Palladium-Catalyzed Site-Selective C−H Arylation of 2,2′-Bipyridine-6-carboxamides via a Rollover Cyclometalation Pathway

Table of Contents

1. General Information S2

2. Experimental Section S3-S28

2.1 Procedure for Synthesis of **S_1-S_3** S3

2.2 Procedure for Synthesis of **1a-1n** S3-S7

2.3 Procedure for Synthesis of **3a-3h**, **3m** S7-S12

2.4 Procedure for Synthesis of **4a-4v** S12-S23

2.5 Procedure for Synthesis of **I-1-I-2** S23-S26

2.6 1 mmol-Scale Experiment of **3a** S27

2.7 Reversibility and KIE Study S27-S28

3. References S28

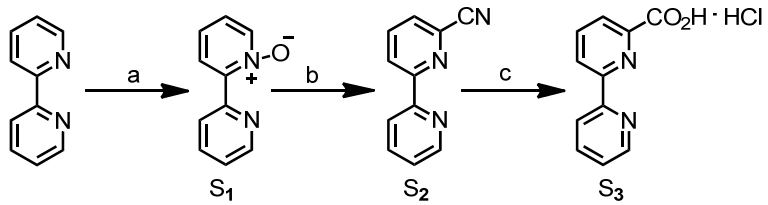
4. ^{1}H and ^{13}C NMR Spectra S28-S71

1. General Information

All solvents and chemicals were from Sigma-Aldrich, Tansoole, Energy Chemical , Acros and Alfa Aesar and used directly without further purification. All reactions were performed under an inert atmosphere of nitrogen in oven-dried glassware, unless otherwise stated. Flash column chromatography was performed over silica gel (300-400 mesh). ^{1}H NMR spectra were recorded on a Bruker AVIII-500M spectrometers, Chemical shifts (in ppm) were referenced to $CHCl_3$ (δ =7.26 ppm) as an internal standard. ^{13}C NMR spectra were obtained by using the same NMR spectrometers and were calibrated with $CDCl_3$ (δ = 77.0 ppm). Chemical shifts (δ) are reported in ppm, and coupling constants (J) are in Hertz (Hz). Multiplicities are reported using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. High-resolution mass spectra (HRMS) were recorded on an Agilent 1290 Mass spectrometer using ESI-TOF (electrospray ionization-time of flight).

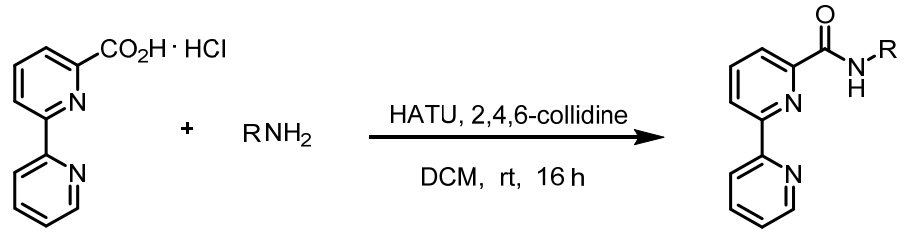
2.1 Procedure for Synthesis of S_1-S_3

S_1 and **S_2** were synthesized following a literature procedure[1]. **S_3** was synthesized following a literature procedure[2].



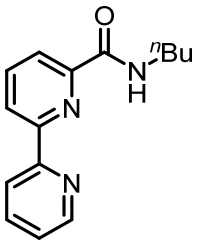
(a) TFA, 1.5 equiv H_2O_2, rt, 2.5 h; (b) 2.5 equiv TMSCN, 1 equiv Benzoyl chloride, DCM, 5 d; (c) 4 equiv NaOH, C_2H_5OH/H_2O = 2:1, reflux, 30 min; then HCl (1 M), pH = 3.8.

2.2 Procedure for Synthesis of 1a-1i



To a 50-mL oven-dried round-bottom flask were added **S_3** (2,2'-bipyridine-6-carboxylic acid hydrochloride) (1 equiv, 4.24 mmol) in dichloromethane (25 mL). The solution was added appropriate amines (1.8 equiv, 7.63 mmol) and 2,4,6-collidine (1 equiv, 4.24 mmol), followed by addition of HATU (2 equiv, 8.48 mmol). The mixture was stirred at room temperature overnight. The crude mixture was quenched with aqueous $NaHCO_3$ and extracted with DCM (3 × 15 mL), dried over Mg_2SO_4, concentrated *in vacuo*. The crude amide product was purified by silica gel column chromatography to afford the pure product.

***N*-butyl-[2,2'-bipyridine]-6-carboxamide (1a)**

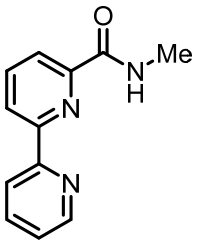


1a

The title compound **1a** was prepared from **S_3** (1 g, 4.24 mmol) and *n*-butylamine (0.56 g, 7.63 mmol) according to the general procedure. Purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a colorless solid (0.99 g, 92% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 – 8.68 (m, 1H), 8.55 (dd, *J* = 7.9, 0.5 Hz, 1H), 8.38 (d, *J* = 7.9 Hz, 1H), 8.24 (dd, *J* = 7.7, 0.5 Hz, 1H), 8.16

(s, 1H), 8.01 – 7.95 (m, 1H), 7.89 – 7.83 (m, 1H), 7.38 – 7.34 (m, 1H), 3.56 – 3.52 (m, 2H), 1.72 – 1.63 (m, 2H), 1.52 – 1.42 (m, 2H), 0.99 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.1, 155.1, 154.6, 149.4, 149.3, 138.3, 136.8, 124.0, 123.5, 122.2, 120.8, 39.2, 31.8, 20.2, 13.8; HRMS (ESI-TOF) calcd for $C_{15}H_{18}N_3O^+$ $[M+H]^+$: 256.1444, found: 256.1444.

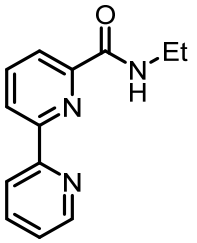
***N*-methyl-[2,2'-bipyridine]-6-carboxamide (1b)**



1b

Synthesized from **S$_3$** (1 g, 4.24 mmol) and methanamine hydrochloride (1.03 g, 7.63 mmol) following general procedure. Purification using preparative TLC (5:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a pale-yellow solid (0.79 g, 87% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.73 – 8.68 (m, 1H), 8.55 (dd, J = 7.9, 1.0 Hz, 1H), 8.40 (d, J = 7.9 Hz, 1H), 8.24 (dd, J = 7.6, 1.0 Hz, 1H), 8.14 (s, 1H), 8.00 – 7.94 (m, 1H), 7.87 – 7.82 (m, 1H), 7.37 – 7.32 (m, 1H), 3.10 (d, J = 5.0, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.9, 155.1, 154.6, 149.3, 149.3, 138.3, 136.8, 124.1, 123.5, 122.1, 120.9, 26.2; HRMS (ESI-TOF) calcd for $C_{12}H_{11}N_3NaO^+$ $[M+Na]^+$: 236.0794, found: 236.0793.

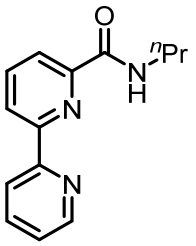
***N*-ethyl-[2,2'-bipyridine]-6-carboxamide (1c)**



1c

Synthesized from **S$_3$** (1 g, 4.24 mmol) and ethylamine (0.34 g, 7.63 mmol) following general procedure. Purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a colorless solid (0.88 g, 92% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.71 (d, J = 4.7 Hz, 1H), 8.55 (dd, J = 7.9, 0.9 Hz, 1H), 8.39 (d, J = 7.9 Hz, 1H), 8.24 (dd, J = 7.7, 0.9 Hz, 1H), 8.12 (s, 1H), 7.99 (t, J = 7.8 Hz, 1H), 7.82 – 7.90 (m, 1H), 7.39 – 7.33 (m, 1H), 3.63 – 3.52 (m, 2H), 1.33 (t, J = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.1, 155.1, 154.6, 149.4, 149.3, 138.3, 136.9, 124.1, 123.5, 122.2, 120.9, 34.3, 15.0; HRMS (ESI-TOF) calcd for $C_{13}H_{14}N_3O^+$ $[M+H]^+$: 228.1131, found: 228.1131.

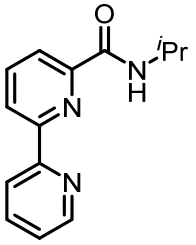
***N*-propyl-[2,2'-bipyridine]-6-carboxamide (1d)**



1d

Synthesized from **S₃** (1 g, 4.24 mmol) and propan-1-amine (0.45 g, 7.63 mmol) following general procedure. Purification using preparative TLC (8:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a colorless solid (0.92 g, 90% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.71 (d, *J* = 4.3 Hz, 1H), 8.58 – 8.47 (m, 1H), 8.38 (d, *J* = 7.9 Hz, 1H), 8.27 – 8.21 (m, 1H), 8.18 (s, 1H), 8.01 – 7.90 (m, 1H), 7.89 – 7.77 (m, 1H), 7.39 – 7.28 (m, 1H), 3.54 – 3.43 (m, 2H), 1.77 – 1.62 (m, 2H), 1.06 – 0.95 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.1, 155.0, 154.5, 149.4, 149.2, 138.2, 136.8, 124.0, 123.4, 122.1, 120.8, 41.1, 23.0, 11.5; HRMS (ESI-TOF) calcd for $C_{14}H_{15}N_3NaO^+$ $[M+Na]^+$: 264.1107, found: 264.1110.

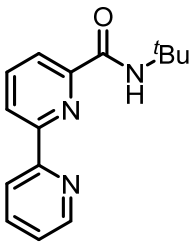
***N*-isopropyl-[2,2'-bipyridine]-6-carboxamide (1e)**



1e

Synthesized from **S₃** (1 g, 4.24 mmol) and isopropylamine (0.45 g, 7.63 mmol) following general procedure. Purification using preparative TLC (4:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a colorless solid (0.91 g, 89% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.72 – 8.70 (m, 1H), 8.55 (d, *J* = 7.9 Hz, 1H), 8.38 (d, *J* = 7.9 Hz, 1H), 8.24 (d, *J* = 7.6 Hz, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 7.95 (d, *J* = 7.5 Hz, 1H), 7.89 – 7.85 (m, 1H), 7.38 – 7.35 (m, 1H), 4.37 – 4.31 (m, 1H), 1.35 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.3, 155.1, 154.6, 149.5, 149.3, 138.3, 136.9, 124.1, 123.5, 122.2, 120.9, 41.4, 22.8; HRMS (ESI-TOF) calcd for $C_{14}H_{15}N_3NaO^+$ $[M+Na]^+$: 264.1107, found: 264.1110.

***N*-(tert-butyl)-[2,2'-bipyridine]-6-carboxamide (1f)**

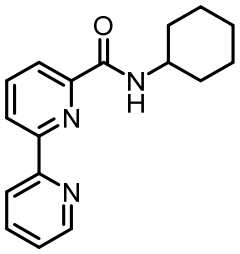


1f

Synthesized from **S₃** (1 g, 4.24 mmol) and tert-butylamine (0.56 g, 7.63 mmol) following general procedure. Purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the

product as a off-white solid (1.06 g, 98% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.70 (d, *J* = 2.3 Hz, 1H), 8.56 – 8.53 (m, 1H), 8.34 (dd, *J* = 7.9, 2.3 Hz, 1H), 8.23 – 8.20 (m, 1H), 8.11 (s, 1H), 7.99 – 7.95 (m, 1H), 7.88 – 7.84 (m, 1H), 7.35 (dd, *J* = 5.5, 1.9 Hz, 1H), 1.55 (d, *J* = 1.8 Hz, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.3, 155.2, 154.4, 150.1, 149.3, 138.3, 136.9, 124.0, 123.3, 121.7, 120.7, 50.9, 28.8; HRMS (ESI-TOF) calcd for $C_{15}H_{17}N_3NaO^+$ $[M+Na]^+$: 278.1264, found: 278.1264.

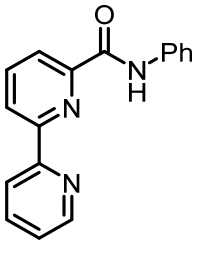
***N*-cyclohexyl-[2,2'-bipyridine]-6-carboxamide (1g)**



1g

Synthesized from **S$_3$** (1 g, .24 mmol) and cyclohexylamine (0.76 g, 7.63 mmol) following general procedure. Purification using preparative TLC (8:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a white solid (1.17 g, 98% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.73 – 8.69 (m, 1H), 8.55 (dd, *J* = 7.9, 1.0 Hz, 1H), 8.37 (d, *J* = 7.9 Hz, 1H), 8.24 (dd, *J* = 7.7, 1.0 Hz, 1H), 8.04 (d, *J* = 7.9 Hz, 1H), 7.98 (t, *J* = 7.8 Hz, 1H), 7.84–7.90 (m, 1H), 7.34 – 7.40 (m, 1H), 3.97 – 4.08 (m, 1H), 2.07 (dd, *J* = 12.2, 3.2 Hz, 2H), 1.85 – 1.77 (m, 2H), 1.72 – 1.64 (m, 1H), 1.53 – 1.43 (m, 2H), 1.43 – 1.34 (m, 2H), 1.32 – 1.23 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.2, 155.2, 154.6, 149.6, 149.3, 138.3, 136.9, 124.1, 123.4, 122.3, 120.8, 48.1, 33.1, 25.6, 24.9; HRMS (ESI-TOF) calcd for $C_{17}H_{19}N_3NaO^+$ $[M+Na]^+$: 304.1420, found: 304.1420.

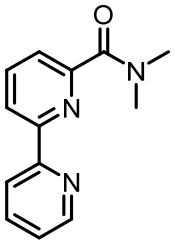
***N*-phenyl-[2,2'-bipyridine]-6-carboxamide (1h)**



1h

Synthesized from **S$_3$** (1 g, 4.24mmol) and aniline (0.71 g, 7.63 mmol) following general procedure. Purification using preparative TLC (2:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a white solid (0.99 g, 85% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.07 (s, 1H), 8.76 – 8.70 (m, 1H), 8.61 (dd, *J* = 7.9, 0.8 Hz, 1H), 8.42 (dd, *J* = 7.9, 0.9 Hz, 1H), 8.33 (d, *J* = 7.7 Hz, 1H), 8.00 – 8.07 (m, 1H), 7.93 – 7.87 (m, 1H), 7.84 – 7.80 (m, 2H), 7.42 (t, *J* = 7.9 Hz, 2H), 7.40 – 7.36 (m, 1H), 7.17 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.9, 154.8, 154.7, 149.4, 149.1, 138.7, 137.6, 137.0, 129.1, 124.4, 124.2, 124.0, 122.4, 120.9, 119.8; HRMS (ESI-TOF) calcd for $C_{17}H_{13}N_3NaO^+$ $[M+Na]^+$: 298.0951, found: 298.0951.

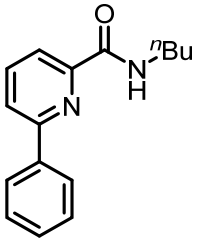
***N*,*N*-dimethyl-[2,2'-bipyridine]-6-carboxamide (1i)**



1i

Synthesized from **S_3** (1 g, 4.24 mmol) and dimethylamine (0.34 g, 7.63 mmol) following general procedure. Purification using preparative TLC (4:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a creamy white solid (0.84 g, 87% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (d, *J* = 1.7 Hz, 1H), 8.49 – 8.43 (m, 1H), 8.43 – 8.38 (m, 1H), 7.95 – 7.88 (m, 1H), 7.85 – 7.78 (m, 1H), 7.70 – 7.64 (m, 1H), 7.29 – 7.35 (m, 1H), 3.21 – 3.16 (m, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.8, 155.5, 154.5, 153.7, 149.1, 137.9, 136.9, 123.9, 123.6, 121.5, 121.2, 39.2, 35.9; HRMS (ESI-TOF) calcd for $C_{13}H_{14}N_3O^+$ $[M+H]^+$: 228.1131, found: 228.1131.

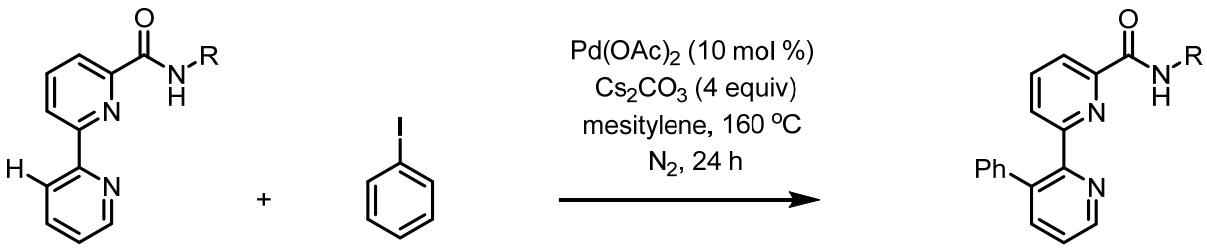
***N*-butyl-6-phenylpicolinamide(1n)**



1n

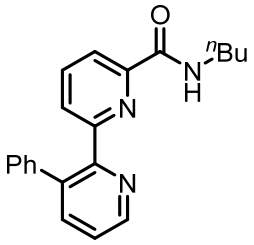
Synthesized from 6-phenylpicolinic acid (0.3 g, 1.51 mmol) and *n*-butylamine (0.2 g, 2.71 mmol) following general procedure. Purification using preparative TLC (20:1 hexane: ethyl acetate) gave the product as a creamy white oil (0.245g, 64% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 (t, *J* = 6.1 Hz, 1H), 8.16 (m, *J* = 7.6, 1.1 Hz, 1H), 8.03 – 7.97 (m, 2H), 7.90 (t, *J* = 7.7 Hz, 1H), 7.84 (m, *J* = 7.9, 1.1 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.48 – 7.43 (m, 1H), 3.52 (m, *J* = 7.3, 6.1 Hz, 2H), 1.71 – 1.61 (m, 2H), 1.45 (m, *J* = 14.7, 7.4 Hz, 2H), 0.98 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.3, 155.8, 149.8, 138.4, 138.1, 129.4, 128.8,126.9, 122.8, 120.5, 39.2, 31.8, 20.2, 13.8; HRMS (ESI-TOF) calcd for $C_{16}H_{18}N_2O^+$ $[M+Na]^+$: 277.1311, found: 277.1314.

2.3 Procedure for Synthesis of 3a-3h



To a dried 10 mL Schlenk tube equipped with a magnetic stir bar were added 2,2'-bipyridin-6-carboxamide (0.2 mmol), iodobenzene (0.6 mmol, 122.4 mg), $Pd(OAc)_2$ (0.02 mmol, 4.4 mg), Cs_2CO_3 (0.8 mmol, 260.6 mg), mesitylene (2 mL). Then the tube was evacuated and back filled with nitrogen (10 times). The mixtures were stirred at 16 °C under a blanket of nitrogen. After 24 hours, the reaction was cooled to room temperature; the crude reaction mixture was diluted with DCM, washed with H_2O and brine, dried over Mg_2SO_4. The organic phase was concentrated and purified, running through a silica flash column chromatography to give pure product.

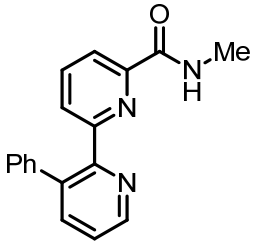
***N*-butyl-3'-phenyl-[2,2'-bipyridine]-6-carboxamide (3a)**



3a

3a was prepared from **1a** (0.2 mmol, 51.0 mg) and iodobenzene (0.6 mmol, 122.4 mg) according to the general procedure. After 24 hours, and purification using preparative TLC (8:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a colorless solid (53.6 mg, 81% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.73 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.16 (dd, *J* = 7.8, 1.0 Hz, 1H), 8.04 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 1H), 7.78 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.43 (dd, *J* = 7.7, 4.7 Hz, 1H), 7.35 – 7.29 (m, 3H), 7.22 – 7.16 (m, 2H), 6.80 (s, 1H), 3.20 – 3.13 (m, 2H), 1.44 – 1.37 (m, 2H), 1.33 –1.25 (m, 2H), 0.93 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.9, 155.9, 153.9, 148.4, 148.2, 141.0, 139.3, 137.9, 137.0, 128.7, 128.3, 126.8, 126.3, 123.3, 121.1, 38.7, 31.6, 20.0, 13.8; HRMS (ESI-TOF) calcd for $C_{21}H_{22}N_3O^+$ $[M+H]^+$: 332.1757, found: 332.1758.

***N*-methyl-3'-phenyl-[2,2'-bipyridine]-6-carboxamide (3b)**

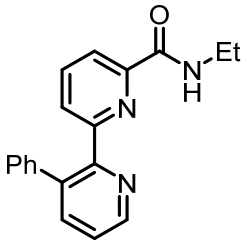


3b

3b was prepared from **1b** (0.2 mmol, 42.6 mg) and iodobenzene (0.6 mmol, 122.4 mg) according to the general procedure. After 24 hours, and purification using preparative TLC (8:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a colorless solid (32.9 mg, 57% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.75 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.21 – 8.19 (m, 1H), 8.03 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.90 (t, *J* = 7.8 Hz, 1H), 7.78 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.45 – 7.41 (m, 1H), 7.37 – 7.32 (m, 3H), 7.22 – 7.17 (m, 2H), 6.62 (s, 1H),

2.72 (d, J = 5.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.6, 155.7, 153.5, 148.3, 148.2, 141.4, 139.4, 138.0, 137.1, 128.8, 128.3, 126.7, 126.2, 123.4, 121.0, 25.6; HRMS (ESI-TOF) calcd for $C_{18}H_{16}N_3O$ $[M+H]^+$: 290.1288, found: 290.1287.

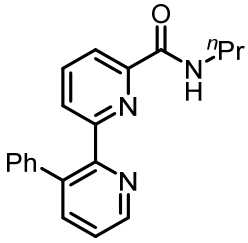
***N*-ethyl-3'-phenyl-[2,2'-bipyridine]-6-carboxamide (3c)**



3c

3c was prepared from **1c** (0.2 mmol, 45.4 mg) and iodobenzene (0.6 mmol, 122.4 mg) according to the general procedure. After 24 hours, and purification using preparative TLC (2:1:20 acetone: DCM: hexanes) gave the product as a off-white solid (41.2 mg, 68% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.72 (dd, J = 4.7, 1.7 Hz, 1H), 8.16 (dd, J = 7.8, 1.0 Hz, 1H), 8.04 (dd, J = 7.7, 1.0 Hz, 1H), 7.90 (t, J = 7.8 Hz, 1H), 7.77 (dd, J = 7.7, 1.7 Hz, 1H), 7.42 (dd, J = 7.7, 4.7 Hz, 1H), 7.34 – 7.29 (m, 3H), 7.20 – 7.18 (m, 2H), 6.80 (s, 1H), 3.25 – 3.17 (m, 2H), 1.07 (t, J = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.8, 155.9, 153.7, 148.3, 148.2, 141.0, 139.3, 137.9, 137.0, 128.7, 128.2, 126.8, 126.3, 123.3, 121.0, 33.8, 14.7; HRMS (ESI-TOF) calcd for $C_{19}H_{18}N_3O^+$ $[M+H]^+$: 304.1444, found: 304.1444.

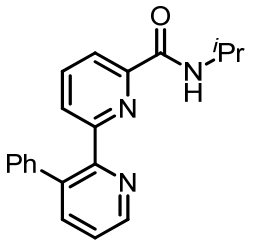
3'-phenyl-*N*-propyl-[2,2'-bipyridine]-6-carboxamide (3d)



3d

3d was prepared from **1d** (0.2 mmol, 48.2 mg) and iodobenzene (0.6 mmol, 122.4 mg) according to the general procedure. After 24 hours, and purification using preparative TLC (8:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a yellow solid (37.4 mg, 59% yield); 1H NMR (500 MHz, CDCl3) δ 8.72 (dd, J = 4.7, 1.6 Hz, 1H), 8.17 – 8.14 (m, 1H), 8.04 (d, J = 7.6 Hz, 1H), 7.90 (t, J = 7.8 Hz, 1H), 7.77 (dd, J = 7.7, 1.6 Hz, 1H), 7.42 (dd, J = 7.7, 4.7 Hz, 1H), 7.33 – 7.29 (m, 3H), 7.18 (dd, J = 7.6, 1.7 Hz, 2H), 6.84 (s, 1H), 3.15 – 3.11 (m, 2H), 1.47 – 1.42 (m, 2H), 0.87 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.0, 155.9, 153.8, 148.4, 148.2, 140.9, 139.3, 137.9, 137.0, 128.7, 128.3, 126.8, 126.3, 123.3, 121.1, 40.7, 22.8, 11.4; HRMS (ESI-TOF) calcd for $C_{20}H_{19}N_3NaO^+$ $[M+Na]^+$: 340.1420, found: 340.1420.

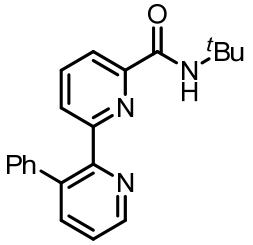
***N*-isopropyl-3'-phenyl-[2,2'-bipyridine]-6-carboxamide (3e)**



3e

3e was prepared from **1e** (0.2 mmol, 48.2 mg) and iodobenzene (0.6 mmol, 122.4 mg) according to the general procedure. After 24 hours, and purification using preparative TLC (8:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a pale-yellow (38.2 mg, 60% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.72 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.10 (dd, *J* = 7.8, 1.1 Hz, 1H), 8.06 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 1H), 7.79 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.44 (dd, *J* = 7.8, 4.7 Hz, 1H), 7.33 – 7.28 (m, 3H), 7.18 – 7.15 (m, 2H), 6.83 (d, *J* = 8.0 Hz, 1H), 4.09 – 4.00 (m, 1H), 1.07 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.1, 156.2, 154.2, 148.5, 148.1, 140.6, 139.2, 137.9, 137.0, 128.8, 128.4, 127.2, 126.5, 123.4, 121.1, 41.0, 22.5; HRMS (ESI-TOF) calcd for $C_{20}H_{20}N_3O^+$ $[M+H]^+$: 318.1601, found: 318.1601.

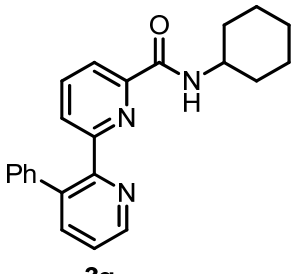
***N*-(tert-butyl)-3'-phenyl-[2,2'-bipyridine]-6-carboxamide (3f)**



3f

3f was prepared from **1f** (0.2 mmol, 51.0 mg) and iodobenzene (0.2 mmol, 122.4 mg) according to the general procedure. After 24 hours, purification using preparative TLC (5:4:1 hexane : DCM : EA) gave the product as a white solid (29.8 mg, 45% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.72 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.06 (dd, *J* = 7.7, 1.1 Hz, 1H), 8.02 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 1H), 7.81 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.45 (dd, *J* = 7.8, 4.7 Hz, 1H), 7.30 – 7.27 (m, 3H), 7.17 – 7.10 (m, 3H), 1.29 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.1, 156.2, 154.6, 149.2, 148.1, 140.2, 139.1, 138.0, 137.1, 128.9, 128.5, 127.0, 126.5, 123.4, 120.6, 50.6, 28.5; HRMS (ESI-TOF) calcd for $C_{21}H_{22}N_3O^+$ $[M+H]^+$: 332.1757, found: 332.1757.

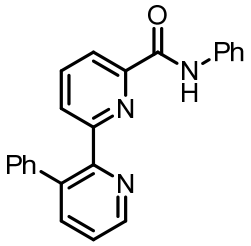
***N*-cyclohexyl-3'-phenyl-[2,2'-bipyridine]-6-carboxamide (3g)**



3g

3g was prepared from **1g** (0.2 mmol, 56.2 mg) and iodobenzene (0.6 mmol, 122.4 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane : EA and 5-10% Et_3N) gave the product as a white solid (52.8 mg, 74% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.71 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.08 (dd, *J* = 4.1, 1.0 Hz, 1H), 8.06 (d, *J* = 3.2 Hz, 1H), 7.90 (t, *J* = 7.8 Hz, 1H), 7.79 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.43 (dd, *J* = 7.7, 4.7 Hz, 1H), 7.32 – 7.27 (m, 3H), 7.18 – 7.14 (m, 2H), 6.93 (d, *J* = 8.3 Hz, 1H), 3.78 – 3.67 (m, 1H), 1.83 – 1.74 (m, 2H), 1.74 – 1.67 (m, 2H), 1.66 – 1.59 (m, 1H), 1.38 – 1.29 (m, 2H), 1.21 – 1.14 (m, 1H), 1.07 – 1.01(m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.0, 156.2, 154.2, 148.6, 148.0, 140.3, 139.1, 137.8, 136.9, 128.7, 128.4, 127.1, 126.5, 123.3, 121.1, 48.0, 32.6, 25.5, 24.8; HRMS (ESI-TOF) calcd for $C_{23}H_{24}N_3O^+$ $[M+H]^+$: 358.1914, found: 358.1914.

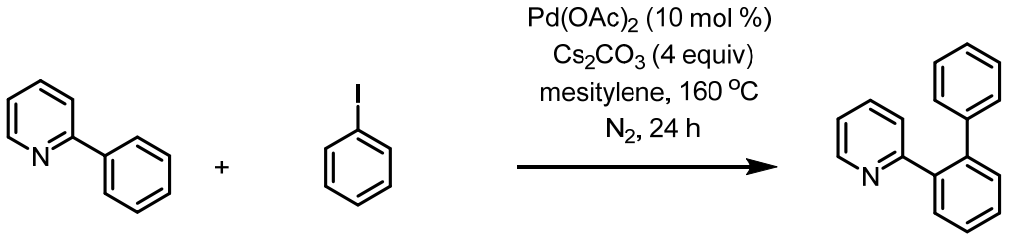
***N*,3'-diphenyl-[2,2'-bipyridine]-6-carboxamide (3h)**



3h

3h was prepared from **1h** (0.2 mmol, 55.0 mg) and iodobenzene (0.6 mmol, 22.4 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a white solid (28.8 mg, 41% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.90 (s, 1H), 8.75 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.20 – 8.13 (m, 2H), 7.98 (dd, *J* = 9.7, 5.9 Hz, 1H), 7.84 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.55 – 7.50 (m, 2H), 7.46 (dd, *J* = 7.8, 4.7 Hz, 1H), 7.34 (dd, *J* = 10.8, 5.1 Hz, 2H), 7.31 – 7.27 (m, 2H), 7.25 – 7.20 (m, 2H), 7.19 – 7.14 (m, 1H), 7.13 – 7.08 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.7, 156.2, 153.9, 148.2, 148.1, 140.3, 139.2, 138.3, 137.4, 137.0, 128.7, 128.7, 128.5, 127.3, 127.0, 124.0, 123.5, 121.3, 120.0; HRMS (ESI-TOF) calcd for $C_{23}H_{17}N_3NaO^+$ $[M+Na]^+$: 374.1264, found: 374.1264.

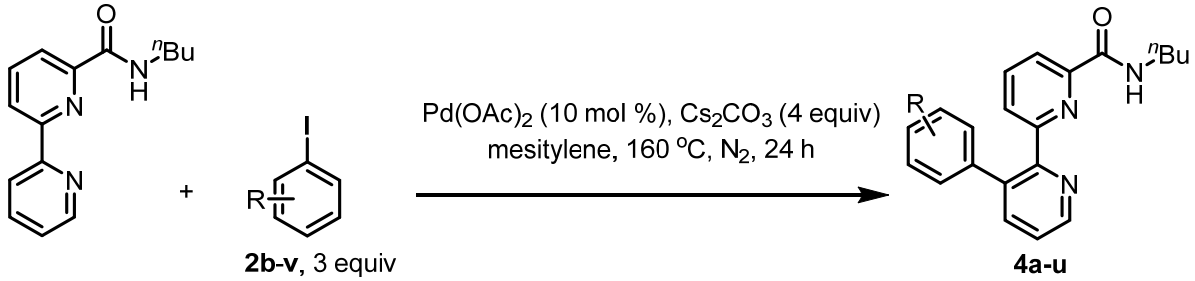
2-(biphenyl-2-yl)pyridine (3m)



To a dried 10 mL Schlenk tube equipped with a magnetic stir bar were added 2-phenylpyridine (0.2 mmol, 31 mg), iodobenzene (0.6 mmol, 122.4 mg), $Pd(OAc)_2$ (0.02 mmol, 4.5 mg), Cs_2CO_3 (0.8 mmol, 260.6 mg), mesitylene (2 mL). Then the tube was evacuated and back filled with nitrogen (10 times). The mixtures were stirred at 160 °C under a blanket of nitrogen. After 24 hours, the reaction was cooled to room temperature; the crude reaction mixture was diluted with DCM, washed with H_2O and brine, dried

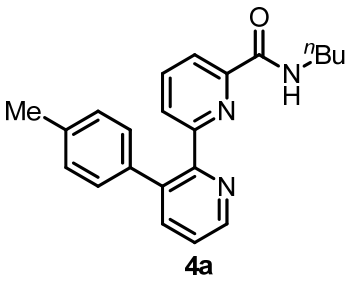
over Mg_2SO_4. The organic phase was concentrated and purification using preparative TLC (15:1 hexane: ethyl acetate) gave the product as a colorless solid (6 mg, 13% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.64-8.62 (m, 1H), 7.71 – 7.69 (m, 1H), 7.48 – 7.43 (m, 3H), 7.39-7.36 (m, 1H), 7.24 – 7.22 (m, 3H), 7.17 – 7.15 (m, 2H), 7.11-7.08 (m, 1H), 6.88 (dd, J = 7.9, 0.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.2, 149.4, 141.3, 140.6, 139.4, 135.2, 130.5, 130.4, 129.7, 128.5, 128.0, 127.6, 126.7, 125.4, 121.3.

2.4 Procedure for Synthesis of 4a-4v



To a dried 10 mL Schlenk tube equipped with a magnetic stir bar were added *N*-butyl-[2,2'-bipyridine]-6-carboxamide （0.2 mmol, 51.0 mg）, iodobenzene (0.6 mmol), $Pd(OAc)_2$ (0.02 mmol, 4.4 mg), Cs_2CO_3 (0.8 mmol, 260.6 mg), mesitylene (2 mL). Then the tube was evacuated and back filled with nitrogen (10 times). The mixtures were stirred at 160 °C under a blanket of nitrogen. After 24-48 hours, the reaction was cooled to room temperature. The crude reaction mixture was diluted with DCM, washed with H_2O and brine, dried over Mg_2SO_4. The organic phase was concentrated and purified, running through a silica flash column chromatography (ethyl acetate / hexane and 5-10% Et_3N) to give pure product.

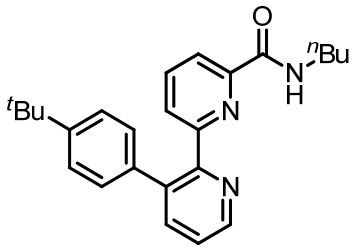
***N*-butyl-3'-(p-tolyl)-[2,2'-bipyridine]-6-carboxamide (4a)**



4a

4a was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-iodo-4-methylbenzene (0.6 mmol, 130.8 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane:ethyl acetate and 5-10% Et_3N) gave the product as a yellow oil (57.3 mg, 82% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.70 (dd, J = 4.7, 1.5 Hz, 1H), 8.16 – 8.11 (m, 1H), 8.04 (d, J = 7.1 Hz, 1H), 7.90 (t, J = 7.8 Hz, 1H), 7.76 (dd, J = 7.7, 1.6 Hz, 1H), 7.41 (dd, J = 7.7, 4.7 Hz, 1H), 7.12 (d, J = 7.9 Hz, 2H), 7.06 (d, J = 8.0 Hz, 2H), 6.92 (d, J = 5.2 Hz, 1H), 3.21 – 3.14 (m, 2H), 2.35 (s, 3H), 1.44 – 1.37 (m, 2H), 1.33 – 1.24 (m, 2H), 0.94 (t, J = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.9, 156.0, 153. 8, 148.3, 147.9, 139.2, 137.9, 137.8, 136.9, 136.4, 128.9, 128.5, 126.2, 123.3, 120.9, 38.7, 31.6, 21.0, 20.0, 13.7; HRMS (ESI-TOF) calcd for $C_{22}H_{24}N_3O^+$ $[M+H]^+$: 346.1914. found: 346.1914.

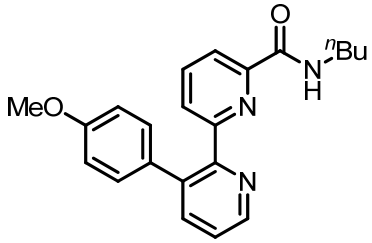
***N*-butyl-3'-(4-(tert-butyl)phenyl)-[2,2'-bipyridine]-6-carboxamide (4b)**



4b

4b was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-(tert-butyl)-4-iodobenzene (0.6 mmol, 156.1 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane:ethyl acetate and 5-10% Et_3N) gave the product as a yellow oil (61.9 mg, 80% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.71 (dd, *J* = 4.7, 1.3 Hz, 1H), 8.05 (d, *J* = 3.3 Hz, 1H), 8.03 (d, *J* = 3.5 Hz, 1H), 7.90 (t, *J* = 7.8 Hz, 1H), 7.79 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.42 (dd, *J* = 7.7, 4.8 Hz, 1H), 7.31 (d, *J* = 8.3 Hz, 2H), 7.09 (d, *J* = 8.3 Hz, 3H), 3.21 – 3.15 (m, 2H), 1.46 – 1.40 (m, 2H), 1.32 – 1.26 (m, 11H), 0.92 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.0, 156.3, 154.4, 150.0, 148.4, 148.0, 139.2, 137.9, 137.6, 137.0, 128.4, 126.4, 125.2, 123.3, 120.9, 38.9, 34.5, 31.5, 31.3, 20.1, 13.8; HRMS (ESI-TOF) calcd for $C_{25}H_{30}N_3O^+$ $[M+H]^+$: 388.2383, found: 388.2387.

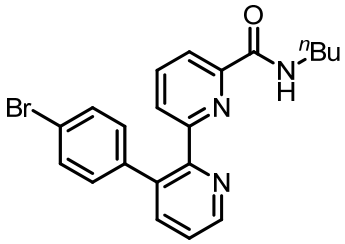
***N*-butyl-3'-(4-methoxyphenyl)-[2,2'-bipyridine]-6-carboxamide (4c)**



4c

4c was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-iodo-4-methoxybenzene (0.6 mmol, 140.4 mg) according to the general procedure. After 24 hours, purification using preparative TLC (4:1 hexane : ethyl acetate and 5-10% Et_3N) gave the product as a scream oil (39.7 mg, 55% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.70 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.09 (dd, *J* = 7.8, 1.1 Hz, 1H), 8.05 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.90 (t, *J* = 7.8 Hz, 1H), 7.76 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.41 (dd, *J* = 7.8, 4.7 Hz, 1H), 7.11 – 7.07 (m, 2H), 7.01 (t, *J* = 5.5 Hz, 1H), 6.86 – 6.83 (m, 2H), 3.79 (s, 3H), 3.23 – 3.20 (m, 2H), 1.45 – 1.39 (m, 2H), 1.35 – 1.29 (m, 2H), 0.94 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.0, 158.7, 156.2, 153.9, 148.5, 147.9, 139.2, 137.9, 136.7, 133.0, 130.0, 126.4, 123.3, 121.0, 113.7, 55.1, 38.8, 31.4, 20.1, 13.7; HRMS (ESI-TOF) calcd for $C_{22}H_{24}N_3O_2^+$ $[M+H]^+$: 362.1863, found: 362.1863.

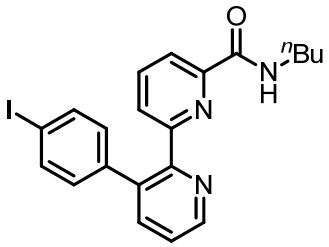
3'-(4-bromophenyl)-*N*-butyl-[2,2'-bipyridine]-6-carboxamide (4d)



4d

4d was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-bromo-4-iodobenzene (0.6 mmol, 169.7 mg) according to the general procedure. After 24 hours , purification using preparative TLC (10:1 hexane:ethyl acetate and 5-10% Et_3N) gave the product as a scream solid (69.7 mg, 85% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.79 –8.71 (m, 1H), 8.22 (t, *J* = 7.2 Hz, 1H), 8.15 – 8.03 (m, 1H), 8.00 – 7.88 (m, 1H), 7.80 – 7.68 (m, 1H),, 7.52 – 7.40 (m, 3H), 7.08 (dd, *J* = 13.5, 5.1 Hz, 2H), 6.82 (s, 1H), 3.31 – 3.18 (m, 2H), 1.50 – 1.41 (m, 2H),, 1.38 – 1.30 (m, 2H), 1.00 – 1.93 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.7, 155.6, 153.5, 148.5, 148.3, 140.0, 139.1, 138.1, 135.7, 131.4, 130.3, 126.3, 123.4, 121.3, 121.1, 38.9, 31.7, 20.1, 13.8; HRMS (ESI-TOF) calcd for $C_{21}H_{20}BrN_3NaO^+$ $[M+Na]^+$: 432.0682, found: 432.0682.

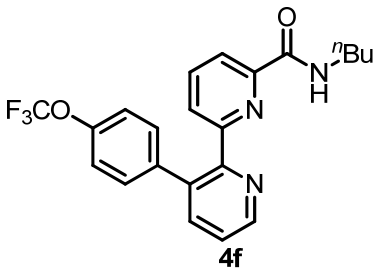
***N*-butyl-3'-(4-iodophenyl)-[2,2'-bipyridine]-6-carboxamide (4e)**



4e

4e was prepared from **1a** (0.2 mmol, 51.0 mg) and 1,4-diiodobenzene (0.6 mmol, 197.9 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane:ethyl acetate and 5-10% Et_3N) gave the product as a scream solid (33.8 mg, 37% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.74 (dd, *J* = 4.7, 1.5 Hz, 1H), 8.21 (d, *J* = 7.8 Hz, 1H), 8.08 (d, *J* = 7.7 Hz, 1H), 7.93 (t, *J* = 7.8 Hz, 1H), 7.73 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.66 (d, *J* = 8.3 Hz, 2H), 7.43 (dd, *J* = 7.7, 4.7 Hz, 1H), 6.94 (d, *J* = 8.3 Hz, 2H), 6.82 (s, 1H), 3.29 – 3.21 (m, 2H), 1.49 – 1.42 (m, 2H), 1.39 – 1.31 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.8, 155.6, 153.6, 148.6, 148.4, 140.7, 139.2, 138.2, 137.5, 135.9, 130.6, 126.4, 123.5, 121.4, 92.6, 39.0, 31.9, 20.2, 13.9; HRMS (ESI-TOF) calcd for $C_{21}H_{20}IN_3KO^+$ $[M+K]^+$: 496.0283, found: 496.0283.

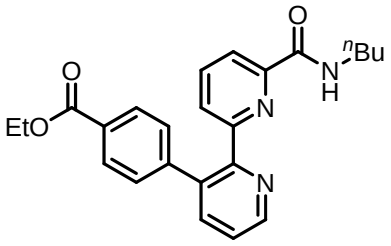
***N*-butyl-3'-(4-(trifluoromethoxy)phenyl)-[2,2'-bipyridine]-6-carboxamide (4f)**



4f

4f was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-iodo-4-(trifluoromethoxy)benzene (0.6 mmol, 172.8 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a scream solid (63.9 mg, 77% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.75 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.14 (dd, *J* = 7.8, 1.0 Hz, 1H), 8.08 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.93 (t, *J* = 7.8 Hz, 1H), 7.77 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.45 (dd, *J* = 7.8, 4.7 Hz, 1H), 7.23 – 7.19 (m, 2H), 7.17 (d, *J* = 8.6 Hz, 2H), 6.94 (t, *J* = 5.5 Hz, 1H), 3.22 – 3.18 (m, 2H), 1.45 – 1.38 (m, 2H), 1.33 – 1.28 (m, 2H), 0.93 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.7, 155.7, 154.0, 148.6, 148.5, 148.27 (q, *J* = 1.9 Hz), 139.4, 139.2, 138.121, 135.6, 130.1, 126.5, 123.4, 121.3, 120.6, 120.4 (q, *J* = 257.7 Hz), 38.8, 31.6, 20.1, 13.6; HRMS (ESI-TOF) calcd for $C_{22}H_{21}F_3N_3O_2^+$ $[M+H]^+$: 416.1580 found: 416.1580.

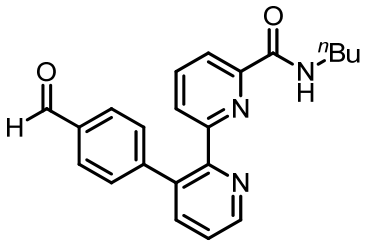
ethyl 4-(6'-(butylcarbamoyl)-[2,2'-bipyridin]-3-yl)benzoate (4g)



4g

4g was prepared from **1a** (0.2 mmol, 51.0 mg) and ethyl 4-iodobenzoate (0.6 mmol, 165.6 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a colorless solid (70.1 mg, 87% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.23 (dd, *J* = 7.8, 1.0 Hz, 1H), 8.06 (dd, *J* = 7.7, 1.0 Hz, 1H), 8.04 – 7.99 (m, 2H), 7.94 (t, *J* = 7.8 Hz, 1H), 7.78 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.46 (dd, *J* = 7.7, 4.7 Hz, 1H), 7.29 – 7.26 (m, 2H), 6.71 (t, *J* = 5.5 Hz, 1H), 4.42 – 4.36 (m, 2H), 3.13 – 3.09 (m, 2H), 1.40 (t, *J* = 7.1 Hz, 3H), 1.37 – 1.32 (m, 2H), 1.30 – 1.24 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.0, 163.7, 155.5, 153.8, 148.7, 148.3, 145.8, 139.1, 138.2, 136.1, 129.6, 129.0, 128.7, 126.3, 123.4, 121.4, 61.1, 38.7, 31.6, 20.0, 14.3, 13.7; HRMS (ESI-TOF) calcd for $C_{24}H_{26}N_3O_3^+$ $[M+H]^+$: 404.1969, found: 404.1969.

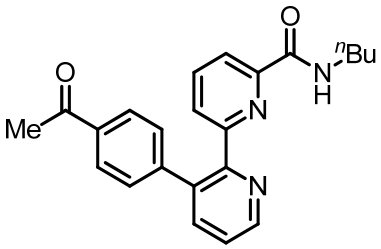
***N*-butyl-3'-(4-formylphenyl)-[2,2'-bipyridine]-6-carboxamide (4h)**



4h

4h was prepared from **1a** (0.2 mmol, 51.0 mg) and 4-iodobenzaldehyde (0.6 mmol, 139.2 mg)according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a yellow oil (65.3 mg, 91% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 10.02 (s, 1H), 8.78 (dd, *J* = 4.7, 1.5 Hz, 1H), 8.23 (dd, *J* = 7.8, 0.9 Hz, 1H), 8.08 (d, *J* = 7.7 Hz, 1H), 7.95 (t, *J* = 7.8 Hz, 1H), 7.86 (d, *J* = 8.1 Hz, 2H), 7.80 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.49 (dd, *J* = 7.7, 4.7 Hz, 1H), 7.38 (d, *J* = 8.1 Hz, 2H), 6.75 (t, *J* = 5.5 Hz, 1H), 3.12 – 3.07 (m, 2H), 1.35 – 1.30 (m, 2H), 1.27 – 1.22 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.2, 163.6, 155.3, 153.7, 148.9, 148.3, 147.4, 139.0, 138.2, 135.6, 134.7, 129.6, 129.4, 126.4, 123.4, 121.4, 38.7, 31.6, 19.9, 13.6; HRMS (ESI-TOF) calcd for $C_{22}H_{21}N_3NaO_2^+$ $[M+Na]^+$: 382.1526, found: 382.1526.

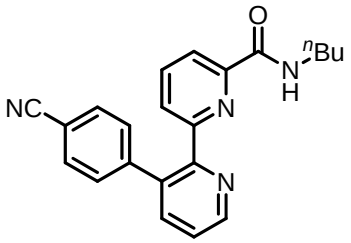
3'-(4-acetylphenyl)-*N*-butyl-[2,2'-bipyridine]-6-carboxamide (4i)



4i

4i was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-(4-iodophenyl)ethanone (0.6 mmol, 147.6 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a white solid (56.0 mg, 75% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.77 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.21 (dd, *J* = 7.8, 1.1 Hz, 1H), 8.07 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.96 – 7.92 (m, 3H), 7.78 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.47 (dd, *J* = 7.8, 4.7 Hz, 1H), 7.32 – 7.29 (m, 2H), 6.77 (t, *J* = 5.7 Hz, 1H), 3.13 – 3.06 (m, 2H), 2.60 (s, 3H), 1.36 – 1.30 (m, 2H), 1.28 – 1.22 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.1, 163.7, 155.5, 153.8, 148.8, 148.4, 146.0, 139.1, 138.2, 135.9, 135.4, 129.0, 128.4, 126.4, 123.4, 121.4 , 38.8, 31.7, 26.5, 20.0, 13.7; HRMS (ESI-TOF) calcd for $C_{23}H_{24}N_3O_2^+$ $[M+H]^+$: 374.1863, found: 374.1863.

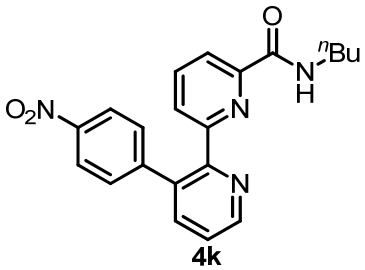
***N*-butyl-3'-(4-cyanophenyl)-[2,2'-bipyridine]-6-carboxamide (4j)**



4j

4j was prepared from **1a** (0.2 mmol, 51.0 mg) and 4-iodobenzonitrile (0.6 mmol, 137.4 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a white solid (58.4 mg , 82% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.22 (dd, *J* = 7.8, 0.9 Hz, 1H), 8.11 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.96 (t, *J* = 7.8 Hz, 1H), 7.76 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.65 – 7.61 (m, 2H), 7.49 (dd, *J* = 7.8, 4.7 Hz, 1H), 7.33 – 7.30 (m, 2H), 6.76 (s, 1H), 3.24 – 3.19 (m, 2H), 1.45 – 1.38 (m, 2H), 1.34 – 1.30 (m, 2H), 0.96 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.6, 155.2, 153.8, 149.2, 148.4, 146.0, 139.0, 138.4, 135.1, 132.1, 130.0, 126.5, 123.5, 121.7, 118.3, 110.9, 38.9, 31.8, 20.1, 13.8; HRMS (ESI-TOF) calcd for $C_{22}H_{20}N_4NaO^+$ $[M+Na]^+$: 379.1529, found: 379.1529.

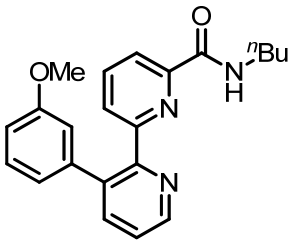
***N*-butyl-3'-(4-nitrophenyl)-[2,2'-bipyridine]-6-carboxamide (4k)**



4k

4k was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-iodo-4-nitrobenzene (0.6 mmol, 149.4 mg) according to the general procedure. After 24 hours, purification using preparative TLC (4:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a colorless solid (60.9 mg, 81% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.81 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.25 (dd, *J* = 7.8, 1.0 Hz, 1H), 8.23 – 8.19 (m, 2H), 8.10 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.97 (t, *J* = 7.8 Hz, 1H), 7.79 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.50 (dd, *J* = 7.8, 4.7 Hz, 1H), 7.40 – 7.35 (m, 2H), 6.75 (s, 1H), 3.15 – 3.10 (m, 2H), 1.35 – 1.29 (m, 2H), 1.27 – 1.21 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.5, 155.2, 153.9, 149.3, 148.4, 148.0, 146.7, 139.0, 138.4, 134.7, 129.6, 126.5, 123.6, 123.5, 121.7, 38.8, 31.7, 20.0, 13.6; HRMS(ESI-TOF) calcd for $C_{21}H_{20}N_4NaO_3^+$ $[M+Na^+]$: 399.1428, found: 399.1428.

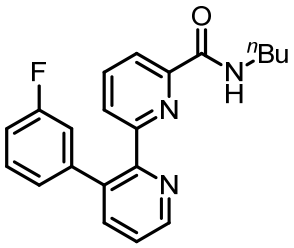
***N*-butyl-3'-(3-methoxyphenyl)-[2,2'-bipyridine]-6-carboxamide (4l)**



4l

4l was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-iodo-3-methoxybenzene (0.6 mmol, 140.4 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a white solid (60.7 mg, 84% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 – 8.66 (m, 1H), 8.14 (dd, *J* = 7.8, 1.2 Hz, 1H), 8.08 – 7.99 (m, 1H), 7.94 – 7.85 (m, 1H), 7.81 – 7.72 (m, 1H), 7.45 – 7.36 (m, 1H), 7.25 – 7.16 (m, 1H), 6.93 (s, 1H), 6.86 – 6.78 (m, 1H), 6.73 (d, *J* = 11.5 Hz, 2H), 3.71 – 3.65 (m, 3H), 3.22 – 3.14 (m, 2H), 1.46 – 1.37 (m, 2H), 1.32 – 1.24 (m, 2H), 0.93 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.0, 159.5, 155.9, 153.9, 148.4, 148.3, 142.4, 139.2, 137.9, 136.9, 129.3, 126.2, 123.3, 121.2, 121.1, 114.3, 112.3, 55.1, 38.9, 31.6, 20.1, 13.8; HRMS (ESI-TOF) calcd for $C_{22}H_{24}N_3O_2^+$ $[M+H]^+$: 362.1863, found: 362.1863.

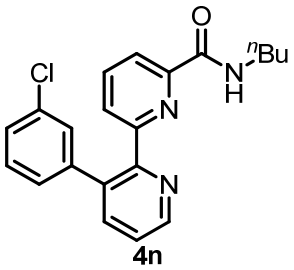
***N*-butyl-3'-(3-fluorophenyl)-[2,2'-bipyridine]-6-carboxamide (4m)**



4m

4m was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-fluoro-3-iodobenzene (0.6 mmol, 133.2 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a colorless solid (54.4 mg, 78% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.20 (dd, *J* = 7.8, 0.9 Hz, 1H), 8.09 (dd, *J* = 7.7, 0.9 Hz, 1H), 7.95 (t, *J* = 7.8 Hz, 1H), 7.78 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.46 (dd, *J* = 7.7, 4.7 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.04 – 6.95 (m, 2H), 6.94 – 6.89 (m, 2H),, 3.25 – 3.21 (m, 2H), 1.47 – 1.42 (m, 2H), 1.35 – 1.30 (m, 2H), 0.96 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.7, 162.5 (d, *J* = 246.9 Hz), 155.6, 153.8, 148.5, 148.3, 143.2 (d, *J* = 7.8 Hz), 139.0, 138.0, 135.7 (d, *J* = 1.9 Hz), 129.7 (d, *J* = 8.3 Hz), 126.3, 124.5 (d, *J* = 2.9 Hz), 123.3, 121.2, 115.6 (d, *J* = 21.9 Hz), 113.7 (d, *J* = 20.9 Hz), 38.8, 31.5, 20.0, 13.7; HRMS (ESI-TOF) calcd for $C_{21}H_{21}FN_3O^+$ $[M+H]^+$: 350.1663, found: 350.1664..

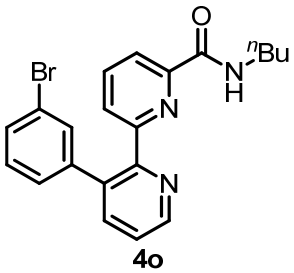
***N*-butyl-3'-(3-chlorophenyl)-[2,2'-bipyridine]-6-carboxamide(4n)**



4n

4n was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-chloro-3-iodobenzene (0.6 mmol, 143.1 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a scream solid (64.2 mg, 88% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.75 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.20 (d, *J* = 7.8 Hz, 1H), 8.08 (d, *J* = 7.7 Hz, 1H), 7.94 (t, *J* = 7.8 Hz, 1H), 7.76 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.44 (dd, *J* = 7.7, 4.7 Hz, 1H), 7.34 – 7.27 (m, 2H), 7.20 (t, *J* = 7.8 Hz, 1H), 6.95 (d, *J* = 7.7 Hz, 1H), 6.86 (s, 1H), 3.26 – 3.18 (m, 2H), 1.48 – 1.41 (m, 2H), 1.36 – 1.28 (m, 2H), 0.94 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.8, 155.5, 153.8, 148.7, 148.4, 142.9, 139.2, 138.1, 135.6, 134.3, 129.4, 128.6, 127.1, 127.0, 126.3, 123.4, 121.3, 39.0, 31.7, 20.1, 13. 8; HRMS (ESI-TOF) calcd for $C_{21}H_{21}ClN_3O^+$ $[M+H]^+$: 366.1368, found: 366.1368.

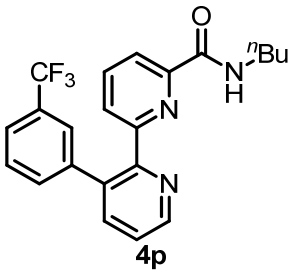
3'-(3-bromophenyl)-*N*-butyl-[2,2'-bipyridine]-6-carboxamide (4o)



4o

4o was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-bromo-3-iodobenzene (0.6 mmol, 169.2 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a scream solid (54.8 mg, 67% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (dd, *J* = 4.7, 1.4 Hz, 1H), 8.21 (d, *J* = 7.7 Hz, 1H), 8.08 (d, *J* = 7.6 Hz, 1H), 7.94 (t, *J* = 7.8 Hz, 1H), 7.75 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.51 – 7.41 (m, 3H), 7.13 (t, *J* = 7.8 Hz, 1H), 6.99 (d, *J* = 7.7 Hz, 1H), 6.85 (s, 1H), 3.26 – 3.17 (m, 2H), 1.49 – 1.41 (m, 2H), 1.36 – 1.28 (m, 2H), 0.95 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.8, 155.5, 153.7, 148.7, 148.3, 143.2, 139.2, 138.1, 135.4, 131.4, 129.9, 129.7, 127.6, 126.3, 123.4, 122.3, 121.3, 39.0, 31.8, 20.1, 13.8; HRMS (ESI-TOF) calcd for $C_{21}H_{20}BrN_3NaO^+$ $[M+Na^+]$: 432.0682, found: 432.0682.

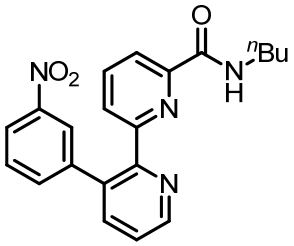
***N*-butyl-3'-(3-(trifluoromethyl)phenyl)-[2,2'-bipyridine]-6-carboxamide (4p)**



4p

4p was prepared from **1a** (0.2mmol, 51.0 mg) and 1-iodo-3-(trifluoromethyl)benzene (o.6 mmol, 163.2 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a yellow oil (33.5 mg, 42% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.77 (dd, *J* = 4.7, 1.3 Hz, 1H), 8.20 (d, *J* = 7.7 Hz, 1H), 8.09 (d, *J* = 7.6 Hz, 1H), 7.95 (t, *J* = 7.8 Hz, 1H), 7.80 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.59 – 7.54 (m, 2H), 7.48 (dd, *J* = 7.7, 4.7 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 6.77 (s, 1H), 3.18 – 3.12 (m, 2H), 1.39 – 1.33 (m, 2H), 1.27 – 1.24 (m, 2H); 0.91 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.7, 155.5, 153.9, 148.8, 148.3, 141.7, 139.2, 138.2, 135.4, 132.3, 130.9 (q, *J* = 32.5 Hz), 128.6, 126.5, 125.4 (q, *J* = 3.7 Hz), 123.8 (q, *J* = 272.3 Hz), 123.6 (q, *J* = 3.6 Hz), 123.5, 121.4, 38.8, 31.6, 20.0, 13.6; HRMS (ESI-TOF) calcd for $C_{22}H_{21}F_3N_3O^+$ $[M+H]^+$: 400.1631, found: 400.1631.

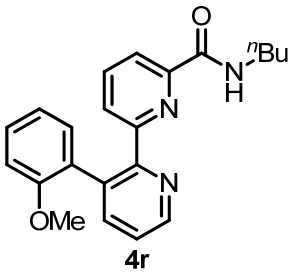
***N*-butyl-3'-(3-nitrophenyl)-[2,2'-bipyridine]-6-carboxamide(4q)**



4q

4q was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-iodo-3-nitrobenzene (0.6 mmol, 149.4 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate) gave the product as a white solid (48.9 mg, 65% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.22 (dd, *J* = 7.8, 1.0 Hz, 1H), 8.20 – 8.15 (m, 2H), 8.09 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.97 (t, *J* = 7.8 Hz, 1H), 7.82 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.51 (dd, *J* = 7.8, 4.7 Hz, 1H), 7.48 –7.40 (m, 2H), 6.81 (s, 1H), 3.19 – 3.11 (m, 2H), 1.35 – 1.28 (m, 2H), 1.27 – 1.20 (m, 2H), 0.90 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.4, 155.2, 153.9, 149.1, 148.2, 148.1, 142.6, 139.0, 138.3, 134.9, 134.4, 129.1, 126.6, 123.5, 123.3, 121.8, 121.5, 38.8, 31.5, 19.9, 13.6.; HRMS (ESI-TOF) calcd for $C_{21}H_{20}N_4NaO_3^+$ $[M+Na]^+$: 399.1428, found: 399.1428.

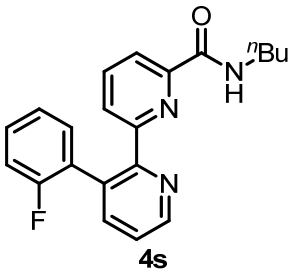
***N*-butyl-3'-(2-methoxyphenyl)-[2,2'-bipyridine]-6-carboxamide (4r)**



4r

4r was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-iodo-2-methoxybenzene (0.6 mmol, 140.4 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a scream oil (32.5 mg, 45% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.71 (dd, *J* = 4.7, 1.5 Hz, 1H), 8.16 (d, *J* = 7.8 Hz, 1H), 8.04 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 1H), 7.75 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.43 (dd, *J* = 7.7, 4.8 Hz, 1H), 7.35 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.33 – 7.28 (m, 1H), 7.10 – 7.05 (m, 1H), 6.83 (s, 1H), 6.72 (d, *J* = 8.1 Hz, 1H), 3.32 – 3.00 (m, 5H), 1.45 – 1.37 (m, 2H), 1.34 – 1.26 (m, 2H), 0.93 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.1, 156.9, 155.4, 154.8, 148.0, 139.8, 137.7, 133.3, 130.2, 130.1, 128.9, 125.4, 123.4, 121.0, 120.8, 110.7, 100.0, 54.8, 38.8, 31.7, 20.1, 13.8; HRMS (ESI-TOF) calcd for $C_{22}H_{24}N_3O_2^+$ $[M+H]^+$: 362.1863; found: 362.1863.

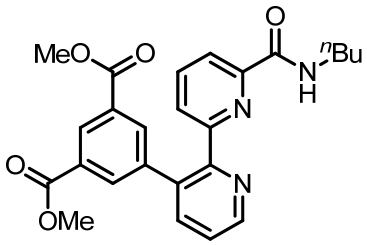
***N*-butyl-3'-(2-fluorophenyl)-[2,2'-bipyridine]-6-carboxamide(4s)**



4s

4s was prepared from **1a** (0.2 mmol, 51.0 mg) and 1-fluoro-2-iodobenzene (0.6 mmol, 133.2 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10%Et_3N) gave the product as a white solid (28.6 mg, 41% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.24 (dd, *J* = 7.9, 0.9 Hz, 1H), 8.07 (dd, *J* = 7.7, 0.9 Hz, 1H), 7.94 (t, *J* = 7.8 Hz, 1H), 7.77 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.45 (dd, *J* = 7.7, 4.7 Hz, 1H), 7.34 – 7.29 (m, 2H), 7.23 – 7.19 (m, 1H), 6.97 (t, *J* = 9.0 Hz, 1H), 6.82 (s, 1H), 3.20 – 3.13 (m, 2H), 1.44 – 1.39 (m, 2H), 1.33 – 1.29 (m, 2H), 0.93 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.0, 159.0 (d, *J* = 246.8 Hz), 156.1, 154.6, 148.8, 148.2, 139.8, 138.1, 130.6 (d, *J* = 2.9 Hz), 129.2 (d, *J* = 8.0 Hz), 128.9 (d, *J* = 15.9 Hz), 125.9, 124.2 (d, *J* = 3.7 Hz), 123.3, 121.4, 115.6 (d, *J* = 22.0 Hz); HRMS (ESI-TOF) calcd for $C_{21}H_{20}FN_3NaO$ $[M+Na]^+$: 372.1483. found: 372.1482.

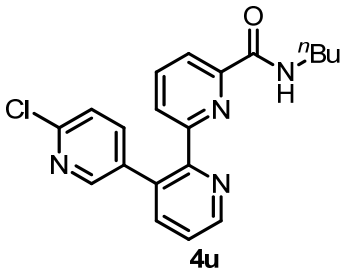
dimethyl 5-(6'-(butylcarbamoyl)-[2,2'-bipyridin]-3-yl)isophthalate (4t)



4t

4t was prepared from **1a** (0.2 mmol, 51.0 mg) and diethyl 5-iodoisophthalate (0.6 mmol, 192.0) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a white solid (42.9 mg, 48% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.82 – 8.76 (m, 1H), 8.63 (d, *J* = 5.4 Hz, 1H), 8.26 (dd, *J* = 7.8, 4.3 Hz, 1H), 8.11 –8.04 (m, 3H), 8.00 – 7.93 (m, 1H), 7.83 – 7.77 (m, 1H), 7.52 – 7.46 (m, 1H), 6.72 (d, *J* = 5.3 Hz, 1H), 3.92 (d, *J* = 6.1 Hz, 6H), 3.14 – 3.07 (m, 2H), 1.31 – 1.26 (m, 2H), 1.25 – 1.18 (m, 2H), 0.90 (t, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.6, 163.6, 155.3, 153.9, 149.0, 148.2, 142.0, 139.2, 138.3, 134.9, 133.8, 130.8, 129.0, 126.6, 123.5, 121.5, 52.5, 38.8, 31.6, 20.0, 13.6; HRMS (ESI-TOF) calcd for $C_{25}H_{26}N_3O_5^+$ $[M+H]^+$: 448.1867; found: 448.1867.

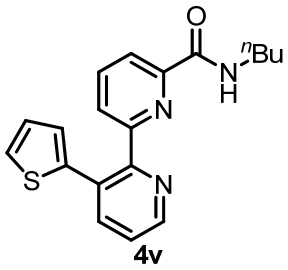
***N*-butyl-6''-chloro-[2,2':3',3''-terpyridine]-6-carboxamide (4u)**



4u

4u was prepared from **1a** (0.2 mmol, 51.0 mg) and 2-chloro-5-iodopyridine (0.6 mmol, 143.7 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a white solid (54.2 mg , 74% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.80 (dd, *J* = 4.7, 1.5 Hz, 1H), 8.35 (d, *J* = 2.4 Hz, 1H), 8.23 (d, *J* = 7.8 Hz, 1H), 8.12 (d, *J* = 7.7 Hz, 1H), 7.97 (t, *J* = 7.8 Hz, 1H), 7.78 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.50 (dd, *J* = 7.7, 4.7 Hz, 1H), 7.36 (dd, *J* = 8.2, 2.5 Hz, 1H), 7.25 (d, *J* = 8.2 Hz, 1H), 6.85 (t, *J* = 5.4 Hz, 1H), 3.31 – 3.24(m, 2H), 1.50 – 1.43 (m, 2H), 1.37 – 1.30 (m, 2H), 0.96 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, CDCl3) δ 163.5, 155.2, 154.0, 150.2, 149.3, 148.9, 148.4, 139.1, 138.8, 138.4, 135.6, 132.0, 126.6, 123.6, 123.6, 121.7. 38.9, 31.6, 20.1, 13.7; HRMS (ESI-TOF) calcd for $C_{20}H_{19}ClN_4NaO^+$ $[M+Na^+]$: 389.1140, found: 389.1140.

***N*-butyl-3'-(thiophen-2-yl)-[2,2'-bipyridine]-6-carboxamide (4v)**

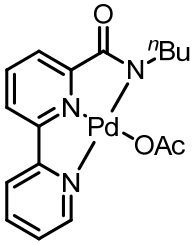


4v

4v was prepared from **1a** (0.2 mmol, 51.0 mg) and 2-iodothiophene (0.6 mmol, 126.0 mg) according to the general procedure. After 24 hours, purification using preparative TLC (10:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a yellow oil (47.8 mg ,71% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.70 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.12 (dd, *J* = 7.7, 0.9 Hz, 1H), 8.00 (dd, *J* = 7.8, 0.9 Hz, 1H), 7.92 (t, *J* = 7.7 Hz, 1H), 7.88 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.41 (dd, *J* = 7.8, 4.7 Hz, 1H), 7.36 (s, 1H), 7.29 (d, *J* = 1.0 Hz, 1H), 6.95 (dd, *J* = 5.1, 3.6 Hz, 1H), 6.78 (dd, *J* = 3.5, 1.0 Hz, 1H), 3.33 – 3.27 (m, 2H), 1.52 – 1.46 (m, 2H), 1.36 – 1.31 (m, 2H), 0.94 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.0, 155.9, 154.7, 148.7, 148.6, 141.6, 139.5, 138.0, 129.9, 127.2, 126.7, 126.4, 126.0, 123.2, 121.4, 38.9, 31.6, 20.1, 13.8; HRMS (ESI-TOF) calcd for $C_{19}H_{20}N_3OS^+$ $[M+H]^+$: 338.1322, found: 338.1322.

2.5 Procedure for Synthesis of I-1 and I-2

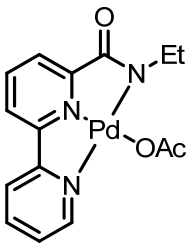
Synthesis of Complex I-1



I-1

To a vial equipped with a magnetic stir bar was charged with $Pd(OAc)_2$ (0.1 mmol ,22.4 mg), 1a (0.1 mmol, 25.5 mg) and MeCN (1 mL). The solution was stirred at room temperature for 2 h. The reaction mixture was filtered, and the filter cake was collected and dried *in vacuo* to afford of complex **I-1 (**35.6 mg, 85%) as a gold powder; ^1H NMR (500 MHz, $CDCl_3$) δ 8.29 (dd, *J* = 5.4, 1.0 Hz, 1H), 8.22 (d, *J* = 7.9 Hz, 1H), 8.12 (dd, *J* = 8.1, 1.8 Hz, 1H), 8.11 – 8.08 (m, 1H), 8.08 – 8.04 (m, 1H), 7.67 (dd, *J* = 7.1, 1.7 Hz, 1H), 7.49 – 7.45 (m, 1H), 3.16 – 3.10 (m, 2H), 2.16 (s, 3H), 1.64 – 1.57 (m, 2H), 1.45 – 1.37 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.1, 170.1, 155.2, 154.6, 152.9, 151.1, 140.6, 140.1, 127.2, 125.0, 123.0, 122.4, 45.7, 32.4, 23.6, 20.7, 14.1; HRMS (ESI-TOF) calcd for $C_{17}H_{19}N_3O_3NaPd^+$ $[M+Na]^+$: 442.0353. found: 442.0357.

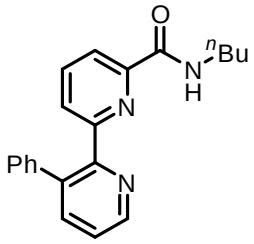
Synthesis of Complex I-2



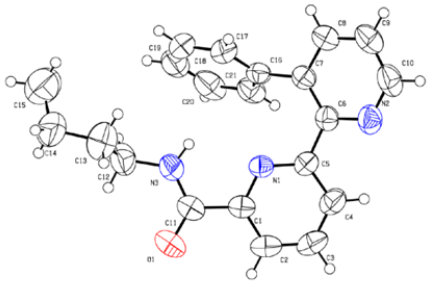
I-2

To a vial equipped with a magnetic stir bar was charged with $Pd(OAc)_2$ (22.5 mg, 0.1 mmol), **1b** (22.7 mg, 0.1 mmol) and MeCN (1 mL). The solution was stirred at room temperature for 2 h. The reaction mixture was filtered, and the filter cake was collected and dried *in vacuo* to afford of complex **I-2 (**36.7 mg, 94%) as a gold powder; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (d, *J* = 5.2 Hz, 1H), 8.13 – 8.08 (m, 3H), 7.98 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.76 (dd, *J* = 7.8, 0.9 Hz, 1H), 7.56 – 7.53 (m, 1H), 3.21 (q, *J* = 7.1 Hz, 2H), 2.18 (s, 3H), 1.21 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.3, 170.0, 155.6, 154.7, 153.0, 151.4, 140.6, 140.1, 127.4, 125.1, 122.5, 121.8, 40.5, 23.6, 15.1; HRMS (ESI-TOF) calcd for $C_{15}H_{15}N_3O_3NaPd^+$ $[M+Na]^+$: 414.0040 found: 414.0042.

Crystal structure and data of N-butyl-3'-phenyl-[2,2'-bipyridine]-6-carboxamide (3a) (CCDC 1840936, Displacement ellipsoids are drawn at the 50% probability level.)

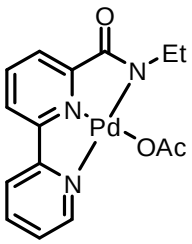


3a



Identification code	exp_5180
Empirical formula	$C_{21}H_{21}N_3O$
Formula weight	331.41
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	12.3246(5)
b/Å	10.4302(5)
c/Å	14.0891(5)
α/°	90
β/°	98.191(4)
γ/°	90
Volume/Å^3	1792.65(13)
Z	4
ρ_{calc}g/cm^3	1.228
μ/mm^{-1}	0.608
F(000)	704.0
Crystal size/mm^3	0.21 × 0.2 × 0.19
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	8.924 to 143.382
Index ranges	$-15 \leq h \leq 14$, $-12 \leq k \leq 12$, $-10 \leq l \leq 17$
Reflections collected	7029
Independent reflections	3420 [R_{int} = 0.0209, R_{sigma} = 0.0286]
Data/restraints/parameters	3420/0/228
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0596, wR_2 = 0.1711
Final R indexes [all data]	R_1 = 0.0764, wR_2 = 0.1892
Largest diff. peak/hole / e Å^{-3}	0.54/-0.25

Crystal structure and data of I-2 (CCDC 1840935, Displacement ellipsoids are drawn at the 50% probability level.)



I-2

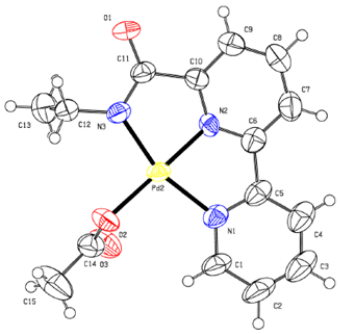


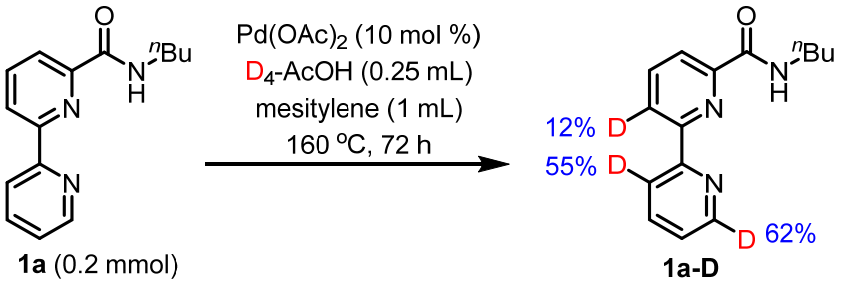
Table S1. Crystal data and structure refinement for I-2

Identification code	exp_5179_pl_sq
Empirical formula	$C_{15}H_{15}N_3O_3Pd$
Formula weight	391.70
Temperature/K	293.15
Crystal system	triclinic
Space group	P-1
a/Å	8.8222(6)
b/Å	10.4866(7)
c/Å	10.6004(6)
α/°	100.088(5)
β/°	108.748(6)
γ/°	97.604(6)
Volume/Å^3	895.39(11)
Z	2
ρ_{calc}g/cm^3	1.453
μ/mm^{-1}	8.485
F(000)	392.0
Crystal size/mm^3	0.22 × 0.21 × 0.2
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	8.746 to 143.332
Index ranges	-10 ≤ h ≤ 6, -12 ≤ k ≤ 12, -10 ≤ l ≤ 13
Reflections collected	5820
Independent reflections	3393 [R_{int} = 0.0585, R_{sigma} = 0.0679]
Data/restraints/parameters	3393/0/201
Goodness-of-fit on F^2	1.083
Final R indexes [I>=2σ (I)]	R_1 = 0.0571, wR_2 = 0.1550
Final R indexes [all data]	R_1 = 0.0629, wR_2 = 0.1629
Largest diff. peak/hole / e Å^{-3}	1.33/-1.77

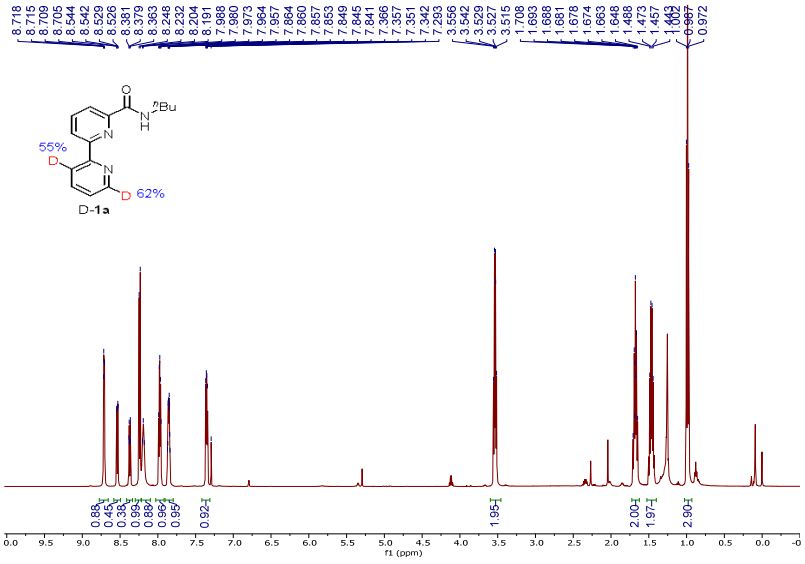
2.6 1 mmol-Scale Experiment of 3a

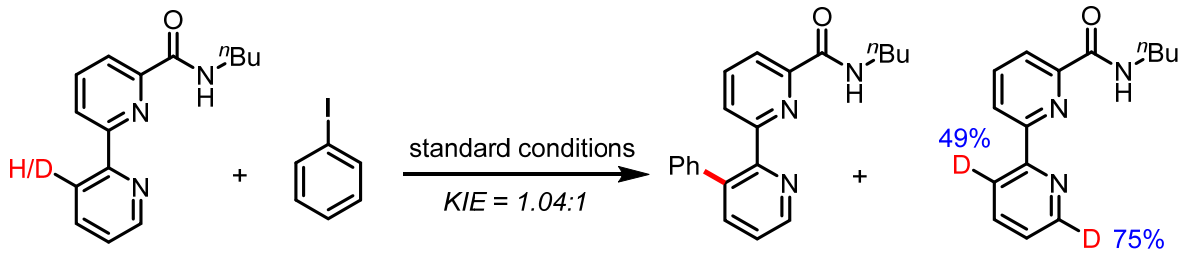
To a dried 10 mL Schlenk tube equipped with a magnetic stir bar were added 2,2'-bipyridin-6-carboxamide (1 mmol, 255 mg), iodobenzene (3 mmol, 612 mg), $Pd(OAc)_2$ (0.1 mmol, 22.5 mg), Cs_2CO_3 (4 mmol, 1.3 g), mesitylene (3 mL). Then the tube was evacuated and back filled with nitrogen (10 times). The mixtures were stirred at 160 °C under a blanket of nitrogen. After 24 hours, the reaction was cooled to room temperature; the crude reaction mixture was diluted with DCM, washed with H_2O and brine, dried over Mg_2SO_4. The organic phase was concentrated and purification using preparative TLC (8:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a colorless solid (245 mg, 74% yield).

2.7 Reversibility and KIE Study

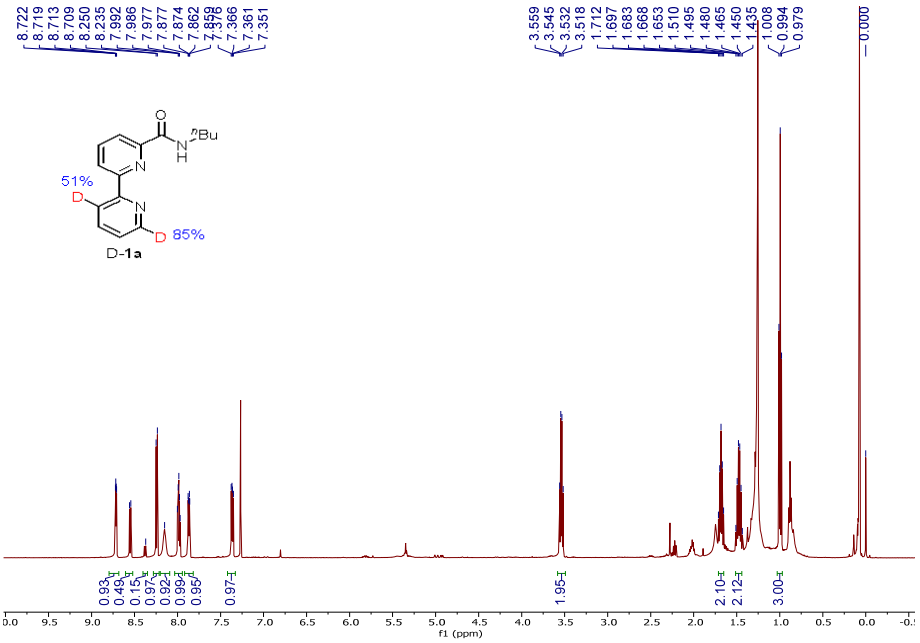


In a clean oven dried tube equipped with a magnetic stir bar were added 2,2'-bipyridin-6-carboxamide (0.2 mmol, 51 mg), $Pd(OAc)_2$ (0.02 mmol, 4.5 mg), 0.25 ml D_4-AcOH, mesitylene (1 mL). Then the tube was evacuated and back filled with nitrogen (10 times). The mixtures were stirred at 160 °C under a blanket of nitrogen. After 72 hours, the reaction was cooled to room temperature; the crude reaction mixture was diluted with DCM, washed with H_2O and brine, dried over Mg_2SO_4. The organic phase was concentrated and purification using preparative TLC (8:1 hexane: ethyl acetate and 5-10% Et_3N) gave the product as a colorless solid (47 mg, 92% yield).





In a clean oven dried tube equipped with a magnetic stir bar were added the mixture of **1a** and D-**1a** (0.2 mmol), iodobenzene (0.6 mmol, 122.4 mg), $Pd(OAc)_2$ (0.02 mmol, 4.5 mg), Cs_2CO_3 (0.8 mmol, 261 mg), mesitylene (2 mL). Then the tube was evacuated and back filled with nitrogen (10 times). The mixtures were stirred at 160 °C under a blanket of nitrogen. After 12 hours, the reaction was cooled to room temperature; the crude reaction mixture was diluted with DCM, washed with H_2O and brine, dried over Mg_2SO_4. The organic phase.was concentrated and dried. After 10 hours, and purification using preparative TLC (8:1 hexane: ethyl acetate and 5-10% Et_3N) gave the starting material (7.1 mg, 14% yield) the product **3a** as a colorless solid (45.7 mg, 69% yield).

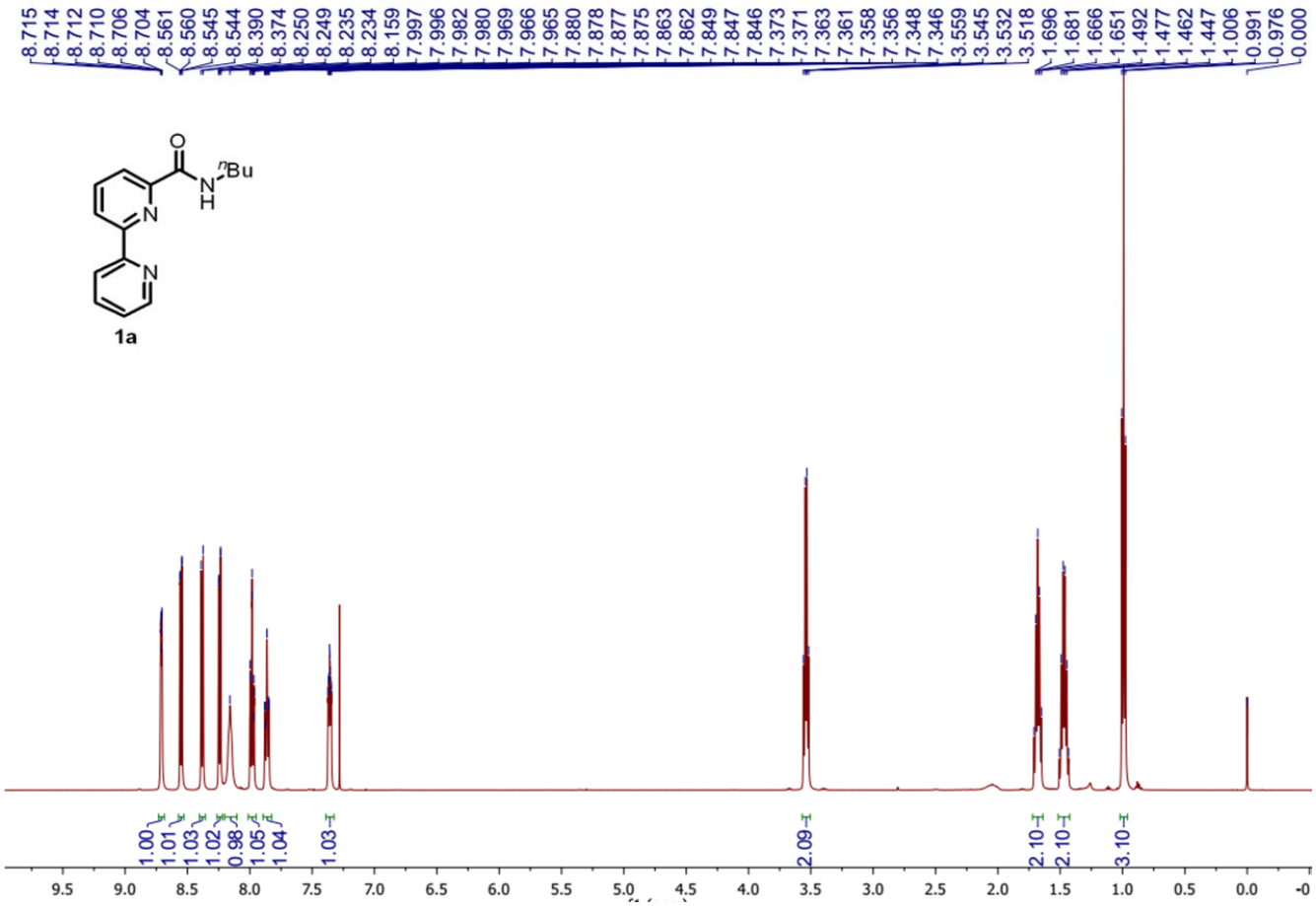


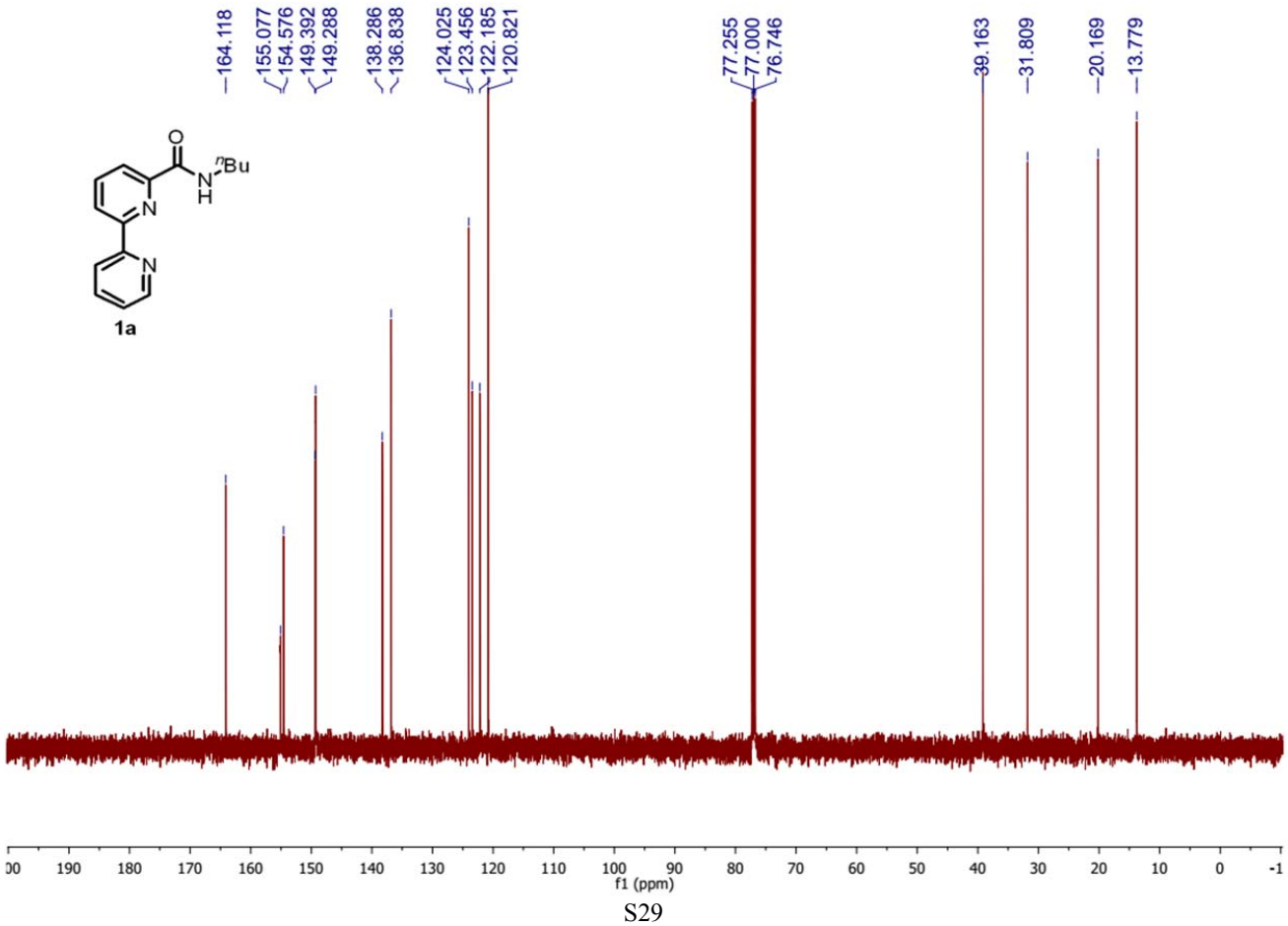
3. References

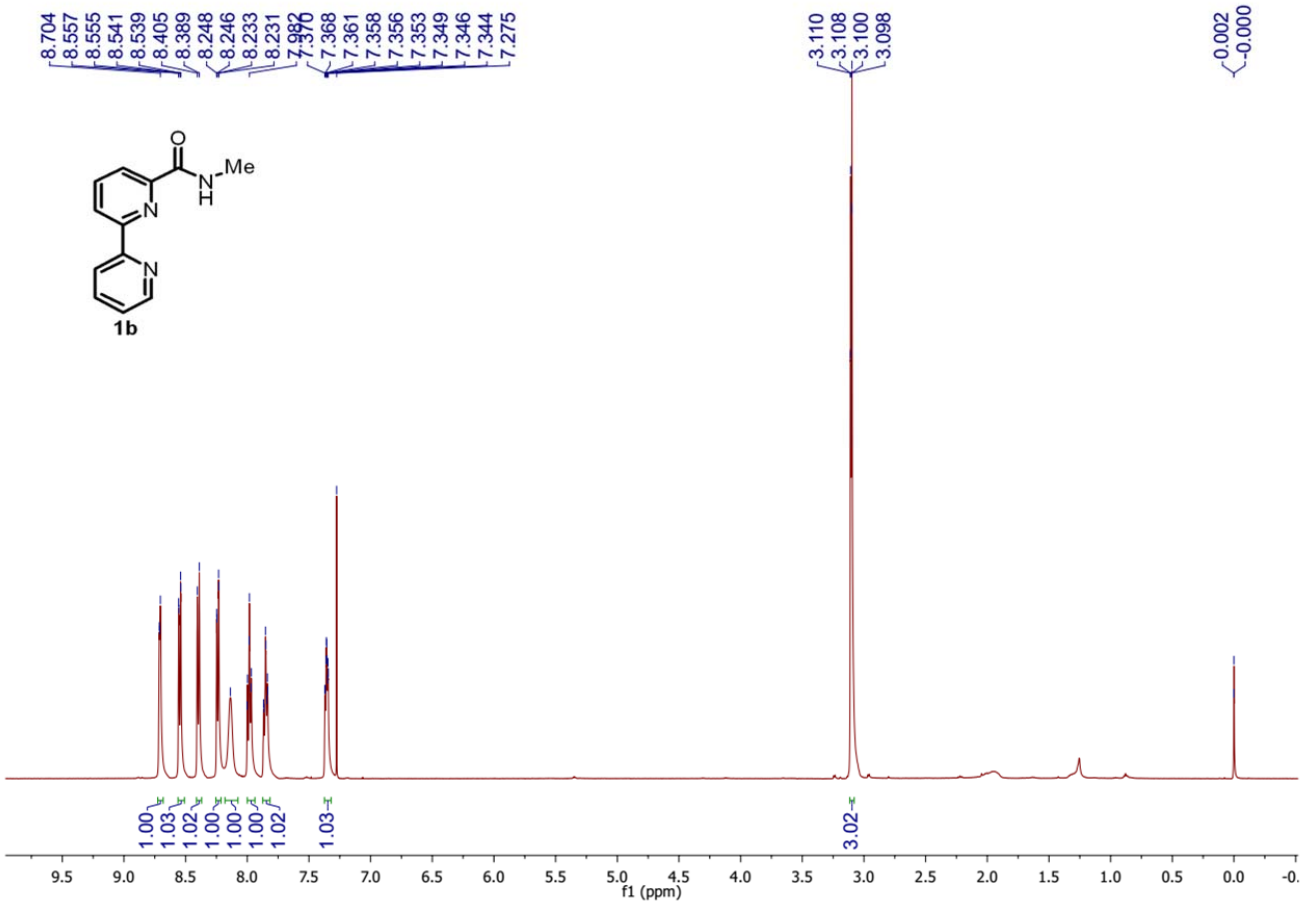
1. Young, M. C.; Liew, E.; Ashby, J.; McCoy, K. E.; Hooley, R. J. *Chem. Commun.* **2013,** *49*, 6331-6333.

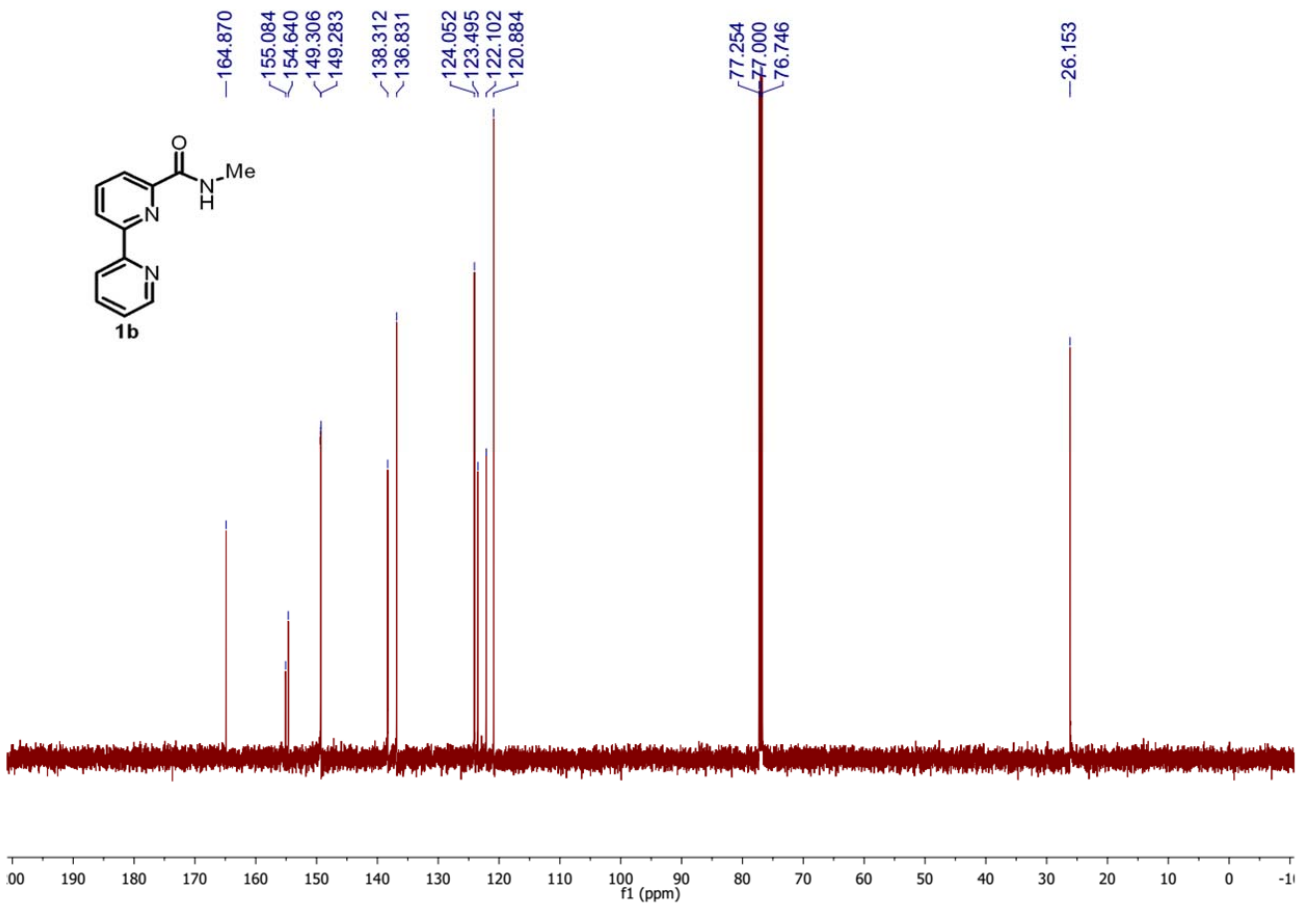
2. O'Duill, M. L.; Matsuura, R.; Wang, Y.; Turnbull, J. L.; Gurak, J. A., Jr.; Gao, D.-W.; Lu, G.; Liu, P.; Engle, K. M. *J. Am. Chem. Soc.* **2017,** *139*, 15576-15579.

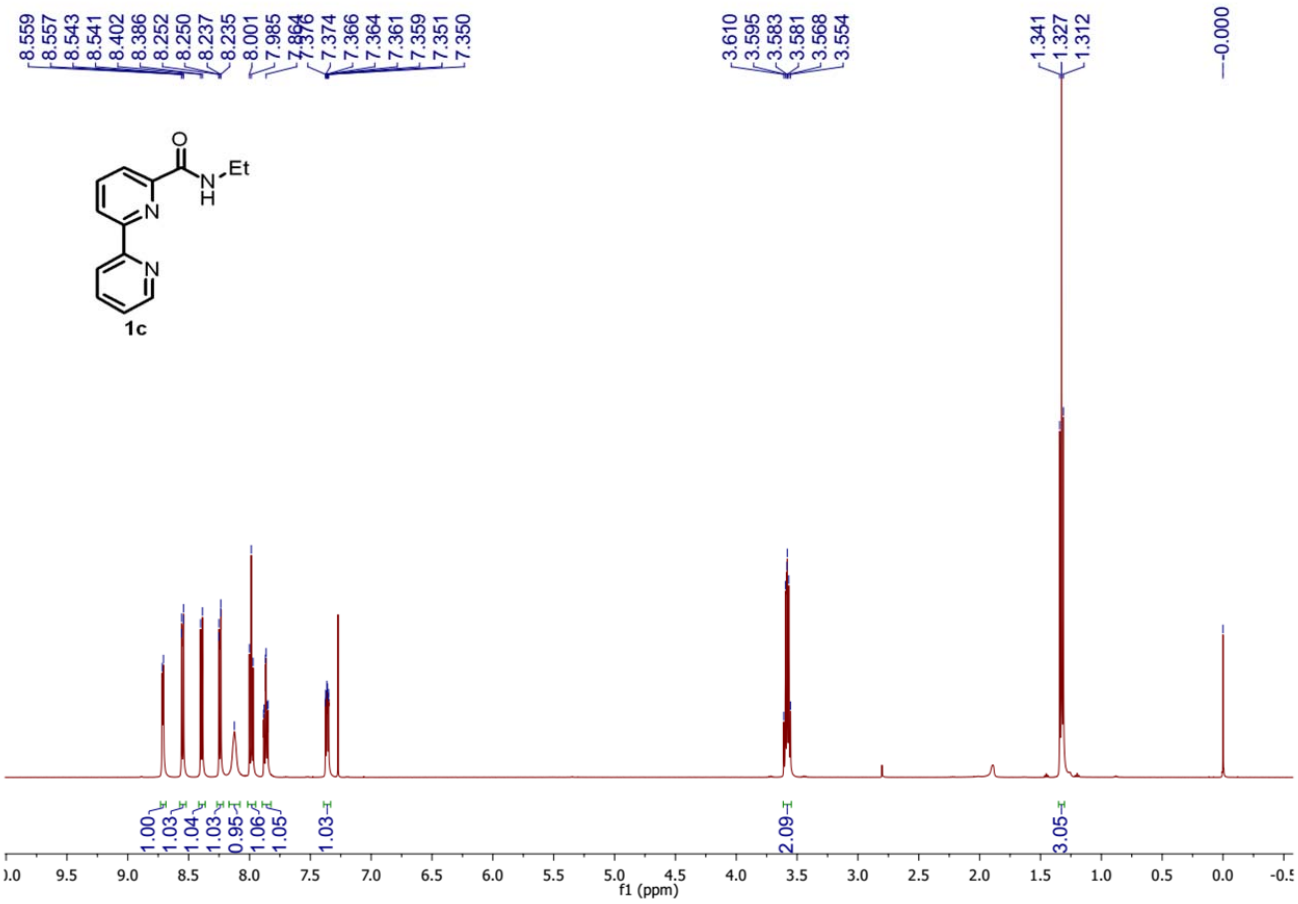
4. ^{1}H and ^{13}C NMR Spectra

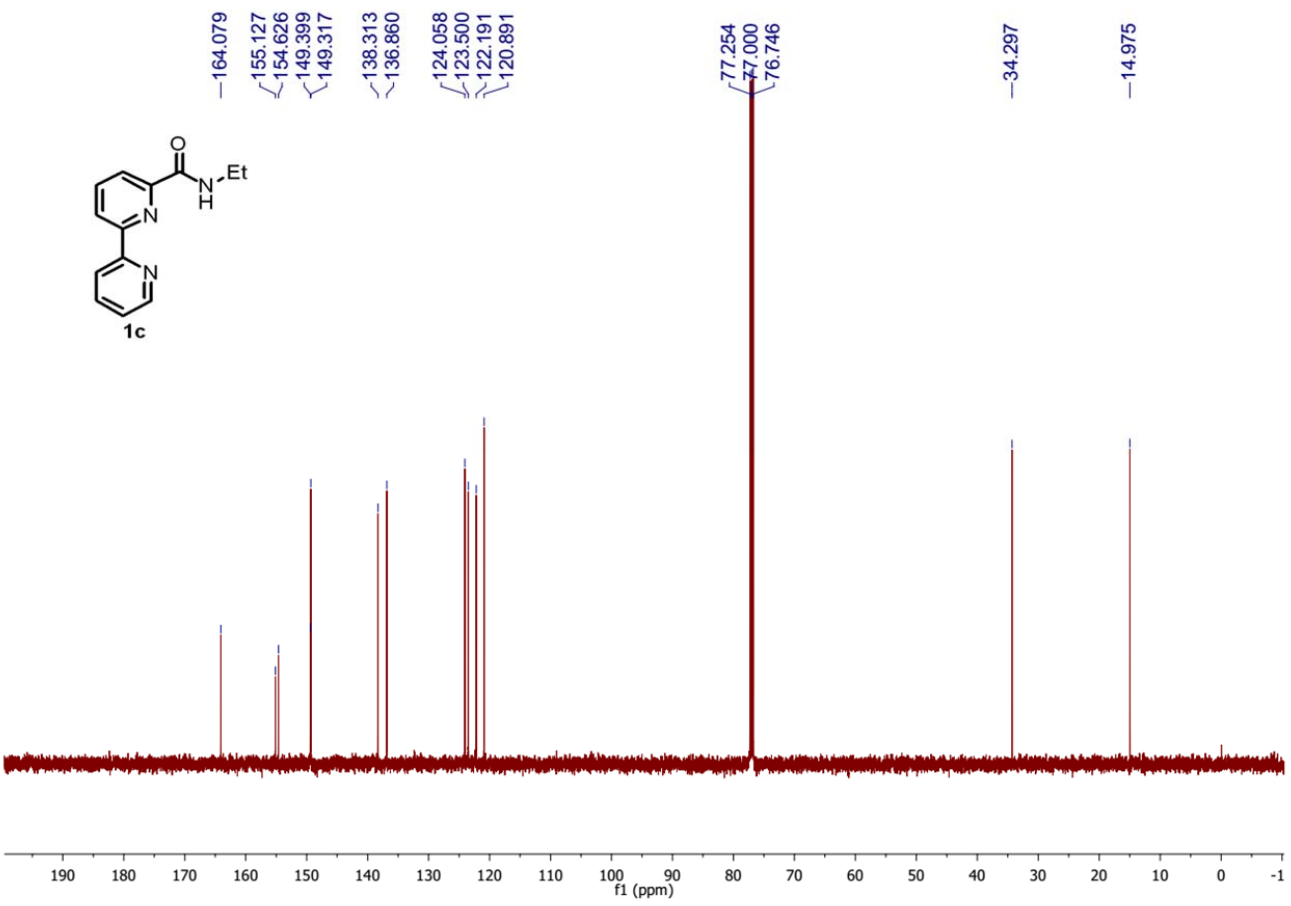

8.715
8.714
8.712
8.710
8.706
8.704
8.561
8.560
8.545
8.544
8.390
8.374
8.250
8.249
8.235
8.234
8.159
7.997
7.996
7.982
7.980
7.969
7.966
7.965
7.880
7.878
7.877
7.875
7.863
7.862
7.849
7.847
7.846
7.373
7.371
7.363
7.361
7.358
7.356
7.348
7.346
3.559
3.545
3.532
3.518
1.696
1.681
1.666
1.651
1.492
1.477
1.462
1.447
1.006
0.991
0.976
0.000
O
N
nBu
H
N
N
1a
1.00
1.01
1.03
1.02
0.98
1.05
1.04
1.03
2.09
2.10
2.10
3.10
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

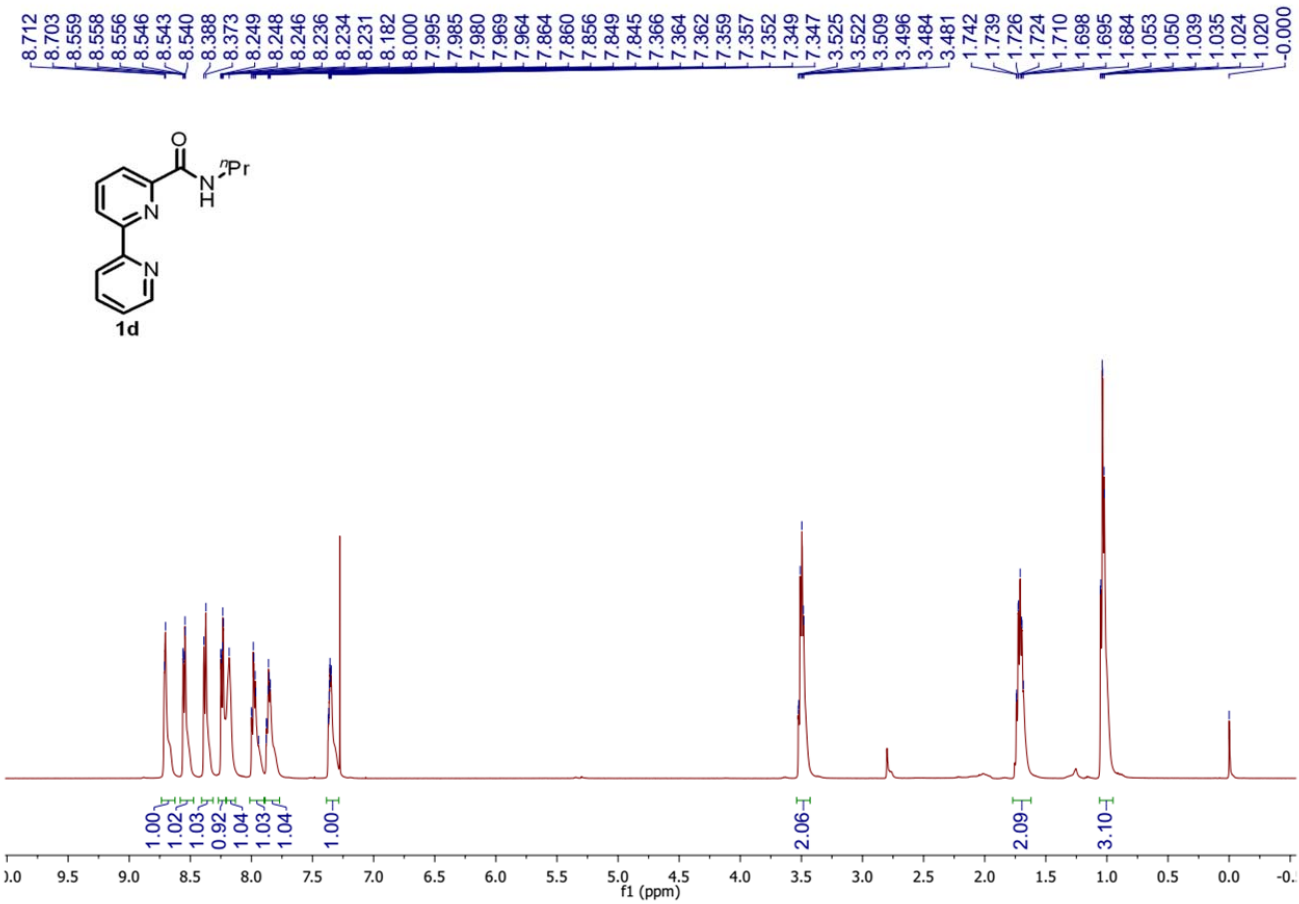

164.118
155.077
154.576
149.392
149.288
138.286
136.838
124.025
123.456
122.185
120.821
77.255
77.000
76.746
39.163
31.809
20.169
13.779
O
N
nBu
H
N
N
1a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

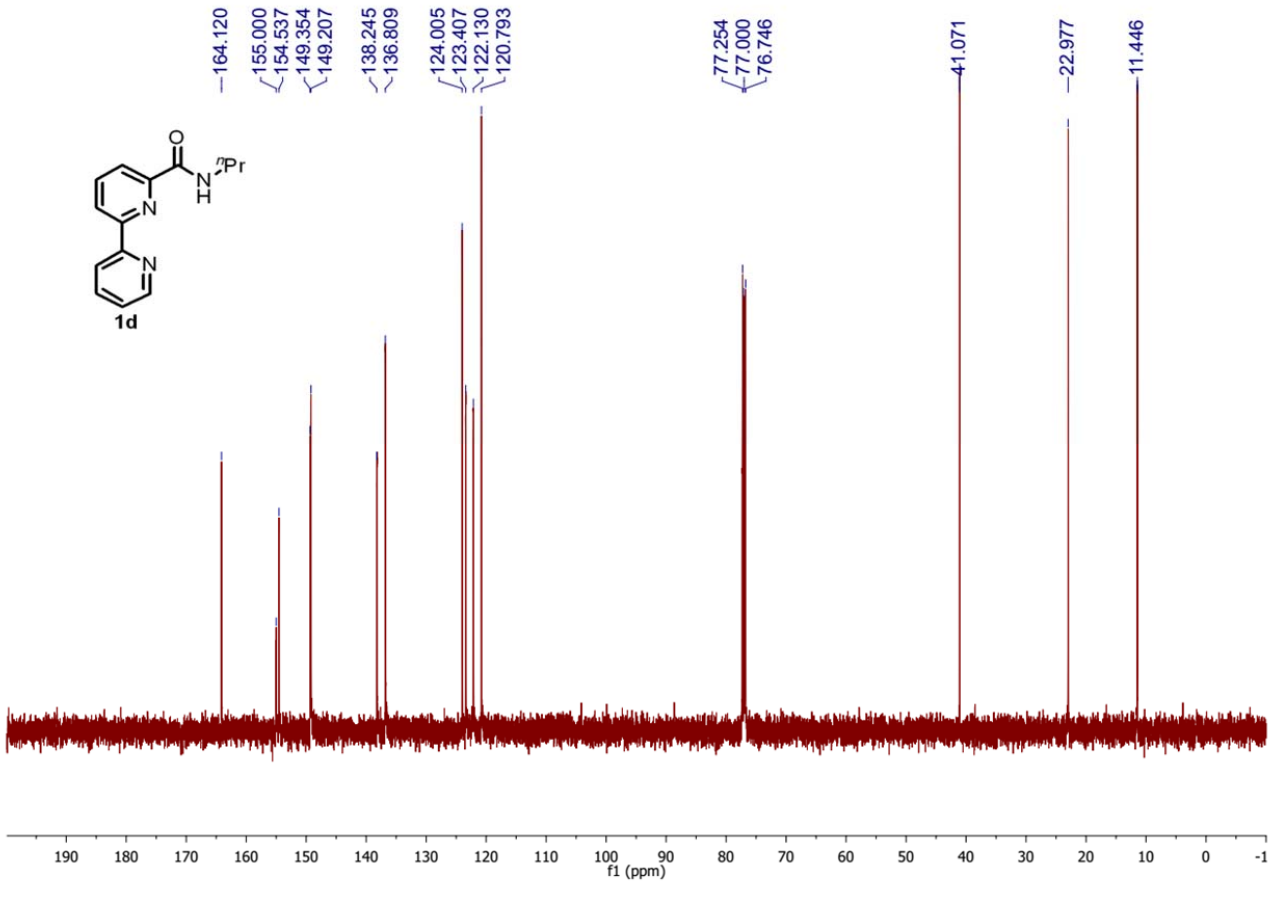

8.704
8.557
8.555
8.541
8.539
8.405
8.389
8.248
8.246
8.233
8.231
7.982
7.370
7.368
7.361
7.358
7.356
7.353
7.349
7.346
7.344
7.275
3.110
3.108
3.100
3.098
0.002
-0.000
O
N
Me
H
N
N
1b
1.00
1.03
1.02
1.00
1.00
1.00
1.02
1.03
3.02
f1 (ppm)

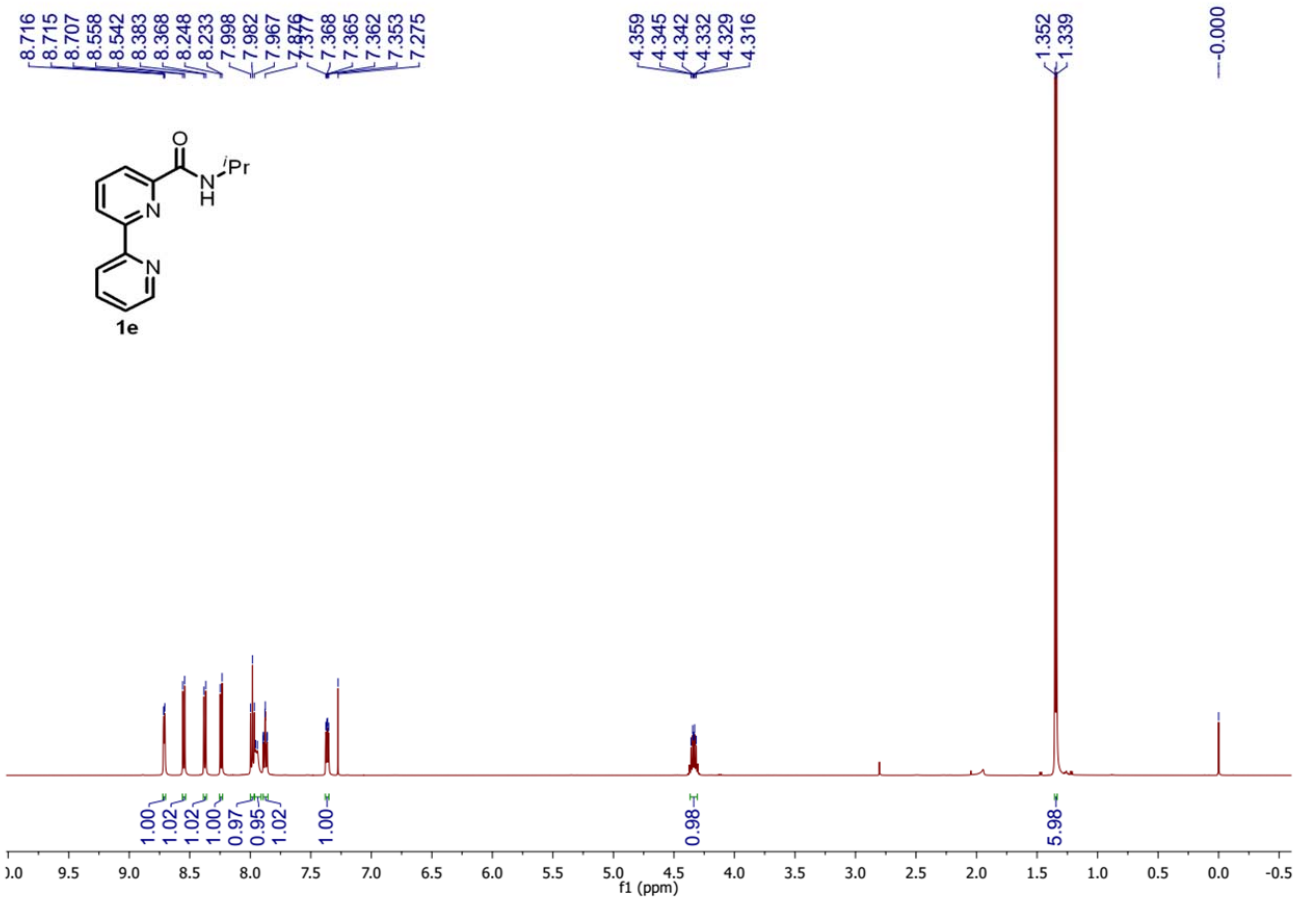

164.870
155.084
154.640
149.306
149.283
138.312
136.831
124.052
123.495
122.102
120.884
77.254
77.000
76.746
26.153
O
N
Me
H
N
N
1b
f1 (ppm)

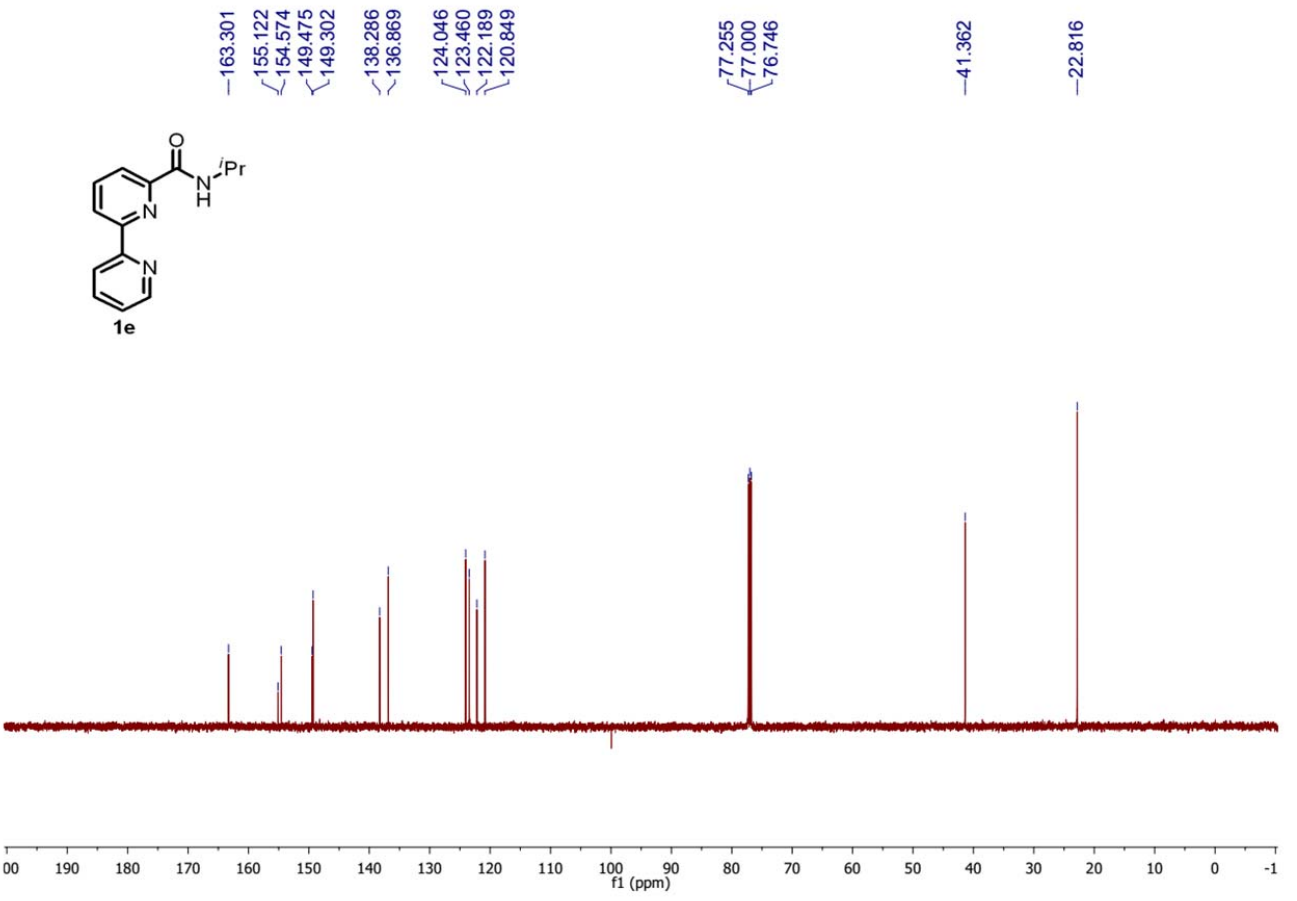

8.559
8.557
8.543
8.541
8.402
8.386
8.252
8.250
8.237
8.235
8.001
7.985
7.864
7.376
7.374
7.366
7.364
7.361
7.359
7.351
7.350
3.610
3.595
3.583
3.581
3.568
3.554
1.341
1.327
1.312
-0.000
Et
N
H
O
N
N
1c
1.00
1.03
1.04
1.03
0.95
1.06
1.05
1.03
2.09
3.05
f1 (ppm)

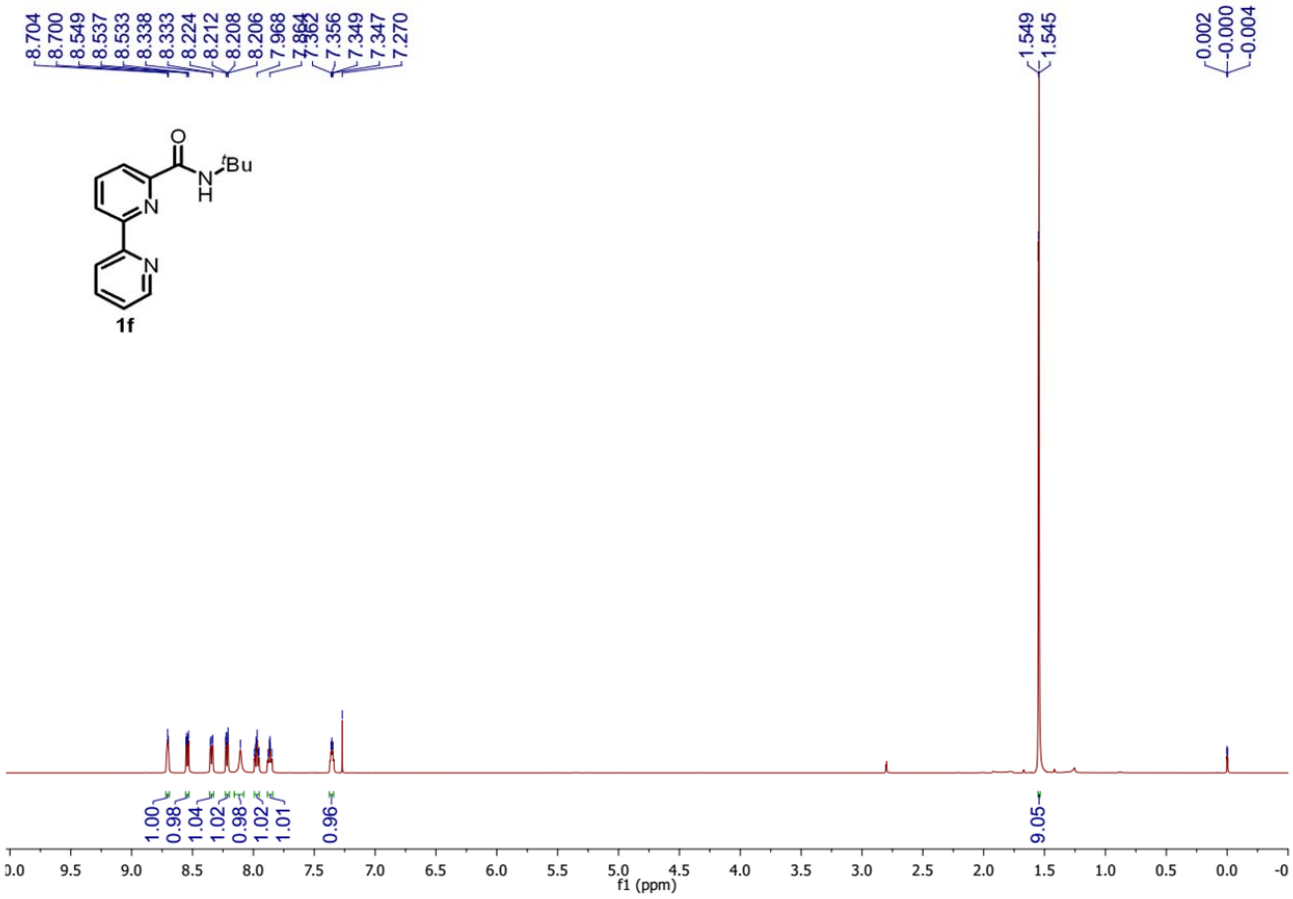

164.079
155.127
154.626
149.399
149.317
138.313
136.860
124.058
123.500
122.191
120.891
77.254
77.000
76.746
34.297
14.975
Et
N
H
O
N
N
1c
f1 (ppm)

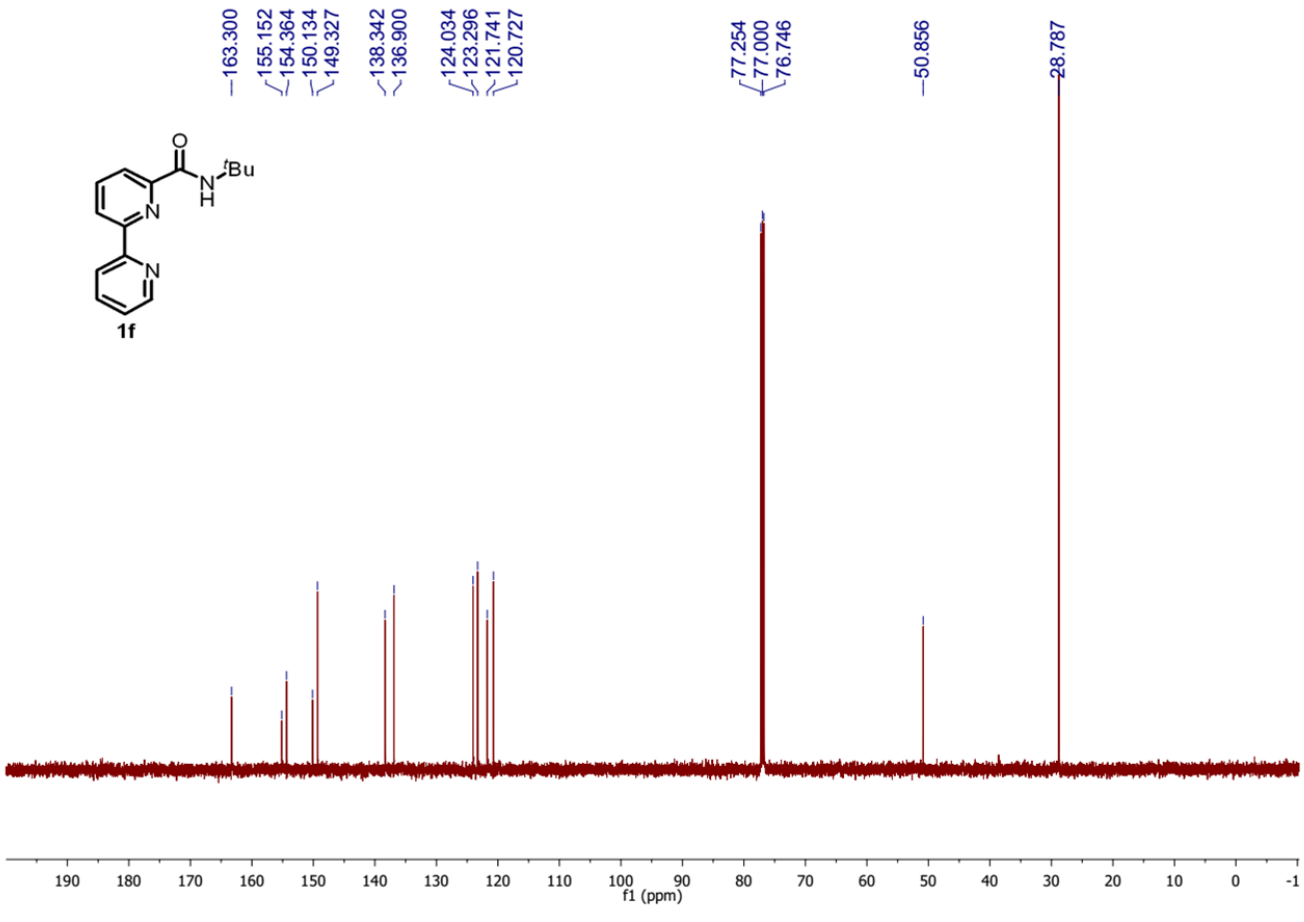

8.712
8.703
8.559
8.558
8.556
8.546
8.543
8.540
8.388
8.373
8.249
8.248
8.246
8.236
8.234
8.231
8.182
8.000
7.995
7.985
7.980
7.969
7.964
7.864
7.860
7.856
7.849
7.845
7.366
7.364
7.362
7.359
7.357
7.352
7.349
7.347
3.525
3.522
3.509
3.496
3.484
3.481
1.742
1.739
1.726
1.724
1.710
1.698
1.695
1.684
1.053
1.050
1.039
1.035
1.024
1.020
-0.000
nPr
1d
1.00
1.02
1.03
0.92
1.04
1.03
1.04
1.00
2.06
2.09
3.10
f1 (ppm)

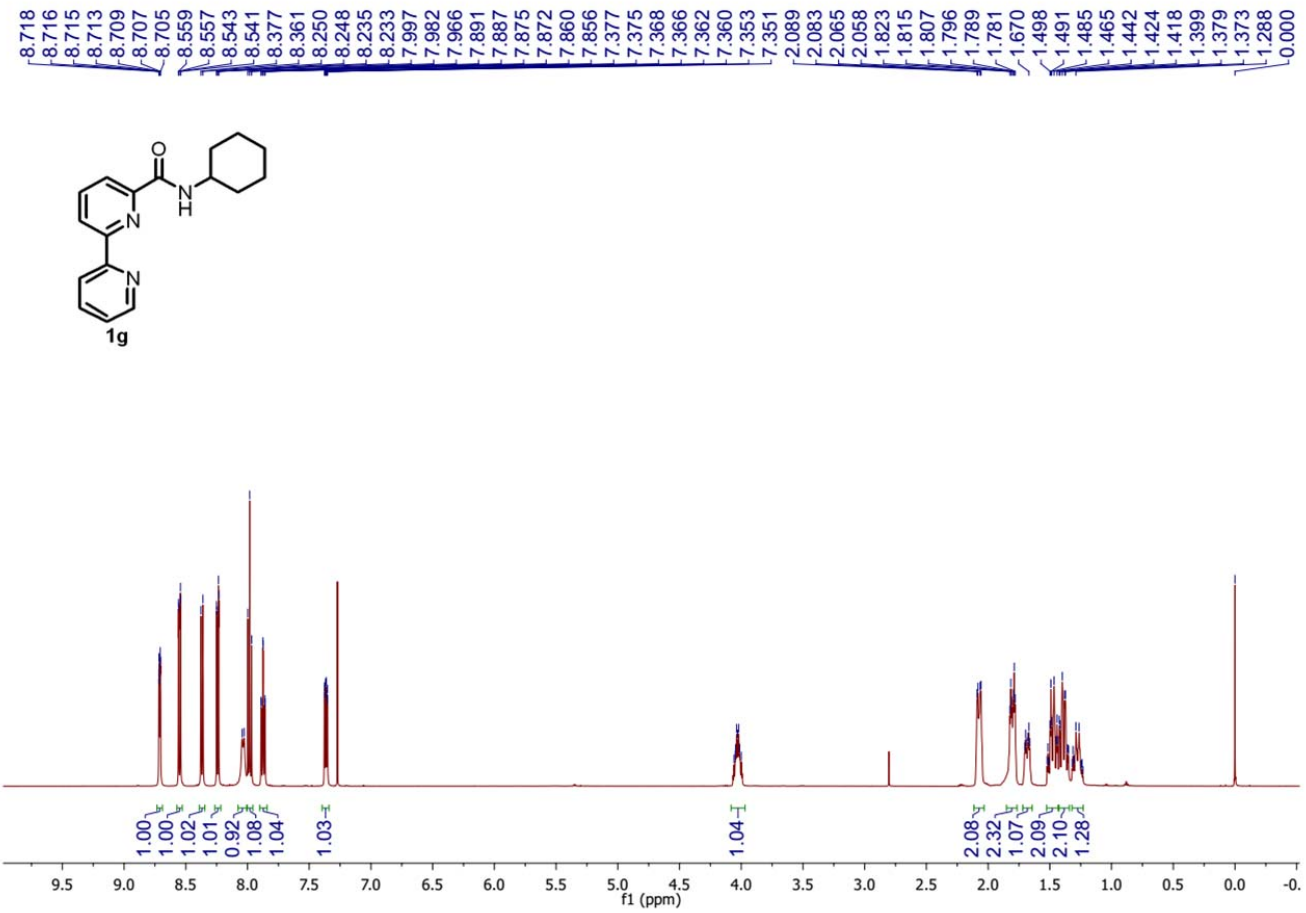

164.120
155.000
154.537
149.354
149.207
138.245
136.809
124.005
123.407
122.130
120.793
77.254
77.000
76.746
41.071
22.977
11.446
nPr
1d
f1 (ppm)

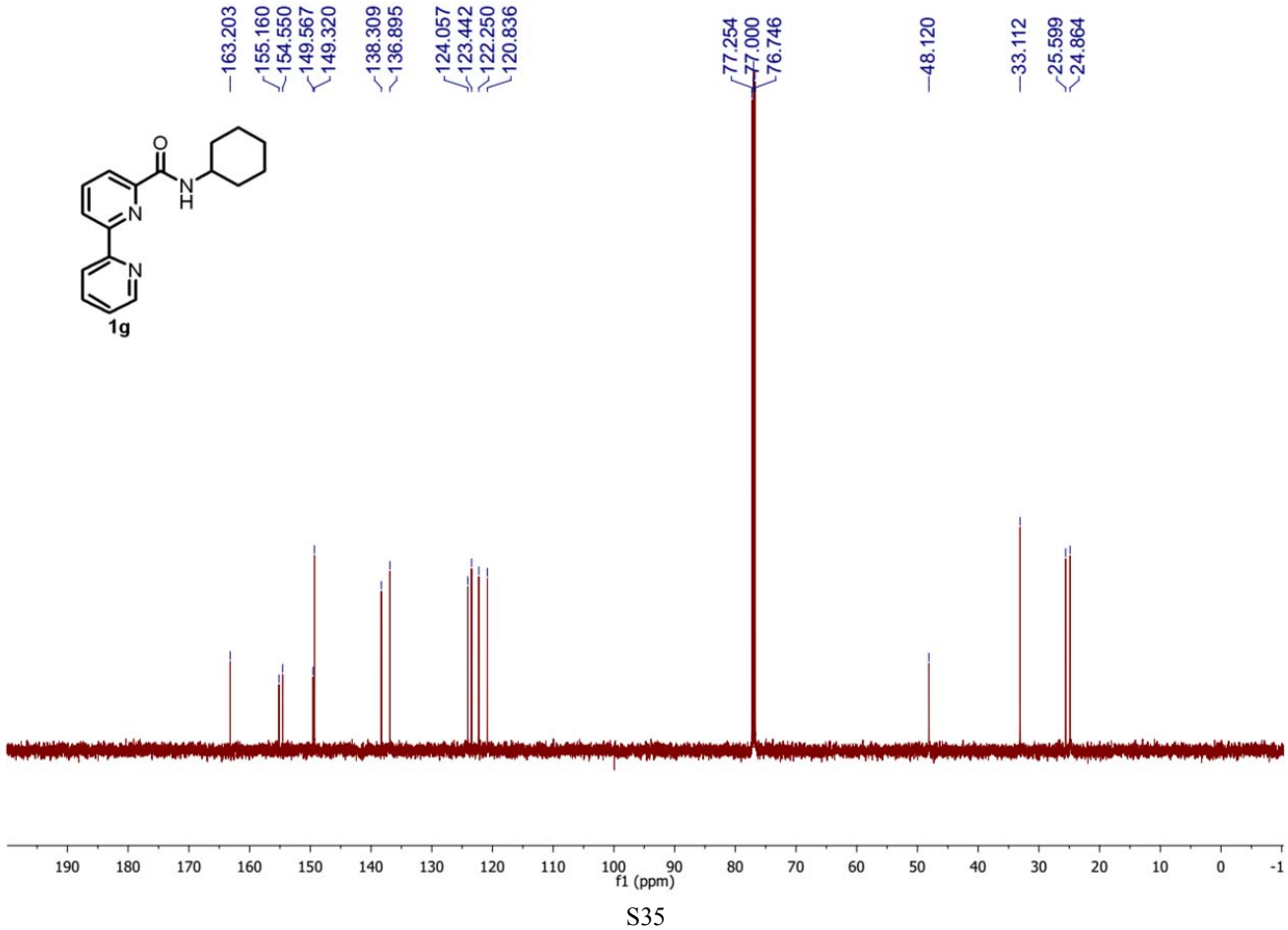

8.716
8.715
8.707
8.558
8.542
8.383
8.368
8.248
8.233
7.998
7.982
7.967
7.876
7.377
7.368
7.365
7.362
7.353
7.275
4.359
4.345
4.342
4.332
4.329
4.316
1.352
1.339
-0.000
1.00
1.02
1.02
1.00
0.97
0.95
1.02
1.00
0.98
5.98
f1 (ppm)

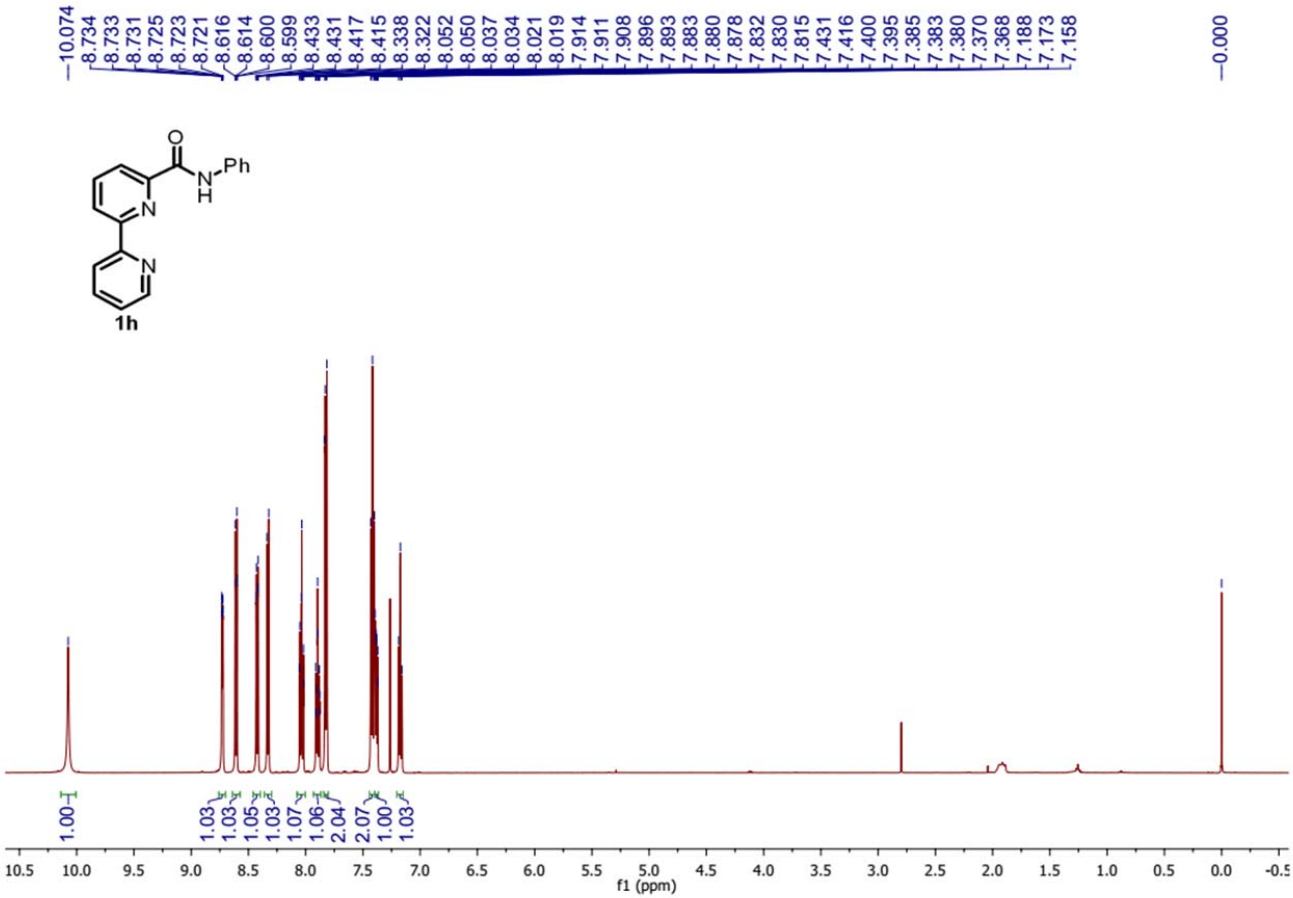

163.301
155.122
154.574
149.475
149.302
138.286
136.869
124.046
123.460
122.189
120.849
77.255
77.000
76.746
41.362
22.816
f1 (ppm)

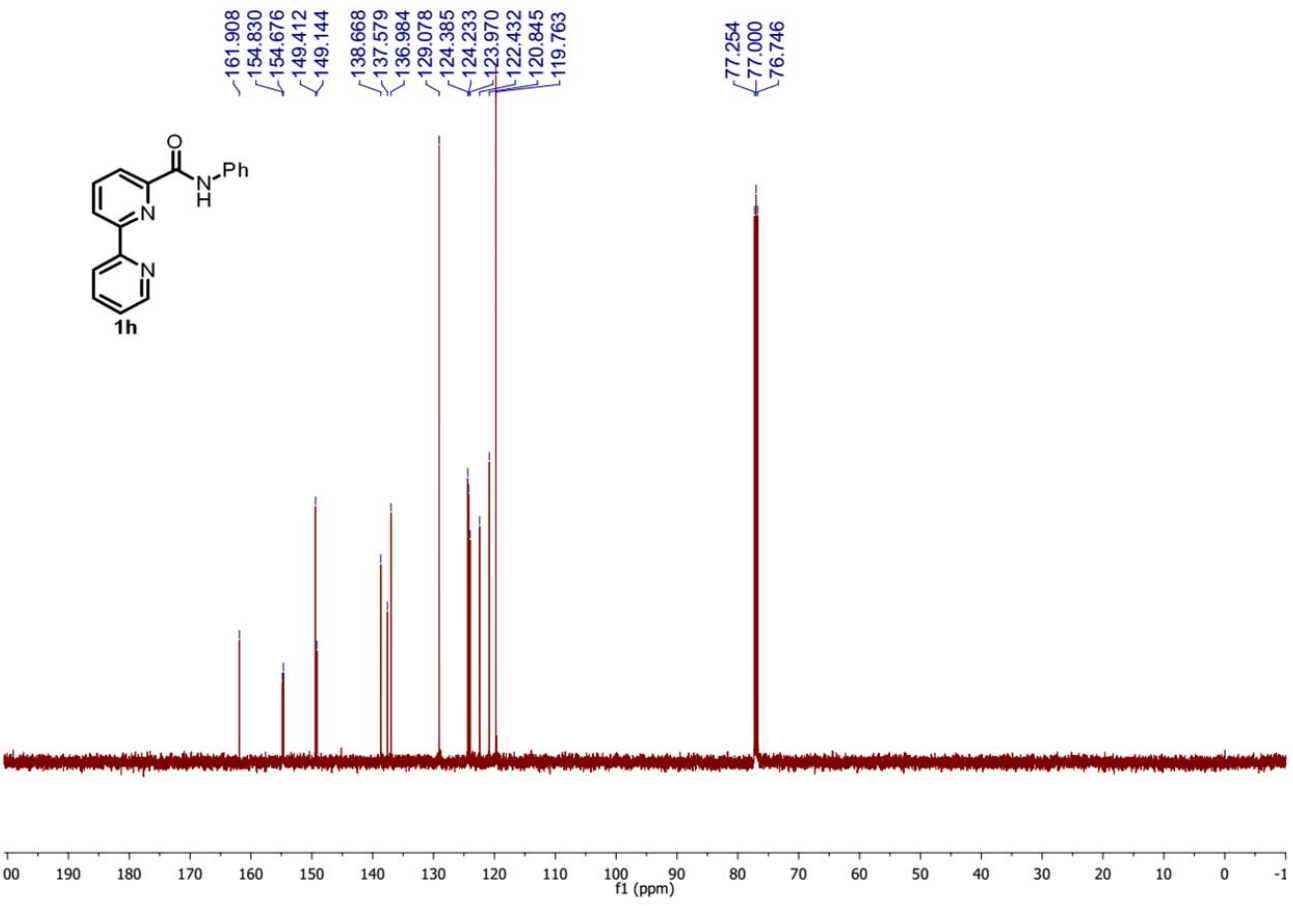

8.704
8.700
8.549
8.537
8.533
8.338
8.333
8.224
8.212
8.208
8.206
7.968
7.356
7.349
7.347
7.270
1.549
1.545
0.002
-0.000
-0.004
1f
1.00
0.98
1.04
1.02
0.98
1.02
1.01
0.96
9.05
f1 (ppm)

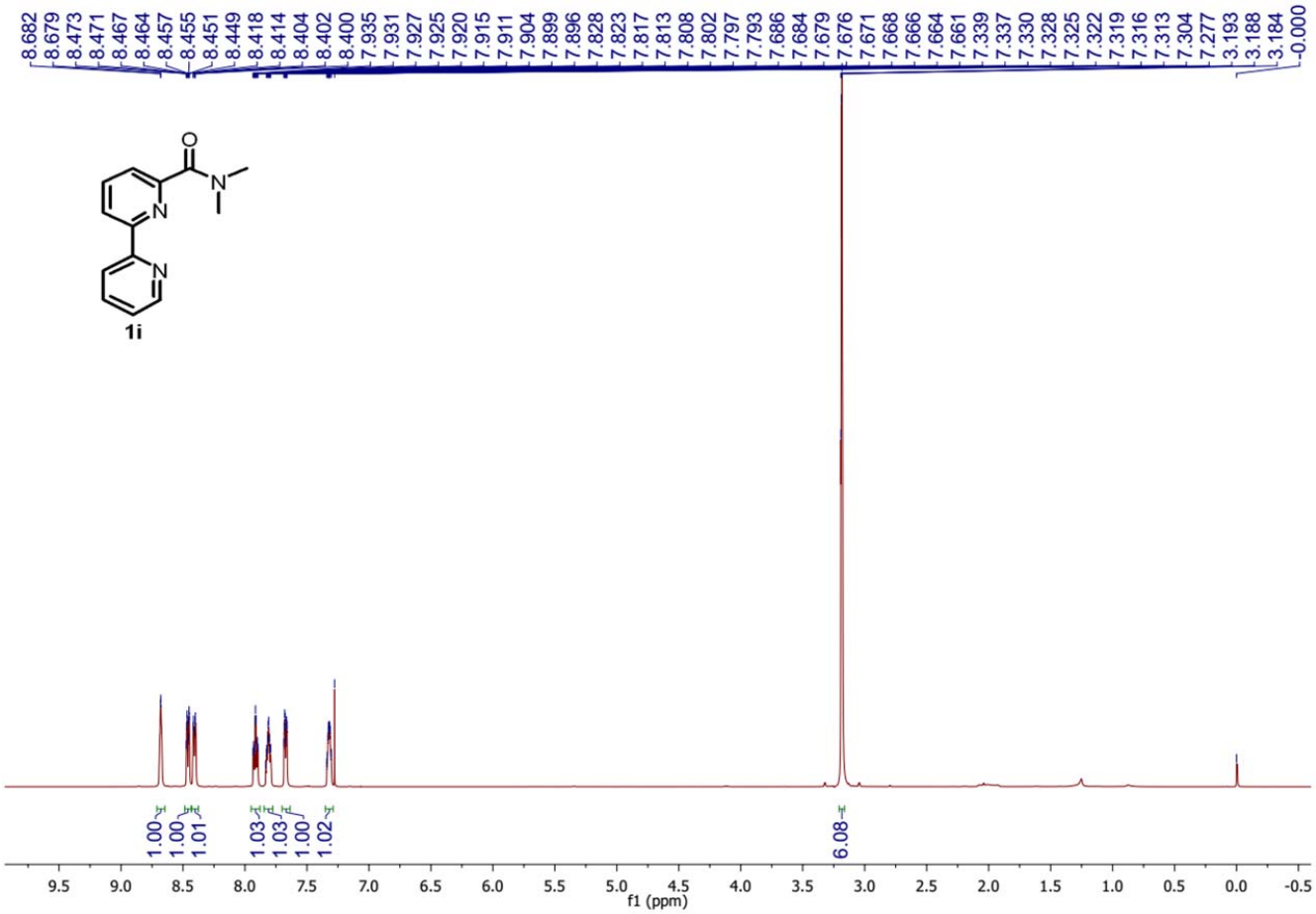

163.300
155.152
154.364
150.134
149.327
138.342
136.900
124.034
123.296
121.741
120.727
77.254
77.000
76.746
50.856
28.787
1f
f1 (ppm)

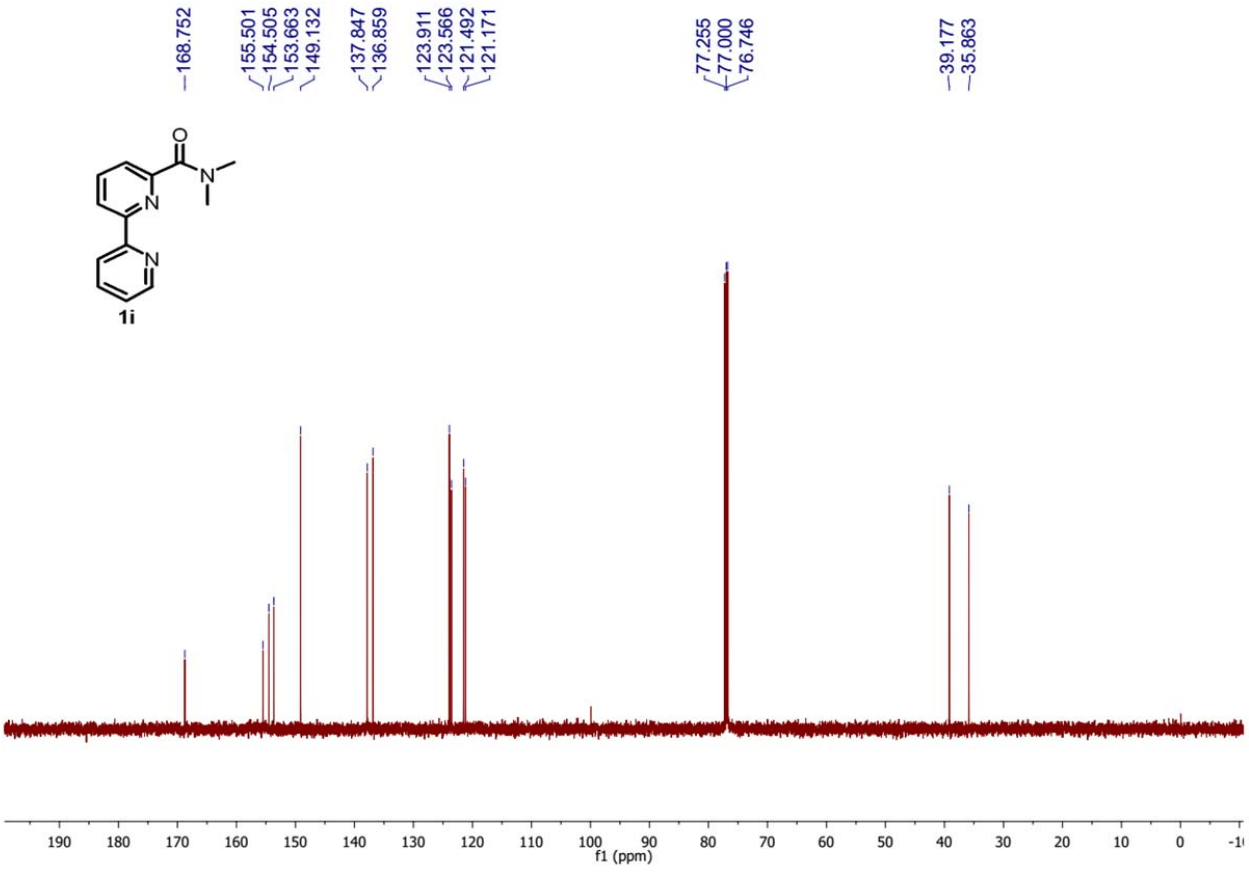

8.718
8.716
8.715
8.713
8.709
8.707
8.705
8.559
8.557
8.543
8.541
8.377
8.361
8.250
8.248
8.235
8.233
7.997
7.982
7.966
7.891
7.887
7.875
7.872
7.860
7.856
7.377
7.375
7.368
7.366
7.362
7.360
7.353
7.351
2.089
2.083
2.065
2.058
1.823
1.815
1.807
1.796
1.789
1.781
1.670
1.498
1.491
1.485
1.465
1.442
1.424
1.418
1.399
1.379
1.373
1.288
0.000
1g
1.00
1.00
1.02
1.01
0.92
1.08
1.04
1.03
1.04
2.08
2.32
1.07
2.09
2.10
1.28
f1 (ppm)

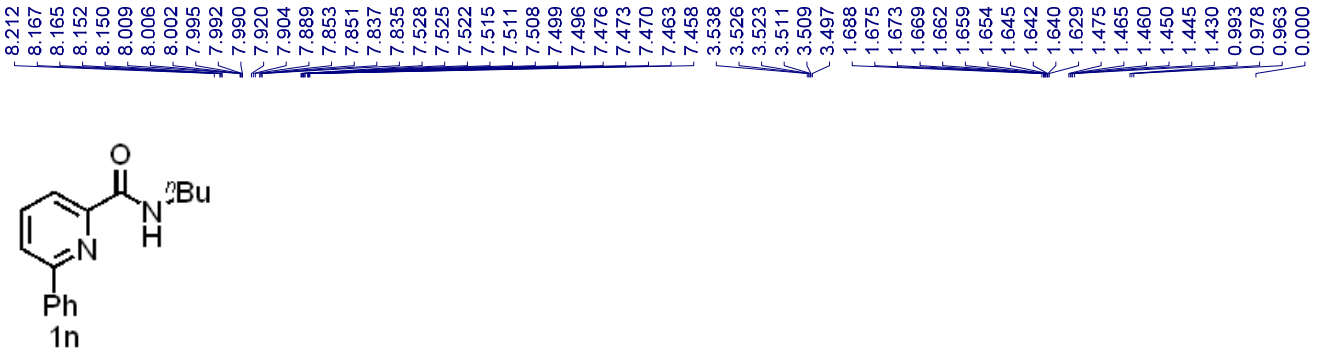

163.203
155.160
154.550
149.567
149.320
138.309
136.895
124.057
123.442
122.250
120.836
77.254
77.000
76.746
48.120
33.112
25.599
24.864
1g
f1 (ppm)


10.074
8.734
8.733
8.731
8.725
8.723
8.721
8.616
8.614
8.600
8.599
8.433
8.431
8.417
8.415
8.338
8.322
8.052
8.050
8.037
8.034
8.021
8.019
7.914
7.911
7.908
7.896
7.893
7.883
7.880
7.878
7.832
7.830
7.815
7.431
7.416
7.400
7.395
7.385
7.383
7.380
7.370
7.368
7.188
7.173
7.158
0.000
Ph
N
H
O
N
N
1h
1.00
1.03
1.03
1.05
1.03
1.07
1.06
2.04
2.07
1.00
1.03
f1 (ppm)


161.908
154.830
154.676
149.412
149.144
138.668
137.579
136.984
129.078
124.385
124.233
123.970
122.432
120.845
119.763
77.254
77.000
76.746
Ph
N
H
O
N
N
1h
f1 (ppm)

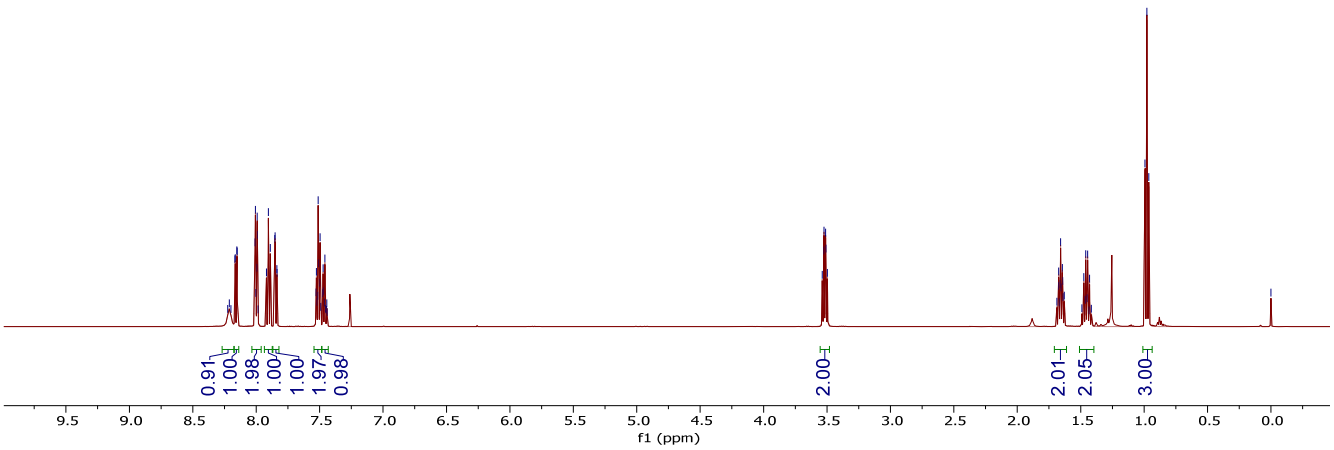

8.682
8.679
8.473
8.471
8.467
8.464
8.457
8.455
8.451
8.449
8.418
8.414
8.404
8.402
8.400
7.935
7.931
7.927
7.925
7.920
7.915
7.911
7.904
7.899
7.896
7.828
7.823
7.817
7.813
7.808
7.802
7.797
7.793
7.686
7.684
7.679
7.676
7.671
7.668
7.666
7.664
7.661
7.339
7.337
7.330
7.328
7.325
7.322
7.319
7.316
7.313
7.304
7.277
3.193
3.188
3.184
-0.000
1i
1.00
1.00
1.01
1.03
1.03
1.00
1.02
6.08
f1 (ppm)


168.752
155.501
154.505
153.663
149.132
137.847
136.859
123.911
123.566
121.492
121.171
77.255
77.000
76.746
39.177
35.863
1i
f1 (ppm)

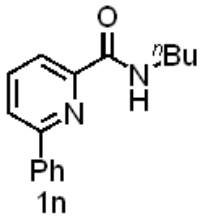

8.212
8.167
8.165
8.152
8.150
8.009
8.006
8.002
7.995
7.992
7.990
7.920
7.904
7.889
7.853
7.851
7.837
7.835
7.528
7.525
7.522
7.515
7.511
7.508
7.499
7.496
7.476
7.473
7.470
7.463
7.458
3.538
3.526
3.523
3.511
3.509
3.497
1.688
1.675
1.673
1.669
1.662
1.659
1.654
1.645
1.642
1.640
1.629
1.475
1.465
1.460
1.450
1.445
1.430
0.993
0.978
0.963
0.000

O
N
H
tBu
N
Ph

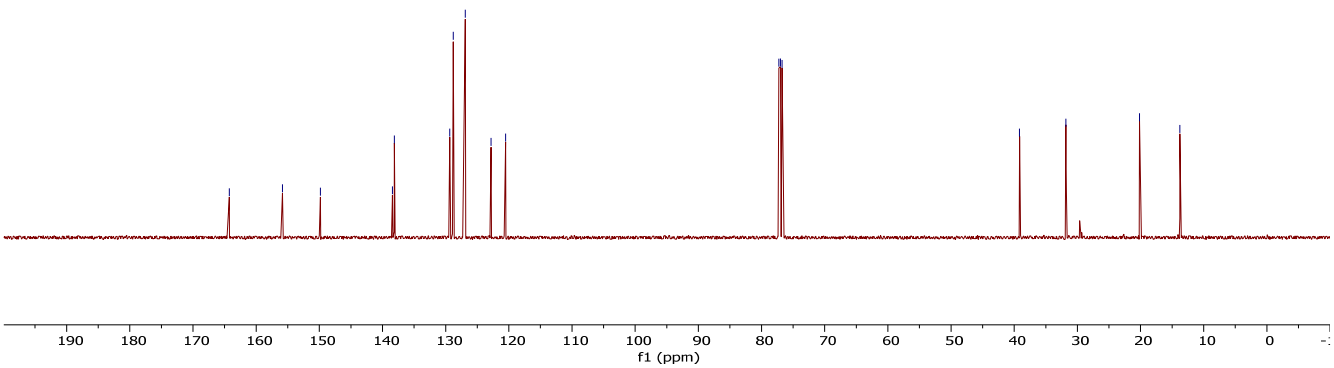
1n

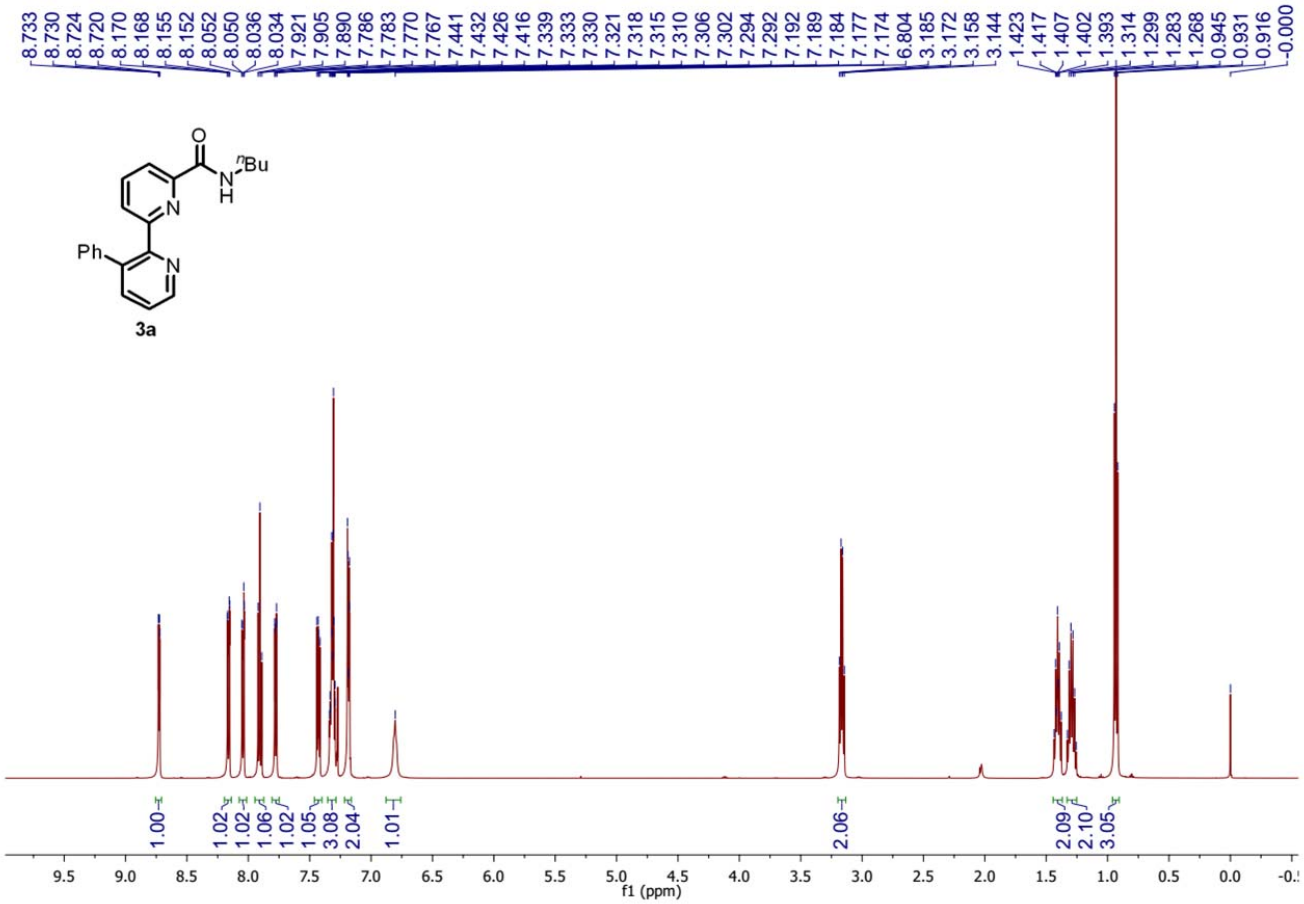

0.91
1.00
1.98
1.00
1.00
1.97
0.98
2.00
2.01
2.05
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

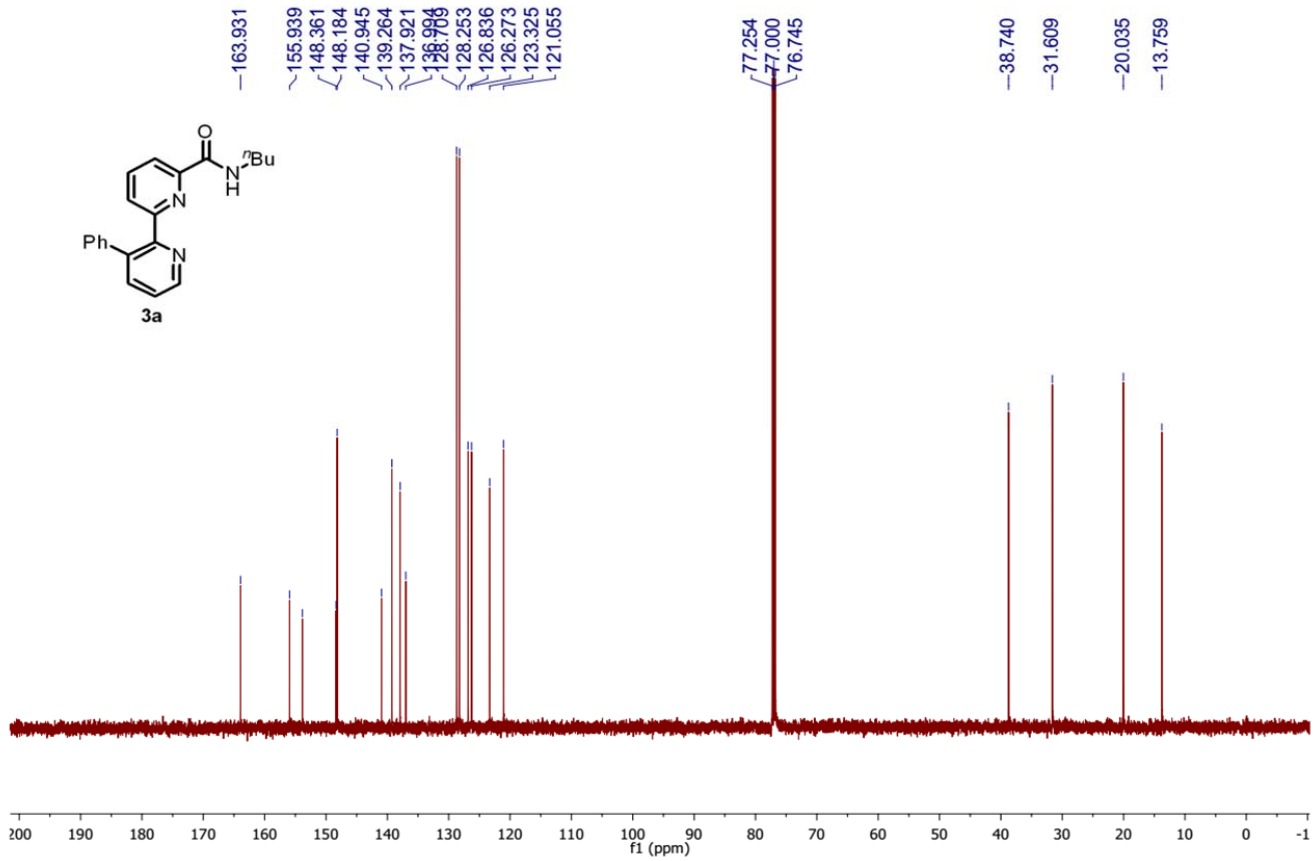

164.257
155.832
149.838
138.437
138.121
129.354
128.792
126.895
122.826
120.520
77.254
77.000
76.746
39.157
31.809
20.171
13.772

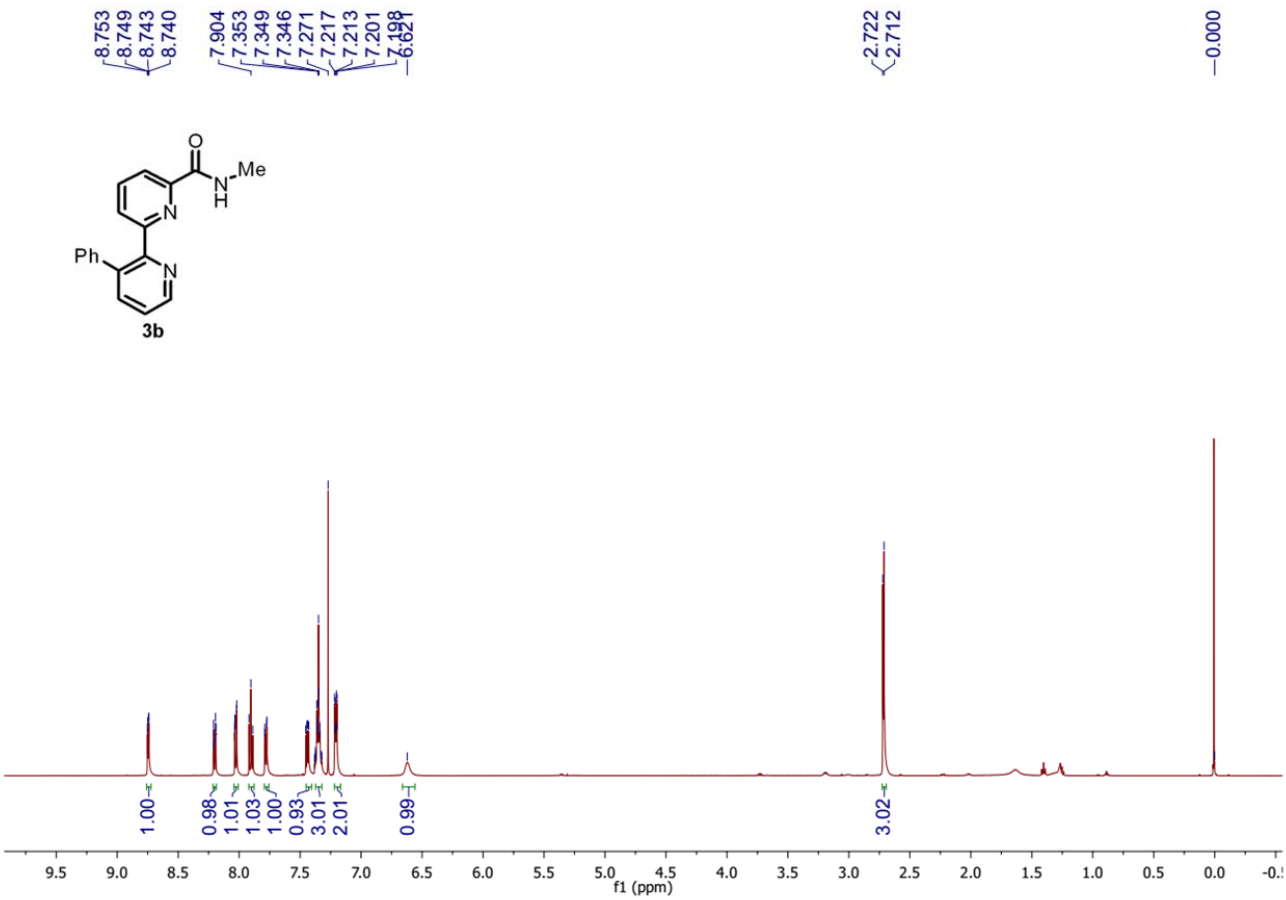

O
N
H
tBu
N
Ph

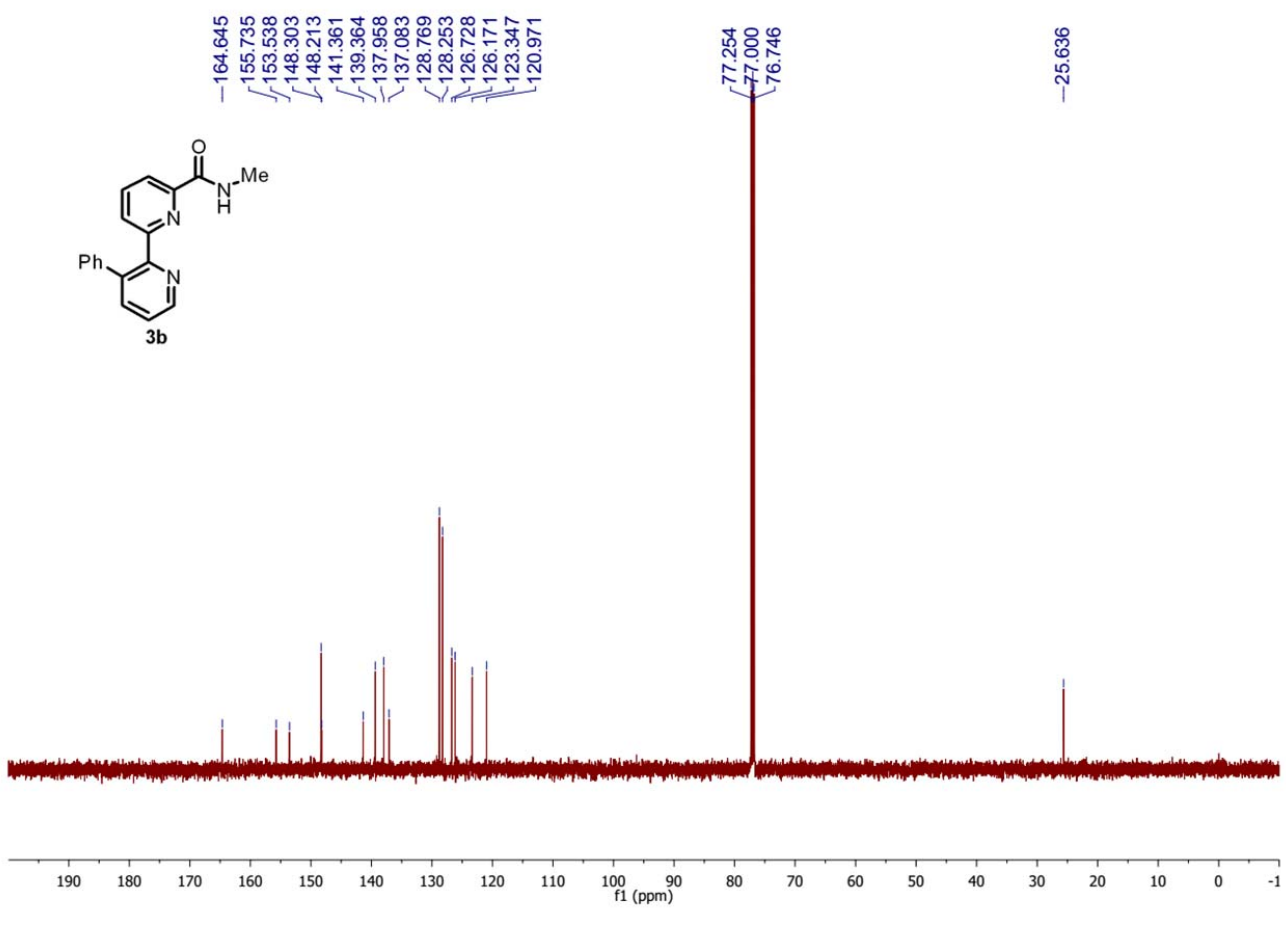
1n

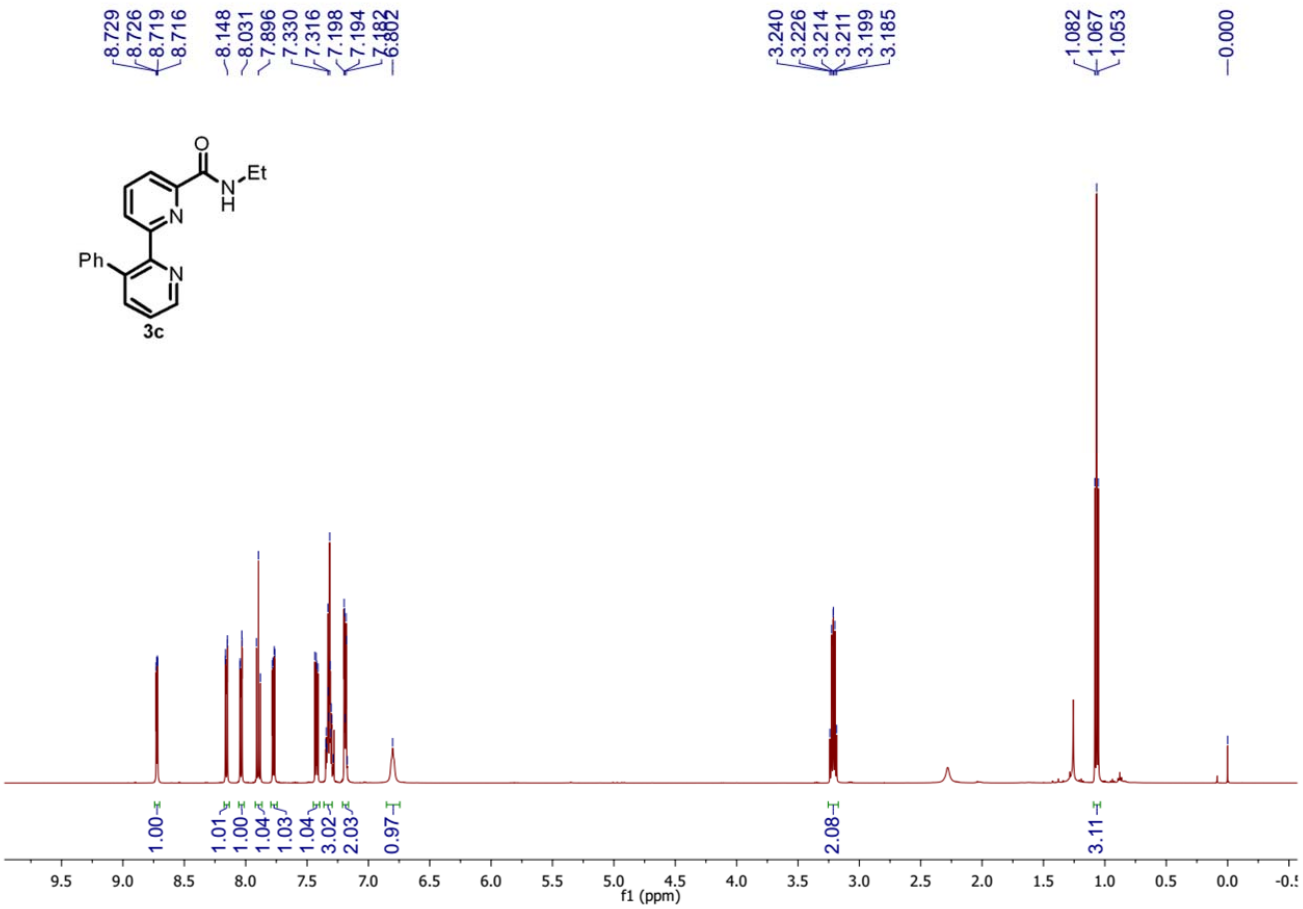

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

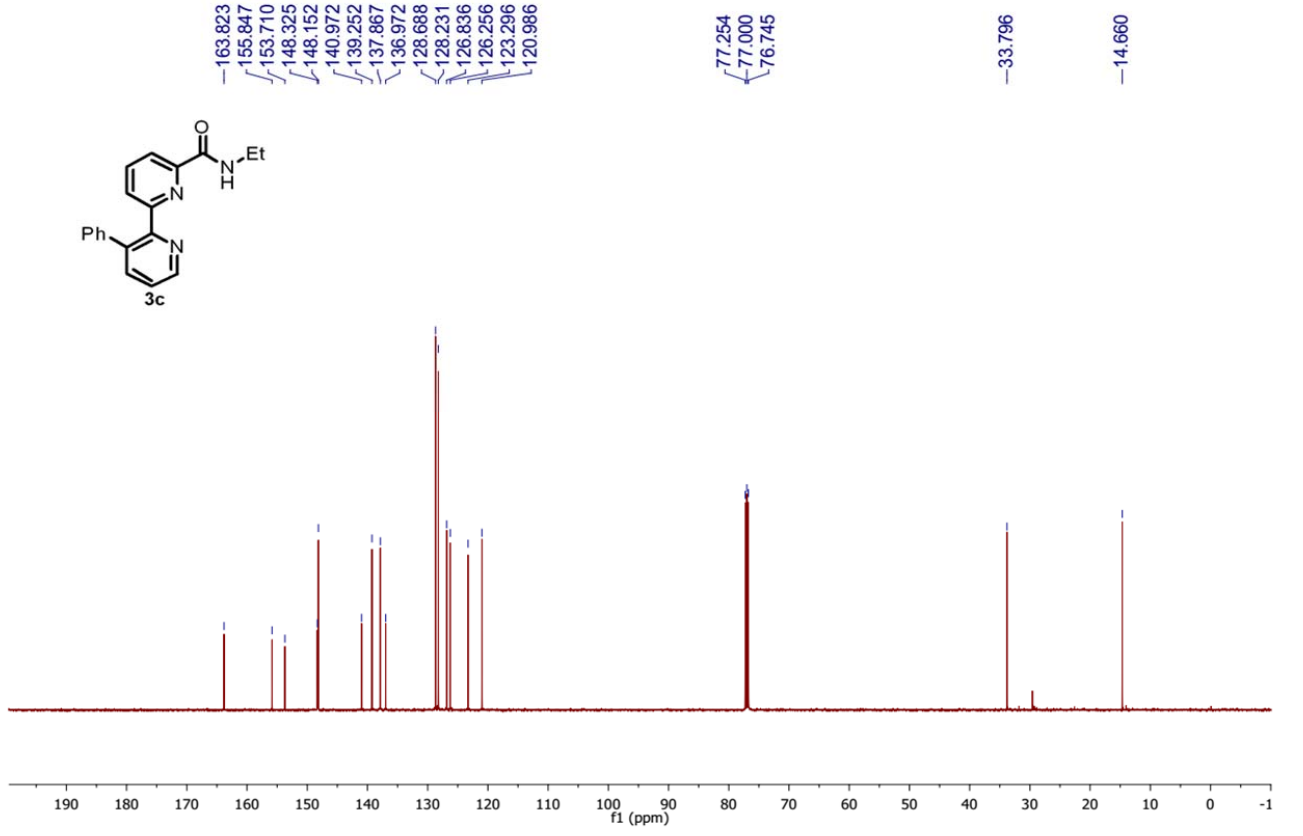

8.733
8.730
8.724
8.720
8.170
8.168
8.155
8.152
8.052
8.050
8.036
8.034
7.921
7.905
7.890
7.786
7.783
7.770
7.767
7.441
7.432
7.426
7.416
7.339
7.333
7.330
7.321
7.318
7.315
7.310
7.306
7.302
7.294
7.292
7.192
7.189
7.184
7.177
7.174
6.804
3.185
3.172
3.158
3.144
1.423
1.417
1.407
1.402
1.393
1.314
1.299
1.283
1.268
0.945
0.931
0.916
-0.000
nBu
Ph
3a
1.00
1.02
1.02
1.06
1.02
1.05
3.08
2.04
1.01
2.06
2.09
2.10
3.05
f1 (ppm)

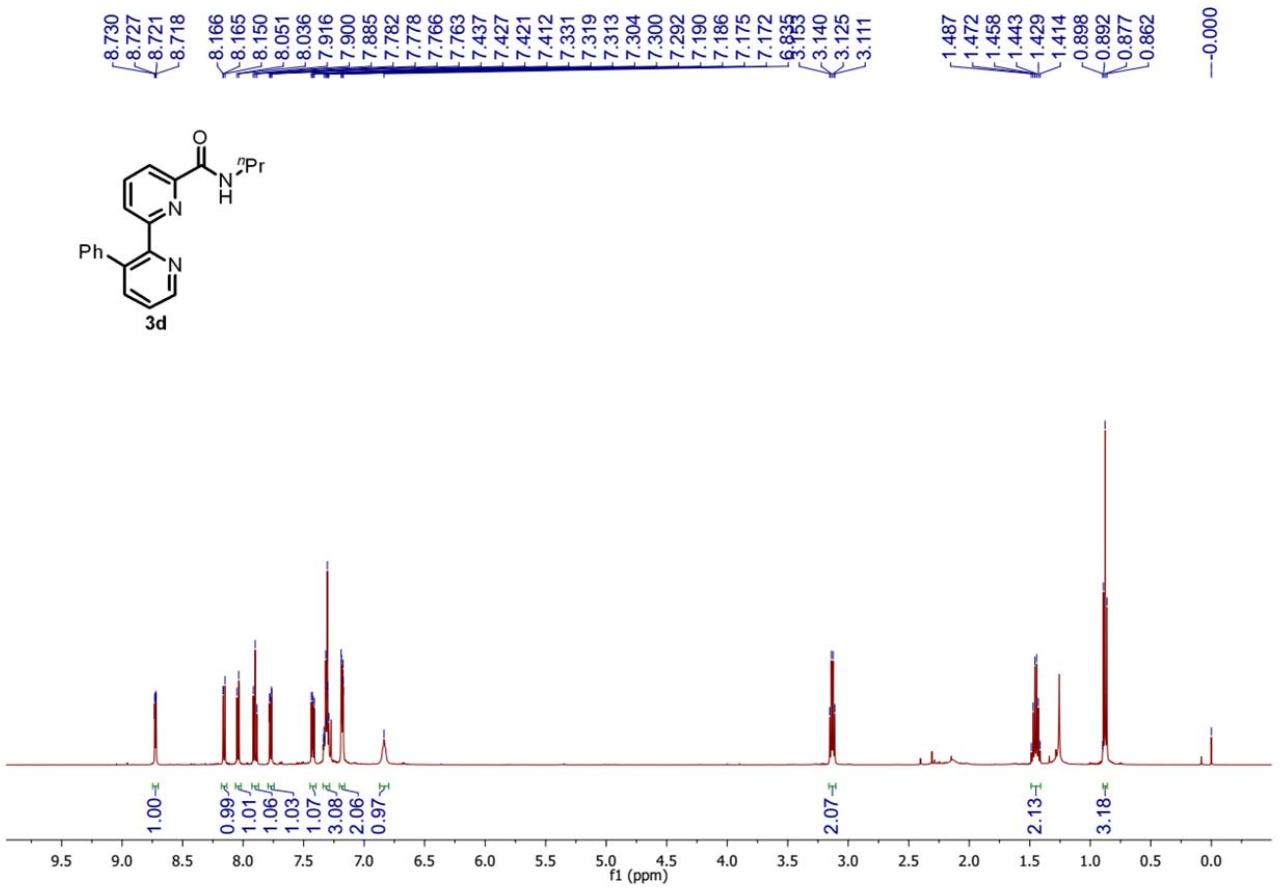

163.931
155.939
148.361
148.184
140.945
139.264
137.921
136.994
128.709
128.253
126.836
126.273
123.325
121.055
77.254
77.000
76.745
38.740
31.609
20.035
13.759
nBu
Ph
3a
f1 (ppm)

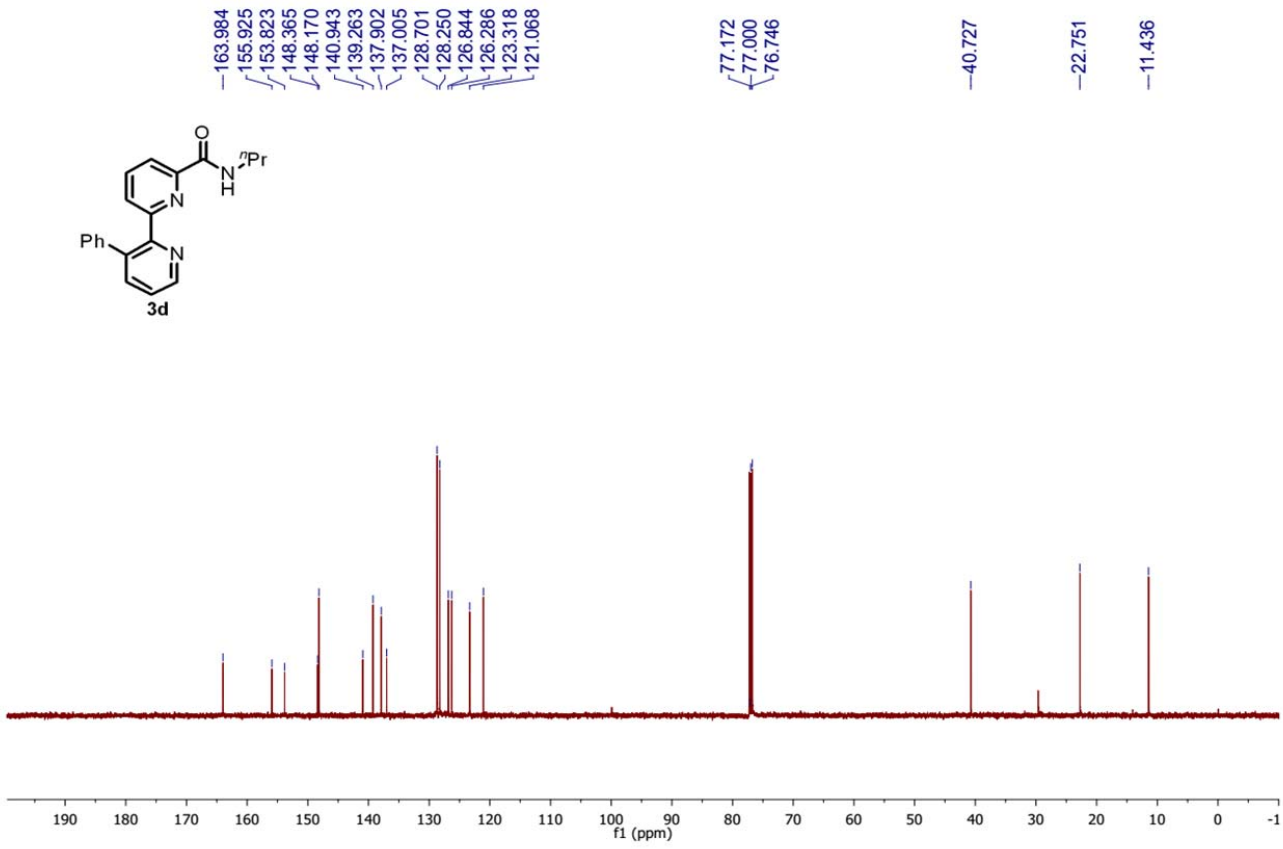

8.753
8.749
8.743
8.740
7.904
7.353
7.349
7.346
7.271
7.217
7.213
7.201
7.198
6.621
2.722
2.712
0.000
Me
N
H
O
N
Ph
N
3b
1.00
0.98
1.01
1.03
1.00
0.93
3.01
2.01
0.99
3.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

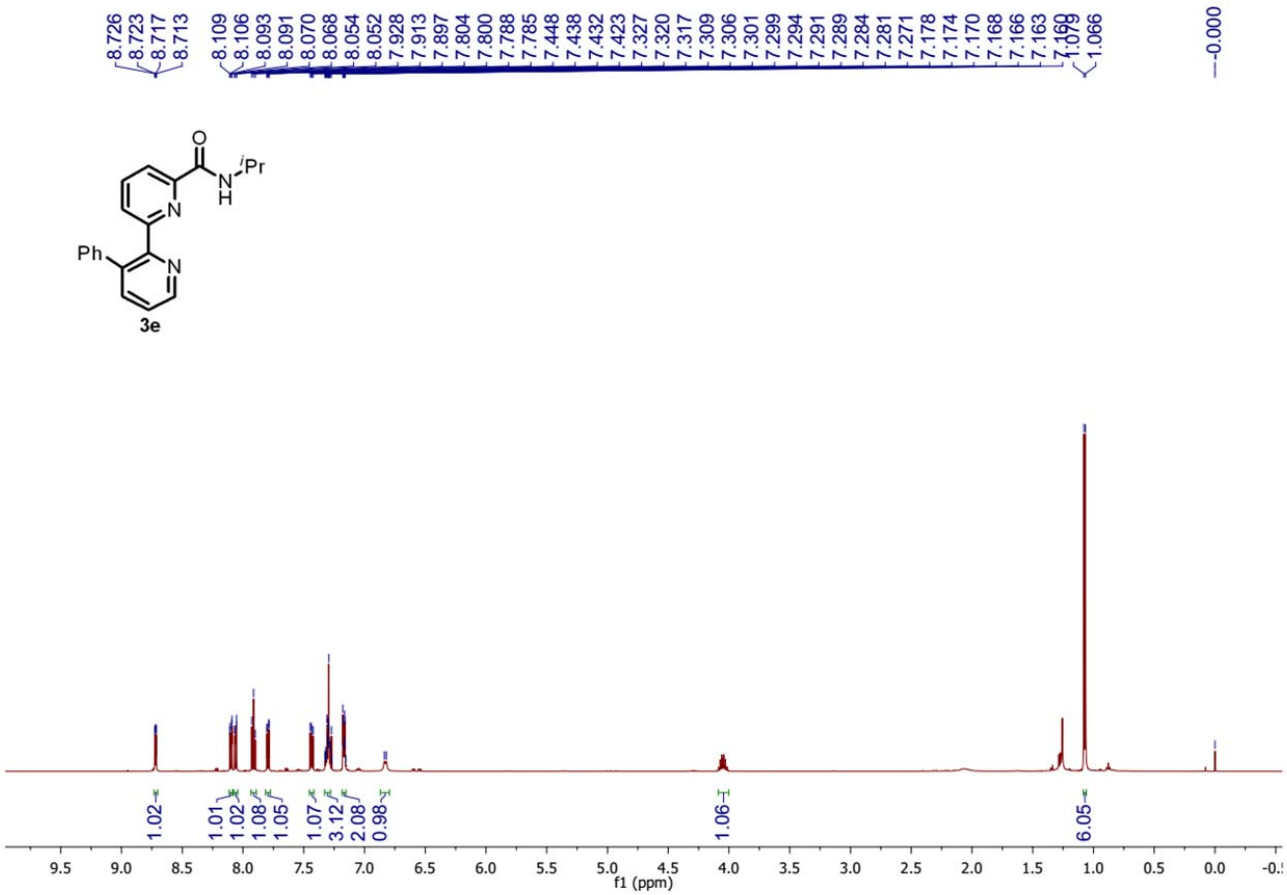

164.645
155.735
153.538
148.303
148.213
141.361
139.364
137.958
137.083
128.769
128.253
126.728
126.171
123.347
120.971
77.254
77.000
76.746
25.636
Me
N
H
O
N
Ph
N
3b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

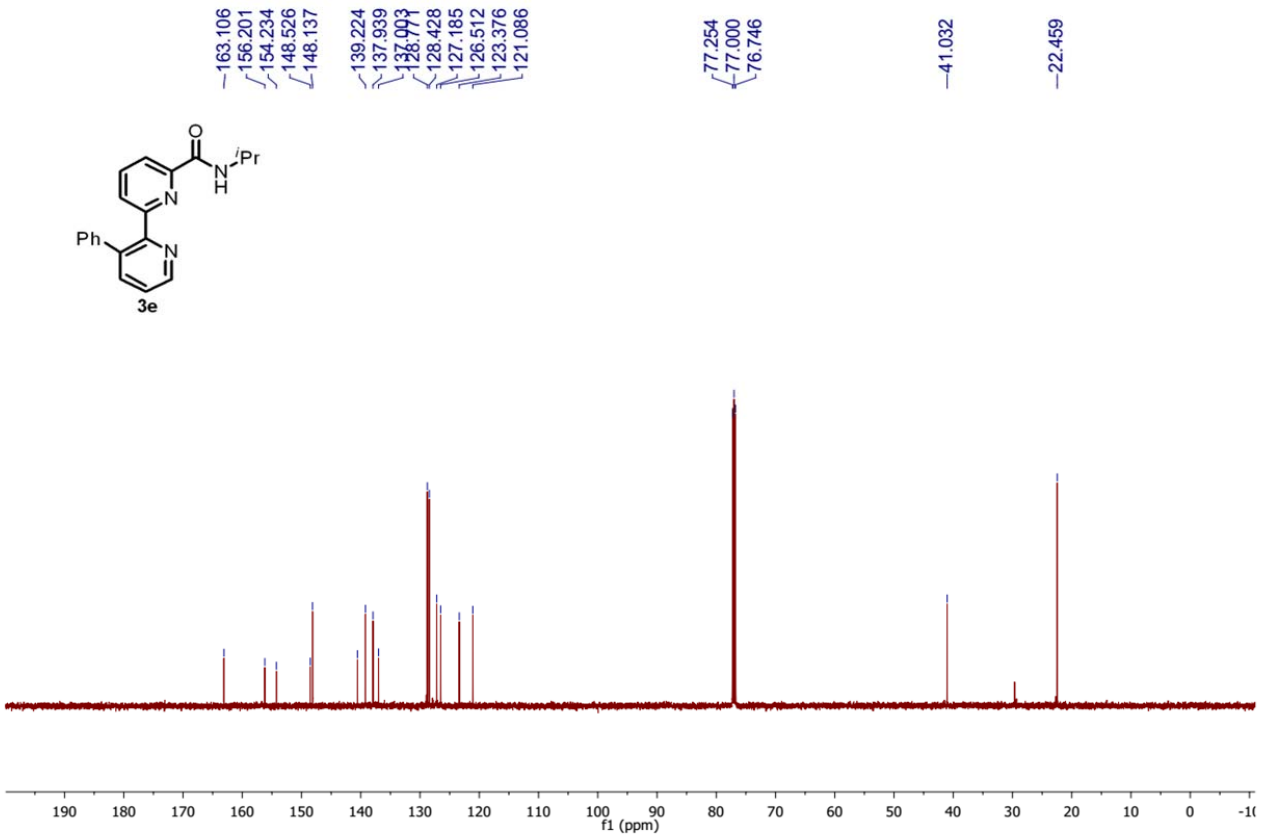

8.729
8.726
8.719
8.716
8.148
8.031
7.896
7.330
7.316
7.198
7.194
6.802
3.240
3.226
3.214
3.211
3.199
3.185
1.082
1.067
1.053
0.000
Et
N
H
O
N
Ph
N
3c
1.00
1.01
1.00
1.04
1.03
1.04
3.02
2.03
0.97
2.08
3.11
f1 (ppm)

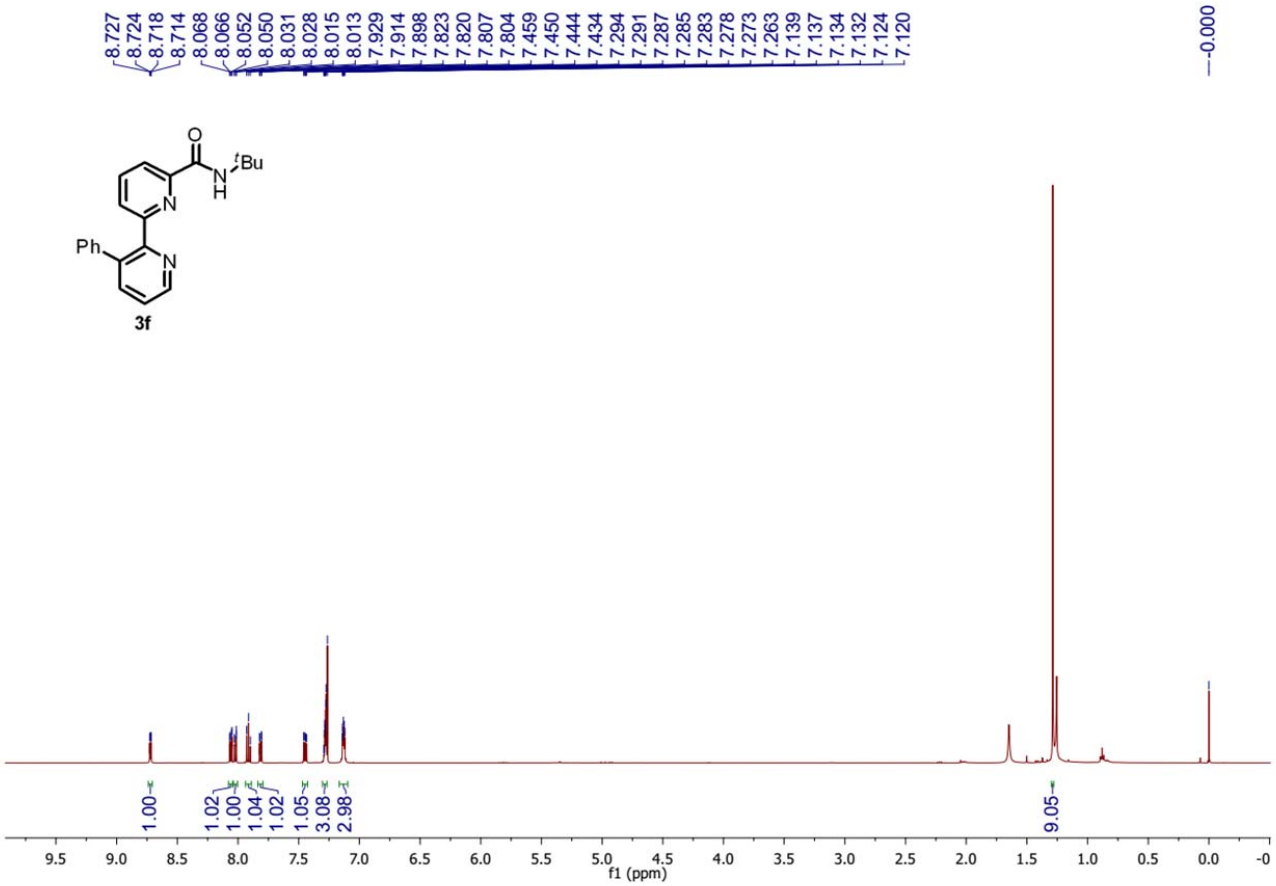

163.823
155.847
153.710
148.325
148.152
140.972
139.252
137.867
136.972
128.688
128.231
126.836
126.256
123.296
120.986
77.254
77.000
76.745
33.796
14.660
Et
N
H
O
N
Ph
N
3c
f1 (ppm)

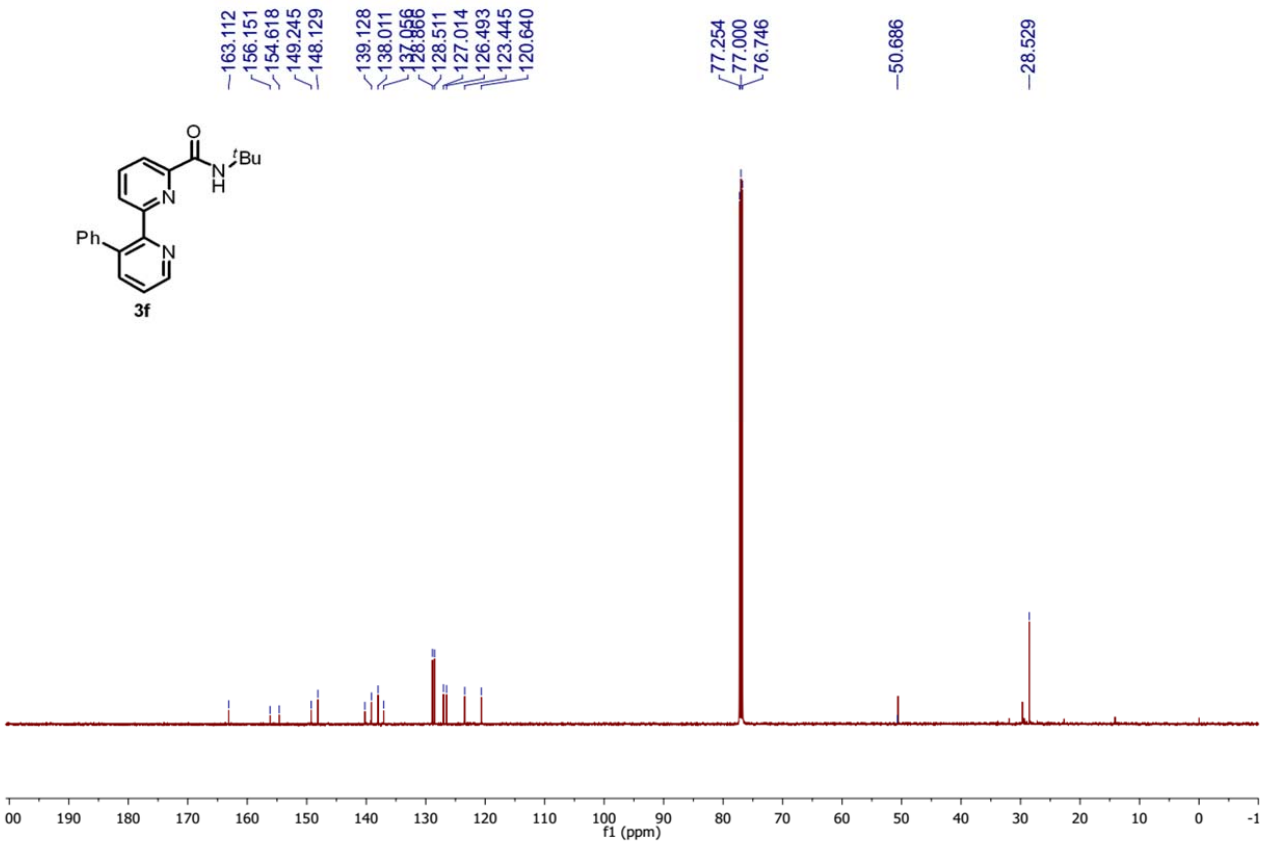

8.730
8.727
8.721
8.718
8.166
8.165
8.150
8.051
8.036
7.916
7.900
7.885
7.782
7.778
7.766
7.763
7.437
7.427
7.421
7.412
7.331
7.319
7.313
7.304
7.300
7.292
7.190
7.186
7.175
7.172
3.140
3.125
3.111
1.487
1.472
1.458
1.443
1.429
1.414
0.898
0.892
0.877
0.862
-0.000
Ph
N
O
N
H
nPr
3d
1.00
0.99
1.01
1.06
1.03
1.07
3.08
2.06
0.97
2.07
2.13
3.18
f1 (ppm)

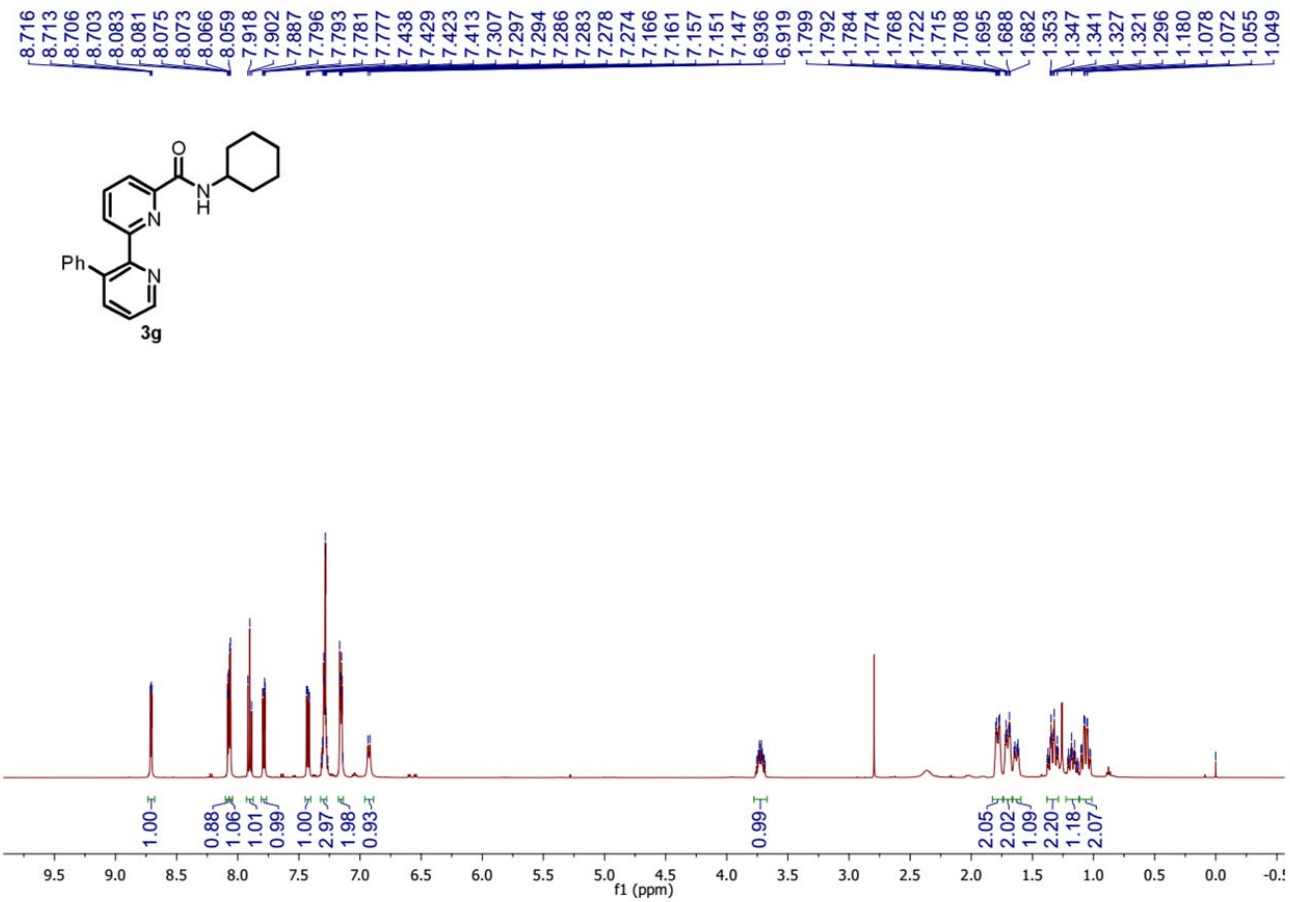

163.984
155.925
153.823
148.365
148.170
140.943
139.263
137.902
137.005
128.701
128.250
126.844
126.286
123.318
121.068
77.172
77.000
76.746
40.727
22.751
11.436
Ph
N
O
N
H
nPr
3d
f1 (ppm)

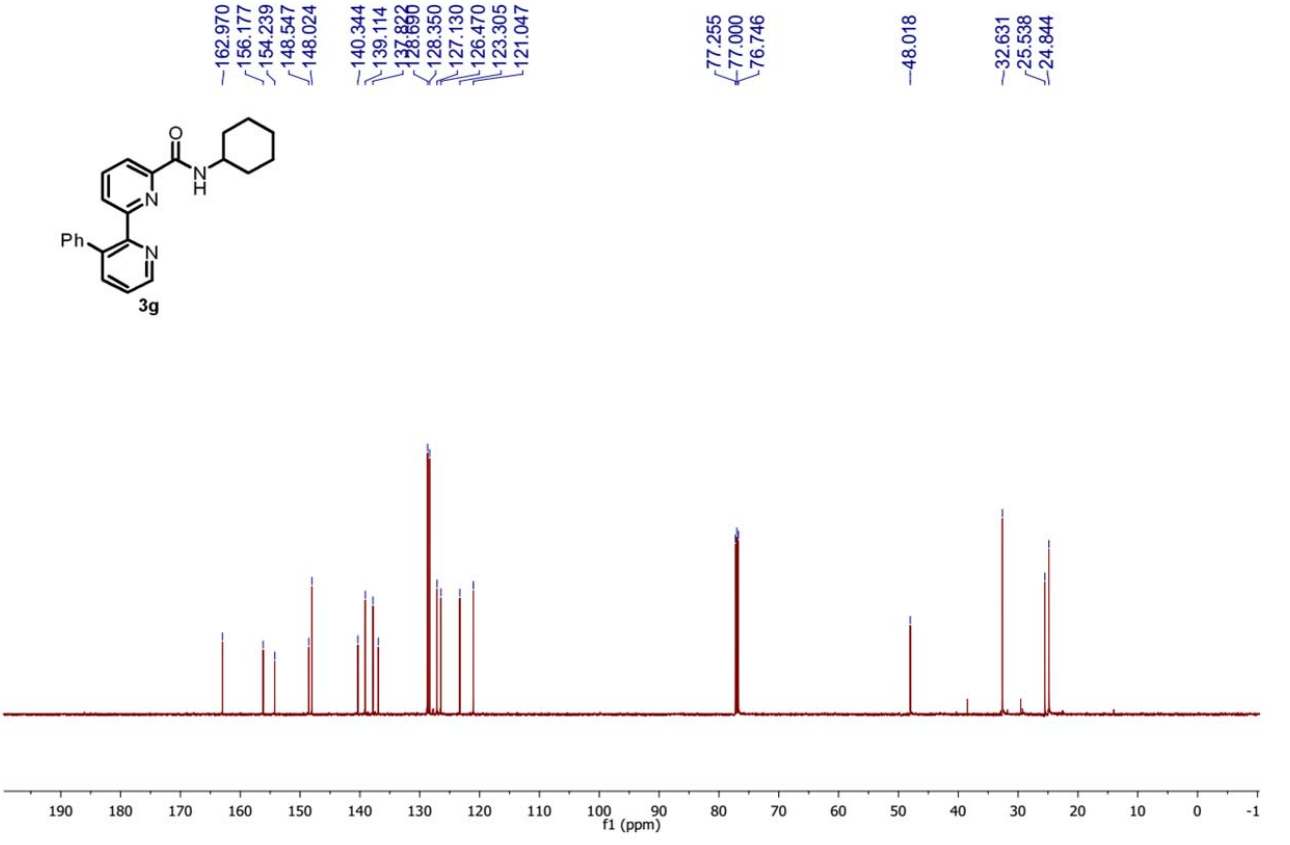

8.726
8.723
8.717
8.713
8.109
8.106
8.093
8.091
8.070
8.068
8.054
8.052
7.928
7.913
7.897
7.804
7.800
7.788
7.785
7.448
7.438
7.432
7.423
7.327
7.320
7.317
7.309
7.306
7.301
7.299
7.294
7.291
7.289
7.284
7.281
7.271
7.178
7.174
7.170
7.168
7.166
7.163
7.079
7.066
-0.000
Ph
N
N
O
N
H
iPr
3e
1.02
1.01
1.02
1.08
1.05
1.07
3.12
2.08
0.98
1.06
6.05
f1 (ppm)

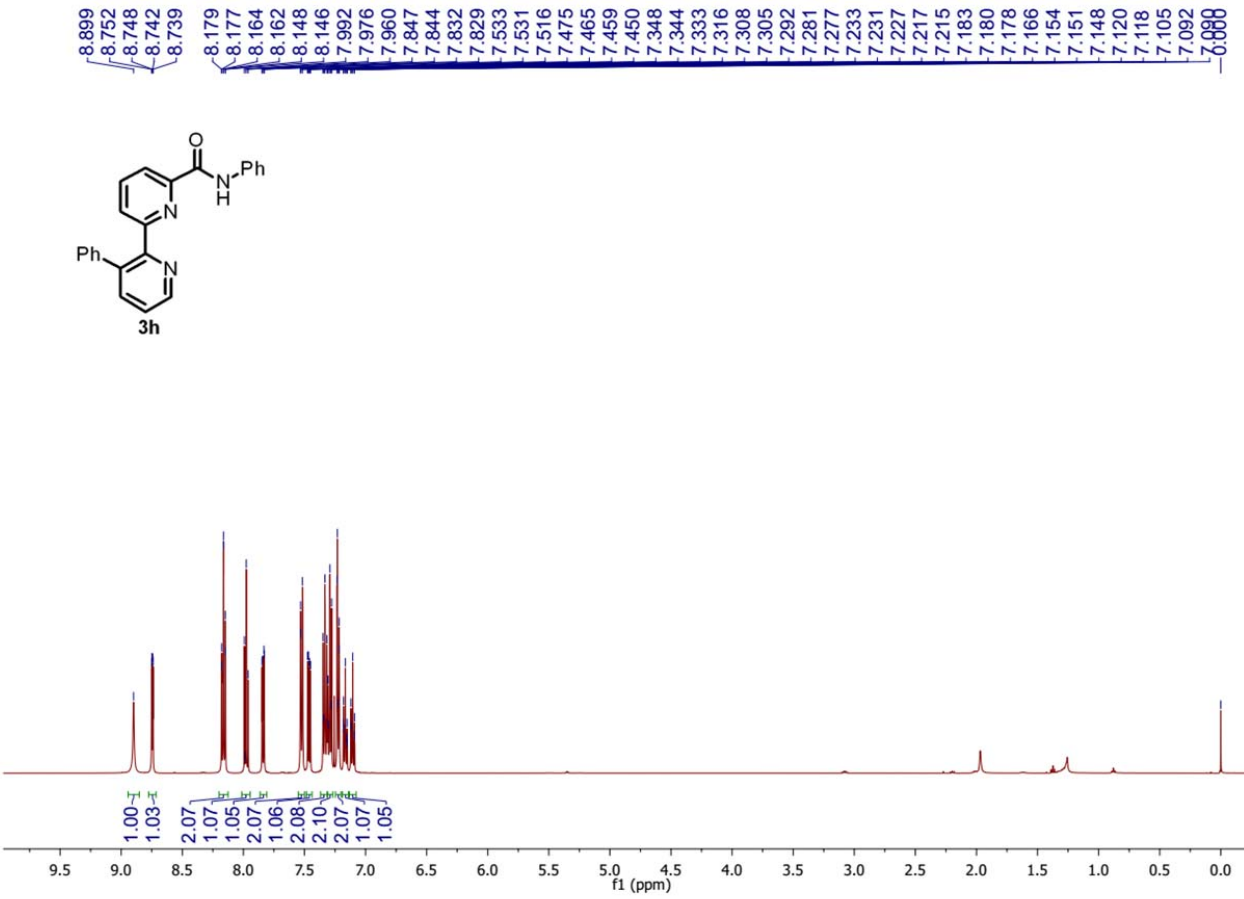

163.106
156.201
154.234
148.526
148.137
139.224
137.939
128.771
128.428
127.185
126.512
123.376
121.086
77.254
77.000
76.746
41.032
22.459
Ph
N
N
O
N
H
iPr
3e
f1 (ppm)

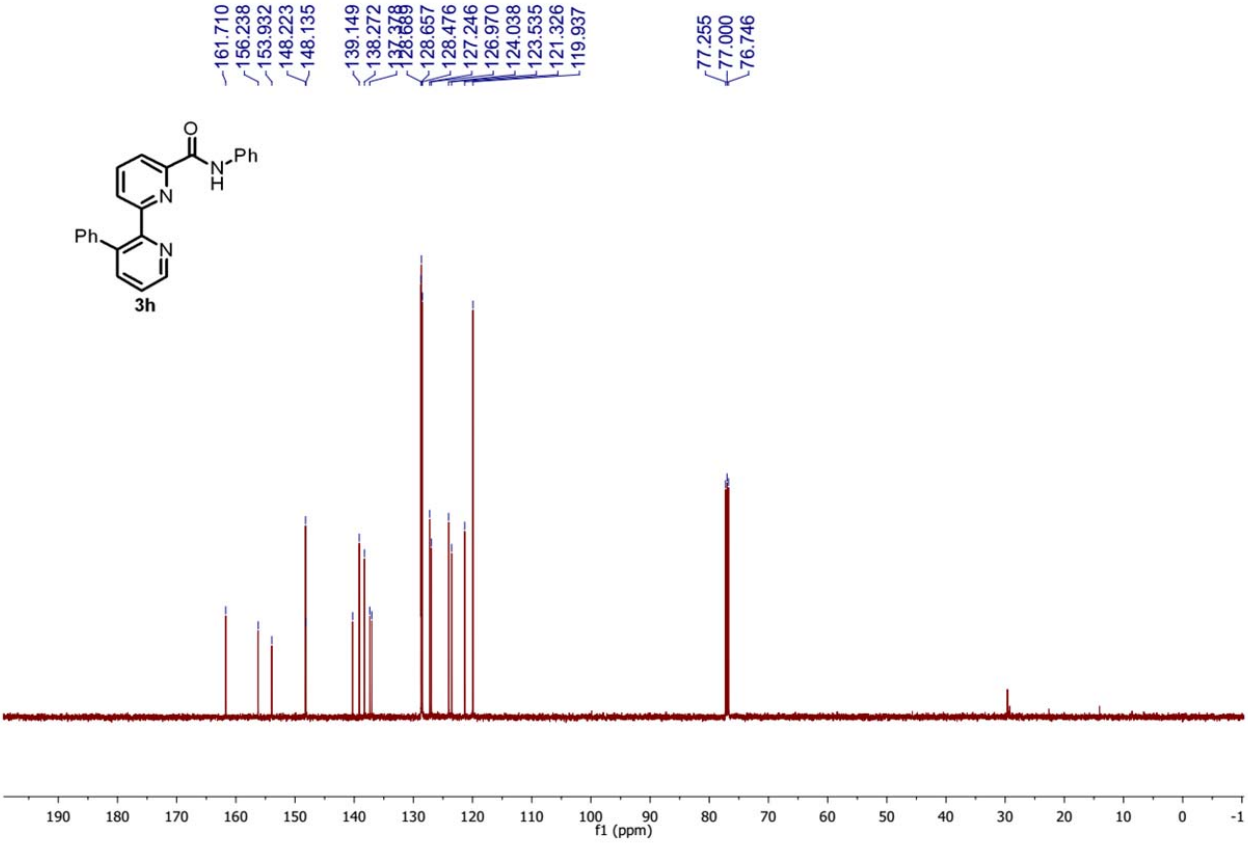

8.727
8.724
8.718
8.714
8.068
8.066
8.052
8.050
8.031
8.028
8.015
8.013
7.929
7.914
7.898
7.823
7.820
7.807
7.804
7.459
7.450
7.444
7.434
7.294
7.291
7.287
7.285
7.283
7.278
7.273
7.263
7.139
7.137
7.134
7.132
7.124
7.120
-0.000
tBu
Ph
3f
1.00
1.02
1.00
1.04
1.02
1.05
3.08
2.98
9.05
f1 (ppm)


163.112
156.151
154.618
149.245
148.129
139.128
138.011
128.511
127.014
126.493
123.445
120.640
77.254
77.000
76.746
50.686
28.529
tBu
Ph
3f
f1 (ppm)

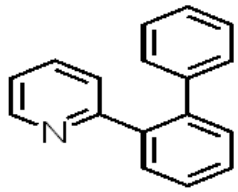

8.716
8.713
8.706
8.703
8.083
8.081
8.075
8.073
8.066
8.059
7.918
7.902
7.887
7.796
7.793
7.781
7.777
7.438
7.429
7.423
7.413
7.307
7.297
7.294
7.286
7.283
7.278
7.274
7.166
7.161
7.157
7.151
7.147
6.936
6.919
1.799
1.792
1.784
1.774
1.768
1.722
1.715
1.708
1.695
1.688
1.682
1.353
1.347
1.341
1.327
1.321
1.296
1.180
1.078
1.072
1.055
1.049
O
N
H
N
Ph
N
3g
1.00
0.88
1.06
1.01
0.99
1.00
2.97
1.98
0.93
0.99
2.05
2.02
1.09
2.20
1.18
2.07
f1 (ppm)


162.970
156.177
154.239
148.547
148.024
140.344
139.114
128.690
128.350
127.130
126.470
123.305
121.047
77.255
77.000
76.746
48.018
32.631
25.538
24.844
O
N
H
N
Ph
N
3g
f1 (ppm)

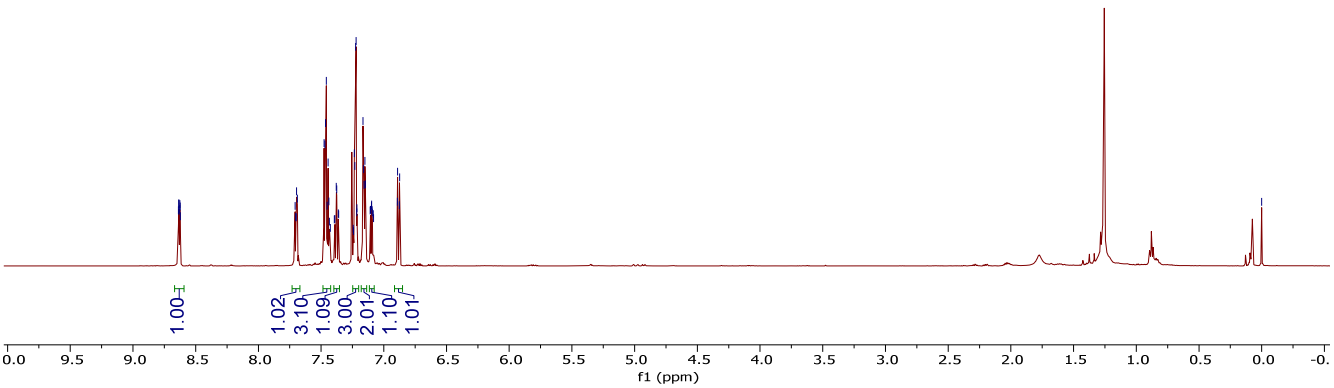

8.899
8.752
8.748
8.742
8.739
8.179
8.177
8.164
8.162
8.148
8.146
7.992
7.976
7.960
7.847
7.844
7.832
7.829
7.533
7.531
7.516
7.475
7.465
7.459
7.450
7.348
7.344
7.333
7.316
7.308
7.305
7.292
7.281
7.277
7.233
7.231
7.227
7.217
7.215
7.183
7.180
7.178
7.166
7.154
7.151
7.148
7.120
7.118
7.105
7.092
7.090
7.088
O
N
Ph
H
N
Ph
N
3h
1.00
1.03
2.07
1.07
1.05
2.07
1.06
2.08
2.10
2.07
1.07
1.05
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
f1 (ppm)


161.710
156.238
153.932
148.223
148.135
139.149
138.272
128.657
128.476
127.246
126.970
124.038
123.535
121.326
119.937
77.255
77.000
76.746
O
N
Ph
H
N
Ph
N
3h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

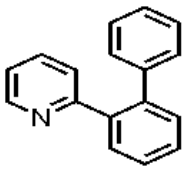

8.637
8.635
8.634
8.632
8.628
8.626
8.624
8.622
7.707
7.702
7.699
7.696
7.689
7.476
7.469
7.465
7.458
7.452
7.444
7.438
7.434
7.426
7.394
7.390
7.378
7.375
7.363
7.359
7.244
7.241
7.235
7.230
7.224
7.220
7.216
7.215
7.166
7.160
7.157
7.151
7.147
7.109
7.107
7.099
7.097
7.094
7.092
7.084
7.082
6.892
6.890
6.876
6.874
0.000



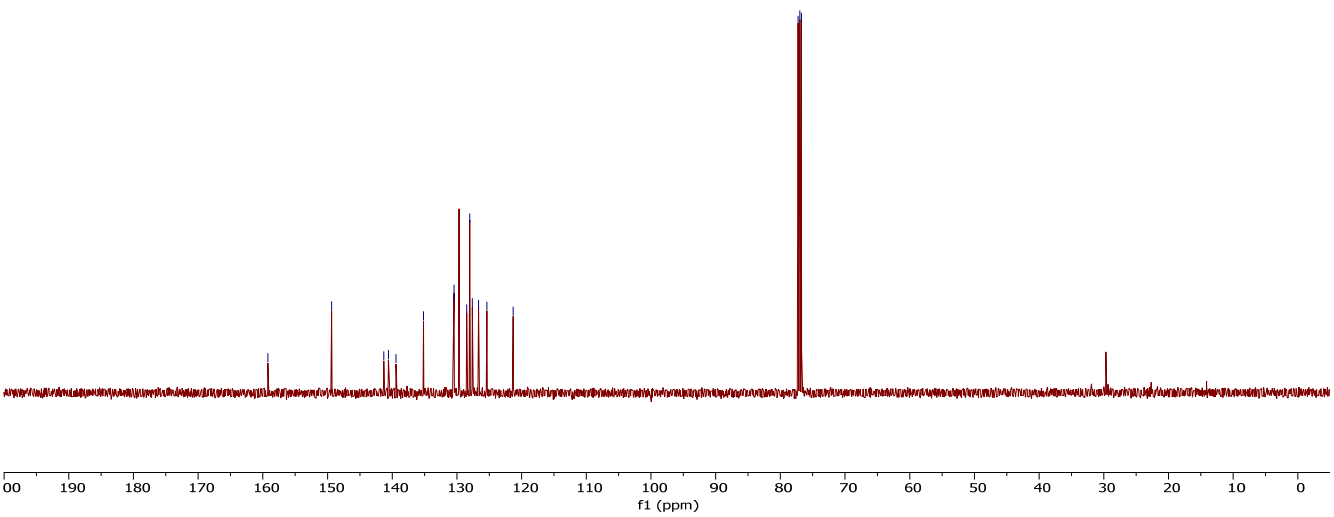
3m

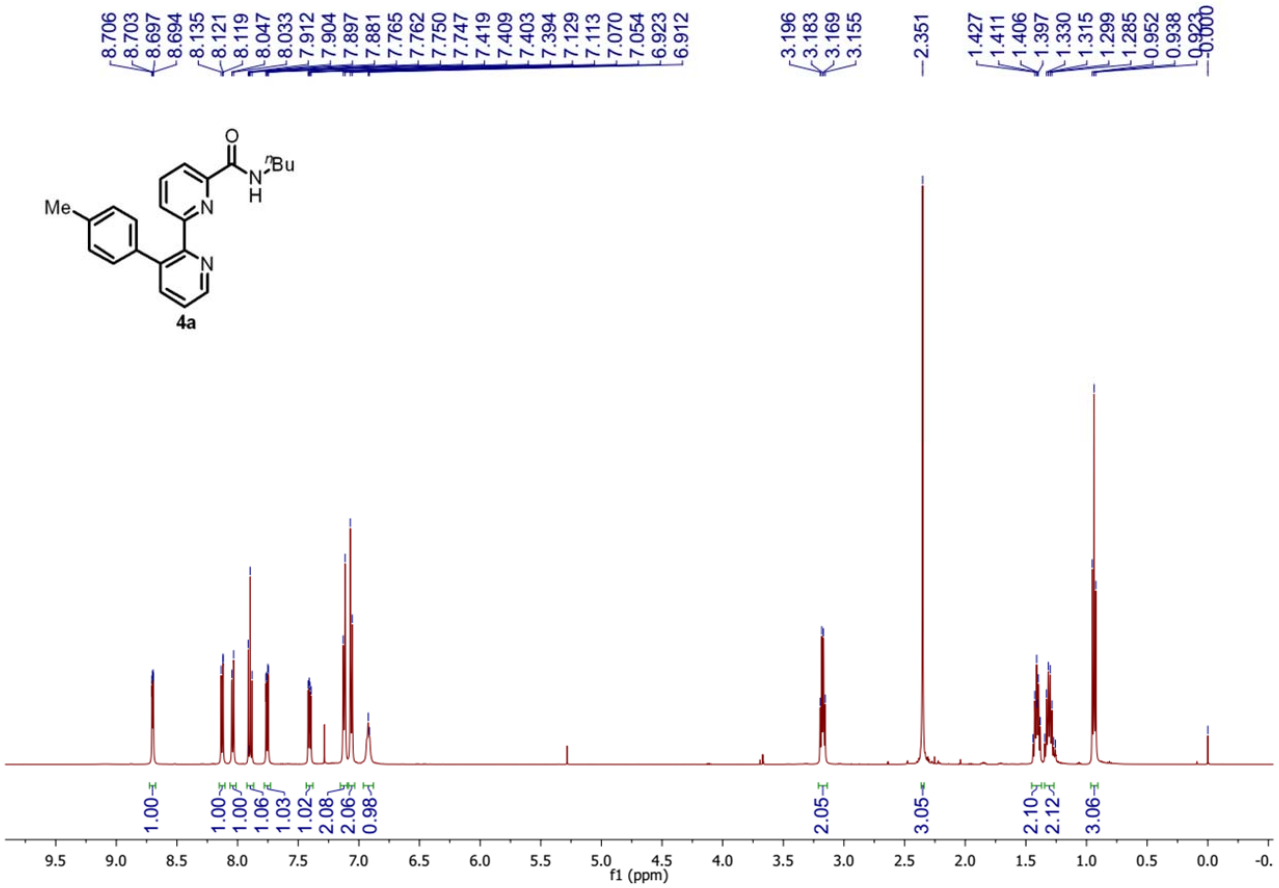

1.00
1.02
3.10
1.09
3.00
2.01
1.10
1.01
f1 (ppm)

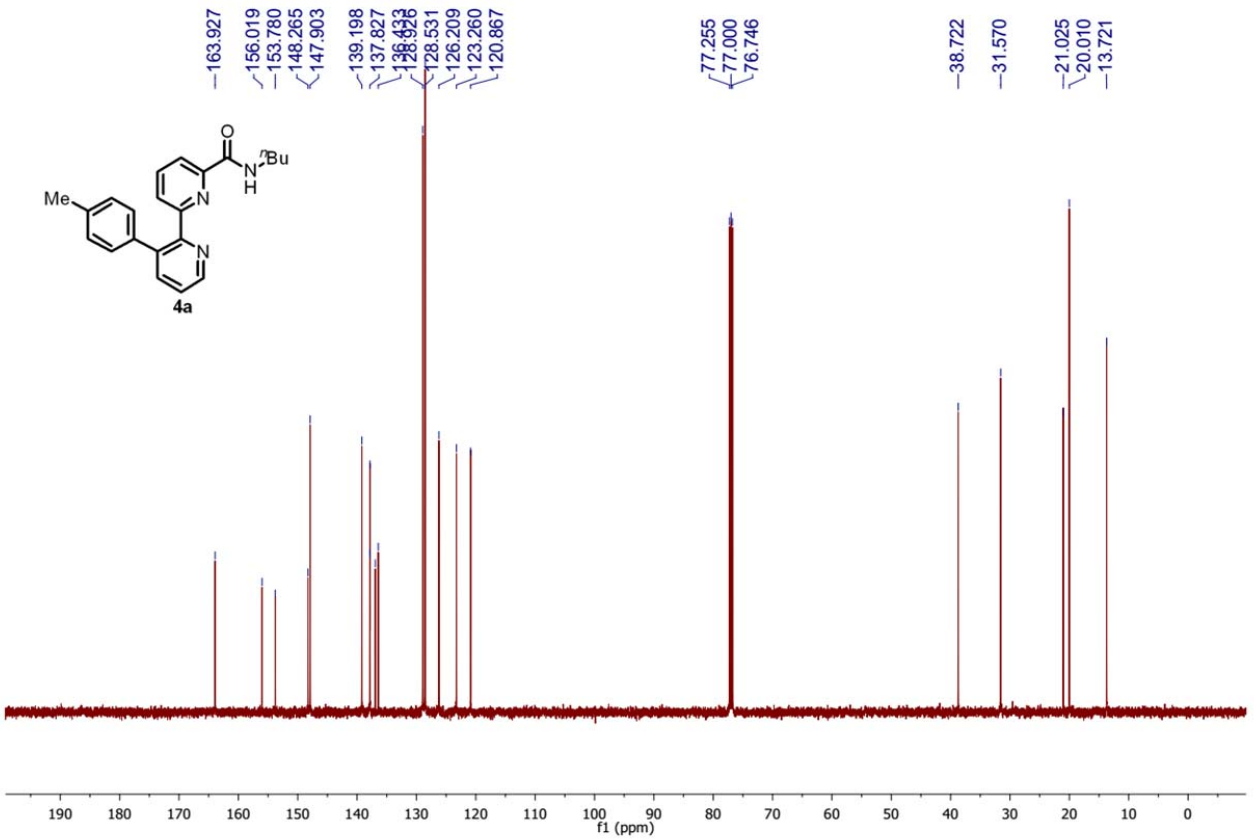

159.213
149.364
141.311
140.586
139.420
135.169
130.457
130.443
128.491
128.018
127.607
126.660
125.377
121.308
77.254
77.000
76.746

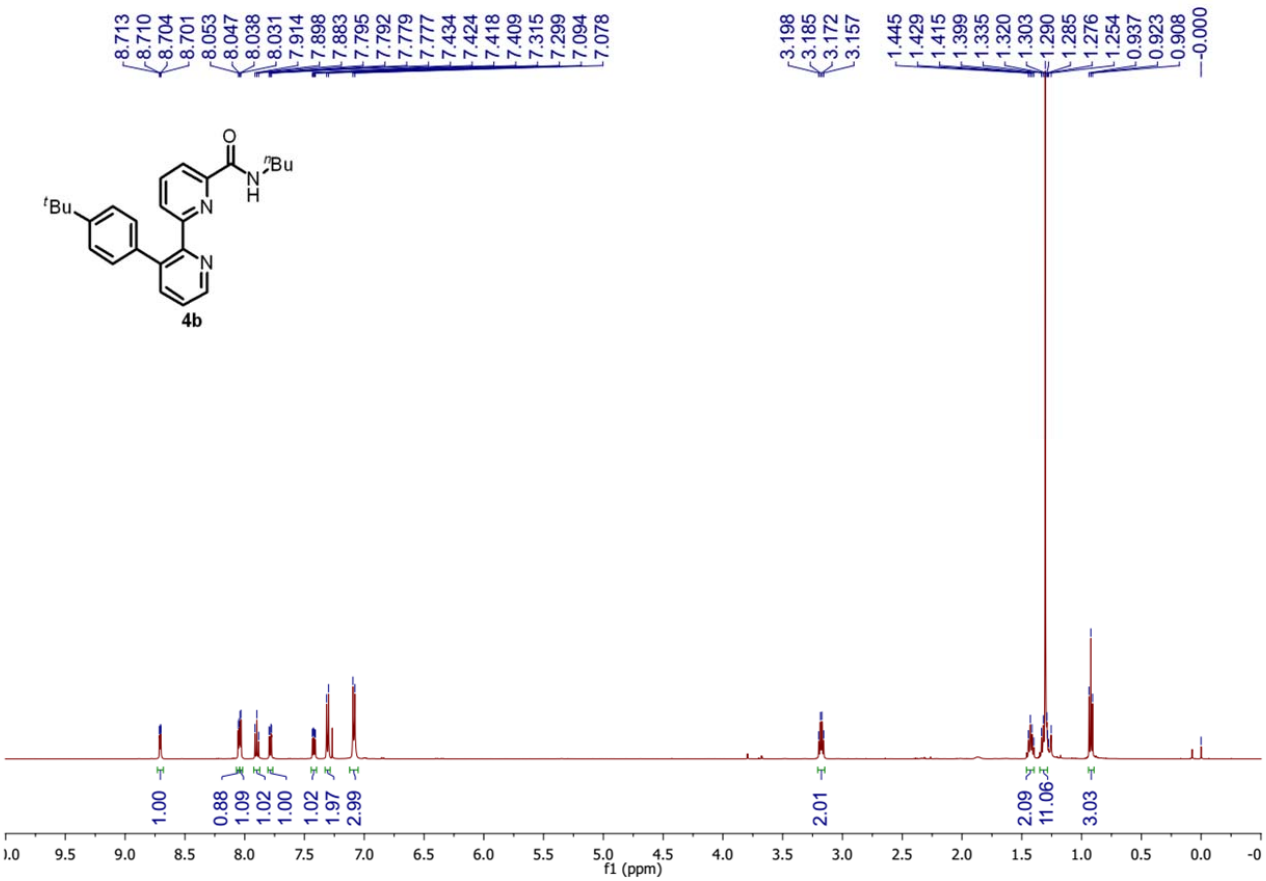


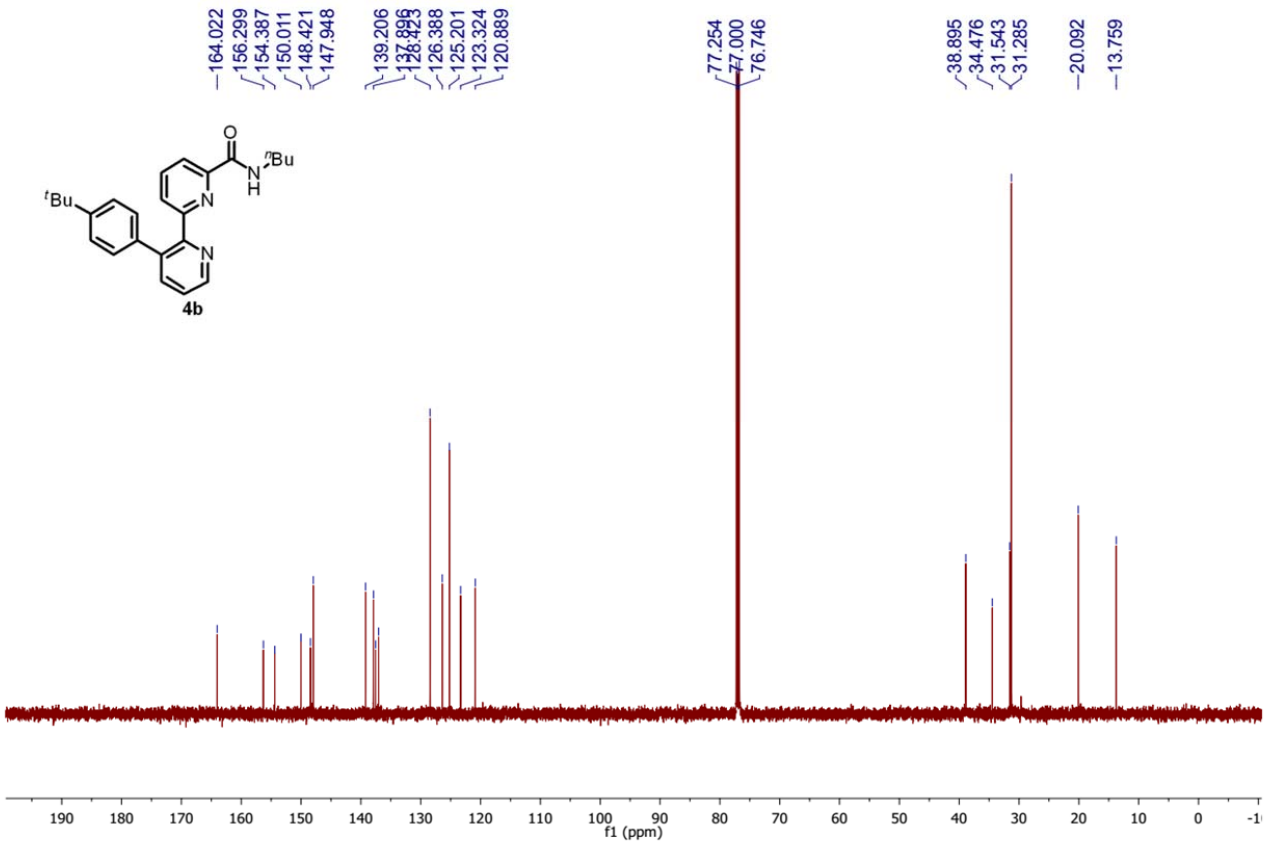
3m

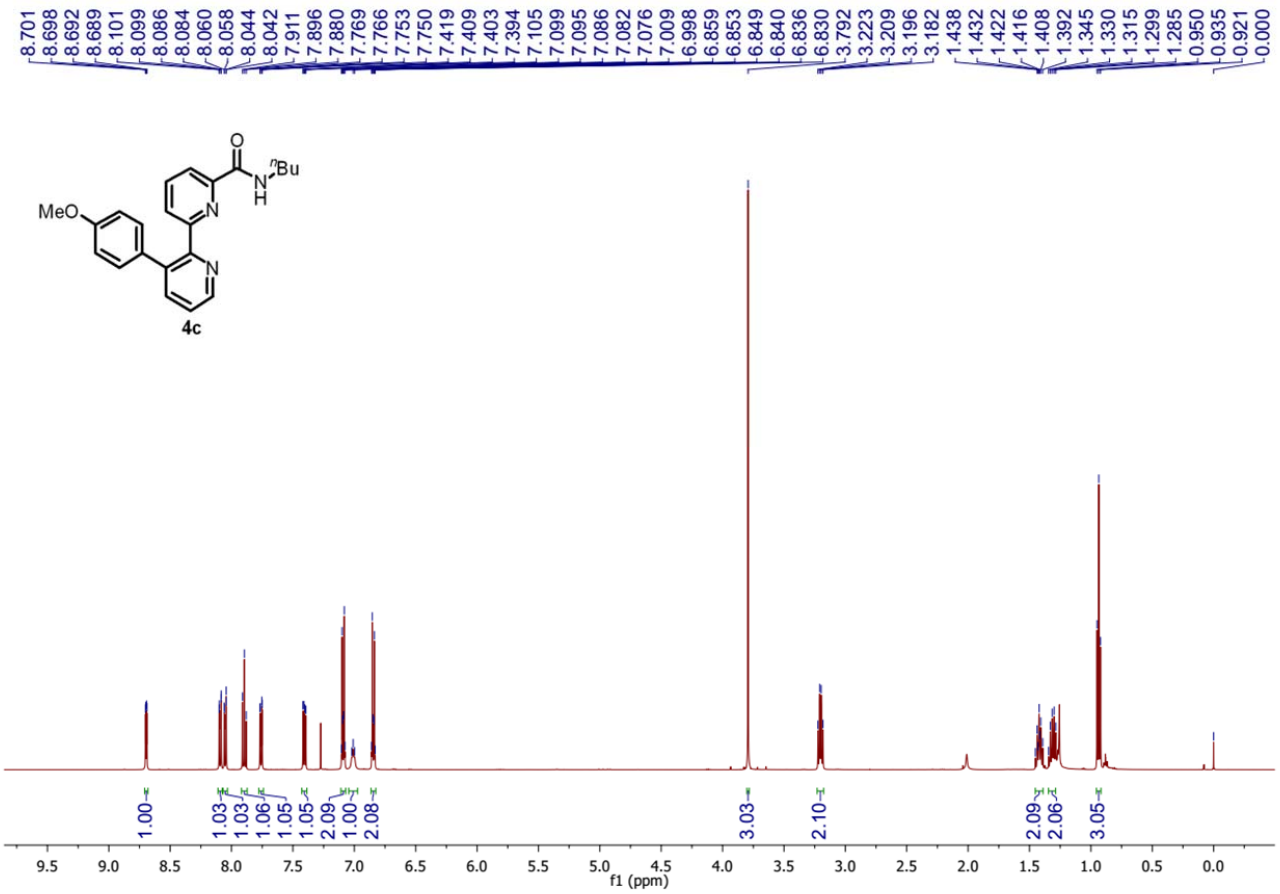

f1 (ppm)

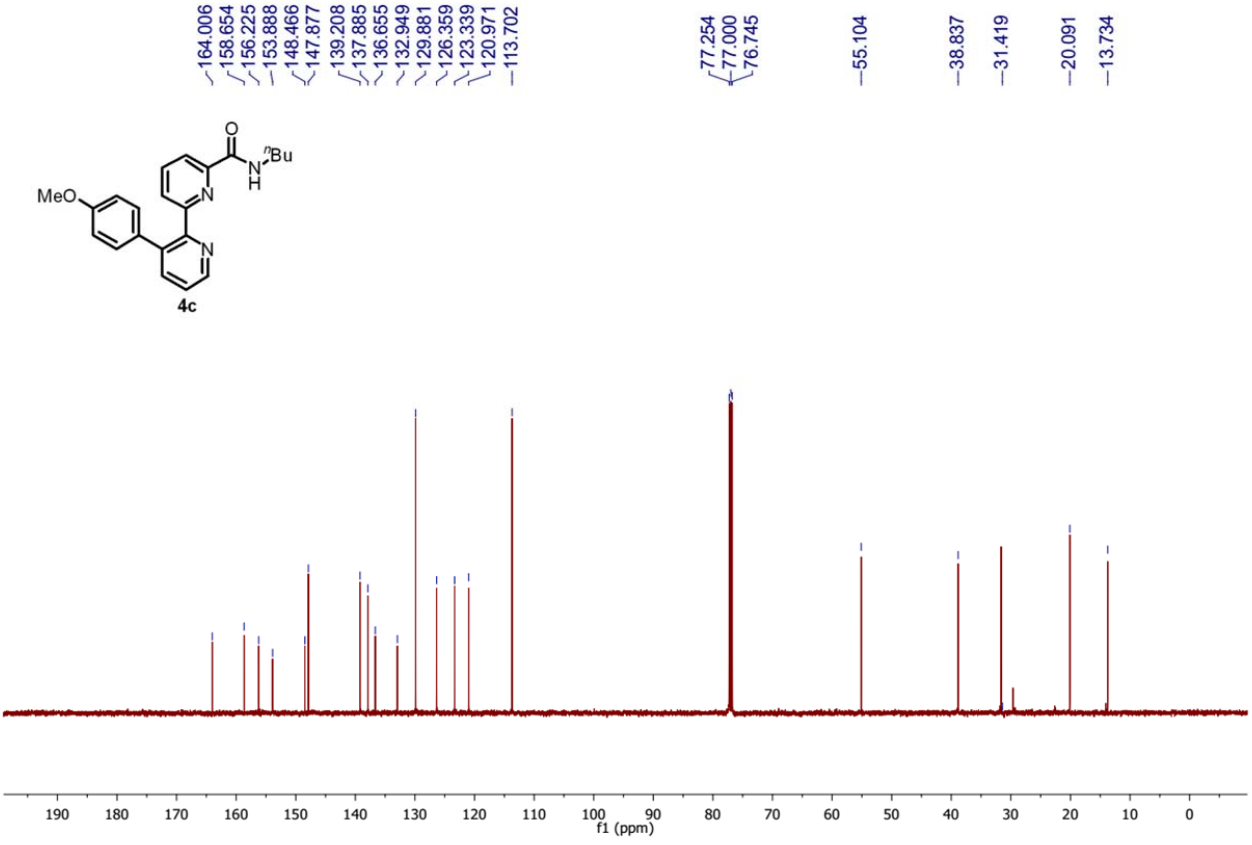

8.706
8.703
8.697
8.694
8.135
8.121
8.119
8.047
8.033
7.912
7.904
7.897
7.881
7.765
7.762
7.750
7.747
7.419
7.409
7.403
7.394
7.129
7.113
7.070
7.054
6.923
6.912
3.196
3.183
3.169
3.155
2.351
1.427
1.411
1.406
1.397
1.330
1.315
1.299
1.285
0.952
0.938
0.923
0.000
Me
O
N
H
nBu
N
N
4a
1.00
1.00
1.00
1.06
1.03
1.02
2.08
2.06
0.98
2.05
3.05
2.10
2.12
3.06
f1 (ppm)

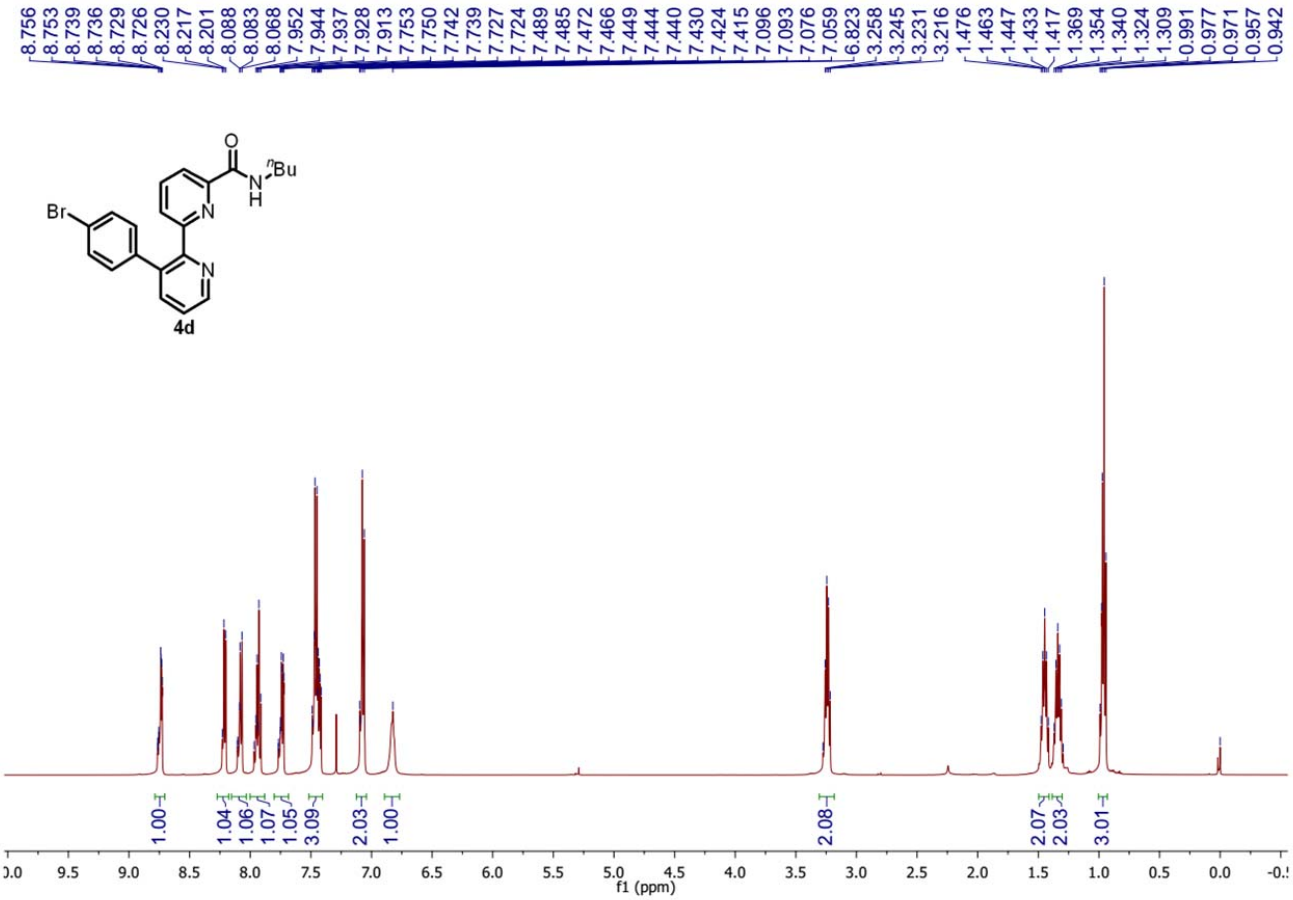

163.927
156.019
153.780
148.265
147.903
139.198
137.827
136.433
128.926
128.531
126.209
123.260
120.867
77.255
77.000
76.746
38.722
31.570
21.025
20.010
13.721
Me
O
N
H
nBu
N
N
4a
f1 (ppm)

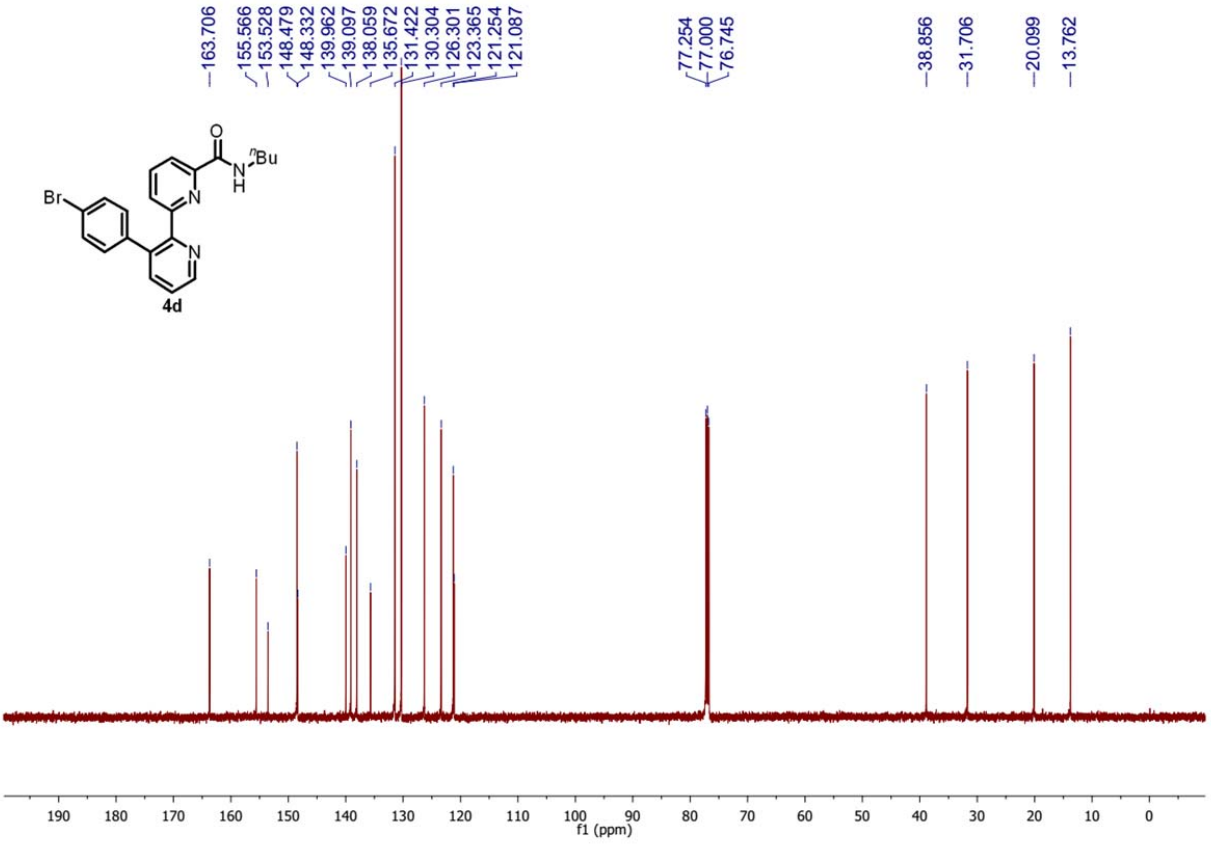

8.713
8.710
8.704
8.701
8.053
8.047
8.038
8.031
7.914
7.898
7.883
7.795
7.792
7.779
7.777
7.434
7.424
7.418
7.409
7.315
7.299
7.094
7.078
3.198
3.185
3.172
3.157
1.445
1.429
1.415
1.399
1.335
1.320
1.303
1.290
1.285
1.276
1.254
0.937
0.923
0.908
-0.000
4b
1.00
0.88
1.09
1.02
1.00
1.02
1.97
2.99
2.01
2.09
11.06
3.03
f1 (ppm)

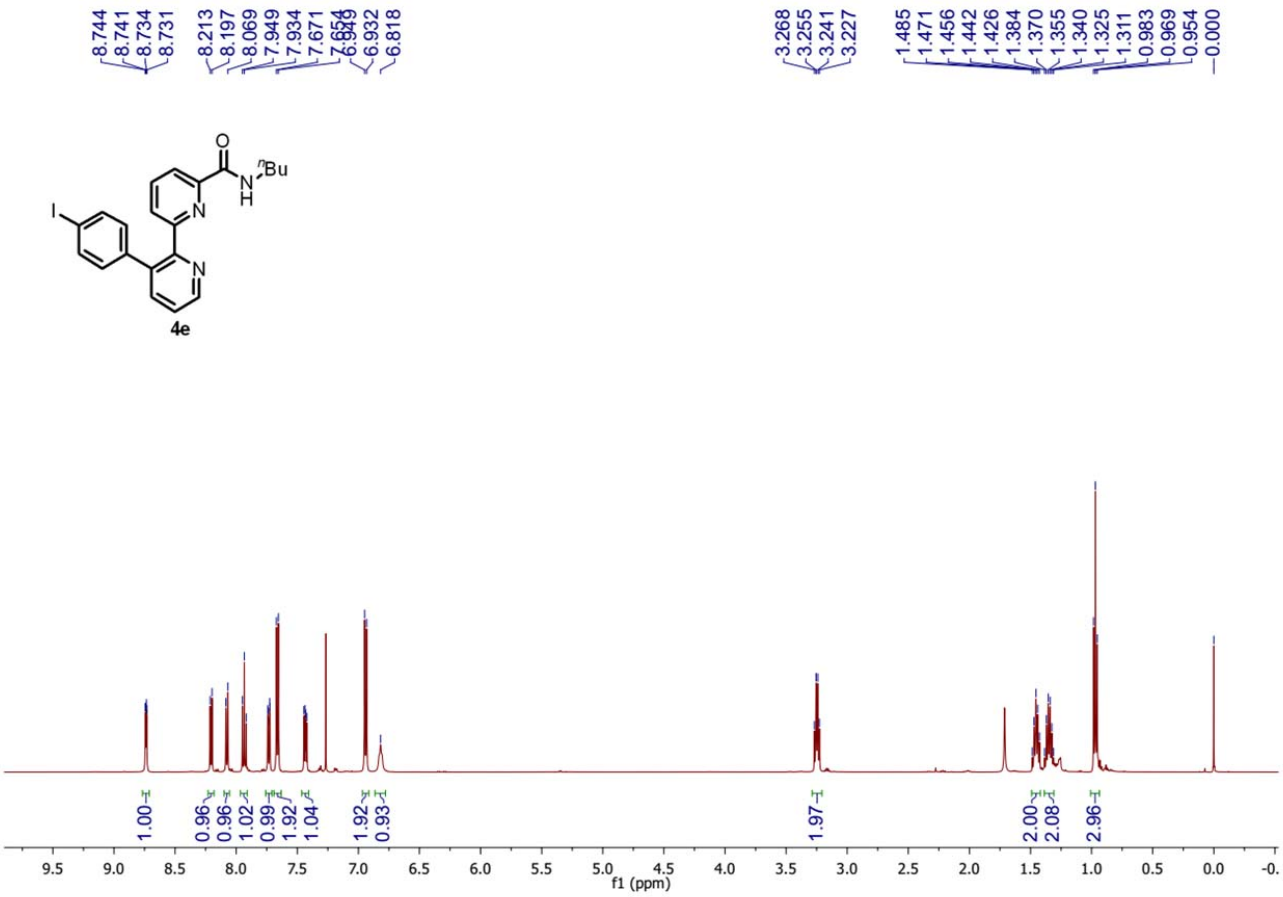

164.022
156.299
154.387
150.011
148.421
147.948
139.206
126.388
125.201
123.324
120.889
77.254
77.000
76.746
38.895
34.476
31.543
31.285
20.092
13.759
4b
f1 (ppm)

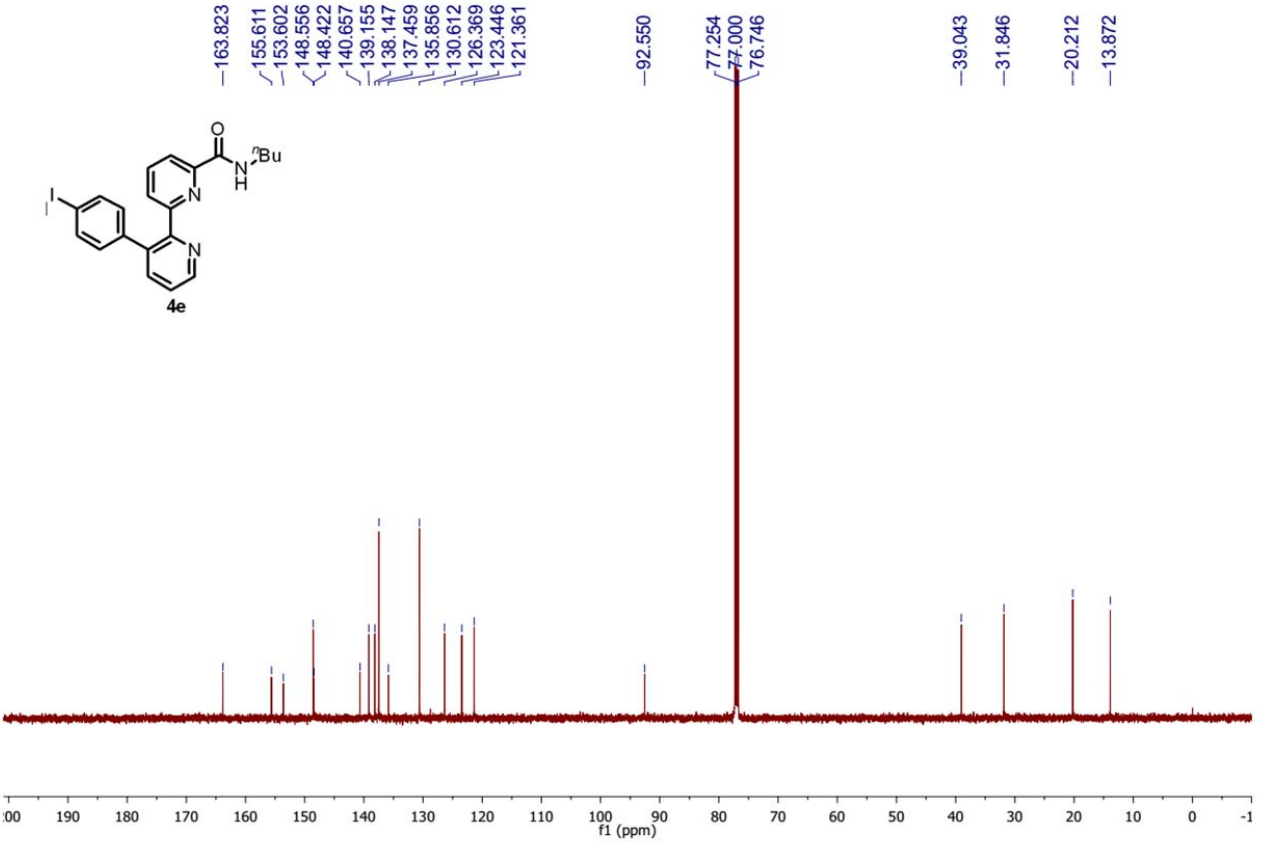

8.701
8.698
8.692
8.689
8.101
8.099
8.086
8.084
8.060
8.058
8.044
8.042
7.911
7.896
7.880
7.769
7.766
7.753
7.750
7.419
7.409
7.403
7.394
7.105
7.099
7.095
7.086
7.082
7.076
7.009
6.998
6.859
6.853
6.849
6.840
6.836
6.830
3.792
3.223
3.209
3.196
3.182
1.438
1.432
1.422
1.416
1.408
1.392
1.345
1.330
1.315
1.299
1.285
0.950
0.935
0.921
0.000
MeO
O
N
H
nBu
4c
1.00
1.03
1.03
1.06
1.05
1.05
2.09
1.00
2.08
3.03
2.10
2.09
2.06
3.05
f1 (ppm)

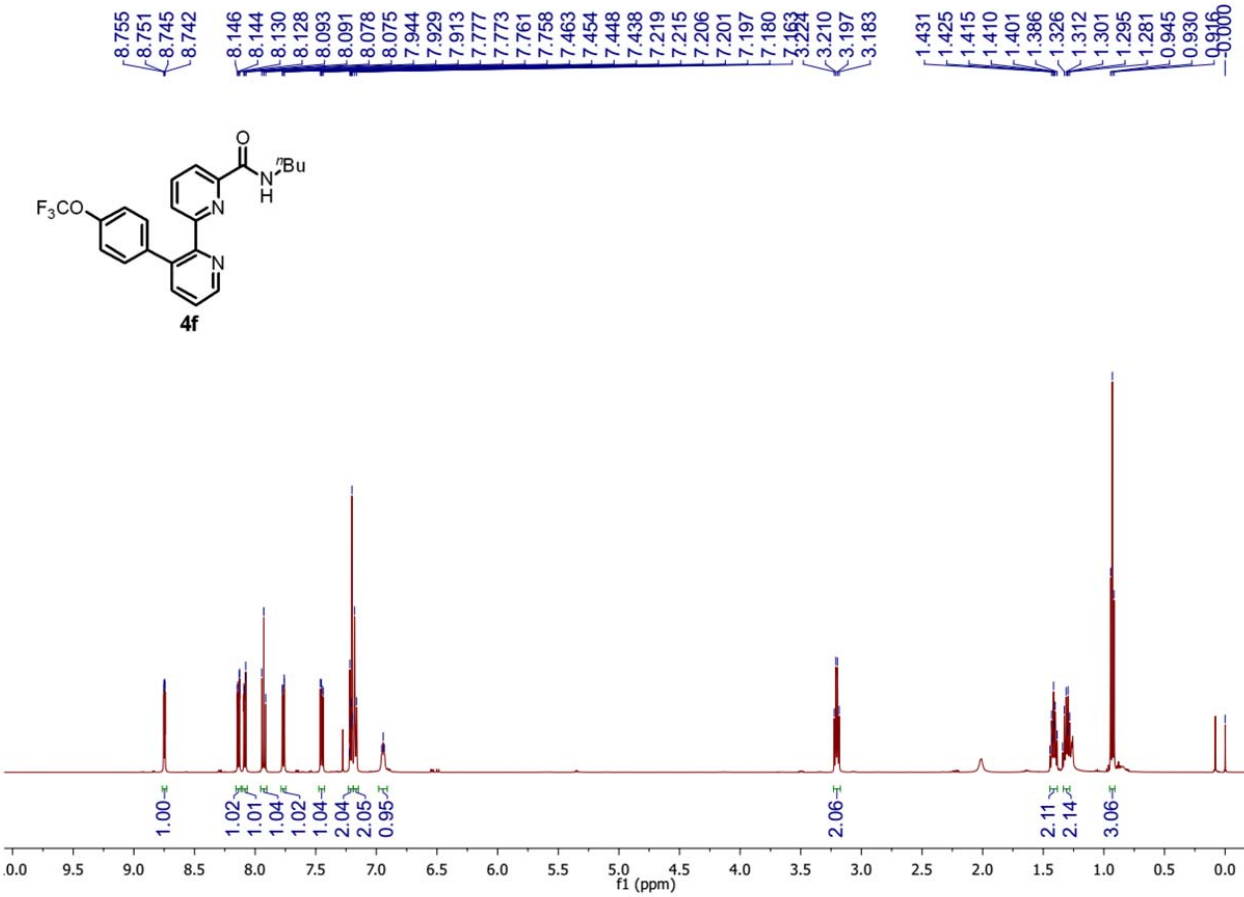

164.006
158.654
156.225
153.888
148.466
147.877
139.208
137.885
136.655
132.949
129.881
126.359
123.339
120.971
113.702
77.254
77.000
76.745
55.104
38.837
31.419
20.091
13.734
MeO
O
N
H
nBu
4c
f1 (ppm)

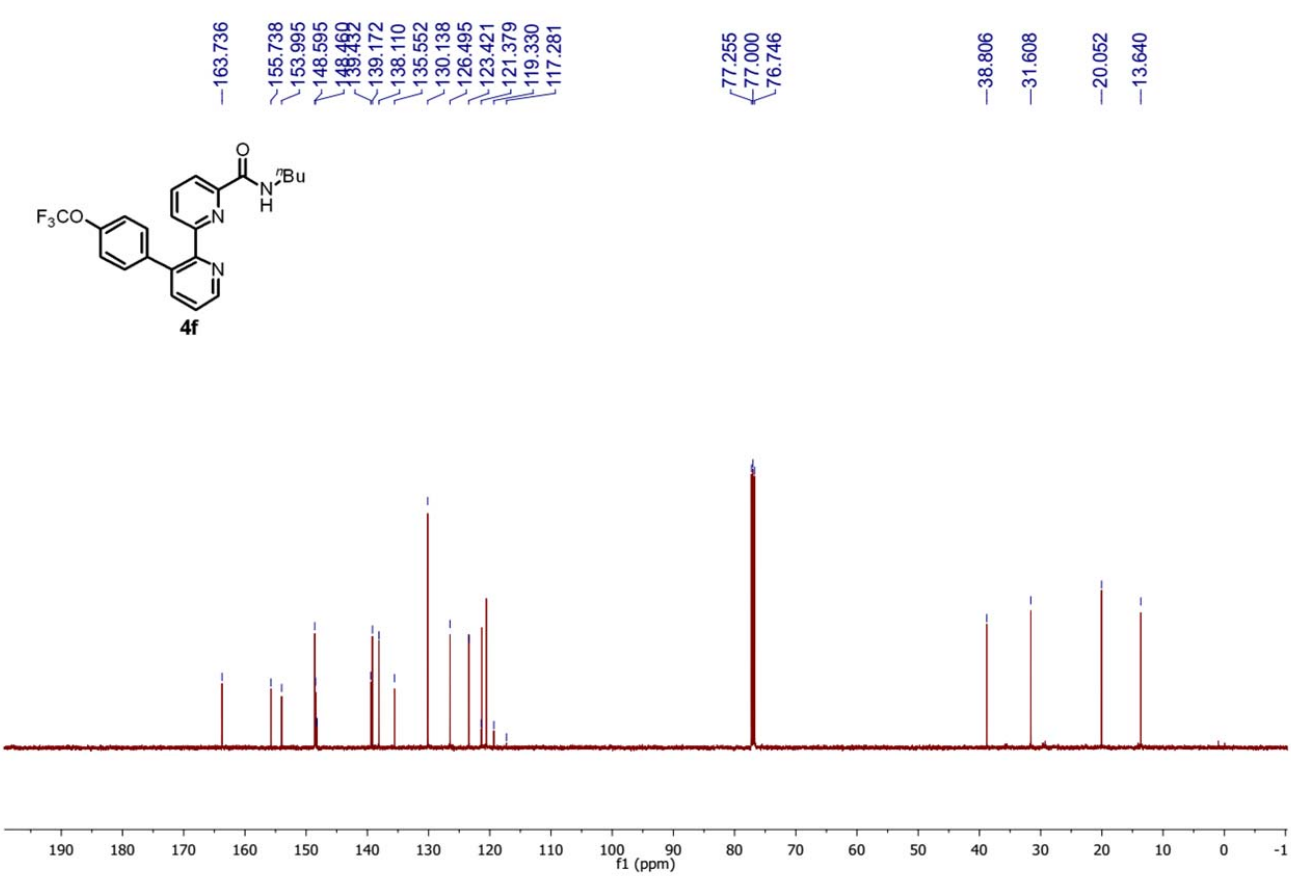

8.756
8.753
8.739
8.736
8.729
8.726
8.230
8.217
8.201
8.088
8.083
8.068
7.952
7.944
7.937
7.928
7.913
7.753
7.750
7.742
7.739
7.727
7.724
7.489
7.485
7.472
7.466
7.449
7.444
7.440
7.430
7.424
7.415
7.096
7.093
7.076
7.059
6.823
3.258
3.245
3.231
3.216
1.476
1.463
1.447
1.433
1.417
1.369
1.354
1.340
1.324
1.309
0.991
0.977
0.971
0.957
0.942
Br
N
H
nBu
O
4d
1.00
1.04
1.06
1.07
1.05
3.09
2.03
1.00
2.08
2.07
2.03
3.01
f1 (ppm)

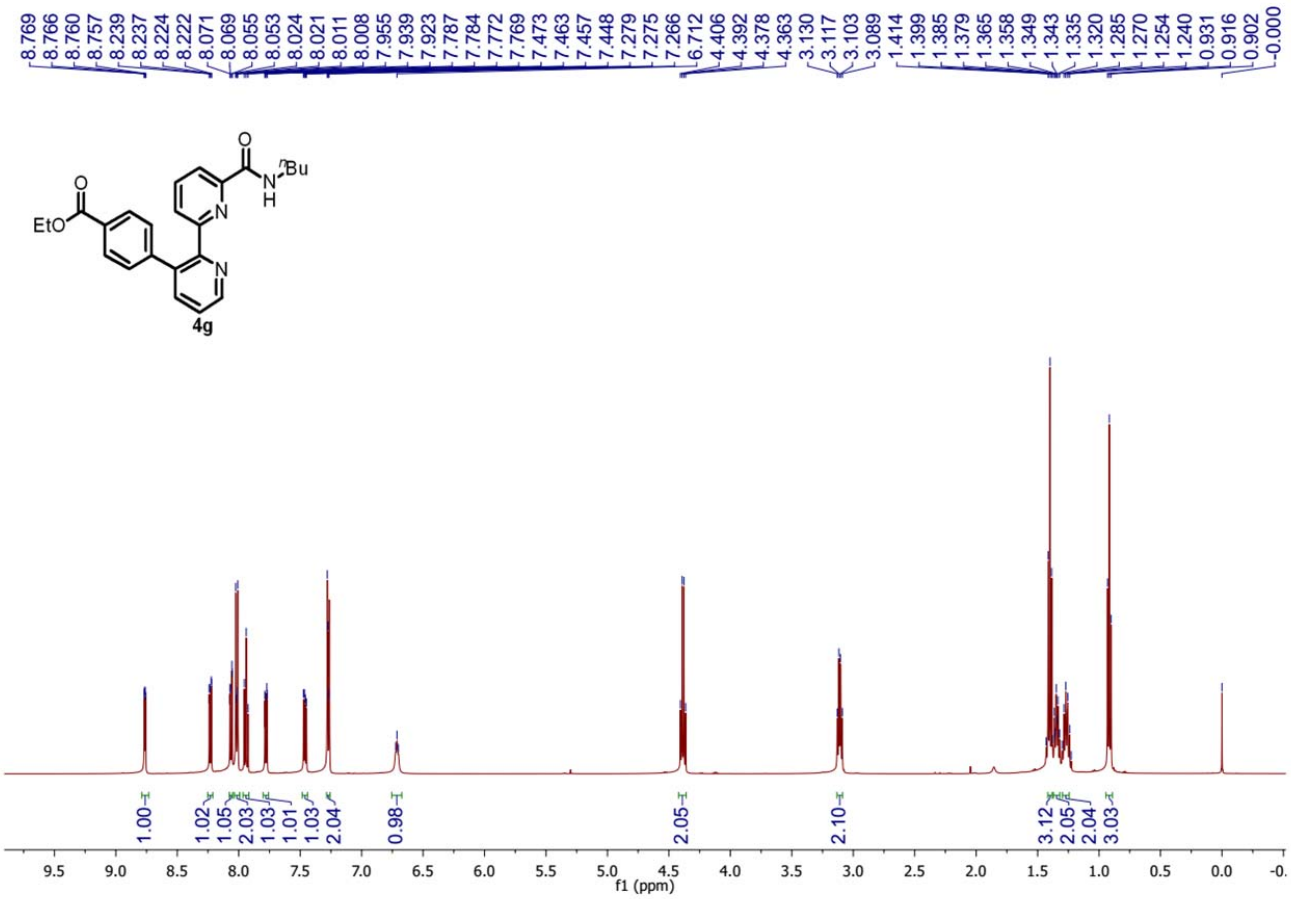

163.706
155.566
153.528
148.479
148.332
139.962
139.097
138.059
135.672
131.422
130.304
126.301
123.365
121.254
121.087
77.254
77.000
76.745
38.856
31.706
20.099
13.762
Br
N
H
nBu
O
4d
f1 (ppm)

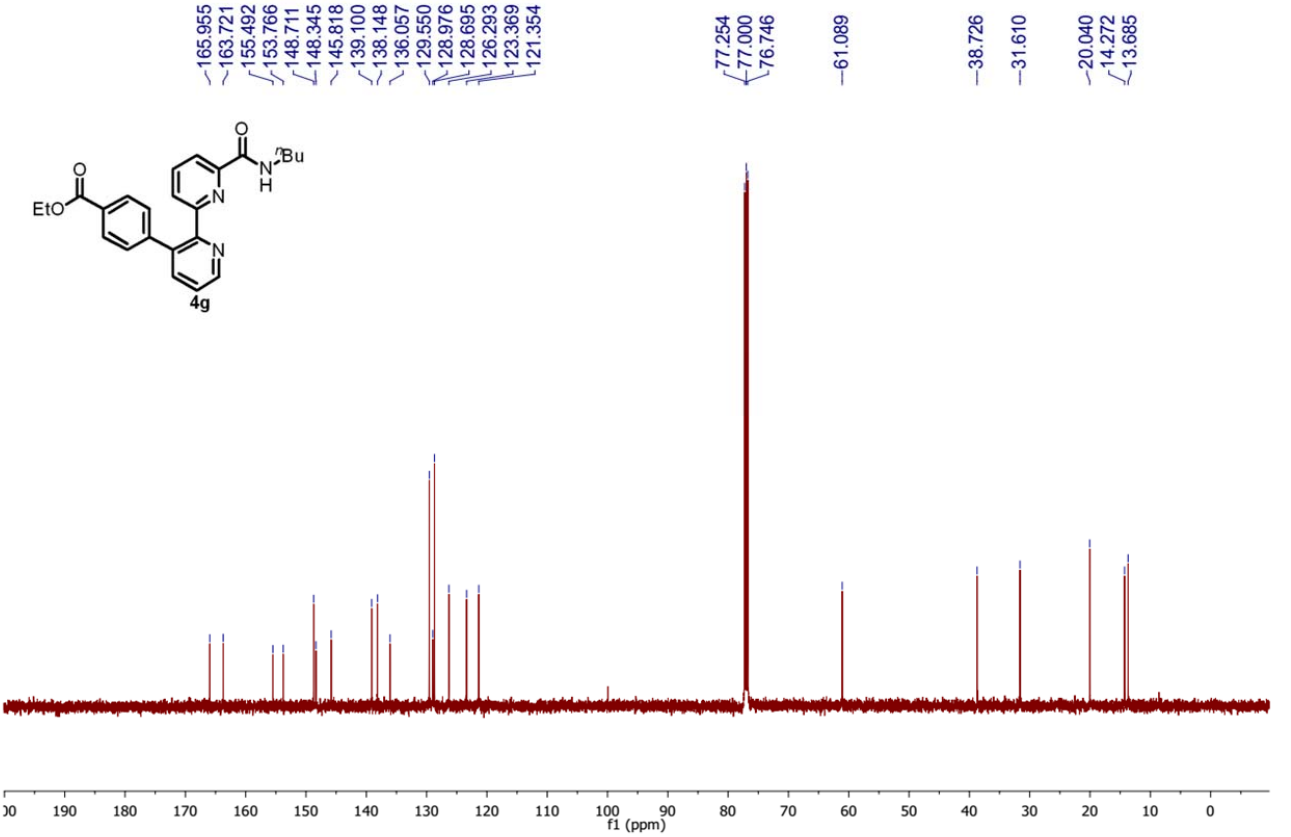

8.744
8.741
8.734
8.731
8.213
8.197
8.069
7.949
7.934
7.671
7.654
6.932
6.818
3.268
3.255
3.241
3.227
1.485
1.471
1.456
1.442
1.426
1.384
1.370
1.355
1.340
1.325
1.311
0.983
0.969
0.954
0.000
4e
1.00
0.96
0.96
1.02
0.99
1.92
1.04
1.92
0.93
1.97
2.00
2.08
2.96
f1 (ppm)

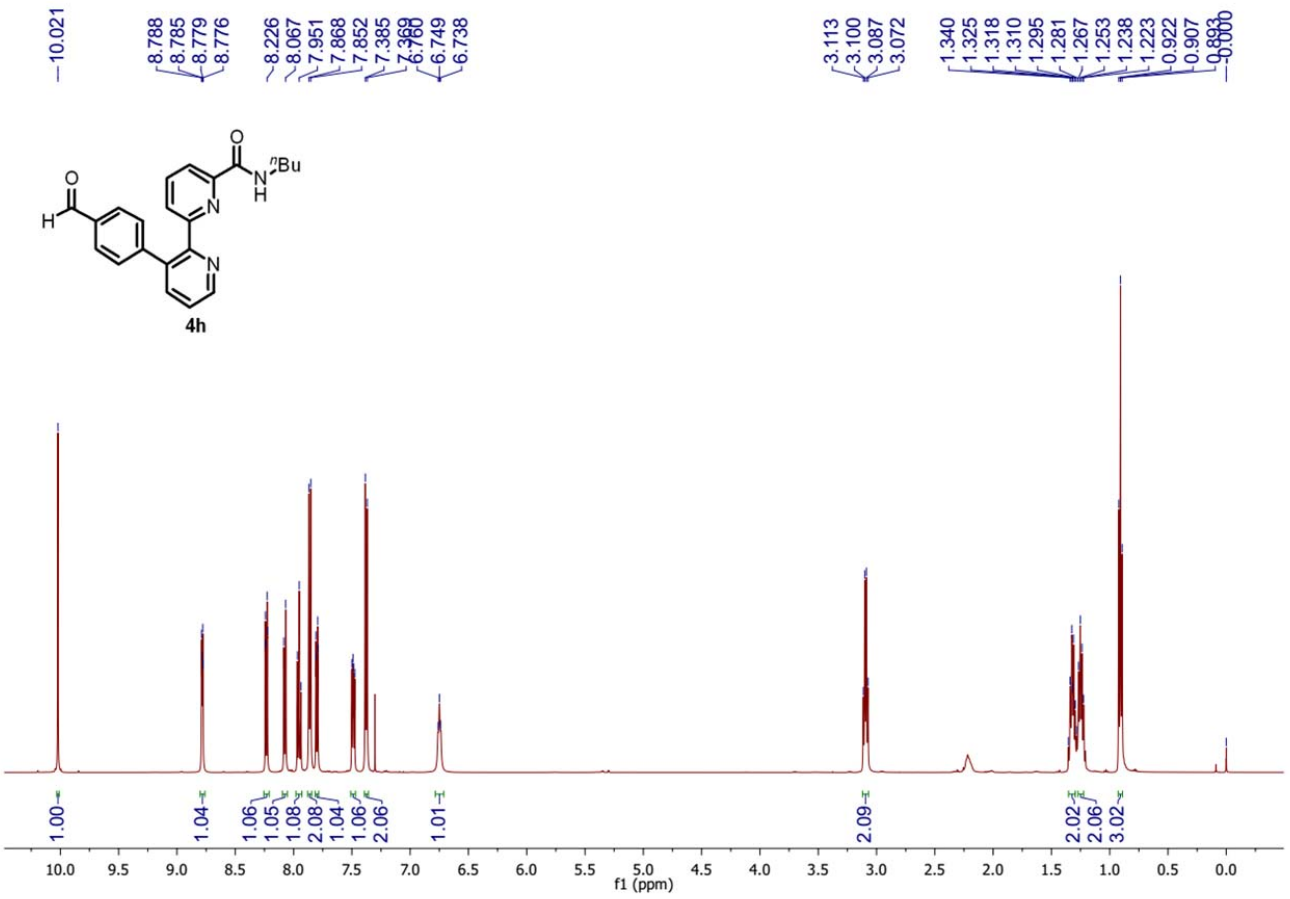

163.823
155.611
153.602
148.556
148.422
140.657
139.155
138.147
137.459
135.856
130.612
126.369
123.446
121.361
92.550
77.254
77.000
76.746
39.043
31.846
20.212
13.872
4e
f1 (ppm)

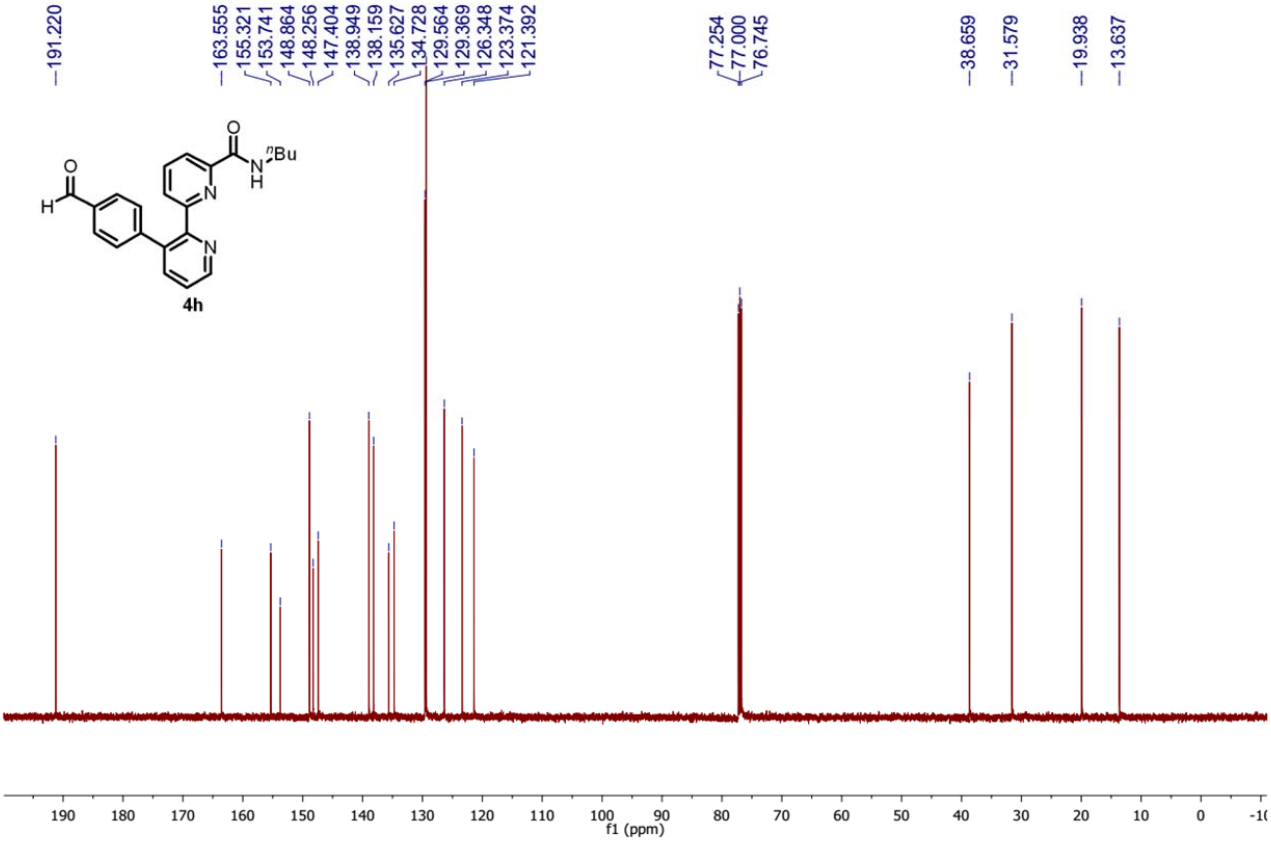

8.755
8.751
8.745
8.742
8.146
8.144
8.130
8.128
8.093
8.091
8.078
8.075
7.944
7.929
7.913
7.777
7.773
7.761
7.758
7.463
7.454
7.448
7.438
7.219
7.215
7.206
7.201
7.197
7.180
3.224
3.210
3.197
3.183
1.431
1.425
1.415
1.410
1.401
1.386
1.326
1.312
1.301
1.295
1.281
0.945
0.930
0.000
O
N
H
nBu
F3CO
N
N
4f
1.00
1.02
1.01
1.04
1.02
1.04
2.04
2.05
0.95
2.06
2.11
2.14
3.06
f1 (ppm)

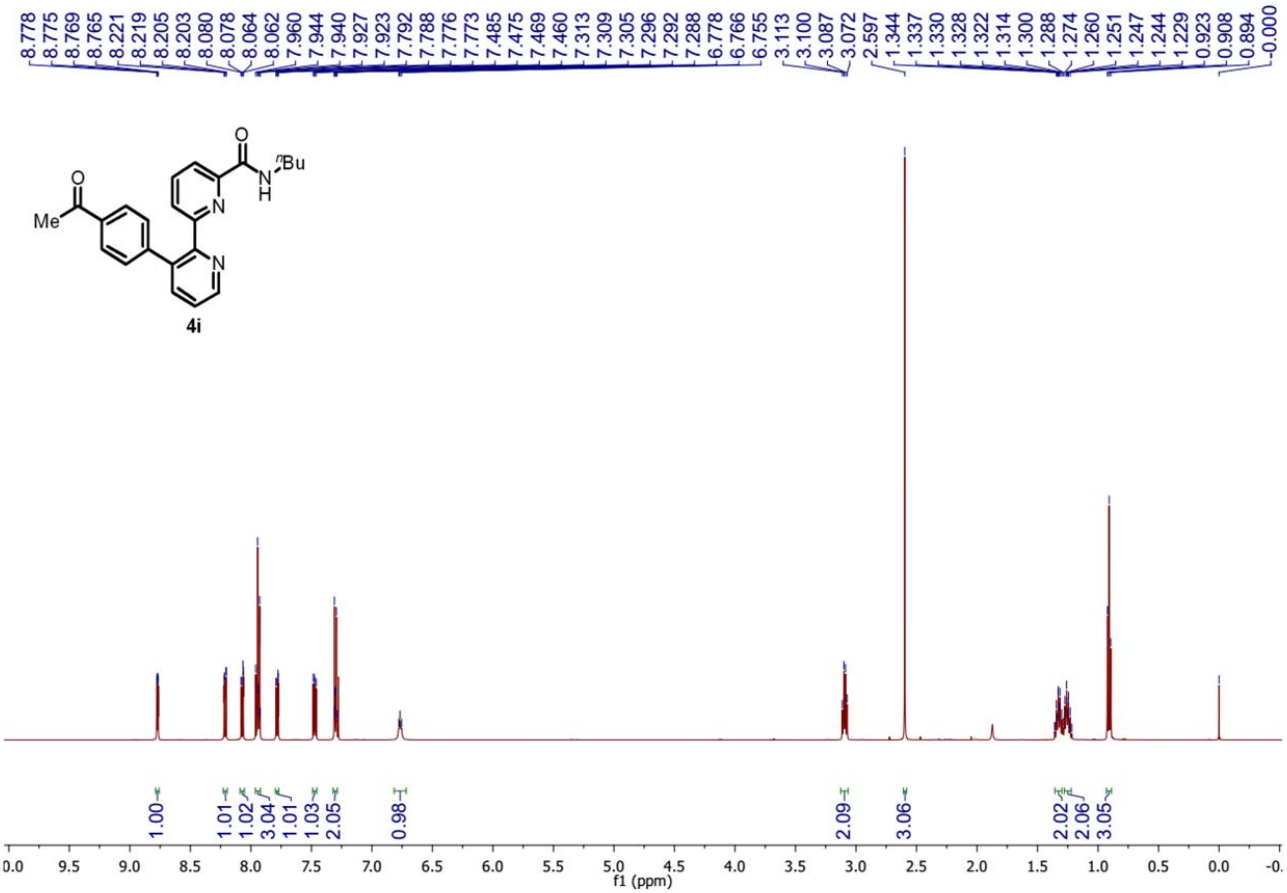

163.736
155.738
153.995
148.595
139.172
138.110
135.552
130.138
126.495
123.421
121.379
119.330
117.281
77.255
77.000
76.746
38.806
31.608
20.052
13.640
O
N
H
nBu
F3CO
N
N
4f
f1 (ppm)

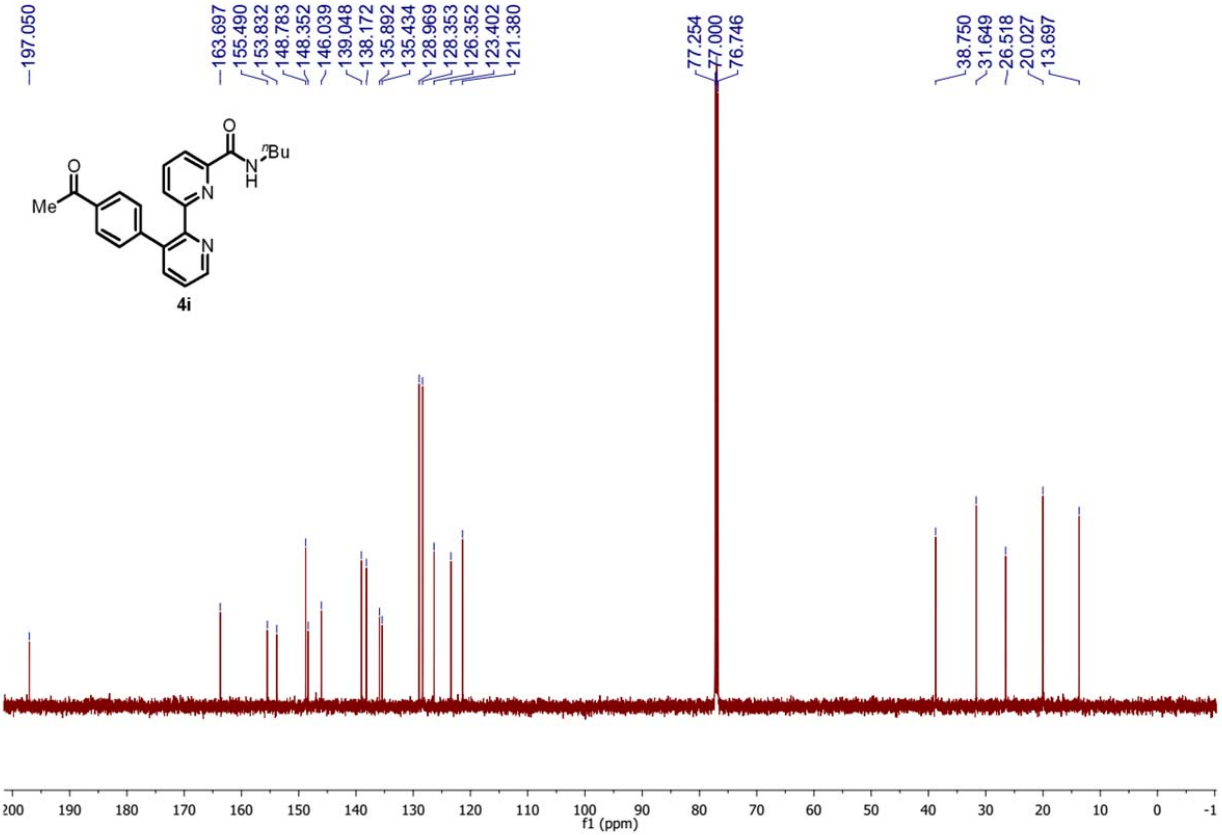

8.769
8.766
8.760
8.757
8.239
8.237
8.224
8.222
8.071
8.069
8.055
8.053
8.024
8.021
8.011
8.008
7.955
7.939
7.923
7.787
7.784
7.772
7.769
7.473
7.463
7.457
7.448
7.279
7.275
7.266
6.712
4.406
4.392
4.378
4.363
3.130
3.117
3.103
3.089
1.414
1.399
1.385
1.379
1.365
1.358
1.349
1.343
1.335
1.320
1.285
1.270
1.254
1.240
0.931
0.916
0.902
-0.000
EtO
O
N
H
nBu
4g
1.00
1.02
1.05
2.03
1.03
1.01
1.03
2.04
0.98
2.05
2.10
3.12
2.05
2.04
3.03
f1 (ppm)

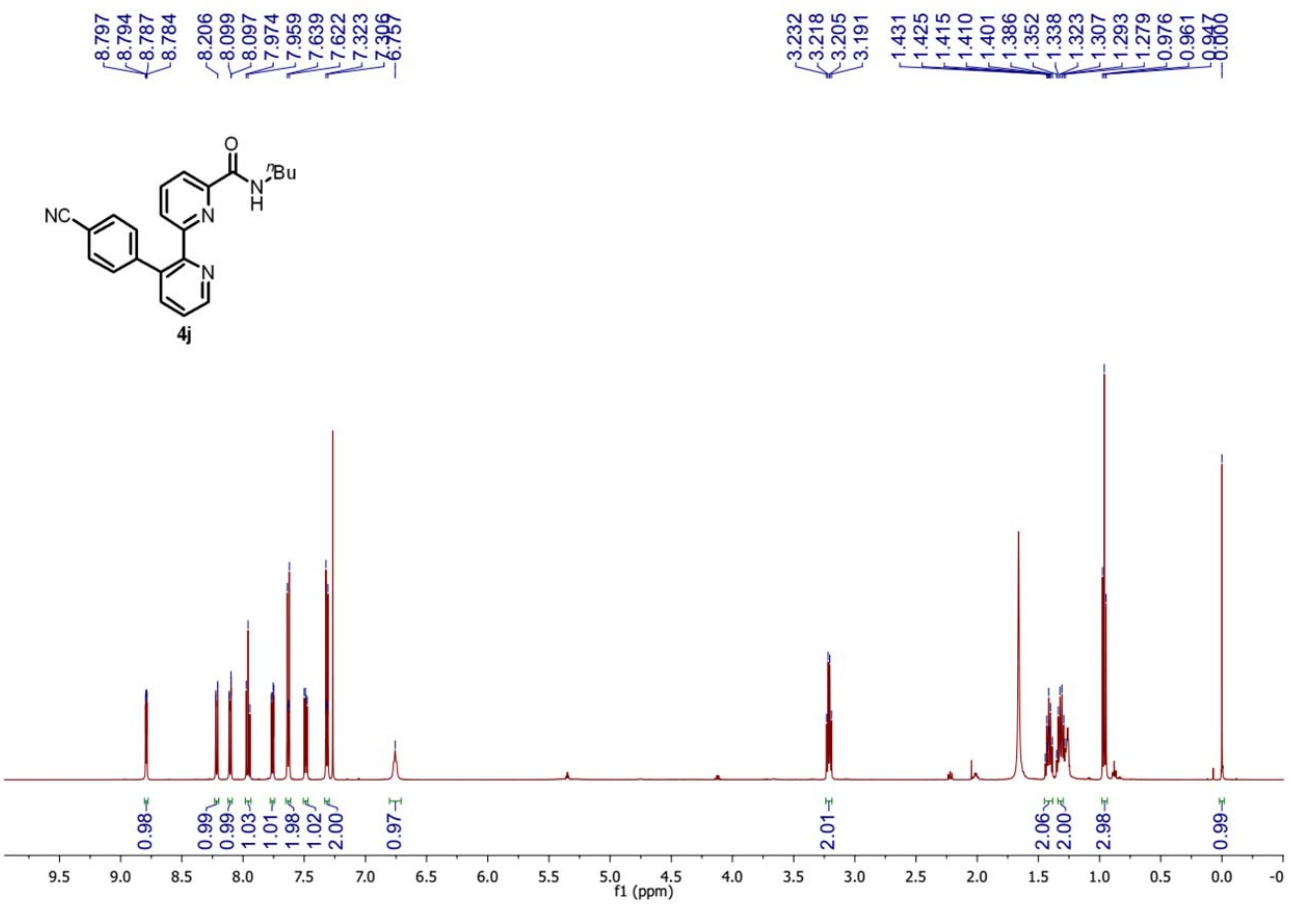

165.955
163.721
155.492
153.766
148.711
148.345
145.818
139.100
138.148
136.057
129.550
128.976
128.695
126.293
123.369
121.354
77.254
77.000
76.746
61.089
38.726
31.610
20.040
14.272
13.685
EtO
O
N
H
nBu
4g
f1 (ppm)

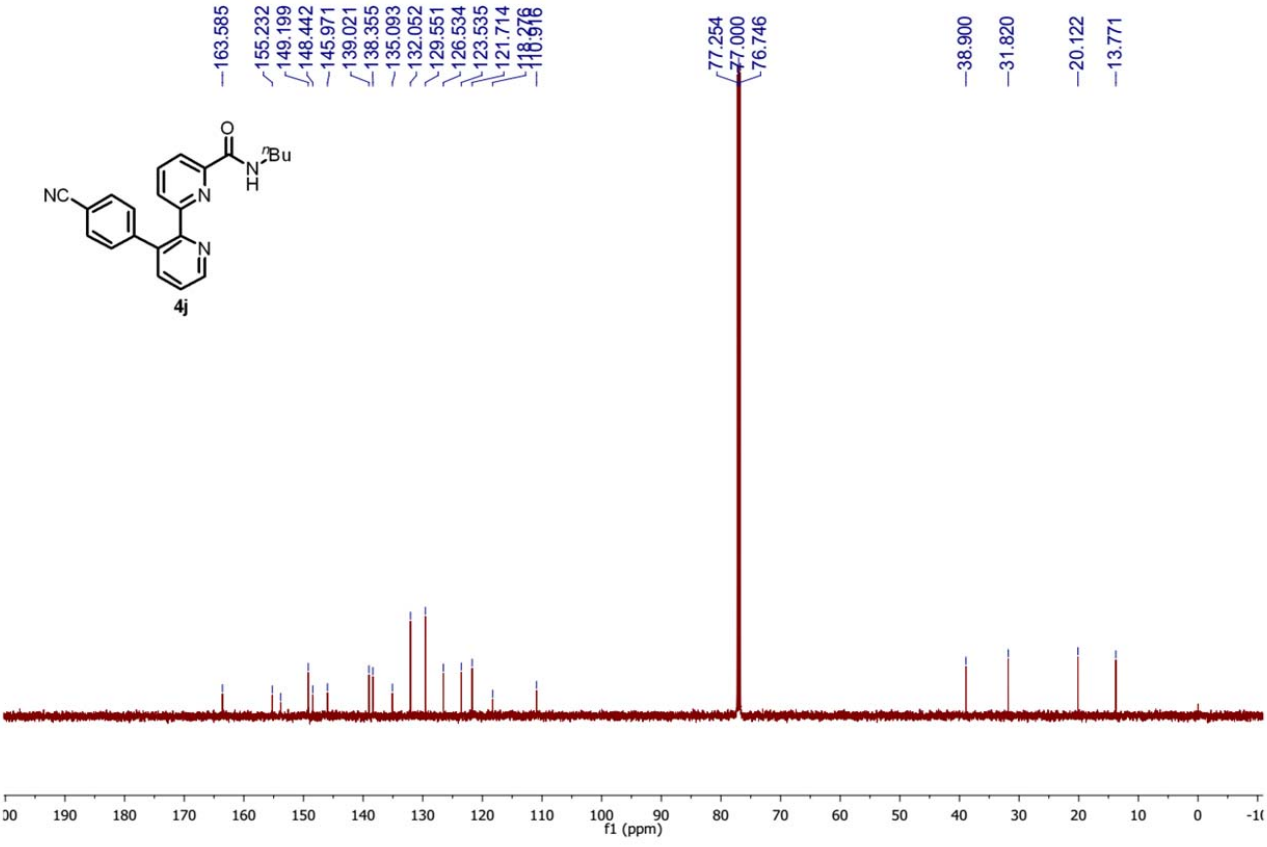

10.021
8.788
8.785
8.779
8.776
8.226
8.067
7.951
7.868
7.852
7.385
7.369
7.360
6.749
6.738
3.113
3.100
3.087
3.072
1.340
1.325
1.318
1.310
1.295
1.281
1.267
1.253
1.238
1.223
0.922
0.907
0.000
nBu
4h
1.00
1.04
1.06
1.05
1.08
2.08
1.04
1.06
2.06
1.01
2.09
2.02
2.06
3.02
f1 (ppm)

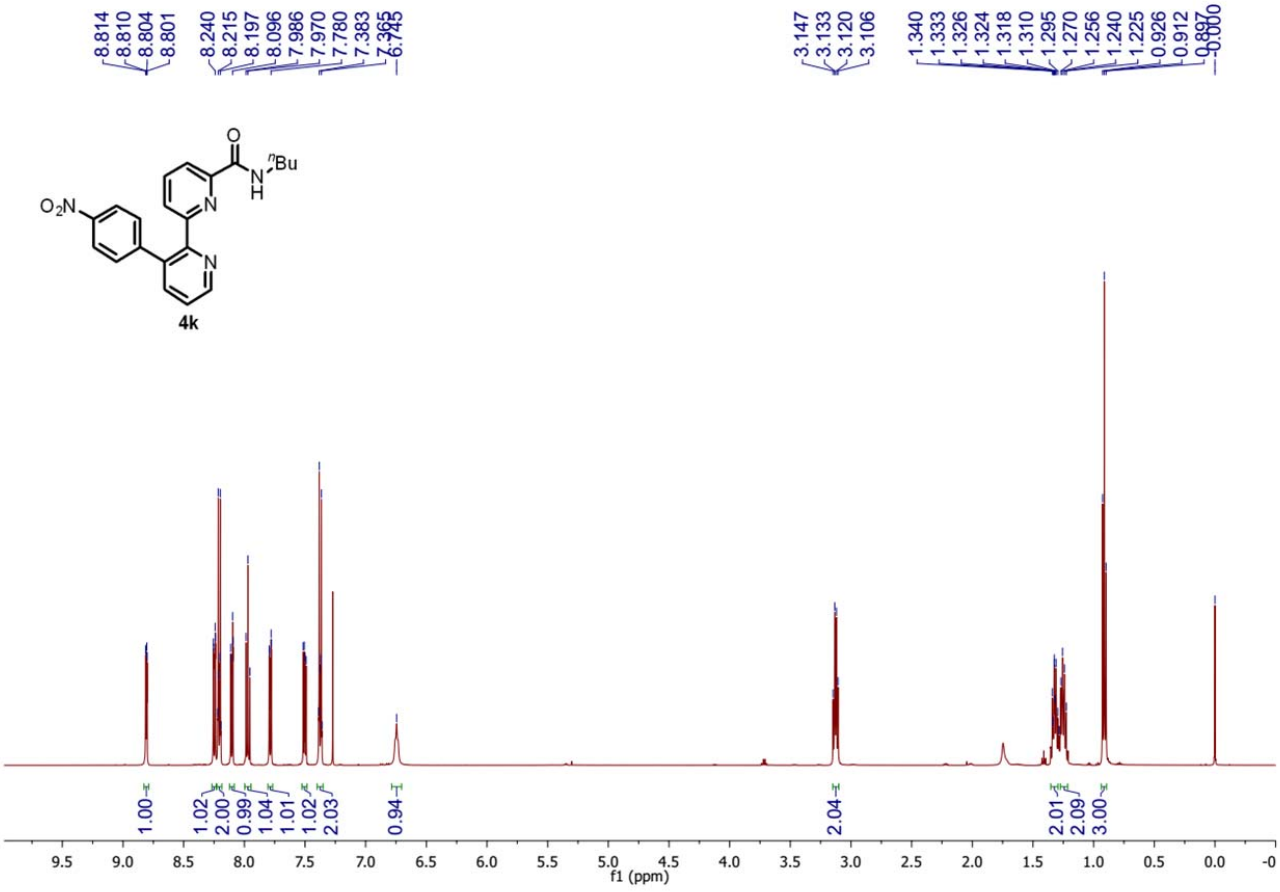

191.220
163.555
155.321
153.741
148.864
148.256
147.404
138.949
138.159
135.627
134.728
129.564
129.369
126.348
123.374
121.392
77.254
77.000
76.745
38.659
31.579
19.938
13.637
nBu
4h
f1 (ppm)

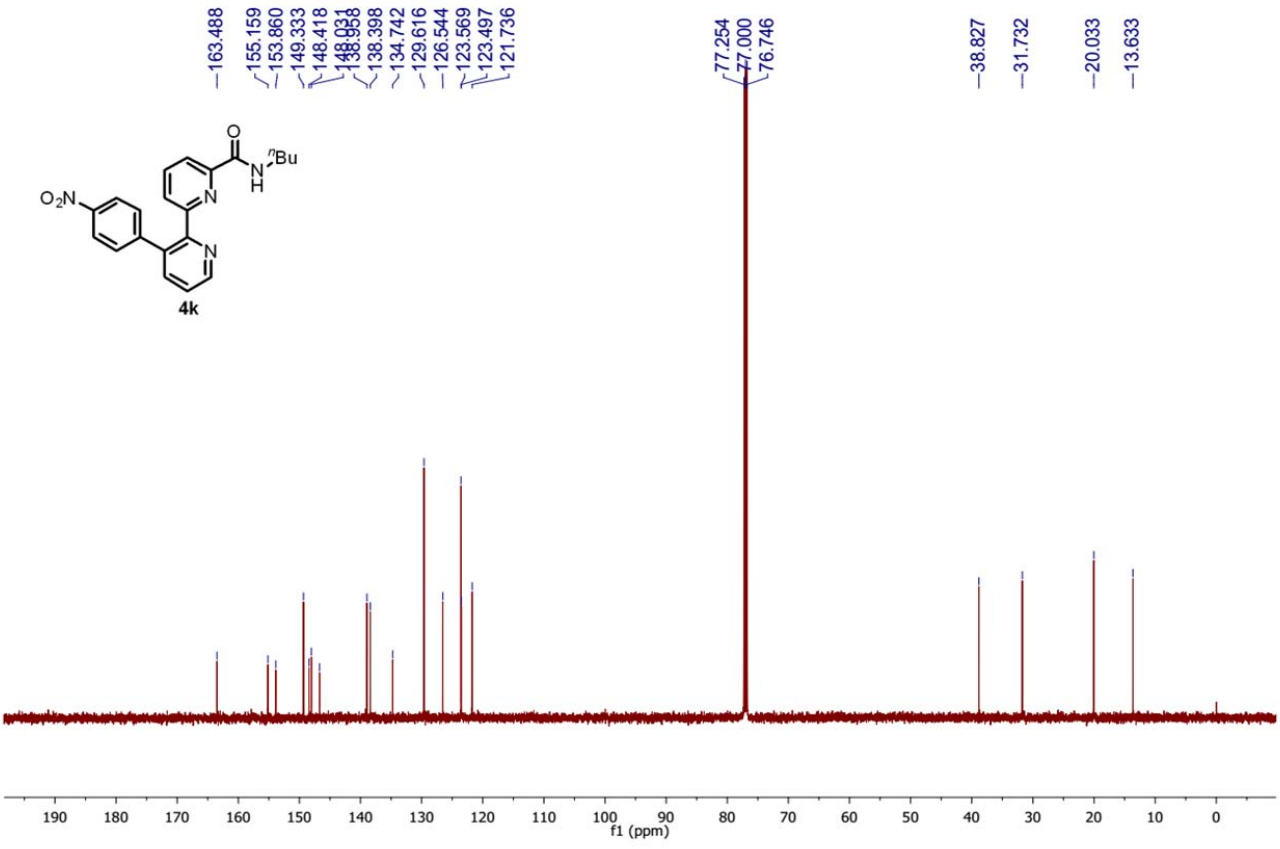

8.778
8.775
8.769
8.765
8.221
8.219
8.205
8.203
8.080
8.078
8.064
8.062
7.960
7.944
7.940
7.927
7.923
7.792
7.788
7.776
7.773
7.485
7.475
7.469
7.460
7.313
7.309
7.305
7.296
7.292
7.288
6.778
6.766
6.755
3.113
3.100
3.087
3.072
2.597
1.344
1.337
1.330
1.328
1.322
1.314
1.300
1.288
1.274
1.260
1.251
1.247
1.244
1.229
0.923
0.908
0.894
-0.000
Me
tBu
4i
1.00
1.01
1.02
3.04
1.01
1.03
2.05
0.98
2.09
3.06
2.02
2.06
3.05
f1 (ppm)

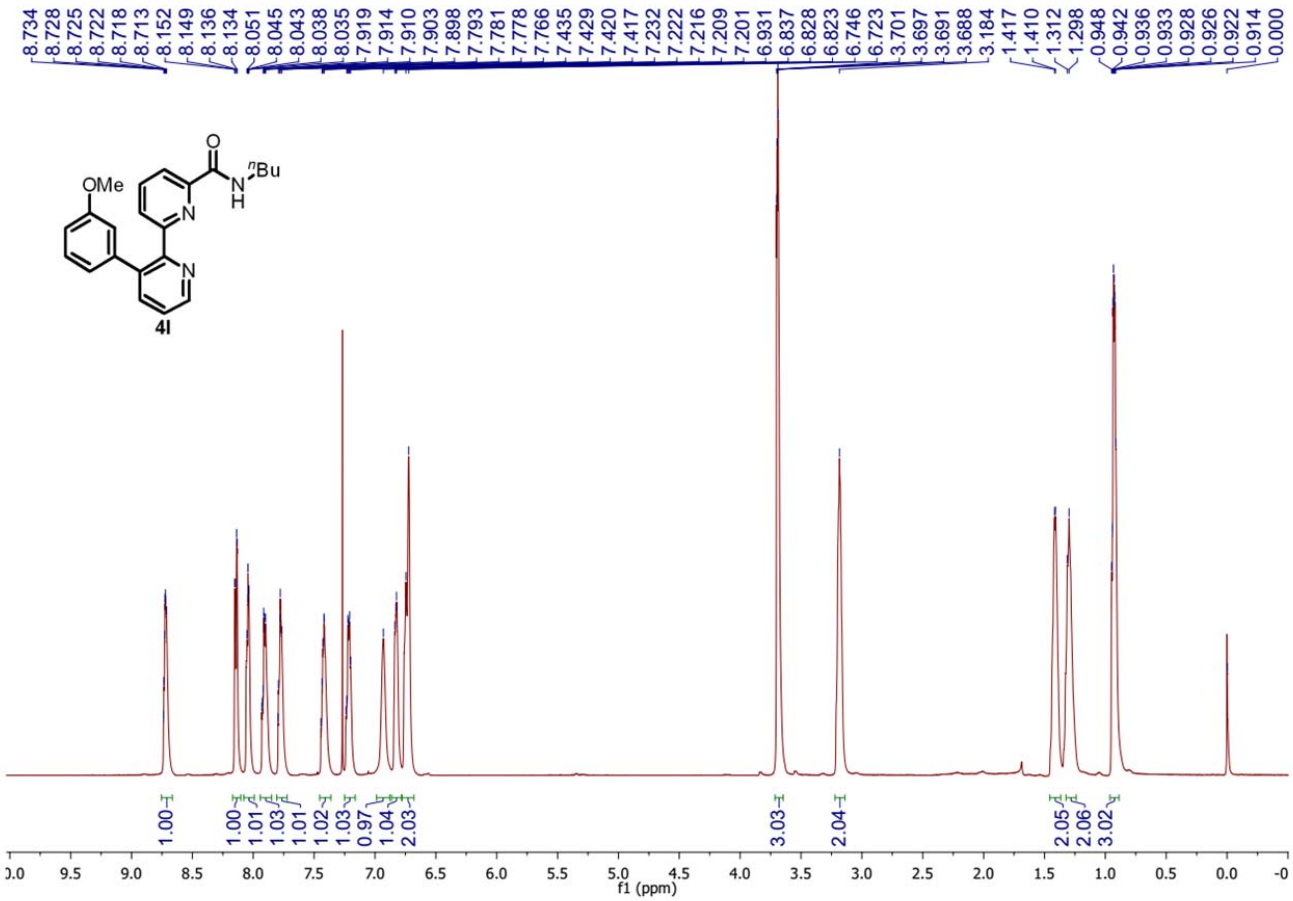

197.050
163.697
155.490
153.832
148.783
148.352
146.039
139.048
138.172
135.892
135.434
128.969
128.353
126.352
123.402
121.380
77.254
77.000
76.746
38.750
31.649
26.518
20.027
13.697
Me
tBu
4i
f1 (ppm)

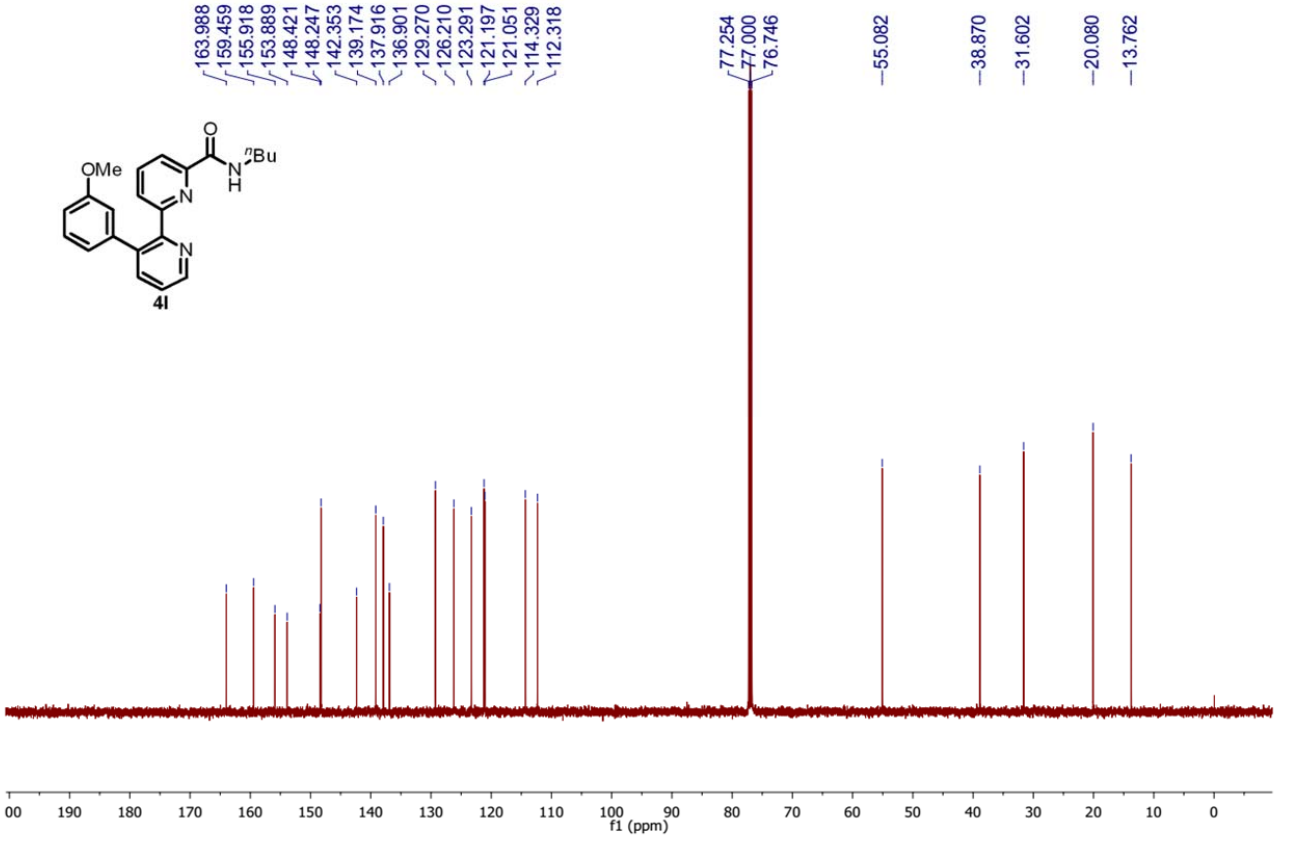

8.797
8.794
8.787
8.784
8.206
8.099
8.097
7.974
7.959
7.639
7.622
7.323
7.306
6.757
3.232
3.218
3.205
3.191
1.431
1.425
1.415
1.410
1.401
1.386
1.352
1.338
1.323
1.307
1.293
1.279
0.976
0.961
0.947
0.000
NC
O
N
H
nBu
N
4j
0.98
0.99
0.99
1.03
1.01
1.98
1.02
2.00
0.97
2.01
2.06
2.00
2.98
0.99
f1 (ppm)

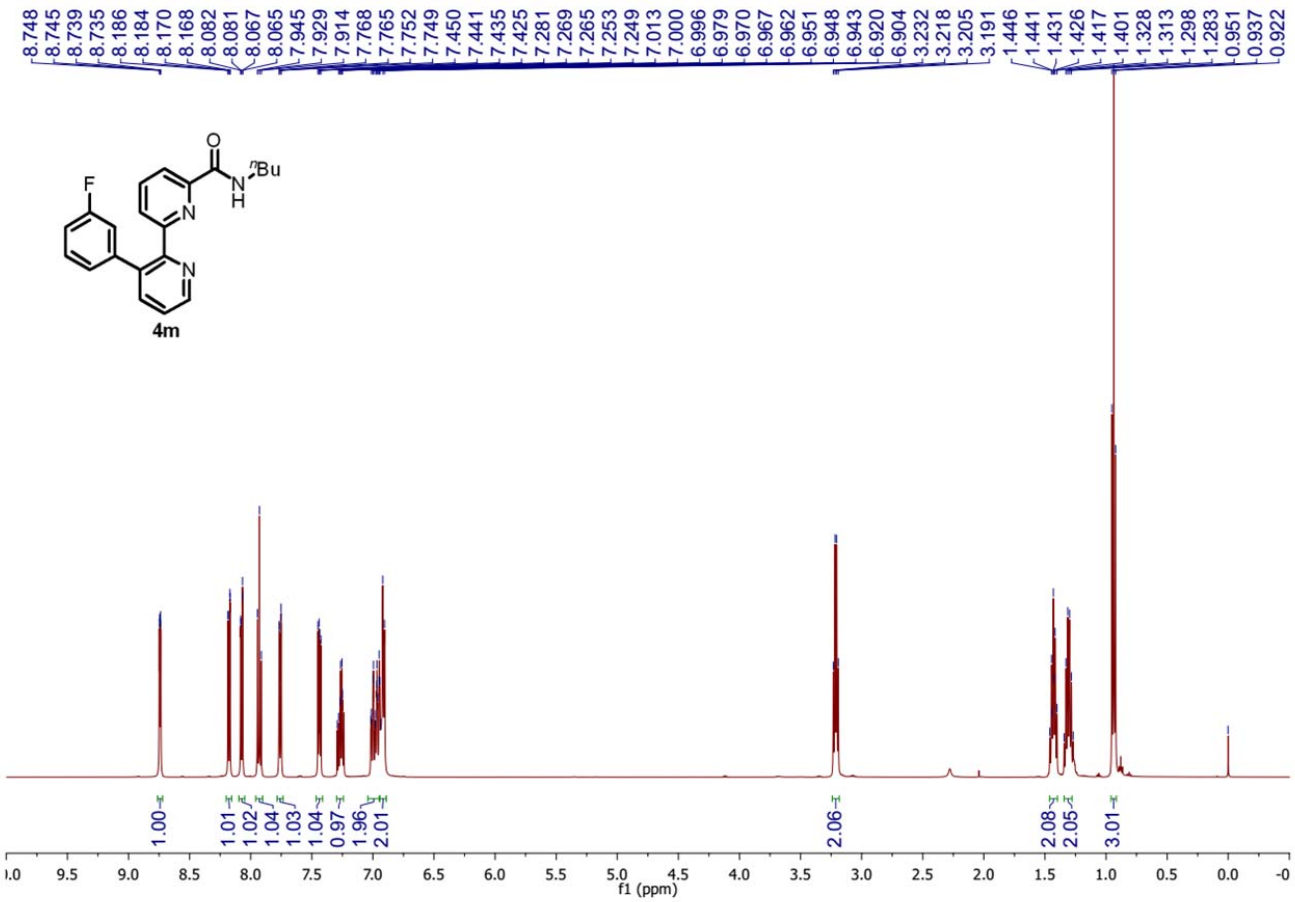

163.585
155.232
149.199
148.442
145.971
139.021
138.355
135.093
132.052
129.551
126.534
123.535
121.714
77.254
77.000
76.746
38.900
31.820
20.122
13.771
NC
O
N
H
nBu
N
4j
f1 (ppm)

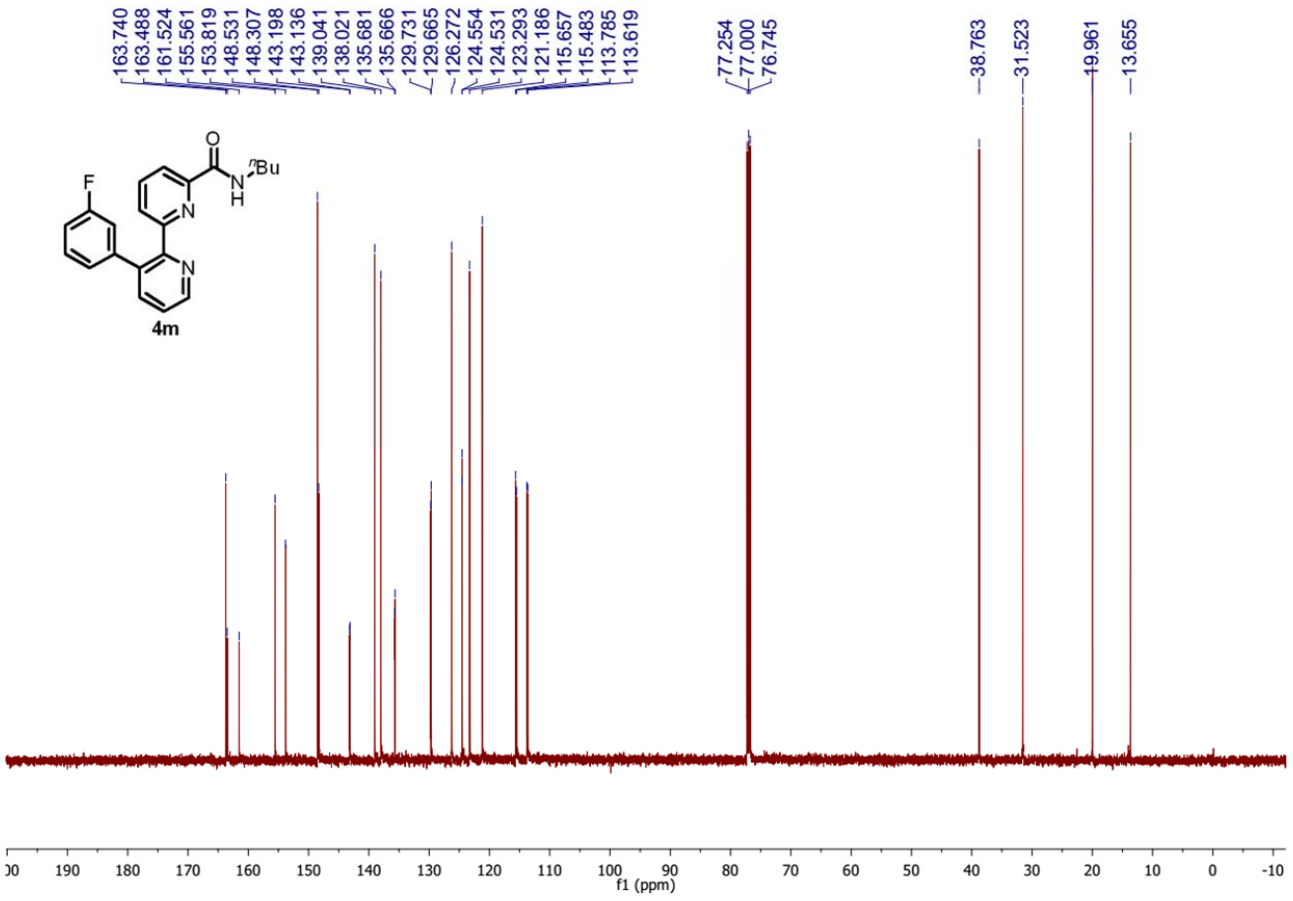

8.814
8.810
8.804
8.801
8.240
8.215
8.197
8.096
7.986
7.970
7.780
7.383
7.365
6.745
3.147
3.133
3.120
3.106
1.340
1.333
1.326
1.324
1.318
1.310
1.295
1.270
1.256
1.240
1.225
0.926
0.912
0.897
0.000
O
N
nBu
H
O2N
N
N
4k
1.00
1.02
2.00
0.99
1.04
1.01
1.02
2.03
0.94
2.04
2.01
2.09
3.00
f1 (ppm)

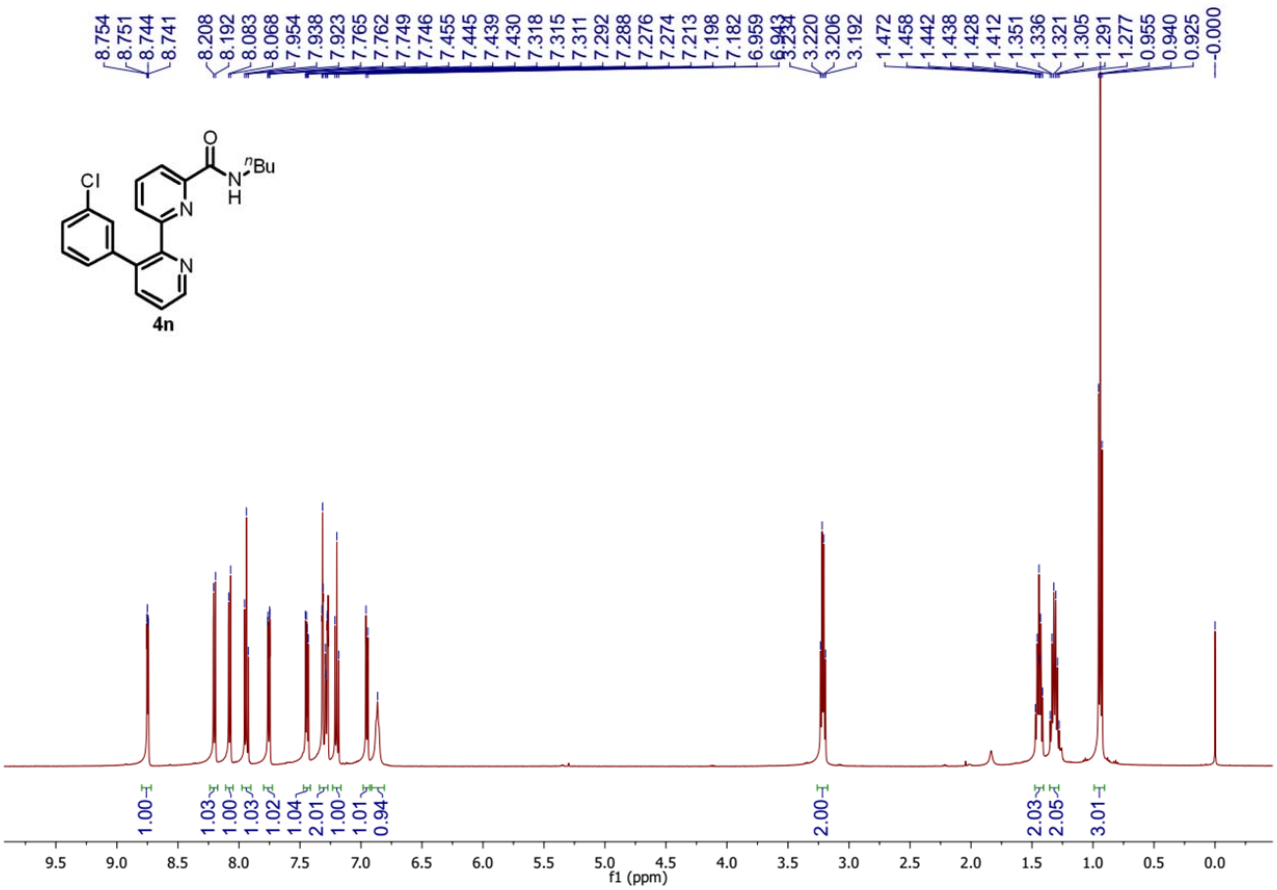

163.488
155.159
153.860
149.333
148.418
138.398
134.742
129.616
126.544
123.569
123.497
121.736
77.254
77.000
76.746
38.827
31.732
20.033
13.633
O
N
nBu
H
O2N
N
N
4k
f1 (ppm)

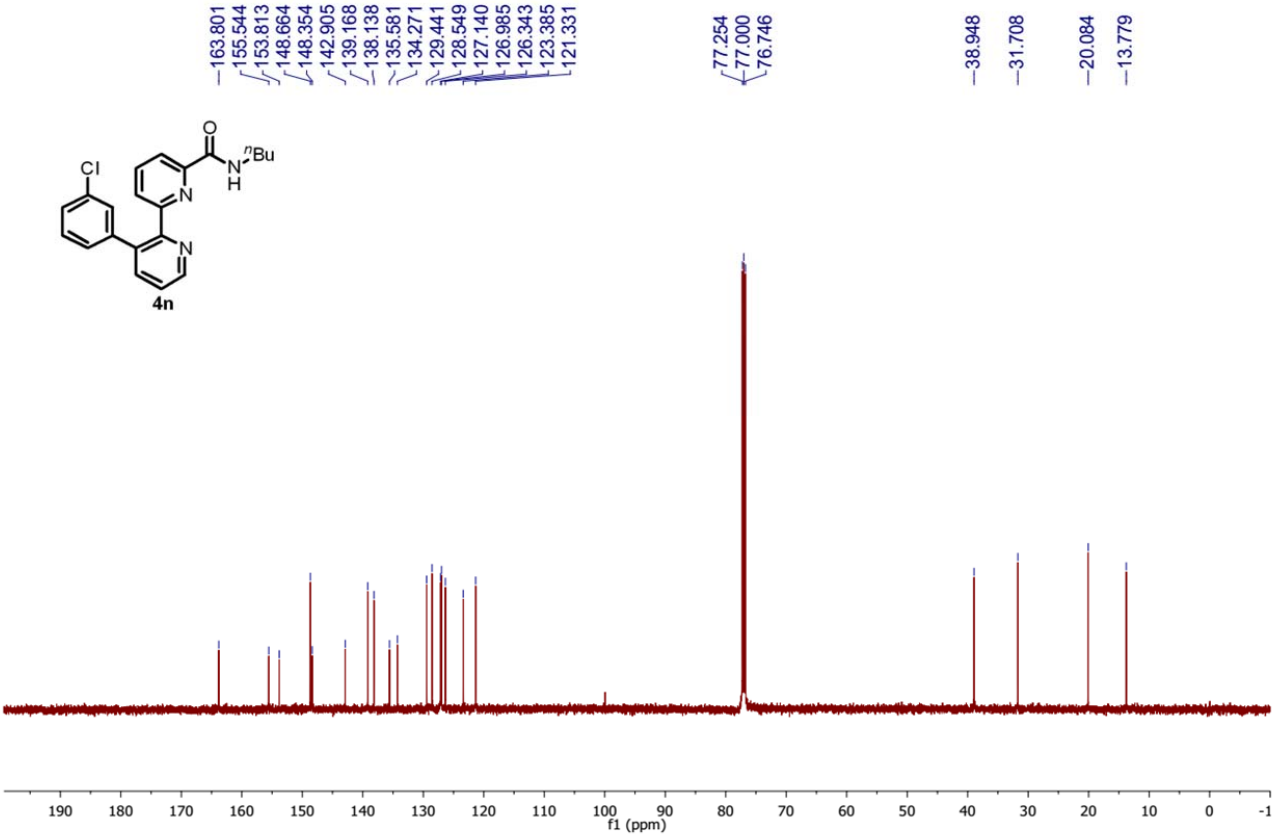

8.734
8.728
8.725
8.722
8.718
8.713
8.152
8.149
8.136
8.134
8.051
8.045
8.043
8.038
8.035
7.919
7.914
7.910
7.903
7.898
7.793
7.781
7.778
7.766
7.435
7.429
7.420
7.417
7.232
7.222
7.216
7.209
7.201
6.931
6.837
6.828
6.823
6.746
6.723
3.701
3.697
3.691
3.688
3.184
1.417
1.410
1.312
1.298
0.948
0.942
0.936
0.933
0.928
0.926
0.922
0.914
0.000
OMe
O
N
H
nBu
N
N
4l
1.00
1.00
1.01
1.03
1.01
1.02
1.03
0.97
1.04
2.03
3.03
2.04
2.05
2.06
3.02
f1 (ppm)

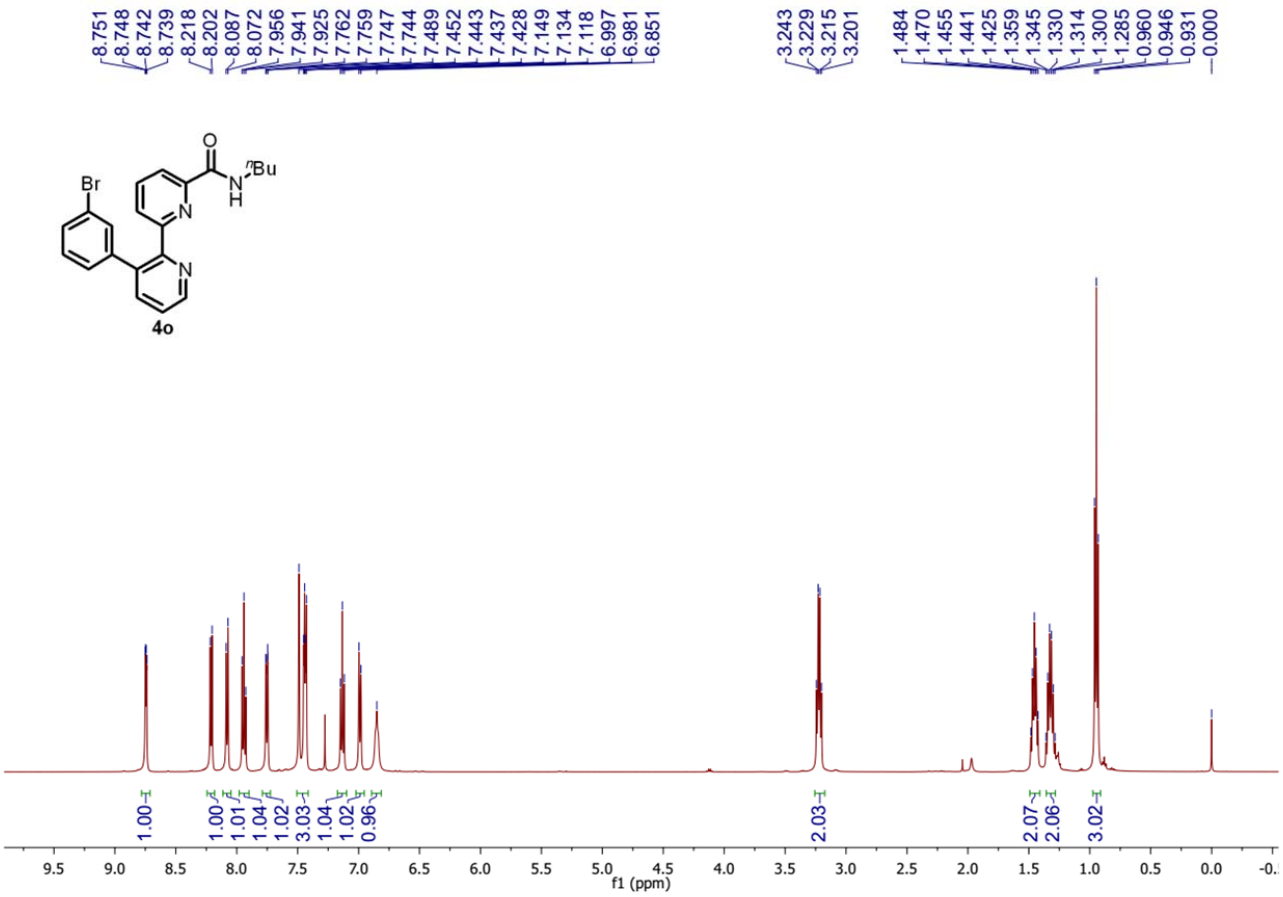

163.988
159.459
155.918
153.889
148.421
148.247
142.353
139.174
137.916
136.901
129.270
126.210
123.291
121.197
121.051
114.329
112.318
77.254
77.000
76.746
55.082
38.870
31.602
20.080
13.762
OMe
O
N
H
nBu
N
N
4l
f1 (ppm)

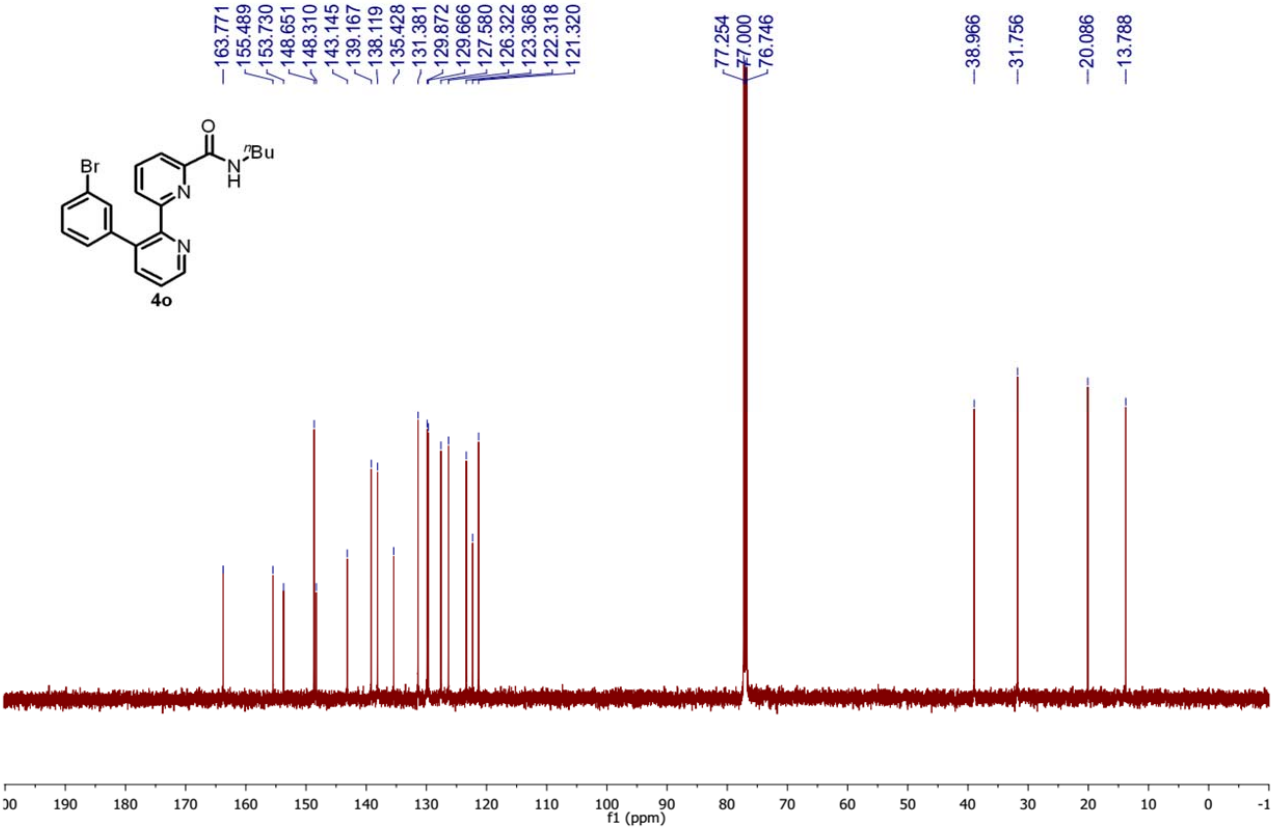

8.748
8.745
8.739
8.735
8.186
8.184
8.170
8.168
8.082
8.081
8.067
8.065
7.945
7.929
7.914
7.768
7.765
7.752
7.749
7.450
7.441
7.435
7.425
7.281
7.269
7.265
7.253
7.249
7.013
7.000
6.996
6.979
6.970
6.967
6.962
6.951
6.948
6.943
6.920
6.904
3.232
3.218
3.205
3.191
1.446
1.441
1.431
1.426
1.417
1.401
1.328
1.313
1.298
1.283
0.951
0.937
0.922
F
O
N
H
nBu
N
N
4m
1.00
1.01
1.02
1.04
1.03
1.04
0.97
1.96
2.01
2.06
2.08
2.05
3.01
f1 (ppm)

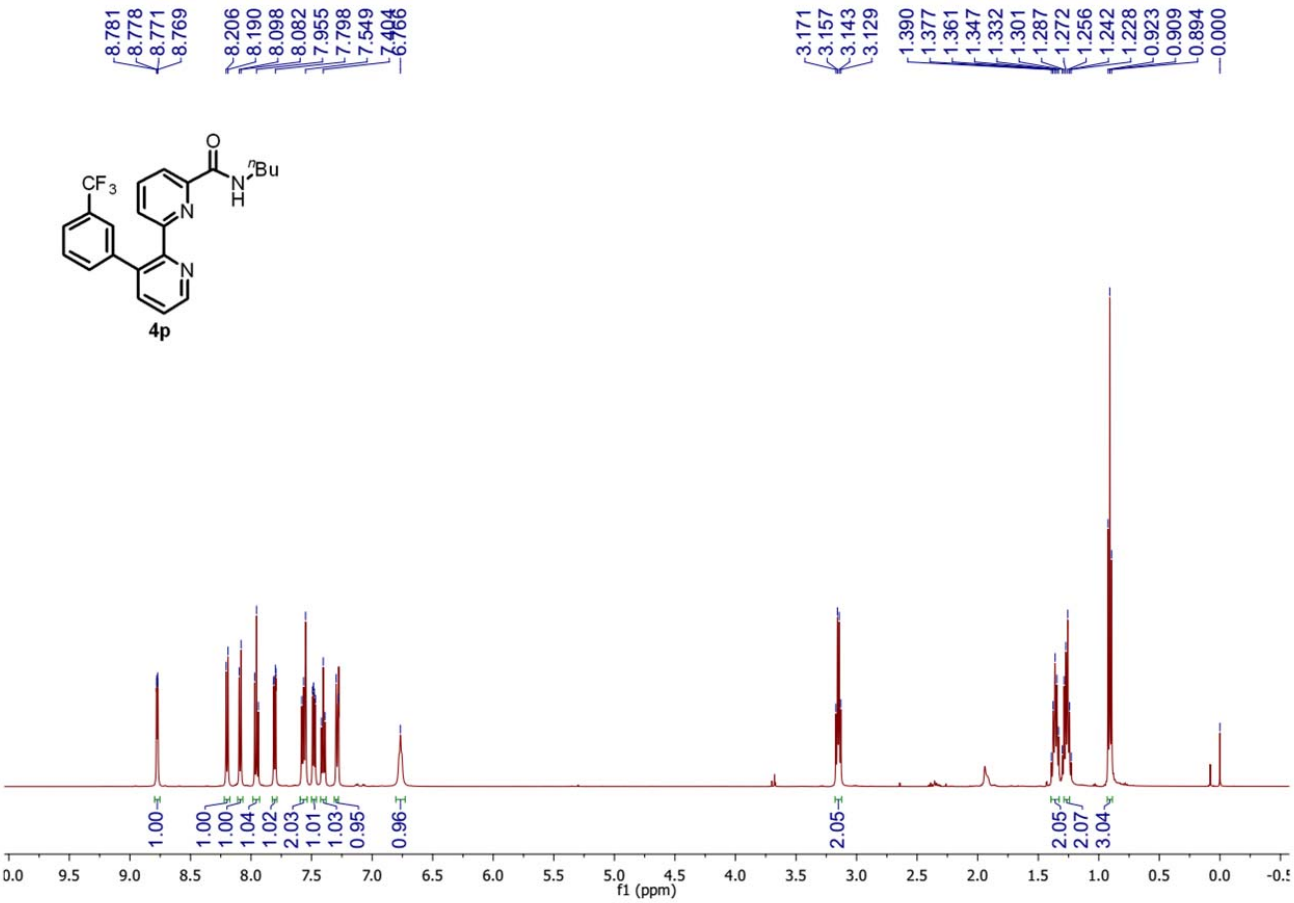

163.740
163.488
161.524
155.561
153.819
148.531
148.307
143.198
143.136
139.041
138.021
135.681
135.666
129.731
129.665
126.272
124.554
124.531
123.293
121.186
115.657
115.483
113.785
113.619
77.254
77.000
76.745
38.763
31.523
19.961
13.655
F
O
N
H
nBu
N
N
4m
f1 (ppm)

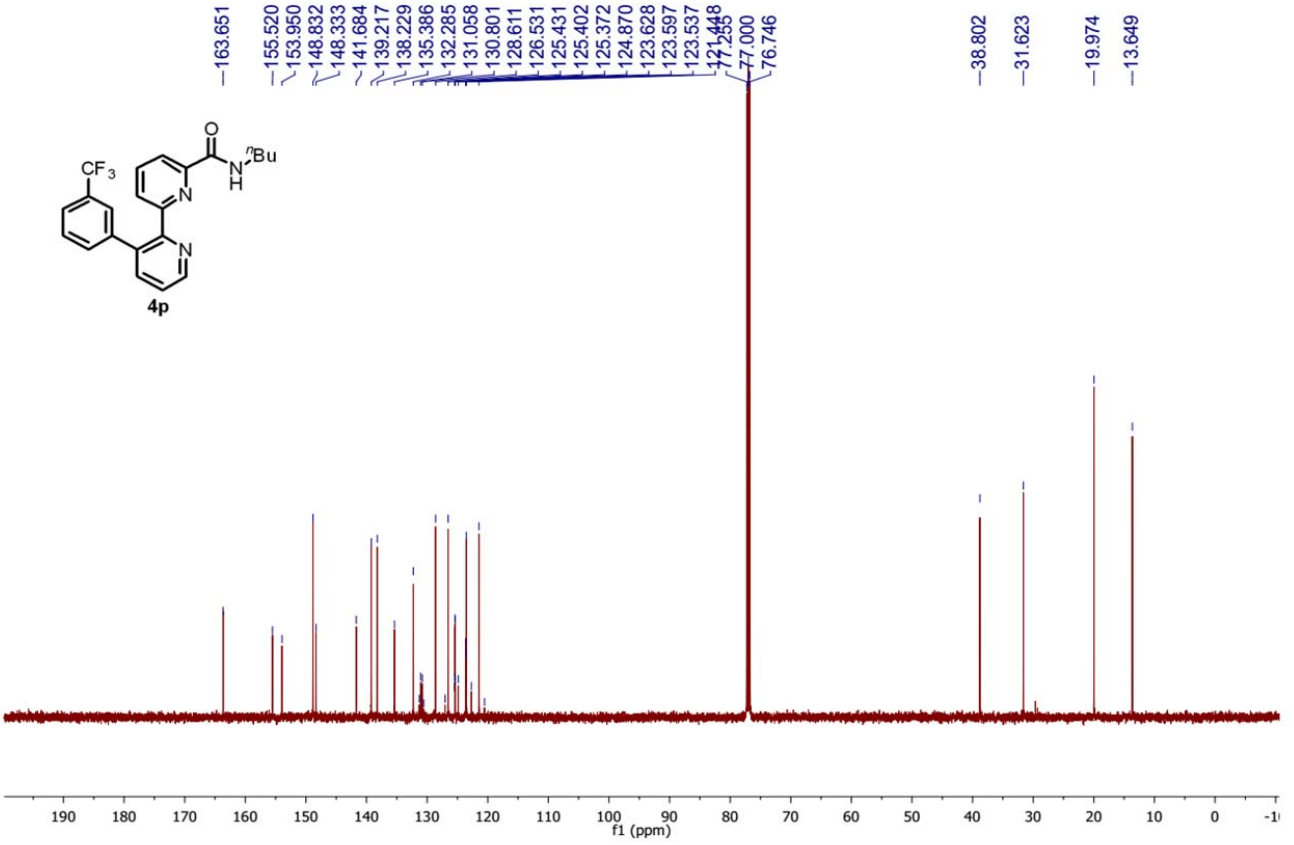

8.754
8.751
8.744
8.741
8.208
8.192
8.083
8.068
7.954
7.938
7.923
7.765
7.762
7.749
7.746
7.455
7.445
7.439
7.430
7.318
7.315
7.311
7.292
7.288
7.276
7.274
7.213
7.198
7.182
6.959
3.234
3.220
3.206
3.192
1.472
1.458
1.442
1.438
1.428
1.412
1.351
1.336
1.321
1.305
1.291
1.277
0.955
0.940
0.925
-0.000
Cl
O
N
nBu
H
N
N
4n
1.00
1.03
1.00
1.03
1.02
1.04
2.01
1.00
1.01
0.94
2.00
2.03
2.05
3.01
f1 (ppm)

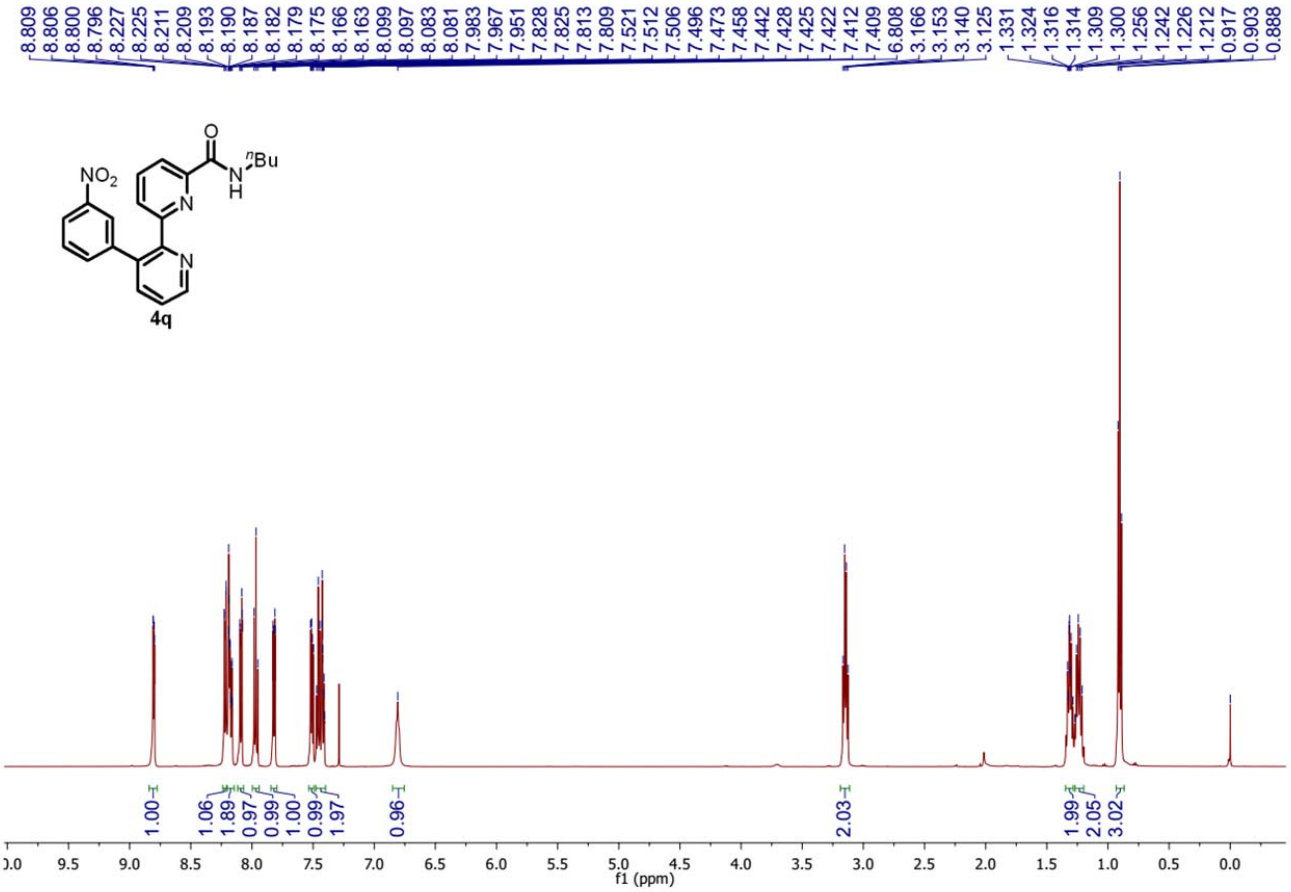

163.801
155.544
153.813
148.664
148.354
142.905
139.168
138.138
135.581
134.271
129.441
128.549
127.140
126.985
126.343
123.385
121.331
77.254
77.000
76.746
38.948
31.708
20.084
13.779
Cl
O
N
nBu
H
N
N
4n
f1 (ppm)

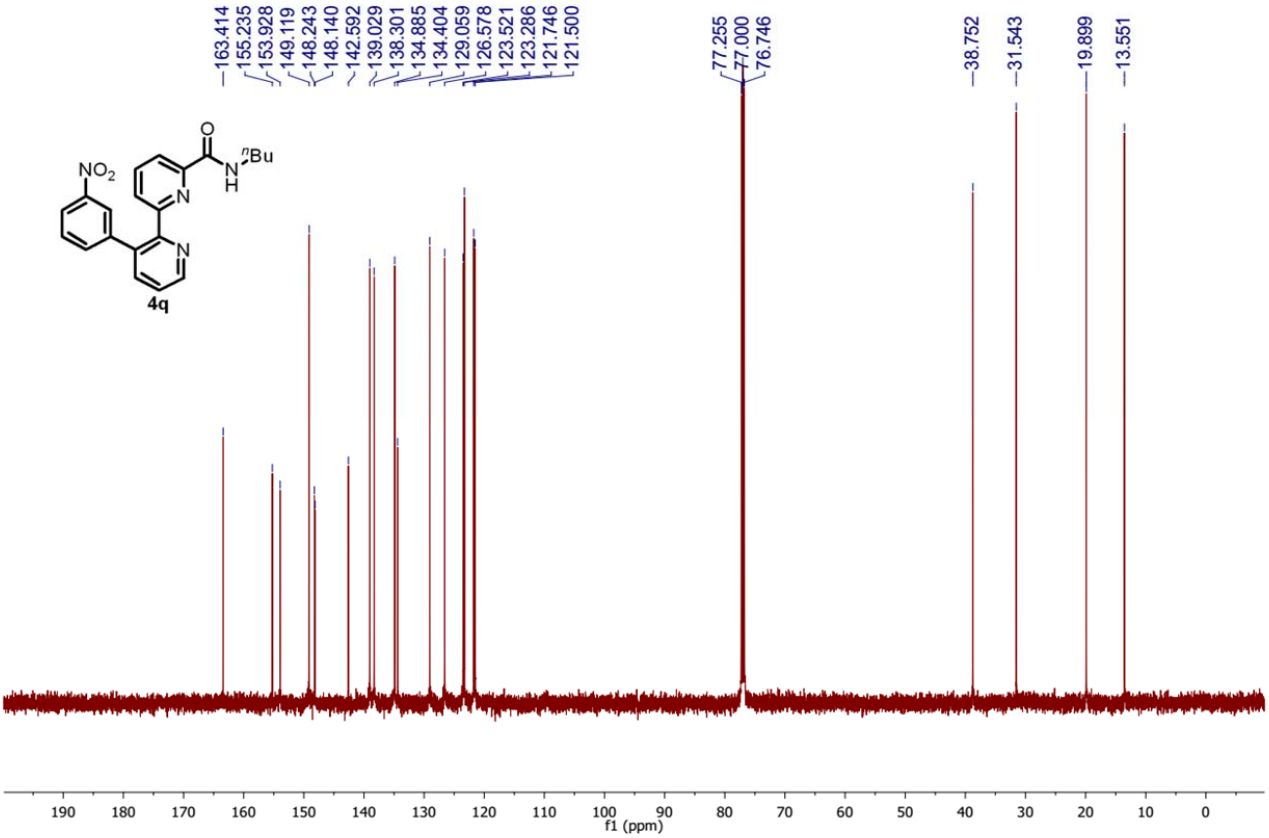

8.751
8.748
8.742
8.739
8.218
8.202
8.087
8.072
7.956
7.941
7.925
7.762
7.759
7.747
7.744
7.489
7.452
7.443
7.437
7.428
7.149
7.134
7.118
6.997
6.981
6.851
3.243
3.229
3.215
3.201
1.484
1.470
1.455
1.441
1.425
1.359
1.345
1.330
1.314
1.300
1.285
0.960
0.946
0.931
0.000
Br
O
N
H
nBu
N
4o
1.00
1.00
1.01
1.04
1.02
3.03
1.04
1.02
0.96
2.03
2.07
2.06
3.02
f1 (ppm)

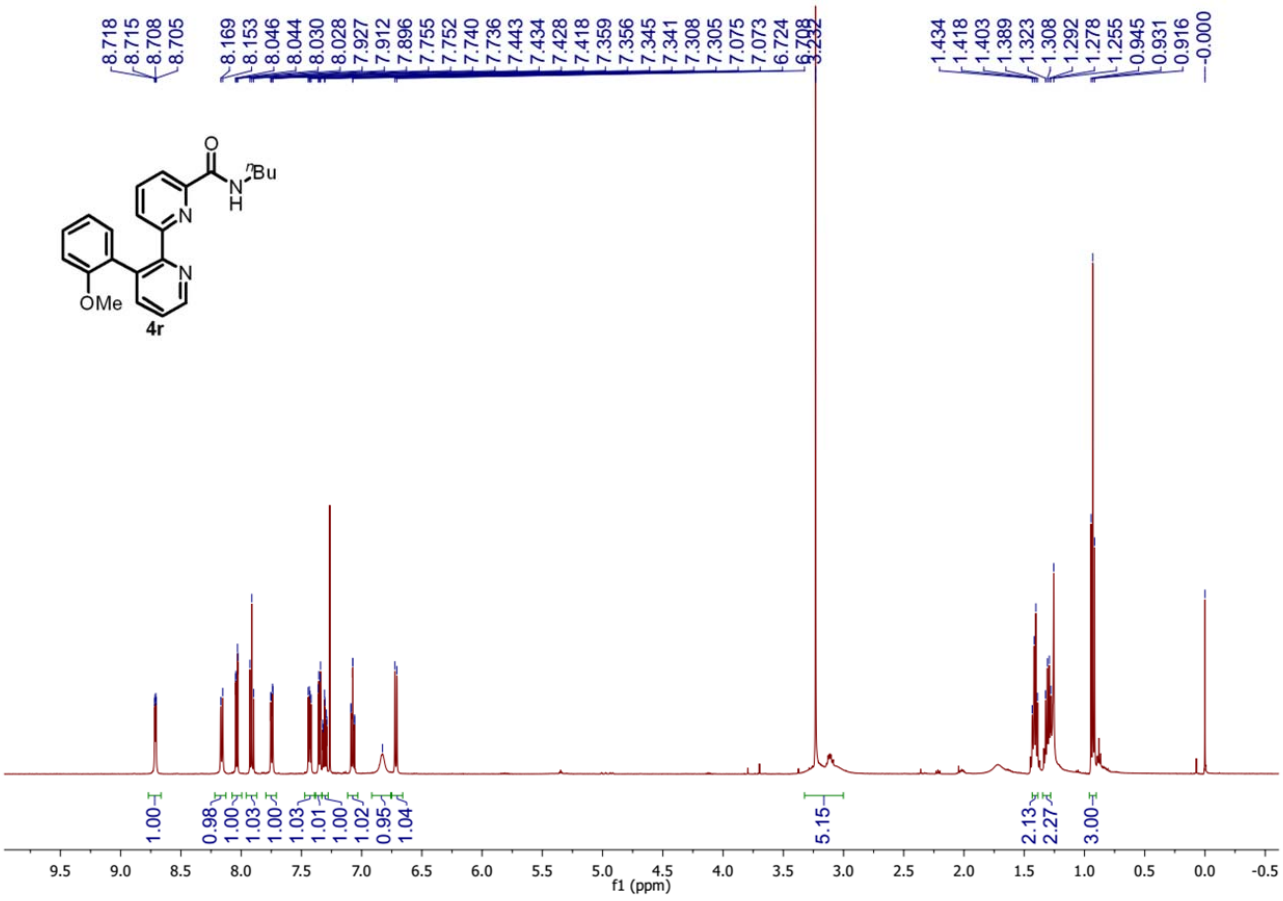

163.771
155.489
153.730
148.651
148.310
143.145
139.167
138.119
135.428
131.381
129.872
129.666
127.580
126.322
123.368
122.318
121.320
77.254
77.000
76.746
38.966
31.756
20.086
13.788
Br
O
N
H
nBu
N
4o
f1 (ppm)

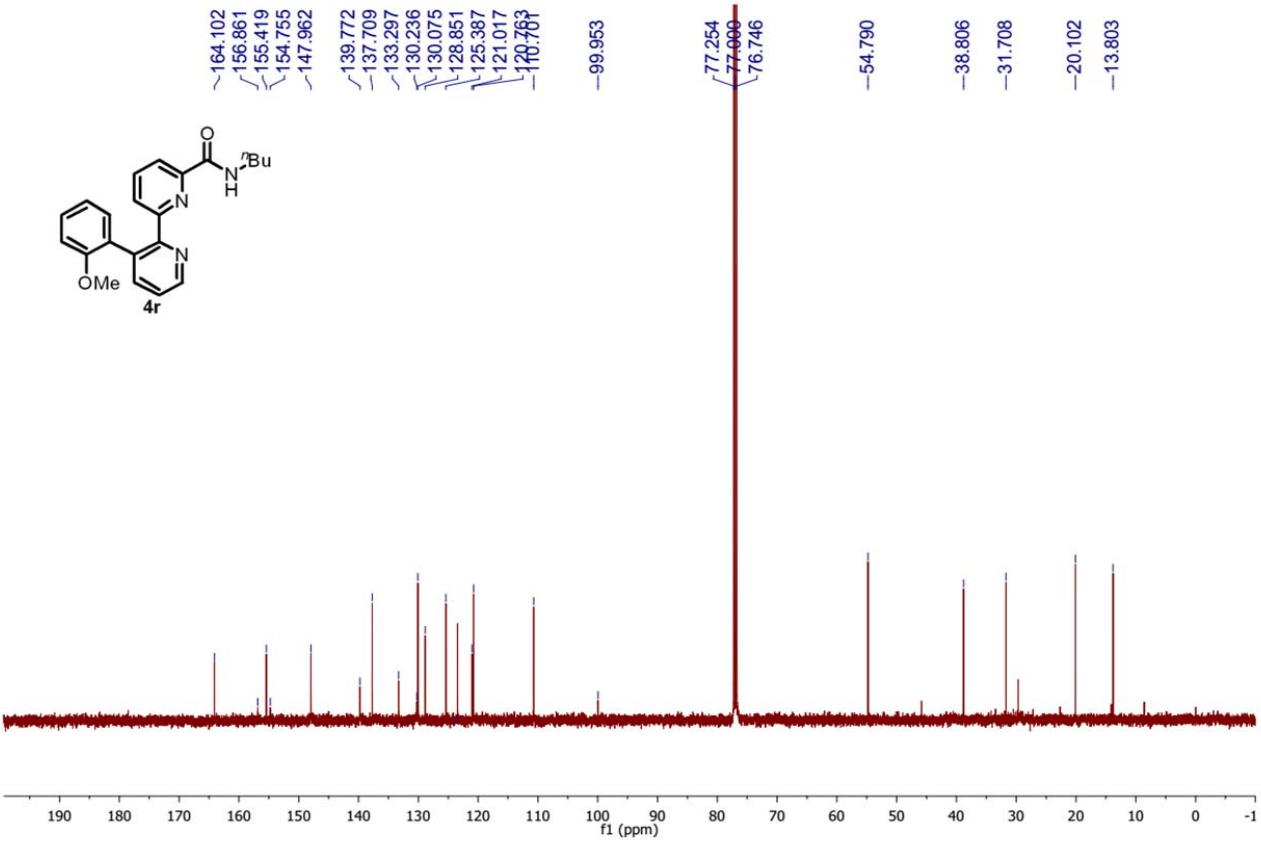

8.781
8.778
8.771
8.769
8.206
8.190
8.098
8.082
7.955
7.798
7.549
7.404
7.388
3.171
3.157
3.143
3.129
1.390
1.377
1.361
1.347
1.332
1.301
1.287
1.272
1.256
1.242
1.228
0.923
0.909
0.894
0.000
CF3
O
N
nBu
H
N
N
4p
1.00
1.00
1.00
1.04
1.02
2.03
1.01
1.03
0.95
0.96
2.05
2.05
2.07
3.04
f1 (ppm)

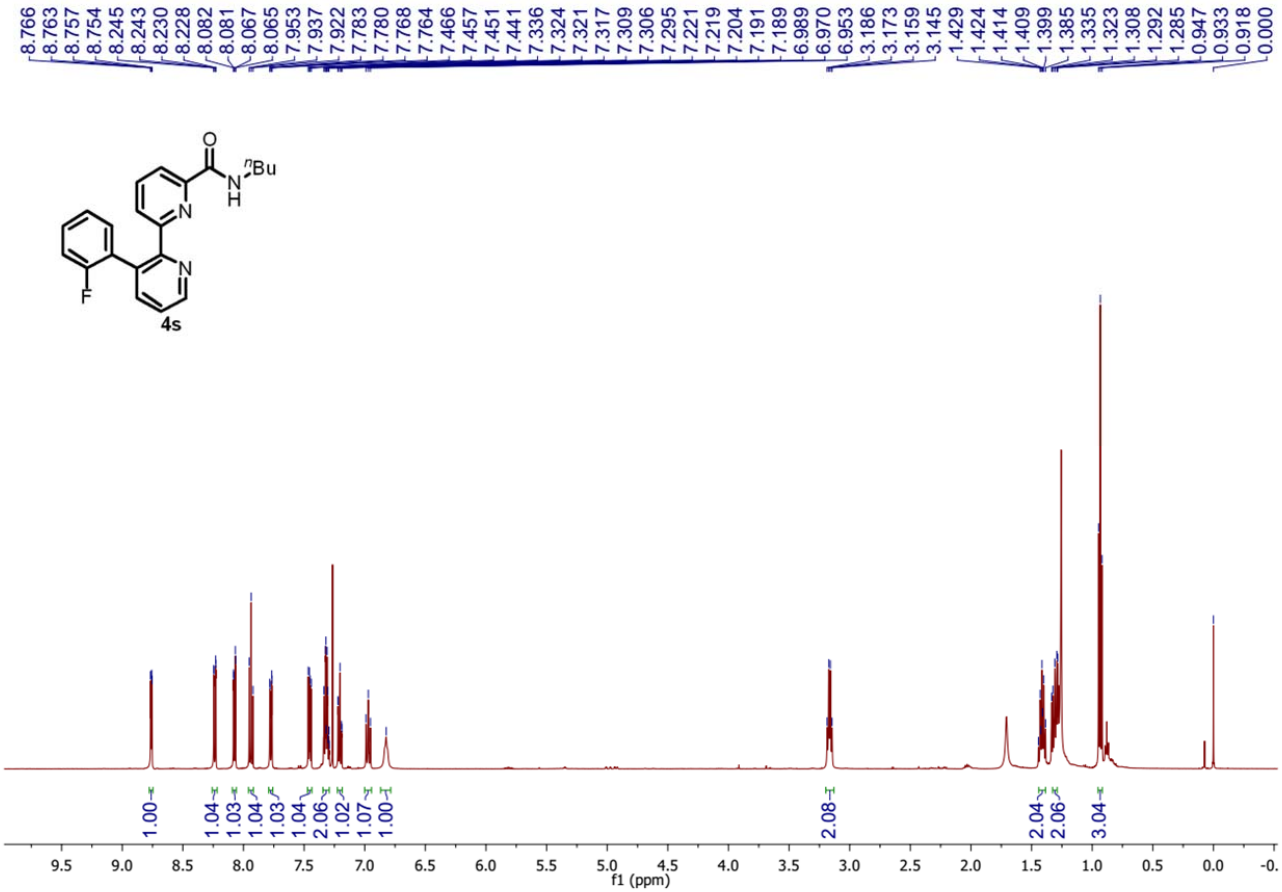

163.651
155.520
153.950
148.832
148.333
141.684
139.217
138.229
135.386
132.285
131.058
130.801
128.611
126.531
125.431
125.402
125.372
124.870
123.628
123.597
123.537
77.000
76.746
38.802
31.623
19.974
13.649
CF3
O
N
nBu
H
N
N
4p
f1 (ppm)

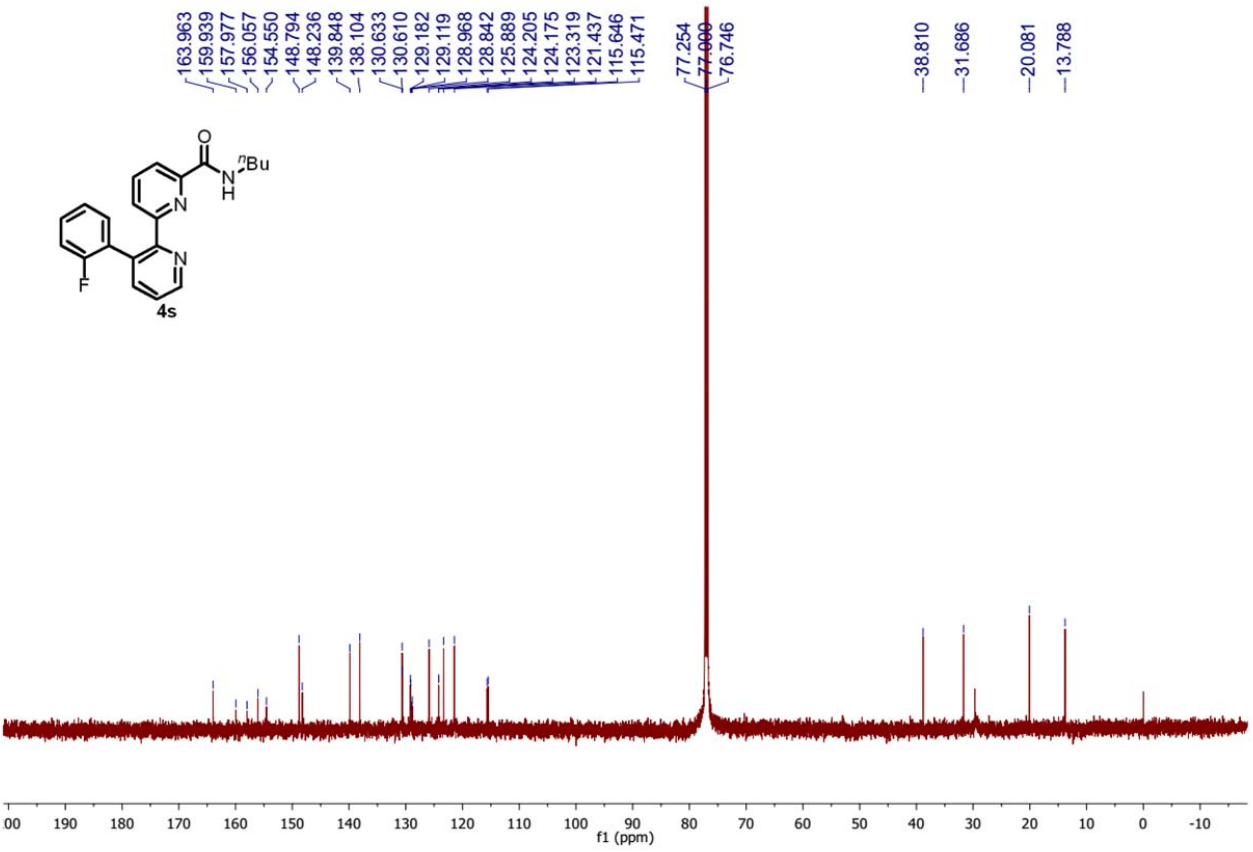

8.809
8.806
8.800
8.796
8.227
8.225
8.211
8.209
8.193
8.190
8.187
8.182
8.179
8.175
8.166
8.163
8.099
8.097
8.083
8.081
7.983
7.967
7.951
7.828
7.825
7.813
7.809
7.521
7.512
7.506
7.496
7.473
7.458
7.442
7.428
7.425
7.422
7.412
7.409
6.808
3.166
3.153
3.140
3.125
1.331
1.324
1.316
1.314
1.309
1.300
1.256
1.242
1.226
1.212
0.917
0.903
0.888
NO2
nBu
4q
1.00
1.06
1.89
0.97
0.99
1.00
0.99
1.97
0.96
2.03
1.99
2.05
3.02
f1 (ppm)

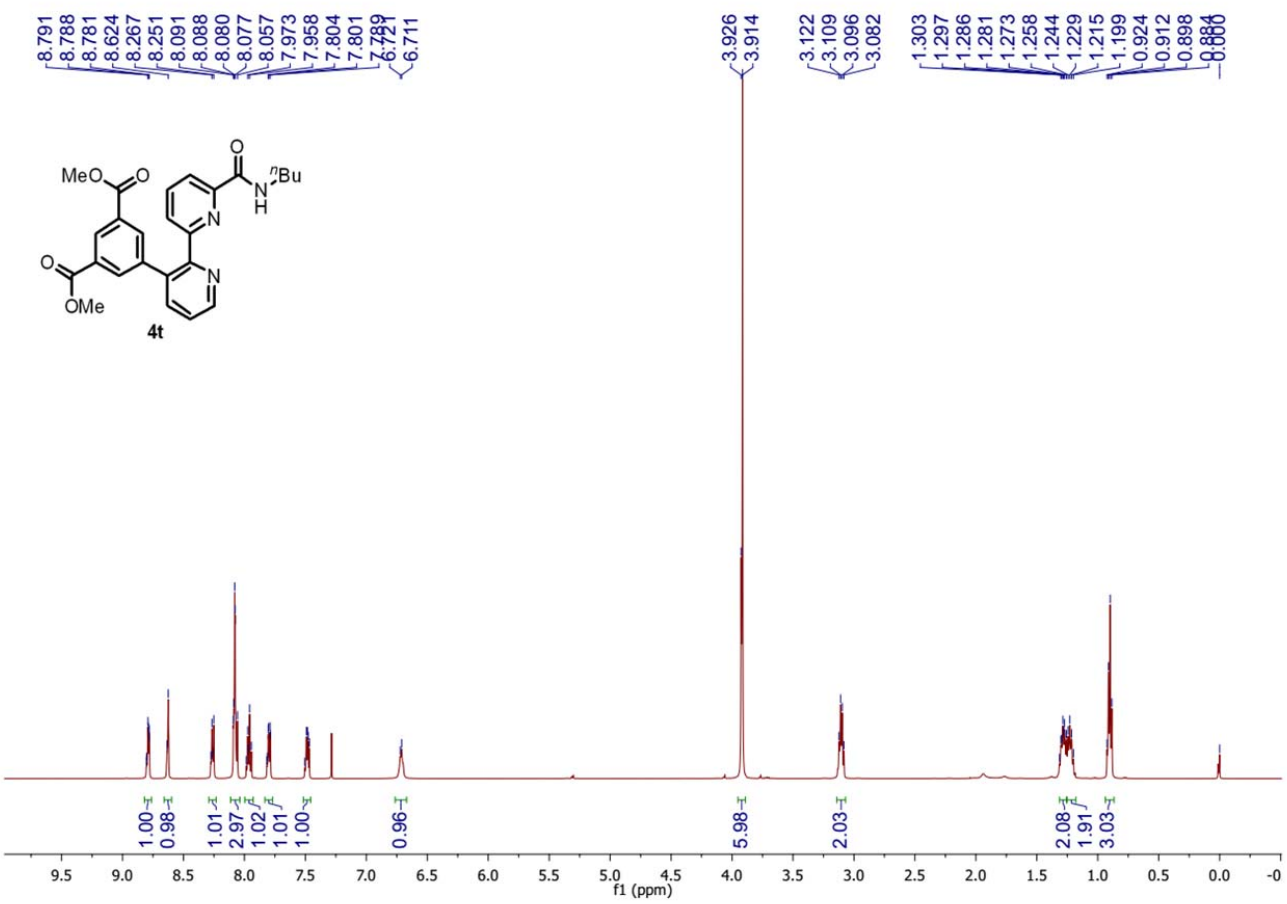

163.414
155.235
153.928
149.119
148.243
148.140
142.592
139.029
138.301
134.885
134.404
129.059
126.578
123.521
123.286
121.746
121.500
77.255
77.000
76.746
38.752
31.543
19.899
13.551
NO2
nBu
4q
f1 (ppm)

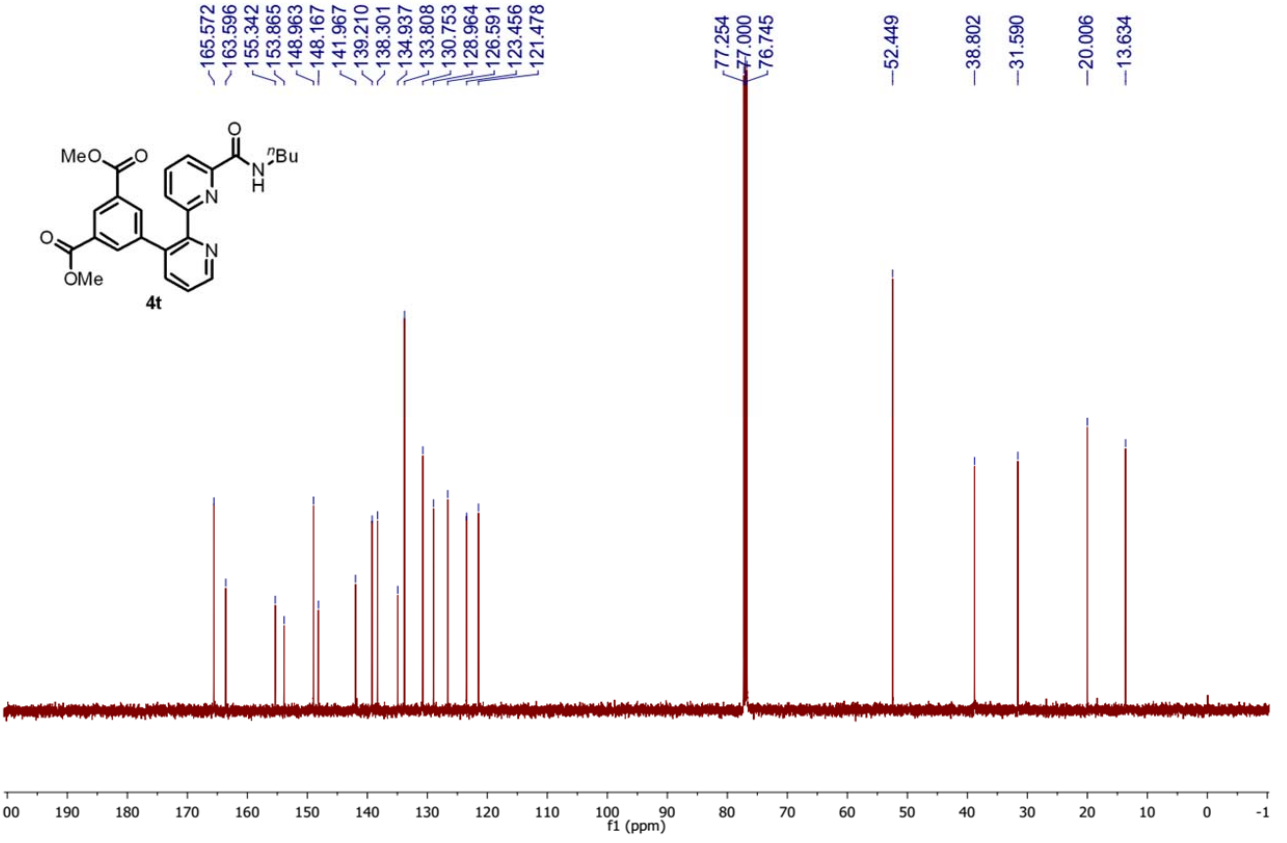

8.718
8.715
8.708
8.705
8.169
8.153
8.046
8.044
8.030
8.028
7.927
7.912
7.896
7.755
7.752
7.740
7.736
7.443
7.434
7.428
7.418
7.359
7.356
7.345
7.341
7.308
7.305
7.075
7.073
6.724
6.708
3.292
1.434
1.418
1.403
1.389
1.323
1.308
1.292
1.278
1.255
0.945
0.931
0.916
-0.000
nBu
N
H
O
N
N
OMe
4r
1.00
0.98
1.00
1.03
1.00
1.03
1.01
1.00
1.02
0.95
1.04
5.15
2.13
2.27
3.00
f1 (ppm)

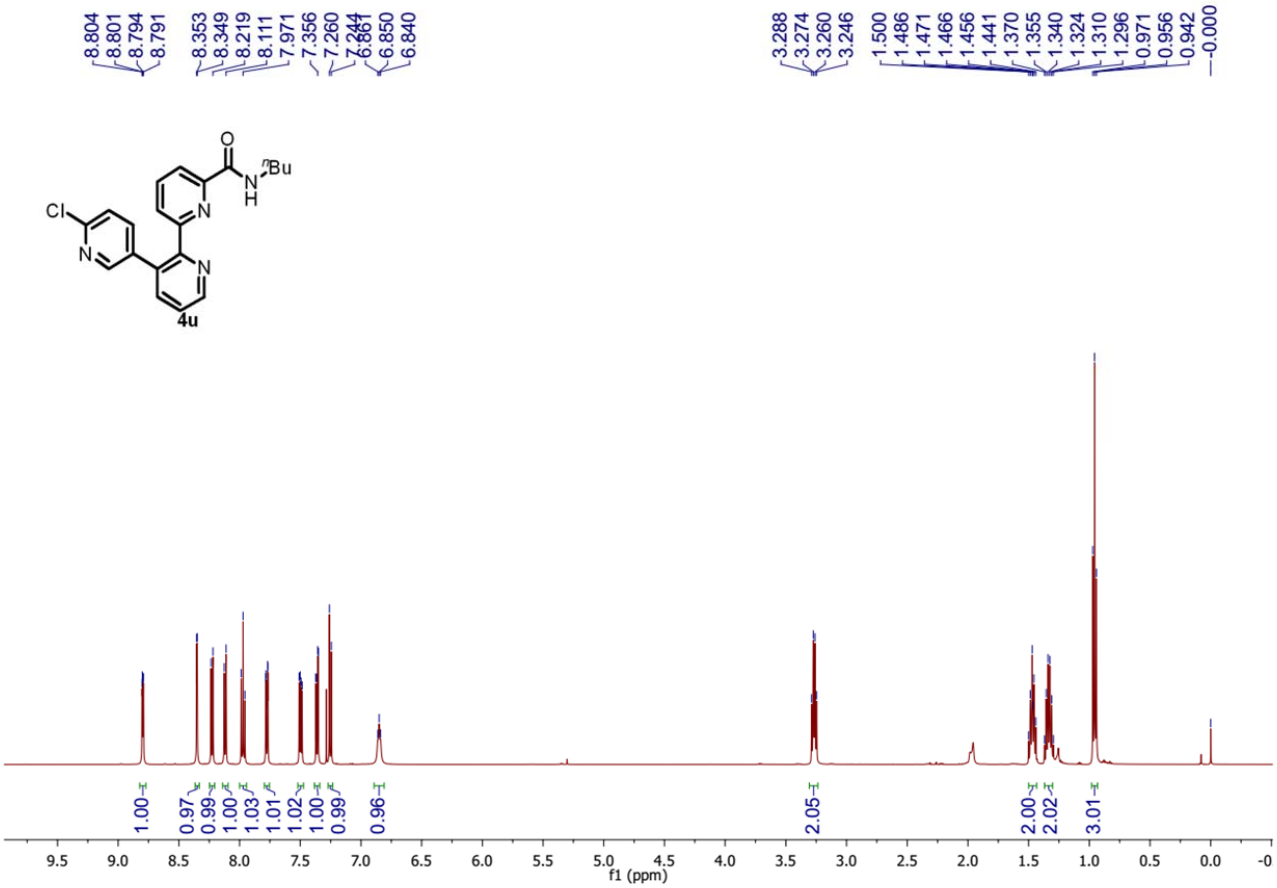

164.102
156.861
155.419
154.755
147.962
139.772
137.709
133.297
130.236
130.075
128.851
125.387
121.017
120.763
110.701
99.953
77.254
77.000
76.746
54.790
38.806
31.708
20.102
13.803
nBu
N
H
O
N
N
OMe
4r
f1 (ppm)

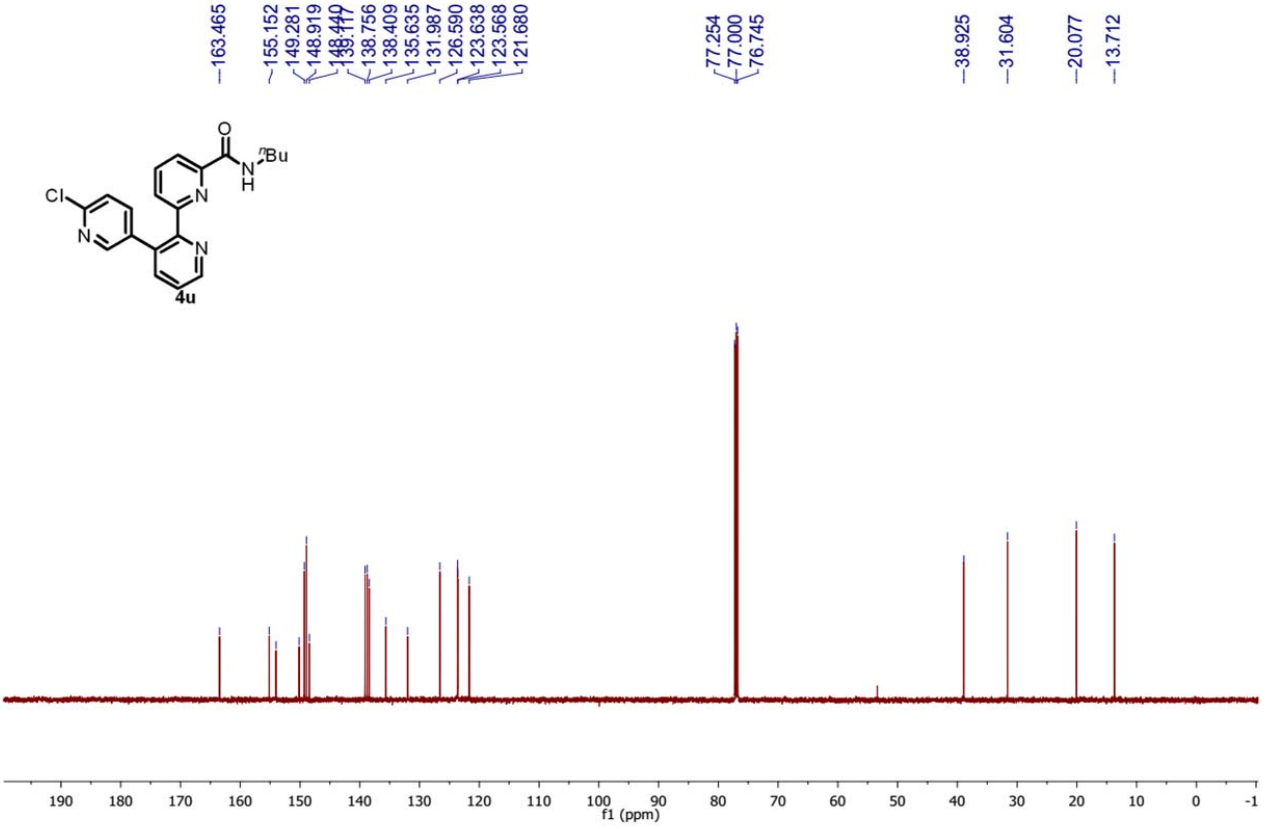

8.766
8.763
8.757
8.754
8.245
8.243
8.230
8.228
8.082
8.081
8.067
8.065
7.953
7.937
7.922
7.783
7.780
7.768
7.764
7.466
7.457
7.451
7.441
7.336
7.324
7.321
7.317
7.309
7.306
7.295
7.221
7.219
7.204
7.191
7.189
6.989
6.970
6.953
3.186
3.173
3.159
3.145
1.429
1.424
1.414
1.409
1.399
1.385
1.335
1.323
1.308
1.292
1.285
0.947
0.933
0.918
0.000
nBu
4s
1.00
1.04
1.03
1.04
1.03
1.04
2.06
1.02
1.07
1.00
2.08
2.04
2.06
3.04
f1 (ppm)

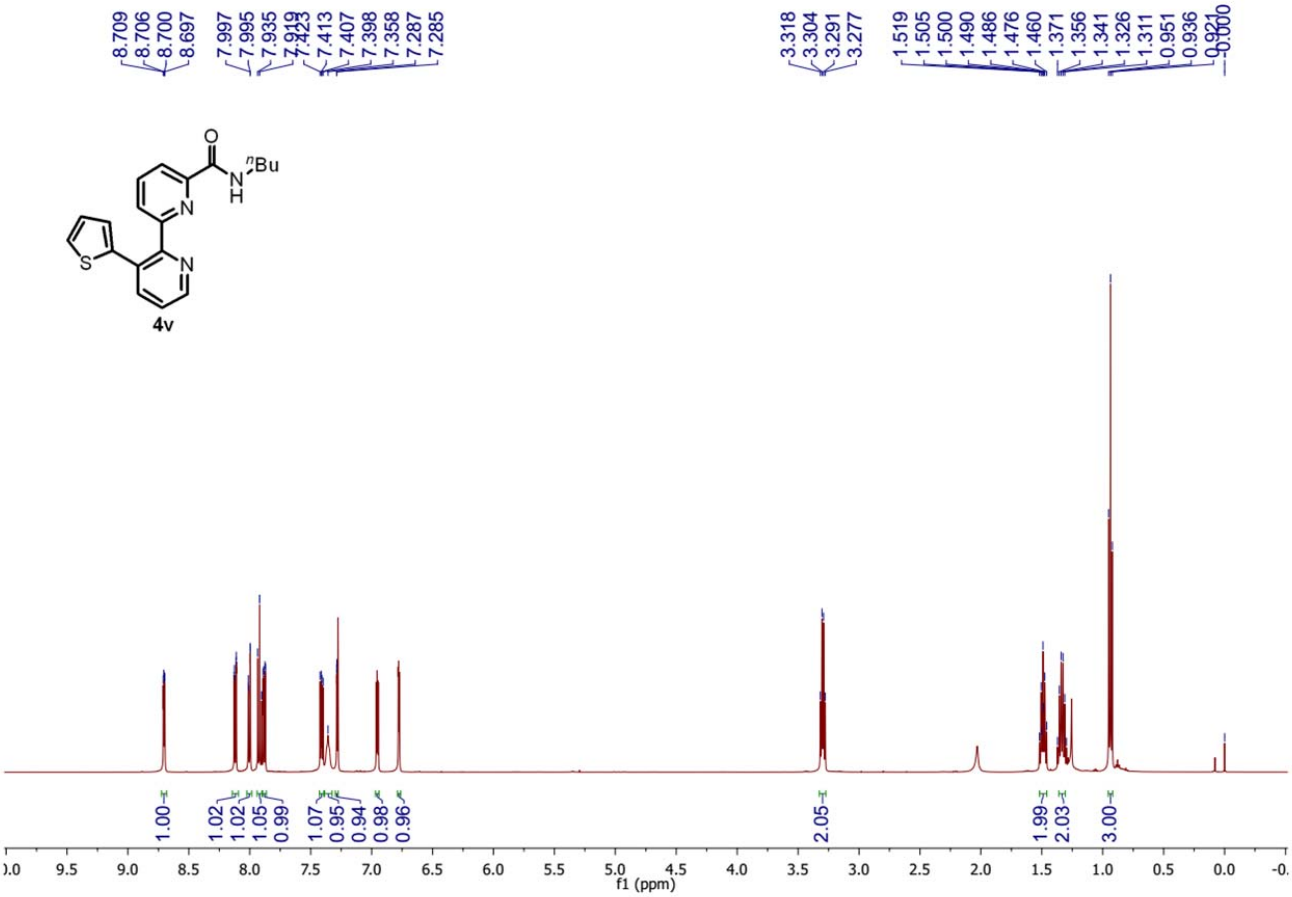

163.963
159.939
157.977
156.057
154.550
148.794
148.236
139.848
138.104
130.633
130.610
129.182
129.119
128.968
128.842
125.889
124.205
124.175
123.319
121.437
115.646
115.471
77.254
77.000
76.746
38.810
31.686
20.081
13.788
nBu
4s
f1 (ppm)

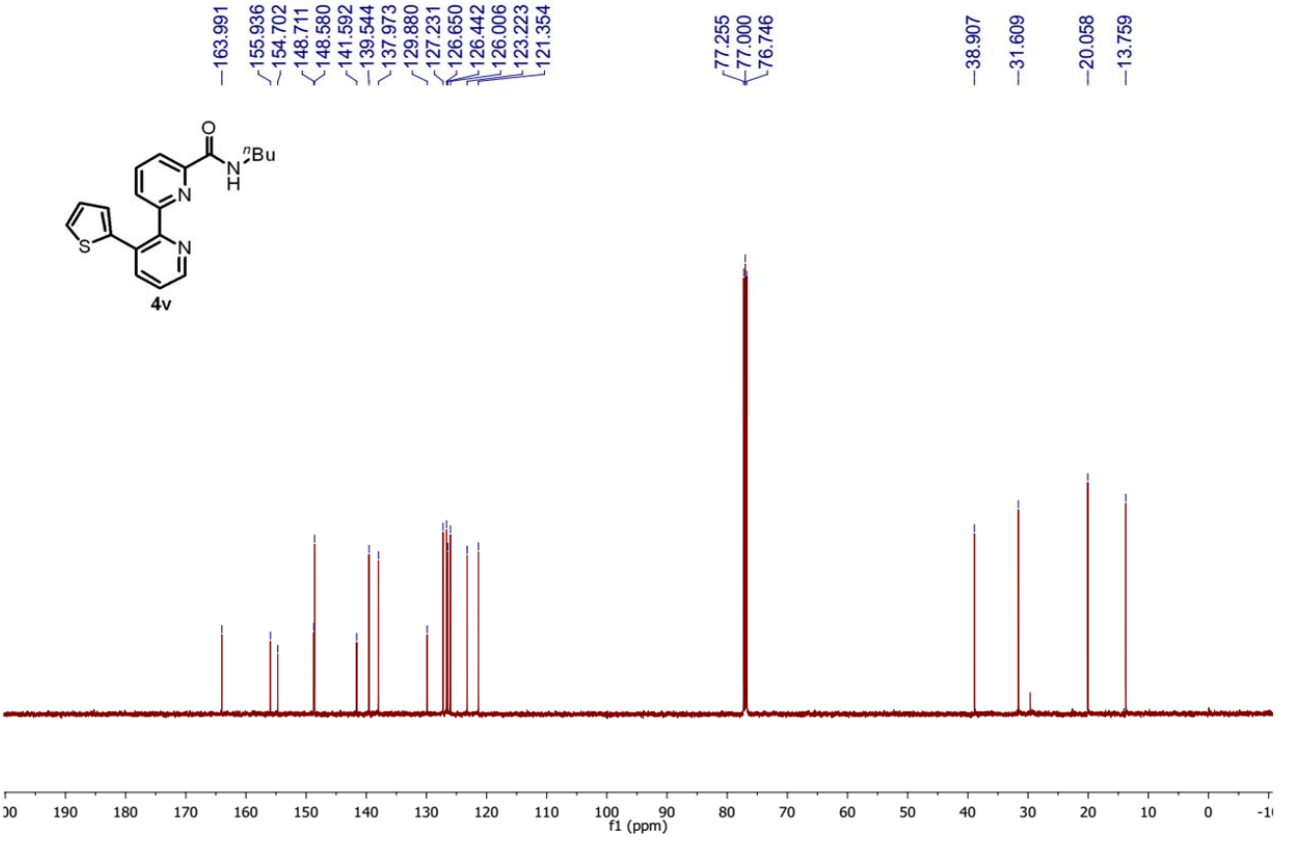

8.791
8.788
8.781
8.624
8.267
8.251
8.091
8.088
8.080
8.077
8.057
7.973
7.958
7.804
7.801
6.721
6.711
3.926
3.914
3.122
3.109
3.096
3.082
1.303
1.297
1.286
1.281
1.273
1.258
1.244
1.229
1.215
1.199
0.924
0.912
0.898
MeO
O
O
OMe
O
N
H
nBu
N
4t
1.00
0.98
1.01
2.97
1.02
1.01
1.00
0.96
5.98
2.03
2.08
1.91
3.03
f1 (ppm)

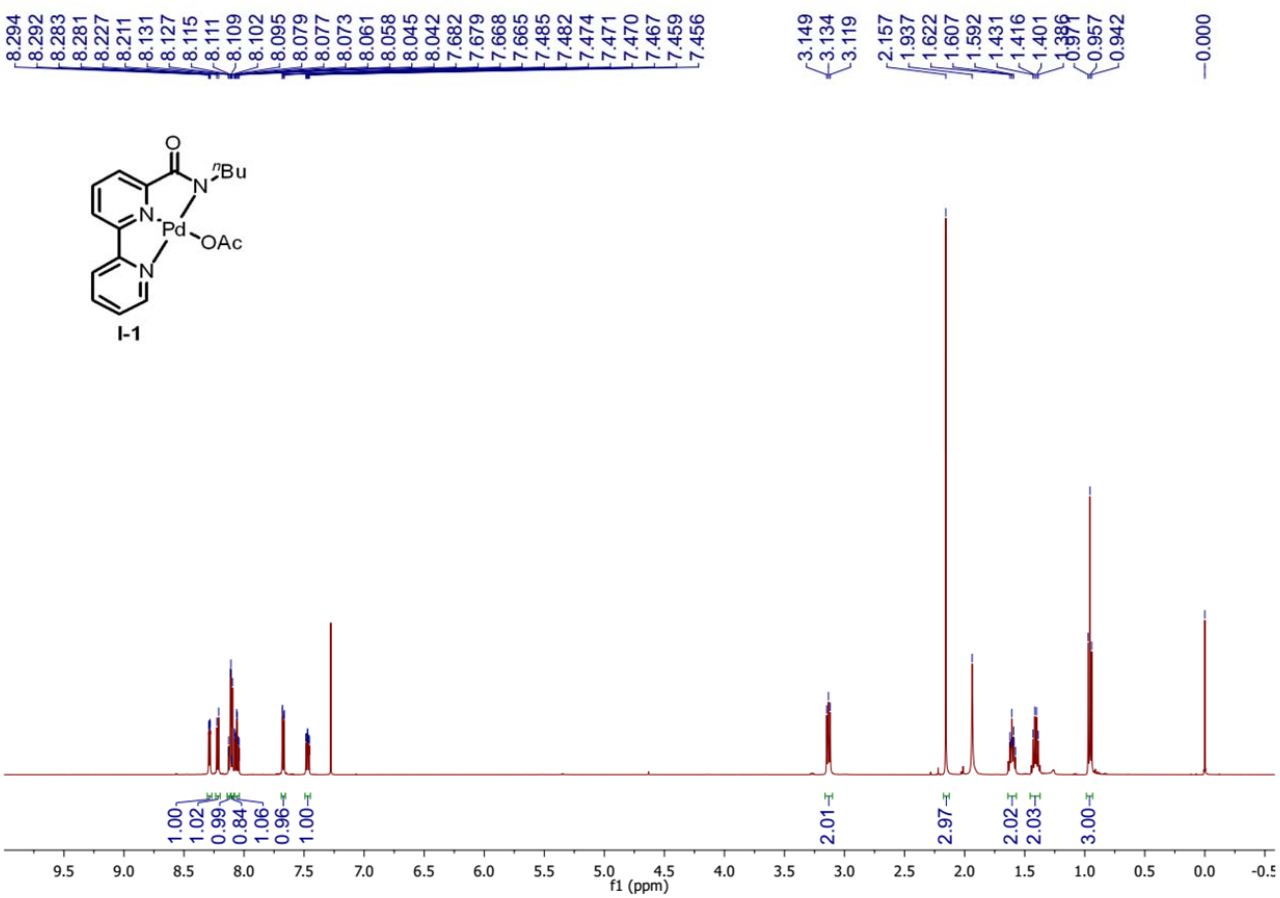

165.572
163.596
155.342
153.865
148.963
148.167
141.967
139.210
138.301
134.937
133.808
130.753
128.964
126.591
123.456
121.478
77.254
77.000
76.745
52.449
38.802
31.590
20.006
13.634
MeO
O
O
OMe
O
N
H
nBu
N
4t
f1 (ppm)

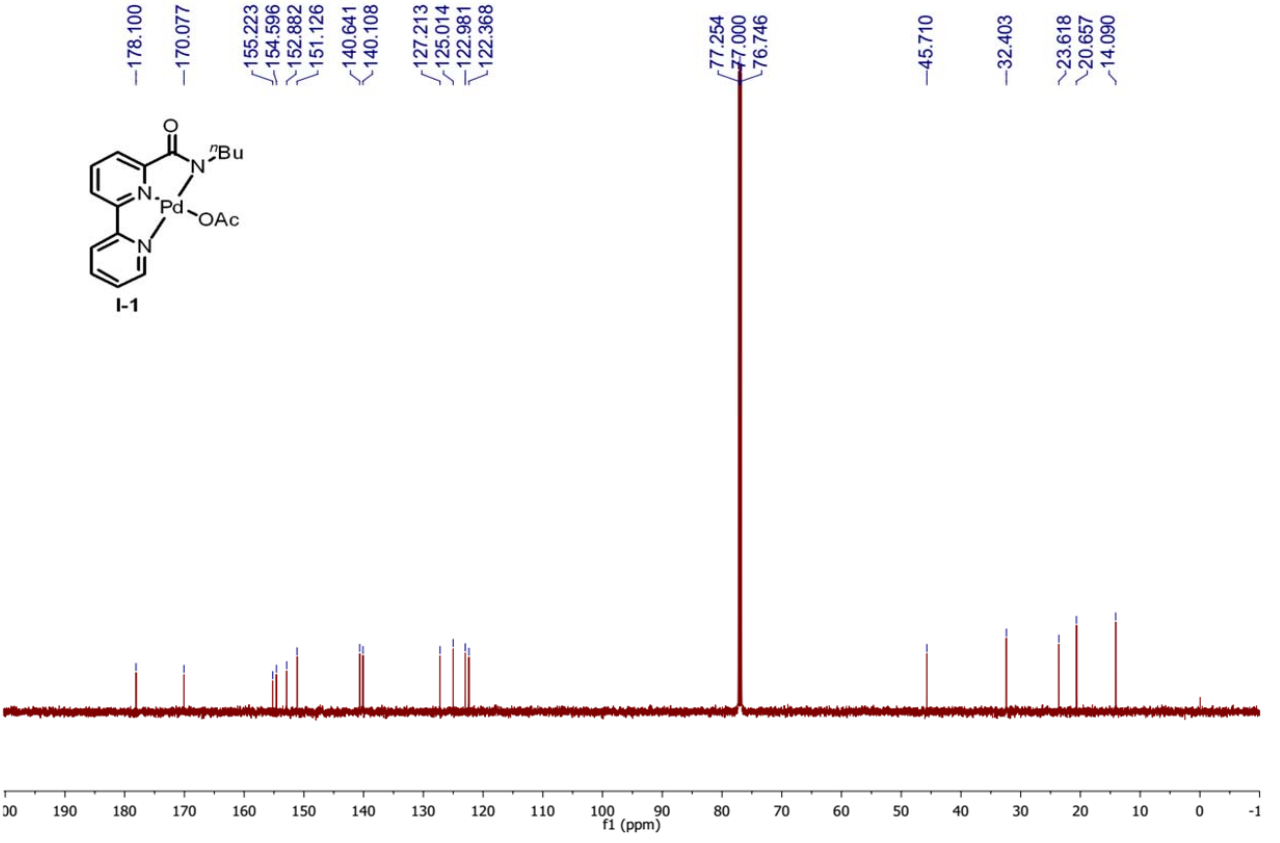

8.804
8.801
8.794
8.791
8.353
8.349
8.219
8.111
7.971
7.356
7.260
6.850
6.840
3.288
3.274
3.260
3.246
1.500
1.486
1.471
1.466
1.456
1.441
1.370
1.355
1.340
1.324
1.310
1.296
0.971
0.956
0.942
-0.000
Cl
N
O
N
H
nBu
4u
1.00
0.97
0.99
1.00
1.03
1.01
1.02
1.00
0.99
0.96
2.05
2.00
2.02
3.01
f1 (ppm)

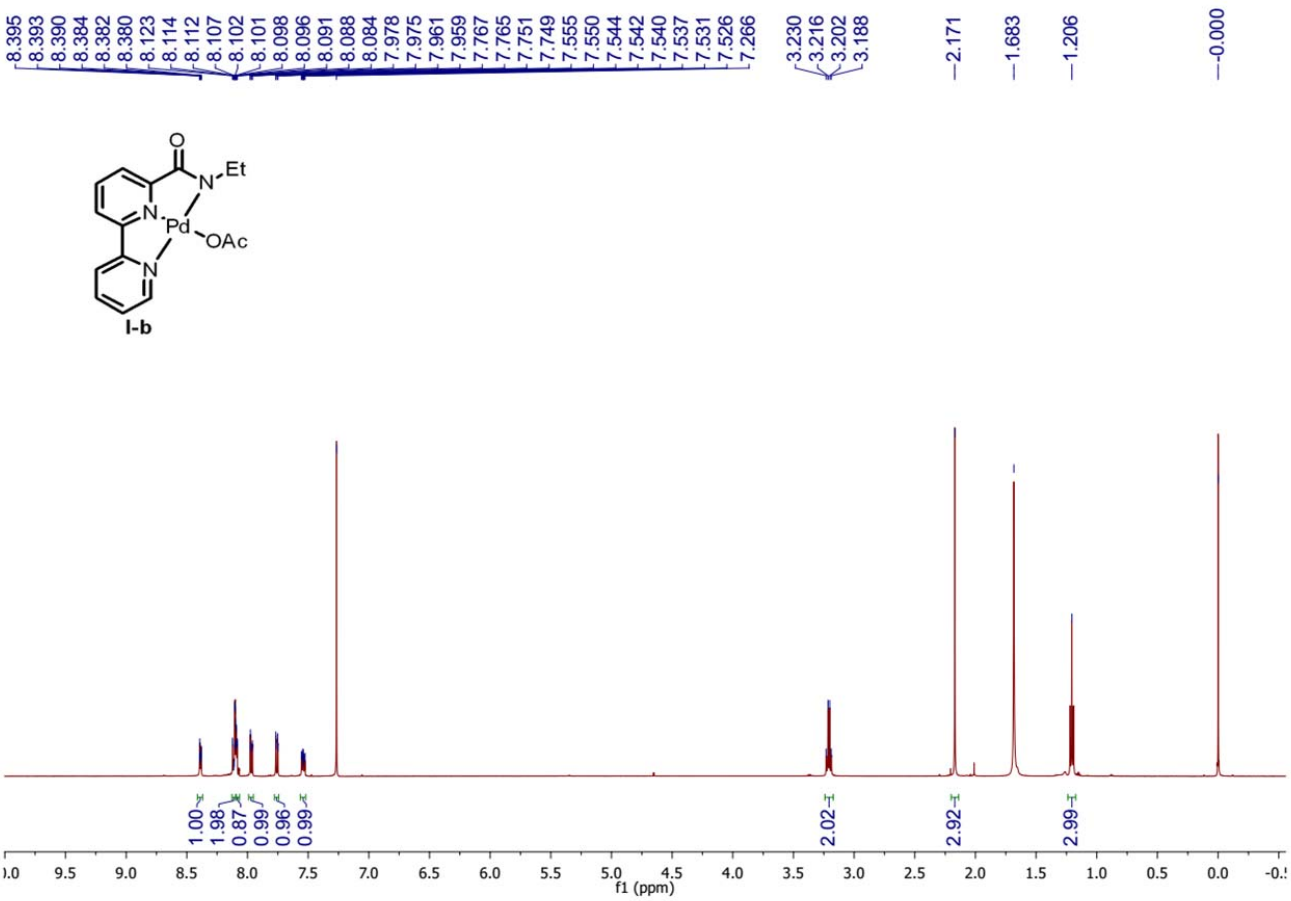

163.465
155.152
149.281
148.919
138.756
138.409
135.635
131.987
126.590
123.638
123.568
121.680
77.254
77.000
76.745
38.925
31.604
20.077
13.712
Cl
N
O
N
H
nBu
4u
f1 (ppm)

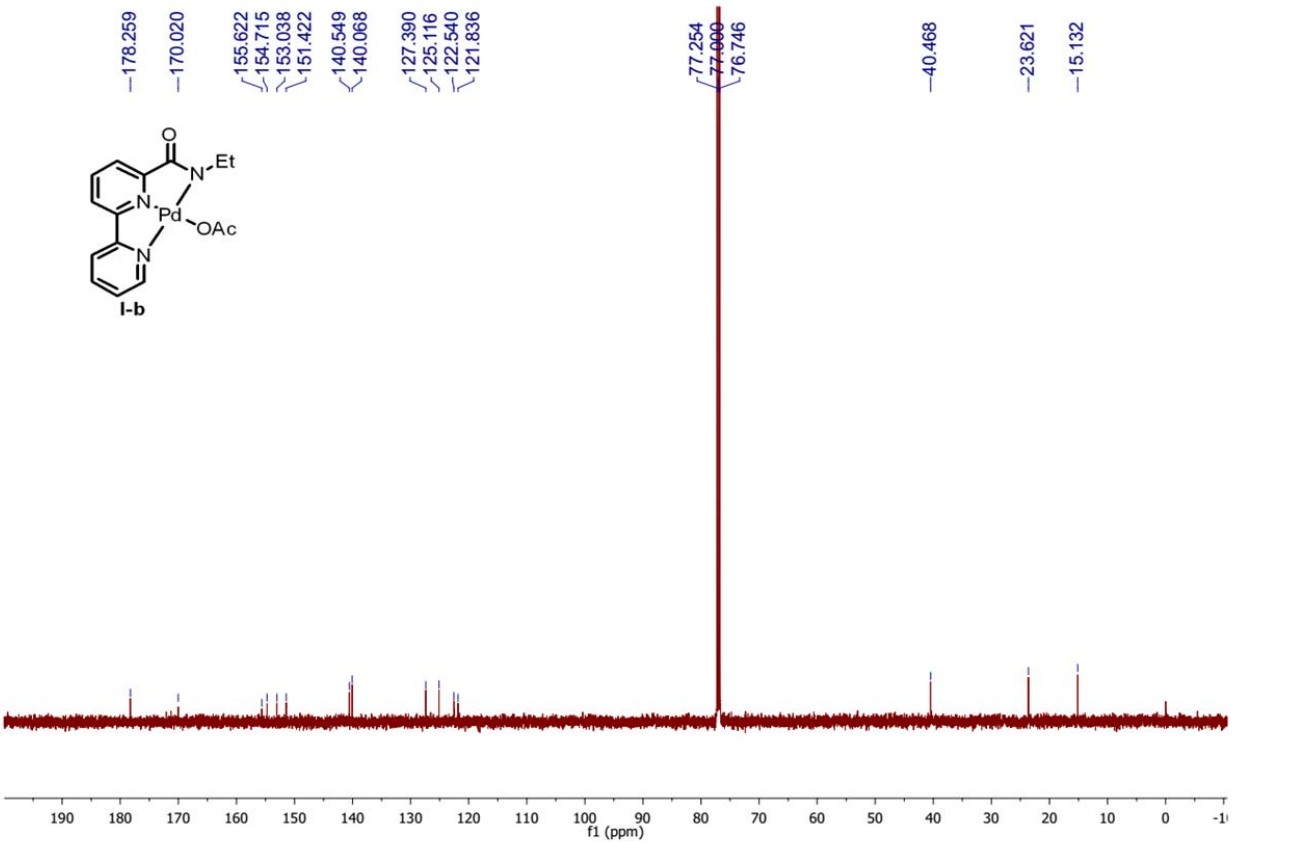

8.709
8.706
8.700
8.697
7.997
7.995
7.935
7.413
7.407
7.398
7.358
7.287
7.285
3.318
3.304
3.291
3.277
1.519
1.505
1.500
1.490
1.486
1.476
1.460
1.371
1.356
1.341
1.326
1.311
0.951
0.936
0.000
nBu
4v
1.00
1.02
1.02
1.05
0.99
1.07
0.95
0.94
0.98
0.96
2.05
1.99
2.03
3.00
f1 (ppm)


163.991
155.936
154.702
148.711
148.580
141.592
139.544
137.973
129.880
127.231
126.650
126.442
126.006
123.223
121.354
77.255
77.000
76.746
38.907
31.609
20.058
13.759
nBu
4v
f1 (ppm)


8.294
8.292
8.283
8.281
8.227
8.211
8.131
8.127
8.115
8.111
8.109
8.102
8.095
8.079
8.077
8.073
8.061
8.058
8.045
8.042
7.682
7.679
7.668
7.665
7.485
7.482
7.474
7.471
7.470
7.467
7.459
7.456
3.149
3.134
3.119
2.157
1.937
1.622
1.607
1.592
1.431
1.416
1.401
0.957
0.942
0.000
nBu
N
Pd
OAc
I-1
1.00
1.02
0.99
0.84
1.06
0.96
1.00
2.01
2.97
2.02
2.03
3.00
f1 (ppm)


178.100
170.077
155.223
154.596
152.882
151.126
140.641
140.108
127.213
125.014
122.981
122.368
77.254
77.000
76.746
45.710
32.403
23.618
20.657
14.090
nBu
N
Pd
OAc
I-1
f1 (ppm)


8.395
8.393
8.390
8.384
8.382
8.380
8.123
8.114
8.112
8.107
8.102
8.101
8.098
8.096
8.091
8.088
8.084
7.978
7.975
7.961
7.959
7.767
7.765
7.751
7.749
7.555
7.550
7.544
7.542
7.540
7.537
7.531
7.526
7.266
3.230
3.216
3.202
3.188
2.171
1.683
1.206
0.000
O
N
Et
N
Pd
OAc
N
I-b
1.00
1.98
0.87
0.99
0.96
0.99
2.02
2.92
2.99
f1 (ppm)


178.259
170.020
155.622
154.715
153.038
151.422
140.549
140.068
127.390
125.116
122.540
121.836
77.254
77.000
76.746
40.468
23.621
15.132
O
N
Et
N
Pd
OAc
N
I-b
f1 (ppm)