

Supporting Information

A Highly Efficient, Ligand-Free and Recyclable SBA-15 Supported Cu₂O Catalyzed Cyanation of Aryl Iodides with Potassium Hexacyanoferrate (II)

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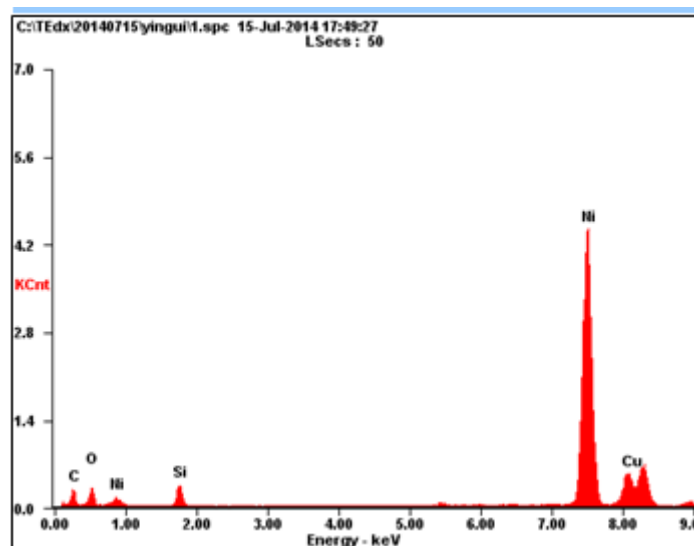


Fig. S1 TEM-EDS pattern of Cu₂O/SBA-15

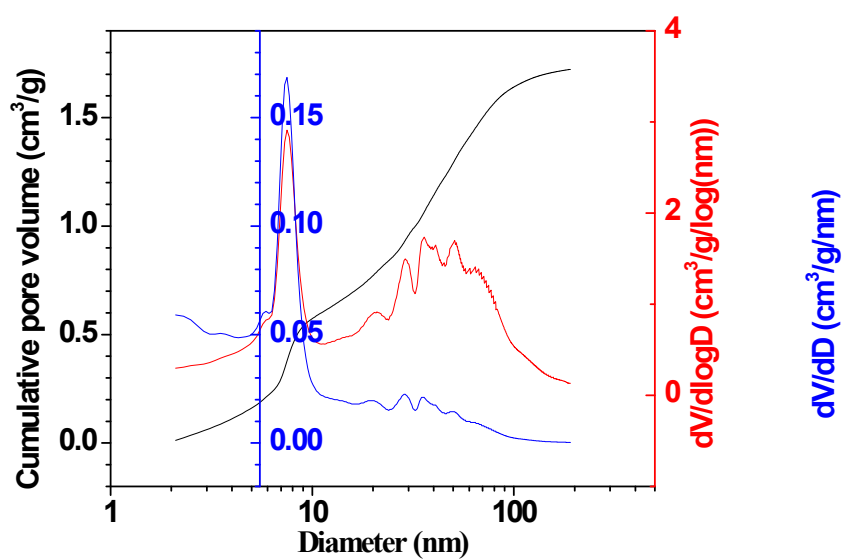


Fig. S2 The pore size distributions.

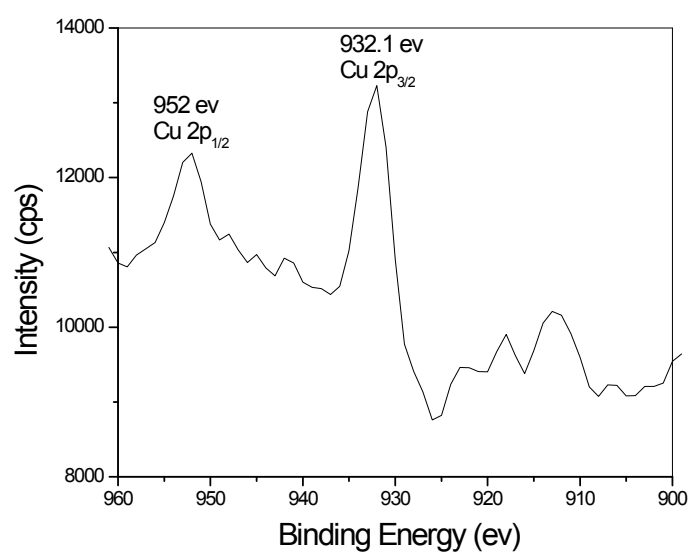


Fig. S3 XPS of Cu₂O/SBA-15

^1H NMR, ^{13}C NMR and GC-MS data

¹H NMR, ¹³C NMR and GC-MS data

4-Nitrobenzonitrile (1a). pale yellow solid; mp 143-145 °C;

¹H NMR (300 MHz, DMSO-d₆) δ 8.36 (d, *J* = 8.9 Hz, 1H), 8.16 (d, *J* = 8.9 Hz, 1H).

¹³C NMR (75 MHz, DMSO-d₆) δ 150.39, 134.60, 124.78, 117.76, 117.65

GC-MS (EI): rt=10.450 min, m/z:148

4-Methoxybenzonitrile (1b). white solid; mp 57-58 °C

¹H NMR (300 MHz, DMSO-d₆) δ 7.75 (d, 9.0 Hz, 2H), 7.09 (d, 9.0Hz, 2H), 3.82 (s, 3H).

¹³C NMR (75 MHz, DMSO-d₆) δ 163.15, 134.63, 119.62, 115.56, 103.26, 56.12.

GC-MS (EI): rt=8.475 min, m/z:133

Terephthalonitrile (1c). white solid; m.p.111-114°C

¹H NMR (300 MHz, DMSO-d₆) δ 8.06 (s, 1H).

¹³C NMR (75 MHz, DMSO-d₆) δ 133.67, 117.99, 116.17.

GC-MS (EI): rt=8.685 min, m/z:128

4-Fluorobenzonitrile (1d). white solid; mp 33-36 °C

¹H NMR (300 MHz, CDCl₃) δ 7.68 (dd, *J* = 8.5, 5.2 Hz, 1H), 7.28 – 6.92 (m, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 166.64 (4-Ar-C, *J*=254.25 Hz), 163.25 (4-Ar-C, *J* =254.25 Hz), 134.74 (3-Ar-C, *J*=9.0 Hz), 134.62 (3-Ar-C, *J*=9.0 Hz), 117.99 (1-Ar-C), 116.94 (2-Ar-C, *J*=23.25 Hz), 116.63 (2-Ar-C, *J*=23.25 Hz), 108.50 (CN).

GC-MS (EI): rt=4.535 min, m/z:121

4-Bromobenzonitrile (1e). white solid; m.p.110-113 °C

¹H NMR (300 MHz, CDCl₃) δ 7.64 (d, *J* = 8.3 Hz, 2H), 7.53 (d, *J* = 8.4 Hz, 2H).

¹³C NMR (75 MHz, CDCl₃) δ 133.43, 132.65, 128.03, 118.07, 111.25.

GC-MS (EI): rt=8.300 min, m/z: 181, 183.

4-Phenylbenzonitrile (1f). white solid; mp 83-84 °C

¹H NMR (300 MHz, DMSO-d₆) δ 7.90 (m, 4H), 7.73 (d, *J* = 7.2 Hz, 2H), 7.60 – 7.30 (m, 3H).

¹³C NMR (75 MHz, DMSO-d₆) δ 145.10, 138.72, 133.32, 129.64, 129.23, 128.04, 127.55, 119.34, 110.

GC-MS (EI): rt=14.970 min, m/z:179

4,4'-Biphenyldicarbonitrile (1g). white solid; m.p.239-241 °C

¹H NMR (300 MHz, DMSO-d₆) δ 7.97 (d, *J* = 0.6 Hz, 1H).

¹³C NMR (75 MHz, DMSO-d₆) δ 143.14, 133.49, 128.55, 119.09, 111.76

GC-MS (EI): rt=19.230 min, EI-MS: m/z:204

4-(4-Bromophenyl)benzonitrile (1h). white solid; mp. 152-155 °C

¹H NMR (300 MHz, CDCl₃) δ 7.73 (d, *J* = 8.5 Hz, 2H), 7.62 (dd, *J* = 11.8, 8.5 Hz, 4H), 7.47 (d, *J*=8.5 Hz, 2H).

¹³C NMR (75 MHz, CDCl₃) δ 144.40, 138.05, 132.74, 132.30, 128.80, 127.55, 123.19, 118.78, 111.34.

GC-MS (EI): rt=18.630 min, m/z:257, 259.

Methyl 4-cyanobenzoate (1i). white solid; mp 65-67 °C

¹H NMR (300 MHz, DMSO-d₆) δ 8.06 (d, *J* = 8.6 Hz, 1H), 7.98 (d, *J* = 8.6 Hz, 1H), 3.88 (s, 1H).

¹³C NMR (75 MHz, DMSO-d₆) δ 165.46, 133.94, 133.26, 130.24, 118.48, 115.93, 53.18

GC-MS (EI): rt=10.075 min, m/z:161

4-Methylbenzonitrile (1j). white solid; mp 28-30 °C

¹H NMR (300 MHz, CDCl₃) δ 7.54 (d, *J* = 7.9 Hz, 2H), 7.27 (d, *J* = 7.6 Hz, 2H), 2.42 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ 143.74, 131.99, 129.86, 119.15, 109.24, 21.81.

GC-MS (EI): rt=6.350 min, m/z:117

3-Nitrobenzonitrile (1k). pale yellow solid; mp 114-115 °C

¹H NMR (300 MHz, DMSO-d₆) δ 8.77 – 8.71 (m, 1H), 8.51 (ddd, *J* = 8.4, 2.3, 1.0 Hz, 1H), 8.38 – 8.23 (m, 1H), 7.86 (t, *J* = 8.1 Hz, 1H).

¹³C NMR (75 MHz, DMSO-d₆) δ 148.35, 138.99, 131.67, 128.47, 127.90, 117.49, 113.30.

GC-MS (EI): rt=10.595 min, m/z:148

3-Fluorobenzonitrile (1l). white solid; mp 14-16 °C

¹H NMR (300 MHz, CDCl₃) δ 7.50-7.47 (m, 2H), 7.39-7.32 (m, 2H).

¹³C NMR (75 MHz, CDCl₃) δ 163.85(3-Ar-C, *J*=248.25 Hz), 160.54(3-Ar-C, *J* =248.25 Hz), 131.25(5-Ar-C, *J*=8.25 Hz), 131.14(5-Ar-C, *J*=8.25 Hz), 128.24(6-Ar-C, *J*=3.75 Hz), 128.19 (6-Ar-C, *J*=3.75 Hz), 120.68 (4-Ar-C, *J*=21 Hz), 120.40 (4-Ar-C,

$J=21$ Hz), 119.31 (2-Ar-C, $J=24$ Hz), 118.99 (2-Ar-C, $J=24$ Hz), 117.53 (CN), 113.96(1-Ar-C, $J=9$ Hz), 113.84(1-Ar-C, $J=9$ Hz).

GC-MS (EI): $rt=4.215$ min, m/z :121

3-Bromobenzonitrile (1m). white solid; m.p.43-46°C

^1H NMR (300 MHz, DMSO- d_6) δ 8.15 (s, 1H), 7.90 (dd, $J = 19.1, 7.4$ Hz, 2H), 7.53 (t, $J = 7.6$ Hz, 1H).

^{13}C NMR (75 MHz, DMSO- d_6) δ 136.89, 135.03, 131.93, 131.63, 122.63, 117.88, 113.83.

GC-MS (EI): $rt=8.155$ min, m/z : 181, 183.

3-Methylbenzonitrile (1n). colorless liquid; b.p.212-215°C

^1H NMR (300 MHz, CDCl_3) δ 7.55 (d, $J = 7.7$ Hz, 1H), 7.46 (td, $J = 7.7, 1.2$ Hz, 1H), 7.26 (dd, $J = 17.9, 7.8$ Hz, 1H), 2.51 (s, 1H).

^{13}C NMR (75 MHz, CDCl_3) δ 141.87, 132.67, 132.46, 130.24, 126.24, 118.12, 112.70, 20.42.

GC-MS (EI): $rt=6.130$ min, m/z :117

2-Nitrobenzonitrile (1o). pale yellow solid; m.p 107-109°C

^1H NMR (300 MHz, DMSO- d_6) δ 8.45 – 8.33 (m, 1H), 8.18 (dd, $J = 5.9, 3.2$ Hz, 1H), 7.98 (dd, $J = 5.9, 3.4$ Hz, 2H).

^{13}C NMR (75 MHz, DMSO- d_6) δ 148.65, 136.28, 135.47, 135.01, 126.19, 116.03, 107.27.

GC-MS (EI): $rt=11.890$ min, m/z :148

Methyl 2-cyanobenzoate (1p).colorless solid. m.p.48-50°C

^1H NMR (300 MHz, DMSO- d_6) δ 8.14 – 8.08 (m, 1H), 8.00 (dd, $J = 5.8, 3.1$ Hz, 1H), 7.87 – 7.77 (m, 1H), 3.90 (s, 2H).

^{13}C NMR (75 MHz, DMSO- d_6) δ 164.57, 135.62, 133.93, 133.81, 132.10, 131.32, 117.84, 112.07, 53.29.

GC-MS (EI): $rt=10.620$ min, m/z :161

2-Fluorobenzonitrile (1q). colorless liquid. b.p. 20-22°C

^1H NMR (300 MHz, CDCl_3) δ 7.74 – 7.52 (m, 1H), 7.24 (dt, $J = 17.9, 8.3$ Hz, 1H).

^{13}C NMR (75 MHz, CDCl_3) δ 164.83 (2-Ar-C, $J=257.25$ Hz), 161.40 (2-Ar-C, $J=257.25\text{Hz}$), 135.24 (4-Ar-C, $J=8.25$ Hz), 135.13 (4-Ar-C, $J=8.25$ Hz), 133.54 (5-Ar-C), 124.93 (3-Ar-C, $J=0.3$ Hz), 124.89 (3-Ar-C, $J=0.3$ Hz), 116.62 (1-Ar-C, $J=19.5$ Hz), 116.36 (1-Ar-C, $J=19.5$ Hz), 113.97 (CN).

GC-MS (EI): $rt=4.810$ min, m/z :121

2-Chlorobenzonitrile (1r). white solid; m.p. 43-46 °C

¹H NMR (300 MHz, DMSO-d₆) δ 8.01 (t, *J* = 1.7 Hz, 1H), 7.80 (tdd, *J* = 8.3, 2.4, 1.1 Hz, 2H), 7.59 (t, *J* = 8.0 Hz, 1H).

¹³C NMR (75 MHz, DMSO-d₆) δ 134.42, 134.03, 132.28, 131.81, 131.60, 117.98, 113.62.

GC-MS (EI): rt=6.415 min, m/z: 187

2-Bromobenzonitrile (1s). white solid; m.p. 54-56 °C

¹H NMR (300 MHz, DMSO-d₆) δ 8.11 – 7.75 (m, 1H), 7.77 – 7.45 (m, 1H).

¹³C NMR (75 MHz, DMSO-d₆) δ 135.56, 135.42, 133.63, 128.97, 124.93, 117.72, 114.88.

GC-MS (EI): rt=8.755 min, m/z: 181, 183.

2-Methylbenzonitrile (1t). colorless liquid; b.p. 203-205 °C

¹H NMR (300 MHz, CDCl₃) δ 7.60 – 7.29 (m, 4H), 2.38 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 139.23, 133.66, 132.47, 129.26, 129.00, 119.04, 112.23, 21.15.

GC-MS (EI): rt=6.335 min, m/z: 117

Benzonitrile (1u). colorless liquid. b.p. 188-191 °C

¹H NMR (300 MHz, DMSO) δ 7.85 (dt, *J* = 3.3, 1.4 Hz, 2H), 7.79 – 7.71 (m, 1H), 7.65 – 7.57 (m, 2H).

¹³C NMR (75 MHz, DMSO-d₆) δ 133.60, 132.57, 129.80, 119.21, 111.89.

GC-MS (EI): rt=4.675 min, m/z: 103

4-Cyanopyridine (1v). white solid; m.p. 82-84 °C

¹H NMR (300 MHz, DMSO-d₆) δ 8.83 (dd, *J* = 8.8 Hz, 1H), 7.85 (dd, *J* = 8.8 Hz, 1H).

¹³C NMR (75 MHz, DMSO-d₆) δ 151.21, 126.08, 119.86, 117.24.

GC-MS (EI): rt=4.505 min, m/z: 104

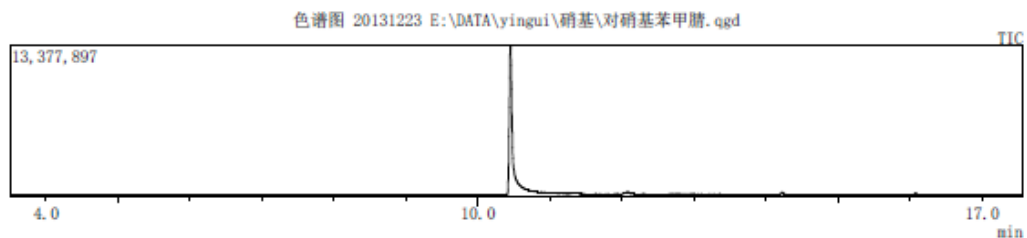
3-Cyanopyridine (1w). white solid; m.p. 50-51 °C

¹H NMR (300 MHz, DMSO-d₆) δ 9.01 (s, 1H), 8.85 (d, *J* = 3.8 Hz, 1H), 8.31 (dt, *J* = 8.0, 1.9 Hz, 1H), 7.61 (dd, *J* = 7.7, 4.8 Hz, 1H).

¹³C NMR (75 MHz, DMSO-d₆) δ 153.72, 152.87, 140.47, 124.56, 117.45, 109.68.

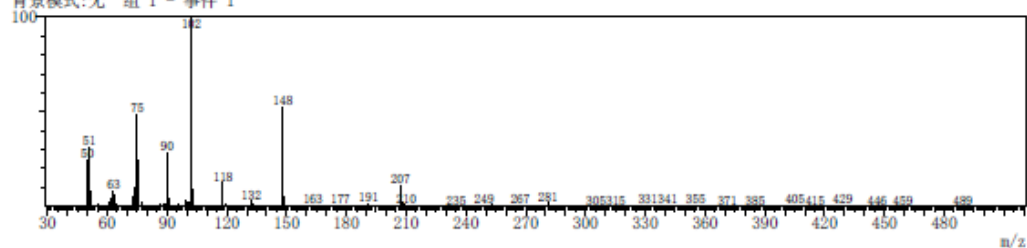
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4-Nitrobenzonitrile (1a)

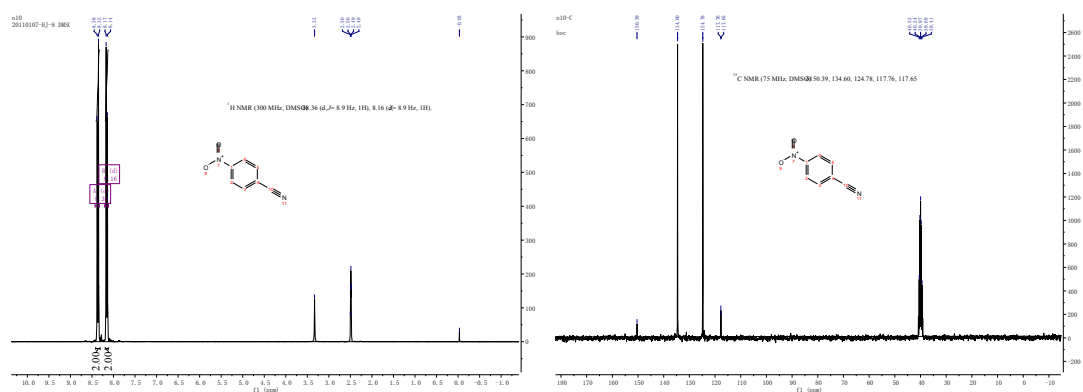
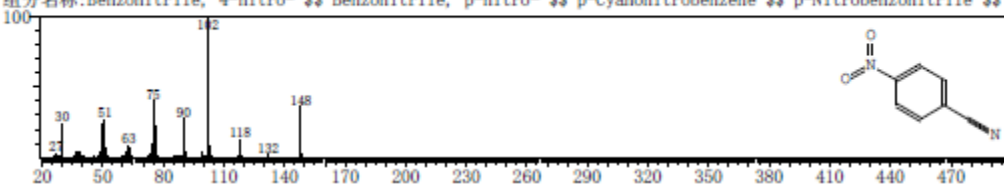


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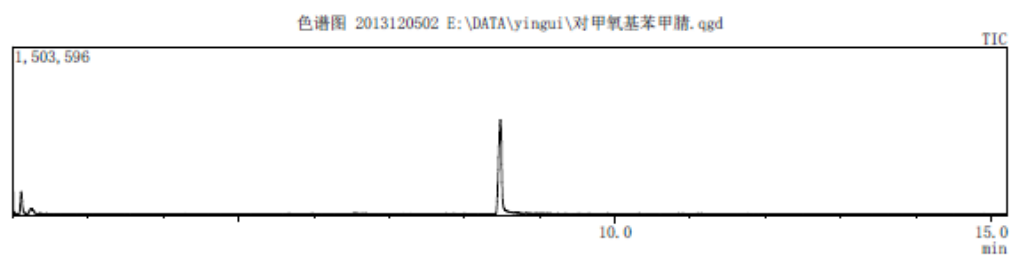
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4-Methoxybenzonitrile (1b)



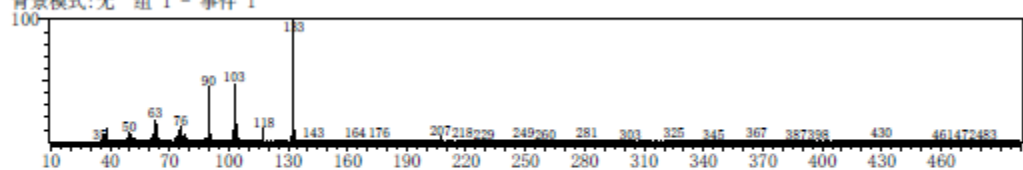
谱库

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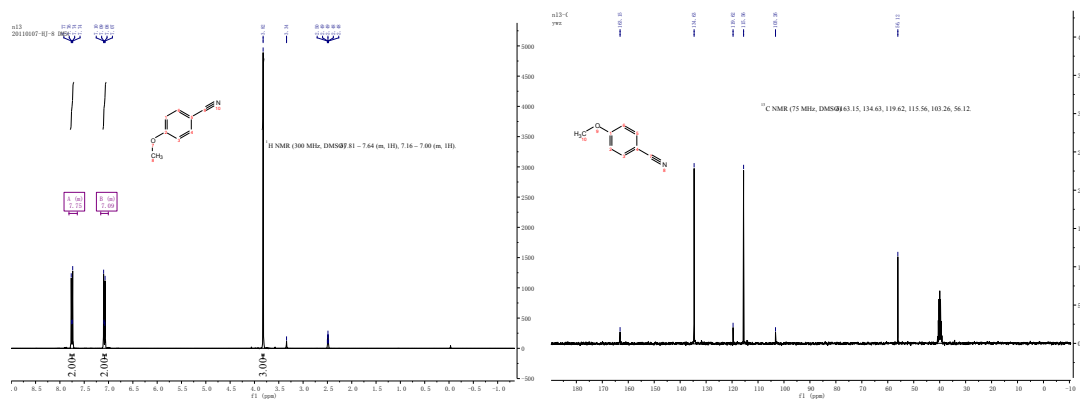
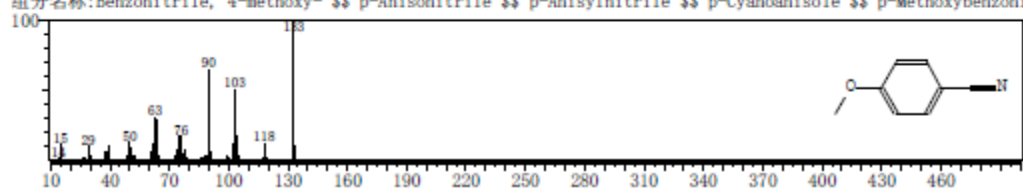
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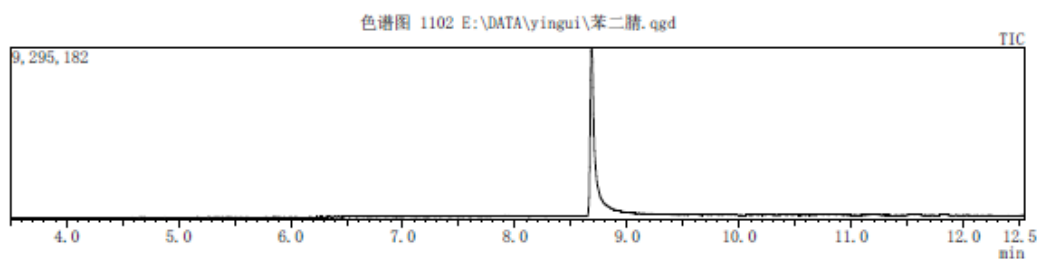
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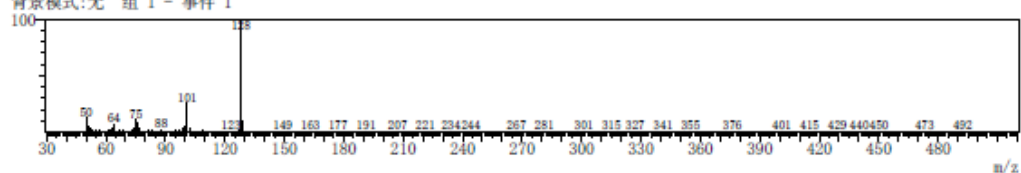


Terephthalonitrile (1c)



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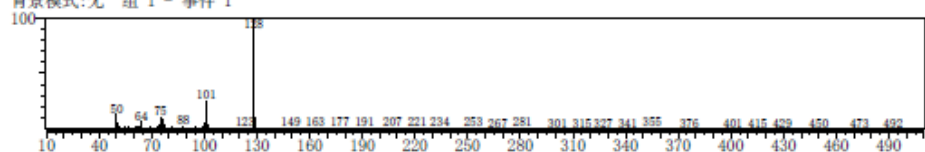
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背景模式:无 组 1 - 事件 1



谱库

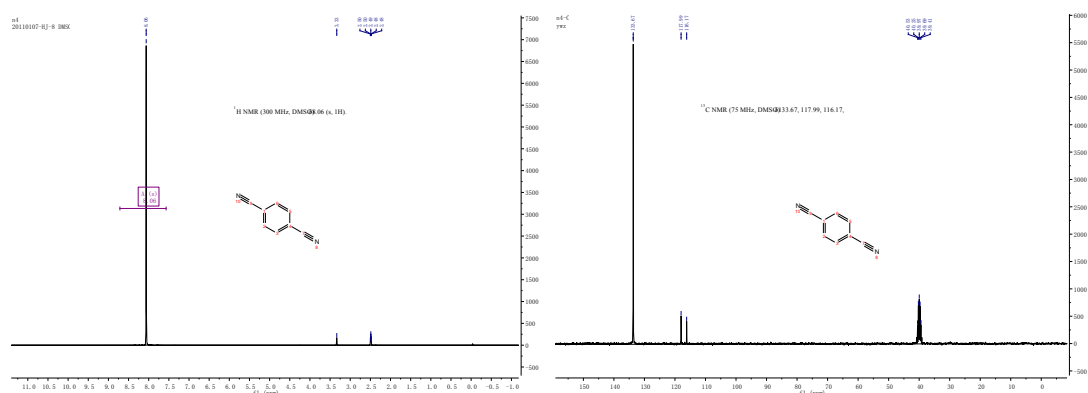
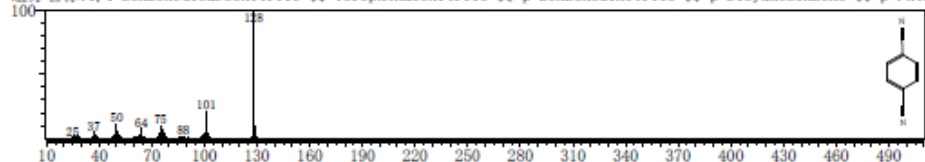
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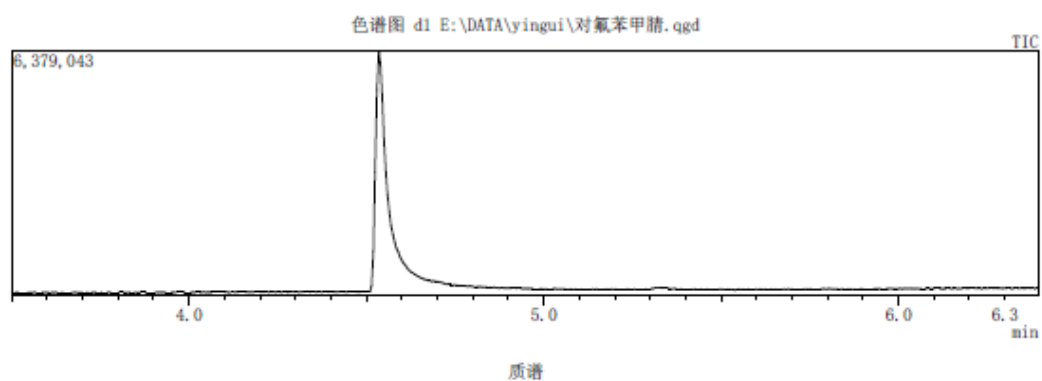


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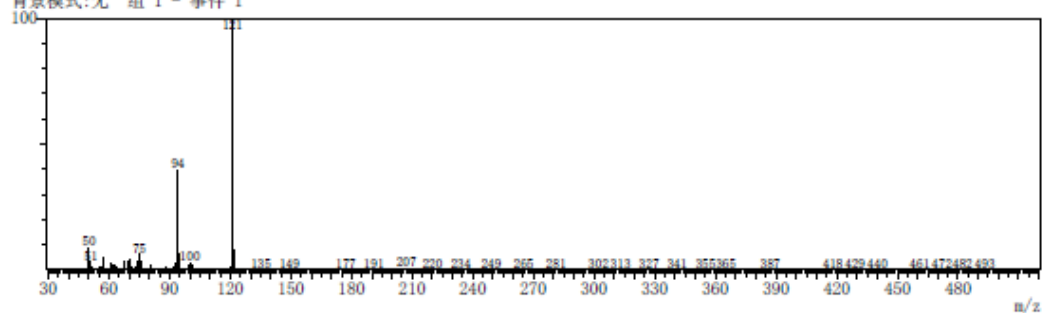
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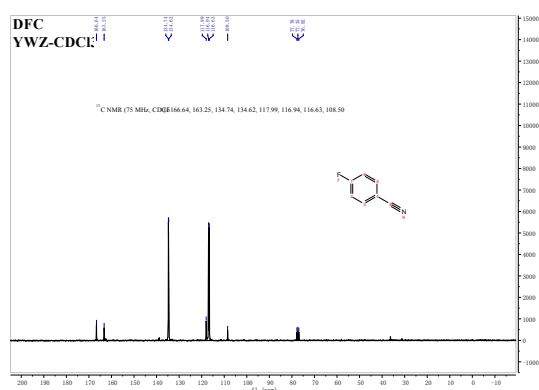
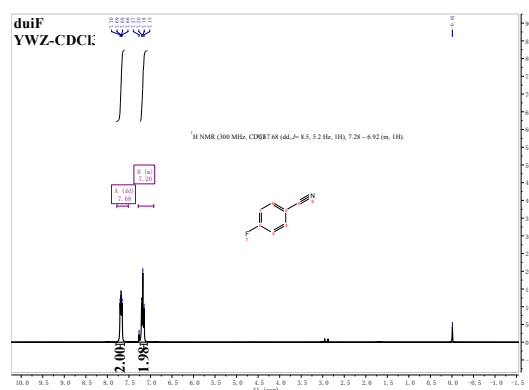
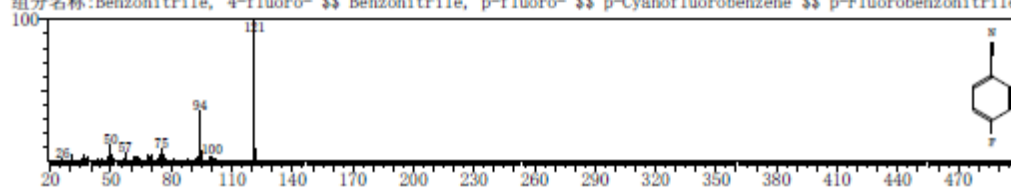
4-Fluorobenzonitrile (1d)



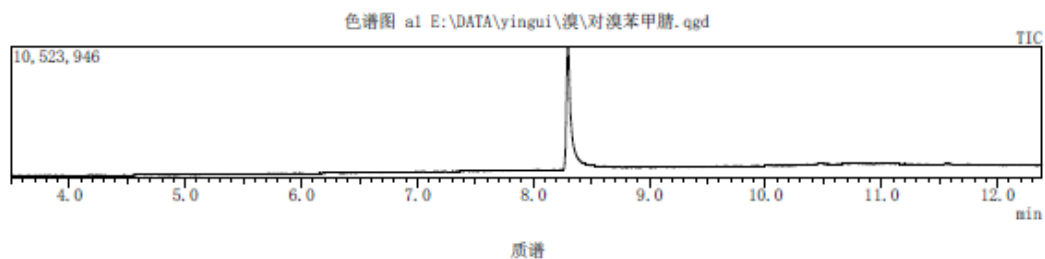
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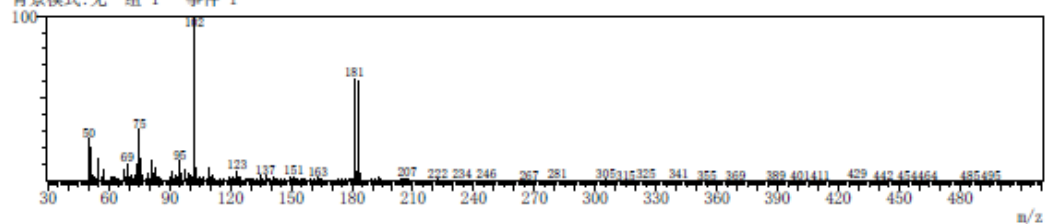
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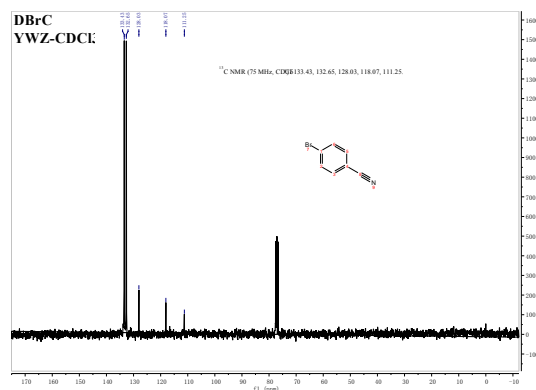
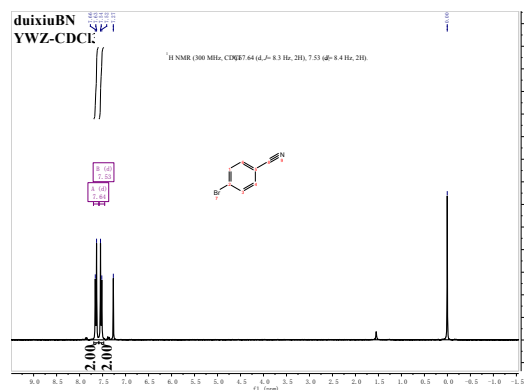
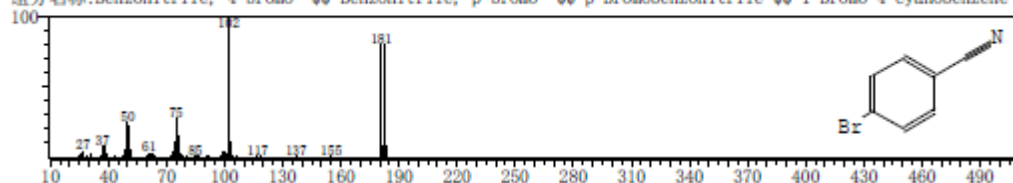
4-Bromobenzonitrile (1e)



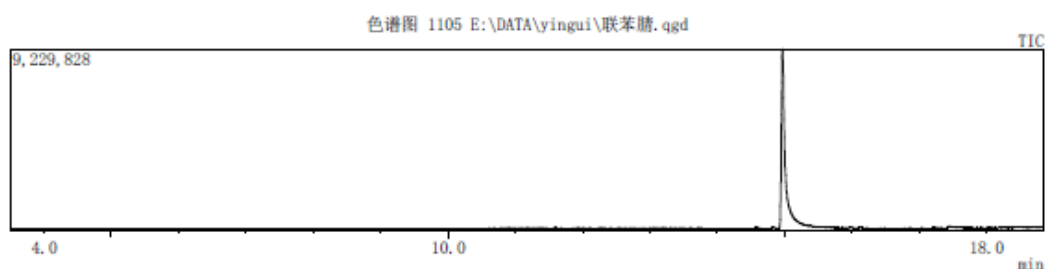
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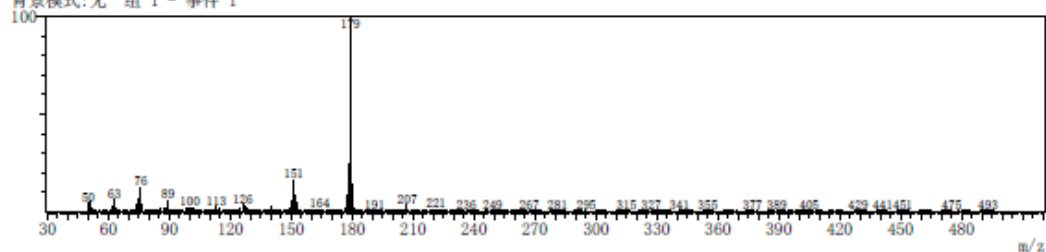


4-Phenylbenzonitrile (1f)

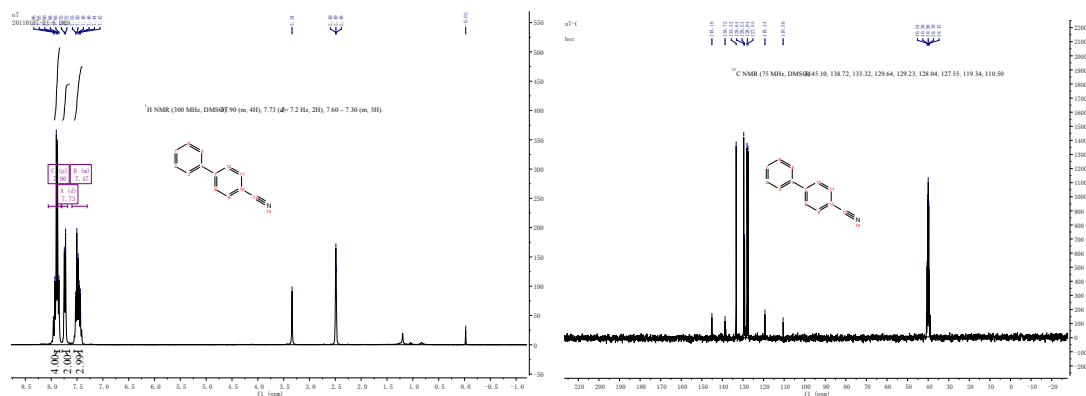
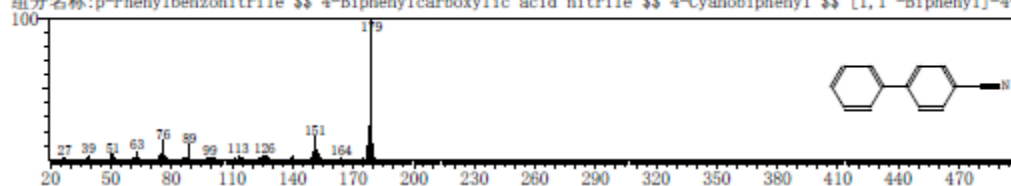


质谱

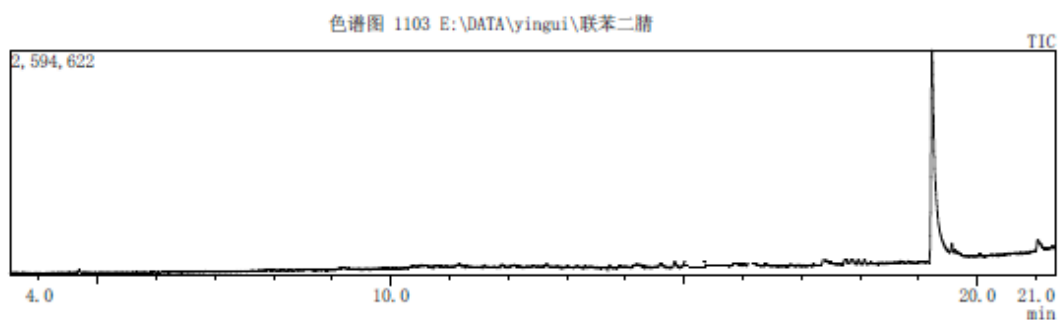
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背景模式:无 组 1 - 事件 1



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组分名称:p-Phenylbenzonitrile 4-Biphenylcarboxylic acid nitrile 4-Cyanobiphenyl [1,1'-Biphenyl]-4-

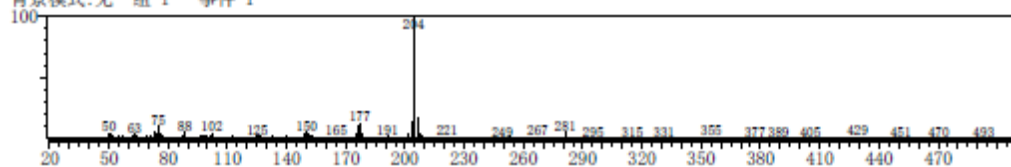


4,4'-Biphenyldicarbonitrile (1g)

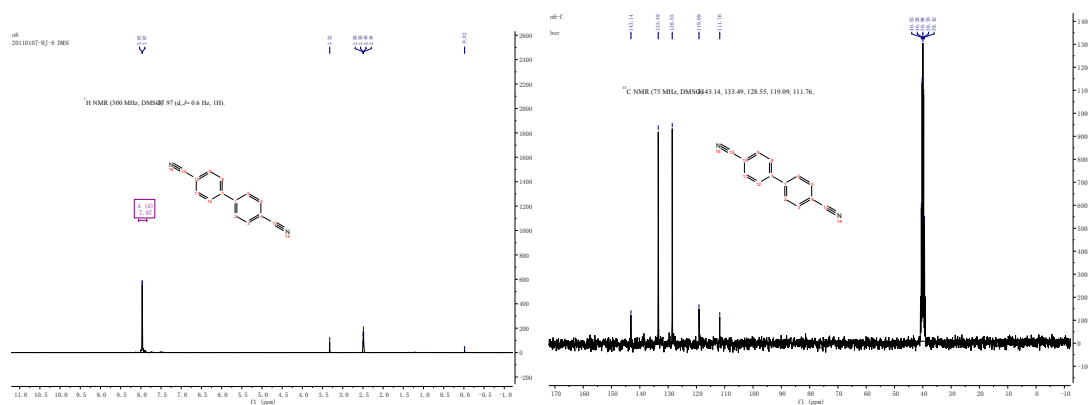
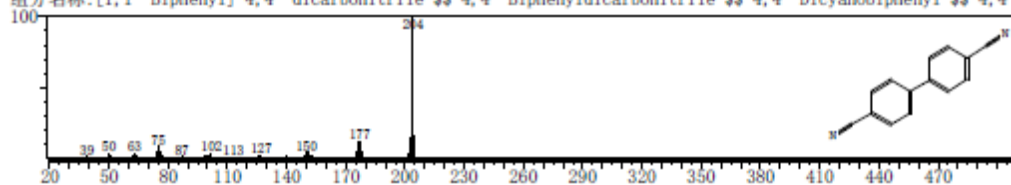


<< 目标组分 >>

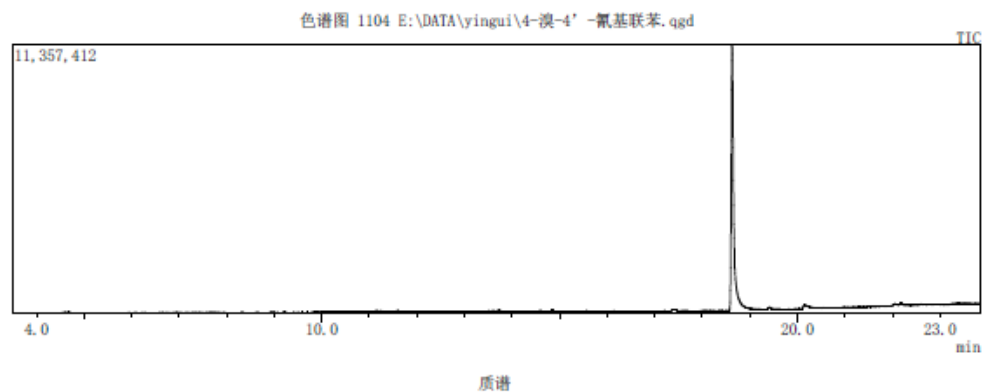
行号#:1 保留时间:19.230(扫描数#:3147) 质量峰:451
 原始模式:平均 18.915-19.700(3084-3241) 基峰:204.05(113213)
 背景模式:无 组 1 - 事件 1



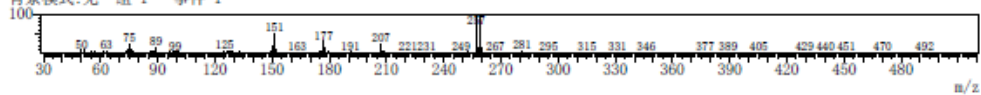
命中#:1 输入:17054 谱库:NIST08s.LIB
 SI:86 分子式:C14H8N2 CAS:1591-30-6 摩尔质量:204 保留指数:1923
 组分名称:[1,1'-Biphenyl]-4,4'-dicarbonitrile \$\$ 4,4'-Biphenyldicarbonitrile \$\$ 4,4'-Dicyanobiphenyl \$\$ 4,4'-



4-(p-bromophenyl)benzonitrile (1h)



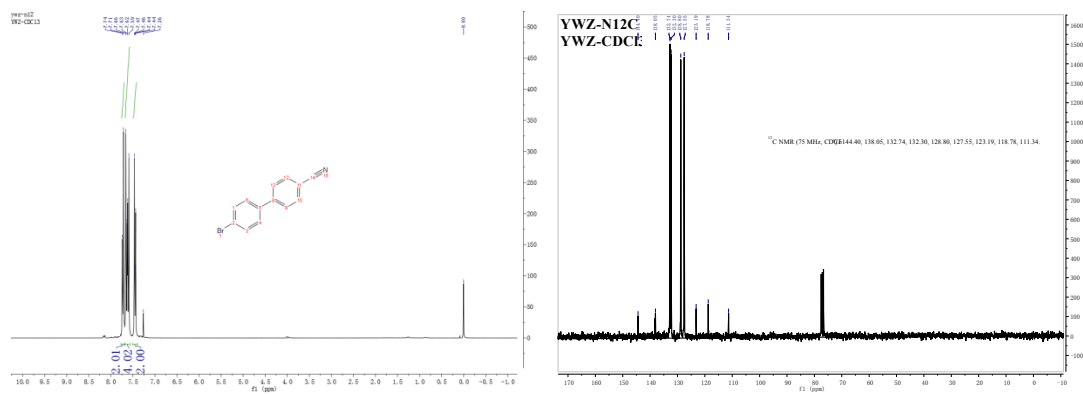
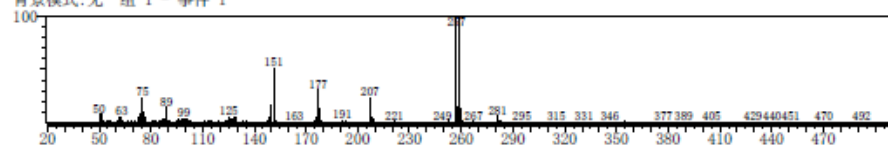
流路号:1 保留时间:18.630(扫描数:3027)
质量峰:451
原始模式:平均 18.140-19.815(2929-3264) 基峰:257(80571)
背景模式:无 组 1 - 事件 1



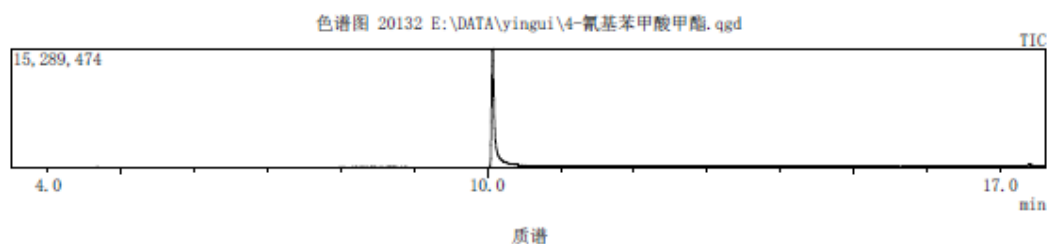
谱库

<< 目标组分 >>

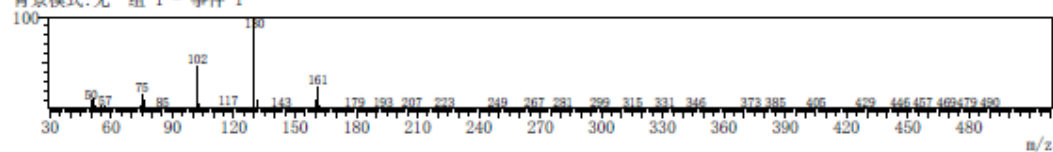
行号#:1 保留时间:18.630(扫描数#:3027) 质量峰:451
原始模式:平均 18.140-19.815(2929-3264) 基峰:257.00(80571)
背景模式:无 组 1 - 事件 1



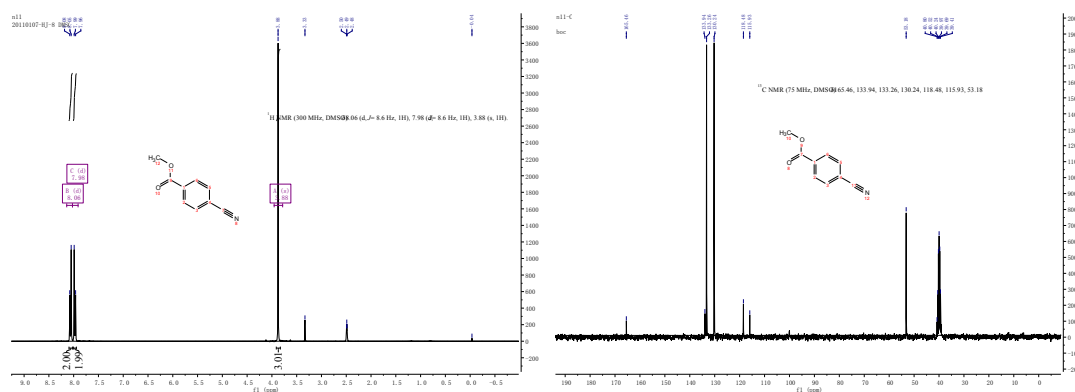
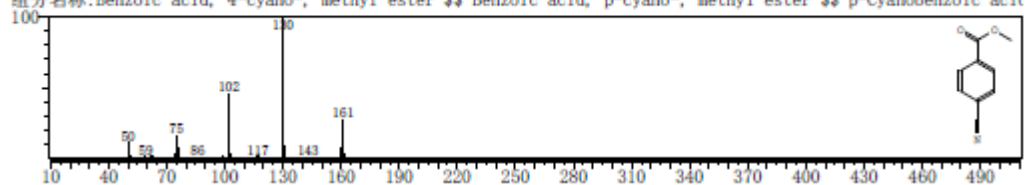
Methyl 4-cyanobenzoate (1i)



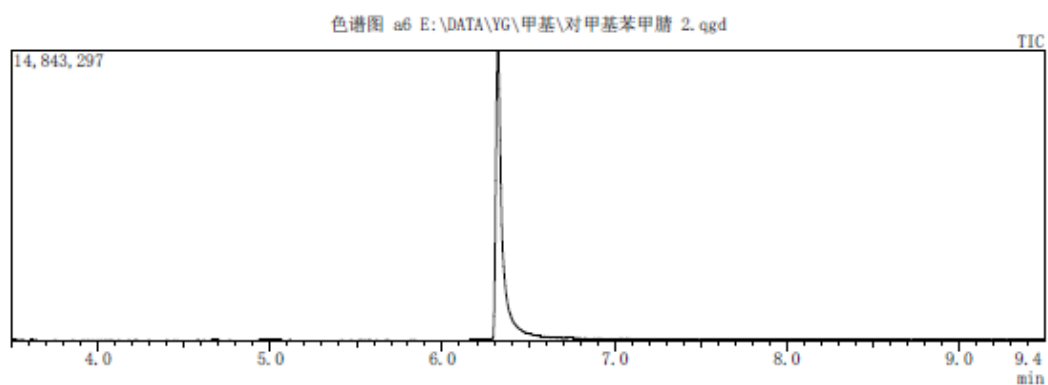
流路号:1 保留时间:10.075(扫描数:1316)
 质量峰:451
 原始模式:平均 9,520-11,445(1205-1590) 基峰:130(177068)
 背景模式:无 组 1 - 事件 1



命中#:1 输入:10608 谱库:NIST08s.LIB
 SI:94 分子式:C9H7NO2 CAS:1129-35-7 摩尔质量:161 保留指数:1338
 组分名称:Benzoic acid, 4-cyano-, methyl ester \$\$ Benzoic acid, p-cyano-, methyl ester \$\$ p-Cyanobenzoic acid

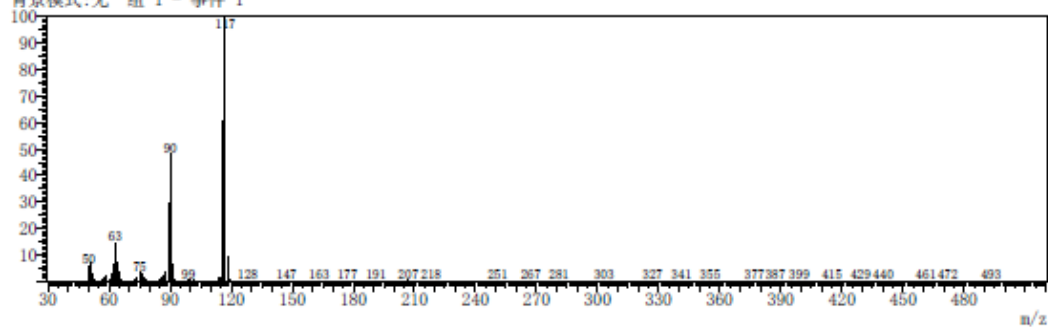


4-Methylbenzonitrile (1j)

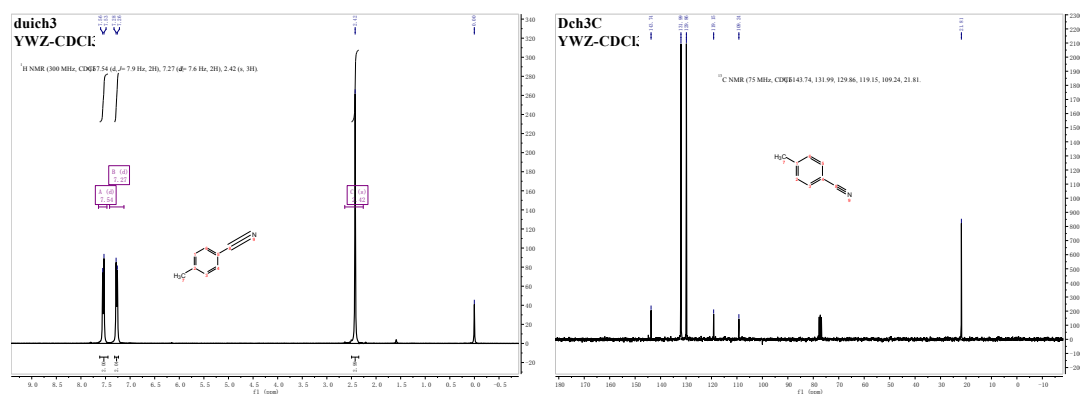
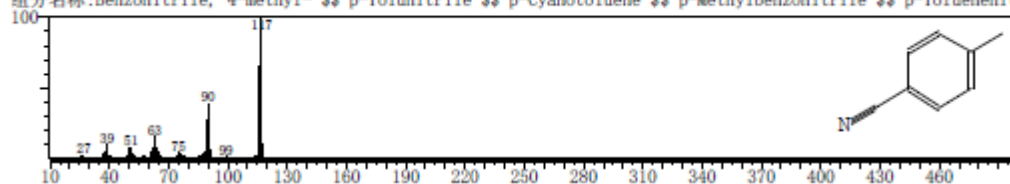


质谱

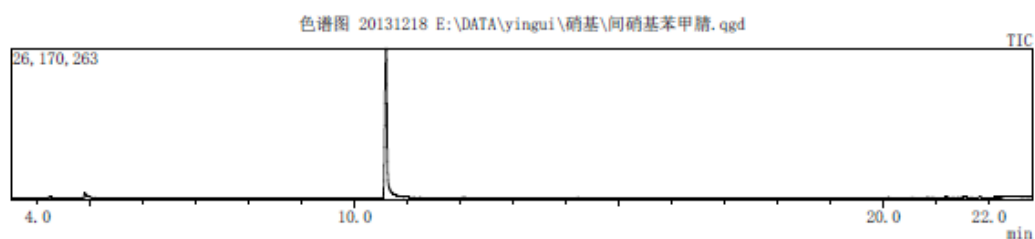
流路号:1 保留时间:6.320(扫描数:565)
 质量峰:451
 原始模式:平均 6.275-6.525(556-606) 基峰:117(783053)
 背景模式:无 组 1 - 事件 1



命中#:3 输入:3679 谱库:NIST08s.LIB
 SI:88 分子式:C8H7N CAS:104-85-8 摩尔质量:117 保留指数:1071
 组分名称:Benzonitrile, 4-methyl- \$\$ p-Tolunitrile \$\$ p-Cyanotoluene \$\$ p-Methylbenzonitrile \$\$ p-Toluenenitrile

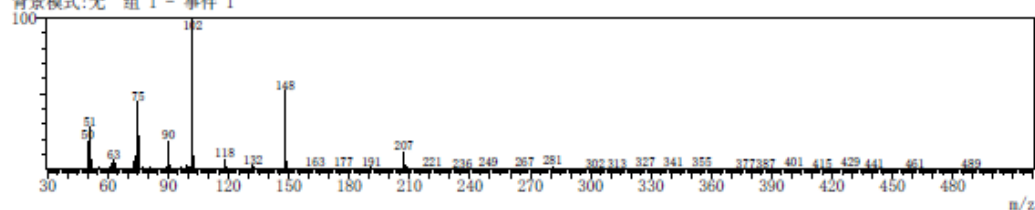


3-Nitrobenzonitrile (1k)

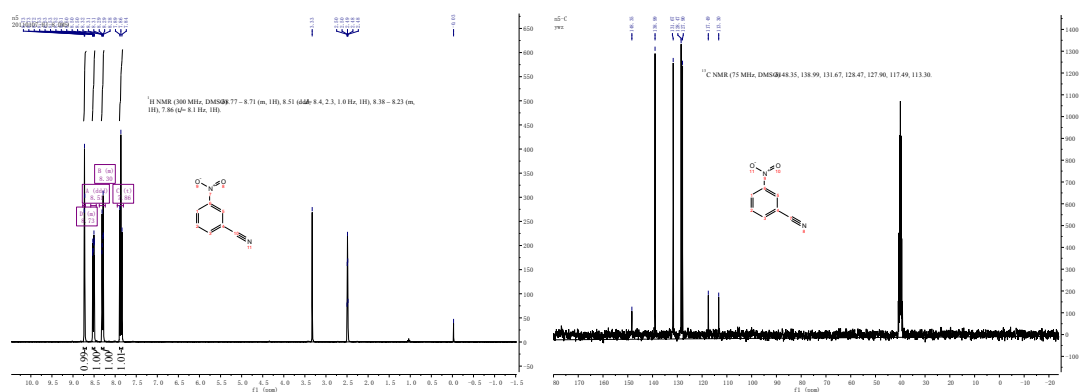
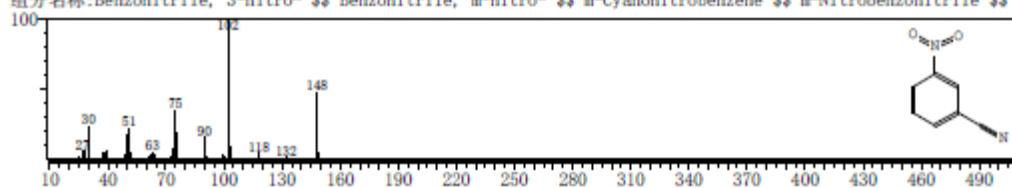


质谱

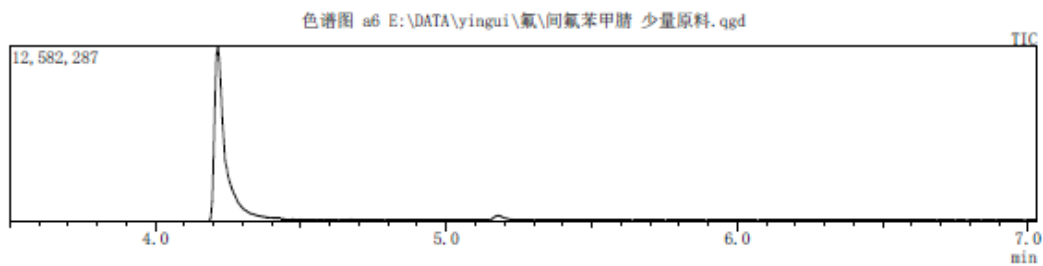
流路号:1 保留时间:10.595(扫描数:1420)
质量峰:451
原始模式:平均 10.315-11.660(1364-1633) 基峰:102(310963)
背景模式:无 组 1 - 事件 1



命中#:1 输入:8191 谱库:NIST08s.LIB
SI:93 分子式:C7H4N2O2 CAS:619-24-9 摩尔质量:148 保留指数:1354
组分名称:Benzonitrile, 3-nitro- \$\$ Benzonitrile, m-nitro- \$\$ m-Cyanonitrobenzene \$\$ m-Nitrobenzonitrile \$:

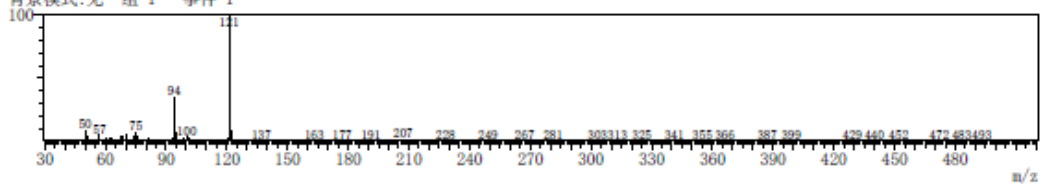


3-Fluorobenzonitrile (1l)

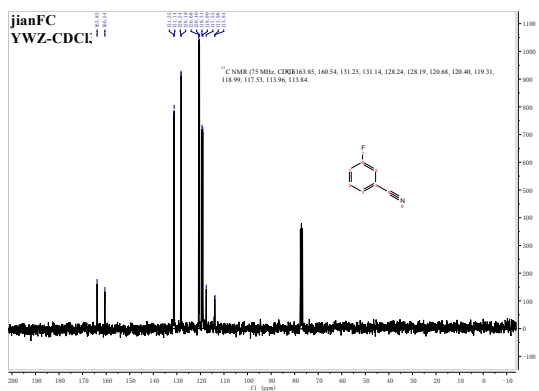
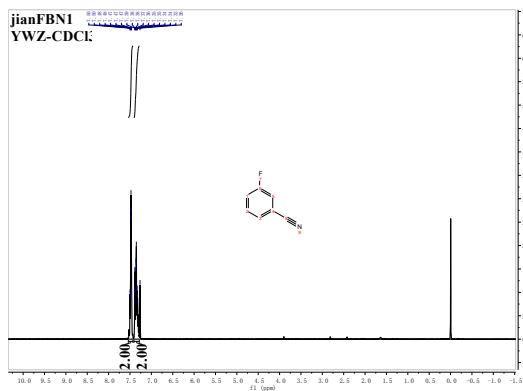
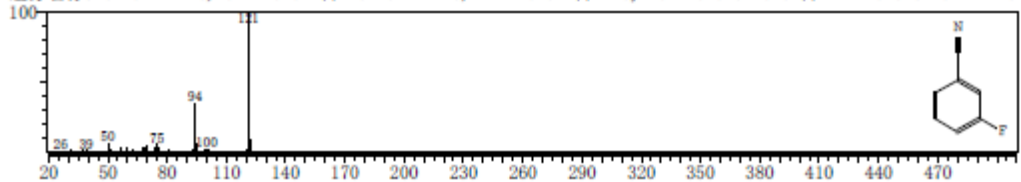


质谱

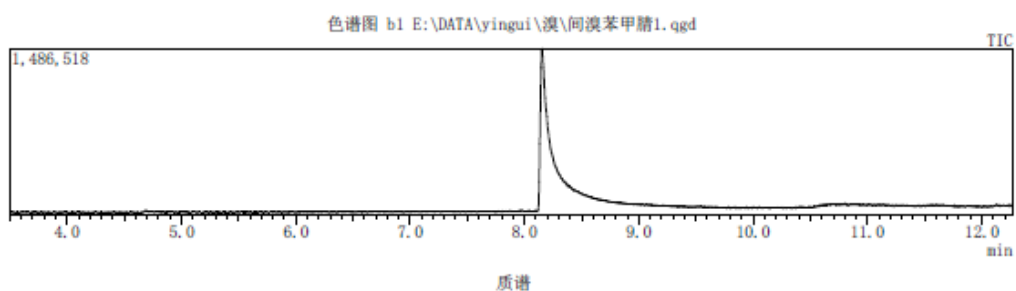
流路号:1 保留时间:4.215(扫描数:144)
 质量峰:451
 原始模式:平均 3.995-4.555(100-212) 基峰:121(466519)
 背景模式:无 组 1 - 事件 1



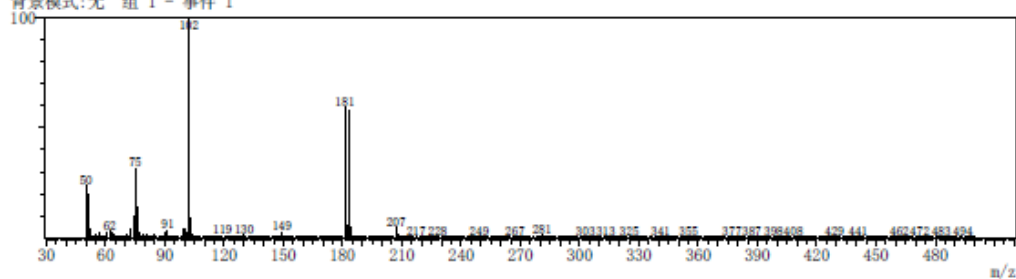
命中#:1 输入:4024 谱库:NIST08s.LIB
SI:98 分子式:C7H4FN CAS:403-54-3 摩尔质量:121 保留指数:933
组分名称:Benzonitrile, 3-fluoro- \$\$ Benzonitrile, m-fluoro- \$\$ m-Cyanofluorobenzene \$\$ m-Fluorobenzonitrile



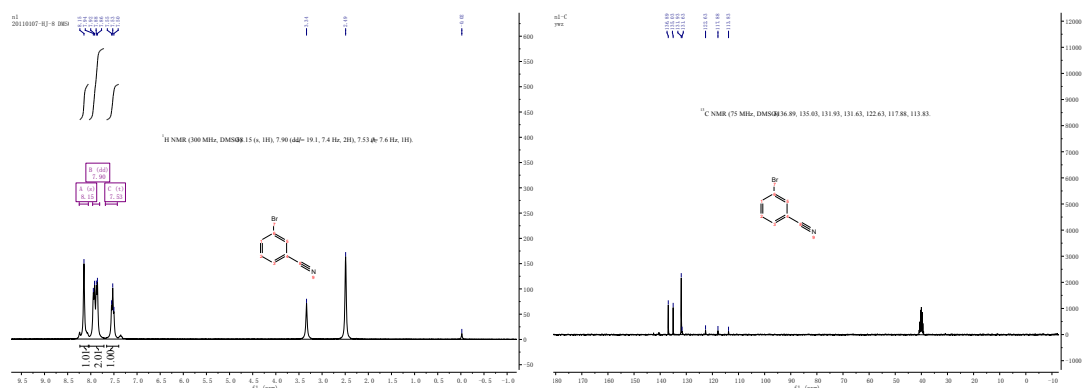
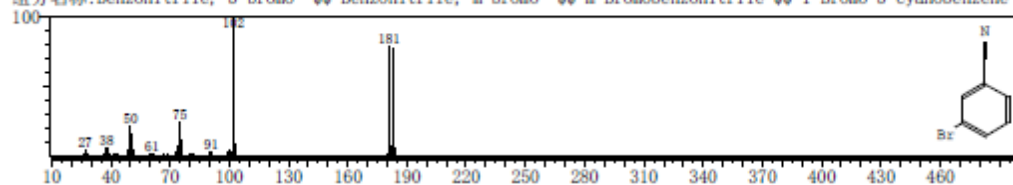
3-Bromobenzonitrile (1m)



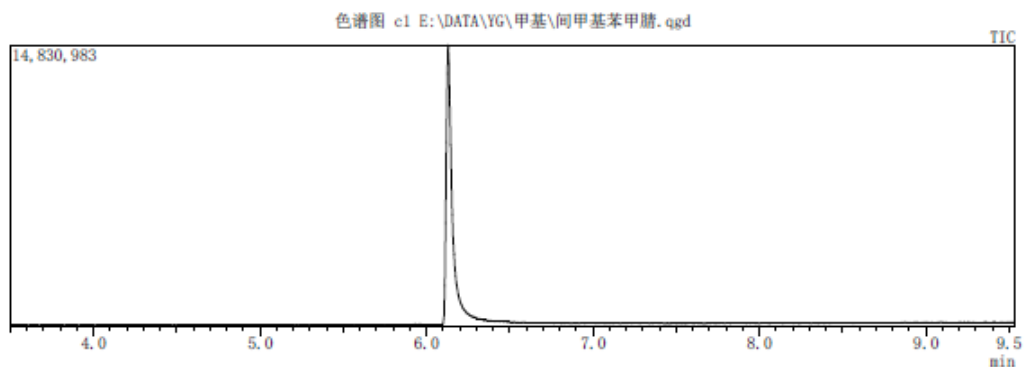
流路号:1 保留时间:8.155(扫描数:932)
质量峰:451
原始模式:平均 7.945-9.100(890-1121) 基峰:102(50611)
背景模式:无 组 1 - 事件 1



命中#:2 输入:13824 谱库:NIST08s.LIB
SI:92 分子式:C7H4BrN CAS:6952-59-6 摩尔质量:181 保留指数:1278
组分名称:Benzonitrile, 3-bromo- \$\$ Benzonitrile, m-bromo- \$\$ m-Bromobenzonitrile \$\$ 1-Bromo-3-cyanobenzene \$

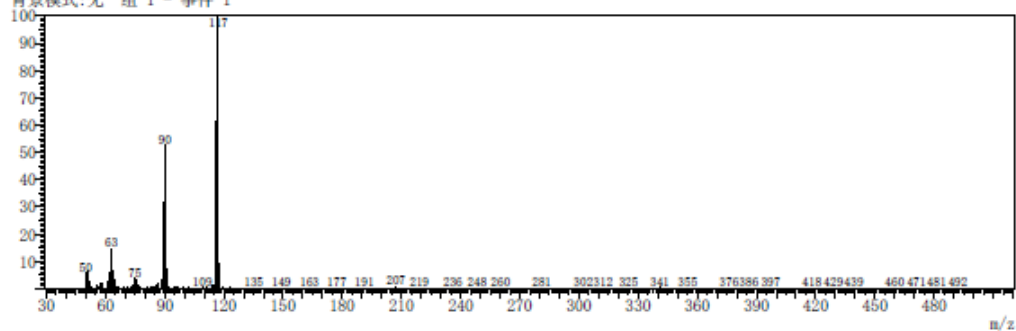


3-Methylbenzonitrile (1n)

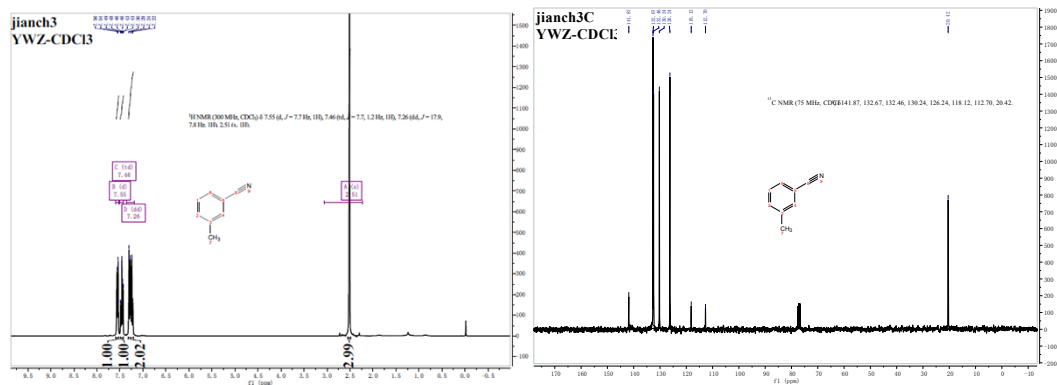
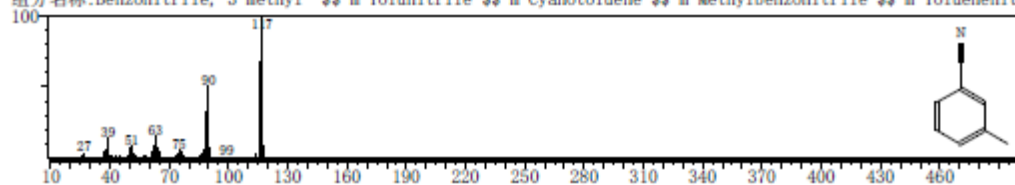


质谱

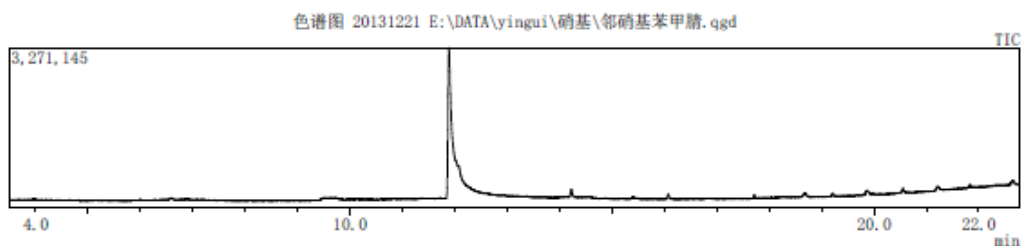
流路号:1 保留时间:6.130(扫描数:527)
 质量峰:451
 原始模式:平均 6.065-6.475(514-596) 基峰:117(479563)
 背景模式:无 组 1 - 事件 1



命文#:2 输入:4815 谱库:NIST08.LIB
 SI:97 分子式:C8H7N CAS:620-22-4 摩尔质量:117 保留指数:1071
 组分名称:Benzonitrile, 3-methyl- \$ \$ m-Tolunitrile \$ \$ m-Cyanotoluene \$ \$ m-Methylbenzonitrile \$ \$ m-Toluenenitrile

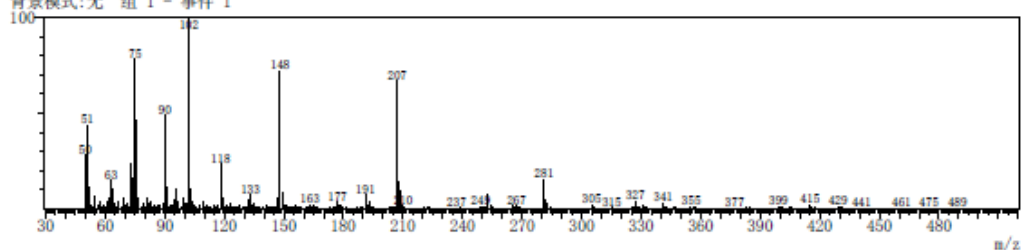


2-Nitrobenzonitrile (1o)

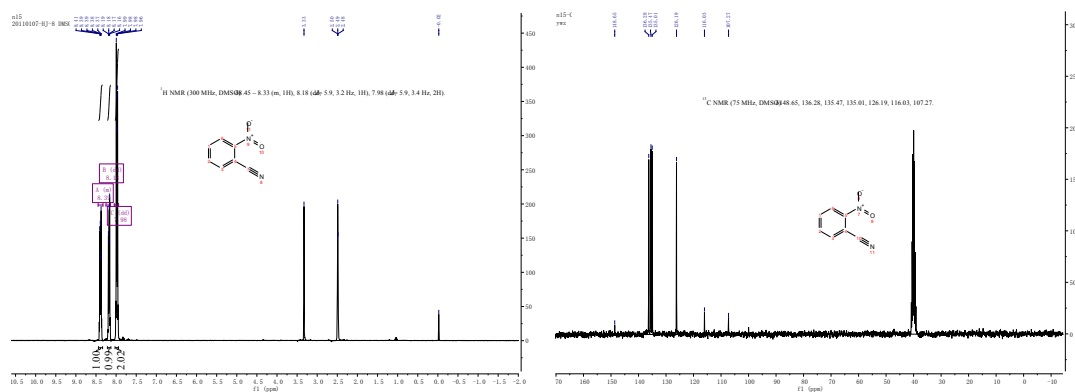
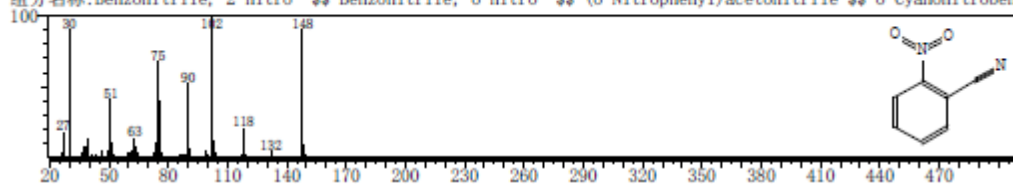


质谱

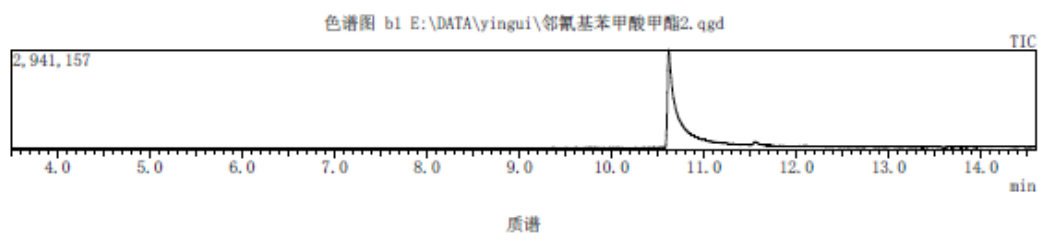
流路号:1 保留时间:11.890(扫描数:1679)
质量峰:451
原始模式:平均 11.510-12.995(1603-1900) 基峰:102(49680)
背景模式:无 组 1 - 事件 1



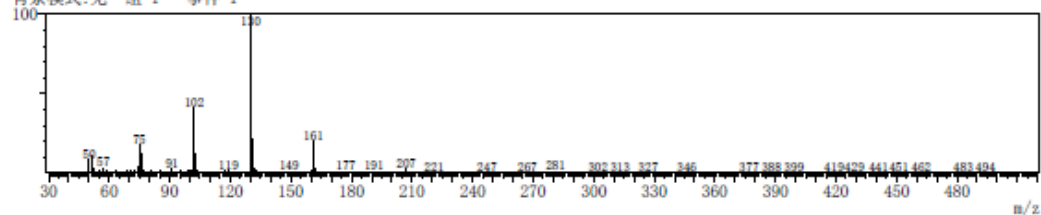
命中#:1 输入:8187 谱库:NIST08s.LIB
SI:80 分子式:C7H4N2O2 CAS:612-24-8 摩尔质量:148 保留指数:1354
组分名称:Benzonitrile, 2-nitro- \$\$ Benzonitrile, o-nitro- \$\$ (o-Nitrophenyl)acetonitrile \$\$ o-Cyanonitrobenz



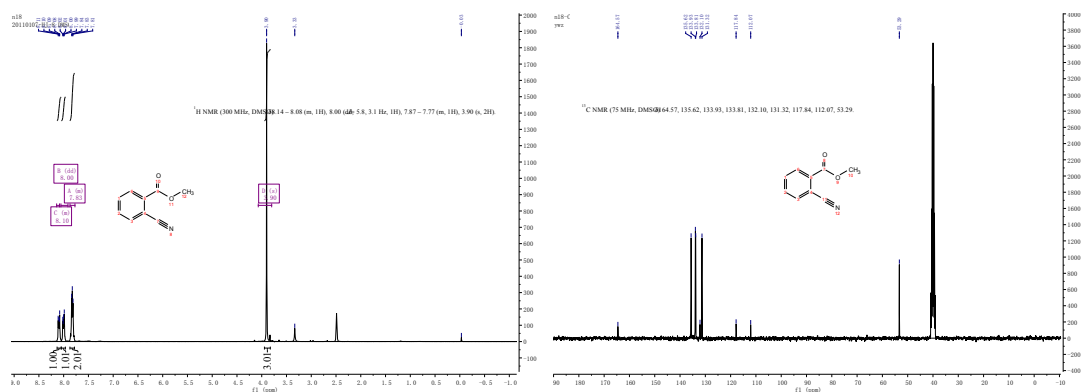
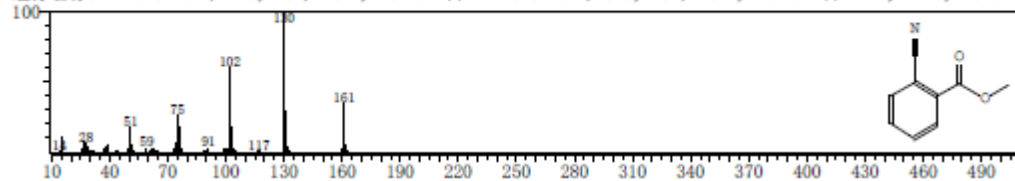
Methyl 2-cyanobenzoate (1p)



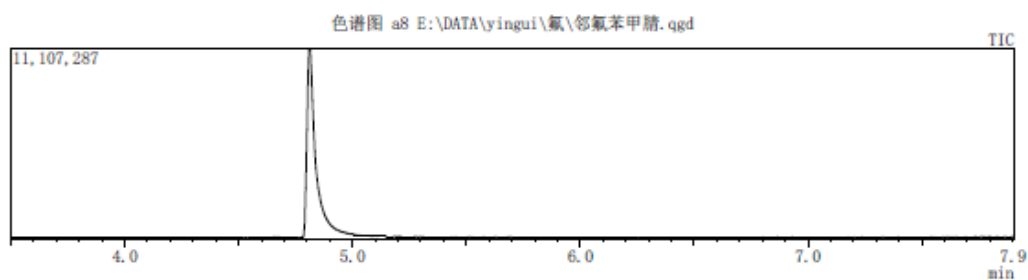
流路号:1 保留时间:10.620(扫描数:1425)
质量峰:451
原始模式:平均 10.170-11.260(1335-1553) 基峰:130(124400)
背景模式:无 组 1 - 事件 1



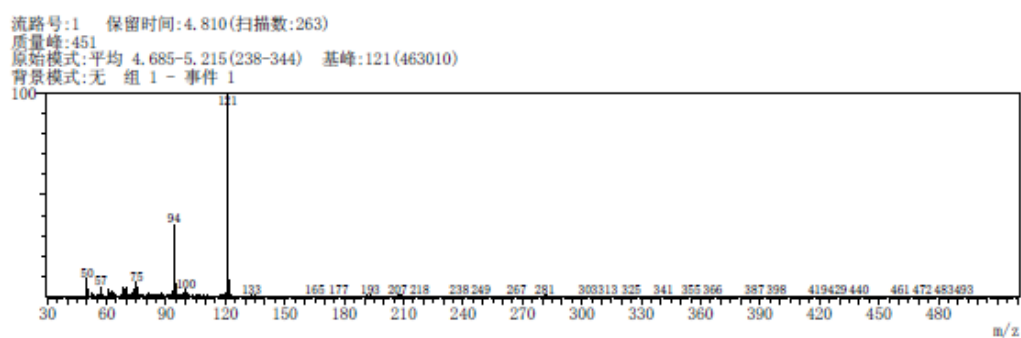
命中#:1 输入:20458 谱库:NIST08.LIB
SI:90 分子式:C9H7N02 CAS:6587-24-2 摩尔质量:161 保留指数:1338
组分名称:Benzoic acid, 2-cyano-, methyl ester \$\$ Benzoic acid, o-cyano-, methyl ester \$\$ Methyl o-cyanobenz



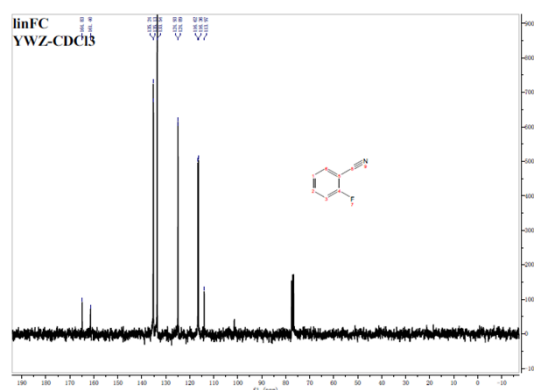
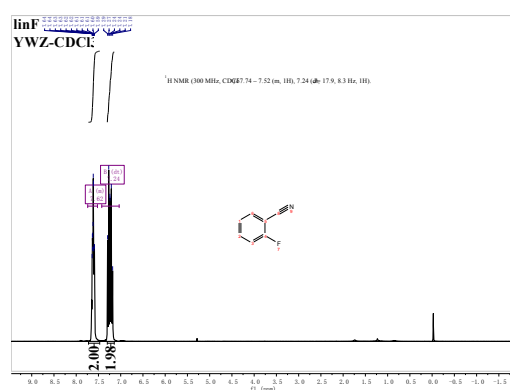
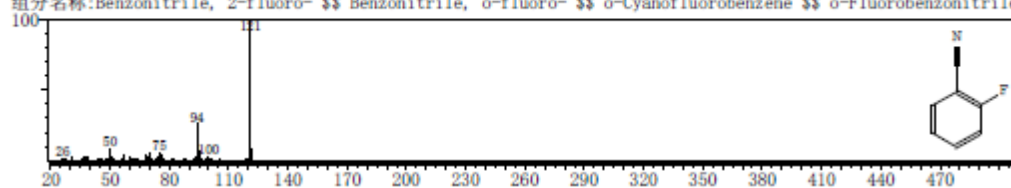
2-Fluorobenzonitrile (1q)



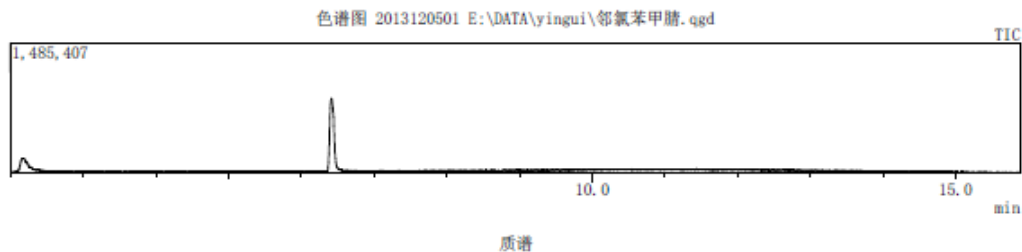
质谱



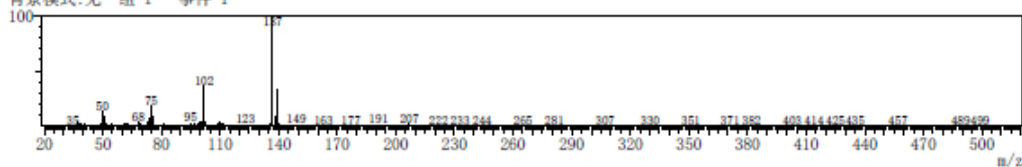
命中#:4 输入:5370 谱库:NIST08.LIB
SI:97 分子式:C7H4FN CAS:394-47-8 摩尔质量:121 保留指数:933
组分名称:Benzonitrile, 2-fluoro- \$\$ Benzonitrile, o-fluoro- \$\$ o-Cyanofluorobenzene \$\$ o-Fluorobenzonitrile



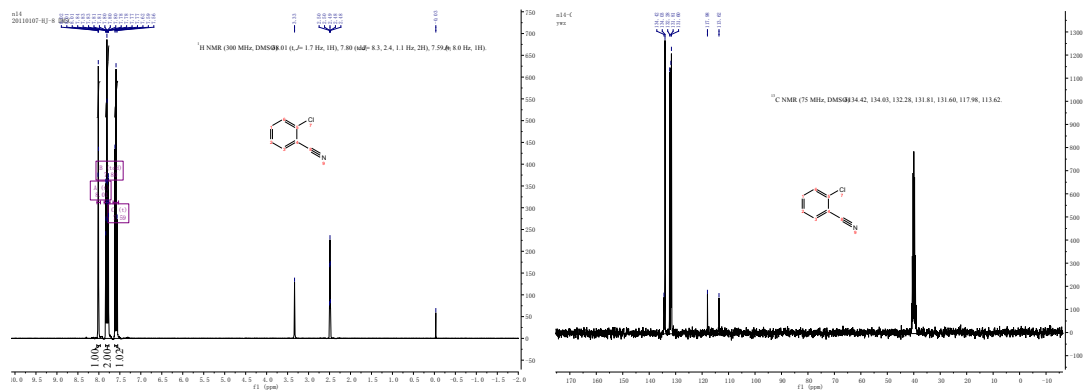
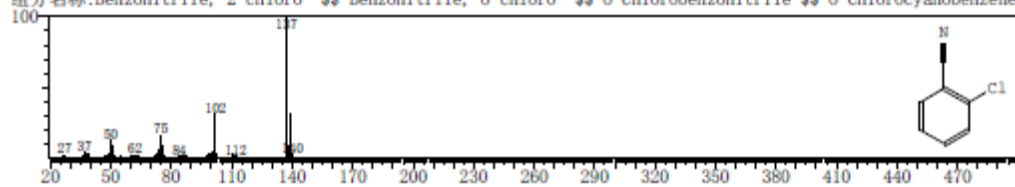
2-Chlorobenzonitrile (1r)



流路号:1 保留时间:6.415(扫描数:884)
质量峰:466
原始模式:平均 6.230-6.860(847-973) 基峰:137(32048)
背景模式:无 组 1 - 事件 1

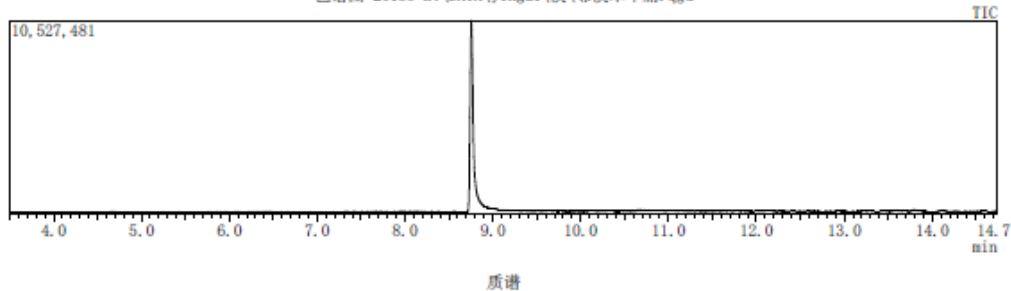


命中#:2 输入:6496 谱库:NIST08s.LIB
SI:94 分子式:C7H4ClN CAS:873-32-5 摩尔质量:137 保留指数:1138
组分名称:Benzonitrile, 2-chloro- \$\$ Benzonitrile, o-chloro- \$\$ o-Chlorobenzonitrile \$\$ o-Chlorocyanobenzene

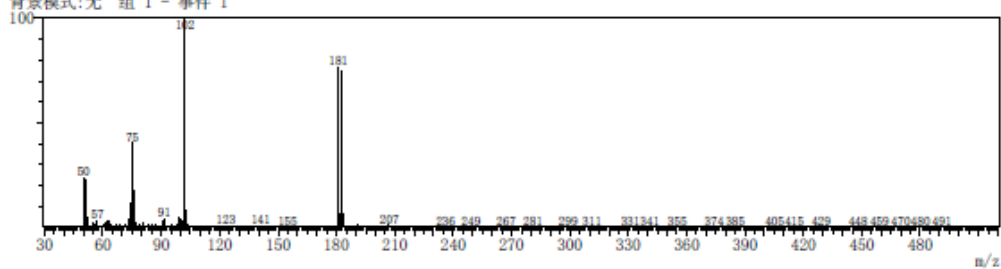


2-Bromobenzonitrile (1s)

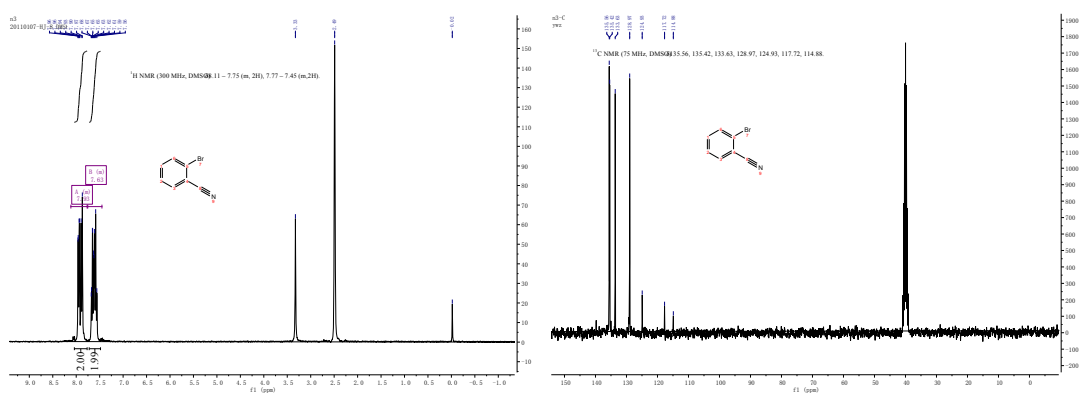
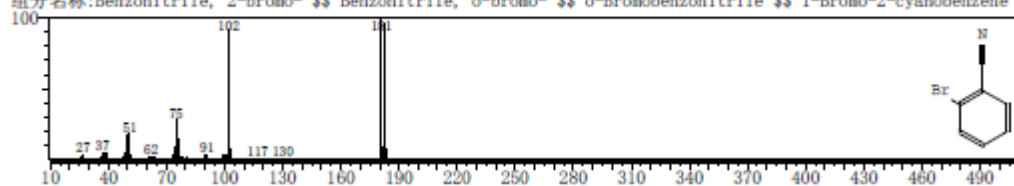
色谱图 20136 E:\DATA\yingui\溴\邻溴苯甲腈.qgd



流路号:1 保留时间:8.755(扫描数:1052)
质量峰:451
原始模式:平均 8.545-9.300(1010-1161) 基峰:102(155473)
背景模式:无 组 1 - 事件 1

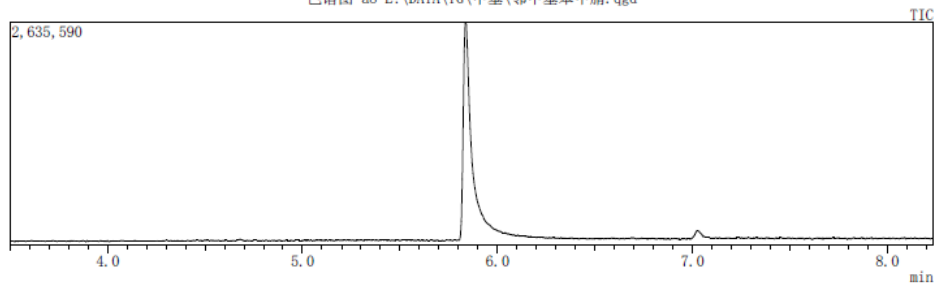


命中#:5 输入:31322 谱库:NIST08.LIB
SI:92 分子式:C7H4BrN CAS:2042-37-7 摩尔质量:181 保留指数:1278
组分名称:Benzonitrile, 2-bromo- \$\$ Benzonitrile, o-bromo- \$\$ o-Bromobenzonitrile \$\$ 1-Bromo-2-cyanobenzene :



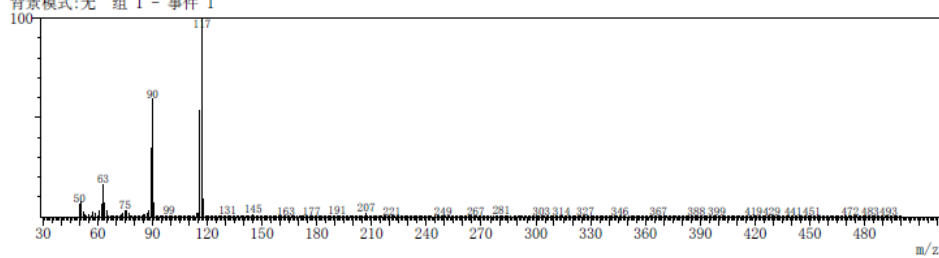
2-Methylbenzonitrile (1t)

色谱图 a8 E:\DATA\YG\甲基\邻甲基苯甲腈. qgd



质谱

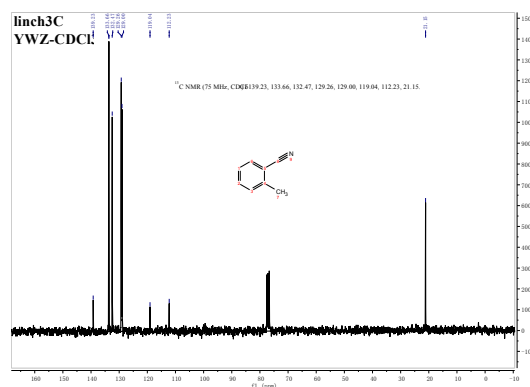
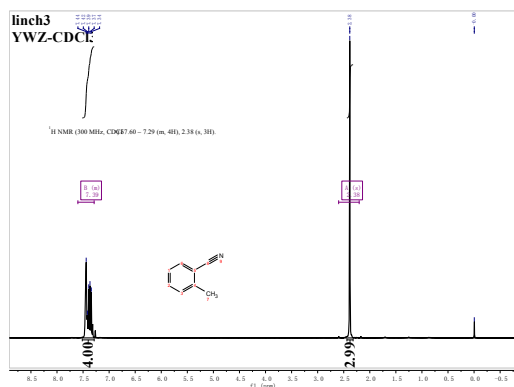
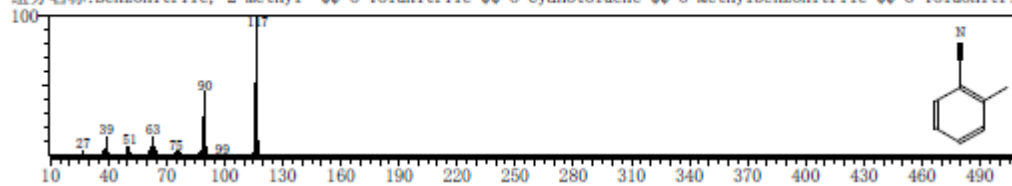
流路号:1 保留时间:5.835(扫描数:468)
质量峰:451
原始模式:平均 5.775-6.030(456-507) 基峰:117(154844)
背景模式:无 组 1 - 事件 1



命中#:1 输入:3675 谱库:NIST08s.LIB

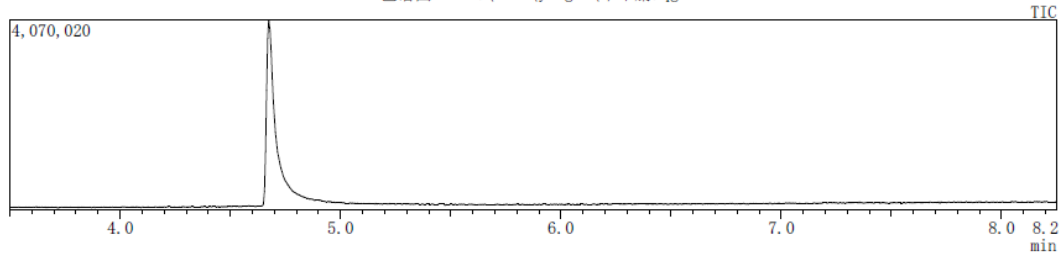
SI:88 分子式:C8H7N CAS:529-19-1 摩尔质量:117 保留指数:1071

组分名称:Benzonitrile, 2-methyl- \$\$ o-Tolunitrile \$\$ o-Cyanotoluene \$\$ o-Methylbenzonitrile \$\$ o-Tolunitri



Benzonitrile (1u)

色谱图 a2 E:\DATA\yingui\苯甲腈.qgd



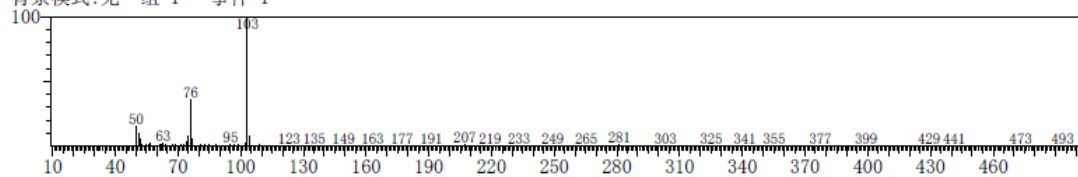
谱库

<< 目标组分 >>

行号#:1 保留时间:4.675(扫描数#:236) 质量峰:451

原始模式:平均 4.605-5.050(222-311) 基峰:103.05(241400)

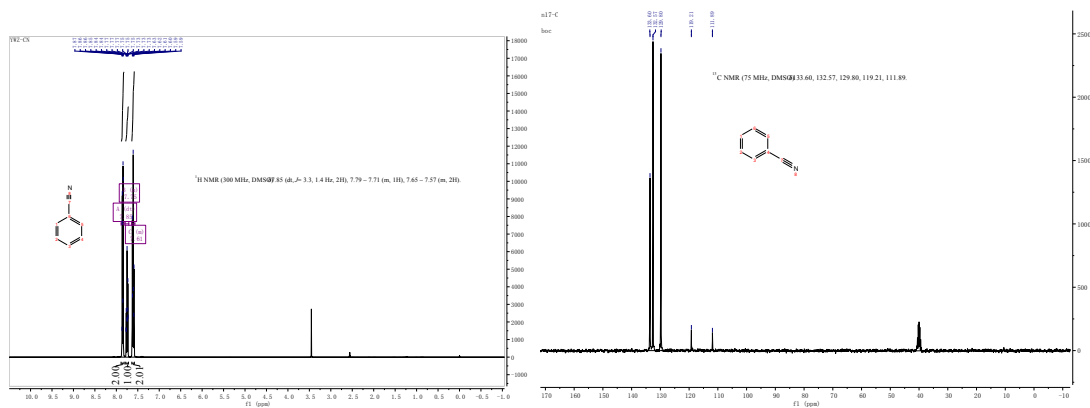
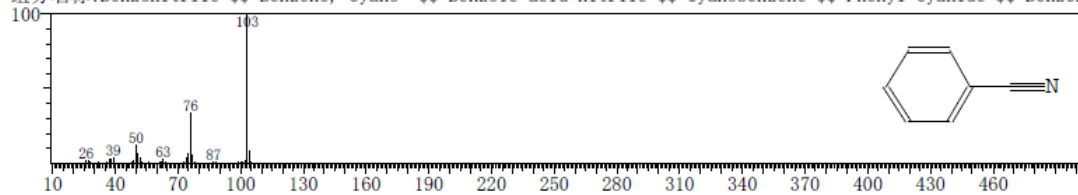
背景模式:无 组 1 - 事件 1



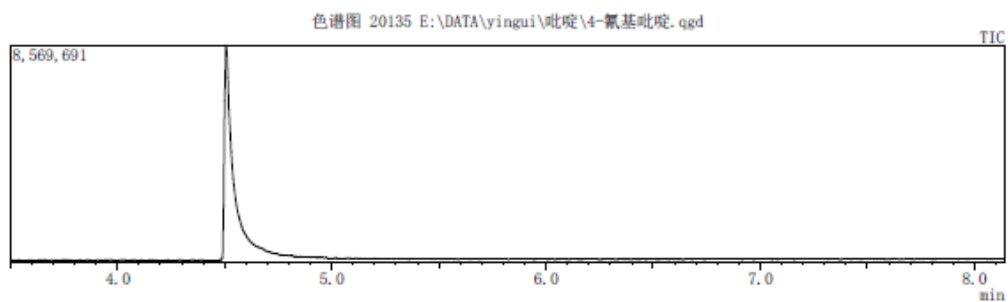
命中#:1 输入:2160 谱库:NIST08s.LIB

SI:95 分子式:C7H5N CAS:100-47-0 摩尔质量:103 保留指数:958

组分名称:Benzonitrile \$\$ Benzene, cyano- \$\$ Benzoic acid nitrile \$\$ Cyanobenzene \$\$ Phenyl cyanide \$\$ Benze



4-Cyanopyridine (1v)



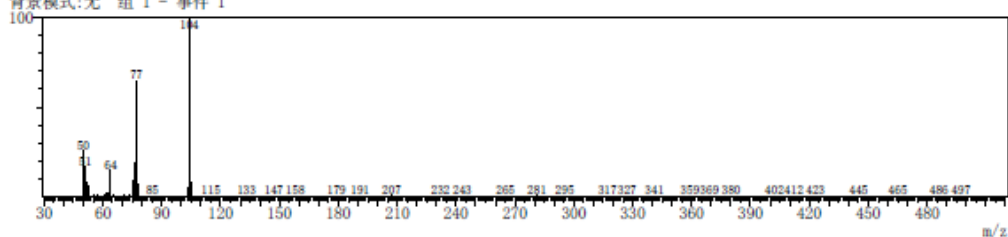
质谱

流路号:1 保留时间:4.505(扫描数:202)

质量峰:451

原始模式:平均 4.435-4.970(188-295) 基峰:104(303190)

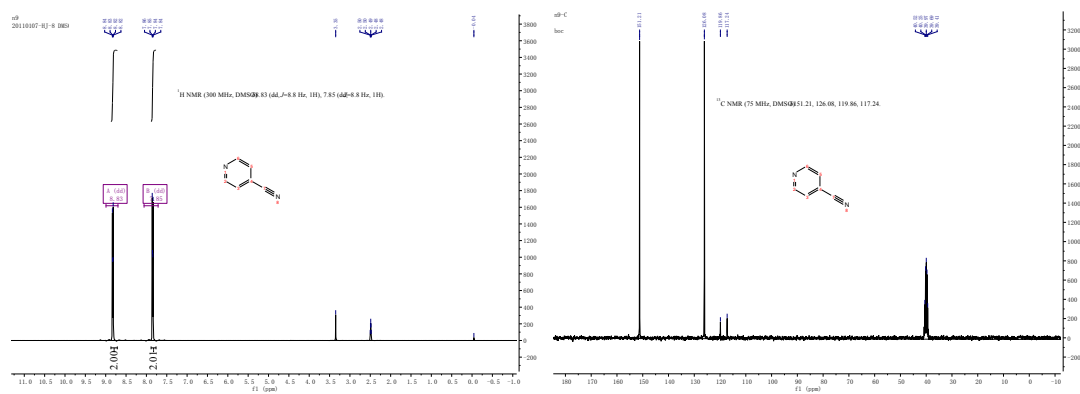
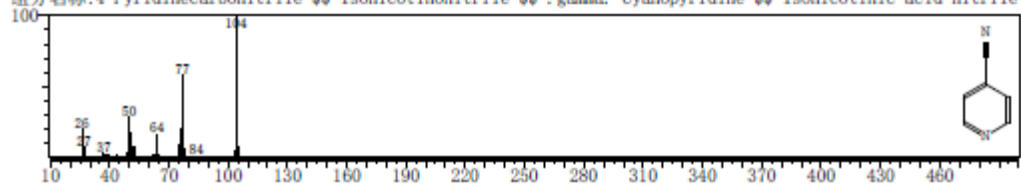
背景模式:无 组 1 - 事件 1



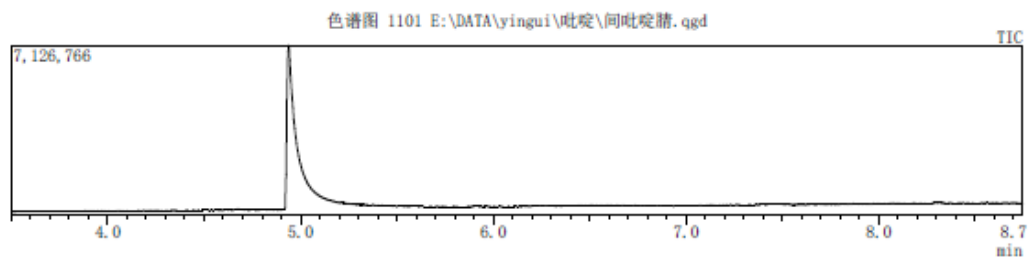
命中#:1 输入:2260 谱库:NIST08s.LIB

SI:98 分子式:C6H4N2 CAS:100-48-1 摩尔质量:104 保留指数:952

组分名称:4-Pyridinecarbonitrile \$\$ Isonicotinonitrile \$\$.gamma.-Cyanopyridine \$\$ Isonicotinic acid nitrile



3-Cyanopyridine (1w)



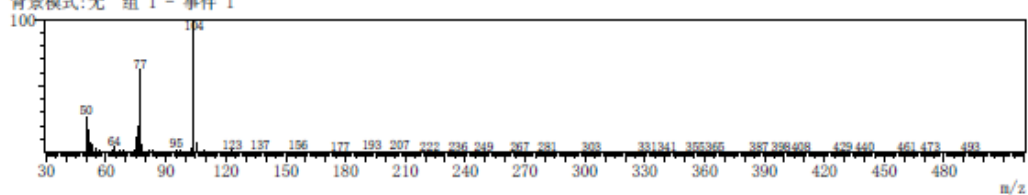
质谱

流路号:1 保留时间:4.940(扫描数:289)

质量峰:451

原始模式:平均 4.840-5.230(269-347) 基峰:104(425526)

背景模式:无 组 1 - 事件 1



命中#:2 输入:2556 谱库:NIST08.LIB

SI:92 分子式:C6H4N2 CAS:100-54-9 摩尔质量:104 保留指数:952

组分名称:3-Pyridinecarbonitrile \$\$ Nicotinonitrile \$\$ Nicotinic acid nitrile \$\$ 3-Cyanopyridine \$\$ 3-Pyridyl

