Supplementary Information

Copper-Catalyzed Domino Coupling Reaction: An Efficient Method to Synthesize Oxindoles

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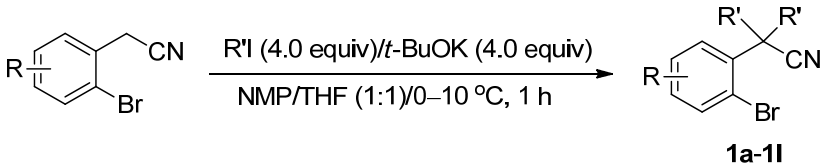
General information: All reagents were purchased from Sigma-Aldrich, Fisher-Acros, TCI, or Alfa-Aesar, and were used without further purification unless otherwise noted. THF and Et_2O were distilled from sodium, and CH_3CN was distilled from CaH_2. All manipulations of oxygen- and moisture-sensitive materials were conducted with a standard Schlenk technique. Flash column chromatography was performed using silica gel (230-400 mesh). Analytical thin layer chromatography (TLC) was performed on 60 F_{254} (0.25 mm) plates and visualization was accomplished with UV light (254 and 354 nm) and/or an aqueous alkaline $KMnO_4$ solution followed by heating. Proton and carbon nuclear magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were recorded on Bruck 300 or Bruck 600 spectrometer with Me_4Si or solvent resonance as the internal standard (^{1}H NMR, Me_4Si at 0 ppm, $CHCl_3$ at 7.26 ppm; ^{13}C NMR, Me_4Si at 0 ppm, $CDCl_3$ at 77.0 ppm). ^{1}H NMR data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sext = sextet, sept = septet, br = broad, m = multiplet), coupling constants (Hz), and integration. IR spectral data were recorded on a Brucker TENSOR 37 spectrometer. Melting points (mp) were determined using a Fargo MP-1D. GC-MS data were obtained from the HP 5890 Series II GC/ HP 5972 GC MASS Spectrometer System. High Resolution Mass spectral data were obtained from the MAT-95XL HRMS by using EI method.

General procedure for the copper-catalyzed domino reactions:

To a screw-capped vial (10-mL) were added CuI (0.015 mmol, 2.9 mg, 3.0 mol %), KI (0.005 mmol, 0.9 mg, 1.0 mol %), *N*-acetylglycine (0.03 mmol, 3.5 mg, 6.0 mol %), NaOH (1.5 mmol, 60 mg, 3.0 equiv) and 2,2-disubstituted 2-(2-bromophenyl)-acetonitrile (**1**, 0.5 mmol, 1.0 equiv) in *t*BuOH (*tert*-butanol, 5.0 mL). The vial was sealed with cap and allowed to stir at 100 °C for the specific reaction time. The crude reaction mixture was diluted with CH_2Cl_2, filtered through a thin Celite pad, and concentrated *in vacuo*. The residue was isolated through a column chromatography by using hexane and ethyl acetate as eluent to give the pure product. Products **2** were obtained according to this procedure. The known structures were characterized by the HRMS, ^{1}H NMR and ^{13}C NMR spectra of reported literatures. Spectral data, melting point, HRMS data and the copies of ^{1}H NMR and ^{13}C NMR spectra for all compounds are listed below.

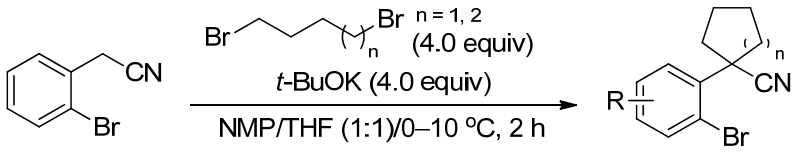
General procedure (A) for the synthesis of starting materials 1a–1l:[1]



1a-1l

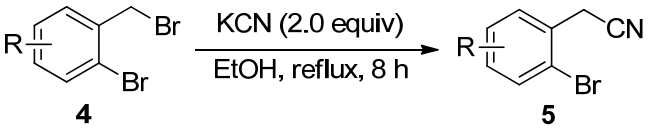
To a suspension of *t*-BuOK (897 mg, 8.0 mmol) in THF and NMP co-solvent (6 mL, 1:1) was added 2-(2-bromoaryl)acetonitrile (**5a**–**5j**, 2.0 mmol). The mixture was allowed to stir at 0 °C for 10 min, and RI (8.0 mmol) was then slowly injected into the reaction mixture over a period of 10 min. The resulting mixture was warmed to 10 °C and stir for an additional 1 hour, quenched with a saturated $NaHCO_3$ aqueous solution, and then extracted with ethyl acetate for three times. The combined organic layers were washed with water and brine, dried over anhydrous Na_2SO_4, filtered through a Celite pad, and concentrated *in vacuo*. The residue was purified by flash column chromatography on silica gel using hexane and ethyl acetate as eluent to give the pure compound. Compounds **1a**–**1l** were obtained according to this procedure.

General procedure (B) for the synthesis of starting materials 1 with spiro ring:[1]



Similar procedure with the synthesis of compounds **1a**–**1l** expects the slight longer reaction time. Compounds **1q, 1r, 1A, 1B, 1C** and **1D** were obtained according to this procedure.

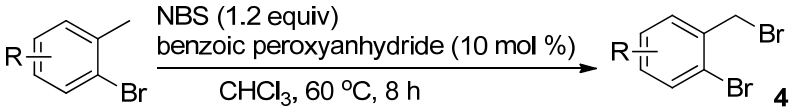
General procedure (C) for the synthesis of 2-(2-bromoaryl)acetonitrile:[2]



4 **5**

To a suspension of KCN (261 mg, 4.0 mmol) in EtOH (16 mL) was added 1-bromo-2-(bromomethyl)arene (2.0 mmol). The mixture was allowed to reflux and stir for 8 h. The residue was filtered to remove salt and isolated through a short flash column chromatography by using ethyl acetate as eluent to give the pure compound. Compounds **5c, 5d, 5e, 5g, 5h, 5i** and **5j** were obtained according to this procedure.

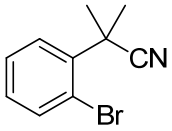
General procedure (D) for the synthesis of 1-bromo-2-(bromomethyl)arene:[3]



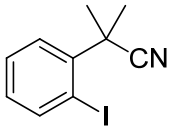
4

The NBS (427 mg, 2.4 mmol) and benzoic peroxyanhydride (49 mg, 0.2 mmol) were dissolved in $CHCl_3$ (6 mL). The substituted 2-bromotoluene (2.0 mmol) was added to the solution and allowed to stir at 60 °C for 8 h. The residue was filtered and isolated through a column chromatography by using hexane and ethyl acetate as eluent to give the pure compound. Compounds **4c** and **4h** were obtained according to this procedure.

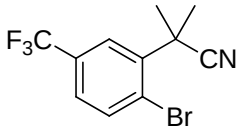
Experimental Details for all substrates:



2-(2-Bromophenyl)-2-methylpropanenitril (1a):[4] Prepared according to the general procedure A, 87% isolated yield; Yellow oil; IR (KBr): 3462, 2984, 2930, 2234, 1647, 1559, 1024, 757 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.67 (dd, J_1 = 8.1 Hz, J_2 = 1.5 Hz, 1H), 7.48 (dd, J_1 = 7.8 Hz, J_2 = 1.5 Hz, 1H), 7.35 (td, J_1 = 7.5 Hz, J_2 = 1.2 Hz, 1H), 7.19 (td, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 1.90 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 138.2, 135.7, 129.6, 127.9, 127.2, 123.4, 122.6, 37.5, 27.5; HRMS: $C_{10}H_{10}BrN$ calculated 222.9997, found 222.9994; Registry Number: [57775-06-1].

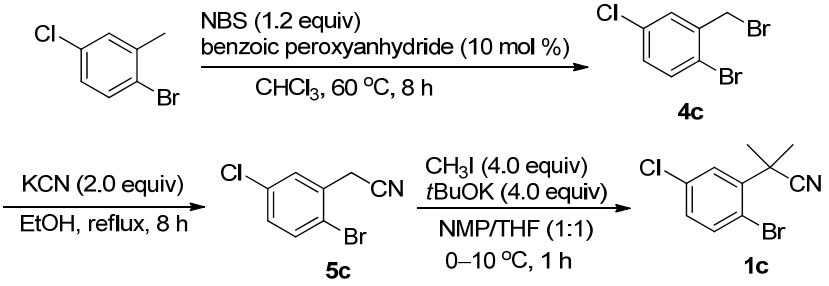


2-(2-Iodophenyl)-2-methylpropanenitril (1a'): Prepared according to the general procedure A, 90% isolated yield; Colorless oil; IR (KBr): 3459, 3061, 2983, 2935, 2232, 1582, 1462, 1230, 1009, 758, 721 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.04 (dd, J_1 = 7.8 Hz, J_2 = 1.5 Hz, 1H), 7.46 (dd, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 7.38 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 6.99 (td, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 1.91 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 143.3, 140.6, 129.6, 128.6, 126.8, 123.3, 95.8, 39.1, 27.9; HRMS: $C_{10}H_{10}IN$ calculated 270.9858, found 270.9855; New compound.



2-(2-Bromo-5-(trifluoromethyl)phenyl)-2-methylpropanenitrile (1b): Prepared according to the general procedure A, 79% isolated yield; Colorless oil; IR (KBr): 3458, 2989, 2236, 1608, 1475, 1330, 1174, 1129, 1027, 831 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.93 (s, 1H), 7.62 (t, J = 1.8 Hz, 2H), 1.92 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 142.2, 132.6 (d, J = 3 Hz), 131.9 (q, J = 33 Hz), 127.8, 124.8 (d, J = 3 Hz), 122.8, 122.8 (q, J = 270 Hz), 122.5, 37.6, 27.3; HRMS: $C_{11}H_9BrF_3N$ calculated 290.9870, found 290.9868; New compound.

Preparation of 2-(2-bromo-5-chlorophenyl)-2-methylpropanenitrile (1c):

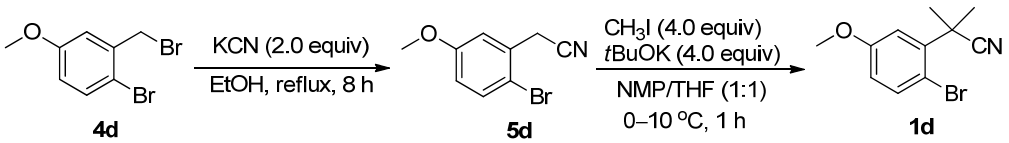


1-Bromo-2-(bromomethyl)-4-chlorobenzene (4c): Prepared according to the general procedure D, 85% isolated yield; White solid, mp: 66–68 °C; IR (KBr): 3474, 2922, 1753, 1656, 1453, 1215, 1104, 1026, 812, 741 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.49 (d, J = 8.4 Hz, 1H), 7.44 (d, J = 2.4 Hz, 1H), 7.15 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 4.53 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 139.3, 135.0, 134.4, 131.7, 130.8, 122.9, 32.9; HRMS: $C_7H_5Br_2Cl$ calculated 281.8447, found 281.8443; Registry Number: [66192-24-3].

2-(2-Bromo-5-chlorophenyl)acetonitrile (5c): Prepared according to the general procedure C, 71% isolated yield; White solid, mp: 112–114 °C; IR (KBr): 3467, 1638, 1385, 1028, 640 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.54–7.52 (m, 2H), 7.21 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 3.81 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 134.2, 134.1, 131.6, 130.0, 129.7, 121.4, 116.2, 24.7; HRMS: C_8H_5BrClN calculated 228.9294, found 228.9297; New compound.

2-(2-Bromo-5-chlorophenyl)-2-methylpropanenitrile (1c): Prepared according to the general procedure A, 86% isolated yield; White solid, mp: 162–164 °C; IR (KBr): 3450, 2986, 2939, 1638, 1459, 1382, 1226, 1109, 1024, 817 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.54 (d, J = 8.4 Hz, 1H), 7.40 (d, J = 2.4 Hz, 1H), 7.14 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 1.83 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.7, 136.4, 133.8, 129.4, 127.3, 122.4, 120.2, 36.9, 27.1; HRMS: $C_{10}H_9BrClN$ calculated 256.9607, found 256.9607; New compound.

Preparation of 2-(2-bromo-5-methoxyphenyl)-2-methylpropanenitrile (1d):

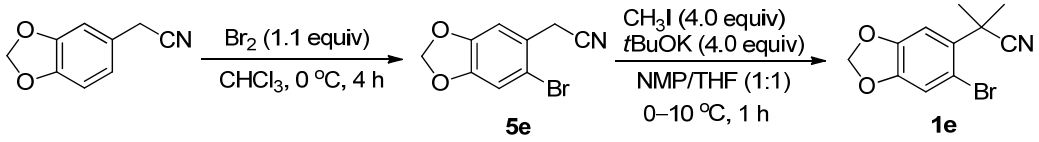


2-(2-Bromo-5-methoxyphenyl)acetonitrile (5d):[3] Prepared according to the general procedure C, 86% isolated yield; White solid, mp: 54–56 °C; IR (KBr): 3531, 3008, 2939, 2839, 2251, 1575, 1475, 1019, 810, 597 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.47 (d, J = 9.0 Hz, 1H), 7.07 (d, J = 3.0 Hz, 1H), 6.77 (dd, J_1 = 9.0 Hz, J_2 = 3.0 Hz, 1H), 3.82 (s, 3H), 3.80 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.4, 133.7, 130.7, 116.8, 115.6, 115.4, 113.7, 55.6, 24.9; HRMS: C_9H_8BrNO calculated 224.9789, found

224.9786; Registry Number: [27387-23-1].

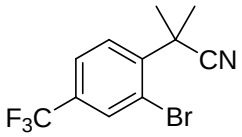
2-(2-Bromo-5-methoxyphenyl)-2-methylpropanenitrile (1d): Prepared according to the general procedure A, 99% isolated yield; Colorless oil; IR (KBr): 3468, 2983, 2937, 2285, 2235, 1468, 1292, 1246, 1047 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.53 (d, J = 8.7 Hz, 1H), 7.02 (d, J = 2.7 Hz, 1H), 6.73 (dd, J_1 = 8.7 Hz, J_2 = 3.0 Hz, 1H), 3.80 (s, 3H), 1.86 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.1, 139.1, 136.1, 123.2, 114.5, 113.9, 112.5, 55.5, 37.3, 27.3; HRMS: $C_{11}H_{12}BrNO$ calculated 253.0102, found 253.0106; Registry Number: [173026-39-6].

Preparation of 2-(6-bromobenzo[*d*][1,3]dioxol-5-yl)-2-methylpropanenitrile (1e):



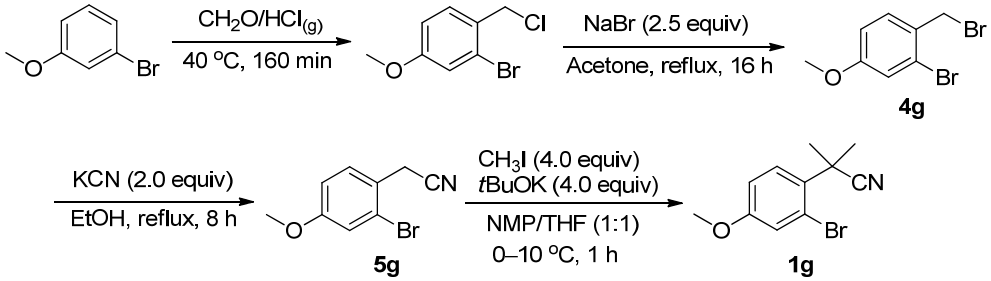
2-(6-Bromobenzo[*d*][1,3]dioxol-5-yl)acetonitrile (5e):[5] To a round bottom flask (25 mL), the commercial source 2-(benzo[*d*][1,3]dioxol-5-yl)-acetonitrile (322 mg, 2.0 mmol) was dissolved in $CHCl_3$ (5 mL) and the flask was sealed by a septum. The reaction mixture was kept stirring at 0 °C and covered by an aluminum foil to make sure that the reaction process in dark. Bromine (352 mg, 2.2 mmol) was then dropwise injected into the solution and allowed to stir at 0 °C for 4 h, quenched by a saturated $NaHCO_3$ aqueous solution, and then extracted with ether for three times. The combined organic layers were washed with water and brine, dried over anhydrous Na_2SO_4, filtered through a Celite pad, and concentrated *in vacuo*. The residue was purified by flash column chromatography on silica gel using hexane and ethyl acetate as eluent to give the pure product **5e** in 55% isolated yield; White solid, mp: 64–66 °C; IR (KBr): 3467, 2917, 2286, 1634, 1503, 1384, 1246, 861, 657 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.04 (s, 1H), 6.98 (s, 1H), 6.02 (s, 2H), 3.75 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 148.5, 147.9, 122.6, 117.0, 114.2, 113.0, 109.5, 102.2, 24.6; HRMS: $C_9H_6BrNO_2$ calculated 238.9582, found 238.9583; Registry Number: [5434-50-4].

2-(6-Bromobenzo[*d*][1,3]dioxol-5-yl)-2-methylpropanenitrile (1e): Prepared according to the general procedure A, 85% isolated yield; Colorless oil; IR (KBr): 3467, 2916, 2233, 1637, 1483, 1242, 1036, 931, 860, 636 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.10 (s, 1H), 6.95 (s, 1H), 6.00 (s, 2H), 1.84 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 147.9, 147.7, 131.4, 123.3, 115.2, 113.5, 107.2, 102.2, 36.9, 27.8; HRMS: $C_{11}H_{10}BrNO_2$ calculated 266.9895, found 266.9889; New compound.



2-(2-Bromo-4-(trifluoromethyl)phenyl)-2-methylpropanenitrile (1f): Prepared according to the general procedure A, 99% isolated yield; Colorless oil; IR (KBr): 3459, 2989, 2237, 1614, 1396, 1327, 1132, 892, 832, 709 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.90 (s, 1H), 7.60 (s, 2H), 1.90 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 142.2, 132.5, 131.7 (q, J = 33 Hz), 127.8, 124.8, 122.9 (q, J = 286 Hz), 122.8, 122.5, 37.5, 27.2; HRMS: $C_{11}H_9BrF_3N$ calculated 290.9870, found 290.9870; New compound.

Preparation of 2-(2-bromo-4-methoxyphenyl)-2-methylpropanenitrile (1g):

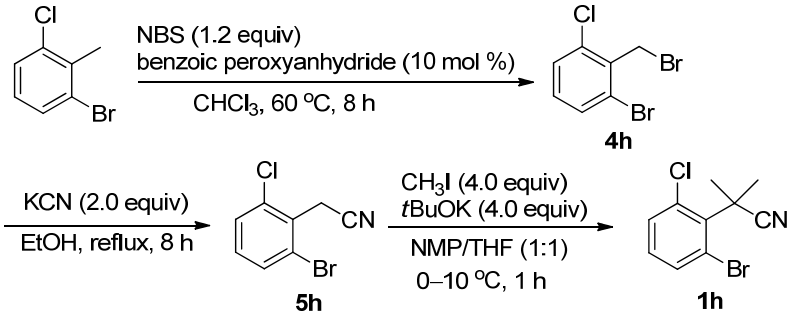


2-Bromo-1-(bromomethyl)-4-methoxybenzene (4g):[6] Preparation and experimental data please see the ref 6 for the detail.

2-(2-Bromo-4-methoxyphenyl)acetonitrile (5g): Prepared according to the general procedure C, 73% isolated yield; Yellow solid, mp: 52–54 °C; IR (KBr): 3461, 2963, 2926, 2851, 2252, 1605, 1495, 1288, 1241, 1031, 862 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.40 (d, J = 8.4 Hz, 1H), 7.15 (d, J = 3.0 Hz, 1H), 6.89 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 3.81 (s, 3H), 3.77 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 160.1, 130.2, 123.9, 121.7, 118.5, 117.2, 114.0, 55.7, 24.0; HRMS: C_9H_8BrNO calculated 224.9789, found 224.9790; Registry Number: [66916-98-1].

2-(2-Bromo-4-methoxyphenyl)-2-methylpropanenitrile (1g): Prepared according to the general procedure A, 87% isolated yield; Colorless oil; IR (KBr): 3468, 2924, 2851, 1603, 1492, 1385, 1298, 1244, 1034, 812 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.35 (d, J = 9.0 Hz, 1H), 7.20 (d, J = 2.4 Hz, 1H), 6.85 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 3.79 (s, 3H), 1.85 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 159.4, 130.2, 127.7, 123.6, 122.8, 120.8, 113.3, 55.5, 36.6, 27.7; HRMS: $C_{11}H_{12}BrNO$ calculated 253.0102, found 253.0109; New compound.

Preparation of 2-(2-bromo-6-chlorophenyl)-2-methylpropanenitrile (1h):

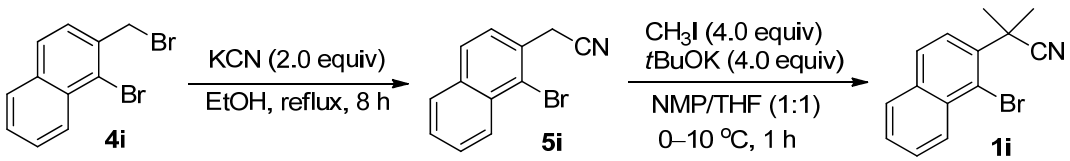


1-Bromo-2-(bromomethyl)-3-chlorobenzene (4h): Prepared according to the general procedure D, 80% isolated yield; White solid, mp: 58–60 °C; IR (KBr): 3465, 2920, 1638, 1571, 1436, 1074, 863, 742 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.48 (dd, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 7.34 (dd, J_1 = 7.8 Hz, J_2 = 0.9 Hz, 1H), 7.08 (t, J = 8.4 Hz, 1H), 4.77 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 135.8, 135.1, 132.0, 130.5, 129.3, 126.0, 30.9; HRMS: $C_7H_5Br_2Cl$ calculated 281.8447, found 281.8442; Registry Number: [75002-98-1].

2-(2-Bromo-6-chlorophenyl)acetonitrile (5h):[3] Prepared according to the general procedure C, 65% isolated yield; White solid, mp: 74–76 °C; IR (KBr): 3488, 1753, 1631, 1520, 1364, 1261, 773, 617, 552, 442 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.54 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 7.41 (d, J = 8.1 Hz, 1H), 7.17 (t, J = 8.1 Hz, 1H), 4.05 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 135.6, 132.1, 130.8, 129.4, 128.8, 125.7, 115.6, 23.0; HRMS: C_8H_5BrClN calculated 228.9294, found 228.9297; Registry Number: [76574-39-5].

2-(2-Bromo-6-chlorophenyl)-2-methylpropanenitrile (1h): Prepared according to the general procedure A, 90% isolated yield; Colorless oil; IR (KBr): 3487, 2980, 2935, 2247, 1682, 1559, 1429, 1195, 793, 753 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.59 (d, J = 7.8 Hz, 1H), 7.39 (d, J = 8.1 Hz, 1H), 7.05 (t, J = 7.8 Hz, 1H), 2.10 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 135.2, 134.6, 132.0, 130.2, 129.4, 124.1, 123.2, 39.9, 29.3; HRMS: $C_{10}H_9BrClN$ calculated 256.9607, found 256.9606; New compound.

Preparation of 2-(1-bromonaphthalen-2-yl)-2-methylpropanenitrile (1i):

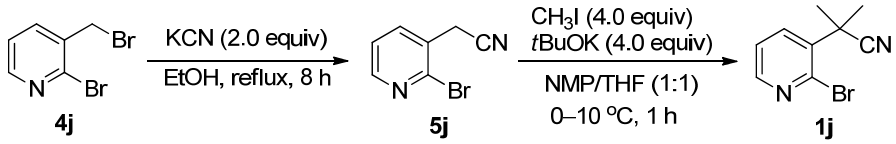


2-(1-Bromonaphthalen-2-yl)acetonitrile (5i):[7] Prepared according to the general procedure C, 48% isolated yield; White solid, mp: 122–123 °C; IR (KBr): 3459, 2905, 2252, 1502, 1384, 1257, 799, 750, 531 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 8.27 (d, J

= 8.4 Hz, 1H), 7.83 (d, J = 8.1 Hz, 2H), 7.65–7.53 (m, 3H), 4.05 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 133.8, 132.2, 128.5, 128.2, 128.1, 127.7, 127.2, 127.1, 126.0, 124.1, 117.0, 25.8; HRMS: $C_{12}H_8BrN$ calculated 244.9840, found 244.9844; Registry Number: [6323-67-7].

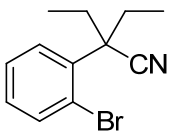
2-(1-Bromonaphthalen-2-yl)-2-methylpropanenitrile (1i): Prepared according to the general procedure A, 90% isolated yield; White solid, mp: 75–77 °C; IR (KBr): 3459, 2982, 2929, 2231, 1637, 1502, 1320, 966, 811, 746 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.47 (d, J = 8.7 Hz, 1H), 7.82 (t, J = 4.8 Hz, 2H), 7.63 (td, J = 4.8 Hz, 1H), 7.58–7.53 (m, 2H), 2.01 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 136.0, 133.7, 133.2, 128.4, 128.0, 127.9, 127.7, 127.2, 123.9, 123.7, 123.5, 38.1, 28.1; HRMS: $C_{14}H_{12}BrN$ calculated 273.0153, found 273.0156; New compound.

Preparation of 2-(2-bromopyridin-3-yl)-2-methylpropanenitrile (1j):



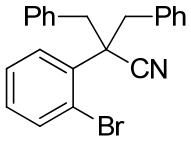
2-(2-Bromopyridin-3-yl)acetonitrile (5j):[8] Prepared according to the general procedure C, 65% isolated yield; Colorless oil; IR (KBr): 3467, 2923, 2852, 2297, 1636, 1406, 1122 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.37 (dd, J_1 = 4.8 Hz, J_2 = 1.8 Hz, 1H), 7.86 (dd, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 7.36 (dd, J_1 = 7.8 Hz, J_2 = 4.8 Hz, 1H), 3.86 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 149.7, 143.1, 137.7, 127.8, 123.3, 115.8, 24.2; HRMS: $C_7H_5BrN_2$ calculated 195.9636, found 195.9635; Registry Number: [1211523-71-5].

2-(2-Bromopyridin-3-yl)-2-methylpropanenitrile (1j): Prepared according to the general procedure A, 83% isolated yield; Yellow oil; IR (KBr): 3449, 2923, 1637, 1572, 1557, 1388, 1041, 743, 643 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.36 (dd, J_1 = 4.8 Hz, J_2 = 1.8 Hz, 1H), 7.81 (dd, J_1 = 7.5 Hz, J_2 = 1.8 Hz, 1H), 7.33 (dd, J_1 = 8.1 Hz, J_2 = 4.8 Hz, 1H), 1.92 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 149.1, 141.7, 136.0, 135.8, 123.0, 122.4, 36.5, 26.9; HRMS: $C_9H_9BrN_2$ calculated 223.9949, found 223.9944; New compound.



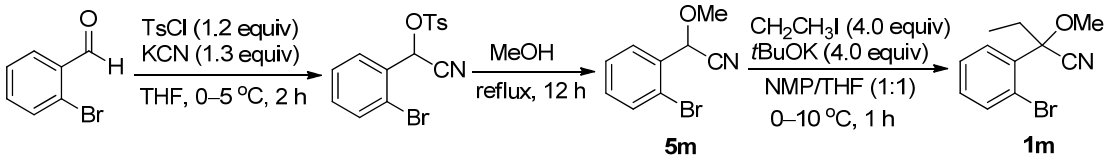
2-(2-Bromophenyl)-2-ethylbutanenitrile (1k):[4] Prepared according to the general procedure A, 95% isolated yield; Colorless oil; IR (KBr): 3450, 2973, 2936, 2879, 2285, 2233, 1637, 893, 755 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.69 (dd, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 7.62 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.33 (td, J_1 = 7.5 Hz, J_2

= 1.2 Hz, 1H), 7.17 (td, J_1 = 7.5 Hz, J_2 = 1.8 Hz, 1H), 2.71–2.59 (m, 2H), 2.13–2.01 (m, 2H), 0.91 (t, J = 7.2 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 135.9, 134.6, 131.7, 129.3, 127.5, 122.5, 120.3, 52.2, 30.0, 9.8; HRMS: $C_{12}H_{14}BrN$ calculated 251.0310, found 251.0315; Registry Number: [212626-87-4].



2-Benzyl-2-(2-bromophenyl)-3-phenylpropanenitrile (1l):[9] Prepared according to the general procedure A, 99% isolated yield; White solid, mp: 92–94 °C; IR (KBr): 3468, 3031, 2930, 2862, 2236, 1604, 1024, 759, 657 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.68 (dd, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 7.23–7.00 (m, 13H), 4.20 (d, J = 13.8 Hz, 2H), 3.36 (d, J = 13.8 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 135.9, 135.3, 133.7, 132.9, 130.2, 129.6, 128.1, 127.8, 127.2, 121.6, 120.5, 54.5, 41.8; HRMS: $C_{22}H_{18}BrN$ calculated 375.0623, found 375.0621; Registry Number: [1312716-88-3].

Preparation of 2-(2-bromophenyl)-2-methoxybutanenitrile (1m):

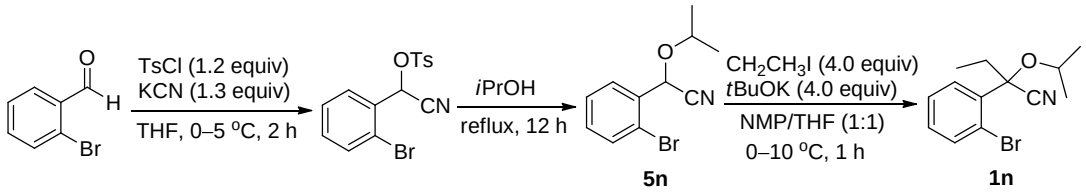


2-(2-Bromophenyl)-2-methoxyacetonitrile (5m): To a solution of TsCl (458 mg, 2.4 mmol) in THF (2 mL) was added to the solution of 2-bromobenzaldehyde (370 mg, 2 mmol) in THF (2 mL) at 0 °C. The mixture was allowed to stir for 15 min; the solution of KCN (169 mg, 2.6 mmol) in H_2O (1.5 mL) was then added into the solution of 2-bromobenzaldehyde. The resulting solution mixture was kept to stir for 2 h, extracted by ether, filtered to remove salt and concentrated *in vacuo*. The crude residue was dissolved in methanol (30 mL), and allowed to keep stirring for 12 h under reflux. The crude reaction mixture was filtered and concentrated *in vacuo,* isolated through a column chromatography to get compound **5m** in 99% isolated yield; Colorless oil; IR (KBr): 3467, 3004, 2933, 2830, 2288, 1629, 1592, 1471, 1438, 1198, 1086, 754 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.70 (dd, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 7.62 (td, J_1 = 7.8 Hz, J_2 = 0.9 Hz, 1H), 7.41 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.28 (td, J_1 = 7.8 Hz, J_2 = 1.5 Hz, 1H), 5.44 (s, 1H), 3.61 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 133.1, 132.8, 131.2, 128.9, 128.0, 122.8, 116.3, 71.6, 57.9; HRMS: C_9H_8BrNO calculated 224.9789, found 224.9791; New compound.

2-(2-Bromophenyl)-2-methoxybutanenitrile (1m): Prepared according to the general procedure A, 91% isolated yield; Yellow oil; IR (KBr): 3458, 2882, 2285,

1638, 1467, 1429, 1027, 758 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.65 (dd, J_1 = 8.1 Hz, J_2 = 1.5 Hz, 2H), 7.38 (td, J_1 = 7.5 Hz, J_2 = 1.2 Hz, 1H), 7.24 (td, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 3.37 (s, 3H), 2.38–2.28 (m, 2H), 0.99 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 135.8, 134.0, 130.4, 130.0, 127.6, 119.9, 117.5, 84.0, 54.2, 32.2, 8.6; HRMS: $C_{11}H_{12}BrNO$ calculated 253.0102, found 253.0101; New compound.

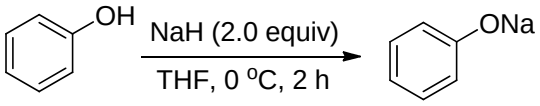
Preparation of 2-(2-bromophenyl)-2-isopropoxybutanenitrile (1n):



2-(2-Bromophenyl)-2-isopropoxyacetonitrile (5n): Procedure was the same with the preparation of **5m**, 99% isolated yield; Colorless oil; IR (KBr): 3459, 2976, 2932, 1636, 1469, 1385, 1116, 1026, 754, 684 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.74 (dd, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 7.60 (dd, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 7.42 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.28 (td, J_1 = 7.5 Hz, J_2 = 1.8 Hz, 1H), 5.58 (s, 1H), 4.14–4.01 (m, 1H), 1.35 (d, J = 6.3 Hz, 3H), 1.29 (d, J = 6.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 133.8, 133.1, 131.1, 129.3, 128.2, 122.7, 117.5, 72.9, 67.7, 22.5, 21.4; HRMS: $C_{11}H_{12}BrNO$ calculated 253.0102, found 253.0105; New compound.

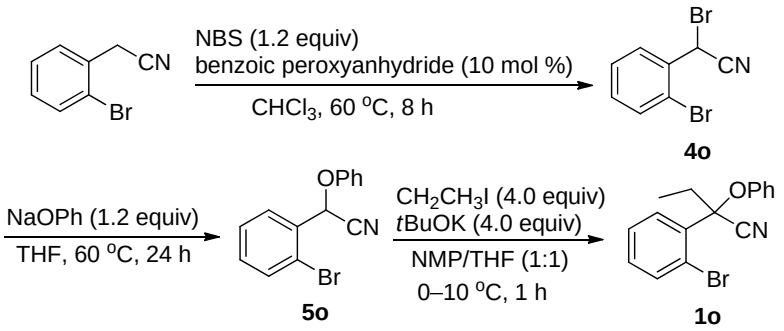
2-(2-Bromophenyl)-2-isopropoxybutanenitrile (1n): Prepared according to the general procedure A, 86% isolated yield; White solid, mp: 30–32 °C; IR (KBr): 3462, 2976, 2937, 1466, 1384, 1077, 923, 757, 453 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.79 (dd, J_1 = 8.4 Hz, J_2 = 1.8 Hz, 1H), 7.64 (dd, J_1 = 7.8 Hz, J_2 = 0.6 Hz, 1H), 7.36 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.22 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 3.94–3.90 (m, 1H), 2.46–2.38 (m, 2H), 1.33 (d, J = 6.0 Hz, 3H), 1.11 (d, J = 6.0 Hz, 3H), 0.93 (t, J = 7.5 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 135.9, 135.3, 130.4, 130.3, 127.3, 120.4, 118.9, 82.4, 71.2, 32.3, 23.2, 23.0, 8.7; HRMS: $C_{13}H_{16}BrNO$ calculated 281.0415, found 281.0419; New compound.

Preparation of 2-(2-bromophenyl)-2-phenoxybutanenitrile (1o):



Preparation of sodium phenoxide: Sodium hydride powder (NaH, 60% in mineral oil, 192 mg, 4.8 mmol) was washed by the dry hexane for several times. The hexane was removed and THF (6 mL) was then added and kept stirring at 0 °C. Phenol (226 mg, 2.4 mmol) was slowly added into the suspension and the reaction mixture was

allowed to stir at 0 °C for 2 h. The crude residue was concentrated *in vacuo* to remove THF. The resulting crude sodium phenoxide was directly used for the synthesis of compound **5o**.

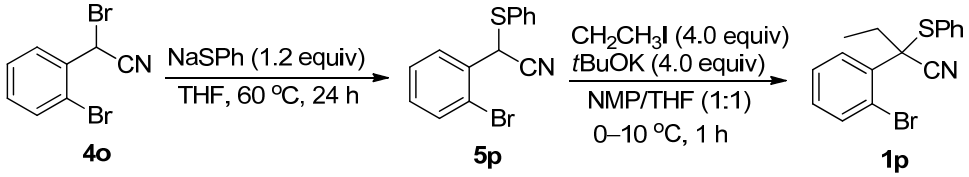


2-Bromo-2-(2-bromophenyl)acetonitrile (4o): Prepared according to the general procedure D, 55% isolated yield; White solid, mp: 67–68 °C; IR (KBr): 3468, 2969, 2924, 2853, 2248, 1639, 1471, 1442, 758, 720, 676, 648, 617 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.84 (dd, J_1 = 7.8 Hz, J_2 = 1.5 Hz, 1H), 7.60 (dd, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 7.43 (t, J = 6.6 Hz, 1H), 7.28 (t, J = 7.8 Hz, 1H), 5.85 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 133.8, 132.9, 131.9, 129.7, 128.8, 123.1, 116.0, 27.5; HRMS: $C_8H_5Br_2N$ calculated 272.8789, found 272.8785; New compound.

2-(2-Bromophenyl)-2-phenoxyacetonitrile (5o): To a solution of **4o** (550 mg, 2.0 mmol) in THF (4 mL) was added the prepared crude sodium phenoxide. The mixture was allowed to stir at 60 °C for 24 h, filtered to remove the salt and isolated by short column to give **5o** in 53% isolated yield; White solid, mp: 116–118 °C; IR (KBr): 3467, 2925, 2854, 1745, 1647, 1636, 1458, 1384, 740 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.85 (dd, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 7.67 (d, J = 6.6 Hz, 1H), 7.47 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.38–7.33 (m, 3H), 7.12 (t, J = 7.8 Hz, 3H), 6.18 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 156.3, 133.4, 132.4, 131.7, 129.9, 129.3, 128.4, 123.6, 122.9, 116.4, 116.1, 68.7; HRMS: $C_{14}H_{10}BrNO$ calculated 286.9946, found 286.9949; New compound.

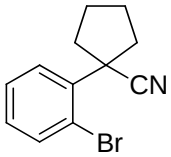
2-(2-Bromophenyl)-2-phenoxybutanenitrile (1o): Prepared according to the general procedure A, 82% isolated yield; Colorless oil; IR (KBr): 3464, 3088, 3957, 1574, 1476, 1408, 1184, 1008, 731 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.71 (dd, J_1 = 7.8 Hz, J_2 = 1.5 Hz, 1H), 7.65 (dd, J_1 = 8.1 Hz, J_2 = 1.5 Hz, 1H), 7.36 (t, J = 6.6 Hz, 1H), 7.26–7.20 (m, 3 H), 7.03 (d, J = 7.5 Hz, 1H), 6.95–6.92 (m, 2H), 2.62–2.49 (m, 2 H), 1.18 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 154.5, 135.9, 134.5, 130.5, 129.6, 129.1, 127.7, 122.9, 119.5, 118.2, 117.1, 81.7, 33.8, 8.7; HRMS: $C_{16}H_{14}BrNO$ calculated 315.0259, found 315.0260; New compound.

Preparation of 2-(2-bromophenyl)-2-(phenylthio)butanenitrile (1p):

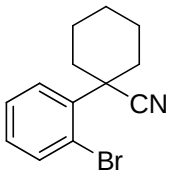


2-(2-Bromophenyl)-2-(phenylthio)acetonitrile (5p): Procedure was the same with the preparation of **5o**, 52% isolated yield; White solid, mp: 53–55 °C; IR (KBr): 3459, 2924, 2853, 2285, 1639, 1384, 727, 707, 623 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.65–7.62 (m, 1H), 7.54–7.50 (m, 2H), 7.44–7.41 (m, 1H), 7.38–7.33 (m, 2H), 7.25–7.21 (m, 3H), 5.34 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 135.9, 133.5, 131.9, 130.6, 130.2, 129.8, 129.6, 129.3, 127.8, 123.2, 117.7, 41.9; HRMS: $C_{14}H_{10}BrNS$ calculated 302.9717, found 302.9721; New compound.

2-(2-Bromophenyl)-2-(phenylthio)butanenitrile (1p): Prepared according to the general procedure A, 80% isolated yield; Yellow oil; IR (KBr): 3460, 2972, 2934, 1637, 1469, 1459, 1025, 749, 691 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.72–7.66 (m, 1H), 7.38–7.30 (m, 4H), 7.23–7.11 (m, 4H), 3.10–3.02 (m, 1H), 2.42–2.35 (m, 1H), 1.04 (t, J = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 136.6, 136.3, 132.6, 131.6, 130.1, 129.9, 129.8, 128.7, 127.1, 121.1, 119.7, 57.5, 30.4, 10.3; HRMS: $C_{16}H_{14}BrNS$ calculated 331.0030, found 331.0035; New compound.



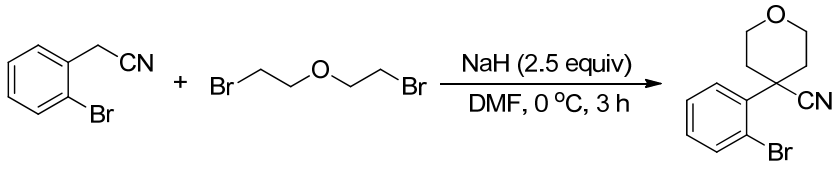
2-(2-Bromophenyl)-2-(phenylthio)butanenitrile (1q):[10] Prepared according to the general procedure B, 90% isolated yield; Colorless oil; IR (KBr): 3467, 2960, 2876, 2231, 1469, 1023, 756 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.67 (dd, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 7.41 (dd, J_1 = 8.1 Hz, J_2 = 1.5 Hz, 1H), 7.31 (td, J_1 = 8.1 Hz, J_2 = 1.5 Hz, 1H), 7.18 (td, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 2.79–2.71 (m, 2H), 2.25–2.15 (m, 2H), 2.07–2.00 (m, 2H), 1.94–1.87 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 137.6, 135.2, 129.5, 127.7, 127.5, 123.7, 122.9, 47.6, 38.2, 23.7; HRMS: $C_{12}H_{12}BrN$ calculated 249.0153, found 249.0148; Registry Number: [143328-17-0].



1-(2-Bromophenyl)cyclohexanecarbonitrile (1r):[11] Prepared according to the

gereral procedure B, 94% isolated yield; Colorless oil; IR (KBr): 3459, 2935, 1637, 1469, 1454, 1385, 1009, 735 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.67 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.45 (dd, J_1 = 8.1 Hz, J_2 = 1.8 Hz, 1H), 7.35 (td, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 7.18 (td, J_1 = 7.2 Hz, J_2 = 1.8 Hz, 1H), 2.57 (d, J = 11.1 Hz, 2H), 2.04–1.77 (m, 7H), 1.33–1.26 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 138.4, 135.8, 129.4, 127.9, 127.4, 123.0, 121.0, 43.8, 35.0, 25.0, 23.2; HRMS: $C_{13}H_{14}BrN$ calculated 263.0310, found 263.0311; Registry Number: [106795-74-8].

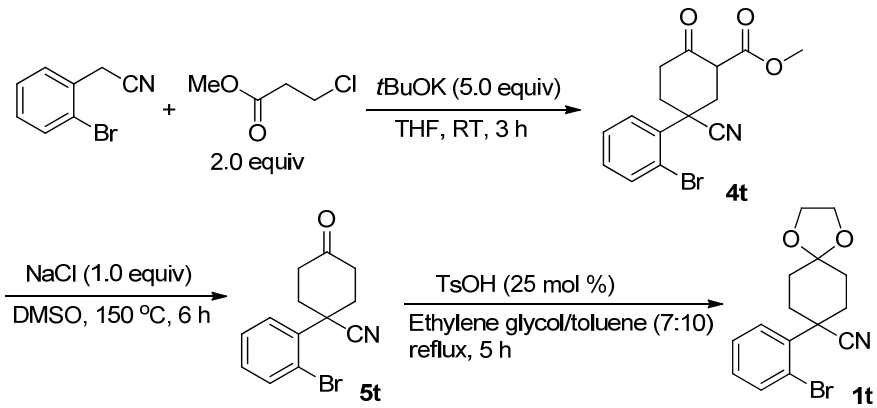
Preparation of 4-(2-bromophenyl)tetrahydro-2*H*-pyran-4-carbonitrile (1s):



1s

Sodium hydride (NaH, 60% in mineral oil, 200 mg, 5 mmol) was washed by dry hexane for several times, the hexane was removed and dry DMF (3 mL) was then added and kept stirring at 0 °C. The solution of 2-(2-bromophenyl)acetonitrile (390 mg, 2 mmol) in DMF (1 mL) was added to the NaH/DMF suspension and kept stirring at 0 °C for 3 h. The reaction mixture was filtered and purified by column chromatography to get compound **1s** in 47% isolated yield; White solid, mp: 95–97 °C; IR (KBr): 3460, 2964, 2931, 2858, 2768, 2703, 2233, 1635, 1469, 1114, 755 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.66 (d, J = 7.8 Hz, 1H), 7.36 (d, J = 4.2 Hz, 2H), 7.23–7.17 (m, 1H), 4.07 (dd, J_1 = 11.4 Hz, J_2 = 4.2 Hz, 2H), 3.96 (td, J_1 = 12.3 Hz, J_2 = 1.5 Hz, 2H), 2.50 (dd, J_1 = 11.7 Hz, J_2 = 1.2 Hz, 2H), 2.11 (td, J_1 = 13.2 Hz, J_2 = 4.5 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 136.7, 135.7, 129.7, 128.0, 127.2, 122.7, 119.9, 64.4, 41.3, 34.5; HRMS: $C_{12}H_{12}BrNO$ calculated 265.0102, found 265.0103; New compound.

Preparation of 8-(2-bromophenyl)-1,4-dioxaspiro[4.5]decane-8-carbonitrile (1t):

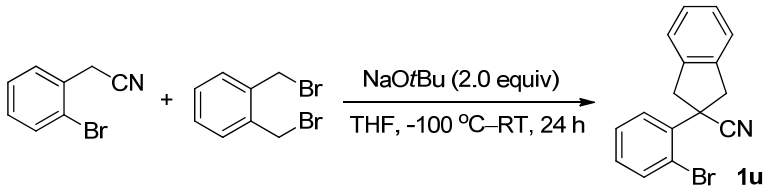


Methyl 5-(2-bromophenyl)-5-cyano-2-oxocyclohexanecarboxylate (4t): To a suspension of potassium *tert*-butoxide (KO*t*Bu, 1122 mg, 10 mmol) in THF (5 mL) was added 2-(2-bromophenyl)acetonitrile (390 mg, 2 mmol) and methyl 3-chloropropanoate (490 mg, 4 mmol). The mixture was kept stirring for 3 h at room temperature, quenched, extracted by HCl/CH_2Cl_2 for three times and collected the combined organic layer. Purification by the column chromatography to provide the compound **4t** in 52% isolated yield; Yellow oil; IR (KBr): 3427, 2923, 1636, 1572, 1470, 1439, 1124, 755 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 12.23 (s, 1H), 7.70 (dd, J_1 = 7.8 Hz, J_2 = 0.9 Hz, 1H), 7.43 (dd, J_1 = 7.8 Hz, J_2 = 1.5 Hz, 1H), 7.36 (td, J_1 = 6.6 Hz, J_2 = 1.2 Hz, 1H), 7.22 (td, J_1 = 7.8 Hz, J_2 = 1.5 Hz, 1H), 3.80 (s, 3H), 3.40 (d, J = 16.2 Hz, 1H), 2.85–2.78 (m, 2H), 2.56–2.48 (m, 2H), 2.45–2.36 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.8, 170.6, 135.9, 130.0, 128.0, 127.7, 122.7, 120.5, 94.4, 51.8, 40.8, 32.1, 29.6, 26.7; HRMS: $C_{15}H_{14}BrNO_3$ calculated 335.0157, found 335.0153; New compound.

1-(2-Bromophenyl)-4-oxocyclohexanecarbonitrile (5t): To a solution of NaCl (117 mg, 2 mmol) in DMSO (4 mL) was added **4t** (670 mg, 2 mmol) and stirred at 150 °C for 6 h under nitrogen atmosphere, quenched, extracted by HCl/CH_2Cl_2 for 3 times and collected the combined organic layer. Purification by the column chromatography to provide the compound **5t** in 94% isolated yield; Yellow solid, mp: 95–96 °C; IR (KBr): 3461, 2924, 1719, 1647, 1637, 1466, 1427, 1339, 758 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.70 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.43 (dd, J_1 = 8.4 Hz, J_2 = 1.8 Hz, 1H), 7.37 (td, J_1 = 8.4 Hz, J_2 = 0.6 Hz, 1H), 7.24 (td, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 2.95 (td, J_1 = 15.0 Hz, J_2 = 6.0 Hz, 2H), 2.90–2.87 (m, 2H), 2.60–2.57 (m, 2H), 2.29 (td, J_1 = 13.8 Hz, J_2 = 4.2 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 207.0, 135.9 (2C), 130.1, 128.2, 127.1, 123.0, 119.5, 42.4, 38.0, 34.4; HRMS: $C_{13}H_{12}BrNO$ calculated 277.0102, found 277.0100; New compound.

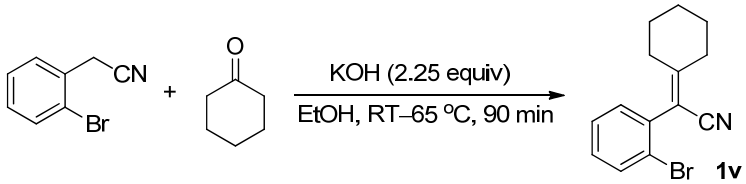
8-(2-Bromophenyl)-1,4-dioxaspiro[4.5]decane-8-carbonitrile (1t): White solid, mp: 114–116 °C; IR (KBr): 3459, 2286, 1638, 1109, 1032, 719 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.67 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.45 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.34 (td, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 7.20 (td, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 4.01 (t, J = 6.0 Hz, 2H), 3.95 (t, J = 6.0 Hz, 2H), 2.59–2.57 (m, 2H), 2.22–2.14 (m, 4H), 1.91–1.88 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 137.3, 135.8, 129.6, 127.9, 127.3, 123.2, 120.3, 107.0, 64.6, 64.3, 42.7, 32.5, 32.1; HRMS: $C_{15}H_{16}BrNO_2$ calculated 321.0364, found 321.0364; New compound.

Preparation of 2-(2-bromophenyl)-2,3-dihydro-1*H*-indene-2-carbonitrile (1u):



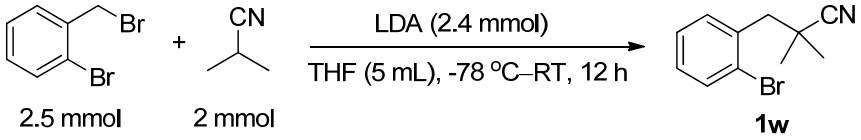
To a suspension of sodium *tert*-butoxide (NaO*t*Bu, 384 mg, 4 mmol) in THF (5 mL) was added 2-(2-bromophenyl)acetonitrile (390 mg, 2 mmol) and kept stirring for a while at -100 °C. The solution of 1,2-bis(bromomethyl)benzene (528 mg, 2 mmol) in THF (1 mL) was then slowly added into the suspension for 30 min at -100 °C. The reaction mixture was then warmed up room temperature and kept stirring for 24 h, quenched, extracted by $NaHCO_3$/toluene for three times and collected the combined organic layer. Purification by the column chromatography to provide the compound **1u** in 42% isolated yield; White solid, mp: 134–135 °C; IR (KBr): 3459, 2922, 2851, 2234, 1636, 1470, 1385, 1023, 757 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.69 (dd, J_1 = 8.4 Hz, J_2 = 1.8 Hz, 1H), 7.49 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.31–7.24 (m, 5H), 7.20 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 3.92 (d, J = 15.6 Hz, 2H), 3.81 (d, J = 15.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 138.9, 136.2, 135.5, 129.8, 128.6, 127.7, 127.6, 124.5, 123.1, 123.1, 47.8, 44.8; HRMS: $C_{16}H_{12}BrN$ calculated 297.0153, found 297.0157; New compound.

Preparation of 2-(2-bromophenyl)-2-cyclohexylideneacetonitrile (1v):

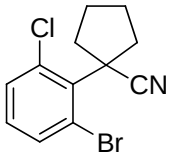


To a solution of potassium hydroxide (KOH, 253 mg, 4.5 mmol) in EtOH (1 mL) was added 2-(2-bromophenyl)acetonitrile (390 mg, 2 mmol) and kept stirring under nitrogen atmosphere for a while at room temperature. Cyclohexanone (216 mg, 2.2 mmol) was then slowly injected into the reaction mixture and kept stirring at 65 °C for 90 min, filtered to remove the salt and isolated by column chromatography to provide **1v** in 47% isolated yield; Colorless oil, IR (KBr): 3499, 3058, 2934, 2857, 2210, 1625, 1470, 1443, 1028, 982, 755 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.61 (d, J = 7.8 Hz, 1H), 7.32 (td, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 7.21 (td, J_1 = 9.6 Hz, J_2 = 1.8 Hz, 2H), 2.73–2.62 (m, 2H), 2.07–1.99 (m, 2H), 1.80–1.75 (m, 2H), 1.62–1.60 (m, 3H), 1.54–1.51 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.9, 134.4, 133.0, 131.3, 130.0, 127.6, 124.1, 117.0, 106.6, 34.4, 31.4, 27.8, 27.3, 25.7; HRMS: $C_{14}H_{14}BrN$ calculated 275.0310, found 275.0313; New compound.

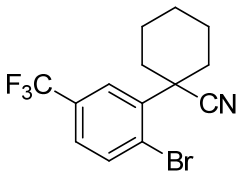
Preparation of 3-(2-bromophenyl)-2,2-dimethylpropanenitrile (1w):[2b]



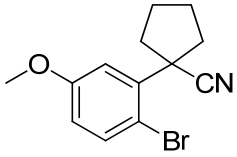
Compound **1w** was prepared according to the ref 2b. Yellow oil; IR (KBr): 3460, 2979, 2934, 2234, 1635, 1469, 1439, 1028, 758, 659 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.59 (dd, J_1 = 7.8 Hz, J_2 = 0.9 Hz, 1H), 7.51 (dd, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1H), 7.32 (td, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 7.15 (td, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 3.08 (s, 2H), 1.43 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 135.6, 133.2, 131.9, 129.0, 127.6, 125.8, 124.7, 44.4, 34.2, 26.6; HRMS: $C_{11}H_{12}BrN$ calculated 237.0153, found 237.0154; Registry Number: [321985-22-2].



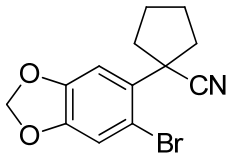
1-(2-Bromo-6-chlorophenyl)cyclopentanecarbonitrile (1A): Prepared according to the general procedure B by using **5h** as starting material, 92% isolated yield; White solid, mp: 59–61 °C; IR (KBr): 3449, 2975, 2951, 2227, 1573, 1554, 1449, 1410, 1193, 1047, 777, 743 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.60 (dd, J_1 = 8.4 Hz, J_2 = 1.8 Hz, 1H), 7.39 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.05 (t, J = 7.8 Hz, 1H), 3.19–3.15 (m, 2H), 2.37–2.35 (m, 2H), 1.98–1.96 (m, 2H), 1.90–1.87 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 135.4, 135.2, 135.1, 132.0, 129.4, 124.3, 122.5, 49.0, 40.7, 23.6; HRMS: $C_{12}H_{11}BrClN$ calculated 282.9763, found 282.9767; New compound.



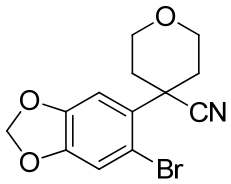
1-(2-Bromo-5-(trifluoromethyl)phenyl)cyclohexanecarbonitrile (1B): Prepared according to the general procedure B, 75% isolated yield; Yellow oil; IR (KBr): 3449, 2932, 2861, 1637, 1385, 1329, 1129, 1093, 1015 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.81 (d, J = 7.8 Hz, 1H), 7.65 (d, J = 1.8 Hz, 1H), 7.45 (dd, J_1 = 8.4 Hz, J_2 = 1.8 Hz, 1H), 2.61 (d, J = 11.4 Hz, 2H), 1.95–1.92 (m, 4H), 1.89–1.85 (m, 1H), 1.79–1.75 (m, 2H), 1.32–1.28 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.6, 136.3, 130.3 (q, J = 33 Hz), 127.0, 126.0, 124.2, 123.5 (q, J = 270 Hz), 120.1, 43.6, 34.9, 24.8, 23.1; HRMS: $C_{14}H_{13}BrF_3N$ calculated 331.0183, found 331.0187; New compound.



1-(2-Bromo-5-methoxyphenyl)cyclopentanecarbonitrile (1C): Prepared according to the general procedure B by using **5d** as starting material, 90% isolated yield; Colorless oil; IR (KBr): 3450, 2960, 2877, 2232, 1594, 1271, 1466, 1293, 1243, 1017, 810, 603 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.55 (d, J = 8.7 Hz, 1H), 6.98 (d, J = 3.0 Hz, 1H), 6.73 (dd, J_1 = 8.7 Hz, J_2 = 3.0 Hz, 1H), 3.80 (s, 3H), 2.74–2.69 (m, 2H), 2.21–2.17 (m, 2H), 2.04–2.00 (m, 2H), 1.92–1.88 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.4, 139.0, 136.2, 123.4, 115.6, 114.4, 114.2, 56.1, 48.1, 38.7, 24.2; HRMS: $C_{13}H_{14}BrNO$ calculated 279.0259, found 279.0263; New compound.



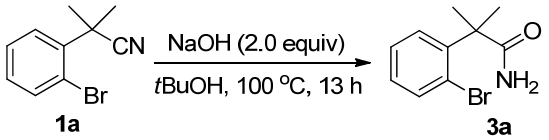
1-(6-Bromobenzo[*d*][1,3]dioxol-5-yl)cyclopentanecarbonitrile (1D): Prepared according to the general procedure B by using **5e** as starting material, 72% isolated yield; White solid, mp: 83–85 °C; IR (KBr): 3458, 2957, 2919, 2877, 2230, 1637, 1506, 1481, 1238, 1038 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.11 (s, 1H), 6.89 (s, 1H), 6.00 (s, 2H), 2.74–2.70 (m, 2H), 2.13–2.08 (m, 2H), 2.03–2.00 (m, 2H), 1.89–1.87 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 147.9, 147.4, 130.8, 122.8, 114.9, 114.7, 107.9, 102.1, 47.3, 38.5, 23.5; HRMS: $C_{13}H_{12}BrNO_2$ calculated 293.0051, found 293.0050; New compound.



4-(6-Bromobenzo[*d*][1,3]dioxol-5-yl)tetrahydro-2*H*-pyran-4-carbonitrile (1E): Prepared according to the general procedure B by using **5e** as starting material, 76% isolated yield; White solid, mp: 120–122 °C; IR (KBr): 3474, 2980, 2909, 2838, 1631, 1474, 1273, 760, 513 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.12 (s, 1H), 6.87 (s, 1H), 6.02 (s, 2H), 4.07 (dd, J_1 = 12 Hz, J_2 = 3.6 Hz, 2H), 3.96 (td, J_1 = 12.6 Hz, J_2 = 1.8 Hz, 2H), 2.50 (dd, J_1 = 12.6 Hz, J_2 = 0.6 Hz, 2H), 2.04 (td, J_1 = 13.2 Hz, J_2 = 4.2 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 148.1, 148.0, 130.1, 120.0, 115.5, 113.8, 107.3, 102.3, 64.6, 41.0, 35.1. HRMS: $C_{13}H_{12}BrNO_3$ calculated 309.0001, found 309.0005; New

compound.

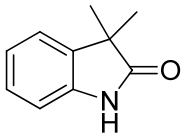
Preparation of 2-(2-bromophenyl)-2-methylpropanamide (3a):[12]



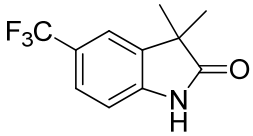
1a **3a**

To a screw-capped vial (25 mL) were added NaOH (400 mg, 10 mmol), *tert*-butanol (*t*BuOH, 10 mL) and **1a** (1.12 g, 5 mmol). The vial was sealed with cap and allowed to stir at 100 °C. The reaction was monitored by TLC every hour until the complete consumption of **1a**. After total conversion of **1a**, the reaction was diluted with CH_2Cl_2, filtered through a thin Celite pad to remove salt, and concentrated *in vacuo*. The residue was isolated through a short flash column chromatography by using ethyl acetate as eluent to give the pure compound **3a** in 92% isolated yield; Colorless oil (high viscosity); IR (KBr): 3472, 2977, 2932, 1669, 1605, 1468, 1427, 1390, 1360, 1022, 756 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.60 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.49 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.34 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.14 (td, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 5.72 (br, 1H), 5.23 (br, 1H), 1.65 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 179.0, 143.0, 134.8, 128.6, 127.7, 127.6, 124.1, 48.3, 26.4; HRMS: $C_{10}H_{12}BrNO$ calculated 241.0102, found 241.0098; Registry Number: [173026-22-7].

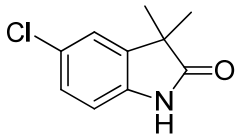
Experimental Details for all products



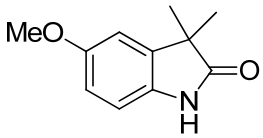
3,3-Dimethylindolin-2-one (2a):[13] White solid, mp: 182–184 °C; IR (KBr): 3450, 3096, 1717, 1676, 1410, 1226, 1172, 738, 618, 492 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 8.62 (br, 1H), 7.20 (t, J = 7.8 Hz, 2H), 7.04 (t, J = 7.8 Hz, 1H), 6.94 (d, J = 7.2 Hz, 1H), 1.41 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 183.9, 139.8, 136.3, 127.6, 122.6, 122.4, 109.8, 44.6, 24.3; HRMS: $C_{10}H_{11}NO$ calculated 161.0841, found 161.0838; Registry Number: [19155-24-9].



3,3-Dimethyl-5-(trifluoromethyl)indolin-2-one (2b): White solid, mp: 152–154 °C; IR (KBr): 3450, 2930, 2880, 1729, 1629, 1339, 1095, 897, 816, 779, 537 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 8.89 (br, 1H), 7.50 (d, J = 8.4 Hz, 1H), 7.43 (s, 1H), 7.02 (d, J = 7.8 Hz, 1H), 1.44 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 183.8, 142.9, 136.7, 125.5, 125.0 (q, J = 31.5 Hz), 124.4 (q, J = 270 Hz), 119.8, 109.7, 44.8, 24.2; HRMS: $C_{11}H_{10}F_3NO$ calculated 229.0714, found 229.0715; New compound.

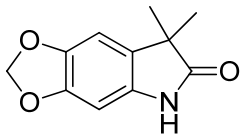


5-Chloro-3,3-dimethylindolin-2-one (2c):[14] White solid, mp: 162–164 °C; IR (KBr): 3468, 3167, 2874, 2926, 2853, 2304, 1731, 1670, 1481, 1204 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 9.14 (br, 1H), 7.18–7.16 (m, 2H), 6.88 (d, J = 8.4 Hz, 1H), 1.40 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 183.9, 138.4, 138.0, 127.9, 127.6, 123.2, 110.9, 45.1, 24.2; HRMS: $C_{10}H_{10}ClNO$ calculated 195.0451, found 195.0453; Registry Number: [74492-46-9].

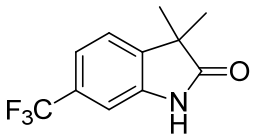


5-Methoxy-3,3-dimethylindolin-2-one (2d): White solid, mp: 154–156 °C; IR(KBr): 3483, 2966, 1702, 1452, 1029, 596 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 8.14 (br, 1H), 6.83–6.79 (m, 2H), 6,73 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 3.79 (s, 3H), 1.39 (s, 6H);

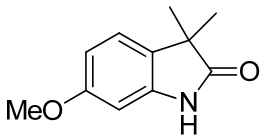
^{13}C NMR (150 MHz, $CDCl_3$): δ 183.5, 155.9, 137.7, 133.0, 111.9, 110.1, 110.0, 55.8, 45.1, 24.4; HRMS: $C_{11}H_{13}NO_2$ calculated 191.0946, found 191.0951; Registry Number: [87234-57-7].



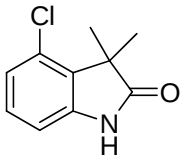
7,7-Dimethyl-5*H*-[1,3]dioxolo[4,5-*f*]indol-6(7*H*)-one (2e): White solid, mp: 244–246 °C; IR (KBr): 3467, 2925, 2284, 1701, 1476, 1118, 1035, 680, 486 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.63 (br, 1H), 6.70 (s, 1H), 6.53 (s, 1H), 5.91 (s, 2H), 1.36 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 184.4, 146.8, 143.2, 133.5, 128.2, 104.1, 100.9, 93.6, 45.0, 24.5; HRMS: $C_{11}H_{11}NO_3$ calculated 205.0739, found 205.0740; New compound.



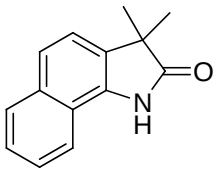
3,3-Dimethyl-6-(trifluoromethyl)indolin-2-one (2f): White solid, mp: 180–181 °C; IR (KBr): 3449, 2970, 2637, 1676, 1460, 1355, 1157, 1052, 640, 519 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.35 (br, 1H), 7.33 (d, J = 7.8 Hz, 1H), 7.29 (d, J = 7.8 Hz, 1H), 7.21 (s, 1H), 1.44 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 184.0, 140.4, 140.0, 130.3 (q, J = 31.5 Hz), 124.0 (q, J = 270 Hz), 122.8, 119.6 (d, J = 3 Hz), 106.9 (d, J = 3 Hz), 44.9, 24.1; HRMS: $C_{11}H_{10}F_3NO$ calculated 229.0714, found 229.0712; New compound.



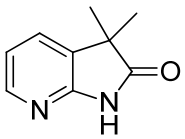
6-Methoxy-3,3-dimethylindolin-2-one (2g): White solid, mp: 167–169 °C; IR (KBr): 3856, 3449, 3192, 2969, 1712, 1672, 1384, 1351, 1157, 740, 572 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.42 (br, 1H), 7.07 (d, J = 7.8 Hz, 1H), 6.56 (dd, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 1H), 6.53 (d, J = 2.4 Hz, 1H), 3.80 (s, 3H), 1.38 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 184.4, 159.7, 140.7, 128.3, 123.2, 107.2, 97.2, 55.5, 44.2, 24.5; HRMS: $C_{11}H_{13}NO_2$ calculated 191.0946, found 191.0948; New compound.



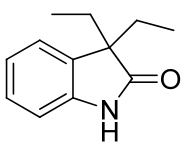
4-Chloro-3,3-dimethylindolin-2-one (2h): White solid, mp: 136–138 °C; IR (KBr): 3469, 3152, 2826, 1723, 1676, 1619, 1247, 1188, 661 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 9.50 (br, 1H), 7.13 (t, J = 7.8 Hz, 1H), 6.97 (dd, J_1 = 7.8 Hz, J_2 = 0.6 Hz, 1H), 6.88 (dd, J_1 = 7.8 Hz, J_2 = 0.6 Hz, 1H), 1.55 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 183.8, 141.7, 132.0, 130.6, 128.9, 123.5, 108.6, 46.3, 21.3; HRMS: $C_{10}H_{10}ClNO$ calculated 195.0451, found 195.0454; New compound.



3,3-Dimethyl-1*H*-benzo[*g*]indol-2(3*H*)-one (2i): White solid, mp: 222–224 °C; IR (KBr): 3468, 2970, 1703, 1459, 1197, 812, 558 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.97 (d, J = 8.4 Hz, 1H), 7.87 (d, J = 8.4 Hz, 1H), 7.61 (d, J = 8.4 Hz, 1H), 7.57 (t, J = 6.6 Hz, 1H), 7.49 (t, J = 6.6 Hz, 1H), 7.38 (d, J = 7.8 Hz, 1H), 2.17 (br, 1H), 1.53 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 185.7, 135.7, 133.3, 130.8, 128.6, 126.1, 125.8, 122.4, 121.6, 120.2, 119.8, 46.0, 24.2; HRMS: $C_{14}H_{13}NO$ calculated 211.0997, found 211.0994; New compound.

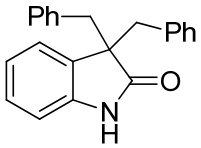


3,3-Dimethyl-1*H*-pyrrolo[2,3-*b*]pyridin-2(3*H*)-one (2j): White solid, mp: 182–184 °C; IR (KBr): 3450, 3114, 2966, 2874, 1731, 1613, 1466, 1200, 1153, 777 cm^{-1}; ^{1} H NMR (600 MHz, $CDCl_3$): δ 8.16 (dd, J_1 = 5.4 Hz, J_2 = 1.8 Hz, 1H), 7.44 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 6.96 (dd, J_1 = 7.2 Hz, J_2 = 5.4 Hz, 1H), 1.87 (br, 1H), 1.42 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 182.1, 155.6, 146.1, 130.5, 130.4, 118.1, 44.6, 23.8; HRMS: $C_9H_{10}N_2O$ calculated 162.0793, found 162.0794; Registry Number: [109535-73-1].

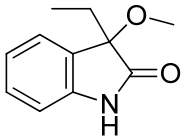


3,3-Diethylindolin-2-one (2k):[15] White solid, mp: 166–168 °C; IR (KBr): 3873, 3449,

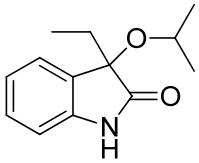
3136, 2969, 2876, 1667, 1344, 1204, 744 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 8.40 (br, 1H), 7.20 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.12 (d, J = 6.6 Hz, 1H), 7.06 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 6.91 (d, J = 7.8 Hz, 1H), 1.96–1.90 (m, 2H), 1.83–1.78 (m, 2H), 0.64 (t, J = 7.8 Hz, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 182.5, 141.3, 132.4, 127.6, 123.1, 122.4, 109.5, 54.9, 30.6, 8.7; HRMS: $C_{12}H_{15}NO$ calculated 189.1154, found 189.1159; Registry Number: [53204-33-4].



3,3-Dibenzylindolin-2-one (2l):[16] White solid, mp: 218–220 °C; IR (KBr): 3450, 3083, 2919, 2854, 1718, 1625, 1241, 754, 696, 556 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.18–7.17 (m, 2H), 7.09–7.00 (m, 8H), 6.93 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 4H), 6.45 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 3.31 (d, J = 13.2 Hz, 2H), 3.17 (d, J = 13.2 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 180.1, 140.5, 135.8, 130.6, 130.1, 127.8, 127.7, 126.5, 124.8, 121.7, 109.2, 56.4, 43.5; HRMS: $C_{22}H_{19}NO$ calculated 313.1467, found 313.1463; Registry Number: [14192-31-5].

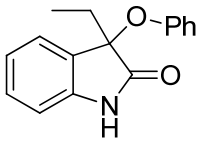


3-Ethyl-3-methoxyindolin-2-one (2m): Yellow solid, mp: 160–161 °C; IR (KBr): 3463, 3274, 2984, 2828, 1729, 1621, 1470, 1210, 1139, 765, 706, 646 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 8.65 (br, 1H), 7.30–7.27 (m, 2H), 7.10 (td, J_1 = 7.2 Hz, J_2 = 0.6 Hz, 1H), 6.93 (d, J = 8.4 Hz, 1H), 3.10 (s, 3H), 2.00 (q, J = 7.2 Hz, 2H), 0.79 (t, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 178.8, 141.3, 129.7, 127.4, 124.6, 123.0, 110.3, 84.0, 53.2, 30.7, 7.3; HRMS: $C_{11}H_{13}NO_2$ calculated 191.0946, found 191.0942; New compound.

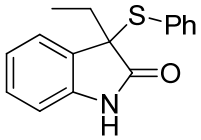


3-Ethyl-3-isopropoxyindolin-2-one (2n): White solid, mp: 171–172 °C; IR (KBr): 3449, 2923, 1754, 1689, 1625, 1384, 1107, 747, 497 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 9.00 (br, 1H), 7.30–7.25 (m, 2H), 7.07 (t, J = 7.8 Hz, 1H), 6.94 (d, J = 7.8 Hz, 1H), 3.46–3.42 (m, 1H), 1.96 (q, J = 7.2 Hz, 2H), 1.12 (d, J = 6.0 Hz, 3H), 0.99 (d, J = 6.6 Hz, 3H), 0.73 (t, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 180.1, 141.0,

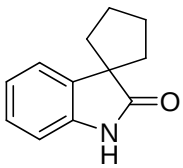
129.4, 128.8, 124.8, 122.7, 110.3, 83.1, 69.2, 31.6, 24.2, 23.3, 7.1; HRMS: $C_{13}H_{17}NO_2$ calculated 219.1259, found 219.1261; New compound.



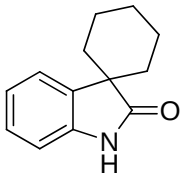
3-Ethyl-3-phenoxyindolin-2-one (2o): White solid, mp: 125–127 °C; IR (KBr): 3449, 2923, 1721, 1619, 1544, 1324, 1115, 691, 489 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 8.42 (br, 1H), 7.28 (d, J = 7.2 Hz, 1H), 7.24 (td, J_1 = 7.8 Hz, J_2 = 0.6 Hz, 1H), 7.07–7.02 (m, 3H), 6.88–6.84 (m, 2H), 6.72 (q, J = 8.4 Hz, 2H), 2.25–2.17 (m, 2H), 0.91 (d, J = 7.8 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 177.6, 155.7, 140.2, 129.7, 129.1, 127.8, 124.8, 123.0, 122.7, 119.0, 110.5, 84.1, 32.2, 7.1; HRMS: $C_{16}H_{15}NO_2$ calculated 253.1103, found 253.1108; New compound.



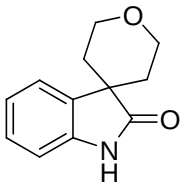
3-Ethyl-3-(phenylthio)indolin-2-one (2p): Yellow solid, mp: 134–136 °C; IR (KBr): 3449, 2923, 2853, 1639, 1384, 1118, 742, 492 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 8.30 (br, 1H), 7.32 (d, J = 7.2 Hz, 1H), 7.24–7.20 (m, 3H), 7.14 (td, J_1 = 7.8 Hz, J_2 = 0.6 Hz, 1H), 7.10–7.06 (m, 3H), 6.67 (d, J = 7.8 Hz, 1H), 2.24–2.17 (m, 1H), 2.16–2.10 (m, 1H), 0.77 (d, J = 7.8 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 178.6, 140.6, 136.4, 129.9, 129.5, 129.3, 128.6, 128.3, 124.6, 122.6, 109.7, 60.1, 28.6, 9.3; HRMS: $C_{16}H_{15}NOS$ calculated 269.0874, found 269.0873; New compound.



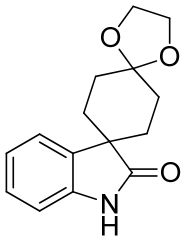
Spiro[cyclopentane-1,3'-indolin]-2'-one (2q):[15] White solid, mp: 122–124 °C; IR (KBr): 3449, 2956, 2928, 2281, 1703, 1619, 1384, 747, 492 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 8.55 (br, 1H), 7.18 (t, J = 7.8 Hz, 2H), 7.02 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 6.90 (dd, J_1 = 7.8 Hz, J_2 = 0.6 Hz, 1H), 2.20–2.17 (m, 2H), 2.09–2.06 (m, 2H), 2.00–1.98 (m, 2H), 1.90–1.87 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 184.6, 140.0, 137.4, 127.3, 122.6, 122.5, 109.5, 54.4, 38.4, 26.7; HRMS: $C_{12}H_{13}NO$ calculated 187.0997, found 187.0993; Registry Number: [41058-67-7].



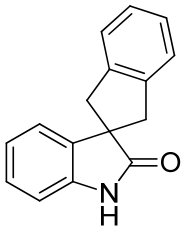
Spiro[cyclohexane-1,3'-indolin]-2'-one (2r):[15] White solid, mp: 115–117 °C; IR (KBr): 3468, 2924, 2852, 1701, 1637, 1619, 1385, 1101, 746 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 8.68 (br, 1H), 7.45 (d, J = 7.2 Hz, 1H), 7.21 (td, J_1 = 7.8 Hz, J_2 = 0.6 Hz, 1H), 7.02 (td, J_1 = 7.2 Hz, J_2 = 0.6 Hz, 1H), 6.94 (d, J = 7.8 Hz, 1H), 1.97–1.92 (m, 2H), 1.90–1.85 (m, 2H), 1.80–1.73 (m, 3H), 1.66–1.60 (m, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 183.3, 140.0, 135.8, 127.4, 124.2, 121.8, 109.7, 48.0, 32.9, 25.2, 21.1; HRMS: $C_{13}H_{15}NO$ calculated 201.1154, found 201.1156; Registry Number: [4933-14-6].



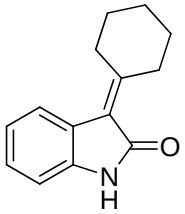
2',3',5',6'-Tetrahydrospiro[indoline-3,4'-pyran]-2-one (2s): White solid, mp: 238–240 °C; IR (KBr): 3568, 3447, 2913, 1700, 1624, 1559, 1092 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 8.17 (br, 1H), 7.36 (d, J = 7.8 Hz, 1H), 7.23 (t, J = 6.6 Hz, 1H), 7.06 (t, J = 7.8 Hz, 1H), 6.92 (d, J = 7.8 Hz, 1H), 4.27–4.23 (m, 2H), 3.96–3.92 (m, 2H), 1.94–1.86 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 181.8, 139.8, 134.6, 128.0, 123.5, 122.5, 109.7, 62.9, 44.6, 32.9; HRMS: $C_{12}H_{13}NO_2$ calculated 203.0946, found 203.0944; Registry Number: [304876-29-7].



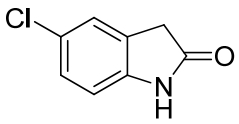
Dispiro[1,3-dioxolane-2,1'-cyclohexane-4',3''-[3*H*]indol]-2''(1''*H*)-one (2t): White solid, mp: 214–215 °C; IR (KBr): 3468, 2958, 2925, 2854, 1700, 1620, 1444, 1094, 750, 488 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 9.34 (br, 1H), 7.35 (d, J = 7.2 Hz, 1H), 7.20 (t, J = 7.8 Hz, 1H), 7.00 (t, J = 7.8 Hz, 1H), 6.96 (d, J = 7.8 Hz, 1H), 4.03 (s, 4H), 2.30–2.24 (m, 2H), 2.05–2.00 (m, 2H), 1.93–1.86 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 183.1, 140.2, 134.9, 127.7, 123.3, 122.0, 109.9, 108.1, 64.3, 46.5, 31.2, 30.1; HRMS: $C_{15}H_{17}NO_3$ calculated 259.1208, found 259.1202; Registry Number: [52140-55-3].



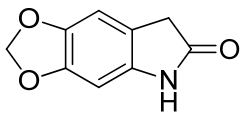
1,3-Dihydrospiro[indene-2,3'-indolin]-2'-one (2u): White solid, mp: 210–212 °C; IR (KBr): 3464, 3187, 1707, 1459, 1225, 1009, 749, 643 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 8.71 (br, 1H), 7.28–7.24 (m, 4H), 7.18 (t, J = 7.8 Hz, 1H), 6.93 (d, J = 7.8 Hz, 1H), 6.89 (t, J = 7.8 Hz, 1H), 6.83 (d, J = 7.8 Hz, 1H), 3.65 (d, J = 16.2 Hz, 2H), 3.13 (d, J = 15.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 182.6, 141.1, 139.6, 136.7, 128.0, 127.0, 124.5, 122.8, 121.9, 109.8, 54.5, 44.0; HRMS: $C_{16}H_{13}NO$ calculated 235.0997, found 235.1001; Registry Number: [114727-61-6].



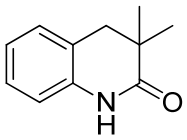
3-Cyclohexylideneindolin-2-one (2v):[17] White solid, mp: 204–206 °C; IR (KBr): 3449, 2926, 2854, 1690, 1618, 1467, 1217, 736 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 8.03 (br, 1H), 7.61 (d, J = 7.8 Hz, 1H), 7.16 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 6.98 (td, J_1 = 7.8 Hz, J_2 = 0.6 Hz, 1H), 6.84 (d, J = 7.2 Hz, 1H), 3.35 (t, J = 6.6 Hz, 2H), 2.87 (t, J = 6.0 Hz, 2H), 1.86–1.82 (m, 2H), 1.80–1.76 (m, 2H), 1.72–1.68 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 169.9, 164.6, 139.3, 127.5, 124.3, 123.8, 121.5, 120.0, 109.3, 33.1, 30.0, 28.1, 27.8, 25.8; HRMS: $C_{14}H_{15}NO$ calculated 213.1154, found 213.1153; Registry Number: [3478-78-2].



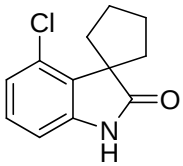
5-Chloroindolin-2-one (2x):[18] White solid, mp: 195–196 °C; IR (KBr): 3444, 2900, 1701 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 8.50 (br, 1H), 7.21–7.18 (m, 2H), 7.01 (d, J = 7.8 Hz, 1H), 3.54 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 176.8, 140.9, 127.9, 127.7, 126.9, 125.1, 110.5, 36.1; HRMS: C_8H_6ClNO calculated 167.0138, found 167.0144; Registry Number: [17630-75-0].



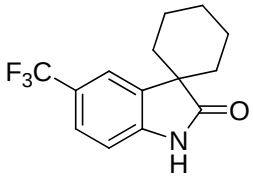
5*H*-[1,3]dioxolo[4,5-*f*]indol-6(7*H*)-one (2y): White solid, mp: 228–229 °C; IR (KBr): 742, 1295, 1475, 1720, 2915 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.91 (br, 1H), 6.74 (s, 1H), 6.47 (s, 1H), 5.92 (s, 2H), 3.46 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 177.6, 147.1, 143.1, 136.0, 116.7, 106.1, 100.1, 93.3, 36.4; HRMS: C_8H_7NO calculated 177.0426, found 177.0429; New compound.



3,3-Dimethyl-3,4-dihydroquinolin-2(1*H*)-one (2y):[19] Yellow solid, mp: 159–161 °C; IR (KBr): 3475, 3195, 3071, 2985, 2923, 1672, 1494, 1389, 762, 670 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 8.22 (br, 1H), 7.18 (t, J = 7.2 Hz, 1H), 7.14 (d, J = 7.2 Hz, 1H), 7.00 (t, J = 7.2 Hz, 1H), 6.78 (d, J = 7.8 Hz, 1H), 2.81 (s, 2H), 1.22 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 176.9, 136.6, 128.5, 127.4, 123.3, 123.2, 114.8, 40.2, 37.3, 24.3; HRMS: $C_{11}H_{13}NO$ calculated 175.0997, found 175.0993; Registry Number: [92367-59-4].

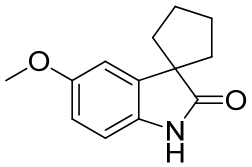


4'-Chlorospiro[cyclopentane-1,3'-indolin]-2'-one (2A): White solid, mp: 168–170 °C; IR (KBr): 3487, 3170, 3134, 2957, 2870, 1706, 1619, 1444, 1178, 661 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 9.25 (br, 1H), 7.11 (t, J = 7.8 Hz, 1H), 6.96 (d, J = 7.8 Hz, 1H), 6.83 (d, J = 7.8 Hz, 1H), 2.33–2.31 (m, 2H), 2.09–2.03 (m, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): 185.4, 142.5, 131.9, 129.8, 128.6, 123.4, 108.2, 54.6, 35.0, 27.6; HRMS: $C_{12}H_{12}ClNO$ calculated 221.0607, found 221.0611; New compound.

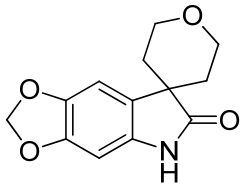


5'-(Trifluoromethyl)spiro[cyclohexane-1,3'-indolin]-2'-one (2B): White solid, mp: 182–184 °C; IR (KBr): 3467, 2933, 1724, 1691, 1113, 825 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 9.11 (br, 1H), 7.64 (s, 1H), 7.51 (d, J = 8.4 Hz, 1H), 7.02 (d, J = 7.8 Hz,

1H), 2.00–1.97 (m, 2H), 1.91–1.86 (m, 2H), 1.77–1.64 (m, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 183.3, 143.1, 136.3, 125.2, 124.5 (q, J = 270 Hz), 124.3 (q, J = 33 Hz), 121.0, 109.5, 48.0, 32.8, 25.0, 21.0; HRMS: $C_{14}H_{14}F_3NO$ calculated 269.1027, found 269.1025; New compound.



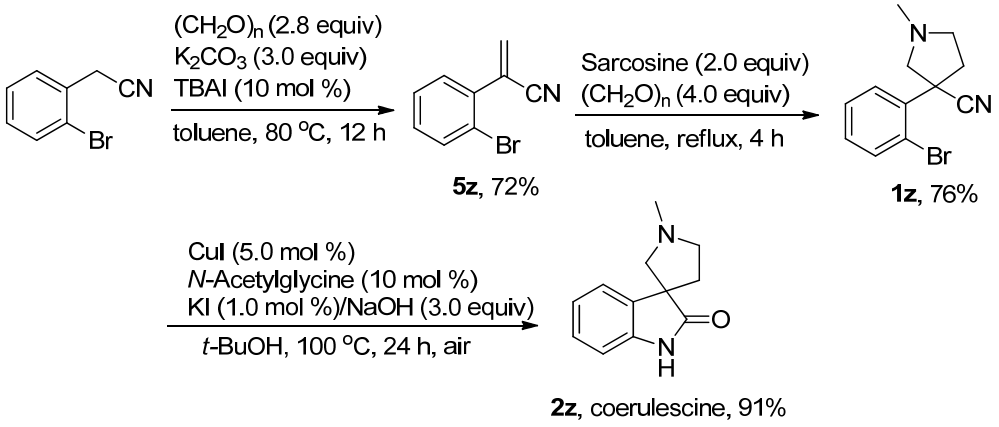
5'-Methoxyspiro[cyclopentane-1,3'-indolin]-2'-one (2C): White solid, mp: 180–182 °C; IR (KBr): 3460, 2956, 2862, 1682, 1652, 1635, 1491, 1209, 1029 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.86 (br, 1H), 6.82 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 6.79 (d, J = 3.0 Hz, 1H), 6.70 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 3.78 (s, 3H), 2.20–2.17 (m, 2H), 2.08–2.05 (m, 2H), 1.98–1.95 (m, 2H), 1.87–1.84 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 184.7, 155.9, 138.8, 133.6, 111.3, 110.2, 109.7, 55.8, 54.9, 38.4, 26.7; HRMS: $C_{13}H_{15}NO_2$ calculated 217.1103, found 217.1100; New compound.



2',3',5',6'-Tetrahydrospiro[[1,3]dioxolo[4,5-*f*]indole-7,4'-pyran]-6(5*H*)-one (2D): White solid, mp: 276–277 °C; IR (KBr): 3461, 2923, 1721, 1631, 1474, 1267, 1176, 1111, 754, 409 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$, bad solubility): δ 7.72 (br, 1H), 6.86 (s, 1H), 6.49 (s, 1H), 5.93 (s, 2H), 4.25–4.21 (m, 2H), 3.91–3.88 (m, 2H), 1.86–1.84 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 182.0, 147.0, 143.2, 133.6, 126.4, 104.9, 101.1, 93.2, 62.8, 44.8, 33.1; HRMS: $C_{13}H_{13}NO_4$ calculated 247.0845, found 247.0844; New compund.

Experimental Details for natural alkaloids

Synthesis of (±)-coerulescine (2z):



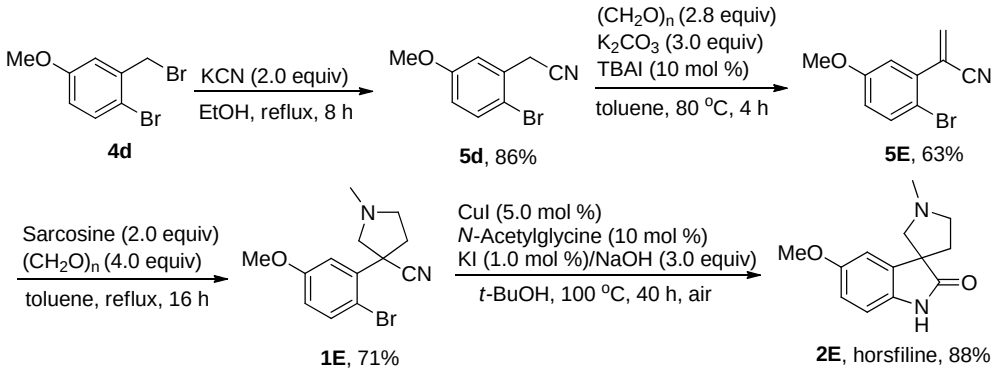
2-(2-Bromophenyl)acrylonitrile (5z): To a suspension of potassium carbonate (K_2CO_3, 830 mg, 6 mmol) and tetrabutyl ammonium iodide (Bu_4NI, 74 mg, 0.2 mmol) in toluene (4 mL) was added 2-(2-bromophenyl)acetonitrile (390 mg, 2 mmol) and allowed to stir for few minutes. The aqueous formaldehyde (CH_2O, 37% in H_2O, 168 mg, 5.6 mmol) was then slowly injected into the solution over a period of 20 min. The resulting reaction mixture was warmed to 80 °C and kept stirring for 12 h, quenched by H_2O and extracted by toluene for several times. The combined organic layer was collected and dried over anhydrous $MgSO_4$, purified by column chromatography to provide pure compound **5z** in 72% isolated yield; Orange oil; IR (KBr): 3459, 2921, 2851, 2227, 1611, 1471, 1430, 1026, 947, 767, 742 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.58 (d, J = 7.8 Hz, 1H), 7.33–7.29 (m, 2H), 7.25–7.21 (m, 1H), 6.28 (s, 1H), 6.08 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 135.1, 134.3, 133.2, 130.7, 130.3, 127.7, 122.5, 121.5, 116.6; HRMS: C_9H_6BrN calculated 206.9684, found 206.9681; New compound.

3-(2-Bromophenyl)-1-methylpyrrolidine-3-carbonitrile (1z): Compound **5z** (416 mg, 2 mmol) was dissolved in toluene (4 mL) and allowed to stir under reflux. The prepared solution of sarcosine (356 mg, 4 mmol) in aqueous formaldehyde (CH_2O, 37% in H_2O, 1 mL) was slowly injected into the solution of **5z** in toluene for the period over 2 h. The reaction mixture was allowed to stir for an additional 2 h, quenched by H_2O and extracted by toluene for several times. The combined organic layer was collected and dried over anhydrous $MgSO_4$, purified by column chromatography to provide pure compound **1z** in 76% isolated yield; Yellow oil; IR (KBr): 3460, 2921, 2850, 2789, 1637, 1471, 1384, 1028, 760 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.66 (dd, J_1 = 8.1 Hz, J_2 = 0.9 Hz, 1H), 7.38 (dd, J_1 = 8.1 Hz, J_2 = 1.8 Hz, 1H), 7.32 (td, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 7.19 (td, J_1 = 7.5 Hz, J_2 = 1.8 Hz, 1H), 3.42 (d, J = 9.9 Hz, 1H), 3.20 (d, J = 9.6 Hz, 1H), 3.04–2.90 (m, 2H), 2.76–2.67

(m, 1H), 2.46 (s, 4H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 137.1, 135.1, 129.7, 127.7, 127.6, 123.6, 122.7, 65.6, 54.6, 46.0, 41.8, 38.3; HRMS: $C_{12}H_{13}BrN_2$ calculated 264.0262, found 264.0267; New compound.

(±)-Coerulescine (2z):[20] Yellow solid, mp: 129–130 °C; IR (KBr): 3465, 3242, 2944, 2791, 1709, 1620, 1472, 1338, 1197, 753 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.04 (br, 1H), 7.38 (d, J = 7.8 Hz, 1H), 7.18 (t, J = 7.8 Hz, 1H), 7.03 (t, J = 7.8 Hz, 1H), 6.91 (d, J = 7.8 Hz, 1H), 3.02–2.98 (m, 1H), 2.90 (d, J = 9.6 Hz, 1H), 2.84–2.78 (m, 2H), 2.46 (s, 3H), 2.44–2.40 (m, 1H), 2.12–2.08 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 183.2, 140.2, 136.3, 127.7, 123.2, 122.7, 109.6, 66.4, 56.8, 53.7, 41.8, 37.9; HRMS: $C_{12}H_{14}N_2O$ calculated 202.1106, found 202.1104; Registry Number: [66859-18-5].

Synthesis of (±)-horsfiline (2E):



2-(2-Bromo-5-methoxyphenyl)acrylonitrile (5E): Procedure is the same with the preparation of **5z**, 63% isolated yield; Colorless oil; IR (KBr): 3467, 2921, 2851, 2298, 1637, 1384 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.47 (d, J = 9.0 Hz, 1H), 6.86 (d, J = 3.0 Hz, 1H), 6.80 (dd, J_1 = 9.0 Hz, J_2 = 3.0 Hz, 1H), 6.30 (s, 1H), 6.12 (s, 1H), 3.77 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.0, 135.2, 135.1, 134.1, 122.6, 116.7, 116.5, 116.0, 111.9, 55.5; HRMS: $C_{10}H_8BrNO$ calculated 236.9789, found 236.9786; New compound.

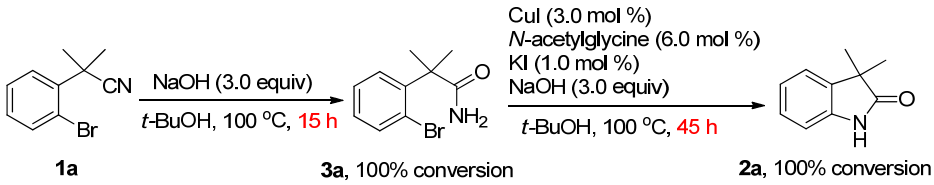
3-(2-Bromo-5-methoxyphenyl)-1-methylpyrrolidine-3-carbonitrile (1E): Prepared according to the preparation of **1z**, 71% isolated yield; Yellow oil; IR (KBr): 3446, 2941, 2842, 2789, 2235, 1635, 1467, 1293, 811 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.53 (d, J = 9.0 Hz, 1H), 6.93 (d, J = 3.0 Hz, 1H), 6.73 (dd, J_1 = 8.7 Hz, J_2 = 3.0 Hz, 1H), 3.79 (s, 3H), 3.41 (d, J = 9.9 Hz, 1H), 3.17 (d, J = 9.9 Hz, 1H), 3.00–2.90 (m, 2H), 2.75–2.69 (m, 1H), 2.46 (s, 3H), 2.45–2.37 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.8, 137.9, 135.5, 122.6, 115.0, 114.0, 113.5, 65.4, 55.5, 54.5, 45.9, 41.6, 38.1; HRMS: $C_{13}H_{15}BrN_2O$ calculated 294.0368, found 294.0363; New compound.

(±)-Horsfiline (2E):[21] Yellow solid, mp: 159–160 °C; IR (KBr): 3449, 2922, 2851, 1702, 1492, 1208, 1032, 811, 669, 618 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.95 (br,

1H), 7.02 (d, J = 2.4 Hz, 1H), 6.78 (d, J = 8.4 Hz, 1H), 6.72 (dd, J_1 = 8.4 Hz, J_2 =2.4 Hz, 1H), 3.79 (s, 3H), 3.03–2.99 (m, 1H), 2.85 (s, 2H), 2.74 (q, J = 7.2 Hz, 1H), 2.45 (s, 3H), 2.43–2.39 (m, 1H), 2.11–2.06 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 182.4, 156.2, 137.7, 133.2, 112.4, 110.4, 109.6, 66.5, 56.7, 55.9, 54.1, 41.8, 38.1; HRMS: $C_{13}H_{16}N_2O_2$ calculated 232.1212, found 232.1211; Registry Number: [136316-07-9].

Control Experiments and Proposed Pathway

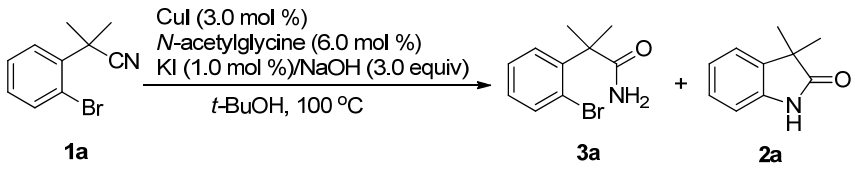
The following two control experiments were preceded for the study of reaction pathway. First, the reaction was processed stepwise by converting all the **1a** to its corresponding amide derivative **3a** and then coupling the C-N bond to form **2a** by using the same reaction condition with the domino process.



Scheme 1. Stepwise formation of oxindole

Second, the reaction was monitored and the ratios of each species were checked at the different reaction time (Table 1).

Table 1. Reaction monitoring for the ratio of all species.



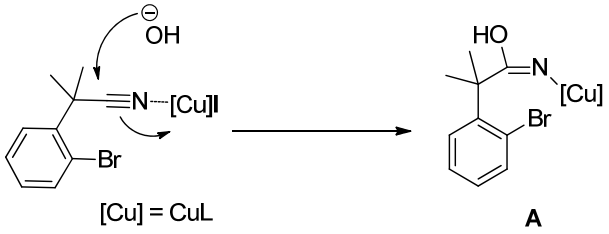
Entry	t (h)	Ratio of **1a**[a]	Ratio of **3a**[a]	Ratio of **2a**[a]
1	4	38	56	6
2	6	22	55	23
3	8	3	53	44
4	10	0	31	69
5	12	0	19	81
6	16	0	12	88
7	20	0	7	93
8	24	0	0	100

[a] The ratios were determined by ^{1}H NMR after working up the reaction.

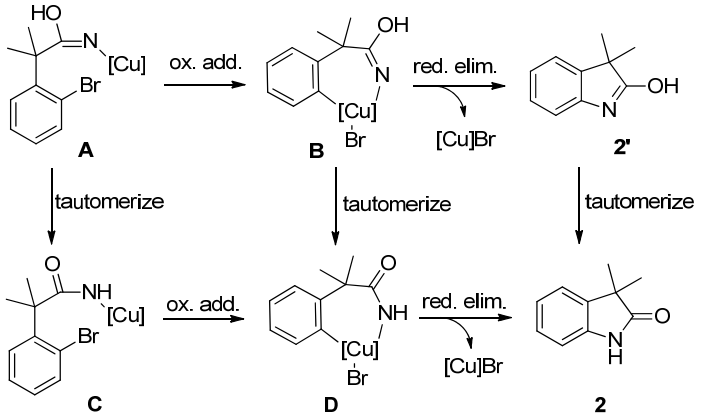
We can conclude and describe the results according to the control experiments:

1. For the stepwise reaction (Scheme 1), the transformation from **3a** to **2a** required much longer time than the overall reaction time of Cu-catalyzed domino reaction. Thus, the reaction pathway of the Cu-catalyzed domino reaction might be not via the directly intramolecular C-N coupling reaction of **3a** to form **2a**.

2. According to the results listed in table 1, we observed that the consumption of **1a** is significantly faster than the stepwise reaction. This is caused by the acceleration of nucleophilic addition by copper complex, which is acting as a Lewis acid.

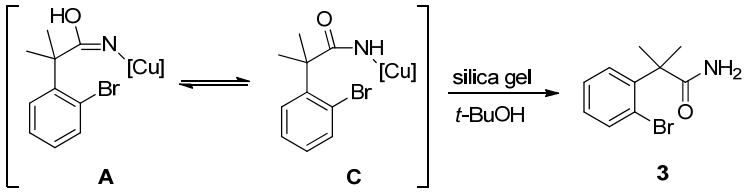


3. The formation of **2a** in the domino reaction is much more facile than the stepwise reaction; more than 80% **2a** was generated within 12 h (Table 1, entry 5). That means the oxidative addition of copper complex to aryl bromide moiety in domino reaction is much easier than the transformation of **2a** from **3a**. This suggests that the oxidative addition occurs in intramolecular manner. The following reductive elimination provides **2'**, and a rapid tautomerization affords product **2**.



Furthermore, we believe that the tautomerization should be much faster than the intramolecular oxidative addition. Thus, the reaction pathway should be decided as **A**→**C**→**D**→**2**.

4. The observation of **3** in table 1 was caused by the direct hydrolysis of **A** or **C**. And the amount of **3** was related to the amount of **A** and **C**.



5. Before the complete consumption of **1a**, the ratio of **3a** is always about 55% (Table 1, entries 1–3). After the consumption of **1a** is complete, the ratio of **3a** is also reduced significantly. This result reveals that the equilibrium between **C** and **D** can be maintained before the complete consumption of **1a**, and the reductive elimination of **D** dominate the formation of **2**. Our proposed mechanism (shown in manuscript) was suggested according to the results described above.

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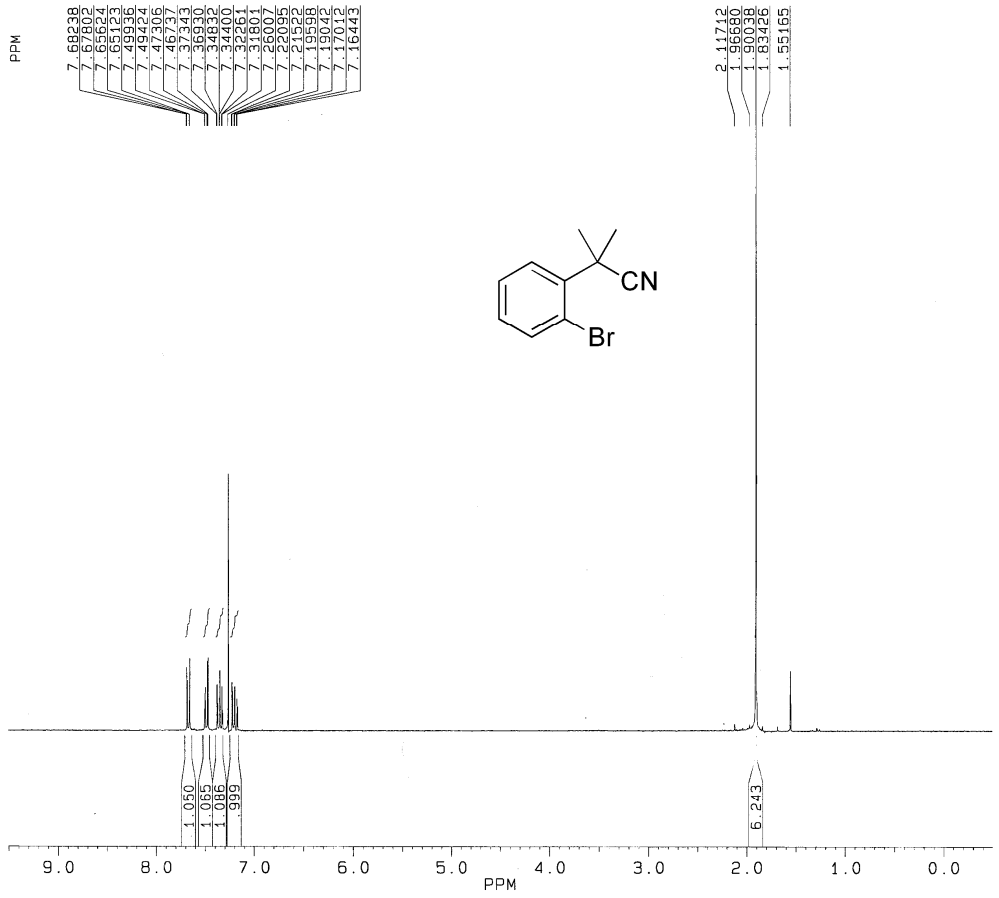
^{1}H and ^{13}C NMR Spectra (300 MHz and 600 MHz, $CDCl_3$) for substrates

2-(2-Bromophenyl)-2-methylpropanenitril (1a)



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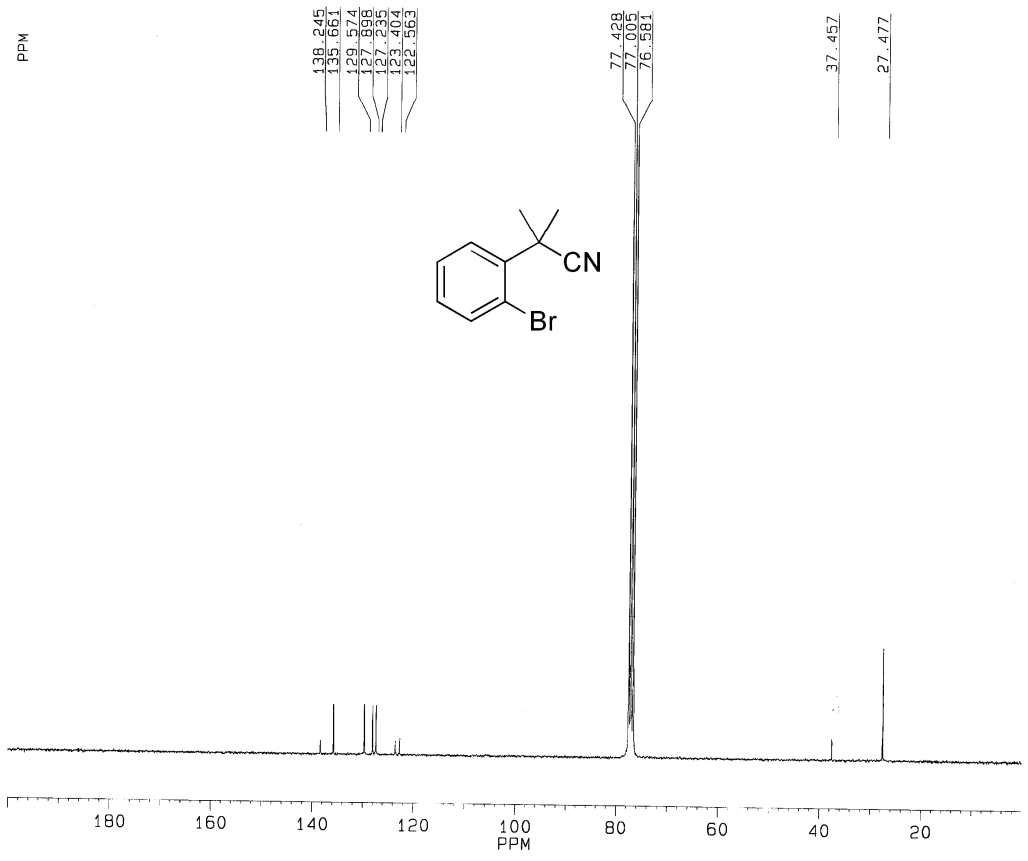

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DATE ??-??-??

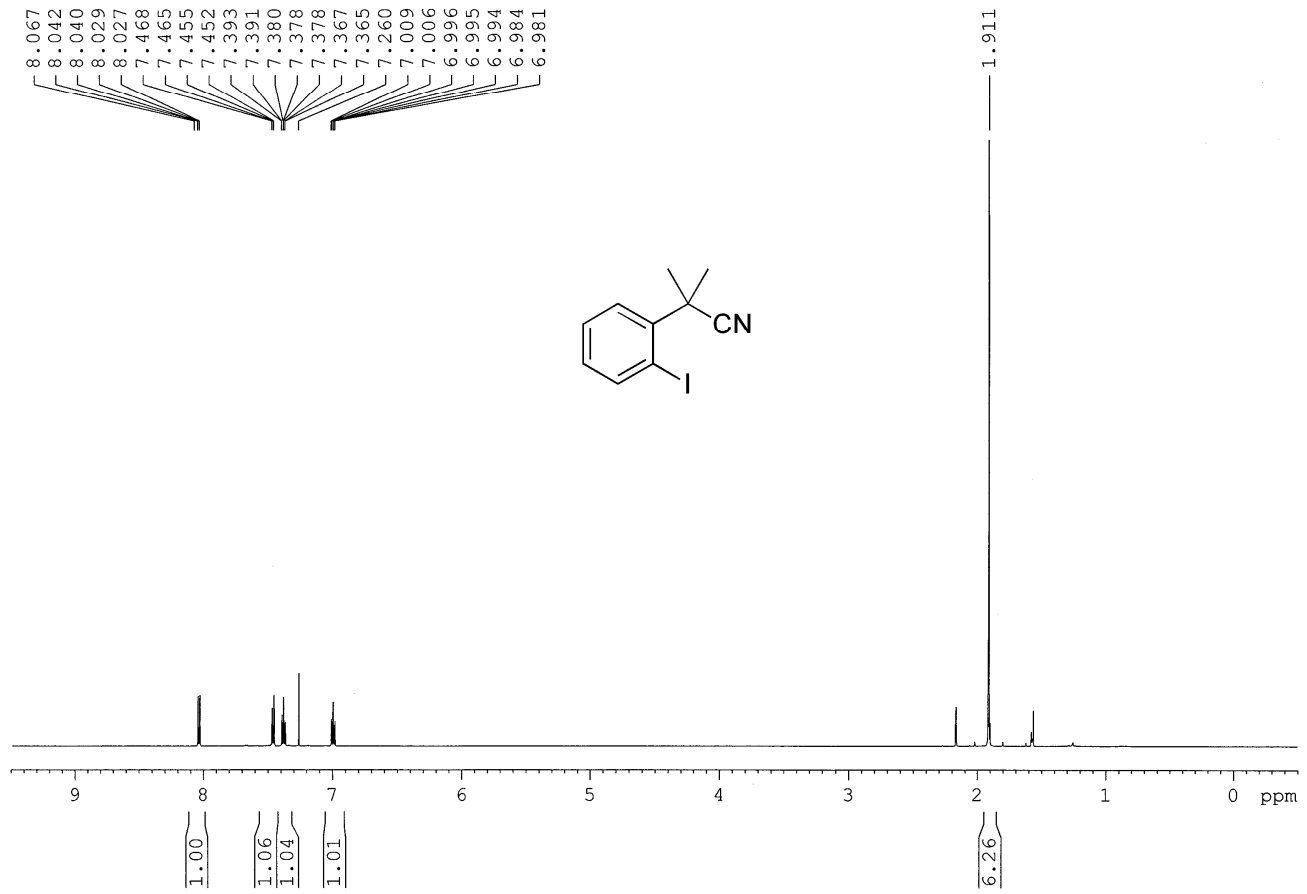
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

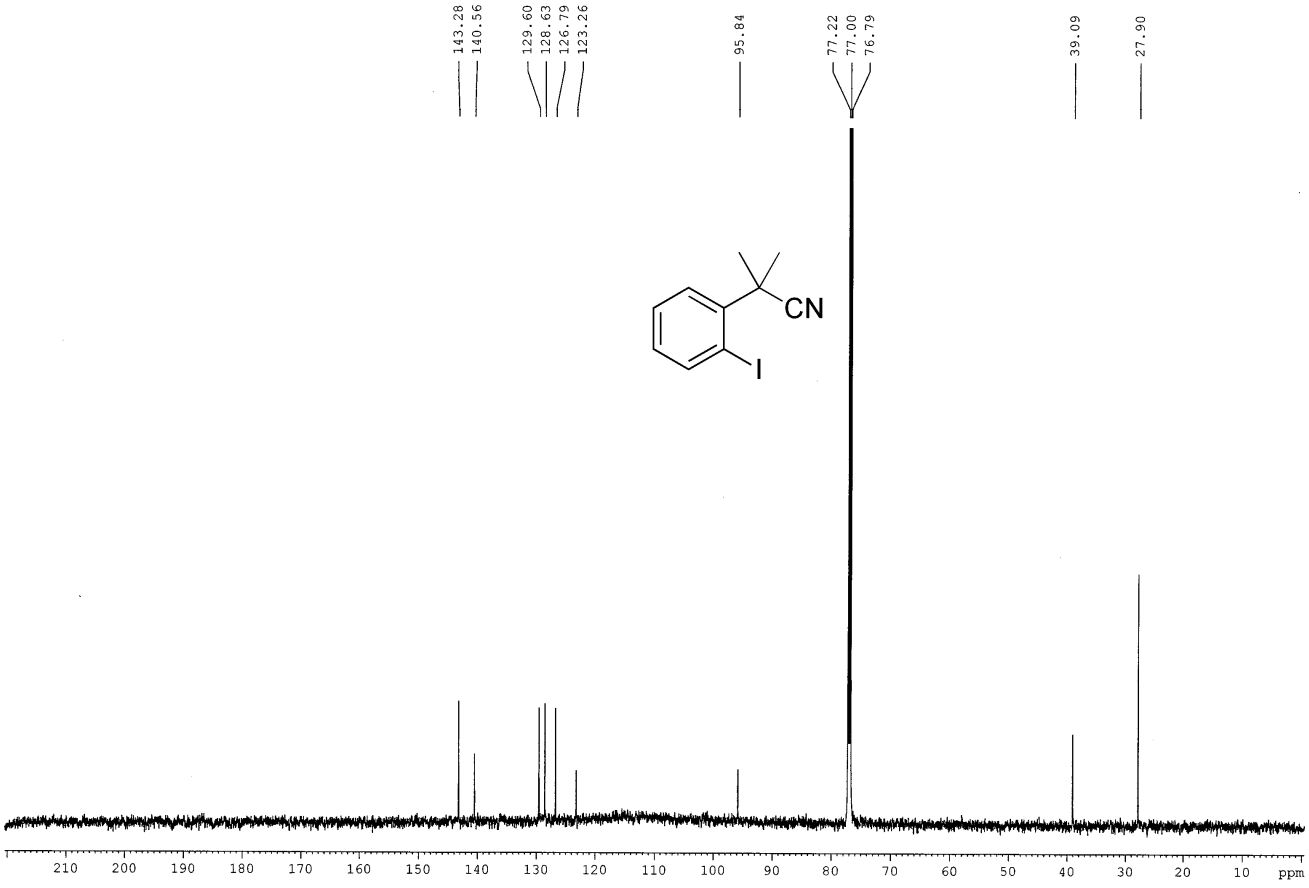
PW 1.4
RD 1.500
AQ .852
RG 200
NS 22397
TE 297

FW 24100
O2 4869.082
DP 15H CPD

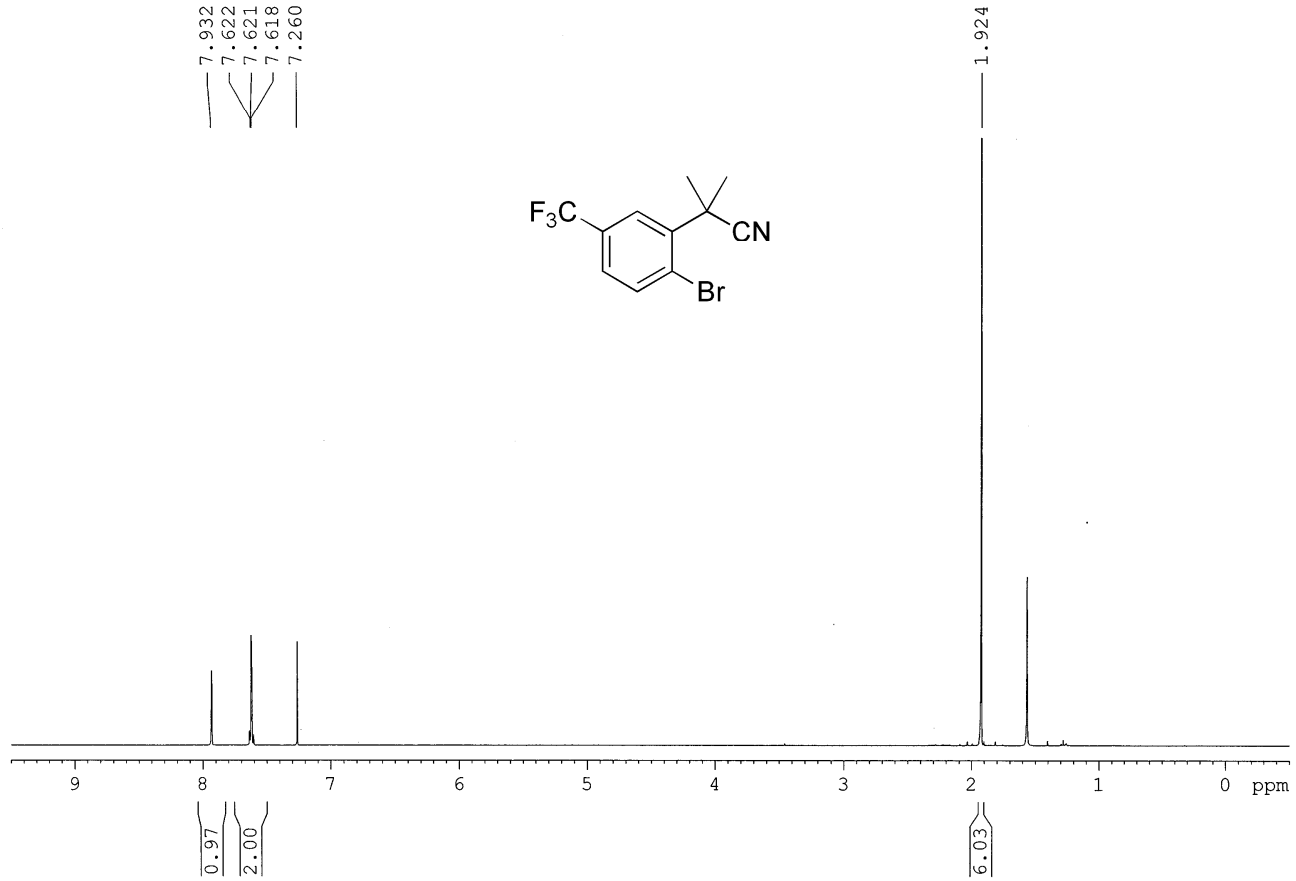
LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 200.008P
F2 .013P
HZ/CM 718.728
PPM/CM 9.524
SR -1406.14

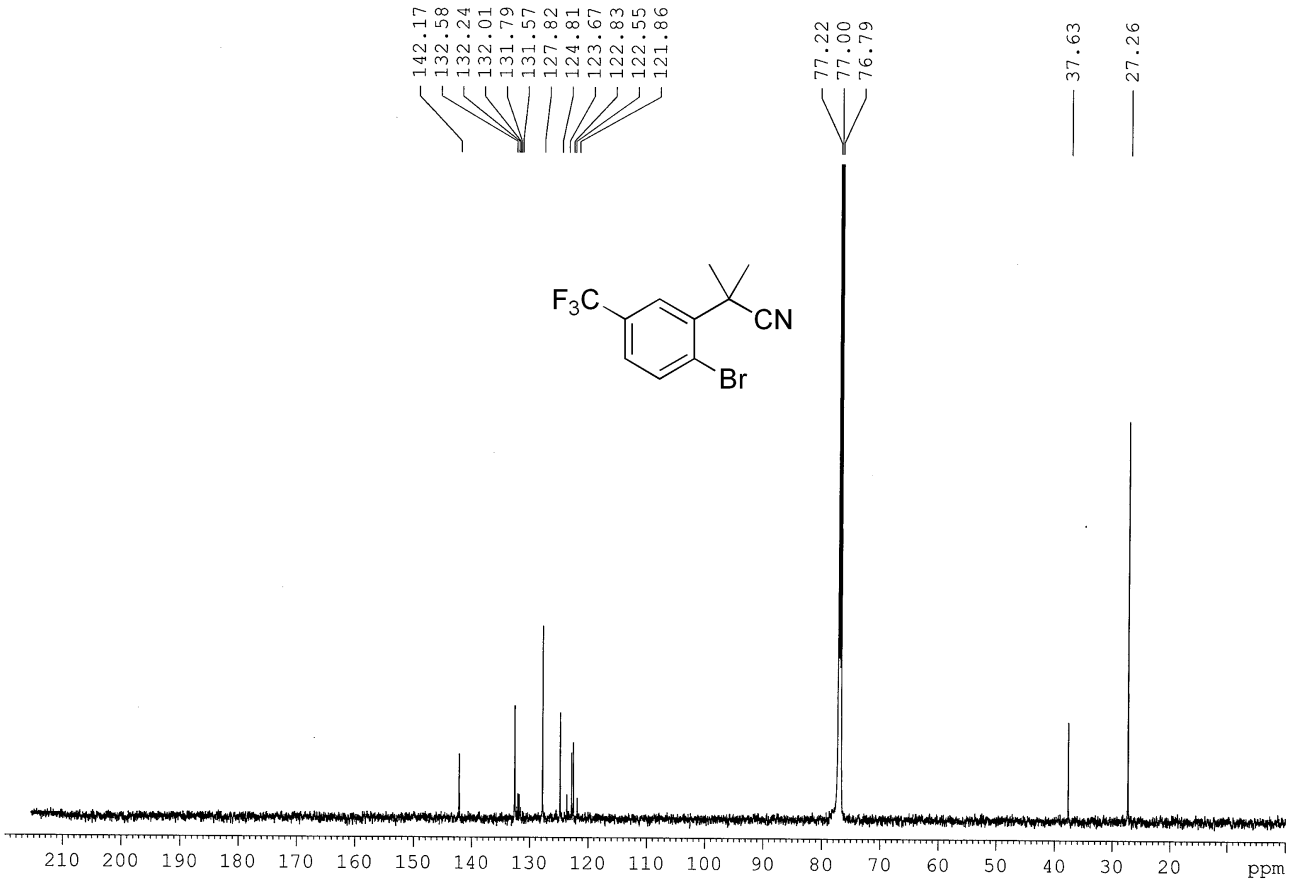
2-(2-Iodophenyl)-2-methylpropanenitril (1a')



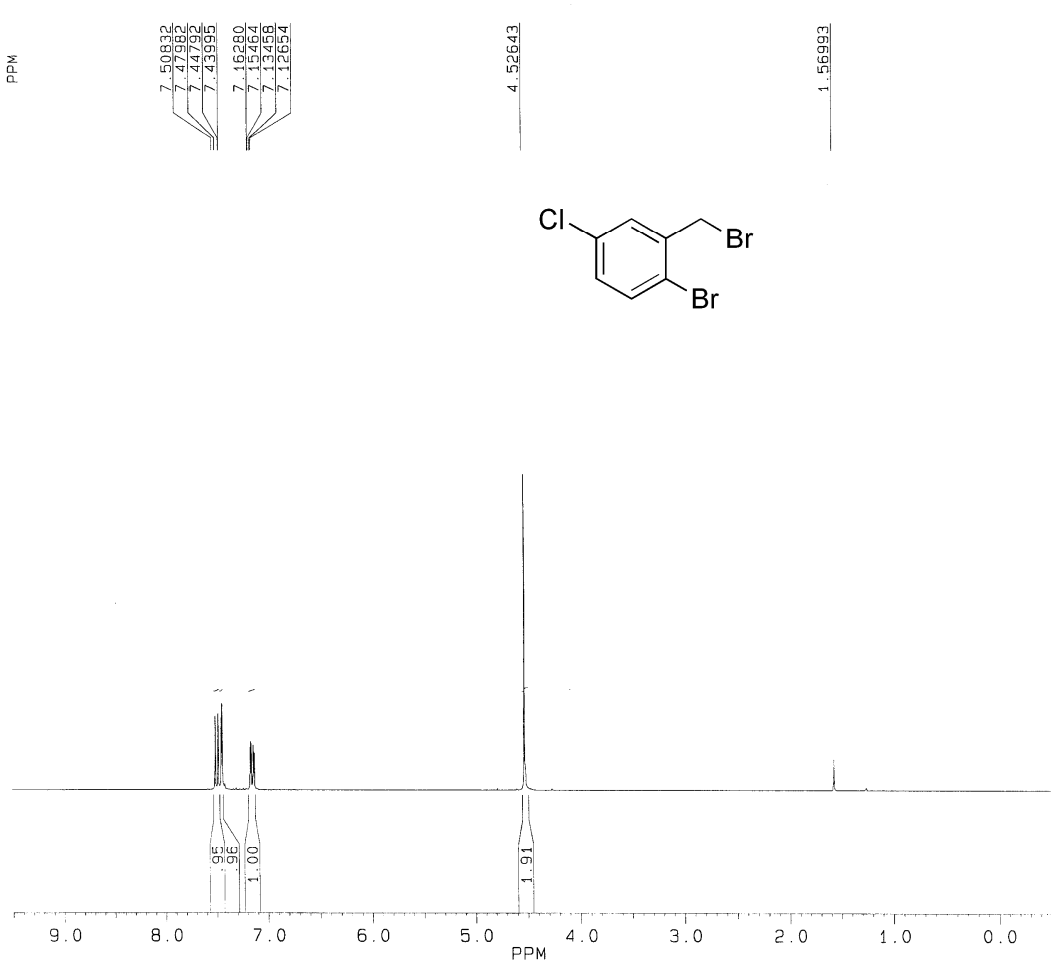


2-(2-Bromo-5-(trifluoromethyl)phenyl)-2-methylpropanenitrile (1b)





1-Bromo-2-(bromomethyl)-4-chlorobenzene (4c)

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D0316.009
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI   16384
TD   16384
SW    4807.692
HZ/PT     .587

PW       1.4
RD       1.000
AQ       1.704
RG      40
NS      16
TE     297

FW    6100
O2       0.0
DP   63L PO

LB       0.0
GB       0.0
CX      21.00
CY       0.0
F1       9.501P
F2       -.499P
HZ/CM 142.918
PPM/CM    .476
SR    3367.55
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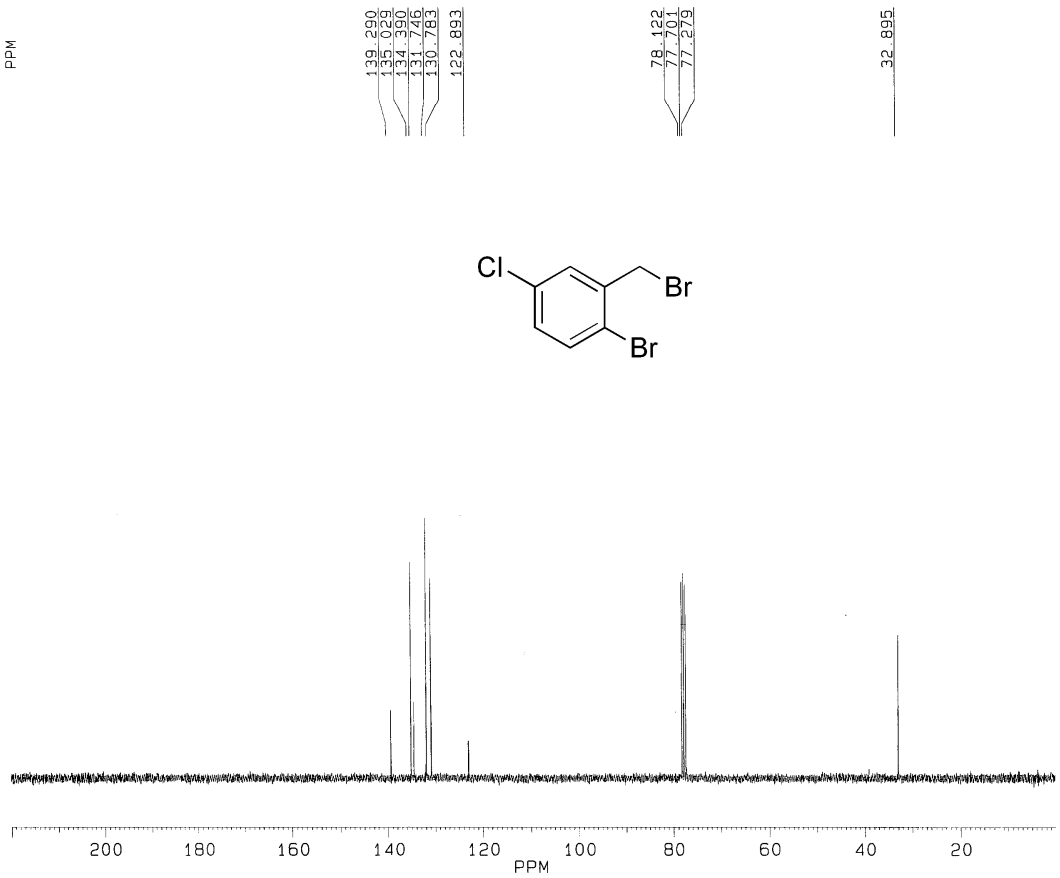


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D0316.902
DATE ??-??-??

SF      75.469
SY   75.0
O1    6517.695
SI   32768
TD   32768
SW   19230.769
HZ/PT    1.174

PW       1.4
RD       1.500
AQ        .852
RG     200
NS     325
TE     297

FW   24100
O2    4869.082
DP   15H CPD

LB       0.0
GB       0.0
CX      21.00
CY       0.0
F1     220.009P
F2        .013P
HZ/CM 790.606
PPM/CM 10.476
SR   -1454.27
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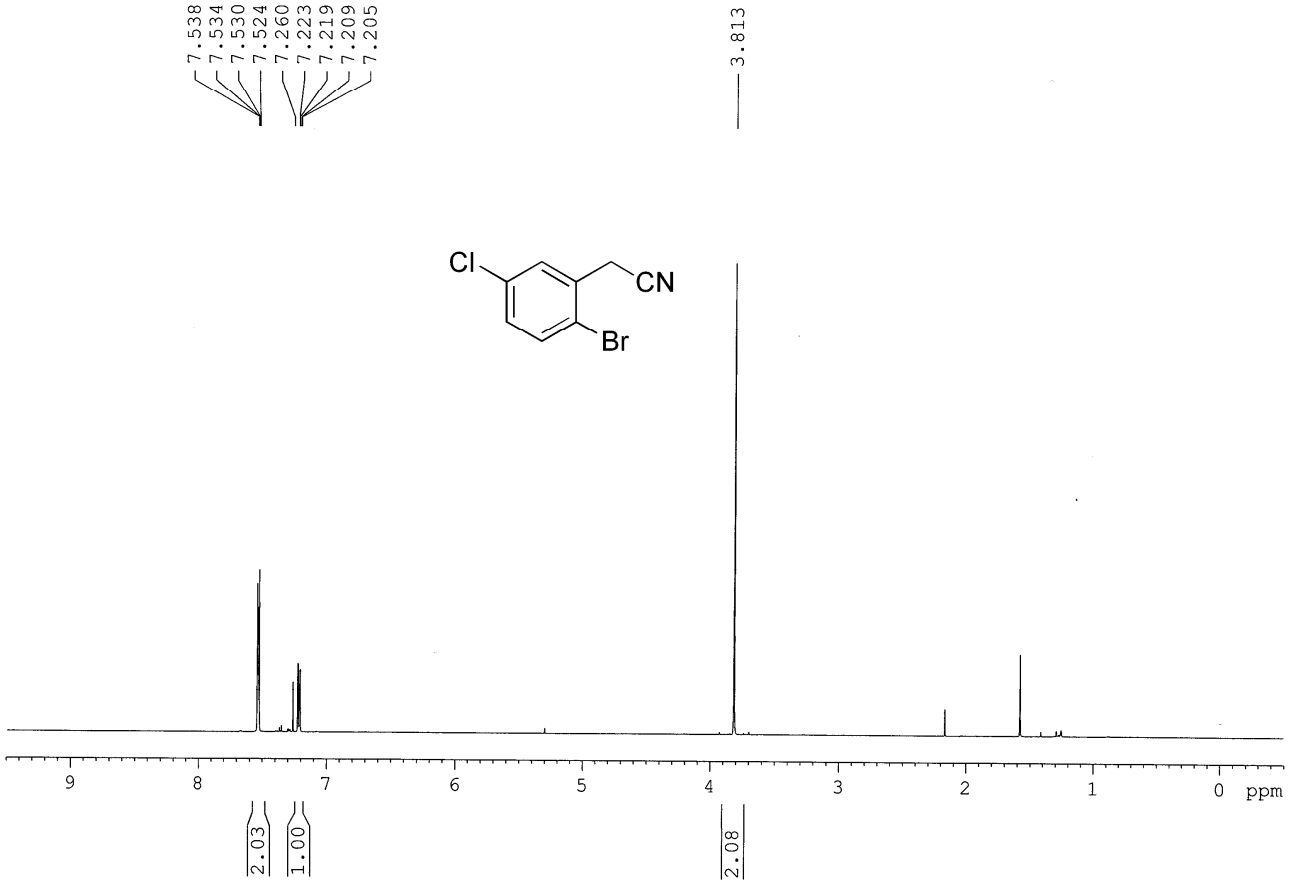
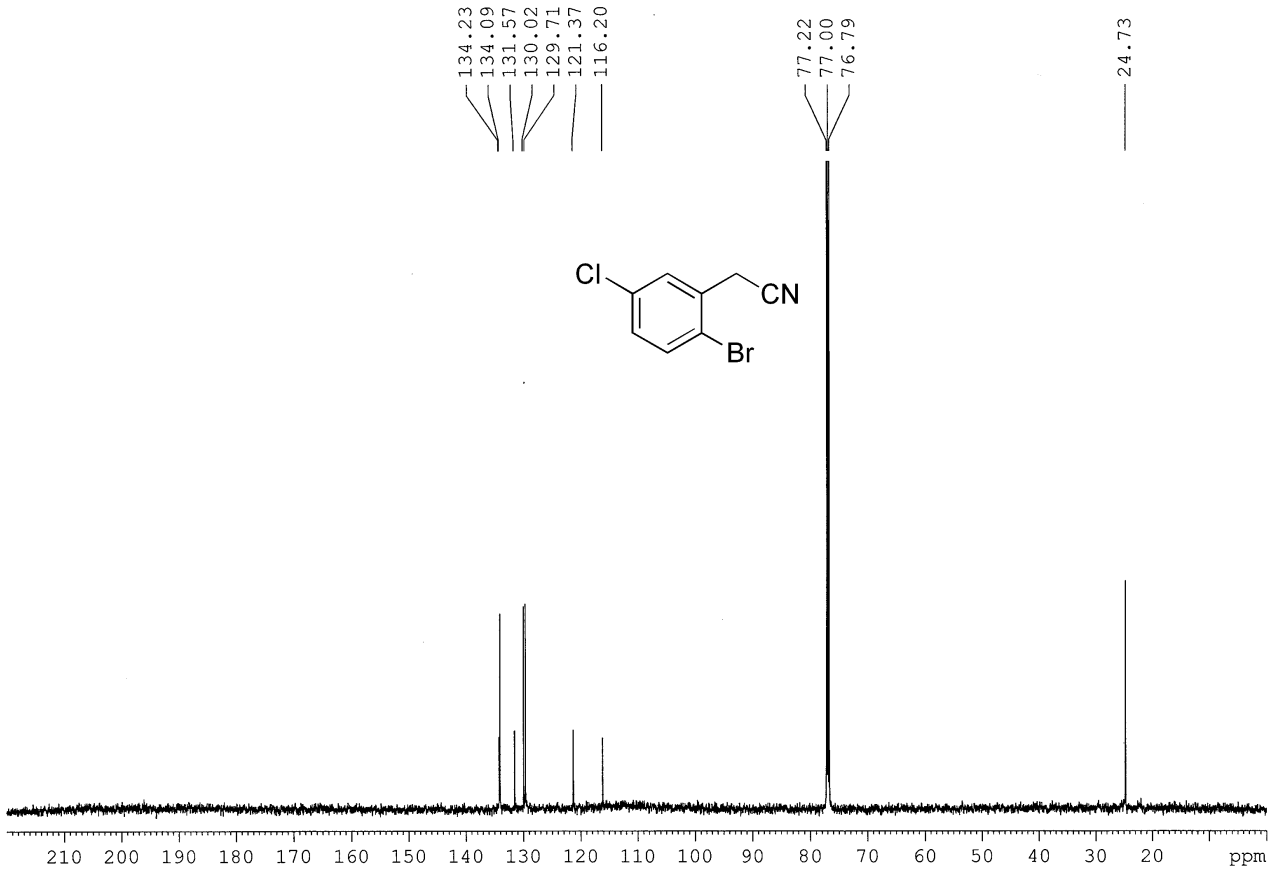
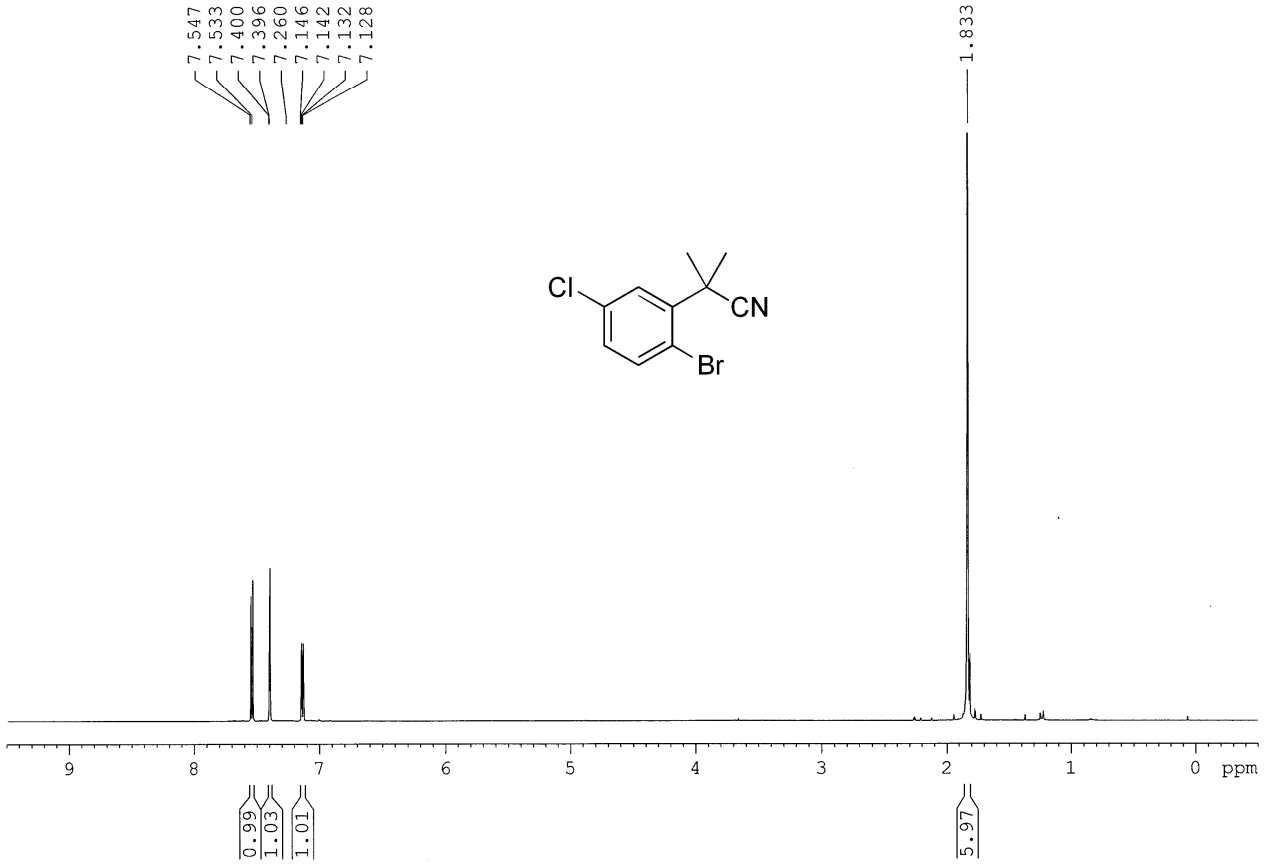
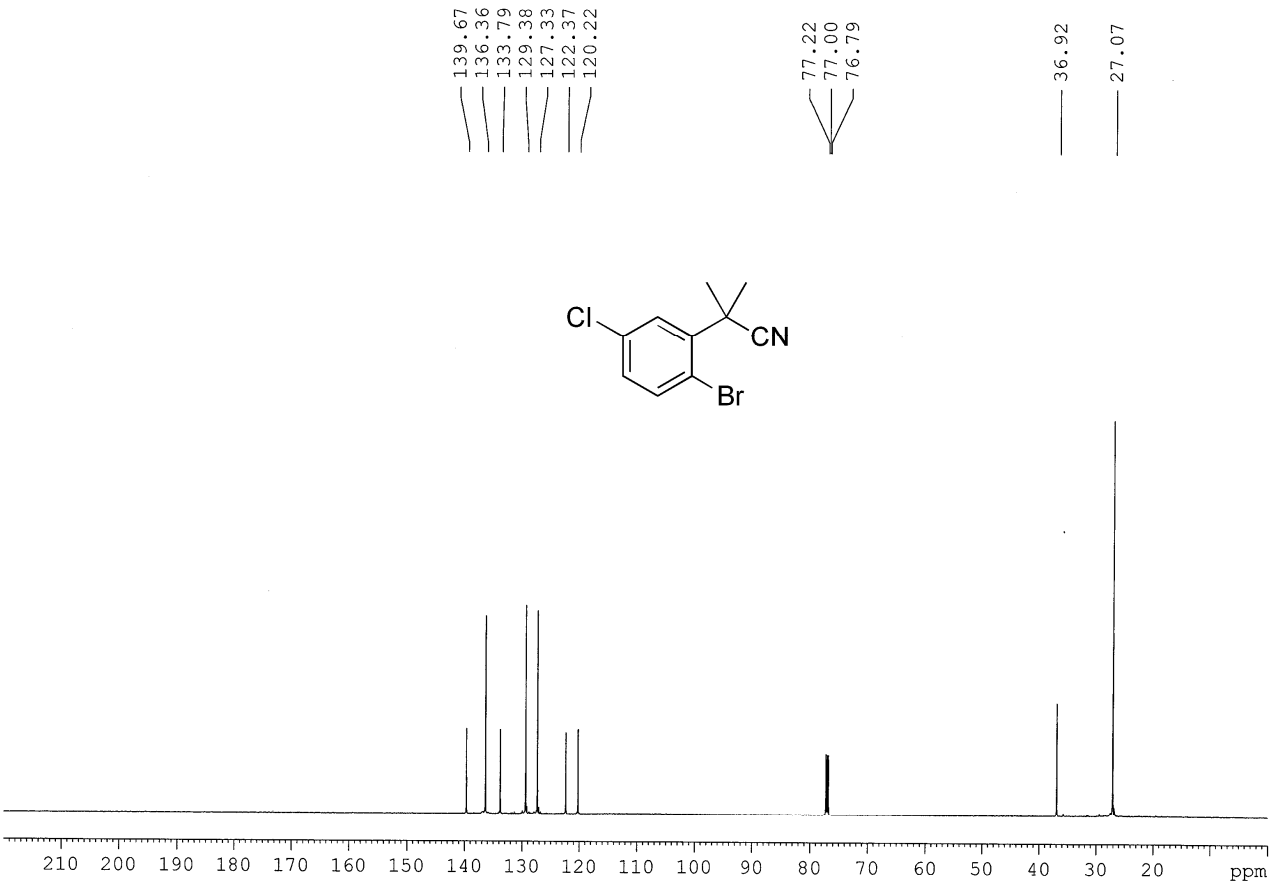
2-(2-Bromo-5-chlorophenyl)acetonitrile (5c)



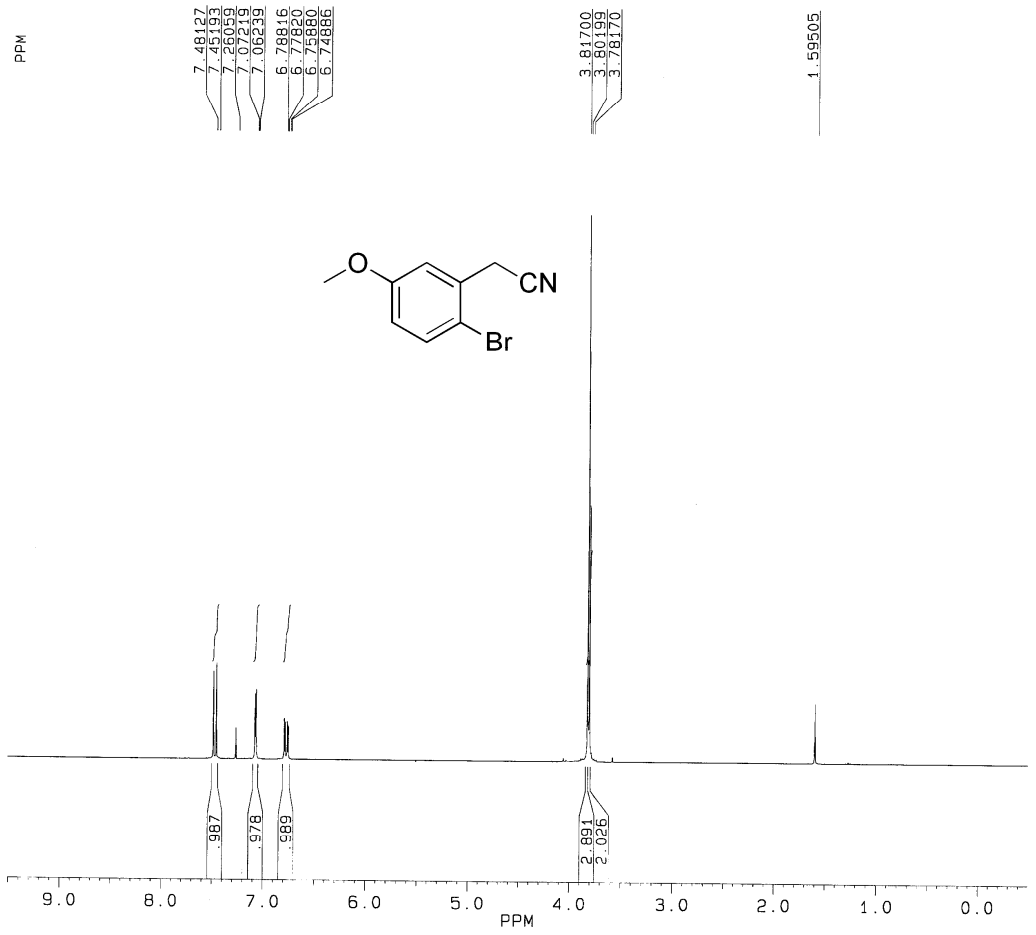


2-(2-Bromo-5-chlorophenyl)-2-methylpropanenitrile (1c)





2-(2-Bromo-5-methoxyphenyl)acetonitrile (5d)

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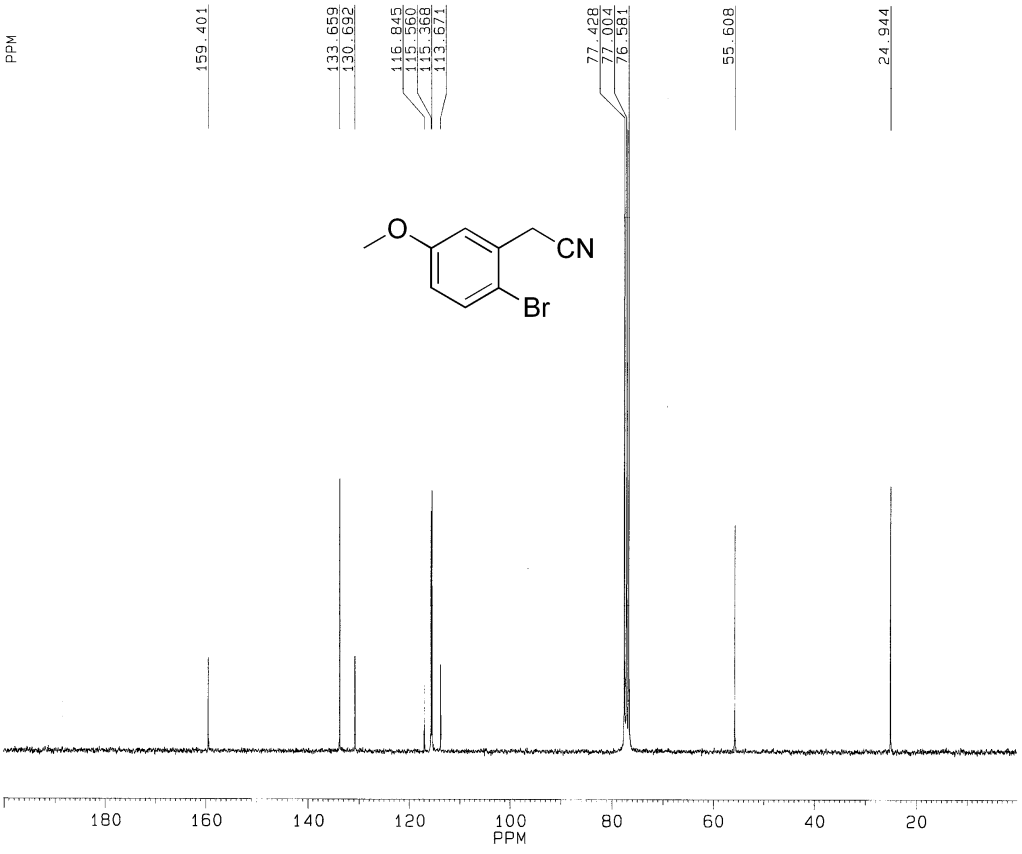
D0729.012
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI   16384
TD   16384
SW    4807.692
HZ/PT     .587

PW        1.4
RD        1.000
AQ        1.704
RG       40
NS       32
TE      297

FW    6100
O2       0.0
DP   63L PO

LB        0.0
GB        0.0
CX       21.00
CY        0.0
F1        9.501P
F2        -.499P
HZ/CM 142.918
PPM/CM    .476
SR    3366.97
```

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D0905.901
DATE ??-??-??

SF      75.469
SY   75.0
O1    6517.695
SI   32768
TD   32768
SW   19230.769
HZ/PT    1.174

PW        1.4
RD        1.500
AQ         .852
RG      200
NS     5105
TE      297

FW   24100
O2    4869.082
DP   15H CPD

LB        2.000
GB        0.0
CX       21.00
CY        0.0
F1      200.008P
F2         .013P
HZ/CM 718.728
PPM/CM   9.524
SR   -1403.80
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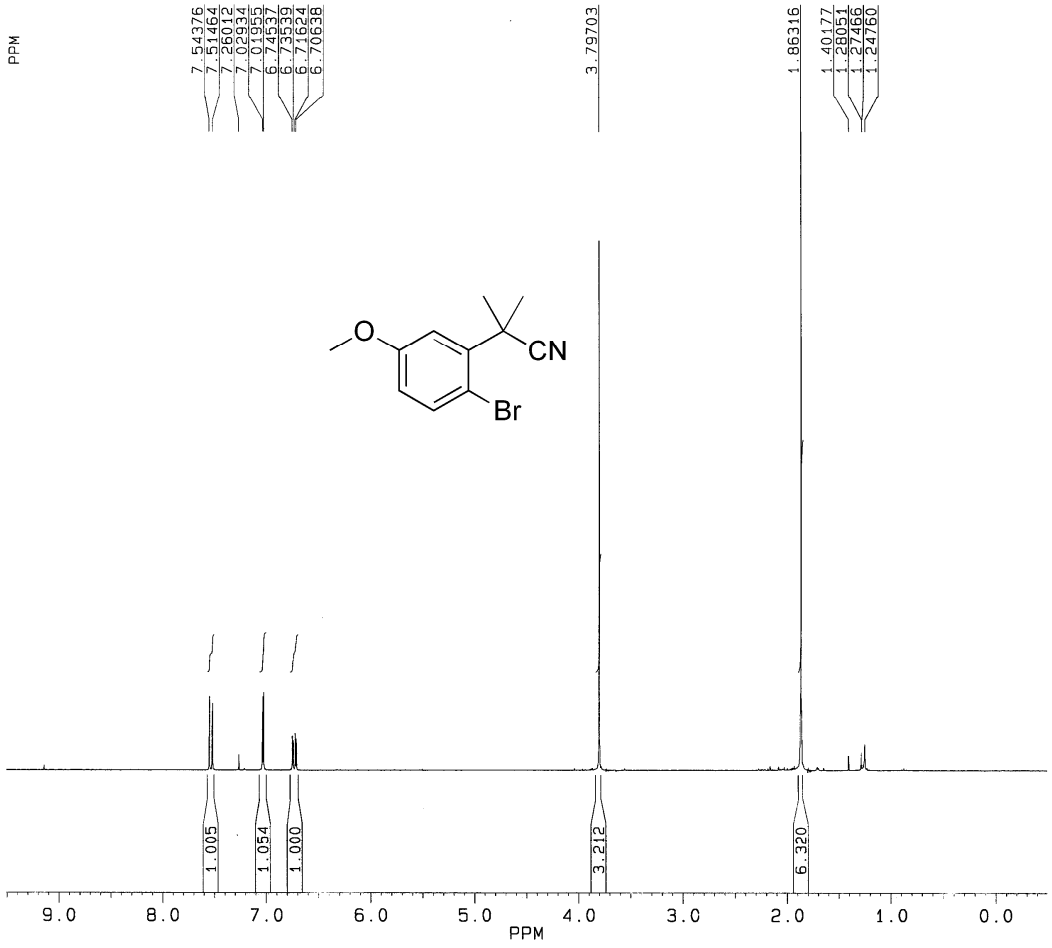
2-(2-Bromo-5-methoxyphenyl)-2-methylpropanenitrile (1d)

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D1213.013
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI   16384
TD   16384
SW    4807.692
HZ/PT     .587

PW       1.4
RD       1.000
AQ       1.704
RG      20
NS       0
TE     297

FW    6100
O2       0.0
DP   63L PO

LB       0.0
GB       0.0
CX      21.00
CY       0.0
F1       9.501P
F2       -.499P
HZ/CM 142.918
PPM/CM    .476
SR    3367.55
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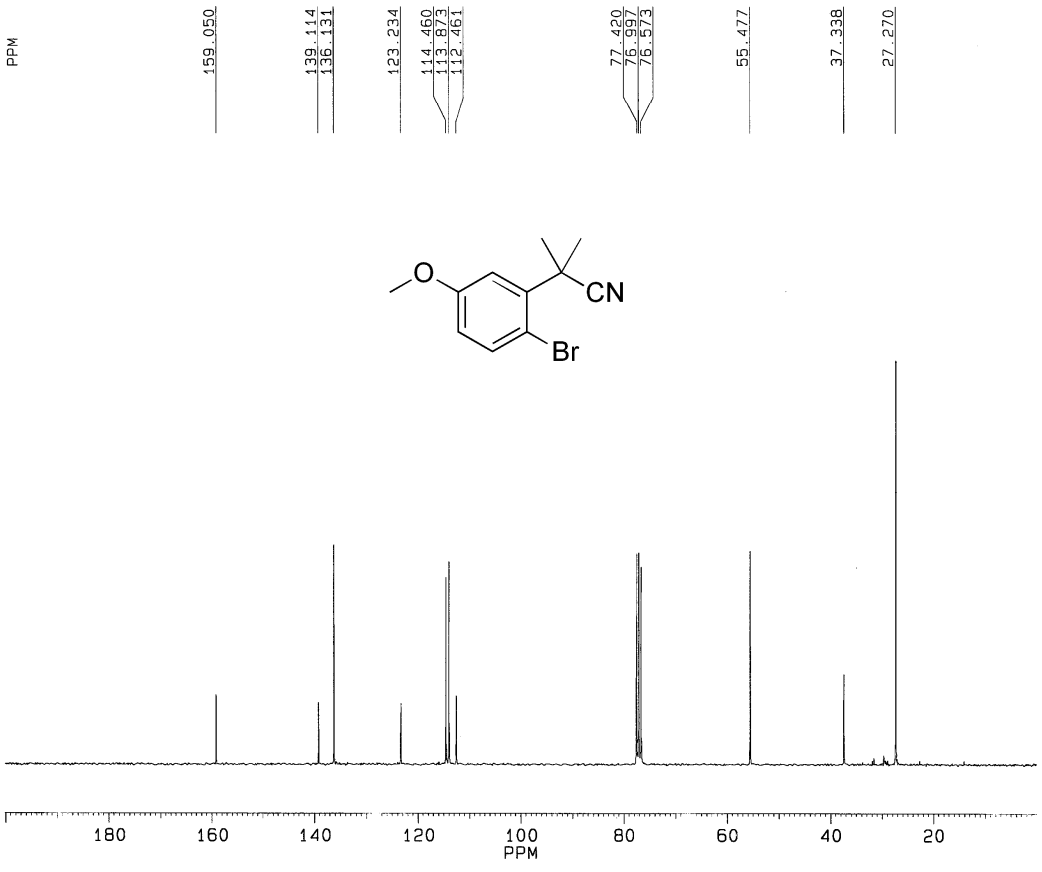


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D1213.901
DATE ??-??-??

SF      75.469
SY  75.0
O1    6517.695
SI   32768
TD   32768
SW   19230.769
HZ/PT    1.174

PW       1.4
RD       1.500
AQ        .852
RG     160
NS    4058
TE     297

FW   24100
O2    4869.082
DP   15H CPD

LB       2.000
GB       0.0
CX      21.00
CY       0.0
F1     200.008P
F2        .013P
HZ/CM 718.728
PPM/CM   9.524
SR   -1399.10
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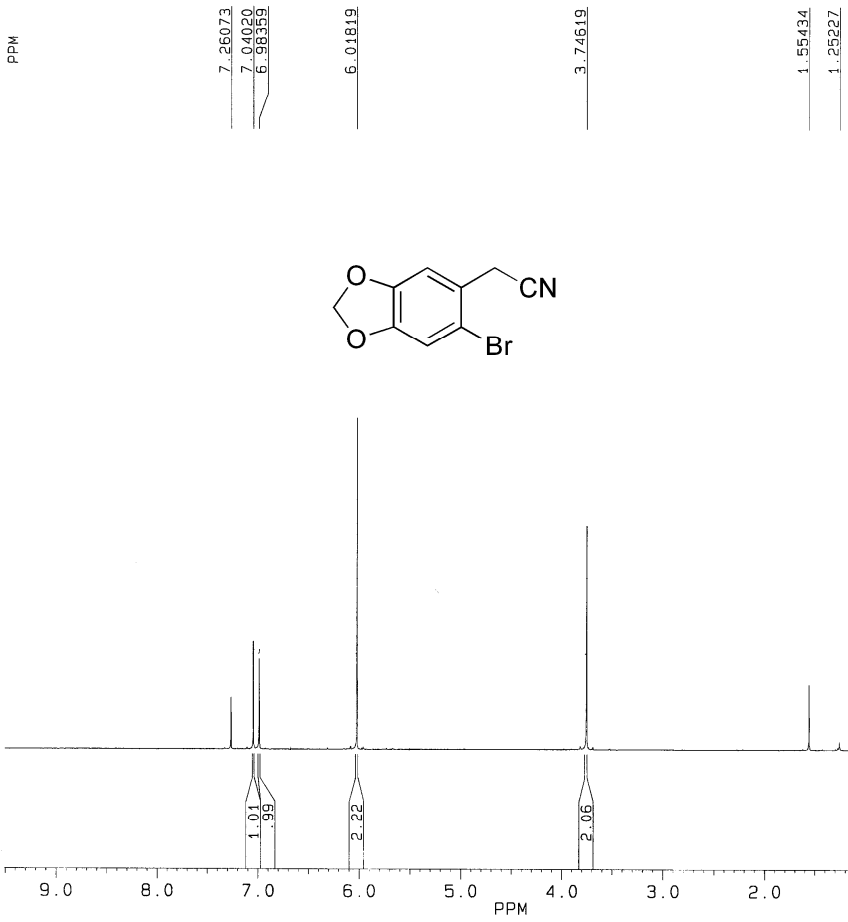
2-(6-Bromobenzo[*d*][1,3]dioxol-5-yl)acetonitrile (5e)

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D0810.039
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI   16384
TD   16384
SW    4807.692
HZ/PT     .587

PW       1.4
RD       1.000
AQ       1.704
RG     400
NS      32
TE     297

FW    6100
O2       0.0
DP   63L PO

LB       0.0
GB       0.0
CX      21.00
CY       0.0
F1       9.501P
F2       -.499P
HZ/CM 142.918
PPM/CM    .476
SR    3367.55
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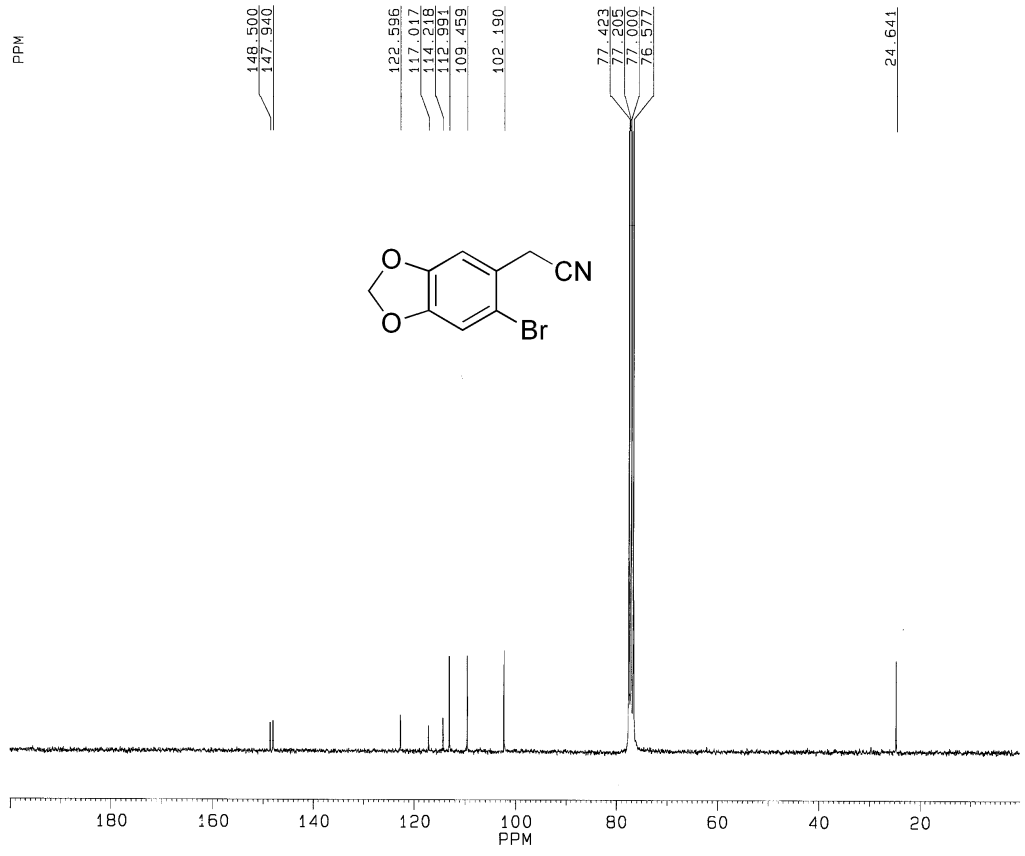


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D0810.902
DATE ??-??-??

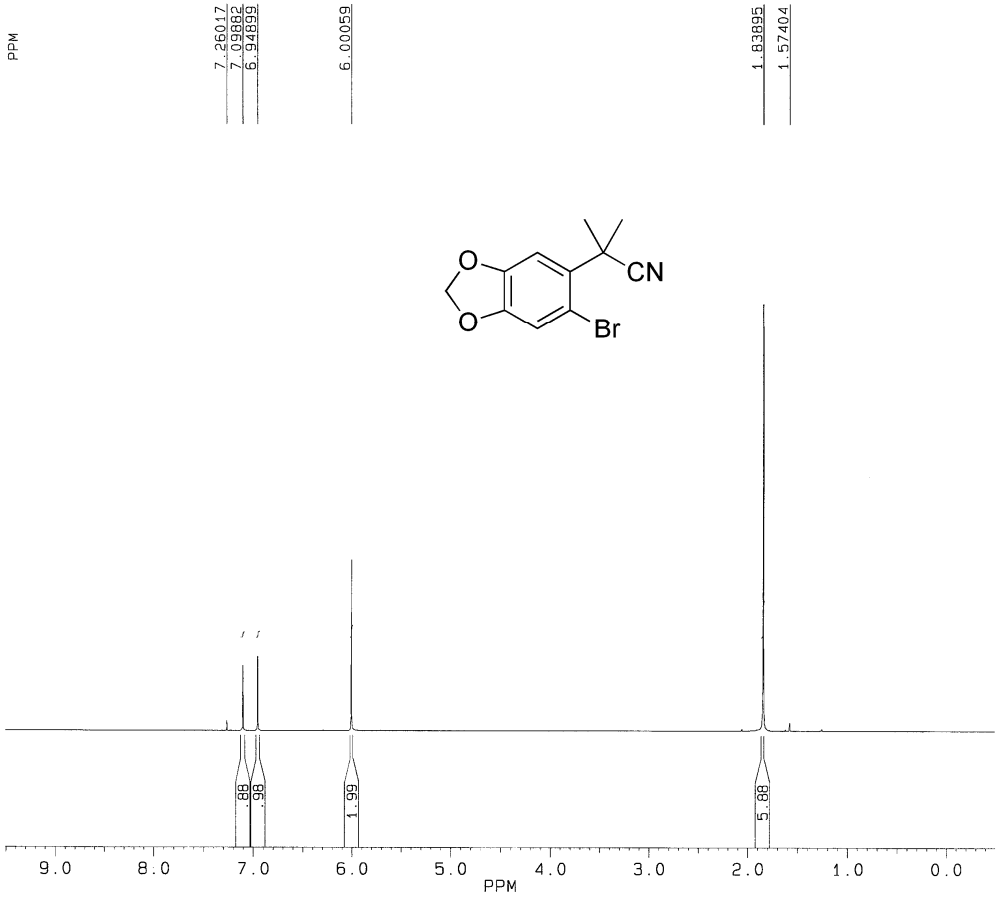
SF      75.469
SY   75.0
O1    6517.695
SI   32768
TD   32768
SW   19230.769
HZ/PT    1.174

PW       1.4
RD       1.500
AQ        .852
RG     200
NS   15928
TE     297

FW   24100
O2    4869.082
DP   15H CPD

LB       2.000
GB       0.0
CX      21.00
CY       0.0
F1     200.008P
F2        .013P
HZ/CM 718.728
PPM/CM   9.524
SR   -1404.97
```

2-(6-Bromobenzo[*d*][1,3]dioxol-5-yl)-2-methylpropanenitrile (1e)

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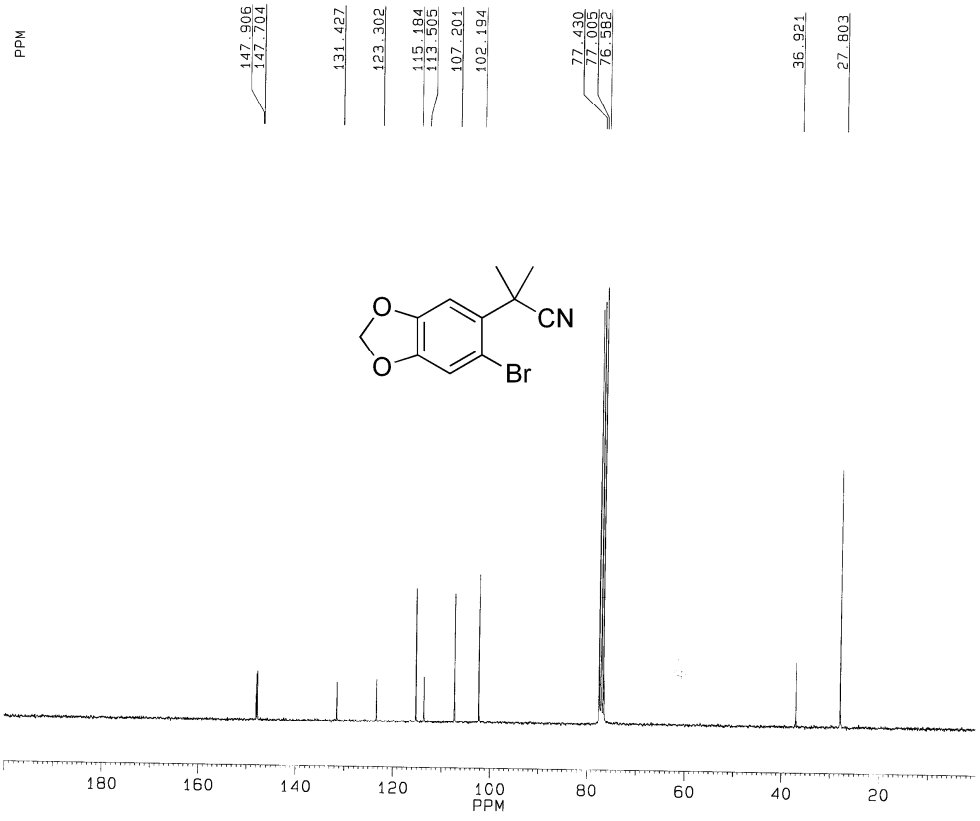
D0815.004
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI   16384
TD   16384
SW    4807.692
HZ/PT     .587

PW       1.4
RD       1.000
AQ       1.704
RG      20
NS      32
TE     297

FW    6100
O2       0.0
DP   63L PO

LB       0.0
GB       0.0
CX      21.00
CY       0.0
F1       9.501P
F2       -.499P
HZ/CM 142.918
PPM/CM    .476
SR    3367.55
```

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D0815.901
DATE ??-??-??

SF      75.469
SY   75.0
O1    6517.695
SI   32768
TD   32768
SW   19230.769
HZ/PT    1.174

PW       1.4
RD       1.500
AQ        .852
RG     160
NS    3356
TE     297

FW   24100
O2    4869.082
DP   15H CPD

LB       2.000
GB       0.0
CX      21.00
CY       0.0
F1     200.008P
F2        .013P
HZ/CM 718.728
PPM/CM   9.524
SR   -1403.80
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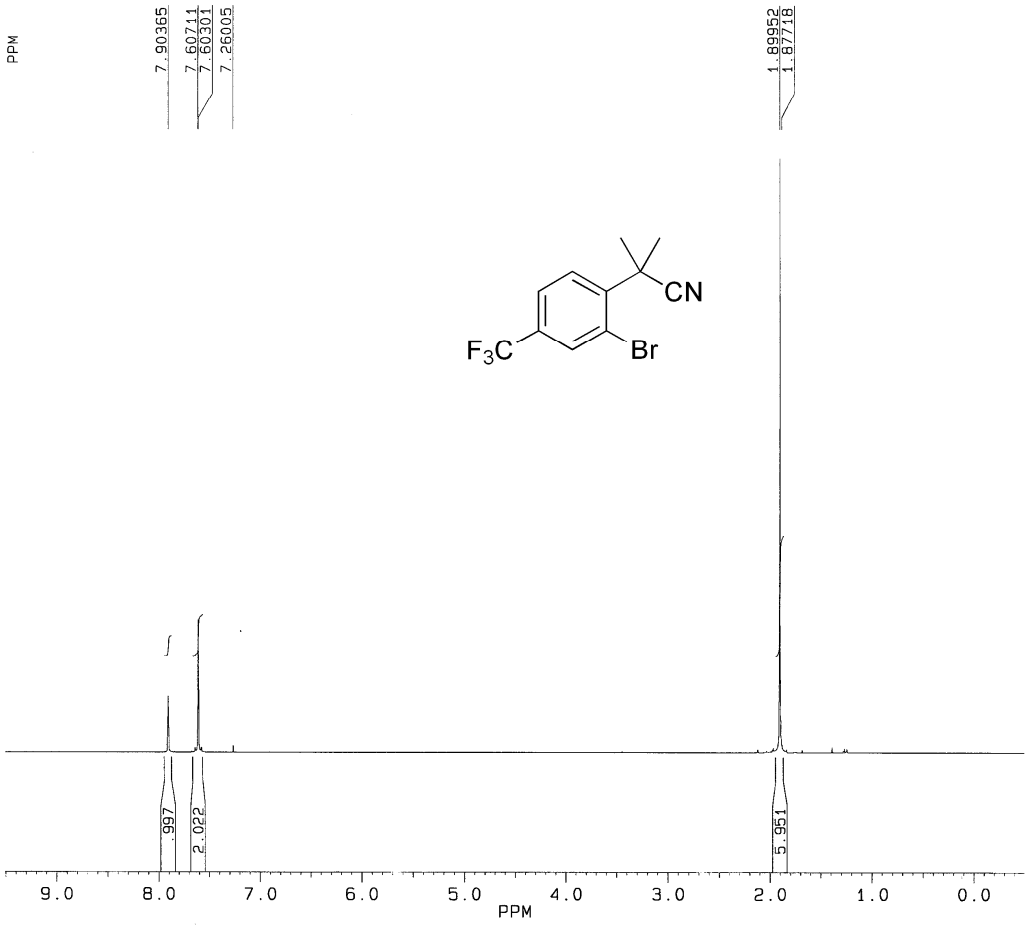
2-(2-Bromo-4-(trifluoromethyl)phenyl)-2-methylpropanenitrile (1f)

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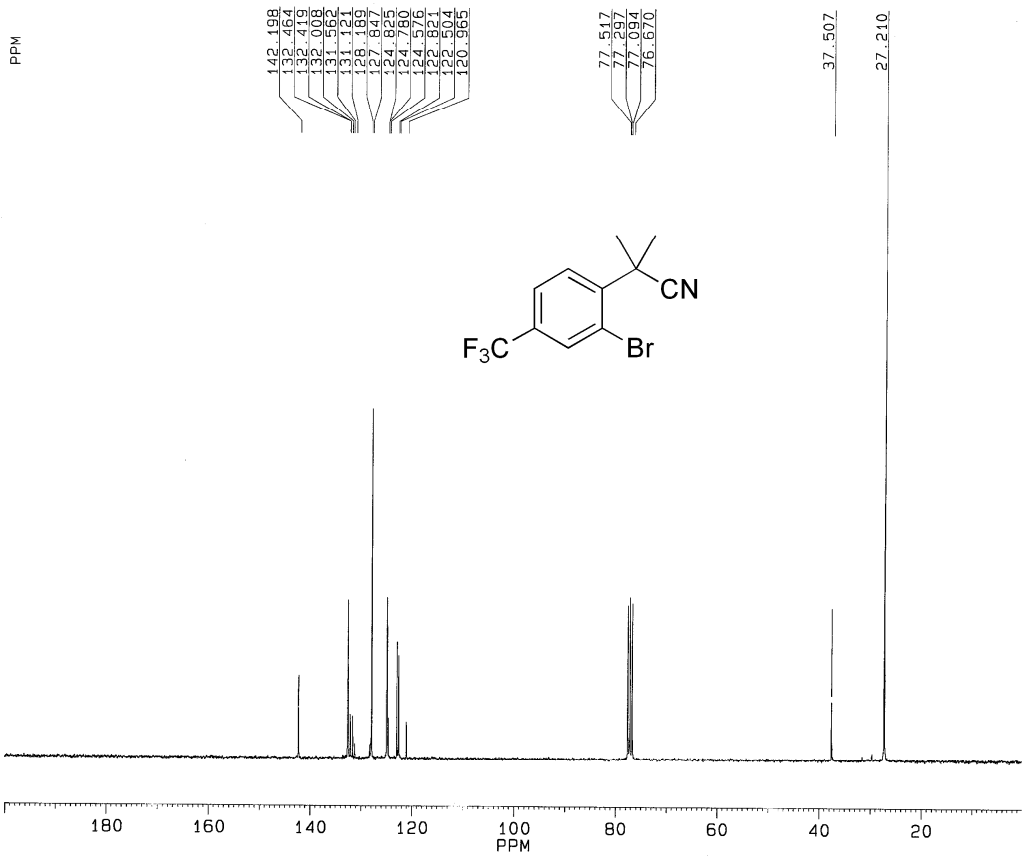
D1222.009
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI   16384
TD   16384
SW    4807.692
HZ/PT     .587

PW       1.4
RD       1.000
AQ       1.704
RG      10
NS      32
TE     297

FW    6100
O2.      0.0
DP   63L PO

LB       0.0
GB       0.0
CX      21.00
CY       0.0
F1       9.501P
F2       -.499P
HZ/CM 142.918
PPM/CM    .476
SR    3367.55
```

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D1221.907
DATE ??-??-??

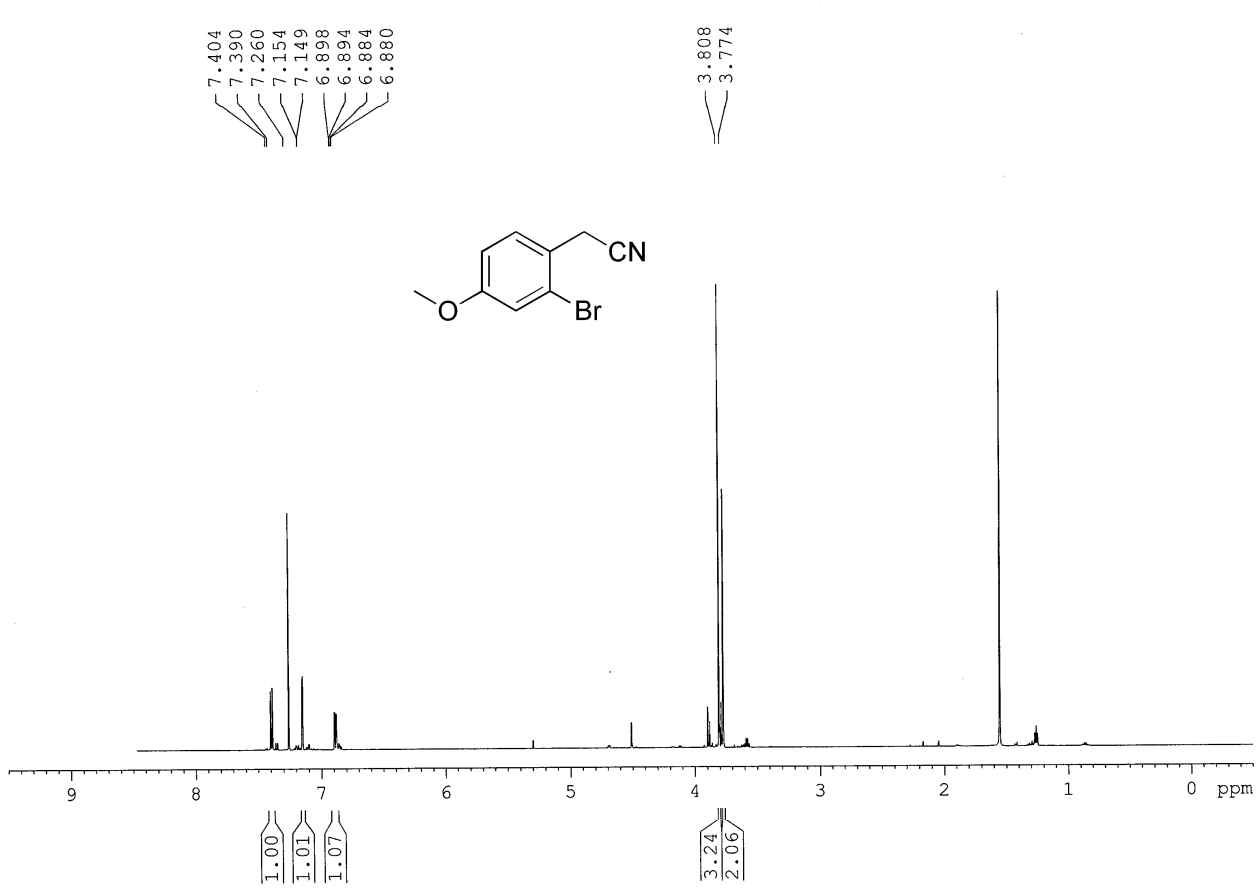
SF      75.469
SY  75.0
O1    6517.695
SI   32768
TD   32768
SW   19230.769
HZ/PT    1.174

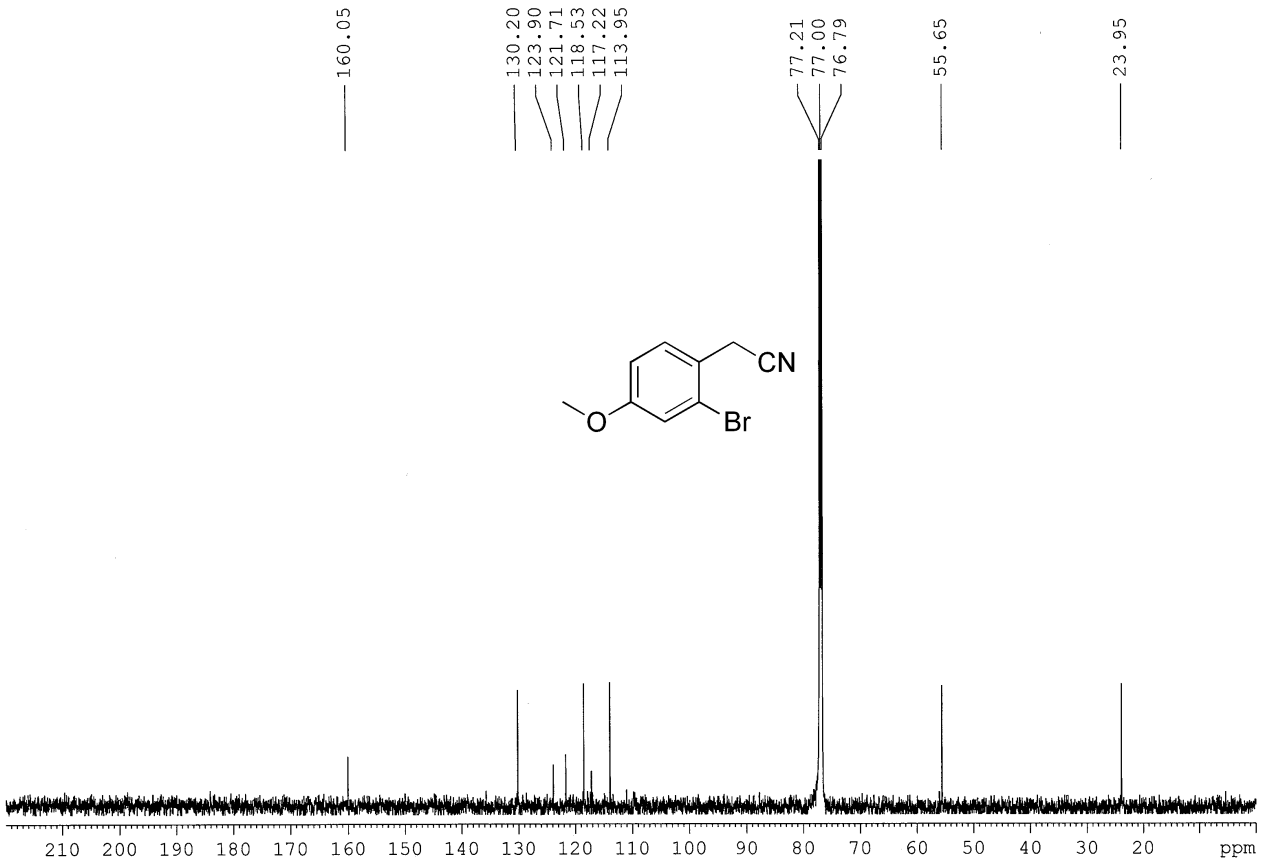
PW       1.4
RD       1.500
AQ        .852
RG     160
NS     800
TE     297

FW   24100
O2    4869.082
DP   15H CPD

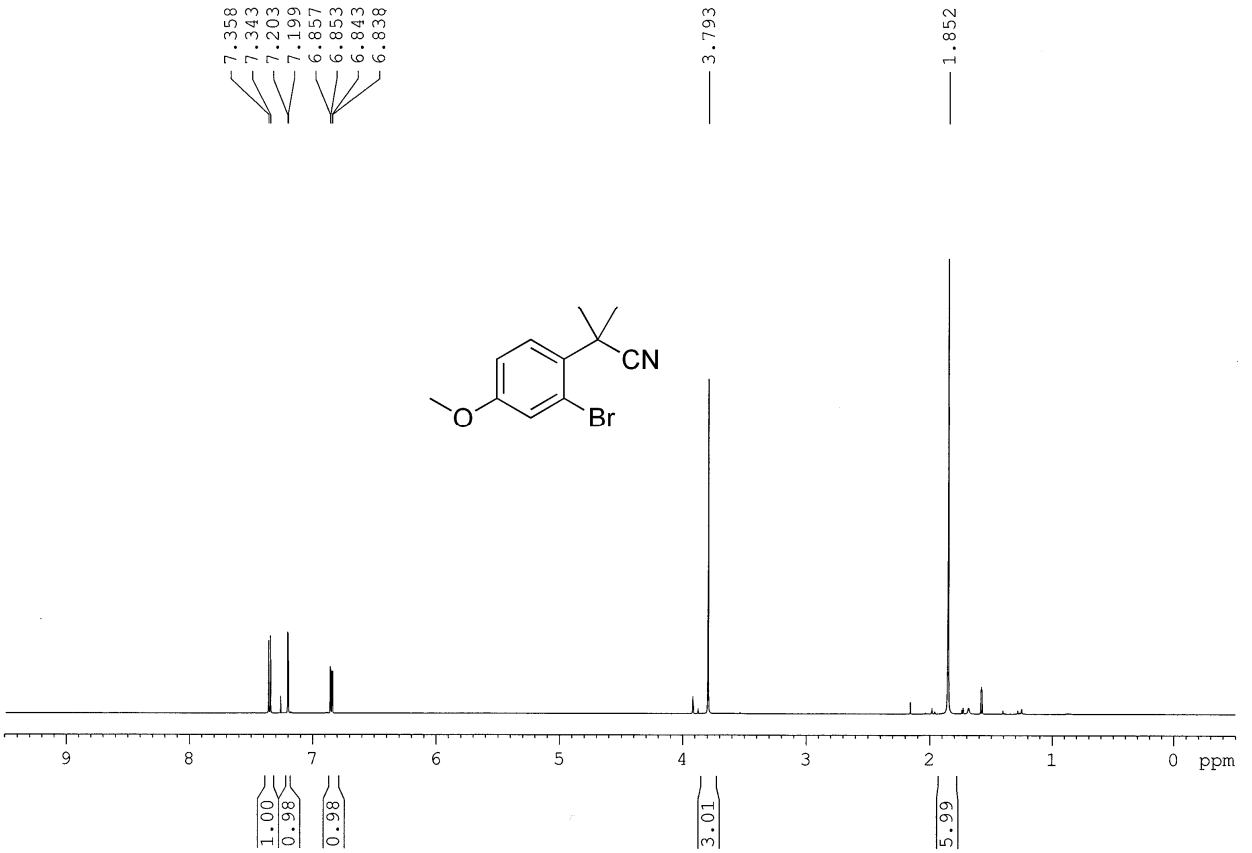
LB       2.000
GB       0.0
CX      21.00
CY       0.0
F1     200.008P
F2        .013P
HZ/CM 718.728
PPM/CM  9.524
SR   -1404.97
```

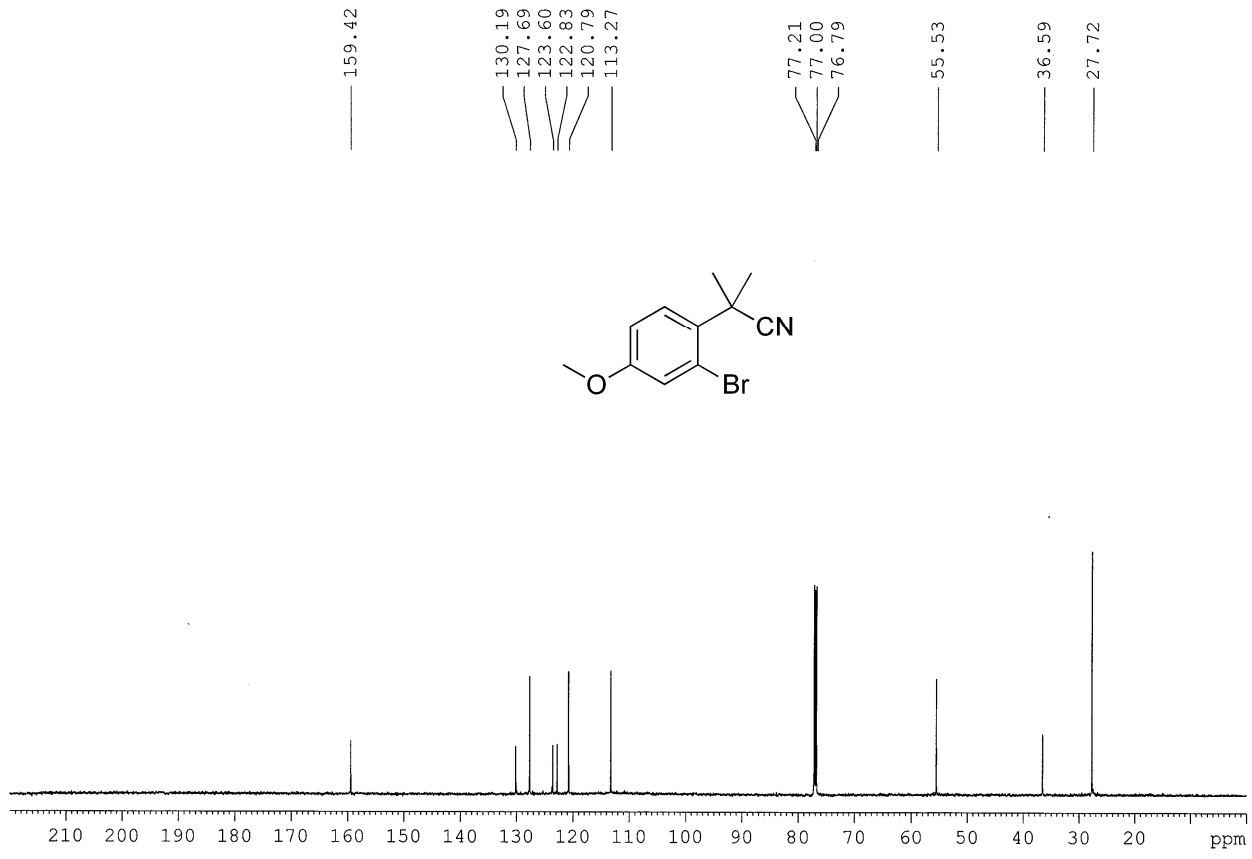
2-(2-Bromo-4-methoxyphenyl)acetonitrile (5g)



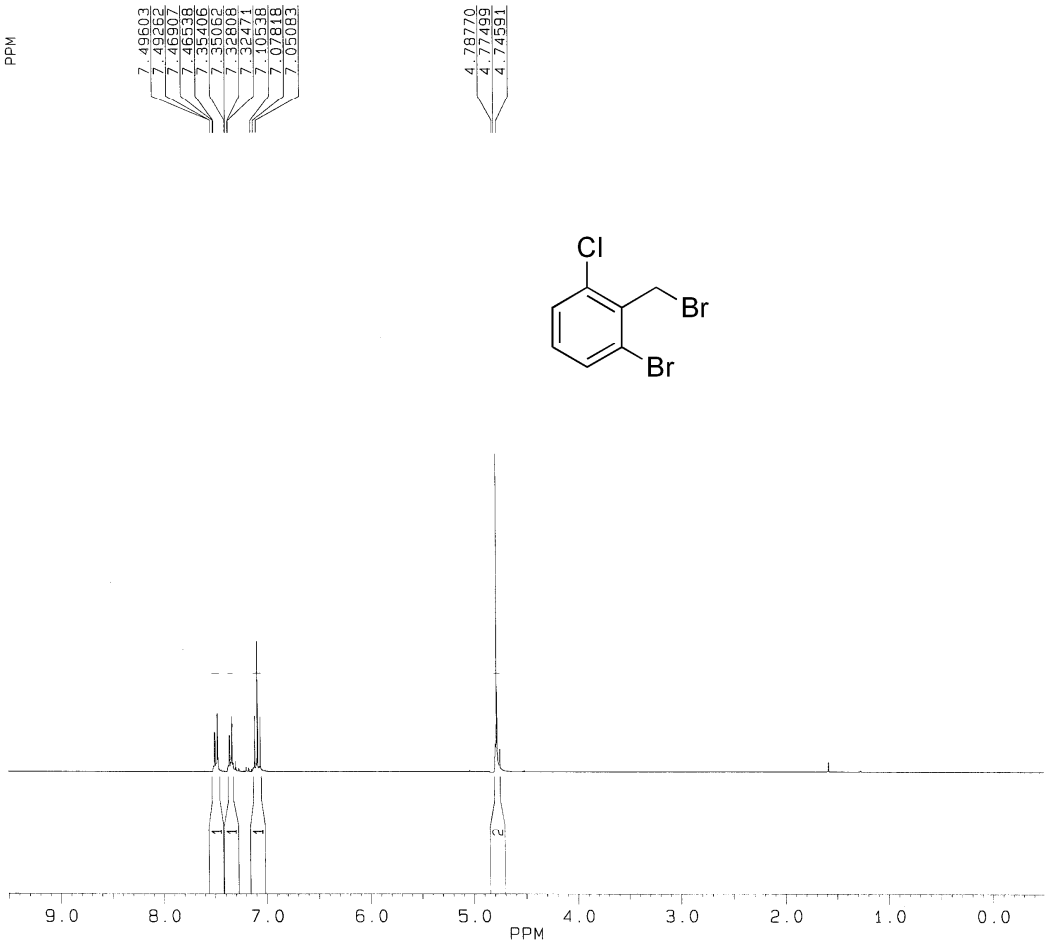


2-(2-Bromo-4-methoxyphenyl)-2-methylpropanenitrile (1g)





1-Bromo-2-(bromomethyl)-3-chlorobenzene (4h)

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D0316.014
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI   16384
TD   16384
SW    4807.692
HZ/PT     .587

PW       1.4
RD       1.000
AQ       1.704
RG      20
NS      32
TE     297

FW    6100
O2       0.0
DP   63L PO

LB       0.0
GB       0.0
CX      21.00
CY       0.0
F1       9.501P
F2       - 499P
HZ/CM 142.918
PPM/CM    .476
SR    3367.55
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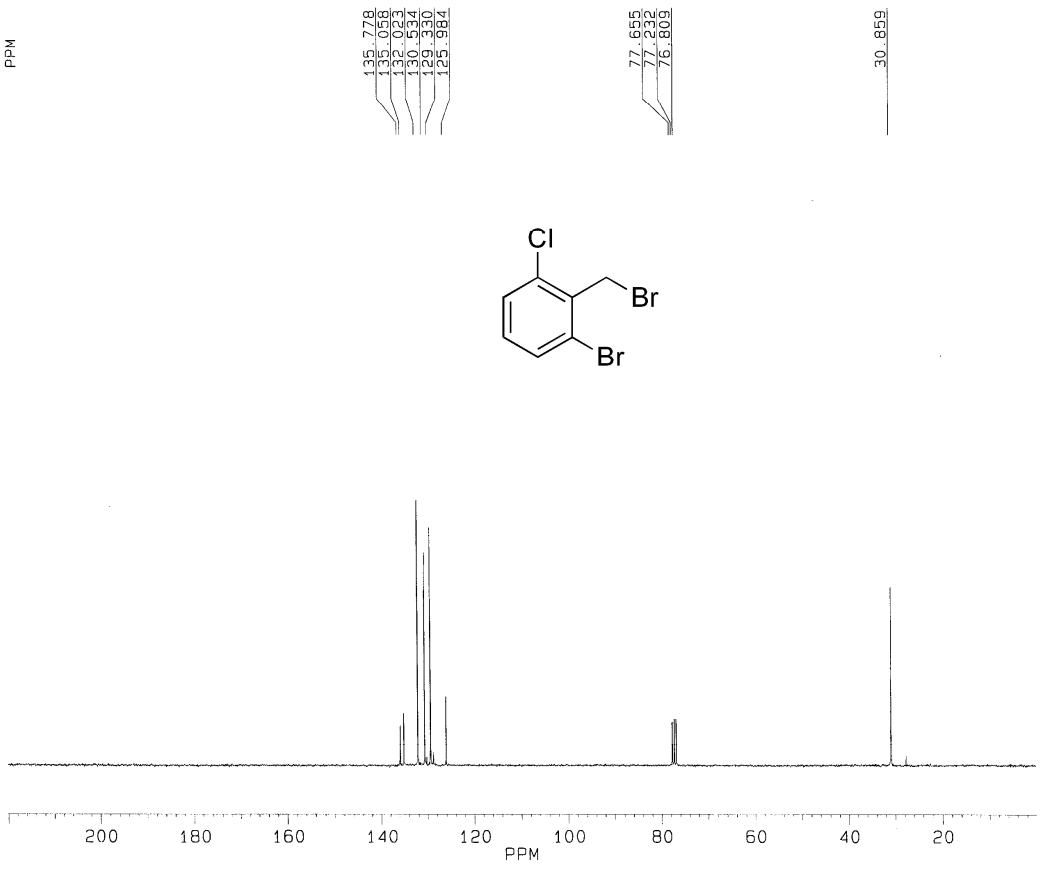


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D0316.903
DATE ??-??-??

SF      75.469
SY  75.0
O1    6517.695
SI   32768
TD   32768
SW  19230.769
HZ/PT    1.174

PW       1.4
RD       1.500
AQ        .852
RG     200
NS     305
TE     297

FW   24100
O2    4869.082
DP   15H CPD

LB       2.000
GB       0.0
CX      21.00
CY       0.0
F1     220.005P
F2        .010P
HZ/CM 790.606
PPM/CM 10.476
SR   -1409.42
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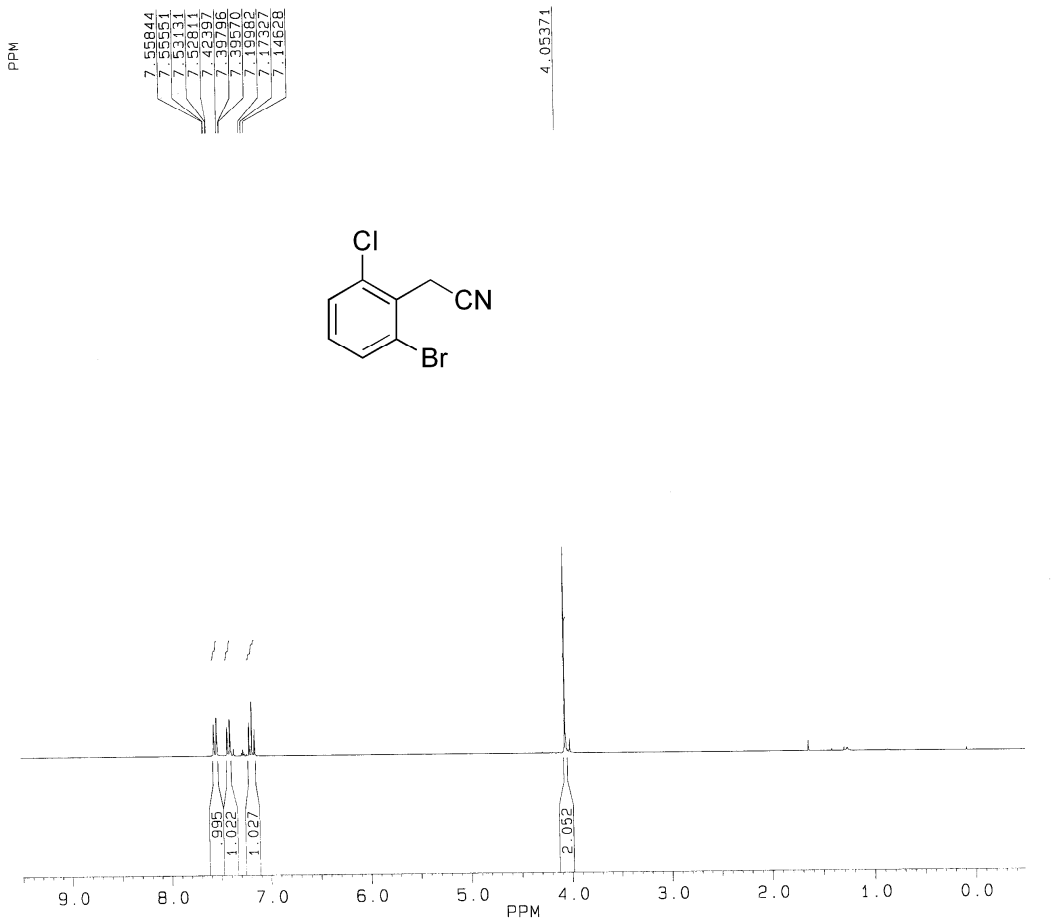
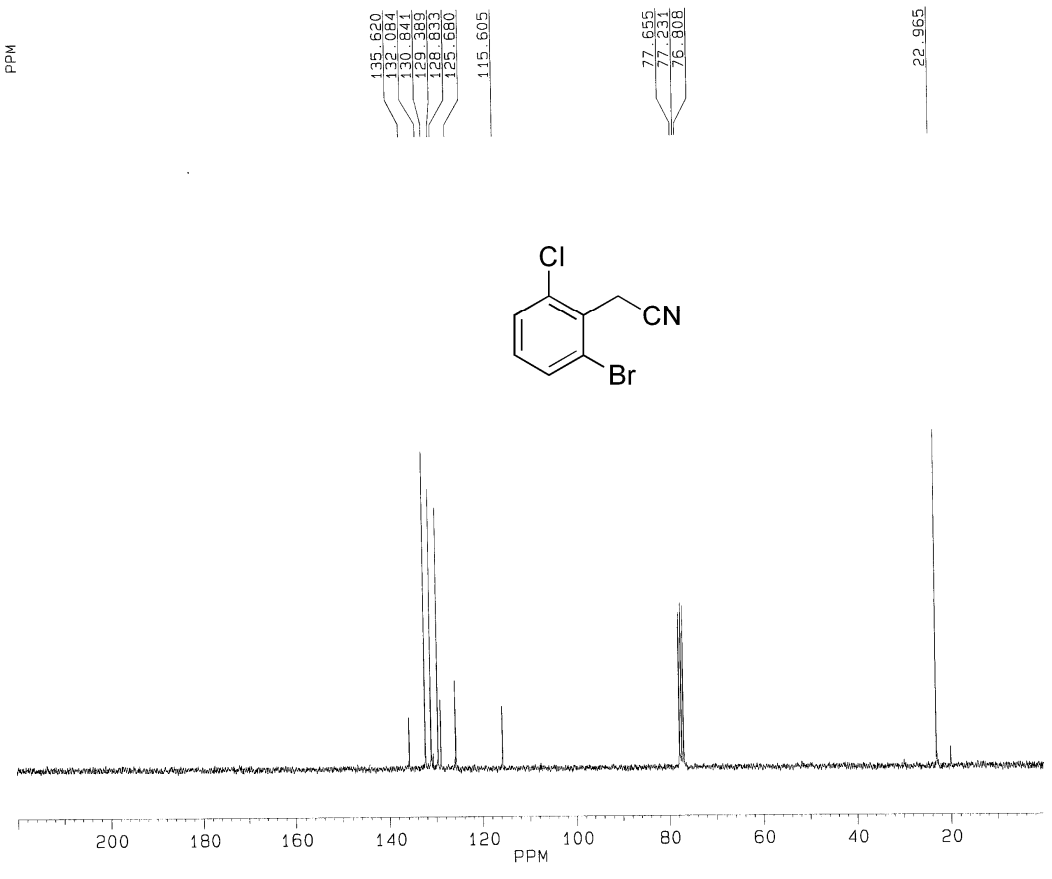
2-(2-Bromo-6-chlorophenyl)acetonitrile (5h)



D0317.001
DATE ??-??-??

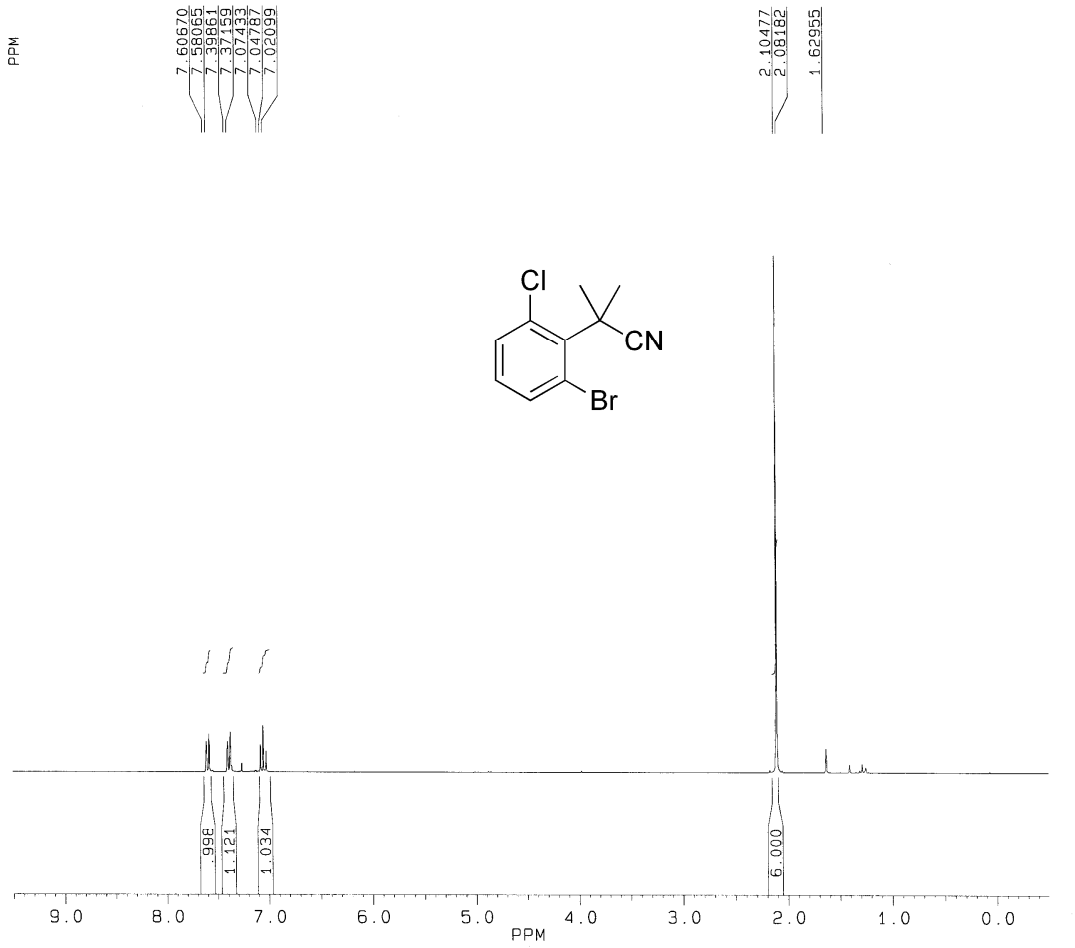
SF	300.133
SY	299.0
O1	5018.332
SI	16384
TD	16384
SW	4807.692
HZ/PT	.587
PW	1.4
RD	1.000
AQ	1.704
RG	40
NS	32
TE	297
FW	6100
O2	0.0
DP	63L PO
LB	0.0
GB	0.0
CX	21.00
CY	0.0
F1	9.501P
F2	-.499P
HZ/CM	142.918
PPM/CM	.476
SR	3367.00



D0317.901
DATE ??-??-??

SF	75.469
SY	75.0
O1	6517.695
SI	32768
TD	32768
SW	19230.769
HZ/PT	1.174
PW	1.4
RD	1.500
AQ	.852
RG	200
NS	501
TE	297
FW	24100
O2	4869.082
DP	15H CPD
LB	2.000
GB	0.0
CX	21.00
CY	0.0
F1	220.021P
F2	.026P
HZ/CM	790.606
PPM/CM	10.476
SR	-1416.46

2-(2-Bromo-6-chlorophenyl)-2-methylpropanenitrile (1h)

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D0316.018
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI    16384
TD    16384
SW    4807.692
HZ/PT     .587

PW        1.4
RD        1.000
AQ        1.704
RG       40
NS       32
TE      297

FW      6100
O2         0.0
DP    63L PO

LB         0.0
GB         0.0
CX        21.00
CY         0.0
F1         9.501P
F2        -.499P
HZ/CM 142.918
PPM/CM    .476
SR     3368.14
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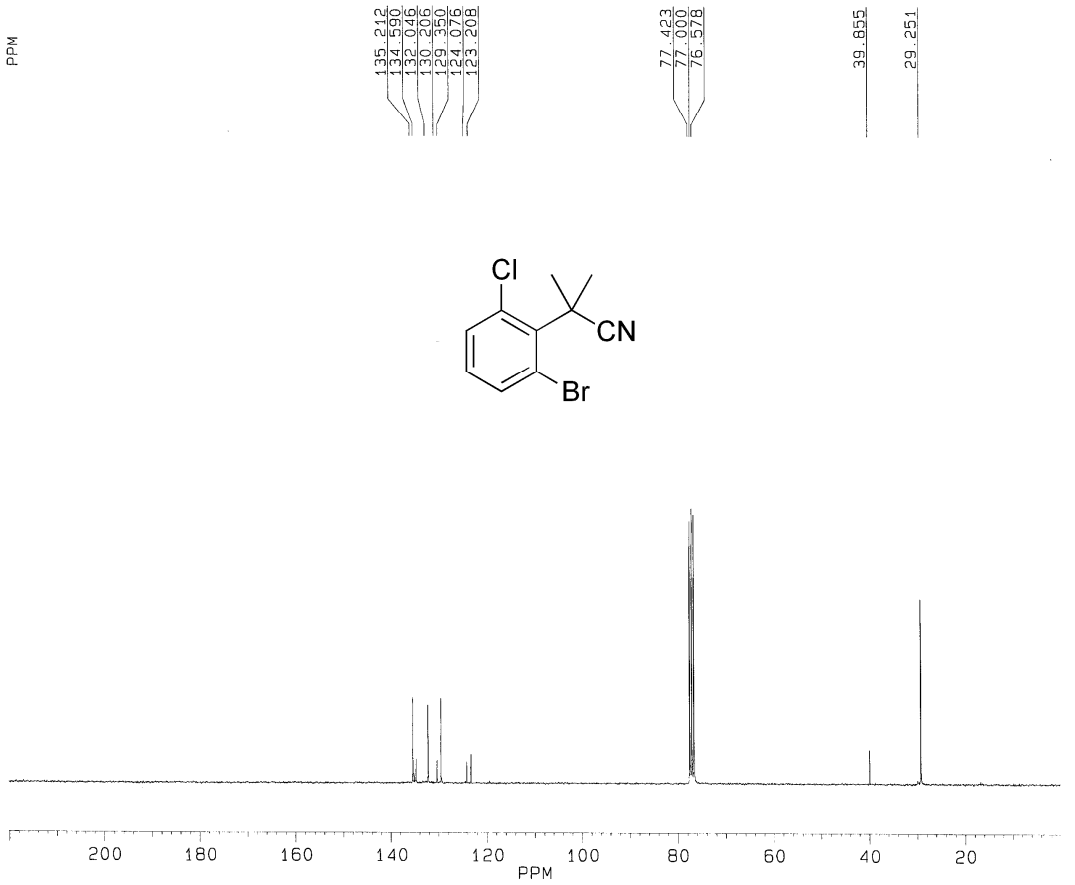


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D0317.902
DATE ??-??-??

SF      75.469
SY   75.0
O1    6517.695
SI    32768
TD    32768
SW    19230.769
HZ/PT     1.174

PW        1.4
RD        1.500
AQ         .852
RG      200
NS     3113
TE      297

FW    24100
O2     4869.082
DP    15H CPD

LB        2.000
GB        0.0
CX       21.00
CY        0.0
F1      220.009P
F2         .013P
HZ/CM 790.606
PPM/CM 10.476
SR   -1402.62
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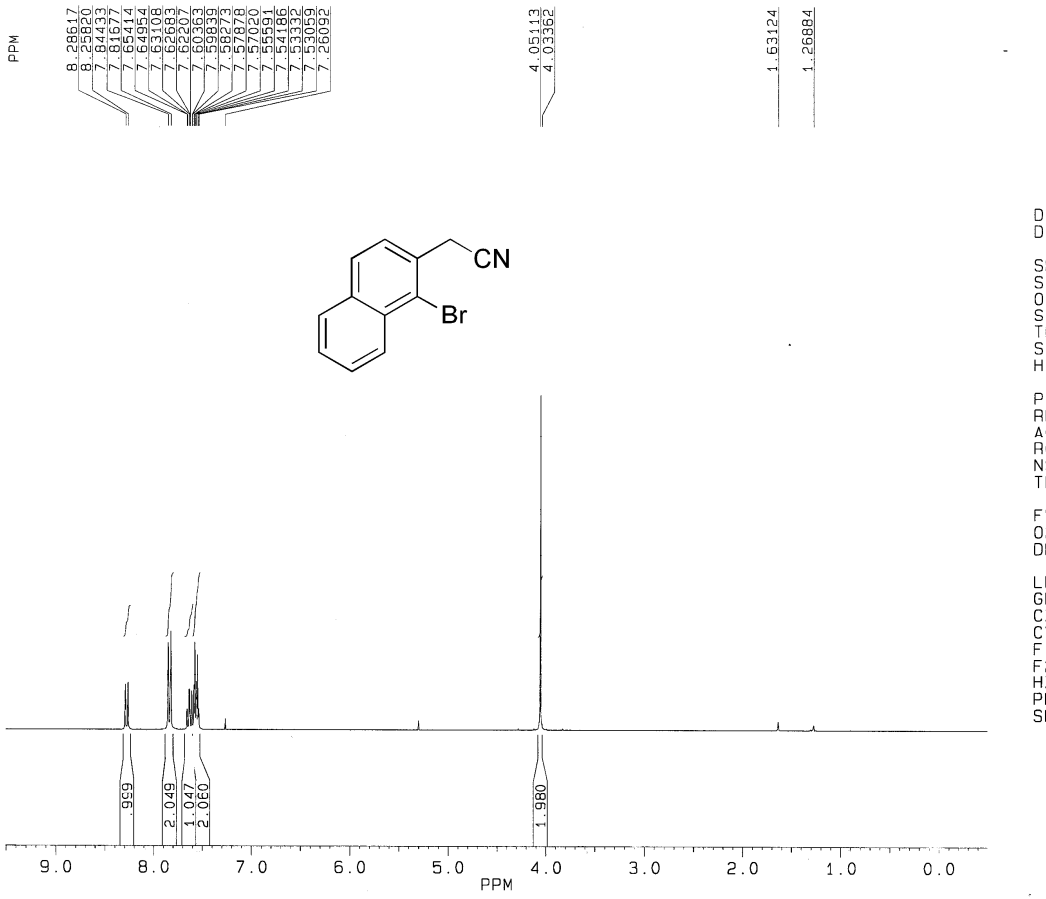
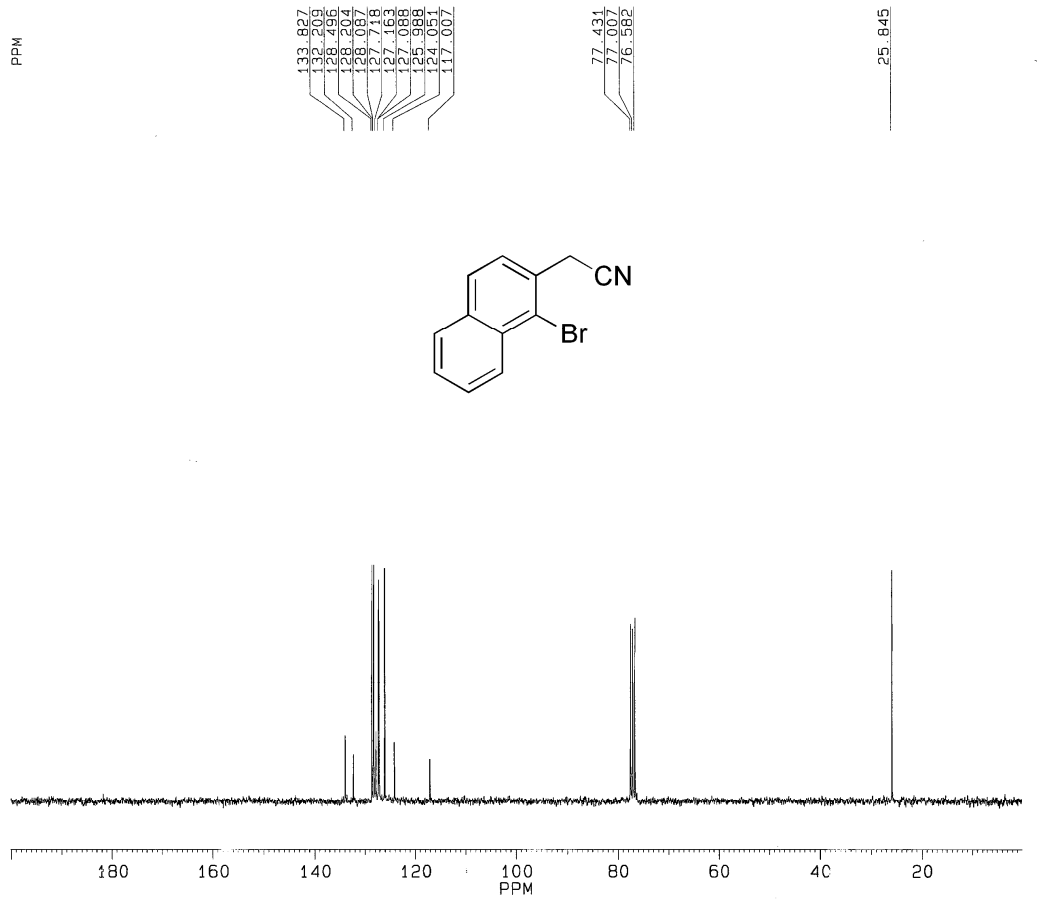
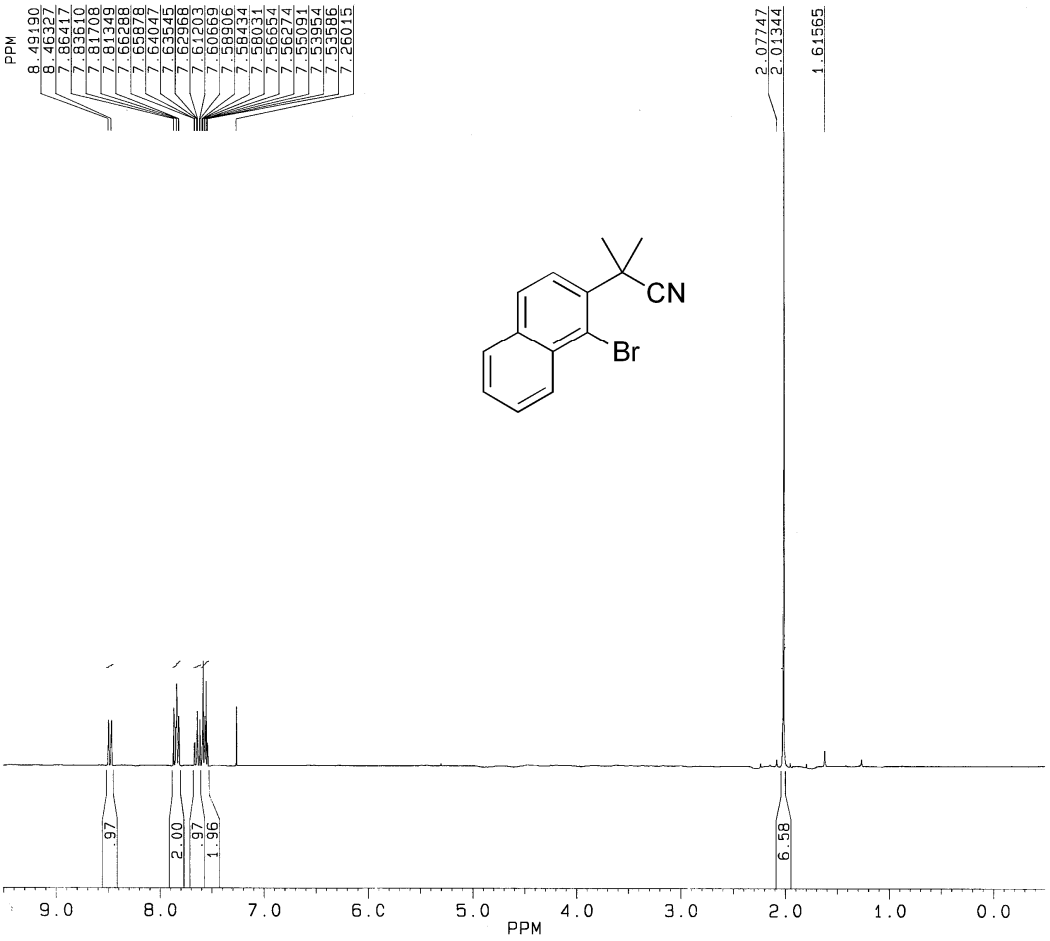
2-(1-Bromonaphthalen-2-yl)acetonitrile (5i)





2-(1-Bromonaphthalen-2-yl)-2-methylpropanenitrile (1i)



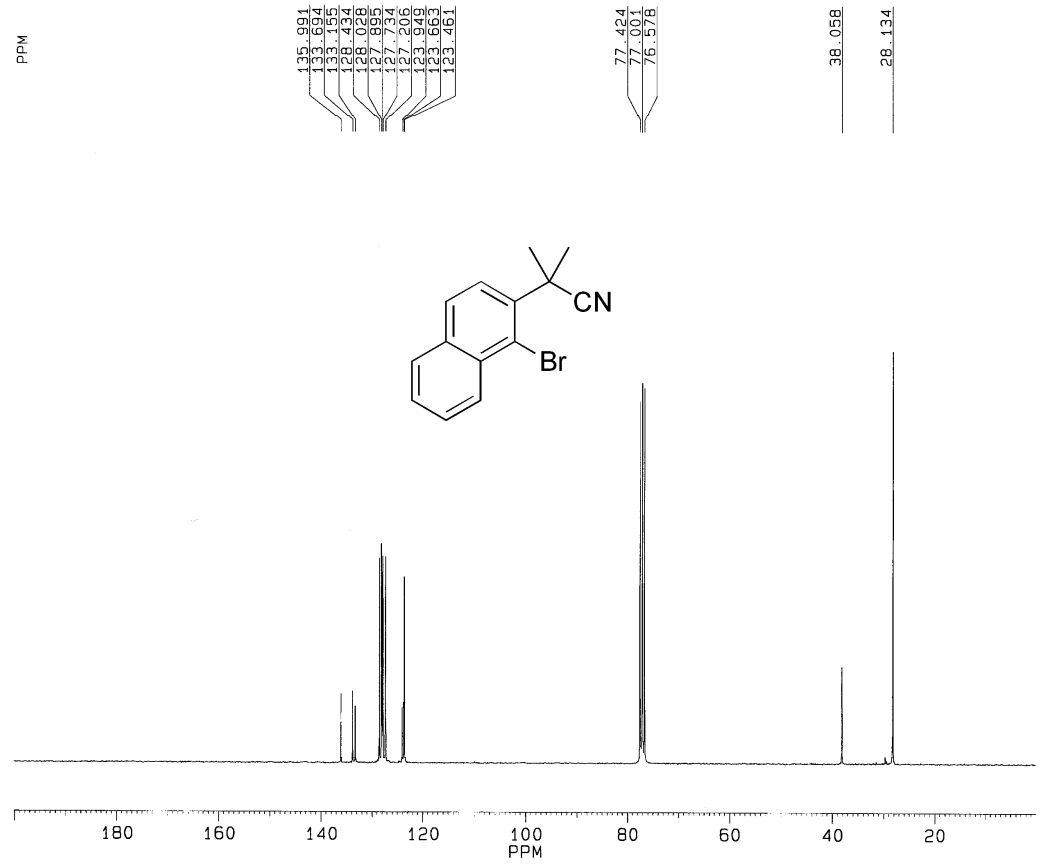
D1021.012
DATE ??-??-??

SF 300.133
SY 299.0
O1 5018.332
SI 16384
TD 16384
SW 4807.692
HZ/PT .587

PW 1.4
RD 1.000
AQ 1.704
RG 160
NS 32
TE 297

FW 6100
O2 0.0
DP 63L PO

LB 0.0
GB 0.0
CX 21.00
CY 0.0
F1 9.501P
F2 -.499P
HZ/CM 142.918
PPM/CM .476
SR 3367.55



D1019.901
DATE ??-??-??

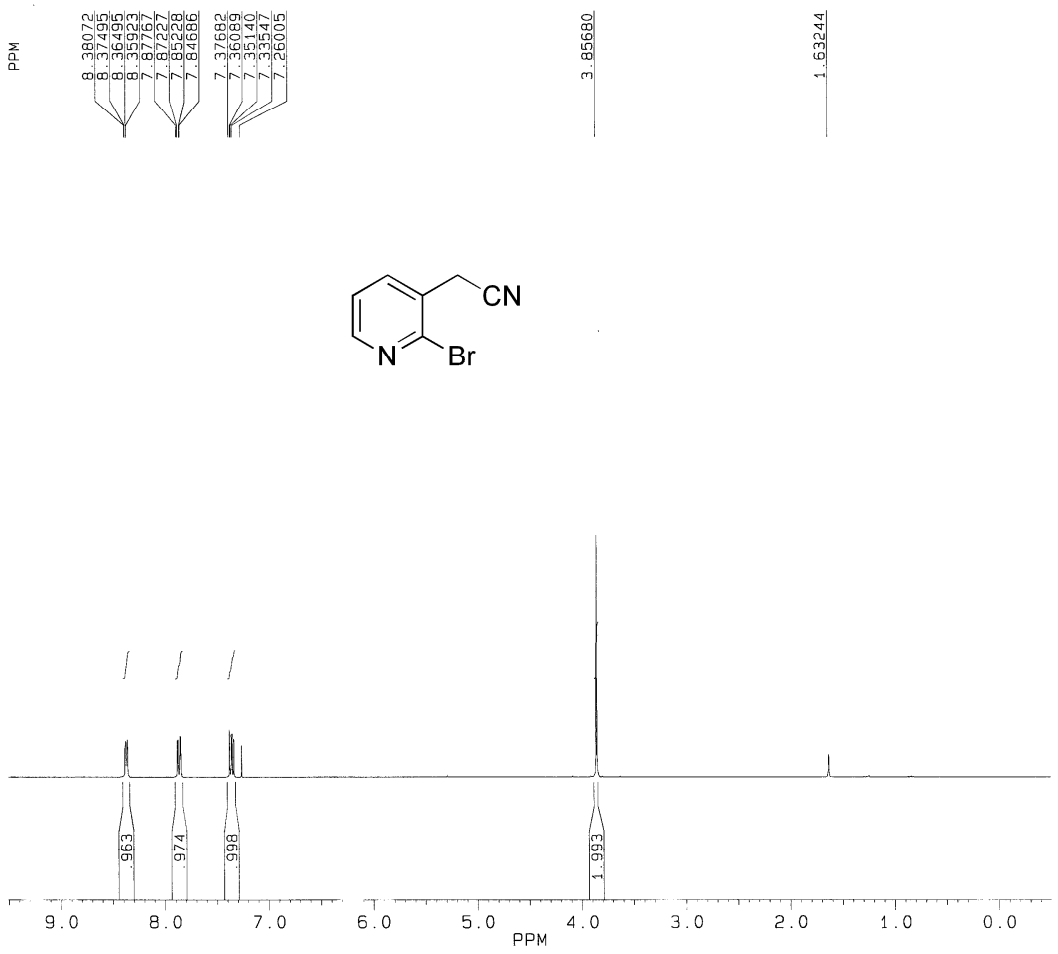
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

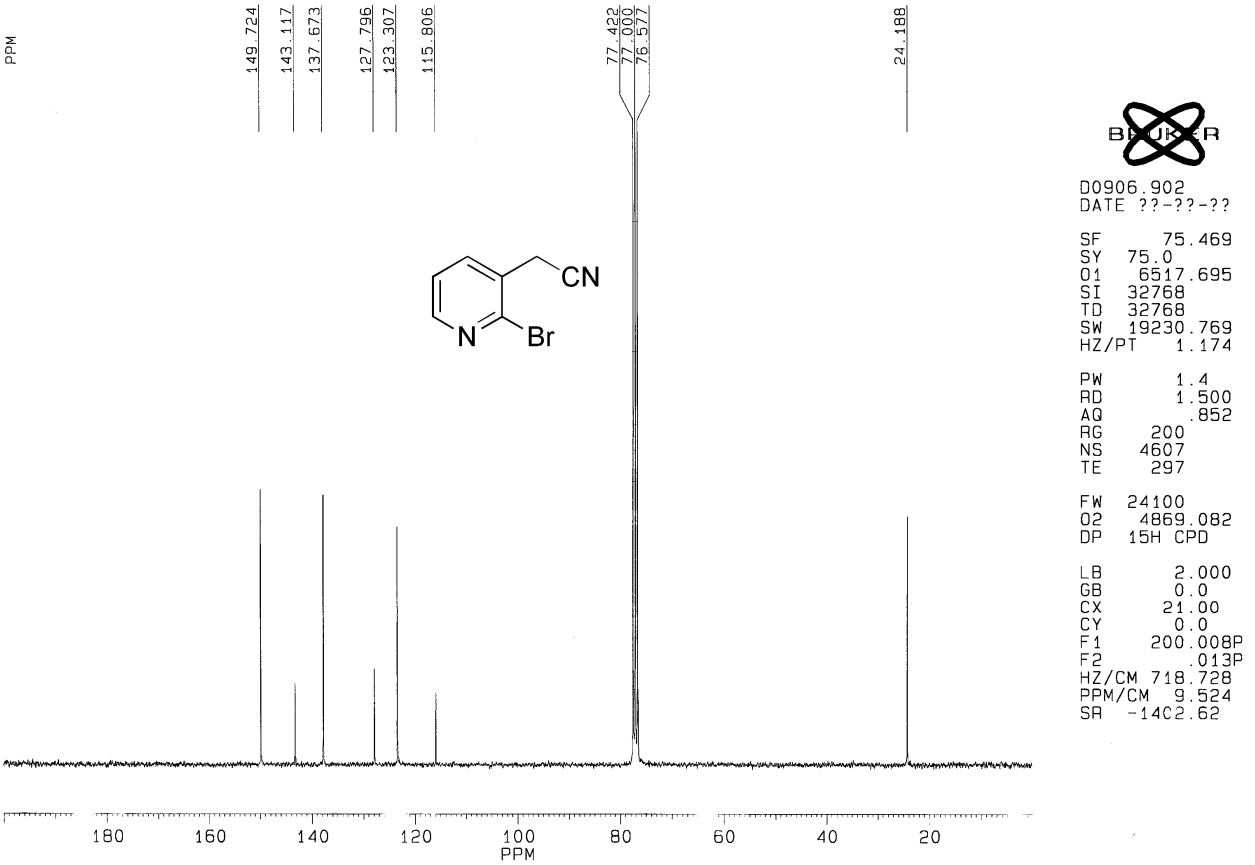
PW 1.4
RD 1.500
AQ .852
RG 200
NS 18955
TE 297

FW 24100
O2 4869.082
DP 15H CPD

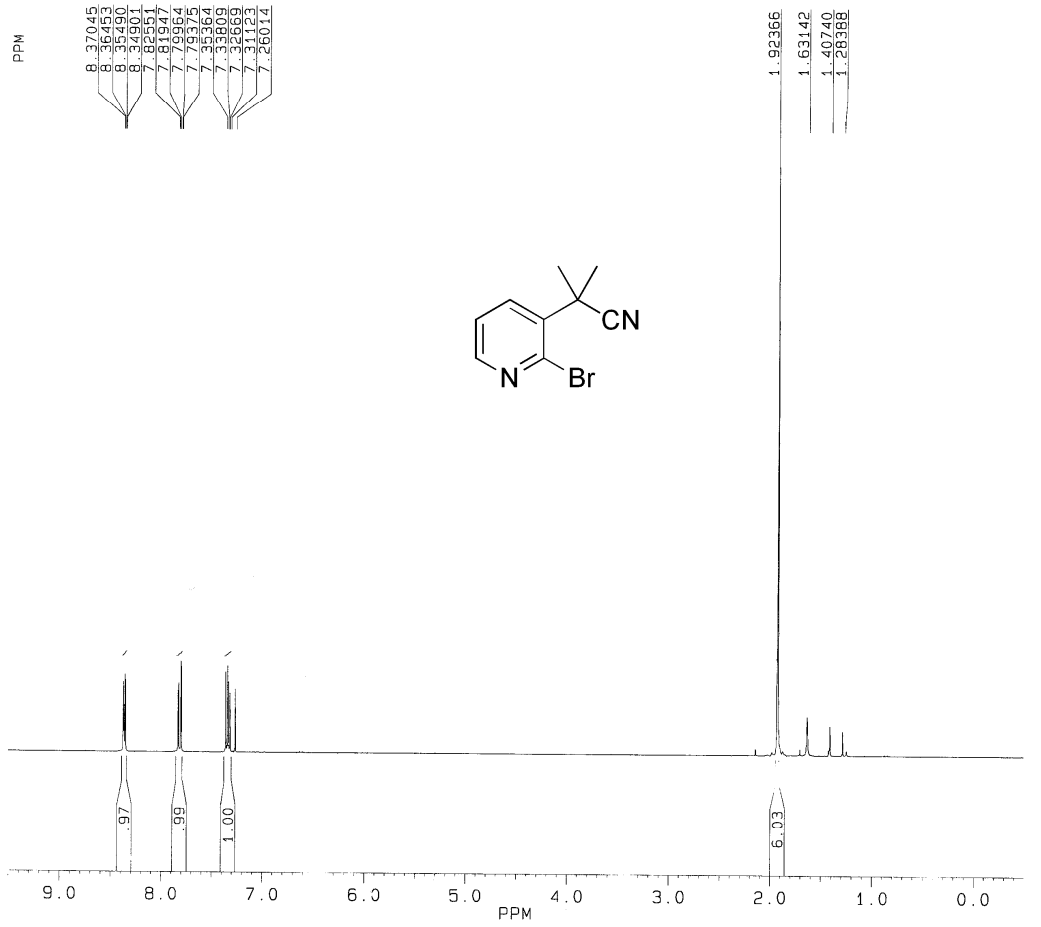
LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 200.008P
F2 .013P
HZ/CM 718.728
PPM/CM 9.524
SR -1400.27

2-(2-Bromopyridin-3-yl)acetonitrile (5j)





2-(2-Bromopyridin-3-yl)-2-methylpropanenitrile (1j)



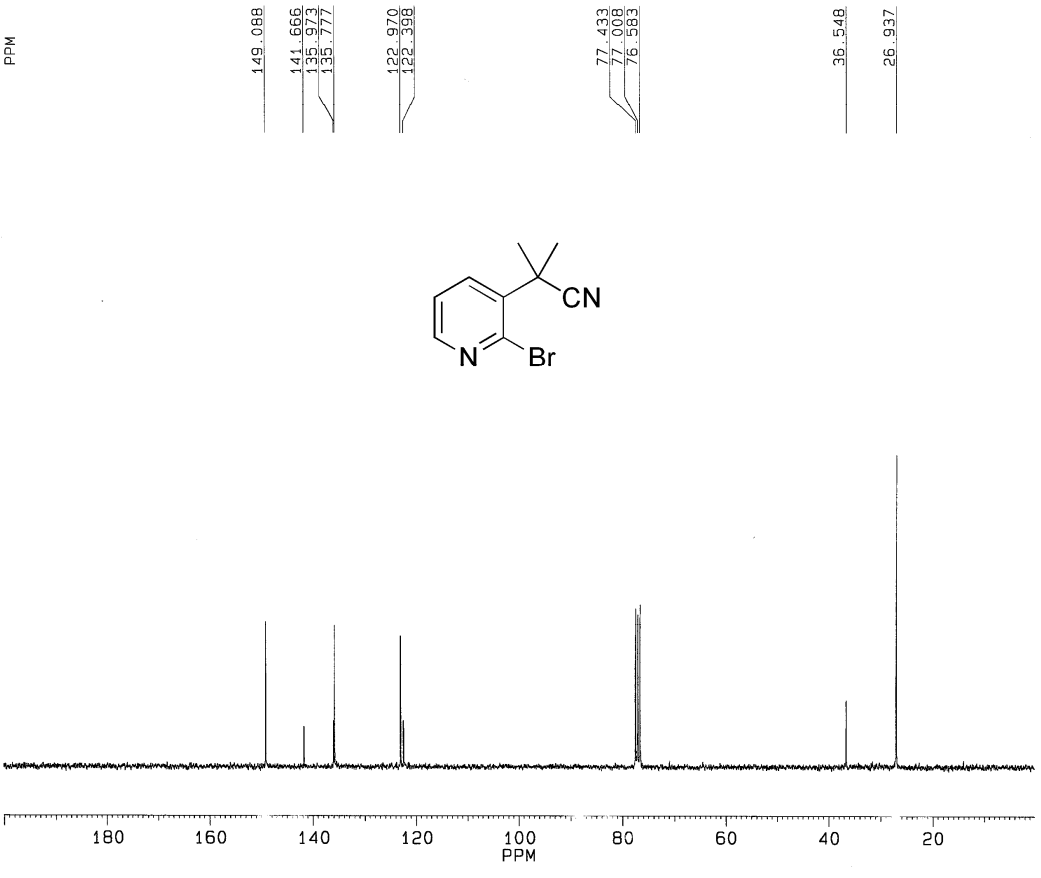
D0908.010
DATE ??-??-??

SF 300.133
SY 299.0
O1 5018.332
SI 16384
TD 16384
SW 4807.692
HZ/PT .587

PW 1.4
RD 1.000
AQ 1.704
RG 160
NS 32
TE 297

FW 6100
O2 0.0
DP 63L PO

LB 0.0
GB 0.0
CX 21.00
CY 0.0
F1 9.501P
F2 -.499P
HZ/CM 142.918
PPM/CM .476
SR 3367.55



D1215.904
DATE ??-??-??

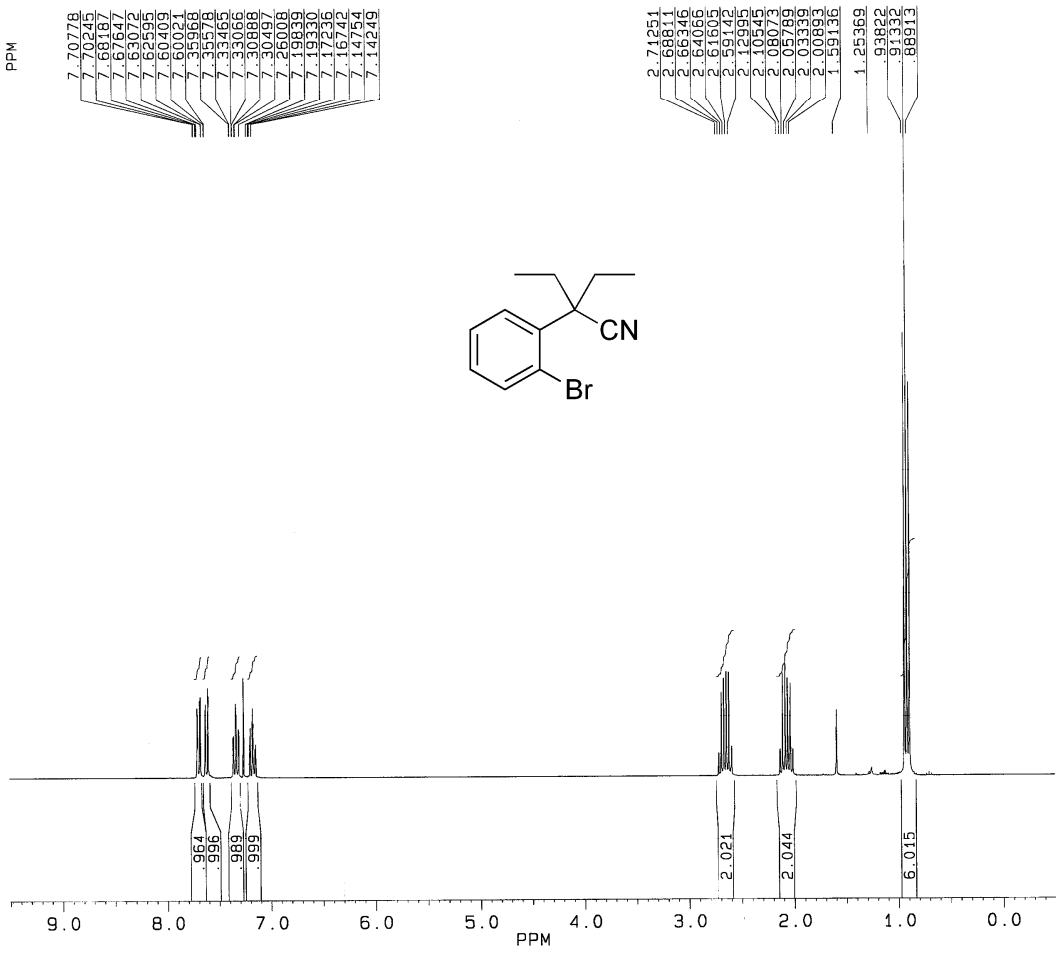
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

PW 1.4
RD 1.500
AQ .852
RG 160
NS 150
TE 297

FW 24100
O2 4869.082
DP 15H CPD

LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 200.008P
F2 .013P
HZ/CM 718.728
PPM/CM 9.524
SR -1396.75

2-(2-Bromophenyl)-2-ethylbutanenitrile (1k)

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D1126.004
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI   16384
TD   16384
SW    4807.692
HZ/PT     .587

PW       1.4
RD       1.000
AQ       1.704
RG        80
NS        32
TE       297

FW.    6100
O2        0.0
DP   63L PO

LB        0.0
GB        0.0
CX       21.00
CY        0.0
F1        9.501P
F2        -.499P
HZ/CM 142.918
PPM/CM    .476
SR    3367.55
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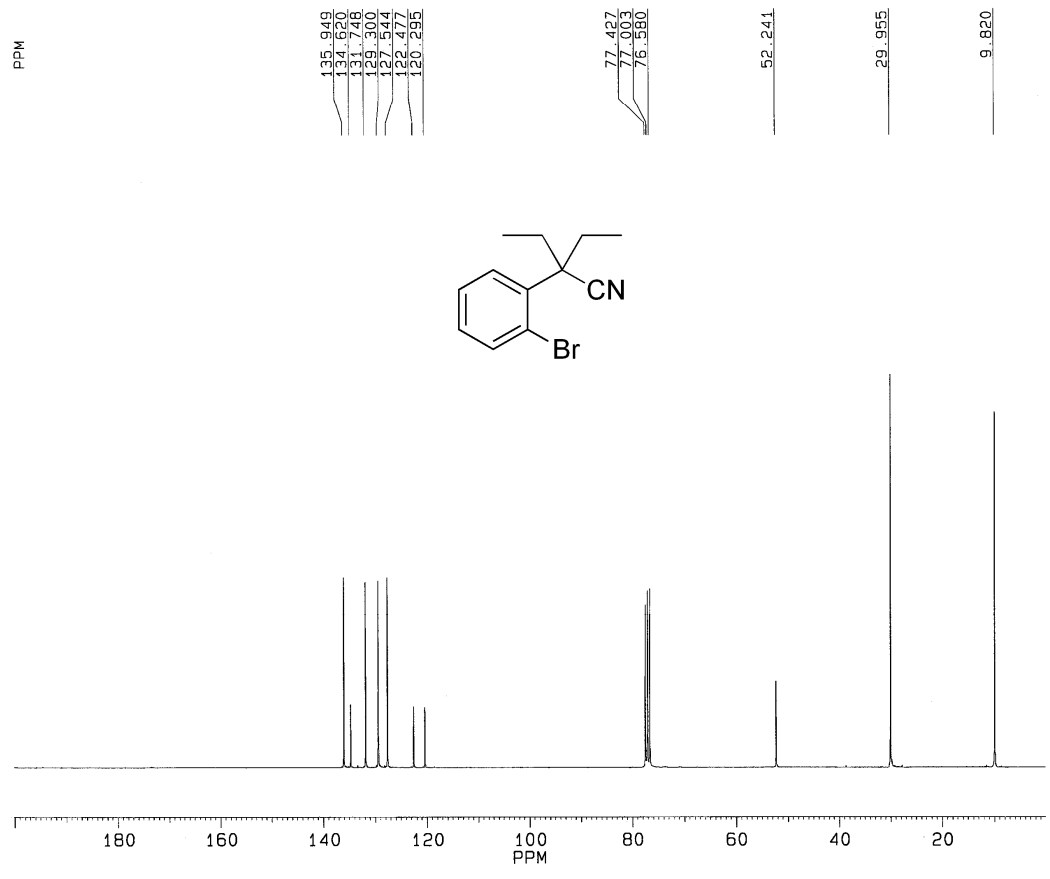


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D1124.903
DATE ??-??-??

SF      75.469
SY   75.0
O1    6517.695
SI   32768
TD   32768
SW   19230.769
HZ/PT    1.174

PW       1.4
RD       1.500
AQ        .852
RG        200
NS.   18563
TE       297

FW   24100
O2    4869.082
DP   15H CPD

LB       2.000
GB       0.0
CX      21.00
CY       0.0
F1     200.008P
F2        .013P
HZ/CM 718.728
PPM/CM   9.524
SR    -1400.27
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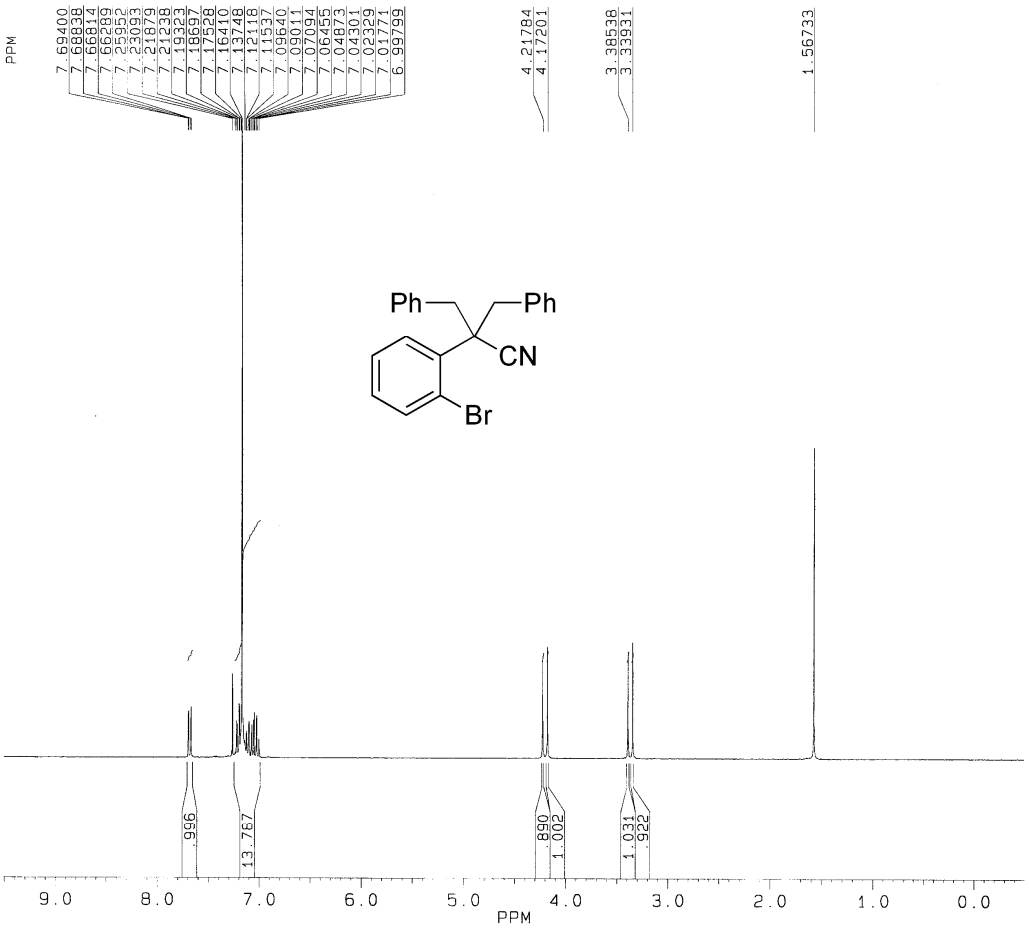
2-Benzyl-2-(2-bromophenyl)-3-phenylpropanenitrile (1l)



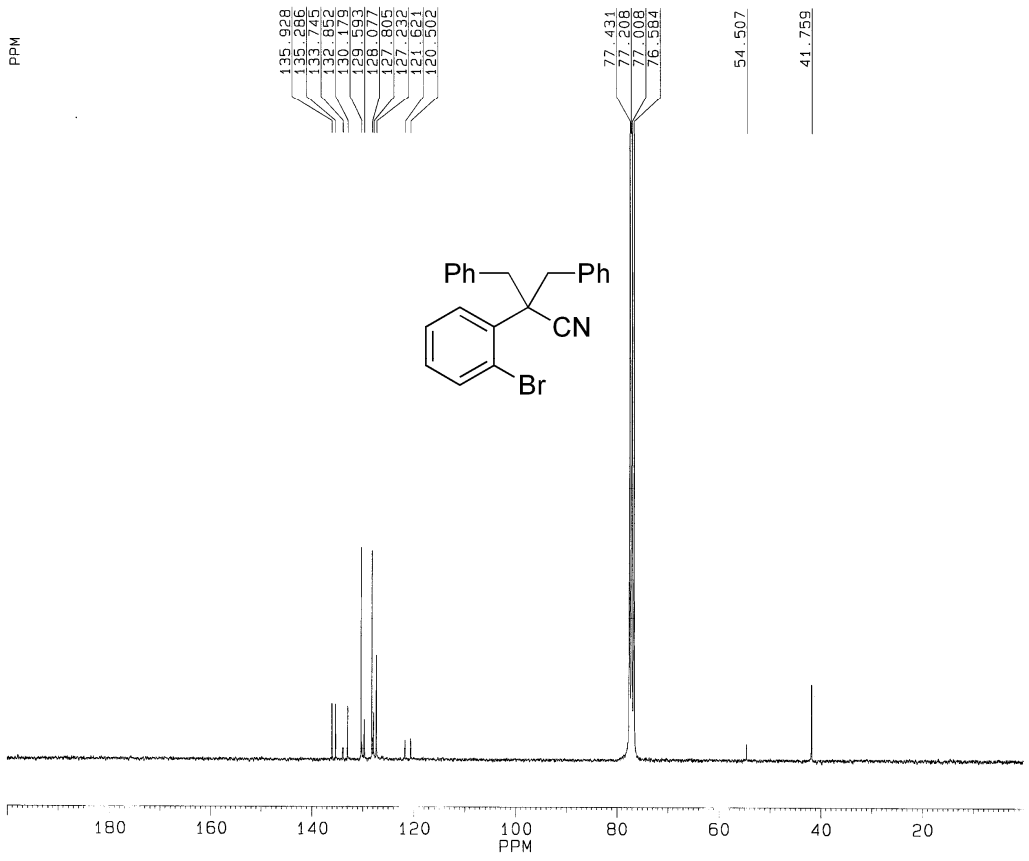
D0919.025
DATE ??-??-??

SF 300.133
SY 299.0
O1 5018.332
SI 16384
TD 16384
SW 4807.692
HZ/PT .587

PW 1.4
RD 1.000
AQ 1.704
RG 160
NS 64
TE 297

FW. 6100
O2 0.0
DP 63L PO

LB 0.0
GB 0.0
CX 21.00
CY 0.0
F1 9.501P
F2 -.499P
HZ/CM 142.918
PPM/CM .476
SR 3368.14



D0816.902
DATE ??-??-??

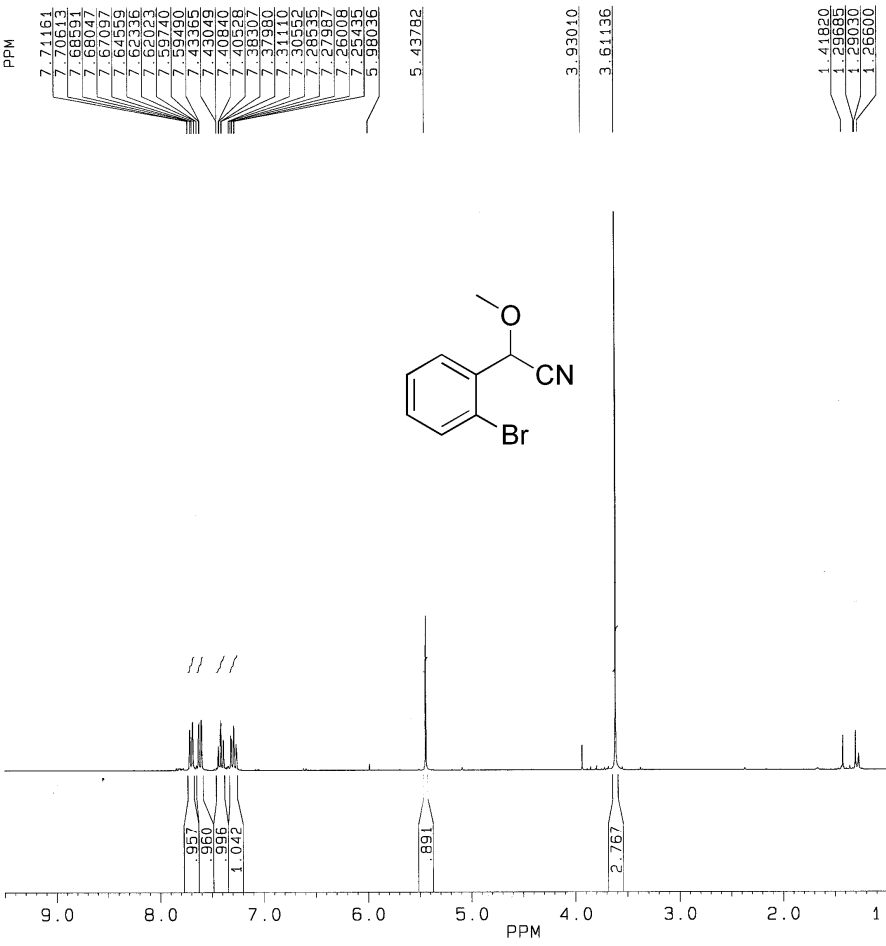
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

PW 1.4
RD 1.500
AQ .852
RG 200
NS 38520
TE. 297

FW 24100
O2 4869.082
DP 15H CPD

LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 200.008P
F2 .013P
HZ/CM 718.728
PPM/CM 9.524
SR -1406.14

2-(2-Bromophenyl)-2-methoxyacetonitrile (5m)



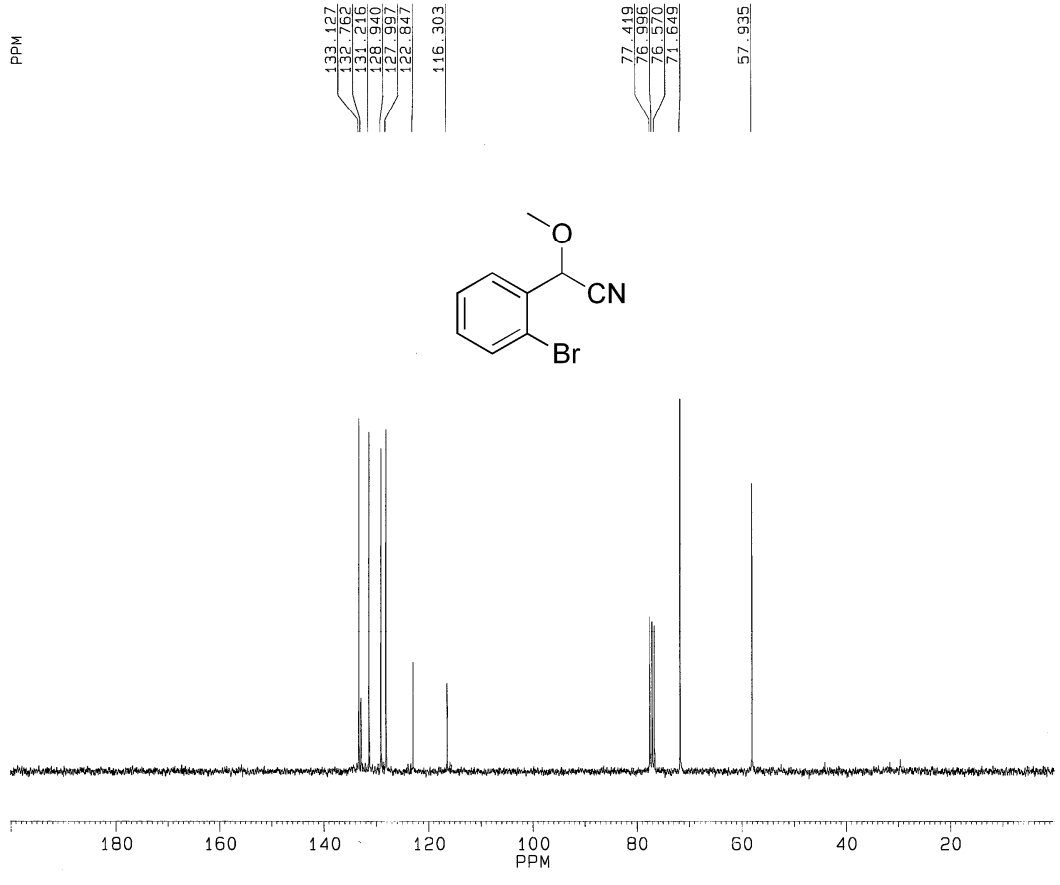
D1222.020
DATE ??-??-??

SF 300.133
SY 299.0
O1 5018.332
SI 16384
TD 16384
SW 4807.692
HZ/PT .587

PW 1.4
RD 1.000
AQ 1.704
RG 20
NS 16
TE 297

FW 6100
O2 0.0
DP 63L PO

LB 0.0
GB 0.0
CX 21.00
CY 0.0
F1 9.501P
F2 -.499P
HZ/CM 142.918
PPM/CM .476
SR 3367.55



D1222.903
DATE ??-??-??

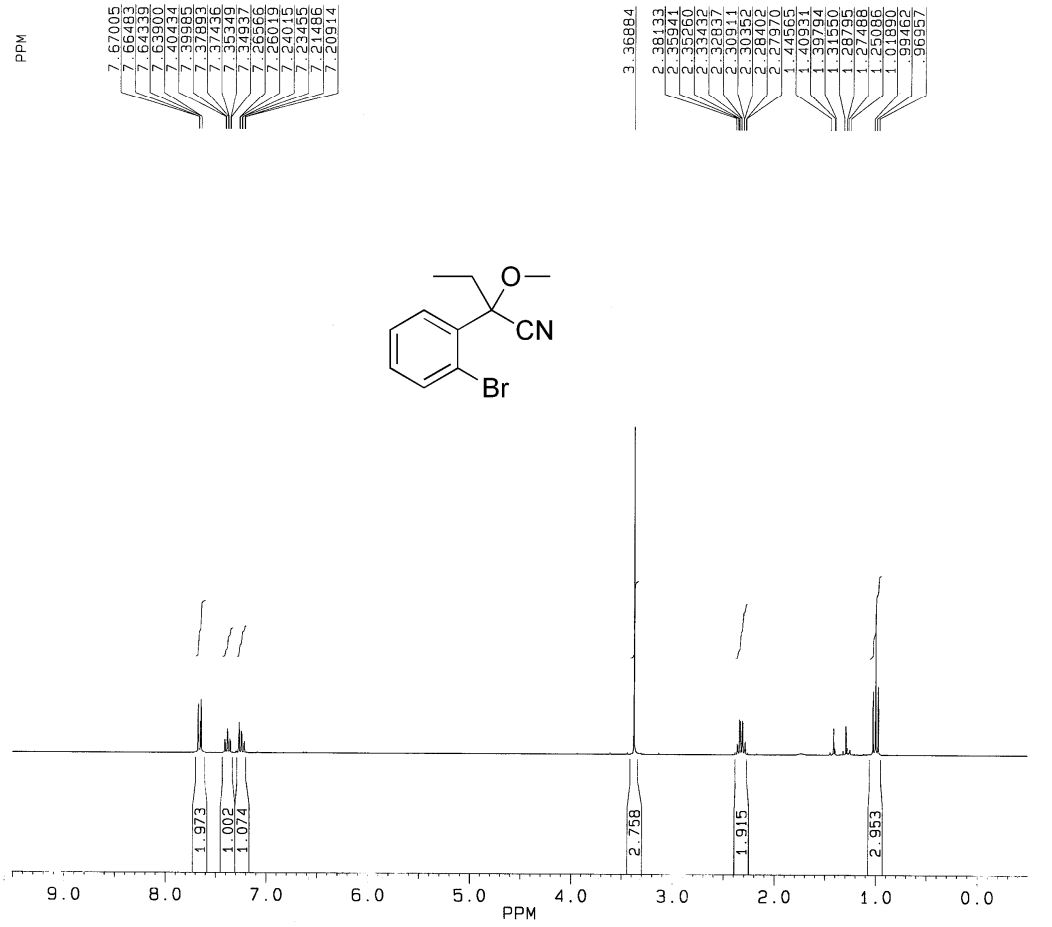
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

PW 1.4
RD 1.500
AQ .852
RG 160
NS 250
TE 297

FW 24100
O2 4869.082
DP 15H CPD

LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 200.008P
F2 .013P
HZ/CM 718.728
PPM/CM 9.524
SR -1395.58

2-(2-Bromophenyl)-2-methoxybutanenitrile (1m)

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D1216.011
DATE ??-??-??

SF    300.133
SY 299.0
O1   5018.332
SI  16384
TD  16384
SW   4807.692
HZ/PT     .587

PW       1.4
RD       1.000
AQ       1.704
RG      40
NS      32
TE     297

FW.   6100
O2       0.0
DP  63L PO

LB       0.0
GB       0.0
CX      21.00
CY       0.0
F1       9.501P
F2       -.499P
HZ/CM 142.918
PPM/CM    .476
SR    3367.55
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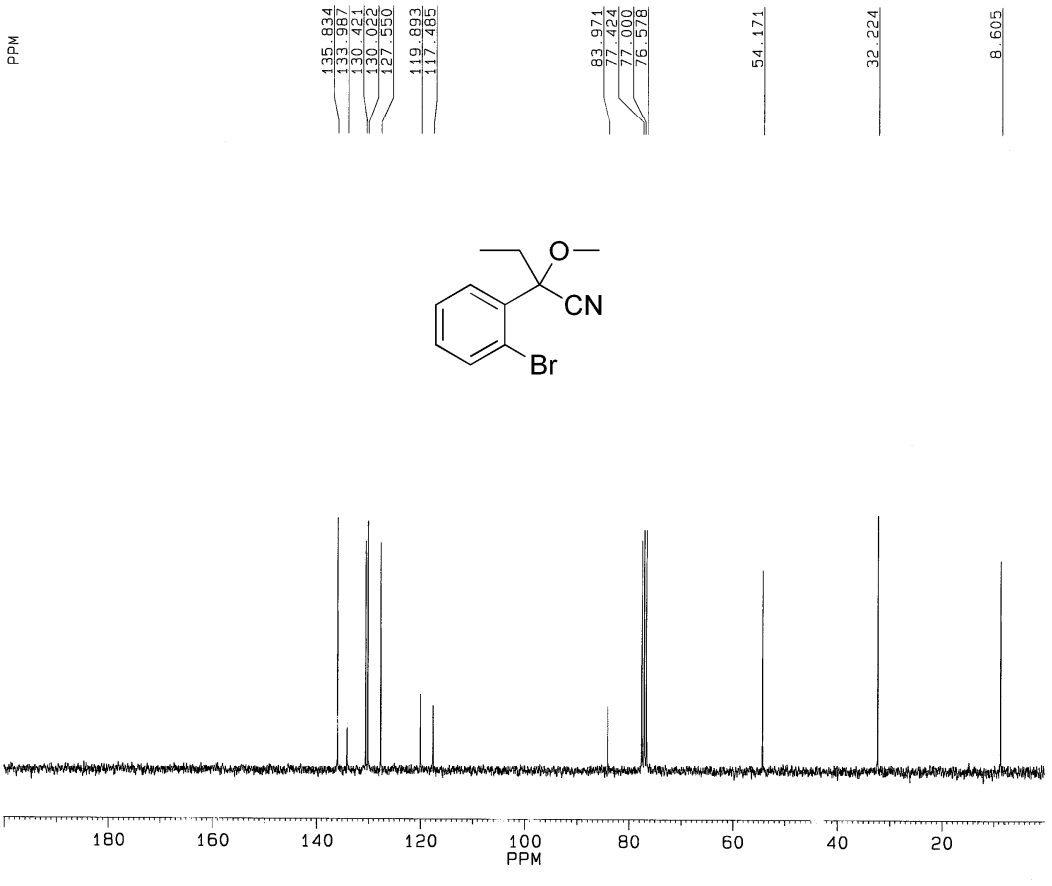


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D1216.901
DATE ??-??-??

SF      75.469
SY   75.0
O1    6517.695
SI   32768
TD   32768
SW  19230.769
HZ/PT    1.174

PW       1.4
RD       1.500
AQ        .852
RG     200
NS     300
TE.    297

FW   24100
O2    4869.082
DP   15H CPD

LB       2.000
GB       0.0
CX      21.00
CY       0.0
F1     200.008P
F2        .013P
HZ/CM 718.728
PPM/CM  9.524
SR   -1402.62
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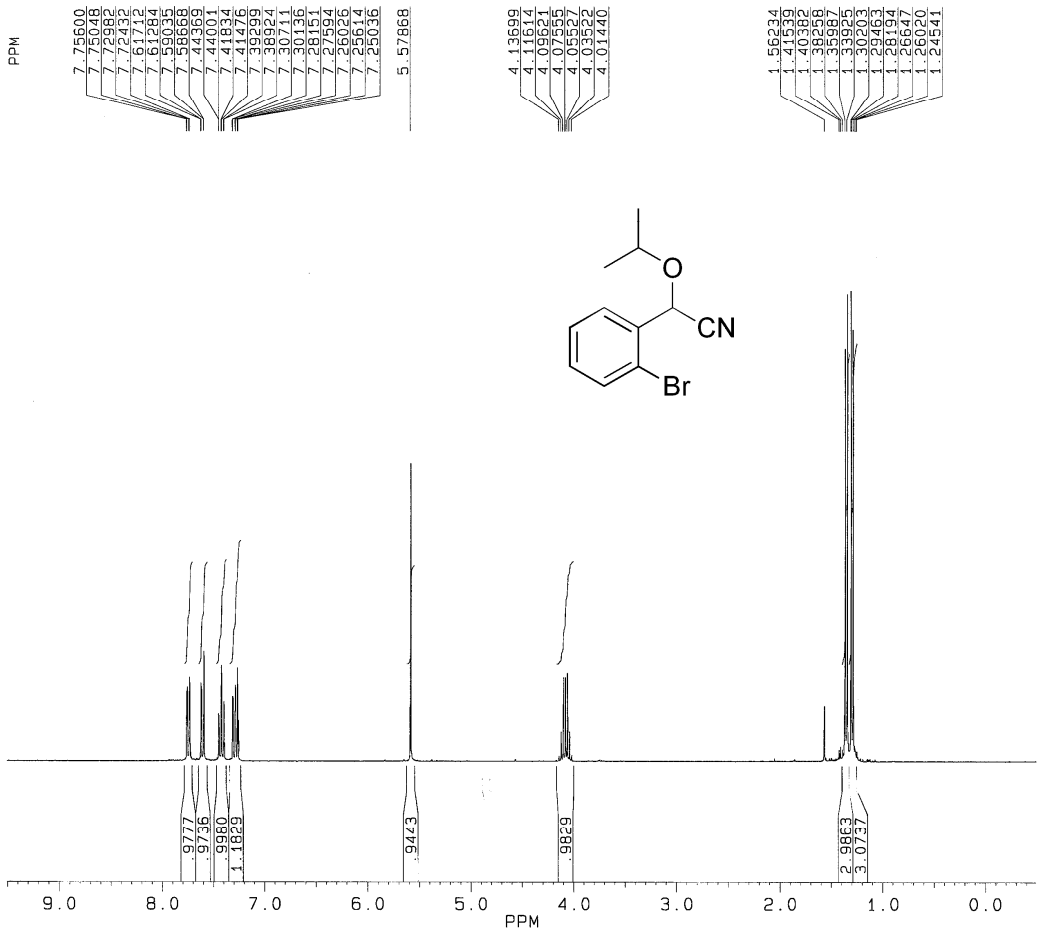
2-(2-Bromophenyl)-2-isopropoxyacetonitrile (5n)



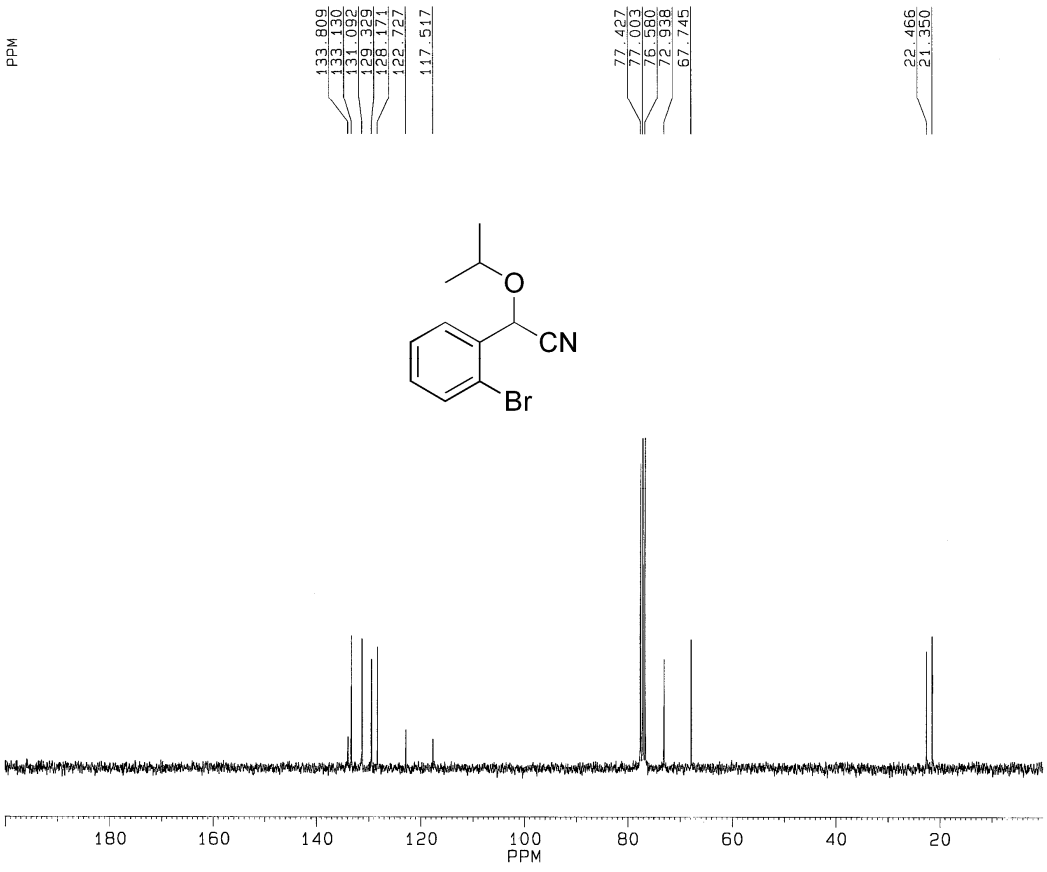
D1231.008
DATE ??-??-??

SF 300.133
SY 299.0
O1 5018.332
SI 16384
TD 16384
SW 4807.692
HZ/PT .587

PW 1.4
RD 1.000
AQ 1.704
RG 100
NS 32
TE 297

FW 6100
O2 0.0
DP 63L PO

LB 0.0
GB 0.0
CX 21.00
CY 0.0
F1 9.501P
F2 -.499P
HZ/CM 142.918
PPM/CM .476
SR 3367.55



D1231.901
DATE ??-??-??

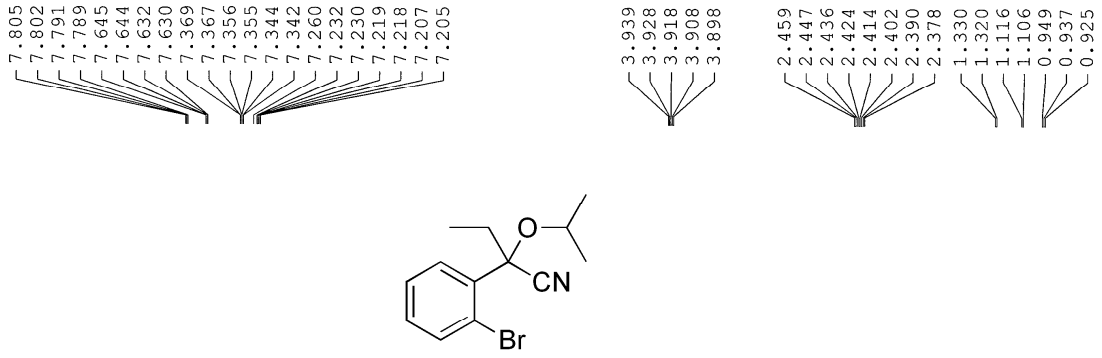
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

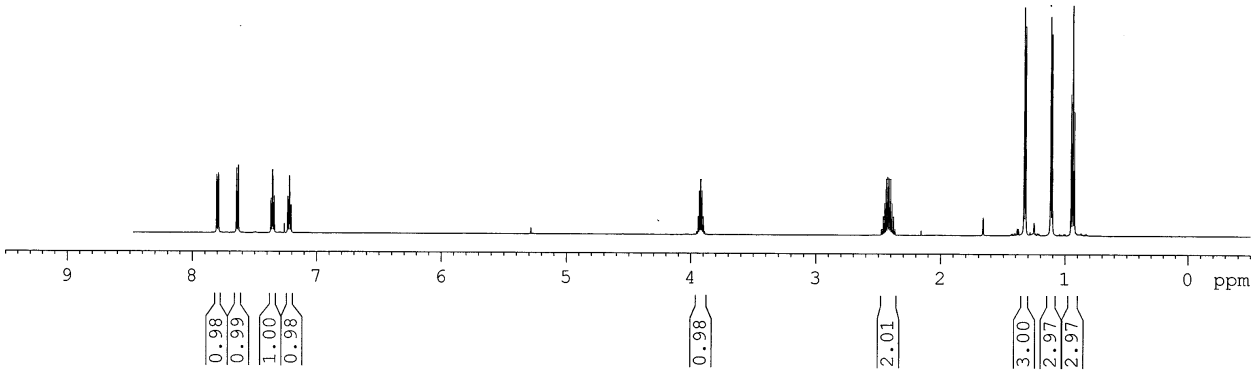
PW 1.4
RD 1.500
AQ .852
RG 160
NS 500
TE 297

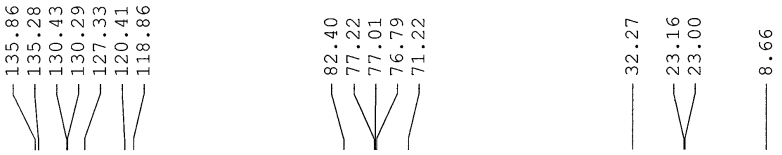
FW 24100
O2 4869.082
DP 15H CPD

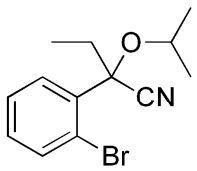
LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 200.008P
F2 .013P
HZ/CM 718.728
PPM/CM 9.524
SR -1404.97

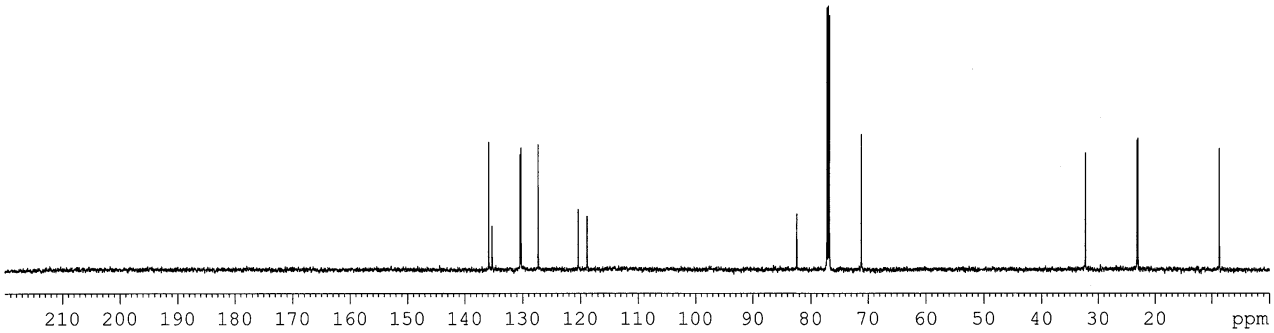
2-(2-Bromophenyl)-2-isopropoxybutanenitrile (1n)



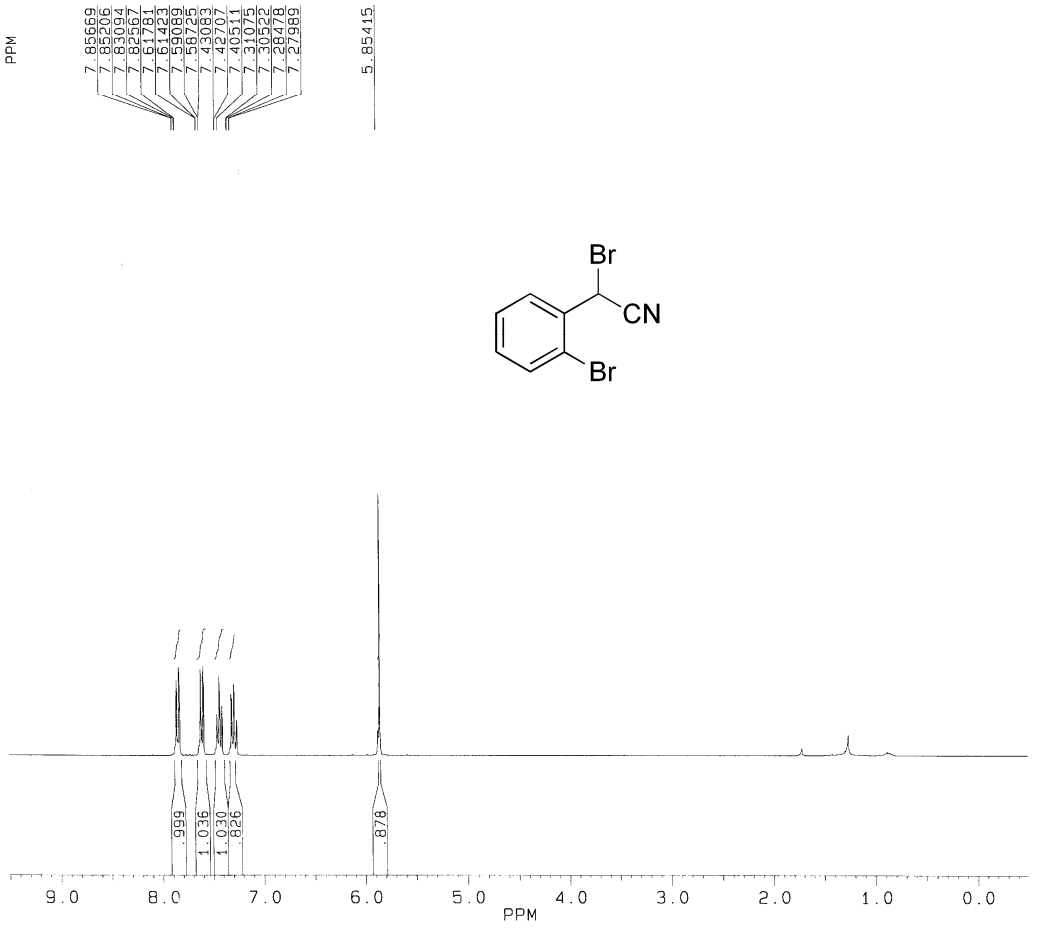








2-Bromo-2-(2-bromophenyl)acetonitrile (4o)

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D0214.019
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI   16384
TD   16384
SW    4807.692
HZ/PT     .587

PW       1.4
RD       1.000
AQ       1.704
RG      20
NS      32
TE     297

FW    6100
O2       0.0
DP   63L PO

LB       0.0
GB       0.0
CX      21.00
CY       0.0
F1       9.501P
F2       -.499P
HZ/CM 142.918
PPM/CM    .476
SR    3367.55
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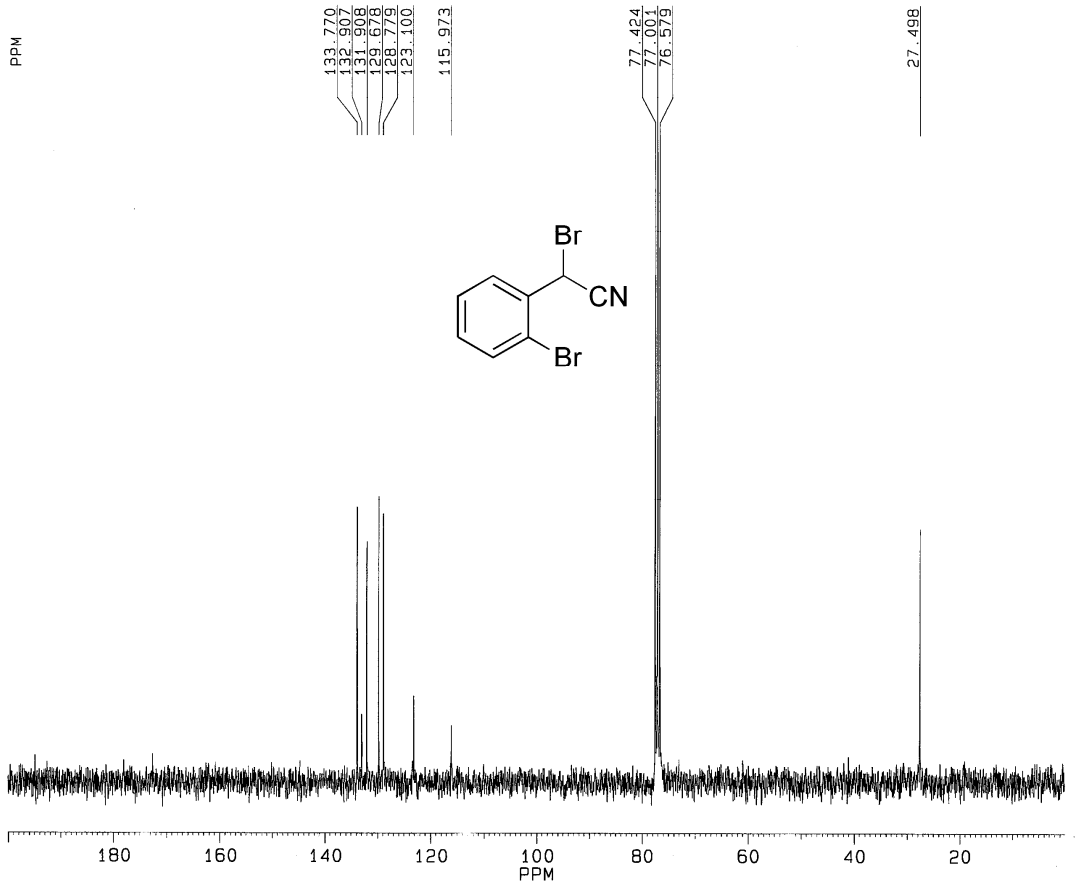


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D1121.903
DATE ??-??-??

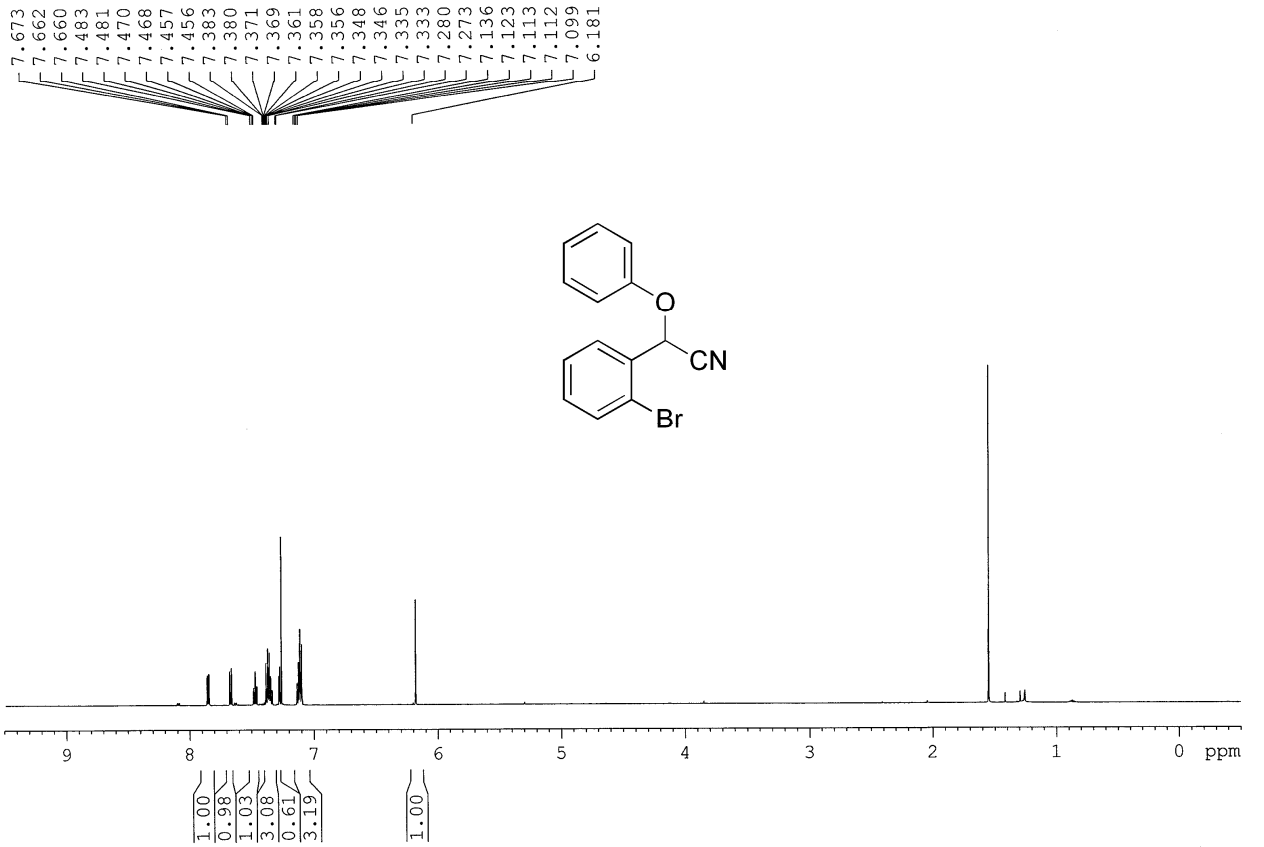
SF      75.469
SY   75.0
O1    6517.695
SI   32768
TD   32768
SW   19230.769
HZ/PT    1.174

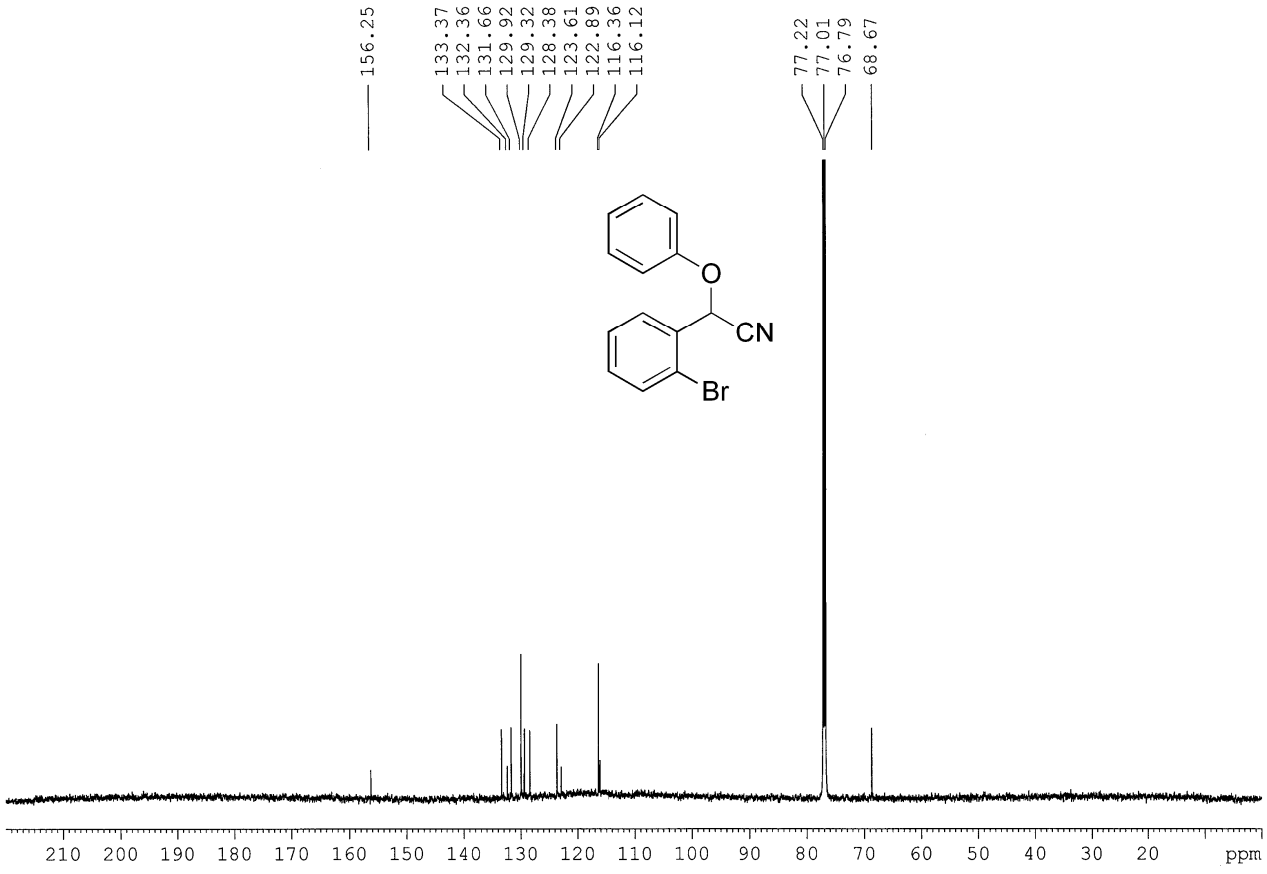
PW       1.4
RD       1.500
AQ        .852
RG     200
NS     500
TE     297

FW   24100
O2    4869.082
DP   15H CPD

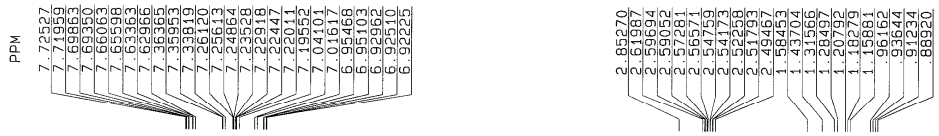
LB       2.000
GB       0.0
CX      21.00
CY       0.0
F1     200.008P
F2        .013P
HZ/CM 718.728
PPM/CM   9.524
SR   -1404.97
```

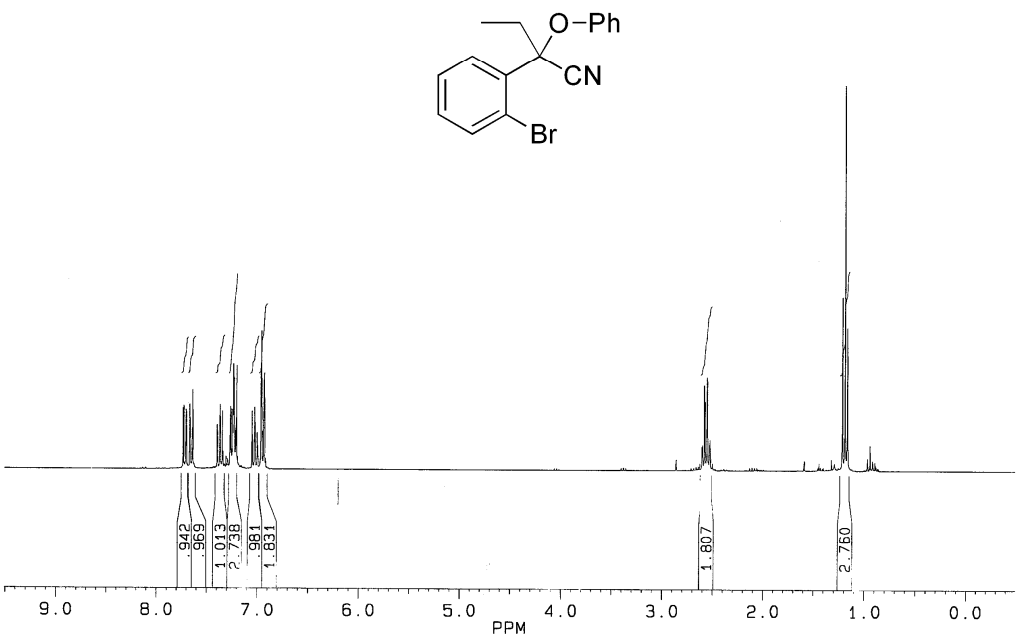
2-(2-Bromophenyl)-2-phenoxyacetonitrile (5o)





2-(2-Bromophenyl)-2-phenoxybutanenitrile (1o)





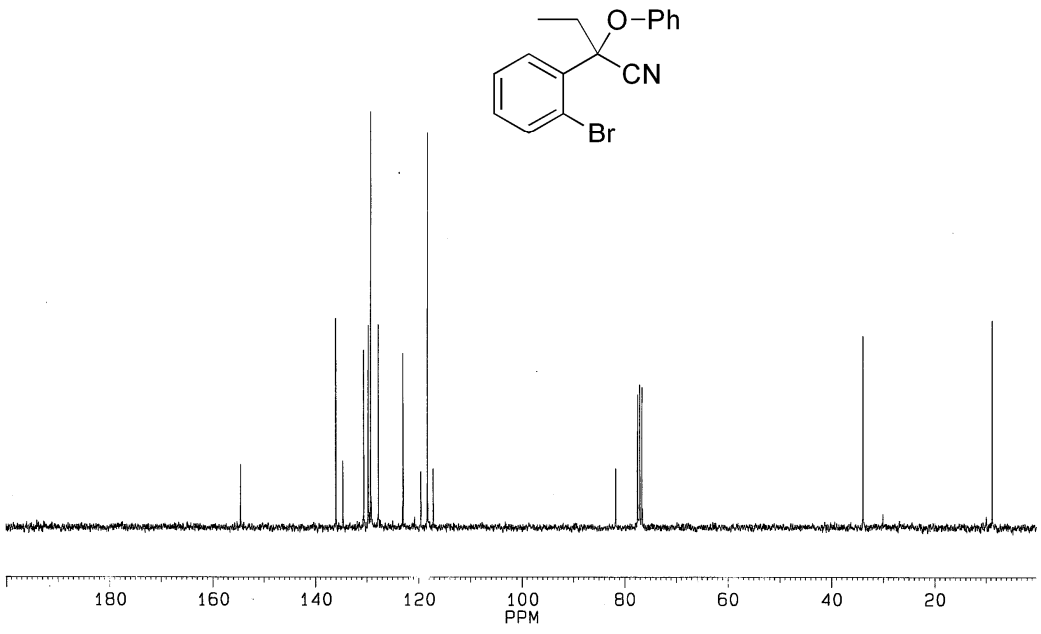
D1215.015
DATE ??-??-??

SF 300.133
SY 299.0
O1 5018.332
SI 16384
TD 16384
SW 4807.692
HZ/PT .587

PW 1.4
RD 1.000
AQ 1.704
RG 20
NS 35
TE 297

FW 6100
O2 0.0
DP 63L PO

LB 0.0
GB 0.0
CX 21.00
CY 0.0
F1 9.501P
F2 -.499P
HZ/CM 142.918
PPM/CM .476
SR 3367.55



D1215.905
DATE ??-??-??

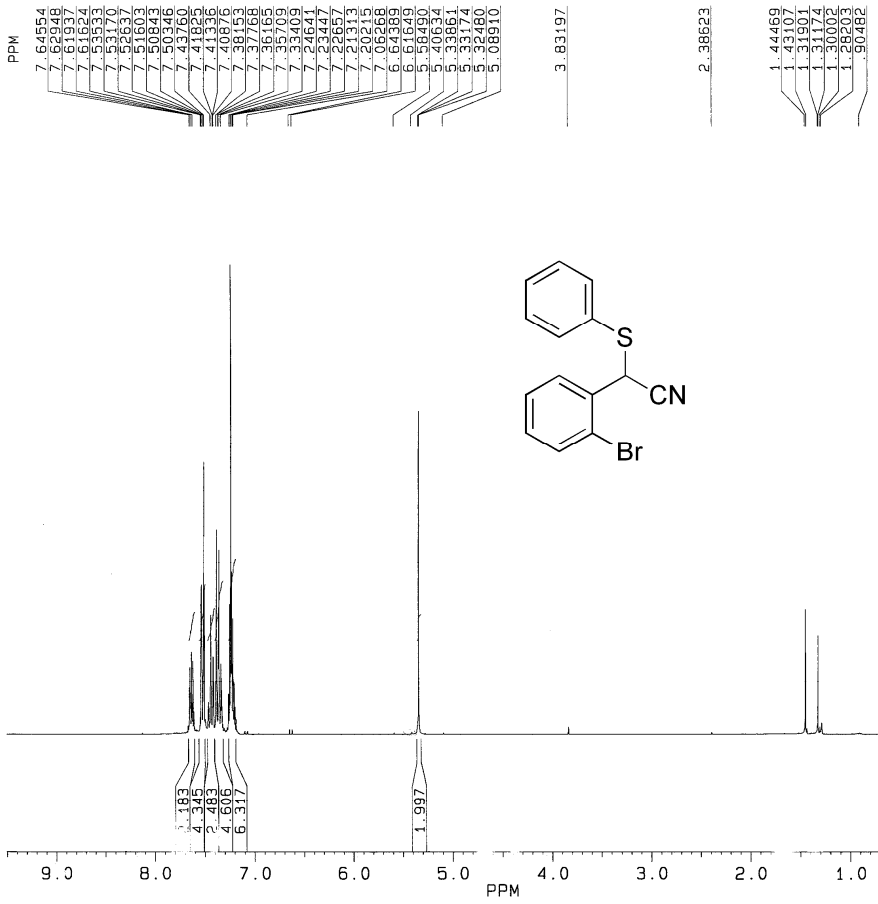
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

PW 1.4
RD 1.500
AQ .852
RG 160
NS 250
TE. 297

FW 24100
O2 4869.082
DP 15H CPD

LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 200.008P
F2 .013P
HZ/CM 718.728
PPM/CM 9.524
SR -1400.27

2-(2-Bromophenyl)-2-(phenylthio)acetonitrile (5p)



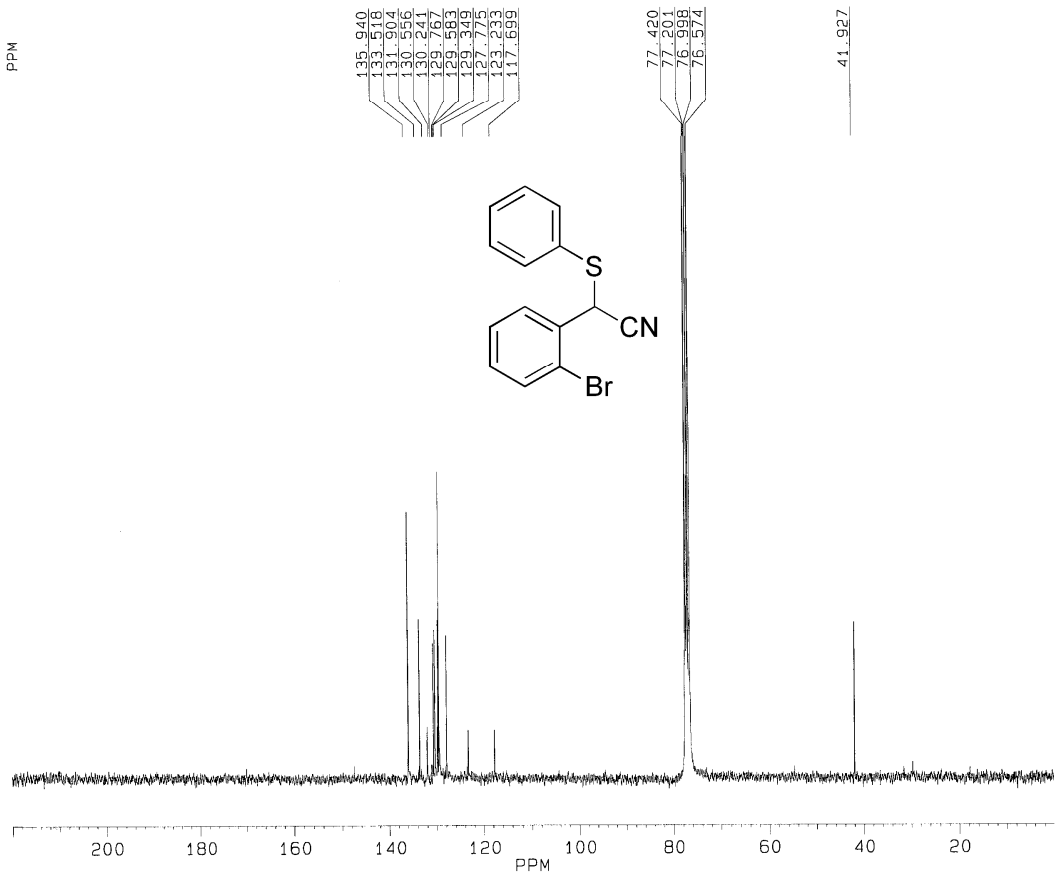
D1209.008
DATE ??-??-??

SF 300.133
SY 299.0
O1 5018.332
SI 16384
TD 16384
SW 4807.692
HZ/PT .587

PW 1.4
RD 1.000
AQ 1.704
RG 20
NS 32
TE 297

FW 6100
O2 0.0
DP 63L PO

LB 0.0
GB 0.0
CX 21.00
CY 0.0
F1 9.501P
F2 -.499P
HZ/CM 142.918
PPM/CM .476
SR 3367.55



D0209.901
DATE ??-??-??

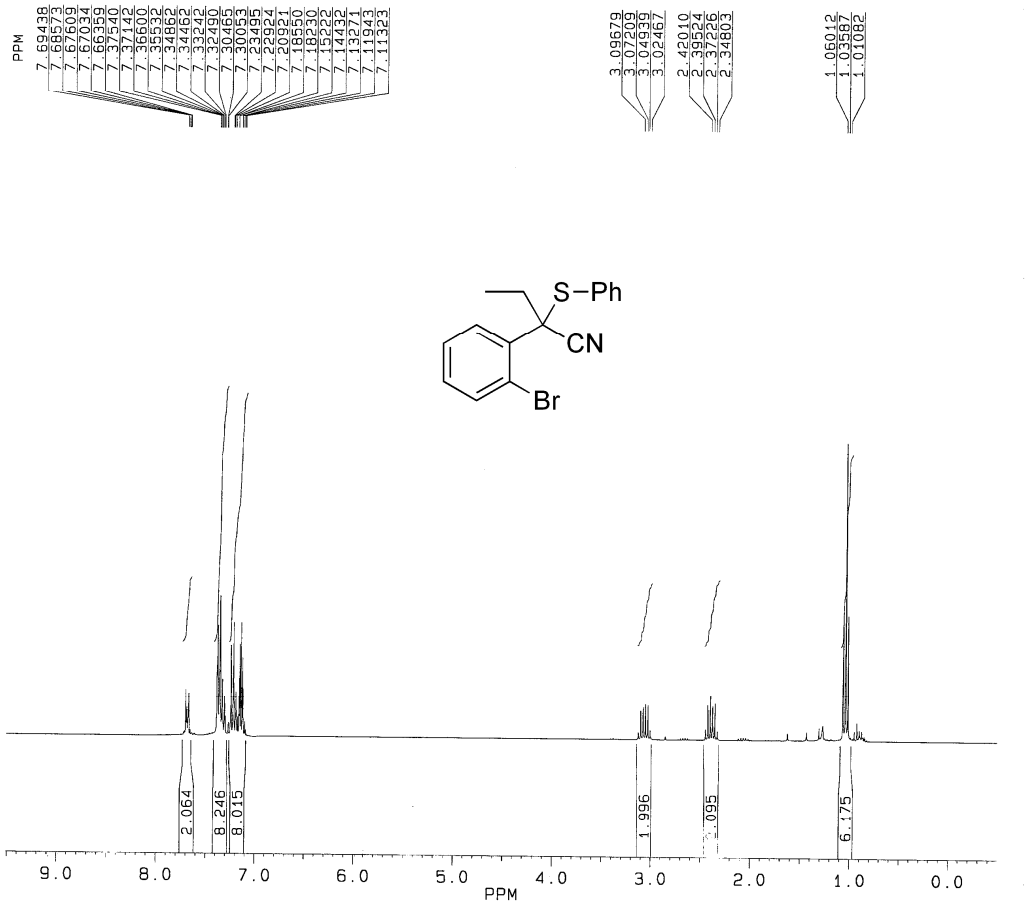
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

PW 1.4
RD 1.500
AQ .852
RG 200
NS 21336
TE 297

FW 24100
O2 4869.082
DP 15H CPD

LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 220.009P
F2 .013P
HZ/CM 790.606
PPM/CM 10.476
SR -1404.97

2-(2-Bromophenyl)-2-(phenylthio)butanenitrile (1p)



BRUKER

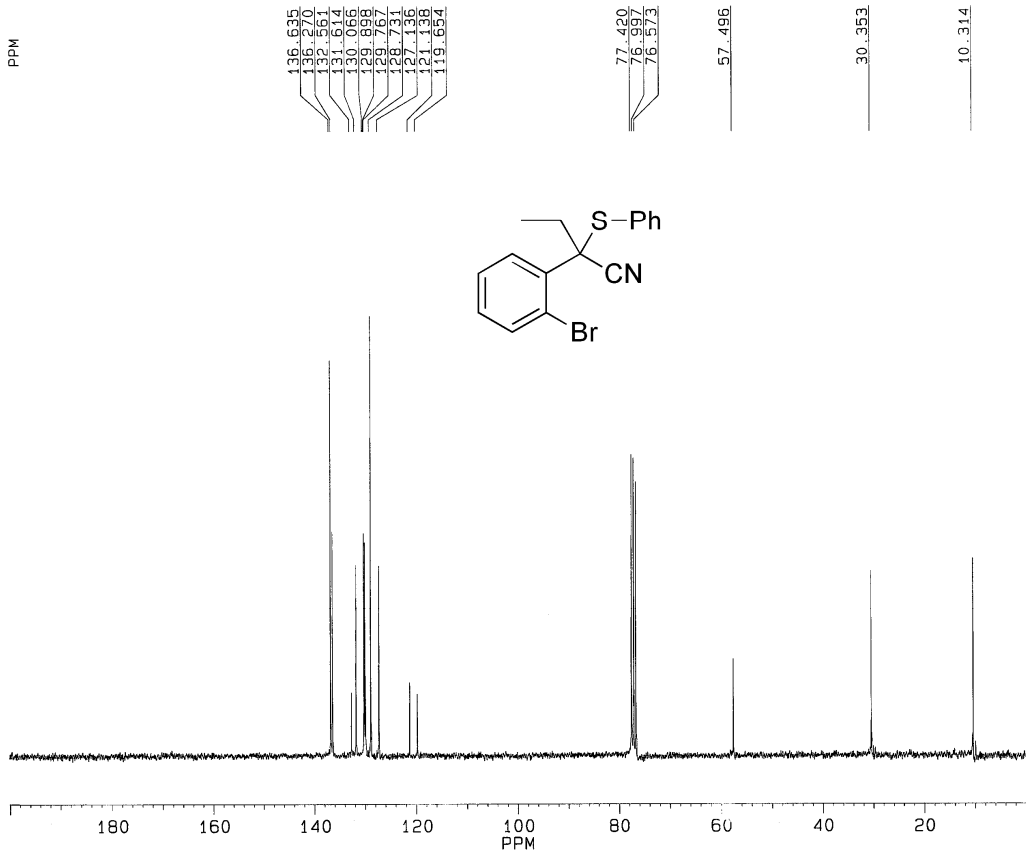
D1224.016
DATE ??-??-??

SF 300.133
SY 299.0
O1 5018.332
SI 16384
TD 16384
SW 4807.692
HZ/PT .587

PW 1.4
RD 1.000
AQ 1.704
RG 20
NS 32
TE 297

FW 6100
O2 0.0
DP 63L PO

LB 0.0
GB 0.0
CX 21.00
CY 0.0
F1 9.501P
F2 -.499P
HZ/CM 142.918
PPM/CM .476
SR 3367.00



BRUKER

D1224.902
DATE ??-??-??

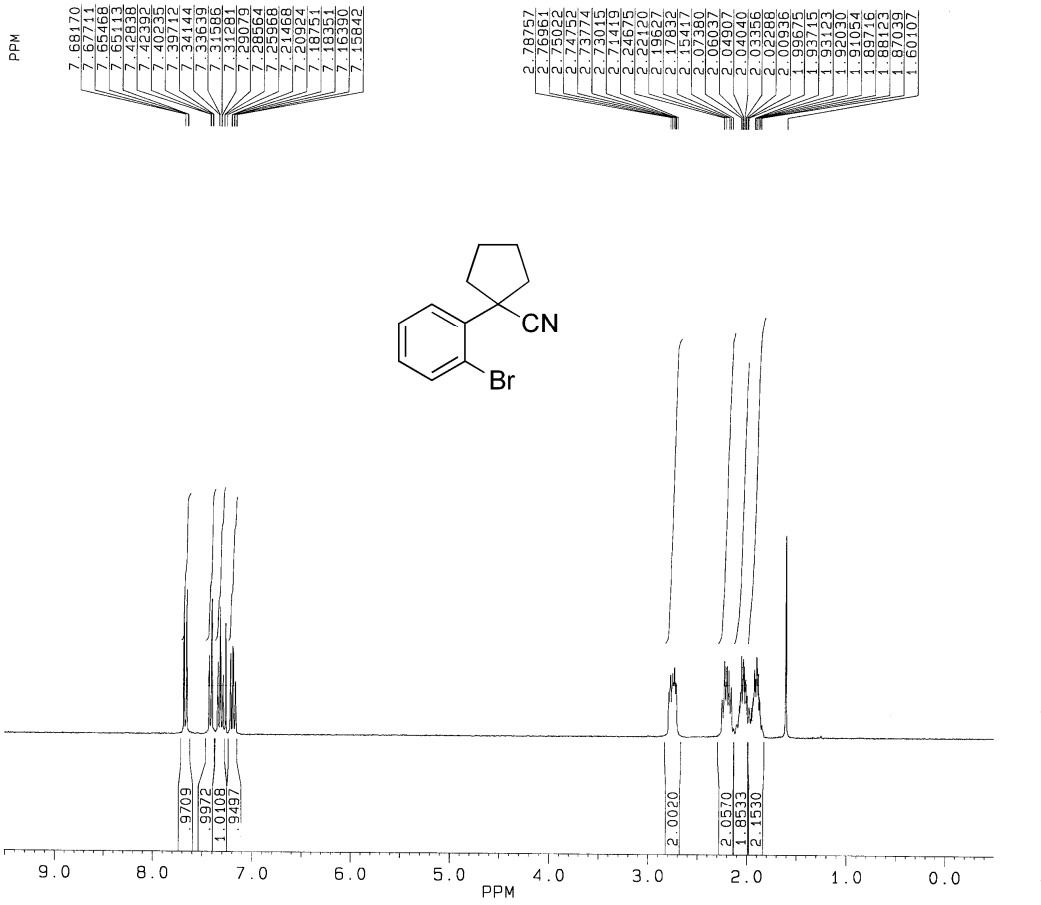
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

PW 1.4
RD 1.500
AQ .852
RG 200
NS 474
TE 297

FW 24100
O2 4869.082
DP 15H CPD

LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 200.008P
F2 .013P
HZ/CM 718.728
PPM/CM 9.524
SR -1399.10

2-(2-Bromophenyl)-2-(phenylthio)butanenitrile (1q)

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D0718.002
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI   16384
TD   16384
SW    4807.692
HZ/PT     .587

PW       1.4
RD       1.000
AQ       1.704
RG     160
NS      32
TE     297

FW.   6100
O2       0.0
DP   63L PO

LB       0.0
GB       0.0
CX      21.00
CY       0.0
F1       9.501P
F2       -.499P
HZ/CM 142.918
PPM/CM    .476
SR    3367.55
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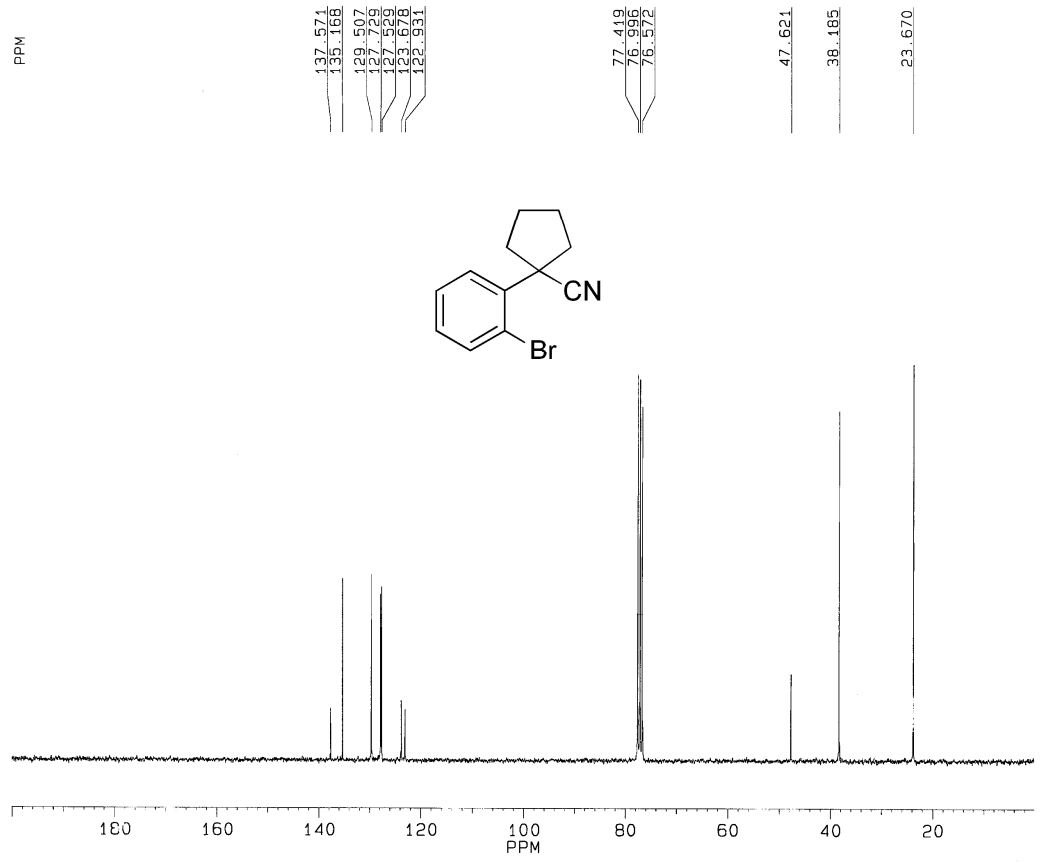


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D0709.901
DATE ??-??-??

SF      75.469
SY   75.0
O1    6517.695
SI   32768
TD   32768
SW   19230.769
HZ/PT    1.174

PW       1.4
RD       1.500
AQ        .852
RG     200
NS    1141
TE·    297

FW   24100
O2    4869.082
DP   15H CPD

LB       2.000
GB       0.0
CX      21.00
CY       0.0
F1     200.008P
F2        .013P
HZ/CM 718.728
PPM/CM   9.524
SR   -1401.45
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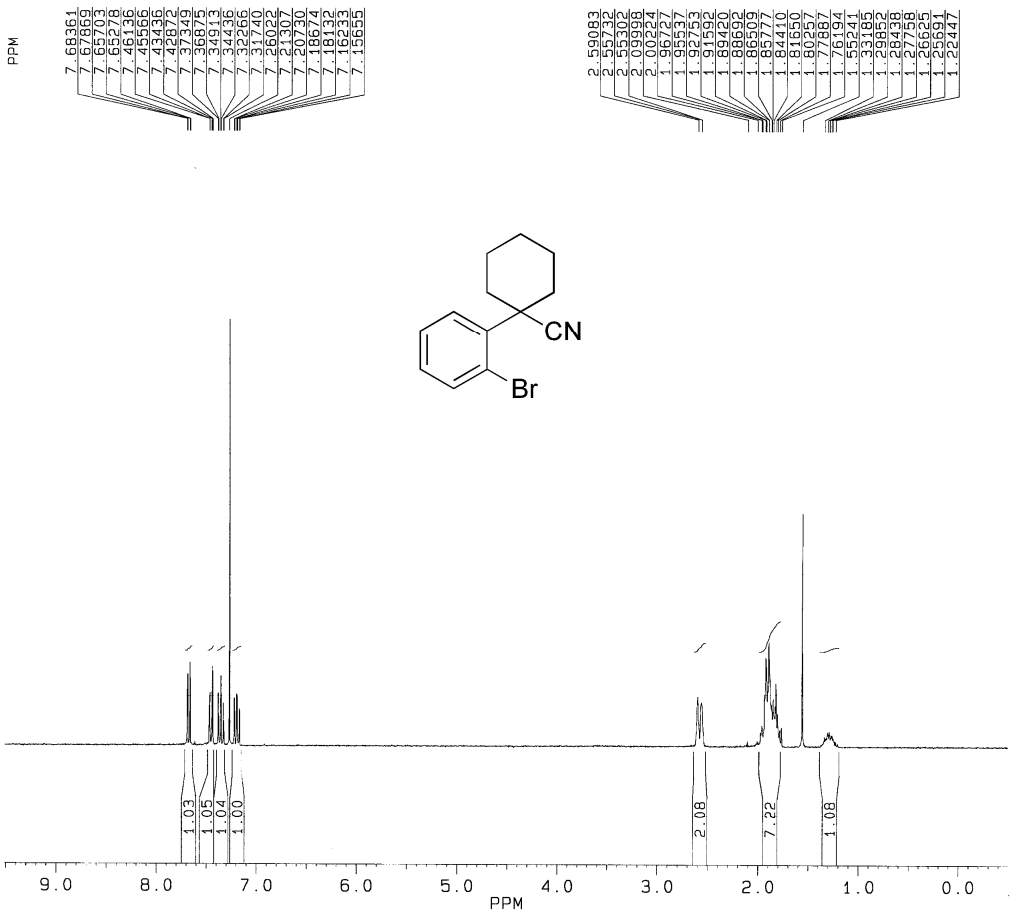
1-(2-Bromophenyl)cyclohexanecarbonitrile (1r)

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D0722.043
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI   16384
TD   16384
SW    4807.692
HZ/PT     .587

PW       1.4
RD       1.000
AQ       1.704
RG      40
NS      64
TE     297

FW.   6100
O2       0.0
DP   63L PO

LB       0.0
GB       0.0
CX      21.00
CY       0.0
F1       9.501P
F2       -.499P
HZ/CM 142.918
PPM/CM    .476
SR    3366.97
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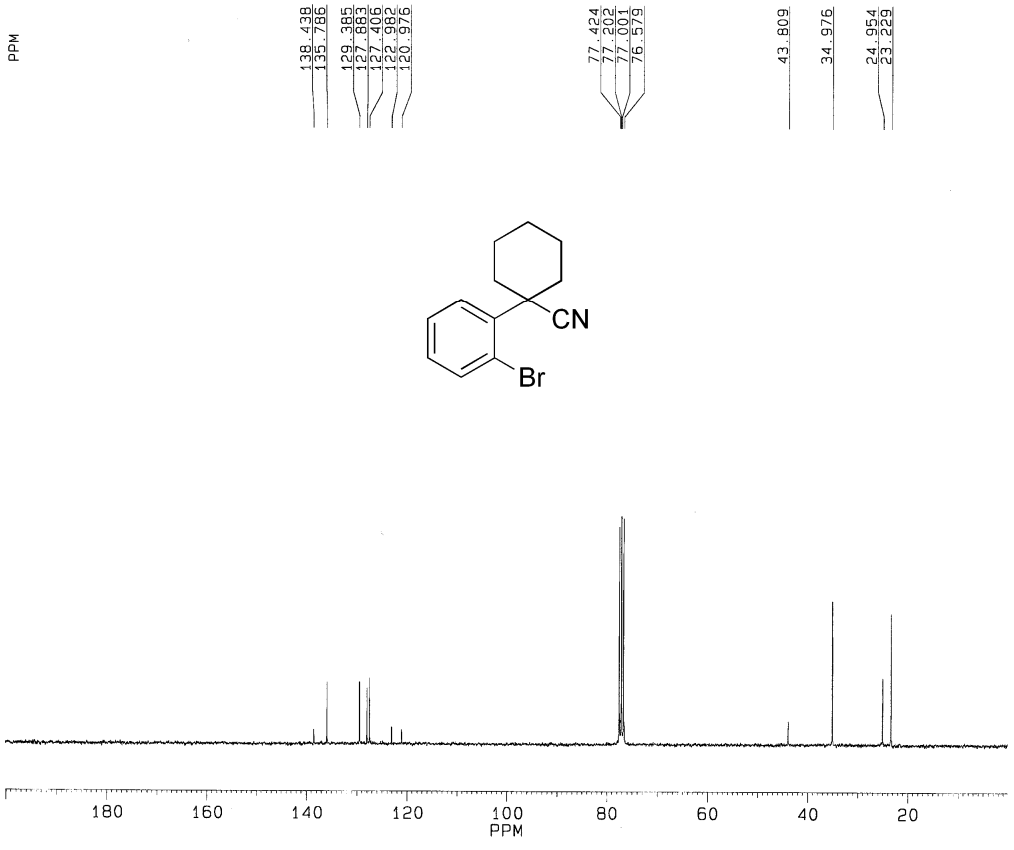


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D0721.904
DATE ??-??-??

SF      75.469
SY   75.0
O1    6517.695
SI   32768
TD   32768
SW   19230.769
HZ/PT    1.174

PW       1.4
RD       1.500
AQ        .852
RG     200
NS    2641
TE.    297

FW   24100
O2    4869.082
DP   15H CPD

LB       2.000
GB       0.0
CX      21.00
CY       0.0
F1     200.008P
F2        .013P
HZ/CM 718.728
PPM/CM   9.524
SR   -1404.97
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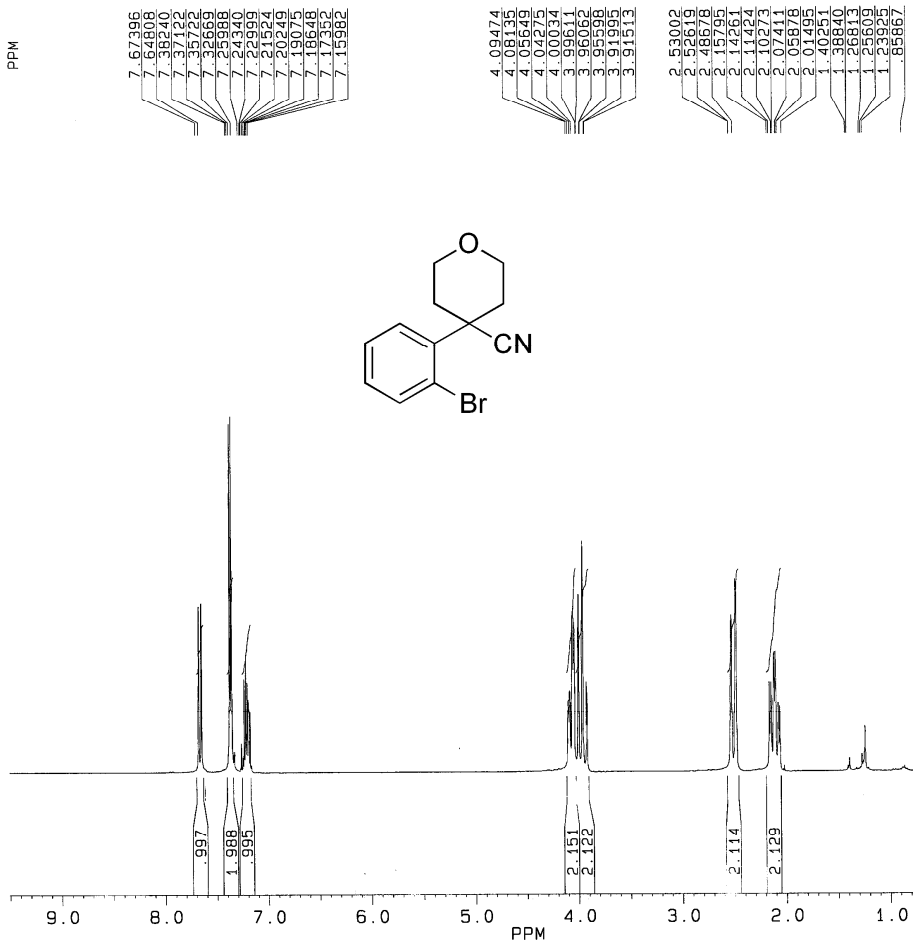
4-(2-Bromophenyl)tetrahydro-2*H*-pyran-4-carbonitrile (1s)



BRUKER

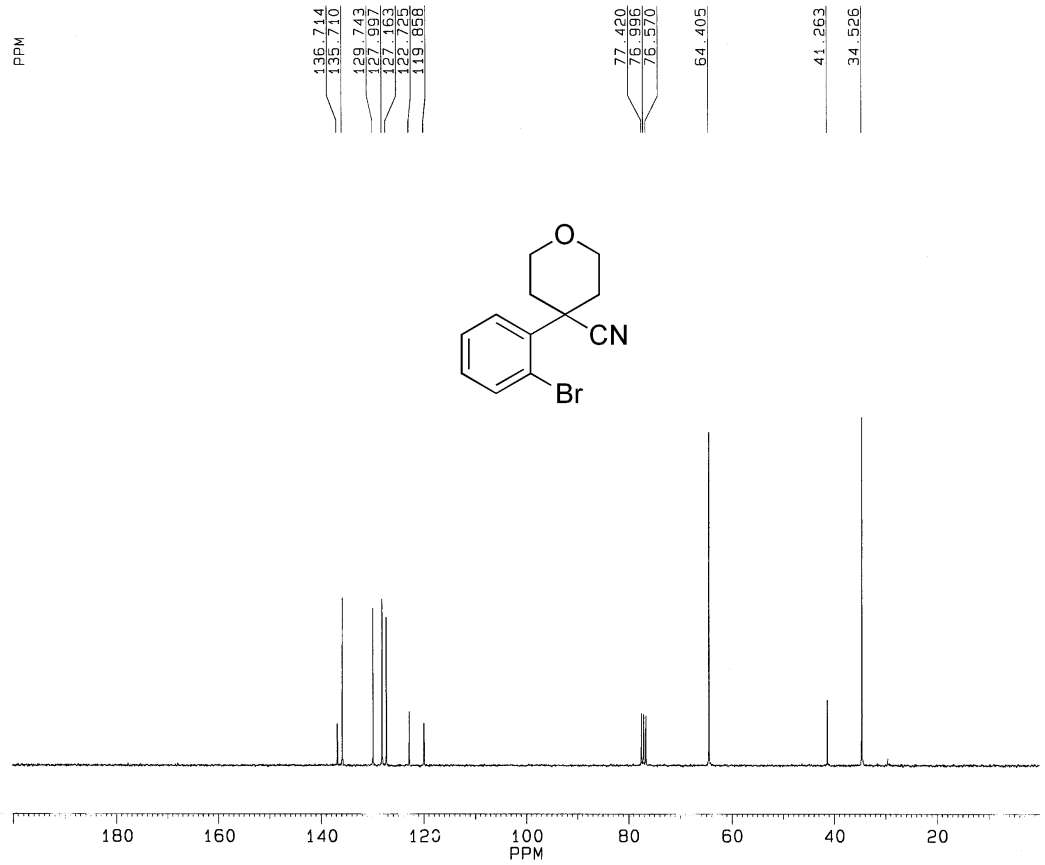
D1201.005
DATE ??-??-??

SF 300.133
SY 299.0
O1 5018.332
SI 16384
TD 16384
SW 4807.692
HZ/PT .587

PW 1.4
RD 1.000
AQ 1.704
RG 16
NS 32
TE 297

FW 6100
O2 0.0
DP 63L PO

LB 0.0
GB 0.0
CX 21.00
CY 0.0
F1 9.501P
F2 -.499P
HZ/CM 142.918
PPM/CM .476
SR 3367.55



BRUKER

D1201.902
DATE ??-??-??

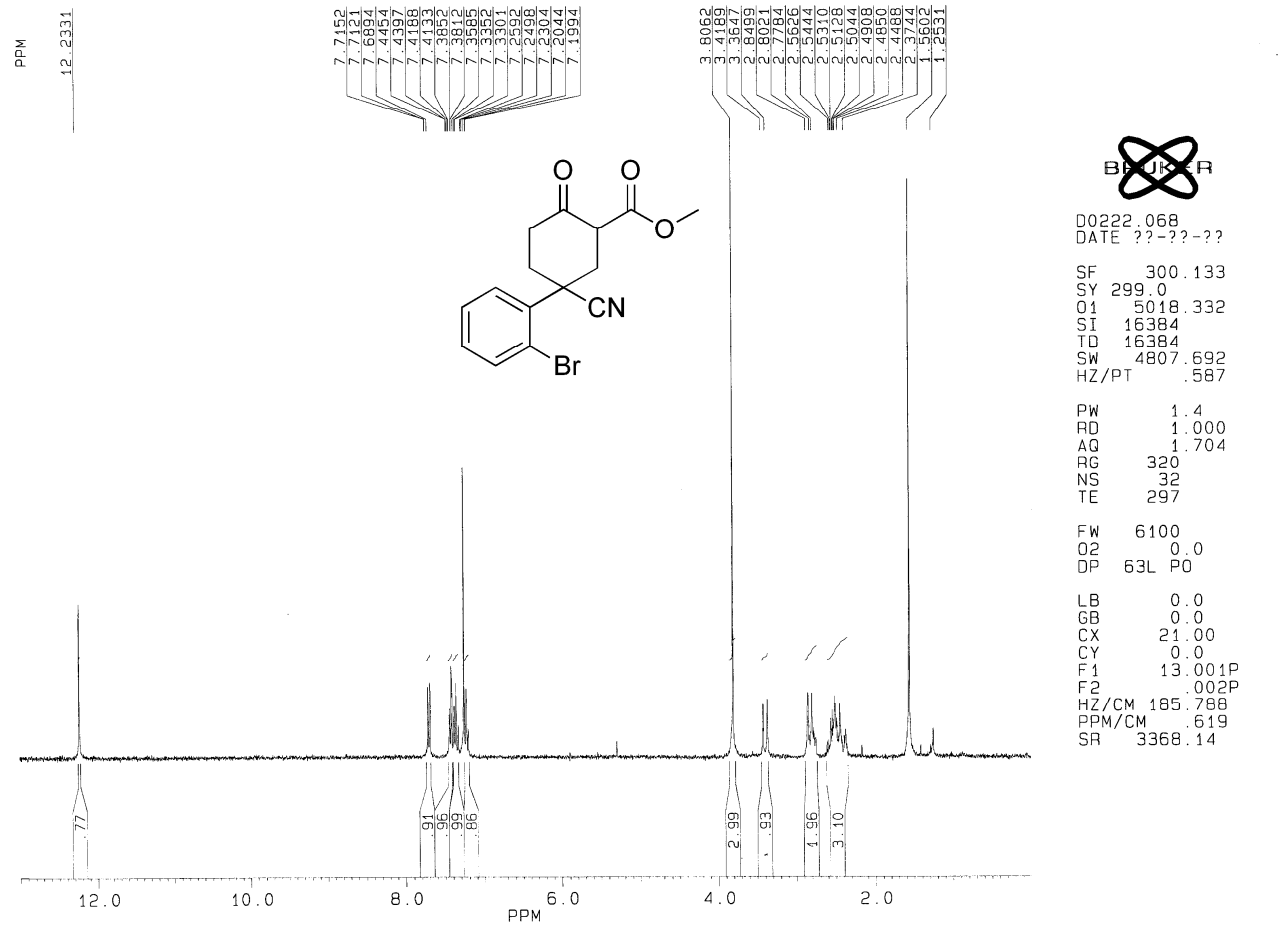
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

PW 1.4
RD 1.500
AQ .852
RG 160
NS 410
TE 297

FW 24100
O2 4869.082
DP 15H CPD

LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 200.008P
F2 .013P
HZ/CM 718.728
PPM/CM 9.524
SR -393.23

Methyl 5-(2-bromophenyl)-5-cyano-2-oxocyclohexanecarboxylate (4t)

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D0222.068
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI   16384
TD   16384
SW    4807.692
HZ/PT     .587

PW       1.4
RD       1.000
AQ       1.704
RG     320
NS      32
TE     297

FW    6100
O2       0.0
DP   63L PO

LB       0.0
GB       0.0
CX      21.00
CY       0.0
F1      13.001P
F2        .002P
HZ/CM 185.788
PPM/CM    .619
SR    3368.14
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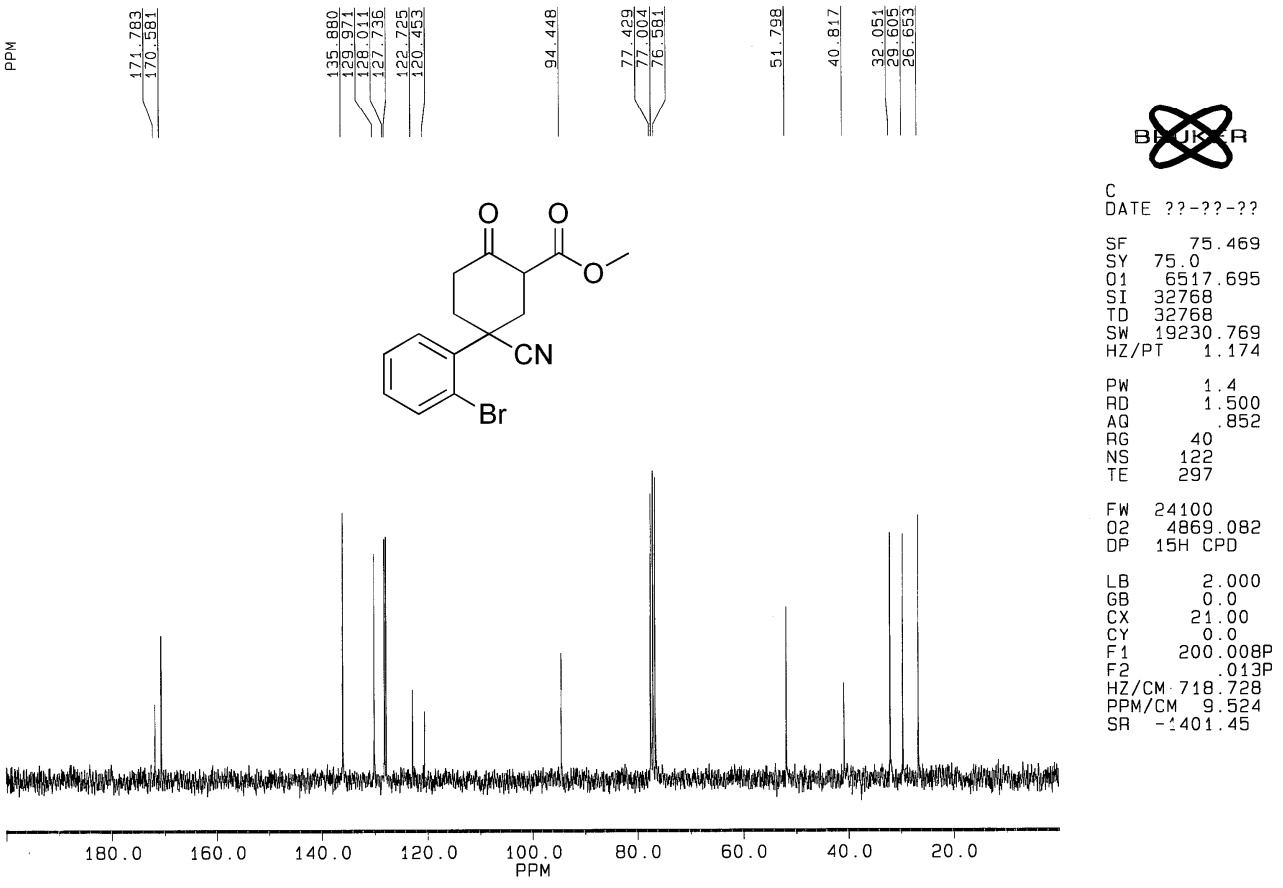


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C
DATE ??-??-??

SF      75.469
SY   75.0
O1    6517.695
SI   32768
TD   32768
SW   19230.769
HZ/PT    1.174

PW       1.4
RD       1.500
AQ        .852
RG      40
NS     122
TE     297

FW   24100
O2    4869.082
DP   15H CPD

LB       2.000
GB       0.0
CX      21.00
CY       0.0
F1     200.008P
F2        .013P
HZ/CM 718.728
PPM/CM  9.524
SR   -1401.45
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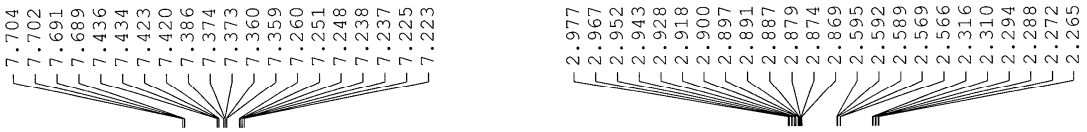
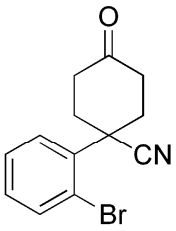
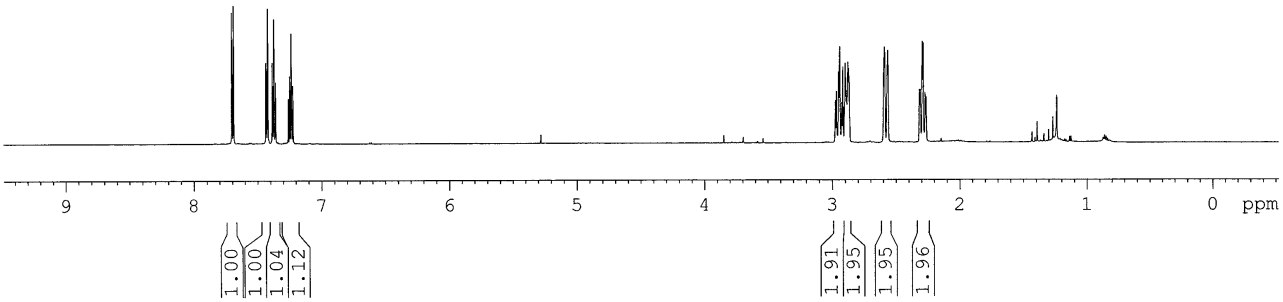
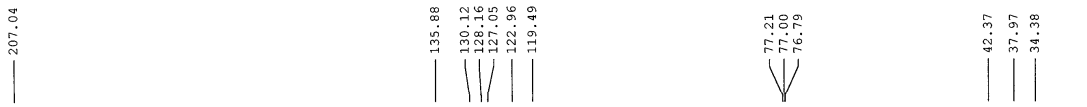
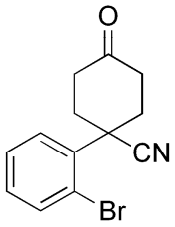
1-(2-Bromophenyl)-4-oxocyclohexanecarbonitrile (5t)

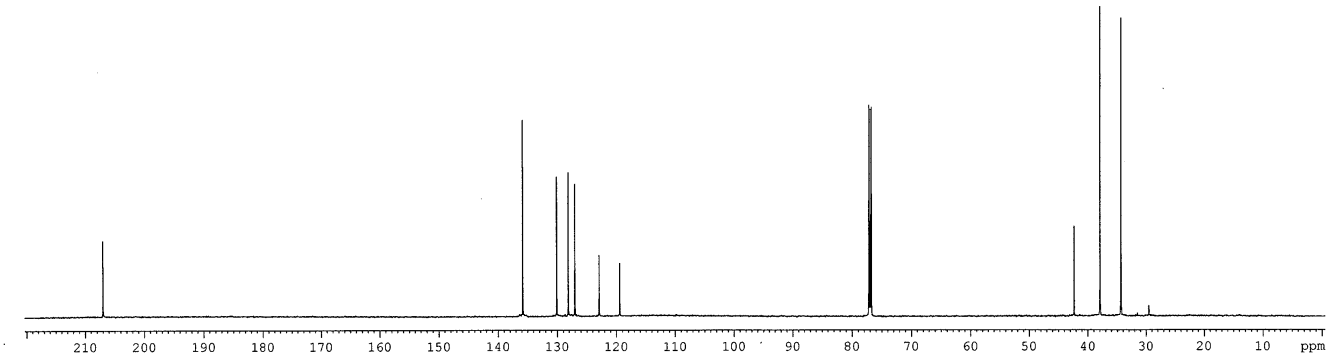




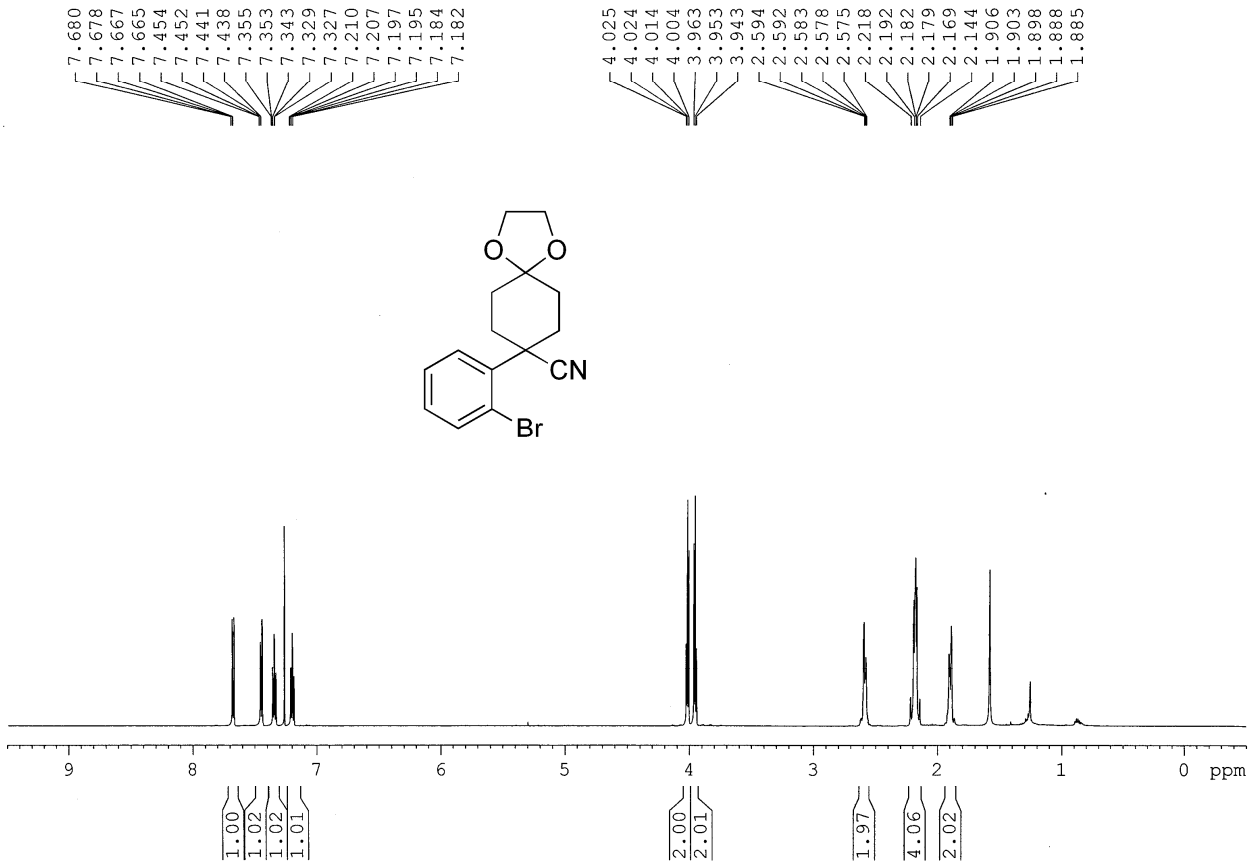


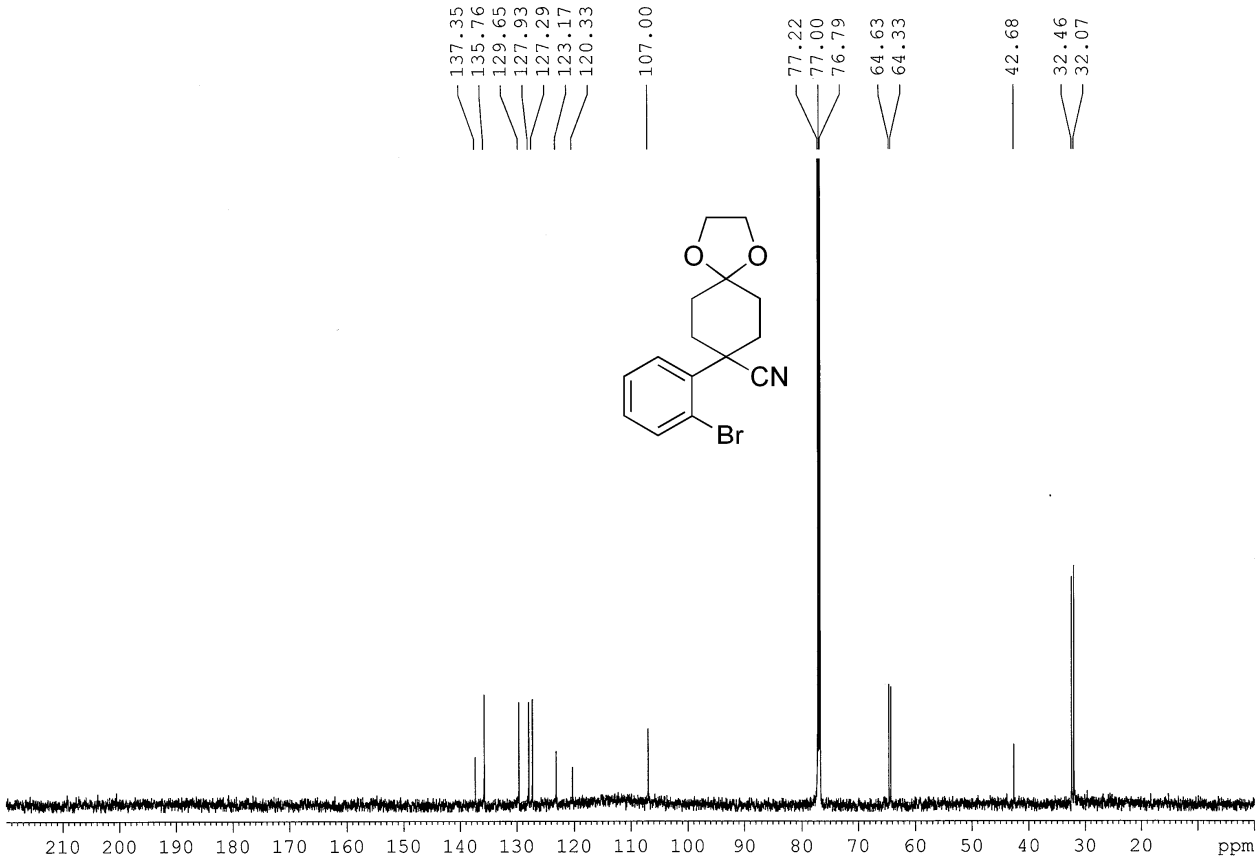




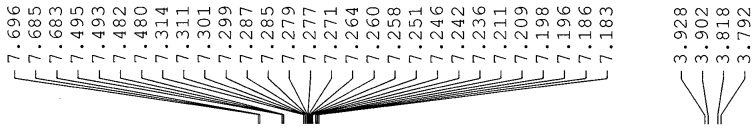


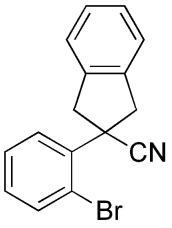
8-(2-Bromophenyl)-1,4-dioxaspiro[4.5]decane-8-carbonitrile (1t)

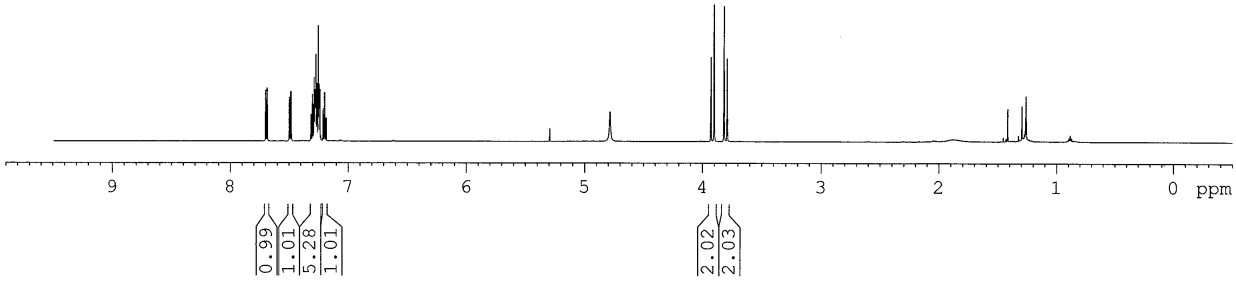


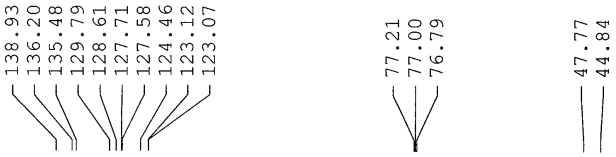


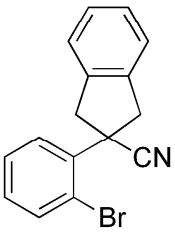
2-(2-Bromophenyl)-2,3-dihydro-1*H*-indene-2-carbonitrile (1u)

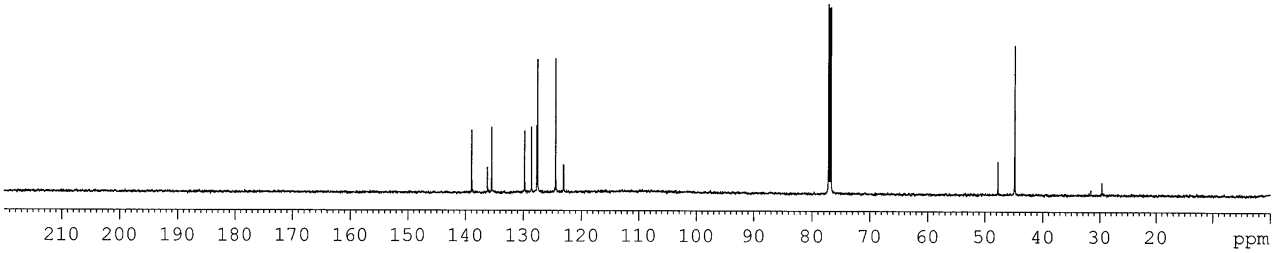




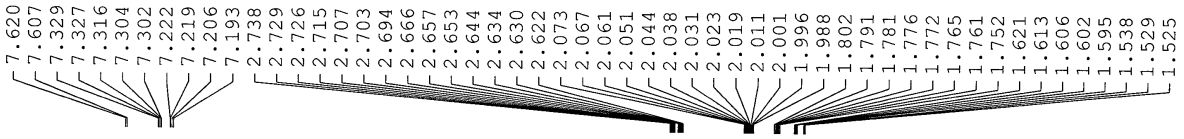


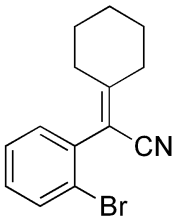


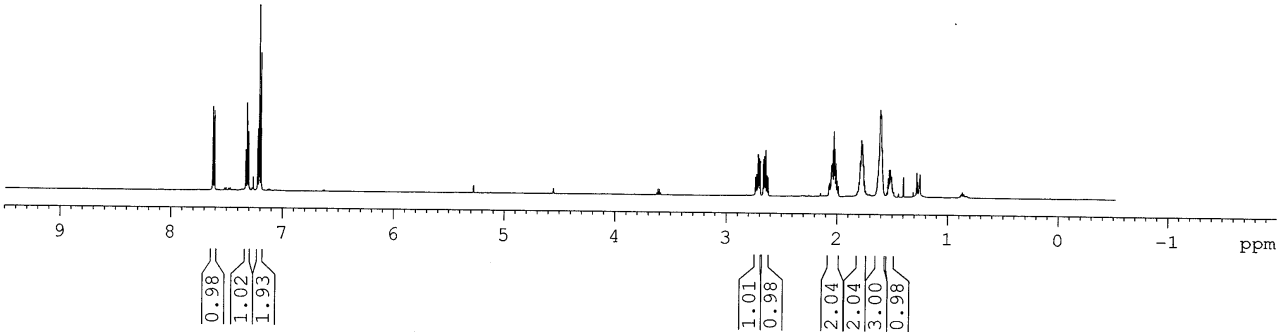


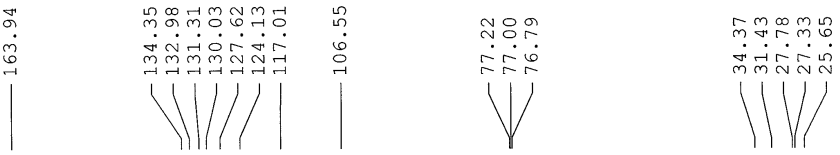


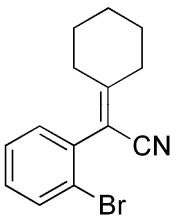
2-(2-Bromophenyl)-2-cyclohexylideneacetonitrile (1v)

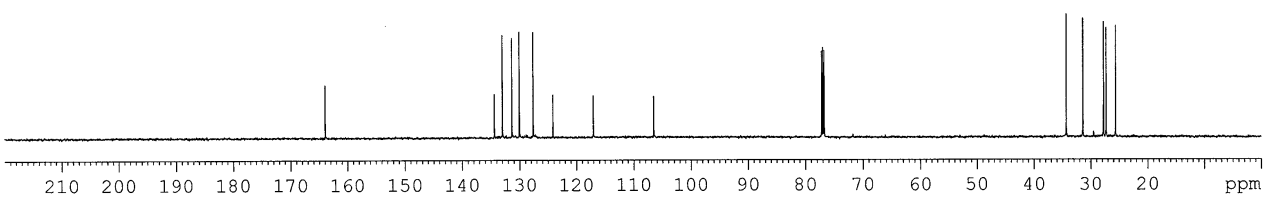




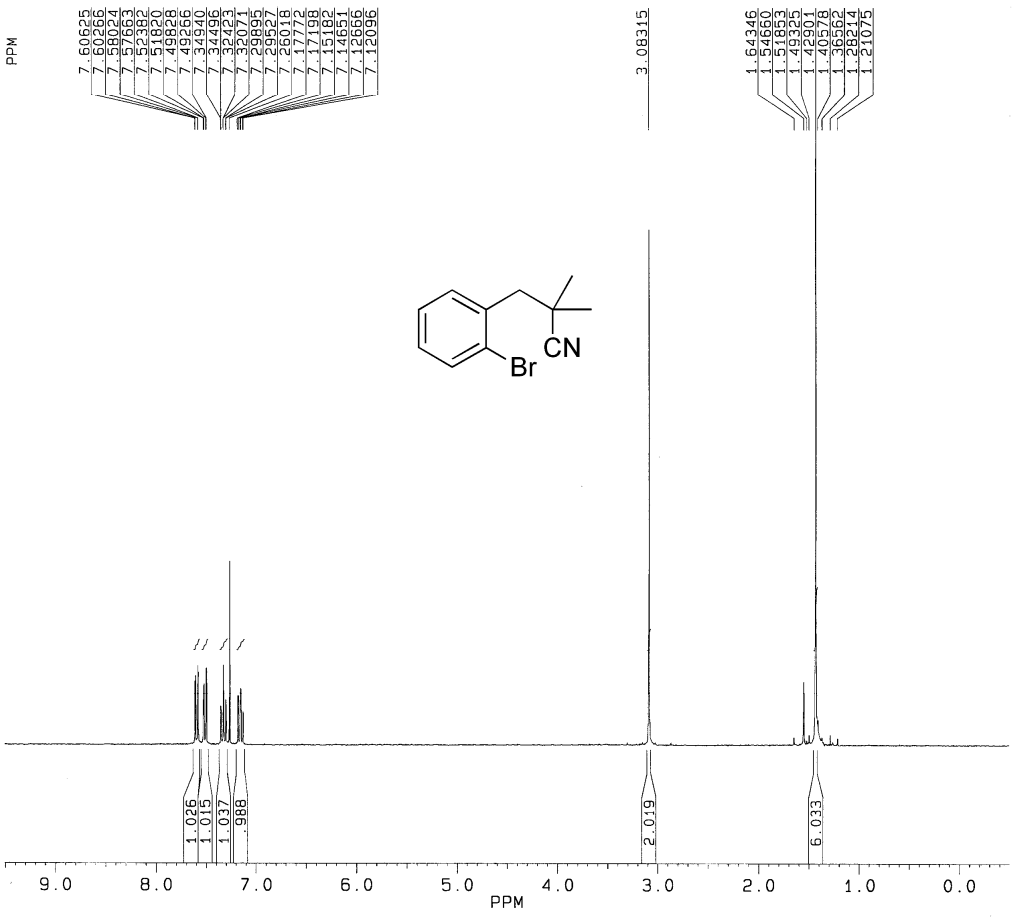








3-(2-Bromophenyl)-2,2-dimethylpropanenitrile (1w)

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D1020.009
DATE ??-??-??

SF     300.133
SY 299.0
O1    5018.332
SI   16384
TD   16384
SW    4807.692
HZ/PT     .587

PW       1.4
RD       1.000
AQ       1.704
RG     160
NS      32
TE     297

FW    6100
O2       0.0
DP   63L PO

LB       0.0
GB       0.0
CX      21.00
CY       0.0
F1       9.501P
F2       -.499P
HZ/CM 142.918
PPM/CM    .476
SR    3367.55
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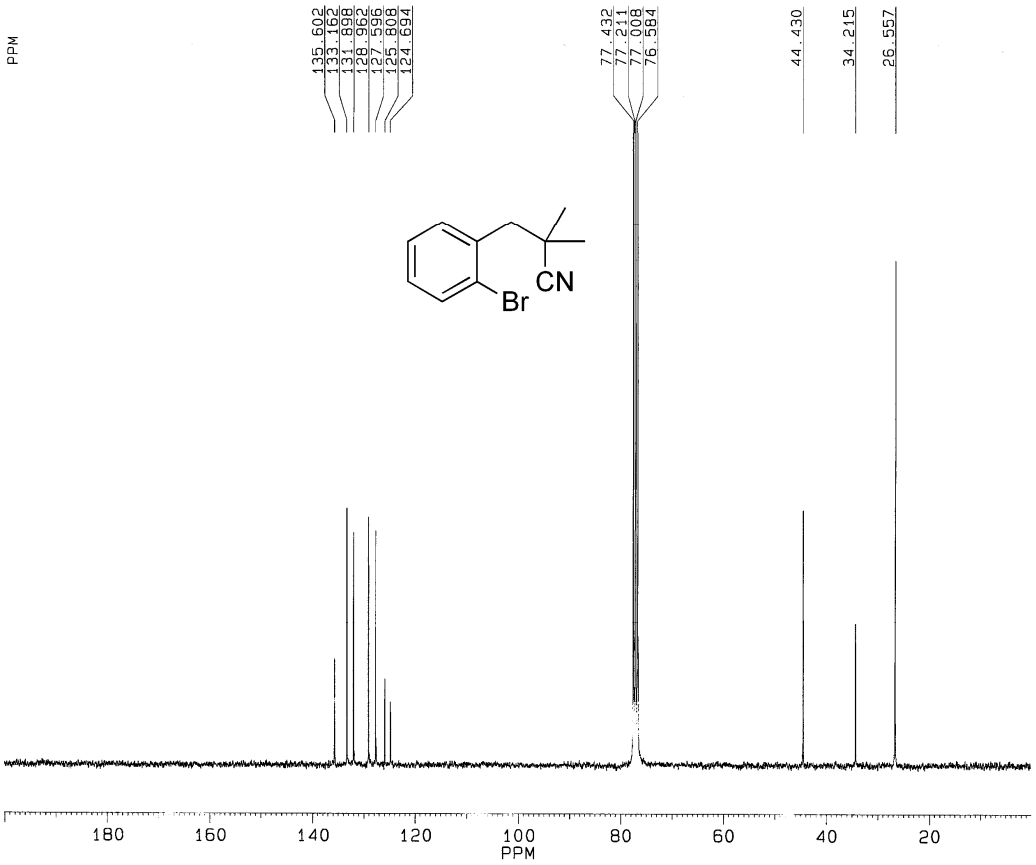


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D1021.901
DATE ??-??-??

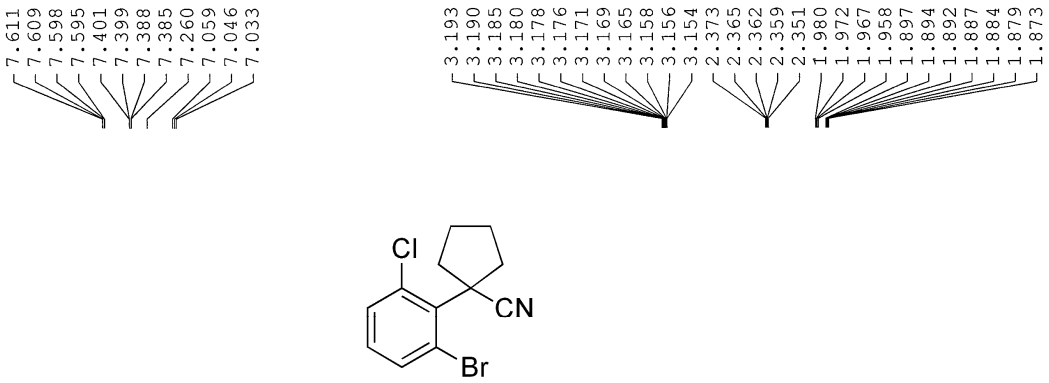
SF      75.469
SY   75.0
O1    6517.695
SI   32768
TD   32768
SW   19230.769
HZ/PT    1.174

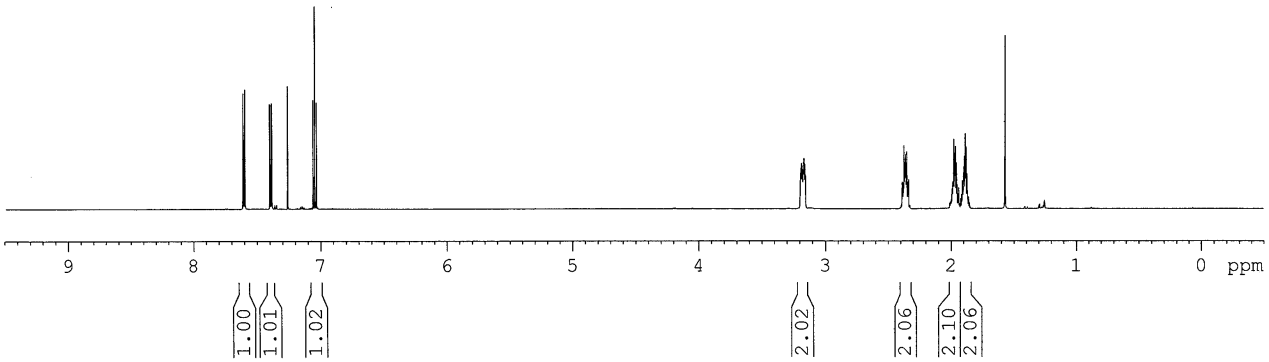
PW       1.4
RD       1.500
AQ        .852
RG     200
NS    8197
TE     297

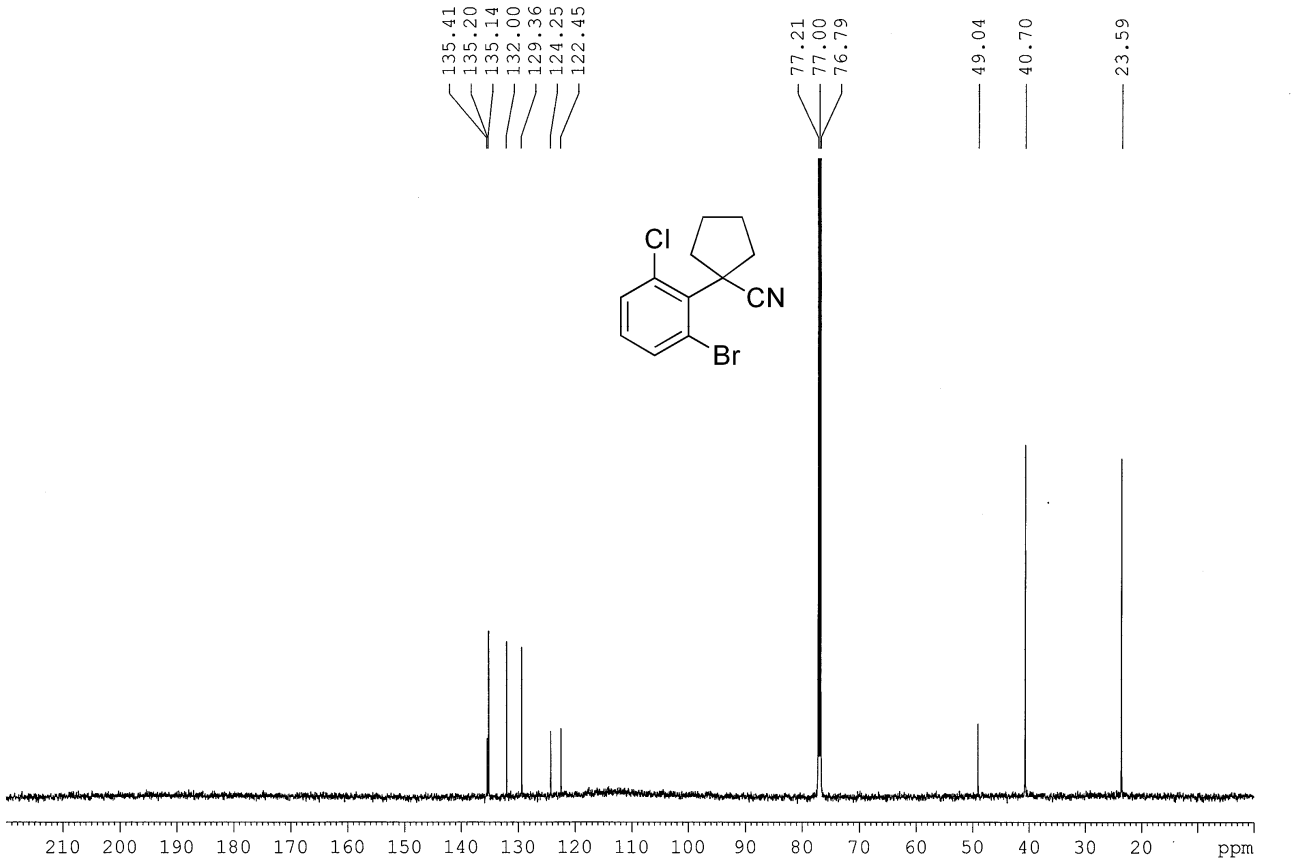
FW   24100
O2    4869.082
DP   15H CPD

LB       2.000
GB       0.0
CX      21.00
CY       0.0
F1     200.008P
F2        .013P
HZ/CM 718.728
PPM/CM   9.524
SR   -1404.97
```

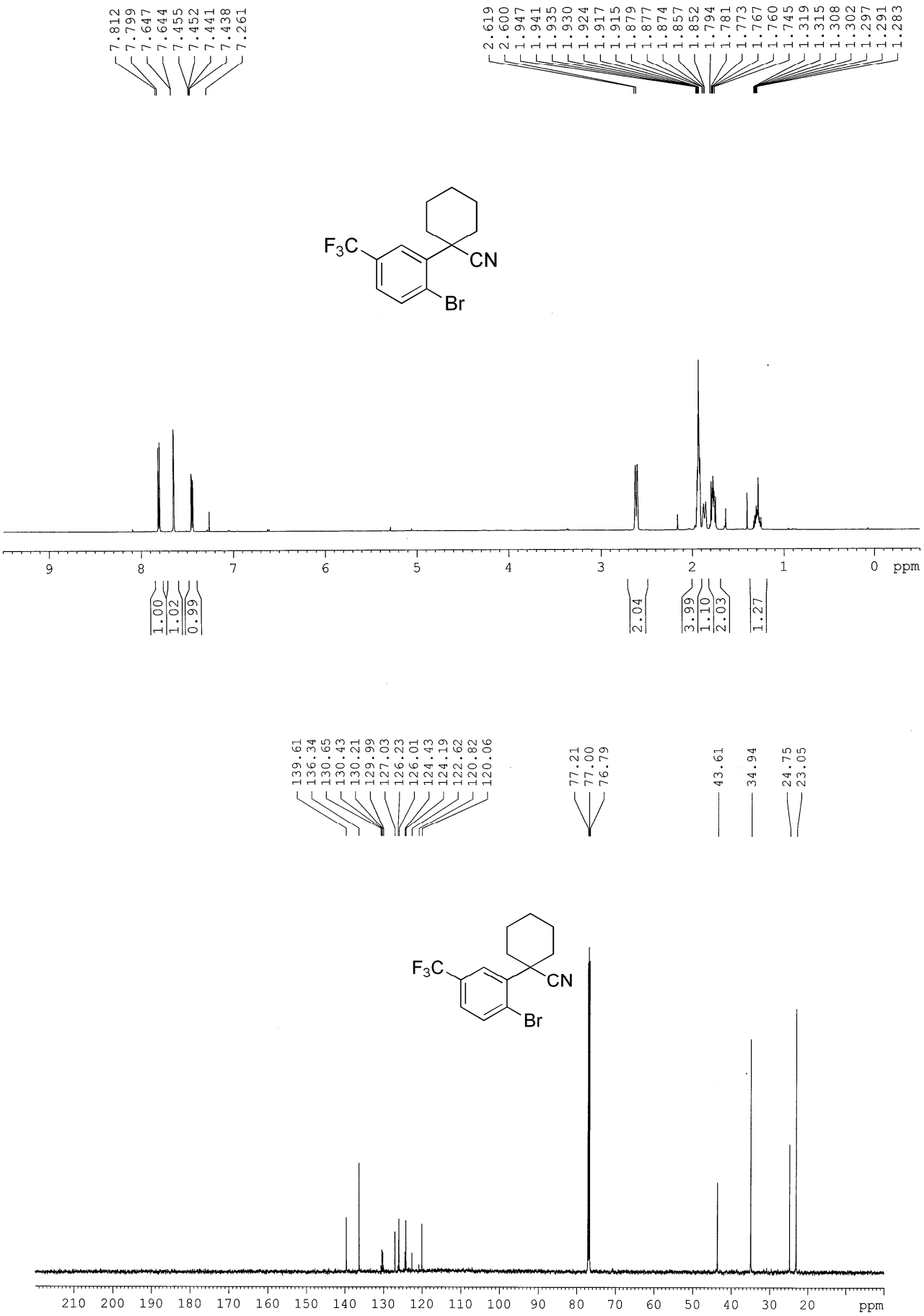
1-(2-Bromo-6-chlorophenyl)cyclopentanecarbonitrile (1A)



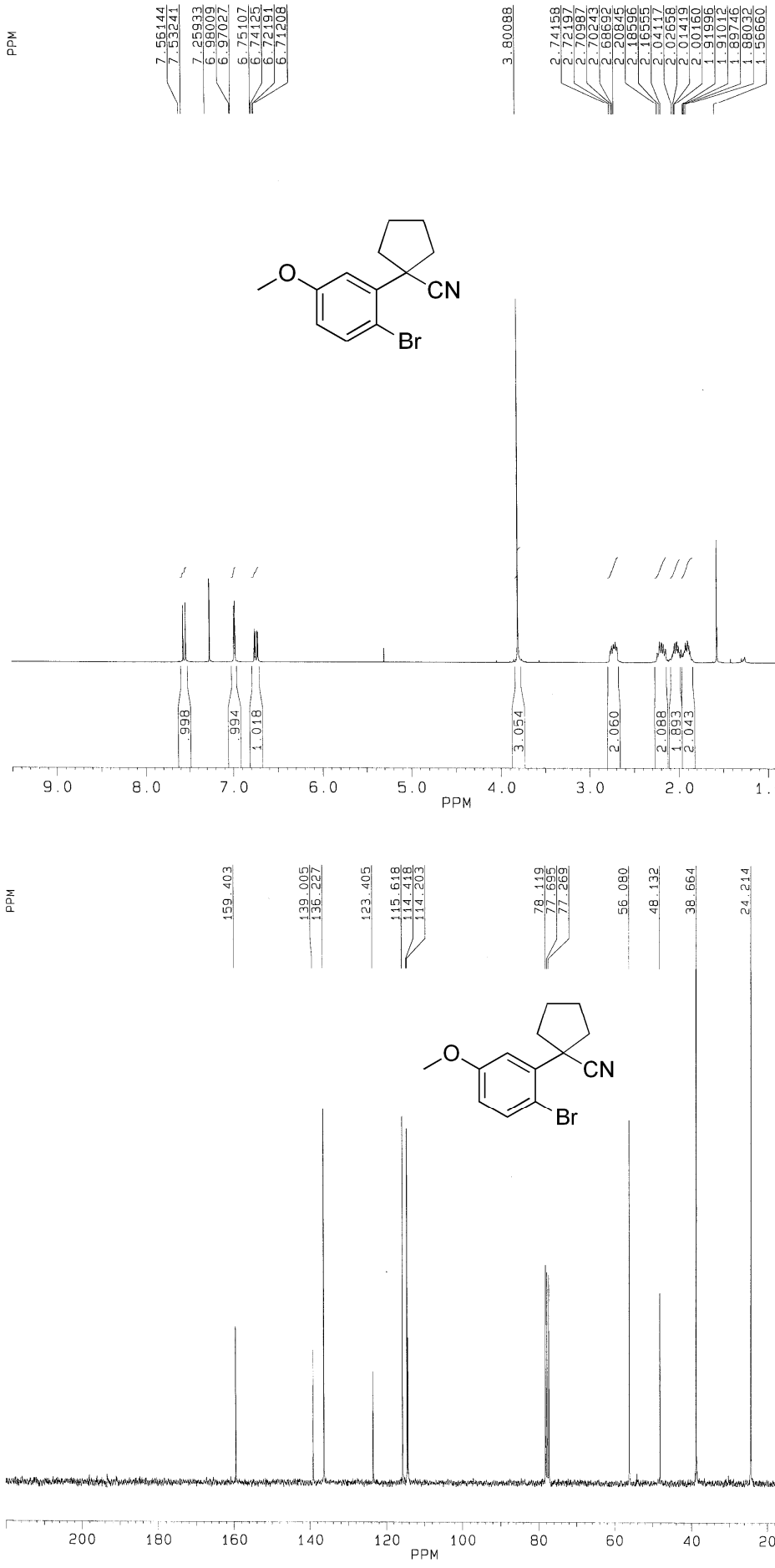




1-(2-Bromo-5-(trifluoromethyl)phenyl)cyclohexanecarbonitrile (1B)



1-(2-Bromo-5-methoxyphenyl)cyclopentanecarbonitrile (1C)



BRUKER

D0229.904
DATE ??-??-??

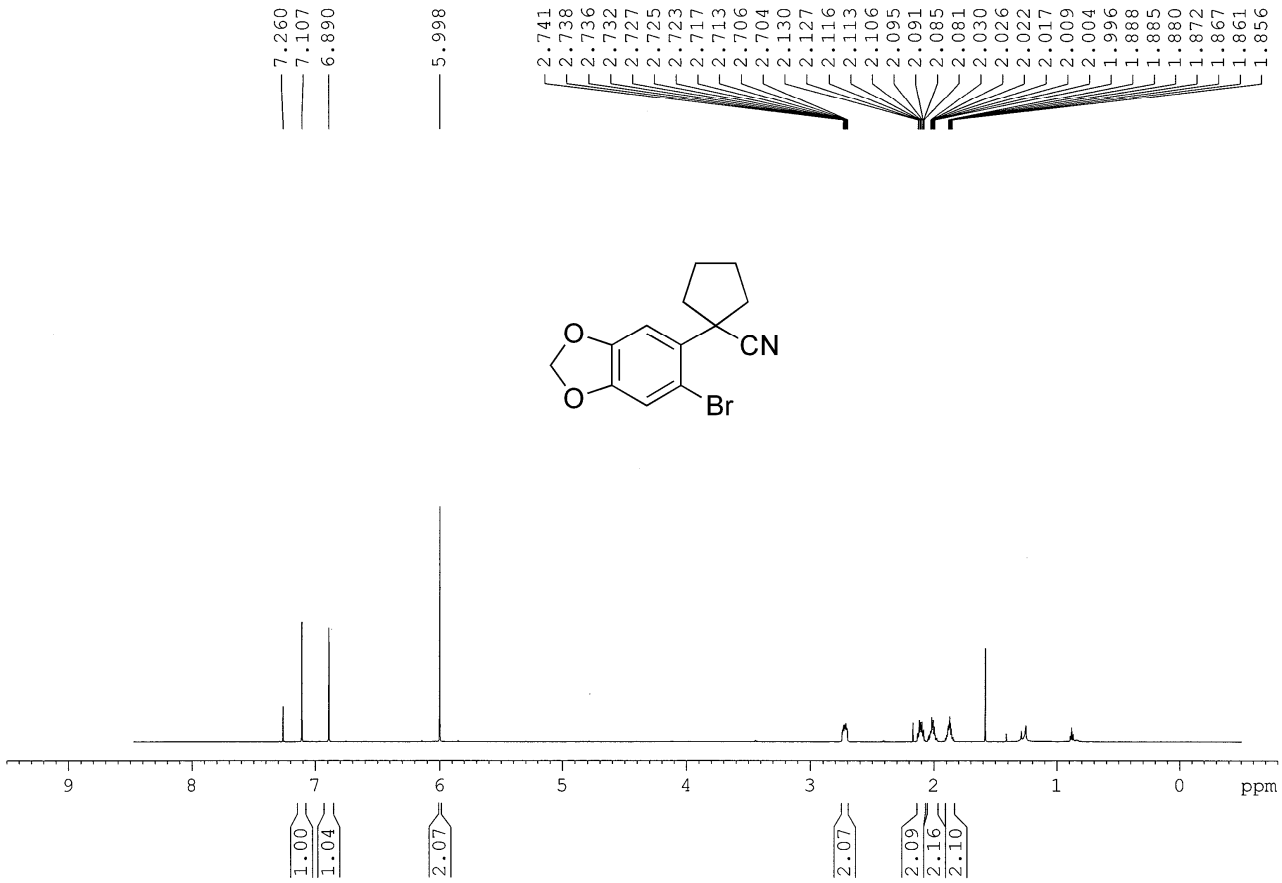
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

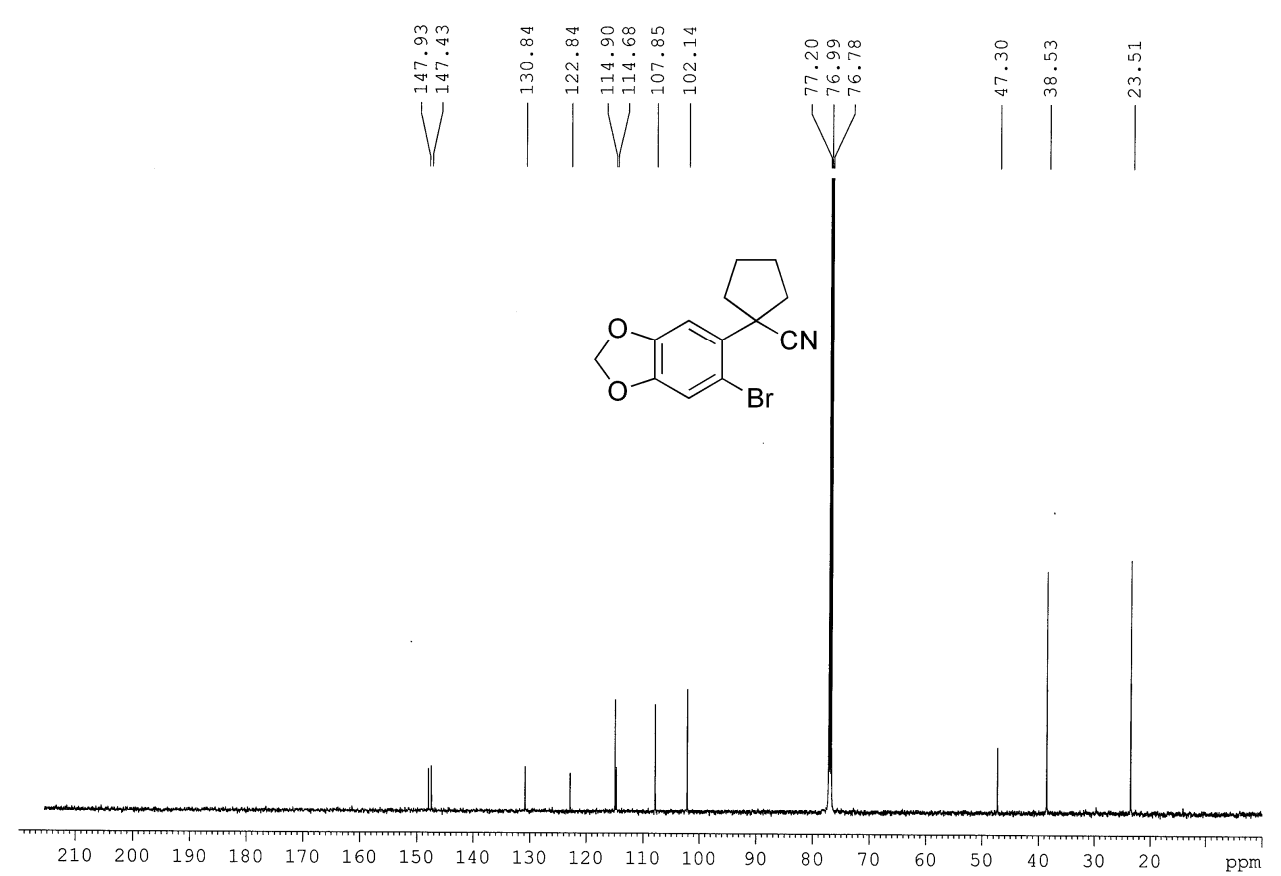
PW 1.4
RD 1.500
AQ .852
RG 200
NS 207
TE 297

FW 24100
O2 4869.082
DP 15H CPD

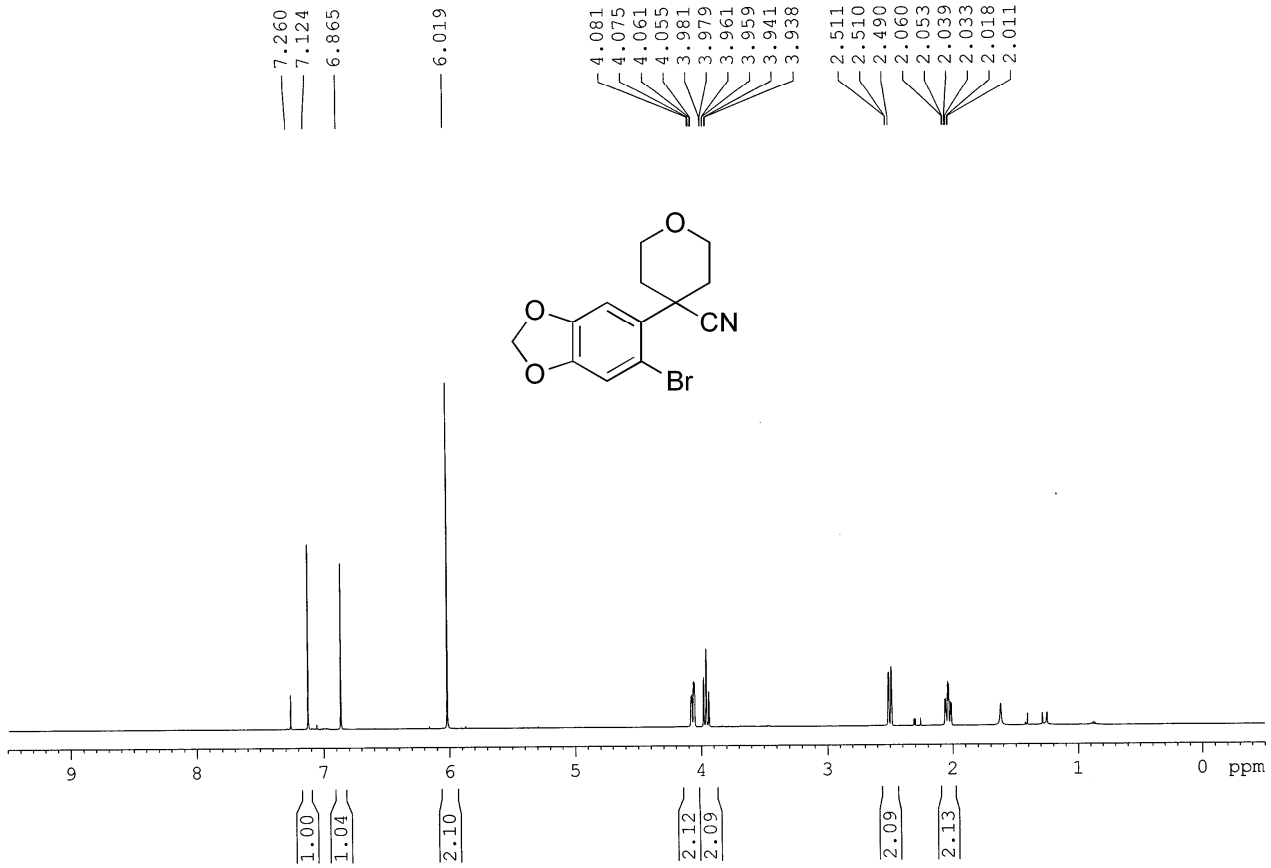
LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 220.009P
F2 .013P
HZ/CM 790.606
PPM/CM 10.476
SR -1443.71

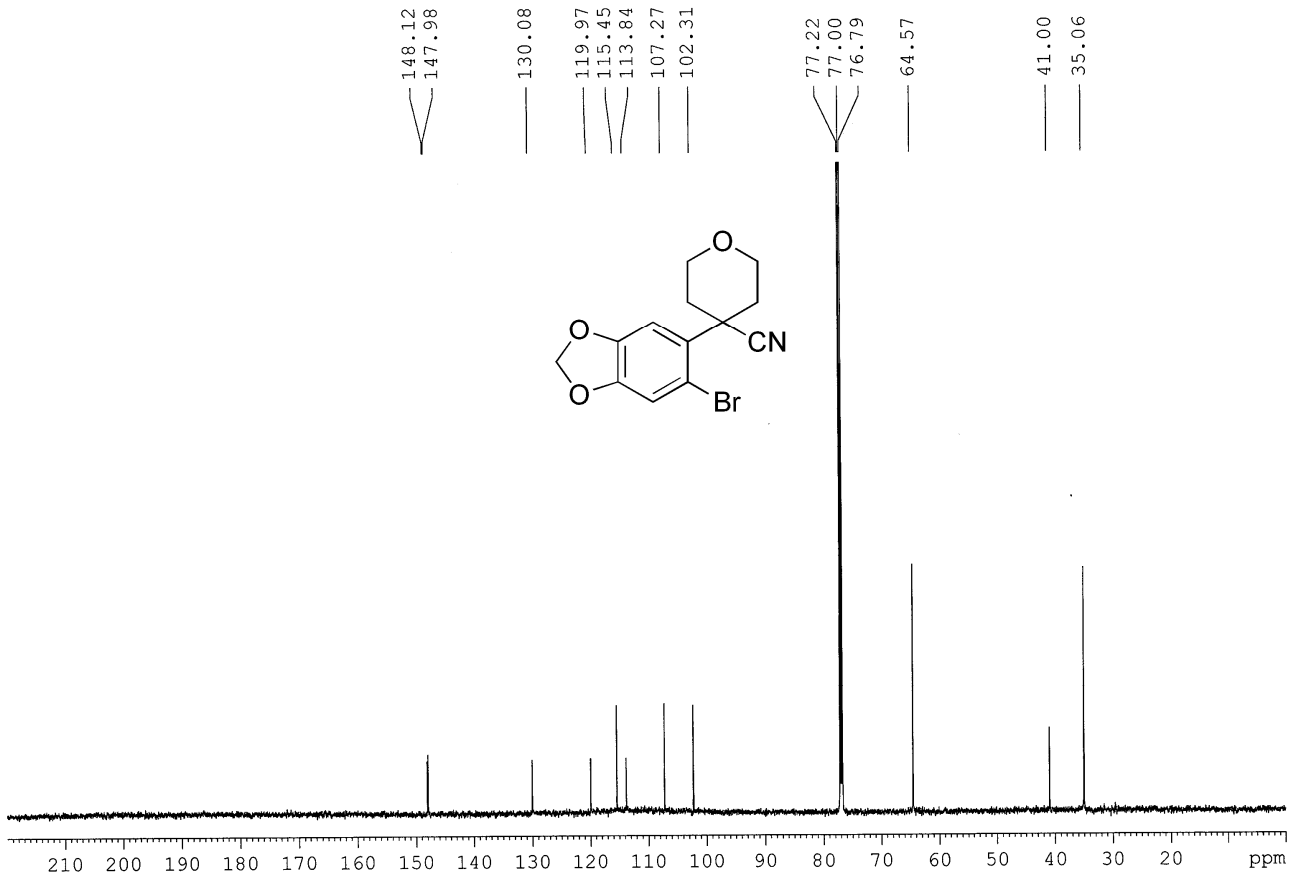
1-(6-Bromobenzo[*d*][1,3]dioxol-5-yl)cyclopentanecarbonitrile (1D)





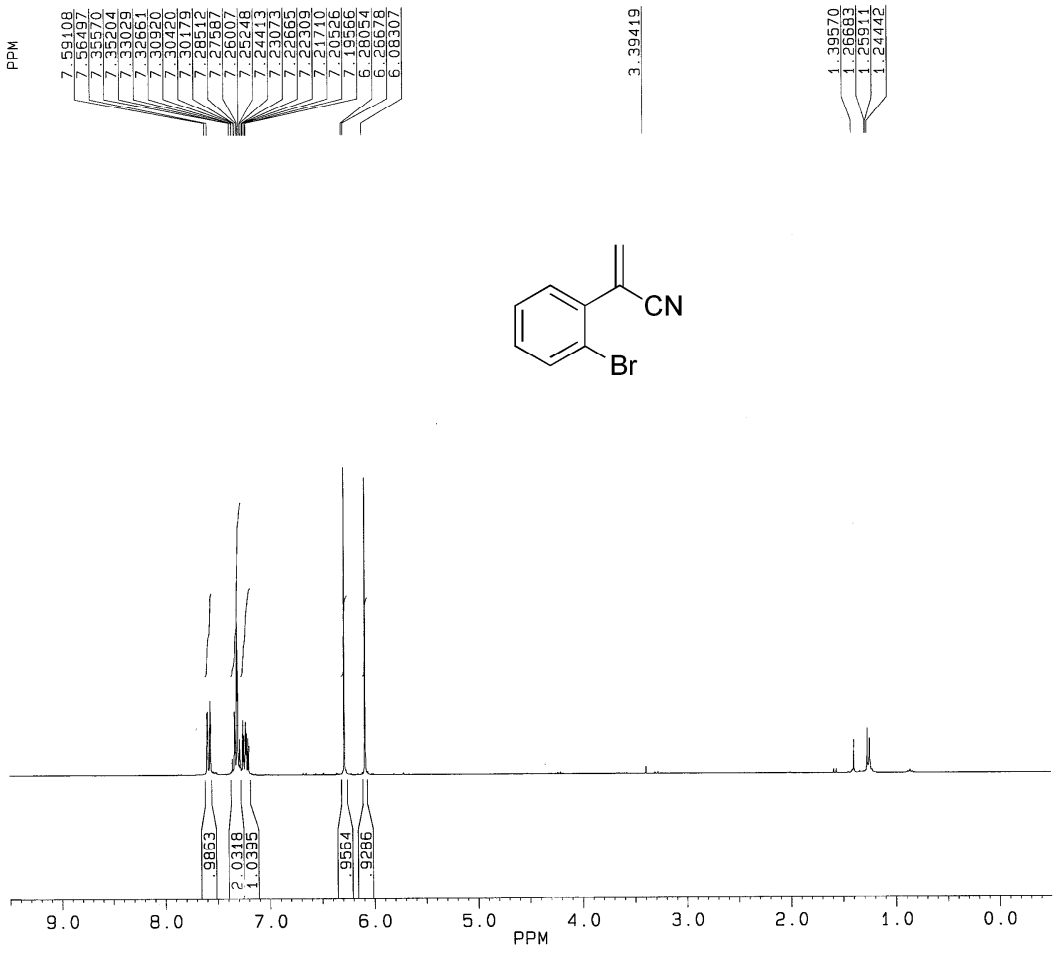
4-(6-Bromobenzo[*d*][1,3]dioxol-5-yl)tetrahydro-2*H*-pyran-4-carbonitrile (1E)





2-(2-Bromophenyl)-2-methylpropanamide (3a)

2-(2-Bromophenyl)acrylonitrile (5x)



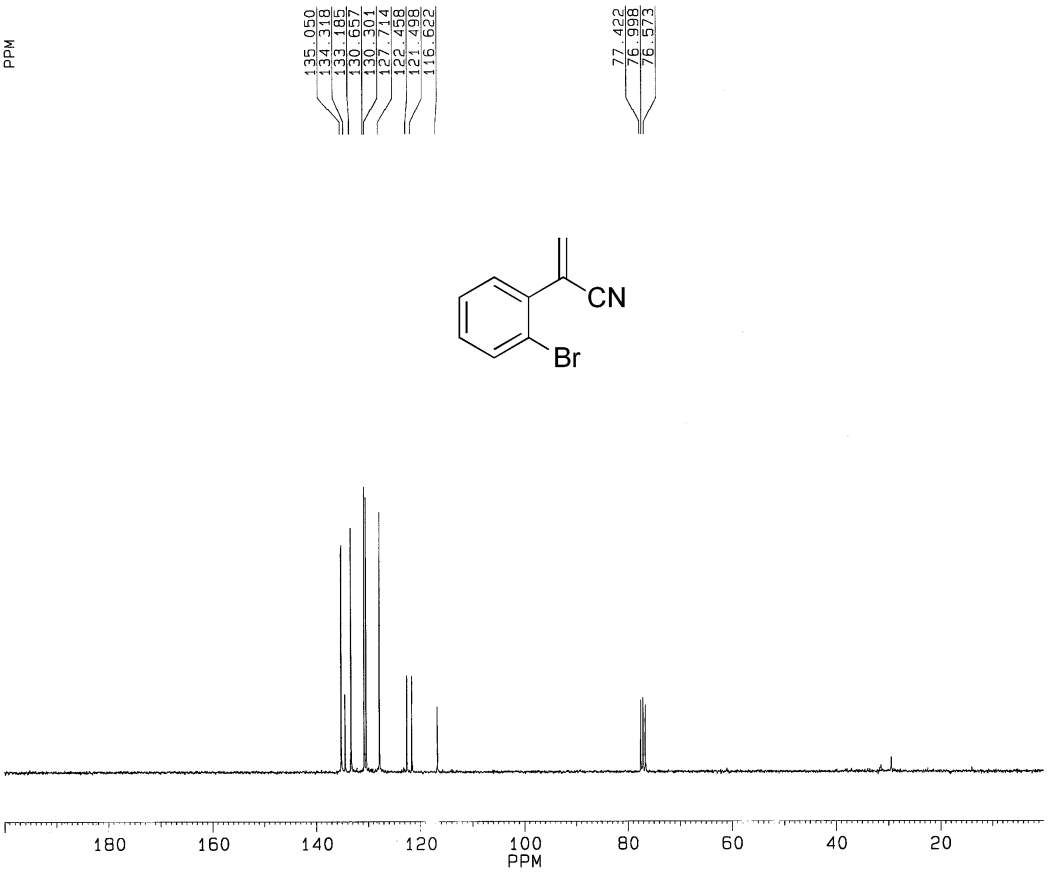
D1222.008
DATE ??-??-??

SF 300.133
SY 299.0
O1 5018.332
SI 16384
TD 16384
SW 4807.692
HZ/PT .587

PW 1.4
RD 1.000
AQ 1.704
RG 10
NS 16
TE 297

FW 6100
O2 0.0
DP 63L PO

LB 0.0
GB 0.0
CX 21.00
CY 0.0
F1 9.501P
F2 -.499P
HZ/CM 142.918
PPM/CM .476
SR 3367.55



D1221.908
DATE ??-??-??

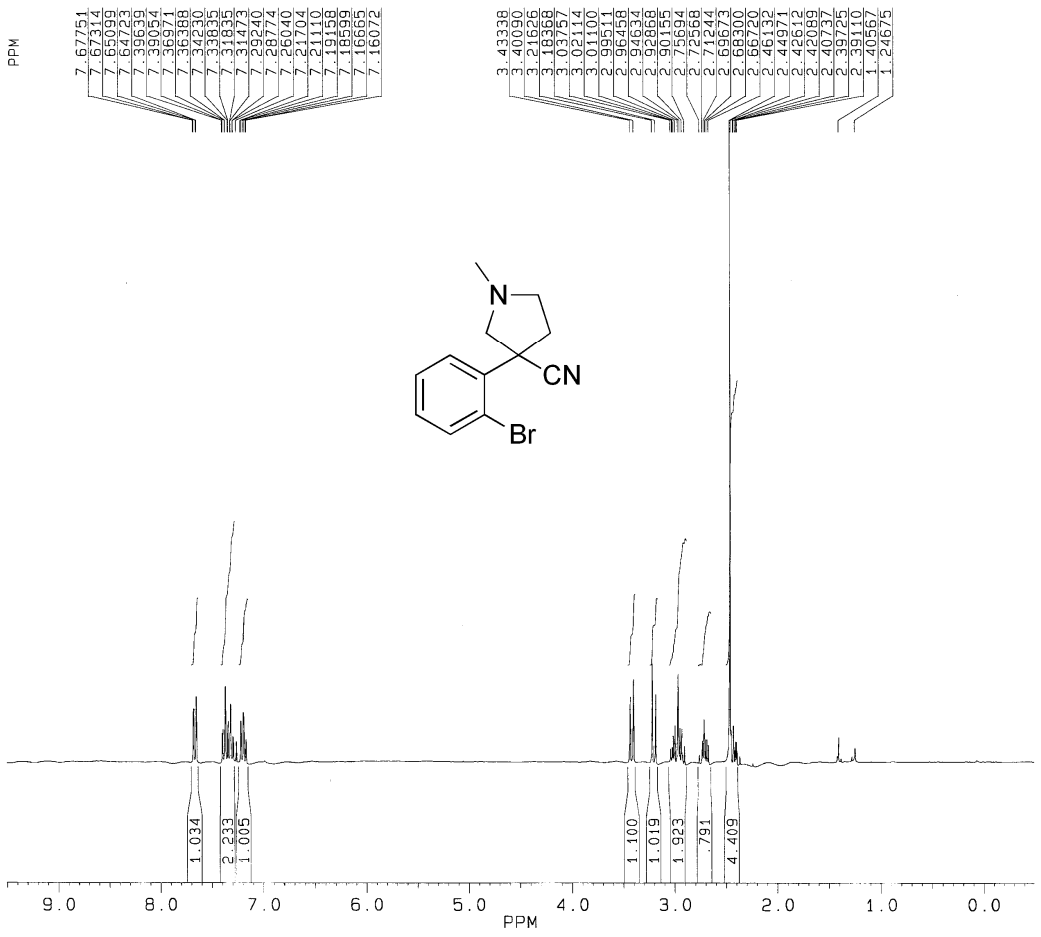
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

PW 1.4
RD 1.500
AQ .852
RG 160
NS 160
TE 297

FW 24100
O2 4869.082
DP 15H CPD

LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 200.008P
F2 .013P
HZ/CM 718.728
PPM/CM 9.524
SR -1379.75

3-(2-Bromophenyl)-1-methylpyrrolidine-3-carbonitrile (1x)



BRUKER

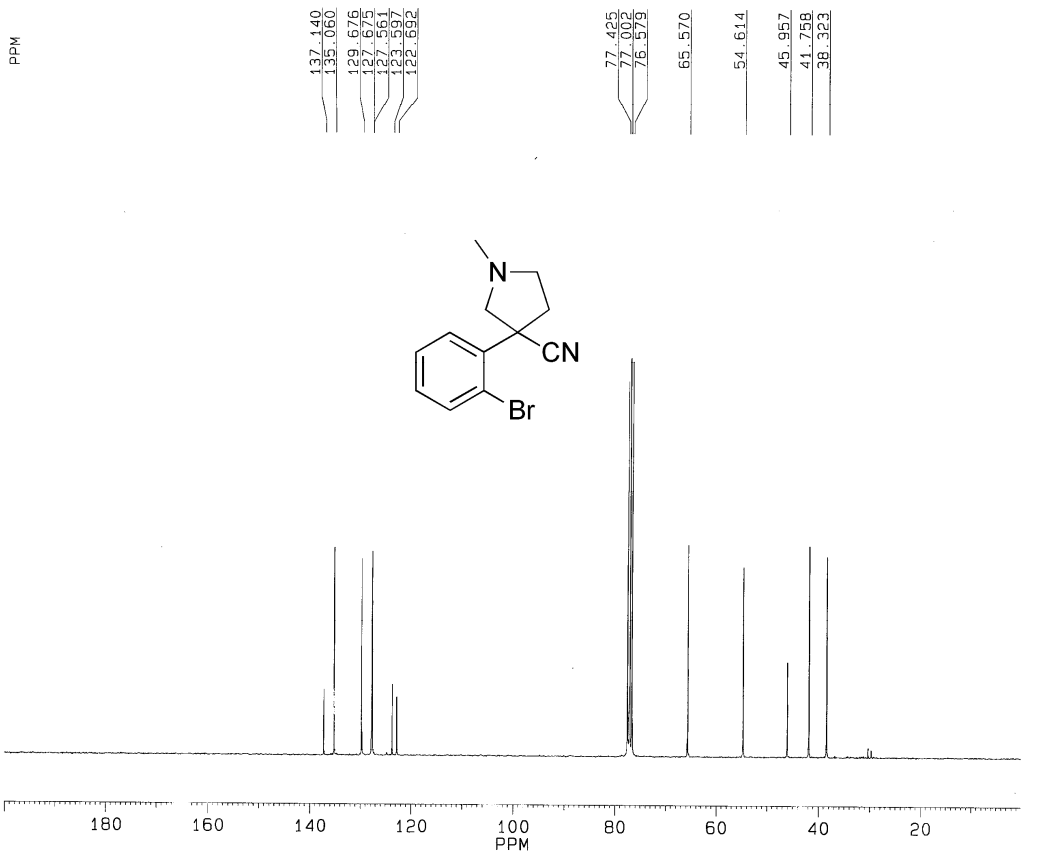
D1004.020
DATE ??-??-??

SF 300.133
SY 299.0
O1 5018.332
SI 16384
TD 16384
SW 4807.692
HZ/PT .587

PW 1.4
RD 1.000
AQ 1.704
RG 160
NS 32
TE 297

FW 6100
O2 0.0
DP 63L PO

LB 0.0
GB 0.0
CX 21.00
CY 0.0
F1 9.501P
F2 -.499P
HZ/CM 142.918
PPM/CM .476
SR 3367.55



BRUKER

D1004.901
DATE ??-??-??

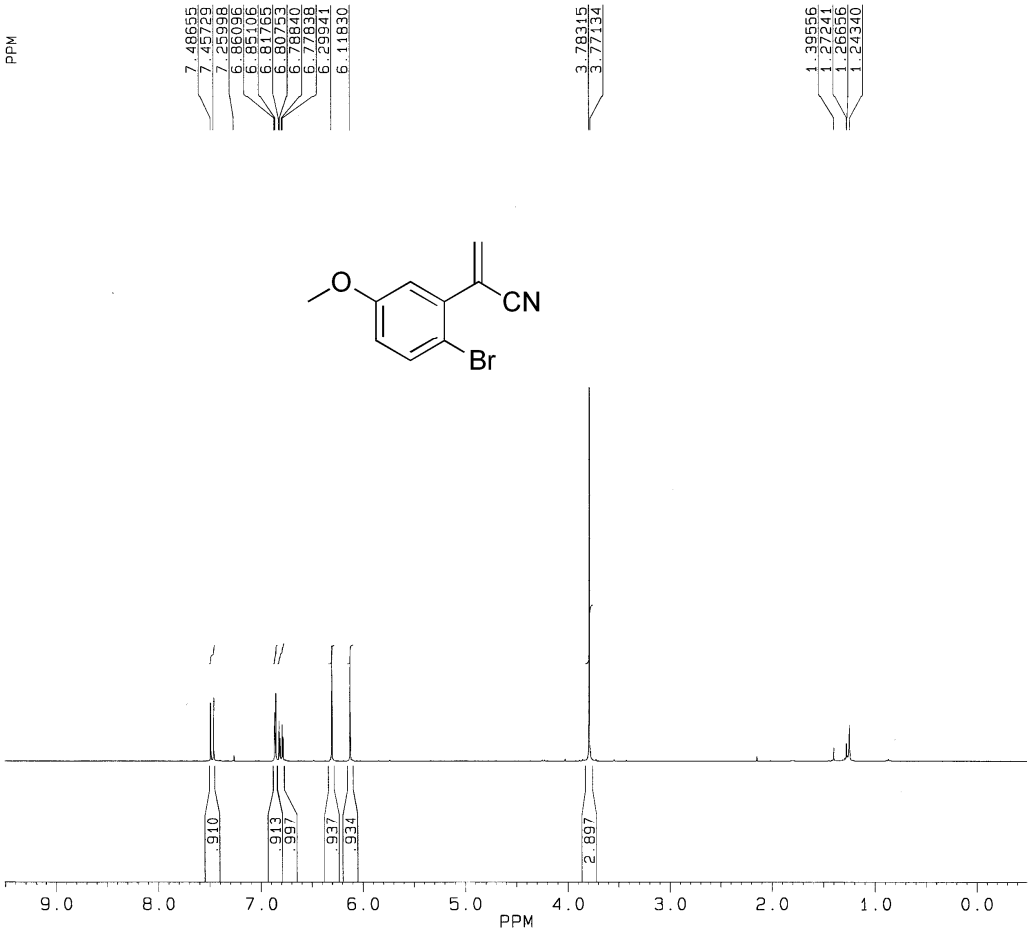
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

PW 1.4
RD 1.500
AQ .852
RG 200
NS 20326
TE 297

FW 24100
O2 4869.082
DP 15H CPD

LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 200.008P
F2 .013P
HZ/CM 718.728
PPM/CM 9.524
SR -1401.45

2-(2-Bromo-5-methoxyphenyl)acrylonitrile (5F)



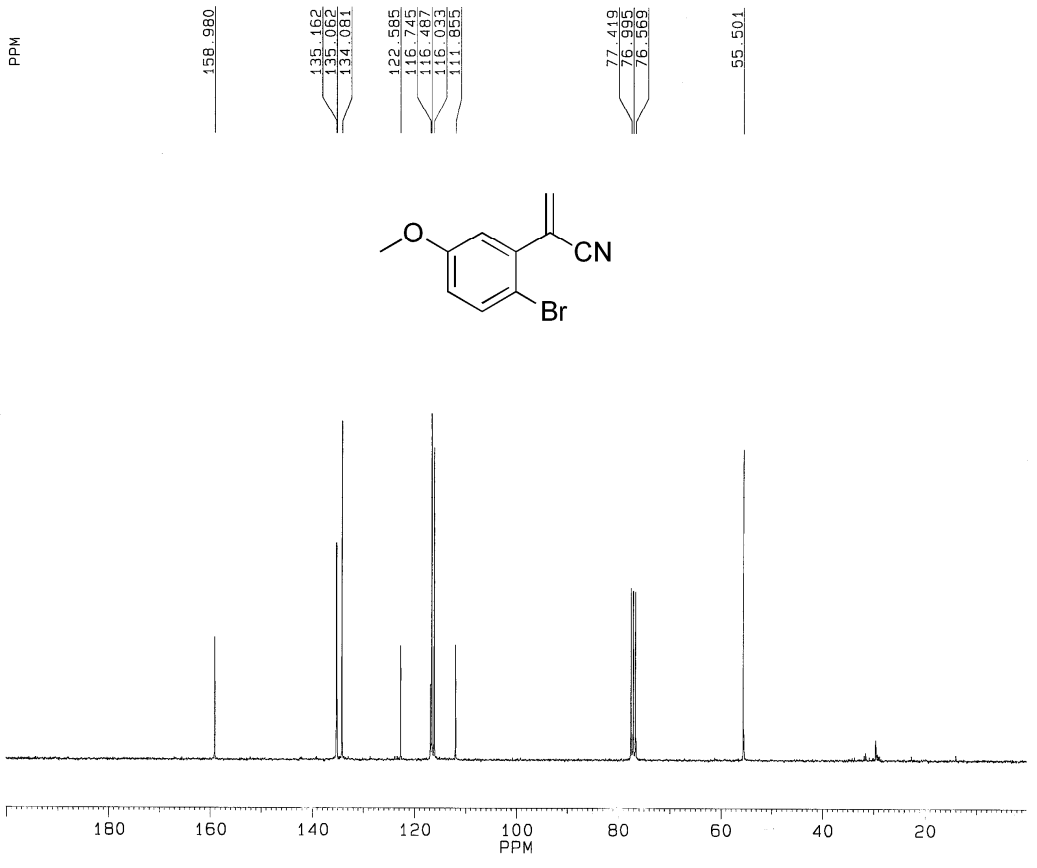
D1222.019
DATE ??-??-??

SF 300.133
SY 299.0
O1 5018.332
SI 16384
TD 16384
SW 4807.692
HZ/PT .587

PW 1.4
RD 1.000
AQ 1.704
RG 20
NS 16
TE 297

FW 6100
O2 0.0
DP 63L PO

LB 0.0
GB 0.0
CX 21.00
CY 0.0
F1 9.501P
F2 -.499P
HZ/CM 142.918
PPM/CM .476
SR 3367.55



D1222.901
DATE ??-??-??

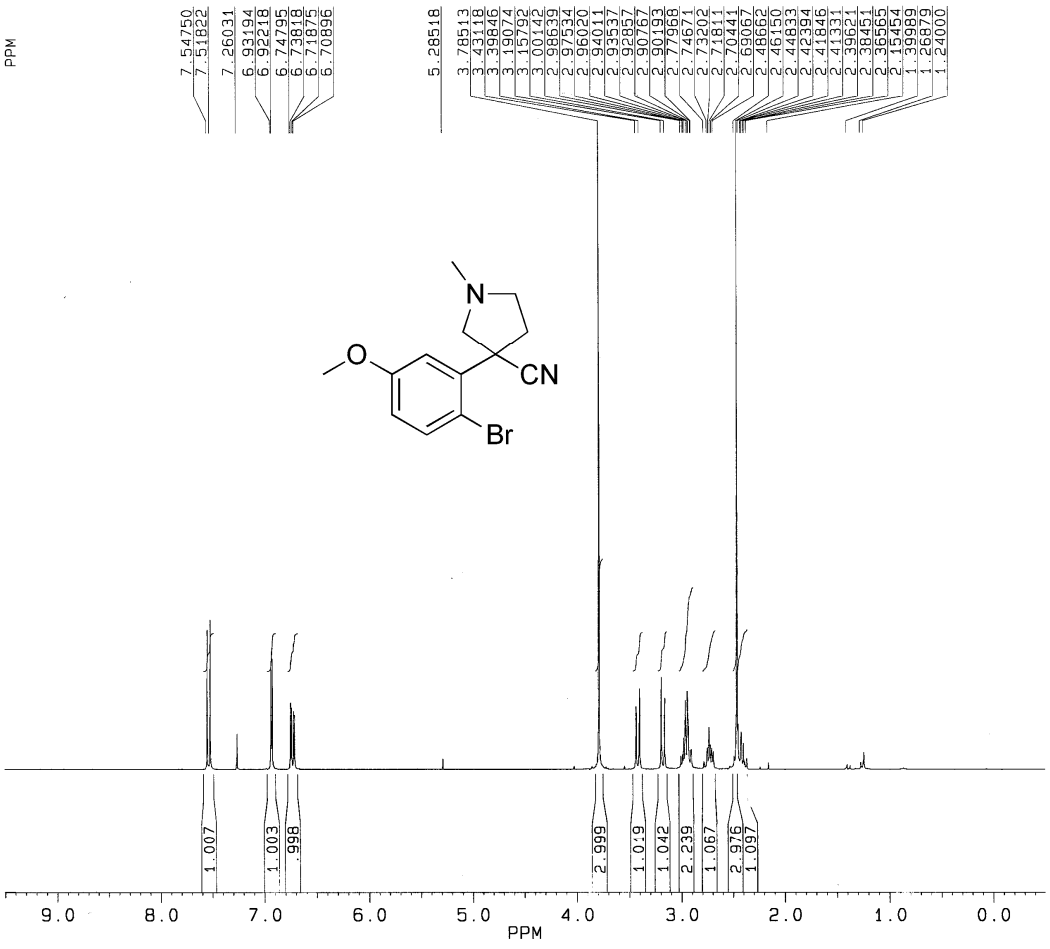
SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

PW 1.4
RD 1.500
AQ .852
RG 200
NS 1200
TE 297

FW 24100
O2 4869.082
DP 15H CPD

LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 200.008P
F2 .013P
HZ/CM 718.728
PPM/CM 9.524
SR -1392.06

3-(2-Bromo-5-methoxyphenyl)-1-methylpyrrolidine-3-carbonitrile (1F)



BRUKER

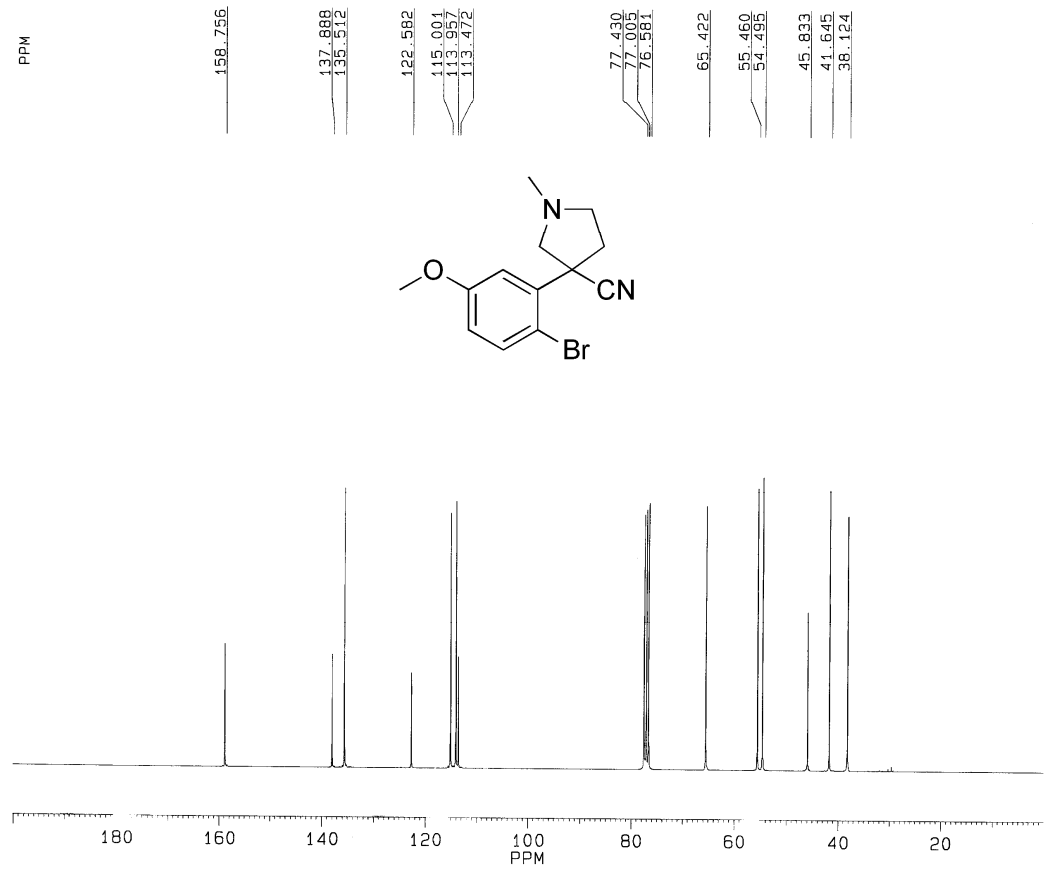
D1215.019
DATE ??-??-??

SF 300.133
SY 299.0
O1 5018.332
SI 16384
TD 16384
SW 4807.692
HZ/PT .587

PW 1.4
RD 1.000
AQ 1.704
RG 32
NS 16
TE 297

FW 6100
O2 0.0
DP 63L PO

LB 0.0
GB 0.0
CX 21.00
CY 0.0
F1 9.501P
F2 -.499P
HZ/CM 142.918
PPM/CM .476
SR 3367.55



BRUKER

D0827.902
DATE ??-??-??

SF 75.469
SY 75.0
O1 6517.695
SI 32768
TD 32768
SW 19230.769
HZ/PT 1.174

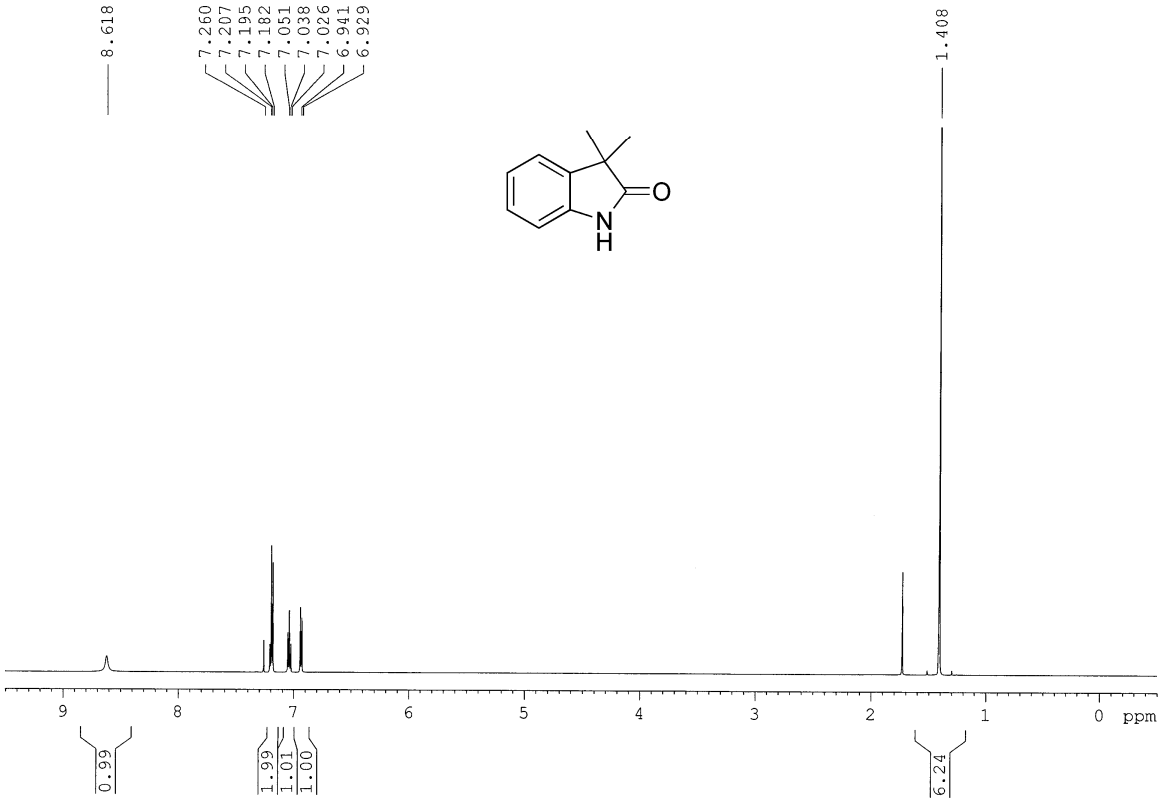
PW 1.4
RD 1.500
AQ .852
RG 200
NS 50290
TE 297

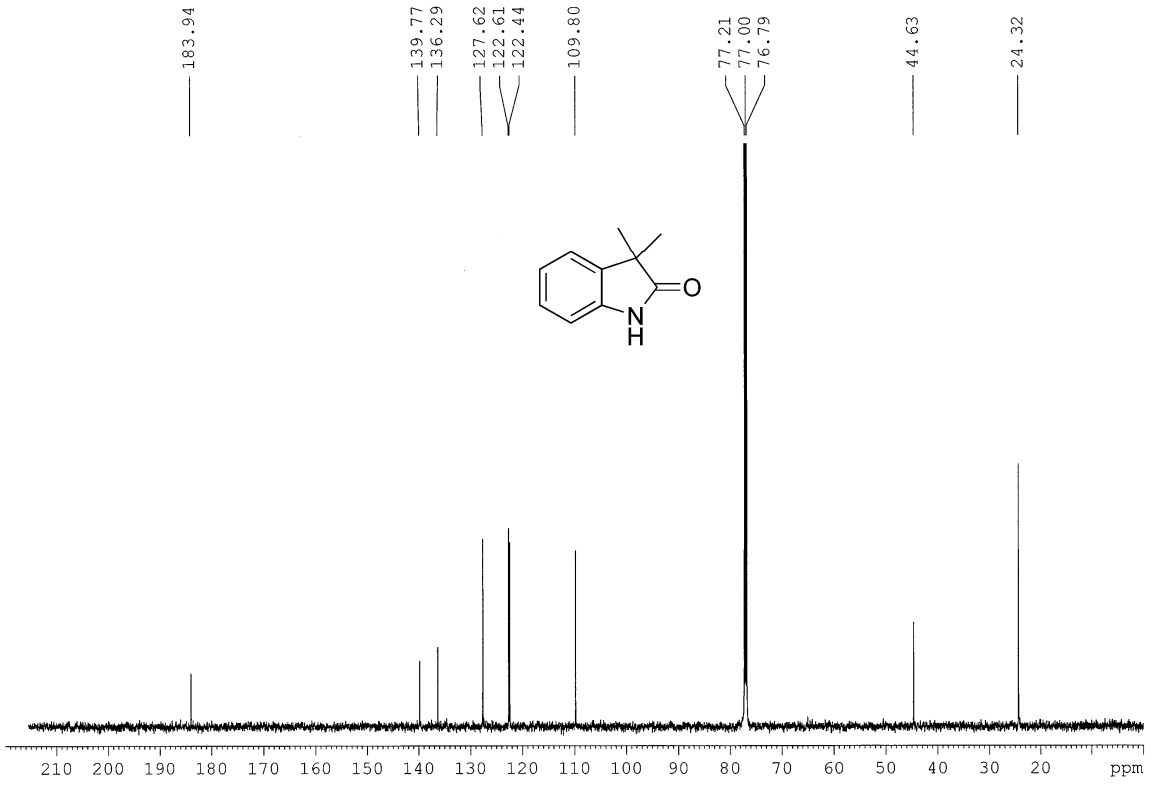
FW 24100
O2 4869.082
DP 15H CPD

LB 2.000
GB 0.0
CX 21.00
CY 0.0
F1 200.008P
F2 .013P
HZ/CM 718.728
PPM/CM 9.524
SR -1395.58

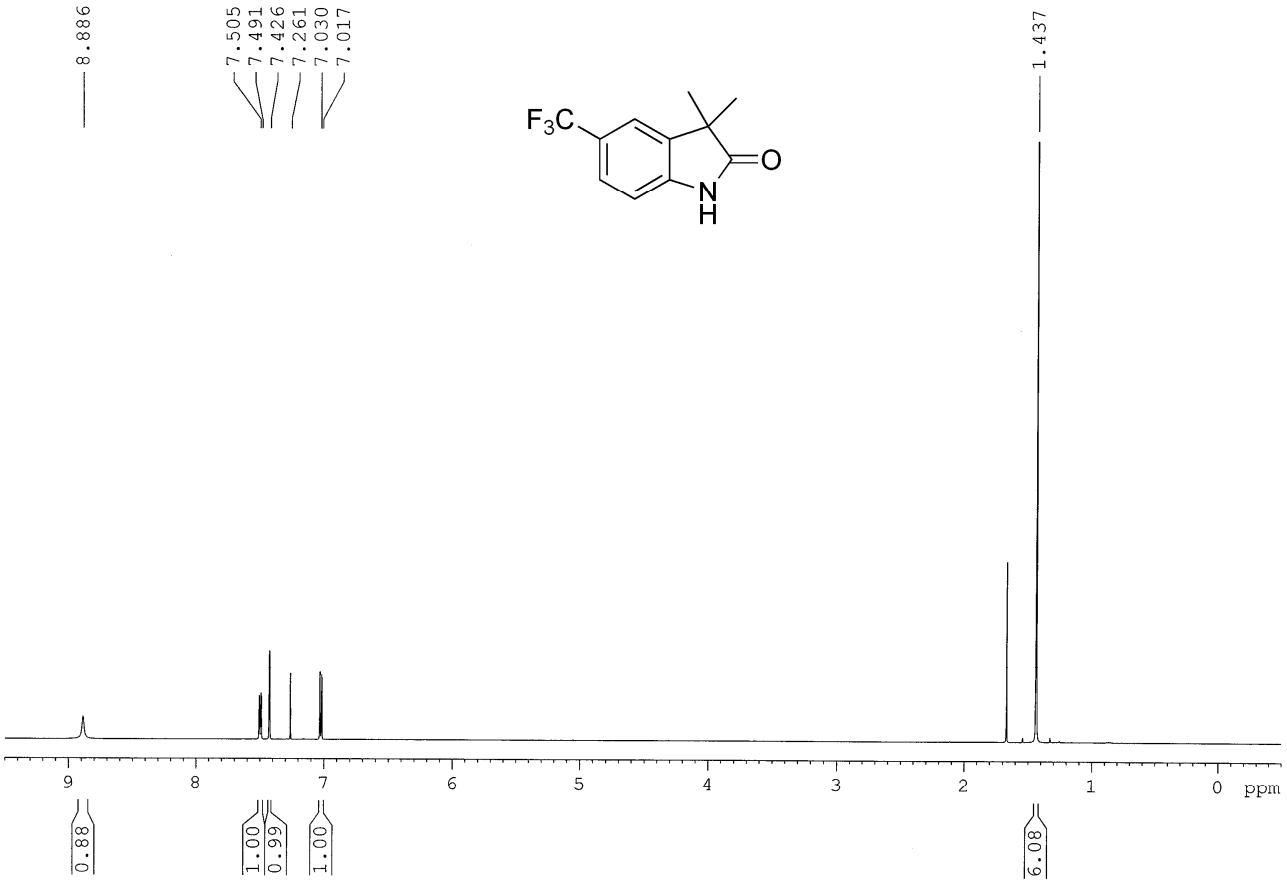
^{1}H and ^{13}C NMR Spectra (600 MHz, $CDCl_3$) for Products

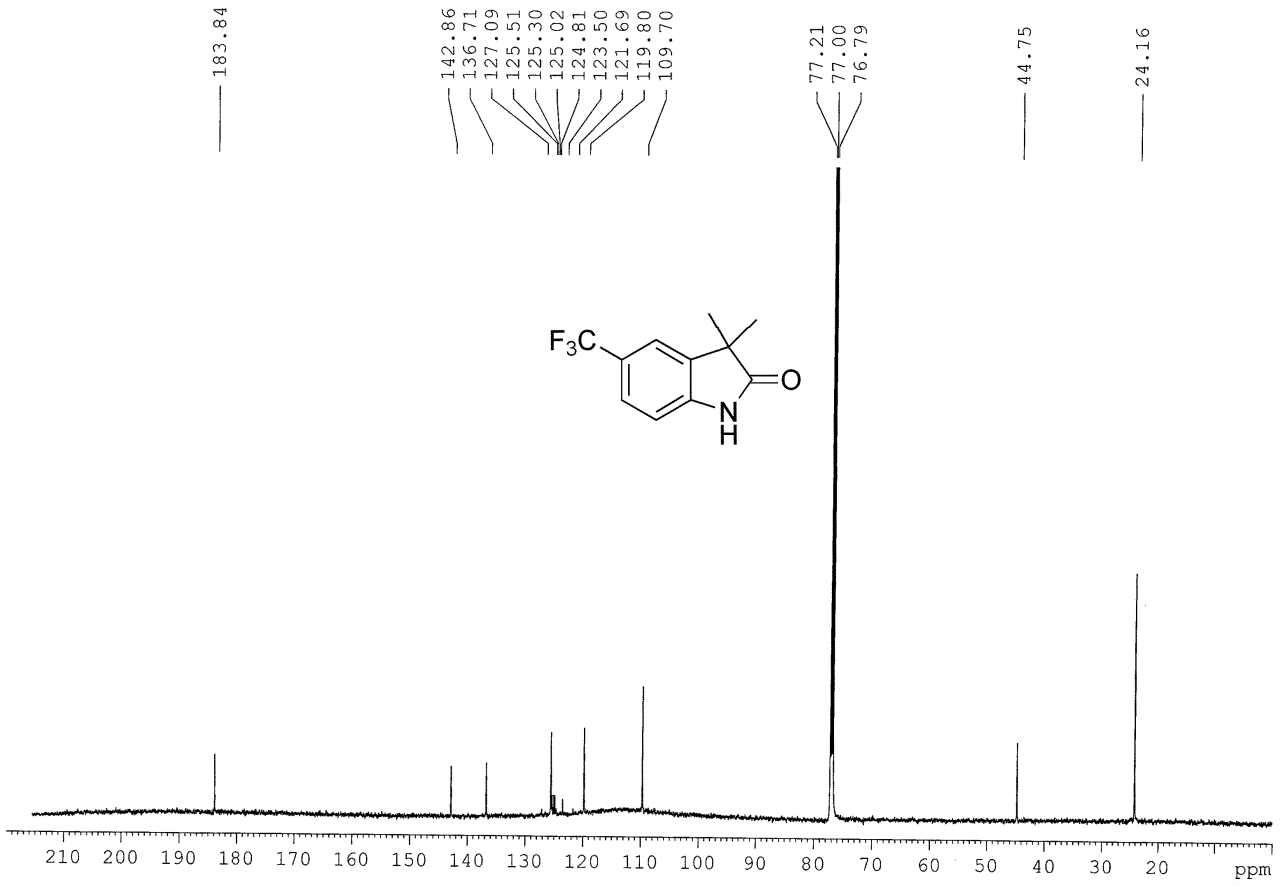
3,3-Dimethylindolin-2-one (2a)



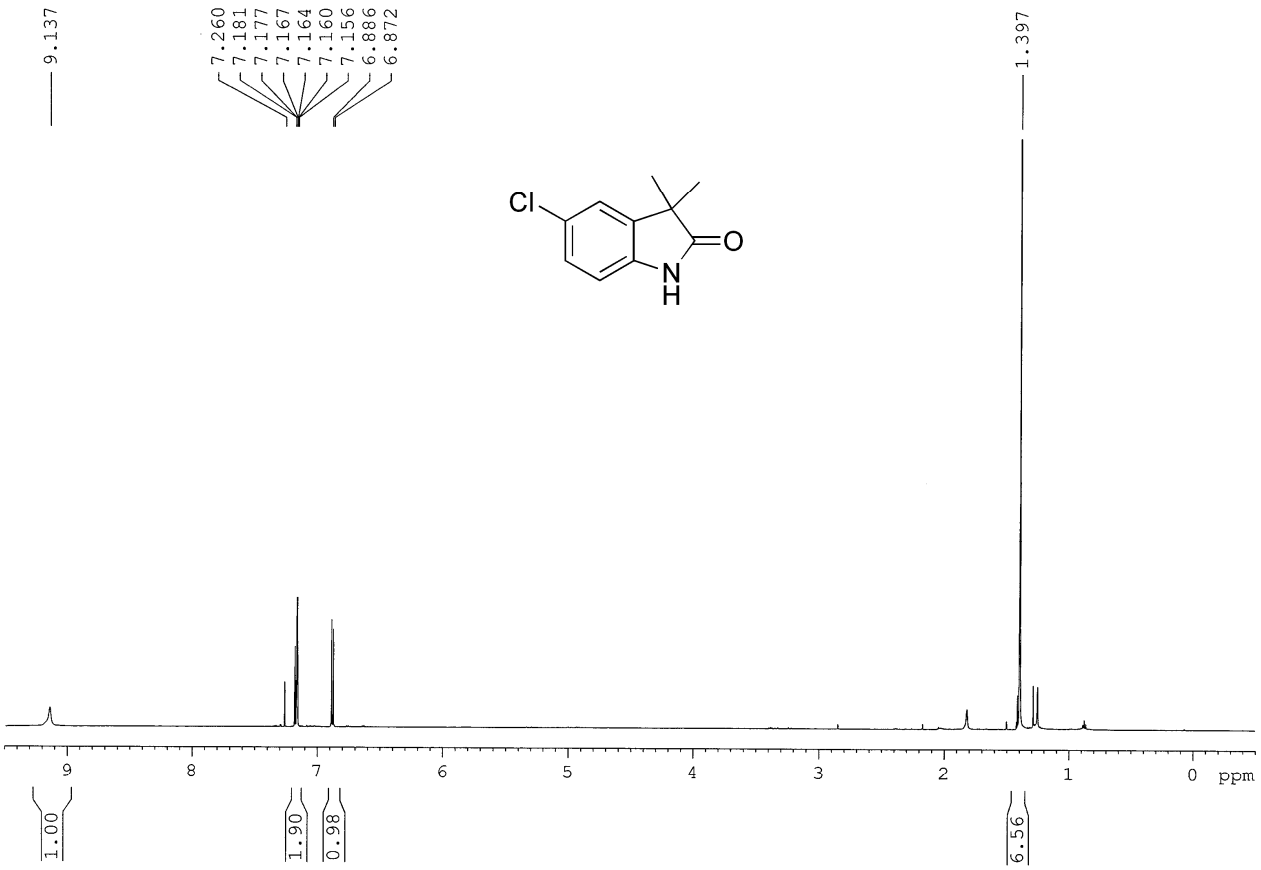


3,3-Dimethyl-5-(trifluoromethyl)indolin-2-one (2b)

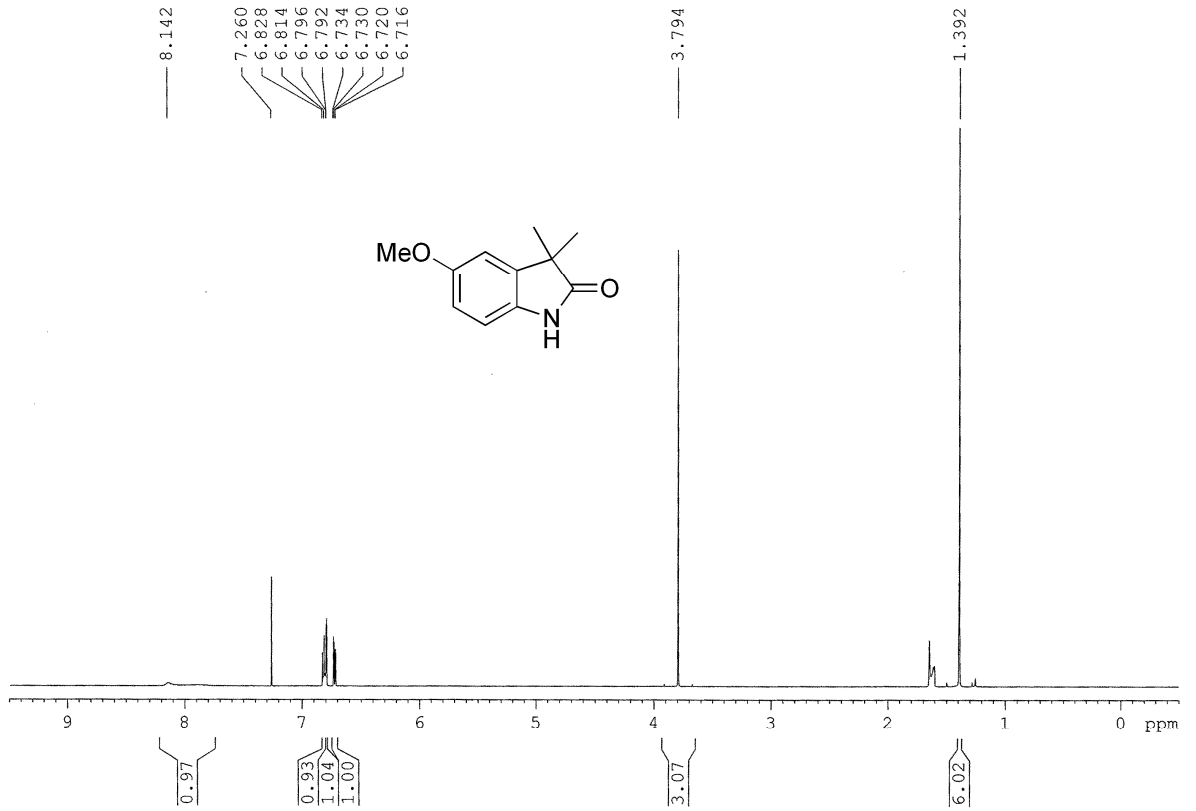


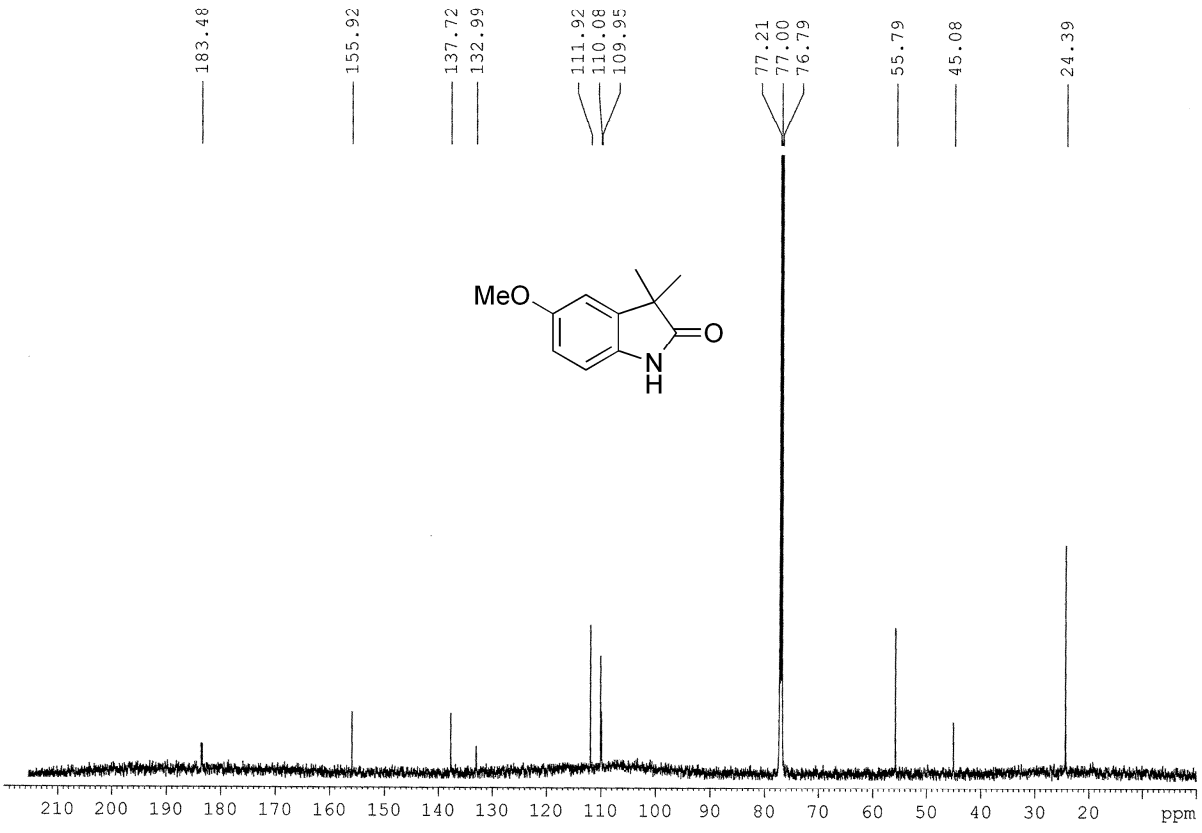


5-Chloro-3,3-dimethylindolin-2-one (2c)

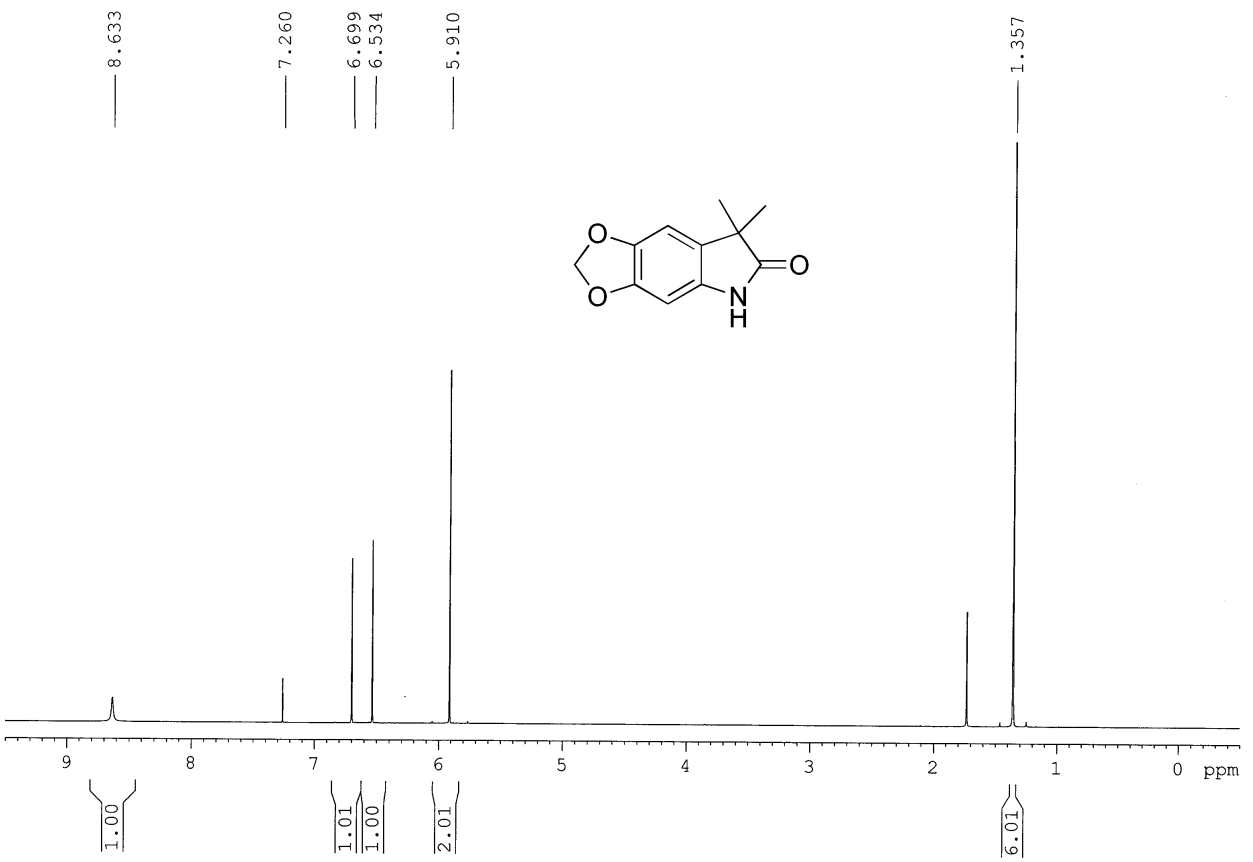


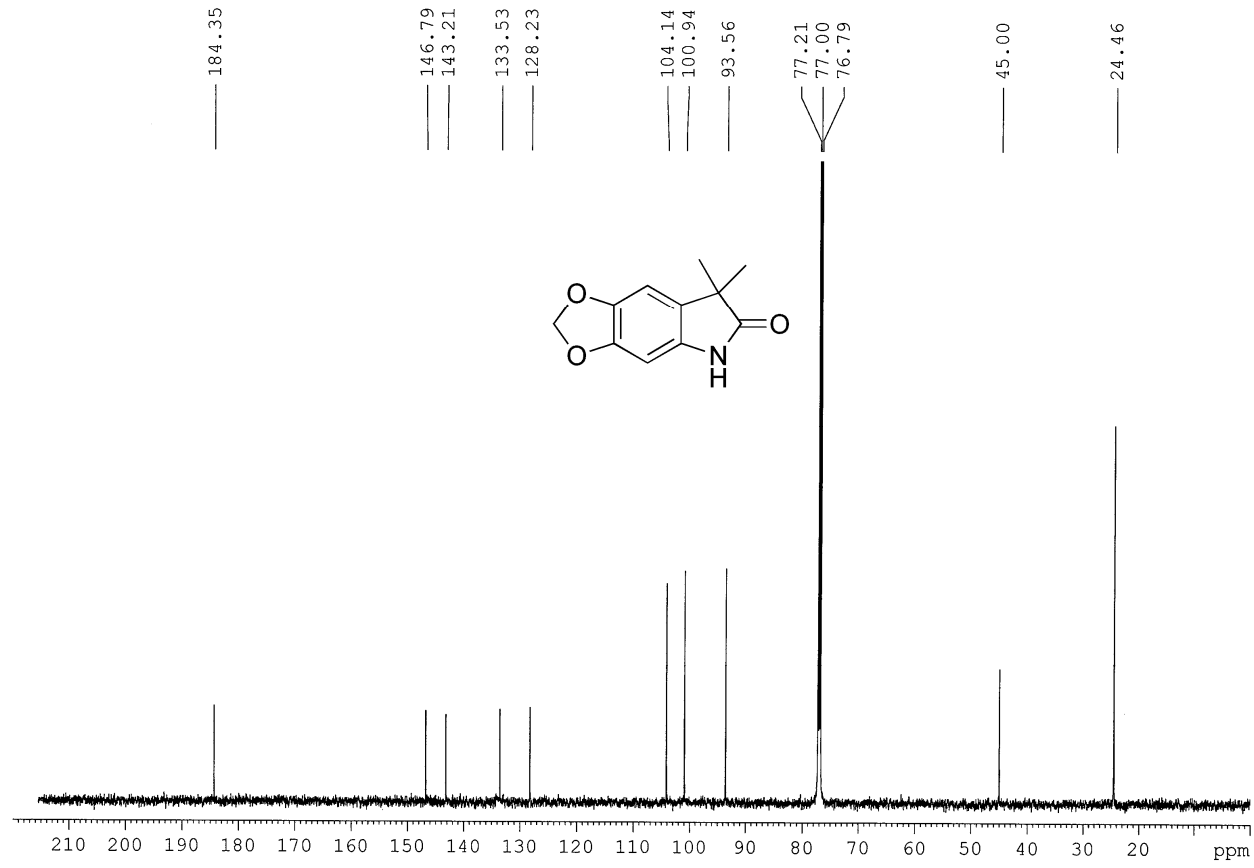
5-Methoxy-3,3-dimethylindolin-2-one (2d)



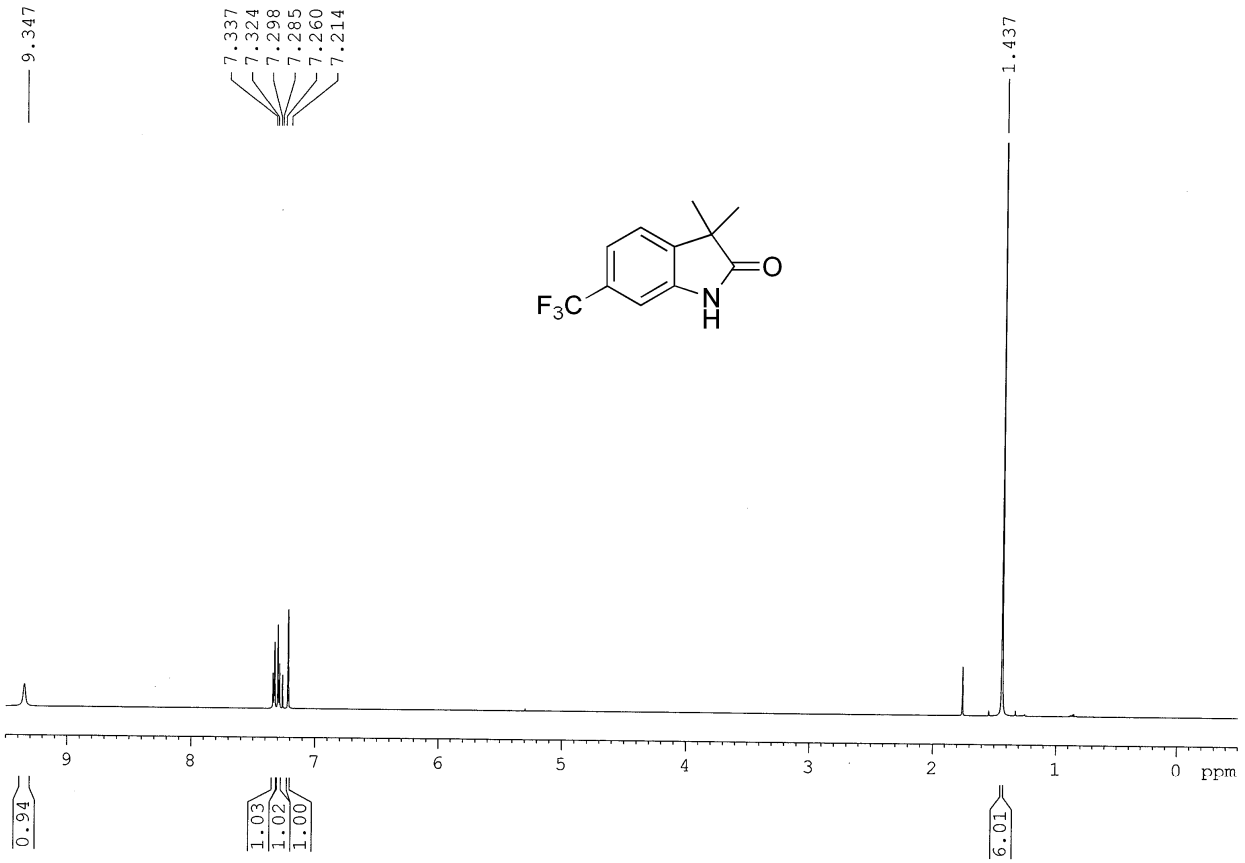


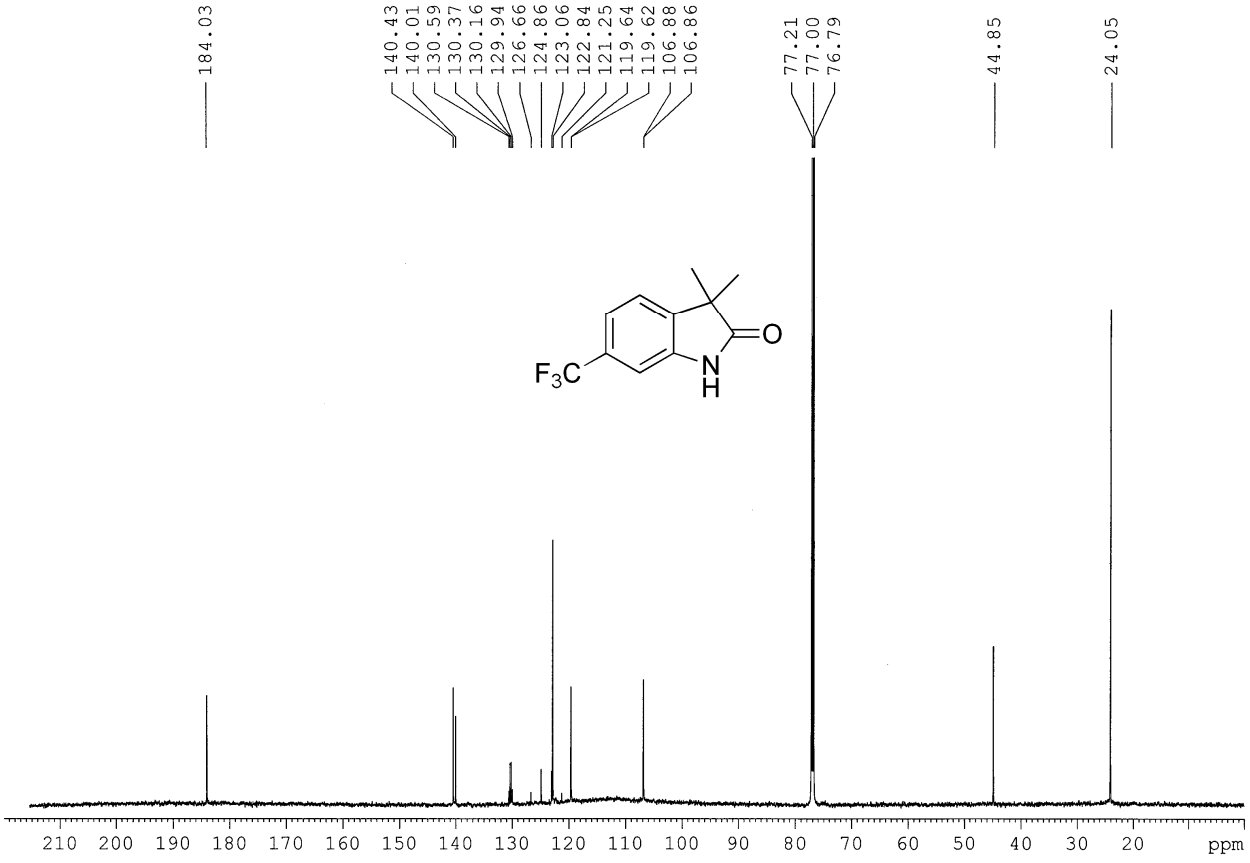
7,7-Dimethyl-5*H*-[1,3]dioxolo[4,5-*f*]indol-6(7*H*)-one (2e)



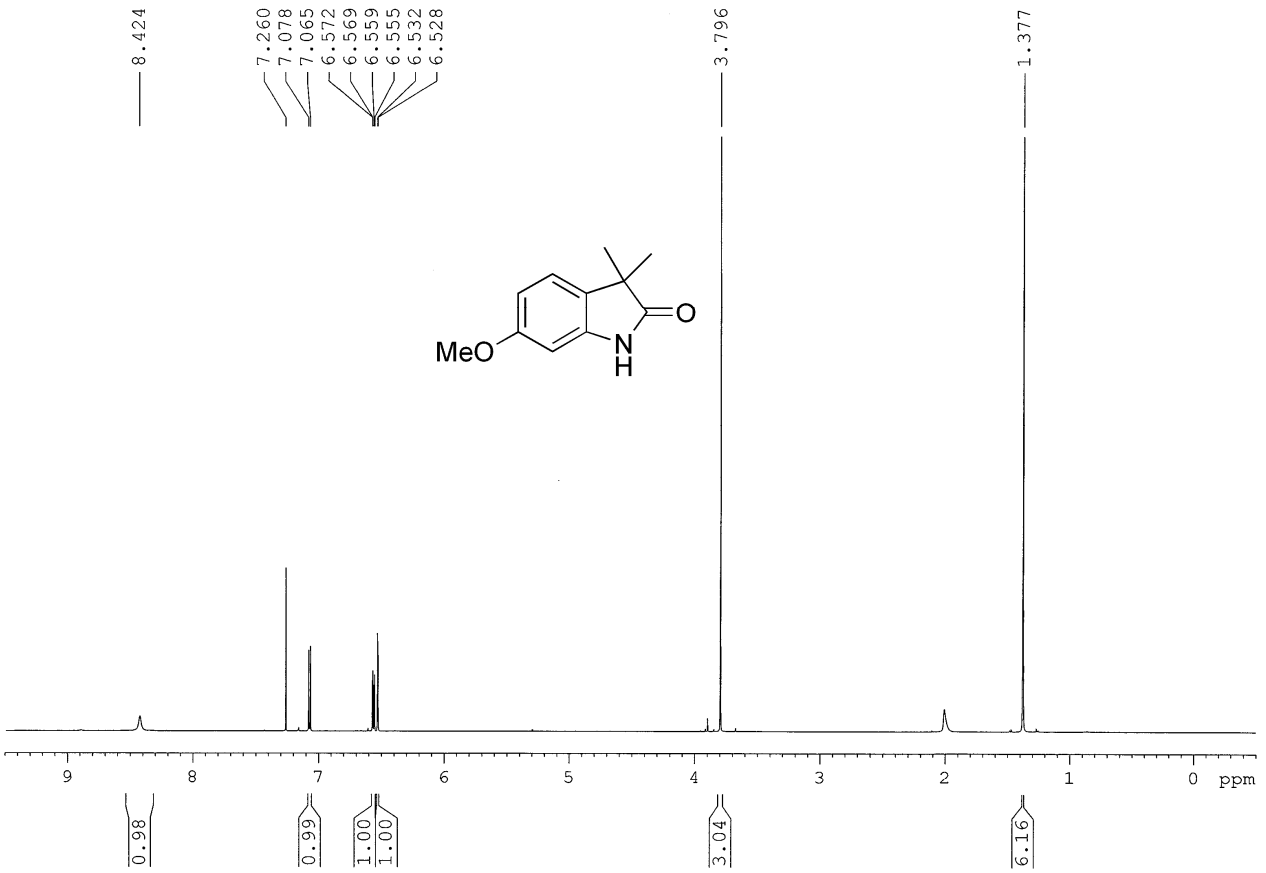


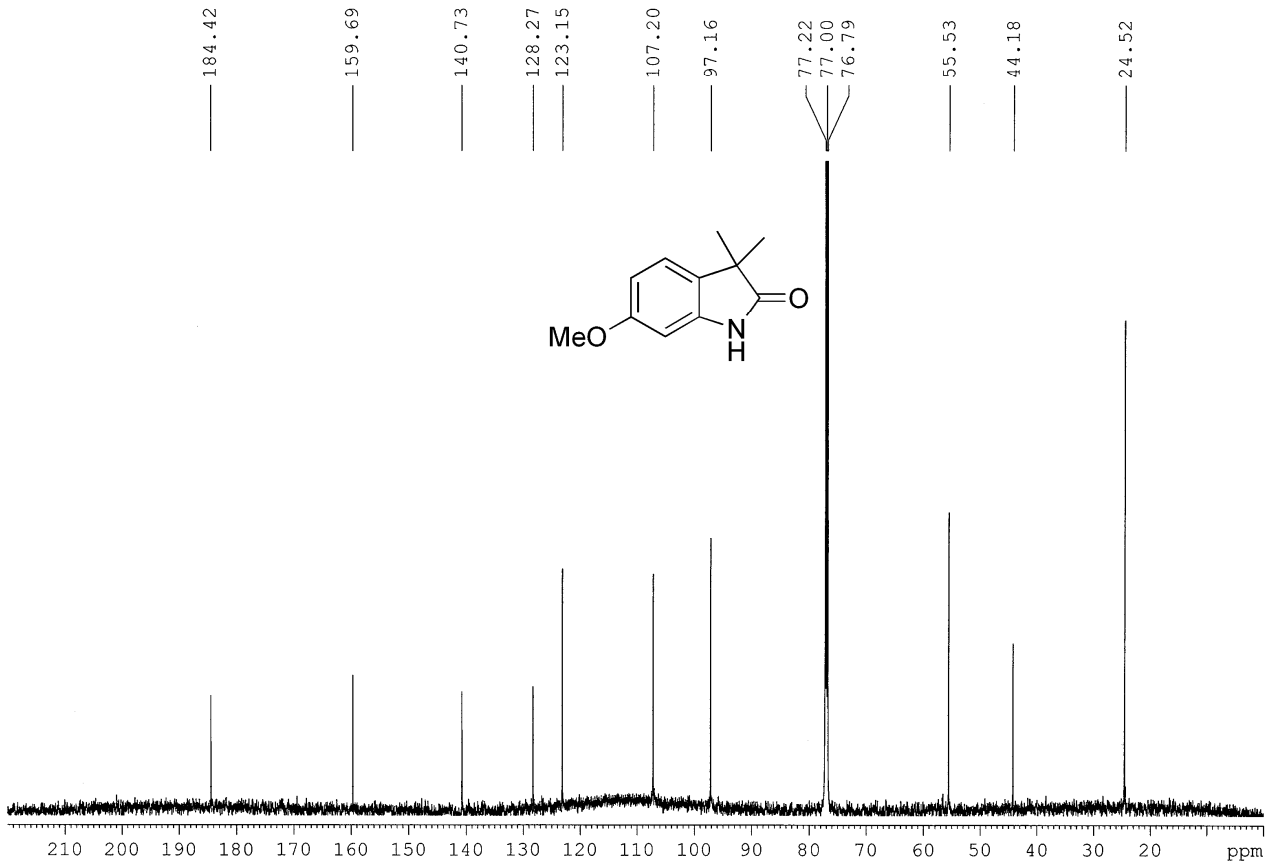
3,3-Dimethyl-6-(trifluoromethyl)indolin-2-one (2f)



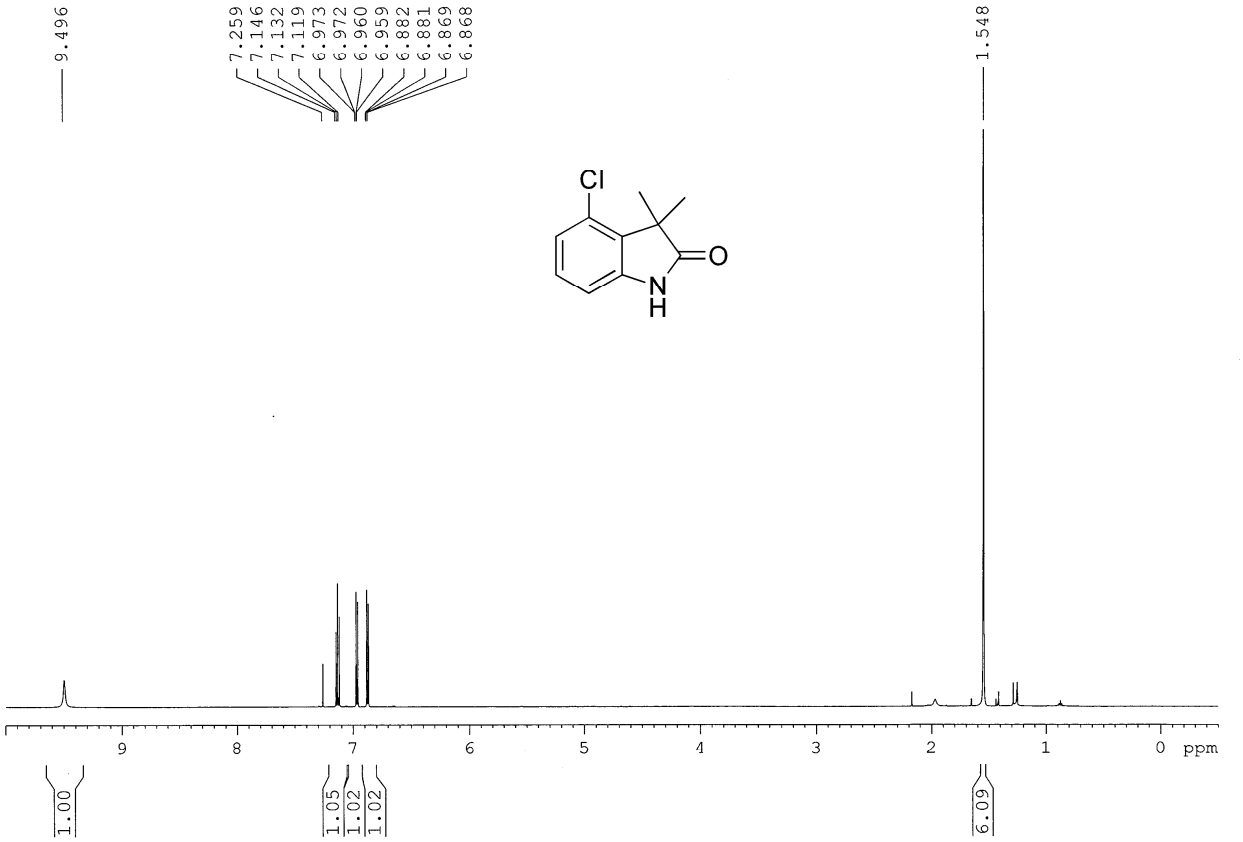


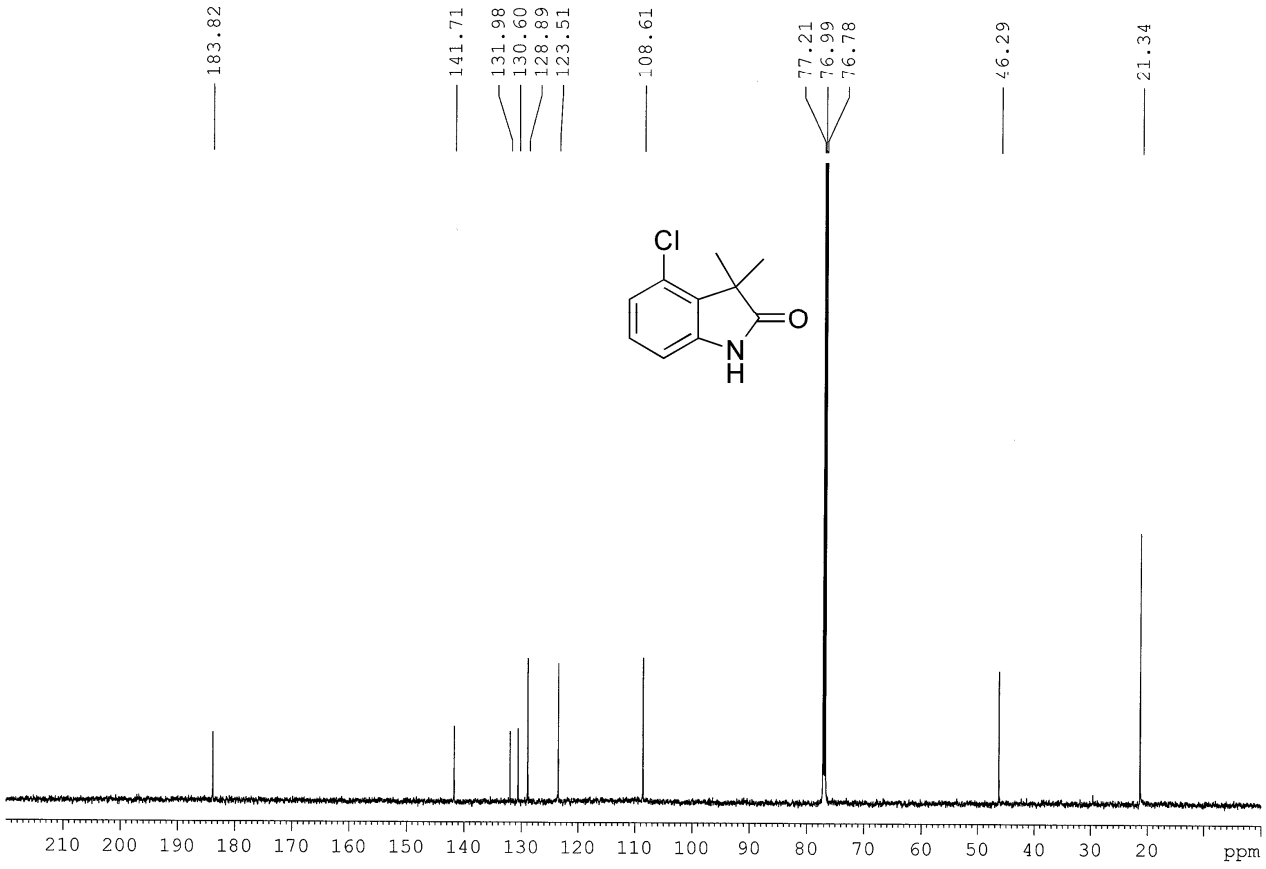
6-Methoxy-3,3-dimethylindolin-2-one (2g)



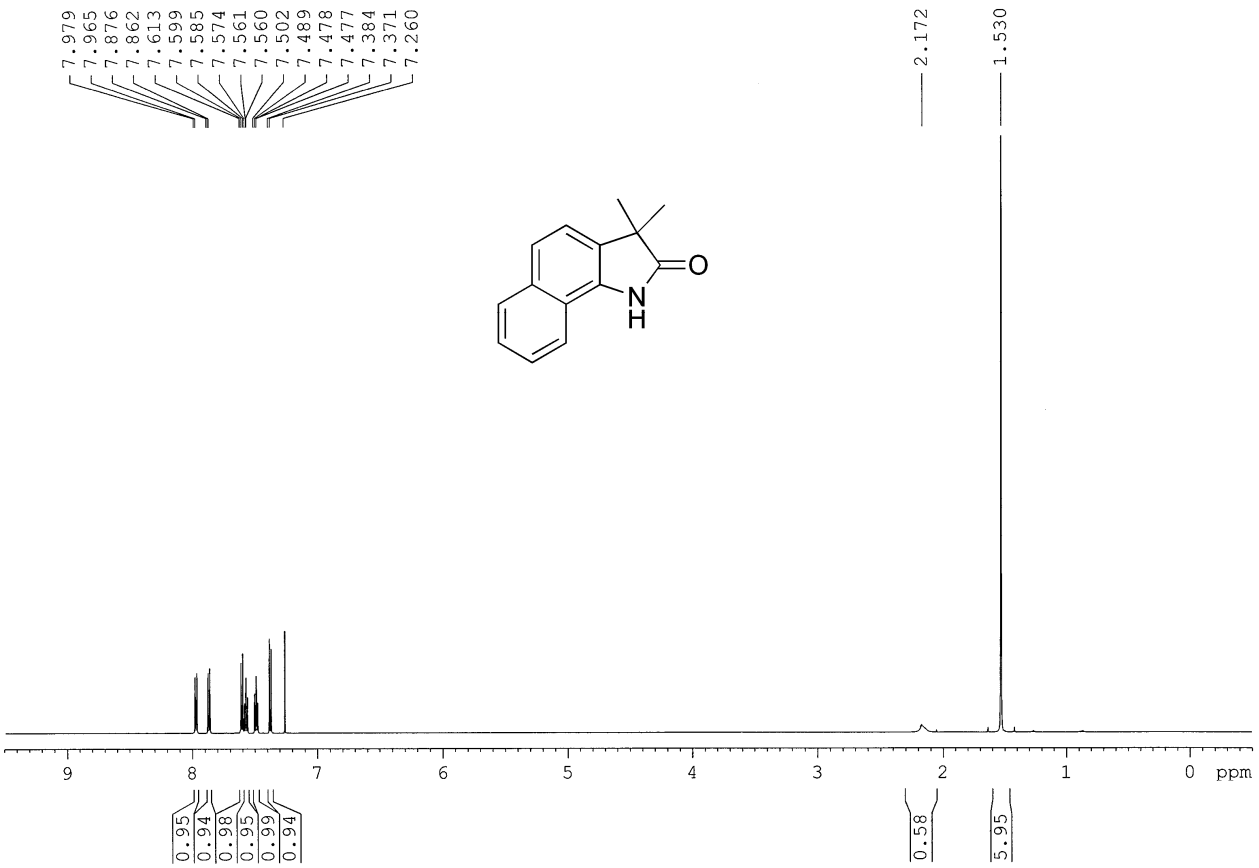


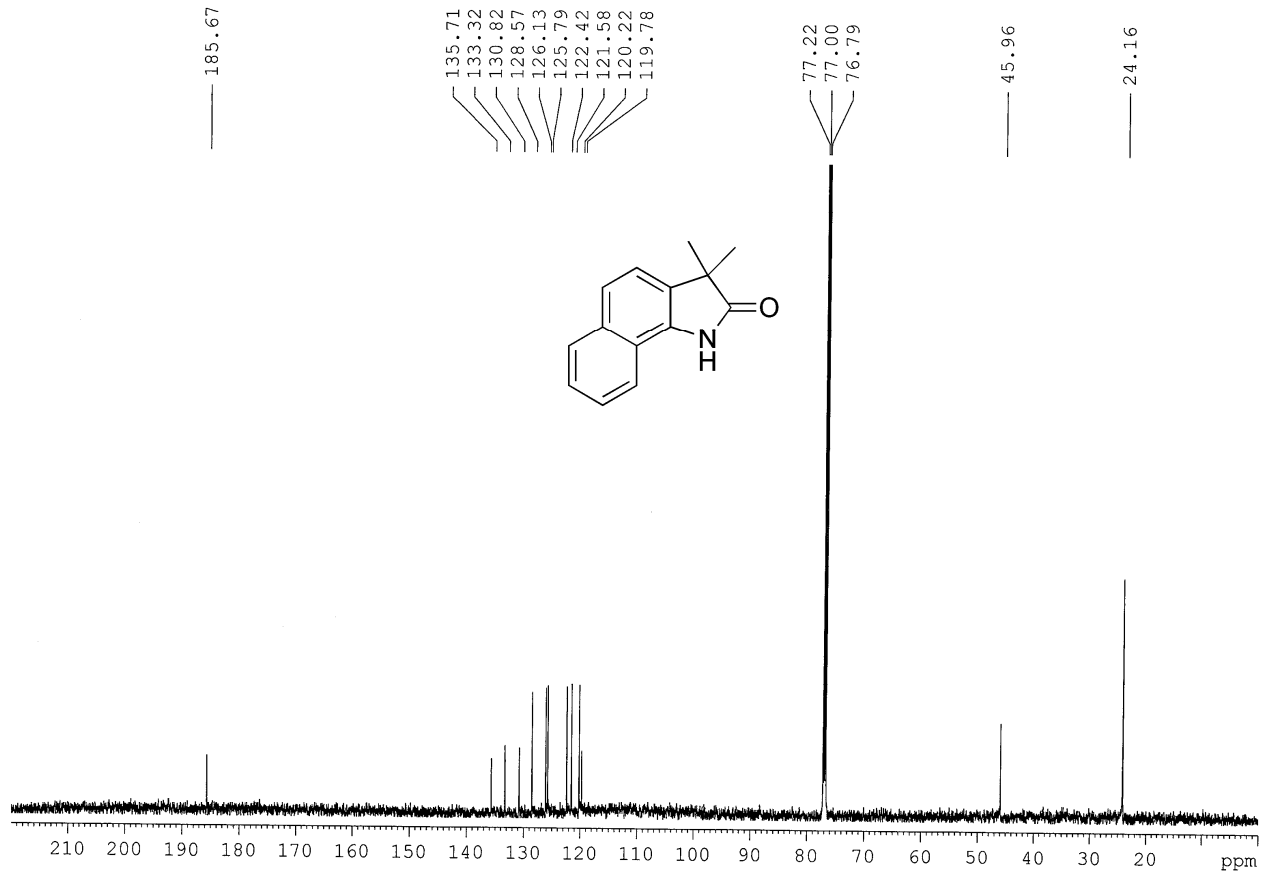
4-Chloro-3,3-dimethylindolin-2-one (2h)



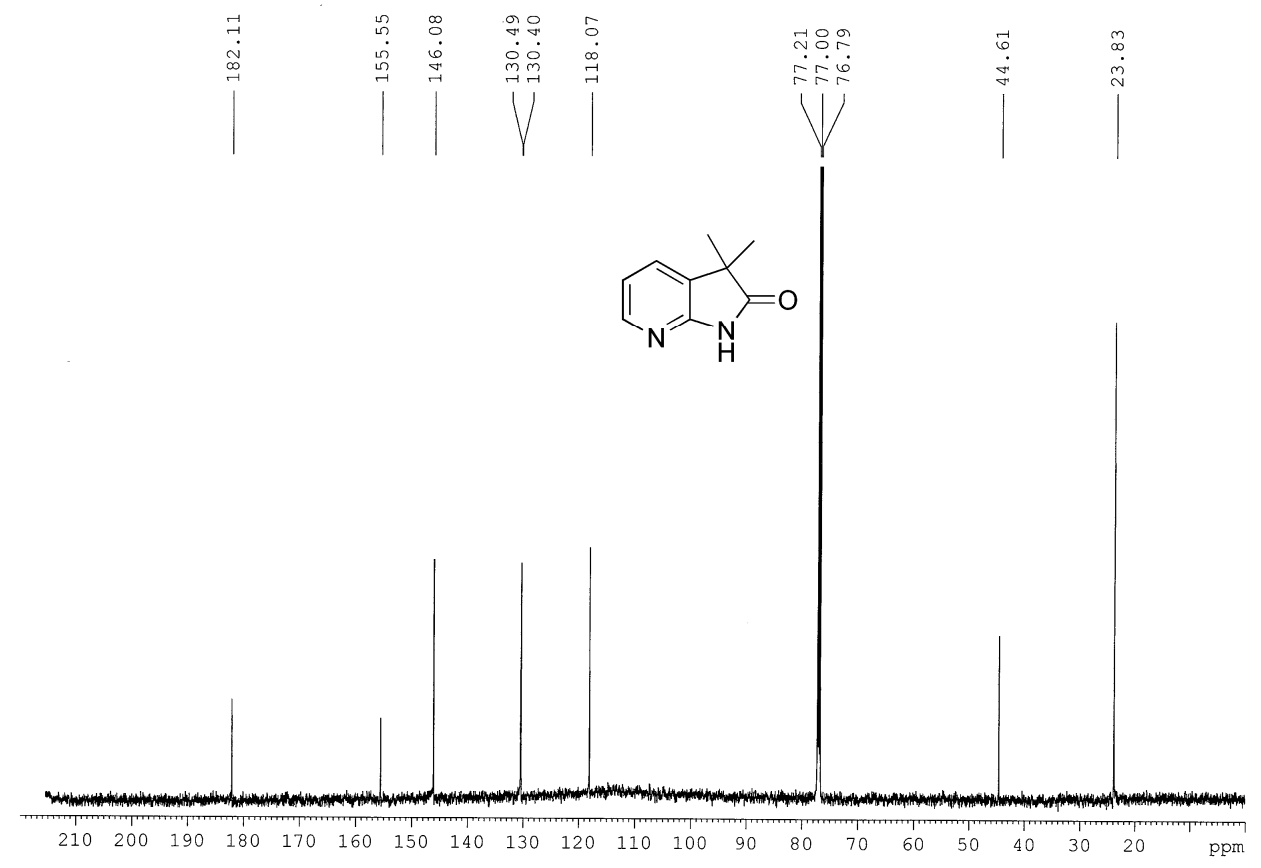


3,3-Dimethyl-1*H*-benzo[*g*]indol-2(3*H*)-one (2i)

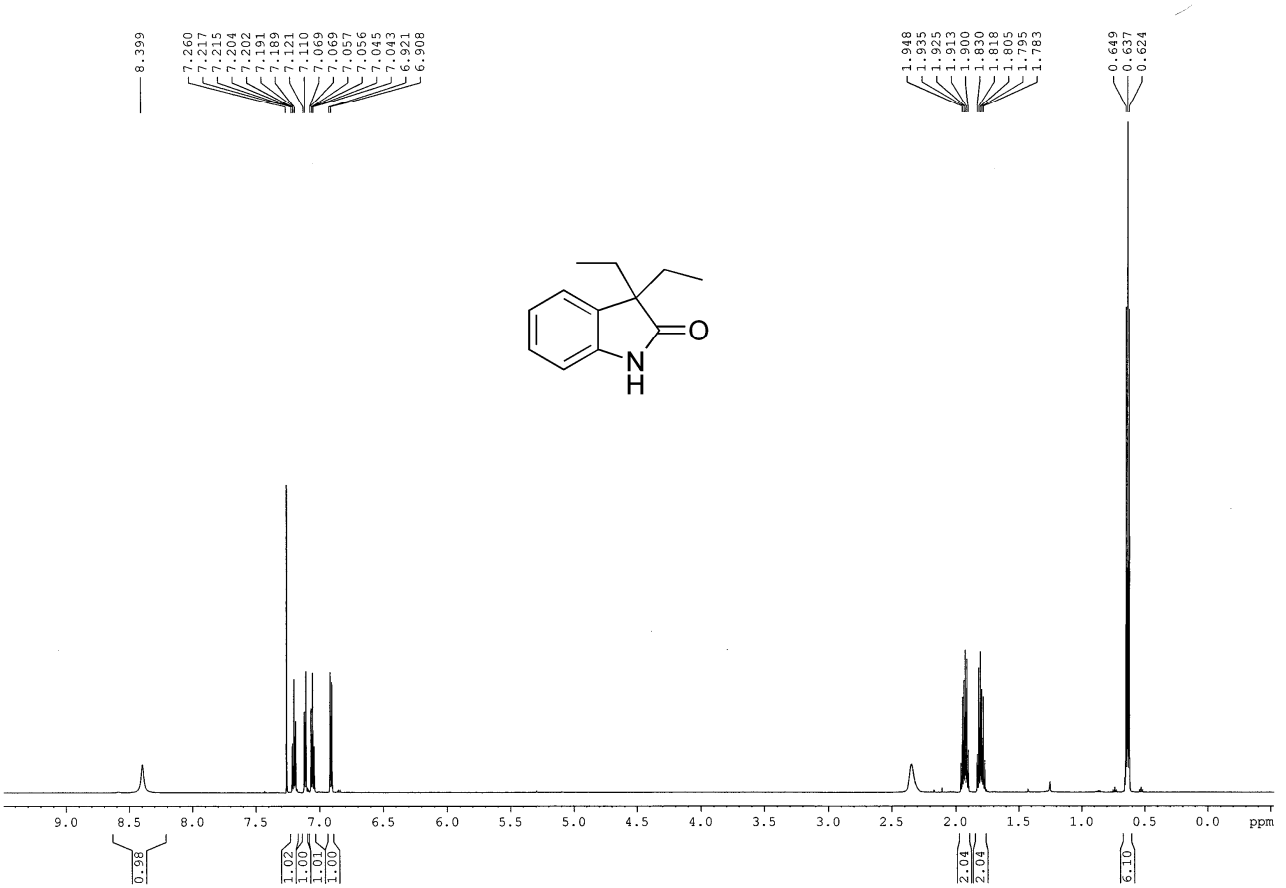


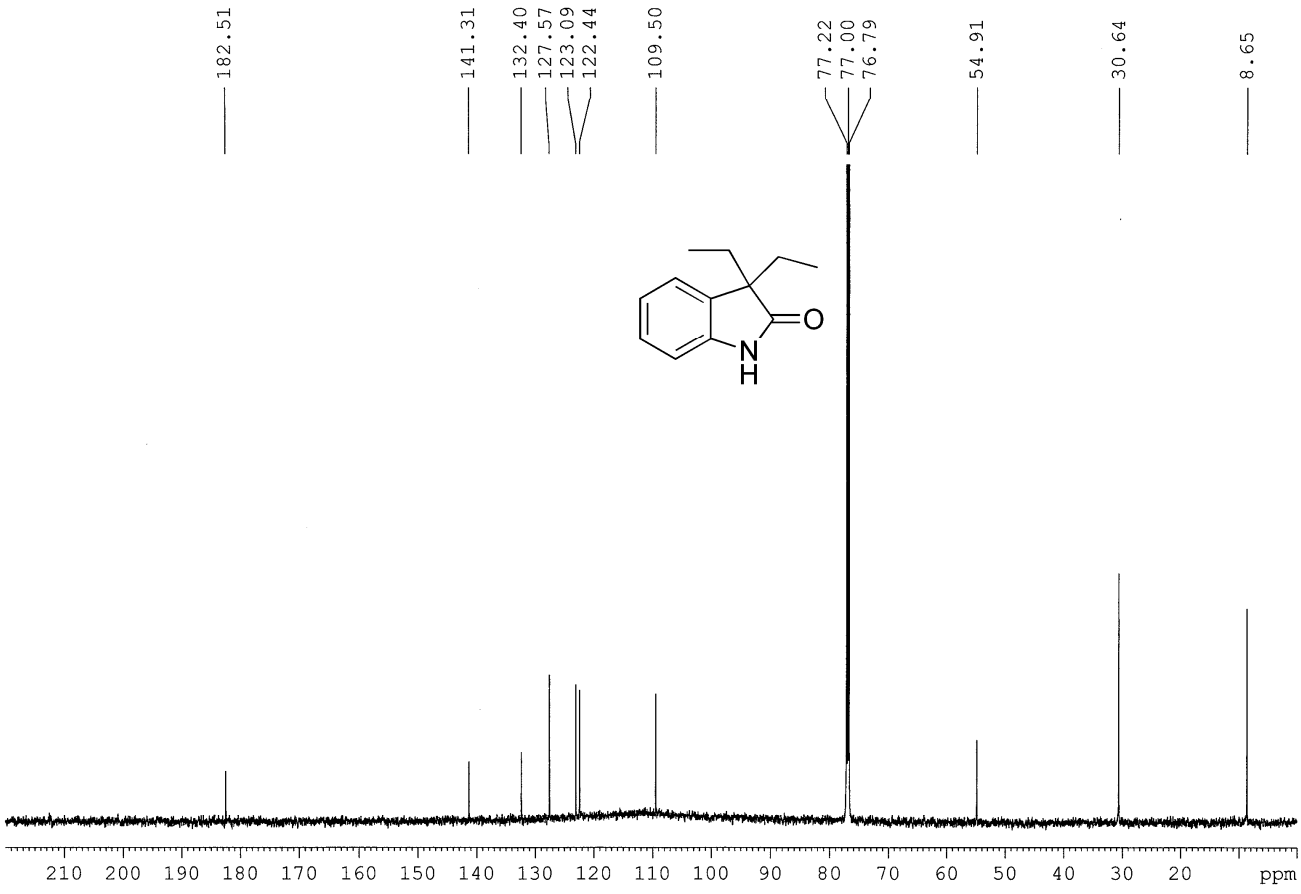


3,3-Dimethyl-1*H*-pyrrolo[2,3-*b*]pyridin-2(3*H*)-one (2j)

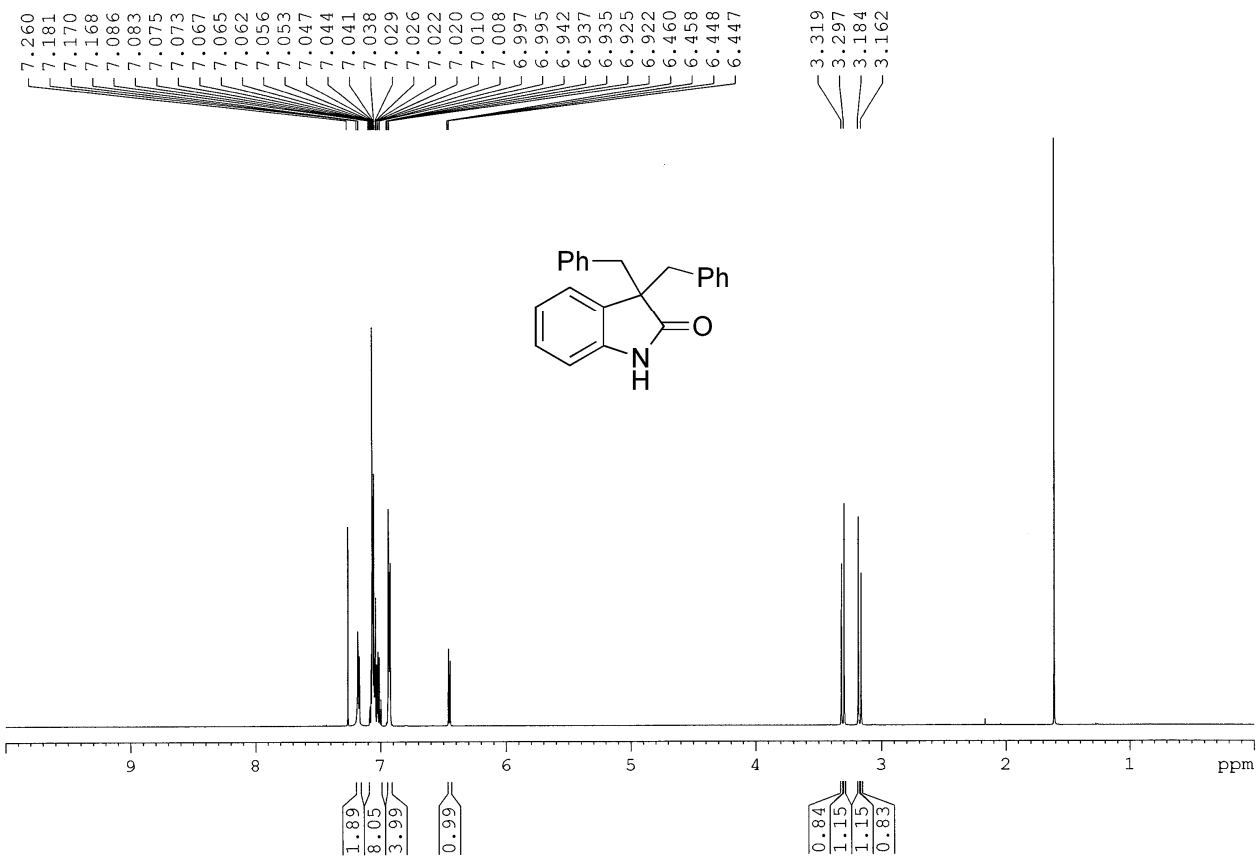


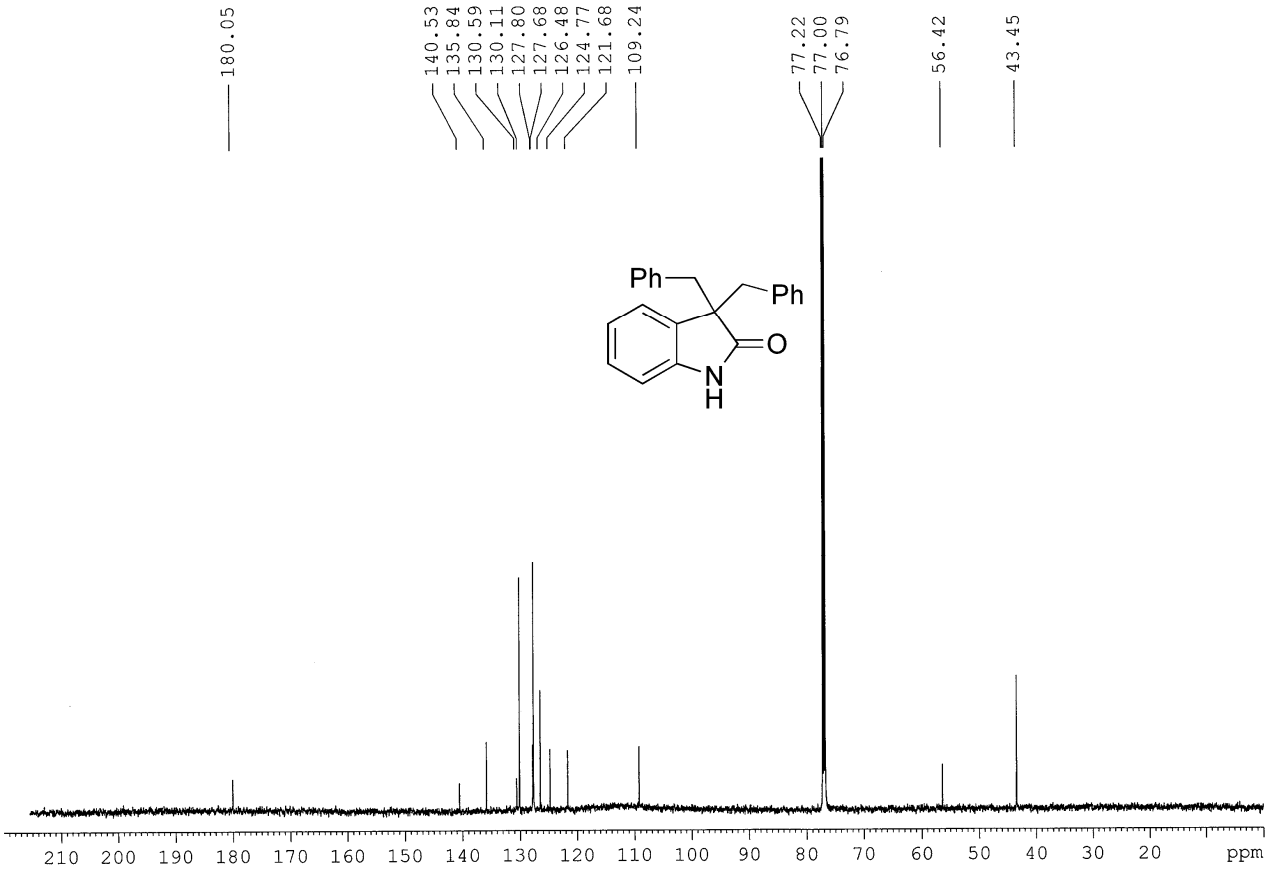
3,3-Diethylindolin-2-one (2k)



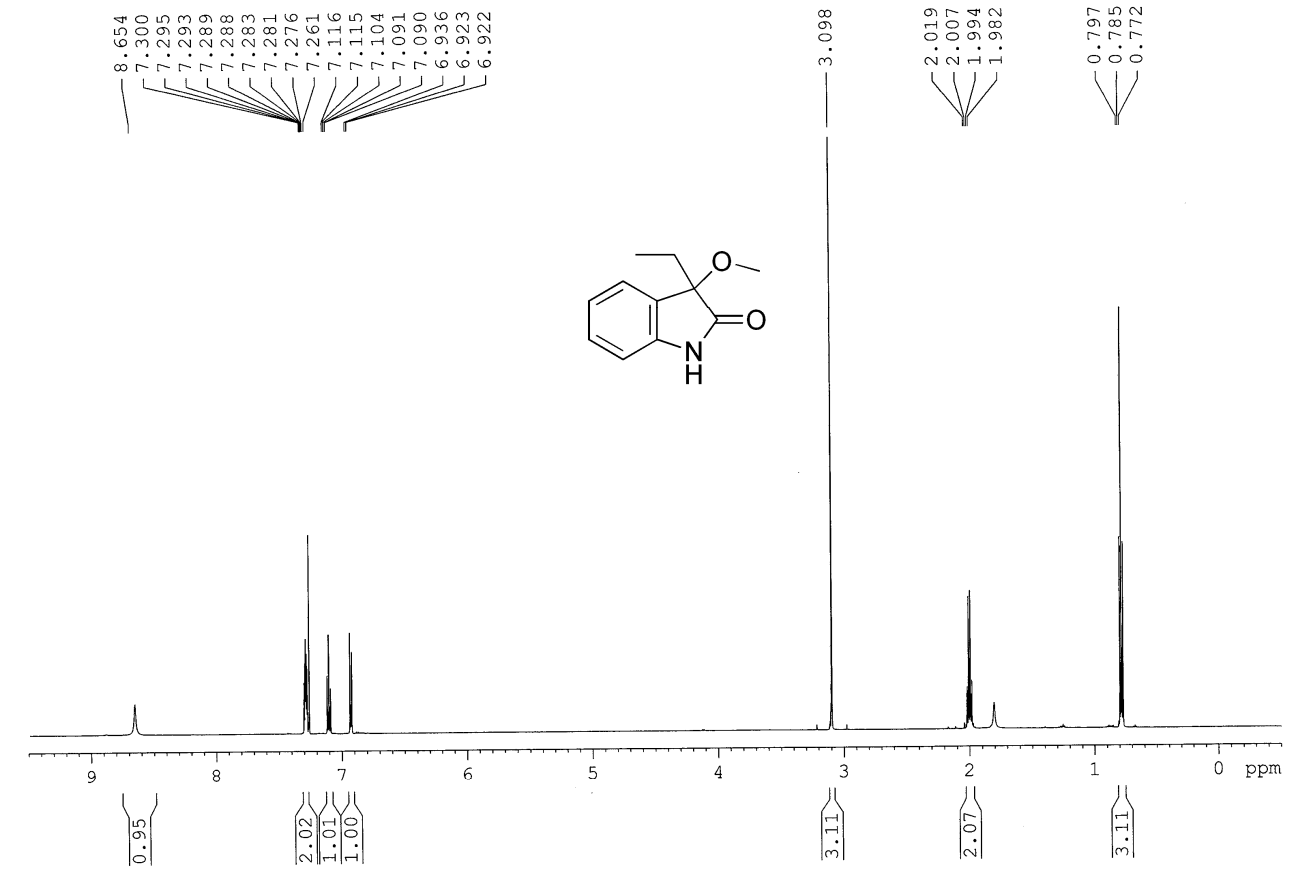


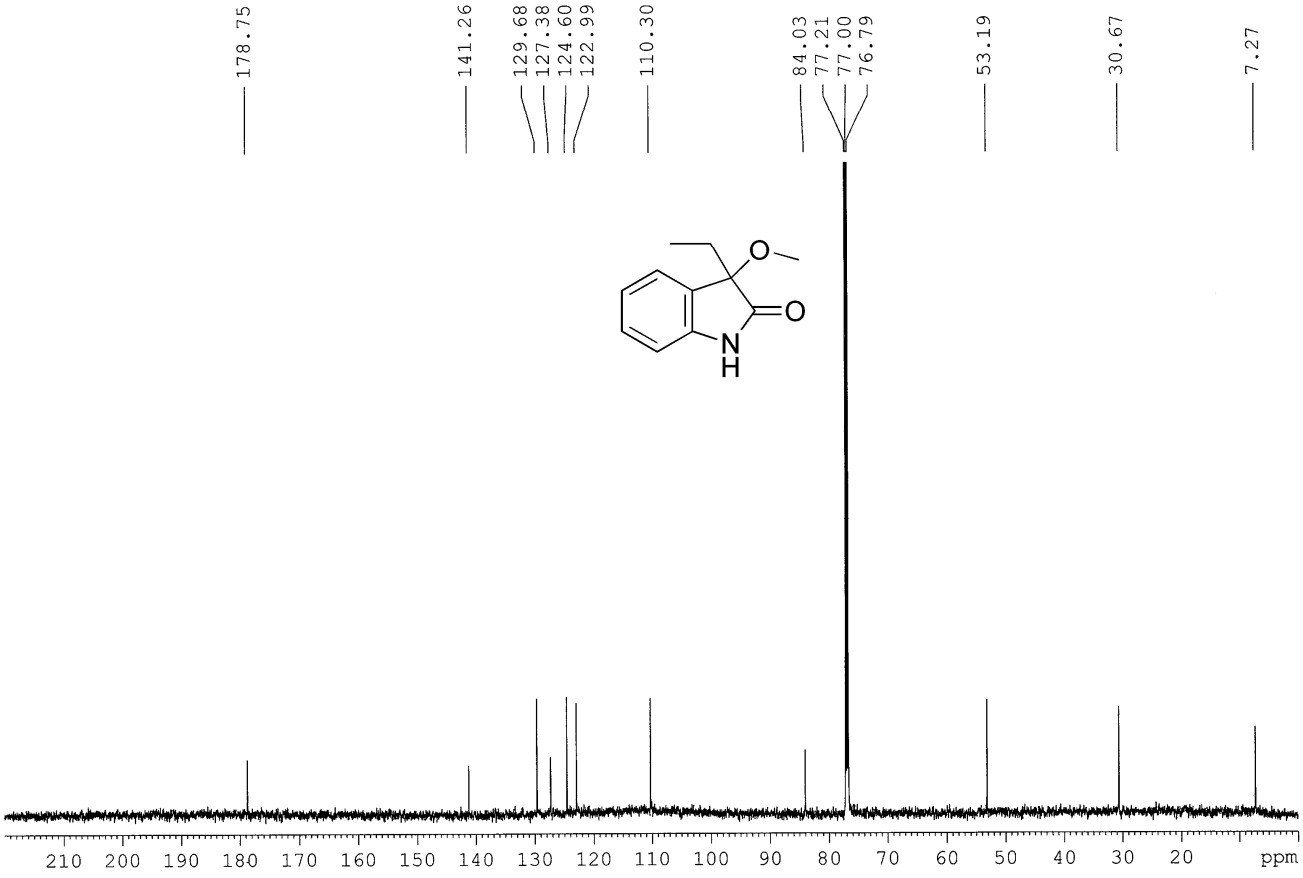
3,3-Dibenzylindolin-2-one (2l)



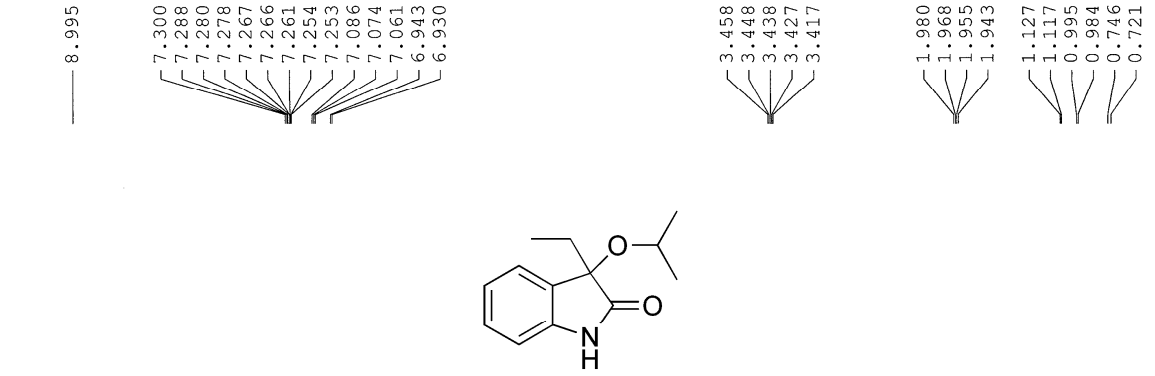


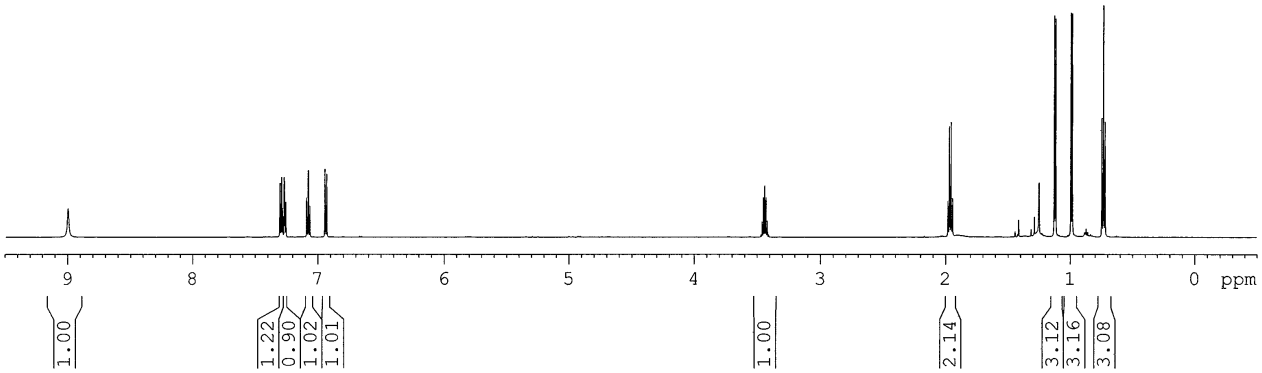
3-Ethyl-3-methoxyindolin-2-one (2m)

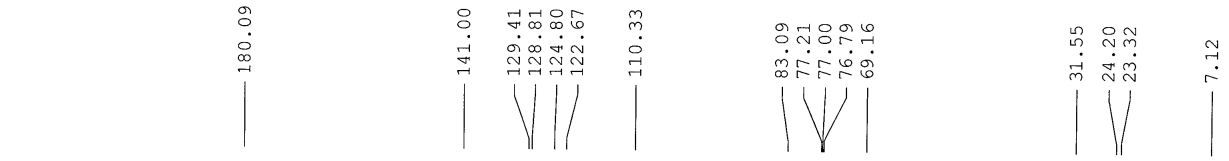


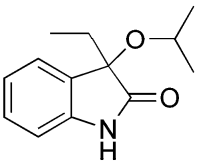


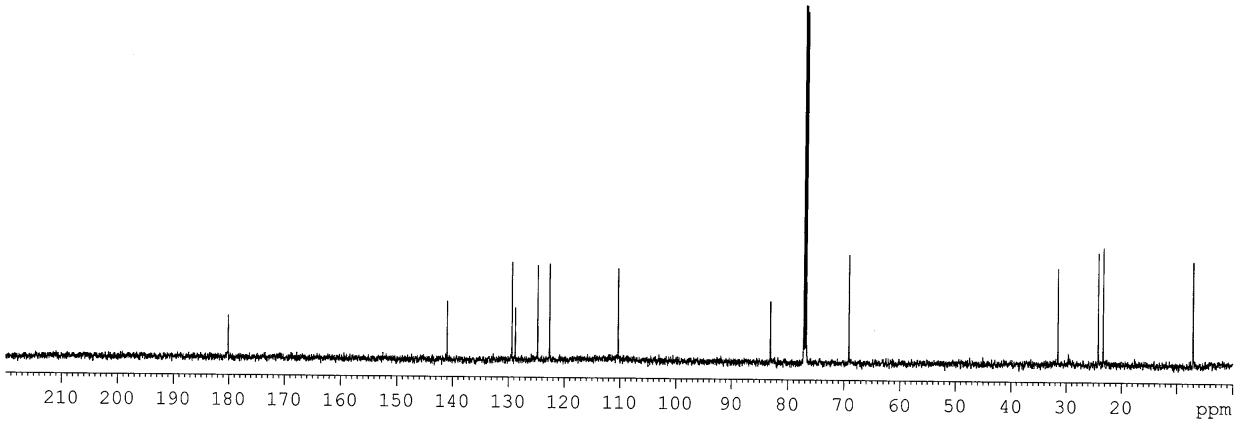
3-Ethyl-3-isopropoxyindolin-2-one (2n)



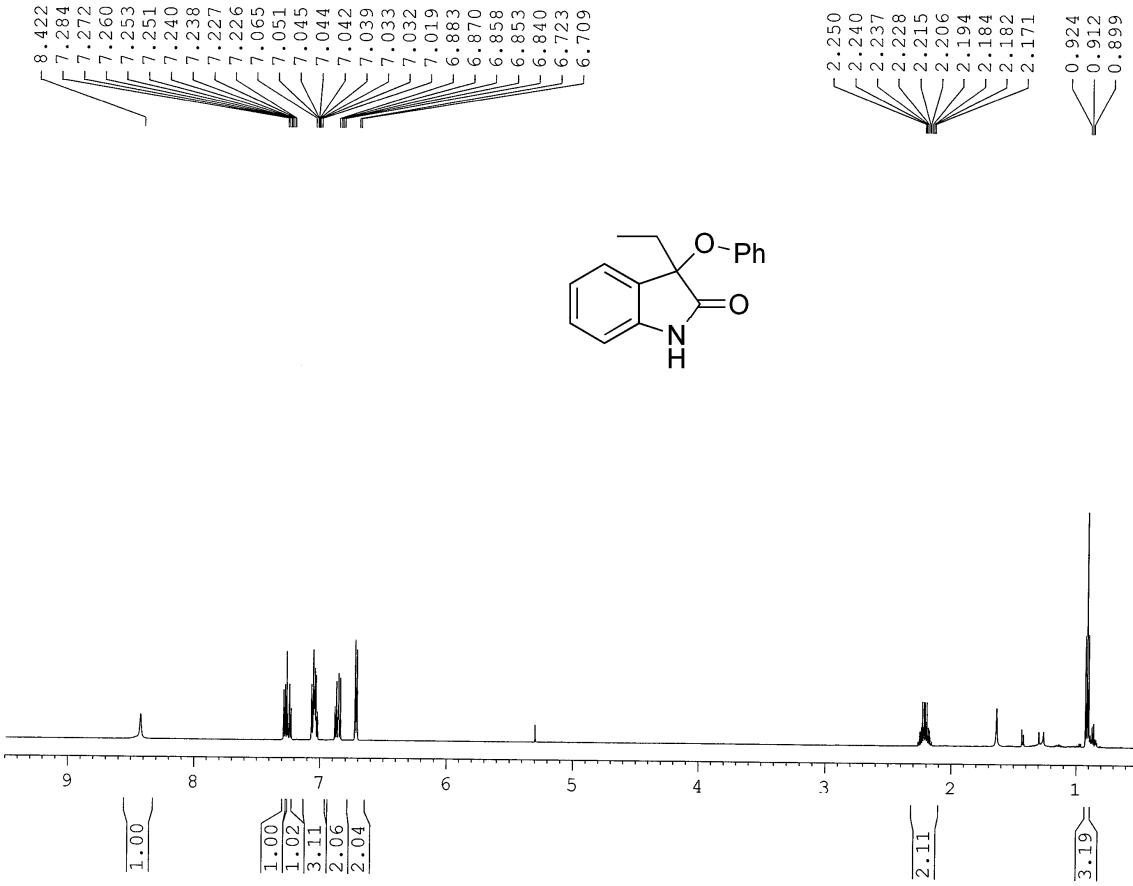


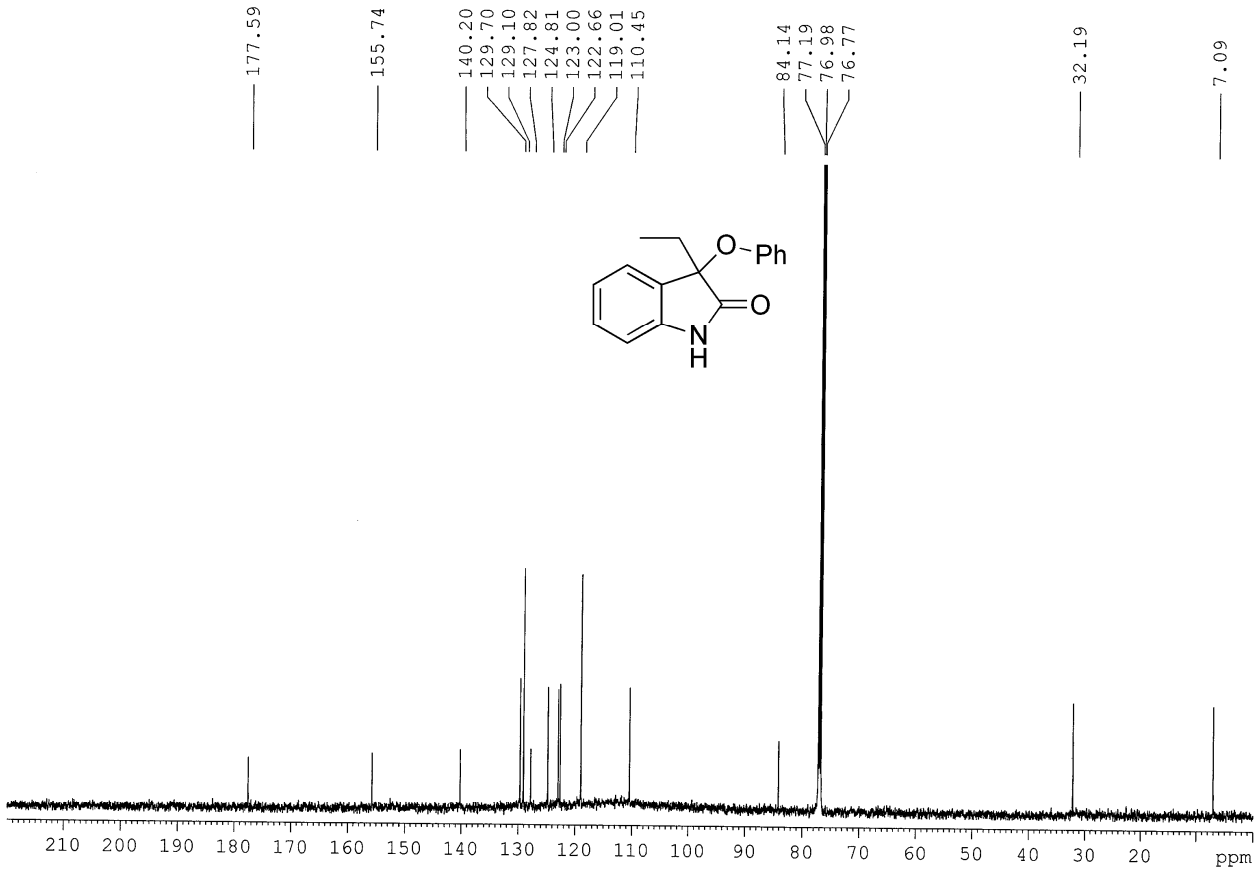




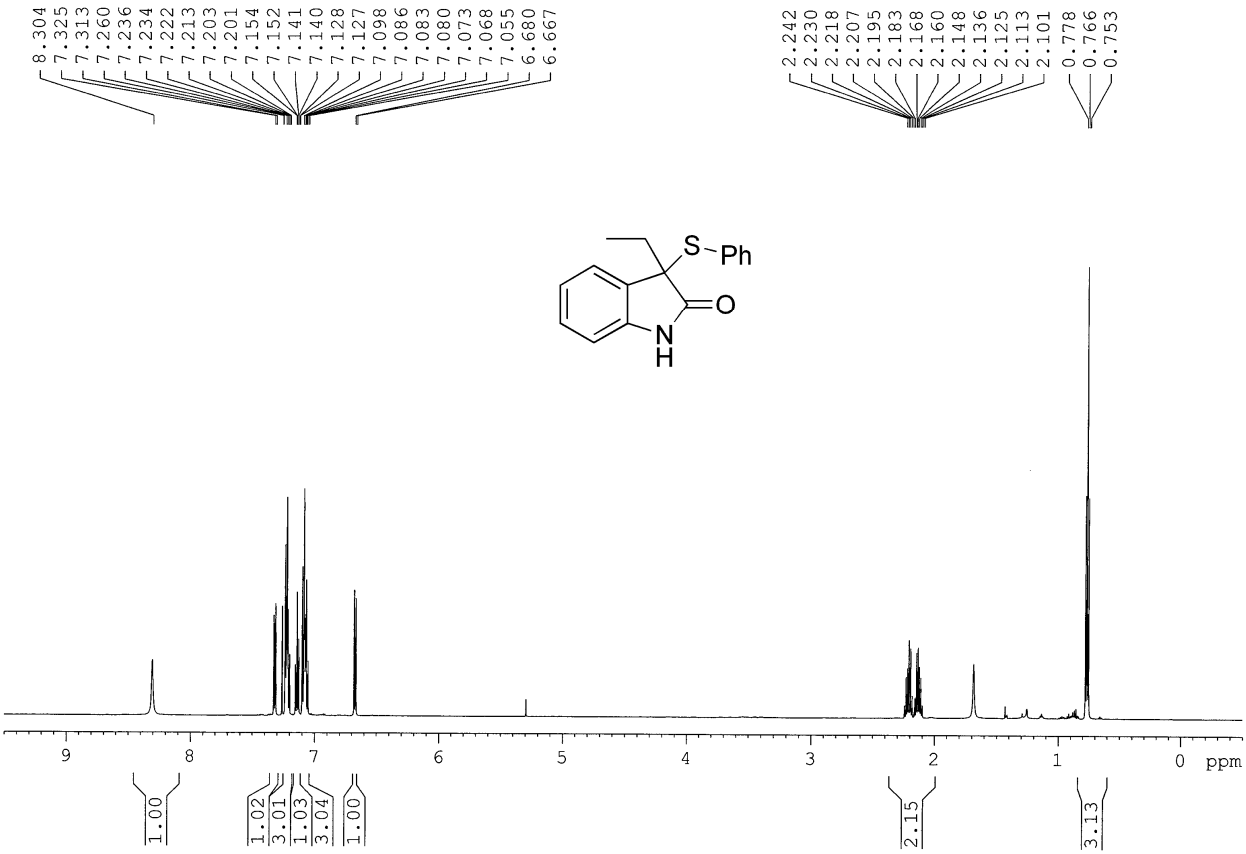


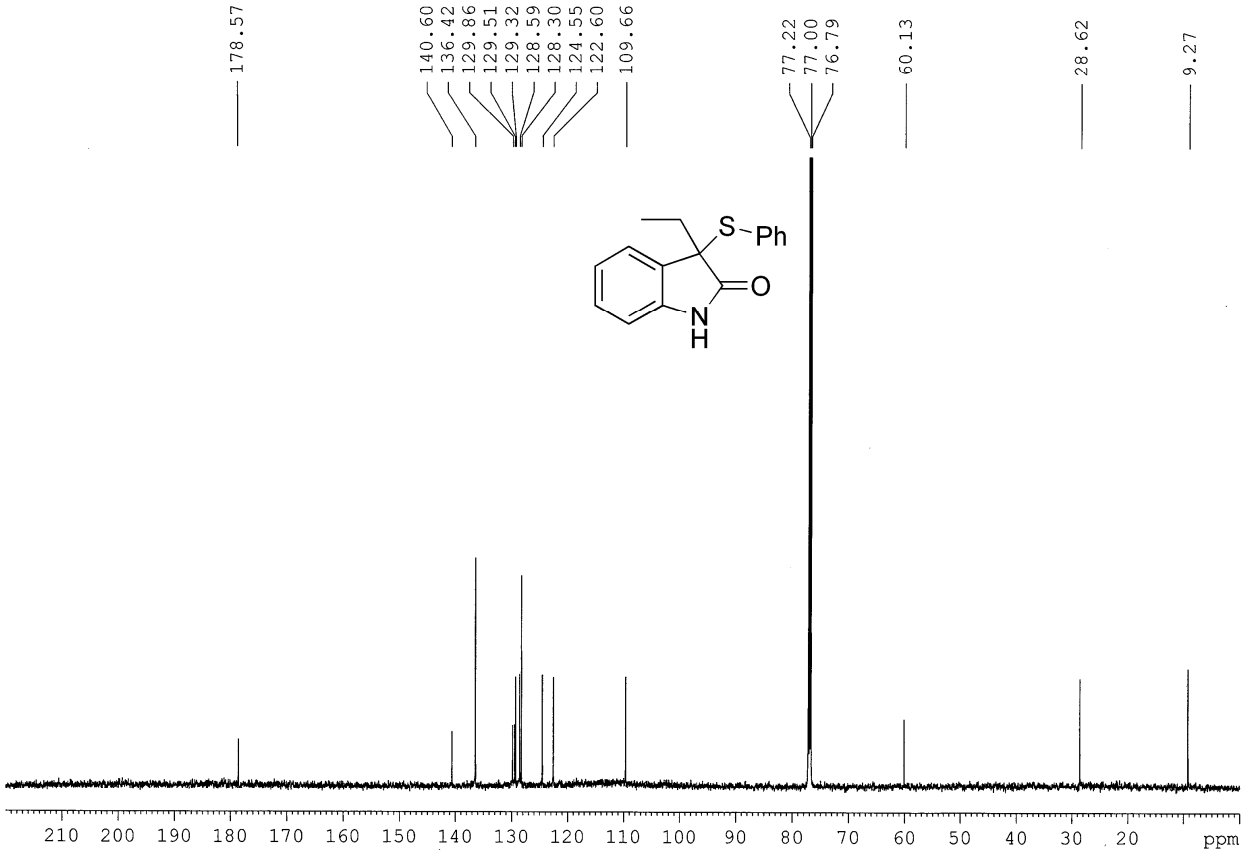
3-Ethyl-3-phenoxyindolin-2-one (2o)



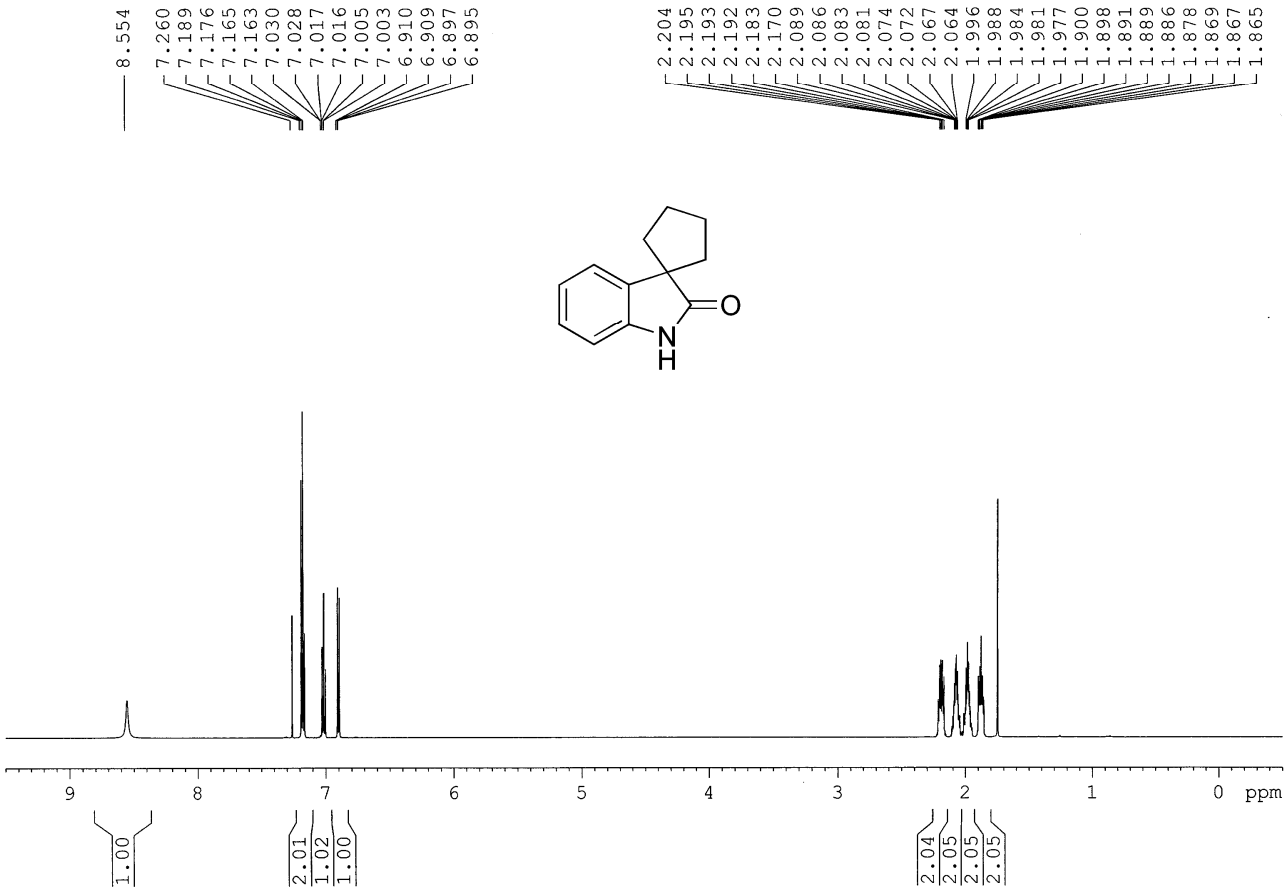


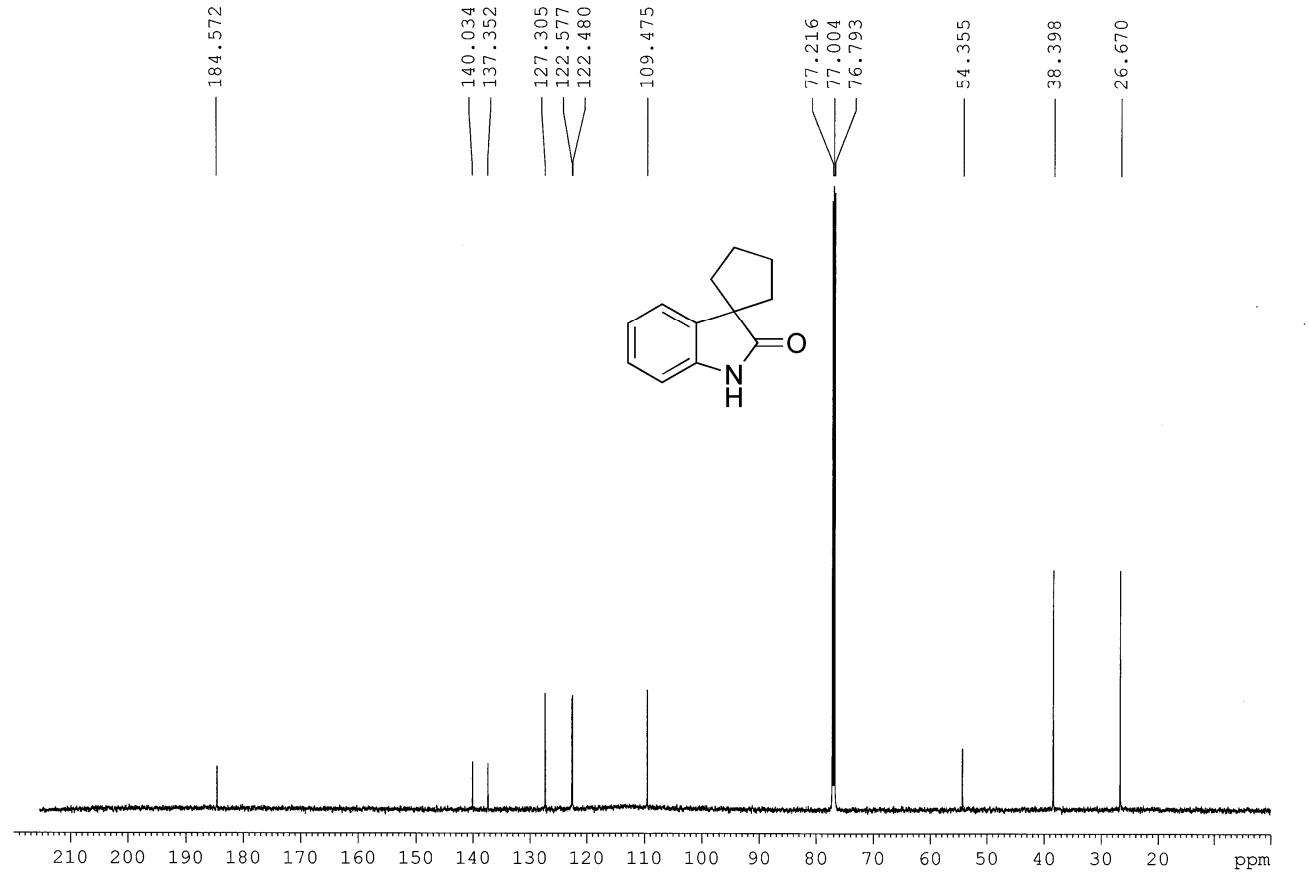
3-Ethyl-3-(phenylthio)indolin-2-one (2p)



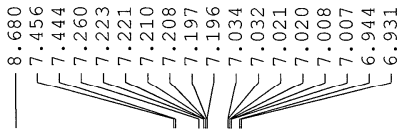


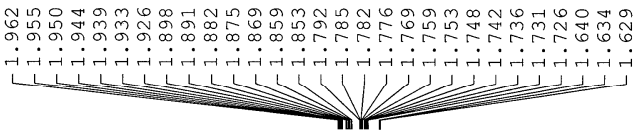
Spiro[cyclopentane-1,3'-indolin]-2'-one (2q)

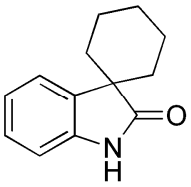


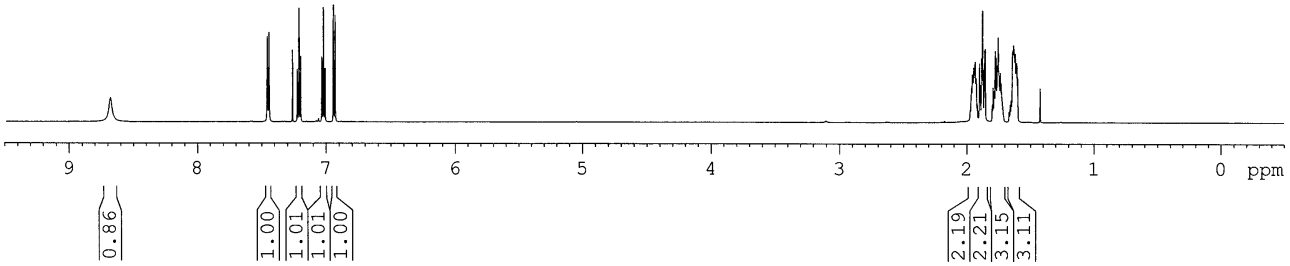


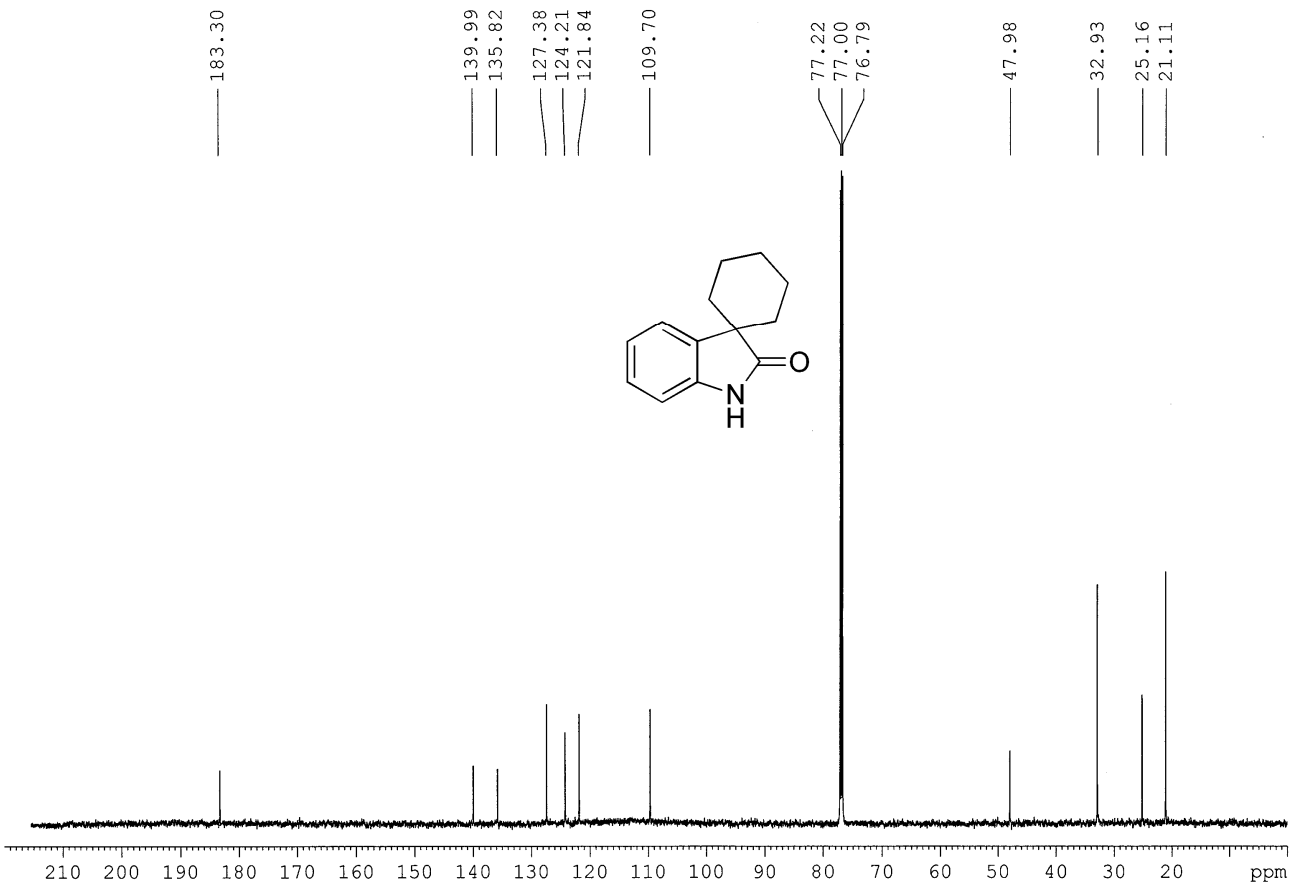
Spiro[cyclohexane-1,3'-indolin]-2'-one (2r)



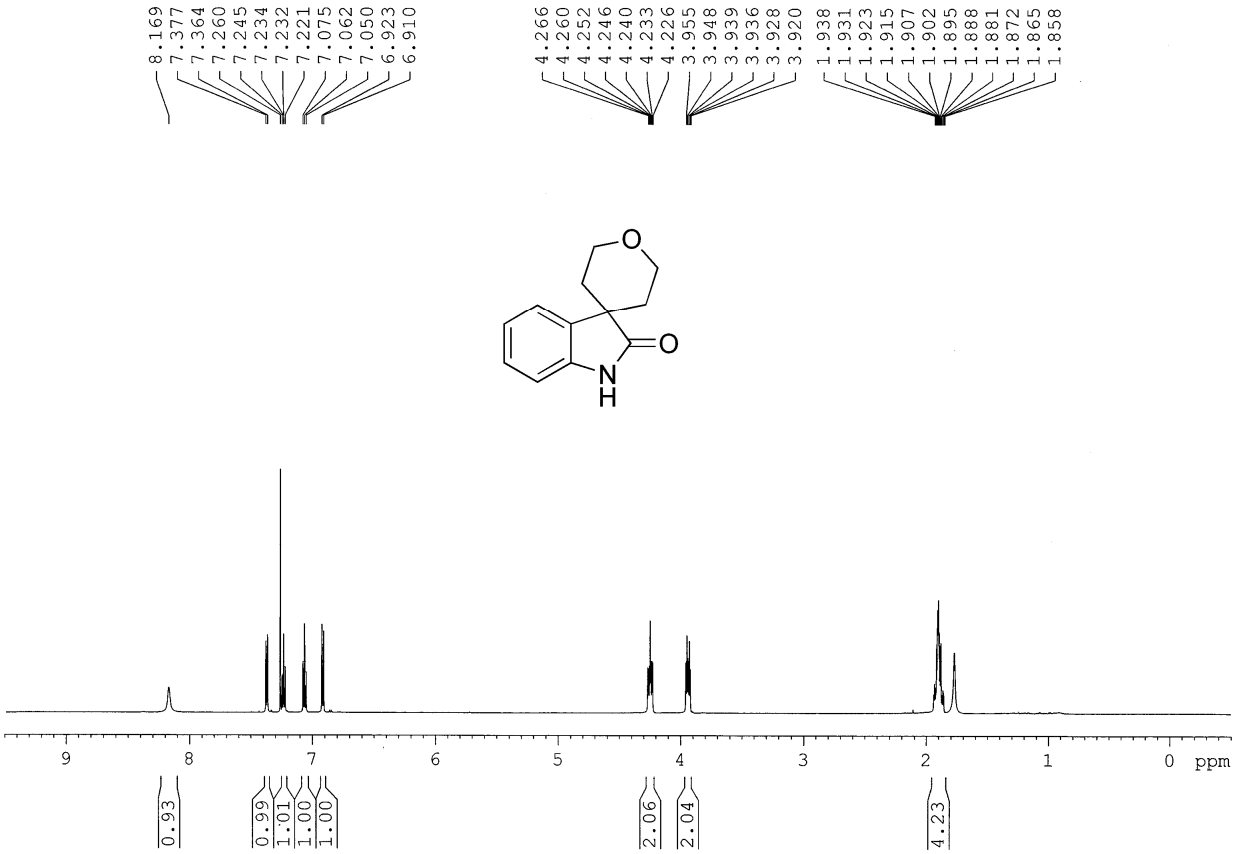


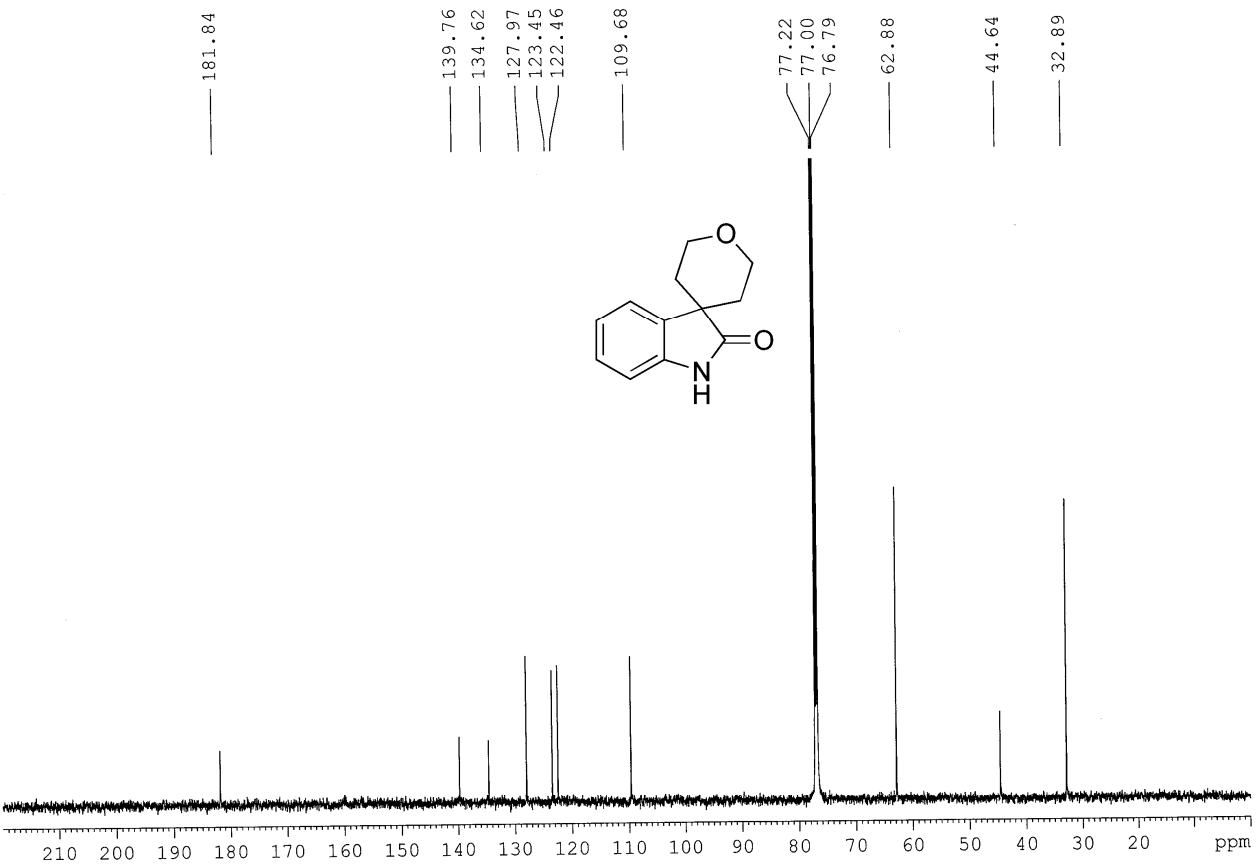




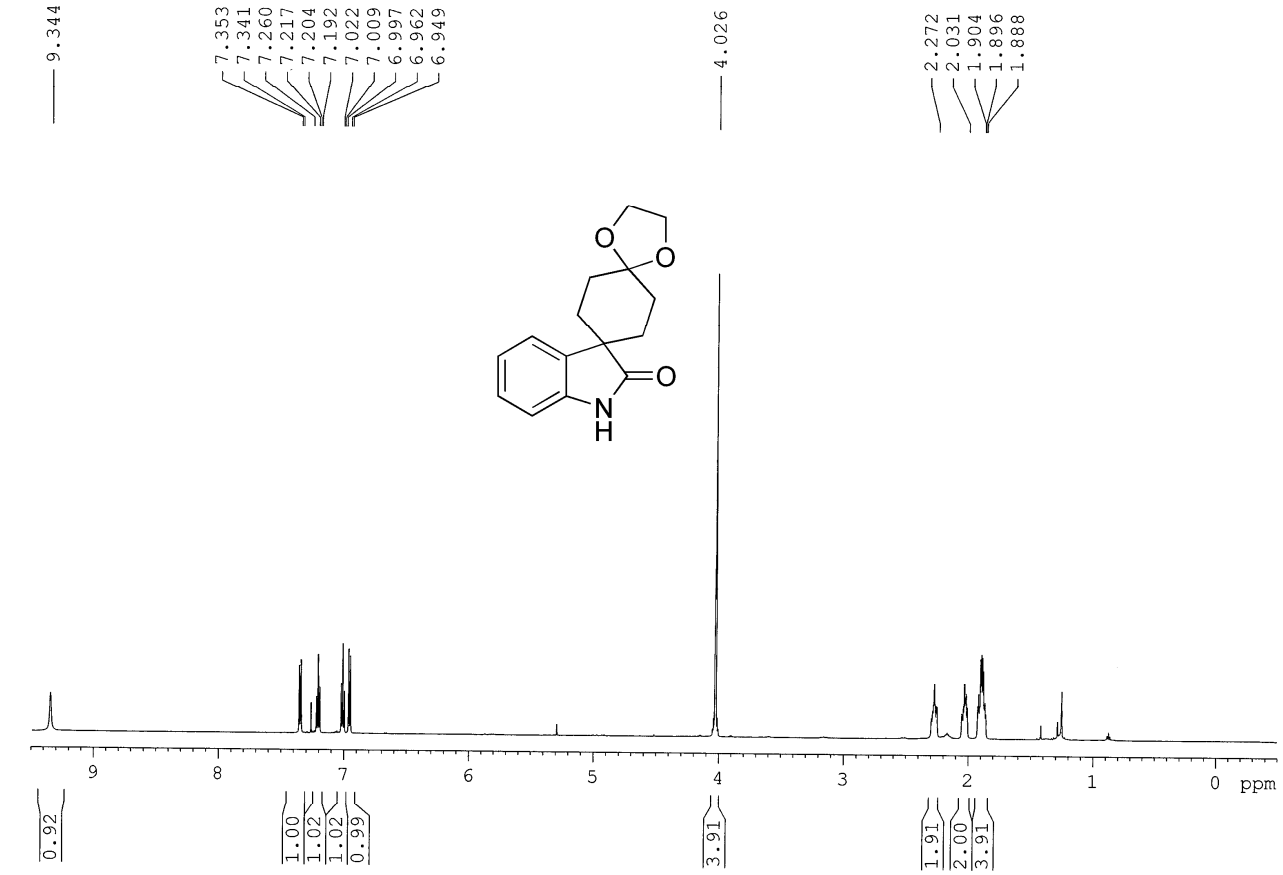


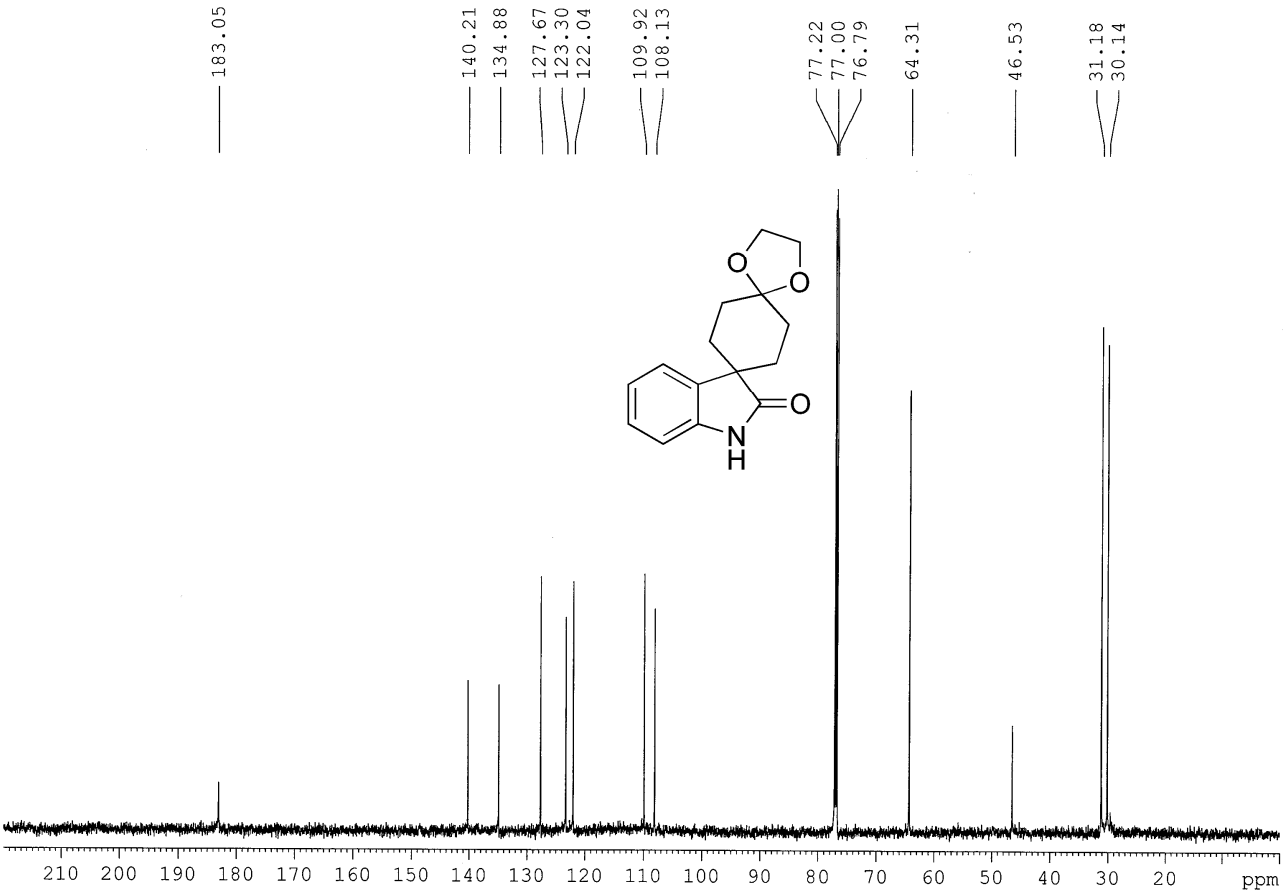
2',3',5',6'-Tetrahydrospiro[indoline-3,4'-pyran]-2-one (2s)



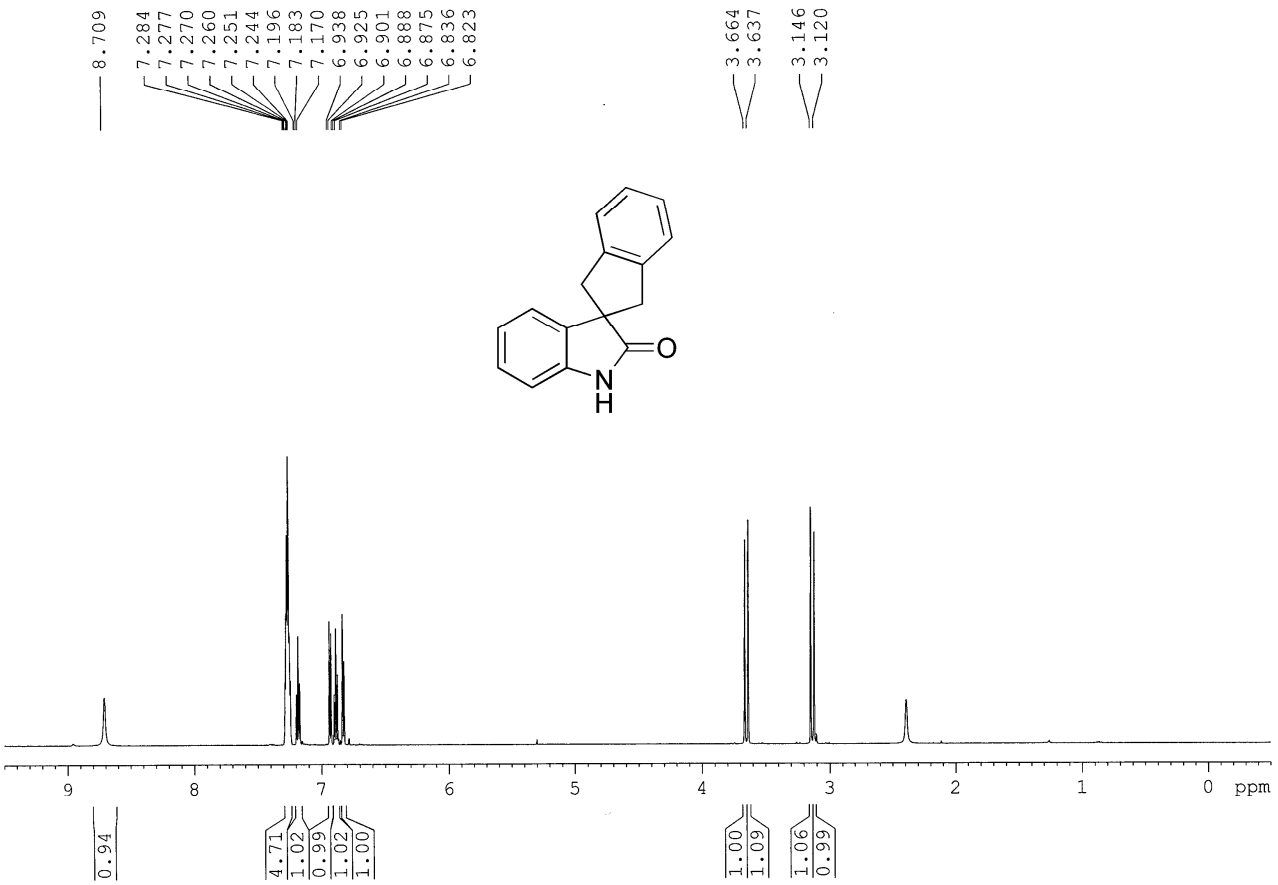


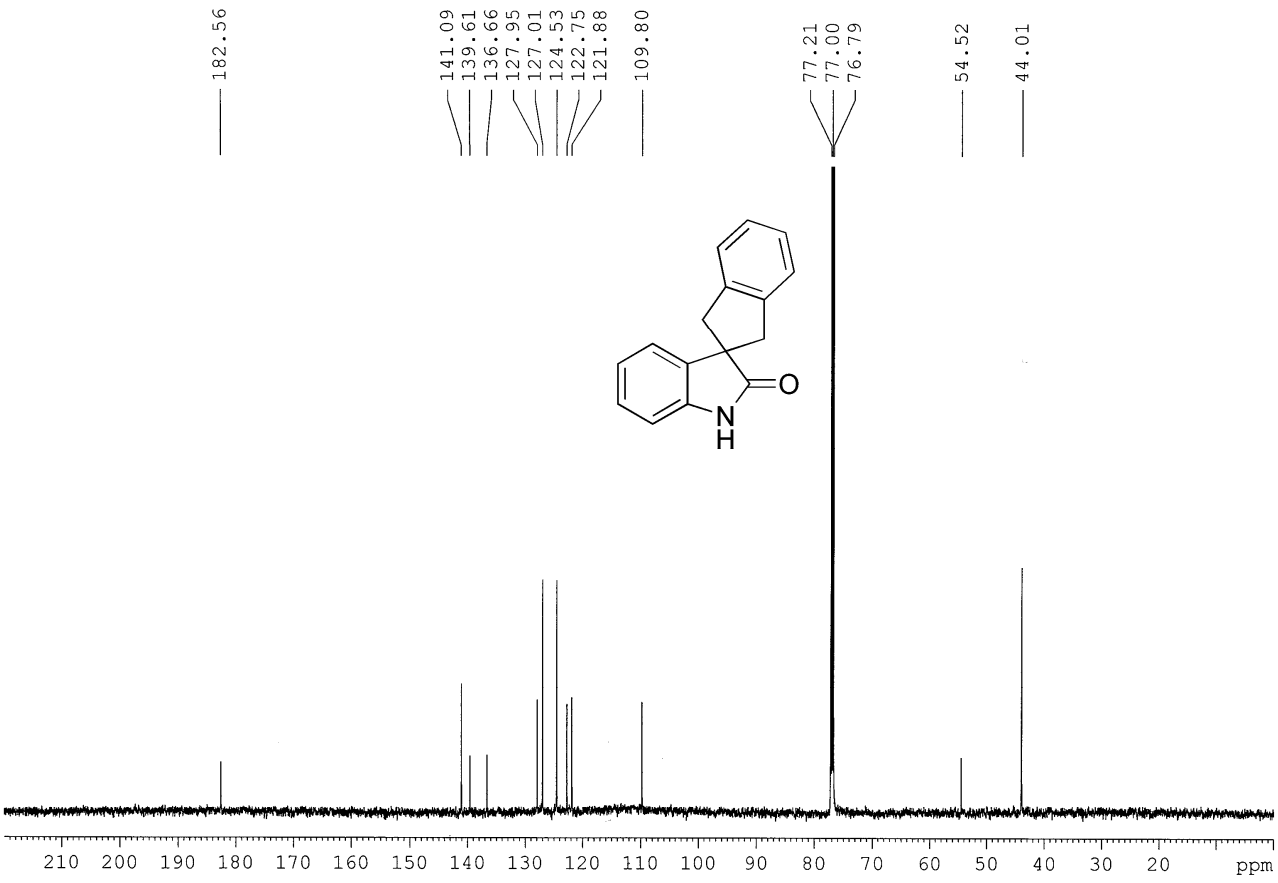
Dispiro[1,3-dioxolane-2,1'-cyclohexane-4',3''-[3*H*]indol]-2''(1''*H*)-one (2t)



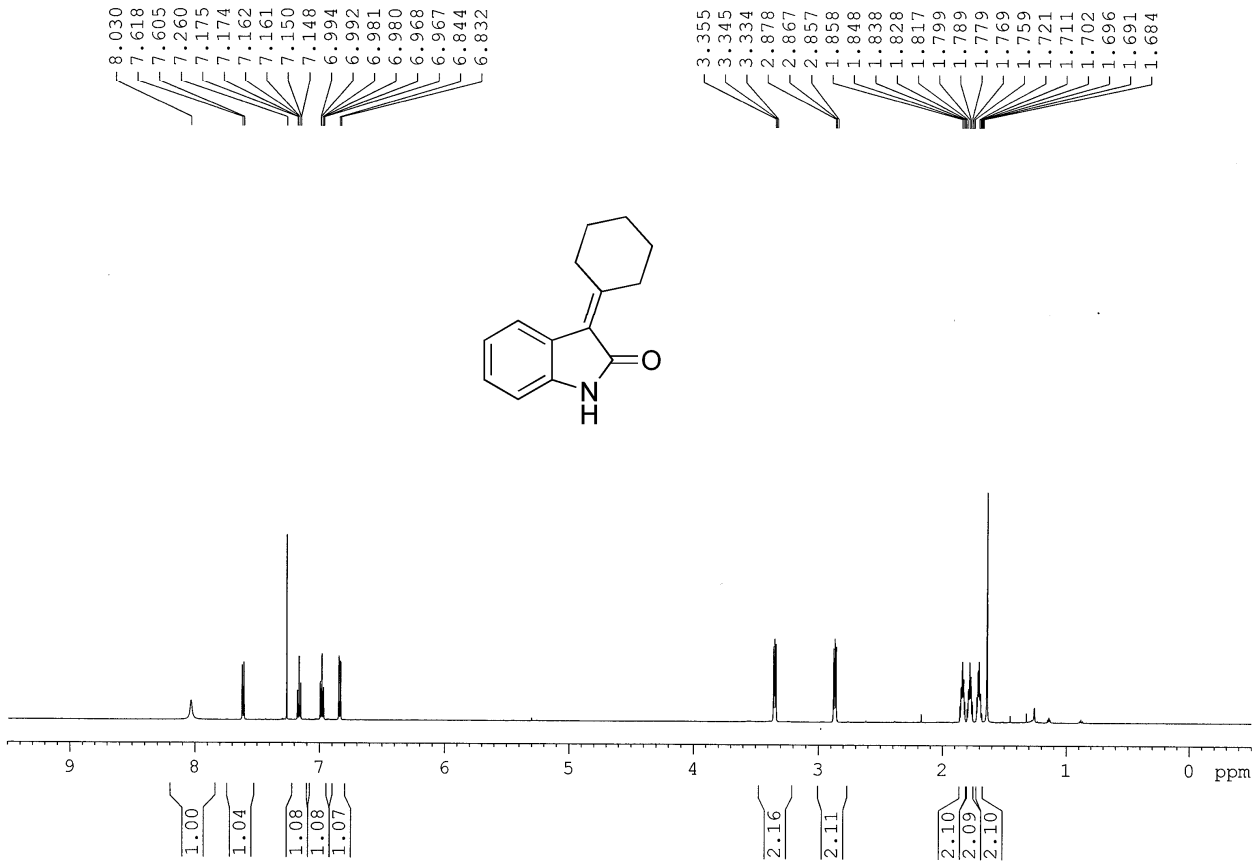


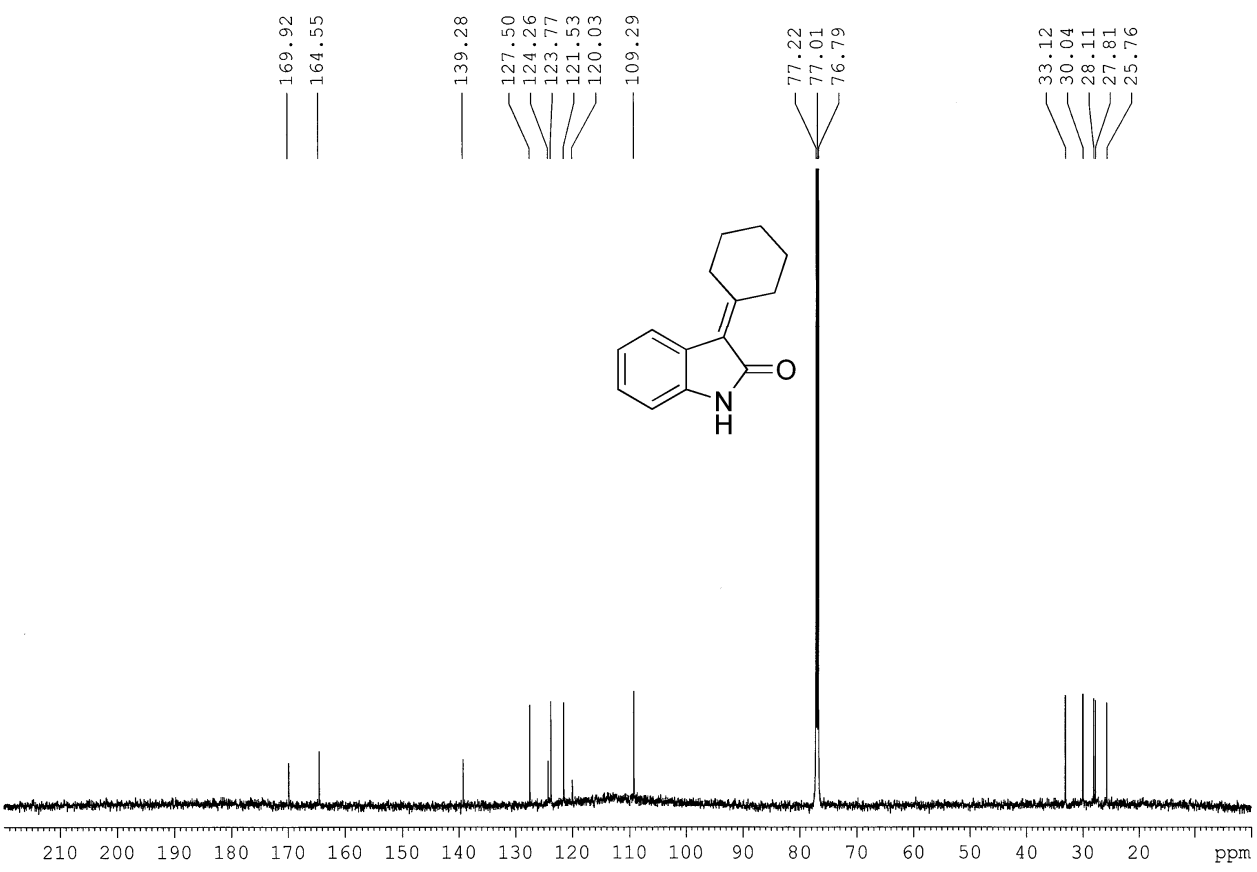
1,3-Dihydrospiro[indene-2,3'-indolin]-2'-one (2u)



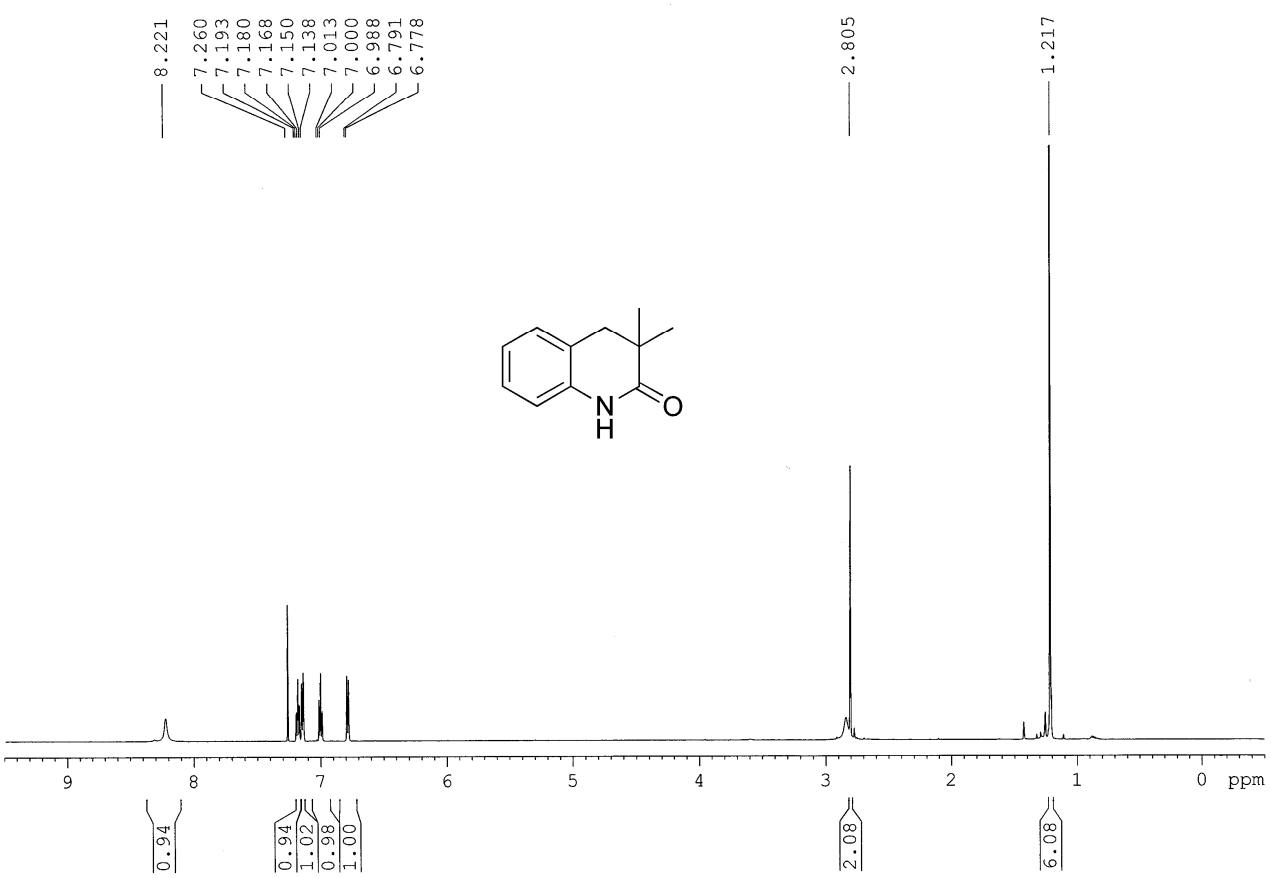


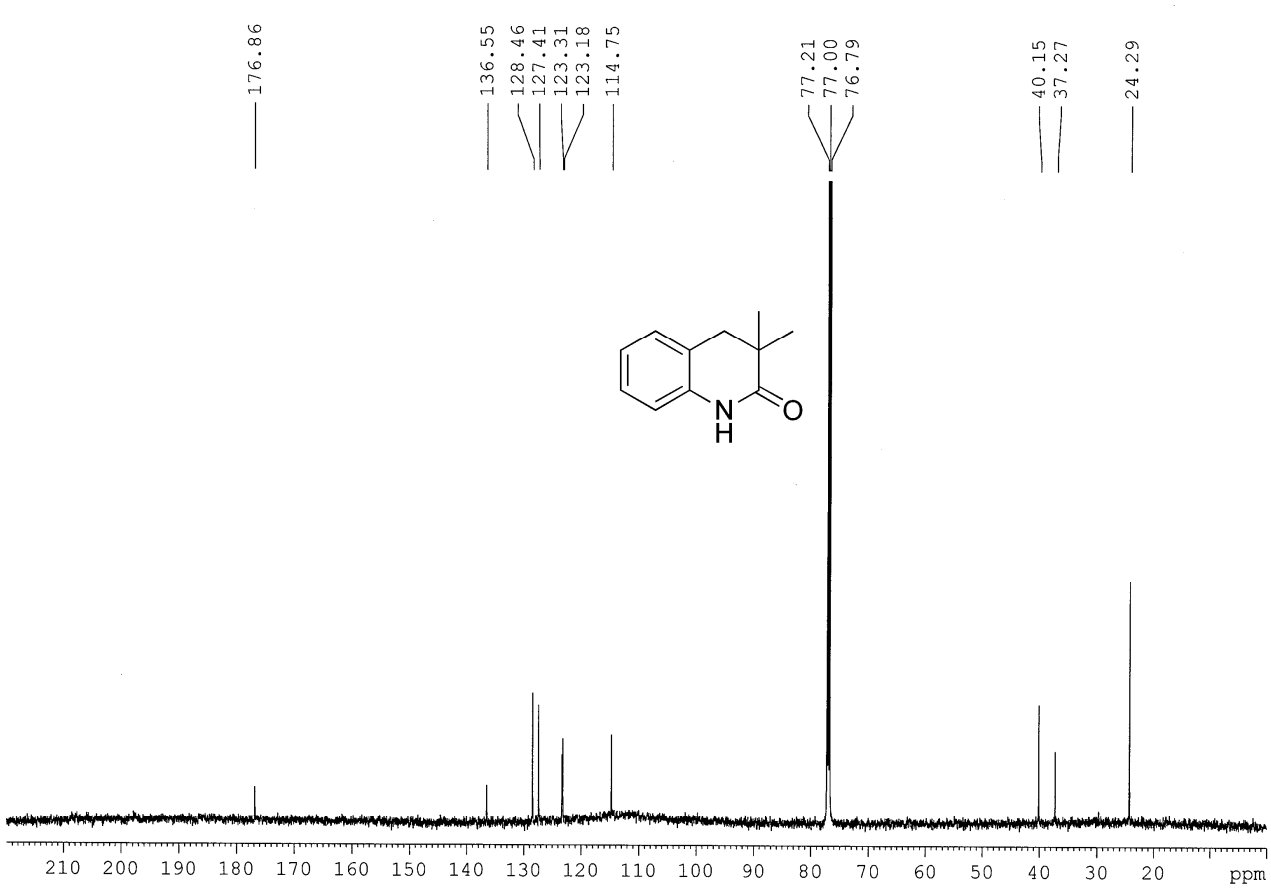
3-Cyclohexylideneindolin-2-one (2v)



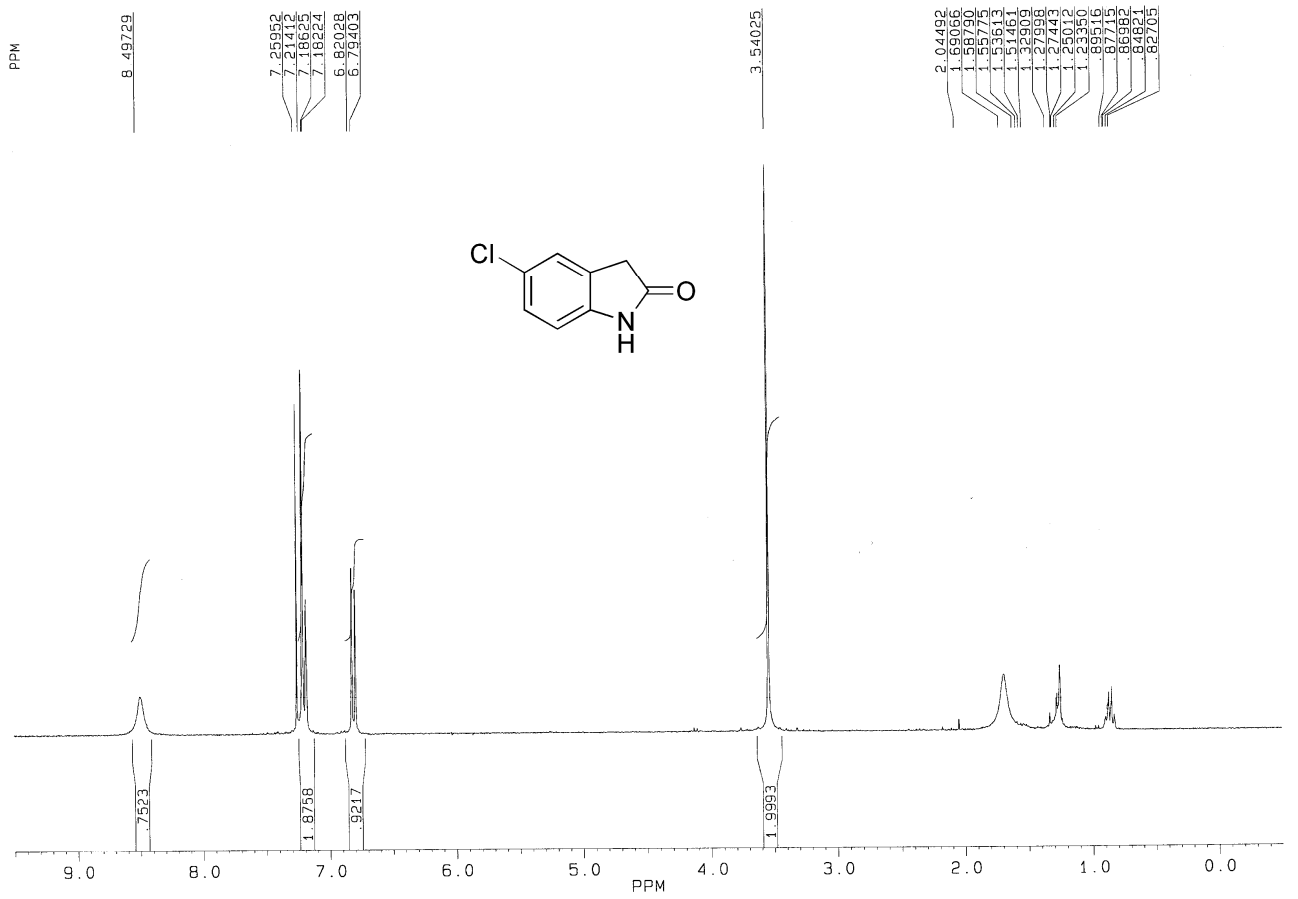


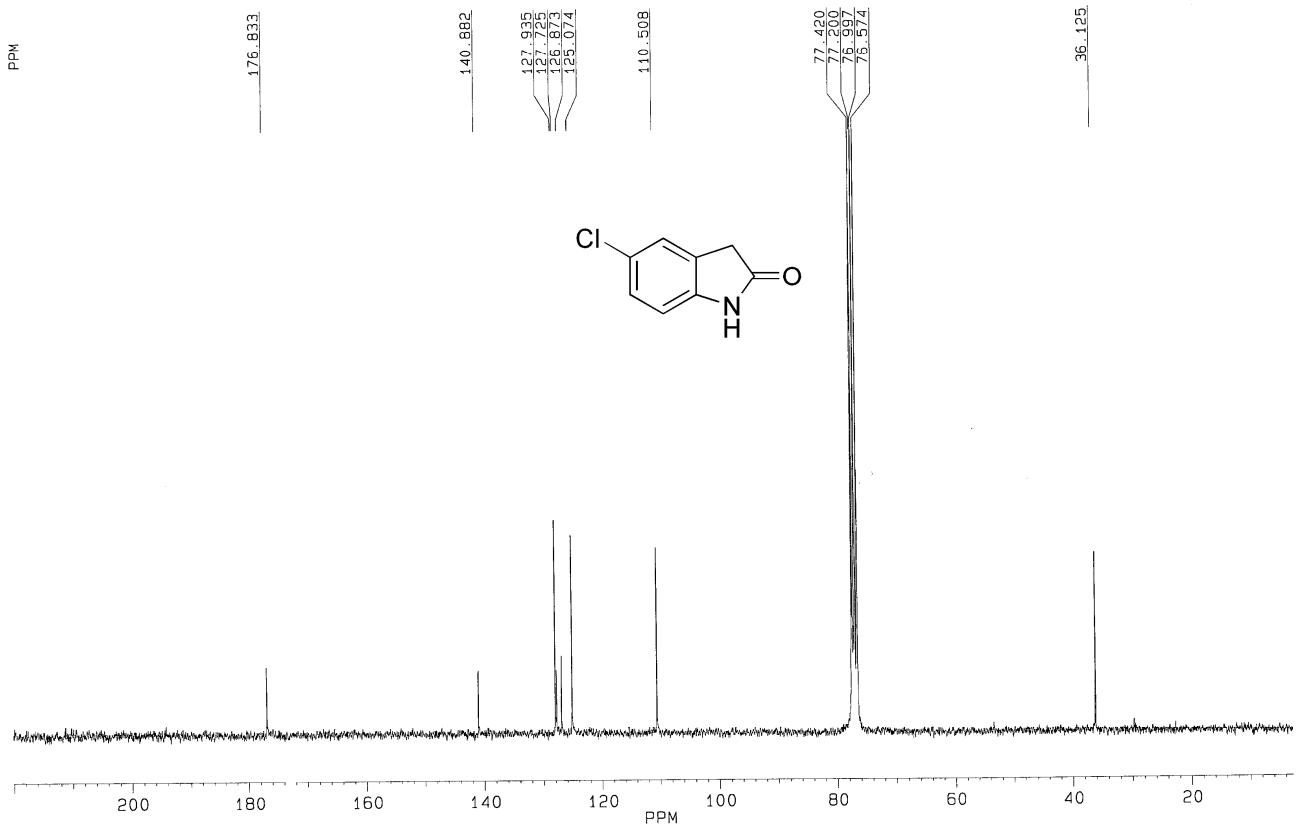
3,3-Dimethyl-3,4-dihydroquinolin-2(1*H*)-one (2y)



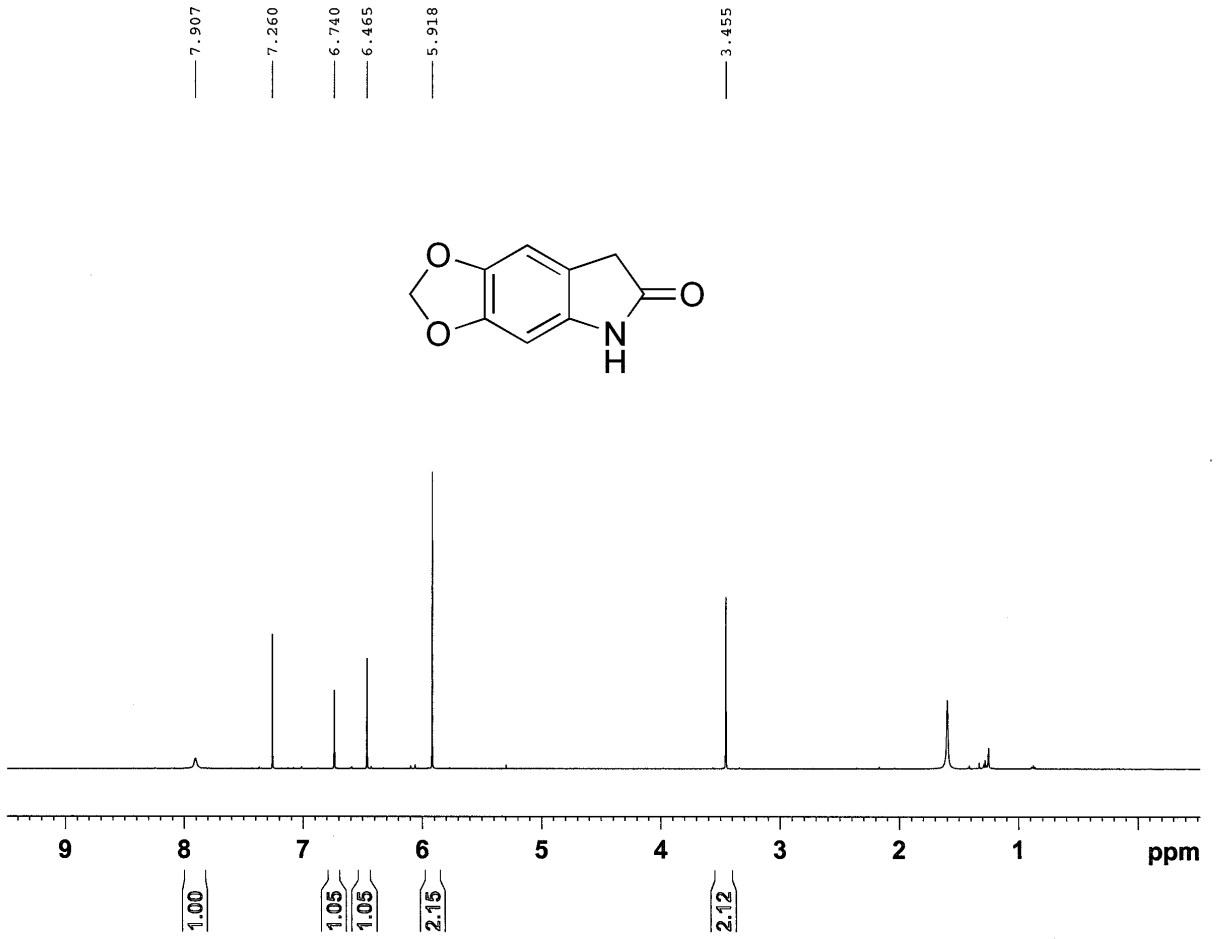


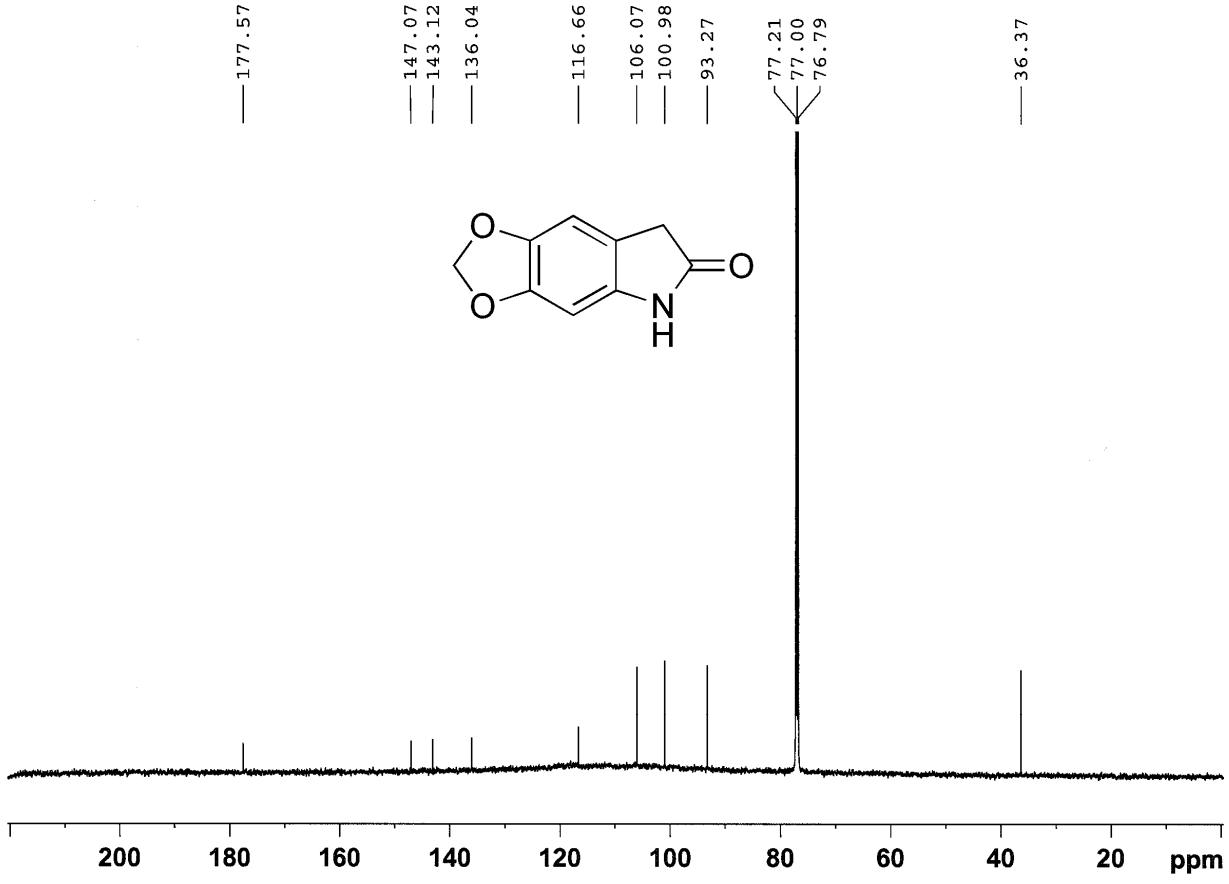
5-Chloroindolin-2-one (2w, 300 MHz, $CDCl_3$)



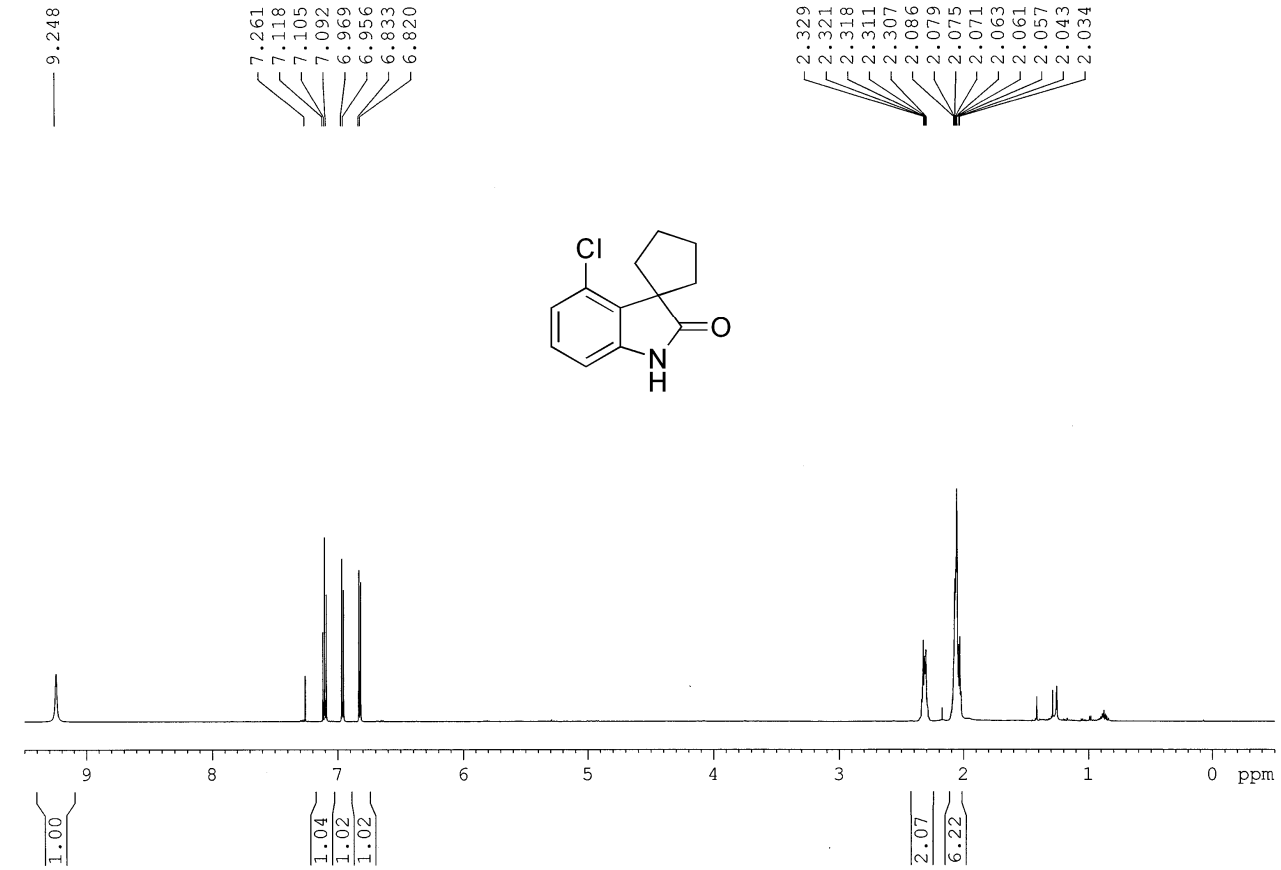


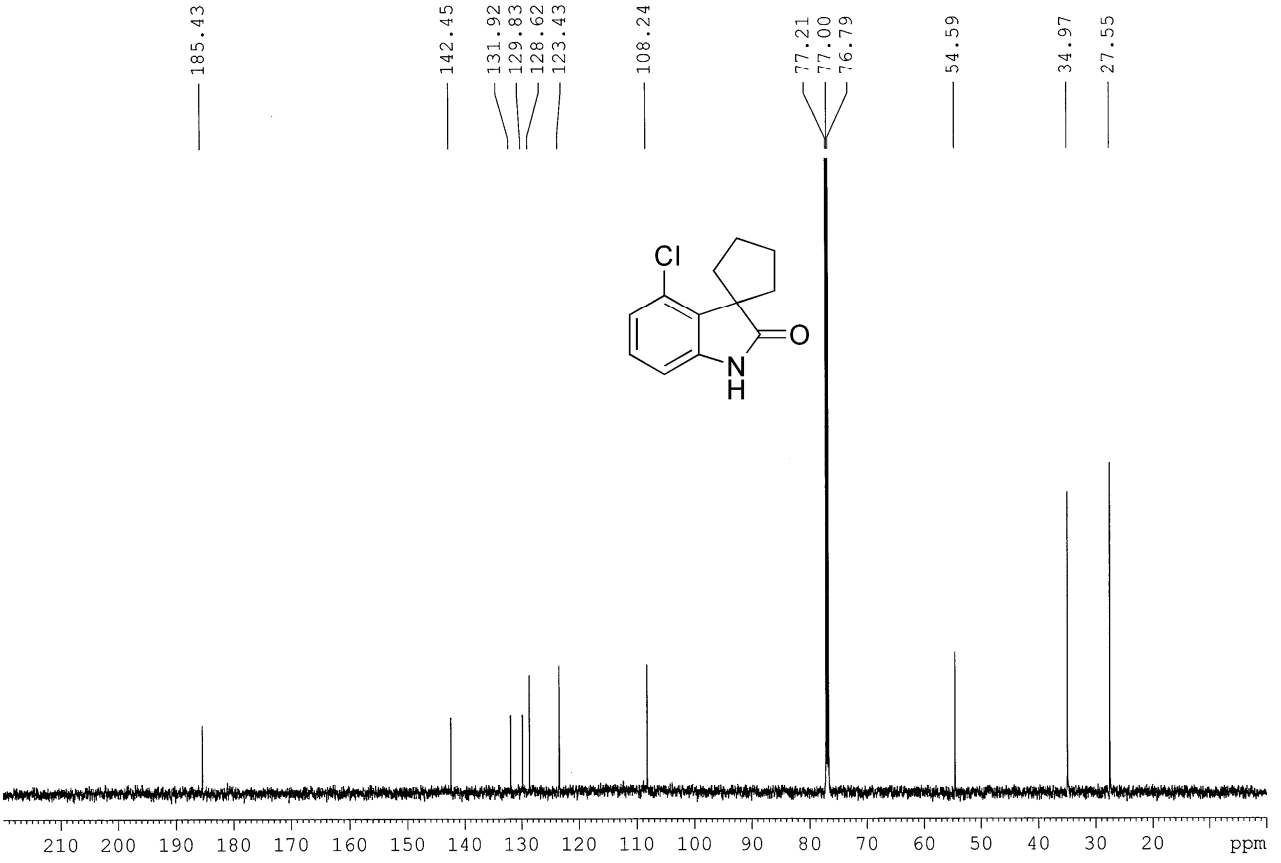
5*H*-[1,3]dioxolo[4,5-*f*]indol-6(7*H*)-one (2x)



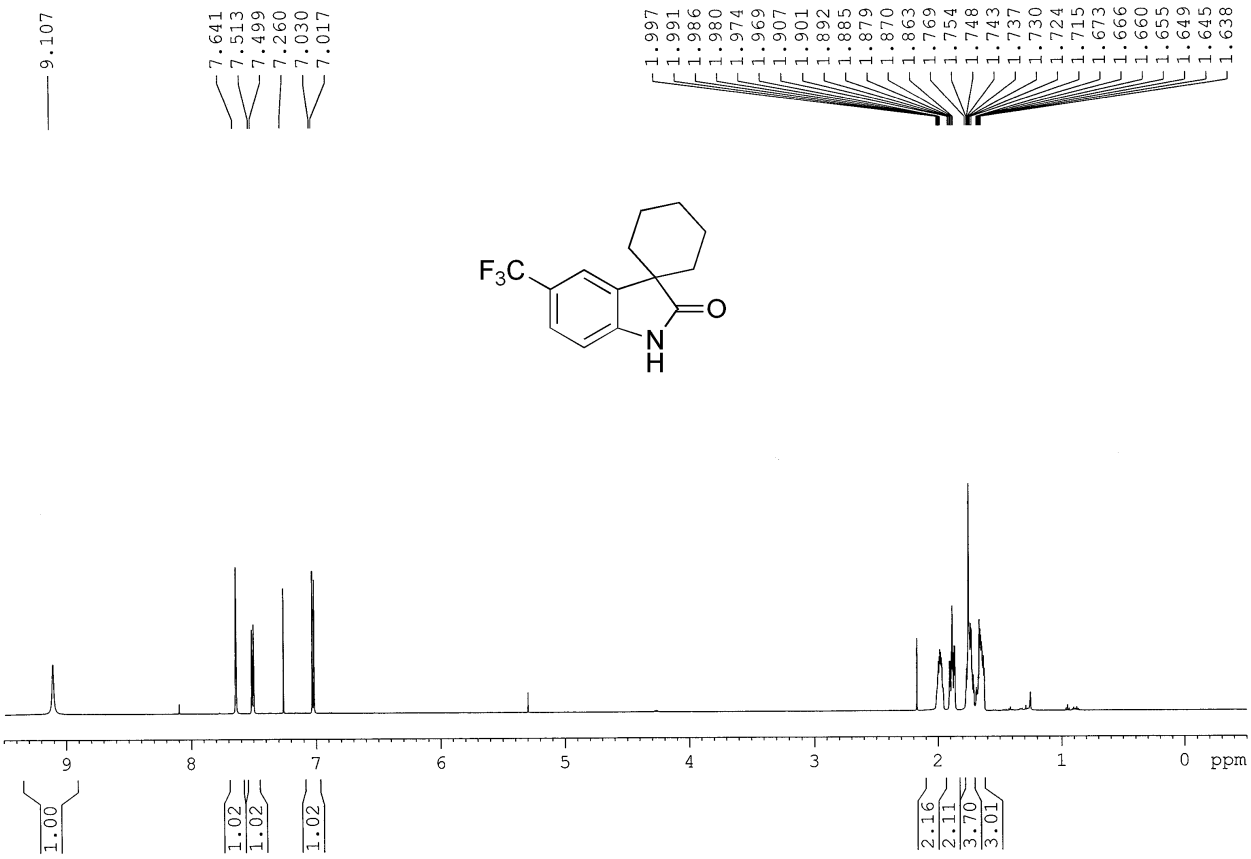


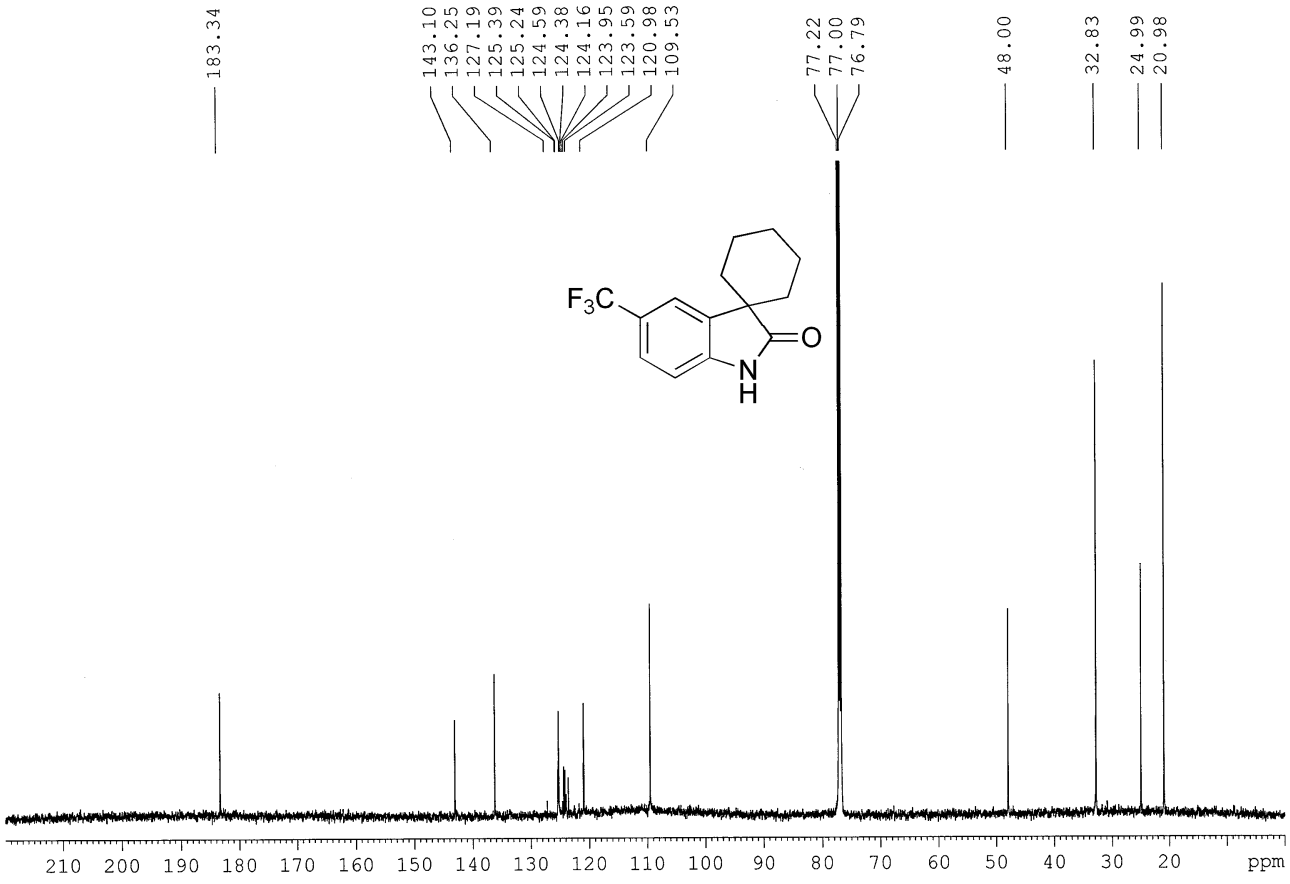
4'-Chlorospiro[cyclopentane-1,3'-indolin]-2'-one (2A)



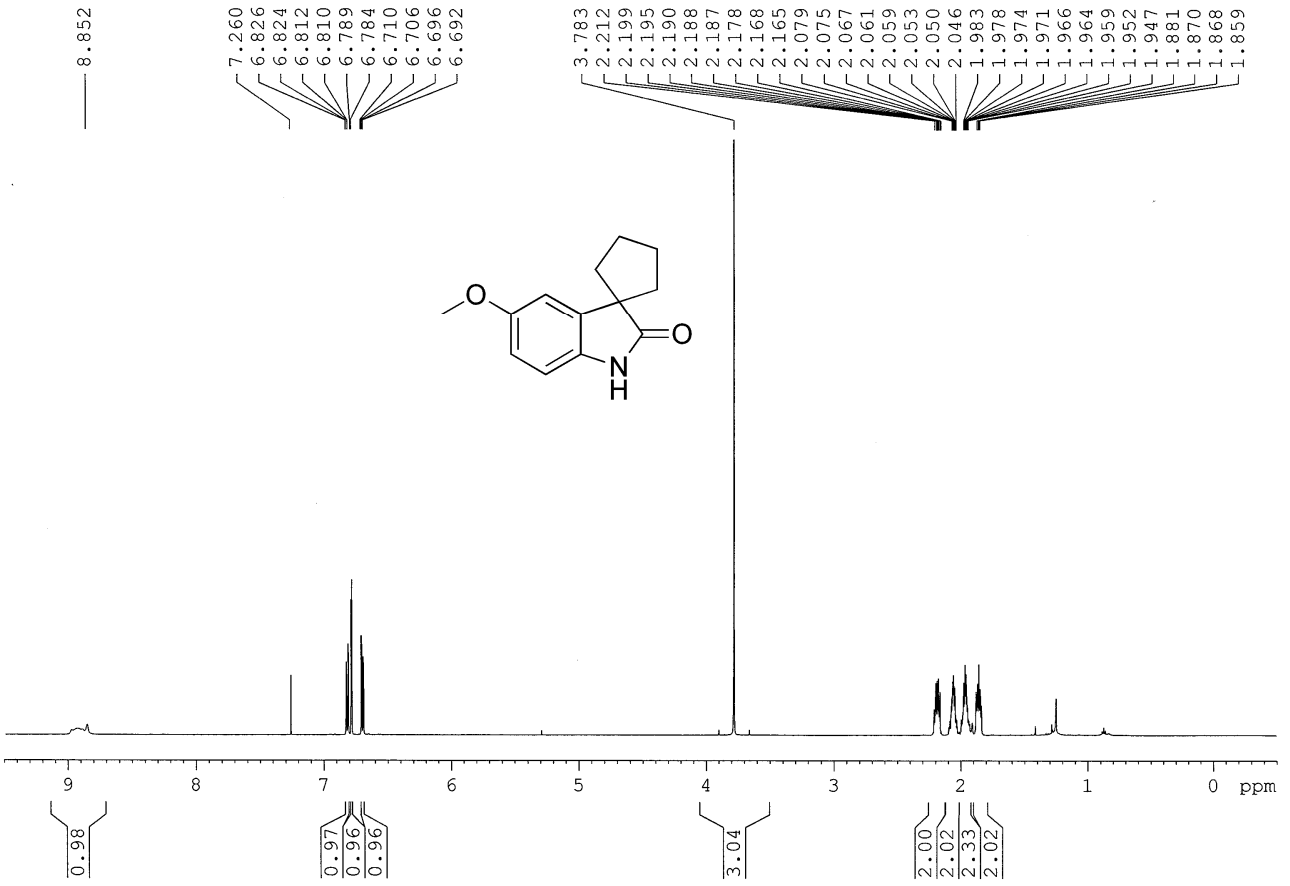


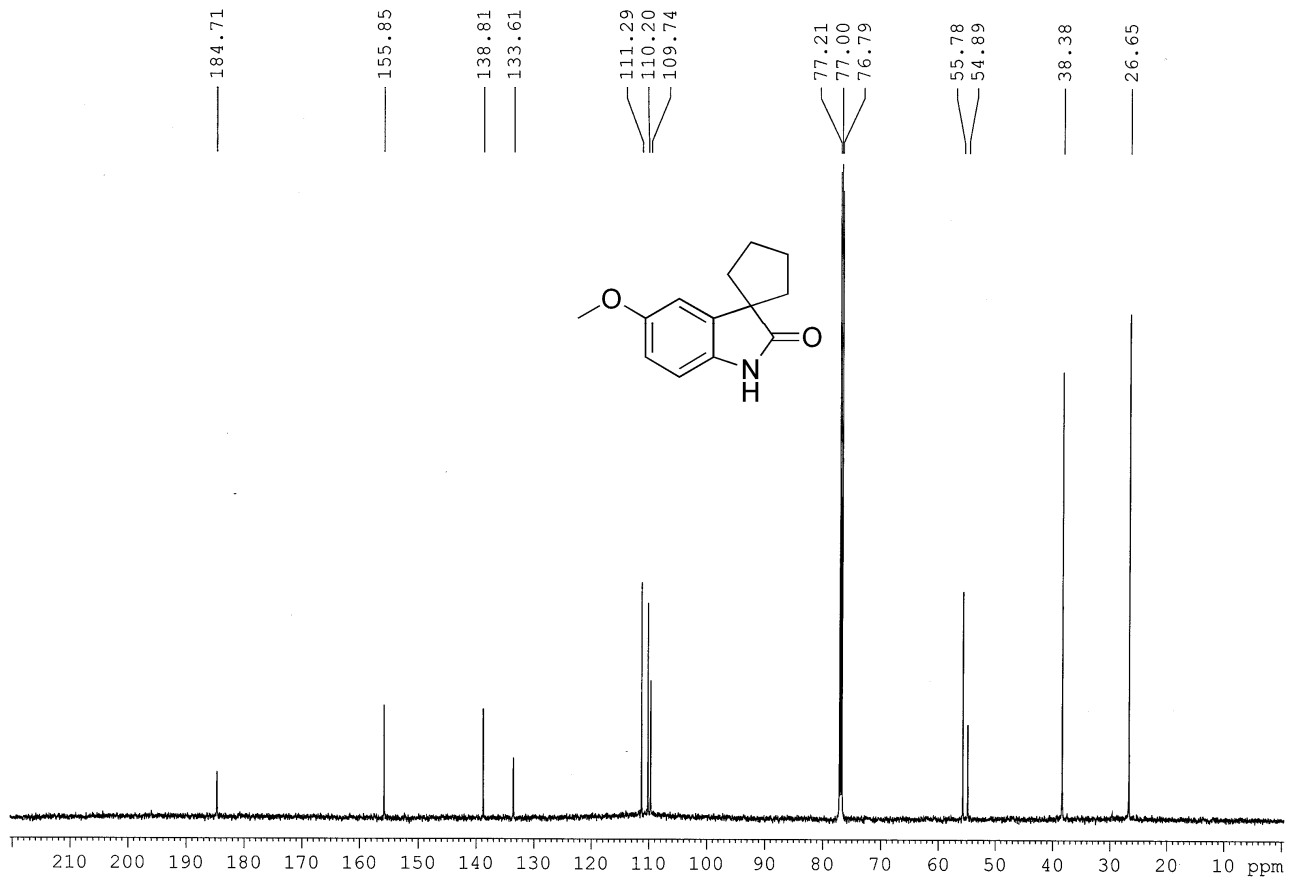
5'-(Trifluoromethyl)spiro[cyclohexane-1,3'-indolin]-2'-one (2B)



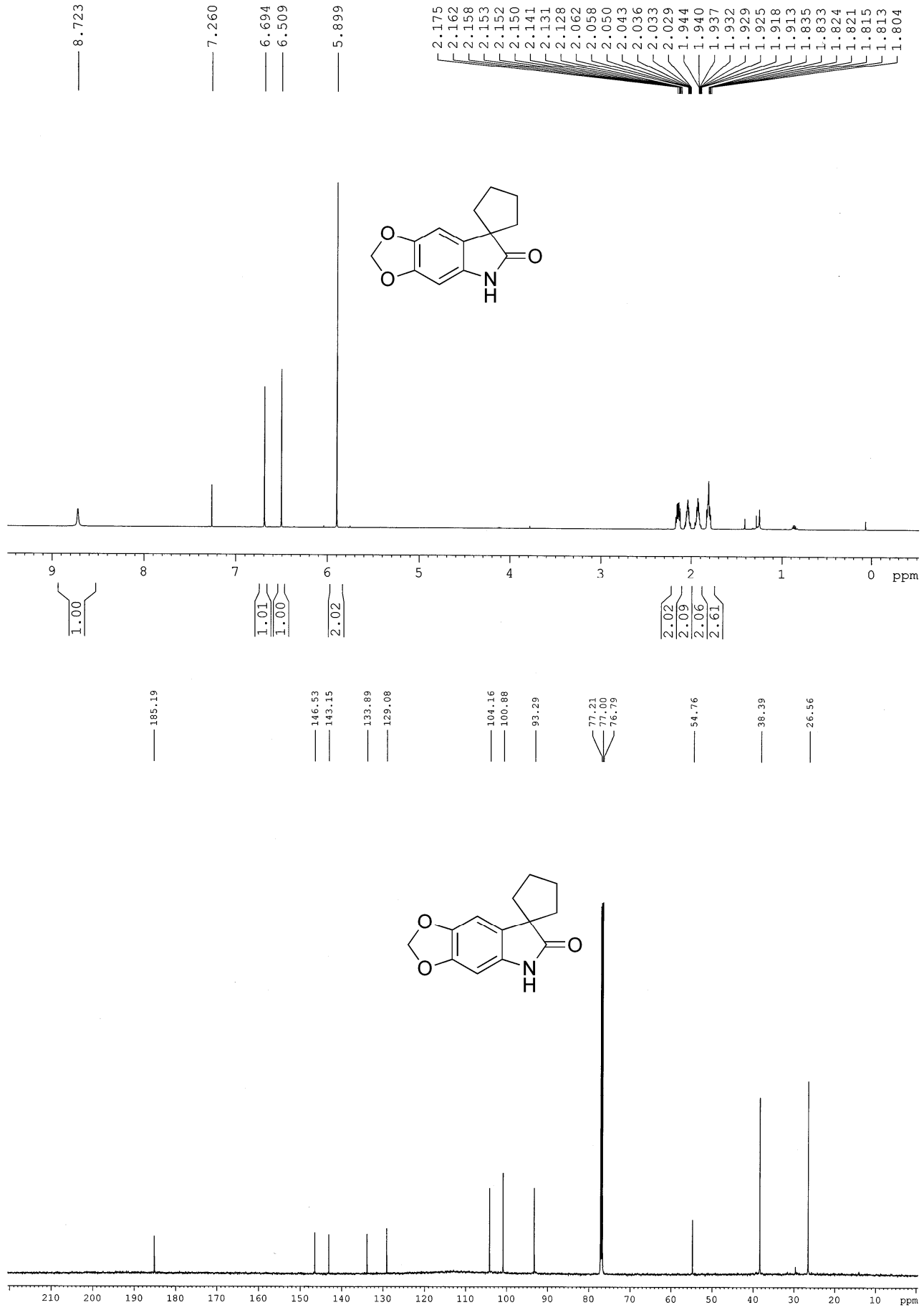


5'-Methoxyspiro[cyclopentane-1,3'-indolin]-2'-one (2C)

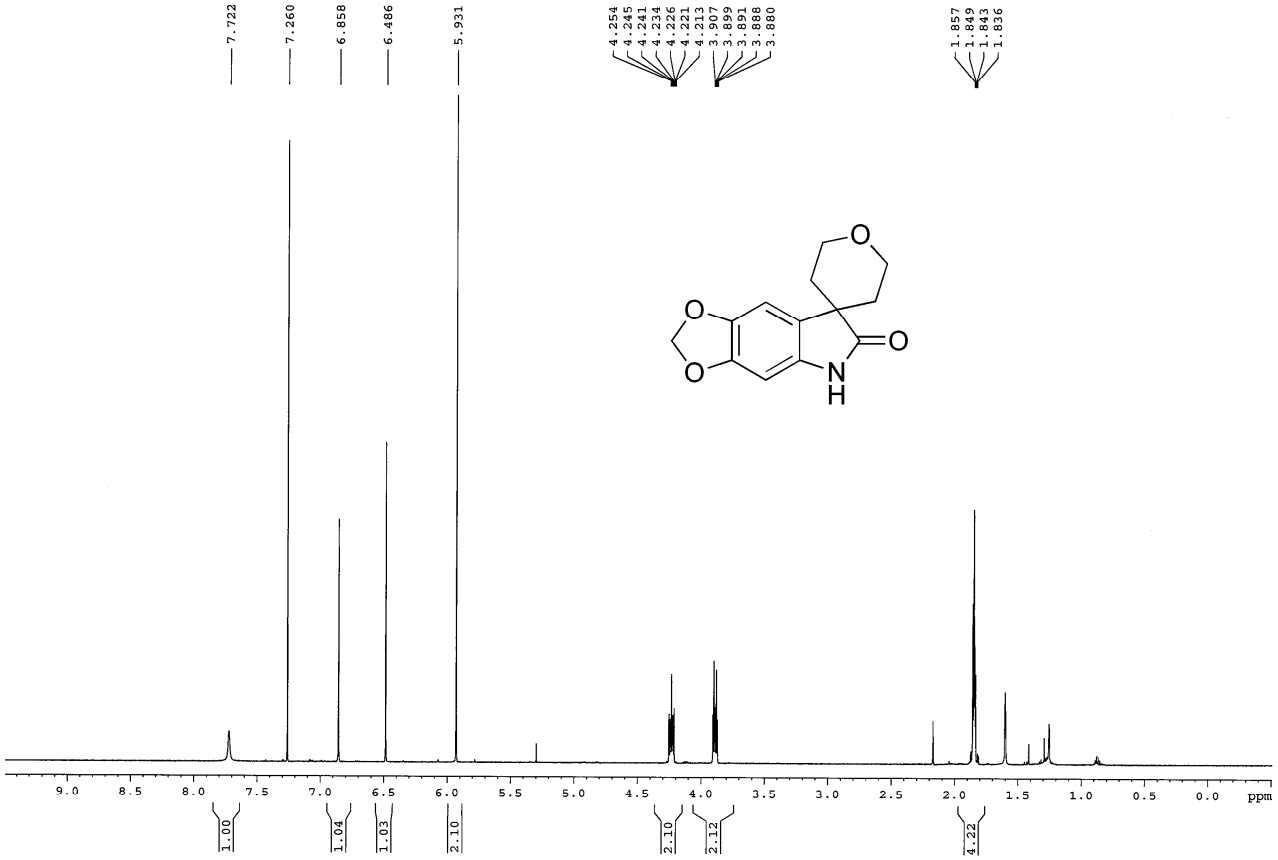


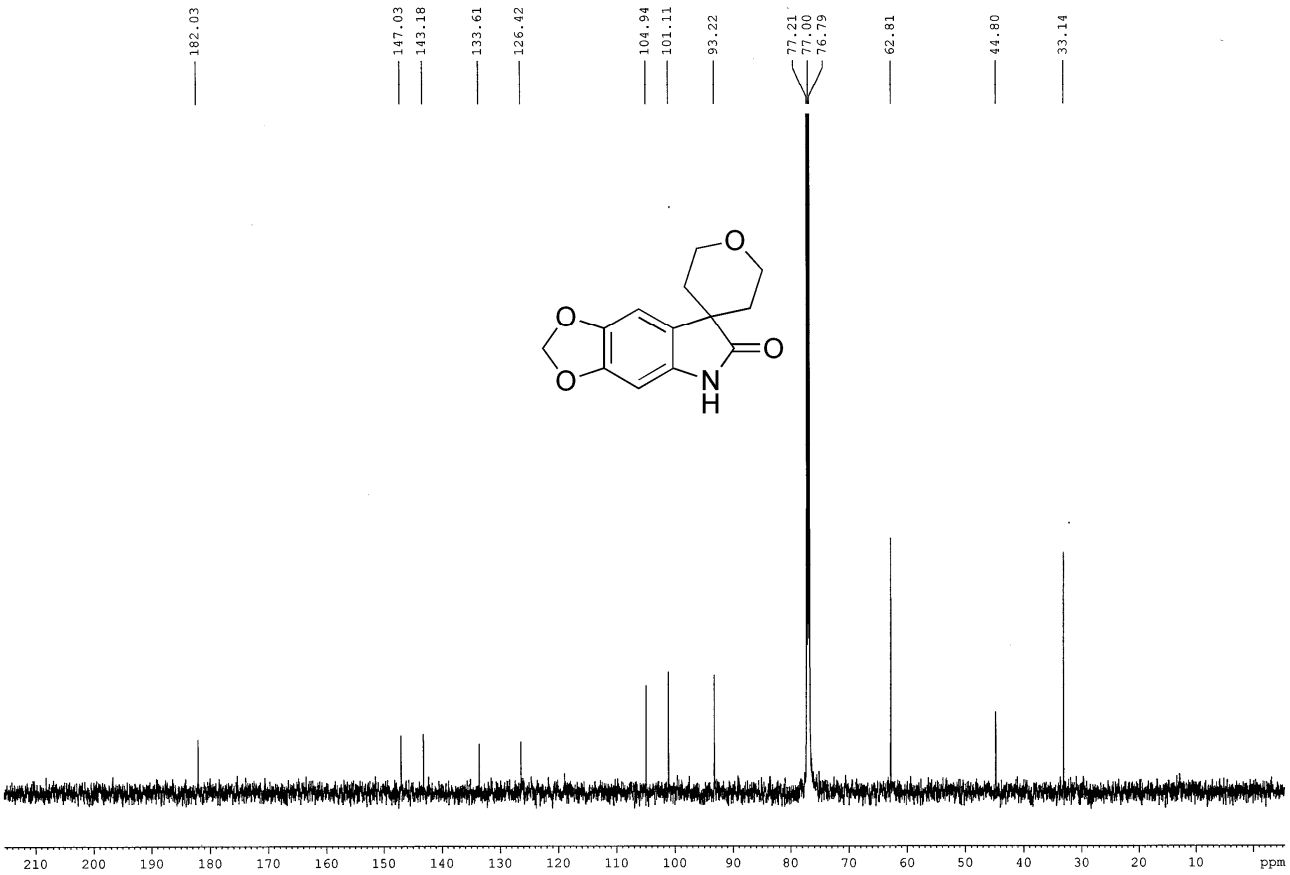


Spiro[[1,3]dioxolo[4,5-*f*]indole-7,1'-cyclopentan]-6(5*H*)-one (2D')

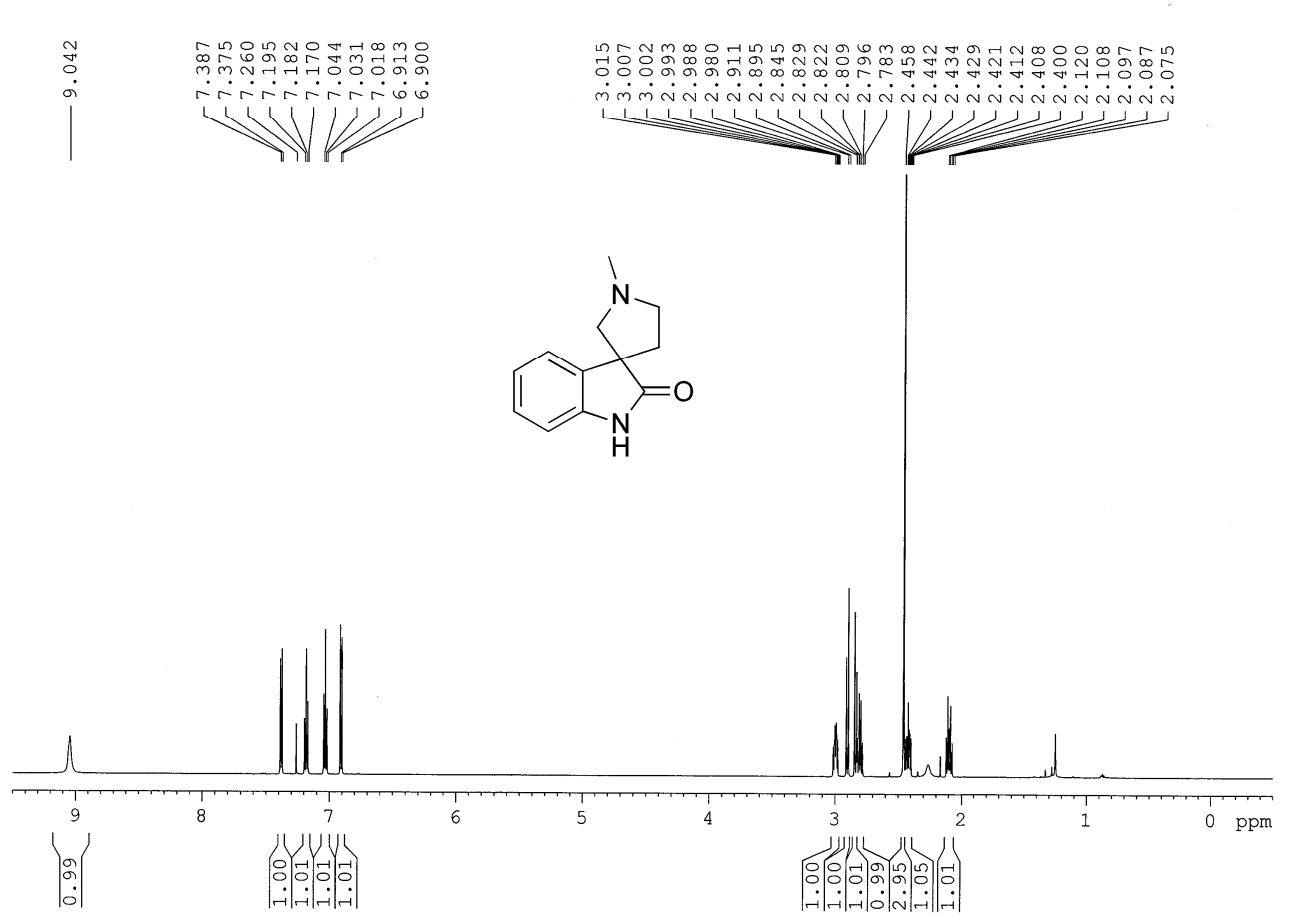


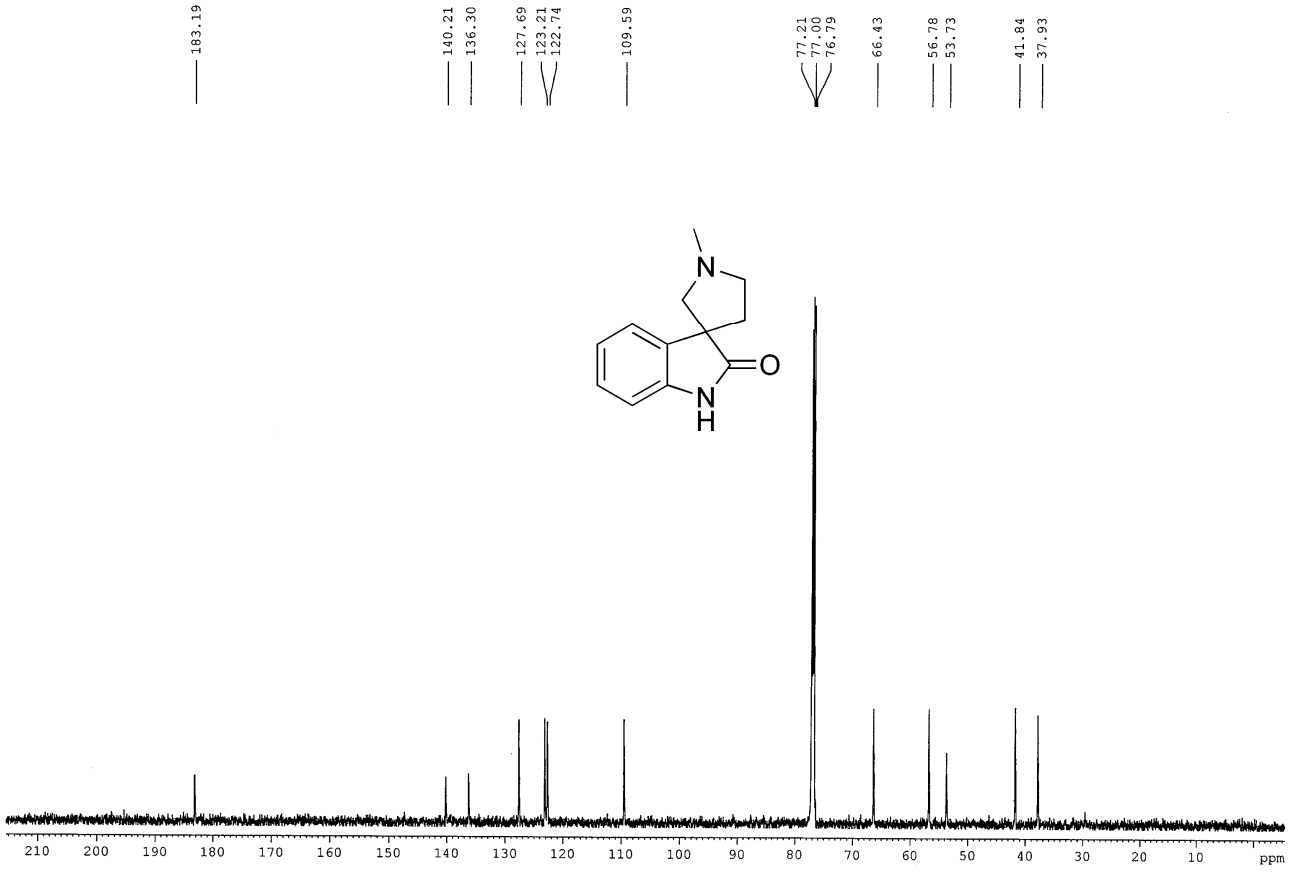
2',3',5',6'-Tetrahydrospiro[[1,3]dioxolo[4,5-*f*]indole-7,4'-pyran]-6(5*H*)-one (2D)





(±)-Coerulescine (2y)





(±)-Horsfiline (2F)