

Synthesis of Benzoylacetonitriles from Pd-Catalyzed Carbonylation of Aryl Iodides and Trimethylsilylacetonitrile

Ahbyeol Park and Sunwoo Lee*

Department of Chemistry, Chonnam National University, Gwangju, 500-757, Republic of Korea

Supporting Information

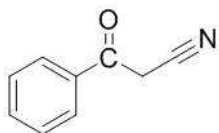
Table of Contents

General Procedure for the Synthesis of Benzoylacetonitriles	-S2-
Reference	-S11-
¹ H and ¹³ C NMR Spectra	-S12-

General Procedure for the Synthesis of Benzoylacetonitriles

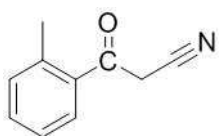
All palladium-catalyzed carbonylation of aryl iodides and trimethylsilylacetonitrile have been employed in a 200 mL autoclave equipped with magnetic stirring and automatic temperature controller. {Pd(2-methylallyl)Cl}₂ (47.3 mg, 0.12 mmol), aryl iodides (3.0 mmol) and trimethylsilylacetonitrile (408 mg, 3.6 mmol), ZnF₂ (186 mg, 1.8 mmol), CuBr₂ (67 mg, 0.3 mmol) and DMF (10.0 mL) was mixed in the 20 mL vial. The reaction mixture was placed in an autoclave. After autoclave was closed, purged CO three times, pressurized to 10 atm with CO and then stirred at 80 °C for 12 h. The reaction mixture was poured into 25 mL of 1 N hydrochloric acid and extracted with ethyl acetate (5 × 20 mL). The combined ethyl acetate extracts were washed with brine (90 mL), dried over MgSO₄, and was passed through a celite. The resulting crude product was purified by flash chromatography on silica gel. The product was eluted with ethyl acetate in hexane.

3-Oxo-3-phenylpropanenitrile (**2a**)¹



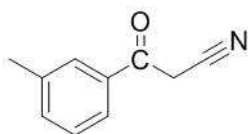
Iodobenzene (**1a**) (612 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 348 mg (2.40 mmol, 80 %) of **2a** as pale yellow solid after chromatography. mp 79-81 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.94 – 7.90 (m, 2H), 7.69 – 7.63 (m, 1H), 7.56 – 7.49 (m, 2H), 4.09 (s, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 187.2, 134.9, 134.4, 129.3, 128.6, 113.9, 29.5; HRMS (APCI) calcd. for C₉H₇NO [M-H]⁻ 144.0449, found 144.0449.

3-Oxo-3-*o*-tolylpropanenitrile (**2b**)



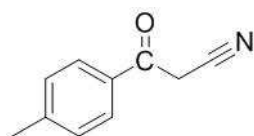
2-Iodotoluene (**1b**) (654 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 348 mg (2.16 mmol, 72 %) of **2b** as pale yellow solid after chromatography. mp 86-88 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.64 – 7.60 (m, 1H), 7.47 (td, *J* = 7.3, 1.3 Hz, 1H), 7.32 (dd, *J* = 7.3, 6.8 Hz, 2H), 4.06 (s, 2H), 2.56 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 189.5, 140.5, 133.9, 133.4, 132.8, 129.4, 126.3, 114.2, 31.6, 21.9; HRMS (APCI) calcd. for C₁₀H₉NO [M-H]⁻ 158.0606, found 158.0606.

3-Oxo-3-*m*-tolylpropanenitrile (**2c**)



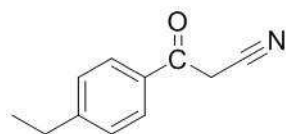
3-Iodotoluene (**1c**) (654 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 310 mg (1.95 mmol, 65 %) of **2c** as yellow-brown solid after chromatography. mp 80-82 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.72 – 7.45 (m, 3H), 7.39 (t, *J* = 7.5 Hz, 1H), 4.08 (s, 2H), 2.42 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 187.4, 139.2, 135.6, 134.4, 129.1, 129.0, 125.8, 114.1, 29.5, 21.4; HRMS (APCI) calcd. for C₁₀H₉NO [M-H]⁻ 158.0606, found 158.0605.

3-Oxo-3-*p*-tolylpropanenitrile (**2d**)¹



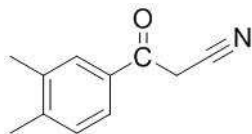
4-Iodotoluene (**1d**) (654 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 358 mg (2.25 mmol, 75 %) of **2d** as pale yellow solid after chromatography. mp 94-99 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.84 – 7.80 (m, 2H), 7.33 – 7.30 (m, 2H), 4.04 (s, 2H), 2.44 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 186.7, 146.1, 132.0, 130.0, 128.7, 114.0, 29.4, 22.0; HRMS (APCI) calcd. for C₁₀H₉NO [M-H]⁻ 158.0606, found 158.0606.

3-(4-Ethylphenyl)-3-oxopropanenitrile (**2e**)



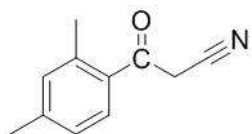
4-EthylIodobenzene (**1e**) (696 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 337 mg (1.95 mmol, 65 %) of **2e** as yellow solid after chromatography. mp 169-174 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.86 – 7.82 (m, 2H), 7.33 (m, 2H), 4.06 (s, 2H), 2.73 (q, *J* = 7.6 Hz, 2H), 1.26 (t, *J* = 7.6 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 186.8, 152.2, 132.1, 128.8, 128.8, 114.1, 29.40, 29.1, 15.1; HRMS (APCI) calcd. for C₁₁H₁₁NO [M-H]⁻ 172.0762, found 172.0764.

3-(3,4-Dimethylphenyl)-3-oxopropanenitrile (**2f**)



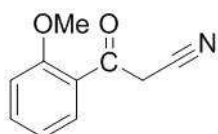
1-Iodo-3,4-dimethylbenzene (**1f**) (696 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 410 mg (2.37 mmol, 79 %) of **2f** as white solid after chromatography. mp 118-120 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.65 – 7.59 (m, 2H), 7.24 (d, *J* = 7.9 Hz, 1H), 4.05 (s, 2H), 2.32 (s, 3H), 2.30 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 187.1, 144.8, 137.7, 132.2, 130.3, 129.5, 126.2, 114.3, 29.3, 20.2, 19.8; HRMS (APCI) calcd. for C₁₁H₁₁NO [M-H]⁻ 172.0762, found 172.0762.

3-(2,4-Dimethylphenyl)-3-oxopropanenitrile (**2g**)



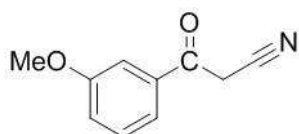
1-Iodo-2,4-dimethylbenzene (**1g**) (696 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 368 mg (2.13 mmol, 71 %) of **2g** as white solid after chromatography. mp 77-80 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.53 (d, *J* = 8.4 Hz, 1H), 7.13 – 7.10 (m, 2H), 4.03 (s, 2H), 2.54 (s, 3H), 2.37 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 188.7, 144.5, 141.0, 133.8, 131.1, 129.9, 126.90, 114.4, 31.3, 22.1, 21.6; HRMS (APCI) calcd. for C₁₁H₁₁NO [M-H]⁻ 172.0762, found 172.0763.

3-(2-Methoxyphenyl)-3-oxopropanenitrile (**2h**)¹



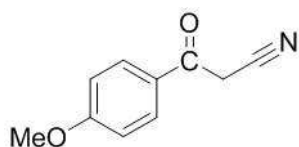
2-Iodoanisole (**1h**) (702 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 378 mg (2.16 mmol, 72 %) of **2h** as white solid after chromatography. mp 87-88 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.86 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.57 (ddd, *J* = 8.4, 7.3, 1.8 Hz, 1H), 7.08 – 7.00 (m, 2H), 4.08 (s, 2H), 3.97 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 188.2, 159.4, 135.9, 131.5, 124.6, 121.3, 114.7, 111.9, 55.9, 34.2; HRMS (APCI) calcd. for C₁₀H₉NO₂ [M-H]⁻ 174.0555, found 174.0554.

3-(3-Methoxyphenyl)-3-oxopropanenitrile (**2i**)



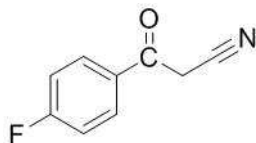
3-Iodoanisole (**1i**) (702 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 362 mg (2.07 mmol, 69 %) of **2i** as pale yellow solid after chromatography. mp 85-87 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.46 – 7.38 (m, 3H), 7.18 (m, 1H), 4.08 (s, 2H), 3.85 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 187.2, 160.2, 135.6, 130.2, 121.3, 121.0, 114.0, 112.8, 55.7, 29.6; HRMS (APCI) calcd. for C₁₀H₉NO₂ [M-H]⁻ 174.0555, found 174.0555.

3-(4-Methoxyphenyl)-3-oxopropanenitrile (**2j**)¹



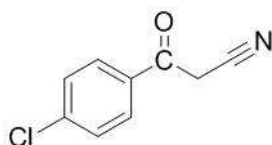
4-Iodoanisole (**1j**) (702 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 383 mg (2.19 mmol, 73 %) of **2j** as pale yellow solid after chromatography. mp 123-126 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.90 (m, 2H), 6.97 (m, 2H), 4.03 (s, 2H), 3.88 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 185.6, 164.8, 131.0, 127.4, 114.4, 114.3, 55.8, 29.2; HRMS (APCI) calcd. for C₁₀H₉NO₂ [M-H]⁻ 174.0555, found 174.0555.

3-(4-Fluorophenyl)-3-oxopropanenitrile (**2k**)



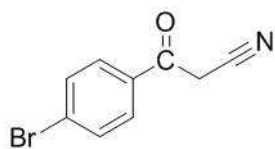
4-Fluoriodobenzene (**1k**) (666 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 318 mg (1.95 mmol, 65 %) of **2k** as pale yellow solid after chromatography. mp 84-86 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.93 (m, 2H), 7.17 (m, 2H), 4.11 (s, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 186.0, 166.6 (d, *J* = 256.4 Hz, 1C), 131.38 (d, *J* = 9.7 Hz, 1C), 130.8 (d, *J* = 2.7 Hz, 1C), 116.5 (d, *J* = 22.1 Hz, 1C), 113.95, 29.56; HRMS (APCI) calcd. for C₉H₆FNO [M-H]⁻ 162.0355, found 162.0354.

3-(4-Chlorophenyl)-3-oxopropanenitrile (**2l**)¹



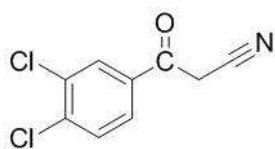
1-Chloro-4-iodobenzene (**1l**) (715 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 397 mg (2.22 mmol, 74 %) of **2l** as yellow solid after chromatography. mp 125-128 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.87 (m, 2H), 7.51 (m, 2H), 4.05 (s, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 186.1, 141.6, 132.7, 130.0, 129.7, 113.6, 29.5; HRMS (APCI) calcd. for C₉H₆ClNO [M-H]⁻ 178.0060, found 178.0060.

3-(4-Bromophenyl)-3-oxopropanenitrile (**2m**)



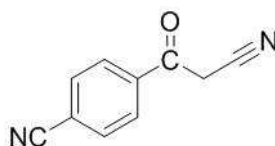
1-Bromo-4-iodobenzene (**1m**) (849 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 548 mg (2.46 mmol, 82 %) of **2m** as yellow solid after chromatography. mp 158-162 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.79 (m, 2H), 7.67 (m, 2H), 4.05 (s, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 186.3, 133.1, 132.7, 130.4, 130.0, 113.6, 29.5; HRMS (APCI) calcd. for C₉H₆BrNO [M-H]⁻ 221.9554, found 221.9554.

3-(3,4-Dichlorophenyl)-3-oxopropanenitrile (**2n**)¹



3,4-Dichloroiodobenzene (**1n**) (819 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 402 mg (1.89 mmol, 63 %) of **2n** as yellow solid after chromatography. mp 104-107 °C; ¹H NMR (300 MHz, CDCl₃) δ 8.00 (d, *J* = 2.1 Hz, 1H), 7.76 – 7.60 (m, 2H), 4.08 (s, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 185.4, 139.8, 134.2, 133.8, 131.4, 130.5, 127.5, 113.3, 29.6; HRMS (APCI) calcd. for C₉H₅Cl₂NO [M-H]⁻ 211.9670, found 211.9669.

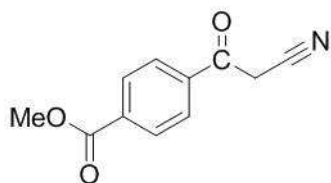
4-(2-Cyanoacetyl)benzonitrile (**2o**)



4-Iodobenzonitrile (**1o**) (687 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 209 mg (1.23 mmol, 41 %) of **2o** as yellow-brown solid after chromatography. mp 122-126

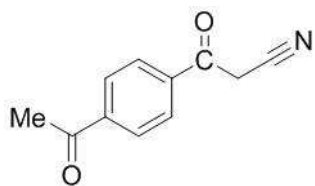
°C; ^1H NMR (300 MHz, CDCl_3) δ 8.03 (m, 2H), 7.85 (m, 2H), 4.12 (s, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 186.2, 137.1, 133.1, 129.0, 118.1, 117.5, 113.1, 29.8; HRMS (APCI) calcd. for $\text{C}_{10}\text{H}_6\text{N}_2\text{O}$ $[\text{M}-\text{H}]^-$ 169.0402, found 169.0402.

Methyl 4-(2-cyanoacetyl)benzoate (**2p**)



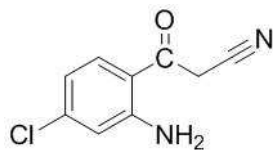
Methyl-4-Iodobenzoate (**1p**) (786 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 505 mg (2.49 mmol, 83 %) of **2p** as yellow solid after chromatography. mp 98-100 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.18 (d, J = 8.4 Hz, 2H), 7.98 (d, J = 8.4 Hz, 2H), 4.12 (s, 2H), 3.97 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 186.8, 165.8, 137.4, 135.5, 130.4, 128.5, 113.4, 52.8, 29.8; HRMS (APCI) calcd. for $\text{C}_{11}\text{H}_9\text{NO}_3$ $[\text{M}-\text{H}]^-$ 202.0504, found 202.0504.

3-(4-Acetylphenyl)-3-oxopropanenitrile (**2q**)



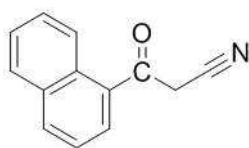
4-Iodoacetophenone (**1q**) (738 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 241 mg (1.29 mmol, 43 %) of **2q** as white solid after chromatography. mp 109-112 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.10 – 8.00 (m, 4H), 4.12 (s, 2H), 2.66 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 197.1, 186.8, 141.5, 137.3, 129.0, 128.9, 113.4, 29.9, 27.1; HRMS (APCI) calcd. for $\text{C}_{11}\text{H}_9\text{NO}_2$ $[\text{M}-\text{H}]^-$ 186.0555, found 186.0556.

3-(2-Amino-4-chlorophenyl)-3-oxopropanenitrile (**2r**)



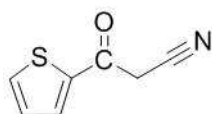
5-Chloro-2-iodoaniline (**1r**) (760 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 390 mg (2.01 mmol, 67 %) of **2r** as white solid after chromatography. mp 139-142 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.40 (d, *J* = 8.7 Hz, 1H), 6.71 (m, 1H), 6.64 (dd, *J* = 8.7, 2.0 Hz, 1H), 6.41 (s, 2H), 4.03 (s, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 187.6, 184.5, 152.0, 142.3, 131.9, 117.0, 114.1, 114.0, 30.2; HRMS (APCI) calcd. for C₉H₇ClN₂O [M-H]⁻ 193.0169, found 193.0170.

3-(Naphthalen-2-yl)-3-oxopropanenitrile (**2s**)¹



1-Iodonaphthalene (**1s**) (762 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 398 mg (2.04 mmol, 68 %) of **2s** as yellow solid after chromatography. mp 95-98 °C; ¹H NMR (300 MHz, CDCl₃) δ 8.81 (dd, *J* = 8.8, 0.9 Hz, 1H), 8.09 (d, *J* = 8.2 Hz, 1H), 7.92 – 7.87 (m, 2H), 7.69 – 7.51 (m, 3H), 4.20 (s, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 189.6, 135.3, 134.2, 131.6, 130.4, 129.7, 129.3, 128.8, 127.2, 125.70, 124.3, 114.2, 31.9; HRMS (APCI) calcd. for C₁₃H₉NO [M-H]⁻ 194.0606, found 194.0608.

3-Oxo-3-(thiophen-2-yl)propanenitrile (**2t**)¹



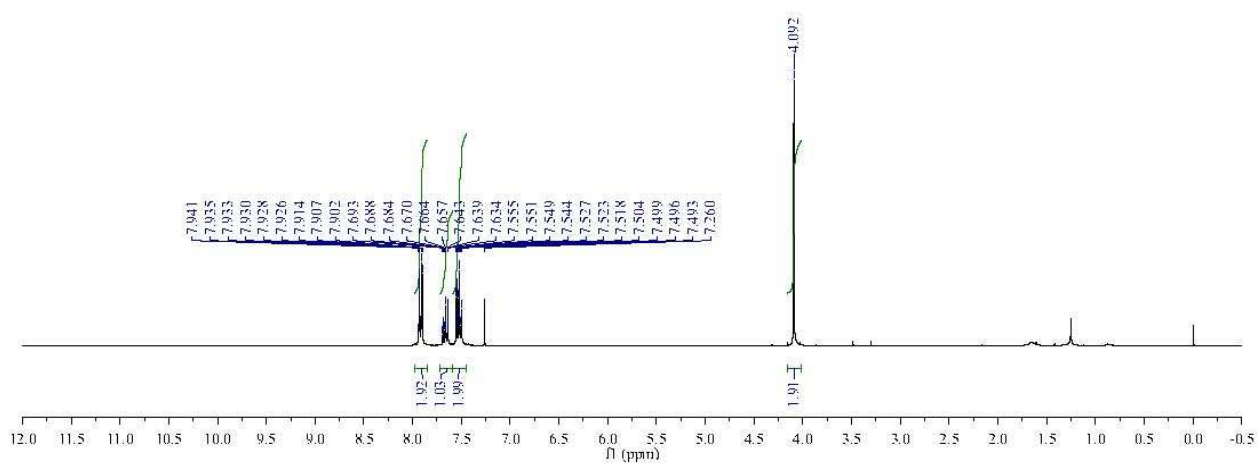
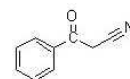
2-Iodothiophene (**1t**) (630 mg, 3.00 mmol) was coupled with trimethylsilylacetonitrile (408 mg, 3.60 mmol) to give 358 mg (2.37 mmol, 79 %) of **2t** as yellow solid after chromatography. mp 131-135 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.80 – 7.78(m, 2H), 7.20 (dd, *J* = 4.8, 0.9 Hz, 1H), 4.01 (s, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 179.7, 141.0, 136.4, 133.8, 128.8, 113.6, 29.70; HRMS (APCI) calcd. for C₇H₅NOS [M-H]⁺ 150.0014, found 150.0013.

Reference

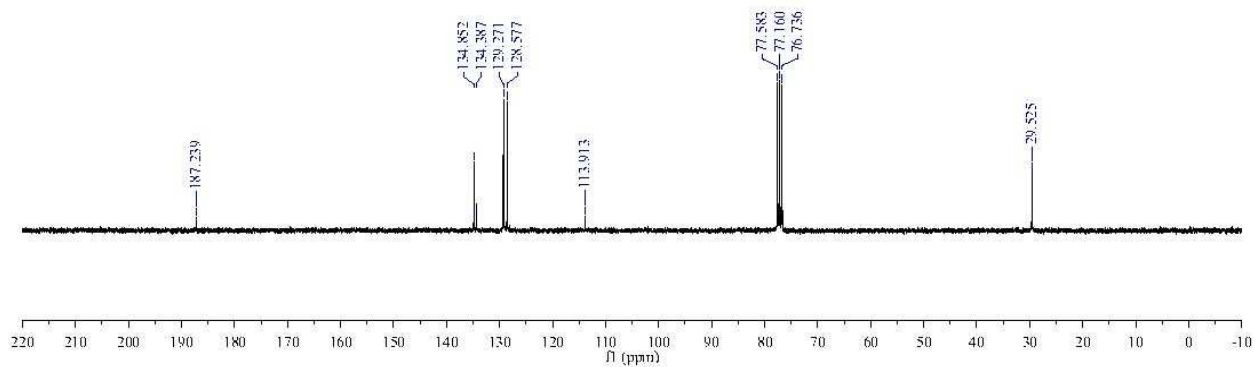
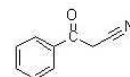
1. Long, R. S. *J. Am. Chem. Soc.* **1947**, *69*, 990-995

3-Oxo-3-phenylpropanenitrile (2a) : ^1H , ^{13}C NMR

CNU_SWLae_PAB244-1_18Aug2011
PAB244-1

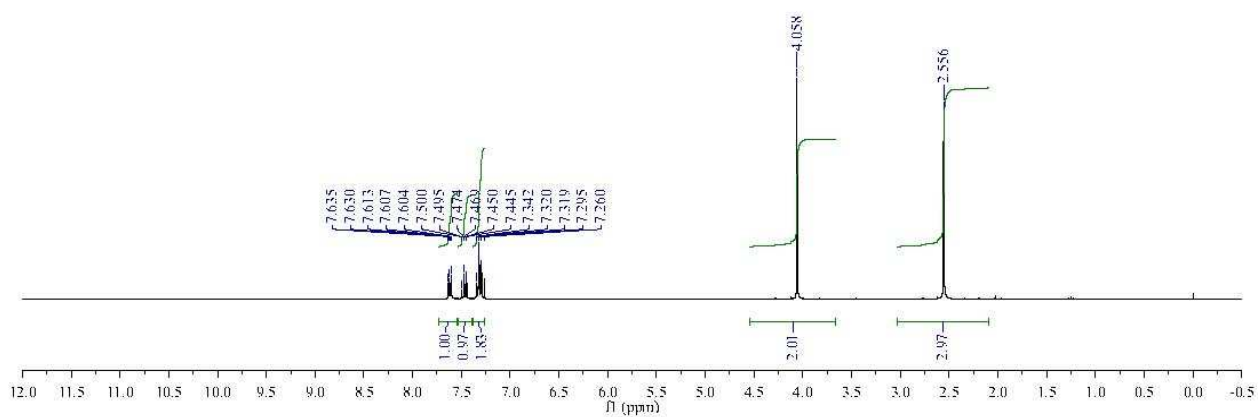
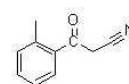


CNU_SWLae_PAB244-1_13C_18Aug2011
PAB244-1,13C

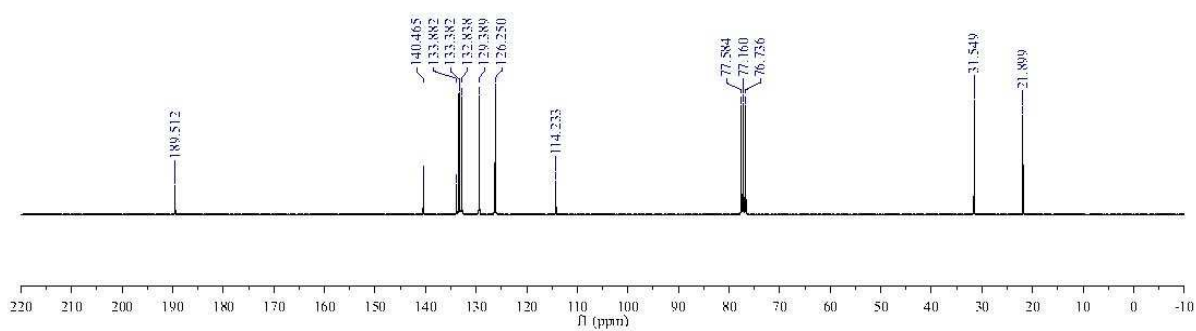
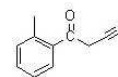


3-Oxo-3-*o*-tolylpropanenitrile (2b) : ^1H , ^{13}C NMR

C:\NU_SW\Lab_PAB240-1r2_19Aug2011
PAB240-1r2

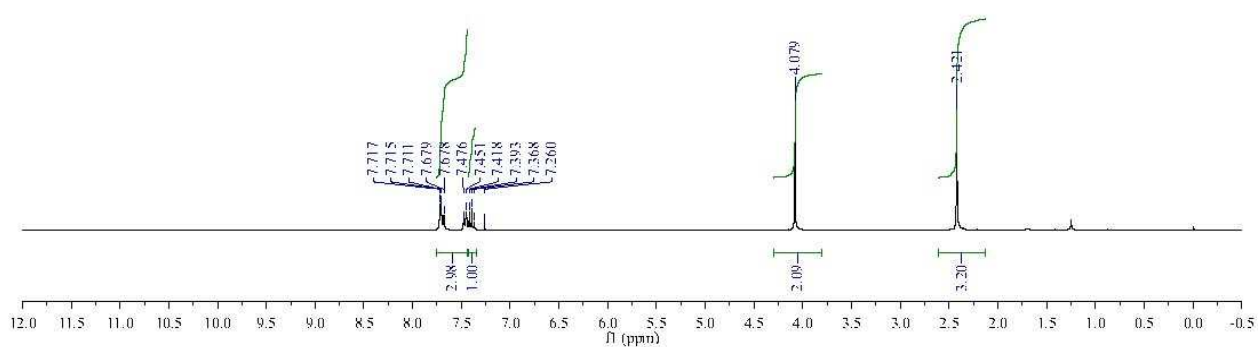
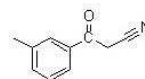


C:\NU_SW\Lab_PAB240-1r2_13C_19Aug2011
PAB240-1r2, 13C

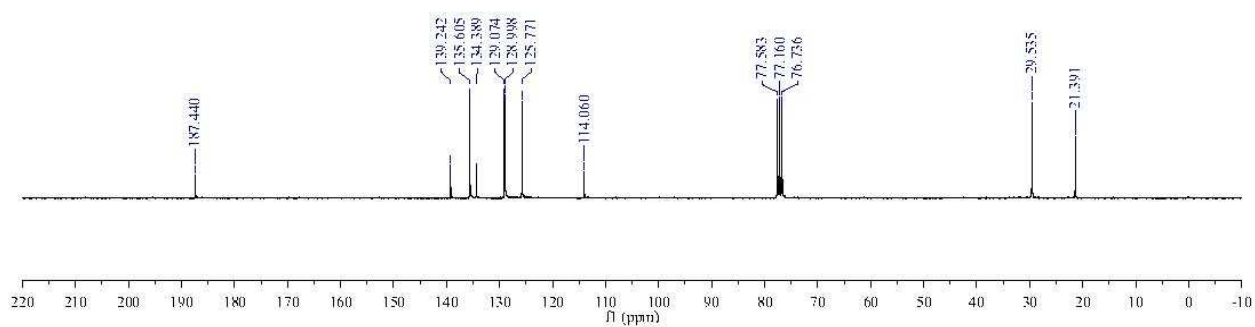
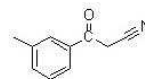


3-Oxo-3-*m*-tolylpropanenitrile (2c) : ^1H , ^{13}C NMR

CNU_SWLac_PAB243-1_18Aug2011
PAB243-1

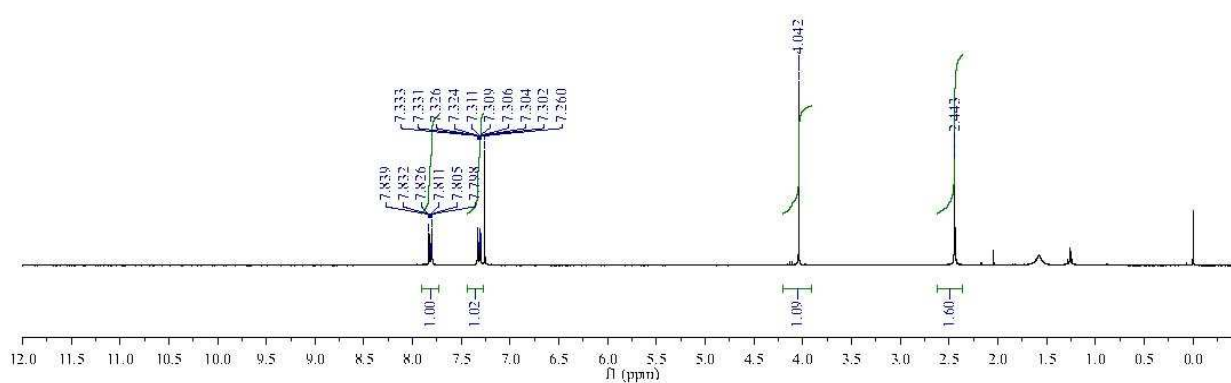
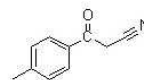


CNU_SWLac_PAB243-1_13C_18Aug2011
PAB243-1,13C

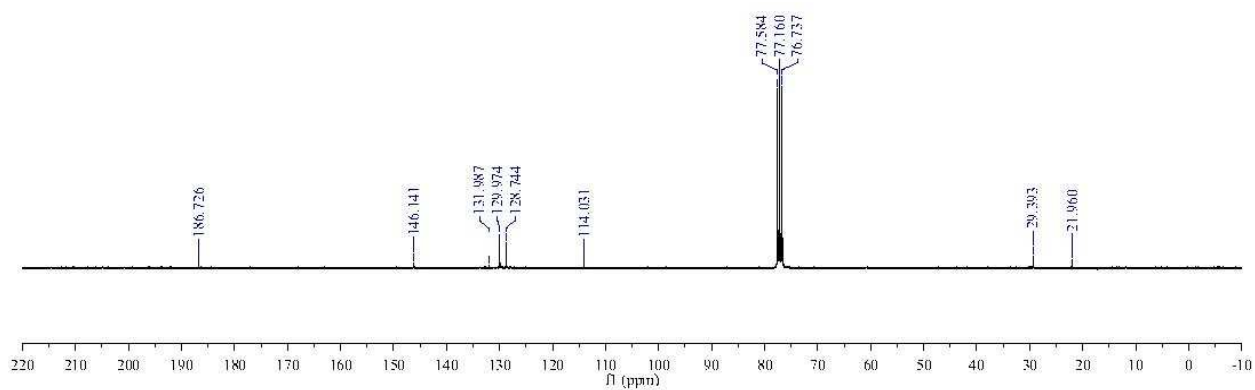
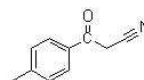


3-Oxo-3-*p*-tolylpropanenitrile (2d) : ^1H , ^{13}C NMR

CNU_SWLac_PAB242-1_08Aug2011
PAB242-1

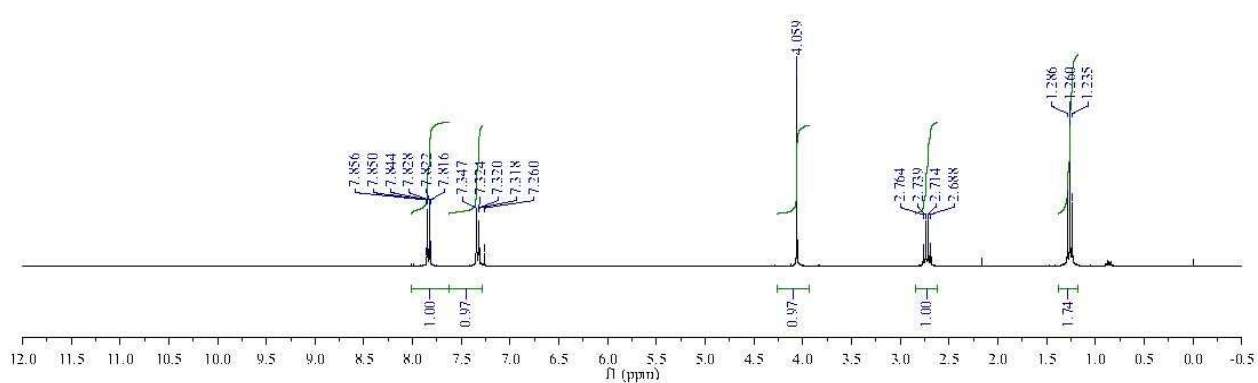
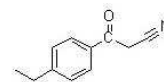


CNU_SWLac_PAB242-1_13C_08Aug2011
standard Carbon parameters

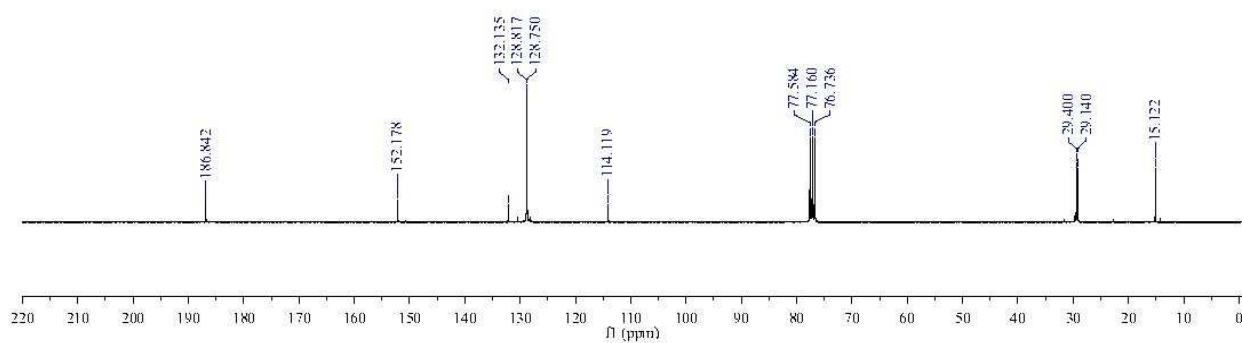
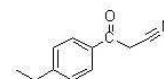


3-(4-Ethylphenyl)-3-oxopropanenitrile (2e) : ^1H , ^{13}C NMR

CNU_SWLac_PAB254-1_22Aug2011
PAB247-1

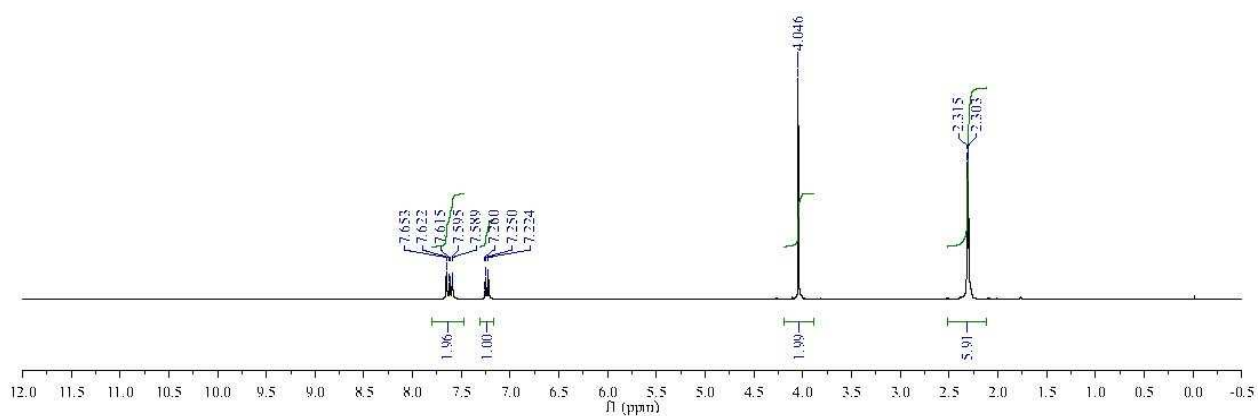
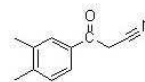


CNU_SWLac_PAB254-1_13C_22Aug2011
PAB247-1,13C

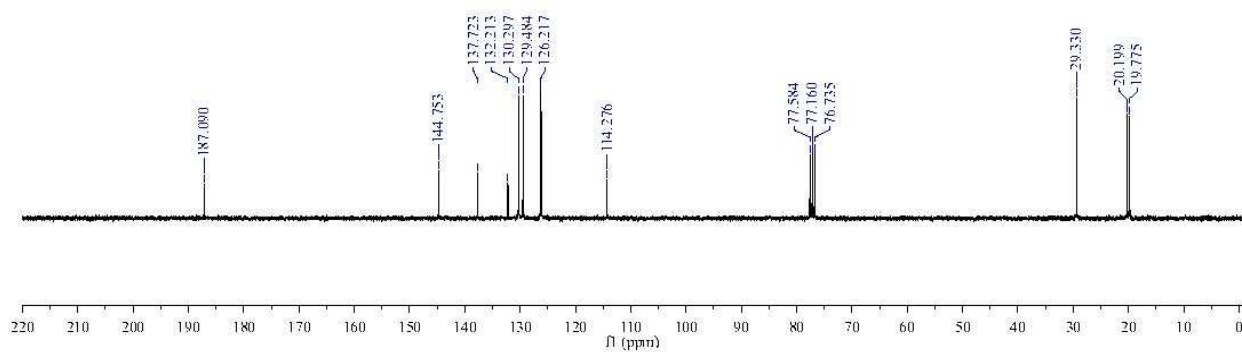
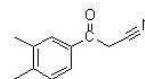


3-(3,4-Dimethylphenyl)-3-oxopropanenitrile (2f) : ^1H , ^{13}C NMR

CNU_SWLac_PAB248-1_06Sep2011
PAB248-1

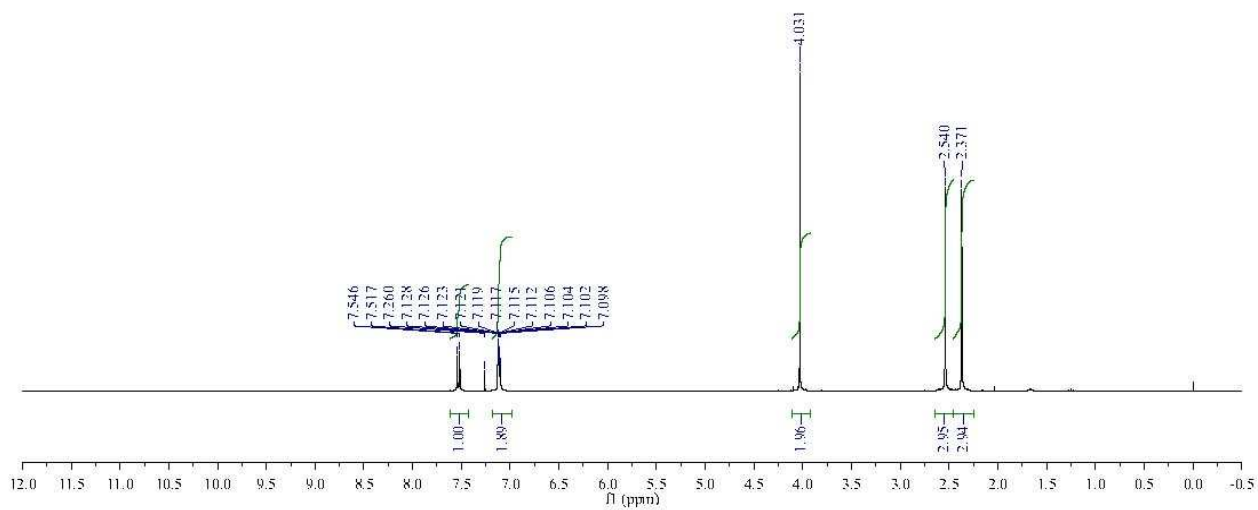
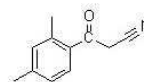


CNU_SWLac_PAB248-1_13C_06Sep2011
PAB248-1,13C

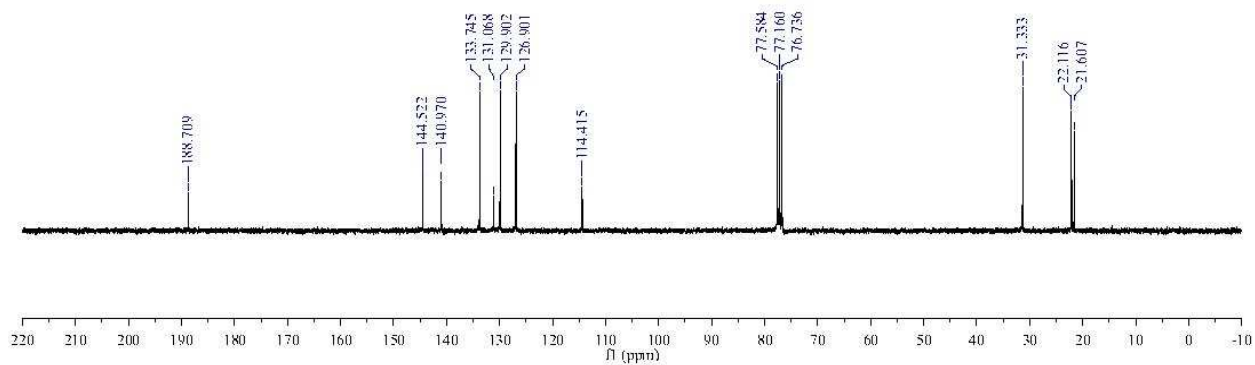
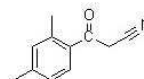


3-(2,4-Dimethylphenyl)-3-oxopropanenitrile (2g) : ^1H , ^{13}C NMR

CNU_SWLac_PAB257-2_15Sep2011
PAB257-2

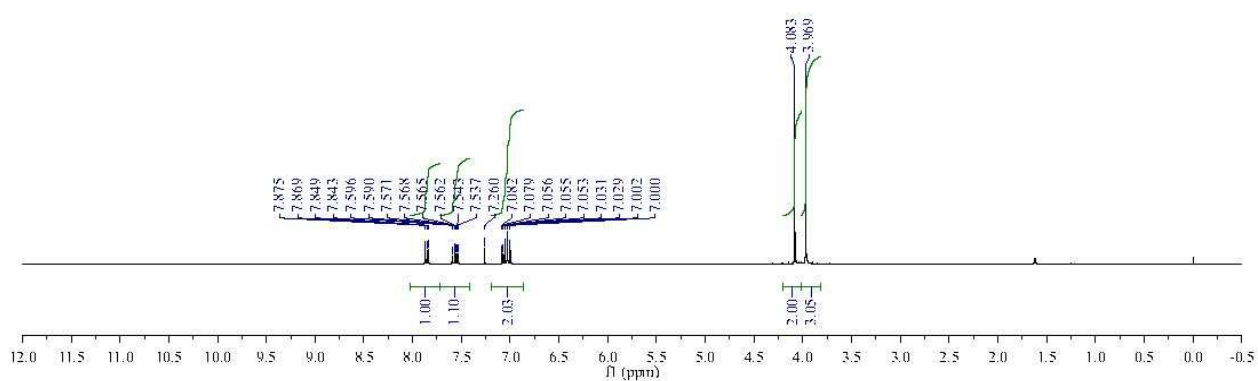
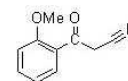


CNU_SWLac_PAB257-2_13C_15Sep2011
PAB257-2,13C

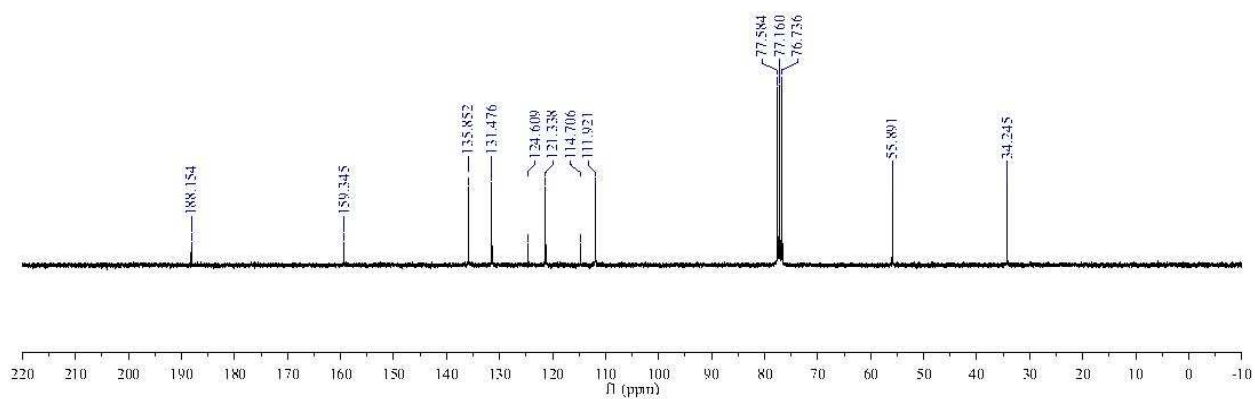
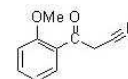


3-(2-Methoxyphenyl)-3-oxopropanenitrile (2h) : ^1H , ^{13}C NMR

CNU_SWLsc_PAB240-2_250d2011
PAB240-2

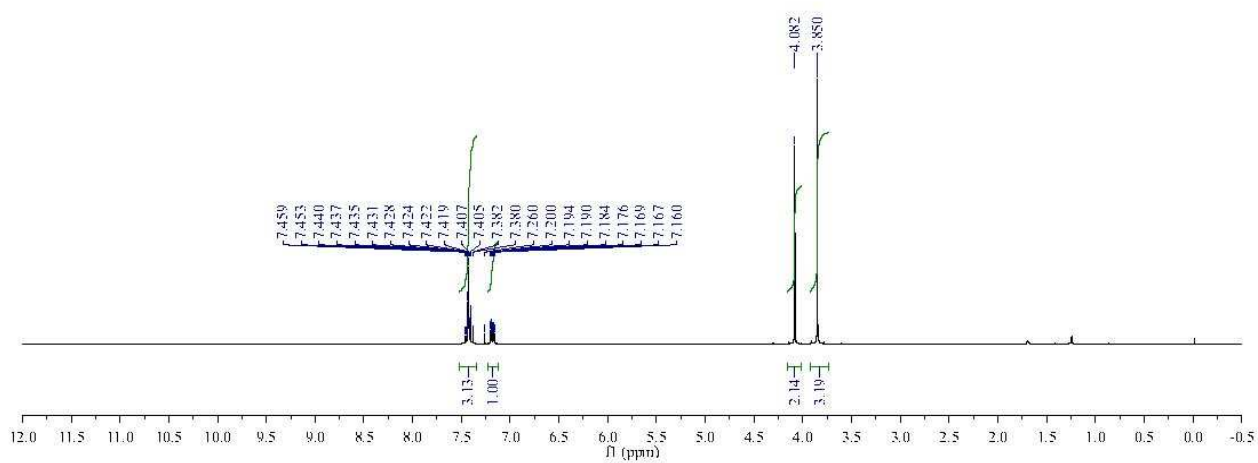
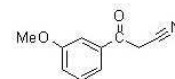


CNU_SWLsc_PAB240-2_13C_250d2011
PAB240-2

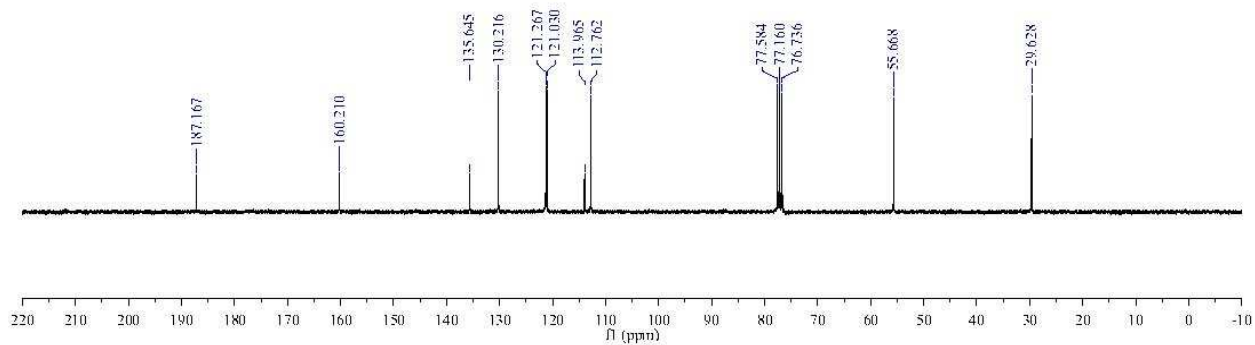
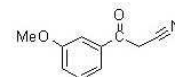


3-(3-Methoxyphenyl)-3-oxopropanenitrile (2i) : ^1H , ^{13}C NMR

CNU_SWLac_PAB243-2_19Aug2011
PAB243-2

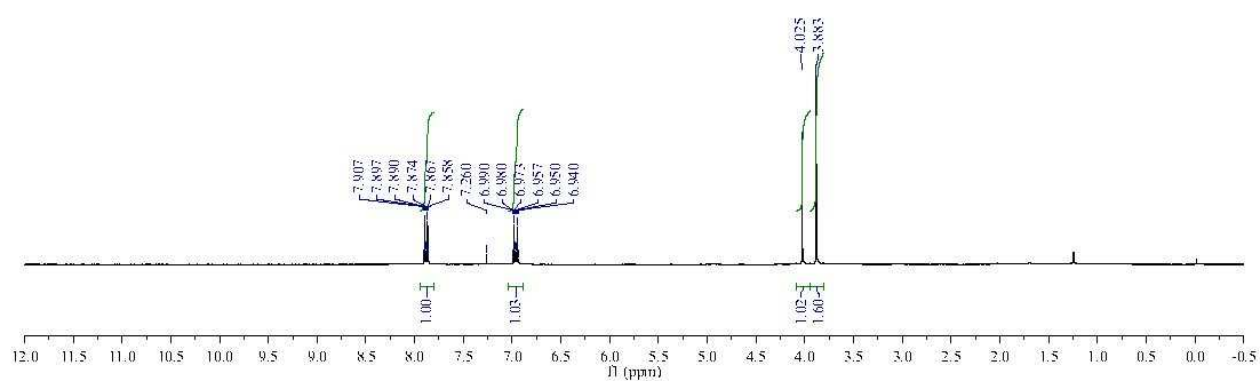
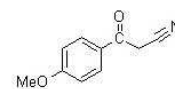


CNU_SWLac_PAB243-2_13C_19Aug2011
PAB243-2,13C

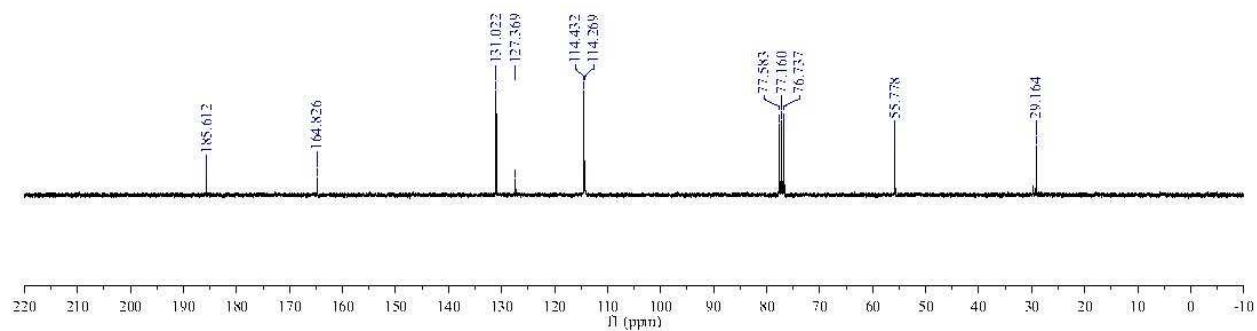
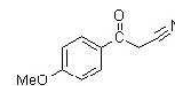


3-(4-Methoxyphenyl)-3-oxopropanenitrile (2j) : ^1H , ^{13}C NMR

CNU_SWLae_PAB242-2_22Aug2011
PAB242-2

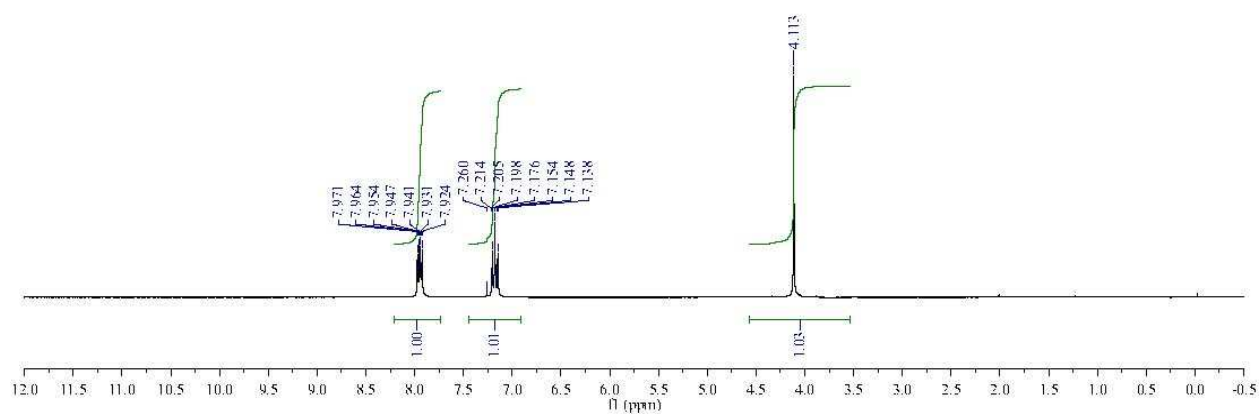
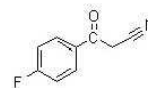


CNU_SWLae_PAB242-2_13C_22Aug2011
PAB242-2,13C

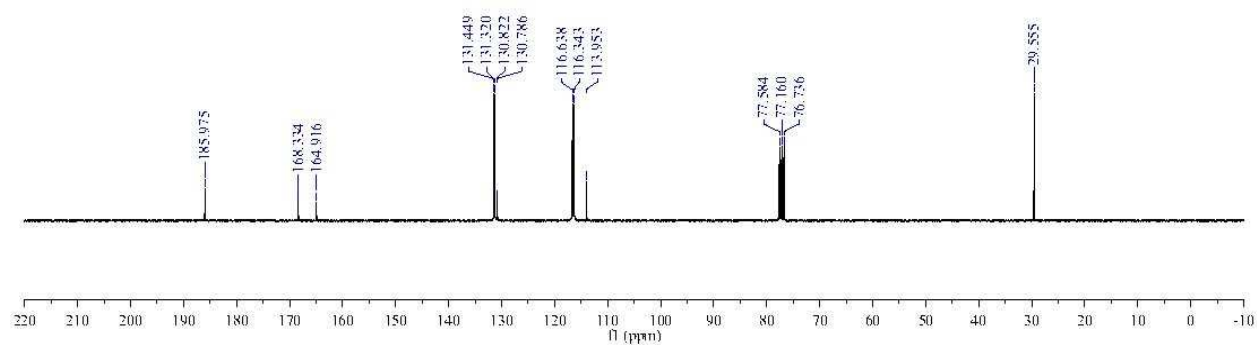
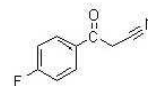


3-(4-Fluorophenyl)-3-oxopropanenitrile (2k) : ^1H , ^{13}C NMR

CNU_SWLae_PAB241-1re_19Aug2011
PAB241-1re

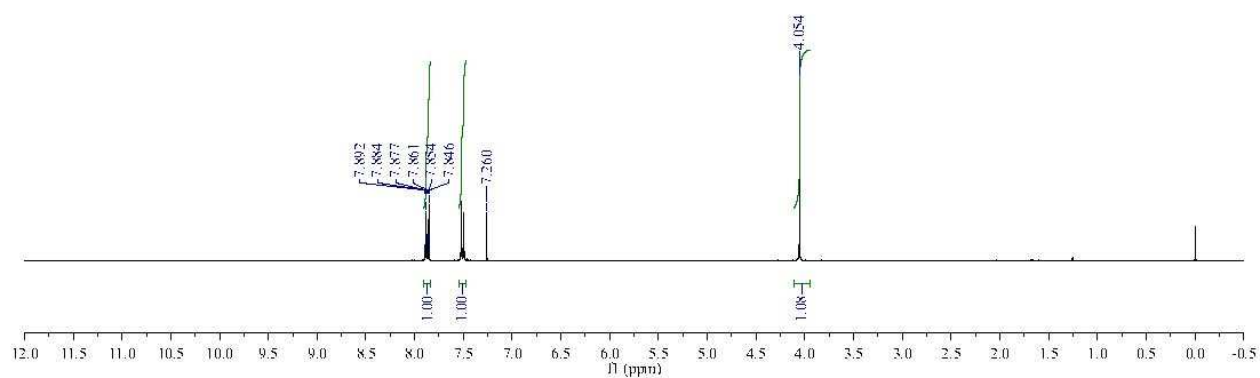
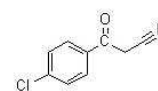


CNU_SWLae_PAB241-1re_13C_30Aug2011
PAB241-1re,13C

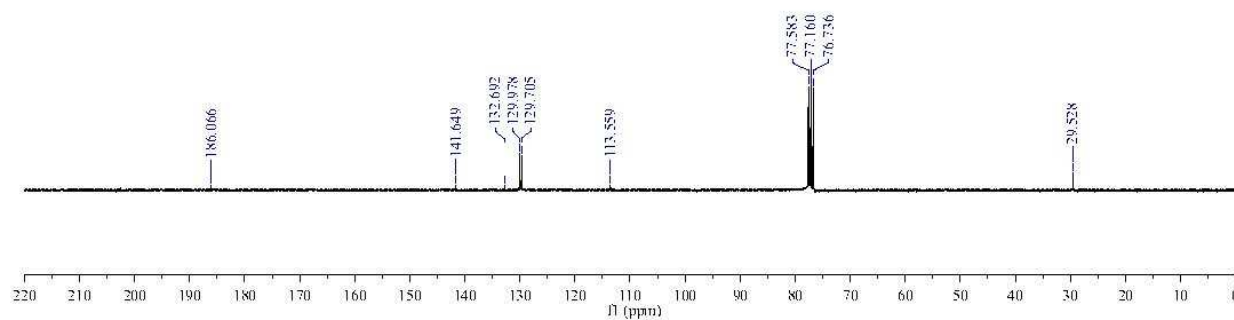
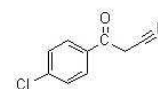


3-(4-Chlorophenyl)-3-oxopropanenitrile (2l) : ^1H , ^{13}C NMR

CNU_SWLae_PAB241-2_08Sep2011
PAB241-2

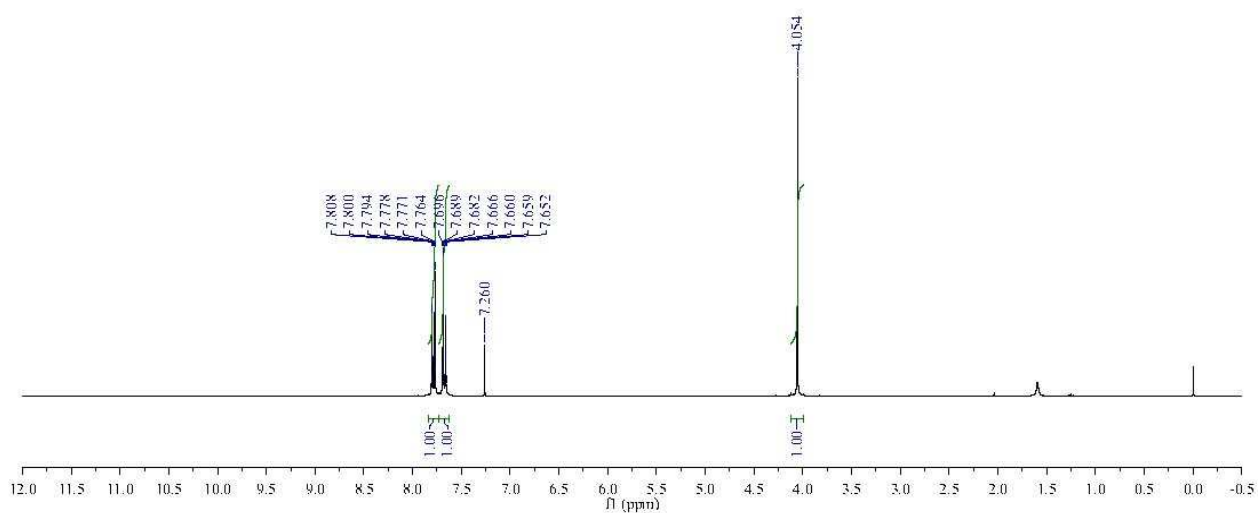
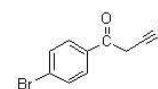


CNU_SWLae_PAB241-2_13C_08Sep2011
PAB241-2,13C

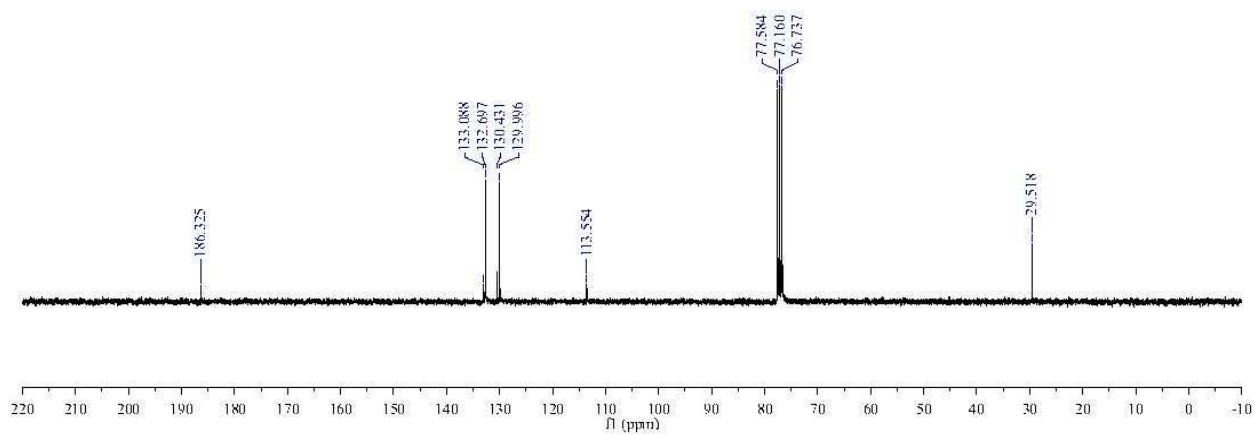
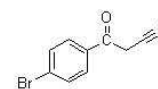


3-(4-Bromophenyl)-3-oxopropanenitrile (2m) : ^1H , ^{13}C NMR

CNU_SWLac_PAB255-1_08Sep2011
PAB255-1

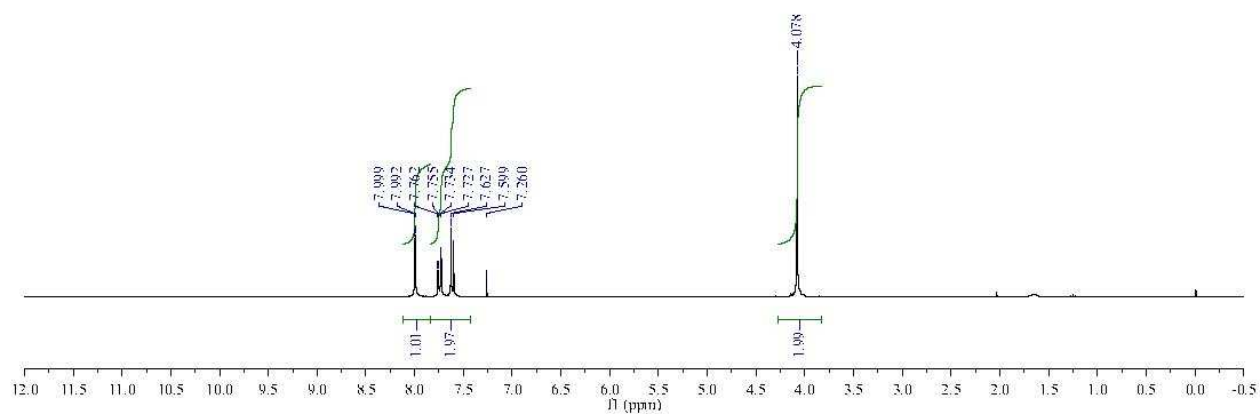
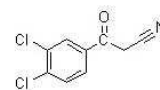


CNU_SWLac_PAB255-1_13C_08Sep2011
PAB255-1,13C

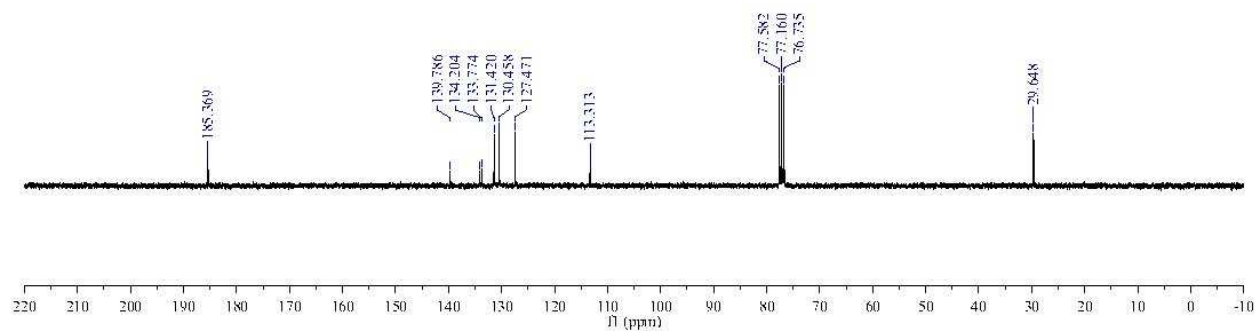
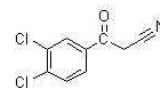


3-(3,4-Dichlorophenyl)-3-oxopropanenitrile (2n) : ^1H , ^{13}C NMR

CNU_SWLae_PAB262-2_19Sep2011
PAB262-2

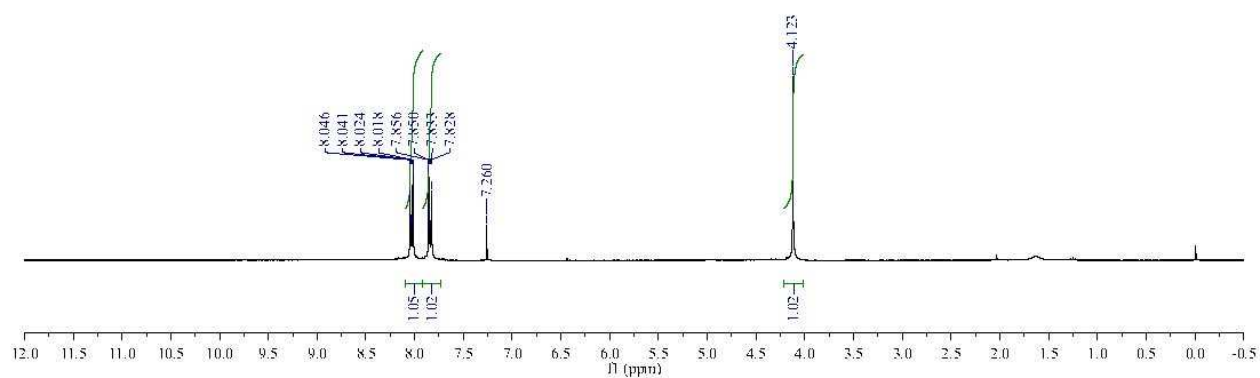
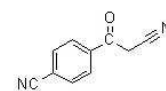


CNU_SWLae_PAB262-2_13C_19Sep2011
PAB262-2,13C

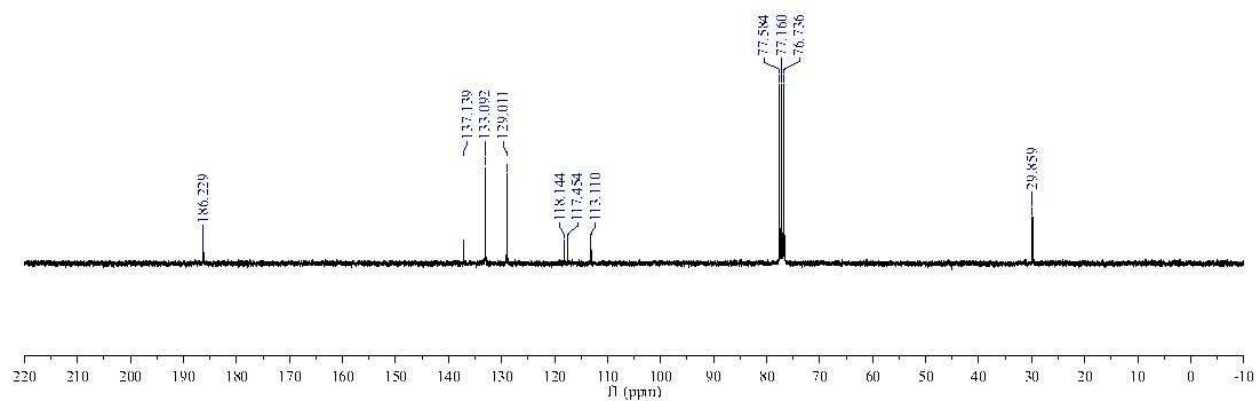
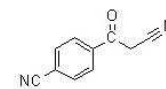


4-(2-Cyanoacetyl)benzonitrile (2o) : ^1H , ^{13}C NMR

CNU_SWLae_PAB256-2_06Sep2011
PAB256-2

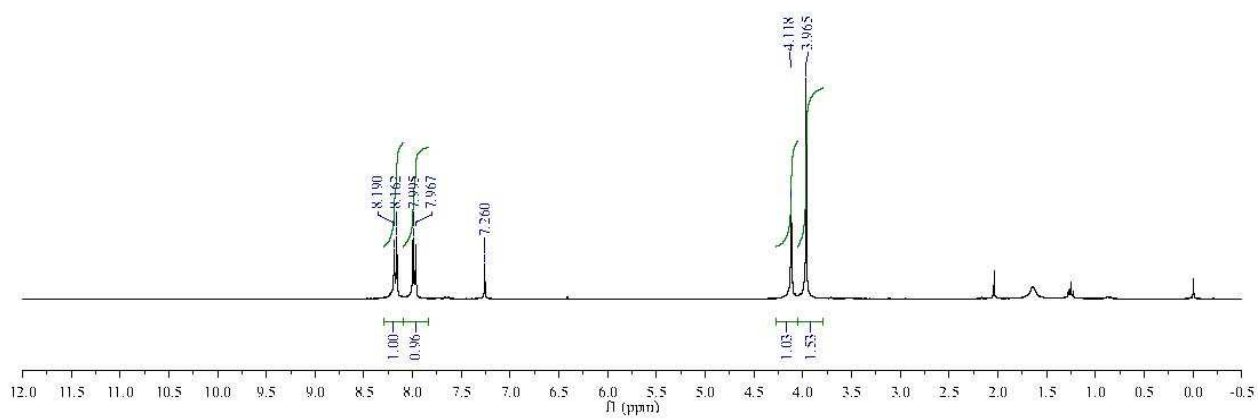
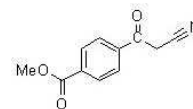


CNU_SWLae_PAB256-2_13C_06Sep2011
PAB256-2,13C

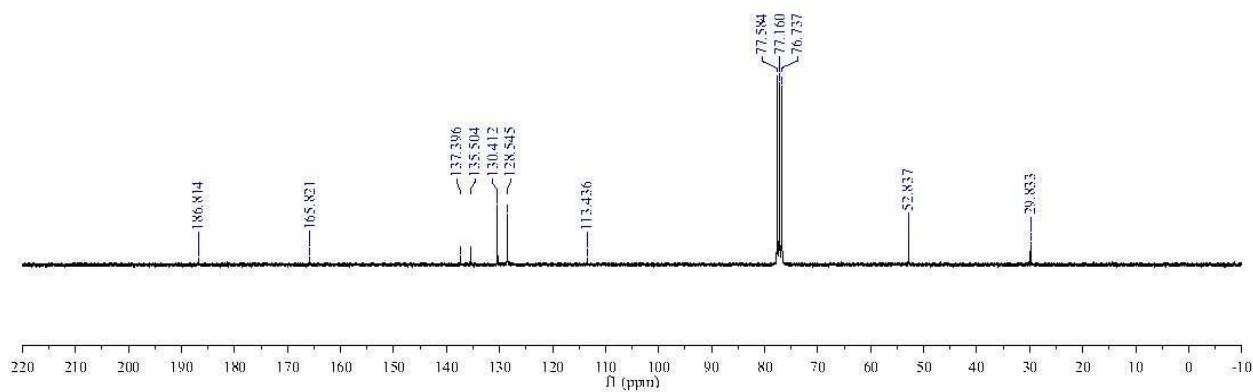
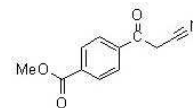


Methyl 4-(2-cyanoacetyl)benzoate (2p)

CNU_SWLac_PAB254-1_22Aug2011
PAB254-1

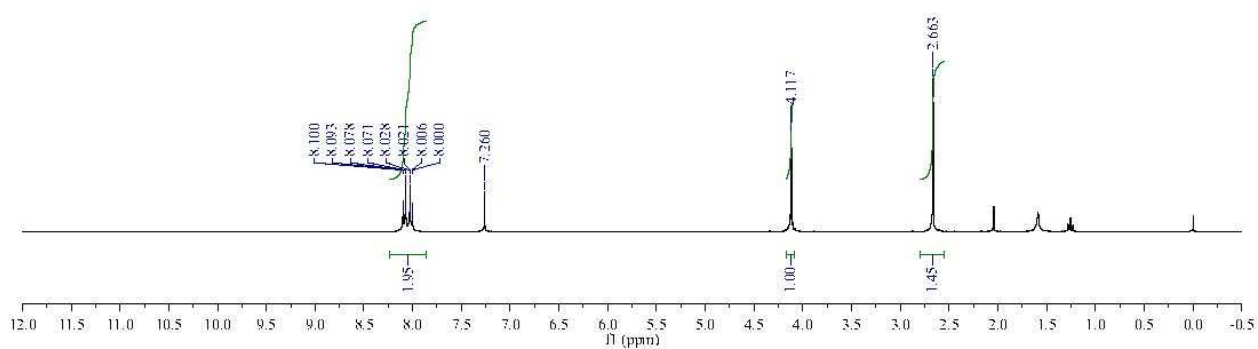
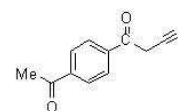


CNU_SWLac_PAB254-1_13C_22Aug2011
PAB254-1,13C

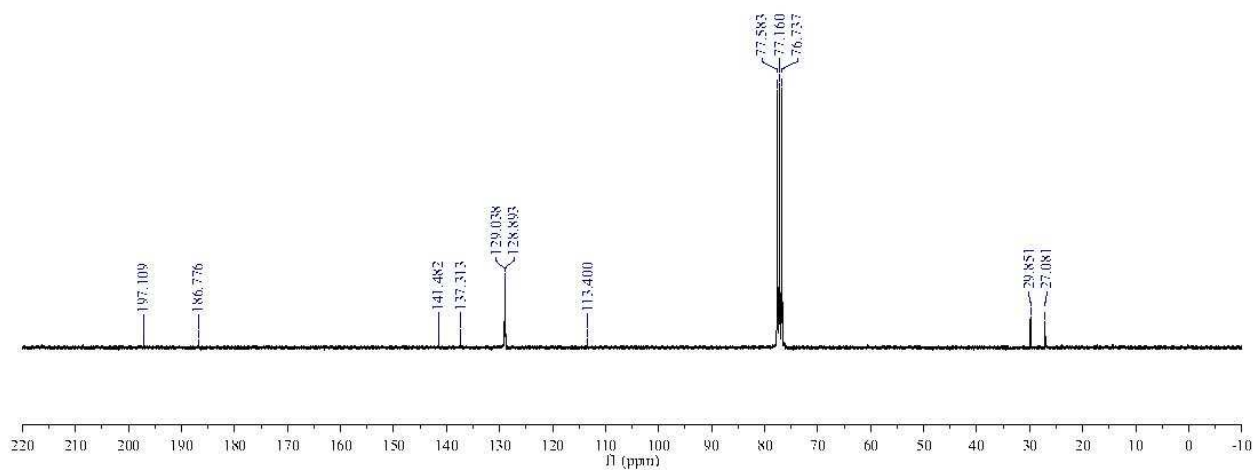
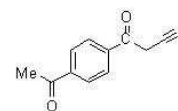


3-(4-Acetylphenyl)-3-oxopropanenitrile (2q)

CNU_SWLac_PAB255-2_09Sep2011
PAB255-2

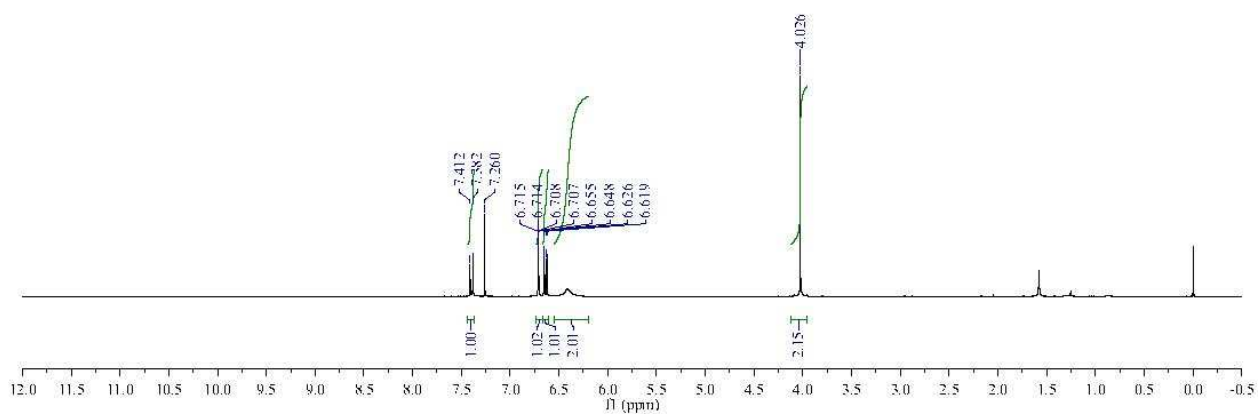
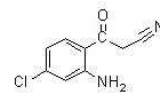


CNU_SWLac_PAB255-2_13C_09Sep2011
PAB255-2,13C

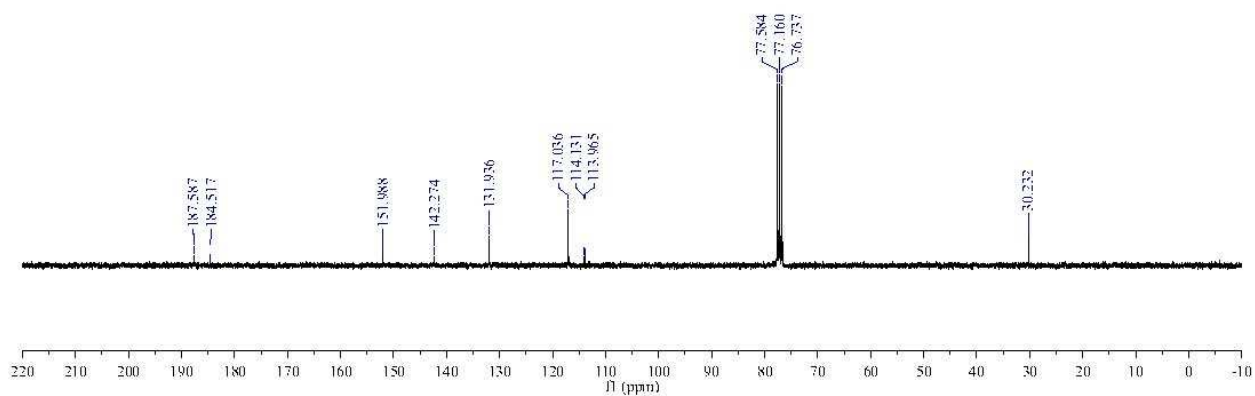
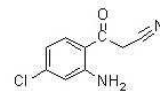


3-(2-Amino-4-chlorophenyl)-3-oxopropanenitrile (2r)

CNU_SWLac_PAB248-2_07Sep2011
PAB248-2

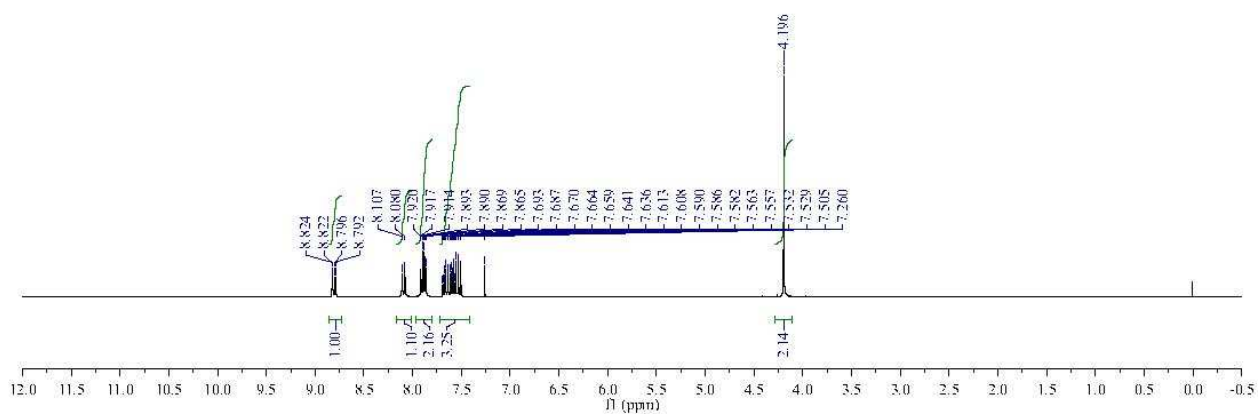
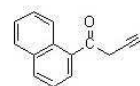


CNU_SWLac_PAB248-2_13C_07Sep2011
PAB248-2

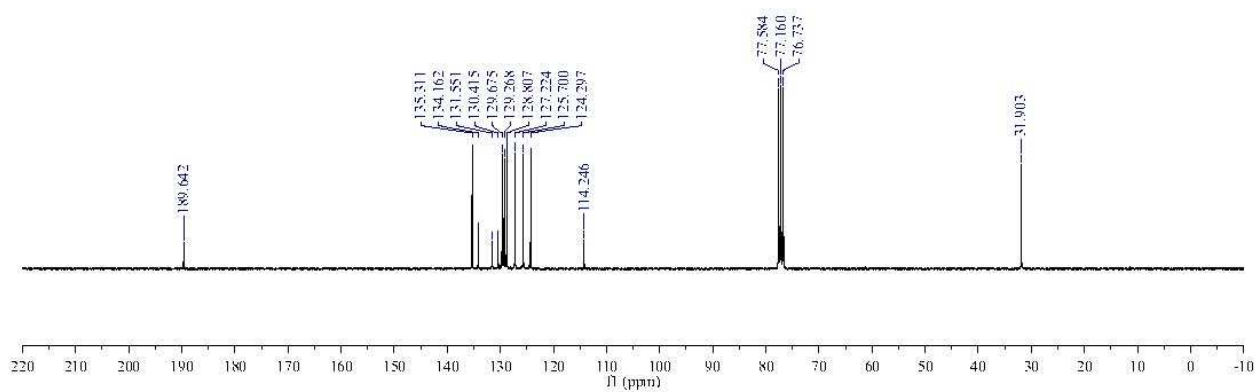
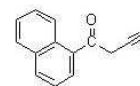


3-(Naphthalen-2-yl)-3-oxopropanenitrile (2s)

CNU_SWLac_PAB254-2_07Sep2011
PAB254-2

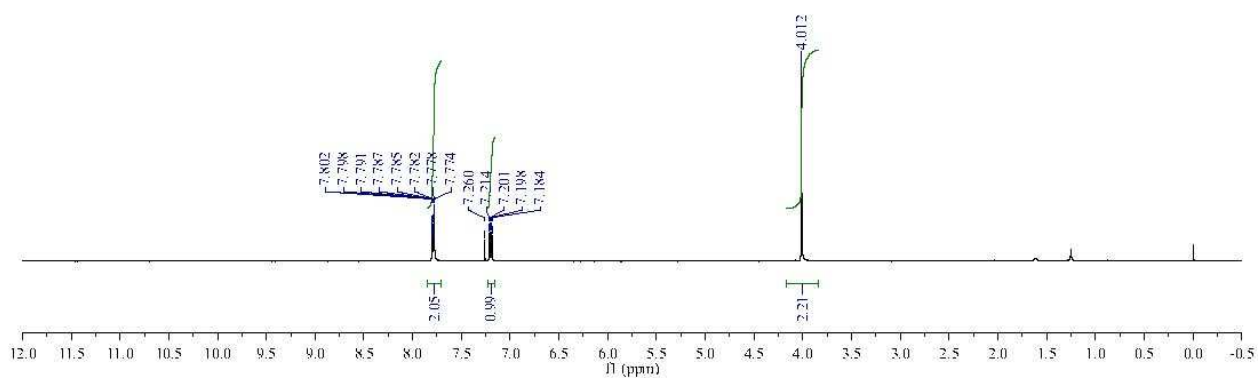
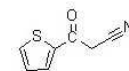


CNU_SWLac_PAB254-2_13C_07Sep2011
PAB254-2,13C



3-Oxo-3-(thiophen-2-yl)propanenitrile (2t)

CNU_SWLac_PAB256-1_06Sep2011
PAB256-1



CNU_SWLac_PAB256-1_13C_06Sep2011
PAB256-1,13C

