Supporting Information

CCC Pincer Ru Complex-Catalyzed C-H Vinylation/6π-E-Cyclization of Aldimines for Constructing 4*H*-Pyrido[1,2-*a*]pyrimidines

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1. General information

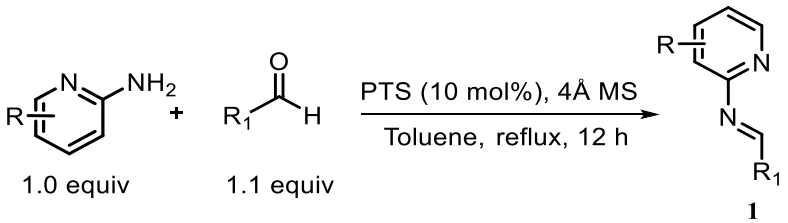
All the Ru-catalyzed C-H vinylation/6π-electrocyclization of aldimines reactions were carried out using oven-dried (120 ºC) schlenk tubes or bottles equipped with a magnetic stir bar in a glove box under argon atmosphere (H_2O < 0.5 ppm, O_2 < 0.5 ppm). 4Å molecular sieve powder was dried in a vacuum oven at 200 ℃ overnight. Unless noted otherwise, all commercial reagents and solvents were used without additional purification. Toluene and tetrahydrofuran (THF) were dried over sodium. Analytical TLC was performed on silica gel plates with F254 indicator. Visualization was accomplished with ultraviolet light (254 nm). Products purifications were conducted with column chromatography on 200-300 mesh silica gel unless specially stated.

^1H, ^{13}C and ^{19}F NMR spectra were recorded on Bruker AM-400 MHz or Bruker AM-600 MHz spectrometers. Chemical shifts (δ) were reported in ppm relative to residual solvent peak or tetramethylsilane as internal standard ($CDCl_3$: δ_H 7.26 ppm and δ_C 77.00 ppm). The following abbreviations were used to describe peak splitting patterns when appropriate: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, td = triplet of doublet, ddd = doublet of doublet of doublet, m = multiplet. Coupling constants, J, were reported in hertz unit (Hz). High-resolution mass spectral analysis (HRMS) data were collected on the Bruker Apex^{II} or Agilent 1290×1290-6560 Ion Mobility QTOF-MS with ESI resource. The FT-IR spectra were recorded on Nicolet Nexus 670 FT-IR spectrometer using neat thin film technique with potassium bromide (KBr) salt plates. The X-ray single-crystal data were recorded on Bruker APEX^{II} X-ray single crystal diffractometer.

2. Preparation of substrates

Substrates **1**, **2** and **4** were prepared according to the following procedures.

2.1. Preparation and identification of aldimines



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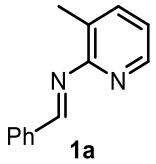
The aldimines used in this study were prepared from the corresponding aldehydes and 2-amino-3-picoline according to the literature procedure.[1-4]

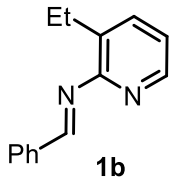
To a dry round-bottom flask equipped with a Dean-Stark apparatus were added anhydrous toluene (15 mL), 2-aminopyridine (5.0 mmol, 1.0 equiv), aldehydes (5.5 mmol, 1.1 equiv), *p*-tosylic acid (PTS, 10 mol%) and 4Å MS (1.0 g). The reaction mixture was refluxed for 12 h under Dean-Stark conditions and then cooled to room temperature. The molecular sieve was removed by filtration. The solvent was evaporated in vacuo, and the residual was purified by silica gel column chromatography to give products **1**.



1a

***N*-(3-methylpyridin-2-yl)-1-phenylmethanimine (1a)** [1]

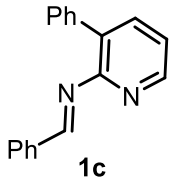
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.07 (s, 1H), 8.30 (d, *J* = 4.0 Hz, 1H), 8.03 – 7.97 (m, 2H), 7.52 (d, *J* = 7.4 Hz, 1H), 7.50 – 7.43 (m, 3H), 7.06 (dd, *J* = 7.3, 4.8 Hz, 1H), 2.45 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.5, 159.4, 146.1, 138.8, 136.2, 131.6, 129.3, 128.7, 128.6, 121.8, 17.3.



1b

***N*-(3-ethylpyridin-2-yl)-1-phenylmethanimine (1b)**

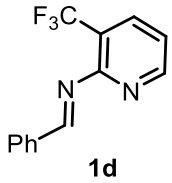
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.10 (s, 1H), 8.32 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.05 – 7.94 (m, 2H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.51 – 7.41 (m, 3H), 7.11 (dd, *J* = 7.5, 4.8 Hz, 1H), 2.89 (q, *J* = 7.5 Hz, 2H), 1.24 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.5, 159.0, 146.1, 137.2, 136.4, 134.5, 131.6, 129.4, 128.6, 122.0, 24.3, 14.6; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{14}H_{15}N_2$, *m/z*: 211.1230, found: 211.1225, Error 2.4 ppm.



1c

1-phenyl-*N*-(3-phenylpyridin-2-yl)methanimine (1c)

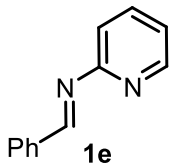
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.21 – 9.13 (m, 1H), 8.45 (dd, *J* = 4.6, 1.2 Hz, 1H), 7.87 (d, *J* = 7.5 Hz, 2H), 7.79 – 7.71 (m, 1H), 7.54 (d, *J* = 7.3 Hz, 2H), 7.43 – 7.36 (m, 5H), 7.33 (t, *J* = 7.3 Hz, 1H), 7.21 – 7.19 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 162.4, 157.8, 147.6, 138.6, 137.7, 136.1, 132.0, 131.6, 130.2, 129.5, 128.6, 127.7, 127.3, 122.0; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{18}H_{15}N_2$, *m/z*: 259.1230, found: 259.1225, Error 1.9 ppm.



1d

1-phenyl-*N*-(3-(trifluoromethyl)pyridin-2-yl)methanimine (1d)

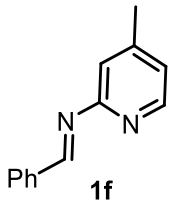
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.11 (s, 1H), 8.60 (d, *J* = 4.1 Hz, 1H), 8.02 (d, *J* = 7.0 Hz, 2H), 7.99 (d, *J* = 7.1 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.48 (t, *J* = 7.3 Hz, 2H), 7.24 (dd, *J* = 7.4, 4.8 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 164.0, 158.6, 151.8, 135.6, 135.4 (q, *J* = 5.0 Hz), 132.5, 130.0, 128.8, 125.2 (q, *J* = 270.9 Hz), 120.6 (q, *J* = 731.6 Hz), 121.0; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -61.1; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{13}H_{10}F_3N_2$, *m/z*: 251.0791, found: 251.0784, Error 2.8 ppm.



1e

1-phenyl-N-(pyridin-2-yl)methanimine (1e) [1]

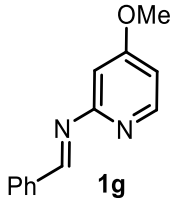
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.15 (s, 1H), 8.50 (dd, *J* = 4.7, 1.0 Hz, 1H), 8.02 – 7.95 (m, 2H), 7.77 – 7.74 (m, 1H), 7.54 – 7.45 (m, 3H), 7.34 (d, *J* = 7.9 Hz, 1H), 7.21 – 7.15 (m, 1H).



1f

***N*-(4-methylpyridin-2-yl)-1-phenylmethanimine (1f)** [1]

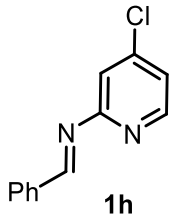
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.14 (s, 1H), 8.35 (d, *J* = 4.8 Hz, 1H), 8.07 – 7.86 (m, 2H), 7.48 (d, *J* = 6.6 Hz, 3H), 7.16 (s, 1H), 7.00 (d, *J* = 4.3 Hz, 1H), 2.39 (s, 3H).



1g

***N*-(4-methoxypyridin-2-yl)-1-phenylmethanimine (1g)** [1]

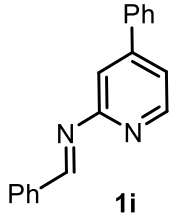
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.30 (d, *J* = 5.7 Hz, 1H), 7.98 (d, *J* = 6.6 Hz, 2H), 7.48 (d, *J* = 7.4 Hz, 3H), 6.86 (d, *J* = 2.4 Hz, 1H), 6.73 (dd, *J* = 5.7, 2.4 Hz, 1H), 3.89 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 167.4, 163.0, 162.9, 149.6, 135.8, 131.9, 129.4, 128.7, 109.1, 104.7, 55.3.



1h

***N*-(4-chloropyridin-2-yl)-1-phenylmethanimine (1h)**

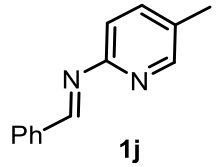
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.12 (s, 1H), 8.39 (s, 1H), 7.98 (d, *J* = 7.2 Hz, 2H), 7.49 (d, *J* = 7.1 Hz, 3H), 7.35 (s, 1H), 7.19 (d, *J* = 4.3 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 164.1, 162.4, 149.5, 145.4, 135.5, 132.3, 129.7, 128.8, 122.0, 120.0; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{12}H_{10}ClN_2$, *m/z*: 217.0527, found: 217.0523, Error 1.8 ppm.



1i

1-phenyl-*N*-(4-phenylpyridin-2-yl)methanimine (1i)

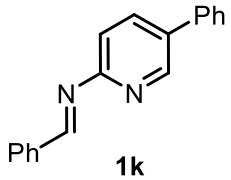
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.23 (s, 1H), 8.74 (d, *J* = 2.3 Hz, 1H), 8.02 (dd, *J* = 7.8, 1.4 Hz, 2H), 7.97 (dd, *J* = 8.2, 2.5 Hz, 1H), 7.66 – 7.60 (m, 2H), 7.55 – 7.47 (m, 5H), 7.45 – 7.39 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 162.7, 160.0, 147.3, 137.5, 136.5, 135.9, 134.9, 132.0, 129.5, 129.1, 128.8, 128.0, 126.9, 119.9; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{18}H_{15}N_2$, *m/z*: 259.1230, found: 259.1225, Error 1.9 ppm.



1j

***N*-(5-methylpyridin-2-yl)-1-phenylmethanimine (1j)** [2]

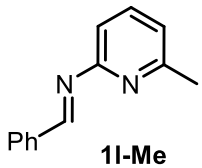
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.16 (s, 1H), 8.31 (s, 1H), 7.98 (d, *J* = 6.5 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.51 – 7.43 (m, 3H), 7.24 (d, *J* = 8.0 Hz, 1H), 2.34 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.9, 158.8, 148.9, 138.7, 136.0, 131.4, 129.4, 129.3, 128.7, 119.4, 18.0.



1k

1-phenyl-*N*-(5-phenylpyridin-2-yl)methanimine (1k)

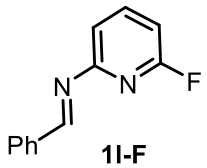
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.22 (s, 1H), 8.53 (d, *J* = 5.0 Hz, 1H), 8.01 (d, *J* = 7.1 Hz, 2H), 7.69 (d, *J* = 7.7 Hz, 2H), 7.58 (s, 1H), 7.54 – 7.46 (m, 5H), 7.44 (d, *J* = 7.1 Hz, 1H), 7.40 (d, *J* = 5.0 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 163.1, 161.7, 150.6, 149.2, 138.0, 135.9, 131.9, 129.5, 129.1, 129.1, 128.7, 127.0, 119.9, 117.7; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{18}H_{15}N_2$, *m/z*: 259.1230, found: 259.1225, Error 1.9 ppm.



1l-Me

***N*-(6-methylpyridin-2-yl)-1-phenylmethanimine (1l-Me)** [2]

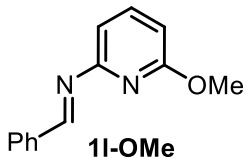
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (s, 1H), 8.04 – 7.91 (m, 2H), 7.61 (t, *J* = 7.7 Hz, 1H), 7.46 (d, *J* = 6.6 Hz, 3H), 7.09 (d, *J* = 7.8 Hz, 1H), 7.02 (d, *J* = 7.5 Hz, 1H), 2.57 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.6, 160.9, 157.8, 138.2, 135.9, 131.68, 129.4, 128.6, 121.2, 115.7, 24.3.



1l-F

***N*-(6-fluoropyridin-2-yl)-1-phenylmethanimine (1l-F)**

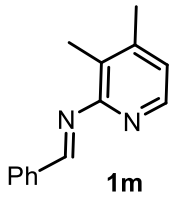
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 7.98 (d, *J* = 6.6 Hz, 2H), 7.82 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.56 – 7.41 (m, 3H), 7.24 (dd, *J* = 7.5, 1.3 Hz, 1H), 6.88 – 6.76 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ163.9, 162.8 (d, *J* = 240.5 Hz), 159.3 (d, *J* = 11.0 Hz), 142.5 (d, *J* = 8.0 Hz), 135.5, 132.2, 129.6, 128.8, 117.3 (d, *J* = 4.5 Hz), 107.0 (d, *J* = 37.0 Hz).



1l-OMe

***N*-(6-methoxypyridin-2-yl)-1-phenylmethanimine (1l-OMe)**

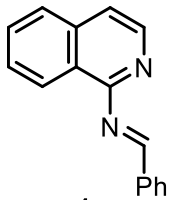
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.22 (s, 1H), 7.98 (dd, *J* = 7.1, 2.1 Hz, 2H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.54 – 7.42 (m, 3H), 6.93 (d, *J* = 7.4 Hz, 1H), 6.64 (d, *J* = 8.1 Hz, 1H), 3.98 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.4, 162.0, 158.6, 140.2, 136.0, 131.7, 129.4, 128.7, 112.5, 108.9, 53.2.



1m

***N*-(3,4-dimethylpyridin-2-yl)-1-phenylmethanimine (1m)**

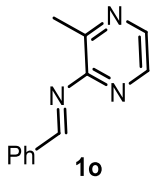
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.05 (s, 1H), 8.17 (d, *J* = 4.8 Hz, 1H), 8.03 – 7.96 (m, 2H), 7.45 (d, *J* = 6.4 Hz, 3H), 6.95 (d, *J* = 4.8 Hz, 1H), 2.40 (s, 3H), 2.29 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.4, 159.1, 147.5, 145.3, 136.3, 131.4, 129.2, 128.6, 127.4, 123.4, 19.5, 13.1. **HRMS (ESI)** calcd for $[M+H]^+$ $C_{14}H_{15}N_2$, *m/z*: 221.1230, found: 221.1225, Error 2.3 ppm.



1n

***N*-(isoquinolin-1-yl)-1-phenylmethanimine (1n)**

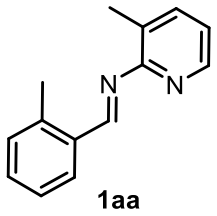
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.18 (s, 1H), 8.63 (d, *J* = 8.3 Hz, 1H), 8.33 (d, *J* = 5.7 Hz, 1H), 8.13 – 8.04 (m, 2H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.51 – 7.43 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.2, 159.5, 141.4, 137.3, 135.9, 132.0, 130.3, 129.6, 128.6, 126.8, 126.0, 125.9, 124.5, 119.5; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{16}H_{13}N_2$, *m/z*: 233.1073, found: 233.1068, Error 2.1 ppm.



1o

***N*-(3-methylpyrazin-2-yl)-1-phenylmethanimine (1o)**

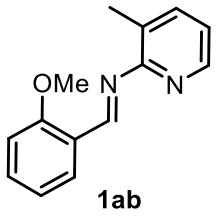
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.07 (s, 1H), 8.33 (d, *J* = 2.4 Hz, 1H), 8.24 (d, *J* = 2.3 Hz, 1H), 8.01 (d, *J* = 7.2 Hz, 2H), 7.53 (t, *J* = 7.1 Hz, 1H), 7.49 (t, *J* = 7.3 Hz, 2H), 2.72 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 163.8, 155.2, 150.8, 141.7, 140.5, 135.7, 132.3, 129.6, 128.7, 20.6; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{12}H_{12}N_3$, *m/z*: 198.1026, found: 198.1022, Error 2.0 ppm.



1aa

***N*-(3-methylpyridin-2-yl)-1-(*o*-tolyl)methanimine (1aa)** [1]

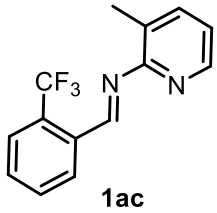
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.36 (s, 1H), 8.29 (dd, *J* = 4.7, 1.3 Hz, 1H), 8.14 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.47 (dd, *J* = 7.4, 0.6 Hz, 1H), 7.32 (td, *J* = 7.4, 1.6 Hz, 1H), 7.27 (t, *J* = 7.0 Hz, 1H), 7.19 (d, *J* = 7.4 Hz, 1H), 7.02 (dd, *J* = 7.4, 4.8 Hz, 1H), 2.65 (s, 3H), 2.43 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.4, 159.7, 146.0, 139.4, 138.5, 134.0, 131.0, 130.9, 129.0, 128.5, 126.0, 121.5, 19.8, 17.4.



1ab

1-(2-methoxyphenyl)-*N*-(3-methylpyridin-2-yl)methanimine (1ab)

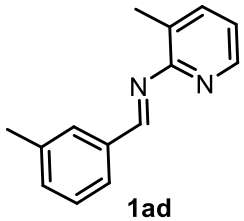
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.48 (s, 1H), 8.29 (d, *J* = 24.2 Hz, 2H), 7.48 (d, *J* = 42.5 Hz, 2H), 7.00 (d, *J* = 57.3 Hz, 3H), 3.89 (s, 3H), 2.44 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 160.4, 160.2, 157.7, 146.2, 138.6, 133.1, 128.5, 127.9, 124.9, 121.4, 120.7, 111.2, 55.5, 17.5; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{14}H_{15}N_2O$, *m/z*: 227.1179, found: 227.1176, Error 1.3 ppm.



1ac

***N*-(3-methylpyridin-2-yl)-1-(2-(trifluoromethyl)phenyl)methanimine (1ac)**

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.46 (d, *J* = 1.3 Hz, 1H), 8.53 (d, *J* = 7.8 Hz, 1H), 8.33 (d, *J* = 4.2 Hz, 1H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.56 (dd, *J* = 14.7, 7.4 Hz, 2H), 7.10 (dd, *J* = 7.3, 4.9 Hz, 1H), 2.46 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.00, 157.71, 146.34, 138.89, 134.22, 131.92, 130.88, 130.3 (q, *J* = 30.9 Hz), 128.91, 128.80, 125.7 (q, *J* = 5.4 Hz), 124.1, 122.32, 17.31; **^{19}F NMR** (565 MHz, $CDCl_3$) δ -56.8; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{14}H_{12}F_3N_2$, *m/z*: 265.0947, found: 265.0940, Error 2.6 ppm.

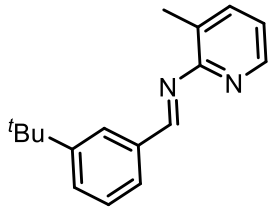


1ad

***N*-(3-methylpyridin-2-yl)-1-(*m*-tolyl)methanimine (1ad)** [2]

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.36 – 8.24 (m, 1H), 7.83 (s, 1H), 7.77 (d, *J* = 7.5 Hz, 1H), 7.51 (dd, *J* = 7.4, 0.6 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.29 (d, *J* = 7.5 Hz, 1H), 7.05 (dd, *J* = 7.4, 4.8

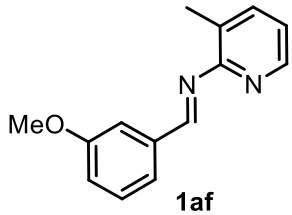
Hz, 1H), 2.45 (s, 3H), 2.40 (d, *J* = 7.6 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.8, 159.5, 146.1, 138.7, 138.28, 136.2, 132.5, 129.5, 128.6, 128.5, 126.9, 121.6, 21.2, 17.3.



1ae

1-(3-(tert-butyl)phenyl)-*N*-(3-methylpyridin-2-yl)methanimine (1ae)

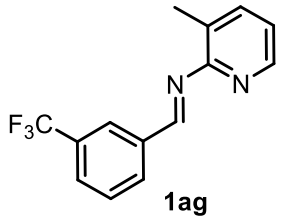
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.06 (s, 1H), 8.31 (d, *J* = 3.7 Hz, 1H), 8.03 (s, 1H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.55 – 7.51 (m, 2H), 7.42 (d, *J* = 7.7 Hz, 1H), 7.08 (dd, *J* = 7.4, 4.8 Hz, 1H), 2.46 (s, 3H), 1.38 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 162.2, 159.7, 151.6, 146.1, 138.8, 136.0, 128.9, 128.6, 128.4, 126.6, 126.5, 121.7, 34.7, 31.3, 17.4; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{17}H_{21}N_2$, *m/z*: 253.1699, found: 253.1696, Error 1.2 ppm.



1af

1-(3-methoxyphenyl)-*N*-(3-methylpyridin-2-yl)methanimine (1af) [2]

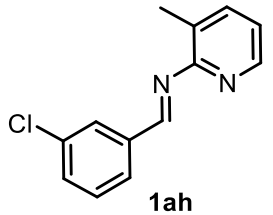
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.30 (d, *J* = 4.3 Hz, 1H), 7.61 (s, 1H), 7.53 (d, *J* = 7.3 Hz, 2H), 7.37 (t, *J* = 7.8 Hz, 1H), 7.07 (dd, *J* = 7.4, 4.8 Hz, 1H), 7.04 (dd, *J* = 8.2, 2.4 Hz, 1H), 3.87 (s, 3H), 2.45 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.5, 159.8, 159.4, 146.1, 138.8, 137.6, 129.6, 128.7, 122.7, 121.8, 118.2, 112.8, 55.3, 17.3.



1ag

***N*-(3-methylpyridin-2-yl)-1-(3-(trifluoromethyl)phenyl)methanimine (1ag)**

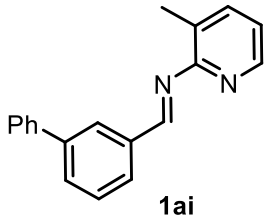
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.13 (d, *J* = 2.5 Hz, 1H), 8.29 (d, *J* = 9.9 Hz, 2H), 8.13 (d, *J* = 4.6 Hz, 1H), 7.76 – 7.69 (m, 1H), 7.63 – 7.48 (m, 2H), 7.15 – 7.04 (m, 1H), 2.46 (d, *J* = 3.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.8, 158.6, 146.1, 139.0, 136.9, 132.5, 131.2 (q, *J* = 32.4 Hz), 129.2, 129.1, 127.8, 125.6, 123.9 (q, *J* = 32.4 Hz) 122.3, 17.2; **^{19}F NMR** (565 MHz, $CDCl_3$) δ -62.8; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{14}H_{12}F_3N_2$, *m/z*: 265.0947, found: 265.0941, Error 2.3 ppm.



1ah

1-(3-chlorophenyl)-*N*-(3-methylpyridin-2-yl)methanimine (1ah)

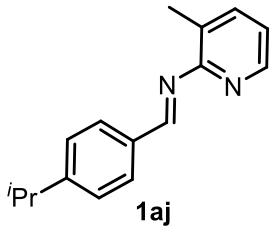
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.34 – 8.25 (m, 1H), 8.03 (s, 1H), 7.80 (d, *J* = 7.6 Hz, 1H), 7.58 – 7.48 (m, 1H), 7.48 – 7.41 (m, 1H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.08 (dd, *J* = 7.4, 4.8 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.9, 158.7, 146.1, 138.9, 138.0, 134.8, 131.4, 129.9, 129.0, 128.5, 127.9, 122.2, 17.3; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{16}H_{19}N_2$, *m/z*: 231.0684, found: 231.0679, Error 2.2 ppm.



1ai

1-([1,1'-biphenyl]-3-yl)-*N*-(3-methylpyridin-2-yl)methanimine (1ai)

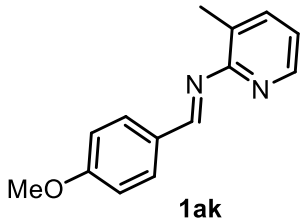
^{1}H NMR δ 9.12 (s, 1H), 8.28 (dd, *J* = 4.7, 1.3 Hz, 1H), 8.22 (s, 1H), 7.93 (d, *J* = 7.7 Hz, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.61 – 7.57 (m, 2H), 7.49 – 7.41 (m, 2H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.3 Hz, 1H), 6.98 (dd, *J* = 7.4, 4.8 Hz, 1H), 2.42 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.3, 159.1, 145.9, 141.4, 140.2, 138.6, 136.6, 130.1, 128.9, 128.6, 128.6, 128.1, 127.7, 127.4, 126.9, 121.7, 17.2; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{19}H_{17}N_2$, *m/z*: 273.1386, found: 273.1382, Error 1.5 ppm.



1aj

1-(4-isopropylphenyl)-*N*-(3-methylpyridin-2-yl)methanimine (1aj)

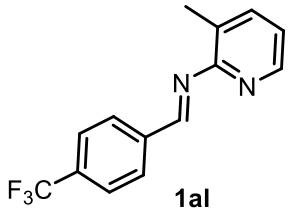
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.34 – 8.25 (m, 1H), 7.93 (d, *J* = 8.1 Hz, 2H), 7.51 (d, *J* = 7.4 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.05 (dd, *J* = 7.4, 4.8 Hz, 1H), 3.03 – 2.90 (m, 1H), 2.44 (s, 3H), 1.28 (d, *J* = 6.9 Hz, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.4, 159.7, 153.0, 146.0, 138.7, 134.1, 129.5, 128.6, 126.8, 121.5, 34.2, 23.7, 17.4; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{16}H_{19}N_2$, *m/z*: 239.1543, found: 239.1538, Error 2.1 ppm.



1ak

1-(4-methoxyphenyl)-*N*-(3-methylpyridin-2-yl)methanimine (1ak) [1]

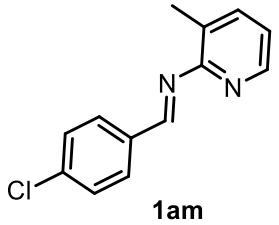
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.00 (s, 1H), 8.29 (d, *J* = 3.5 Hz, 1H), 7.95 (d, *J* = 8.7 Hz, 2H), 7.52 (d, *J* = 7.3 Hz, 1H), 7.05 (dd, *J* = 7.4, 4.8 Hz, 1H), 6.98 (d, *J* = 8.7 Hz, 2H), 3.86 (s, 3H), 2.44 (s, 3H).



1al

***N*-(3-methylpyridin-2-yl)-1-(4-(trifluoromethyl)phenyl)methanimine (1al)** [1]

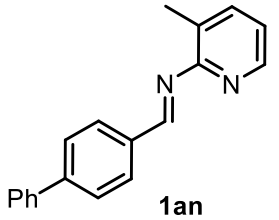
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.12 (s, 1H), 8.29 (d, *J* = 4.4 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 2H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 7.4 Hz, 1H), 7.06 (dd, *J* = 7.3, 4.8 Hz, 1H), 2.43 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.6, 158.4, 146.0, 139.2, 138.9, 132.7 (q, *J* = 32.3 Hz), 129.3, 129.2, 125.4 (q, *J* = 3.5 Hz), 123.8 (q, *J* = 270.8 Hz), 122.3, 17.1.



1am

1-(4-chlorophenyl)-*N*-(3-methylpyridin-2-yl)methanimine (1ab) [1]

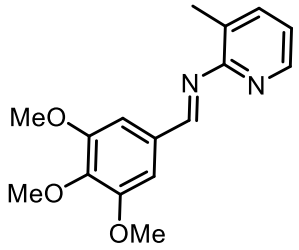
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.29 (d, *J* = 4.4 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 2H), 7.51 (d, *J* = 7.3 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.14 – 6.96 (m, 1H), 2.44 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 160.0, 158.9, 146.1, 138.8, 137.6, 134.7, 130.4, 128.9, 128.9, 122.0, 17.3.



1an

1-([1,1'-biphenyl]-4-yl)-*N*-(3-methylpyridin-2-yl)methanimine (1an)

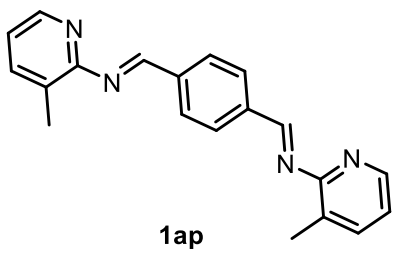
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.11 (s, 1H), 8.30 (d, *J* = 4.5 Hz, 1H), 8.05 (d, *J* = 8.2 Hz, 2H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.62 (d, *J* = 7.3 Hz, 2H), 7.50 (d, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.05 (dd, *J* = 7.1, 5.0 Hz, 1H), 2.46 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.0, 159.4, 146.1, 144.2, 140.2, 138.7, 135.2, 129.8, 128.8, 128.8, 127.8, 127.3, 127.1, 121.7, 17.4.



1ao

***N*-(3-methylpyridin-2-yl)-1-(3,4,5-trimethoxyphenyl)methanimine (1ao)**

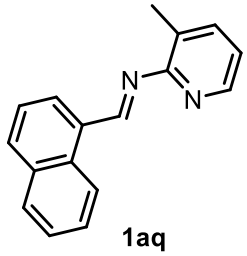
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.96 (s, 1H), 8.30 (s, 1H), 7.54 (s, 1H), 7.27 (s, 2H), 7.08 (s, 1H), 3.94 (s, 9H), 2.46 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.1, 159.4, 153.4, 146.1, 141.2, 138.8, 131.7, 128.5, 121.7, 106.3, 60.9, 56.1, 17.3; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{16}H_{19}N_2O_3$, *m/z*: 287.1390, found: 287.1384, Error 2.5 ppm.



1ap

1,1'-(1,4-phenylene)bis(*N*-(3-methylpyridin-2-yl)methanimine) (1ap) [3]

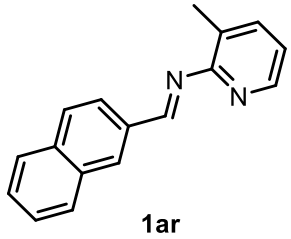
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.15 (s, 2H), 8.32 (d, *J* = 4.3 Hz, 2H), 8.11 (s, 4H), 7.55 (d, *J* = 7.3 Hz, 2H), 7.15 – 7.05 (m, 2H), 2.48 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 160.7, 159.1, 146.1, 139.0, 138.9, 129.6, 129.1, 122.1, 17.3.



1aq

***N*-(3-methylpyridin-2-yl)-1-(naphthalen-1-yl)methanimine (1aq)** [1]

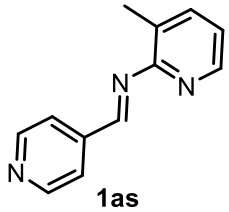
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.70 (s, 1H), 9.35 (d, *J* = 8.6 Hz, 1H), 8.36 (d, *J* = 3.7 Hz, 1H), 8.19 (d, *J* = 7.0 Hz, 1H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.71 – 7.62 (m, 1H), 7.61 – 7.53 (m, 3H), 7.11 (dd, *J* = 7.4, 4.8 Hz, 1H), 2.54 (s, 3H).



1ar

***N*-(3-methylpyridin-2-yl)-1-(naphthalen-2-yl)methanimine (1ar)** [1]

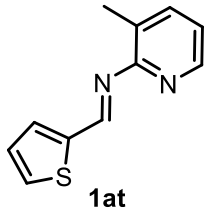
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.23 (s, 1H), 8.33 (dd, *J* = 4.7, 1.3 Hz, 1H), 8.29 – 8.25 (m, 2H), 7.94 – 7.88 (m, 3H), 7.57 – 7.51 (m, 3H), 7.09 (dd, *J* = 7.4, 4.8 Hz, 1H), 2.50 (s, 3H).



1as

***N*-(3-methylpyridin-2-yl)-1-(pyridin-4-yl)methanimine (1as)** [4]

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.07 (s, 1H), 8.79 – 8.69 (m, 2H), 8.29 (d, *J* = 4.0 Hz, 1H), 7.83 – 7.71 (m, 2H), 7.51 (d, *J* = 7.3 Hz, 1H), 7.12 – 7.05 (m, 1H), 2.44 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.9, 157.6, 150.1, 145.8, 142.3, 138.7, 129.1, 122.4, 122.2, 16.8.

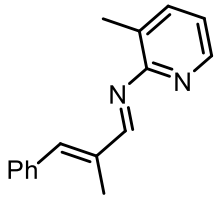


1at

***N*-(3-methylpyridin-2-yl)-1-(thiophen-2-yl)methanimine (1at)** [1]

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.23 (d, *J* = 0.5 Hz, 1H), 8.27 (dd, *J* = 4.7, 1.2 Hz, 1H), 7.56 (dd, *J* = 3.6, 0.9 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.12 (dd, *J* = 5.0, 3.7 Hz, 1H), 7.05 (dd, *J* = 7.4, 4.8 Hz, 1H), 2.44 (s,

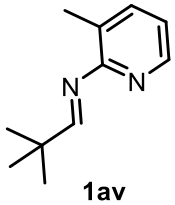
3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.7, 154.1, 146.0, 143.2, 138.8, 133.3, 130.8, 128.9, 127.8, 121.8, 17.3.



1au

2-methyl-*N*-(3-methylpyridin-2-yl)-3-phenylprop-2-en-1-imine (1au)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (s, 1H), 8.28 (dd, *J* = 4.8, 1.3 Hz, 1H), 7.49 (dd, *J* = 12.0, 4.2 Hz, 3H), 7.40 (dd, *J* = 10.4, 4.8 Hz, 2H), 7.30 (t, *J* = 7.3 Hz, 1H), 7.12 (s, 1H), 7.03 (dd, *J* = 7.4, 4.8 Hz, 1H), 2.40 (s, 3H), 2.32 (d, *J* = 0.9 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.4, 159.9, 146.1, 143.1, 138.5, 137.5, 136.5, 129.6, 128.3, 128.3, 128.1, 121.3, 17.3, 12.9; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{16}H_{17}N_2$, *m/z*: 237.1386, found: 237.1380, Error 2.5 ppm.

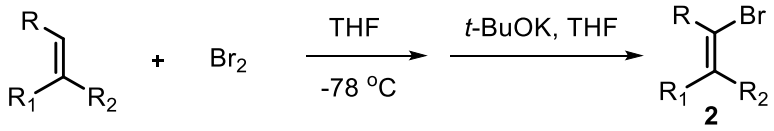


1av

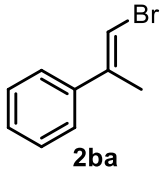
2,2-dimethyl-*N*-(3-methylpyridin-2-yl)propan-1-imine (1av) [1]

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (dd, *J* = 4.8, 1.2 Hz, 1H), 8.15 (s, 1H), 7.50 – 7.42 (m, 1H), 7.02 (dd, *J* = 7.4, 4.9 Hz, 1H), 2.30 (s, 3H), 1.23 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 174.8, 160.6, 146.1, 138.4, 126.7, 121.0, 37.1, 26.7, 17.2.

2.2 Preparation and identification of vinyl bromides



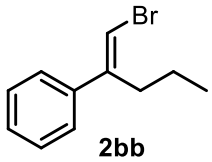
At -78 °C, a solution of the above olefin in THF (20 mL) was added Br_2 (12 mmol, 1.2 equiv), after 5 mins, the reaction was quenched with saturated $Na_2S_2O_3$ aqueous solution. The residue was washed with brine, dried over anhydrous Na_2SO_4. The solution was added potassium tert-butoxide (15 mmol, 1.5 equiv). After stirred for 3 h, the mixture was washed by water and brine successively. The organic layer was dried over anhydrous Na_2SO_4 and concentrated carefully to get corresponding vinyl bromine **2**.



2ba

(1-bromoprop-1-en-2-yl)benzene (2ba) [5]

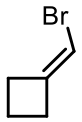
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.33 (d, *J* = 4.3 Hz, 4H), 7.34 – 7.27 (m, 1H), 6.44 (s, 1H), 2.22 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 141.5, 140.9, 128.5, 127.8, 126.0, 105.4, 19.6



2bb

(1-bromopent-1-en-2-yl)benzene (2bb) [6]

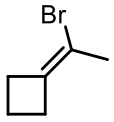
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.23 (m, 5H), 6.34 (s, 1H), 2.73 – 2.62 (m, 2H), 1.53 – 1.36 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.3, 140.3, 128.5, 127.7, 126.6, 105.1, 35.0, 20.6, 13.7.



2bd

(bromomethylene)cyclobutene (2bd)

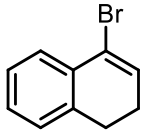
^{1}H NMR (400 MHz, $CDCl_3$) δ 5.80 – 5.71 (m, 1H), 3.51 (d, *J* = 10.4 Hz, 2H), 2.69 – 2.61 (m, 4H), 2.05 – 1.91 (m, 2H), 0.93 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.2, 95.9, 31.3, 30.7, 15.7; **HRMS (ESI)** calcd for $[M+H]^+$ C_5H_8Br, *m/z*: 146.9804, found: 146.9804, Error 0 ppm.



2be

(1-bromoethylidene)cyclobutene (2be)

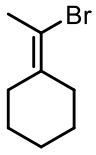
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62 (d, *J* = 8.0 Hz, 4H), 2.08 (s, 3H), 1.98 – 1.82 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.6, 110.6, 31.9, 29.31, 22.8, 14.6; **HRMS (ESI)** calcd for $[M+H]^+$ $C_6H_{10}Br$, *m/z*: 160.9960, found: 160.9960, Error 0 ppm.



2bj

4-bromo-1,2-dihydronaphthalene (2bj) [8]

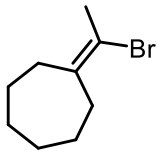
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.7 Hz, 1H), 7.21 (t, *J* = 7.4 Hz, 1H), 7.18 – 7.13 (m, 1H), 7.06 (d, *J* = 7.3 Hz, 1H), 6.40 (t, *J* = 4.8 Hz, 1H), 2.80 (t, *J* = 8.1 Hz, 2H), 2.36 – 2.27 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 136.2, 133.0, 130.6, 128.2, 127.2, 126.7, 126.4, 121.3, 27.5, 25.4.



2bk

(1-bromoethylidene)cyclohexane (2bk)

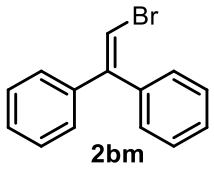
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.42 – 2.34 (m, 2H), 2.30 (s, 3H), 2.26 – 2.19 (m, 2H), 1.57 – 1.45 (m, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.3, 113.0, 35.1, 30.8, 27.4, 27.1, 26.3, 24.6; **HRMS (ESI)** calcd for $[M+H]^+$ $C_8H_{14}Br$, *m/z*: 189.0273, found: 189.0270, Error 1.6 ppm.



2bl

(1-bromoethylidene)cycloheptane (2bl)

^{1}H NMR (600 MHz, $CDCl_3$) δ 2.45 – 2.39 (m, 2H), 2.33 – 2.26 (m, 5H), 1.64 – 1.56 (m, 4H), 1.53 – 1.47 (m, 4H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 138.9, 116.0, 36.5, 31.6, 28.9, 28.8, 27.5, 26.6, 24.9; **HRMS (ESI)** calcd for $[M+H]^+$ $C_9H_{16}Br$, *m/z*: 203.0430, found: 203.0432, Error 1.0 ppm.

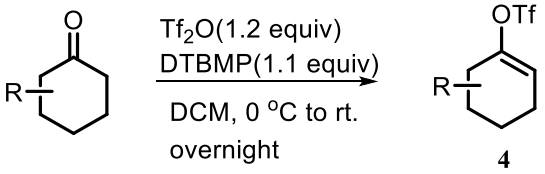


2bm

(2-bromoethene-1,1-diyl)dibenzene (2bm) [7]

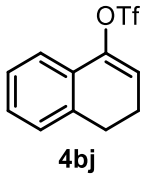
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.34 (m, 3H), 7.31 – 7.26 (m, 5H), 7.22 – 7.15 (m, 2H), 6.75 (s, 1H).

2.3 Preparation and identification of vinyl triflates



4

To a solution of ketone (10.0 mmol) in DCM (30 mL) was added 2,6-di-tert-butyl-4-methylpyridine (DTBMP, 11.0 mmol, 1.1 equiv) at 0 °C. Tf_2O (12.0 mmol, 1.2 equiv) was added dropwise. The reaction mixture was then allowed to warm to room temperature, stirred overnight and evaporated to dryness. Petroleum ether was added and the mixture was filtered to remove pyridinium triflate. The petroleum ether solution was washed with cool HCl/H_2O (1.0 M), brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel to give the resulting alkenyl triflate. Substrates **4** were prepared with this method.



4bj

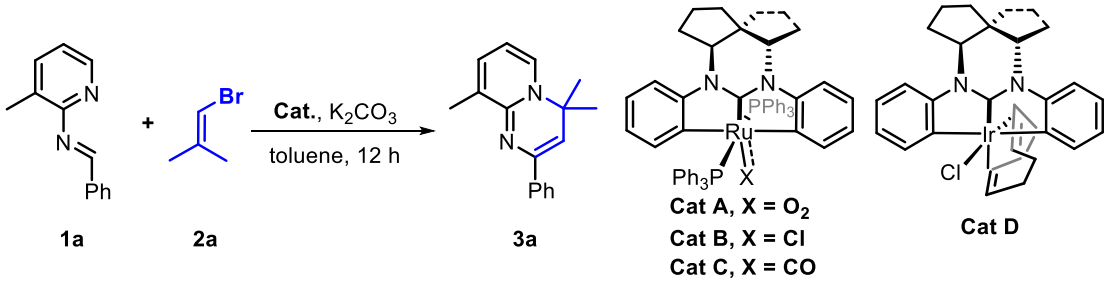
3,4-dihydronaphthalen-1-yl trifluoromethanesulfonate(4bj) [10]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.31 (m, 1H), 7.28 – 7.21 (m, 2H), 7.19 – 7.12 (m, 1H), 6.00 (t, *J* = 4.8 Hz, 1H), 2.85 (t, *J* = 8.2 Hz, 2H), 2.53 – 2.44 (m, 2H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.7.

3. Experimental procedures

3.1 Screening of reaction conditions

Table S1. Investigation of the catalysts



1a **2a** **3a**

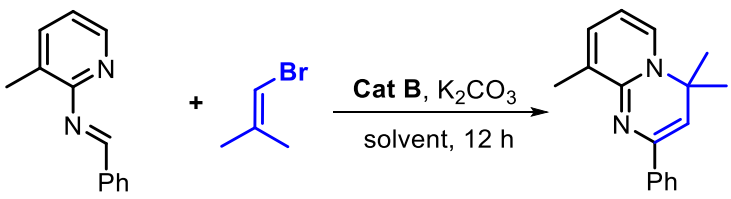
Cat A, X = O_2
Cat B, X = Cl
Cat C, X = CO

Cat D

Entry	Catalysts	Yield/%
1	A	40
2	**B**	**43**
3	C	NR
4	D	NR
5	$Ru(bpy)_3Cl_2$	NR
6	$Cp(PPh_3)_2RuCl$	NR
7	$RuCl_3$	NR
8	$Ru(acac)_3$	NR
9	RuO_2	NR
10	None	NR

[a]General conditions: **1a** (0.1 mmol), **2a** (0.2 mmol), **Cat.** (3 mol%), K_2CO_3 (0.15 mmol) and toluene (1.0 mL) at 110 °C for 12 h under argon atmosphere. Yields were determined by ^1H NMR with 1,3,5-trimethoxybenzene as internal standard.

Table S2. Investigation of the solvent



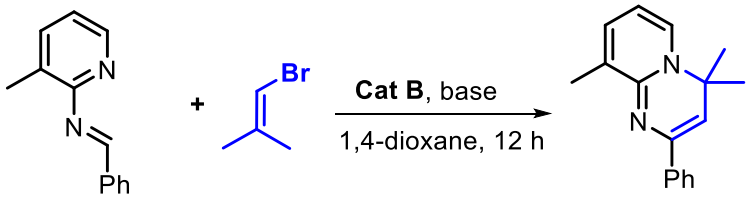
1a **2a** **3a**

Entry	Solvent	Yield/%
1	THF	48
2	**1,4-dioxane**	**51**
3	toluene	43

4	DMF	trace
5	NMP	trace
6	MeCN	12
7	DMSO	NR
8	DCE	NR

[a]General conditions: **1a** (0.1 mmol), **2a** (0.2 mmol), **Cat B** (3 mol%), K_2CO_3 (0.15 mmol) and solvent (1.0 mL) at 110 °C for 12 h under argon atmosphere. Yields were determined by ^{1}H NMR with 1,3,5-trimethoxybenzene as internal standard.

Table S3. Investigation of the bases

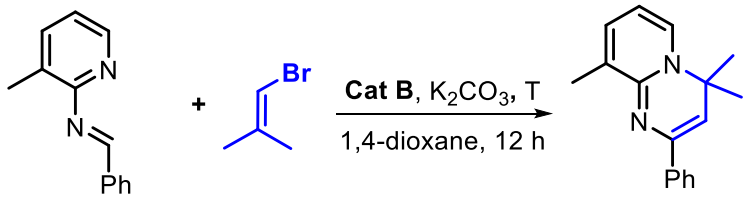


1a **2a** **3a**

Entry	Base	Yield/%
1	**K_2CO_3**	**51**
2	Na_2CO_3	trace
3	Cs_2CO_3	45
4	K_3PO_4	23
5	KO^{t}Bu	NR
6	KOH	NR
7	CH_3ONa	trace

[a]General conditions: **1a** (0.1 mmol), **2a** (0.2 mmol), **Cat B** (3 mol%), base (0.15 mmol) and 1,4-dioxane (1.0 mL) at 110 °C for 12 h under argon atmosphere. Yields were determined by ^{1}H NMR with 1,3,5-trimethoxybenzene as internal standard.

Table S4. Investigation of temperature and amount of 2a



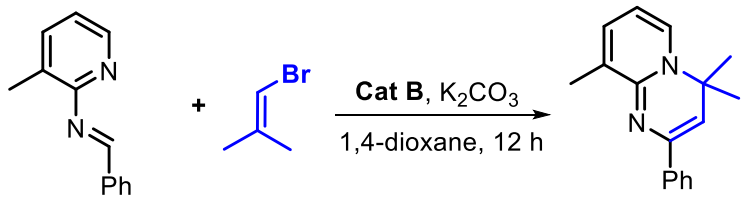
1a **2a** **3a**

Entry	T/°C	Yield/%
1	110	51
2	120	60
3	130	89
4	140	88
5 [b]	**130**	**96**

6[b,c]	130	89
7[b, d]	130	95

[a]General conditions: **1a** (0.1 mmol), **2a** (0.2 mmol), **Cat B** (3 mol%), base (0.15 mmol) and 1,4-dioxane (1.0 mL) at T °C for 12 h under argon atmosphere. [b] **Cat B** (5 mol%). [c]**2a** (0.15 mmol), [d]**2a** (0.25 mmol). Yields were determined by ^{1}H NMR with 1,3,5-trimethoxybenzene as internal standard.

Table S5. Investigation of the amount of base

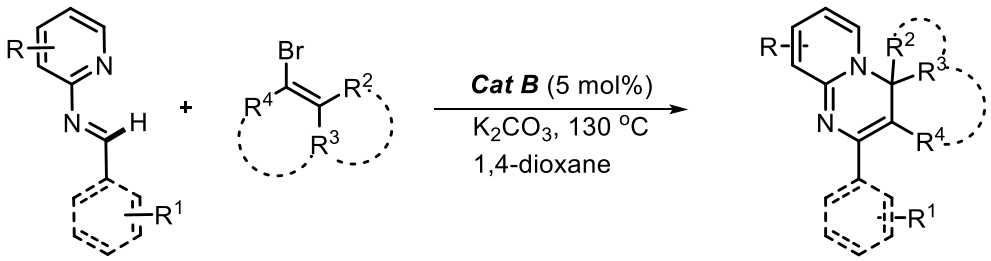


1a **2a** **3a**

Entry	K_2CO_3 (x equiv)	Yield/%
1	1.0	88
2	**1.5**	**96**
3	2.0	96

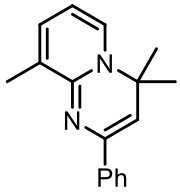
[a]General conditions: **1a** (0.1 mmol), **2a** (0.2 mmol), **Cat B** (5 mol%), K_2CO_3 (x equiv) and 1,4-dioxane (1.0 mL) at 130 °C for 12 h under argon atmosphere. Yields were determined by ^{1}H NMR with 1,3,5-trimethoxybenzene as internal standard.

3.2 Substrate expansion and product identification



1 **2** **3**

In glove box, to dry 1,4-dioxane (2 mL) were added substrate **1** (0.2 mmol, 1.0 equiv), substrate **2** (0.4 mmol, 2.0 equiv), K_2CO_3 (0.3 mmol, 1.5 equiv) and **Cat. B** (5 mol%) in a 10 mL oven-dried Schlenk tube. Then the tube was sealed and the mixture was stirred at 130 °C for 24 h. After the reaction was completed, the resulting mixture was concentrated in vacuo, and the residual was purified by silica gel column chromatography to give the product **3**.



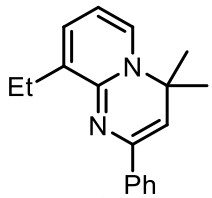
3a

4,4,9-trimethyl-2-phenyl-4H-pyrido[1,2-a]pyrimidine (3a)

Obtained as yellow liquid (44.9 mg, 90% yield);**^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.9 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.25 (dd, *J* = 14.0, 6.6 Hz, 1H), 7.16 (d, *J* = 7.1 Hz, 1H), 6.86 (d, *J* = 6.3 Hz, 1H), 6.04 (t, *J* = 6.8 Hz, 1H), 5.09 (s, 1H), 2.24 (s, 3H), 1.61 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.0, 141.5, 139.1, 131.7, 131.7, 129.0, 127.9, 127.4, 125.5, 107.9, 102.9, 59.0, 31.2, 18.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{17}H_{19}N_2$, *m/z*: 251.1543, found: 251.1548, Error -2.1 ppm.

IR (KBr): 2972, 1626, 1519, 1389, 742, 696 cm^{-1}.



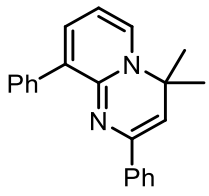
3b

9-ethyl-4,4-dimethyl-2-phenyl-4H-pyrido[1,2-a]pyrimidine (3b)

Obtained as yellow liquid (48.2 mg, 91% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.92 – 7.81 (m, 2H), 7.37 – 7.30 (m, 2H), 7.27 – 7.23 (m, 1H), 7.15 (d, *J* = 6.6 Hz, 1H), 6.84 (dd, *J* = 6.5, 1.2 Hz, 1H), 6.07 (t, *J* = 6.9 Hz, 1H), 5.10 (s, 1H), 2.71 (q, *J* = 7.4 Hz, 2H), 1.60 (s, 6H), 1.25 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.4, 141.5, 139.2, 136.9, 129.4, 128.7, 127.9, 127.4, 125.5, 107.9, 102.8, 59.0, 31.2, 24.3, 12.4.

HRMS (ESI) calcd for $[M+H]^+$ $C_{18}H_{21}N_2$, *m/z*: 265.1699, found: 265.1702, Error -0.9 ppm.

IR (KBr): 2967, 1634, 1515, 1448, 749, 669 cm^{-1}.



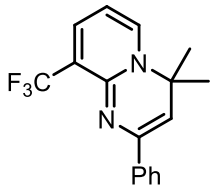
3c

4,4-dimethyl-2,9-diphenyl-4H-pyrido[1,2-a]pyrimidine (3c)

Obtained as yellow liquid (42.3 mg, 68% yield) at 150 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 6.7, 4.4 Hz, 4H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.30 – 7.23 (m, 3H), 7.23 – 7.18 (m, 1H), 6.99 (d, *J* = 6.1 Hz, 1H), 6.15 (t, *J* = 6.8 Hz, 1H), 5.15 (s, 1H), 1.65 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 149.8, 141.4, 138.8, 138.3, 134.4, 133.4, 130.8, 129.60, 127.9, 127.5, 127.4, 127.3, 125.4, 108.2, 102.9, 59.3, 31.2.

HRMS (ESI) calcd for $[M+H]^+$ $C_{22}H_{21}N_2$, *m/z*: 313.1699, found: 313.1698, Error 0.3 ppm.

IR (KBr): 2972, 1628, 1518, 757, 696 cm^{-1}.



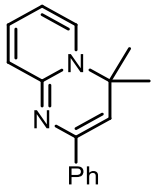
3d

4,4-dimethyl-2-phenyl-9-(trifluoromethyl)-4H-pyrido[1,2-a]pyrimidine (3d)

Obtained as yellow liquid (40.6 mg, 67% yield) at 150 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88 – 7.80 (m, 2H), 7.33 (dd, *J* = 12.6, 4.9 Hz, 4H), 7.26 (t, *J* = 7.3 Hz, 1H), 6.04 (t, *J* = 7.0 Hz, 1H), 5.17 (s, 1H), 1.62 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 146.3, 140.5, 138.1, 135.4, 134.0 (q, *J* = 5.5 Hz), 128.0, 127.8, 125.5, 122.8 (q, *J* = 270.8 Hz), 122.0 (q, *J* = 30.0 Hz), 105.6, 103.9, 59.4, 31.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -66.1.

HRMS (ESI) calcd for $[M+H]^+$ $C_{17}H_{16}N_2F_3$, *m/z*: 305.1260, found: 305.1266, Error-1.9 ppm.

IR (KBr): 1646, 1541, 1309, 1137, 1050, 749 cm^{-1}.



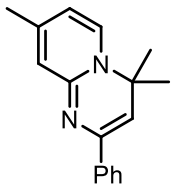
3e

4,4-dimethyl-2-phenyl-4H-pyrido[1,2-a]pyrimidine (3e)

Obtained as yellow liquid (31.3 mg, 66% yield) at 150 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 – 7.70 (m, 2H), 7.36 – 7.30 (m, 2H), 7.28 – 7.23 (m, 1H), 7.22 (dd, *J* = 7.1, 0.9 Hz, 1H), 6.94 – 6.90 (m, 1H), 6.70 (dd, *J* = 9.1, 0.8 Hz, 1H), 6.17 – 6.02 (m, 1H), 5.00 (s, 1H), 1.64 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.5, 142.2, 139.1, 133.5, 131.4, 128.0, 127.5, 125.6, 124.3, 108.8, 103.3, 59.0, 31.3.

HRMS (ESI) calcd for $[M+H]^+$ $C_{16}H_{17}N_2$, *m/z*: 237.1386, found: 237.1388, Error -0.8 ppm.

IR (KBr): 2971, 1641, 1527, 1447, 1385, 755 cm^{-1}.



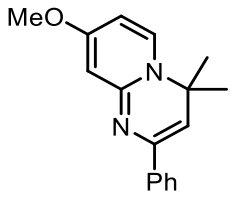
3f

4,4,8-trimethyl-2-phenyl-4H-pyrido[1,2-a]pyrimidine (3f)

Obtained as yellow liquid (37.5 mg, 75% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.4 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.26 (d, *J* = 7.0 Hz, 1H), 7.15 (d, *J* = 7.2 Hz, 1H), 6.56 (s, 1H), 5.98 (d, *J* = 7.1 Hz, 1H), 4.99 (s, 1H), 2.10 (s, 3H), 1.62 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.5, 144.8, 142.1, 139.1, 130.7, 127.9, 127.4, 125.5, 121.9, 111.6, 102.8, 58.8, 31.3, 20.7.

HRMS (ESI) calcd for $[M+H]^+$ $C_{17}H_{19}N_2$, *m/z*: 251.1543, found: 251.1543, Error 0 ppm.

IR (KBr): 2971, 1652, 1520, 1357, 770, 731 cm^{-1}.

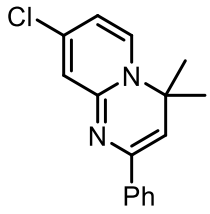


3g

8-methoxy-4,4-dimethyl-2-phenyl-4H-pyrido[1,2-a]pyrimidine (3g)

Obtained as yellow liquid (42.9 mg, 81% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.26 (d, *J* = 7.3 Hz, 1H), 7.15 (d, *J* = 7.8 Hz, 1H), 6.04 (d, *J* = 2.7 Hz, 1H), 5.86 (dd, *J* = 7.7, 2.8 Hz, 1H), 4.99 (s, 1H), 3.76 (s, 3H), 1.60 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 163.1, 153.2, 142.2, 139.4, 132.5, 128.0, 127.3, 125.5, 103.9, 102.6, 99.1, 58.6, 55.3, 31.3.

HRMS (ESI) calcd for $[M+H]^+$ $C_{17}H_{19}N_2O$, *m/z*: 267.1492, found: 267.1503, Error -4.3 ppm.



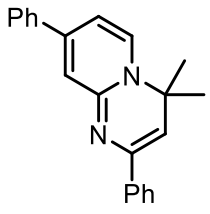
3h

8-chloro-4,4-dimethyl-2-phenyl-4H-pyrido[1,2-a]pyrimidine (3h)

Obtained as yellow liquid (22.2 mg, 41% yield) at 150 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.4 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.28 (d, *J* = 7.2 Hz, 1H), 7.14 (d, *J* = 7.6 Hz, 1H), 6.71 (d, *J* = 2.2 Hz, 1H), 6.06 (dd, *J* = 7.5, 2.3 Hz, 1H), 5.04 (s, 1H), 1.63 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.9, 141.9, 140.2, 138.7, 132.4, 128.1, 127.7, 125.5, 122.3, 110.0, 103.9, 59.1, 31.3.

HRMS (ESI) calcd for $[M+H]^+$ $C_{16}H_{16}ClN_2$, *m/z*: 271.0997, found: 271.1002, Error -2.1 ppm.

IR (KBr): 2927, 1631, 1531, 1349, 1085, 762 cm^{-1}.



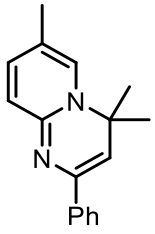
3i

4,4-dimethyl-2,8-diphenyl-4H-pyrido[1,2-a]pyrimidine (3i)

Obtained as yellow solid (27.5 mg, 44% yield, m.p. = 144-146 ºC); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.7 Hz, 2H), 7.46 – 7.38 (m, 5H), 7.34 (dd, *J* = 16.2, 8.5 Hz, 3H), 7.27 (dd, *J* = 15.2, 7.6 Hz, 2H), 6.81 (d, *J* = 9.3 Hz, 1H), 5.06 (s, 1H), 1.71 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.5, 142.3, 139.1, 137.0, 133.4, 129.0, 129.0, 128.1, 127.6, 127.2, 125.6, 125.3, 124.6, 122.6, 103.6, 59.5, 31.5.

HRMS (ESI) calcd for $[M+H]^+$ $C_{22}H_{21}N_2$, *m/z*: 313.1699, found: 313.1706, Error -2.1 ppm.

IR (KBr): 1647, 1537, 1495, 1428, 756, 696 cm^{-1}.



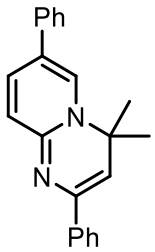
3j

4,4,7-trimethyl-2-phenyl-4H-pyrido[1,2-a]pyrimidine (3j)

Obtained as yellow liquid (35.7 mg, 71% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.26 (d, *J* = 6.7 Hz, 1H), 7.00 (s, 1H), 6.82 (d, *J* = 9.0 Hz, 1H), 6.69 (d, *J* = 9.2 Hz, 1H), 4.97 (s, 1H), 2.02 (s, 3H), 1.63 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.9, 142.3, 139.2, 136.4, 128.5, 128.0, 127.4, 125.5, 124.1, 117.8, 102.8, 59.0, 31.4, 17.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{17}H_{19}N_2$, *m/z*: 251.1534, found: 251.1543, Error -3.6 ppm.

IR (KBr): 2972, 1690, 1527, 1433, 726, 696 cm^{-1}.



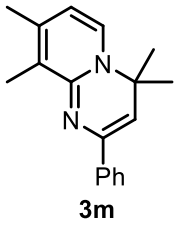
3k

4,4-dimethyl-2,7-diphenyl-4H-pyrido[1,2-a]pyrimidine (3k)

Obtained as red solid (34.6 mg, 55% yield, m.p. = 144-146 ºC); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82 – 7.74 (m, 2H), 7.62 – 7.55 (m, 2H), 7.47 – 7.38 (m, 3H), 7.35 (t, *J* = 7.4 Hz, 2H), 7.31 – 7.24 (m, 2H), 6.97 (d, *J* = 2.0 Hz, 1H), 6.39 (dd, *J* = 7.4, 2.1 Hz, 1H), 5.03 (s, 1H), 1.67 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.7, 145.3, 142.5, 139.2, 137.2, 131.7, 129.0, 128.8, 128.0, 127.5, 126.2, 125.6, 120.7, 108.1, 103.3, 58.9, 31.4.

HRMS (ESI) calcd for $[M+H]^+$ $C_{22}H_{21}N_2$, *m/z*: 313.1699, found: 313.1704, Error -1.5 ppm.

IR (KBr): 2970, 1642, 1520, 1356, 758, 695 cm^{-1}.



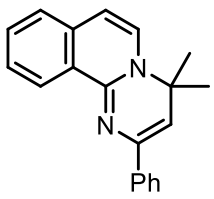
3m

4,4,8,9-tetramethyl-2-phenyl-4H-pyrido[1,2-a]pyrimidine (3m)

Obtained as yellow liquid (48.1 mg, 91% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.25 (t, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 7.2 Hz, 1H), 5.99 (d, *J* = 7.2 Hz, 1H), 5.08 (s, 1H), 2.24 (s, 3H), 2.12 (s, 3H), 1.61 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.0, 141.9, 140.1, 139.4, 127.9, 127.7, 127.5, 127.4, 125.6, 111.8, 102.2, 59.0, 31.1, 19.6, 13.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{18}H_{21}N_2$, *m/z*: 265.1699, found: 265.1709, Error -3.8 ppm.

IR (KBr): 2973, 1689, 1551, 1515, 1447, 736 cm^{-1}.



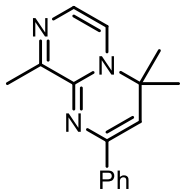
3n

4,4-dimethyl-2-phenyl-4H-pyrimido[2,1-a]isoquinoline (3n)

Obtained as yellow solid (27.9 mg, 49% yield, m.p. = 95-97 ºC); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.75 (d, *J* = 8.1 Hz, 1H), 7.94 (d, *J* = 7.6 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.41 (d, *J* = 7.7 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 2H), 7.30 (t, *J* = 8.6 Hz, 2H), 7.05 (d, *J* = 7.6 Hz, 1H), 6.36 (d, *J* = 7.6 Hz, 1H), 5.27 (s, 1H), 1.64 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 148.9, 140.6, 138.9, 134.1, 130.9, 128.0, 127.6, 127.5, 127.1, 127.0, 126.6, 125.5, 125.2, 107.8, 106.0, 58.4, 31.4.

HRMS (ESI) calcd for $[M+H]^+$ $C_{20}H_{19}N_2$, *m/z*: 287.1543, found: 287.1541, Error 0.8 ppm.

IR (KBr): 2970, 1636, 1561, 1538, 1345, 781, 677 cm^{-1}.



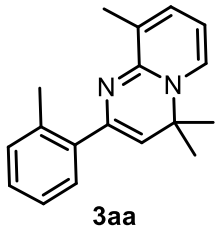
3o

4,4,9-trimethyl-2-phenyl-4H-pyrazino[1,2-a]pyrimidine (3o)

Obtained as yellow liquid (27.2 mg, 54% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.85 – 7.78 (m, 2H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.32 – 7.27 (m, 1H), 7.06 (d, *J* = 4.8 Hz, 1H), 6.88 (d, *J* = 4.8 Hz, 1H), 5.17 (s, 1H), 2.52 (s, 3H), 1.61 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.6, 144.3, 141.3, 138.2, 128.1, 127.9, 125.4, 124.2, 120.7, 105.4, 58.6, 30.8, 21.8.

HRMS (ESI) calcd for $[M+H]^+$ $C_{16}H_{18}N_3$, *m/z*: 252.1495, found: 252.1496, Error -0.3 ppm.

IR (KBr): 2972, 1537, 1370, 1182, 745, 697 cm^{-1}.



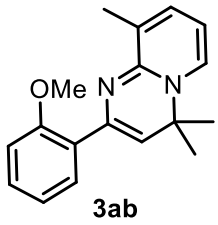
3aa

4,4,9-trimethyl-2-(o-tolyl)-4H-pyrido[1,2-a]pyrimidine (3aa)

Obtained as yellow liquid (51.9 mg, 98% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.40 (d, *J* = 6.5 Hz, 1H), 7.19 – 7.11 (m, 4H), 6.82 (d, *J* = 6.4 Hz, 1H), 6.03 (t, *J* = 6.8 Hz, 1H), 4.64 (s, 1H), 2.46 (s, 3H), 2.13 (s, 3H), 1.61 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.3, 144.5, 140.6, 136.2, 131.5, 131.4, 130.3, 129.1, 128.8, 127.1, 125.3, 107.7, 106.9, 58.9, 31.2, 20.6, 18.7.

HRMS (ESI) calcd for $[M+H]^+$ $C_{18}H_{21}N_2$, *m/z*: 265.1699, found: 265.1696, Error 1.1 ppm.

IR (KBr): 2971, 1637, 1514, 1459, 1081, 744 cm^{-1}.



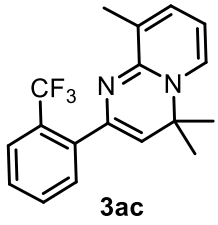
3ab

2-(2-methoxyphenyl)-4,4,9-trimethyl-4H-pyrido[1,2-a]pyrimidine (3ab)

Obtained as yellow liquid (30.4mg, 54% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.23 – 7.18 (m, 1H), 7.17 (d, *J* = 7.1 Hz, 1H), 7.00 (t, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 8.2 Hz, 1H), 6.82 (d, *J* = 6.4 Hz, 1H), 6.01 (t, *J* = 6.8 Hz, 1H), 5.50 (s, 1H), 3.84 (s, 3H), 2.20 (s, 3H), 1.62 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.6, 150.5, 138.1, 131.5, 131.2, 129.8, 129.0, 128.2, 128.1, 120.7, 111.7, 108.7, 107.5, 58.6, 55.8, 31.0, 18.7.

HRMS (ESI) calcd for $[M+H]^+$ $C_{18}H_{21}N_2O$, *m/z*: 281.1648, found: 281.1649, Error -0.1 ppm.

IR (KBr): 2971, 1638, 1525, 1488, 1238, 756 cm^{-1}.



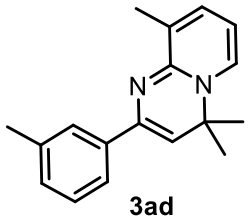
3ac

4,4,9-trimethyl-2-(2-(trifluoromethyl)phenyl)-4H-pyrido[1,2-a]pyrimidine (3ac)

Obtained as yellow liquid (47.5mg, 75% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.9 Hz, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 7.1 Hz, 1H), 6.85 (d, *J* = 6.5 Hz, 1H), 6.07 (t, *J* = 6.8 Hz, 1H), 4.66 (s, 1H), 2.12 (s, 3H), 1.61 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.6, 142.7, 140.9, 131.8, 131.5, 131.2, 131.0, 129.1, 128.2 (q, *J* = 29.9 Hz), 127.2, 126.2 (q, *J* = 5.4 Hz), 124.5 (q, *J* = 272.3 Hz), 108.1, 106.8 (q, *J* = 1.9 Hz), 59.1, 30.7, 18.7; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -56.7.

HRMS (ESI) calcd for $[M+H]^+$ $C_{18}H_{18}F_3N_2$, *m/z*: 319.1417, found: 319.1414, Error 0.9 ppm.

IR (KBr): 2975, 1637, 1513, 1313, 1165, 1130, 769 cm^{-1}.



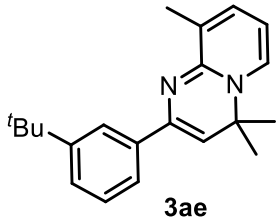
3ad

4,4,9-trimethyl-2-(m-tolyl)-4H-pyrido[1,2-a]pyrimidine (3ad)

Obtained as yellow liquid (50.1 mg, 95% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.68 (s, 1H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 7.0 Hz, 1H), 7.07 (d, *J* = 7.4 Hz, 1H), 6.84 (d, *J* = 6.4 Hz, 1H), 6.02 (t, *J* = 6.8 Hz, 1H), 5.08 (s, 1H), 2.37 (s, 3H), 2.24 (s, 3H), 1.60 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.9, 141.6, 139.1, 137.3, 131.6, 131.6, 129.0, 128.2, 127.8, 126.2, 122.6, 107.8, 102.9, 58.9, 31.1, 21.5, 18.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{18}H_{21}N_2$, *m/z*: 265.1699, found: 265.1696, Error 1.1 ppm.

IR (KBr): 2971, 2910, 1519, 1176, 1083, 745 cm^{-1}.



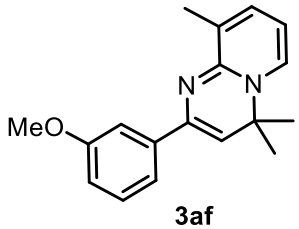
3ae

2-(3-(tert-butyl)phenyl)-4,4,9-trimethyl-4H-pyrido[1,2-a]pyrimidine (3ae)

Obtained as yellow liquid (53.9 mg, 88% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.98 (t, *J* = 1.7 Hz, 1H), 7.66 – 7.59 (m, 1H), 7.32 – 7.29 (m, 1H), 7.27 (t, *J* = 7.6 Hz, 1H), 7.17 (d, *J* = 7.0 Hz, 1H), 6.86 (d, *J* = 6.4 Hz, 1H), 6.03 (t, *J* = 6.8 Hz, 1H), 5.08 (s, 1H), 2.25 (s, 3H), 1.61 (s, 6H), 1.35 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.9, 150.5, 141.9, 138.7, 131.6, 131.6, 129.0, 127.6, 124.5, 122.7, 122.6, 107.8, 102.7, 59.0, 34.6, 31.3, 31.1, 18.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{21}H_{27}N_2$, *m/z*: 307.2169, found: 307.2166, Error 1.0 ppm.

IR (KBr): 2963, 1638, 1521, 1489, 744 cm^{-1}.



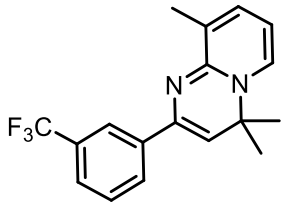
3af

2-(3-methoxyphenyl)-4,4,9-trimethyl-4H-pyrido[1,2-a]pyrimidine (3af)

Obtained as yellow liquid (49.3 mg, 88% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.54 – 7.50 (m, 1H), 7.42 (d, *J* = 7.7 Hz, 1H), 7.24 (t, *J* = 7.9 Hz, 1H), 7.16 (d, *J* = 7.1 Hz, 1H), 6.86 (d, *J* = 6.4 Hz, 1H), 6.82 (dd, *J* = 8.1, 2.5 Hz, 1H), 6.04 (t, *J* = 6.8 Hz, 1H), 5.10 (s, 1H), 3.83 (s, 3H), 2.23 (s, 3H), 1.61 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.5, 150.9, 141.3, 140.7, 131.7, 131.6, 129.0, 128.8, 117.9, 113.2, 111.0, 107.9, 103.1, 59.0, 55.1, 31.1, 18.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{18}H_{21}N_2O$, *m/z*: 281.1648, found: 281.1652, Error -1.4 ppm.

IR (KBr): 2970, 1638, 1519, 1489, 1271, 1045, 746 cm^{-1}.



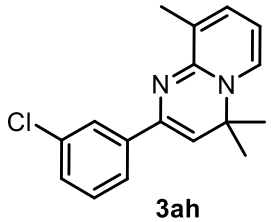
3ag

4,4,9-trimethyl-2-(3-(trifluoromethyl)phenyl)-4H-pyrido[1,2-a]pyrimidine (3ag)

Obtained as yellow liquid (54.3 mg, 85% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.14 (s, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 7.7 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.19 (d, *J* = 7.1 Hz, 1H), 6.89 (d, *J* = 6.5 Hz, 1H), 6.08 (t, *J* = 6.8 Hz, 1H), 5.14 (s, 1H), 2.24 (s, 3H), 1.63 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.2, 140.6, 140.0, 132.1, 131.6, 130.2 (q, *J* = 31.6 Hz), 129.0, 128.8, 128.3, 124.4 (q, *J* = 270.6 Hz), 124.0 (q, *J* = 3.8 Hz), 122.4 (q, *J* = 4.0 Hz), 108.4, 103.6, 59.1, 31.1, 18.6.; **^{19}F NMR** (565 MHz, $CDCl_3$) δ -62.4.

HRMS (ESI) calcd for $[M+H]^+$ $C_{18}H_{18}F_3N_2$, *m/z*: 319.1417, found: 319.1424, Error -2.5 ppm.

IR (KBr): 3074, 1698, 1519, 1518, 1330, 1124, 700 cm^{-1}.



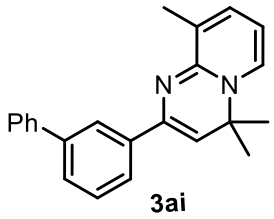
3ah

2-(3-chlorophenyl)-4,4,9-trimethyl-4H-pyrido[1,2-a]pyrimidine (3ah)

Obtained as yellow liquid (53.8 mg, 94% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.73 (d, *J* = 7.5 Hz, 1H), 7.24 (dt, *J* = 14.3, 7.8 Hz, 2H), 7.18 (d, *J* = 7.1 Hz, 1H), 6.88 (d, *J* = 6.3 Hz, 1H), 6.07 (t, *J* = 6.8 Hz, 1H), 5.09 (s, 1H), 2.23 (s, 3H), 1.62 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.1, 141.2, 140.6, 134.0, 132.0, 131.7, 129.1, 129.0, 127.4, 125.8, 123.6, 108.2, 103.5, 59.1, 31.1, 18.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{17}H_{18}ClN_2$, *m/z*: 285.1153, found: 285.1157, Error -1.4 ppm.

IR (KBr): 2974, 1639, 1517, 1374, 1082, 741 cm^{-1}.



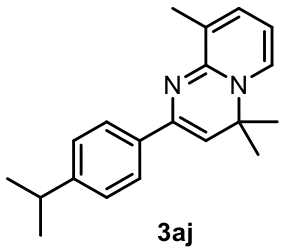
3ai

2-([1,1'-biphenyl]-3-yl)-4,4,9-trimethyl-4H-pyrido[1,2-a]pyrimidine (3ai)

Obtained as yellow liquid (52.3 mg, 80% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.85 (d, *J* = 7.7 Hz, 1H), 7.65 (d, *J* = 7.3 Hz, 2H), 7.50 (d, *J* = 7.7 Hz, 1H), 7.43 (dt, *J* = 9.7, 7.6 Hz, 3H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.20 (d, *J* = 7.0 Hz, 1H), 6.88 (d, *J* = 6.5 Hz, 1H), 6.07 (t, *J* = 6.8 Hz, 1H), 5.15 (s, 1H), 2.25 (s, 3H), 1.64 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.1, 141.8, 141.7, 140.9, 139.7, 131.8, 129.1, 128.6, 128.4, 127.2, 127.0, 126.4, 124.7, 124.6, 108.0, 103.2, 59.1, 31.2, 18.7.

HRMS (ESI) calcd for $[M+H]^+$ $C_{23}H_{23}N_2$, *m/z*: 327.1856, found: 327.1856, Error 0 ppm.

IR (KBr): 2972, 1638, 1518, 759, 745, 700 cm^{-1}.



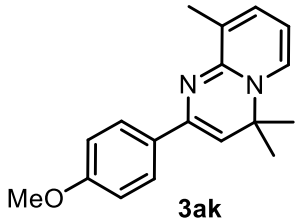
3aj

2-(4-isopropylphenyl)-4,4,9-trimethyl-4H-pyrido[1,2-a]pyrimidine (3aj)

Obtained as yellow liquid (55.7 mg, 95% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 7.1 Hz, 1H), 6.83 (d, *J* = 6.3 Hz, 1H), 6.01 (t, *J* = 6.8 Hz, 1H), 5.04 (s, 1H), 2.95 – 2.85 (m, 1H), 2.22 (s, 3H), 1.59 (s, 6H), 1.24 (d, *J* = 6.9 Hz, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.9, 148.1, 141.6, 136.9, 131.7, 131.5, 129.0, 126.0, 125.5, 107.7, 102.4, 58.9, 33.8, 31.2, 24.0, 18.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{20}H_{25}N_2$, *m/z*: 293.2012, found: 293.2013, Error -0.2 ppm.

IR (KBr): 2961, 1638, 1522, 1388, 1178, 774 cm^{-1}.



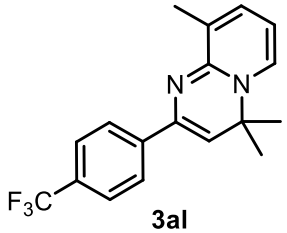
3ak

2-(4-methoxyphenyl)-4,4,9-trimethyl-4H-pyrido[1,2-a]pyrimidine (3ak)

Obtained as yellow liquid (55.4 mg, 99% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.8 Hz, 2H), 7.16 (d, *J* = 7.1 Hz, 1H), 6.87 (d, *J* = 8.8 Hz, 2H), 6.85 (d, *J* = 6.4 Hz, 1H), 6.03 (t, *J* = 6.8 Hz, 1H), 5.00 (s, 1H), 3.80 (s, 3H), 2.23 (s, 3H), 1.60 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.2, 150.9, 141.1, 131.9, 131.6, 129.0, 126.7, 113.3, 107.8, 101.4, 58.9, 55.2, 31.2, 18.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{18}H_{21}N_2O$, *m/z*: 281.1648, found: 281.1637, Error 3.9 ppm.

IR (KBr): 2970, 1925, 1518, 1249, 1171, 745 cm^{-1}.



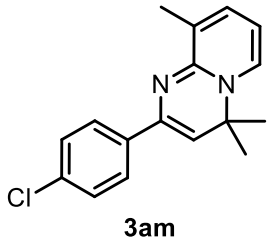
3al

4,4,9-trimethyl-2-(4-(trifluoromethyl)phenyl)-4H-pyrido[1,2-a]pyrimidine (3al)

Obtained as yellow liquid (51.7 mg, 81% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.2 Hz, 2H), 7.59 (d, *J* = 8.2 Hz, 2H), 7.20 (d, *J* = 7.1 Hz, 1H), 6.90 (d, *J* = 6.5 Hz, 1H), 6.10 (t, *J* = 6.8 Hz, 1H), 5.16 (s, 1H), 2.24 (s, 3H), 1.64 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.2, 142.6, 140.6, 132.3, 131.6, 129.3 (q, *J* = 31.8 Hz), 129.1, 125.8, 124.9 (q, *J* = 3.5 Hz), 124.4 (q, *J* = 270.3 Hz), 108.5, 104.4, 59.2, 31.2, 18.6; **^{19}F NMR** (565 MHz, $CDCl_3$) δ -62.3.

HRMS (ESI) calcd for $[M+H]^+$ $C_{18}H_{18}F_3N_2$, *m/z*: 319.1417, found: 319.1409, Error 2.5 ppm.

IR (KBr): 2975, 1522, 1325, 1163, 1122, 855 cm^{-1}.



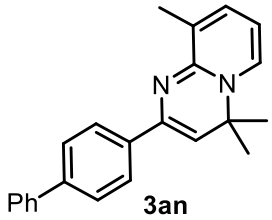
3am

2-(4-chlorophenyl)-4,4,9-trimethyl-4H-pyrido[1,2-a]pyrimidine (3am)

Obtained as yellow liquid (54.1 mg, 95% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.5 Hz, 2H), 7.29 (d, *J* = 8.5 Hz, 2H), 7.16 (d, *J* = 7.0 Hz, 1H), 6.87 (d, *J* = 6.4 Hz, 1H), 6.05 (t, *J* = 6.8 Hz, 1H), 5.06 (s, 1H), 2.22 (s, 3H), 1.60 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.0, 140.6, 137.7, 133.0, 131.9, 131.5, 129.0, 128.0, 126.8, 108.1, 102.9, 59.0, 31.1, 18.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{17}H_{18}ClN_2$, *m/z*: 285.1153, found: 285.1165, Error -4.4 ppm.

IR (KBr): 2973, 1638, 1519,1491, 1086, 848, 744 cm^{-1}.



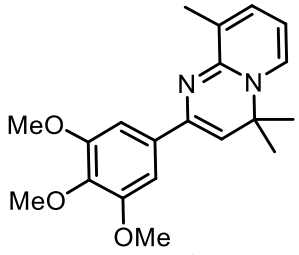
3an

2-([1,1'-biphenyl]-4-yl)-4,4,9-trimethyl-4H-pyrido[1,2-a]pyrimidine (3an)

Obtained as yellow solid (64.0 mg, 98% yield, m.p. = 116-118 ºC); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.6 Hz, 2H), 7.62 (d, *J* = 7.7 Hz, 2H), 7.59 (d, *J* = 7.6 Hz, 2H), 7.41 (t, *J* = 7.4 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.15 (d, *J* = 7.1 Hz, 1H), 6.85 (d, *J* = 6.3 Hz, 1H), 6.03 (t, *J* = 6.7 Hz, 1H), 5.13 (s, 1H), 2.25 (s, 3H), 1.61 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.0, 141.2, 141.1, 140.0, 138.2, 131.7, 131.7, 129.1, 128.6, 127.0, 126.9, 126.6, 125.9, 107.9, 103.0, 59.0, 31.2, 18.7.

HRMS (ESI) calcd for $[M+H]^+$ $C_{23}H_{23}N_2$, *m/z*: 327.1856, found: 327.1864, Error -2.6 ppm.

IR (KBr): 2972, 1636, 1522, 763, 745, 698 cm^{-1}.



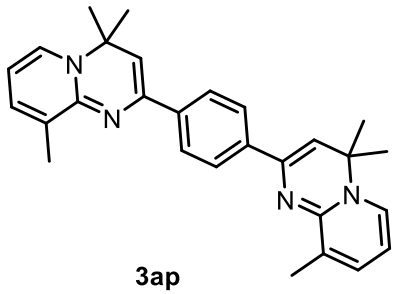
3ao

4,4,9-trimethyl-2-(3,4,5-trimethoxyphenyl)-4H-pyrido[1,2-a]pyrimidine (3ao)

Obtained as yellow solid (61.3 mg, 90% yield, m.p. = 110-112 ºC); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.20 (d, *J* = 7.0 Hz, 1H), 7.16 (s, 2H), 6.89 (d, *J* = 6.4 Hz, 1H), 6.07 (t, *J* = 6.8 Hz, 1H), 5.04 (s, 1H), 3.91 (s, 6H), 3.85 (s, 3H), 2.24 (s, 3H), 1.63 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.8, 150.9, 141.3, 137.8, 134.9, 131.8, 131.4, 129.0, 108.0, 102.8, 102.4, 60.7, 59.0, 55.9, 31.0, 18.5.

HRMS (ESI) calcd for $[M+H]^+$ $C_{20}H_{25}N_2O_3$, *m/z*: 341.1860, found: 341.1859, Error 0.1 ppm.

IR (KBr): 2938, 1581, 1519, 1339, 1126, 734 cm^{-1}.



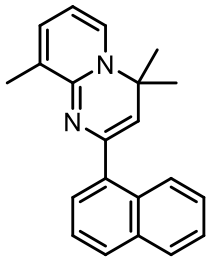
3ap

1,4-bis(4,4,9-trimethyl-4H-pyrido[1,2-a]pyrimidin-2-yl)benzene (3ap)

Obtained as yellow solid (70.7 mg, 84% yield, m.p. = 201-203 ºC); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86 (s, 4H), 7.16 (d, *J* = 7.0 Hz, 2H), 6.85 (d, *J* = 6.4 Hz, 2H), 6.02 (s, 2H), 5.13 (s, 2H), 2.25 (s, 6H), 1.61 (s, 12H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.9, 141.3, 138.1, 131.7, 131.5, 129.0, 125.0, 107.7, 102.6, 58.9, 31.1, 18.6.

HRMS (ESI) calcd for $[M+Na]^+$ $C_{28}H_{30}N_4Na$, *m/z*: 445.2363, found: 445.2367, Error -0.9 ppm.

IR (KBr): 2966, 1631, 1517, 1175, 1086, 738 cm^{-1}.



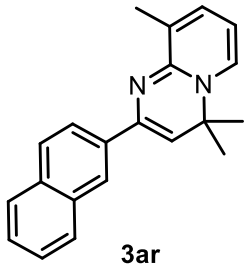
3aq

4,4,9-trimethyl-2-(naphthalen-1-yl)-4H-pyrido[1,2-a]pyrimidine (3aq)

Obtained as yellow liquid (38.2 mg, 64% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.49 (d, *J* = 3.4 Hz, 1H), 7.84 – 7.78 (m, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.60 (d, *J* = 6.6 Hz, 1H), 7.43 (t, *J* = 7.2 Hz, 3H), 7.21 (d, *J* = 7.1 Hz, 1H), 6.87 (d, *J* = 6.4 Hz, 1H), 6.08 (t, *J* = 6.8 Hz, 1H), 4.84 (s, 1H), 2.15 (s, 3H), 1.68 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.5, 144.0, 139.0, 133.9, 131.8, 131.7, 131.6, 129.2, 128.0, 127.8, 126.8, 126.1, 125.2, 125.1, 108.0, 108.0, 59.2, 31.2, 18.8.

HRMS (ESI) calcd for $[M+H]^+$ $C_{21}H_{21}N_2$, *m/z*: 301.1699, found: 301.1696, Error 1.1 ppm.

IR (KBr): 2972, 1696, 1511, 1458, 779, 744 cm^{-1}.



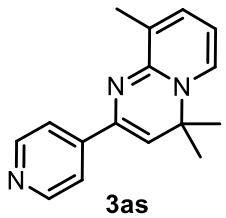
3ar

4,4,9-trimethyl-2-(naphthalen-2-yl)-4H-pyrido[1,2-a]pyrimidine (3ar)

Obtained as yellow solid (54.0 mg, 90% yield, m.p. = 150-152 ºC); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.84 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.80 (d, *J* = 7.8 Hz, 1H), 7.71 (dd, *J* = 8.1, 4.5 Hz, 2H), 7.39 – 7.30 (m, 2H), 7.10 (d, *J* = 7.0 Hz, 1H), 6.80 (d, *J* = 6.4 Hz, 1H), 5.97 (t, *J* = 6.8 Hz, 1H), 5.17 (s, 1H), 2.23 (s, 3H), 1.56 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.1, 141.4, 136.4, 133.5, 133.1, 131.8, 131.7, 129.1, 128.5, 127.4, 127.3, 125.6, 125.4, 124.6, 123.8, 108.0, 103.7, 59.1, 31.2, 18.7.

HRMS (ESI) calcd for $[M+H]^+$ $C_{21}H_{21}N_2$, *m/z*: 301.1699, found: 301.1694, Error 1.6 ppm.

IR (KBr): 2973, 1693, 1624, 1519, 1487, 748 cm^{-1}.



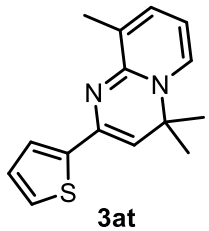
3as

4,4,9-trimethyl-2-(pyridin-4-yl)-4H-pyrido[1,2-a]pyrimidine (3as)

Obtained as yellow liquid (25.5 mg, 51% yield) at 150 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.57 (d, *J* = 4.6 Hz, 2H), 7.80 – 7.70 (m, 2H), 7.20 (d, *J* = 7.1 Hz, 1H), 6.91 (d, *J* = 6.4 Hz, 1H), 6.11 (t, *J* = 6.8 Hz, 1H), 5.25 (s, 1H), 2.24 (s, 3H), 1.64 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.3, 149.6, 146.5, 139.7, 132.2, 131.7, 129.1, 119.9, 108.5, 105.2, 59.2, 31.1, 18.5.

HRMS (ESI) calcd for $[M+H]^+$ $C_{16}H_{18}N_3$, *m/z*: 252.1495, found: 252.1486, Error 3.6 ppm.

IR (KBr): 2972, 1637, 1595, 1517,1086, 744 cm^{-1}.



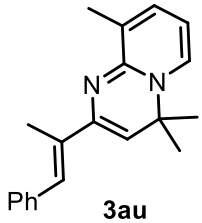
3at

4,4,9-trimethyl-2-(thiophen-2-yl)-4H-pyrido[1,2-a]pyrimidine (3at)

Obtained as yellow liquid (29.8 mg, 58% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.34 (dd, *J* = 3.6, 1.1 Hz, 1H), 7.23 – 7.15 (m, 2H), 7.00 (dd, *J* = 5.0, 3.6 Hz, 1H), 6.91 – 6.85 (m, 1H), 6.08 (t, *J* = 6.8 Hz, 1H), 5.05 (s, 1H), 2.22 (s, 3H), 1.62 (s, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.1, 145.5, 137.7, 132.0, 131.5, 129.0, 127.2, 124.6, 122.1, 108.2, 100.7, 59.0, 31.2, 18.5.

HRMS (ESI) calcd for $[M+H]^+$ $C_{15}H_{17}N_2S$, *m/z*: 257.1107, found: 257.1101, Error 2.3 ppm.

IR (KBr): 2973, 1638, 1373, 1241, 745 cm^{-1}.



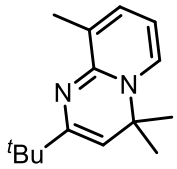
3au

4,4,9-trimethyl-2-(1-phenylprop-1-en-2-yl)-4H-pyrido[1,2-a]pyrimidine (3au)

Obtained as yellow liquid (28.9 mg, 50% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.37 – 7.30 (m, 4H), 7.22 – 7.17 (m, 1H), 7.14 (d, *J* = 6.6 Hz, 1H), 6.88 – 6.78 (m, 1H), 6.00 (t, *J* = 6.8 Hz, 1H), 4.87 (s, 1H), 2.21 (s, 3H), 2.04 (d, *J* = 1.2 Hz, 3H), 1.59 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.3, 142.3, 139.1, 134.0, 131.6, 131.5, 129.4, 128.9, 127.8, 127.4, 125.9, 107.5, 105.3, 58.8, 31.2, 18.6, 14.2.

HRMS (ESI) calcd for $[M+H]^+$ $C_{20}H_{23}N_2$, *m/z*: 291.1856, found: 291.1851, Error 1.7 ppm.

IR (KBr): 2972, 1638, 1528, 1092, 743 cm^{-1}.



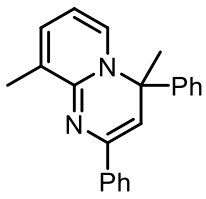
3av

2-(*tert*-butyl)-4,4,9-trimethyl-4H-pyrido[1,2-a]pyrimidine (3av)

Obtained as yellow liquid (17.3 mg, 38% yield) at 150 °C with 10mol% **Cat B**; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.08 (d, *J* = 7.1 Hz, 1H), 6.73 (d, *J* = 6.4 Hz, 1H), 5.90 (t, *J* = 6.8 Hz, 1H), 4.38 (s, 1H), 2.08 (s, 3H), 1.49 (s, 6H), 1.13 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 152.3, 150.1, 131.7, 130.6, 129.1, 106.6, 100.2, 58.4, 35.2, 31.4, 28.6, 18.5.

HRMS (ESI) calcd for $[M+H]^+$ $C_{15}H_{23}N_2$, *m/z*: 231.1856, found: 231.1864, Error -3.7 ppm.

IR (KBr): 2954, 2867, 1639, 1701, 1526, 1103, 740 cm^{-1}.



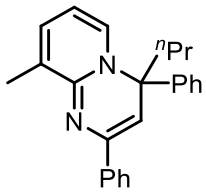
3ba

4,9-dimethyl-2,4-diphenyl-4H-pyrido[1,2-a]pyrimidine (3ba)

Obtained as yellow liquid (48.7 mg, 78% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.90 – 7.83 (m, 2H), 7.60 – 7.53 (m, 2H), 7.35 (t, *J* = 7.8 Hz, 2H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.28 – 7.22 (m, 2H), 6.81 (d, *J* = 6.4 Hz, 1H), 6.71 (d, *J* = 7.0 Hz, 1H), 5.85 (t, *J* = 6.8 Hz, 1H), 5.13 (s, 1H), 2.27 (s, 3H), 2.01 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.5, 147.1, 139.8, 139.0, 132.0, 131.8, 131.7, 128.5, 127.9, 127.6, 127.5, 126.9, 125.5, 107.6, 103.7, 65.0, 28.9, 18.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{22}H_{21}N_2$, *m/z*: 313.1699, found: 313.1692, Error 2.3 ppm.

IR (KBr): 2920, 2850, 1643, 1480, 1448, 697 cm^{-1}.



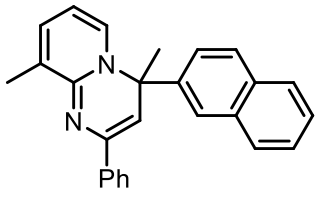
3bb

9-methyl-2,4-diphenyl-4-propyl-4H-pyrido[1,2-a]pyrimidine (3bb)

Obtained as yellow solid (51.6 mg, 76% yield, m.p. = 132-134 ºC); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.5 Hz, 2H), 7.59 (d, *J* = 7.7 Hz, 2H), 7.36 (t, *J* = 7.7 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.25 (dd, *J* = 9.9, 4.6 Hz, 2H), 6.80 (d, *J* = 6.2 Hz, 1H), 6.68 (d, *J* = 7.0 Hz, 1H), 5.84 (t, *J* = 6.7 Hz, 1H), 4.98 (s, 1H), 2.45 (td, *J* = 13.2, 4.5 Hz, 1H), 2.26 (s, 3H), 1.97 (td, *J* = 13.4, 3.9 Hz, 1H), 1.92 – 1.81 (m, 1H), 1.45 – 1.36 (m, 1H), 0.99 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.4, 147.8, 140.4, 139.1, 132.0, 131.9, 131.7, 128.5, 128.0, 127.5, 127.4, 127.1, 125.5, 107.5, 102.3, 68.4, 43.9, 18.7, 17.2, 14.3.

HRMS (ESI) calcd for $[M+H]^+$ $C_{24}H_{25}N_2$, *m/z*: 341.2012, found: 341.2007, Error 1.6 ppm.

IR (KBr): 2957, 1639, 1520, 1307, 740, 695 cm^{-1}.



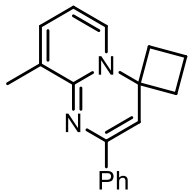
3bc

4,9-dimethyl-4-(naphthalen-2-yl)-2-phenyl-4H-pyrido[1,2-a]pyrimidine (3bc)

Obtained as yellow solid (63.7 mg, 88% yield, m.p. = 121-123 ºC); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.88 (d, *J* = 7.4 Hz, 2H), 7.86 – 7.83 (m, 1H), 7.83 – 7.75 (m, 3H), 7.53 – 7.46 (m, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.25 (t, *J* = 7.3 Hz, 1H), 6.81 (d, *J* = 6.4 Hz, 1H), 6.71 (d, *J* = 7.0 Hz, 1H), 5.82 (t, *J* = 6.8 Hz, 1H), 5.16 (s, 1H), 2.30 (s, 3H), 2.12 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.6, 144.0, 140.0, 139.0, 132.7, 132.5, 132.1, 131.8, 128.7, 128.3, 128.0, 127.6, 127.5, 126.5, 126.2, 125.5, 124.2, 107.7, 103.4, 65.2, 28.9, 18.7.

HRMS (ESI) calcd for $[M+H]^+$ $C_{26}H_{23}N_2$, *m/z*: 363.1856, found: 363.1856, Error 0 ppm.

IR (KBr): 3056, 2974, 1638, 1518, 1178, 745 cm^{-1}.



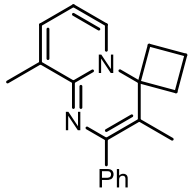
3bd

9'-methyl-2'-phenylspiro[cyclobutane-1,4'-pyrido[1,2-a]pyrimidine] (3bd)

Obtained as yellow liquid (33.6 mg, 64% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.7 Hz, 2H), 7.41 (d, *J* = 7.1 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.27 (t, *J* = 7.3 Hz, 1H), 6.82 (d, *J* = 6.4 Hz, 1H), 6.05 (t, *J* = 6.8 Hz, 1H), 5.60 (s, 1H), 2.96 (dd, *J* = 22.3, 10.7 Hz, 2H), 2.33 – 2.25 (m, 2H), 2.18 (s, 3H), 1.97 – 1.90 (m, 1H), 1.89 – 1.80 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.1, 140.4, 139.2, 131.8, 131.5, 129.7, 128.0, 127.4, 125.4, 107.8, 102.6, 63.2, 41.7, 18.6, 12.1.

HRMS (ESI) calcd for $[M+H]^+$ $C_{18}H_{19}N_2$, *m/z*: 263.1543, found: 263.1540, Error 1.1 ppm.

IR (KBr): 2947, 1676, 1623, 1598, 1485, ,1259, 738, 693 cm^{-1}.



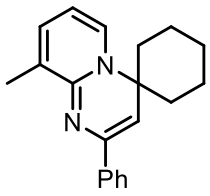
3be

3',9'-dimethyl-2'-phenylspiro[cyclobutane-1,4'-pyrido[1,2-a]pyrimidine] (3be)

Obtained as yellow liquid (36.6 mg, 66% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.52 – 7.45 (m, 2H), 7.34 (dd, *J* = 14.3, 7.0 Hz, 3H), 7.23 (dd, *J* = 10.3, 4.3 Hz, 1H), 6.75 (d, *J* = 6.4 Hz, 1H), 6.04 (t, *J* = 6.8 Hz, 1H), 2.82 – 2.70 (m, 4H), 2.07 (s, 3H), 1.98 (s, 3H), 1.95 – 1.82 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 148.7, 141.6, 139.5, 131.0, 130.4, 129.5, 129.2, 127.5, 126.6, 107.4, 107.0, 66.7, 36.4, 18.4, 15.0, 13.1.

HRMS (ESI) calcd for $[M+H]^+$ $C_{19}H_{21}N_2$, *m/z*: 277.1699, found: 277.1702, Error -1.0 ppm.

IR (KBr): 2949, 1641, 1535, 1263, 737, 701 cm^{-1}.



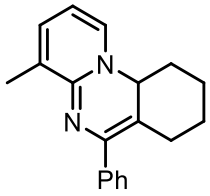
3bf

9'-methyl-2'-phenylspiro[cyclohexane-1,4'-pyrido[1,2-a]pyrimidine] (3bf)

Obtained as yellow liquid (27.8 mg, 48% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 – 7.85 (m, 2H), 7.39 – 7.31 (m, 2H), 7.29 – 7.25 (m, 2H), 6.90 (dd, *J* = 5.3, 1.2 Hz, 1H), 6.11 (t, *J* = 6.8 Hz, 1H), 5.50 (s, 1H), 2.27 (s, 3H), 2.22 (d, *J* = 7.2 Hz, 2H), 1.77 – 1.70 (m, 5H), 1.71 – 1.64 (m, 2H), 1.29 – 1.14 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.7, 142.5, 139.6, 131.5, 128.2, 128.0, 127.5, 125.9, 108.0, 97.5, 61.4, 36.9, 25.4, 21.6, 18.7.

HRMS (ESI) calcd for $[M+H]^+$ $C_{20}H_{23}N_2$, *m/z*: 291.1856, found: 291.1847, Error 3.1 ppm.

IR (KBr): 2930, 1634, 1514, 1173, 739, cm^{-1}.



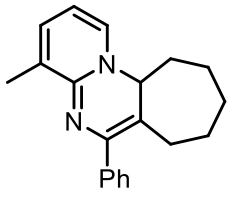
3bg

4-methyl-6-phenyl-8,9,10,10a-tetrahydro-7H-pyrido[1,2-a]quinazoline (3bg)

Obtained as yellow liquid (38.0 mg, 69% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.27 – 7.23 (m, 1H), 6.76 (d, *J* = 6.4 Hz, 1H), 6.70 (d, *J* = 6.8 Hz, 1H), 5.96 (t, *J* = 6.7 Hz, 1H), 4.77 (dd, *J* = 10.4, 4.5 Hz, 1H), 2.80 – 2.70 (m, 1H), 2.07 (s, 3H), 2.06 – 2.01 (m, 2H), 2.00 – 1.95 (m, 1H), 1.70 (td, *J* = 13.6, 4.1 Hz, 2H), 1.63 – 1.52 (m, 1H), 1.43 – 1.34 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 149.0, 140.6, 136.8, 131.9, 131.5, 131.4, 128.9, 127.6, 126.8, 111.3, 107.1, 64.0, 35.8, 30.1, 27.1, 26.0, 18.3.

HRMS (ESI) calcd for $[M+H]^+$ $C_{19}H_{21}N_2$, *m/z*: 277.1699, found: 277.1692, Error 2.5 ppm.

IR (KBr): 2939, 1667, 1554, 1448, 734, 702 cm^{-1}.



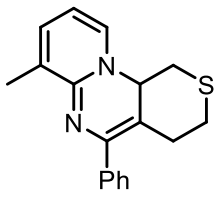
3bh

4-methyl-6-phenyl-7,8,9,10,11,11a-hexahydrocyclohepta[*e*]pyrido[1,2-a]pyrimidine (3bh)

Obtained as yellow liquid (55.2 mg, 95% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.8 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.25 (t, *J* = 7.3 Hz, 1H), 6.82 (d, *J* = 6.4 Hz, 1H), 6.79 (d, *J* = 6.7 Hz, 1H), 6.03 (t, *J* = 6.7 Hz, 1H), 4.37 (dd, *J* = 11.3, 4.1 Hz, 1H), 2.76 – 2.65 (m, 1H), 2.17 (s, 3H), 2.06 – 1.99 (m, 1H), 1.99 – 1.92 (m, 1H), 1.90 – 1.83 (m, 1H), 1.82 – 1.75 (m, 1H), 1.73 – 1.63 (m, 3H), 1.60 – 1.54 (m, 1H), 1.45 – 1.35 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 148.6, 140.8, 140.6, 132.4, 131.0, 130.8, 129.0, 127.5, 126.8, 108.9, 107.6, 64.8, 35.2, 29.9, 28.9, 26.3, 25.8, 18.0.

HRMS (ESI) calcd for $[M+H]^+$ $C_{20}H_{23}N_2$, *m/z*: 291.1856, found: 291.1865, Error -3.2 ppm.

IR (KBr): 2925, 1635, 1525, 1445, 740, 701 cm^{-1}.



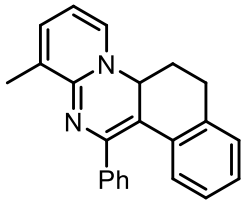
3bi

7-methyl-5-phenyl-1,3,4,11a-tetrahydropyrido[1,2-a]thiopyrano[4,3-e]pyrimidine (3bi)

Obtained as yellow liquid (24.7 mg, 42% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.8 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 2H), 7.30 – 7.25 (m, 1H), 6.82 (d, *J* = 6.3 Hz, 1H), 6.74 (d, *J* = 6.8 Hz, 1H), 6.07 (t, *J* = 6.7 Hz, 1H), 5.20 (dd, *J* = 10.9, 2.5 Hz, 1H), 3.34 (t, *J* = 11.7 Hz, 1H), 3.05 (d, *J* = 13.8 Hz, 1H), 2.81 (td, *J* = 12.7, 2.4 Hz, 1H), 2.61 (d, *J* = 12.0 Hz, 1H), 2.44 (d, *J* = 12.8 Hz, 1H), 2.24 (td, *J* = 13.2, 3.5 Hz, 1H), 2.08 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 148.8, 140.1, 139.3, 131.9, 131.8, 131.6, 128.7, 127.8, 127.2, 108.5, 108.1, 65.2, 34.2, 33.5, 29.0, 18.2.

HRMS (ESI) calcd for $[M+H]^+$ $C_{18}H_{19}N_2S$, *m/z*: 295.1263, found: 295.1255, Error 2.7 ppm.

IR (KBr): 2927, 1643, 1553, 1377, 1061, 735, 701 cm^{-1}.



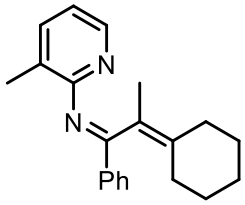
3bj

1-methyl-12-phenyl-5a,6-dihydro-7H-benzo[f]pyrido[1,2-a]quinazoline (3bj)

Obtained as yellow solid (54.5 mg, 84% yield) **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.54 – 7.45 (m, 2H), 7.25 – 7.19 (m, 3H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.98 – 6.91 (m, 3H), 6.77 – 6.68 (m, 2H), 6.15 (t, *J* = 6.7 Hz, 1H), 4.73 (dd, *J* = 11.8, 4.1 Hz, 1H), 3.05 – 2.96 (m, 2H), 2.54 – 2.46 (m, 1H), 2.41 – 2.32 (m, 1H), 2.23 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.4, 141.8, 141.0, 136.1, 134.7, 132.4, 131.4, 130.6, 130.0, 129.2, 128.0, 127.8, 127.4, 125.2, 124.9, 108.9, 104.1, 59.9, 30.6, 28.8, 18.3.

HRMS (ESI) calcd for $[M+H]^+$ $C_{23}H_{21}N_2$, *m/z*: 325.1699, found: 325.1689, Error 4.7 ppm.

IR (KBr): 2926, 1640, 1518, 1449, 736, 701 cm^{-1}.



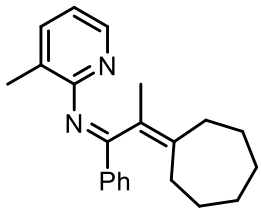
3bk

2-cyclohexylidene-*N*-(3-methylpyridin-2-yl)-1-phenylpropan-1-imine (3bk)

Obtained as yellow liquid (45.8 mg, 75% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.22 – 8.13 (m, 1H), 8.07 – 7.93 (m, 2H), 7.44 (dd, *J* = 16.3, 8.8 Hz, 4H), 6.89 (dd, *J* = 7.4, 4.9 Hz, 1H), 2.21 (s, 3H), 2.06 (d, *J* = 5.8 Hz, 2H), 1.89 (t, *J* = 5.8 Hz, 2H), 1.77 (s, 3H), 1.60 – 1.10 (m, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.1, 162.0, 145.4, 137.7, 137.6, 136.9, 130.7, 128.6, 128.3, 124.5, 123.0, 119.1, 32.7, 29.2, 27.5, 27.2, 3.43, 17.7, 17.3.

HRMS (ESI) calcd for $[M+H]^+$ $C_{21}H_{25}N_2$, *m/z*: 305.2012, found: 305.2026, Error -4.5 ppm.

IR (KBr): 2926, 2853, 1617, 1578, 1446, 1413, 700 cm^{-1}.



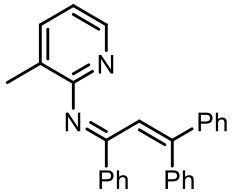
3bl

2-cycloheptylidene-N-(3-methylpyridin-2-yl)-1-phenylpropan-1-imine (3bl)

Obtained as yellow liquid (51.5 mg, 81% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 4.8, 1.2 Hz, 1H), 7.99 (dd, *J* = 7.8, 1.6 Hz, 2H), 7.51 – 7.36 (m, 4H), 6.88 (dd, *J* = 7.4, 4.9 Hz, 1H), 2.23 (s, 3H), 2.15 (s, 2H), 2.04 (s, 2H), 1.79 (s, 3H), 1.53 – 1.13 (m, 8H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.0, 161.8, 145.4, 138.8, 137.7, 137.6, 130.7, 128.6, 128.3, 126.3, 124.7, 119.1, 33.4, 30.5, 30.5, 28.2, 27.1, 27.0, 18.4, 17.4.

HRMS (ESI) calcd for $[M+H]^+$ $C_{22}H_{27}N_2$, *m/z*: 319.2169, found: 319.2178, Error -3.0 ppm.

IR (KBr): 2922, 1616, 1577, 1446, 1413, 785, 701 cm^{-1}.



3bm

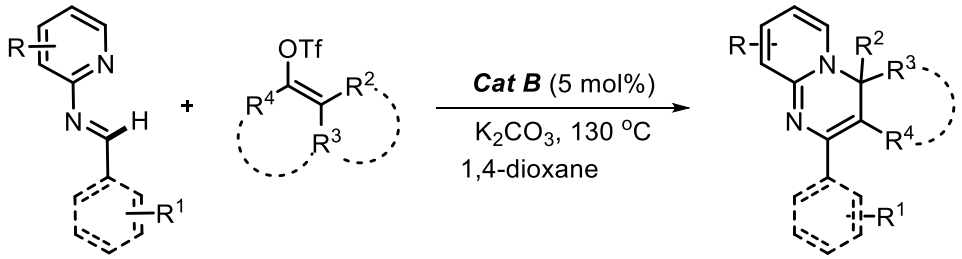
***N*-(3-methylpyridin-2-yl)-1,3,3-triphenylprop-2-en-1-imine (3bm)**

Obtained as yellow solid (47.2 mg, 63% yield, m.p. = 162-164 ºC) at 150 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.24 (d, *J* = 4.1 Hz, 1H), 8.00 (d, *J* = 7.2 Hz, 2H), 7.42 – 7.38 (m, 1H), 7.36 (t, *J* = 7.3 Hz, 2H), 7.32 (t, *J* = 4.1 Hz, 1H), 7.29 – 7.26 (m, 3H), 7.25 – 7.23 (m, 1H), 7.22 (d, *J* = 7.4 Hz, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 7.05 (t, *J* = 7.6 Hz, 2H), 6.85 – 6.80 (m, 2H), 6.77 (d, *J* = 7.3 Hz, 2H), 1.63 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 166.9, 161.2, 146.3, 145.2, 141.9, 139.3, 138.9, 137.7, 130.6, 129.5, 128.5, 128.4, 128.1, 128.1, 127.9, 127.8, 126.2, 124.5, 119.4, 16.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{27}H_{23}N_2$, *m/z*: 375.1856, found: 375.1856, Error -0.1 ppm.

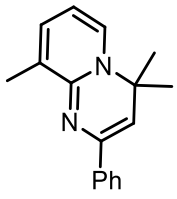
IR (KBr): 2924, 1613, 1574, 1445, 1228, 737, 697 cm^{-1}.

3.2.1 General procedure for C-H vinylation/6π-electrocyclization of 2-pyridyl aldimines with vinyl triflates 4



1 **4** **3**

In glove box, to dry 1,4-dioxane (2 mL) were added substrate **1** (0.2 mmol, 1.0 equiv), substrate **4** (0.4 mmol, 2.0 equiv), K_2CO_3 (0.3 mmol, 1.5 equiv) and **Cat B** (5 mol%) in a 10 mL oven-dried Schlenk tube. Then the tube was sealed and the mixture was stirred at 130 °C for 24 h. After the reaction was completed, the resulting mixture was concentrated in vacuo, and the residual was purified by silica gel column chromatography to give the product **3**.

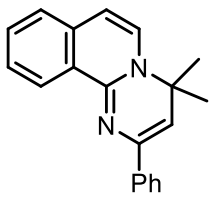


3a

4,4,9-trimethyl-2-phenyl-4H-pyrido[1,2-a]pyrimidine (3a)

Obtained as yellow liquid (49.3 mg, 98% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.1 Hz, 2H), 7.34 (t, *J* = 7.7 Hz, 2H), 7.26 (t, *J* = 7.3 Hz, 1H), 7.16 (d, *J* = 7.1 Hz, 1H), 6.90 – 6.81 (m, 1H), 6.03 (t, *J* = 6.8 Hz, 1H), 5.09 (s, 1H), 2.24 (s, 3H), 1.60 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.0, 141.5, 139.1, 131.6, 131.6, 129.0, 127.9, 127.4, 125.5, 107.9, 102.9, 58.9, 31.1, 18.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{17}H_{19}N_2$, *m/z*: 251.1543, found: 251.1554, Error -4.7 ppm.



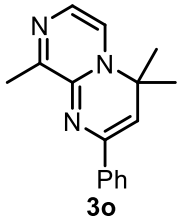
3n

4,4-dimethyl-2-phenyl-4H-pyrimido[2,1-a]isoquinoline (3n)

Obtained as yellow solid (42.1 mg, 74% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.75 (d, *J* = 8.1 Hz, 1H), 7.94 (d, *J* = 7.4 Hz, 2H), 7.49 (t, *J* = 7.0 Hz, 1H), 7.42 (d, *J* = 7.4 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 2H), 7.34 – 7.27 (m, 2H), 7.06 (d, *J* = 7.6 Hz, 1H), 6.36 (d, *J* = 7.6 Hz, 1H), 5.27 (s, 1H), 1.64 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 148.9, 140.6, 138.9, 134.1, 130.9, 128.0, 127.6, 127.5, 127.1, 127.0, 126.6, 125.5, 125.2, 107.8, 106.0, 58.4, 31.4.

HRMS (ESI) calcd for $[M+H]^+$ $C_{20}H_{19}N_2$, *m/z*: 287.1543, found: 287.1549, Error -2.3 ppm.

IR (KBr): 2971, 1636, 1561, 1537, 1344, 781, 677 cm^{-1}.

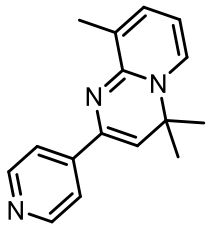


3o

4,4,9-trimethyl-2-phenyl-4H-pyrazino[1,2-a]pyrimidine (3o)

Obtained as yellow liquid (38.4 mg, 76% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.86 – 7.76 (m, 2H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.32 – 7.27 (m, 1H), 7.06 (d, *J* = 4.8 Hz, 1H), 6.88 (d, *J* = 4.8 Hz, 1H), 5.17 (s, 1H), 2.52 (s, 3H), 1.60 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.6, 144.3, 141.3, 138.2, 128.1, 127.9, 125.4, 124.1, 120.7, 105.4, 58.6, 30.8, 21.8.

IR (KBr): 2972, 1537, 1342, 1182, 745, 663 cm^{-1}.



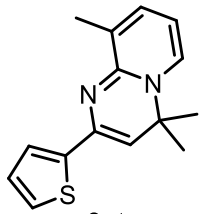
3as

4,4,9-trimethyl-2-(pyridin-4-yl)-4H-pyrido[1,2-a]pyrimidine (3as)

Obtained as yellow liquid (47.9 mg, 95% yield) at 150 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.57 (d, *J* = 4.7 Hz, 2H), 7.79 – 7.71 (m, 2H), 7.21 (d, *J* = 7.1 Hz, 1H), 6.92 (d, *J* = 6.4 Hz, 1H), 6.12 (t, *J* = 6.8 Hz, 1H), 5.26 (s, 1H), 2.24 (s, 3H), 1.65 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.3, 149.7, 146.5, 139.6, 132.3, 131.7, 129.1, 119.9, 108.5, 105.2, 59.2, 31.1, 18.6.

HRMS (ESI) calcd for $[M+H]^+$ $C_{16}H_{18}N_3$, *m/z*: 252.1495, found: 252.1497, Error -0.6 ppm.

IR (KBr): 2972, 1637, 1595, 1517, 1086, 744 cm^{-1}.



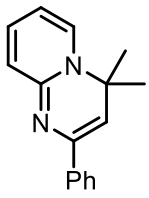
3at

4,4,9-trimethyl-2-(thiophen-2-yl)-4H-pyrido[1,2-a]pyrimidine (3at)

Obtained as yellow liquid (35.2 mg, 69% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.36 – 7.32 (m, 1H), 7.21 –7.14 (m, 2H), 7.02 –6.97 (m, 1H), 6.87 (d, *J* = 6.2 Hz, 1H), 6.06 (t, *J* = 6.6 Hz, 1H), 5.04 (s, 1H), 2.21 (s, 3H), 1.61 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.1, 145.5, 137.6, 132.0, 131.5, 129.0, 127.2, 124.6, 122.1, 108.2, 100.7, 59.0, 31.2, 18.5.

HRMS (ESI) calcd for $[M+H]^+$ $C_{15}H_{17}N_2S$, *m/z*: 257.1107, found: 257.1113, Error -2.3 ppm.

IR (KBr): 2974, 1638, 1535, 1372, 744 cm^{-1}.



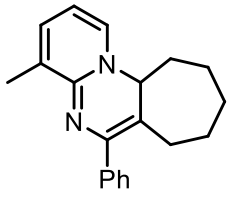
3e

4,4-dimethyl-2-phenyl-4H-pyrido[1,2-a]pyrimidine (3e)

Obtained as yellow liquid (20.4 mg, 43% yield) at 150 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.80 – 7.70 (m, 2H), 7.36 – 7.31 (m, 2H), 7.28 – 7.25 (m, 1H), 7.24 (dd, *J* = 7.1, 0.8 Hz, 1H), 6.96 – 6.89 (m, 1H), 6.73 (d, *J* = 9.1 Hz, 1H), 6.17 – 6.05 (m, 1H), 5.01 (s, 1H), 1.65 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 151.5, 142.1, 139.0, 133.6, 131.4, 128.0, 127.5, 125.6, 124.3, 108.9, 103.3, 59.1, 31.3.

HRMS (ESI) calcd for $[M+H]^+$ $C_{16}H_{17}N_2$, *m/z*: 237.1386, found: 237.1387, Error -0.4 ppm.

IR (KBr): 2971, 1641, 1527, 1395, 754 cm^{-1}.



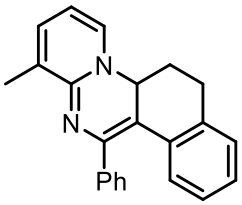
3bh

4-methyl-6-phenyl-7,8,9,10,11,11a-hexahydrocyclohepta[e]pyrido[1,2-a]pyrimidine (3bh)

Obtained as yellow liquid (38.5 mg, 66% yield); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.7 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.25 (t, *J* = 7.4 Hz, 1H), 6.86 (d, *J* = 6.6 Hz, 2H), 6.08 (t, *J* = 6.7 Hz, 1H), 4.42 (dd, *J* = 11.3, 4.1 Hz, 1H), 2.74 – 2.66 (m, 1H), 2.18 (s, 3H), 2.08 – 1.99 (m, 1H), 1.99 – 1.92 (m, 1H), 1.89 – 1.83 (m, 1H), 1.82 – 1.76 (m, 1H), 1.74 – 1.64 (m, 3H), 1.61 – 1.53 (m, 1H), 1.47 – 1.37 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 148.6, 140.5, 140.3, 132.5, 131.5, 130.7, 129.0, 127.6, 126.9, 109.1, 108.0, 64.9, 35.3, 29.9, 28.9, 26.3, 25.9, 18.0.

HRMS (ESI) calcd for $[M+H]^+$ $C_{20}H_{23}N_2$, *m/z*: 291.1856, found: 291.1842, Error 4.7 ppm.

IR (KBr): 2925, 1635, 1525, 743, 701 cm^{-1}.



3bj

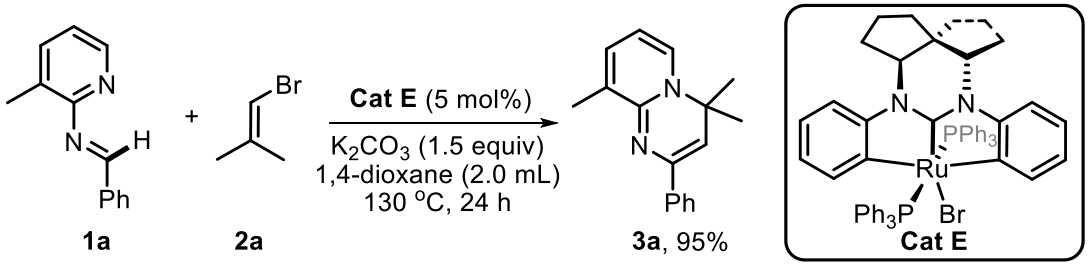
1-methyl-12-phenyl-5a,6-dihydro-7H-benzo[f]pyrido[1,2-a]quinazoline (3bj)

Obtained as yellow solid (48.2 mg, 74% yield) **^{1}H NMR** (400 MHz, CD_2Cl_2) δ 7.43 – 7.36 (m, 2H), 7.28 – 7.20 (m, 3H), 7.05 (d, *J* = 7.5 Hz, 1H), 7.00 (d, *J* = 6.9 Hz, 1H), 6.98 – 6.90 (m, 2H), 6.69 (t, *J* = 7.5 Hz, 1H), 6.62 (d, *J* = 7.7 Hz, 1H), 6.17 (t, *J* = 6.8 Hz, 1H), 4.78 (dd, *J* = 11.7, 4.0 Hz, 1H), 3.09 – 2.98 (m, 2H), 2.56 – 2.48 (m, 1H), 2.45 – 2.33 (m, 1H), 2.15 (s, 3H); **^{13}C NMR** (100 MHz, CD_2Cl_2) δ 150.1, 141.7, 141.3, 136.2, 134.8, 132.6, 131.2, 131.1, 129.8, 128.9, 128.2, 127.8, 127.2, 125.2, 124.6, 108.7, 104.8, 60.1, 31.2, 28.7, 18.1.

HRMS (ESI) calcd for $[M+H]^+$ $C_{23}H_{21}N_2$, *m/z*: 325.1699, found: 325.1711, Error -3.7 ppm.

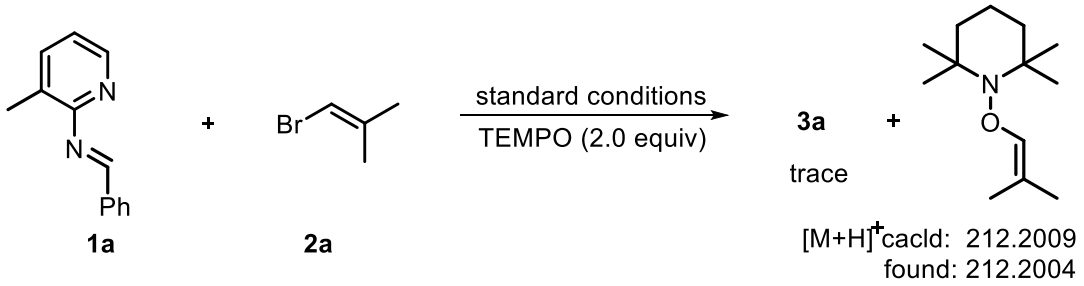
4. Mechanistic studies

4.1 Cat E catalyzed C-H vinylation/6π-electrocyclization of 1a with 2a



In glove box, to dry 1,4-dioxane (2 mL) were added substrate **1** (39.3mg, 0.2 mmol), substrate **2** (54.0 mg, 0.4 mmol), K_2CO_3 (41.2 mg, 0.3 mmol) and **Cat E** (10.2 mg, 5 mol%) in a 10 mL oven-dried Schlenk tube. Then the tube was sealed and the mixture was stirred at 130 °C for 24 h. After the reaction was completed, the resulting solution was concentrated in vacuo, and the residual was purified by silica gel column chromatography to give the product **3a** (47.5 mg, 95% yield). (**Note**: The **Cat E** was prepared according to our reported methods [9]).

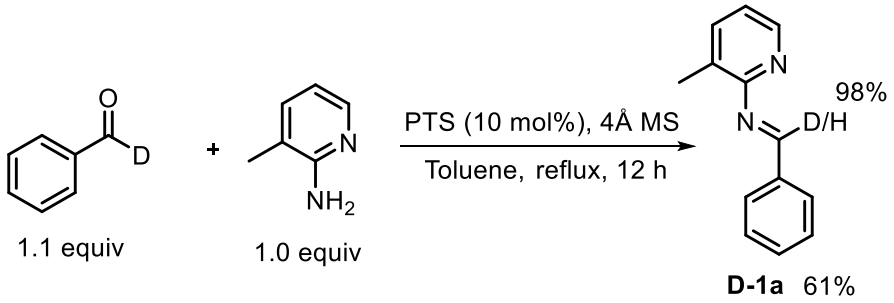
4.2 Radical inhibition experiment



In glove box, to dry 1,4-dioxane (2 mL) were added substrate **1a** (39.3 mg, 0.2 mmol), substrate **2a** (54.0 mg, 0.4 mmol), K_2CO_3 (41.5 mg, 0.3 mmol), **Cat B** (5 mol%) and TEMPO (62.5 mg, 0.4 mmol, 2.0

equiv) in a 10 mL oven-dried Schlenk tube. Then the tube was sealed and the mixture was stirred at 130 °C for 24 h. The reaction mixture was then analyzed by HRMS and the result is shown above.

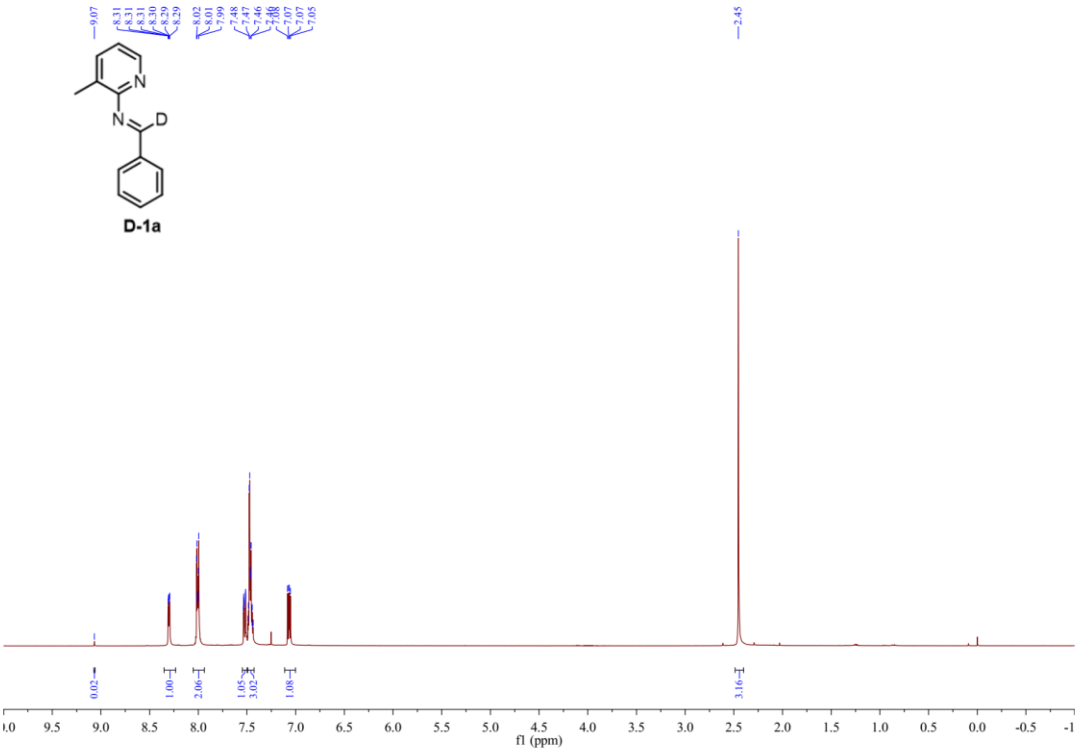
4.3 Synthesis of *N*-(3-methylpyridin-2-yl)-1-phenylmethanimine-*d* (D-1a)



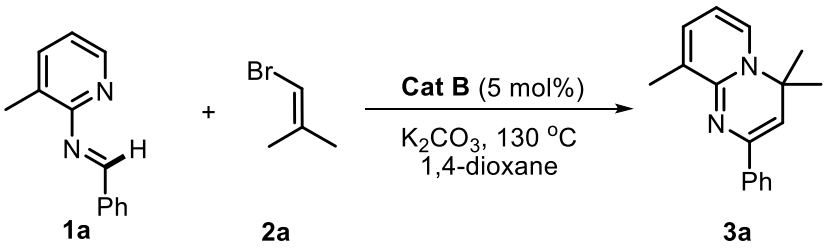
To a dry round-bottom flask equipped with a Dean-Stark apparatus were added anhydrous toluene (10 mL), 3-methylpyridin-2-amine (324.4 mg, 3.0 mmol, 1.0 equiv), D-benzaldehyde (353.5 mg, 3.3 mmol, 1.1 equiv), *p*-toluenesulfonic acid (PTS, 51.7 mg, 10 mol%) and 4Å MS (0.5 g). The reaction mixture was refluxed for 12 h under Dean-Stark conditions and then cooled to room temperature. The molecular sieve was removed by filtration. The solvent was evaporated in vacuo, and the residual was purified by silica gel column chromatography to give the product **D-1a** (98% D).

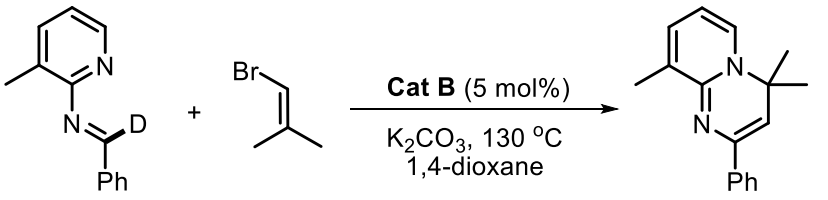
N-(3-methylpyridin-2-yl)-1-phenylmethanimine-*d* (**D-1a**) [2]

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 – 8.23 (m, 1H), 8.05 – 7.94 (m, 2H), 7.54 – 7.51 (M, 1H), 7.49 – 7.43 (m, 3H), 7.07 (dd, *J* = 7.4, 4.8 Hz, 1H), 2.45 (s, 3H).



4.4 KIE determined from parallel reactions





K_H/K_D = 1.05

In glove box, to dry 1,4-dioxane (2 mL) were added K_2CO_3 (41.5 mg, 0.3 mmol, 1.5 equiv), **Cat B** (9.8 mg, 5 mol%), substrate **1a** (39.3 mg, 0.2 mmol, 1.0 equiv) or **D-1a** (39.5 mg, 0.2 mmol, 1.0 equiv), and **2a** (54.0 mg, 0.4 mmol, 2.0 equiv) in a 10 mL oven-dried Schlenk tube. The reaction system was stirred at 130 °C and quenched after reacting for 0.5 h, 1 h, 1.5 h and 2 h respectively. Yield was determined by ^{1}H NMR with 1,3,5-trimethoxybenzene as internal standard.

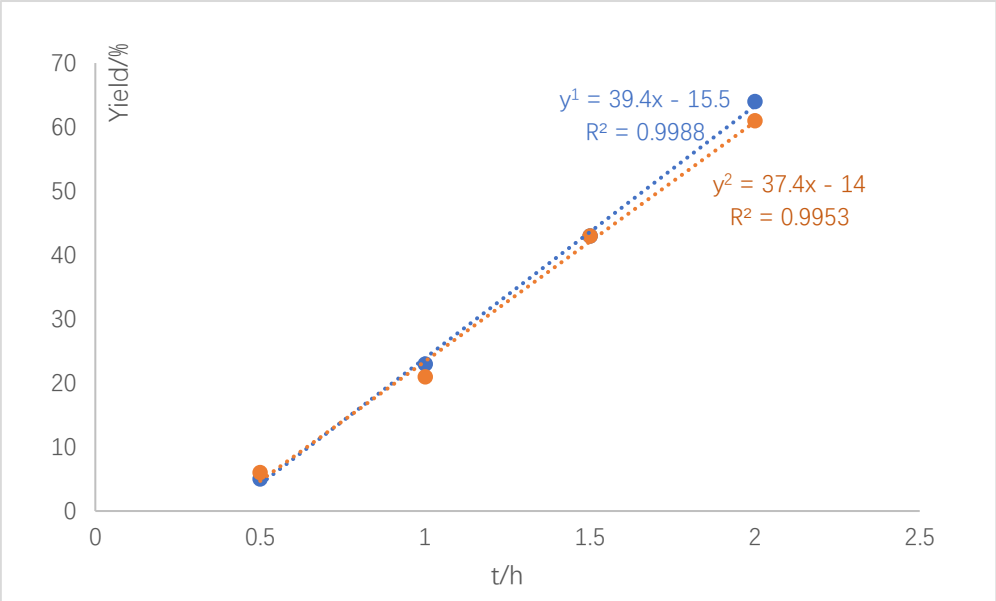
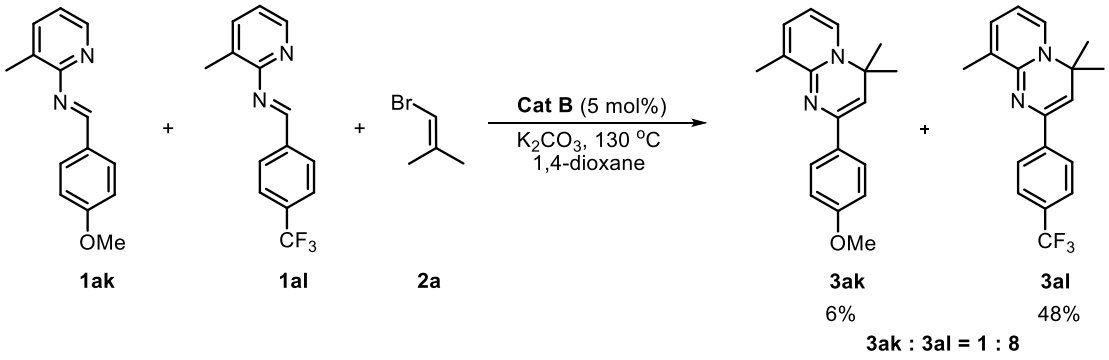


Figure S1 KIE from parallel reactions of **1a**/**D-1a** was determined to k_H / k_D = 1.05

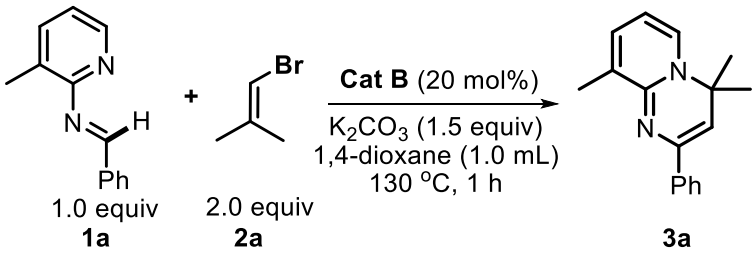
4.5 Competition experiment



In glove box, to dry 1,4-dioxane (2 mL) were added **1ak** (45.3 mg, 0.2 mmol), **1al** (52.9 mg, 0.2 mmol), **2a** (54.0 mg, 0.4 mmol) K_2CO_3 (41.5 mg, 0.3 mmol) and **Cat B** (9.8 mg, 5 mol%) in a 10 mL oven-dried Schlenk tube. The tube was taken out from the glove box, placed in a preheated oil bath (130 °C) and reacted for 3 h under stirring. After that, the mixture was cooled to room temperature. Analysis of the crude using ^{1}H NMR with 1,3,5-trimethoxybenzene as internal standard, with reference to the spectra of pure compounds, showed the formation of **3ak** (6%) and **3al** (48%).

5. In Situ HRMS experiments

5.1 In situ HRMS analysis of the reaction system of 1a with 2a and Cat B



In glove box, to dry 1,4-dioxane (1.0 mL) were added *N*-(3-methylpyridin-2-yl)-1-phenylmethanimine **1a** (19.6 mg, 0.1 mmol, 1.0 equiv), **2a** (27.0 mg, 0.2 mmol, 2.0 equiv), K_2CO_3 (20.8 mg, 0.15 mmol, 1.5 equiv) and **Cat B** (19.5 mg, 0.02 mmol, 0.2 equiv) in a 10 mL oven-dried Schlenk tube. Then the tube was sealed and the mixture was stirred at 130 °C for 1 h. The reaction was cooled to room temperature and diluted with MeOH prior to the injection into the mass spectrometer.

The positive-ion mode of ESI-MS showed the peaks corresponding to the **Cat E** (m/z calcd: 1019.1833, found:1019.1825), **I** (m/z calcd: 757.0921, found:757.0916), **III** (m/z calcd: 611.1749, found: 611.1755), **IV** (m/z calcd: 873.2660, found:873.2666) and **VI** (m/z calcd: 667.2375, found: 667.2376).

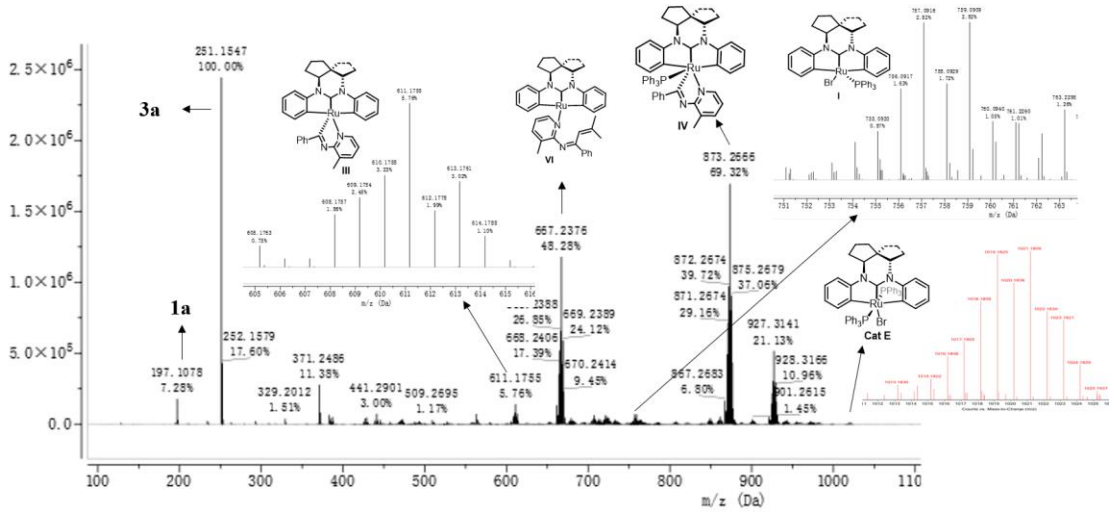
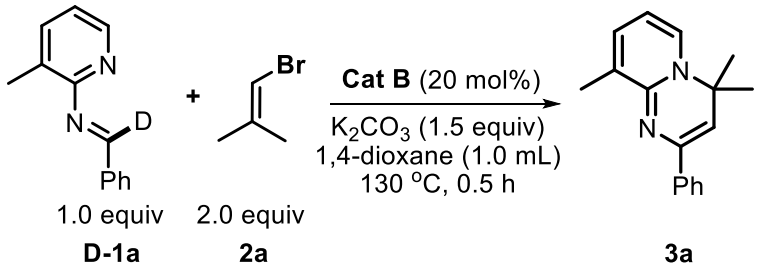


Figure S2 In situ ESI-MS of the reaction system of **1a** with **2a** and **Cat B**

5.2 In situ HRMS analysis of the reaction system of D-1a with 2a and Cat B



In glove box, to dry 1,4-dioxane (1.0 mL) were added *N*-(3-methylpyridin-2-yl)-1-phenylmethanimine-*d* **D-1a** (19.7 mg, 0.1 mmol, 1.0 equiv), **2a** (27.0 mg, 0.2 mmol, 2.0 equiv), K_2CO_3 (20.8 mg, 0.15 mmol, 1.5 equiv) and **Cat B** (19.5 mg, 0.02 mmol, 0.2 equiv) in a 10 mL oven-dried Schlenk tube. Then the tube was sealed and the mixture was stirred at 130 °C for 0.5 h. The reaction was cooled to room temperature and diluted with MeOH prior to the injection into the mass spectrometer.

The positive-ion mode of ESI-MS showed the peaks corresponding to the **D-IV** (m/z calcd: 874.2723, found:875.2723) and **2D-IV** (m/z calcd: 875.2786, found:875.2771).

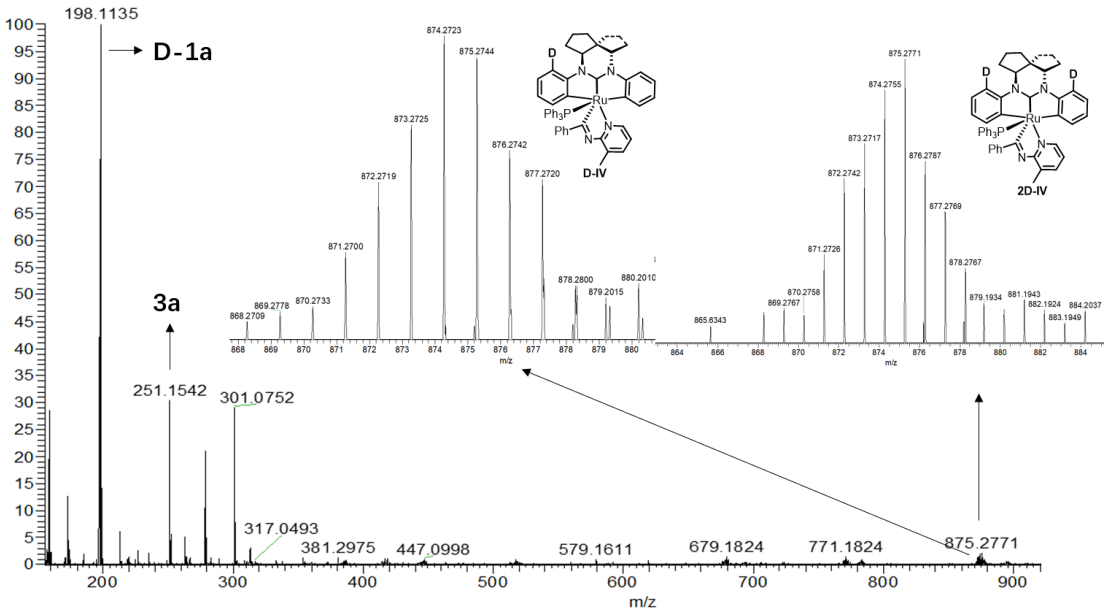
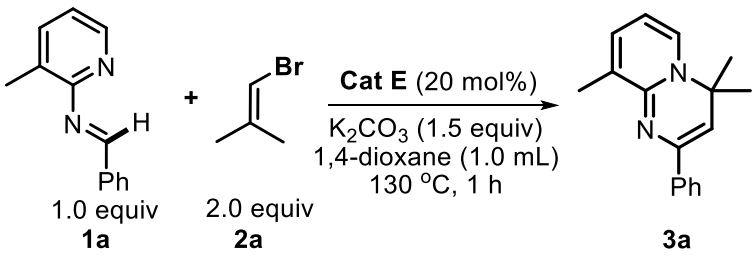


Figure S3 In situ ESI-MS of the reaction system of **D-1a** with **2a** and **Cat B**

5.3 In situ HRMS analysis of the reaction system of 1a with 2a and Cat E



In glove box, to dry 1,4-dioxane (1.0 mL) were added *N*-(3-methylpyridin-2-yl)-1-phenylmethanimine **1a** (9.8 mg, 0.05 mmol, 1.0 equiv), **2a** (13.5 mg, 0.1 mmol, 2.0 equiv), K_2CO_3 (10.4 mg, 0.075 mmol, 1.5 equiv) and **Cat E** (10.3 mg, 0.01 mmol, 0.2 equiv) in a 10 mL oven-dried Schlenk tube. Then the tube was sealed and the mixture was stirred at 130 °C for 1 h. The reaction was cooled to room temperature and diluted with MeOH prior to the injection into the mass spectrometer.

The positive-ion mode of ESI-MS showed the peaks corresponding to the, **I** (m/z calcd: 757.0921, found:757.0948), **III** (m/z calcd: 611.1749, found: 611.1792), **IV** (m/z calcd: 873.2660, found:873.2689) and **VI** (m/z calcd: 667.2375, found: 667.2393)

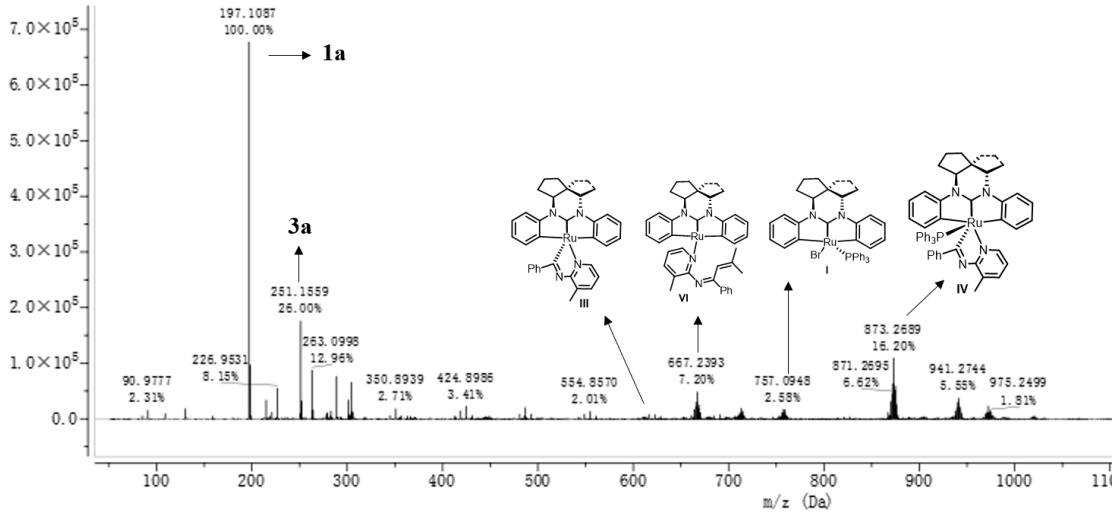
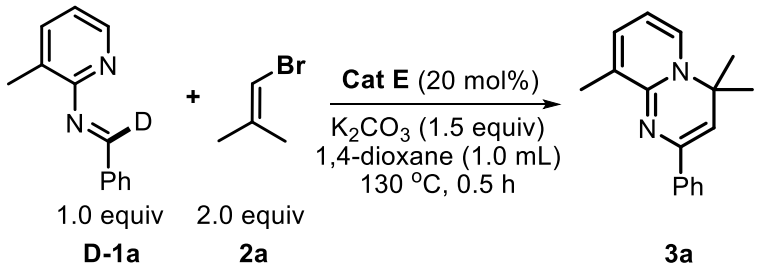


Figure S4 In situ ESI-MS of the reaction system of **1a** with **2a** and **Cat E**

5.4 In situ HRMS analysis of the reaction system of D-1a with 2a and Cat E



In glove box, to dry 1,4-dioxane (1.0 mL) were added *N*-(3-methylpyridin-2-yl)-1-phenylmethanimine-*d* **D-1a** (9.8 mg, 0.05 mmol, 1.0 equiv), **2a** (13.5 mg, 0.1 mmol, 2.0 equiv), K_2CO_3 (10.4 mg, 0.075 mmol, 1.5 equiv) and **Cat E** (10.3 mg, 0.01 mmol, 0.2 equiv) in a 10 mL oven-dried Schlenk tube. Then the tube was sealed and the mixture was stirred at 130 °C for 0.5 h. The reaction was cooled to room temperature and diluted with MeOH prior to the injection into the mass spectrometer.

The positive-ion mode of ESI-MS showed the peaks corresponding to the **D-IV** (m/z calcd: 874.2723, found:875.2732) and **2D-IV** (m/z calcd: 875.2786, found:875.2773).

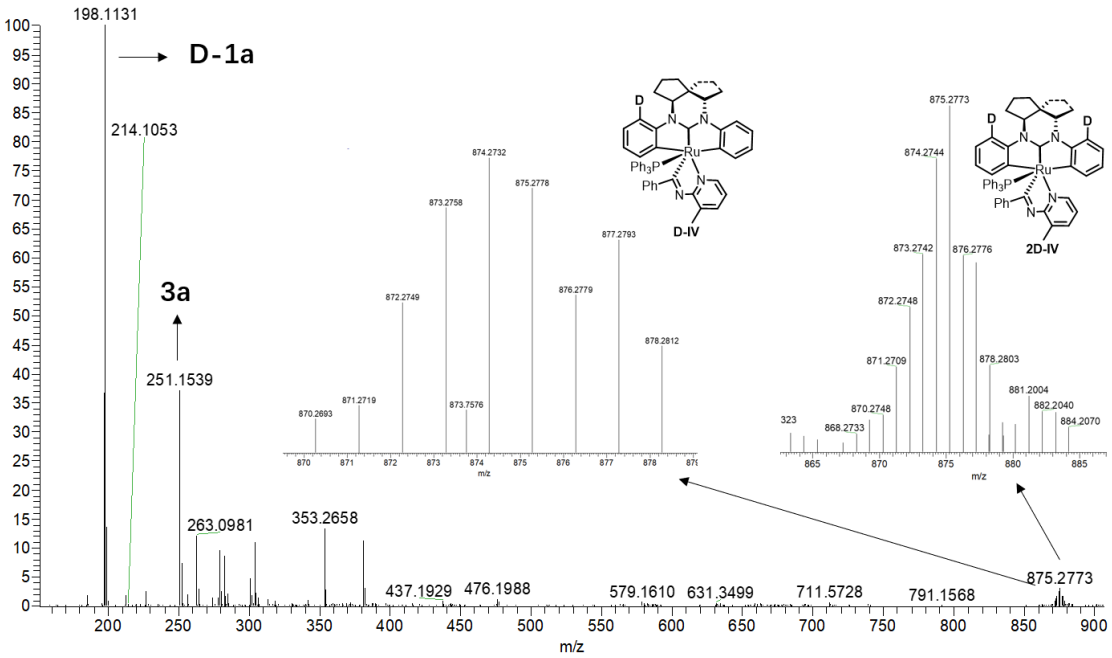


Figure S5 In situ ESI-MS of the reaction system of **D-1a** with **2a** and **Cat E**

5.5 In situ HRMS analysis of the reaction system of 1a with Cat E

In glove box, to dry 1,4-dioxane (0.5 mL) were added *N*-(3-methylpyridin-2-yl)-1-phenylmethanimine **1a** (3.9 mg, 0.02 mmol, 1.0 equiv), K_2CO_3 (4.1 mg, 0.03 mmol, 1.5 equiv) and **Cat E** (20.4 mg, 0.02 mmol, 1.0 equiv) in a 10 mL oven-dried Schlenk tube. Then the tube was sealed and the mixture was stirred at 130 °C for 3 h. The reaction was cooled to room temperature and diluted with MeOH prior to the injection into the mass spectrometer.

The positive-ion mode of ESI-MS showed the peaks corresponding to the **IV** (m/z calcd: 873.2660, found:873.2660).

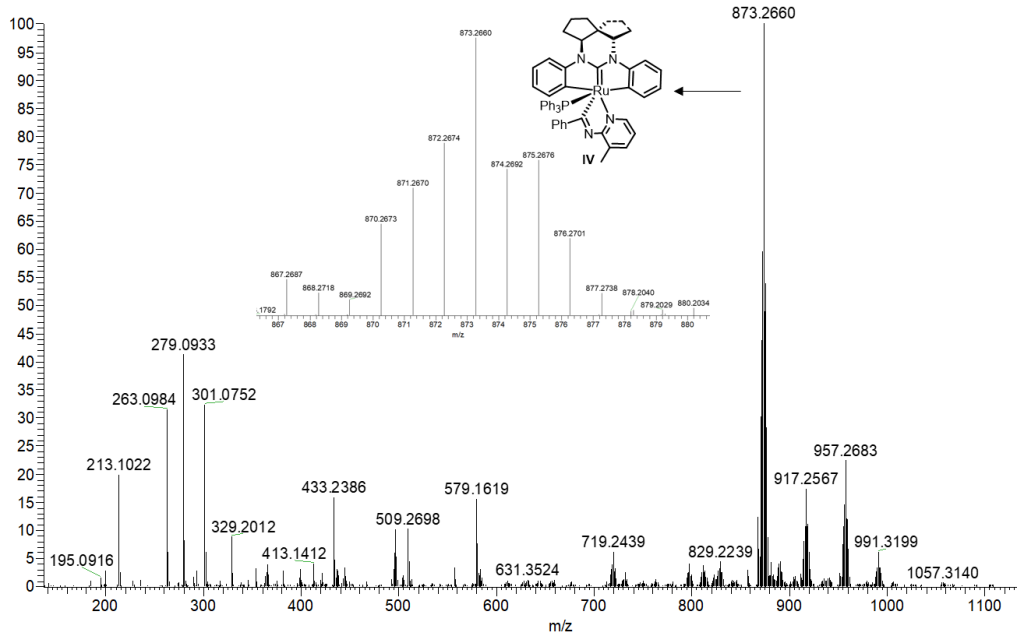


Figure S6 In situ ESI-MS of the reaction system of **1a** with **Cat E**

5.6 In situ HRMS analysis of the reaction system of D-1a with Cat E

In glove box, to dry 1,4-dioxane (0.5 mL) were added *N*-(3-methylpyridin-2-yl)-1-phenylmethanimine-*d* **D-1a** (3.9 mg, 0.02 mmol, 1.0 equiv), K_2CO_3 (4.1 mg, 0.03 mmol, 1.5 equiv) and **Cat E** (20.4 mg, 0.02 mmol, 1.0 equiv) in a 10 mL oven-dried Schlenk tube. Then the tube was sealed and the mixture was stirred at 130 °C for 3 h. The reaction was cooled to room temperature and diluted with MeOH prior to the injection into the mass spectrometer.

The positive-ion mode of ESI-MS showed the peaks corresponding to the **D-IV** (m/z calcd: 874.2723, found:874.2731).

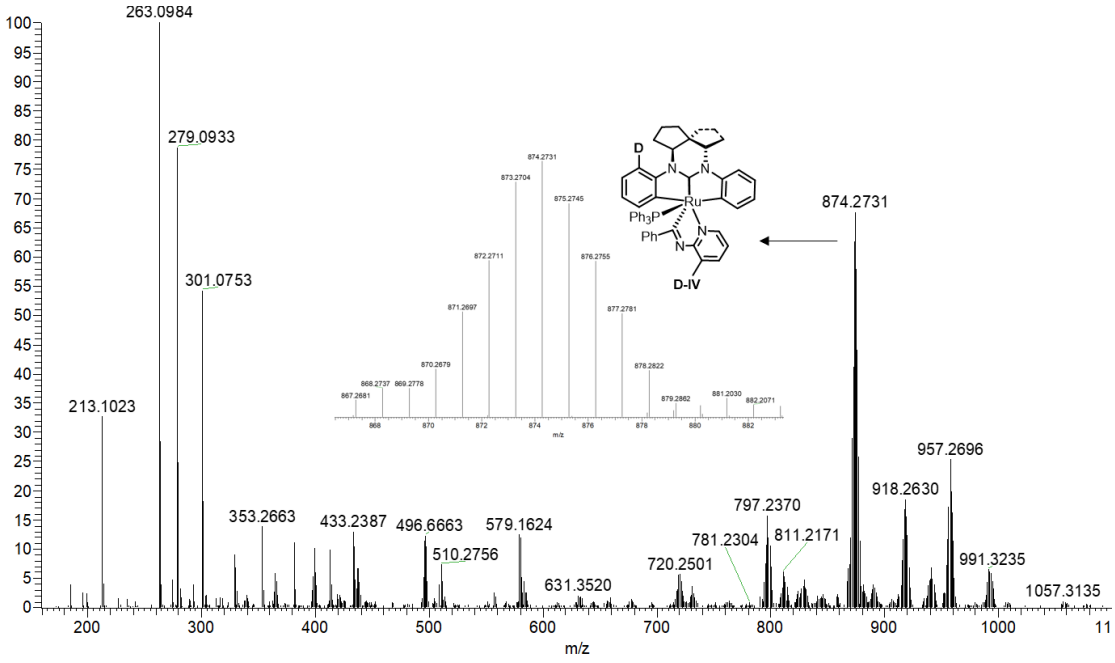


Figure S7 In situ ESI-MS of the reaction system of **D-1a** with **Cat E**

6. DFT calculations

6.1. Computational methods

All the DFT calculations were carried out by using Gaussian 09, Rev. D01.[11] The B3LYP functional [12] was applied to execute the structural optimizations and single point energy calculations, notably Grimme's D3 empirical dispersion term [13] was used during the single point energy calculations. C, H, N, O, K, P, Br and Ru atoms were described by Def2-SVP [14,15] basis set to obtain the optimized geometries and thermal correction of free energy data, while Def2-TZVP [16] basis set was used to get single point energy. The solvation effect of 1,4-Dioxane was stimulated by using SMD [17] continuum solvation model. In addition, the temperature was set to 403.15 K during the calculations according to the experimental condition. For all the geometry optimizations, analysis of vibrational frequency was done to ensure there were no imaginary frequencies for the intermediates and only one imaginary frequency for each transition state.

6.2. Cartesian Coordinates and energies

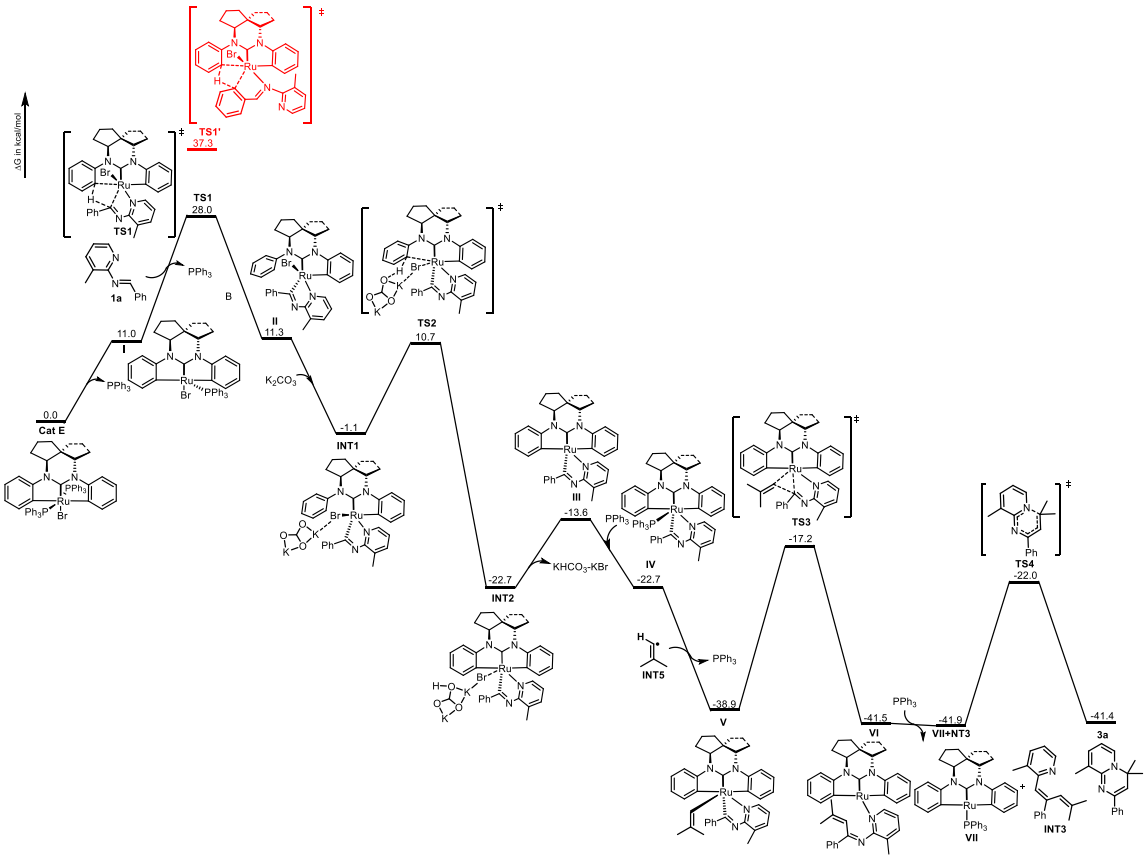


Figure S8 Energy profile of the Ru-catalyzed C–H vinylation/6π-electrocyclization of **1a**

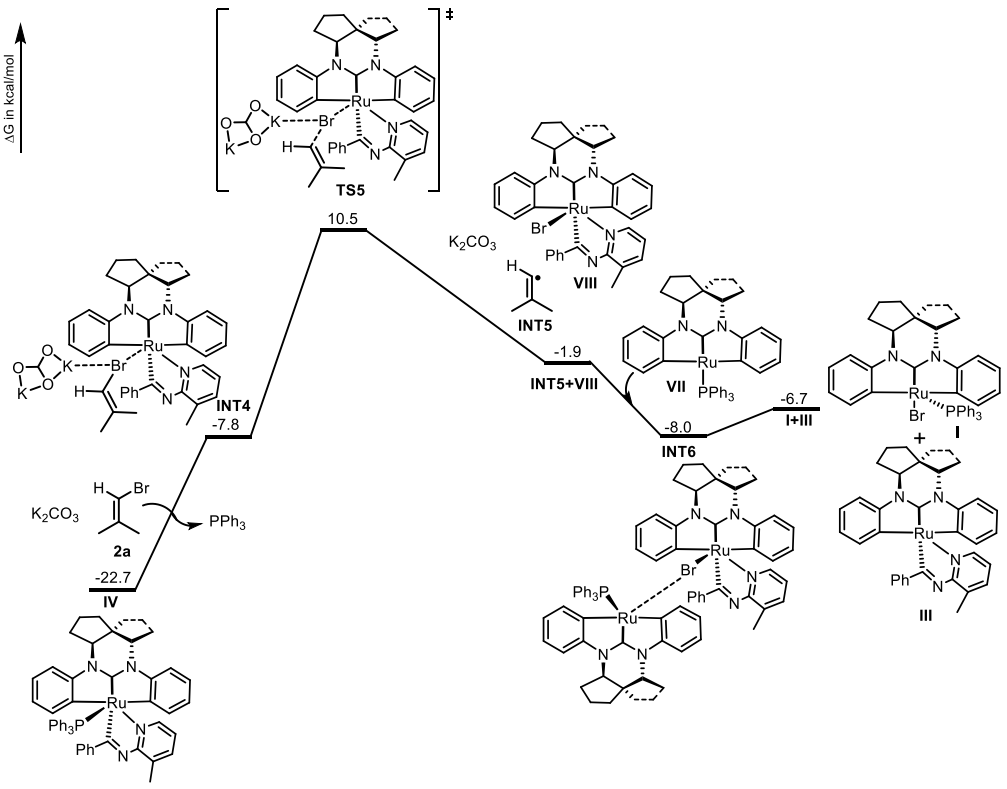


Figure S9 Energy profile for generation of the vinyl radical

Cartesian Coordinates

Cat E

Ru	0.00475900	-0.54369300	-0.02867200
P	-2.42559500	-0.81682000	0.03231800
P	2.47273800	-0.70006500	-0.19342100
N	0.11372700	2.03201600	1.43621100
N	-0.13204100	2.31679800	-0.86846800
C	-0.35807800	4.34002300	0.62663900
C	0.41545300	5.66983300	0.78532600
H	0.00512800	6.20794500	1.65700400
H	0.30743800	6.33829600	-0.08270500
C	1.87483700	5.26408100	1.05054200
H	2.41952400	5.14988100	0.10095100
H	2.41410200	6.02950300	1.62914000
C	1.79754100	3.90339000	1.78282100
H	2.11122600	3.97923100	2.83467500
H	2.45096600	3.15671000	1.31256700
C	0.31048000	3.45701600	1.68756000
H	-0.19329300	3.68305500	2.63766700
C	-1.87755100	4.50517500	0.80471600
H	-2.12658300	5.12894700	1.67822400
H	-2.34666300	3.51892100	0.95940500
C	-2.32757700	5.10056800	-0.52855000
H	-2.12130800	6.18310200	-0.54728700
H	-3.40389400	4.97406000	-0.71618900
C	-1.46617300	4.36005100	-1.57246200
H	-2.03330100	3.52925600	-2.00823400
H	-1.17339900	5.01821300	-2.40377400
C	-0.21270100	3.79730000	-0.82260800
H	0.71540700	4.17370200	-1.28205100
C	-0.01625500	1.49364200	0.20282500
C	0.19502300	1.08888900	2.49589500
C	0.32817900	1.45833100	3.84154900
H	0.40636200	2.50364400	4.14428400
C	0.36424300	0.45757000	4.82144800
H	0.46652900	0.73599700	5.87395100
C	0.26938500	-0.88243700	4.44467000
H	0.29197900	-1.66961800	5.20402500
C	0.15319000	-1.22924000	3.09019700
H	0.09393000	-2.28455700	2.81937500
C	0.12185600	-0.25608400	2.07927000
C	-0.09297800	1.63562200	-2.11846700
C	-0.01737200	2.30160000	-3.34927100
H	0.01829700	3.38855300	-3.40819600

C	0.02456700	1.55550900	-4.53406200
H	0.07903500	2.07204300	-5.49607100
C	-0.00040000	0.16342400	-4.47502100
H	0.02813200	-0.42871100	-5.39425200
C	-0.04170100	-0.48365200	-3.22930900
H	-0.03039100	-1.57416500	-3.22319800
C	-0.07809100	0.22457500	-2.01846100
C	-3.52056800	0.65572200	-0.33468400
C	-3.51627800	1.12764700	-1.66134900
H	-2.84166900	0.68476500	-2.39624100
C	-4.39433600	2.13467100	-2.06637000
H	-4.38464700	2.46963000	-3.10688100
C	-5.28724400	2.70337500	-1.15150200
H	-5.98095700	3.48563400	-1.47077900
C	-5.29108200	2.25375000	0.17001800
H	-5.98856500	2.68201100	0.89498400
C	-4.41894900	1.23549900	0.57510900
H	-4.47546600	0.87969000	1.60317200
C	-3.23351600	-1.97457100	-1.19669200
C	-4.64060600	-2.03651600	-1.24514200
H	-5.24139800	-1.43142400	-0.56305200
C	-5.28974500	-2.86685100	-2.15928600
C	-4.54586100	-3.64566300	-3.05282900
H	-5.05349000	-4.29308300	-3.77301200
C	-3.15255200	-3.58986100	-3.01566700
H	-2.55916100	-4.19620000	-3.70515500
C	-2.50111500	-2.76319200	-2.09200800
H	-1.41527800	-2.75508400	-2.05142100
C	3.17328300	-1.52975500	-1.71792600
C	2.47031100	-2.55420100	-2.37152300
H	1.49807300	-2.86594200	-1.99173400
C	3.02091400	-3.20690200	-3.47930900
H	2.45426500	-4.00331800	-3.96925500
C	4.28287200	-2.84740900	-3.95648300
H	4.71085500	-3.35528100	-4.82502700
C	4.99686300	-1.83511000	-3.30958300
H	5.98960000	-1.54726300	-3.66608300
C	4.44957300	-1.18422300	-2.20104900
H	5.03407400	-0.40452100	-1.71166200
C	3.30631700	-1.65902500	1.16217700
C	3.92721700	-2.89431200	0.91110500
H	3.93883700	-3.31005300	-0.09641500
C	4.53506400	-3.61192100	1.94530300
H	5.00844900	-4.57275000	1.72634300

C	4.53821200	-3.10716600	3.24752600
C	3.91921700	-1.88255000	3.51067200
H	3.90307100	-1.47962500	4.52650600
C	3.30012400	-1.16921200	2.48086500
H	2.81061000	-0.22441500	2.71610200
C	3.45028500	0.88941500	-0.25590100
C	4.47990200	1.21966700	0.63997200
H	4.73052300	0.55432800	1.46559600
C	5.22191800	2.39610000	0.47609300
H	6.02067000	2.62931200	1.18527000
C	4.95720100	3.25662900	-0.59069800
H	5.54451700	4.16911600	-0.72315200
C	3.93986300	2.93321400	-1.49518900
H	3.73065700	3.58732200	-2.34607300
C	3.19232800	1.76564500	-1.32732600
H	2.42388900	1.51987700	-2.06120000
H	-6.38236700	-2.90205100	-2.17575300
H	5.01618900	-3.66782500	4.05533500
C	-3.06749400	-1.46963800	1.64551400
C	-3.52282500	-2.79356100	1.76579700
C	-3.03041300	-0.66826500	2.80109100
C	-3.96268700	-3.28807300	2.99741100
H	-3.53263800	-3.45224100	0.89732400
C	-3.48794800	-1.15784800	4.02675900
H	-2.62837500	0.34453300	2.75747100
C	-3.95869400	-2.46955600	4.12904300
H	-4.30978700	-4.32237400	3.06749300
H	-3.45501900	-0.51354900	4.90890100
H	-4.30889400	-2.85560600	5.09010100
Br	0.06695100	-3.14801000	0.16965000

I

Ru	-0.35755800	-0.01478600	-1.31870800
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N	2.04732300	1.28781500	-0.19192200
N	2.22217700	-1.03704300	-0.28902900
C	4.32427600	0.32962900	0.10676700
C	5.31294500	0.36809800	1.29370200
H	5.98942700	1.22879300	1.15537000
H	5.94632200	-0.53025300	1.35915900
C	4.43644800	0.57902000	2.54082800
H	4.09089800	-0.39031900	2.93346400
H	4.99317200	1.06483500	3.35641000
C	3.22776900	1.41537900	2.05597600

H	3.24736500	2.44322300	2.44883400
H	2.27630200	0.97225200	2.37887400
C	3.32180200	1.42686400	0.50385600
H	3.76236700	2.37696200	0.17621400
C	4.99563800	0.57030800	-1.25883700
H	5.74895500	1.37292500	-1.21327100
H	4.23527300	0.87619900	-1.99871100
C	5.56727300	-0.79590300	-1.63044400
H	6.49595400	-0.98441200	-1.06677300
H	5.81524700	-0.89005000	-2.69886500
C	4.45919200	-1.77300600	-1.20194700
H	3.76617000	-1.94558900	-2.03775400
H	4.85644800	-2.75643900	-0.91416100
C	3.68056000	-1.08577800	-0.02878800
H	3.81289900	-1.65119100	0.90696100
C	1.48780100	0.08521800	-0.45531800
C	1.30461600	2.40225300	-0.67190700
C	1.70822700	3.73275800	-0.51615500
H	2.60572000	4.00028600	0.04448900
C	0.93829200	4.74760900	-1.10350300
H	1.24994100	5.78985100	-0.99354700
C	-0.20825300	4.42492000	-1.82948400
H	-0.80041400	5.21503600	-2.30032500
C	-0.61392400	3.08492500	-1.94522900
H	-1.52834400	2.85190900	-2.49573100
C	0.11906900	2.04725100	-1.35186300
C	1.51823900	-2.23892200	-0.60480800
C	2.03340500	-3.51686400	-0.36094800
H	3.00460600	-3.65952900	0.11384000
C	1.28313600	-4.63763900	-0.74198700
H	1.68003600	-5.63974500	-0.55929900
C	0.04518800	-4.46836100	-1.36181200
H	-0.53430600	-5.34050200	-1.67829200
C	-0.46627600	-3.17758800	-1.57200900
H	-1.44156600	-3.07030500	-2.05109500
C	0.24441500	-2.03414100	-1.17732600
C	-2.67567800	-1.43085800	0.88532800
C	-3.38136500	-1.92518000	-0.22376200
H	-3.18733100	-1.51957000	-1.21839300
C	-4.34498800	-2.92542800	-0.06499600
H	-4.88290700	-3.29583500	-0.94160000
C	-4.61622900	-3.45066000	1.20069900
H	-5.36555200	-4.23744000	1.32188600
C	-3.92389400	-2.96132200	2.31144500

H	-4.13074700	-3.35975100	3.30827100
C	-2.96348000	-1.95778400	2.15773000
H	-2.44550500	-1.58616700	3.04245200
C	-2.53005600	1.46115500	0.92970400
C	-3.93162600	1.36094700	0.94985800
H	-4.41836900	0.39276900	0.83093300
C	-4.72434700	2.50029100	1.12006800
H	-5.81285000	2.40075100	1.12731500
C	-4.13165200	3.75413300	1.28066100
C	-2.73811500	3.86525700	1.26124200
H	-2.26096800	4.84168200	1.37582800
C	-1.94383200	2.73192400	1.07718600
H	-0.86034900	2.84639300	1.04496900
C	-0.49184300	-0.17622100	2.26262100
C	-0.57214200	0.75881000	3.30693100
H	-1.19687200	1.64640600	3.20929400
C	0.13271700	0.55613300	4.49955600
H	0.05667200	1.29626300	5.30042900
C	0.91625100	-0.58645000	4.67123100
H	1.45868200	-0.74693000	5.60665600
C	0.99330900	-1.52990700	3.64059300
H	1.59000800	-2.43696500	3.76846200
C	0.29946800	-1.32600800	2.44635700
H	0.35276200	-2.08431800	1.66358600
H	-4.75247000	4.64380100	1.41543300
Br	-2.12145600	-0.05552500	-3.11317800

TS1

Ru	-0.80754900	-0.51638300	-0.17295300
N	1.70188000	0.80262700	-0.95742600
N	1.96889400	-0.72083200	0.79296800
C	4.02778600	0.05057200	-0.46909200
C	5.27419400	0.83008300	0.00911800
H	5.85572100	1.13904700	-0.87634200
H	5.94539300	0.22718000	0.64027100
C	4.71430700	2.06636500	0.73049100
H	4.47113000	1.81790500	1.77645800
H	5.44215800	2.89103200	0.76708800
C	3.42798400	2.43393000	-0.04489500
H	3.57056700	3.32560000	-0.67356200
H	2.58817200	2.65840700	0.62748800
C	3.10787900	1.19586600	-0.93457100
H	3.39109300	1.41547100	-1.97267200
C	4.33178700	-0.98327500	-1.57111000

H	5.03826800	-0.59037400	-2.31968400
H	3.40017800	-1.24657500	-2.10080700
C	4.85378600	-2.19566600	-0.80315500
H	5.89973100	-2.03063200	-0.49503400
H	4.83357900	-3.12546200	-1.39185600
C	3.92695800	-2.26554700	0.42247800
H	3.05063400	-2.88880900	0.19314200
H	4.42188900	-2.71350100	1.29591100
C	3.44436400	-0.80260600	0.70315000
H	3.83965500	-0.44091300	1.66511600
C	1.16733600	-0.07300900	-0.08790700
C	0.76083700	1.41108200	-1.82755600
C	1.09601900	2.35779300	-2.80194200
H	2.12467700	2.69306700	-2.94366600
C	0.08285700	2.88845700	-3.60951400
H	0.33777900	3.62724000	-4.37388200
C	-1.24178000	2.48450200	-3.43440800
H	-2.03104500	2.90075700	-4.06670900
C	-1.56313000	1.54978800	-2.43806400
H	-2.60772900	1.25588100	-2.30479000
C	-0.56898400	0.98649700	-1.63265200
C	1.26996100	-1.48252300	1.76088300
C	1.89524600	-2.17105700	2.80838700
H	2.97673100	-2.14329100	2.93725200
C	1.11947400	-2.91501100	3.70559300
H	1.61331800	-3.45144500	4.51990400
C	-0.26721700	-2.97411700	3.56538500
H	-0.86900800	-3.56404600	4.26154700
C	-0.89034500	-2.25744900	2.53417100
H	-1.97961100	-2.28565500	2.44487900
C	-0.13609600	-1.51627400	1.61756000
C	-5.12437600	-0.22054200	0.20763400
C	-3.71142100	-0.07977500	0.19815800
C	-3.43538000	-2.13474200	-0.89277400
C	-4.80660500	-2.34470600	-0.92085700
C	-5.65282200	-1.37623700	-0.36363700
H	-2.72489900	-2.84580200	-1.31991400
H	-5.20718300	-3.25351100	-1.37359300
H	-6.73633400	-1.52384700	-0.37507600
N	-3.12615800	1.03222900	0.74427900
N	-2.89820200	-1.02853900	-0.34431500
C	-5.98610300	0.84789200	0.81922900
H	-5.84883800	1.81393400	0.30694400
H	-5.72114500	1.01979600	1.87465400

H	-7.05060800	0.57536600	0.76624800
C	-1.82289800	1.07763100	0.78266700
H	-1.04723400	-0.15879400	1.39558800
C	-1.21824700	2.30041600	1.37484500
C	-0.00544000	2.26682900	2.08558000
C	-1.89447300	3.53195700	1.26010600
C	0.50929400	3.42435000	2.67543100
H	0.52749700	1.32273200	2.20354300
C	-1.36629400	4.69089100	1.82624900
H	-2.83853800	3.56149300	0.71442900
C	-0.16365900	4.64184700	2.54076200
H	1.44158500	3.37369500	3.24405700
H	-1.89767600	5.63973200	1.71382000
H	0.24593100	5.54946800	2.99201400
Br	-0.09649600	-2.39679900	-1.78759600

TS1'

Ru	-0.59360100	0.18826200	0.09391200
N	2.13391500	0.90566500	-0.66237900
N	2.02128800	-0.99848700	0.68584100
C	4.13940300	-0.55313100	-0.61722700
C	5.60143900	-0.30940900	-0.18158900
H	6.17750500	0.00857900	-1.06652300
H	6.09067700	-1.21532300	0.20792200
C	5.54453300	0.83449600	0.85499200
H	5.51296200	0.43271400	1.87954800
H	6.44222300	1.46838900	0.80017500
C	4.24432300	1.62017800	0.54509800
H	4.42765700	2.67838000	0.30772400
H	3.55809100	1.60452700	1.40542500
C	3.59143400	0.88144200	-0.65242200
H	3.93543400	1.33071400	-1.59436000
C	4.00691800	-1.31603100	-1.94801400
H	4.73138900	-0.96485800	-2.70006900
H	2.99626800	-1.16393500	-2.36377400
C	4.19056600	-2.77990700	-1.54879100
H	5.26032600	-3.00300900	-1.40150500
H	3.81539800	-3.48507900	-2.30600600
C	3.42112400	-2.89345100	-0.21913100
H	2.38612000	-3.21055200	-0.40896700
H	3.86695600	-3.63743700	0.45675600
C	3.40282500	-1.46194000	0.41571800
H	3.93495000	-1.45279900	1.37956100
C	1.39986800	0.02009700	0.03771200

C	1.37989100	1.96208600	-1.23614100
C	1.94210800	3.00441400	-1.98103600
H	3.01472900	3.05212100	-2.17743600
C	1.10549000	4.01136900	-2.47796900
H	1.53672800	4.82852500	-3.06228900
C	-0.26566100	3.97786700	-2.21714800
H	-0.91594800	4.77024800	-2.59884500
C	-0.80874100	2.93143900	-1.45568900
H	-1.88182400	2.93347600	-1.24667000
C	-0.00618700	1.89180000	-0.97206700
C	1.18662700	-1.71663400	1.57618900
C	1.63287400	-2.78480200	2.36545300
H	2.67312800	-3.10832700	2.34642500
C	0.72386900	-3.45831500	3.19073400
H	1.07806700	-4.29137900	3.80366100
C	-0.61899700	-3.08211900	3.22851600
H	-1.32763600	-3.62469700	3.85962000
C	-1.05512200	-1.99441800	2.45907500
H	-2.10652000	-1.69671200	2.49250700
C	-0.16533900	-1.30336100	1.62948900
C	-4.12923700	-0.46508100	-1.69645500
C	-3.74880500	-0.58087400	-0.34013400
C	-5.10392400	-2.39956900	0.02452000
C	-5.53580700	-2.40611900	-1.30009800
C	-5.04492600	-1.41801200	-2.15629100
H	-5.47168800	-3.14395200	0.73972200
H	-6.24358600	-3.15986400	-1.65204600
H	-5.37518100	-1.37978800	-3.19821400
N	-2.79199100	0.31361700	0.23463900
N	-4.23368700	-1.50067700	0.49230100
C	-3.62062500	0.63740300	-2.58122300
H	-2.52287900	0.61264800	-2.64988500
H	-3.90847800	1.62902300	-2.19380400
H	-4.03141300	0.54344600	-3.59733500
C	-3.22320700	1.13124900	1.14816700
H	-0.56002300	0.19781600	1.77006800
C	-2.27064200	1.92306000	1.88542100
C	-0.89608600	1.61293000	1.67340900
C	-2.66185900	2.95350900	2.76272900
C	0.05482600	2.36565700	2.38809800
C	-1.69664100	3.69477300	3.43543100
H	-3.72506800	3.16847400	2.90416700
C	-0.33780300	3.39702100	3.24265900
H	1.11871500	2.14587700	2.27119900

H	-1.99181400	4.49997900	4.11243500
H	0.42351900	3.97700200	3.77195800
Br	-0.59091300	-1.41236500	-1.90700700
H	-4.29612100	1.19846400	1.37725800

II

Ru	-0.81812000	-0.49471500	-0.24472400
N	1.56308800	0.96516600	-0.97555700
N	2.04002700	-0.56087700	0.72382700
C	3.96116200	0.38542500	-0.70038100
C	5.15310600	1.19815500	-0.14667500
H	5.65845000	1.70269900	-0.98838500
H	5.90791100	0.57180400	0.35431600
C	4.50996400	2.24066800	0.78002300
H	4.30115000	1.79370400	1.76613300
H	5.16733100	3.10496900	0.95963400
C	3.18869400	2.62451400	0.07670200
H	3.27166900	3.59223300	-0.44089200
H	2.35150500	2.71870000	0.78050900
C	2.92520100	1.49221100	-0.96152200
H	3.12849400	1.87497500	-1.96822800
C	4.29804500	-0.44033400	-1.96001400
H	5.01438300	0.08189700	-2.61389800
H	3.37891200	-0.61241500	-2.54613500
C	4.80454000	-1.77359600	-1.41608700
H	5.83698700	-1.67042200	-1.03966800
H	4.81141400	-2.57739300	-2.16861400
C	3.82796700	-2.05947100	-0.26950300
H	2.90099700	-2.49979200	-0.66887000
H	4.23575600	-2.76806800	0.46448000
C	3.48119500	-0.66988400	0.35310100
H	4.04392200	-0.51095100	1.28296500
C	1.11791800	0.03165300	-0.09930600
C	0.57312100	1.46810000	-1.84917800
C	0.80647200	2.43835200	-2.83258200
H	1.79055800	2.88859100	-2.96858800
C	-0.24538700	2.84142000	-3.66077500
H	-0.06172500	3.59614900	-4.42980900
C	-1.52114600	2.28987100	-3.50698200
H	-2.33844700	2.60634900	-4.16060700
C	-1.75529700	1.34242100	-2.50525000
H	-2.75829700	0.92807200	-2.38467600
C	-0.71819700	0.91087700	-1.66352100
C	1.58728400	-1.35086200	1.81742400

C	2.47013500	-2.15349600	2.56804700
H	3.53113400	-2.18668400	2.33797000
C	2.00798800	-2.94393200	3.62297900
H	2.72727100	-3.55642300	4.17298600
C	0.65723000	-2.96860400	3.97161100
H	0.30121900	-3.59831100	4.78990700
C	-0.22563100	-2.15315900	3.26210700
H	-1.28484600	-2.11691800	3.52827500
C	0.23306500	-1.34933600	2.21808600
C	-5.13633300	-0.49923900	0.20607300
C	-3.73525000	-0.27281800	0.17630600
C	-3.36910700	-2.22462900	-1.06338600
C	-4.72733000	-2.51391000	-1.08120900
C	-5.61304800	-1.64003300	-0.43799700
H	-2.62766500	-2.87140200	-1.53808400
H	-5.08498800	-3.41110400	-1.58977500
H	-6.68652300	-1.84963200	-0.43743100
N	-3.20354800	0.83441600	0.78706700
N	-2.88389100	-1.12955000	-0.45144600
C	-6.04405500	0.47120100	0.90876900
H	-5.97482600	1.47687700	0.46341800
H	-5.76379100	0.58650100	1.96789100
H	-7.09216900	0.14020000	0.85819800
C	-1.90305500	0.98026200	0.74529900
H	-0.49487000	-0.62395800	1.81765000
C	-1.40936900	2.23537600	1.38852700
C	-0.16710800	2.32037900	2.04177300
C	-2.22796900	3.38527300	1.37552600
C	0.23366200	3.49902100	2.67795400
H	0.48647600	1.44932100	2.07888900
C	-1.81534300	4.57069100	1.98190400
H	-3.19516800	3.32738700	0.87450300
C	-0.58364700	4.63174900	2.64358600
H	1.19257700	3.53193700	3.20211000
H	-2.46063700	5.45274000	1.94401600
H	-0.26324200	5.55740900	3.12924000
Br	0.04570800	-2.66261600	-1.38906800

INT1

C	-2.47739200	4.39883300	0.08112900
C	-1.49399300	3.37657800	-0.02680000
C	-2.76207100	2.22289600	-1.62360000
C	-3.75360400	3.19545900	-1.59852100
C	-3.61007400	4.28281000	-0.72073100

H	-2.81381700	1.35240700	-2.28374800
H	-4.61711300	3.11505800	-2.26248300
H	-4.38407400	5.05393400	-0.67492500
N	-0.32433000	3.46598500	0.67688000
N	-1.67004100	2.29760100	-0.83899600
C	-2.26419100	5.54886500	1.02314000
H	-1.31891400	6.07029400	0.80517800
H	-2.18722700	5.19795300	2.06521500
H	-3.09036300	6.27249100	0.96096100
C	0.54706400	2.49528500	0.52099300
C	1.82223400	2.68705300	1.26814600
C	3.05700000	2.24518800	0.76119700
C	1.81189300	3.35828400	2.50892400
C	4.24316100	2.47438900	1.46388400
H	3.08949100	1.74971700	-0.20795700
C	2.99183200	3.56015900	3.22411200
H	0.85804300	3.71094800	2.90400200
C	4.21472400	3.12185800	2.70288300
H	5.19639400	2.14764600	1.03953600
H	2.95991600	4.06777800	4.19209800
H	5.14160700	3.28857900	3.25837300
C	0.68098500	-0.90735100	2.04701900
C	1.32396800	-0.34017900	3.15797500
C	0.57714400	0.00150200	4.28680600
C	-0.80706200	-0.21556700	4.31232500
C	-1.44976800	-0.78313500	3.20989500
C	-0.70066800	-1.13546400	2.07813800
H	1.08014700	0.44795700	5.14872400
H	-1.38292300	0.05139100	5.20281400
H	-2.52748200	-0.99620900	3.17536200
H	-1.20961100	-1.63022700	1.25085600
N	1.47504200	-1.28268100	0.89483800
C	1.38312200	-0.50410800	-0.19432000
N	2.27216000	-0.67088600	-1.21204000
C	2.15360900	0.28383700	-2.24221900
C	2.98080700	0.33061800	-3.36960500
C	1.13800800	1.26018800	-2.03869500
C	2.80617500	1.35836800	-4.30427400
H	3.76069000	-0.41507800	-3.53121100
C	1.00279800	2.28983500	-2.98274600
C	1.82492300	2.33611300	-4.11460900
H	3.45298000	1.39503800	-5.18466300
H	0.23882700	3.05718700	-2.84075400
H	1.70267100	3.13955200	-4.84564900

C	3.34262000	-1.66298200	-1.18323200
H	3.48505700	-2.02356500	-2.21343500
C	2.38388000	-2.45106100	1.05030000
C	2.96893300	-2.87977300	-0.31941800
C	4.34877900	-3.55219100	-0.14215600
C	4.69096800	-1.15476900	-0.61822900
H	4.49651300	-0.39869600	0.15662300
H	5.29841400	-0.66528300	-1.39358500
C	5.37600300	-2.40522200	-0.00977400
H	6.31548100	-2.65533100	-0.52501700
H	5.64030300	-2.22543500	1.04330600
H	4.55769600	-4.14438900	-1.04802600
H	4.37232400	-4.25492100	0.70473300
H	3.17163100	-2.17682100	1.77064400
C	1.60828000	-3.69878900	1.50141000
H	2.33934300	-4.44176500	1.85858600
H	0.91376900	-3.50648700	2.33054400
C	0.91687100	-4.18928100	0.22026800
H	-0.03749300	-3.65432600	0.10130300
H	0.69117700	-5.26601300	0.25879900
C	1.88148700	-3.81204900	-0.93072900
H	2.35763300	-4.69993800	-1.37502300
H	1.34267300	-3.30079100	-1.74328700
Ru	-0.07854400	0.85910300	-0.52539300
Br	-1.52983800	-1.09714700	-1.71801300
H	2.39959200	-0.15418400	3.13037400
K	-2.83749500	-4.13568700	-0.70698800
C	-4.03054100	-2.50081200	1.29159200
O	-4.23412200	-1.42535000	1.97346300
O	-4.66887300	-2.64983600	0.14434400
K	-4.64873800	-0.16260400	-0.16549900
O	-3.18348700	-3.39028600	1.65832800

TS2

C	5.04910500	0.99639700	-0.00417100
C	3.62416500	0.96730400	0.04280800
C	3.64168400	-1.11594800	1.11384600
C	5.02768900	-1.15317100	1.12170600
C	5.73294300	-0.08685800	0.53492100
H	3.03392800	-1.88859300	1.59441800
H	5.55226300	-1.98462100	1.59741000
H	6.82656500	-0.09472300	0.52443700
N	2.89519000	2.03557900	-0.38402400
N	2.95021900	-0.10197200	0.55466200

C	5.75034700	2.18571100	-0.59551000
H	5.48061500	3.10895500	-0.05801400
H	5.45177900	2.34716700	-1.64388200
H	6.84316800	2.06288200	-0.55866600
C	1.58637700	1.94729800	-0.25144100
C	0.85272400	3.18468100	-0.65138500
C	-0.27736900	3.64423500	0.04656800
C	1.32346700	3.95397900	-1.73531300
C	-0.91199600	4.83431000	-0.32021800
H	-0.63512200	3.08267800	0.90794000
C	0.67235200	5.12615400	-2.11984600
H	2.20847400	3.61158100	-2.27322000
C	-0.44763200	5.57464000	-1.41118800
H	-1.77284300	5.18775500	0.25411600
H	1.04467400	5.69809900	-2.97441700
H	-0.95236600	6.49908400	-1.70509300
C	-1.07998900	0.51039600	-2.07341900
C	-1.59360800	1.17146100	-3.19987000
C	-0.74812500	1.48204200	-4.26475500
C	0.61082100	1.14301100	-4.21695300
C	1.09753200	0.44962000	-3.11380100
C	0.27345600	0.08831200	-2.02171500
H	-1.15324000	2.00754600	-5.13380800
H	1.26966700	1.39125800	-5.05316600
H	2.13679600	0.10963800	-3.11400400
H	0.56003000	-1.07719200	-1.72571700
N	-1.87021700	0.36227100	-0.90142800
C	-1.17536500	0.44937900	0.25476900
N	-1.83644100	0.67776600	1.41498900
C	-0.98304400	0.96569400	2.50722900
C	-1.44135400	1.27775400	3.79108000
C	0.40033500	0.95546000	2.18702700
C	-0.51072900	1.60585000	4.78512500
H	-2.50606300	1.27363800	4.03146000
C	1.30078900	1.30558400	3.20195900
C	0.85466700	1.62425500	4.49286200
H	-0.86295900	1.85558200	5.78956400
H	2.37349800	1.31763800	2.99577800
H	1.57750900	1.89059500	5.26917700
C	-3.28533200	0.82933800	1.48731600
H	-3.61592600	0.41760400	2.45405900
C	-3.34387900	0.25309000	-1.01296900
C	-3.99983400	0.04263800	0.37754500
C	-5.41952400	0.66009700	0.40712400

C	-3.79559400	2.27987000	1.33766900
H	-3.17244000	2.79845100	0.59363800
H	-3.71230100	2.84781300	2.27556500
C	-5.25069500	2.14214800	0.83282100
H	-5.97821000	2.40344800	1.61633900
H	-5.43977100	2.83035400	-0.00461400
H	-6.02182100	0.11710700	1.15352600
H	-5.94207100	0.55366000	-0.55533200
H	-3.71368000	1.18307200	-1.47040400
C	-3.74278200	-1.00140500	-1.84777800
H	-4.40350000	-0.73248400	-2.68533800
H	-2.83744900	-1.46918600	-2.26187200
C	-4.42892000	-1.97797200	-0.86305400
H	-4.15092100	-3.02407000	-1.06982100
H	-5.52624100	-1.92737800	-0.95277500
C	-4.00412900	-1.48944600	0.52872800
H	-4.66959900	-1.82573300	1.34045000
H	-2.98216800	-1.82611700	0.77629500
Ru	0.81246400	0.17999200	0.34580600
Br	0.32899600	-2.32977500	1.52544600
H	-2.63858800	1.47930000	-3.24371200
K	-1.70567900	-4.46644400	0.00441400
C	0.02233100	-3.33599000	-1.88236900
O	0.98455400	-2.44516100	-2.00400800
O	0.36405600	-4.53869900	-1.53724400
K	2.57801000	-3.76612900	-0.54756300
O	-1.19433700	-3.00844700	-2.02849900

INT2

C	-4.17093000	-3.47428500	-0.00296600
C	-3.30839100	-2.34040900	-0.00366800
C	-1.61677100	-3.55245800	-1.09222900
C	-2.40063800	-4.69371300	-1.13114200
C	-3.69142500	-4.64707400	-0.57512700
H	-0.60615800	-3.52768200	-1.50648100
H	-2.01441400	-5.60615700	-1.58966800
H	-4.32728100	-5.53707900	-0.59368500
N	-3.70787700	-1.15607100	0.53745300
N	-2.05287700	-2.40109400	-0.53850600
C	-5.54113400	-3.36745300	0.60471800
H	-6.13225000	-2.57423400	0.11975800
H	-5.48440100	-3.09278200	1.67076500
H	-6.08999700	-4.31756200	0.51748900
C	-2.84108000	-0.16207700	0.45732800

C	-3.31602200	1.09951200	1.10325800
C	-3.16572900	2.35963600	0.50035000
C	-3.97259000	1.03177100	2.34886900
C	-3.66177900	3.51243200	1.11689100
H	-2.68918200	2.42812000	-0.47692500
C	-4.44005000	2.18605900	2.97869200
H	-4.10892200	0.05497000	2.81645800
C	-4.29097700	3.43344900	2.36282600
H	-3.55869900	4.47942700	0.61658000
H	-4.93304600	2.11121800	3.95224900
H	-4.66866900	4.33743000	2.84866700
C	0.52507000	0.56436000	1.96934400
C	1.10913400	0.70452900	3.23744400
C	0.81621600	-0.23471800	4.23909400
C	-0.06906700	-1.28474000	3.98003800
C	-0.66690000	-1.39258500	2.70974900
C	-0.37108500	-0.49646800	1.66919900
H	1.27083000	-0.12467800	5.22717100
H	-0.31314600	-2.00508900	4.76651900
H	-1.37909000	-2.20522800	2.53535000
H	5.37356100	-0.40616800	2.04931600
N	0.75637500	1.46387700	0.89684200
C	-0.03664000	1.21810300	-0.18512500
N	-0.05475600	2.10611100	-1.20208300
C	-0.90787100	1.73992600	-2.27908000
C	-1.08319600	2.52165200	-3.42635700
C	-1.58681800	0.51239300	-2.08592900
C	-1.95365900	2.07212700	-4.42839900
H	-0.56182800	3.47191300	-3.55805900
C	-2.45980500	0.10468900	-3.10496000
C	-2.63736000	0.86535700	-4.27181000
H	-2.09740100	2.67701000	-5.32789900
H	-3.01417300	-0.83254400	-3.00184600
H	-3.31922900	0.51639400	-5.05306900
C	0.63891200	3.38589200	-1.13862700
H	0.89883200	3.67619000	-2.16710100
C	1.79040600	2.51822300	0.99157600
C	1.95293400	3.28531900	-0.35311000
C	2.28633700	4.77413700	-0.09605100
C	-0.15092500	4.52822400	-0.46204000
H	-0.73690100	4.11339700	0.37120600
H	-0.86739900	4.99719400	-1.15262200
C	0.92842600	5.50807000	0.05866200
H	0.93219100	6.45193600	-0.50743800

H	0.73245500	5.77948500	1.10702200
H	2.83134000	5.16469300	-0.97089500
H	2.94593200	4.91579600	0.77366300
H	1.48344800	3.20440400	1.79751900
C	3.21449600	1.93252400	1.27446000
H	3.64234600	2.35184200	2.19766800
H	3.14620700	0.84809800	1.42760500
C	4.09093900	2.23894100	0.03976400
H	4.77640200	1.40885500	-0.19011300
H	4.71107400	3.13263400	0.21743600
C	3.07724800	2.51866200	-1.07169800
H	3.49327100	3.08881500	-1.91772100
H	2.67733800	1.57148000	-1.47291500
Ru	-1.04107500	-0.52404100	-0.33673300
Br	1.36788500	-1.57553900	-1.33887400
H	1.77788600	1.53346300	3.46991900
K	4.39762700	-2.23773900	-2.04101300
C	5.08570900	-1.76866500	0.73548900
O	4.87437400	-1.23689100	2.00593400
O	4.47118500	-2.84373500	0.53294600
K	2.20214500	-2.26821500	1.77382800
O	5.79303800	-1.11544800	-0.05326700

III

C	-5.14249400	0.00411000	-0.27195900
C	-3.72234000	0.01600100	-0.18249600
C	-3.51420300	0.18955900	-2.51925500
C	-4.88798700	0.17716000	-2.68531700
C	-5.70380400	0.08474600	-1.54175000
H	-2.83140000	0.26350800	-3.37110800
H	-5.32043900	0.24066100	-3.68531500
H	-6.79211400	0.07716500	-1.65009500
N	-3.08022600	-0.06707700	1.01469400
N	-2.94223200	0.11302100	-1.29942100
C	-5.96503500	-0.09038800	0.98144000
H	-5.74173500	0.74522800	1.66446000
H	-5.73192200	-1.01000200	1.54254300
H	-7.04167900	-0.08092400	0.75489200
C	-1.76339300	-0.01795300	0.96875300
C	-1.07656400	-0.15751900	2.28618900
C	-0.09350800	0.74366100	2.72646000
C	-1.45873600	-1.20745600	3.14391600
C	0.48690900	0.60257600	3.99054800
H	0.19022600	1.57905800	2.08622900

C	-0.85705900	-1.36402500	4.39345200
H	-2.23357800	-1.90199800	2.81426000
C	0.11665000	-0.45677400	4.82442200
H	1.23150000	1.32912900	4.32735400
H	-1.15640200	-2.19452400	5.03892800
H	0.58016600	-0.57152500	5.80811500
C	0.97073200	-2.22422000	-0.43386000
C	1.45730000	-3.52434500	-0.26357700
C	0.55321400	-4.59621100	-0.26277600
C	-0.81236300	-4.36190700	-0.42057600
C	-1.28344700	-3.04572200	-0.55851200
C	-0.40963000	-1.94900200	-0.57932000
H	0.92838200	-5.61492200	-0.13292900
H	-1.51708300	-5.19858700	-0.42342700
H	-2.36119400	-2.88364300	-0.65296700
N	1.81066000	-1.06830500	-0.43717400
C	1.11993000	0.09370800	-0.41242600
N	1.78591900	1.26188000	-0.28644100
C	0.95484300	2.41775100	-0.33080300
C	1.43996100	3.72184400	-0.19143400
C	-0.42263700	2.13771300	-0.51354400
C	0.53719200	4.79362600	-0.24932500
H	2.50096900	3.92566000	-0.03514400
C	-1.29445900	3.23629300	-0.54854800
C	-0.82476100	4.55529900	-0.43250700
H	0.91018600	5.81574900	-0.14223100
H	-2.36908100	3.07198000	-0.67134800
H	-1.52819700	5.39196700	-0.47301900
C	3.21412400	1.31893100	0.00405900
H	3.59829100	2.26018000	-0.41339400
C	3.27957200	-1.20183800	-0.55406400
C	3.98321700	0.18216400	-0.68695300
C	5.31680800	0.19265500	0.09298400
C	3.58076700	1.23196900	1.50820300
H	2.80382500	0.66948700	2.04510100
H	3.62060200	2.23193200	1.96510100
C	4.94074600	0.48996500	1.56099100
H	5.72353800	1.07952300	2.06144900
H	4.84246000	-0.44353200	2.13600500
H	5.94726700	1.00305300	-0.30989400
H	5.88848500	-0.74131600	-0.01988900
H	3.62890500	-1.72719500	0.34884300
C	3.69030500	-1.98352700	-1.84791900
H	4.22052600	-2.91632100	-1.60730100

H	2.78432300	-2.27237200	-2.39863400
C	4.55511000	-1.02816100	-2.69596600
H	4.39576100	-1.16960100	-3.77599700
H	5.62683200	-1.20145200	-2.50631200
C	4.15709400	0.36425100	-2.20549900
H	4.89281600	1.14764700	-2.44774900
H	3.19649700	0.66942400	-2.65628900
Ru	-0.88996000	0.10010500	-0.78626200
H	2.52033700	-3.72428100	-0.12452000

IV

C	-1.41621100	0.08806500	2.32925200
C	-0.43330100	1.01557400	1.91338200
C	0.13425900	1.82695400	2.90825100
C	-0.21832000	1.69139300	4.26035600
C	-1.15511800	0.73120700	4.64443500
C	-1.76155700	-0.08038200	3.67614700
H	0.88824100	2.57114900	2.64095900
H	0.24889800	2.33469500	5.01184600
H	-1.42813500	0.61110000	5.69639500
H	-2.49350200	-0.82628000	3.98746200
N	-1.99134700	-0.67048700	1.27340900
C	-1.36546200	-0.49777100	0.08263800
N	-1.77826300	-1.22198400	-0.98390100
C	-1.16118400	-0.85862000	-2.20815800
C	-1.42743100	-1.49250900	-3.42754000
C	-0.26070600	0.22775600	-2.10150800
C	-0.81703000	-1.01285300	-4.59431600
H	-2.09899300	-2.35044700	-3.49051600
C	0.29822000	0.70364100	-3.29669300
C	0.03665800	0.08924500	-4.53317100
H	-1.02260600	-1.50230400	-5.55015400
H	0.95820600	1.57570700	-3.28167300
H	0.50039100	0.47731300	-5.44478100
C	-2.73540000	-2.32061600	-0.88024500
H	-3.27050600	-2.36969500	-1.83835400
C	-3.22244800	-1.45892300	1.50984300
C	-3.80101400	-2.07012800	0.19965900
C	-4.32885800	-3.49932300	0.45873700
C	-2.10876200	-3.70891100	-0.56871800
H	-1.11740800	-3.58309100	-0.11559900
H	-1.95795300	-4.28369900	-1.49381300
C	-3.08830400	-4.40749500	0.40507700
H	-3.34409700	-5.43102000	0.09150700

H	-2.63210700	-4.49485000	1.40399400
H	-5.02856000	-3.76333500	-0.35254000
H	-4.88681500	-3.58913000	1.40379600
H	-2.95528600	-2.26023100	2.21755000
C	-4.38435900	-0.58002000	2.08540100
H	-4.65390300	-0.87881500	3.10879000
H	-4.05231900	0.46553700	2.13560100
C	-5.56974200	-0.70940800	1.10957600
H	-6.15911100	0.21776200	1.04879900
H	-6.25684400	-1.50965400	1.43113300
C	-4.90597700	-1.08328700	-0.21463600
H	-5.59782600	-1.52299900	-0.95109700
H	-4.45672200	-0.18996900	-0.67760200
Ru	0.13311700	0.87265900	-0.11068900
C	1.49978700	4.98526400	-0.34588400
C	2.83224800	5.01542500	0.04836400
C	3.48226700	3.83109100	0.43244200
C	2.78122800	2.63869700	0.37498000
C	0.83919500	3.72386800	-0.35073300
H	3.36835800	5.96848700	0.07262000
H	4.52103100	3.83455300	0.76731800
H	3.25816900	1.70402600	0.66794300
C	0.74031100	6.22366800	-0.73092000
H	1.39458200	7.10867700	-0.72457800
H	0.29115300	6.12328000	-1.73168200
H	-0.09937300	6.40394000	-0.04010400
N	1.49453300	2.56609100	-0.03373800
N	-0.49274700	3.65253800	-0.63902600
C	-1.03568100	2.45886100	-0.53811900
C	-2.51723400	2.46287800	-0.76074000
C	-3.07859300	2.16298400	-2.01357500
C	-3.37218700	2.86136500	0.28264800
C	-4.45762900	2.27211700	-2.21922700
H	-2.42722700	1.86505900	-2.83672400
C	-4.75113400	2.96326700	0.07578700
H	-2.94469100	3.10977000	1.25709300
C	-5.30024100	2.67243500	-1.17763500
H	-4.87423400	2.04917900	-3.20564900
H	-5.39866300	3.28522700	0.89647800
H	-6.37744700	2.76171600	-1.34252600
P	2.03961400	-0.91760000	0.11465700
C	3.45512700	-0.73530800	-1.08237000
C	4.45343400	-1.72522500	-1.17691100
C	3.53570600	0.37903600	-1.92973200

C	5.50751300	-1.59130300	-2.08163600
H	4.40777700	-2.61209900	-0.54114700
C	4.59128800	0.51174600	-2.83981500
H	2.76473300	1.14689700	-1.88955600
C	5.57981600	-0.47012100	-2.91651900
H	6.27401000	-2.36887900	-2.13818900
H	4.63217600	1.38683700	-3.49351500
H	6.40273200	-0.36840500	-3.62907500
C	2.88249400	-0.90904100	1.77173600
C	2.09091400	-1.09090000	2.92179800
C	4.25765600	-0.66771900	1.93966400
C	2.66356600	-1.06850900	4.19577200
H	1.01399400	-1.24008700	2.82925500
C	4.82556600	-0.62907600	3.21755500
H	4.89983000	-0.50670900	1.07310700
C	4.03349100	-0.83684300	4.34880900
H	2.02775700	-1.21562600	5.07218900
H	5.89660400	-0.43684900	3.32414600
H	4.47940500	-0.80902400	5.34647800
C	1.68150700	-2.72465200	-0.17188400
C	1.43270600	-3.13467000	-1.49579900
C	1.68392000	-3.69472600	0.84285100
C	1.21908700	-4.48118700	-1.79612200
H	1.42420100	-2.40133500	-2.30465400
C	1.45850400	-5.04296300	0.53924100
H	1.88480800	-3.41332500	1.87743900
C	1.23334000	-5.44223300	-0.77990400
H	1.04050400	-4.77836900	-2.83289700
H	1.47450000	-5.78461400	1.34253700
H	1.07014600	-6.49706000	-1.01614200

INT5

C	-0.01756800	0.18682600	-0.00000500
C	-0.33305000	1.46982800	-0.00003300
H	-1.24231100	2.07452000	-0.00002300
C	1.41633000	-0.29222800	0.00002500
H	1.61719800	-0.92018300	-0.88612700
H	2.12837200	0.54553900	0.00009700
H	1.61712800	-0.92027900	0.88612400
C	-1.07961200	-0.89818200	-0.00000200
H	-0.96884600	-1.54602200	-0.88749000
H	-0.96909900	-1.54575600	0.88771400
H	-2.09904500	-0.48528600	-0.00020600

V

C	-1.08438700	-0.82920600	-2.28354200
C	0.29358900	-0.93222900	-1.95758800
C	1.13584800	-1.54286400	-2.89516600
C	0.64581400	-2.01574700	-4.12274300
C	-0.70714000	-1.86868400	-4.43061400
C	-1.58253200	-1.26971200	-3.51517400
H	2.20088300	-1.65226400	-2.67504000
H	1.32291000	-2.49441500	-4.83566500
H	-1.09529500	-2.22204400	-5.38977100
H	-2.63394300	-1.15074000	-3.77940700
N	-1.89803100	-0.22971700	-1.27910000
C	-1.17292700	0.30798300	-0.26999700
N	-1.79049200	0.87980500	0.78099100
C	-0.91612900	1.17783300	1.85752600
C	-1.34242000	1.63317000	3.11047500
C	0.44538500	0.91846800	1.58591200
C	-0.40225200	1.79120000	4.13573000
H	-2.39339800	1.85198800	3.30834100
C	1.35499300	1.05260300	2.63744300
C	0.94066900	1.48750800	3.90643400
H	-0.73066400	2.14195200	5.11761700
H	2.41320200	0.83464500	2.47020900
H	1.67468900	1.60037200	4.70934800
C	-3.20326000	1.24018600	0.77036200
H	-3.56043200	1.18250300	1.80648900
C	-3.37172500	-0.32464500	-1.32675500
C	-4.06290600	0.24595200	-0.04134200
C	-5.26918300	1.12762000	-0.44107600
C	-3.49187500	2.66665600	0.20805800
H	-2.59282800	3.08693700	-0.26593600
H	-3.76182300	3.34665800	1.03017200
C	-4.65676100	2.49196000	-0.79061100
H	-5.39396900	3.30757900	-0.73800900
H	-4.27445500	2.48068600	-1.82449100
H	-5.94006500	1.22571700	0.42995700
H	-5.86607600	0.69735800	-1.26040200
H	-3.69487700	0.25200900	-2.20811500
C	-3.87220600	-1.80302000	-1.43557100
H	-4.28888000	-2.02593500	-2.42793800
H	-3.01941300	-2.48264400	-1.29442800
C	-4.90238000	-2.00521300	-0.31082400
H	-4.93336000	-3.04648000	0.04552000
H	-5.91763900	-1.75701400	-0.66212600

C	-4.45820300	-1.01016800	0.75884700
H	-5.23105300	-0.79128800	1.51281500
H	-3.57629300	-1.39933000	1.29649200
Ru	0.83365500	0.38144600	-0.41376700
C	4.97315400	-0.91133700	-0.20877000
C	5.72113900	-0.02225100	-0.97363000
C	5.09664800	1.05827000	-1.61694800
C	3.72878600	1.22419300	-1.46754400
C	3.57276000	-0.67765600	-0.11542300
H	6.80016600	-0.17022300	-1.07360700
H	5.66838100	1.76494700	-2.22138000
H	3.20223300	2.06030700	-1.93119100
C	5.58226000	-2.08972100	0.49739500
H	6.66812900	-2.13790200	0.32578300
H	5.40126500	-2.04138300	1.58334300
H	5.13047400	-3.03501500	0.15612900
N	2.97873800	0.37863900	-0.73410400
N	2.77361200	-1.52686800	0.59661700
C	1.48552700	-1.29760500	0.57077700
C	0.66643500	-2.24145300	1.38920800
C	1.16676900	-2.69947400	2.62475500
C	-0.57432900	-2.73330200	0.95287500
C	0.44068400	-3.59976500	3.40404200
H	2.13686500	-2.33335200	2.96435700
C	-1.29016400	-3.65683200	1.72082900
H	-0.96069500	-2.41368100	-0.01386400
C	-0.79163700	-4.08603300	2.95382900
H	0.84056800	-3.92934800	4.36707500
H	-2.24148300	-4.04906500	1.35093800
H	-1.35738100	-4.79952100	3.55918900
C	1.20178500	3.66610500	-0.31631100
C	0.93700400	2.37717200	-0.56345500
H	0.53148500	2.12140000	-1.59545600
C	1.77595400	4.17569400	0.98358000
H	1.08737100	4.89416400	1.46482300
H	1.97702500	3.36877700	1.69749100
H	2.71894600	4.72397300	0.80237100
C	0.96263600	4.73831600	-1.36093900
H	0.26838200	5.51158700	-0.98285600
H	1.90134200	5.26481800	-1.61509300
H	0.53959900	4.33279900	-2.29311200

TS3

C	1.10558400	-1.82413700	-1.29158600

C	-0.24647500	-1.41833900	-1.43211900
C	-1.11075500	-2.30249900	-2.09012600
C	-0.67258200	-3.54567800	-2.57346400
C	0.65157100	-3.93500800	-2.37744500
C	1.55059500	-3.07389000	-1.73308800
H	-2.16401600	-2.03484400	-2.21226700
H	-1.37311100	-4.21499700	-3.08111500
H	0.99899000	-4.91194600	-2.72436400
H	2.58263100	-3.39484300	-1.58863500
N	1.98073200	-0.86741100	-0.67411800
C	1.34112400	0.23926800	-0.23743300
N	2.05452700	1.27658400	0.26459900
C	1.35296400	2.52440400	0.27347400
C	1.93452800	3.71845900	0.70908700
C	0.02579300	2.47600800	-0.23911700
C	1.21065800	4.91639700	0.59644300
H	2.93933900	3.74834600	1.13438100
C	-0.65756000	3.69409900	-0.33278600
C	-0.07555600	4.91239100	0.06238800
H	1.66828600	5.85108800	0.93216700
H	-1.68345300	3.70906000	-0.71456100
H	-0.63509800	5.84741300	-0.03372400
C	3.43060800	1.11411900	0.71868100
H	3.90635200	2.10082100	0.68014700
C	3.44608700	-0.99975800	-0.82649500
C	4.25529500	0.20078600	-0.21767200
C	5.35307600	-0.32099300	0.73683400
C	3.57541500	0.53776000	2.16220000
H	2.60790600	0.17904900	2.54223800
H	3.90860400	1.32978200	2.85033700
C	4.61881700	-0.59555500	2.05682900
H	5.30188500	-0.63369600	2.91895900
H	4.11451700	-1.57487300	2.01073700
H	6.10454700	0.47427000	0.88224600
H	5.88602400	-1.20100300	0.34383500
H	3.73243400	-1.92966200	-0.31073800
C	3.87898800	-1.06624200	-2.32741600
H	4.07436700	-2.09255700	-2.66614100
H	3.05771100	-0.67738700	-2.94901700
C	5.10499600	-0.15407600	-2.45898100
H	5.24370100	0.21689900	-3.48640600
H	6.02675900	-0.69363300	-2.18255700
C	4.81165800	0.94944200	-1.44657400
H	5.68499400	1.57009100	-1.19002700

H	4.03601800	1.62449300	-1.84972000
Ru	-0.61891600	0.47875100	-0.57723500
C	-4.89996500	0.00370800	-0.87447800
C	-5.30644600	0.80707800	-1.92928400
C	-4.37766600	1.60184800	-2.63182100
C	-3.05306500	1.56897700	-2.23238000
C	-3.50843200	0.00648100	-0.52997000
H	-6.36150900	0.82048000	-2.21824300
H	-4.68624300	2.23589400	-3.46468100
H	-2.29059600	2.17496900	-2.73119500
C	-5.85025200	-0.86719000	-0.10521400
H	-6.87820900	-0.77271800	-0.48698300
H	-5.55257500	-1.92734700	-0.16261400
H	-5.85232700	-0.61083100	0.96788500
N	-2.62707900	0.80052400	-1.20879200
N	-3.02670100	-0.77292500	0.45108900
C	-1.70619500	-0.75816200	0.71933400
C	-1.24729700	-1.93946000	1.54989700
C	0.09727400	-2.18741000	1.88086600
C	-2.20764300	-2.85930700	2.01654100
C	0.46723900	-3.29668800	2.64356500
H	0.87437500	-1.51061000	1.53228100
C	-1.84053800	-3.96752600	2.78200400
H	-3.25225500	-2.68425400	1.76263700
C	-0.49972500	-4.19566100	3.10226500
H	1.52290900	-3.46079800	2.87771800
H	-2.61225100	-4.66092900	3.12846100
H	-0.21062100	-5.06503500	3.69889000
C	-1.78019900	1.48456200	2.24684500
C	-0.95885200	0.67503300	1.49867600
H	-0.06335400	0.36718700	2.03996800
C	-3.11360300	1.99397900	1.81615600
H	-3.46676800	2.81093600	2.46317200
H	-3.12622100	2.33066700	0.77173600
H	-3.84485600	1.16441000	1.89001200
C	-1.39090300	1.81758800	3.66181200
H	-1.24520200	2.90797000	3.77179700
H	-2.19763100	1.54198100	4.36604800
H	-0.46547600	1.31483700	3.97753700

VI

C	1.02924000	-1.87846900	-1.20307900
C	-0.20076800	-1.31190200	-1.62650100
C	-1.02723700	-2.09168700	-2.44946600

C	-0.68576600	-3.41327100	-2.76767000
C	0.48442500	-3.98162100	-2.25379200
C	1.35058400	-3.21444300	-1.46648000
H	-1.96659600	-1.67965300	-2.82698200
H	-1.34936600	-4.00773400	-3.40246000
H	0.73421400	-5.02311500	-2.47328500
H	2.26742300	-3.65933300	-1.07663000
N	1.88294100	-0.95897400	-0.53435100
C	1.23988800	0.21026500	-0.30837900
N	1.97139300	1.33727500	-0.06324200
C	1.30005100	2.48857400	-0.53090300
C	1.76770700	3.79992700	-0.38954300
C	0.08249400	2.19362400	-1.21309000
C	1.05279600	4.84273800	-0.99500100
H	2.67522100	4.02312000	0.17552700
C	-0.60176700	3.26589600	-1.80158700
C	-0.11883600	4.58155200	-1.70945100
H	1.42134300	5.86816400	-0.90236100
H	-1.53579200	3.08259600	-2.34042100
H	-0.66525500	5.40084000	-2.18498600
C	3.33027600	1.31257300	0.45514300
H	3.80907800	2.24662900	0.13399400
C	3.35243000	-1.13937100	-0.54450700
C	4.17074300	0.14997300	-0.14381400
C	5.14204200	-0.18440000	1.01357000
C	3.42932200	1.19611500	2.00909300
H	2.43285400	1.13306600	2.46745900
H	3.91808200	2.09641700	2.41488600
C	4.28492500	-0.05468400	2.27702200
H	4.88620000	0.02128500	3.19643000
H	3.63699000	-0.93952300	2.39064800
H	5.95087900	0.56707300	1.03225400
H	5.61955200	-1.17097500	0.90439200
H	3.57206700	-1.93698900	0.18310600
C	3.90039400	-1.54324700	-1.95023600
H	4.03437500	-2.62781000	-2.05738100
H	3.17365400	-1.23298100	-2.71637700
C	5.20422900	-0.76110900	-2.13899500
H	5.47556100	-0.64946100	-3.20045700
H	6.04639300	-1.27038300	-1.64007300
C	4.89259100	0.56045900	-1.44528300
H	5.77696300	1.18561500	-1.24314000
H	4.20779100	1.15326000	-2.07693600
Ru	-0.69322600	0.38464300	-0.65648500

C	-4.44876300	-1.27969600	-0.50857800
C	-5.32942600	-0.76608400	-1.46015700
C	-4.98691300	0.35183300	-2.23724300
C	-3.72776800	0.91336900	-2.06287900
C	-3.21041300	-0.59745900	-0.34996900
H	-6.29878600	-1.25197600	-1.60661200
H	-5.67360800	0.75512700	-2.98359100
H	-3.38145800	1.74766100	-2.67973300
C	-4.75647500	-2.50415300	0.30535300
H	-5.69106100	-2.97860900	-0.02964900
H	-3.93954900	-3.23957400	0.22883000
H	-4.86080200	-2.27008500	1.37773700
N	-2.86789300	0.43710300	-1.15348300
N	-2.23975100	-1.04227800	0.51845600
C	-1.47492400	-0.21004100	1.28945400
C	-0.54468300	-0.91104900	2.24549700
C	-0.00164200	-0.24506700	3.35934800
C	-0.23124600	-2.27245700	2.06907900
C	0.83340600	-0.91284900	4.26095600
H	-0.24699100	0.80339100	3.53724500
C	0.59974800	-2.93818700	2.96981600
H	-0.65788300	-2.80110300	1.21632300
C	1.13953200	-2.26281700	4.07161000
H	1.23780700	-0.37400500	5.12229300
H	0.82440100	-3.99706000	2.81368300
H	1.78597600	-2.78751000	4.78030700
C	-3.12124400	1.51974300	2.24439200
C	-1.93848900	1.16611300	1.69687500
H	-1.19891200	1.96566200	1.56507500
C	-4.20610300	0.54898800	2.62195100
H	-4.51452000	0.71910900	3.66864500
H	-5.10987800	0.70322000	2.00633200
H	-3.89366600	-0.49804700	2.52479800
C	-3.42035400	2.96423100	2.55171400
H	-4.33183900	3.29368400	2.02070500
H	-3.62247600	3.10904700	3.62822700
H	-2.59731000	3.63331700	2.26025600

VII

C	-2.00068700	-2.19025900	-0.01069200
C	-0.68510600	-1.82779200	0.42244300
C	0.14002700	-2.88058000	0.86166900
C	-0.28058100	-4.21867900	0.81579200
C	-1.54650300	-4.53973800	0.31879700

C	-2.41420600	-3.52320300	-0.09940200
H	1.13967500	-2.65830300	1.24266600
H	0.39037400	-5.01132900	1.15962500
H	-1.86891000	-5.58294300	0.26088800
H	-3.40456300	-3.77784200	-0.48240900
N	-2.84541100	-1.08418000	-0.31200200
C	-2.12070200	0.06015700	-0.32500000
N	-2.75452000	1.25734000	-0.22505800
C	-1.89832600	2.24233600	0.32238900
C	-2.26221400	3.57937900	0.51166400
C	-0.62272800	1.73393800	0.73338700
C	-1.38270200	4.43763100	1.18589200
H	-3.22166200	3.95982100	0.15378600
C	0.21413600	2.62749400	1.42135500
C	-0.15594500	3.96229800	1.65256500
H	-1.66652700	5.48170900	1.34471800
H	1.19183200	2.29029200	1.77486500
H	0.52722700	4.63226000	2.18227600
C	-4.14690000	1.44239900	-0.59219200
H	-4.51263800	2.32398800	-0.04926600
C	-4.31043600	-1.16206200	-0.14478900
C	-5.03415300	0.24279300	-0.15349500
C	-6.14758300	0.25602800	-1.22704900
C	-4.38292100	1.64681900	-2.12412000
H	-3.43872600	1.56643700	-2.68181900
H	-4.77769900	2.65863300	-2.30738400
C	-5.41124000	0.57519600	-2.53331700
H	-6.08818300	0.90857000	-3.33513900
H	-4.89584900	-0.32623900	-2.90535100
H	-6.86183100	1.06535700	-0.99389500
H	-6.72312800	-0.68231800	-1.26499800
H	-4.69542900	-1.76052400	-0.98655600
C	-4.72804600	-1.82821100	1.20293300
H	-4.94592900	-2.89978400	1.09623400
H	-3.89235000	-1.73994400	1.91426000
C	-5.92410100	-1.02037900	1.71794900
H	-6.06784600	-1.12728900	2.80455200
H	-6.85960600	-1.34780900	1.23261700
C	-5.56839200	0.39934200	1.28618200
H	-6.40761300	1.11121900	1.33731100
H	-4.76553100	0.78920000	1.93630100
Ru	-0.16535100	0.00811500	-0.21603900
P	2.34559500	-0.02493500	-0.13410300
C	3.14204400	1.63299200	-0.37878100

C	4.15915300	2.14277700	0.44271600
C	2.65964200	2.43136400	-1.43211100
C	4.68603300	3.41896800	0.21094000
H	4.54604000	1.54735300	1.27194700
C	3.19298400	3.69914000	-1.66885900
H	1.85478700	2.05927000	-2.07347800
C	4.20826000	4.19798000	-0.84512100
H	5.47563700	3.80295400	0.86253600
H	2.80707900	4.30453700	-2.49317700
H	4.62068500	5.19450500	-1.02375600
C	3.15271900	-1.03173500	-1.47559300
C	4.33178800	-0.63503900	-2.13061000
C	2.54116600	-2.23817800	-1.86192000
C	4.88776000	-1.42885700	-3.13880300
H	4.82232800	0.30139800	-1.85768200
C	3.10095900	-3.03224400	-2.86660800
H	1.62108200	-2.56515600	-1.37204700
C	4.27539400	-2.62953700	-3.50890000
H	5.80481500	-1.10403800	-3.63780300
H	2.61087300	-3.96714000	-3.15085500
H	4.71015900	-3.24753400	-4.29900200
C	3.13764100	-0.65956100	1.41704800
C	2.44308000	-0.48791300	2.62760800
C	4.38683100	-1.30282300	1.43539600
C	2.99623200	-0.93140800	3.83215600
H	1.45404800	-0.02264600	2.62010000
C	4.93381400	-1.75318300	2.64088700
H	4.93798300	-1.45962800	0.50568600
C	4.24235900	-1.56513900	3.84152700
H	2.44362000	-0.79105300	4.76483000
H	5.90465600	-2.25603200	2.63987300
H	4.67084000	-1.92018800	4.78262500

INT3

C	-2.43399100	-1.40155800	0.59111800
C	-3.79976100	-1.33987300	0.30549700
C	-4.25508600	-0.65186600	-0.82340500
C	-3.30524900	-0.04150600	-1.64349000
C	-1.56059500	-0.72269900	-0.30418300
H	-4.51070500	-1.84462100	0.96654500
H	-5.31849900	-0.60173100	-1.06784800
H	-3.61604100	0.49240400	-2.55004200
C	-1.89285600	-2.14824800	1.77810400
H	-2.67800600	-2.74461200	2.26697600

H	-1.07101100	-2.81843700	1.47850900
H	-1.47094000	-1.46462300	2.53467500
N	-1.99676700	-0.06939500	-1.38965600
N	-0.18932700	-0.83686400	-0.08977900
C	0.66680800	0.11347500	-0.23798900
C	2.11623200	-0.25161300	-0.20152400
C	3.11639800	0.73124800	-0.09110700
C	2.50608600	-1.60324700	-0.27740300
C	4.46691500	0.37432200	-0.05630200
H	2.83527600	1.78374200	-0.01991500
C	3.85277700	-1.95806200	-0.24377100
H	1.72859700	-2.36385100	-0.36643600
C	4.83946400	-0.96992400	-0.13350700
H	5.23097400	1.15102900	0.03297400
H	4.13884000	-3.01135500	-0.30758000
H	5.89623200	-1.24917100	-0.10954800
C	-0.29291100	2.37210500	0.40812000
C	0.33520700	1.55095200	-0.45513500
H	0.69195900	1.96609900	-1.40508400
C	-0.78277500	1.94999200	1.76743500
H	-1.88557100	1.99612900	1.81382800
H	-0.47383900	0.93232800	2.04184000
H	-0.41137900	2.64174800	2.54385500
C	-0.55551200	3.81140100	0.05070900
H	-1.63986500	4.02340900	0.06801400
H	-0.09509900	4.49644100	0.78501300
H	-0.17517800	4.06950600	-0.94873600

TS4

C	-2.02698500	-1.96635800	0.07965400
C	-3.36327500	-2.01734300	-0.29497400
C	-4.08730800	-0.83954200	-0.55218900
C	-3.43248300	0.36914900	-0.38495200
C	-1.40542200	-0.67445100	0.20804300
H	-3.85241600	-2.98989200	-0.40218400
H	-5.14119800	-0.86721400	-0.83621300
H	-3.95145900	1.32295300	-0.53100000
C	-1.22137400	-3.21407900	0.30465500
H	-1.86672400	-4.10572700	0.30341800
H	-0.45850400	-3.34374300	-0.48107400
H	-0.67623300	-3.16971700	1.25984000
N	-2.15746400	0.43772000	0.02004700
N	-0.06225800	-0.65538500	0.46116700
C	0.73552300	0.32989900	0.05116200

C	2.19393900	0.01668800	-0.03647500
C	3.14885300	1.04483700	-0.14667700
C	2.64900000	-1.31449000	0.00225700
C	4.51190300	0.75204700	-0.22960800
H	2.81815900	2.08593400	-0.14303500
C	4.01058900	-1.60765100	-0.07284800
H	1.90964800	-2.11125600	0.09003800
C	4.94853200	-0.57570800	-0.19296800
H	5.23818300	1.56539100	-0.31115900
H	4.34452900	-2.64853600	-0.04218500
H	6.01580500	-0.80581900	-0.25278200
C	-0.93392800	2.14338800	0.10238300
C	0.25260100	1.58659500	-0.40270200
H	0.71963000	2.04424900	-1.28099300
C	-1.13224700	2.26054000	1.59758300
H	-2.19510200	2.33183500	1.87289400
H	-0.67443300	1.42613700	2.14468300
H	-0.63385900	3.18865800	1.93305200
C	-1.62484200	3.21657100	-0.69976000
H	-2.68309800	3.31720300	-0.41401600
H	-1.15038500	4.19203800	-0.49169300
H	-1.56294700	3.03060700	-1.78160100

3a

C	-2.08433500	1.96804100	-0.07107800
C	-3.45157900	1.88044200	-0.06699500
C	-4.10351000	0.61562400	-0.02483600
C	-3.33446300	-0.50954500	0.01323600
C	-1.27436400	0.75480700	-0.03590400
H	-4.04982100	2.79543800	-0.09551300
H	-5.19061000	0.53212700	-0.02207400
H	-3.78144200	-1.50175500	0.04785000
C	-1.35863500	3.28013500	-0.10881100
H	-2.06596400	4.12102900	-0.16072500
H	-0.72364300	3.40573100	0.78391400
H	-0.67585000	3.33200600	-0.97229500
N	-1.96342300	-0.46729900	0.00984200
N	0.02694300	0.86338900	-0.04625600
C	0.80205600	-0.28422000	-0.00269200
C	2.27856100	-0.05540600	-0.00898200
C	3.20370300	-1.08913400	-0.25208100
C	2.78202400	1.23569300	0.23309000
C	4.57717700	-0.84388200	-0.23625300
H	2.85165200	-2.09834100	-0.47577600

C	4.15702400	1.48152600	0.25081900
H	2.06981100	2.04205300	0.40857400
C	5.06295800	0.44354900	0.01828000
H	5.27420300	-1.66325600	-0.43256800
H	4.52239600	2.49365700	0.44641400
H	6.13929100	0.63530900	0.02807300
C	-1.23030500	-1.78826700	0.06050900
C	0.25612800	-1.52187200	0.06351800
H	0.87901000	-2.41409600	0.13599700
C	-1.59675000	-2.63139900	-1.18065100
H	-2.65486000	-2.93821800	-1.19083100
H	-1.38311400	-2.07428900	-2.10526100
H	-0.98950600	-3.55017000	-1.19025700
C	-1.61466700	-2.54475200	1.35080700
H	-2.67093500	-2.85688400	1.36581000
H	-1.00319200	-3.45685900	1.43363600
H	-1.41820600	-1.92415900	2.23806600

INT4

Ru	1.53967300	0.10279900	-0.40852700
N	-0.98913800	-0.98920100	0.68375500
N	0.25471800	0.19576400	2.26304800
C	-2.13517600	-0.47236200	2.88323100
C	-2.61289000	-1.47193100	3.96333300
H	-3.69623200	-1.63732000	3.83179800
H	-2.46873800	-1.08202200	4.98462000
C	-1.85277500	-2.76671200	3.67339300
H	-0.81342600	-2.69041200	4.03480400
H	-2.29690200	-3.64693300	4.16445700
C	-1.87917200	-2.85812100	2.13769500
H	-2.74349900	-3.45435600	1.80554600
H	-0.97955700	-3.33769700	1.72618400
C	-2.03831800	-1.38934500	1.62839400
H	-2.98354200	-1.26549300	1.08330800
C	-3.12495500	0.72532000	2.70438300
H	-3.85448200	0.70331000	3.53186500
H	-3.68681300	0.65599200	1.75846700
C	-2.28343200	1.99817000	2.81020900
H	-2.85752600	2.87066500	3.16126700
H	-1.85684500	2.26762200	1.83016300
C	-1.16146700	1.60154600	3.76752000
H	-0.31403900	2.29940900	3.77261100
H	-1.54793300	1.54748600	4.80014500
C	-0.77164300	0.16935400	3.32525200

H	-0.33646500	-0.39749800	4.16370700
C	0.11280000	-0.28789000	1.00791300
C	-1.01770300	-1.44131400	-0.66164500
C	-2.05272000	-2.22581700	-1.18603900
H	-2.89743700	-2.53706700	-0.57282100
C	-2.01564500	-2.58790400	-2.54128200
H	-2.82462700	-3.19541000	-2.95495100
C	-0.95636800	-2.17173900	-3.35243600
H	-0.92817300	-2.45386200	-4.40919600
C	0.09024100	-1.41087000	-2.79766600
H	0.92544900	-1.12137000	-3.44295300
C	0.08676900	-1.02881000	-1.44646500
C	1.55107700	0.73504100	2.51665600
C	2.40156400	0.77557000	1.38539600
C	3.70633000	1.25242300	1.57670000
H	4.40134500	1.28839800	0.73254900
C	4.15405000	1.68793700	2.83518400
H	5.17403200	2.06539700	2.95320900
C	3.30171200	1.61199000	3.93646900
H	3.64760500	1.92105500	4.92658500
C	1.99403300	1.12705100	3.78636100
C	4.94829900	-0.67418100	-2.92102600
C	3.85945800	-0.64547200	-2.00363500
C	3.30145600	1.54224600	-2.64607900
C	4.34430100	1.58987900	-3.55472300
C	5.17301700	0.46161000	-3.68981100
H	2.63312400	2.39467100	-2.50756200
H	4.51087600	2.49035500	-4.14869100
H	6.00195400	0.47537300	-4.40323300
N	3.59621600	-1.71154300	-1.19987100
N	3.05469500	0.45417300	-1.88452100
C	5.79824700	-1.90881400	-3.02176700
H	5.19161400	-2.78565800	-3.30077900
H	6.25658800	-2.15489100	-2.05043400
H	6.59816300	-1.78385600	-3.76709100
C	2.59481300	-1.56499800	-0.35560400
H	1.35134700	1.05771900	4.66415900
C	2.31631100	-2.76674600	0.48766000
C	2.18193000	-4.02123600	-0.13871000
C	2.23134500	-2.70533700	1.88877800
C	1.94938700	-5.17449500	0.61255600
H	2.25880400	-4.07835700	-1.22622800
C	2.02939900	-3.86598900	2.64171900
H	2.36144600	-1.74753200	2.39274200

C	1.87737000	-5.10302300	2.00789200
H	1.83337700	-6.13696300	0.10627100
H	1.99525100	-3.80261800	3.73296000
H	1.70852500	-6.00790600	2.59805800
C	0.23851400	4.72136300	0.58557100
C	-0.56638600	3.91799400	-0.12070600
H	-1.65549100	3.95501500	-0.09443300
C	1.73817400	4.68697000	0.58131700
H	2.15236800	3.97556300	-0.14375300
H	2.11328100	4.40582300	1.58000700
H	2.14162200	5.69015500	0.36097500
C	-0.39645200	5.75225800	1.48642900
H	-0.07717100	6.76816000	1.19521800
H	-0.06688800	5.60258100	2.52909200
H	-1.49514900	5.71513300	1.46363100
Br	0.03942300	2.54121200	-1.32353700
K	-2.78190100	0.57005400	-2.45859700
C	-5.24402200	0.09081400	-0.92043100
O	-6.29096000	-0.25367700	-0.27133800
O	-5.28821800	0.14758500	-2.24627100
K	-7.68741000	-0.54724600	-2.27995400
O	-4.13690100	0.38077700	-0.33235000

TS5

Ru	1.48325700	0.18271500	-0.32563200
N	-1.00371900	-1.06672200	0.66786200
N	0.23356000	-0.00016700	2.32683100
C	-2.18232300	-0.61370500	2.85744400
C	-2.70938300	-1.62822100	3.89752100
H	-3.78440200	-1.79147200	3.71001600
H	-2.61454200	-1.25436100	4.93042700
C	-1.93293800	-2.91898900	3.62639200
H	-0.92031800	-2.85259900	4.06010800
H	-2.40998000	-3.80688000	4.06993500
C	-1.85812200	-2.98276900	2.08864600
H	-2.66653400	-3.61272600	1.68721800
H	-0.91173100	-3.41188900	1.72895900
C	-2.05480900	-1.51514200	1.59328000
H	-3.00160300	-1.41442100	1.04140000
C	-3.14539300	0.60160800	2.66445300
H	-3.86751600	0.60998700	3.49897000
H	-3.72560000	0.50913300	1.73341000
C	-2.27573800	1.85865600	2.74425900
H	-2.83591100	2.75433100	3.05613500

H	-1.81822300	2.09183900	1.76828400
C	-1.19107400	1.46108600	3.74667200
H	-0.32170600	2.13322900	3.75384100
H	-1.60691000	1.44873500	4.76906200
C	-0.82653900	0.00906600	3.35297900
H	-0.43430100	-0.55294900	4.21489100
C	0.08443800	-0.37670100	1.03513900
C	-0.93075600	-1.52300600	-0.66516500
C	-1.91804800	-2.29344300	-1.29315700
H	-2.83544700	-2.56129000	-0.77029700
C	-1.73002400	-2.67061200	-2.62860200
H	-2.49724000	-3.26740700	-3.12849500
C	-0.57013600	-2.29425500	-3.31559700
H	-0.42713200	-2.59337000	-4.35773300
C	0.42097700	-1.54256000	-2.66520100
H	1.32878700	-1.27197200	-3.20976100
C	0.24477900	-1.12630400	-1.34010800
C	1.55889300	0.39520300	2.61144900
C	2.43277500	0.32790700	1.49622600
C	3.78882500	0.61156300	1.69353200
H	4.49332200	0.52826800	0.86307300
C	4.26279700	1.00703400	2.95386500
H	5.32158400	1.24396800	3.08782800
C	3.38408000	1.07728100	4.03601200
H	3.75255000	1.36643000	5.02385000
C	2.02668900	0.76898000	3.87698600
C	5.03656800	0.23011500	-2.80973800
C	3.91855800	-0.02998100	-1.97162700
C	3.12272800	2.15656200	-2.23571200
C	4.18993100	2.49017900	-3.05520800
C	5.15209600	1.51071300	-3.34373300
H	2.33826600	2.87618900	-1.99590900
H	4.26641700	3.49886300	-3.46507100
H	6.00166200	1.75087200	-3.98925000
N	3.75811100	-1.25529000	-1.38868800
N	2.98504300	0.92586400	-1.70320000
C	6.04203500	-0.85421800	-3.07750200
H	5.57153900	-1.72552600	-3.56150600
H	6.48361800	-1.22810700	-2.13993000
H	6.85296400	-0.49151700	-3.72675500
C	2.75123900	-1.40157900	-0.56462300
H	1.35943700	0.81708400	4.73792100
C	2.60818900	-2.77333600	0.00724100
C	3.02490200	-3.88308000	-0.75875700

C	2.10392800	-3.01414600	1.29671400
C	2.92488100	-5.18057100	-0.25916000
H	3.42693900	-3.70532800	-1.75714200
C	2.02794900	-4.31274100	1.80823600
H	1.79746900	-2.17555200	1.91850100
C	2.42894000	-5.40212300	1.03057500
H	3.23943100	-6.02580700	-0.87755400
H	1.65269500	-4.47255200	2.82260400
H	2.35708200	-6.41856200	1.42692400
C	-0.13308400	5.21014900	0.66354800
C	-0.87112600	4.38460300	-0.06511400
H	-1.90271000	4.45312900	-0.41675400
C	1.29421300	4.94290300	1.07242000
H	1.64511500	3.95920300	0.73461200
H	1.39852600	4.98756700	2.17070300
H	1.96767800	5.71623900	0.66157800
C	-0.71249700	6.52849500	1.14751300
H	-0.09968400	7.37539200	0.79055000
H	-0.70549800	6.57120300	2.25126600
H	-1.74614800	6.68334400	0.80496000
Br	-0.10653400	2.16953900	-0.99316200
K	-2.88893100	0.62465500	-2.11083300
C	-5.42118200	-0.35763500	-0.92957700
O	-6.50810000	-0.84923000	-0.47254900
O	-5.40377800	0.16735700	-2.14775600
K	-7.83514100	-0.30464900	-2.47520000
O	-4.32731600	-0.35336200	-0.24876000

VIII

Ru	-0.73596400	-0.56275900	-0.18125600
N	1.85626900	0.42768400	-1.13704200
N	1.94989900	-0.50426700	1.00052300
C	4.08865300	-0.25900900	-0.29519800
C	5.40425200	0.52326800	-0.09048800
H	5.99770100	0.44125500	-1.01623000
H	6.02338600	0.10687400	0.71979100
C	4.99164100	1.98997400	0.14613700
H	4.88881400	2.19841900	1.22243700
H	5.75266000	2.68864100	-0.23237000
C	3.62548700	2.15780100	-0.56877900
H	3.65621100	2.90648100	-1.37376800
H	2.84280700	2.48703200	0.12947100
C	3.27879000	0.75357900	-1.12929300
H	3.63633100	0.67558400	-2.16640000

C	4.27700300	-1.64589000	-0.98600100
H	5.32571000	-1.75560300	-1.30508100
H	3.65977800	-1.72439100	-1.89396900
C	3.88713800	-2.72383900	0.04414400
H	4.55542400	-3.59815600	0.02264700
H	2.86786200	-3.08743700	-0.15632800
C	3.92289900	-1.99995400	1.39331200
H	3.33898900	-2.50832700	2.17149100
H	4.95818800	-1.91657900	1.76503000
C	3.42343000	-0.57253000	1.08250200
H	3.74118400	0.14316200	1.85789400
C	1.23846200	-0.16360100	-0.09961700
C	0.94832200	0.90823200	-2.09819300
C	1.30469600	1.52615700	-3.30099900
H	2.35174200	1.67513700	-3.57088900
C	0.29190800	1.95652200	-4.16430000
H	0.55971400	2.44106500	-5.10671700
C	-1.05183800	1.77914000	-3.82437600
H	-1.83888800	2.11980300	-4.50225600
C	-1.39882600	1.17800700	-2.60593900
H	-2.45359300	1.07008200	-2.34574000
C	-0.40403600	0.71066600	-1.74006000
C	1.10477500	-0.72266300	2.10881500
C	-0.27294700	-0.57759400	1.80924800
C	-1.20147300	-0.70213300	2.84807000
H	-2.26684100	-0.56471400	2.65423300
C	-0.77715700	-1.00424300	4.15007500
H	-1.51589500	-1.11953200	4.94746200
C	0.58480900	-1.13088100	4.42945800
H	0.91862200	-1.33591500	5.44993400
C	1.53738400	-0.98565400	3.41422900
C	-5.07225400	-0.37545000	0.12199000
C	-3.66523000	-0.19038900	0.08631900
C	-3.32195300	-2.37720600	-0.67806100
C	-4.68545100	-2.63526300	-0.67236400
C	-5.56255400	-1.62080400	-0.26670200
H	-2.58919000	-3.12647600	-0.98510900
H	-5.05421700	-3.61515500	-0.98061100
H	-6.64099800	-1.80250600	-0.25274700
N	-3.11377600	1.00764800	0.45137600
N	-2.82179200	-1.18407700	-0.30620400
C	-5.96995500	0.74567000	0.56458500
H	-5.85642100	1.62780100	-0.08617900
H	-5.71731900	1.08180400	1.58292000

H	-7.02591400	0.43693400	0.55030800
C	-1.80974200	1.10668500	0.42791700
H	2.59750400	-1.06645700	3.65504000
C	-1.28570100	2.46031700	0.78186700
C	-2.13469400	3.58266300	0.66375400
C	0.02326100	2.67694600	1.24631600
C	-1.68814500	4.86309800	0.98427300
H	-3.15363000	3.42417800	0.30940300
C	0.46629600	3.95713200	1.58899000
H	0.69588200	1.83091300	1.36508100
C	-0.38390300	5.05734700	1.45328900
H	-2.36199300	5.71679100	0.87052200
H	1.48304800	4.09516800	1.96652400
H	-0.03397800	6.06039900	1.71188300
Br	0.04758500	-2.82715500	-1.14321500

INT6

C	2.65121800	2.33309200	0.93389200
C	1.86472100	1.22040500	1.35676700
C	1.13081500	1.42012600	2.53896200
C	1.16347600	2.62135200	3.26829500
C	1.93945600	3.68618000	2.81332700
C	2.68721300	3.54721000	1.63372200
H	0.49752500	0.60990900	2.91859700
H	0.58009500	2.72151100	4.18936400
H	1.97180100	4.63011700	3.36510900
H	3.28170900	4.39378100	1.28707900
N	3.37429700	2.14298200	-0.29155800
C	3.08515100	0.96487700	-0.92353600
N	3.44020200	0.78442400	-2.22598600
C	3.02805700	-0.45729300	-2.81035200
C	3.30079200	-0.77654600	-4.14670600
C	2.34400500	-1.34060400	-1.92623500
C	2.91234100	-2.02860000	-4.64632700
H	3.80551000	-0.07571000	-4.81542300
C	1.98021600	-2.58098800	-2.47867200
C	2.25681400	-2.93338800	-3.81074100
H	3.12338600	-2.28312500	-5.68895800
H	1.45647200	-3.31027900	-1.84987400
H	1.95428000	-3.91318100	-4.19510100
C	4.00795900	1.86597200	-3.01583900
H	4.65400700	1.41421500	-3.78306600
C	4.24568300	3.20379200	-0.82849900
C	4.90205900	2.78770100	-2.17497100

C	5.05045800	4.01128700	-3.10707600
C	2.97753600	2.79808400	-3.70060400
H	2.07561200	2.86553000	-3.07359400
H	2.65324300	2.39644100	-4.67169400
C	3.68343200	4.17352000	-3.81538900
H	3.81670300	4.48786700	-4.86177200
H	3.07979900	4.95833400	-3.33396800
H	5.83786800	3.79083500	-3.84705900
H	5.36344000	4.92181600	-2.57292600
H	3.62014300	4.10166100	-0.96647100
C	5.45478600	3.52391600	0.11216800
H	5.48260000	4.59326700	0.37051100
H	5.33490600	2.98196500	1.05921600
C	6.73917900	3.08551900	-0.62970200
H	7.46242400	2.59349100	0.03880500
H	7.25164300	3.96017200	-1.06228100
C	6.24209200	2.16516300	-1.74785100
H	6.94653100	2.07460400	-2.59030400
H	6.06802600	1.14738100	-1.35982600
Ru	2.02126900	-0.36078400	-0.06042300
P	3.59793700	-1.45305300	1.13114900
C	5.20541500	-2.14188300	0.48397900
C	6.16072800	-2.68788600	1.36269000
C	5.48102000	-2.13993400	-0.89172000
C	7.35575600	-3.22067000	0.87446900
H	5.97488900	-2.69904500	2.43846400
C	6.68217000	-2.66866300	-1.37871000
H	4.74717400	-1.73493400	-1.58704900
C	7.62174400	-3.20999800	-0.49908500
H	8.08442800	-3.64266700	1.57200100
H	6.87672000	-2.65629200	-2.45436700
H	8.55997700	-3.62260300	-0.88011300
C	2.60442300	-2.95644300	1.55992700
C	2.94784100	-4.24610800	1.11749600
C	1.39171900	-2.77935300	2.25622900
C	2.10728800	-5.33204400	1.37598000
H	3.87519800	-4.40626400	0.56481700
C	0.55436500	-3.86933500	2.51256000
H	1.10269300	-1.78610900	2.60801100
C	0.91025400	-5.14857600	2.07556900
H	2.39182700	-6.32873300	1.02787700
H	-0.37776200	-3.71050500	3.06040600
H	0.25831100	-6.00211900	2.28064600
C	4.18751900	-0.79716600	2.77015700

C	4.93612800	0.39211500	2.76540400
C	3.93071500	-1.42354000	3.99928200
C	5.41434800	0.94174800	3.95525400
H	5.14631300	0.89451600	1.81893900
C	4.40689200	-0.86969900	5.19400700
H	3.36090100	-2.35341600	4.03655300
C	5.14800600	0.31302700	5.17651700
H	5.99112400	1.87014700	3.93073000
H	4.19596300	-1.37176800	6.14230400
H	5.51736200	0.74568500	6.11012600
Ru	-2.88807100	0.86936900	-0.06999000
N	-3.49443700	-1.95236100	0.53978200
N	-3.92655400	-1.37286300	-1.67819400
C	-3.70899000	-3.80784400	-1.09778900
C	-4.64398100	-5.03614400	-1.15109000
H	-4.13778500	-5.87298500	-0.64178600
H	-4.84853400	-5.37002500	-2.18046300
C	-5.91216500	-4.63365100	-0.37471700
H	-6.66441000	-4.20284300	-1.05392900
H	-6.38878600	-5.50350000	0.10165600
C	-5.44674100	-3.57320100	0.65654600
H	-5.58483700	-3.90583800	1.69568300
H	-6.01098400	-2.63543200	0.55494500
C	-3.94502500	-3.32831400	0.34844900
H	-3.32828300	-3.96319200	1.00129600
C	-2.21824700	-4.13307200	-1.42341500
H	-2.08787400	-5.22514100	-1.48511400
H	-1.55034400	-3.78233000	-0.62202500
C	-1.88387200	-3.44550400	-2.76198500
H	-1.27915100	-4.07708200	-3.42950700
H	-1.30521200	-2.52740400	-2.58406700
C	-3.24388300	-3.09488700	-3.37259700
H	-3.18387600	-2.29178500	-4.11819300
H	-3.68719400	-3.97145100	-3.87464300
C	-4.14137200	-2.75268000	-2.16365700
H	-5.21037300	-2.84456300	-2.41614300
C	-3.50650400	-1.03129800	-0.43860200
C	-3.22962500	-1.38915200	1.80113800
C	-3.12459000	-2.10698300	2.99668200
H	-3.25305300	-3.19052300	3.01714900
C	-2.85945200	-1.40924500	4.18045300
H	-2.77756900	-1.95952700	5.12127100
C	-2.71103400	-0.01979100	4.16708300
H	-2.50316100	0.51925900	5.09490200

C	-2.84695700	0.69427200	2.96754800
H	-2.75211800	1.78165400	2.97959600
C	-3.08198000	0.01426500	1.76776100
C	-4.25783500	-0.23097500	-2.43918600
C	-4.03559200	0.98909200	-1.75526900
C	-4.39847400	2.18692000	-2.37976400
H	-4.27074100	3.14030300	-1.86446900
C	-4.93101400	2.17814300	-3.67712600
H	-5.18689900	3.12279200	-4.16379600
C	-5.15751200	0.96600800	-4.33091500
H	-5.60262900	0.95594500	-5.32909600
C	-4.83109600	-0.24833900	-3.71598500
C	-2.80319800	5.09141700	0.90189600
C	-3.06506500	3.71475500	0.69413800
C	-0.88006000	3.32987200	-0.06068500
C	-0.54729500	4.66686100	0.11399600
C	-1.52065400	5.54811000	0.59676400
H	-0.15656500	2.59699500	-0.41805300
H	0.46406500	5.00500900	-0.11209200
H	-1.27833300	6.60447500	0.74360100
N	-4.30232700	3.19068100	0.96400800
N	-2.11273400	2.86676100	0.21529000
C	-3.87890400	5.99796400	1.43168000
H	-4.21467800	5.67832600	2.43162800
H	-4.77287100	5.98132200	0.78821200
H	-3.52018500	7.03565400	1.50385300
C	-4.49267000	1.92778700	0.69819400
H	-5.03615600	-1.18529800	-4.23295100
C	-5.84144800	1.40812700	1.07272000
C	-6.55283200	2.04072800	2.11556300
C	-6.45688600	0.32550400	0.42112600
C	-7.81887400	1.59960200	2.49576400
H	-6.08611000	2.88566600	2.62319600
C	-7.73709700	-0.10149400	0.78443800
H	-5.94308000	-0.16957800	-0.39936000
C	-8.42096000	0.52728600	1.82787100
H	-8.34274600	2.09756300	3.31630200
H	-8.20422400	-0.93062100	0.24616200
H	-9.41772200	0.18531900	2.11931700
Br	-0.57002100	-0.06571500	-0.98689300

1a

C	-2.63967100	0.94734100	0.07084900
C	-3.98637500	0.56844800	0.07476700

C	-4.34029600	-0.77758500	-0.03636800
C	-3.31419100	-1.71900100	-0.15192300
C	-1.68219800	-0.09475100	-0.04495400
H	-4.76095100	1.33605400	0.16114600
H	-5.38654800	-1.09135700	-0.04019200
H	-3.54762600	-2.78632900	-0.24898400
C	-2.21663600	2.38574100	0.18298400
H	-3.09016000	3.05500300	0.19347500
H	-1.63600200	2.56591500	1.10225300
H	-1.56300800	2.67470400	-0.65490300
N	-2.02681200	-1.38385400	-0.15565700
N	-0.32839200	0.27529200	-0.05826800
C	0.58380100	-0.61566900	0.07957800
C	2.01543000	-0.29785200	0.03538800
C	2.95508000	-1.33178500	0.20310300
C	2.47656600	1.01751400	-0.17403000
C	4.32424700	-1.06106900	0.16259400
H	2.60264100	-2.35449800	0.36533700
C	3.84227700	1.28532800	-0.21395000
H	1.74138900	1.81416600	-0.30339400
C	4.76994900	0.24744800	-0.04609300
H	5.04554400	-1.87179500	0.29342900
H	4.19235500	2.30803100	-0.37746500
H	5.84152900	0.46182900	-0.07862500
H	0.31937800	-1.67643700	0.23373700

2a

C	-1.44949500	-0.02921300	0.00007500
C	-0.31452100	-0.74209300	0.00000000
H	-0.29916900	-1.83353600	-0.00000900
C	-1.53238400	1.47002200	0.00011900
H	-2.09024200	1.82426600	0.88482200
H	-0.54454200	1.94910700	-0.00027600
H	-2.09096400	1.82428900	-0.88411400
C	-2.76896800	-0.76150000	0.00016100
H	-3.36868000	-0.48471800	0.88545600
H	-3.36875100	-0.48480500	-0.88511100
H	-2.64361000	-1.85438600	0.00021200
Br	1.45137600	-0.01610000	-0.00008900

K_2CO_3

K	2.49260700	-0.61429800	0.00422200
C	-0.00006600	0.80879900	-0.00024600
O	-1.12223600	1.42133900	0.02201300

O	-0.00018700	-0.53083300	-0.00023900
K	-2.49256700	-0.61434400	-0.00410000
O	1.12237600	1.42091800	-0.02187900

PPh_3

P	-0.00110400	0.00013400	-1.19873100
C	0.96332200	-1.36722900	-0.39804200
C	0.88416900	-2.63684200	-1.00042300
H	0.26459500	-2.77517600	-1.89173200
C	1.58951500	-3.72287200	-0.47716300
H	1.51154700	-4.70279000	-0.95582400
C	2.40406500	-3.55324800	0.64726900
H	2.96468100	-4.39990400	1.05227200
C	2.50324500	-2.29390800	1.24516800
H	3.14129600	-2.15252900	2.12190100
C	1.78697800	-1.20865700	0.72899900
H	1.87348700	-0.23195700	1.21001300
C	-1.66733700	-0.14994000	-0.39745000
C	-1.94343400	-0.94551400	0.72700600
H	-1.14164900	-1.51050400	1.20735300
C	-3.24187400	-1.02328500	1.24203700
C	-4.28173400	-0.30492200	0.64561600
H	-5.29552600	-0.36743600	1.04985200
C	-4.01953200	0.48895900	-0.47584600
H	-4.82808900	1.04893600	-0.95344100
C	-2.72590600	0.55718700	-0.99777400
H	-2.53437700	1.16637600	-1.88644100
H	-3.43939600	-1.64870800	2.11698800
C	0.70203400	1.51844600	-0.39851300
C	0.15055700	2.15724400	0.72455400
C	1.84626600	2.07801900	-0.99719700
C	0.73482000	3.31917200	1.24015500
H	-0.74133300	1.74729500	1.20348000
C	2.43653400	3.23083700	-0.47456400
H	2.27772200	1.60556900	-1.88496600
C	1.87975000	3.85675900	0.64567700
H	0.29215500	3.80487900	2.11412300
H	3.32808400	3.64814500	-0.95041700
H	2.33472800	4.76456000	1.05075200

$KHCO_3$-KBr

H	2.83562500	-0.86641200	1.61885000
Br	-2.07282600	0.00722900	0.27085100
K	0.15272900	2.10305700	-0.39563800

C	2.16399200	0.09909900	0.10796000
O	2.45739900	-1.10511000	0.75771100
O	1.62191000	-0.05767400	-1.01336900
K	0.10248600	-2.09704500	-0.41846500
O	2.40572200	1.15085800	0.72085600

7. X-ray structural characterization of 3ar, 3au, 3bb, 3bc, 3bf, and 3bm

7.1 X-ray ellipsoid plots of 3ar (CCDC 2340956)

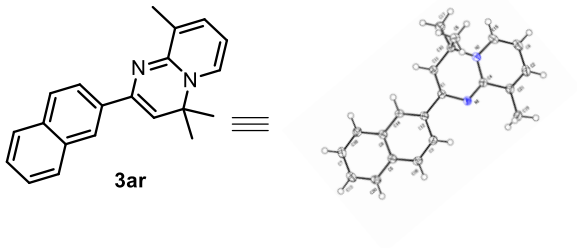
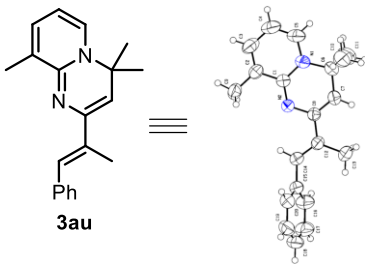


Table S6 Crystal data and structure refinement for 3ar.

Identification code	**3ar**
Empirical formula	$C_{21}H_{20}N_2$
Formula weight	300.39
Temperature/K	150.00(11)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	5.9659(2)
b/Å	12.6239(5)
c/Å	21.0785(8)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1587.48(10)
Z	4
ρ_{calc}mg/mm^3	1.257
μ/mm^{-1}	0.074
F(000)	640.0
Crystal size/mm^3	0.15 × 0.13 × 0.12
2Θ range for data collection	3.76 to 61.18°
Index ranges	-7 ≤ h ≤ 7, -15 ≤ k ≤ 15, -29 ≤ l ≤ 27
Reflections collected	12585
Independent reflections	3833[R(int) = 0.0341]

Data/restraints/parameters	3833/0/211
Goodness-of-fit on F^2	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0376, wR_2 = 0.0901
Final R indexes [all data]	R_1 = 0.0459, wR_2 = 0.0943
Largest diff. peak/hole / e $Å^{-3}$	0.19/-0.21
Flack parameter	-0.2(10)

7.2 X-ray ellipsoid plots of 3au (CCDC 2340957)



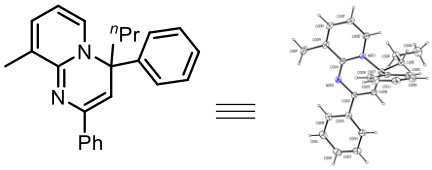
3au

Table S7 Crystal data and structure refinement for 3au.

Identification code	**3au**
Empirical formula	$C_{20}H_{22}N_2$
Formula weight	290.39
Temperature/K	303.64(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	10.02211(19)
b/Å	10.3152(2)
c/Å	16.3908(3)
α/°	90
β/°	90
γ/°	90
Volume/$Å^3$	1694.48(6)
Z	4
ρ_{calc}g/cm^3	1.138
μ/mm^{-1}	0.510
F(000)	624.0
Crystal size/mm^3	0.21 × 0.17 × 0.15
Radiation	Cu *K*α (λ = 1.54184)
2Θ range for data collection/°	10.132 to 151.466
Index ranges	-11 ≤ h ≤ 12, -12 ≤ k ≤ 9, -20 ≤ l ≤ 20
Reflections collected	10954
Independent reflections	3369 [R_{int} = 0.0281, R_{sigma} = 0.0252]
Data/restraints/parameters	3369/0/203
Goodness-of-fit on F^2	1.059

Final R indexes [I>=2σ (I)]	R_1 = 0.0427, wR_2 = 0.1116
Final R indexes [all data]	R_1 = 0.0444, wR_2 = 0.1138
Largest diff. peak/hole / e Å^{-3}	0.14/-0.14
Flack parameter	0.01(19)

7.3 X-ray ellipsoid plots of 3bb (CCDC 2340961)

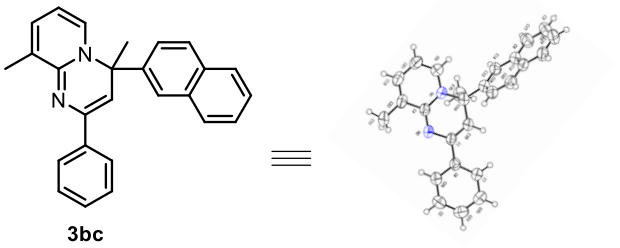


3bb

Table S8 Crystal data and structure refinement for 3bb.

Identification code	**3bb**
Empirical formula	$C_{24}H_{24}N_2$
Formula weight	340.45
Temperature/K	300.77(10)
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	9.3172(3)
b/Å	13.2929(4)
c/Å	15.5466(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1925.49(11)
Z	4
ρ_{calc}g/cm^3	1.174
μ/mm^{-1}	0.523
F(000)	728.0
Crystal size/mm^3	0.15 × 0.14 × 0.12
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.752 to 154.752
Index ranges	-9 ≤ h ≤ 11, -16 ≤ k ≤ 13, -17 ≤ l ≤ 19
Reflections collected	7964
Independent reflections	3184 [R_{int} = 0.0315, R_{sigma} = 0.0352]
Data/restraints/parameters	3184/1/237
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0440, wR_2 = 0.1208
Final R indexes [all data]	R_1 = 0.0477, wR_2 = 0.1241
Largest diff. peak/hole / e Å^{-3}	0.13/-0.13
Flack parameter	-0.2(6)

7.4 X-ray ellipsoid plots of 3bc (CCDC 2340961)

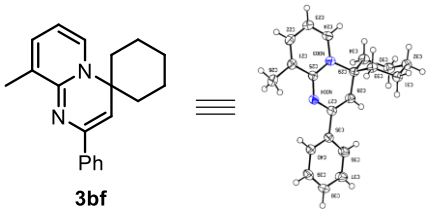


3bc

Table S9 Crystal data and structure refinement for 3bc.

Identification code	**3bc**
Empirical formula	$C_{26}H_{22}N_2$
Formula weight	362.45
Temperature/K	302.03(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.8920(3)
b/Å	20.1165(7)
c/Å	9.3605(3)
α/°	90
β/°	104.195(3)
γ/°	90
Volume/Å^3	1988.35(11)
Z	4
ρ_{calc}g/cm^3	1.211
μ/mm^{-1}	0.543
F(000)	768.0
Crystal size/mm^3	0.18 × 0.15 × 0.12
Radiation	Cu *K*α (λ = 1.54184)
2Θ range for data collection/°	8.374 to 154.156
Index ranges	-13 ≤ h ≤ 13, -24 ≤ k ≤ 19, -11 ≤ l ≤ 11
Reflections collected	13973
Independent reflections	3970 [R_{int} = 0.0459, R_{sigma} = 0.0459]
Data/restraints/parameters	3970/0/255
Goodness-of-fit on F^2	1.072
Final R indexes [I>=2σ (I)]	R_1 = 0.0497, wR_2 = 0.1327
Final R indexes [all data]	R_1 = 0.0687, wR_2 = 0.1529
Largest diff. peak/hole / e Å^{-3}	0.17/-0.20

7.5 X-ray ellipsoid plots of 3bf (CCDC 2340955)

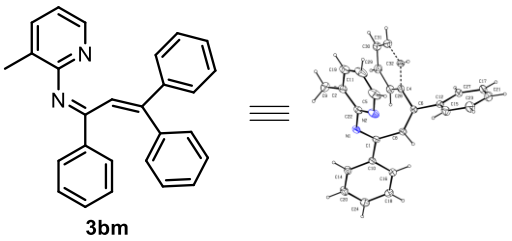


3bf

Table S10 Crystal data and structure refinement for 3bf.

Identification code	**3bf**
Empirical formula	$C_{20}H_{22}N_2$
Formula weight	290.39
Temperature/K	149.99(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.1803(2)
b/Å	12.0750(2)
c/Å	28.1968(4)
α/°	90
β/°	96.3230(10)
γ/°	90
Volume/Å^3	3106.66(10)
Z	8
ρ_{calc}g/cm^3	1.242
μ/mm^{-1}	0.556
F(000)	1248.0
Crystal size/mm^3	0.15 × 0.13 × 0.07
Radiation	Cu *K*α (λ = 1.54184)
2Θ range for data collection/°	6.308 to 153.226
Index ranges	-9 ≤ h ≤ 11, -15 ≤ k ≤ 15, -35 ≤ l ≤ 35
Reflections collected	6789
Independent reflections	6789 [R_{int} = ?, R_{sigma} = 0.0191]
Data/restraints/parameters	6789/0/400
Goodness-of-fit on F^2	1.079
Final R indexes [I>=2σ (I)]	R_1 = 0.0647, wR_2 = 0.1855
Final R indexes [all data]	R_1 = 0.0696, wR_2 = 0.1892
Largest diff. peak/hole / e Å^{-3}	0.34/-0.28

7.6 X-ray ellipsoid plots of 3bm (CCDC 2340960)



3bm

Table S11 Crystal data and structure refinement for 3bm.

Identification code	**3bm**
Empirical formula	$C_{27}H_{22}N_2$
Formula weight	374.46
Temperature/K	301.84(10)
Crystal system	triclinic
Space group	*P*-1
a/Å	9.0020(2)
b/Å	10.8545(2)
c/Å	12.0854(2)
α/°	109.707(2)
β/°	101.745(2)
γ/°	98.816(2)
Volume/Å^3	1056.43(4)
Z	2
ρ_{calc}g/cm^3	1.177
μ/mm^{-1}	0.528
F(000)	396.0
Crystal size/mm^3	0.17 × 0.14 × 0.12
Radiation	Cu *K*α (λ = 1.54184)
2Θ range for data collection/°	8.082 to 152.07
Index ranges	-11 ≤ h ≤ 11, -13 ≤ k ≤ 13, -15 ≤ l ≤ 14
Reflections collected	11830
Independent reflections	4181 [R_{int} = 0.0256, R_{sigma} = 0.0271]
Data/restraints/parameters	4181/60/308
Goodness-of-fit on F^2	1.072
Final R indexes [I>=2σ (I)]	R_1 = 0.0461, wR_2 = 0.1288
Final R indexes [all data]	R_1 = 0.0543, wR_2 = 0.1368
Largest diff. peak/hole / e Å^{-3}	0.11/-0.14

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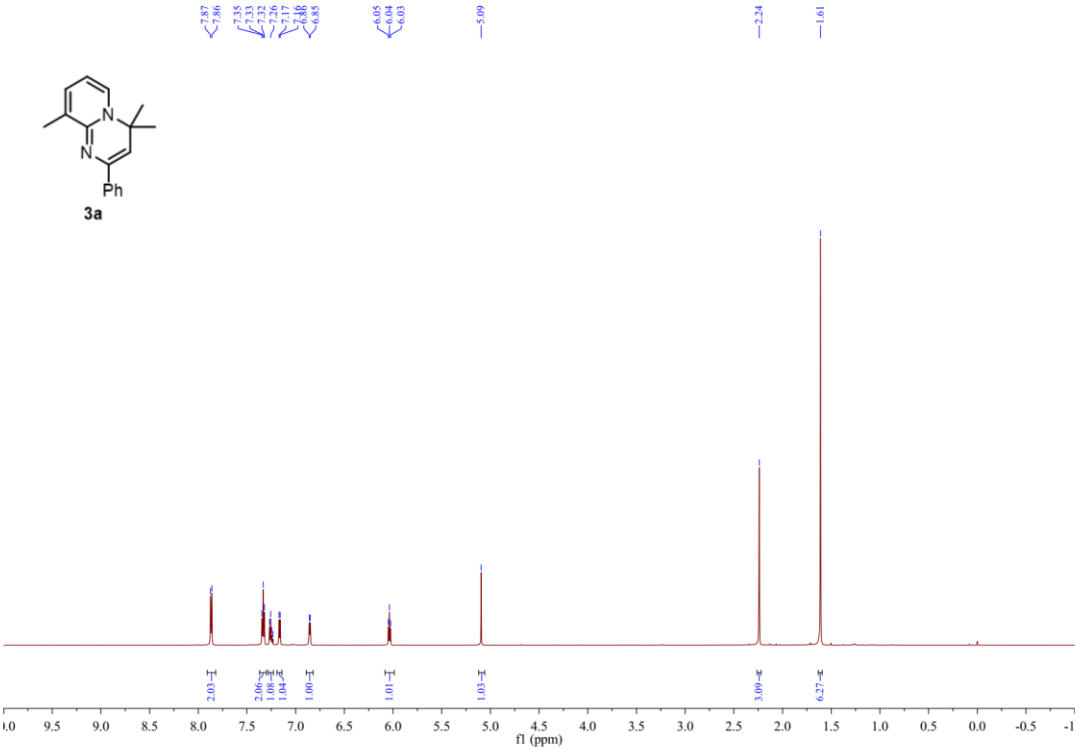
9. Copies of NMR spectra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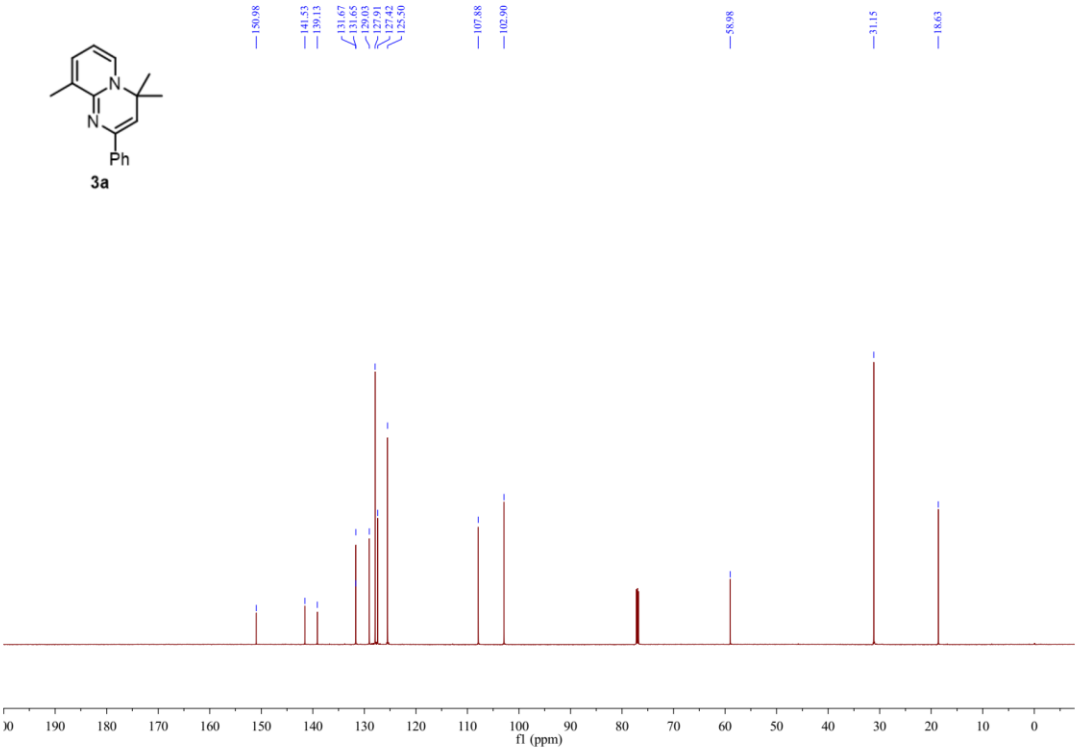
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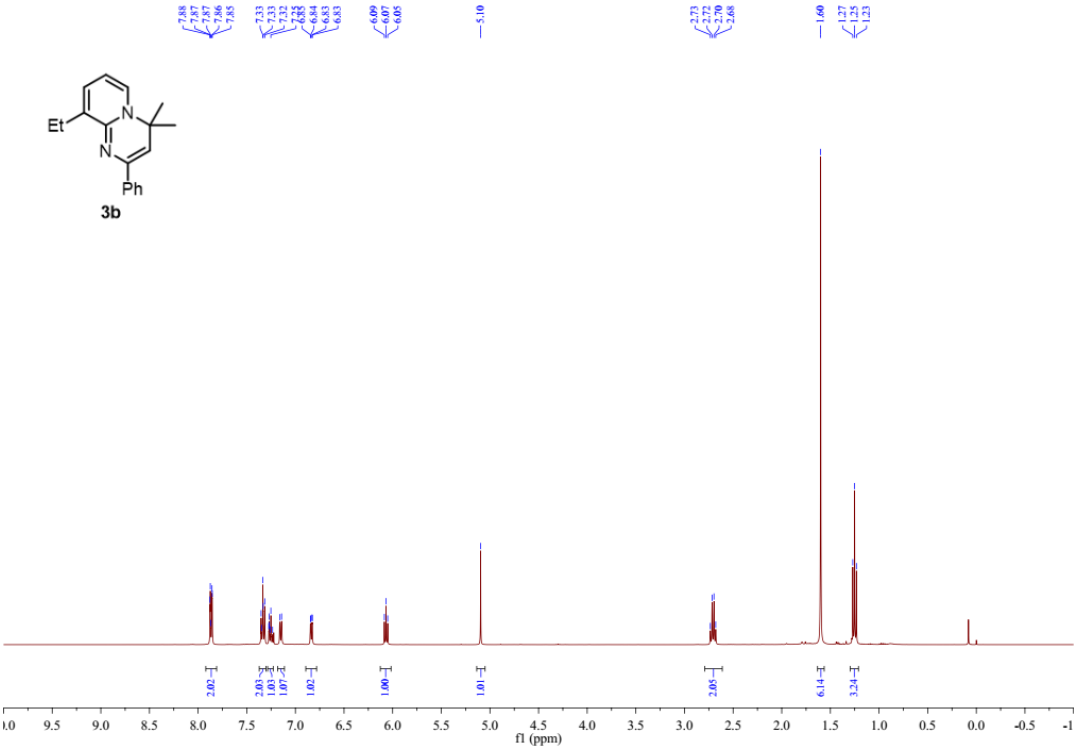
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1.25
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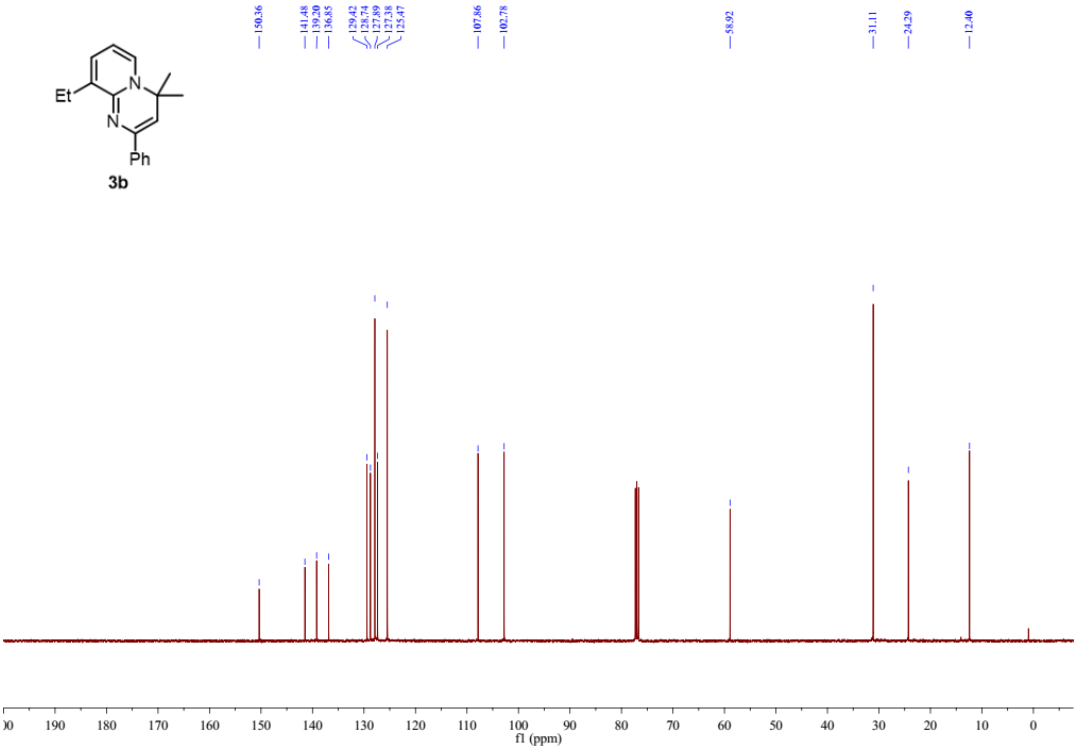
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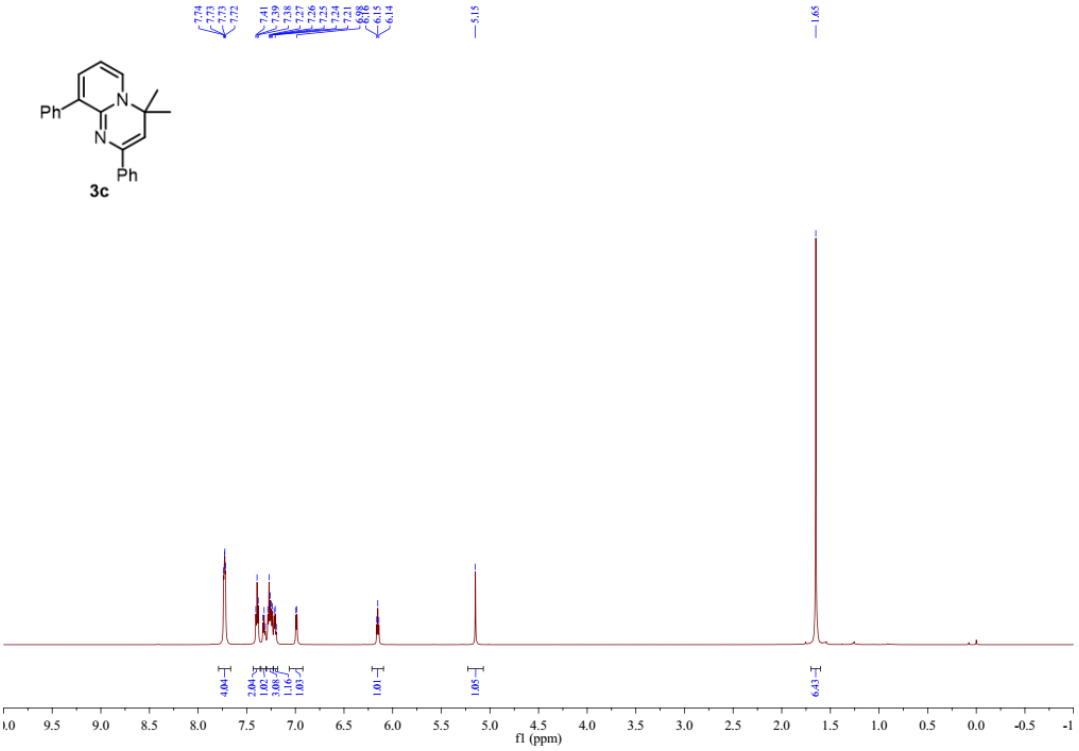
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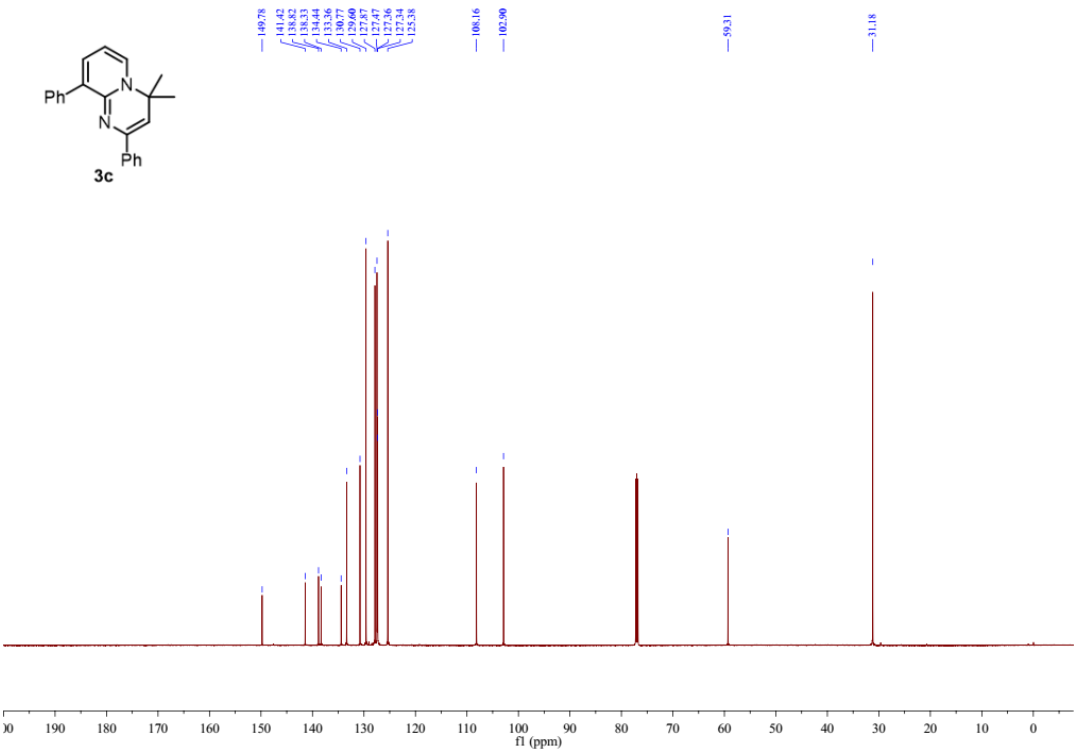
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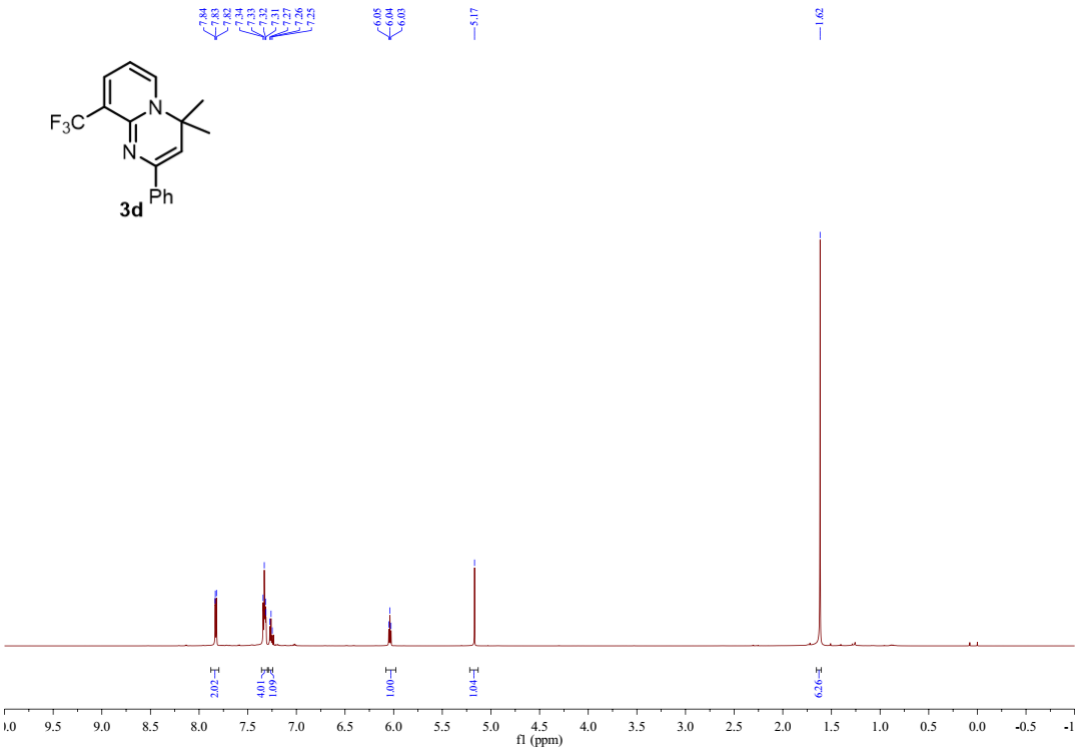
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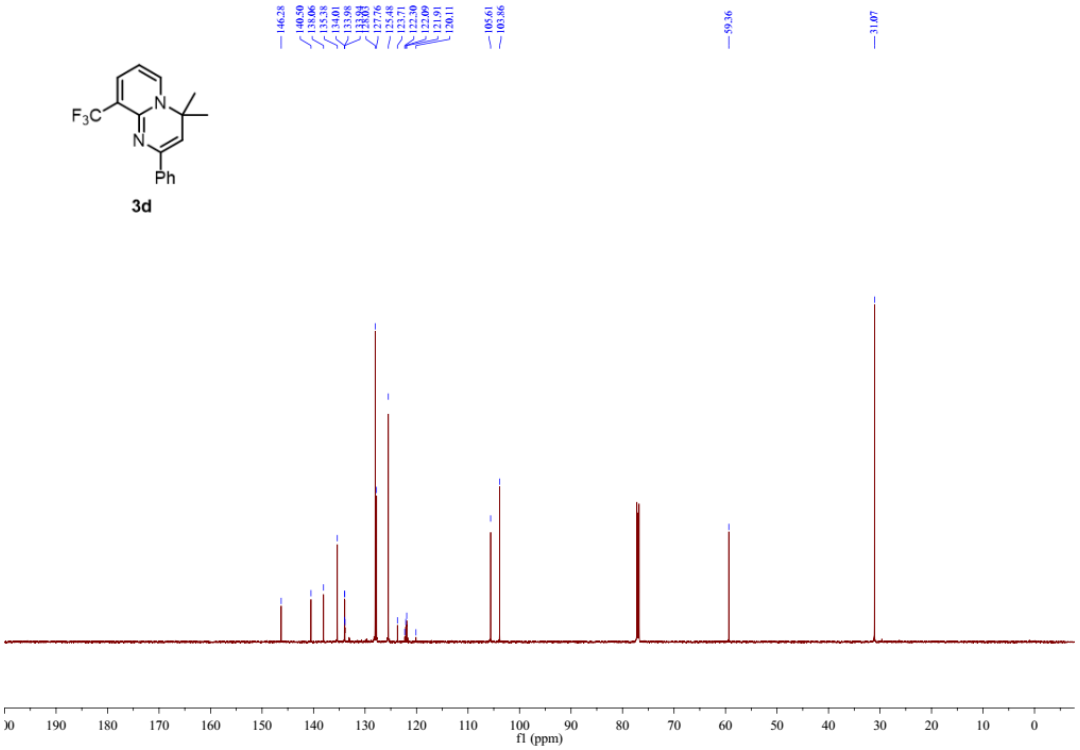
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f1 (ppm)

F3C
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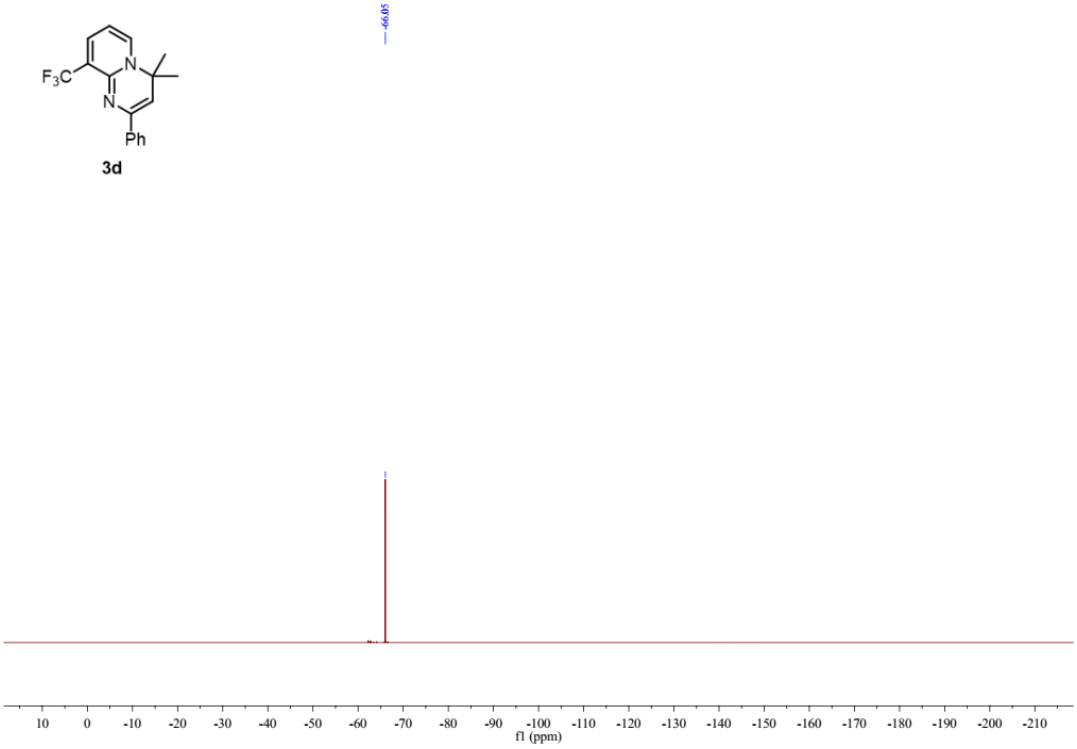
N
Ph

3d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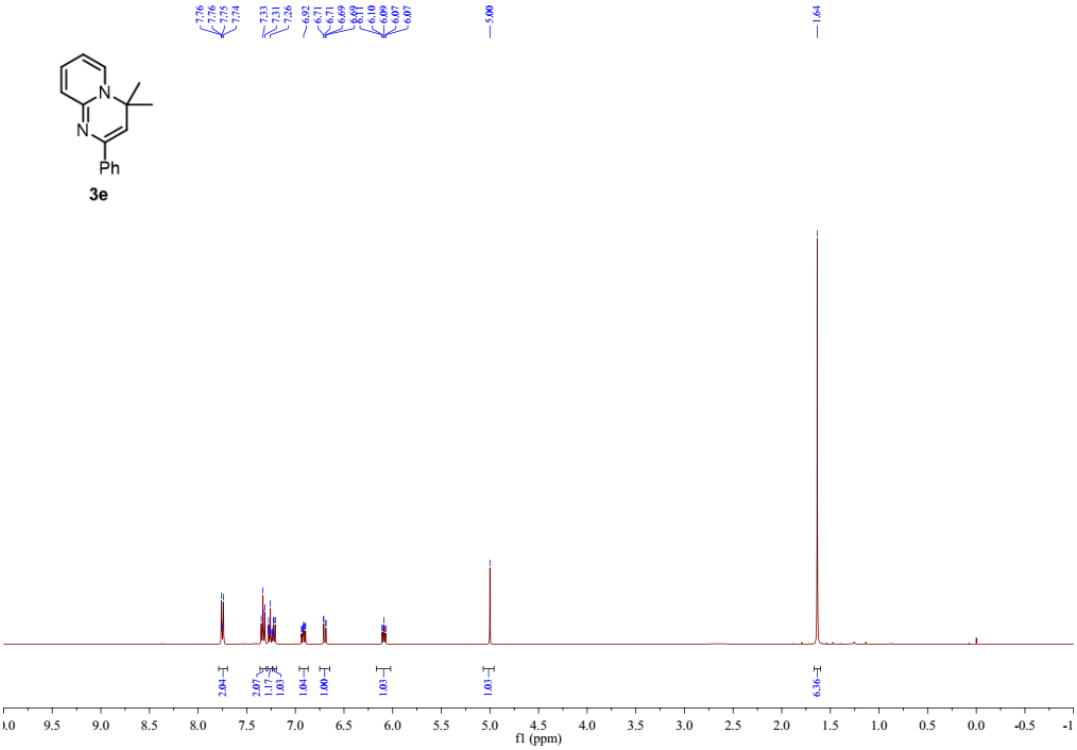
Ph

3e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6.07
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1.03
1.04
1.00
1.03
1.03
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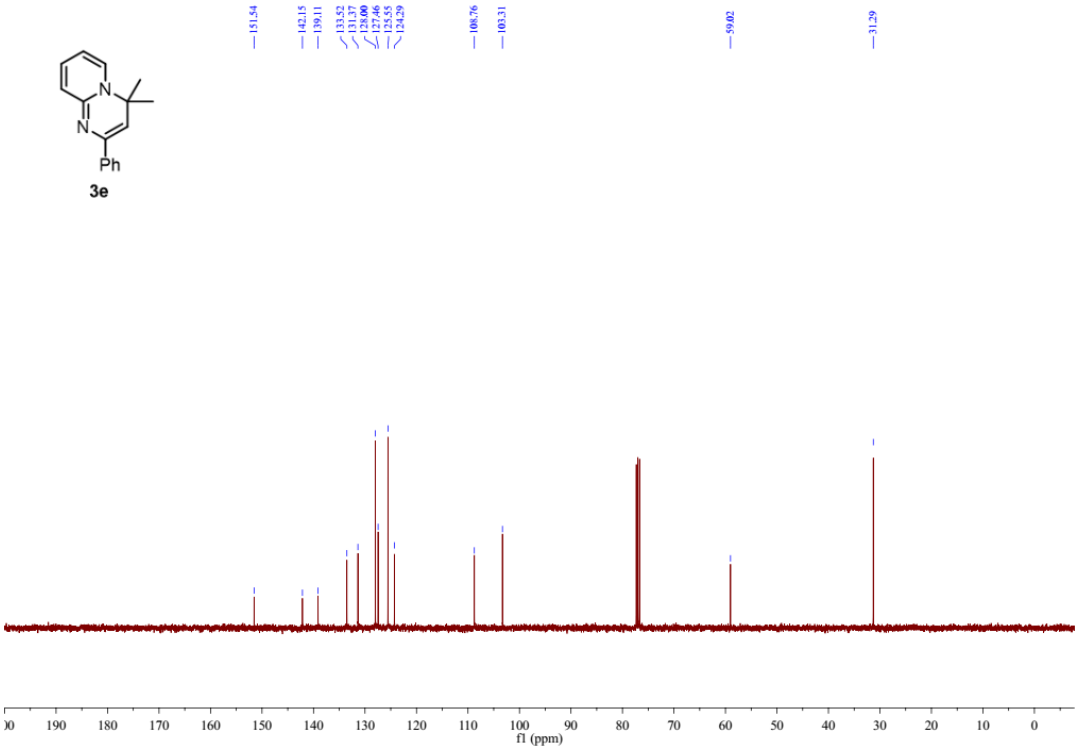
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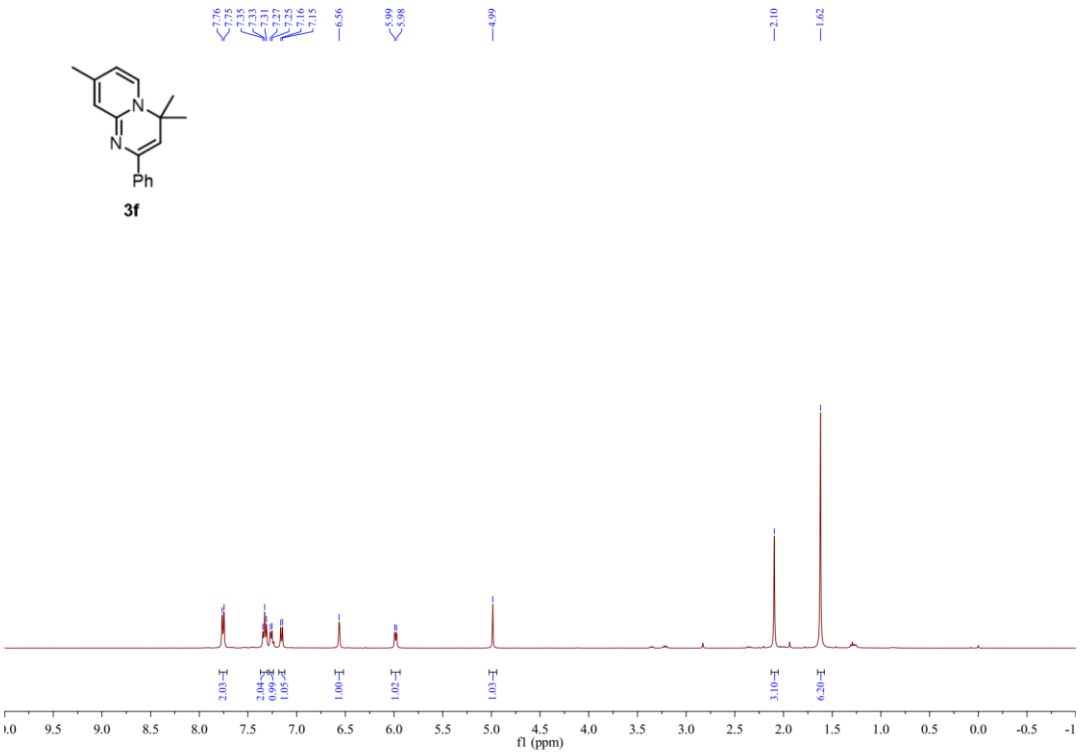
fl (ppm)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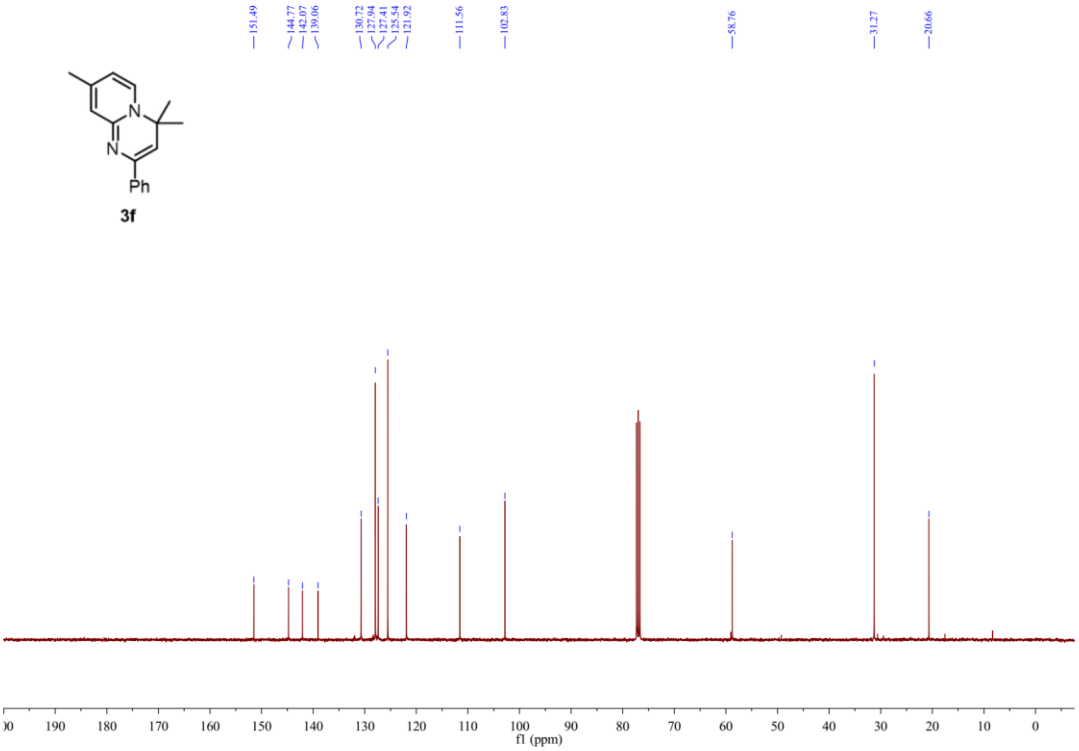
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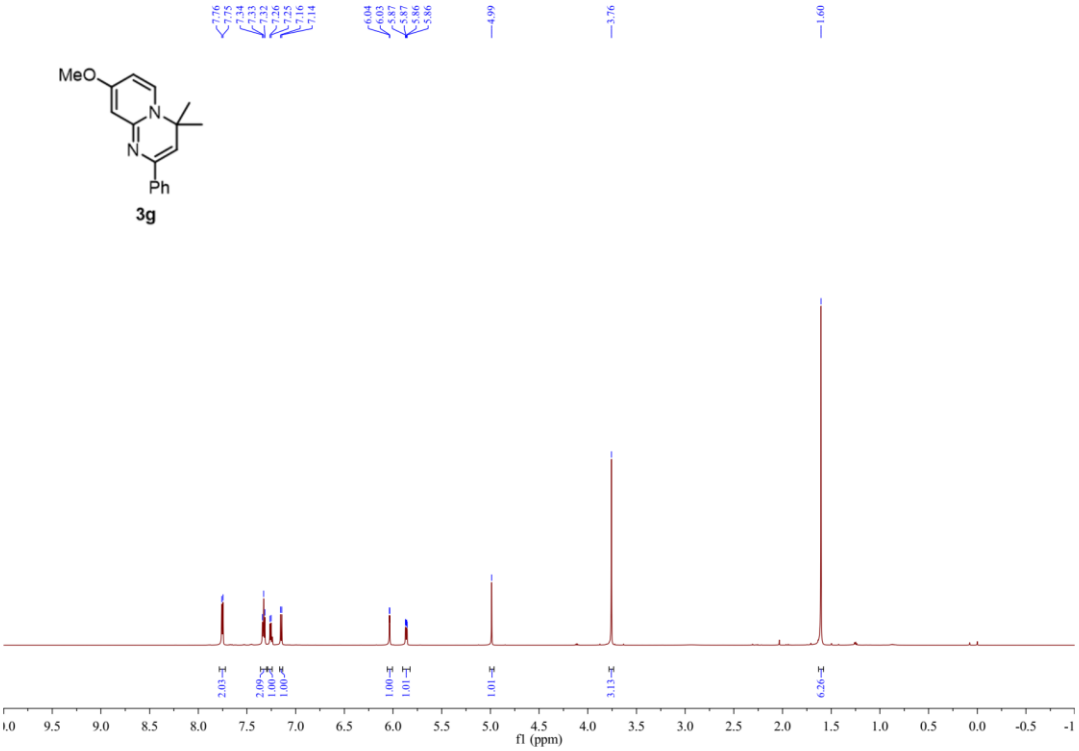
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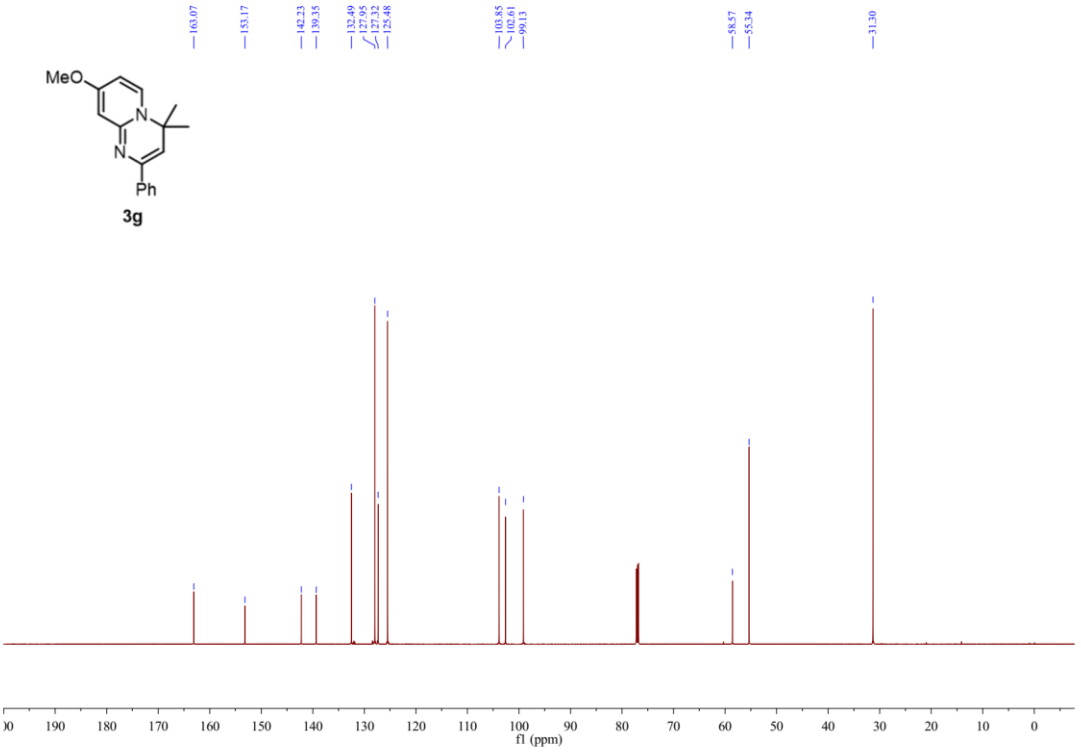
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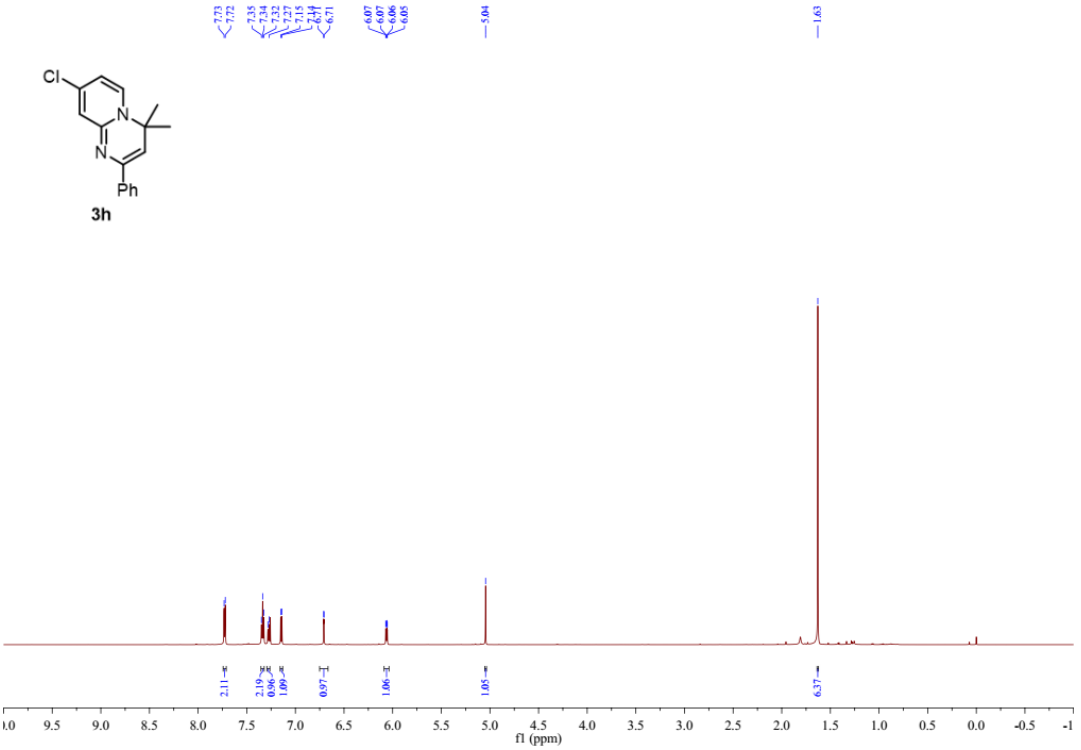
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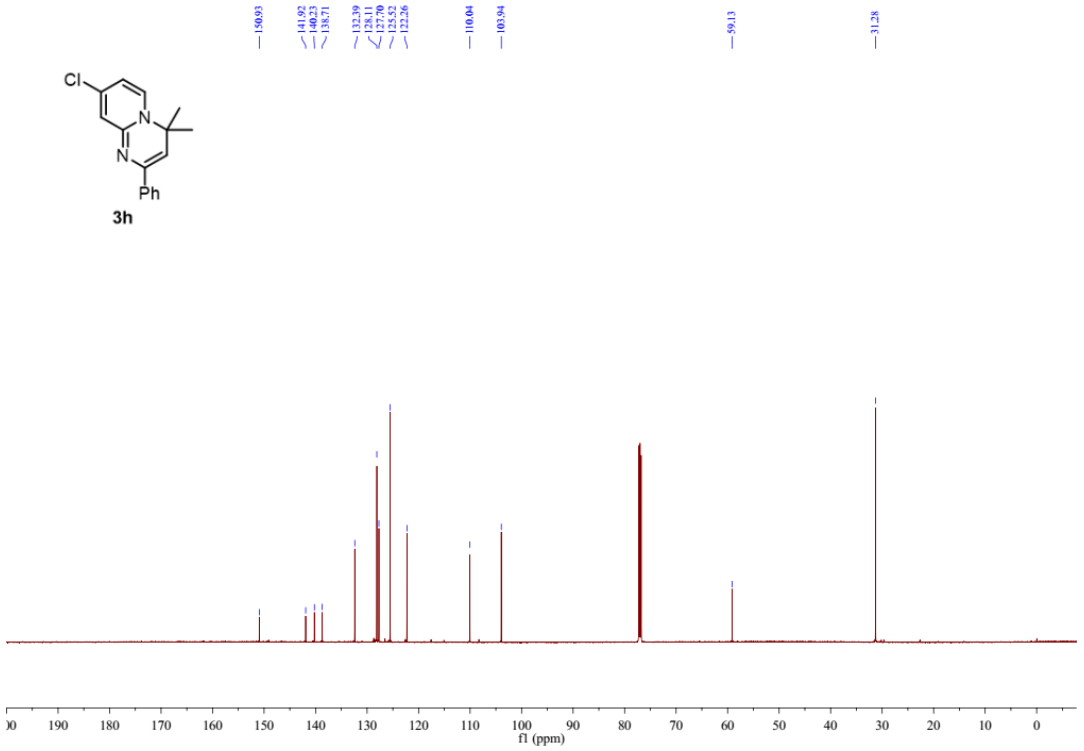
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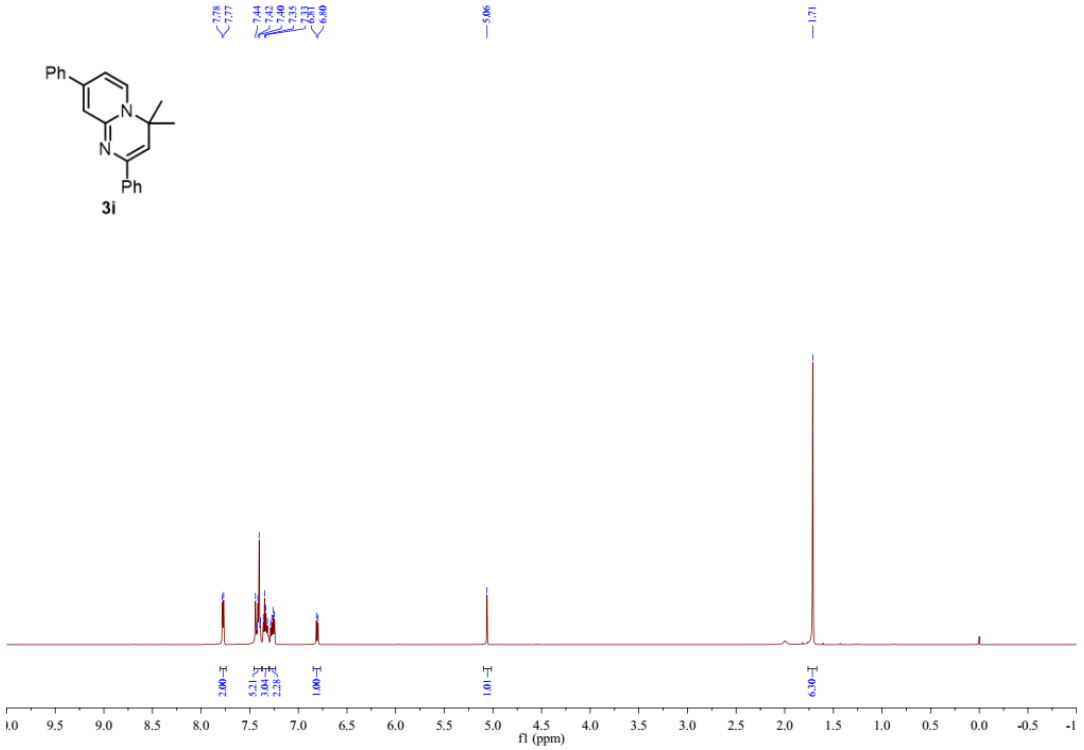
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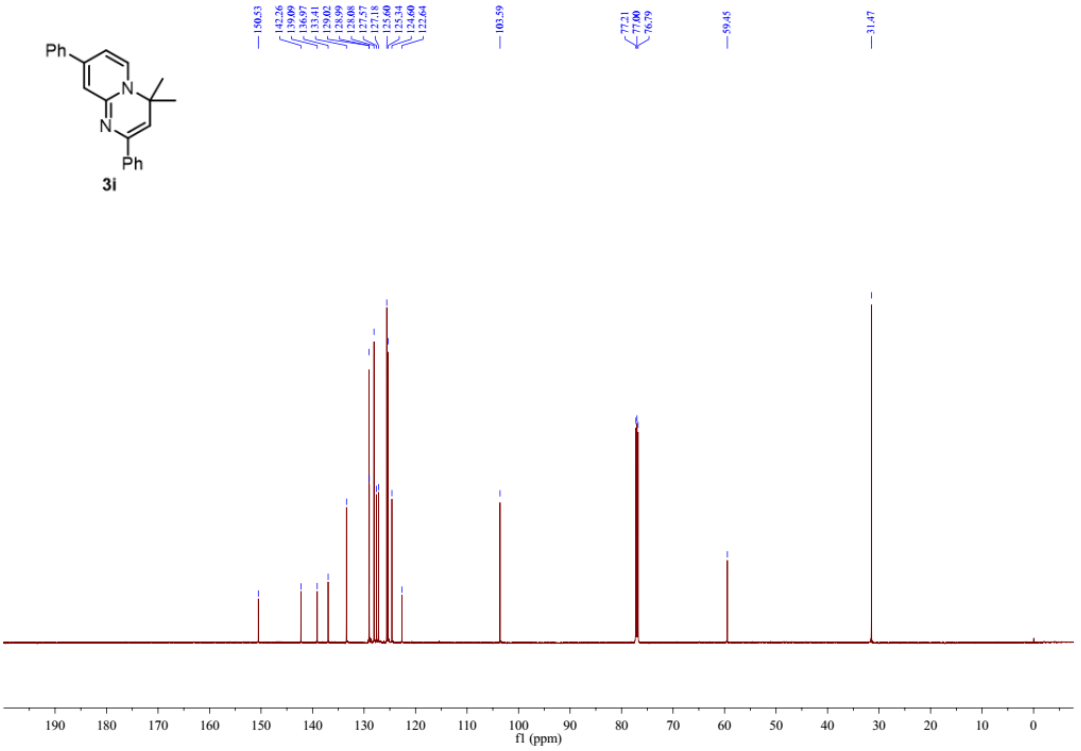
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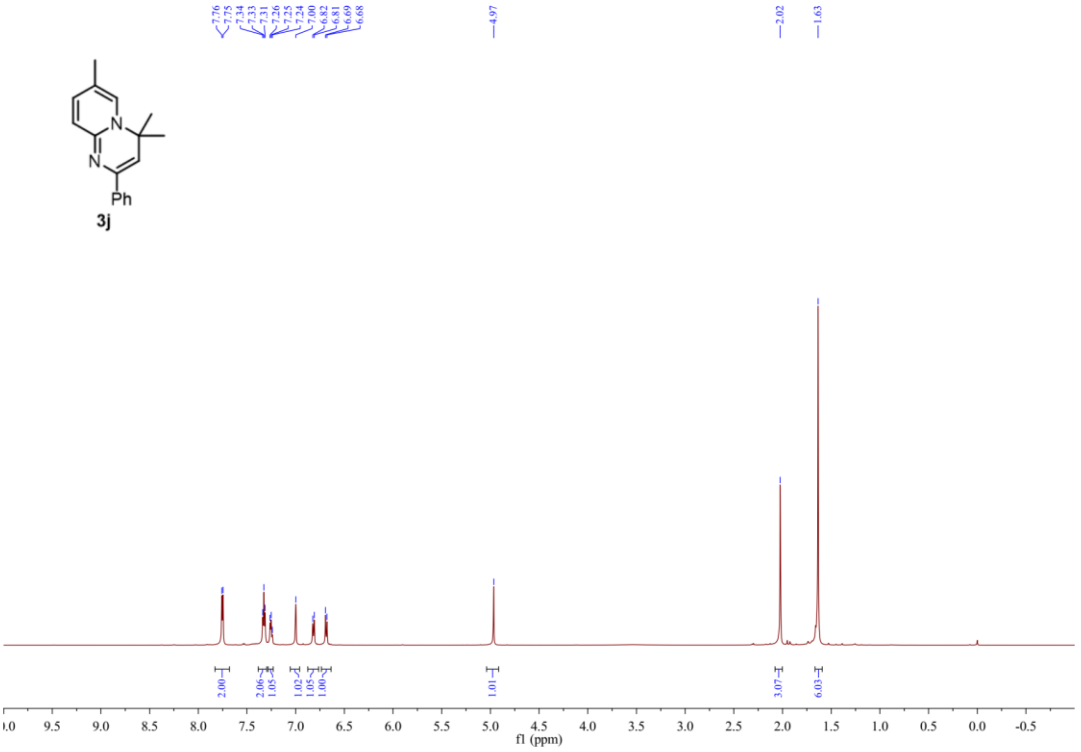
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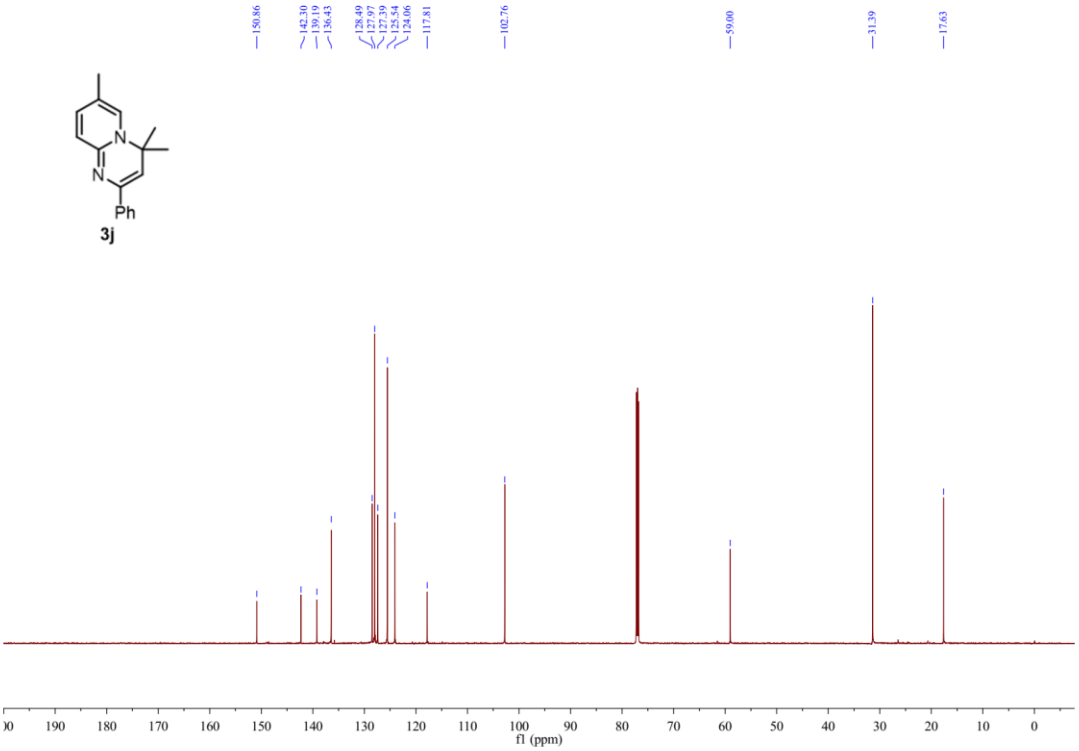
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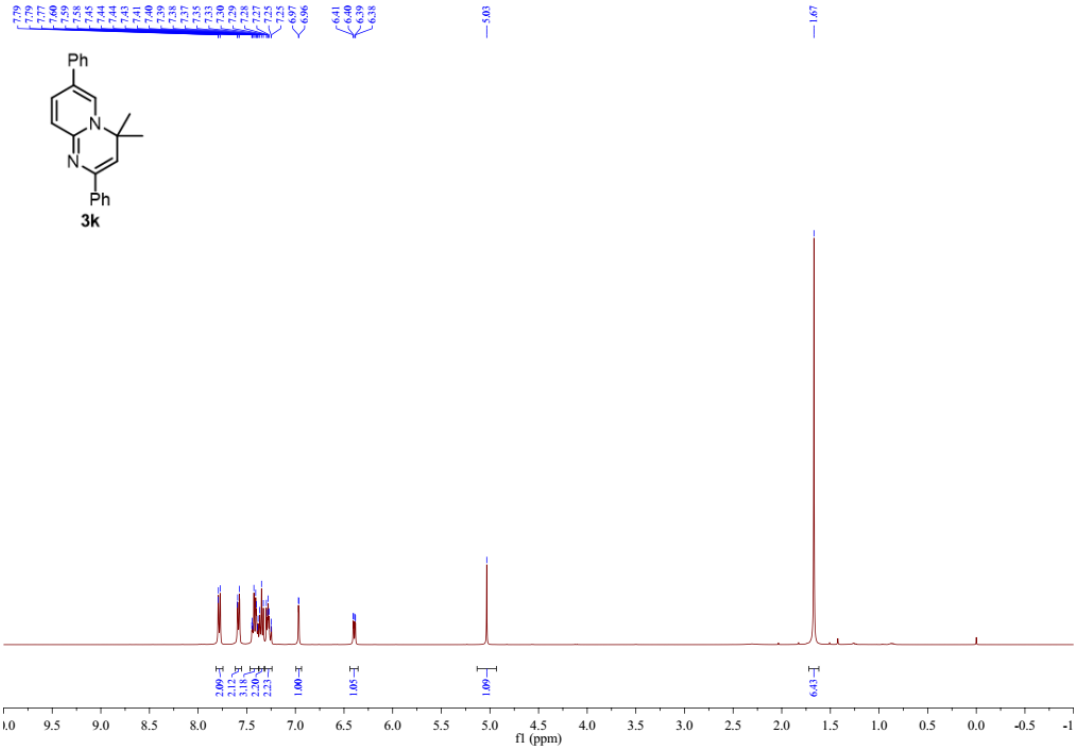
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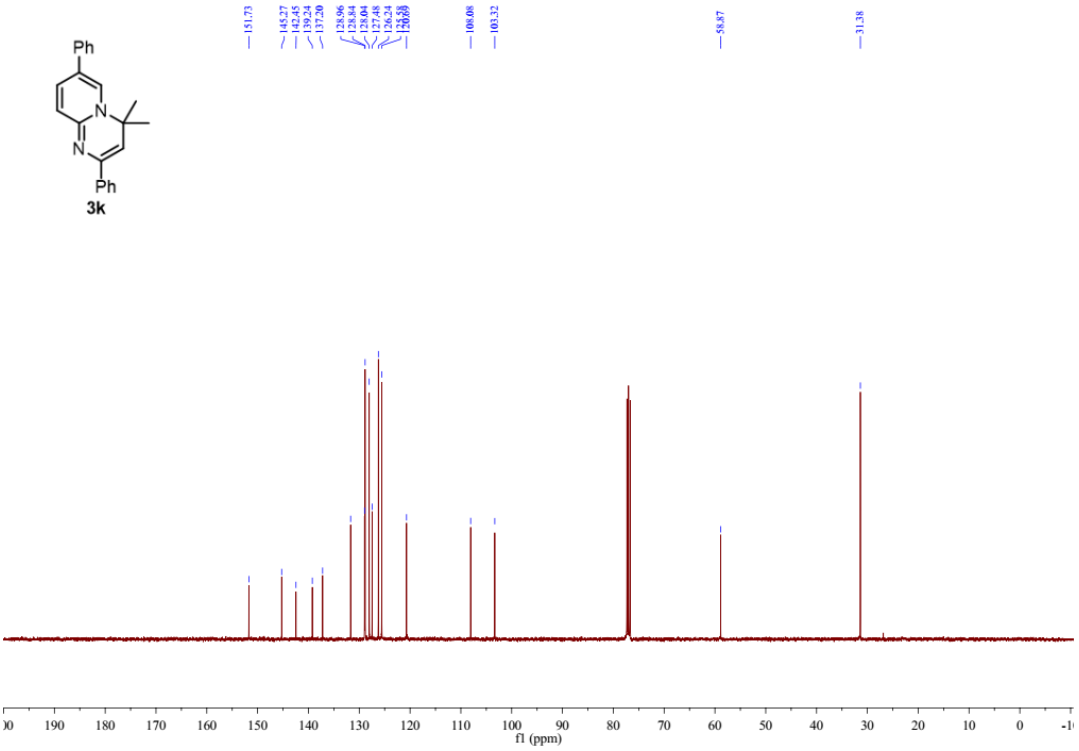
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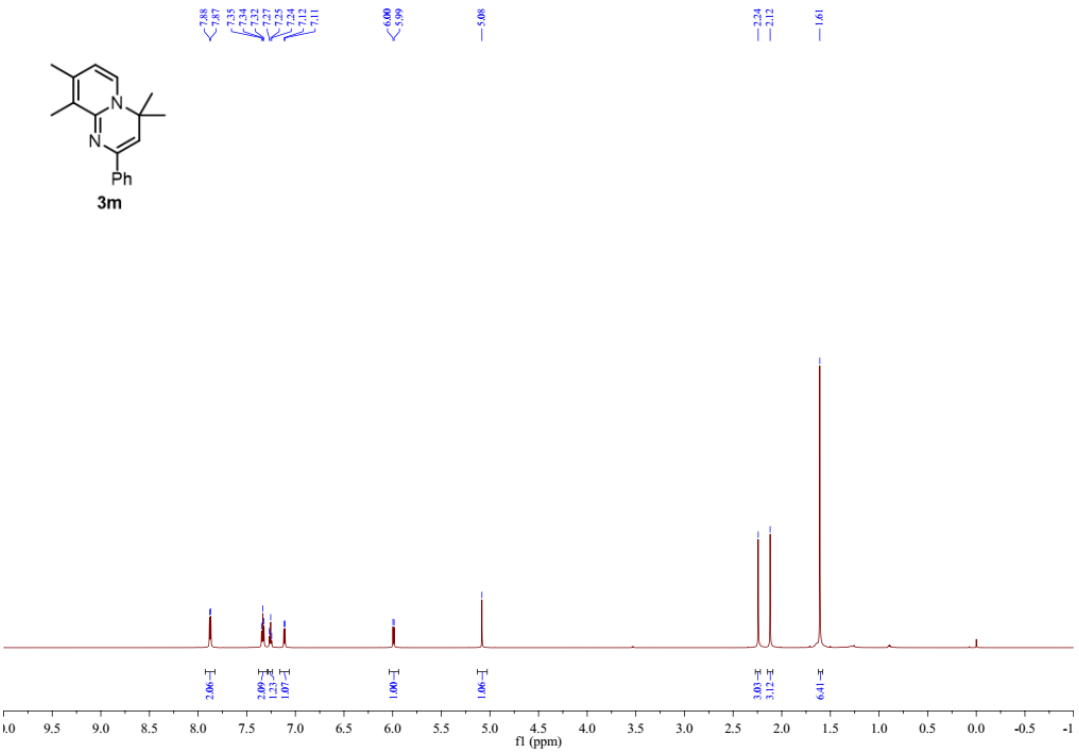
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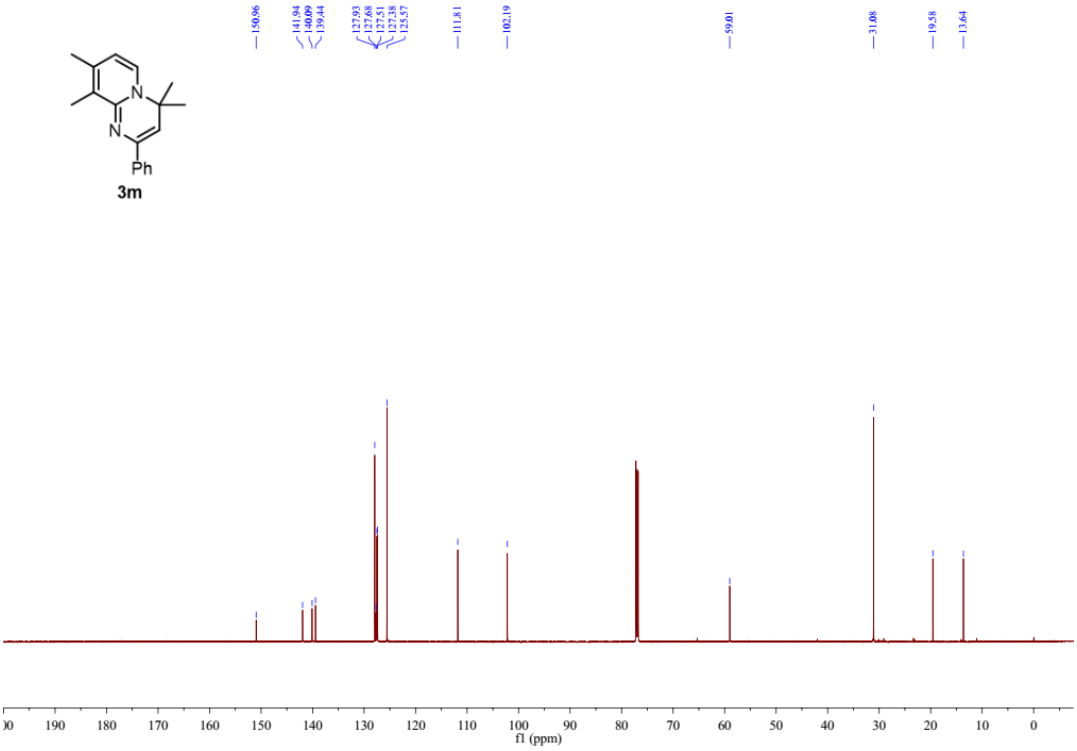
Ph

3m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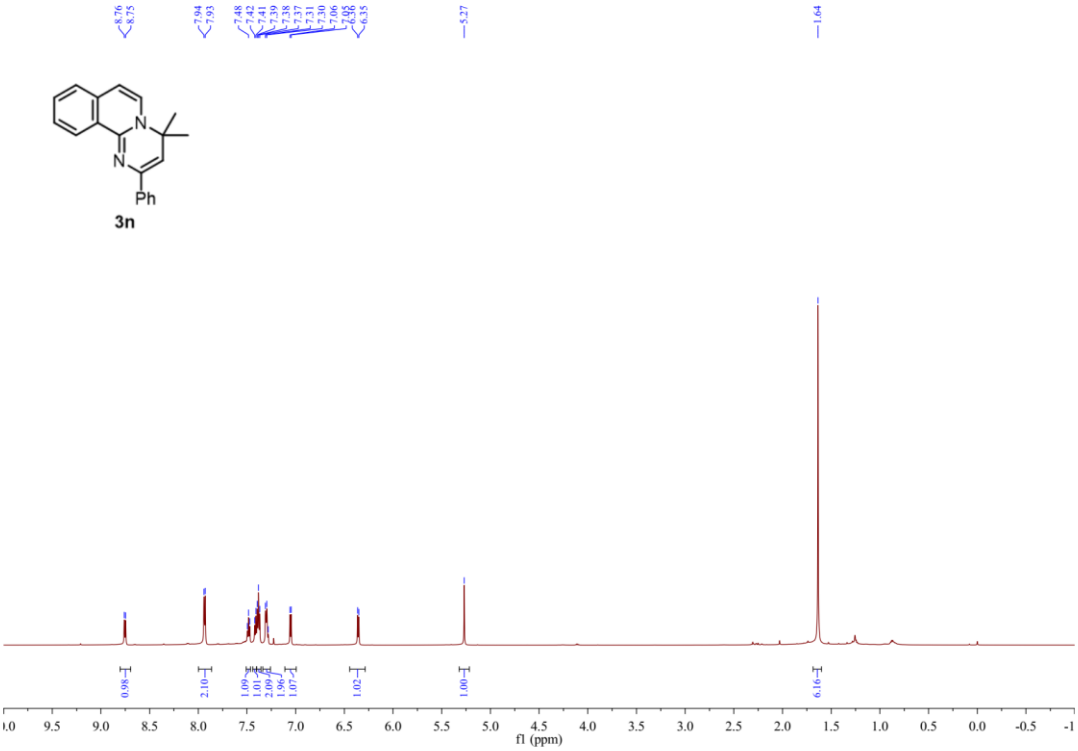
Ph

3n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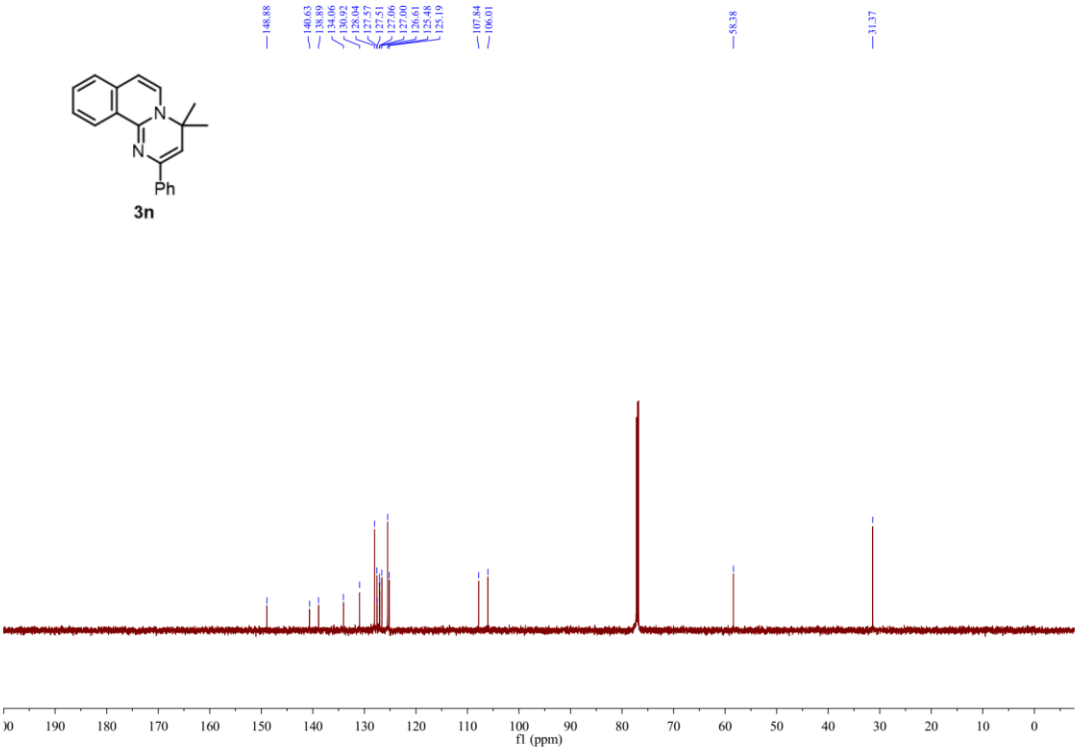
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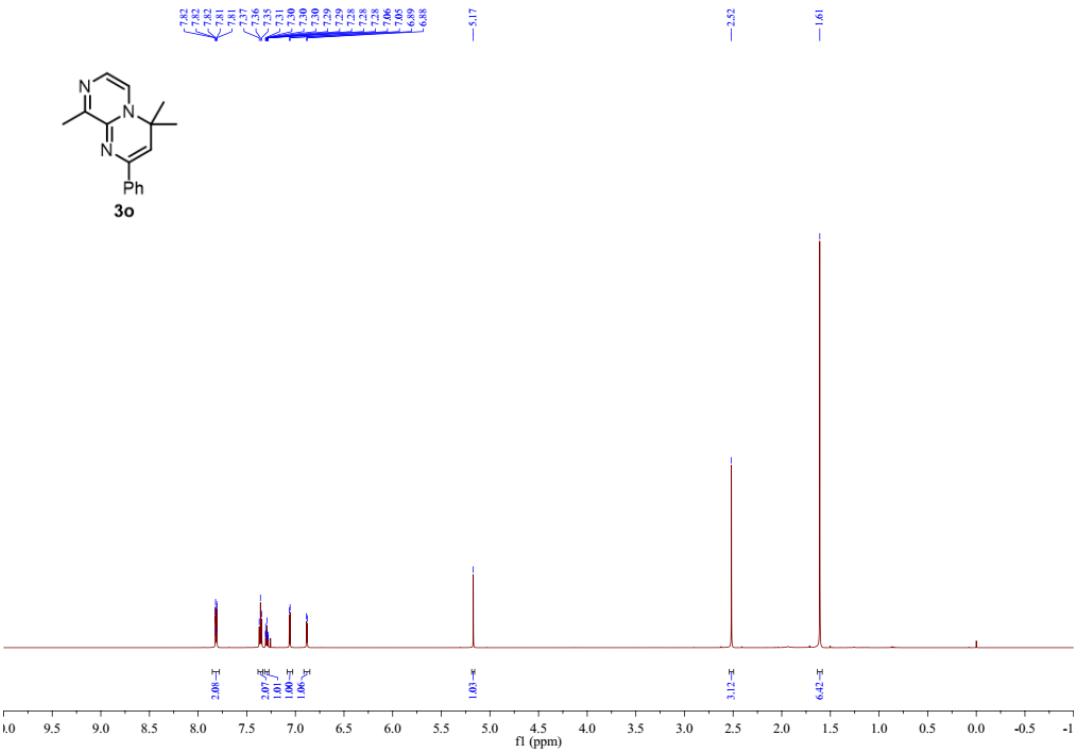
fl (ppm)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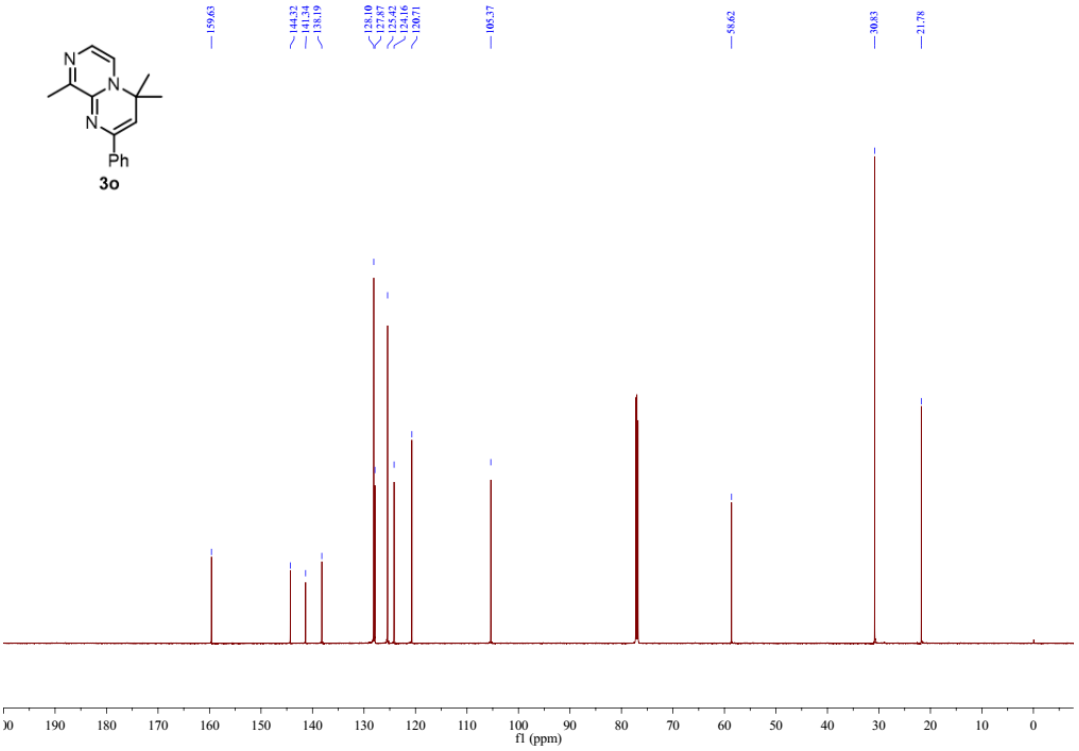
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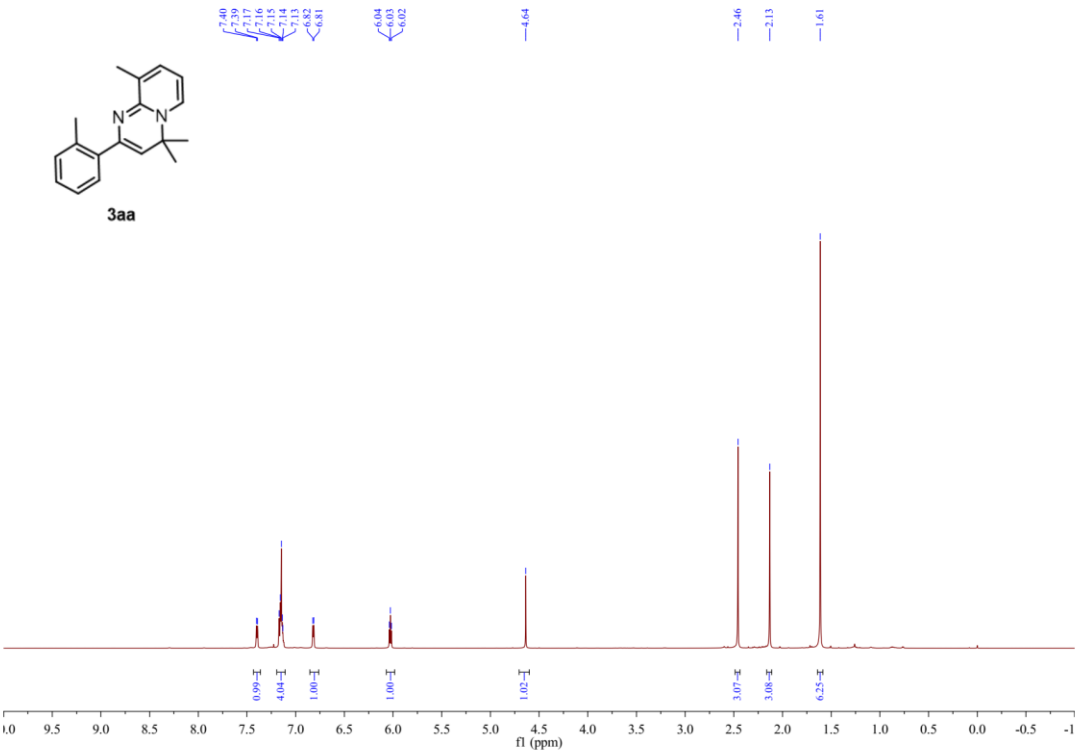
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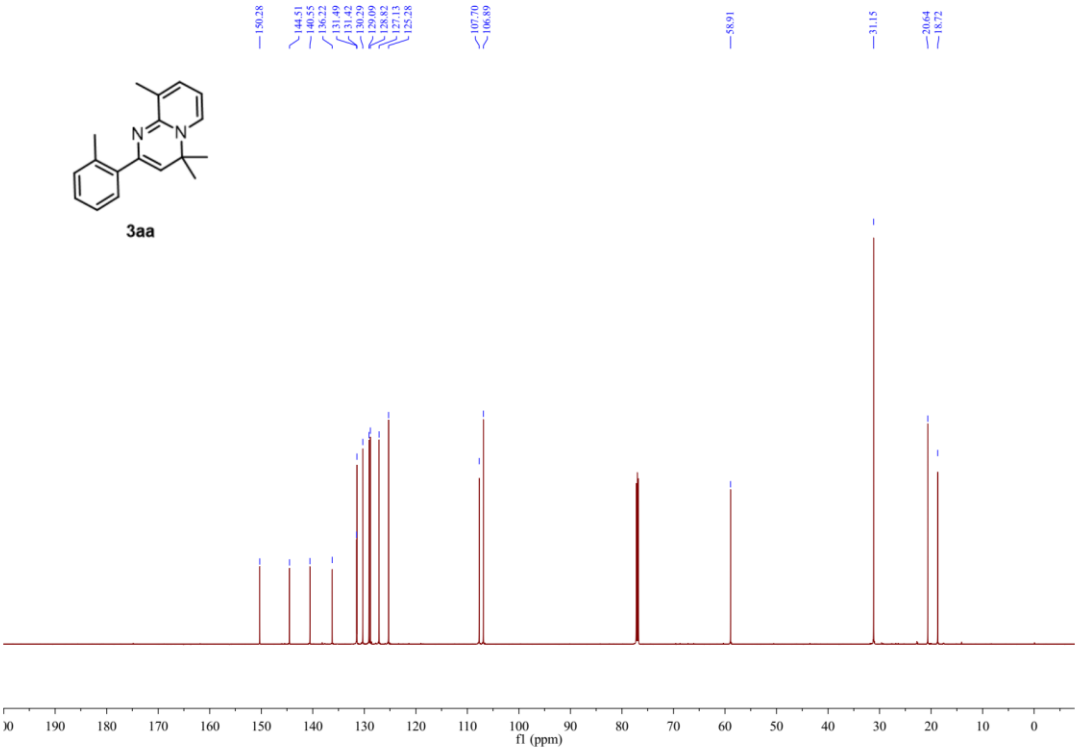
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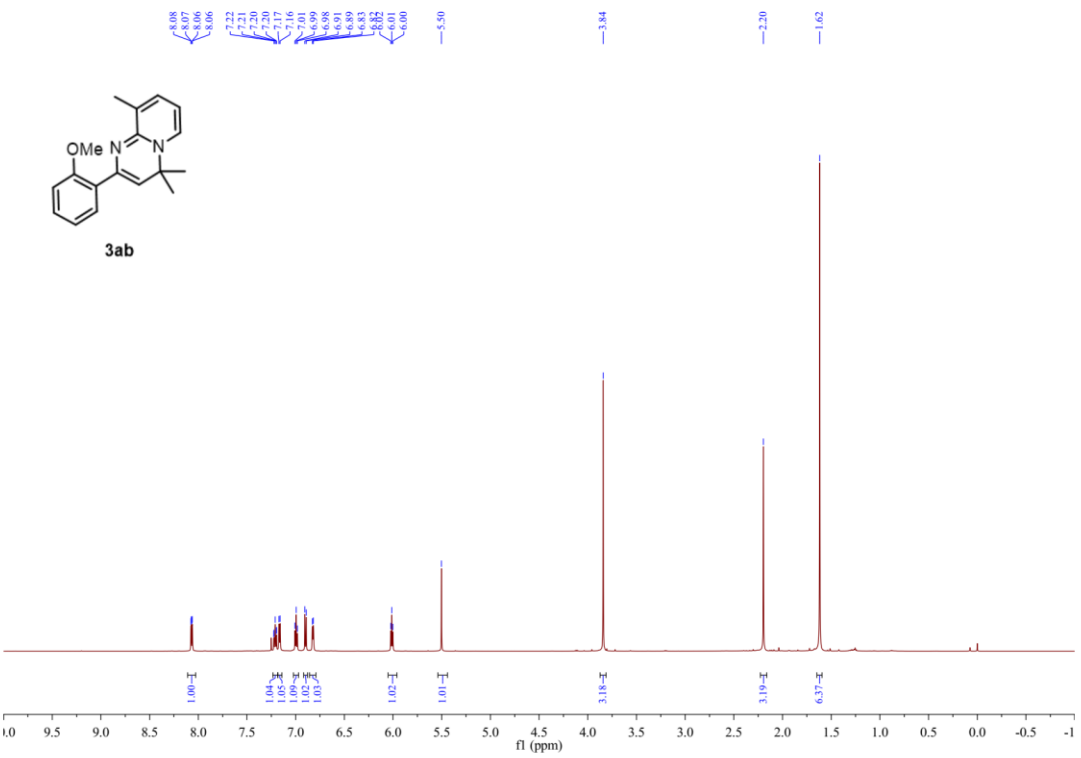
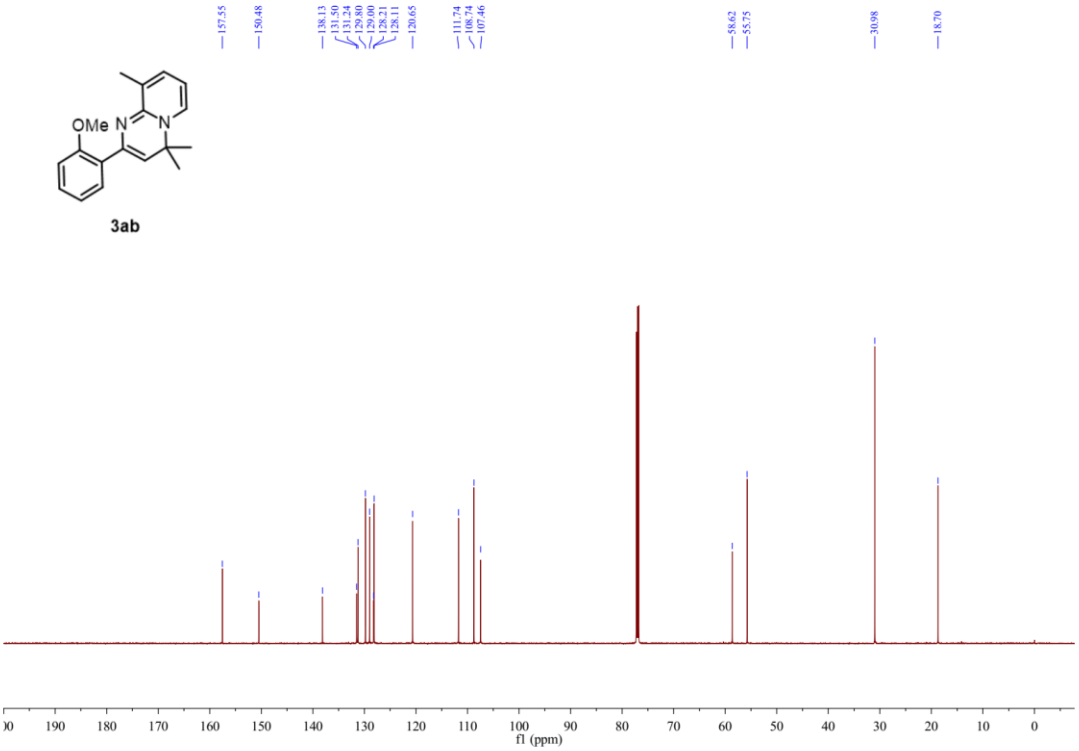
fl (ppm)


8.08
8.07
8.06
8.06
7.22
7.21
7.20
7.20
7.17
7.16
7.01
6.99
6.98
6.91
6.89
6.83
6.82
6.02
6.01
6.00
5.50
3.84
2.20
1.62
OMe
N
N
3ab
1.00
1.04
1.05
1.09
1.02
1.03
1.02
1.01
3.18
3.19
6.37
fl (ppm)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129.80
129.00
128.21
128.11
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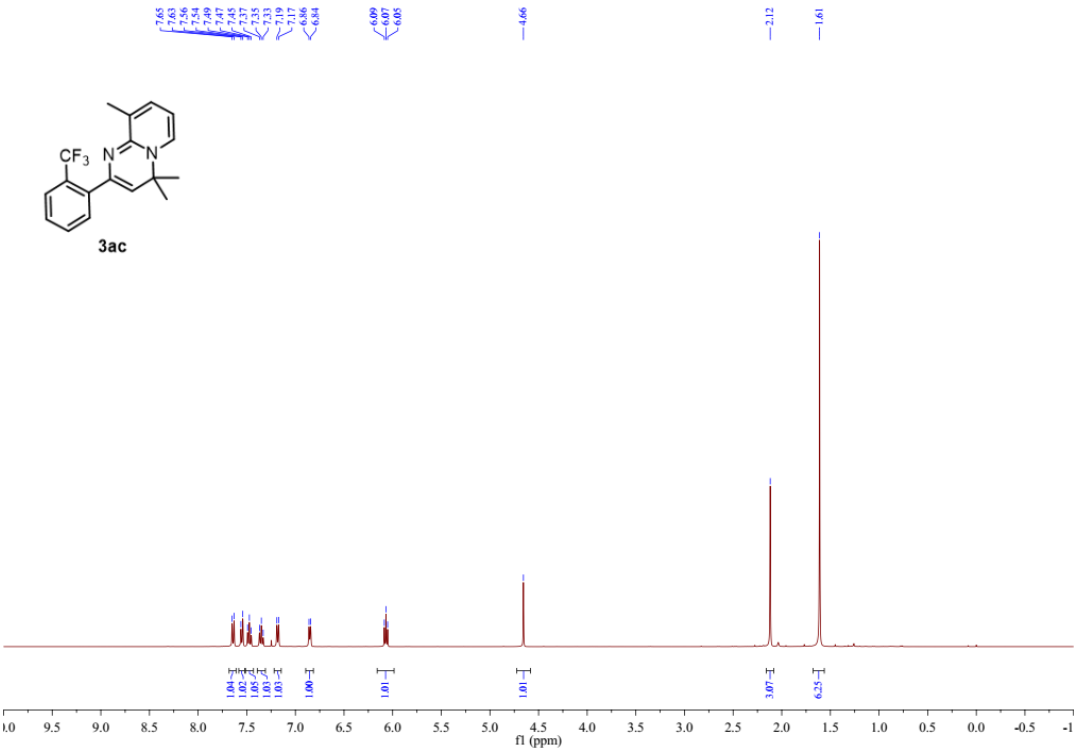
111.74
108.74
107.46
58.62
55.75
30.98
18.70
OMe
N
N
3ab
f1 (ppm)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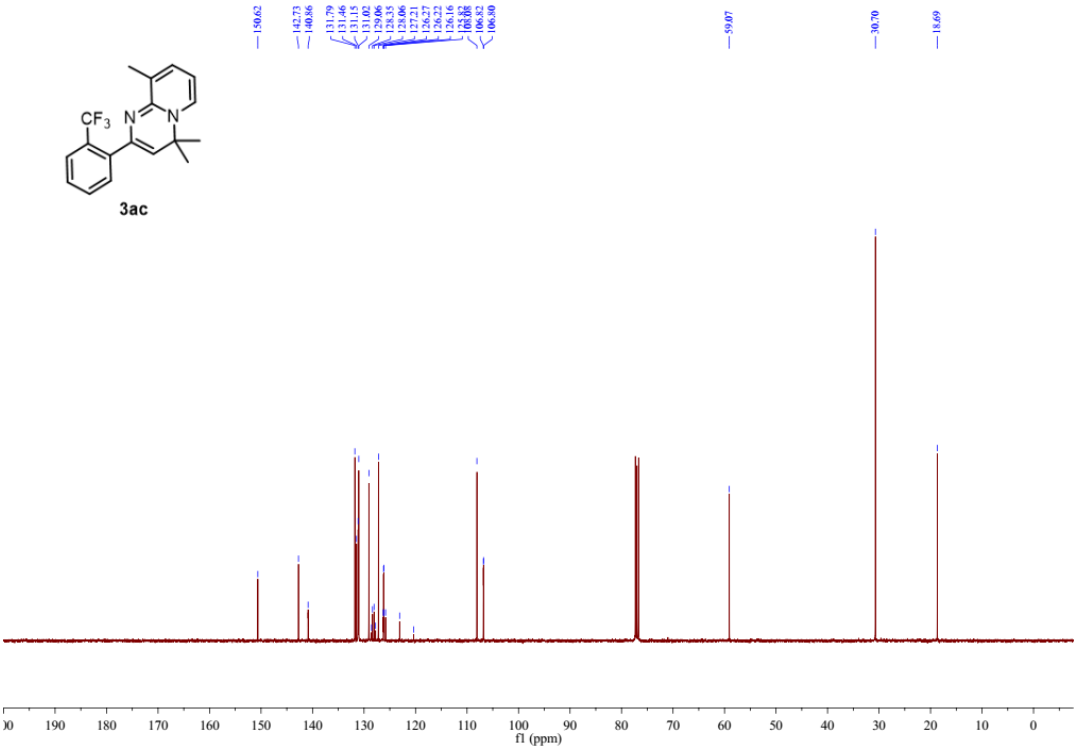
7.63
7.56
7.54
7.49
7.47
7.45
7.37
7.35
7.33
7.19
7.17
6.86
6.84
6.09
6.07
6.05
4.66
2.12
1.61
CF3
N
N
3ac
1.04
1.02
1.05
1.03
1.03
1.00
1.01
1.01
3.07
6.25
f1 (ppm)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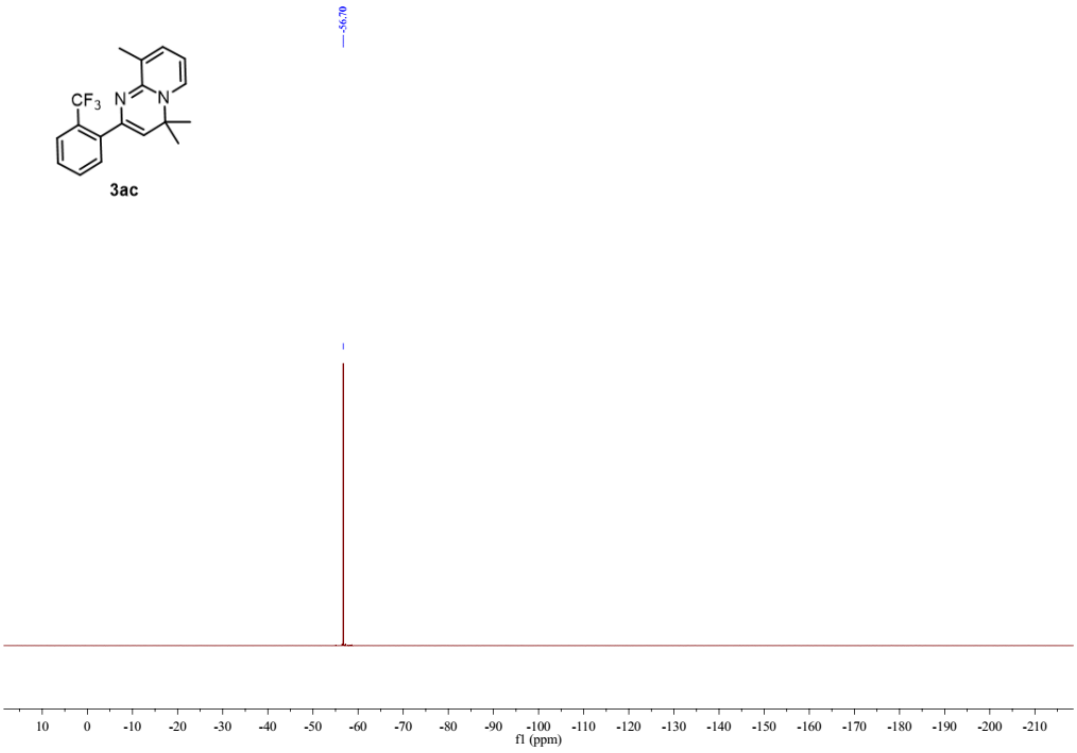
140.86
131.79
131.46
131.15
131.02
129.06
128.35
124.66
127.21
126.27
126.22
126.16
106.82
106.80
59.07
30.70
18.69
CF3
N
N
3ac
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-56.70
CF3
N
N
3ac
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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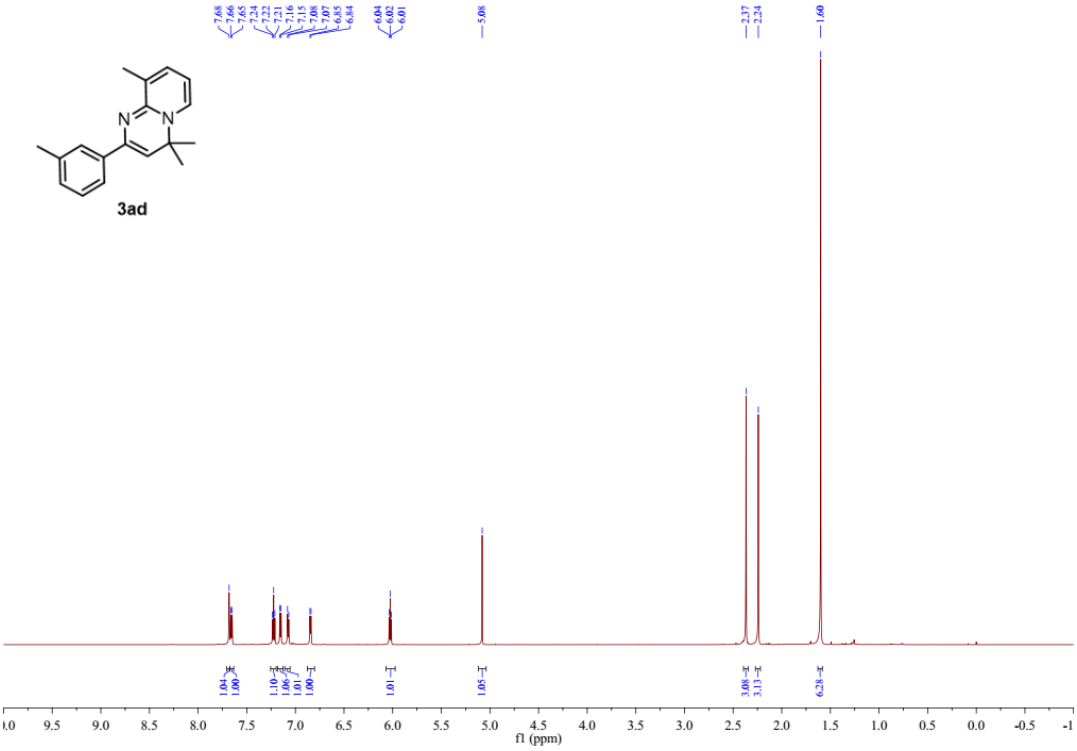
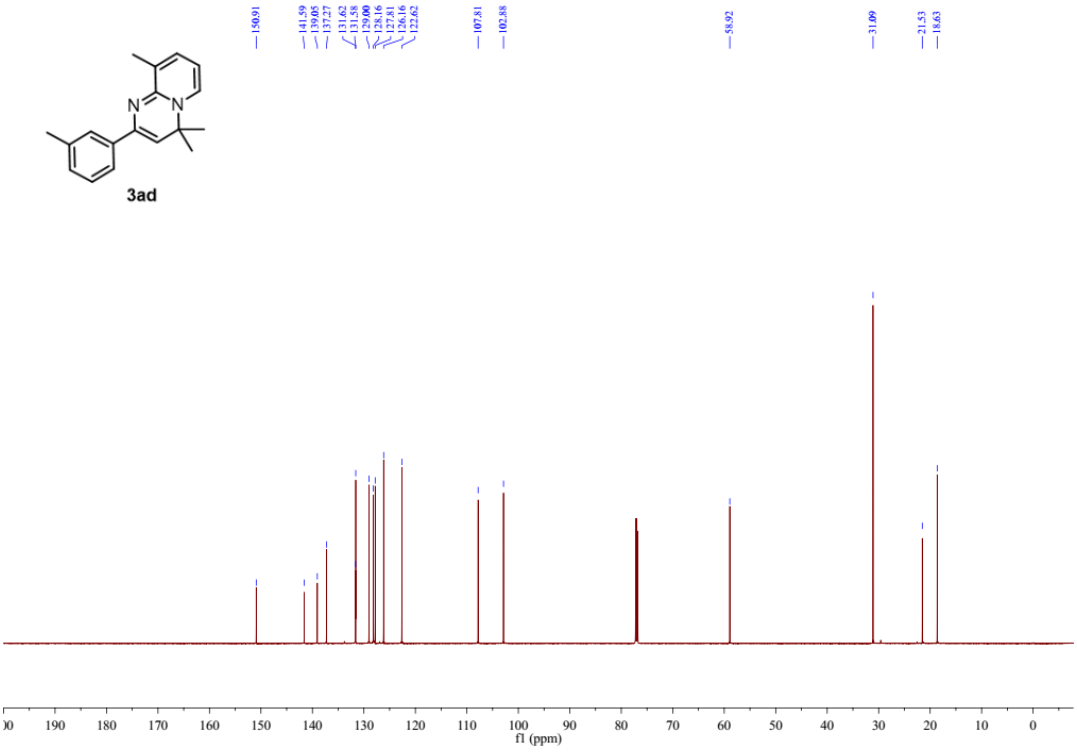
-160
-170
-180
-190
-200
-210
f1 (ppm)


7.68
7.66
7.65
7.24
7.22
7.21
7.16
7.15
7.08
7.07
6.85
6.84
6.04
6.02
6.01
5.08
2.37
2.24
1.60
1.04
1.00
1.10
1.06
1.01
1.00
1.01
1.05
3.08
3.13
6.28
f1 (ppm)

3ad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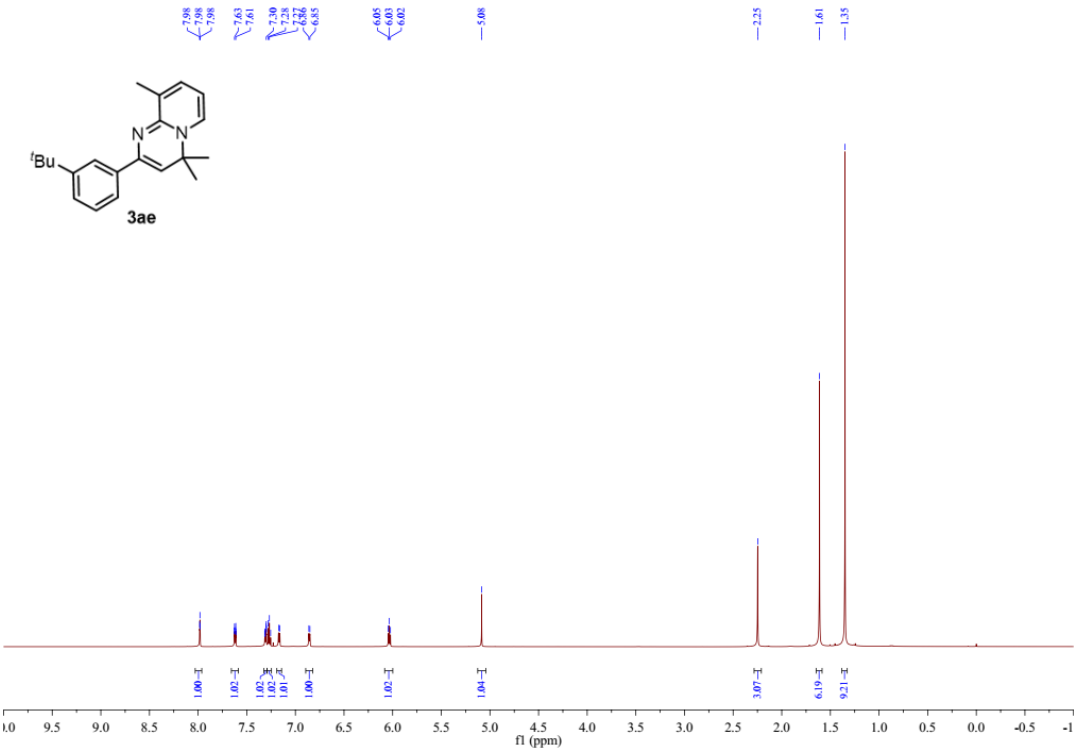
141.59
139.05
137.27
131.62
131.58
129.00
128.16
127.81
126.16
122.62
107.81
102.88
58.92
31.09
21.53
18.63
f1 (ppm)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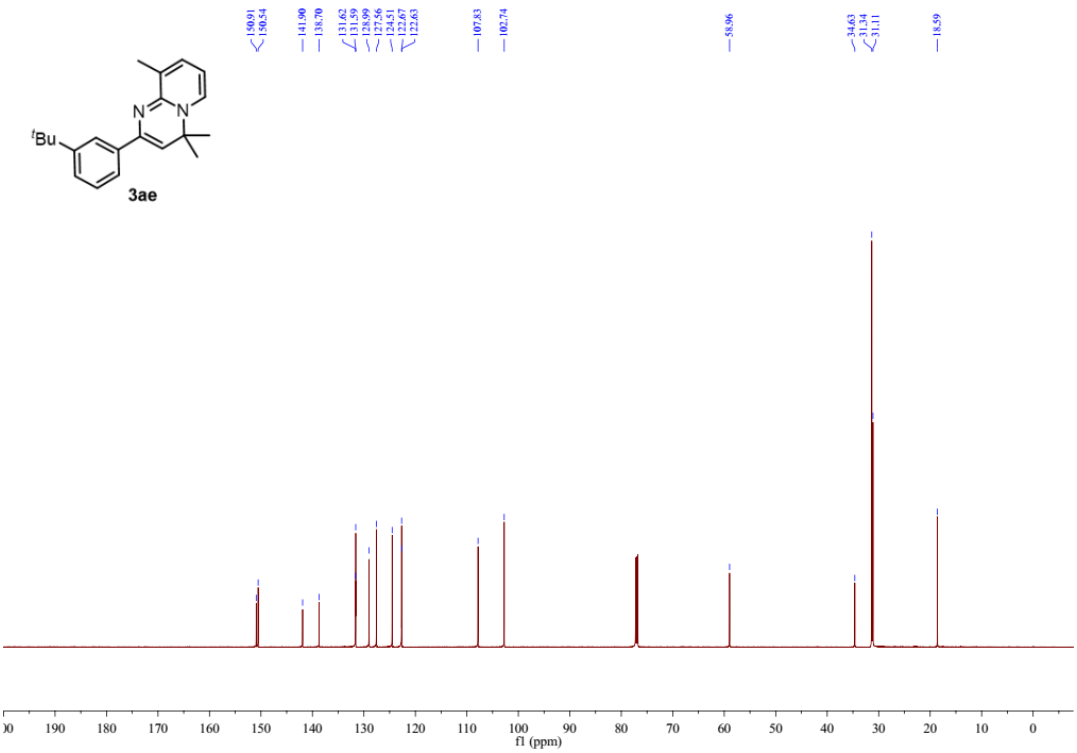
7.98
7.98
7.63
7.61
7.39
7.28
7.27
7.26
6.85
6.05
6.03
6.02
5.08
2.25
1.61
1.35
tBu
N
N
3ae
1.00
1.02
1.02
1.02
1.01
1.00
1.02
1.04
3.07
6.19
9.21
fl (ppm)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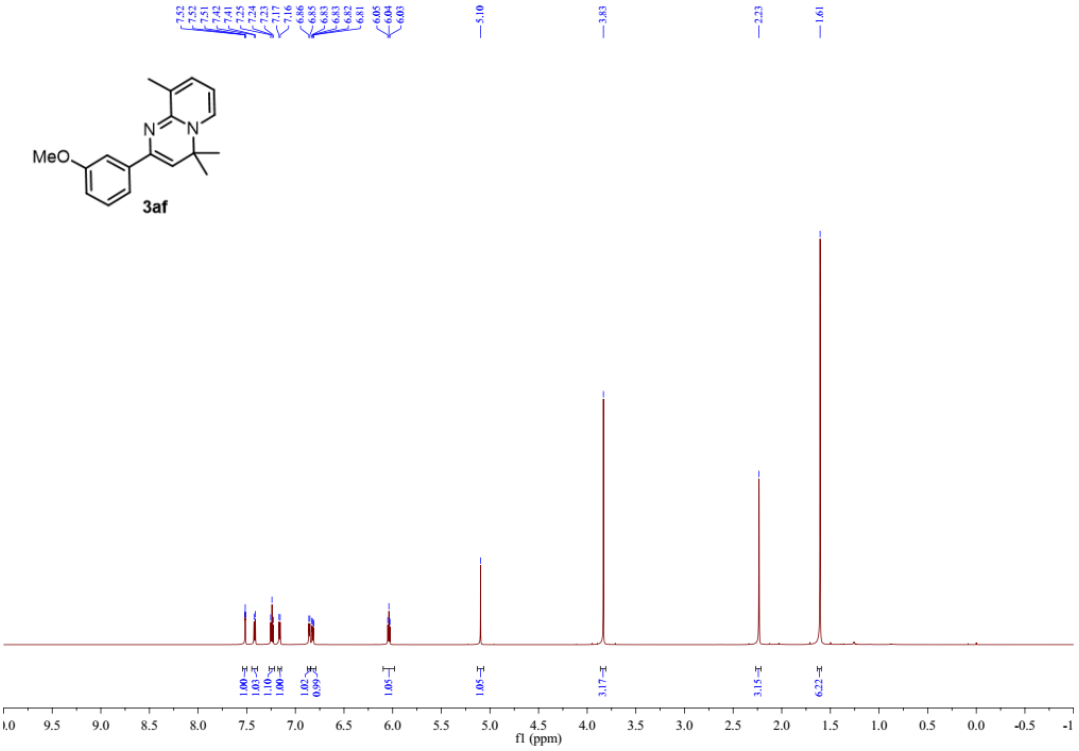
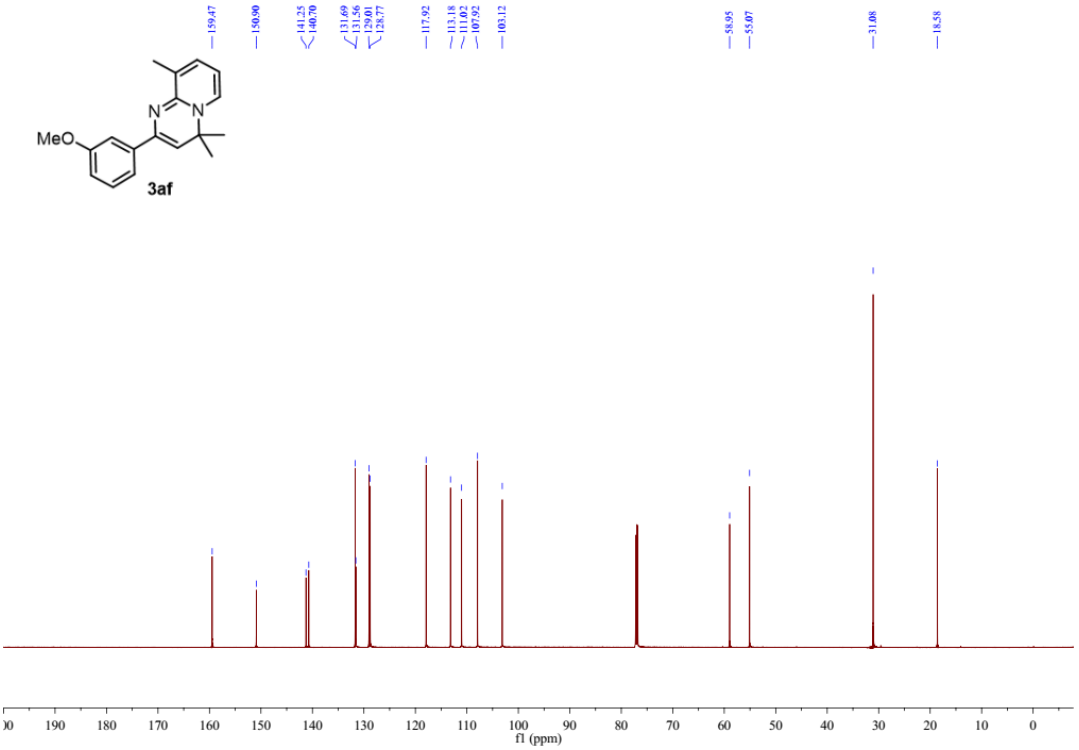
150.54
141.90
138.70
131.62
131.59
128.99
127.56
124.51
122.67
122.63
107.83
102.74
58.96
34.63
31.34
31.11
18.59
tBu
N
N
3ae
fl (ppm)


7.52
7.52
7.51
7.42
7.41
7.25
7.24
7.23
7.17
7.16
6.86
6.85
6.83
6.83
6.82
6.61
6.05
6.04
6.03
5.10
3.83
2.23
1.61
MeO
N
N
3af
1.00
1.03
1.10
1.00
1.02
0.99
1.05
1.05
3.17
3.15
6.22
fl (ppm)


159.47
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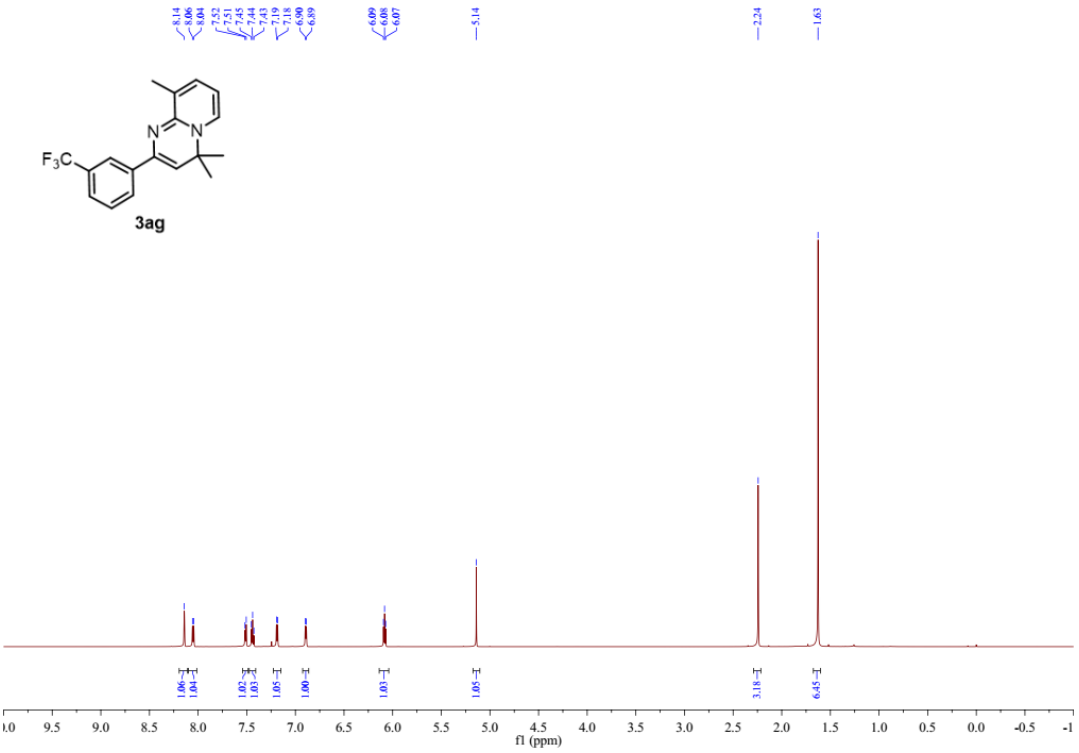
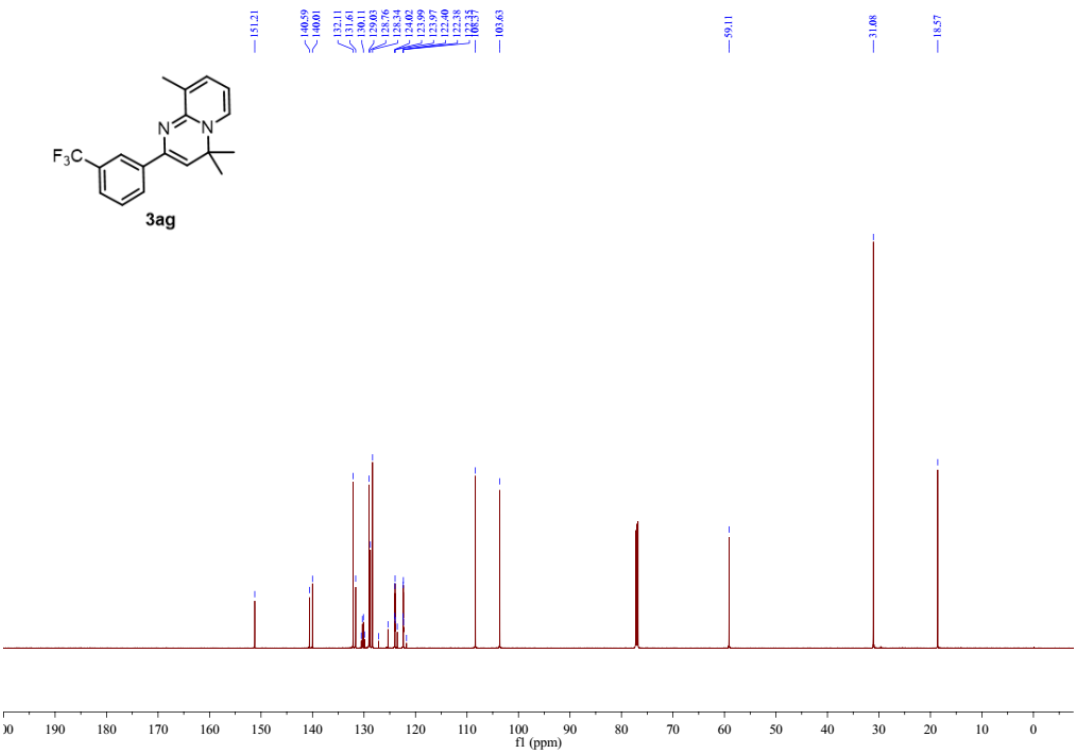
140.70
131.69
131.56
129.01
128.77
117.92
113.18
111.02
107.92
103.12
58.95
55.07
31.08
18.58
MeO
N
N
3af
fl (ppm)


8.14
8.06
8.04
7.52
7.51
7.45
7.44
7.43
7.19
7.18
6.90
6.89
6.09
6.08
6.07
5.14
2.24
1.63
F3C
N
N
3ag
1.06
1.04
1.02
1.03
1.05
1.00
1.03
1.05
3.18
6.45
f1 (ppm)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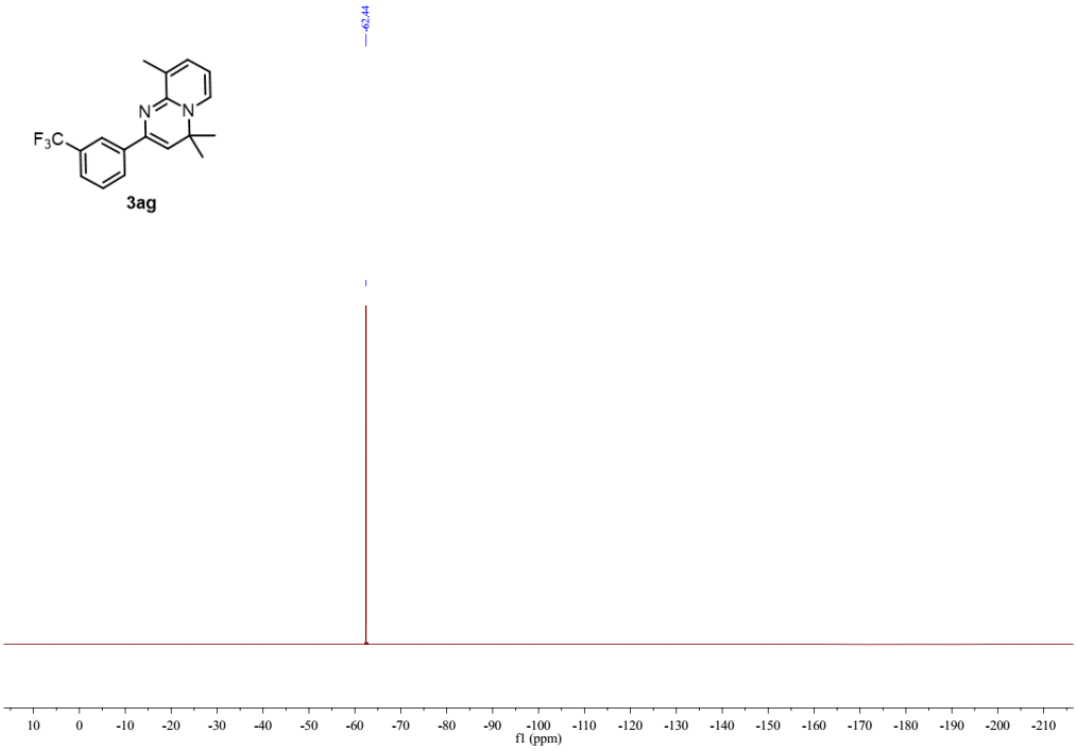
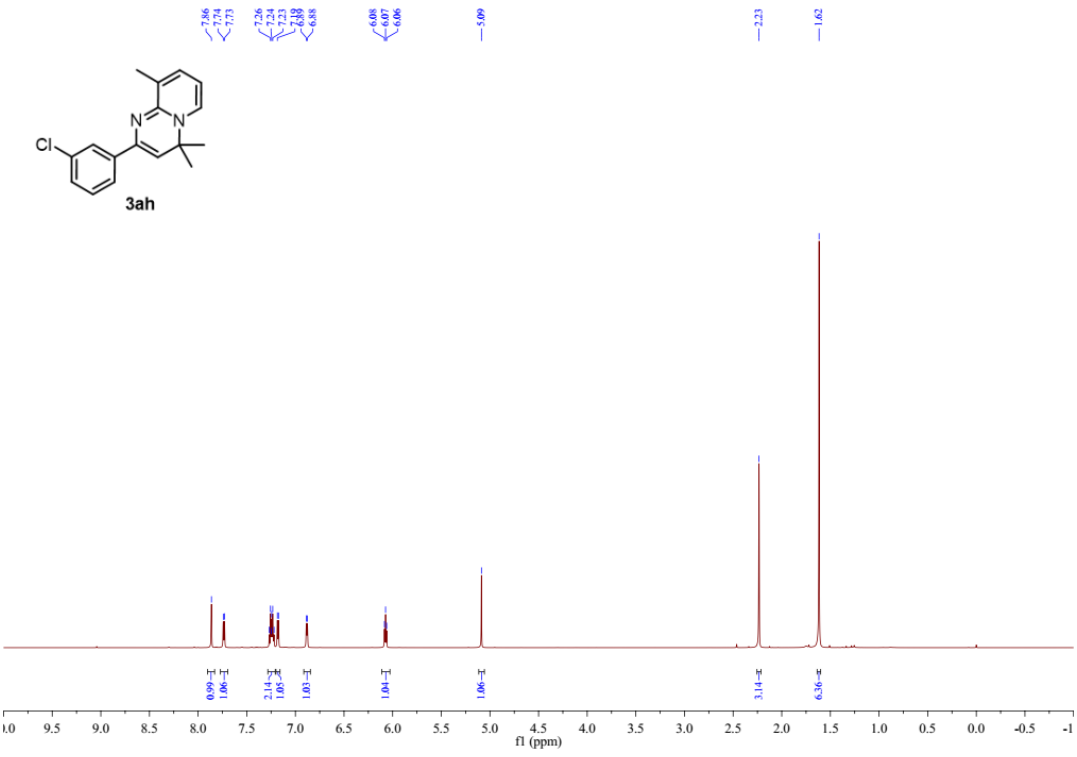
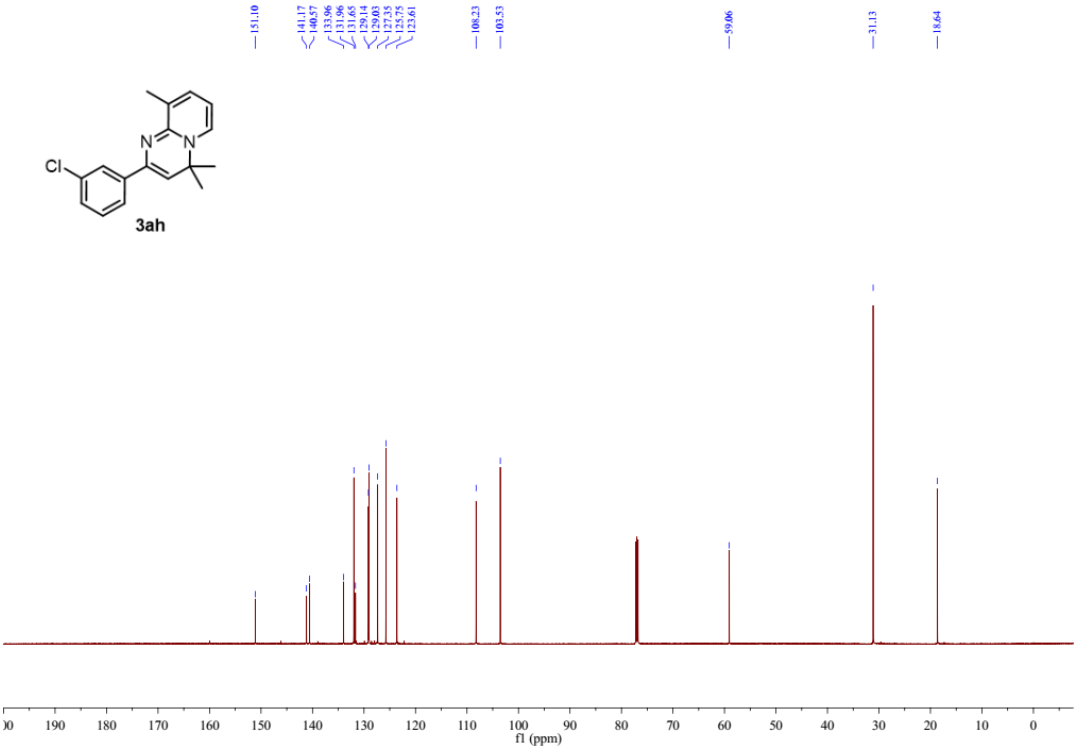
140.59
140.01
132.11
131.61
130.11
129.03
128.76
128.34
124.02
123.99
123.97
123.60
122.38
122.35
122.37
103.63
59.11
31.08
18.57
F3C
N
N
3ag
f1 (ppm)


-62.44
F3C
N
N
3ag
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


7.86
7.74
7.73
7.26
7.24
7.23
6.88
6.08
6.07
6.06
5.09
2.23
1.62
Cl
N
N
3ah
0.99
1.06
2.14
1.03
1.04
1.06
3.14
6.36
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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141.17
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131.96
131.65
129.14
129.03
127.35
125.75
123.61
108.23
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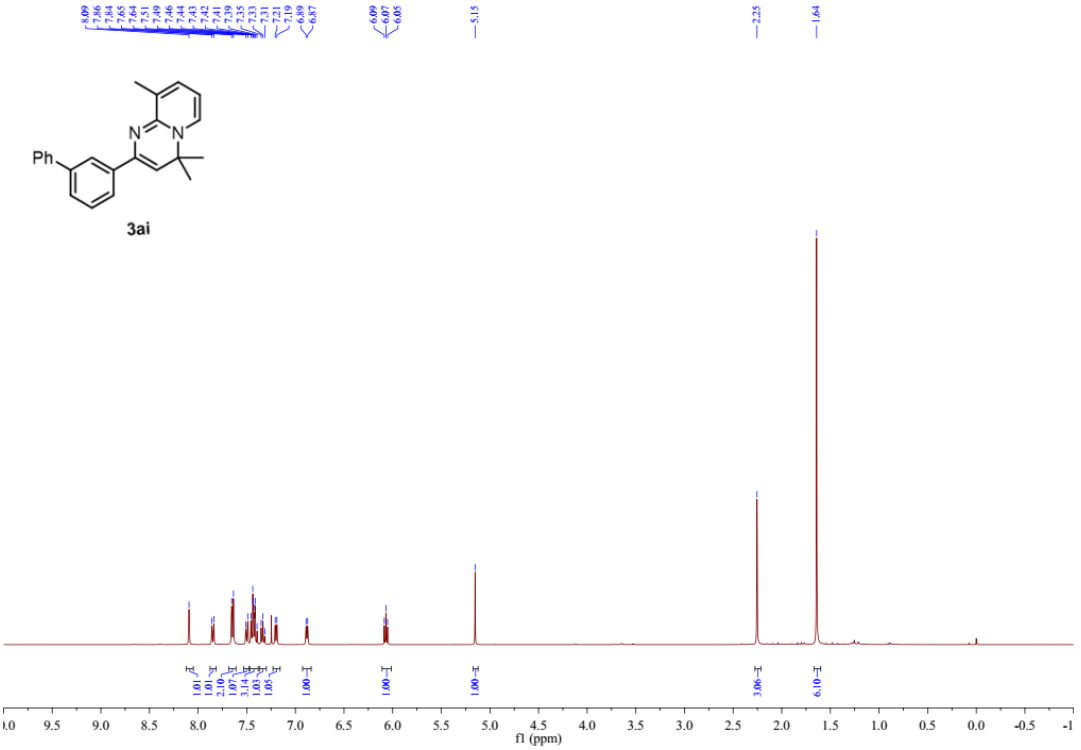
31.13
18.64
Cl
N
N
3ah
f1 (ppm)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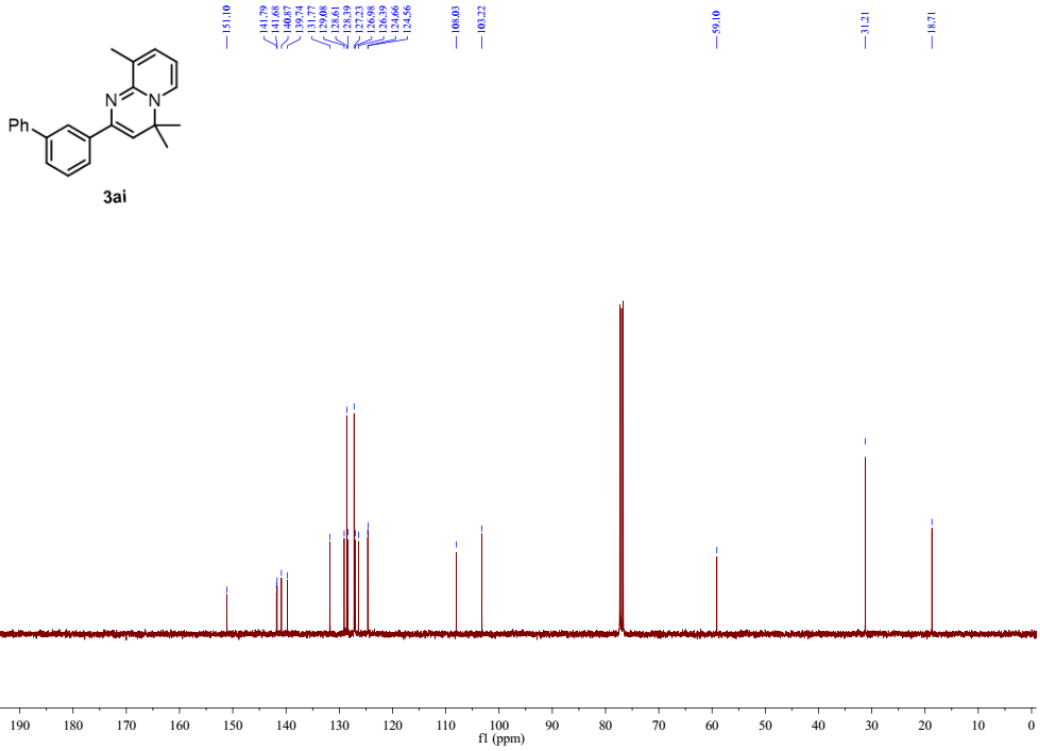
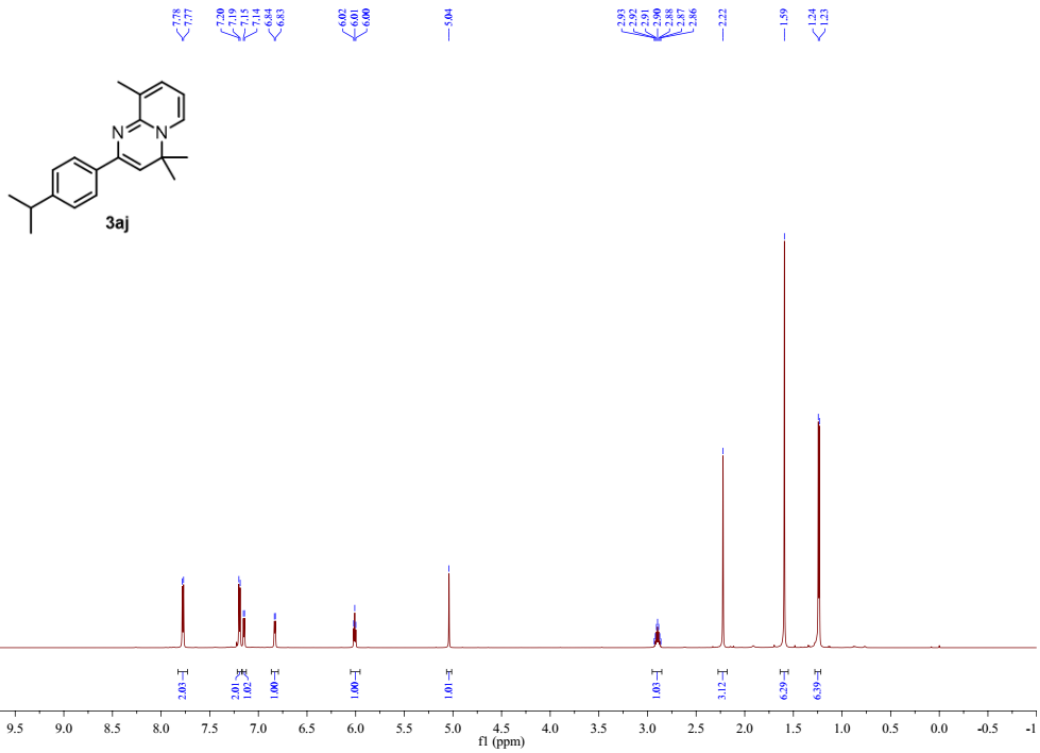
7.86
7.84
7.65
7.64
7.51
7.49
7.46
7.44
7.43
7.42
7.41
7.39
7.35
7.33
7.31
7.21
7.19
6.89
6.87
6.09
6.07
6.05
5.15
2.25
1.64
Ph
N
N
3ai
1.01
1.01
2.10
1.07
3.14
1.03
1.05
1.00
1.00
1.00
3.06
6.10
f1 (ppm)


Ph
N
N
3ai
151.10
141.79
141.68
140.87
139.74
131.77
129.98
128.61
128.39
127.23
126.98
126.39
124.66
124.56
108.03
103.22
59.10
31.21
18.71
f1 (ppm)


N
N
3aj
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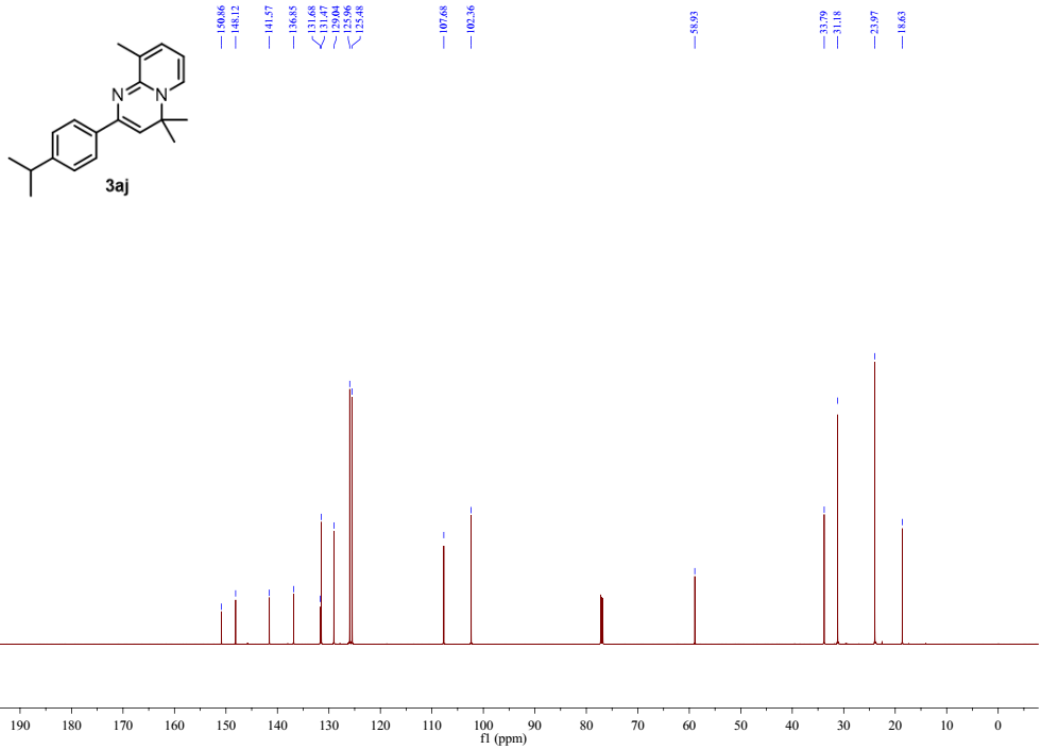
7.77
7.20
7.19
7.15
7.14
6.84
6.83
6.02
6.01
6.00
5.04
2.93
2.92
2.91
2.90
2.88
2.87
2.86
2.22
1.59
1.24
1.23
2.03
2.01
1.02
1.00
1.00
1.01
1.03
3.12
6.29
6.39
f1 (ppm)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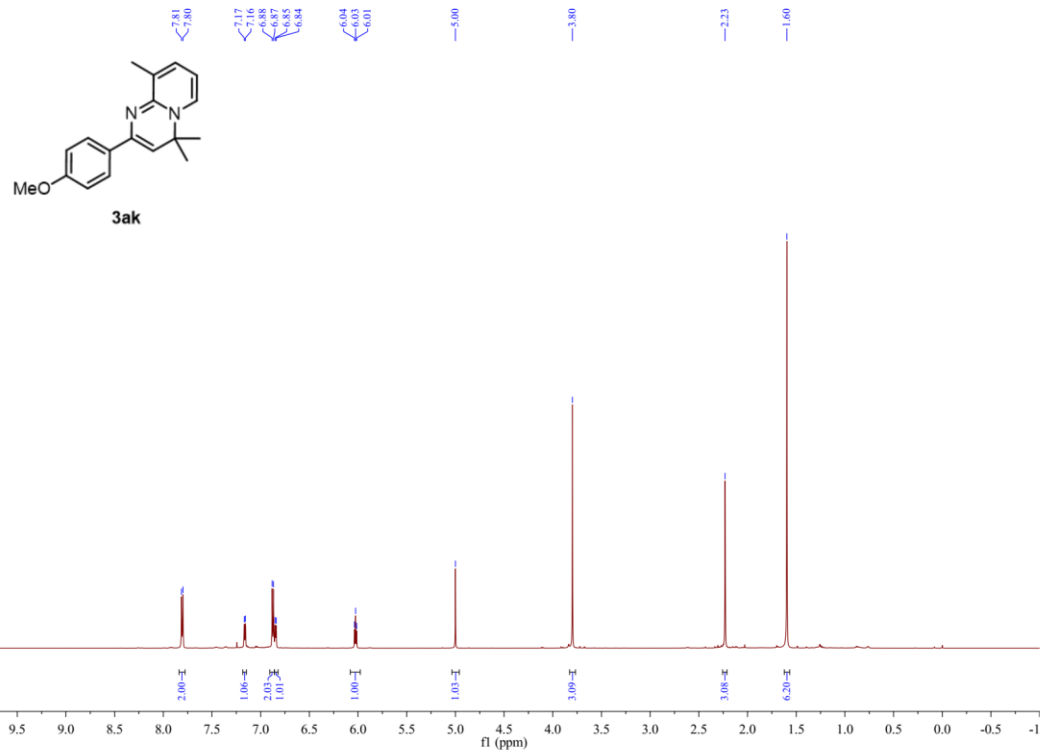
148.12
141.57
136.85
131.68
131.47
129.04
125.96
125.48
107.68
102.36
58.93
33.79
31.18
23.97
18.63
3aj
f1 (ppm)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6.87
6.85
6.84
6.04
6.03
6.01
5.00
3.80
2.23
1.60
MeO
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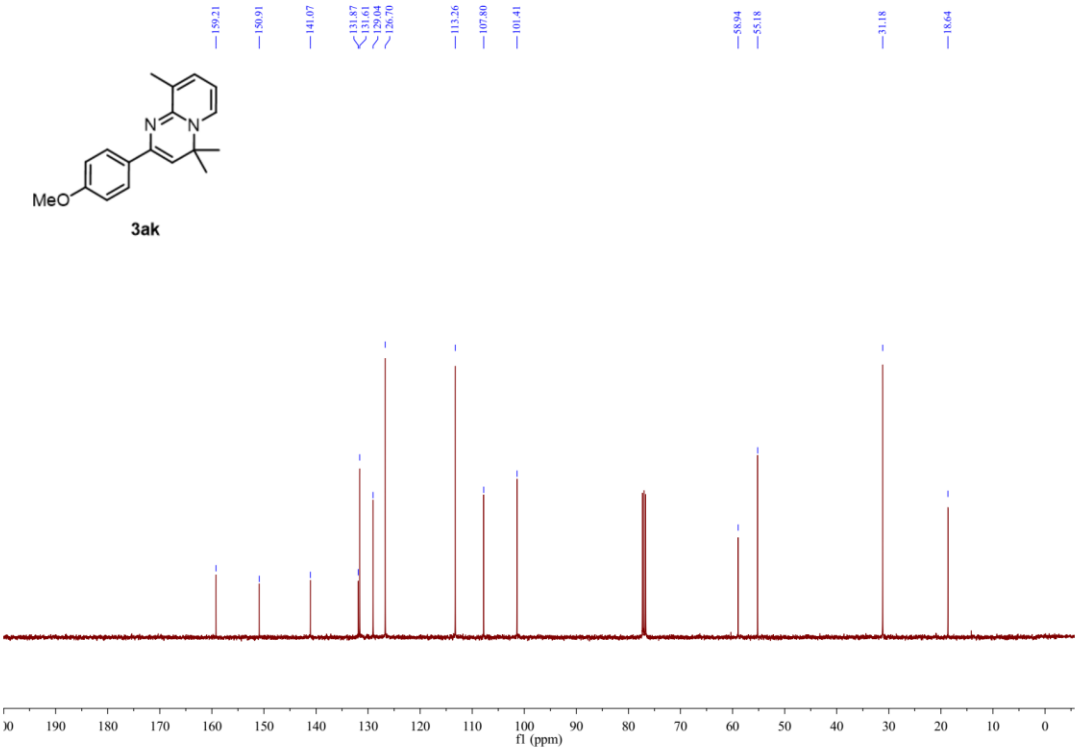
2.00
1.06
2.03
1.01
1.00
1.03
3.09
3.08
6.20
f1 (ppm)


159.21
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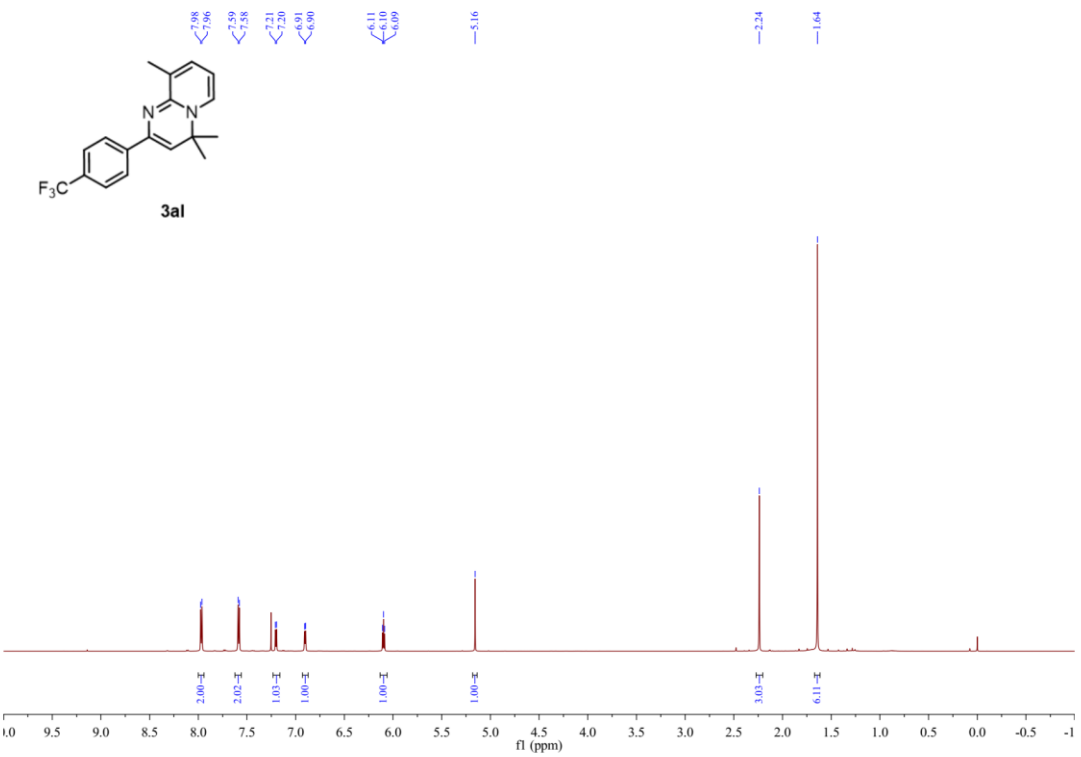
131.61
129.04
126.70
113.26
107.80
101.41
58.04
55.18
31.18
18.64
MeO
3ak
f1 (ppm)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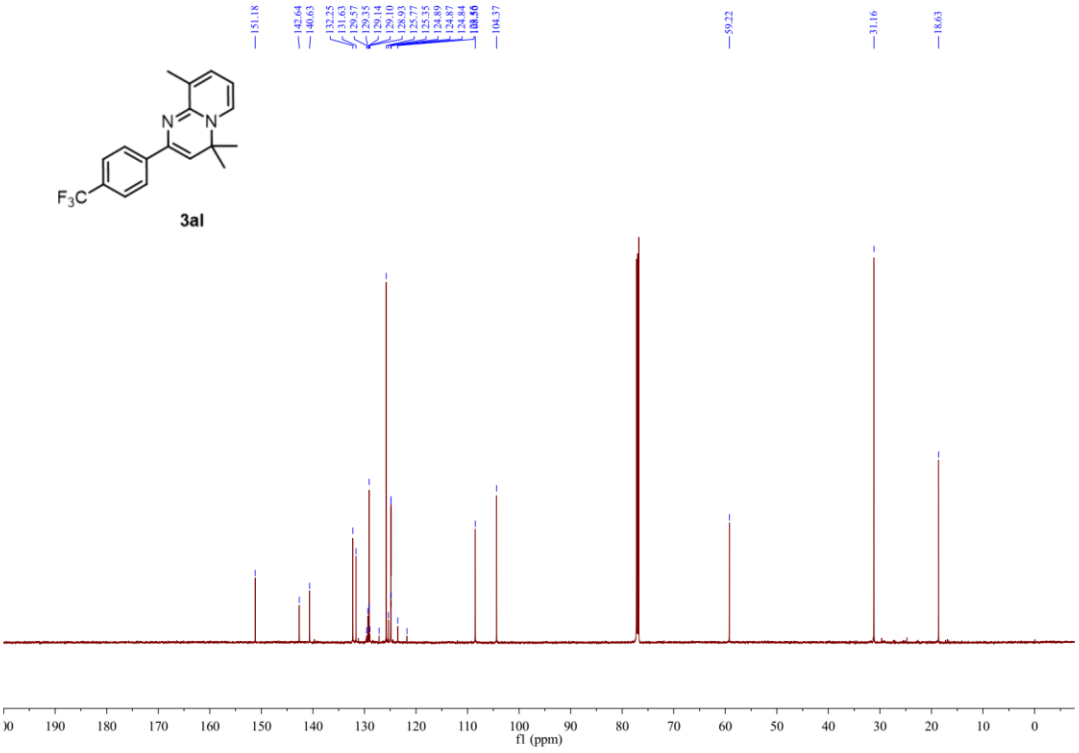
7.96
7.59
7.58
7.21
7.20
6.91
6.90
6.11
6.10
6.09
5.16
2.24
1.64
F3C
3al
2.00
2.02
1.03
1.00
1.00
1.00
3.03
6.11
f1 (ppm)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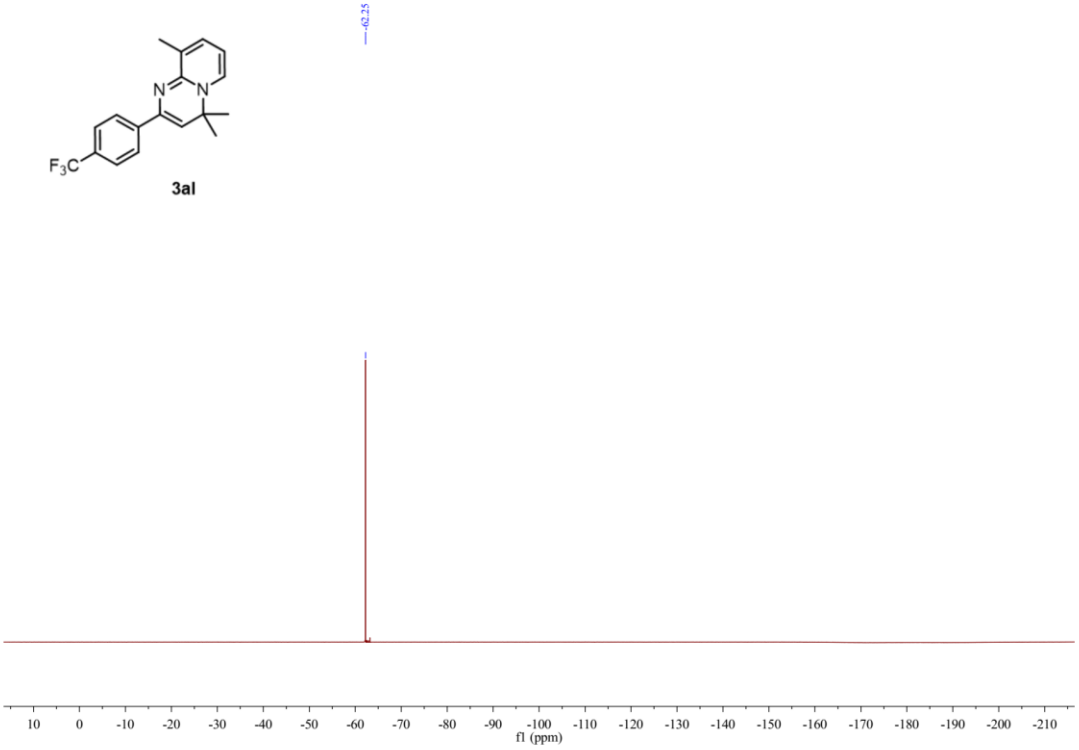
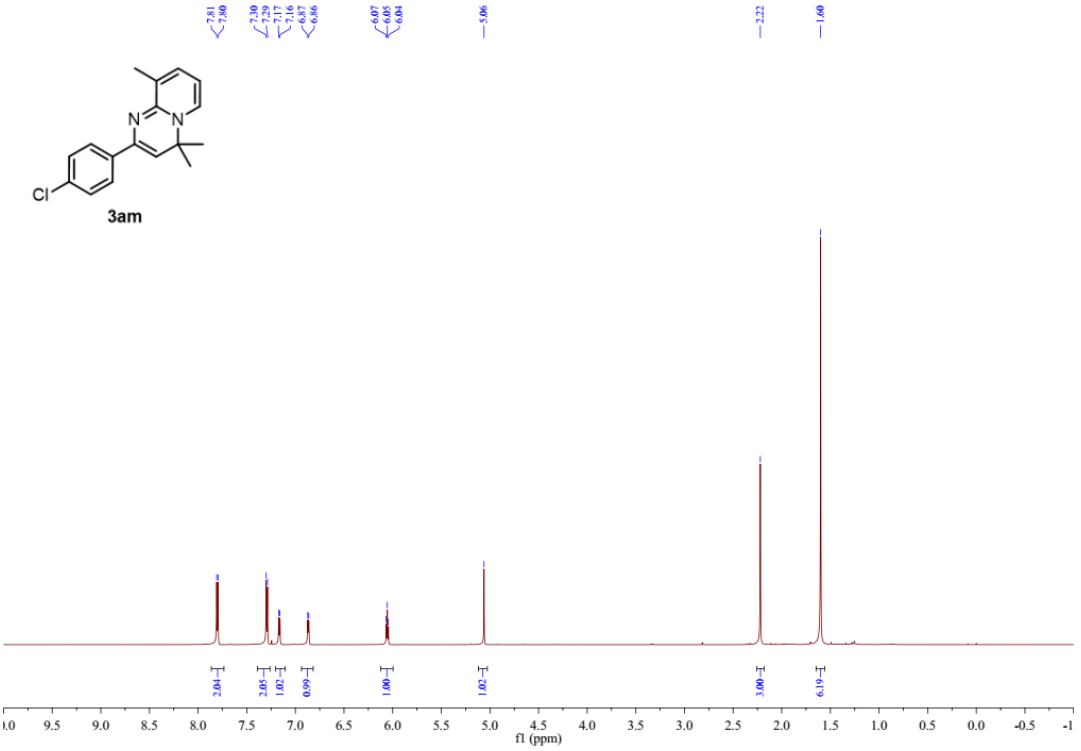
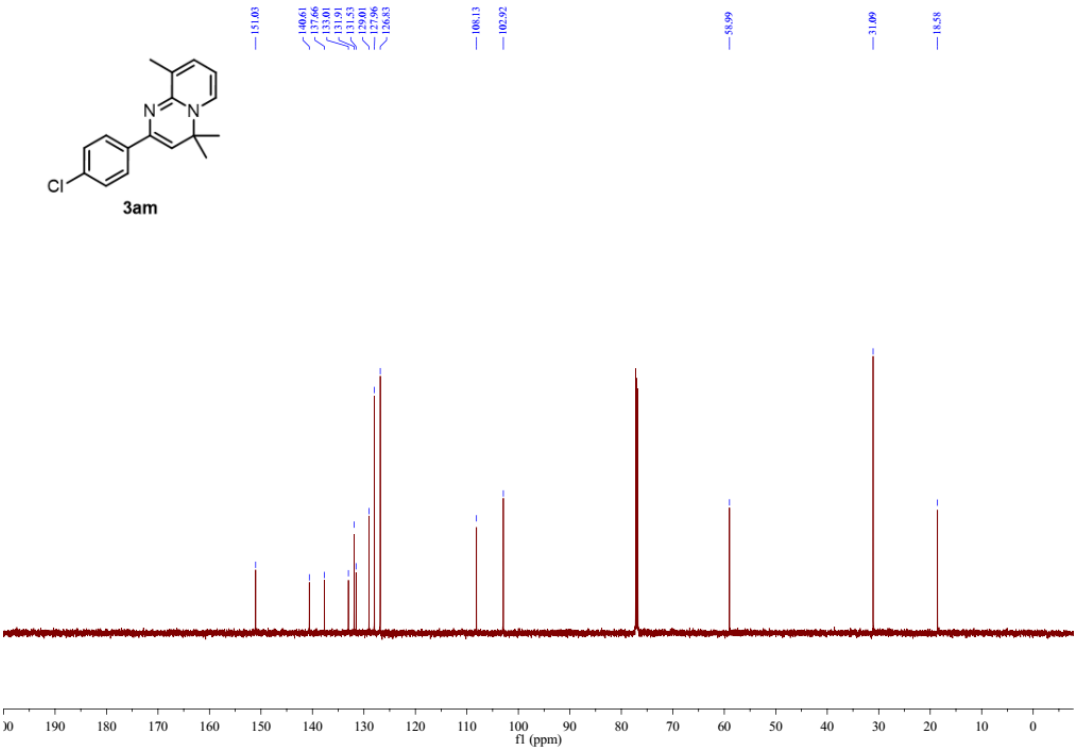
129.57
129.35
129.14
129.10
128.95
125.77
125.35
124.89
124.87
124.84
104.56
104.37
59.22
31.16
18.63
F3C
N
N
3al
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-62.25
F3C
N
N
3al
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


7.81
7.80
7.39
7.29
7.17
7.16
6.87
6.86
6.07
6.05
6.04
5.06
2.22
1.60
Cl
3am
2.04
2.05
1.02
0.99
1.00
1.02
3.00
6.19
f1 (ppm)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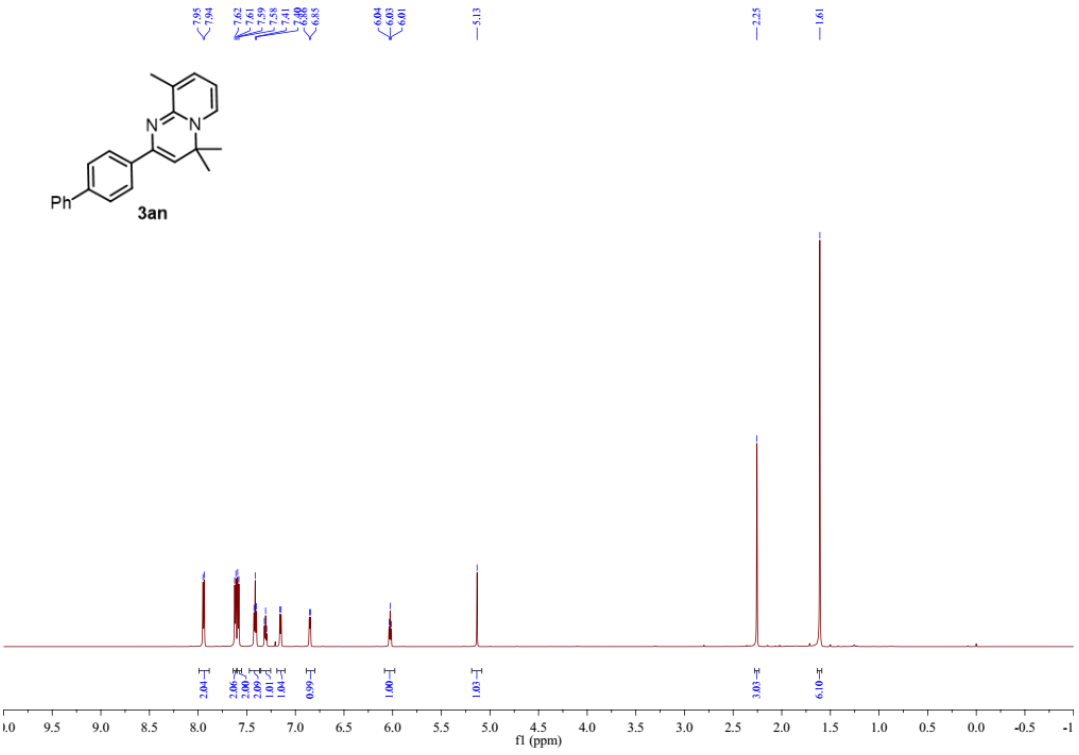
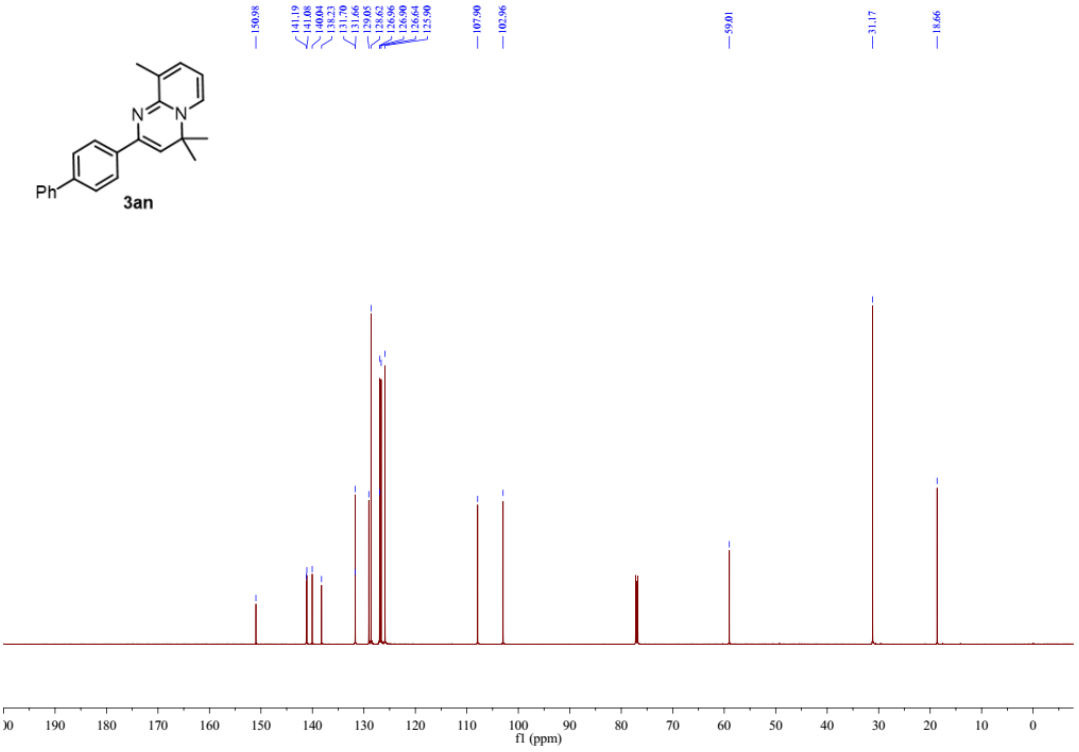
140.61
137.66
133.01
131.91
131.53
129.01
127.96
126.83
100.13
102.92
58.99
31.09
18.58
Cl
3am
f1 (ppm)


7.95
7.94
7.62
7.61
7.59
7.58
7.41
6.85
6.04
6.03
6.01
5.13
2.25
1.61
Ph
N
N
3an
2.04
2.06
2.00
2.09
1.01
1.04
0.99
1.00
1.03
3.03
6.10
fl (ppm)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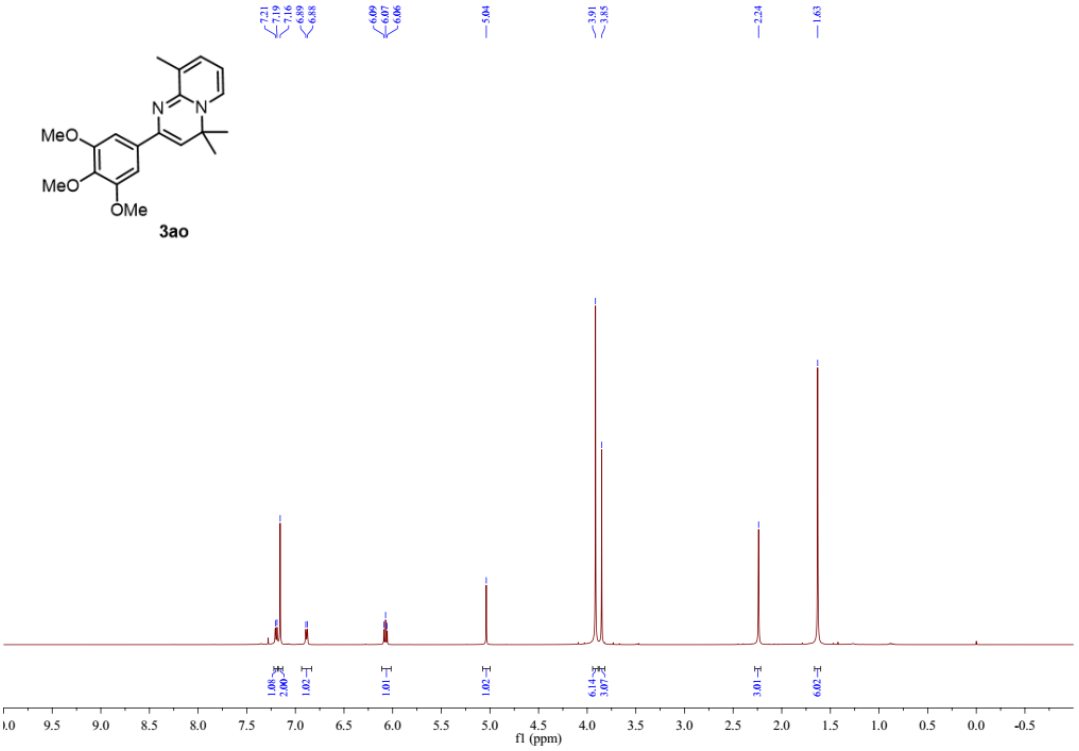
141.08
140.04
138.23
131.70
131.66
129.05
128.62
126.96
126.90
126.64
125.90
107.90
102.96
59.01
31.17
18.66
Ph
N
N
3an
fl (ppm)


7.21
7.19
7.16
6.89
6.88
6.09
6.07
6.06
5.04
3.91
3.85
2.24
1.63
MeO
MeO
OMe
N
N
3ao
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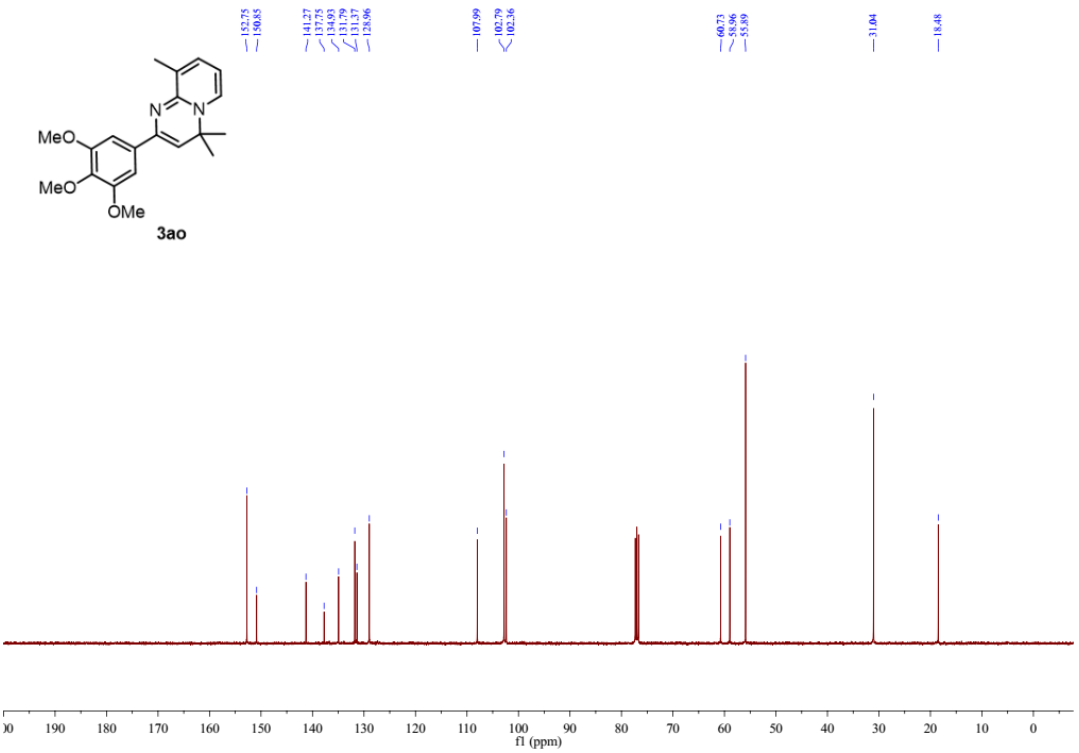
2.00
1.02
1.01
1.02
6.14
3.07
3.01
6.02
f1 (ppm)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141.27
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134.93
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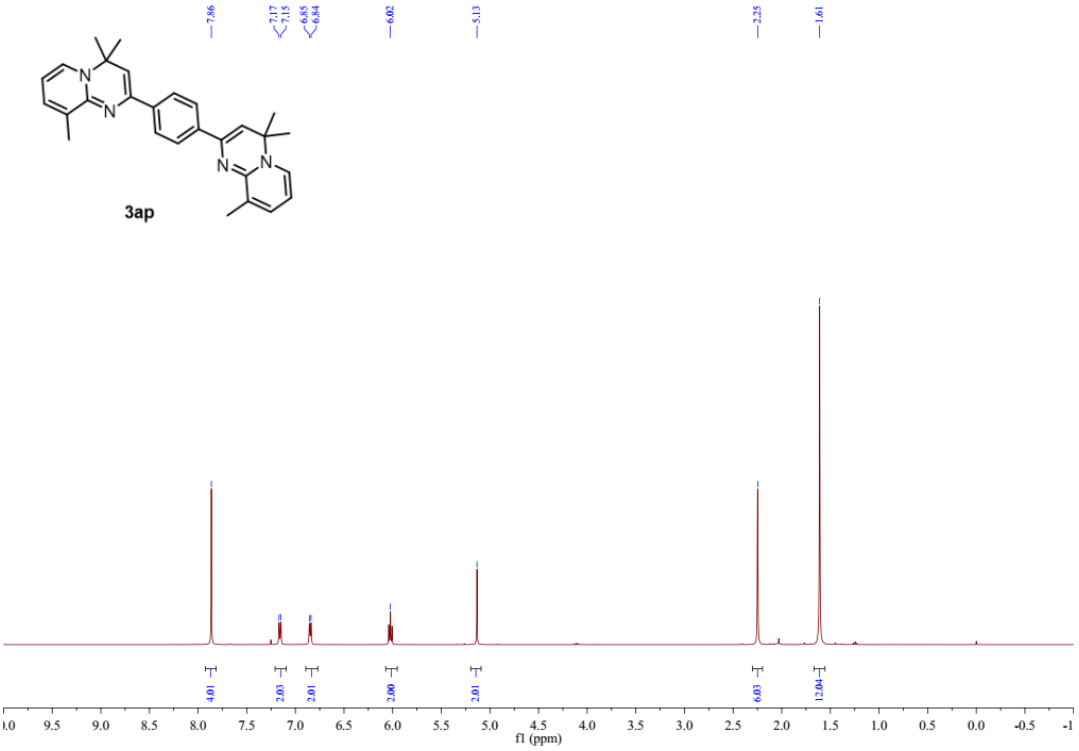
131.37
128.96
107.99
102.79
102.36
60.73
58.96
55.89
31.04
18.48
MeO
MeO
OMe
N
N
3ao
f1 (ppm)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7.17
7.15
6.85
6.84
6.02
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2.25
1.61
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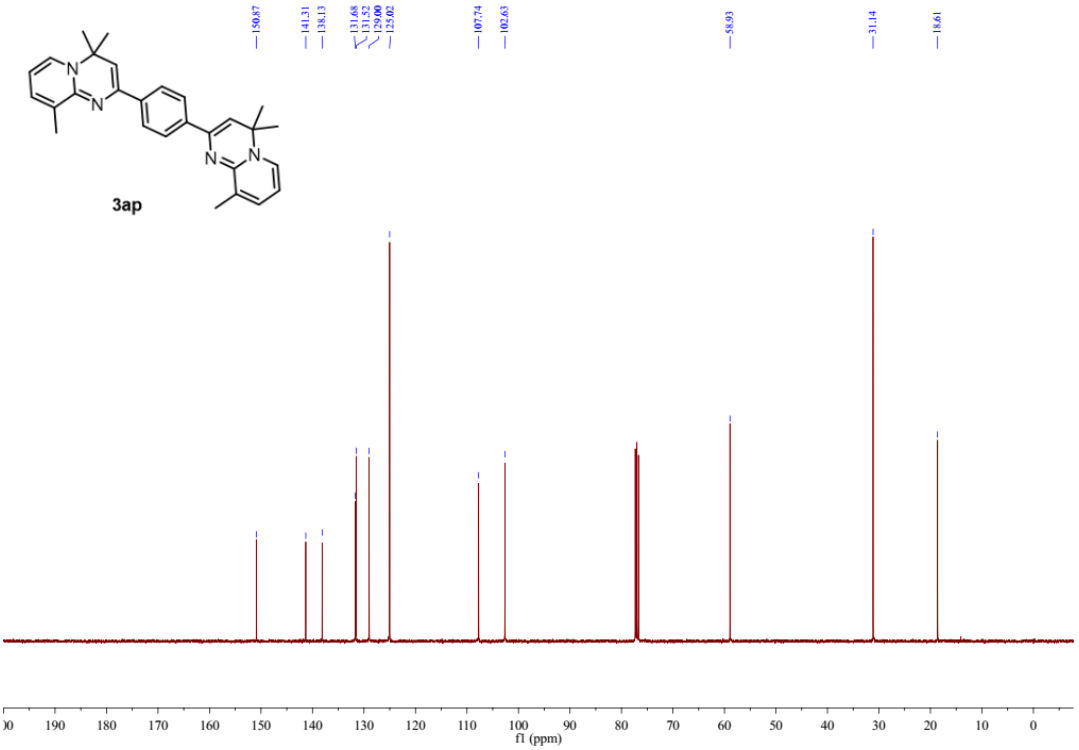
4.01
2.03
2.01
2.00
2.01
6.03
12.04
f1 (ppm)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141.31
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131.52
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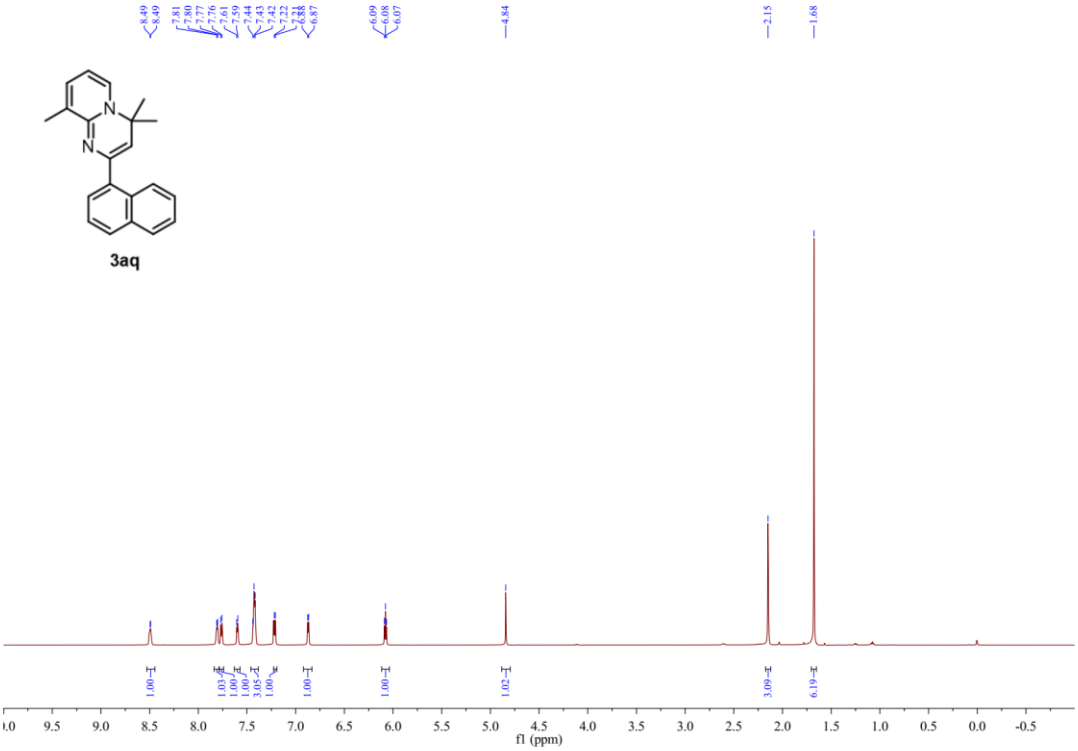
125.02
107.74
102.63
58.93
31.14
18.61
3ap
f1 (ppm)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7.76
7.61
7.59
7.44
7.43
7.42
7.22
7.18
6.87
6.09
6.08
6.07
4.84
2.15
1.68
3aq
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1.03
1.00
1.00
3.05
1.00
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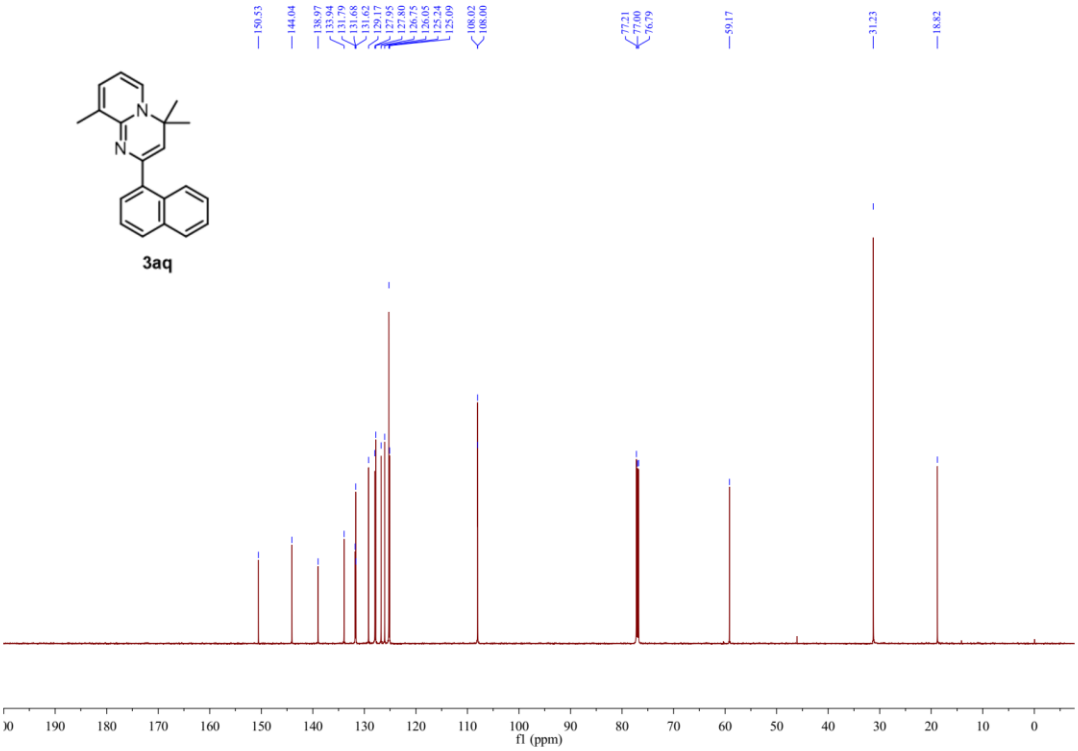
1.00
1.02
3.09
6.19
fl (ppm)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127.80
126.75
126.05
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108.02
108.00
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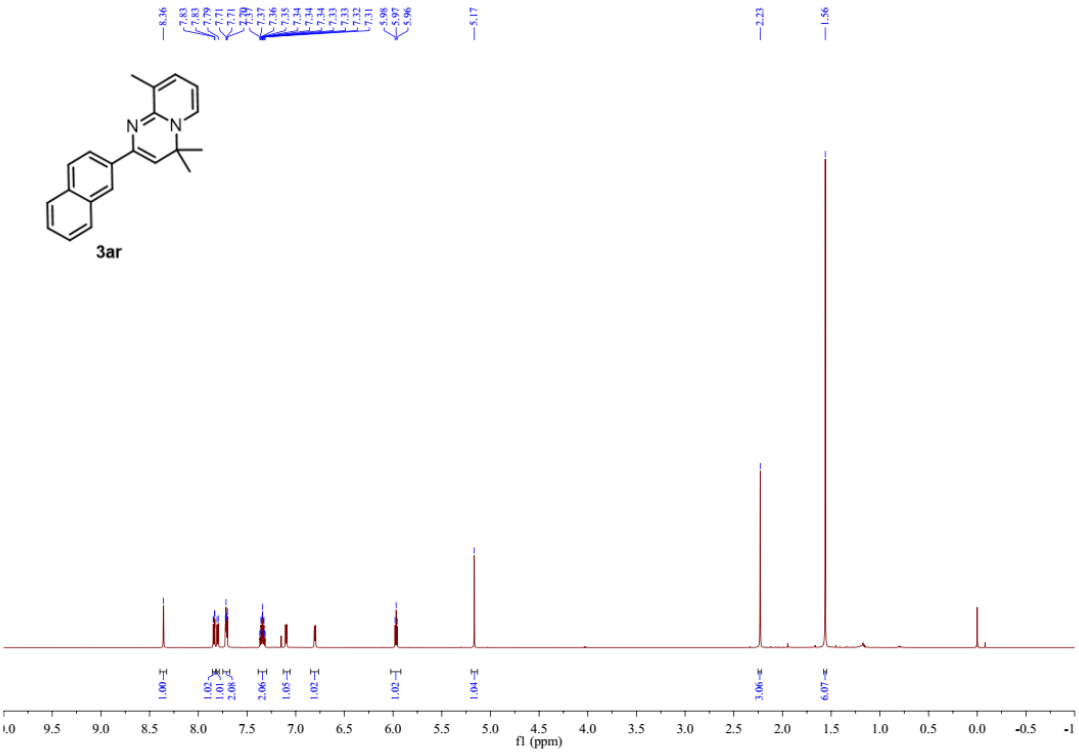
77.00
76.79
59.17
31.23
18.82
3aq
fl (ppm)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7.35
7.34
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7.33
7.33
7.32
7.31
5.98
5.97
5.96
5.17
2.23
1.56
3ar
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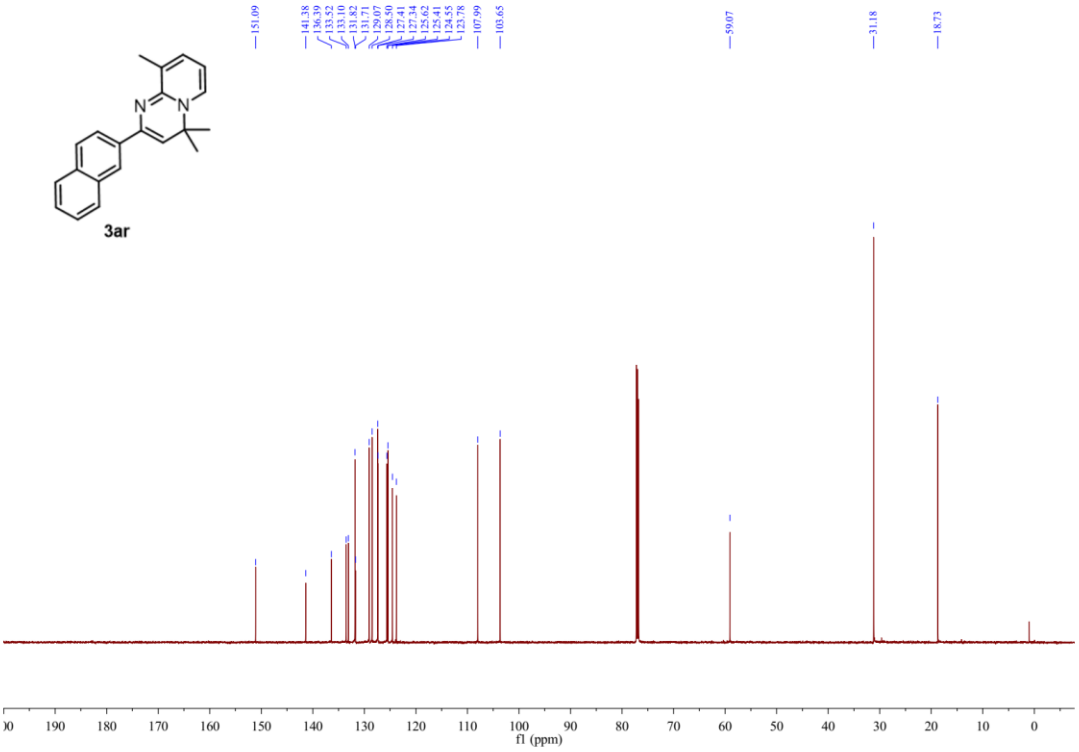
1.02
1.01
2.00
2.06
1.05
1.02
1.02
1.04
3.06
6.07
f1 (ppm)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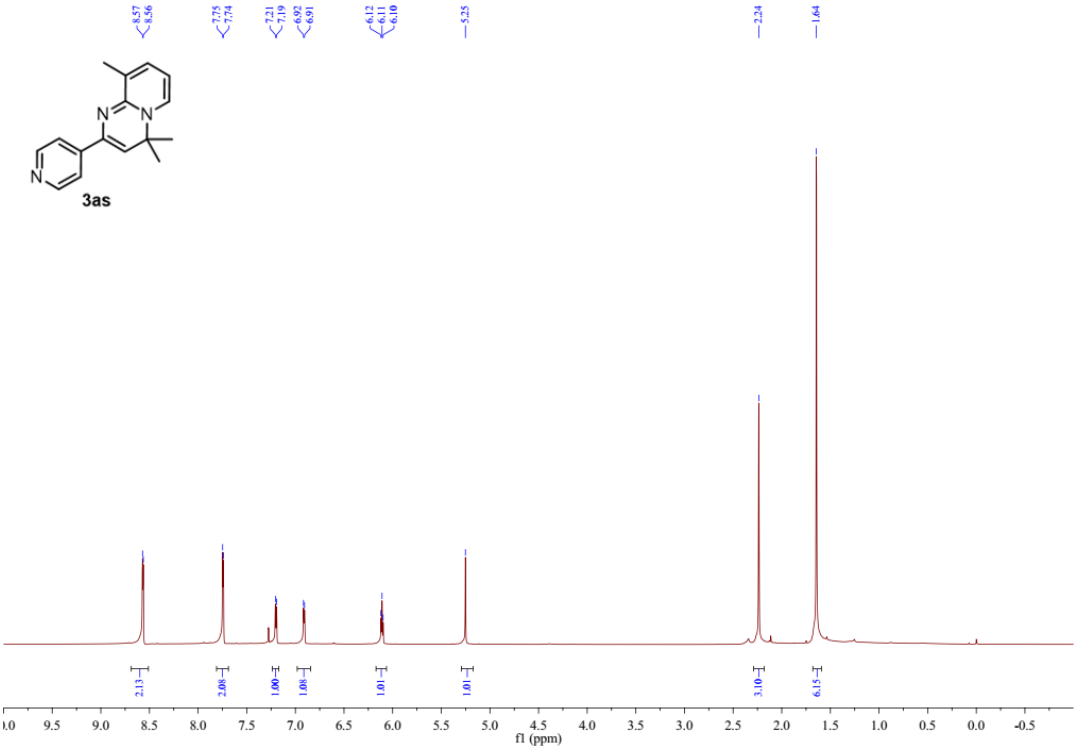
133.10
131.82
131.71
129.07
128.90
127.41
127.34
125.62
125.41
124.55
123.78
107.99
103.65
59.07
31.18
18.73
3ar
f1 (ppm)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6.92
6.91
6.12
6.11
6.10
5.25
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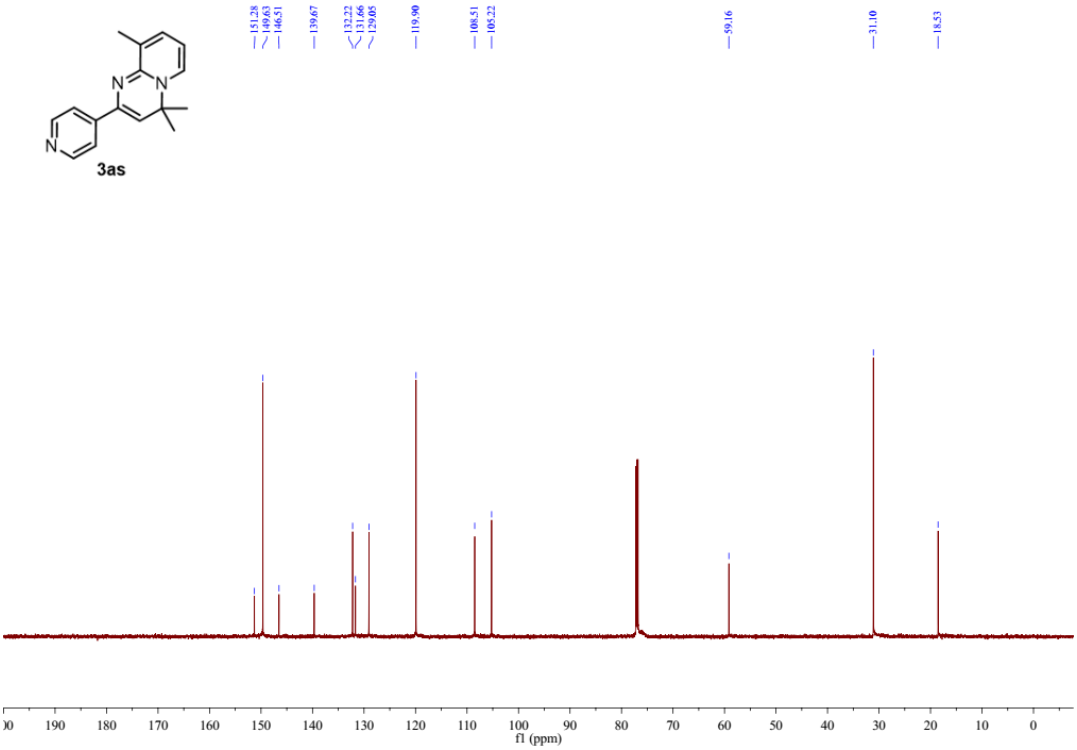
1.00
1.08
1.01
1.01
3.10
6.15
f1 (ppm)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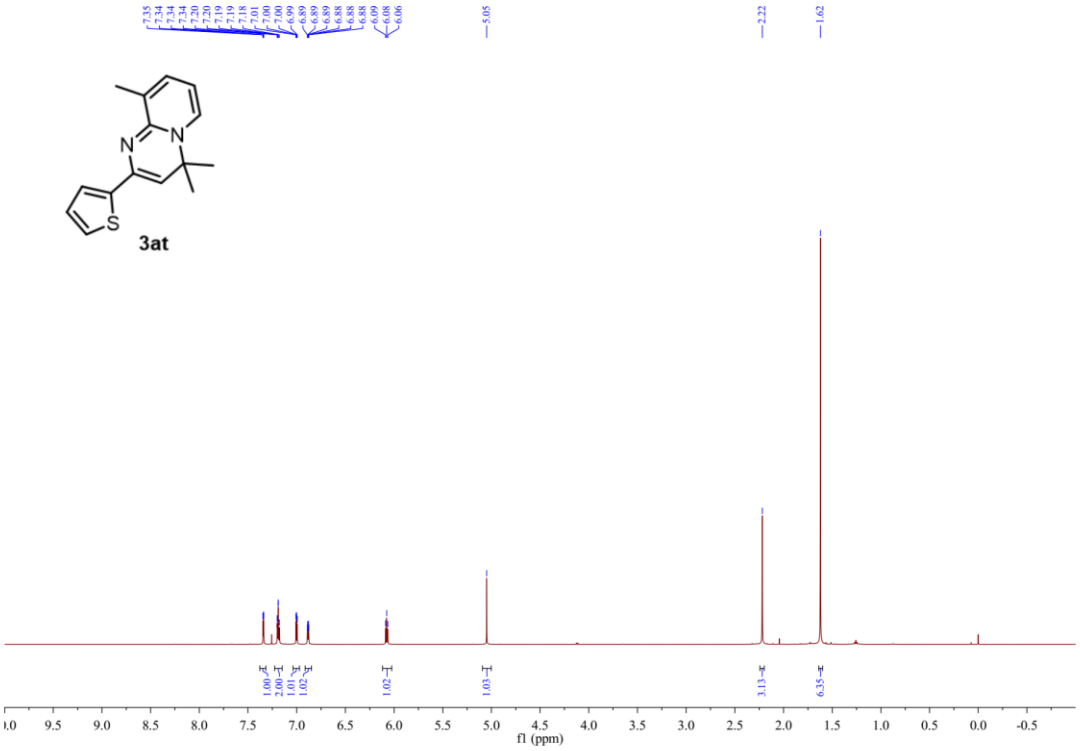
105.22
59.16
31.10
18.53
3as
f1 (ppm)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7.19
7.19
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7.01
7.00
7.00
6.99
6.89
6.89
6.89
6.88
6.88
6.88
6.87
6.08
6.06
5.05
2.22
1.62
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N
S
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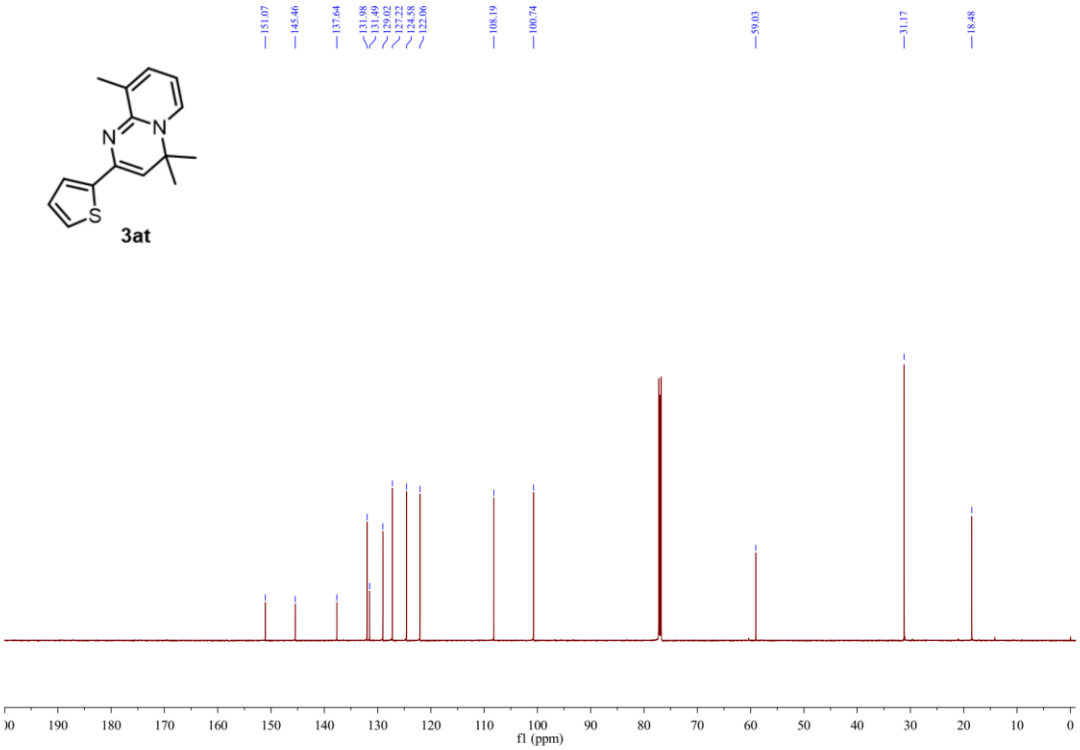
1.00
2.00
1.01
1.02
1.02
1.03
3.13
6.35
fl (ppm)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145.46
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131.98
131.49
129.02
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108.19
100.74
59.03
31.17
18.48
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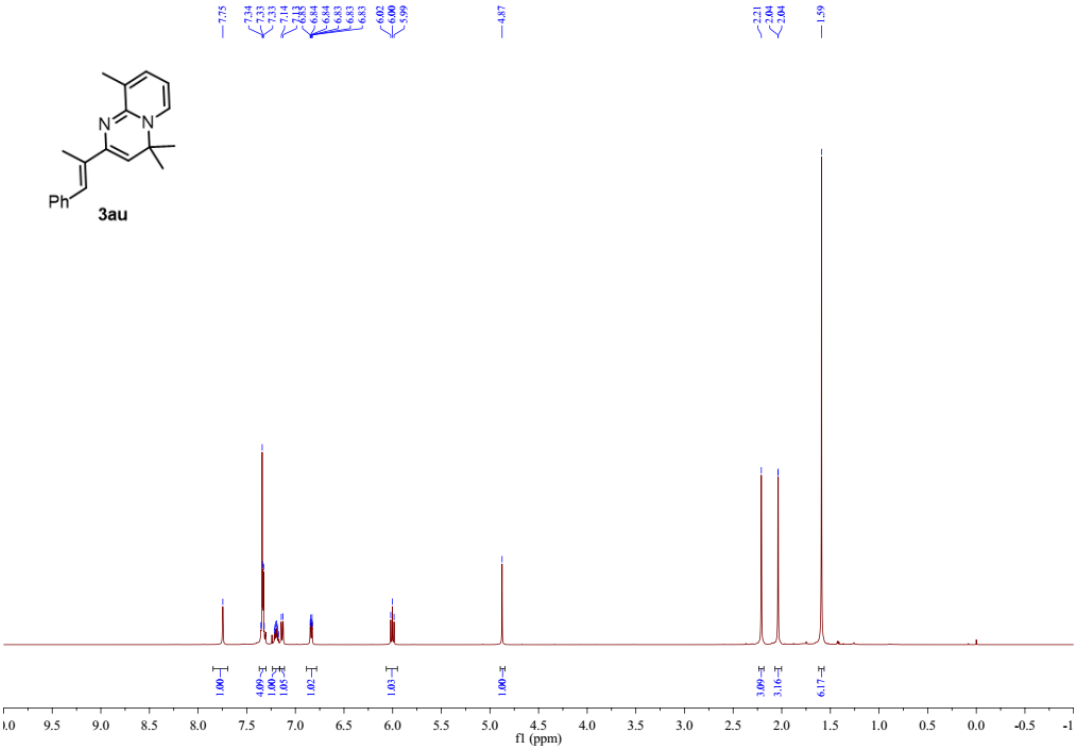
N
S
3at
fl (ppm)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7.33
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7.14
6.84
6.84
6.84
6.83
6.83
6.83
6.02
6.00
5.99
4.87
2.21
2.04
2.04
1.59
N
N
Ph
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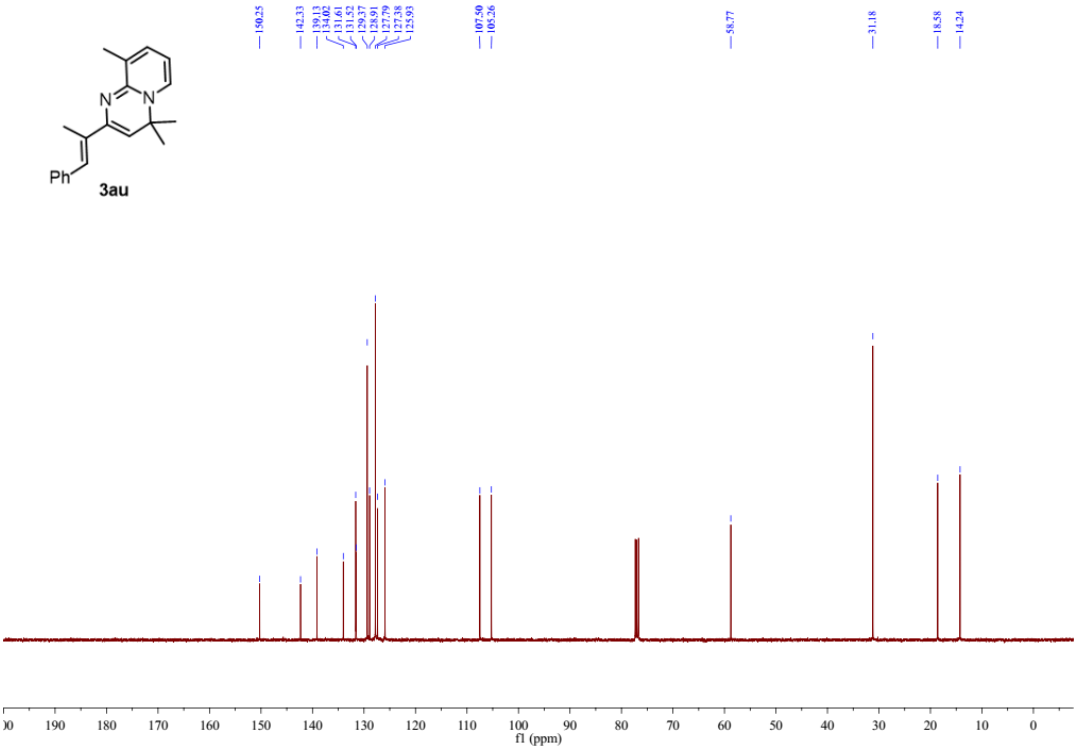
4.09
1.00
1.05
1.02
1.03
1.00
3.09
3.16
6.17
f1 (ppm)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131.52
129.37
128.91
127.79
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125.93
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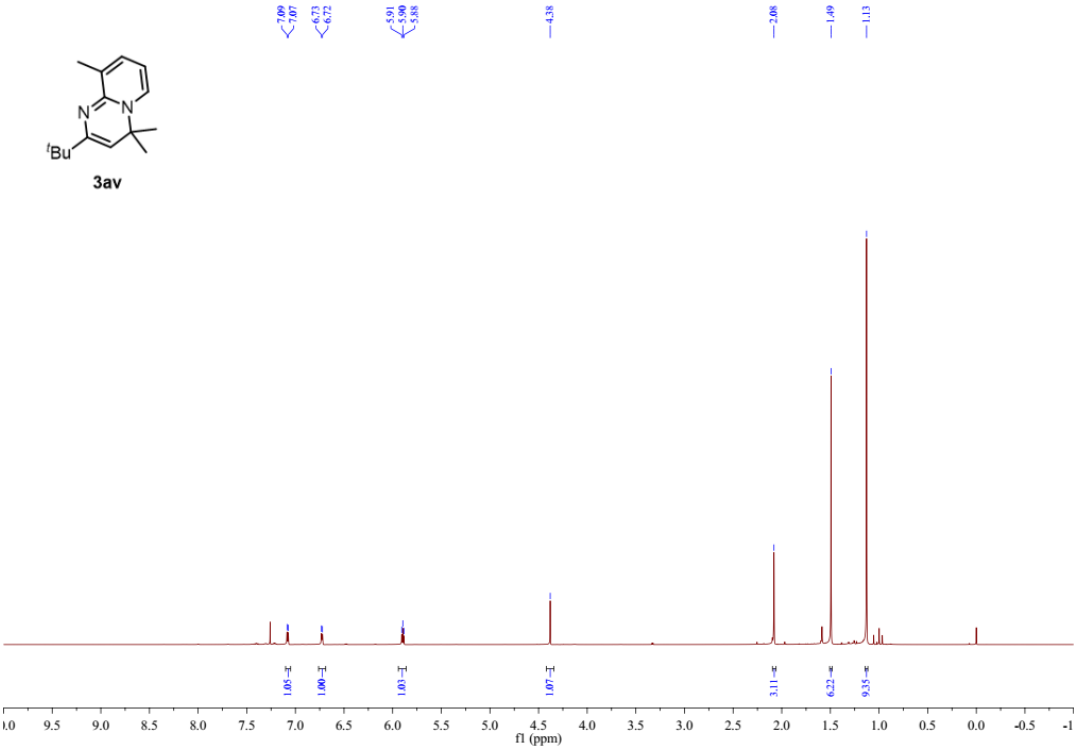
105.26
58.77
31.18
18.58
14.24
N
N
Ph
3au
f1 (ppm)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7.07
6.73
6.72
5.91
5.90
5.88
4.38
2.08
1.49
1.13
1.05
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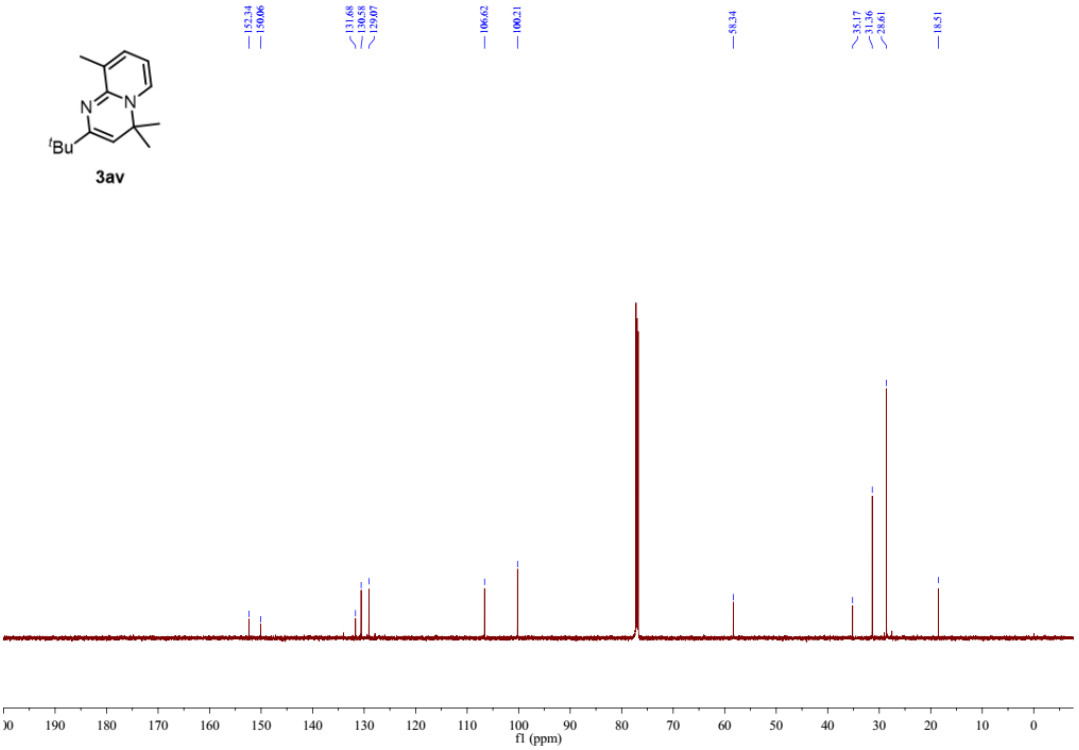
1.03
1.07
3.11
6.22
9.35
fl (ppm)

3av


152.34
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131.68
130.58
129.07
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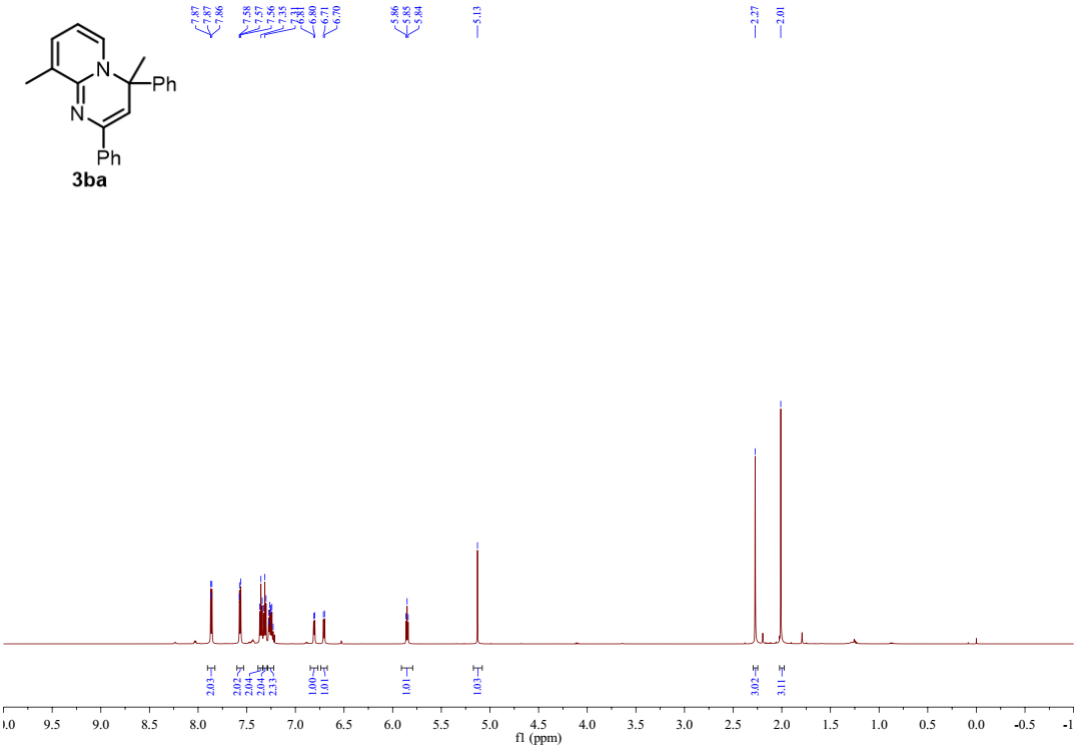
58.34
35.17
31.36
28.61
18.51
fl (ppm)

3av

Ph
N
N
Ph

3ba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7.58
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7.56
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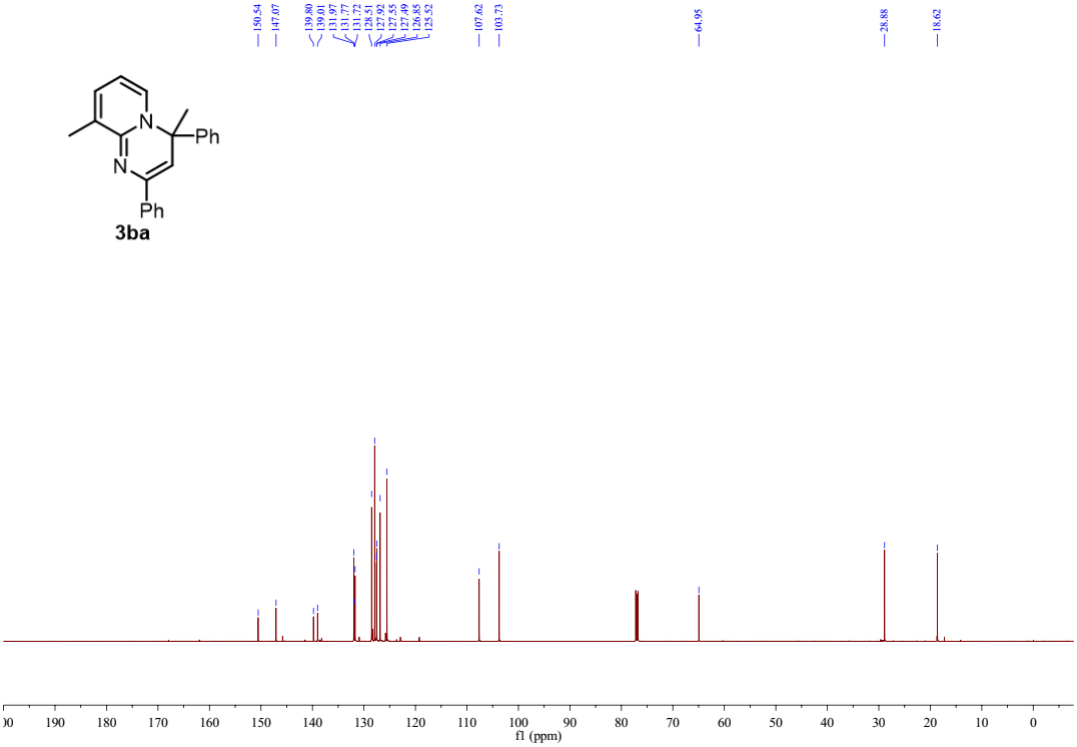
6.81
6.80
6.71
6.70
5.86
5.85
5.84
5.13
2.27
2.01
2.03
2.02
2.04
2.33
1.00
1.01
1.01
1.03
3.02
3.11
f1 (ppm)

Ph
N
N
Ph

3ba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131.77
131.72
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127.92
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127.49
126.85
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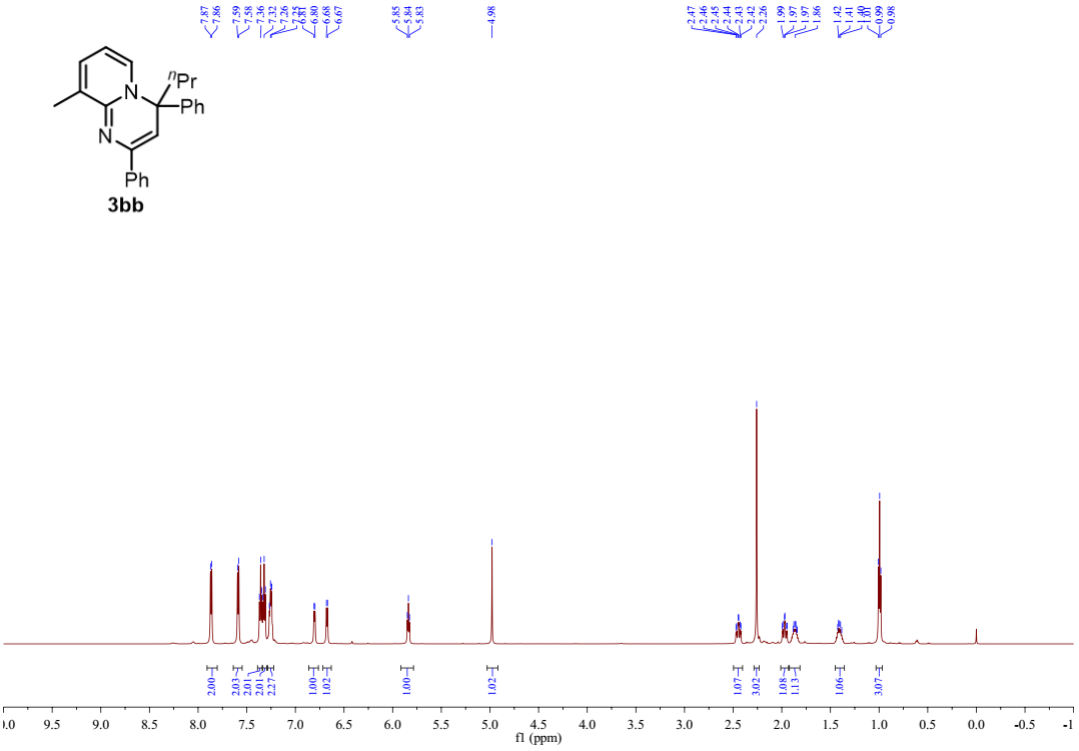
103.73
64.95
28.88
18.62
f1 (ppm)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Ph
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N
Ph
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7.58
7.36
7.32
7.26
6.80
6.68
6.67
5.85
5.84
5.83
4.98
2.47
2.46
2.45
2.44
2.43
2.32
2.26
1.99
1.97
1.97
1.86
1.42
1.41
1.00
0.99
0.98
2.00
2.03
2.01
2.27
1.00
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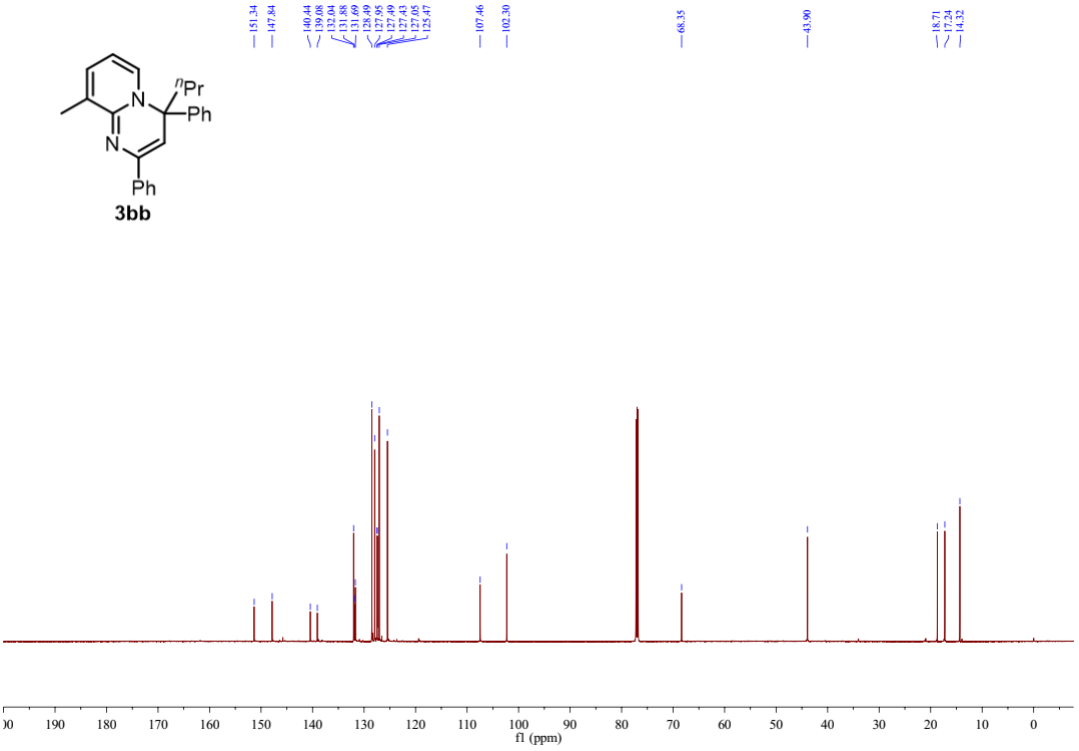
1.00
1.02
1.07
3.02
1.08
1.13
1.06
3.07
f1 (ppm)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Ph
N
N
Ph
3bb
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147.84
140.44
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131.88
131.69
128.49
127.95
127.49
127.43
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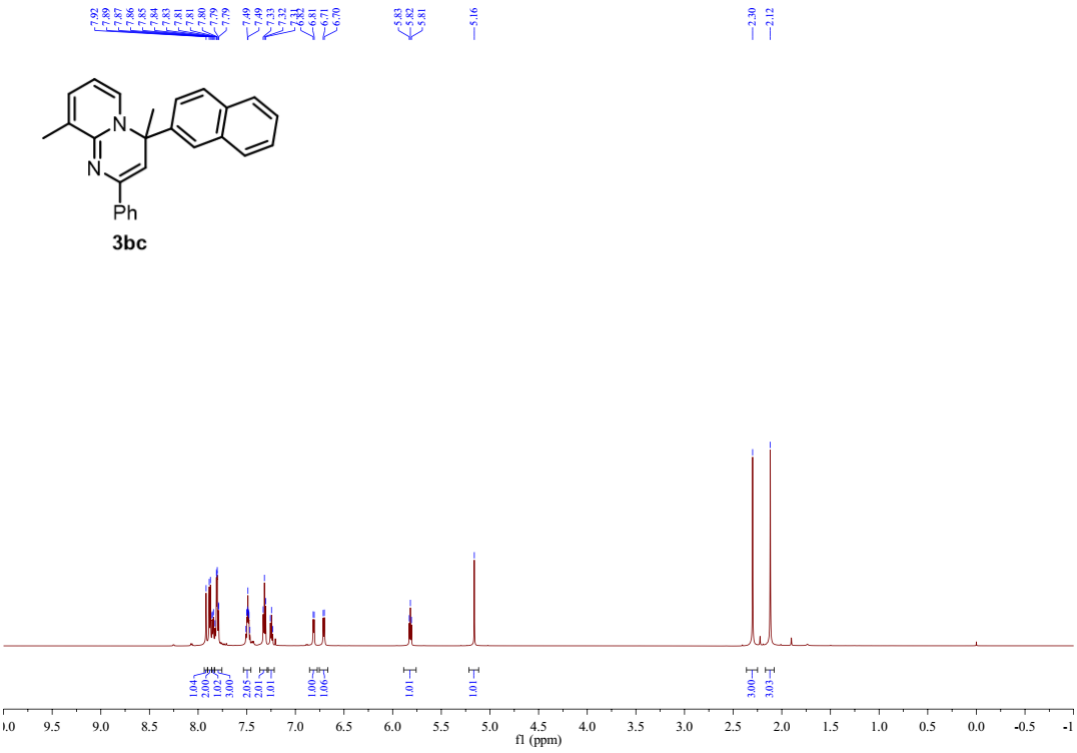
125.47
107.46
102.30
68.35
43.90
18.71
17.24
14.32
f1 (ppm)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7.79
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7.49
7.33
7.32
6.81
6.81
6.71
6.70
5.83
5.82
5.81
5.16
2.30
2.12
N
N
Ph
3bc
1.04
2.00
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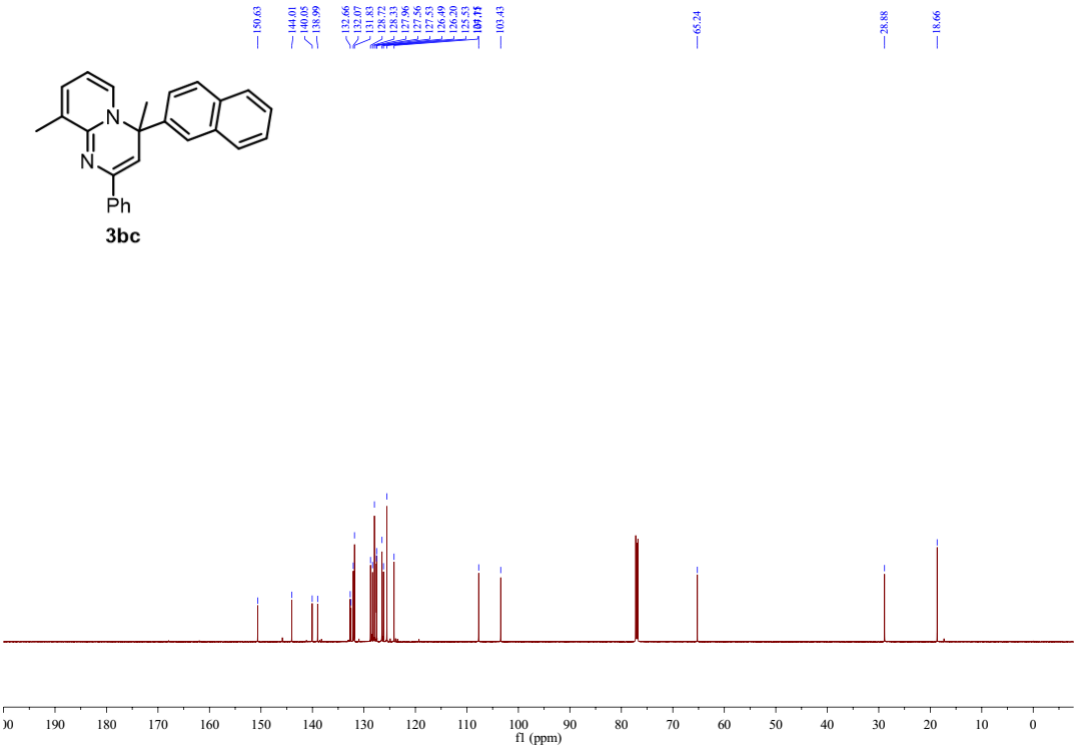
2.01
1.01
1.00
1.06
1.01
1.01
3.00
3.03
f1 (ppm)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127.56
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125.53
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65.24
28.88
18.66
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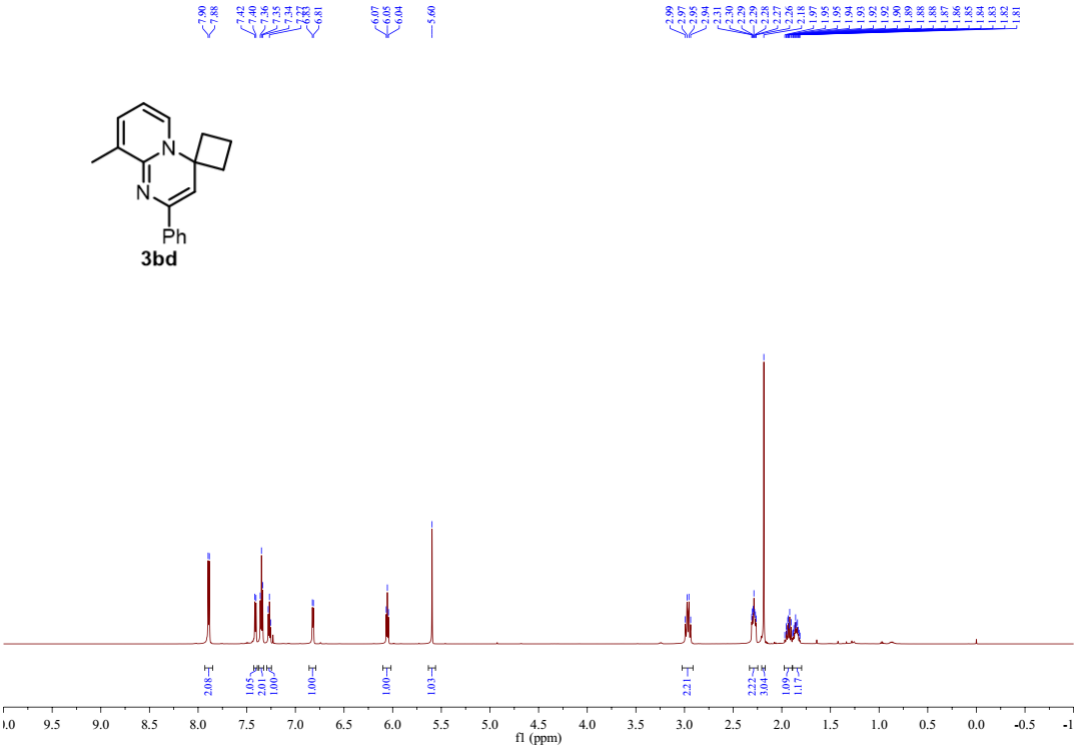
N
Ph
3bc
f1 (ppm)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7.27
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6.81
6.07
6.05
6.04
5.60
3.99
3.97
3.95
3.94
2.31
2.30
2.29
2.28
2.27
2.26
2.18
1.97
1.95
1.95
1.94
1.93
1.92
1.92
1.90
1.89
1.88
1.88
1.87
1.86
1.85
1.84
1.83
1.82
1.81
N
N
Ph
3bd
2.08
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1.00
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2.22
3.04
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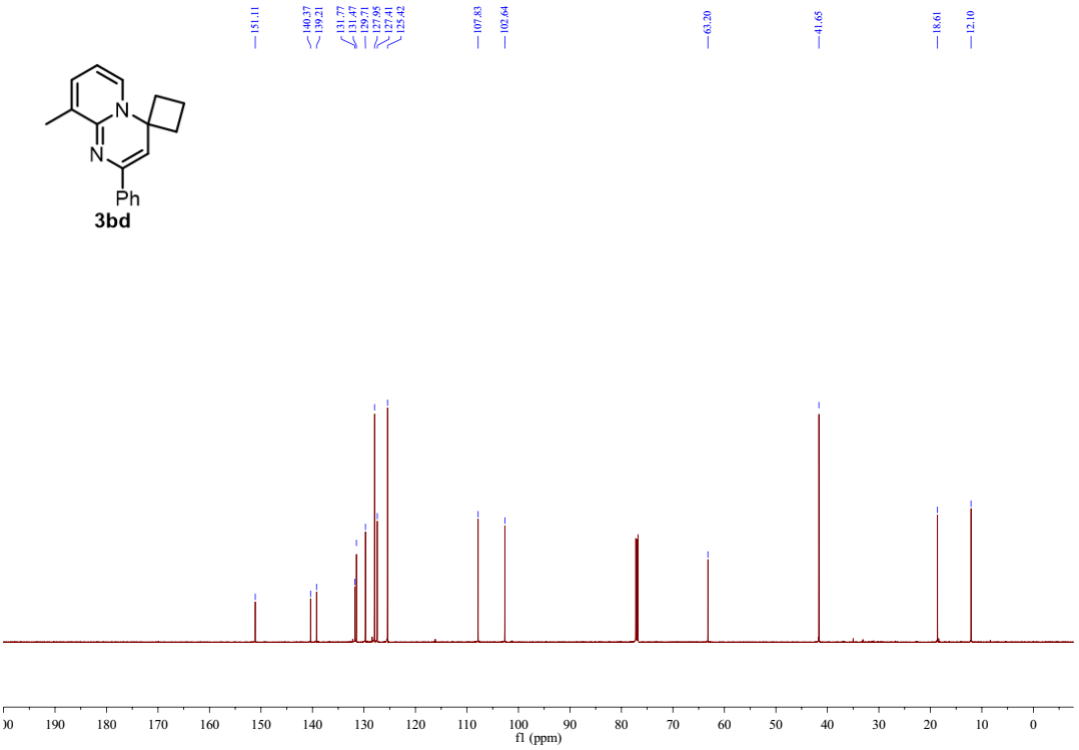
1.17
fl (ppm)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127.95
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107.83
102.64
63.20
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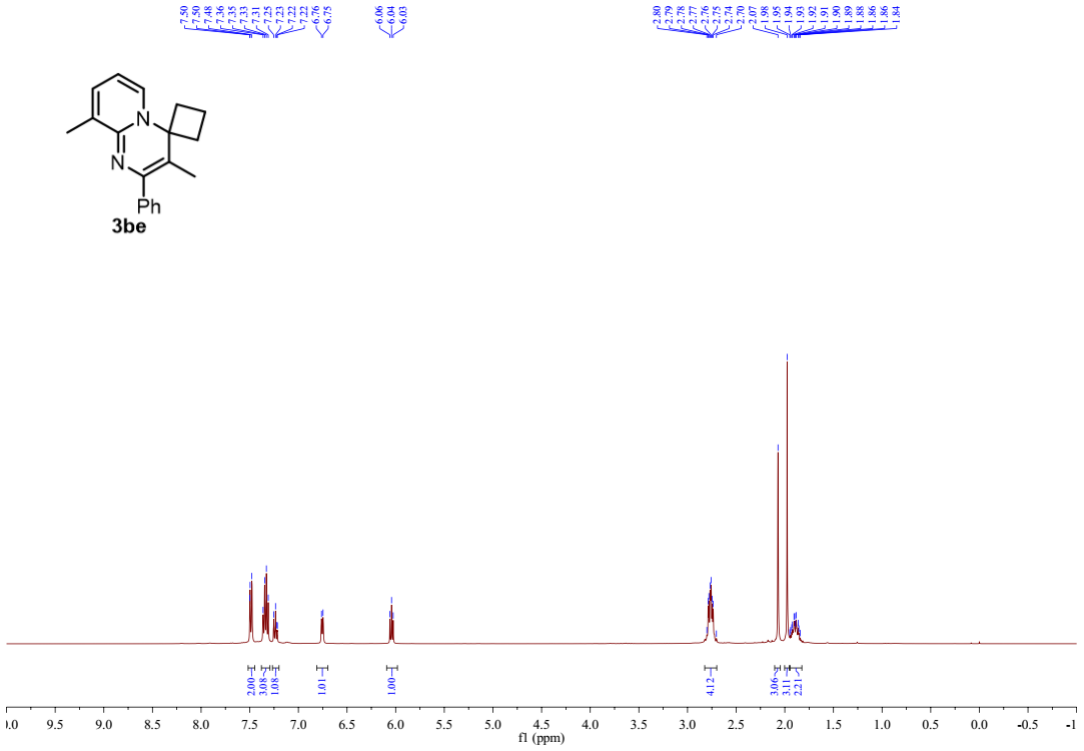
18.61
12.10
N
N
Ph
3bd
fl (ppm)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7.25
7.23
7.22
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6.75
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6.03
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1.95
1.94
1.93
1.92
1.91
1.90
1.89
1.88
1.86
1.86
1.84
N
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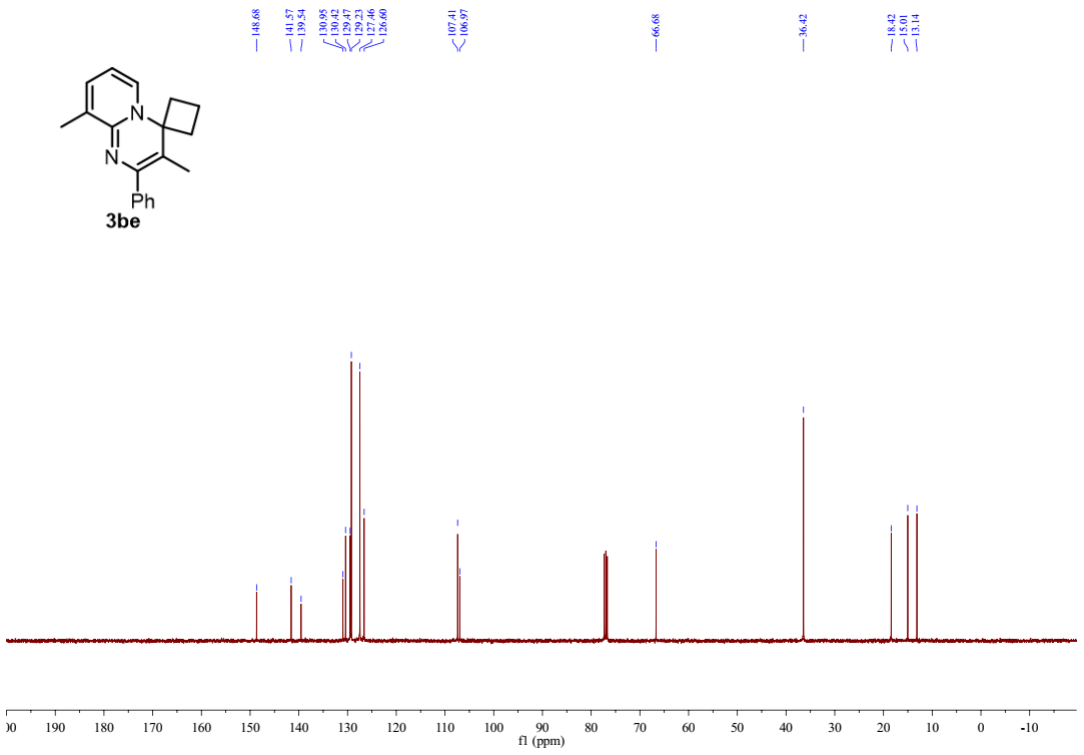
1.00
4.12
3.06
3.11
2.21
f1 (ppm)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129.47
129.23
127.46
126.60
107.41
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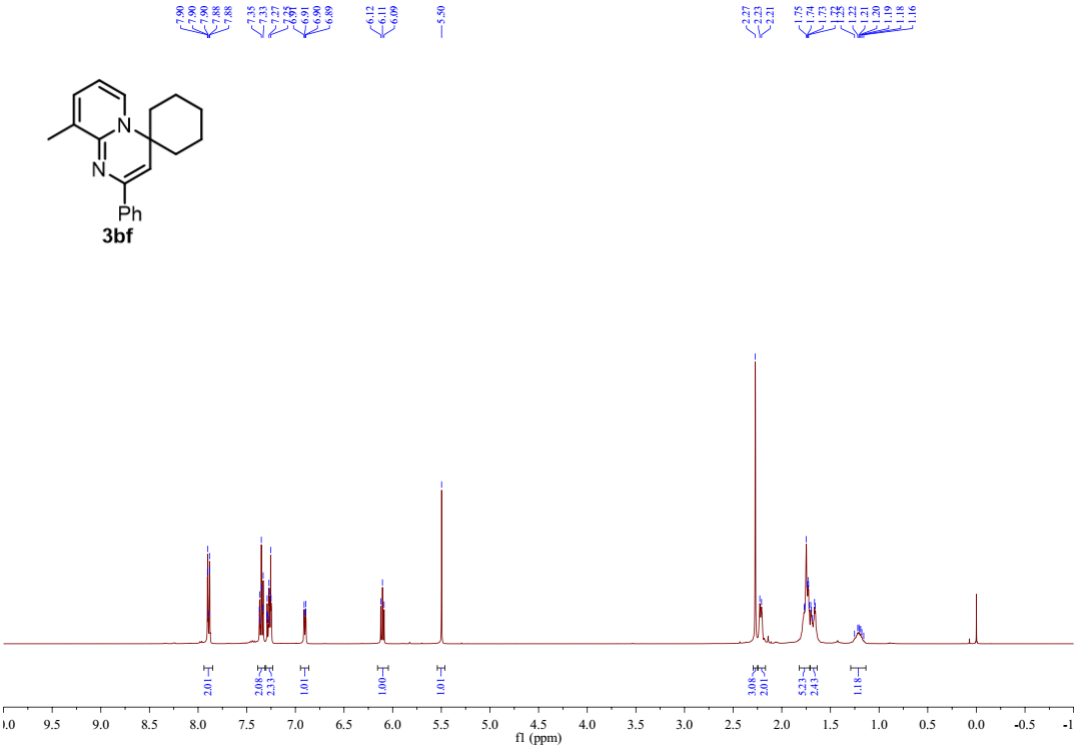
18.42
15.01
13.14
N
N
Ph
3be
f1 (ppm)

N
N
Ph

3bf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6.91
6.90
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6.11
6.09
5.50
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2.23
2.21
1.75
1.74
1.73
1.25
1.22
1.21
1.20
1.19
1.18
1.16
2.01
2.08
2.33
1.01
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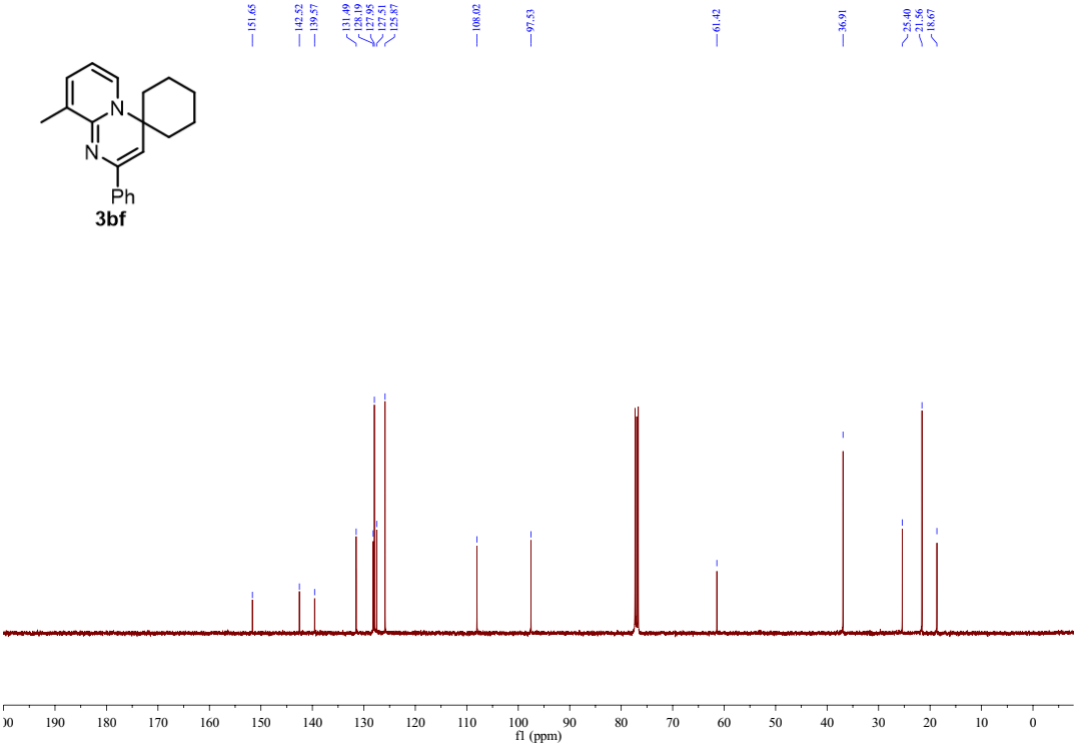
1.01
3.08
2.01
5.23
2.43
1.18
f1 (ppm)

N
N
Ph

3bf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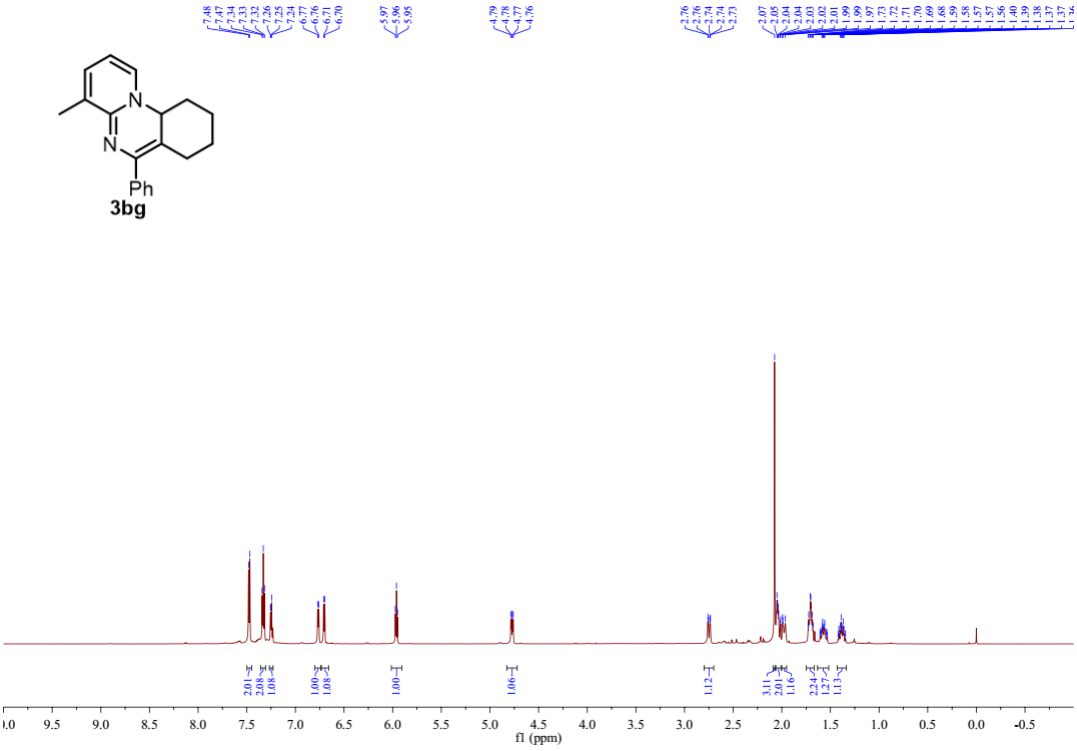
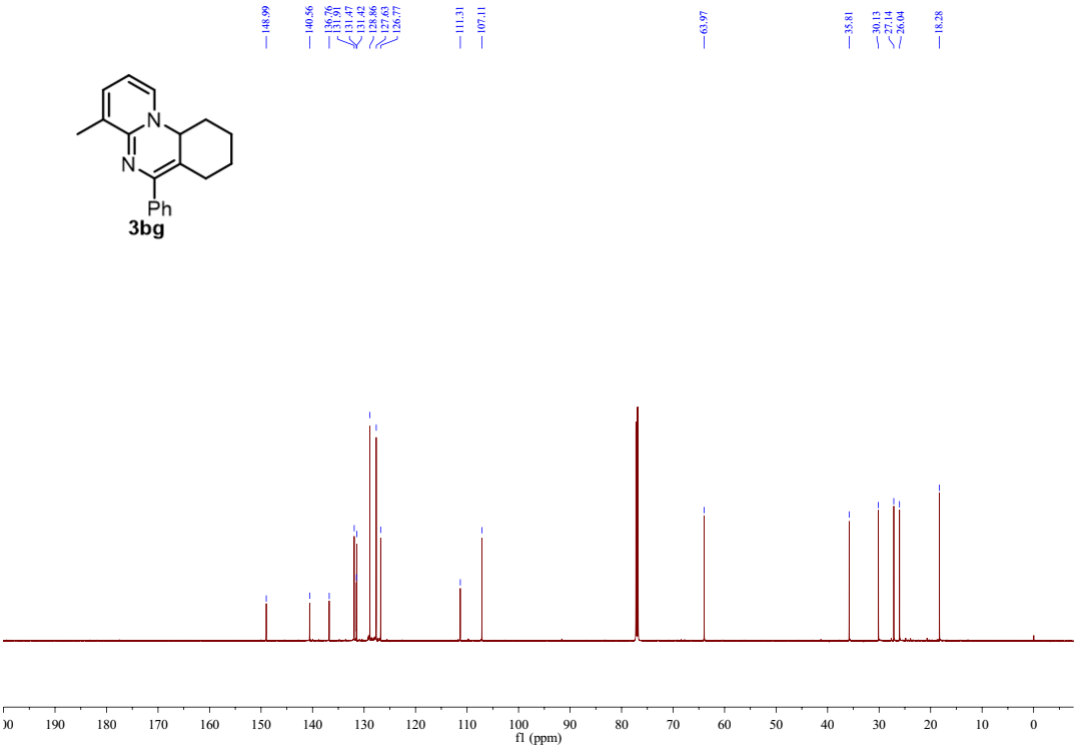
25.40
21.56
18.67
f1 (ppm)


3bg
fl (ppm)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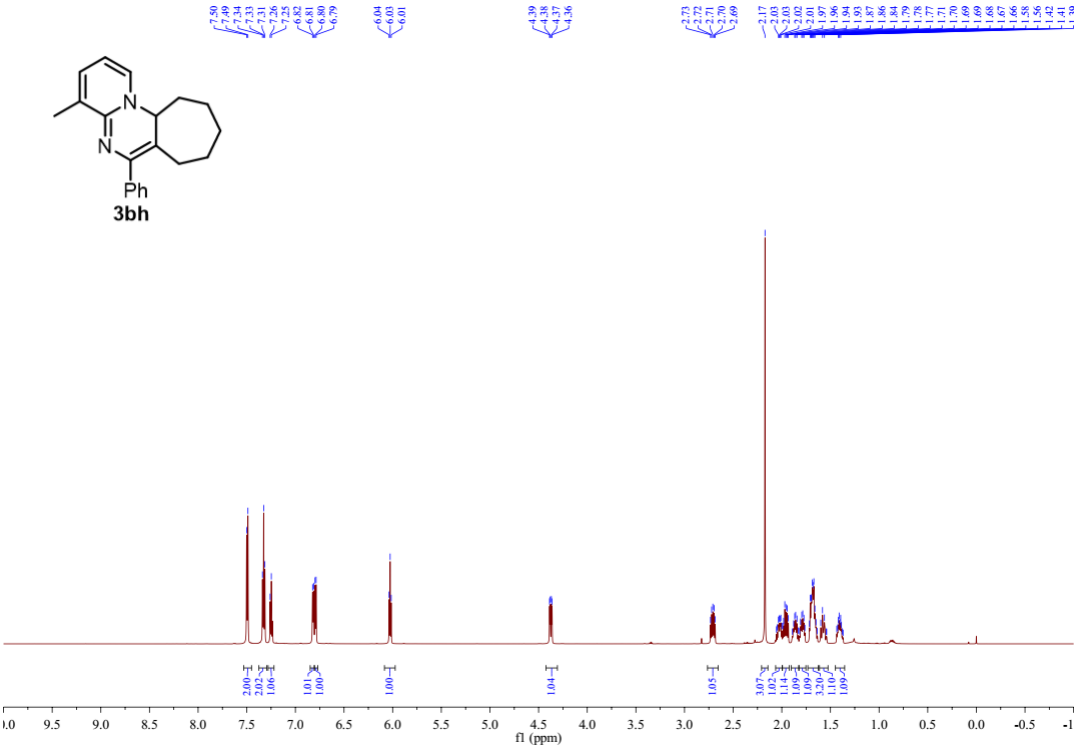
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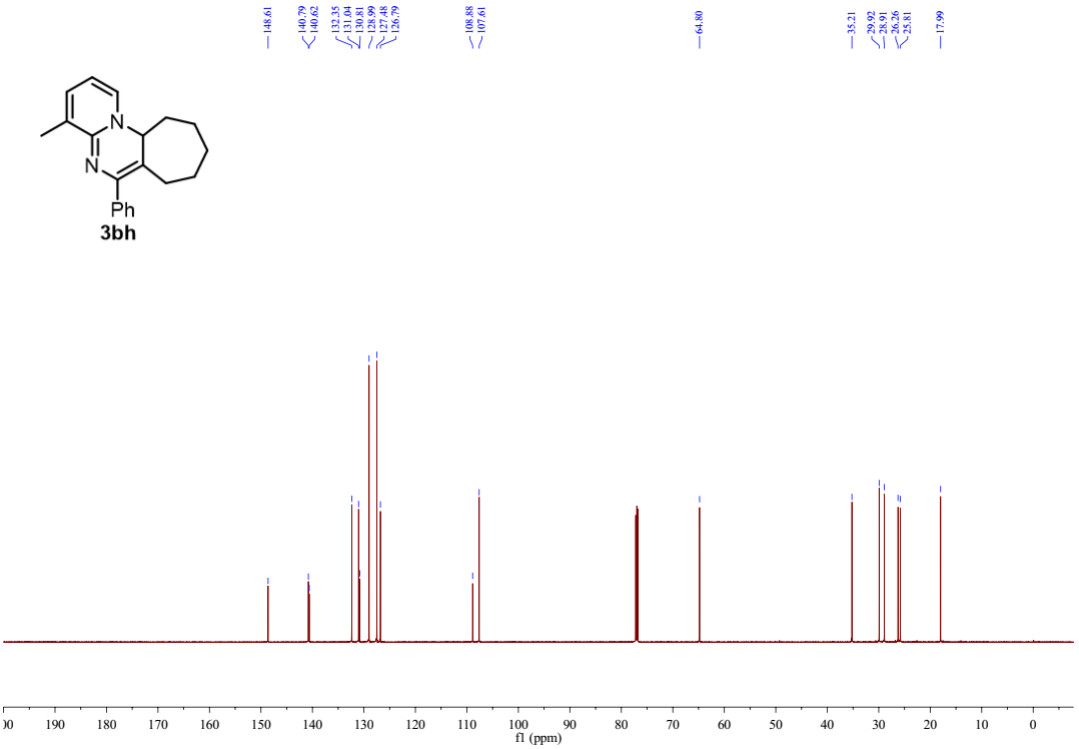
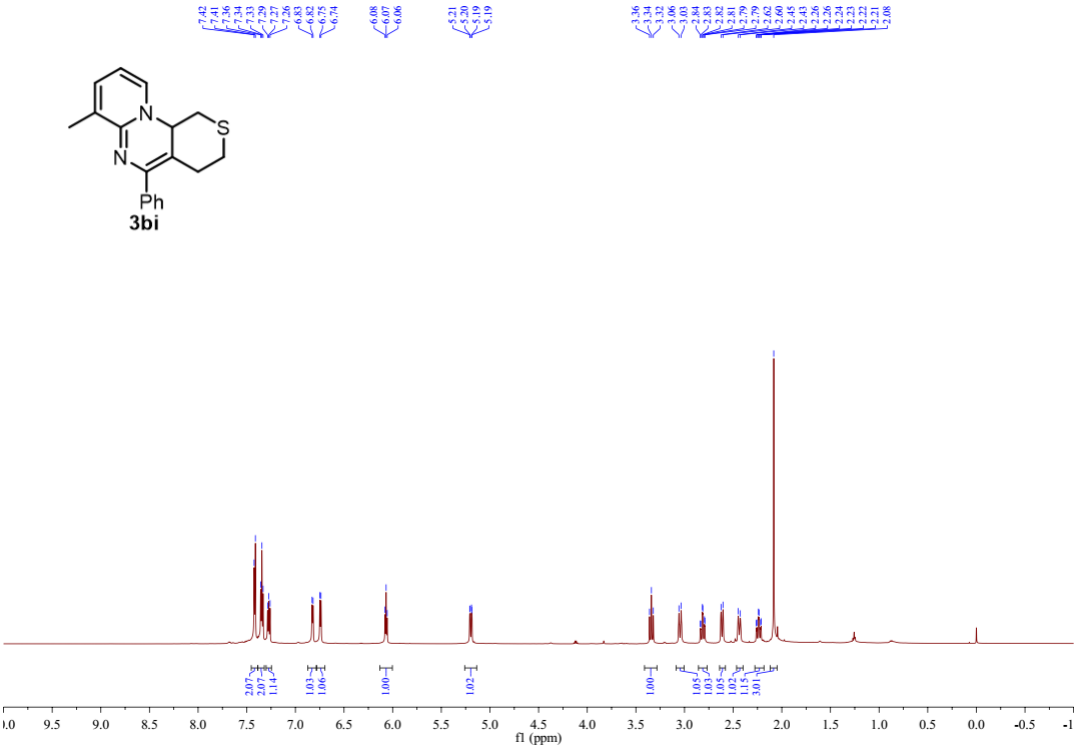
3bh
fl (ppm)


Ph
3bh
fl (ppm)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6.74
6.08
6.07
6.06
5.21
5.20
5.19
5.19
3.36
3.34
3.32
3.06
3.03
3.01
2.83
2.82
2.81
2.79
2.79
2.62
2.60
2.45
2.43
2.26
2.26
2.24
2.23
2.22
2.21
2.08
N
S
N
Ph
3bi
2.07
2.07
1.14
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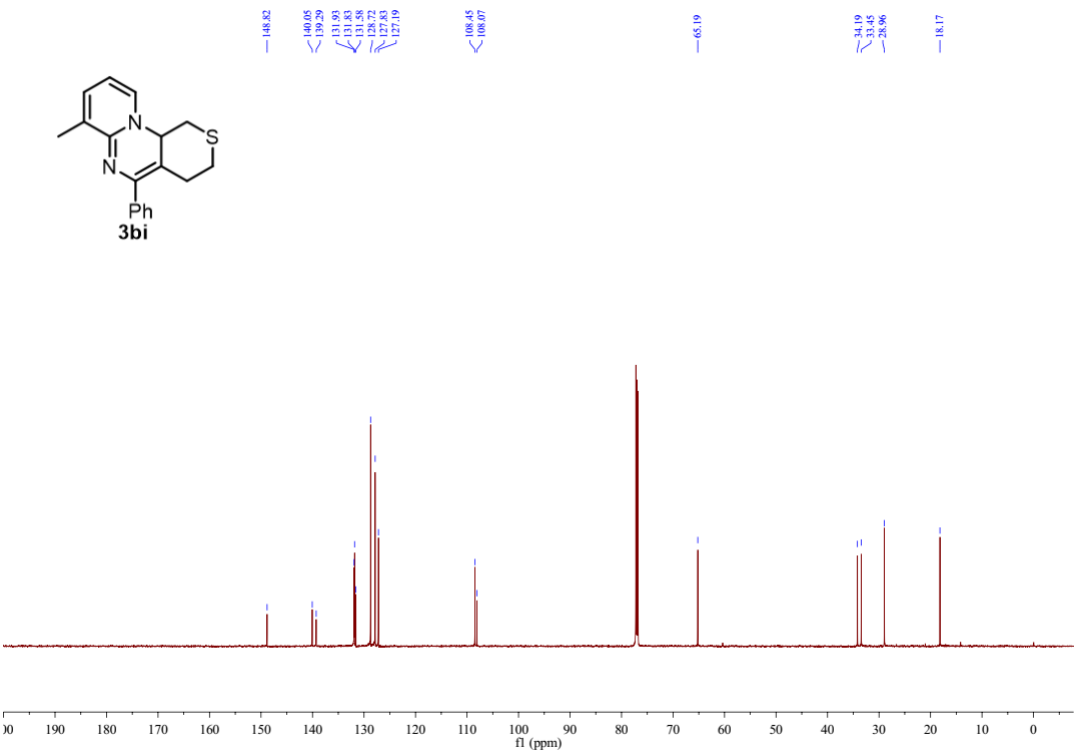
3.01
f1 (ppm)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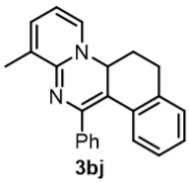
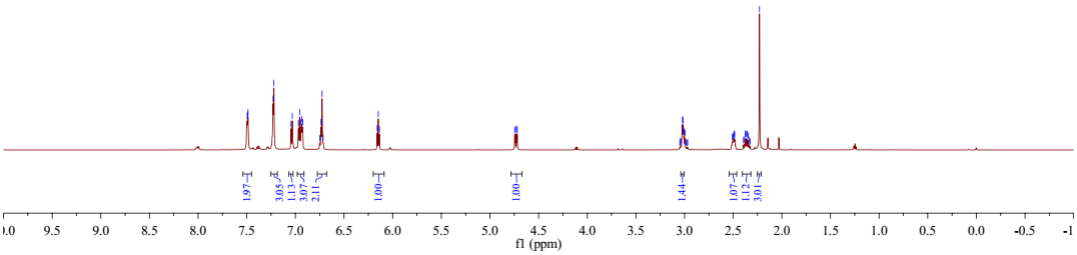
127.19
108.45
108.07
65.19
34.19
33.45
28.96
18.17
N
S
N
Ph
3bi
f1 (ppm)


N
N
Ph

3bj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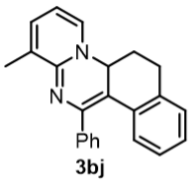
1.13
3.07
2.11
1.00
1.00
1.44
1.07
1.12
3.01
f1 (ppm)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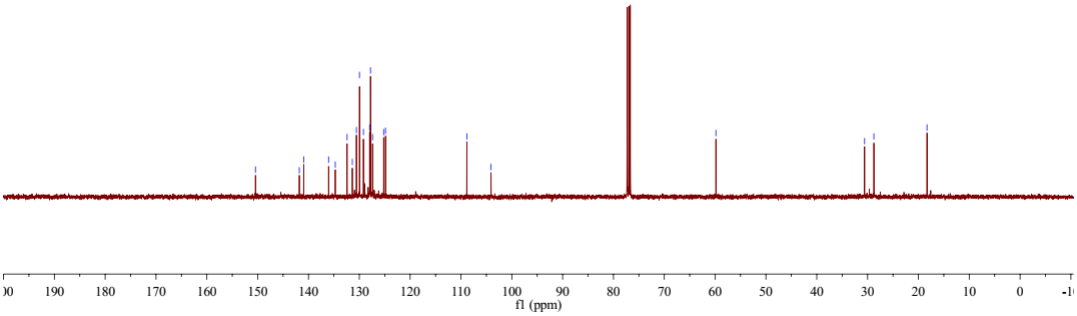
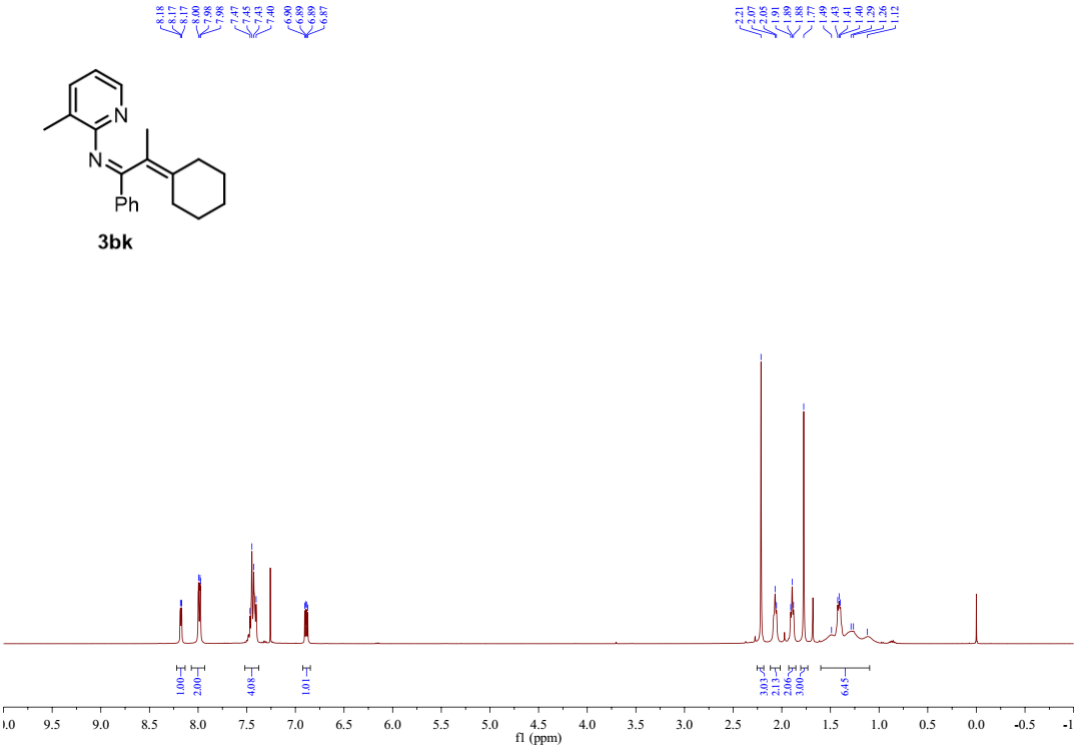
N
Ph

3bj


f1 (ppm)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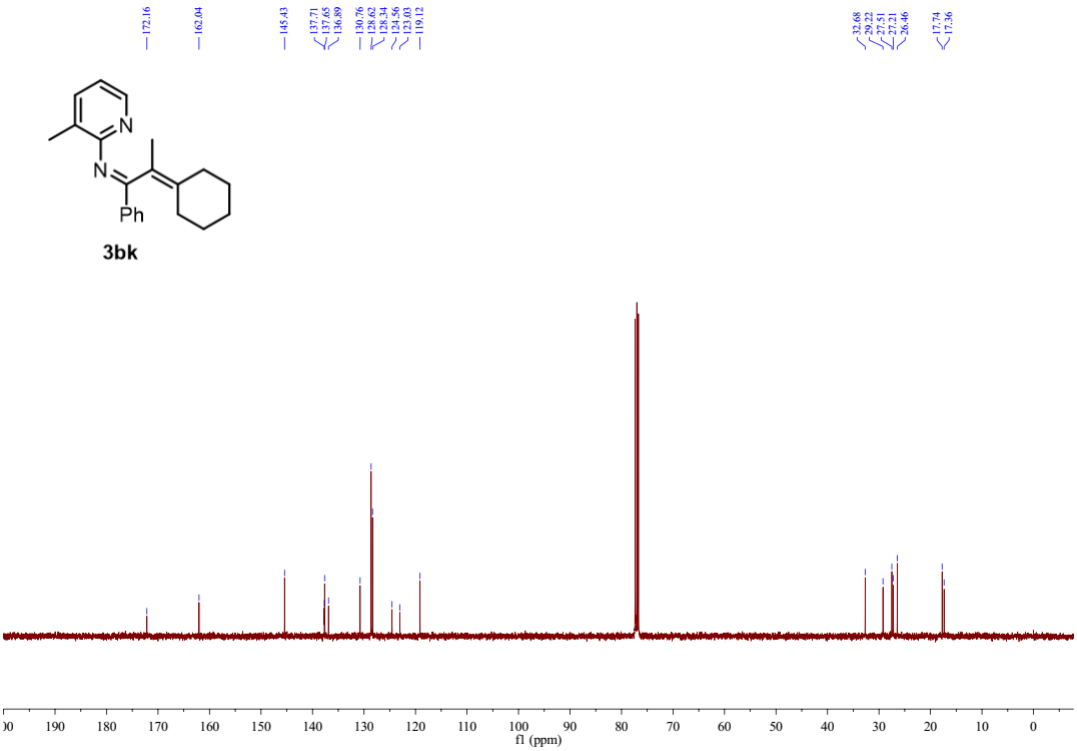
8.17
8.17
8.00
7.98
7.98
7.47
7.45
7.43
7.40
6.90
6.89
6.89
6.87
2.21
2.07
2.05
1.91
1.89
1.88
1.77
1.49
1.45
1.41
1.40
1.29
1.26
1.12
N
N
Ph
3bk
1.00
2.00
4.08
1.01
3.03
2.13
2.06
3.00
6.45
f1 (ppm)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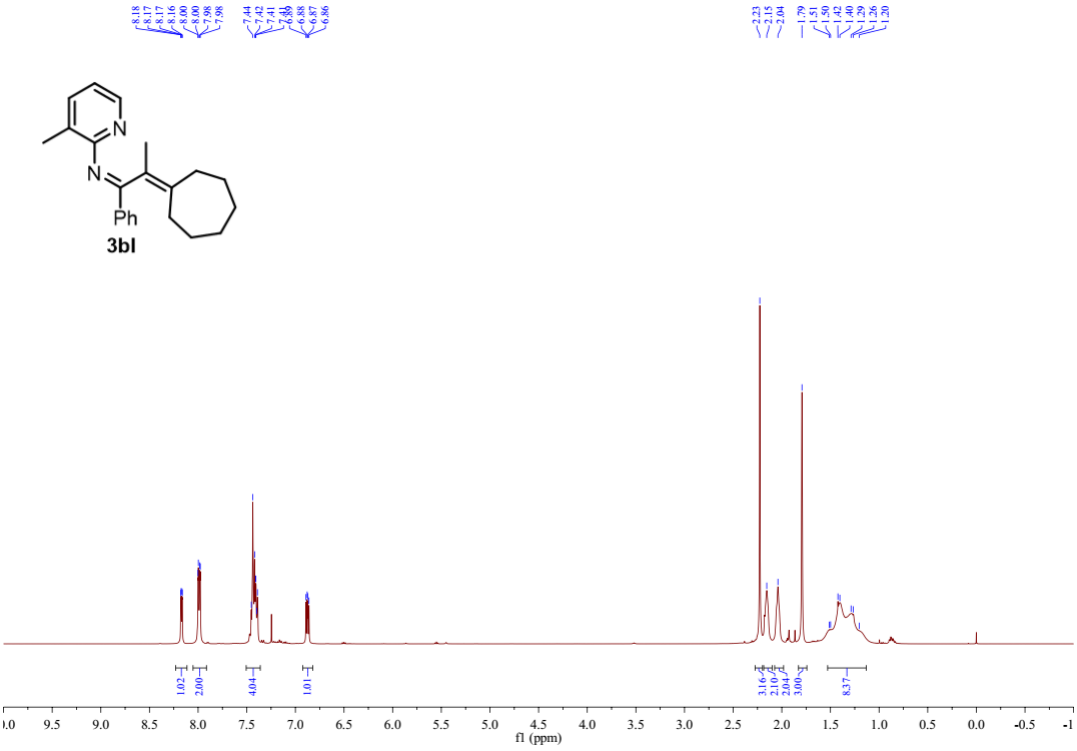
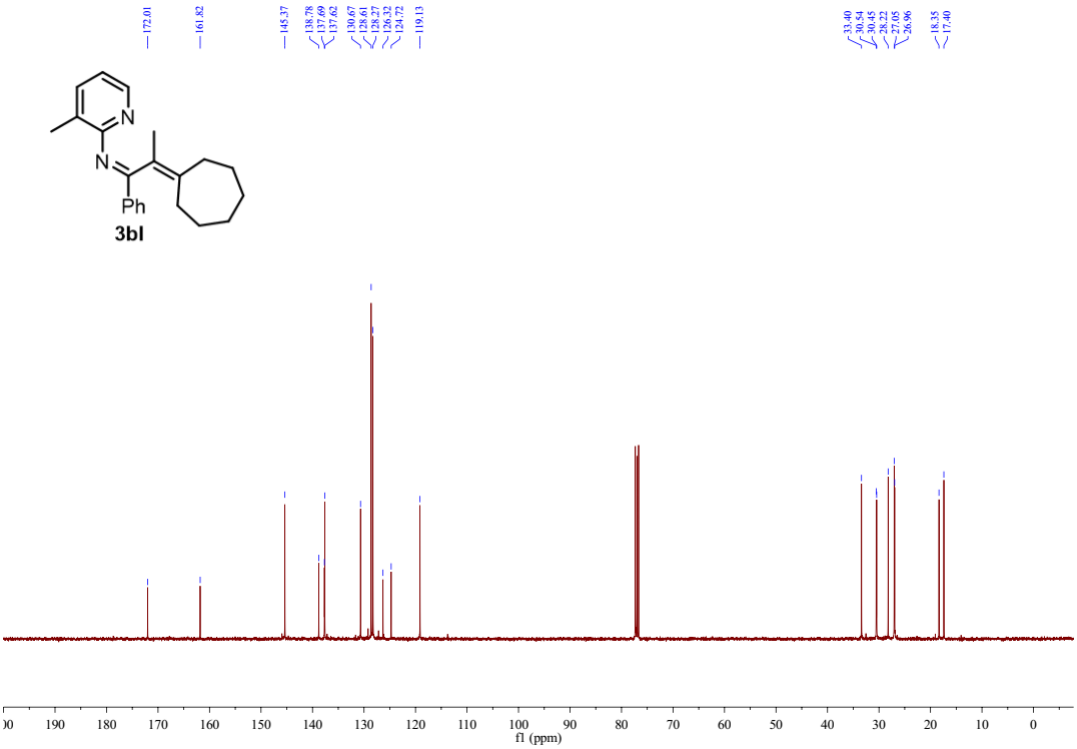
162.04
145.43
137.71
137.65
136.89
130.76
128.62
128.34
124.56
123.03
119.12
32.68
29.22
27.51
27.21
26.46
17.74
17.36
N
N
Ph
3bk
f1 (ppm)


8.18
8.17
8.17
8.16
8.00
8.00
7.98
7.98
7.44
7.42
7.41
6.88
6.88
6.87
6.86
2.23
2.15
2.04
1.79
1.51
1.50
1.42
1.40
1.29
1.26
1.20
N
N
Ph
3bl
1.02
2.00
4.04
1.01
3.16
2.10
2.04
3.00
8.37
f1 (ppm)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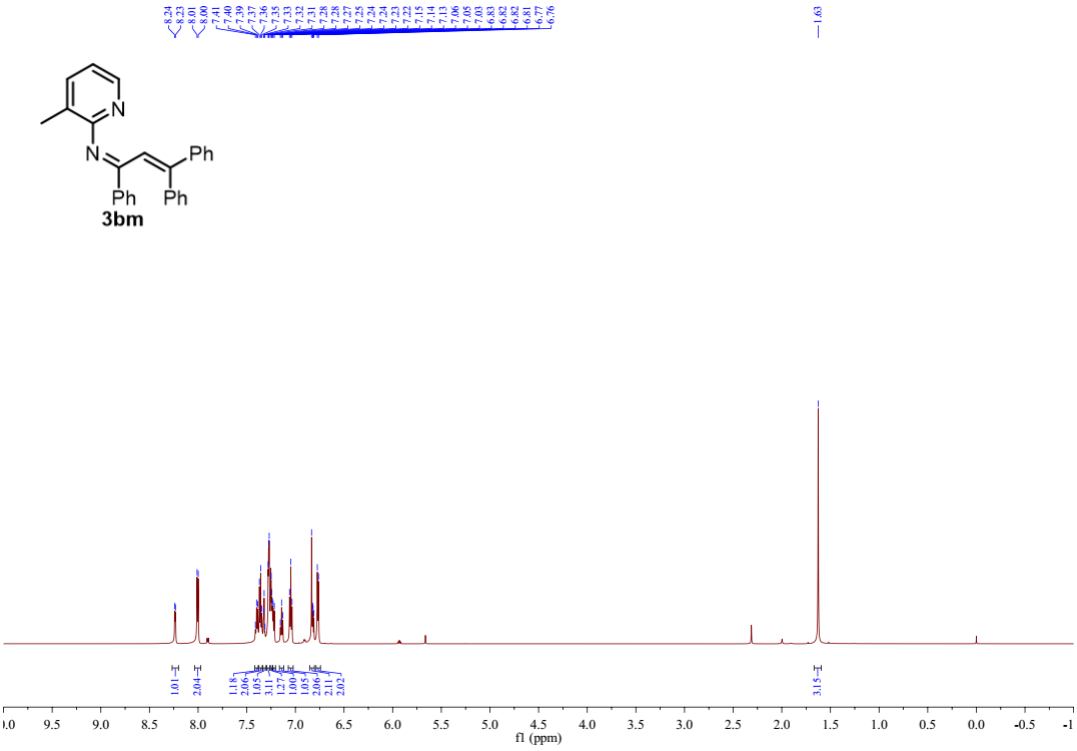
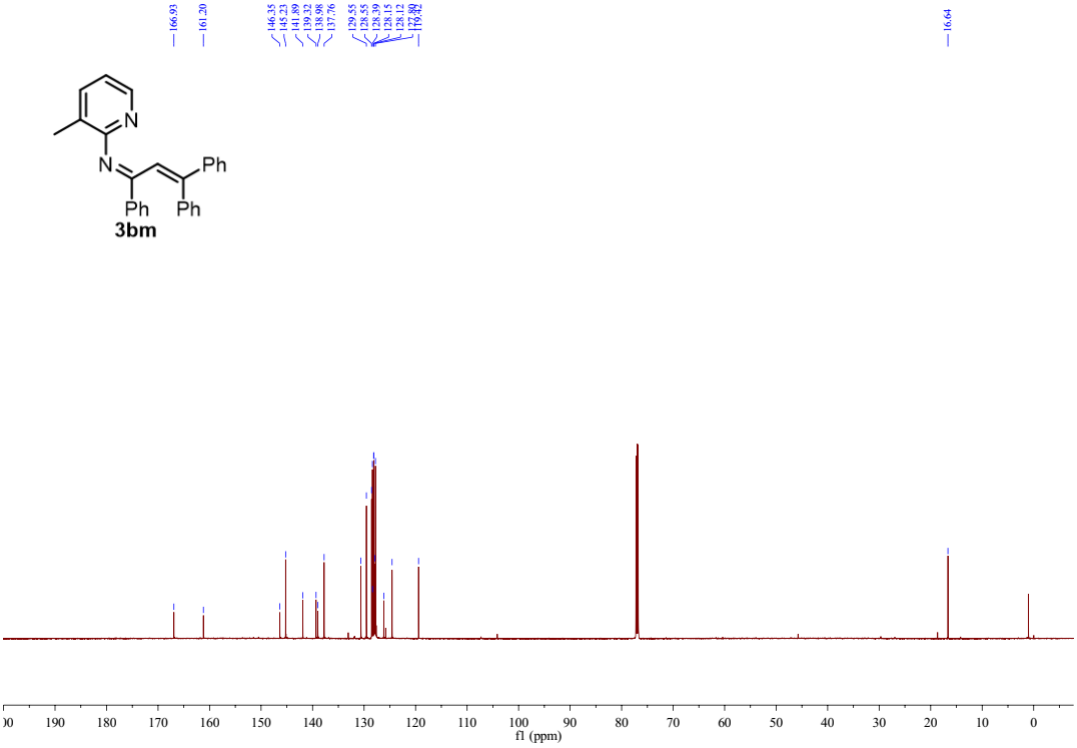
145.37
138.78
137.69
137.62
130.67
128.61
128.27
126.23
124.72
119.13
33.40
30.54
30.45
28.22
27.05
26.96
18.35
17.40
N
N
Ph
3bl
f1 (ppm)


8.24
8.23
8.01
8.00
7.41
7.40
7.39
7.37
7.36
7.35
7.33
7.32
7.31
7.28
7.27
7.25
7.24
7.24
7.23
7.22
7.15
7.14
7.13
7.06
7.05
7.03
6.83
6.82
6.82
6.81
6.77
6.76
1.63
N
N
Ph
Ph
Ph
3bm
1.01
2.04
1.18
2.06
1.03
3.11
1.27
1.00
1.04
2.06
2.11
2.02
3.15
f1 (ppm)


166.93
161.20
146.35
145.23
141.89
139.32
138.98
137.76
129.55
128.55
128.39
128.15
128.12
119.42
16.64
N
N
Ph
Ph
Ph
3bm
f1 (ppm)