One-Pot Synthesis of 2-Amino-indole-3-carboxamide and Analogous

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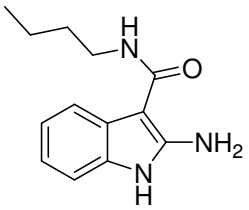
Supporting Information

General Information. All reactions were under air atmosphere. All cyanoacetamides are prepared as the procedure described in the reference. [1] All other reagents and solvents are purchased without further purification. Analytical thin-layer chromatography (TLC) was preformed on SiO_2 plates on Alumina available from Whatman. Visualization was accomplished by UV irradiation at 254 nm, or by staining with any one of the following reagents: iodine, ninhydrin (0.3% w/v in glacial acetic acid/*n*-butyl alcohol 3:97), Vaughn's reagent (4.8 g of $(NH_4)_6Mo_7O_{24}\bullet 4H_2O$ and 0.2 g of $Ce(SO_4)_2\bullet 4H_2O$ in 10 mL of conc. H_2SO_4 and 90 mL of H_2O). Flash column chromatography was performed using SiO_2 60 (particle size 0.040-0.055 mm, 230-400 mesh, EMD science distributed by Bioman), Preparative TLC was conducted using Preparative Silica gel TLC plates (1000 μm, 20cm×20cm).
Proton and carbon NMR spectra were obtained on Bruker Avance™ 600 MHz NMR spectrometer. Chemical shifts are reported as δ values in parts per million (ppm) as referenced to residual solvent. 1H NMR spectra are tabulated as follows: chemical shift, multiplicity (s = singlet, bs = broad singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant(s), and number of protons. High Resolution Mass spectra were obtained at the University of Pittsburgh Mass Spectrometry facility. LC-MS analysis was performed on an SHIMADZU instrument, using an analytical C18 column (Dionex Acclaim 120 Å, 2.1 × 50 mm, 3.0 μm, 0.2 mL/min).

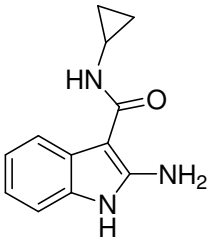
One-pot procedure for preparation of 2-amino-1H-indole-3-carboxamide (3-n, n = 1-23): In a 50 ml flask equipped with stir bar added cyanoacetamide (2a-n, 1.0 mmol, 1.0

[1] Wang, K.; Nguyen, K.; Huang, Y. J.; Doemling, A. *J. Comb. Chem.* **2009**, *11*, 920-927.

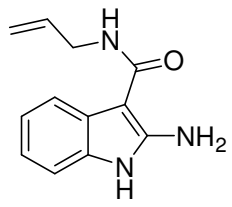
equiv.) in dry DMF (0.2 M) and NaH (60% dispersion in mineral oil, 1.0 equiv.). After 10 min, 2-fluoronitrobenzene or analogous (1.0 equiv.) was added and the reaction was stir at room temperature for 24 h. The reaction becomes deep purple. Then 0.2 N HCl (1.0 equiv.) was added following $FeCl_3$ (3 equiv.) and Zn dust (10 equiv.). The reaction was heated to 100 ^oC for 1 h. Cool the reaction down and the crude reaction was added 20 ml water. The crude reaction was filtered, washed with 25 ml ethyl acetate. The solution was extracted with ethyl acetate (20 ml X 2). The combined organic phase was washed by 0.2 N HCl 10 ml and brine 10 ml. The organic phase was dried with anhydrous sodium sulfate and the solvent was removed. The crude product was purified with chromatography.



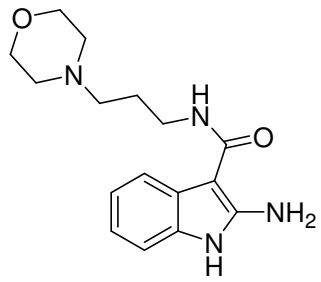
2-Amino-*N*-butyl-1H-indole-3-carboxamide (3-1): The crude product was purified by short silica gel column chromatography with 5% methanol in ethyl acetate as yellow oil. HRMS ESL-TOF for $C_{13}H_{17}N_3ONa$ ($M+Na^+$) found: *m/z*: 254.1288; Calc. Mass 254.1269; ^1H NMR (*DMSO-d*$_6$, 600 MHz): δ 10.54 (s, 1H), 7.53 (d, J = 7.8 Hz, 1H), 7.10 (d, J = 7.8 Hz, 1H), 6.93 (t, J = 7.8 Hz, 1H), 6.85 (t, J = 7.8 Hz, 1H), 6.70 (s, 2H), 6.67 (t, J = 6.6 Hz, 1H), 3.27 (m, 2H), 1.51 (m, 2H), 1.32 (m, 2H), 0.91 (t, J = 7.2 Hz, 3H) ppm; ^{13}C NMR (*DMSO-d*$_6$, 150 MHz): δ 167.2, 152.8, 132.7, 125.7, 120.2, 118.8, 116.8, 110.1, 86.8, 38.5, 32.5, 20.2, 14.3 ppm.



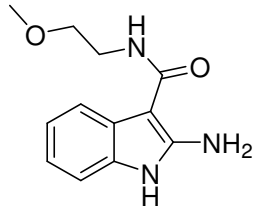
2-Amino-*N*-cyclopropyl-1H-indole-3-carboxamide (3-2): The crude product was purified by short silica gel column chromatography with 5% methanol in ethyl acetate as light yellow oil. HRMS ESL-TOF for $C_{12}H_{14}N_3O$ ($M+H^+$) found: *m/z*: 216.1128; Calc. Mass 216.1137. ^1H NMR ($CDCl_3$, 600 MHz): δ 9.95 (s, 1H), 7.12 (d, J = 7.8 Hz, 1H), 7.02 (d, J = 7.8 Hz, 1H), 6.98 (t, J = 7.8 Hz, 1H), 6.89 (t, J = 7.8 Hz, 1H), 6.26 (s, 2H), 5.92 (s, 1H), 2.80 (m, 1H), 0.72-0.75 (m, 2H), 0.55-0.58 (m, 1H) ppm; ^{13}C NMR ($CDCl_3$, 150 MHz): δ 169.7, 152.6, 132.5, 125.1, 121.0, 119.9, 115.7, 110.3, 87.1, 22.4, 7.1 ppm.



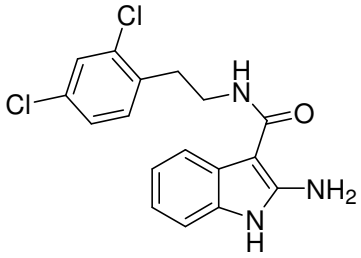
***N*-Allyl-2-amino-1H-indole-3-carboxamide (3-3):** The crude product was purified by silica gel chromatography with 5% methanol in ethyl acetate light yellow oil. HRMS ESL-TOF for $C_{12}H_{13}N_3ONa$ ($M+Na^+$) found: *m/z*: 238.0967; Calc. Mass 238.0956; ^1H NMR (*DMSO-d*$_6$, 600 MHz): δ 10.64 (s, 1H), 7.63 (d, J = 7.8 Hz, 1H), 7.17 (d, J = 7.8 Hz, 1H), 6.99 (t, J = 7.8 Hz, 1H), 6.80-6.94 (m, 2H), 6.90 (s, 2H), 5.95-6.01 (m, 1H), 5.16 (d, J = 17.2 Hz, 1H), 5.14 (d, J = 10.2 Hz, 1H), 3.96 (s, 2H) ppm; ^{13}C NMR (*DMSO-d*$_6$, 150 MHz): δ 166.5, 152.5, 136.9, 132.2, 125.1, 119.8, 118.4, 116.3, 114.2, 109.6, 86.1, 40.7 ppm.



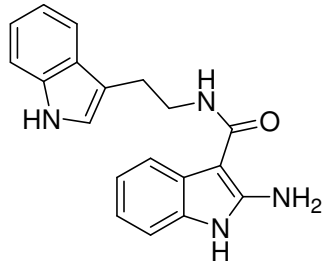
2-Amino-*N*-(3-morpholinopropyl)-1H-indole-3-carboxamide (3-4): The crude product was purified by silica gel chromatography with 50% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{16}H_{23}N_4O_2$ ($M+H^+$) found: *m/z*: 303.1835; Calc. Mass 303.1821; ^{1}H NMR (*DMSO-d*$_6$, 600 MHz): δ 10.56 (s, 1H), 7.53 (d, J = 7.8 Hz, 1H), 7.10 (d, J = 7.8 Hz, 1H), 6.93 (t, J = 7.8 Hz, 1H), 6.85 (t, J = 7.8 Hz, 1H), 6.76 (t, J = 5.4 Hz, 1H), 6.70 (s, 2H), 3.56 (t, J = 4.2 Hz, 4H), 3.31 (m, 2H), 2.34 (m, 6H), 1.69 (m, 2H) ppm; ^{13}C NMR (*DMSO-d*$_6$, 150 MHz): δ 167.2, 152.8, 132.7, 125.6, 120.2, 118.9, 116.8, 110.1, 86.8, 66.6, 57.1, 53.9, 37.7, 26.9 ppm.



2-Amino-*N*-(2-methoxyethyl)-1H-indole-3-carboxamide (3-5): The crude product was purified by silica gel chromatography with 5% methanol in ethyl acetate as yellow solid. ESL-TOF for $C_{12}H_{16}N_3O_2$ ($M+H^+$) found: *m/z*: 234.1232; Calc. Mass 234.1243; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 8.60 (s, 1H), 7.34 (d, J = 7.8 Hz, 1H), 7.13 (t, J = 7.8 Hz, 1H), 7.12 (d, J = 7.8 Hz, 1H), 7.02 (d, J = 7.8 Hz, 1h), 6.22 (t, J = 5.4 Hz, 1H), 6.03 (s, 2H), 3.68 (q, J = 5.4 Hz, 2H), 3.59 (t, J = 5.4 Hz, 2H), 3.43 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 150 MHz): δ 167.8, 151.7, 132.2, 125.2, 121.2, 119.9, 116.0, 110.1, 87.8, 71.7, 58.9, 38.8 ppm.

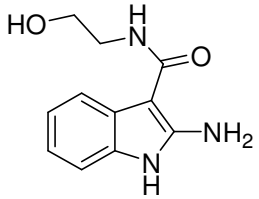


2-Amino-*N*-(2,4-dichlorophenethyl)-1H-indole-3-carboxamide (3-6): The crude product was purified by silica gel chromatography with 5% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{17}H_{15}Cl_2N_3ONa$ ($M+Na^+$) found: *m/z*: 370.0467; Calc. Mass 370.0490; ^{1}H NMR (*DMSO-d*$_6$, 600 MHz): δ 10.56 (s, 1H), 7.57 (s, 1H), 7.48 (d, J = 7.8 Hz, 1H), 7.32-7.40 (m, 2H), 7.10 (d, J = 7.2 Hz, 1H), 6.92 (t, J = 7.8 Hz, 1H), 6.85 (t, J = 7.8 Hz, 1H), 6.82 (t, J = 6.0 Hz, 1H), 6.71 (s, 2H), 3.52 (q, J = 6.0 Hz, 2H), 2.97 (t, J = 7.2 Hz, 2H) ppm; ^{13}C NMR (*DMSO-d*$_6$, 150 MHz): δ 167.2, 152.9, 137.1, 134.6, 132.8, 132.7, 131.9, 129.1, 127.7, 125.6, 120.2, 118.9, 116.8, 110.1, 86.7, 38.5, 33.5 ppm;

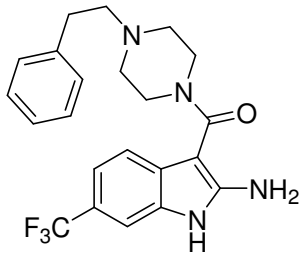


***N*-(2-(1H-indol-3-yl)ethyl)-2-amino-1H-indole-3-carboxamide (3-7):** The crude product was purified by silica gel chromatography with 10% methanol in ethyl acetate as dark yellow solid. HRMS ESL-TOF for $C_{19}H_{18}N_4ONa$ ($M+Na^+$) found: *m/z*: 341.1365; Calc. Mass 341.1378. ^{1}H NMR (*DMSO-d*$_6$, 600 MHz): δ 10.95 (s, 1H), 10.73 (s, 1H), 7.71 (d, J = 7.2 Hz, 1H), 7.49 (d, J = 7.2 Hz, 1H), 7.40 (d, J = 7.2 Hz, 1H), 7.26 (s, 1H), 7.16 (d, J = 7.2 Hz, 1H), 7.13 (t, J = 7.2 Hz, 1H), 7.05 (t, J = 7.2 Hz, 1H), 6.97 (t, J = 7.2 Hz, 1H), 6.91 (t, J = 7.2 Hz, 1H),

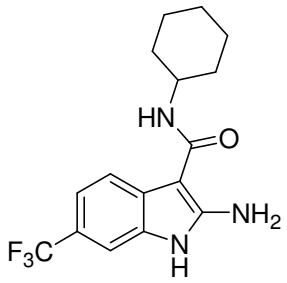
6.81 (s, 3H), 3.63 (s, 2H), 3.03 (t, J = 6.0 Hz, 2H) ppm; ^{13}C NMR (*DMSO-d*$_6$, 150 MHz): δ 166.7, 152.4, 136.2, 132.2, 127.9, 125.1, 122.5, 120.9, 119.7, 118.5, 118.3, 118.1, 116.2, 112.2, 111.3, 109.6, 86.3, 25.9 ppm.



2-Amino-*N*-(2-hydroxyethyl)-1H-indole-3-carboxamide (3-8): The crude product was purified by silica gel chromatography with 15% methanol in ethyl acetate as yellow oil. HRMS ESL-TOF for $C_{11}H_{13}N_3O_2Na$ (M+Na$^+$) found: *m/z*: 242.0916; Calc. Mass 242.0905; ^{1}H NMR (*DMSO-d*$_6$, 600 MHz): δ 10.58 (s, 1H), 7.49 (d, J = 7.2 Hz, 1H), 7.12 (d, J = 7.2 Hz, 1H), 6.95 (t, J = 7.2 Hz, 1H), 6.86 (t, J = 7.2 Hz, 1H), 6.73 (s, 2H), 6.63 (t, J = 6.0 Hz, 1H), 4.80 (t, J = 5.4 Hz, 1H), 3.52 (q, J = 6.0 Hz, 2H), 3.37 (q, J = 6.0 Hz, 2H) ppm; ^{13}C NMR (*DMSO-d*$_6$, 150 MHz): δ 167.5, 152.9, 132.8, 125.6, 120.3, 118.9, 116.6, 110.2, 86.6, 61.0, 41.7 ppm.

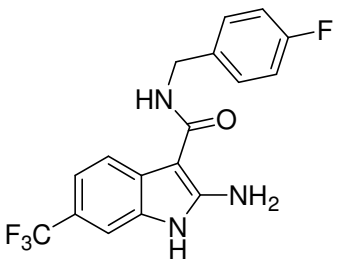


(2-Amino-6-(trifluoromethyl)-1H-indol-3-yl)(4-phenethylpiperazin-1-yl)methanone: (3-9): The crude product was purified by silica gel chromatography with 20% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{22}H_{24}F_3N_4O$ (M+H$^+$) found: *m/z*: 417.1895; Calc. Mass 417.1902; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 10.08 (s, 1H), 7.28-7.33 (m, 3H), 7.19-7.26 (m, 4H), 7.10 (s, 1H), 5.44 (s, 2H), 3.70 (m, 4H), 2.83 (m, 2H), 2.67 (m, 2H), 2.59 (s, 4H) ppm; ^{13}C NMR ($CDCl_3$, 150 MHz): δ 169.0, 152.8, 139.9, 131.1, 128.6, 128.4, 128.2, 126.2, 126.1, 125.0 (q, J = 270 Hz), 121.4 (q, J = 29 Hz), 117.8, 116.7, 107.1, 87.7, 53.4, 45.7, 33.4 ppm.

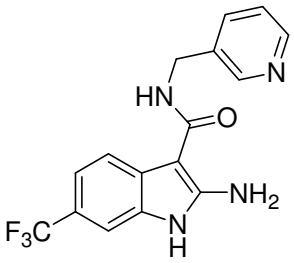


2-Amino-*N*-cyclohexyl-6-(trifluoromethyl)-1H-indole-3-carboxamide (3-10): The crude product was purified by silica gel chromatography with 5% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{16}H_{18}F_3N_3ONa$ (M+Na$^+$) found: *m/z*: 348.1326; Calc. Mass 348.1300; ^{1}H NMR (*DMSO-d*$_6$, 600 MHz): δ 10.84 (s, 1H), 7.59 (d, J = 7.8 Hz, 1H), 7.40 (s, 1H), 7.23 (d, J = 7.8 Hz, 1H), 6.97 (s, 2H), 6.50 (d, J = 8.4 Hz, 1H), 3.75-3.83 (m, 1H), 1.82 (d, J = 12.0 Hz, 2H), 1.73 (d, J = 13.2 Hz, 2H), 1.60 (d, J = 12.6 Hz, 1H), 1.42 (q, J = 12.0 Hz, 2H), 1.31 (q, J = 12.6 Hz, 2H), 1.17 (q, J = 13.2 Hz, 1H) ppm; ^{13}C NMR (*DMSO-d*$_6$, 150 MHz): δ 166.0, 154.4, 132.0, 128.9, 126.1 (q, J = 270 Hz), 118.6 (q, J = 30 Hz), 116.9, 116.7, 106.7, 87.5, 47.8, 33.1, 25.8, 25.5 ppm.

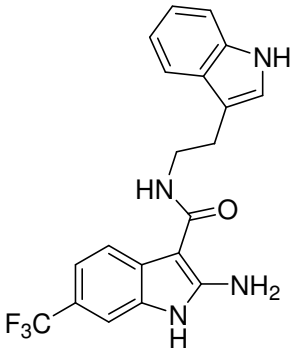
2-Amino-*N*-(4-fluorobenzyl)-6-(trifluoromethyl)-1H-indole-3-carboxamide (3-11): The crude product was purified by silica gel chromatography with 5% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{17}H_{13}F_4N_3ONa$ (M+Na$^+$) found: *m/z*: 374.0876; Calc. Mass 374.0892; ^{1}H NMR (*DMSO-d*$_6$, 600 MHz): δ 10.87 (s, 1H), 7.79 (d,



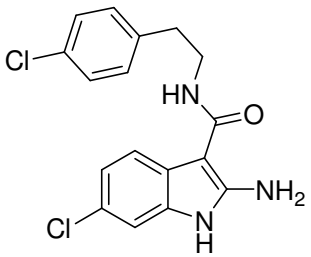
J = 7.8 Hz, 1H), 7.53 (t, J = 7.8 Hz, 1H), 7.42 (s, 1H), 7.37 (dd. J = 9.0, 6.0 Hz, 2H), 7.24 (d, J = 7.8 Hz, 1H), 7.13 (t, J = 9.0 Hz, 2H), 7.07 (s, 2H), 4.47 (d, J = 6.0 Hz, 2H) ppm; ^{13}C NMR (*DMSO-d*$_6$, 150 MHz): δ 166.6, 161.6 (d, J = 240 Hz), 154.8, 137.6 (d, J = 3 Hz), 132.1, 129.5, 129.4, 128.8, 126.1 (q, J = 240 Hz), 118.8 (q, J = 32 Hz), 116.9 (d, J = 4.5 Hz), 116.6, 115.3, 115.2, 106.8 (d, J = 3 Hz), 87.0, 47.7 ppm;



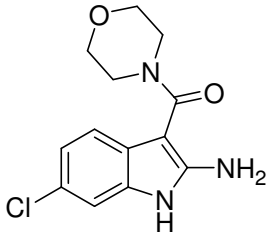
2-Amino-*N*-(pyridin-3-ylmethyl)-6-(trifluoromethyl)-1H-indole-3-carboxamide (3-12): The crude product was purified by silica gel chromatography with 10% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{16}H_{13}F_3N_4ONa$ ($M+Na^+$) found: *m/z*: 357.0952; Calc. Mass 357.0939; ^{1}H NMR (*DMSO-d*$_6$, 600 MHz): δ 10.88 (s, 1H), 8.57 (s, 1H), 8.42 (d, J = 4.2 Hz, 1H), 7.79 (d, J = 8.4 Hz, 1H), 7.74 (d, J = 7.8 Hz, 1H), 7.59 (t, J = 6.0 Hz, 1H), 7.42 (s, 1H), 7.33 (dd, J = 7.8, 4.8 Hz, 1H), 7.25 (d, J = 7.8 Hz, 1H), 7.08 (s, 2H), 4.50 (d, J = 6.0 Hz, 2H) ppm; ^{13}C NMR (*DMSO-d*$_6$, 150 MHz): δ 170.8, 166.7, 154.8, 149.3, 148.2, 136.8, 135.5, 132.1, 128.8, 126.1 (q, J = 270 Hz), 123.8, 118.9 (q, J = 30 Hz), 117.0, 116.6, 40.5 ppm;



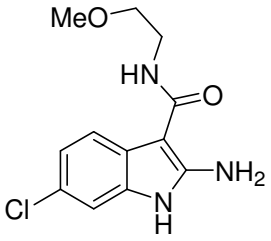
***N*-(2-(1H-Indol-3-yl)ethyl)-2-amino-6-(trifluoromethyl)-1H-indole-3-carboxamide (3-13):** The crude product was purified by silica gel chromatography with 10% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{20}H_{17}F_3N_4ONa$ ($M+Na^+$) found: *m/z*: 409.1235; Calc. Mass 409.1252; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 9.48 (s, 1H), 8.28 (s, 1H), 7.61 (s, 1H), 7.36 (s, 1H), 7.19 (s, 2H), 7.09 (s, 2H), 6.98 (s, 1H), 6.76 (s, 1H), 6.23 (s, 2H), 5.85 (s, 1H), 3.78 (s, 2H), 3.05 (s, 2H) ppm; ^{13}C NMR ($CDCl_3$, 150 MHz): δ 167.6, 153.4, 136.5, 131.5, 127.8, 127.1, 125.1 (q, J = 270 Hz), 122.4, 121.2 (q, J = 31 Hz), 119.6, 118.7, 117.9, 115.3, 112.7, 111.5, 107.0, 87.7, 39.5, 25.3 ppm.



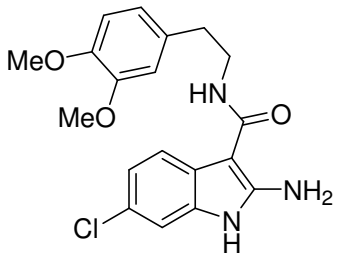
2-Amino-6-chloro-*N*-(4-chlorophenethyl)-1H-indole-3-carboxamide (3-14): The crude product was purified by silica gel chromatography with 5% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{17}H_{16}Cl2N_3O$ ($M+H^+$) found: *m/z*: 348.0672; Calc. Mass 348.0670. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 9.72 (s, 1H), 7.22 (d, J = 7.8 Hz, 2H), 7.08 (d, J = 7.8 Hz, 2H), 6.98 (s, 1H), 6.94 (d, J = 7.8 Hz, 1H), 6.76 (d, J = 7.8 Hz, 1H), 6.13 (s, 2H), 5.68 (s, 1H), 3.66 (m, 2H), 2.84 (m, 2H) ppm; ^{13}C NMR ($CDCl_3$, 150 MHz): δ 167.7, 152.6, 137.1, 133.1, 132.6, 130.1, 128.9, 125.4, 123.5, 121.2, 116.2, 110.5, 87.1, 40.4, 35.4 ppm.



(2-Amino-6-chloro-1H-indol-3-yl)(morpholino)methanone (3-15): The crude product was purified by silica gel chromatography with 20% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{13}H_{15}ClN_3O_2$ ($M+H^+$) found: *m/z*: 280.0825; Calc. Mass 280.0853. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 9.74 (s, 1H), 7.03 (d, J = 7.8 Hz, 1H), 7.00 (dd, J = 7.8, 1.2 Hz, 1H), 6.89 (s, 1H), 5.54 (s, 2H), 3.73 (m, 4H), 3.62 (m, 4H) ppm; ^{13}C NMR ($CDCl_3$, 150 MHz): δ 169.6, 152.2, 132.4, 125.0, 124.1, 121.0, 117.7, 110.2, 87.1, 67.1, 46.2 ppm.

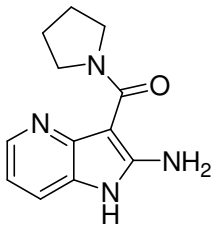


2-Amino-6-chloro-*N*-(2-methoxyethyl)-1H-indole-3-carboxamide (3-16): The crude product was purified by silica gel chromatography with 5% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{12}H_{14}ClN_3O_2Na$ ($M+Na^+$) found: *m/z*: 290.0670; Calc. Mass 290.0672. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 9.74 (s, 1H), 7.16 (s, 1H), 7.00-7.05 (m, 2H), 6.20 (s, 2H), 6.13 (s, 1H), 3.65 (t, J = 7.2 Hz, 2H), 3.57 (t, J = 7.2 Hz, 2H), 3.41 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 150 MHz): δ 167.7, 152.6, 133.1, 125.1, 123.7, 121.1, 116.3, 110.3, 87.1, 71.4, 58.8, 38.9 ppm.



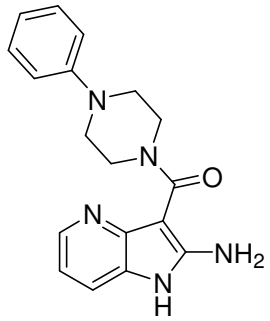
2-Amino-6-chloro-*N*-(3,4-dimethoxyphenethyl)-1H-indole-3-carboxamide (3-17): The crude product was purified by silica gel chromatography with 5% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{19}H_{20}ClN_3O_3$ ($M+Na^+$) found: *m/z*: 396.1120; Calc. Mass 396.1091; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 9.62 (s, 1H), 7.03 (s, 1H), 6.93 (d, J = 8.4 Hz, 1H), 6.82 (d, J = 3.6 Hz, 1H), 6.80 (s, 1H), 6.77 (d, J = 7.8 Hz, 1H), 6.74 (s, 1H), 3.85 (s, 3H), 3.77 (s, 3H), 3.70 (q, J = 6.6 Hz, 2H), 2.86 (t, J = 6.6 Hz, 2H) ppm; ^{13}C NMR ($CDCl_3$, 150 MHz): δ 167.6, 152.5, 149.1, 147.8, 133.0, 131.4, 125.1, 123.7, 121.0, 120.8, 116.3, 111.9, 111.5, 110.4, 87.2, 55.9, 55.8, 40.5, 35.6 ppm.

.

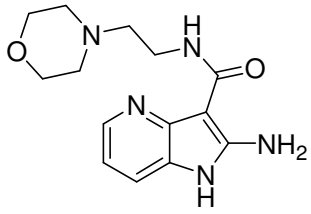


(2-Amino-1H-pyrrolo[3,2-b]pyridin-3-yl)(pyrrolidin-1-yl)methanone (3-18): The crude product was purified by silica gel chromatography with 33% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{12}H_{14}N_4ONa$ ($M+Na^+$) found: *m/z*: 253.1076; Calc. Mass 253.1065; ^{1}H NMR (*DMSO-d*$_6$, 600 MHz): δ 10.84 (s, 1H), 8.01 (d, J = 4.8 Hz, 1H), 7.40 (s, 1H), 6.80 (s, 3H), 3.61 (m, 4H), 1.81

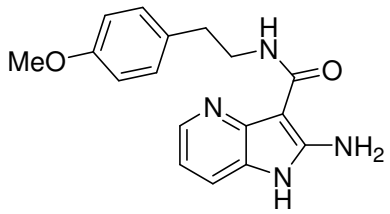
(m, 4H) ppm; ^{13}C NMR (*DMSO-d_6*, 150 MHz): δ166.1, 154.5, 126.6, 115.9, 113.3, 88.9, 68.2, 55.4, 47.2, 25.3, 19.6 ppm.



(2-Amino-1H-pyrrolo[3,2-b]pyridin-3-yl)(4-phenylpiperazin-1-yl)methanone (3-19): The crude product was purified by silica gel chromatography with 33% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{18}H_{19}N_5O$ Na (M+Na$^+$) found: *m/z*: 344.1484; Calc. Mass 344.1487; ^{1}H NMR (*acetone-d_6*, 600 MHz): δ 8.16 (s, 1H), 7.40 (d, J = 7.2 Hz, 1H), 7.24 (s, 2H), 7.02 (s, 2H), 6.83 (m, 2H), 6.68 (s, 1H), 3.87 (s, 4H), 3.29 (s, 4H) ppm; ^{13}C NMR (*acetone-d_6*, 150 MHz): δ 167.5, 155.5, 151.9, 144.9, 141.3, 128.9, 125.6, 119.3, 116.1, 115.0, 113.5, 88.1, 49.5, 45.1 ppm.

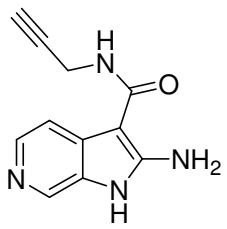


2-Amino-*N*-(2-morpholinoethyl)-1H-pyrrolo[3,2-b]pyridine-3-carboxamide (3-20): The crude product was purified by silica gel chromatography with 50% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{14}H_{20}N_5O_2$ (M+H$^+$) found: *m/z*: 290.1614; Calc. Mass 290.1617; ^{1}H NMR (*DMSO-d_6*, 600 MHz): δ 10.68 (s, 1H), 8.52 (s, 1H), 8.05 (s, 1H), 7.37 (s, 1H), 6.97 (s, 2H), 6.82 (t, J = 6.0 Hz, 1H), 3.59 9m, 4H), 3.43 (s, m, 2H), 2.38-2.50 (m, 6H) ppm; ^{13}C NMR (*DMSO-d_6*, 150 MHz): δ 166.1, 154.0, 146.0, 141.0, 126.5, 115.7, 114.1, 86.3, 66.8, 58.3, 53.7, 35.3 ppm. Crystal structure of X-ray is described later.

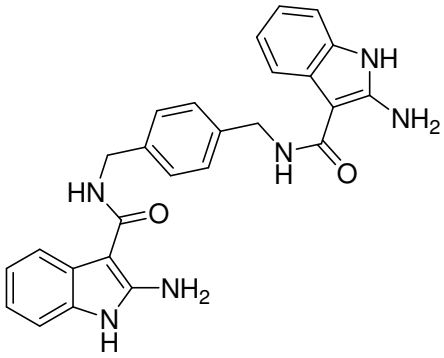


2-Amino-*N*-(4-methoxyphenethyl)-1H-pyrrolo[3,2-b]pyridine-3-carboxamide (3-21): The crude product was purified by silica gel chromatography with 10% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{17}H_{18}N_4O_2Na$ (M+Na$^+$) found: *m/z*: 333.1327; Calc. Mass 333.1327; ^{1}H NMR (*DMSO-d_6*, 600 MHz): δ 10.67 (s, 1H), 8.01 (s, 1H), 7.95 (s, 1H), 7.36 (s, 1H), 7.18 (s, 2H), 6.98 (s, 2H), 6.83 (s, 3H), 3.72 (s, 3H), 3.49 (q, J = 6.6 Hz, 2H), 2.75 (t, J = 6.6 Hz, 2H) ppm; ^{13}C NMR (*DMSO-d_6*, 150 MHz): δ 166.1, 162.8, 158.1, 154.0, 145.9, 140.9, 132.0, 130.2, 126.5, 115.7, 114.2, 114.1, 86.2, 55.4, 36.2, 31.2 ppm.

2-Amino-*N*-(prop-2-yn-1-yl)-1H-pyrrolo[2,3-c]pyridine-3-carboxamide (3-22): The crude product was purified by silica gel chromatography with 2 % triethylamine in methanol as yellow solid. HRMS ESL-TOF for $C_{11}H_{11}N_4O$ (M+H$^+$) found: *m/z*: 215.0926;



Calc. Mass 215.0933; ^{1}H NMR (*DMSO-d_6*, 600 MHz): δ 11.08 (brs, 1H), 8.31 (s, 1H), 8,01 (s, 1H), 7.40 (t, J = 4.8 Hz, 1H), 7.09 (s, 2H), 4.52 (s, 2H), 2.64 (s, 1H) ppm; ^{13}C NMR (*DMSO-d_6*, 150 MHz): δ 161.7, 158.9, 139.4, 137.0, 131.4, 113.0, 112.1, 83.1, 56.1, 41.5, 27.0 ppm.



***N,N′*-(1,4-phenylenebis(methylene))bis(2-amino-1H-indole-3-carboxamide) (3-23):** The crude product was purified by silica gel chromatography with 10% methanol in ethyl acetate as yellow solid. HRMS ESL-TOF for $C_{26}H_{24}N_6O_2Na$ ($M+Na^+$) found: *m/z*: 475.1855; Calc. Mass 475.1858; ^{1}H NMR (*DMSO-d_6*, 600 MHz): δ 10.57 (s, 2H), 7.60 (d, J = 7.8 Hz, 2H), 7.27 (s, 4H), 7.23 (t, J = 6.6 Hz, 2H), 7.10 (d, J = 7.8 Hz, 2H), 6.93 (t, J = 7.2 Hz, 2H), 6.85 (t, J = 7.8 Hz, 2H), 6.72 (s, 4H), 4.45 (d, J = 6.0 Hz, 4H) ppm; ^{13}C NMR (*DMSO-d_6*, 150 MHz): δ 167.0, 153.0, 139.7, 132.8, 127.4, 125.6, 120.3, 118.9, 116.9, 110.1, 86.6, 42.1 ppm.

Crystal Structure Determination

Compound 3-20 May 28th 2010

Operator:	*** Herdtweck ***
Molecular Formula:	C_{14} H_{19} N_5 O_2
Crystal Color / Shape	Colorless fragment
Crystal Size	Approximate size of crystal fragment used for data collection: 0.25 × 0.41 × 0.41 mm
Molecular Weight:	289.34 a.m.u.
F_{000}:	1232
Systematic Absences:	h0l: h+l≠2n; 0k0: k≠2n
Space Group:	Monoclinic $P\,2_1/n$ (I.T.-No.: 14)
Cell Constants:	Least-squares refinement of 9937 reflections with the programs "APEX suite" and "SAINT" [1,2]; theta range 1.65° < θ < 25.39°; Mo($K\overline{\alpha}$); λ = 71.073 pm
	a = 1564.65(3) pm
	b = 957.00(2) pm β = 91.6774(8)°
	c = 1949.60(3) pm
	V = 2918.02(9)· 10^6 pm^3; Z = 8; D_{calc} = 1.317 g cm^{-3}; Mos. = 0.74
Diffractometer:	Kappa APEX II (Area Diffraction System; BRUKER AXS); rotating anode; graphite monochromator; 50 kV; 40 mA; λ = 71.073 pm; Mo($K\overline{\alpha}$)
Temperature:	(-150±1) °C; (123±1) K
Measurement Range:	1.65° < θ < 25.39°; h: -18/18, k: -11/10, l: -23/23
Measurement Time:	2 × 5 s per film
Measurement Mode:	measured: 9 runs; 2660 films / scaled: 4 runs; 1149 films
	φ– and ω–movement; Increment: $\Delta\varphi/\Delta\omega$ = 0.50°; dx = 45.0 mm
LP - Correction:	Yes [2]
Intensity Correction	No/Yes; during scaling [2]
Absorption Correction:	Multi-scan; during scaling; μ = 0.092 mm^{-1} [2]
	Correction Factors: T_{min} = 0.6442 T_{max} = 0.7452
Reflection Data:	24863 reflections were integrated and scaled
	1000 reflections systematic absent and rejected
	23863 reflections to be merged
	5363 independent reflections
	0.022 R_{int}: (basis F_o^2)
	5363 independent reflections (all) were used in refinements
	4749 independent reflections with $I_o > 2\sigma(I_o)$
	99.9 % completeness of the data set
	411 parameter full-matrix refinement
	13.0 reflections per parameter
Solution:	Direct Methods [3]; Difference Fourier syntheses
Refinement Parameters:	In the asymmetric unit:

	42 Non-hydrogen atoms with anisotropic displacement parameters	
	8 Hydrogen atoms with isotropic displacement parameters	
Hydrogen Atoms:	All hydrogen atom positions bound to the nitrogen atoms were found in the difference maps. The hydrogen positions were refined with individual isotropic displacement parameters. All other hydrogen atoms were placed in calculated positions (d_{C-H} = 95, 99 pm). Isotropic displacement parameters were calculated from the parent carbon atom (U_H = 1.2 U_C). The hydrogen atoms were included in the structure factor calculations but not refined.	
Atomic Form Factors:	For neutral atoms and anomalous dispersion [4]	
Extinction Correction:	no	
Weighting Scheme:	$w^{-1} = \sigma^2(F_o^2)+(a*P)^2+b*P$	
	with a: 0.0436; b: 1.0629; P: [Maximum(0 or F_o^2)+2$*F_c^2$]/3	
Shift/Err:	Less than 0.001 in the last cycle of refinement:	
Resid. Electron Density:	+0.22 $e_{0;}^-/Å^3$; -0.20 $e_{0;}^-/Å^3$	
R1:	$\Sigma(\|\|F_o\|-\|F_c\|\|)/\Sigma\|F_o\|$	
[$F_o > 4\sigma(F_o)$; N=4749]:		= 0.0338
[all reflctns; N=5363]:		= 0.0393
wR2:	$[\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$	
[$F_o > 4\sigma(F_o)$; N=4749]:		= 0.0869
[all reflctns; N=5363]:		= 0.0912
Goodness of fit:	$[\Sigma w(F_o^2-F_c^2)^2/(NO-NV)]^{1/2}$	= 1.045
Remarks:	Refinement expression $\Sigma w(F_o^2-F_c^2)^2$ [5,6,7]	

References:

[1] APEX suite of crystallographic software. APEX 2 Version 2008.4. Bruker AXS Inc., Madison, Wisconsin, USA (2008).

[2] SAINT, Version 7.56a and SADABS Version 2008/1. Bruker AXS Inc., Madison, Wisconsin, USA (2008).

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[4] International Tables for Crystallography, Vol. C, Tables 6.1.1.4 (pp. 500-502), 4.2.6.8 (pp. 219-222), and 4.2.4.2 (pp. 193-199), Wilson, A. J. C., Ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1992.

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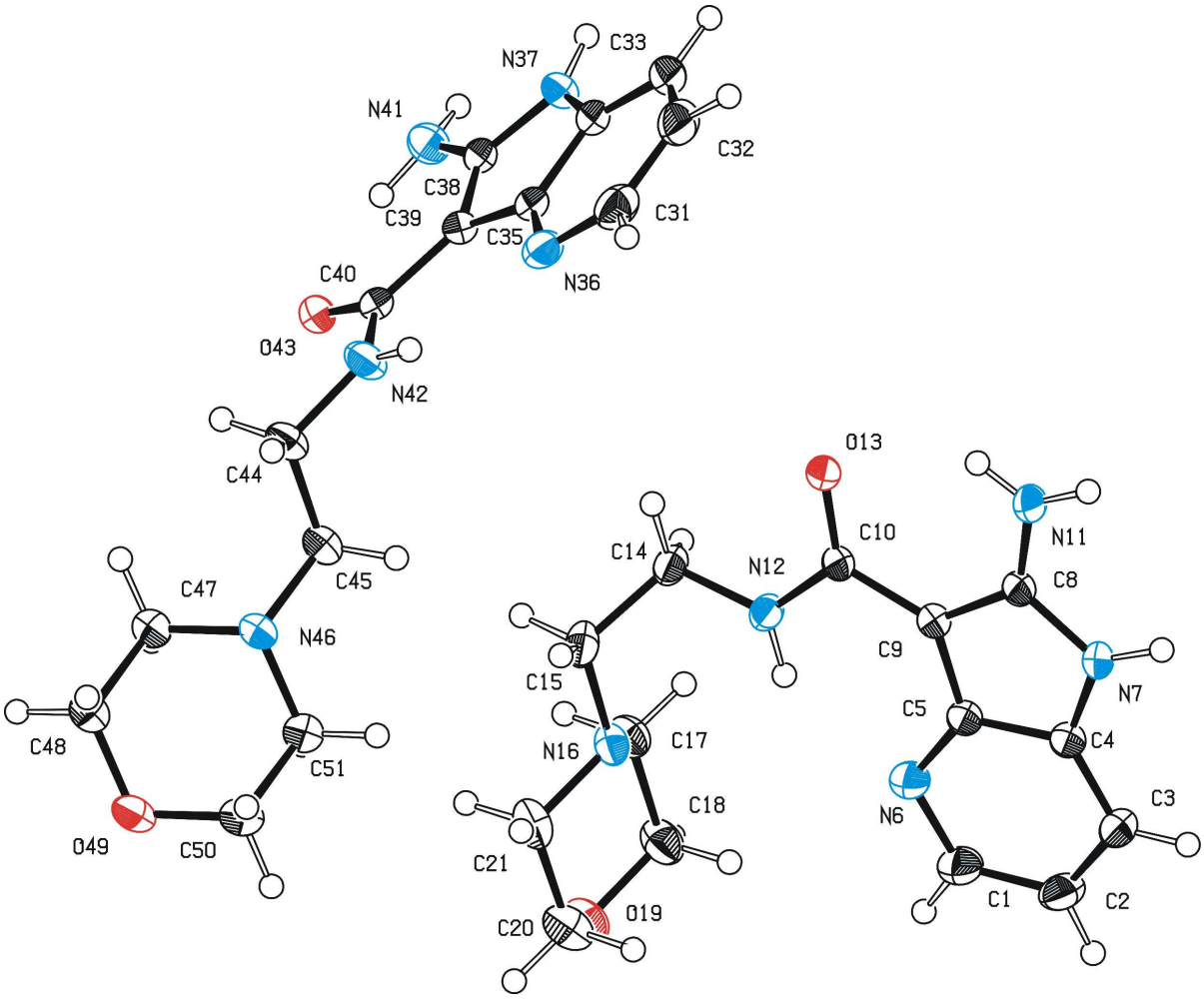
[6] Spek, A. L. "**PLATON**", A Multipurpose Crystallographic Tool, Utrecht University, Utrecht, The Netherlands, (2010).

[7] L. J. Farrugia, "**WinGX** (Version 1.70.01 January 2005) ", *J. Appl. Cryst.* **1999**, *32*, 837-838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N41
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C38
C39
C31
C35
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N42
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C48
C51
O49
C50
O13
C10
N11
C14
N12
C8
C9
C15
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C17
C4
C18
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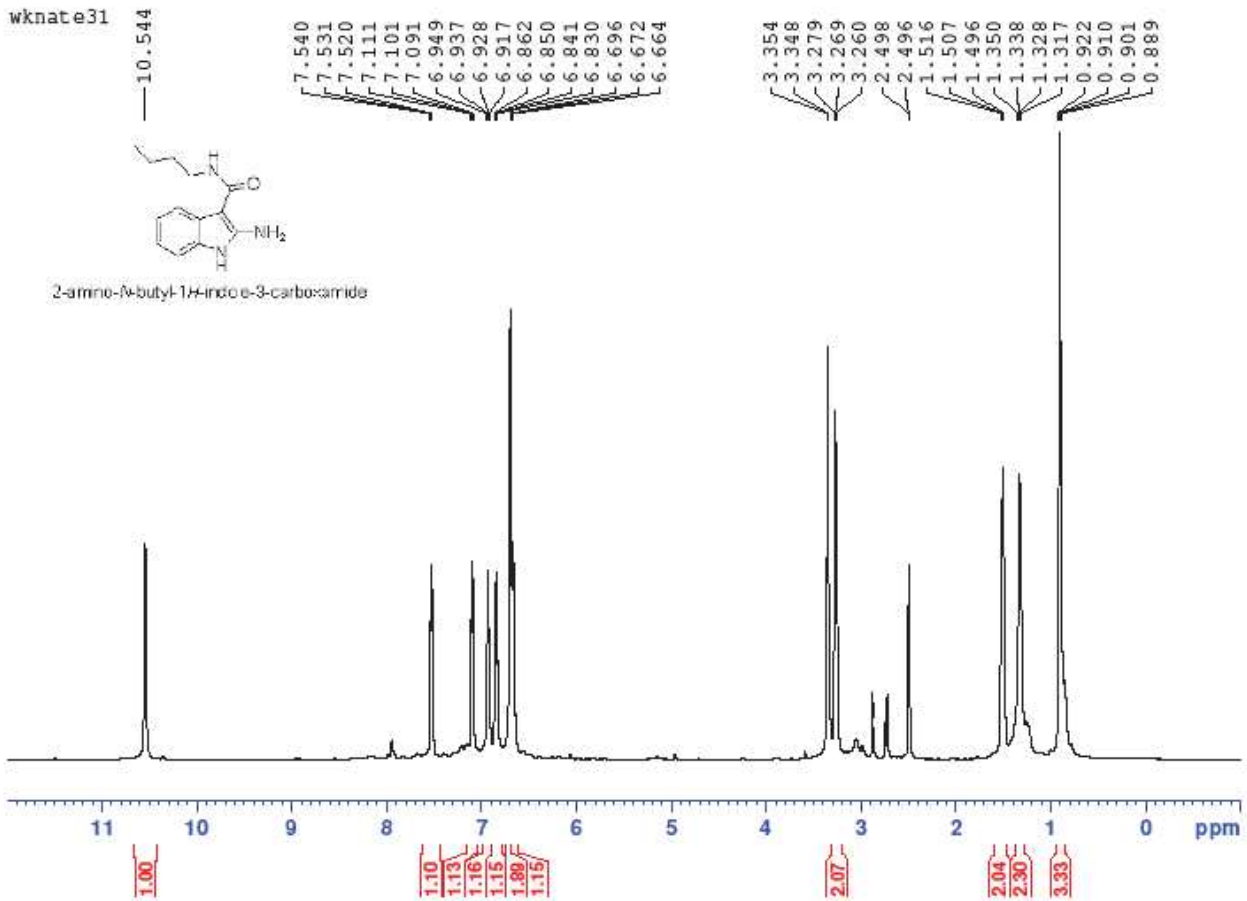
C3
C21
C1
C2
C20
O19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6.664
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0.889
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9
8
7
6
5
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ppm
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3.33

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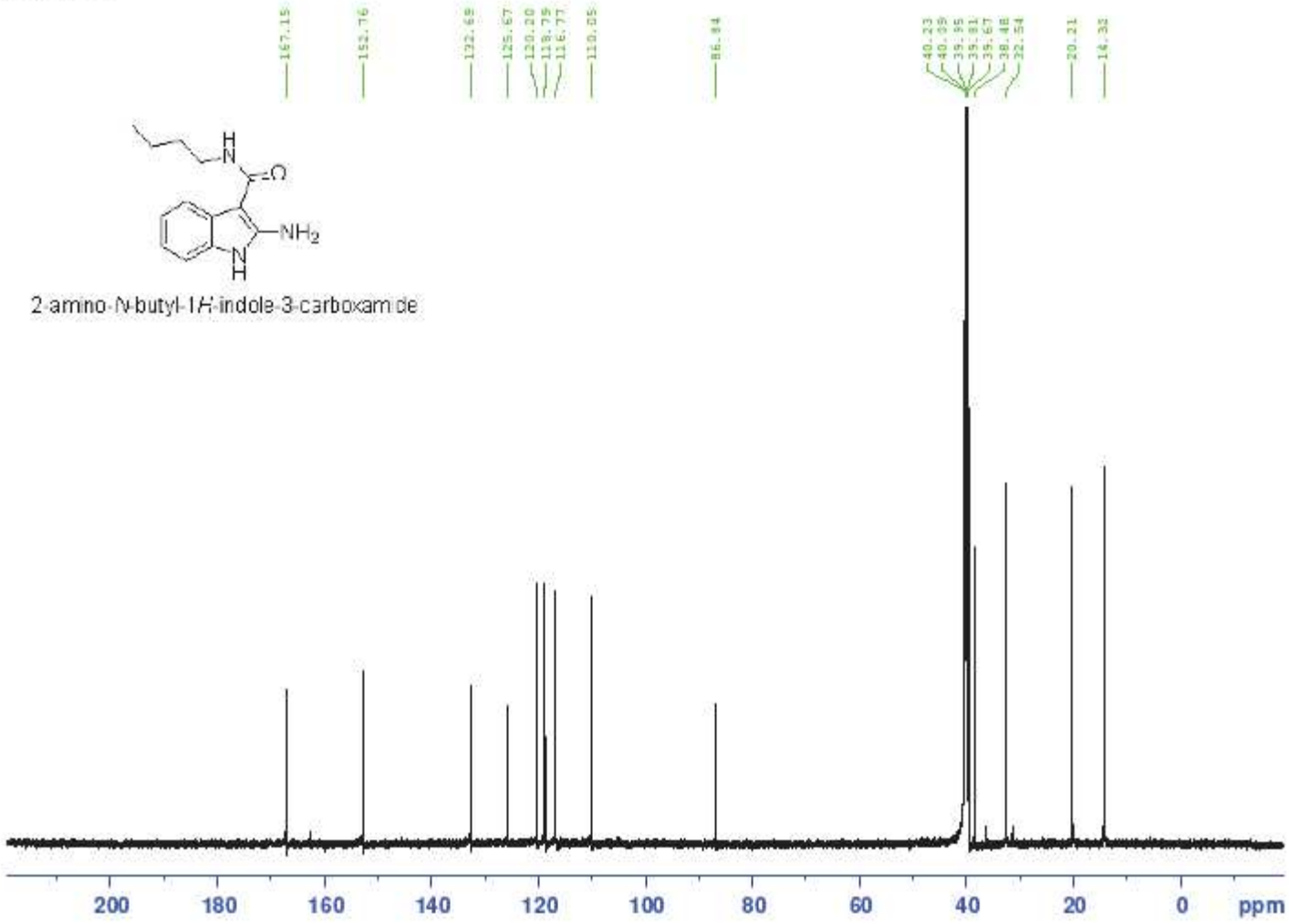
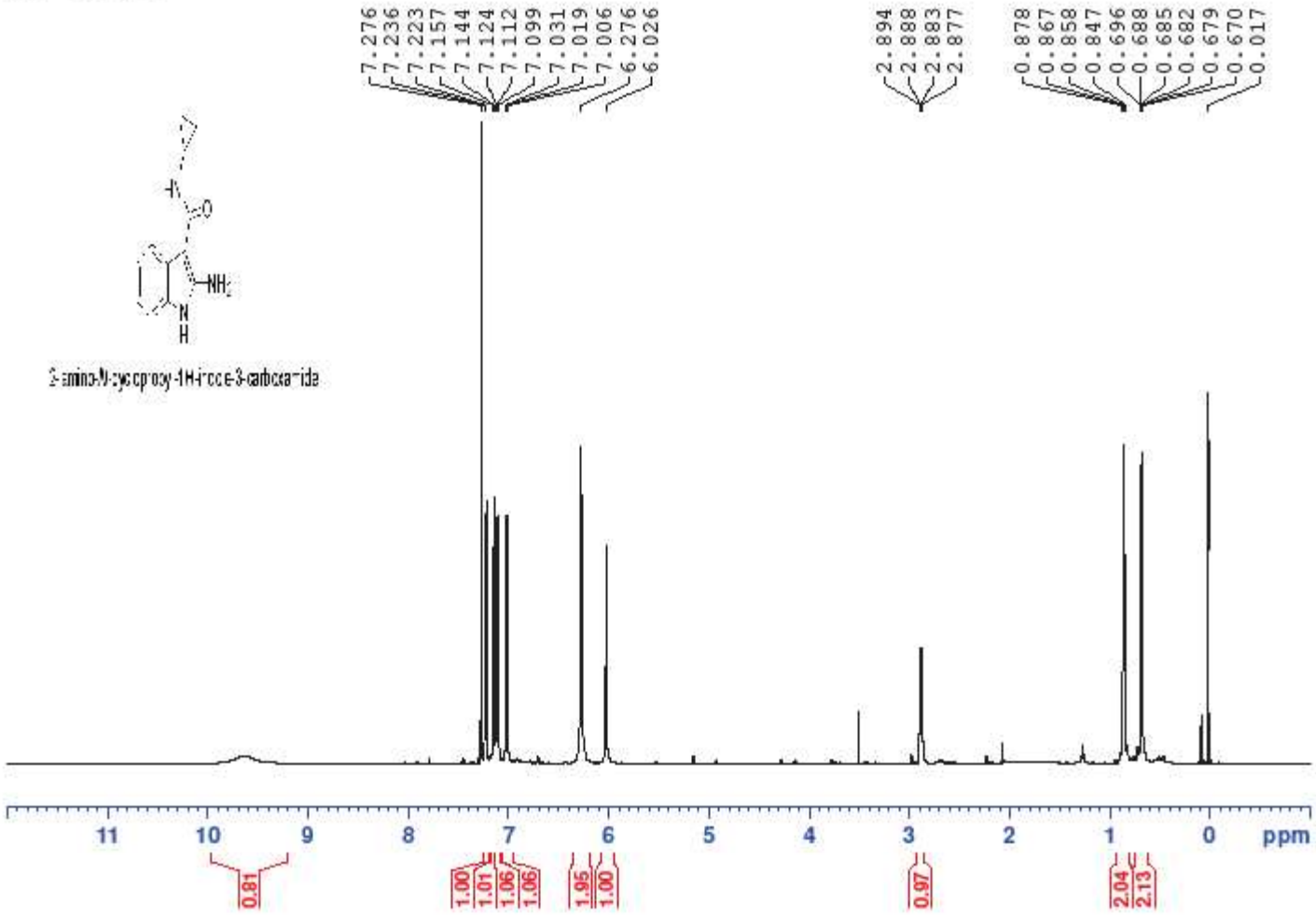


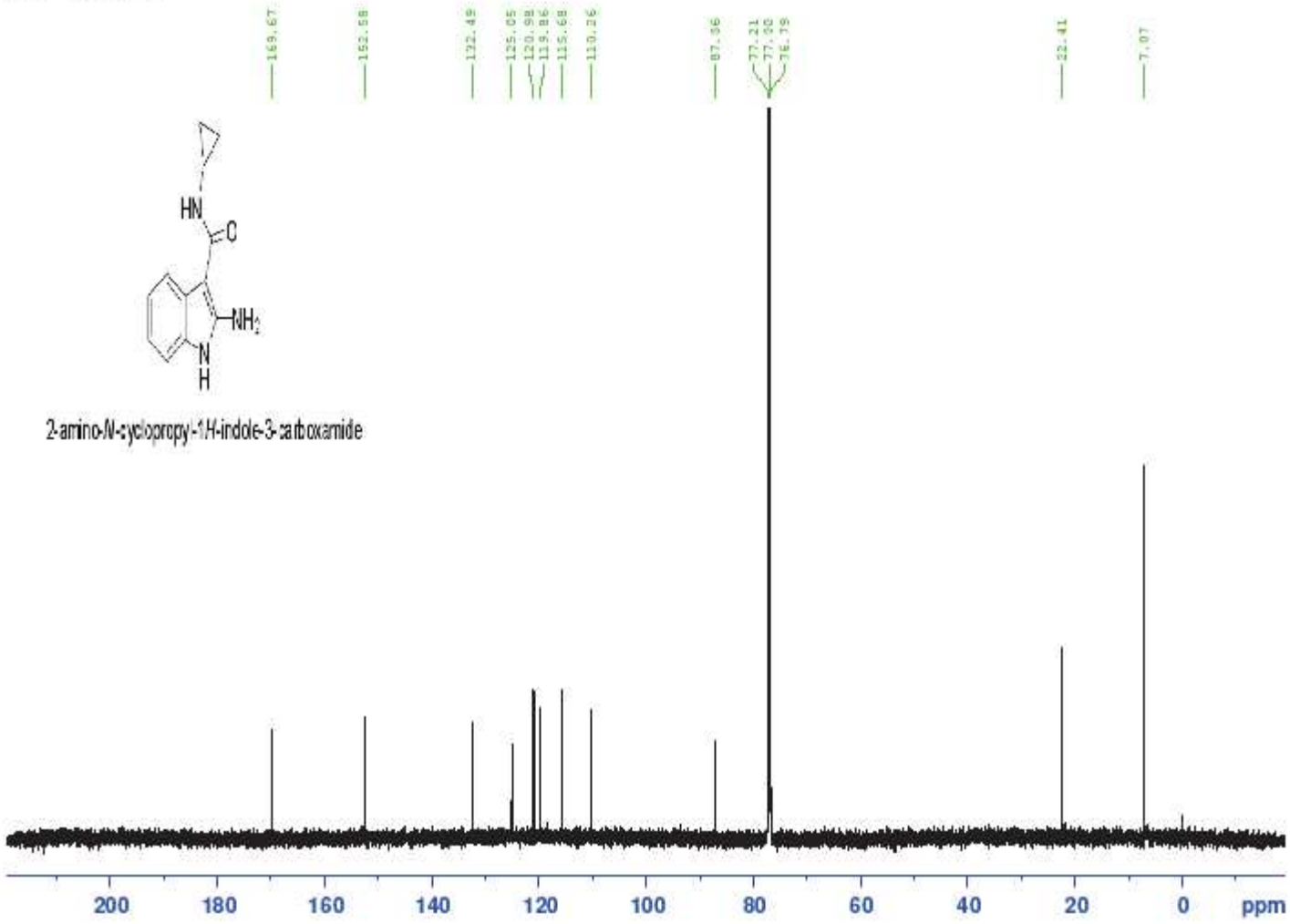
2-amino-*N*-butyl-1*H*-indole-3-carboxamide

wk4-162-2-1



3-amino-N-cyclopropyl-1H-indole-3-carboxamide

wk4-162-2-1



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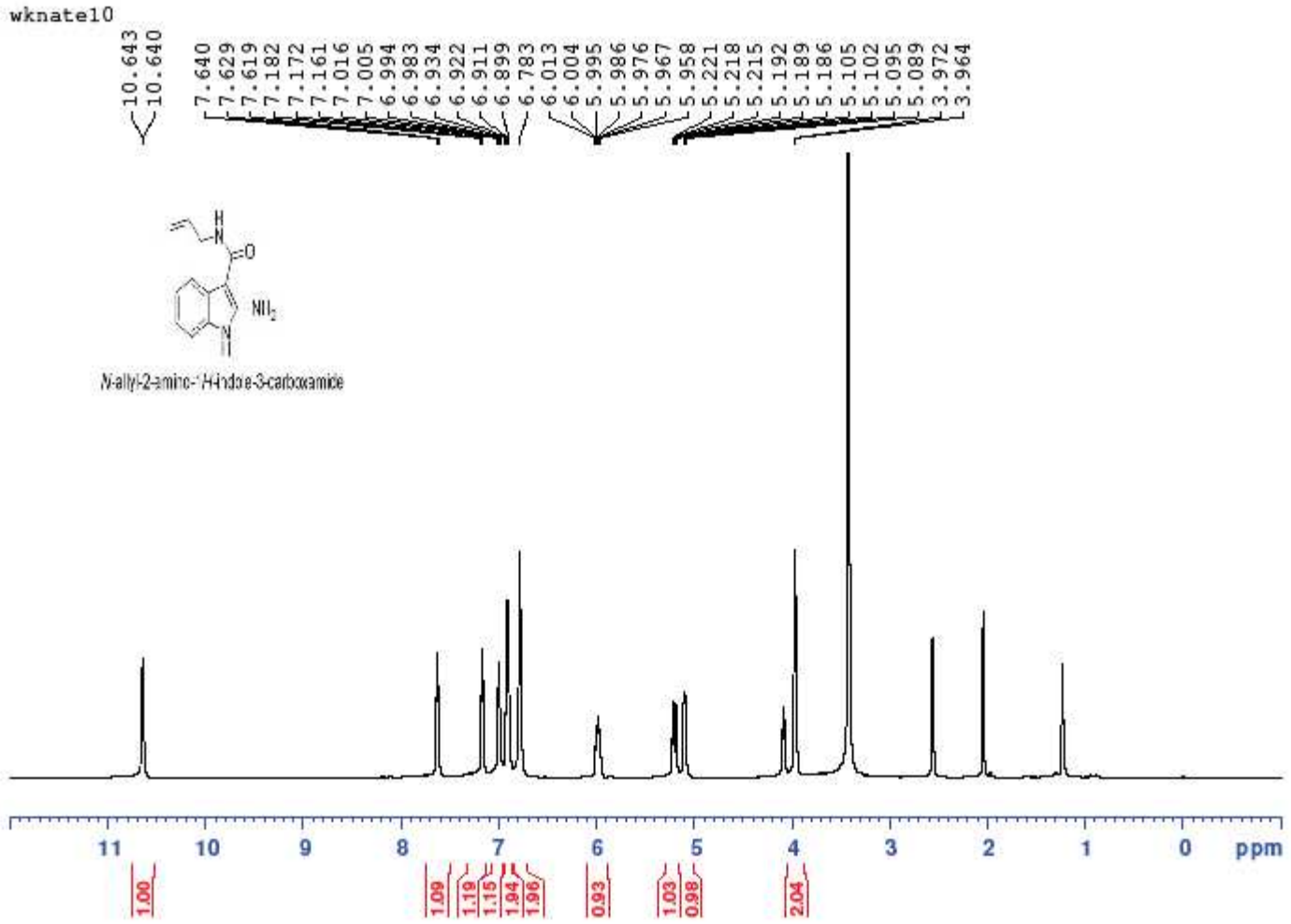
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N-allyl-2-amino-1H-indole-3-carboxamide
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10
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8
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5
4
3
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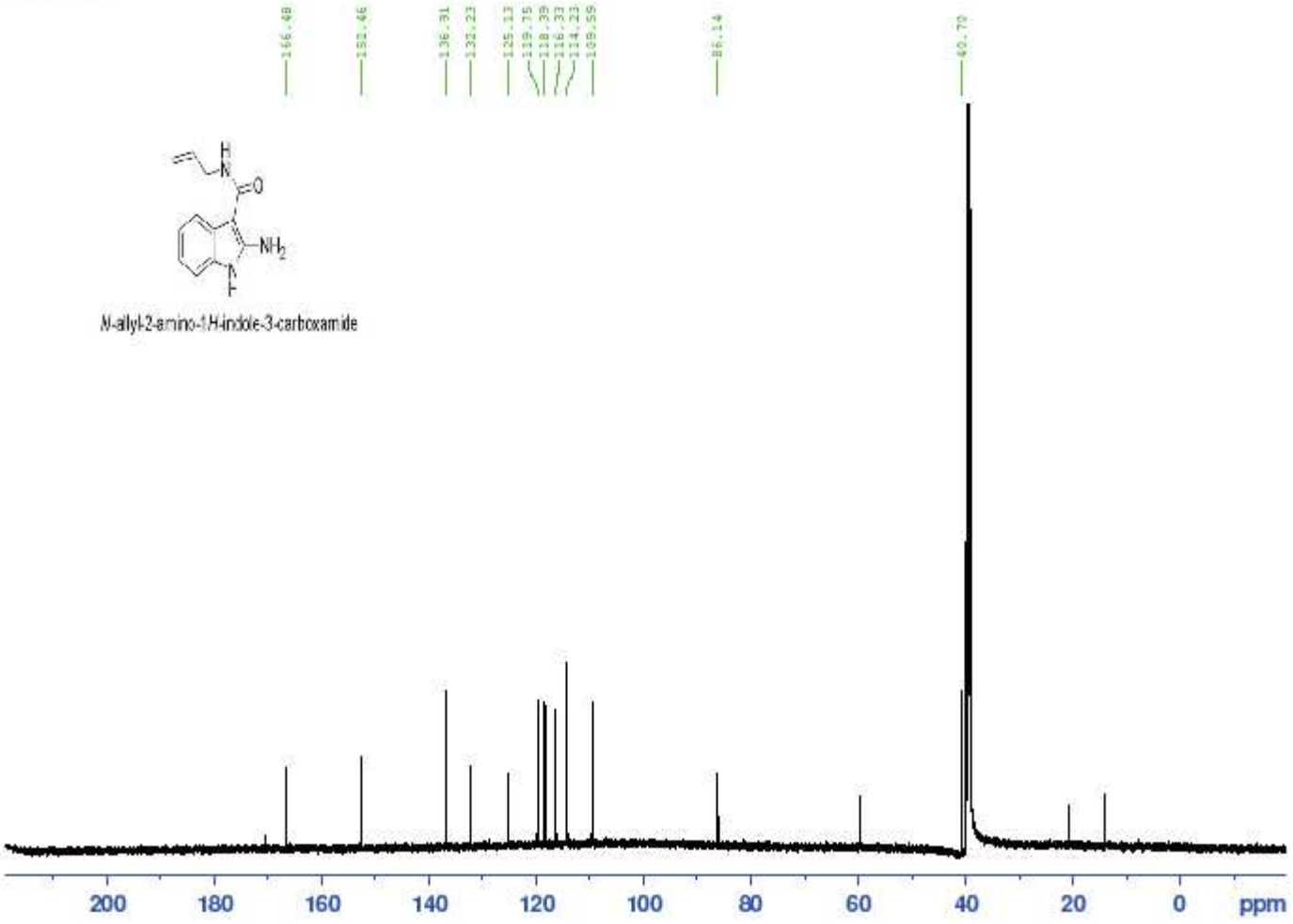
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O
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N
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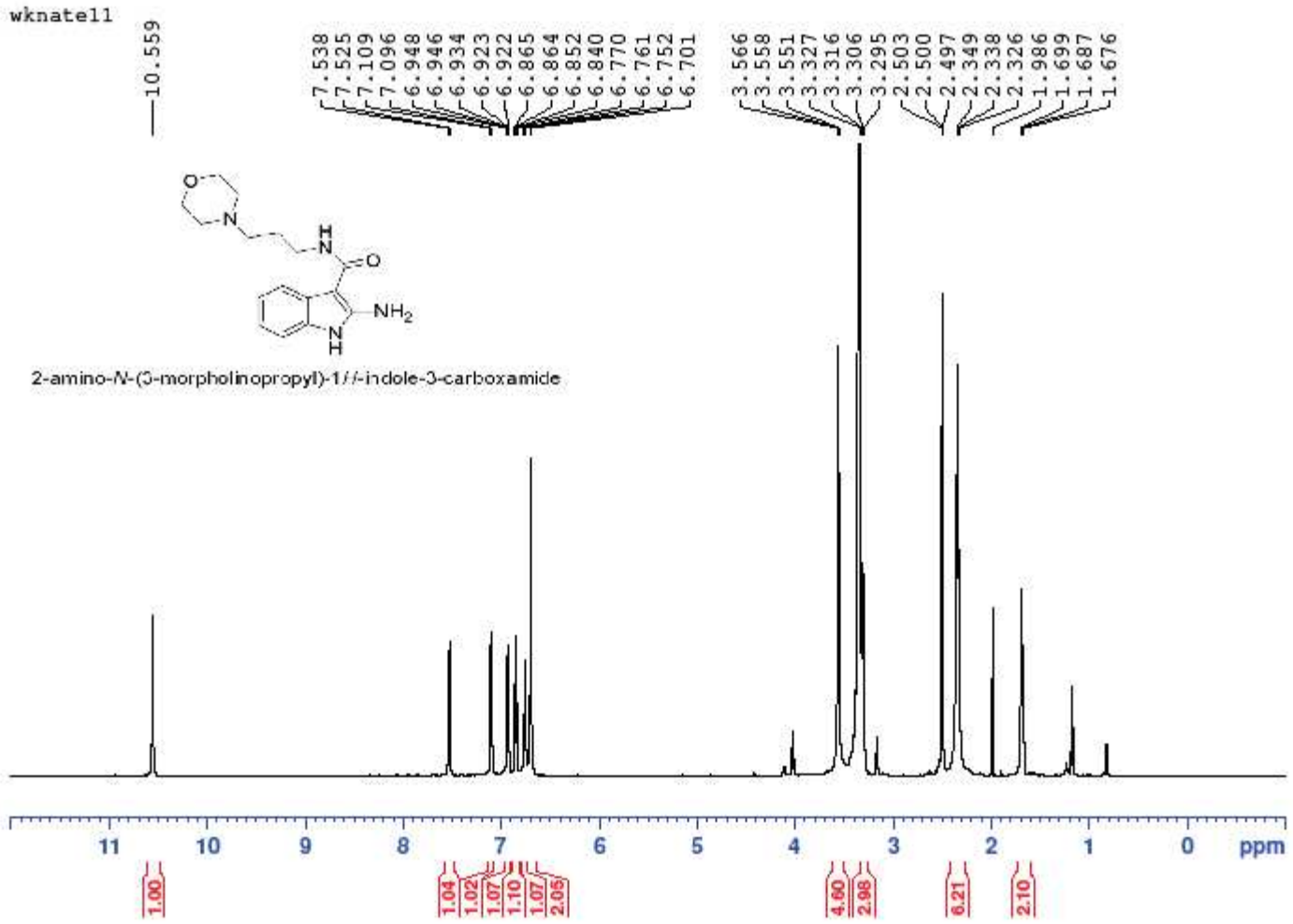
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6.701
3.566
3.558
3.551
3.327
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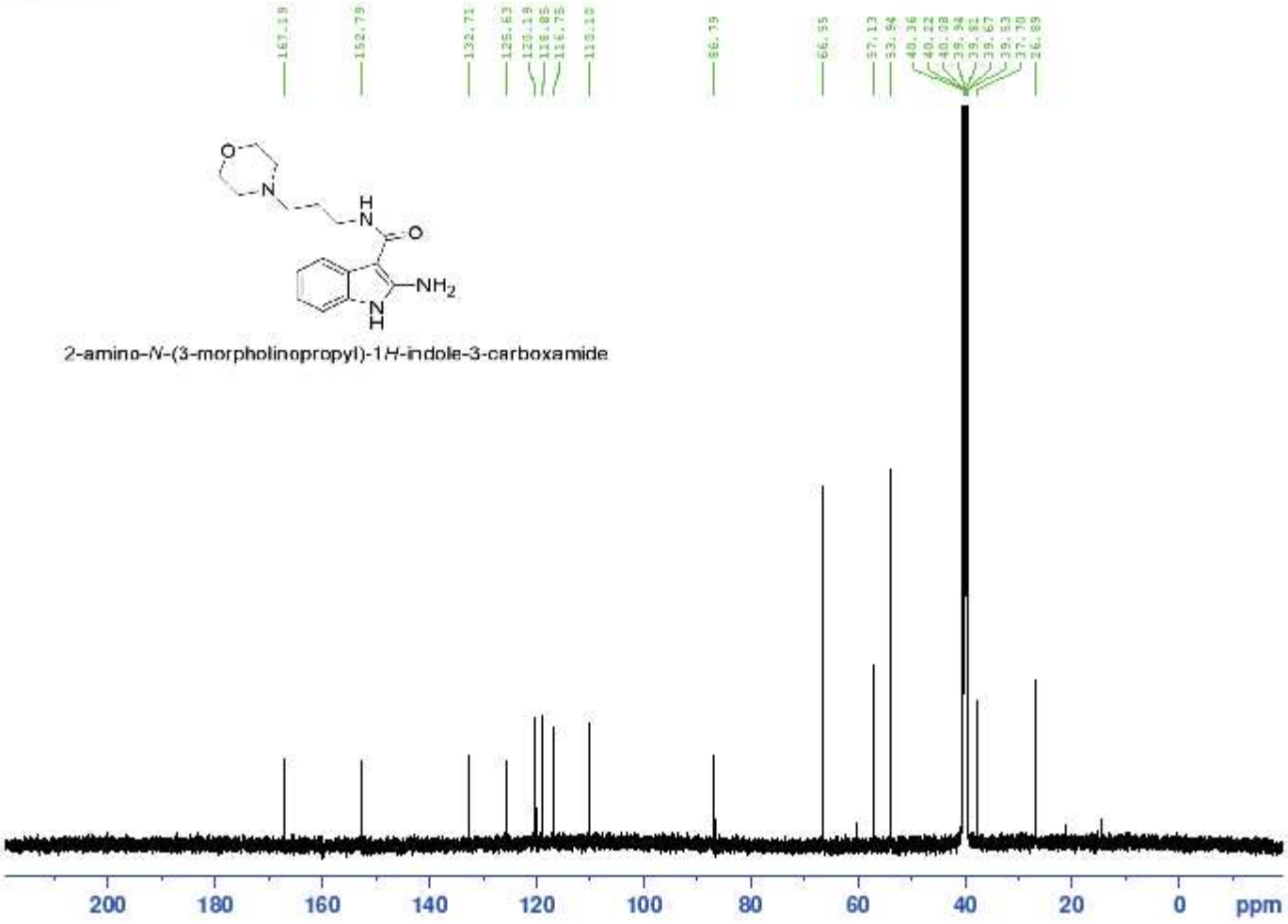
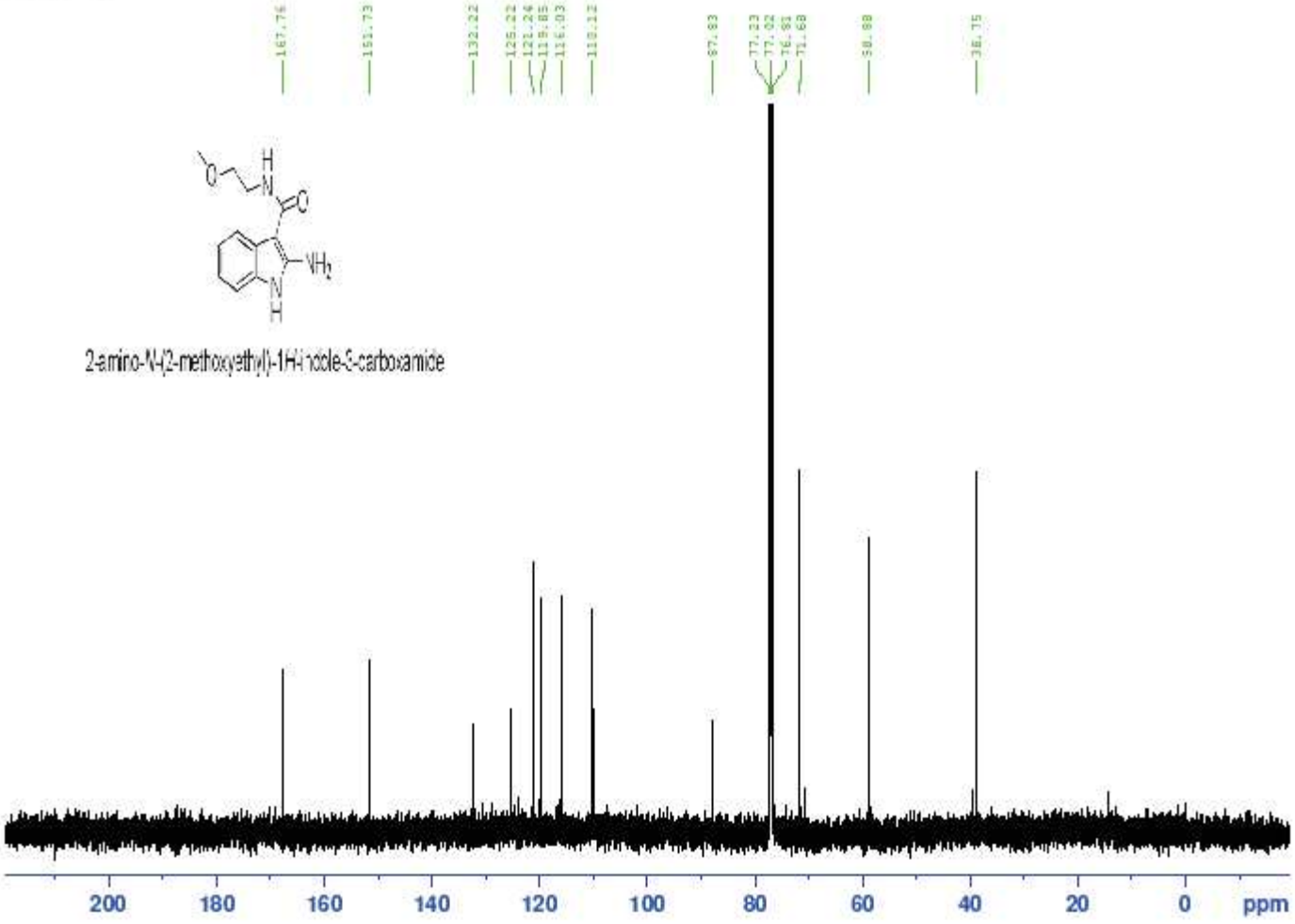
wknate11



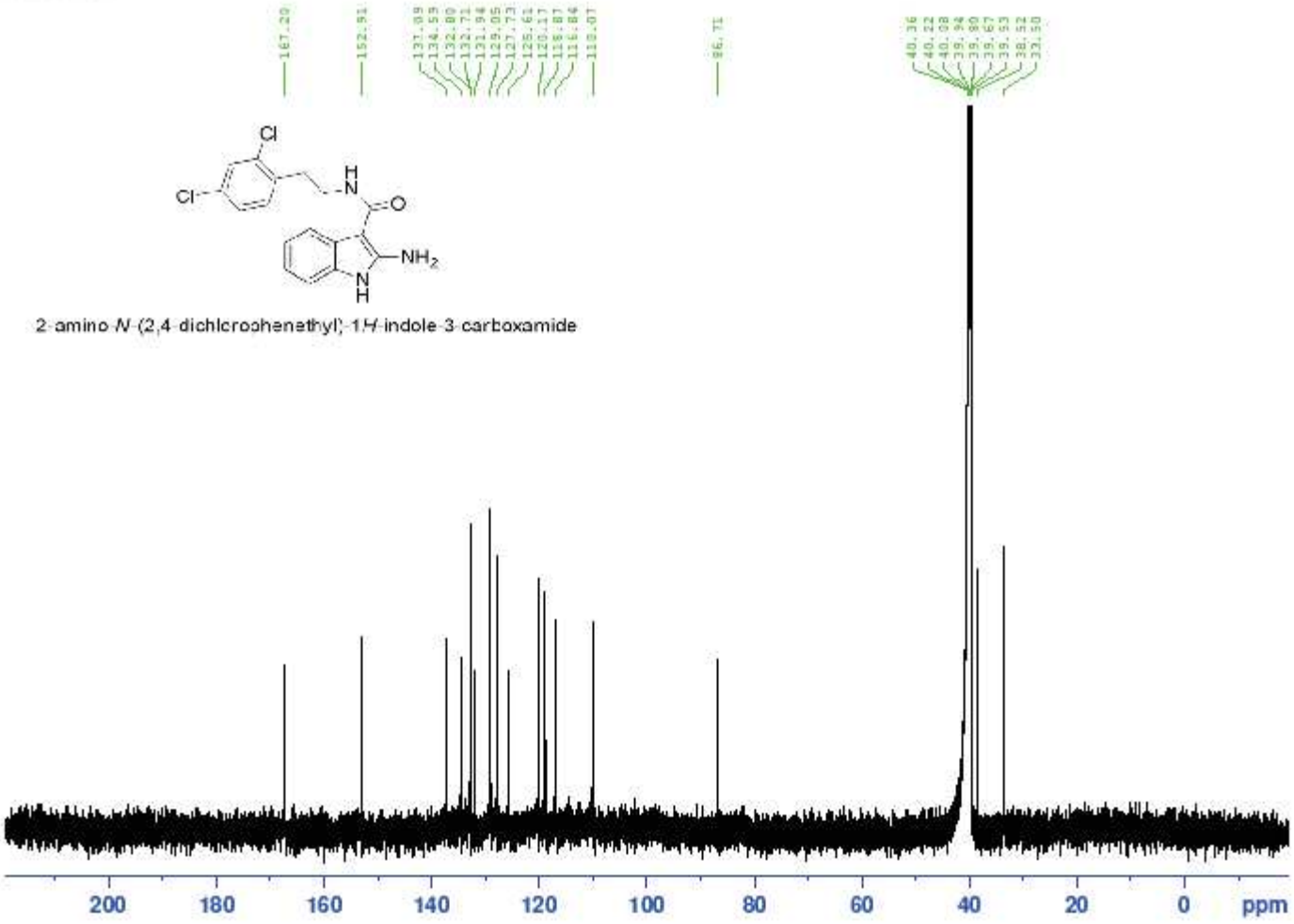
2-amino-*N*-(3-morpholinopropyl)-1*H*-indole-3-carboxamide

WKNATE12

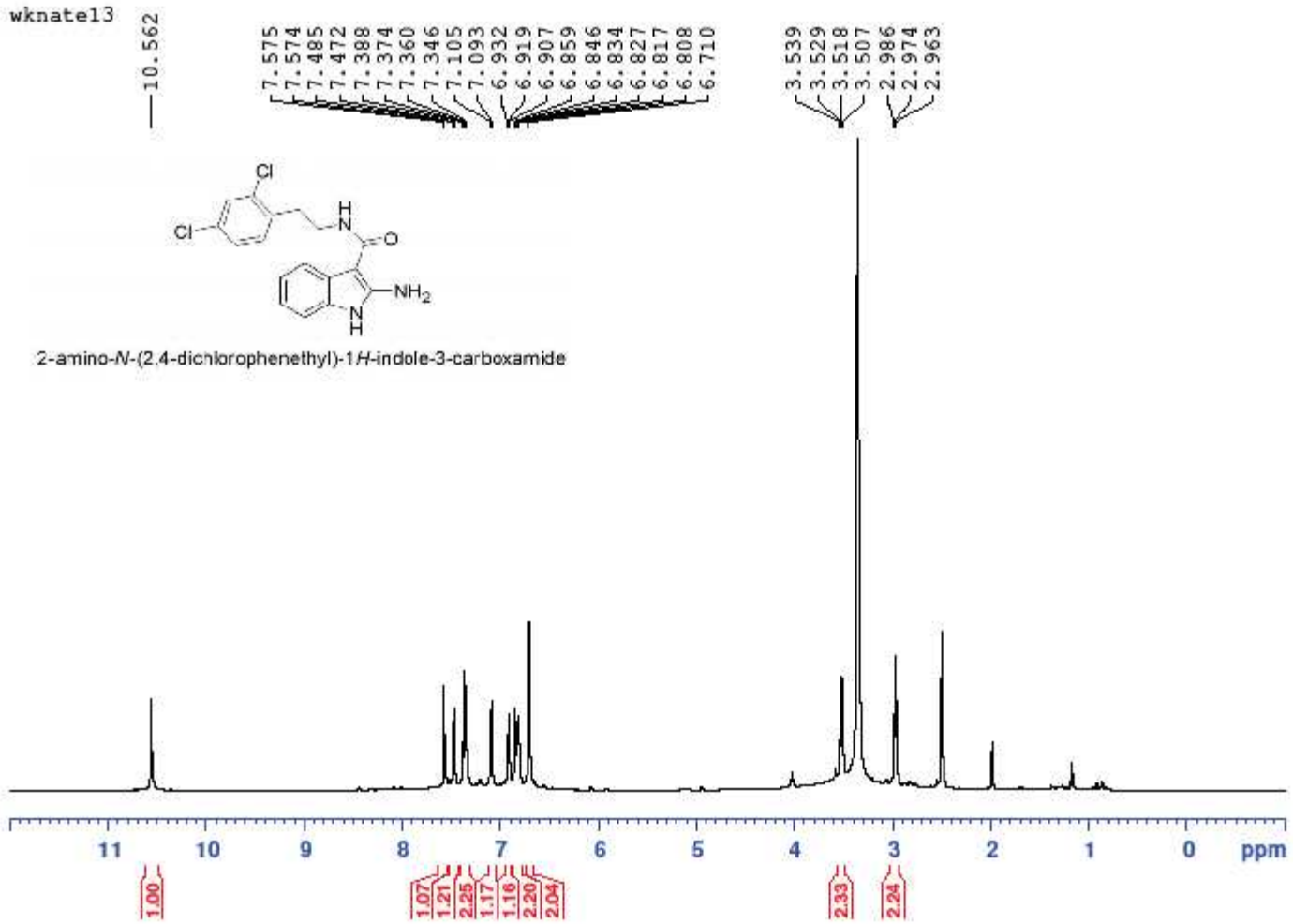


2-amino-N-(2-methoxyethyl)-1H-indole-3-carboxamide

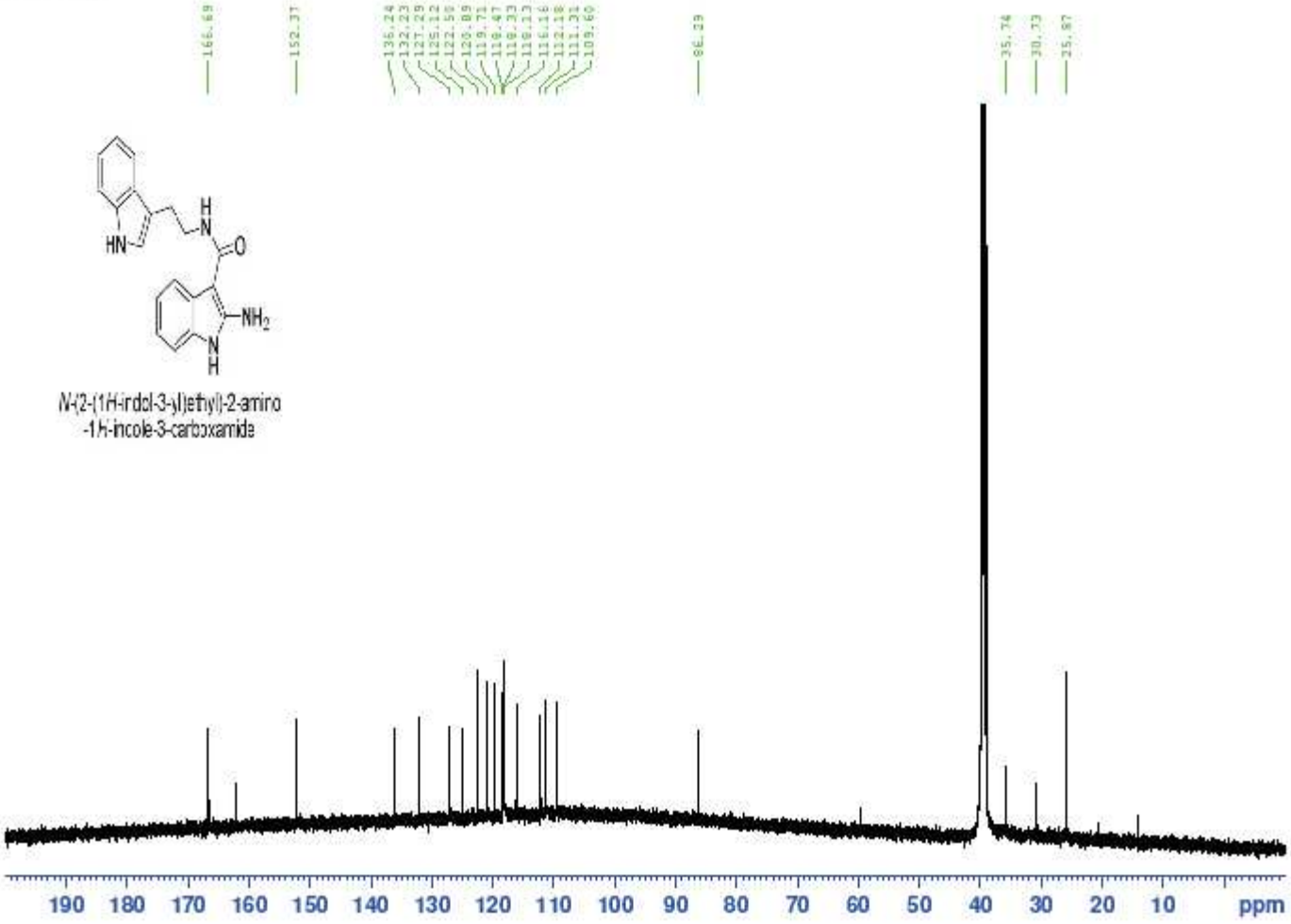
wknate13



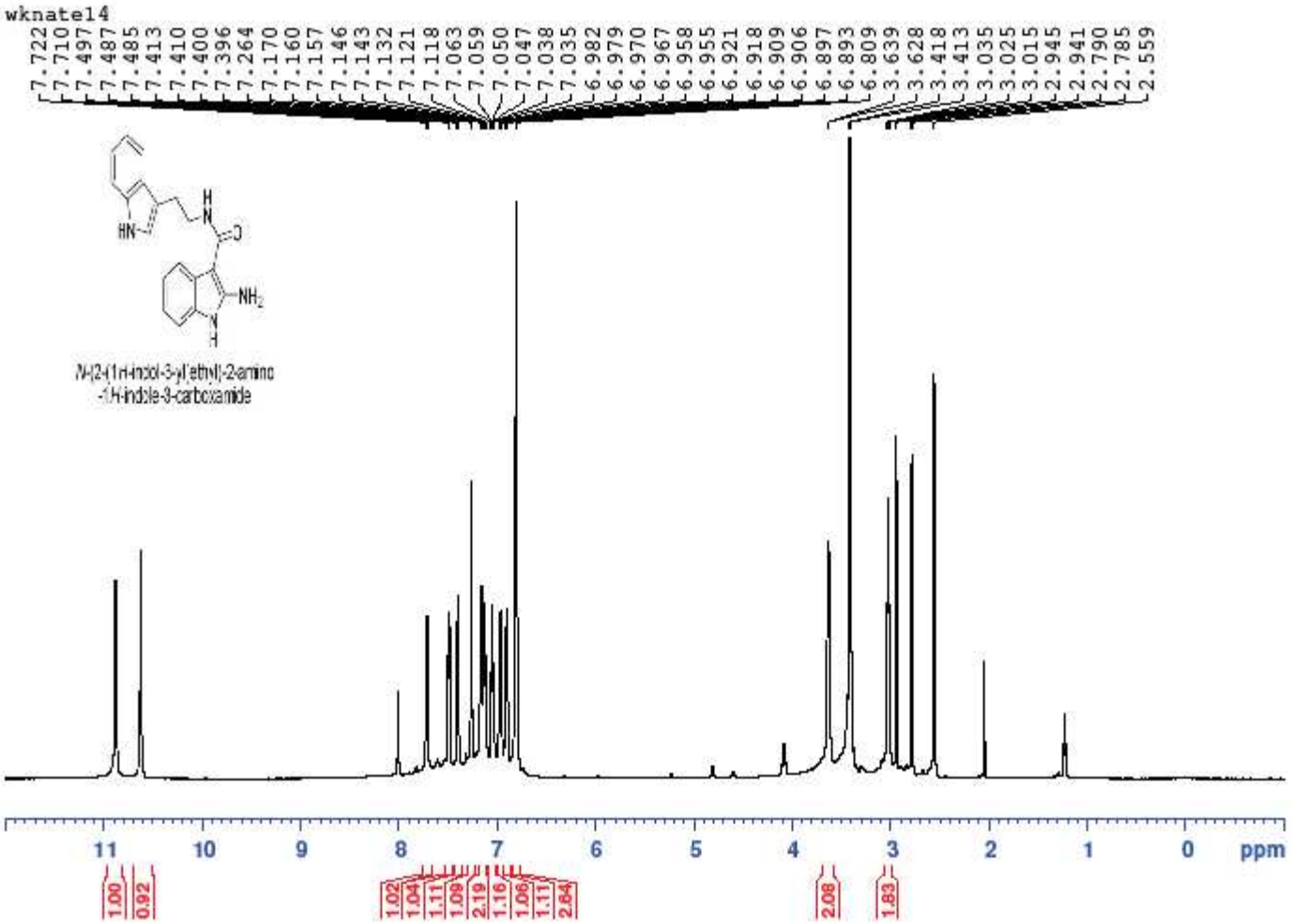
2-amino-*N*-(2,4-dichlorophenethyl)-1*H*-indole-3-carboxamide


wknate13
10.562
7.575
7.574
7.485
7.472
7.388
7.374
7.360
7.346
7.105
7.093
6.932
6.919
6.907
6.859
6.846
6.834
6.827
6.817
6.808
6.710
3.539
3.529
3.518
3.507
2.986
2.974
2.963
Cl
Cl
H
N
O
NH2
N
H
2-amino-N-(2,4-dichlorophenethyl)-1H-indole-3-carboxamide
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.07
1.21
2.25
1.17
1.16
2.20
2.04
2.33
2.24

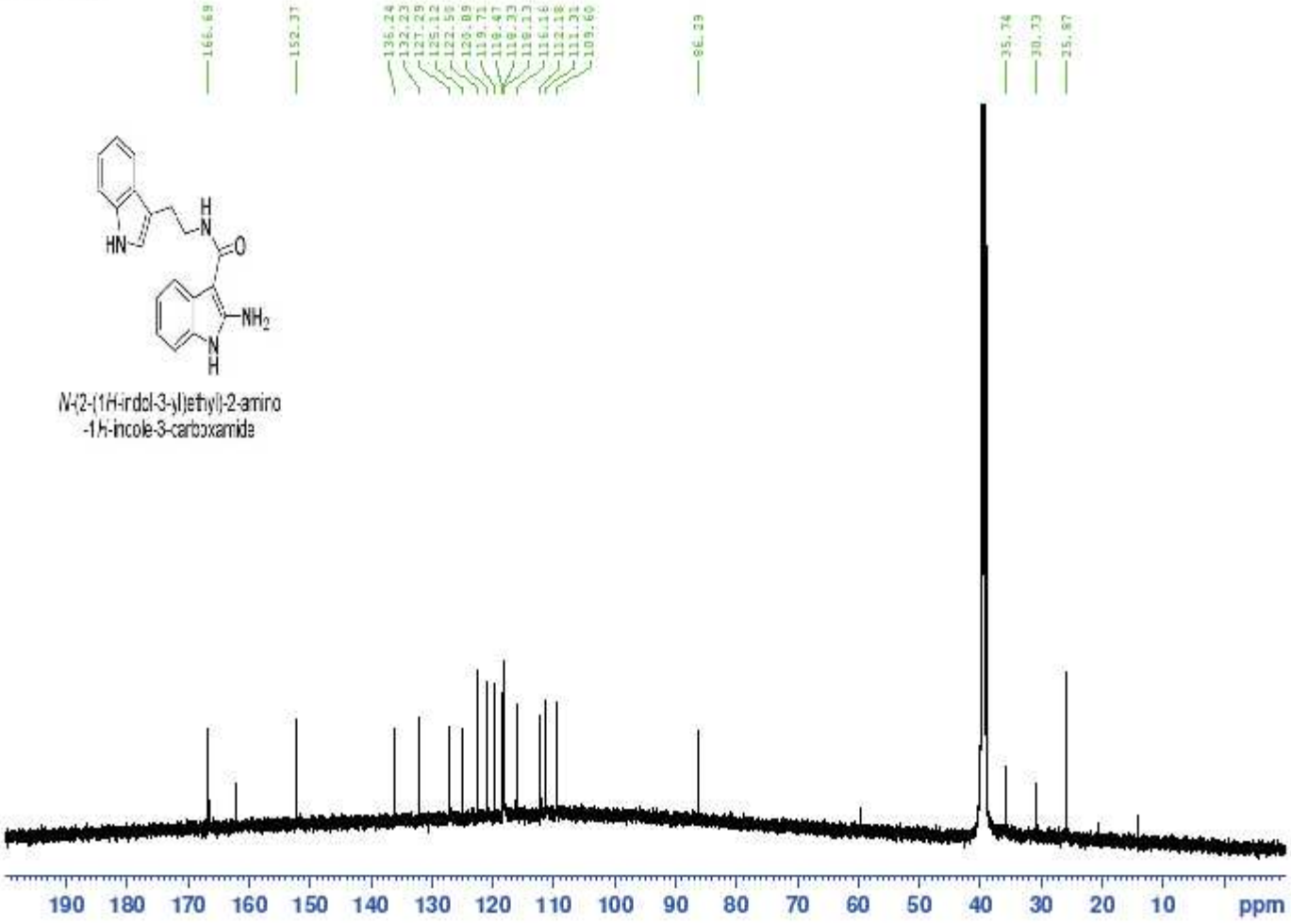
wknate14



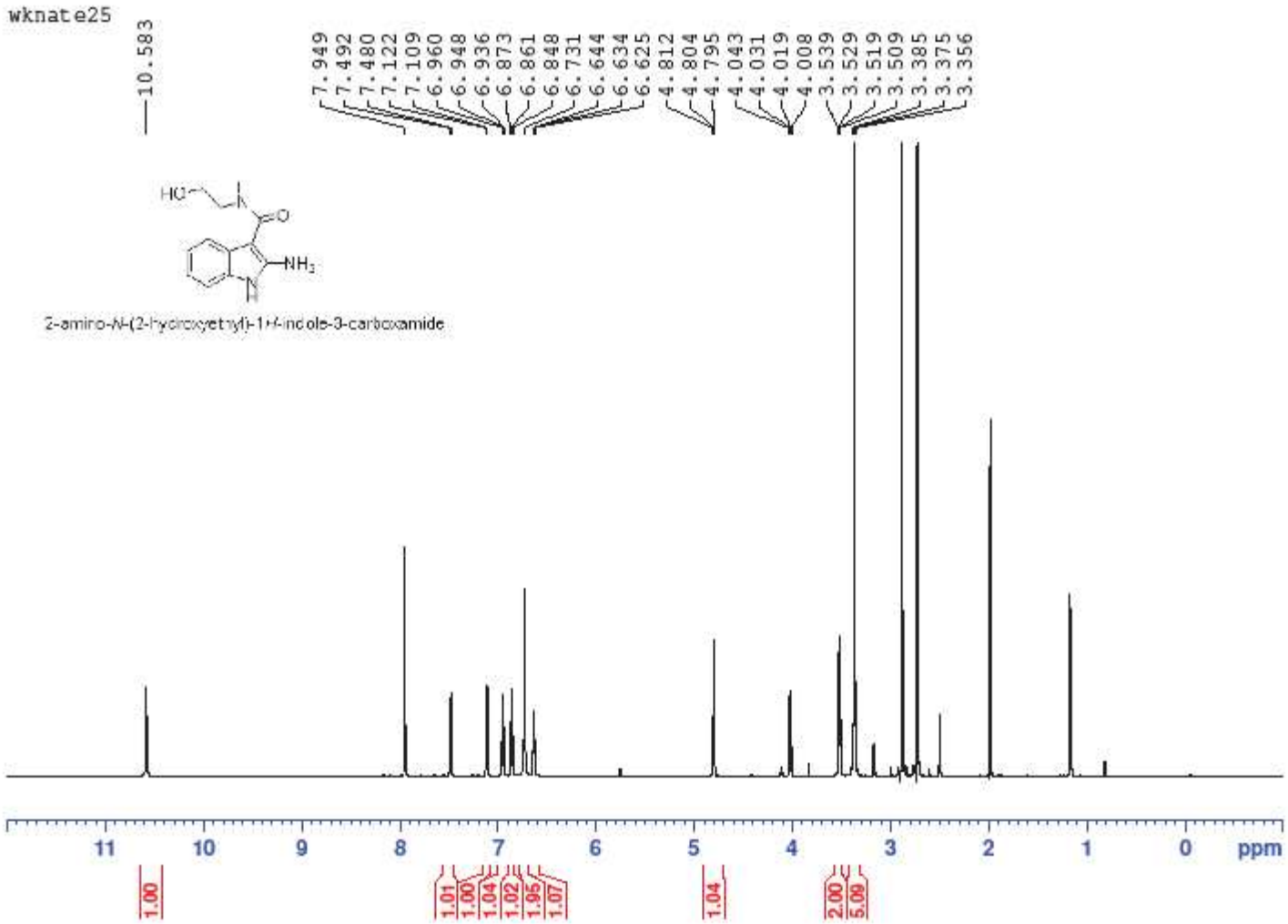
N-(2-(1*H*-indol-3-yl)ethyl)-2-amino-1*H*-incole-3-carboxamide


wknate14
7.722
7.710
7.497
7.487
7.485
7.413
7.410
7.400
7.396
7.264
7.170
7.160
7.157
7.146
7.143
7.132
7.121
7.118
7.063
7.059
7.050
7.047
7.038
7.035
6.982
6.979
6.970
6.967
6.958
6.955
6.921
6.918
6.909
6.906
6.897
6.893
6.809
3.639
3.628
3.418
3.413
3.035
3.025
3.015
2.945
2.941
2.790
2.785
2.559
HN
H
N
O
NH2
N
H
N-(2-(1H-indol-3-yl)ethyl)-2-amino
-1H-indole-3-carboxamide
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.92
1.02
1.04
1.11
1.08
2.19
1.16
1.06
1.11
2.84
2.08
1.83

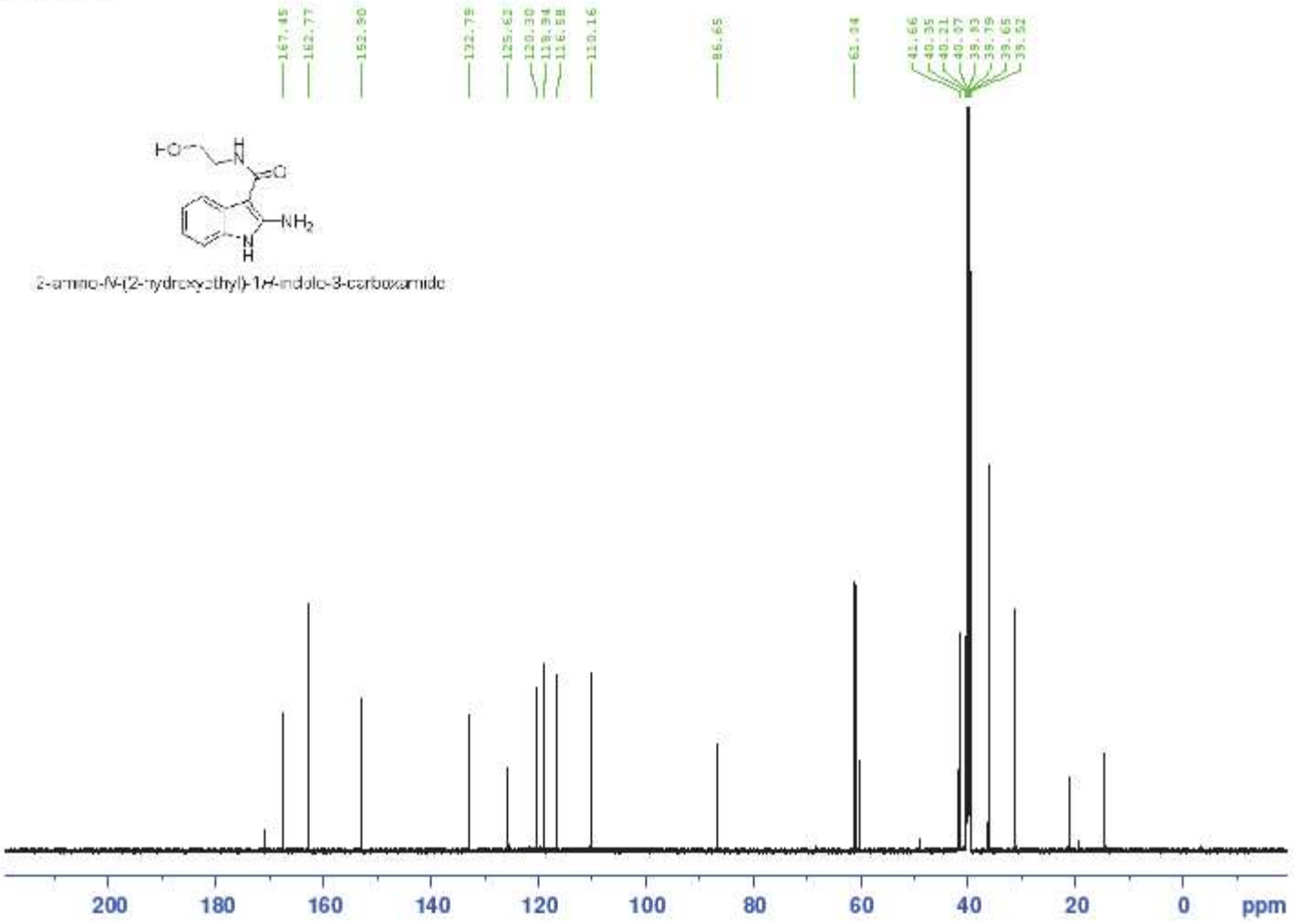
wknate14



N-(2-(1*H*-indol-3-yl)ethyl)-2-amino-1*H*-incole-3-carboxamide

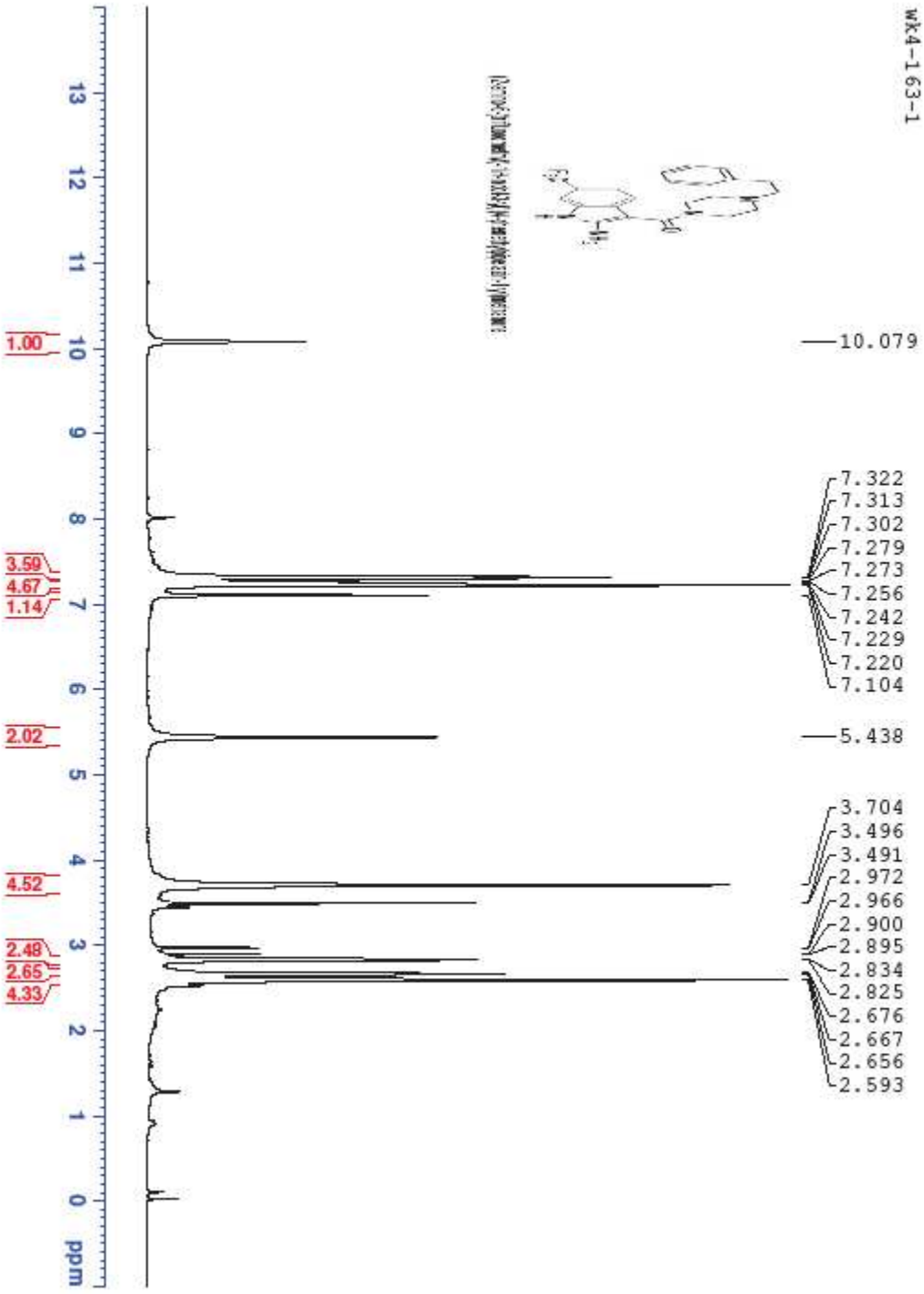

wknate25
10.583
7.949
7.492
7.480
7.122
7.109
6.960
6.948
6.936
6.873
6.861
6.848
6.731
6.644
6.634
6.625
4.812
4.804
4.795
4.043
4.031
4.019
4.008
3.539
3.529
3.519
3.509
3.385
3.375
3.356
HO
O
NH2
2-amino-N-(2-hydroxyethyl)-1H-indole-3-carboxamide
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.00
1.04
1.02
1.95
1.07
1.04
2.00
5.00

wknate25

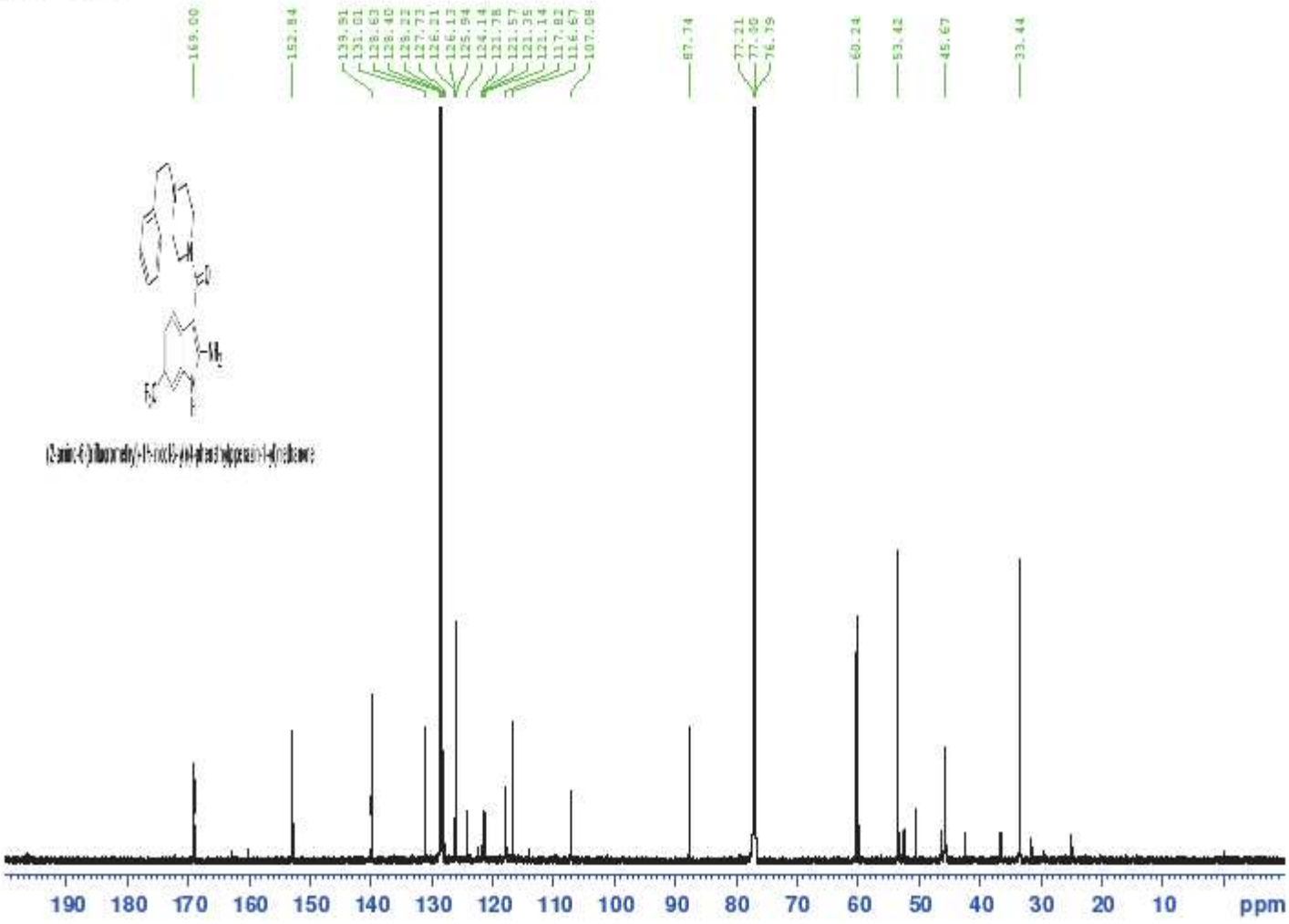


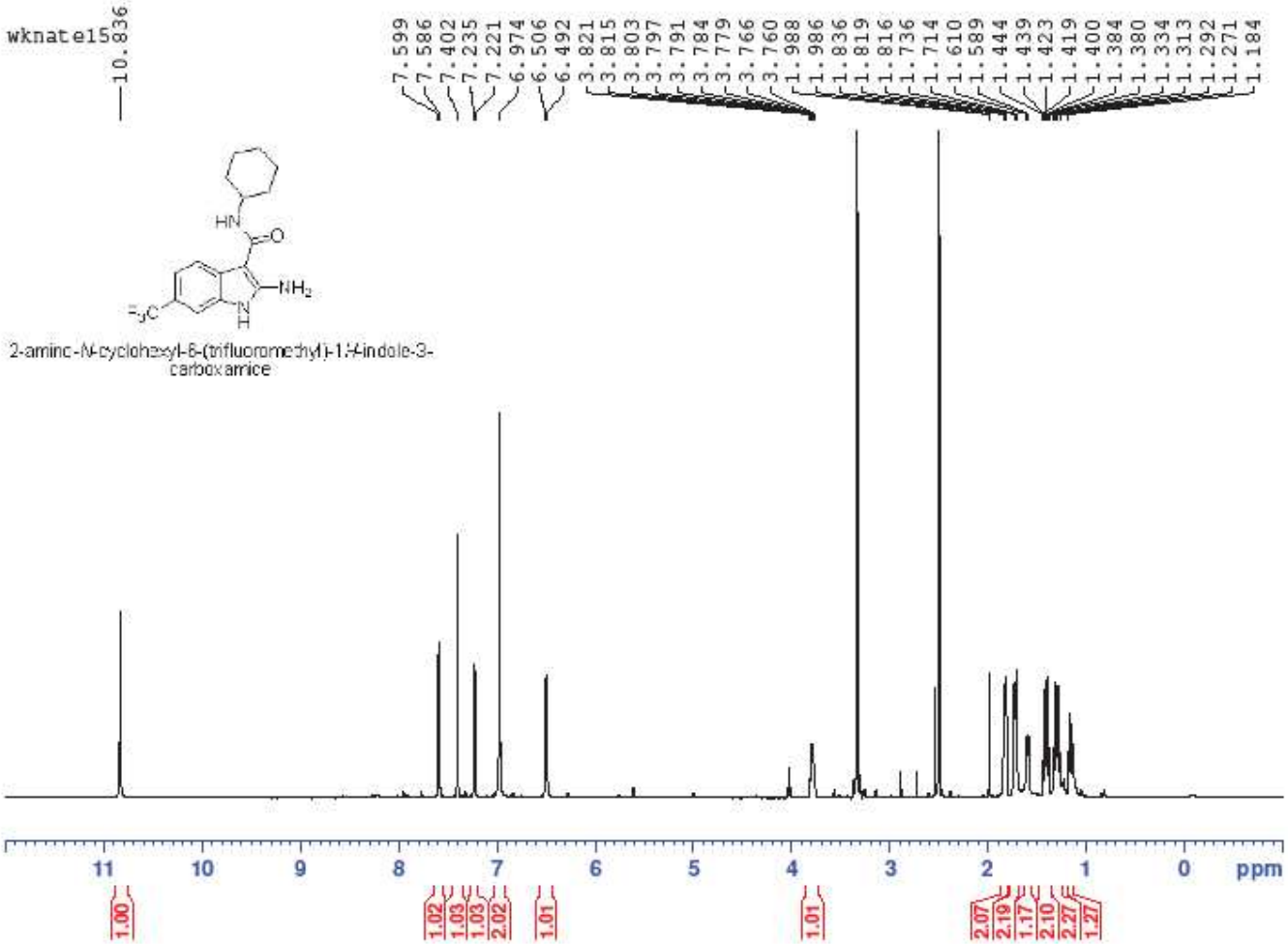
2-amino-*N*-(2-hydroxyethyl)-1*H*-indole-3-carboxamide

3-9

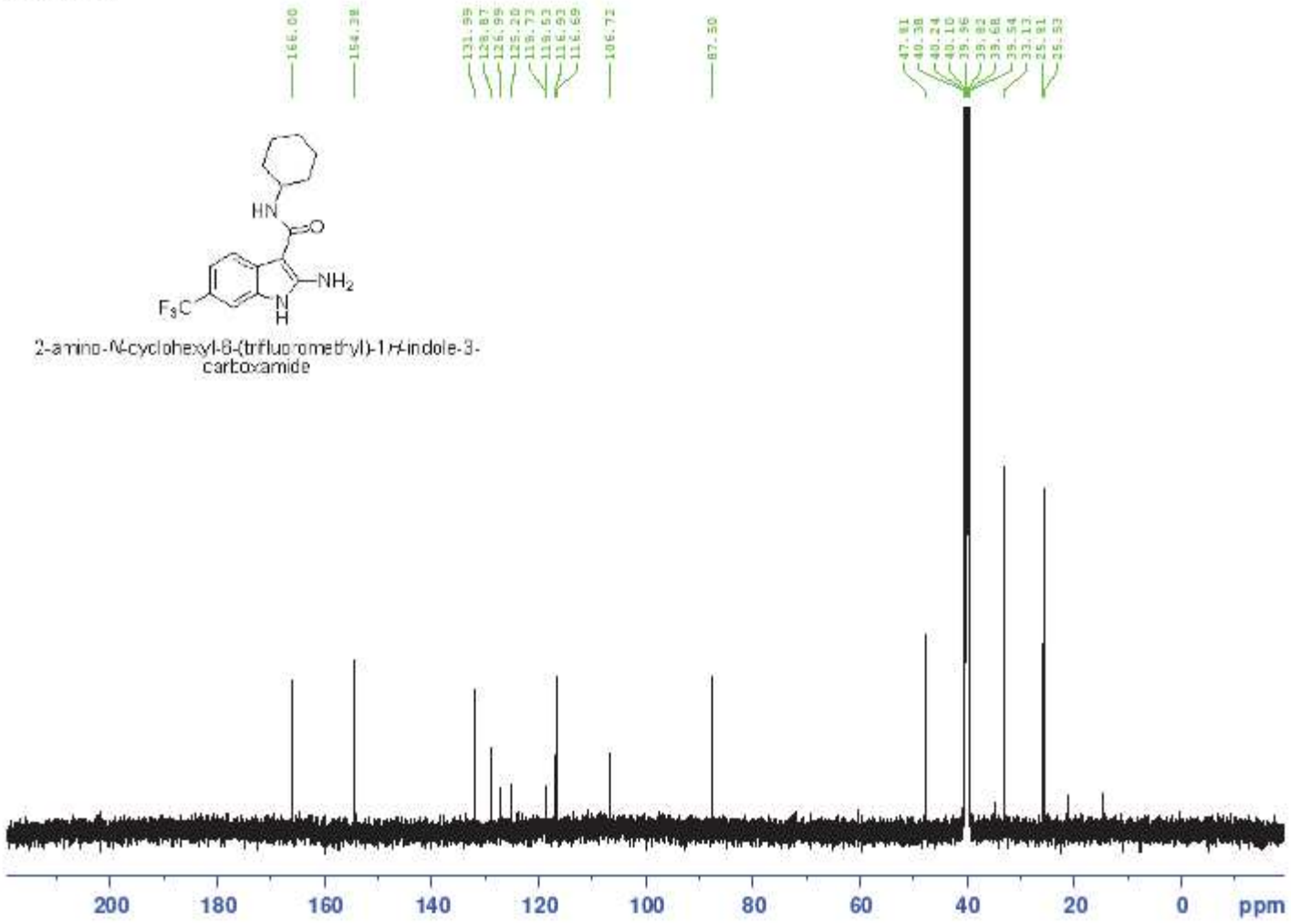

wk4-163-1
10.079
7.322
7.313
7.302
7.279
7.273
7.256
7.242
7.229
7.220
7.104
5.438
3.704
3.496
3.491
2.972
2.966
2.900
2.895
2.834
2.825
2.676
2.667
2.656
2.593
1.00
3.59
4.67
1.14
2.02
4.52
2.49
2.65
4.33
ppm

wk4-163-1


169.00
152.84
139.91
131.01
129.63
128.40
128.22
127.73
126.21
126.13
125.94
124.14
121.78
121.57
121.35
121.14
117.82
116.67
107.08
87.74
77.21
77.00
76.79
60.24
53.42
45.67
33.44
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

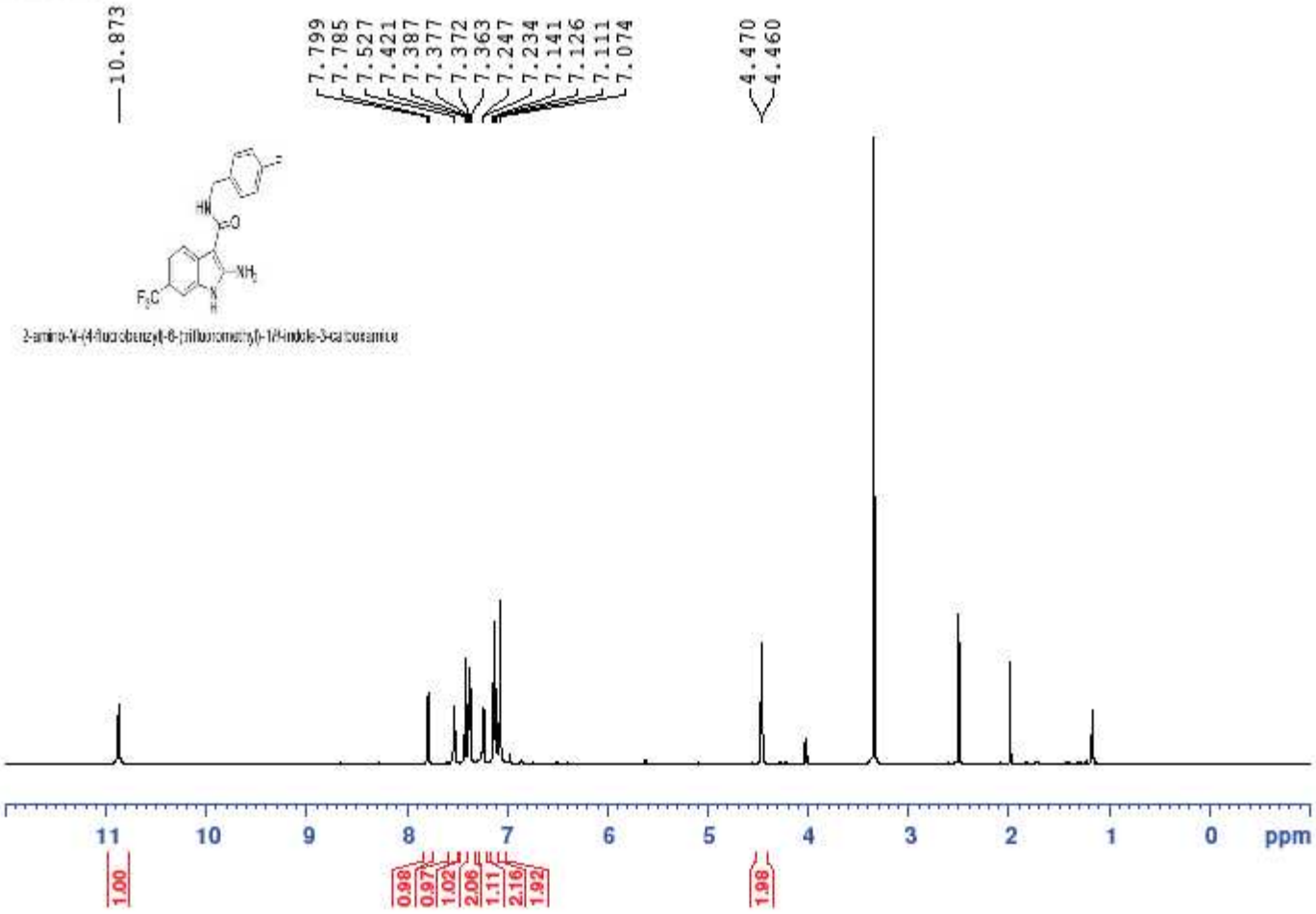

wknate15
10.836
7.599
7.586
7.402
7.235
7.221
6.974
6.506
6.492
3.821
3.815
3.803
3.797
3.791
3.784
3.779
3.766
3.760
1.988
1.986
1.836
1.819
1.816
1.736
1.714
1.610
1.589
1.444
1.439
1.423
1.419
1.400
1.384
1.380
1.334
1.313
1.292
1.271
1.184
HN
O
NH2
F3C
H
2-amino-N-cyclohexyl-6-(trifluoromethyl)-1H-indole-3-carboxamide
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.02
1.03
1.03
2.02
1.01
1.01
2.07
2.19
1.17
2.10
2.27
1.27

wknate15

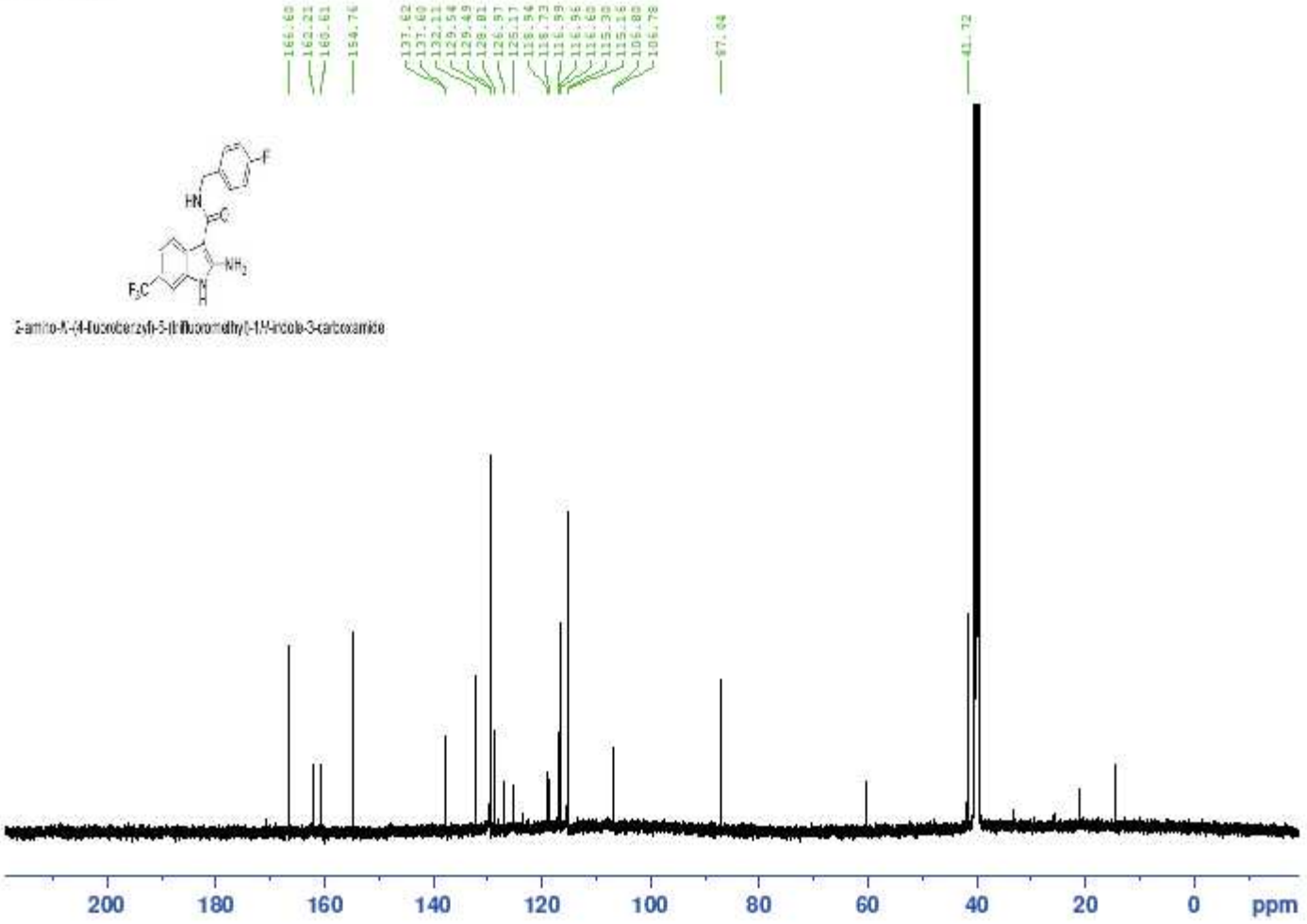


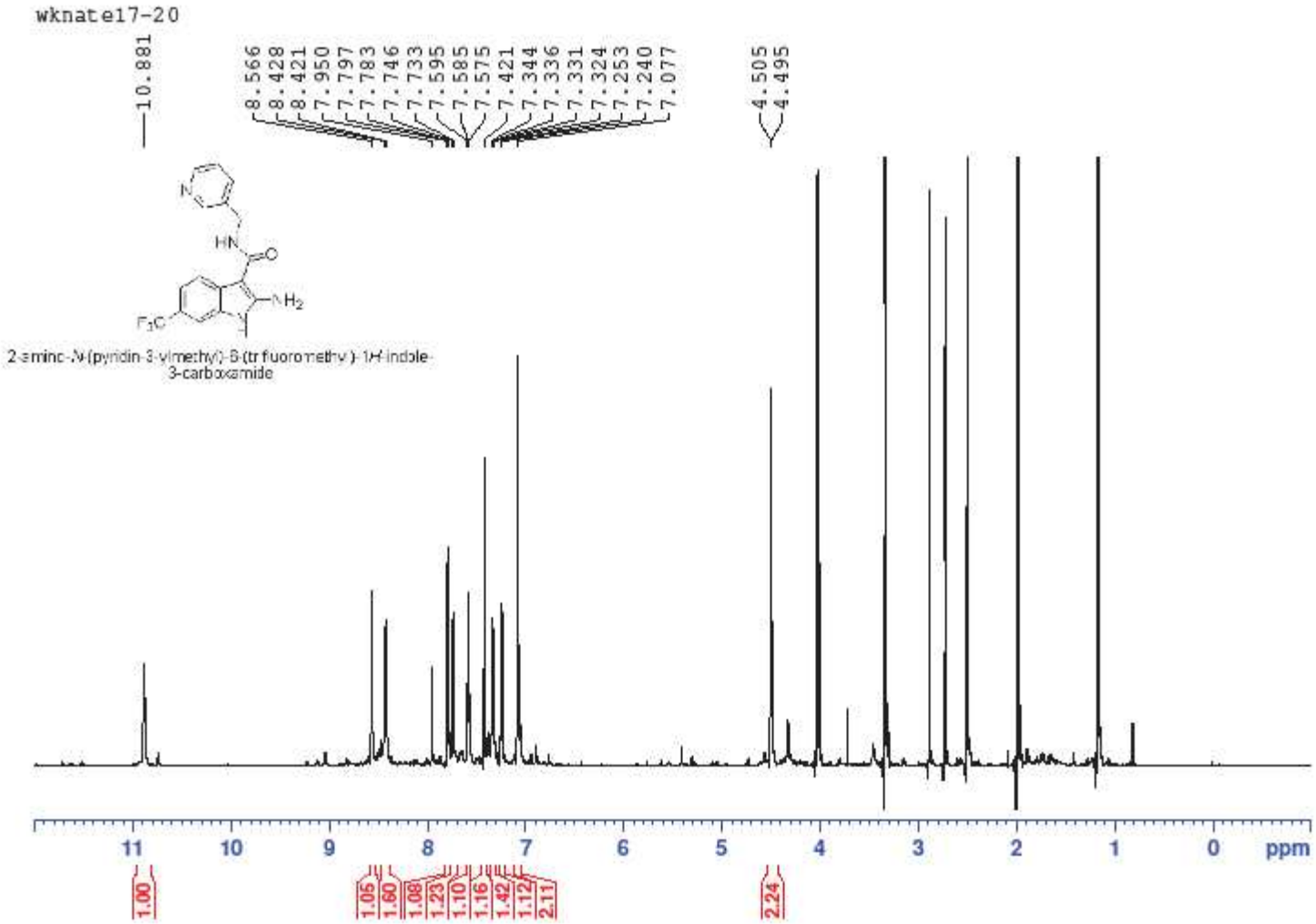
2-amino-N-cyclohexyl-6-(trifluoromethyl)-1*H*-indole-3-carboxamide

wknate16

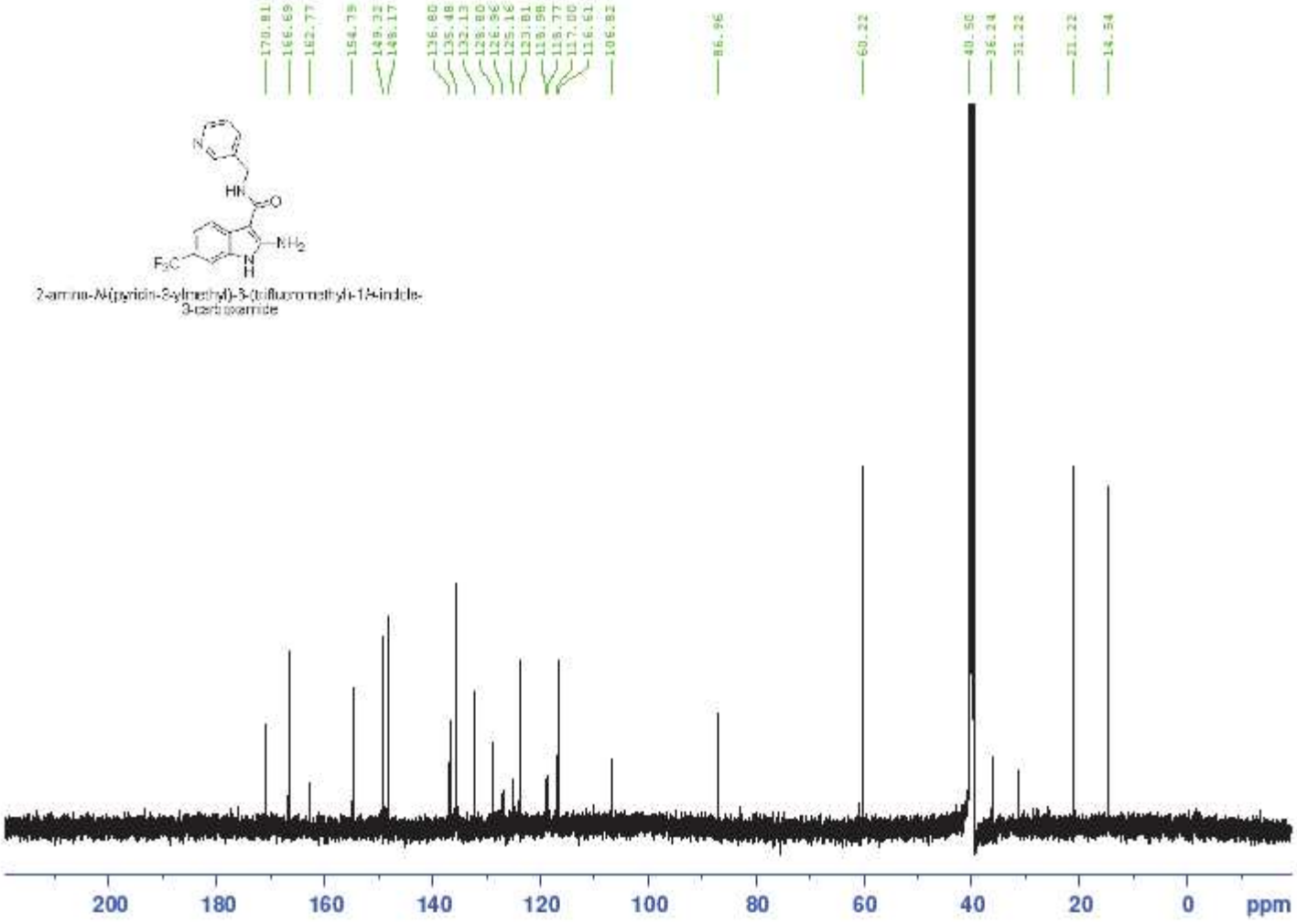

10.873
7.799
7.785
7.527
7.421
7.387
7.377
7.372
7.363
7.247
7.234
7.141
7.126
7.111
7.074
4.470
4.460
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.98
0.97
1.02
2.06
1.11
2.16
1.92
1.98

wknate16

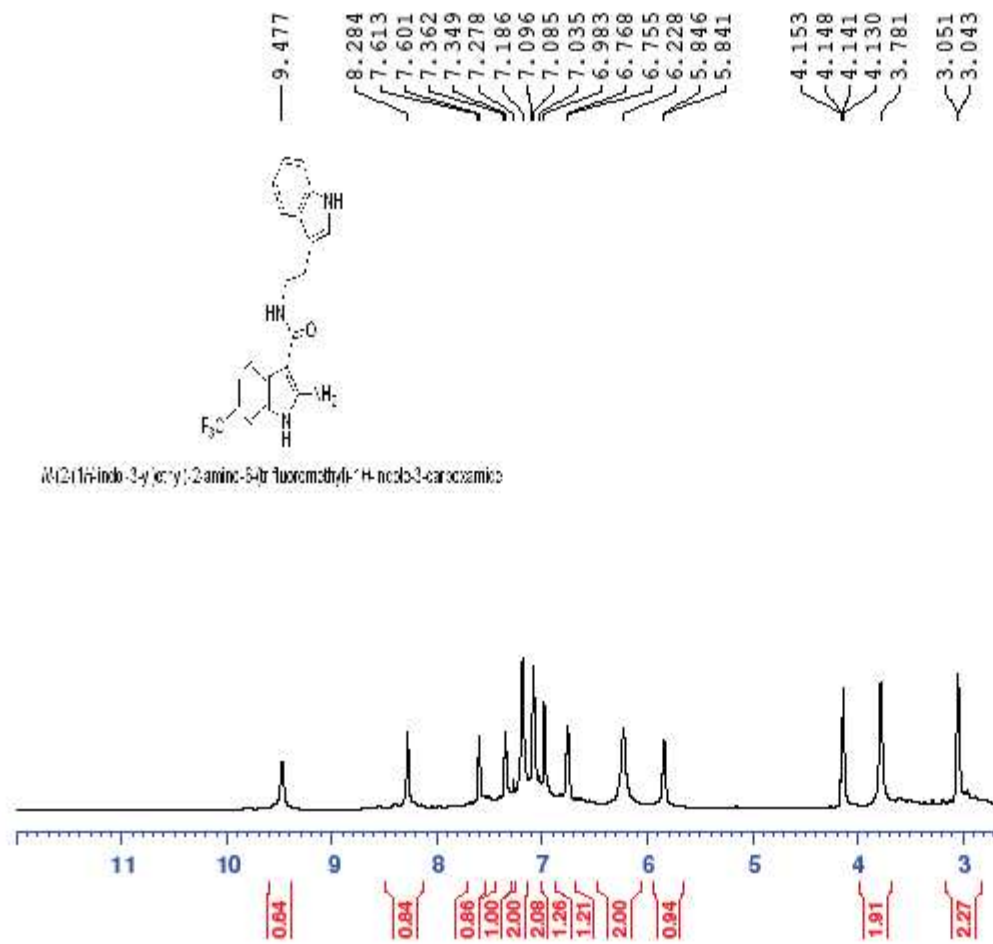

166.60
162.21
160.61
154.76
137.62
137.60
132.11
129.54
129.49
128.81
126.97
125.17
118.54
118.73
111.99
111.96
116.60
115.30
115.16
105.80
105.78
67.04
41.72
F
HN
C=O
NH2
F3C
N
H
200
180
160
140
120
100
80
60
40
20
0
ppm


wknate17-20
10.881
8.566
8.428
8.421
7.950
7.797
7.783
7.746
7.733
7.595
7.585
7.575
7.421
7.344
7.336
7.331
7.324
7.253
7.240
7.077
4.505
4.495
HN
O
NH2
F3C
2-amino-N-(pyridin-3-ylmethyl)-5-(trifluoromethyl)-1H-indole-3-carboxamide
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.05
1.60
1.08
1.23
1.10
1.16
1.42
1.12
2.11
2.24

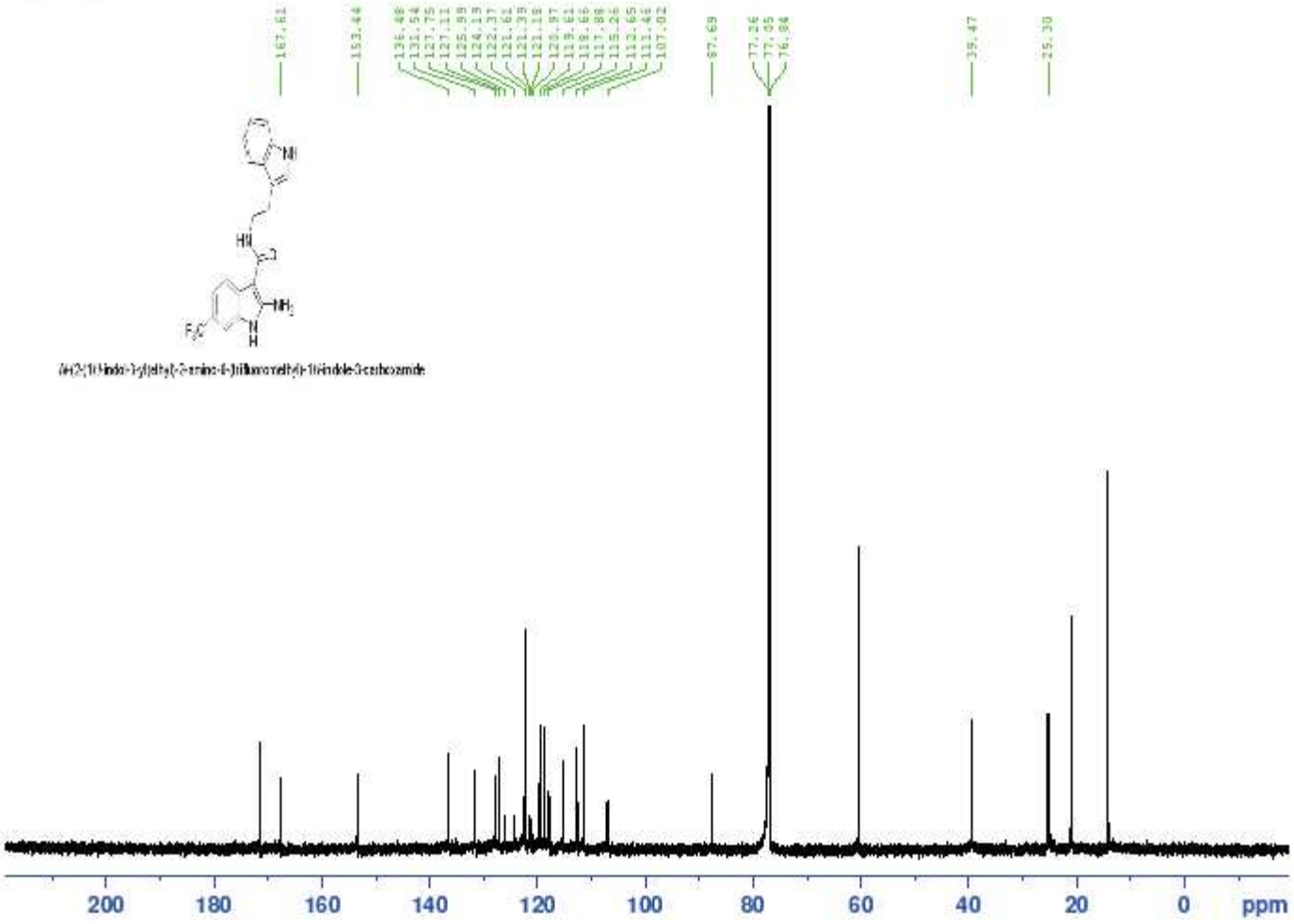
wknate17-20

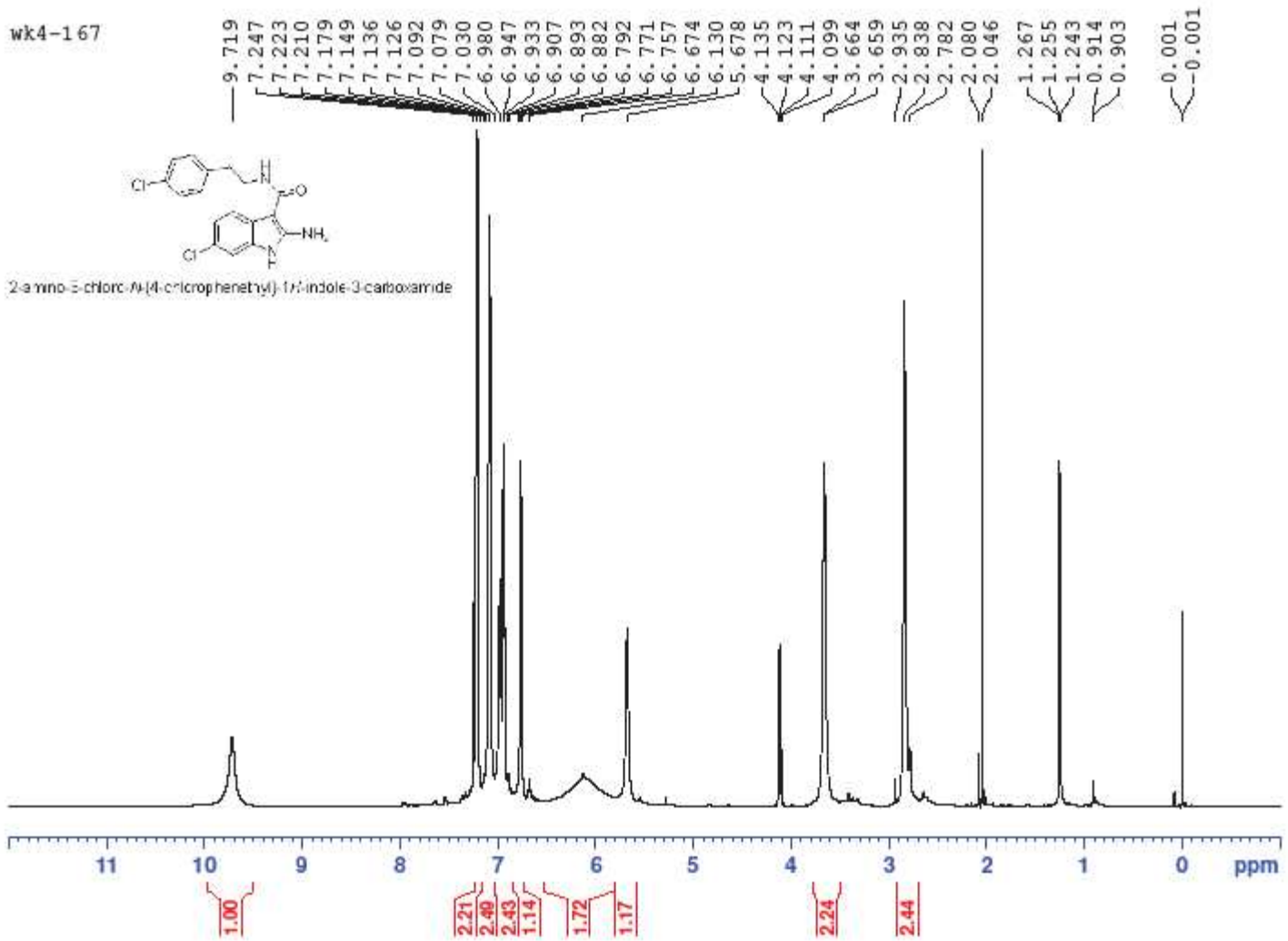

170.81
166.69
162.77
154.79
149.32
148.17
136.80
135.48
132.13
128.80
126.96
125.16
123.81
119.58
118.77
117.00
116.61
106.82
86.96
60.22
40.50
36.24
31.22
21.22
14.54
HN
O
NH2
F3C
N
H
2-amino-N-(pyridin-2-ylmethyl)-3-(trifluoromethyl)-1H-indole-3-carboxamide
200
180
160
140
120
100
80
60
40
20
0
ppm

wknate18

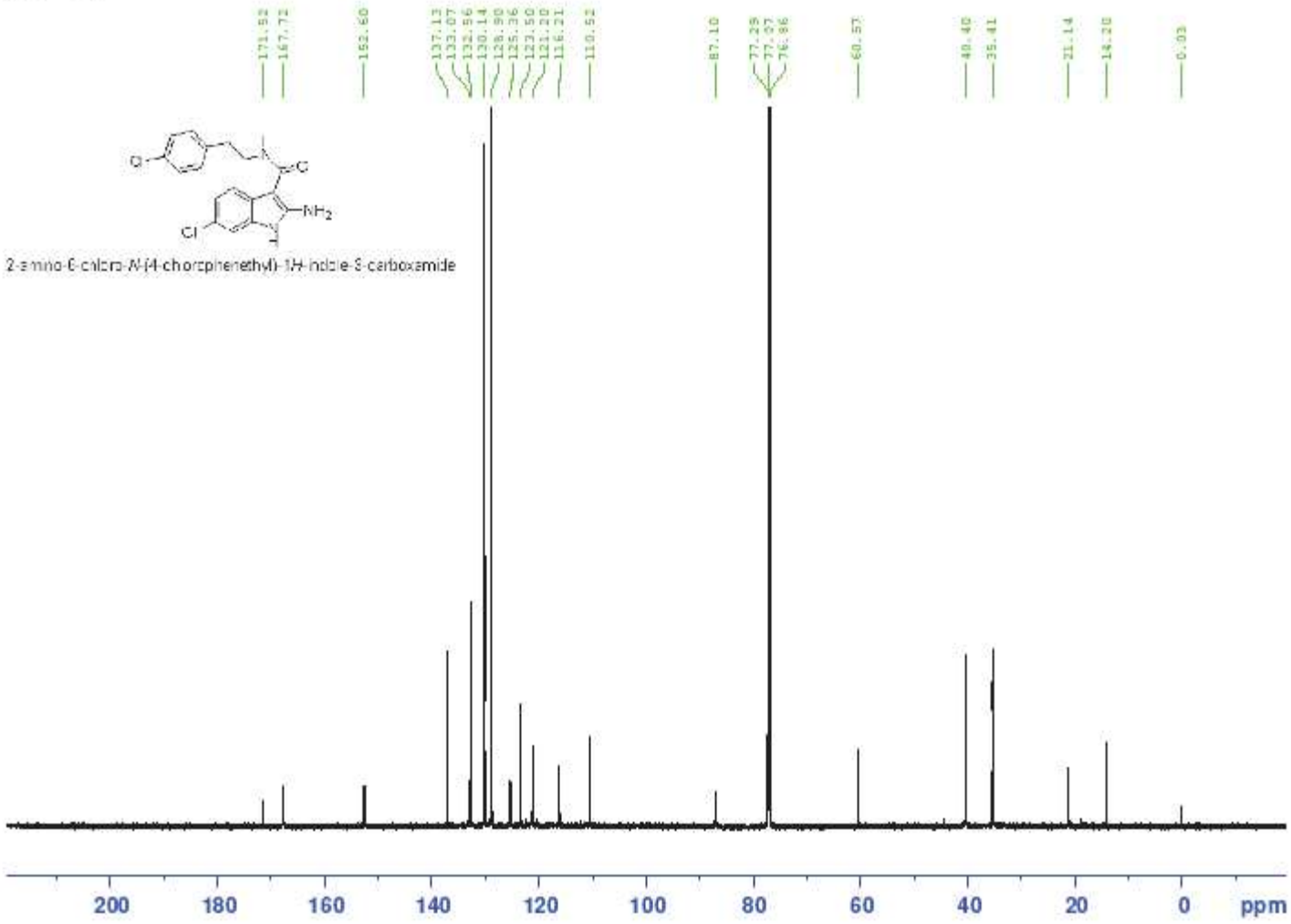

9.477
8.284
7.613
7.601
7.362
7.349
7.278
7.186
7.096
7.085
7.035
6.983
6.768
6.755
6.228
5.846
5.841
4.153
4.148
4.141
4.130
3.781
3.051
3.043
NH
HN
O
NH2
F3C
N
H
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.64
0.84
0.86
1.00
2.00
2.08
1.26
1.21
2.00
0.94
1.91
2.27

wknate18


167.61
153.44
136.48
131.54
127.75
127.11
125.99
124.19
122.37
121.61
121.38
121.18
120.97
119.61
118.66
117.88
116.26
113.65
111.48
107.02
87.69
77.26
77.05
76.84
39.47
25.30
200
180
160
140
120
100
80
60
40
20
0
ppm

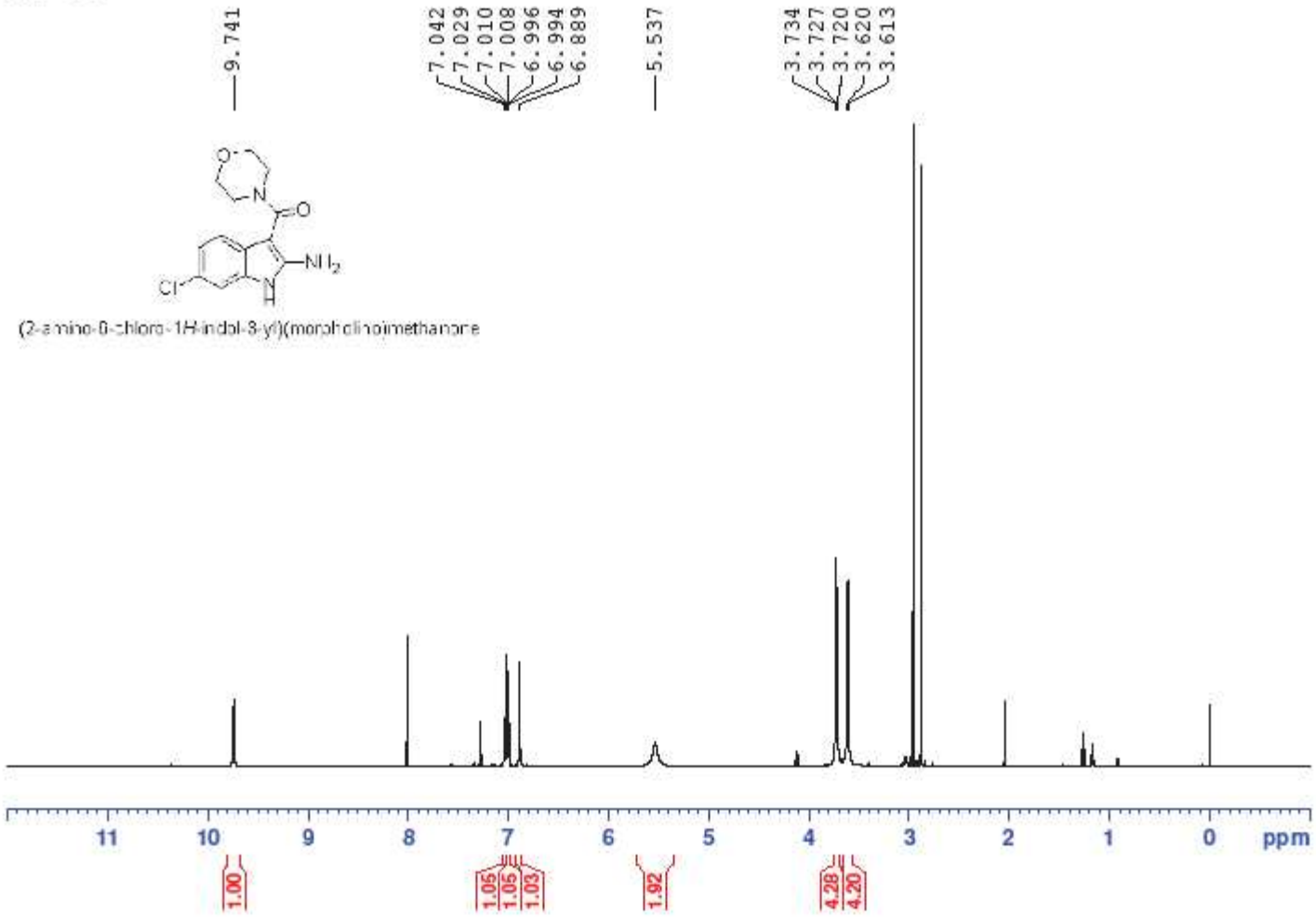

wk4-167
9.719
7.247
7.223
7.210
7.179
7.149
7.136
7.126
7.092
7.079
7.030
6.980
6.947
6.933
6.907
6.893
6.882
6.792
6.771
6.757
6.674
6.130
5.678
4.135
4.123
4.111
4.099
3.664
3.659
2.935
2.838
2.782
2.080
2.046
1.267
1.255
1.243
0.914
0.903
0.001
-0.001
Cl
NH
O
NH2
Cl
2-amino-5-chloro-N-(4-chlorophenethyl)-1H-indole-3-carboxamide
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.21
2.49
2.43
1.14
1.72
1.17
2.24
2.44

wk4-167



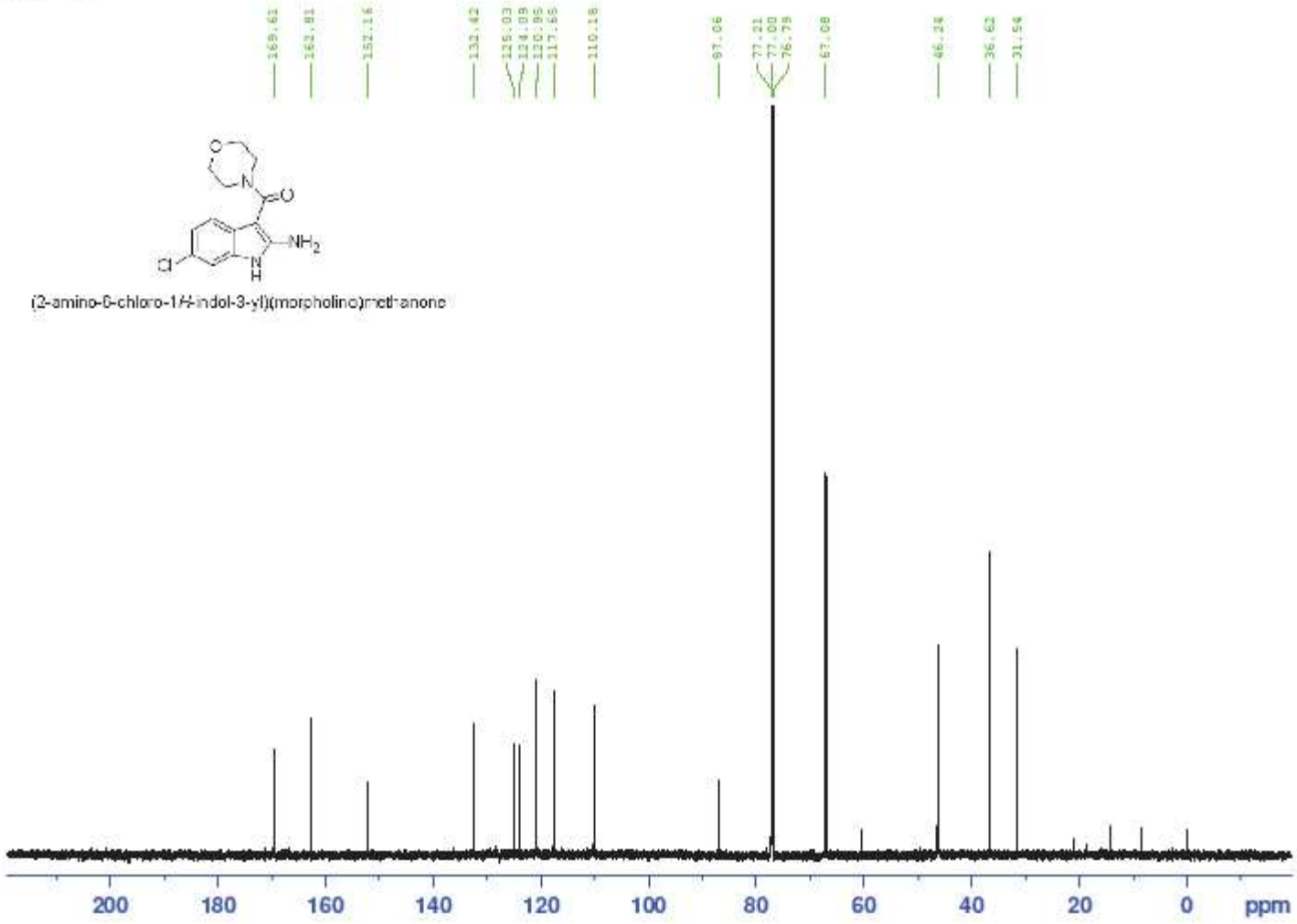
2-amino-6-chloro-N-(4-chlorophenethyl)-1H-indole-3-carboxamide

WK4-168

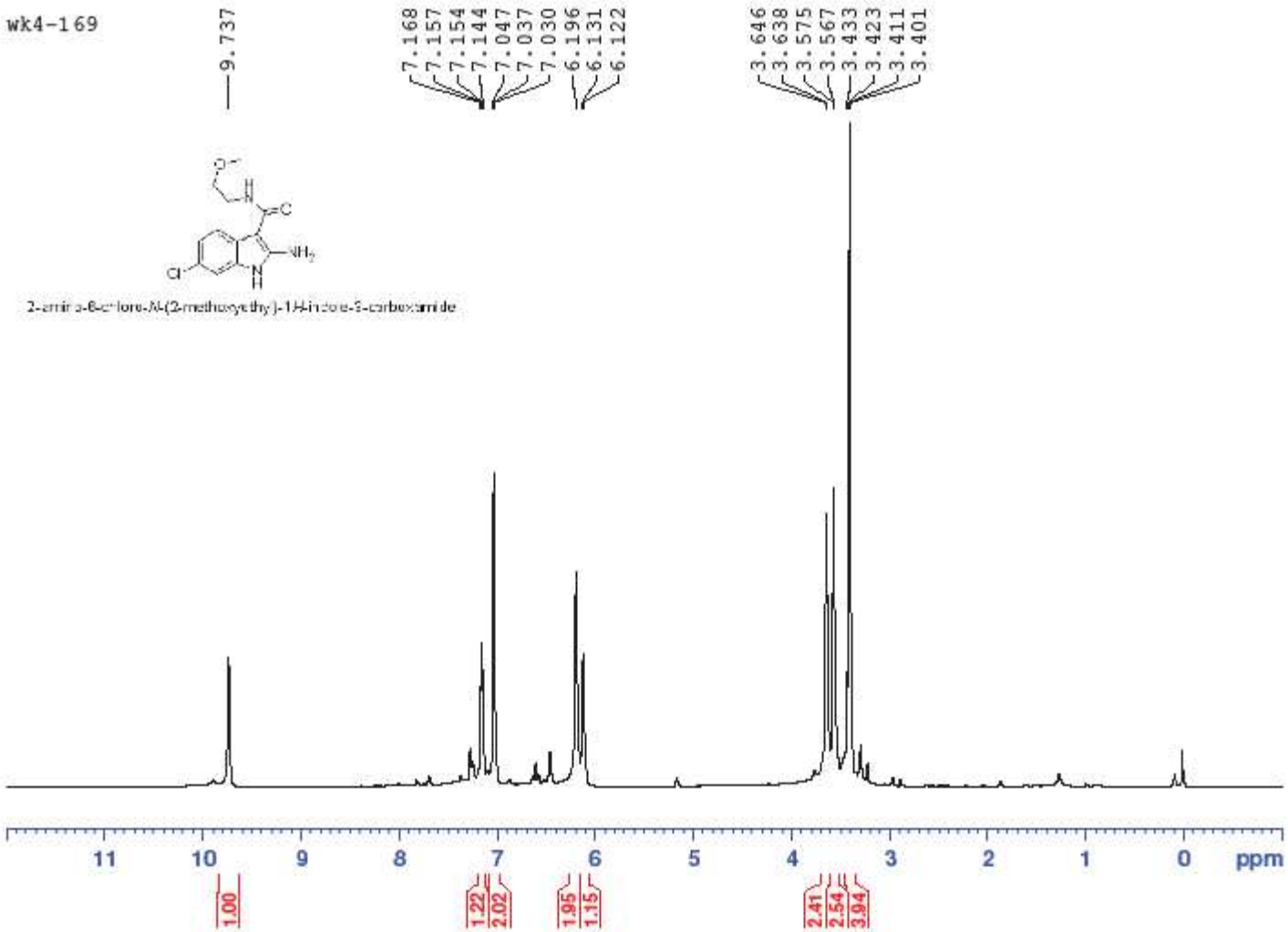


(2-amino-6-chloro-1H-indol-3-yl)(morpholino)methanone

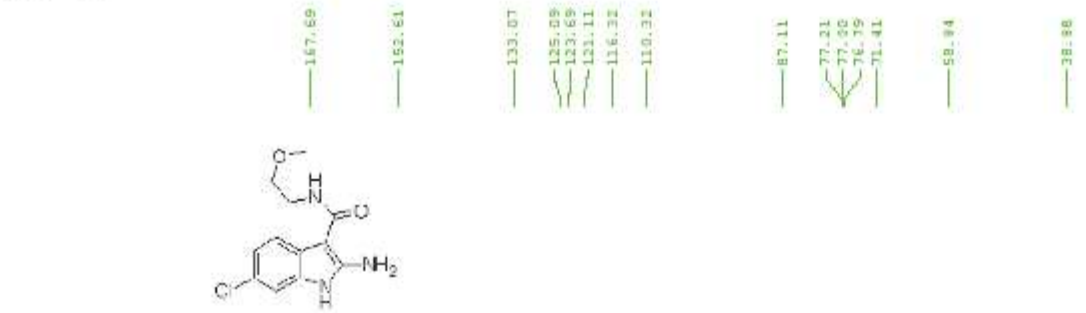
WK4-168



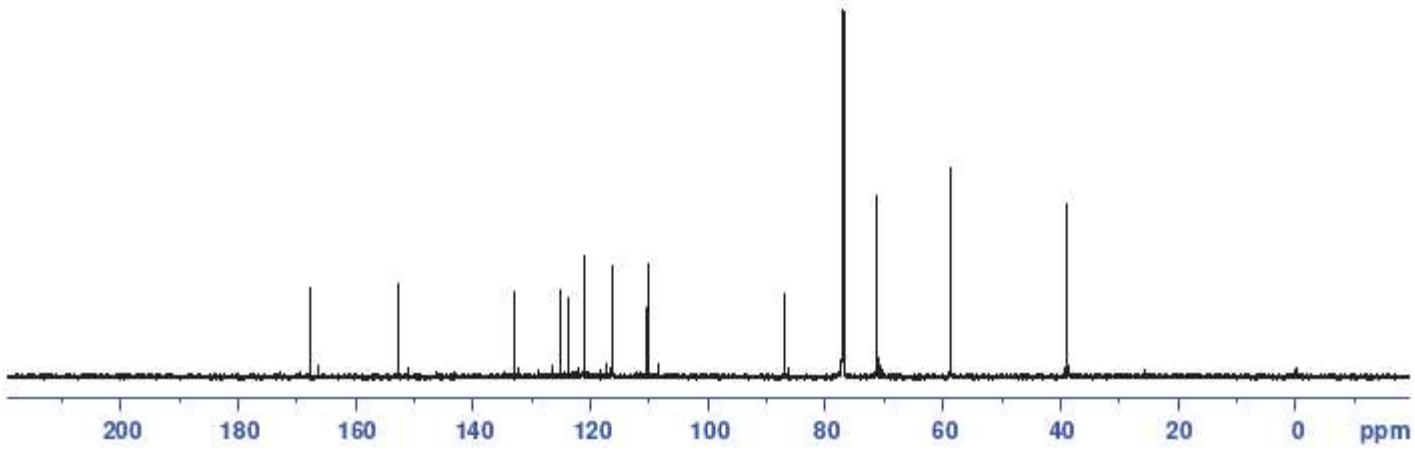
(2-amino-6-chloro-1*H*-indol-3-yl)(morpholino)methanone

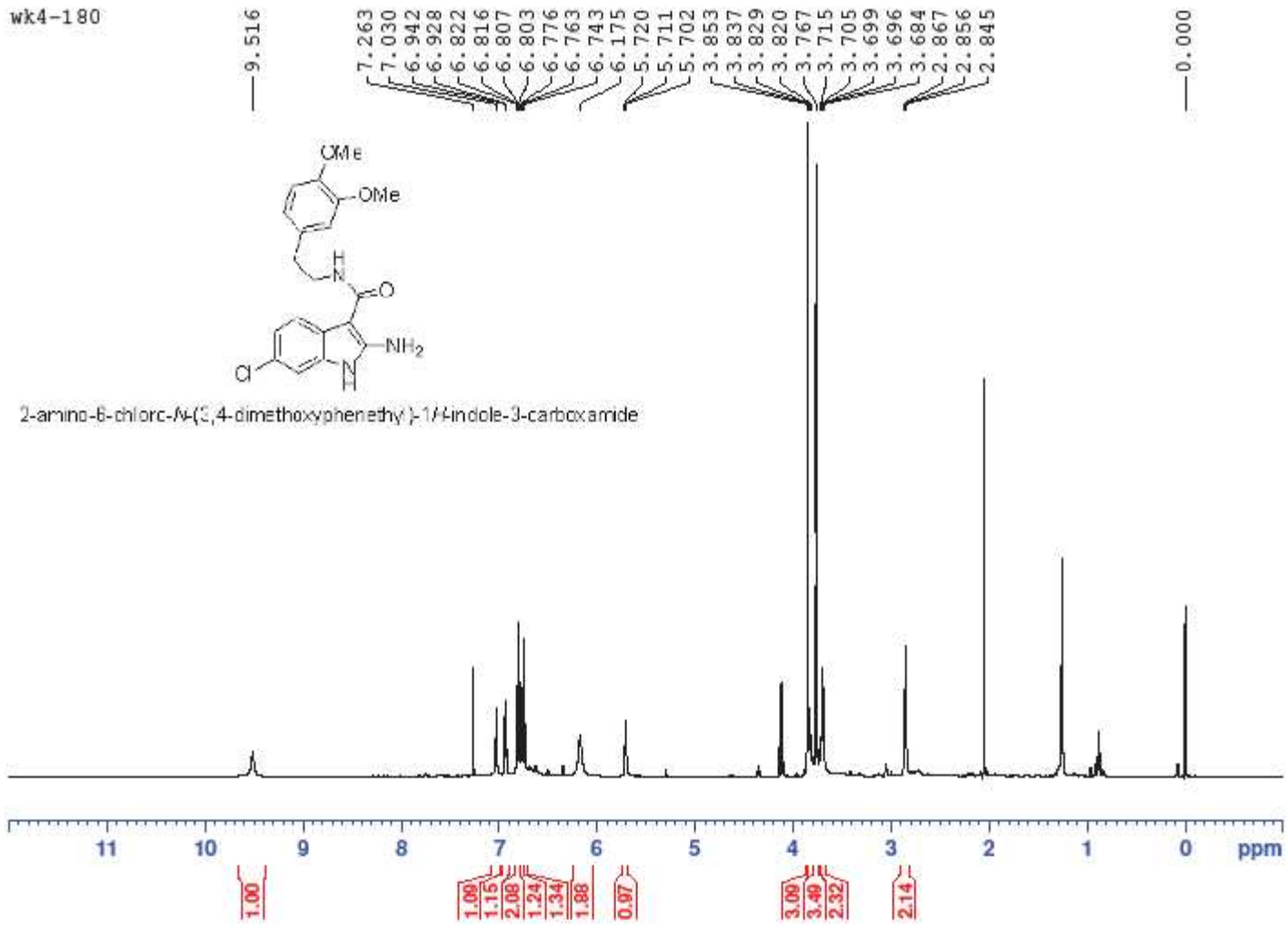

wk4-169
9.737
7.168
7.157
7.154
7.144
7.047
7.037
7.030
6.196
6.131
6.122
3.646
3.638
3.575
3.567
3.433
3.423
3.411
3.401
2-amino-6-chloro-N-(2-methoxyethyl)-1H-indole-3-carboxamide
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.22
2.02
1.95
1.15
2.41
2.54
3.94

wk4-169

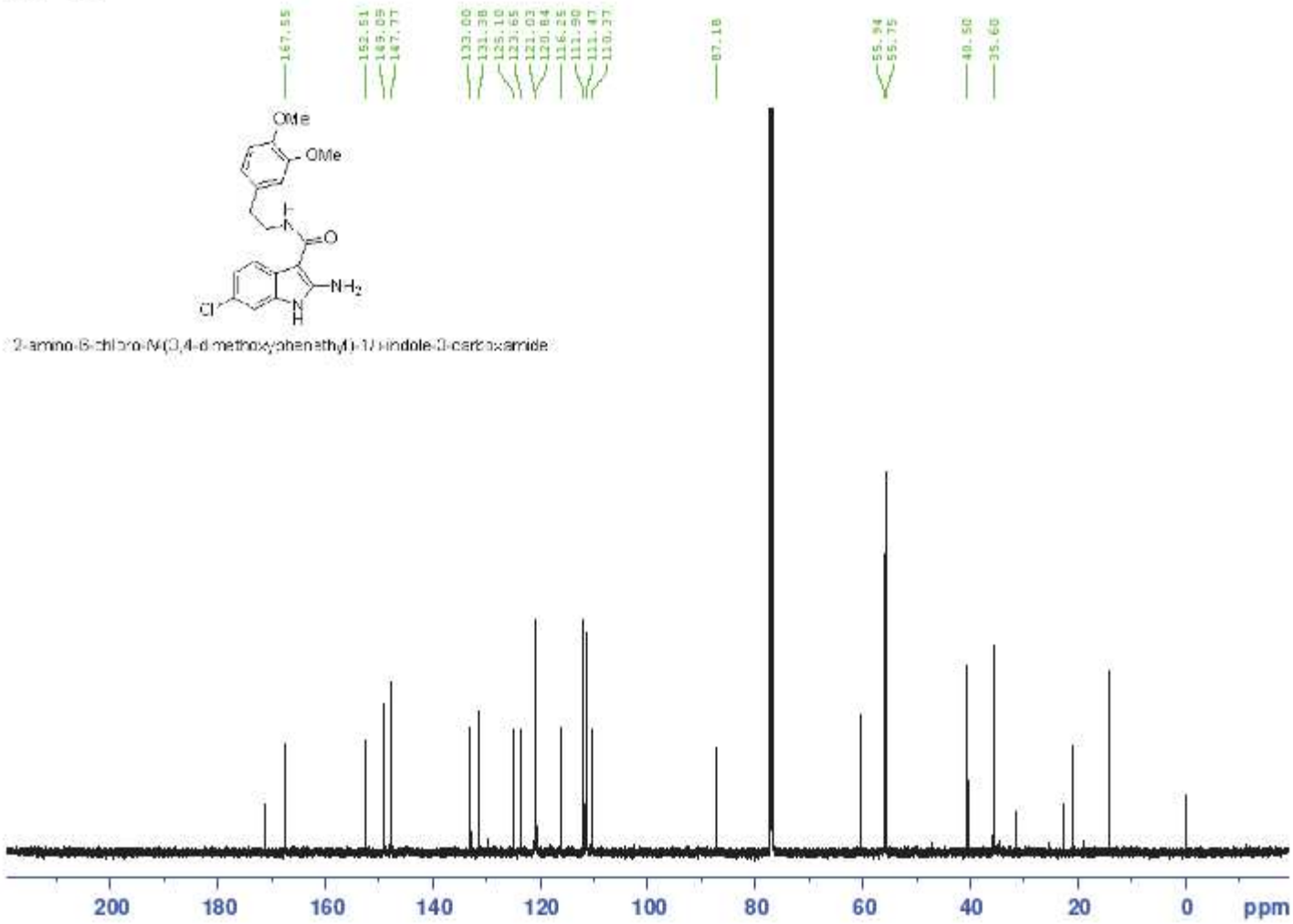


2-amino-6-chloro-N-(2-methoxyethyl)-1H-indole-3-carboxamide

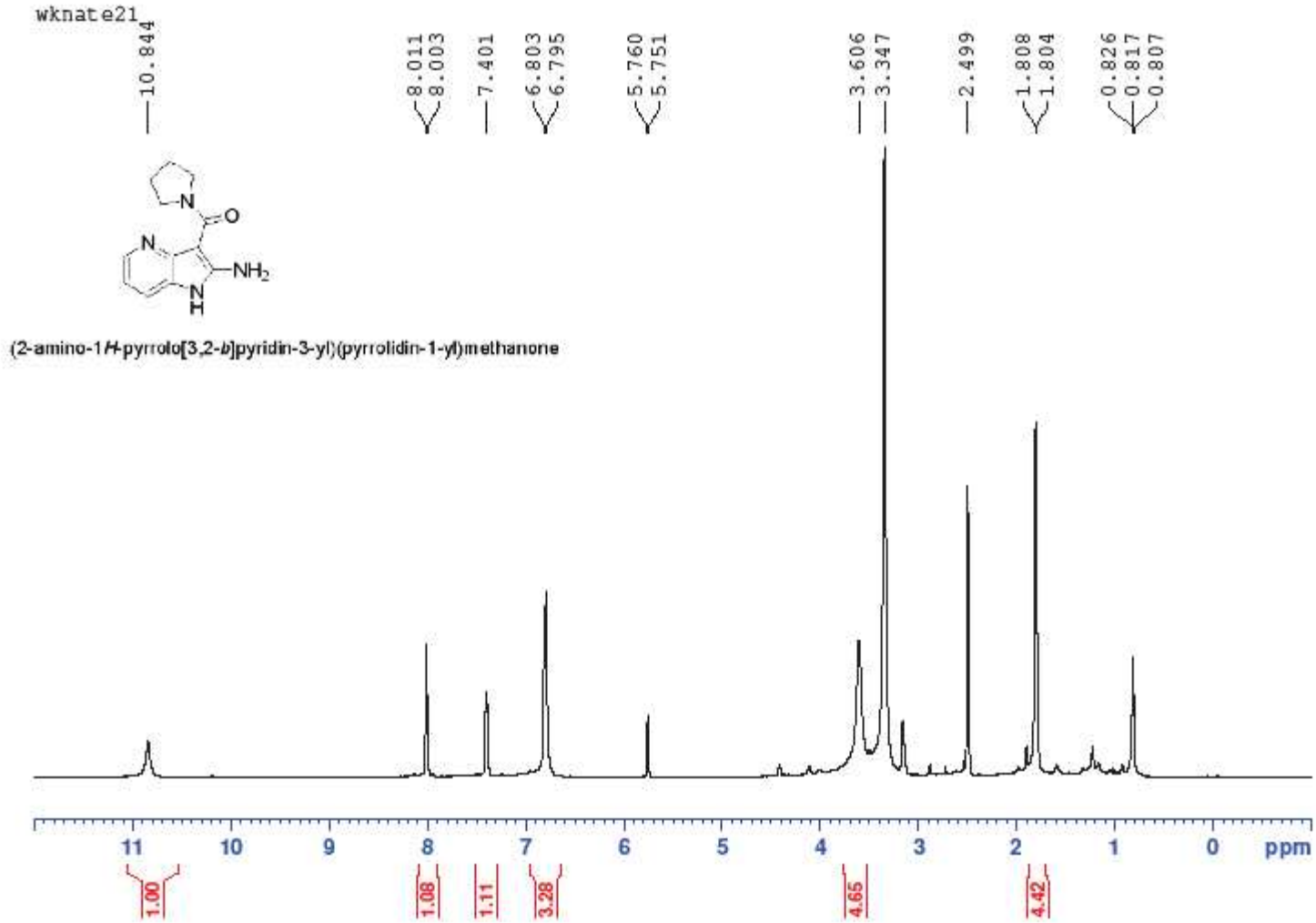



wk4-180
9.516
7.263
7.030
6.942
6.928
6.822
6.816
6.807
6.803
6.776
6.763
6.743
6.175
5.720
5.711
5.702
3.853
3.837
3.829
3.820
3.767
3.715
3.705
3.699
3.696
3.684
2.867
2.856
2.845
0.000
OMe
OMe
H
N
O
NH2
Cl
N
H
2-amino-6-chloro-N-(3,4-dimethoxyphenethyl)-1H-indole-3-carboxamide
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.15
2.08
1.24
1.34
1.88
0.97
3.09
3.49
2.32
2.14

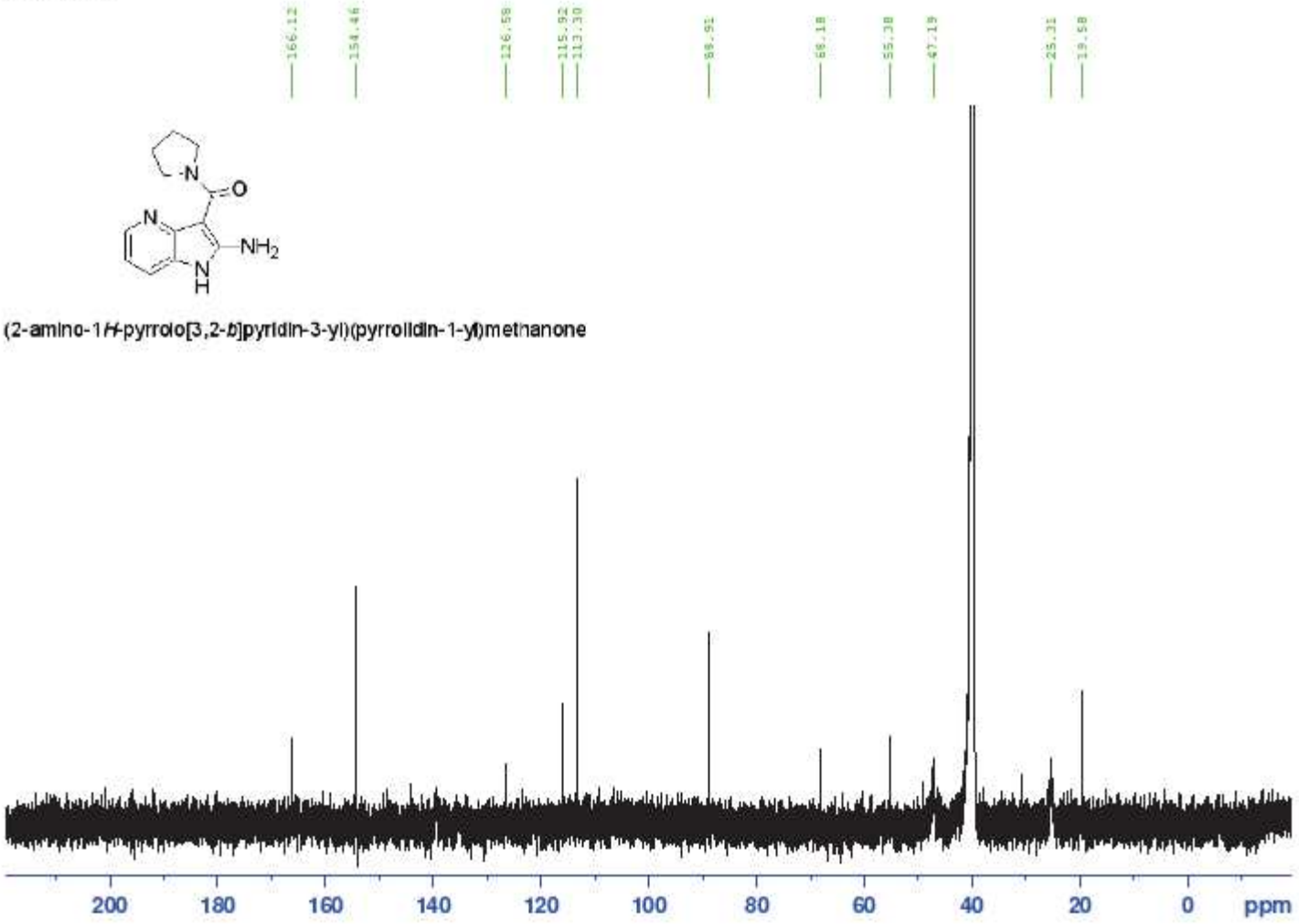
wk4-180



2-amino-6-chloro-N-(3,4-dimethoxyphenethyl)-1H-indole-3-carboxamide

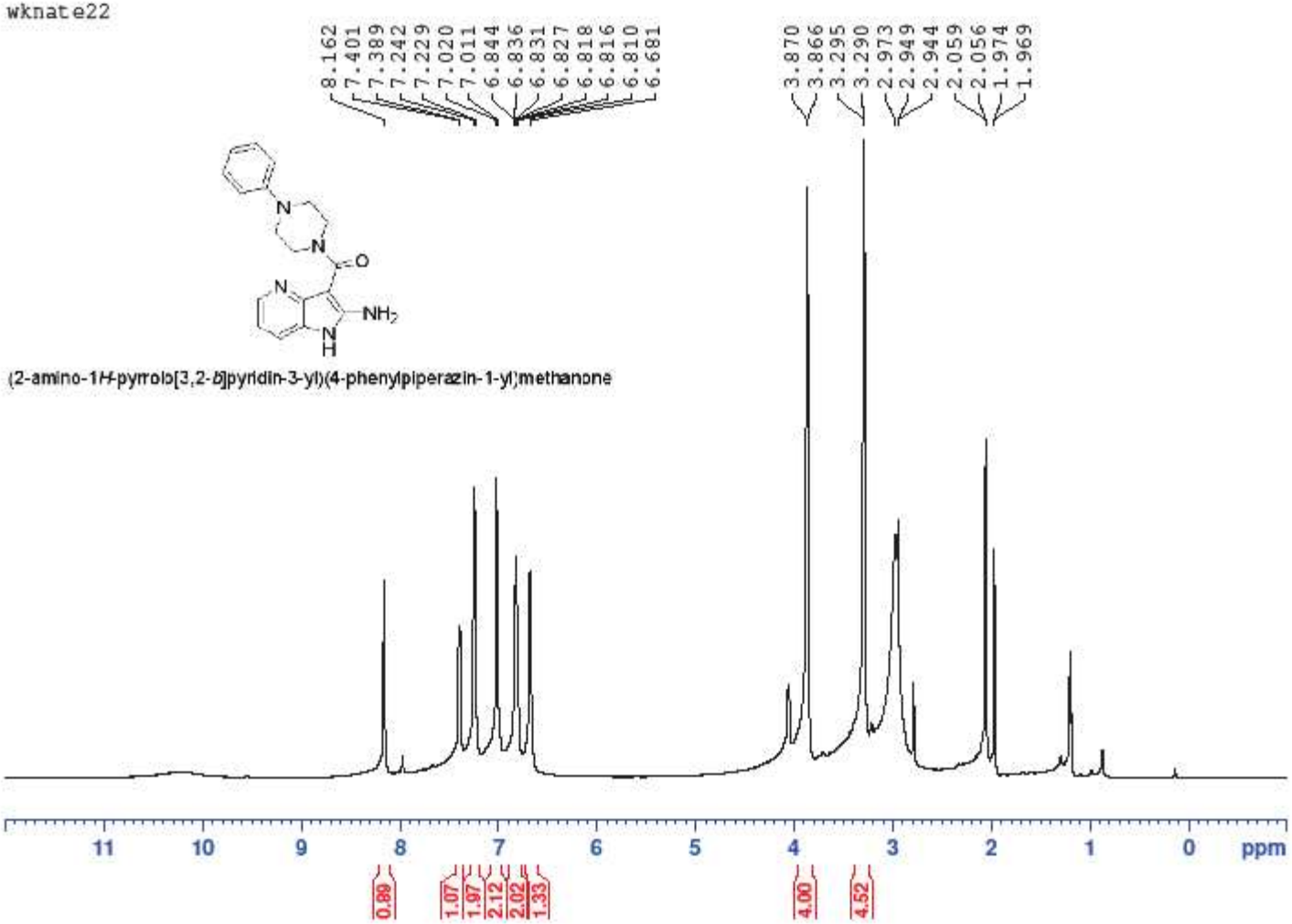

wknate21
10.844
8.011
8.003
7.401
6.803
6.795
5.760
5.751
3.606
3.347
2.499
1.808
1.804
0.826
0.817
0.807
(2-amino-1H-pyrrolo[3,2-b]pyridin-3-yl)(pyrrolidin-1-yl)methanone
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.08
1.11
3.28
4.65
4.42

wknate21



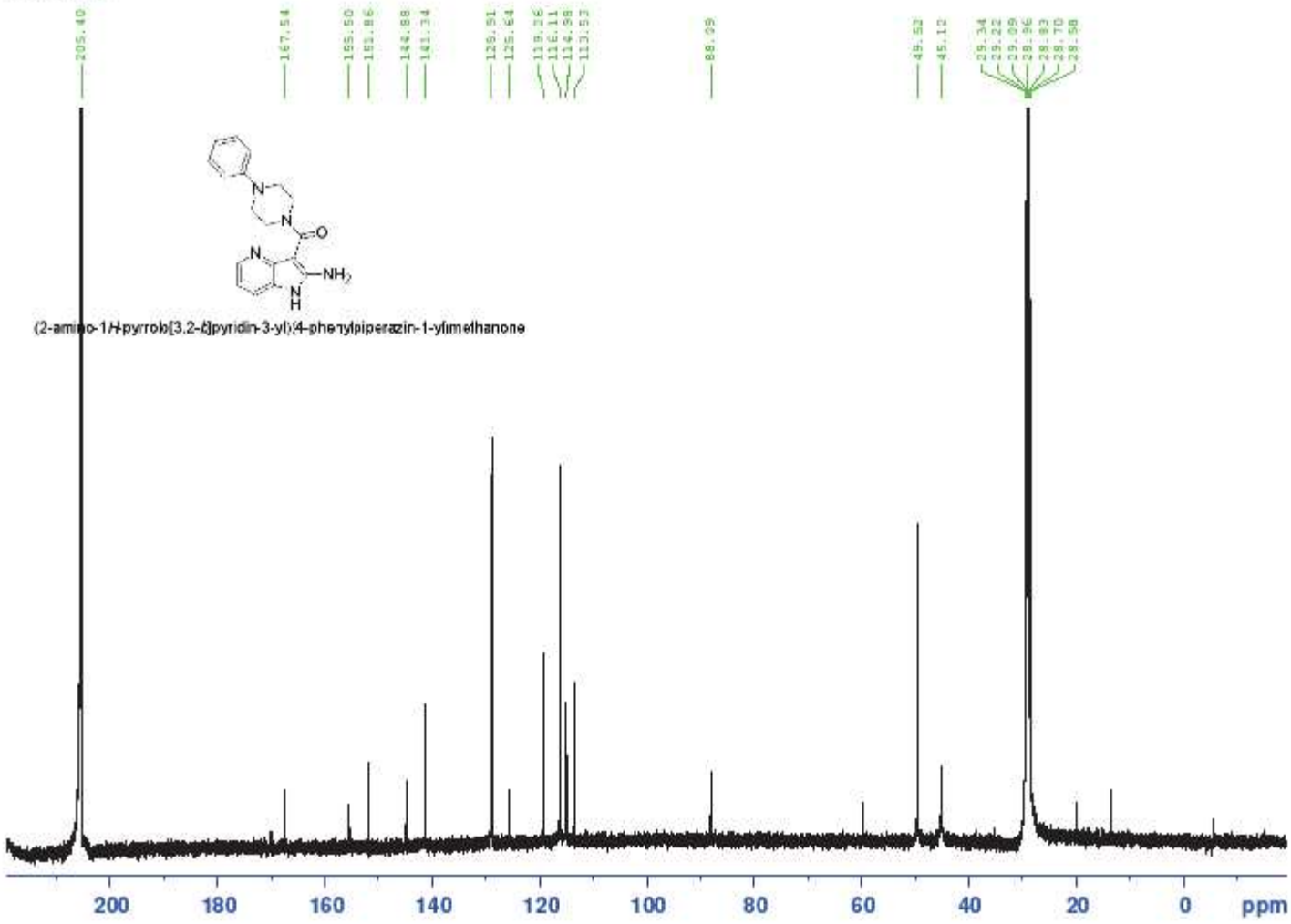
(2-amino-1*H*-pyrrolo[3,2-*b*]pyridin-3-yl)(pyrrolidin-1-yl)methanone

wknate22

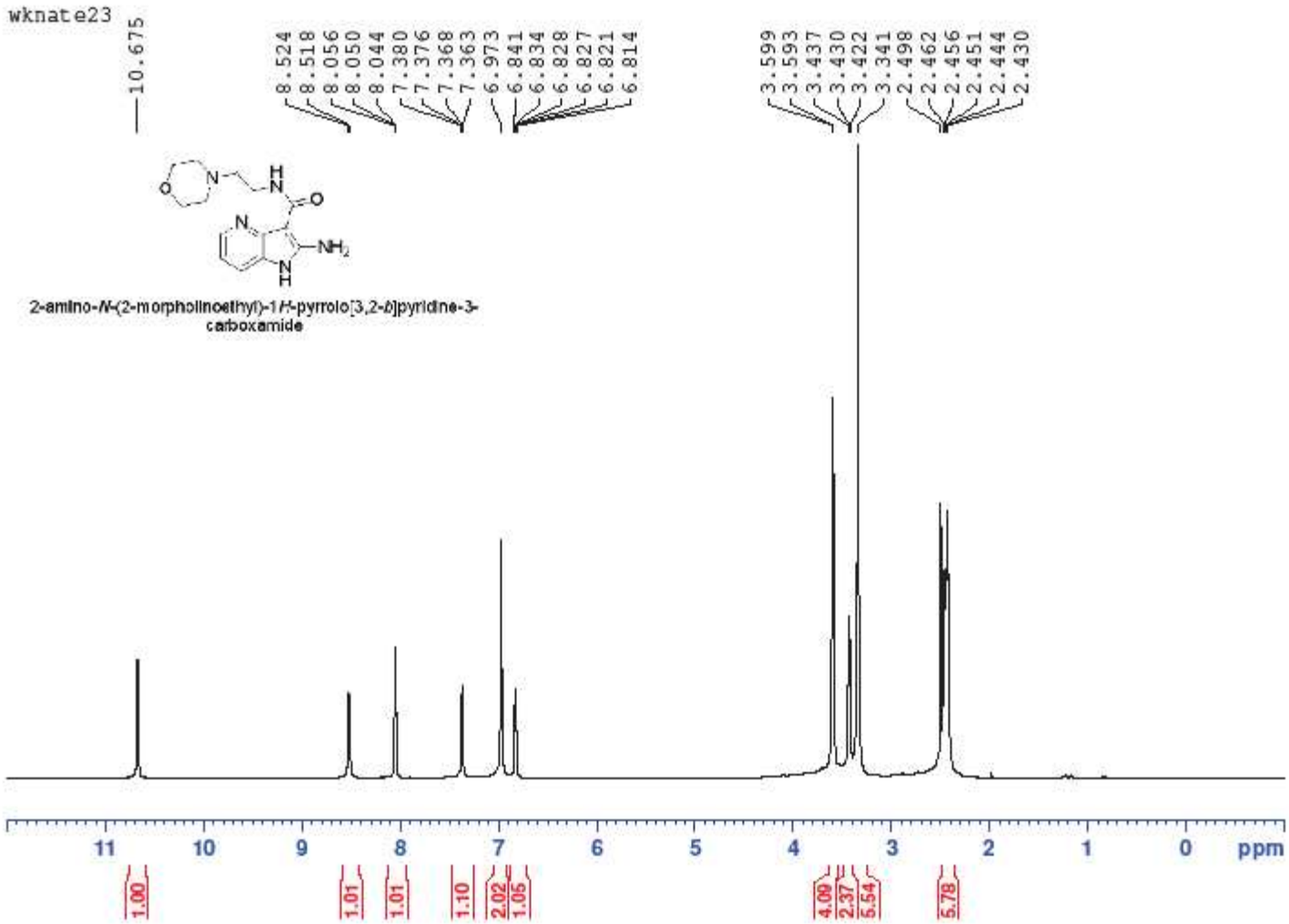


(2-amino-1*H*-pyrrolo[3,2-*b*]pyridin-3-yl)(4-phenylpiperazin-1-yl)methanone

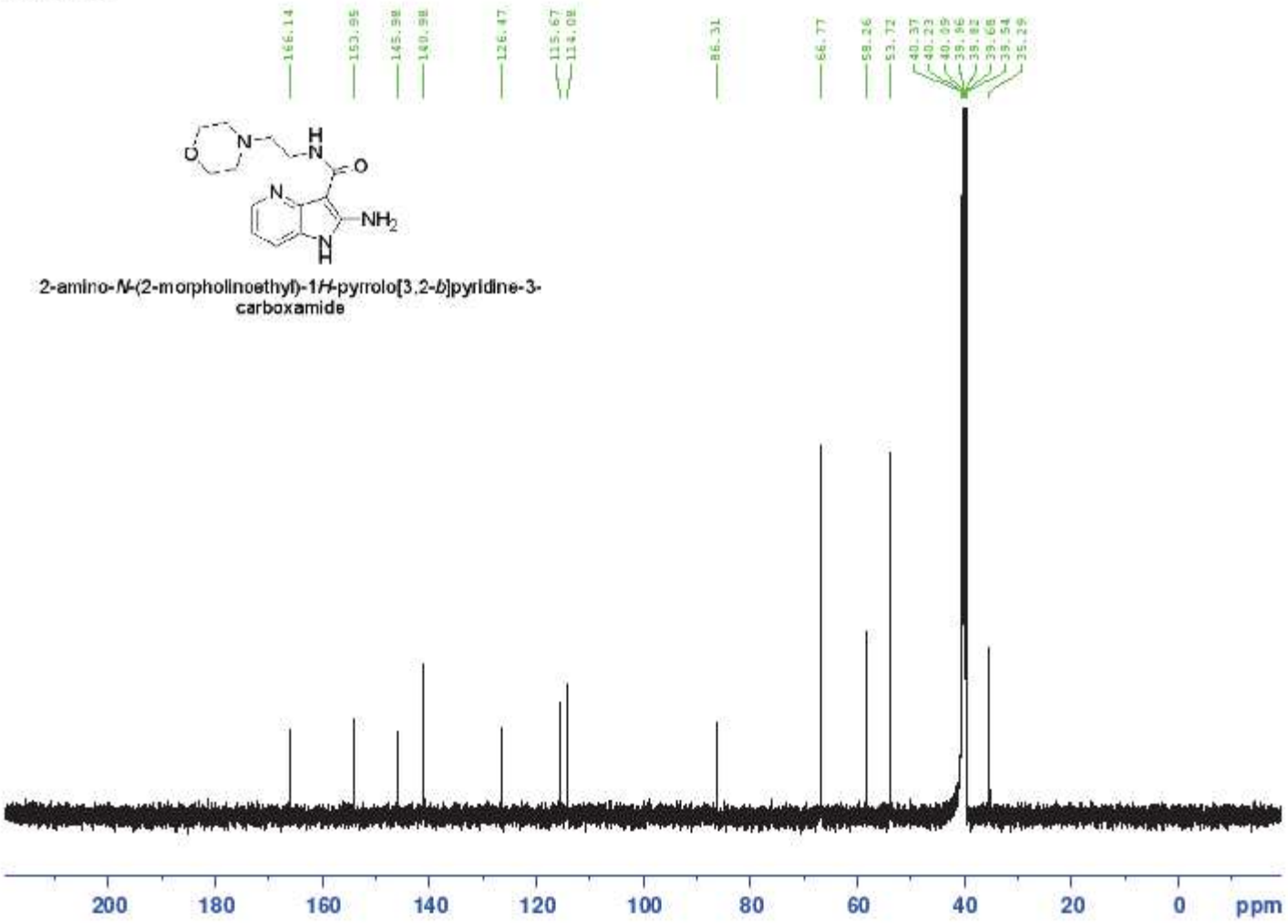
wknate22



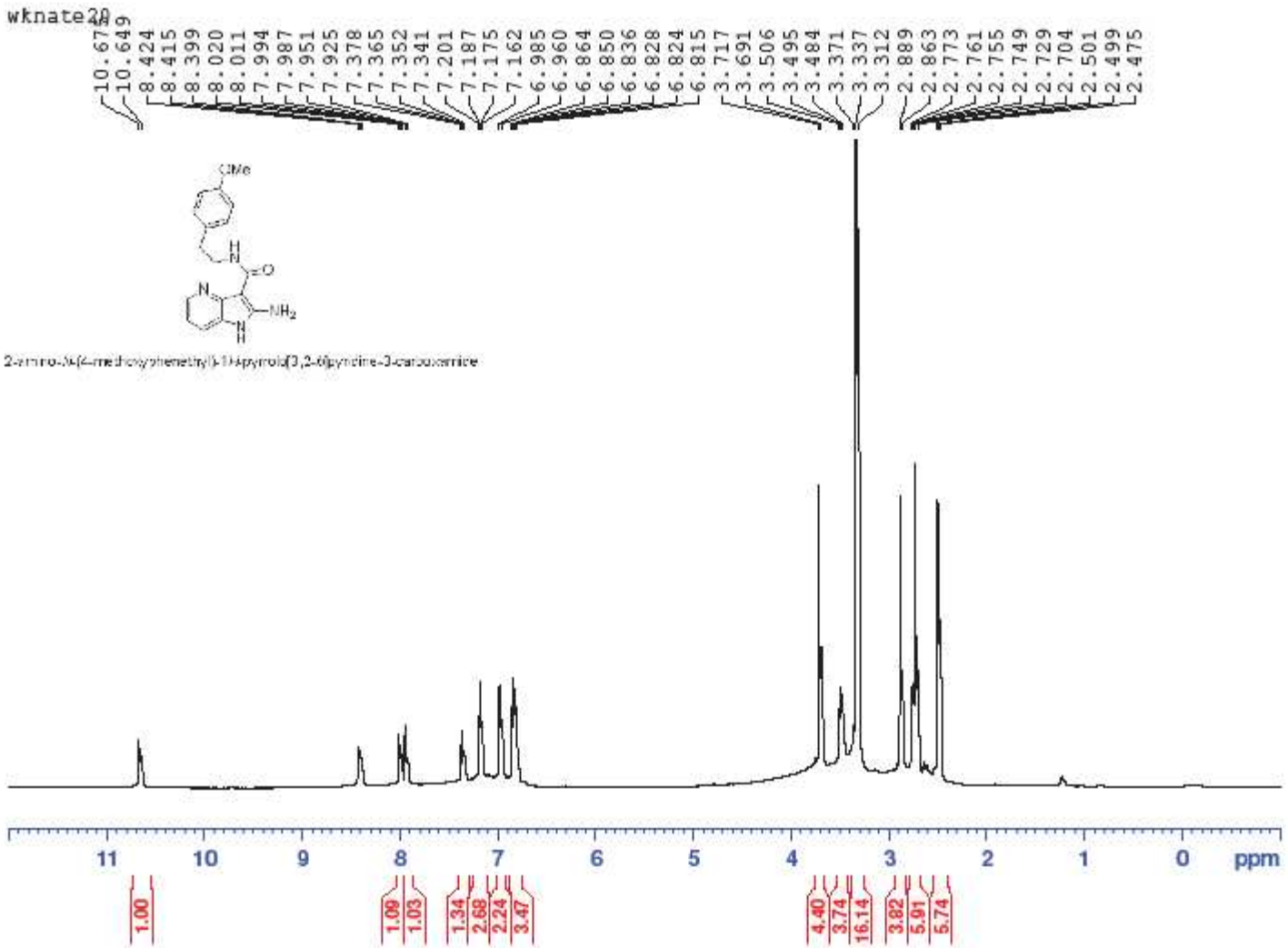
(2-amino-1*H*-pyrrolo[3,2-*b*]pyridin-3-yl)(4-phenylpiperazin-1-yl)methanone


wknate23
10.675
8.524
8.518
8.056
8.050
8.044
7.380
7.376
7.368
7.363
6.973
6.841
6.834
6.828
6.827
6.821
6.814
3.599
3.593
3.437
3.430
3.422
3.341
2.498
2.462
2.456
2.451
2.444
2.430
2-amino-N-(2-morpholinoethyl)-1H-pyrrolo[3,2-b]pyridine-3-carboxamide
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.01
1.10
2.02
1.05
4.09
2.37
5.54
5.78

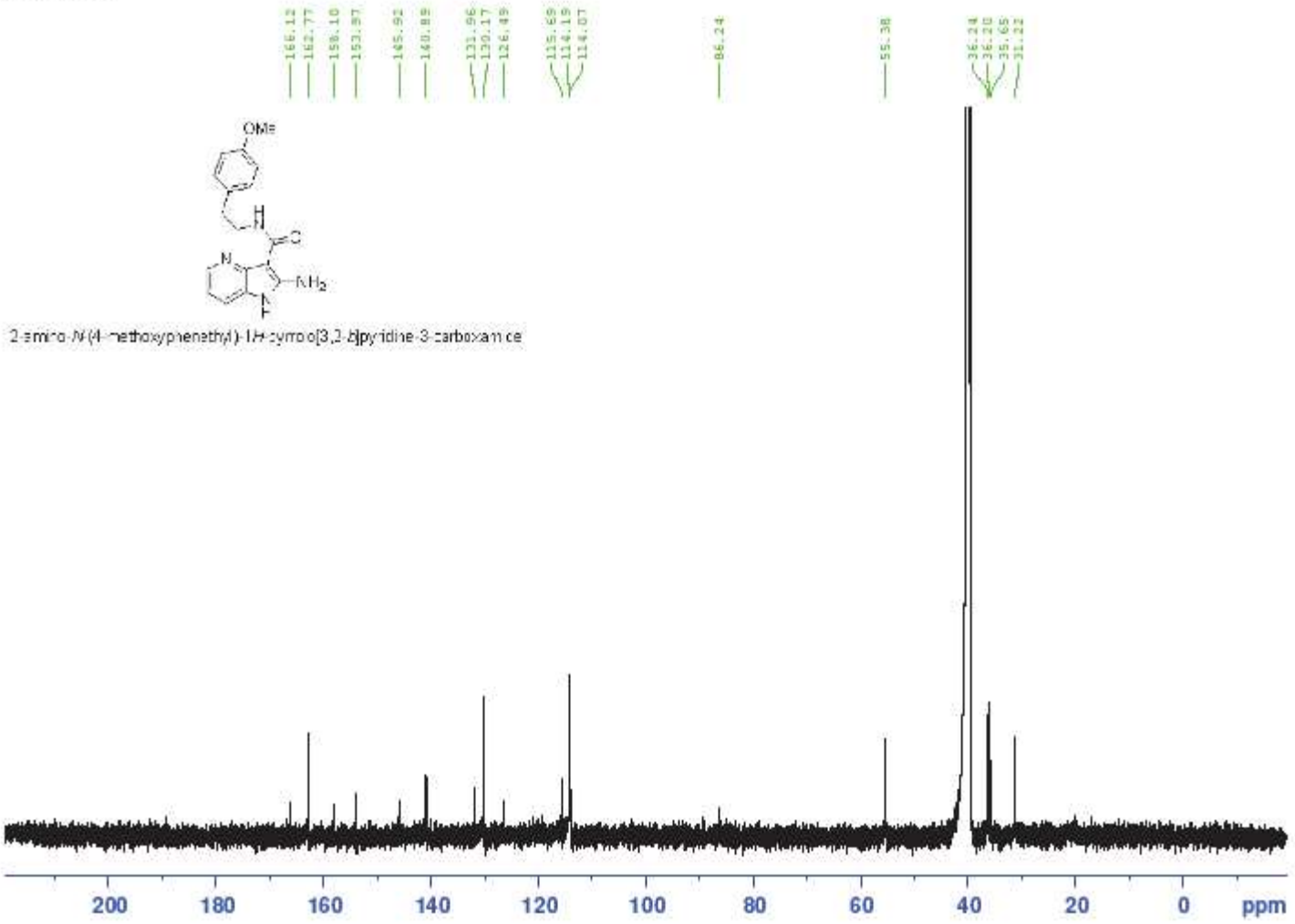
wknate23



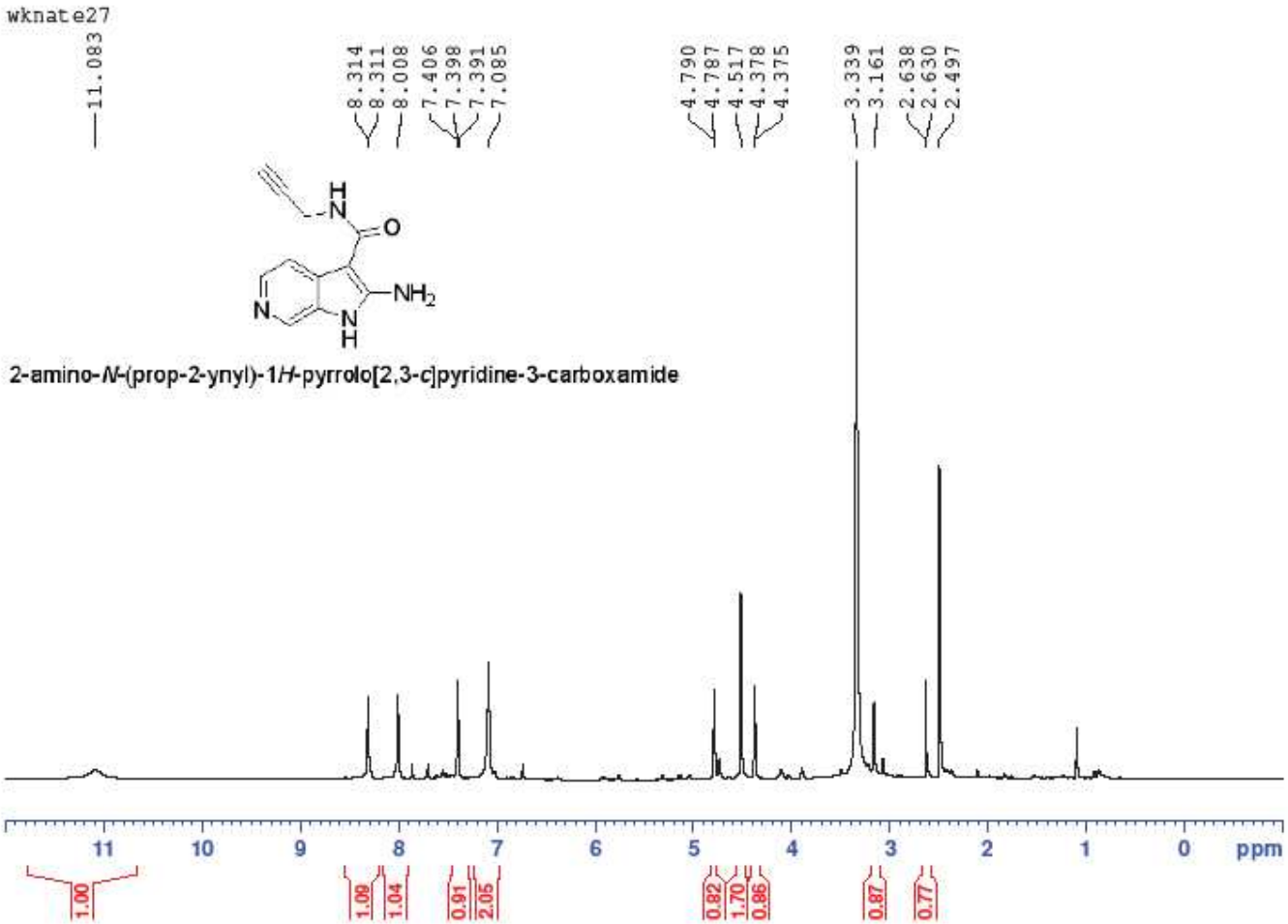
2-amino-*N*-(2-morpholinoethyl)-1*H*-pyrrolo[3,2-*b*]pyridine-3-carboxamide


wknate20
10.675
10.649
8.424
8.415
8.399
8.020
8.011
7.994
7.987
7.951
7.925
7.378
7.365
7.352
7.341
7.201
7.187
7.175
7.162
6.985
6.960
6.864
6.850
6.836
6.828
6.824
6.815
3.717
3.691
3.506
3.495
3.484
3.371
3.337
3.312
2.889
2.863
2.773
2.761
2.755
2.749
2.729
2.704
2.501
2.499
2.475
OMe
H
N
O
N
NH2
H
2-amino-N-(4-methoxyphenethyl)-1H-pyrrolo[3,2-b]pyridine-3-carboxamide
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.09
1.03
1.34
2.68
2.24
3.47
4.40
3.74
16.14
3.82
5.91
5.74

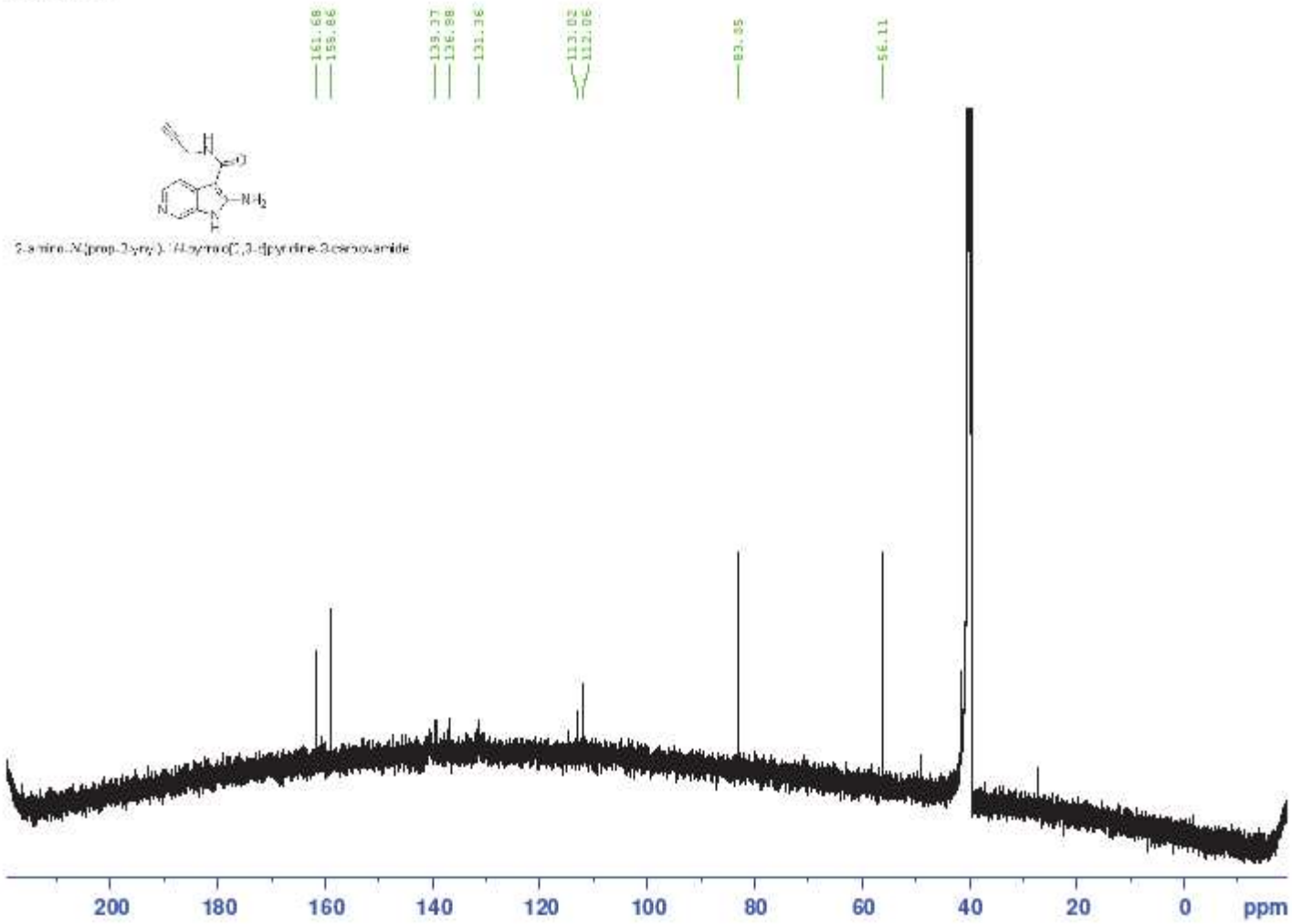
wknate24

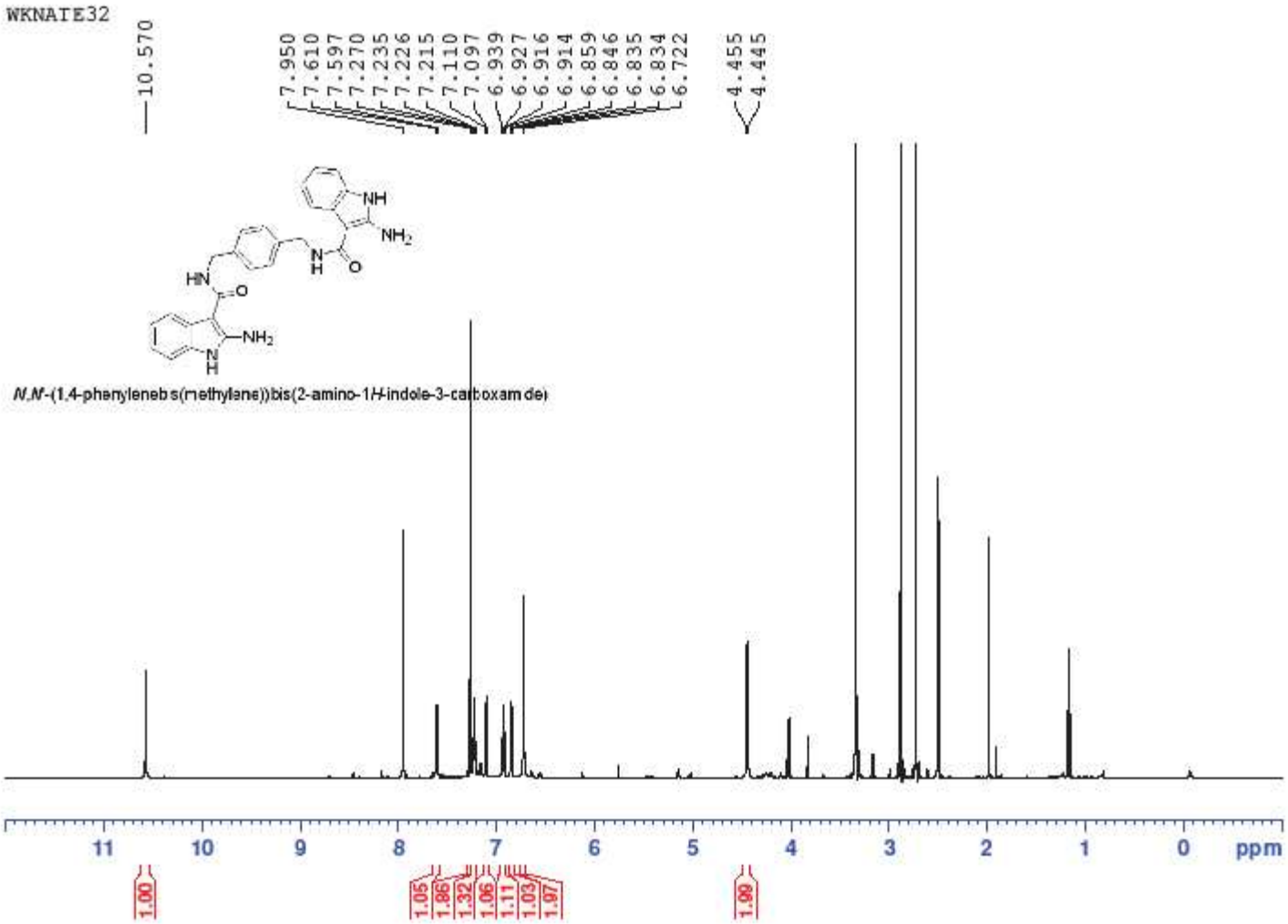


2-amino-*N*-(4-methoxyphenethyl)-1*H*-pyrrolo[3,2-*b*]pyridine-3-carboxamide

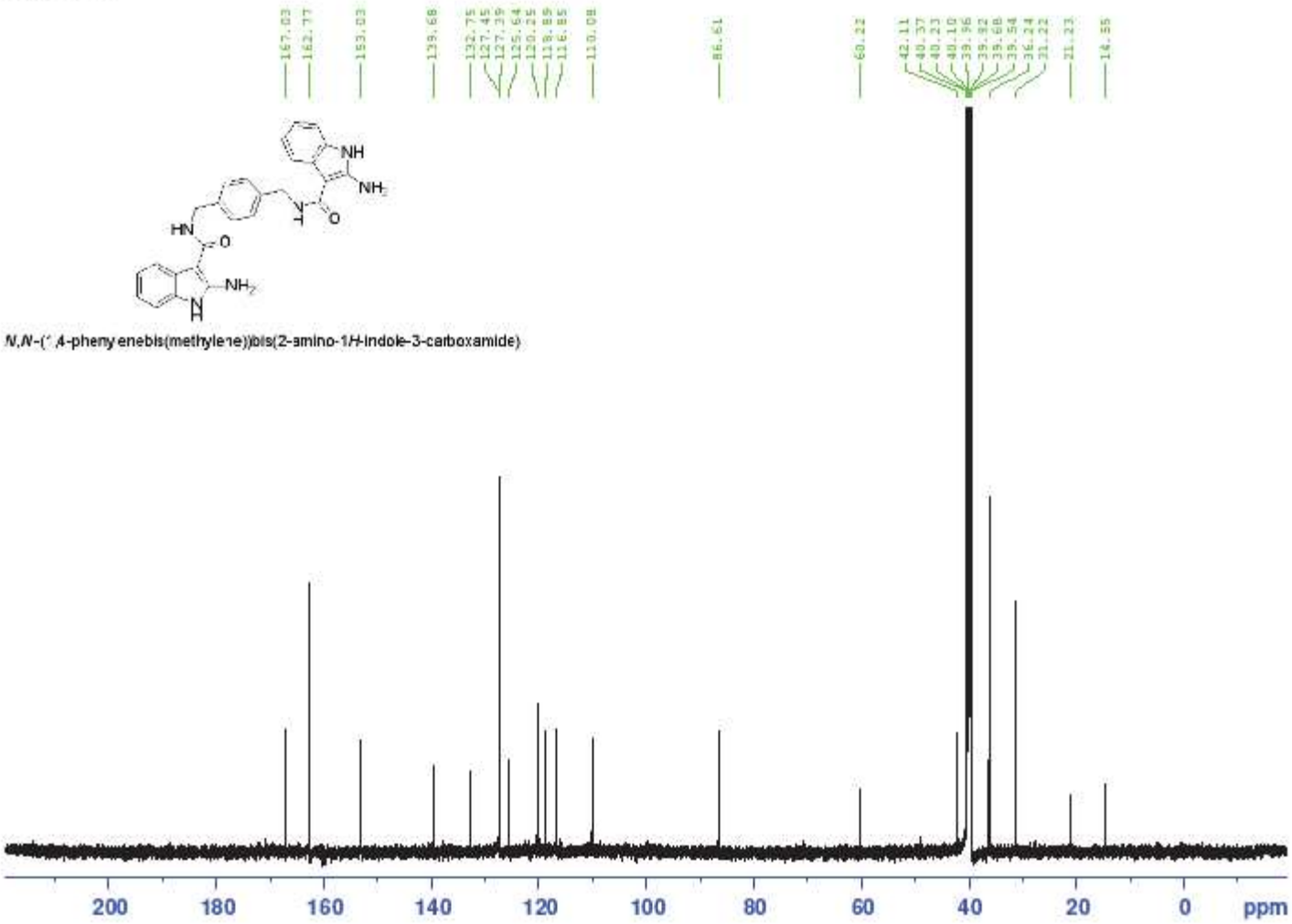

wknate27
11.083
8.314
8.311
8.008
7.406
7.398
7.391
7.085
4.790
4.787
4.517
4.378
4.375
3.339
3.161
2.638
2.630
2.497
NH2
2-amino-N-(prop-2-ynyl)-1H-pyrrolo[2,3-c]pyridine-3-carboxamide
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.09
1.04
0.91
2.05
0.82
1.70
0.86
0.87
0.77

wknate27


161.68
159.86
139.37
136.88
131.36
113.02
112.06
83.35
56.11
200
180
160
140
120
100
80
60
40
20
0
ppm


WKNATE32
10.570
7.950
7.610
7.597
7.270
7.235
7.226
7.215
7.110
7.097
6.939
6.927
6.916
6.914
6.859
6.846
6.835
6.834
6.722
4.455
4.445
NH
NH2
N
H
O
HN
O
NH2
N
H
N,N'-(1,4-phenylenebis(methylene))bis(2-amino-1H-indole-3-carboxamide)
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.05
1.86
1.32
1.06
1.11
1.03
1.97
1.99

WKNATE32



N,N-(*1,4*-phenylenebis(methylene))bis(2-amino-1*H*-indole-3-carboxamide)