# Supporting Information

## Palladium Catalyzed Norbornene Mediated Tandem *Ortho* C-H Amination/ *Ipso* C-I Cyanation of Iodoarenes: Regiospecific Synthesis of 2-Amino Benzonitrile

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## General Procedure for the Synthesis of *O*-Benzoyl Hydroxylamines (2a-2h):

To a 50 mL round bottom flask with stir bar and a rubber septum was charged with benzoyl peroxide (3.46 g, 70% purity 10 mmol, 1 equiv), dipotassium hydrogen phosphate (3.50 g, 20 mmol, 2 equiv) and N,N-dimethylformamide (25 mL). A solution of morpholine (1.3 g, 15 mmol, 1.5 equiv) was added dropwise at 0 $^{o}$C temperature. After complete addition, the reaction was further stirred at room temperature for 24 h. After monitored by TLC to see the full conversion of benzoyl peroxide, water (100 mL) was added, and the product was extracted with ethyl acetate (5 × 30 mL). The combined organic extract was washed with brine (2 × 20 mL), dried over anhydrous sodium sulphate, filtered and concentrated under vacuum. The residue was purified by column chromatography on silica gel (hexane/ethyl acetate = 9:1) to give morpholino benzoate (**2a**) as a white solid.

Piperidine-1-yl benzoate (**2b**), 4-methylpiperidine-1-yl benzoate (**2c**), 2-methylpiperidine-1-yl benzoate (**2d**), ethyl-1-(benzoyloxy)piperidine-4-carboxylate (**2e**), pyrroidine-1-yl benzoate (**2f**), *O*-benzoyl-N,N-diethylhydroxyl amine (**2g**) and *O*-benzoyl-N-benzyl-N-methylhydroxylamine (**2h**) were prepared according to the same procedure.

## Representative Experimental Procedure for the Synthesis of Compound 3aa

An oven dried 10 mL round-bottom flask was charged with 1-iodo-2-methylbenzene (**1a**, 0.5 mmol, 109 mg, 1 equiv.), morpholine benzoate (**2a**, 0.75 mmol, 155 mg, 1.5 equiv.), $K_4[Fe(CN)_6].3H_2O$ (2.5 mmol, 1.0 g, 5 equiv.), norbornene (1.0 mmol, 94 mg, 2 equiv.), $PPh_3$ (0.1 mmol, 26 mg, 20 mol %), $Cs_2CO_3$ (1.0 mmol, 326 mg, 2 equiv.), $Pd(OAc)_2$ (0.05 mmol, 11 mg, 10 mol %) and anhydrous toluene in an argon atmosphere. The resulting mixture was stirred at room temperature for 30 minutes and was further stirred at 100 $^{o}$C for 14 h. After the reaction was complete (TLC), it was allowed to cool to room temperature and was extracted with ethyl acetate (60 mL). The extract was washed with water (10 mL) and then brine solution (10 mL). The organic layer was dried over anhydrous $Na_2SO_4$. After evaporation of the solvent, the residue (crude product) was purified by column chromatography over silica gel (100-200 mesh) using petroleum ether/ethyl acetate to afford the pure product, 2-methyl-6-morpholinobenzonitrile (**3aa**, 92 mg, 91 %) as a white solid, m.p. 68-70 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 2.50 (s, 3H), 3.14-3.17 (m, 4H), 3.87-3.90 (m, 4H), 6.83 (d, $J$ = 8.1 Hz, 1H), 6.91 (d, $J$ = 7.5 Hz, 1H), 7.36 (t, $J$ = 8.1 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 21.0, 52.2 (2C), 67.1 (2C), 107.3, 115.9, 117.3, 123.8, 133.2, 144.1, 156.2; IR (KBr): 2960, 2855, 2216, 1583, 1473, 1449, 1243, 1117 cm$^{-1}$; HRMS: m/z calcd. for $C_{12}H_{15}N_2O$ $[M+H]^+$ 203.1179, found 203.1178.

This procedure was followed for all the reactions listed in Scheme 2 and Scheme 6.

## Representative Experimental Procedure for the Synthesis of Compounds 5aa

An oven dried 10 mL round-bottom flask was charged with iodobenzene (**4a**, 0.5 mmol, 109 mg, 1 equiv.), morpholine benzoate (**2a**, 1.25 mmol, 259 mg, 2.5 equiv.), $K_4[Fe(CN)_6].3H_2O$ (2.5 mmol, 1.0 g, 5 equiv.), norbornene (1.5 mmol, 141 mg, 3 equiv.), $PPh_3$ (0.1 mmol, 26 mg, 20 mol %), $Cs_2CO_3$ (1.5 mmol, 489 mg, 3 equiv.), $Pd(OAc)_2$ (0.05 mmol, 11 mg, 10 mol %) and anhydrous toluene in an argon atmosphere. The resulting mixture was stirred at room temperature for 30 minutes and was further stirred at 100 $^{o}$C for 16 h. After the reaction was complete (TLC), it was allowed to cool to room temperature and was extracted with ethyl acetate (60 mL). The extract was washed with water (10 mL) and then brine solution (10 mL). The organic layer was dried over anhydrous $Na_2SO_4$. After evaporation of the solvent, the residue (crude product) was purified by column chromatography over silica gel (100-200 mesh) using petroleum ether/ethyl acetate to afford the pure product, 2,6-dimorpholinobenzonitrile (**5aa**, 118 mg, 86 %) as a white solid : mp 88-90 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 3.15-3.18 (m, 8H), 3.86 (t, $J$ = 4.5 Hz, 8H), 6.60 (d, $J$ = 8.4 Hz, 2H), 7.37 (t, $J$ = 8.4 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 52.1 (4C), 67.0 (4C), 100.2, 111.9 (2C), 117.6, 134.3, 157.8 (2C);

IR (KBr): 2854, 2210, 1576, 1448, 1235, 1116 $cm^{-1}$; HRMS: m/z calcd. for $C_{15}H_{20}N_3O_2$ $[M+H]^+$ 274.1550, found 274.1553.

This procedure was followed for all the reactions listed in Scheme 3 and Scheme 5.

All the products were not reported earlier and are characterized by $^1H$ NMR, $^{13}C$ NMR, $^{19}F$ NMR, IR, and HRMS or elemental analysis. These data are given below in the order of their entries in Scheme 2, Scheme 3, Scheme 4, Scheme 5 and Scheme 6.

## Characterization Data of Products:

**2-Methoxy-6-morpholinobenzonitrile (3ba, Scheme 2):** White solid (77.43 mg, 71%); m.p. 117-119 $^oC$; $^1H$ NMR (300 MHz, $CDCl_3$): δ 3.19 (t, $J$ = 4.2 Hz, 4H), 3.88 (t, $J$ = 4.5 Hz, 4H), 3.90 (s, 3H), 6.57 (d, $J$ = 8.1 Hz, 2H), 7.40 (t, $J$ = 8.4 Hz, 1H); $^{13}C$ NMR (75 MHz, $CDCl_3$): δ 51.9 (2C), 56.3, 67.1 (2C), 104.6, 110.6 (2C), 115.9, 134.5, 157.3, 163.2; IR (KBr): 2858, 2216, 1587, 1477, 1273, 1234, 1109 $cm^{-1}$; HRMS: m/z calcd. for $C_{12}H_{15}N_2O_2$ $[M+H]^+$ 219.1128, found 219.1125.

**2-Fluoro-6-morpholinobenzonitrile (3ca, Scheme 2):** White solid (71.1 mg, 69%); m.p. 81-83 $^oC$; $^1H$ NMR (300 MHz, $CDCl_3$): δ 3.23-3.26 (m, 4H), 3.86-3.89 (m, 4H), 6.74-6.79 (m, 2H), 7.41-7.49 (m, 1H); $^{13}C$ NMR (75 MHz, $CDCl_3$): δ 51.7 (2C), 66.9 (2C), 95.1 (d, $J_{C-F}$ = 16.5 Hz, 1C), 108.8 (d, $J_{C-F}$ = 20.3 Hz, 1C), 113.5 (d, $J_{C-F}$ = 1.5 Hz, 1C), 113.8 (d, $J_{C-F}$ = 3 Hz, 1C), 135.0 (d, $J_{C-F}$ = 10.5 Hz, 1C), 156.9 (d, $J_{C-F}$ = 3 Hz, 1C), 164.9 (d, $J_{C-F}$ = 255.7 Hz, 1C); IR (KBr): 2959, 2219, 1614, 1497, 1453 $cm^{-1}$; anal. calcd. for $C_{11}H_{11}FN_2O$: C 64.07, H 5.38, N 13.58; found C 64.01, H 5.42, N 13.61%.

**2-Chloro-6-morpholinobenzonitrile (3da, Scheme 2):** White solid (69.95 mg, 63%); m.p. 84-86 $^oC$; $^1H$ NMR (300 MHz, $CDCl_3$): δ 3.19-3.22 (m, 4H), 3.87-3.90 (m, 4H), 6.90 (dd, $J_1$ = 8.4 Hz, $J_2$ = 0.6 Hz, 1H), 7.09 (d, $J$ = 8.1 Hz, 1H), 7.40 (t, $J$ = 8.4 Hz, 1H); $^{13}C$ NMR (75 MHz, $CDCl_3$): δ 51.9 (2C), 66.9 (2C), 107.2, 115.5, 116.8, 123.0, 134.1, 138.6, 157.5; IR (KBr): 2866, 2845, 2228, 1589, 1556, 1443, 1244, 1113 $cm^{-1}$; anal. calcd. for $C_{11}H_{11}ClN_2O$: C 59.33, H 4.98, N 12.58; found C 59.30, H 4.95, N 12.63%.

**2,4-Difluoro-6-morpholinobenzonitrile (3ea, Scheme 2):** White solid (68.34 mg, 61%); m.p. 98-100 $^oC$; $^1H$ NMR (300 MHz, $CDCl_3$): δ 3.25-3.28 (m, 4H), 3.85-3.89 (m, 4H); 6.43-6.53 (m, 2H); $^{13}C$ NMR (75 MHz, $CDCl_3$): δ 51.4 (2C), 66.7 (2C), 90.8 (dd, $J_1$ = 17.25 Hz, $J_2$ = 3.75 Hz, 1C), 97.6 (t, $J_{C-F}$ = 24.75 Hz, 1C), 101.7 (dd, $J_1$ = 24 Hz, $J_2$ = 3 Hz, 1C), 113.0, 158.0 (dd, $J_1$ = 12 Hz, $J_2$ = 4.5 Hz, 1C), 165.9 (dd, $J_1$ = 257.25 Hz, $J_2$ = 16.5 Hz, 1C), 166.4 (dd, $J_1$ = 255.75 Hz, $J_2$ = 15.75 Hz, 1C); $^{19}F$ NMR (470 MHz, $CDCl_3$, $C_6F_6$ as standard compound): δ -101.2 (d, $J$ = 10.8 Hz, 1F), -104.2 (d, $J$ = 11.7 Hz, 1F); IR (KBr): 2976, 2869, 2229, 1616, 1580, 1442, 1115 $cm^{-1}$; anal calcd. for $C_{11}H_{10}F_2N_2O$ : C 58.93, H 4.50, N 12.49; found C 58.95, H 4.52, N 12.46%.

**3-Chloro-2-methyl-6-morpholinobenzonitrile (3fa, Scheme 2):** White solid (105.33 mg, 89%); m.p. 99-101 $^oC$; $^1H$ NMR (300 MHz, $CDCl_3$): δ 2.53 (s, 3H), 3.10-3.13 (m, 4H), 3.86 (t, $J$ = 4.5 Hz, 4H), 6.79 (d, $J$ = 8.7 Hz, 1H), 7.42 (d, $J$ = 9 Hz, 1H); $^{13}C$ NMR (75 MHz, $CDCl_3$): δ 19.1, 52.1 (2C), 66.9 (2C), 109.0, 116.6, 117.3, 128.1, 133.9, 141.3, 155.0; IR (KBr): 2859, 2828, 2220, 1573, 1445, 1238, 1114 $cm^{-1}$; HRMS: m/z calcd. for $C_{12}H_{14}ClN_2O$ $[M+H]^+$ 237.0789, found 237.0788.

**Methyl 2-cyano-3-morpholinobenzoate (3ga, Scheme 2):** Light yellow solid (86.19 mg, 70%); m.p. 120-122 $^oC$; $^1H$ NMR (300 MHz, $CDCl_3$): δ 3.18-3.21 (m, 4H), 3.90 (t, $J$ = 4.8 Hz, 4H), 3.96 (s, 3H), 7.23 (dd, $J_1$ = 8.1 Hz, $J_2$ = 0.9 Hz, 1H), 7.55 (t, $J$ = 7.8 Hz, 1H), 7.68 (dd, $J_1$ = 7.5 Hz, $J_2$ = 0.9 Hz, 1H); $^{13}C$ NMR (75 MHz, $CDCl_3$): δ 52.2 (2C), 52.9, 67.0 (2C), 106.7, 116.2, 123.0, 124.5, 133.1, 134.8, 157.6, 165.1; IR (KBr): 2963, 2216, 1720, 1584, 1451, 1273 $cm^{-1}$; anal. calcd. for $C_{13}H_{14}N_2O_3$: C 63.40, H 5.73, N 11.38; found C 63.45, H 5.70, N 11.33%.

**2-(Dimethylamino)-6-morpholinobenzonitrile (3ha, Scheme 2):** White solid (61.29 mg, 53%); m.p. 84-86 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 3.00 (s, 6H), 3.15-3.18 (m, 4H), 3.87-3.89 (m, 4H), 6.44 (dd, $J_1$ = 8.1 Hz, $J_2$ = 0.6 Hz, 1H), 6.53 (dd, $J_1$ = 8.4 Hz, $J_2$ = 0.6 Hz, 1H), 7.29 (t, $J$ = 8.4 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 43.5 (2C), 52.4 (2C), 67.1 (2C), 96.6, 109.0, 110.7, 118.7, 133.9, 158.1, 158.3; IR (KBr): 2952, 2206, 1571, 1493, 1437, 1236, 1113 cm$^{-1}$; HRMS: m/z calcd. for $C_{13}H_{17}N_3NaO$ $[M+Na]^+$ 254.1264, found 254.1268.

**2-Methyl-6-(piperidin-1-yl)benzonitrile (3ab, Scheme 2):** White solid (88.12 mg, 88%); m.p. 49-51 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 1.56-1.62 (m, 2H), 1.73-1.81 (m, 4H), 2.48 (s, 3H), 3.11 (t, $J$ = 5.4 Hz, 4H), 6.80-6.84 (m, 2H), 7.31 (t, $J$ = 8.1 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 21.0, 24.2, 26.3 (2C), 53.5 (2C), 107.1, 116.1, 117.6, 122.8, 132.9, 143.7, 157.7; IR (KBr): 2933, 2848, 2215, 1584, 1470, 1246 cm$^{-1}$; HRMS: m/z calcd. for $C_{13}H_{17}N_2$ $[M+H]^+$ 201.1386, found 201.1384.

**2-(Piperidin-1-yl)-6-(trifluoromethoxy)benzonitrile (3ib, Scheme 2):** Colorless gummy liquid (98.59 mg, 73%); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 1.59-1.65 (m, 2H), 1.73-1.80 (m, 4H), 3.21 (t, $J$ = 5.4 Hz, 4H), 6.83-6.90 (m, 2H), 7.43 (t, $J$ = 8.7 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 24.0, 26.0 (2C), 53.0 (2C), 99.8, 112.1, 114.1, 116.7, 120.4 (q, $J$ = 258.75, 1C), 134.1, 151.6, 158.5; $^{19}$F NMR (470 MHz, $CDCl_3$, $C_6F_6$ as standrad compound): δ -60.82; IR (KBr): 2973, 2871, 2207, 1572, 1463, 1250 cm$^{-1}$; anal. calcd. for $C_{13}H_{13}F_3N_2O$: C 57.78, H 4.85, N 10.37; found C 57.83, H 4.90, N 10.35%.

**2-Methyl-6-(4-methylpiperidin-1-yl)benzonitrile (3ac, Scheme 2):** White solid (86.79 mg, 81%), m.p. 83-85 $^{o}$C, $^{1}$H NMR (300 MHz, $CDCl_3$): δ 0.99 (d, $J$ = 5.7 Hz, 3H), 1.44-1.51 (m, 3H), 1.73-1.76 (m, 2H), 2.49 (s, 3H), 2.71-2.78 (m, 2H), 3.51 (dd, $J_1$ = 10.8 Hz, $J_2$ = 1.2 Hz, 2H), 6.81 (d, $J$ = 3.3 Hz, 1H), 6.84 (d, $J$ = 2.7 Hz, 1H), 7.31 (t, $J$ = 7.8 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 21.0, 21.9, 30.7, 34.6 (2C), 52.9 (2C), 107.1, 116.1, 117.7, 122.7, 132.9, 143.7, 157.6; IR (KBr): 2950, 2922, 2808, 2215, 1584, 1467, 1382, 1238 cm$^{-1}$; HRMS: m/z calcd. for $C_{14}H_{19}N_2$ $[M+H]^+$ 215.1543, found 215.1545.

**2-Ethyl-6-(4-methylpiperidin-1-yl)benzonitrile (3jc, Scheme 2):** Colorless gummy liquid (102.75 mg, 90%); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 0.99 (d, $J$ = 2.7 Hz, 3H), 1.27 (t, $J$ = 7.5 Hz, 3H), 1.45-1.52 (m, 3H), 1.73-1.76 (m, 2H), 2.70-2.86 (m, 4H), 3.48-3.53 (m, 2H), 6.84 (t, $J$ = 7.5 Hz, 2H), 7.35 (t, $J$ = 8.1 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 15.1, 21.9, 28.1, 30.7, 34.6 (2C), 52.9 (2C), 106.4, 116.3, 117.5, 121.3, 133.1, 149.9, 157.7; IR (KBr): 2925, 2808, 2215, 1581, 1465, 1381, 1235 cm$^{-1}$; HRMS: m/z calcd. for $C_{15}H_{21}N_2$ $[M+H]^+$ 229.1699, found 229.1697.

**2,4-Dimethyl-6-(4-methylpiperidin-1-yl)benzonitrile (3kc, Scheme 2):** White solid (100 mg, 88%); m.p. 74-76 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 0.99 (d, $J$ = 5.7 Hz, 3H), 1.43-1.51 (m, 3H), 1.72-1.75 (m, 2H), 2.30 (s, 3H), 2.44 (s, 3H), 2.68-2.76 (m, 2H), 3.49 (dd, $J_1$ = 10.8 Hz, $J_2$ = 1.5 Hz, 2H), 6.62-6.66 (m, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 20.9, 21.9, 22.0, 30.8, 34.6 (2C), 52.8 (2C), 104.1, 116.9, 118.0, 123.8, 143.4, 143.7, 157.5; IR (KBr): 2922, 2807, 2213, 1601, 1569, 1453 cm$^{-1}$; anal. calcd. for $C_{15}H_{20}N_2$ : C 78.90, H 8.83, N 12.27; found C 78.93, H 8.80, N 12.31%.

**2-(4-Methylpiperidin-1-yl)-6-(trifluoromethyl)benzonitrile (3lc, Scheme 2):** White solid (103.29 mg, 77%); m.p. 78-80 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 1.01 (d, $J$ = 6 Hz, 3H), 1.45-1.55 (m, 3H), 1.76-1.80 (m, 2H), 2.82-2.89 (m, 2H), 3.55-3.60 (m, 2H), 7.21 (d, $J$ = 8.4 Hz, 1H), 7.27 (d, $J$ = 7.8 Hz, 1H), 7.49-7.55 (m, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 21.8, 30.8, 34.4 (2C), 52.8 (2C), 103.0, 115.1, 118.5 (q, $J_{C-F}$ = 5.3 Hz, 1C), 122.6, 122.7 (q, $J_{C-F}$ = 272.2 Hz, 1C), 133.2, 134.6 (d, $J_{C-F}$ = 32.2 Hz, 1C), 158.9; $^{19}$F NMR (470 MHz, $CDCl_3$, $C_6F_6$ as standrad compound): δ -65.2; IR (KBr): 2960, 2924, 2218, 1595, 1458, 1315, 1128 cm$^{-1}$; anal. calcd. for $C_{14}H_{15}F_3N_2$: C 62.68, H 5.64, N 10.44; found C 62.64, H 5.61, N 10.48%.

**Methyl-4-cyano-3-methyl-5-(4-methylpiperidin-1-yl)benzoate (3mc, Scheme 2):** Off white solid (93.96 mg, 69%); m.p. 72-74 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 0.99 (d, $J$ = 5.7 Hz, 3H), 1.43-1.50 (m, 3H), 1.73-1.77 (m, 2H), 2.51 (s, 3H), 2.79 (t, $J$ = 11.4 Hz, 2H), 3.53 (d, $J$ = 12 Hz, 2H), 3.89 (s,

3H), 7.45 (d, $J$ = 2.4 Hz, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 21.0, 21.8, 30.6, 34.4 (2C), 52.6, 52.7 (2C), 110.8, 116.9, 117.0, 123.2, 133.9, 143.9, 157.4, 166.3; IR (KBr): 2952, 2218, 1727, 1573, 1435, 1230 cm$^{-1}$; anal. calcd. for $C_{16}H_{20}N_2O_2$ : C 70.56, H 7.40, N 10.29; found C 70.58, H 7.43, N 10.25%.

**2-(4-Methylpiperidin-1-yl)-6-nitrobenzonitrile (3nc, Scheme 2):** Yellow solid (96.88 mg, 79%), m.p. 112-114 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 1.02 (d, $J$ = 6 Hz, 3H), 1.47-1.60 (m, 3H), 1.78-1.82 (m, 2H), 2.88-2.96 (m, 2H), 3.62-3.67 (m, 2H), 7.30 (dd, $J_1$ = 8.4 Hz, $J_2$ = 0.9 Hz, 1H), 7.56 (t, $J$ = 8.4 Hz, 1H), 7.69 (dd, $J_1$ = 8.1 Hz, $J_2$ = 1.2 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 21.8, 30.5, 34.3 (2C), 52.8 (2C), 99.9, 114.3, 116.9 (2C), 124.4, 133.2, 151.4, 159.2; IR (KBr): 2928, 2222, 1538, 1452, 1345, 1245 cm$^{-1}$; HRMS: m/z calcd. for $C_{13}H_{16}N_3O_2$ $[M+H]^+$ 246.1237, found 246.1235.

**2-Methyl-6-(2-methylpiperidin-1-yl)benzonitrile (3ad, Scheme 2):** Colorless gummy liquid (38.58 mg, 36%); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 0.96 (d, $J$ = 6.3 Hz, 3H), 1.49-1.55 (m, 2H), 1.69-1.77 (m, 3H), 1.87-1.94 (m, 1H), 2.50 (s, 3H), 2.76-2.83 (m, 1H), 3.16-3.23 (m, 1H), 3.52-3.57 (m, 1H), 6.90-6.92 (m, 2H), 7.33 (t, $J$ = 7.8 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 16.8, 21.0, 21.7, 26.5, 32.9, 51.1, 54.7, 110.2, 117.5, 119.5, 123.9, 132.5, 143.6, 157.0; IR (KBr): 2934, 2856, 2217, 1582, 1468, 1256 cm$^{-1}$; HRMS: m/z calcd. for $C_{14}H_{19}N_2$ $[M+H]^+$ 215.1543, found 215.1544.

**Ethyl 1-(2-cyano-3-methylphenyl)piperidine-4-carboxylate (3ae, Scheme 2):** White solid (117.12 mg, 86%); m.p. 72-74 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 1.24 (t, $J$ = 7.2 Hz, 3H), 1.94-2.07 (m, 4H), 2.37-2.44 (m, 1H), 2.46 (s, 3H), 2.77-2.86 (m, 2H), 3.44-3.50 (m, 2H), 4.13 (q, $J$ = 7.2 Hz, 2H), 6.79-6.86 (m, 2H), 7.30 (t, $J$ = 8.1 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 14.4, 21.0, 28.5 (2C), 40.8, 51.9 (2C), 60.6, 107.4, 116.2, 117.4, 123.3, 133.0, 143.8, 157.0, 174.7; IR (KBr): 2956, 2215, 1730, 1584, 1469, 1172 cm$^{-1}$; HRMS: m/z calcd. for $C_{16}H_{21}N_2O_2$ $[M+H]^+$ 273.1598, found 273.1597.

**Ethyl 1-(1-cyanonaphthalen-2-yl)piperidine-4-carboxylate (3oe, Scheme 2):** Colorless gummy liquid (127.97, 83%); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 1.26 (t, $J$ = 7.2 Hz, 3H), 1.99-2.11 (m, 4H), 2.45-2.55 (m, 1H), 3.04-3.12 (m, 2H), 3.73-3.77 (m, 2H), 4.16 (q, $J$ = 7.2 Hz, 2H), 7.16 (d, $J$ = 9.3 Hz, 1H), 7.37 (t, $J$ = 7.5 Hz, 1H), 7.55 (t, $J$ = 8.1 Hz, 1H), 7.72 (d, $J$ = 8.1 Hz, 1H), 7.85 (d, $J$ = 9 Hz, 1H), 8.06 (d, $J$ = 8.7 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 14.3, 28.5 (2C), 40.7, 51.4 (2C), 60.5, 98.1, 117.8, 118.6, 124.0, 124.9, 128.1, 128.2, 128.7, 133.8, 134.2, 156.2, 174.5; IR (KBr): 2963, 2216, 1721, 1583, 1272 cm$^{-1}$; anal. calcd. for $C_{19}H_{20}N_2O_2$ : C 74.00, H 6.54, N 9.08; found C 74.06, H 6.60, N 9.02%.

**Ethyl 1-(3-(benzyloxy)-2-cyanophenyl)piperidine-4-carboxylate (3pe, Scheme 2):** Colorless gummy liquid (142.13 mg, 78%); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 1.27 (t, $J$ = 7.2 Hz, 3H), 1.92-2.08 (m, 4H), 2.40-2.50 (m, 1H), 2.83-2.92 (m, 2H), 3.54-3.60 (m, 2H), 4.16 (q, $J$ = 7.2 Hz, 2H), 5.18 (s, 2H), 6.53-6.57 (m, 2H), 7.27-7.40 (m, 4H), 7.43-7.46 (m, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 14.2, 28.3 (2C), 40.8, 51.4 (2C), 60.5, 70.6, 96.0, 105.4, 111.1, 115.8, 126.9 (2C), 128.0, 128.7 (2C), 134.0, 136.0, 157.9, 161.9, 174.6; IR (KBr): 2959, 2925, 2214, 1719, 1582, 1454, 1382, 1274 cm$^{-1}$; HRMS: m/z calcd. for $C_{22}H_{25}N_2O_3$ $[M+H]^+$ 365.1860, found 365.1862.

**2-Methyl-6-(pyrrolidin-1-yl)benzonitrile (3af, Scheme 2):** Colorless gummy liquid (59.60 mg, 64%); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 1.96-2.01 (m, 4H), 2.46 (s, 3H), 3.57-3.61 (m, 4H), 6.49 (d, $J$ = 8.7 Hz, 1H), 6.55 (d, $J$ = 7.5 Hz, 1H), 7.16-7.22 (m, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 21.6, 25.9 (2C), 50.3 (2C), 96.1, 111.8, 117.7, 120.0, 132.9, 144.3, 151.5; IR (KBr): 2969, 2873, 2204, 1591, 1482, 1379 cm$^{-1}$; HRMS: m/z calcd. for $C_{12}H_{15}N_2$ $[M+H]^+$ 187.1230, found 187.1232.

**2-(Diethylamino)-6-methylbenzonitrile (3ag, Scheme 2):** Colorless gummy liquid (45.18 mg, 48%); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 1.13 (t, $J$ = 7.2 Hz, 6H), 2.49 (s, 3H), 3.33 (q, $J$ = 7.2 Hz, 4H), 6.80 (d, $J$ = 7.5 Hz, 2H), 7.29 (t, $J$ = 7.8 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 12.6 (2C), 21.3, 47.1 (2C), 106.2, 117.5, 118.0, 122.1, 132.6 (2C), 144.2; IR (KBr): 2974, 2932, 2212, 1584, 1469, 1381, 1262 cm$^{-1}$; HRMS: m/z calcd. for $C_{12}H_{17}N_2$ $[M+H]^+$ 189.1386, found 189.1387.

**2-(Benzyl(methyl)amino)-6-methylbenzonitrile (3ah, Scheme 2):** Colorless gummy liquid (91.16 mg, 78 %); $^1$H NMR (300 MHz, $CDCl_3$): δ 2.54 (s, 3H), 2.87 (s, 3H), 4.45 (s, 2H), 6.81-6.85 (m, 2H), 7.27-7.30 (m, 2H), 7.31-7.35 (m, 4H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 21.2, 40.5, 60.2, 105.0, 116.3, 118.0, 122.2, 127.4, 128.2 (2C), 128.5 (2C), 132.9, 137.6, 144.1, 156.2; IR (KBr): 2954, 2212, 1583, 1477, 1450, 1362 cm$^{-1}$; HRMS: m/z calcd. for $C_{16}H_{16}N_2Na$ $[M+Na]^+$ 259.1206, found 259.1213.

**2-(Benzyl(methyl)amino)-6-fluorobenzonitrile (3ch, Scheme 2):** Colorless gummy liquid (79.29 mg, 66%); $^1$H NMR (300 MHz, $CDCl_3$): δ 3.03 (s, 3H), 4.60 (s, 2H), 6.58-6.67 (m, 2H), 7.26-7.36 (m, 6H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 40.3, 59.1, 91.1, 105.8 (d, $J_{C\text{-}F}$ = 20.25 Hz, 1C), 113.1 (d, $J_{C\text{-}F}$ = 3 Hz, 1C), 114.5 (d, $J_{C\text{-}F}$ = 2.25 Hz, 1C), 127.6 (2C), 127.7, 128.8 (2C), 134.4 (d, $J_{C\text{-}F}$ = 11.25 Hz, 1C), 137.0, 155.9 (d, $J_{C\text{-}F}$ = 3 Hz, 1C), 165.3 (d, $J_{C\text{-}F}$ = 254.25 Hz, 1C); $^{19}$F NMR (470 MHz, $CDCl_3$, $C_6F_6$ as standrad compound): δ -108.1; IR (KBr): 2958, 2219, 1613, 1560, 1496, 1453 cm$^{-1}$; anal. calcd. for $C_{15}H_{13}FN_2$: C 74.98, H 5.45, N 11.66; found C 74.95, H 5.49, N 11.60%.

**2-(Benzyl(methyl)amino)-1-naphthonitrile (3oh, Scheme 2):** Colorless gummy liquid (100.77 mg, 74%); $^1$H NMR (300 MHz, $CDCl_3$): δ 3.23 (s, 3H), 4.73 (s, 2H), 7.11 (d, $J$ = 9 Hz, 1H), 7.24-7.38 (m, 6H), 7.54-7.60 (m, 1H), 7.70 (d, $J$ = 8.1 Hz, 1H), 7.77 (d, $J$ = 9.3 Hz, 1H), 8.10 (dd, $J_1$ = 8.7 Hz, $J_2$ = 0.6 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 40.9, 59.0, 92.7, 118.3, 119.0, 123.9, 124.4, 127.4, 127.5 (2C), 127.6, 128.3, 128.9 (2C), 129.0, 133.8, 134.9, 137.3, 154.9; IR (KBr): 2201, 1620, 1597, 1509, 1449, 1356 cm$^{-1}$; HRMS: m/z calcd. for $C_{19}H_{17}N_2$ $[M+H]^+$ 273.1386, found 273.1389.

**4-Methyl-2,6-dimorpholinobenzonitrile (5ba, Scheme 3):** White solid (109.19 mg, 76%); m.p. 69-71 $^o$C; $^1$H NMR (300 MHz, $CDCl_3$): δ 2.32 (s, 3H), 3.13-3.16 (m, 8H), 3.86 (t, $J$ = 4.5 Hz, 8H), 6.41 (s, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 22.6, 52.2 (4C), 67.0 (4C), 97.3, 109.2, 112.8 (2C), 117.9, 145.4, 157.6; IR (KBr): 2854, 2209, 1596, 1563, 1445, 1230, 1116 cm$^{-1}$; HRMS: m/z calcd. for $C_{16}H_{22}N_3O_2$ $[M+H]^+$ 288.1707, found 288.1709.

**4-(*Tert*-butyl)-2,6-dimorpholinobenzonitrile (5ca, Scheme 3):** White solid (126.83, 77%); m.p. 103-105 $^o$C; $^1$H NMR (300 MHz, $CDCl_3$): δ 1.30 (s, 9H), 3.17-3.20 (m, 8H), 3.87-3.90 (m, 8H), 6.63 (s, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 31.2 (3C), 35.9, 52.3 (4C), 67.2 (4C), 97.7, 109.4 (2C), 117.9, 157.5 (2C), 158.6; IR (KBr): 2963, 2209, 1592, 1561, 1430, 1235, 1113 cm$^{-1}$; HRMS: m/z calcd. for $C_{19}H_{28}N_3O_2$ $[M+H]^+$ 330.2176, found 330.2177.

**4-Methoxy-2,6-dimorpholinobenzonitrile (5da, Scheme 3):** White solid (104.66 mg, 69%); m.p. 75-77 $^o$C; $^1$H NMR (300 MHz, $CDCl_3$): δ 3.16 (t, $J$ = 4.5 Hz, 8H), 3.82 (s, 3H), 3.87 (t, $J$ = 4.5 Hz, 8H), 6.10 (s, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 52.1 (4C), 55.6, 67.0 (4C), 92.1, 97.9 (2C), 118.3, 159.4 (2C), 164.7; IR (KBr): 2956, 2857, 2195, 1590, 1568, 1438, 1114 cm$^{-1}$; HRMS: m/z calcd. for $C_{16}H_{22}N_3O_3$ $[M+H]^+$ 304.1656, found 304.2234.

**3,5-Dimorpholino-[1,1'-biphenyl]-4-carbonitrile (5ea, Scheme 3):** Off white solid (127.54 mg, 73%), m.p. 165-167 $^o$C, $^1$H NMR (300 MHz, $CDCl_3$): δ 3.25 (t, $J$ = 4.5 Hz, 8H), 3.90 (t, $J$ = 4.5 Hz, 8H), 6.78 (s, 2H), 7.41-7.48 (m, 3H), 7.54 (d, $J$ = 7.2 Hz, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 52.2 (4C), 67.0 (4C), 98.7, 110.9 (2C), 117.8, 127.3 (2C), 128.7, 129.0 (2C), 140.4, 147.6, 158.0 (2C); IR (KBr): 2964, 2848, 2207, 1591, 1552, 1418, 1232 cm$^{-1}$; HRMS: m/z calcd. for $C_{21}H_{24}N_3O_2$ $[M+H]^+$ 350.1863, found 350.1864.

**4-(Allyloxy)-2,6-dimorpholinobenzonitrile (5fa, Scheme 3):** Light brown gummy liquid (118.58 mg, 72%); $^1$H NMR (300 MHz, $CDCl_3$): δ 3.14-3.17 (m, 8H), 3.86-3.88 (m, 8H), 4.54-4.56 (m, 2H), 5.29-5.44 (m, 2H), 5.95-6.08 (m, 1H), 6.12 (s, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 52.1 (4C), 67.0 (5C), 69.1, 98.7 (2C), 118.2, 118.5, 132.5, 159.3 (2C), 163.7; IR (KBr): 2960, 2856, 2207, 1592, 1443, 1266, 1116 cm$^{-1}$; HRMS: m/z calcd. for $C_{18}H_{24}N_3O_3$ $[M+H]^+$ 330.1812, found 330.1813.

**4-Acetyl-2,6-dimorpholinobenzonitrile (5ga, Scheme 3):** Light yellow solid (108.80 mg, 69%); m.p. 108-110 $^o$C, $^1$H NMR (300 MHz, $CDCl_3$): δ 2.57 (s, 3H), 3.19-3.23 (m, 8H), 3.86-3.89 (m, 8H),

7.09 (s, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 26.9, 52.0 (4C), 66.9 (4C), 103.5, 111.0 (2C), 117.0, 141.6, 157.9 (2C), 197.3; IR (KBr): 2854, 2212, 1688, 1562, 1430, 1264, 1116 cm$^{-1}$; HRMS: m/z calcd. for $C_{17}H_{22}N_3O_3$ $[M+H]^+$ 316.1656, found 316.1655.

**2,6-Dimorpholino-4-nitrobenzonitrile (5ha, Scheme 3):** Yellow solid (100.27 mg, 63%); m.p. 121-123 °C; $^1$H NMR (300 MHz, $CDCl_3$): δ 3.26-3.29 (m, 8H), 3.87-3.90 (m, 8H), 7.34 (s, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 51.8 (4C), 66.7 (4C), 103.4, 105.7 (2C), 116.5, 151.8, 158.4 (2C); IR (KBr): 2859, 2216, 1577, 1526, 1438, 1116 cm$^{-1}$; anal. calcd. for $C_{15}H_{18}N_4O_4$ : C 56.60, H 5.70, N 17.60; found C 56.62, H 5.73, N 17.57 %.

**2,6-Di(piperidin-1-yl)benzonitrile (5ab, Scheme 3):** White solid (103.71 mg, 77%); m.p. 84-86 °C; $^1$H NMR (300 MHz, $CDCl_3$): δ 1.54-1.62 (m, 4H), 1.72-1.79 (m, 8H), 3.12 (t, $J$ = 5.4 Hz, 8H), 6.51 (d, $J$ = 8.1 Hz, 2H), 7.26 (t, $J$ = 8.1 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 24.3 (2C), 26.3 (4C), 53.5 (4C), 100.1, 111.1 (2C), 118.2, 133.7, 159.1 (2C); IR (KBr): 2934, 2209, 1574, 1469, 1453, 1218 cm$^{-1}$; anal. calcd. for $C_{17}H_{23}N_3$: C 75.80, H 8.61, N 15.60; found C 75.83, H 8.66, N 15.56%.

**2,6-Bis(4-methylpiperidin-1-yl)benzonitrile (5ac, Scheme 3):** White solid (117 mg, 79%); m.p. 93-95 °C; $^1$H NMR (300 MHz, $CDCl_3$): δ 0.98 (d, $J$ = 5.7 Hz, 6H), 1.41-1.50 (m, 6H), 1.72 (d, $J$ = 9 Hz, 4H), 2.74 (t, $J$ = 11.1 Hz, 4H), 3.50-3.54 (m, 4H), 6.51 (d, $J$ = 8.1 Hz, 2H), 7.26 (t, $J$ = 8.4 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 21.9 (2C), 30.8 (2C), 34.5 (4C), 52.8 (4C), 99.9, 111.1 (2C), 118.3, 133.7, 158.8 (2C); IR (KBr): 2918, 2799, 2210, 1576, 1455, 1379, 1231 cm$^{-1}$; HRMS: m/z calcd. for $C_{19}H_{28}N_3$ $[M+H]^+$ 298.2278, found 298.2276.

**2,6-Bis(4-methylpiperidin-1-yl)-4-(trifluoromethoxy)benzonitrile (5ic, Scheme 3):** White solid (118.24 mg, 62%); m.p. 95-97 °C; $^1$H NMR (300 MHz, $CDCl_3$): δ 0.99 (d, $J$ = 6 Hz, 6H), 1.42-4.54 (m, 6H), 1.71-1.76 (m, 4H), 2.74-2.82 (m, 4H), 3.56 (d, $J$ = 12.6 Hz, 4H), 6.28 (d, $J$ = 0.6 Hz, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 21.8 (2C), 30.8 (2C), 34.3 (4C), 52.6 (4C), 96.6, 102.7 (2C), 117.8, 120.4 (q, $J_{C\text{-}F}$ = 256.5 Hz, 1C), 153.6, 160.0 (2C); $^{19}$F NMR (470 MHz, $CDCl_3$, $C_6F_6$ as standrad compound): δ -60.4; IR (KBr): 2925, 2815, 2212, 1584, 1448, 1381, 1256, 1222 cm$^{-1}$; HRMS: m/z calcd. for $C_{20}H_{27}F_3N_3O$ $[M+H]^+$ 382.2101, found 382.2102.

**Ethyl 4-cyano-3,5-bis(4-methylpiperidin-1-yl)benzoate (5jc, Scheme 3):** Light yellow gummy liquid (109.0 mg, 59%); $^1$H NMR (300 MHz, $CDCl_3$): δ 0.99 (d, $J$ = 5.7 Hz, 6H), 1.37 (t, $J$ = 6.9 Hz, 3H), 1.47-1.50 (m, 6H), 1.74 (d, $J$ = 9.3 Hz, 4H), 2.80 (t, $J$ = 11.4 Hz, 4H), 3.55 (d, $J$ = 12.3 Hz, 4H, 4.35 (q, $J$ = 7.2 Hz, 2H), 7.14 (s, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 14.4, 21.9 (2C), 30.7 (2C), 34.4 (4C), 52.7 (4C), 61.6, 103.2, 111.7 (2C), 117.7, 135.0, 158.6 (2C), 166.1; IR (KBr): 2923, 2812, 2212, 1722, 1564, 1436, 1380, 1260 cm$^{-1}$; HRMS: m/z calcd. for $C_{22}H_{32}N_3O_2$ $[M+H]^+$ 370.2489, found 370.2487.

**2,6-Bis(4-methylpiperidin-1-yl)-4-(trifluoromethyl)benzonitrile (5kc, Scheme 3):** White solid (135.21 mg, 74%); m.p. 136-138 °C; $^1$H NMR (300 MHz, $CDCl_3$): δ 0.99 (d, $J$ = 5.7 Hz, 6H), 1.43-1.53 (m, 6H), 1.73-1.77 (m, 4H), 2.82 (t, $J$ = 12 Hz, 4H), 3.57 (d, $J$ = 12.3 Hz, 4H), 6.67 (s, 2H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 21.8 (2C), 30.7 (2C), 34.3 (4C), 52.6 (4C), 101.5, 107.1 (d, $J_{C\text{-}F}$ = 3.7 Hz, 2C), 117.5, 123.7 (q, $J_{C\text{-}F}$ = 272.3 Hz, 1C), 135.3 (d, $J_{C\text{-}F}$ = 31.5 Hz, 1C), 159.0 (2C); IR (KBr): 2951, 2818, 2210, 1572, 1444, 1377, 1288 cm$^{-1}$; anal. calcd. for $C_{20}H_{26}F_3N_3$: C 65.73, H 7.17, N 11.50; found C 65.75, H 7.16, N 11.54%.

**2,6-Bis(diethylamino)benzonitrile (5ag, Scheme 3):** Colorless gummy liquid (46.62 mg, 38%); $^1$H NMR (300 MHz, $CDCl_3$): δ 1.14 (t, $J$ = 7.2 Hz, 12H), 3.30 (q, $J$ = 6.9 Hz, 8H), 6.49 (d, $J$ = 8.1 Hz, 2H), 7.22 (t, $J$ = 8.1 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 12.7 (4C), 46.8 (4C), 99.5, 111.7 (2C), 119.2, 132.7, 156.8 (2C); IR (KBr): 2973, 2931, 2870, 2207, 1573, 1462, 1380, 1251 cm$^{-1}$; HRMS: m/z calcd. for $C_{15}H_{24}N_3$ $[M+H]^+$ 246.1965, found 246.1966.

**Diethyl 1,1'-(2-cyano-1,3-phenylene)bis(piperidine-4-carboxylate) (5ae, Scheme 3):** White solid (173.67 mg, 84%); m.p. 83-85 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 1.25 (t, $J$ = 7.2 Hz, 6H), 1.94-2.04 (m, 8H), 2.37-2.47 (m, 2H), 2.79-2.88 (m, 4H), 3.46-3.53 (m, 4H), 4.14 (q, $J$ = 7.2 Hz, 4H), 6.53 (d, $J$ = 8.1 Hz, 2H), 7.28 (t, $J$ = 8.4 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 14.4 (2C), 28.5 (4C), 40.9 (2C), 51.9 (4C), 60.6 (2C), 100.5, 111.8 (2C), 117.9, 133.9, 158.4 (2C), 174.8 (2C); IR (KBr): 2960, 2926, 2214, 1719, 1583, 1275 cm$^{-1}$; HRMS: m/z calcd. for $C_{23}H_{32}N_3O_4$ $[M+H]^+$ 414.2387, found 414.2385.

**Diethyl 1,1'-(2-cyano-5-formyl-1,3-phenylene)bis(piperidine-4-carboxylate) (5ke, Scheme 3):** Light yellow solid (183.23 mg, 83%); mp 79-81 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 1.25 (t, $J$ = 6.9 Hz, 6H), 1.91-2.08 (m, 8H), 2.41-2.49 (m, 2H), 2.88-2.97 (m, 4H), 3.53-3.59 (m, 4H), 4.14 (q, $J$ = 7.2 Hz, 4H), 6.98 (s, 2H), 9.89 (s, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 14.3 (2C), 28.3 (4C), 40.6 (2C), 51.6 (4C), 60.6 (2C), 104.3, 111.7 (2C), 117.1, 140.0, 158.8 (2C, 174.5 (2C), 191.7; IR (KBr): 2957, 2819, 2211, 1729, 1565, 1444, 1171 cm$^{-1}$; HRMS: m/z calcd. for $C_{24}H_{31}N_3NaO_5$ $[M+H]^+$ 464.2156, found 464.2163.

**Diethyl 1,1'-(5-(benzyloxy)-2-cyano-1,3-phenylene)bis(piperidine-4-carboxylate) (5me, Scheme 3):** Colorless gummy liquid (202 mg, 78%); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 1.26 (t, $J$ = 6.9 Hz, 6H), 1.90-2.06 (m, 8H), 2.39-2.48 (m, 2H), 2.78-2.87 (m, 4H), 3.48-3.54 (m, 4H), 4.15 (q, $J$ = 7.2 Hz, 4H), 5.04 (s, 2H), 6.14 (s, 2H), 7.35-7.40 (m, 5H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 14.4 (2C), 28.4 (4C), 40.9 (2C), 51.7 (4C), 60.6 (2C), 70.3, 92.5, 98.6 (2C), 118.4, 127.7 (2C), 128.5, 128.9 (2C), 136.2, 159.8 (2C), 163.5, 174.8; IR (KBr): 2955, 2814, 2206, 1729, 1588, 1446, 1168 cm$^{-1}$; anal. calcd. for $C_{30}H_{37}N_3O_5$: C 69.34, H 7.18, N 8.09; found C 69.32, H 7.20, N 8.05%.

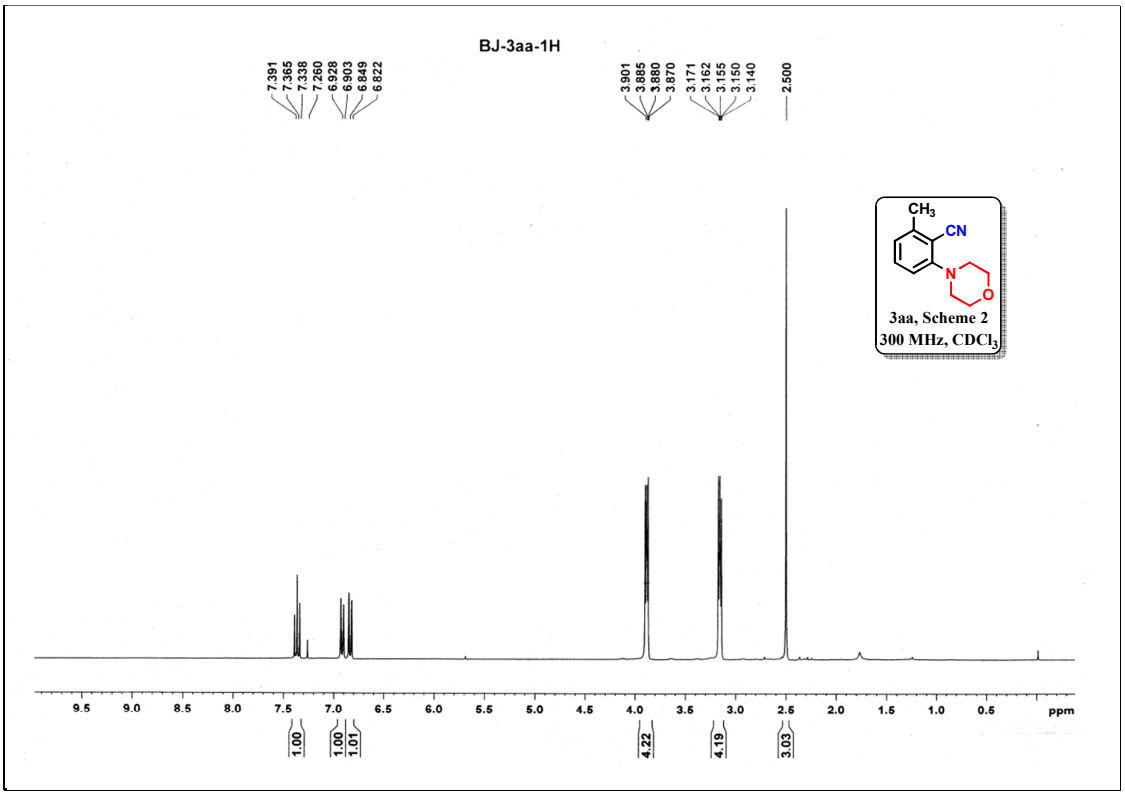
**2,6-Bis(1-phenylpropan-2-yl)benzonitrile (5ah, Scheme 3):** Colorless gummy liquid (129.0 mg, 76%); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 2.89 (s, 6H), 4.49 (s, 4H), 6.50 (d, $J$ = 8.1 Hz, 2H), 7.21-7.30 (m, 4H), 7.33-7.36 (m, 7H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 40.6 (2C), 60.2 (2C), 96.0, 110.5 (2C), 118.9, 127.4 (2C), 128.1 (4C), 128.6 (4C), 133.7, 137.8 (2C), 158.0 (2C); IR (KBr): 2954, 2804, 2206, 1725, 1571, 1449, 1361 cm$^{-1}$; anal. calcd. for $C_{25}H_{25}N$: C 88.45, H 7.42, N 4.13; found C 88.49, H 7.45, N 4.10%.

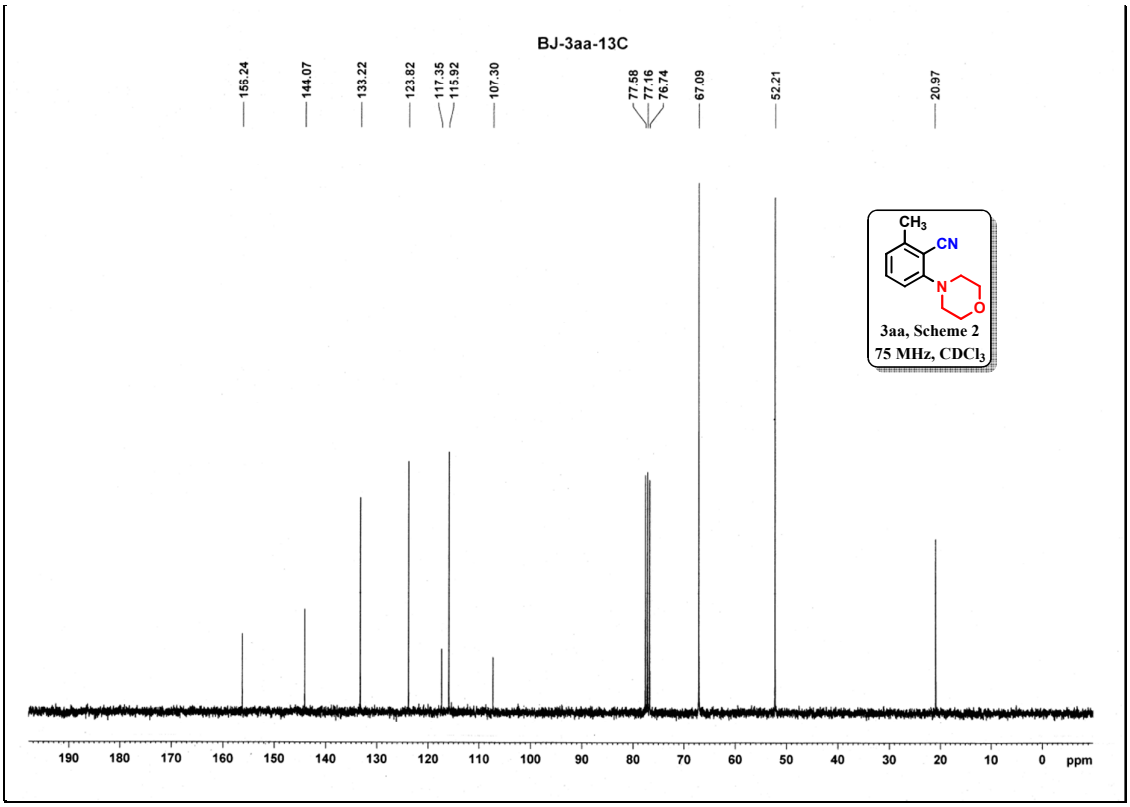
**(1S,2R,4R)-3-(4-Cyano-3,5-bis(4-methylpiperidin-1-yl)phenyl)bicyclo[2.2.1]heptane-2-carbonitrile (7ac, Scheme 4):** Colorless gummy liquid (147.89 mg, 71%); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 0.98 (d, $J$ = 5.4 Hz, 6H), 1.33-1.38 (m, 3H), 1.43-1.56 (m, 6H), 1.67-1.73 (m, 6H), 1.99 (d, $J$ = 10.5 Hz, 1H), 2.60 (s, 1H), 2.72-2.75 (m, 5H), 3.53 (d, $J$ = 11.7 Hz, 4H), 6.38 (s, 2H); $^{13}$C NMR (75 MHz, CDCl3): δ = 21.9 (2C), 27.7, 30.6, 30.8 (2C), 34.5 (4C), 37.2, 41.1, 41.4, 42.6, 50.8, 52.8 (4C), 98.5, 110.7 (2C), 118.2, 120.0, 132.9, 147.2, 158.8; IR (KBr): 2953, 2924, 2874, 2808, 2235, 2208, 1713, 1594, 1560, 1441, 1381, 1227 cm$^{-1}$; anal. calcd. for $C_{27}H_{36}N_4$: C 77.84, H 8.71, N 13.45; found C 77.88, H 8.74, N 13.47%.

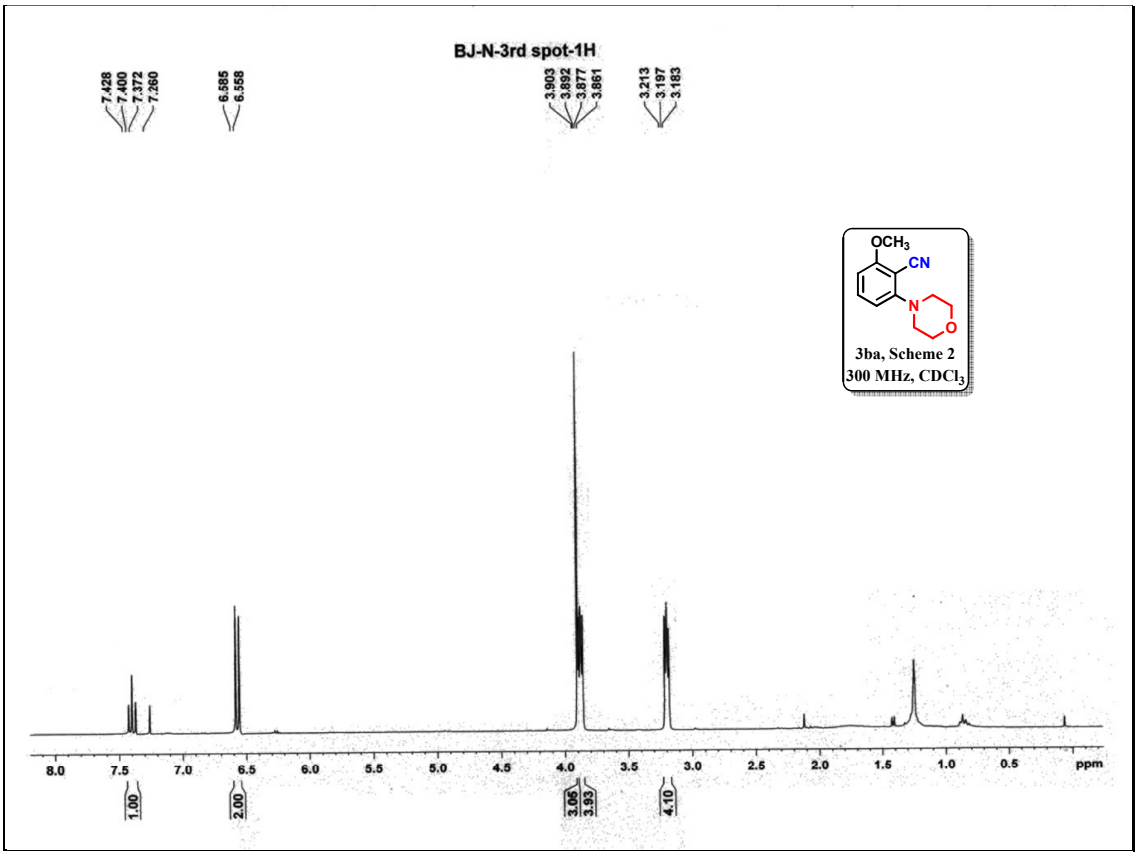
**2,3,5,6-Tetrakis(benzyl(methyl)amino)terephthalonitrile (7ah, Scheme 4):** Colorless gummy liquid (211.67 mg, 70%); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 2.88 (s, 12H), 4.50 (s, 8H), 6.31 (s, 4H), 7.32 (d, $J$ = 4.5 Hz, 16H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 27.6, 30.4, 37.1, 40.4, 40.7, 42.6, 50.5, 60.1, 93.9, 109.8, 119.9, 127.3, 128.1 (2C), 128.6 (2C), 132.6, 137.7, 147.2, 157.9; IR (KBr): 2960, 2876, 2233, 2204, 1593, 1556, 1450, 1219 cm$^{-1}$; anal. calcd. for $C_{40}H_{40}N_6$ : C 79.44, H 6.67, N 13.90; found C 79.47, H 6.69, N 13.87%.

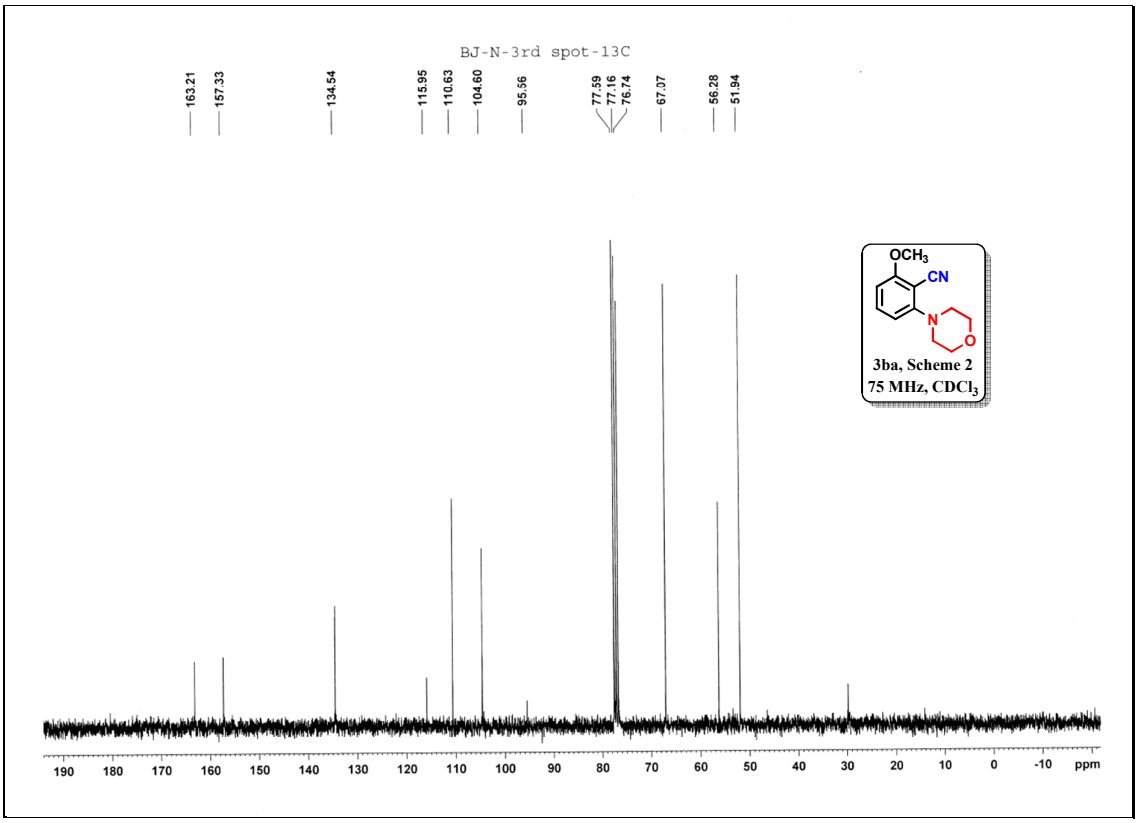
**1-Methyl-4,6-dimorpholino-1H-indole-5-carbonitrile (9aa, Scheme 5):** Off white solid (88.13 mg, 54%); m.p. 163-165 $^{o}$C; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 3.13-3.16 (m, 4H), 3.56 (t, $J$ = 4.5 Hz, 4H), 3.72 (s, 3H), 3.89-3.94 (m, 8H), 6.52 (s, 1H), 6.59 (dd, $J_1$ = 3.3 Hz, $J_2$ = 0.3 Hz, 1H), 6.96 (d, $J$ = 3.3 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 33.3, 52.9 (2C), 53.3 (2C), 67.3 (2C), 67.8 (2C), 93.8, 94.2, 101.7, 117.8, 119.6, 128.5, 140.6, 151.8, 152.2; IR (KBr): 2956, 2200, 1597, 1444, 1267, 1112 cm$^{-1}$; HRMS: m/z calcd. for $C_{18}H_{22}N_4NaO_2$ $[M+Na]^+$ 349.1635, found 349.1642.

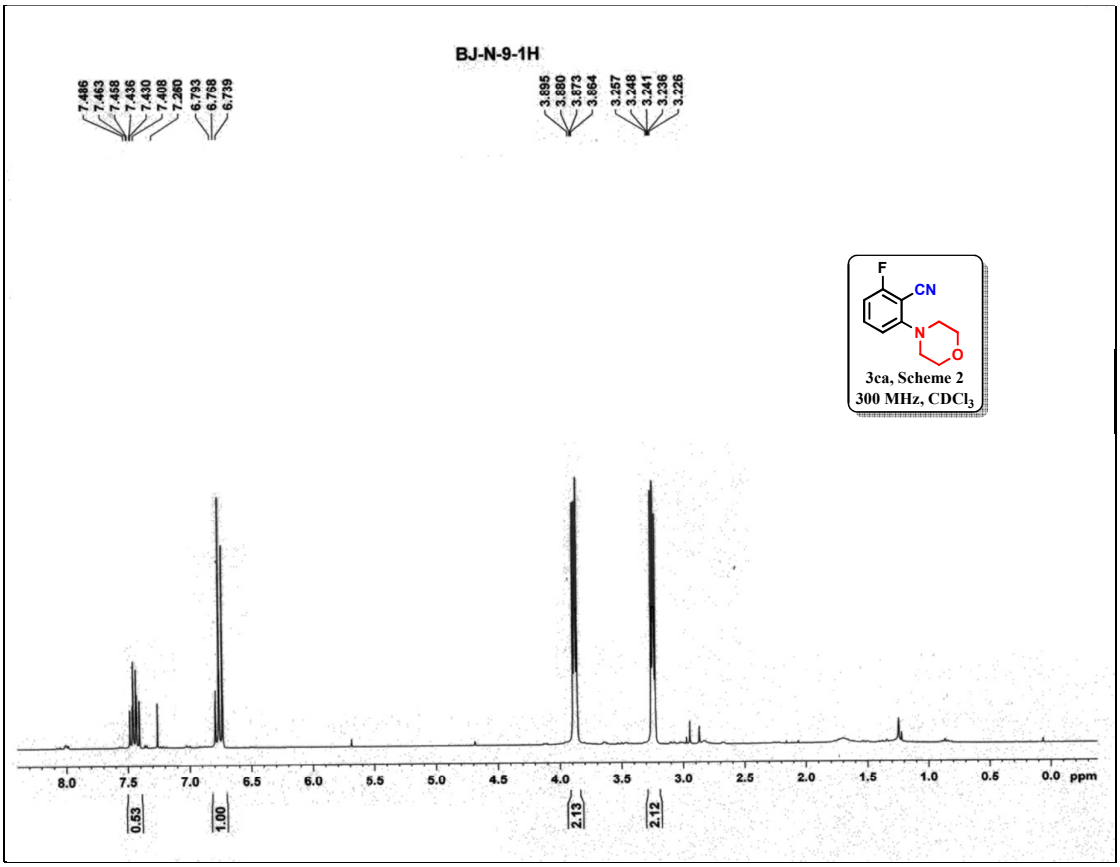
**2-(4-Methylpiperidin-1-yl)-5-(trifluoromethyl)benzonitrile (11ac, Scheme 6):** Colorless gummy liquid (97.86 mg, 73%); $^{1}$H NMR (300 MHz, $CDCl_3$): δ 1.01 (d, $J$ = 6.3 Hz, 3H), 1.40-1.54 (m, 2H), 1.55-1.61 (m, 1H), 1.79 (dd, $J_1$ = 12.6 Hz, $J_2$ = 1.8 Hz, 2H), 2.87-2.95 (m, 2H), 3.71-3.76 (m, 2H), 7.02 (d, $J$ = 9 Hz, 1H), 7.62 (dd, $J_1$ = 8.7 Hz, $J_2$ = 2.1 Hz, 1H), 7.75 (d, $J$ = 2.1 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ 21.8, 30.6, 34.2 (2C), 51.8 (2C), 103.9, 117.9, 118.6, 122.2 (q, $J_{C\text{-}F}$ = 33.7 Hz, 1C), 123.6 (q, $J_{C\text{-}F}$ = 270 Hz, 1C), 130.5 (q, $J_{C\text{-}F}$ = 3.75 Hz, 1C), 132.0 (q, $J_{C\text{-}F}$ = 3.75 Hz, 1C), 158.2; $^{19}$F NMR (470 MHz, $CDCl_3$, $C_6F_6$ as standrad compound): δ -65.4; IR (KBr): 2955, 2928, 2222, 1616, 1510, 1462, 1384, 1333, 1126 cm$^{-1}$; HRMS: m/z calcd. for $C_{14}H_{16}F_3N_2$ $[M+H]^+$ 269.1260, found 269.1261.

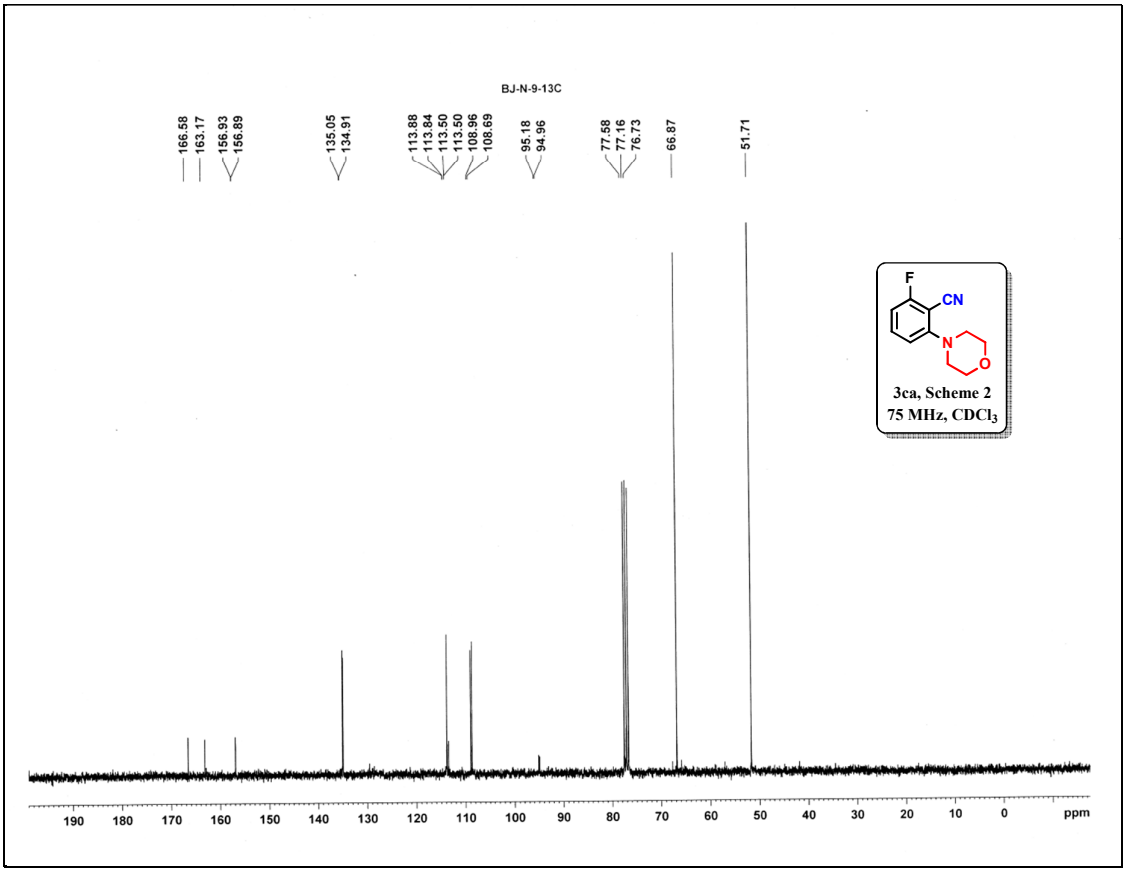

BJ-3aa-1H
7.391
7.365
7.338
7.260
6.928
6.903
6.849
6.822
3.901
3.885
3.880
3.870
3.171
3.162
3.155
3.150
3.140
2.500
CH3
CN
N
O
3aa, Scheme 2
300 MHz, CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
1.00
1.01
4.22
4.19
3.03

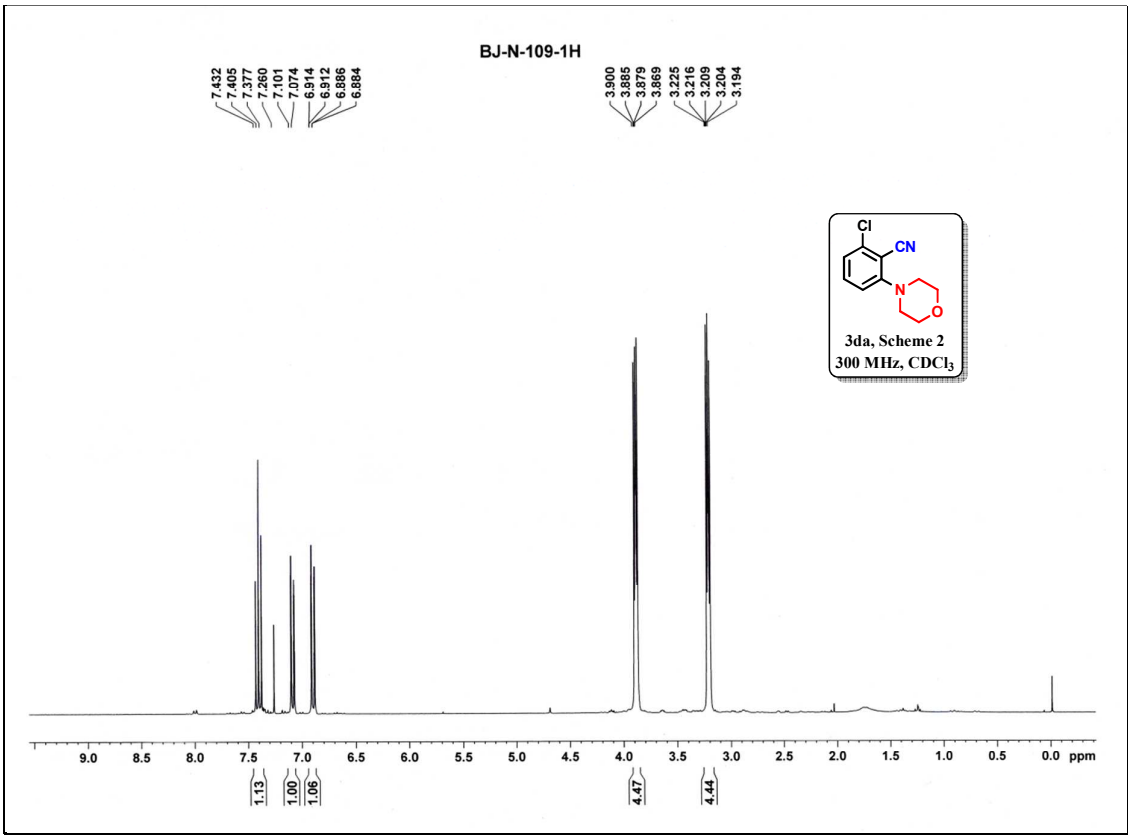

BJ-3aa-13C
155.24
144.07
133.22
123.82
117.35
115.92
107.30
77.58
77.16
76.74
67.09
52.21
20.97
CH3
CN
N
O
3aa, Scheme 2
75 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

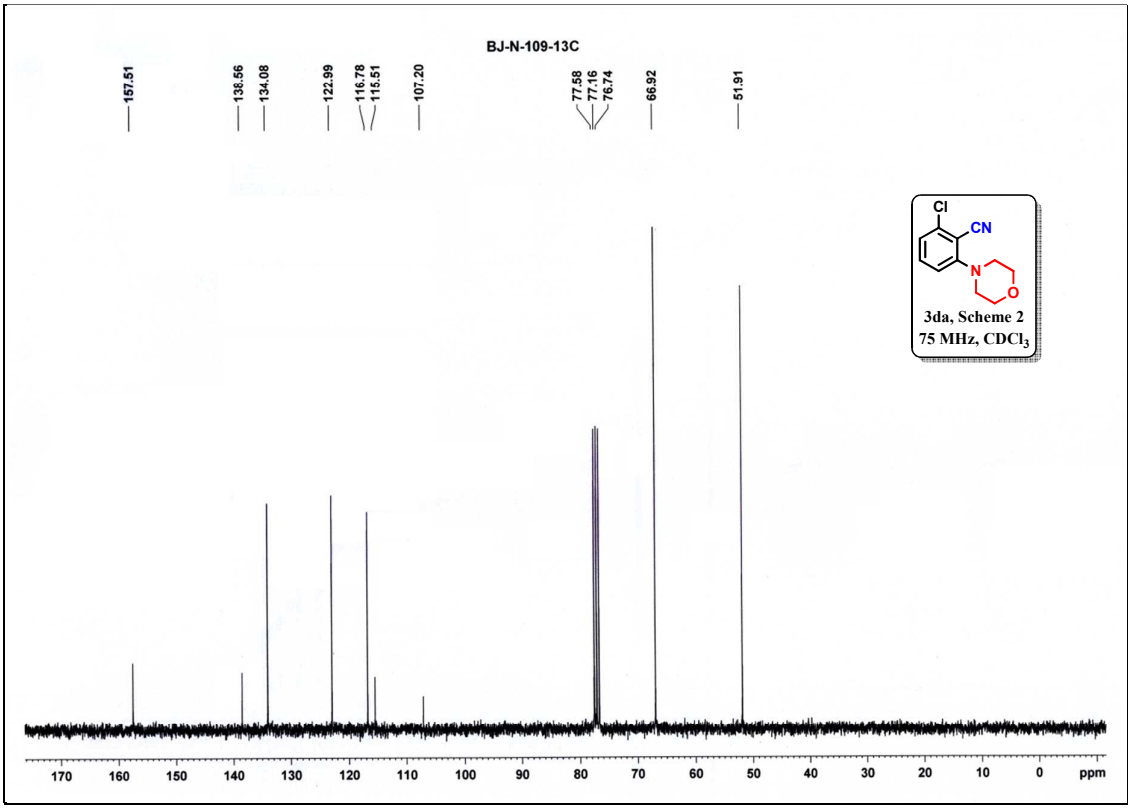

BJ-N-3rd spot-1H
7.428
7.400
7.372
7.260
6.585
6.558
3.903
3.892
3.877
3.861
3.213
3.197
3.183
OCH3
CN
N
O
3ba, Scheme 2
300 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
2.00
3.06
3.93
4.10

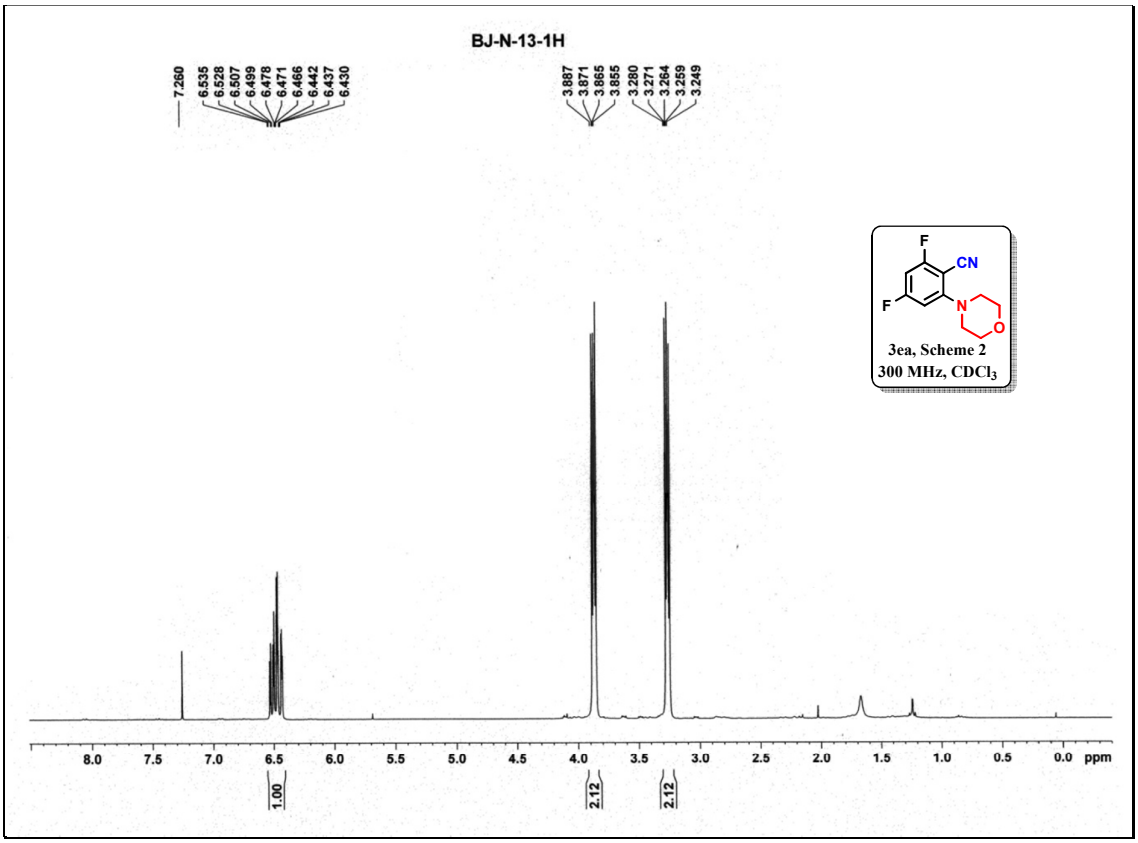

BJ-N-3rd spot-13C
163.21
157.33
134.54
115.95
110.63
104.60
95.56
77.59
77.16
76.74
67.07
56.28
51.94
OCH3
CN
N
O
3ba, Scheme 2
75 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm

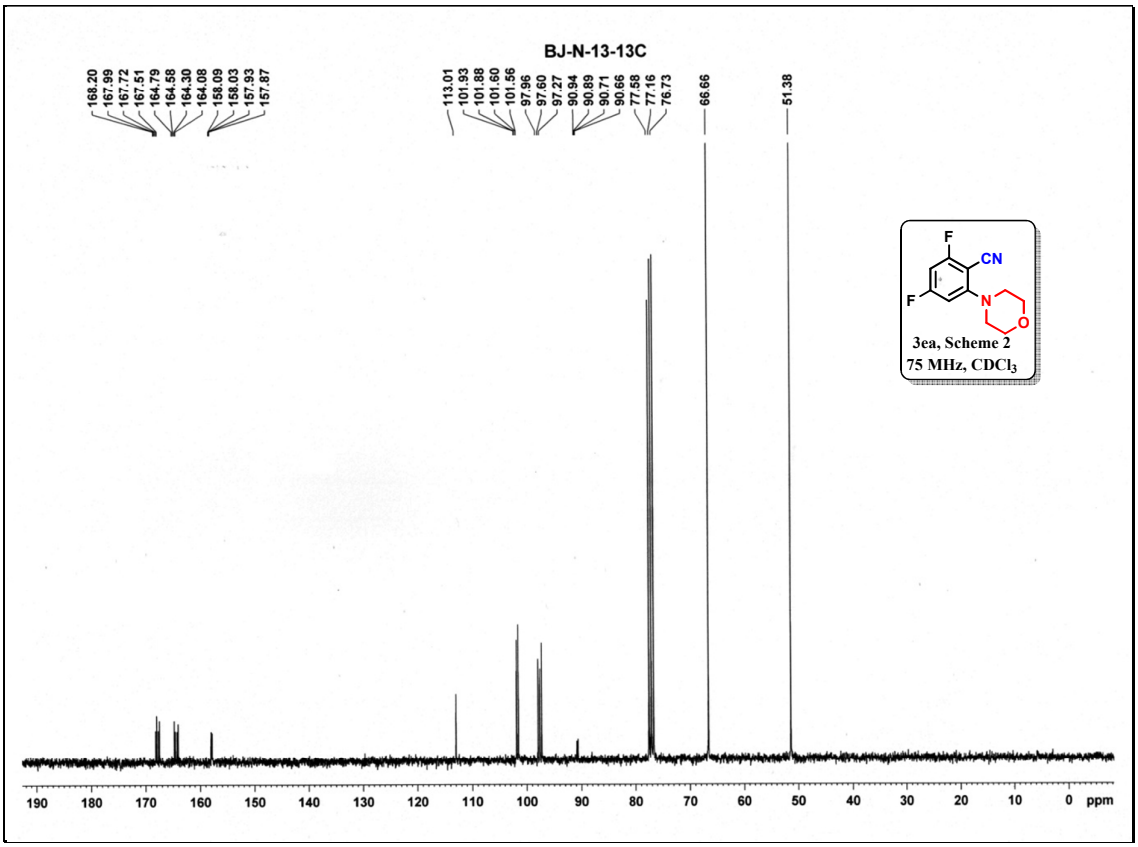

BJ-N-9-1H
7.486
7.463
7.458
7.436
7.430
7.408
7.260
6.793
6.768
6.739
3.895
3.880
3.873
3.864
3.257
3.248
3.241
3.236
3.226
F
CN
N
O
3ca, Scheme 2
300 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.53
1.00
2.13
2.12

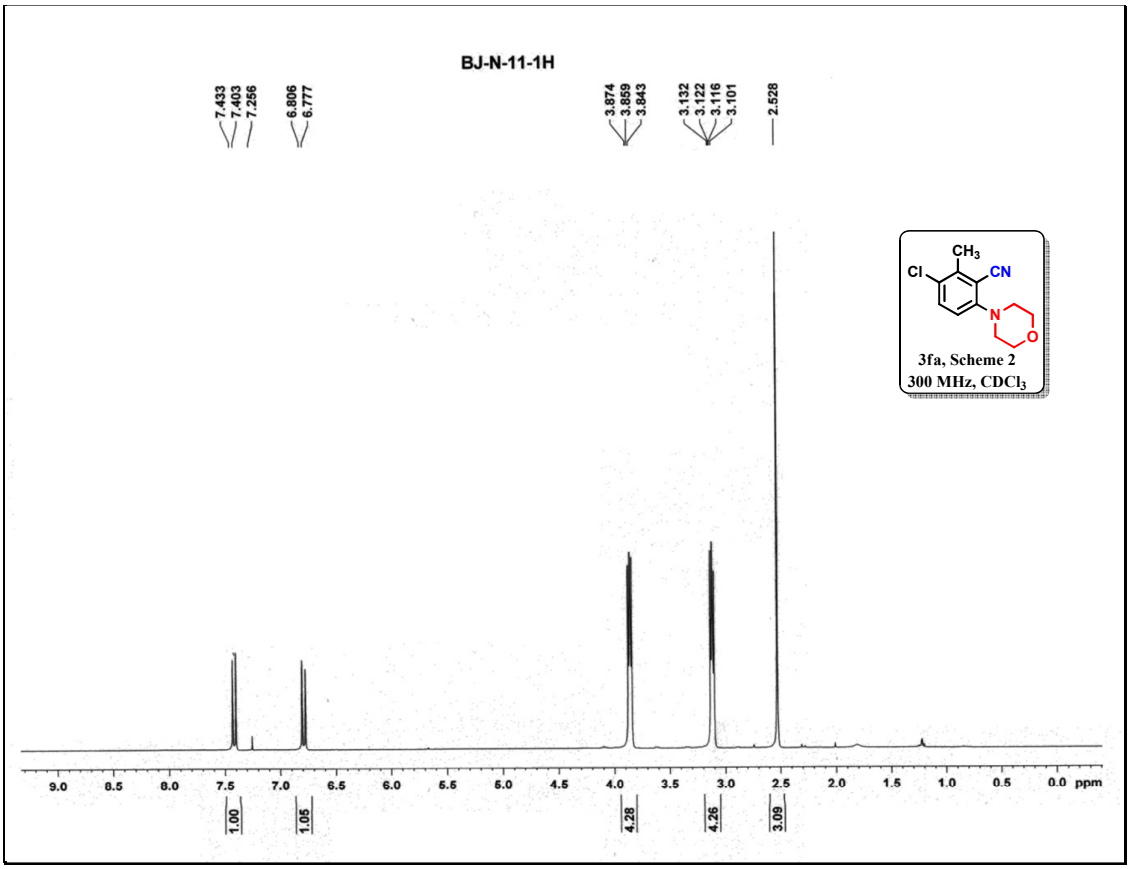

BJ-N-9-13C
166.58
163.17
156.93
156.89
135.05
134.91
113.88
113.84
113.50
113.50
108.96
108.69
95.18
94.96
77.58
77.16
76.73
66.87
51.71
F
CN
N
O
3ca, Scheme 2
75 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

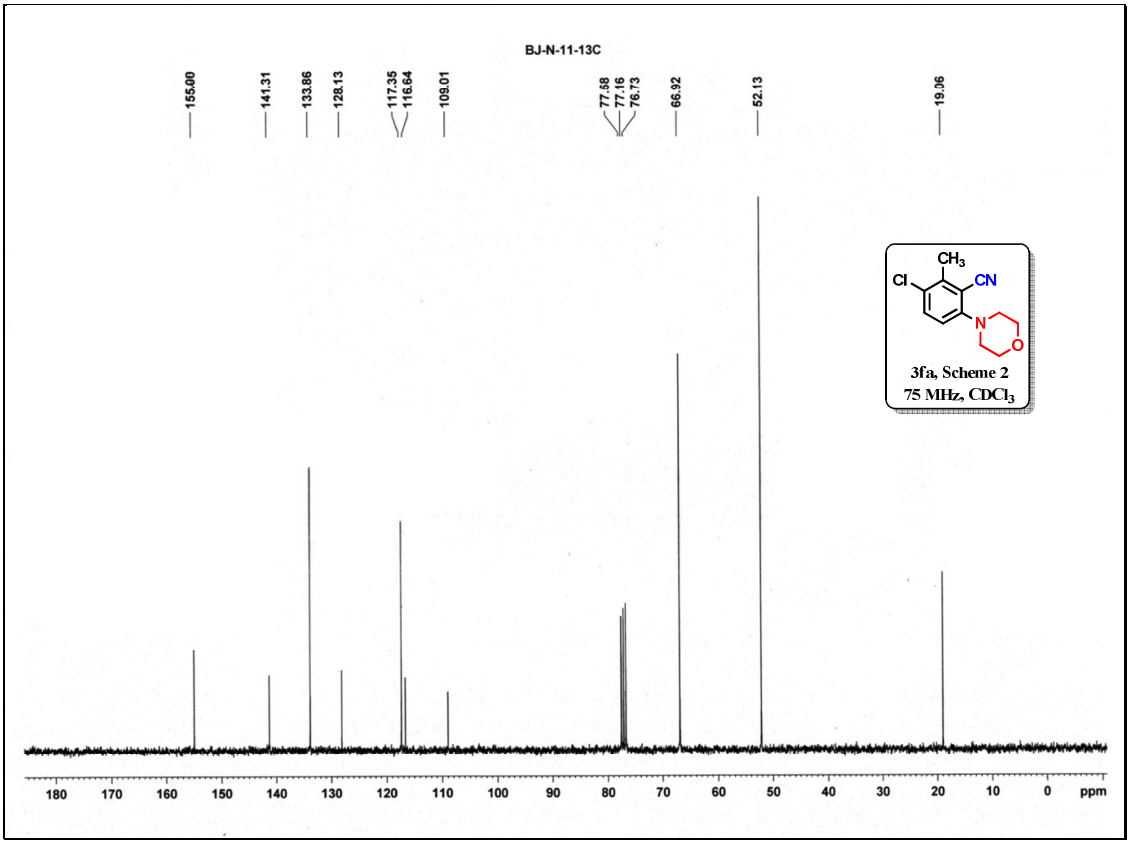

BJ-N-109-1H
7.432
7.405
7.377
7.260
7.101
7.074
6.914
6.912
6.886
6.884
3.900
3.885
3.879
3.869
3.225
3.216
3.209
3.204
3.194
Cl
CN
N
O
3da, Scheme 2
300 MHz, CDCl3
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.13
1.00
1.06
4.47
4.44

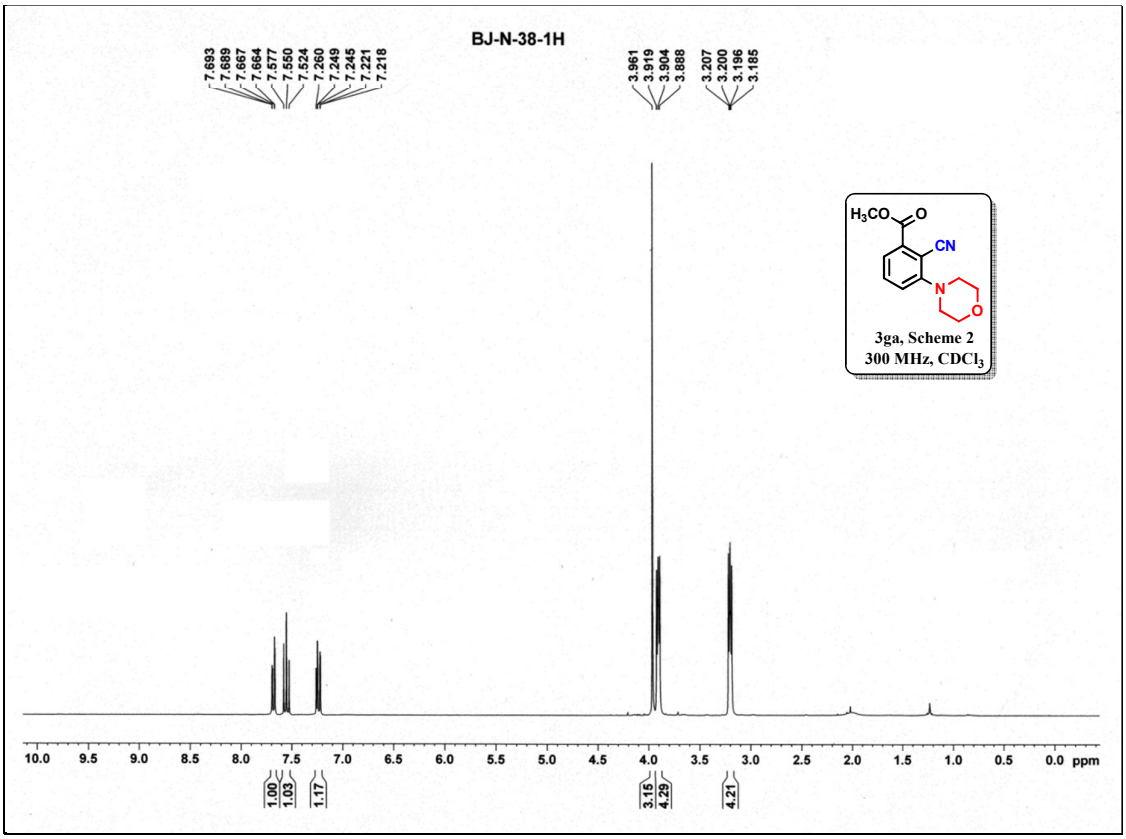

BJ-N-109-13C
157.51
136.56
134.08
122.99
116.78
115.51
107.20
77.58
77.16
76.74
66.92
51.91
Cl
CN
N
O
3da, Scheme 2
75 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

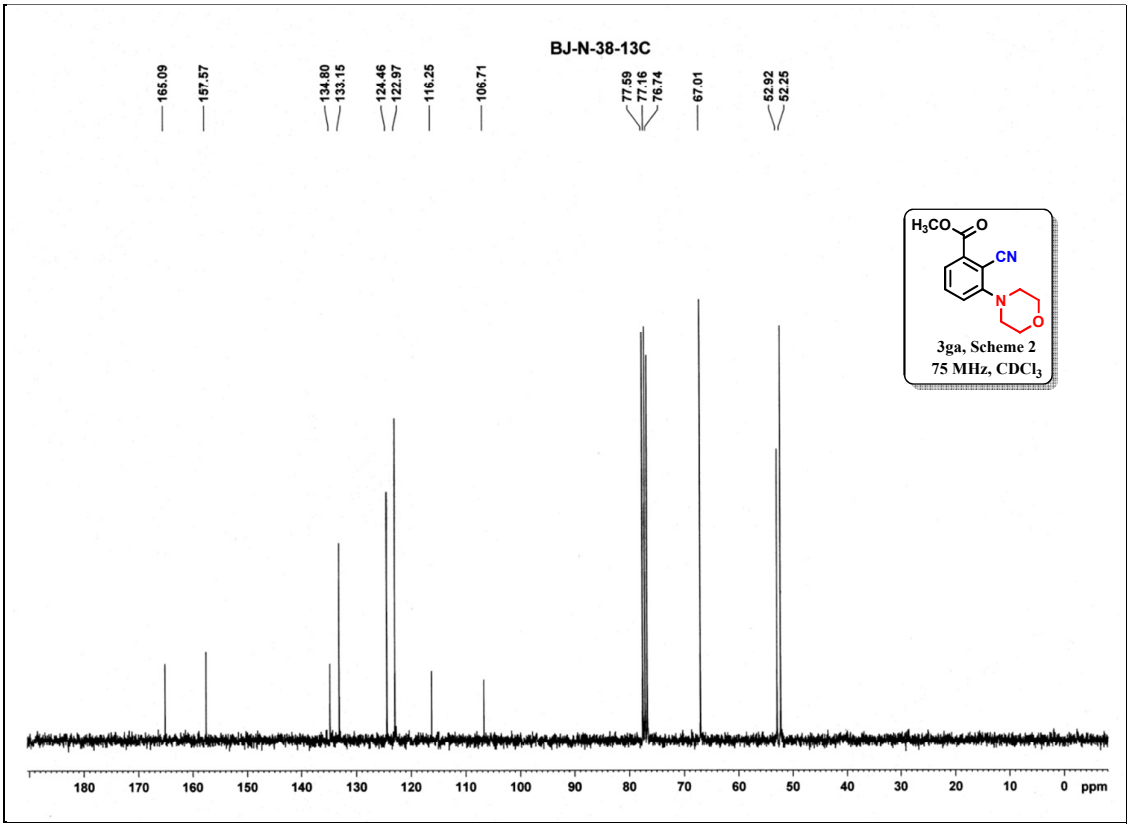

BJ-N-13-1H
7.260
6.535
6.528
6.507
6.499
6.478
6.471
6.466
6.442
6.437
6.430
3.887
3.871
3.865
3.855
3.280
3.271
3.264
3.259
3.249
F
CN
F
N
O
3ea, Scheme 2
300 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.12
2.12

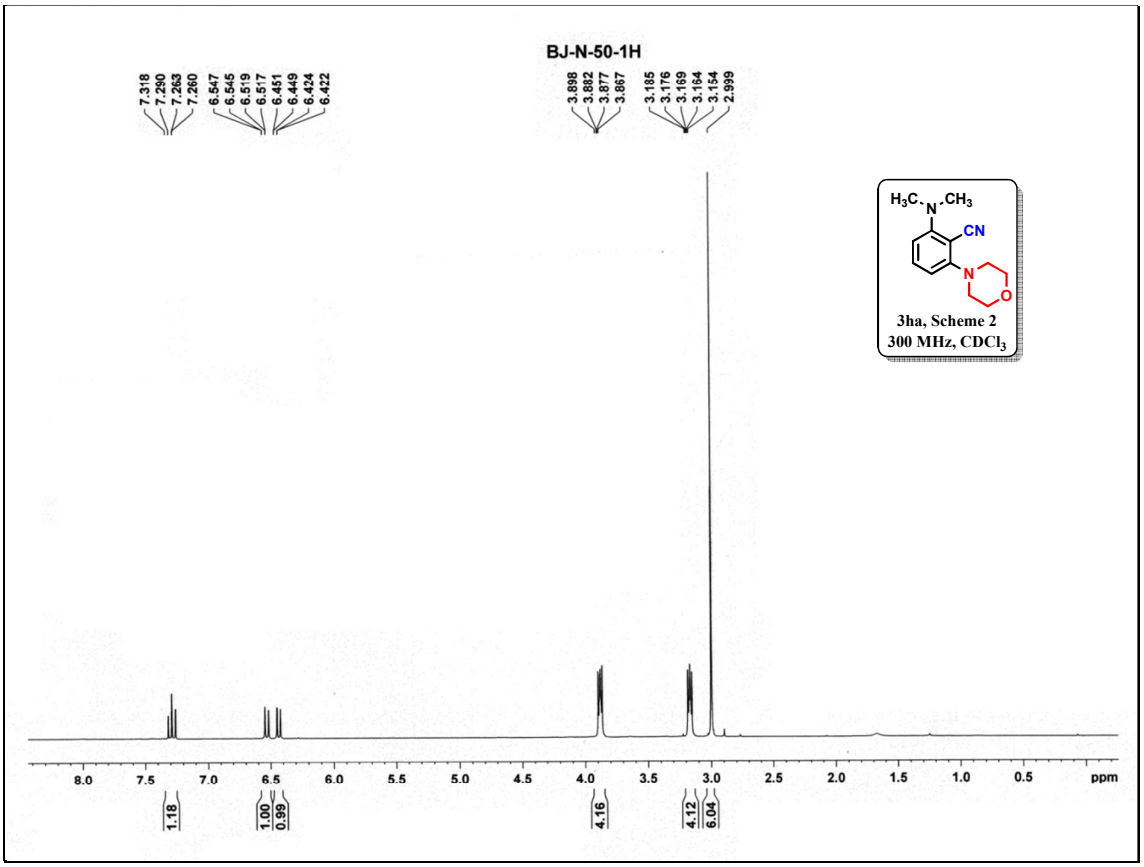

BJ-N-13-13C
168.20
167.99
167.72
167.51
164.79
164.58
164.30
164.08
158.09
158.03
157.93
157.87
113.01
101.93
101.88
101.60
101.56
97.96
97.60
97.27
90.94
90.89
90.71
90.66
77.58
77.16
76.73
66.66
51.38
F
CN
F
N
O
3ea, Scheme 2
75 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

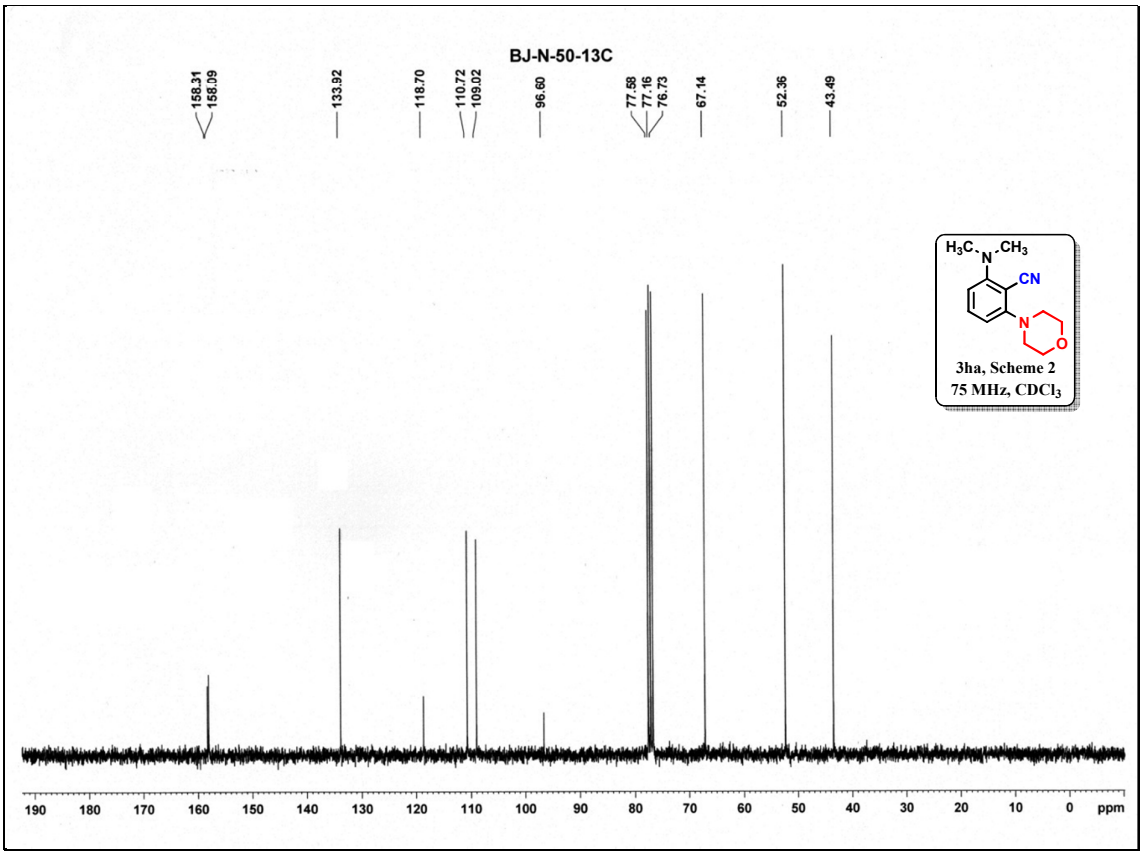

BJ-N-11-1H
7.433
7.403
7.256
6.806
6.777
3.874
3.859
3.843
3.132
3.122
3.116
3.101
2.528
CH3
Cl
CN
N
O
3fa, Scheme 2
300 MHz, CDCl3
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
1.00
1.05
4.28
4.26
3.09

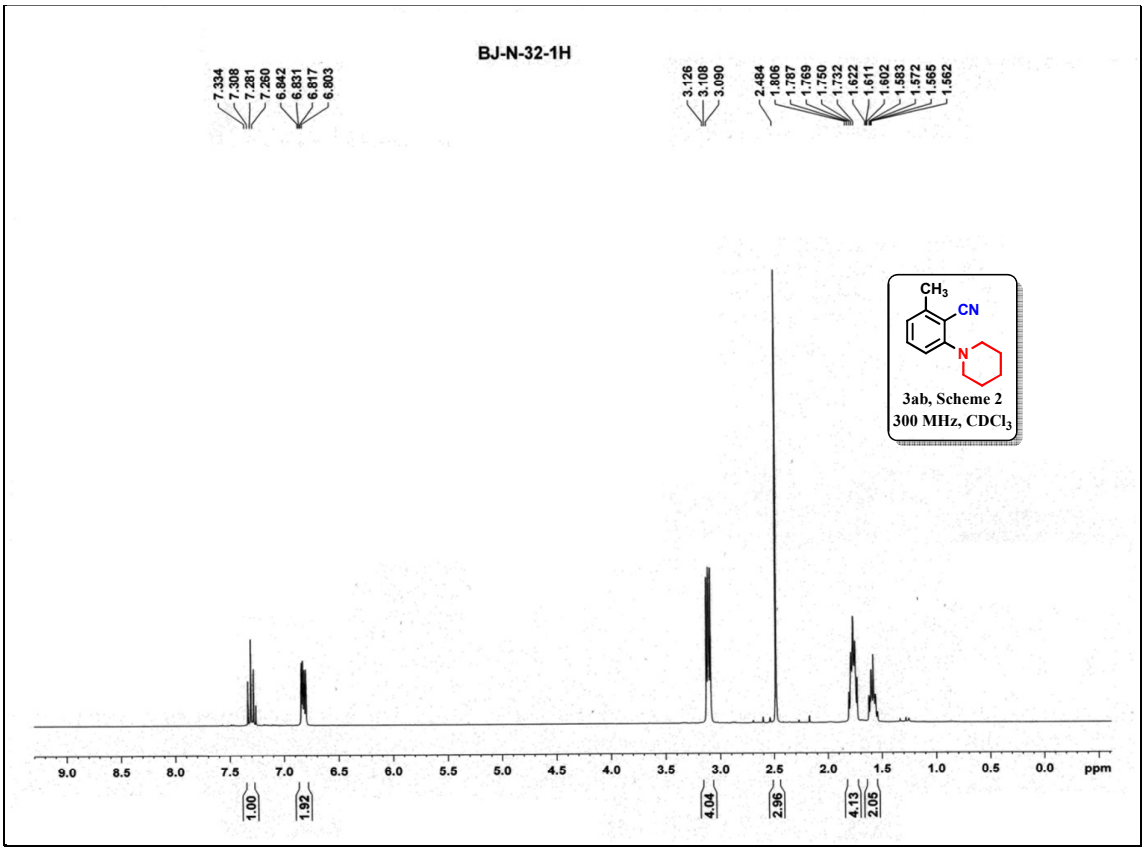

BJ-N-11-13C
155.00
141.31
133.86
128.13
117.35
116.64
109.01
77.58
77.16
76.73
66.92
52.13
19.06
CH3
Cl
CN
N
O
3fa, Scheme 2
75 MHz, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

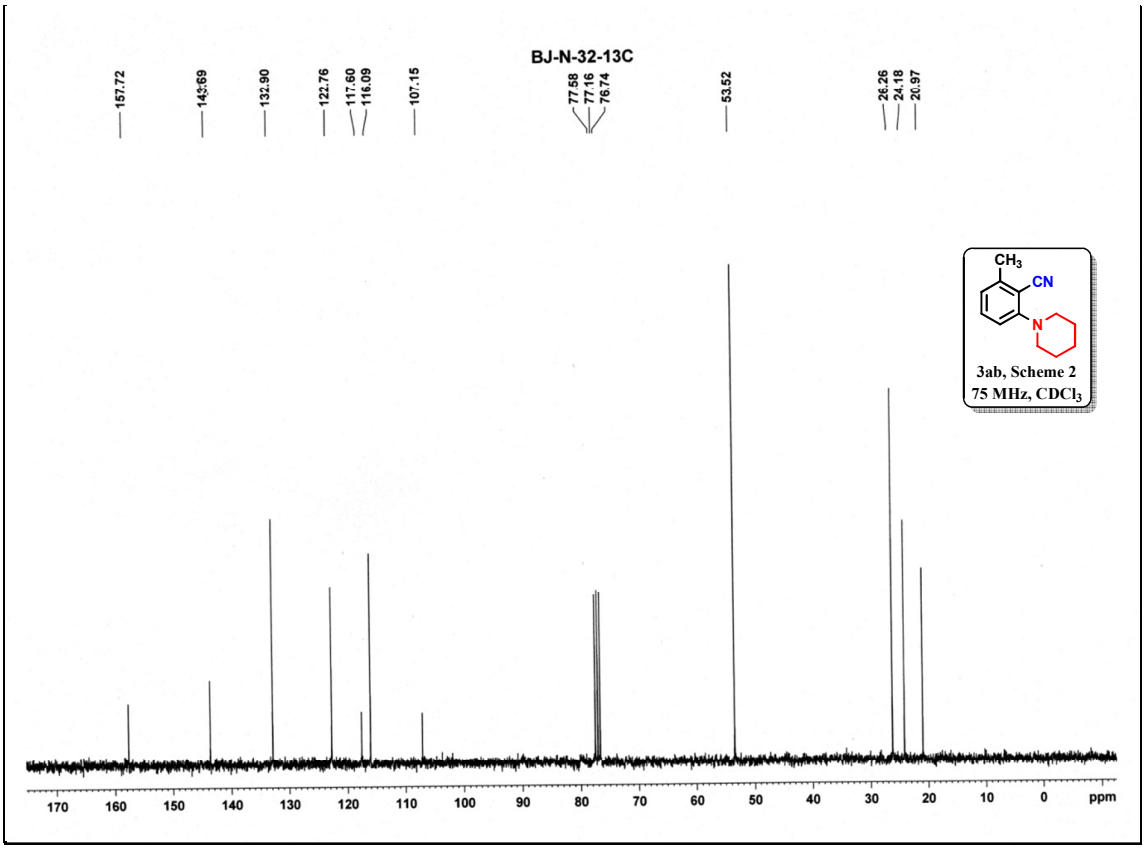

BJ-N-38-1H
7.693
7.689
7.687
7.664
7.577
7.550
7.524
7.260
7.249
7.245
7.221
7.218
3.961
3.919
3.904
3.888
3.207
3.200
3.196
3.185
H3CO
O
CN
N
O
3ga, Scheme 2
300 MHz, CDCl3
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
1.03
1.17
3.15
4.29
4.21

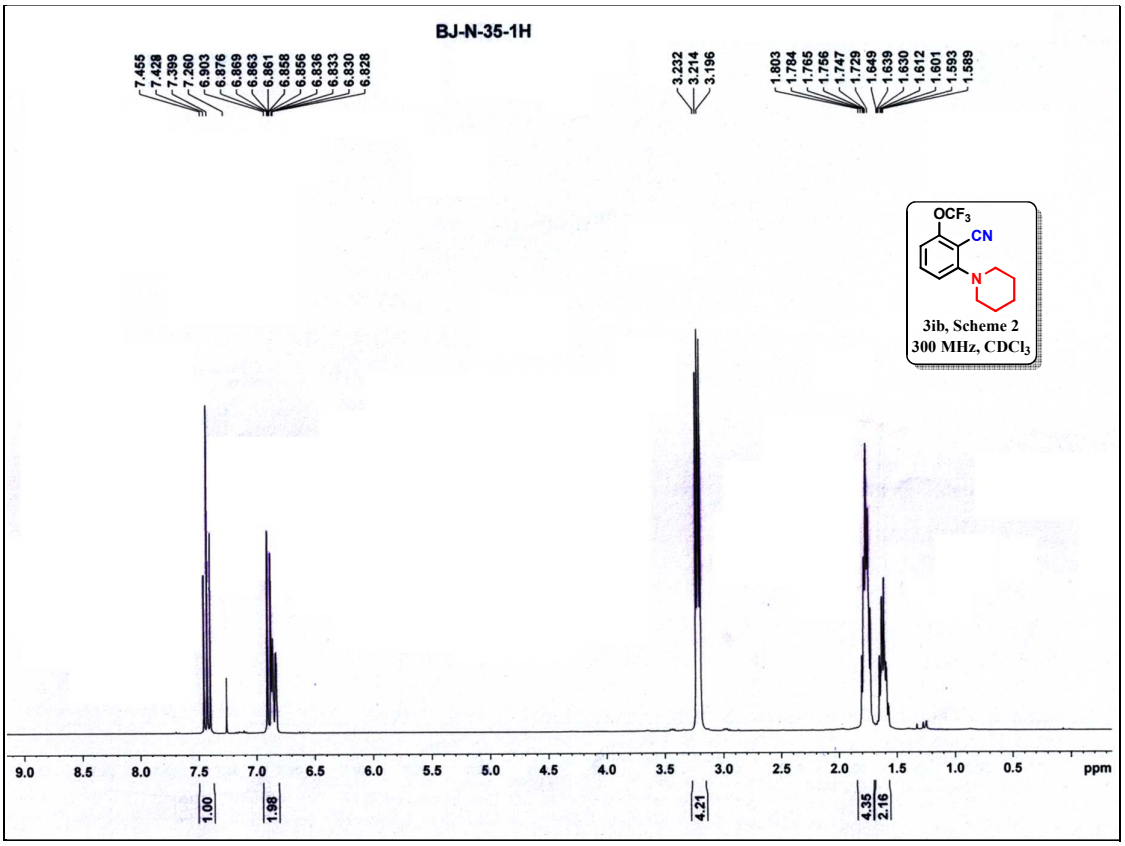

BJ-N-38-13C
165.09
157.57
134.80
133.15
124.46
122.97
116.25
106.71
77.59
77.16
76.74
67.01
52.92
52.25
H3CO
O
CN
N
O
3ga, Scheme 2
75 MHz, CDCl3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

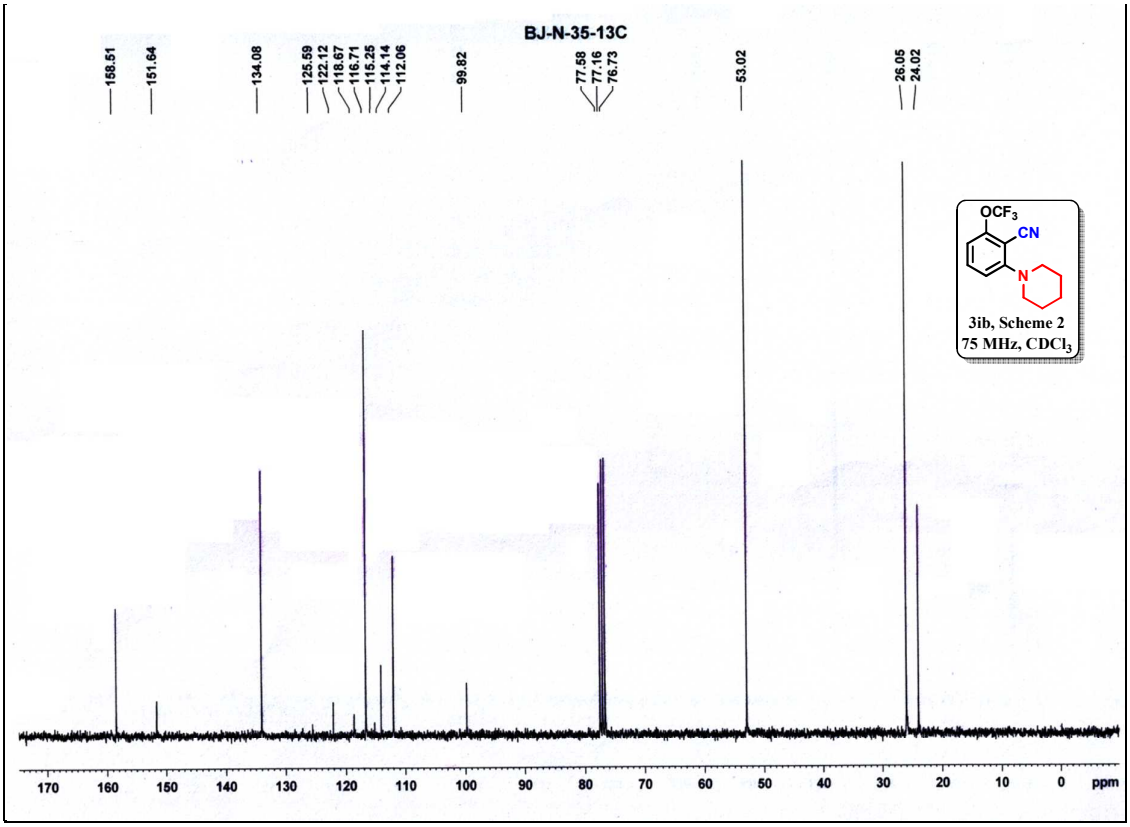

BJ-N-50-1H
7.318
7.290
7.263
7.260
6.547
6.545
6.519
6.517
6.451
6.449
6.424
6.422
3.898
3.882
3.877
3.867
3.185
3.176
3.169
3.164
3.154
2.999
3ha, Scheme 2
300 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.18
1.00
0.99
4.16
4.12
6.04

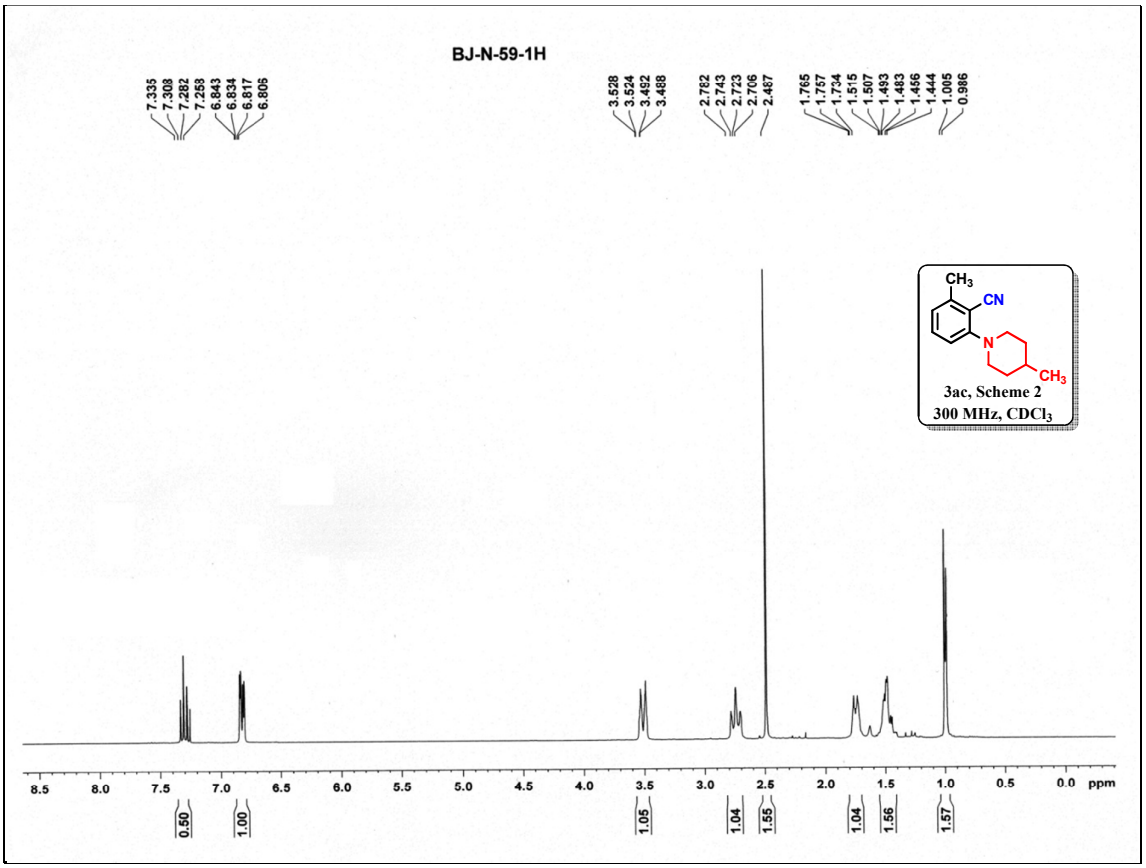

BJ-N-50-13C
158.31
158.09
133.92
118.70
110.72
109.02
96.60
77.58
77.16
76.73
67.14
52.36
43.49
3ha, Scheme 2
75 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

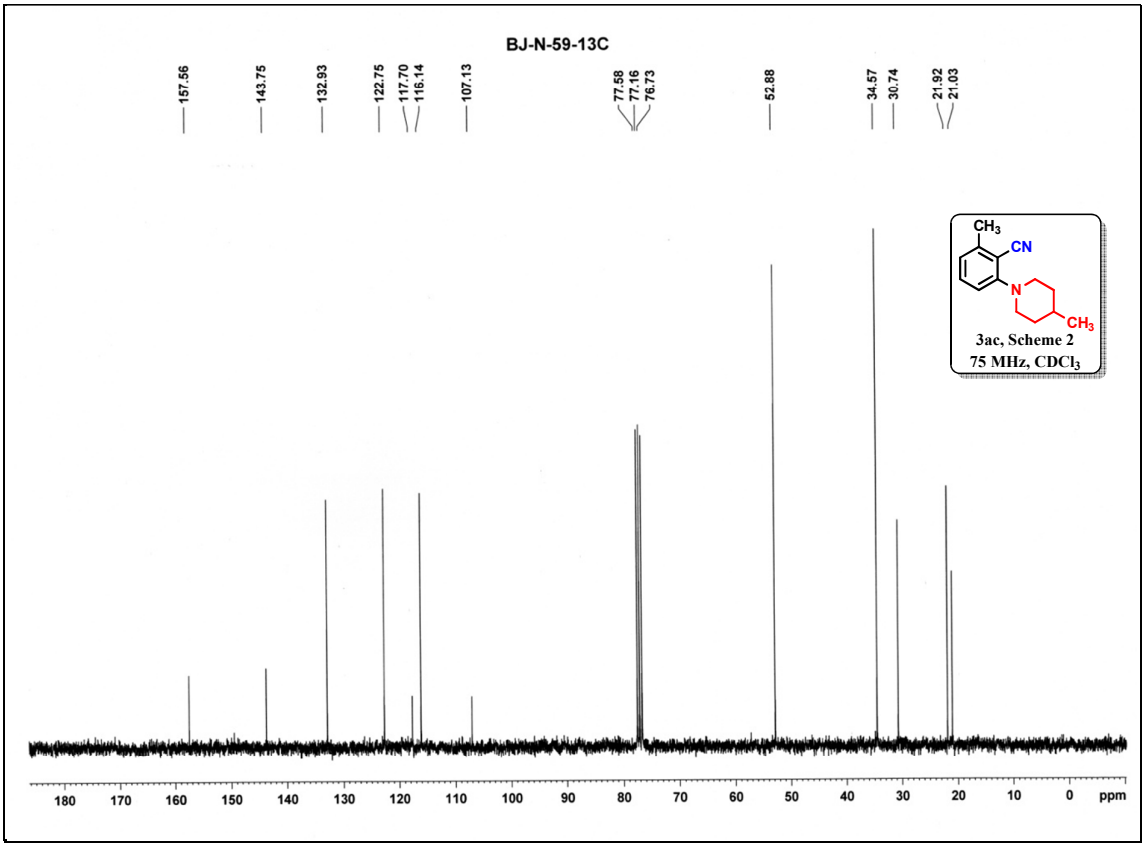

BJ-N-32-1H
7.334
7.308
7.281
7.260
6.842
6.831
6.817
6.803
3.126
3.108
3.090
2.484
1.806
1.787
1.769
1.750
1.732
1.622
1.611
1.602
1.583
1.572
1.565
1.562
CH3
CN
N
3ab, Scheme 2
300 MHz, CDCl3
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.92
4.04
2.96
4.13
2.05

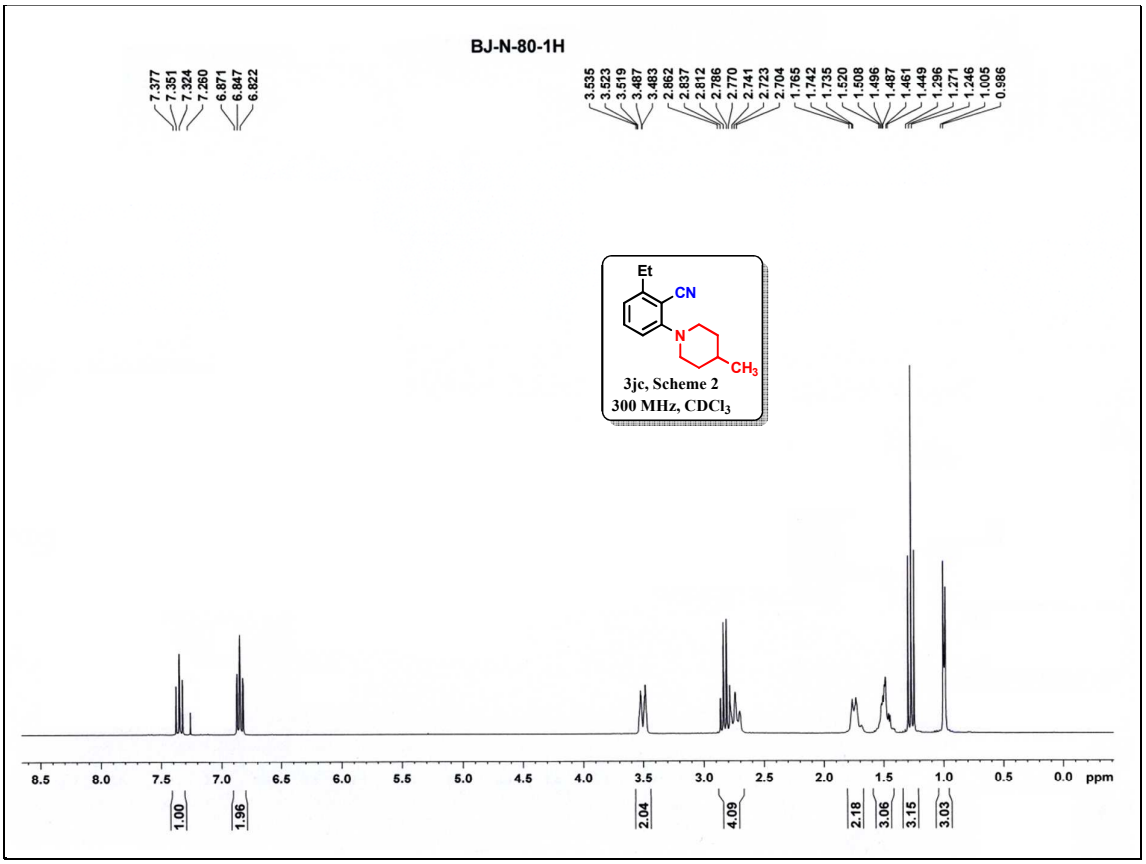

BJ-N-32-13C
157.72
143.69
132.90
122.76
117.60
116.09
107.15
77.58
77.16
76.74
53.52
26.26
24.18
20.97
CH3
CN
N
3ab, Scheme 2
75 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

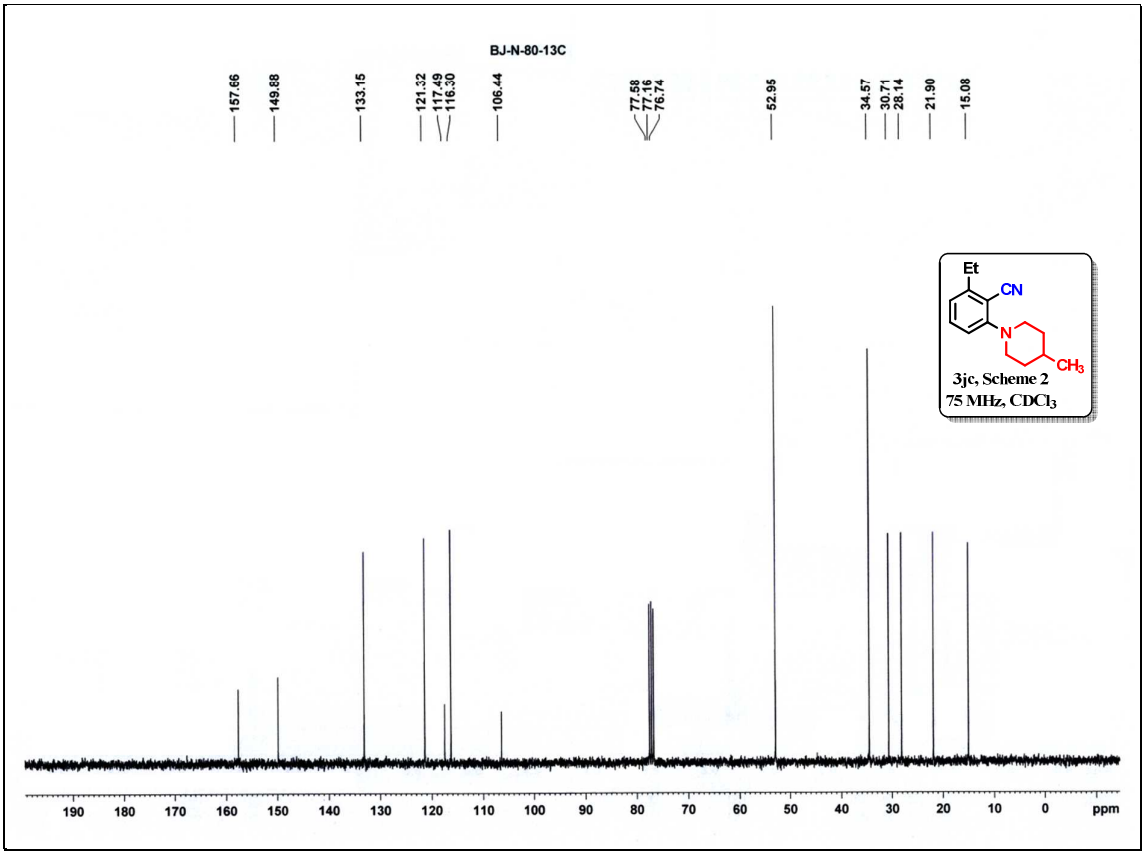

BJ-N-35-1H
7.455
7.428
7.399
7.260
6.903
6.876
6.869
6.863
6.861
6.858
6.856
6.836
6.833
6.830
6.828
3.232
3.214
3.196
1.803
1.784
1.765
1.756
1.747
1.729
1.649
1.639
1.630
1.612
1.601
1.593
1.589
OCF3
CN
N
3ib, Scheme 2
300 MHz, CDCl3
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
1.98
4.21
4.35
2.16

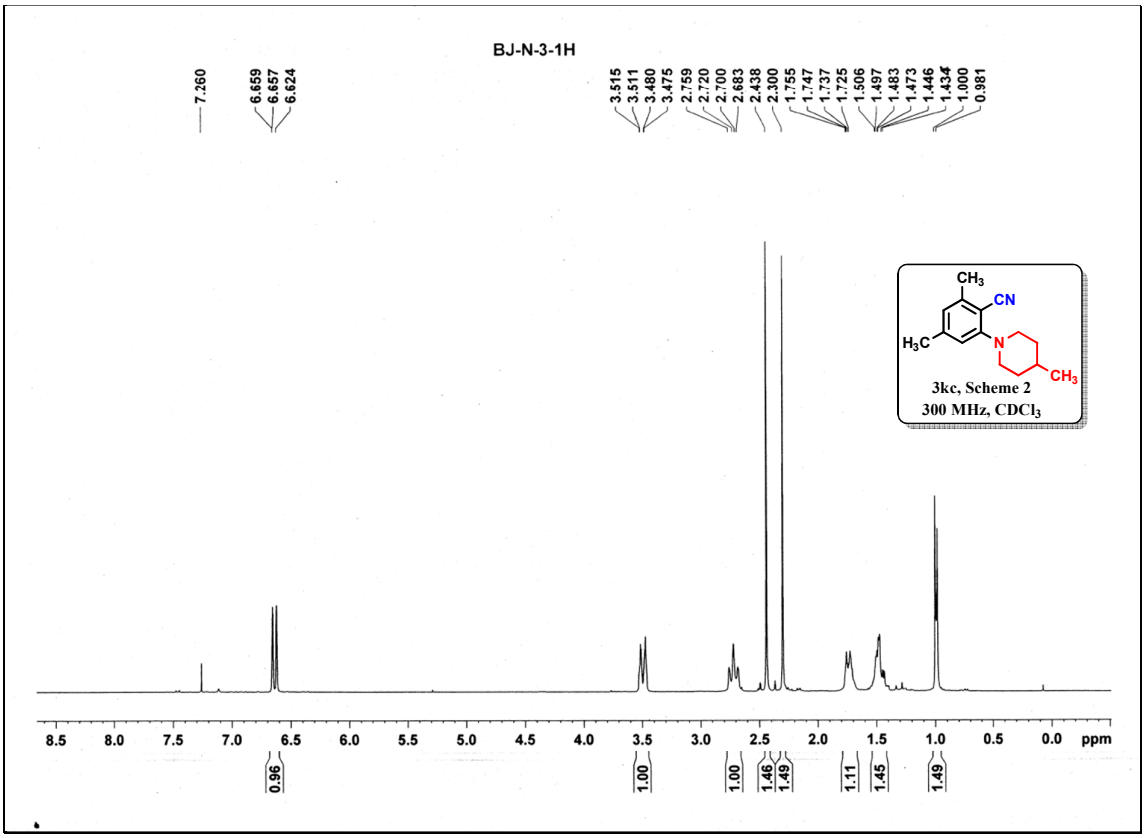

BJ-N-35-13C
158.51
151.64
134.08
125.59
122.12
118.67
116.71
115.25
114.14
112.06
99.82
77.58
77.16
76.73
53.02
26.05
24.02
OCF3
CN
N
3ib, Scheme 2
75 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

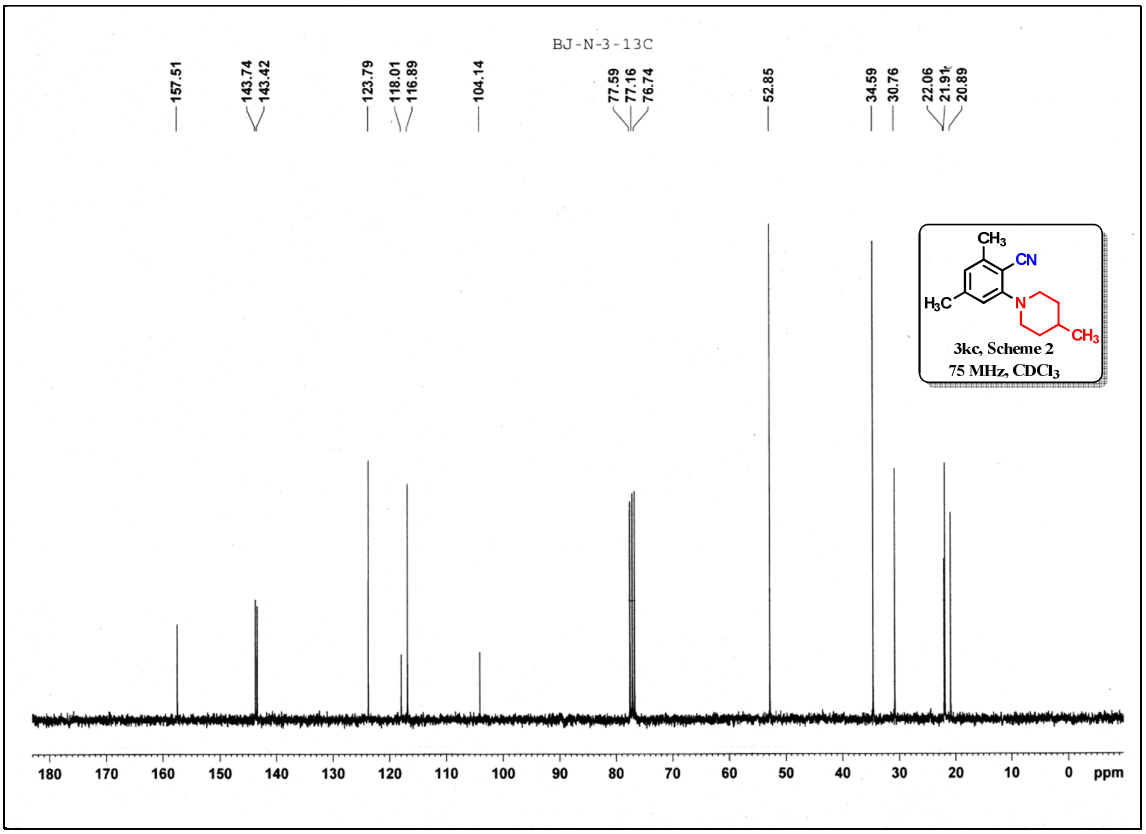

BJ-N-59-1H
7.335
7.308
7.282
7.258
6.843
6.834
6.817
6.806
3.528
3.524
3.492
3.488
2.762
2.743
2.723
2.706
2.467
1.765
1.757
1.734
1.515
1.507
1.493
1.483
1.456
1.444
1.005
0.986
CH3
CN
N
CH3
3ac, Scheme 2
300 MHz, CDCl3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.50
1.00
1.05
1.04
1.55
1.04
1.56
1.57

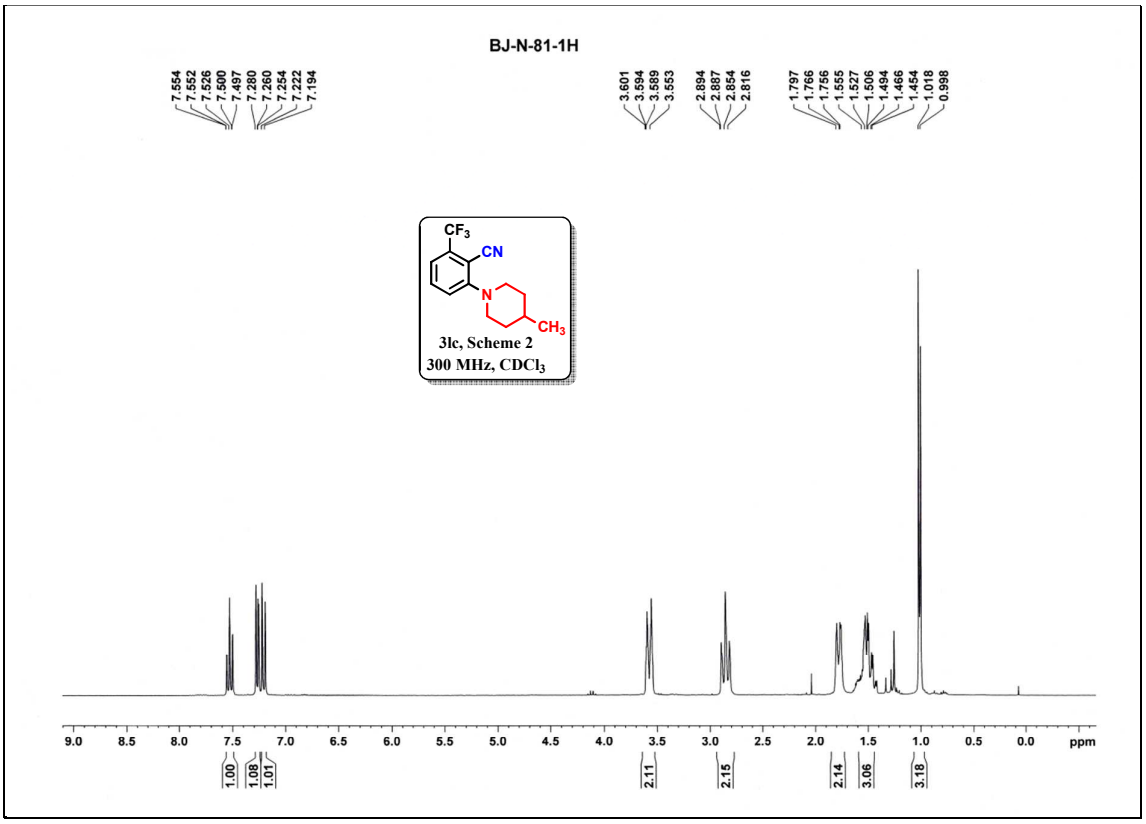

BJ-N-59-13C
157.56
143.75
132.93
122.75
117.70
116.14
107.13
77.58
77.16
76.73
52.88
34.57
30.74
21.92
21.03
CH3
CN
N
CH3
3ac, Scheme 2
75 MHz, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

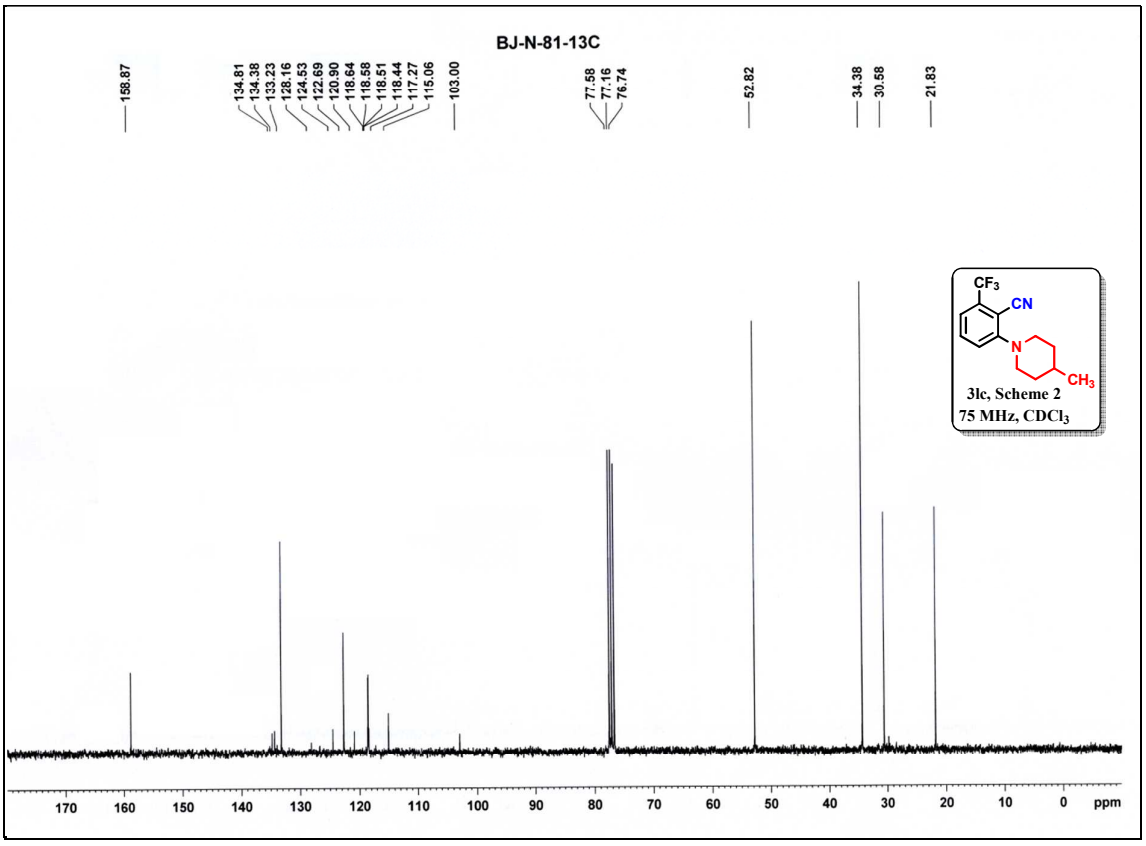

BJ-N-80-1H
7.377
7.351
7.324
7.260
6.871
6.847
6.822
3.535
3.523
3.519
3.487
3.483
2.862
2.837
2.812
2.786
2.770
2.741
2.723
2.704
1.765
1.742
1.735
1.520
1.508
1.496
1.487
1.461
1.449
1.296
1.271
1.246
1.005
0.986
Et
CN
N
CH3
3jc, Scheme 2
300 MHz, CDCl3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.96
2.04
4.09
2.18
3.06
3.15
3.03

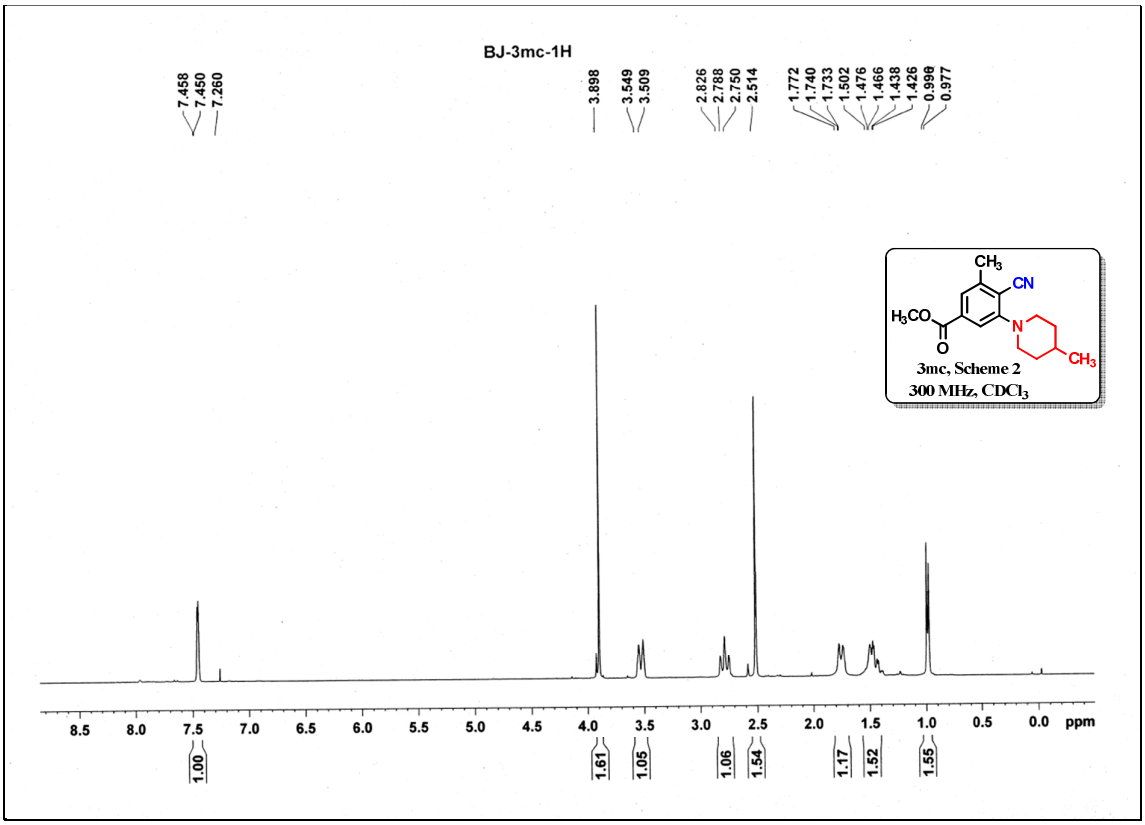

BJ-N-80-13C
157.66
149.88
133.15
121.32
117.49
116.30
106.44
77.58
77.16
76.74
52.95
34.57
30.71
28.14
21.90
15.08
Et
CN
N
CH3
3jc, Scheme 2
75 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

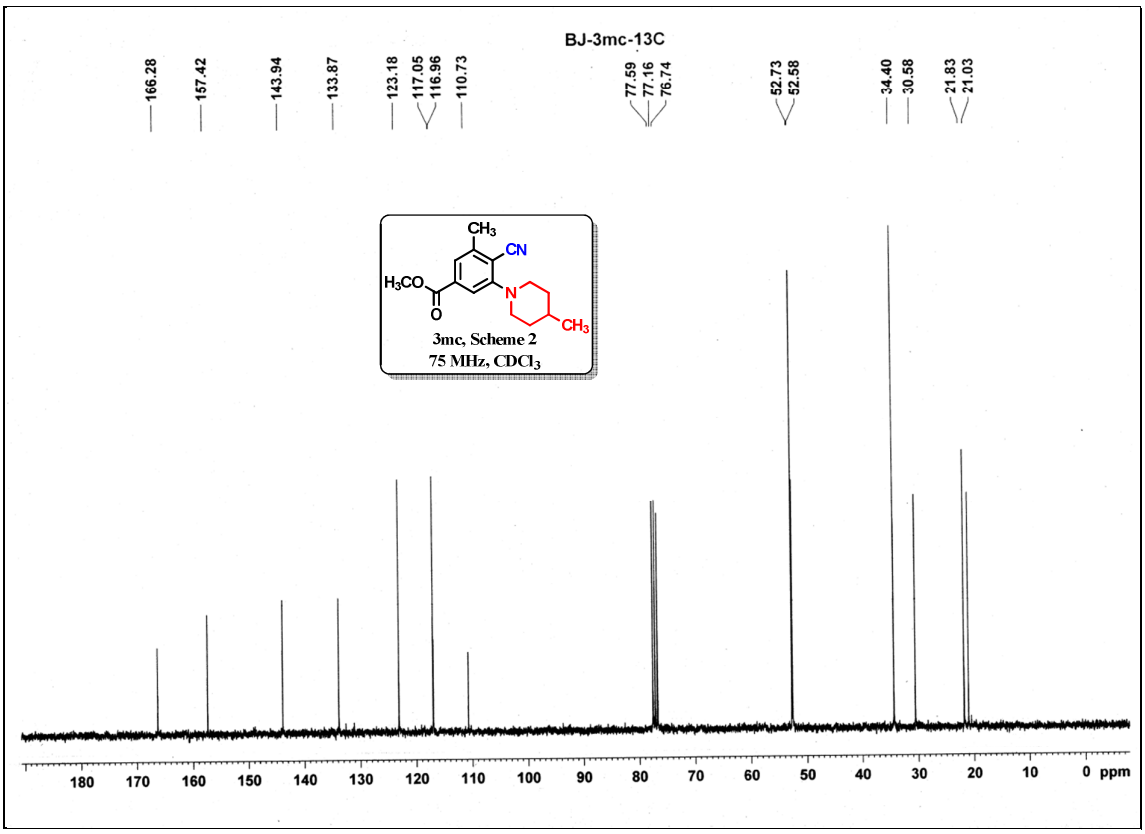

BJ-N-3-1H
7.260
6.659
6.657
6.624
3.515
3.511
3.480
3.475
2.759
2.720
2.700
2.683
2.438
2.300
1.755
1.747
1.737
1.725
1.506
1.497
1.483
1.473
1.446
1.434
1.000
0.981
3kc, Scheme 2
300 MHz, CDCl3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.96
1.00
1.00
1.46
1.49
1.11
1.45
1.49

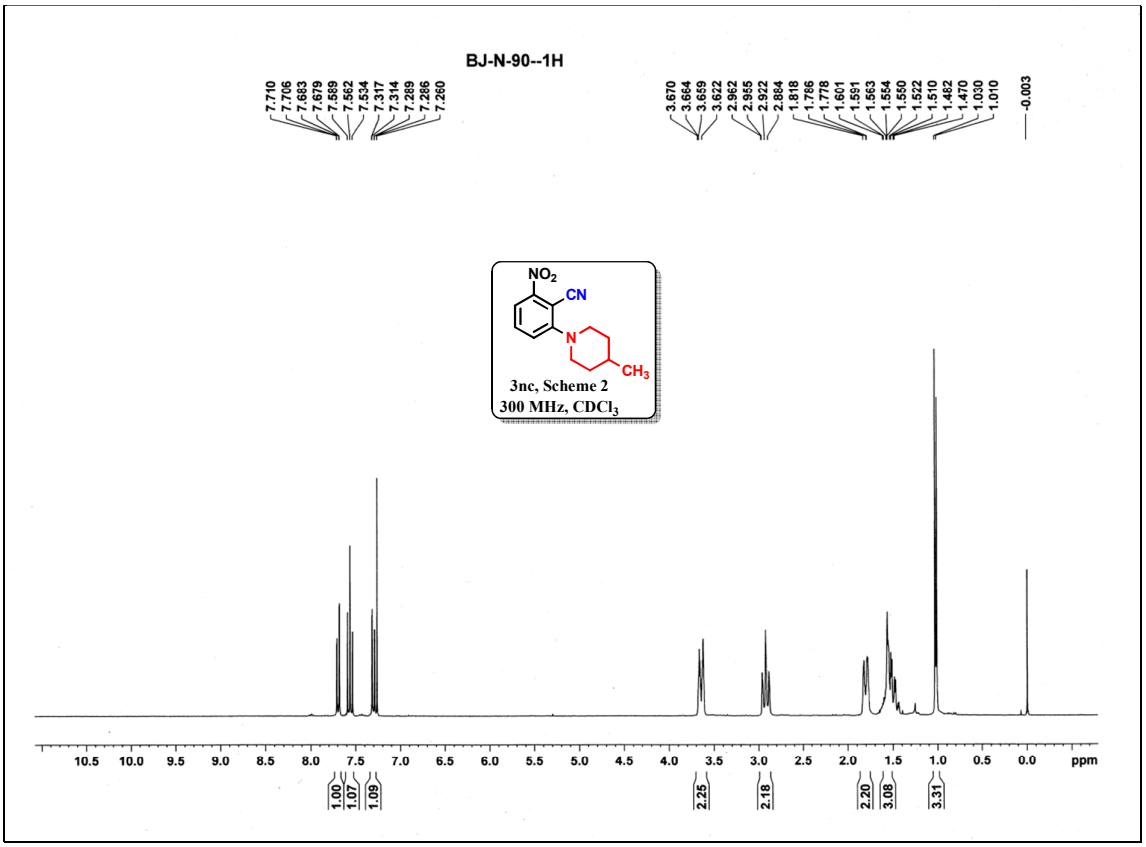

BJ-N-3-13C
157.51
143.74
143.42
123.79
118.01
116.89
104.14
77.59
77.16
76.74
52.85
34.59
30.76
22.06
21.91
20.89
3kc, Scheme 2
75 MHz, CDCl3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

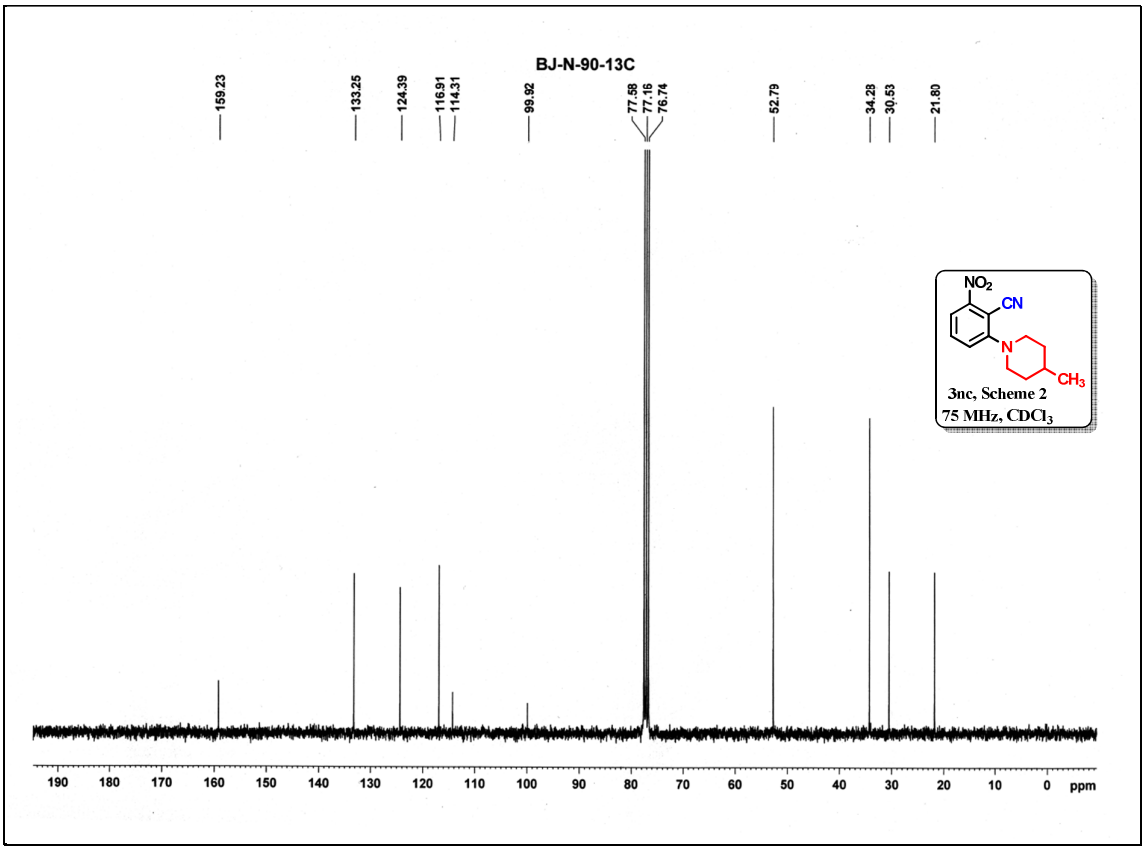

BJ-N-81-1H
7.554
7.552
7.526
7.500
7.497
7.280
7.260
7.254
7.222
7.194
3.601
3.594
3.589
3.553
2.894
2.887
2.854
2.816
1.797
1.766
1.756
1.555
1.527
1.506
1.494
1.466
1.454
1.018
0.998
CF3
CN
N
CH3
3lc, Scheme 2
300 MHz, CDCl3
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.08
1.01
2.11
2.15
2.14
3.06
3.18

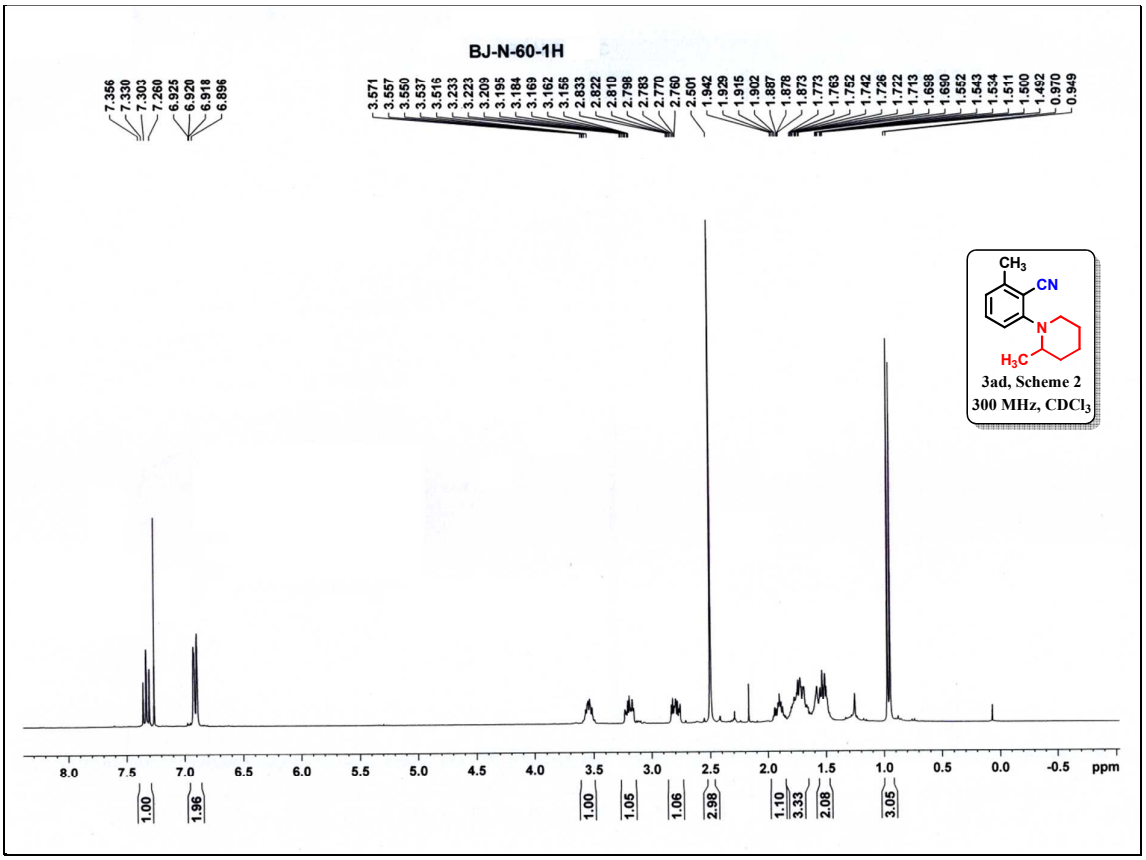

BJ-N-81-13C
158.87
134.81
134.38
133.23
128.16
124.53
122.69
120.90
118.64
118.58
118.51
118.44
117.27
115.06
103.00
77.58
77.16
76.74
52.82
34.38
30.58
21.83
CF3
CN
N
CH3
3lc, Scheme 2
75 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

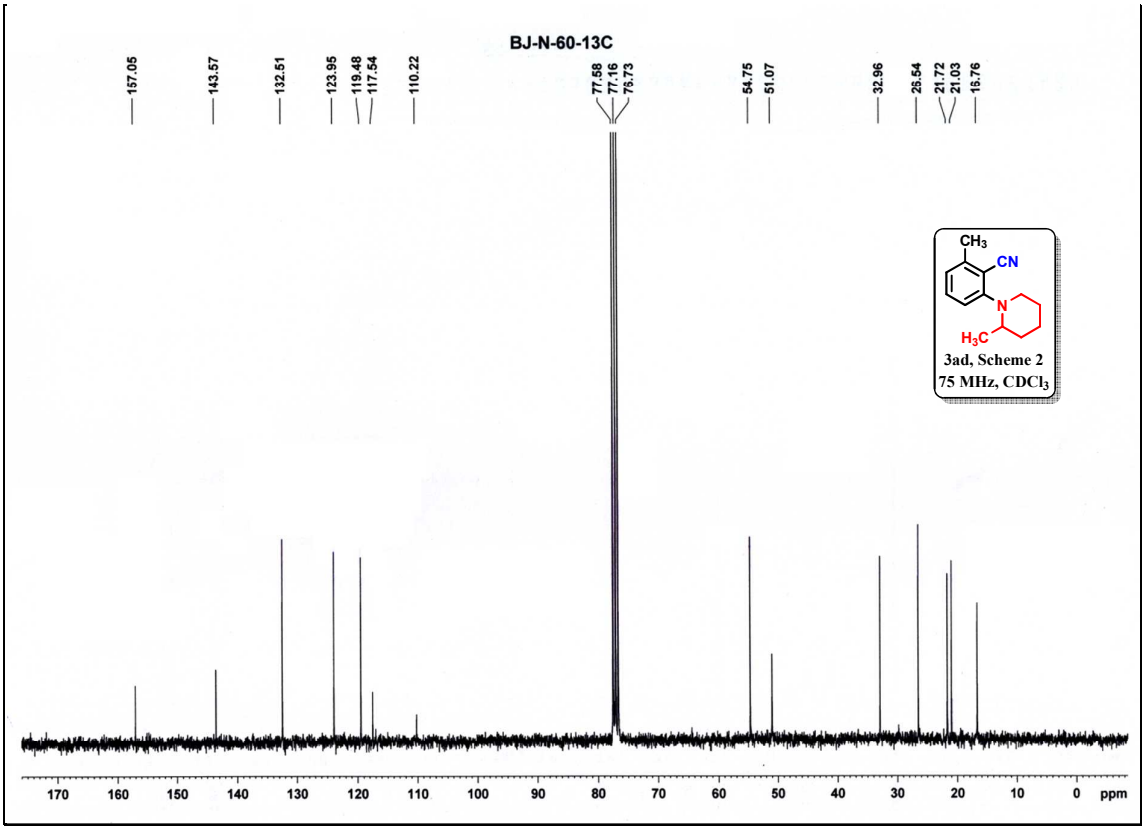

BJ-3mc-1H
7.458
7.450
7.260
3.898
3.549
3.509
2.826
2.788
2.750
2.514
1.772
1.740
1.733
1.502
1.476
1.466
1.438
1.426
0.998
0.977
CH3
CN
H3CO
O
N
CH3
3mc, Scheme 2
300 MHz, CDCl3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
1.61
1.05
1.06
1.54
1.17
1.52
1.55

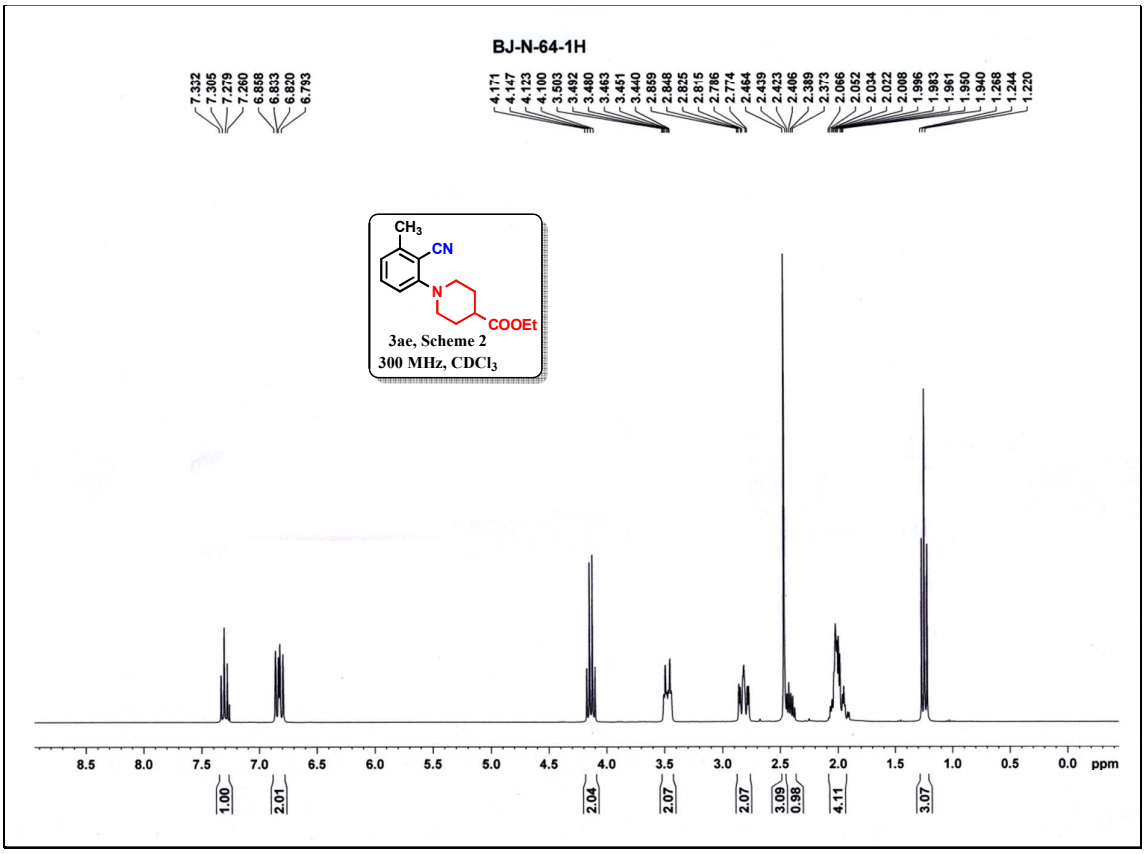

BJ-3mc-13C
166.28
157.42
143.94
133.87
123.18
117.05
116.96
110.73
77.59
77.16
76.74
52.73
52.58
34.40
30.58
21.83
21.03
CH3
CN
H3CO
O
N
CH3
3mc, Scheme 2
75 MHz, CDCl3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

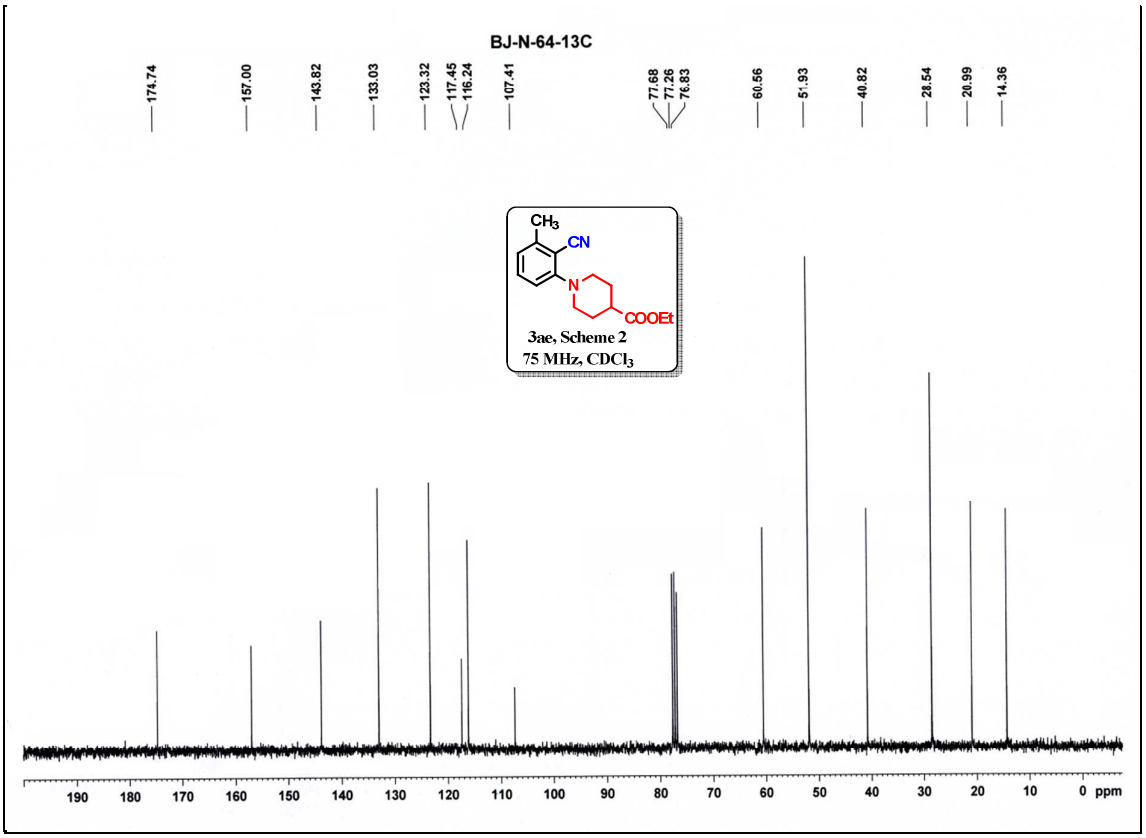

BJ-N-90--1H
7.710
7.706
7.683
7.679
7.589
7.562
7.534
7.317
7.314
7.289
7.286
7.260
3.670
3.664
3.659
3.622
2.962
2.955
2.922
2.884
1.818
1.786
1.778
1.601
1.591
1.563
1.554
1.550
1.522
1.510
1.482
1.470
1.030
1.010
-0.003
NO2
CN
N
CH3
3nc, Scheme 2
300 MHz, CDCl3
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
1.07
1.09
2.25
2.18
2.20
3.08
3.31

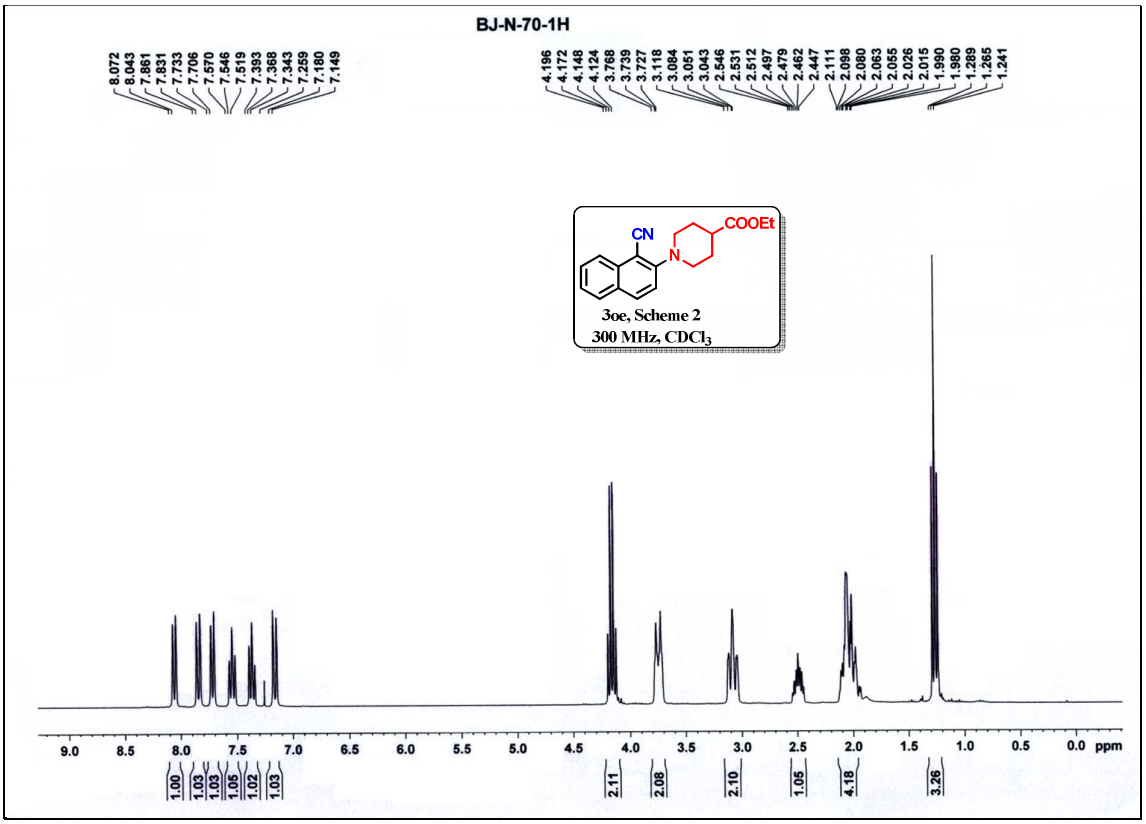

BJ-N-90-13C
159.23
133.25
124.39
116.91
114.31
99.92
77.68
77.16
76.74
52.79
34.28
30.53
21.80
NO2
CN
N
CH3
3nc, Scheme 2
75 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

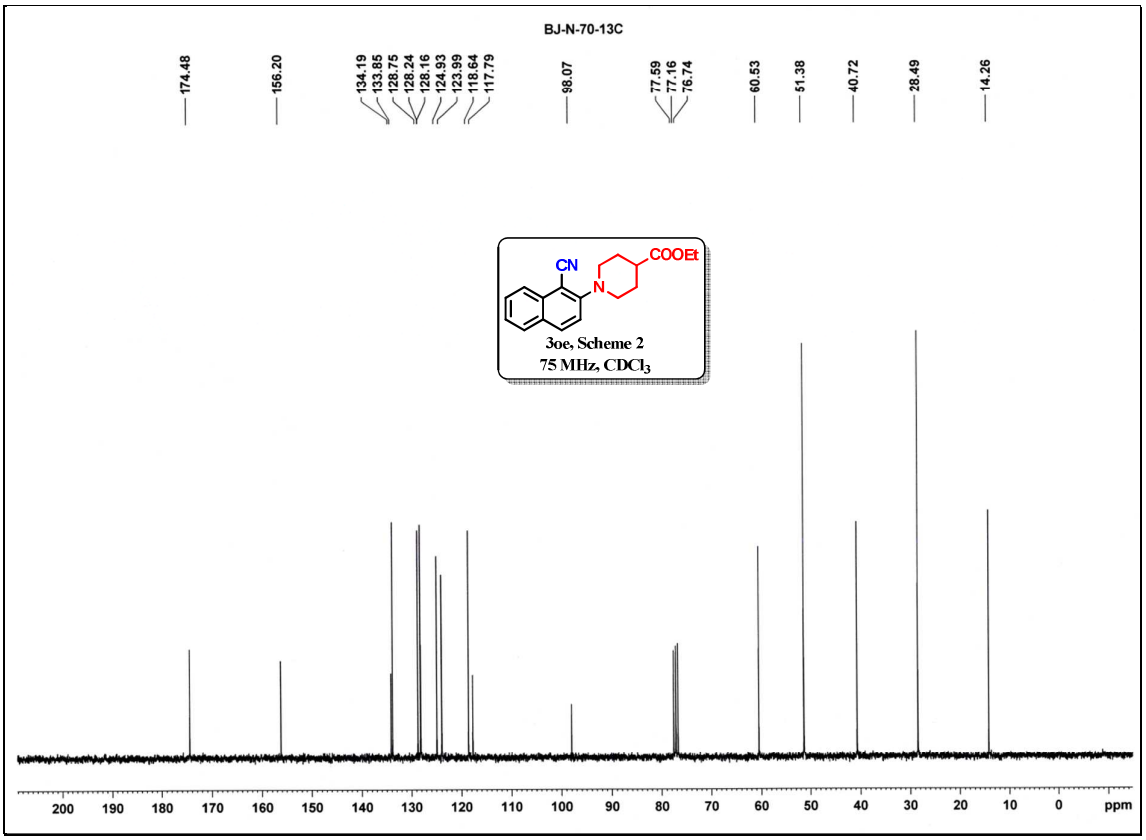

BJ-N-60-1H
7.356
7.330
7.303
7.260
6.925
6.920
6.918
6.896
3.571
3.557
3.550
3.537
3.516
3.233
3.223
3.209
3.195
3.184
3.169
3.162
3.155
2.833
2.822
2.810
2.798
2.783
2.770
2.760
2.501
1.942
1.929
1.915
1.902
1.887
1.878
1.873
1.773
1.763
1.752
1.742
1.726
1.722
1.713
1.688
1.680
1.552
1.543
1.534
1.511
1.500
1.492
0.970
0.949
CH3
CN
N
H3C
3ad, Scheme 2
300 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
1.00
1.96
1.00
1.05
1.06
2.98
1.10
3.33
2.08
3.05

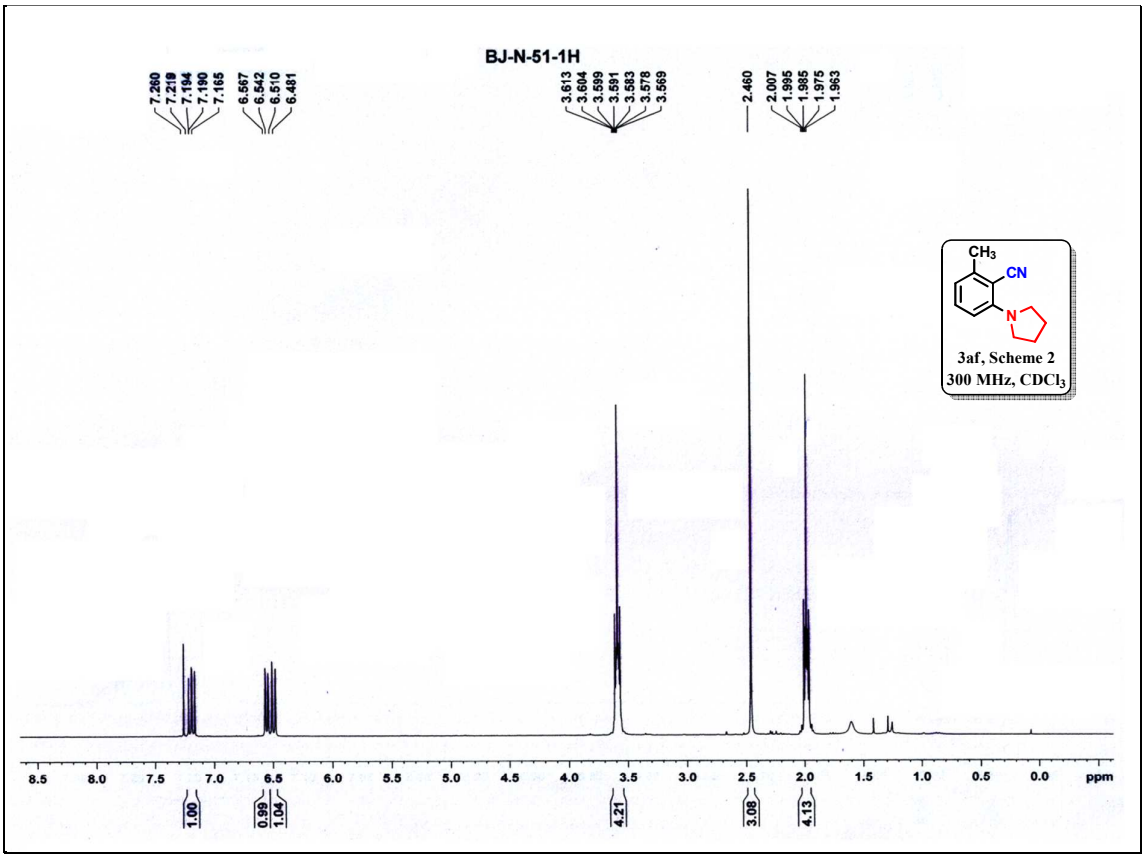

BJ-N-60-13C
157.05
143.57
132.51
123.95
119.48
117.54
110.22
77.58
77.16
76.73
54.75
51.07
32.96
28.54
21.72
21.03
16.76
CH3
CN
N
H3C
3ad, Scheme 2
75 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

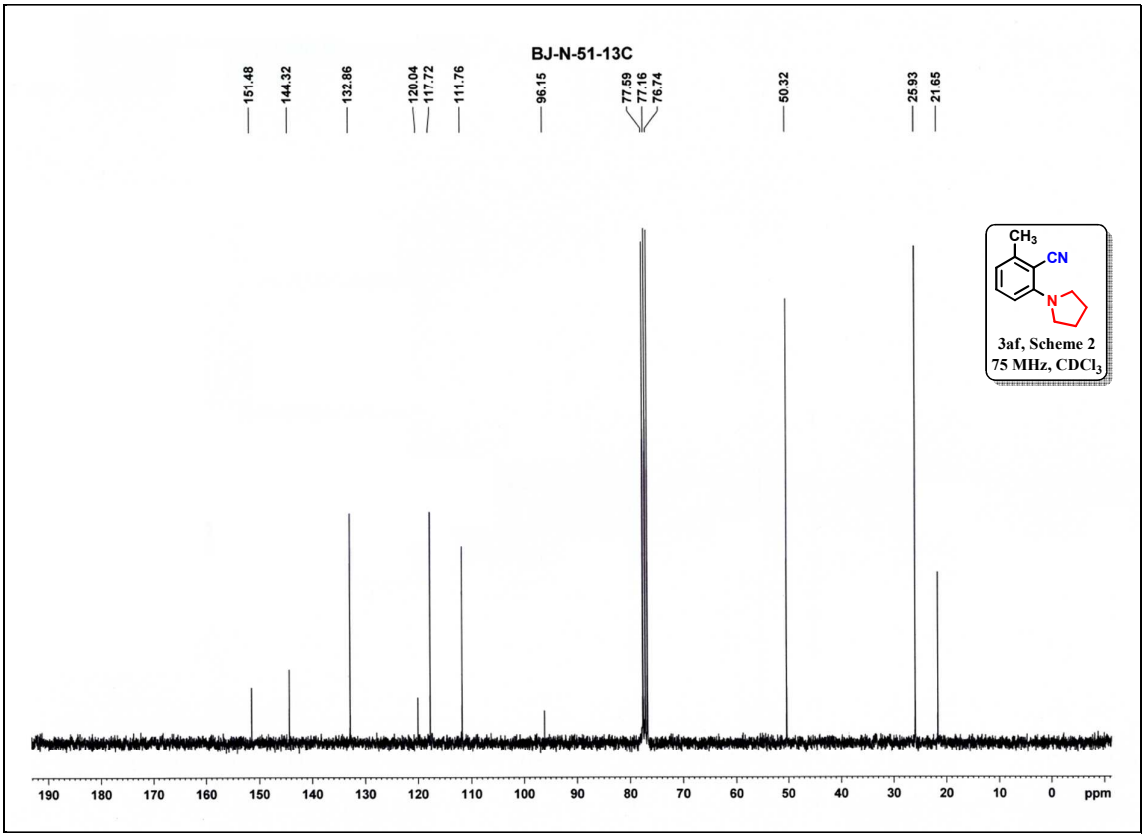

BJ-N-64-1H
7.332
7.305
7.279
7.260
6.858
6.833
6.820
6.793
4.171
4.147
4.123
4.100
3.503
3.492
3.480
3.463
3.451
3.440
2.859
2.848
2.825
2.815
2.786
2.774
2.464
2.439
2.423
2.406
2.389
2.373
2.066
2.052
2.034
2.022
2.008
1.996
1.983
1.961
1.950
1.940
1.268
1.244
1.220
CH3
CN
N
COOEt
3ae, Scheme 2
300 MHz, CDCl3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.01
2.04
2.07
2.07
3.09
0.98
4.11
3.07

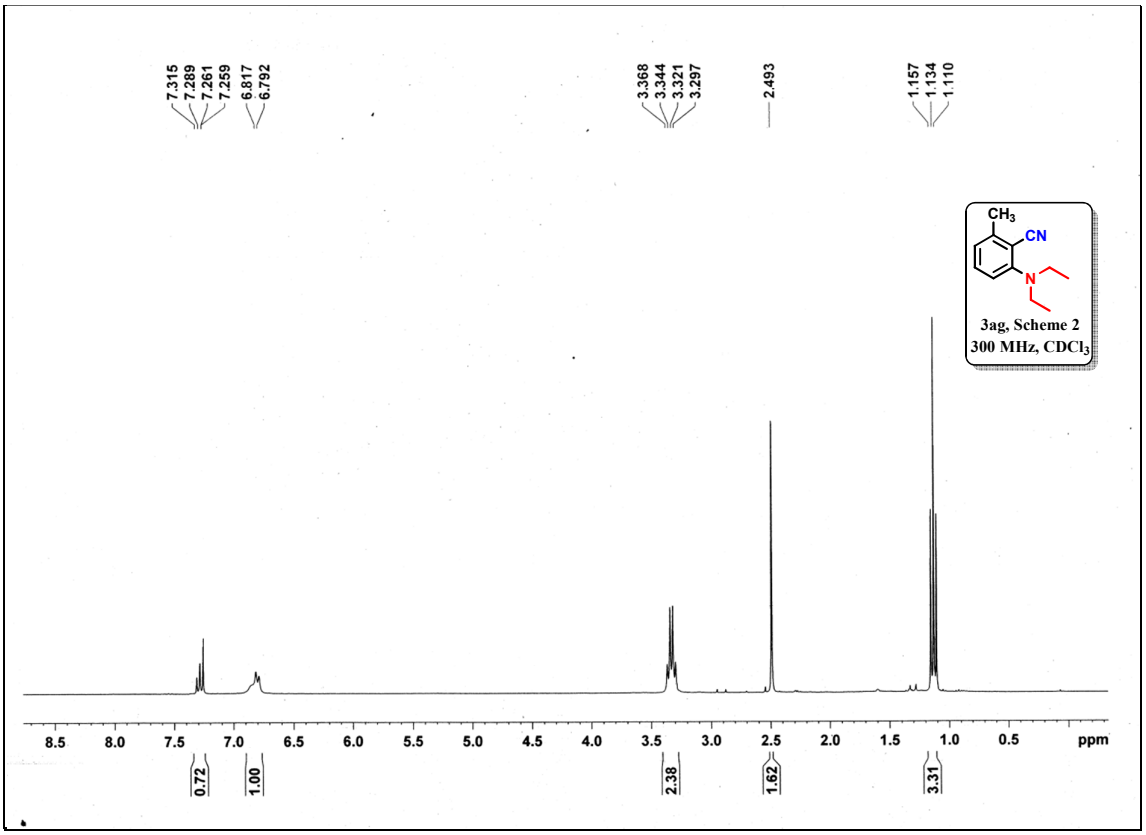

BJ-N-64-13C
174.74
157.00
143.82
133.03
123.32
117.45
116.24
107.41
77.68
77.26
76.83
60.56
51.93
40.82
28.54
20.99
14.36
CH3
CN
N
COOEt
3ae, Scheme 2
75 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

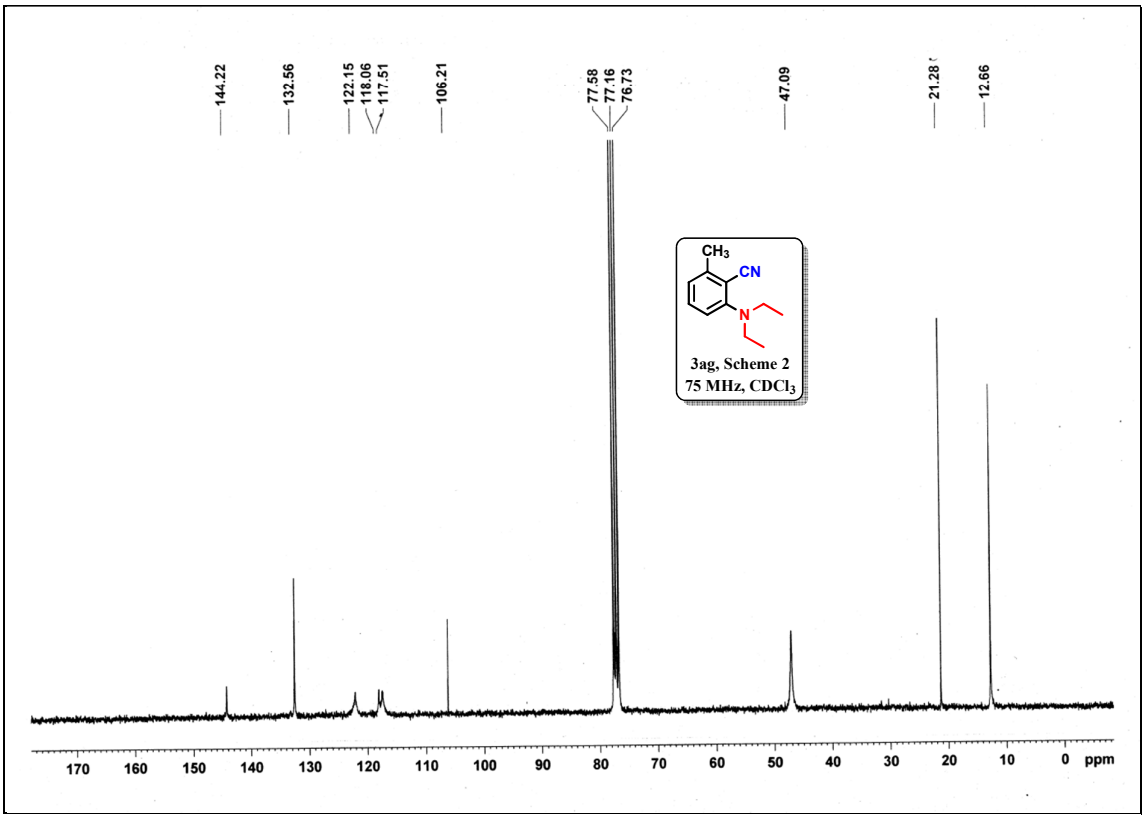

BJ-N-70-1H
8.072
8.043
7.861
7.831
7.733
7.706
7.570
7.546
7.519
7.393
7.368
7.343
7.259
7.180
7.149
4.196
4.172
4.148
4.124
3.768
3.739
3.727
3.118
3.084
3.051
3.043
2.546
2.531
2.512
2.497
2.479
2.462
2.447
2.111
2.098
2.080
2.063
2.055
2.026
2.015
1.990
1.980
1.289
1.265
1.241
CN
COOEt
N
3oe, Scheme 2
300 MHz, CDCl3
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.03
1.03
1.05
1.02
1.03
2.11
2.08
2.10
1.05
4.18
3.26

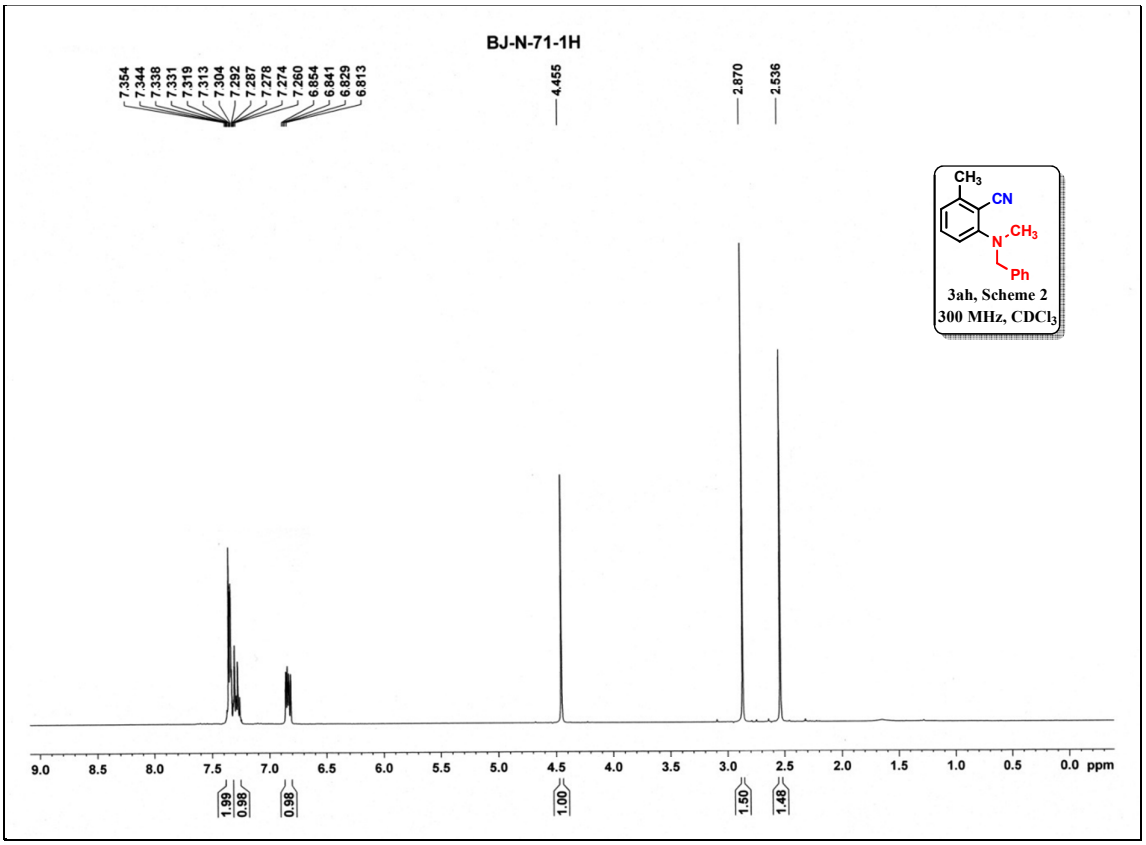

BJ-N-70-13C
174.48
156.20
134.19
133.85
128.75
128.24
128.16
124.93
123.99
118.64
117.79
98.07
77.59
77.16
76.74
60.53
51.38
40.72
28.49
14.26
CN
COOEt
N
3oe, Scheme 2
75 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

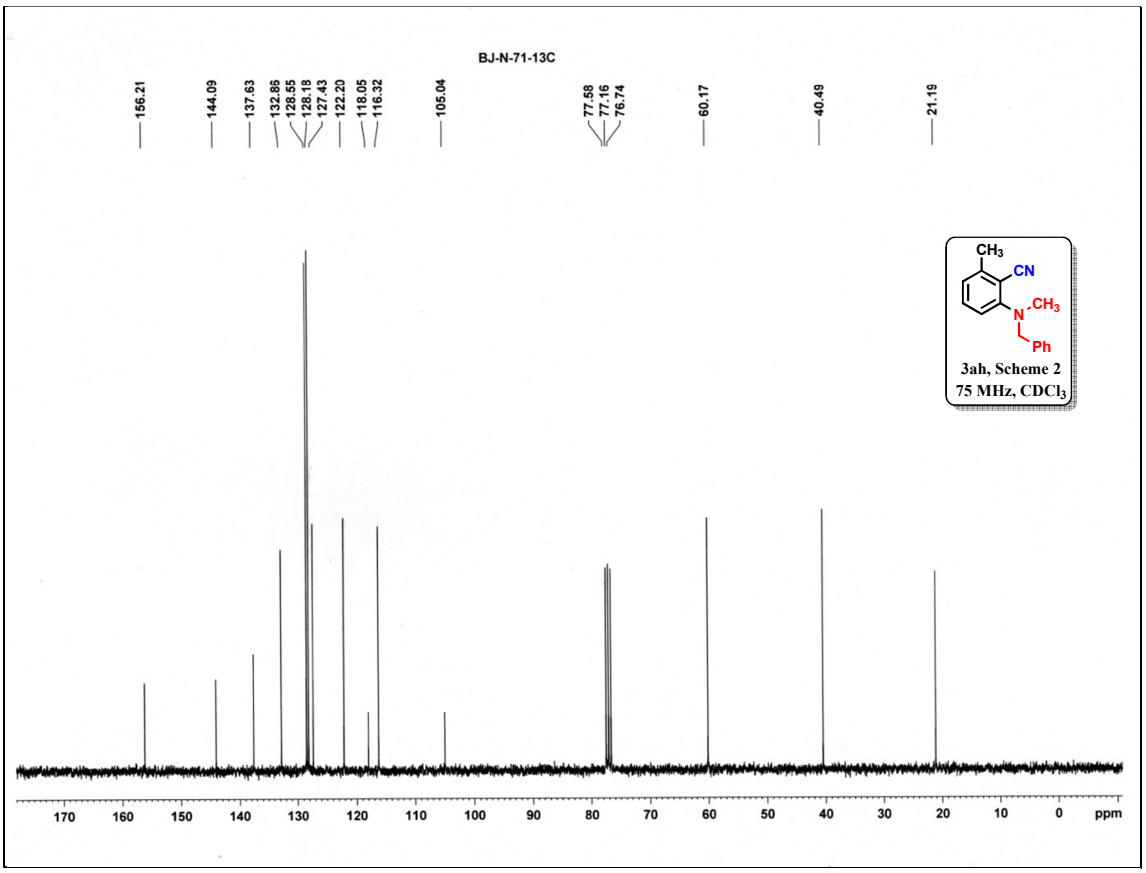

BJ-N-51-1H
7.260
7.219
7.194
7.190
7.165
6.567
6.542
6.510
6.481
3.613
3.604
3.599
3.591
3.583
3.578
3.569
2.460
2.007
1.995
1.985
1.975
1.963
CH3
CN
N
3af, Scheme 2
300 MHz, CDCl3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
0.99
1.04
4.21
3.08
4.13

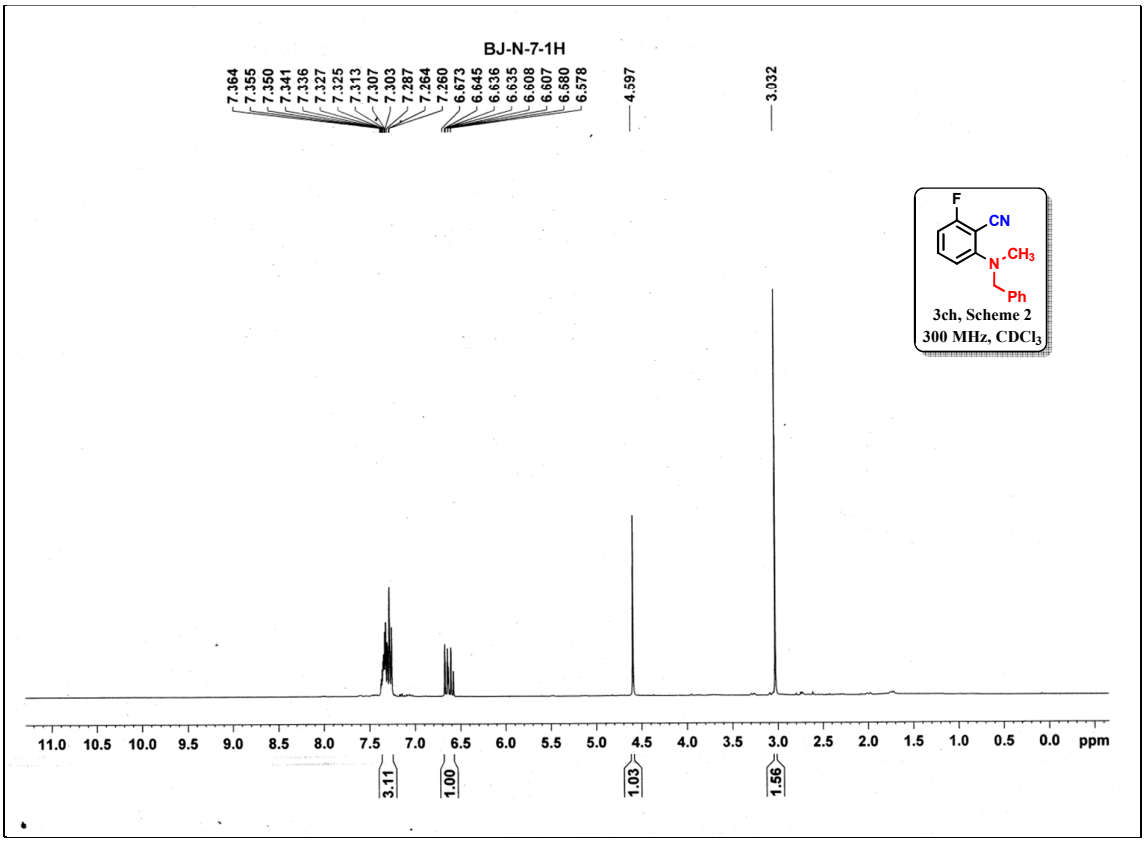

BJ-N-51-13C
151.48
144.32
132.86
120.04
117.72
111.76
96.15
77.59
77.16
76.74
50.32
25.93
21.65
CH3
CN
N
3af, Scheme 2
75 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

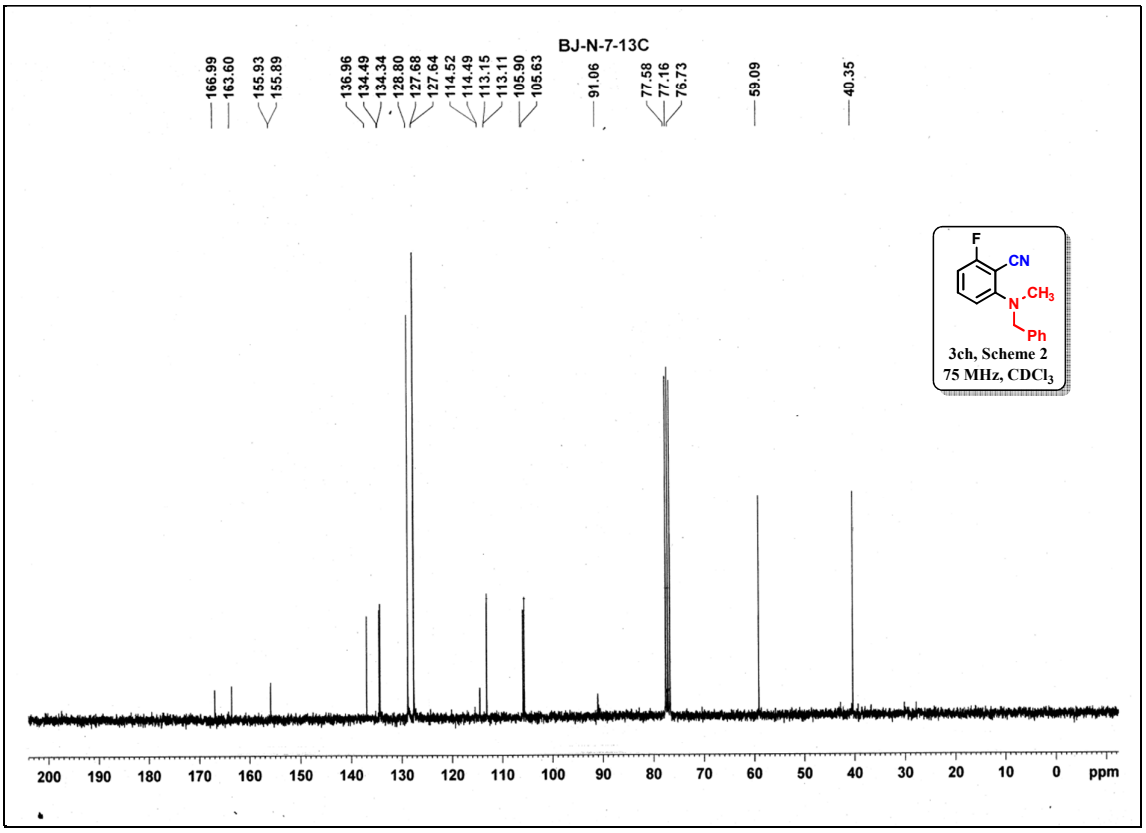

7.315
7.289
7.261
7.259
6.817
6.792
3.368
3.344
3.321
3.297
2.493
1.157
1.134
1.110
CH3
CN
N
3ag, Scheme 2
300 MHz, CDCl3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.72
1.00
2.38
1.62
3.31

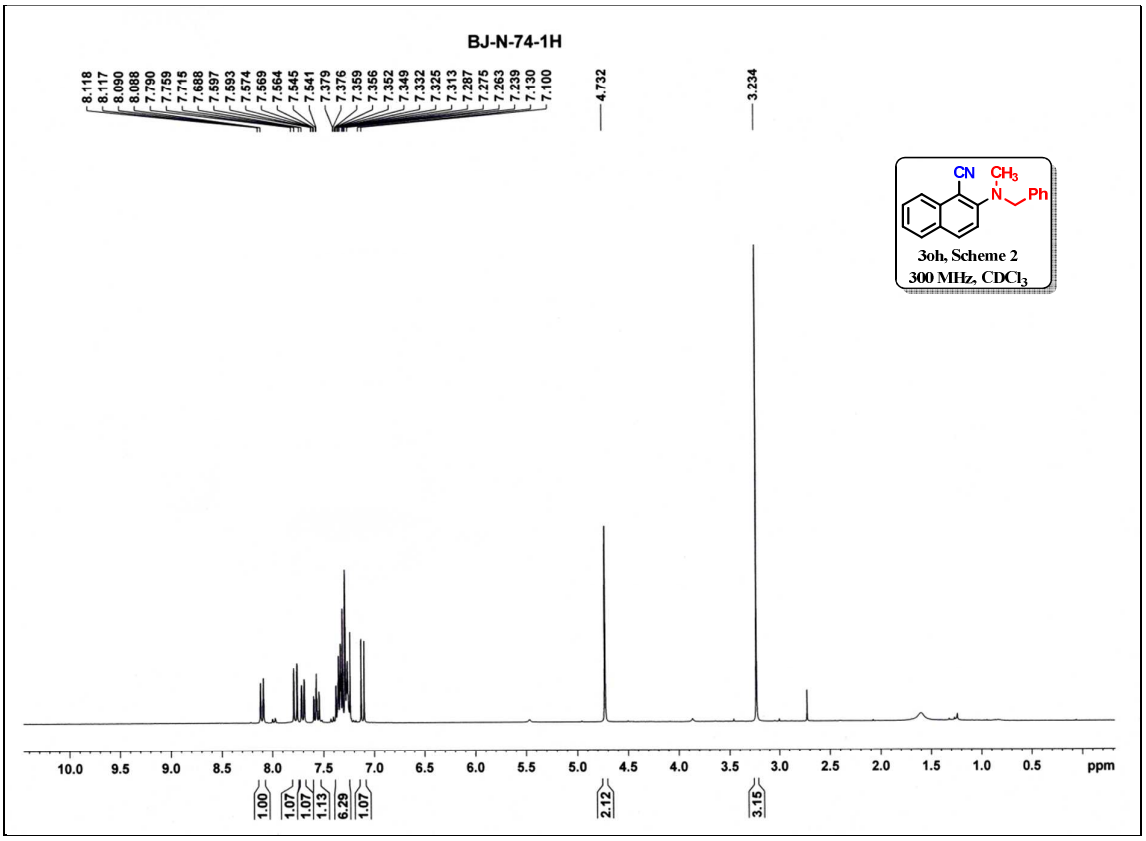

144.22
132.56
122.15
118.06
117.51
106.21
77.58
77.16
76.73
47.09
21.28
12.66
CH3
CN
N
3ag, Scheme 2
75 MHz, CDCl3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

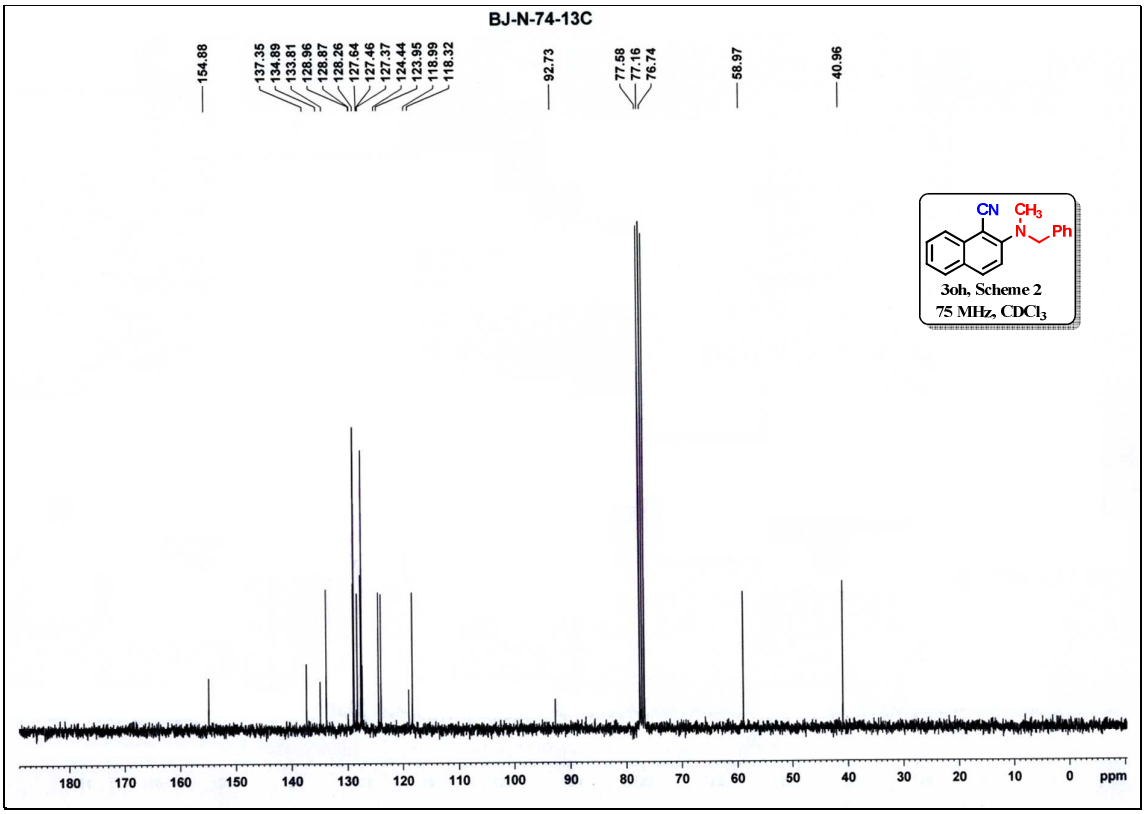

BJ-N-71-1H
7.354
7.344
7.338
7.331
7.319
7.313
7.304
7.292
7.287
7.278
7.274
7.260
6.854
6.841
6.829
6.813
4.455
2.870
2.536
CH3
CN
N
CH3
Ph
3ah, Scheme 2
300 MHz, CDCl3
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.99
0.98
0.98
1.00
1.50
1.48

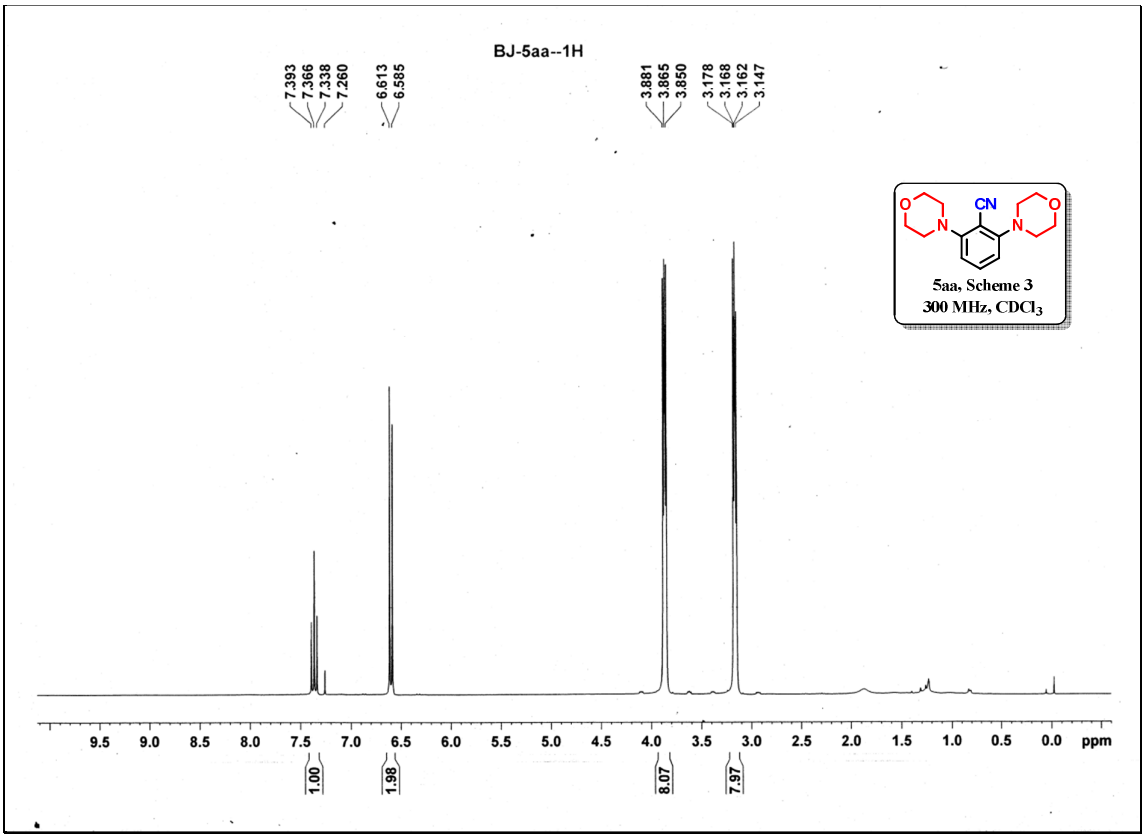

BJ-N-71-13C
156.21
144.09
137.63
132.86
128.55
128.18
127.43
122.20
118.05
116.32
105.04
77.58
77.16
76.74
60.17
40.49
21.19
CH3
CN
N
CH3
Ph
3ah, Scheme 2
75 MHz, CDCl3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

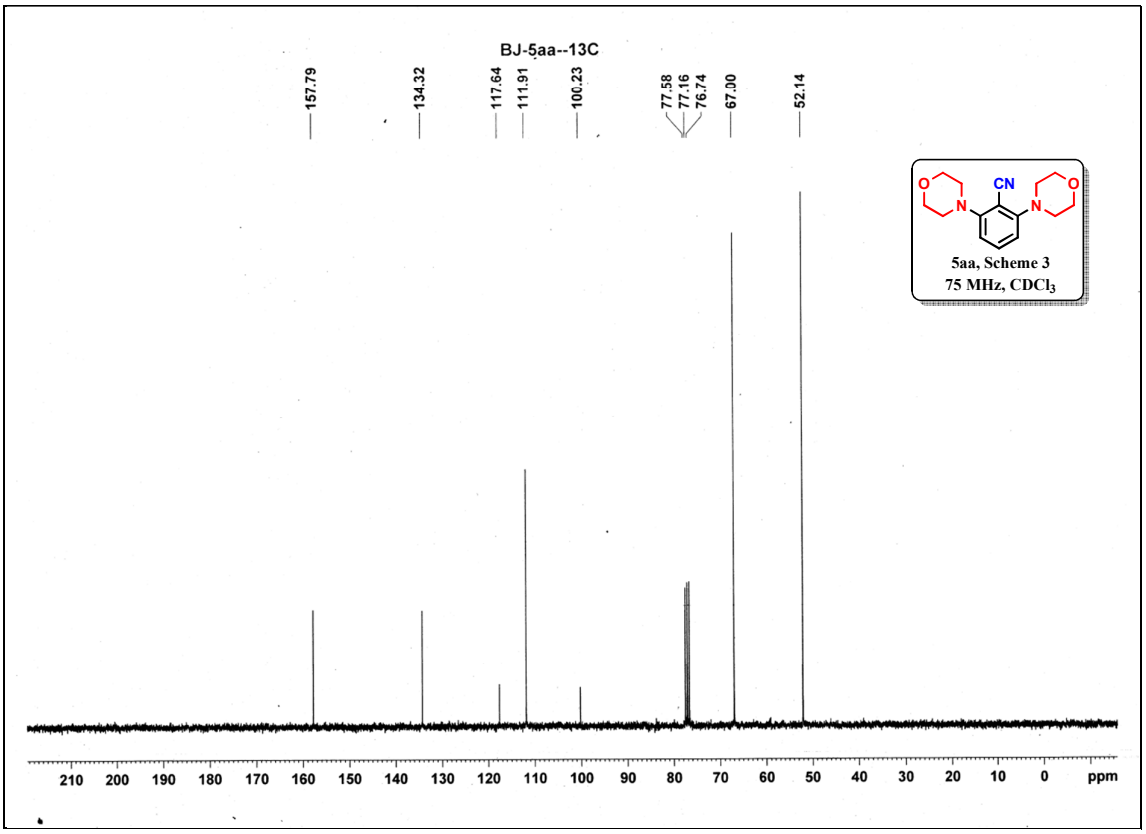

BJ-N-7-1H
7.364
7.355
7.350
7.341
7.336
7.327
7.325
7.313
7.307
7.303
7.287
7.264
7.260
6.673
6.645
6.636
6.635
6.608
6.607
6.580
6.578
4.597
3.032
F
CN
N
CH3
Ph
3ch, Scheme 2
300 MHz, CDCl3
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
3.11
1.00
1.03
1.56

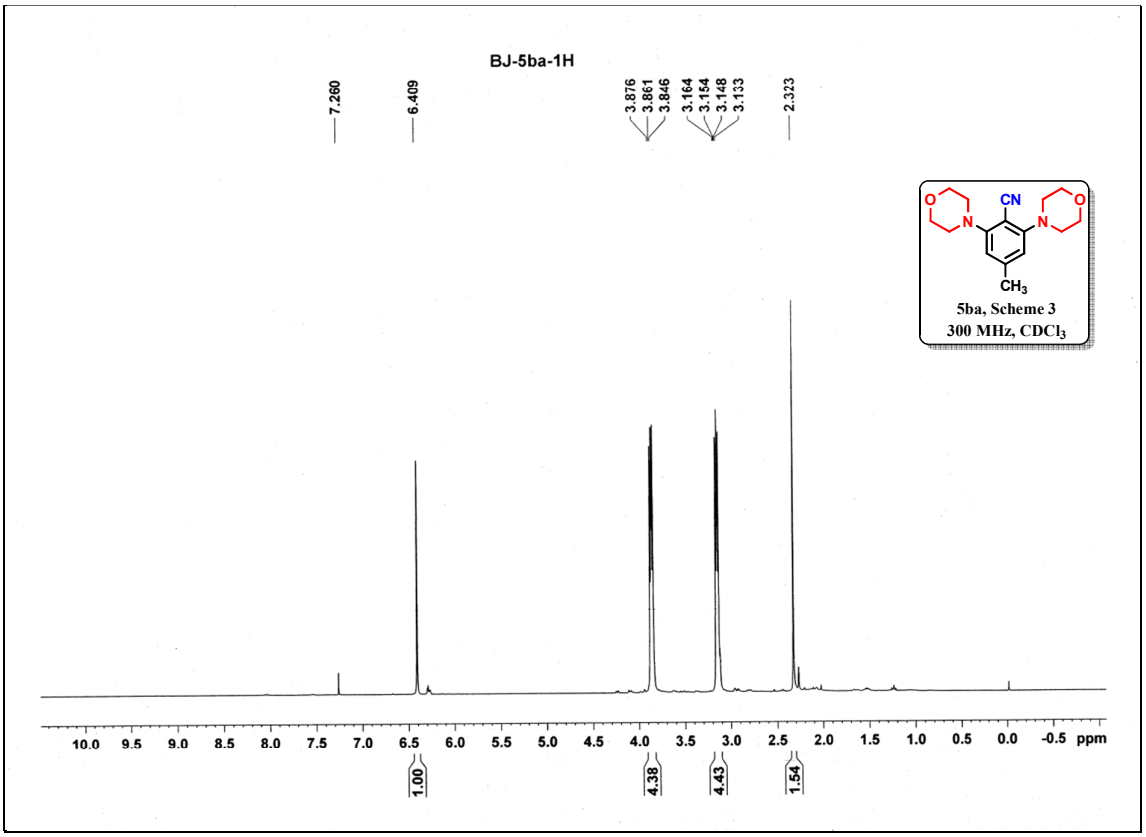

BJ-N-7-13C
166.99
163.60
155.93
155.89
136.96
134.49
134.34
128.80
127.68
127.64
114.52
114.49
113.15
113.11
105.90
105.63
91.06
77.58
77.16
76.73
59.09
40.35
F
CN
N
CH3
Ph
3ch, Scheme 2
75 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

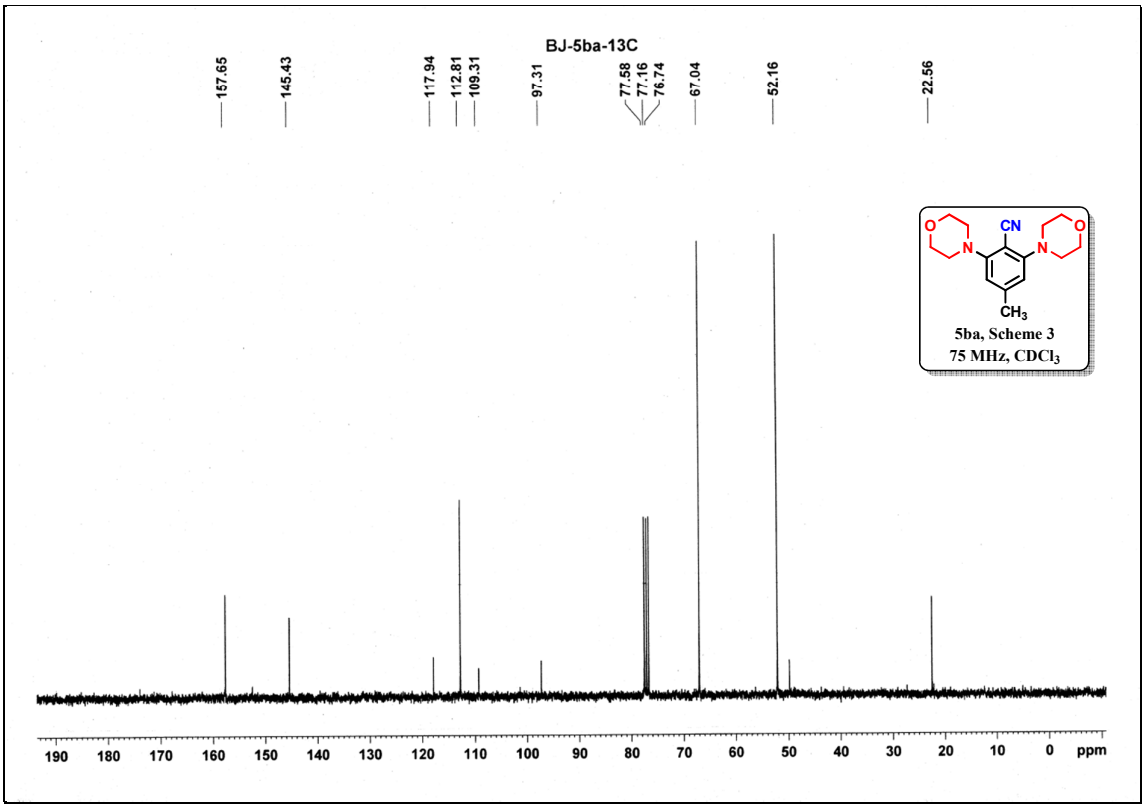

BJ-N-74-1H
8.118
8.117
8.090
8.088
7.790
7.759
7.715
7.688
7.597
7.593
7.574
7.569
7.564
7.545
7.541
7.379
7.376
7.359
7.356
7.352
7.349
7.332
7.325
7.313
7.287
7.275
7.263
7.239
7.130
7.100
4.732
3.234
CN
CH3
N
Ph
3oh, Scheme 2
300 MHz, CDCl3
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
1.07
1.07
1.13
6.29
1.07
2.12
3.15

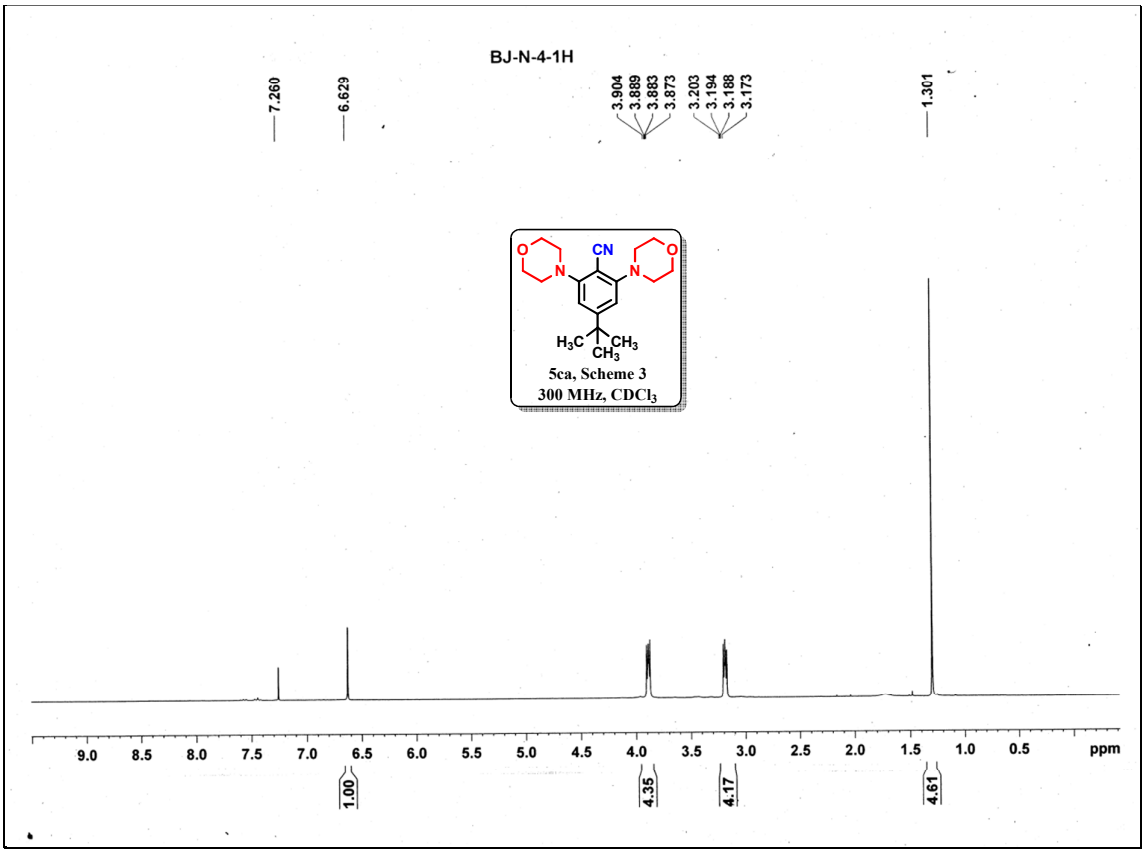

BJ-N-74-13C
154.88
137.35
134.89
133.81
128.96
128.87
128.26
127.64
127.46
127.37
124.44
123.95
118.99
118.32
92.73
77.58
77.16
76.74
58.97
40.96
CN
CH3
N
Ph
3oh, Scheme 2
75 MHz, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

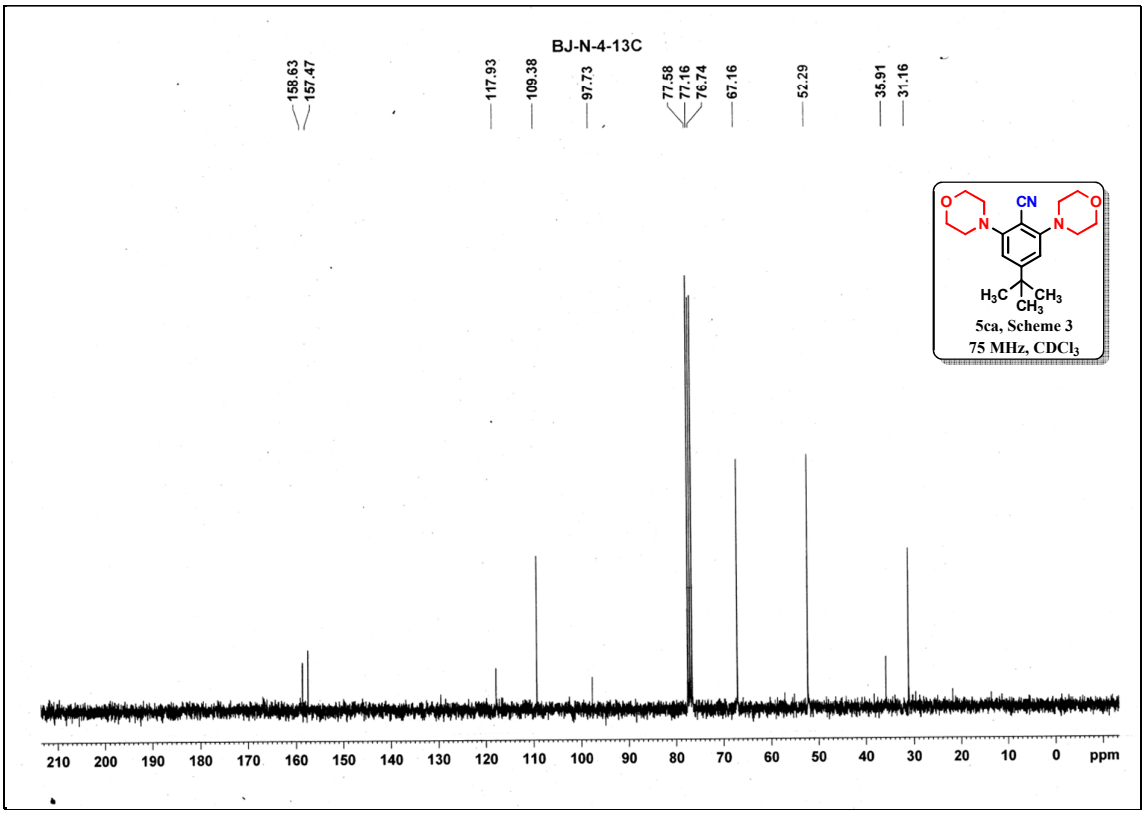

BJ-5aa--1H
7.393
7.366
7.338
7.260
6.613
6.585
3.881
3.865
3.850
3.178
3.168
3.162
3.147
CN
5aa, Scheme 3
300 MHz, CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
1.98
8.07
7.97

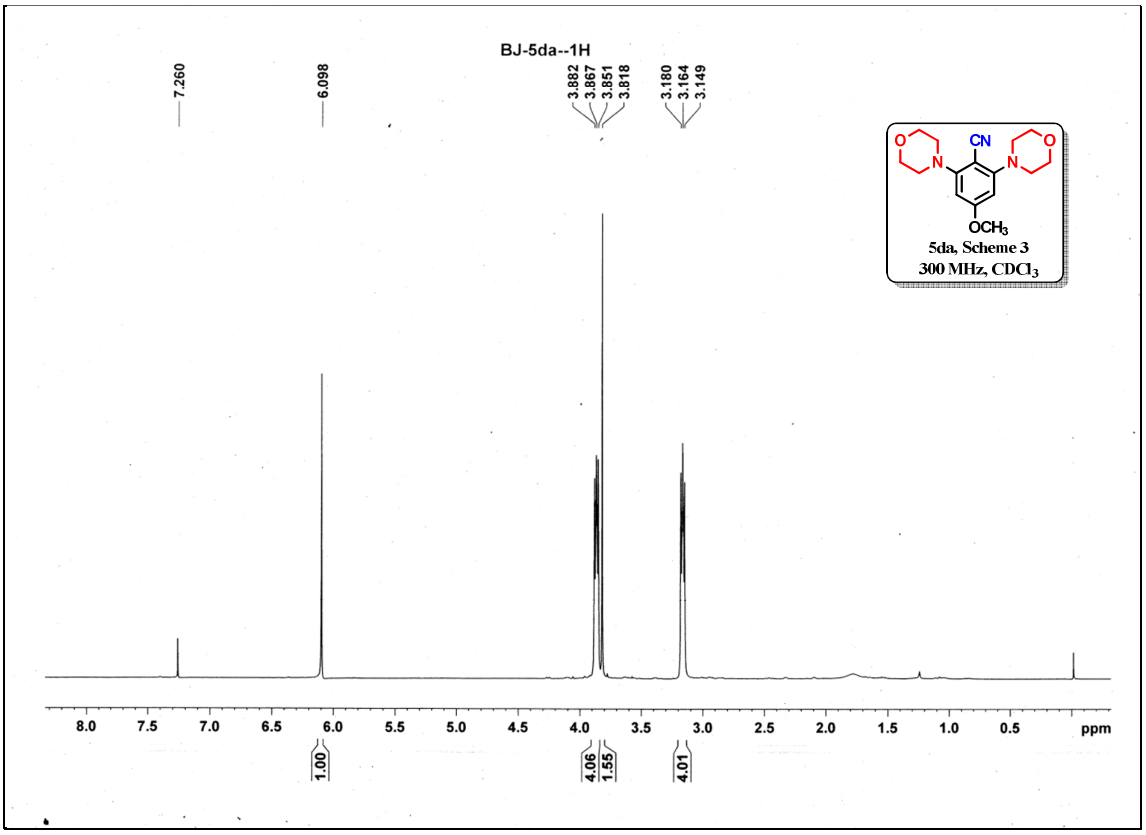

BJ-5aa--13C
157.79
134.32
117.64
111.91
106.23
77.58
77.16
76.74
67.00
52.14
CN
5aa, Scheme 3
75 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

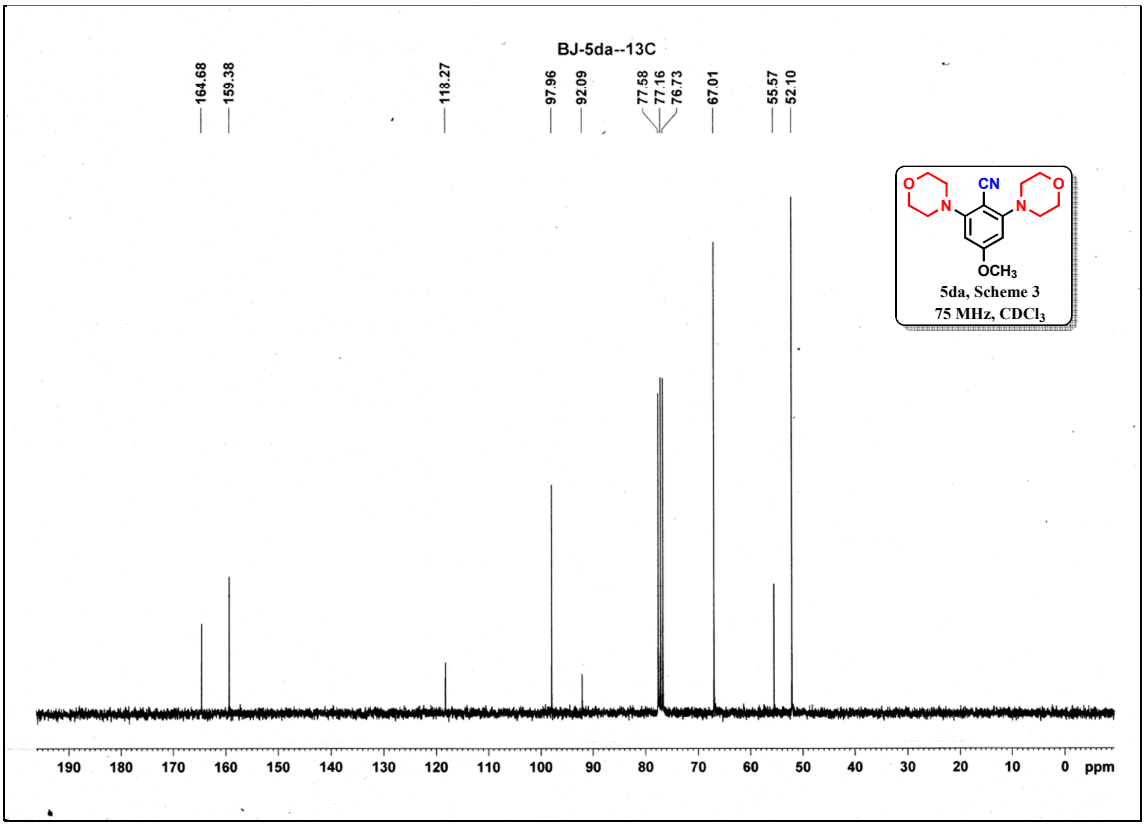

BJ-5ba-1H
7.260
6.409
3.876
3.861
3.846
3.164
3.154
3.148
3.133
2.323
CN
CH3
5ba, Scheme 3
300 MHz, CDCl3
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 ppm
1.00
4.38
4.43
1.54

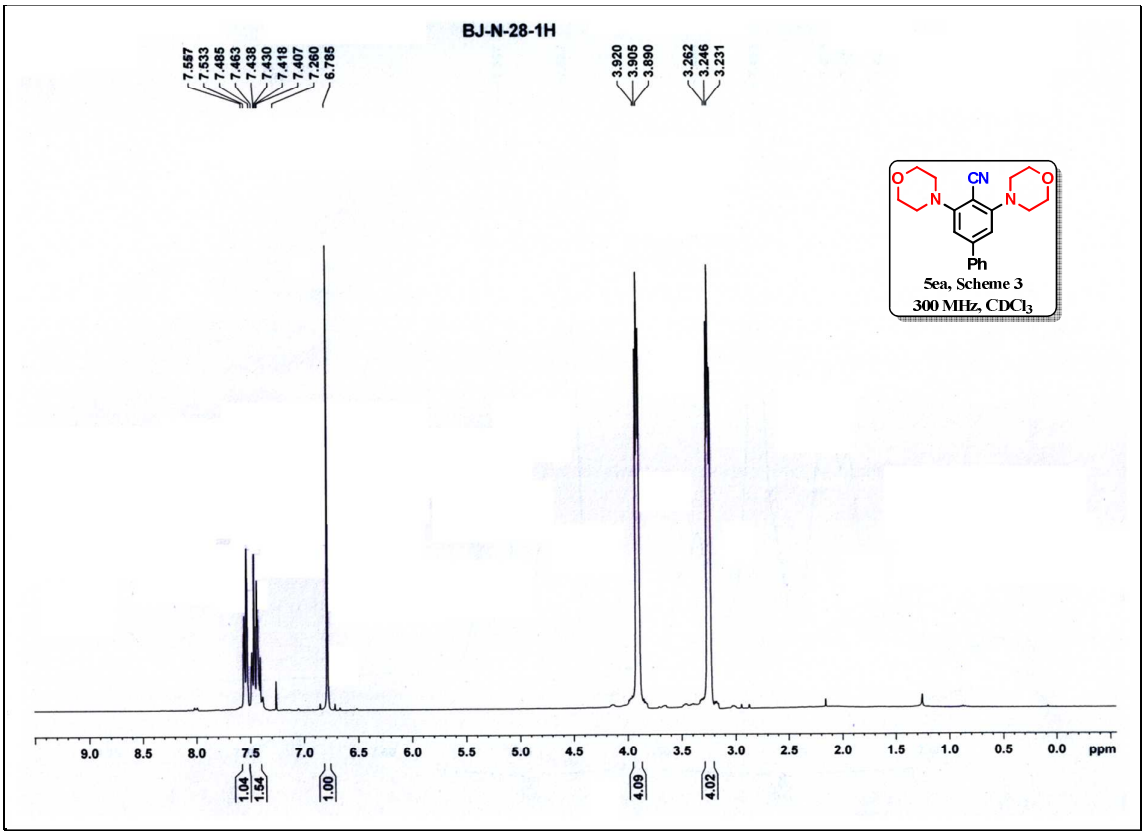

BJ-5ba-13C
157.65
145.43
117.94
112.81
109.31
97.31
77.58
77.16
76.74
67.04
52.16
22.56
CN
CH3
5ba, Scheme 3
75 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

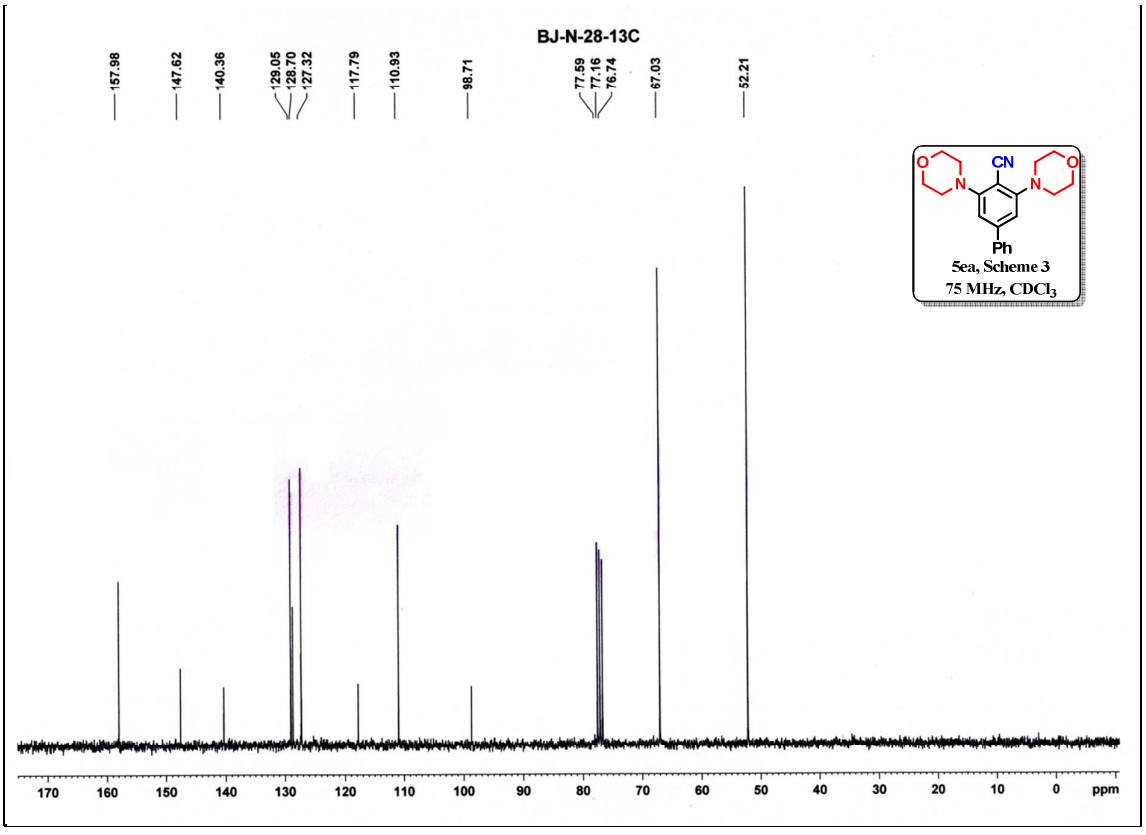

BJ-N-4-1H
7.260
6.629
3.904
3.889
3.883
3.873
3.203
3.194
3.188
3.173
1.301
CN
5ca, Scheme 3
300 MHz, CDCl3
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
4.35
4.17
4.61

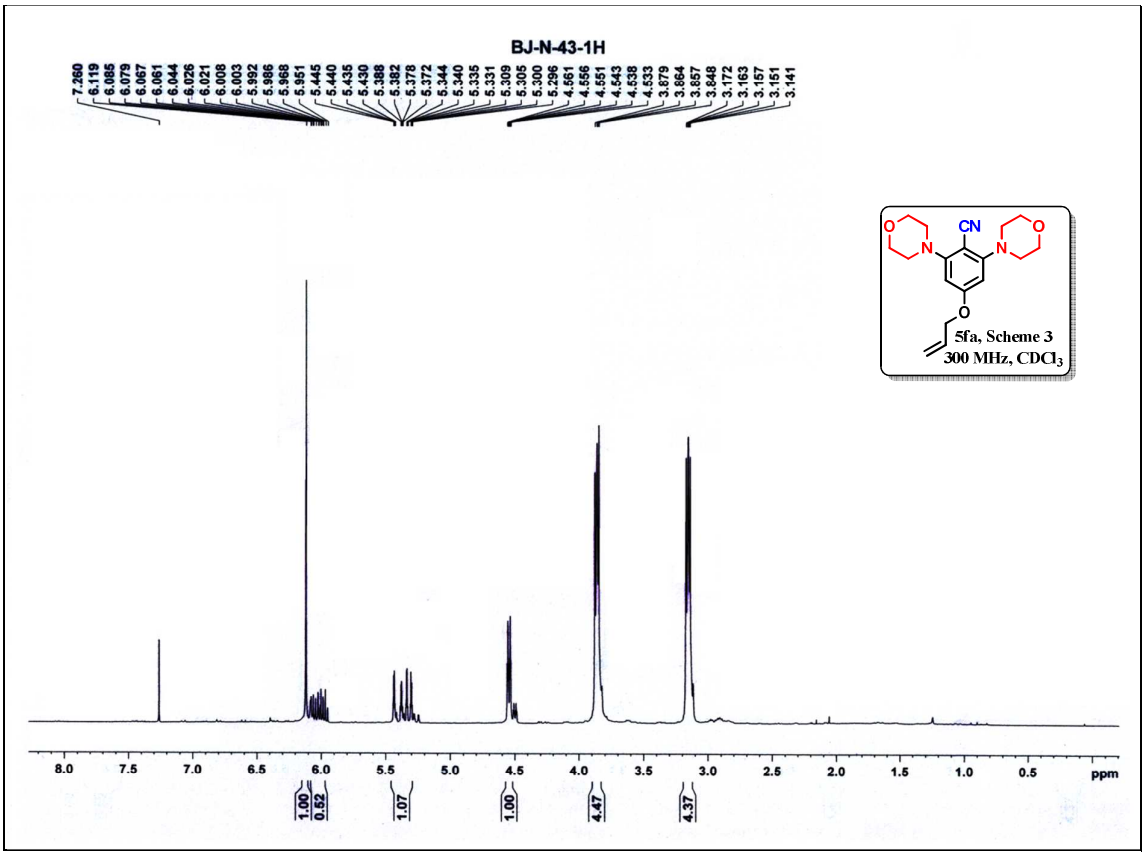

BJ-N-4-13C
158.63
157.47
117.93
109.38
97.73
77.58
77.16
76.74
67.16
52.29
35.91
31.16
CN
5ca, Scheme 3
75 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

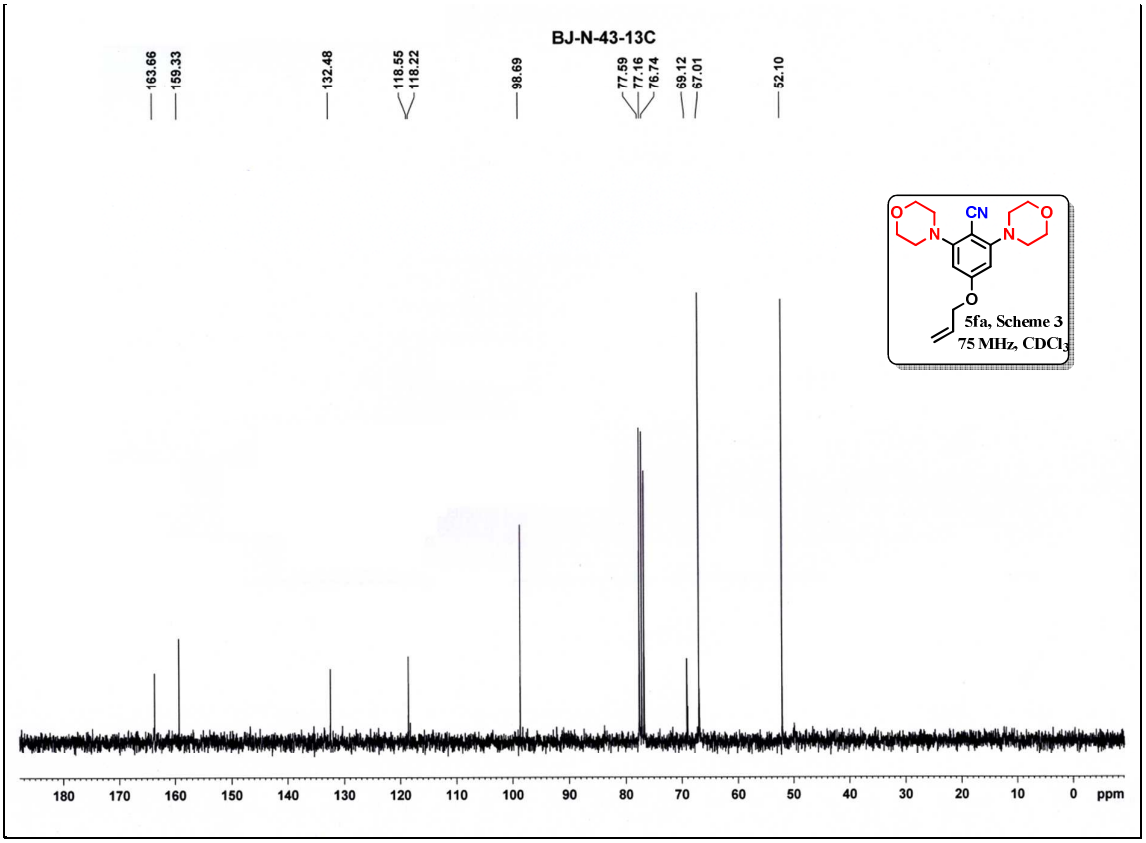

BJ-5da--1H
7.260
6.098
3.882
3.867
3.851
3.818
3.180
3.164
3.149
CN
OCH3
5da, Scheme 3
300 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
4.06
1.55
4.01

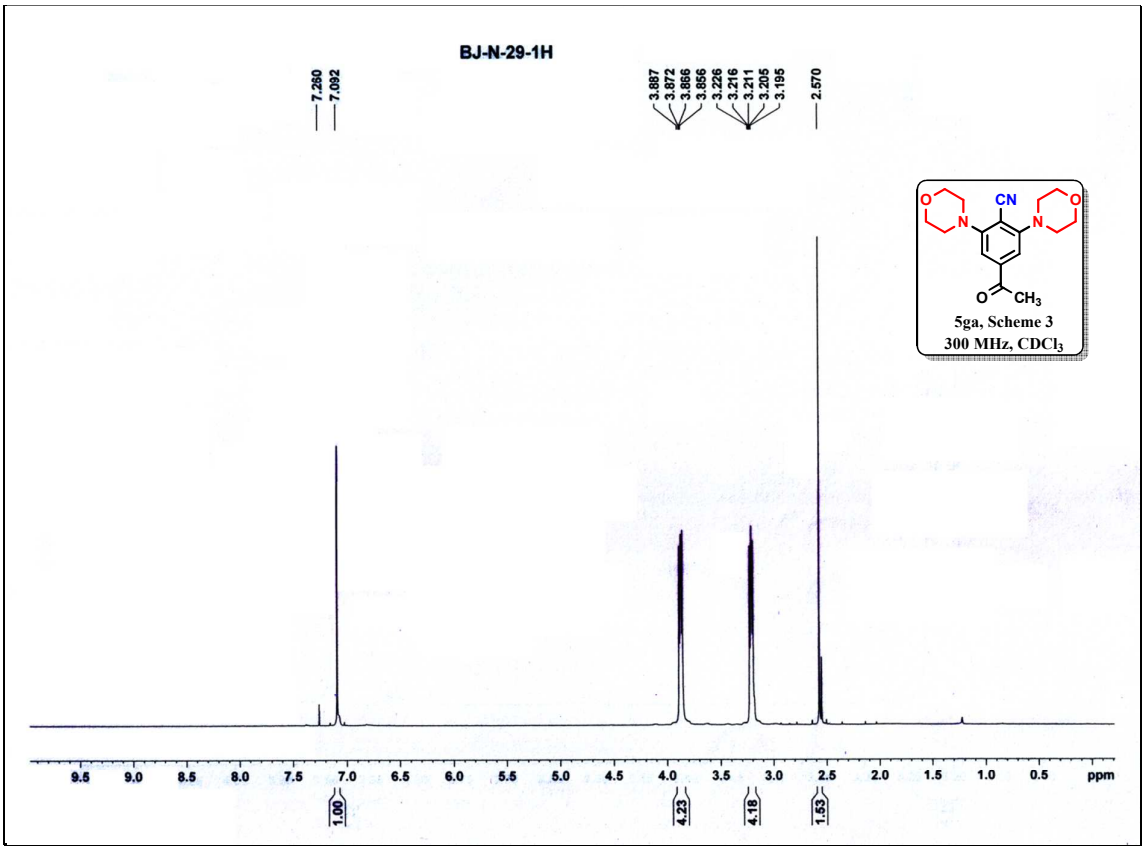

BJ-5da--13C
164.68
159.38
118.27
97.96
92.09
77.58
77.16
76.73
67.01
55.57
52.10
CN
OCH3
5da, Scheme 3
75 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

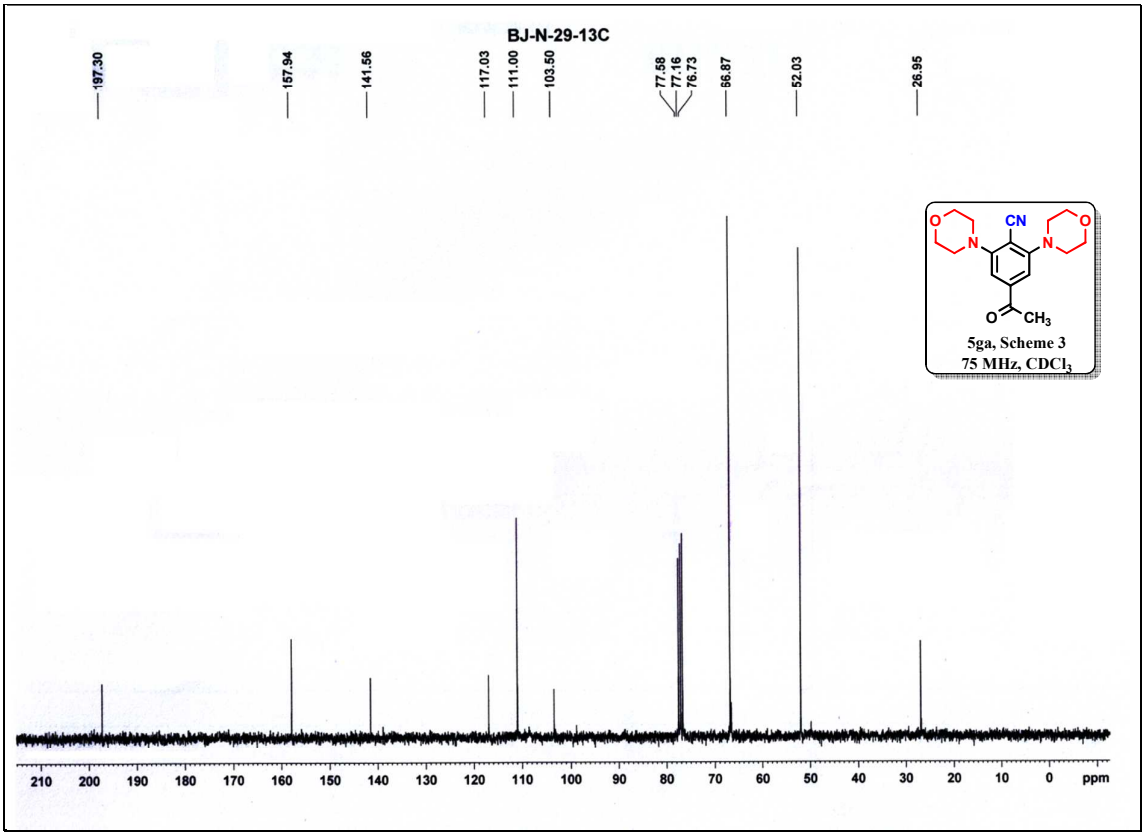

BJ-N-28-1H
7.587
7.533
7.485
7.463
7.438
7.430
7.418
7.407
7.260
6.785
3.920
3.905
3.890
3.262
3.246
3.231
CN
Ph
5ea, Scheme 3
300 MHz, CDCl3
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.04
1.54
1.00
4.09
4.02

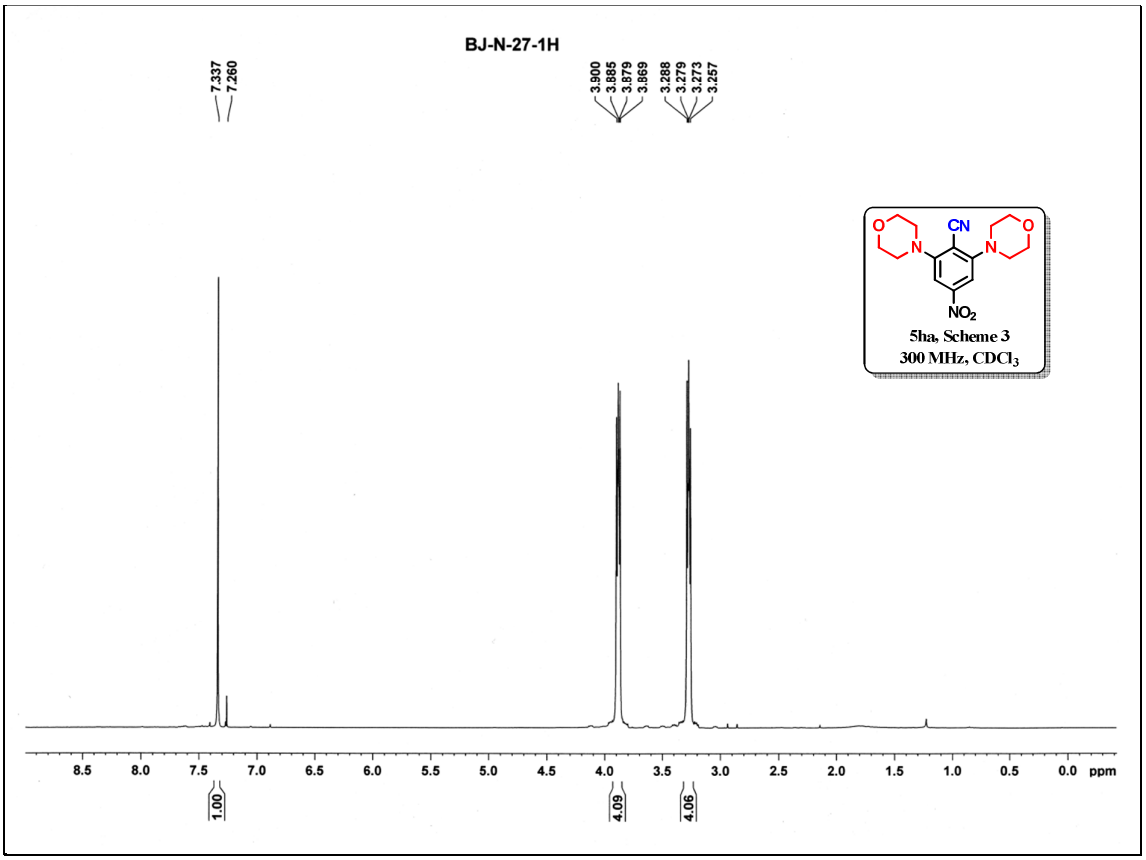

BJ-N-28-13C
157.98
147.62
140.36
129.05
128.70
127.32
117.79
110.93
98.71
77.59
77.16
76.74
67.03
52.21
CN
Ph
5ea, Scheme 3
75 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

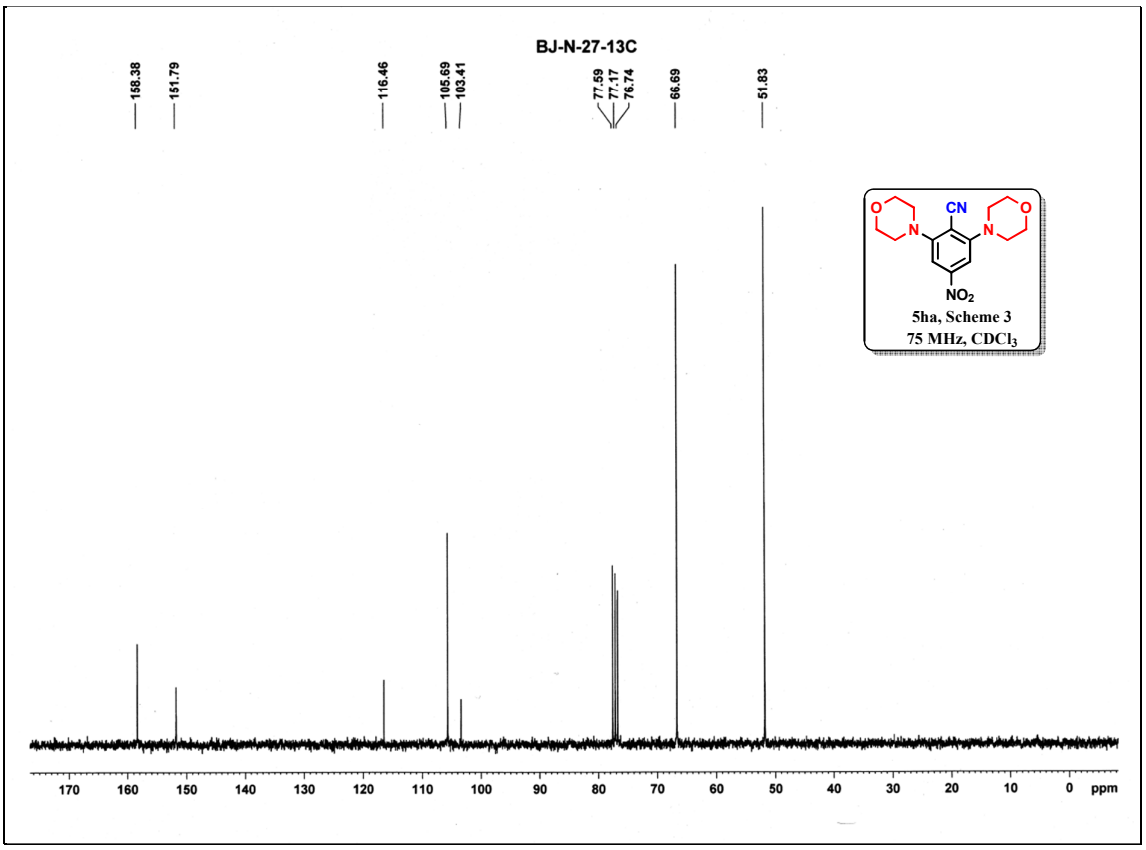

BJ-N-43-1H
7.260
6.119
6.085
6.079
6.067
6.061
6.044
6.026
6.021
6.008
6.003
5.992
5.986
5.968
5.951
5.445
5.440
5.435
5.430
5.388
5.382
5.378
5.372
5.344
5.340
5.335
5.331
5.309
5.305
5.300
5.296
4.561
4.556
4.551
4.543
4.538
4.533
3.879
3.864
3.857
3.848
3.172
3.163
3.157
3.151
3.141
CN
5fa, Scheme 3
300 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
0.52
1.07
1.00
4.47
4.37

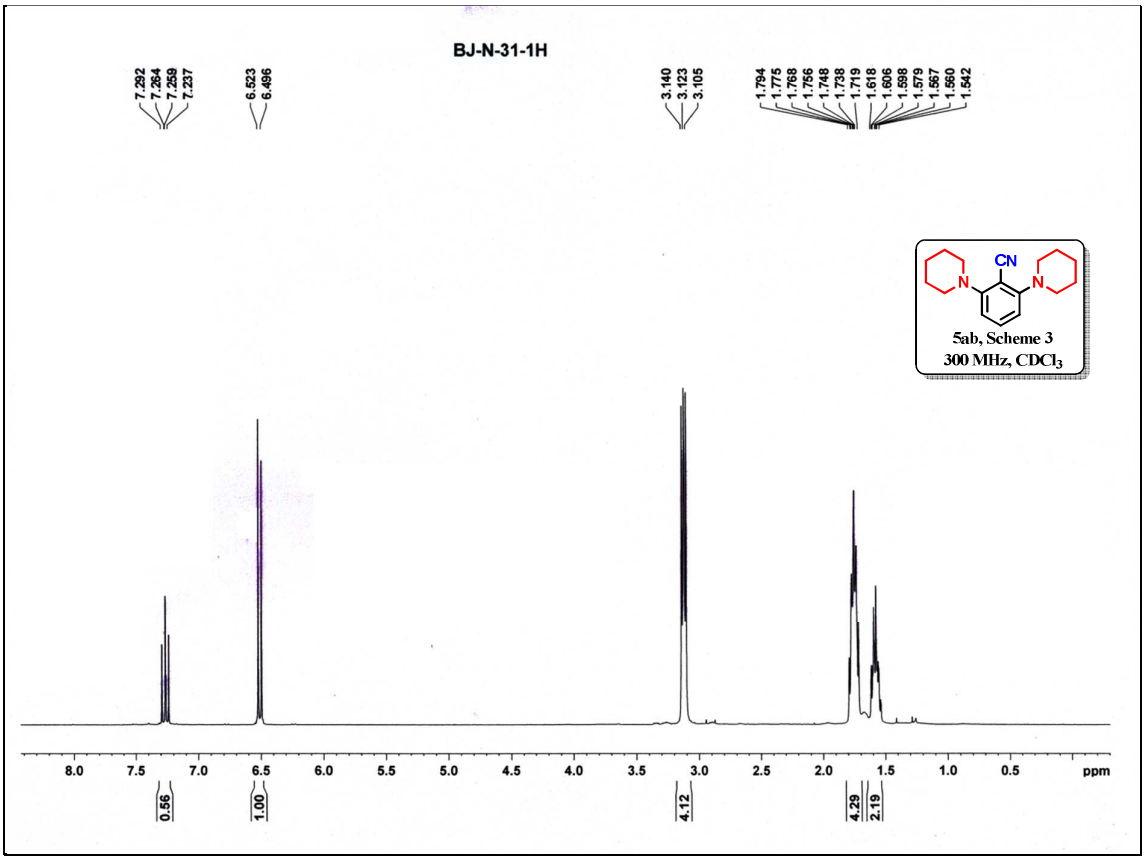

BJ-N-43-13C
163.66
159.33
132.48
118.55
118.22
98.69
77.59
77.16
76.74
69.12
67.01
52.10
CN
5fa, Scheme 3
75 MHz, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

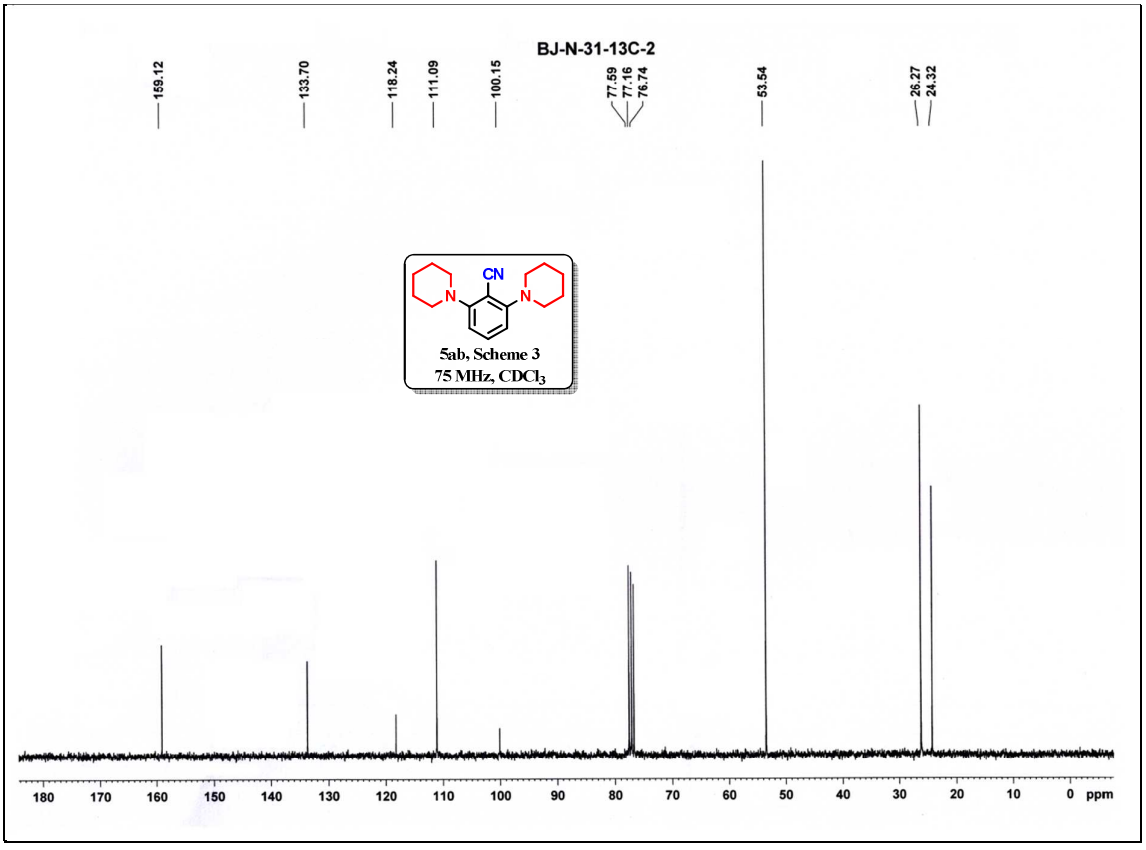

BJ-N-29-1H
7.280
7.092
3.887
3.872
3.866
3.856
3.226
3.216
3.211
3.205
3.195
2.570
CN
O
N
N
O
O
CH3
5ga, Scheme 3
300 MHz, CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
4.23
4.18
1.53

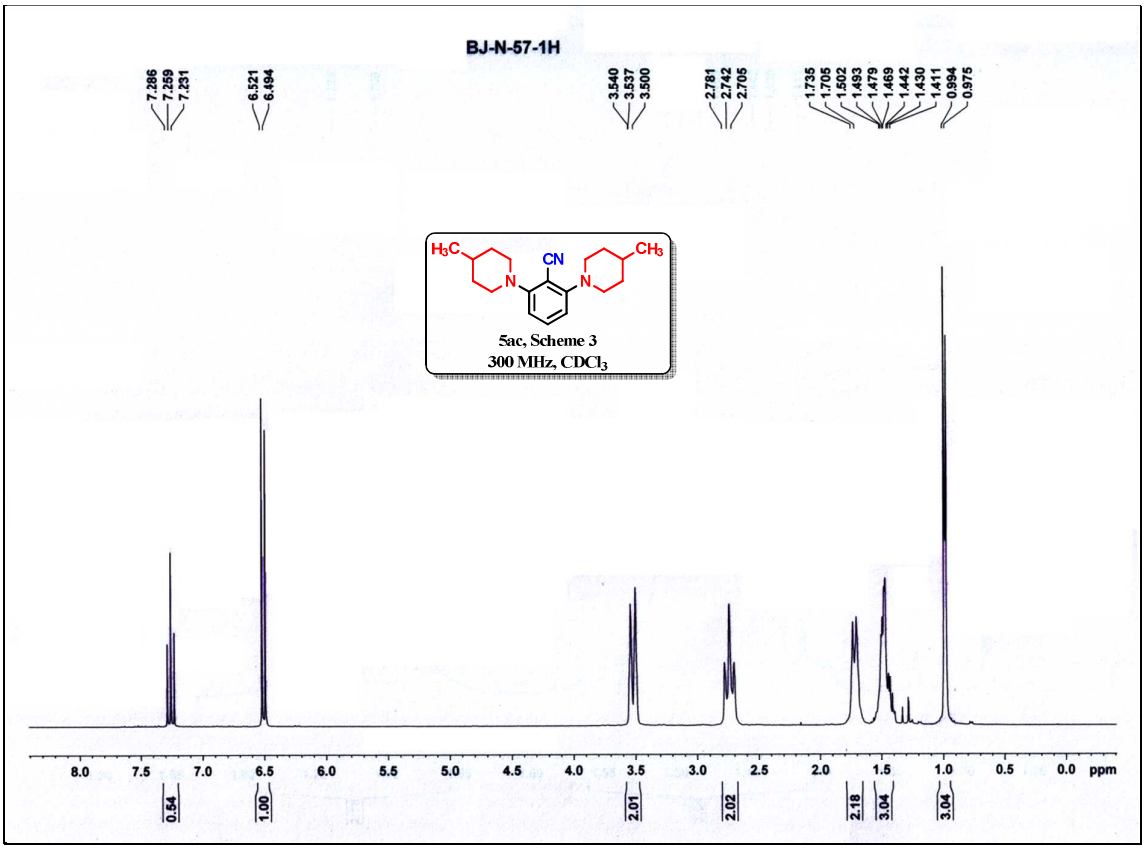

BJ-N-29-13C
197.30
157.94
141.56
117.03
111.00
103.50
77.58
77.16
76.73
66.87
52.03
26.95
CN
O
N
N
O
O
CH3
5ga, Scheme 3
75 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

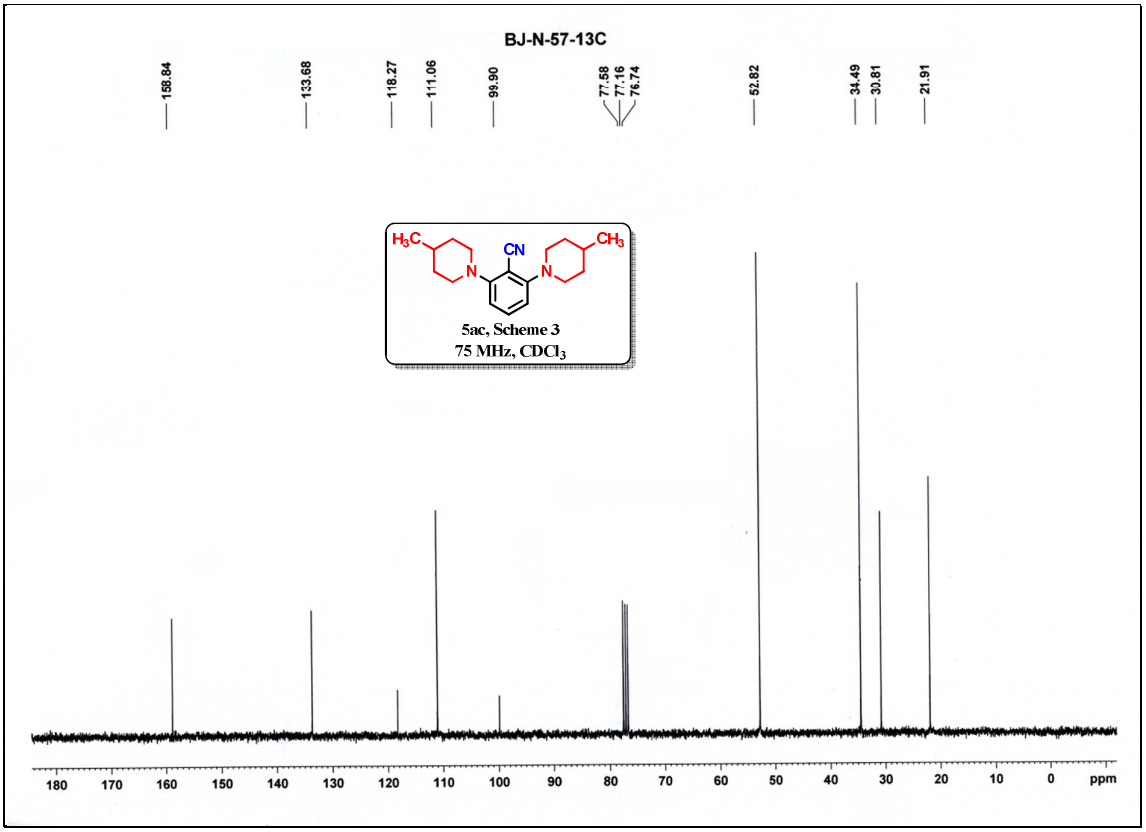

BJ-N-27-1H
7.337
7.260
3.900
3.885
3.879
3.869
3.288
3.279
3.273
3.257
CN
O
N
NO2
5ha, Scheme 3
300 MHz, CDCl3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
4.09
4.06

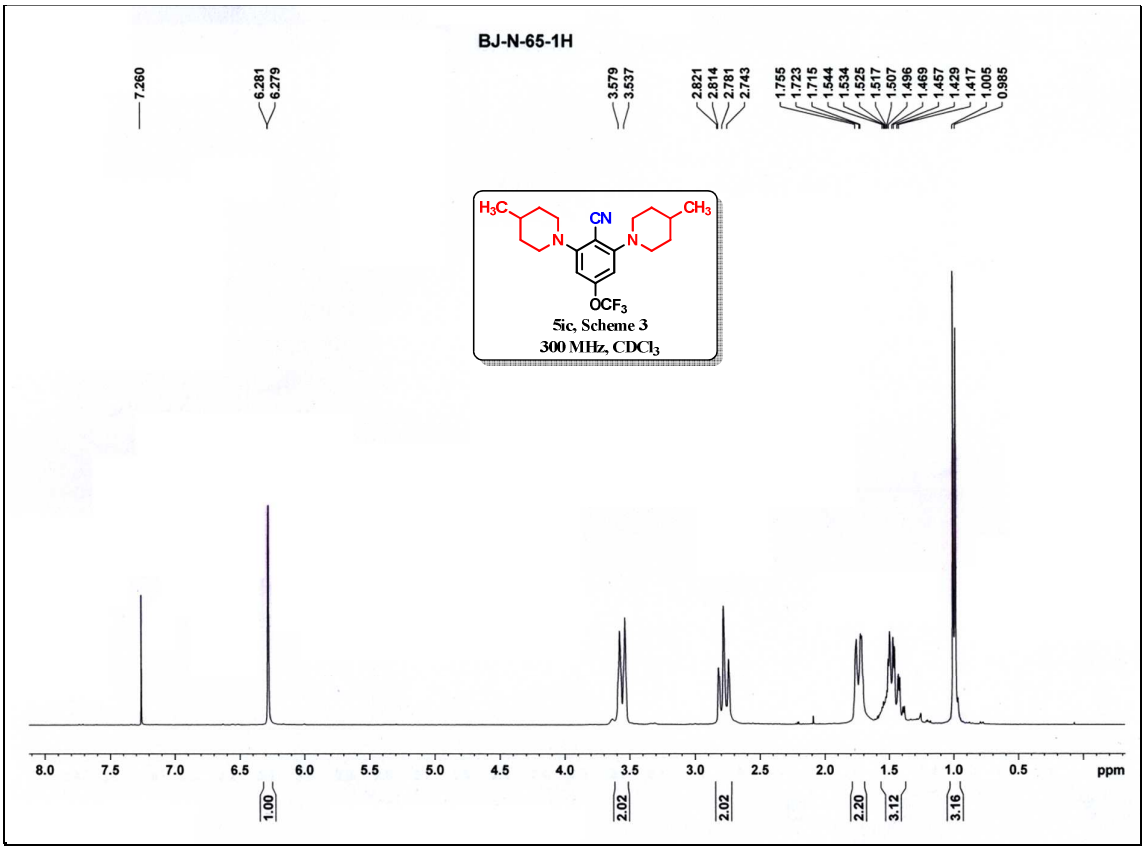

BJ-N-27-13C
168.38
151.79
116.46
105.69
103.41
77.59
77.17
76.74
66.69
51.83
CN
O
N
NO2
5ha, Scheme 3
75 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

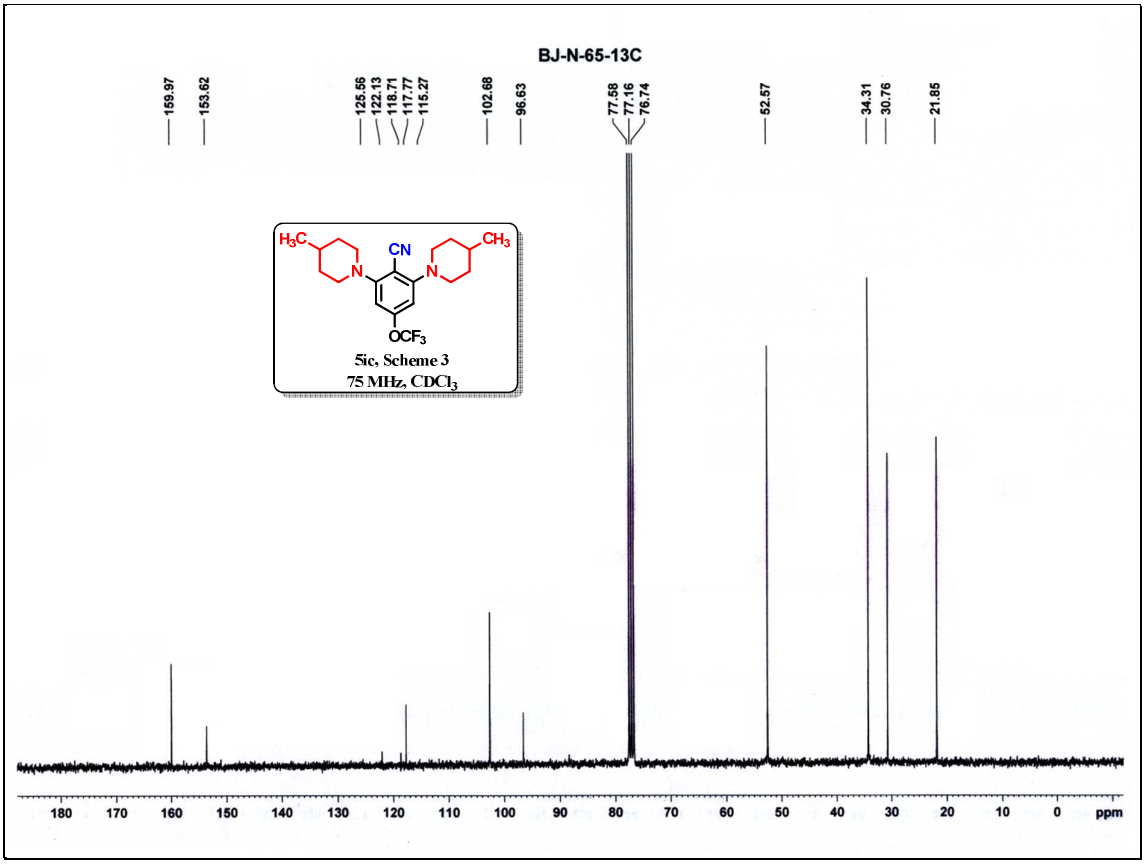

BJ-N-31-1H
7.292
7.264
7.259
7.237
6.523
6.496
3.140
3.123
3.105
1.794
1.775
1.768
1.756
1.748
1.738
1.719
1.618
1.606
1.598
1.579
1.567
1.560
1.542
CN
N
N
5ab, Scheme 3
300 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.56
1.00
4.12
4.29
2.19

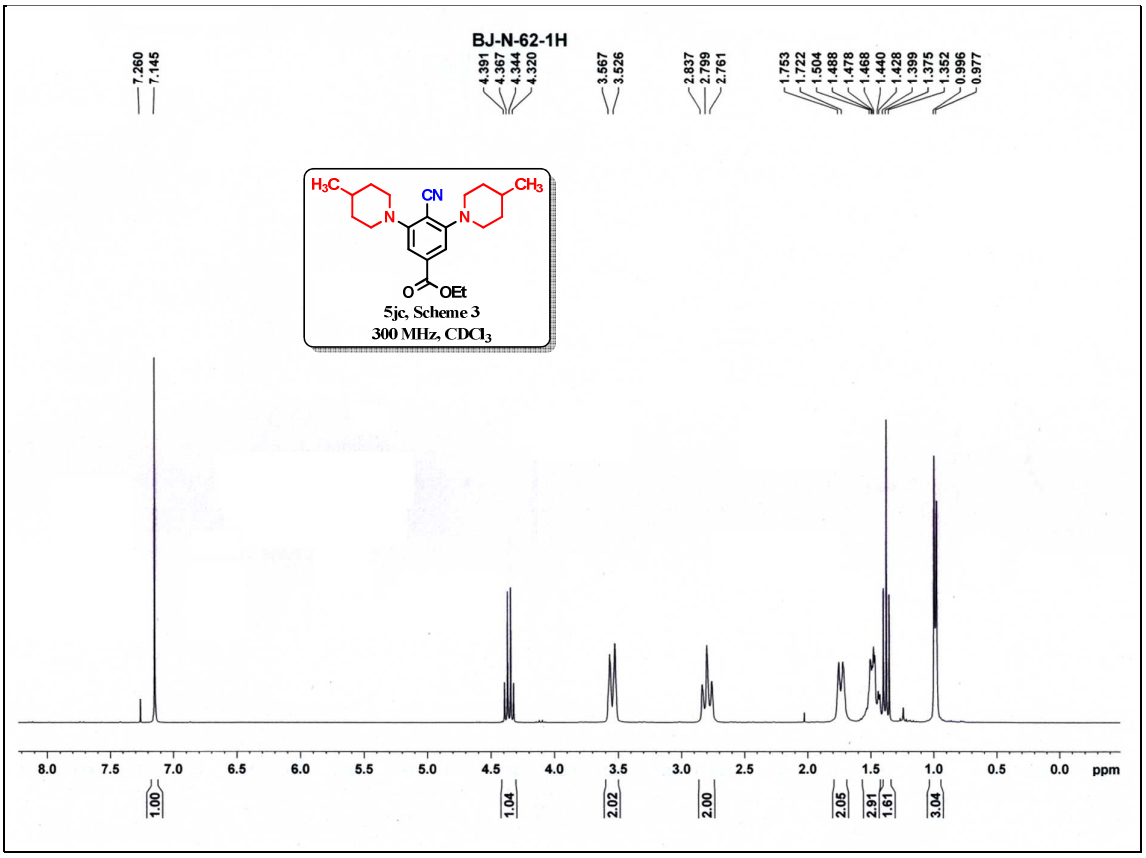

BJ-N-31-13C-2
159.12
133.70
118.24
111.09
100.15
77.59
77.16
76.74
53.54
26.27
24.32
CN
N
N
5ab, Scheme 3
75 MHz, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

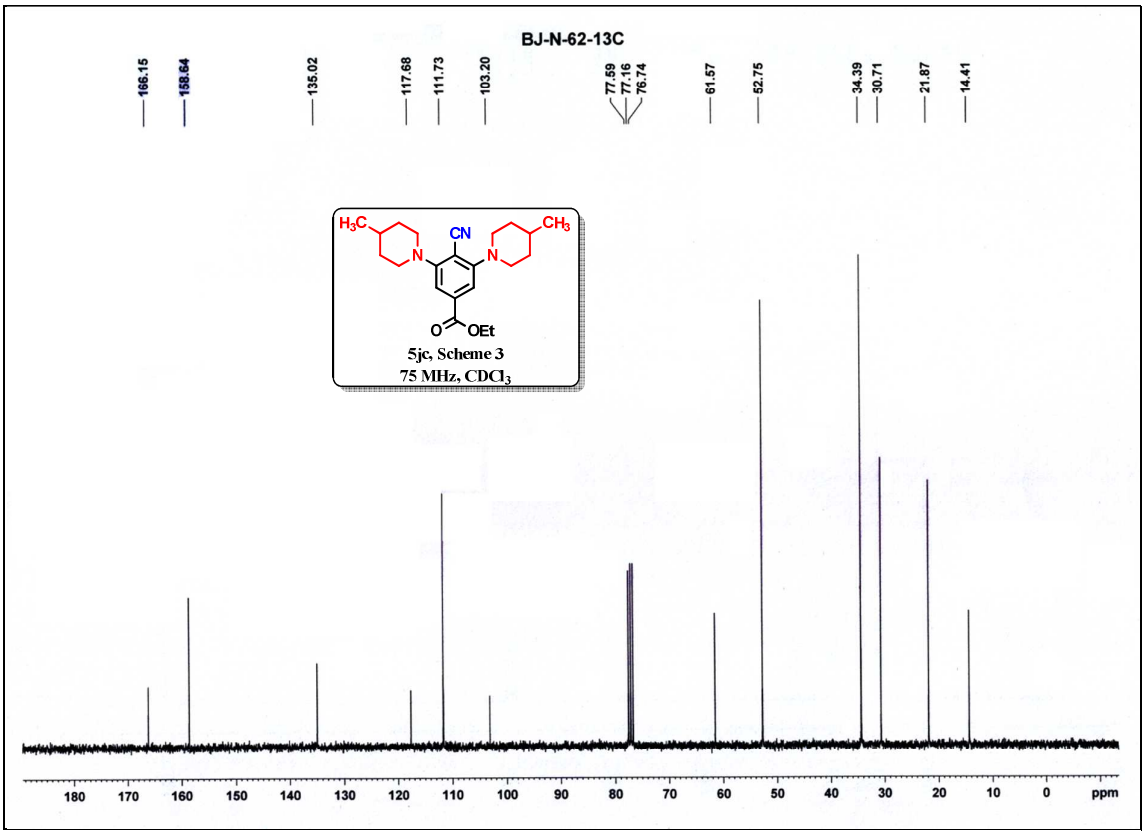

BJ-N-57-1H
7.286
7.259
7.231
6.521
6.494
3.540
3.537
3.500
2.781
2.742
2.705
1.735
1.705
1.502
1.493
1.479
1.469
1.442
1.430
1.411
0.994
0.975
H3C
CN
CH3
N
N
5ac, Scheme 3
300 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.54
1.00
2.01
2.02
2.18
3.04
3.04

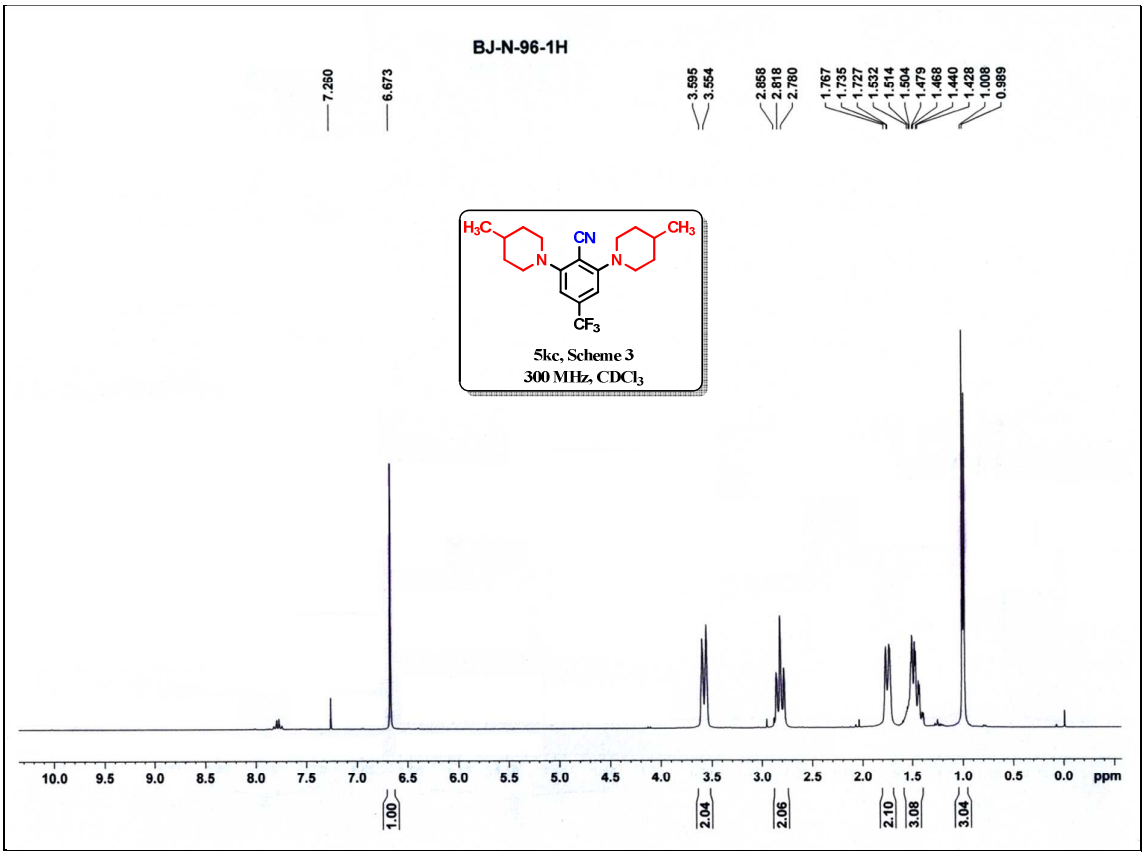

BJ-N-57-13C
158.84
133.68
118.27
111.06
99.90
77.68
77.16
76.74
52.82
34.49
30.81
21.91
H3C
CN
CH3
N
N
5ac, Scheme 3
75 MHz, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

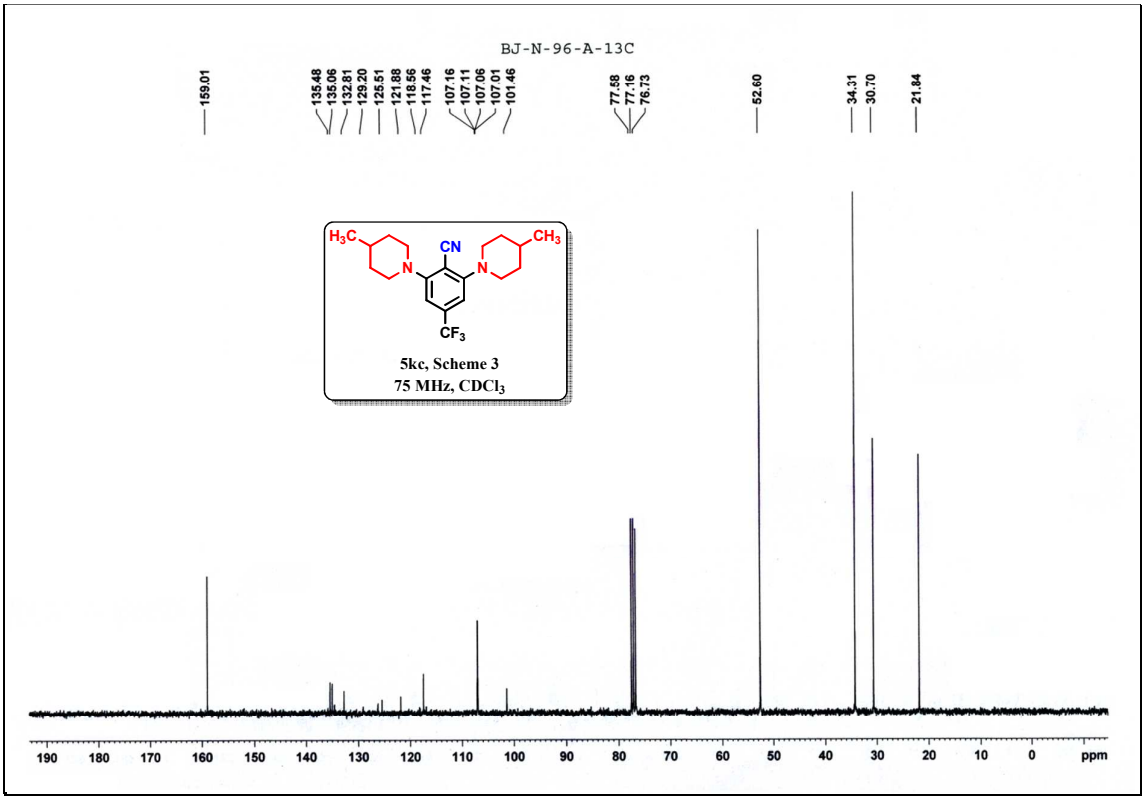

BJ-N-65-1H
7.260
6.281
6.279
3.579
3.537
2.821
2.814
2.781
2.743
1.755
1.723
1.715
1.544
1.534
1.525
1.517
1.507
1.496
1.469
1.457
1.429
1.417
1.005
0.985
5ic, Scheme 3
300 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
2.02
2.02
2.20
3.12
3.16

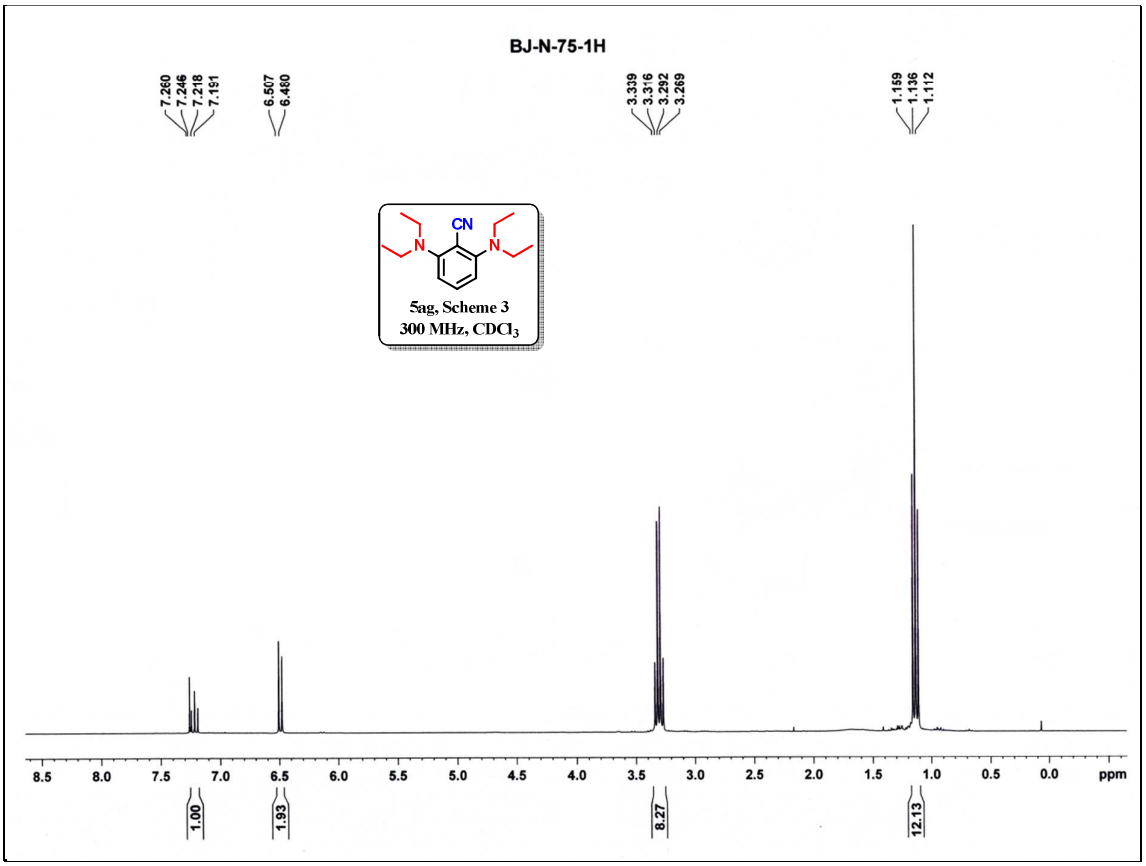

BJ-N-65-13C
159.97
153.62
125.56
122.13
118.71
117.77
115.27
102.68
96.63
77.58
77.16
76.74
52.57
34.31
30.76
21.85
5ic, Scheme 3
75 MHz, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

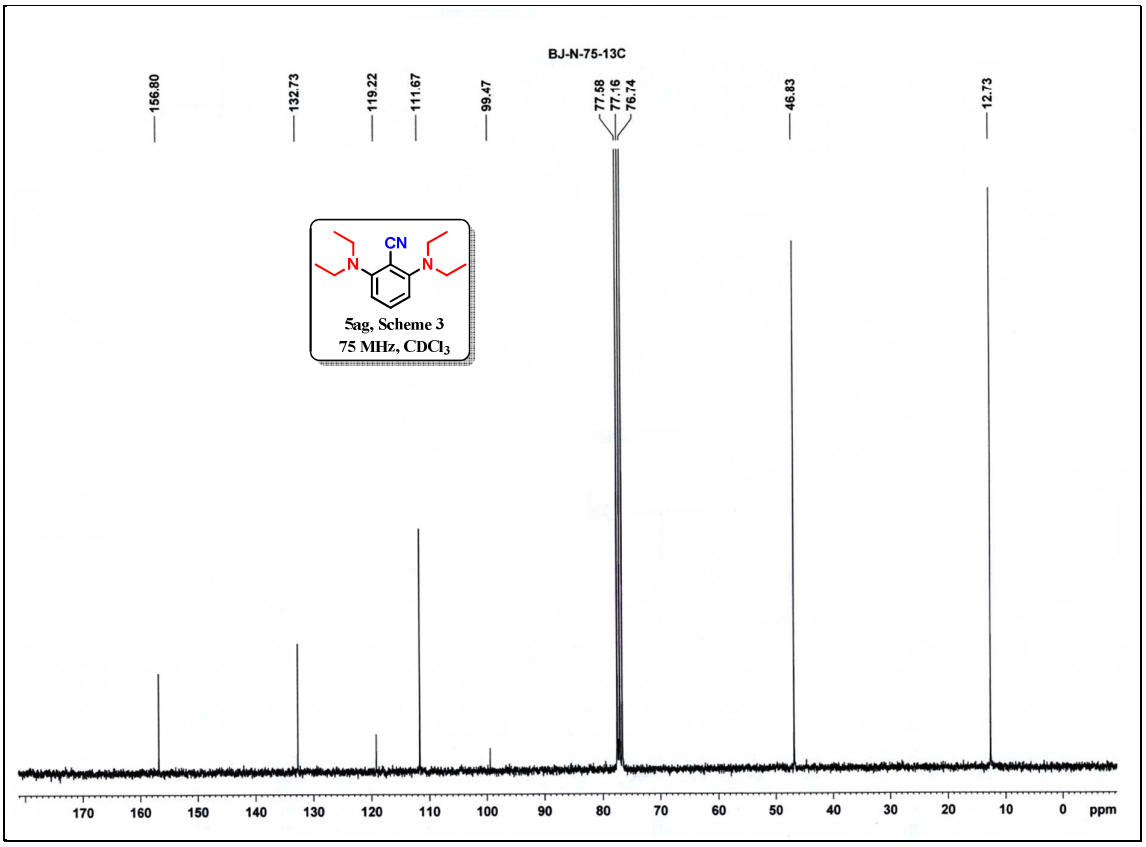

BJ-N-62-1H
7.260
7.145
4.391
4.367
4.344
4.320
3.567
3.526
2.837
2.799
2.761
1.753
1.722
1.504
1.488
1.478
1.468
1.440
1.428
1.399
1.375
1.352
0.996
0.977
5jc, Scheme 3
300 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.04
2.02
2.00
2.05
2.91
1.61
3.04

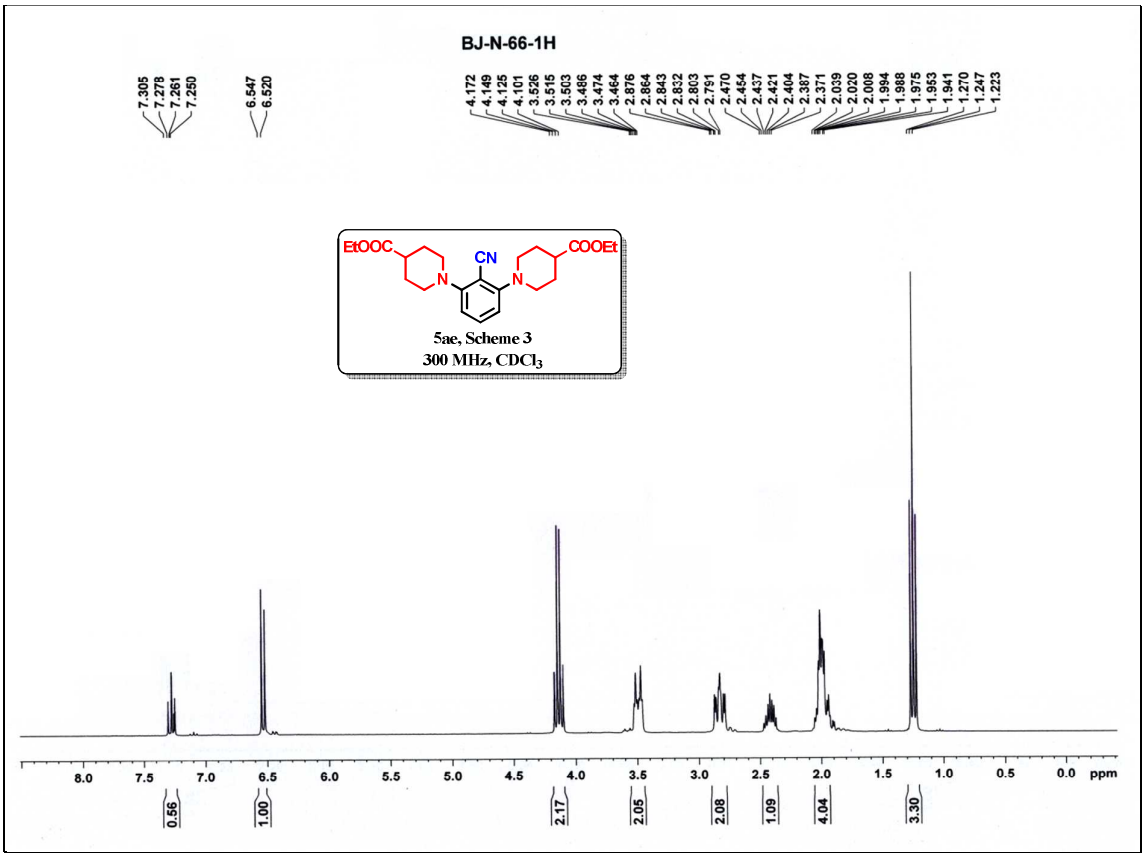

BJ-N-62-13C
166.15
158.64
135.02
117.68
111.73
103.20
77.59
77.16
76.74
61.57
52.75
34.39
30.71
21.87
14.41
5jc, Scheme 3
75 MHz, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

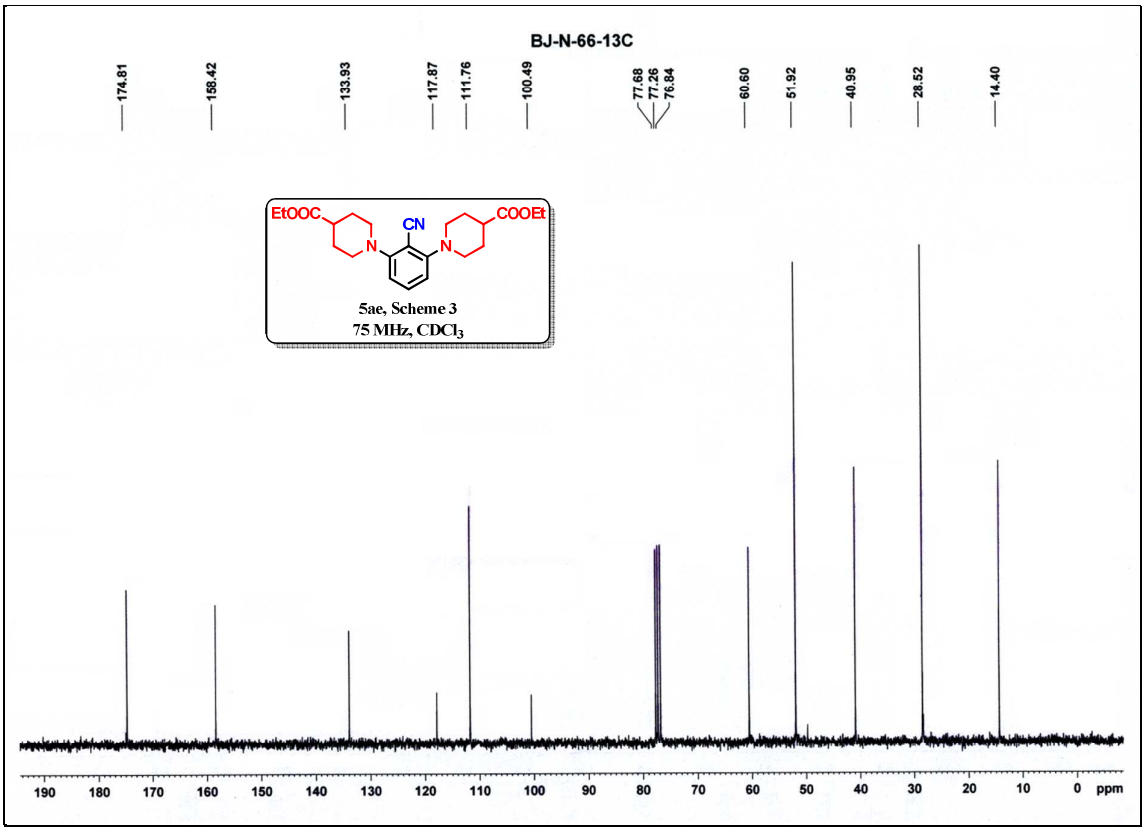

BJ-N-96-1H
7.260
6.673
3.595
3.554
2.858
2.818
2.780
1.767
1.735
1.727
1.532
1.514
1.504
1.479
1.468
1.440
1.428
1.008
0.989
5kc, Scheme 3
300 MHz, CDCl3
1.00
2.04
2.06
2.10
3.08
3.04
ppm

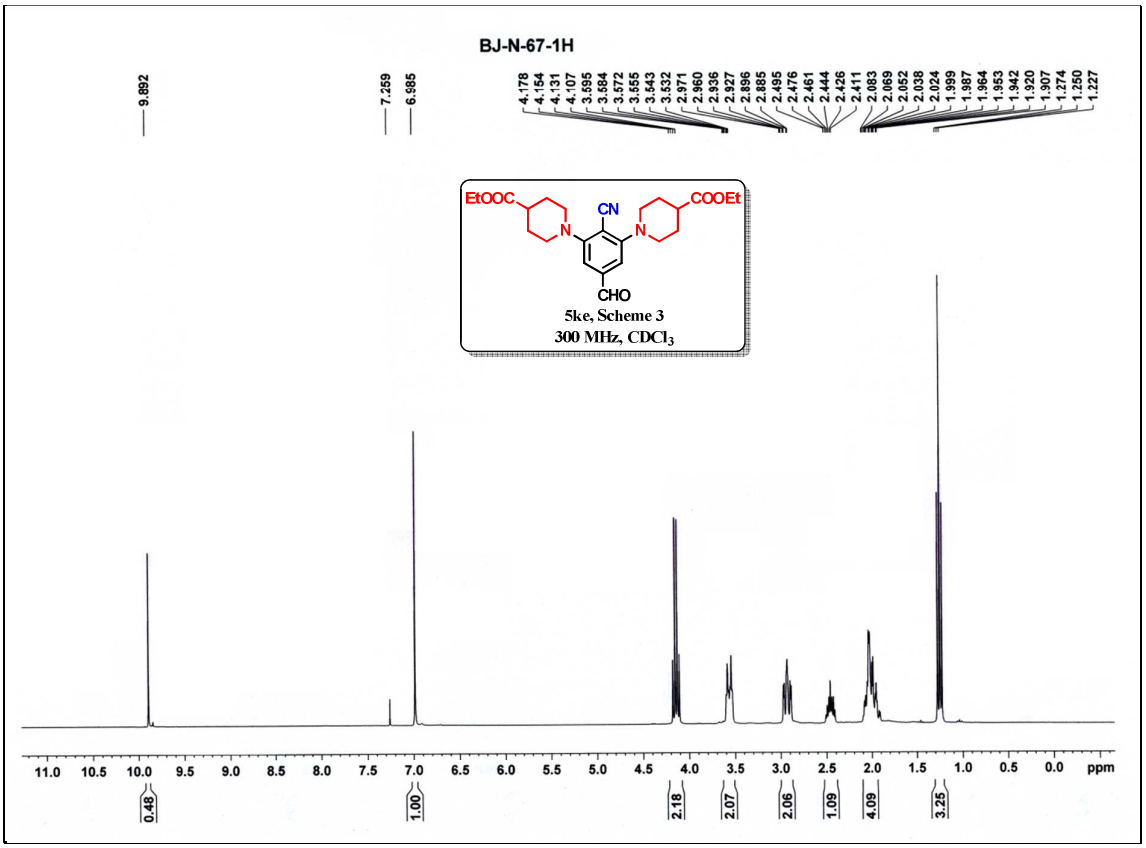

BJ-N-96-A-13C
159.01
135.48
135.06
132.81
129.20
125.51
121.88
118.56
117.46
107.16
107.11
107.06
107.01
101.46
77.58
77.16
76.73
52.60
34.31
30.70
21.84
5kc, Scheme 3
75 MHz, CDCl3
ppm

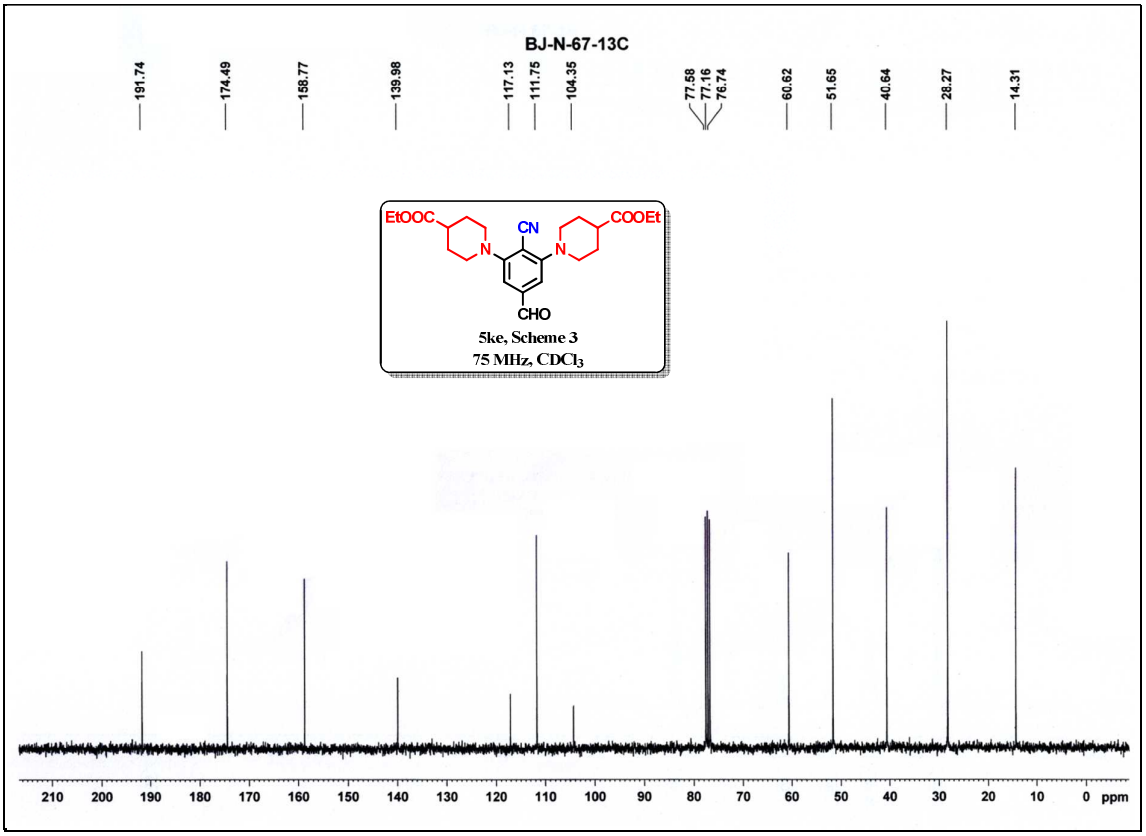

BJ-N-75-1H
7.260
7.246
7.218
7.191
6.507
6.480
3.339
3.316
3.292
3.269
1.159
1.136
1.112
CN
N
N
5ag, Scheme 3
300 MHz, CDCl3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.93
8.27
12.13

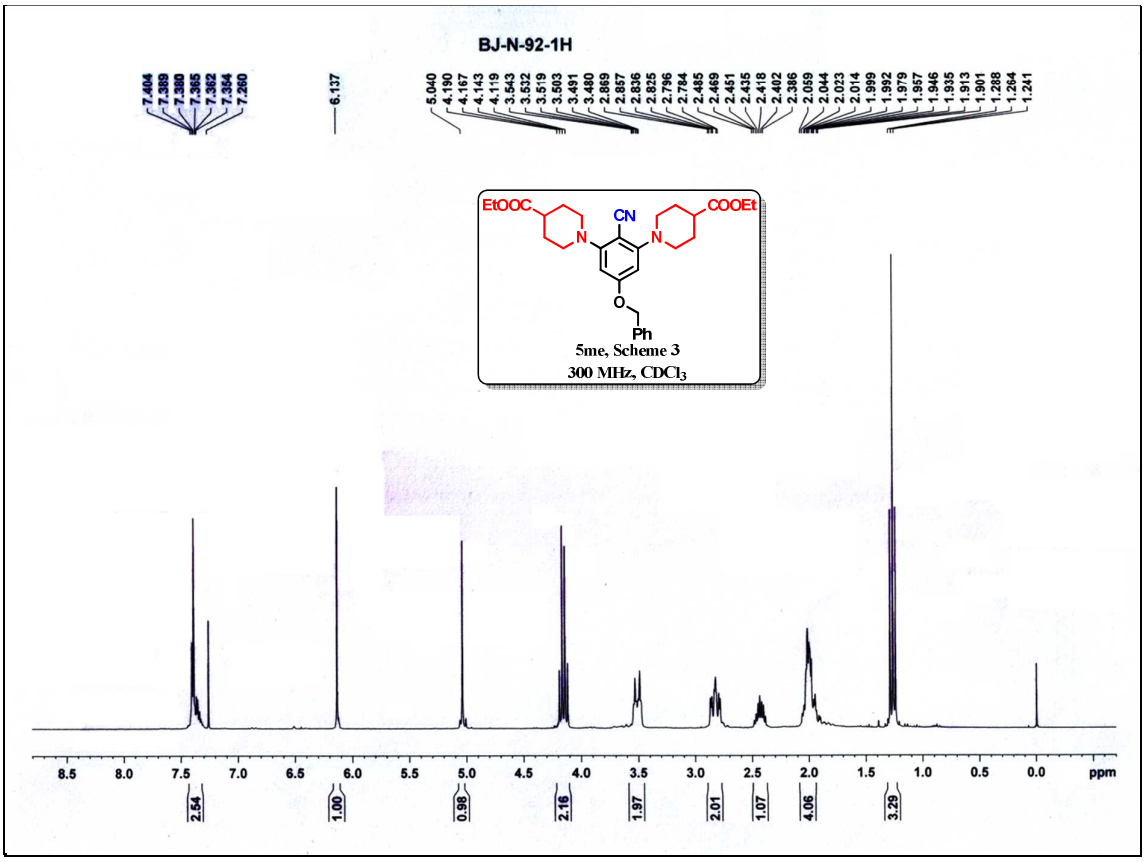

BJ-N-75-13C
156.80
132.73
119.22
111.67
99.47
77.58
77.16
76.74
46.83
12.73
CN
N
N
5ag, Scheme 3
75 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

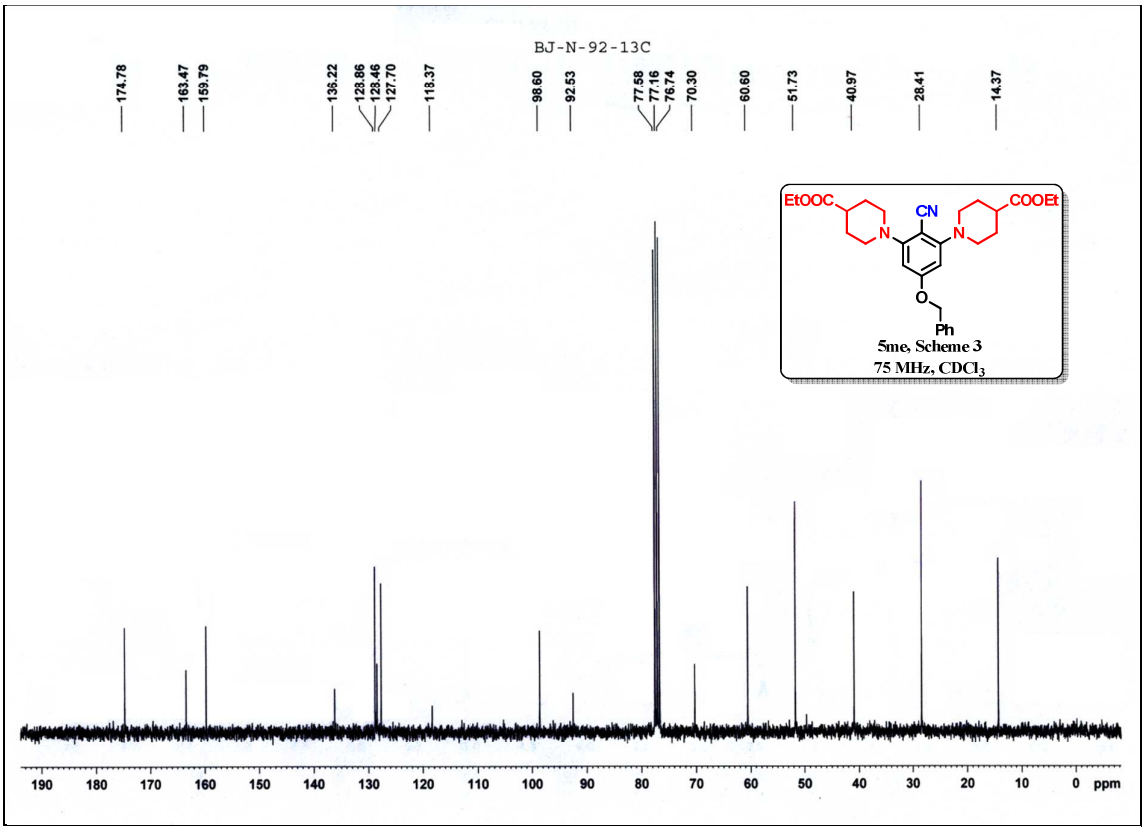

BJ-N-66-1H
7.305
7.278
7.261
7.250
6.547
6.520
4.172
4.149
4.125
4.101
3.526
3.515
3.503
3.486
3.474
3.464
2.876
2.864
2.843
2.832
2.803
2.791
2.470
2.454
2.437
2.421
2.404
2.387
2.371
2.039
2.020
2.008
1.994
1.988
1.975
1.953
1.941
1.270
1.247
1.223
EtOOC
CN
COOEt
N
N
5ae, Scheme 3
300 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.56
1.00
2.17
2.05
2.08
1.09
4.04
3.30

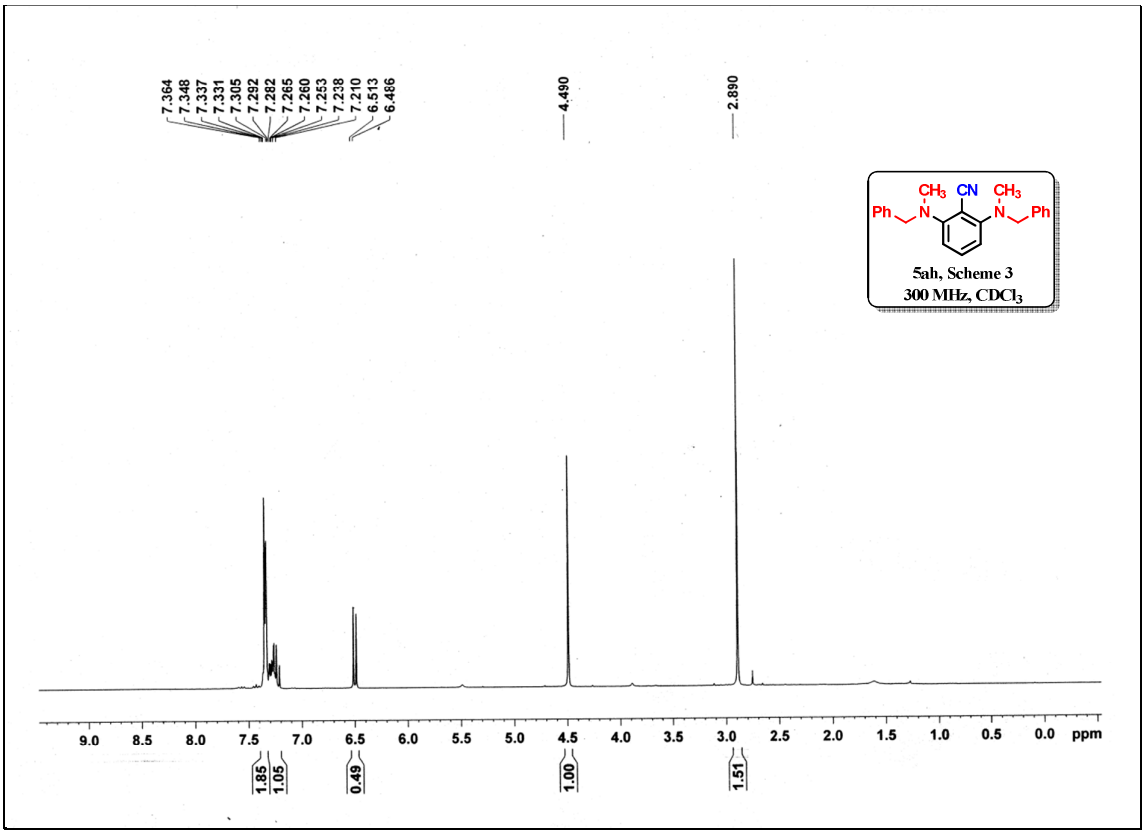

BJ-N-66-13C
174.81
158.42
133.93
117.87
111.76
100.49
77.68
77.26
76.84
60.60
51.92
40.95
28.52
14.40
EtOOC
CN
COOEt
N
N
5ae, Scheme 3
75 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

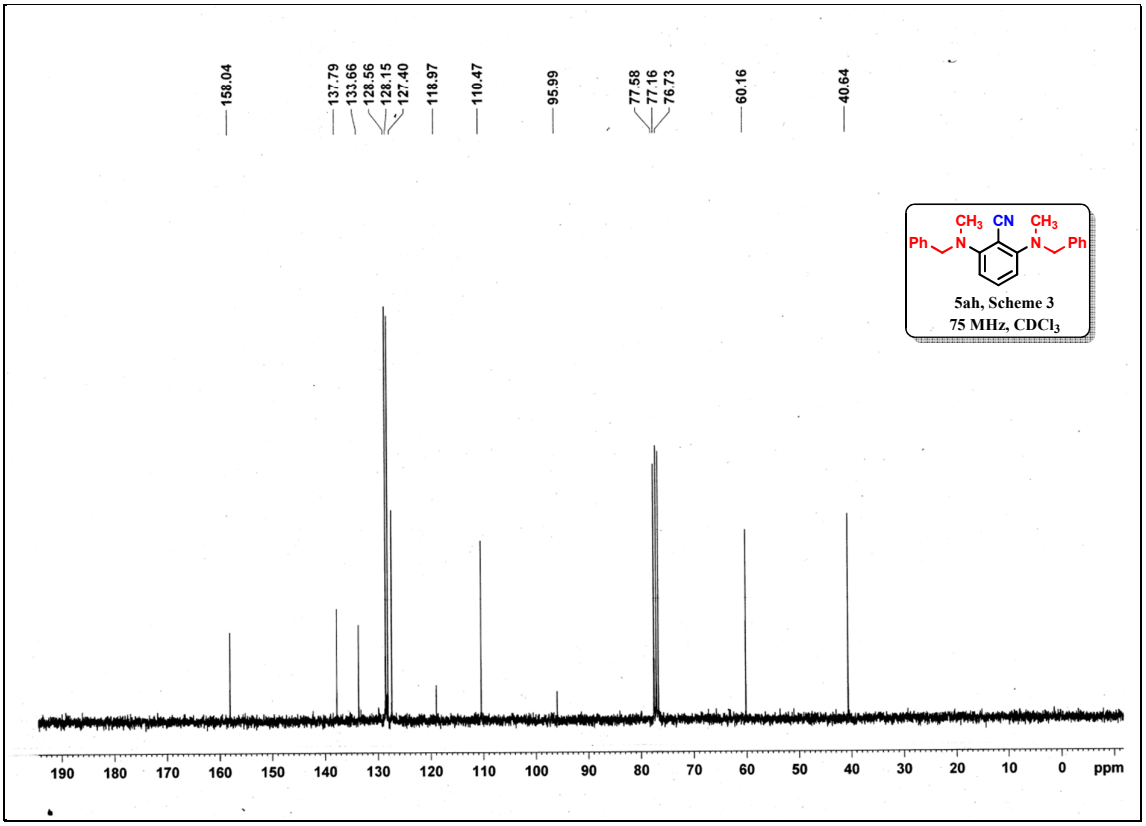

BJ-N-67-1H
9.892
7.459
6.585
4.178
4.154
4.131
4.107
3.595
3.584
3.572
3.555
3.543
3.532
2.971
2.960
2.936
2.927
2.896
2.885
2.495
2.476
2.461
2.444
2.426
2.411
2.083
2.069
2.052
2.038
2.024
1.999
1.987
1.964
1.953
1.942
1.920
1.907
1.274
1.250
1.227
EtOOC
CN
COOEt
N
N
CHO
5ke, Scheme 3
300 MHz, CDCl3
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.48
1.00
2.18
2.07
2.06
1.09
4.09
3.25

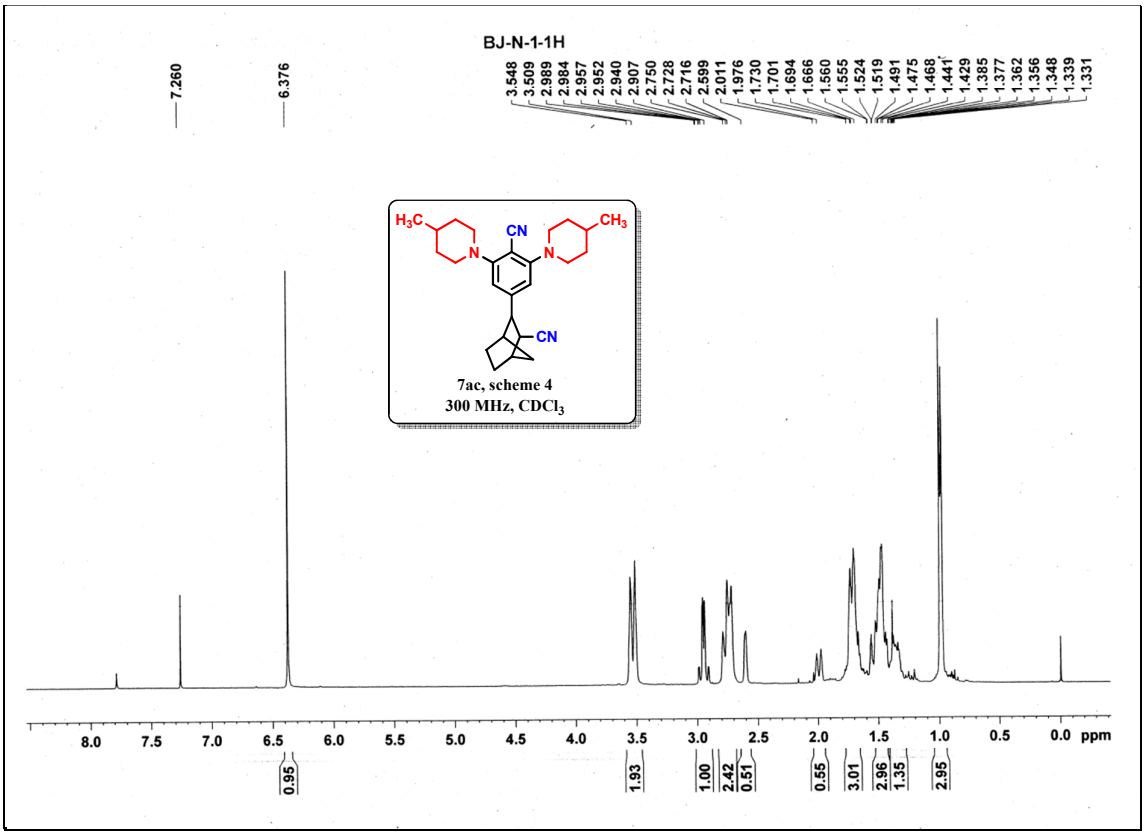

BJ-N-67-13C
191.74
174.49
158.77
139.98
117.13
111.75
104.35
77.58
77.16
76.74
60.62
51.65
40.64
28.27
14.31
EtOOC
CN
COOEt
N
N
CHO
5ke, Scheme 3
75 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

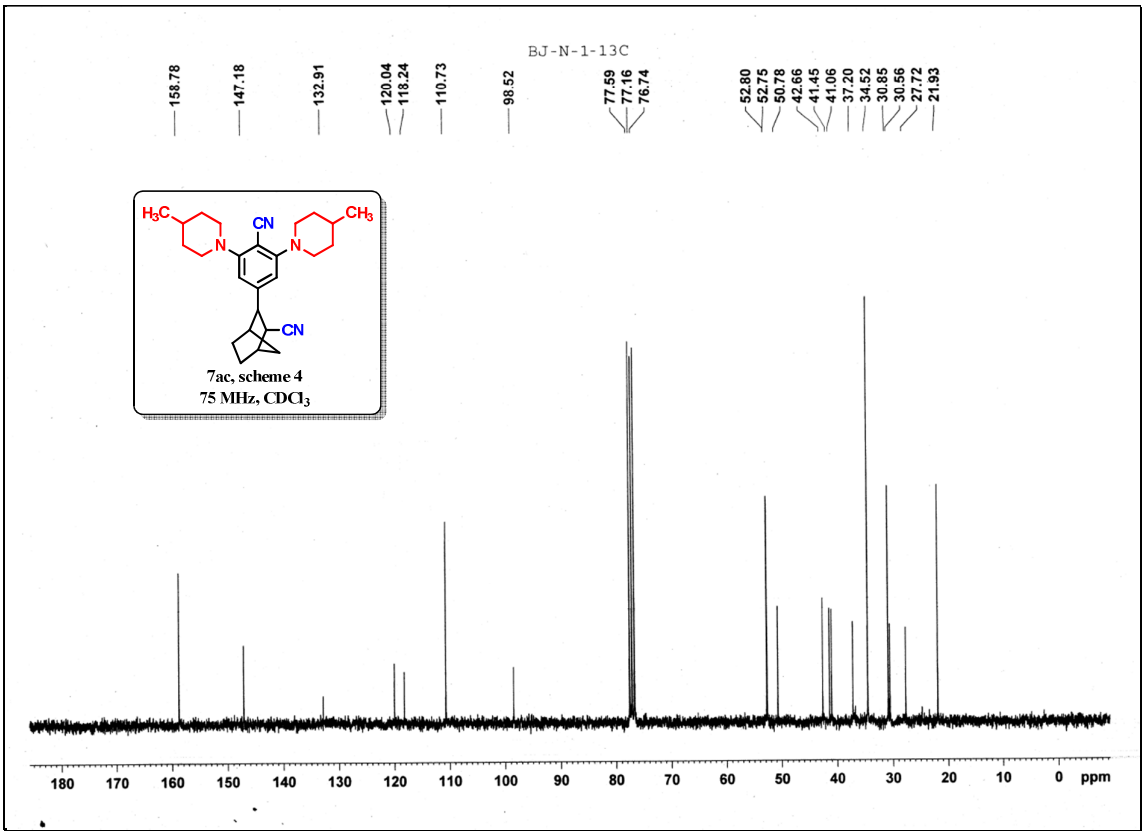

BJ-N-92-1H
7.404
7.389
7.380
7.365
7.362
7.354
7.260
6.137
5.040
4.190
4.167
4.143
4.119
3.543
3.532
3.519
3.503
3.491
3.480
2.869
2.857
2.836
2.825
2.796
2.784
2.485
2.469
2.451
2.435
2.418
2.402
2.386
2.059
2.044
2.023
2.014
1.999
1.992
1.979
1.957
1.946
1.935
1.913
1.901
1.288
1.264
1.241
EtOOC
CN
COOEt
N
N
O
Ph
5me, Scheme 3
300 MHz, CDCl3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.54
1.00
0.98
2.16
1.97
2.01
1.07
4.06
3.29

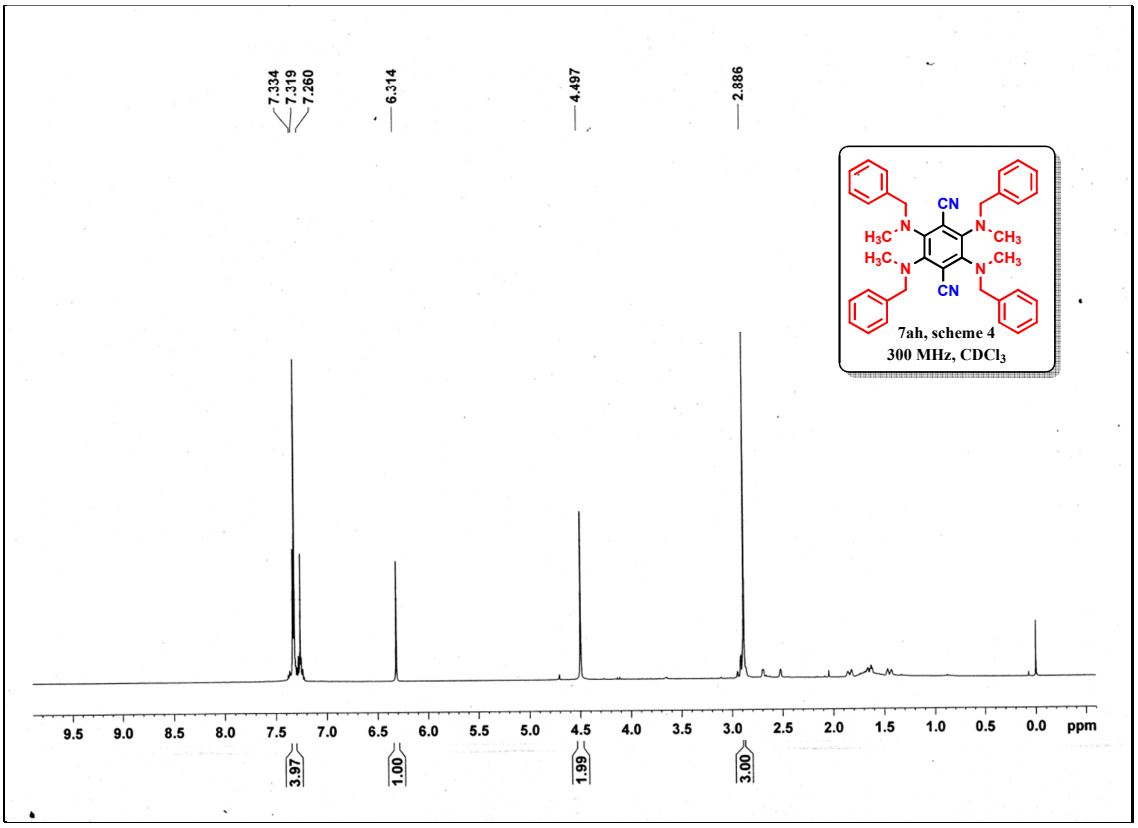

BJ-N-92-13C
174.78
163.47
159.79
136.22
128.86
128.46
127.70
118.37
98.60
92.53
77.58
77.16
76.74
70.30
60.60
51.73
40.97
28.41
14.37
EtOOC
CN
COOEt
N
N
O
Ph
5me, Scheme 3
75 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

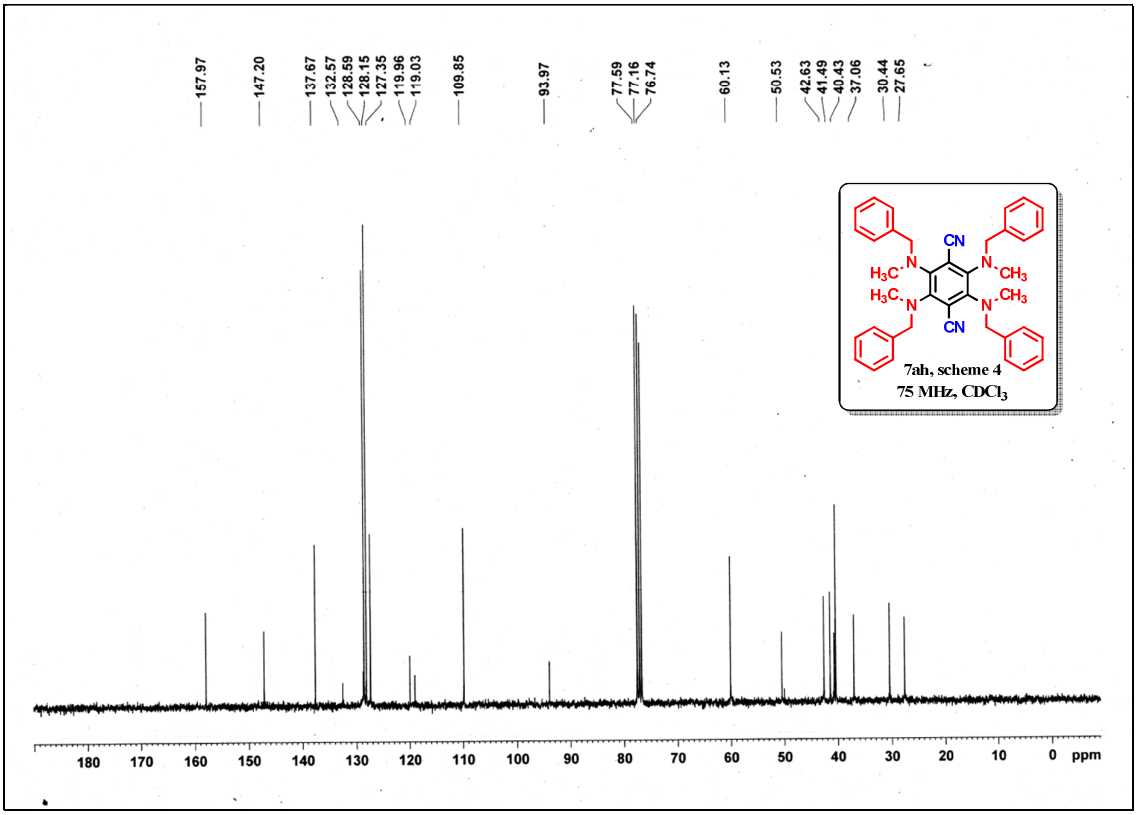

7.364
7.348
7.337
7.331
7.305
7.292
7.282
7.265
7.260
7.253
7.238
7.210
6.513
6.486
4.490
2.890
5ah, Scheme 3
300 MHz, CDCl3
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.85
1.05
0.49
1.00
1.51

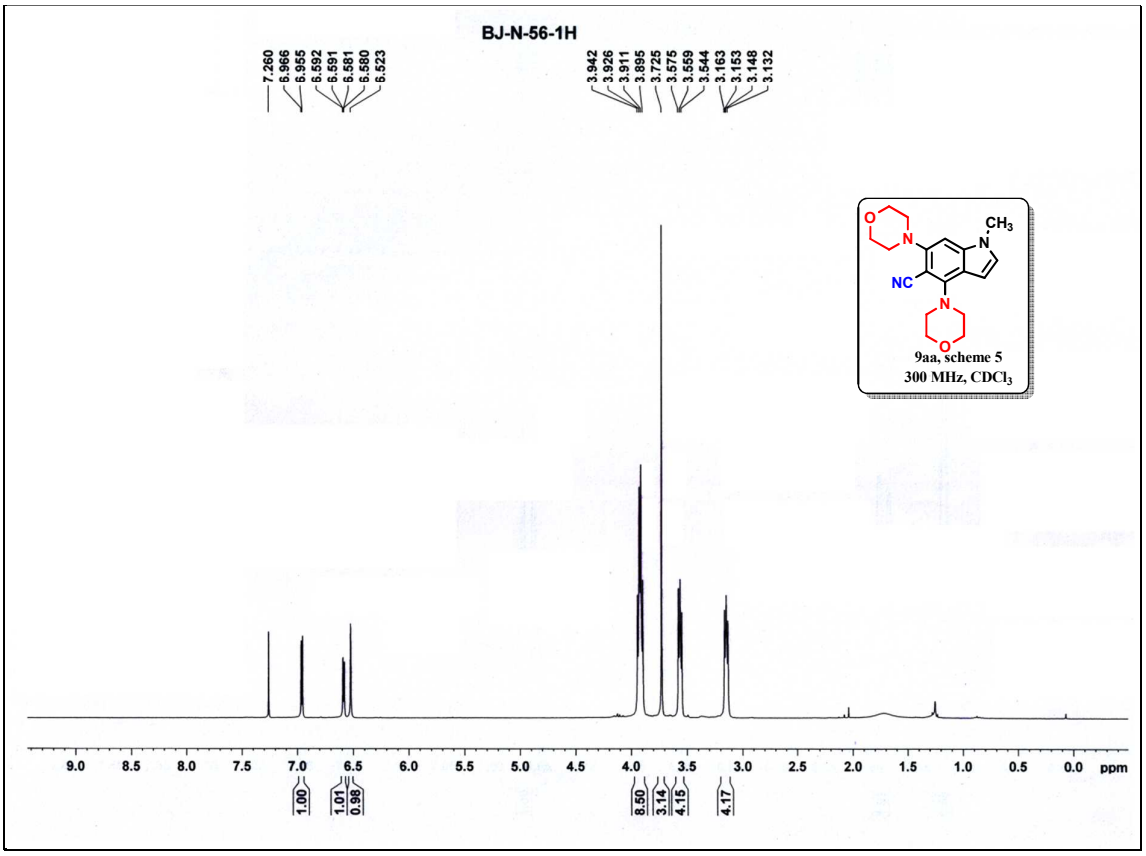

158.04
137.79
133.66
128.56
128.15
127.40
118.97
110.47
95.99
77.58
77.16
76.73
60.16
40.64
5ah, Scheme 3
75 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

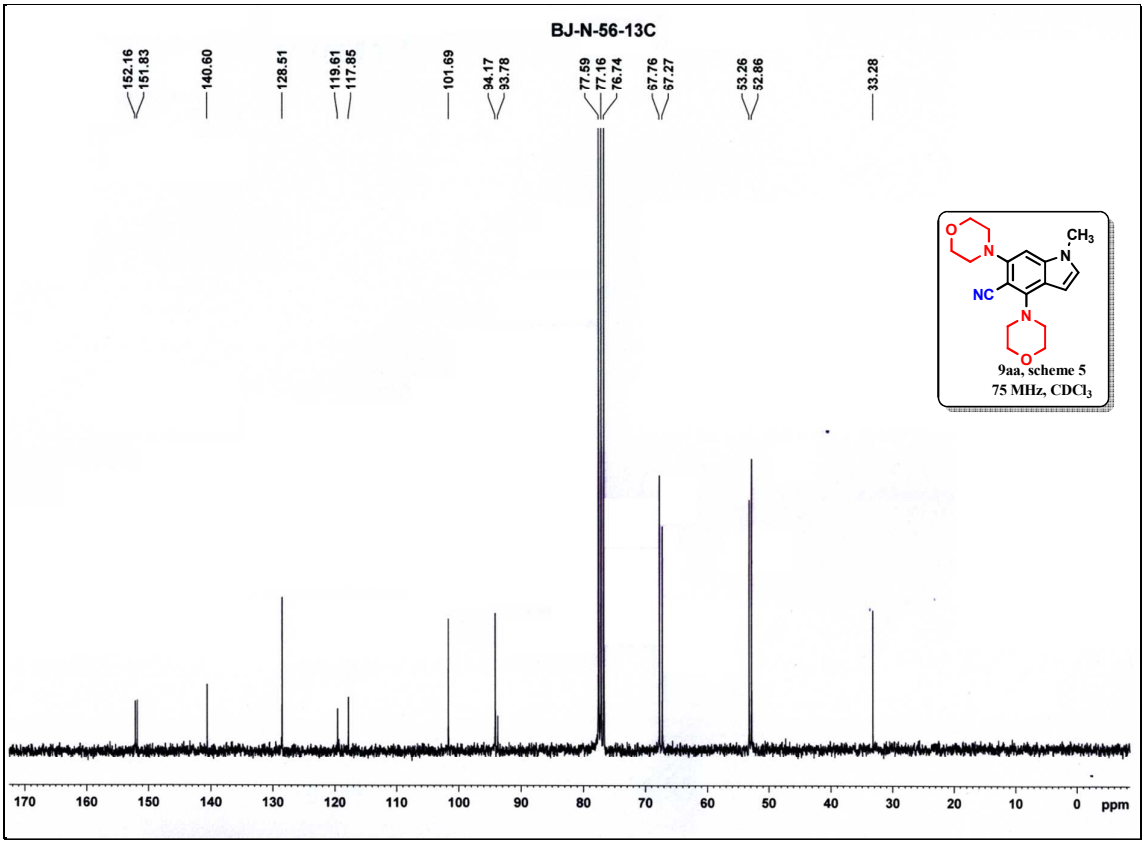

BJ-N-1-1H
7.260
6.376
3.548
3.509
2.989
2.984
2.957
2.952
2.940
2.907
2.750
2.728
2.716
2.599
2.011
1.976
1.730
1.701
1.694
1.666
1.560
1.555
1.524
1.519
1.491
1.475
1.468
1.441
1.429
1.385
1.377
1.362
1.356
1.348
1.339
1.331
7ac, scheme 4
300 MHz, CDCl3
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.95
1.93
1.00
2.42
0.51
0.55
3.01
2.96
1.35
2.95

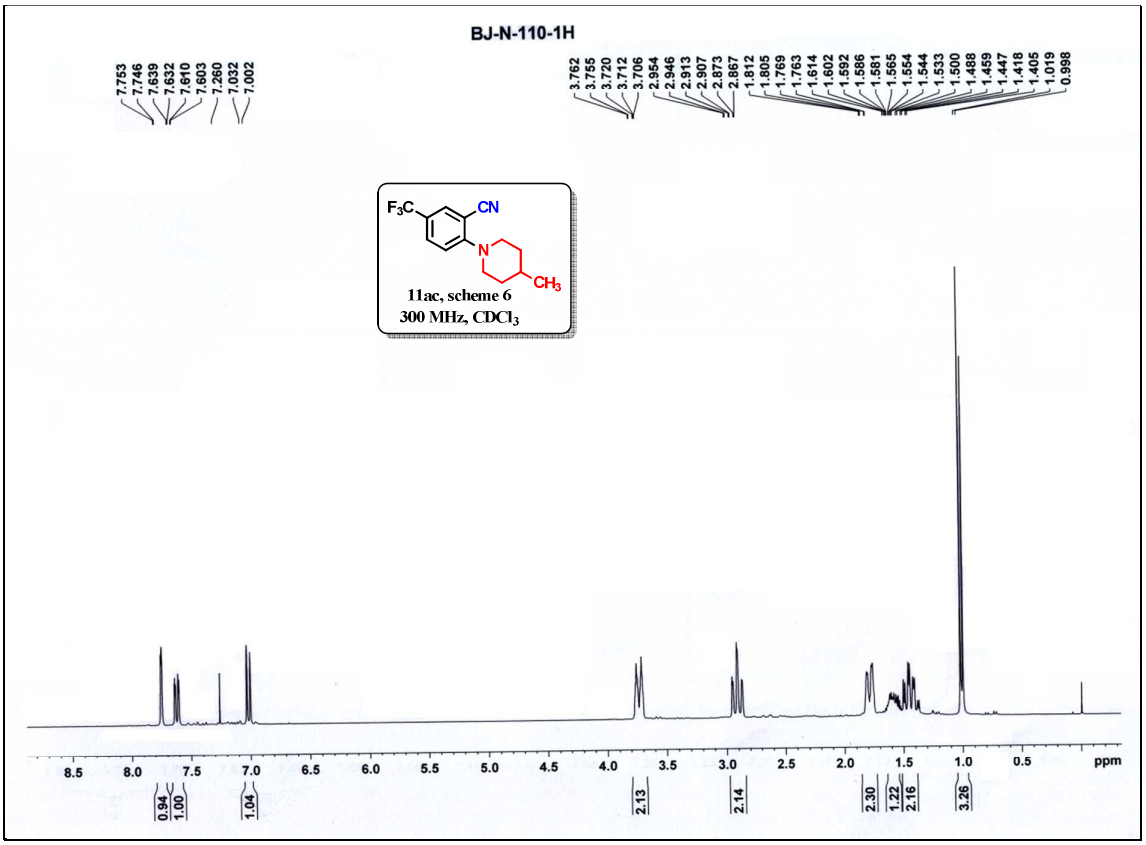

BJ-N-1-13C
158.78
147.18
132.91
120.04
118.24
110.73
98.52
77.59
77.16
76.74
52.80
52.75
50.78
42.66
41.45
41.06
37.20
34.52
30.85
30.56
27.72
21.93
7ac, scheme 4
75 MHz, CDCl3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

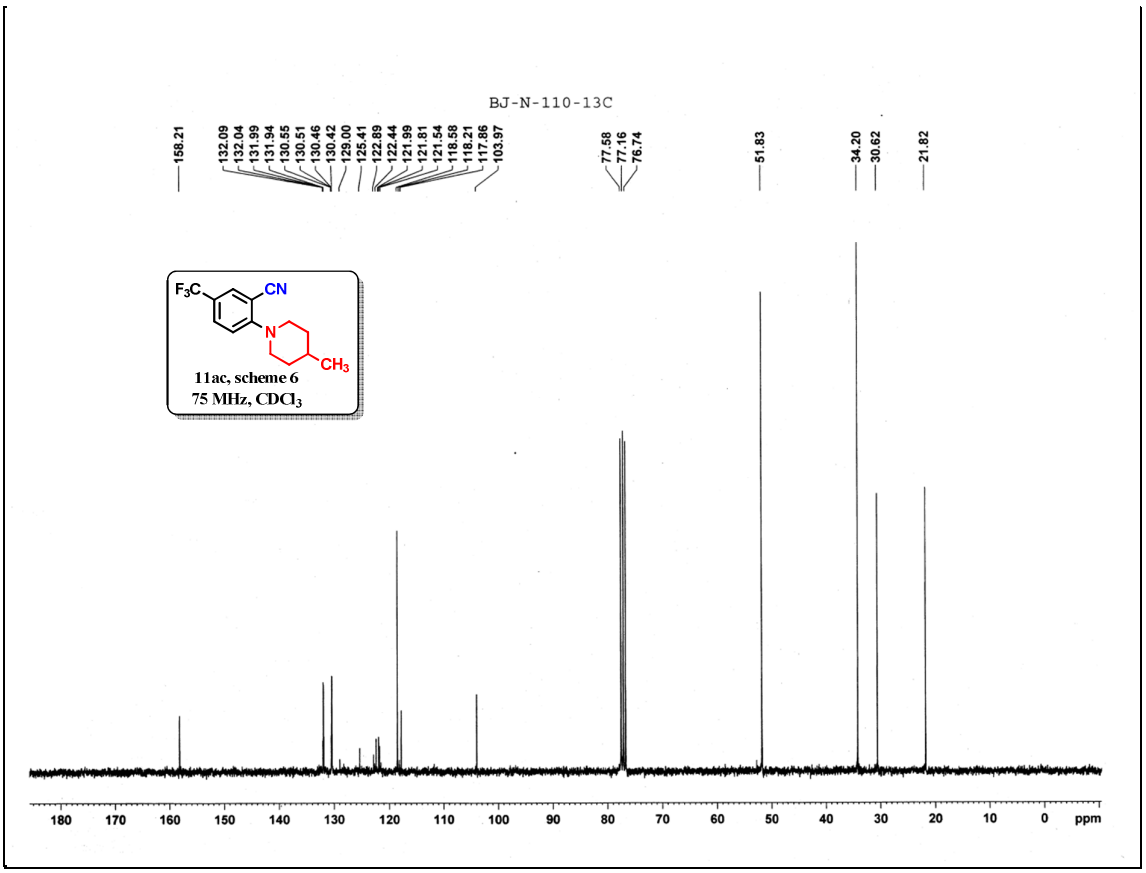

7.334
7.319
7.260
6.314
4.497
2.886
7ah, scheme 4
300 MHz, CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
3.97
1.00
1.99
3.00

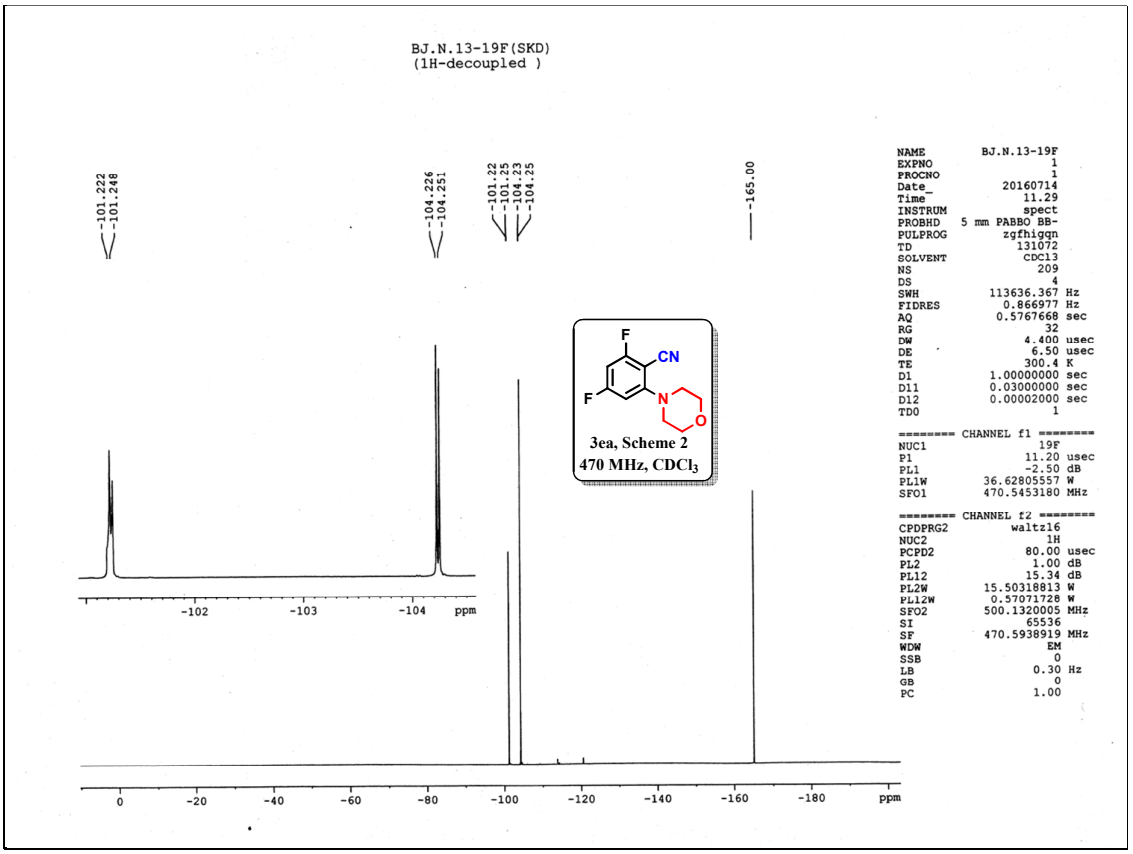

157.97
147.20
137.67
132.57
128.59
128.15
127.35
119.96
119.03
109.85
93.97
77.59
77.16
76.74
60.13
50.53
42.63
41.49
40.43
37.06
30.44
27.65
7ah, scheme 4
75 MHz, CDCl3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

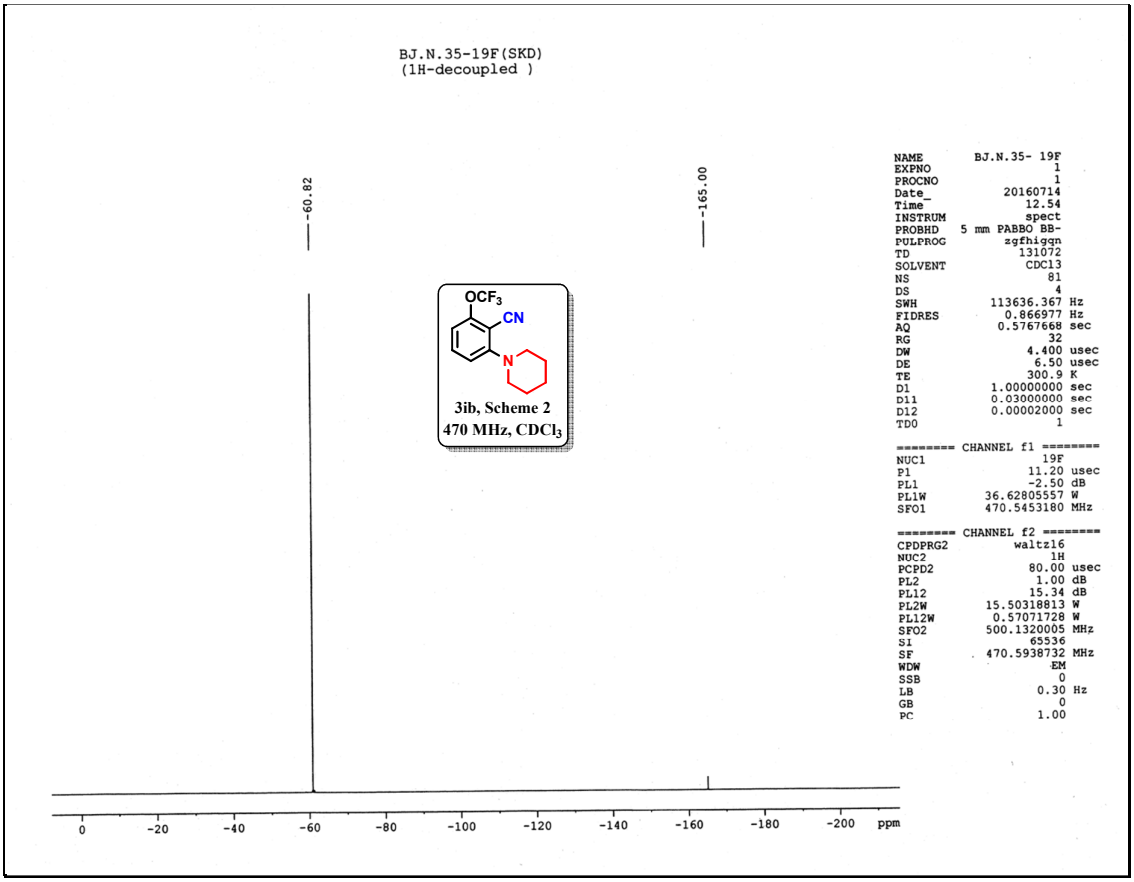

BJ-N-56-1H
7.260
6.966
6.955
6.592
6.591
6.581
6.580
6.523
3.942
3.926
3.911
3.895
3.725
3.575
3.559
3.544
3.163
3.153
3.148
3.132
9aa, scheme 5
300 MHz, CDCl3
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
1.01
0.98
8.50
3.14
4.15
4.17

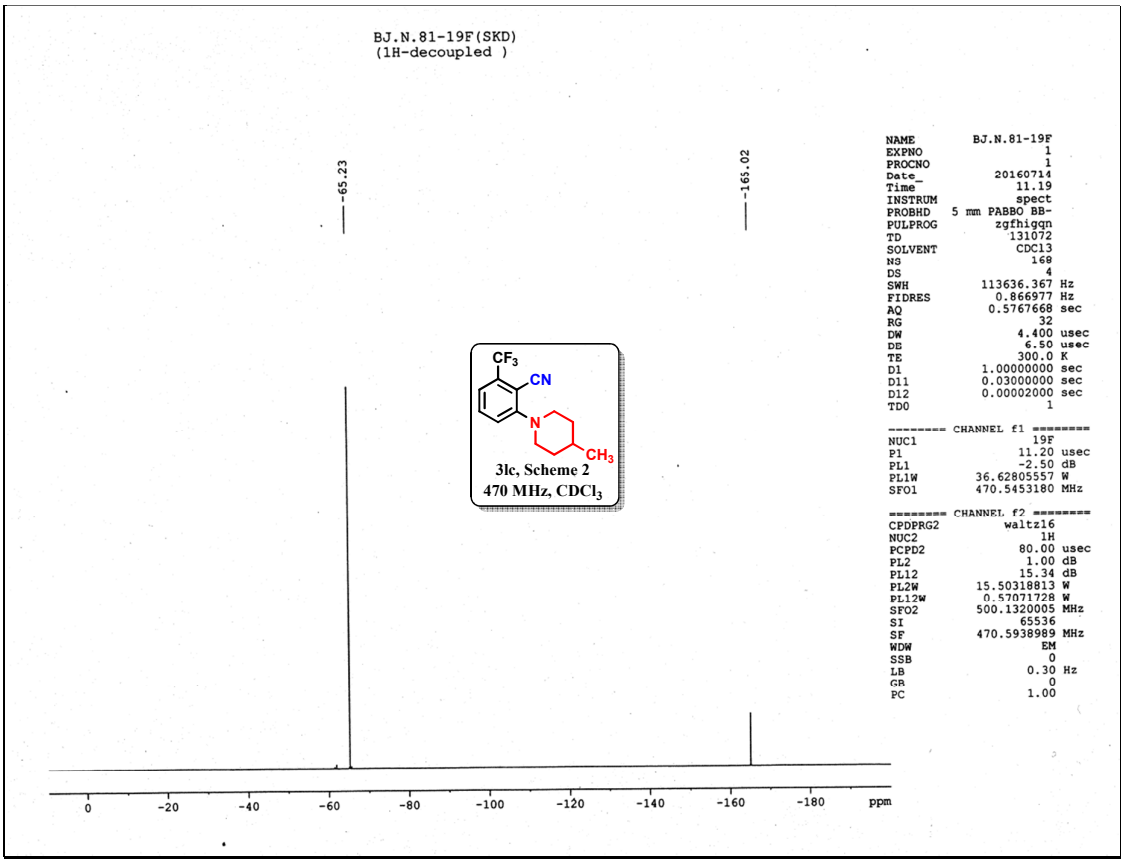

BJ-N-56-13C
152.16
151.83
140.60
128.51
119.61
117.85
101.69
94.17
93.78
77.59
77.16
76.74
67.76
67.27
53.26
52.86
33.28
9aa, scheme 5
75 MHz, CDCl3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


BJ-N-110-1H
11ac, scheme 6
300 MHz, CDCl3

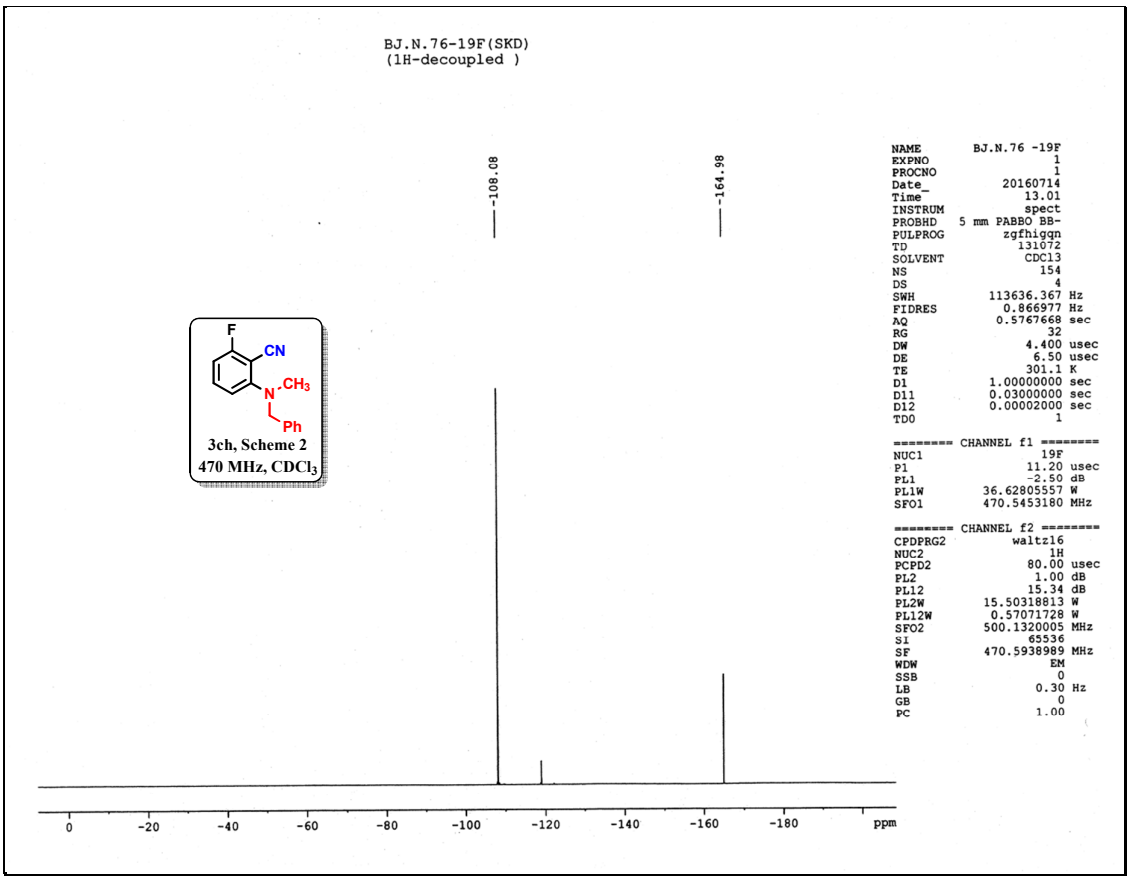

BJ-N-110-13C
11ac, scheme 6
75 MHz, CDCl3


BJ.N.13-19F(SKD)
(1H-decoupled )
-101.222
-101.248
-104.226
-104.251
-101.22
-101.25
-104.23
-104.25
-165.00
F
CN
F
N
O
3ea, Scheme 2
470 MHz, CDCl3
-102
-103
-104
ppm
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm
NAME BJ.N.13-19F
EXPNO 1
PROCNO 1
Date_ 20160714
Time 11.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 209
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 32
DW 4.400 usec
DE 6.50 usec
TE 300.4 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 11.20 usec
PL1 -2.50 dB
PL1W 36.62805557 W
SFO1 470.5453180 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 15.34 dB
PL2W 15.50318813 W
PL12W 0.57071728 W
SFO2 500.1320005 MHz
SI 65536
SF 470.5938919 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

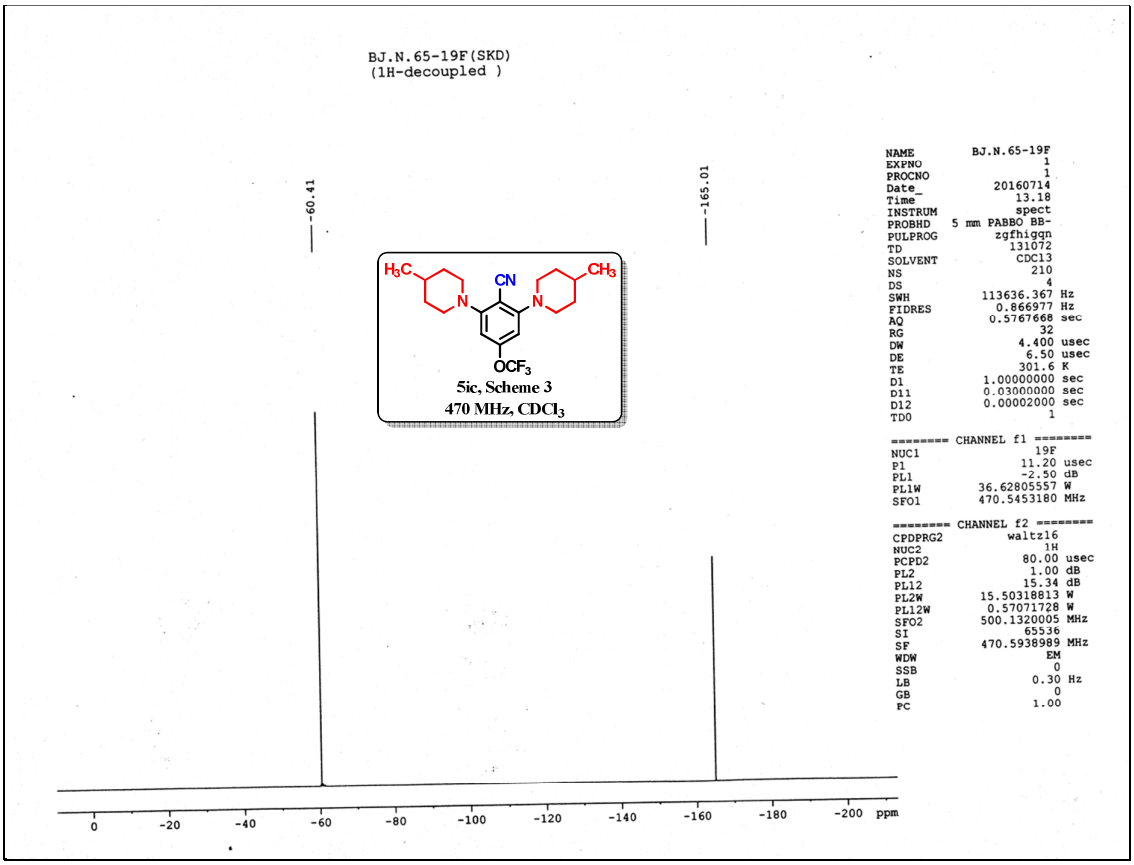

BJ.N.35-19F(SKD)
(1H-decoupled )
-60.82
-165.00
OCF3
CN
N
3ib, Scheme 2
470 MHz, CDCl3
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
NAME BJ.N.35- 19F
EXPNO 1
PROCNO 1
Date_ 20160714
Time 12.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 81
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 32
DW 4.400 usec
DE 6.50 usec
TE 300.9 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 11.20 usec
PL1 -2.50 dB
PL1W 36.62805557 W
SFO1 470.5453180 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 15.34 dB
PL2W 15.50318813 W
PL12W 0.57071728 W
SFO2 500.1320005 MHz
SI 65536
SF 470.5938732 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



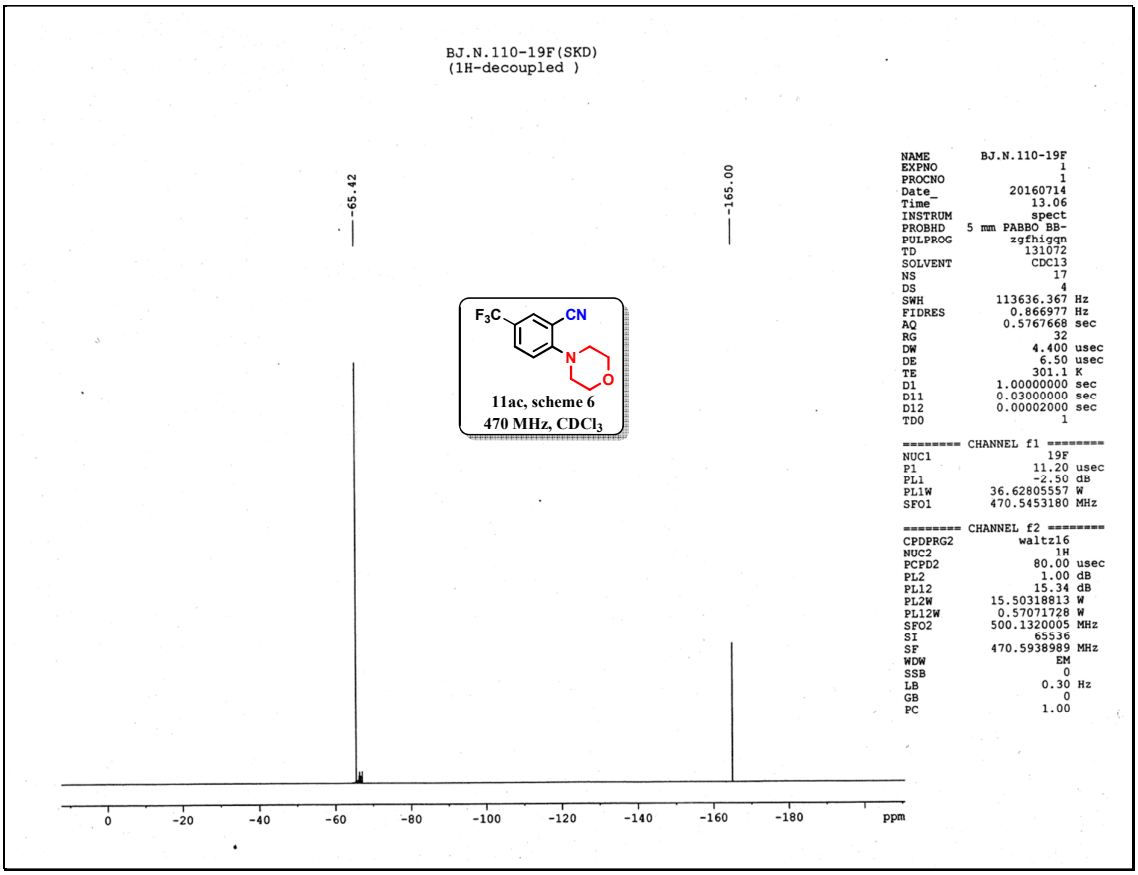

```
NAME          BJ.N.81-19F
EXPNO                   1
PROCNO                  1
Date_            20160714
Time                11.19
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                     168
DS                       4
SWH           113636.367 Hz
FIDRES          0.866977 Hz
AQ             0.5767668 sec
RG                      32
DW                4.400 usec
DE                6.50 usec
TE                300.0 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  19F
P1                11.20 usec
PL1               -2.50 dB
PL1W          36.62805557 W
SFO1          470.5453180 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                1.00 dB
PL12              15.34 dB
PL2W          15.50318813 W
PL12W          0.57071728 W
SFO2          500.1320005 MHz
SI                 65536
SF            470.5938989 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```




```
NAME          BJ.N.76 -19F
EXPNO                   1
PROCNO                  1
Date_            20160714
Time                13.01
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                     154
DS                       4
SWH           113636.367 Hz
FIDRES          0.866977 Hz
AQ             0.5767668 sec
RG                      32
DW                4.400 usec
DE                6.50 usec
TE                301.1 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  19F
P1                11.20 usec
PL1               -2.50 dB
PL1W          36.62805557 W
SFO1          470.5453180 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                1.00 dB
PL12              15.34 dB
PL2W          15.50318813 W
PL12W          0.57071728 W
SFO2          500.1320005 MHz
SI                 65536
SF            470.5938989 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```




| | |
|---|---|
| NAME | BJ.N.65-19F |
| EXPNO | 1 |
| PROCNO | 1 |
| Date_ | 20160714 |
| Time | 13.18 |
| INSTRUM | spect |
| PROBHD | 5 mm PABBO BB- |
| PULPROG | zgfhigqn |
| TD | 131072 |
| SOLVENT | CDCl3 |
| NS | 210 |
| DS | 4 |
| SWH | 113636.367 Hz |
| FIDRES | 0.866977 Hz |
| AQ | 0.5767668 sec |
| RG | 32 |
| DW | 4.400 usec |
| DE | 6.50 usec |
| TE | 301.6 K |
| D1 | 1.00000000 sec |
| D11 | 0.03000000 sec |
| D12 | 0.00002000 sec |
| TD0 | 1 |
| ======== CHANNEL f1 ======== | |
| NUC1 | 19F |
| P1 | 11.20 usec |
| PL1 | -2.50 dB |
| PL1W | 36.62805557 W |
| SFO1 | 470.5453180 MHz |
| ======== CHANNEL f2 ======== | |
| CPDPRG2 | waltz16 |
| NUC2 | 1H |
| PCPD2 | 80.00 usec |
| PL2 | 1.00 dB |
| PL12 | 15.34 dB |
| PL2W | 15.50318813 W |
| PL12W | 0.57071728 W |
| SFO2 | 500.1320005 MHz |
| SI | 65536 |
| SF | 470.5938989 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |




| | |
|---|---|
| NAME | BJ.N.110-19F |
| EXPNO | 1 |
| PROCNO | 1 |
| Date_ | 20160714 |
| Time | 13.06 |
| INSTRUM | spect |
| PROBHD | 5 mm PABBO BB- |
| PULPROG | zgfhigqn |
| TD | 131072 |
| SOLVENT | CDCl3 |
| NS | 17 |
| DS | 4 |
| SWH | 113636.367 Hz |
| FIDRES | 0.866977 Hz |
| AQ | 0.5767668 sec |
| RG | 32 |
| DW | 4.400 usec |
| DE | 6.50 usec |
| TE | 301.1 K |
| D1 | 1.00000000 sec |
| D11 | 0.03000000 sec |
| D12 | 0.00002000 sec |
| TD0 | 1 |
| ======== CHANNEL f1 ======== | |
| NUC1 | 19F |
| P1 | 11.20 usec |
| PL1 | -2.50 dB |
| PL1W | 36.62805557 W |
| SFO1 | 470.5453180 MHz |
| ======== CHANNEL f2 ======== | |
| CPDPRG2 | waltz16 |
| NUC2 | 1H |
| PCPD2 | 80.00 usec |
| PL2 | 1.00 dB |
| PL12 | 15.34 dB |
| PL2W | 15.50318813 W |
| PL12W | 0.57071728 W |
| SFO2 | 500.1320005 MHz |
| SI | 65536 |
| SF | 470.5938989 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |