Supporting Information

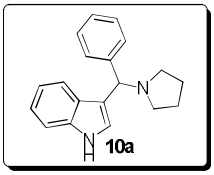
L-Proline catalysed multicomponent synthesis of 3-amino alkylated indole *via* Mannich type reaction under solvent free conditions

General Considerations.

1. Reagent grade solvents were used for extraction and flash chromatography. Whereas, HPLC grade solvent were used for HPLC. All the reagents and chemicals were purchased from Sigma–Aldrich Chemical Co, Lancaster and were used directly without further purification.The progress of reactions was checked by analytical thin-layer chromatography (TLC, Merck silica gel 60 F-254 plates). The plates were visualized first with UV illumination followed by iodine. Flash column chromatography was performed using silica gel (230-400 mesh). The solvent compositions reported for all chromatographic separations are on a volume/volume (v/v) basis. ^{1}H-NMR spectra were recorded at either 200 or 300 MHz and are reported in parts per million (ppm) on the δ scale relative to tetramethylsilane as an internal standard.^{13}C-NMR spectra were recorded at either 50 or 75 MHz and are reported in parts per million (ppm) on the δ scale relative to $CDCl_3$ (δ 77.00). Mass spectra were obtained using JEOL SX-102 (ESI) instrument. Melting points were determined on a Mel Temp II melting point apparatus and are uncorrected.

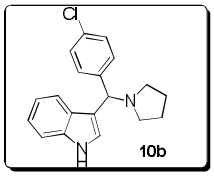
2. **General procedure for the synthesis of compound (10).** In a typical experiment, the aldehyde (1 mmol), secondry amine (1 mmol), indole (1 mmol) and L-proline (30 mol %) were taken in 25 ml round-bottom flask. the reaction mixture was stirred at room temerature till the completion of the reaction (monitored by TLC). After completion the reaction mixturewas diluted with water and extracted with ethyl acetate,dried over sodium sulphateand evoprated under vacuum to give crude product, which was purified by silica gel (230-400 mesh) coloum chromatography to afford the correponding product.

3-(phenyl(pyrrolidin-1-yl)methyl)-1H-indole (10a).



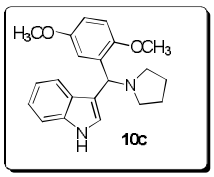
White solid; mp: 145-147 ^{0}C;^{1}H NMR (300 MHz, $CDCl_3$) δ1.75 (s, 4H), 2.51 (d, 4H, *J*=6.5 Hz), 4.59 (s, 1H), 7.04-7.15(m, 4H), 7.21-7.26 (m, 3H), 7.54 (d, 2H, *J*=7.2Hz), 7.82 (d, 1H,*J*=7.5Hz), 8.10 (br, s, 1H);**^{13}C, 50MHz ($CDCl_3$)**: 144.41, 136.08, 128.16, 127.69, 126.53, 122.0, 121.79, 119.73, 119.39, 119.30, 111.01, 67.97, 53.68, 23.51. ESIMS: m/z 276 (M+H).IR (KBr): 3417, 3063, 2824, 1494, 1392, 1213, 1164, 754 cm^{-1}; Analysis calculated for $C_{19}H_{20}N_2$: C, 82.57; H, 7.29; N, 10.14%; found: C, 82.50; H, 7.21; N, 10.05%; HRMS (ES): calculated 276.1626; found:276.1632;HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 ml/min); t_1 = 5.94 min, t_2 = 6.41 min.

3-((4-chlorophenyl)(pyrrolidin-1-yl)methyl)-1H-indole (10b).



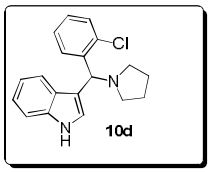
White solid; mp: 152-155 ^{0}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.76 (s, 4H), 2.51(d, 4H, *J*=5.1 Hz), 4.57 (s, 1H), 7.07-7.19 (m, 5H), 7.21-7.30(m, 1H), 7.48(d, 2H, *J*=7.1Hz), 7.78 (d, 1H, J=7.7 Hz) 8.05 (br, s, 1H); **^{13}C, 50 MHz ($CDCl_3$)**: 144.41, 136.08, 128.16, 127.69, 126.53, 122.0, 121.79, 119.73, 119.39, 119.30, 111.01, 67.97, 53.68, 23.51; ESIMS: m/z 311 (M+H).IR (KBr): 3415, 3061, 2820, 1498, 1389, 1217, 1165, 752 cm^{-1}; Analysis calculated for $C_{19}H_{19}ClN_2$: C, 73.42; H, 6.16; N, 9.01; found: C, 73.35; H, 6.08; N, 8.89 %; HRMS (ES): calculated310.1237; found: 310.1245;HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 ml/min); t_1 = 16.20 min, t_2 = 20.29 min.

3-((2,5-dimethoxyphenyl)(pyrrolidin-1-yl)methyl)-1H-indole (10c).



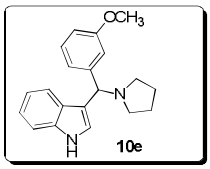
White solid; mp: 161-164 ^{0}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.75 (s, 4H), 2.57 (t, 4H, *J*= 6.4 Hz), 3.72 (s, 3H), 3.74 (s, 3H) 5.12 (s, 1H), 6.61-6.65 (m, 1H), 6.73 (d, 1H, *J*=8.8 Hz), 7.04-7.26 (m, 4H), 7.42 (d, 1H, *J*=5.7 Hz), 7.90 (d, 1H, *J*=7.2 Hz), 8.09 (br, s, 1H); **^{13}C, 50 MHz ($CDCl_3$):** 153.82, 150.80, 135.96, 133.90, 126.78, 122.36, 121.59, 120.02, 119.16, 114.40, 111.95, 111.74, 110.88, 59.10, 56.23, 55.67, 53.55, 23.57; **ESI-MS:** m/z 337 (M+H); **IR** (KBr): 3418, 3062, 2819, 1492, 1393, 1220, 1165, 750 cm^{-1}; Analysis calculated for $C_{21}H_{24}N_2O_2$: C, 74.97; H, 7.19; N, 8.33; found: C, 74.90; H, 7.11; N, 8.22%;HRMS (ES): calculated 336.1838;found:336.1829; HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 13.49 min, t_2 = 16.69 min.

3-((2-chlorophenyl)(pyrrolidin-1-yl)methyl)-1H-indole (10d).



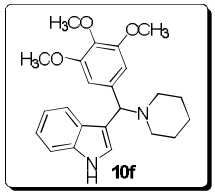
White solid; mp: 154-156 ^{0}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.72 (s, 4H), 2.53 (d, 4H,*J*=3.2 Hz), 5.15 (s, 1H), 6.98-7.23(m, 7H), 7.93(d, 2H, *J*=7.2 Hz), 8.07 (br, s, 1H); **^{13}C, 50 MHz ($CDCl_3$):** 141.25, 135.89, 132.81, 129.40, 129.33, 127.39, 126.83, 126.42, 122.83, 121.74, 119.73, 119.33, 117.75, 111.05, 62.89, 53.41, 23.47; **ESIMS**: m/z 311 (M+H); **IR** (KBr): 3415, 3061, 2821, 1490, 1398, 1209, 1164, 754 cm^{-1}; Analysis calculated for $C_{19}H_{19}ClN_2$: C, 73.42; H, 6.16; N, 9.01; found: C, 73.35; H, 6.11; N, 8.92%; HRMS (ES): calculated 310.1237;found:310.1244; HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 9.59 min, t_2 = 11.98 min.

3-((3-methoxyphenyl)(pyrrolidin-1-yl)methyl)-1H-indole (10e).



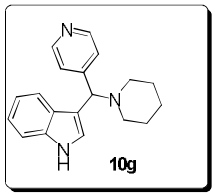
White solid; mp: 159 ^{0}C; ^{1}H, ^{1}H NMR (300 MHz, CDCl$_3$) δ 1.75 (s, 4H), 2.52 (s, 4H), 3.72 (s, 3H), 4.55 (s, 1H), 6.67-6.69 (m, 1H), 7.04-7.17 (m, 6H), 7.24 (d, 1H, J=7.5 Hz), 7.84 (d, 1H, *J*=7.4 Hz), 8.17 (br, s, 1H); **^{13}C, 50 MHz (CDCl$_3$)**: 159.47, 146.02, 136.08, 129.08, 126.50, 122.09, 121.76, 120.17, 119.70, 119.29, 119.21, 113.45, 111.73, 111.05, 67.94, 55.09, 53.67, 23.51 ; **ESIMS**: m/z 307 (M+H); IR (KBr): 3411, 3059, 2822, 1491, 1395, 1211, 1166, 751 cm^{-1}; Analysis calculated for $C_{20}H_{22}N_2O$: C, 78.40; H, 7.24; N, 9.14; found: C, 78.36; H, 7.20; N, 9.08%. HRMS (ES): calculated 306.1732;found:306.1724; HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 16.49 min, t_2 = 21.07 min.

3-(piperidin-1-yl(3,4,5-trimethoxyphenyl)methyl)-1H-indole (10f).



White solid; mp: 112-115 ^{0}C, ^{1}H NMR (300 MHz, CDCl$_3$) δ 1.42 (s, 2H), 1.56 (s, 4H), 1.24, (s, 4H), 3.78 (s, 9H), 4.58 (s, 1H), 6.78(s, 2H), 7.03-7.14 (m, 3H), 7.29 (d, 1H, *J*= 7.2 Hz), 7.85 (d, 1H,*J*= 7.0 Hz), 8.32 (br, s, 1H);**^{13}C, 50 MHz (CDCl$_3$):** 152.78, 139.32, 136.32, 136.22, 126.98, 123.03, 121.71, 120.26, 119.17, 117.18, 111.12, 104.88, 68.59, 60.72, 55.95, 52.80, 26.32, 24.68; **ESIMS**: m/z 381 (M+H); **IR** (KBr): 3413, 3062, 2820, 1495, 1397, 1218, 1161, 758 cm^{-1}; Analysis calculated for $C_{23}H_{28}N_2O_3$: C, 72.60; H, 7.42; N, 7.36%; found: C, 72.54; H, 7.38; N, 7.29%. HRMS (ES): calculated 380.2100;found:380.2109; HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 7.20 min, t_2 = 7.95 min.

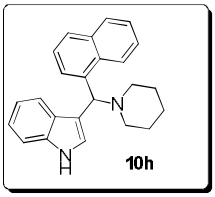
3-(piperidin-1-yl(pyridin-4-yl)methyl)-1H-indole (10g).



White solid; mp: 135-137 ^{0}C; ^{1}H NMR (300 MHz, CDCl$_3$) δ 1.54-1.61 (m, 6H), 2.37-2.46 (m, 4H), 4.68 (s, 1H), 7.03-7.31(m, 4H), 7.46 (d, 2H, *J*= 5.7 Hz), 7.73 (d, 1H, *J*=7.7Hz), 8.48 (d, 2H, *J*=5.9 Hz), 8.94 (br, s, 1H); **^{13}C, 50 MHz (CDCl$_3$):** 152.69, 149.38, 136.43, 126.65, 123.57, 123.40, 123.22, 121.93, 120.09, 119.40, 115.26, 111.23, 67.51, 52.62, 26.26, 24.53; **ESIMS**: m/z 292 (M+H); **IR** (KBr): 3420, 3069, 2829, 1489, 1393, 1217, 1158, 748 cm^{-1}; Analysis calculated for $C_{19}H_{21}N_3$:

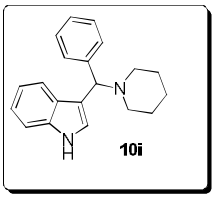
C, 78.32; H, 7.26; N, 14.42; found: C, 78.25; H, 7.19; N, 14.33%; HRMS (ES): calculated 291.1735;found:291.1722; HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 6.75 min, t_2 = 7.84 min.

3-(naphthalen-1-yl(piperidin-1-yl)methyl)-1H-indole(10h).



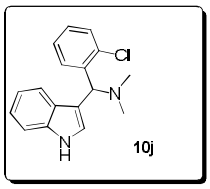
White solid; mp: 119-121 ^{0}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.42-1.46 (m, 2H), 1.54 (s, 4H), 2.50 (d, 4H, *J*= 4.9 Hz), 5.08 (s, 1H), 7.09-7.16(m, 3H), 7.33-7.36 (m, 2H), 7.67 (d, 1H, *J*=8.1Hz), 7.74-7.90 (m, 4H), 8.05 (d, 1H, *J*= 8.2 Hz), 8.37 (br, s, 1H); **^{13}C NMR (50 MHz, $CDCl_3$):** 137.32, 134.39, 132.55, 130.91, 130.50, 129.37, 128.84, 127.96, 127.49, 127.26, 127.00, 126.74, 126.59, 122.12, 121.14, 115.51, 113.48, 72.18, 51.09, 24.68, 23.42; **ESIMS**: m/z 341 (M+H); **IR** (KBr): 3419, 3059, 2820, 1509, 1392, 1213, 1163, 754 cm^{-1}; Analysis calculated for $C_{24}H_{24}N_2$: C, 84.67; H, 7.11; N, 8.23; found: C, 84.61; H, 7.04; N, 8.18%; HRMS (ES): calculated 340.1939;found340.1948; HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 11.00 min, t_2 = 18.01 min.

3-(phenyl(piperidin-1-yl)methyl)-1H-indole (10i).



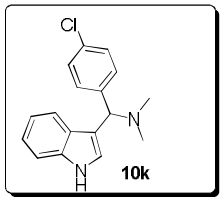
White solid; mp: 112 ^{0}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.38 (s, 2H), 1.54 (s, 4H), 2.40 (s, 4H), 4.65 (s, 1H), 6.92 (d, 2H, *J*= 7.5Hz), 7.21-7.46 (m, 7H),7.76 (br, s, 1H), 7.92 (br, s, 1H); **^{13}C, 50 MHz ($CDCl_3$):** 142.97, 136.49, 136.18, 128.10, 128.04, 126.45, 122.85, 121.71, 120.25, 119.19, 117.44, 111.01, 68.58, 52.83, 26.24, 24.66; **ESIMS**: m/z 291 (M+H); **IR** (KBr): 3400, 3066, 2821, 1493, 1395, 1219, 1164, 753 cm^{-1}; Analysis calculated for $C_{20}H_{22}N_2$: C, 82.72; H, 7.64; N, 9.65; found: C, 82.60; H, 7.54; N, 9.59%; HRMS (ES): calculated 290.1783;found:290.1791; HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 10.99 min, t_2 = 18.61 min.

1-(2-chlorophenyl)-1-(1H-indol-3-yl)-N,N-dimethylmethanamine(10j).



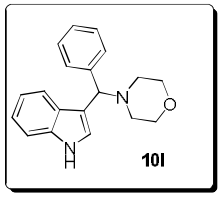
White solid; mp: 85-87 ^{0}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.27 (s, 6H), 5.05 (s, 1H), 7.03-7.26 (m, 7H), 7.87(br, s, 2H), 8.19 (br, s, 1H); **^{13}C, 50 MHz ($CDCl_3$):** 137.32, 136.89, 133.97, 132.19, 130.41, 130.30, 128.35, 127.71, 127.00, 122.13, 121.14, 120.14, 115.97, 113.48, 73.71, 41.64. **ESIMS**: m/z 285 (M+H); **IR** (KBr): 3410, 3065, 2819, 1494, 1391, 1220, 1161, 757 cm^{-1}; Analysis calculated for $C_{17}H_{17}ClN_2$: C, 71.70; H, 6.02; N, 9.84%; found: C, 71.64; H, 5.91; N, 9.77%; HRMS (ES): calculated 284.1080;found:284.1071; HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 7.13 min, t_2 = 8.21 min.

1-(4-chlorophenyl)-1-(1H-indol-3-yl)-N,N-dimethylmethanamine(10k).



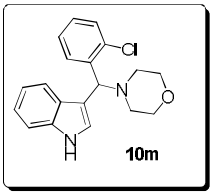
White solid; mp: 89-91 ^{0}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.25 (s, 6H), 4.53 (s, 1H), 7.09-7.44 (m, 8H), 7.68 (d, 1H, *J*=7.7 Hz), 8.13 (br, s, 1H);**^{13}C, 50 MHz ($CDCl_3$):** 137.32, 135.47, 133.18, 131.15., 131.01, 129.66, 129.45, 128.11, 127.00, 122.13, 121.14, 120.14, 115.35, 113.48, 74.27, 41.64; **ESIMS**: m/z 285(M+H); **IR** (KBr): 3415, 3060, 2822, 1497, 1395, 1215, 1165, 753 cm^{-1}; Analysis calculated for $C_{17}H_{17}ClN_2$: C, 71.70; H, 6.02; N, 9.84%; found: C, 71.62; H, 5.91; N, 9.77%; HRMS (ES): calculated 284.1080;found:284.1086; HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 6.65 min, t_2 = 8.43 min.

4-((1H-indol-3-yl)(phenyl)methyl)morpholine(10l).



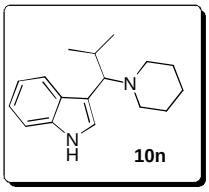
White solid; mp: 129-130 ^{0}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.44 (s, 4H), 3.67-3.68(m, 4H), 4.58(s, 1H), 6.94 (s, 1H), 7.08-7.23 (m, 6H), 7.51 (d, 2H, *J*=6.8Hz), 7.88 (d, 1H, *J*=6.2Hz) 8.11(br, s, 1H);**^{13}C, 50 MHz:** 142.49, 136.30, 128.25, 127.98, 126.71, 126.43, 122.82, 121.87, 120.10, 119.38, 116.82, 111.11, 68.76, 67.24, 52.37; **ESIMS**: m/z 293 (M+H); **IR** (KBr): 3420, 3060, 2821, 1490, 1391, 1212, 1161, 750 cm^{-1}; Analysis calculated for $C_{19}H_{20}N_2O$: C, 78.05; H, 6.89; N, 9.58%; found: C, 78.01; H, 6.81; N, 9.47%; HRMS (ES): calculated 292.1576;found:292.1584; HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 6.60 min, t_2 = 8.10 min.

4-((2-chlorophenyl)(1H-indol-3-yl)methyl)morpholine(10m).



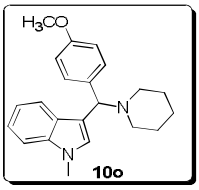
White solid; mp: 134-139 ^{0}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.44 (s, 4H), 3.66 (s, 4H), 5.11 (s, 1H), 7.01-7.15 (m, 7H), 7.94 (s, 2H), 8.12 (br, s, 1H); **^{13}C, 50 MHz ($CDCl_3$):** 139.74, 136.14, 133.69, 129.57, 128.87, 127.53, 126.79, 126.23, 123.53, 121.87, 120.09, 119.47, 115.15, 111.16, 67.17, 63.73,52.32; **ESIMS**: m/z 327 (M+H); **IR** (KBr): 3415, 3061, 2822, 1492, 1389, 1214, 1164, 749 cm^{-1}; Analysis calculated for $C_{19}H_{19}ClN_2O$: C, 69.83; H, 5.86; N, 8.57;found: C, 69.77; H, 5.75; N, 8.51%; HRMS (ES): calculated 326.1186;found:326.1172;HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 6.67 min, t_2 = 8.28 min.

3-(2-methyl-1-(piperidin-1-yl)propyl)-1H-indole (10n).



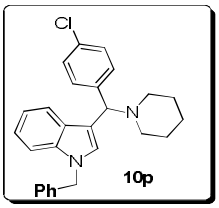
White solid; mp: 87-89 ^{0}C; ^{1}H NMR(200 MHz, $CDCl_3$) δ 0.75 (s, 3H), 0.82 (s, 3H), 1.29-1.48(m, 6H), 1.96-2.23 (m, 3H), 2.23-2.51 (m, 2H), 3.45 (d, 1H, *J*=9.6 Hz), 6.65(s, 1H), 6.77-7.08 (m, 5H); **^{13}C, 50 MHz ($CDCl_3$):** 137.16, 130.64, 127.69, 121.57, 120.67, 118.80, 112.41, 109.39, 68.92, 51.46, 30.13, 27.09, 25.32, 21.51, 20.90; **ESIMS**: m/z 257 (M+H); **IR** (KBr): 3417, 3063, 2830, 1491, 1397, 1211, 1161, 753 cm^{-1}; Analysis calculated for $C_{17}H_{24}N_2$: C, 79.64; H, 9.44; N, 10.93%; found: C, 79.58; H, 9.36; N, 10.81%, HRMS (ES): calculated 256.1939; found:256.1947;HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 4.93 min, t_2 = 5.74 min.

3-((4-methoxyphenyl)(piperidin-1-yl)methyl)-1-methyl-1H-indole (10o).



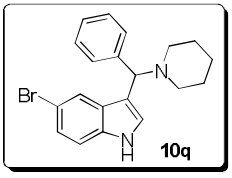
White solid; mp: 124 ^{0}C; ^{1}H NMR (200 MHz, $CDCl_3$) δ 0.84-1.07 (m, 6H), 1.65-1.79 (m, 2H), 1.98-2.11 (m, 2H), 3.06 (s, 3H), 3.13 (s, 3H), 4.58 (s, 1H), 6.16-6.25 (2H), 6.57-6.75 (m, 6H),7.37-7.58 (m, 1H).; **^{13}C, 50 MHz ($CDCl_3$):** 159.99, 139.88, 139.69, 130.17, 130.07, 124.77, 122.15, 113.86, 112.84, 112.51, 111.74, 71.94, 56.03, 51.09, 35.89, 24.68, 23.42; **ESIMS**: m/z 335(M+H). **IR** (KBr): 3058, 2821, 1492, 1397, 1213, 1161, 759 cm^{-1}; Analysis calculated for $C_{22}H_{26}N_2O$: C, 79.00; H, 7.84; N, 8.38; found: C, 69.89; H, 7.76; N, 8.31%; HRMS (ES): calculated 334.2045;found:334.2059;HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 4.98 min, t_2 = 5.77 min.

1-benzyl-3-((4-chlorophenyl)(piperidin-1-yl)methyl)-1H-indole (10p).



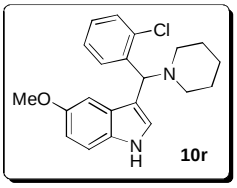
White solid; mp: 155-157 ^{0}C; ^{1}H NMR (200 MHz, $CDCl_3$) δ 0.86-1.14 (m, 6H), 1.67-1.81 (m, 2H), 1.98-2.11 (m, 2H), 4.46 (s, 2H), 4.58 (s, 1H), 6.49-6.76 (m, 11H), 6.79-6.92 (m, 1H), 7.07 (s, 1H), 7.26-7.37 (m, 1H); **^{13}C, 50 MHz ($CDCl_3$):** 139.88, 139.77, 137.46, 135.62, 133.20, 131.43, 131.28, 129.35, 129.19, 128.67, 128.59, 128.47, 128.35, 127.73, 123.82, 123.51, 121.86, 113.99,112.71, 71.94, 52.88, 24.68, 23.42;**ESIMS**: m/z 415 (M+H); **IR** (KBr): 3048, 2883, 2951, 2790, 1395, 1217, 1166, 754 cm^{-1}; Analysis calculated for $C_{27}H_{27}ClN_2$: C, 78.15; H, 6.56; N, 6.75%; found: C, 78.05; H, 6.42; N, 6.66%; HRMS (ES): calculated 414.1863;found:414.1871;HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 19.02 min, t_2 = 22.09 min.

5-bromo-3-(phenyl(piperidin-1-yl)methyl)-1H-indole (10q).



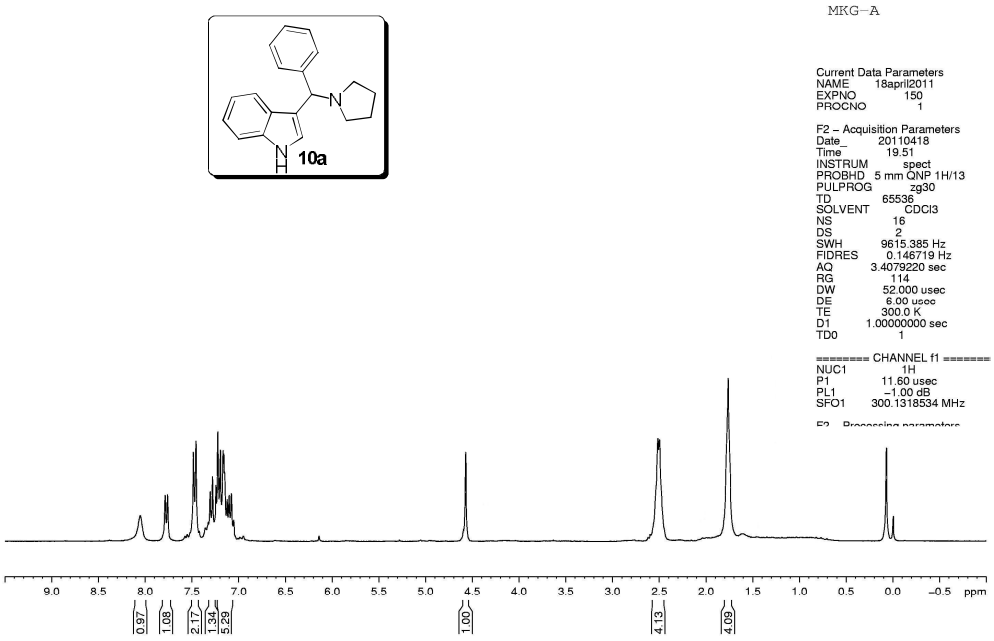
White solid; mp: 89 ^{0}C; ^{1}H NMR (200 MHz, $CDCl_3$) δ 1.12-1.48 (m, 6H), 2.00-2.18 (m, 2H), 2.21-2.39 (m, 2H), 4.88 (s, 1H), 6.65 (s, 1H), 6.83 (s, 4H), 6.93-7.13 (m, 4H);**^{13}C, 50 MHz ($CDCl_3$):** 137.66, 136.73, 129.78, 129.63, 128.91, 128.27, 127.34, 127.02, 124.28, 123.14, 116.52, 115.13, 113.99, 72.58, 51.09, 24.68, 23.42; **ESIMS**: m/z 369 (M+H). **IR** (KBr): 3413, 3062, 2821, 1490, 1392, 1210, 1165, 752 cm^{-1}; Analysis calculated for $C_{20}H_{21}BrN_2$: C, 65.05; H, 5.73; N, 7.59%; found: C, 64.94; H, 5.67; N, 7.50%; HRMS (ES): calculated 368.0888;found:368.0895; HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 17.57 min, t_2 = 21.33 min.

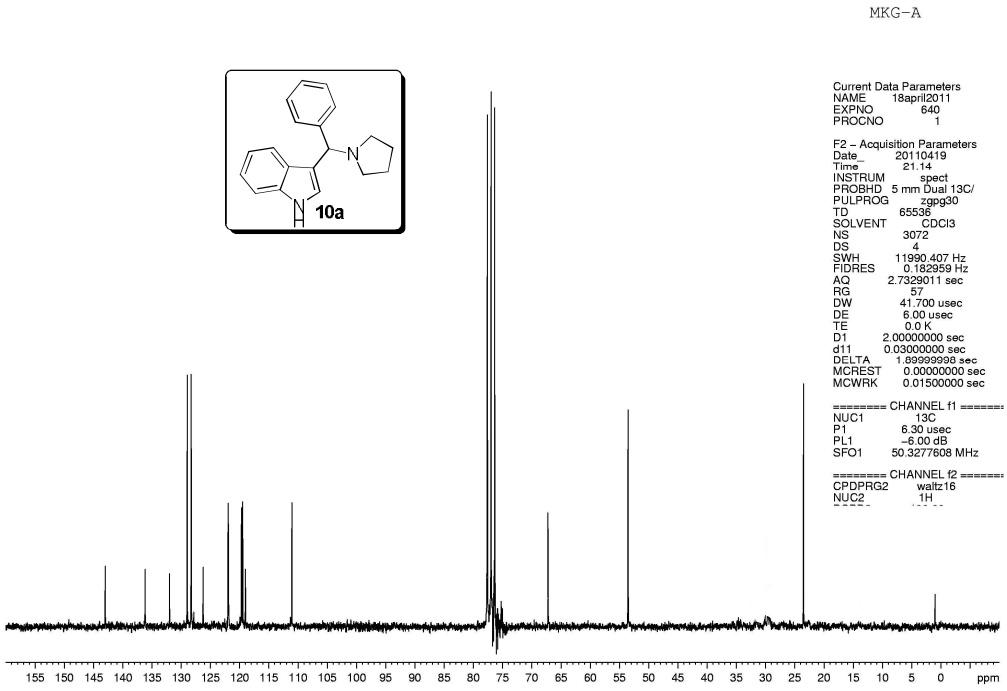
3-((2-chlorophenyl)(piperidin-1-yl)methyl)-5-methoxy-1H-indole (10r).



White solid; mp: 109-113 ^{0}C; ^{1}H NMR (200 MHz, $CDCl_3$) δ 0.93-1.14 (m, 6H),1.71-1.82 (m, 2H), 1.89-2.07 (m, 2H), 4.58 (s, 1H), 6.21 (s, 1H), 6.41-6.55 (m, 5H), 6.58-6.87 (m, 2H), 7.12 (d, 1H, *J*= 3.3Hz); **^{13}C, 50 MHz ($CDCl_3$):** 153.94, 134.05, 132.49, 132.45, 130.46, 130.02, 127.34, 127.28, 125.97, 114.52, 113.36, 113.29, 103.83, 71.28, 56.03, 51.03, 24.68, 23.42;**ESIMS**: m/z 355 (M+H); **IR** (KBr): 3419, 3061, 2829, 1489, 1392, 1212, 1160, 749 cm^{-1}; Analysis calculated for $C_{21}H_{23}ClN_2O$: C, 71.07; H, 6.53; N, 7.89%; found: C, 71.01; H, 6.48; N, 7.78%; HRMS (ES): calculated

354.1499;found:354.1483; HPLC analysis by using a Chiralpak IA column (25 ^{0}C, 254 nm, 4:1 hexane/2-propanol, 0.7 mL/min); t_1 = 15.13 min, t_2 = 18.28 min.




MKG-A
10a
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NAME 18april2011
EXPNO 640
PROCNO 1
F2 – Acquisition Parameters
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Time 21.14
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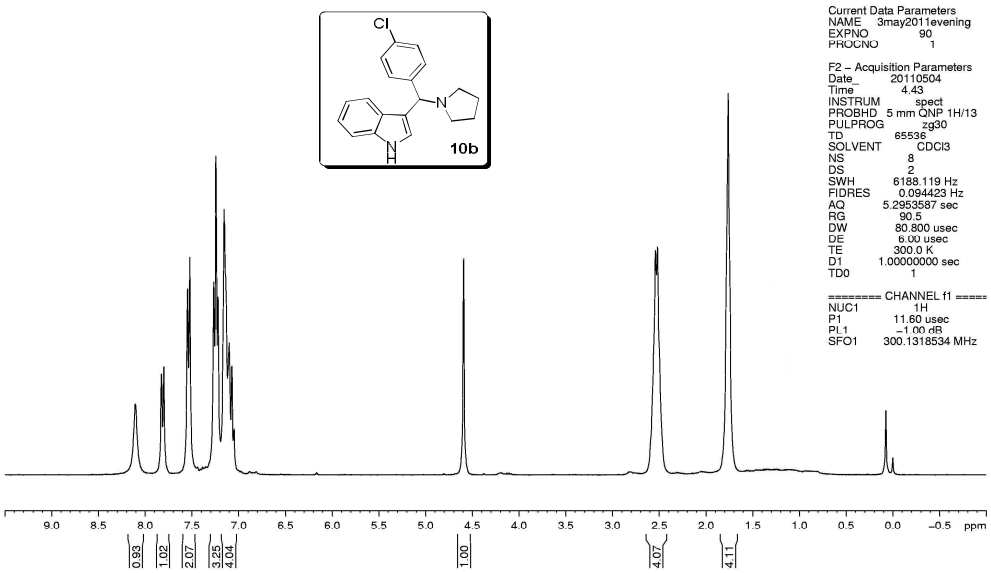
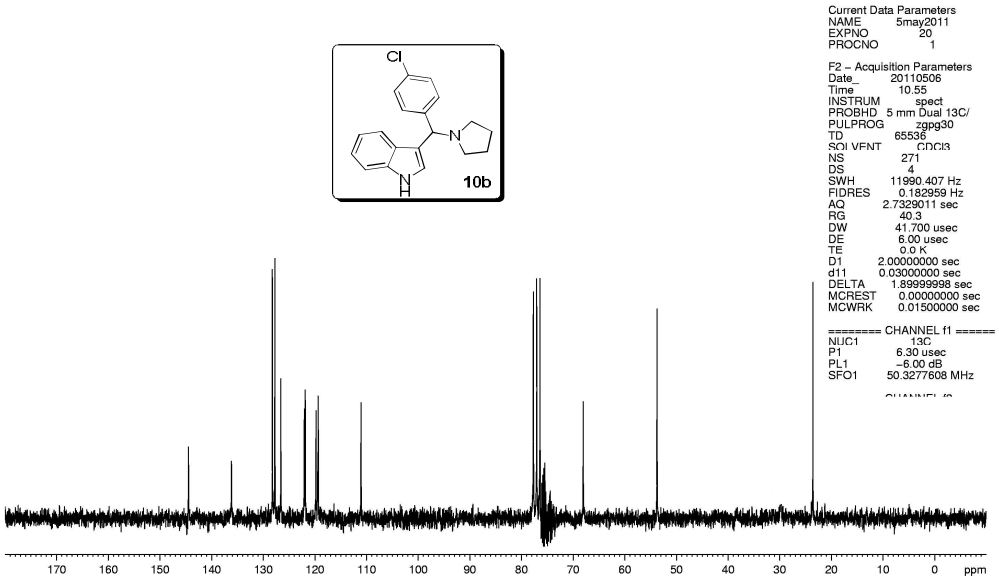
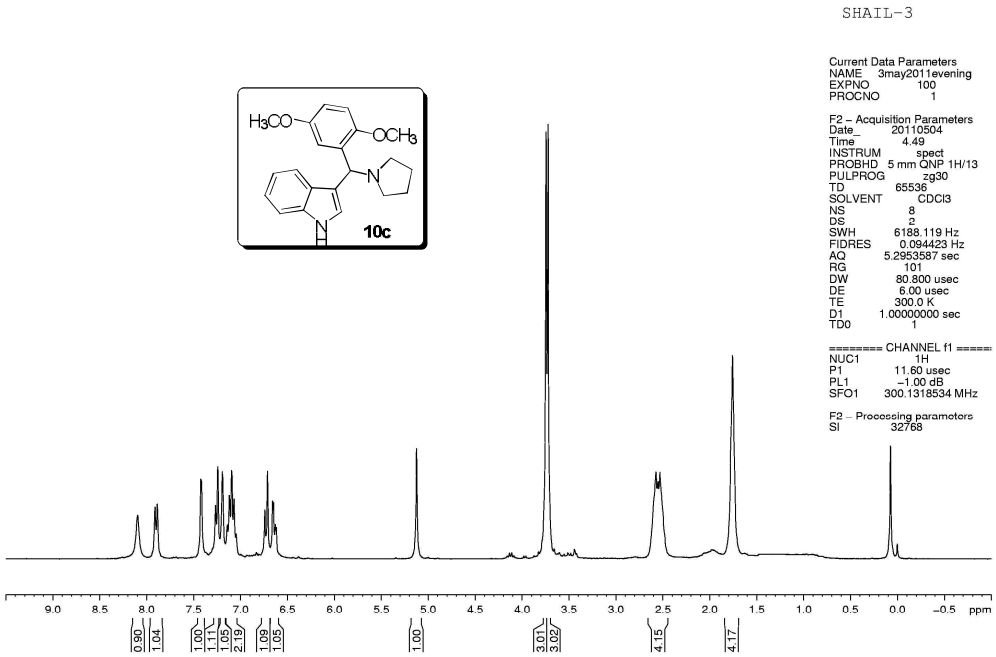
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 11990.407 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 57
DW 41.700 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.30 usec
PL1 -6.00 dB
SFO1 50.3277608 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 ppm

SHAIL-2

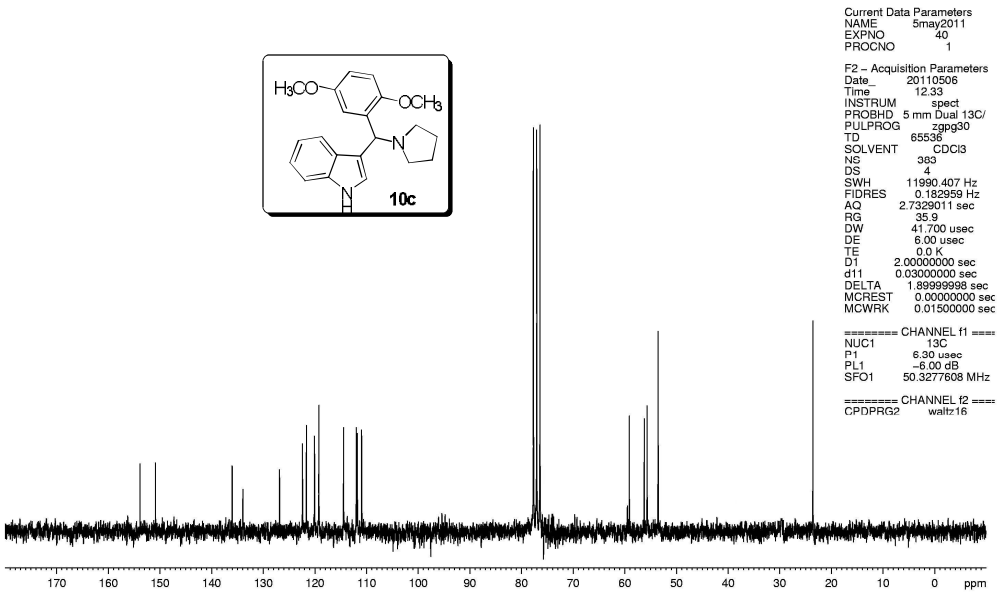


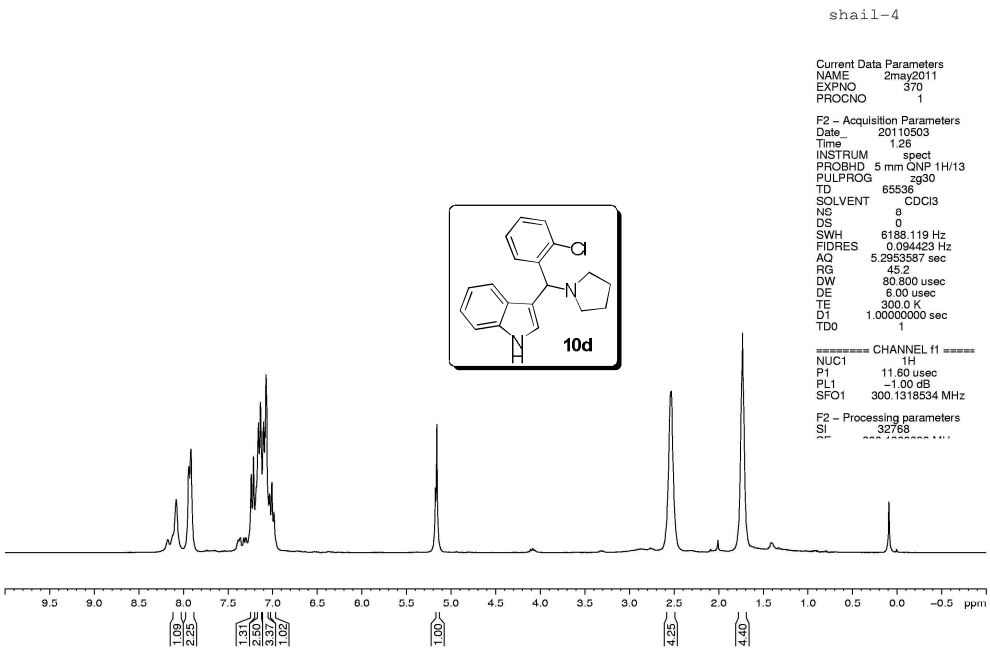
SHAIL-2

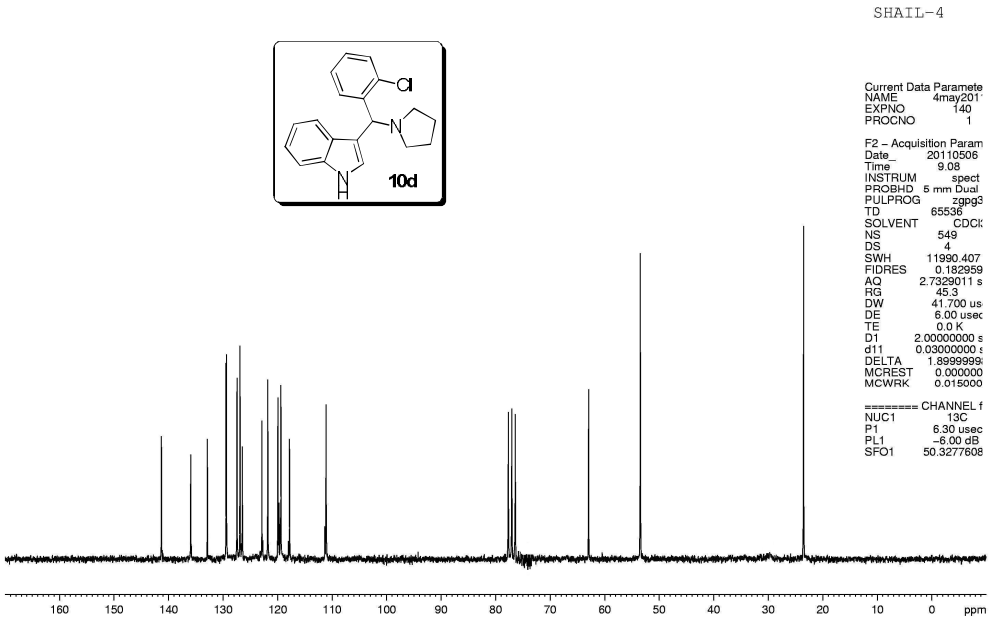




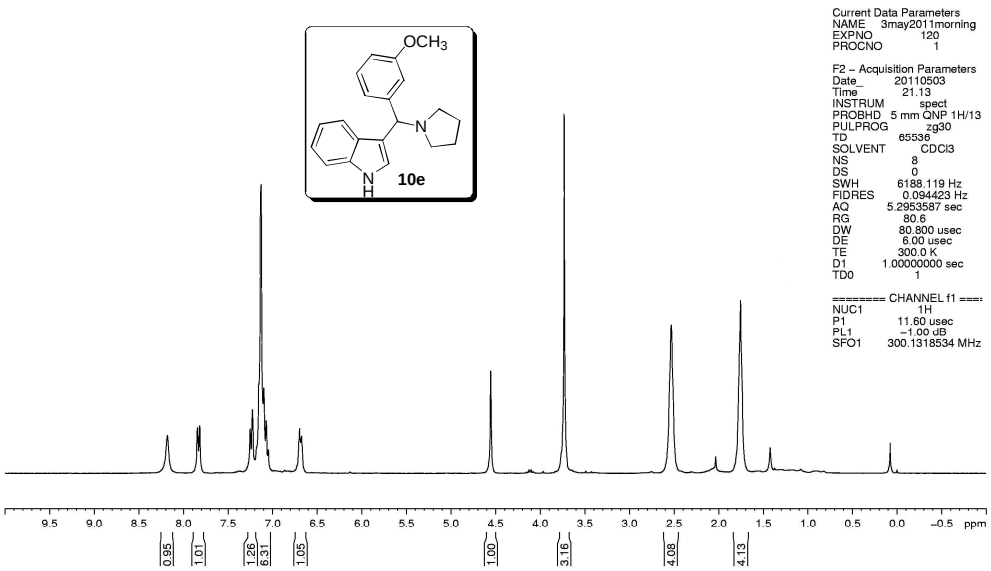
SHAIL-3

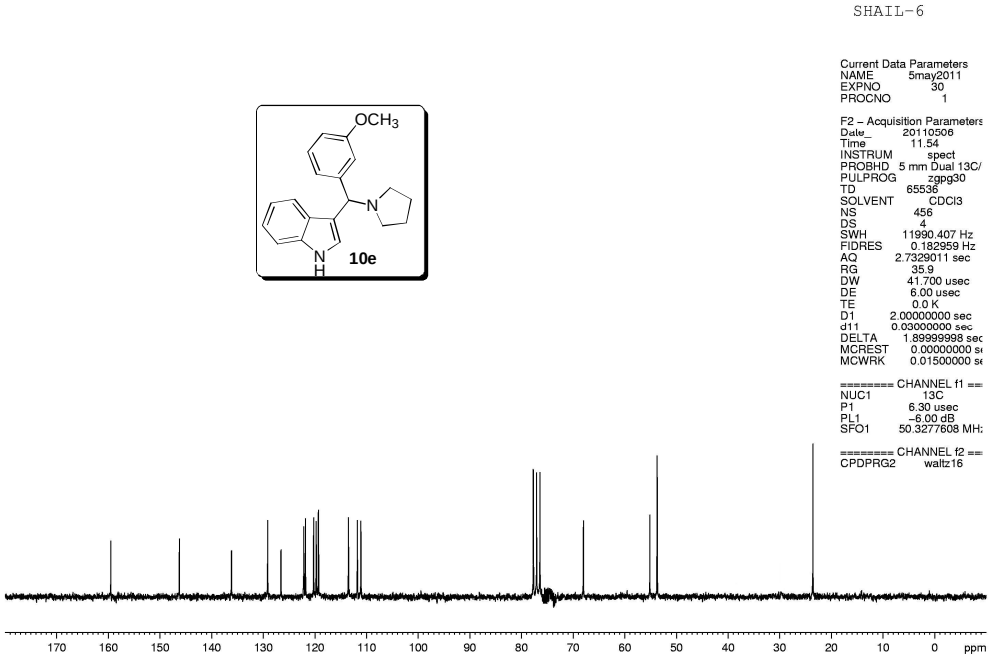


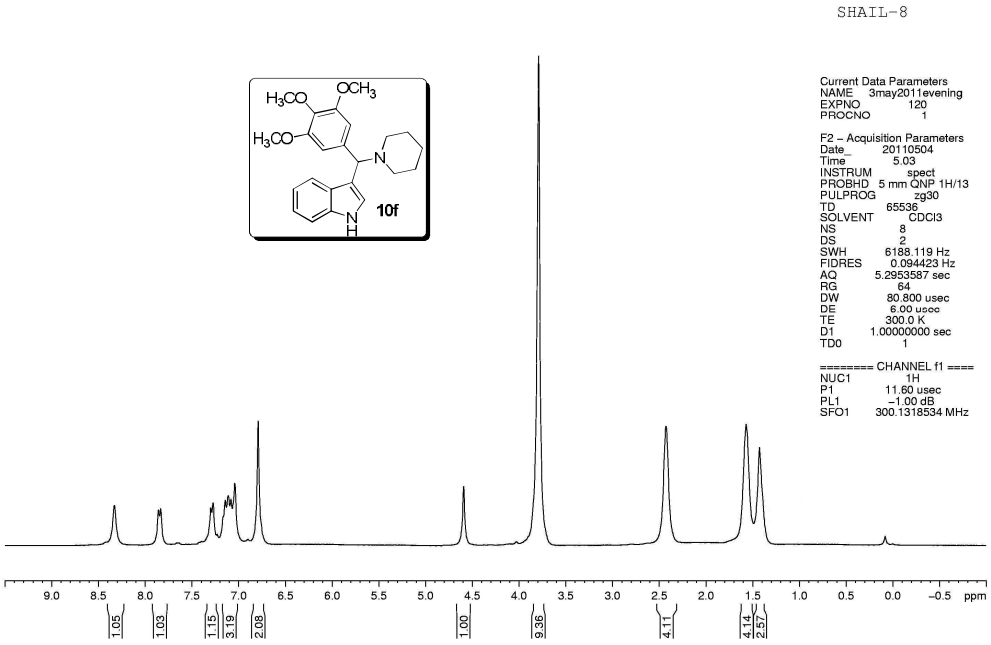




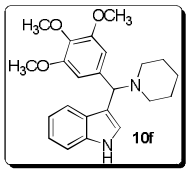
SHAIL-6


OCH3
N
N
H
10e
Current Data Parameters
NAME 3may2011morning
EXPNO 120
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110503
Time 21.13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 80.6
DW 80.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ====
NUC1 1H
P1 11.60 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz
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
0.95
1.01
1.26
6.31
1.05
1.00
3.16
4.08
4.13




SHAIL-8
10f
Current Data Parameters
NAME 3may2011evening
EXPNO 120
PROCNO 1
F2 – Acquisition Parameters
Date_ 20110504
Time 5.03
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 64
DW 80.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ====
NUC1 1H
P1 11.60 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz
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
1.05 1.03 1.15 3.19 2.08 1.00 9.36 4.11 4.14 2.57

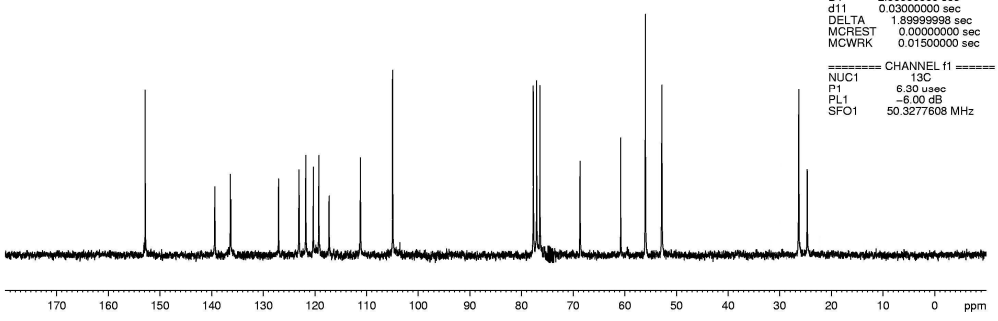
SHAIL-8

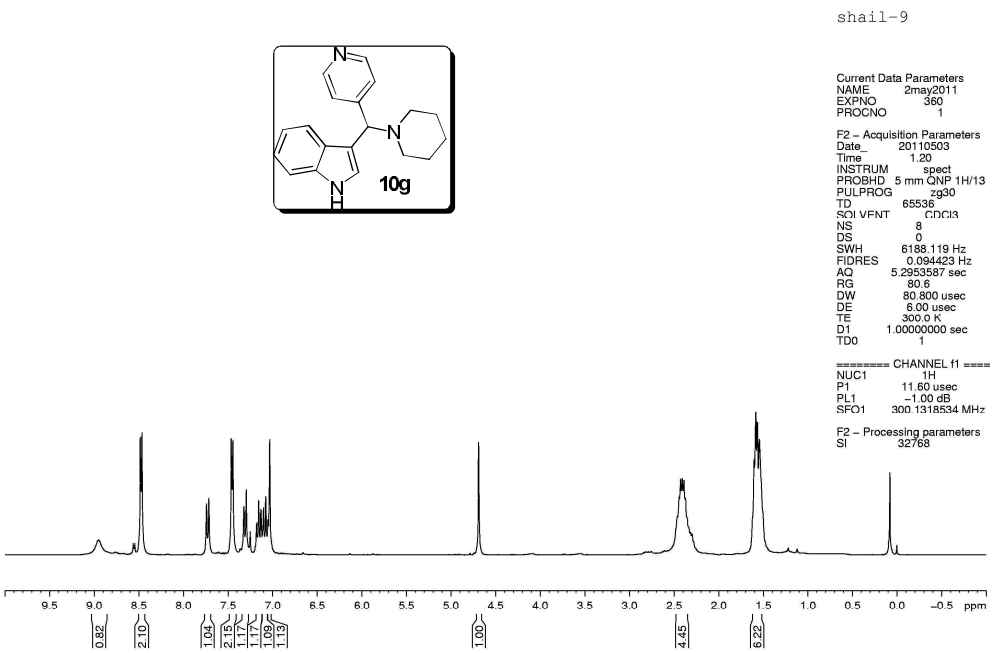


Current Data Parameters
NAME 5may2011
EXPNO 50
PROCNO 1

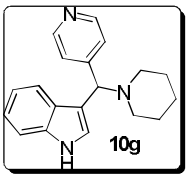
F2 – Acquisition Parameters
Date_ 20110506
Time 13.00
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 782
DS 4
SWH 11990.407 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 64
DW 41.700 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ======
NUC1 13C
P1 6.30 usec
PL1 -6.00 dB
SFO1 50.3277608 MHz





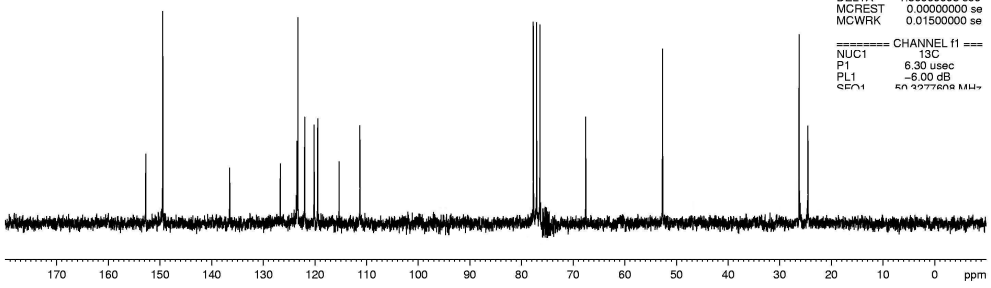
SHAIL-9



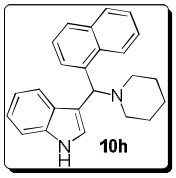
Current Data Parameters
NAME 4may2011
EXPNO 150
PROCNO 1

F2 – Acquisition Parameters
Date_ 20110506
Time 9.33
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 255
DS 4
SWH 11990.407 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 71.8
DW 41.700 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 se
MCWRK 0.01500000 se

======== CHANNEL f1 ===
NUC1 13C
P1 6.30 usec
PL1 –6.00 dB
SFO1 50.3277608 MHz



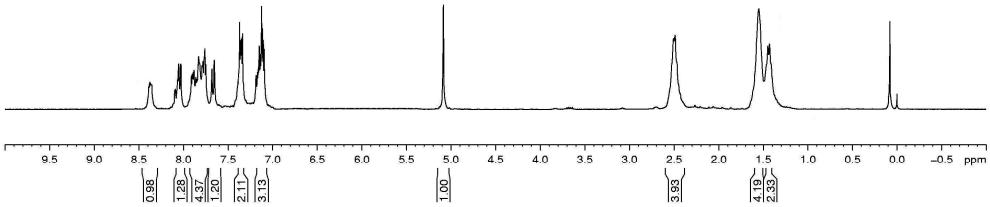
SHAIL-10

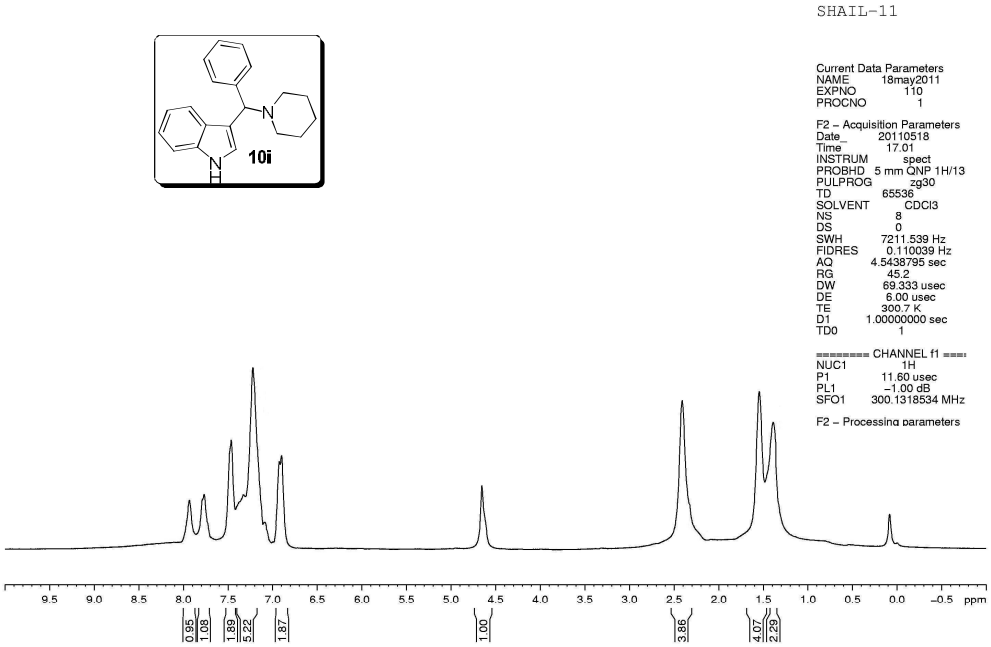


Current Data Parameters
NAME 11may2011
EXPNO 70
PROCNO 1

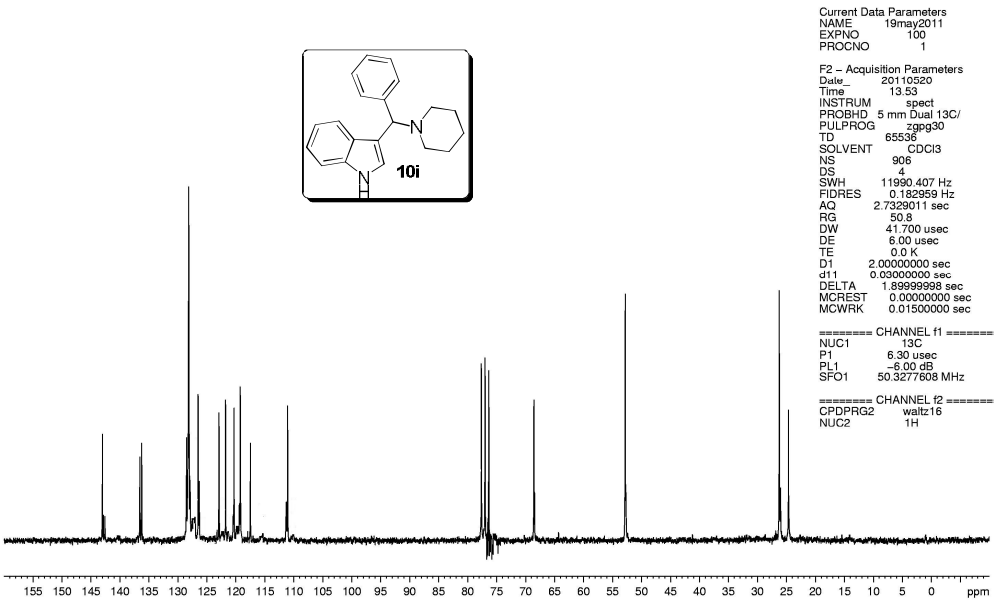
F2 – Acquisition Paramet
Date_ 20110511
Time 22.51
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6188.119 Hz
FIDRES 0.094423 H
AQ 5.2953587 sec
RG 57
DW 80.800 usec
DE 6.00 usec
TE 298.4 K
D1 1.00000000 sec
TD0 1

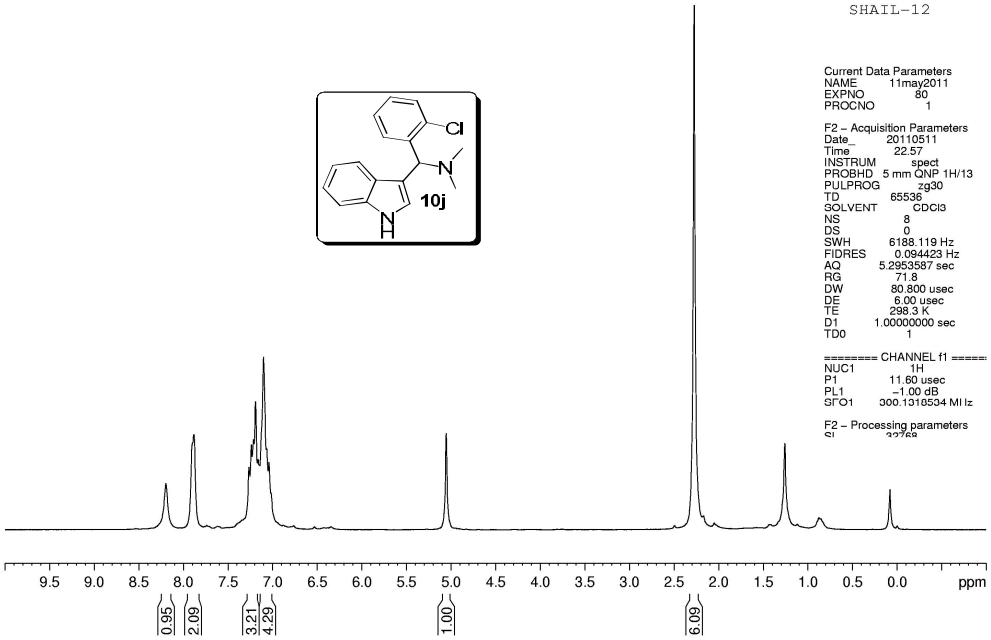
======== CHANNEL f1 =
NUC1 1H
P1 11.60 usec
PL1 –1.00 dB
SFO1 300.1318534 M

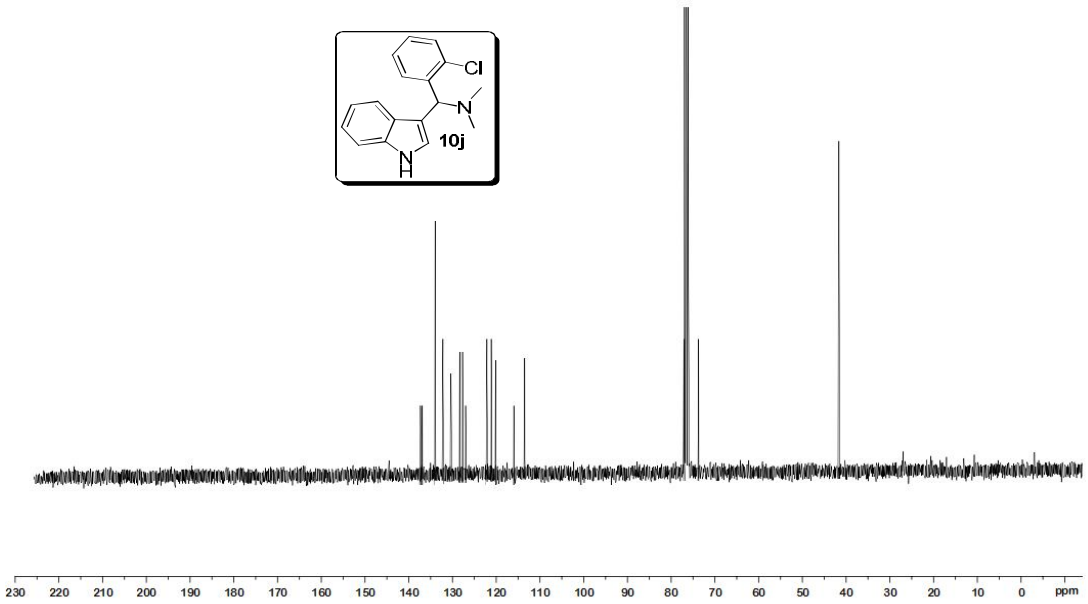




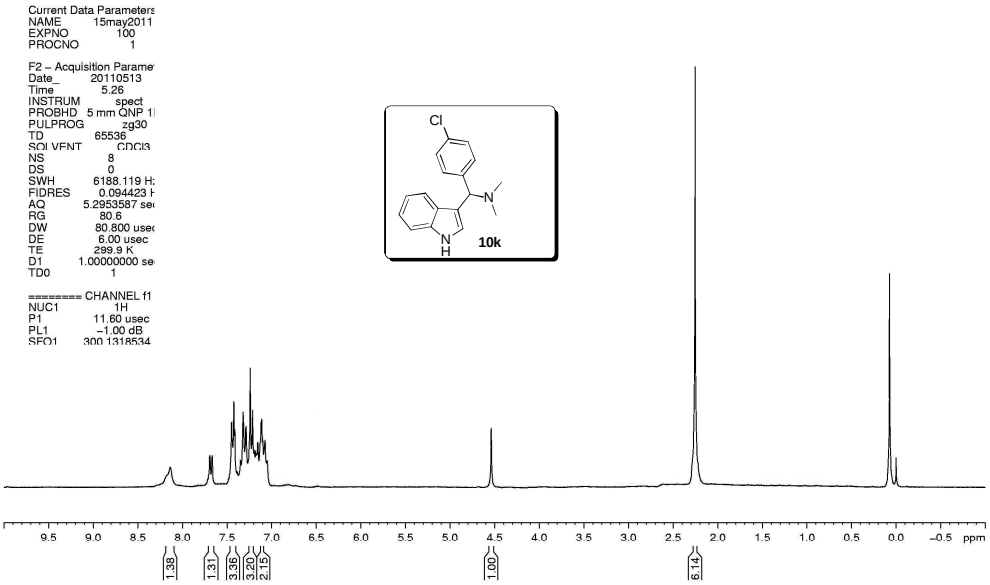
SHAIL-11



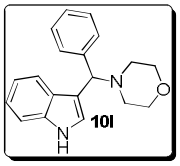




SHAIL-15



SHAIL-18



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NAME 18may2011
EXPNO 40
PROCNO 1

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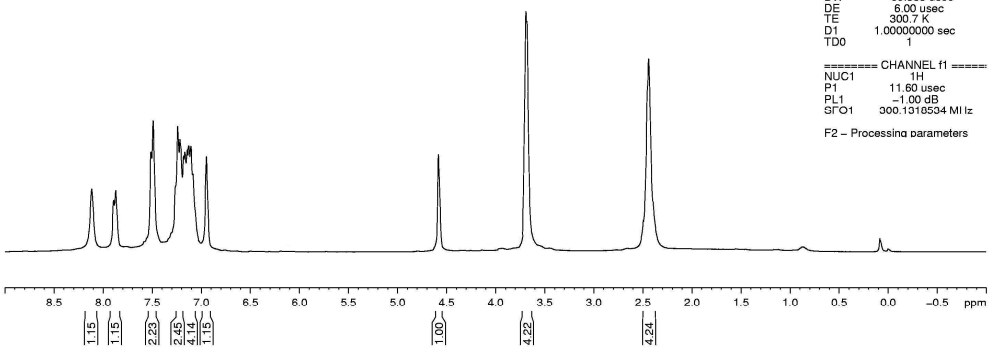
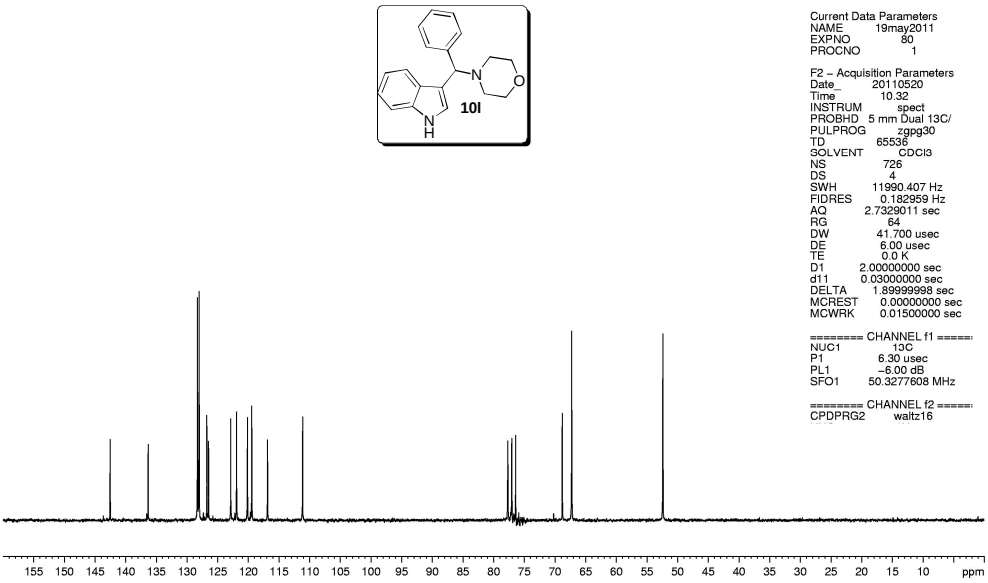
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 7211.539 Hz
FIDRES 0.110039 Hz
AQ 4.5438795 sec
RG 57
DW 69.333 usec
DE 6.00 usec
TE 300.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ======
NUC1 1H
P1 11.60 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz

F2 – Processing parameters



Sahil-18


10l
Current Data Parameters
NAME 19may2011
EXPNO 80
PROCNO 1
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Time 10.32
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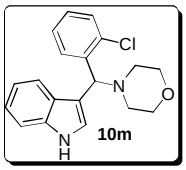
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 726
DS 4
SWH 11990.407 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 64
DW 41.700 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ======
NUC1 13C
P1 6.30 usec
PL1 -6.00 dB
SFO1 50.3277608 MHz
======== CHANNEL f2 ======
CPDPRG2 waltz16
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 ppm

SHAIL-19

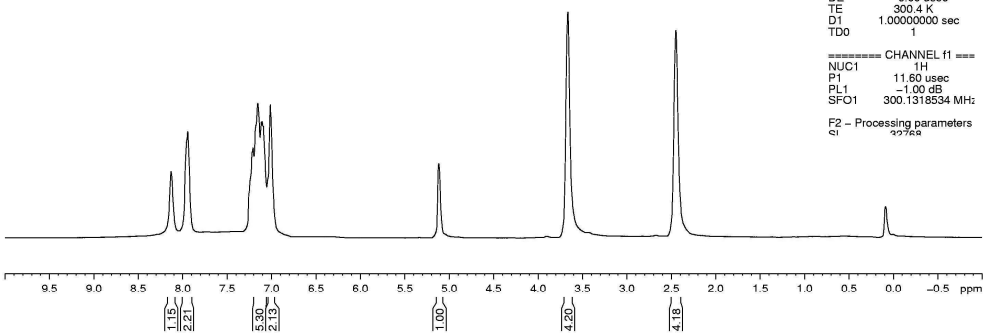


Current Data Parameters
NAME 18may2011
EXPNO 50
PROCNO 1

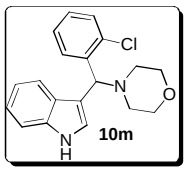
F2 – Acquisition Parameters
Date_ 20110518
Time 16.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 7211.539 Hz
FIDRES 0.110039 Hz
AQ 4.5438795 sec
RG 50.8
DW 69.333 usec
DE 6.00 usec
TE 300.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ===
NUC1 1H
P1 11.60 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz

F2 – Processing parameters



Shail-19

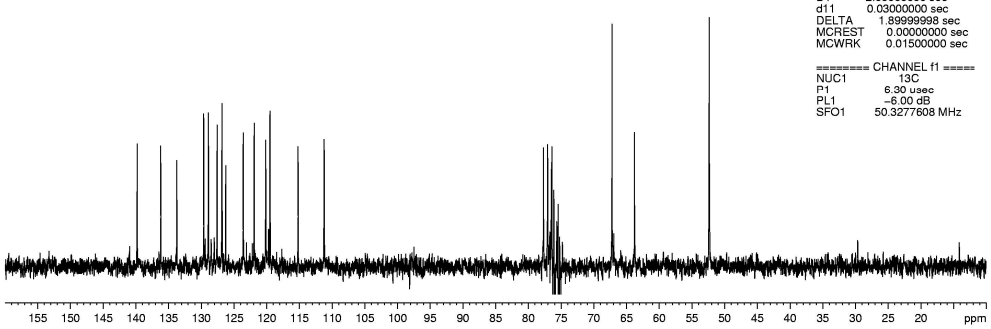


10m

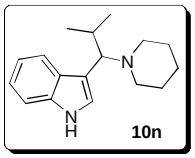
Current Data Parameters
NAME 19may2011
EXPNO 90
PROCNO 1

F2 – Acquisition Parameters
Date_ 20110520
Time 11.14
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 11990.407 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 90.5
DW 41.700 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

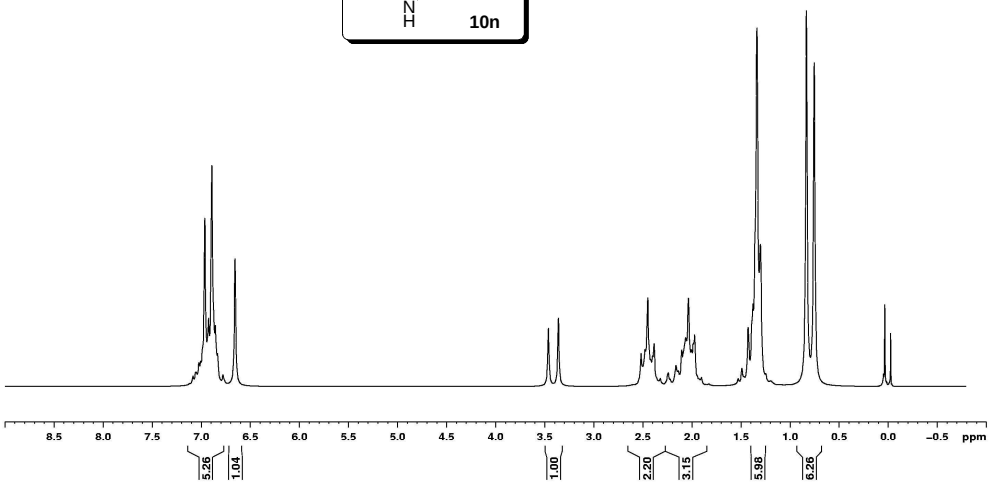
======== CHANNEL f1 =====
NUC1 13C
P1 6.30 usec
PL1 -6.00 dB
SFO1 50.3277608 MHz



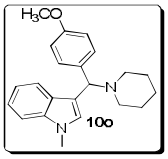
mkg-4n

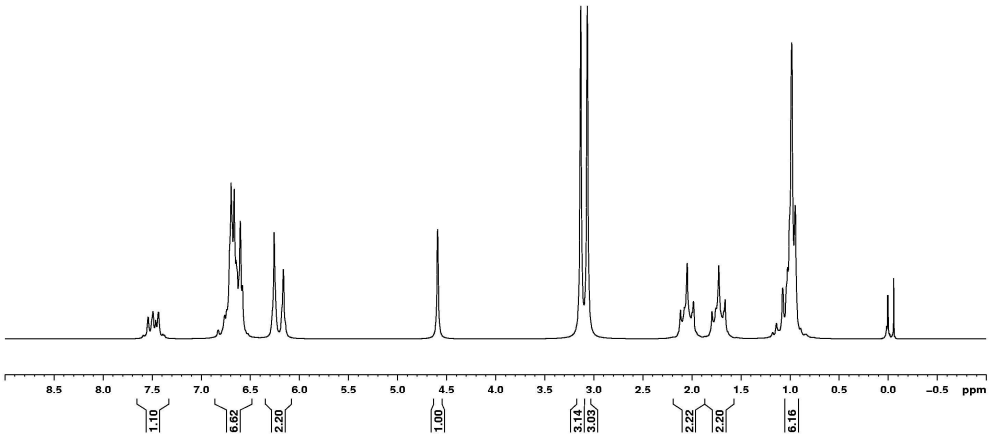


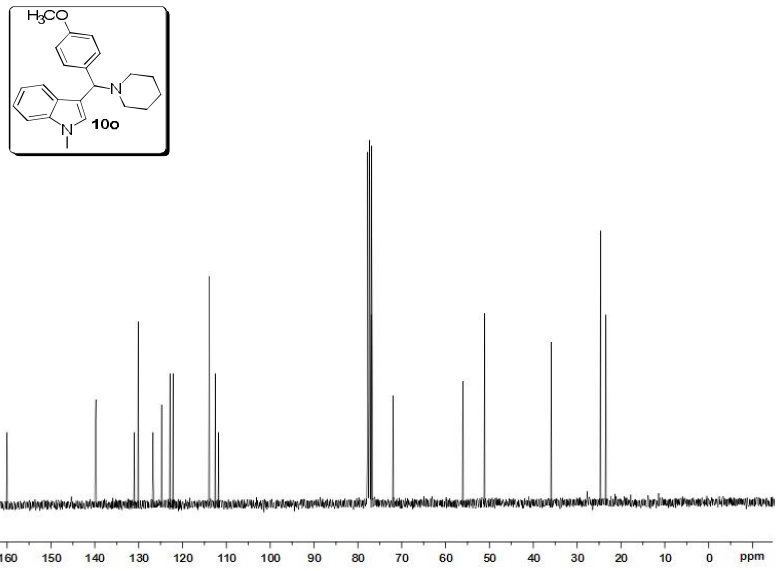
10n

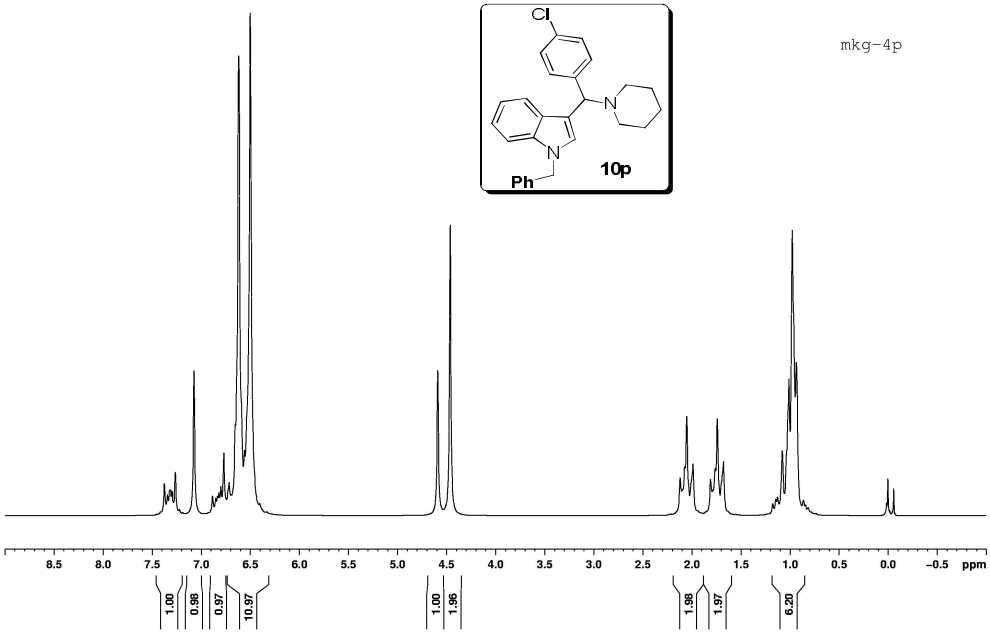


mkg-4o

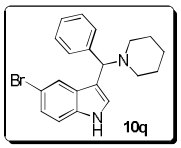


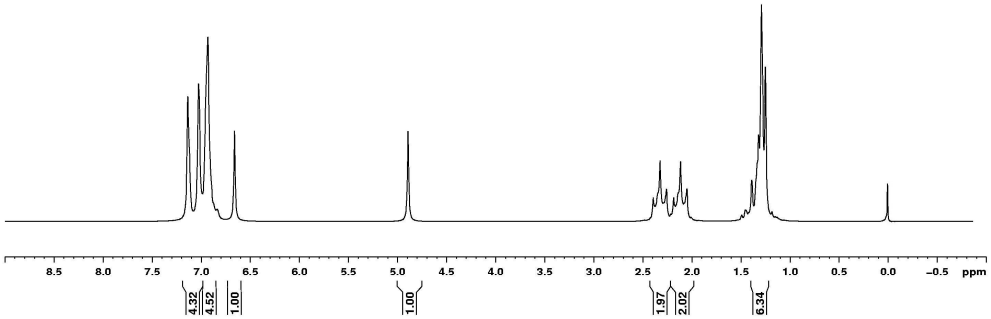


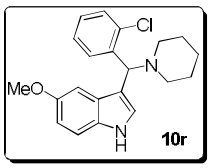




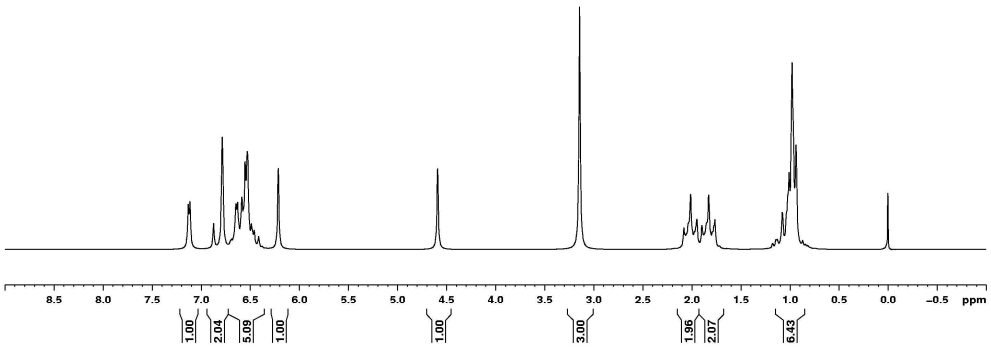
mkg-4q

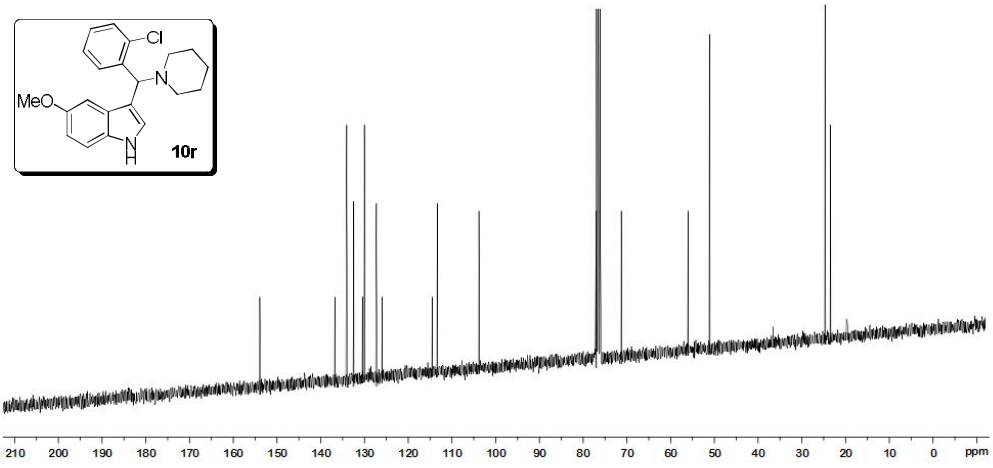




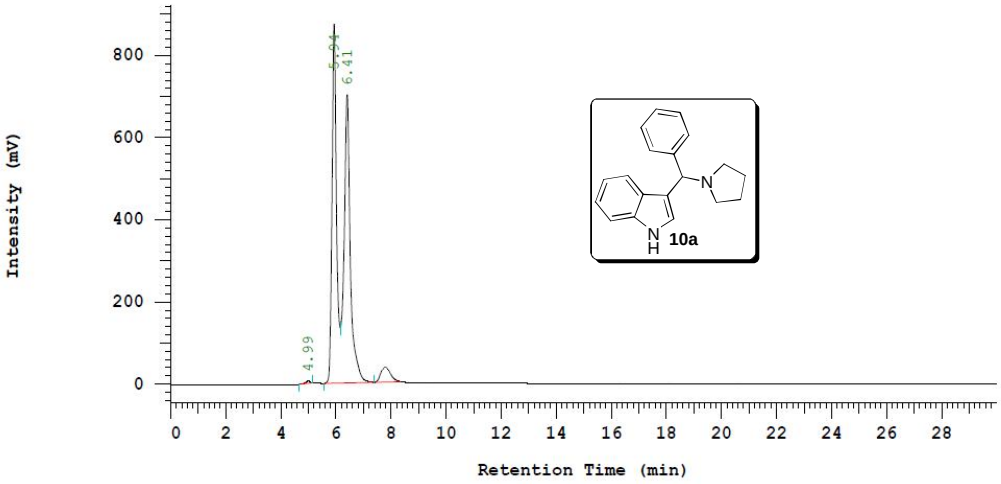


mkg-4r

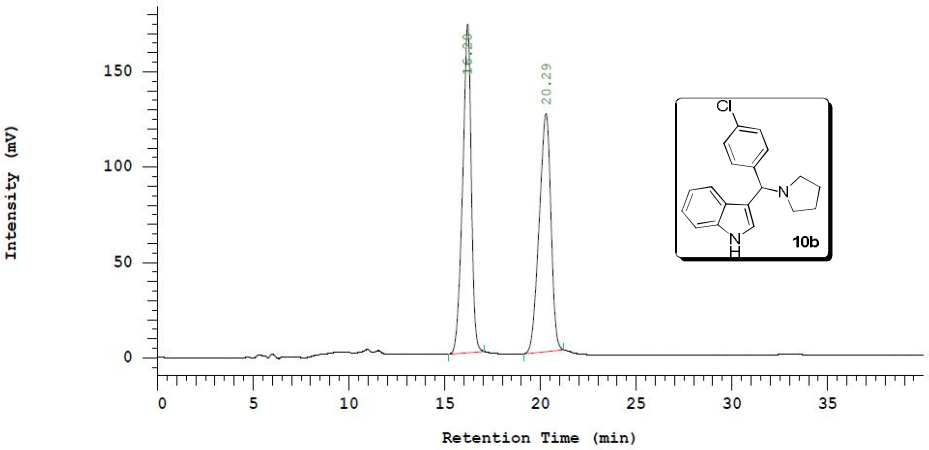




Chrom Type: HPLC Channel : 1

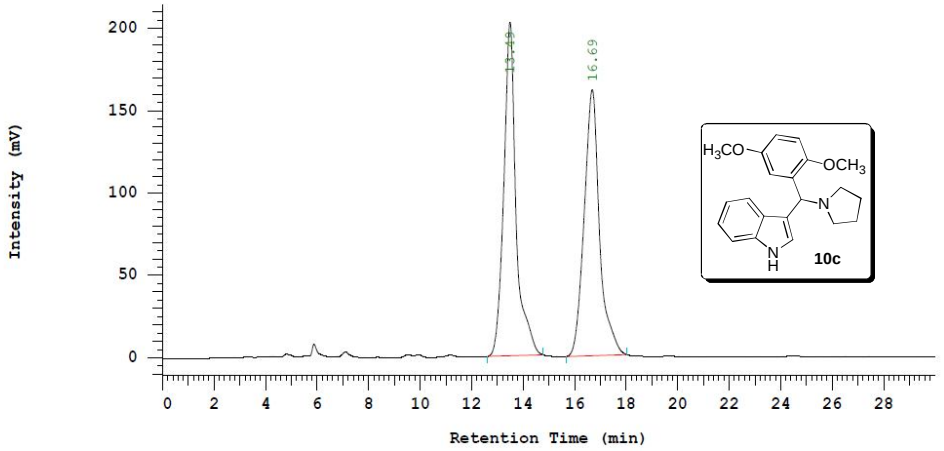


Chrom Type: HPLC Channel : 1



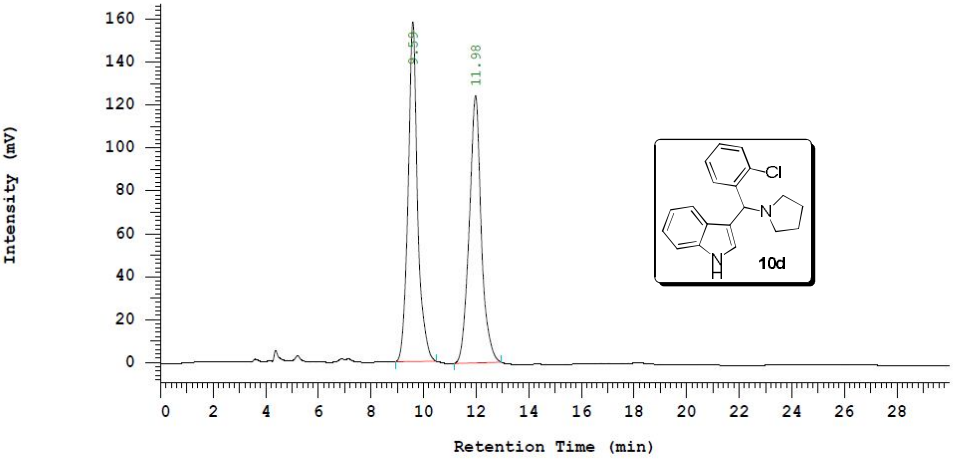
No.	RT	Area	Conc 1	BC
1	16.20	5320817	50.218	BB
2	20.29	5274708	49.782	BB
		10595525	100.000	

Chrom Type: HPLC Channel : 1



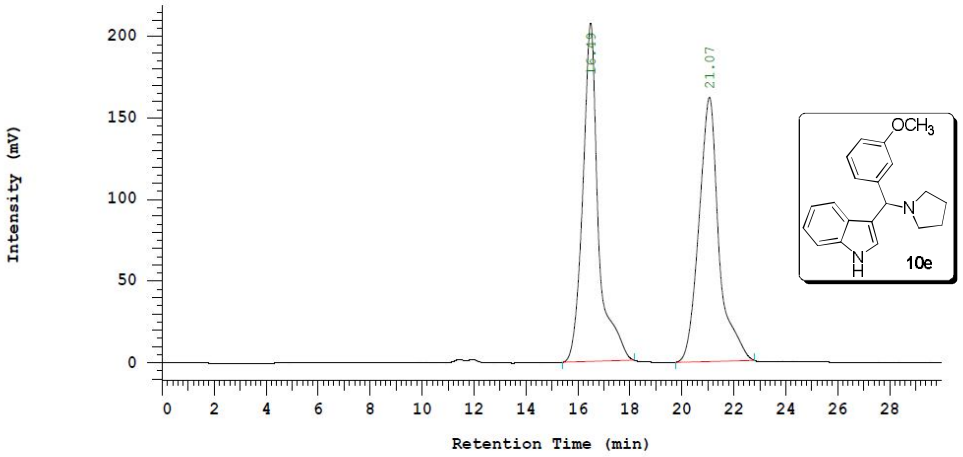
No.	RT	Area	Conc 1	BC
1	13.49	6666199	50.009	BB
2	16.69	6663874	49.991	BB
		13330073	100.000	

Chrom Type: HPLC Channel : 1



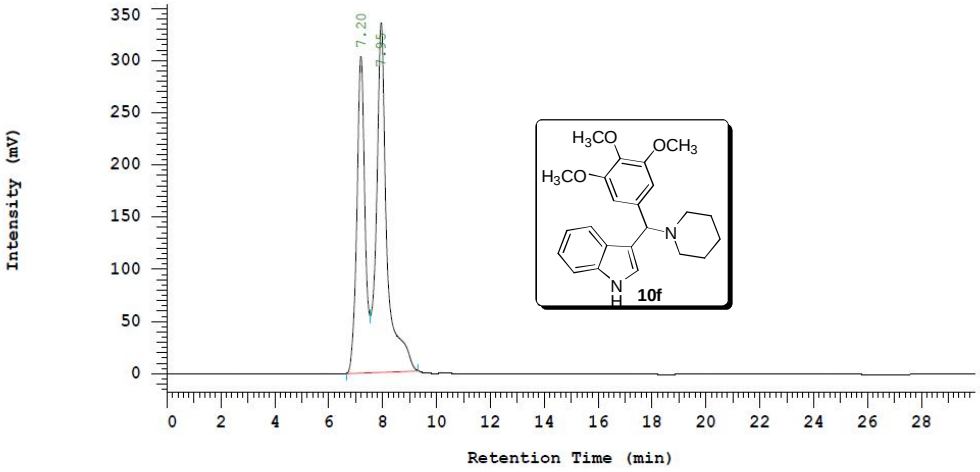
No.	RT	Area	Conc 1	BC
1	9.59	3916225	49.830	BB
2	11.98	3942993	50.170	BB
		7859218	100.000	

Chrom Type: HPLC Channel : 1



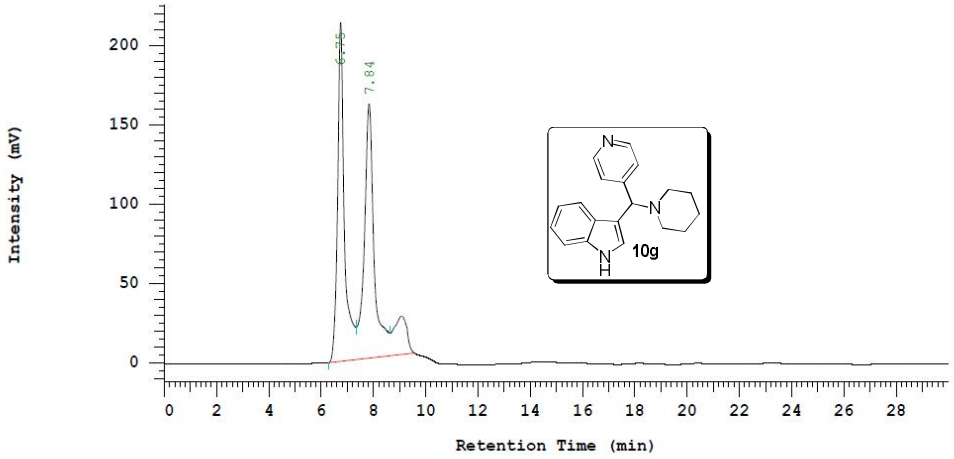
No.	RT	Area	Conc 1	BC
1	16.49	8597367	49.899	BB
2	21.07	8632014	50.101	BB
		17229381	100.000	

Chrom Type: HPLC Channel : 1



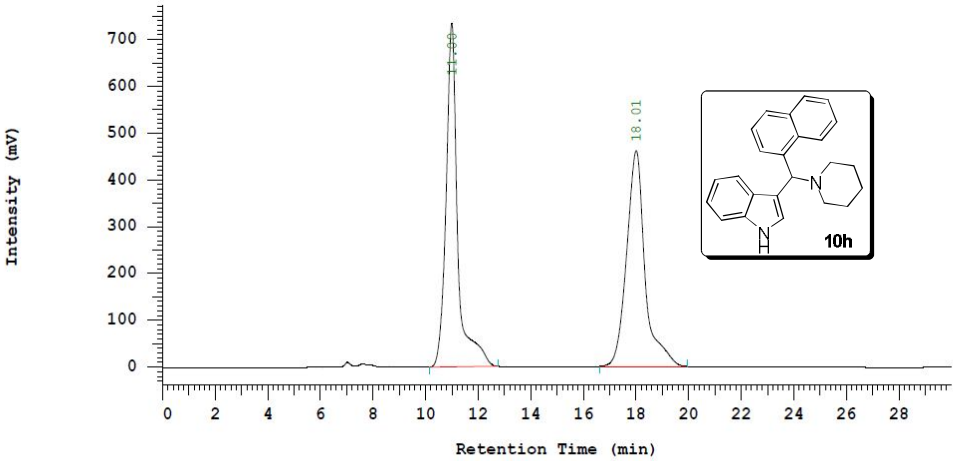
No.	RT	Area	Conc 1	BC
1	7.20	6232911	41.082	BV
2	7.95	8939055	58.918	VB
		15171966	100.000	

Chrom Type: HPLC Channel : 1



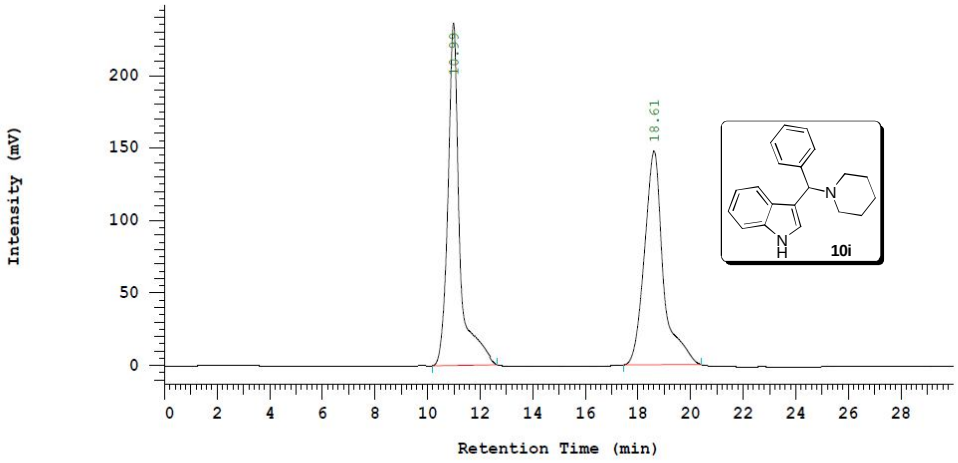
No.	RT	Area	Conc 1	BC
1	6.75	3818369	47.909	BV
2	7.84	4151602	52.091	VV
		7969971	100.000	

Chrom Type: HPLC Channel : 1



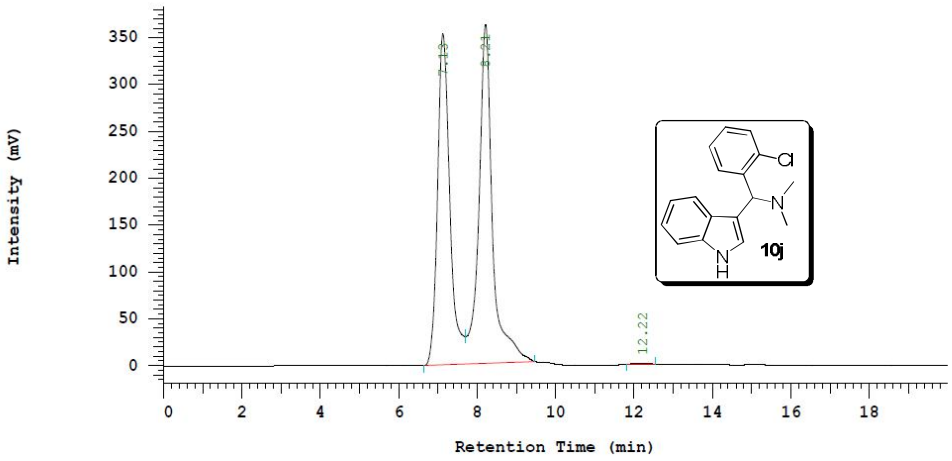
No.	RT	Area	Conc 1	BC
1	11.00	22378180	50.048	BB
2	18.01	22335691	49.952	BB
		44713871	100.000	

Chrom Type: HPLC Channel : 1



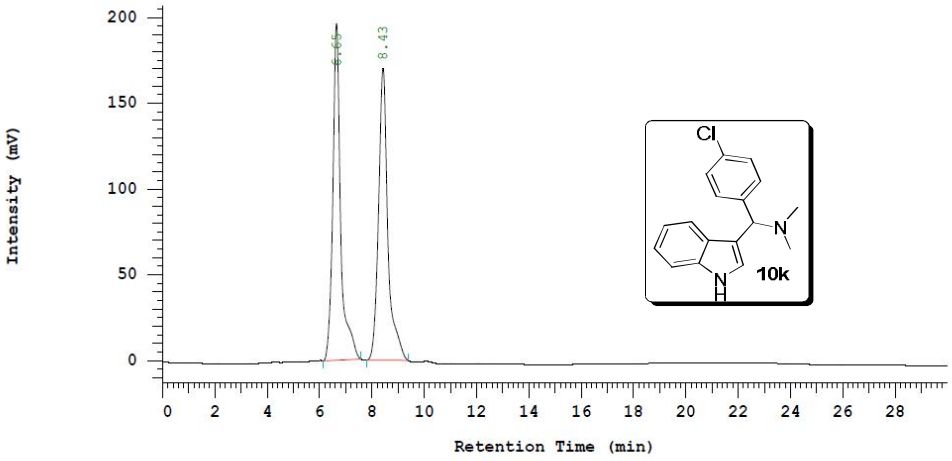
No.	RT	Area	Conc 1	BC
1	10.99	7361176	50.164	BB
2	18.61	7313133	49.836	BB
		14674309	100.000	

Chrom Type: HPLC Channel : 1



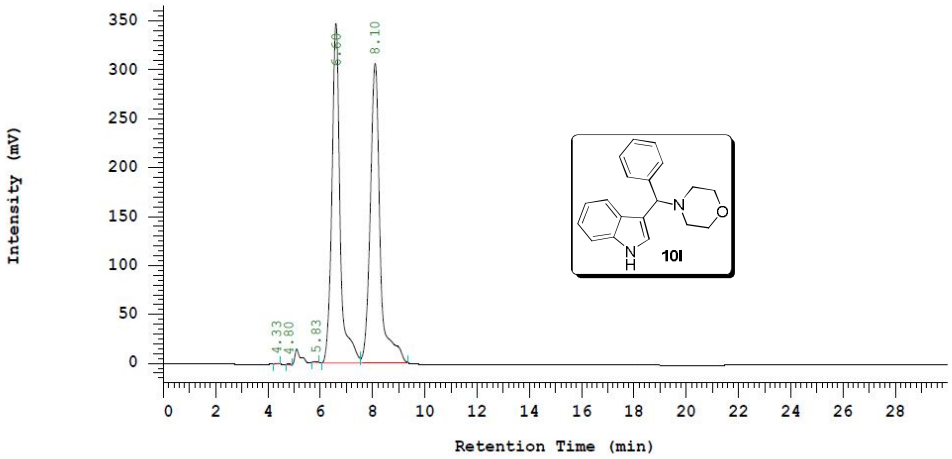
No.	RT	Area	Conc 1	BC
1	7.13	7675517	46.867	BV
2	8.21	8678729	52.993	VB
3	12.22	22872	0.140	BB
		16377118	100.000	

Chrom Type: HPLC Channel : 1

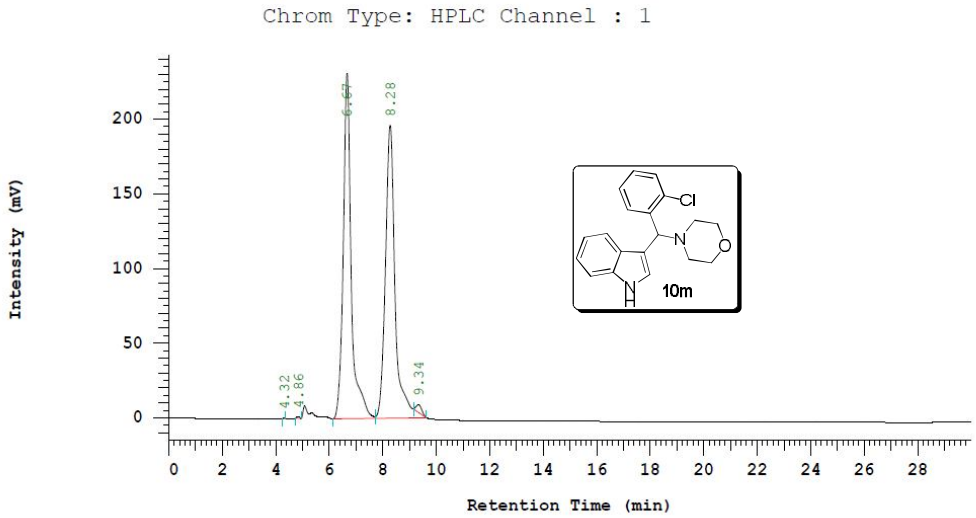


No.	RT	Area	Conc 1	BC
1	6.65	4013698	49.092	BB
2	8.43	4162221	50.908	BB
		8175919	100.000	

Chrom Type: HPLC Channel : 1

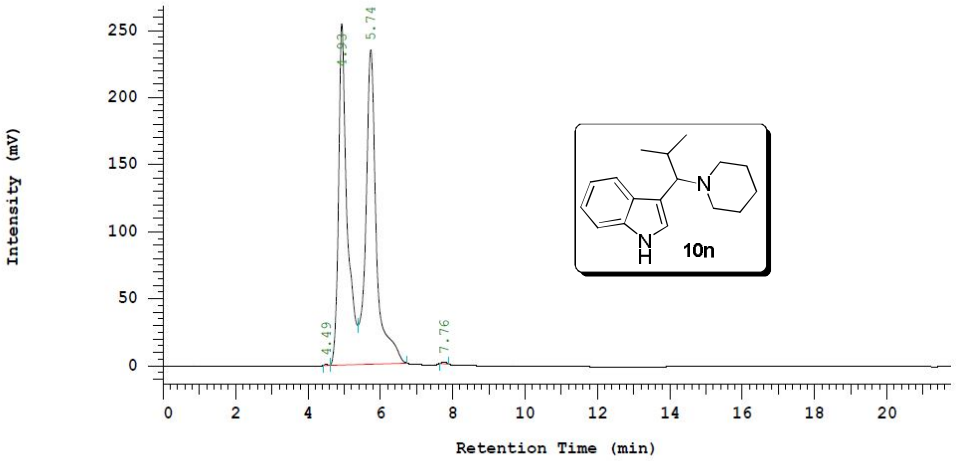


No.	RT	Area	Conc 1	BC
1	4.33	6342	0.041	BB
2	4.80	5810	0.038	BB
3	5.83	8124	0.053	BB
4	6.60	7491757	48.605	BV
5	8.10	7901364	51.263	VB
		15413397	100.000	



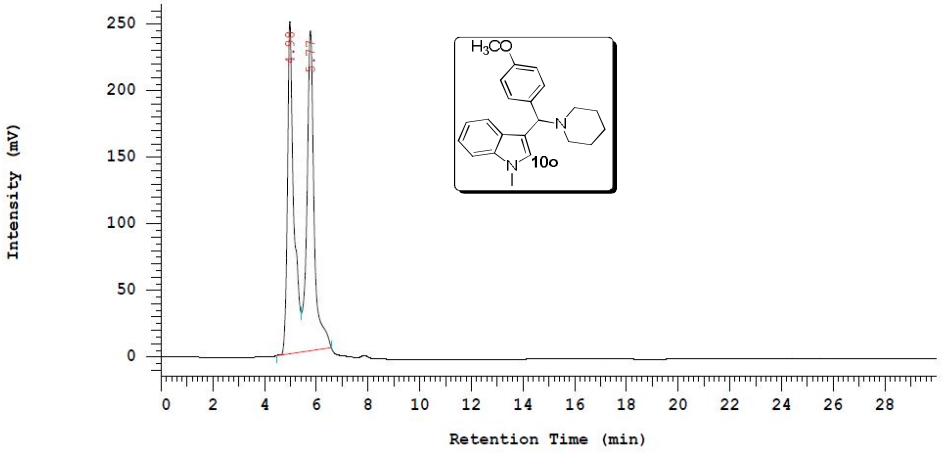
No.	RT	Area	Conc 1	BC
1	4.32	1449	0.015	BB
2	4.86	6964	0.072	BB
3	6.67	4730462	48.850	BV
4	8.28	4870999	50.301	VV
5	9.34	73737	0.761	TBB
		9683611	100.000	

Chrom Type: HPLC Channel : 1



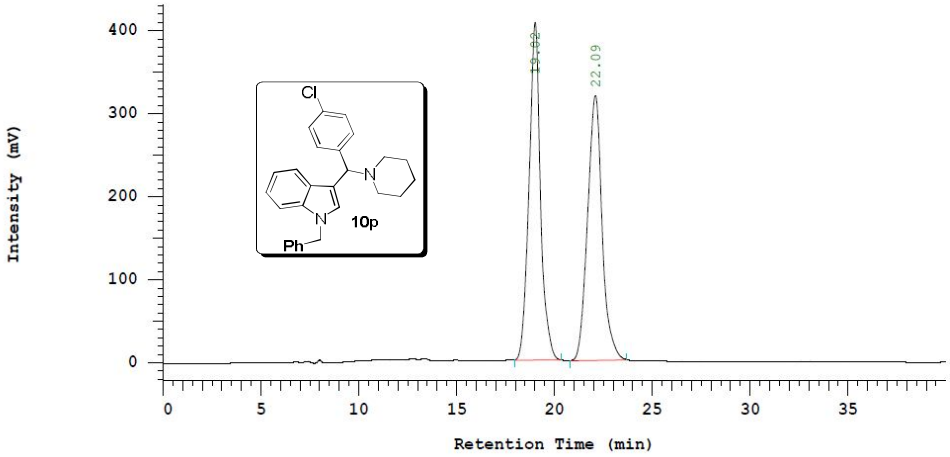
No.	RT	Area	Conc 1	BC
1	4.49	4959	0.056	BB
2	4.93	4138192	46.463	BV
3	5.74	4751185	53.346	VB
4	7.76	12092	0.136	BB
		8906428	100.000	

Chrom Type: HPLC Channel : 1



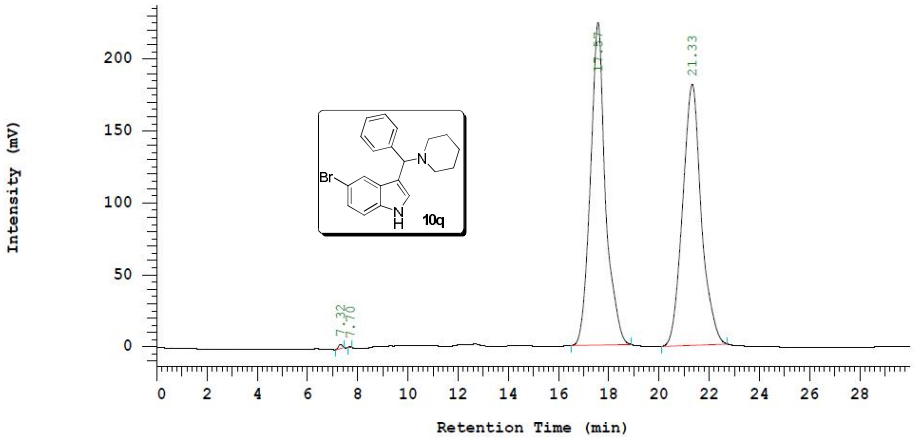
No.	RT	Area	Conc 1	BC
1	4.98	4179458	47.685	MC
2	5.77	4585186	52.315	MC
		8764644	100.000	

Chrom Type: HPLC Channel : 1

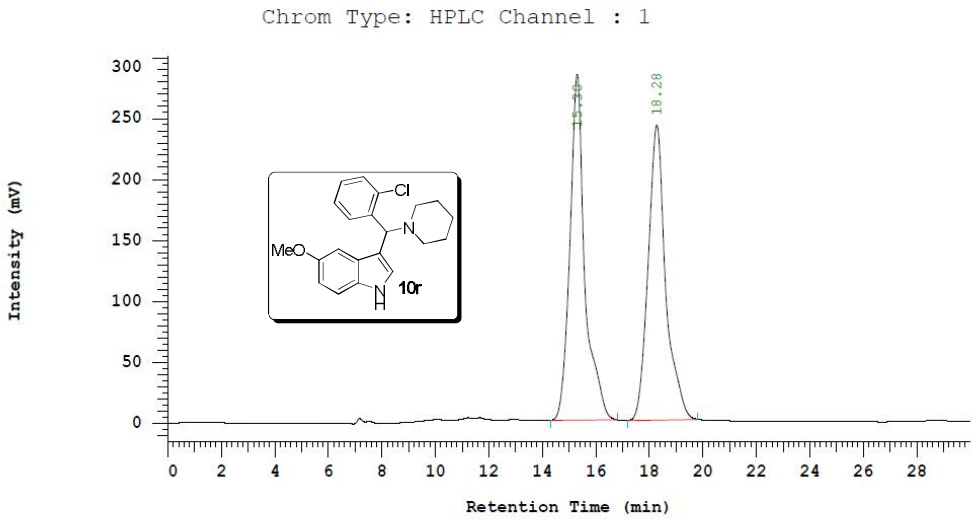


No.	RT	Area	Conc 1	BC
1	19.02	16386747	50.032	BB
2	22.09	16365948	49.968	BB
		32752695	100.000	

Chrom Type: HPLC Channel : 1



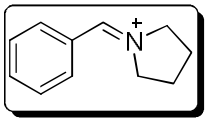
No.	RT	Area	Conc 1	BC
1	7.32	29646	0.159	BB
2	7.70	1726	0.009	BB
3	17.57	9279700	49.731	BB
4	21.33	9348710	50.101	BB
		18659782	100.000	



No.	RT	Area	Conc 1	BC
1	15.30	10975654	49.933	BB
2	18.28	11005227	50.067	BB
		21980881	100.000	

Computational study

Intermediate imine with pyrrolidine

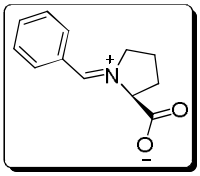


Symbolic Z-matrix:

C	1.4862	-1.3448	3.0805
C	2.5215	-0.8478	3.8706
C	3.4154	0.076	3.3244
C	3.2569	0.5074	2.0082
C	2.2014	0.04	1.2013
C	1.3373	-0.9138	1.7592
C	2.1082	0.5562	-0.1747
N	1.1953	0.4207	-1.122
C	1.3354	1.0667	-2.4924
C	0.3133	0.2957	-3.3388
C	-0.8381	0.073	-2.3503
C	-0.1187	-0.3315	-1.0531
H	0.7887	-2.0891	3.4988
H	2.6406	-1.1892	4.9115
H	4.2447	0.465	3.9377
H	3.9811	1.2384	1.612
H	0.5223	-1.3628	1.1774

H	2.9524	1.1875	-0.5055
H	2.3674	0.9787	-2.9014
H	1.0514	2.1428	-2.4177
H	0.0016	0.8535	-4.2508
H	0.7381	-0.6885	-3.6499
H	-1.5642	-0.6971	-2.6971
H	-1.3881	1.0329	-2.2006
H	-0.7207	-0.0417	-0.1624
H	0.0845	-1.428	-1.065

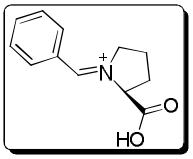
Intermediate imine with L-Proline



Symbolic Z-matrix:

C	3.49413	-0.81005	-0.53837
C	3.93498	-0.02399	0.51513
C	3.07941	0.89646	1.09058
C	1.78263	1.03476	0.62129
C	1.34324	0.24739	-0.42577
C	2.20283	-0.67245	-1.00864
C	-0.05254	0.37513	-0.96425
N	-0.9191	-0.78813	-0.77159
C	-2.29538	-0.24055	-0.70183
C	-3.03781	-1.0611	0.36219
C	-1.90303	-1.42065	1.34273
C	-0.71094	-1.69219	0.40126
C	-2.0796	1.18729	-0.20185
O	-2.89505	1.94212	0.23816
O	-0.7516	1.47999	-0.29929
H	4.15431	-1.52315	-0.99047
H	4.93784	-0.12784	0.87891
H	3.41783	1.51062	1.90122
H	1.11644	1.75298	1.04849
H	1.85625	-1.28237	-1.82059
H	-0.0298	0.61907	-2.01529
H	-2.78912	-0.22973	-1.66344
H	-3.4531	-1.95673	-0.08141
H	-3.82863	-0.47884	0.81273
H	-1.69003	-0.57391	1.98529
H	-2.14057	-2.27474	1.96133
H	-0.73265	-2.71493	0.05143
H	0.2405	-1.50083	0.8671

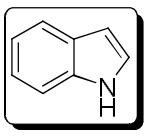
Intermediate imine with L-Proline



Symbolic Z-matrix:

C	-1.3802	2.8823	-0.6024
C	-1.8041	1.4037	-0.5499
N	-0.7538	0.7299	0.3165
C	0.2617	1.796	0.7537
C	-0.5713	3.084	0.685
C	-0.6966	-0.5126	0.7219
C	-1.4521	-1.611	0.5103
C	-1.0952	-2.763	1.1183
C	-1.7927	-3.8992	0.9611
C	-2.8799	-3.9165	0.1784
C	-3.2543	-2.7872	-0.438
C	-2.5484	-1.6572	-0.2704
C	1.4544	1.809	-0.1865
O	2.2124	2.7204	-0.4128
O	1.4876	0.6589	-0.8718
H	-0.7203	3.0606	-1.485
H	-2.2484	3.5761	-0.6775
H	-2.799	1.3274	-0.0515
H	-1.8283	0.9734	-1.5772
H	0.6282	1.6007	1.7873
H	-1.2654	3.1326	1.5581
H	0.0459	4.0099	0.6743
H	0.1816	-0.652	1.3795
H	-0.2096	-2.8111	1.7763
H	-1.4738	-4.8214	1.4757
H	-3.4577	-4.8456	0.0434
H	-4.1475	-2.7909	-1.0857
H	-2.9187	-0.7779	-0.8116
H	2.0696	0.6994	-1.6461

Indole



Symbolic Z-matrix:

C	2.3299	1.9116	-0.6445
C	3.3352	0.9033	-0.6971
C	3.0616	-0.4015	-0.3444
C	1.7402	-0.7015	0.073
C	0.7499	0.2863	0.126
C	1.0431	1.6249	-0.2391

N	1.1562	-1.8828	0.4822
C	-0.175	-1.6541	0.7889
C	-0.4562	-0.3262	0.5796
H	2.5877	2.9437	-0.9345
H	4.3523	1.1725	-1.0266
H	3.8327	-1.1857	-0.3825
H	0.2661	2.4035	-0.1983
H	1.6462	-2.804	0.5486
H	-0.8311	-2.4585	1.1366
H	-1.4226	0.1686	0.7319