- Supporting Information -

Nucleopalladation strategy towards regioselective *N*-alkylation of indoles with unactivated olefins

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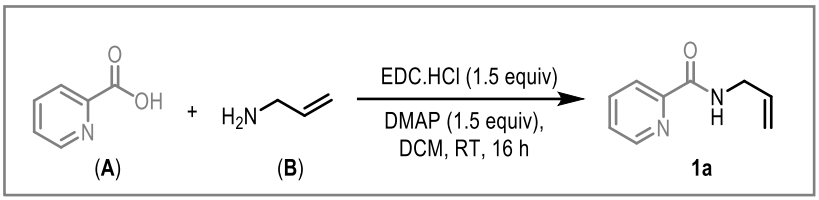
1. General information:

All non-aqueous reactions were carried out under an atmosphere of nitrogen in flame-dried glassware and were stirred using a magnetic stir plate. All reactions were carried out using commercial-grade solvent unless otherwise noted. CH_3CN, DCE, and CH_2Cl_2 were dried over calcium hydride. Dry THF was prepared by distilling over sodium ketyl.

All reactions were monitored by thin layer chromatography (TLC) on WhatmanPartisil® K6F TLC plates (silica gel 60 Å, 0.25 mm thickness) and visualized using a UV lamp (366 or 254 nm) or by use of one of the following visualization reagents: PMA: 10g phosphomolybdic acid/ 100 mL ethanol; $KMnO_4$: 0.75g potassium permanganate, 5g K_2CO_3, / 100 mL water. Products were isolated by column chromatography (Merck silica gel 100-200μm). Yields refer to chromatographically and spectroscopically homogeneous materials unless noted otherwise. ^1H, ^{13}C, and ^{19}F NMR spectra were recorded on Bruker 400 or Bruker 500 MHz spectrometers. Chemical shift values (δ) are reported in ppm and calibrated to the residual solvent peak $CDCl_3$ δ = 7.2600 ppm for ^1H, δ = 77.16 for ^{13}C, DMSO-d6 δ = 2.500 ppm for ^1H, δ = 39.500 ppm for ^{13}C; or calibrated to tetramethylsilane (δ = 0.00 ppm). All NMR spectra were recorded at ambient temperature (290 K) unless otherwise noted. ^1H NMR spectra are reported as follows: chemical shift (multiplicity, coupling constant, integration). The following abbreviations are used to indicate multiplicities: s, singlet; d, doublet; t, triplet; q, quartet; quint, quintet; sext, sextet; sept, septet; m, multiplet; dd, doublet of doublet; dt, doublet of triplet; dq, doublet of quartet; td, triplet of doublet; tt, triplet of triplet; dq, doublet of quartet; br, broad; app, apparent.

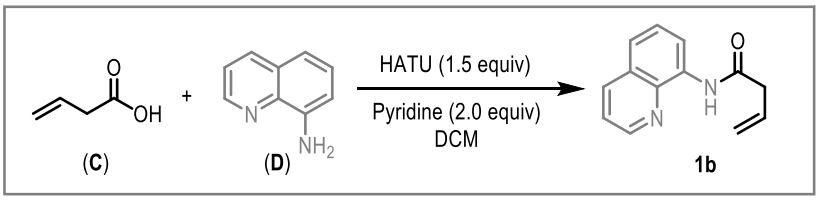
Mass spectra were recorded by electrospray ionization (ESI) method on a Q-TOF Micro with lock spray source.

2. Procedure for the synthesis of *N*-allylpicolinamide (1a):



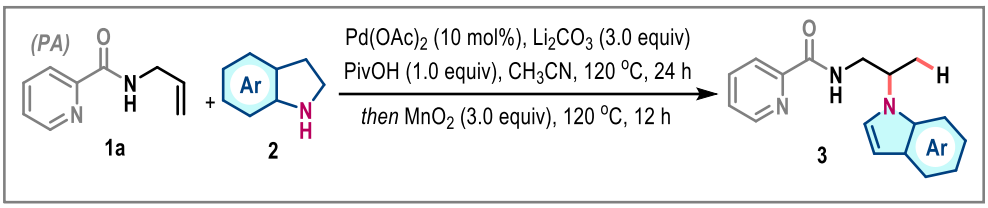
Picolinic acid (**A**) (1.0 equiv, 10 mmol) and 4-*N*,*N*-dimethylaminopyridine (DMAP, 1.5 equiv) were taken in a 50 mL round bottom flask under nitrogen. Anhydrous DCM (30 mL) was added and the mixture was cooled to 0 °C. The *N*'-(3- dimethylaminopropyl)-*N*-ethylcarbodiimide hydrochloride salt (EDC·HCl, 1.5 equiv) was added under nitrogen and the mixture was stirred for 10 minutes at the same temperature. Then, allyl amine (**B**) (1.5 equiv) was added dropwise and the mixture was stirred at room temperature for overnight. Upon completion (TLC monitored), 10% aqueous $NaHCO_3$ solution (30 mL) was added to the reaction mixture and extracted with CH_2Cl_2. The combined extracts were washed with brine, dried over Na_2SO_4, and evaporated under reduced pressure. The crude residue was purified through column chromatography on silica gel using ethyl acetate in hexane to get the pure product **1a** (1.44 g, 89%).

3. Procedure for the synthesis of *N*-(quinolin-8-yl)but-3-enamide (1b):



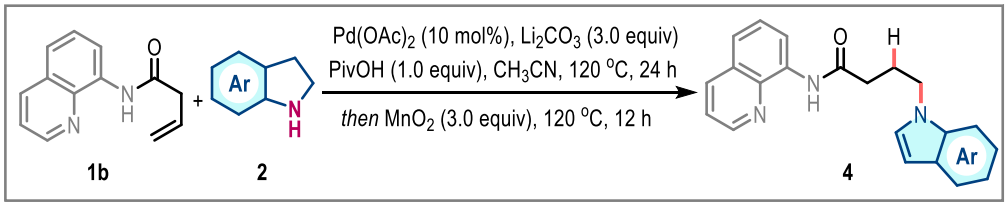
Vinyl acetic acid (**C**) (1.0 equiv, 10 mmol) was taken into a 100 mL RB flask containing dry DCM (20 mL) under nitrogen. 8-Aminoquinoline (**D**) (1.3 g, 9 mmol), pyridine (1.6 mL, 20 mmol), and HATU (5.7 g, 15 mmol) were added sequentially, and the reaction mixture was stirred at ambient temperature for 16 h. Next, 10% aqueous $NaHCO_3$ solution (30 mL) was added to the reaction mixture and extracted with CH_2Cl_2. The combined extracts were washed with brine, dried over Na_2SO_4, and evaporated under reduced pressure. The crude residue was purified through column chromatography on silica gel using ethyl acetate in hexane to get the pure product **1b** (1.80 g, 85%).

4. General procedure for the synthesis of *N*-alkylated indoles with *N*-allylpicolinamide (GP 1):



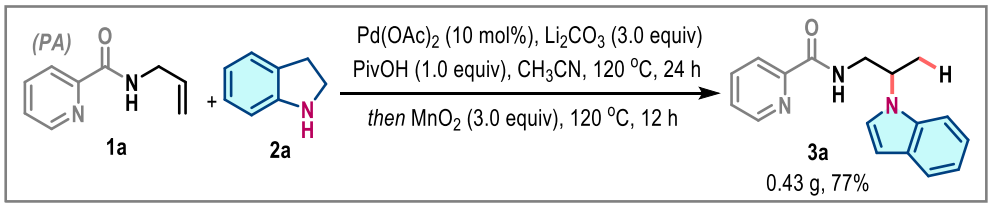
To an oven-dried screw cap reaction tube, *N*-allylpicolinamide **1a** (0.2 mmol), corresponding indoline derivatives **2** (1.1 equiv), $Pd(OAc)_2$ (10 mol%), Li_2CO_3 (3.0 equiv) and PivOH (1.0 equiv) were taken. Acetonitrile (1 mL) was added, the reaction tube was capped, and placed it in a preheated oil bath at 120 °C for 24 h. After 24 h, MnO_2 (3.0 equiv) was added and further heated at 120 °C for 12 h. After completion of the reaction (monitored by TLC), the crude mixture was diluted with DCM and concentrated on a rota vapour. The crude residue was purified through column chromatography on silica gel using ethyl acetate in hexane to get pure product **3**.

5. General procedure for the synthesis of *N*-alkylated indoles with *N*-(quinolin-8-yl)but-3-enamide (GP 2):



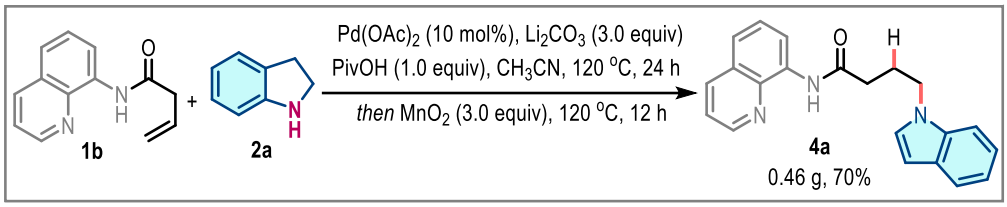
To an oven-dried screw cap reaction tube, *N*-(quinolin-8-yl)but-3-enamide **1b** (0.2 mmol), corresponding indoline derivatives **2** (1.1 equiv), $Pd(OAc)_2$ (10 mol%), Li_2CO_3 (3.0 equiv) and PivOH (1.0 equiv) were taken. Acetonitrile (1 mL) was added, the reaction tube was capped, and placed it in a preheated oil bath at 120 °C for 24 h. After 24 h, MnO_2 (3.0 equiv) was added and further heated at 120 °C for 12 h. After completion of the reaction (monitored by TLC), the crude mixture was diluted with DCM and concentrated on a rota vapour. The crude residue was purified through column chromatography on silica gel using ethyl acetate in hexane to get pure product **4**.

6. Procedure for the scale-up synthesis of compound 3a:



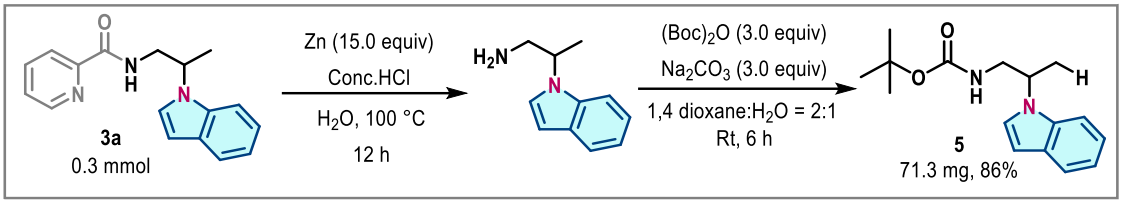
To an oven-dried screw cap reaction tube, *N*-allylpicolinamide **1a** (2.0 mmol), corresponding indoline **2a** (1.1 equiv), $Pd(OAc)_2$ (10 mol%), Li_2CO_3 (3.0 equiv) and PivOH (1.0 equiv) were taken. Acetonitrile (5 mL) was added, the reaction tube was capped, and placed it in a preheated oil bath at 120 °C for 24 h. Then, MnO_2 (3.0 equiv) was added and further heated at 120 °C for 12 h. After completion of the reaction (monitored by TLC), the crude mixture was diluted with DCM and concentrated on a rota vapour. The crude residue was purified through column chromatography on silica gel using ethyl acetate in hexane to get pure product **3a** (0.43 g, 77%).

7. Procedure for the scale-up synthesis of 4a:



To an oven-dried screw cap reaction tube, *N*-(quinolin-8-yl)but-3-enamide **1b** (2.0 mmol), corresponding indoline **2a** (1.1 equiv), $Pd(OAc)_2$ (10 mol%), Li_2CO_3 (3.0 equiv) and PivOH (1.0 equiv) were taken. Acetonitrile (5 mL) was added, the reaction tube was capped, and placed it in a preheated oil bath at 120 °C for 24 h. Then, MnO_2 (3.0 equiv) was added and further heated at 120 °C for 12 h. After completion of the reaction (monitored by TLC), the crude mixture was diluted with DCM and concentrated on a rota vapour. The crude residue was purified through column chromatography on silica gel using ethyl acetate in hexane to get pure product **4a** (0.46 g, 70%).

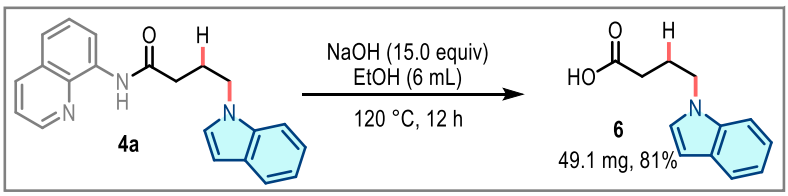
8. Procedure for the removal of the picolinamide directing group:



To a suspension of compound **3a** (0.3 mmol, 1.0 equiv) in H_2O (6 mL) was added conc. HCl (0.7 mL) and the mixture was stirred for 5 minutes at room temperature. Zinc dust (292 mg, 4.5 mmol, 15 equiv) was then carefully added portion wise and the mixture was stirred at 100 °C for 12 h. Upon completion (TLC monitored), the reaction mixture was filtered through a celite plug. The filtrate was neutralized with 2M NaOH solution and then extracted with DCM. The volatiles were evaporated under reduced pressure and the crude residue was directly used for the next step.

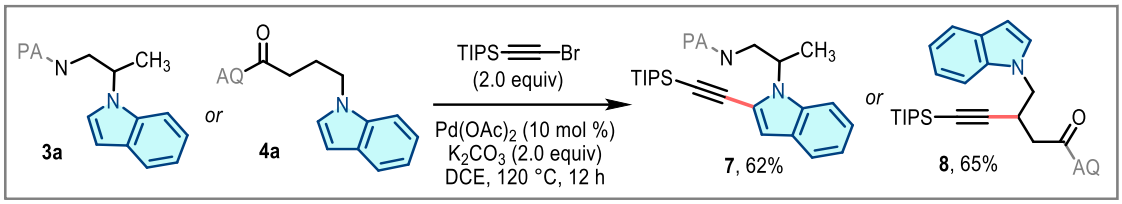
The crude residue was taken in a 50 ml round bottom flask. Then, 1,4 dioxane (5.0 mL), Na_2CO_3 (3.0 equiv), H_2O (2.5 mL) and $(Boc)_2O$ (3.0 equiv) were added. The mixture was allowed to stirred at rt for 6 h. After completion of the reaction (TLC monitored), the crude reaction mixture was quenched with water and extracted with DCM. The crude residue was purified through column chromatography on silica gel using 10% ethyl acetate in hexane to get pure product **5** (71.3 mg, 86%).

9. Procedure for the removal of the 8-aminoquinoline directing group:



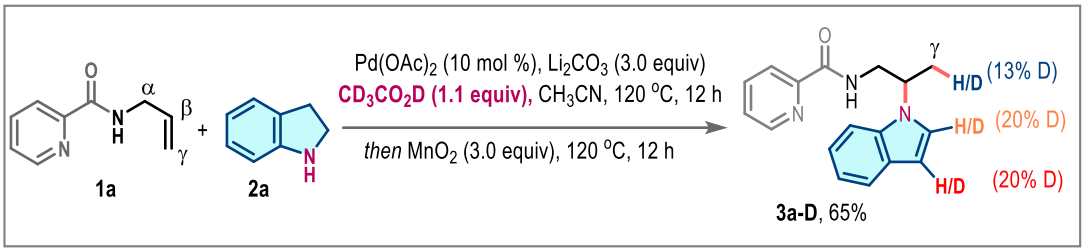
To a solution of compound **4a** (0.3 mmol, 1.0 equiv) in EtOH (6 mL) was added NaOH (15.0 equiv) and the mixture was placed in a preheated oil bath at 120 °C for 12 h. Upon completion (TLC monitored), the reaction mixture was acidified with HCl and extracted with ethyl acetate (20 ml x 3 times). The volatiles were evaporated under reduced pressure. The crude residue was purified through column chromatography on silica gel using 20% ethyl acetate in hexane to get pure product **6** (49.1 mg, 81%).

10. Procedure for directed sp^2 and sp^3 C–H activation reaction

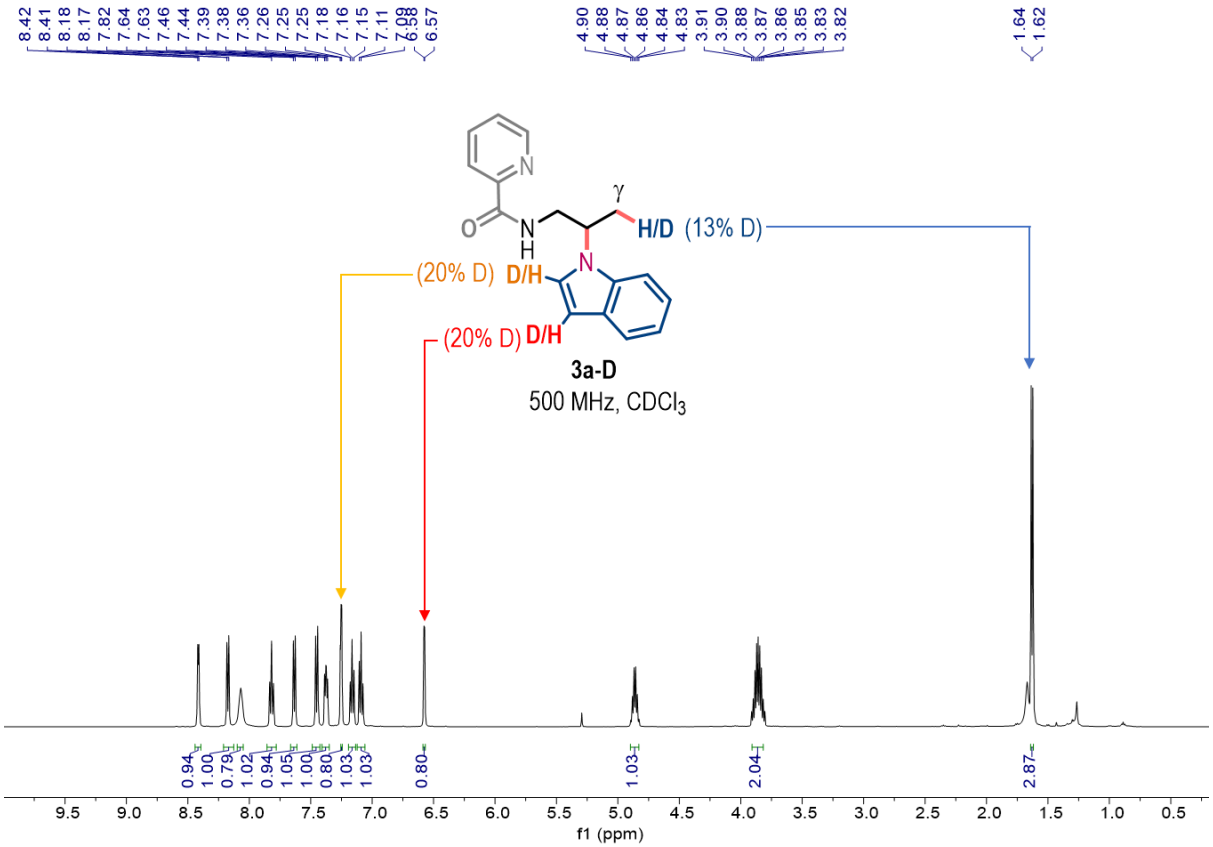


An oven-dried screw cap reaction tube equipped with a magnetic stirrer bar was charged with compound **3a** or **4a** (0.15 mmol, 1.0 equiv), (bromoethynyl)triisopropylsilane (2.0 equiv), $Pd(OAc)_2$ (10 mol %), and K_2CO_3 (2.0 equiv). Then, DCE (1.5 mL, 1M) solvent was added. The reaction tube was capped and placed in a preheated oil bath at 120 °C for 12 h. After completion of the reaction (TLC monitored), the crude mixture was diluted with DCM and concentrated under reduced pressure. The crude residue was purified through column chromatography on silica gel using ethyl acetate in hexane to get pure product **7** or **8**.

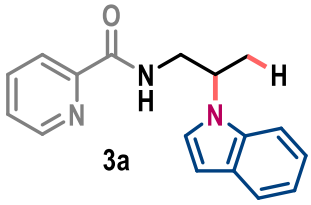
11. H/D Exchange experiment:



To an oven-dried screw cap reaction tube, *N*-allylpicolinamide **1a** (0.2 mmol), indoline **2a** (1.1 equiv), $Pd(OAc)_2$ (10 mol%), Li_2CO_3 (3.0 equiv) and CD_3CO_2D (1.1 equiv) were taken. Acetonitrile (1 mL) was added, the reaction tube was capped, and placed it in a preheated oil bath at 120 °C for 12 h. After 12 h, MnO_2 (3.0 equiv) was added and further heated at 120 °C for 12 h. After completion of the reaction (monitored by TLC), the crude mixture was diluted with DCM and concentrated on a rota vapour. The crude residue was purified through column chromatography on silica gel using ethyl acetate in hexane to get pure product **3a-D** (36.2 mg, 65%).

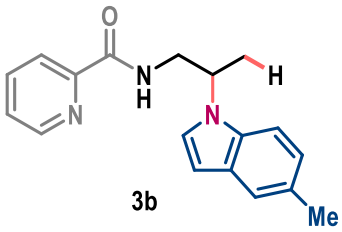


12. Characterization data of synthesized compounds



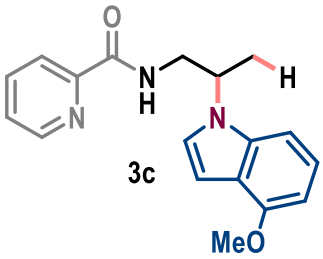
***N*-(2-(1H-indol-1-yl)propyl)picolinamide (3a):**

Compound **3a** was synthesized according to GP-1 as colorless sticky solid; eluent (20% ethyl acetate in hexane); **Yield:** 85% (48 mg); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.42 – 8.41 (m, 1H), 8.18 (d, *J* = 7.8 Hz, 1H), 8.07 (t, *J* = 6.5 Hz, 1H), 7.81 (td, *J* = 7.7, 1.7 Hz, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.46 (d, *J* = 8.3 Hz, 1H), 7.38 – 7.36 (m, 1H), 7.25 (d, *J* = 3.3 Hz, 1H), 7.18 – 7.15 (m, 1H), 7.09 (t, *J* = 7.4 Hz, 1H), 6.58 (d, *J* = 3.3 Hz, 1H), 4.90 – 4.83 (m, 1H), 3.91 – 3.82 (m, 2H), 1.63 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 164.9, 149.5, 148.2, 137.4, 136.2, 128.8, 126.3, 124.0, 122.3, 121.7, 121.1, 119.7, 109.8, 102.3, 51.3, 44.9, 18.5; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{17}H_{17}N_3OH^+$ 280.1444; Found 280.1447.



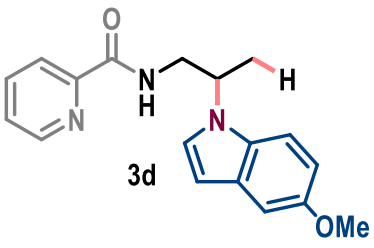
***N*-(2-(5-methyl-1H-indol-1-yl)propyl)picolinamide (3b):**

Compound **3b** was synthesized according to GP-1 as colorless sticky solid; eluent (20% ethyl acetate in hexane); **Yield:** 84% (49 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.42 (d, *J* = 4.7 Hz, 1H), 8.17 (d, *J* = 7.8 Hz, 1H), 8.06 (brs, 1H), 7.84 – 7.80 (m, 1H), 7.42 (s, 1H), 7.39 – 7.36 (m, 1H), 7.34 (d, *J* = 8.8 Hz, 1H), 7.21 – 7.19 (m, 1H), 7.00 (d, *J* = 8.4 Hz, 1H), 6.49 – 6.47 (m, 1H), 4.85 – 4.77 (m, 1H), 3.91 – 3.81 (m, 2H), 2.43 (s, 3H), 1.61 (d, *J* = 8.4 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 164.9, 149.6, 148.2, 137.4, 134.6, 129.1, 128.9, 126.3, 124.2, 123.3, 122.3, 120.7, 109.5, 101.7, 51.4, 44.7, 21.5, 18.5; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{18}H_{19}N_3OH^+$ 294.1601; Found 294.1607.



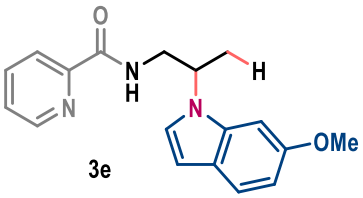
***N*-(2-(4-methoxy-1H-indol-1-yl)propyl)picolinamide (3c):**

Compound **3c** was synthesized according to GP-1 as brown gummy solid; eluent (25% ethyl acetate in hexane); **Yield:** 86% (53 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.42 – 8.41 (m, 1H), 8.18 – 8.15 (m, 1H), 8.06 (brs, 1H), 7.84 – 7.79 (m, 1H), 7.39 – 7.36 (m, 1H), 7.15 (d, *J* = 3.3 Hz, 1H), 7.11 – 7.06 (m, 2H), 6.67 (d, *J* = 3.2 Hz, 1H), 6.52 – 6.50 (m, 1H), 4.84 – 4.77 (m, 1H), 3.95 (s, 3H), 3.88 – 3.80 (m, 2H), 1.61 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, CDCl3)** δ 164.9, 153.6, 149.5, 148.2, 137.7, 137.4, 126.4, 122.6 (2xC), 122.3, 119.3, 103.3, 99.6, 99.5, 55.4, 51.6, 44.8, 18.5; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{18}H_{19}N_3O_2H^+$ 310.1550; Found 310.1556.



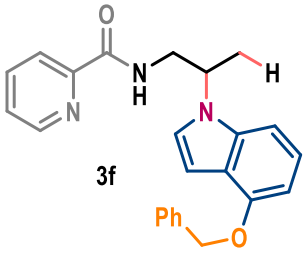
***N*-(2-(5-methoxy-1H-indol-1-yl)propyl)picolinamide (3d):**

Compound **3d** was synthesized according to GP-1 as colorless gummy liquid; eluent (25% ethyl acetate in hexane); **Yield:** 85% (52 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.42 – 8.41 (m, 1H), 8.18 – 8.16 (m, 1H), 8.07 (brs, 1H), 7.83 – 7.79 (m, 1H), 7.39 – 7.36 (m, 1H), 7.34 (d, *J* = 9.1 Hz, 1H), 7.21 (d, *J* = 3.2 Hz, 1H), 7.09 (d, *J* = 2.5 Hz, 1H), 6.84 – 6.81 (m, 1H), 6.49 – 6.48 (m, 1H), 4.83 – 4.75 (m, 1H), 3.85 – 3.83 (m, 4H), 3.82 – 3.78 (m, 1H), 1.61 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 164.9, 154.2, 149.5, 148.2, 137.4, 131.5, 129.1, 126.4, 124.6, 122.3, 112.1, 110.5, 102.7, 101.8, 56.0, 51.4, 44.9, 18.4; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{18}H_{19}N_3O_2H^+$ 310.1550; Found 310.1551.



***N*- (2-(6-methoxy-1H-indol-1-yl)propyl)picolinamide (3e):**

Compound **3e** was synthesized according to GP-1 as colorless gummy solid; eluent (25% ethyl acetate in hexane); **Yield:** 86% (53 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.42 – 8.40 (m, 1H), 8.18 – 8.16 (m, 1H), 8.08 (brs, 1H), 7.82 (td, *J* = 7.7, 1.7 Hz, 1H), 7.48 (d, *J* = 8.6 Hz, 1H), 7.39 – 7.36 (m, 1H), 7.14 (d, *J* = 3.3 Hz, 1H), 6.90 (d, *J* = 2.2 Hz, 1H), 6.75 (dd, *J* = 8.6, 2.2 Hz, 1H), 6.50 (dd, *J* = 3.3, 0.8 Hz, 1H), 4.83 – 4.75 (m, 1H), 3.93 – 3.86 (m, 1H), 3.79 – 3.72 (m, 4H), 1.62 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, CDCl3)** δ 164.9, 156.4, 149.5, 148.2, 137.4, 137.1, 126.4, 122.9, 122.6, 122.3, 121.6, 109.9, 102.3, 93.3, 55.8, 51.1, 45.0, 18.4; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{18}H_{19}N_3O_2H^+$ 310.1550; Found 310.1555.

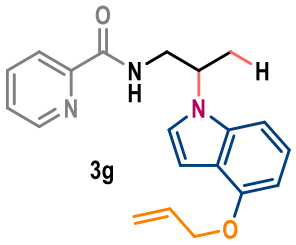


***N*-(2-(4-(benzyloxy)-1H-indol-1-yl)propyl)picolinamide (3f):**

Compound **3f** was synthesized according to GP-1 as colorless gummy liquid; eluent (25% ethyl acetate in hexane); **Yield:** 82% (63 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.42 – 8.41 (m, 1H), 8.19 – 8.17 (m, 1H), 8.09 (brs, 1H), 7.83 – 7.79 (m, 1H), 7.54 – 7.51 (m, 2H), 7.43 – 7.33 (m, 4H), 7.17 (d, *J* = 3.3 Hz, 1H), 7.09 – 7.07 (m, 2H), 6.76 – 6.75 (m, 1H), 6.58 (dd, *J* = 6.6, 1.9 Hz, 1H), 5.24 (s, 2H), 4.86 – 4.81 (m, 1H), 3.91 – 3.82 (m, 2H), 1.62 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 164.9, 152.7, 149.5, 148.2, 137.8, 137.7, 137.4, 128.6, 127.8, 127.4, 126.3, 122.6, 122.5, 122.3, 119.7, 103.5, 101.0, 99.8, 70.0, 51.5, 44.8, 18.5; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{24}H_{23}N_3O_2H^+$ 386.1863; Found 386.1859.

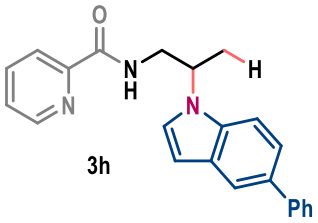
***N*-(2-(4-(allyloxy)-1H-indol-1-yl)propyl)picolinamide (3g):**

Compound **3g** was synthesized according to GP-1 as off brown gummy liquid; eluent (20% ethyl acetate in hexane); **Yield:** 80% (53 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.42 – 8.41 (m, 1H), 8.17 (dt, *J* = 7.9, 1.1 Hz, 1H), 8.06 (brs, 1H), 7.81 (td, *J* = 7.7, 1.7 Hz, 1H), 7.39 – 7.35 (m, 1H), 7.15 (d, *J* = 3.3 Hz, 1H), 7.07 – 7.06



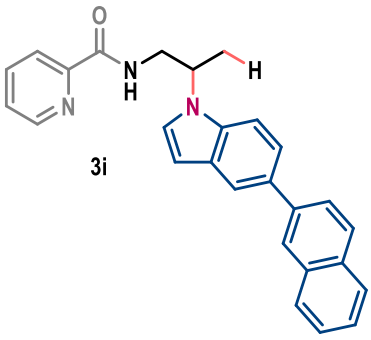
(m, 2H), 6.71 (d, *J* = 3.3 Hz, 1H), 6.51 (dd, *J* = 5.2, 3.2 Hz, 1H), 6.20 – 6.11 (m, 1H), 5.51 – 5.45 (m, 1H), 5.31 – 5.28 (m, 1H), 4.84 – 4.79 (m, 1H), 4.70 – 4.68 (m, 2H), 3.91 – 3.80 (m, 2H), 1.61 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 164.9, 152.5, 149.5, 148.2, 137.8, 137.4, 133.9, 126.3, 122.6, 122.5, 122.3, 119.6, 117.3, 103.4, 100.9, 99.7, 69.0, 51.6, 44.8, 18.5; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{20}H_{21}N_3O_2H^+$ 336.1707; Found 336.1718.

***N*-(2-(5-phenyl-1H-indol-1-yl)propyl)picolinamide (3h):**



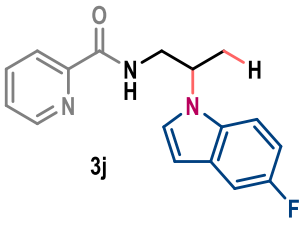
Compound **3h** was synthesized according to GP-1 as colorless sticky solid; eluent (20% ethyl acetate in hexane); **Yield:** 83% (59 mg); **^{1}H NMR (400 MHz, CDCl3)** δ 8.42 – 8.41 (m, 1H), 8.20 – 8.17 (m, 1H), 8.10 (brs, 1H), 7.85 – 7.80 (m, 2H), 7.64 – 7.61 (m, 2H), 7.51 (d, J = 8.6 Hz, 1H), 7.46 – 7.40 (m, 3H), 7.39 – 7.36 (m, 1H), 7.33 – 7.30 (m, 1H), 7.29 – 7.28 (m, 1H), 6.63 (d, J = 3.2 Hz, 1H), 4.93 – 4.86 (m, 1H), 3.93 – 3.82 (m, 2H), 1.65 (d, J = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, CDCl3)** δ 165.0, 149.5, 148.2, 142.6, 137.4, 135.8, 133.3, 129.3, 128.8, 127.5 (2xC), 126.4, 124.7, 122.3, 121.6, 119.6, 110.0, 102.8, 51.5, 44.9, 18.5; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{23}H_{21}N_3OH^+$ 356.1757; Found 356.1757.

***N*-(2-(5-(naphthalen-2-yl)-1H-indol-1-yl)propyl)picolinamide (3i):**



Compound **3i** was synthesized according to GP-1 as off brown gummy liquid; eluent (20% ethyl acetate in hexane); **Yield:** 81% (66 mg); **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.46 – 8.44 (m, 1H), 8.22 – 8.19 (m, 1H), 8.15 (brs, 1H), 7.96 – 7.90 (m, 2H), 7.86 – 7.81 (m, 2H), 7.76 – 7.75 (m, 1H), 7.56 – 7.51 (m, 2H), 7.50 – 7.46 (m, 2H), 7.41 – 7.37 (m, 2H), 7.34 (d, *J* = 3.2 Hz, 1H), 7.31 – 7.29 (m, 1H), 6.65 – 6.64 (m, 1H), 4.97 – 4.92 (m, 1H), 4.00 – 3.94 (m, 1H), 3.92 – 3.85 (m, 1H), 1.70 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 165.0, 149.5, 148.2, 141.5, 137.5, 135.6, 134.0, 132.4, 128.8, 128.3, 127.3, 127.1, 126.7, 126.4, 125.8, 125.7, 125.5, 124.6, 124.3, 122.4, 122.3, 117.0, 109.4, 102.6, 51.4, 45.1, 18.5; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{27}H_{23}N_3OH^+$ 406.1914; Found 406.1923.

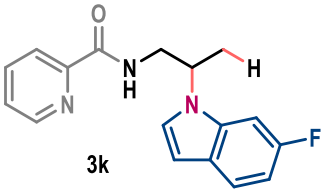
***N*-(2-(5-fluoro-1H-indol-1-yl)propyl)picolinamide (3j):**



Compound **3j** was synthesized according to GP-1 as colorless sticky solid; eluent (25% ethyl acetate in hexane); **Yield:** 76% (45 mg); **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.42 – 8.40 (m, 1H), 8.18 – 8.15 (m, 1H), 8.06 (brs, 1H), 7.82 (td, *J* = 7.7, 1.7 Hz, 1H), 7.39 – 7.34 (m, 2H), 7.28 – 7.24 (m, 2H), 6.88 (td, *J* = 9.1, 2.5 Hz, 1H), 6.53 – 6.52 (m, 1H), 4.84 – 4.79 (m, 1H), 3.86 – 3.76 (m, 2H), 1.62 (d, *J* = 6.9 Hz, 3H);**^{13}C NMR (101 MHz, CDCl3)** δ 164.9, δ 158.0 (d, *J* = 234.0 Hz), 149.4, 148.2, 137.4, 132.9, 128.9 (d, *J* = 10.1 Hz), 126.4, 125.4, 122.3, 110.3 (d, *J* = 7.2 Hz), 110.2 (d, *J* = 43.2 Hz), 105.7 (d, *J* = 23.2 Hz), 102.3 (d, *J* = 4.5 Hz), 51.4, 45.1,

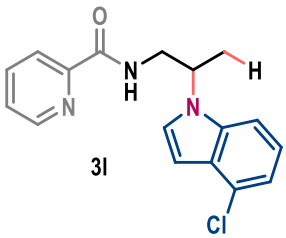
18.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -125.30 (d, *J* = 1.7 Hz); **HRMS** (ESI/TOF-Q) m/z: $[M+Na]^+$ Calculated for $C_{17}H_{16}FN_3ONa^+$ 320.1170; Found 320.1182.

***N*-(2-(6-fluoro-1H-indol-1-yl)propyl)picolinamide (3k):**



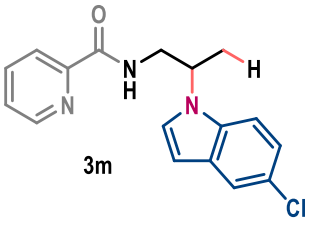
Compound **3k** was synthesized according to GP-1 as colorless sticky solid; eluent (25% ethyl acetate in hexane); **Yield:** 78% (46 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.41 – 8.39 (m, 1H), 8.18 – 8.15 (m, 1H), 8.07 (brs, 1H), 7.83 – 7.79 (m, 1H), 7.53 – 7.49 (m, 1H), 7.38 – 7.35 (m, 1H), 7.22 (d, *J* = 3.3 Hz, 1H), 7.13 – 7.10 (m, 1H), 6.86 – 6.81 (m, 1H), 6.54 (d, *J* = 3.3 Hz, 1H), 4.79 – 4.70 (m, 1H), 3.91 – 3.84 (m, 1H), 3.80 – 3.73 (m, 1H), 1.61 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 164.9, 159.9 (d, *J* = 237.5 Hz), 149.4, 148.2, 137.4, 136.3 (d, *J* = 12.0 Hz), 126.4, 125.1, 124.3 (d, *J* = 3.7 Hz), 122.3, 121.7 (d, *J* = 10.0 Hz), 108.4 (d, *J* = 24.6 Hz), 102.5, 96.2 (d, *J* = 26.7 Hz), 51.4, 44.9, 18.3; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -120.92; **HRMS** (ESI/TOF-Q) m/z: $[M+Na]^+$ Calculated for $C_{17}H_{16}FN_3ONa^+$ 320.1170; Found 320.1176.

***N*-(2-(4-chloro-1H-indol-1-yl)propyl)picolinamide (3l):**

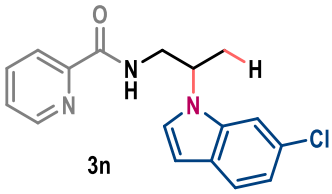


Compound **3l** was synthesized according to GP-1 as colorless gummy solid; eluent (20% ethyl acetate in hexane); **Yield:** 81% (51 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.43 – 8.41 (m, 1H), 8.16 (dd, *J* = 7.9, 1.0 Hz, 1H), 8.05 (brs, 1H), 7.82 (td, *J* = 7.8, 1.7 Hz, 1H), 7.40 – 7.37 (m, 1H), 7.34 (d, *J* = 7.6, 1H), 7.28 (d, *J* = 3.3 Hz, 1H), 7.09 – 7.03 (m, 2H), 6.68 (d, *J* = 3.3 Hz, 1H), 4.89 – 4.80 (m, 1H), 3.90 – 3.83 (m, 1H), 3.83 – 3.76 (m, 1H), 1.63 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 165.0, 149.4, 148.2, 137.5, 137.1, 127.5, 126.5, 126.3, 124.6, 122.34, 122.30, 119.5, 108.5, 101.1, 51.7, 45.0, 18.5; **HRMS** (ESI/TOF-Q) m/z: $[M+Na]^+$ Calculated for $C_{17}H_{16}ClN_3ONa^+$ 336.0874; Found 336.0879.

***N*-(2-(5-chloro-1H-indol-1-yl)propyl)picolinamide (3m):**



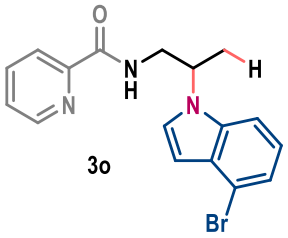
Compound **3m** was synthesized according to GP-1 as off white gummy liquid; eluent (20% ethyl acetate in hexane); **Yield:** 80% (50 mg); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.41 (d, *J* = 4.7 Hz, 1H), 8.16 (d, *J* = 7.9 Hz, 1H), 8.05 (brs, 1H), 7.82 (t, *J* = 7.6 Hz, 1H), 7.57 (s, 1H), 7.39 – 7.38 (m, 1H), 7.36 – 7.34 (m, 1H), 7.27 – 7.25 (m, 1H), 7.08 (d, *J* = 8.8 Hz, 1H), 6.50 (d, *J* = 5.7 Hz, 1H), 4.86 – 4.79 (m, 1H), 3.87 – 3.82 (m, 1H), 3.80 – 3.74 (m, 1H), 1.62 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 165.0, 149.4, 148.2, 137.5, 134.7, 129.7, 126.4, 125.3, 125.2, 122.3, 122.0, 120.4, 110.7, 102.0, 51.4, 45.0, 18.4; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{17}H_{16}ClN_3OH^+$ 314.1055; Found 314.1056.



3n

***N* -(2-(6-chloro-1H-indol-1-yl)propyl)picolinamide (3n):**

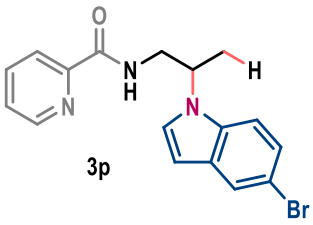
Compound **3n** was synthesized according to GP-1 as brown gummy liquid; eluent (20% ethyl acetate in hexane); **Yield:** 82% (51 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.42 (d, 7.0 Hz, 1H), 8.19 – 8.16 (m, 1H), 8.06 (brs, 1H), 7.84 (td, *J* = 7.7, 1.7 Hz, 1H), 7.50 (dd, *J* = 8.5, 0.5 Hz, 1H), 7.41 – 7.38 (m, 2H), 7.23 (d, *J* = 3.3 Hz, 1H), 7.02 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.54 (dd, *J* = 3.3, 0.9 Hz, 1H), 4.81 – 4.76 (m, 1H), 3.94 – 3.87 (m, 1H), 3.78 – 3.71 (m, 1H), 1.62 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 165.0, 149.4, 148.2, 137.5, 136.7, 127.8, 127.2, 126.4, 124.7, 122.4, 121.9, 120.4, 109.9, 102.6, 51.5, 45.0, 18.5; **HRMS** (ESI/TOF-Q) m/z: $[M+Na]^+$ Calculated for $C_{17}H_{16}ClN_3ONa^+$ 336.0874; Found 336.0879.



3o

***N*-(2-(4-bromo-1H-indol-1-yl)propyl)picolinamide (3o):**

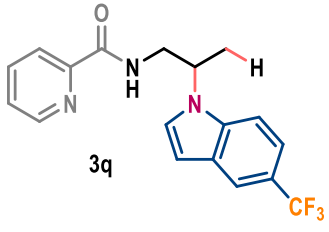
Compound **3o** was synthesized according to GP-1 as brown gummy liquid; eluent (20% ethyl acetate in hexane); **Yield:** 76% (54 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.42 – 8.40 (m, 1H), 8.17 – 8.15 (m, 1H), 8.10 (brs, 1H), 7.82 (td, *J* = 7.7, 1.7 Hz, 1H), 7.40 – 7.37 (m, 2H), 7.30 (d, *J* = 3.3 Hz, 1H), 7.25 – 7.23 (m, 1H), 7.01 – 6.97 (m, 1H), 6.62 – 6.61 (m, 1H), 4.86 – 4.80 (m, 1H), 3.88 – 3.76 (m, 2H), 1.62 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 164.9, 149.2, 148.1, 137.6, 136.6, 129.3, 126.5, 124.6, 122.6 (2xC), 122.4, 115.0, 109.0, 102.7, 51.6, 45.0, 18.5; **HRMS** (ESI/TOF-Q) m/z: $[M+Na]^+$ Calculated for $C_{17}H_{16}BrN_3ONa^+$ 380.0369; Found 380.0372.



3p

***N*-(2-(5-bromo-1H-indol-1-yl)propyl)picolinamide (3p):**

Compound **3p** was synthesized according to GP-1 as off brown gummy liquid; eluent (20% ethyl acetate in hexane); **Yield:** 74% (53 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.41 – 8.39 (m, 1H), 8.16 – 8.14 (m, 1H), 8.05 (brs, 1H), 7.84 – 7.79 (m, 1H), 7.74 – 7.72 (m, 1H), 7.39 – 7.36 (m, 1H), 7.31 (d, *J* = 8.8 Hz, 1H), 7.24 (d, *J* = 3.2 Hz, 1H), 7.21 – 7.18 (m, 1H), 6.51 – 6.49 (m, 1H), 4.84 – 4.77 (m, 1H), 3.87 – 3.74 (m, 2H), 1.61 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 165.0, 149.3, 148.2, 137.4, 135.0, 130.3, 126.4, 125.1, 124.5, 123.5, 122.3, 112.9, 111.2, 101.9, 51.4, 45.0, 18.4; **HRMS** (ESI/TOF-Q) m/z: $[M+Na]^+$ Calculated for $C_{17}H_{16}BrN_3ONa^+$ 380.0369; Found 380.0377



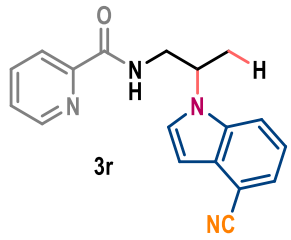
3q

***N*-(2-(5-(trifluoromethyl)-1H-indol-1-yl)propyl)picolinamide (3q):**

Compound **3q** was synthesized according to GP-1 as colorless gummy liquid; eluent (30% ethyl acetate in hexane); **Yield:** 63% (44 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** *δ* 8.38 (d, *J* = 4.7 Hz, 1H), 8.15 (d, *J* = 7.8 Hz, 1H), 8.04 (brs, 1H), 7.91 – 7.90 (m, 1H), 7.84 – 7.79 (m, 1H), 7.50 (d, *J* = 8.7 Hz, 1H), 7.39 – 7.32 (m, 3H), 6.66 – 6.65 (m, 1H), 4.93 – 4.88 (m, 1H), 3.91 – 3.85 (m, 1H), 3.80 – 3.74 (m, 1H), 1.65 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 165.0, 149.3, 148.2, 137.6,

137.5, 128.0, 125.6, 124.3 (q, J = 271.1 Hz), 122.28, 122.25, 121.9, 118.8 (q, J = 4.2 Hz), 118.4 (q, J = 3.4 Hz).110.0, 103.5, 51.5, 45.1, 18.4; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -60.33; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{18}H_{16}F_3N_3OH^+$ 348.1318; Found 348.1317.

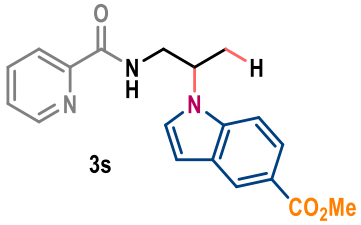
***N*-(2-(4-cyano-1H-indol-1-yl)propyl)picolinamide (3r):**



3r

Compound **3r** was synthesized according to GP-1 as off white gummy liquid; eluent (30% ethyl acetate in hexane); **Yield:** 70% (42 mg); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.44 – 8.40 (m, 1H), 8.16 – 8.14 (m, 1H), 8.05 (brs, 1H), 7.85 – 7.81 (m, 1H), 7.69 – 7.67 (m, 1H), 7.44 – 7.39 (m, 3H), 7.17 – 7.13 (m, 1H), 6.79 (d, J = 3.8 Hz, 1H), 4.94 – 4.90 (m, 1H), 3.87 – 3.75 (m, 2H), 1.66 (d, J = 10.1 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 165.1, 149.3, 148.3, 137.5, 136.1, 129.9, 126.60, 126.56, 125.3, 122.3, 121.4, 118.9, 114.6, 103.4, 101.5, 51.5, 45.3, 18.5; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{18}H_{16}N_4OH^+$ 305.1397; Found 305.1410.

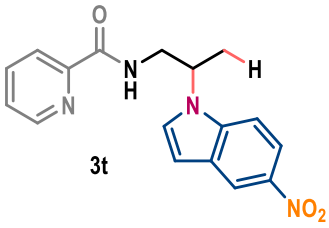
methyl 1-(1-(picolinamido)propan-2-yl)-1H-indole-5-carboxylate (3s):



3s

Compound **3s** was synthesized according to GP-1 as brown gummy liquid; eluent (30% ethyl acetate in hexane); **Yield:** 75% (50 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.39 – 8.37 (m, 2H), 8.16 (d, J = 8.0 Hz, 1H), 8.04 (brs, 1H), 7.84 – 7.79 (m, 2H), 7.42 (d, J = 8.8 Hz, 1H), 7.39 – 7.36 (m, 1H), 7.31 (d, J = 3.3 Hz, 1H), 6.67 – 6.66 (m, 1H), 4.94 – 4.85 (m, 1H), 3.91 (s, 3H), 3.89 – 3.86 (m, 1H), 3.81 – 3.74 (m, 1H), 1.64 (d, J = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 168.3, 165.0, 149.3, 148.2, 138.8, 137.5, 128.2, 126.5, 125.3, 124.2, 123.1, 122.3, 121.8, 109.4, 104.0, 51.9, 51.5, 45.1, 18.5; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{19}H_{19}N_3O_3H^+$ 338.1499; Found 338.1508.

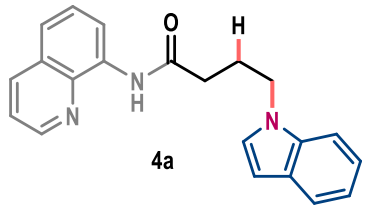
***N*-(2-(5-nitro-1H-indol-1-yl)propyl)picolinamide (3t):**



3t

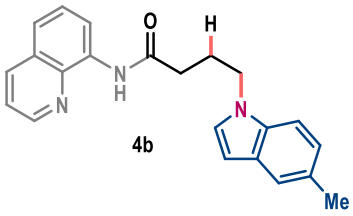
Compound **3t** was synthesized according to GP-1 as yellow sticky solid; eluent (35% ethyl acetate in hexane); **Yield:** 62% (40 mg); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.55 (d, J = 2.2 Hz, 1H), 8.39 – 8.38 (m, 1H), 8.14 (d, J = 7.8 Hz, 1H), 8.06 (t, J = 6.6 Hz, 1H), 8.00 (dd, J = 9.1, 2.2 Hz, 1H), 7.82 (td, J = 7.7, 1.7 Hz, 1H), 7.45 (d, J = 9.1 Hz, 1H), 7.40 – 7.37 (m, 2H), 6.75 (d, J = 3.3 Hz, 1H), 4.97 – 4.91 (m, 1H), 3.90 – 3.85 (m, 1H), 3.78 – 3.72 (m, 1H), 1.67 (d, J = 6.9 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 165.1, 149.2, 148.2, 141.8, 139.3, 137.6, 127.8, 127.0, 126.6, 122.3, 118.3, 117.4, 109.6, 105.2, 51.7, 45.3, 18.4; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{17}H_{16}N_4OH^+$ 325.1295; Found 325.1301.

4-(1H-indol-1-yl)-*N*-(quinolin-8-yl)butanamide (4a):



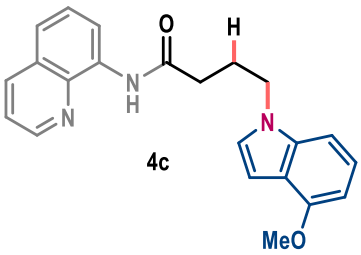
Compound **4a** was synthesized according to GP-2 as brown sticky solid; eluent (20% ethyl acetate in hexane); **Yield:** 73% (48 mg); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.76 (brs, 1H), 8.80 – 8.77 (m, 2H), 8.16 (d, *J* = 8.3 Hz, 1H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.58 – 7.51 (m, 2H), 7.47 – 7.42 (m, 2H), 7.21 – 7.17 (m, 2H), 7.12 – 7.09 (m, 1H), 6.53 – 6.52 (m, 1H), 4.33 – 4.30 (m, 2H), 2.55 – 2.52 (m, 2H), 2.39 – 2.33 (m, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.6, 148.2, 138.3, 136.6, 136.1, 134.4, 128.8, 128.1, 128.0, 127.5, 121.8, 121.73, 121.68, 121.1, 119.5, 116.7, 109.6, 101.4, 45.5, 34.5, 25.9; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{21}H_{19}N_3OH^+$ 330.1601; Found 330.1611.

4-(5-methyl-1H-indol-1-yl)-*N*-(quinolin-8-yl)butanamide (4b):



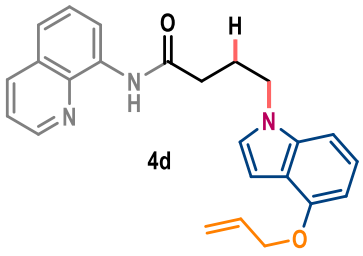
Compound **4b** was synthesized according to GP-2 as off white gummy solid; eluent (20% ethyl acetate in hexane); **Yield:** 75% (51 mg); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.73 (brs, 1H), 8.77 (d, *J* = 5.6 Hz, 2H), 8.16 (d, *J* = 8.3 Hz, 1H), 7.57 – 7.50 (m, 2H), 7.46 – 7.44 (m, 1H), 7.41 (s, 1H), 7.30 (d, *J* = 8.3 Hz, 1H), 7.13 – 7.12 (m, 1H), 7.00 (d, *J* = 8.4 Hz, 1H), 6.43 – 6.42 (m, 1H), 4.30 – 4.27 (m, 2H), 2.53 – 2.50 (m, 2H), 2.43 (s, 3H), 2.38 – 2.34 (m, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.7, 148.3, 138.4, 136.5, 134.6, 134.5, 129.1, 128.7 (2xC), 128.1, 127.5, 123.3, 121.8, 121.7, 120.7, 116.7, 109.3, 100.9, 45.6, 34.5, 25.9, 21.5; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{22}H_{21}N_3OH^+$ 344.1757; Found 344.1759.

4-(4-methoxy-1H-indol-1-yl)-*N*-(quinolin-8-yl)butanamide (4c):



Compound **4c** was synthesized according to GP-2 as colorless gummy liquid; eluent (20% ethyl acetate in hexane); **Yield:** 78% (56 mg); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.84 (brs, 1H), 8.80 – 8.78 (m, 2H), 8.22 (d, *J* = 8.2 Hz, 1H), 7.59 – 7.53 (m, 2H), 7.50 – 7.48 (m, 1H), 7.11 (t, *J* = 8.0 Hz, 1H), 7.08 (d, *J* = 3.2 Hz, 1H), 7.05 – 7.03 (m, 1H), 6.61 – 6.60 (m, 1H), 6.51 – 6.50 (m, 1H), 4.29 (t, *J* = 6.8 Hz, 2H), 3.95 (s, 3H), 2.56 (t, *J* = 7.1 Hz, 2H), 2.38 – 2.32 (m, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.8, 153.6, 147.8, 137.7, 134.2, 128.2, 127.9, 126.6, 122.5 (2xC), 121.8, 121.7, 119.3, 103.2 (2xC), 99.4 (2xC), 98.7, 55.4, 45.8, 34.5, 26.0; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{22}H_{21}N_3O_2H^+$ 360.1707; Found 360.1716.

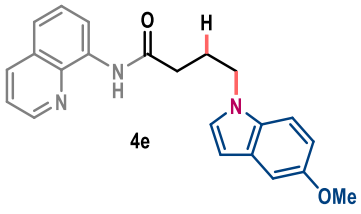
4-(4-(allyloxy)-1H-indol-1-yl)-*N*-(quinolin-8-yl)butanamide (4d):



Compound **4d** was synthesized according to GP-2 as brown gummy liquid; eluent (25% ethyl acetate in hexane); **Yield:** 74% (57 mg); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.73 (brs, 1H), 8.77 (d, *J* = 5.5 Hz, 2H), 8.16 (d, *J* = 8.4 Hz, 1H), 7.55 – 7.50 (m, 2H), 7.46 – 7.43 (m, 1H), 7.10 – 7.02 (m, 3H), 6.67 – 6.64 (m, 1H), 6.52 – 6.50 (m, 1H), 6.19 – 6.13 (m, 1H), 5.48 (d, *J* = 17.2 Hz, 1H), 5.30 (d, *J* = 10.6 Hz, 1H), 4.69 (d, *J* = 5.2 Hz, 2H), 4.30 – 4.27 (m, 2H), 2.53 – 2.50 (m, 2H), 2.38 – 2.33 (m, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.7, 152.6, 148.3, 138.4, 137.8, 136.5, 134.5, 134.0, 128.1, 127.5, 126.6, 122.5, 121.8, 121.7, 119.6, 117.3, 116.7, 103.2, 100.8, 98.9, 69.0, 45.8, 34.5, 25.9; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{22}H_{21}N_3O_2H^+$ 386.1863; Found 386.1863.

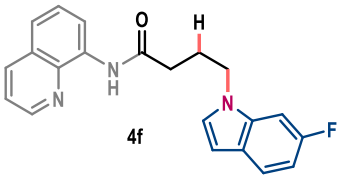
4-(5-methoxy-1H-indol-1-yl)-*N*-(quinolin-8-yl)butanamide (4e):



4e

Compound **4e** was synthesized according to GP-2 as off white gummy liquid; eluent (25% ethyl acetate in hexane); **Yield:** 80% (57 mg); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.73 (brs, 1H), 8.78 – 8.76 (m, 2H), 8.18 – 8.16 (m, 1H), 7.55 – 7.51 (m, 2H), 7.47 – 7.44 (m, 1H), 7.31 – 7.29 (m, 1H), 7.14 (d, *J* = 3.1 Hz, 1H), 7.09 (d, *J* = 2.3 Hz, 1H), 6.85 – 6.83 (m, 1H), 6.43 – 6.42 (m, 1H), 4.29 – 4.27 (m, 2H), 3.84 (s, 3H), 2.53 – 2.51 (m, 2H), 2.37 – 2.33 (m, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.7, 154.1, 148.3, 138.4, 136.5, 134.5, 131.5, 129.1, 128.6, 128.1, 127.5, 121.8, 121.7, 116.7, 112.1, 110.3, 102.7, 101.0, 56.0, 45.7, 34.5, 26.0; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{22}H_{21}N_3O_2H^+$ 360.1707; Found 360.1712.

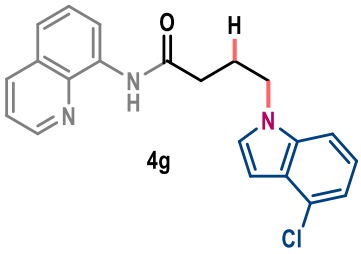
4-(6-fluoro-1H-indol-1-yl)-N-(quinolin-8-yl)butanamide (4f):



4f

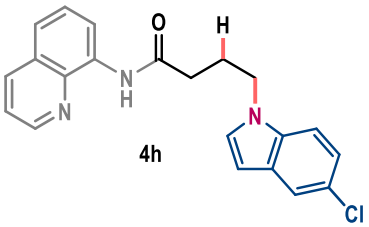
Compound **4f** was synthesized according to GP-2 as colorless gummy liquid; eluent (25% ethyl acetate in hexane); **Yield:** 56% (39 mg); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.78 (brs, 1H), 8.78 (d, *J* = 5.7 Hz, 2H), 8.18 (d, *J* = 8.3 Hz, 1H), 7.58 – 7.50 (m, 3H), 7.48 – 7.45 (m, 1H), 7.15 – 7.14 (m, 1H), 7.09 (d, *J* = 10.1 Hz, 1H), 6.87 – 6.82 (m, 1H), 6.49 – 6.48 (m, 1H), 4.26 – 4.23 (m, 2H), 2.56 – 2.53 (m, 2H), 2.37 – 2.31 (m, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.5, 159.9 (d, *J* = 237.5 Hz), 148.1, 138.2, 136.8, 136.2 (d, *J* = 11.9 Hz), 134.3, 128.44, 128.41, 128.1, 127.6, 125.2, 121.78 (d, *J* = 9.7 Hz), 121.75 (d, *J* = 10.1 Hz), 117.0, 108.3 (d, *J* = 24.6 Hz), 101.7, 96.0 (d, *J* = 26.4 Hz), 45.7, 34.4, 25.7; ^{19}F NMR (471 MHz, $CDCl_3$) δ -120.98; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{21}H_{18}FN_3OH^+$ 348.1507; Found 348.1509.

4-(4-chloro-1H-indol-1-yl)-*N*-(quinolin-8-yl)butanamide (4g):



4g

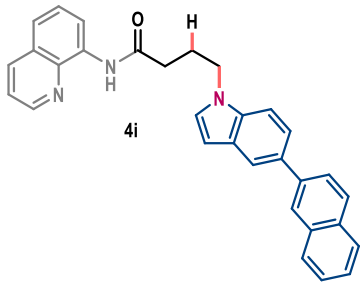
Compound **4g** was synthesized according to GP-2 as pale yellow gummy liquid; eluent (25% ethyl acetate in hexane); **Yield:** 71% (52 mg); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.72 (brs, 1H), 8.78 – 8.74 (m, 2H), 8.18 – 8.15 (m, 1H), 7.57 – 7.51 (m, 2H), 7.47 – 7.44 (m, 1H), 7.32 – 7.30 (m, 1H), 7.21 – 7.20 (m, 1H), 7.08 – 7.06 (m, 2H), 6.62 – 6.61 (m, 1H), 4.33 – 4.30 (m, 2H), 2.54 – 2.50 (m, 2H), 2.38 – 2.32 (m, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.5, 148.3, 138.4, 137.0, 136.5, 134.4, 128.6, 128.1, 127.52, 127.49, 126.4, 122.3, 121.8 (2xC), 119.3, 116.7, 108.3, 100.2, 45.9, 34.3, 25.9; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{21}H_{18}ClN_3OH^+$ 364.1211; Found 364.1209.



4h

4-(5-chloro-1H-indol-1-yl)-*N*-(quinolin-8-yl)butanamide (4h):

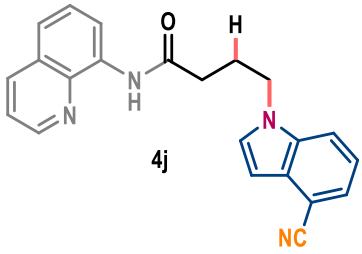
Compound **4h** was synthesized according to GP-2 as off white gummy liquid; eluent (25% ethyl acetate in hexane); **Yield:** 70% (51 mg); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.73 (brs, 1H), 8.78 – 8.76 (m, 2H), 8.18 – 8.16 (m, 1H), 7.57 (d, *J* = 2.0 Hz, 1H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.52 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.46 (dd, *J* = 8.2, 4.3 Hz, 1H), 7.31 (d, *J* = 8.7 Hz, 1H), 7.18 (d, *J* = 3.1 Hz, 1H), 7.10 – 7.08 (m, 1H), 6.45 – 6.44 (m, 1H), 4.28 (t, *J* = 6.8 Hz, 2H), 2.52 (t, *J* = 7.0 Hz, 2H), 2.36 – 2.31(m, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.5, 148.2, 138.2, 136.7, 134.6, 134.3, 129.7, 129.3, 128.1, 127.5, 125.2, 122.0, 121.84, 121.79, 120.4, 116.8, 110.6, 101.2, 45.7, 34.3, 25.9; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{21}H_{18}ClN_3OH^+$ 364.1211; Found 408.177.



4i

4-(5-(naphthalen-2-yl)-1H-indol-1-yl)-*N*-(quinolin-8-yl)butanamide (4i):

Compound **4i** was synthesized according to GP-2 as brown sticky liquid; eluent (25% ethyl acetate in hexane); **Yield:** 68% (62 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.80 (brs, 1H), 8.82 – 8.78 (m, 2H), 8.18 – 8.15 (m, 1H), 8.02 – 7.99 (m, 1H), 7.92 – 7.89 (m, 1H), 7.86 – 7.83 (m, 1H), 7.77 – 7.75 (m, 1H), 7.59 – 7.51 (m, 4H), 7.48 – 7.43 (m, 3H), 7.41 – 7.37 (m, 1H), 7.35 – 7.32 (m, 1H), 7.25 (d, *J* = 3.2 Hz, 1H), 6.59 – 6.58 (m, 1H), 4.39 (t, *J* = 6.8 Hz, 2H), 2.61 (t, *J* = 7.0 Hz, 2H), 2.45 (q, *J* = 6.9 Hz, 2H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.6, 148.3, 141.6, 138.5, 136.6, 135.6, 134.5, 134.0, 132.4, 132.2, 128.8, 128.7, 128.3, 128.1, 127.6, 127.4, 127.1, 126.8, 125.8, 125.7, 125.5, 124.4, 122.5, 121.8 (2xC), 116.7, 109.2, 101.7, 45.8, 34.6, 26.0; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{31}H_{25}N_3OH^+$ 456.2070; Found 456.2076.



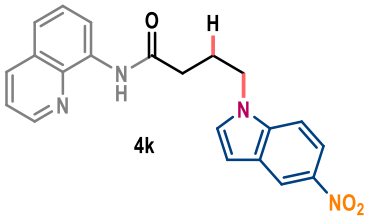
4j

4-(4-cyano-1H-indol-1-yl)-*N*-(quinolin-8-yl)butanamide (4j):

Compound **4j** was synthesized according to GP-2 as gummy liquid; eluent (30% ethyl acetate in hexane); **Yield:** 51% (36 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.84 (brs, 1H), 8.80 – 8.76 (m, 2H), 8.25 (d, *J* = 8.2 Hz, 1H), 7.67 – 7.64 (m, 1H), 7.61 – 7.55 (m, 2H), 7.53 – 7.50 (m, 1H), 7.42 – 7.40 (m, 1H), 7.35 – 7.34 (m, 1H), 7.20 – 7.15 (m, 1H), 6.72 – 6.70 (m, 1H), 4.39 – 4.35 (m, 2H), 2.58 (t, *J* = 6.9 Hz, 2H), 2.36 (p, *J* = 6.9 Hz, 2H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.2, 148.4, 138.4, 136.6, 135.9, 134.3, 130.7, 130.0, 128.1, 127.5, 125.1, 121.92, 121.86, 121.3, 118.9, 116.7, 114.4, 103.4, 100.7, 45.8, 34.1, 25.9; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{22}H_{18}N_4OH^+$ 355.1553; Found 355.1557.

4-(5-nitro-1H-indol-1-yl)-*N*-(quinolin-8-yl)butanamide (4k):

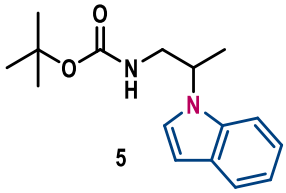
Compound **4k** was synthesized according to GP-2 as off white gummy liquid; eluent (35% ethyl acetate in hexane); **Yield:** 55% (41 mg) **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.76 (brs, 1H), 8.76 – 8.74 (m, 2H), 8.53 (d, *J* = 2.2 Hz, 1H), 8.22 – 8.20



4k

(m, 1H), 8.01 – 7.99 (m, 1H), 7.58 – 7.53 (m, 2H), 7.49 – 7.47 (m, 1H), 7.42 (d, *J* = 9.0 Hz, 1H), 7.32 (d, *J* = 3.2 Hz, 1H), 6.68 – 6.67 (m, 1H), 4.37 (t, *J* = 6.9 Hz, 2H), 2.57 (t, *J* = 6.8 Hz, 2H), 2.40 – 2.34 (m, 2H); **^{13}C NMR (126 MHz, CDCl$_3$)** δ 170.3, 148.0, 141.7, 139.1, 134.1, 131.1 (2xC), 128.2, 127.8, 127.7, 122.0, 121.8, 118.3 (2xC), 117.4 (2xC), 109.5, 104.4, 45.9, 34.1, 25.9; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{21}H_{18}N_4OH^+$ 375.1452; Found 375.1461.

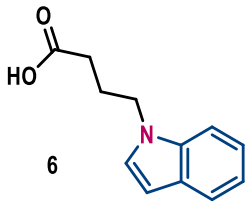
tert-butyl (2-(1H-indol-1-yl)propyl)carbamate (5):



5

Compound **5** was synthesized as off white sticky solid; eluent (15% ethyl acetate in hexane); **Yield:** 86% (71 mg); **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.64 – 7.62 (m, 1H), 7.39 (d, *J* = 8.3 Hz, 1H), 7.22 – 7.18 (m, 1H), 7.17 (d, *J* = 3.2 Hz, 1H), 7.13 – 7.09 (m, 1H), 6.56 (d, *J* = 3.3 Hz, 1H), 4.75 – 4.71 (m, 1H), 4.44 (brs, 1H), 3.65 – 3.60 (m, 1H), 3.37 – 3.31 (m, 1H), 1.53 (d, *J* = 6.9 Hz, 3H), 1.39 (s, 9H); **^{13}C NMR (126 MHz, CDCl$_3$)** δ 156.1, 136.5, 128.6, 123.8, 121.8, 121.1, 119.7, 109.7, 102.3, 79.8, 51.4, 46.4, 28.4, 18.5; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{16}H_{22}N_2O_2H^+$ 275.1754; Found 275.1755.

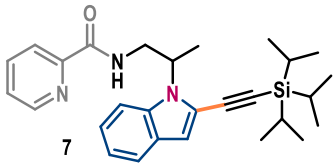
4-(1H-indol-1-yl)butanoic acidamate (6):



6

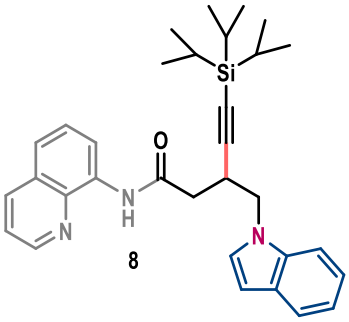
Compound **6** was synthesized as brown gummy liquid; eluent (35% ethyl acetate in hexane); **Yield:** 81% (49 mg); **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.65 – 7.62 (m, 1H), 7.37 – 7.34 (m, 1H), 7.24 – 7.20 (m, 1H), 7.13 – 7.07 (m, 2H), 6.51 – 6.50 (m, 1H), 4.24 – 4.20 (m, 2H), 2.35 (t, *J* = 7.1 Hz, 2H), 2.22 – 2.16 (m, 2H) (H of COOH signal is missing) ; **^{13}C NMR (101 MHz, CDCl$_3$)** δ 178.3, 136.1, 128.8, 127.9, 121.8, 121.2, 119.6, 109.4, 101.6, 45.3, 30.9, 25.3; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{12}H_{13}NO_2H^+$ 204.1019; Found 204.1025.

***N*-(2-(2-((triisopropylsilyl)ethynyl)-1H-indol-1-yl)propyl)picolinamide (7):**



7

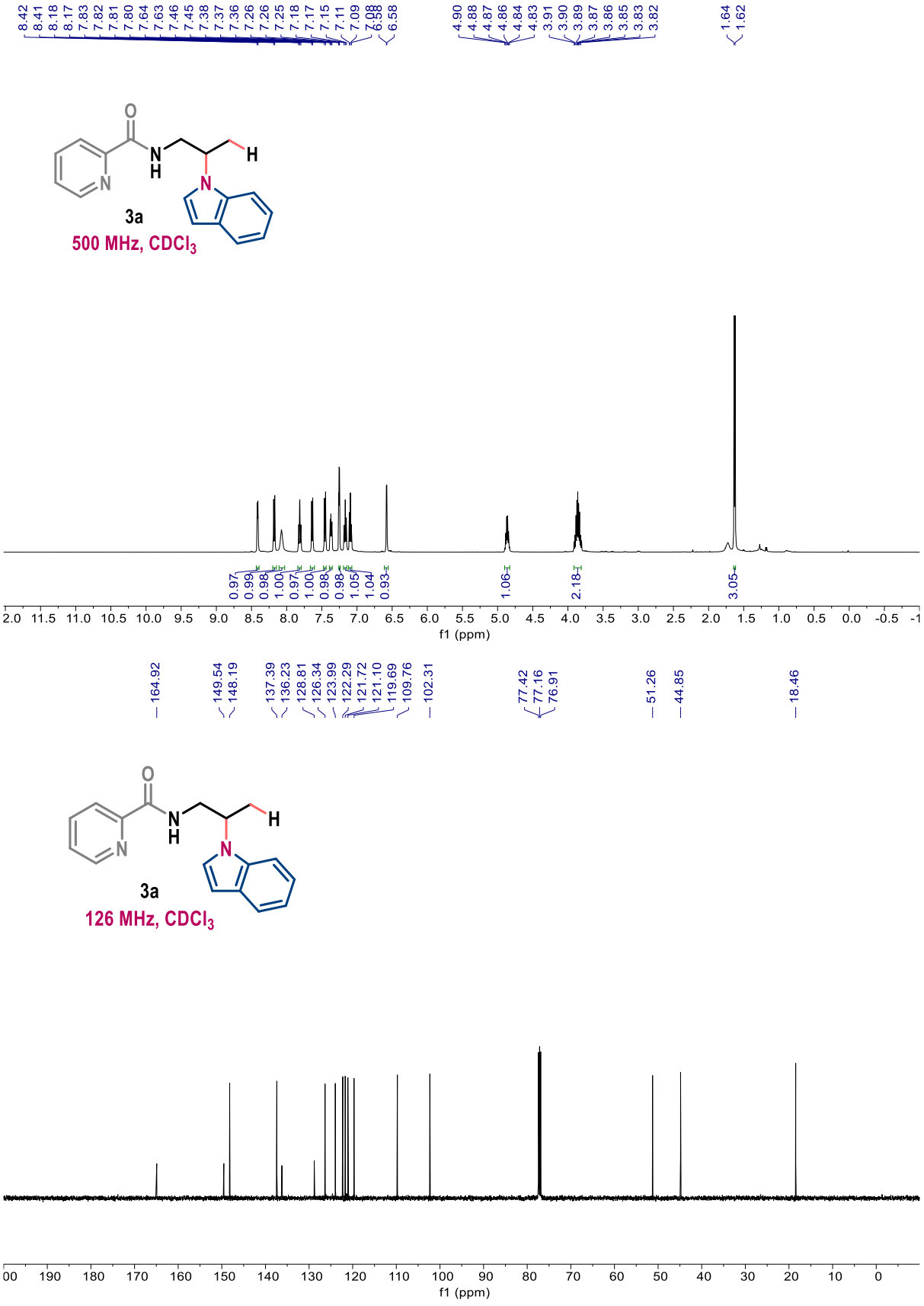
Compound **7** was synthesized as off brown sticky solid; eluent (15% ethyl acetate in hexane); **Yield:** 62% (43 mg); **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.37 (d, *J* = 4.4 Hz, 1H), 8.13 (d, *J* = 7.8 Hz, 1H), 8.00 (brs, 1H), 7.80 – 7.76 (m, 1H), 7.55 (d, *J* = 7.9 Hz, 1H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.35 – 7.32 (m, 1H), 7.18 – 7.14 (m, 1H), 7.08 – 7.04 (m, 1H), 6.85 (s, 1H), 5.16 – 5.07 (m, 1H), 4.24 – 4.17 (m, 1H), 4.07 – 4.00 (m, 1H), 1.76 (d, *J* = 7.1 Hz, 3H), 1.13 – 1.06 (m, 21H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 164.8, 149.6, 148.2, 137.2, 136.3, 127.8, 126.2, 123.2, 122.2, 121.3 (2xC), 120.2, 110.6 (2xC), 98.9 (2xC), 52.7, 43.6, 18.8, 17.9, 11.5; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{28}H_{37}N_3OSiH^+$ 460.2779; Found 460.2784.

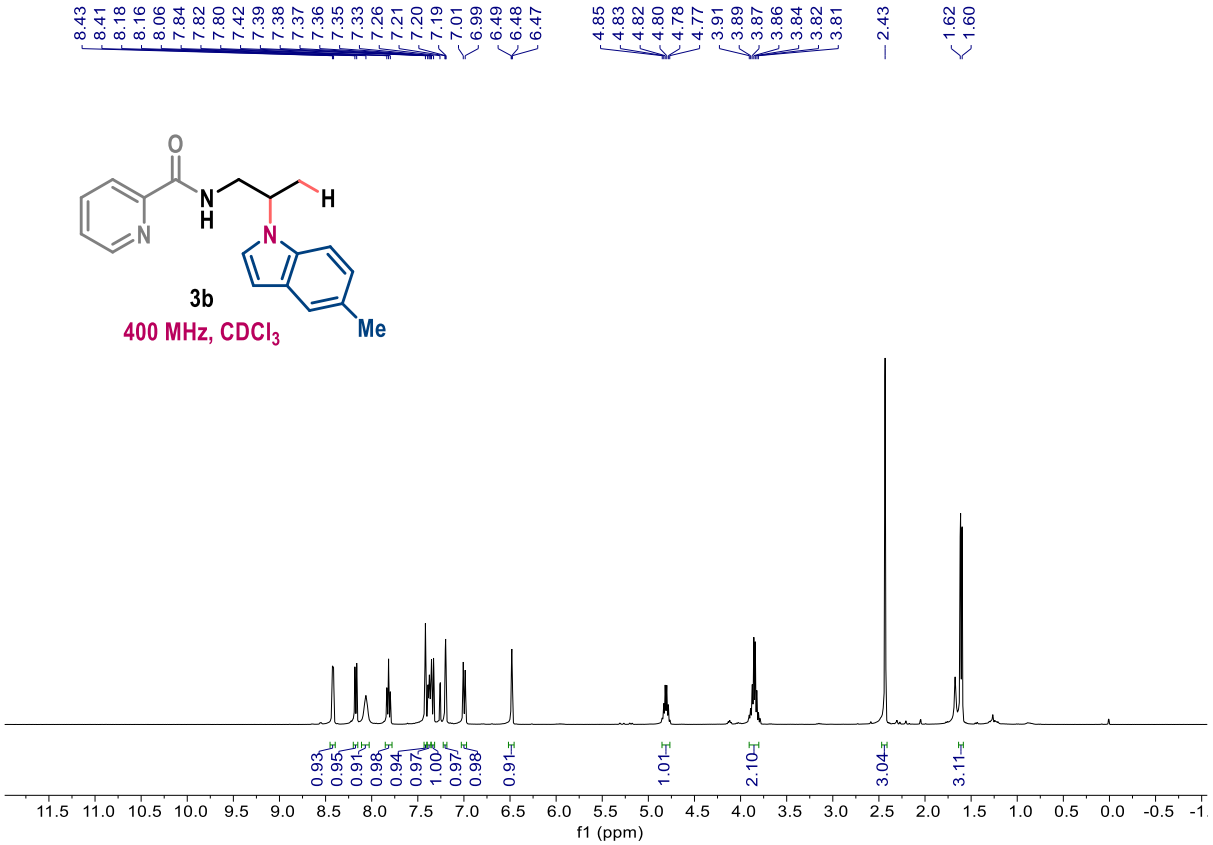


(S)-3-((1H-indol-1-yl)methyl)-*N*-(quinolin-8-yl)-5-(triisopropylsilyl)pent-4-ynamide (8):

Compound **8** was synthesized as pale yellow liquid; eluent (15% ethyl acetate in hexane); **Yield:** 65% (50 mg); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.80 (brs, 1H), 8.80 – 8.76 (m, 2H), 8.18 – 8.15 (m, 1H), 7.62 – 7.59 (m, 1H), 7.57 – 7.51 (m, 2H), 7.50 – 7.48 (m, 1H), 7.46 – 7.43 (m, 1H), 7.32 (d, *J* = 3.3 Hz, 1H), 7.18 – 7.14 (m, 1H), 7.09 – 7.05 (m, 1H), 6.50 – 6.49 (m, 1H), 4.53 – 4.48 (m, 1H), 4.41 – 4.36 (m, 1H), 3.72 – 3.65 (m, 1H), 2.78 – 2.65 (m, 2H), 0.94 – 0.91 (m, 21H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 168.7, 148.2, 138.5, 136.5, 134.4, 128.9, 128.8, 128.0, 127.5, 121.8, 121.76, 121.72, 121.0, 119.6, 116.9, 109.7, 107.5 (2xC), 101.6, 85.0, 49.6, 40.8, 31.5, 18.6, 11.2; **HRMS** (ESI/TOF-Q) m/z: $[M+H]^+$ Calculated for $C_{32}H_{39}N_3OSiH^+$ 510.2935; Found 510.2940.

13. NMR spectra of synthesized compounds

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4.77
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3.81
2.43
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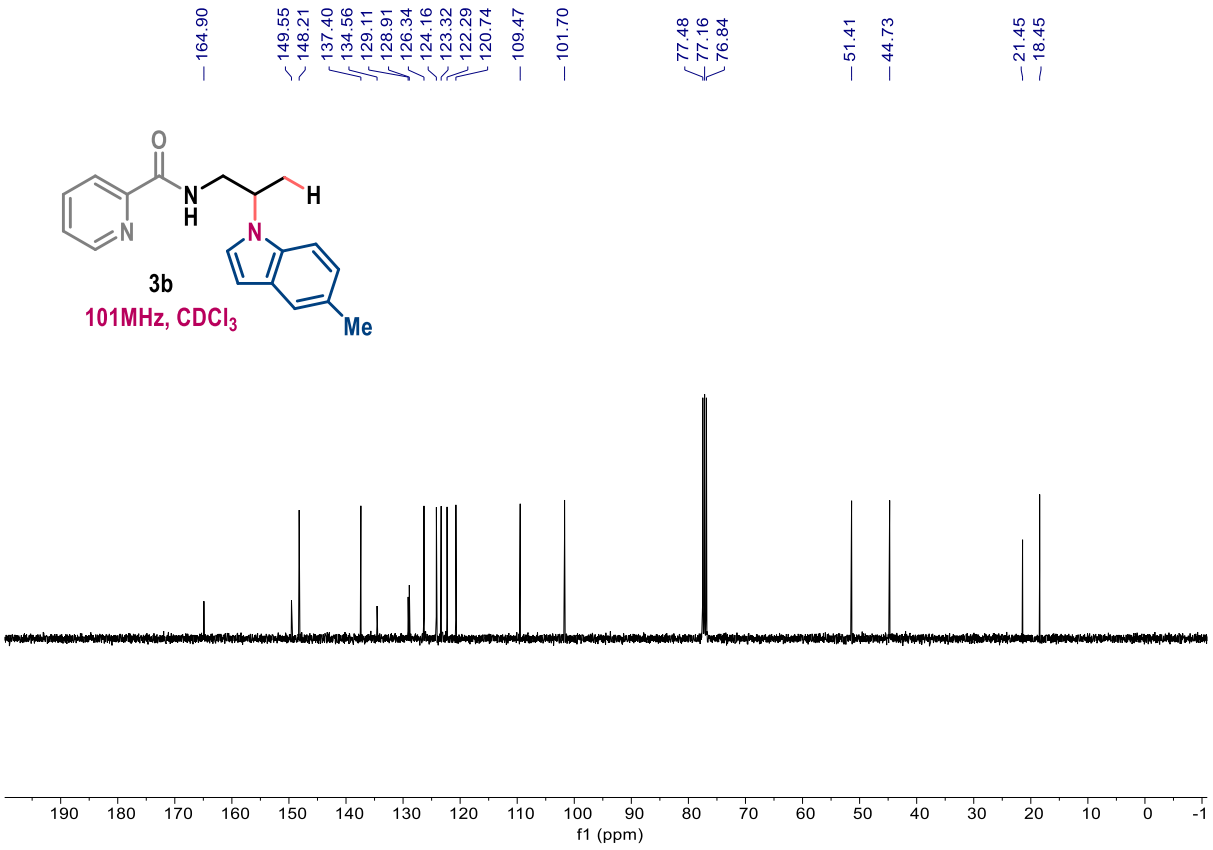
N
H
N
H
3b
400 MHz, CDCl3
Me
0.93
0.95
0.91
0.98
0.94
0.97
1.00
0.97
0.98
0.91
1.01
2.10
3.04
3.11
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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77.16
76.84
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18.45
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101MHz, CDCl3
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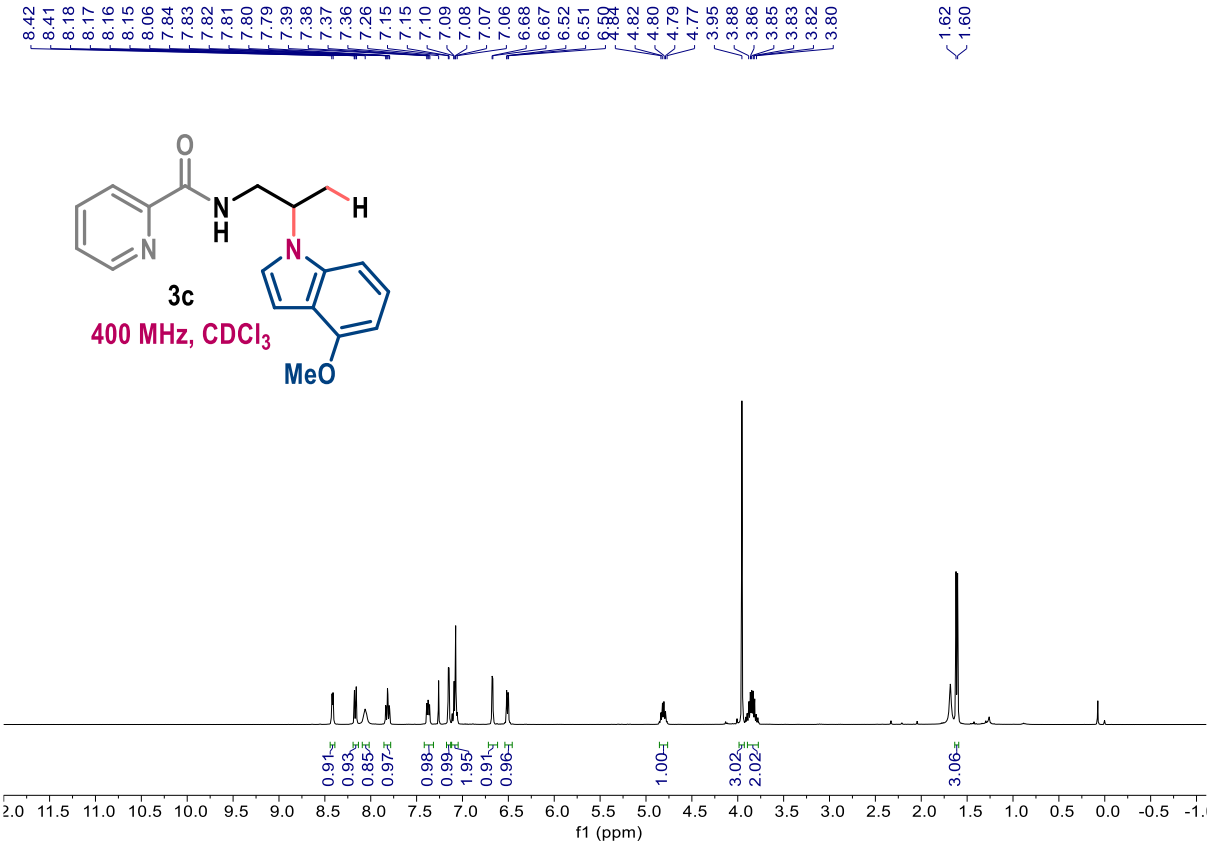
f1 (ppm)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H
N
H
3c
400 MHz, CDCl3
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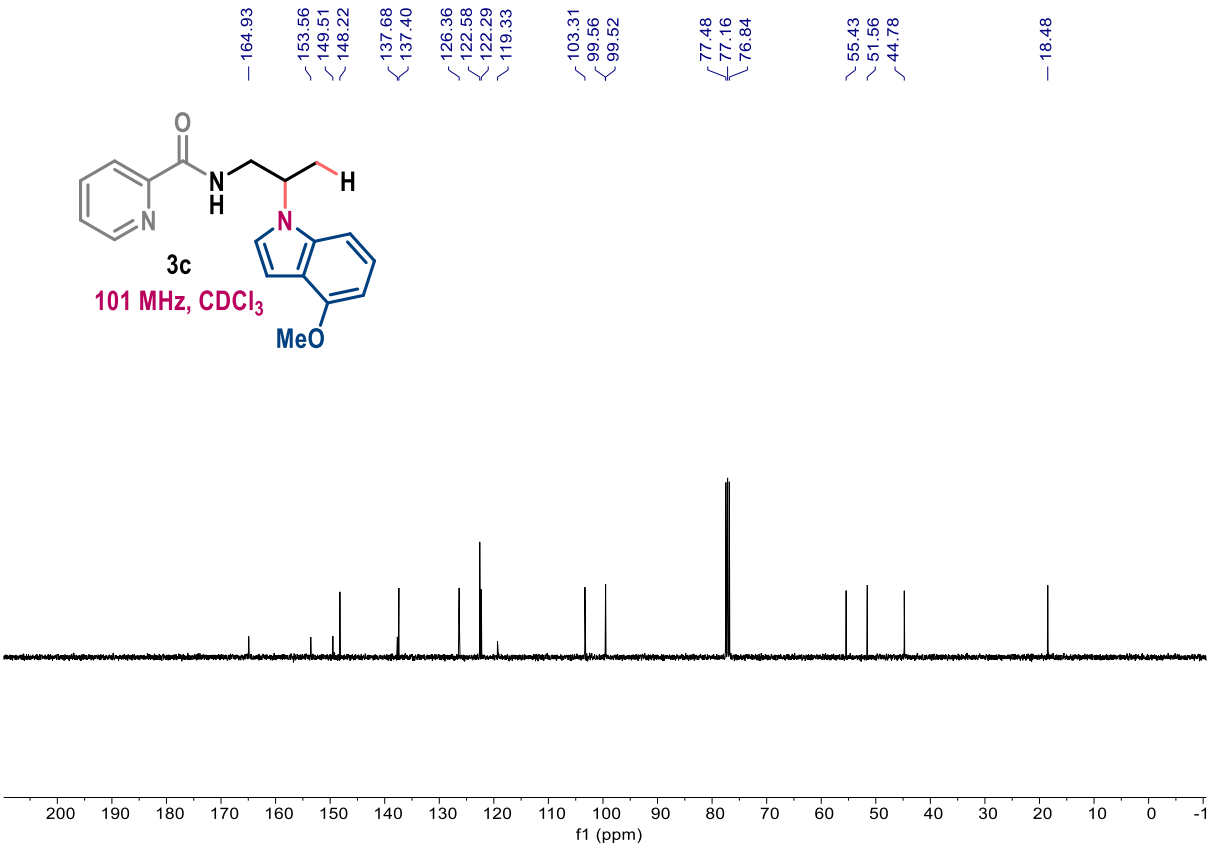
3.06
f1 (ppm)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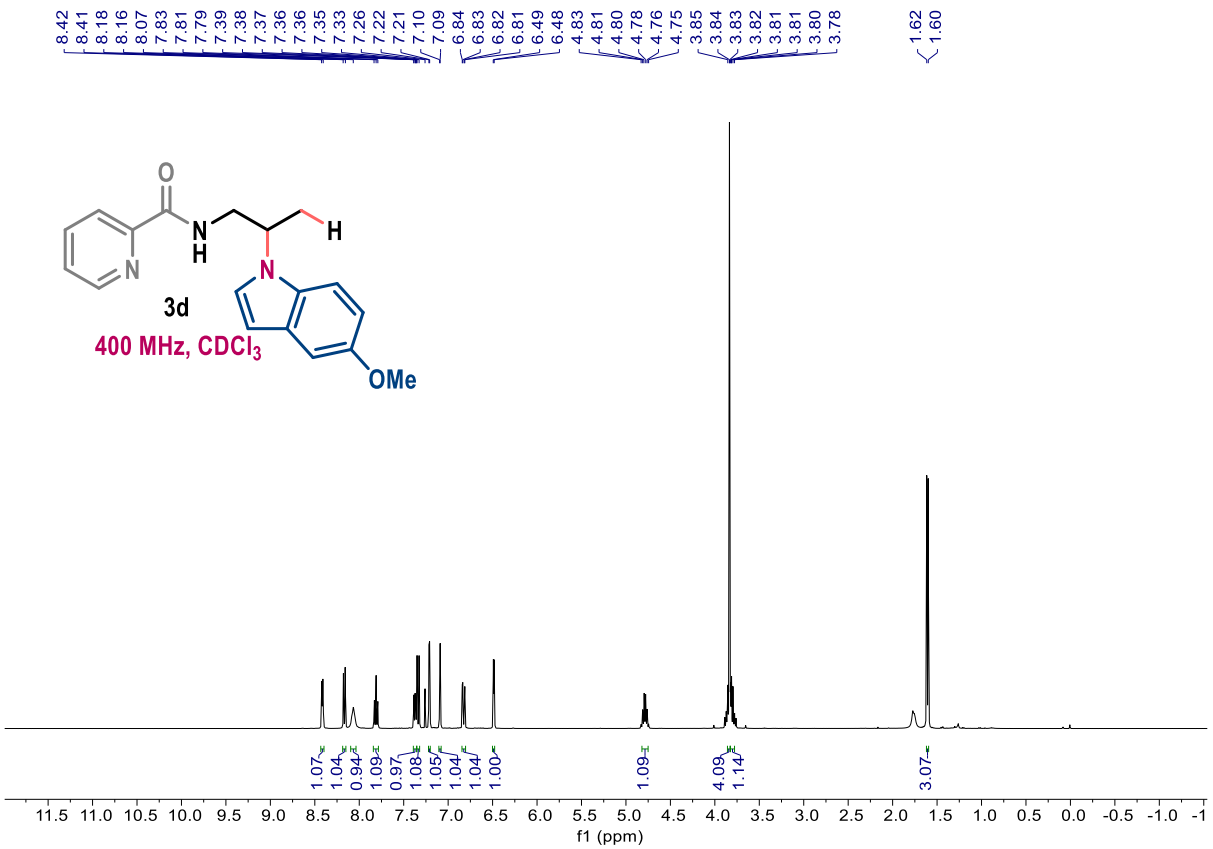
101 MHz, CDCl3
MeO
f1 (ppm)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3d
400 MHz, CDCl3
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1.08
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1.09
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1.14
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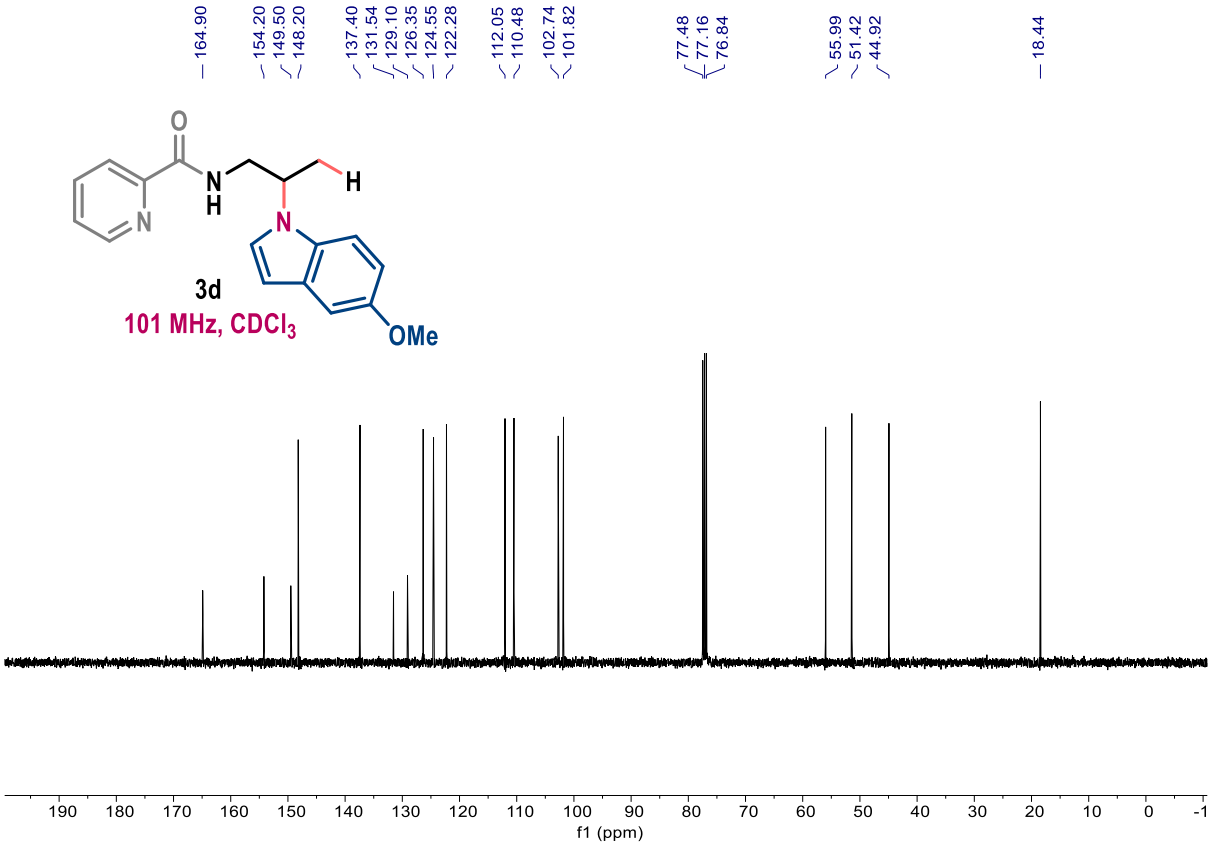
f1 (ppm)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44.92
18.44
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N
H
N
H
3d
101 MHz, CDCl3
OMe
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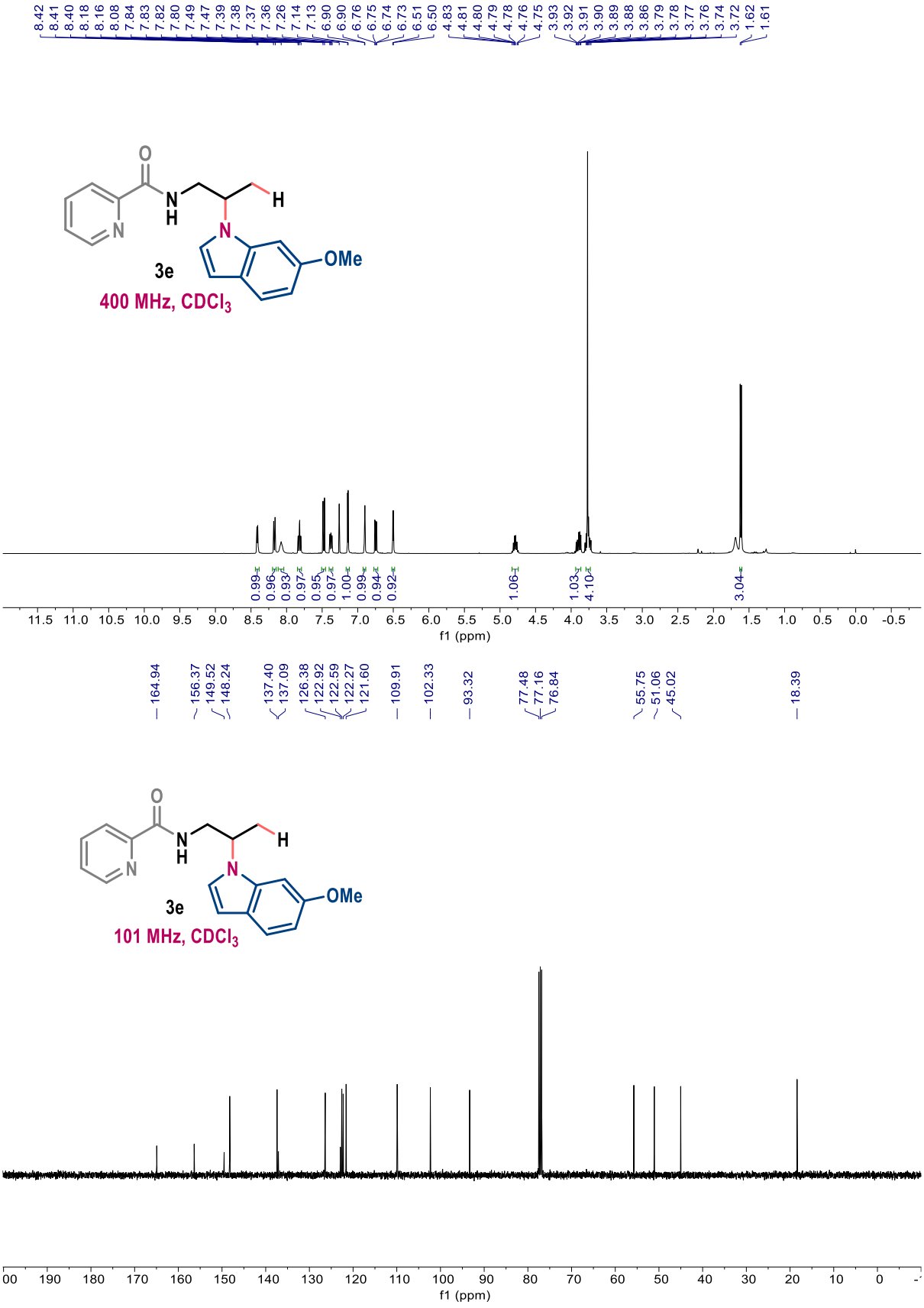
f1 (ppm)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O
N
H
N
H
N
OMe
3e
400 MHz, CDCl3
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11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
164.94 156.37 149.52 148.24 137.40 137.09 126.38 122.92 122.59 122.27 121.60 109.91 102.33 93.32 77.48 77.16 76.84 55.75 51.06 45.02 18.39
O
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N
OMe
3e
101 MHz, CDCl3
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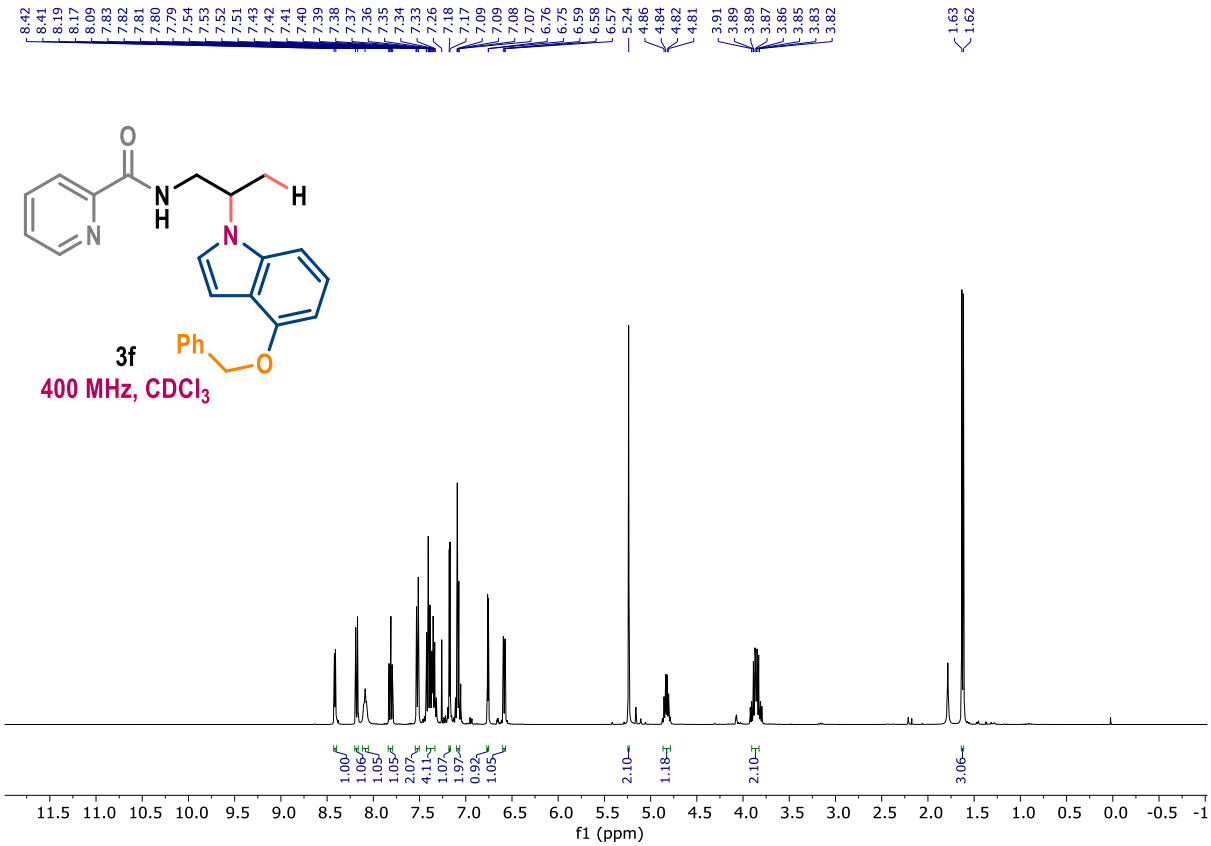
f1 (ppm)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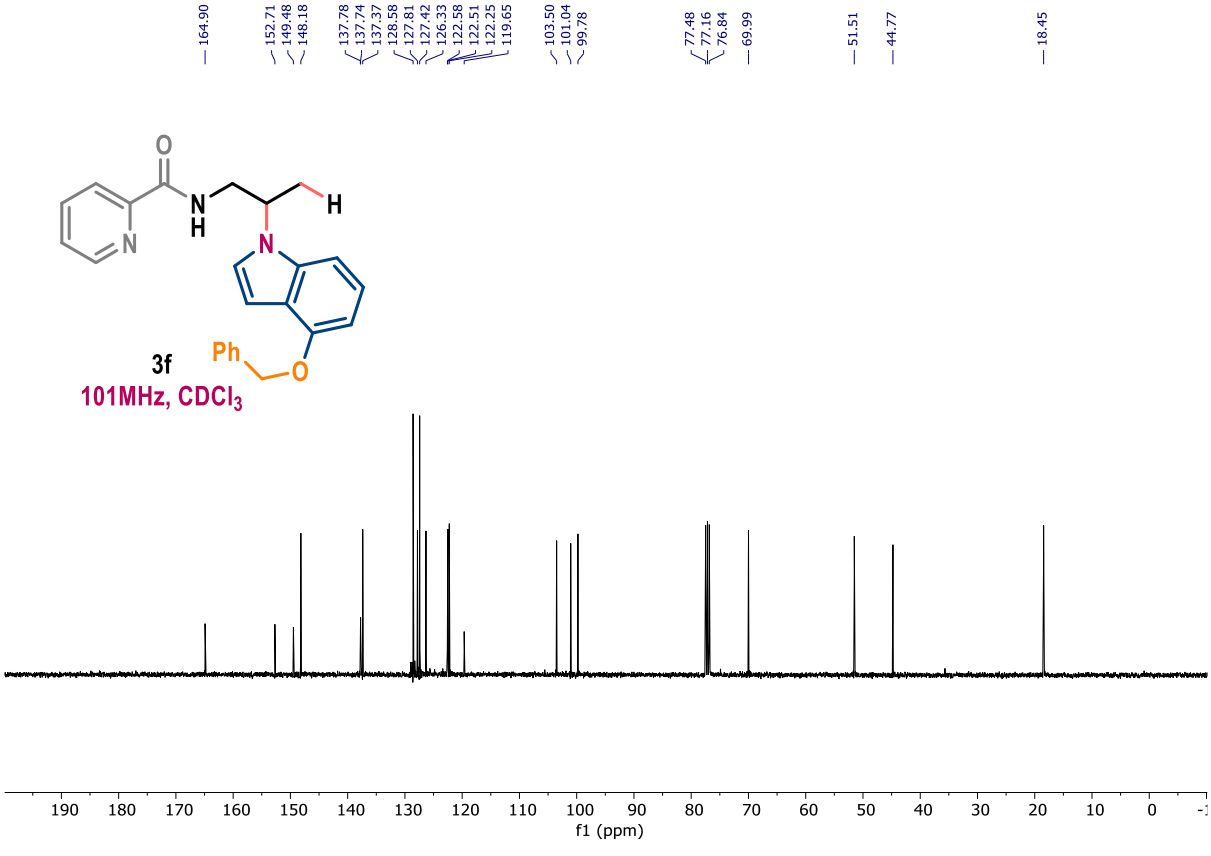
O
N
H
N
H
Ph
O
3f
400 MHz, CDCl3
1.00 1.06 1.05 1.05 2.07 4.11 1.07 1.97 0.92 1.05 2.10 1.18 2.10 3.06
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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H
Ph
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3f
101MHz, CDCl3
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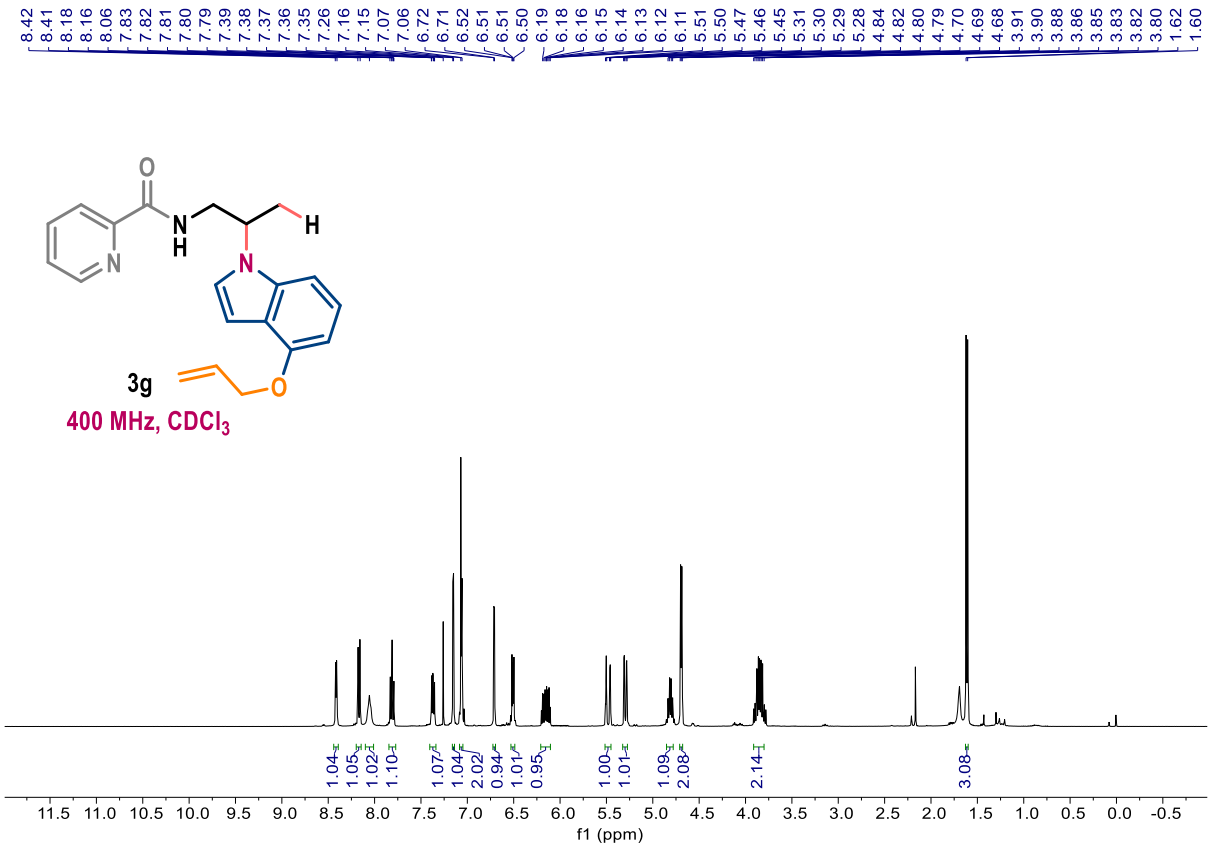
f1 (ppm)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400 MHz, CDCl3
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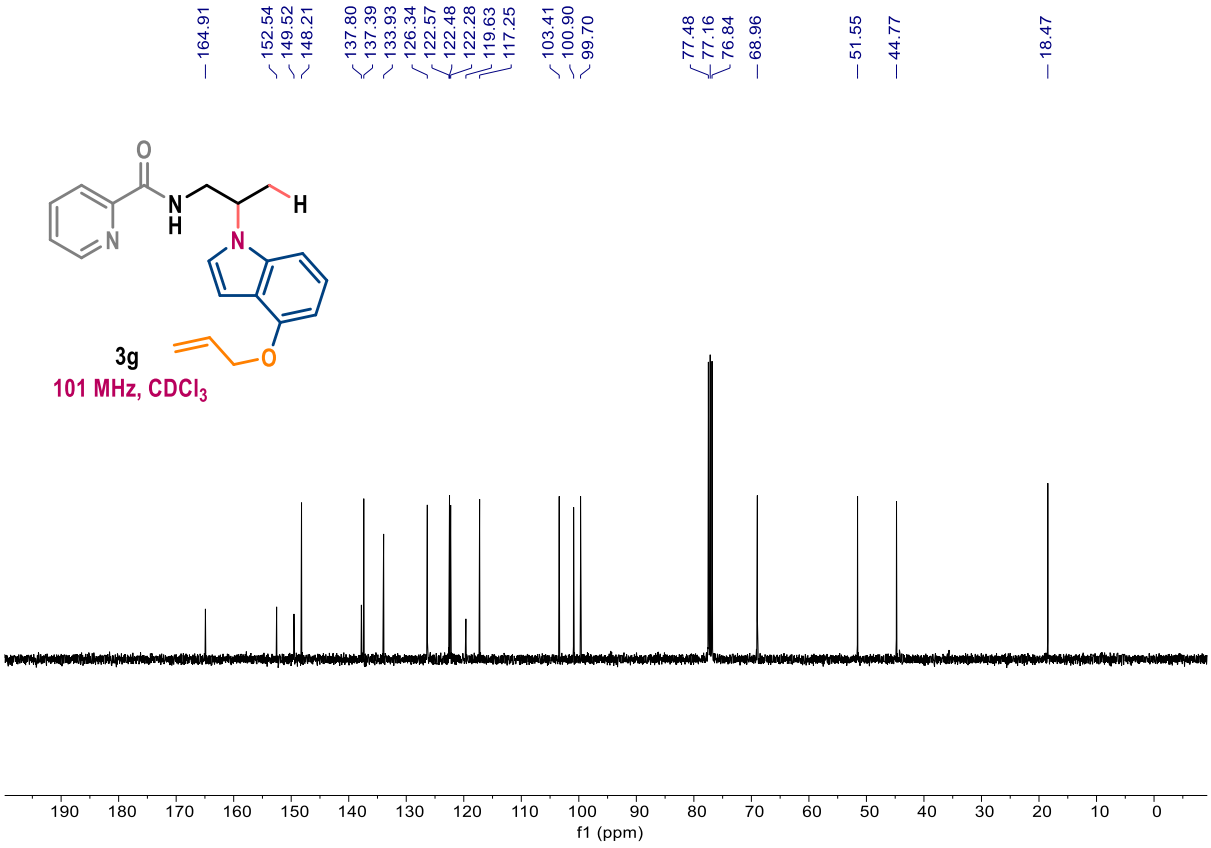
f1 (ppm)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101 MHz, CDCl3
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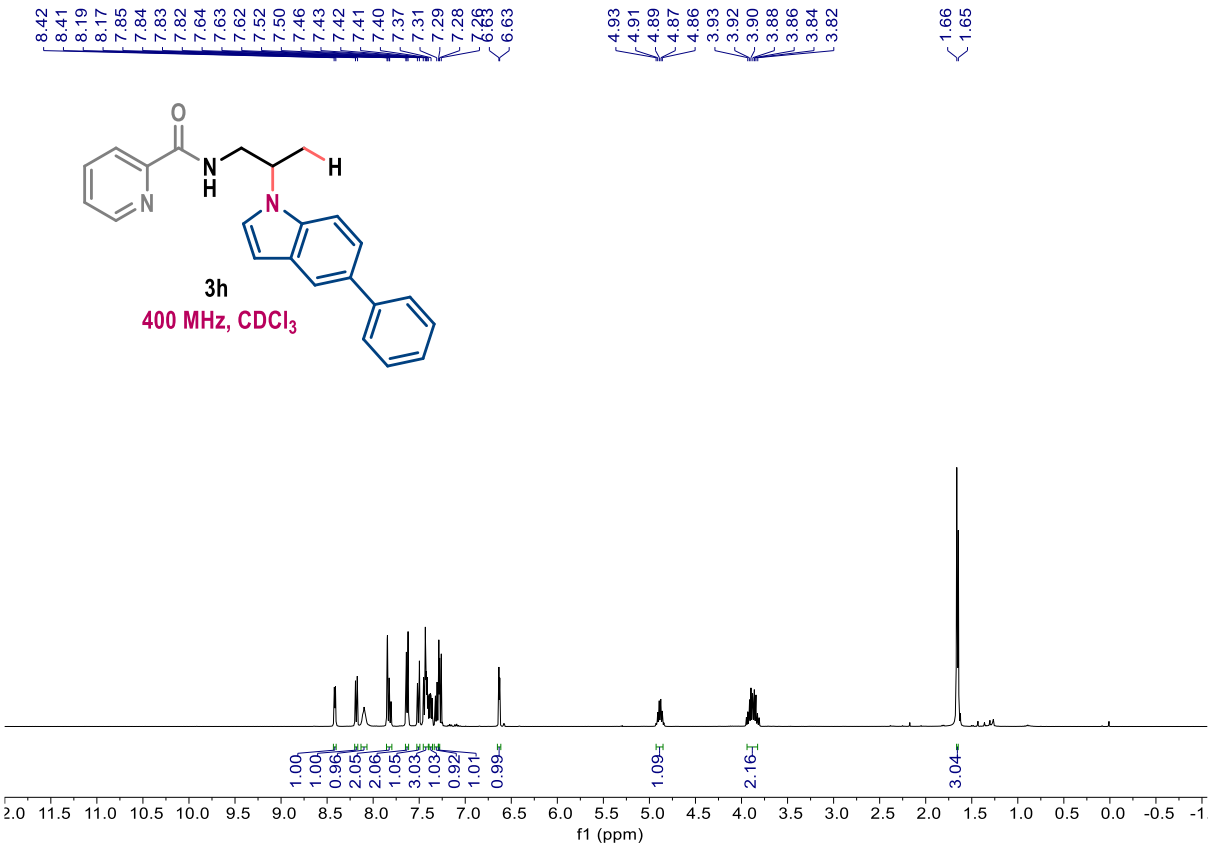
f1 (ppm)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3.86
3.84
3.82
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O
N
H
N
H
3h
400 MHz, CDCl3
1.00
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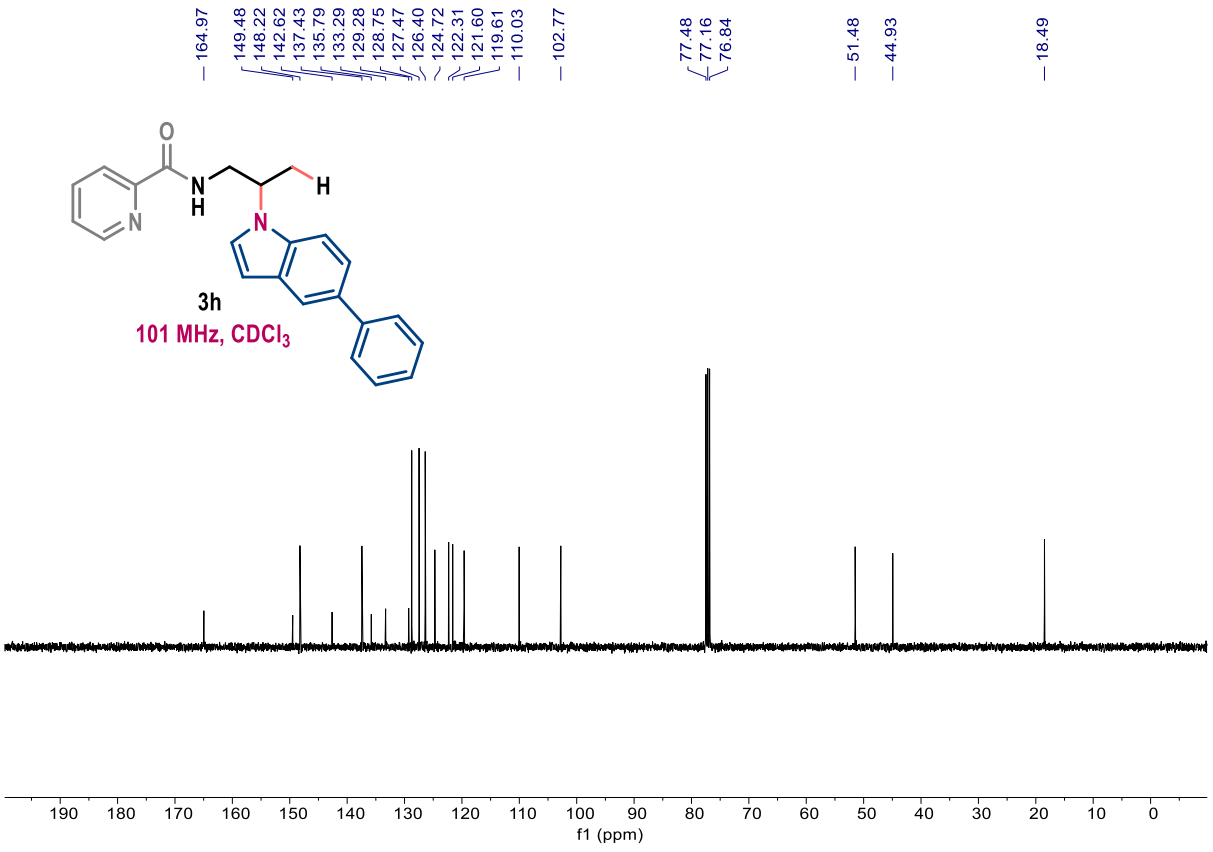
0.96
2.05
2.06
1.05
3.03
1.03
0.92
1.01
0.99
1.09
2.16
3.04
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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3h
101 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.45
8.45
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8.22
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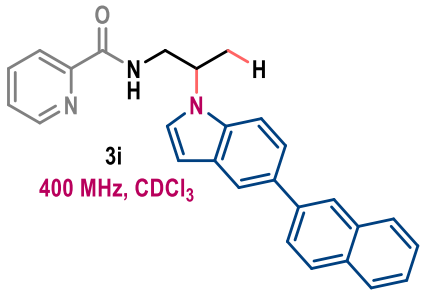
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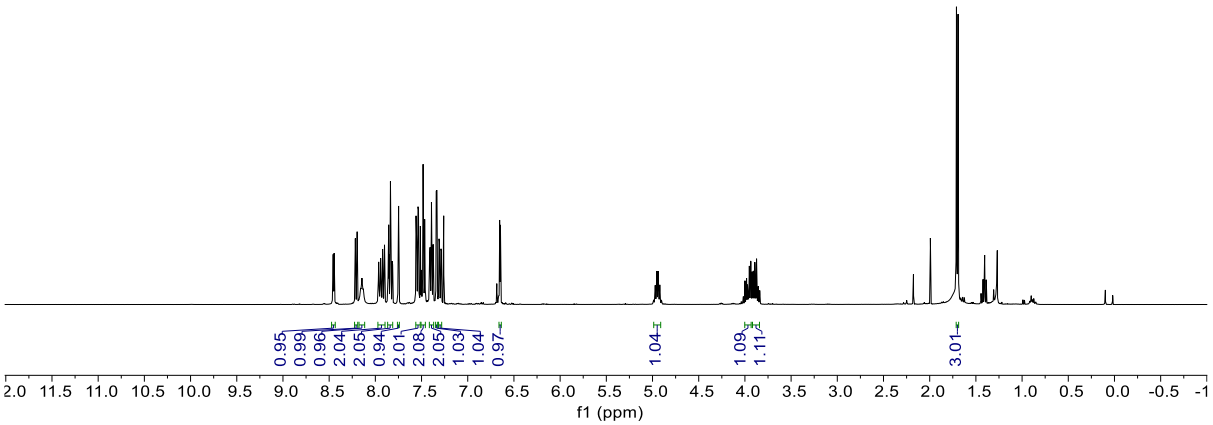
400 MHz, CDCl3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1.09
1.11
3.01
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


164.97
149.51
148.20
141.52
137.45
135.64
133.95
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128.76
128.26
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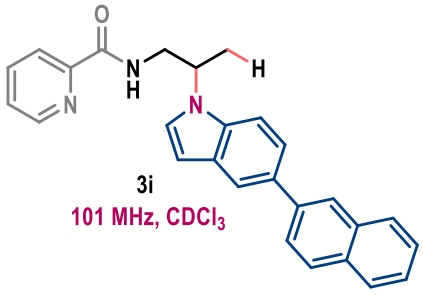
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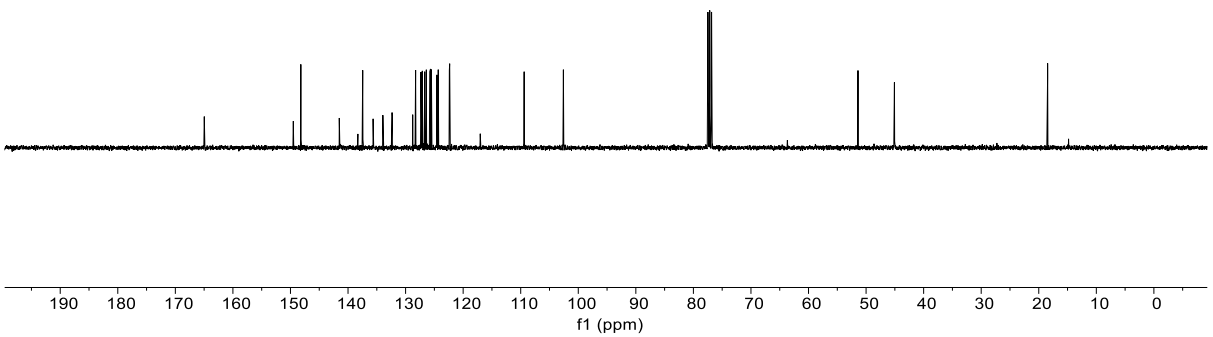
3i
101 MHz, CDCl3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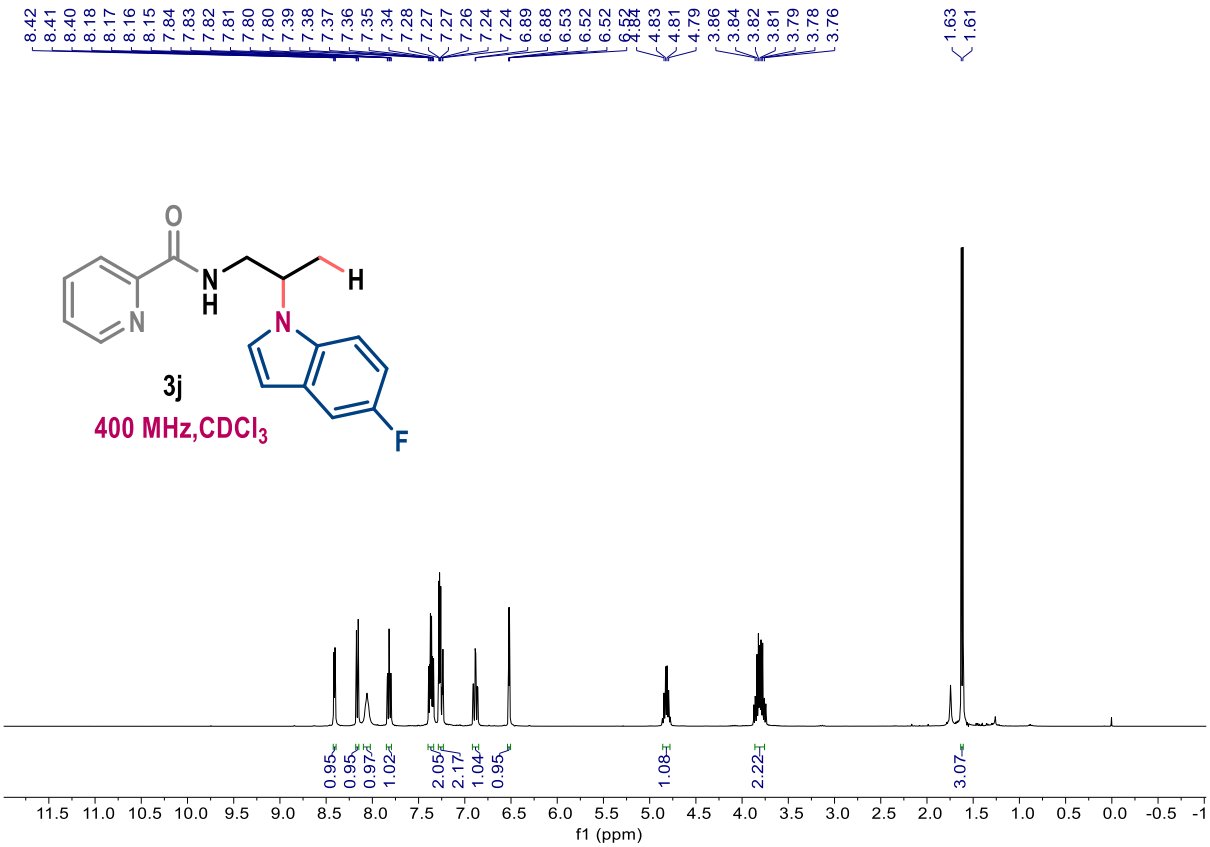
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F
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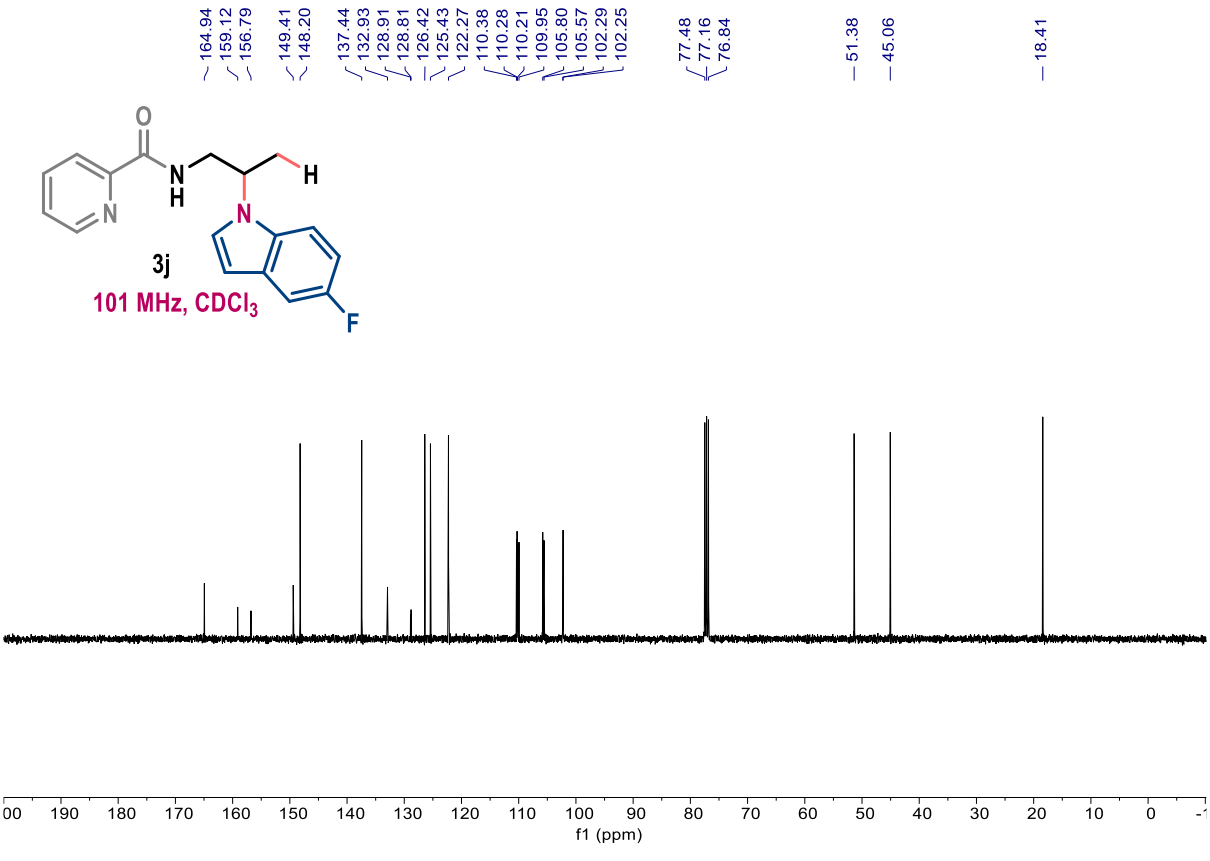
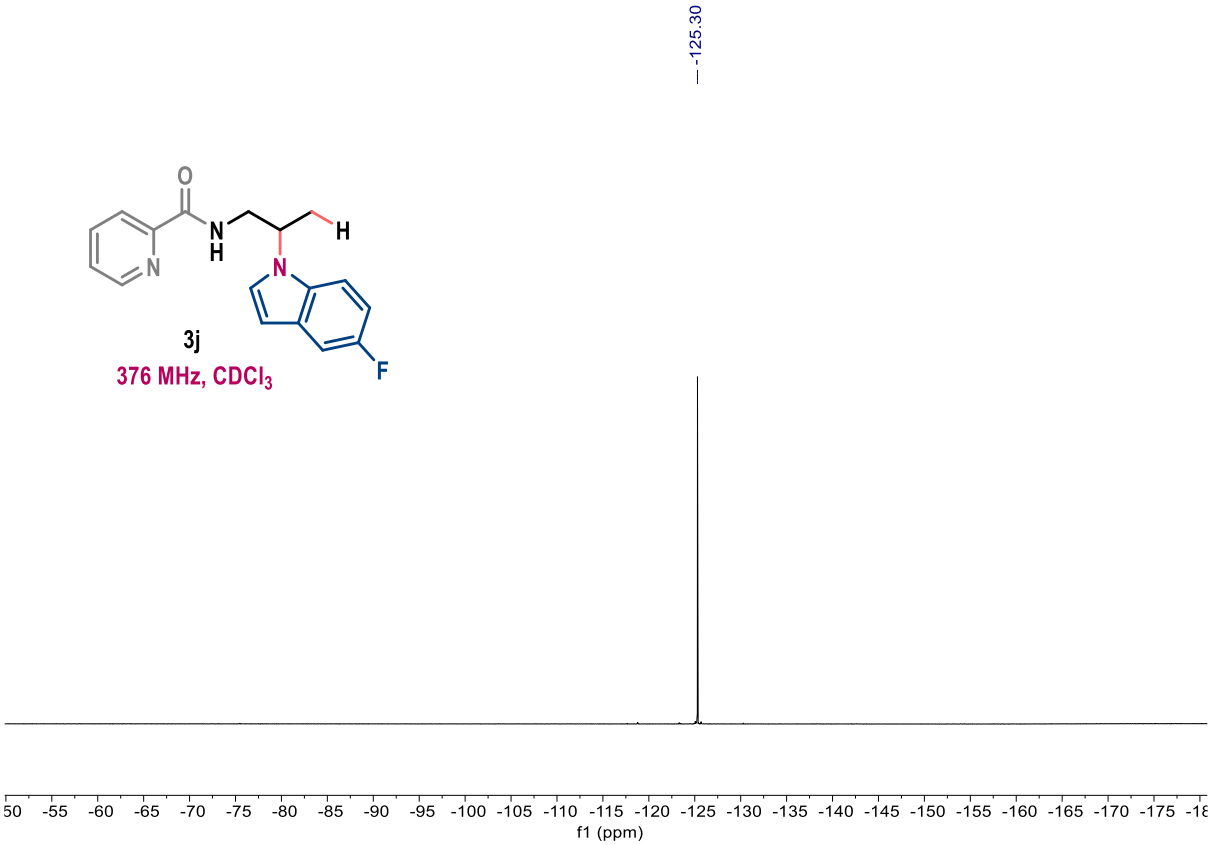
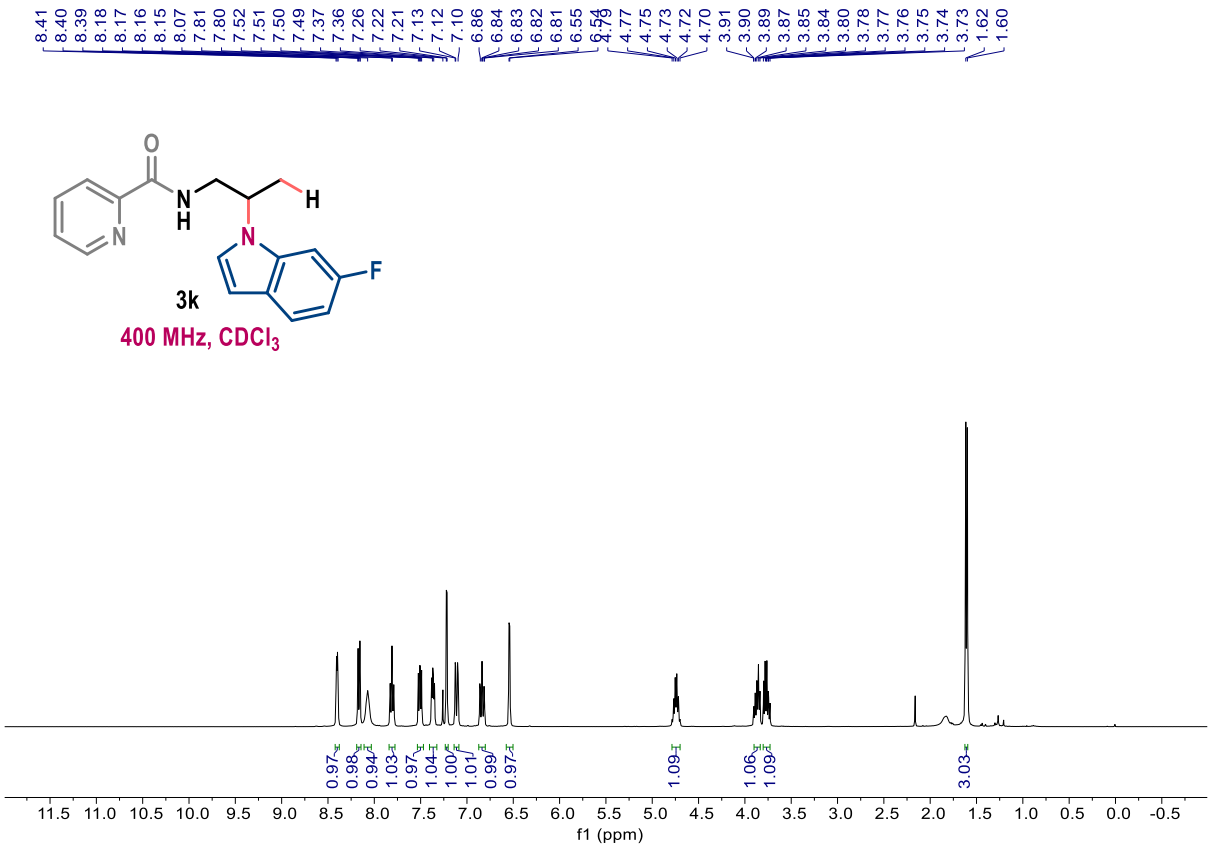
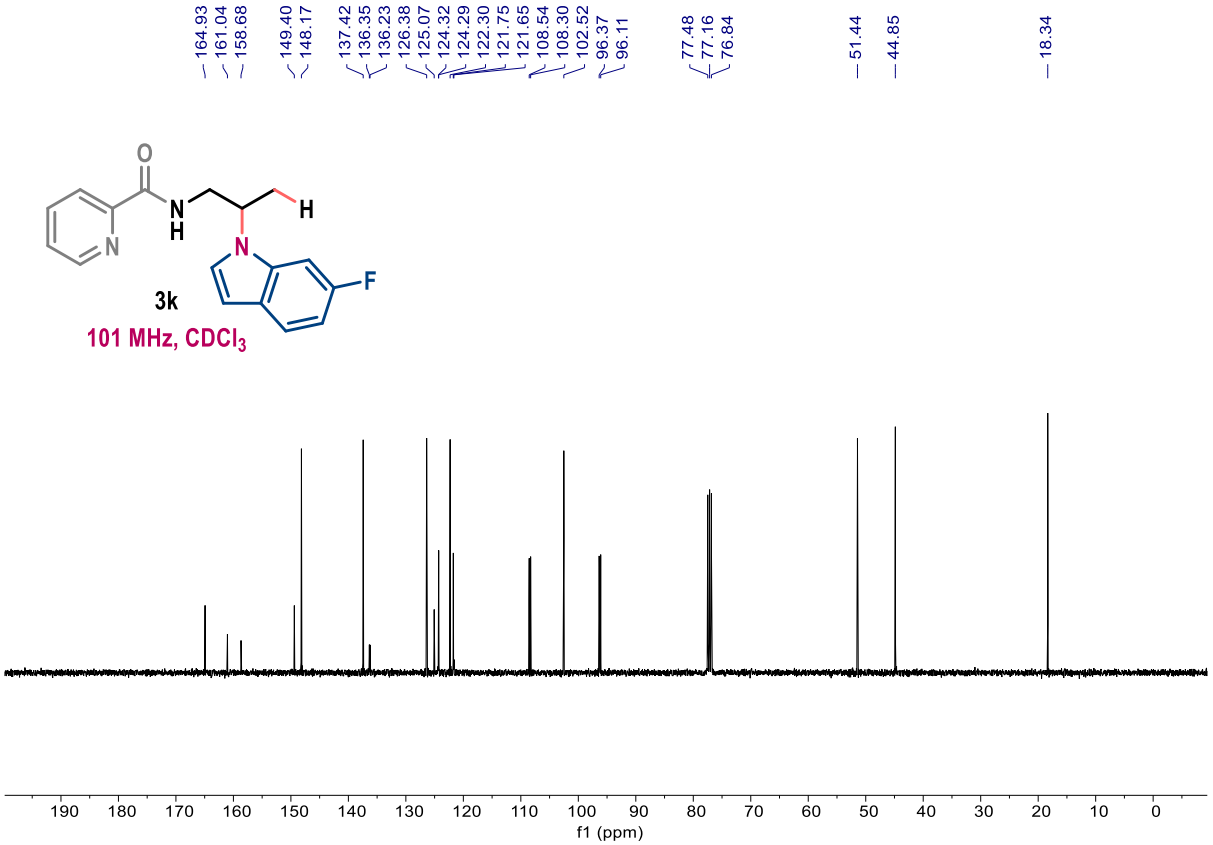
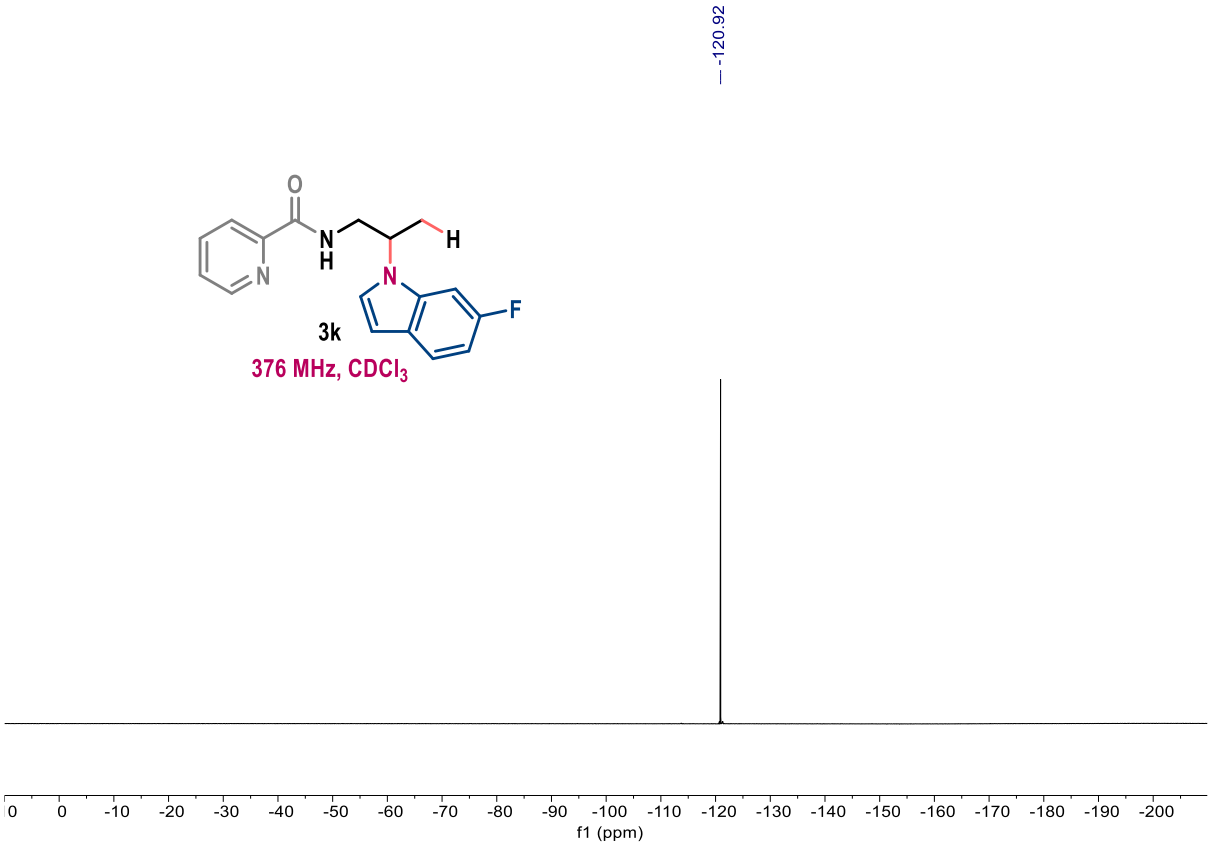
0.97
1.02
2.05
2.17
1.04
0.95
1.08
2.22
3.07
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

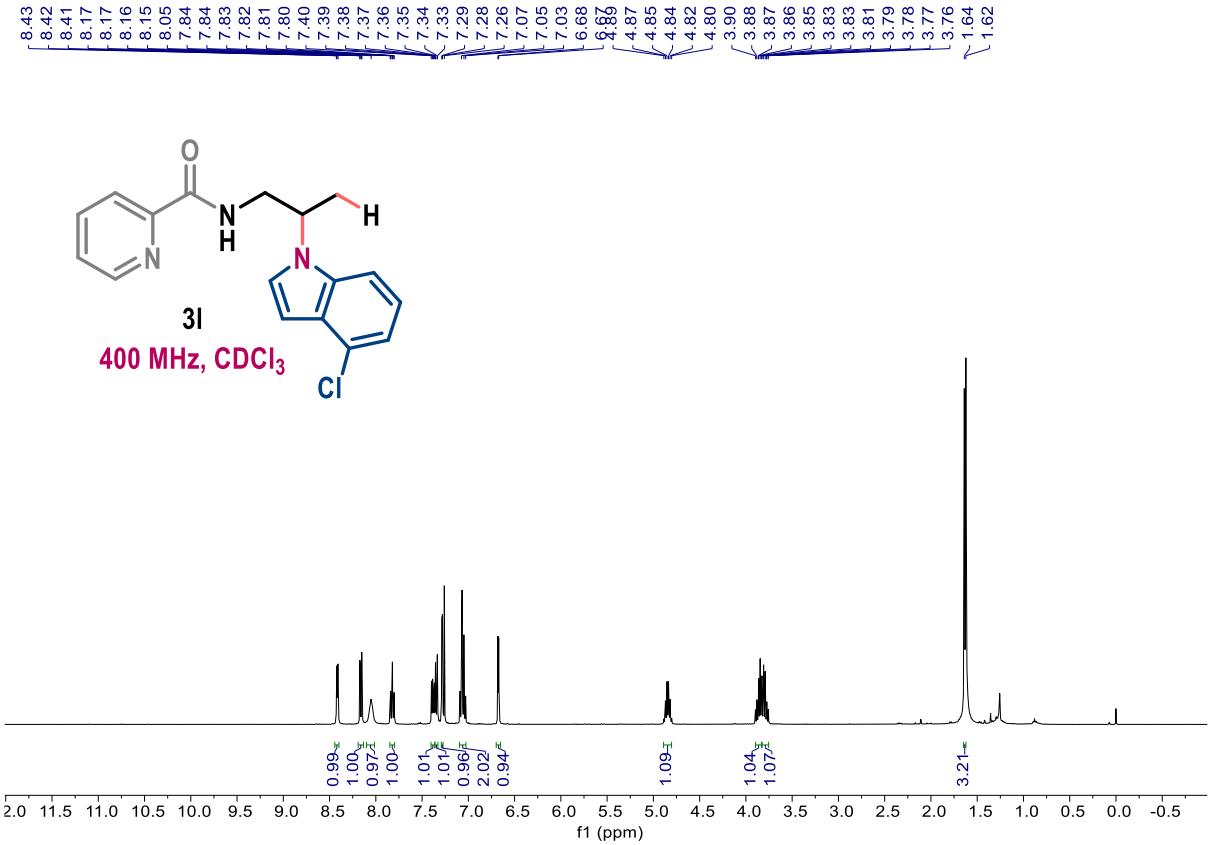

164.94
159.12
156.79
149.41
148.20
137.44
132.93
128.91
128.81
126.42
125.43
122.27
110.38
110.28
110.21
109.95
105.80
105.57
102.29
102.25
77.48
77.16
76.84
51.38
45.06
18.41
O
N
H
N
H
3j
101 MHz, CDCl3
F
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

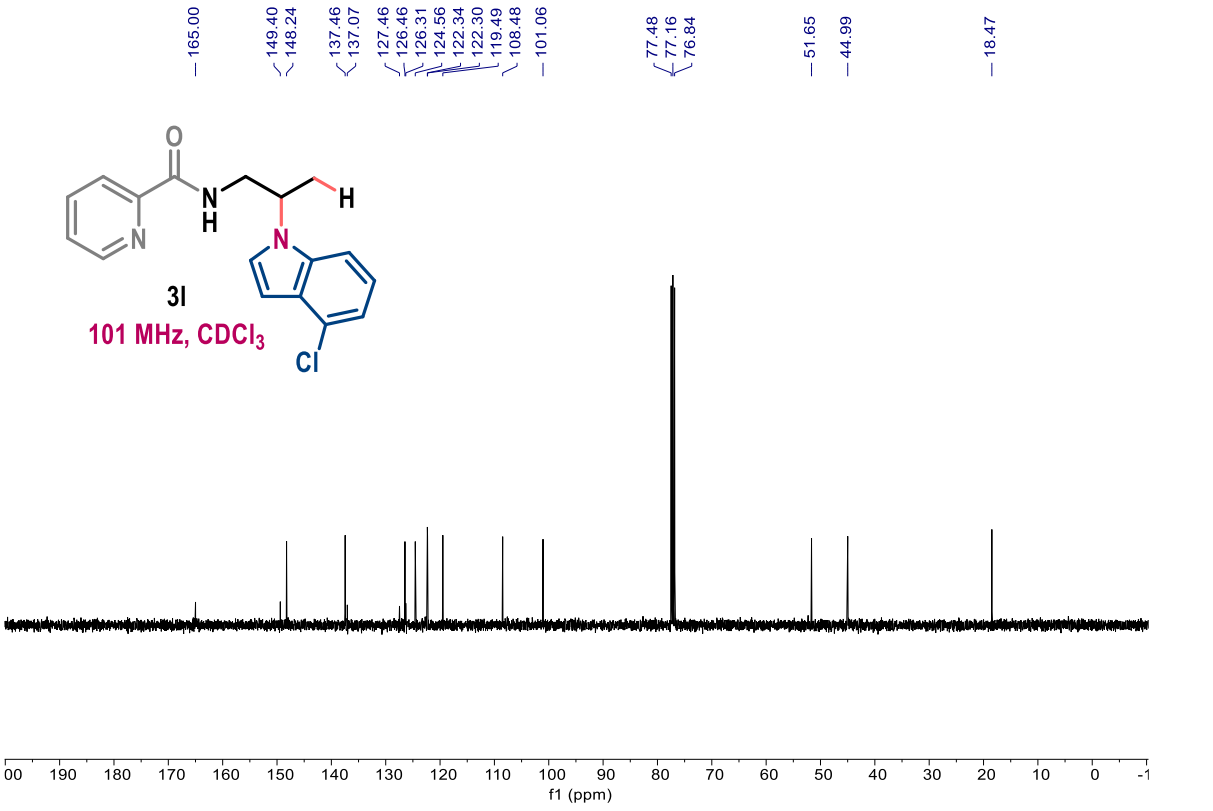

-125.30
3j
376 MHz, CDCl3
f1 (ppm)

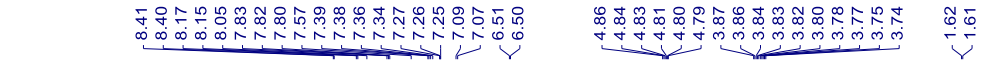

3k
400 MHz, CDCl3
f1 (ppm)

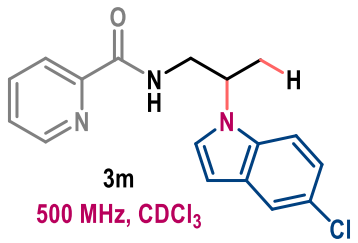

164.93
161.04
158.68
149.40
148.17
137.42
136.35
136.23
126.38
125.07
124.32
124.29
122.30
121.75
121.65
108.54
108.30
102.52
96.37
96.11
77.48
77.16
76.84
51.44
44.85
18.34
O
N
H
N
H
F
3k
101 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-120.92
O
N
H
N
H
F
3k
376 MHz, CDCl3
0 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


8.43 8.42 8.41 8.17 8.17 8.16 8.15 8.05 7.84 7.84 7.83 7.82 7.81 7.80 7.40 7.39 7.38 7.37 7.36 7.35 7.34 7.33 7.29 7.28 7.26 7.07 7.05 7.03 6.68 6.67 4.89 4.87 4.85 4.84 4.82 4.80 3.90 3.88 3.87 3.86 3.85 3.83 3.81 3.79 3.78 3.77 3.76 1.64 1.62
O
N
H
N
H
N
Cl
3l
400 MHz, CDCl3
0.99 1.00 0.97 1.00 1.01 1.01 0.96 2.02 0.94 1.09 1.04 1.07 3.21
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

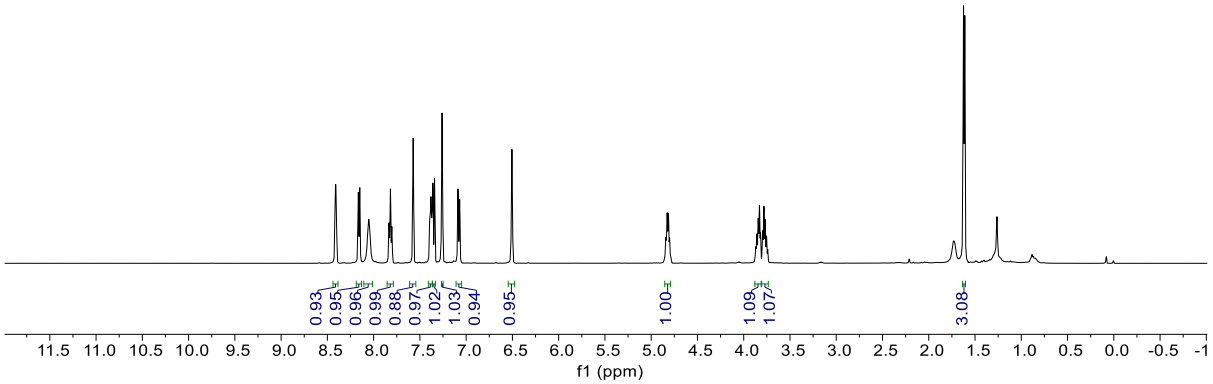

165.00 149.40 148.24 137.46 137.07 127.46 126.46 126.31 124.56 122.34 122.30 119.49 108.48 101.06 77.48 77.16 76.84 51.65 44.99 18.47
O
N
H
N
H
N
Cl
3l
101 MHz, CDCl3
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

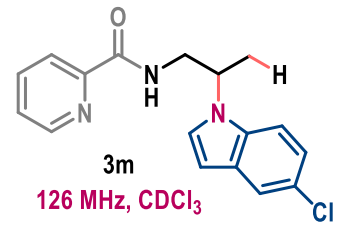




3m

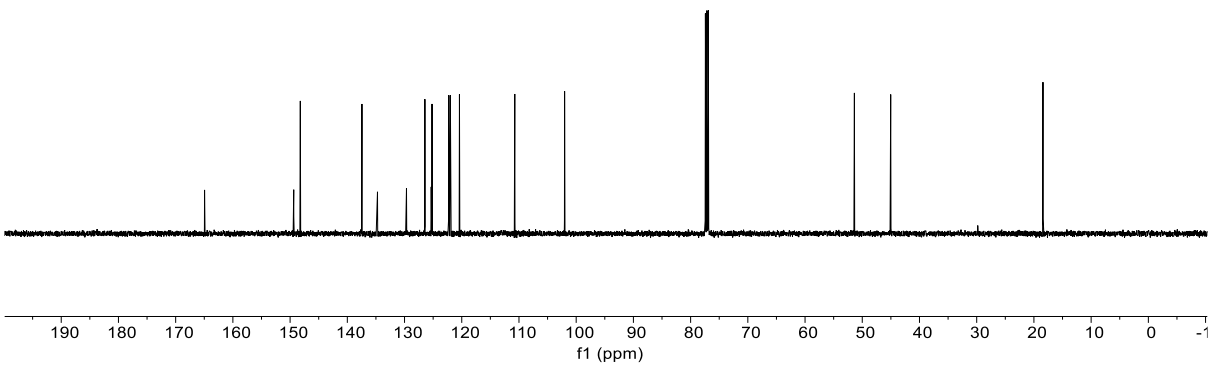
500 MHz, $CDCl_3$

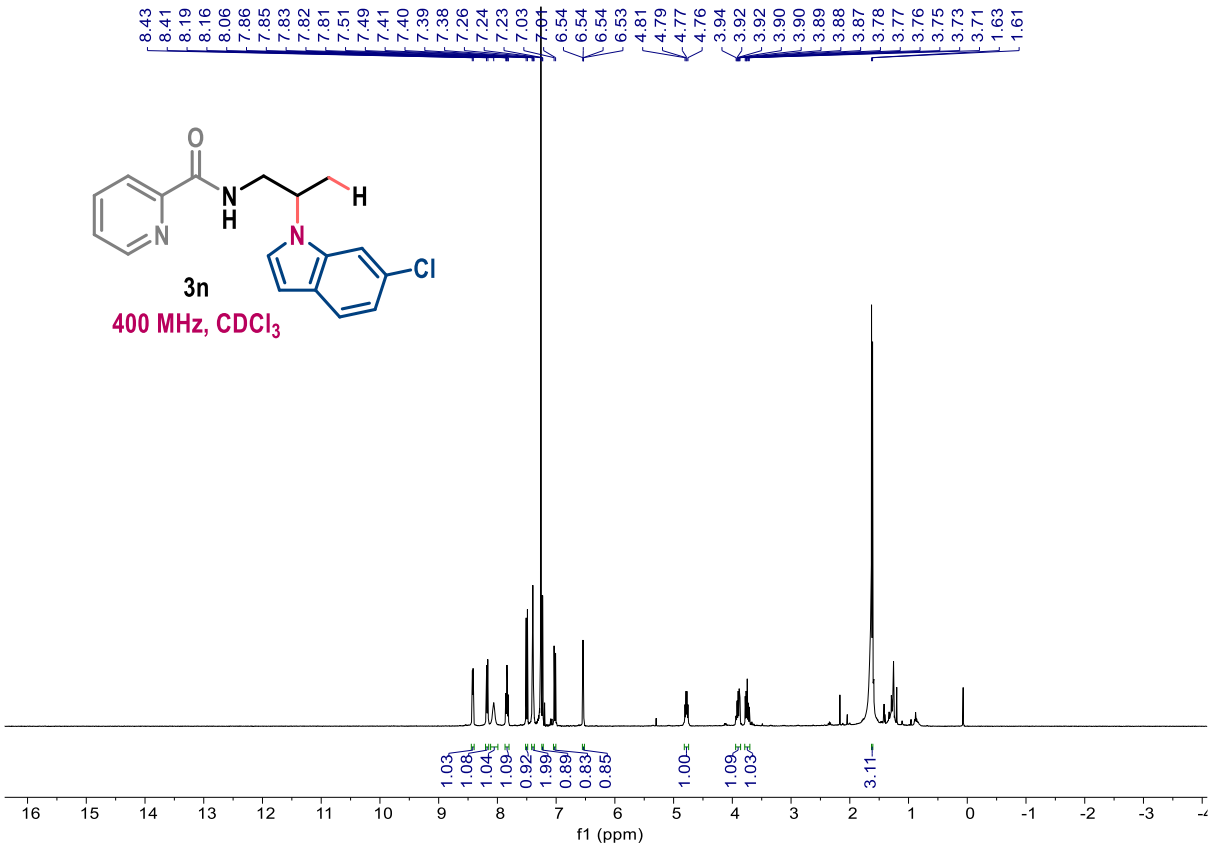


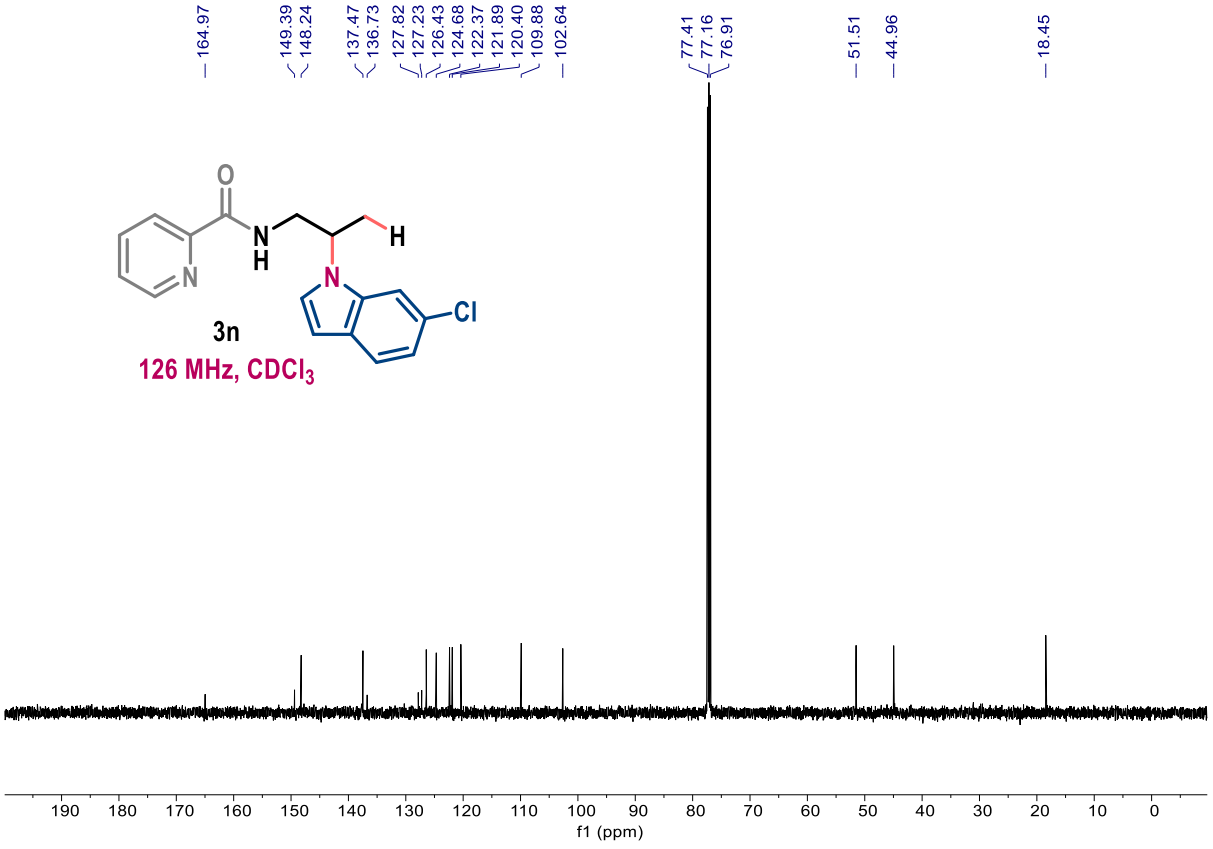


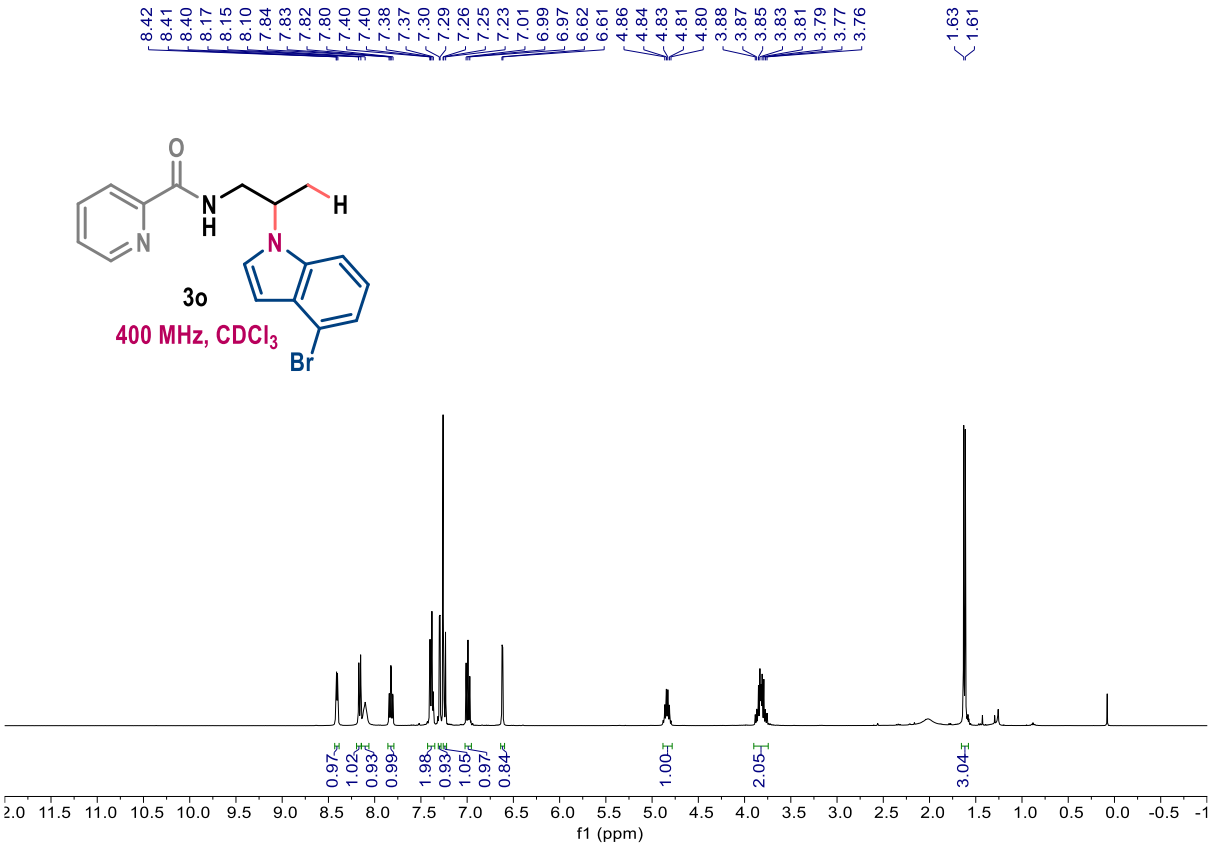
3m

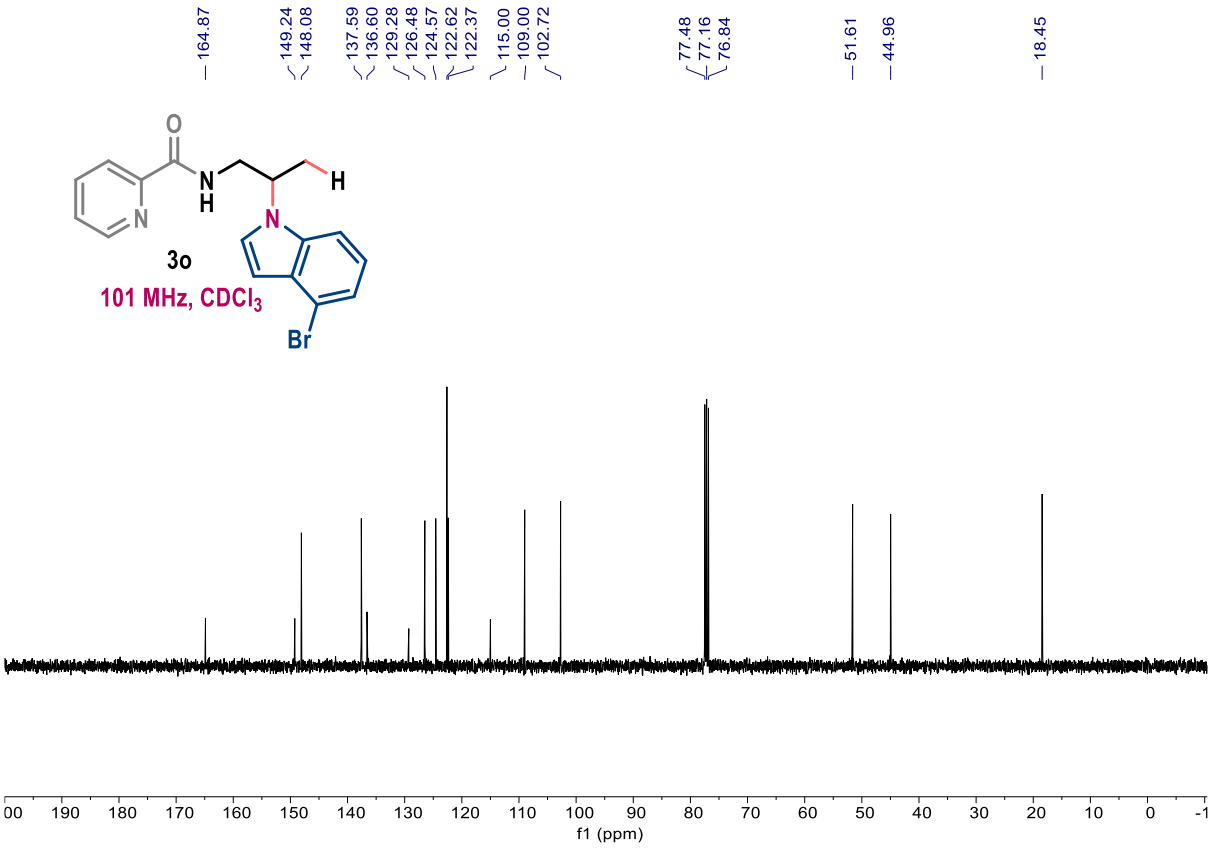
126 MHz, $CDCl_3$

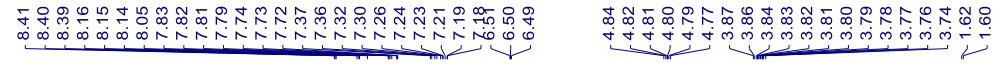


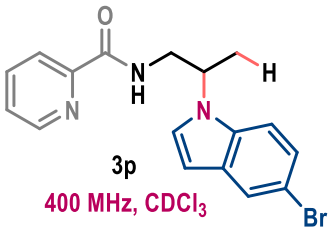

8.43
8.41
8.19
8.16
8.06
7.86
7.85
7.83
7.82
7.81
7.51
7.49
7.41
7.40
7.39
7.38
7.26
7.24
7.23
7.03
7.01
6.54
6.54
6.54
6.53
4.81
4.79
4.77
4.76
3.94
3.92
3.92
3.90
3.90
3.89
3.88
3.87
3.78
3.77
3.76
3.75
3.73
3.71
1.63
1.61
O
N
H
N
H
Cl
3n
400 MHz, CDCl3
1.03
1.08
1.04
1.09
0.92
1.99
0.89
0.83
0.85
1.00
1.09
1.03
3.11
f1 (ppm)


164.97
149.39
148.24
137.47
136.73
127.82
127.23
126.43
124.68
122.37
121.89
120.40
109.88
102.64
77.41
77.16
76.91
51.51
44.96
18.45
O
N
H
N
H
Cl
3n
126 MHz, CDCl3
f1 (ppm)


8.42
8.41
8.40
8.17
8.15
8.10
7.84
7.83
7.82
7.80
7.40
7.40
7.38
7.37
7.30
7.29
7.26
7.25
7.23
7.01
6.99
6.97
6.62
6.61
4.86
4.84
4.83
4.81
4.80
3.88
3.87
3.85
3.83
3.81
3.79
3.77
3.76
1.63
1.61
3o
400 MHz, CDCl3
Br
0.97
1.02
0.93
0.99
1.98
0.93
1.05
0.97
0.84
1.00
2.05
3.04
f1 (ppm)

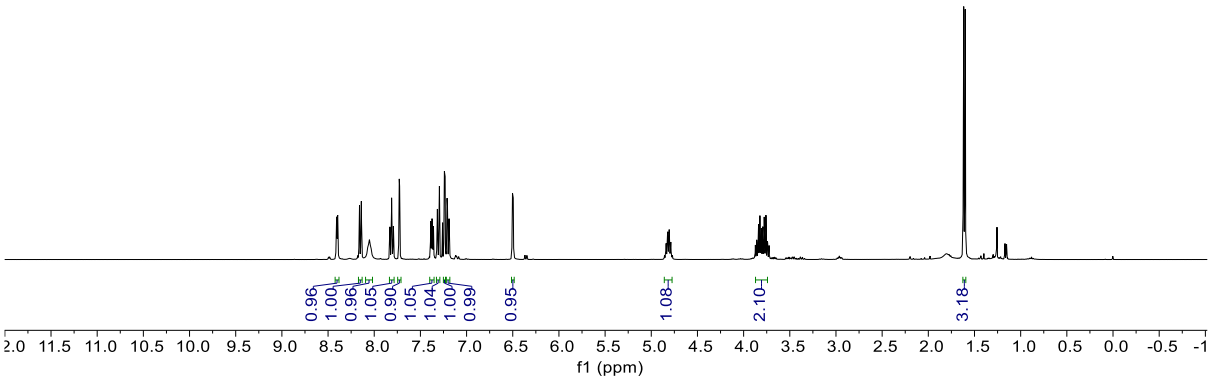

164.87
149.24
148.08
137.59
136.60
129.28
126.48
124.57
122.62
122.37
115.00
109.00
102.72
77.48
77.16
76.84
51.61
44.96
18.45
3o
101 MHz, CDCl3
Br
f1 (ppm)

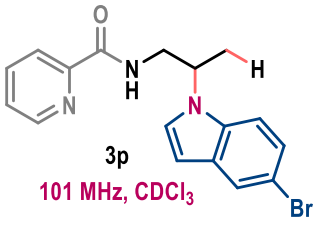




3p

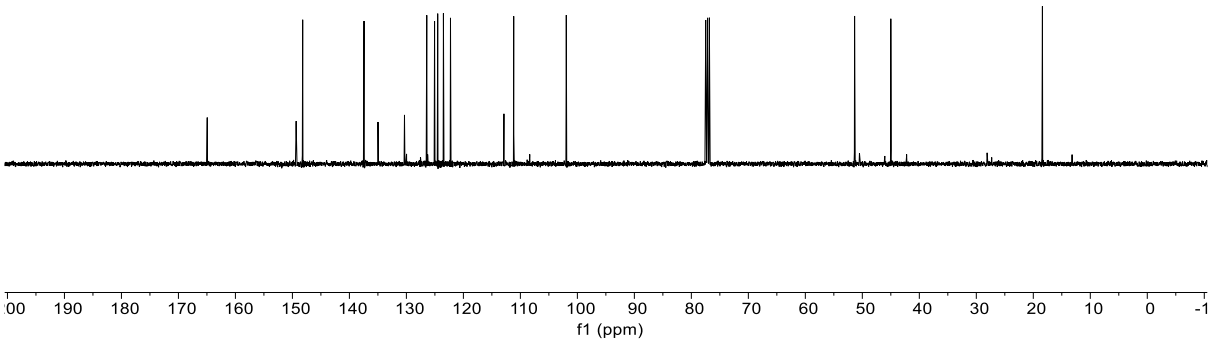
400 MHz, $CDCl_3$





3p

101 MHz, $CDCl_3$




8.39
8.38
8.16
8.14
8.04
7.91
7.90
7.84
7.83
7.82
7.81
7.80
7.79
7.51
7.48
7.39
7.38
7.37
7.36
7.35
7.34
7.33
7.32
7.26
6.66
6.65
4.93
4.91
4.91
4.90
4.89
4.88
3.91
3.90
3.89
3.88
3.88
3.86
3.86
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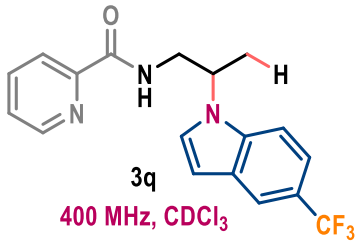
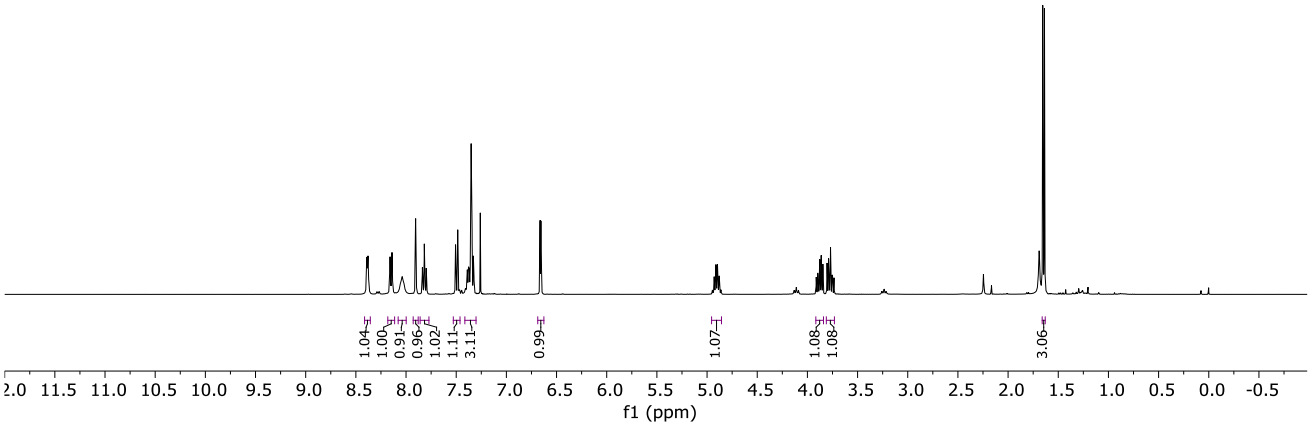
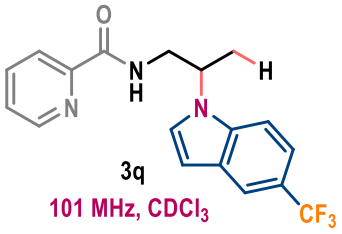
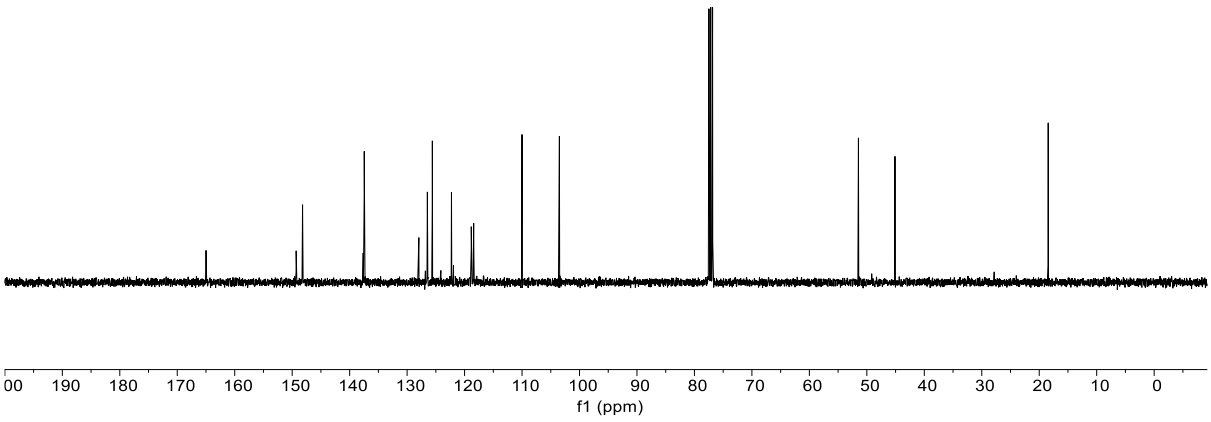
3.80
3.79
3.78
3.77
3.75
3.75
3.74
1.65
1.64

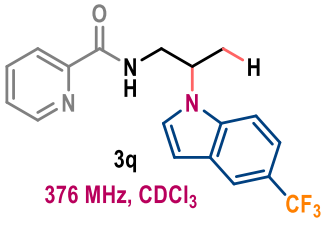

O
N
H
N
H
N
3q
400 MHz, CDCl3
CF3


1.04
1.00
0.91
0.96
1.02
1.11
3.11
0.99
1.07
1.08
1.08
3.06
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


164.99
149.31
148.19
137.64
137.46
127.95
126.82
126.48
125.61
124.12
122.28
121.93
118.88
118.84
118.79
118.75
118.48
118.45
118.42
118.38
110.00
103.50
51.46
45.10
18.44

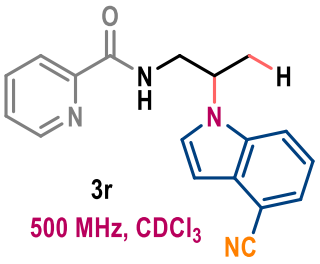

O
N
H
N
H
N
3q
101 MHz, CDCl3
CF3

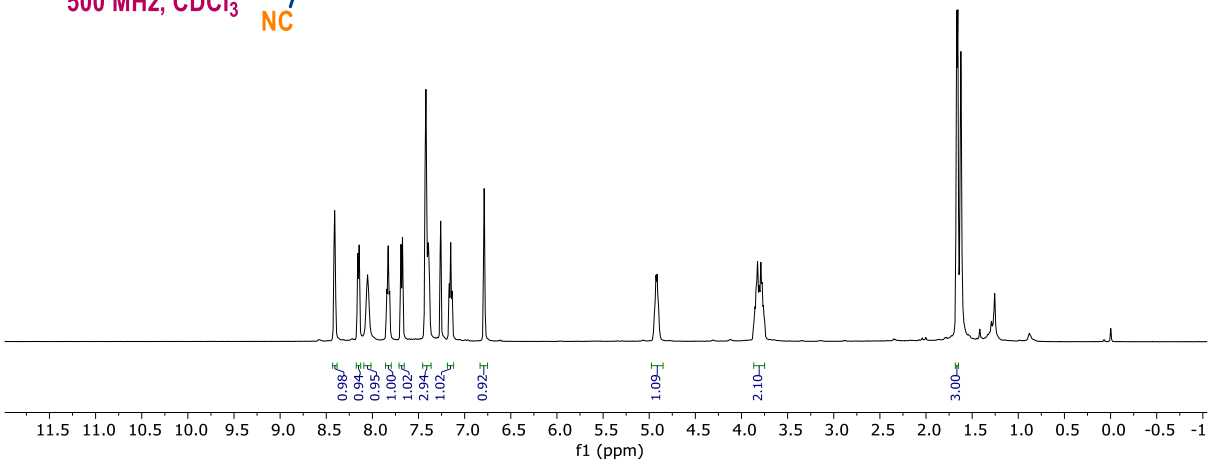

00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

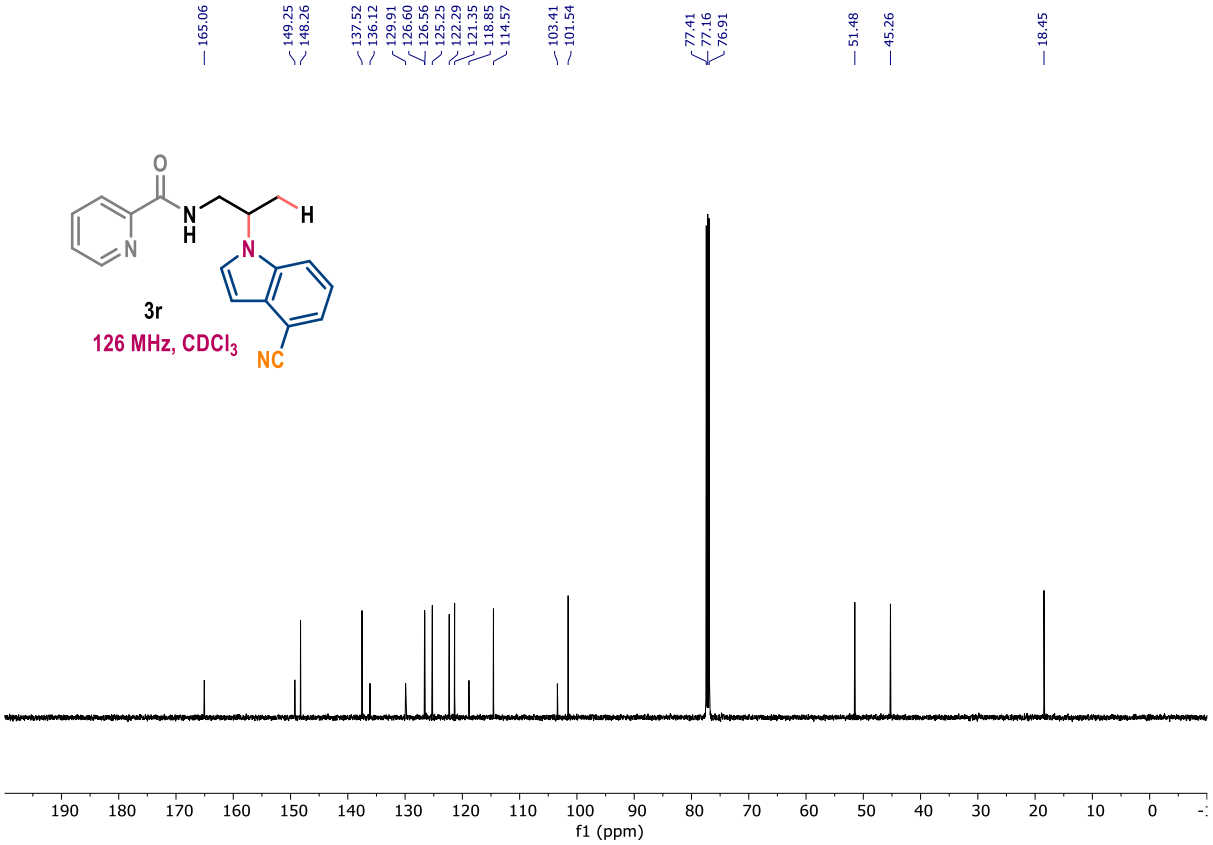

O
N
H
N
H
3q
376 MHz, CDCl3
CF3

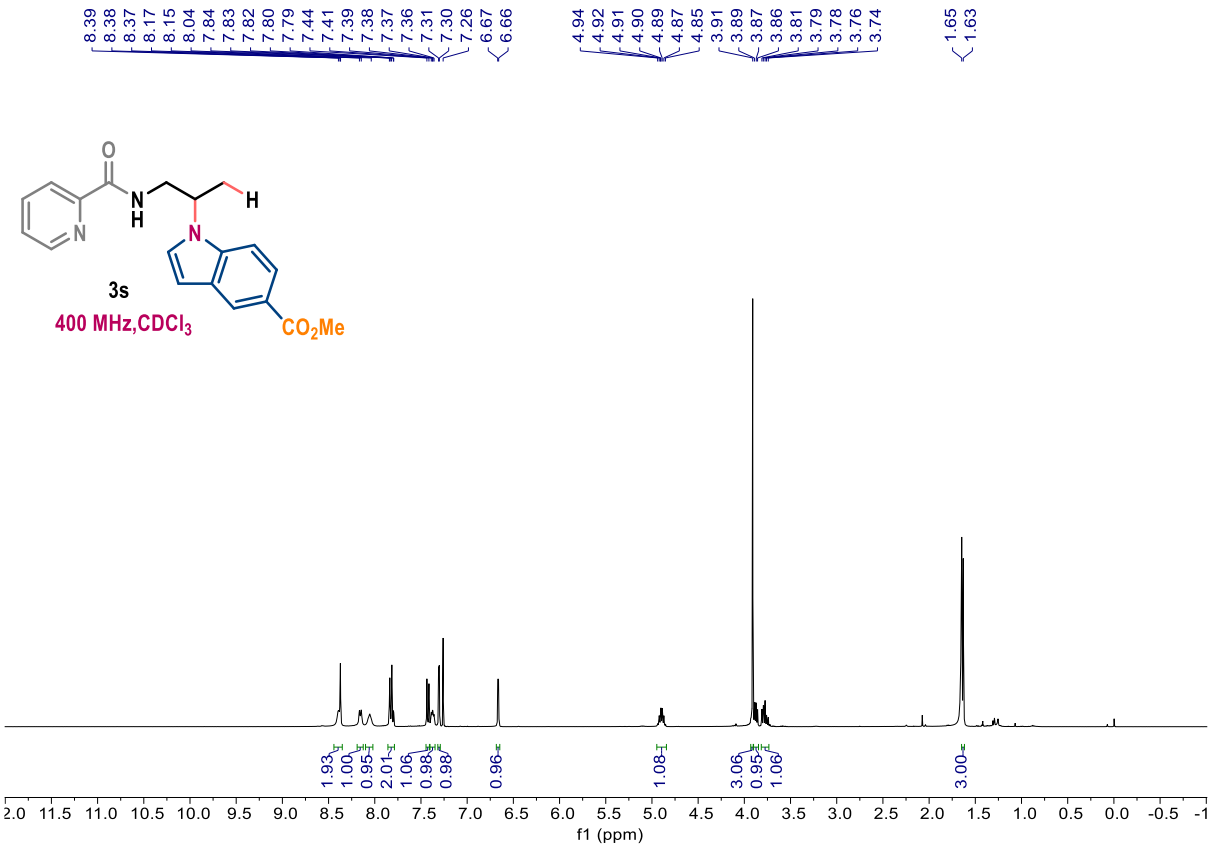
-60.33
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130
f1 (ppm)

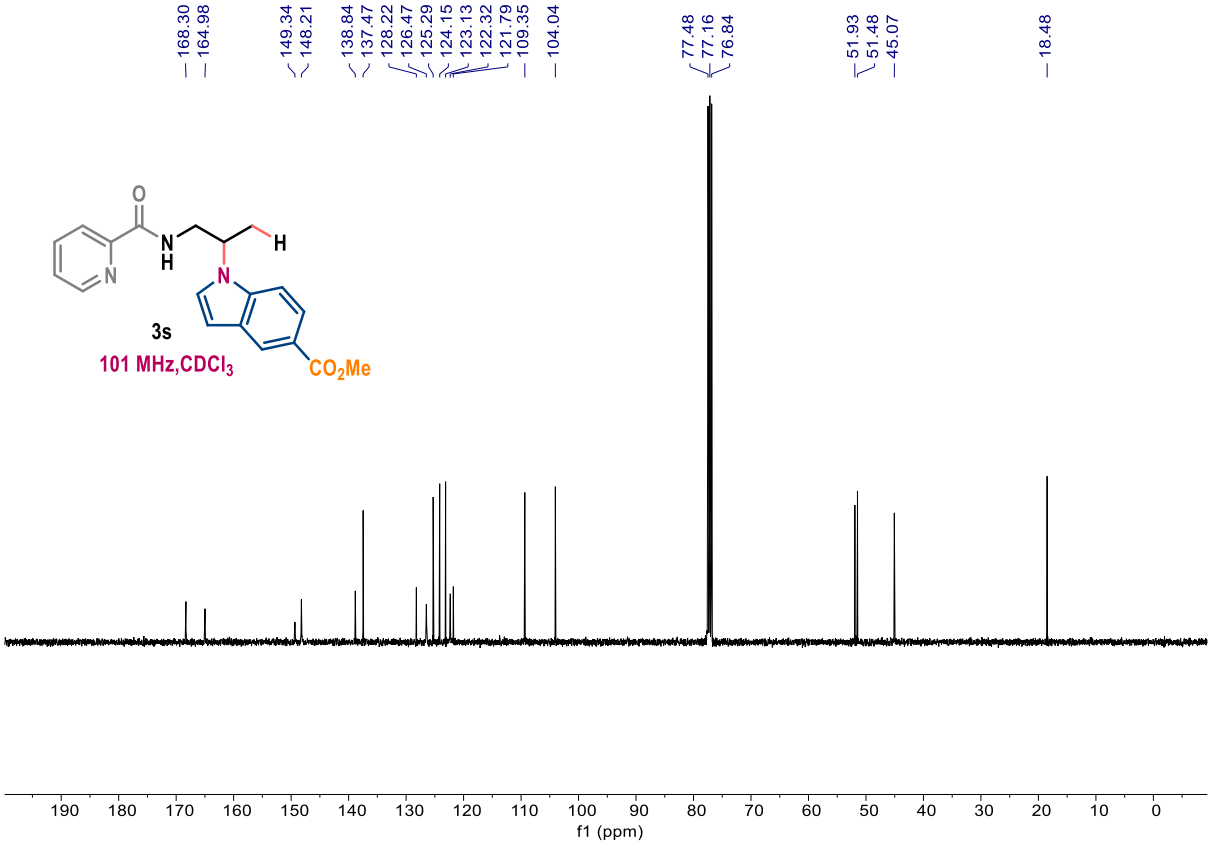

8.42 8.41 8.40 8.16 8.14 8.05 7.85 7.84 7.83 7.81 7.69 7.69 7.68 7.67 7.44 7.43 7.42 7.41 7.40 7.39 7.26 7.17 7.16 7.15 7.14 7.13 6.80 6.78 4.94 4.93 4.91 4.90 3.87 3.86 3.85 3.84 3.83 3.81 3.80 3.79 3.78 3.76 3.75
1.67 1.65

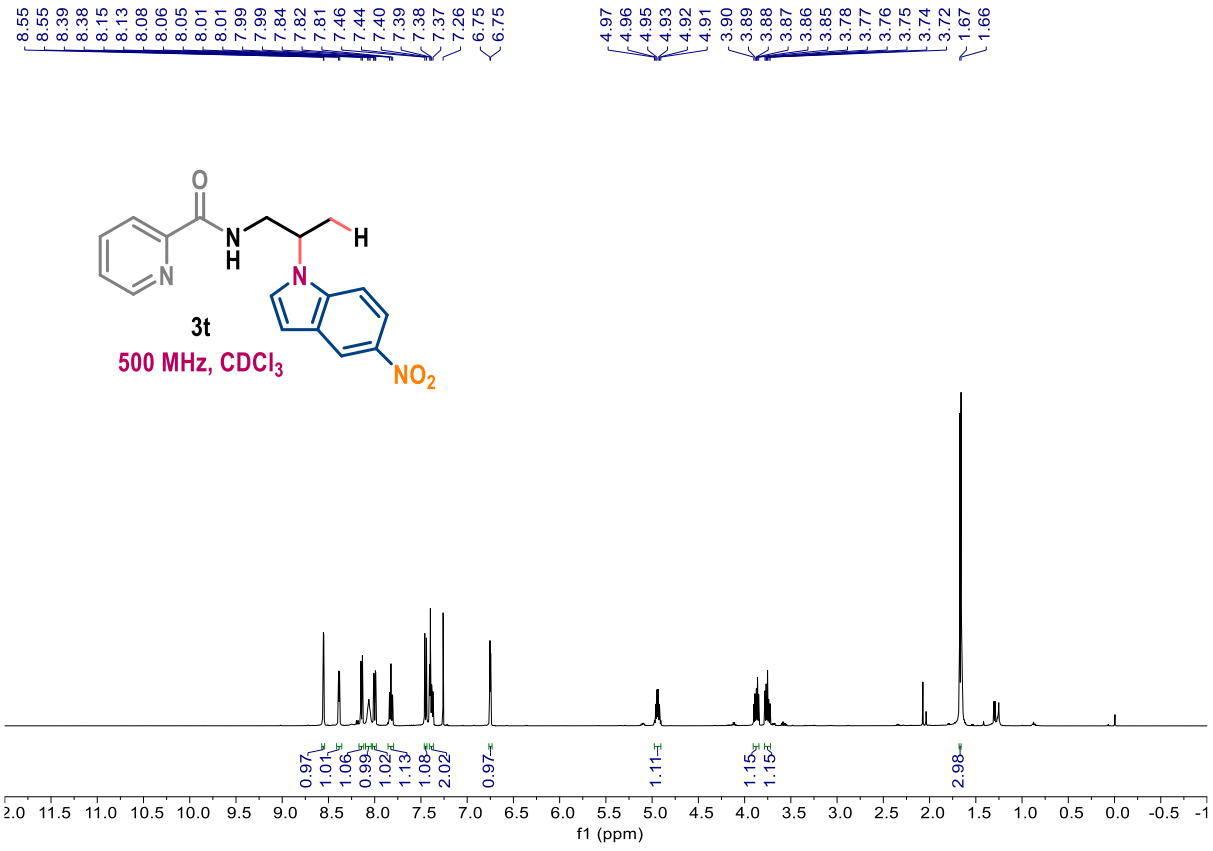

O
N
H
N
H
3r
500 MHz, CDCl3
NC

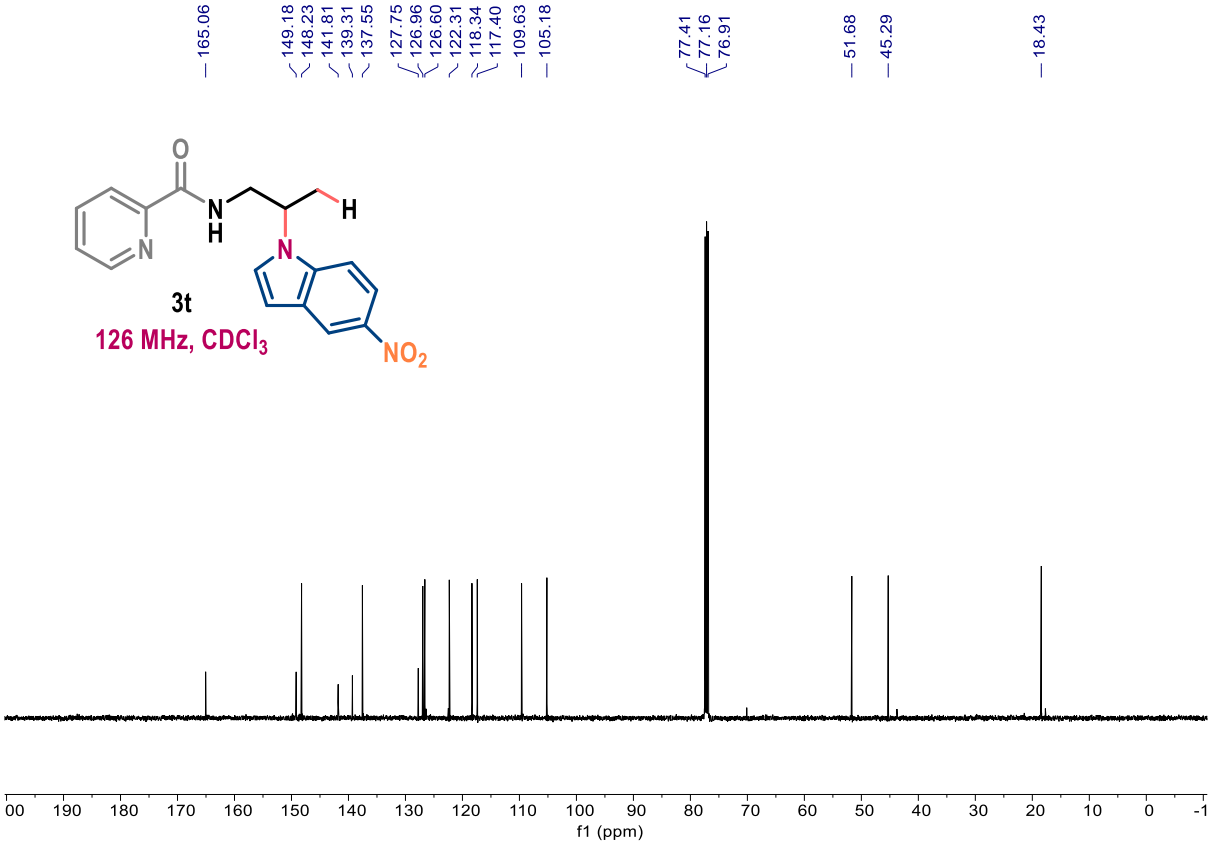

0.98 0.94 0.95 1.00 1.02 2.94 1.02 0.92 1.09 2.10 3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


165.06
149.25
148.26
137.52
136.12
129.91
126.60
126.56
125.25
122.29
121.35
118.85
114.57
103.41
101.54
77.41
77.16
76.91
51.48
45.26
18.45
3r
126 MHz, CDCl3
NC
f1 (ppm)


8.39
8.38
8.37
8.17
8.15
8.04
7.84
7.83
7.82
7.80
7.79
7.44
7.41
7.39
7.38
7.37
7.36
7.31
7.30
7.26
6.67
6.66
4.94
4.92
4.91
4.90
4.89
4.87
4.85
3.91
3.89
3.87
3.86
3.81
3.79
3.78
3.76
3.74
1.65
1.63
3s
400 MHz,CDCl3
CO2Me
1.93
1.00
0.95
2.01
1.06
0.98
0.98
0.96
1.08
3.06
0.95
1.06
3.00
f1 (ppm)


168.30
164.98
149.34
148.21
138.84
137.47
128.22
126.47
125.29
124.15
123.13
122.32
121.79
109.35
104.04
77.48
77.16
76.84
51.93
51.48
45.07
18.48
O
N
H
N
H
3s
101 MHz,CDCl3
CO2Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.55
8.55
8.39
8.38
8.15
8.13
8.08
8.06
8.05
8.01
8.01
7.99
7.99
7.84
7.82
7.81
7.46
7.44
7.40
7.39
7.38
7.37
7.26
6.75
6.75
4.97
4.96
4.95
4.93
4.92
4.91
3.90
3.89
3.88
3.87
3.86
3.85
3.78
3.77
3.76
3.75
3.74
3.72
1.67
1.66
O
N
H
N
H
3t
500 MHz, CDCl3
NO2
0.97
1.01
1.06
0.99
1.02
1.13
1.08
2.02
0.97
1.11
1.15
1.15
2.98
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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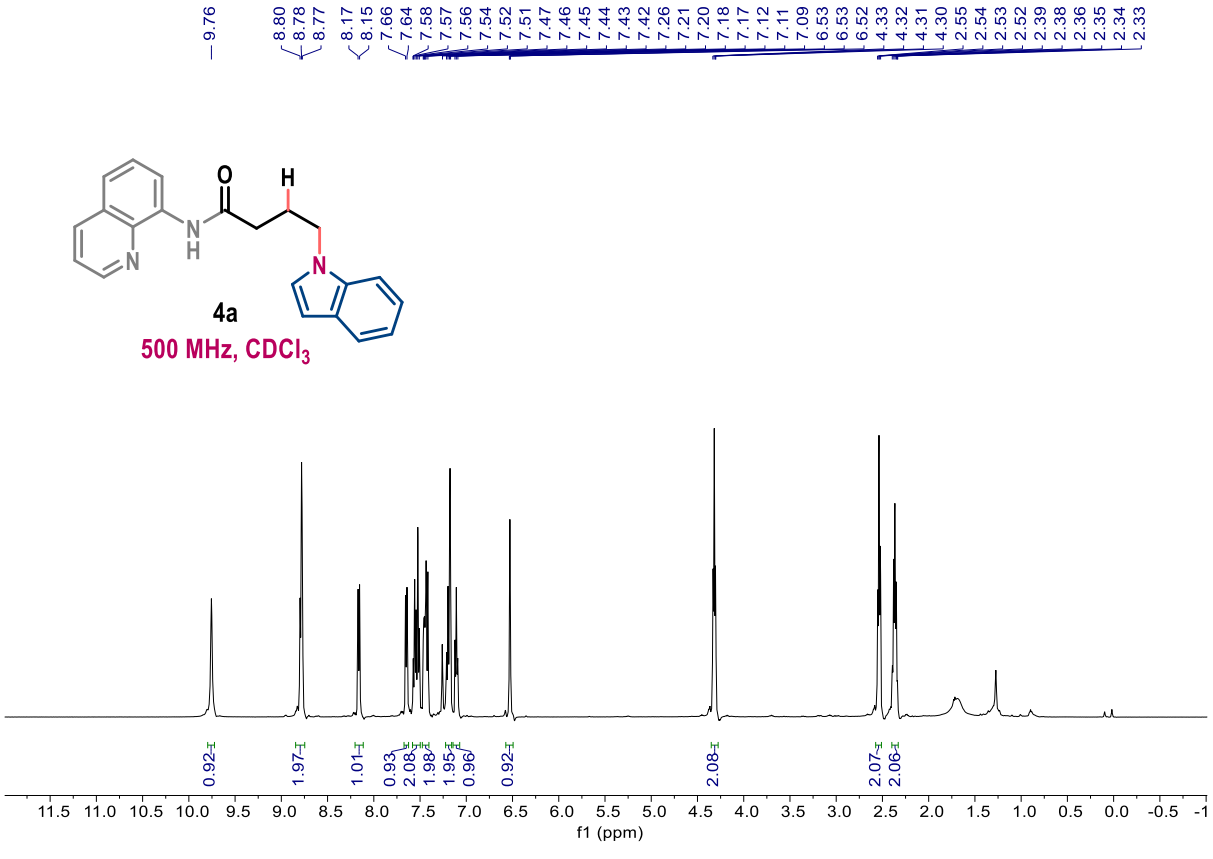
149.18
148.23
141.81
139.31
137.55
127.75
126.96
126.60
122.31
118.34
117.40
109.63
105.18
77.41
77.16
76.91
51.68
45.29
18.43
3t
126 MHz, CDCl3
NO2
f1 (ppm)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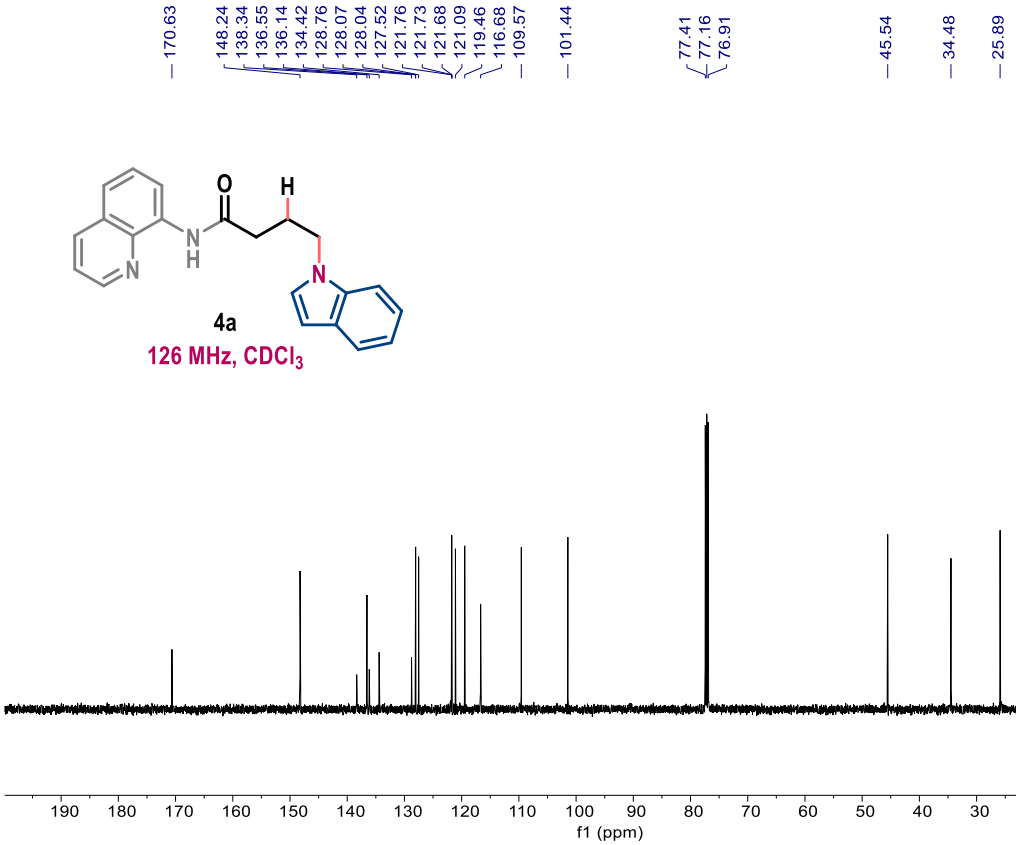
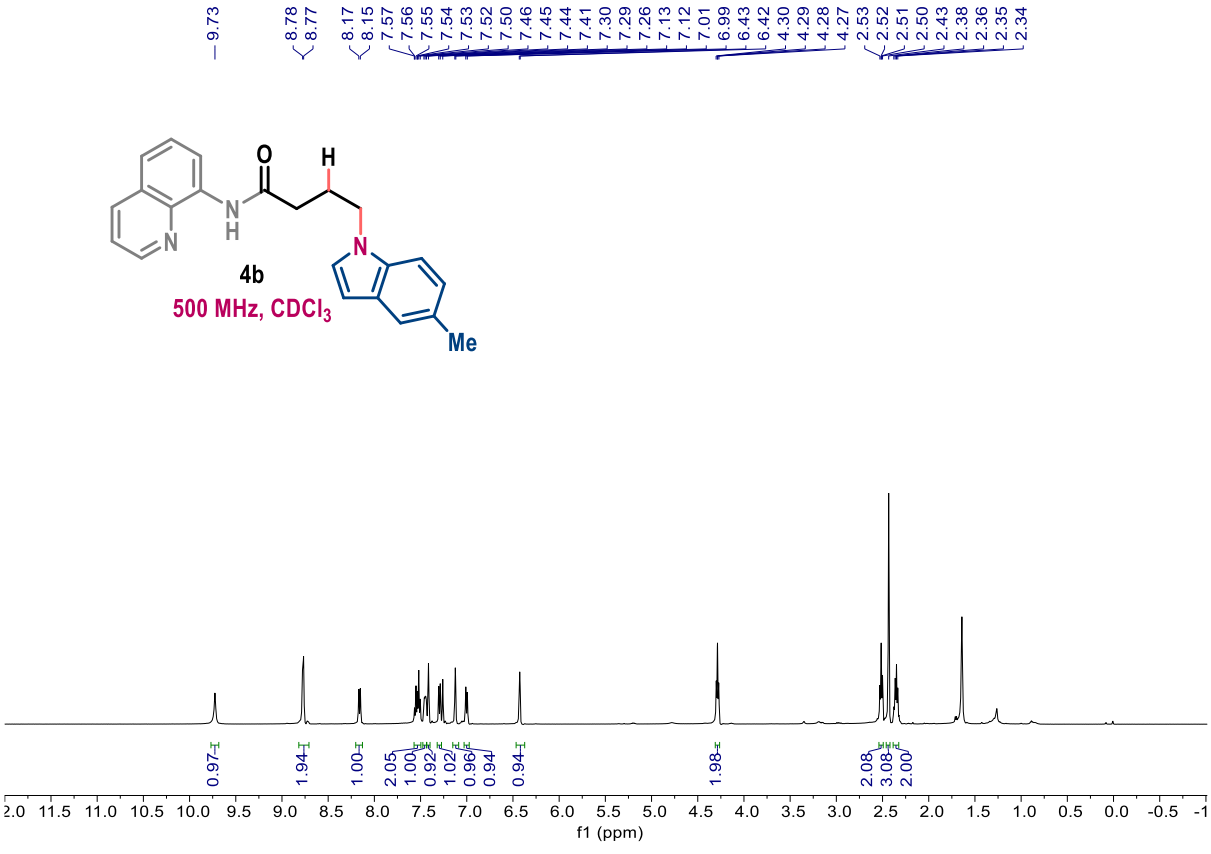
8.80
8.78
8.77
8.17
8.15
7.66
7.64
7.58
7.57
7.56
7.54
7.52
7.51
7.47
7.46
7.45
7.44
7.43
7.42
7.26
7.21
7.20
7.18
7.17
7.12
7.11
7.09
6.53
6.53
6.52
4.33
4.32
4.31
4.30
2.55
2.54
2.53
2.52
2.39
2.38
2.36
2.35
2.34
2.33
4a
500 MHz, CDCl3
0.92
1.97
1.01
0.93
2.08
1.98
1.95
0.96
0.92
2.08
2.07
2.06
f1 (ppm)


170.63
148.24
138.34
136.55
136.14
134.42
128.76
128.07
128.04
127.52
121.76
121.73
121.68
121.09
119.46
116.68
109.57
101.44
77.41
77.16
76.91
45.54
34.48
25.89
O
H
N
H
N
N
4a
126 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)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8.77
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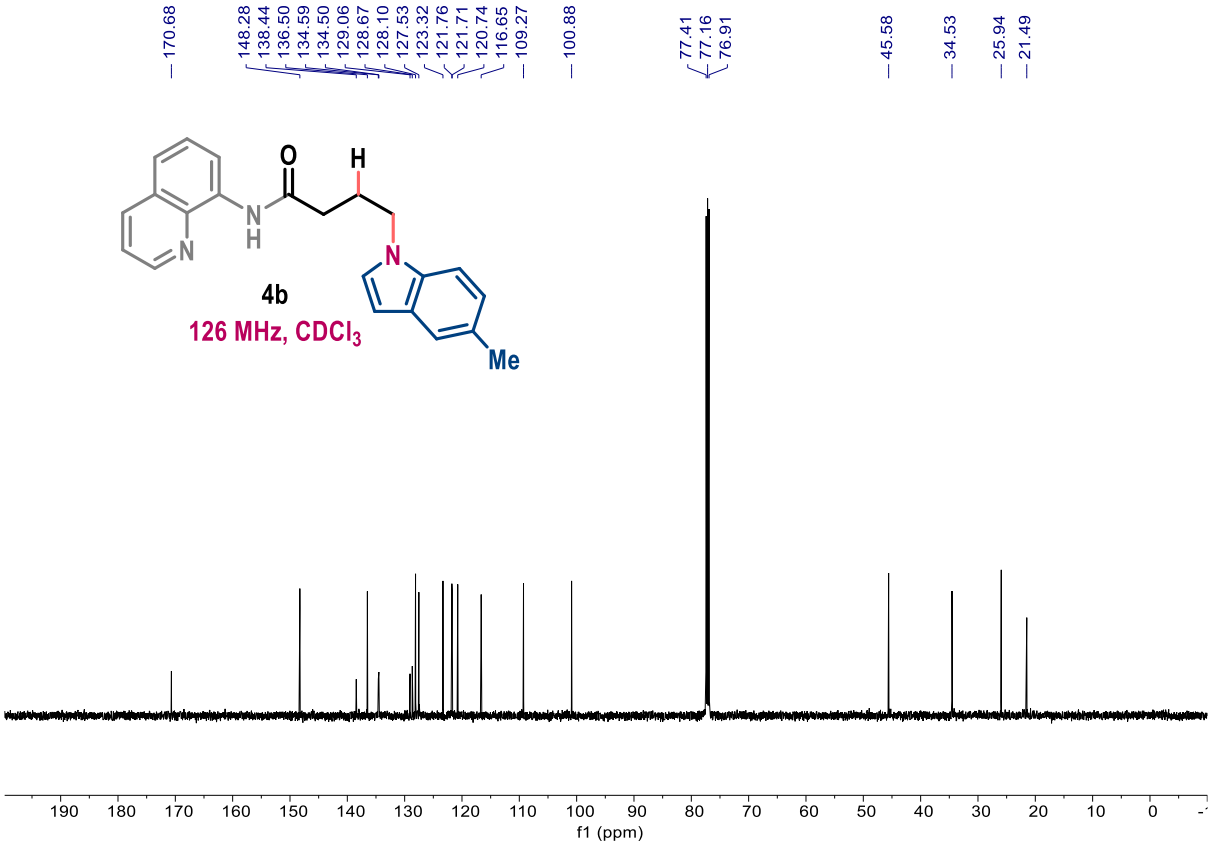
7.56
7.55
7.54
7.53
7.52
7.50
7.46
7.45
7.44
7.41
7.30
7.29
7.26
7.13
7.12
7.01
6.99
6.43
6.42
4.30
4.29
4.28
4.27
2.53
2.52
2.51
2.50
2.43
2.38
2.36
2.35
2.34
O
H
N
H
N
N
4b
500 MHz, CDCl3
Me
0.97
1.94
1.00
2.05
1.00
0.92
1.02
0.96
0.94
0.94
1.98
2.08
3.08
2.00
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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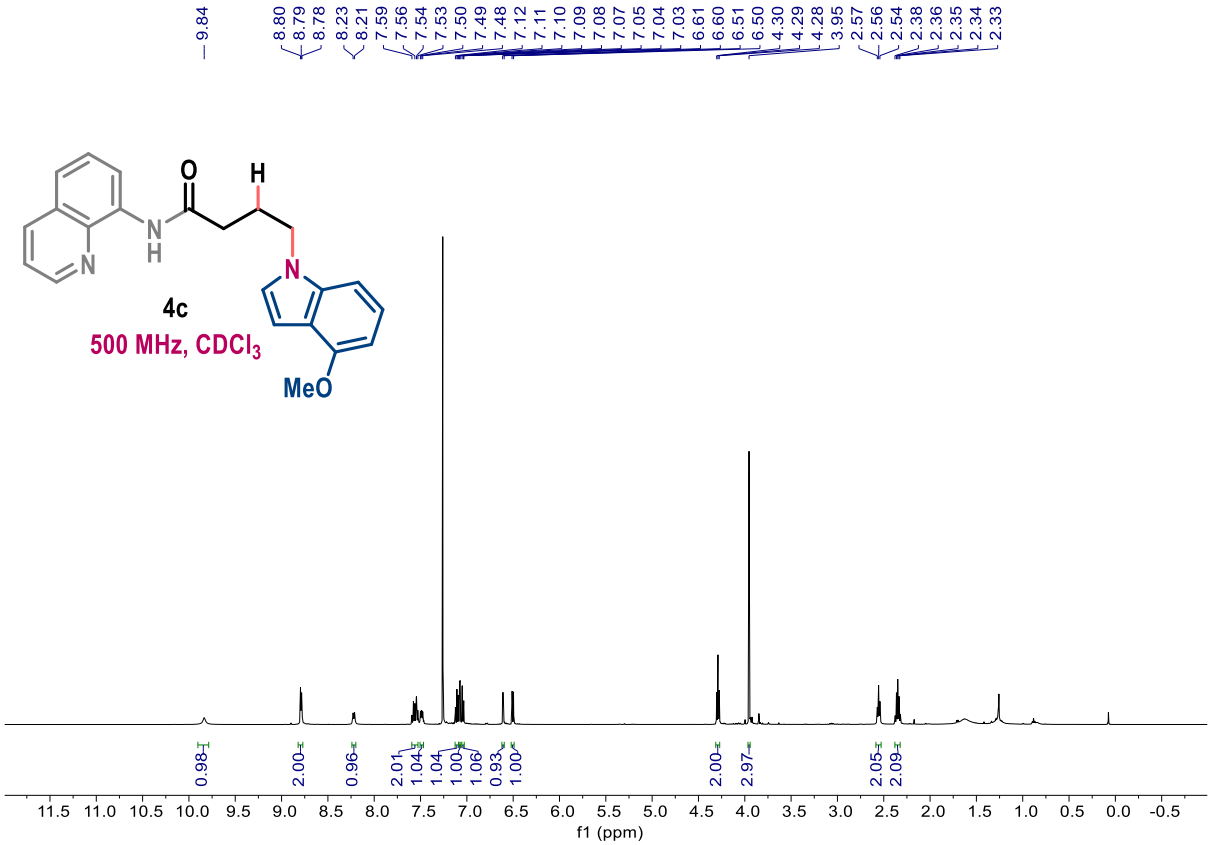
148.28
138.44
136.50
134.59
134.50
129.06
128.67
128.10
127.53
123.32
121.76
121.71
120.74
116.65
109.27
100.88
77.41
77.16
76.91
45.58
34.53
25.94
21.49
O
H
N
H
N
N
4b
126 MHz, CDCl3
Me
f1 (ppm)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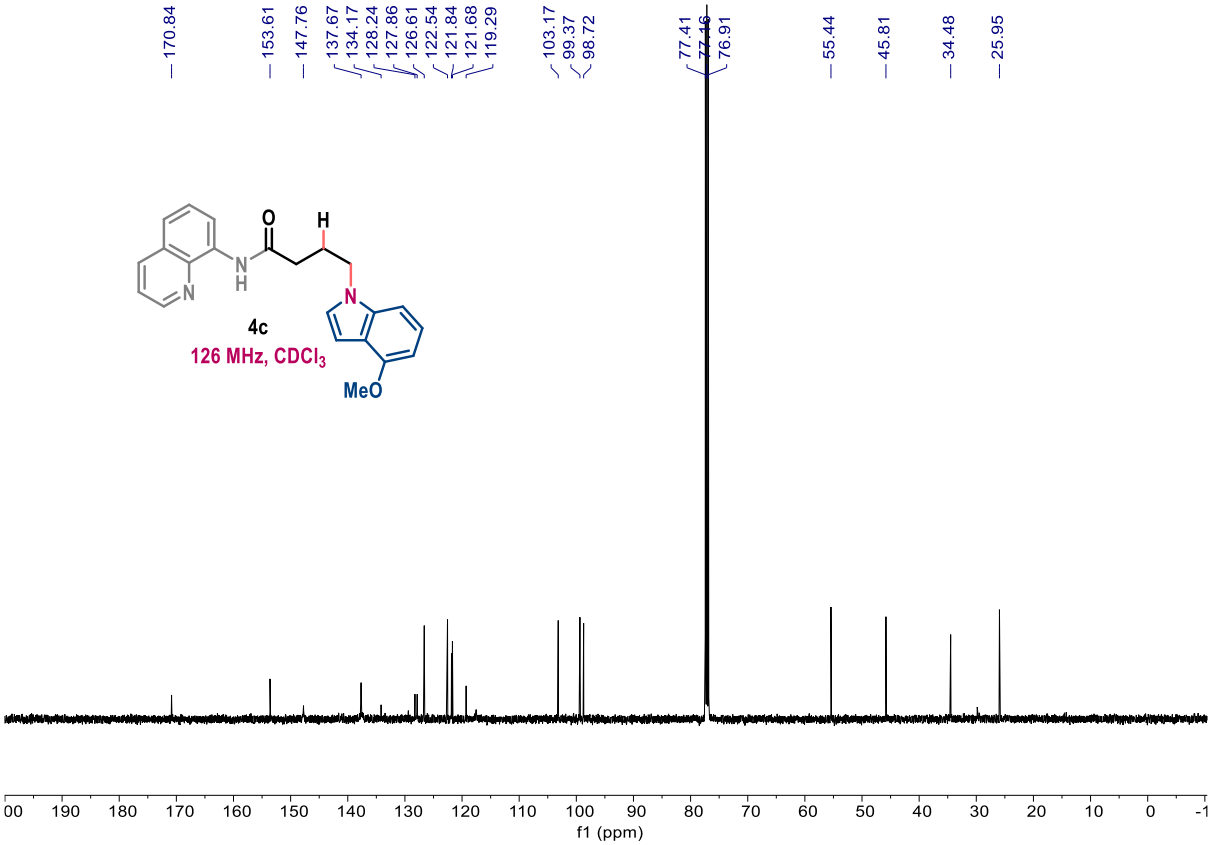
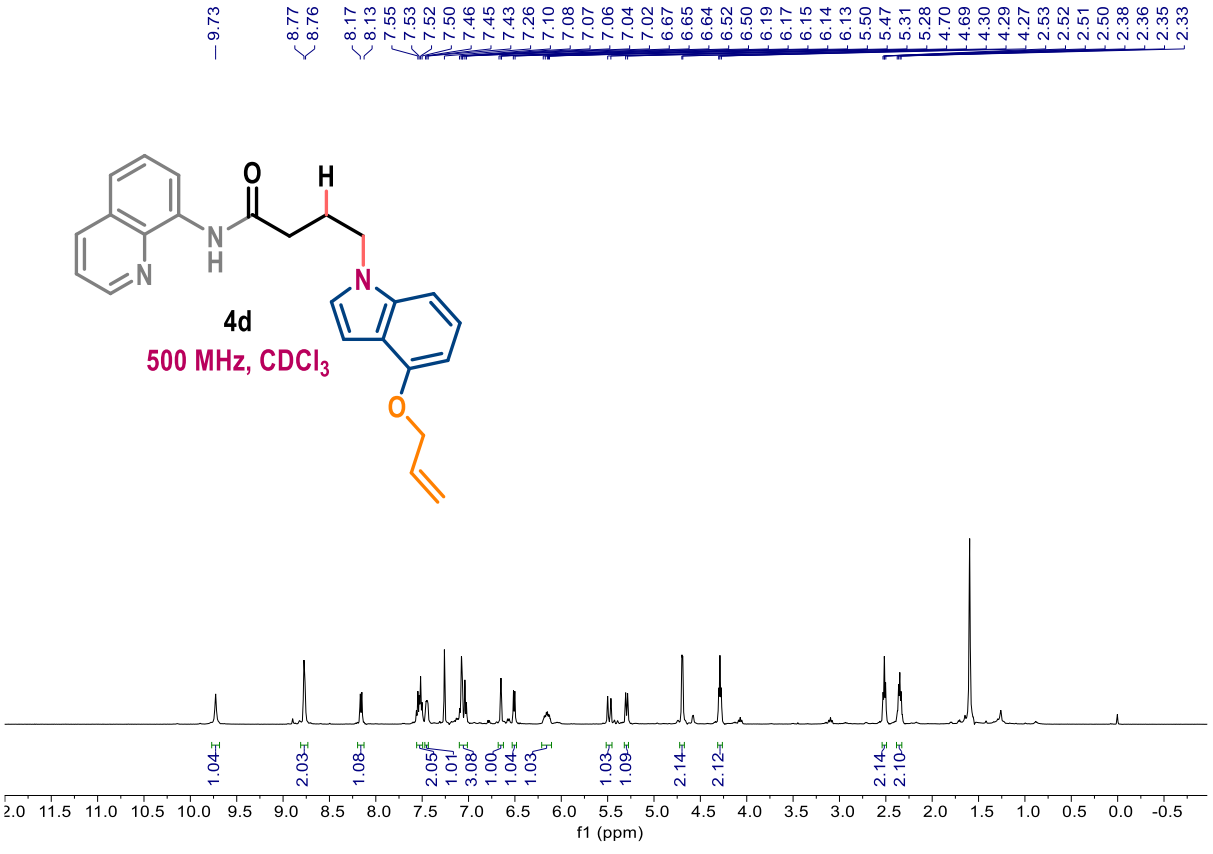
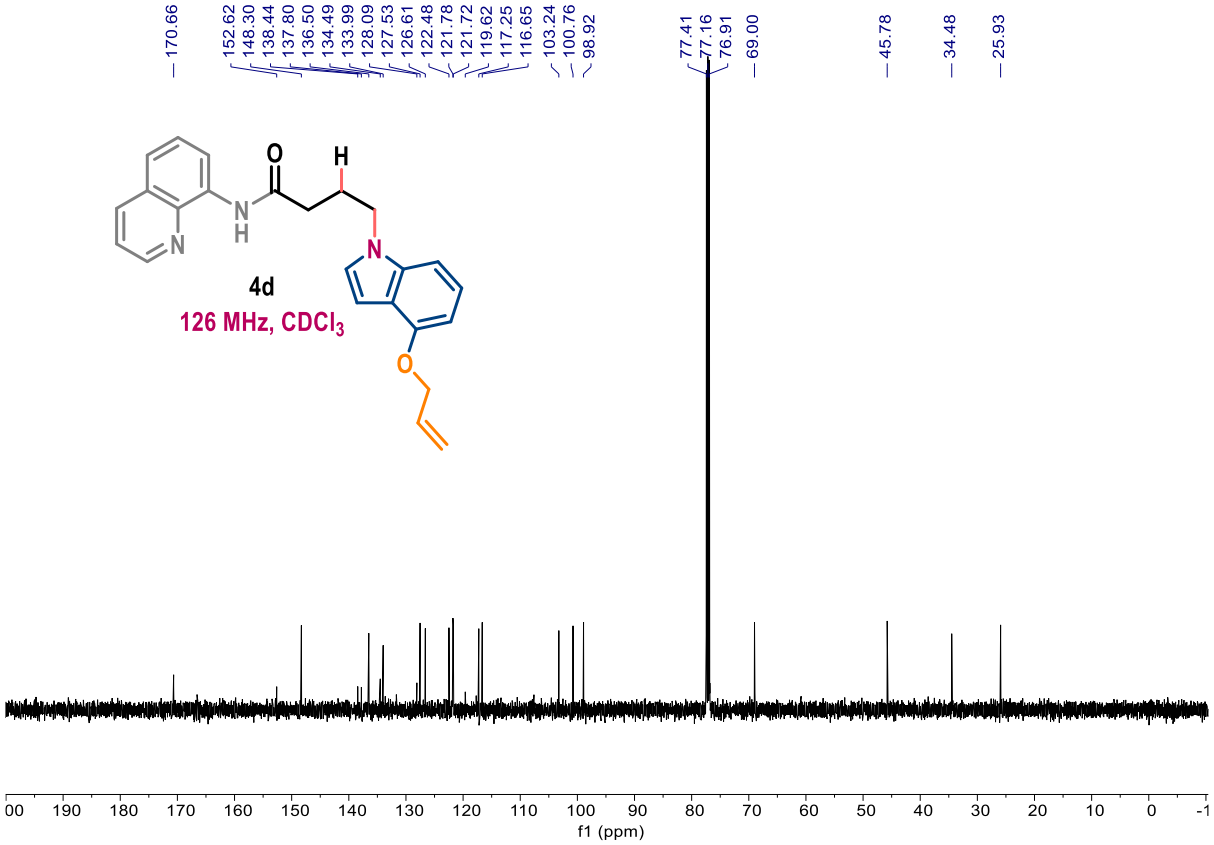
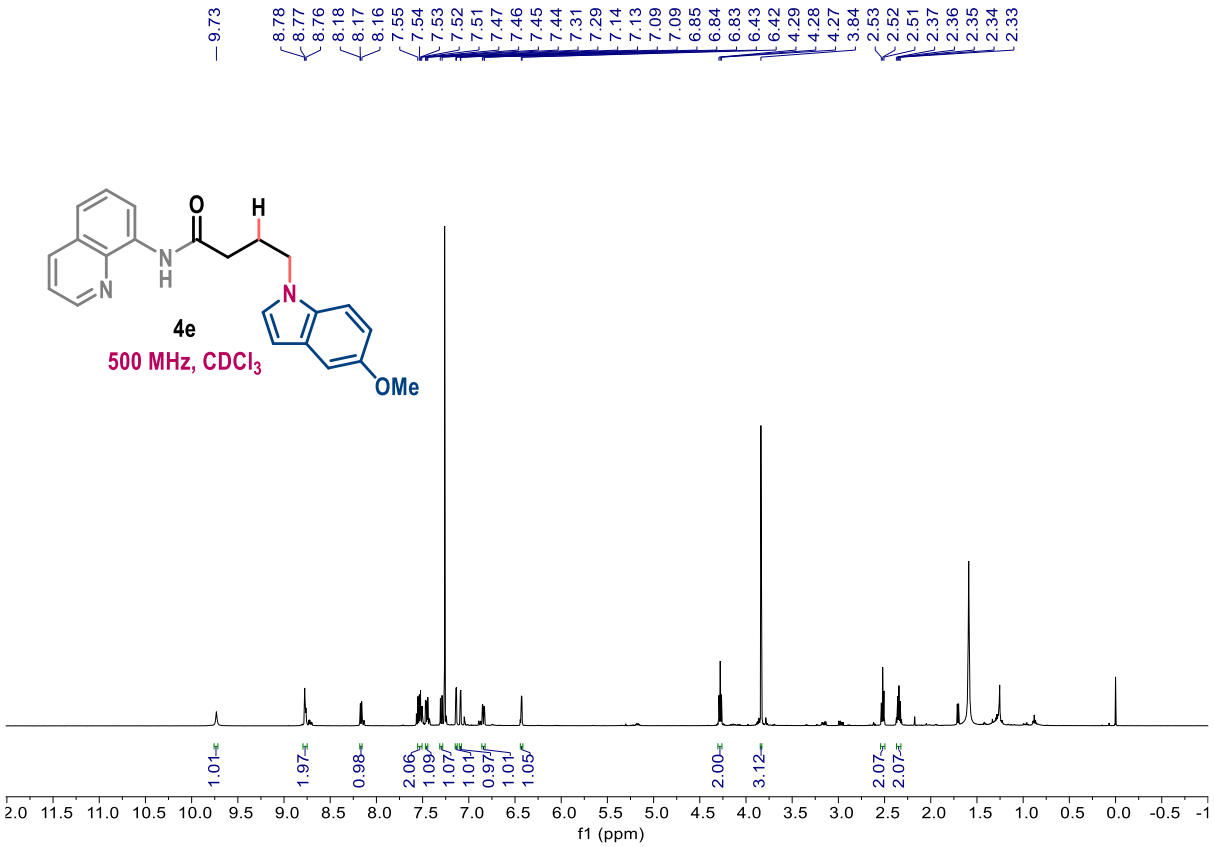
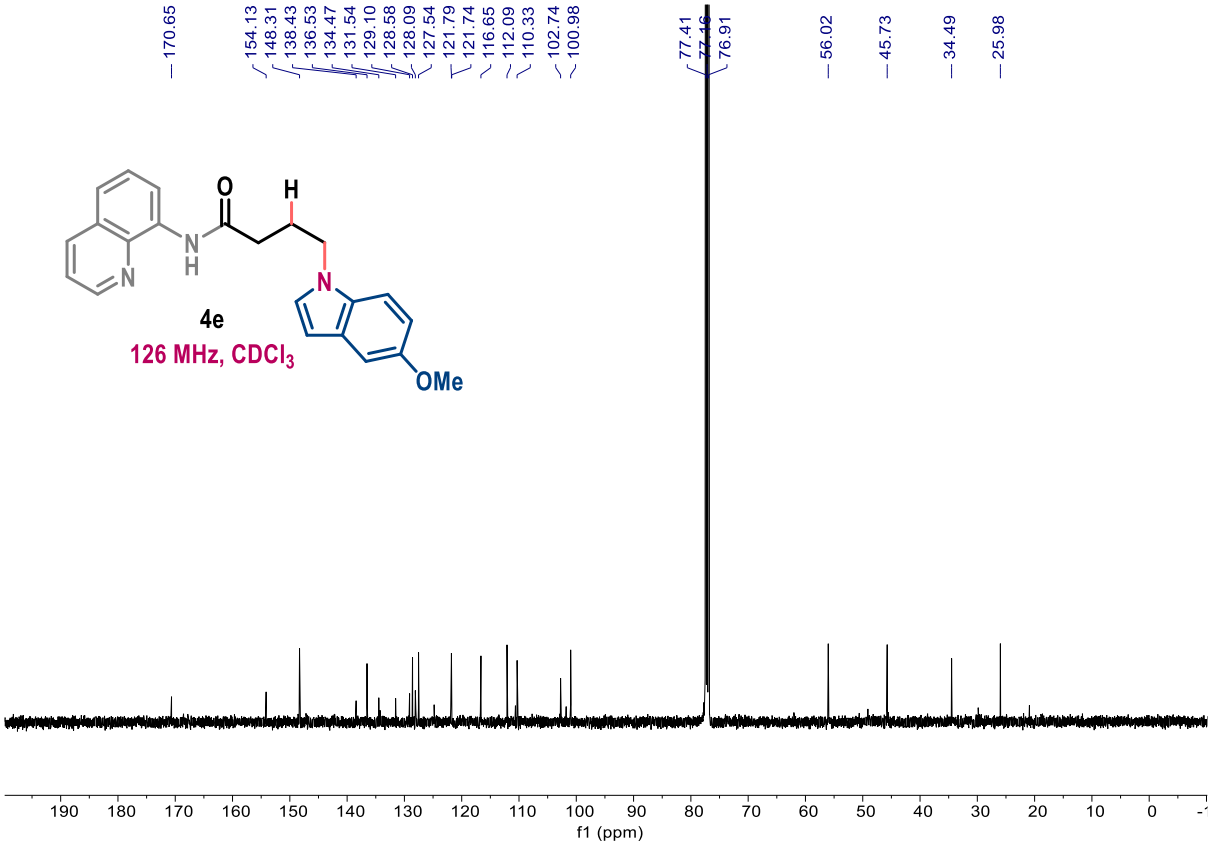
8.80
8.79
8.78
8.23
8.21
7.59
7.56
7.54
7.53
7.50
7.49
7.48
7.12
7.11
7.10
7.09
7.08
7.07
7.05
7.04
7.03
6.61
6.60
6.51
6.50
4.30
4.29
4.28
3.95
2.57
2.56
2.54
2.38
2.36
2.35
2.34
2.33
O
H
N
H
N
N
4c
500 MHz, CDCl3
MeO
0.98
2.00
0.96
2.01
1.04
1.04
1.00
1.06
0.93
1.00
2.00
2.97
2.05
2.09
f1 (ppm)

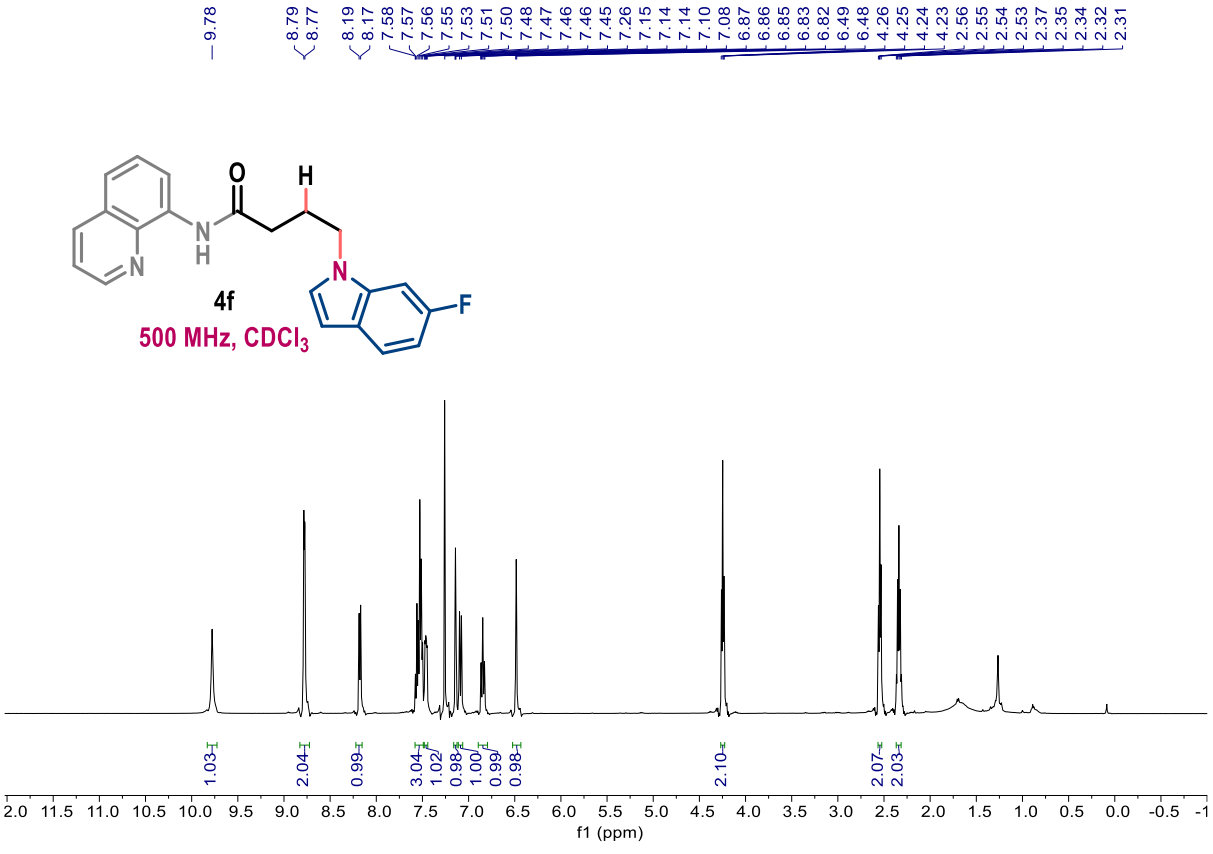

170.84
153.61
147.76
137.67
134.17
128.24
127.86
126.61
122.54
121.84
121.68
119.29
103.17
99.37
98.72
77.41
77.16
76.91
55.44
45.81
34.48
25.95
O
H
N
H
N
N
4c
126 MHz, CDCl3
MeO
f1 (ppm)

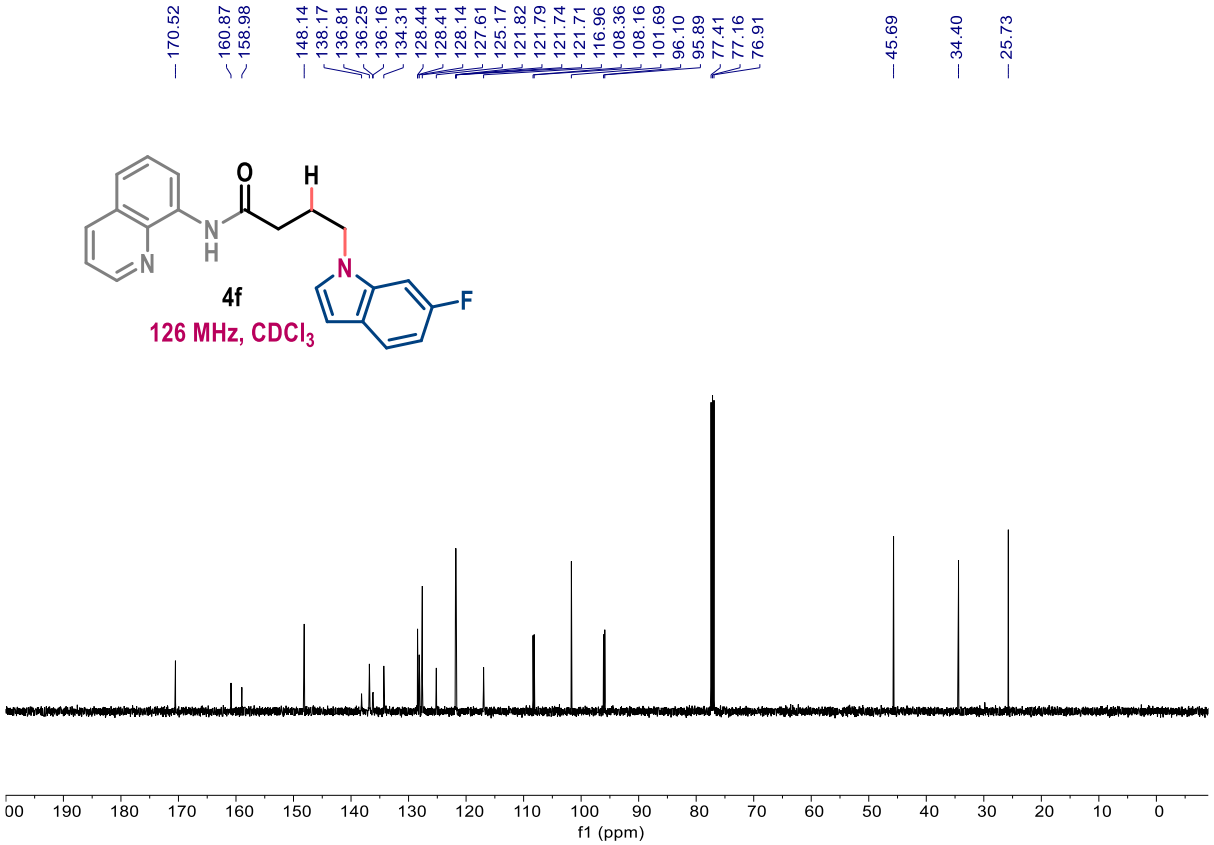

9.73
8.77
8.76
8.17
8.13
7.55
7.53
7.52
7.50
7.46
7.45
7.43
7.26
7.10
7.08
7.07
7.06
7.04
7.02
6.67
6.65
6.64
6.52
6.50
6.19
6.17
6.15
6.14
6.13
5.50
5.47
5.31
5.28
4.70
4.69
4.30
4.29
4.27
2.53
2.52
2.51
2.50
2.38
2.36
2.35
2.33
O
H
N
H
N
N
4d
500 MHz, CDCl3
O
1.04
2.03
1.08
2.05
1.01
3.08
1.00
1.04
1.03
1.03
1.09
2.14
2.12
2.14
2.10
f1 (ppm)

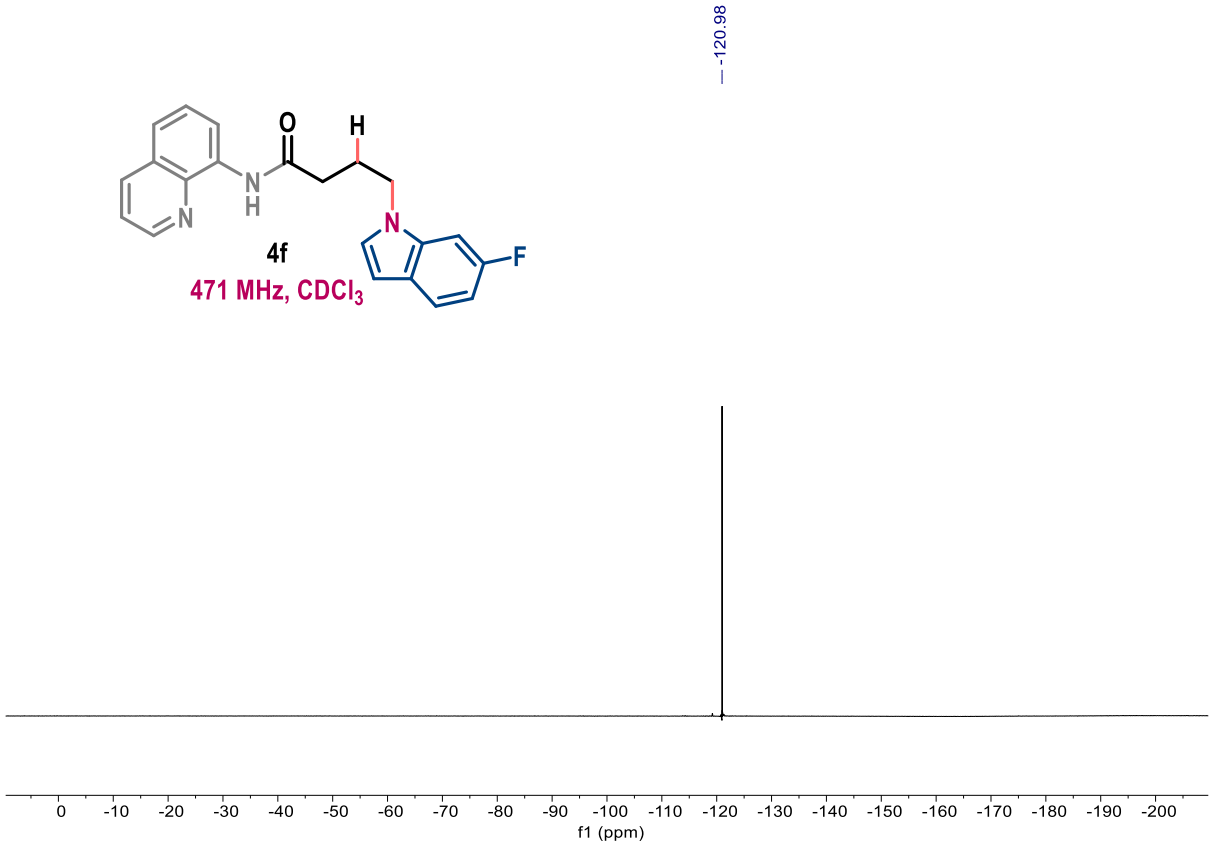

170.66
152.62
148.30
138.44
137.80
136.50
134.49
133.99
128.09
127.53
126.61
122.48
121.78
121.72
119.62
117.25
116.65
103.24
100.76
98.92
77.41
77.16
76.91
69.00
45.78
34.48
25.93
O
H
N
H
N
N
O
4d
126 MHz, CDCl3
f1 (ppm)

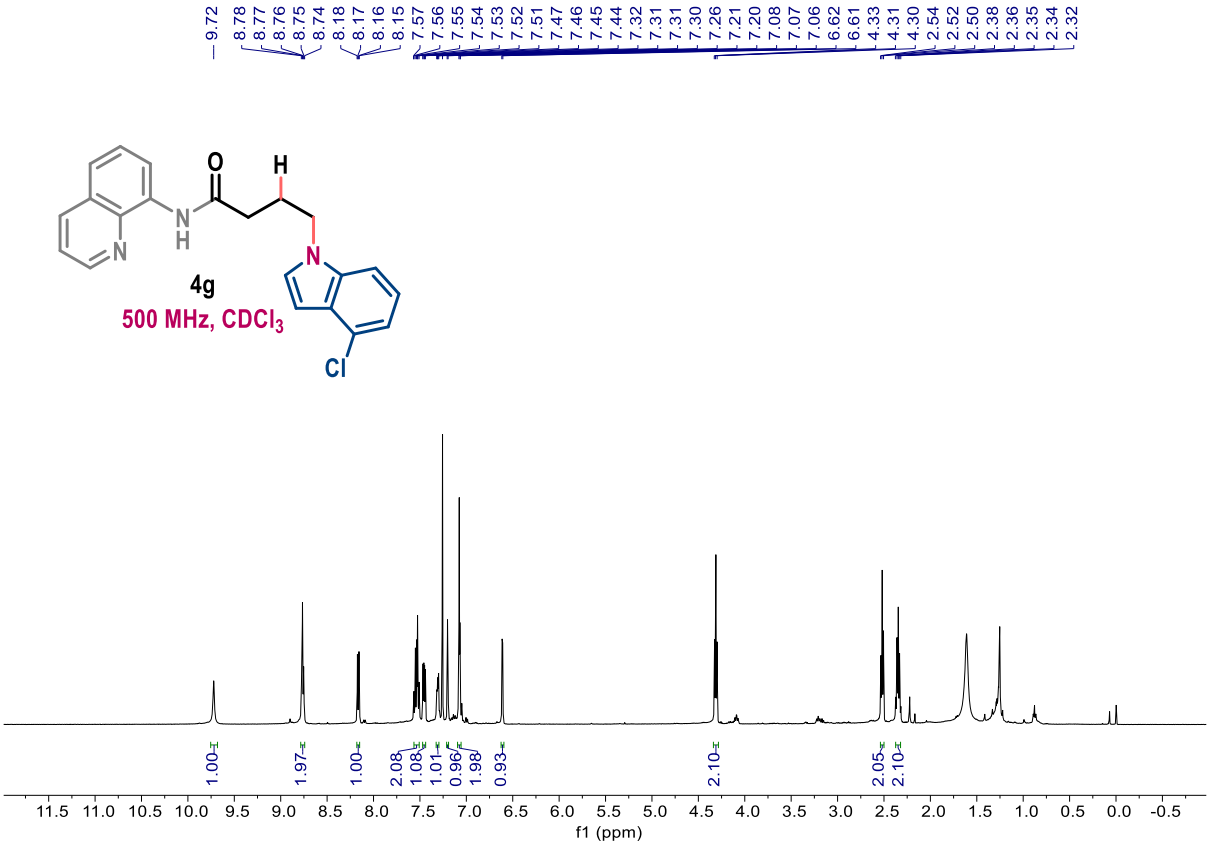

9.73
8.78
8.77
8.76
8.18
8.17
8.16
7.55
7.54
7.53
7.52
7.51
7.47
7.46
7.45
7.44
7.31
7.29
7.14
7.13
7.09
7.09
6.85
6.84
6.83
6.43
6.42
4.29
4.28
4.27
3.84
2.53
2.52
2.51
2.37
2.36
2.35
2.34
2.33
O
H
N
H
N
N
OMe
4e
500 MHz, CDCl3
1.01
1.97
0.98
2.06
1.09
1.07
1.01
0.97
1.01
1.05
2.00
3.12
2.07
2.07
f1 (ppm)

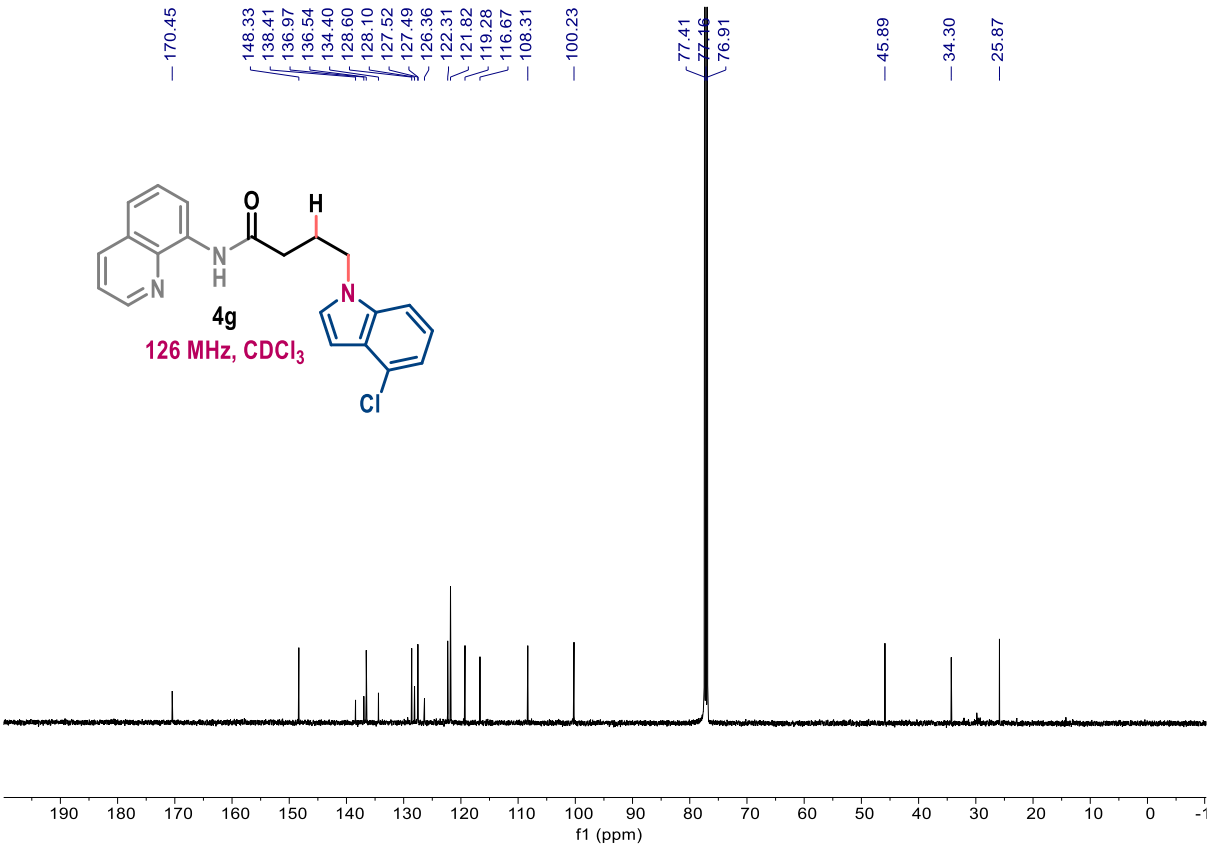

170.65
154.13
148.31
138.43
136.53
134.47
131.54
129.10
128.58
128.09
127.54
121.79
121.74
116.65
112.09
110.33
102.74
100.98
77.41
77.16
76.91
56.02
45.73
34.49
25.98
O
H
N
H
N
N
4e
126 MHz, CDCl3
OMe
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

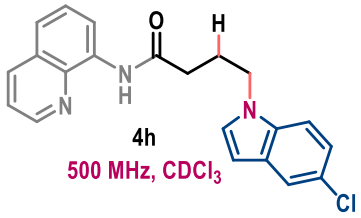

9.78
8.79
8.77
8.19
8.17
7.58
7.57
7.56
7.55
7.53
7.51
7.50
7.48
7.47
7.46
7.46
7.45
7.26
7.15
7.14
7.14
7.10
7.08
6.87
6.86
6.85
6.83
6.82
6.49
6.48
4.26
4.25
4.24
4.23
2.56
2.55
2.54
2.53
2.37
2.35
2.34
2.32
2.31
O
H
N
H
N
N
4f
500 MHz, CDCl3
F
1.03
2.04
0.99
3.04
1.02
0.98
1.00
0.99
0.98
2.10
2.07
2.03
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


170.52
160.87
158.98
148.14
138.17
136.81
136.25
136.16
134.31
128.44
128.41
128.14
127.61
125.17
121.82
121.79
121.74
121.71
116.96
108.36
108.16
101.69
96.10
95.89
77.41
77.16
76.91
45.69
34.40
25.73
O
H
N
H
N
N
F
4f
126 MHz, CDCl3
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-120.98
O
H
N
H
N
N
F
4f
471 MHz, CDCl3
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

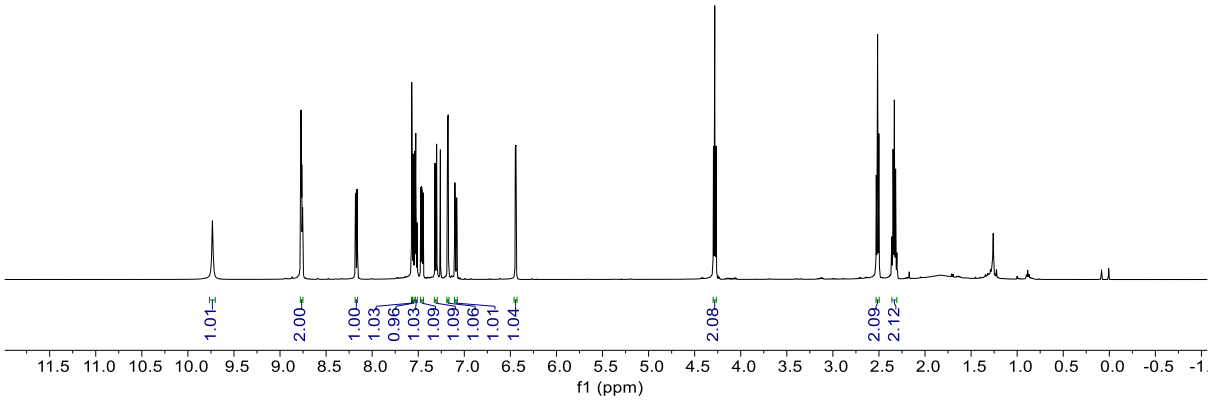

9.72
8.78
8.77
8.76
8.75
8.74
8.18
8.17
8.16
8.15
7.57
7.56
7.55
7.54
7.53
7.52
7.51
7.47
7.46
7.45
7.44
7.32
7.31
7.31
7.30
7.26
7.21
7.20
7.08
7.07
7.06
6.62
6.61
4.33
4.31
4.30
2.54
2.52
2.50
2.38
2.36
2.35
2.34
2.32
O
H
N
H
N
N
4g
500 MHz, CDCl3
Cl
1.00
1.97
1.00
2.08
1.08
1.01
0.96
1.98
0.93
2.10
2.05
2.10
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

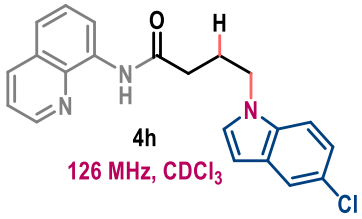

170.45
148.33
138.41
136.97
136.54
134.40
128.60
128.10
127.52
127.49
126.36
122.31
121.82
119.28
116.67
108.31
100.23
77.41
77.16
76.91
45.89
34.30
25.87
O
H
N
H
N
N
4g
126 MHz, CDCl3
Cl
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)



4h

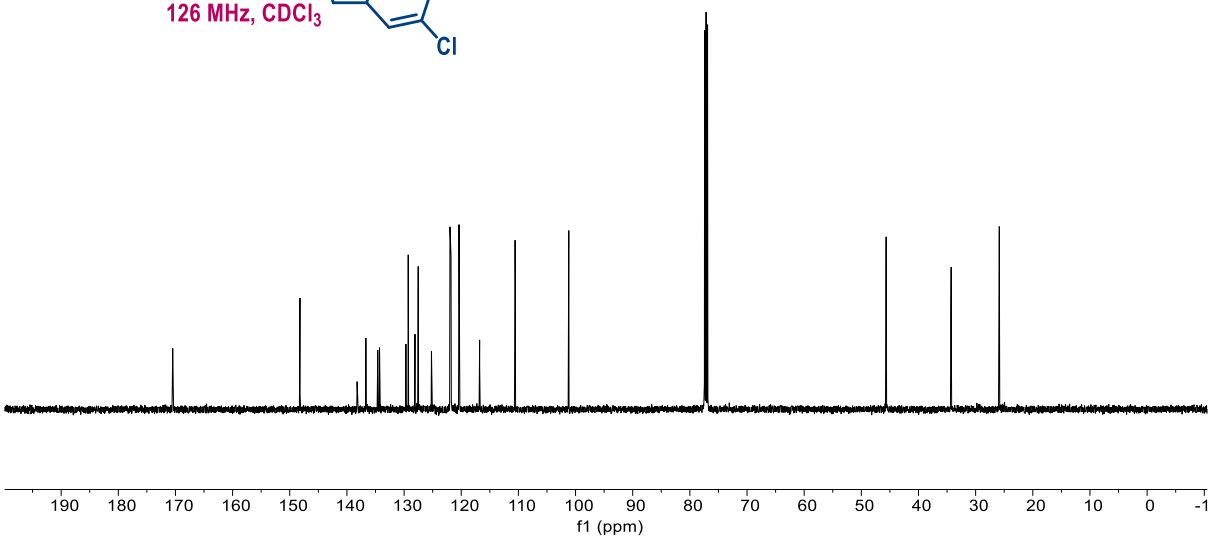
500 MHz, $CDCl_3$

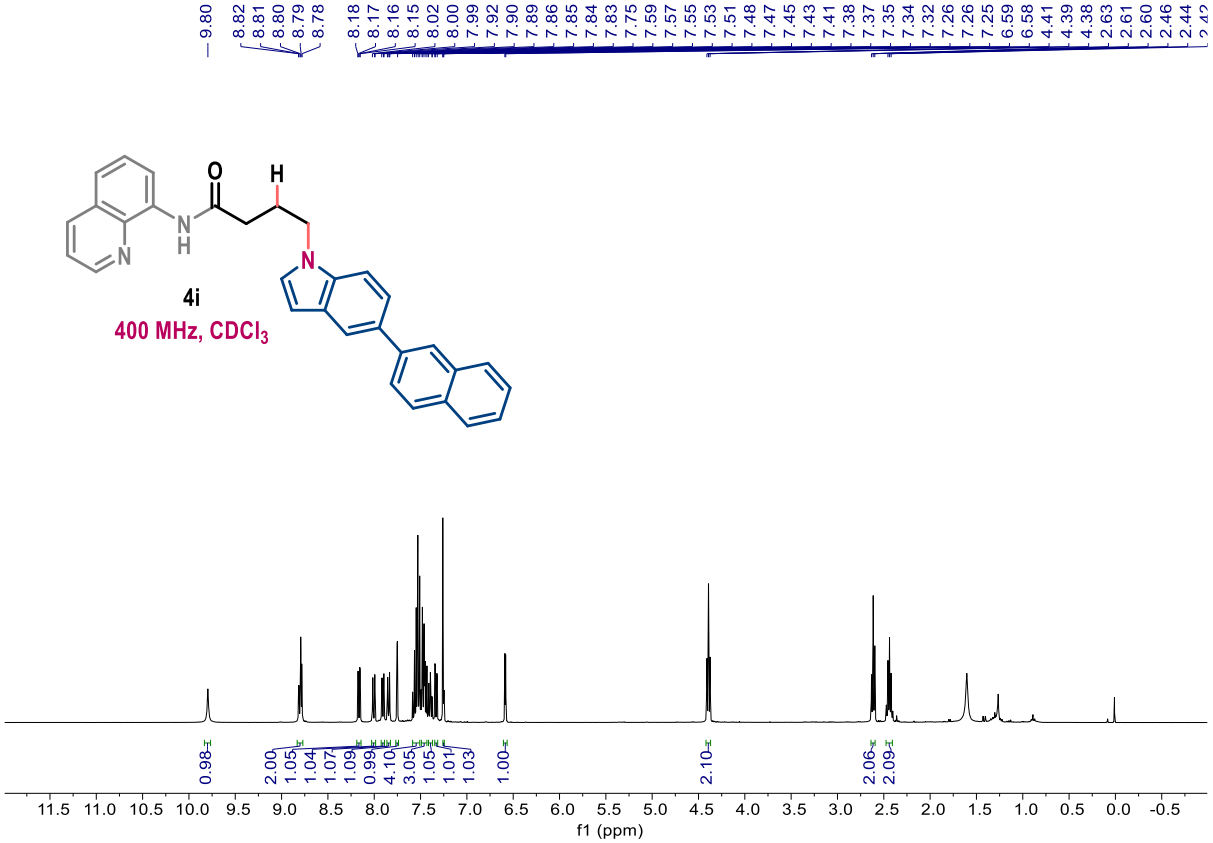


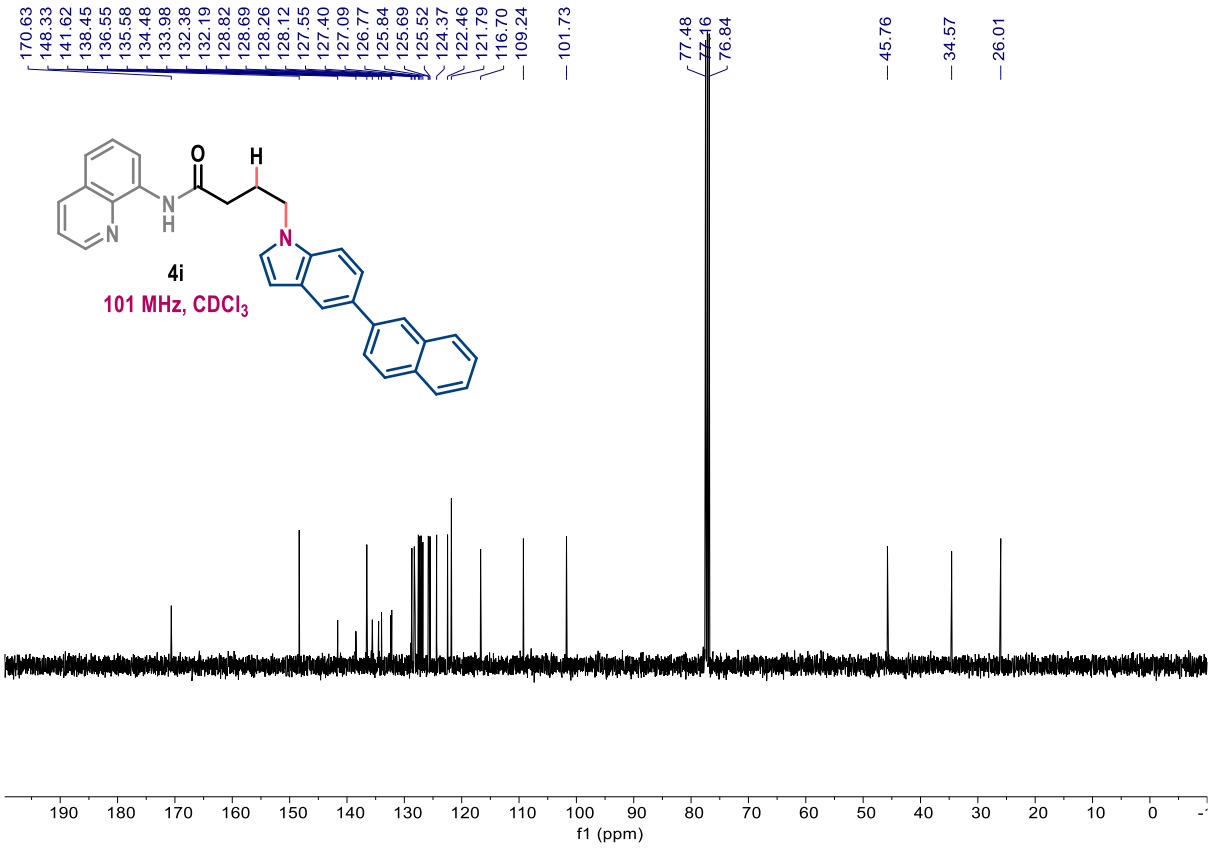


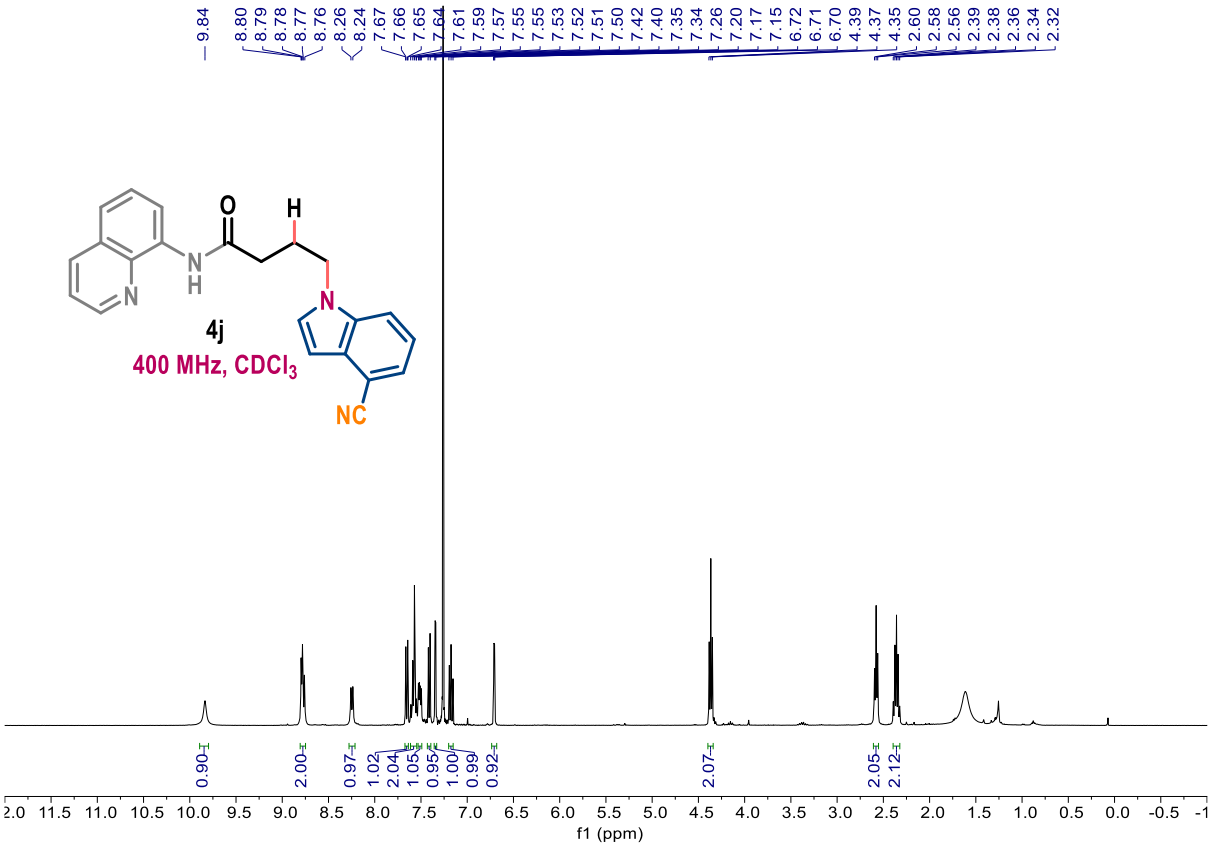
4h

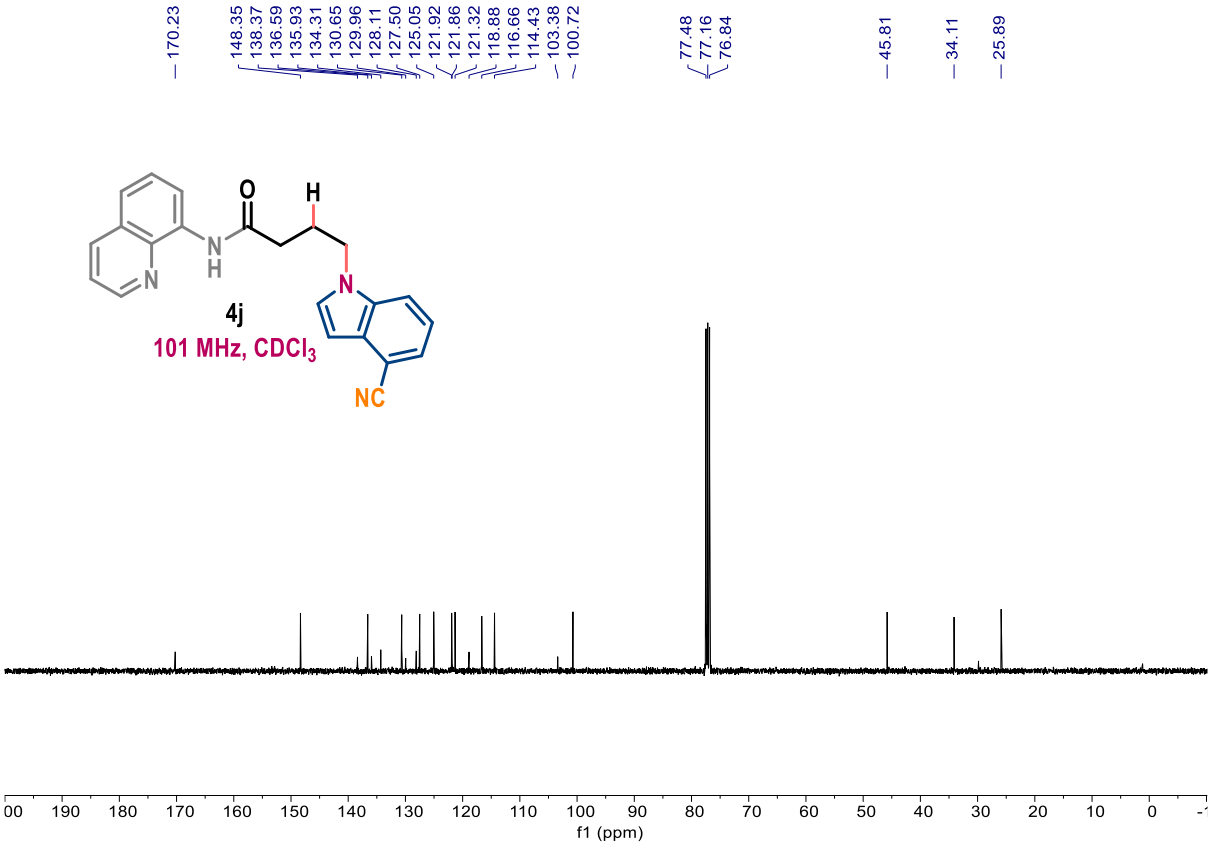
126 MHz, $CDCl_3$

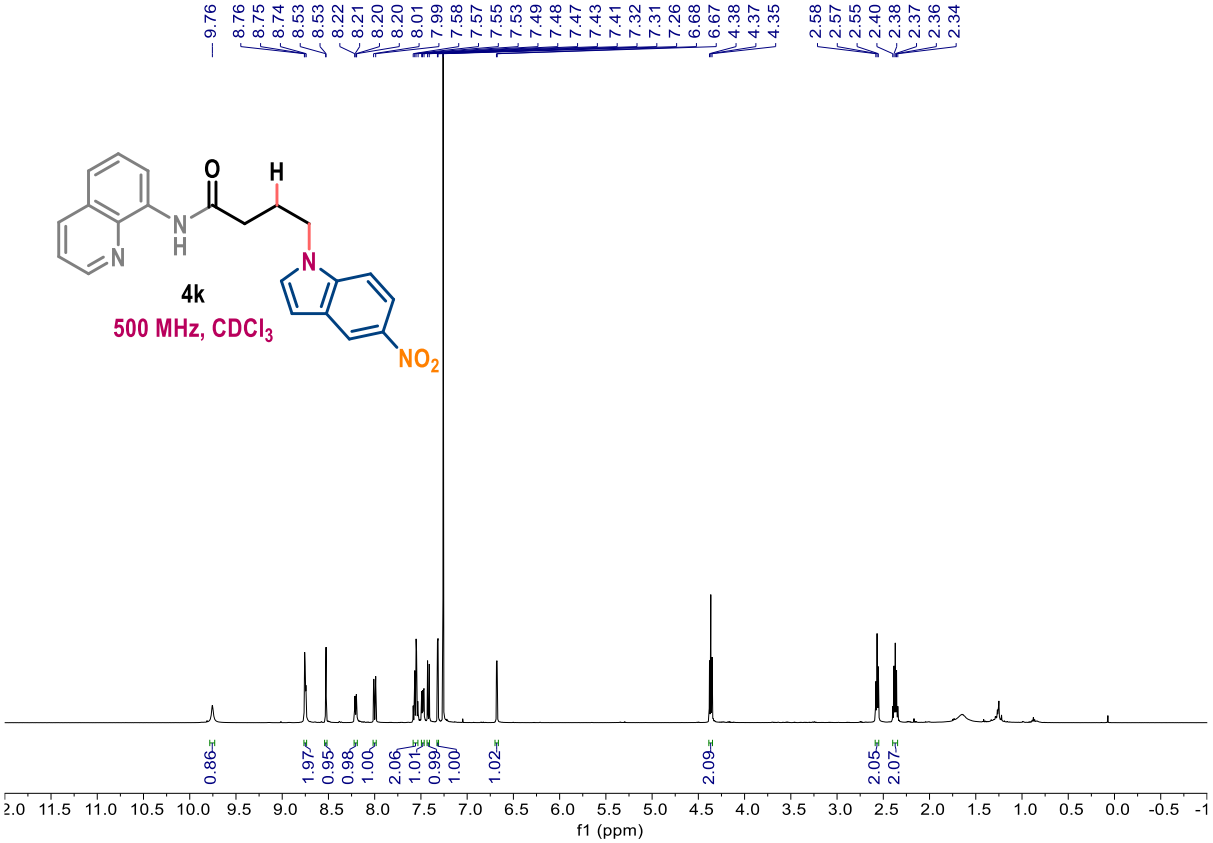


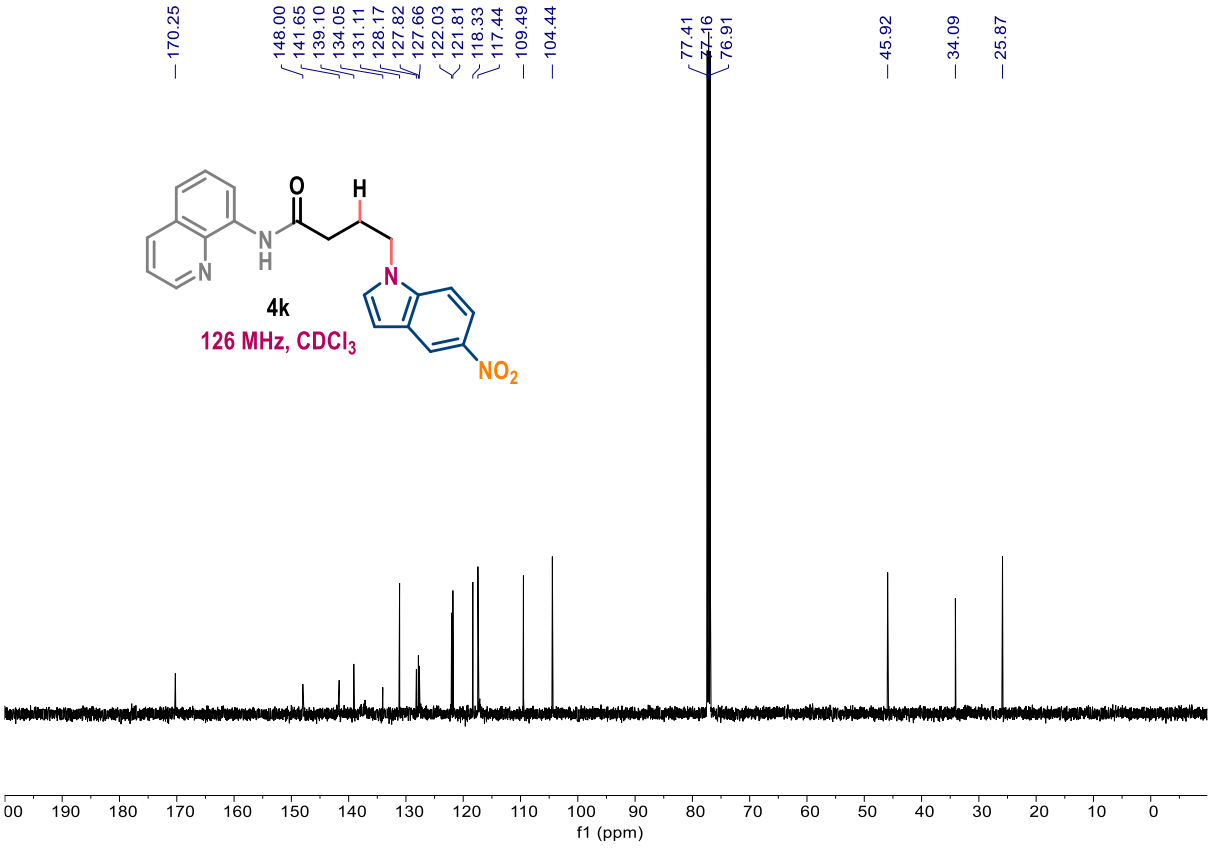

9.80
8.82
8.81
8.80
8.79
8.78
8.18
8.17
8.16
8.15
8.02
8.00
7.99
7.92
7.90
7.89
7.86
7.85
7.84
7.83
7.75
7.59
7.57
7.55
7.53
7.51
7.48
7.47
7.45
7.43
7.41
7.38
7.37
7.35
7.34
7.32
7.26
7.26
7.25
6.59
6.58
4.41
4.39
4.38
2.63
2.61
2.60
2.46
2.44
O
H
N
H
N
N
4i
400 MHz, CDCl3
0.98
2.00
1.05
1.04
1.07
1.09
0.99
4.10
3.05
1.05
1.01
1.03
1.00
2.10
2.06
2.09
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

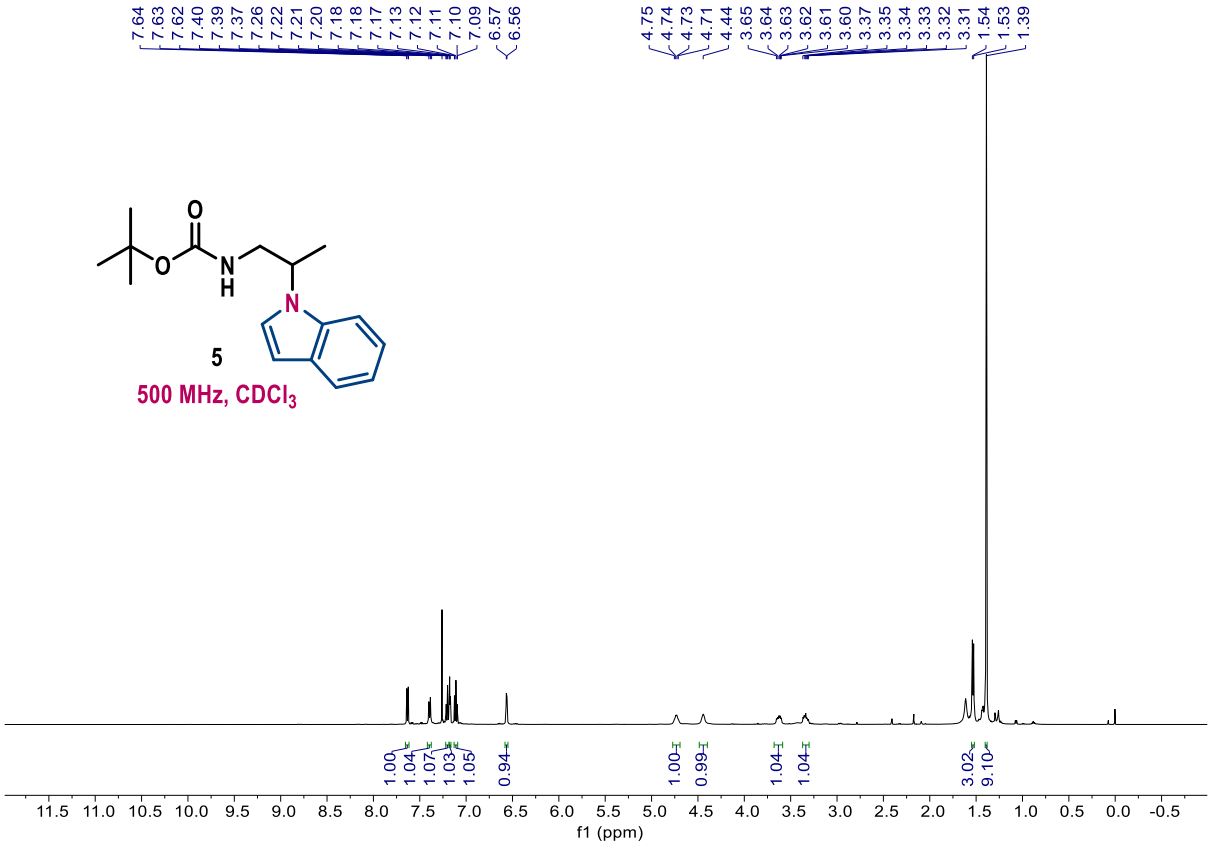

170.63
148.33
141.62
138.45
136.55
135.58
134.48
133.98
132.38
132.19
128.82
128.69
128.26
128.12
127.55
127.40
127.09
126.77
125.84
125.69
125.52
124.37
122.46
121.79
116.70
109.24
101.73
77.48
77.16
76.84
45.76
34.57
26.01
O
H
N
H
N
N
4i
101 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

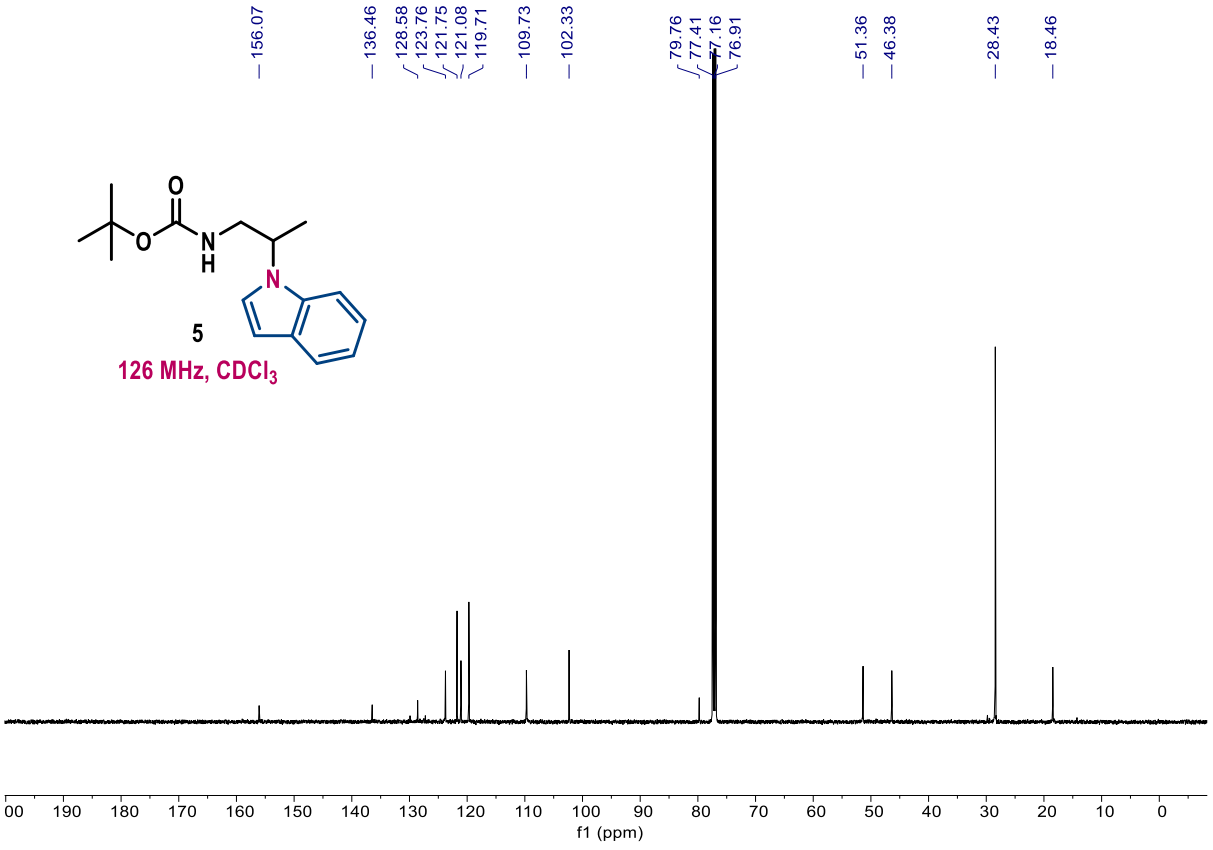

9.84
8.80
8.79
8.78
8.77
8.76
8.26
8.24
7.67
7.66
7.65
7.64
7.61
7.59
7.57
7.55
7.55
7.53
7.52
7.51
7.50
7.42
7.40
7.35
7.34
7.26
7.20
7.17
7.15
6.72
6.71
6.70
4.39
4.37
4.35
2.60
2.58
2.56
2.39
2.38
2.36
2.34
2.32
O
H
N
H
N
N
4j
400 MHz, CDCl3
NC
0.90
2.00
0.97
1.02
2.04
1.05
0.95
1.00
0.99
0.92
2.07
2.05
2.12
f1 (ppm)

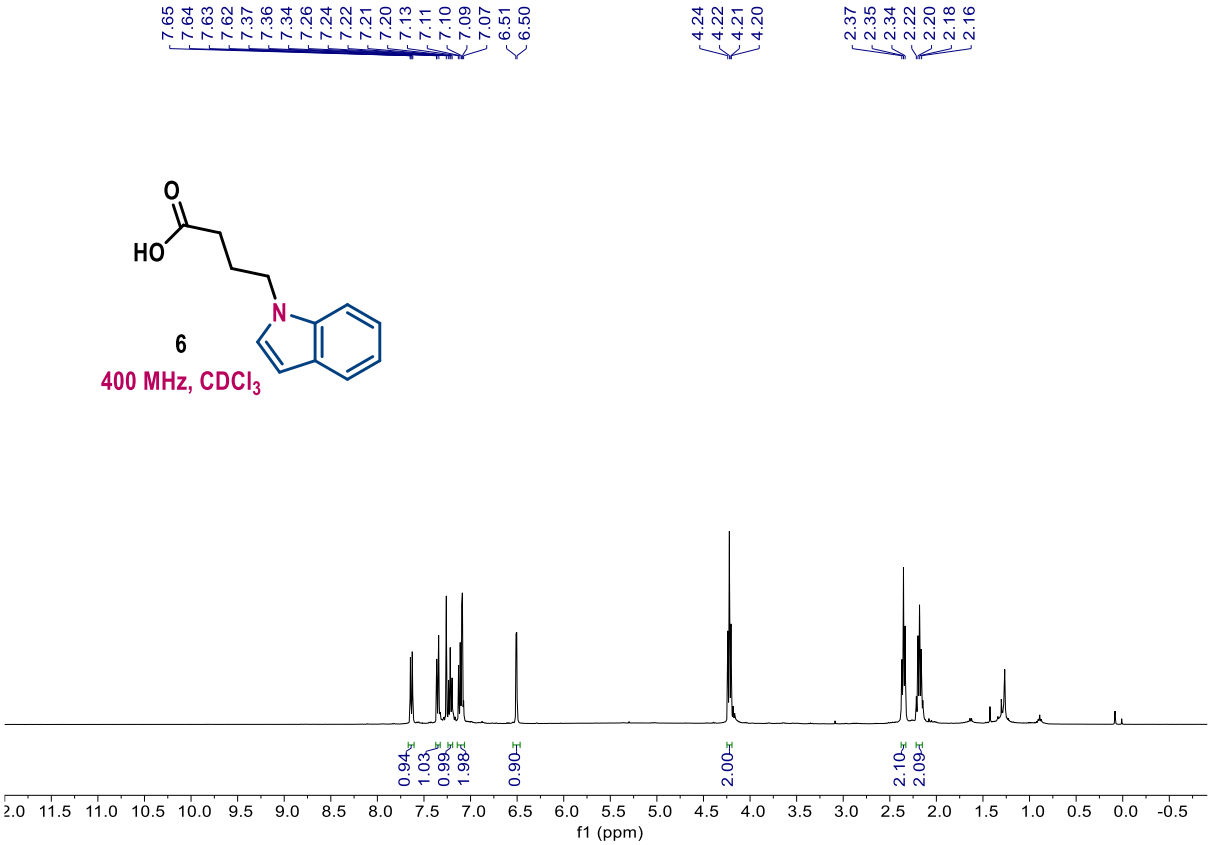

170.23
148.35
138.37
136.59
135.93
134.31
130.65
129.96
128.11
127.50
125.05
121.92
121.86
121.32
118.88
116.66
114.43
103.38
100.72
77.48
77.16
76.84
45.81
34.11
25.89
O
H
N
H
N
N
4j
101 MHz, CDCl3
NC
f1 (ppm)

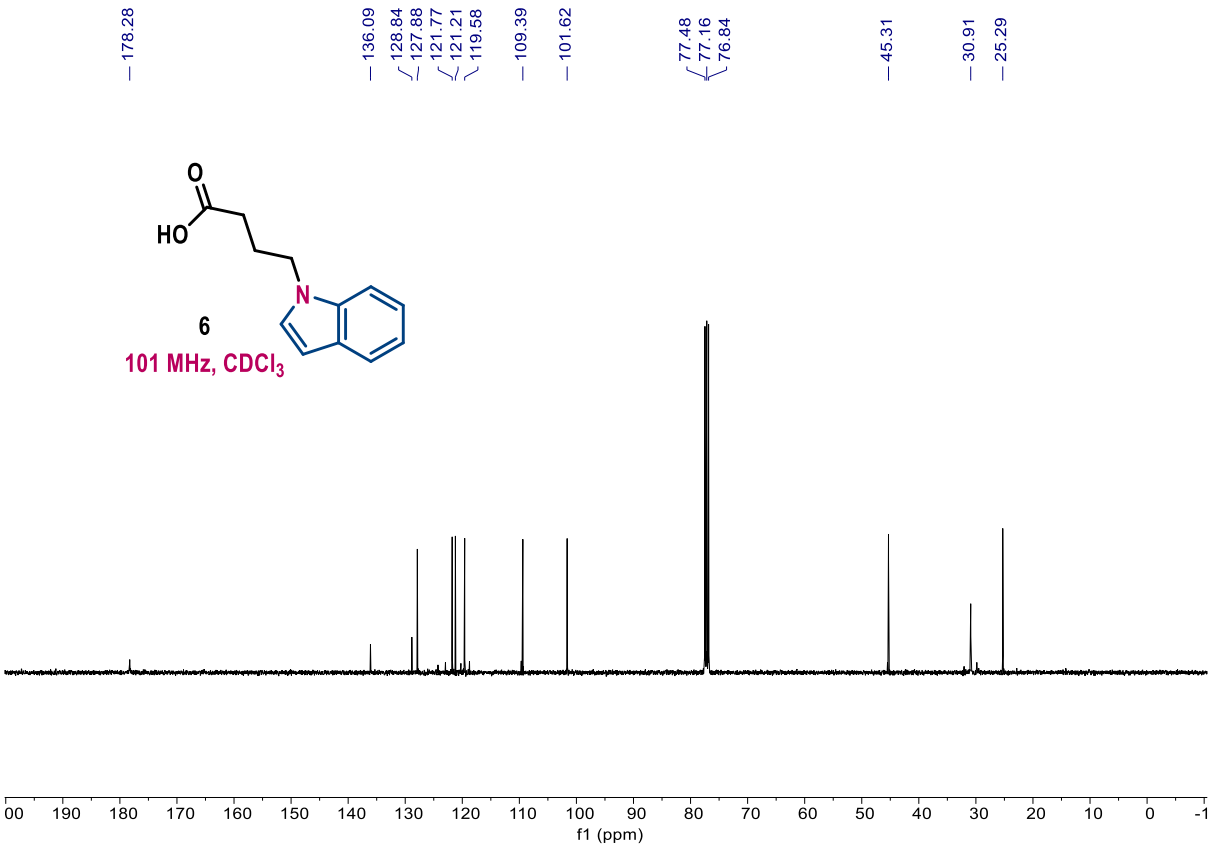

9.76
8.76
8.75
8.74
8.53
8.22
8.21
8.20
8.20
8.01
7.99
7.58
7.57
7.55
7.53
7.49
7.48
7.47
7.43
7.41
7.32
7.31
7.26
6.68
6.67
4.38
4.37
4.35
2.58
2.57
2.55
2.40
2.38
2.37
2.36
2.34
O
H
N
H
N
N
4k
500 MHz, CDCl3
NO2
0.86
1.97
0.95
0.98
1.00
2.06
1.01
0.99
1.00
1.02
2.09
2.05
2.07
f1 (ppm)

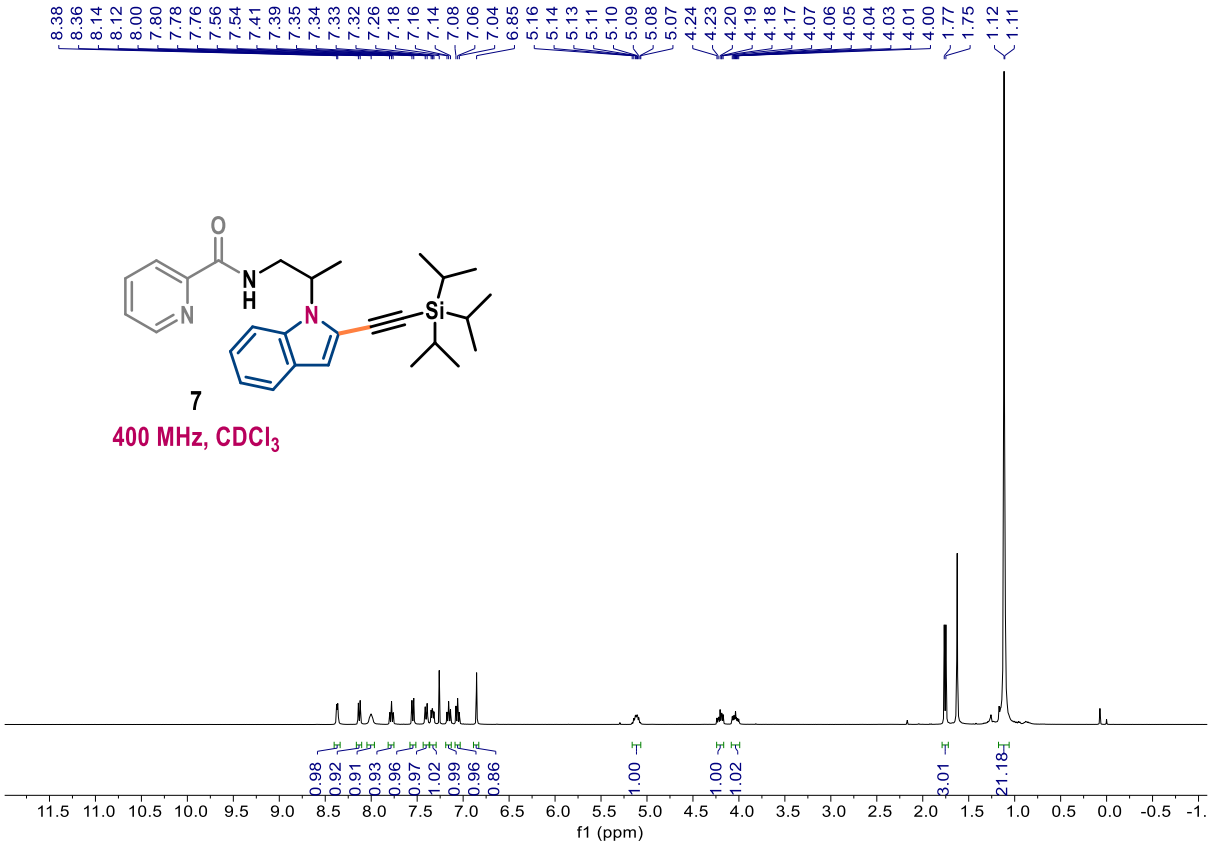

170.25
148.00
141.65
139.10
134.05
131.11
128.17
127.82
127.66
122.03
121.81
118.33
117.44
109.49
104.44
77.41
77.16
76.91
45.92
34.09
25.87
O
H
N
H
N
N
4k
126 MHz, CDCl3
NO2
f1 (ppm)

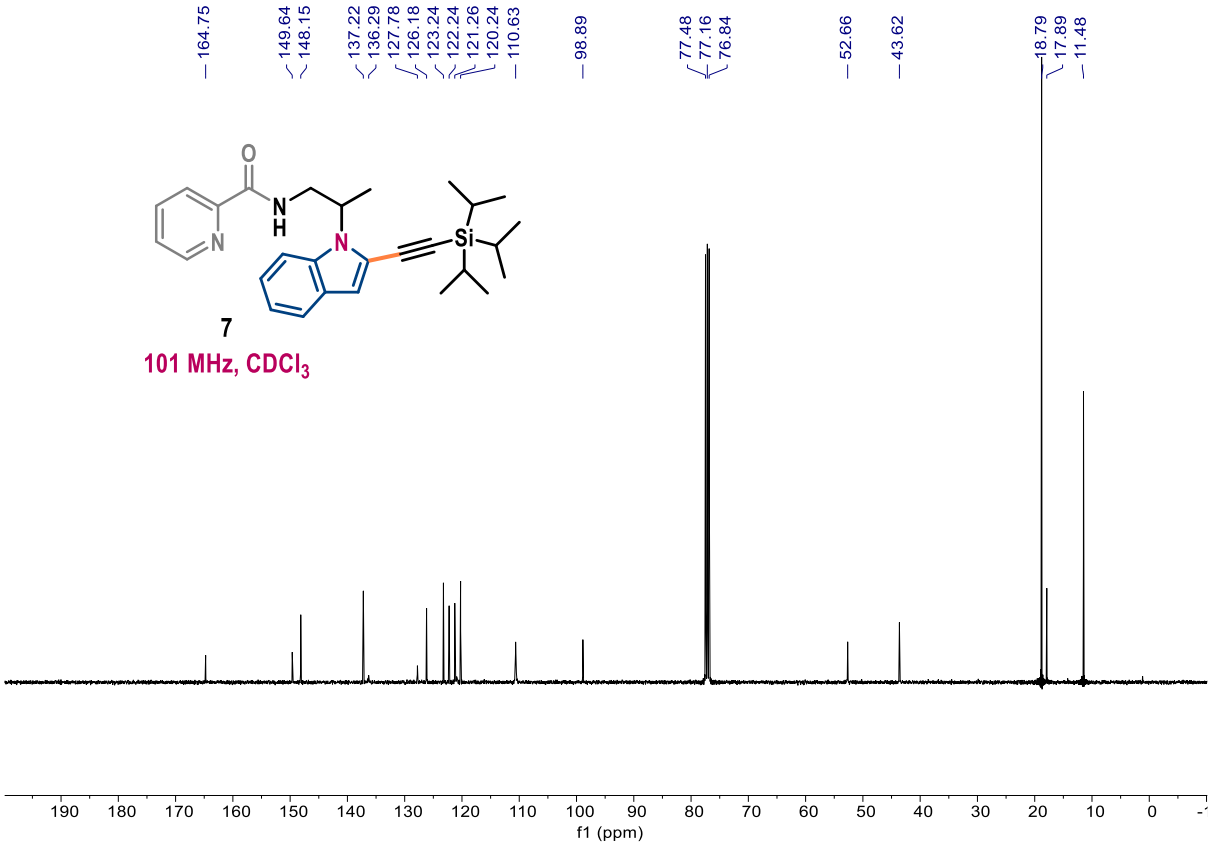

7.64
7.63
7.62
7.40
7.39
7.37
7.26
7.22
7.21
7.20
7.18
7.18
7.17
7.13
7.12
7.11
7.10
7.09
6.57
6.56
4.75
4.74
4.73
4.71
4.44
3.65
3.64
3.63
3.62
3.61
3.60
3.37
3.35
3.34
3.33
3.32
3.31
1.54
1.53
1.39
O
O
N
H
N
5
500 MHz, CDCl3
1.00
1.04
1.07
1.03
1.05
0.94
1.00
0.99
1.04
1.04
3.02
9.10
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

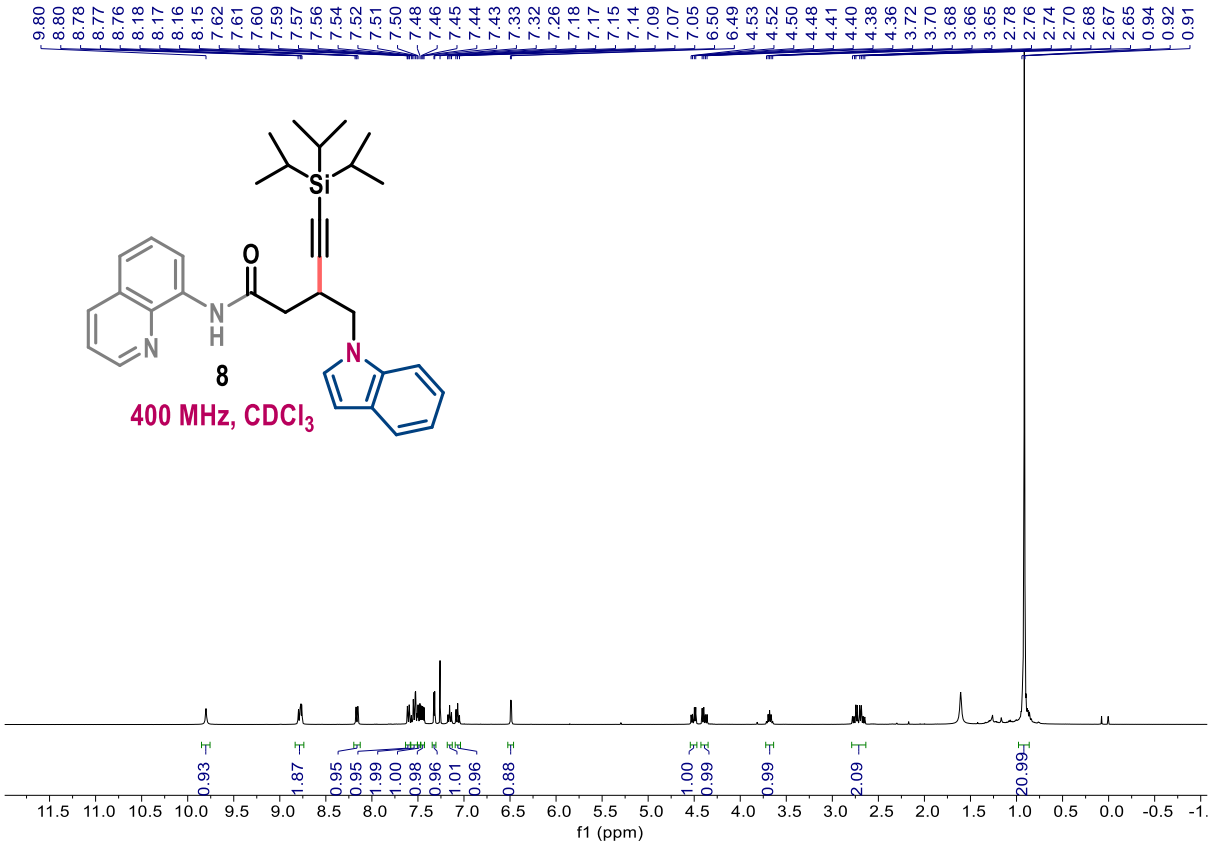

156.07
136.46
128.58
123.76
121.75
121.08
119.71
109.73
102.33
79.76
77.41
77.16
76.91
51.36
46.38
28.43
18.46
O
O
N
H
N
5
126 MHz, CDCl3
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

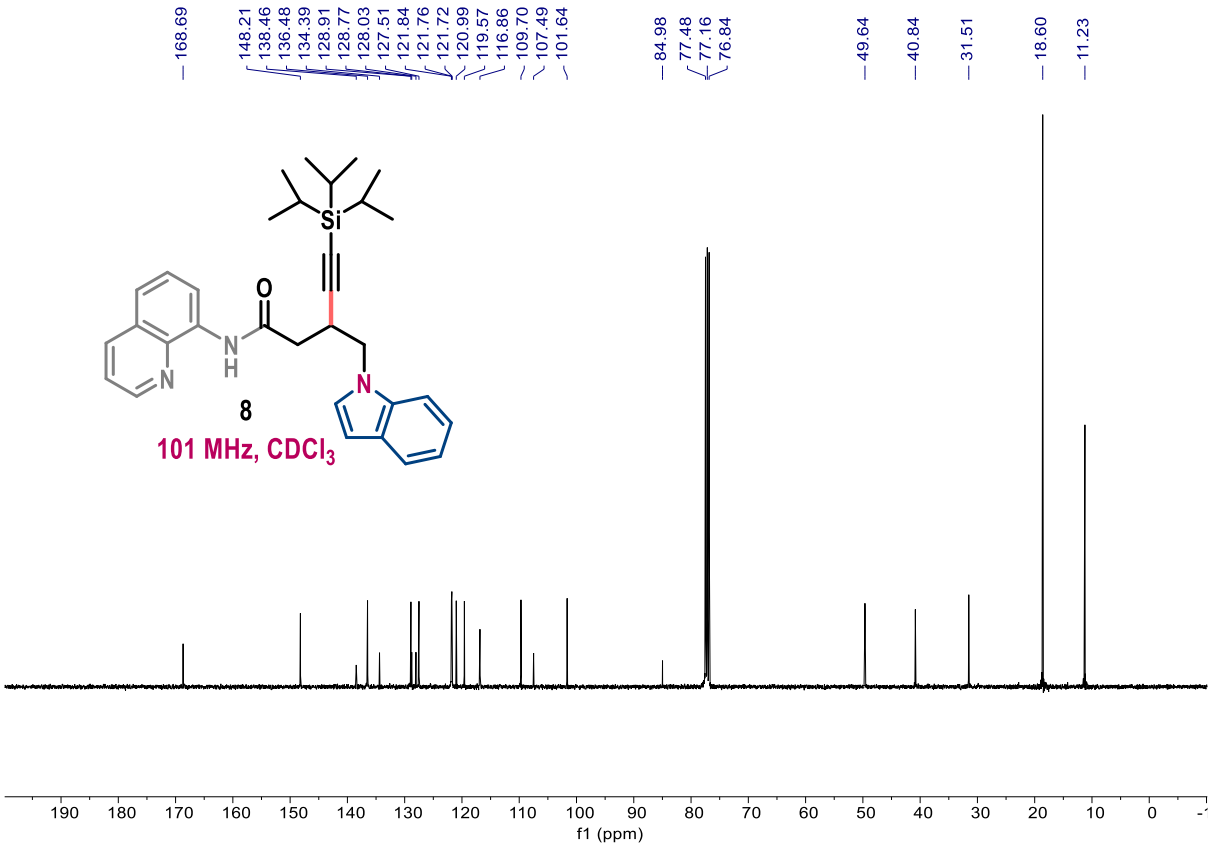

7.65
7.64
7.63
7.62
7.37
7.36
7.34
7.26
7.24
7.22
7.21
7.20
7.13
7.11
7.10
7.09
7.07
6.51
6.50
4.24
4.22
4.21
4.20
2.37
2.35
2.34
2.22
2.20
2.18
2.16
O
HO
N
6
400 MHz, CDCl3
0.94
1.03
0.99
1.98
0.90
2.00
2.10
2.09
f1 (ppm)


178.28
136.09
128.84
127.88
121.77
121.21
119.58
109.39
101.62
77.48
77.16
76.84
45.31
30.91
25.29
O
HO
N
6
101 MHz, CDCl3
f1 (ppm)


8.38 8.36 8.14 8.12 8.00 7.80 7.78 7.76 7.56 7.54 7.41 7.39 7.35 7.34 7.33 7.32 7.26 7.18 7.16 7.14 7.08 7.06 7.04 6.85 5.16 5.14 5.13 5.11 5.10 5.09 5.08 5.07 4.24 4.23 4.20 4.19 4.18 4.17 4.07 4.06 4.05 4.04 4.03 4.01 4.00 1.77 1.75 1.12 1.11
O
N
H
N
Si
7
400 MHz, CDCl3
0.98 0.92 0.91 0.93 0.96 0.97 1.02 0.99 0.96 0.86 1.00 1.00 1.02 3.01 21.18
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)


164.75 149.64 148.15 137.22 136.29 127.78 126.18 123.24 122.24 121.26 120.24 110.63 98.89 77.48 77.16 76.84 52.66 43.62 18.79 17.89 11.48
O
N
H
N
Si
7
101 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.80
8.80
8.78
8.77
8.76
8.18
8.17
8.16
8.15
7.62
7.61
7.60
7.59
7.57
7.56
7.54
7.52
7.51
7.50
7.48
7.46
7.45
7.44
7.43
7.33
7.32
7.26
7.18
7.17
7.15
7.14
7.09
7.07
7.05
6.50
6.49
4.53
4.52
4.50
4.48
4.41
4.40
4.38
4.36
3.72
3.70
3.68
3.66
3.65
2.78
2.76
2.74
2.70
2.68
2.67
2.65
0.94
0.92
0.91
Si
O
N
H
N
N
8
400 MHz, CDCl3
0.93
1.87
0.95
0.95
1.99
1.00
0.98
0.96
1.01
0.96
0.88
1.00
0.99
0.99
2.09
20.99
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)


168.69
148.21
138.46
136.48
134.39
128.91
128.77
128.03
127.51
121.84
121.76
121.72
120.99
119.57
116.86
109.70
107.49
101.64
84.98
77.48
77.16
76.84
49.64
40.84
31.51
18.60
11.23
Si
O
N
H
N
N
8
101 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)