Supporting Information

A General and Convenient Catalytic Synthesis of Nitriles from Amides and Silanes

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General information: Unless otherwise stated, reactions were run under an argon atmosphere with exclusion of moisture from reagents and glassware using standard techniques for manipulating air-senstive compounds. Toluene, 1,4-dioxane and dibutylether were distilled from sodium. NMR spectra were recorded on Bruker AV 300 (^{1}H and ^{13}C) and AV 400 (^{29}Si) spectrometers at 300 MHz (^{1}H), 75 MHz (^{13}C) and 79.5 MHz (^{29}Si). All chemical shift (δ) are reported in ppm and coupling constants (*J*) in Hz; All chemical shifts are relative to tetramethylsilane; the resonance of the residual protons of the solvent was used as the internal standard (7.26 ppm, chloroform; 2.20 ppm, o-xylene) and all *d*-solvent peaks (77.00 ppm, chloroform; 19.60 ppm, o-xylene), respectively. All measurements were carried out at room temperature unless otherwise stated. Mass spectra were in general recorded on an AMD

402/3 or a HP 5989A mass selective detector. Gas chromatography was performed on a HP 6890 chromatography with a HP5 column.

Reagents: $[Et_3NH][HFe_3(CO)_{11}]$[1] was prepared by the method reported preciously. All other chemicals were obtained commercially and were used as received.

General procedure for the dehydration of primary amides to nitriles: A 25 mL oven dried schlenk tube containing a stir bar was charged with primary amides (1.0 mmol), and $[Et_3NH][HFe_3(CO)_{11}]$ (0.02-0.05 mmol). $(EtO)_2MeSiH$ (3.0 mmol; for amide **1k** and **1m**, 4.0 mmol) and dry toluene or 1,4-dioxane (2mL) were added respectively after purging the schlenk tube with argon. The mixture was stirred for the time indicated in table 3 at 100°C. The cooled reaction mixture was diluted with diethyl ether (5 mL) and quenched by addition of 2M HCl (5 mL). The reaction mixture was vigorously stirred for 3h at room temperature and was then extracted with diethyl ether (3 x 20 mL) (for amide **1k**, about 5 M NaOH (2 mL) was used to adjust the PH value to 7 before extracting). The combined organic layers were washed with brine (10 mL), dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure (900 mbar, 40°C). the residue was Purified by silica gel column chromatography and gave the corresponding nitriles.

4-Methylbenzonitrile (**2b**): ^{1}H NMR (300.1 MHz, $CDCl_3$): δ = 2.26 (s, 3 H), 7.10 (d, J = 7.9 Hz, 2 H), 7.37 (d, J = 8.3 Hz, 2 H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 21.75, 109.22, 119.07, 129.76, 131.96, 143.63. MS (EI): m/z (rel. int.) 118 (11), 117 (100), 116 (74), 91 (7), 90 (44), 89 (30), 64 (6), 63 (13), 62 (6), 51 (5), 50 (5), 39 (7).

3-Methylbenzonitrile (**2c**): ^{1}H NMR (300.1 MHz, $CDCl_3$): δ = 2.38 (s, 3 H), 7.08-7.44 (m, 4 H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 20.36, 112.66, 118.04, 126.13, 130.14, 132.40, 133.56, 141.83. MS (EI): m/z (rel. int.) 118 (16), 117 (98), 116 (100), 91 (10), 90 (67), 89 (47), 76 (6), 75 (7), 63 (22), 62 (10), 51 (9), 50 (9), 39 (15), 38 (6). HRMS (EI, m/z) calcd. for C_8H_7N, 117.0573; found 117.0571.

2-Methylbenzonitrile (**2d**): ^{1}H NMR (300.1 MHz, $CDCl_3$): δ = 2.37 (s, 3 H), 7.31-7.46 (m, 4H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 21.04, 112.14, 118.94, 128.90, 129.17, 132.38, 132.56, 139.13. MS (EI): m/z (rel. int.) 118 (12), 117 (100), 116 (66), 91 (7), 90 (54), 89 (36), 64 (6), 63 (14), 51 (6), 50 (6).

4-Methoxylbenzonitrile (**2e**): ^{1}H NMR (300.1 MHz, CDCl$_3$): δ = 3.85 (s, 3 H), 6.92-6.97 (m, 2 H), 7.55-7.60 (m, 2 H); ^{13}C NMR (75.5 MHz, CDCl$_3$): δ = 55.48, 103.88, 114.69, 119.17, 133.91, 162.78. MS (EI): m/z (rel. int.) 134 (9), 133 (100), 118 (10), 104 (11), 103 (38), 102 (9), 90 (45), 76 (10), 75 (7), 64 (12), 63 (14), 62 (5) 39 (7).

4-tert-Butylbenzonitrile (**2f**): ^{1}H NMR (300.1 MHz, CDCl$_3$): δ = 1.32 (s, 9 H), 7.56-7.57 (m, 2 H), 7.59-7.60 (m, 2 H); ^{13}C NMR (75.5 MHz, CDCl$_3$): δ = 30.86, 35.18, 109.23, 119.08, 126.10, 131.88, 156.56. MS (EI): m/z (rel. int.) 159 (19), 145 (12), 144 (100), 128 (59, 117 (7), 116 (59), 115 (5), 104 (12), 89 (7), 77 (5), 51 (4), 39 (6). HRMS (EI, m/z) calcd. for $C_{11}H_{13}N$, 159.1043; found 159.1045.

4-Chlorobenzonitrile (**2g**): ^{1}H NMR (300.1 MHz, CDCl$_3$): δ = 7.26-7.48 (m, 2 H), 7.58-7.62 (m, 2 H); ^{13}C NMR (75.5 MHz, CDCl$_3$): δ = 110.74, 117.92, 129.65, 133.33, 139.50. MS (EI): m/z (rel. int.) 139 (34), 138 (8), 137 (100), 102 (30), 75 (14), 74 (79, 73 (4), 51 (6), 50 (11).

4-Bromobenzonitrile (**2h**): ^{1}H NMR (300.1 MHz, CDCl$_3$): δ = 7.34-7.39 (m, 2 H), 7.46-8.31 (m, 2 H); ^{13}C NMR (75.5 MHz, CDCl$_3$): δ = 111.20, 118.00, 127.97, 132.61, 133.37. MS (EI): m/z (rel. int.) 182 (98), 180 (100), 103 (8), 102 (93), 76 (12), 75 (26), 74 (10), 51 (13), 50 (17).

1-Cyanonaphthalene (**2i**): ^{1}H NMR (300.1 MHz, CDCl$_3$): δ = 7.52 (dd, J = 8.4 Hz, J = 7.4 Hz, 1 H), 7.60-7,72 (m, 2 H), 7.90-7.94 (m, 2 H), 8.08 (d, J = 7.4 Hz, 1 H), 8.22-8.25 (m, 1 H); ^{13}C NMR (75.5 MHz, CDCl$_3$): δ = 110.15, 117.78, 124.89, 124.91, 125,10, 127.51, 128.55, 128.61, 132.32, 132.59, 132.88, 133.23. MS (EI): m/z (rel. int.) 154 (13), 153 (100), 152 (6), 127 (5), 126 (18), 76 (7), 75 (5), 63 (9).

2-Cyanonaphthalene (**2j**): ^{1}H NMR (300.1 MHz, CDCl$_3$): δ = 7.45-7.56 (m, 3 H), 7.84-7.90 (m, 4 H); ^{13}C NMR (75.5 MHz, CDCl$_3$): δ = 109.31, 114.43, 122.33, 125.24, 125.69, 127.83, 134.94, 137.39, 141.24. MS (EI): m/z (rel. int.) 154 (13), 153 (100), 152 (7), 127 (6), 126 (18), 76 (6), 63 (9).

4-Aminobenzonitrile (**2k**): ^{1}H NMR (300.1 MHz, CDCl$_3$): δ = 4.20 (bs, 2 H), 6.61-6.66 (m, 2 H), 7.37-7.42 (m, 2 H); ^{13}C NMR (75.5 MHz, CDCl$_3$): δ = 99.98, 114.36, 120.13, 133.72, 150.42. MS (EI): m/z (rel. int.) 119 (9), 118 (100), 117 (6), 91 (30), 90 (9), 64 (11), 63 (9), 52 (5). HRMS (ESI, m/z) $[M-H]^-$, calcd. for $C_7H_5N_2$, 117.0458; found 117.0459.

Methyl 4-cyanobenzoate (**2l**): ^{1}H NMR (300.1 MHz, CDCl$_3$): δ = 3.95 (s, 3 H), 7.72-7.76 (m, 2 H), 8.11-8.15 (m, 2 H); ^{13}C NMR (75.5 MHz, CDCl$_3$): δ = 52.69, 116.36, 117.92, 130.06, 132.19, 133.89, 165.38. HRMS (ESI, m/z) $[M+H]^+$, calcd. for $C_9H_8O_2N$, 161.0471; found 161.07107.

Cinnamonitrile (**2m**) and **3-Phenylpropionitrile** (**2m'**): ^{1}H NMR (300.1 MHz, CDCl$_3$): δ = 2.52 (t, J = 7.5 Hz, 2 H), 2.86 (t, J = 7.5 Hz, 2 H), 5.36 (d, J = 12.2 Hz, 0.47 H), 5.76-7.39 (m, 8H); ^{13}C NMR (75.5 MHz, CDCl$_3$): δ = 19.24, 31.46, 94.99, 96.25, 118.08, 119.07, 128.18, 128.78, 128.85, 128.93, 129.03, 130.89, 131.13, 133.43, 137.98, 148.64, 150.50. cinnamonitrile (2m) MS (EI): m/z (rel. int.) 130 (11), 129 (100), 128 (27), 103 (14), 102 (32), 78 (8),77 (7), 76 (9), 75 (7), 74 (4), 63 (6), 51 (10); HRMS (EI, m/z) [M], calcd. for C_9H_7N, 129.0573; found 129.0576. **3-phenylpropionitrile** (**2m'**) MS (EI): m/z (rel. int.) 131 (25), 92 (8), 91 (100), 77 (4), 65 (11), 63 (4), 51 (6), 39 (5). HRMS (EI, m/z) [M], calcd. for C_9H_9N, 131.0729; found 131.0733.

Benzo[b]thiophene-carbonitrile (**2n**): ^{1}H NMR (300.1 MHz, CDCl$_3$): δ = 7.45-7.56 (m, 2 H), 7.85-7.90 (m, 3 H); ^{13}C NMR (75.5 MHz, CDCl$_3$): δ = 109.61, 114.42, 122.33, 125.23, 125.68, 127.83, 134.94, 137.38, 141.22. MS (EI): m/z (rel. int.) 161 (5), 160 (11), 159 (100), 133 (2), 132 (5), 115 (5), 114 (4), 79 (2), 69 (5), 63 (3). HRMS (EI, m/z) calcd. for C_9H_5NS, 159.0137; found 159.0140.

Benzyl nitrile (**2p**): ^{1}H NMR (300.1 MHz, $CDCl_3$): δ = 3.76 (s, 2 H), 7.30-7.42 (m, 5 H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 23.50, 117.80, 127.84, 127.97, 129.06, 129.85. MS (EI): m/z (rel. int.) 118 (16), 117 (100), 116 (76), 77 (11), 74 (5), 65 (8), 64 (7), 63 (21), 62 (10), 61 (5), 51 (20), 50 (15), 39 (13), 38 (6). HRMS (EI, m/z) calcd. for C_8H_7N, 117.0573; found 117.0571.

Decanonitrile (**2q**): ^{1}H NMR (300.1 MHz, $CDCl_3$): δ = 0.86 (t, J = 6.5 Hz, 3 H), 1.20-1.31 (m, 10 H), 1.38-1.47 (m, 2 H), 1.59-1.69 (m, 2 H), 2.32 (t, J = 7.0 Hz, 2 H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 13.98, 17.02, 22.55, 25.29, 28.57, 28.67, 29.07, 29.17, 31.71, 119.77. MS (EI): m/z (rel. int.) 152 (3), 138 (6), 125 (5), 124 (36), 111 (21), 110 (83), 98 (8), 97 (75), 96 (100), 93 (5), 84 (11), 83 (69), 82 (96), 81 (8), 71 (12), 70 (18), 69 (62), 68 (13), 67 (8), 57 (37), 56 (19), 55 (50), 54 (49), 53 (9), 43 (47), 42 (17), 41 (80), 40 (57), 39 (25), 29 (26), 28 (8), 27 (20).

Adamantanecarbonitrile (**2r**): ^{1}H NMR (300.1 MHz, $CDCl_3$): δ = 1.72 (bs, 6 H), 2.03 (bs, 9 H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 27.04, 30.14, 35.70, 39.86, 125.22. MS (EI): m/z (rel. int.) 161 (33), 160 (12), 131 (11), 130 (100), 103 (4), 102 (48), 76 (9), 75 (14), 51 (7), 50 (7). HRMS (EI, m/z) [M], calcd. for $C_{11}H_{15}N$, 161.1199; found 161.1206.

Reaction of 1a with $(EtO)_2MeSiH$ in o-xylene-d_{10} in the presence of $[Et_3NH][HFe_3(CO)_{11}]$

A 10 mL oven dried schlenk tube containing a stir bar was charged with benzamide (121 mg, 1.0 mmol), and $[Et_3NH]$ $[HFe_3(CO)_{11}]$ (11.6 mg, 0.02 mmol). $(EtO)_2MeSiH$ (0.48 mL, 3.0 mmol), o-xylene-d_{10} (2 mL) and mesitylene (0.5 mmol, as an internal standard) were added respectively after purging the schlenk tube with argon. The mixture was stirred for 3h at 100 °C. The cooled reaction mixture was directly measured by ^{29}Si NMR and GC-MS. ^{29}Si NMR (79.5 MHz, $[D_{10}]$o-xylene) & = -43.8, -50.4, -51.3; MS [m/z, 267 (M-15), 237 (M-45)].

References

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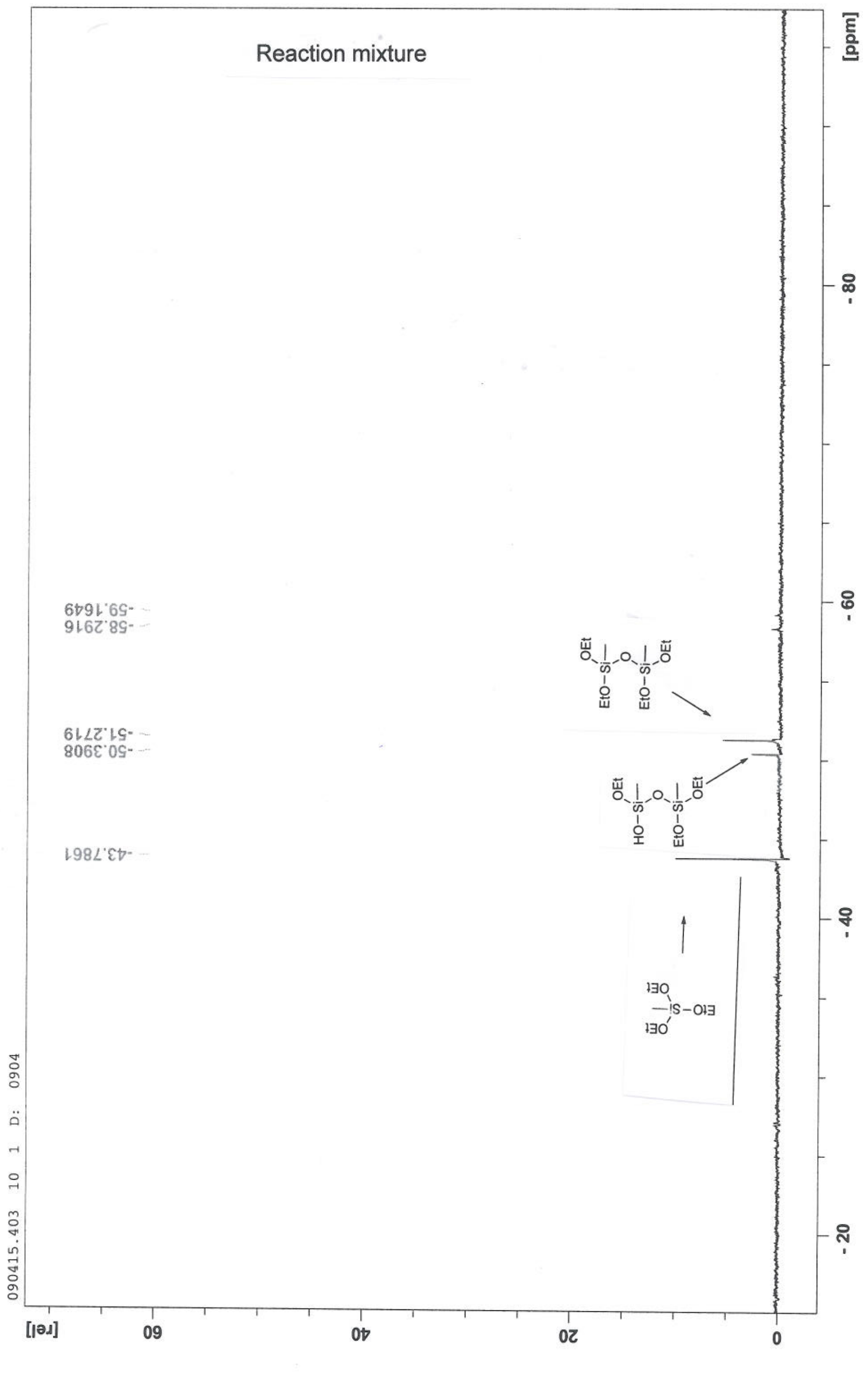
1 F. Henry, J. R. Holtzelow. *Inorganic Synthesis*, Vol, **8**, John Wiley & Sons, New York, London, 1966, pp146-148.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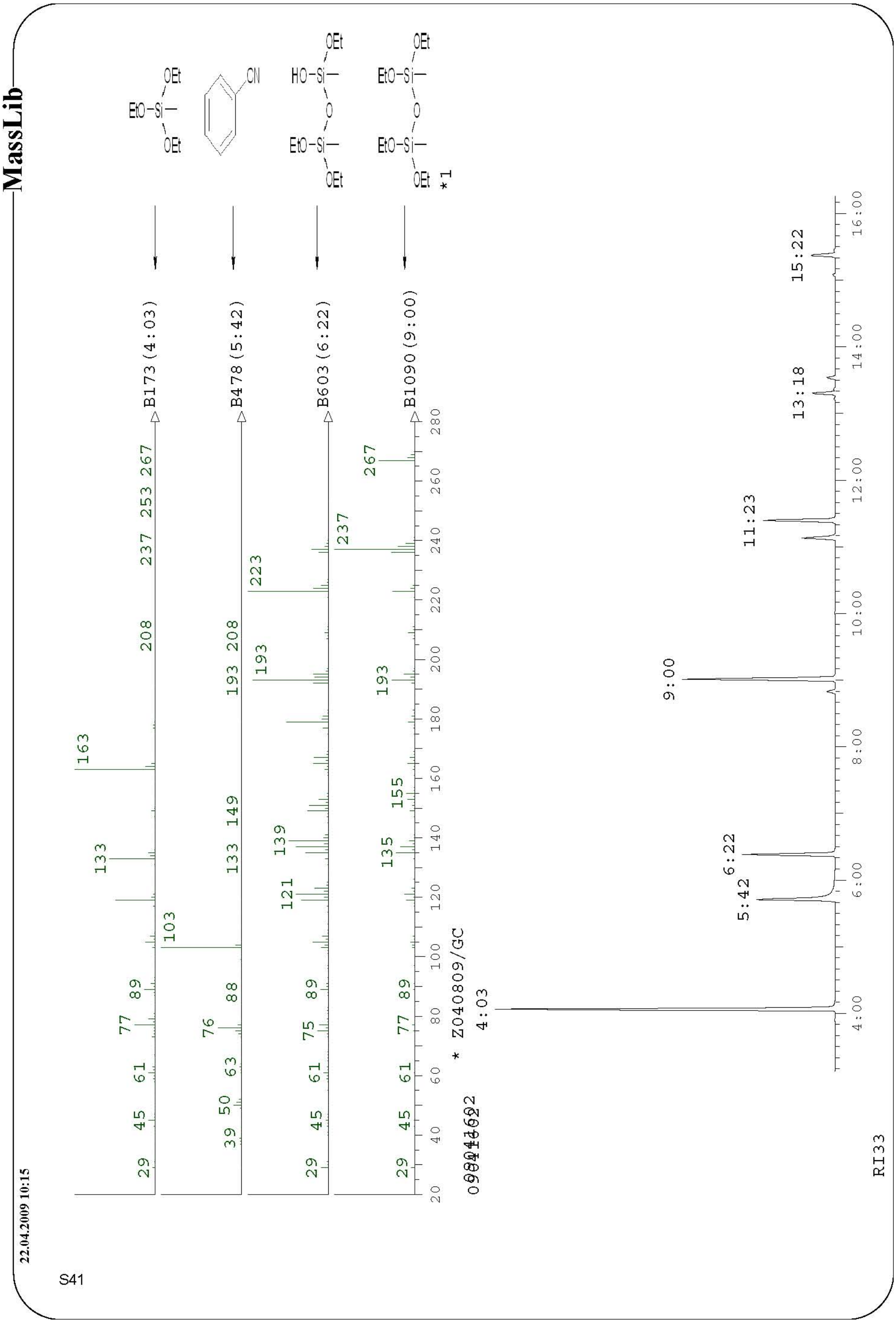
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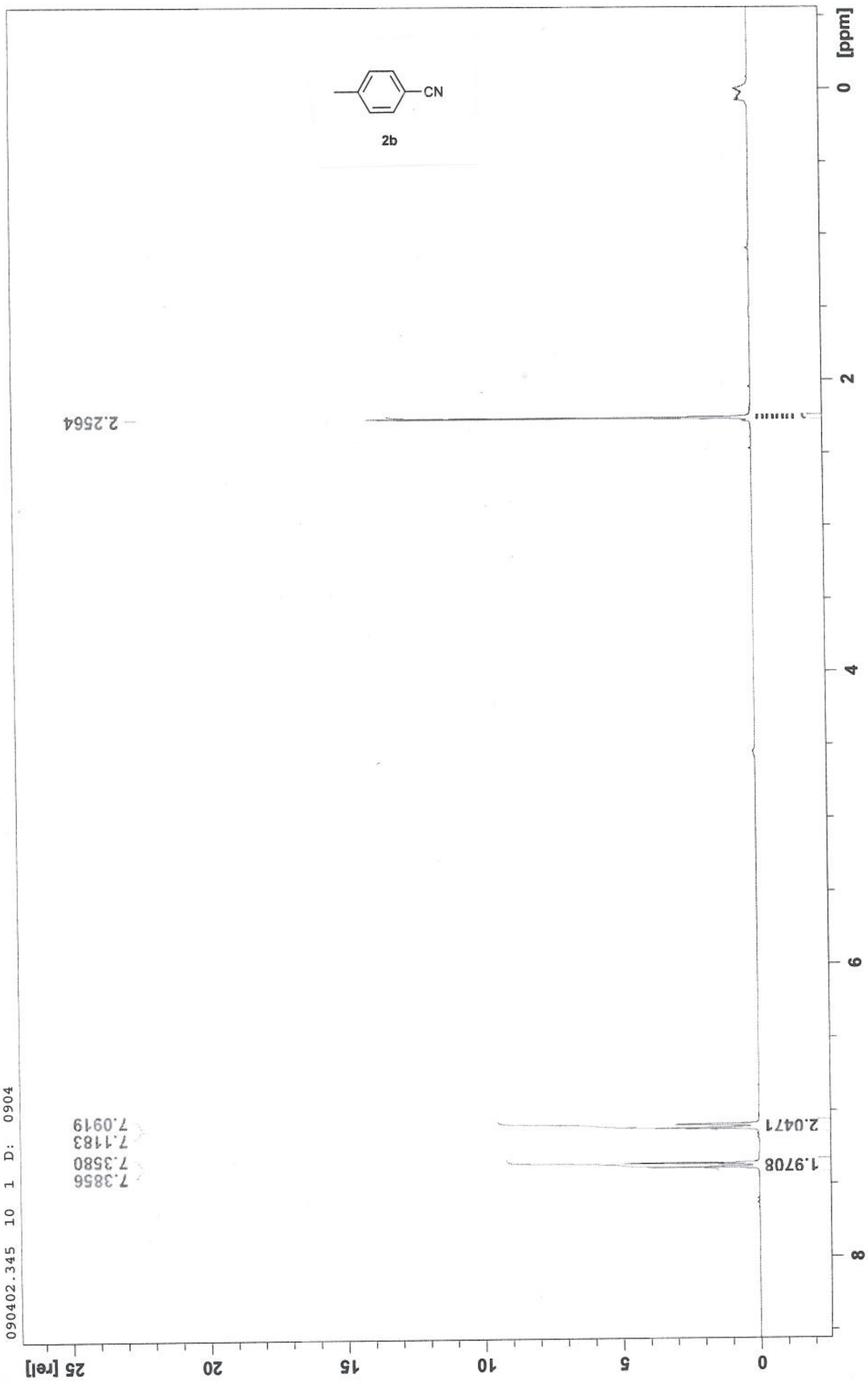
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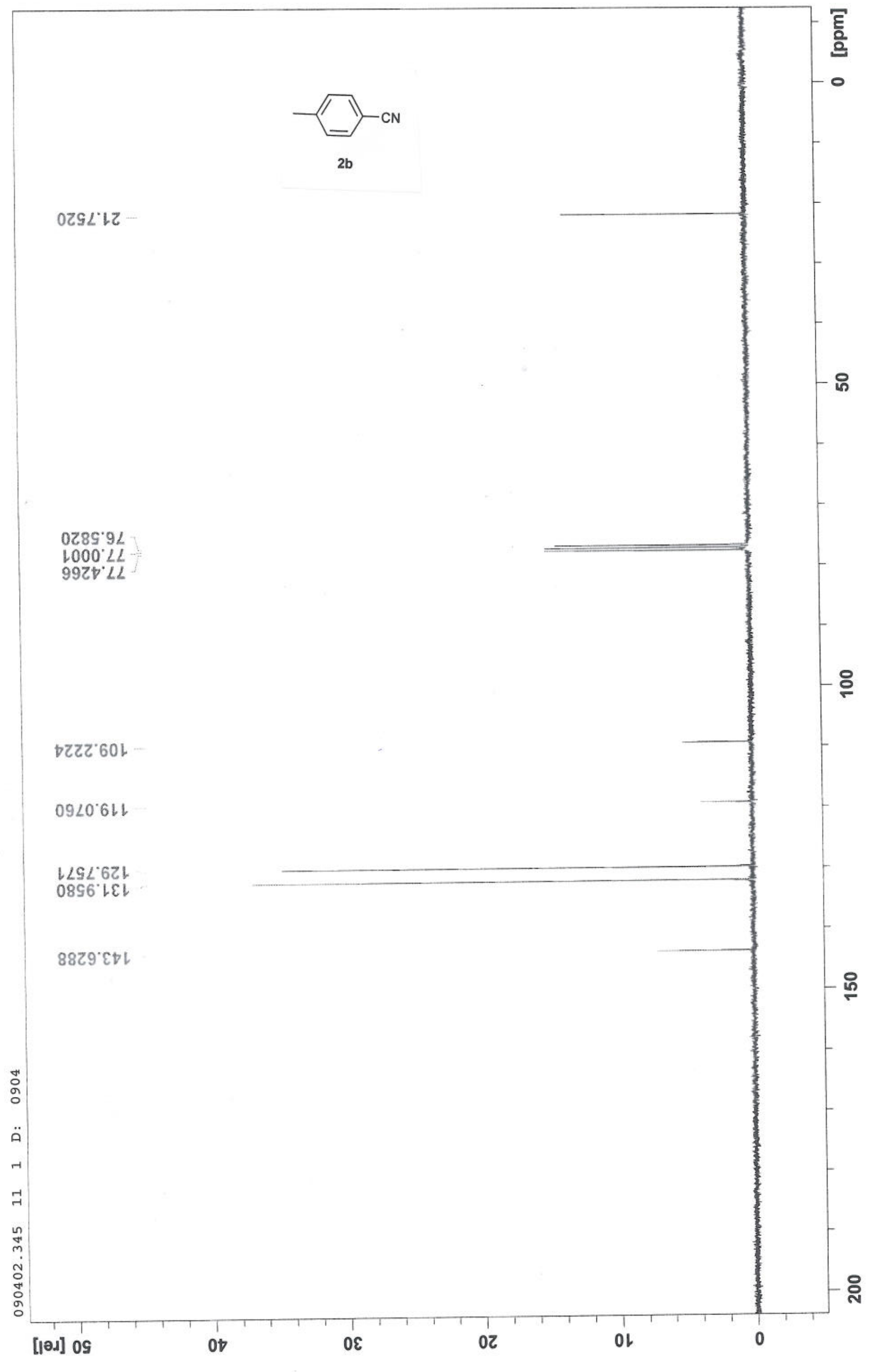
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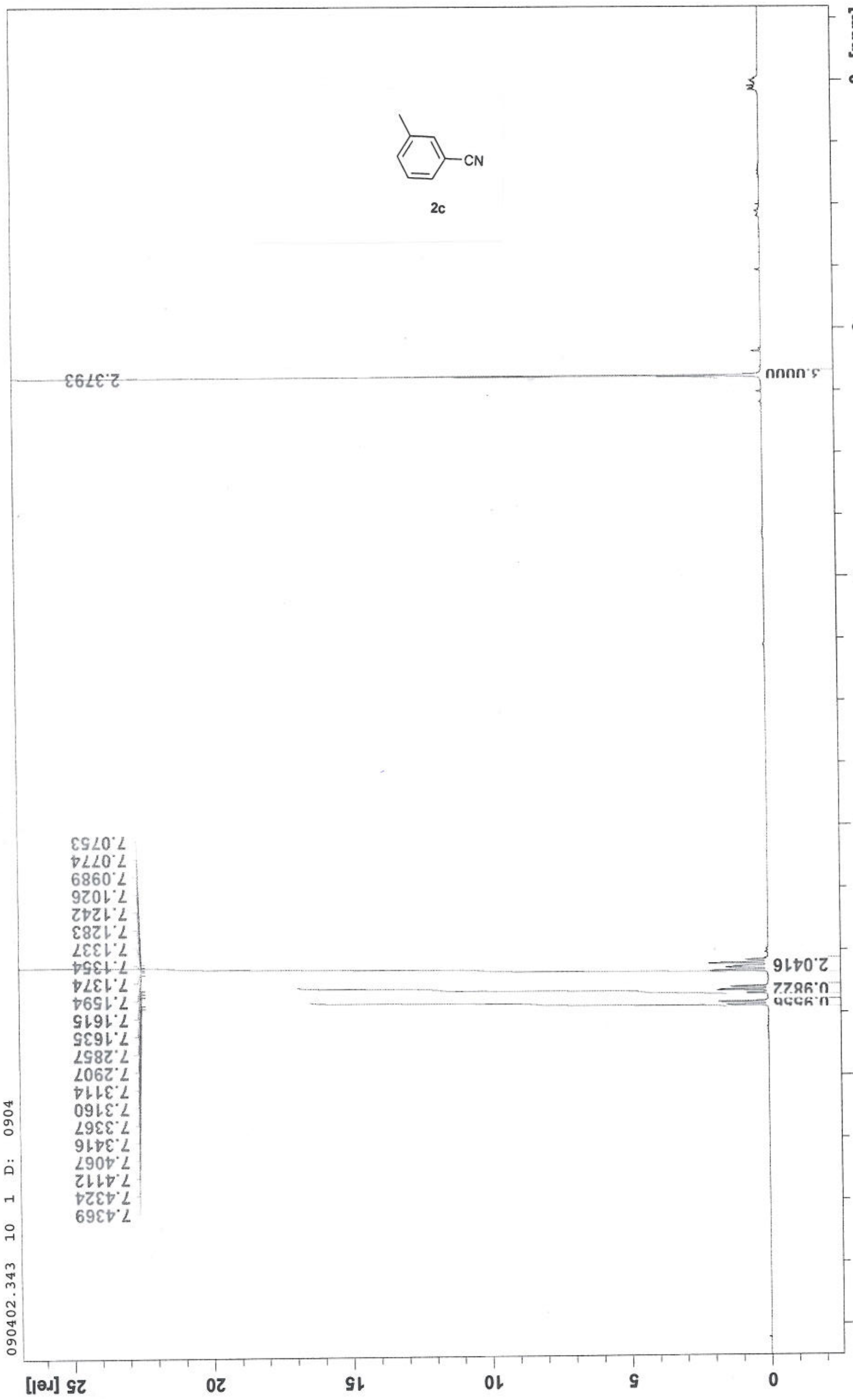
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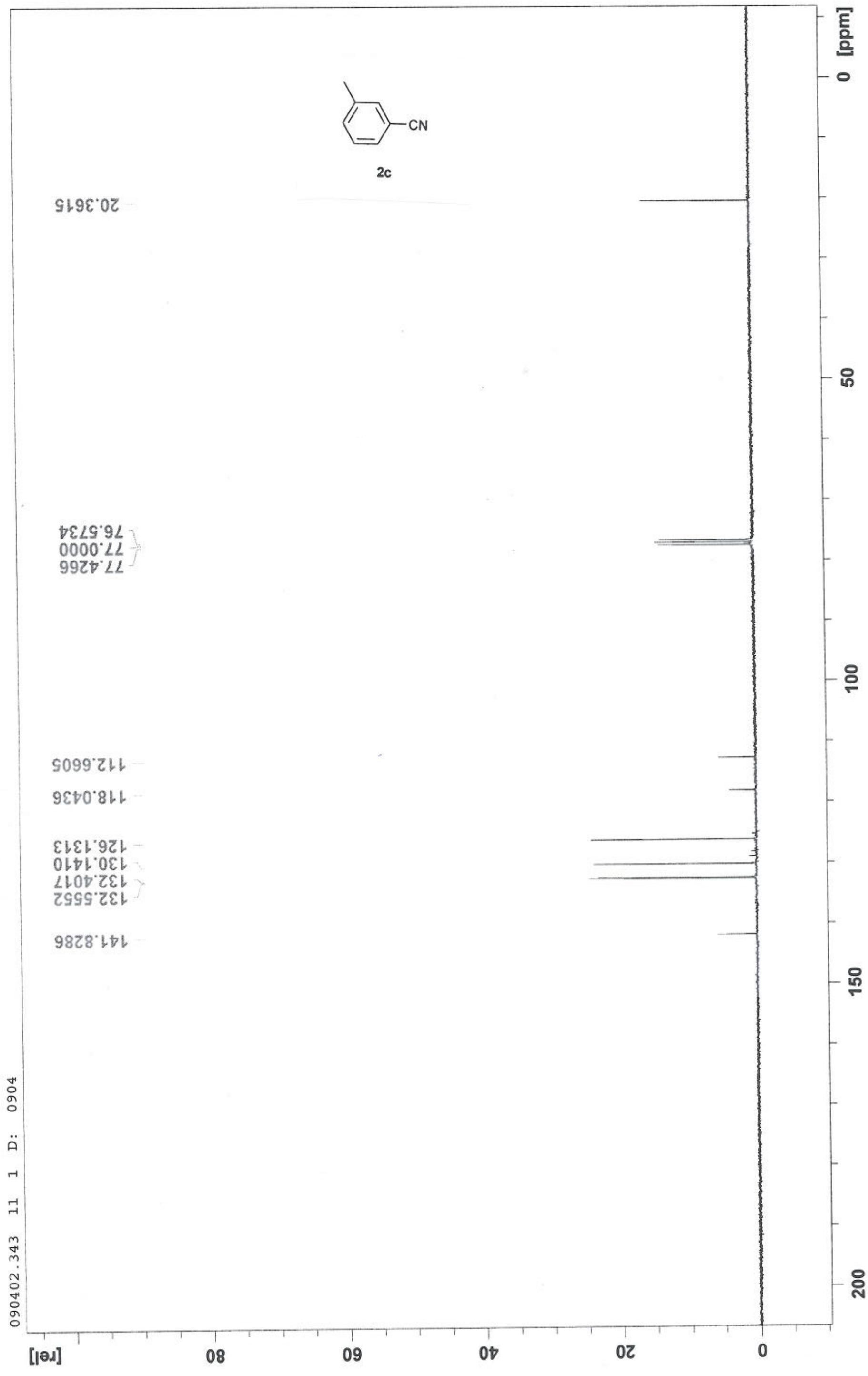
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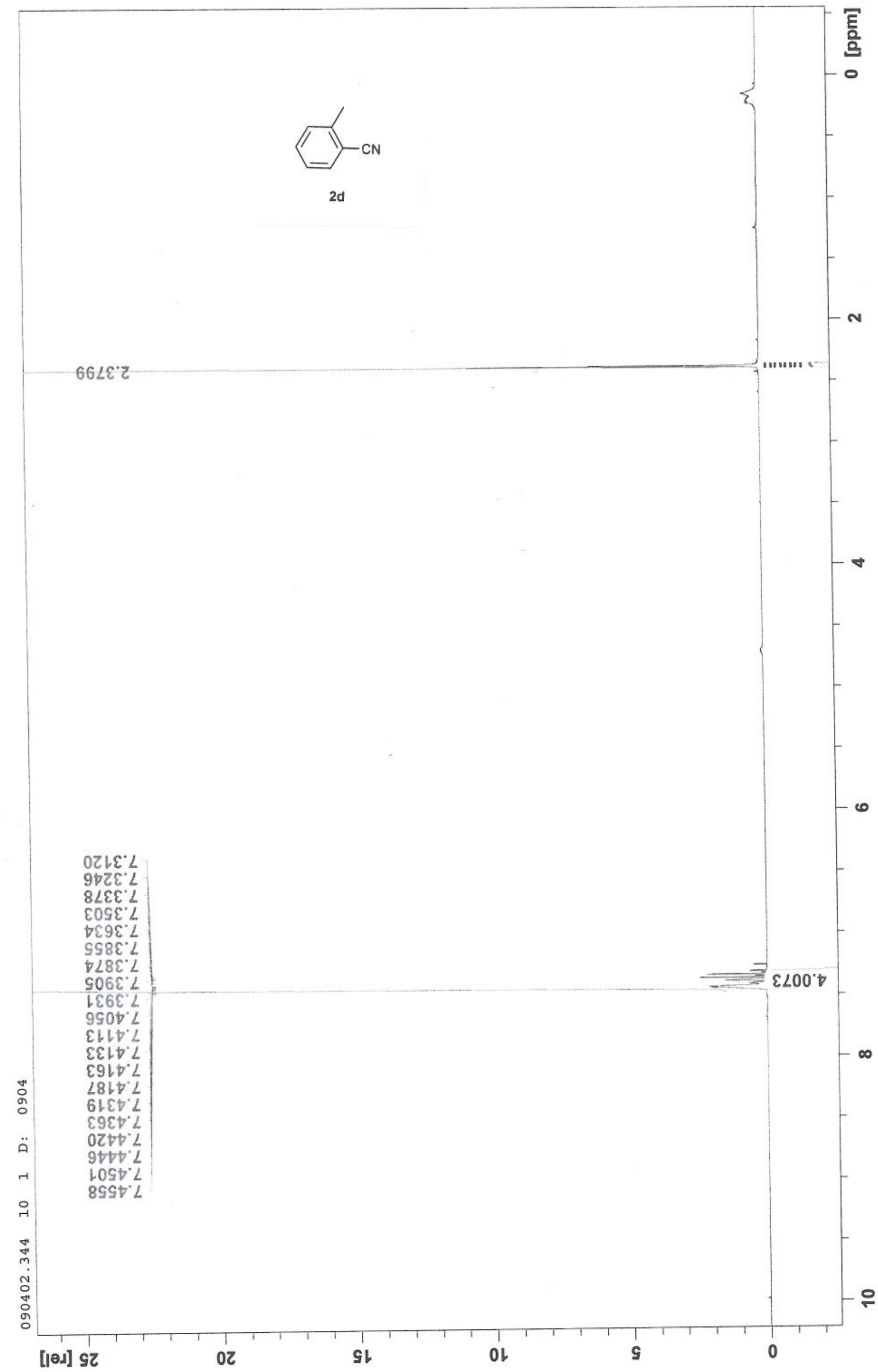
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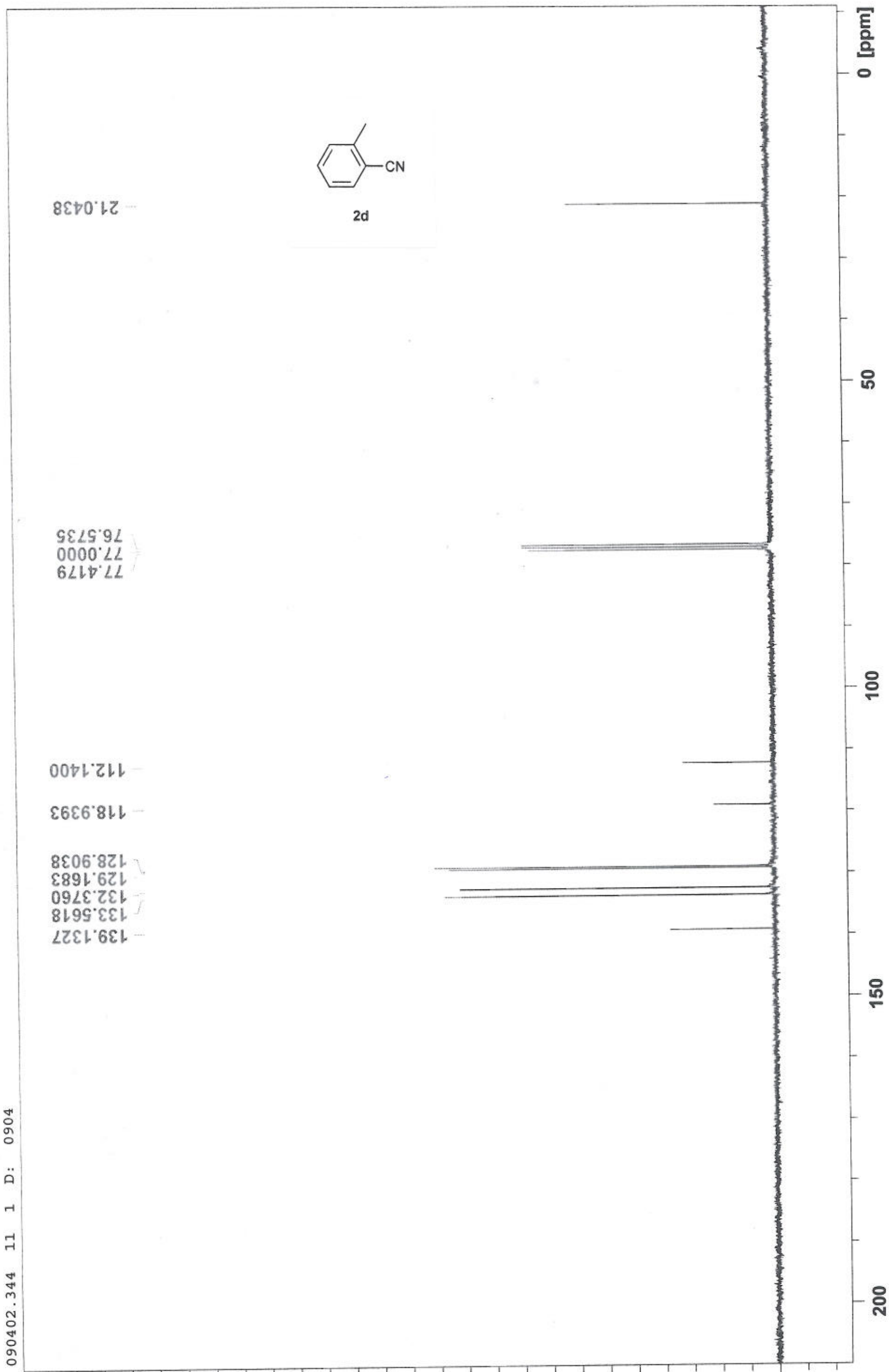
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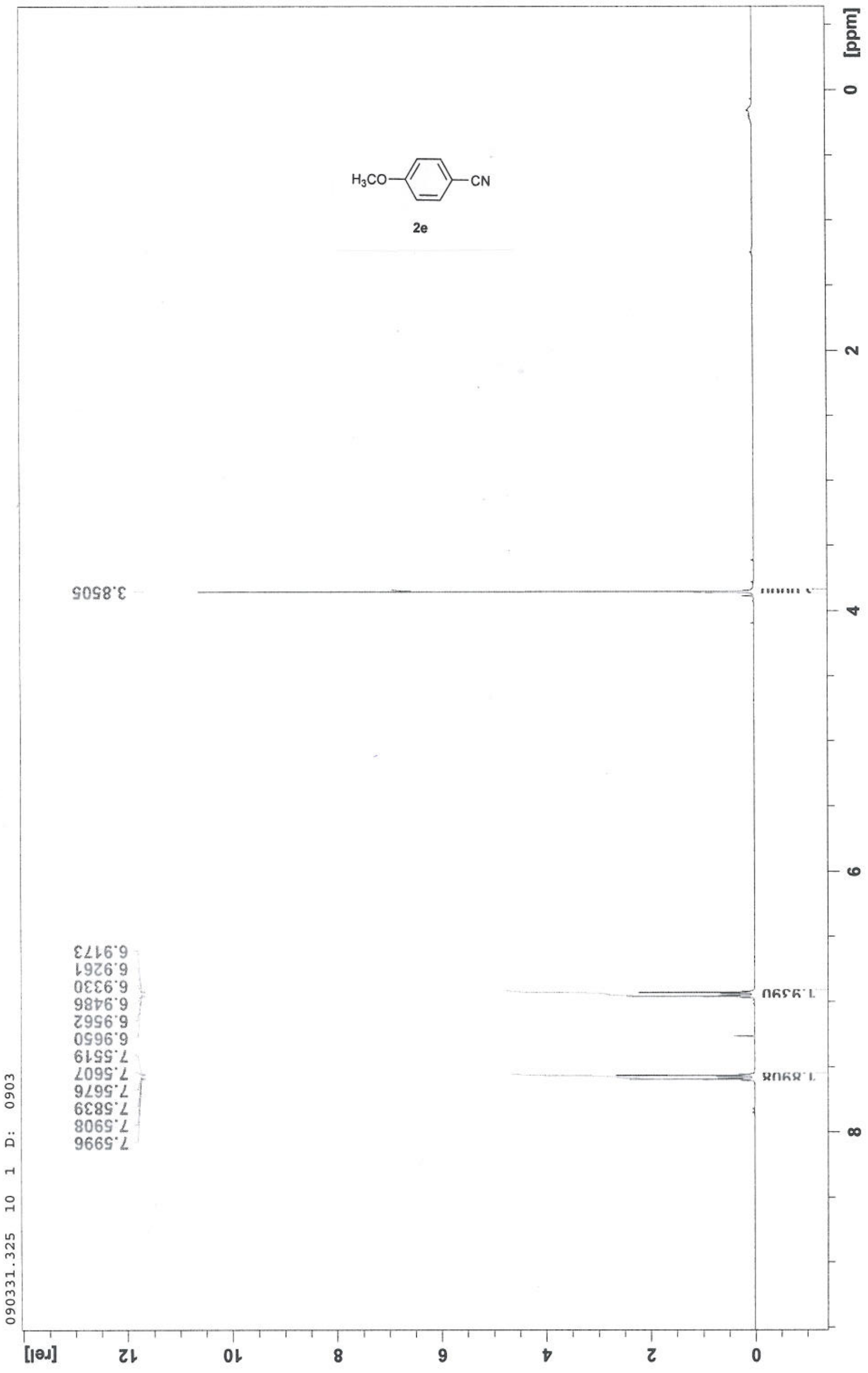
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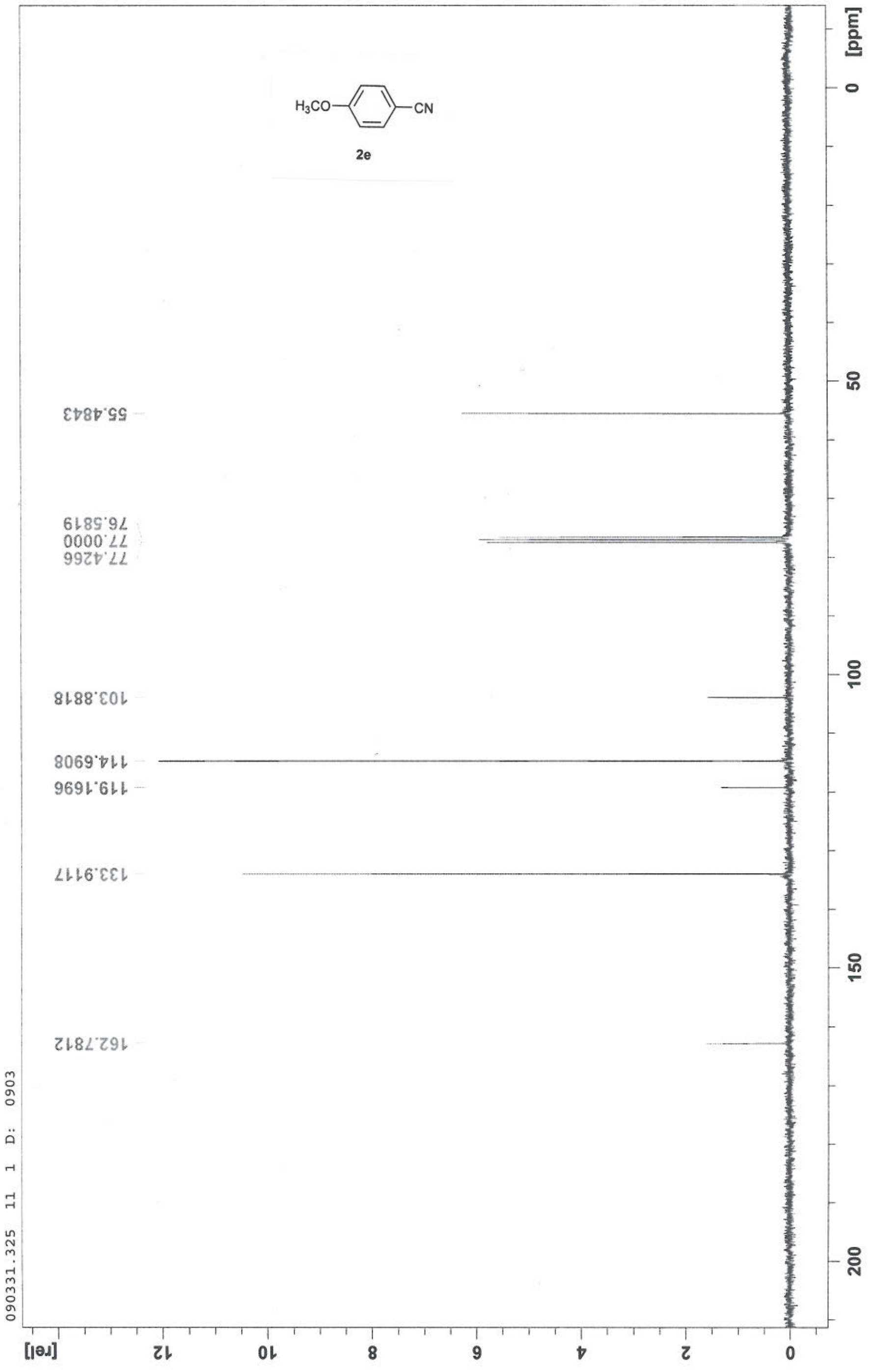
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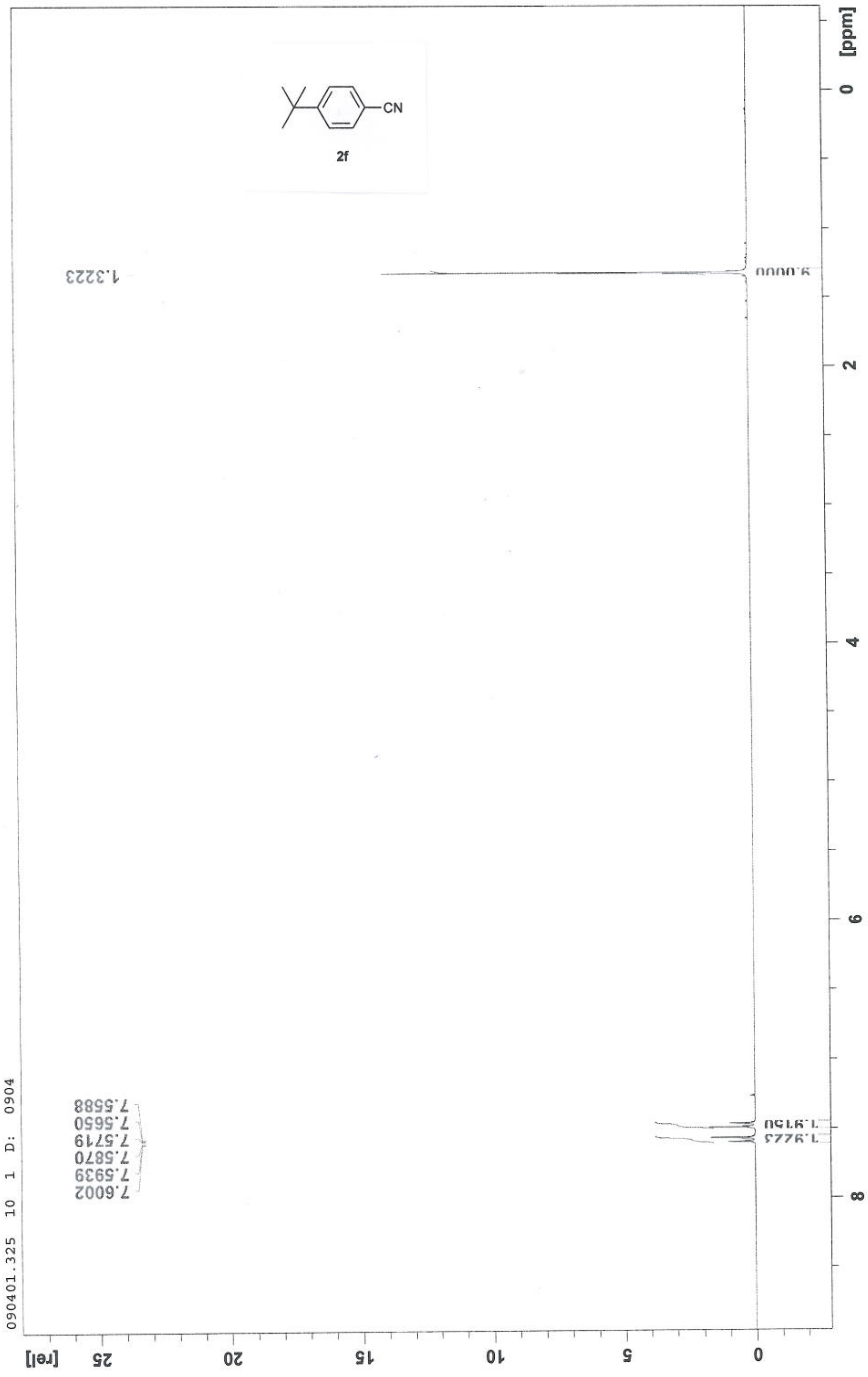
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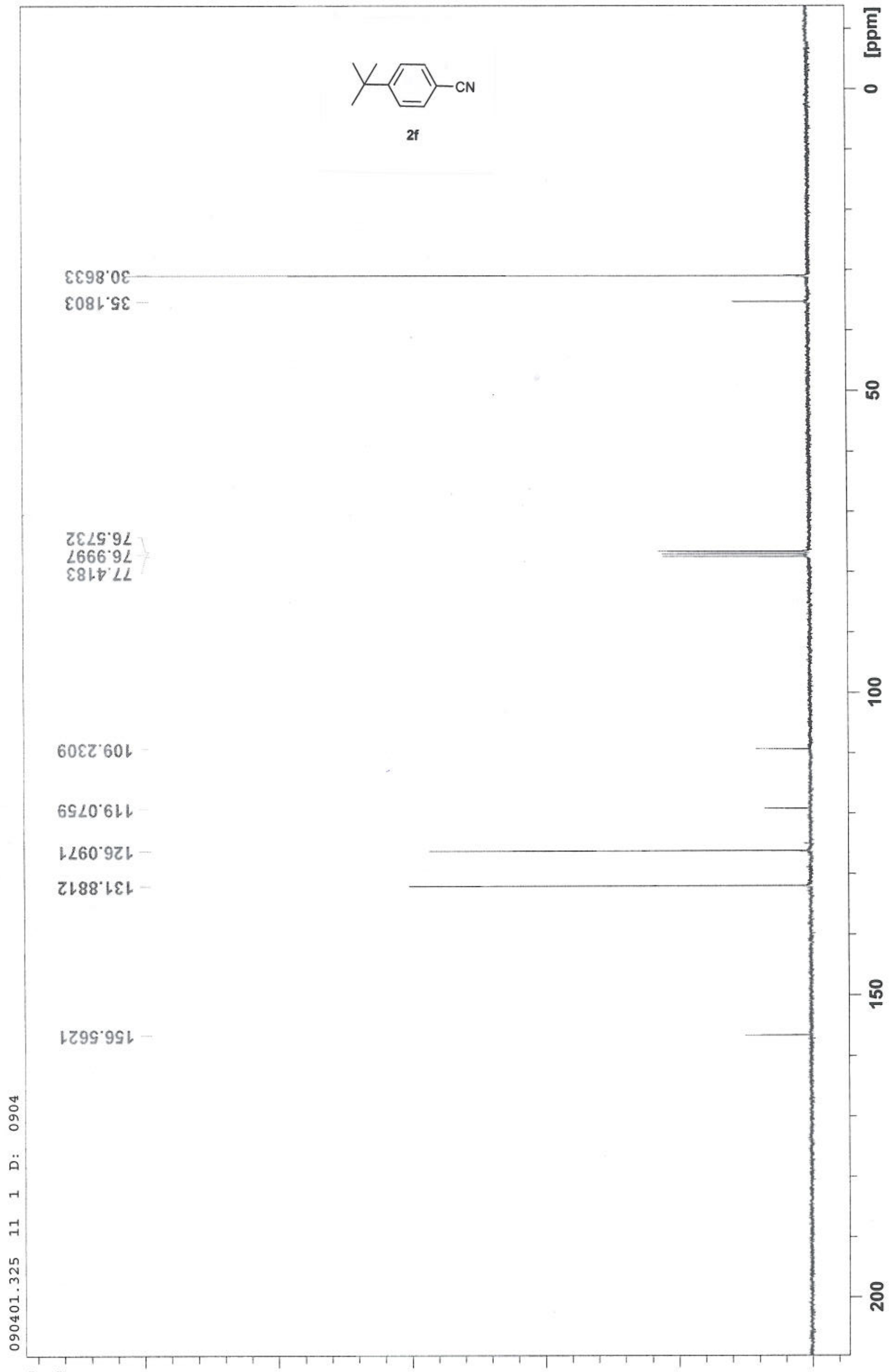
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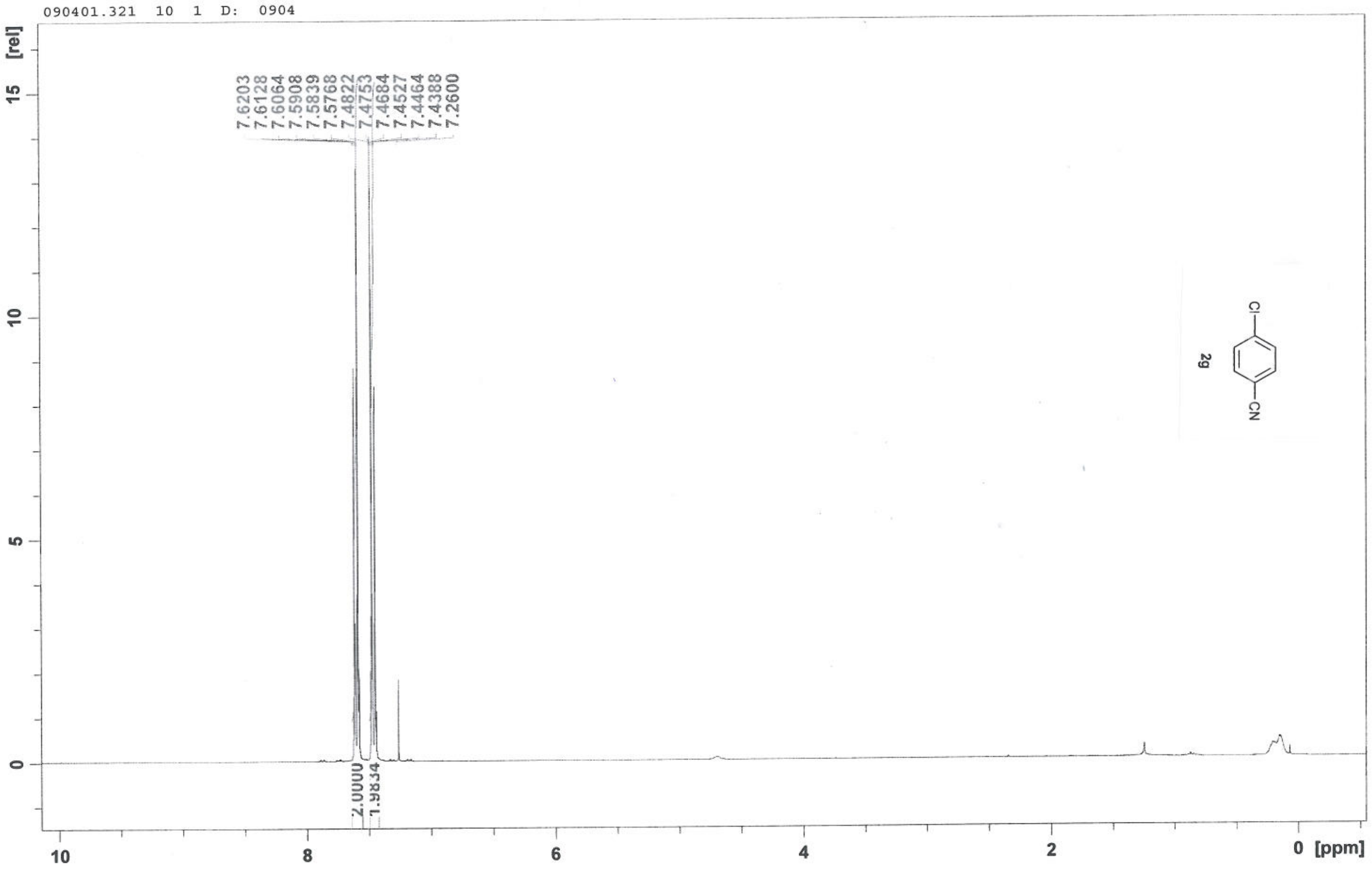

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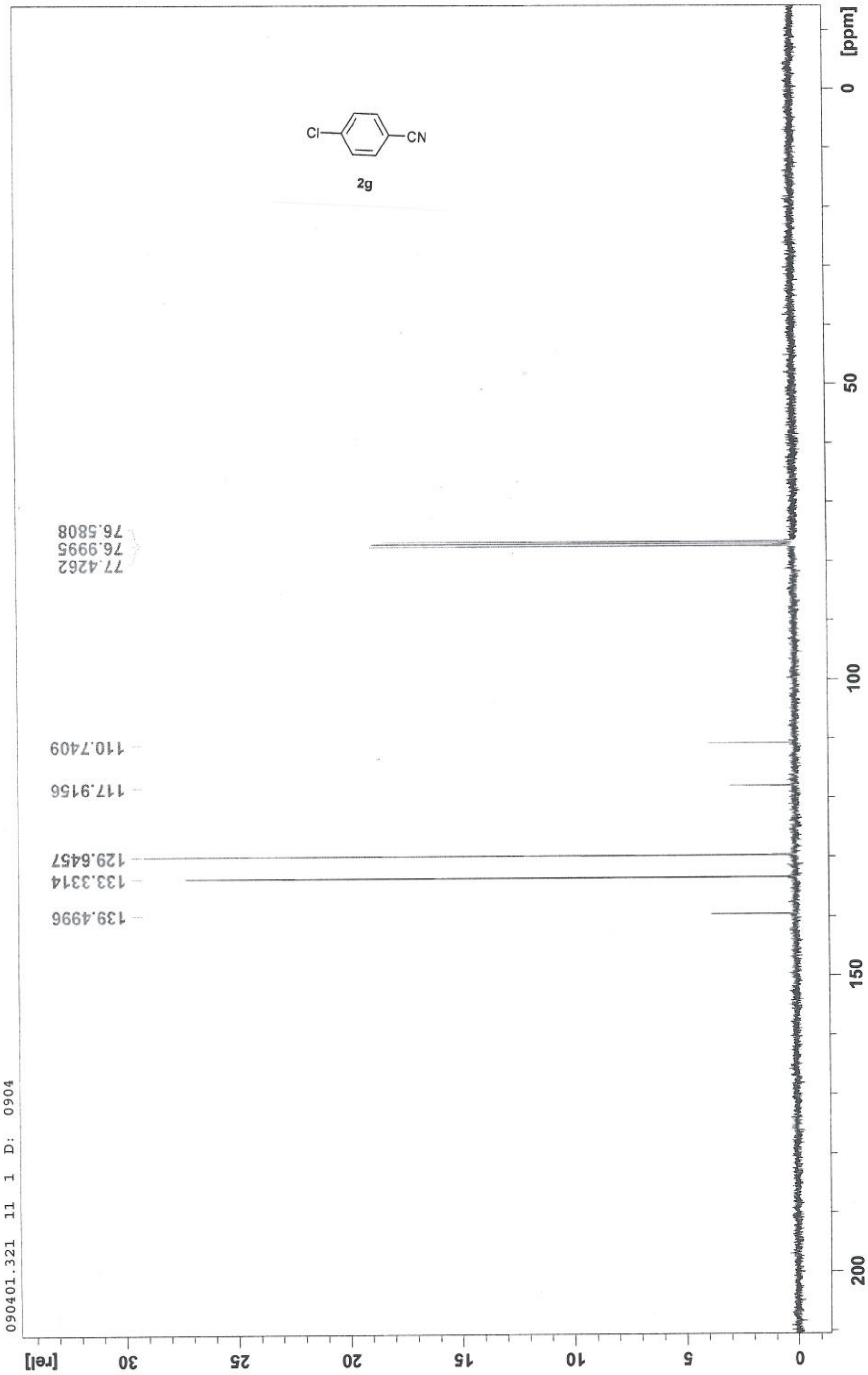
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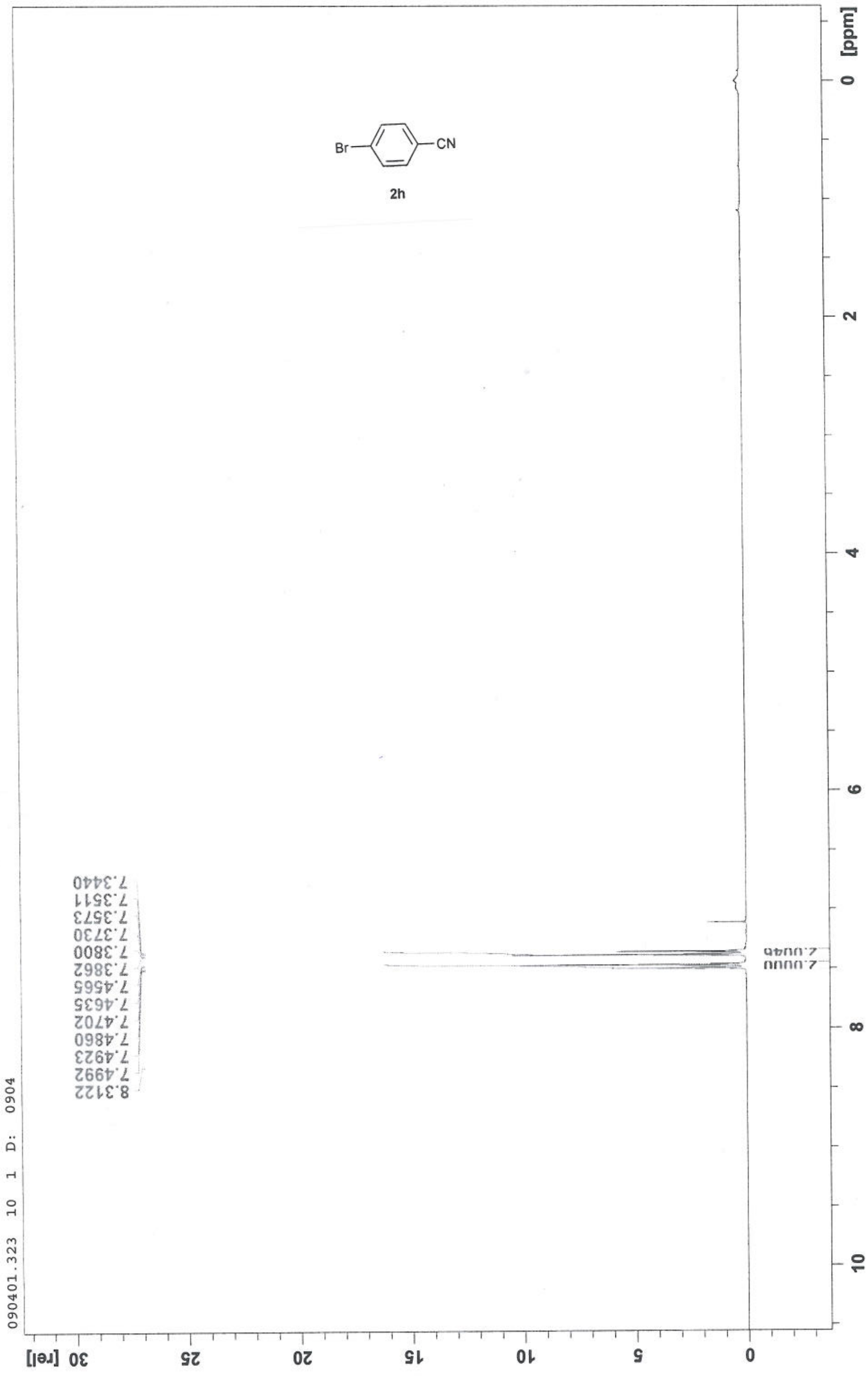
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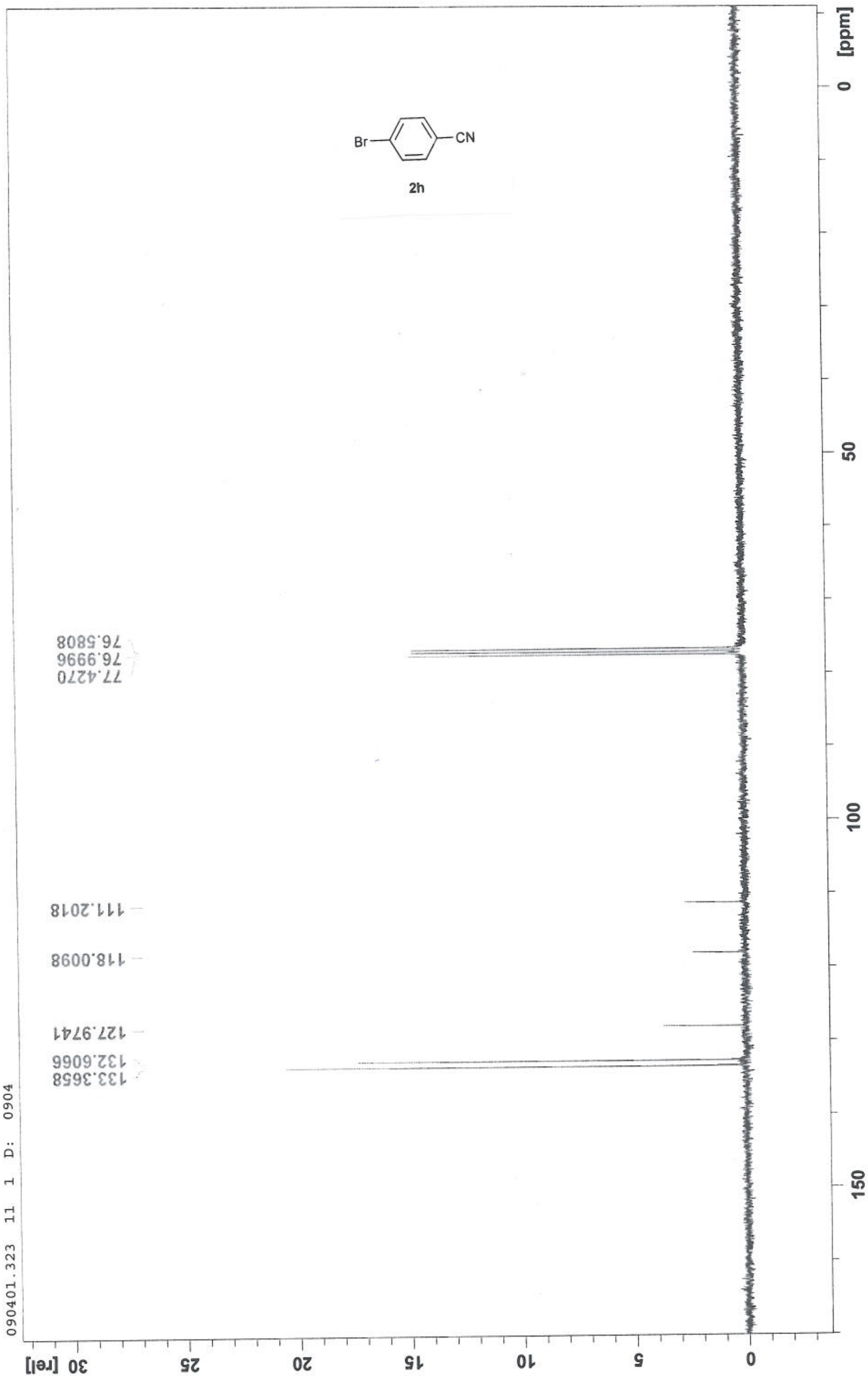
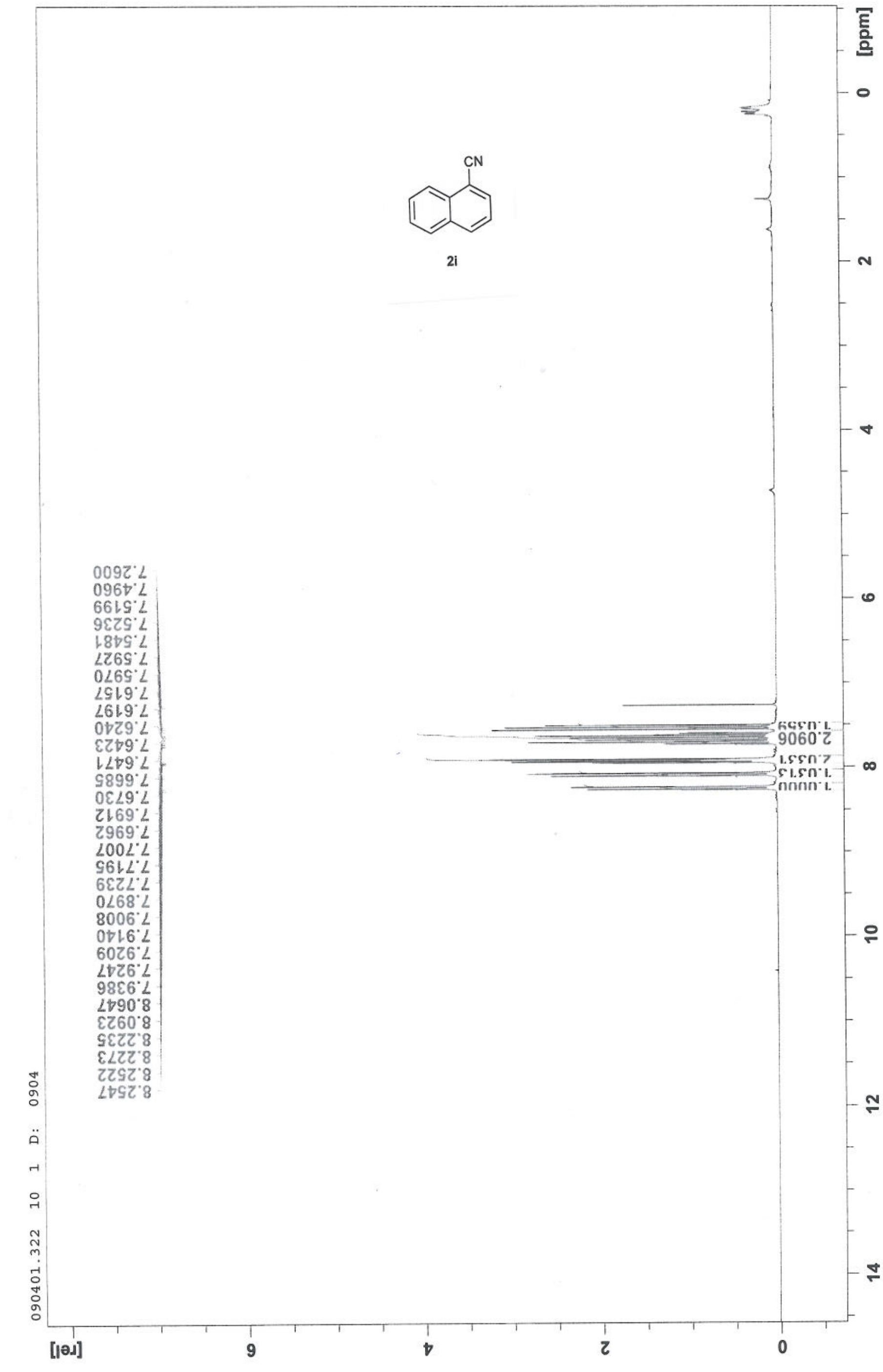
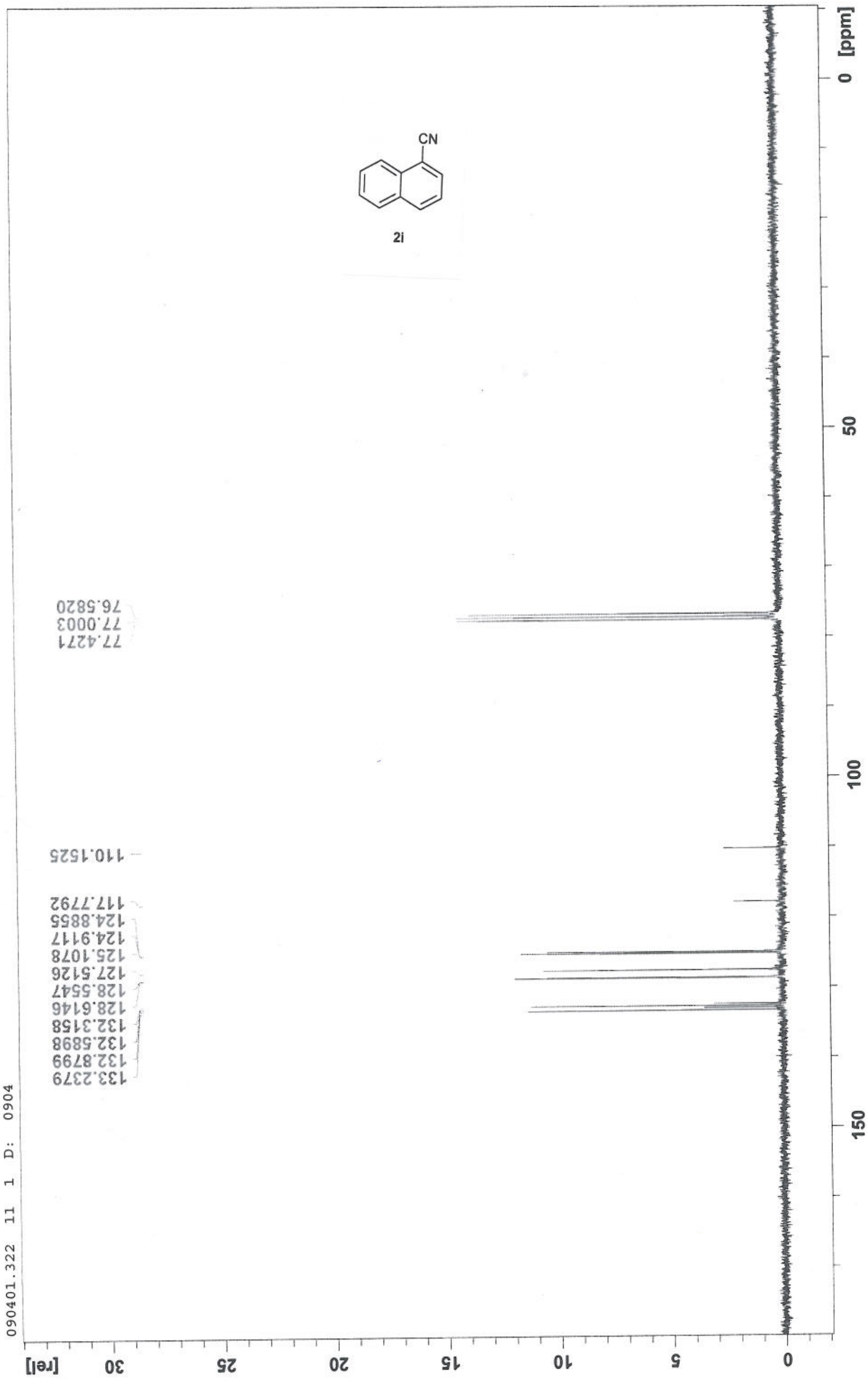
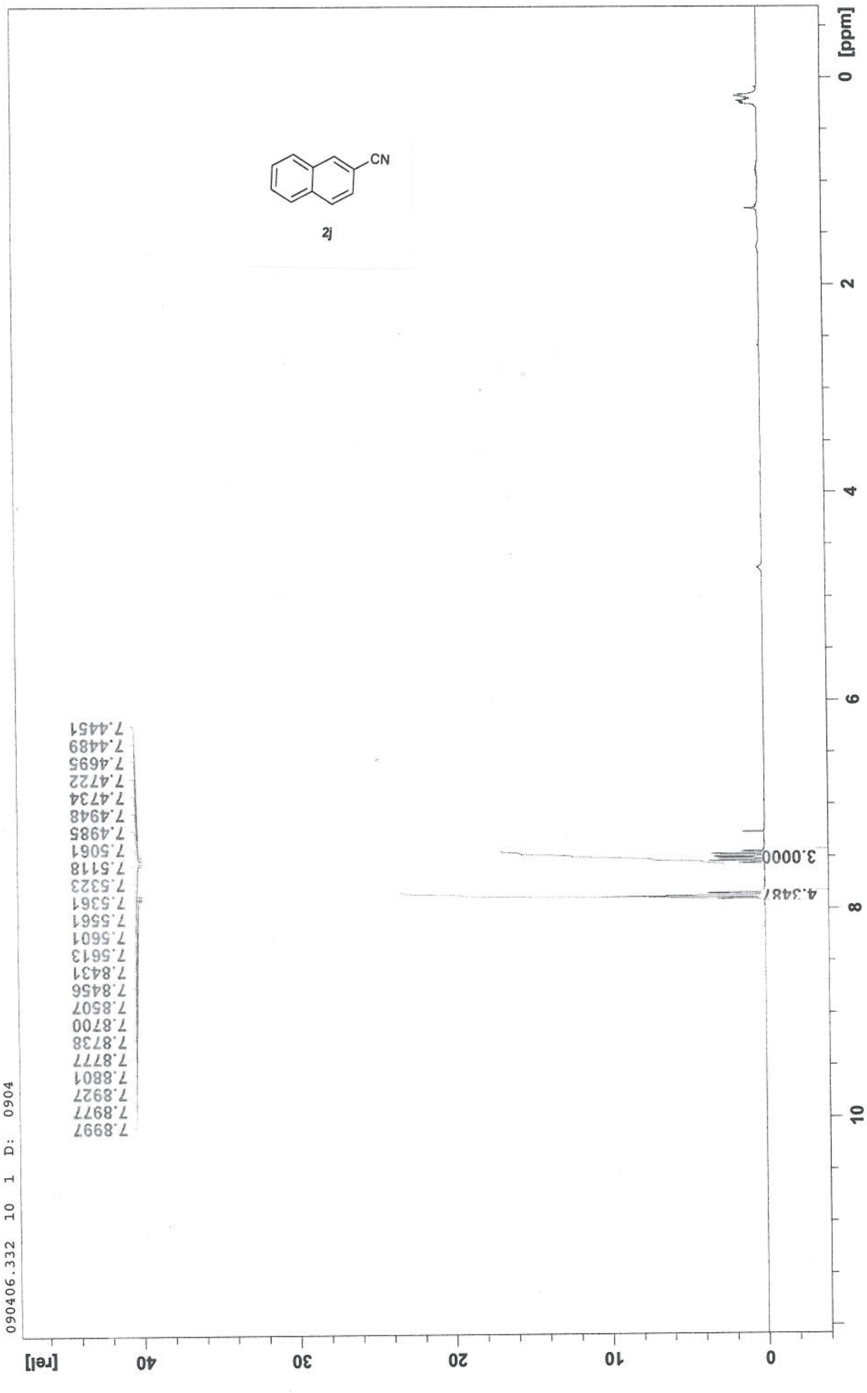
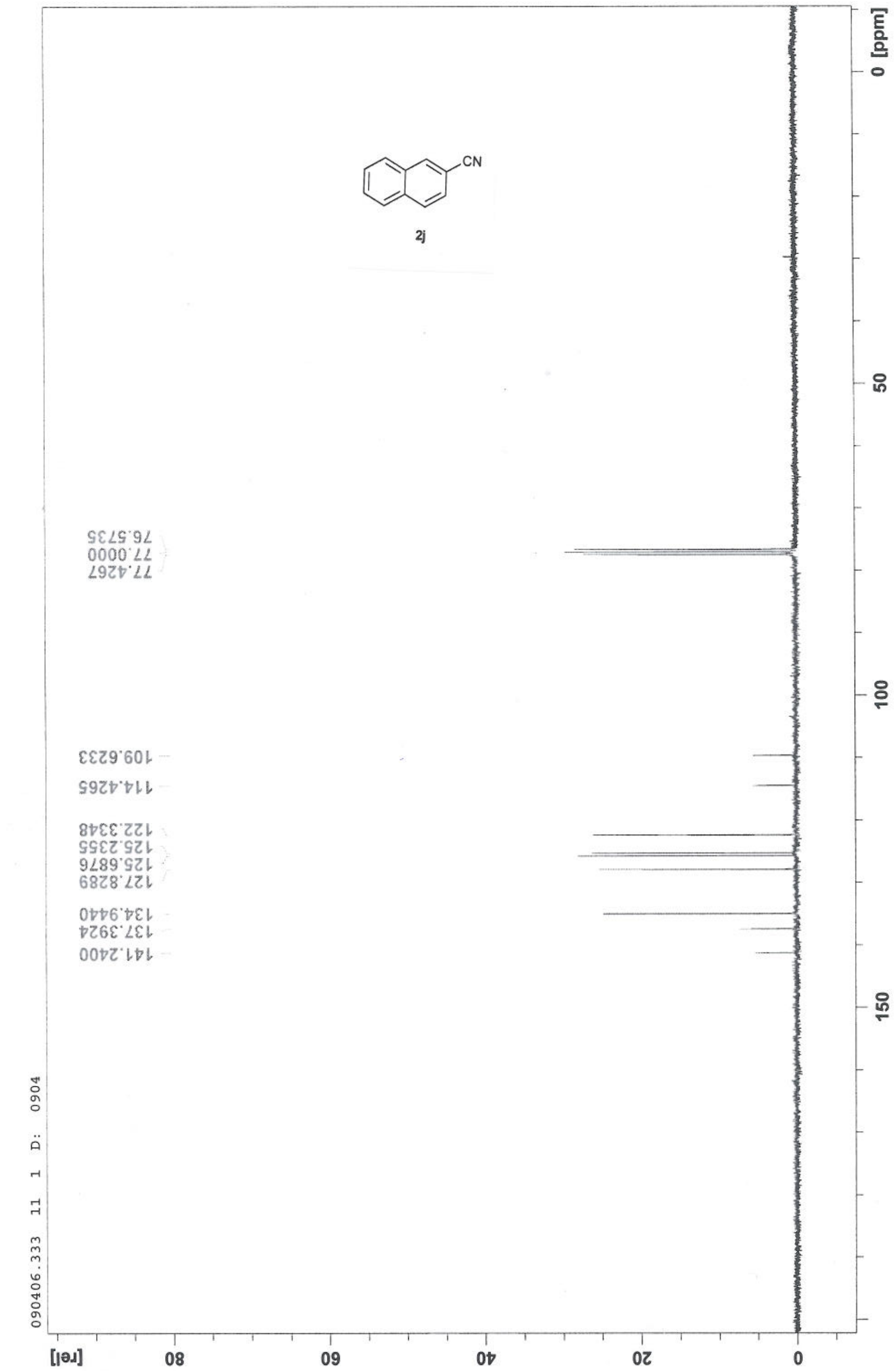
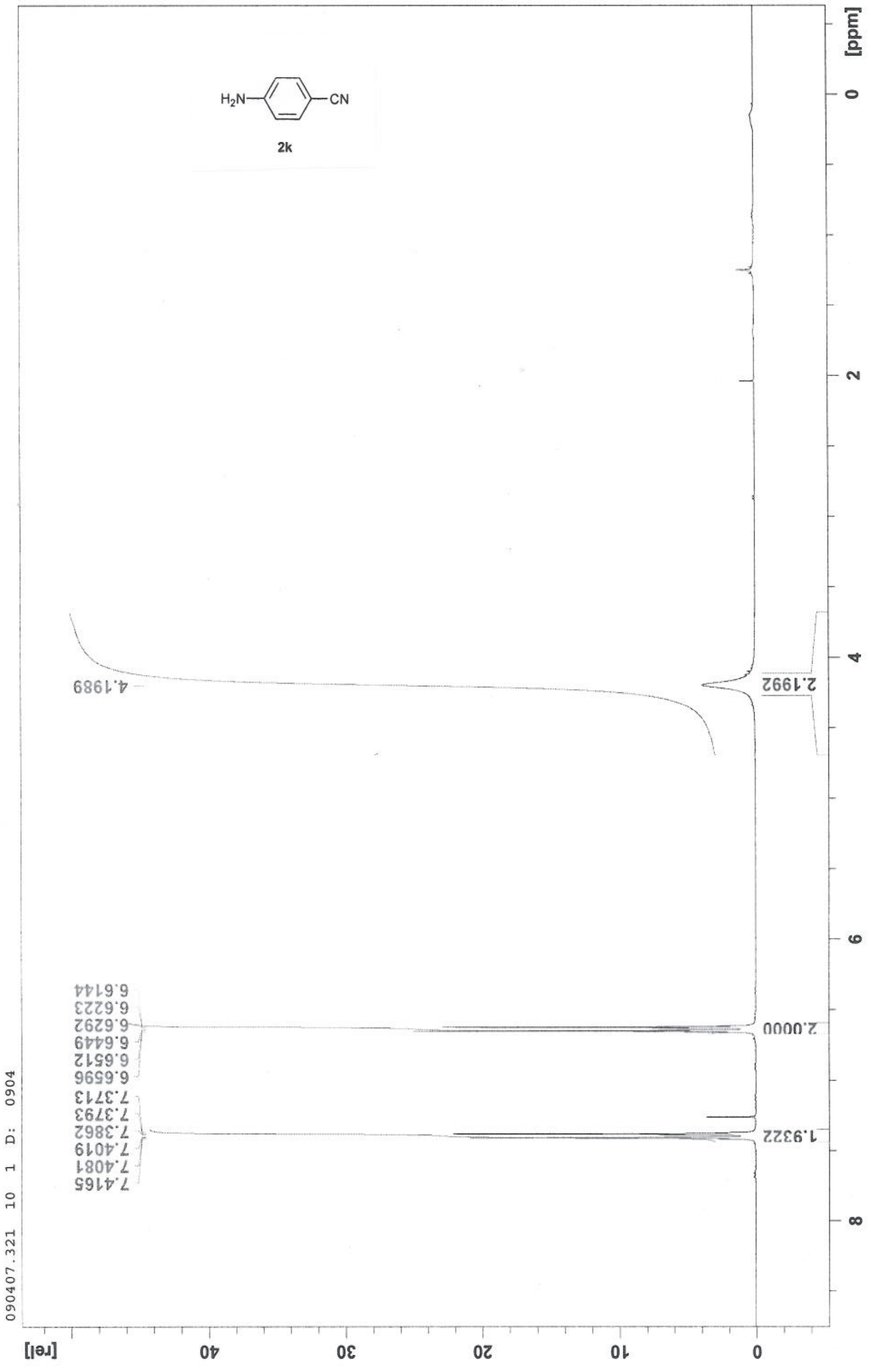

Br
CN
2h
76.5808
76.9996
77.4270
111.2018
118.0098
127.9741
132.6066
133.3658
090401.323 11 1 D: 0904
0
50
100
150
[ppm]
30 [rel]
25
20
15
10
5
0

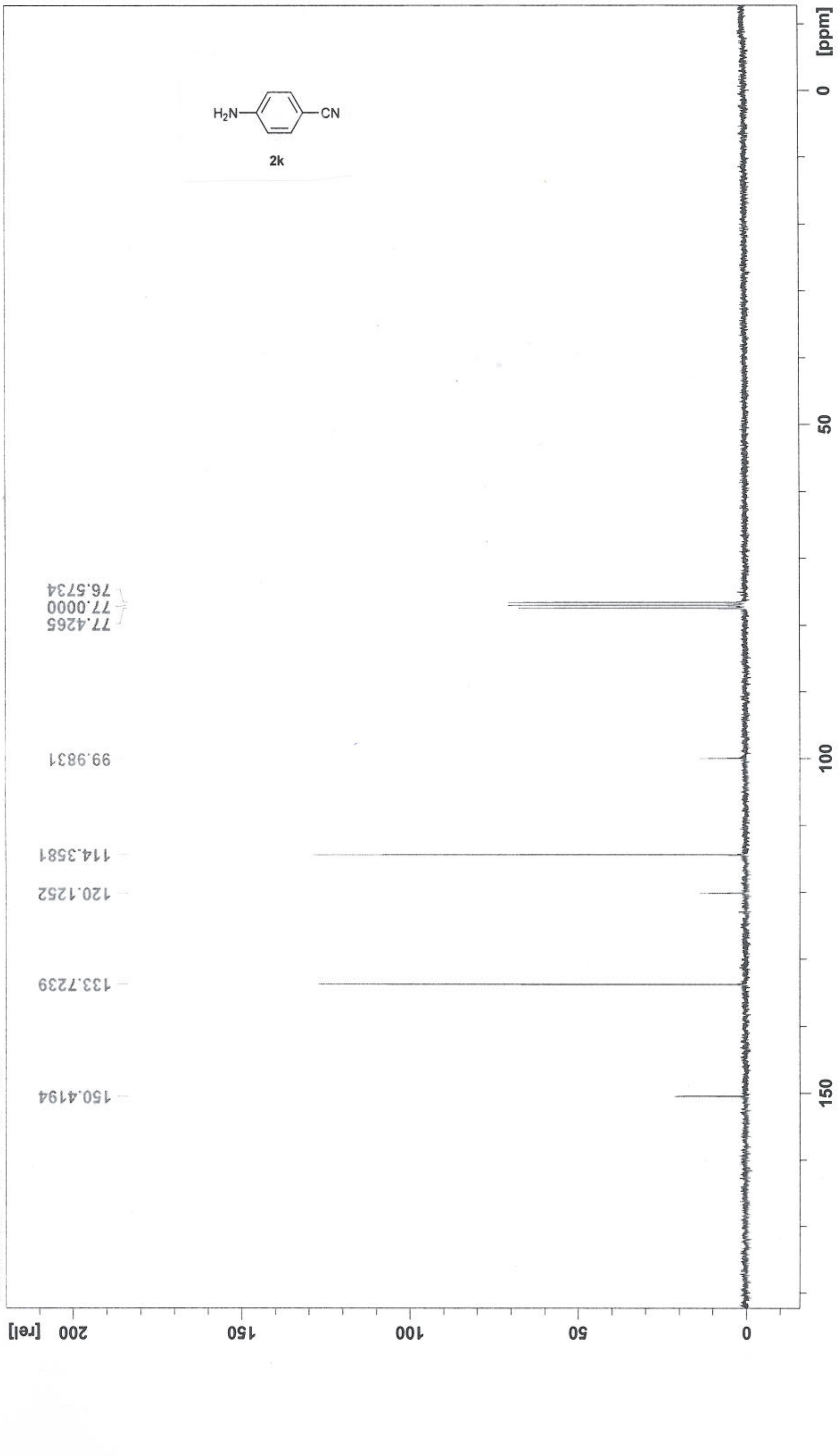

CN
2i
090401.322 10 1 D: 0904
8.2547
8.2522
8.2273
8.2235
8.0923
8.0647
7.9386
7.9247
7.9209
7.9140
7.9008
7.8970
7.7239
7.7195
7.7007
7.6962
7.6912
7.6730
7.6685
7.6471
7.6423
7.6240
7.6197
7.6157
7.5970
7.5927
7.5481
7.5236
7.5199
7.4960
7.2600
1.0559
2.0906
2.0531
1.0515
1.0000
[ppm]
0
2
4
6
8
10
12
14
[rel]
0
2
4
6

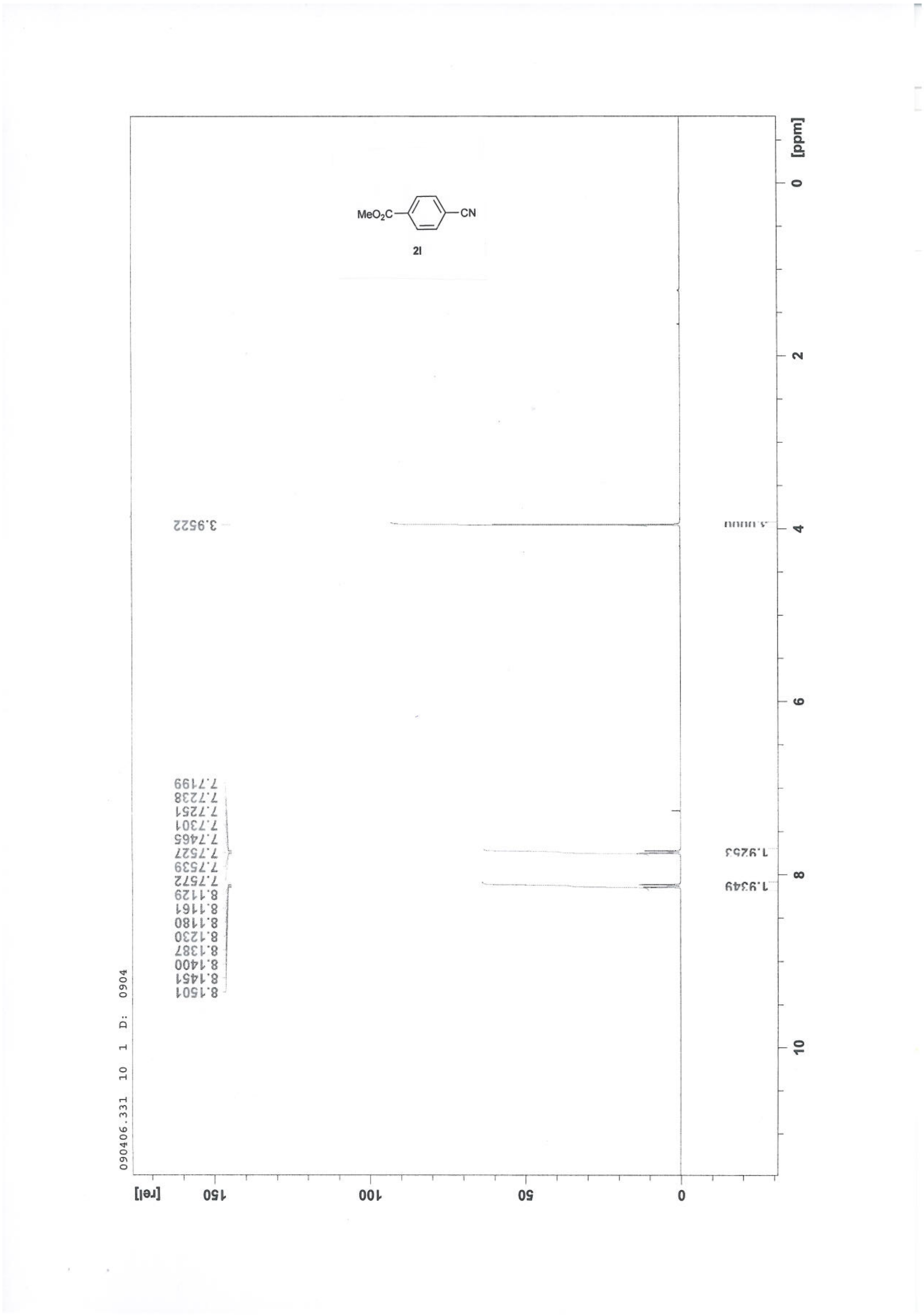

090401.322 11 1 D: 0904
CN
2i
133.2379
132.8799
132.5898
132.3158
128.6146
128.5547
127.5126
125.1078
124.9117
124.8855
117.7792
110.1525
77.4271
77.0003
76.5820
[ppm]
0
50
100
150
[rel]
30
25
20
15
10
5
0

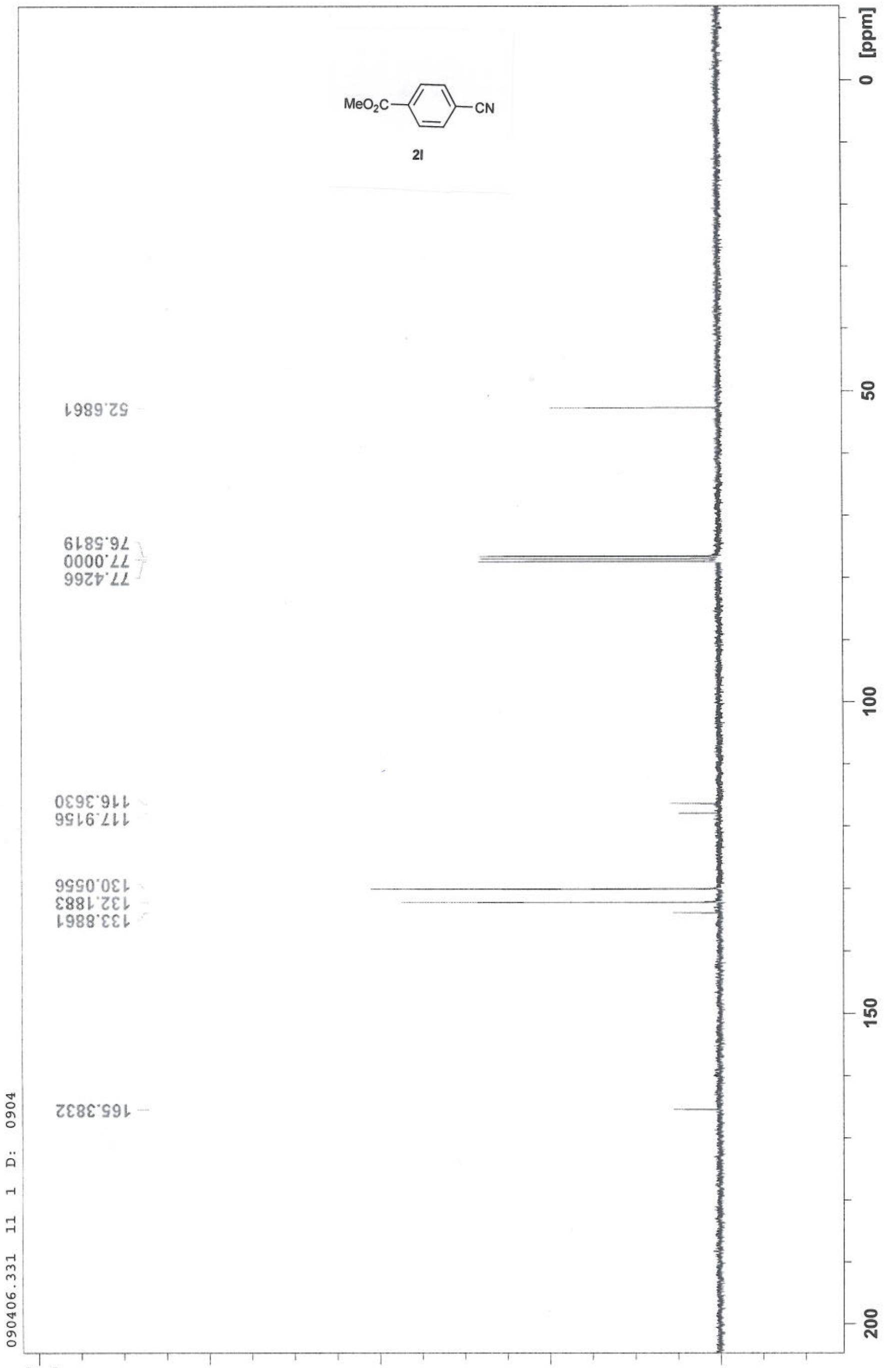

090406.332 10 1 D: 0904
7.8997
7.8977
7.8927
7.8801
7.8777
7.8738
7.8700
7.8507
7.8456
7.8431
7.5613
7.5601
7.5561
7.5361
7.5323
7.5118
7.5061
7.4985
7.4948
7.4734
7.4722
7.4695
7.4489
7.4451
CN
2j
3.0000
4.348
[ppm]
0
2
4
6
8
10
[rel]
40
30
20
10
0

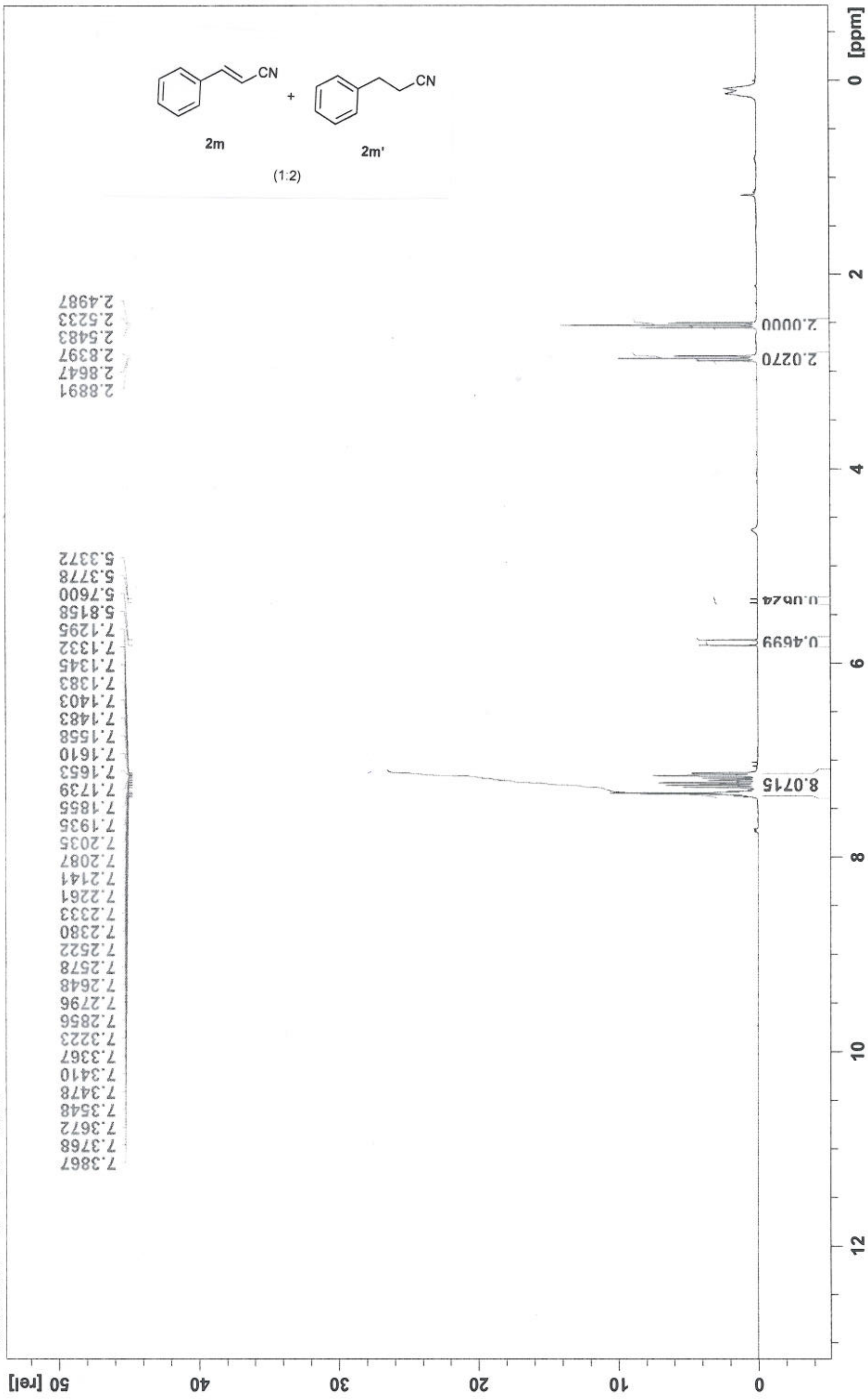

CN
2j
76.5735
77.0000
77.4267
109.6233
114.4265
122.3348
125.2355
125.6876
127.8289
134.9440
137.3924
141.2400
090406.333 11 1 D: 0904
0 [ppm]
50
100
150
[rel]
0
20
40
60
80

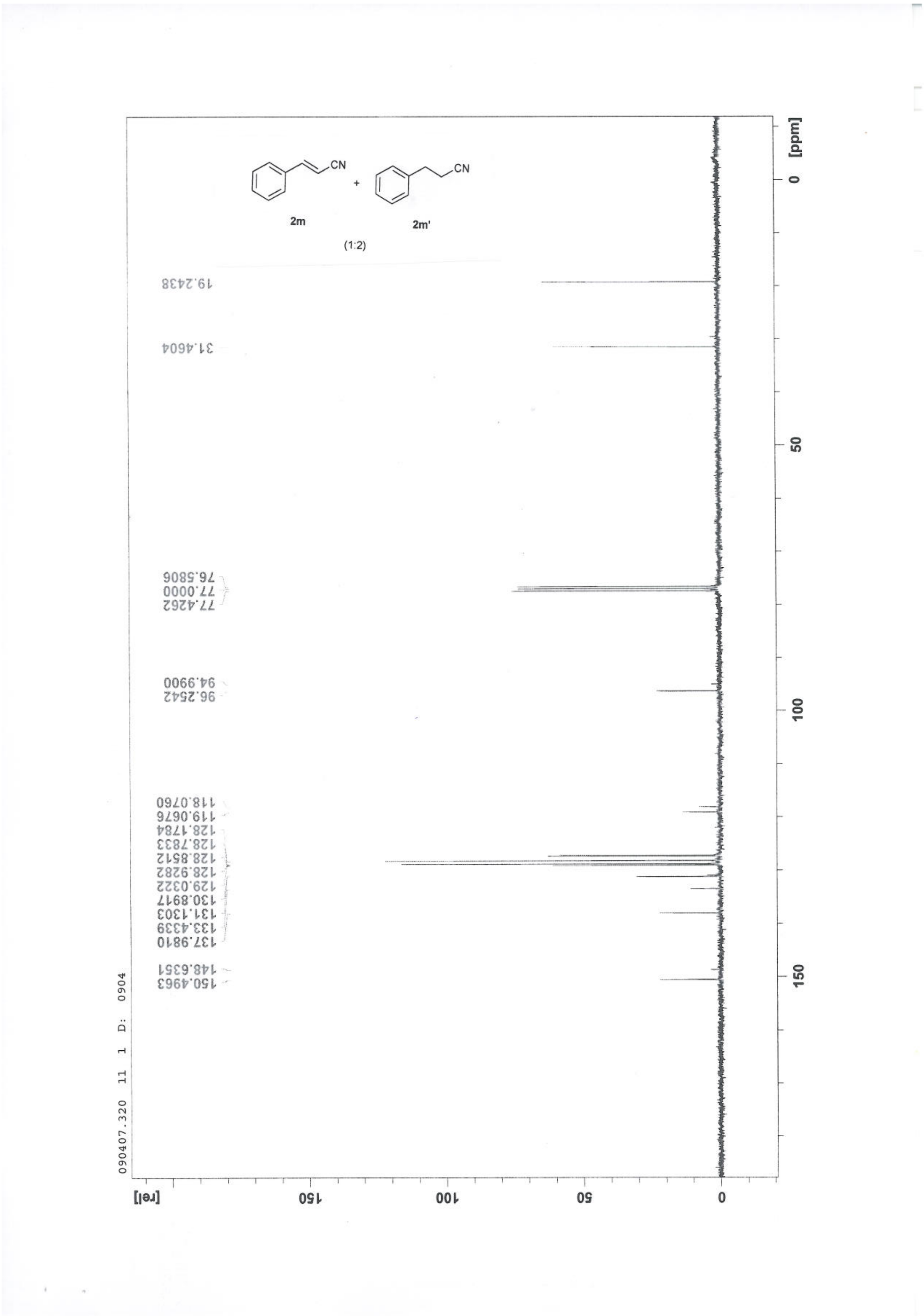

H2N
CN
2k
090407.321 10 1 D: 0904
4.1989
6.6144
6.6223
6.6292
6.6449
6.6512
6.6596
7.3713
7.3793
7.3862
7.4019
7.4081
7.4165
2.1992
2.0000
1.9322
[ppm]
0
2
4
6
8
[rel]
40
30
20
10
0

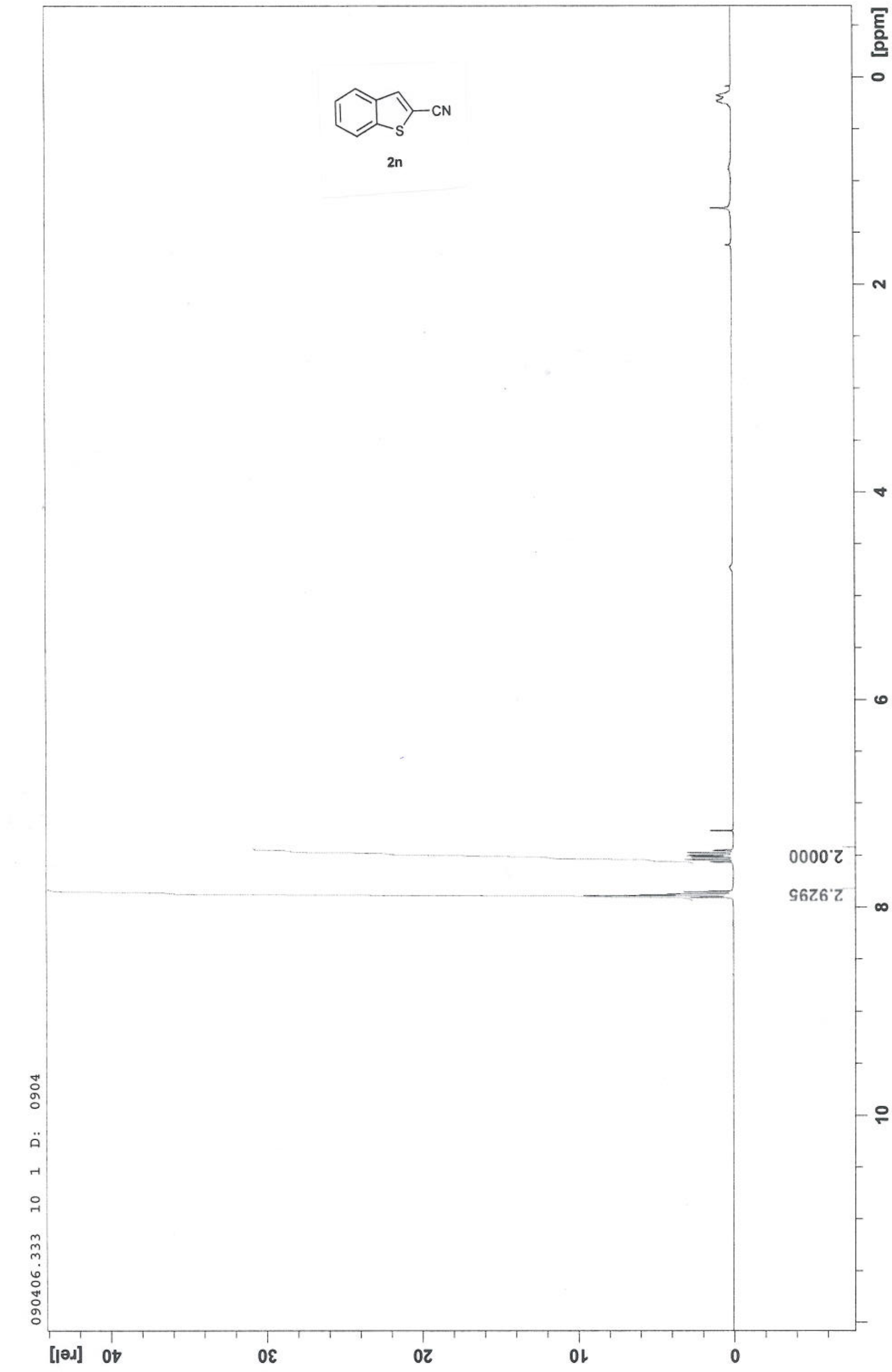

H2N
CN
2k
150.4194
133.7239
120.1252
114.3581
99.9831
77.4265
77.0000
76.5734
0
50
100
150
[ppm]
200
150
100
50
0
[rel]
090407.321 11 1 D: 0904

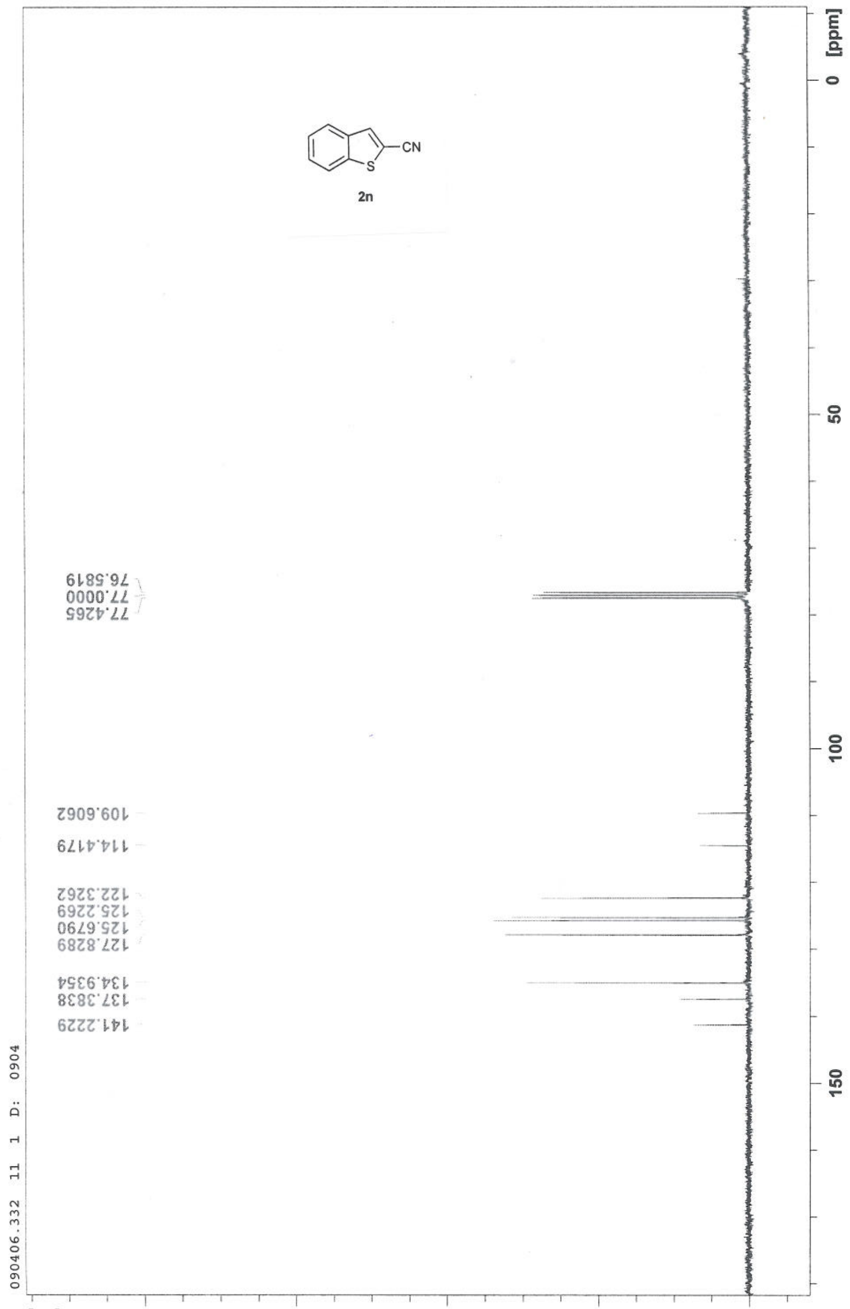

MeO$_2$C
CN
2l
3.9522
7.7199
7.7238
7.7251
7.7301
7.7465
7.7527
7.7539
7.7572
8.1129
8.1161
8.1180
8.1230
8.1387
8.1400
8.1451
8.1501
3.0000
1.9253
1.9349
[ppm]
0
2
4
6
8
10
[rel]
150
100
50
0
090406.331 10 1 D: 0904

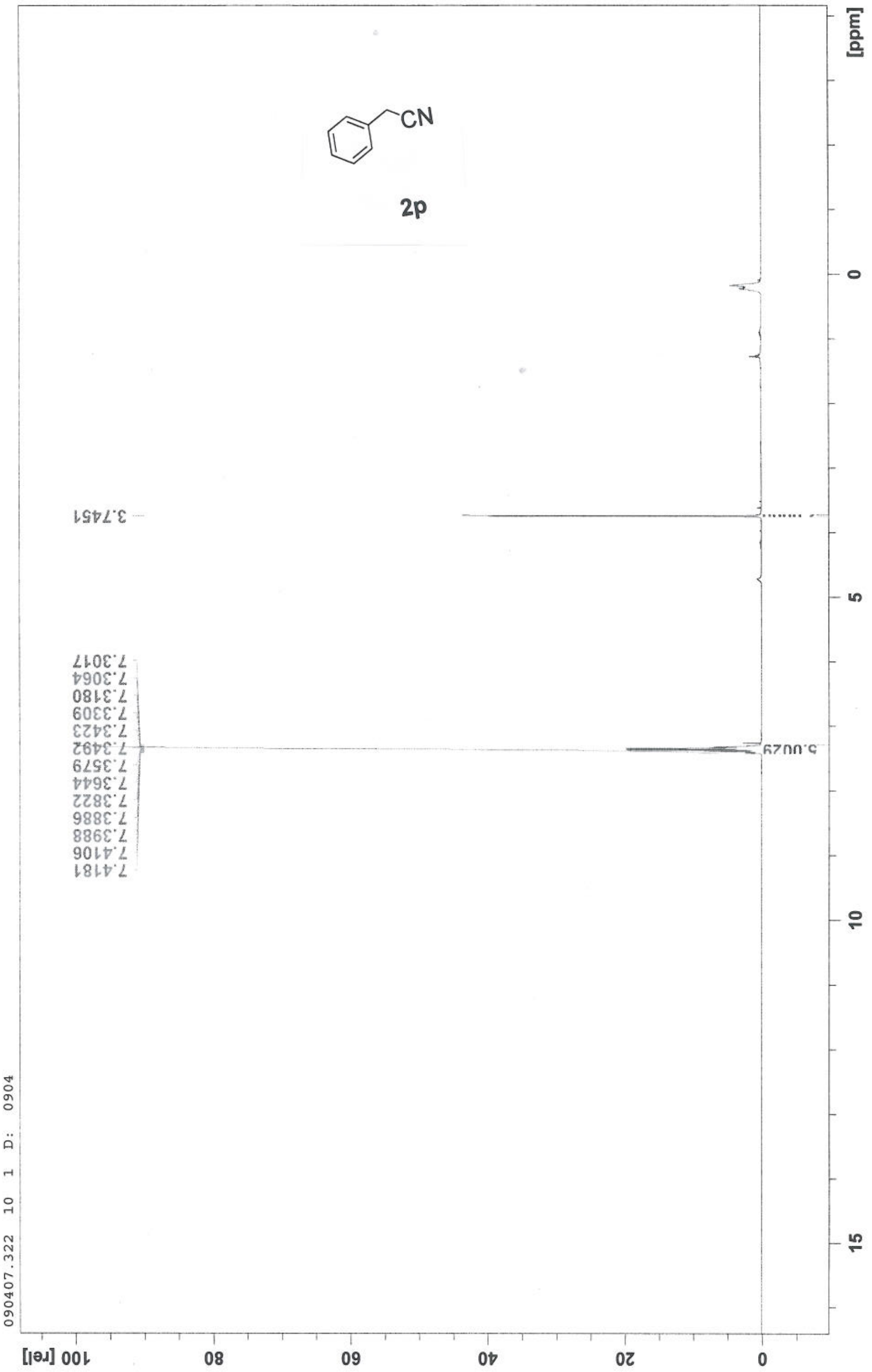

MeO2C
CN
2l
165.3832
133.8861
132.1883
130.0556
117.9156
116.3630
77.4266
77.0000
76.5819
52.6861
090406.331 11 1 1 D: 0904
[ppm]
0
50
100
150
200
[rel]
0
20
40
60

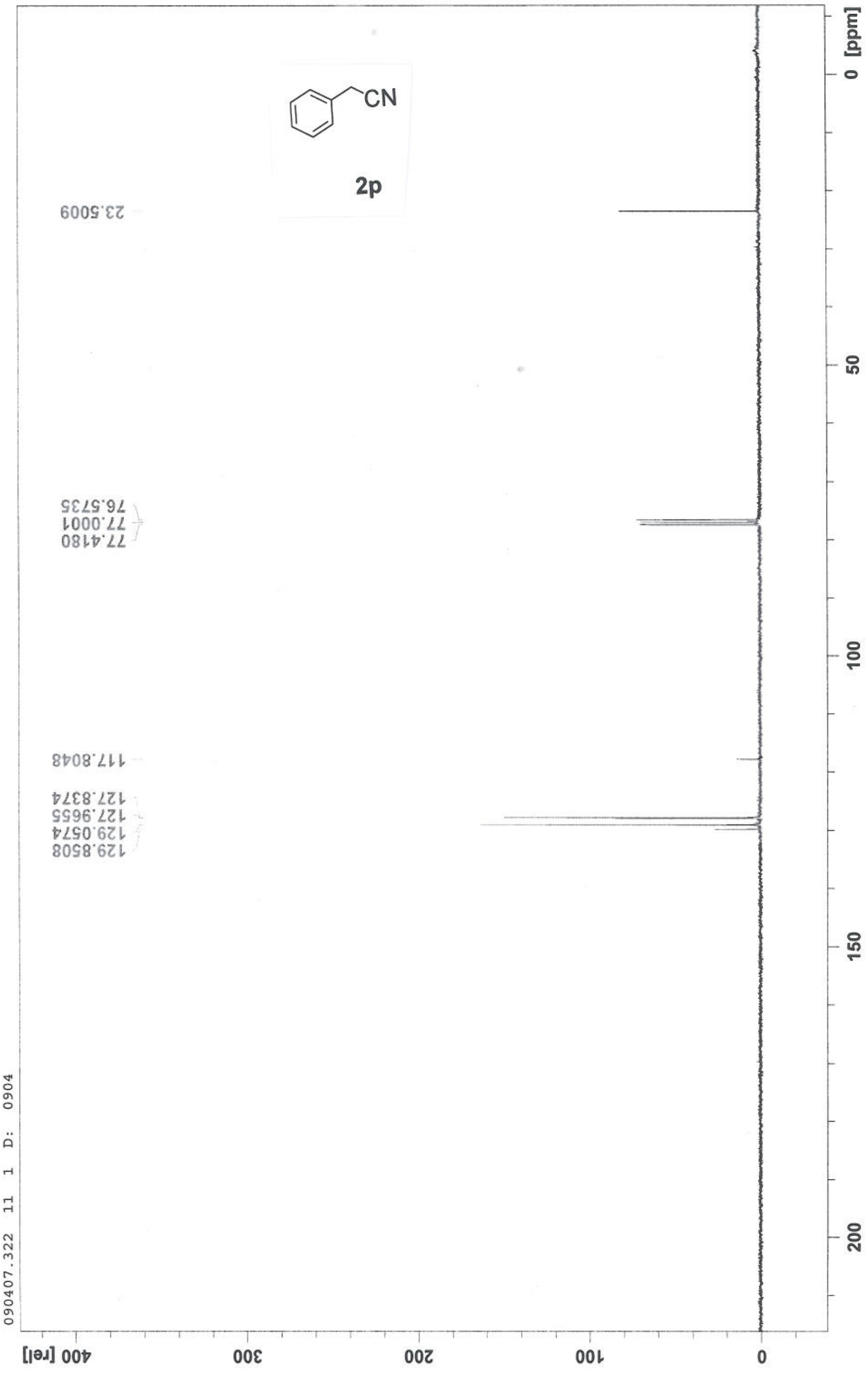

CN
+
CN
2m
2m'
(1:2)
2.4987
2.5233
2.5483
2.8397
2.8647
2.8891
5.3372
5.3778
5.7600
5.8158
7.1295
7.1332
7.1345
7.1383
7.1403
7.1483
7.1558
7.1610
7.1653
7.1739
7.1855
7.1935
7.2035
7.2087
7.2141
7.2261
7.2333
7.2380
7.2522
7.2578
7.2648
7.2796
7.2856
7.3223
7.3367
7.3410
7.3478
7.3548
7.3672
7.3768
7.3867
2.0000
2.0270
0.0624
0.4699
8.0715
090407.320 10 1 D: 0904
[ppm]
0
2
4
6
8
10
12
50 [rel]
40
30
20
10
0

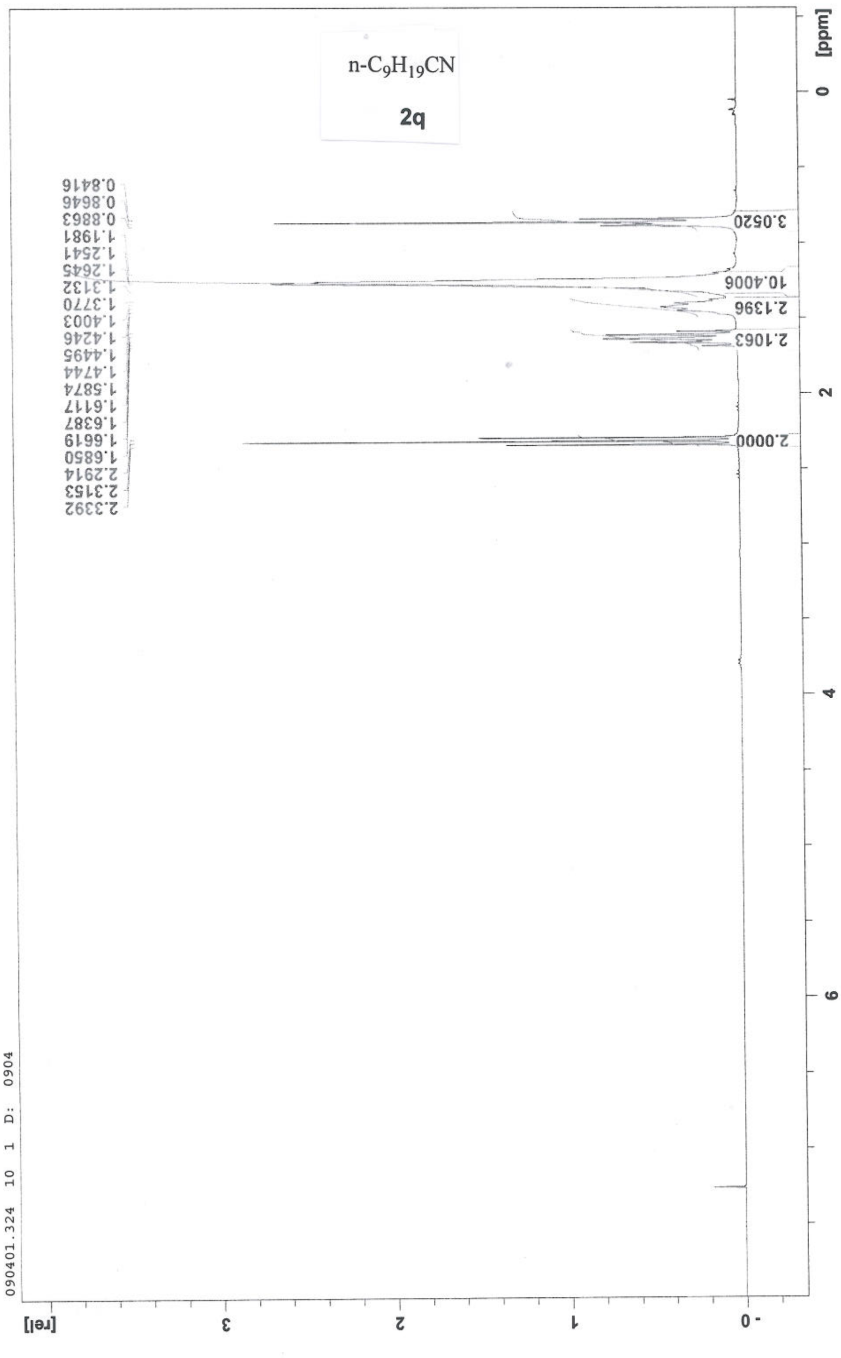

CN
+
CN
2m
2m'
(1:2)
19.2438
31.4604
76.5806
77.0000
77.4262
94.9900
96.2542
118.0760
119.0676
128.1784
128.7833
128.8512
128.9282
129.0322
130.8917
131.1303
133.4339
137.9810
148.6351
150.4963
090407.320 11 1 D: 0904
0
50
100
150
[ppm]
[rel]
0
50
100
150

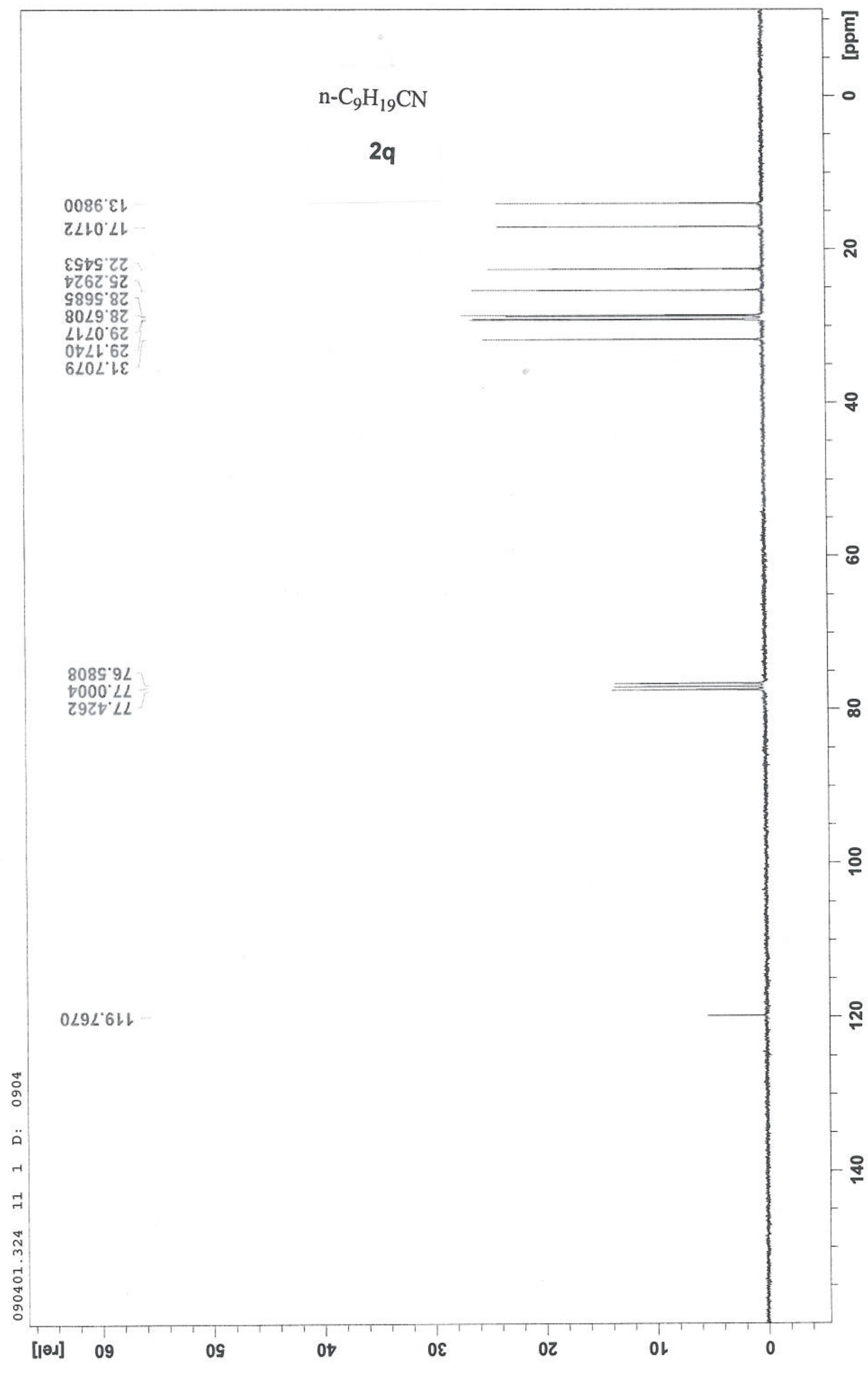

CN
S
2n
[ppm]
0
2
4
6
8
10
2.0000
2.9295
090406.333 10 1 D: 0904
[rel]
40
30
20
10
0

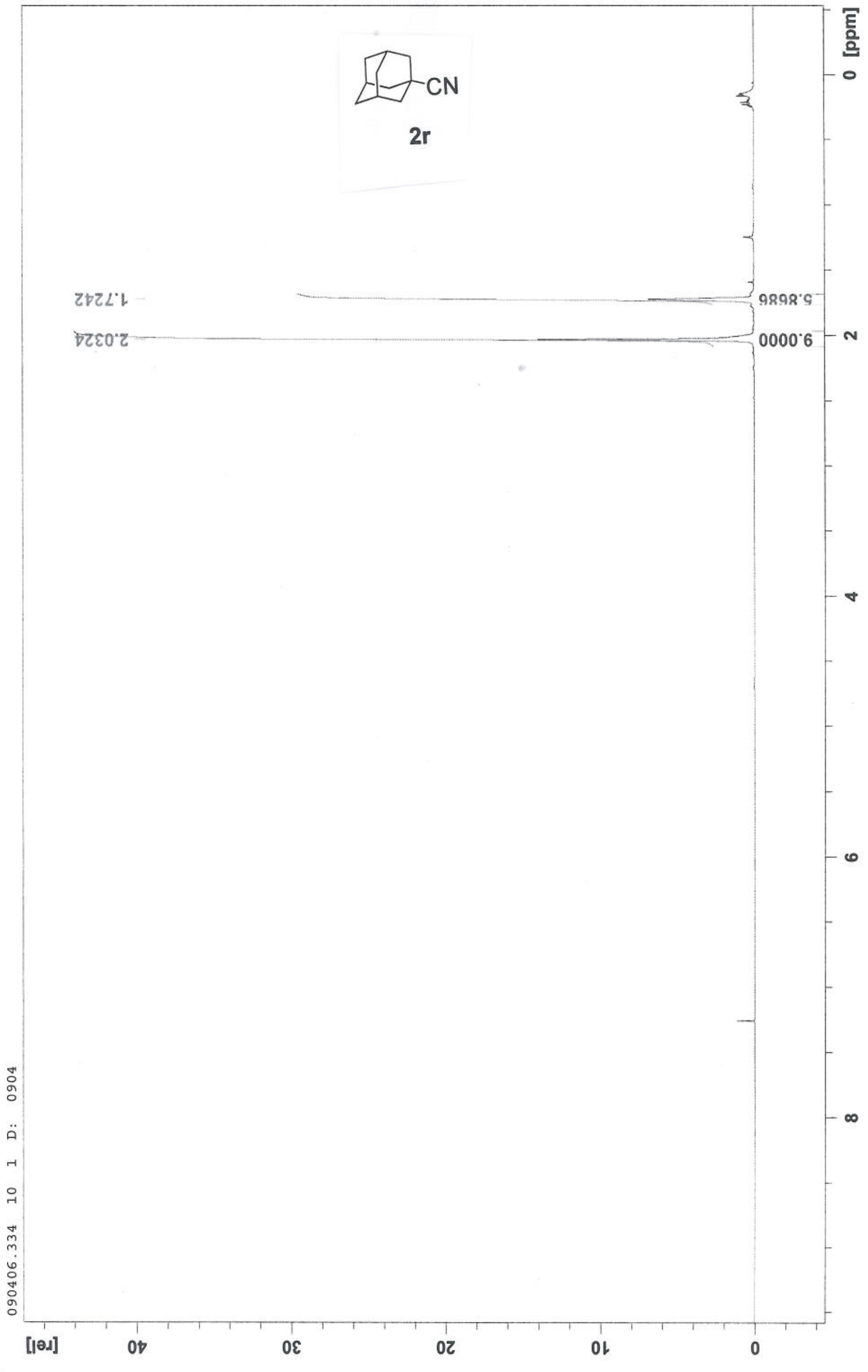

CN
S
2n
76.5819
77.0000
77.4265
109.6062
114.4179
122.3262
125.2269
125.6790
127.8289
134.9354
137.3838
141.2229
090406.332 11 1 D: 0904
0
50
100
150
[ppm]
[rel]
80
60
40
20
0


CN
2p
3.7451
7.3017
7.3064
7.3180
7.3309
7.3423
7.3492
7.3579
7.3644
7.3822
7.3886
7.3988
7.4106
7.4181
5.0029
090407.322 10 1 D: 0904
[ppm]
0
5
10
15
100 [rel]
80
60
40
20
0

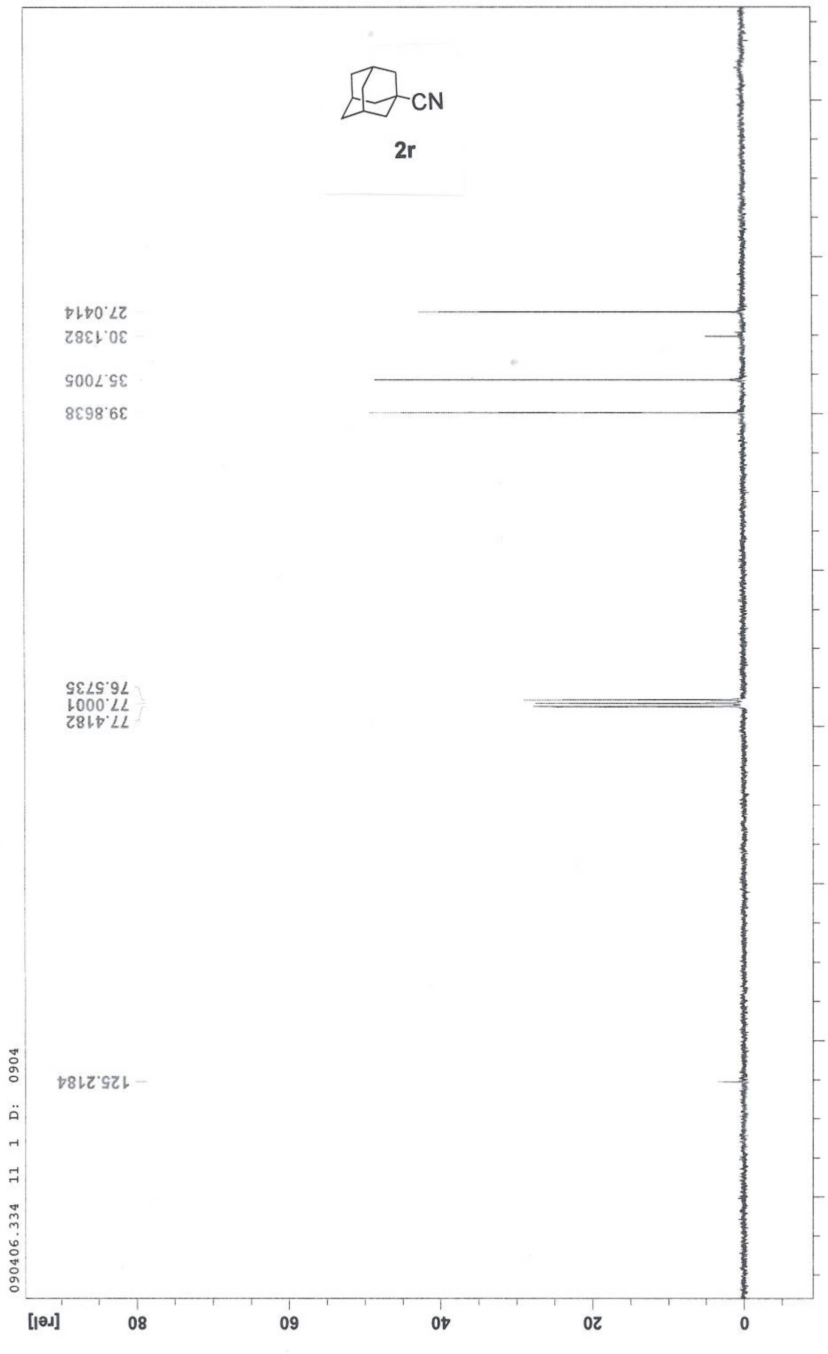

CN
2p
23.5009
76.5735
77.0001
77.4180
117.8048
127.8374
127.9655
129.0574
129.8508
090407.322 11 1 D: 0904
0 [ppm]
50
100
150
200
400 [rel]
300
200
100
0


n-$C_9H_{19}CN$
2q
0.8416
0.8646
0.8883
1.1981
1.2541
1.2645
1.3132
1.3770
1.4003
1.4246
1.4495
1.4744
1.5874
1.6117
1.6387
1.6619
1.6850
2.2914
2.3153
2.3392
3.0520
10.4006
2.1396
2.1063
2.0000
[ppm]
0
2
4
6
[rel]
0
1
2
3
090401.324 10 1 D: 0904


n-$C_9H_{19}CN$
2q
13.9800
17.0172
22.5453
25.2924
28.5685
28.6708
29.0717
29.1740
31.7079
76.5808
77.0004
77.4262
119.7670
090401.324 11 1 D: 0904
[ppm]
0
20
40
60
80
100
120
140
[rel]
60
50
40
30
20
10
0



CN
2r
1.7242
2.0324
5.8686
9.0000
090406.334 10 1 D: 0904
0
2
4
6
8
[ppm]
0
10
20
30
40
[rel]


CN
2r
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30.1382
35.7005
39.8638
76.5735
77.0001
77.4182
125.2184
090406.334 11 1 D: 0904
[ppm]
0
20
40
60
80
100
120
140
[rel]
80
60
40
20
0