Supplementary Material (ESI) for Chemical Communications

Strained Azetidinium Ylides: New Reagents for Epoxidation
The peculiar reactivity of 1-(aminoethyl)-1-cyano epoxides

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General comments

^{1}H and ^{13}C spectra were recorded on a Bruker Avance 300 spectrometer at 300 and 75 MHz respectively; chemical shifts are reported in ppm from TMS. Optical rotations were determined with a Perkin Elmer 141 instrument. All the reactions were carried out under argon. Column chromatography was performed on a silica gel 230-400 mesh. The TLCs were run on Merck Kieselgel $60F_{254}$ plates. The melting points are uncorrected. THF and ether were distilled from sodium/benzophenone ketyl. Dichloromethane was distilled from calcium hydride.

2-[2-(Benzyl-methyl-amino)-ethyl]-3-phenyl-oxirane-2-carbonitrile, **4a**

A 50 mL flask was charged with 148 mg of azetidinium salt **3** (0.41 mmol, M = 358.47), 25 mL of dry THF were added. After complete dissolution, the mixture was cool to -78°C with acetone/dry ice. At this temperature benzaldehyde (42 µL, 1 equiv., 0.41 mmol, M = 106.12, d = 1.044) was added immediately followed by LiHMDS in THF (620 µL, 1.5 equiv., 0.62 mmol, c = 1 $mol.L^{-1}$) The reaction was completed after a period of 15 min, at which point 20 mL of a saturated solution of ammonium chloride were added (the temperature was still of -78°C). The mixture was partitioned between water and dichloromethane, the organic phases were dried over $MgSO_4$ and the solvent evaporated under vacuum. The brown residue was rapidly purified by chromatography over silica gel (eluent Et_2O/PE : 1/1, *Rf* 0.3) to give epoxide **4a** as a colourless oil (119 mg, 98 %, M = 292.37). ν_{max} (KBr)/cm^{-1} 3405, 3352, 2238. δ_H (300 MHz; $CDCl_3$) 2.11-2.24 (2H, m), 2.29 (3H, s), 2.73-2.90 (2H, m), 3.55-3.66 (2H, m), 4.12 (1H, s), 7.31-7.35 (6H, m), 7.39-7.47 (4H, m). δ_C (75 MHz; $CDCl_3$) 32.59, 41.82, 52.80, 56.50, 62.66, 63.59, 116.54, 126.40, 127.22, 127.88, 128.30, 129.06, 129.45, 132.26, 138.50.

2-[2-(Benzyl-methyl-amino)-ethyl]-3-(3-nitro-phenyl)-oxirane-2-carbonitrile, **4b**

The procedure employed for compound **4a** was reproduced using 3-nitrobenzaldehyde with azetidinium salt **3**. The residue was purified by chromatography over silica gel (eluent Et_2O/PE : 1/1, *Rf* 0.1) to give epoxide **4b** as a colourless oil (177 mg, 77 %, M = 337.37). ν_{max} (KBr)/cm^{-1} 3411, 3348, 2242. δ_H (300 MHz; $CDCl_3$) 2.00-2.07 (1H, m), 2.12-2.20 (1H, m), 2.17 (3H, s), 2.61-2.73 (2H, m), 3.43 (1H, d, *J* 13 Hz), 3.52 (1H, d, *J* 13 Hz), 4.10 (1H, s), 7.17-7.20 (5H, m), 7.50-7.63 (2H, m), 8.17-8.20 (2H, m). δ_C (75 MHz; $CDCl_3$) 32.22, 41.85, 52.66, 56.74, 62.23, 62.71, 115.97, 121.90, 124.35, 127.34, 128.40, 129.05, 129.84, 132.10, 134.73, 138.38, 148.34.

2-[2-(Benzyl-methyl-amino)-ethyl]-3-ethyl-oxirane-2-carbonitrile, **4e**

The procedure employed for compound **4a** was reproduced using propanal with azetidinium salt **3**. The residue was purified by chromatography over silica gel (eluent Et_2O/PE : 1/1, *Rf* 0.2) to give epoxide **4e** as a colourless oil (115 mg, 94 %, M = 244.3). ν_{max} (KBr)/cm^{-1} 3405, 3345, 2239. δ_H (300 MHz; $CDCl_3$) 1.02 (3H, t, *J* 7.5 Hz), 1.65-1.72 (2H, m), 1.74-1.98 (2H, m), 2.10 (3H, s), 2.53-2.65 (2H, m), 2.86 (1H, t, *J* 6.1 Hz), 3.38 (1H, d, *J* 13.1 Hz), 3.49 (1H, d, *J* 13.1 Hz), 7.16-7.24 (5H, m). δ_C (75 MHz; $CDCl_3$) 9.84, 23.59, 32.10, 41.84, 52.86, 53.04, 62.55, 64.38, 117.48, 127.19, 128.33, 129.01, 138.59,

2-[2-(Benzyl-methyl-amino)-ethyl]-3-methyl-3-phenyl-oxirane-2-carbonitrile, **4f**

The procedure employed for compound **4a** was reproduced using acetophenone with azetidinium salt **3**. The residue was purified by chromatography over silica gel (eluent Et_2O/PE : 1/1, *Rf* 0.4) to give epoxide **4f** as a colourless oil (179 mg, 99 %, M = 306.40). ν_{max} (KBr)/cm^{-1} 3419, 3355, 2245. δ_H (300 MHz; $CDCl_3$) 1.40-1.59 (2H, m), 1.80 (3H, s), 1.92, (3H, s), 2.35-2.52 (2H, m), 3.22 (1H, d, *J* 13 Hz), 3.36 (1H, d, *J* 13 Hz), 7.07-7.25 (10H, m). δ_C (75 MHz; $CDCl_3$) 22.69, 28.77, 41.89, 52.55, 58.13, 62.40, 67.33, 118.06, 126.39, 127.16, 128.34, 128.52, 128.54, 129.07, 136.61, 138.86.

2-[2-(Benzyl-methyl-amino)-ethyl]-3,3-dimethyl-oxirane-2-carbonitrile, **4g**

The procedure employed for compound **4a** was reproduced using acetone with azetidinium salt **3**. The residue was purified by chromatography over silica gel (eluent Et_2O/PE : 1/1, *Rf* 0.4) to give epoxide

4g as a colourless oil (120 mg, 99 %, M = 244.33). δ_H (300 MHz; $CDCl_3$) 1.32 (3H, s), 1.58 (3H, s), 1.89-2.07 (2H, m), 2.25 (3H, s), 2.72 (2H, t, *J* 7.2 Hz), 3.51 (1H, d, *J* 12.9 Hz), 3.60 (1H, d, *J* 12.9 Hz), 7.22-7.33 (5H, m). δ_C (75 MHz; $CDCl_3$) 19.19, 22.82, 29.26, 42.13, 52.98, 57.02, 62.53, 63.71, 118.35, 127.21, 128.36, 129.03, 138.68. MS (ESI) [MNa^+] $C_{15}H_{20}N_2NaO$ requires 267.15, found 267.20.

2-[2-(Benzyl-methyl-amino)-1-phenyl-ethyl]-3-methyl-3-phenyl-oxirane-2-carbonitrile, **8**
The procedure employed for compound **4a** was reproduced using acetophenone with azetidinium salt **7**. The residue was purified by chromatography over silica gel (eluent Et_2O/PE : 3/7, *Rf* 0.3) to give epoxide **8** as a colourless oil (83 mg, 61 %, M = 382.49). $[\alpha]_D^{25}$ +37.8 (*c* 0.85 in $CHCl_3$). ν_{max} (KBr)/cm^{-1} 3420, 3353, 2242. δ_H (300 MHz; $CDCl_3$) 1.56 (3H, s), 1.92 (3H, s), 2.47 (1H, dd, *J* 6.7 and 9.2 Hz), 2.55-2.61 (1H, m), 2.91 (1H, dd, *J* 9.2 and 12.7 Hz), 3.14 (1H, d, *J* 13 Hz), 3.40 (1H, d, *J* 13 Hz), 7.13-7.29 (15H, m). δ_C (75 MHz; $CDCl_3$) 22.56, 41.99, 42.79, 59.77, 63.01, 69.33, 117.48, 127.11, 127.24, 127.80, 128.34, 128.37, 128.45, 128.77, 128.82, 129.04, 136.61, 137.48, 138.90.

2-[2-(Benzyl-methyl-amino)-1-phenyl-ethyl]-3-phenyl-oxirane-2-carboxylic acid ethyl ester, **10**
The procedure employed for compound **4a** was reproduced using benzaldehyde with azetidinium salt **9**. The residue was purified by chromatography over silica gel (eluent Et_2O/PE : 3/7, *Rf* 0.3) to give epoxide **10** as a colourless oil (125 mg, 85%, M = 415.52). $[\alpha]_D^{25}$ +26.3 (*c* 1.35 in $CHCl_3$). ν_{max} (KBr)/cm^{-1} 3425, 3356, 1745. δ_H (300 MHz; $CDCl_3$) 1.06 (3H, t, *J* 7.1 Hz), 1.37 (3H, s), 2.33 (1H, dd, *J* 4 and 12.5 Hz), 2.74 (1H, dd, *J* 4 and 10.5 Hz), 2.91 (1H, d, *J* 13.1 Hz), 3.09 (1H, d, *J* 13.1 Hz), 3.35 (1H, dd, *J* 10.5 and 12.5 Hz), 4.31 (1H, s), 6.96-7.21 (15H, m). δ_C (75 MHz; $CDCl_3$) 13.94, 41.30, 42.02, 57.04, 61.53, 62.45, 62.88, 65.45, 126.82, 127.04, 128.02, 128.14, 128.41, 128.56, 128.58, 128.94, 129.00, 133.61, 137.96, 138.63, 169.19.

2-Benzyl-1-methyl-2-phenyl-pyrrolidin-3-one **13a**
The crude epoxide **4a**, prepared as describe above is heated without solvent under reduced pressure for a period of 4 hours (Precautions should be taken due to the formation of hydrogen cyanide!) The yellow oil was purified by chromatography on silica gel (eluent Et_2O/PE : 1/1, *Rf* 0.6) to give pyrrolidinone **13a** as a colourless oil (89 mg, 81%, M = 265.35). ν_{max} (KBr)/cm^{-1} 3057, 2924, 1746. δ_H (300 MHz; $CDCl_3$) 1.81-1.92 (1H, m), 2.23-2.26 (1H, m), 2.31 (3H, s), 2.69-2.82 (2H, m), 3.22 (1H, d, *J* 11.6 Hz), 3.30 (1H, d, *J* 11.6 Hz), 7.12-7.29 (10H, m). δ_C (75 MHz; $CDCl_3$) 35.49, 37.88, 39.11, 48.36, 73.81, 126.43, 127.42, 127.51, 127.90, 128.32, 131.18, 137.34, 139.45, 217.89. HRMS (TOF MS ES+) [MH^+] $C_{18}H_{20}NO$ requires 266.1545, found 266.1551.

2-Benzyl-1-methyl-2-(3-nitro-phenyl)-pyrrolidin-3-one, **13b**
The crude epoxide **4b**, prepared as describe above is heated without solvent under reduced pressure for a period of 12 hours (Precautions should be taken due to the formation of hydrogen cyanide!) The yellow oil was purified by chromatography on silica gel (eluent Et_2O/PE : 1/1, *Rf* 0.4) to give pyrrolidinone **13b** as a colourless oil (76 mg, 71%, M = 310.34). ν_{max} (KBr)/cm^{-1} 3083, 2919, 1746. δ_H (300 MHz; $CDCl_3$) 2.02 (1H, ddd, *J* 4.6 and 7.7 and 18.7 Hz), 2.38 (1H, ddd, *J* 6.5 and 8.3 and 18.7 Hz), 2.49 (3H, s), 2.54-2.61 (1H, m), 2.93-3.00 (1H, m), 3.20 (1H, d, *J* 13.6 Hz), 3.47 (1H, d, *J* 13.6 Hz), 7.15-7.19 (5H, m), 7.47 (1H, t, *J* 8.1 Hz), 7.67-7.70 (1H, m), 8.05-8.09 (1H, m), 8.24 (1H, br s). δ_C (75 MHz; $CDCl_3$) 35.29, 37.44, 39.73, 48.35, 73.52, 122.47, 122.53, 127.07, 128.37, 129.40, 130.97, 133.80, 136.44, 143.08, 148.07, 216.30. HRMS (TOF MS ES+) [MH^+] $C_{18}H_{19}N_2O_3$ requires 311.1396, found 311.1402

2-Benzyl-2-(4-methoxy-phenyl)-1-methyl-pyrrolidin-3-one, **13c**
The crude epoxide **4c**, prepared as describe above is heated without solvent under reduced pressure for a period of 2 hours (Precautions should be taken due to the formation of hydrogen cyanide!) The yellow oil was purified by chromatography on silica gel (eluent Et_2O/PE : 1/1, *Rf* 0.5) to give pyrrolidinone **13c** as a colourless oil (117 mg, 58%, M = 295.37). ν_{max} (KBr)/cm^{-1} 3073, 2960, 1751. δ_H (300 MHz; $CDCl_3$) 1.82-1.93 (1H, m), 2.23-2.33 (1H, m), 2.32 (3H, s), 2.71-2.79 (2H, m), 3.20

(1H, d, *J* 9 Hz), 3.29 (1H, d, *J* 9 Hz), 3.72 (3H, s), 6.81 (2H, d, *J* 6 Hz), 7.11-7.14 (7H, m). δ_C (75 MHz; $CDCl_3$) 35.42, 37.79, 39.24, 48.29, 55.29, 73.34, 113.63, 126.37, 127.86, 128.63, 131.12, 131.61, 137.42, 158.73, 218.15. HRMS (TOF MS ES+) $[MH^+]$ $C_{19}H_{22}NO_2$ requires 296.1651, found 296.1657

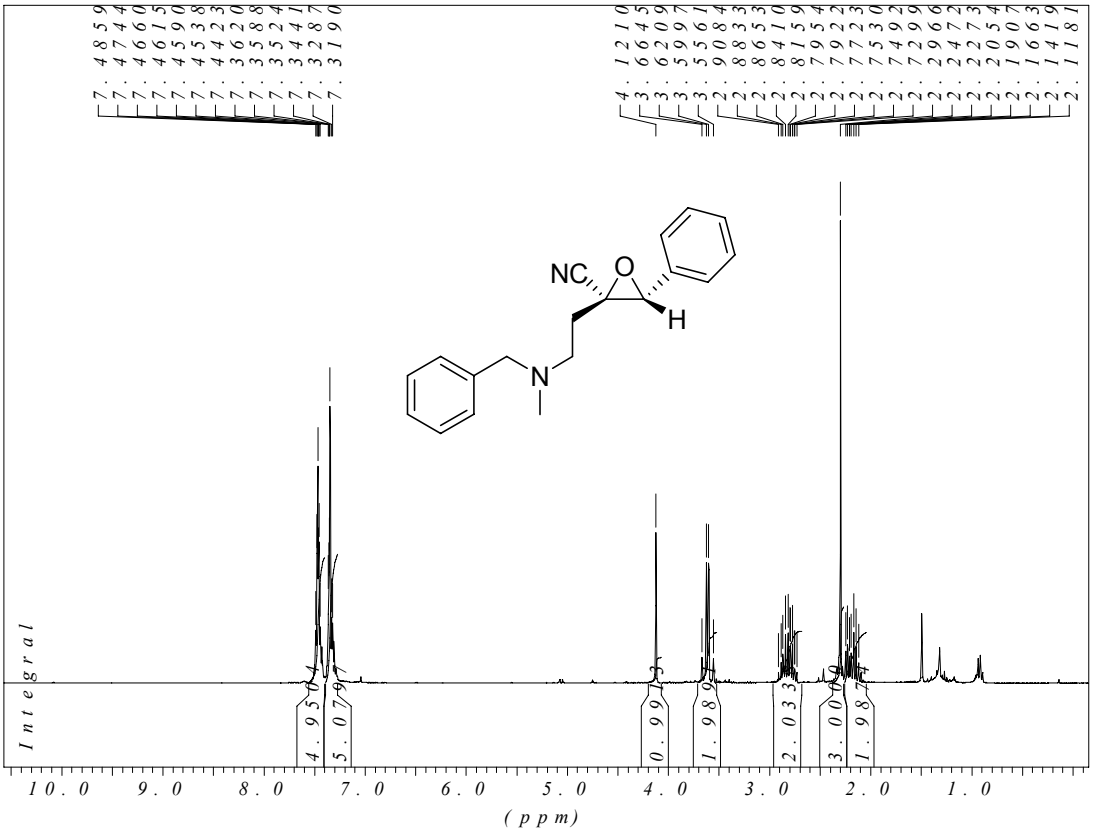
2-Benzyl-2-ethyl-1-methyl-pyrrolidin-3-one, **13d**
The crude epoxide **4d**, prepared as describe above is heated without solvent under reduced pressure for a period of 8 hours (Precautions should be taken due to the formation of hydrogen cyanide!) The yellow oil was purified by chromatography on silica gel (eluent Et_2O/PE : 1/1, *Rf* 0.5) to give pyrrolidinone **13c** as a colourless oil (17 mg, 20%, M = 217.30). ν_{max} (KBr)/cm^{-1} 3057, 3027, 2924, 1746. δ_H (300 MHz; $CDCl_3$) 0.72 (3H, t, *J* 7.3 Hz), 1.48-1.68 (2H, m), 1.89-1.97 (1H, m), 2.10-2.19 (1H, m), 2.46 (3H, s), 2.62-2.75 (3H, m), 2.82-2.90 (1H, m), 6.99-7.02 (2H, m), 7.08-7.18 (3H, m). δ_C (75 MHz; $CDCl_3$) 9.08, 26.12, 34.19, 37.29, 39.01, 48.26, 71.05, 126.19, 127.84, 130.59, 137.62, 218.41. HRMS (TOF MS ES+) $[MH^+]$ $C_{14}H_{20}NO$ requires 218.1545, found 218.1555

2-Benzyl-1-methyl-2-((E)-styryl)-pyrrolidin-3-one, **13e**
The crude epoxide **4e**, prepared as describe above is heated without solvent under reduced pressure for a period of 8 hours (Precautions should be taken due to the formation of hydrogen cyanide!) The yellow oil was purified by chromatography on silica gel (eluent Et_2O/PE : 1/1, *Rf* 0.5) to give pyrrolidinone **13e** as a colourless oil (38 mg, 20%, M = 277.36). δ_H (300 MHz; $CDCl_3$) 2.02-2.15 (1H, m), 2.30-2.44 (1H, m), 2.57 (3H, s), 2.77-2.90 (1H, m), 2.95-3.06 (1H, m), 3.04 and 3.23 (2 x 1H, AB system, *J* 13.8 Hz), 6.26 (1H, d, *J* 16.2), 6.57 (1H, d, *J* 16.2), 7.21-7.39 (10H, m). δ_C (75 MHz; $CDCl_3$) 35.28, 36.82, 39.30, 48.34, 72.30, 125.38, 126.24, 126.40, 127.78, 128.53, 130.71, 132.60, 136.50, 136.88, 215.39. MS (ESI) $[MNa^+]$ $C_{20}H_{21}NNaO$ requires 314.15, found 314.20

Aziridination of phenyl-N-tosylimine.
A 50 mL flask was charged with 359 mg of azetidinium salt **3** (1.0 mmol, M = 358.47), 25 mL of dry THF were added. After complete dissolution, the mixture was cool to -78°C with acetone/dry ice. At this temperature tosylimine (311 mg, 1.2 equiv., 1.2 mmol, M = 259.32) was added immediately followed by LiHMDS in THF (2.2 mL, 2.2 equiv., 2.2 mmol, c = 1 $mol.L^{-1}$) The reaction was completed after a period of 50 min, at which point 20 mL of a saturated solution of ammonium chloride were added (the temperature was still of -78°C). The mixture was partitioned between water and dichloromethane, the organic phases were dried over $MgSO_4$ and the solvent evaporated under vacuum. The TLC (eluent Et_2O/PE : 1/1) showed the presence of two products **18a** and **18b**, with $Rf_{\mathbf{18a}}$ 0.22 and $Rf_{\mathbf{18b}}$ 0.33. Heating at 50°C for 30 min performed the conversion of compound **18b** into product **19** with $Rf_{\mathbf{19}}$ 0.46, while compound **18a** were still present as indicated by the spot with $Rf_{\mathbf{18a}}$ 0.22.
Chromatographic separation using silica gel allowed the isolation of **19** as a pale yellow solid (134 mg, 30 %, M = 418.55) followed by **18a** as a pale yellow oil (144 mg, 30 %, M = 445.57).

2-[2-(Benzyl-methyl-amino)-ethyl]-3-phenyl-1-(toluene-4-sulfonyl)-aziridine-2-carbonitrile, **18a**
ν_{max} (KBr)/cm^{-1} 3078, 3027, 1634, 1593. δ_H (300 MHz; $CDCl_3$) 1.33-1.44 (1H, m), 1.54-1.64 (1H, m), 1.79 (3H, s), 2.24-2.38 (2H, m), 2.33 (3H, s), 3.15 (1H, d, *J* 13.8 Hz), 3.22 (1H, d, *J* 13.8 Hz), 4.43 (1H, s), 7.05-7.24 (12H, m), 7.83 (2H, d, *J* 8.28 Hz). δ_C (75 MHz; $CDCl_3$) 21.81, 28.32, 40.37, 41.55, 51.01, 53.14, 62.26, 116.21, 127.13, 127.60, 128.29, 128.54, 128.80, 128.97, 129.28, 128.84, 130.04, 134.32, 138.45, 145.72.

N-[2-Benzyl-1-methyl-2-phenyl-pyrrolidin-(3E)-ylidene]-4-methyl-benzenesulfonamide, **19**
ν_{max} (KBr)/cm^{-1} 3283, 3062, 2238. δ_H (300 MHz; $CDCl_3$) 2.19 (3H, s), 2.35 (3H, s), 2.39-2.51 (1H, m), 2.60-2.68 (1H, m), 2.83-2.89 (1H, m), 3.06-3.18 (1H, m), 3.16 (1H, d, *J* 13.7 Hz), 3.40 (1H, d, *J* 13.7 Hz), 6.98-7.08 (7H, m), 7.17-7.28 (5H, m), 7.66 (2H, d, *J* 8.3 Hz). δ_C (75 MHz; $CDCl_3$) 21.67, 34.72, 34.96, 39.62, 50.39, 75.01, 126.31, 127.46, 127.50, 127.58, 127.65, 128.44, 129.47, 131.32, 136.92, 137.23, 139.27, 143.97, 198.70.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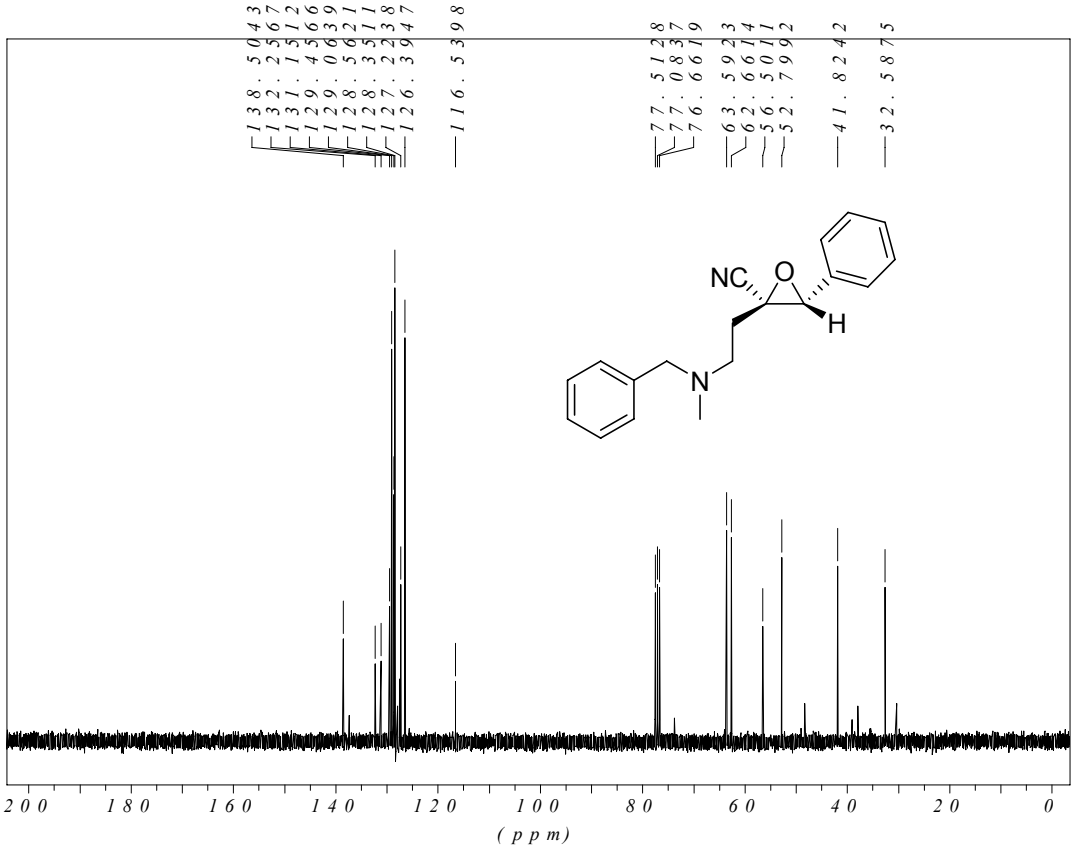
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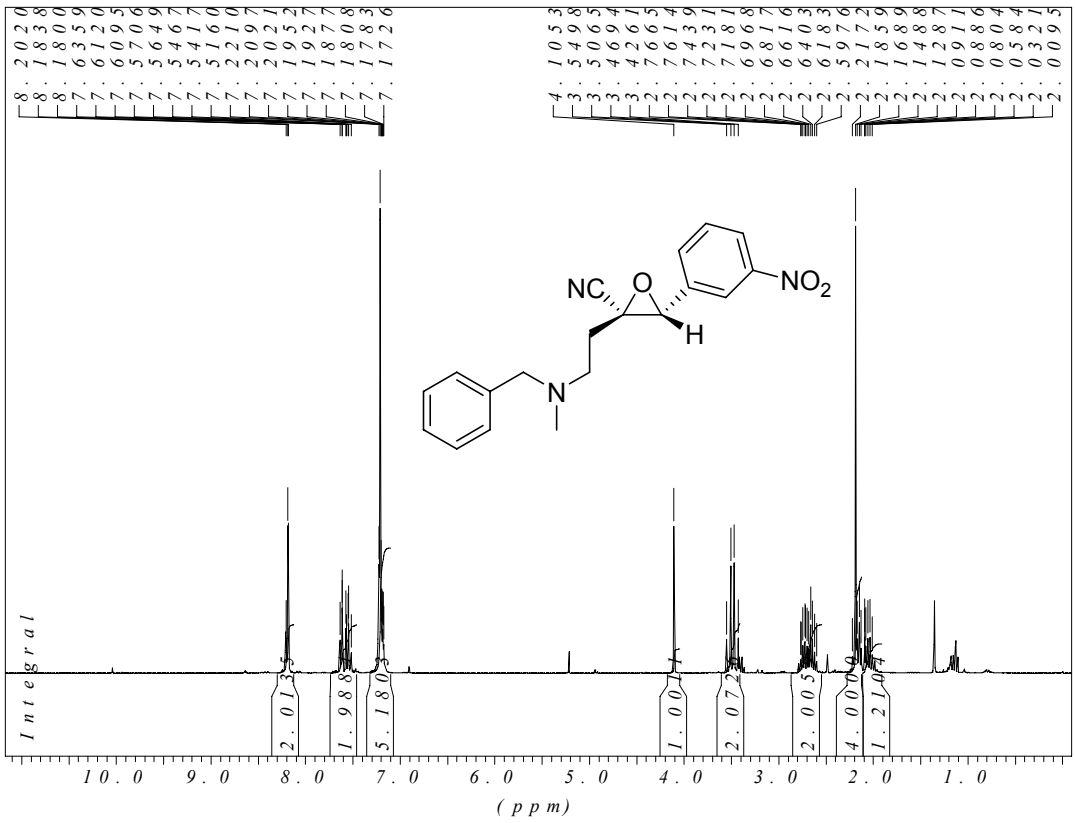
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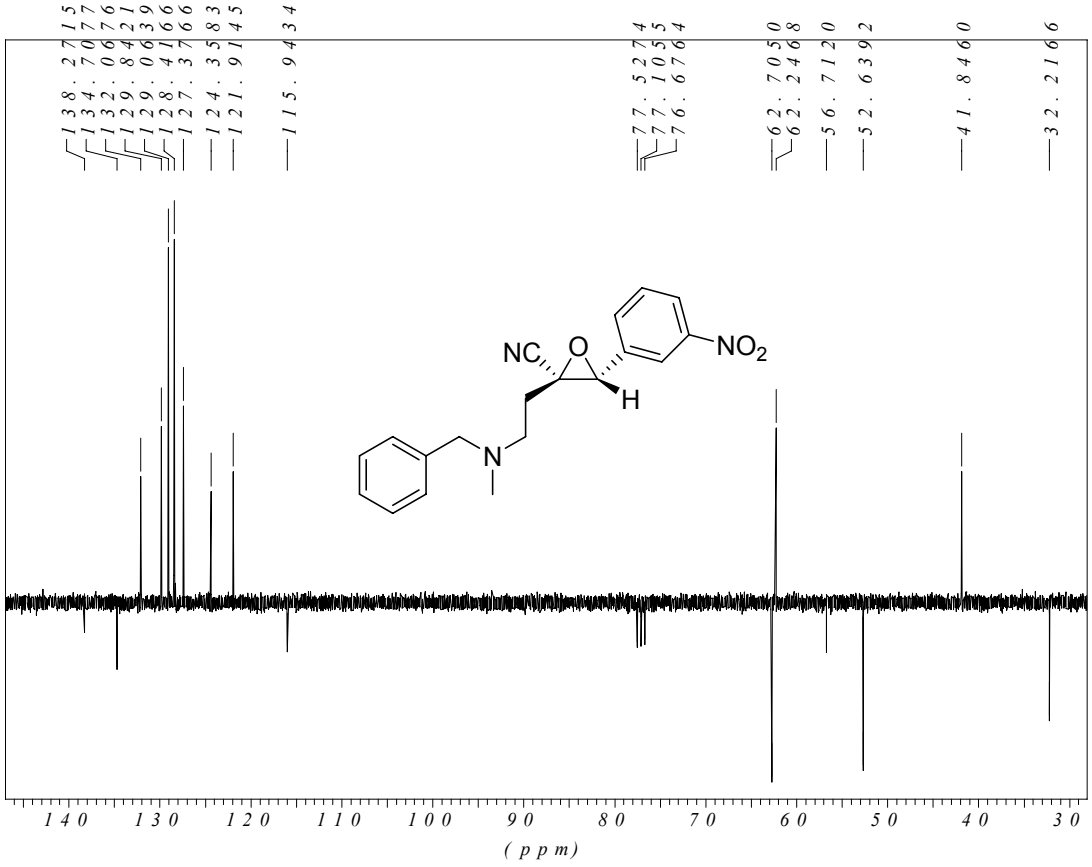

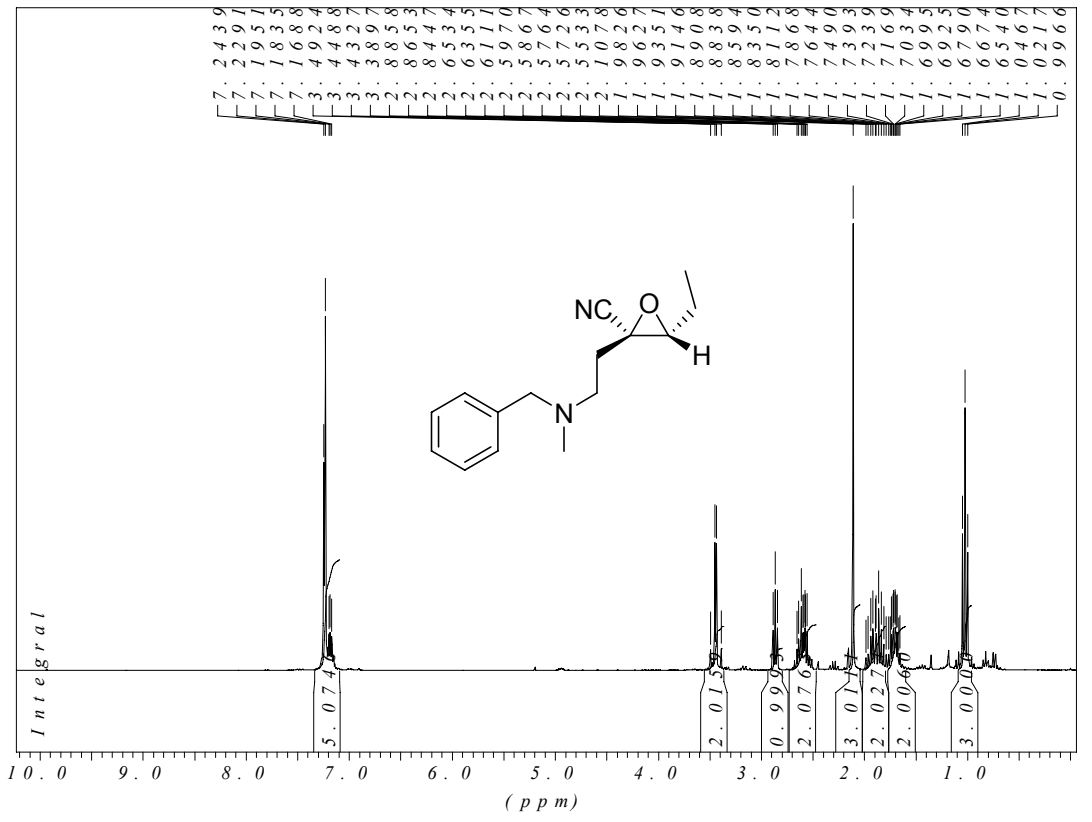

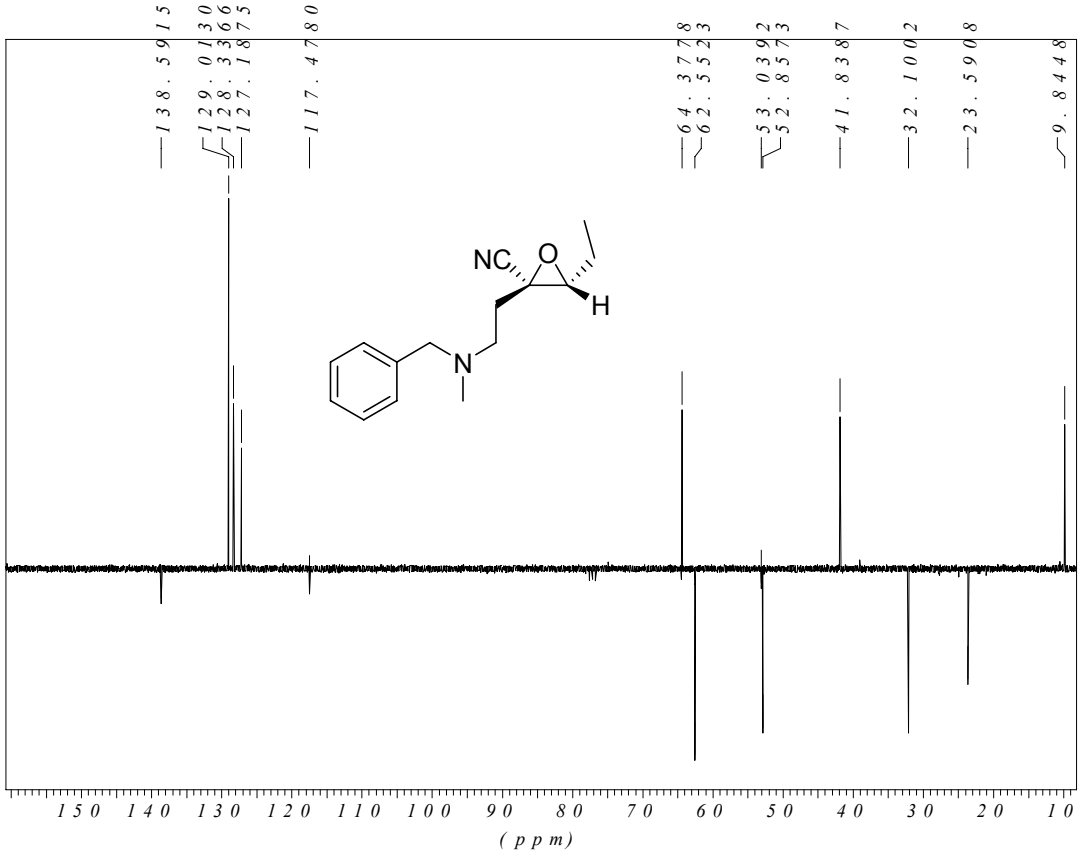

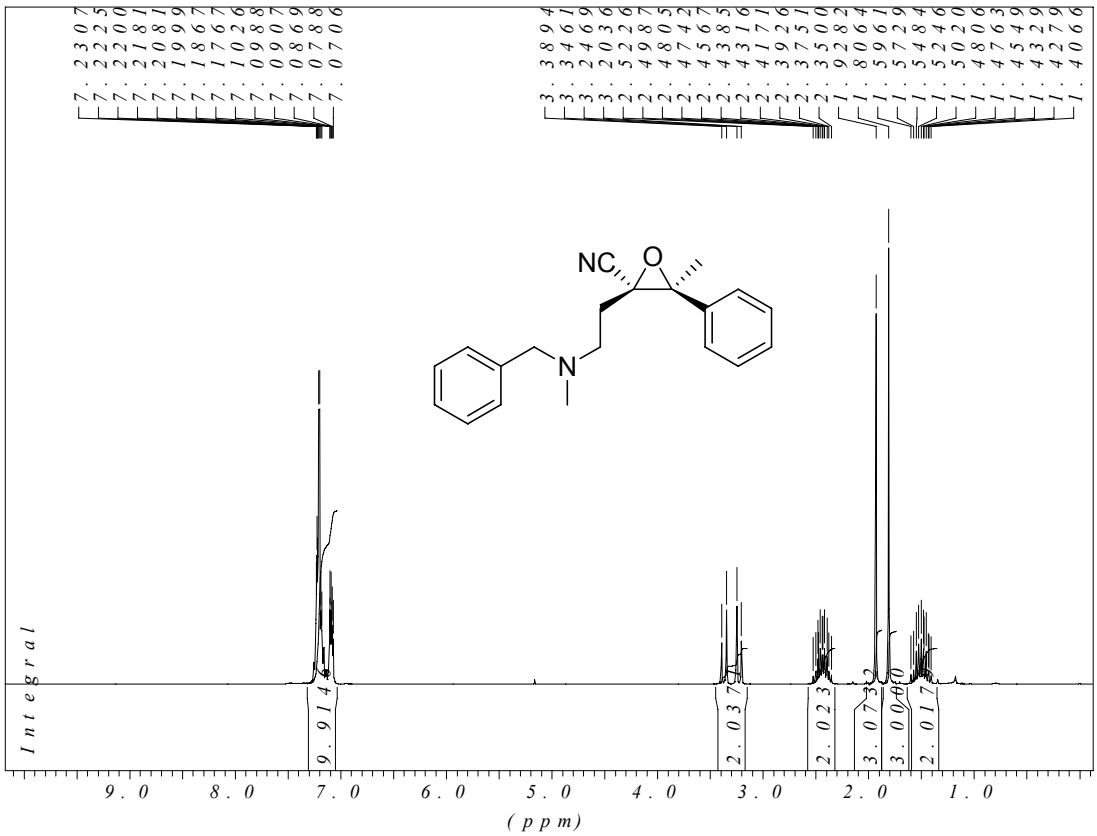

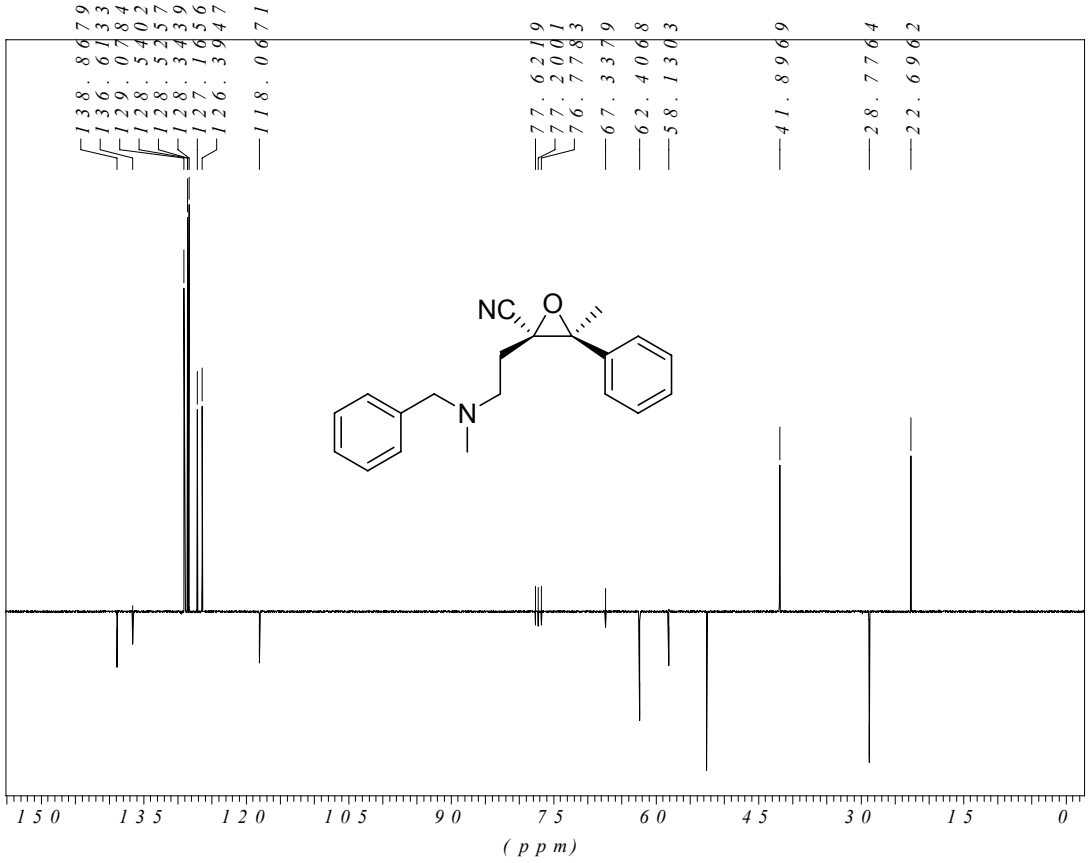

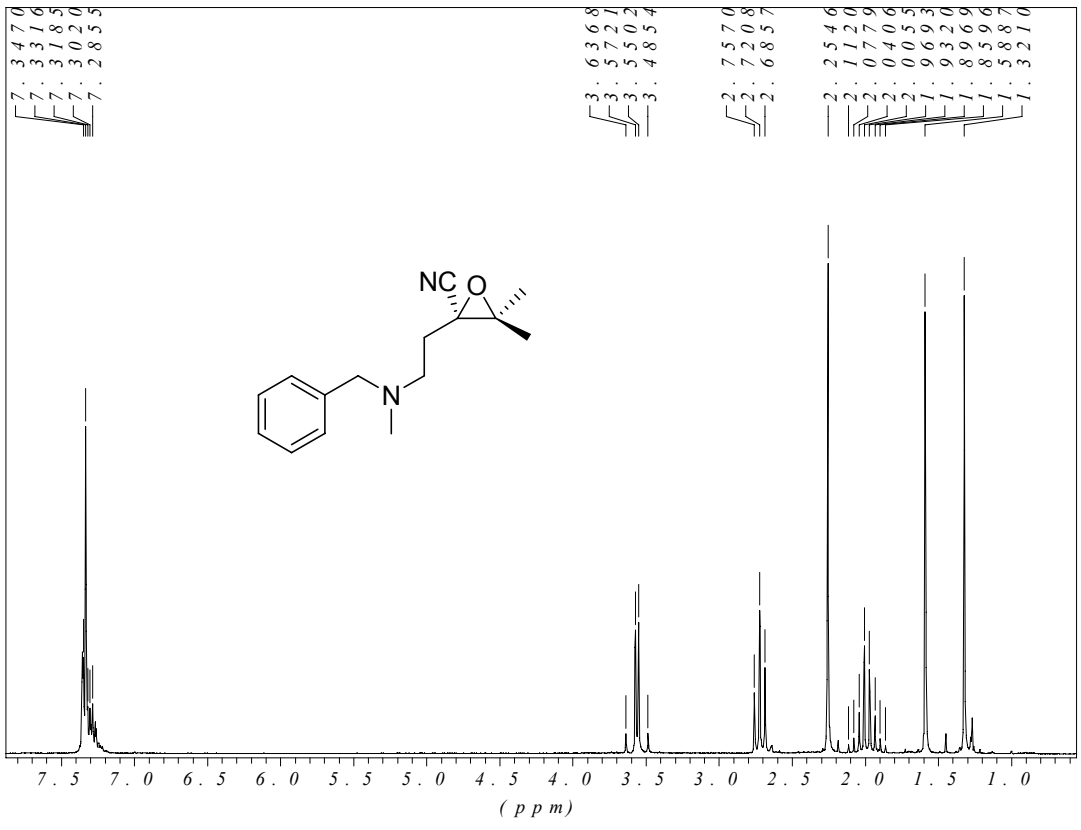

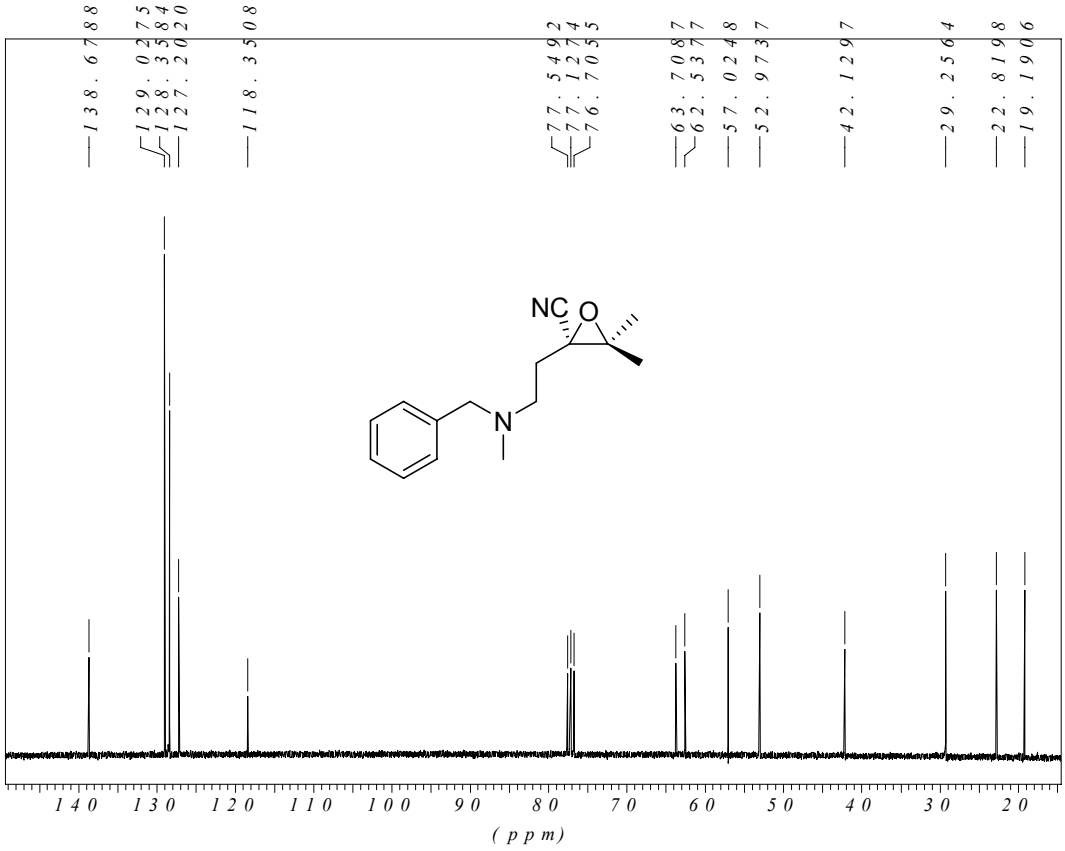
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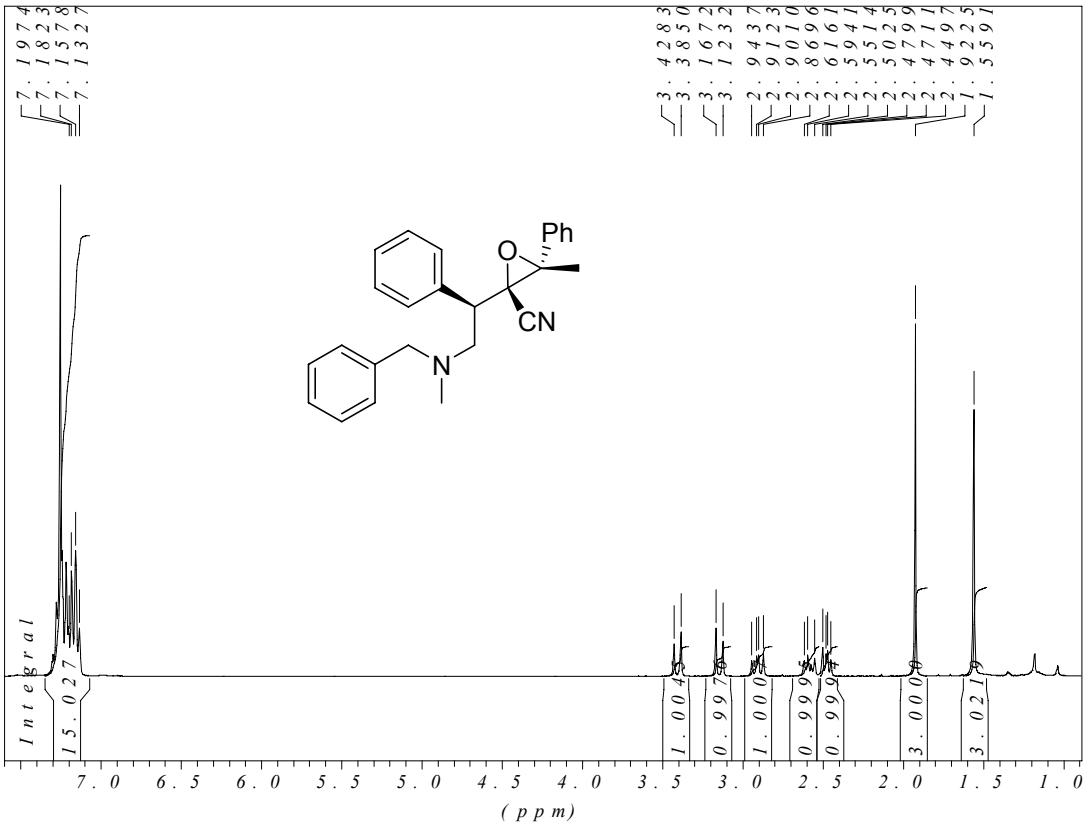
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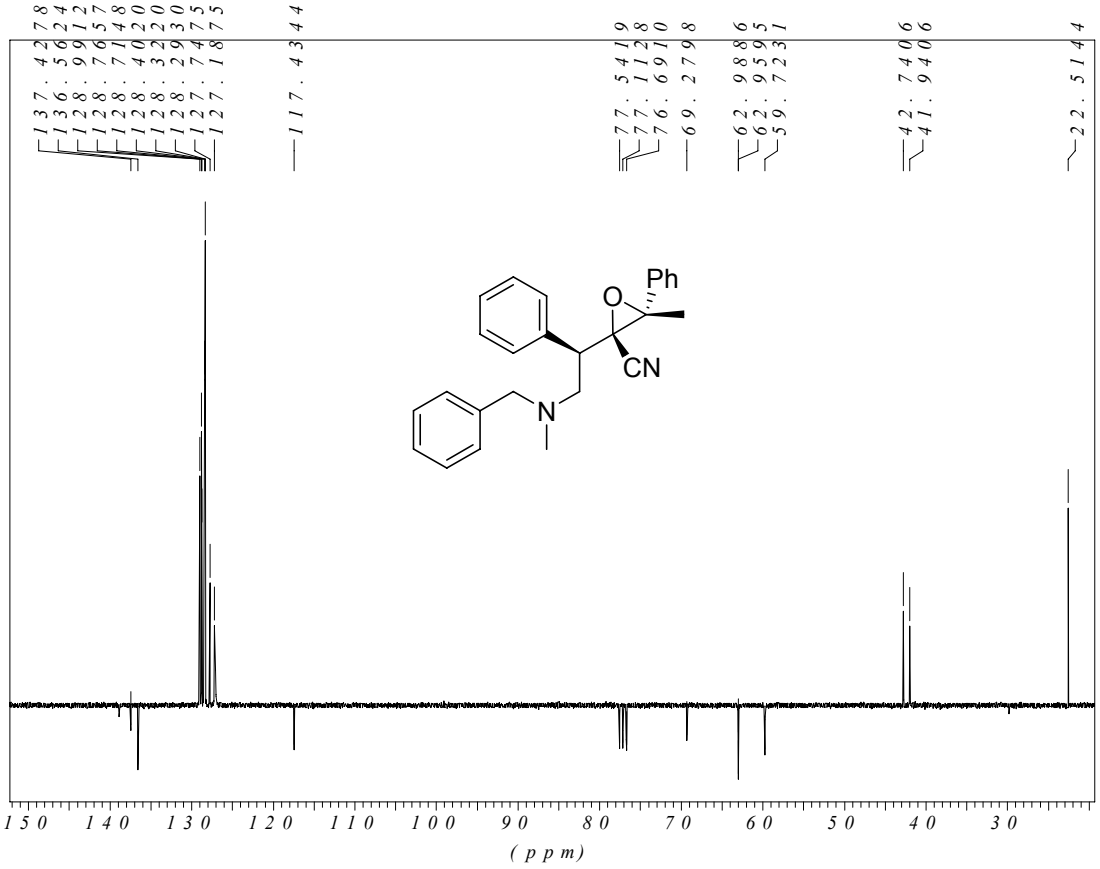
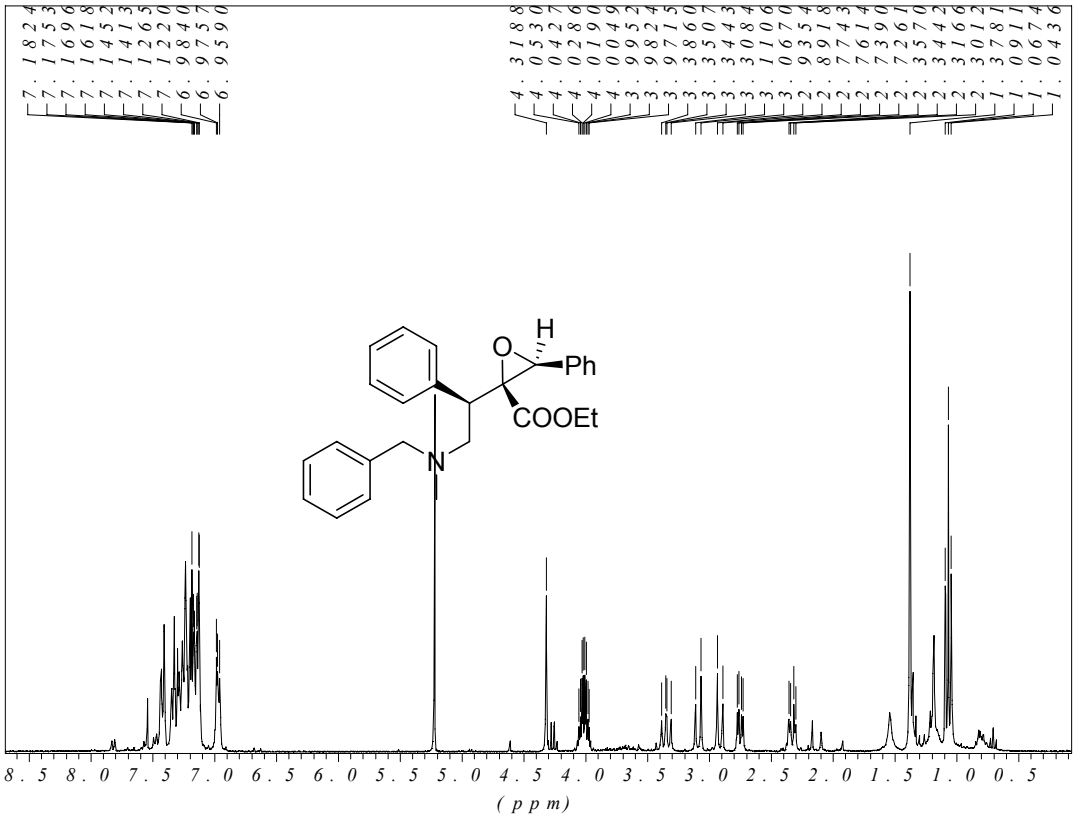
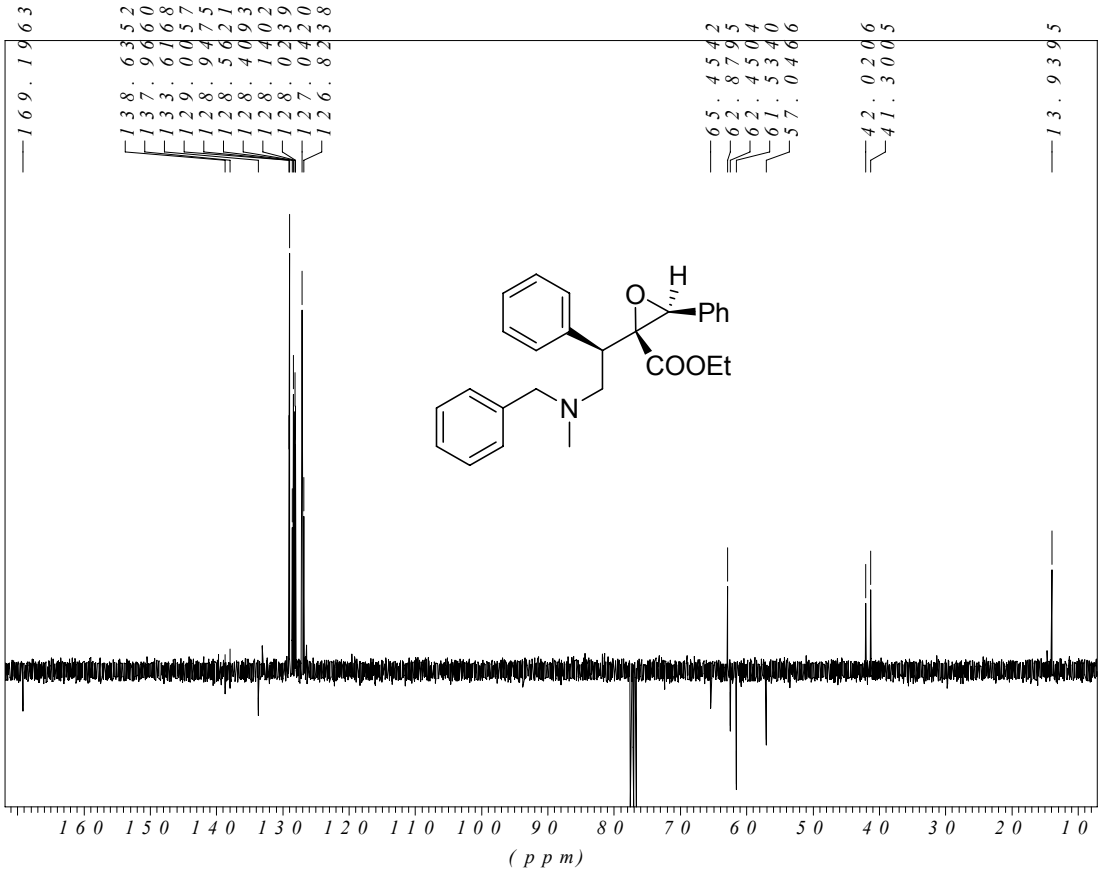
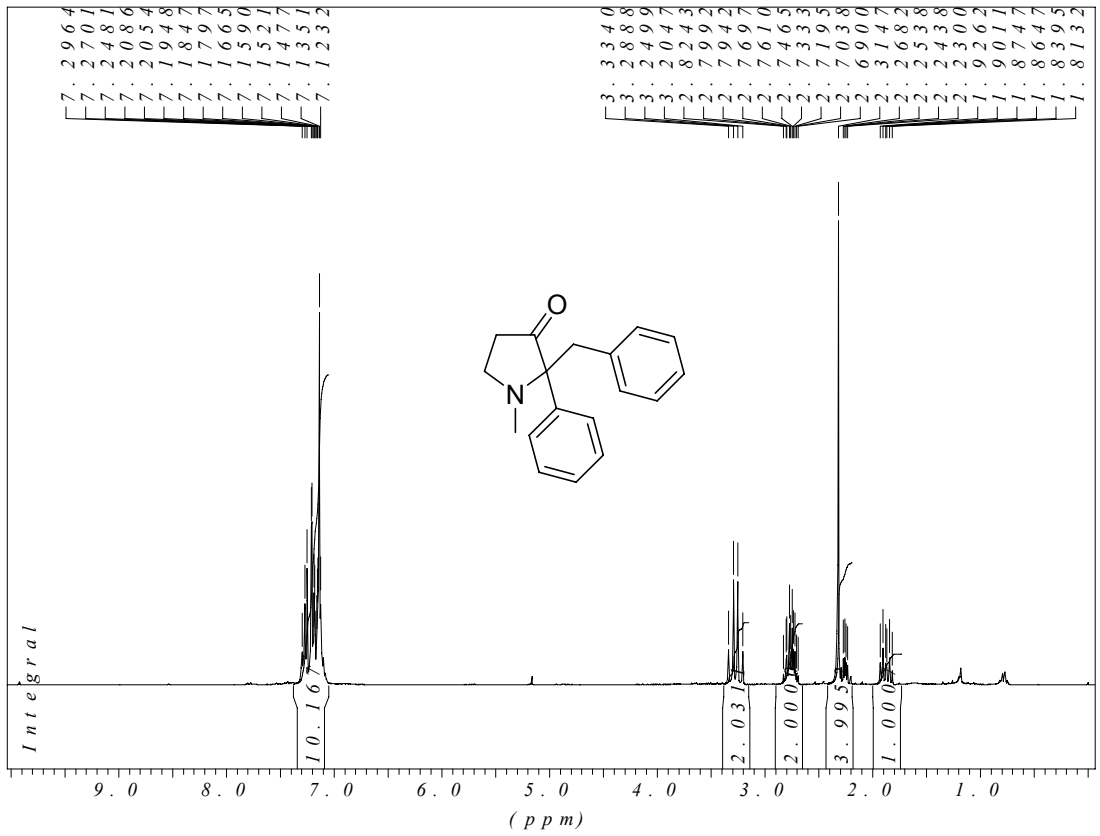
2.5025
2.4799
2.4711
2.4497
1.9225
1.5591
Ph
O
CN
N
Integral
15.027
1.004
0.997
1.000
0.999
0.999
3.000
3.021
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
(ppm)


137.4278
136.5624
128.9912
128.7657
128.7148
128.4020
128.3220
128.2930
127.7475
127.1875
117.4344
77.5419
77.1128
76.6910
69.2798
62.9886
62.9595
59.7231
42.7406
41.9406
22.5144
Ph
O
CN
N
150 140 130 120 110 100 90 80 70 60 50 40 30
(ppm)


7.1824
7.1753
7.1696
7.1618
7.1452
7.1413
7.1265
7.1220
6.9840
6.9757
6.9590
4.3188
4.0530
4.0427
4.0286
4.0190
4.0049
3.9952
3.9824
3.9715
3.8607
3.5507
3.4443
3.3084
3.1106
3.1067
3.0935
2.8918
2.7743
2.7614
2.7390
2.7261
2.3570
2.3442
2.3166
2.3012
2.3781
1.0911
1.0674
1.0436
H
O
Ph
COOEt
N
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)


169.1963
138.6352
137.9660
133.6168
129.0057
128.9475
128.5621
128.4093
128.1402
128.0239
127.0420
126.8238
65.4542
62.8795
62.4504
61.5340
57.0466
42.0206
41.3005
13.9395
H
O
Ph
COOEt
N
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)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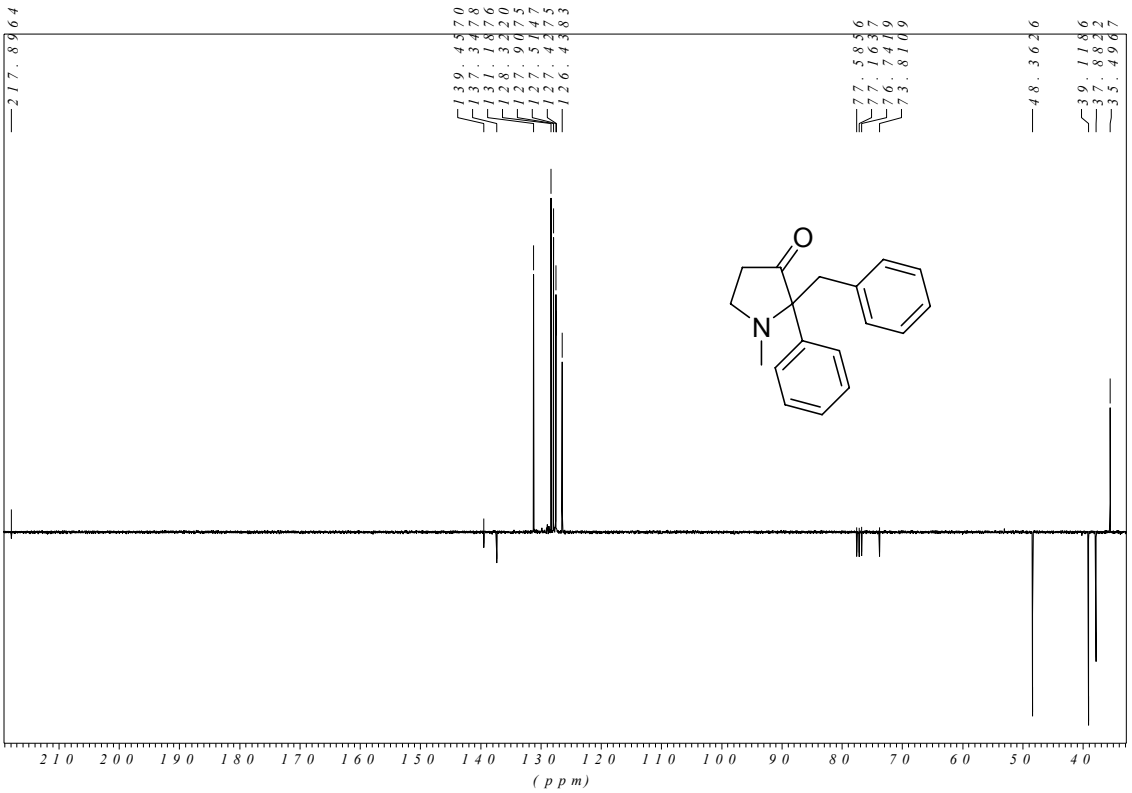
7.2701
7.2481
7.2086
7.2054
7.1948
7.1847
7.1795
7.1665
7.1590
7.1521
7.1477
7.1351
7.1232
3.3340
3.2888
3.2499
3.2043
2.8243
2.7992
2.7694
2.7610
2.7465
2.7333
2.7195
2.7038
2.6900
2.3147
2.2682
2.2538
2.2438
2.2300
1.9262
1.9011
1.8747
1.8647
1.8395
1.8132
O
N
Integral
10.167
2.031
2.000
3.995
1.000
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0
(ppm)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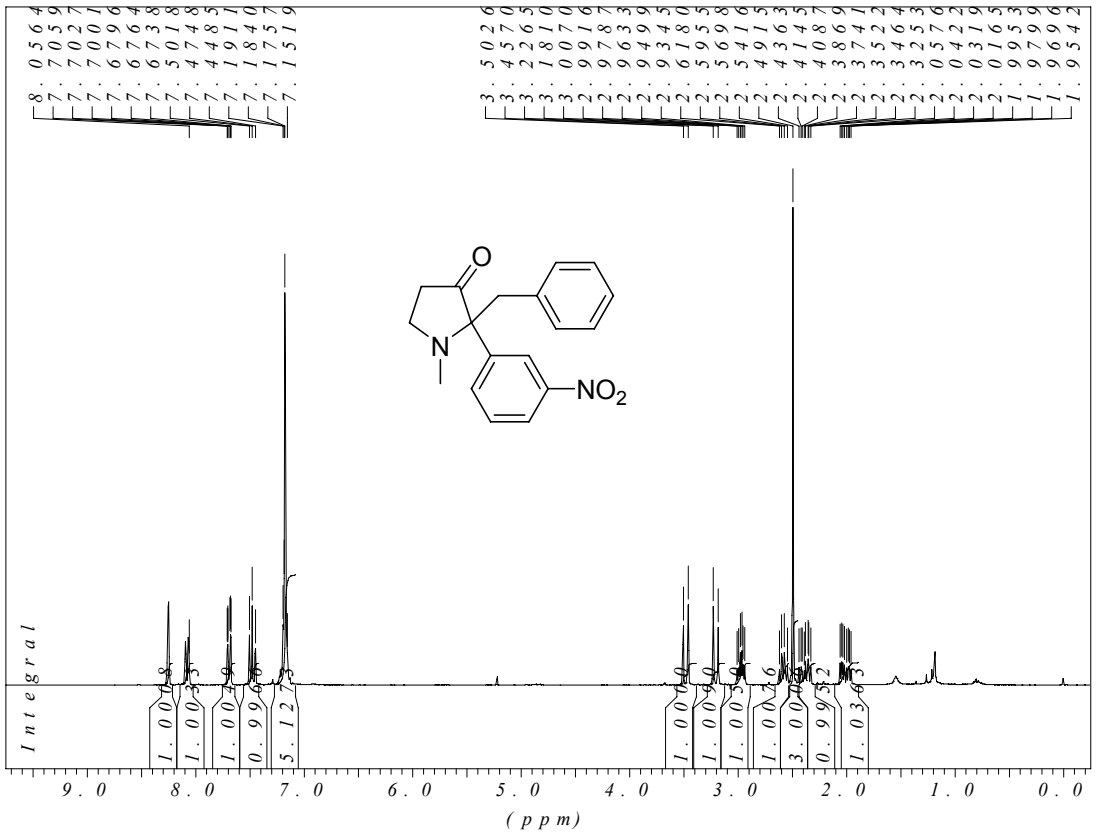
139.4570
137.3478
131.1876
128.3220
127.9075
127.5147
127.4175
126.4383
77.5856
77.1637
76.7419
73.8109
48.3626
39.1186
37.8822
35.4967
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40
(ppm)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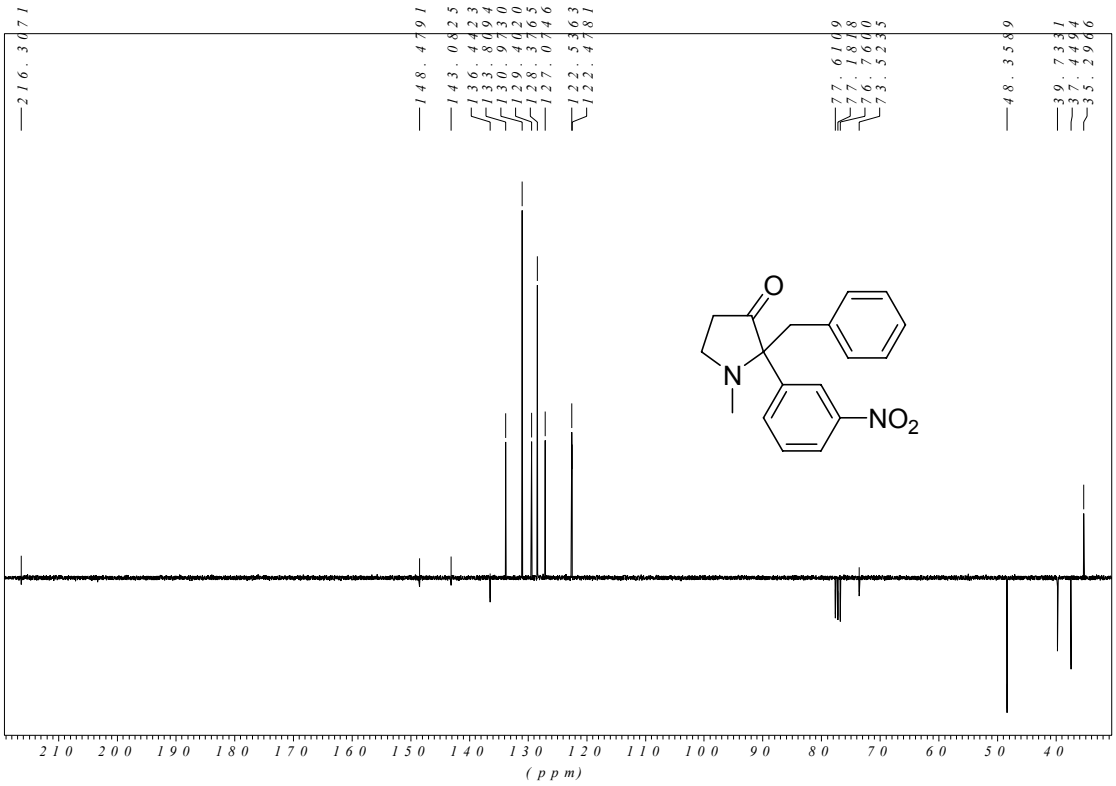
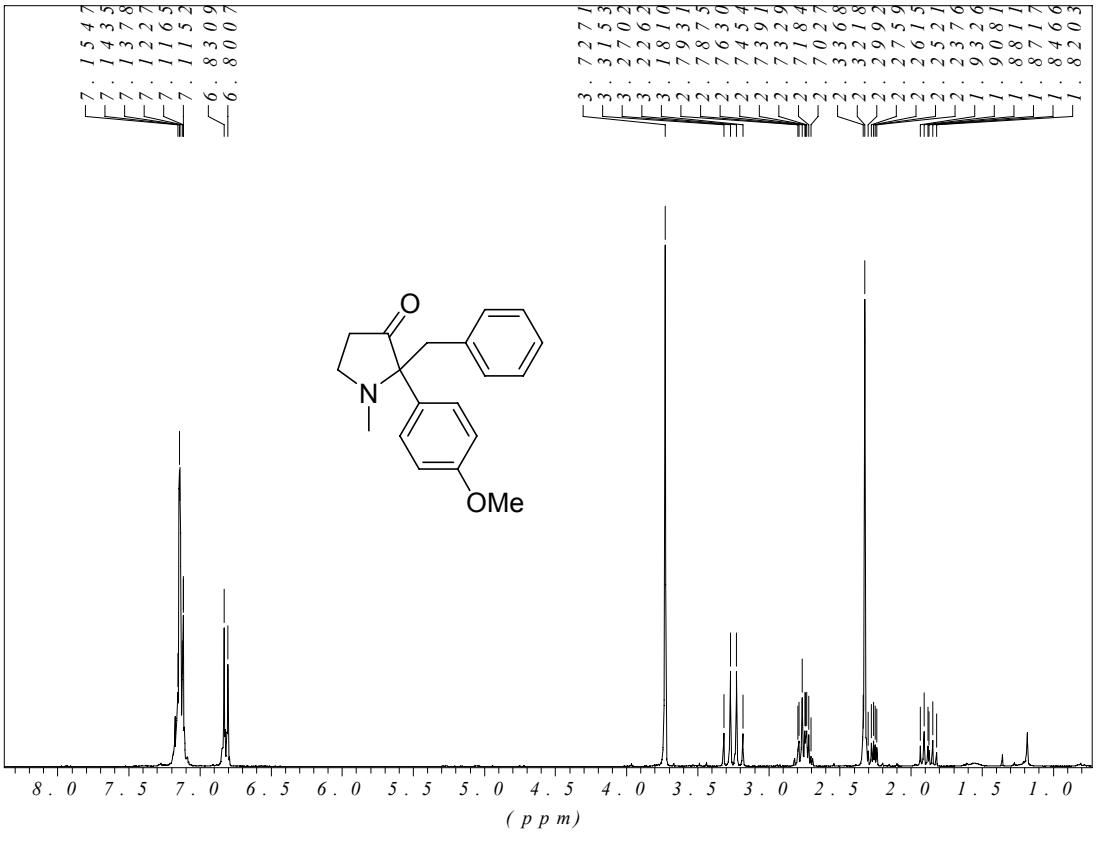
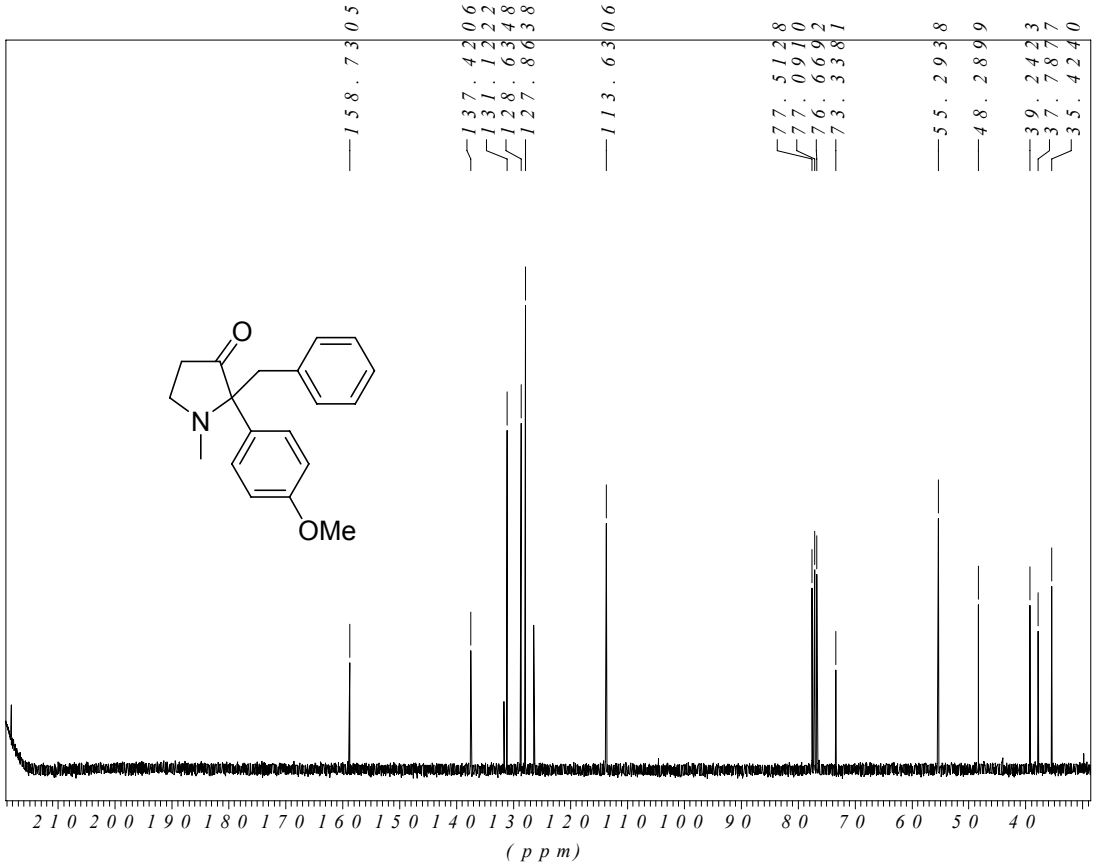
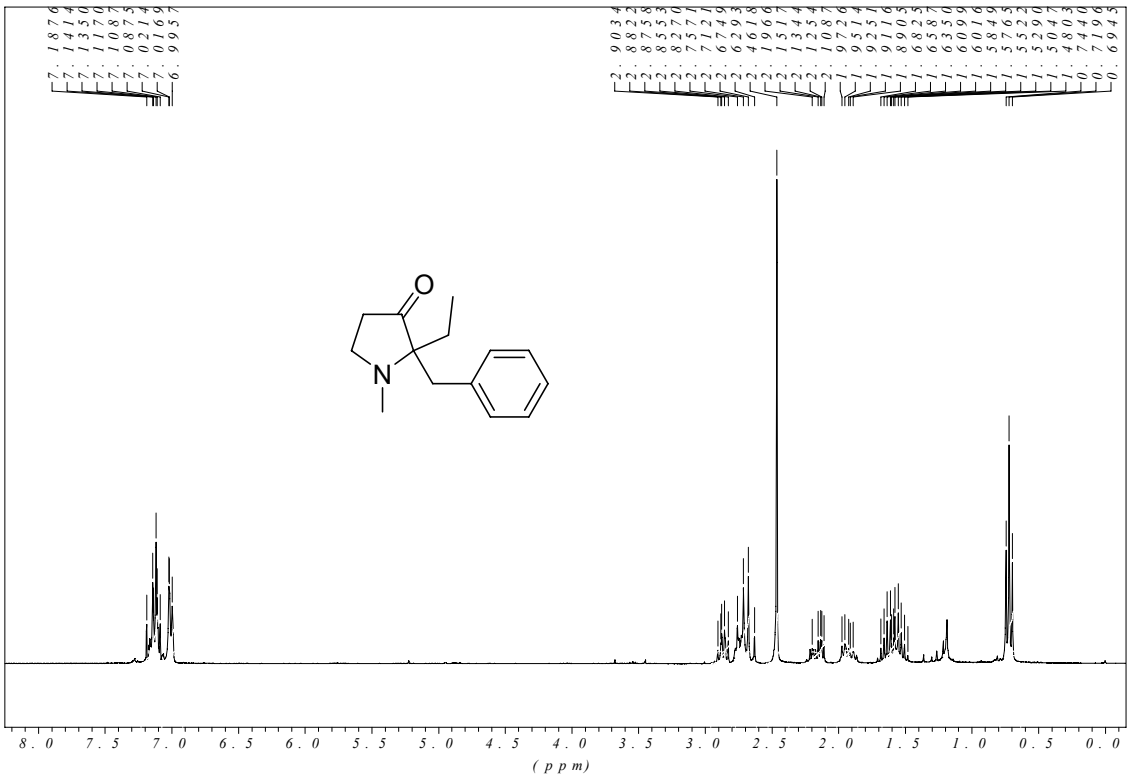
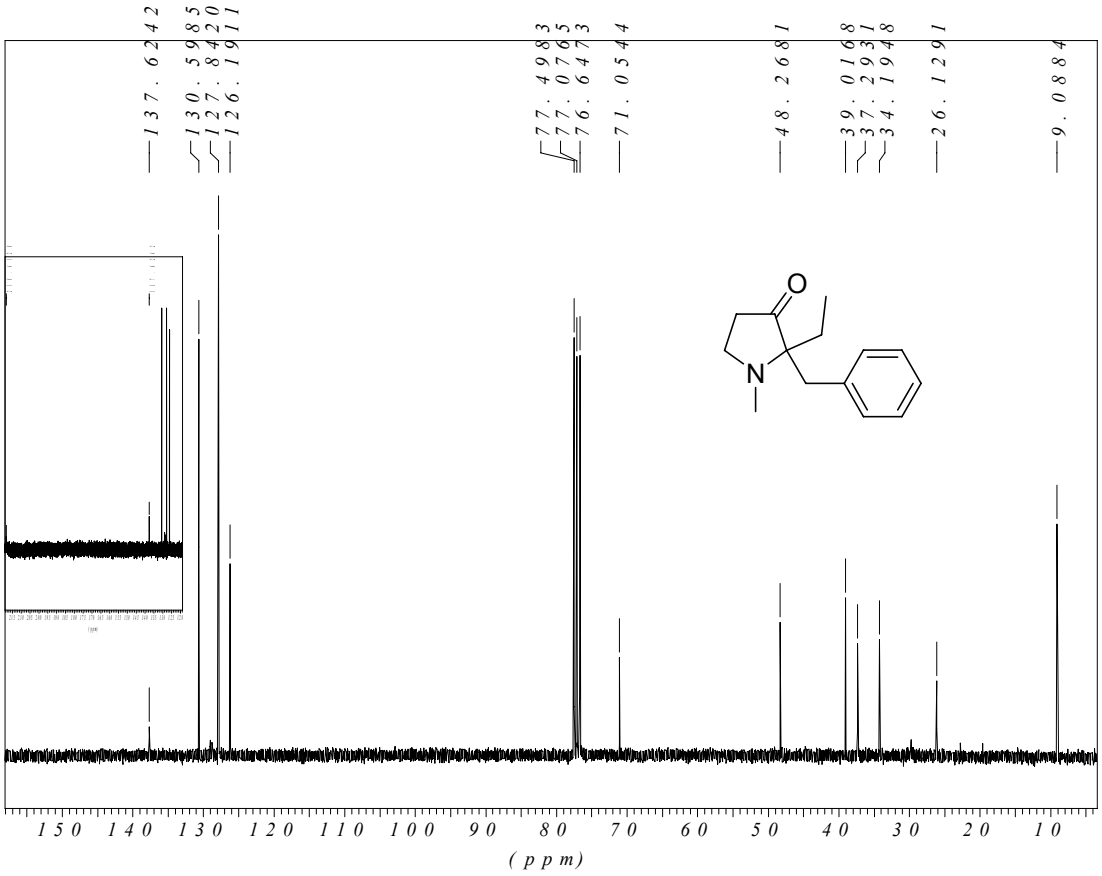
7.7059
7.7027
7.7001
7.6796
7.6764
7.6738
7.5018
7.4748
7.4485
7.1911
7.1840
7.1757
7.1519
3.5026
3.4570
3.2265
3.1810
3.0070
2.9916
2.9787
2.9633
2.9499
2.9345
2.6180
2.5955
2.5698
2.5416
2.4915
2.4363
2.4145
2.4087
2.3869
2.3741
2.3522
2.3464
2.3253
2.0576
2.0422
2.0319
2.0165
1.9953
1.9799
1.9696
1.9542
O
N
NO2
Integral
1.00
1.00
1.00
0.99
5.12
1.00
1.00
1.00
1.00
3.00
0.99
1.03
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
(ppm)

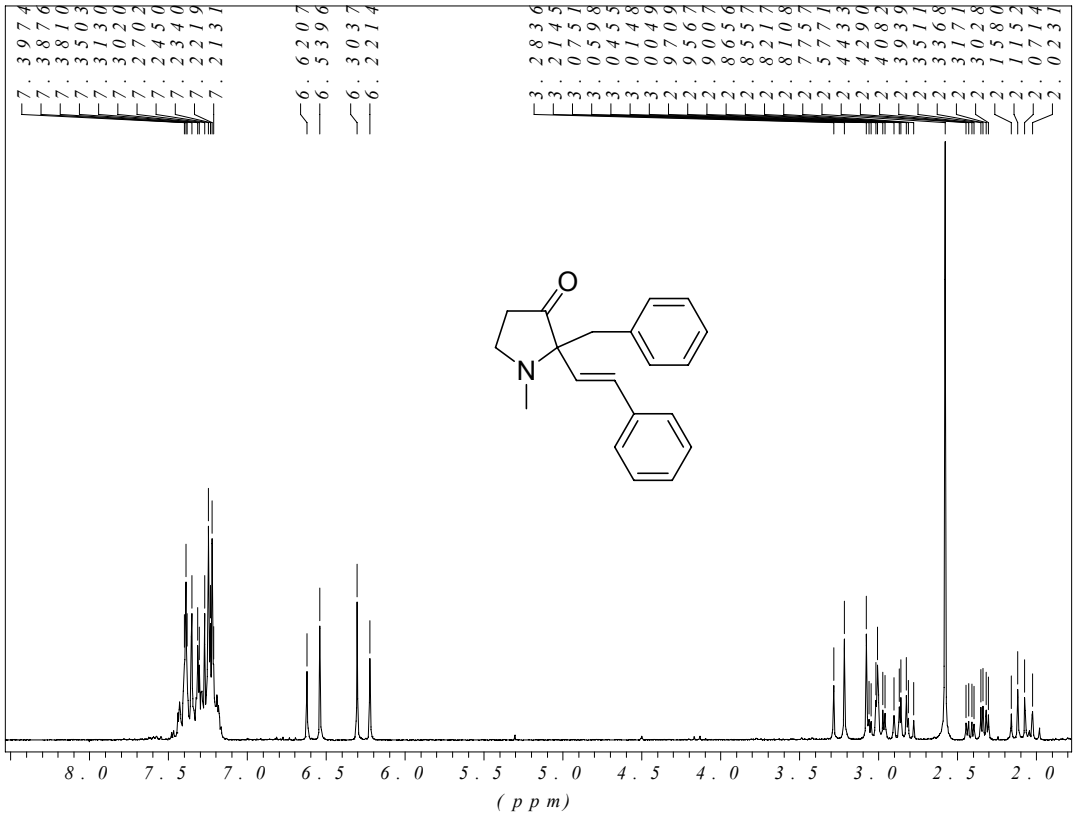

O
N
NO2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40
(ppm)

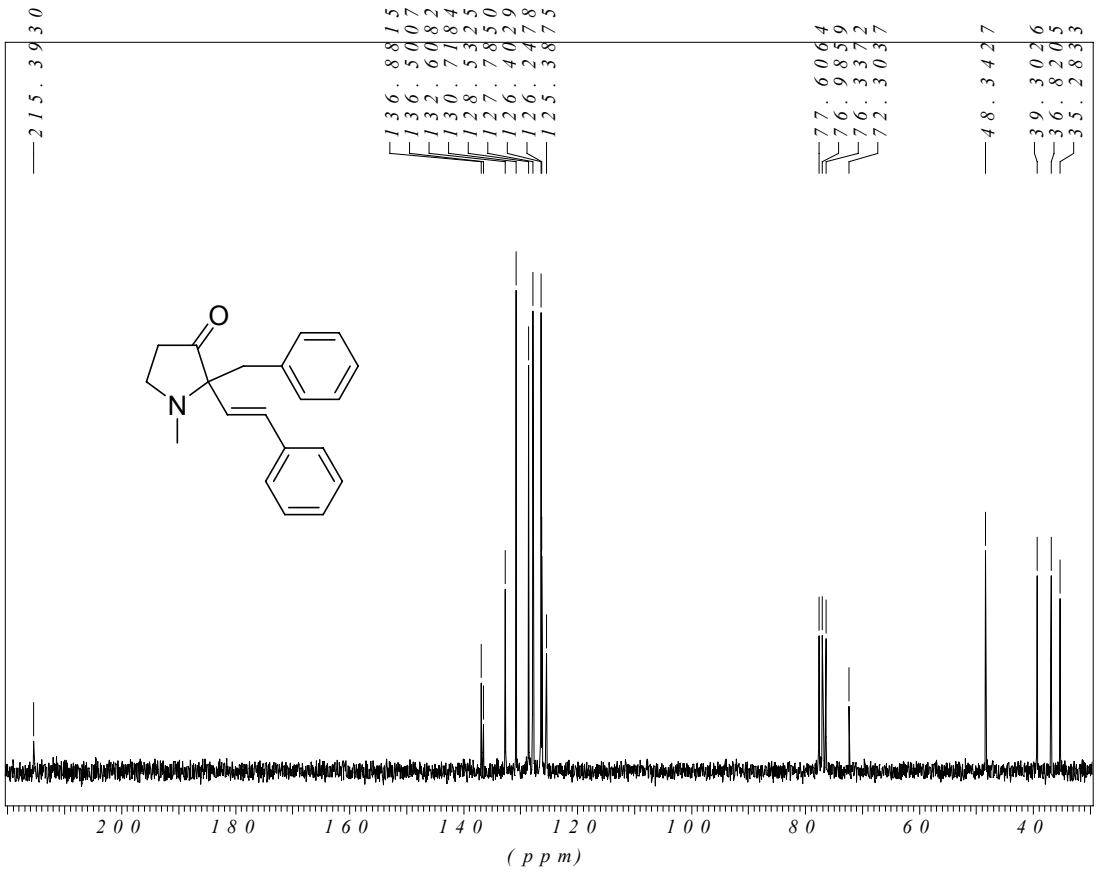

O
N
OMe
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
(ppm)

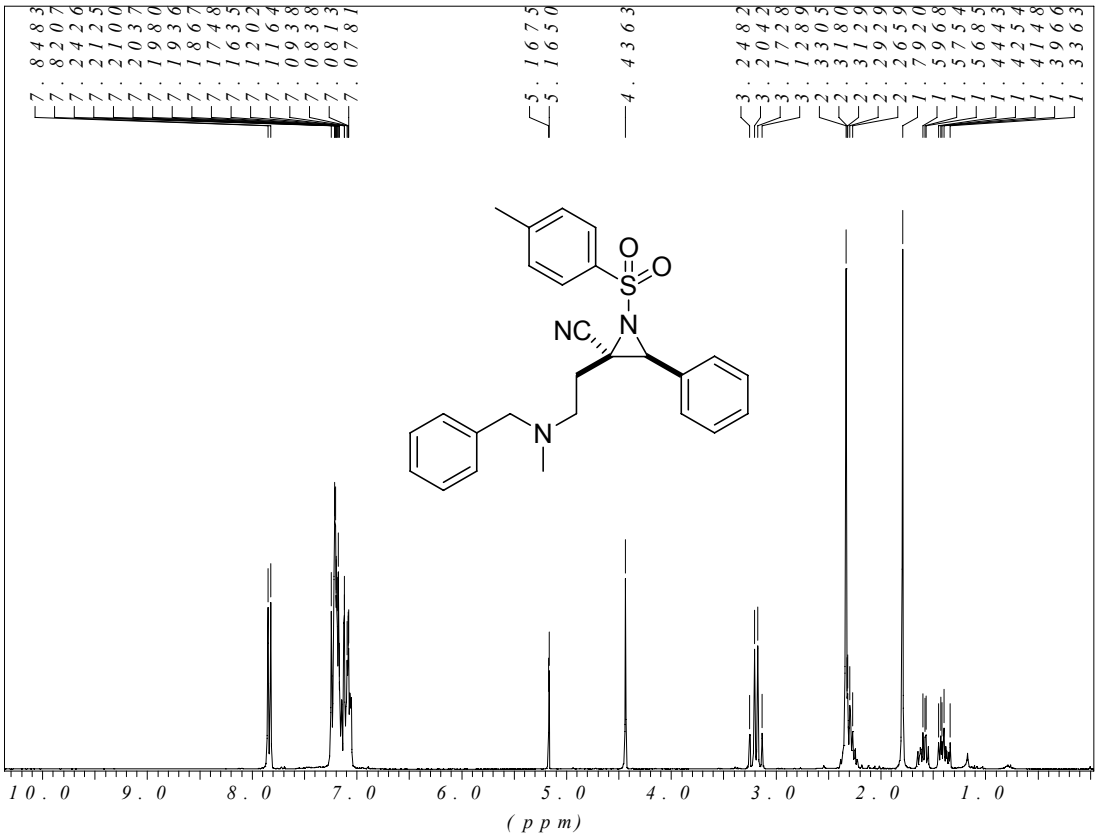





137.6242
130.5985
127.8420
126.1911
77.4983
77.0765
76.6473
71.0544
48.2681
39.0168
37.2931
34.1948
26.1291
9.0884
O
N
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)



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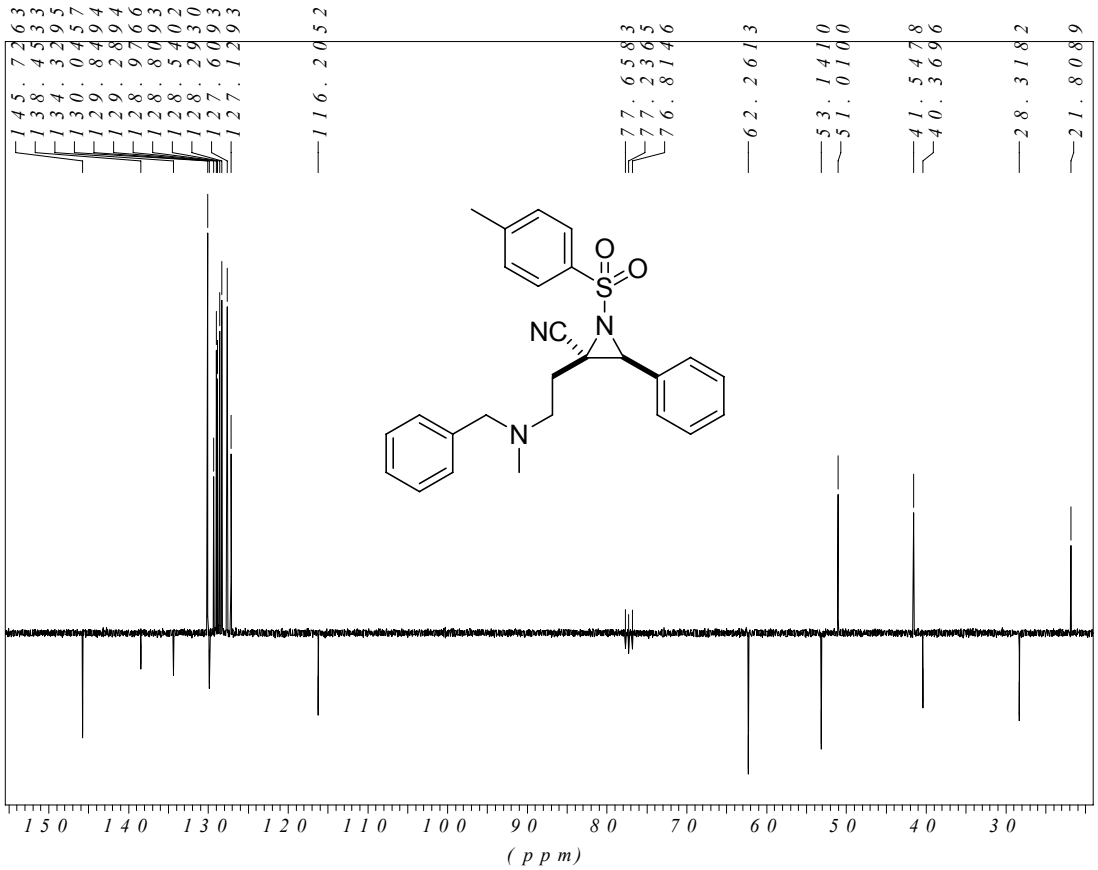
7.8207
7.2426
7.2125
7.2100
7.2037
7.1980
7.1936
7.1867
7.1748
7.1635
7.1202
7.1164
7.0938
7.0838
7.0813
7.0781
5.1675
5.1650
4.4363
3.2482
3.2042
3.1728
3.1289
3.1305
3.1180
3.1129
2.9259
2.7920
1.5968
1.5754
1.5685
1.4443
1.4254
1.4148
1.3966
1.3363
O
O
S
N
NC
N
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
(ppm)


145.7263
138.4533
134.3295
130.0457
129.8494
129.2866
128.8093
128.5402
128.2930
127.6093
127.1293
116.2052
77.6583
77.2365
76.8146
62.2613
53.1410
51.0100
41.5478
40.3696
28.3182
21.8089
O
O
S
N
NC
N
150
140
130
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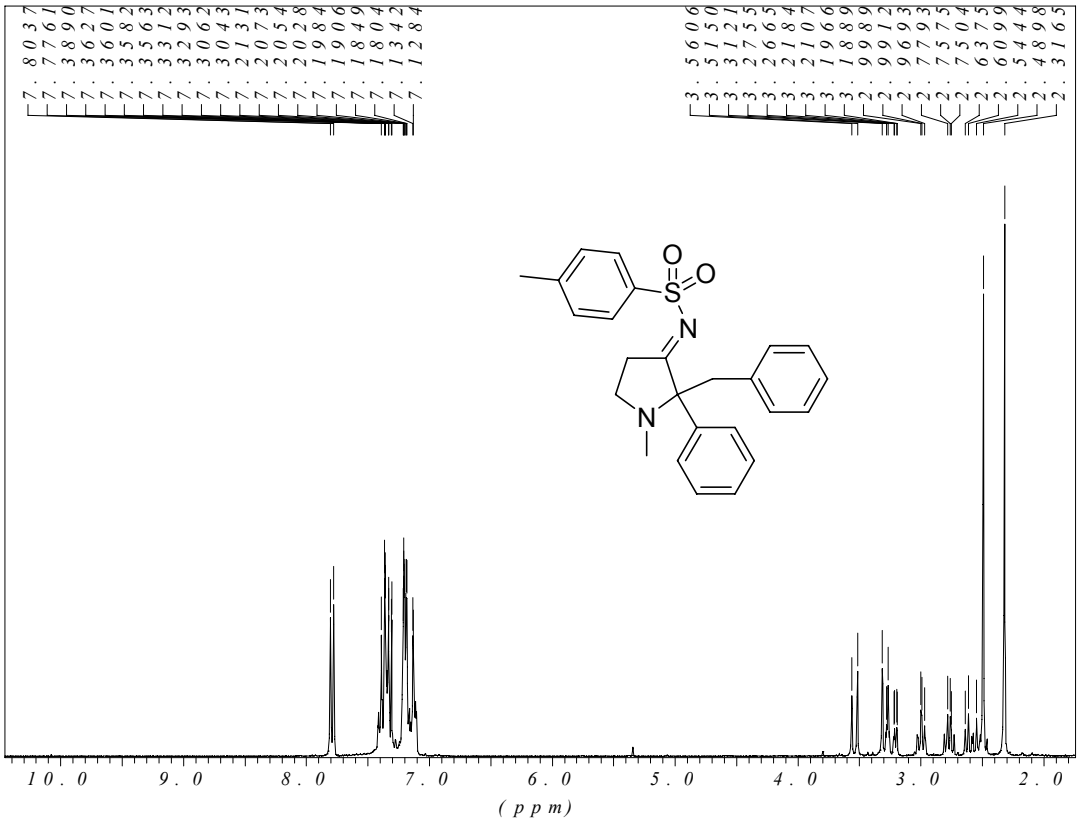
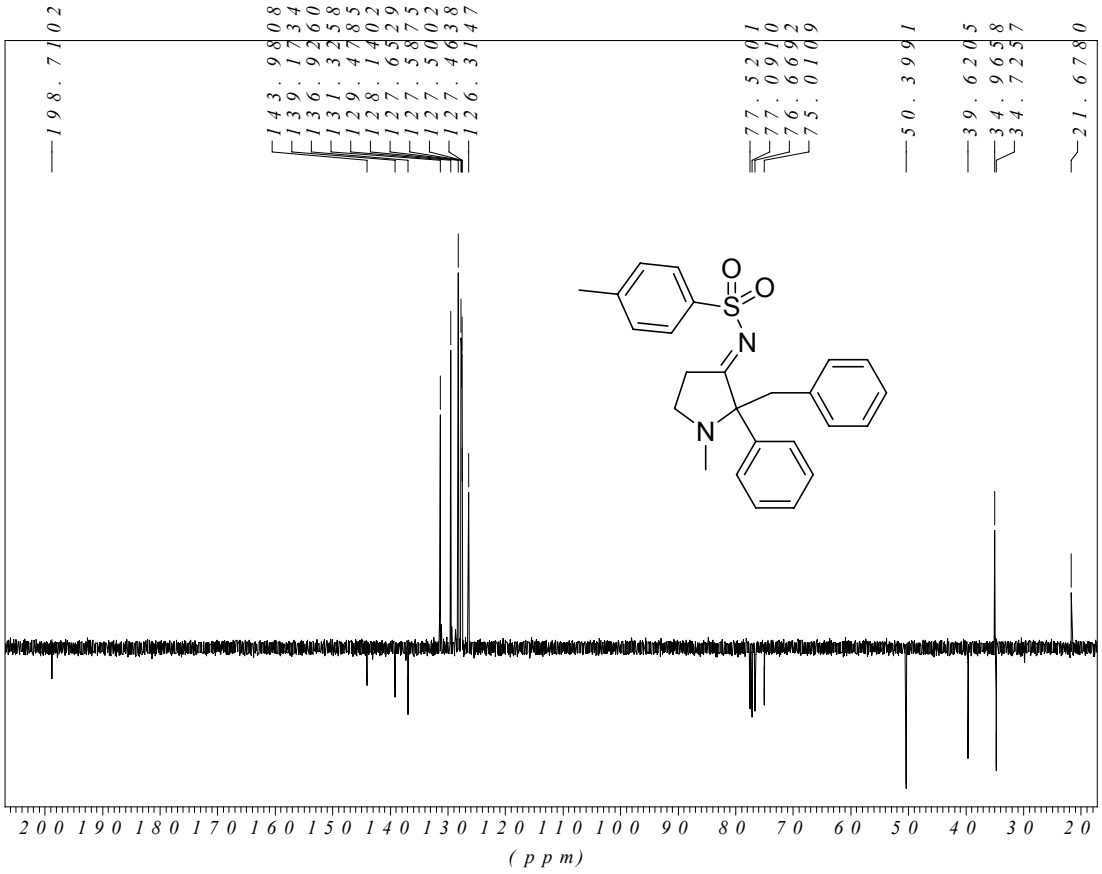
100
90
80
70
60
50
40
30
(ppm)





ORTEP diagram of compound 19