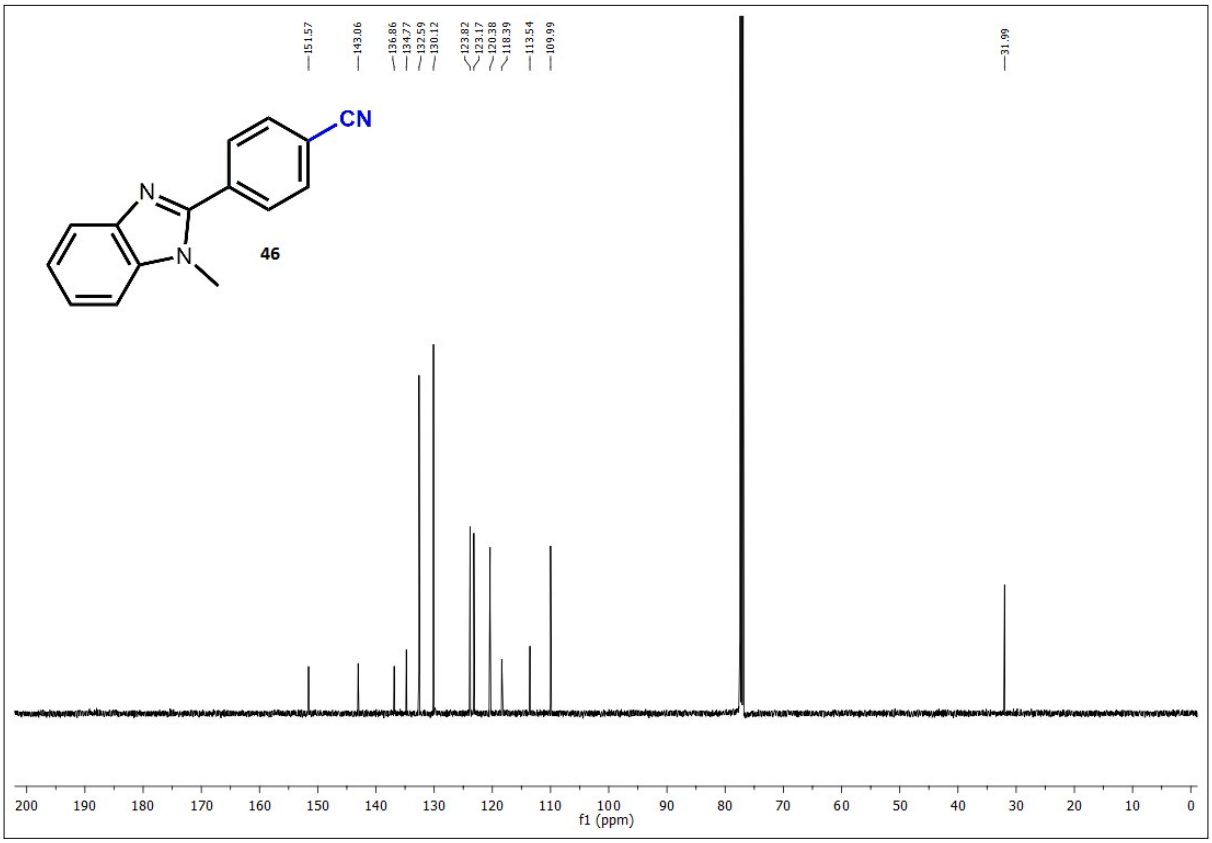

NC
N
Ph
44
7.98
7.37
7.33
7.32
7.31
7.26
7.25
7.10
7.03
6.83
6.63
5.34
1.00
1.06
4.17
1.13
2.09
1.04
2.27
f1 (ppm)

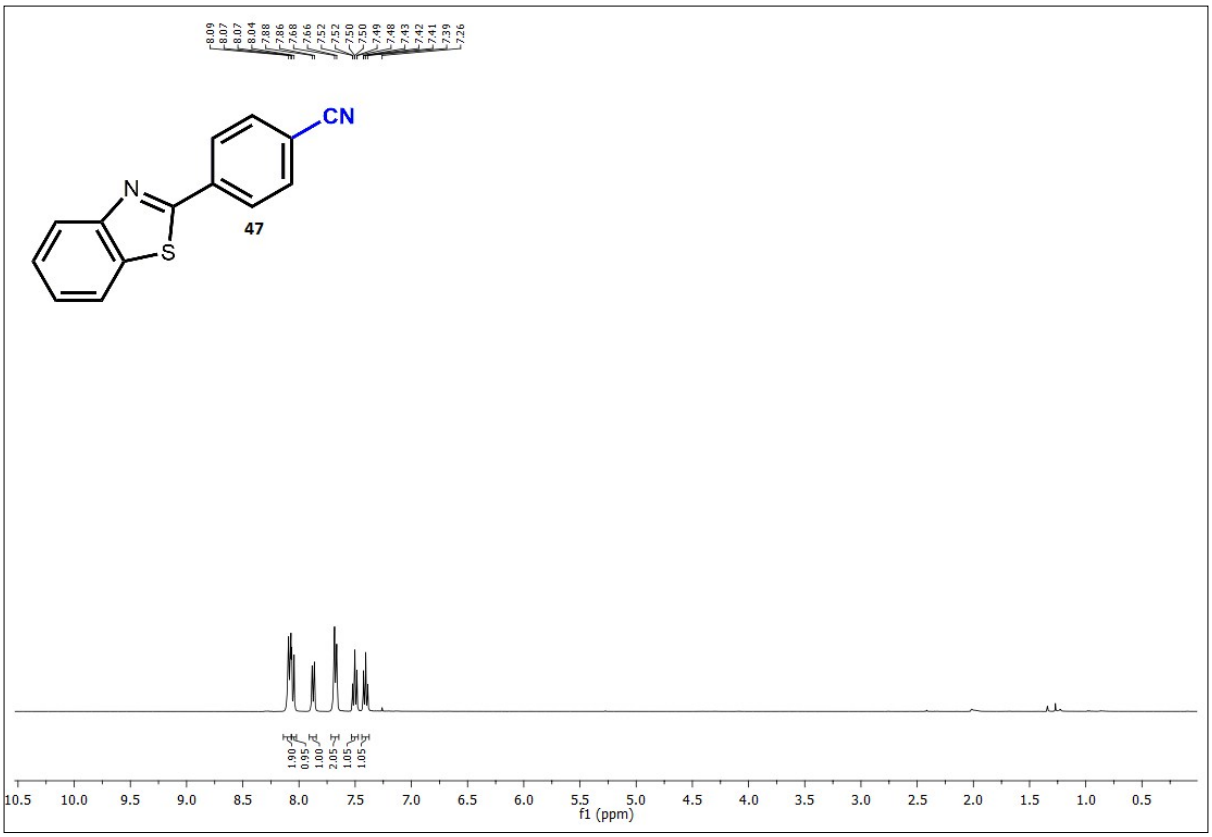

NC
N
Ph
44
137.87
136.49
130.71
129.07
128.55
128.15
126.84
126.67
124.74
120.84
110.67
102.87
102.77
50.48
f1 (ppm)

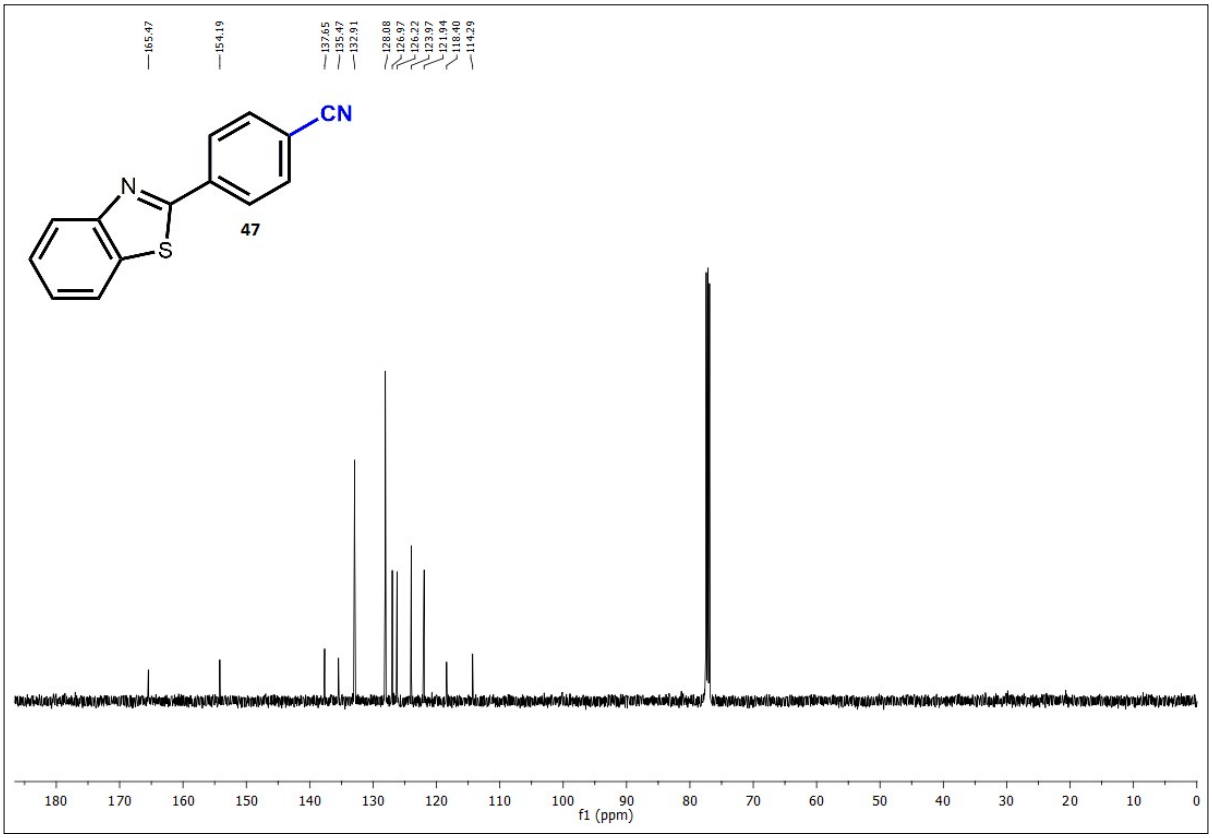

8.40
8.12
8.11
7.72
7.72
7.70
7.69
7.58
7.56
7.54
7.48
7.46
7.44
7.35
7.33
7.31
7.26
4.43
4.41
4.39
4.38
1.58
1.48
1.46
1.44
CN
N
45
1.00
1.04
1.03
1.09
2.18
1.07
2.17
3.23
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

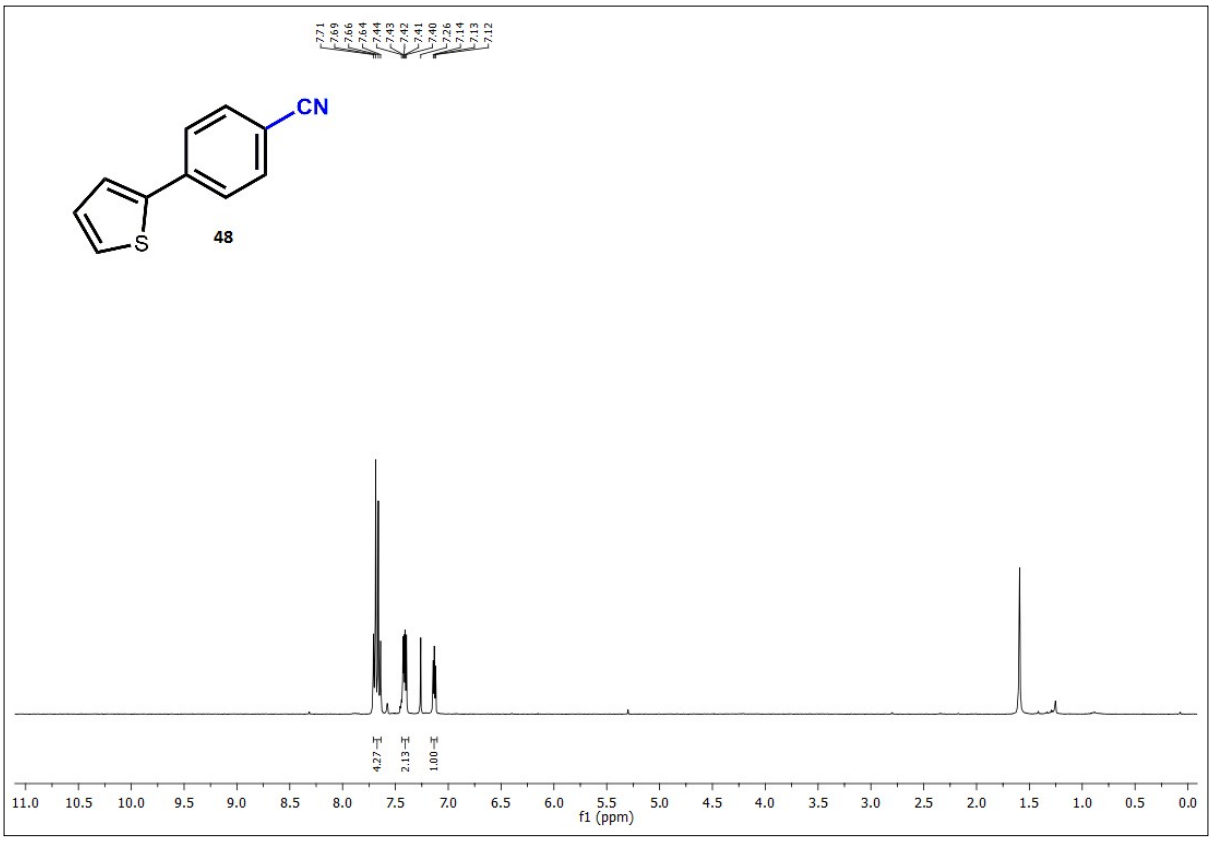

141.79
140.69
129.10
127.29
125.48
123.30
122.22
120.98
120.77
120.52
109.26
109.24
101.71
38.05
13.91
CN
N
45
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

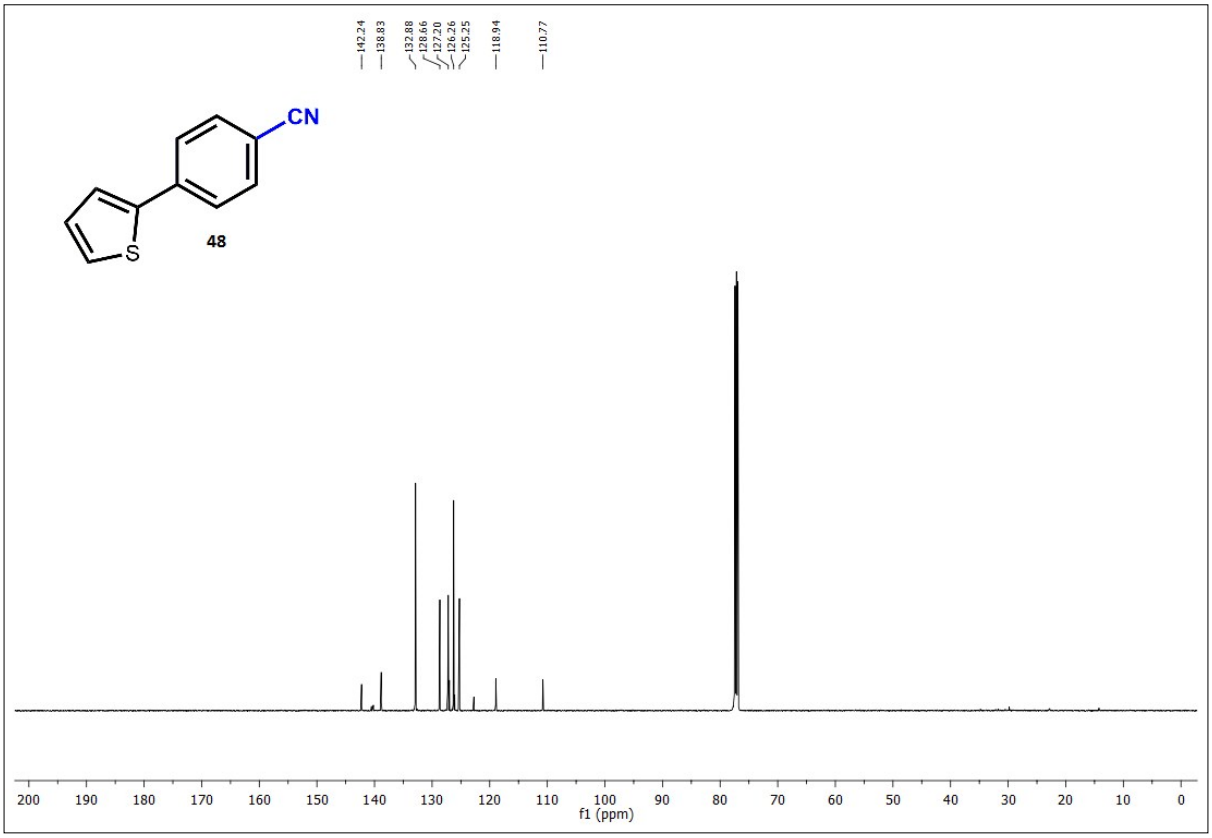

7.93
7.91
7.85
7.83
7.81
7.44
7.42
7.40
7.38
7.36
7.35
7.34
7.33
7.26
3.90
CN
N
N
46
1.98
2.92
0.93
2.01
2.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

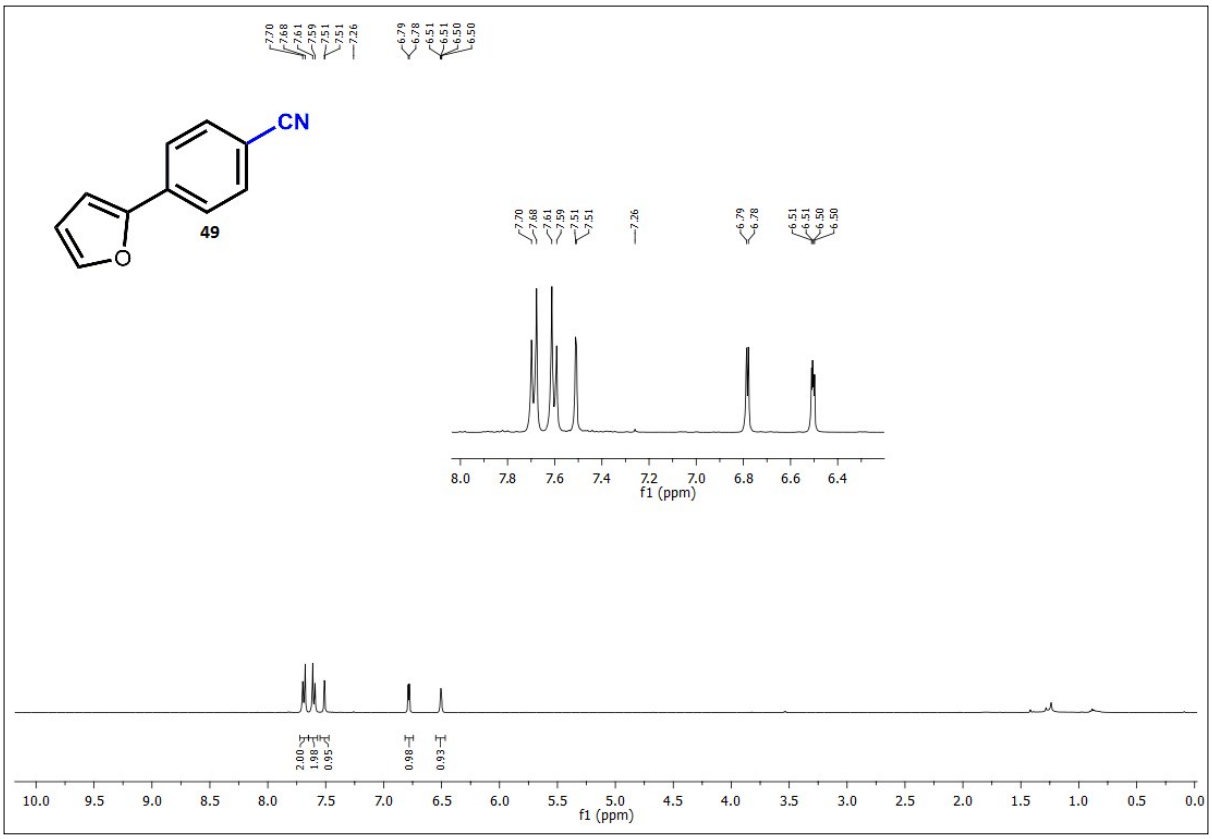

151.57
143.06
136.86
134.77
132.59
130.12
123.82
123.17
120.38
118.39
113.54
109.99
31.99
CN
N
N
46
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

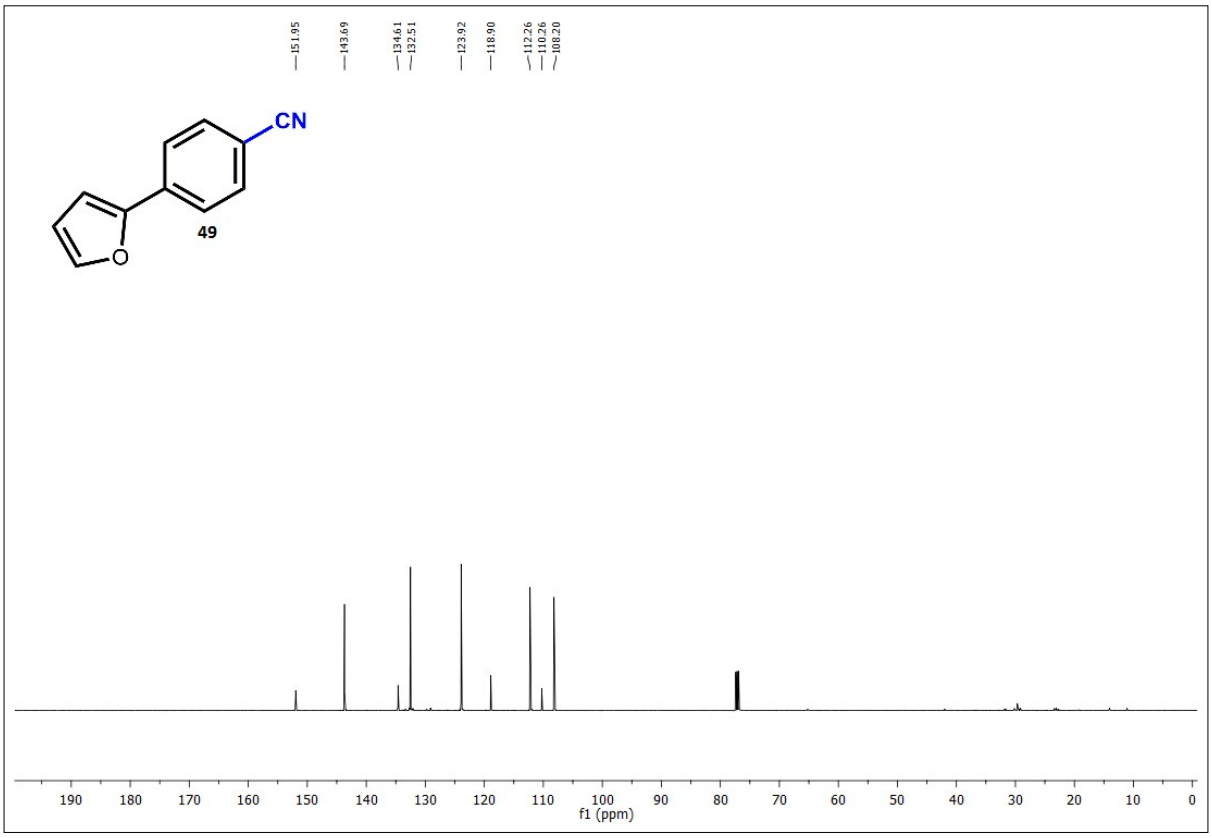

8.09
8.07
8.07
8.04
7.88
7.86
7.68
7.66
7.52
7.52
7.50
7.50
7.49
7.48
7.43
7.42
7.41
7.39
7.26
CN
N
S
47
1.90
0.95
1.00
2.05
1.05
1.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

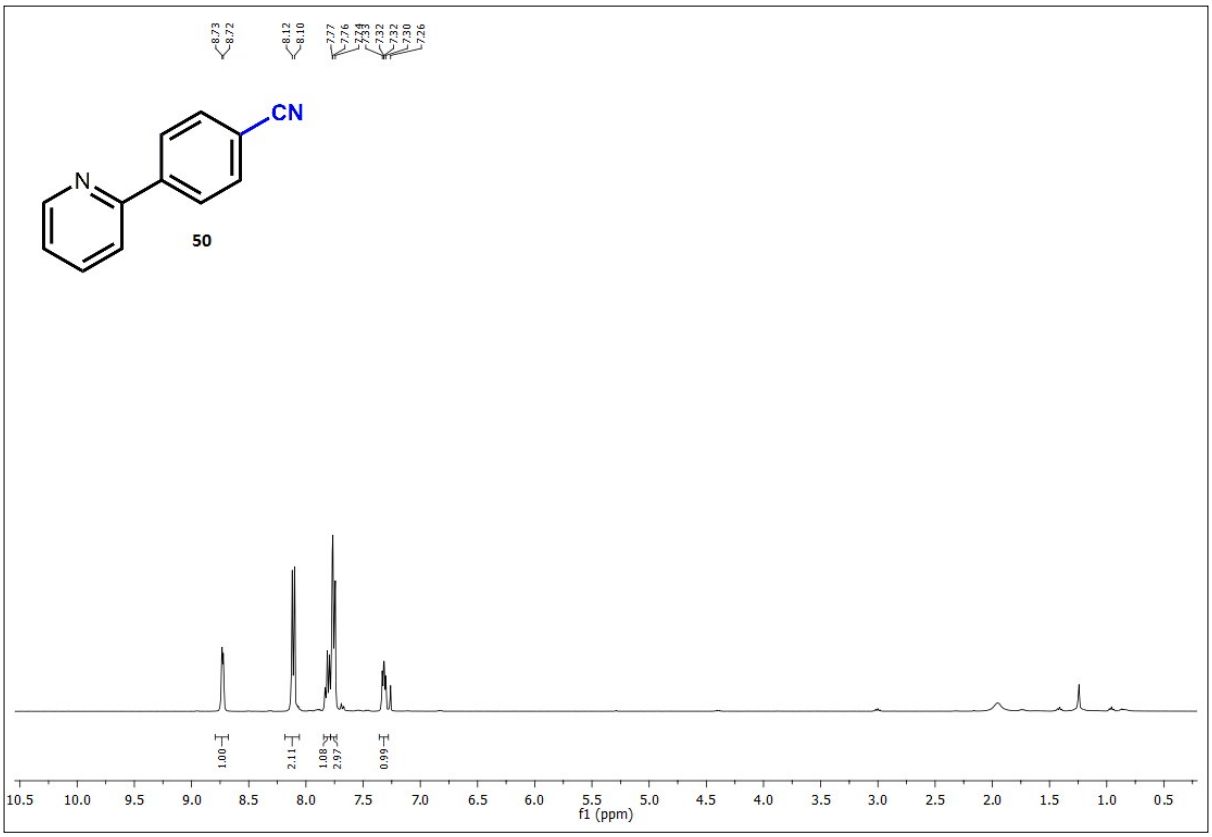

165.47
154.19
137.65
135.47
132.91
128.08
126.97
126.22
123.97
121.94
118.40
114.29
CN
N
S
47
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

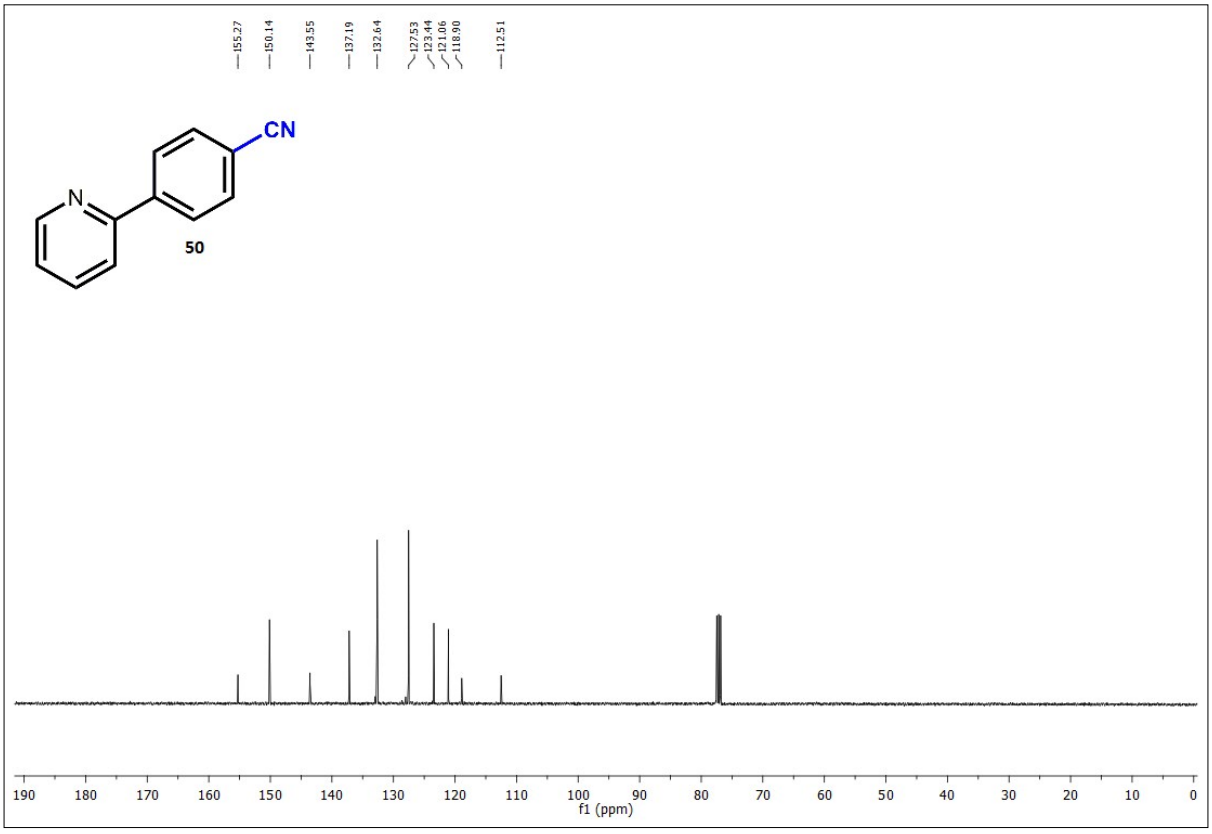

7.71
7.69
7.66
7.64
7.44
7.43
7.42
7.41
7.40
7.26
7.14
7.13
7.12
CN
S
48
4.27
2.13
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


142.24
138.83
132.88
128.66
127.20
126.26
125.25
118.94
110.77
CN
S
48
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.70
7.68
7.61
7.59
7.51
7.51
7.26
6.79
6.78
6.51
6.51
6.50
6.50
CN
O
49
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
f1 (ppm)
2.00
1.98
0.95
0.98
0.93
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


151.95
143.69
134.61
132.51
123.92
118.90
112.26
110.26
108.20
CN
O
49
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.73
8.72
8.12
8.10
7.77
7.76
7.34
7.33
7.32
7.32
7.30
7.26
CN
N
50
1.00
2.11
1.08
2.97
0.99
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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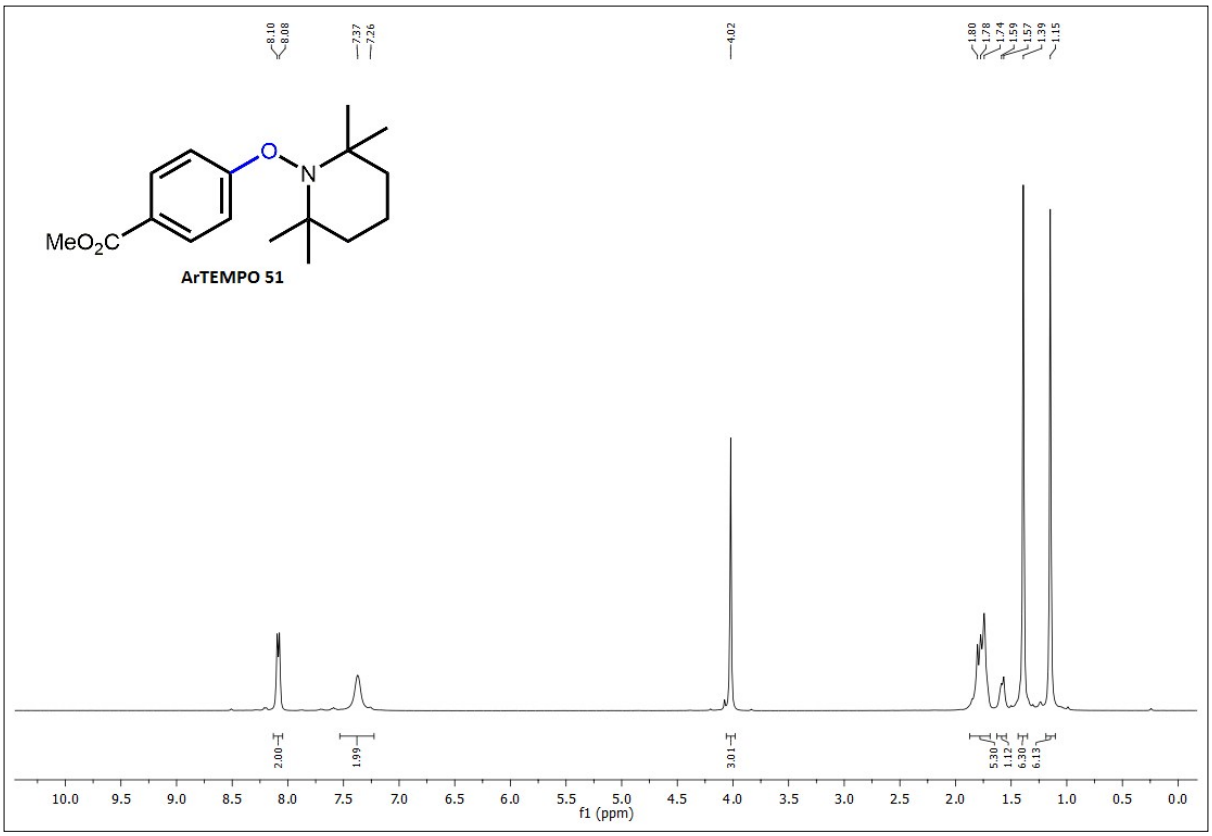
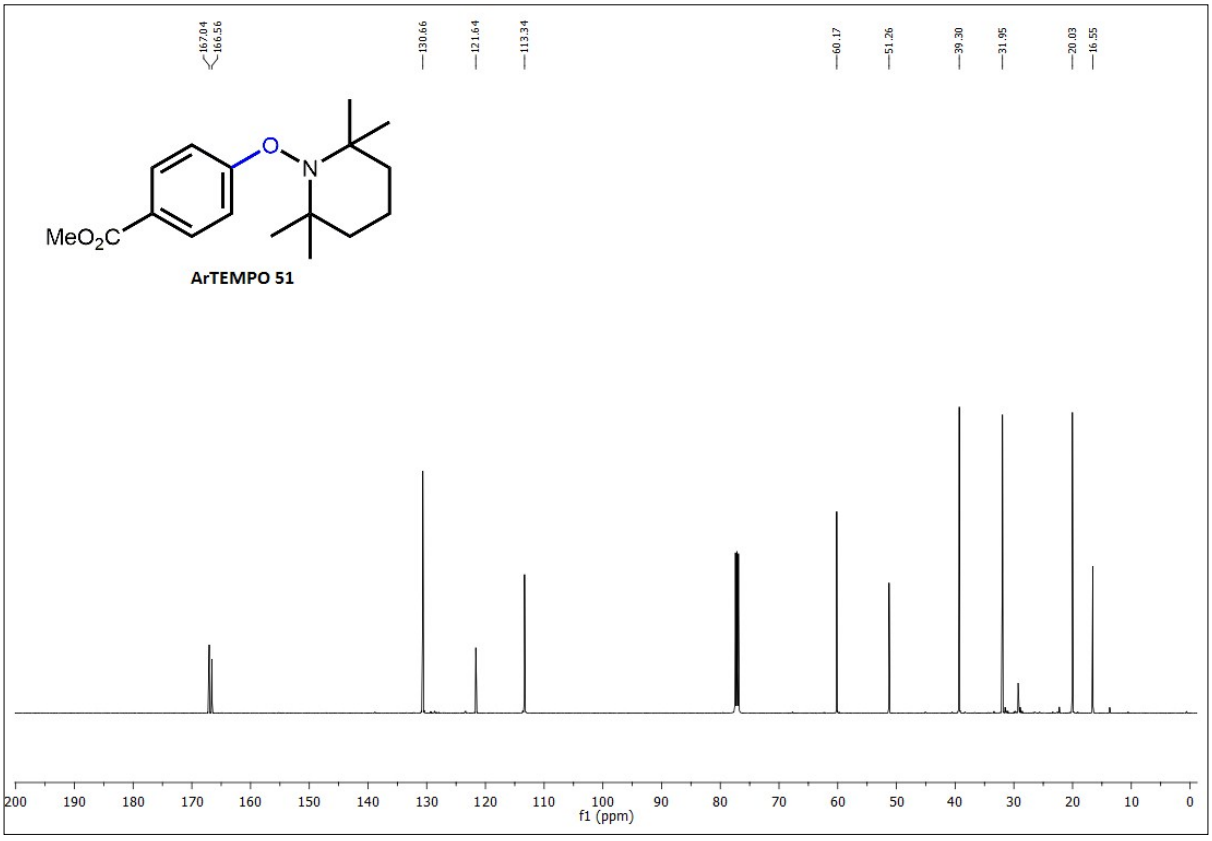
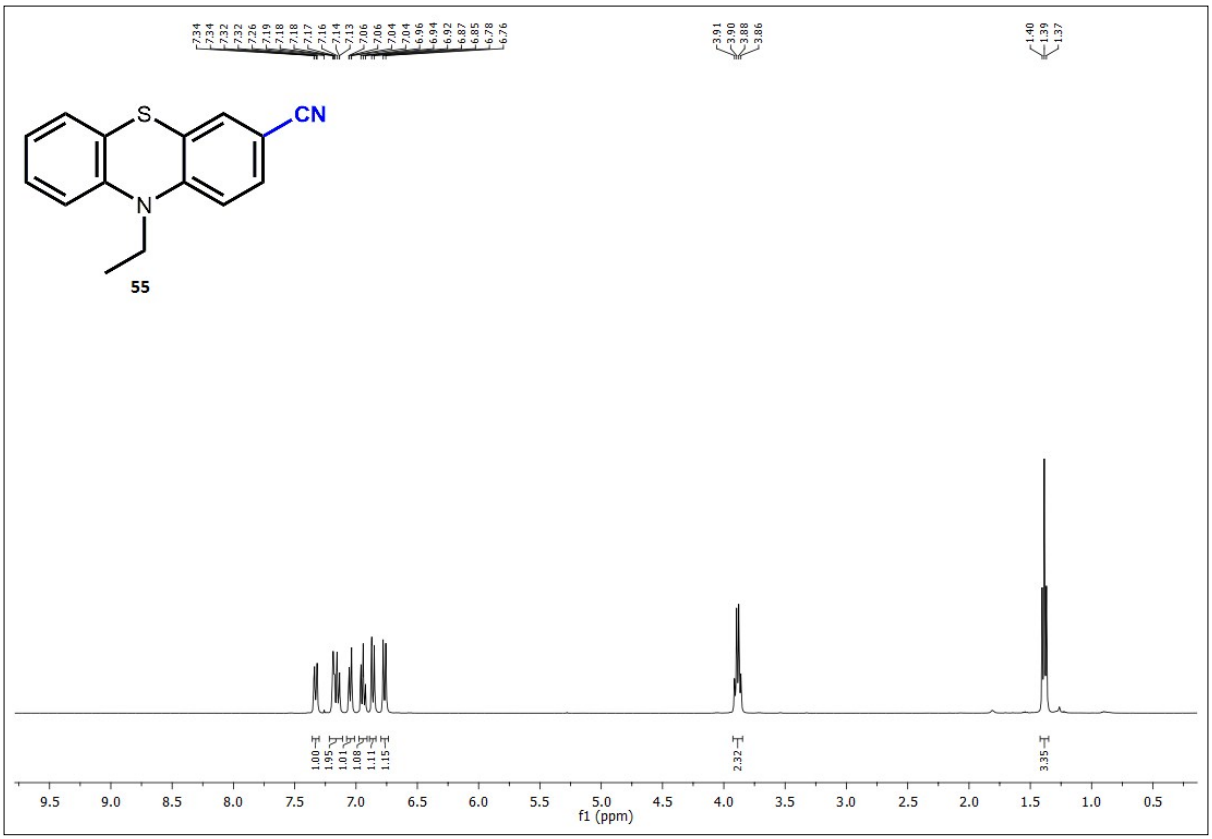
150.14
143.55
137.19
132.64
127.53
123.44
121.06
118.90
112.51
CN
N
50
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.10
8.08
7.37
7.26
4.02
1.80
1.78
1.74
1.59
1.57
1.39
1.15
O
N
MeO2C
ArTEMPO 51
2.00
1.99
3.01
5.30
1.12
6.30
6.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


167.04
166.56
130.66
121.64
113.34
60.17
51.26
39.30
31.95
20.03
16.55
O
N
MeO2C
ArTEMPO 51
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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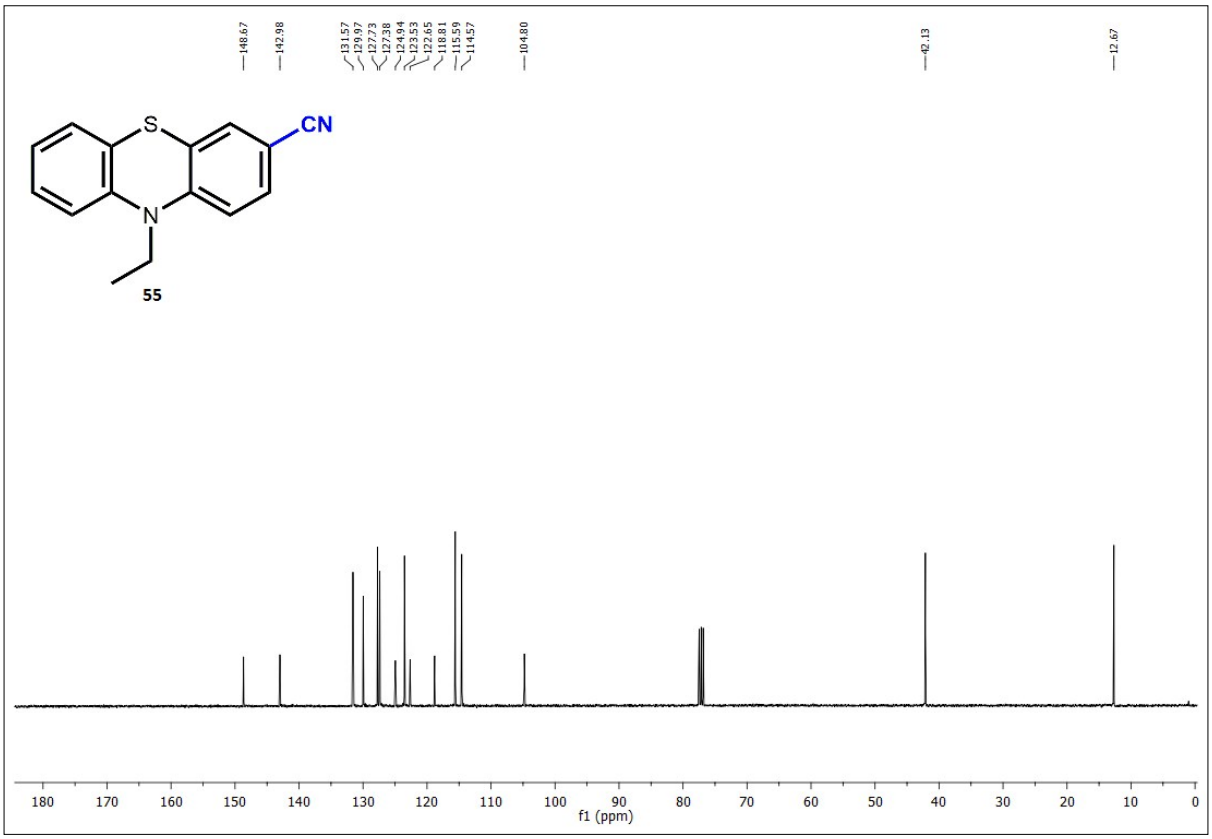
7.34
7.32
7.32
7.26
7.19
7.18
7.18
7.17
7.16
7.14
7.13
7.06
7.06
7.04
7.04
6.96
6.94
6.92
6.87
6.85
6.78
6.76
3.91
3.90
3.88
3.86
1.40
1.39
1.37
S
CN
N
55
1.00
1.95
1.01
1.08
1.11
1.15
2.32
3.35
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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142.98
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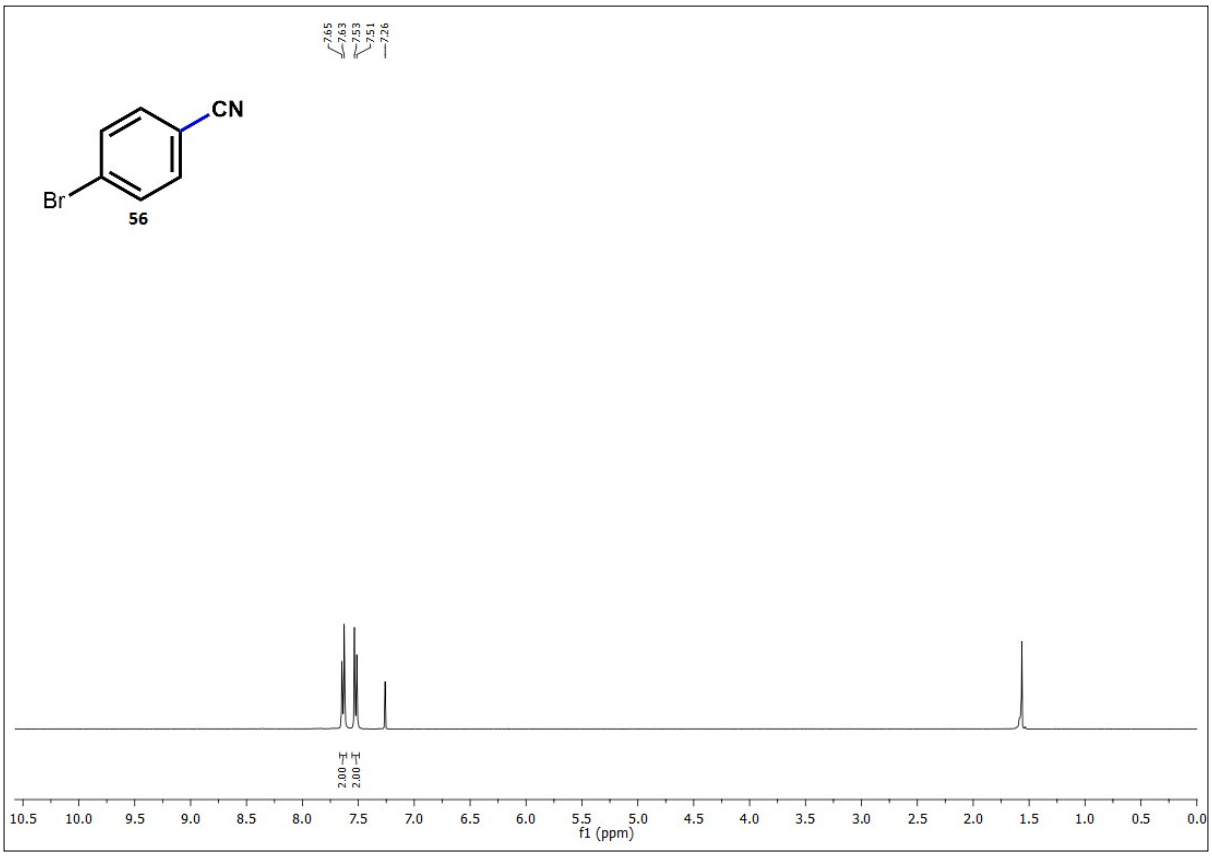
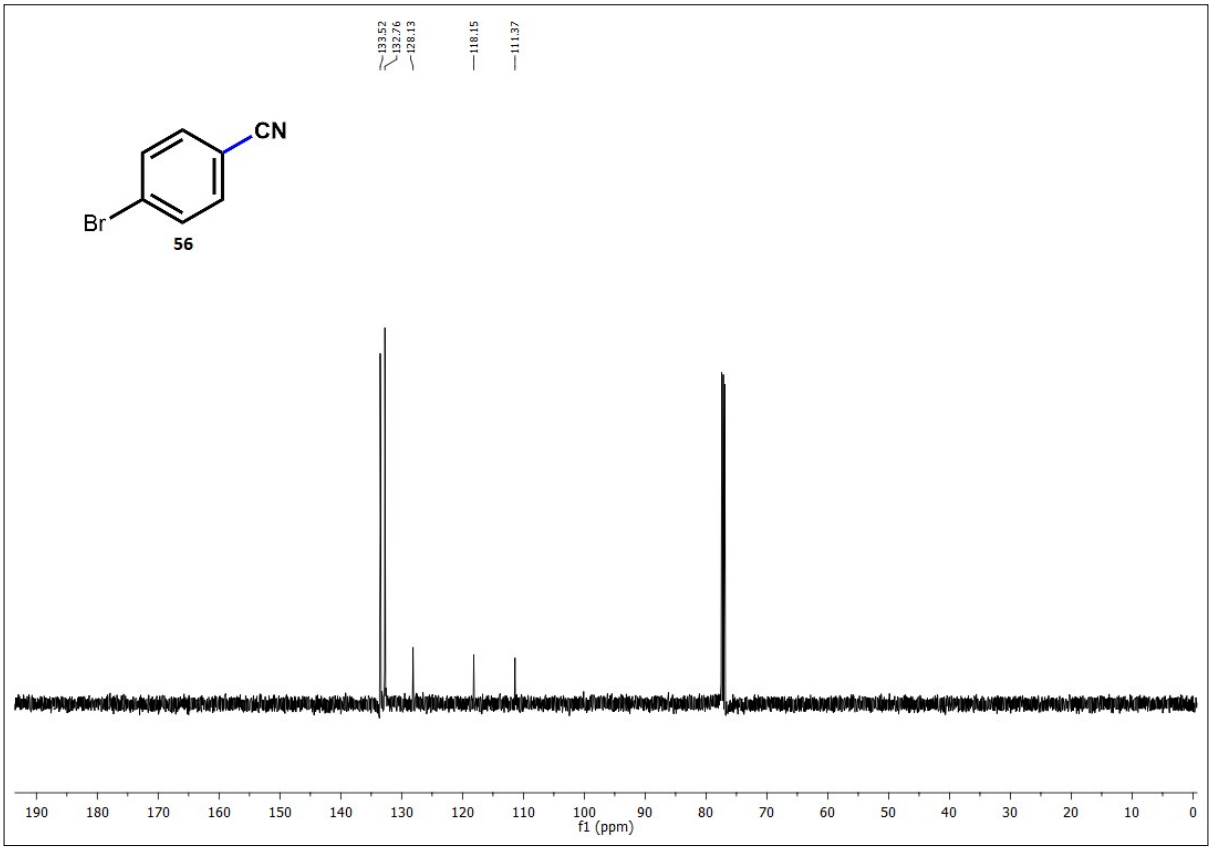
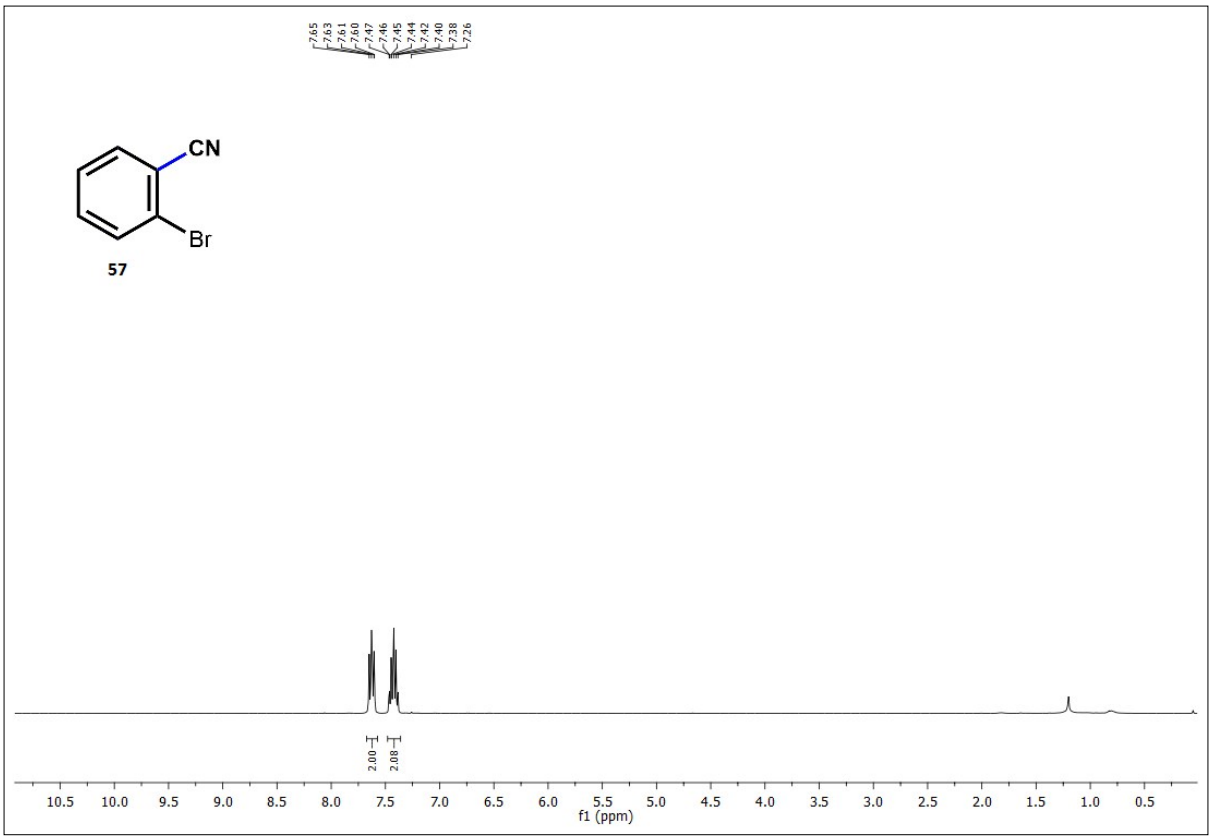
129.97
127.73
127.38
124.94
123.53
122.65
118.81
115.59
114.57
104.80
42.13
12.67
S
CN
N
55
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.65
7.63
7.53
7.51
7.26
CN
Br
56
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


133.52
132.76
128.13
118.15
111.37
CN
Br
56
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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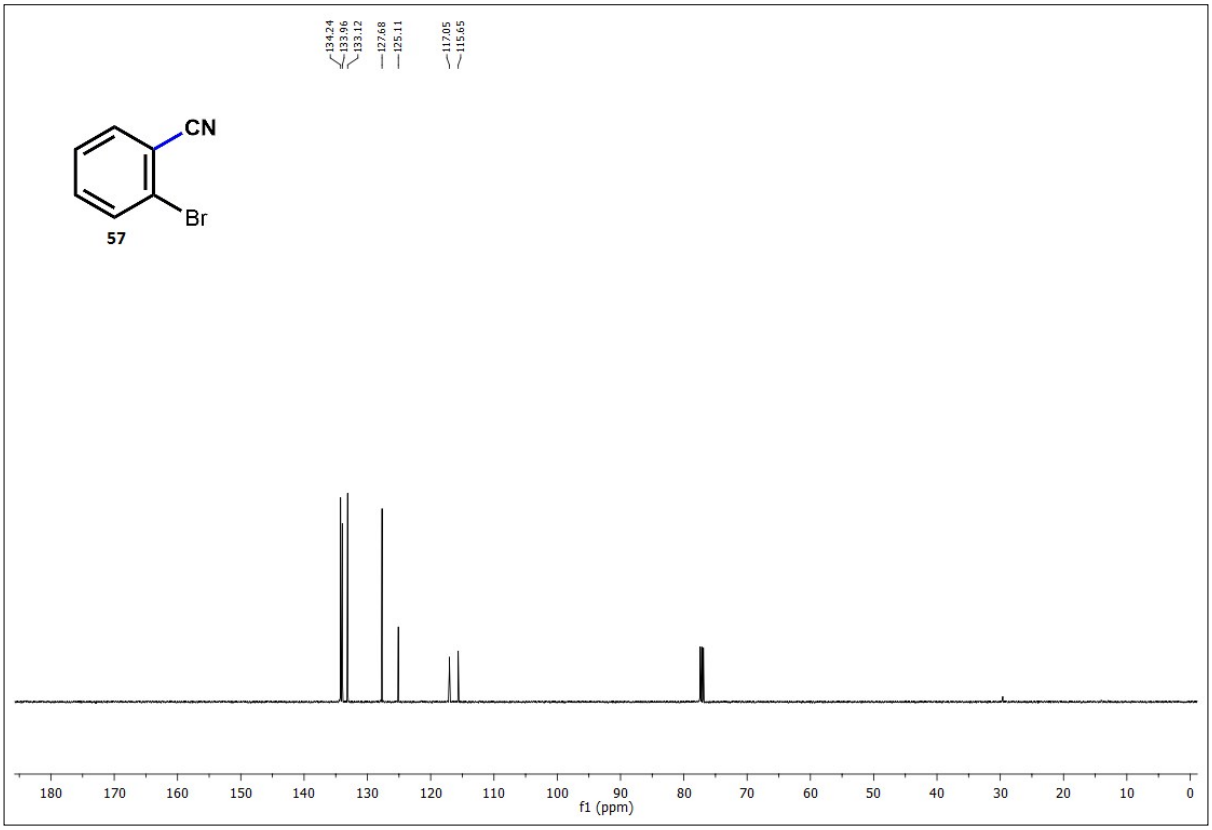
7.63
7.61
7.60
7.47
7.46
7.45
7.44
7.42
7.40
7.38
7.26
CN
Br
57
2.00
2.08
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


134.24
133.96
133.12
127.68
125.11
117.05
115.65
CN
Br
57
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)