

SUPPORTING INFORMATION

Cu(OAc)₂ Catalysed Aerobic Oxidation of Aldehydes to Nitriles under Ligand-Free Condition

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Experimental Section

Materials and methods

All reactants were purchased from SRL, AVRA Chemicals, Alfa-aesar, Spectrochem, and Sigma Aldrich and used as received without further purification. ¹H and ¹³C NMR spectra were obtained on a Bruker-300 spectrometer (300 MHz and 400 MHz) and JEOL Spectrometer (500 MHz) in CDCl₃ and DMSO-*d*₆ solutions with TMS as an internal reference. Melting points were determined in open capillary on electrical bath which is uncorrected. Column chromatography was performed on silica gel (60-120 mesh) from SRL, India. Thin layer chromatographic separations were performed on pre-coated silica gel plates using silica gel G for TLC (E. Merck).

General experimental procedure for the Cu(OAc)₂ catalyzed oxidative transformation of aldehydes to nitriles:

To a stirred suspension of aldehyde **1** (1.0 mmol) and ammonium acetate (1.5 mmol) in DMSO (3 mL), Cu(OAc)₂ (10 mol %) was added. The reaction mixture was stirred for an appropriate time at 60°C under ambient atmosphere. The progress of the reaction was monitored with TLC. Then the reaction mixture was cooled to room temperature, ethyl acetate (15 mL) was

added to dissolve the product. The reaction mixture was repeatedly extracted with ethyl acetate (3×5 mL). The combined organic extracts were washed with water (3×5 mL) and dried over anhydrous Na₂SO₄. The crude product **2** was obtained by removal of the solvent under reduced pressure which was further purified by column chromatography on a short column of silica gel using 1-10% ethyl acetate-hexane as eluent.

Procedure for the Cu(OAc)₂ catalyzed gram-scale synthesis of nitrile (2a):

To a stirred suspension of 4-methoxybenzaldehyde **1a** (20.0 mmol, 2.723 g) and ammonium acetate (30.0 mmol, 2.310 g) in DMSO (60 mL), Cu(OAc)₂ (0.336 g, 10 mol %) was added and the reaction mixture was stirred for the appropriate time at 60°C under ambient atmosphere. The progress of the reaction was monitored with TLC. Then the reaction mixture was cooled to room temperature, ethyl acetate (300 mL) was added to dissolve the product. The reaction mixture was repeatedly extracted with ethyl acetate (3×100 mL). The combined organic extracts were washed with water (3× 100 mL). After drying with anhydrous sodium sulfate, the solvent was removed under reduced pressure to furnish the crude product **2a**, which was further purified by column chromatography of silica gel using ethyl acetate-hexane as eluent. (Yield: 89%, 2.370 g).

Determination of Reaction Order:

To determine the order of the reaction, two identical experiments were carried out following the general procedure varying only the concentration of 4-methoxybenzaldehyde **1a**. The initial rate of the reaction for the different run was calculated to determine the order with respect to aldehyde **1a**.

Table S1 Experimental details to determine the reaction order

| Run | 4-methoxybenzaldehyde 1a | NH ₄ OAc | Cu(OAc) ₂ | DMSO |
|-------|---------------------------------|---------------------|----------------------|------|
| Run 1 | 1 mmol | 1.5 mmol | 10 mol% | 3 mL |
| Run 2 | 2 mmol | 1.5 mmol | 10 mol% | 3 mL |

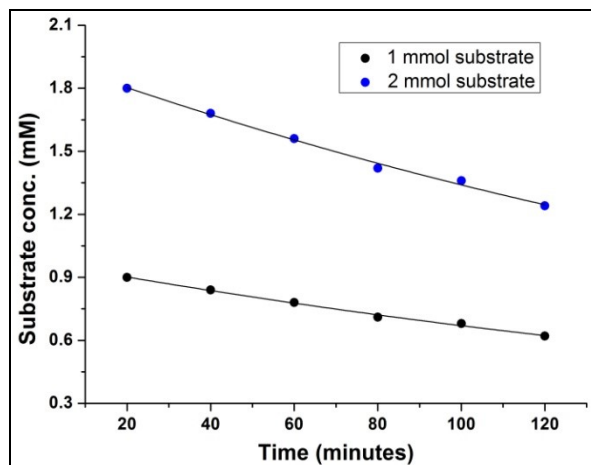


Figure S1 Dependence of [4-methoxybenzaldehyde] on the initial rate of the reaction using $\text{Cu}(\text{OAc})_2$ (10 mol%), NH_4OAc (1.5 mmol), DMSO (3 mL), 60°C , under ambient condition.

Initial slope for Run 1 at 60 minutes = $0.0135 = 13.5 \times 10^{-3}$ (mM)/min

Initial slope for Run 2 at 60 minutes = $0.0269 = 26.9 \times 10^{-3}$ (mM)/min

Simplified rate equation for this system $(r) = k [\text{4-methoxybenzaldehyde}]^a [\text{NH}_4\text{OAc}]^b [\text{Cu}(\text{OAc})_2]^c [\text{DMSO}]^d$
(all terms have their usual significance)

Now for Run 1, $r_1 = 13.5 \times 10^{-3}$ (mM)/min = $k [1]^a [\text{NH}_4\text{OAc}]^b [\text{Cu}(\text{OAc})_2]^c [\text{DMSO}]^d$
.....(1)

Now for Run 2, $r_2 = 26.9 \times 10^{-3}$ (mM)/min = $k [2]^a [\text{NH}_4\text{OAc}]^b [\text{Cu}(\text{OAc})_2]^c [\text{DMSO}]^d$
.....(2)

Comparing the initial rate,

$$r_1/r_2 = (13.5/26.9) = (1/2)^a$$

$$\text{or, } 0.502 = 0.5^a$$

$$\text{or, } \log 0.502 = a \log 0.5$$

$$\text{or, } a = \log 0.502 / \log 0.5$$

$$\text{or, } a = -0.299 / -0.301$$

$$\text{or, } a = 0.99 - 1$$

So, Rate = $k [\text{4-methoxybenzaldehyde}]^1$

The kinetic studies showed that the reaction rate depends on the concentration of 4-methoxybenzaldehyde **1a** only. Therefore, the aforesaid oxidative protocol follows first order kinetics.

Spectral and analytical data of the compounds:

4-methoxybenzonitrile (2a)¹: Yield: 90%; White solid; Mp 57-59 °C (Lit.¹⁰ 58-60 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.57 (2H, d, *J* = 8.4 Hz); 6.93 (2H, d, *J* = 8.4 Hz); 3.84 (3H, s). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 159.3, 131.5, 119.6, 117.1, 114.0, 56.1.

4-tolunitrile (2b)¹: Yield: 91%; Colorless liquid; ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.50 (2H, d, *J* = 7.8 Hz); 7.24 (2H, d, *J* = 7.8 Hz); 2.38 (3H, s). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 145.1, 132.6, 128.9, 119.8, 111.6, 22.5.

2-tolunitrile (2c)¹: Yield: 89%; Colorless liquid; ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.44-7.59 (2H, m); 7.23-7.31 (2H, m); 2.53 (3H, s). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 141.9, 132.6, 132.4, 130.2, 126.2, 118.1, 112.7, 20.4.

Benzonitrile (2d)²: Yield: 90%; Colorless liquid; ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.57-7.64 (3H, m); 7.43-7.48 (2H, m). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 133.9, 133.1, 129.6, 119.5, 113.4.

3, 4-dimethoxybenzonitrile (2e)²: Yield: 90%; White solid; Mp 70-72 °C (Lit.¹⁰ 69-71 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.24 (1H, d, *J* = 1.5 Hz); 7.04 (1H, s); 6.87 (1H, d, *J* = 8.1 Hz); 3.94 (3H, s); 3.90 (3H, s). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 152.8, 149.4, 126.5, 119.1, 113.8, 111.2, 103.6, 56.0, 55.8.

4-hydroxy-3-methoxybenzonitrile (2f)³: Yield: 89%; White solid; Mp 88-90 °C (Lit.¹⁰ 87-89 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.19 (1H, d, *J* = 7.5 Hz); 7.06 (1H, s); 6.92 (1H, d, *J* = 7.8 Hz); 3.89 (3H, s). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 150.1, 146.8, 127.5, 119.3, 113.9, 109.0, 103.1, 56.2.

4-hydroxybenzotrile (2g)³: Yield: 87%; White solid; Mp 110-112 °C (Lit.¹⁰ 111-112 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.54 (2H, d, *J* = 8.4 Hz); 6.94 (2H, d, *J* = 8.4 Hz). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 160.5, 134.3, 119.3, 116.5, 102.7.

3-hydroxybenzotrile (2h)⁴: Yield: 89%; White solid; Mp 79-81 °C; ¹H NMR (DMSO-d₆, 300 MHz); δ (ppm): 7.28-7.33 (2H, m); 7.19 (1H, s); 7.09-7.17 (1H, m). ¹³C NMR (DMSO-d₆, 75 MHz); δ (ppm): 156.5, 131.2, 124.7, 121.2, 119.5, 117.8, 110.4.

2-hydroxybenzotrile (2i)³: Yield: 88%; White solid; Mp 97-99 °C (Lit.¹¹ 96-98 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.48-7.51 (2H, m); 6.95-6.98 (2H, m); 4.89 (1H, br s). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 158.8, 134.7, 132.9, 120.7, 119.1, 116.7, 102.8.

4-(dimethylamino)benzotrile (2j)³: Yield: 88%; White solid; Mp 70-72 °C (Lit.⁵ 71-73 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.45 (2H, d, *J* = 8.7 Hz); 6.63 (2H, d, *J* = 8.7 Hz). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 152.5, 133.6, 120.6, 111.8, 97.4, 39.8.

2-aminobenzotrile (2k)⁵: Yield: 89%; Yellow solid; Mp 48-50 °C (Lit.⁵ 49-51 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.29-7.38 (2H, m); 6.70-6.75 (2H, m); 4.41 (2H, br s). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 149.7, 134.0, 132.4, 117.9, 117.6, 115.2, 95.9.

4-chlorobenzotrile (2l)¹: Yield: 93%; White solid; Mp 92-94 °C (Lit.⁵ 91-93 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.60 (2H, d, *J* = 8.4 Hz); 7.46 (2H, d, *J* = 8.4 Hz). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 139.3, 132.8, 129.2, 118.8, 110.3.

4-bromobenzotrile (2m)¹: Yield: 91%; White solid; Mp 108-110 °C (Lit.⁵ 109-111 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.62 (2H, d, *J* = 8.4 Hz); 7.51 (2H, d, *J* = 8.4 Hz). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 133.4, 132.6, 127.9, 118.0, 111.3.

4-nitrobenzotrile (2n)¹: Yield: 95%; Yellow solid; Mp 147-150 °C (Lit.⁵ 146-148 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 8.36 (2H, d, *J* = 8.7 Hz); 7.88 (2H, d, *J* = 8.7 Hz). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 150.1, 133.5, 124.2, 118.3, 116.8.

3-nitrobenzotrile (2o)³: Yield: 94%; White solid; Mp 114-116 °C (Lit.¹¹ 115-116 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.18-7.25 (1H, m); 7.00 (1H, d, *J* = 7.5 Hz); 6.84-6.89 (2H, m). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 147.0, 130.1, 121.9, 119.2, 117.4, 112.8.

4-formylbenzotrile (2p)⁵: Yield: 88%; White solid; Mp 98-100 °C (Lit.⁵ 100-101 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 10.1 (1H, s); 7.98 (2H, d, *J* = 8.1 Hz); 7.84 (2H, d, *J* = 8.1 Hz). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 190.6, 138.7, 132.9, 130.6, 129.9, 117.6.

Terephthalonitrile (2q)⁵: Yield: 87%; White solid; Mp 225-227 °C (Lit.⁵ 224-226 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.52 (s, 4H). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 132.7, 118.2, 116.6.

4-acetylbenzotrile (2r)⁵: Yield: 88%; Light yellow solid; Mp 56-58 °C (Lit.⁵ 55-57 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 8.03 (2H, d, *J* = 8.1 Hz); 7.77 (2H, d, *J* = 8.1 Hz); 2.64 (3H, s). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 196.6, 139.9, 132.5, 128.7, 117.9, 116.3, 26.7.

1-naphthonitrile (2s)⁶: Yield: 86%; White solid; Mp 33-35 °C (Lit.⁵ 35-37 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 8.21 (1H, d, *J* = 8.4 Hz), 8.02 (1H, d, *J* = 8.6 Hz), 7.76–7.83 (4H, m), 7.48 (1H, t, *J* = 7.8 Hz). ¹³C NMR (75 MHz, CDCl₃); δ (ppm): 133.5, 132.9, 132.1, 131.8, 128.7, 128.1, 127.0, 125.6, 124.7, 118.1, 110.2.

Benzo[d][1,3]dioxole-5-carbonitrile (2t)¹: Yield: 88%; White solid; Mp 92-94 °C; ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.41 (1H, s); 7.14-7.20 (1H, m), 6.98 (1H, d, *J* = 8.2 Hz), 6.01 (2H, s). ¹³C NMR (75 MHz, CDCl₃); δ (ppm): 150.6, 148.2, 127.9, 119.0, 111.1, 108.8, 105.7, 101.3.

Cinnamonitrile (2u)²: Yield: 83%; Colorless oil; ¹H NMR (CDCl₃, 400 MHz); δ (ppm): 7.37-7.49 (6H, m), 5.83 (1H, d, *J* = 16.3 Hz). ¹³C NMR (100 MHz, CDCl₃); δ (ppm): 150.1, 132.9, 131.4, 129.3, 127.5, 118.8, 95.8.

Furan-2-carbonitrile (2v)¹: Yield: 79%; Viscous oil; ¹H NMR (CDCl₃, 400 MHz); δ (ppm): 7.58 (1H, d, *J* = 1.5 Hz), 6.96-7.02 (2H, m). ¹³C NMR (100 MHz, CDCl₃); δ (ppm): 147.5, 132.2, 125.3, 119.8, 111.6.

Thiophene-2-carbonitrile (2w)¹: Yield: 81%; Colorless liquid; ¹H NMR (CDCl₃, 400 MHz); δ (ppm): 7.60 (2H, d, *J* = 4.3 Hz), 7.01-7.06 (1H, m). ¹³C NMR (100 MHz, CDCl₃); δ (ppm): 138.2, 131.4, 126.5, 118.1, 109.2.

Picolinonitrile (2x)⁶: Yield: 83%; Colorless liquid; ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 8.72 (1H, d, *J* = 4.5 Hz), 7.62-7.71 (3H, m). ¹³C NMR (75 MHz, CDCl₃); δ (ppm): 151.3, 135.7, 133.3, 127.6, 124.9, 117.6.

Isonicotinonitrile (2y)⁷: Yield: 80%; White solid; Mp 78-79 °C (Lit.¹⁰ 77-78 °C); ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 8.82 (2H, d, *J* = 13.5 Hz); 7.55 (2H, d, *J* = 13.5 Hz). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 152.3, 126.8, 120.7, 117.3.

4-(benzyloxy)benzonitrile (2z)⁶: Yield: 86%; White solid; Mp 95-98 °C; ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.59-7.63 (2H, m); 7.38-7.44 (5H, m); 7.00-7.07 (2H, m); 5.14 (2H, s). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 161.9, 135.7, 134.0, 128.7, 128.4, 127.5, 119.2, 115.6, 104.3, 70.3.

4-(allyloxy)-3-methoxybenzonitrile (2za)⁸: Yield: 84%; Light yellow liquid; ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.24 (1H, d, *J* = 9.0 Hz); 7.08 (1H, s); 6.88 (1H, d, *J* = 8.4 Hz); 6.00-6.11 (1H, m); 5.31-5.45 (2H, m); 4.65 (2H, d, *J* = 4.8 Hz); 3.88 (3H, s). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 151.9, 149.5, 132.1, 126.2, 119.2, 118.8, 114.3, 112.9, 104.0, 69.7, 56.2.

4-((tert-butyldimethylsilyloxy)-3-methoxybenzonitrile (2zb)⁹: Yield: 85%; Colorless liquid; ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 7.05 (1H, s); 6.94 (2H, m); 3.89 (3H, s); 0.88 (9H, s); 0.06 (6H, s). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 150.2, 146.9, 126.9, 119.2, 115.4, 113.9, 103.1, 56.2, 25.6, 17.9, -3.64.

Heptanenitrile (2zc)³: Yield: 78%; Colorless liquid; ¹H NMR (CDCl₃, 300 MHz); δ (ppm): 1.56 (3H, t); 1.24-1.30 (7H, m); 0.88 (3H, t). ¹³C NMR (CDCl₃, 75 MHz); δ (ppm): 119.2, 31.9, 30.5, 29.3, 28.8, 22.6, 14.0.

Pentanenitrile (2zd)¹²: Yield: 79%; Colorless liquid; ¹H NMR (CDCl₃, 500 MHz); δ (ppm): 2.32 (2H, t, *J* = 7.2 Hz); 1.61-1.63 (2H, m); 1.46-1.47 (2H, m); 0.93 (3H, t, *J* = 7.4 Hz). ¹³C NMR (CDCl₃, 125 MHz); δ (ppm): 119.9, 27.4, 21.9, 16.9, 13.3.

2-Phenylacetonitrile (2ze)⁶: Yield: 84%; Colorless liquid; ¹H NMR (CDCl₃, 500 MHz); δ (ppm): 7.32-7.36 (5H, m); 3.74 (2H, s). ¹³C NMR (CDCl₃, 125 MHz); δ (ppm): 130.0, 129.2, 128.1, 128.0, 117.9, 23.7.

¹H NMR & ¹³C NMR Spectra of the Representative Compounds

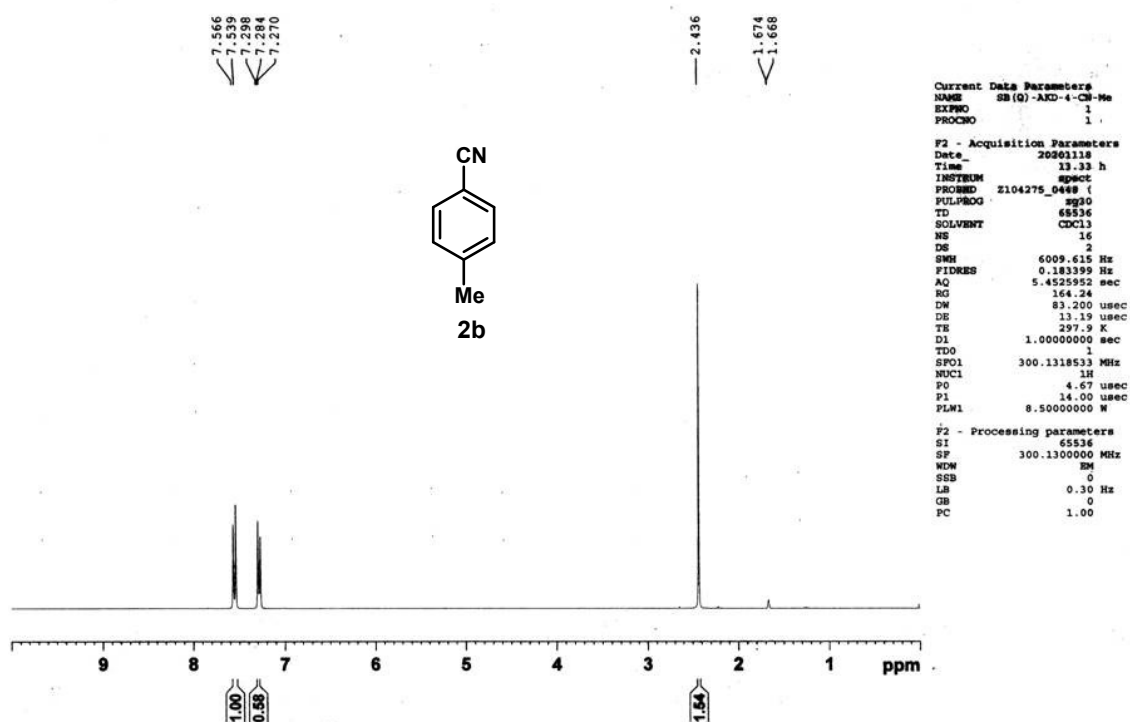


Figure 1 ¹H NMR of 4-tolunitrile (2b)

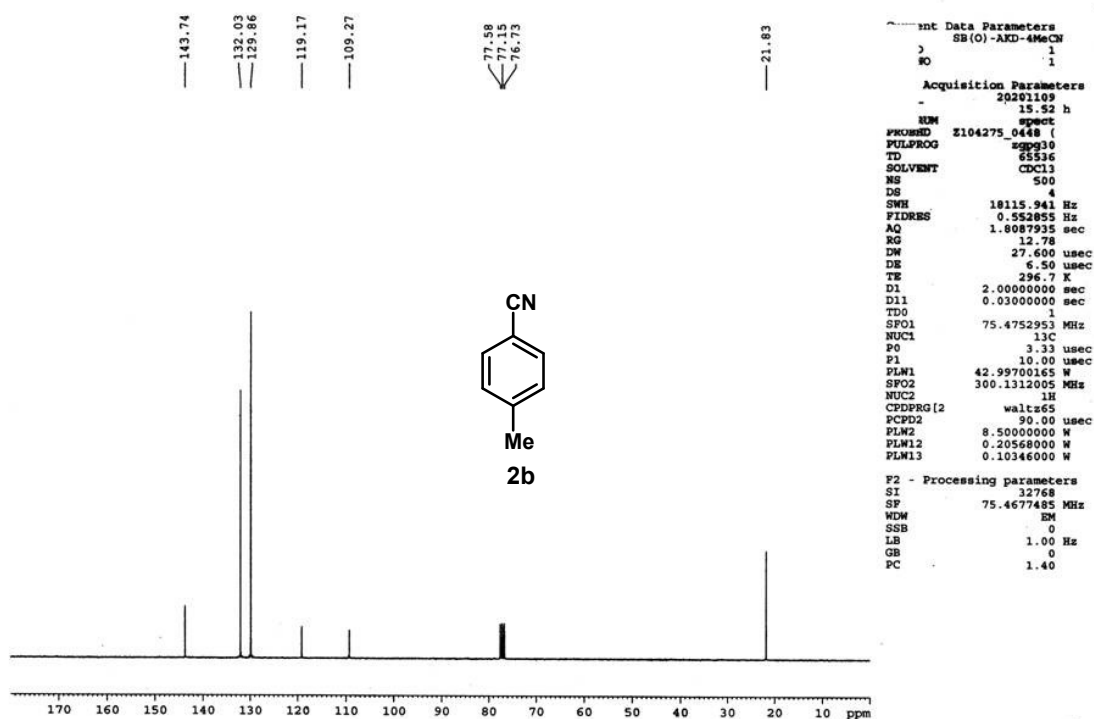


Figure 2 ¹³C NMR of 4-tolunitrile (2b)

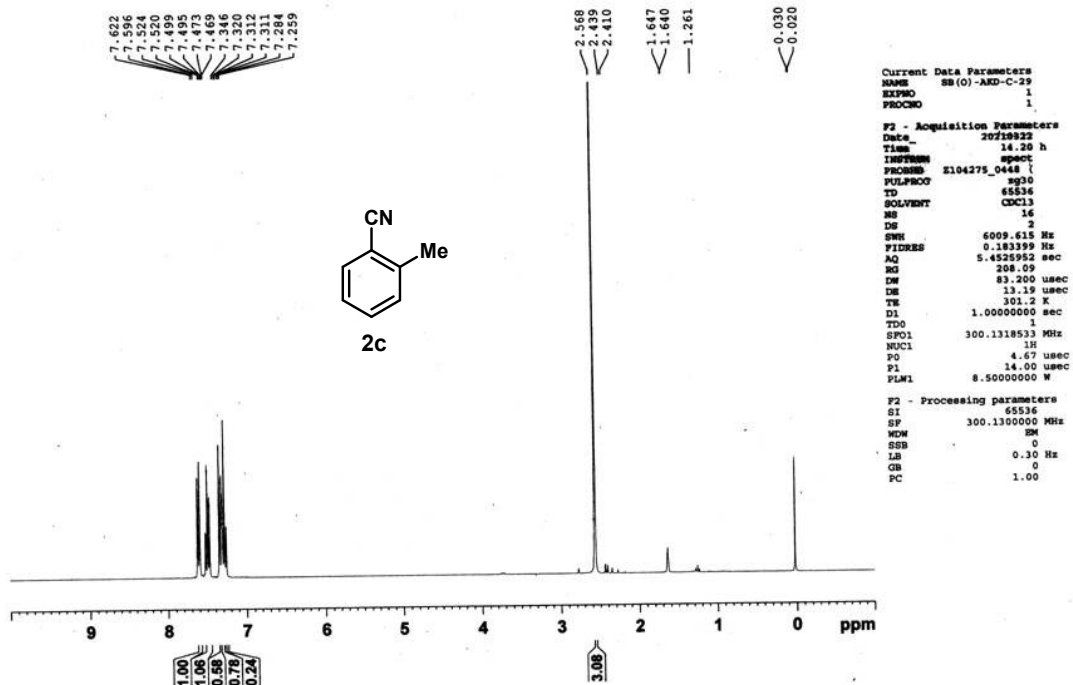


Figure 3 ^1H NMR of 2-tolunitrile (2c)

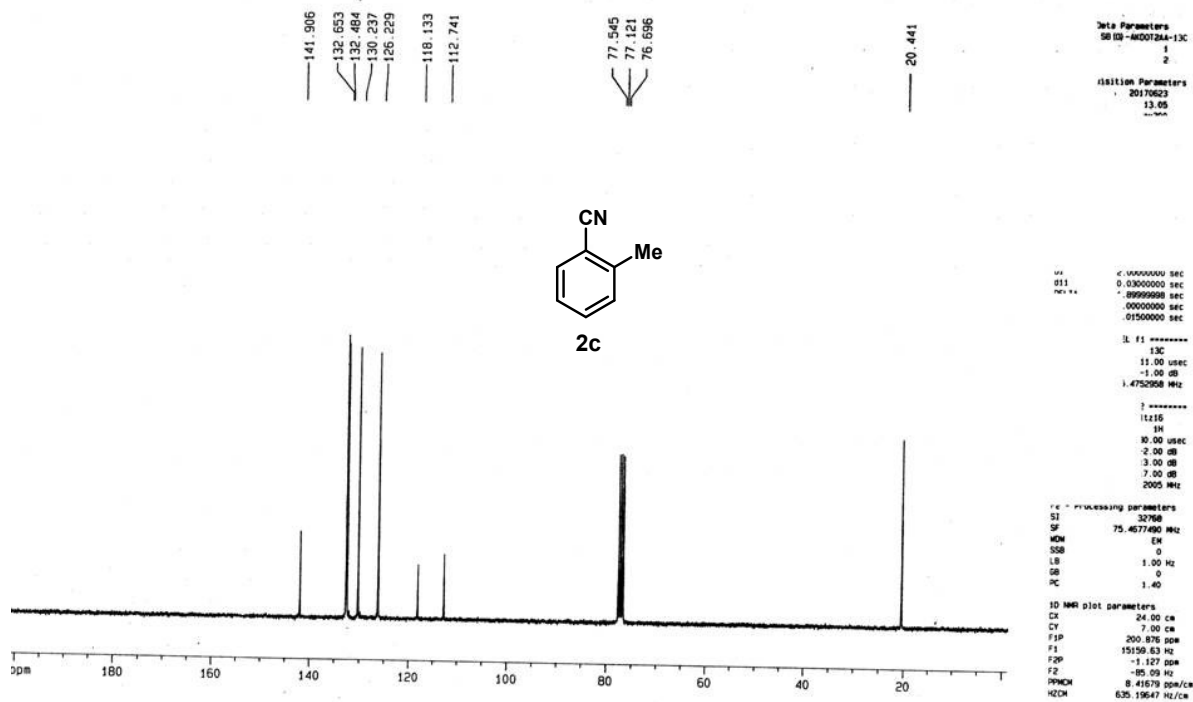


Figure 4 ^{13}C NMR of 2-tolunitrile (2c)

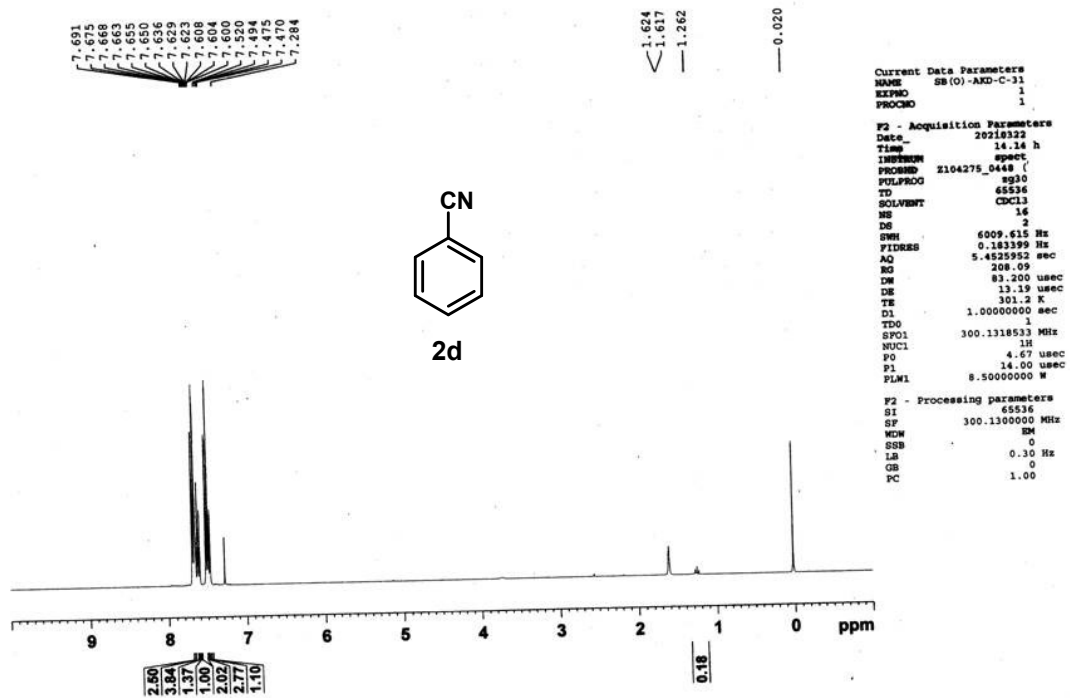


Figure 5 ¹H NMR of Benzonitrile (2d)

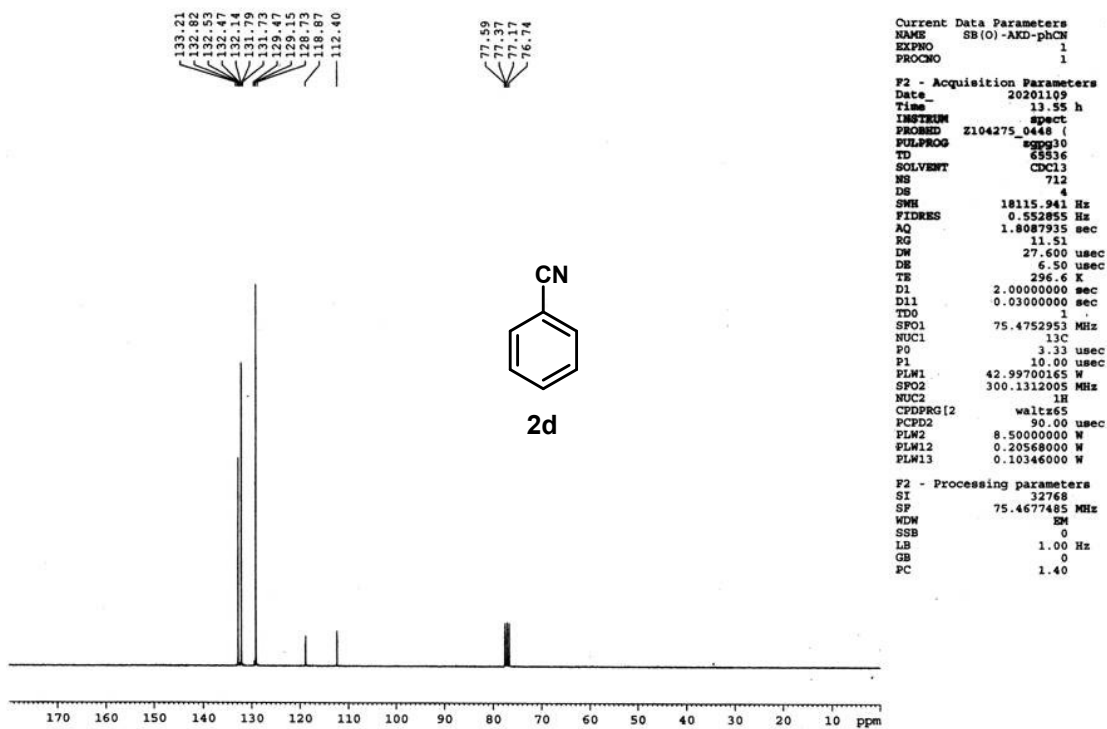


Figure 6 ¹³C NMR of Benzonitrile (2d)

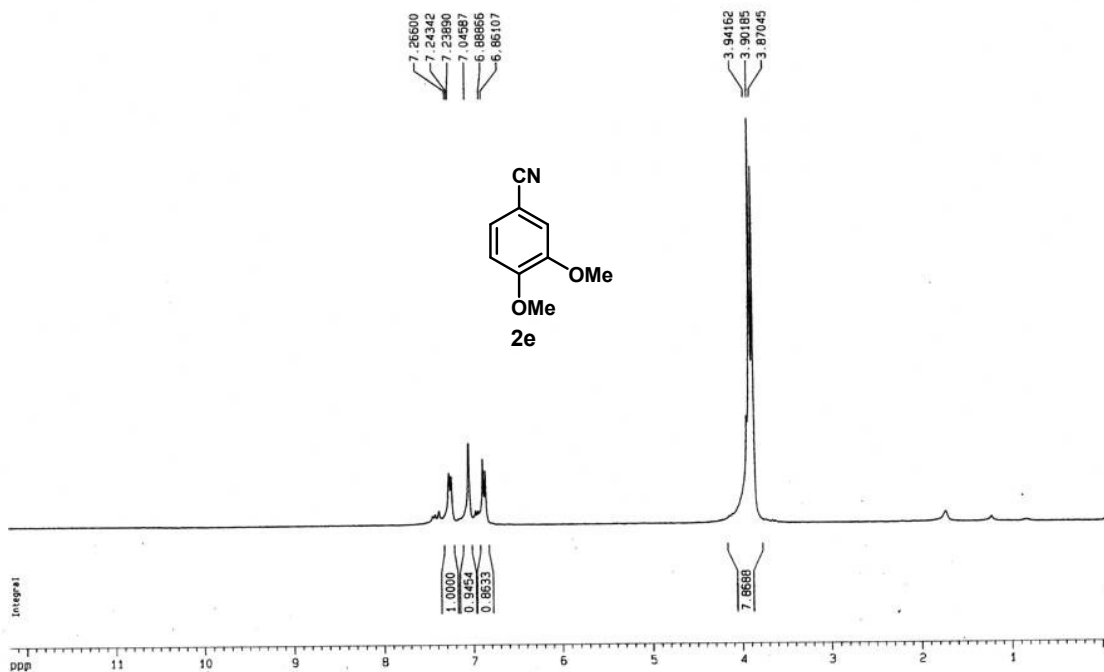


Figure 7 ^1H NMR of 3, 4-dimethoxybenzonitrile (2e)

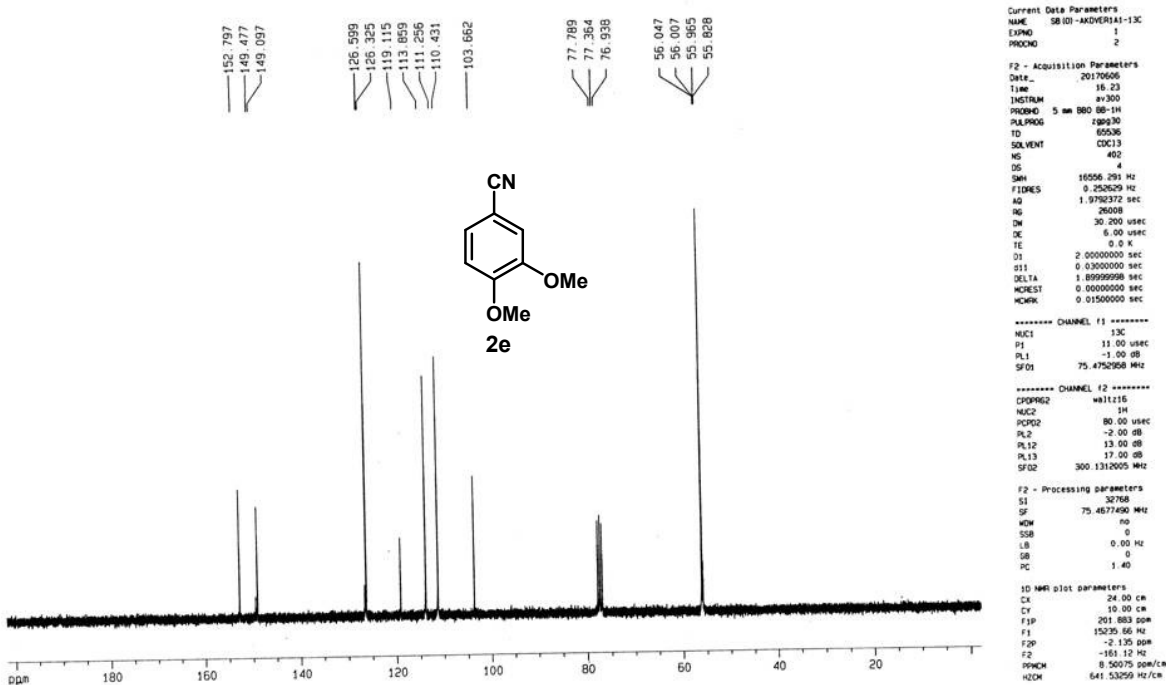


Figure 8 ^{13}C NMR of 3, 4-dimethoxybenzonitrile (2e)

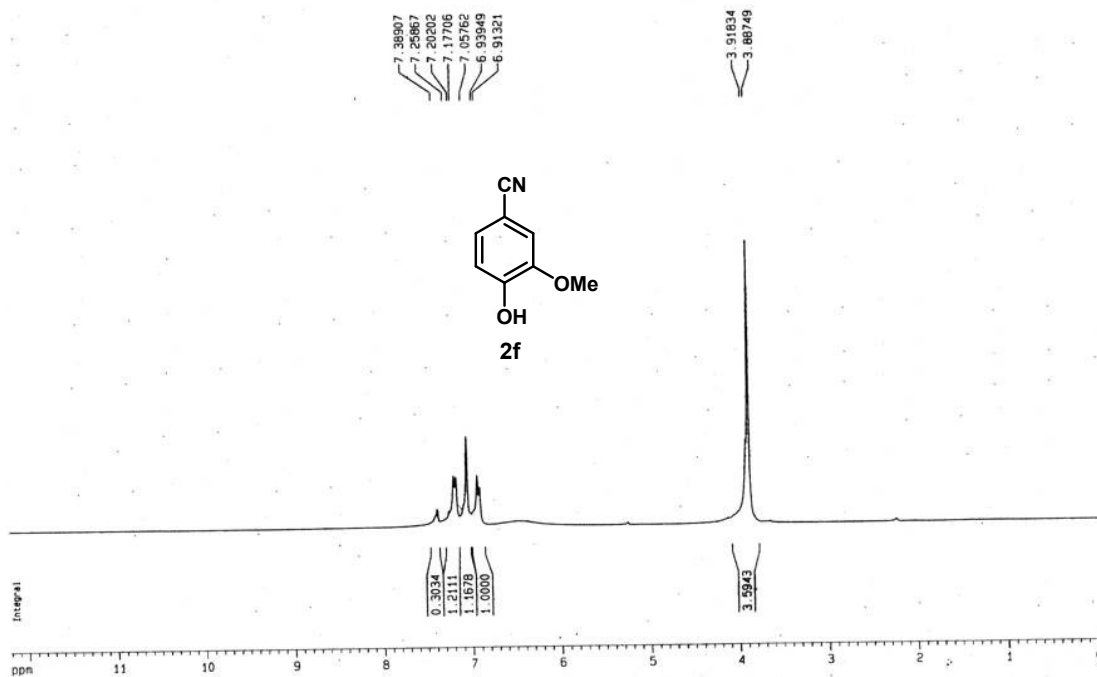


Figure 9 ^1H NMR of 4-hydroxy-3-methoxybenzonitrile (2f)

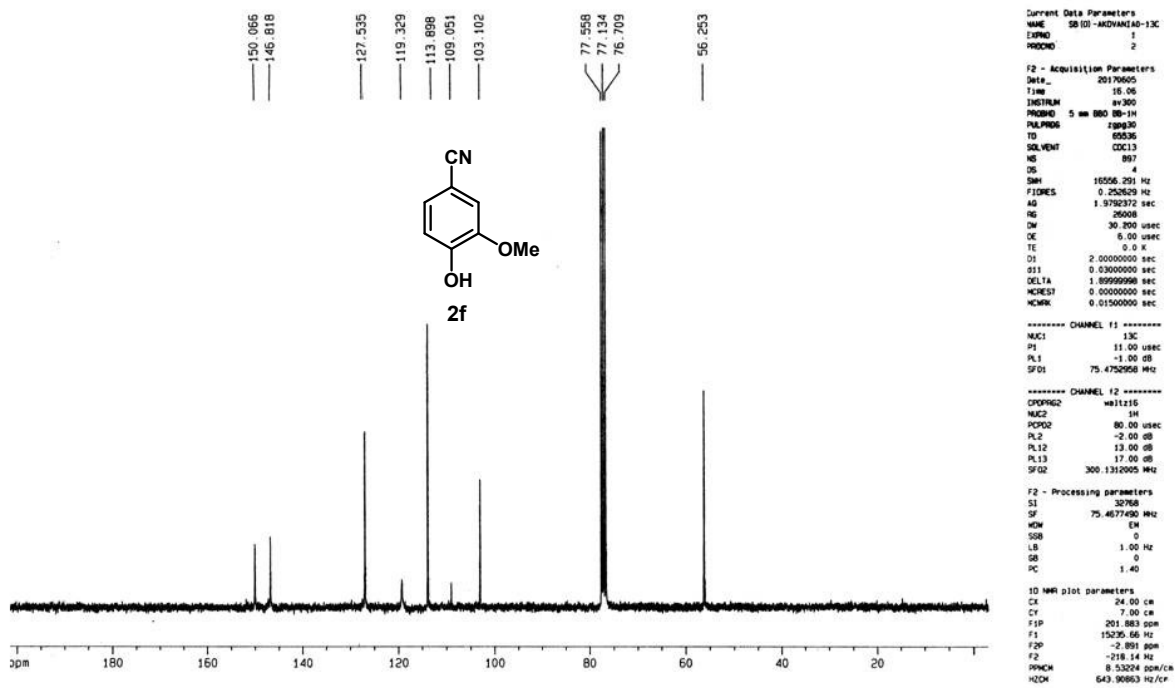


Figure 10 ^{13}C NMR of 4-hydroxy-3-methoxybenzonitrile (2f)

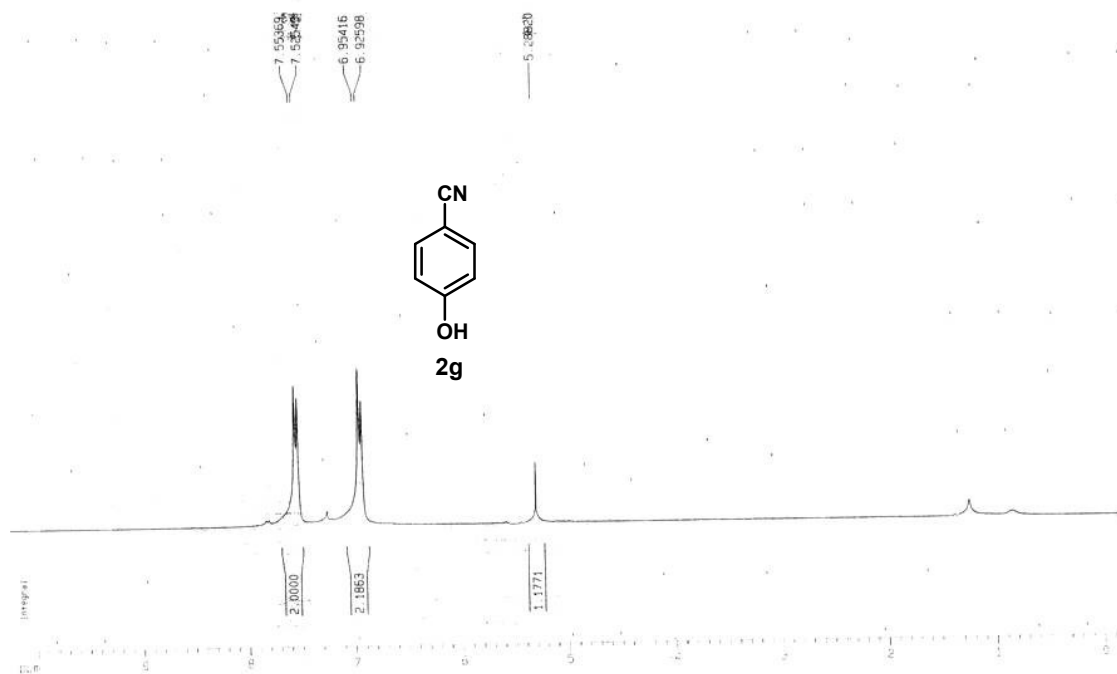


Figure 11 ¹H NMR of 4-hydroxybenzonitrile (2g)

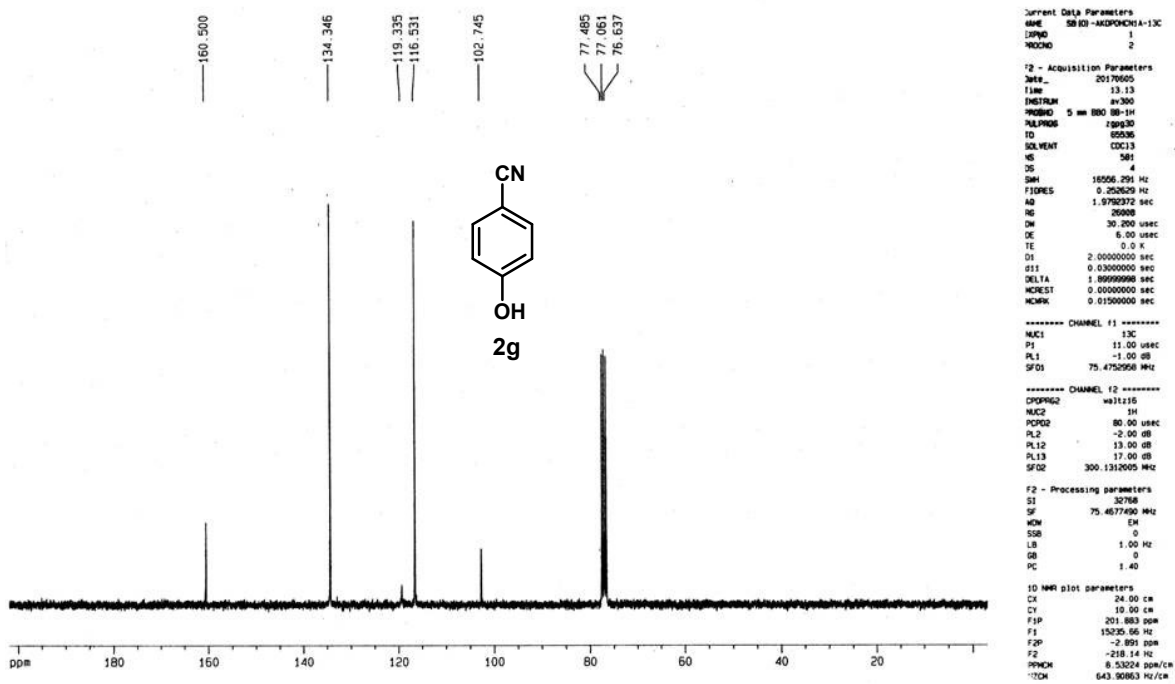


Figure 12 ¹³C NMR of 4-hydroxybenzonitrile (2g)

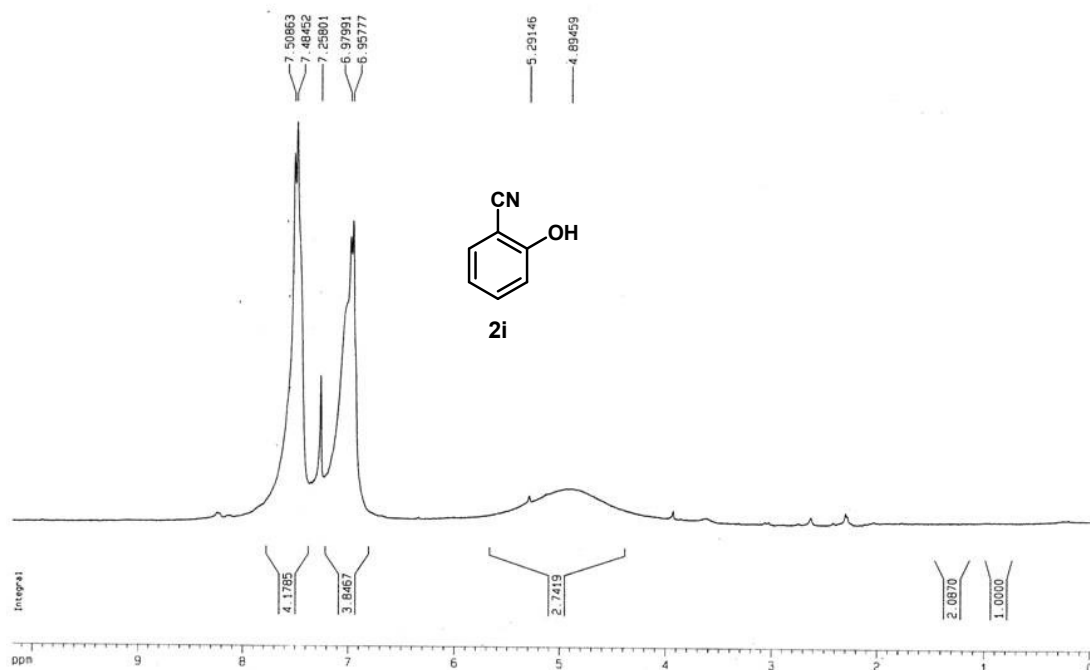
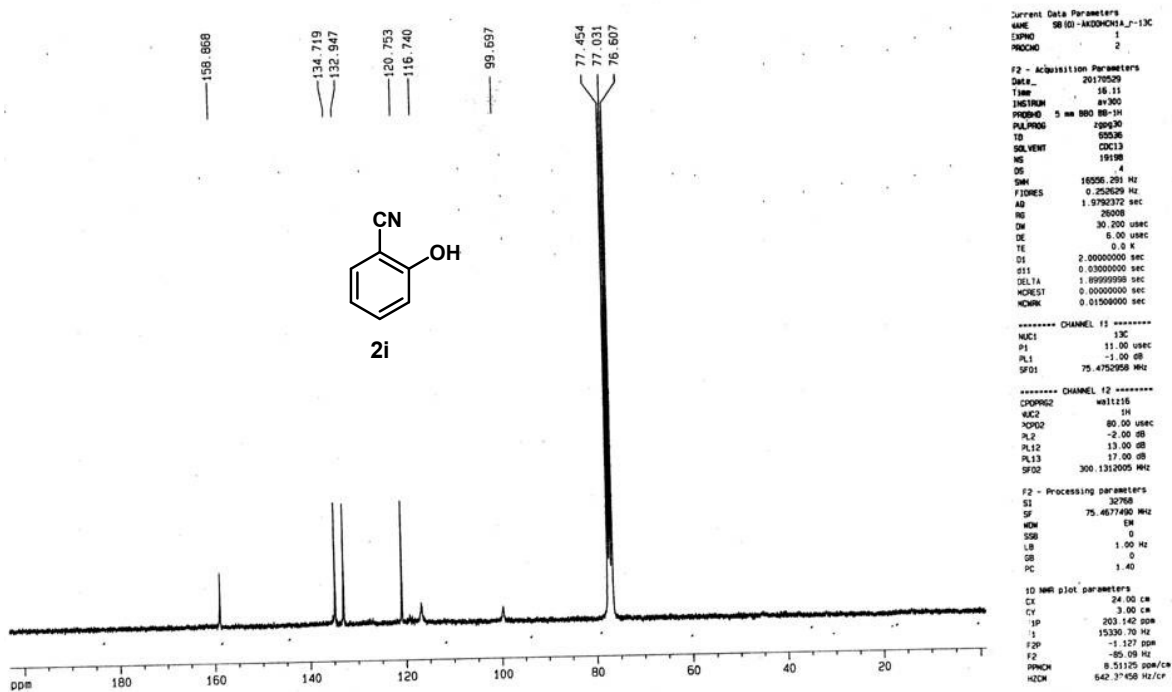


Figure 13 ^1H NMR of 2-hydroxybenzonitrile (2i)



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PROCNO 2

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Figure 14 ^{13}C NMR of 2-hydroxybenzonitrile (2i)

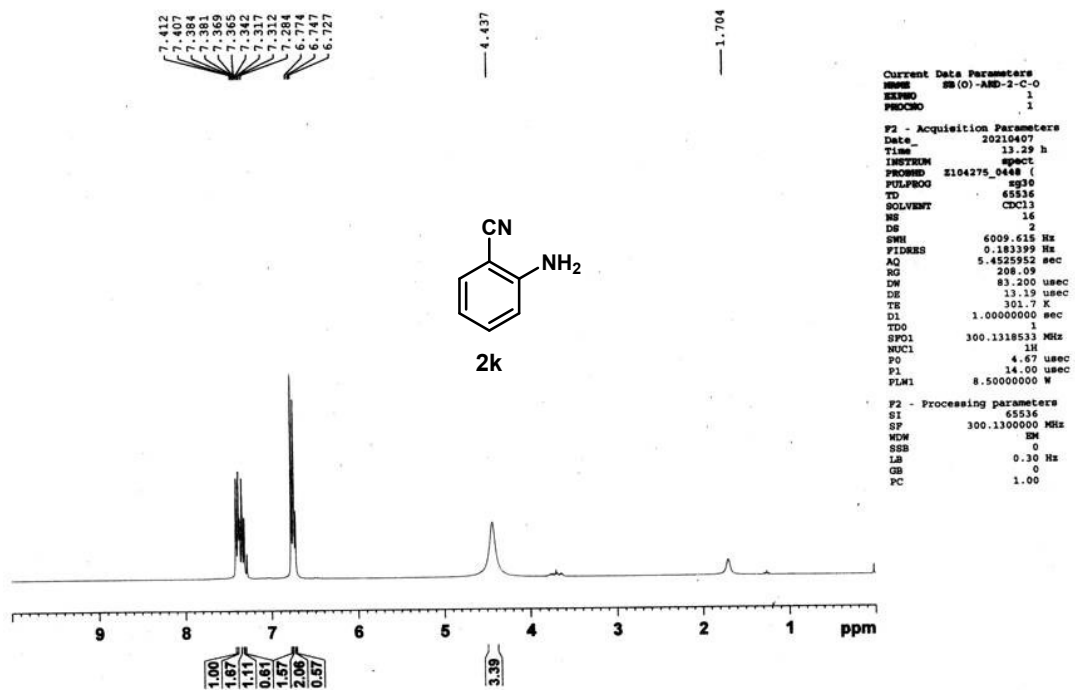


Figure 17 ¹H NMR of 2-aminobenzonitrile (2k)

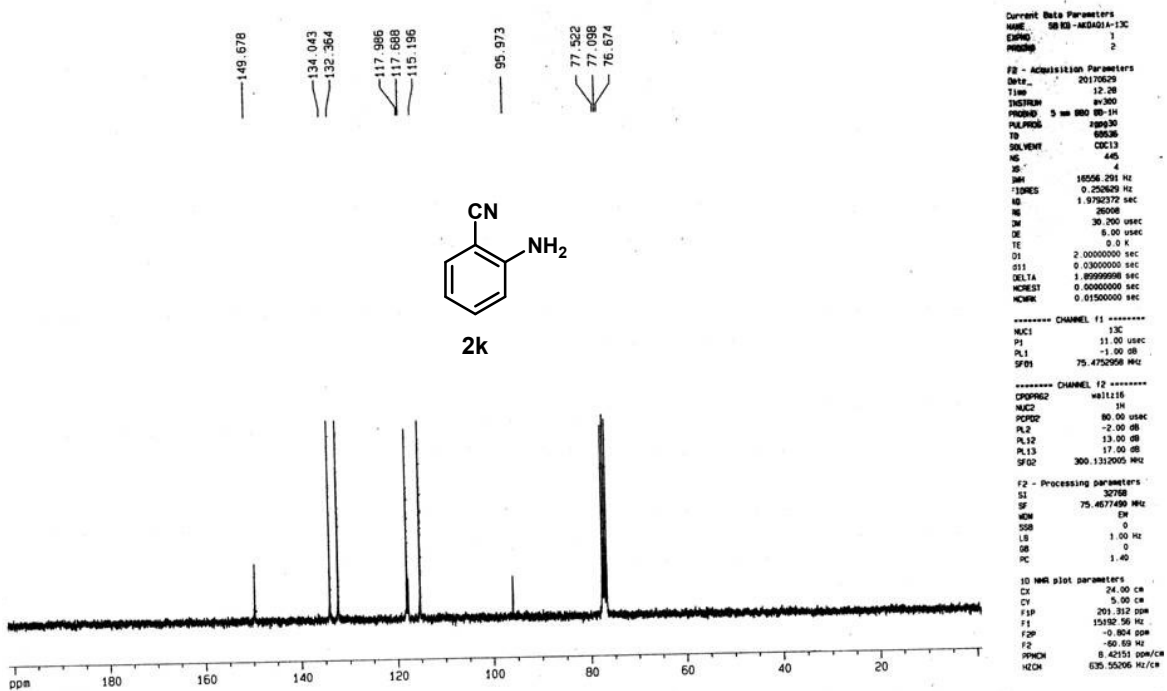


Figure 18 ¹³C NMR of 2-aminobenzonitrile (2k)

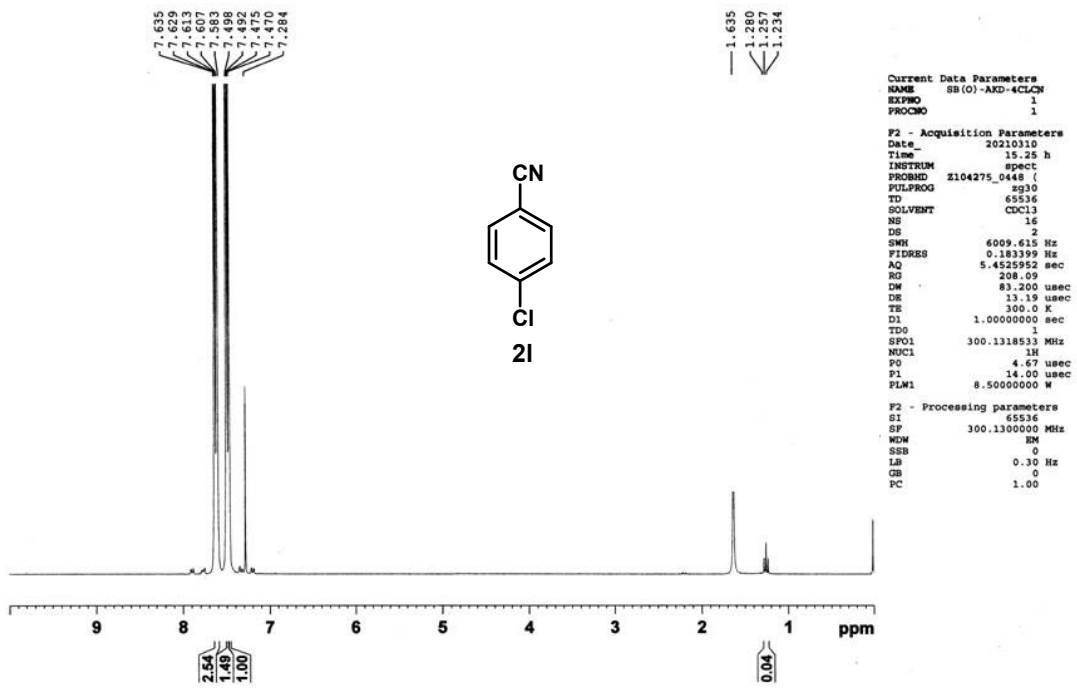


Figure 19 ¹H NMR of 4-chlorobenzonitrile (21)

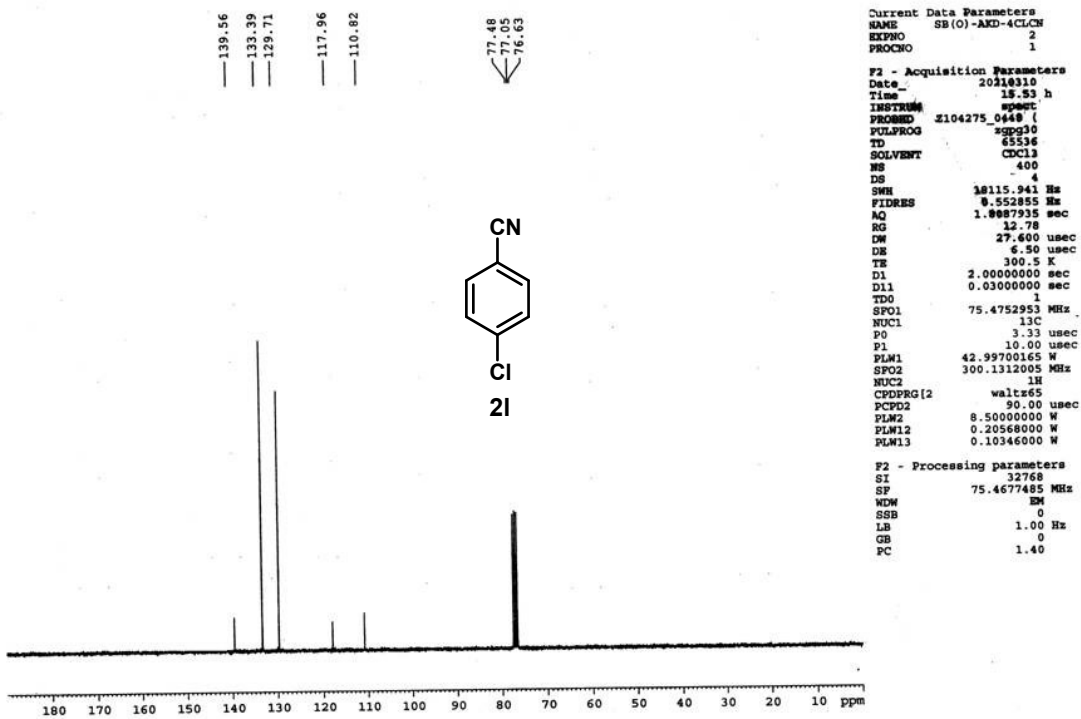


Figure 20 ¹³C NMR of 4-chlorobenzonitrile (21)

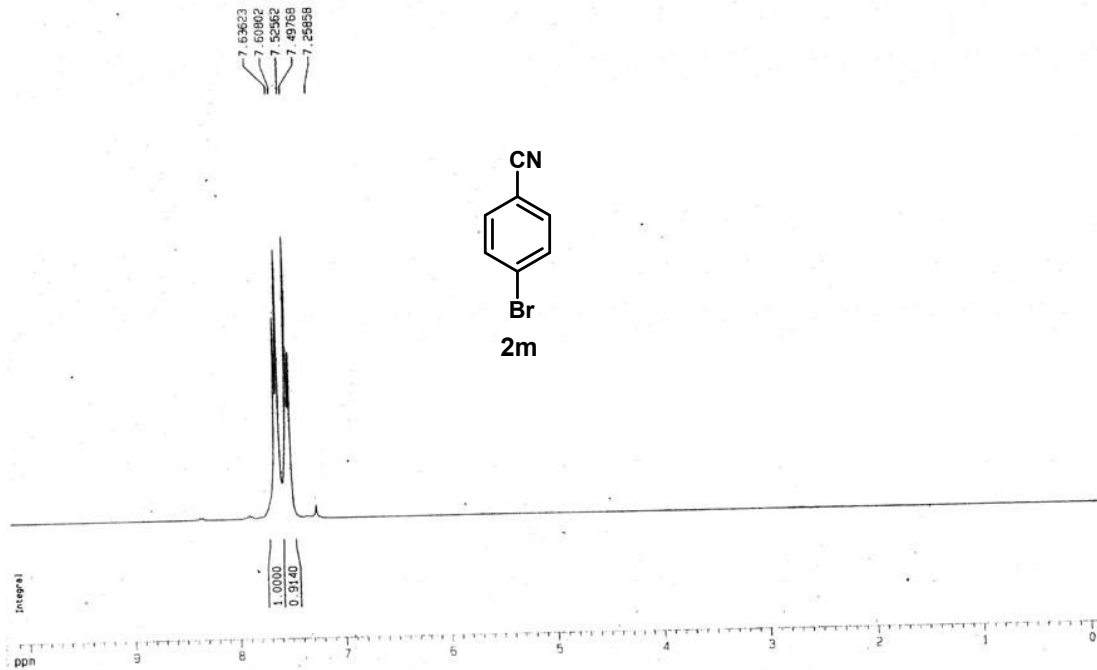


Figure 21 ¹H NMR of 4-bromobenzonitrile (2m)

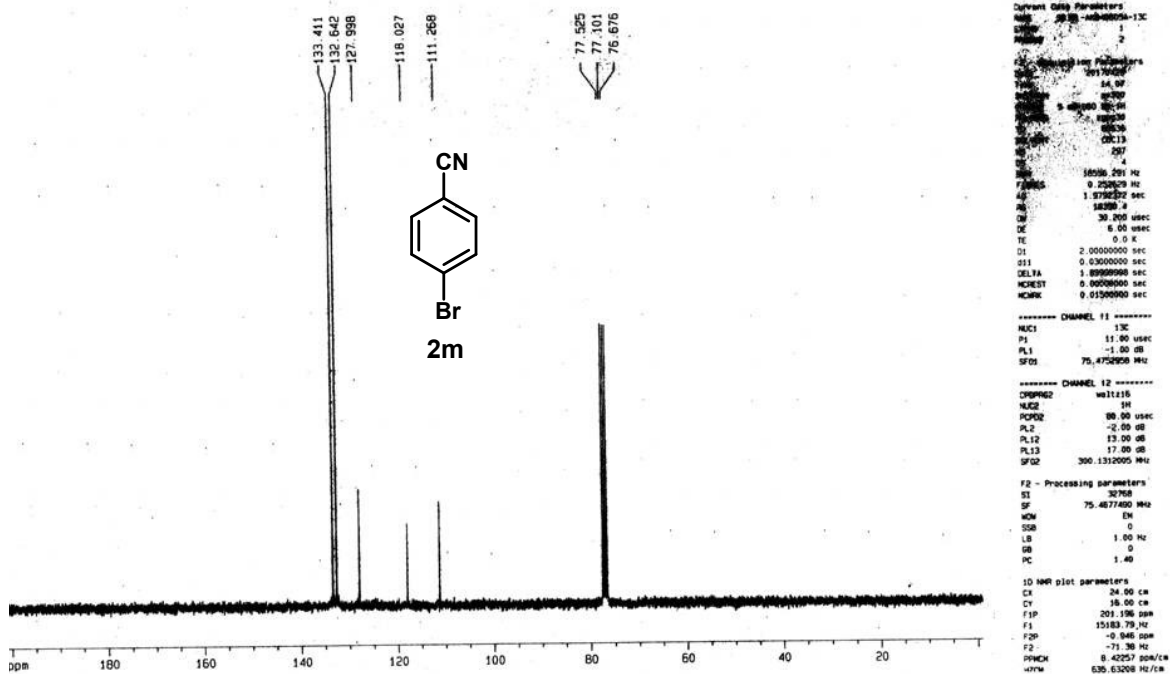


Figure 22 ¹³C NMR of 4-bromobenzonitrile (2m)

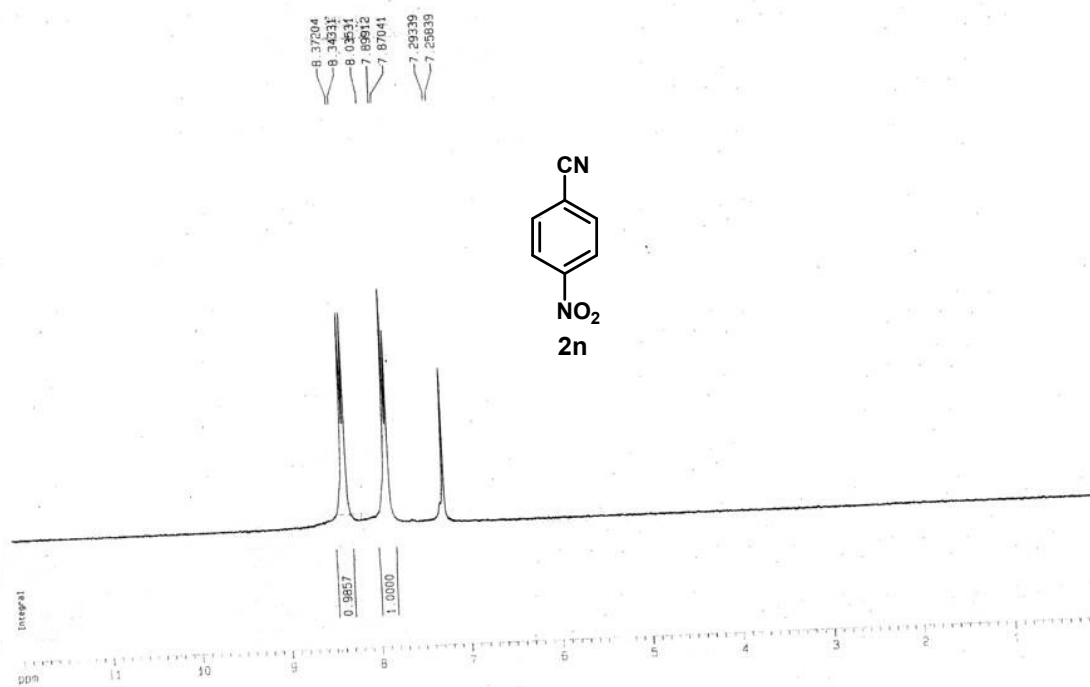
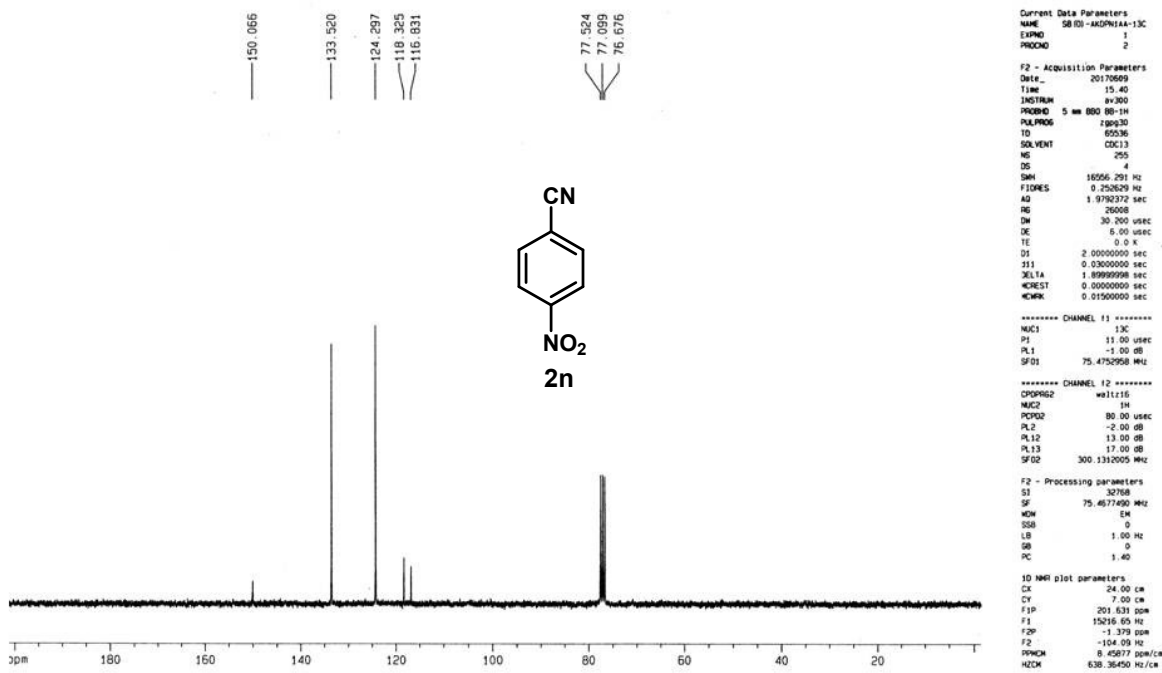


Figure 23 ¹H NMR of 4-nitrobenzonitrile (2n)



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EXPNO 1
PROCNO 2

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NS 255
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FIDRES 0.262629 MHz
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RG 26008
DE 30.200 usec
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KMR 0.01500000 sec

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PL1 -1.00 dB
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***** CHANNEL f2 *****
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PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SFO2 300.131005 MHz

F2 - Processing parameters
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WDW EM
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LB 1.00 Hz
GB 0
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1D NMR plot parameters
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CY 7.00 cm
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F1 15218.60 Hz
F2P -1.379 ppm
F2 -104.09 Hz
FREQ 6.45877 ppm/cm
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Figure 24 ¹³C NMR of 4-nitrobenzonitrile (2n)

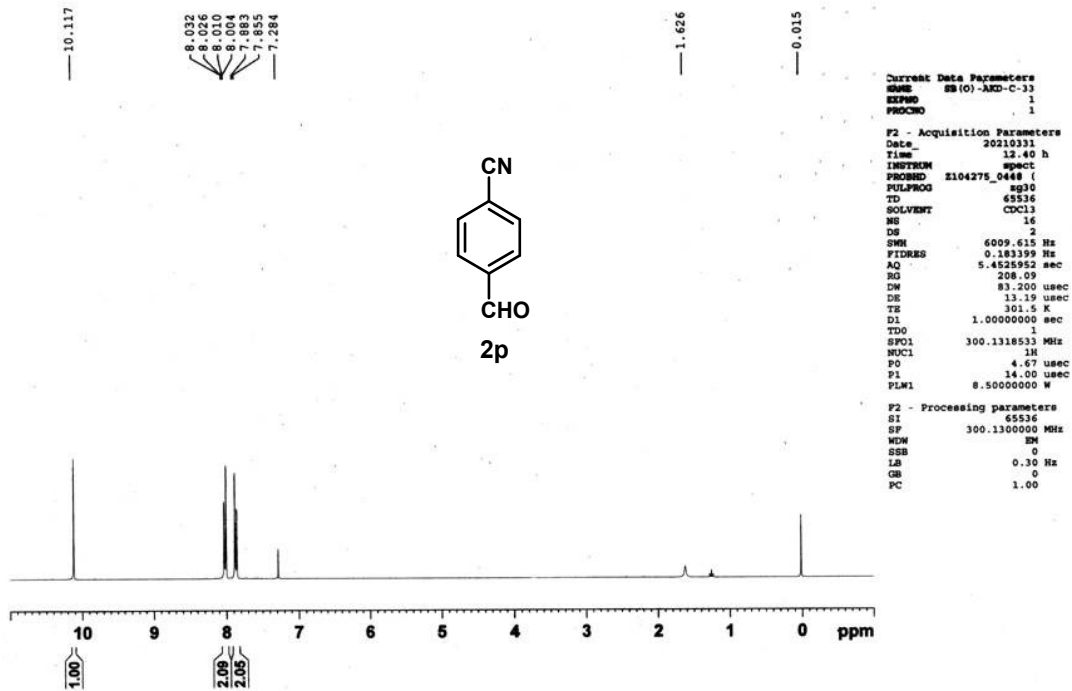


Figure 25 ¹H NMR of 4-formylbenzonitrile (2p)

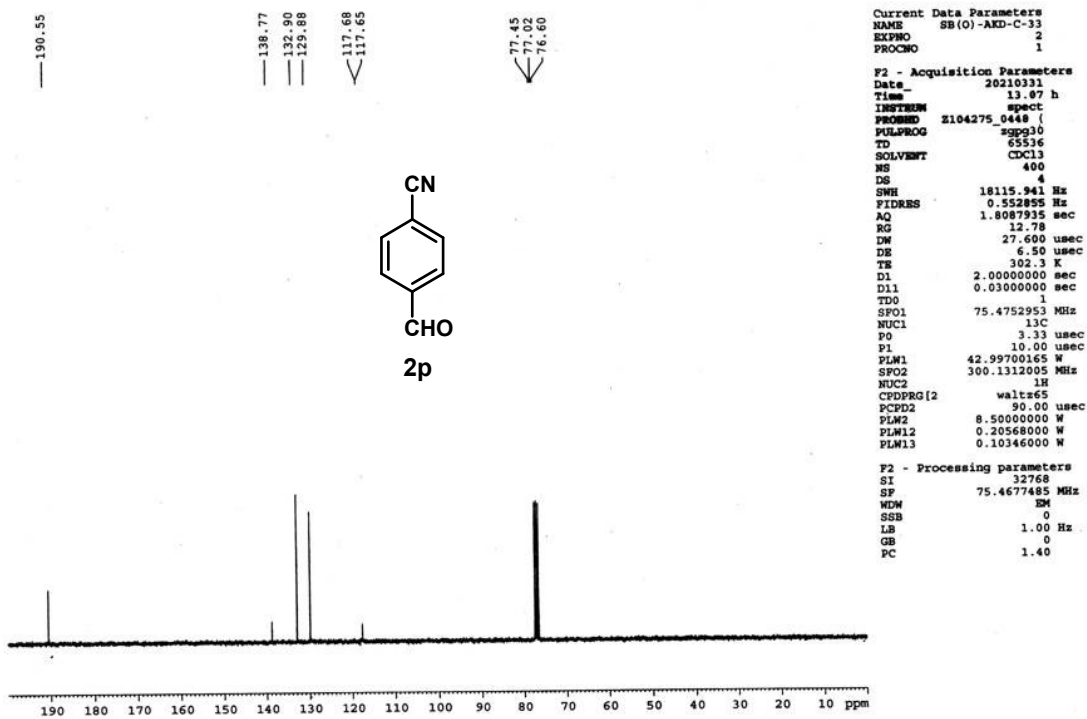


Figure 26 ¹³C NMR of 4-formylbenzonitrile (2p)

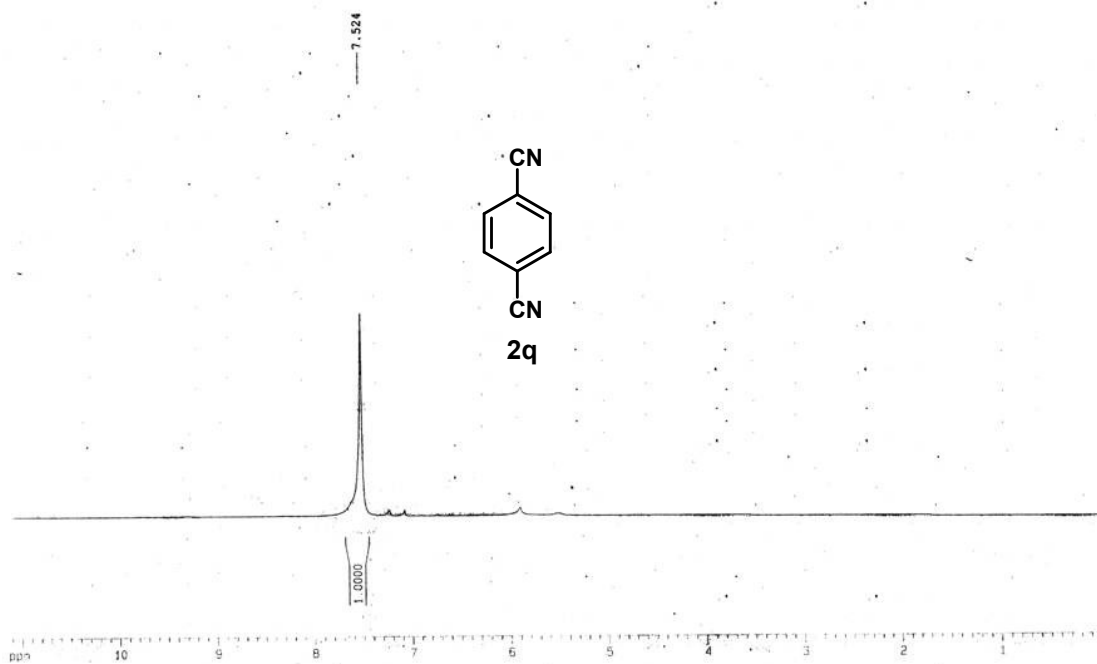


Figure 27 ¹H NMR of Terephthalonitrile (2q)

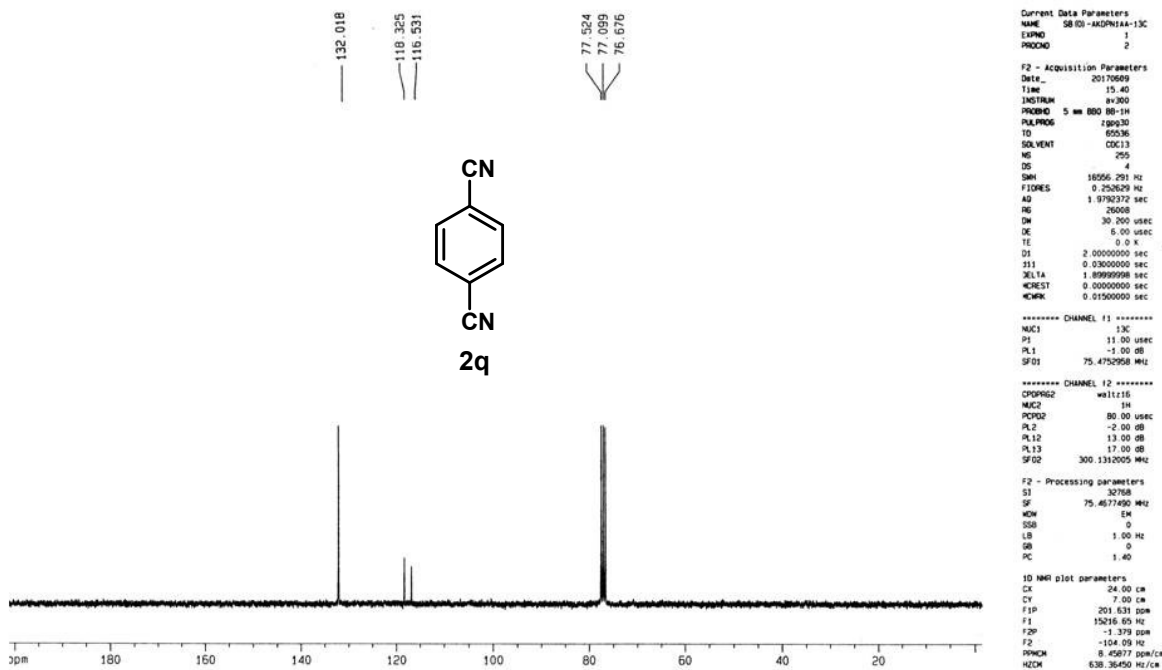


Figure 28 ¹³C NMR of Terephthalonitrile (2q)

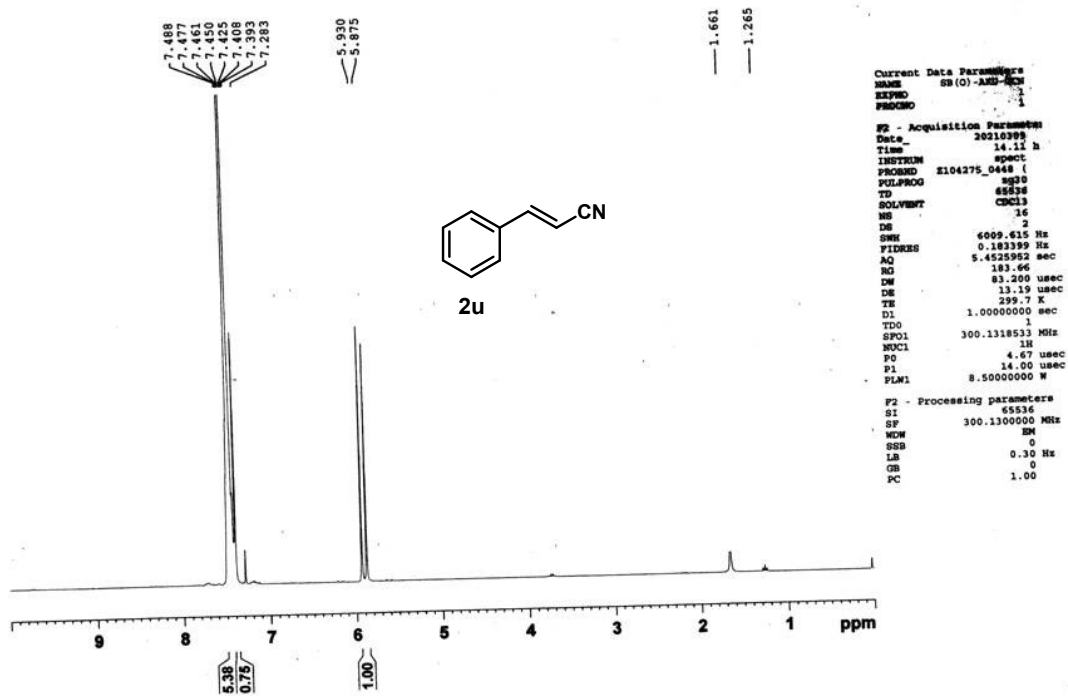


Figure 29 ¹H NMR of Cinnamitrile (2u)

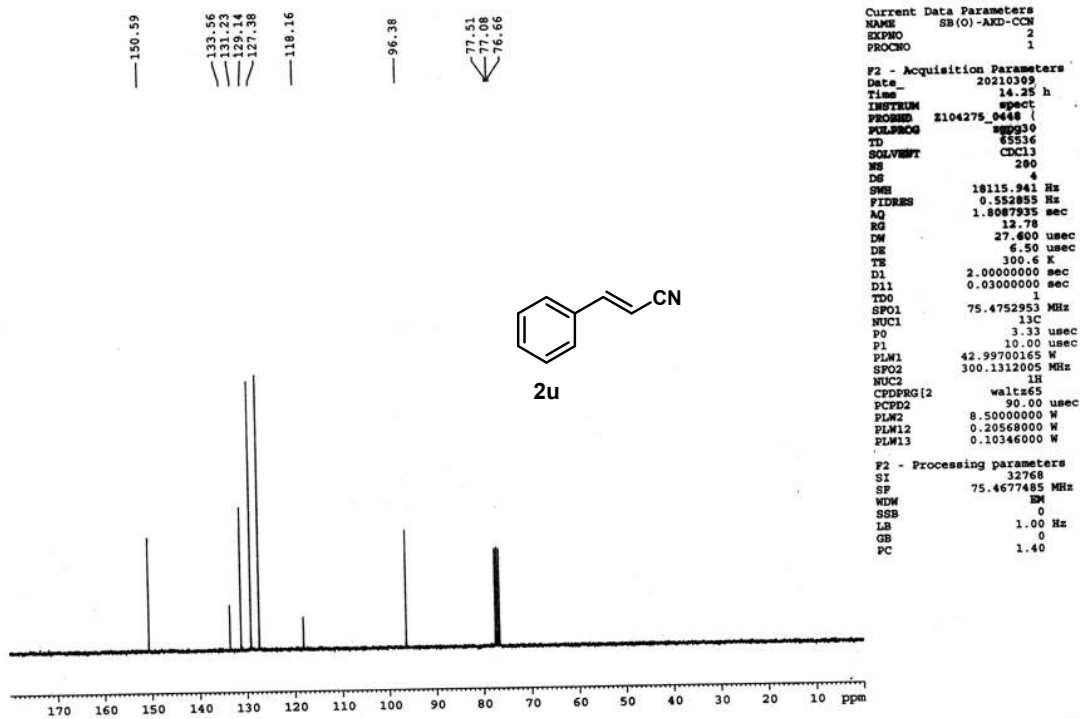


Figure 30 ¹³C NMR of Cinnamitrile (2u)

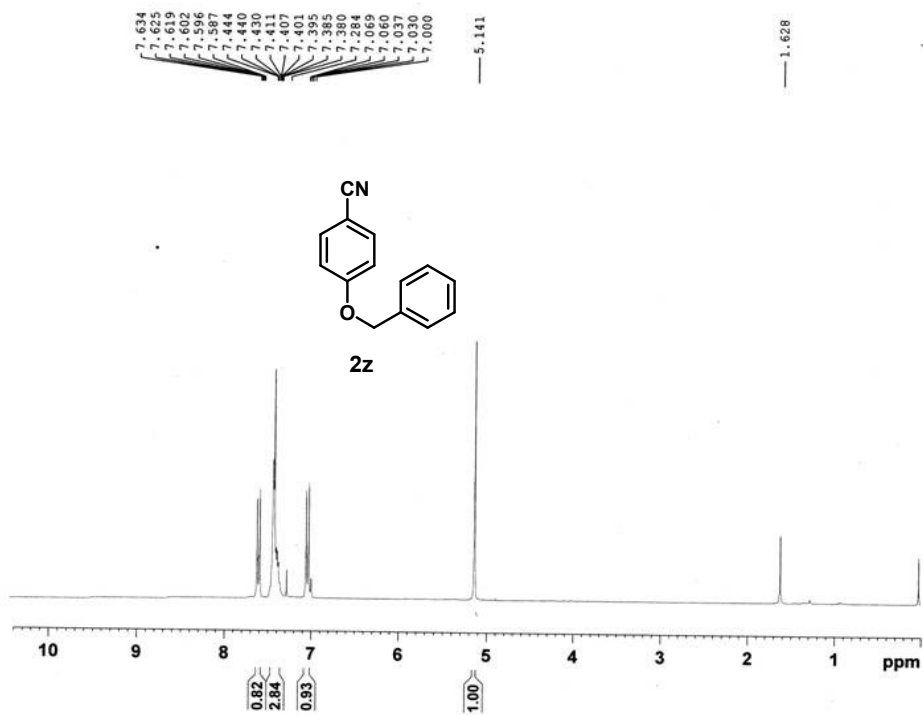


Figure 31 ¹H NMR of 4-(benzyloxy)benzonitrile (2z)

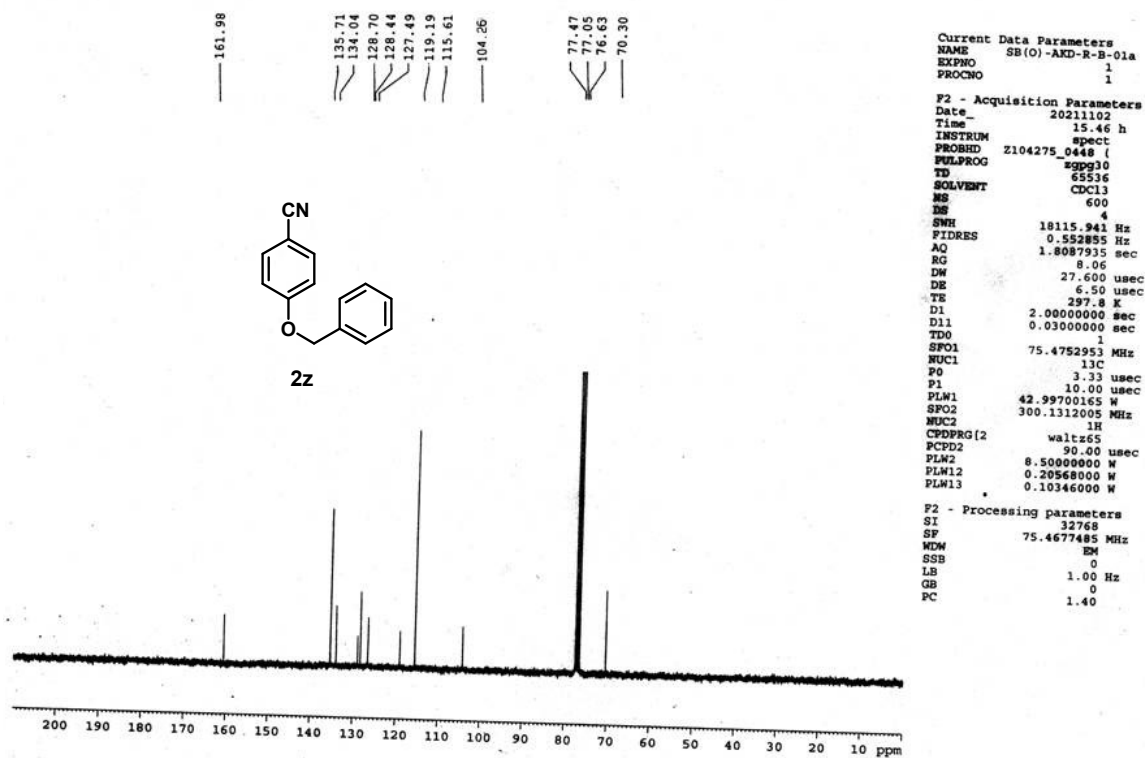


Figure 32 ¹³C NMR of 4-(benzyloxy)benzonitrile (2z)

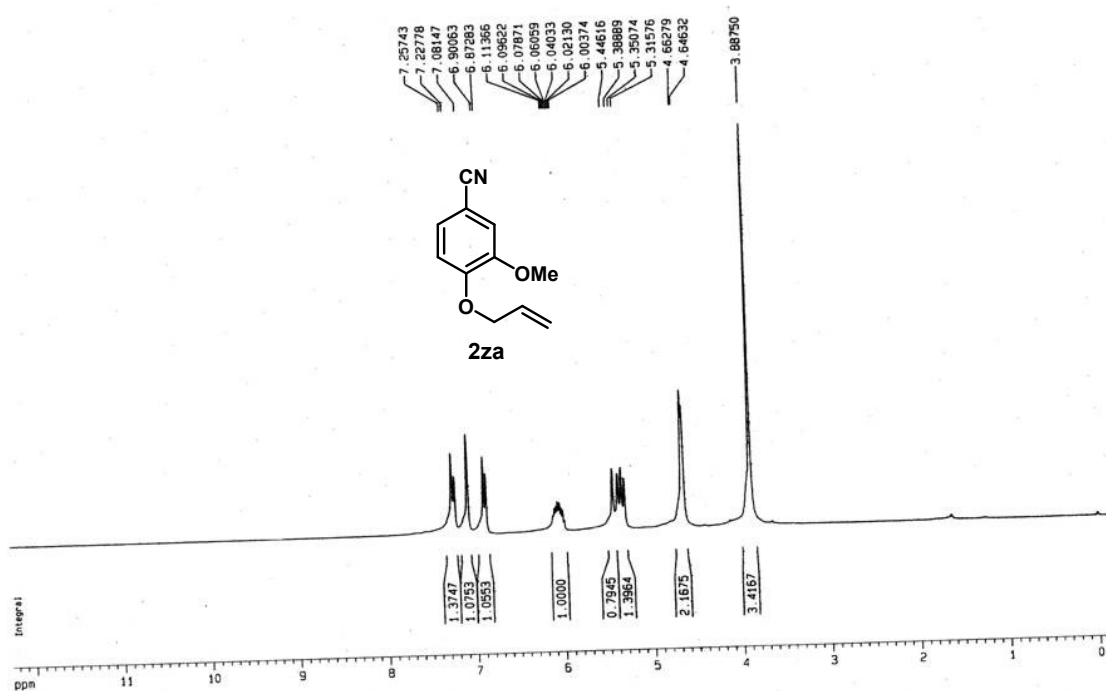


Figure 33 ^1H NMR of 4-(allyloxy)-3-methoxybenzonitrile (2za)

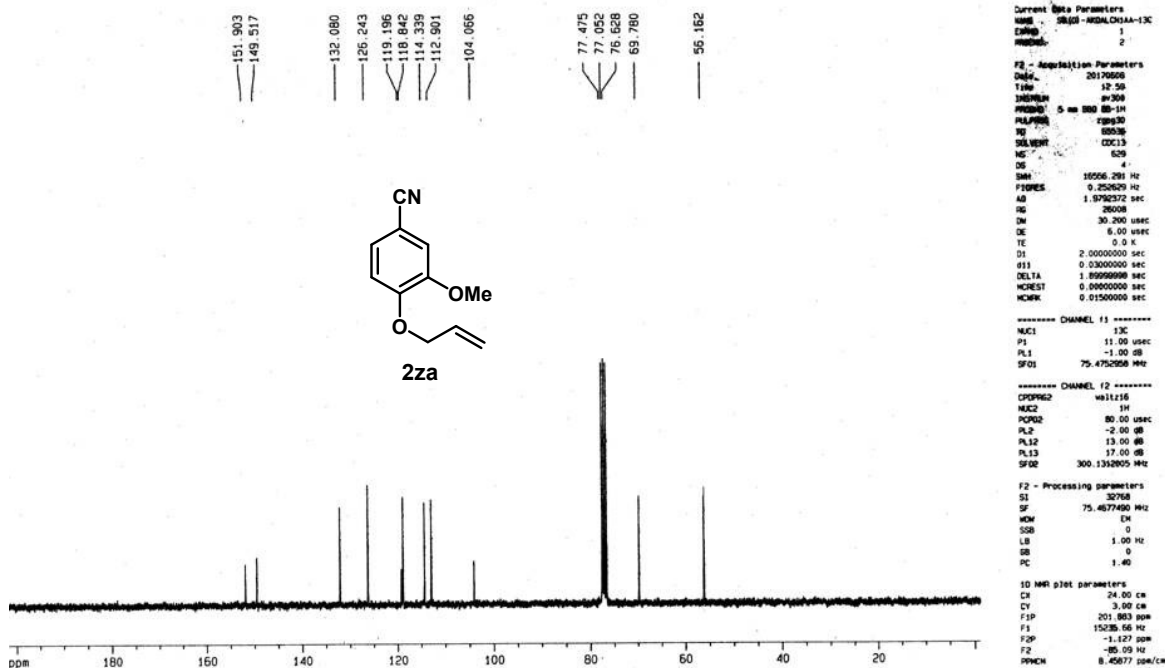


Figure 34 ^{13}C NMR of 4-(allyloxy)-3-methoxybenzonitrile (2za)

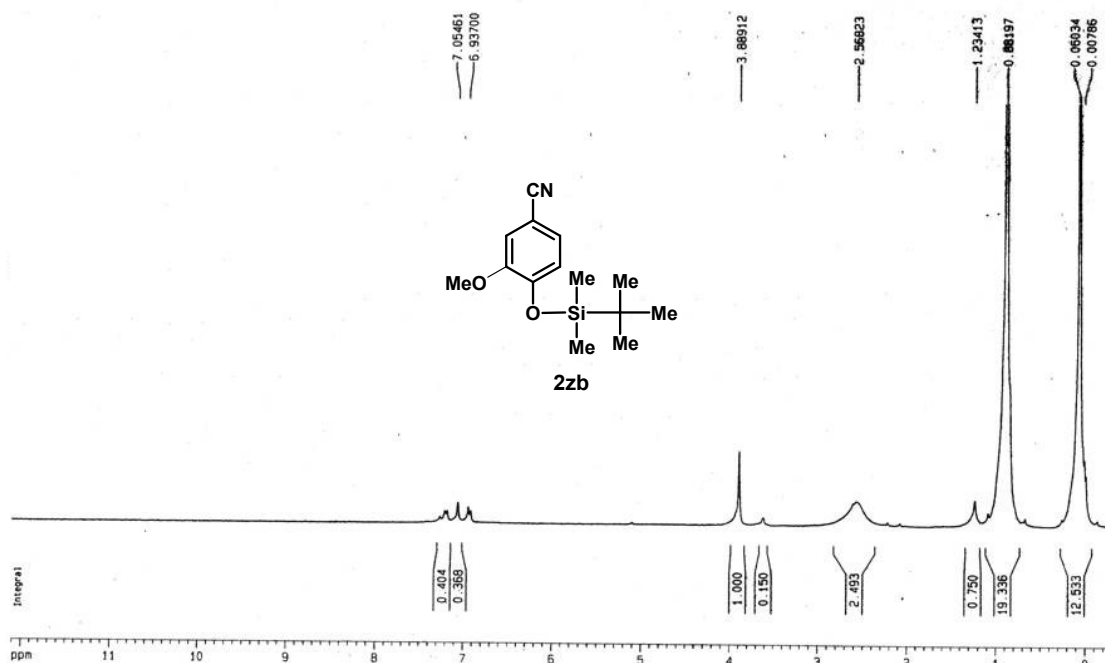


Figure 35 ^1H NMR of 4-((tert-butyl dimethylsilyl)oxy)-3-methoxybenzonitrile (2zb)

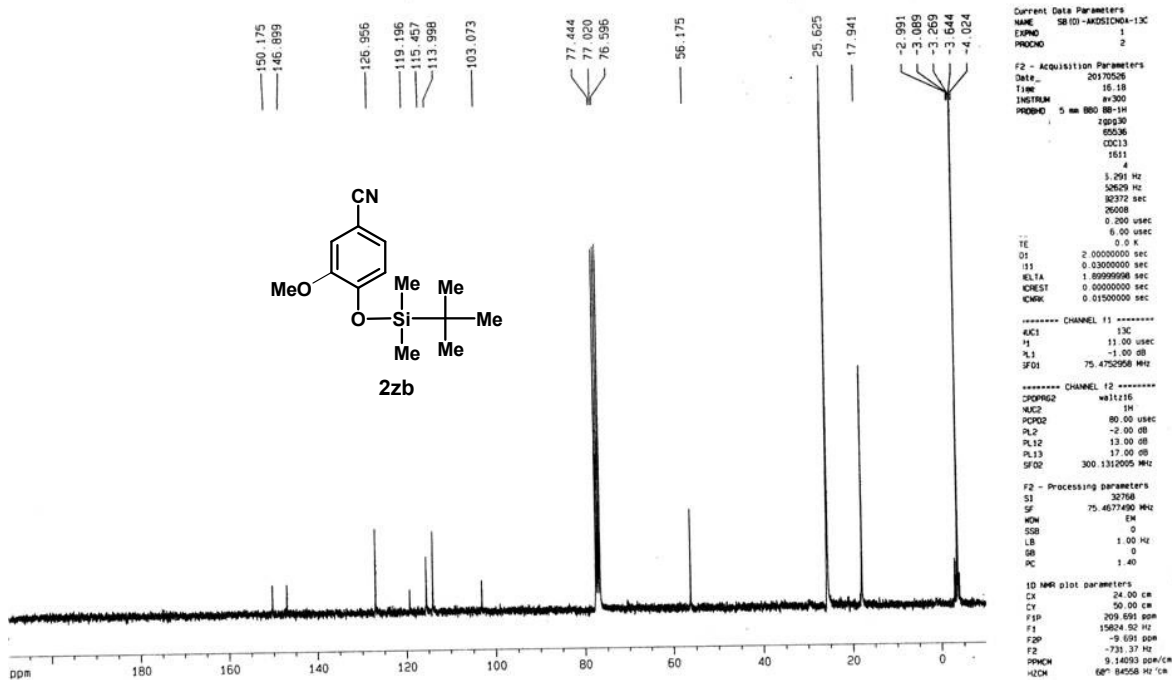
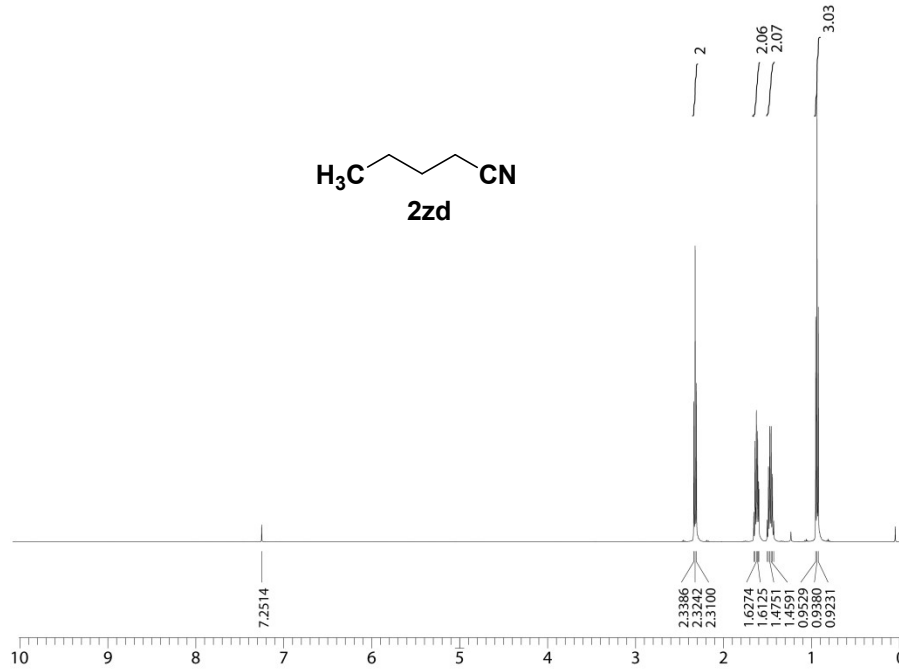


Figure 36 ^{13}C NMR of 4-((tert-butyl dimethylsilyl)oxy)-3-methoxybenzonitrile (2zb)



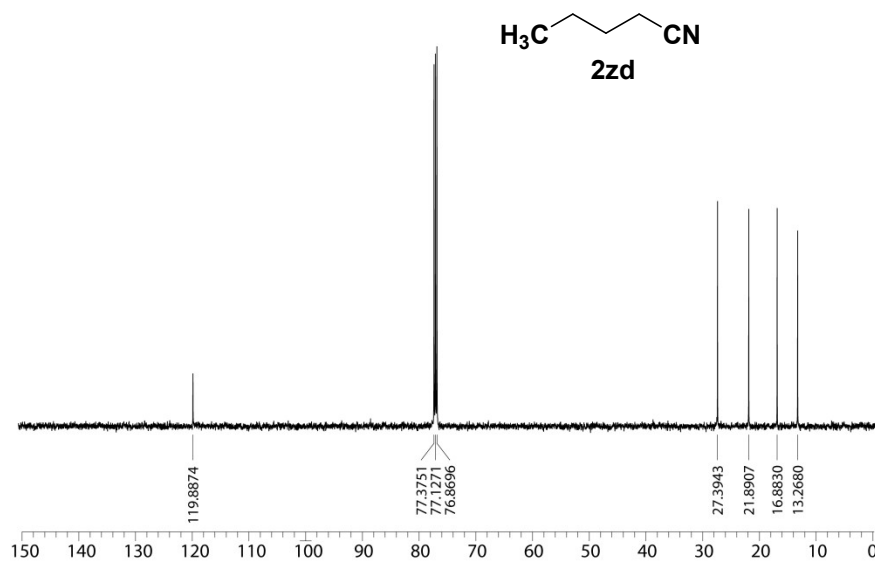
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 Initial_wait = 1[s]
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 Relaxation_delay = 1[s]
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Figure 37 ¹H NMR of Pentanenitrile (2zd)



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 X_sweep = 39.3081761[kHz]
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 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
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 Noe_time = 1[s]
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Figure 38 ¹³C NMR of Pentanenitrile (2zd)

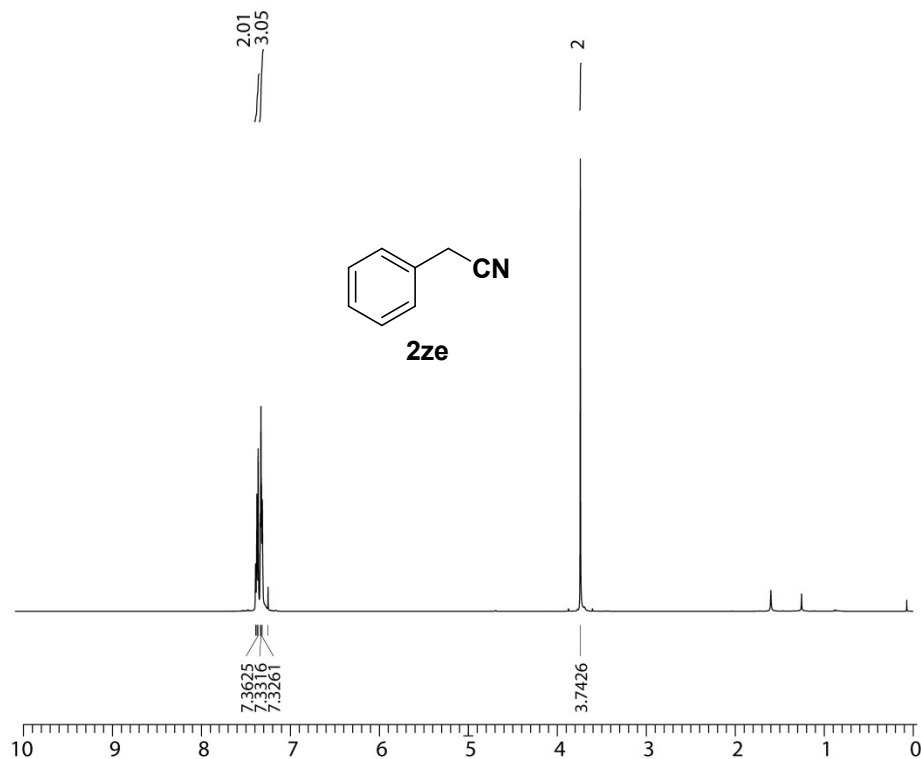


Figure 39 ^1H NMR of 2-Phenylacetonitrile (2ze)



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 Irr_freq = 500.15991521[MHz]
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 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 15.75[us]
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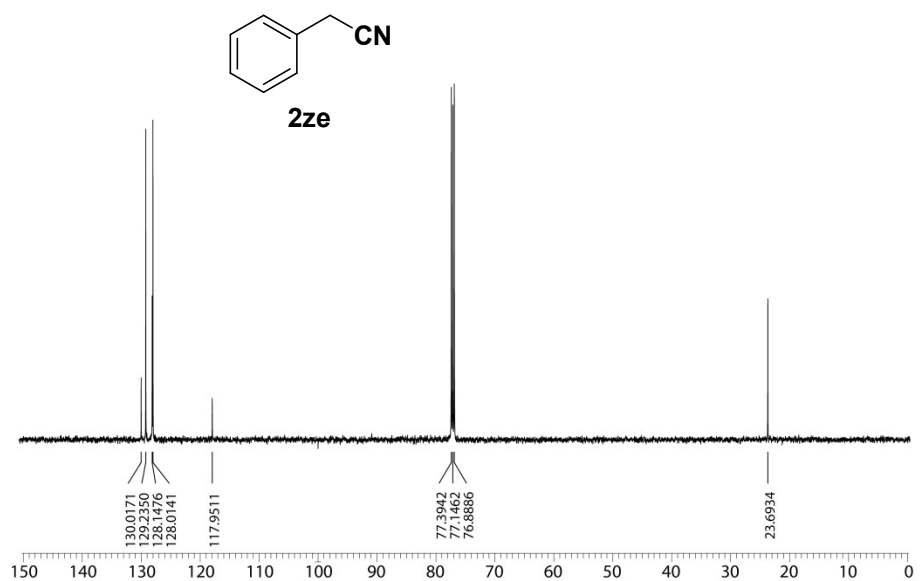


Figure 40 ^{13}C NMR of 2-Phenylacetonitrile (2ze)



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 X_domain = 13C
 X_freq = 125.76529768[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.19959034[Hz]
 X_sweep = 39.3081761[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
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 Total_scans = 512

X_90_width = 11.75[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 7.1[dB]
 X_pulse = 3.91666667[us]
 Irr_atn_dec = 19.32[dB]
 Irr_atn_noe = 19.32[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 1[s]
 Recvr_gain = 58
 Relaxation_delay = 1[s]
 Repetition_time = 1.83361792[s]
 Temp_get = 396.6[dC]

References:

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