Supplementary Material (ESI) for Chemical Communications

A general and mild domino approach to substituted 1-aminoindoles

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Supporting information

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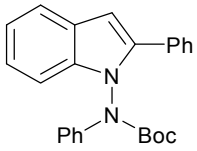
General: The ^{1}H and ^{13}C-NMR spectra were recorded at 500 and 100 MHz respectively using TMS as an internal standard. All hydrazines, alkynes and 1,2-dihalobenzenes were commercially available and used as received without further purification. Transition metal salts, ligands, bases and other reagents as well as anhydrous solvents were also obtained from commercial sources and used as received. Flash chromatography was carried out on silica gel 60 (15-40μm).

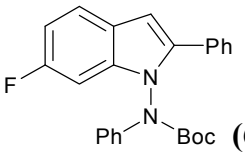
General procedure for the Pd/Cu catalyzed preparation 2-chlorophenylacetylenes 1 from 1-chloro-2-iodobenzenes and terminal alkynes.[1] To a solution of $PdCl_2(PPh_3)_2$ (2.8 mol%), CuI (5.6 mol%), PPh_3 (5.6 mol%) in diisopropylamine was added the 1-chloro-2-iodobenzene (1.0 equiv.) and alkyne (1.1 equiv.) and the mixture stirred for 1-6 h at rt to 50°C. Then the reaction mixture was filtered and evaporated, dissolved in EtOAc and washed with $NaHCO_3$ (aq, sat.) solution. After drying over Na_2SO_4 and evaporation the crude product was purified FC on silica gel using EtOAc/heptane as the eluent. This procedure usually afforded >90% yield of the desired 2-chlorophenylcetylene in high purity.

General procedure for the one-pot domino formation of 1-aminoindoles 3: To a screw-cap test tube was added $PdCl_2$ (5 mol%), tBu_3PHBF_4 (10 mol%), Cs_2CO_3 (1.4 equiv.) a magnetic stirring bar and commercially available anhydrous DMF (2.5 mL) and the mixture was stirred under argon at ambient temperature for 15 min. Then the 2-chlorophenylacetylene **1** (0.5mmol) and the hydrazine (1.4 equiv.) were added and the mixture was heated to 110°C for 3h. After cooling, the reaction mixture was diluted with $NaHCO_3$ (aq, sat) and extracted with EtOAc (x2) and the organic phase dried over Na_2SO_4 and evaporated. The crude product was purified by FC on silica gel using EtOAc/heptane as the eluent.

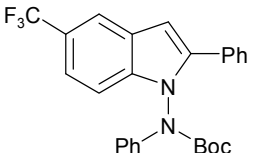
[1] I. Bytschkov, H. Siebeneicher, S. Doye, *Eur. J. Org. Chem*. **2003**, 2888.



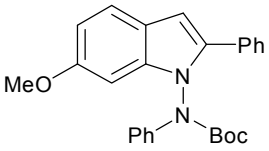
Phenyl-(2-phenyl-indol-1-yl)-carbamic acid tert-butyl ester 3a was prepared as described in the general procedure above and obtained as a slightly yellowish oil. ^{1}H-NMR (DMSO-d_6) δ 1.25 (s, 9H), 6.85 (s, 1H), 7.10-7.14 (m, 3H), 7.15-7.18 (m, 1H), 7.23 (d, 2H, *J* = 4.0 Hz), 7.26-7.30 (m, 2H), 7.39-7.41 (m, 1H), 7.44 (t, *J* = 7.2 Hz, 2H), 7.52 (d, 2H, *J* = 7.9 Hz), 7.65 (d, 1H, *J* = 7.8 Hz); ^{13}C-NMR (DMSO-d_6) δ 27.3, 82.5, 101.4, 109.2, 120.8, 121.0, 123.1, 125.3, 125.7, 127.4, 128.4, 128,7, 128.8, 130.5, 136.7, 139.7, 140.9, 152.0; HRMS (FAB): Calculated for $C_{25}H_{25}N_2O_2$ ($M+H^+$) 385.1916, found 385.1917.



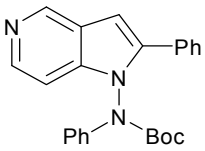
(6-Fluoro-2-phenyl-indol-1-yl)-phenyl-carbamic acid tert-butyl ester 3b was prepared as described in the general procedure above and obtained as a colorless oil. ^{1}H-NMR (DMSO-d_6) δ 1.27 (s, 9H), 6.87 (s, 1H), 7.03 (ddd, 1H, *J* = 9.8, 8.6, 2.3 Hz), 7.07-7.16 (m, 4H), 7.29 (t, 2H, *J* = 7.9 Hz), 7.39-7.42 (m, 1H), 7.43-7.47 (m, 2H), 7.49-7.52 (m, 2H), 7.66 (dd, 1H, *J* = 8.7, 5.3 Hz); ^{13}C-NMR (DMSO-d_6) δ 27.3, 82.7, 95.9 (d, *J* = 27.2 Hz), 101.4, 109.7 (d, *J* = 24.3 Hz), 121.2, 122.2 (d, *J* = 9.9 Hz), 122.3, 125.5, 127.4, 128.5, 128.8, 128.9, 136.9 (d, *J* = 11.9 Hz), 140.5 (d, *J* = 4.3 Hz), 140.6, 151.8, 159.7 (d, *J* = 238.6 Hz); HRMS (FAB): Calculated for $C_{25}H_{24}N_2O_2F$ ($M+H^+$) 403.1822, found 403.1815.



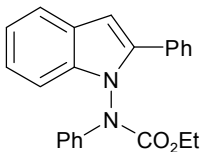
Phenyl-(2-phenyl-5-trifluoromethyl-indol-1-yl)-carbamic acid tert-butyl ester 3c was prepared as described in the general procedure above and obtained as a colorless oil. ^{1}H-NMR (DMSO-d_6) δ 1.25 (s, 9H), 7.03 (s, 1H), 7.11-7.17 (m, 3H), 7.30 (t, 2H, *J* = 7.9 Hz), 7.41-7.49 (m, 4H), 7.52-7.56 (m, 3H), 8.08 (s, 1H); ^{13}C-NMR (DMSO-d_6) δ 27.3, 83.0, 102.1, 110.1, 118.5, 119.7, 122.2 (q, *J* = 31.3 Hz), 125.1 (q, *J* = 271.6 Hz), 125.2, 125.6, 127.6, 128.3 (q, *J* = 39.0 Hz), 128.9, 129.0, 129.8, 138.1, 140.6, 141.7, 151.7; HRMS (FAB): Calculated for $C_{26}H_{24}N_2O_2F_3$ ($M+H^+$) 453.1790, found 453.1785.



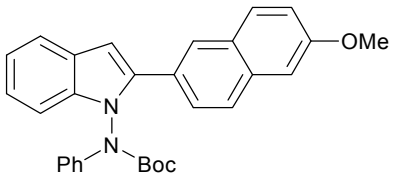
(6-Methoxy-2-phenyl-indol-1-yl)-phenyl-carbamic acid tert-butyl ester 3d was prepared as described in the general procedure above and obtained as a colorless oil. ^{1}H-NMR (DMSO-d_6) δ 1.27 (s, 9H), 3.74 (s, 3H), 6.67 (d, 1H, *J* = 1.9 Hz), 6.76 (d, 1H, *J* = 0.6 Hz), 6.83 (dd, 1H, *J* = 8.5, 2.2 Hz), 7.10-7.13 (m, 3H), 7.27 (t, 2H, *J* = 7.8 Hz), 7.33-7.37 (m, 1H), 7.41 (t, 2H, *J* = 7.6 Hz), 7.45-7.48 (m, 2H), 7.53 (d, 1H, *J* = 8.5 Hz); ^{13}C-NMR (DMSO-d_6) δ 27.3, 55.3, 82.4, 92.8, 101.3, 110.5, 119.7, 121.0, 121.6, 125.2, 127.1, 127.9, 128.6, 128.8, 130.8, 137.8, 138.5, 140.8, 151.9, 156.8; HRMS (FAB): Calculated for $C_{26}H_{27}N_2O_3$ (M+H$^+$) 415.2022, found 415.2028.



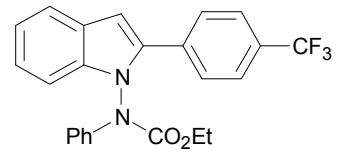
Phenyl-(2-phenyl-pyrrolo[3,2-c]pyridin-1-yl)-carbamic acid tert-butyl ester 3e was prepared as described in the general procedure above and obtained as a colorless oil. ^{1}H-NMR (DMSO-d_6) δ 1.26 (br s, 9H), 7.00 (s, 1H), 7.10-7.17 (m, 3H), 7.26-7.36 (m, 3H), 7.42-7.51 (m, 3H), 7.51-7.55 (m, 2H), 8.32 (d, 1H, *J* = 5.5 Hz), 8.94 (br s, 1H); ^{13}C-NMR (DMSO-d_6) δ 27.3, 82.9, 100.3, 104.6, 121.2, 122.3, 125.7, 127.7, 128.8, 129.0, 129.7, 140.4, 140.5, 140.7, 142.2, 143.4, 151.5; HRMS (FAB): Calculated for $C_{24}H_{24}N_3O_2$ (M+H$^+$) 386.1869, found 386.1882.



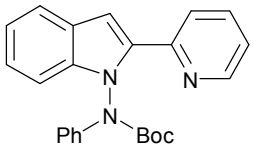
Phenyl-(2-phenyl-indol-1-yl)-carbamic acid ethyl ester 3f was prepared as described in the general procedure above and obtained as a colorless oil. ^{1}H-NMR (DMSO-d_6) δ 1.06 (br t, 3H, *J* = 6.7 Hz), 4.21 (m, 2H), 6.86 (s, 1H), 7.06 (d, 2H, *J* = 7.8 Hz), 7.12 (t, 1H, *J* = 7.4 Hz), 7.17 (t, 1H, *J* = 7.4 Hz), 7.22-7.28 (m, 3H), 7.33 (d, 1H, *J* = 8.0 Hz), 7.38-7.42 (m, 1H), 7.45 (t, 1H, *J* = 7.4 Hz), 7.50-7.53 (m, 2H), 7.65 (d, 1H, *J* = 7.8 Hz); ^{13}C-NMR (DMSO-d_6) δ 14.0, 62.8, 101.7, 109.4, 120.8, 121.3, 121.4, 123.2, 125.6, 125.8, 127.4, 128.4, 128.8, 128.9, 130.4, 136.5, 139.3, 140.6, 153.6; HRMS (FAB): Calculated for $C_{23}H_{21}N_2O_2$ (M+H$^+$) 357.1603, found 357.1595.



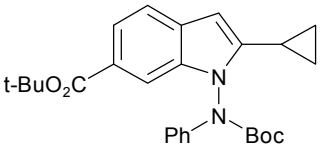
[2-(6-Methoxy-naphthalen-2-yl)-indol-1-yl]-phenyl-carbamic acid tert-butyl ester 3g was prepared as described in the general procedure above and obtained as a yellowish solid. ^{1}H-NMR (DMSO-d_6) δ 1.30 (s, 9H), 3.92 (s, 3H), 6.95 (s, 1H), 7.11-7.17 (m, 3H), 7.19-7.35 (m, 6H), 7.39 (d, 1H, *J* = 2.3 Hz), 7.66 (dd, 1H, *J* = 8.7, 1.6 Hz), 7.70 (d, 1H, *J* = 7.8 Hz), 7.74 (d, 1H, *J* = 9.2 Hz), 7.93 (d, 1H, *J* = 8.9 Hz), 7.98 (s, 1H); ^{13}C-NMR (DMSO-d_6) δ 27.6, 55.2, 82.5, 101.5, 105.9, 109.2, 119.3, 120.7, 121.2, 123.1, 125.4, 125.6, 125.8, 126.1, 127.1, 128.1, 128.5, 128.8, 129.4, 133.8, 136.9, 139.8, 141.0, 152.1, 157.8; HRMS (ESI): Calculated for $C_{30}H_{29}N_2O_3$ (M+H$^+$) 465.2178, found 465.2175.



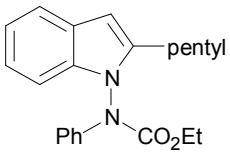
Phenyl-[2-(4-trifluoromethyl-phenyl)-indol-1-yl]-carbamic acid ethyl ester 3h was prepared as described in the general procedure above and obtained as a colourless crystalline solid. ^{1}H-NMR (DMSO-d_6) δ 1.08 (t, 3H, *J* = 7.1 Hz), 4.26 (m, 2H), 7.08 (s, 1H), 7.11 (d, 2H, *J* = 8.6 Hz), 7.17 (t, 1H, *J* = 7.6 Hz), 7.25 (t, 1H, *J* = 7.6 Hz), 7.28-7.35 (m, 3H), 7.41 (d, 1H, *J* = 8.6 Hz), 7.75 (d, 1H, *J* = 7.9 Hz), 7.80 (d, 2H, *J* = 8.31 Hz), 7.91 (d, 2H, *J* = 8.6 Hz) ; ^{13}C-NMR (DMSO-d_6) δ 14.0, 63.1, 103.5, 109.6, 121.2, 121.3, 121.6, 124.0, 124.0, (q, *J* = 272.6 Hz), 125.4, 125.8 (q, *J* = 3.6 Hz), 125.9, 127.9, 128.4 (q, *J* = 32.1 Hz), 129.0, 134.3, 136.9, 137.5, 140.4, 153.5; HRMS (ESI): Calculated for $C_{24}H_{20}N_2O_2F_3$ (M+H$^+$) 425.1477, found 425.1476.



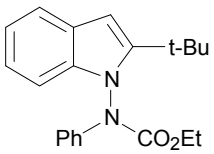
Phenyl-(2-pyridin-2-yl-indol-1-yl)-carbamic acid tert-butyl ester 3i was prepared as described in the general procedure above and obtained as a colorless oil. ^{1}H-NMR (DMSO-d_6) δ 1.23 (br s, 9H), 7.05-7.09 (m, 1H), 7.15 (t, 1H, *J* = 7.4 Hz), 7.22-7.31 (m, 8H), 7.67 (d, 1H, *J* = 7.8 Hz), 7.86 (dt, 1H, *J* = 1,7, 7.4 Hz), 7.92 (d, 1H, *J* = 8.0 Hz), 8.53 (d, 1H, *J* = 4.7 Hz);); ^{13}C-NMR (DMSO-d_6) δ 27.4, 81.5, 102.9, 109.1, 121.1, 121.6, 121.8, 122.5, 123.9, 124.7, 124.8, 128.4, 136.7, 136.8, 137.2, 141.4, 149.1, 149.8, 151.9; HRMS (FAB): Calculated for $C_{24}H_{24}N_3O_2$ (M+H$^+$) 386.1869, found 386.1874.



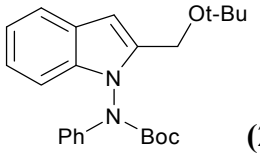
1-(tert-Butoxycarbonyl-phenyl-amino)-2-cyclopropyl-1H-indole-6-carboxylic acid tert-butyl ester 3j was prepared as described in the general procedure above and obtained as a colorless oil. ^{1}H-NMR (DMSO-d_6) δ 0.67-0.77 (m, 2H), 0.85-0.92 (m, 1H), 1.01-1.07 (m, 1H), 1.35 (s, 9H), 1.52 (s, 9H), 1.71-1.77 (m, 1H), 6.28 (s, 1H), 7.21 (t, 1H, *J* = 7.4 Hz), 7.30 (d, 2H, *J* = 7.5 Hz), 7.38 (d, 1H, *J* = 7.4 Hz), 7.40 (d, 1H, *J* = 7.3 Hz), 7.55 (d, 1H, *J* = 8.2 Hz), 7.64 (dd, 1H, *J* = 8.3, 1.5 Hz), 7.68 (s, 1H);); ^{13}C-NMR (DMSO-d_6) δ 6.5, 7.4, 7.9, 27.4, 27.8, 80.1, 82.7, 96.1, 109.0, 119.7, 121.3, 124.6, 125.5, 129.0, 129.1, 135.1, 140.9, 147.1, 151.7, 165.5; HRMS (FAB): Calculated for $C_{27}H_{33}N_2O_4$ ($M+H^+$) 449.2440, found 449.2459.



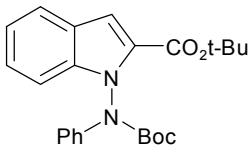
(2-Pentyl-indol-1-yl)-phenyl-carbamic acid ethyl ester 3k was prepared as described in the general procedure above and obtained as a brown oil. ^{1}H-NMR (DMSO-d_6) δ 0.82 (t, 3H, *J* = 7.3 Hz), 1.11 (t, 3H, *J* = 7.3 Hz), 1.21-1.34 (m, 4H), 1.53-1.66 (m, 2H), 2.56 (t, 2H, *J* = 7.7 Hz), 4.19-4.28 (m, 2H), 6.40 (s, 1H), 7.12 (dt, 1H, *J* = 1.2, 7.7 Hz), 7.14-7.18 (m, 1H), 7.20-7.28 (m, 4H), 7.37-7.42 (m, 2H), 7.57 (d, 1H, *J* = 7.6 Hz); ^{13}C-NMR (DMSO-d_6) δ 13.7, 14.1, 21.7, 24.8, 26.8, 30.7, 62.8, 98.6, 108.4, 120.0, 120.5, 121.0, 121.9 125.5, 125.6, 129.0, 135.3, 140.6, 140.8, 153.3; HRMS (ESI): Calculated for $C_{22}H_{27}N_2O_2$ ($M+H^+$) 351.2073, found 351.2072.



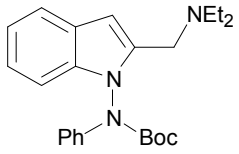
(2-tert-Butyl-indol-1-yl)-phenyl-carbamic acid ethyl ester 3l was prepared as described in the general procedure above and obtained as a brown oil. ^{1}H-NMR (DMSO-d_6) δ 1.03 (t, 3H, *J* = 7.3 Hz), 1.12 (s, 9H), 4.16 (q, 2H, *J* = 7.3 Hz), 6.43 (s, 1H), 7.06 (d, 1H, *J* = 8.1 Hz), 7.15 (t, 1H, *J* = 7.4 Hz), 7.17-7.24 (m, 4H), 7.37-7.42 (m, 2H), 7.61 (d, 1H, *J* = 7.8 Hz); ^{13}C-NMR (DMSO-d_6) δ 14.0, 29.4, 31.9, 62.8, 98.7, 108.2, 119.8, 120.4, 120.7, 122.4, 124.7, 124.8, 128.8, 137.3, 141.4, 147.7, 153.6; HRMS (ESI): Calculated for $C_{21}H_{25}N_2O_2$ ($M+H^+$) 337.1916, found 337.1918.



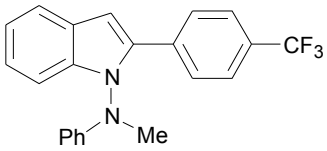
(2-tert-Butoxymethyl-indol-1-yl)-phenyl-carbamic acid tert-butyl ester 3m was prepared as described in the general procedure above and obtained as a yellowish oil. ^{1}H-NMR (DMSO-d_6) δ 1.11 (s, 9H), 1.34 (s, 9H), 4.41 (s, 2H), 6.58 (s, 1H), 7.10-7.14 (m, 4H), 7.32-7.43 (m, 4H), 7.62 (d, 2H, *J* = 7.9 Hz); ^{13}C-NMR (DMSO-d_6) δ 26.9, 27.4, 55.1, 73.1, 82.1, 101.3, 108.4, 120.5, 120.7, 121.3, 122.6, 124.9, 125.1, 128.4, 136.0, 137.8, 141.1, 151.8; HRMS (ESI): Calculated for $C_{24}H_{31}N_2O_3$ ($M+H^+$) 395.2335, found 395.2329.



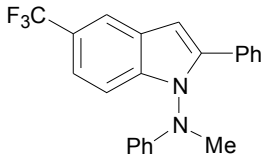
1-(tert-Butoxycarbonyl-phenyl-amino)-1H-indole-2-carboxylic acid tert-butyl ester 3n was prepared as described in the general procedure above and obtained as a brown oil. ^{1}H-NMR (DMSO-d_6) δ 1.32 (br s, 9H), 1.46 (s, 9H), 7.15 (t, 1H, *J* = 7.2 Hz), 7.20 (t, 1H, *J* = 7.4 Hz), 7.26-7.30 (m, 3H), 7.33 (d, 1H, *J* = 8.0 Hz), 7.36 (d, 1H, *J* = 8.5 Hz), 7.75 (d, 1H, *J* = 8.0 Hz); ^{13}C-NMR (DMSO-d_6) δ 27.5, 27.7, 81.4, 82.0, 109.4, 109.9, 120.9, 121.7, 122.6, 123.2, 124.9, 126.3, 128.3, 128.5, 137.4, 141.0, 151.6, 158.8; HRMS (FAB): Calculated for $C_{24}H_{28}N_2O_4Na$ ($M+Na^+$) 431.1947, found 431.1952.



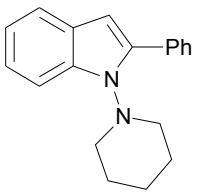
(2-Diethylaminomethyl-indol-1-yl)-phenyl-carbamic acid tert-butyl ester 3o was prepared as described in the general procedure above and obtained as a black oil. ^{1}H-NMR (DMSO-d_6) δ 1.04 (t, 6H, *J* = 7.4 Hz), 1.34 (s, 9H), 2.57 (q, 4H, *J* = 7.4 Hz), 3.71 (s, 2H), 6.68 (d, 1H, *J* = 8.4 Hz), 6.78 (dt, 1H, *J* = 1.0, 7.7 Hz), 7.17 (t, 1H, *J* = 7.5 Hz), 7.23 (t, 1H, *J* = 7.9 Hz), 7.31 (dd, 1H, *J* = 1.4, 7.9 Hz), 7.36-7.41 (m, 2H), 7.60 (d, 2H, *J* = 8.1 Hz), 8.16 (s, 1H); ^{13}C-NMR (DMSO-d_6) δ 12.5, 27.6, 41.3, 46.7, 80.0, 81.0, 91.4, 106.8, 110.5, 118.9, 122.1, 124.4, 128.2, 129.2, 132.1, 142.7, 148.9, 153.1; HRMS (ESI): Calculated for $C_{24}H_{32}N_3O_2$ ($M+H^+$) 394.2495, found 394.2492.



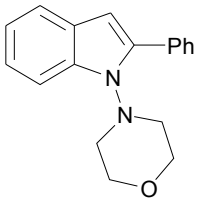
Methyl-phenyl-[2-(4-trifluoromethyl-phenyl)-indol-1-yl]-amine 3p was prepared as described in the general procedure above and obtained as a brown oil. ^{1}H-NMR (DMSO-d_6) δ 3.48 (s, 3H), 6.50 (d, 2H, *J* = 8.1 Hz), 6.84 (t, 1H, *J* = 7,6 Hz), 7.01-7.04 (m, 1H), 7.04 (s, 1H), 7.16 (dd, 2H, *J* = 2.9, 6.3 Hz), 7.23 (dd, 2H, *J* = 7.6, 8.9 Hz), 7.71-7.75 (m, 1H), 7.82 (d, 2H, *J* = 8.6 Hz), 7.93 (d, 2H, *J* = 8.6 Hz); ^{13}C-NMR (DMSO-d_6) δ 39.8, 101.8, 110.6, 112.0, 119.5, 121.1, 121.4, 124.1 (q, *J* = 273 Hz), 123.1, 125.5 (q, *J* = 3.7 Hz), 126.1, 128.0, 128.1 (q, *J* = 32 Hz), 129.4, 134.8, 135.2, 137.7, 148.5; HRMS (FAB): Calculated for $C_{22}H_{18}F_3N_2$ ($M+H^+$) 367.1422, found 367.1410.



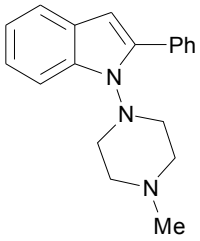
Methyl-phenyl-(2-phenyl-5-trifluoromethyl-indol-1-yl)-amine 3q was prepared as described in the general procedure above and obtained as a brown oil. ^{1}H-NMR (DMSO-d_6) δ 3.50 (s, 3H), 6.50 (d, 2H, *J* = 7.9 Hz), 6.87 (t, 1H, *J* = 7.6 Hz), 7.06 (s, 1H), 7.23-7.29 (m, 3H), 7.43-7.52 (m, 4H), 7.72 (d, 2H, *J* = 7.7 Hz), 8.14 (s, 1H); ^{13}C-NMR (DMSO-d_6) δ 39.8, 101.0, 111.1, 111.9, 118.5, 118.7, 119.6, 121,8 (q, *J* = 31 Hz), 125.2 (q, *J* = 270 Hz), 125.6, 127.8, 128.6, 128.7, 129.5, 130.2, 136.5, 141.6, 148.2; HRMS (FAB): Calculated for $C_{22}H_{18}F_3N_2$ ($M+H^+$) 367.1422, found 367.1426.



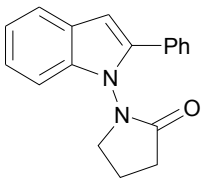
2-Phenyl-1-piperidin-1-yl-1H-indole 3r was prepared as described in the general procedure above and obtained as a brown oil. ^{1}H-NMR (DMSO-d_6) δ 1.41 (br s, 2H), 1.65 (quintet, 4H, *J* = 5.6 Hz), 2.75 (br s, 4H), 6.06 (s, 1H), 6.72 (t, 1H, *J* = 7.5 Hz), 7.19 (d, 1H, *J* = 8.5 Hz), 7.29 (t, 1H, *J* = 7.8 Hz), 7.37 (t, 1H, *J* = 7.8 Hz), 7.46-7.56 (m, 3H), 7.67 (d, 2H, *J* = 7.8 Hz); ^{13}C-NMR (DMSO-d_6) δ 23.1, 25.6, 55.8, 85.7, 94.9, 105.0, 112.0, 117.3, 122.6, 128.4, 128.5, 130.0, 131.2, 132.0, 148.3; HRMS (ESI): Calculated for $C_{19}H_{21}N_2$ ($M+H^+$) 277.1705, found 277.1700.



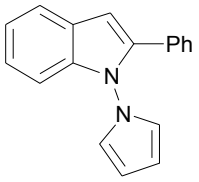
1-Morpholin-4-yl-2-phenyl-1H-indole 3s was prepared as described in the general procedure above and obtained as a brown oil. ^{1}H-NMR (DMSO-d_6) δ 2.83 (br s, 4H), 3.75 (br s, 4H), 6.34 (s, 1H), 6.75 (dt, 1H, *J* = 1.2, 7.5 Hz), 7.24 (d, 1H, *J* = 8.2 Hz), 7.39 (dd, 1H, *J* = 1.4, 7.8 Hz), 7.47-7.54 (m, 3H), 7.70 (dd, 2H, *J* = 1.7, 8.2 Hz); ^{13}C-NMR (DMSO-d_6) δ 54.8, 66.3, 85.7, 94.9, 105.3, 112.1, 117.5, 122.7, 128.4, 128.5, 130.0, 131.3, 132.1, 148.0; HRMS (ESI): Calculated for $C_{18}H_{19}N_2O$ ($M+H^+$) 279.1497, found 279.1497.



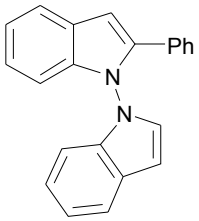
1-(4-Methyl-piperazin-1-yl)-2-phenyl-1H-indole 3t was prepared as described in the general procedure above and obtained as a brown oil. ^{1}H-NMR (DMSO-d_6) δ 2.22 (s, 3H), 2.48 (br s, 4H), 2.83 (s, 4H), 6.18 (s, 1H), 6.72 (dt, 1H, *J* = 1.1, 7.6 Hz), 7.18 (d, 1H, *J* = 8.6 Hz), 7.28 (t, 1H, *J* = 8.2 Hz), 7.36 (dd, 1H, *J* = 1.4, 7.8 Hz), 7.44-7.53 (m, 3H), 7.68 (dd, 2H, *J* = 1.8, 8.3 Hz); ^{13}C-NMR (DMSO-d_6) δ 45.5, 54.1, 54.7, 85.8, 94.9, 105.2, 112.1, 117.4, 122.7, 128.4, 128.5, 130.0, 131.3, 132.1, 148.2; HRMS (ESI): Calculated for $C_{19}H_{22}N_3$ ($M+H^+$) 292.1814, found 292.1812.



1-(2-Phenyl-indol-1-yl)-pyrrolidin-2-one 3u was prepared as described in the general procedure above and obtained as a colourless crystalline solid. ^{1}H-NMR (DMSO-d_6) δ 1.92-2.04 (m, 1H), 2.15-2.25 (m, 1H), 2.37-2.45 (m, 1H), 2.63-2.72 (m, 1H), 3.27-3.32 (m, 1H), 3.76 (m, 1H), 6.82 (s, 1H), 7.21 (t, 1H, *J* = 7.6 Hz), 7.28 (t, 1H, *J* = 7.6 Hz), 7.40 (d, 1H, *J* = 8.3 Hz), 7.48 (m, 1H), 7.55 (t, 2H, *J* = 7.5 Hz), 7.59-7.62 (m, 2H), 7.68 (d, 1H, *J* = 8.5 Hz); ^{13}C-NMR (DMSO-d_6) δ 16.6, 27.9, 47.6, 101.3, 109.5, 120.7, 121.1, 122.7, 125.9, 127.3, 128.3, 128.8, 130.3, 135.8, 139.3, 173.4; HRMS (ESI): Calculated for $C_{18}H_{17}N_2O$ ($M+H^+$) 277.1341, found 277.1340.

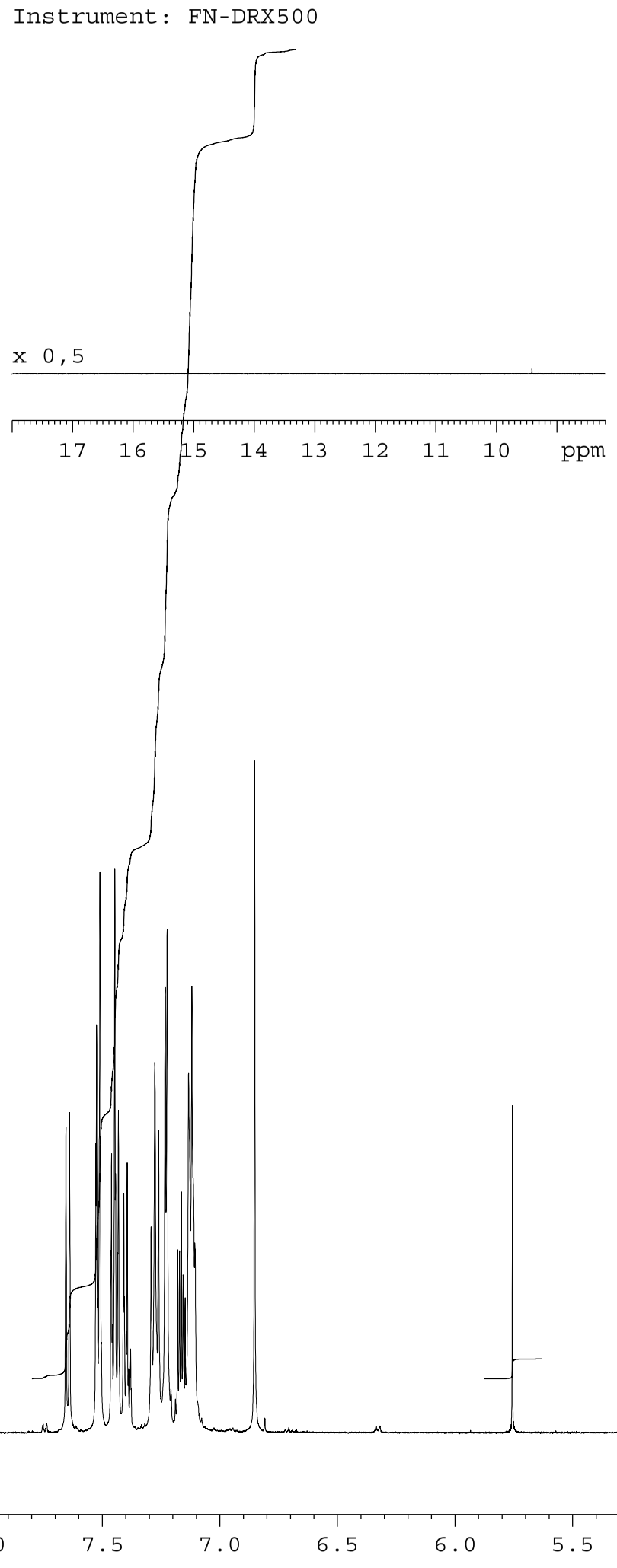


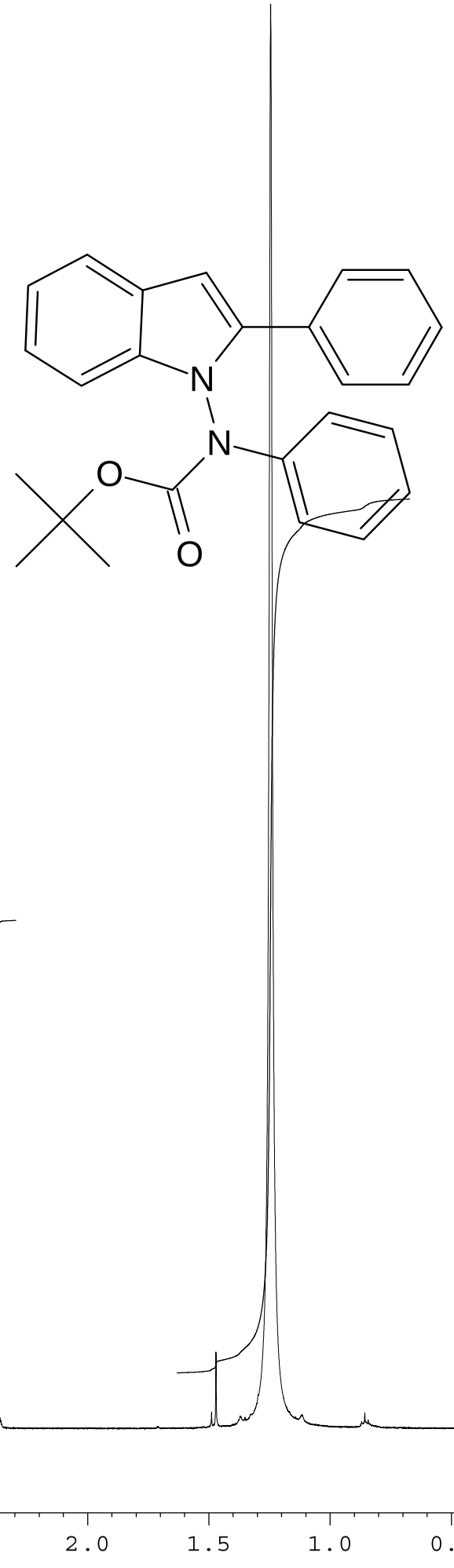
2-Phenyl-1-pyrrol-1-yl-1H-indole 3v was prepared as described in the general procedure above and obtained as a colourless crystalline solid. ^{1}H-NMR (DMSO-d_6) δ 6.28 (t, 2H, *J* = 2.3 Hz), 6.89 (d, 1H, *J* = 8.0 Hz), 6.99 (s, 1H), 7.15 (t, 2H, *J* = 2.3 Hz), 7.20-7.28 (m, 2H), 7.36, (br s, 5H), 7.72 (d, 1H, *J* = 7.6 Hz); ^{13}C-NMR (DMSO-d_6) δ 101.1, 108.1, 108.6, 120.6, 121.5, 122.5, 123.3, 125.0, 126.6, 128.1, 128.5, 129.8, 138.7, 139.2; HRMS (ESI): Calculated for $C_{18}H_{15}N_2$ ($M+H^+$) 259.1235, found 259.1232.



2-Phenyl-[1,1']biindolyl 3w was prepared as described in the general procedure above and obtained as a brown oil. ^{1}H-NMR (DMSO-d_6) δ 6.64 (d, 1H, *J* = 8.3 Hz), 6.67 (d, 1H, *J* = 8.0 Hz), 6.74 (dd, 1H, *J* = 0.8, 3.5 Hz), 7.08 (s, 1H), 7.09-7.15 (m, 2H), 7.17 (dt, 1H, *J* = 1.0, 8.3 Hz), 7.24 (dt, 1H, *J* = 1.0, 7.6 Hz), 7.27-7.32 (m, 3H), 7.40-7.44 (m, 2H), 7.71 (d, 1H, *J* = 8.0 Hz), 7.78 (d, 1H, *J* = 8.0 Hz), 7.92 (d, 1H, *J* = 3.5 Hz); ^{13}C-NMR (DMSO-d_6) δ 101.8, 102.1, 108.4, 108.8, 120.9, 121.2, 121.7, 123.1, 123.4, 125.6, 125.9, 126.9, 128.2, 128.5, 129.5, 129.9, 136.0, 138.5, 140.2; HRMS (ESI): Calculated for $C_{22}H_{17}N_2$ ($M+H^+$) 309.1392, found 309.1390.

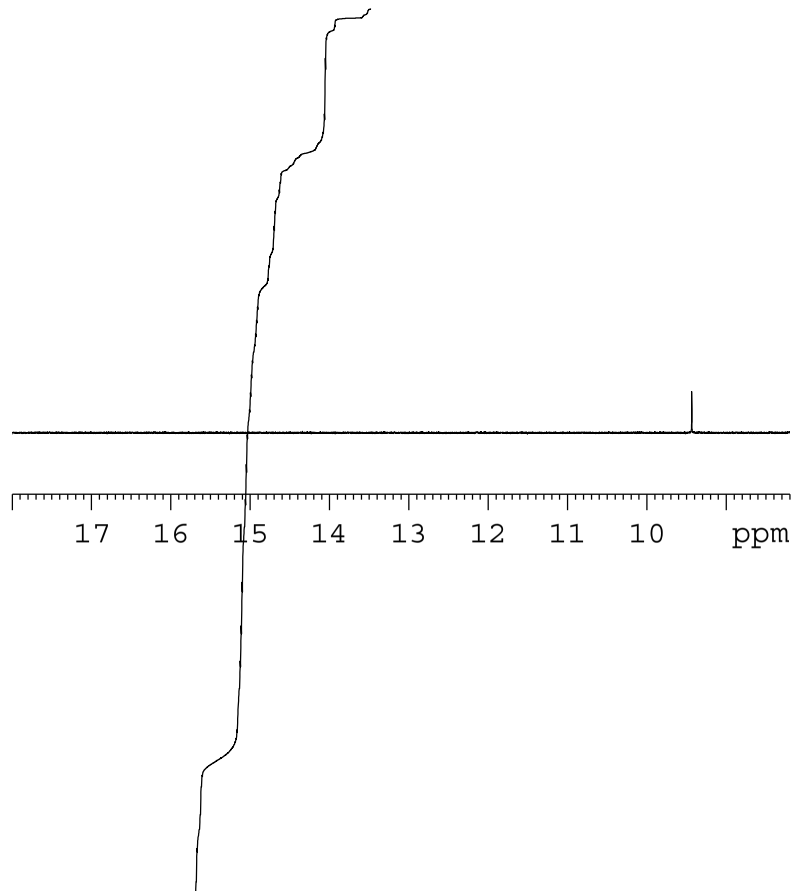
3a

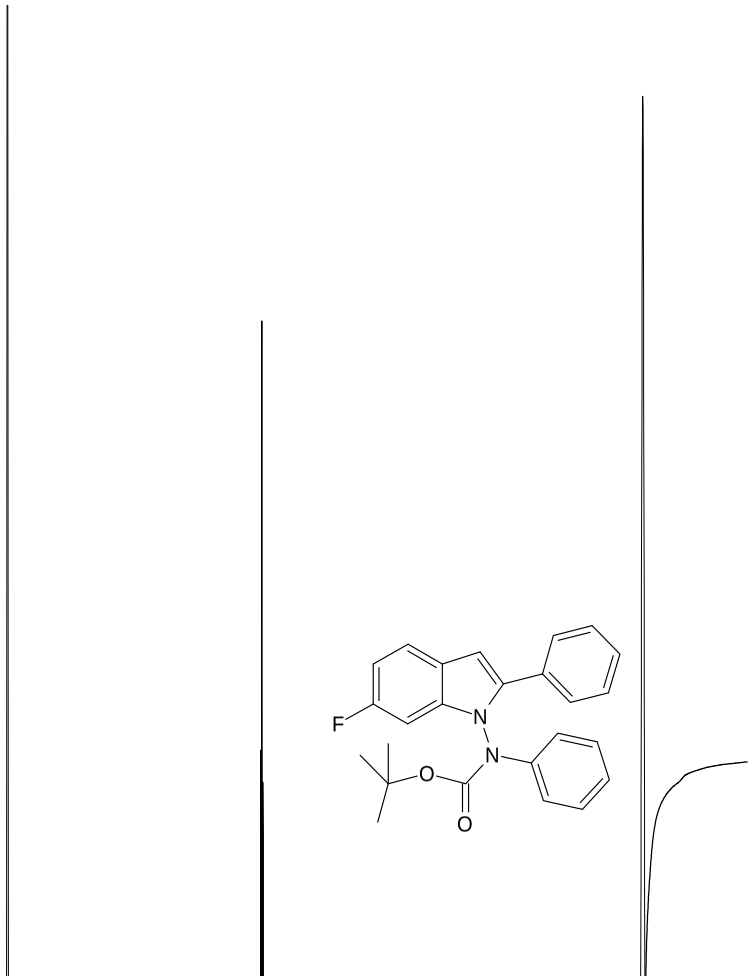


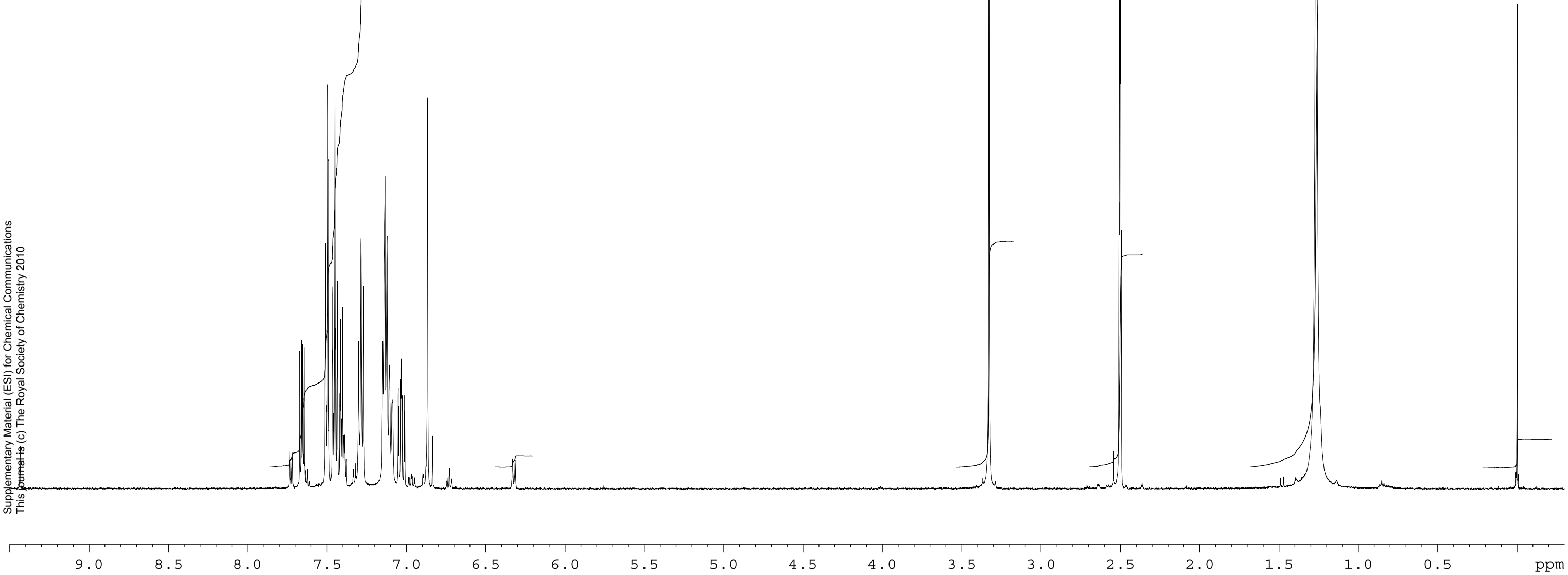


3b

Instrument: FN-ARX500

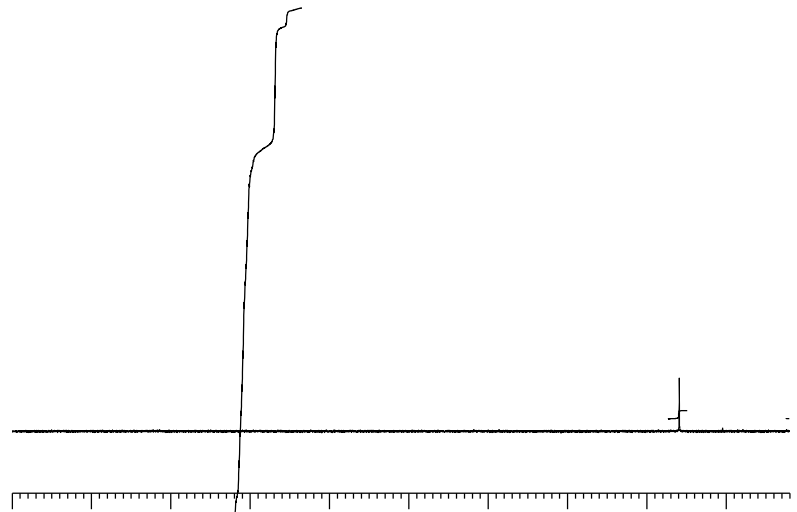


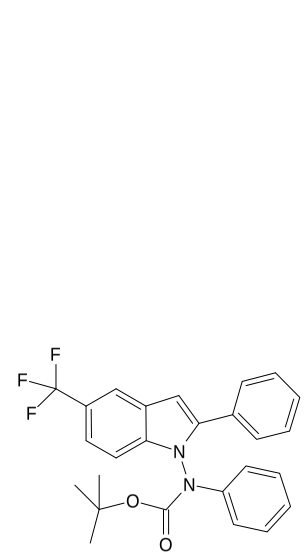




3c

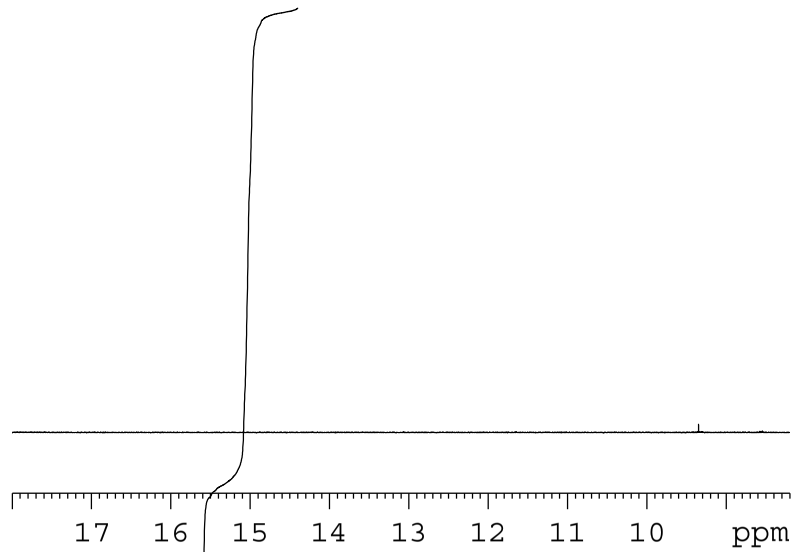
Instrument: FN-ARX500

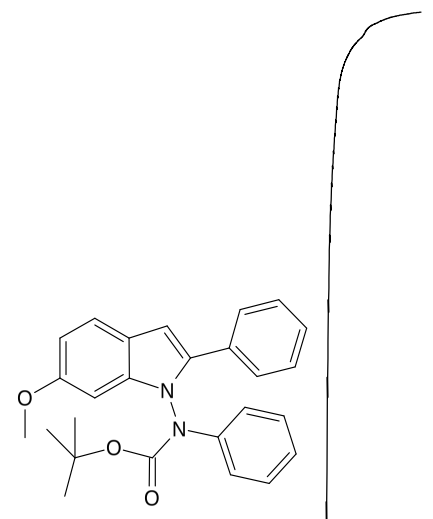




3d

Instrument: FN-ARX500





3e

Instrument: FN-DRX400

x 0,5

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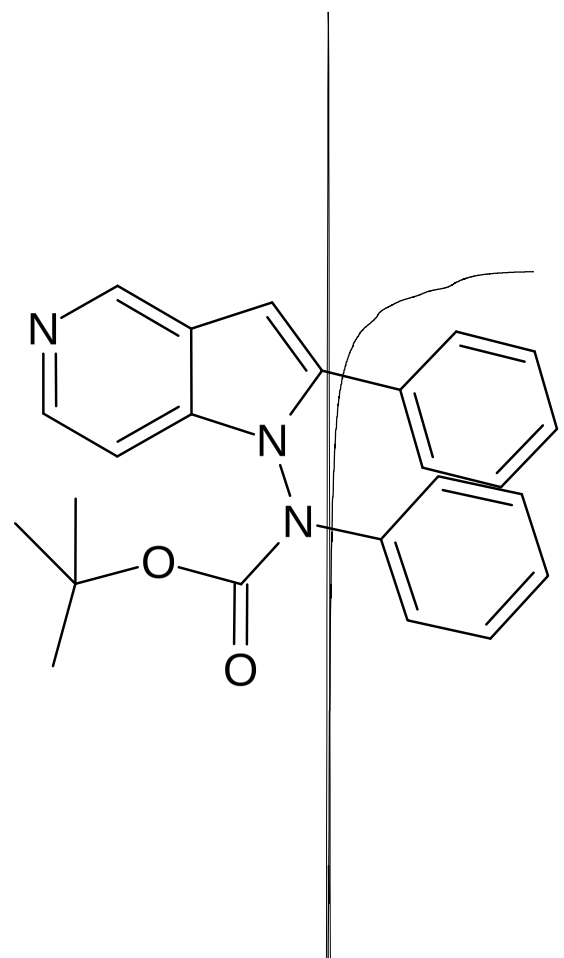

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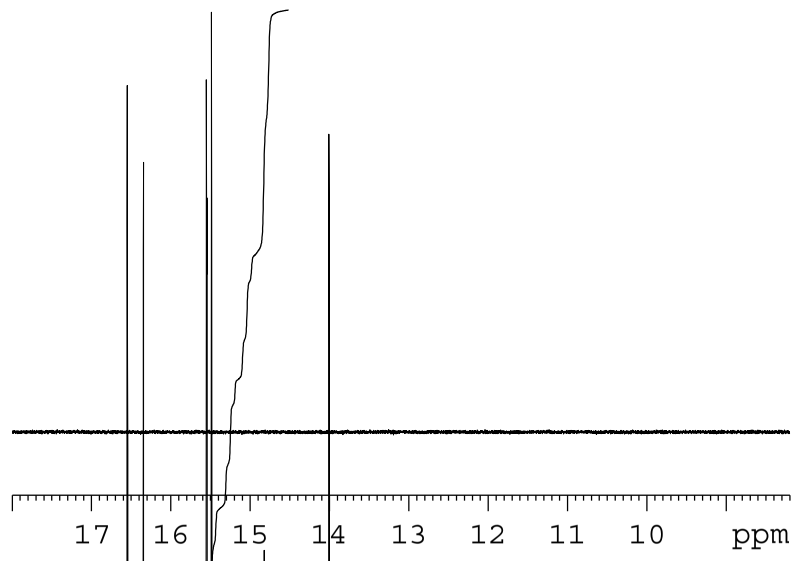
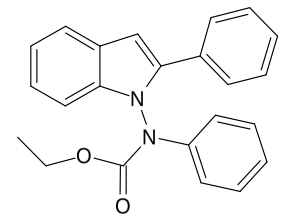
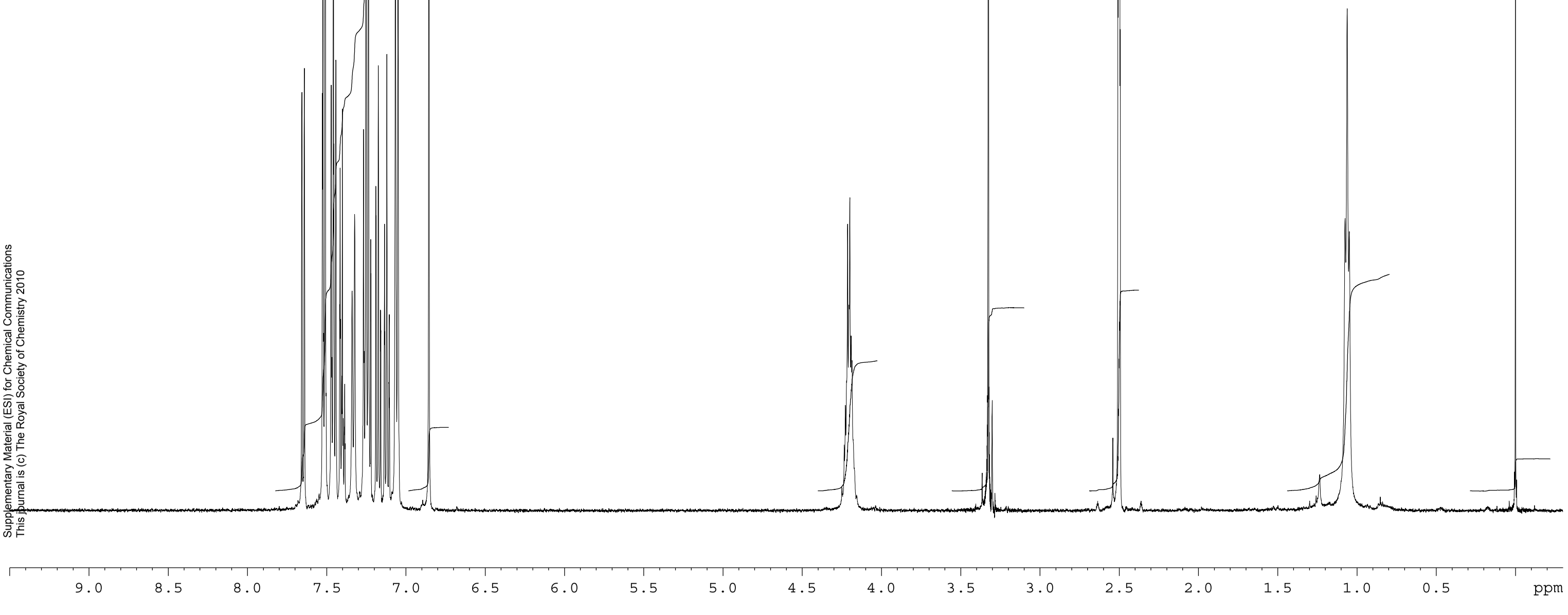
3t

Instrument: FN-ARX500

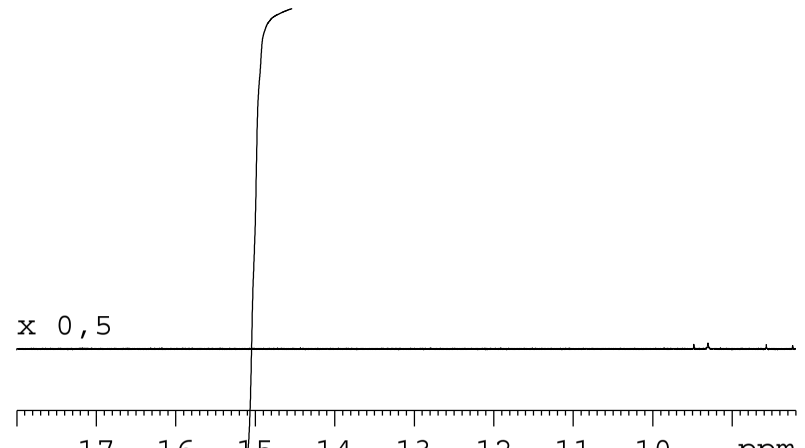


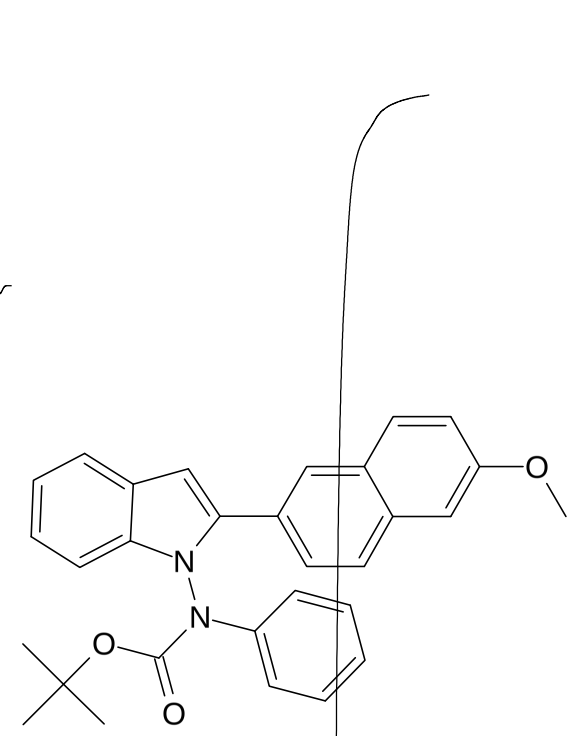




Instrument: FN-DRX500

3g

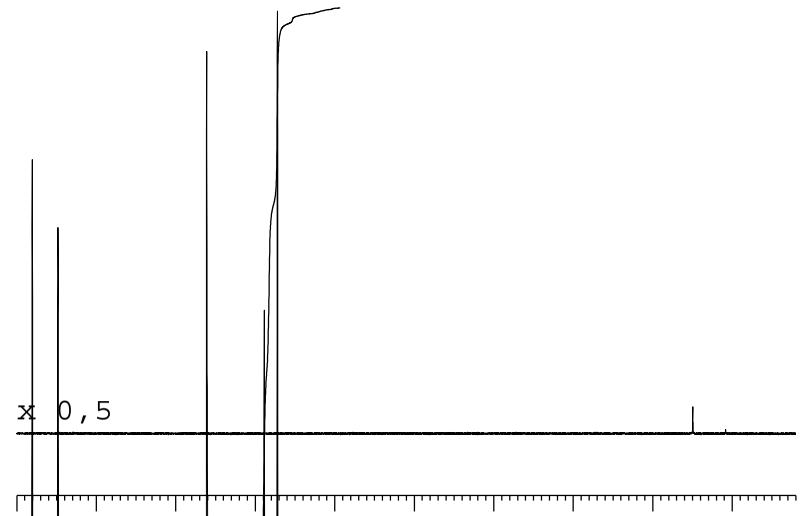


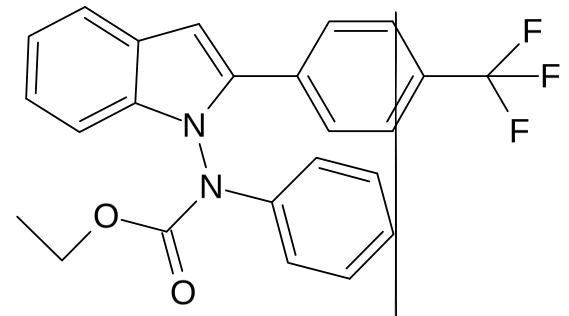


9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

3h

Instrument: FN-DRX500

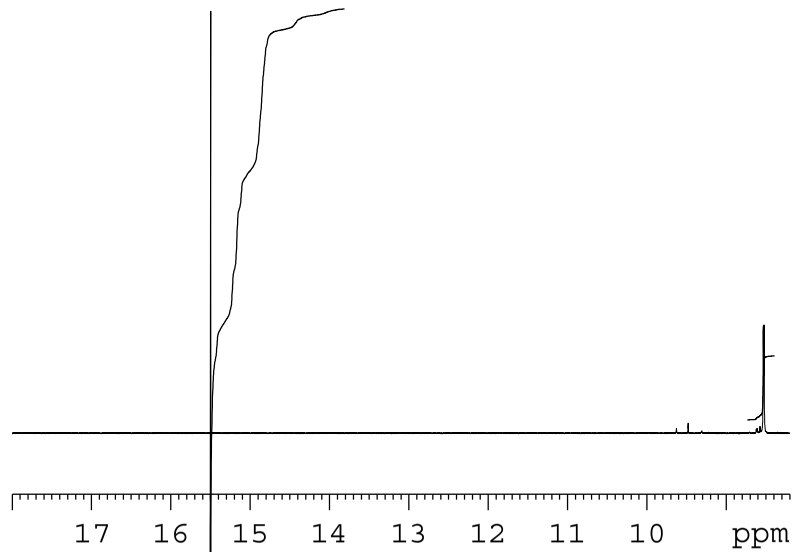


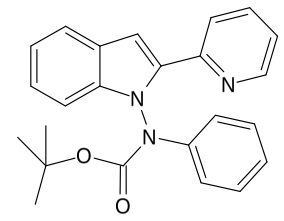


9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

3i

Instrument: FN-ARX500

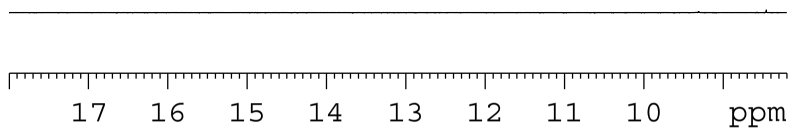


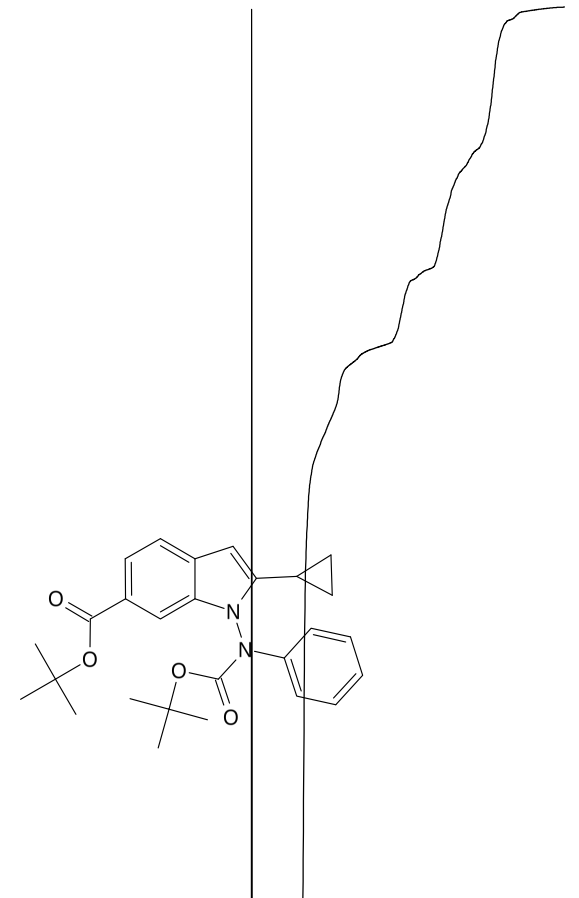


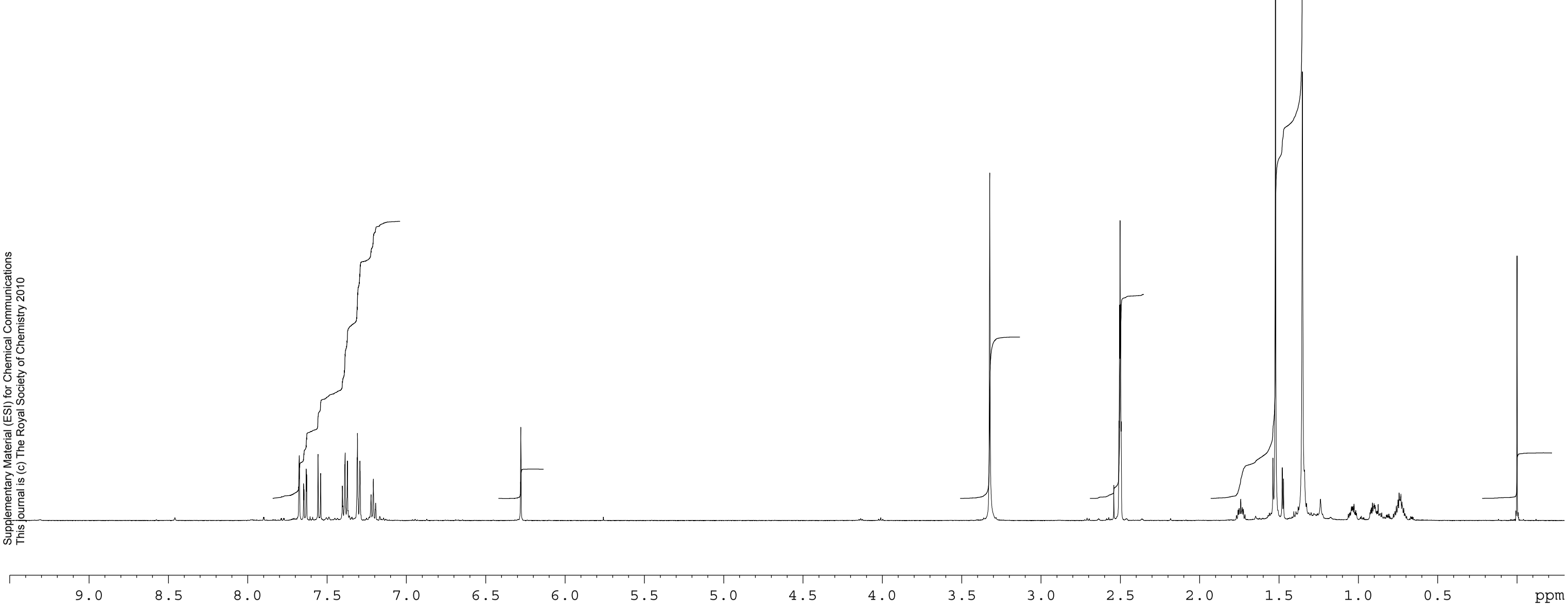
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

Instrument: FN-ARX500

3j

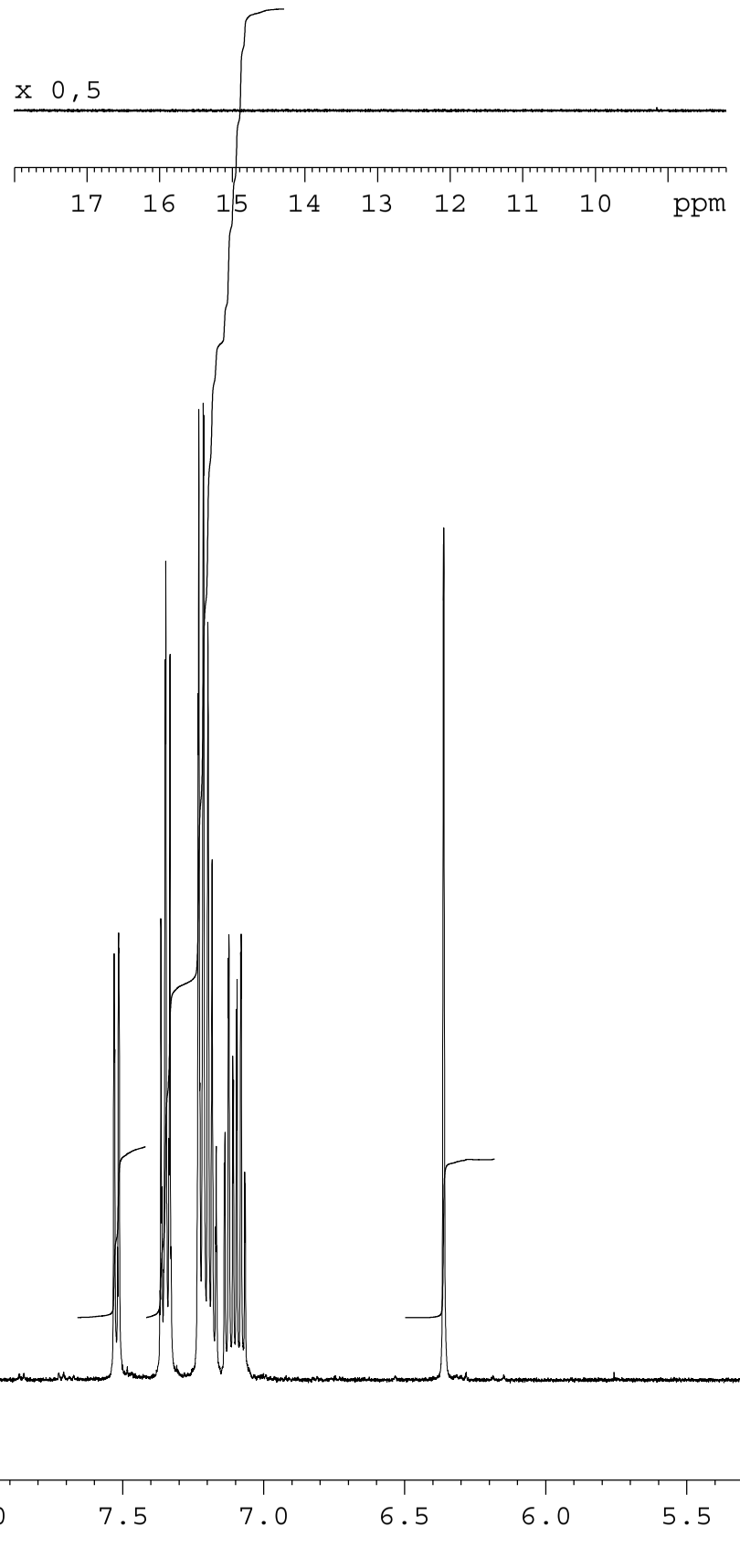


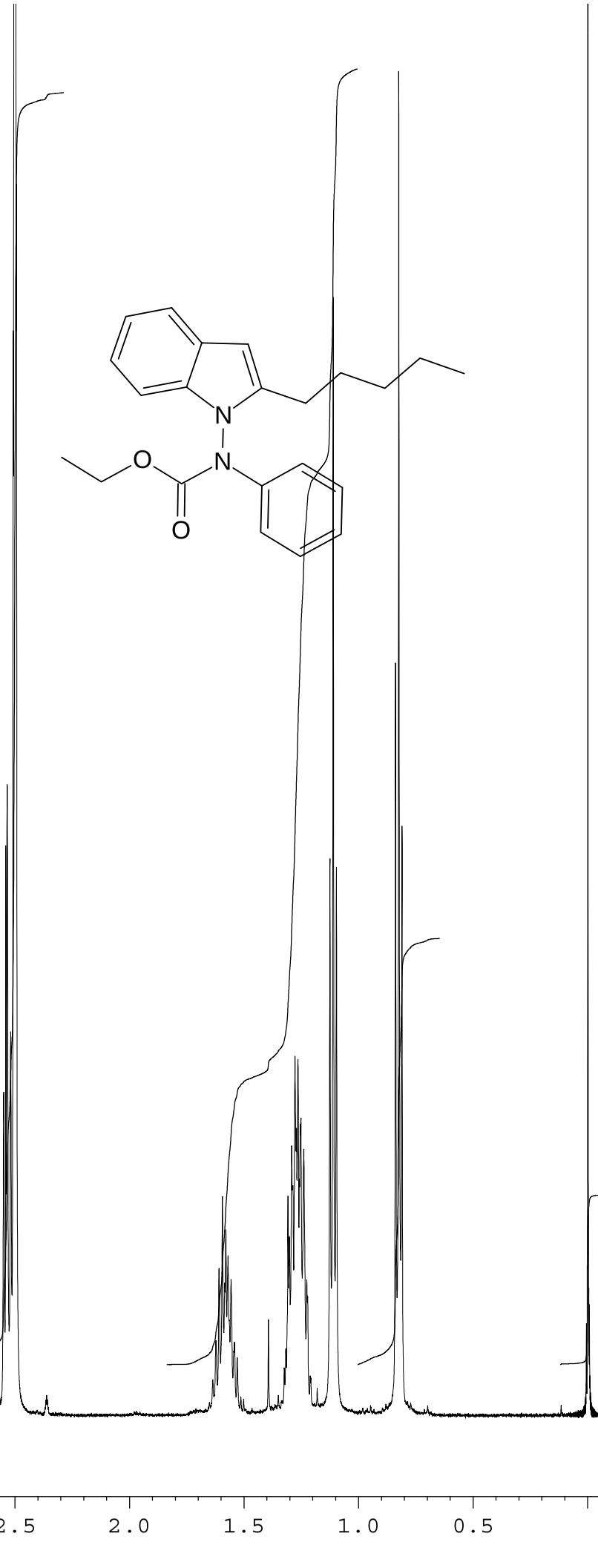




Instrument: FN-DRX500

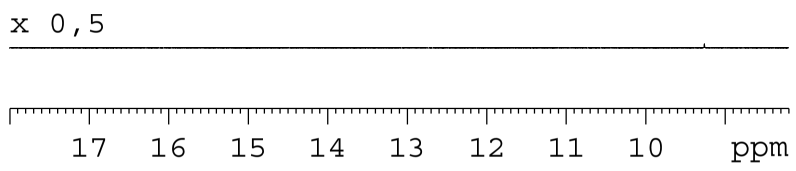
3k

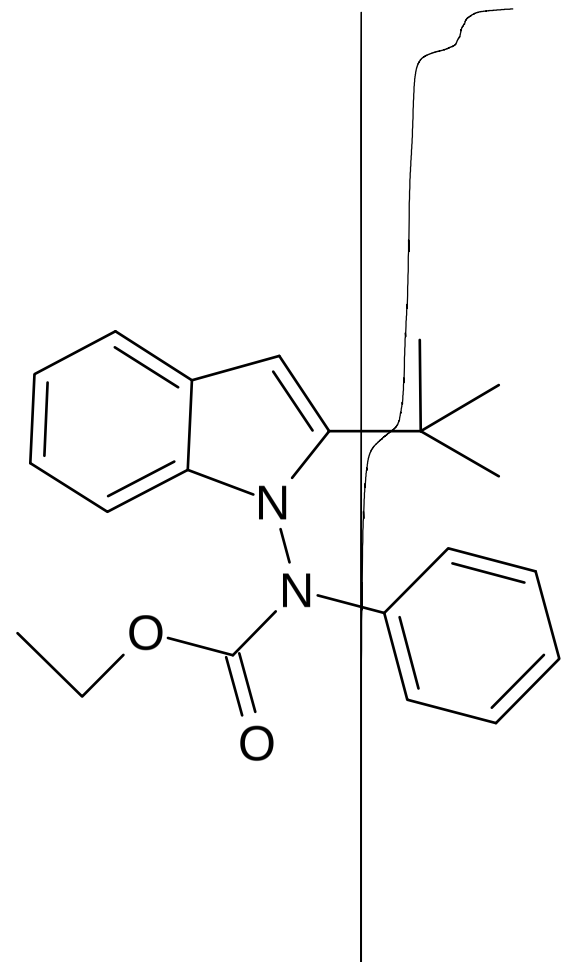


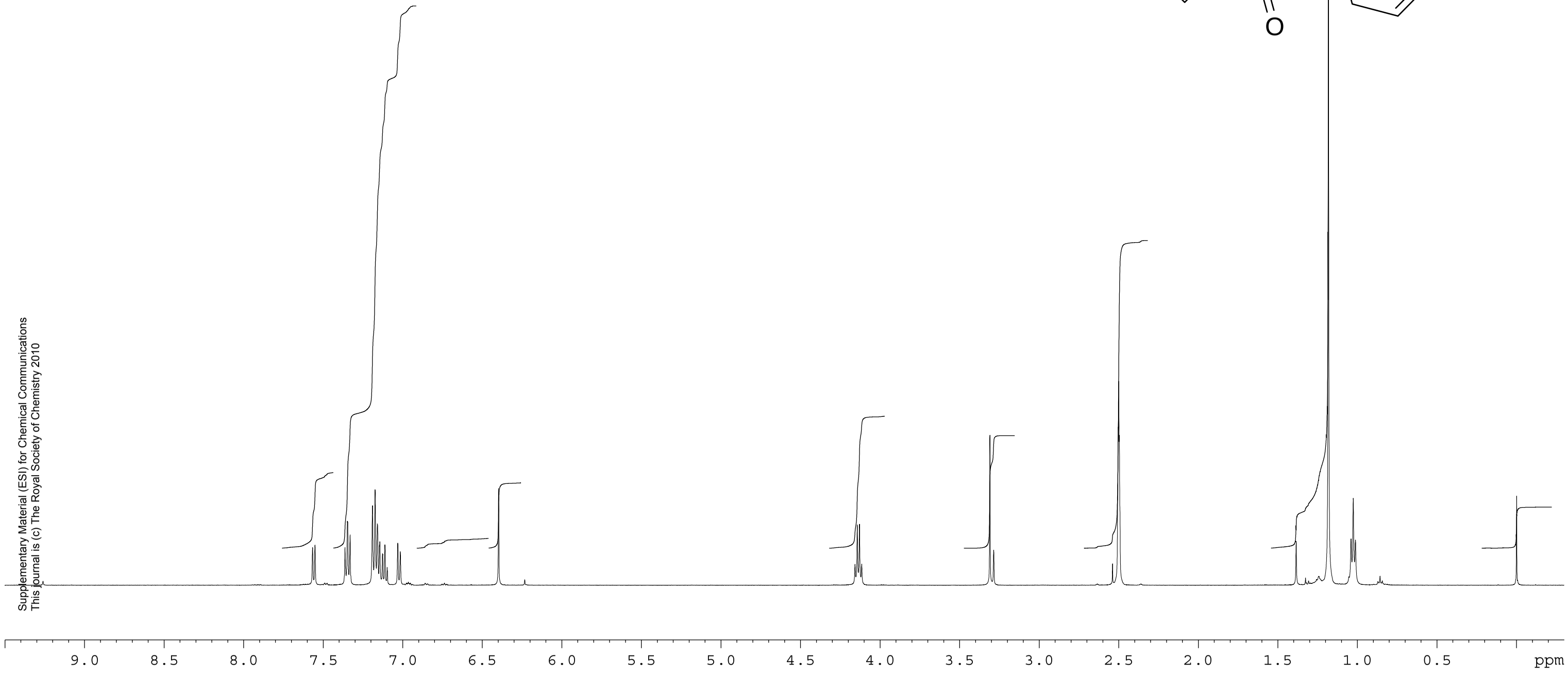


Instrument: FN-DRX500

3 L







Instrument: FN-DRX500

3m

x 0,5

17 16 15 14 13 12 11 10 ppm

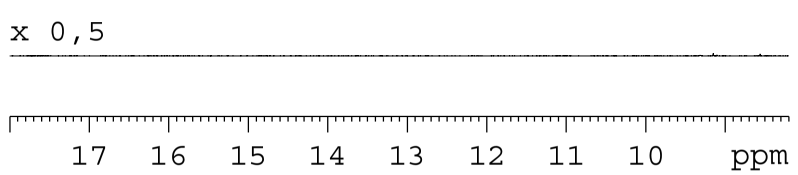
No Structure Found

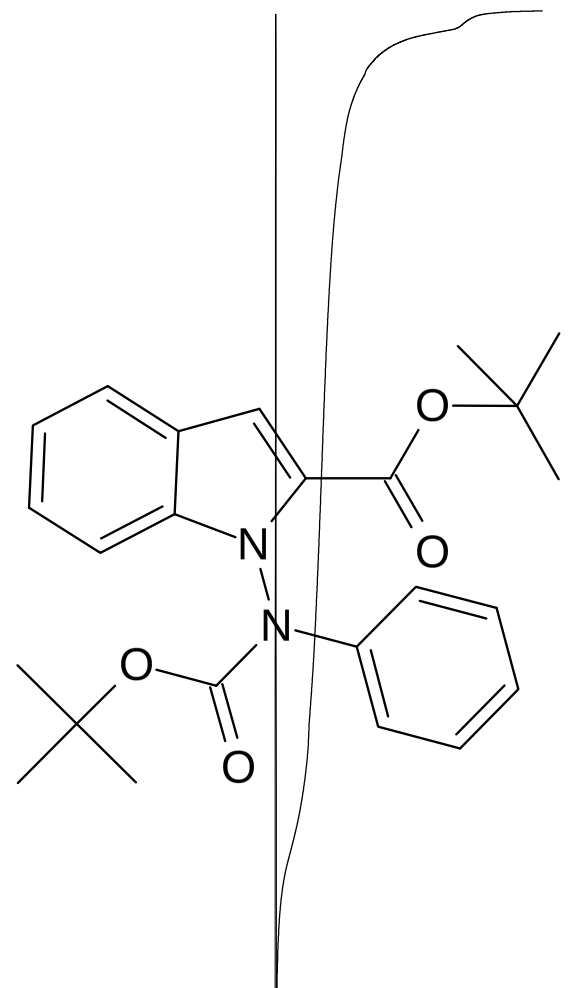
Strukturvorschlag MedChem

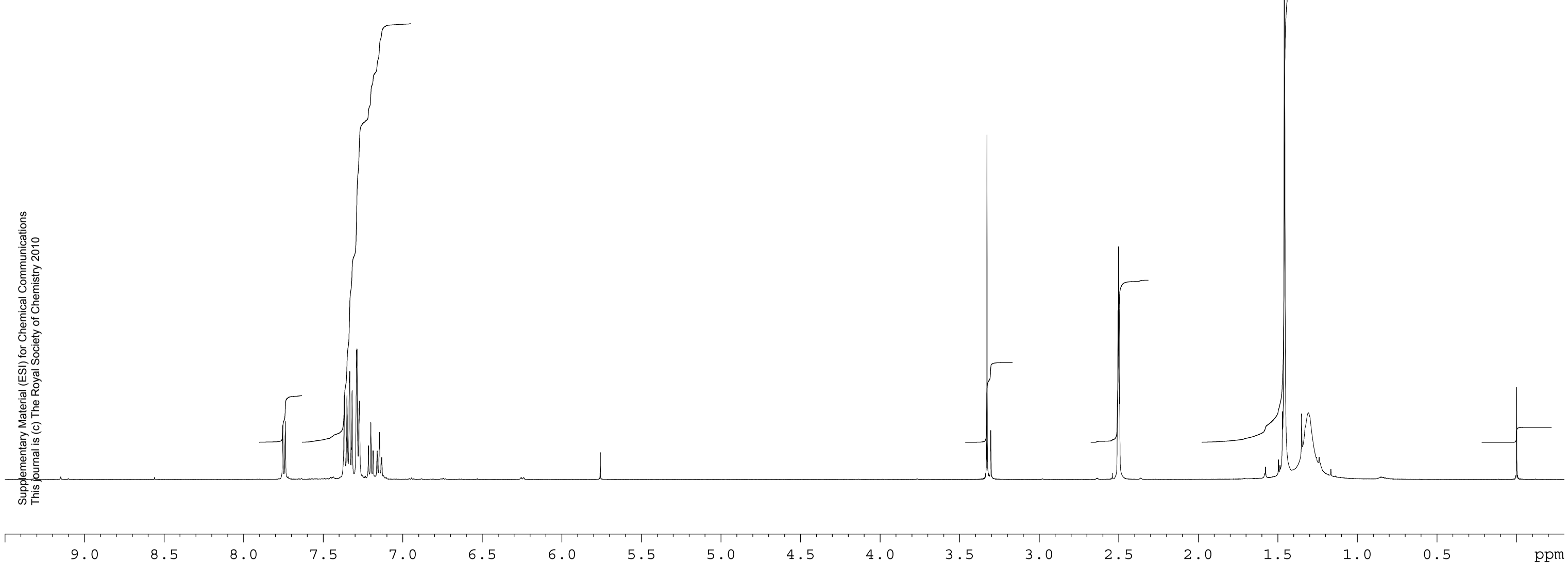
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

Instrument: FN-DRX500

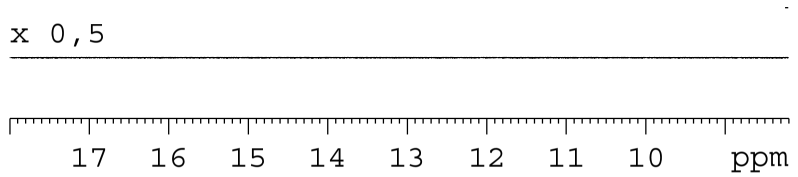
3n





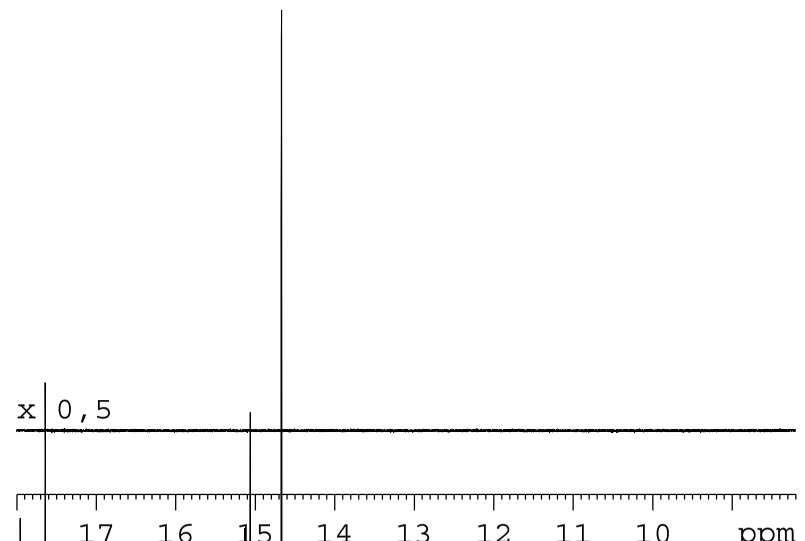


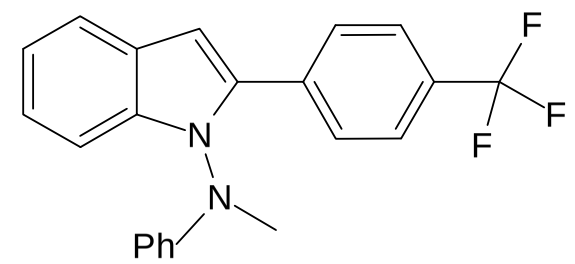
Instrument: FN-DRX500



3p

Instrument: FN-DRX500





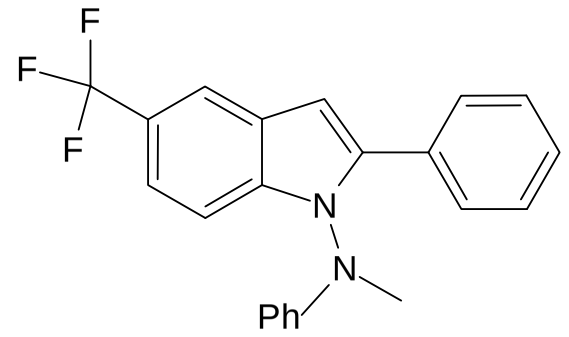
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

3q

Instrument: FN-DRX500

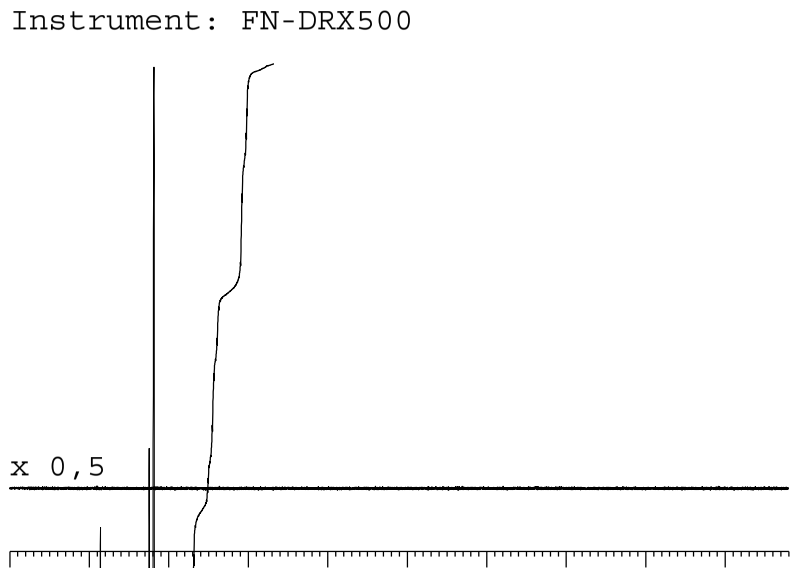
x 0,5

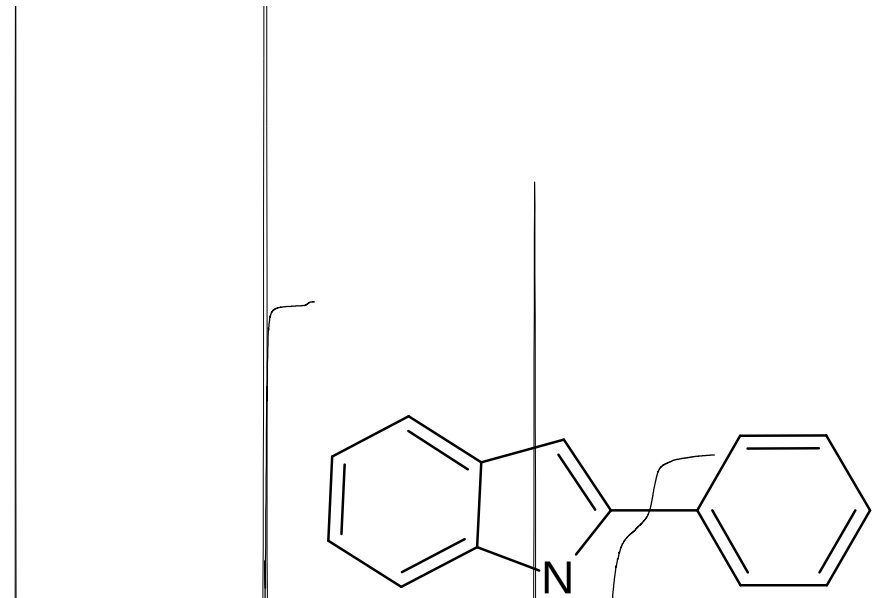
17 16 15 14 13 12 11 10 ppm

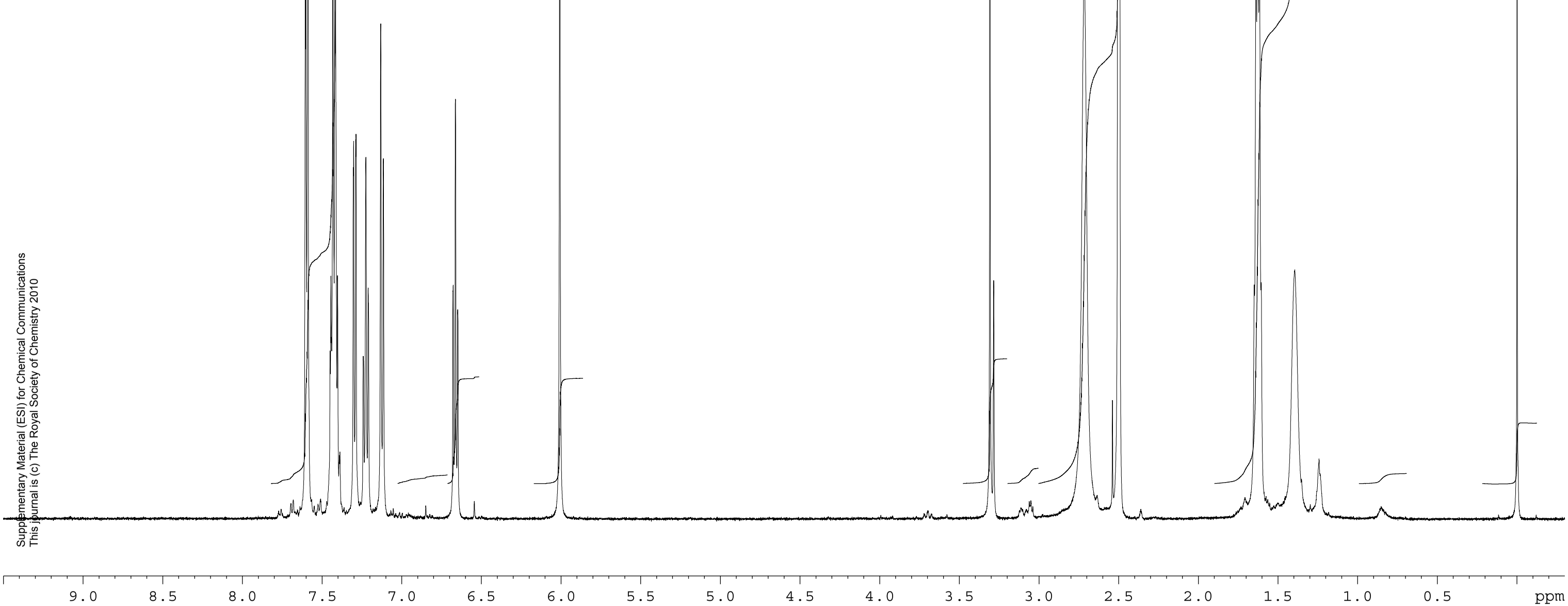


9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

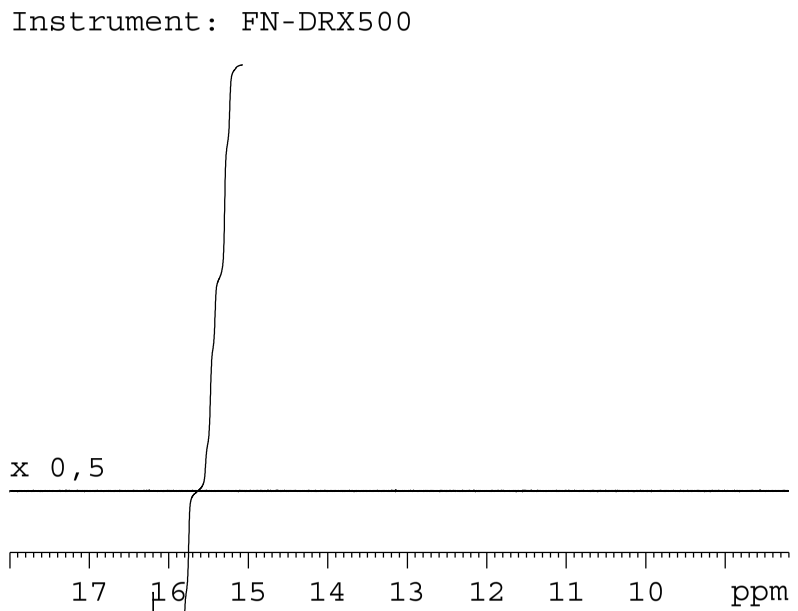
3r

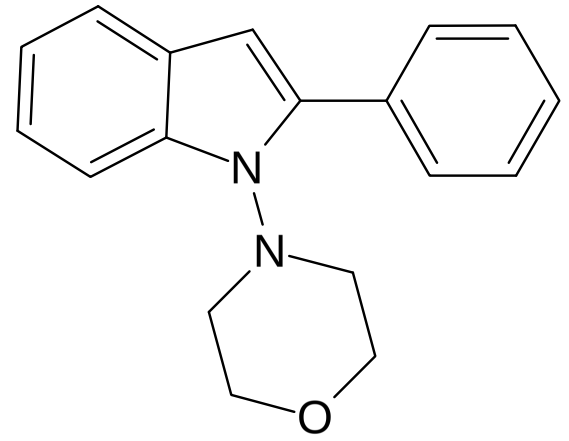






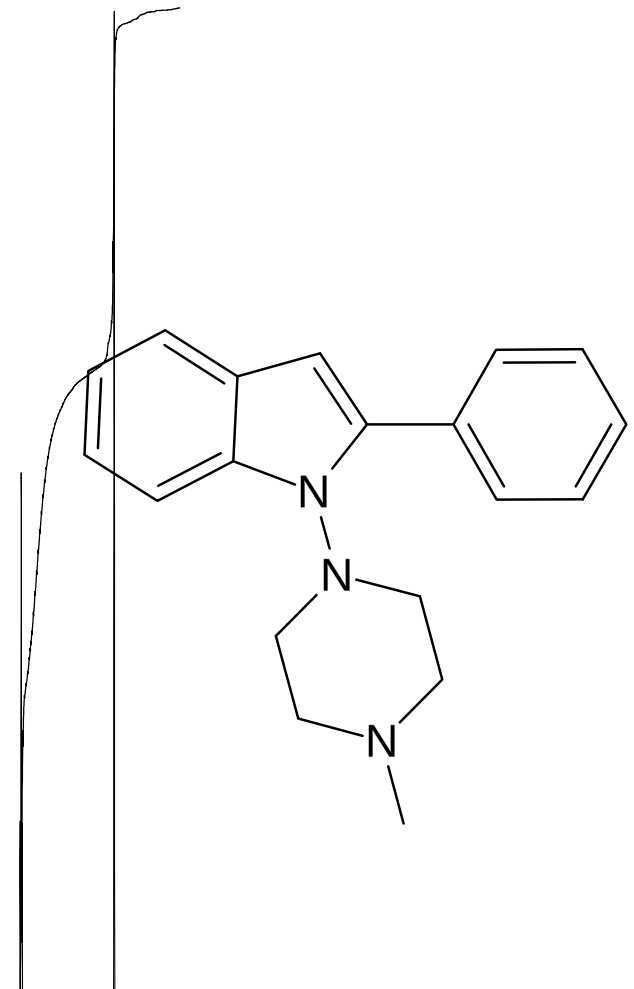
3s





Instrument: FN-DRX500

3t

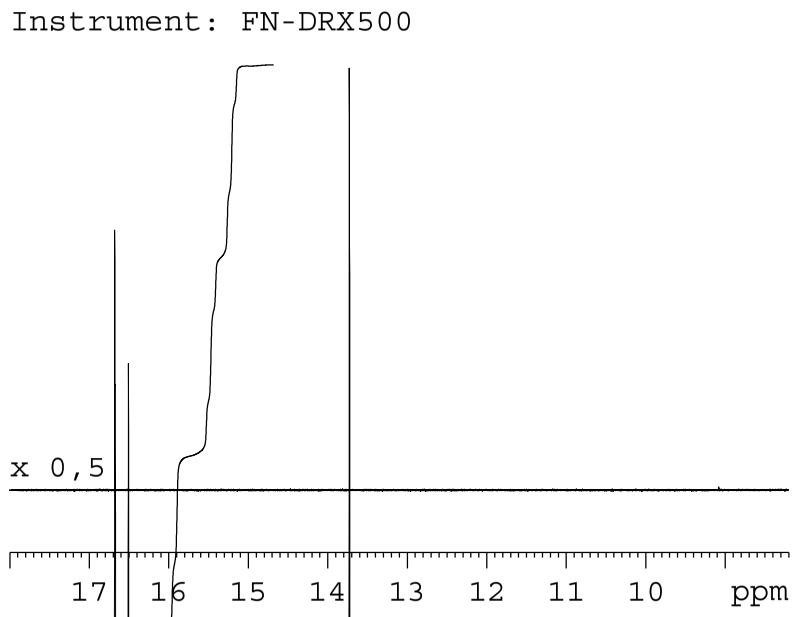


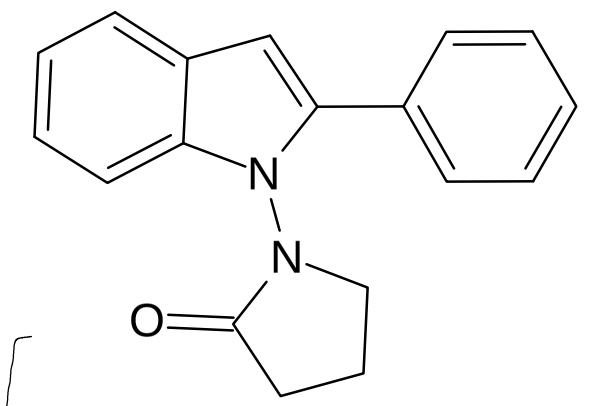
x 0,5

17 16 15 14 13 12 11 10 ppm

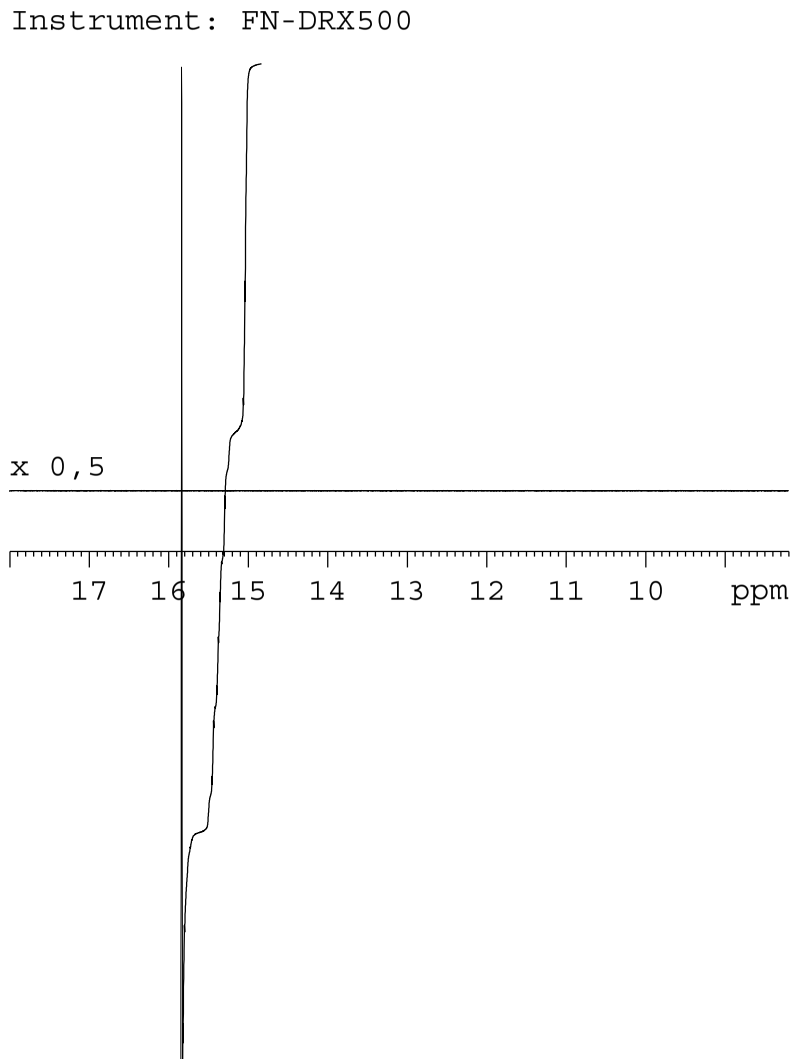
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

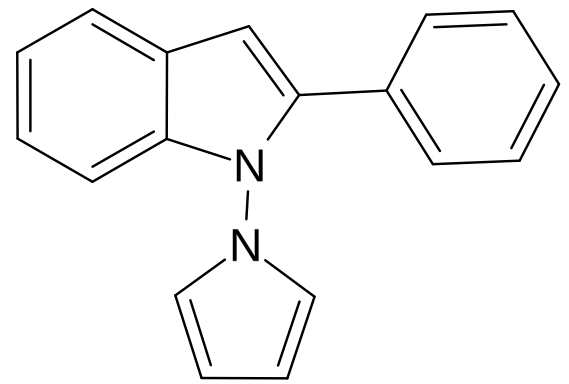
3u

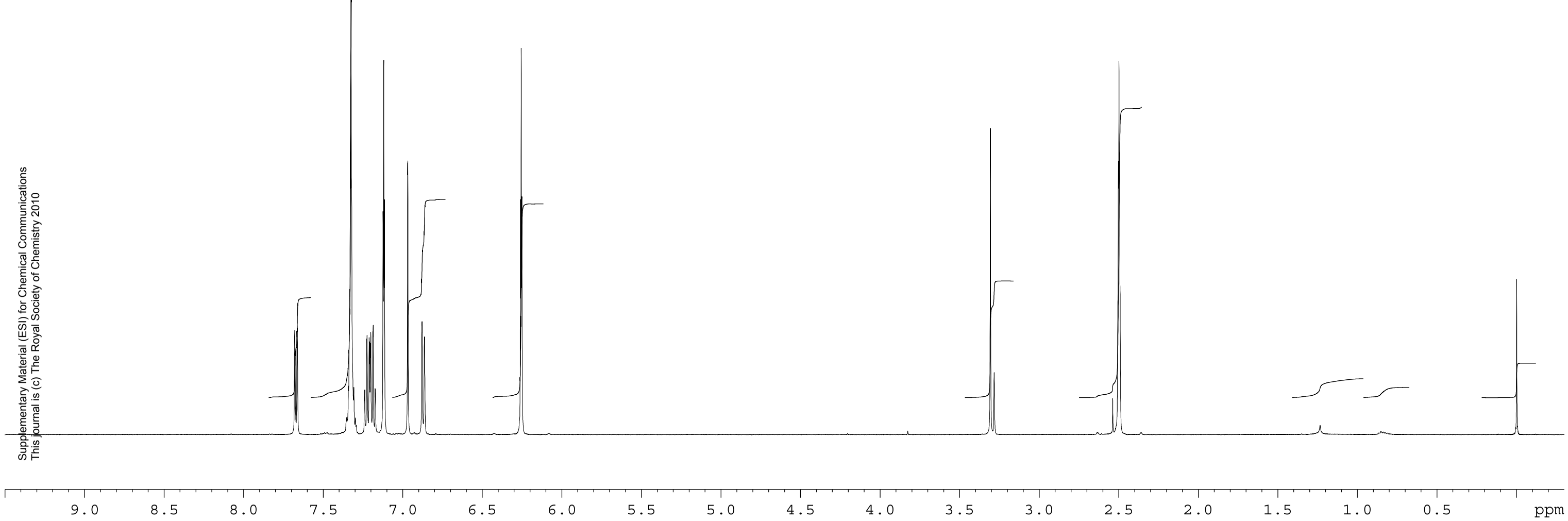




3v





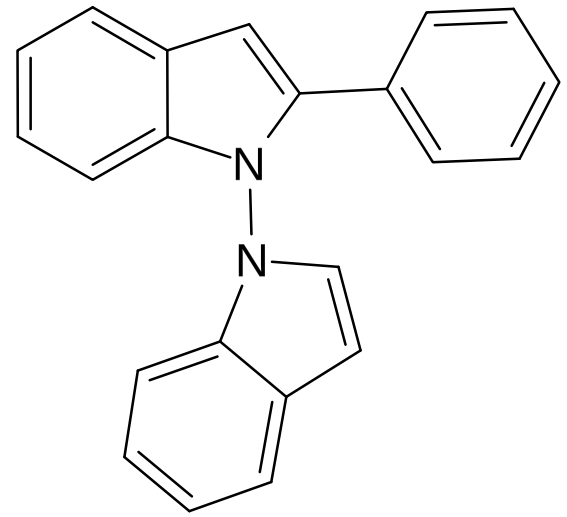


3w

Instrument: FN-DRX500

x 0,5

17 16 15 14 13 12 11 10 ppm



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