Supporting Information

Regioselective access to di- and trisubstituted pyridines via a metal-oxidant-solvent-free domino reaction involving 3-chloropropiphenones

Ashvani Kumar Patel[a], Shikha Singh Rathor[a] and Sampak Samanta*[,a]

[a]Department of Chemistry, Indian Institute of Technology Indore, Simrol, 453552, Indore, India.

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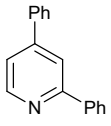
General Information: All reactions were carried out either under inert atmosphere or air and monitored by TLC using Merck 60 F254 pre coated silica gel plates (0.25 mm thickness) and the products were visualized by UV detection. Flash chromatography was carried out with silica gel (200-300 mesh). ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance (III) 500 MHz spectrometer. Data for ^{1}H NMR are reported as a chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, q = quartet, m = multiplet), coupling constant J (Hz), integration, and assignment, data for ^{13}C are reported as a chemical shift (δ ppm). High resolutions mass spectral analyses (HRMS) were carried out using ESI-TOF-MS. Melting points were recorded on an Electrothermal melting points apparatus and are uncorrected.

Starting materials: 3-chloropropiophenones(**1a-1i**)[11] and 3-bromopropiophenone[11] were prepared according to literature procedures. Cyclic and acyclic ketones and ammonium salts were purchased from commercial suppliers and used without further purification unless otherwise stated.

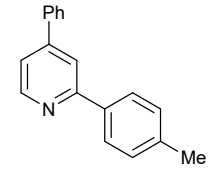
Representative procedure for the synthesis of (3aa): A mixture of compounds **1a** (0.3 mmol), **2a** (0.36 mmol) and NH_4OAc was heated at 70 °C in an open atmosphere. Upon completion of the reaction, the reaction mixture was extracted with ethyl acetate (3 × 10 mL), washed with water and brine, respectively, and dried over Na_2SO_4. The combined organic phases were evaporated under reduced pressure to afford the crude product. Finally, the product was obtained in pure form (72% yield) through column chromatography over silica gel using a mixture of EtOAc/hexane (1:19, v/v) as the eluent. The product was fully characterized by its spectroscopic data (^{1}HNMR, ^{13}C NMR, and HRMS).

The prepared pyridines in Schemes 2-4 were followed the above procedure and characterized by their corresponding spectroscopic data (^{1}H NMR, ^{13}C NMR, and HRMS).

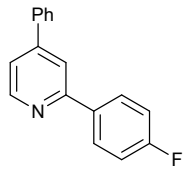
2,4-Diphenylpyridine (3aa):[1,2] Gummy liquid; yield = 72%; time = 24h; R_f = 0.33 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (d, J = 5.0 Hz, 1H), 8.05 (d, J = 7.2 Hz, 2H), 7.94 (s, 1H), 7.70 (d, J = 7.2 Hz, 2H), 7.53 – 7.43 (m, 7H) ppm;^{13}C NMR (125 MHz, $CDCl_3$ δ 158.2, 150.2, 149.4, 139.6, 138.6, 129.2, 129.19, 129.17, 128.9, 127.2, 127.1, 120.4, 118.9 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{14}N^+$ 232.1121, found 232.1119.



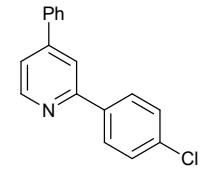
4-Phenyl-2-(4-methylphenyl)pyridine (3ab):[1,2] Gummy liquid; yield = 70%; time = 24h; R_f = 0.34 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.73 (d, *J* = 5.1 Hz, 1H), 7.96 (d, *J* = 8.1 Hz, 2H), 7.91 (s, 1H), 7.70 (d, *J* = 7.0 Hz, 2H), 7.51 (t, *J* = 7.3 Hz, 2H), 7.47 – 7.41 (m, 2H), 7.31 (d, *J* = 7.9 Hz, 2H), 2.43 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.2, 150.1, 149.3, 139.1, 138.7, 136.7, 129.6, 129.2, 129.1, 127.2, 127.0, 120.1, 118.5, 21.4 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{18}H_{16}N^+$ 246.1277, found 246.1279.



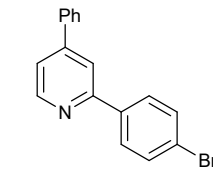
2-(4-Fluorophenyl)-4-phenylpyridine (3ag):[1,2] Yellow oil; yield = 63%; time = 24h; R_f = 0.45 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.72 (d, *J* = 5.1 Hz, 1H), 8.06 – 8.02 (m, 2H), 7.87 (s, 1H), 7.69 (d, *J* = 7.0 Hz, 2H), 7.53 – 7.43 (m, 4H), 7.18 (t, *J* = 8.7 Hz, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.7 (d, J_{C-F} = 247.2 Hz), 157.2, 150.2, 149.5, 138.5, 135.7, 129.28, 129.25, 128.9 (d, J_{C-F} = 8.2 Hz), 127.2, 120.3, 118.5, 115.8 (d, J_{C-F} = 21.3 Hz) ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{13}FN^+$ 250.1027, found 250.1028.



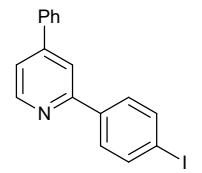
2-(4-Chlorophenyl)-4-phenylpyridine (3ae):[1,2] Light yellow solid; yield =65%; mp 52-54 ℃; time = 24h; R_f = 0.41 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.73 (d, *J* = 5.1 Hz, 1H), 8.00 (d, *J* = 8.5 Hz, 2H), 7.89 (s, 1H), 7.69 (d, *J* = 7.1 Hz, 2H), 7.52 (t, *J* = 7.3 Hz, 2H), 7.48 – 7.45 (m, 4H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9, 150.3, 149.6, 138.5, 138.0, 135.3, 129.3, 129.1, 128.6, 128.4, 127.2, 120.6, 118.6 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{13}ClN^+$ 266.0731, found 266.0729.



2-(4-Bromophenyl)-4-phenylpyridine (3af):[1,2] Pale yellow solid; yield= 66%; mp 66-68 ℃; time = 24h; R_f = 0.41 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.73 (d, *J* = 5.1 Hz, 1H), 7.94 (d, *J* = 8.5 Hz, 2H), 7.89 (s, 1H), 7.68 (d, *J* = 7.1 Hz, 2H), 7.62 (d, *J* = 8.5 Hz, 2H), 7.53–7.45 (m, 4H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.0, 150.3, 149.6, 138.4, 138.2, 132.0, 129.3 (2C, one overlap peak), 128.7, 127.2, 123.6, 120.7, 118.6 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{13}{}^{79}BrN^+$ 310.0226, found 310.0234; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{13}{}^{81}BrN^+$ 312.0211, found 312.0206.

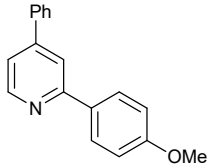


2-(4-Iodophenyl)-4-phenylpyridine (3ah):[1] Colorless solid; yield = 61%; mp 81-83 ℃; time = 24h; R_f = 0.45 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.73 (d, *J* = 5.1 Hz, 1H), 7.89 (s, 1H), 7.85 – 7.77 (m, 4H), 7.68 (d, *J* = 7.1 Hz, 2H), 7.53 – 7.40 (m, 4H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1,

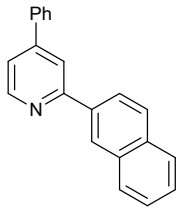


150.3, 149.6, 139.0, 138.4, 138.08, 138.04, 129.3, 128.9, 127.2, 120.8, 118.6, 95.5 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{13}IN^+$ 358.0087, found 358.0081.

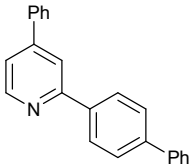
2-(4-Methoxyphenyl)-4-phenylpyridine (3ac):[1] Pale yellow solid; yield=73%; mp 52-54 ℃; time = 24h; R_f = 0.31 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.69 (d, *J* = 5.1 Hz, 1H), 8.01 (d, *J* = 8.8 Hz, 2H), 7.87 (s, 1H), 7.69 (d, *J* = 7.2 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 2H), 7.46 (t, *J* = 7.3 Hz, 1H), 7.40 (dd, *J* = 5.1, 1.5 Hz, 1H), 7.02 (d, *J* = 8.8 Hz, 2H), 3.87 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.6, 157.8, 150.0, 149.3, 138.8, 132.2, 129.2, 129.1, 128.4, 127.2, 119.7, 118.2, 114.3, 55.5 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{18}H_{16}NO^+$ 262.1226, found 262.1224.



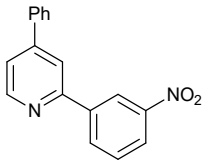
2-(Naphthalen-2-yl)-4-phenylpyridine(3aj):[1,2] Yellow oil; yield = 69%; time = 24h; R_f = 0.28 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (d, *J* = 5.1 Hz, 1H), 8.55 (s, 1H), 8.21 (dd, *J* = 8.6, 1.7 Hz, 1H), 8.08 (s, 1H), 7.98 (d, *J* = 8.7 Hz, 2H), 7.90 – 7.88 (m, 1H), 7.74 (d, *J* = 7.1 Hz, 2H), 7.55 – 7.47 (m, 6H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.0, 150.3, 149.5, 138.6, 136.8, 133.8, 133.6, 129.3, 129.2, 128.8, 128.6, 127.8, 127.2, 126.7, 126.6, 126.4, 124.8, 120.4, 119.1 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{21}H_{16}N^+$ 282.1277, found 182.1286.



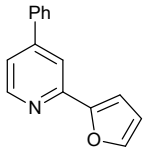
2-([1, 1′-Biphenyl]-4-yl)-4-phenylpyridine (3ad):[1] Light yellow solid; yield = 67%; time = 24h; mp 88-90 ℃; R_f = 0.38 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 (d, *J* = 5.1 Hz, 1H), 8.15 (d, *J* = 8.3 Hz, 2H), 7.99 (s, 1H), 7.75 – 7.71 (m, 4H), 7.68 (d, *J* = 7.3 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 2H), 7.49 – 7.46 (m, 4H), 7.38 (t, *J* = 7.3 Hz, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.7, 150.2, 149.5, 141.9, 140.7, 138.6, 138.4, 129.3, 129.2, 128.9, 128.0, 127.7, 127.6, 127.5, 127.2, 120.4, 118.8 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{23}H_{18}N^+$ 308.1434, found 308.1439.



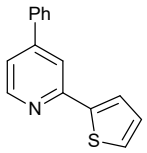
2-(3-Nitrophenyl)-4-phenylpyridine (3ai):[1] Yellow solid; yield = 59% ; mp 109-111 ℃; time = 24h; R_f = 0.33 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.91 (s, 1H), 8.77 (d, *J* = 5.0 Hz, 1H), 8.43 (d, *J* = 7.7 Hz, 1H), 8.28 (d, *J* = 8.1 Hz, 1H), 7.98 (s, 1H), 7.71–7.64 (m, 3H), 7.54–7.47 (m, 4H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.4, 150.5, 149.9, 148.9, 141.2, 138.1, 132.9, 129.8, 129.5, 129.3, 127.2, 123.7, 122.0, 121.4, 118.8 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{13}N_2O_2^+$ 277.0972, found 277.0970.



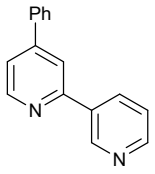
2-(Furan-2-yl)-4-phenylpyridine (3al):[1] Yellow oil; yield = 68%; time = 24h; R_f = 0.32 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 5.1 Hz, 1H), 7.92 (br s, 1H), 7.69 (d, *J* = 7.2 Hz, 2H), 7.55 (br s, 1H), 7.50 (t, *J* = 7.3 Hz, 2H), 7.45 (t, *J* = 7.2 Hz, 1H), 7.37 (dd, *J* = 5.1, 1.5 Hz, 1H), 7.12 (d, *J* = 3.3 Hz, 1H), 6.56 (dd, *J* = 3.2, 1.7 Hz, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.7, 150.1, 149.9, 149.2, 143.4, 138.3, 129.2, 129.2, 127.1, 120.0, 116.6, 112.2, 108.9 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{15}H_{12}NO^+$ 222.0913, found 222.0932.



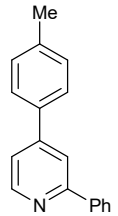
4-Phenyl-2-(thiophen-2-yl)pyridine(3am):[1,2] Colorless oil; yield = 70%; time = 24h; R_f =0.32 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (d, *J* = 5.2 Hz, 1H), 7.86 (br s, 1H), 7.68 (d, *J* = 7.0 Hz, 3H), 7.52 (t, *J* = 7.3 Hz, 2H), 7.47 (t, *J* = 7.3 Hz, 1H), 7.43 (d, *J* = 5.0 Hz, 1H), 7.37 (dd, *J* = 5.2, 1.6 Hz, 1H), 7.14 (dd, *J* = 5.0, 3.7 Hz, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.2, 150.1, 149.4, 144.9, 138.4, 129.2, 128.2, 128.0, 127.8, 127.2, 124.8, 120.2, 117.0 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{15}H_{12}NS^+$ 238.0685, found 238.0690.



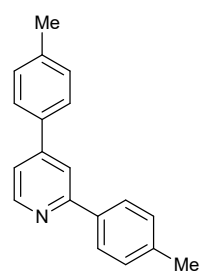
4-Phenyl-2,3′-bipyridine (3ak):[1] Pale yellow solid; yield = 55%; mp 51-53 ℃; time = 24h; R_f = 0.20 (EtOAc/Hexane = 20:80); ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.25 (s, 1H), 8.76 (d, *J* = 5.0 Hz, 1H), 8.68 (br s, 1H), 8.38 (d, *J* = 7.8 Hz, 1H), 7.94 (s, 1H), 7.69 (d, *J* = 7.2 Hz, 2H), 7.55 – 7.42 (m, 5H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.5, 150.6, 150.0, 149.7, 148.3, 138.2, 135.1, 134.7, 129.4, 129.3, 127.2, 123.7, 121.1, 118.9 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{16}H_{13}N_2^+$ 233.1073, found 233.1084.



2-Phenyl-4-(4-methylphenyl)pyridine (3ba):[4] Pale yellow solid; yield = 73%; mp 73-75 ℃; time = 24h; R_f = 0.31 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.72 (d, *J* = 4.0 Hz, 1H), 8.04 (d, *J* = 7.0 Hz, 2H), 7.92 (s, 1H), 7.61 (d, *J* = 7.1 Hz, 2H), 7.49 (t, *J* = 6.7 Hz, 2H), 7.44 (d, *J* = 5.0 Hz, 2H), 7.32 (d, *J* = 7.2 Hz, 2H), 2.43 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.2, 150.2, 149.3, 139.7, 139.3, 135.7, 130.0, 129.1, 128.9, 127.2, 127.0, 120.1, 118.7, 21.3 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{18}H_{16}N^+$ 246.1277, found 246.1295.

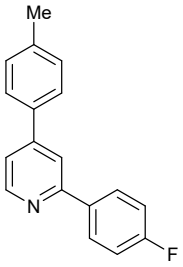


2,4-Di-(4-methylphenyl)pyridine (3bb):[2,4] Colorless solid; yield = 70% ; mp 112-114 ℃; time = 24h; R_f = 0.34 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.70 (d, *J* = 4.9 Hz, 1H), 7.95 (d, *J* = 7.9 Hz, 2H), 7.89 (s, 1H), 7.60 (d, *J* = 7.8 Hz, 2H), 7.41 (d, *J* = 4.7 Hz, 1H), 7.32-7.28 (m, 4H), 2.43 (s, 3H), 2.42 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.1, 150.1,

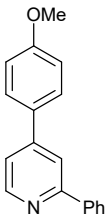


149.2, 139.2, 139.1, 136.9, 135.8, 129.9, 129.6, 127.05, 127.03, 119.9, 118.3, 21.4, 21.3 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{19}H_{18}N^+$ 260.1434, found 260.1440.

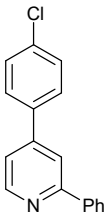
2-(4-Fluorophenyl)-4-(4-methylphenyl)pyridine (3bg): Pale yellow oil; yield = 63% ; time = 24h; R_f = 0.35 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.69 (d, *J* = 5.1 Hz, 1H), 8.03 (dd, *J* = 8.6, 5.5 Hz, 2H), 7.86 (s, 1H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.43 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.32 (d, *J* = 7.8 Hz, 2H), 7.18 (t, *J* = 8.7 Hz, 2H), 2.43 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.5 (d, $J_{C\text{-}F}$ = 246.7 Hz), 157.0, 150.0, 149.3, 139.2, 135.7, 135.4, 129.8, 128.8 (d, $J_{C\text{-}F}$ = 8.2 Hz), 126.9, 120.0, 118.2, 115.6 (d, $J_{C\text{-}F}$ = 21.3 Hz), 21.2 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{18}H_{15}FN^+$ 264.1183, found 264.1184.



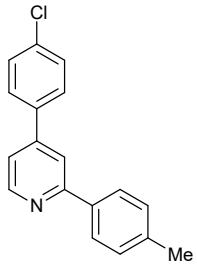
4-(4-Methoxyphenyl)-2-phenylpyridine (3ca):[1,3,4] Yellow oil; yield = 71%; time = 24h; R_f = 0.31 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.70 (d, *J* = 5.1 Hz, 1H), 8.04 (d, *J* = 7.3 Hz, 2H), 7.89 (s, 1H), 7.66 (d, *J* = 8.7 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.45 – 7.41 (m, 2H), 7.04 (d, *J* = 8.7 Hz, 2H), 3.88 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.7, 158.1, 150.0, 148.9, 139.6, 130.8, 129.1, 128.9, 128.4, 127.2, 119.8, 118.4, 114.7, 55.5 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{18}H_{16}NO^+$ 262.1226, found 262.1229.



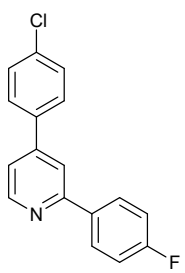
4-(4-Chlorophenyl)-2-phenylpyridine (3ea):[4] Yellow oil; yield = 66%; time = 24h; R_f = 0.33 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (d, *J* = 5.0 Hz, 1H), 8.04 (d, *J* = 7.2 Hz, 2H), 7.88 (s, 1H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.51 – 7.39 (m, 6H) ppm;^{13}C NMR (125 MHz, $CDCl_3$) δ 158.4, 150.3, 148.1, 139.4, 137.1, 135.4, 129.4, 129.3, 128.9, 128.4, 127.1, 120.1, 118.6 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{13}ClN^+$ 266.0731, found 266.0741.



4-(4-Chlorophenyl)-2-(4-methylphenyl)pyridine (3eb):[4] Colorless solid; yield = 68%; mp 96-98 ℃; time = 24h; R_f = 0.37 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.72 (d, *J* = 4.9 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 2H), 7.86 (s, 1H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 3.9 Hz, 1H), 7.31 (d, *J* = 7.9 Hz, 2H), 2.42 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.4, 150.2, 148.1, 139.3, 137.2, 136.6, 135.3, 129.6, 129.4, 128.5, 127.0, 119.8, 118.3, 21.4 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{18}H_{15}ClN^+$ 280.0888, found 280.0894.

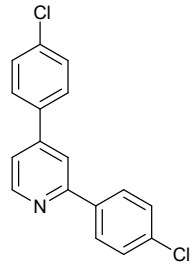


4-(4-Chlorophenyl)-2-(4-fluorophenyl)pyridine (3eg): Colorless solid; yield =56%; mp 61-63 ℃; time = 24h; R_f = 0.39 (EtOAc/Hexane = 10:90);

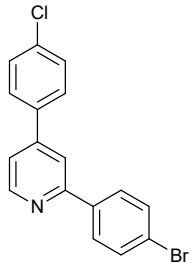


^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 5.1 Hz, 1H), 7.94 (dd, *J* = 8.7, 5.4 Hz, 2H), 7.74 (s, 1H), 7.53 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.31 (dd, *J* = 5.1, 1.5 Hz, 1H), 7.09 (t, *J* = 8.6 Hz, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.7 (d, $J_{C\text{-}F}$ = 247.3 Hz), 157.3, 150.3, 148.2, 136.9, 135.57 (d, $J_{C\text{-}F}$ = 2.8 Hz), 135.50, 129.5, 128.9 (d, $J_{C\text{-}F}$ = 8.4 Hz), 128.4, 120.0, 118.2, 115.8 (d, $J_{C\text{-}F}$ = 21.3 Hz) ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{12}ClFN^+$ 284.0637, found 284.0635.

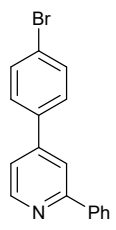
2, 4-Bis(4-chlorophenyl)pyridine (3ee):[2] Colorless solid; yield=61% ; mp 97-99 ℃; R_f = 0.46 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.73 (d, *J* = 5.1 Hz, 1H), 7.99 (d, *J* = 8.6 Hz, 2H), 7.85 (s, 1H), 7.62 (d, *J* = 8.5 Hz, 2H), 7.48 (dd, *J* = 10.4, 8.6 Hz, 4H), 7.42 (dd, *J* = 5.1, 1.6 Hz, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 150.4, 148.4, 137.8, 136.9, 135.5, 135.4, 129.5, 129.1, 128.5, 128.4, 120.4, 118.4 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{12}Cl_2N^+$ 300.0341, found 300.0347.



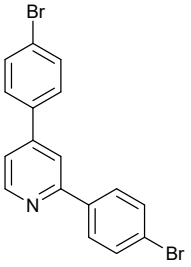
2-(4-Bromophenyl)-4-(4-chlorophenyl)pyridine (3ef): Colorless solid; yield = 58%; mp 112-114 ℃; time = 24h; R_f = 0.47 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.73 (d, *J* = 5.1 Hz, 1H), 7.92 (d, *J* = 8.5 Hz, 2H), 7.85 (s, 1H), 7.62 (dd, *J* = 8.5, 3.6 Hz, 4H), 7.49 (d, *J* = 8.5 Hz, 2H), 7.42 (dd, *J* = 5.1, 1.5 Hz, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 150.4, 148.4, 138.3, 136.9, 135.5, 132.1, 129.5, 128.7, 128.5, 123.8, 120.4, 118.3 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{12}{}^{79}BrClN^+$ 343.9836, found 3343.9844; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{12}{}^{81}BrClN^+$ 345.9815, found 345.9817.



4-(4-Bromophenyl)-2-phenylpyridine (3fa):[4] Yellow oil; yield = 64%; time = 24h; R_f = 0.39 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.75 (d, *J* = 5.1 Hz, 1H), 8.04 (d, *J* = 7.3 Hz, 2H), 7.88 (s, 1H), 7.65 (d, *J* = 8.5 Hz, 2H), 7.56 (d, *J* = 8.5 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 2H), 7.45 (t, *J* = 7.3 Hz, 1H), 7.41 (dd, *J* = 5.1, 1.6 Hz, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.4, 150.3, 148.3, 139.3, 137.5, 132.4, 129.3, 128.9, 128.8, 127.2, 123.7, 120.1, 118.6 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{13}{}^{79}BrN^+$ 310.0226, found 310.0230; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{13}{}^{81}BrN^+$ 312.0207, found 312.0211.

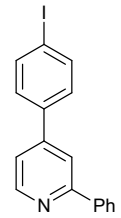


2,4-bis(4-bromophenyl)pyridine (3ff):[2] Colorless solid ; yield = 60%; mp 128-131 ℃; time = 24h; R_f = 0.44 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.72 (d, *J* = 5.1 Hz, 1H), 7.92 (d, *J* = 8.5 Hz, 2H), 7.83 (s, 1H), 7.63 (dd, *J*

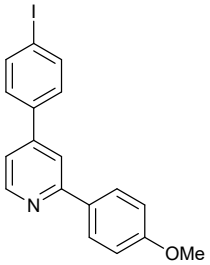


= 10.3, 8.6 Hz, 4H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.41 (dd, *J* = 5.0, 1.3 Hz, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 150.4, 148.4, 138.2, 137.3, 132.4, 132.0, 128.7, 128.7, 123.8, 123.7, 120.3, 118.2 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{12}{}^{79}Br_2N^+$ 387.9331, found 387.9349; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{12}{}^{79}Br\ {}^{81}BrN^+$ 389.9311, found 389.9325; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{12}{}^{81}Br_2N^+$ 391.9293, found 391.9291.

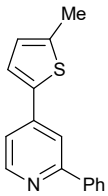
4-(4-Iodophenyl)-2-phenylpyridine (3ga): Gummy; yield = 63%; time = 24h; R_f = 0.40 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.75 (d, *J* = 5.1 Hz, 1H), 8.04 (d, *J* = 7.1 Hz, 2H), 7.88 (s, 1H), 7.86 – 7.83 (m, 2H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.46 – 7.40 (m, 4H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.4, 150.3, 148.4, 139.3, 138.4, 138.1, 129.3, 128.9, 128.9, 127.2, 120.0, 118.5, 95.4 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{13}IN^+$ 358.0087, found 358.0087.



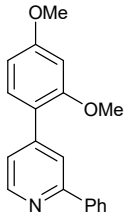
4-(4-Iodophenyl)-2-(4-methoxyphenyl)pyridine (3gb): Gummy**;** yield = 60%; time = 24h; R_f = 0.36 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.69 (d, *J* = 5.1 Hz, 1H), 8.00 (d, *J* = 8.8 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.81 (s, 1H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.34 (dd, *J* = 5.1, 1.5 Hz, 1H), 7.02 (d, *J* = 8.8 Hz, 1H), 3.87 (s, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.7, 158.0, 150.2, 148.2, 138.3, 138.3, 131.9, 128.9, 128.4, 119.3, 117.7, 114.3, 95.2, 55.5 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{18}H_{15}INO^+$ 388.0193, found 388.0197.



4-(5-Methylthiophen-2-yl)-2-phenylpyridine (3ha): Pale yellow solid; yield = 68%; mp 84-86 ℃; time = 24h; R_f = 0.37 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 5.2 Hz, 1H), 8.02 (d, *J* = 7.2 Hz, 2H), 7.82 (s, 1H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.44 (t, *J* = 7.3 Hz, 1H), 7.37 – 7.34 (m, 2H), 6.80 (dd, *J* = 3.5, 0.9 Hz, 1H), 2.55 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.2, 150.2, 142.5, 142.3, 139.5, 139.0, 129.1, 128.8, 127.1, 126.8, 125.5, 118.1, 116.6, 15.7 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{16}H_{14}NS^+$ 352.0841, found 352.0847.

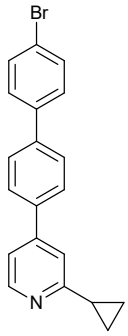


4-(2,4-Dimethoxyphenyl)-2-phenylpyridine (3da): Pale yellow oil; yield = 66%; time = 24h; R_f = 0.21 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (d, *J* = 5.1 Hz, 1H), 8.01 (d, *J* = 7.7 Hz, 2H), 7.88 (s, 1H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.43 – 7.40 (m, 2H), 7.35 (d, *J* = 8.3 Hz, 1H), 6.62 – 6.59 (m, 2H), 3.87 (s, 3H), 3.84 (s, 3H) ppm;^{13}C NMR (125 MHz, $CDCl_3$) δ 161.6, 157.9, 157.3, 149.3,

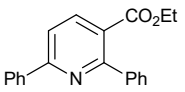


147.2, 139.9, 131.2, 128.9, 128.8, 127.2, 122.8, 121.4, 120.8, 105.2, 99.2, 55.7, 55.6 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{19}H_{18}NO_2^+$ 292.1332, found 292.1343.

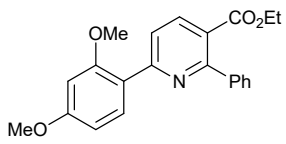
4-(4′-Bromo-[1,1′-biphenyl]-4-yl)-2-cyclopropylpyridine (3in): Pale Yellow oil; yield = 76%; time = 30h; R_f = 0.32 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (d, *J* = 5.2 Hz, 1H), 7.72 – 7.70 (m, 2H), 7.67 – 7.66 (m, 2H), 7.60 – 7.58 (m, 2H), 7.51 – 7.49 (m, 2H), 7.38 (s, 1H), 7.31 (dd, *J* = 5.2, 1.5 Hz, 1H), 2.18 – 2.13 (m, 1H), 1.13 – 1.04 (m, 4H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.4, 149.1, 148.4, 140.8, 139.2, 137.6, 132.2, 128.8, 127.7, 127.7, 122.2, 119.2, 118.7, 17.2, 10.3 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{20}H_{17}{}^{79}BrN^+$ 350.0539, found 350.0539; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{20}H_{17}{}^{81}BrN^+$ 352.0520, found 352.0525.



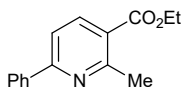
Ethyl 2, 6-diphenylnicotinate (4ay):[7,9] Pale yellow oil; yield =84%; time = 24h; R_f = 0.34 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.1 Hz, 1H), 8.14-8.12 (m, 2H), 7.78 (d, *J* = 8.2 Hz, 1H), 7.66 – 7.63 (m, 2H), 7.50 – 7.43 (m, 6H), 4.18 (q, *J* = 7.1 Hz, 2H), 1.08 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.4, 158.8, 158.5, 140.6, 139.0, 138.4, 129.8, 128.98, 128.92, 128.7, 128.1, 127.4, 125.4, 117.9, 61.5, 13.8 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{20}H_{18}NO_2^+$ 304.1332, found 304.1341.



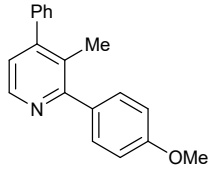
Ethyl 6-(2,4-dimethoxyphenyl)-2-phenylnicotinate (4dy): Yellow oil; yield = 77%; time = 24h; R_f = 0.26 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.2 Hz, 1H), 8.02 (d, *J* = 8.6 Hz, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.61 (dd, *J* = 7.6, 1.4 Hz, 2H), 7.44 – 7.38 (m, 3H), 6.62 (dd, *J* = 8.6, 2.3 Hz, 1H), 6.56 (d, *J* = 2.2 Hz, 1H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.89 (s, 3H), 3.86 (s, 3H), 1.06 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.5, 162.0, 158.8, 158.5, 157.1, 141.0, 137.9, 132.7, 128.9, 128.4, 128.0, 124.2, 122.3, 121.1, 105.4, 98.9, 61.3, 55.7, 55.6 13.8 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{22}H_{22}NO_4^+$ 364.1543, found 364.1541.



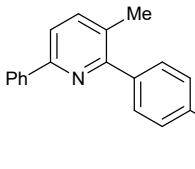
\Ethyl 2-methyl-6-phenylnicotinate (4az):[7] Yellow oil; yield =75%; time = 24h; R_f = 0.58 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.2 Hz, 1H), 8.06 – 8.04 (m, 2H), 7.60 (d, *J* = 8.2 Hz, 1H), 7.49-7.41 (m, 3H), 4.39 (q, *J* = 7.1 Hz, 2H), 2.92 (s, 3H), 1.41 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.6, 159.9, 159.0, 139.3, 138.5, 129.6, 128.8, 127.3, 123.6, 117.3, 61.1, 25.3, 14.3 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{15}H_{16}NO_2^+$ 242.1176, found 242.1182.



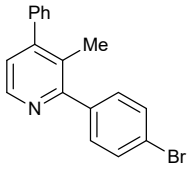
2-(4-Methoxyphenyl)-3-methyl-4-phenylpyridine (3ao, major isomer): Colorless oil; yield = 61%; time = 36h; R_f = 0.24 (EtOAc/Hexane = 20:80); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (d, *J* = 4.9 Hz, 1H), 7.52 (d, *J* = 8.7 Hz, 2H), 7.47 (t, *J* = 7.3 Hz, 2H), 7.42 (d, *J* = 7.3 Hz, 1H), 7.37-7.36 (m, 2H), 7.13 (d, *J* = 4.9 Hz, 1H), 6.99 (d, *J* = 8.7 Hz, 2H), 3.86 (s, 3H), 2.23 (s, 3H).ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.5, 159.4, 151.2, 146.3, 140.0, 130.6, 129.9, 128.8, 128.7, 128.5, 128.0, 123.0, 113.7, 55.4, 18.4 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{19}H_{18}NO^+$ 276.1383, found 276.1382.



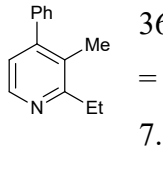
2-(4-Methoxyphenyl)-3-methyl-6-phenylpyridine (4ao, minor isomer): Colorless oil; yield = 9%; time = 36h; R_f = 0.28 (EtOAc/Hexane = 20:80); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (d, *J* = 7.4 Hz, 2H), 7.66-7.60 (m, 4H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.39 (t, *J* = 7.2 Hz, 1H), 7.01 (d, *J* = 8.5 Hz, 2H), 3.88 (s, 3H), 2.42 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.5, 157.5, 154.3, 139.7, 130.6, 129.3, 128.7, 128.6, 128.2, 127.9, 126.9, 118.5, 113.5, 55.3, 20.0 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{19}H_{18}NO^+$ 276.1383, found 276.1388.



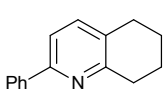
2-(4-Bromophenyl)-3-methyl-4-phenylpyridine (3ap): Yellow oil; yield = 57%; time = 36h; R_f = 0.21 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (d, *J* = 4.9 Hz, 1H), 7.60 (d, *J* = 8.2 Hz, 2H), 7.48 – 7.40 (m, 5H), 7.36 (d, *J* = 7.1 Hz, 2H), 7.16 (d, *J* = 4.9 Hz, 1H), 2.20 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.6, 151.3, 146.7, 140.0, 139.7, 131.4, 131.0, 128.8, 128.7, 128.6, 128.1, 123.6, 122.3, 18.1 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{18}H_{15}{}^{79}BrN^+$ 324.0382, found 324.0383; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{18}H_{15}{}^{81}BrN^+$ 326.0364, found 326.0366.



2-Ethyl-3-methyl-4-phenylpyridine (3aq): Pale yellow oil; yield = 64%; time = 36h; R_f = 0.31 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41 (d, *J* = 5.0 Hz, 1H), 7.45 – 7.42 (m, 2H), 7.40 – 7.37 (m, 1H), 7.29 – 7.27 (m, 2H), 7.00 (d, *J* = 5.0 Hz, 1H), 2.91 (q, *J* = 7.5 Hz, 2H), 2.22 (s, 3H), 1.35 (t, *J* = 7.5 Hz, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.1, 149.9, 146.0, 140.1, 129.1, 128.8, 128.3, 127.7, 122.3, 29.2, 15.6, 12.9 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{14}H_{15}N^+$ 198.1277, found 198.1285.

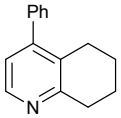


2-Phenyl-5,6,7,8-tetrahydroquinoline (4ar, major isomer):[5,6] Pale yellow oil; yield = 40% ; time = 24h; R_f = 0.52 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 – 7.93 (m, 2H), 7.46-7.35 (m, 5H), 3.01 (t, *J* = 6.4 Hz, 2H), 2.80 (t, *J* = 6.3 Hz, 2H), 1.95-1.91 (m, 2H), 1.86 – 1.81 (m, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ

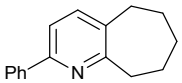


157.3, 154.8, 139.9, 137.6, 130.9, 128.7, 128.5, 126.9, 118.1, 32.9, 28.7, 23.3, 22.9 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{15}H_{15}N^+$ 210.1277, found 210.1281.

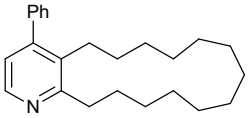
4-Phenyl-5,6,7,8-tetrahydroquinoline (3ar, minor isomer):[3] Pale yellow oil; yield = 33%; time = 24h; R_f = 0.24 (EtOAc/Hexane = 15:85); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, *J* = 4.9 Hz, 1H), 7.44 – 7.37 (m, 3H), 7.29 – 7.27 (m, 2H), 6.99 (d, *J* = 4.9 Hz, 1H), 3.03 (t, *J* = 6.6 Hz, 2H), 2.63 (t, *J* = 6.3 Hz, 2H), 1.93 – 1.88 (m, 2H), 1.75-1.70 (m, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.5, 150.2, 146.0, 139.3, 130.3, 128.6, 128.4, 128.0, 122.2, 32.8, 27.5, 22.9, 22.9 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{15}H_{15}N^+$ 210.1277, found 210.1278.



2-Phenyl-6,7,8,9-tetrahydro-5*H*-cyclohepta[*b*]pyridine (4as, minor):[6] Pale yellow oil; yield =30%; time = 24h; R_f = 0.56 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 – 7.96 (m, 2H), 7.46 – 7.43 (m, 4H), 7.37 (t, *J* = 7.3 Hz, 1H), 3.15 – 3.12 (m, 2H), 2.82 - 2.79 (m, 2H), 1.92 – 1.87 (m, 2H), 1.75 – 1.69 (m, 4H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.2, 154.1, 139.9, 137.3, 136.7, 128.7, 128.4, 126.9, 118.0, 39.8, 35.1, 32.7, 28.2, 26.8 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{16}H_{18}N^+$ 224.1434, found 224.1433.

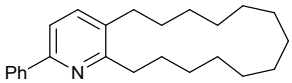


4-Phenyl-6,7,8,9-tetrahydro-5*H*-cyclohepta[*b*]pyridine (3as, major): Pale yellow oil; yield = 39%; time = 24h; R_f = 0.30 (EtOAc/Hexane = 15:85); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (d, *J* = 5.1 Hz, 1H), 7.37 – 7.29 (m, 3H), 7.18 (d, *J* = 6.9 Hz, 2H), 6.91 (d, *J* = 5.1 Hz, 1H), 3.07 – 3.04 (m, 2H), 2.67 – 2.64 (m, 2H), 1.82-1.77 (m, 2H), 1.71 – 1.67 (m, 2H), 1.57-1.52 (m, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.0, 149.1, 145.2, 140.0, 135.7, 128.9, 128.4, 127.74, 122.79, 39.4, 32.3, 29.7, 27.8, 26.5 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{16}H_{18}N^+$ 224.1434, found 224.1443.

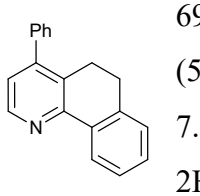


4-Phenyl-6,7,8,9,10,11,12,13,14,15,16,17-dodecahydro-5*H*-cyclopentadeca[*b*]pyridine (3at, major isomer): Yellow oil; yield = 48%; time = 30h; R_f = 0.22 (EtOAc/Hexane = 05:95); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.35 (d, *J* = 4.9 Hz, 1H), 7.41 – 7.33 (m, 3H), 7.24 - 7.22 (m, 2H), 6.90 (d, *J* = 4.9 Hz, 1H), 2.84 – 2.80 (m, 2H), 2.51 – 2.48 (m, 2H), 1.83 – 1.77 (m, 2H), 1.60 – 1.55 (m, 2H), 1.46 – 1.39 (m, 4H), 1.36 – 1.31 (m, 4H), 1.28 – 1.20 (m, 10H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.2, 150.3, 146.1, 140.4, 133.5, 128.4, 128.2, 127.6, 122.6, 35.3, 29.1, 29.0, 28.3, 27.7, 27.6, 26.9, 26.7, 26.5, 26.2, 26.1, 25.4, 25.2 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{24}H_{34}N^+$ 336.2686, found 336.2694.

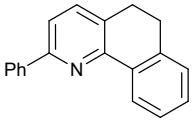
2-[Phenyl-6,7,8,9,10,11,12,13,14,15,16,17-dodecahydro-5*H*-cyclopentadeca[*b*]pyridine (4at, minor isomer):[5] Colorless solid; yield = 24%; mp 39-41 ℃; time = 30h; R_f = 0.69 (EtOAc/Hexane = 05:95); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 – 7.97 (m, 2H), 7.46 – 7.42 (m, 4H), 7.36 (t, *J* = 7.3 Hz, 1H), 2.88 – 2.84 (m, 2H), 2.65 – 2.62 (m, 2H), 1.86 – 1.80 (m, 2H), 1.67 – 1.61 (m, 2H), 1.59 – 1.55 (m, 2H), 1.54 – 1.48 (m, 2H), 1.44 – 1.42 (m, 4H), 1.38 – 1.34 (m, 10H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.3, 154.4, 140.0, 137.9, 134.2, 128.7, 128.4, 126.9, 118.0, 35.1, 32.3, 29.7, 28.2, 27.6, 27.5, 27.1, 27.0, 26.8, 26.17, 26.13, 25.7 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{24}H_{34}N^+$ 336.2686, found 336.2699.



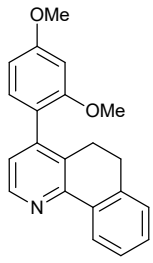
4-Phenyl-5,6-dihydrobenzo[*h*]quinoline (3au, major isomer):[1,5] Yellow solid; yield = 69%; mp 89-91 ℃; time = 24h; R_f = 0.45 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 (d, *J* = 4.9 Hz, 1H), 8.38 (d, *J* = 7.6 Hz, 1H), 7.49 – 7.32 (m, 7H), 7.23 (d, *J* = 7.3 Hz, 1H), 7.14 (d, *J* = 4.9 Hz, 1H), 2.92 (t, *J* = 7.0, 2H), 2.82 (t, *J* =6.9, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.1, 148.6, 147.2, 138.9, 138.2, 135.0, 129.5, 129.2, 128.8, 128.5, 128.1, 127.6, 127.2, 125.5, 123.4, 28.1, 25.5 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{19}H_{16}N^+$ 258.1277, found 258.1278.



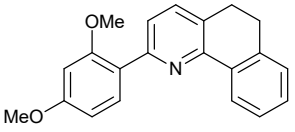
2-Phenyl-5,6-dihydrobenzo[*h*]quinoline (4au, minor isomer):[5,6] Pale yellow oil; yield = 14% ; time = 24h; R_f = 0.60 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.53 (d, *J* = 7.0 Hz, 1H), 8.16 – 8.14 (m, 2H), 7.61 – 7.55 (m, 2H), 7.50 (t, *J* = 7.5 Hz, 2H), 7.42 – 7.38 (m, 2H), 7.34 – 7.30 (m, 1H), 7.23 (d, *J* = 7.1 Hz, 1H), 2.98 – 2.95 (m, 4H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.2, 152.1, 139.7, 138.3, 136.4, 134.9, 130.4, 129.1, 128.7, 127.8, 127.2, 126.9, 125.4, 118.8, 28.2, 27.9 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{19}H_{16}N^+$ 258.1277, found 258.1260.



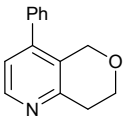
4-(2,4-Dimethoxyphenyl)-5,6-dihydrobenzo[*h*]quinoline (3du, major isomer): Colorless oil; yield =68%; time = 30h; R_f = 0.58 (EtOAc/Hexane = 15:85); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.46 (d, *J* = 4.9 Hz, 1H), 8.28 (d, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.23 (t, *J* = 7.3 Hz, 1H), 7.13 (d, *J* = 7.3 Hz, 1H), 7.05 (d, *J* = 8.3 Hz, 1H), 6.99 (d, *J* = 4.9 Hz, 1H), 6.52 (dd, *J* = 8.3, 2.2 Hz, 1H), 6.49 (d, *J* = 2.1 Hz, 1H), 3.80 (s, 3H), 3.67 (s, 3H), 2.73-2.71 (m, 3H), 2.61 – 2.57 (m, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.2, 157.6, 152.4, 147.0, 145.7, 138.5, 135.2, 131.5, 131.1, 129.0, 127.5, 127.2, 125.5, 124.3, 120.7, 104.6, 98.7, 55.6, 55.5, 28.1, 25.4 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{21}H_{20}NO_2^+$ 318.1489, found 318.1495.



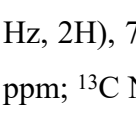
2-(2,4-Dimethoxyphenyl)-5,6-dihydrobenzo[*h*]quinoline (4du): Pale yellow oil; yield = 10%; time = 30h; R_f = 0.69 (EtOAc/Hexane = 15:85); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.46 (d, *J* = 7.5 Hz, 1H), 8.01 (d, *J* = 8.5 Hz, 1H), 7.71 (d, *J* = 7.9 Hz, 1H), 7.50 (d, *J* = 7.9 Hz, 1H), 7.36 (t, *J* = 7.1 Hz, 1H), 7.31 – 7.28 (m, 1H), 7.23 (d, *J* = 7.3 Hz, 1H), 6.67 (dd, *J* = 8.5, 2.3 Hz, 1H), 6.57 (d, *J* = 2.3 Hz, 1H), 3.88 (s, 3H), 3.87 (s, 3H), 2.96 (s, 4H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.1, 158.3, 153.4, 151.6, 138.0, 135.3, 132.1, 129.2, 128.7, 127.6, 127.0, 125.1, 123.2, 105.1, 98.9, 55.6, 55.4, 28.2, 27.7 ppm; HRMS (ESI-TOF): *m/z* [M + H]$^+$ calcd for $C_{21}H_{20}NO_2^+$ 318.1489, found 318.1496.



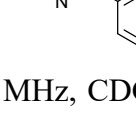
4-Phenyl-7,8-dihydro-5*H*-pyrano[4,3-*b*]pyridine (3aw, minor isomer):[10] Yellow oil; yield = 25%; time = 30h; R_f = 0.16 (EtOAc/Hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41 (d, *J* = 4.9 Hz, 1H), 7.39 – 7.34 (m, 4H), 7.20 (bs, 1H), 6.97 (d, *J* = 4.9 Hz, 1H), 4.60 (s, 2H), 4.03 (t, *J* = 5.9 Hz, 2H), 3.05 (t, *J* = 5.9 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.9, 147.6, 147.3, 137.6, 128.8, 128.5, 128.29, 128.25 122.4, 66.5, 65.8, 32.0 ppm; HRMS (ESI-TOF): *m/z* [M + H]$^+$ calcd for $C_{14}H_{14}NO^+$ 212.1070, found 212.1068.



2-Phenyl-7,8-dihydro-5*H*-pyrano[4,3-*b*]pyridine (4aw, major isomer): Yellow oil; yield = 47%; time = 30h; R_f = 0.70 (EtOAc/Hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.4 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.41 – 7.36 (m, 2H), 4.81 (s, 2H), 4.11 (t, *J* = 5.8 Hz, 2H), 3.11 (t, *J* = 5.7 Hz, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.9, 153.6, 139.5, 133.1, 128.9, 128.8, 127.0 (2C, one overlap peak), 118.4, 67.2, 65.9, 32.1 ppm; HRMS (ESI-TOF): *m/z* [M + H]$^+$ calcd for $C_{14}H_{14}NO^+$ 212.1070, found 212.1072.



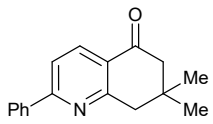
4-phenyl-5*H*-chromeno[4,3-*b*]pyridine (3av, major isomer): Pale yellow solid; yield = 66% ; time = 30h; R_f = 0.62 (EtOAc/Hexane = 15:85); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (d, *J* = 5.0 Hz, 1H), 8.29 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.52 – 7.43 (m, 3H), 7.32 (ddd, *J* = 10.8, 8.2, 4.0 Hz, 3H), 7.17 (d, *J* = 5.0 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 6.96 (d, *J* = 8.1 Hz, 1H), 5.22 (s, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.5, 149.3, 149.0, 146.8, 137.3, 131.5, 128.9, 128.8, 128.6, 125.2, 124.0, 123.8, 123.5, 122.7, 117.0, 66.0 ppm; HRMS (ESI-TOF): *m/z* [M + H]$^+$ calcd for $C_{18}H_{14}NO^+$ 260.1070, found 260.1082.



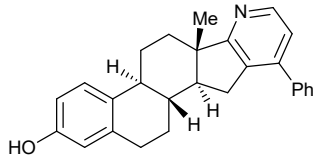
2-Phenyl-5*H*-chromeno[4,3-*b*]pyridine (4av, minor isomer): Pale yellow oil; yield = 13% ; time = 30h; R_f = 0.70 (EtOAc/Hexane = 15:85); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (dd, *J* = 7.7, 1.3 Hz, 1H), 8.13 (d, *J* = 7.4 Hz, 2H), 7.64 (d, *J*

= 7.9 Hz, 1H), 7.51 – 7.48 (m, 3H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.34 – 7.31 (m, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 6.98 (d, *J* = 8.1 Hz, 1H), 5.27 (s, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9, 156.6, 148.4, 139.3, 132.9, 131.3, 129.2, 128.8, 127.0, 125.0, 124.5, 123.5, 122.4, 119.1, 117.0, 68.0 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{18}H_{14}NO^+$ 260.1070, found 260.1071.

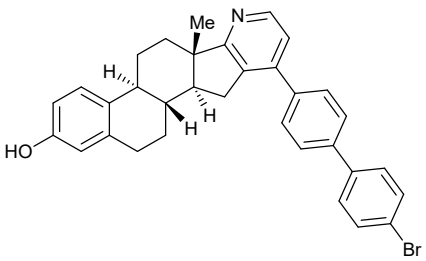
7,7-Dimethyl-2-phenyl-7,8-dihydroquinolin-5(6*H*)-one (4azz):[8] Colorless solid; yield = 81%; mp 58-60 ℃; time = 24h; R_f = 0.38 (EtOAc/Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.2 Hz, 1H), 8.03 (dd, *J* = 8.1, 1.4 Hz, 2H), 7.66 (d, *J* = 8.2 Hz, 1H), 7.47 – 7.40 (m, 3H), 3.08 (s, 2H), 2.53 (s, 2H), 1.11 (s, 6H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.8, 162.4, 161.0, 138.4, 135.3, 129.9, 128.8, 127.4, 125.5, 118.8, 52.0, 46.7, 32.9, 28.3 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{17}H_{18}NO^+$ 252.1383, found 252.1383.



(6b*S*,8a*S*,13a*S*,13b*R*)-8a-Methyl-12-phenyl-2,6b,7,8,8a,13,13a,13b-octahydro-1*H*-naphtho[2′,1′:4,5]indeno[1,2-*b*]pyridin-4-ol (3ax): Pale yellow solid; yield = 68% ; mp 211-213 ℃; time = 30h; R_f = 0.47 (EtOAc/Hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, *J* = 5.3 Hz, 1H), 7.51 – 7.42 (m, 5H), 7.17 (t, *J* = 7.2 Hz, 2H), 6.71 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.64 (d, *J* = 2.0 Hz, 1H), 2.94 – 2.79 (m, 4H), 2.52–2.44 (m, 2H), 2.36 –2.32 (m, 1H), 2.00 –1.96 (m, 1H), 1.86 – 1.67 (m, 4H), 1.48 –1.39 (m, 1H), 1.14 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.5, 154.5, 146.6, 146.4, 138.3, 137.8, 134.3, 131.7, 128.7, 128.5, 128.3, 126.2, 120.9, 115.5, 113.0, 55.1, 46.2, 44.3, 37.6, 33.7, 30.3, 29.5, 27.4, 26.3, 17.6 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{27}H_{28}NO^+$ 382.2165 , found 382.2163.

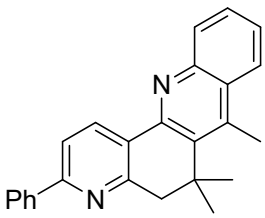


(6b*S*,8a*S*,13a*S*,13b*R*)-12-(4′-Bromo-[1,1′-biphenyl]-4-yl)-8a-methyl-2,6b,7,8,8a,13,13a,13b-octahydro-1*H*-naphtho[2′,1′:4,5]indeno[1,2-*b*]pyridin-4-ol (3ix): Yellow solid; yield =71%; mp 220-222 ℃; time = 30h; R_f = 0.43 (EtOAc/Hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (d, *J* = 5.0 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.60 (t, *J* = 8.7 Hz, 4H), 7.52 (d, *J* = 8.3 Hz, 2H), 7.20 - 7.17 (m, 2H), 6.69 (d, *J* = 8.1 Hz, 1H), 6.62 (s, 1H), 6.41 (br s, 1H), 2.91 – 2.82 (m, 4H), 2.48

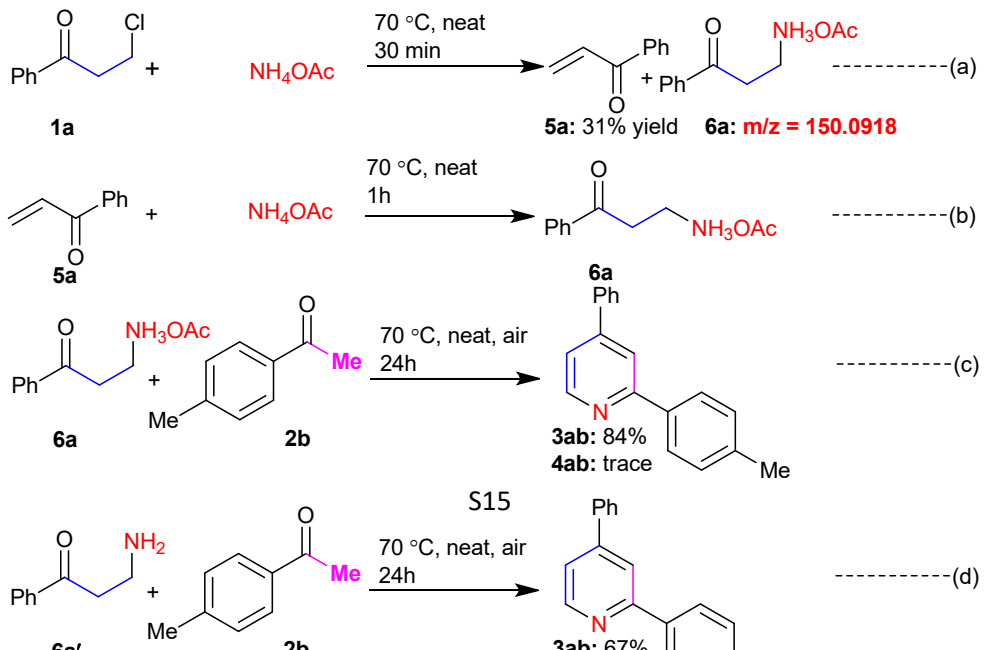


(d, *J* = 10.2 Hz, 2H), 2.37 - 2.33 (m, 1H), 2.01 – 2.00 (m, 1H), 1.86 – 1.72 (m, 4H), 1.49 – 1.40 (m, 1H), 1.15 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.8, 154.2, 147.1, 145.8, 140.3, 139.5, 138.2, 137.9, 134.3, 132.4, 132.3, 129.1, 128.9, 127.4, 126.5, 122.2, 120.9, 115.6, 113.1, 55.4, 46.4, 44.6, 37.8, 34.0, 30.6, 29.7, 27.6, 26.5, 17.8 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{33}H_{31}{}^{79}BrNO^+$ 536.1584, found 536.1586. HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{33}H_{31}{}^{81}BrNO^+$ 538.1569, found 538.1574.

6,6,7-Trimethyl-3-phenyl-5,6-dihydrobenzo[*b*][1,7]phenanthroline: Colorless solid; yield = 61%; mp 141-143 °C; time = 30h; R_f = 0.48 (EtOAc/ Hexane = 10:90); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.71 (d, *J* = 8.0 Hz, 1H), 8.10-8.05 (m, 4H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.67 (t, *J* = 7.3 Hz, 1H), 7.54 – 7.48 (m, 3H), 7.43 (t, *J* = 7.1 Hz, 1H), 3.18 (s, 2H), 2.88 (s, 3H), 1.61 (s, 6H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.8, 157.2, 151.2, 146.5, 141.6, 139.5, 136.5, 135.0, 129.8, 129.2, 129.1, 128.9, 128.8, 128.7, 127.2, 126.3, 123.6, 119.8, 49.4, 37.5, 28.4, 18.0 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_{25}H_{23}N_2^+$ 351.1856, found 351.1860.



3-Bromo-1-phenylpropan-1-one:[12] White solid; mp 47-50°C; R_f = 0.73 (EtOAc/Hexane = 15:85); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 – 7.94 (m, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 3.74 (t, *J* = 6.9 Hz, 2H), 3.58 (t, *J* = 6.9 Hz, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.1, 136.3, 133.7, 128.8, 128.1, 41.6, 25.8 ppm; HRMS (ESI-TOF): *m/z* $[M + Na]^+$ calcd for $C_9H_9{}^{79}BrONa^+$ 234.9729, found 234.9725; HRMS (ESI-TOF): *m/z* $[M + Na]^+$ calcd for $C_9H_9{}^{81}BrONa^+$ 236.9709, found 236.9699.



Scheme S1. Control experiment:

Scheme S1a: A mixture of compounds **1a** (1.0 mmol), **2a** (1.2 mmol) and NH_4OAc (2.5 mmol) was heated at 70 °C for 30 min. Afterwards, we have recorded the MS for the crude reaction mixture in MeCN. The MS indicated that both compounds **5a** and **6a**: (m/z = 150.0918) were formed. Next, the crude reaction mixture was extracted with ether (3 × 10 mL) and dried over Na_2SO_4. Evaporation of the solvent left the crude product which was purified by column chromatography over silica-gel using a mixture of diethyl ether/hexane (1:10) as an eluent give 31% yield of vinyl ketone **5a**.

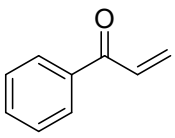
Scheme S1b: A mixture of compounds **5a** (0.1 mmol) and NH_4OAc (2.5 mmol) was heated at 70 °C for 1h. Afterwards, we have recorded the MS for the crude reaction mixture in MeCN. The mass value indicated that **6a**: (m/z = 150.0918) was formed. It is not possible to isolate this product.

Scheme S1c: The white solid compound **6a** (0.2 mmol, prepared by 1:1 mixture of β-amino ketone **6a′**[14] and AcOH) was treated with **2b** (0.24 mmol) under standard conditions in an open-atmosphere. After usual work-up, the desired pyridine derivative **3ab** in 84% yield was purified through column chromatography over silica gel using a mixture of EtOAc/hexane (1:19, v/v) as the eluent. The product was fully characterized by its spectroscopic data (^{1}HNMR, ^{13}C NMR, and HRMS).

Scheme S1d: The yellowish liquid compound **6a′** (0.2 mmol) was treated with **2b** (0.24 mmol) under standard conditions in an open atmosphere. After usual work-up, the desired pyridine derivative **3ab** in 67% yield was purified through column chromatography over silica gel using a mixture of EtOAc/hexane (1:19, v/v) as the eluent.

Scheme S1e: A mixture of vinyl ketone **5a** (0.2 mmol), ketone **2b** (0.24 mmol) and NH_4OAc (0.5 mmol) was heated at 70 °C for 24 h in an open atmosphere. After that, the desired pyridine derivative **3ab** in 73% yield was isolated by using purification technique as described in Scheme S1c.

1-Phenylprop-2-en-1-one:[13] Colorless liquid; R_f = 0.66 (EtOAc/Hexane = 10:90); ^1H NMR



(500 MHz, $CDCl_3$) δ 7.92-7.90 (m, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.13 (dd, *J* = 17.1, 10.6 Hz, 1H), 6.41 (dd, *J* = 17.1, 1.6 Hz, 1H), 5.89 (dd, *J* = 10.6, 1.6 Hz, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.9, 137.2, 132.9, 132.3, 130.0, 128.6, 128.62 ppm; HRMS (ESI-TOF): *m/z* $[M + H]^+$ calcd for $C_9H_8O^+$ 133.0648, found 133.0665.

1-Phenylpropanone-3-ammonium acetate (6a): Colorless solid: ^1H NMR (500 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.5 Hz, 2H), 7.54-7.56 (m, 1H), 7.43-7.46 (m, 2H), 6.23 (br s, 3H), 3.24-3.32 (m, 4H), 1.87 (s, 3H) ppm; HRMS (ESI-TOF): *m/z* $[M]^+$ calcd for $C_9H_{12}NO^+$ 150.0913, found 150.0918.

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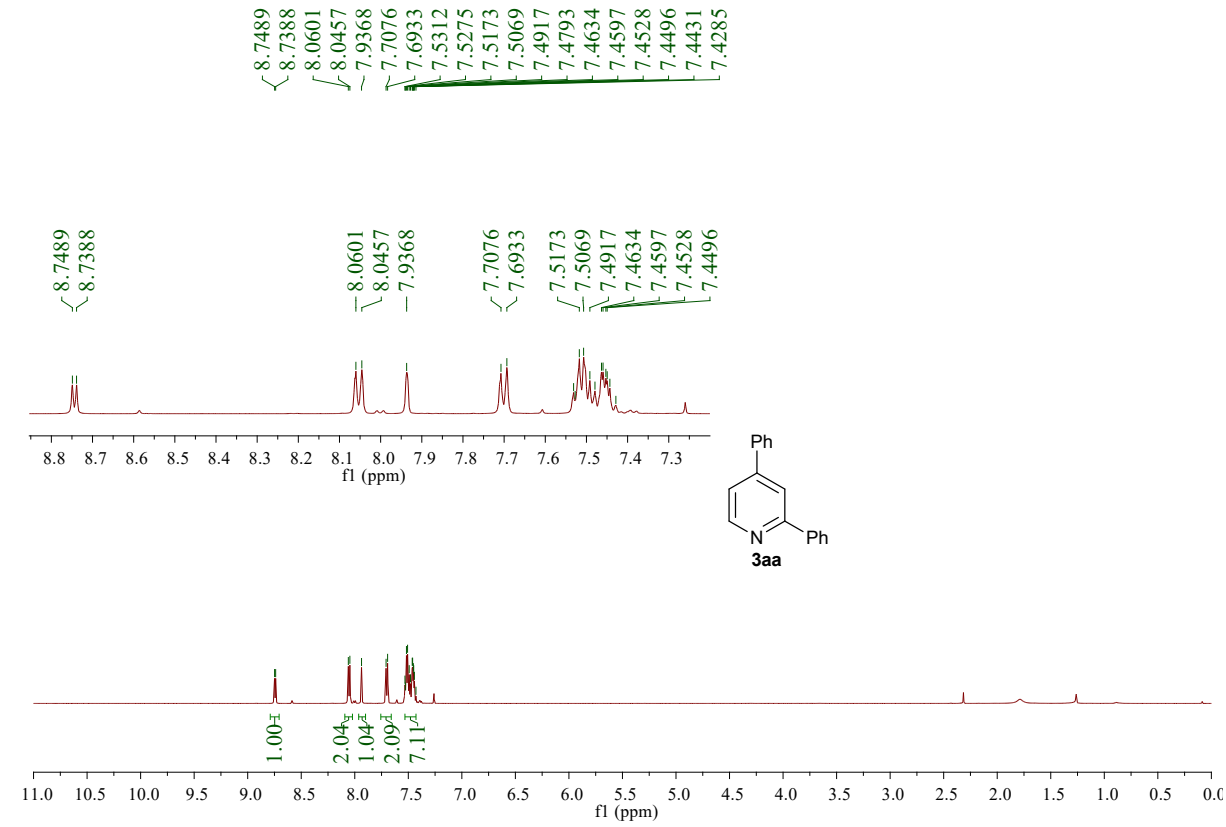

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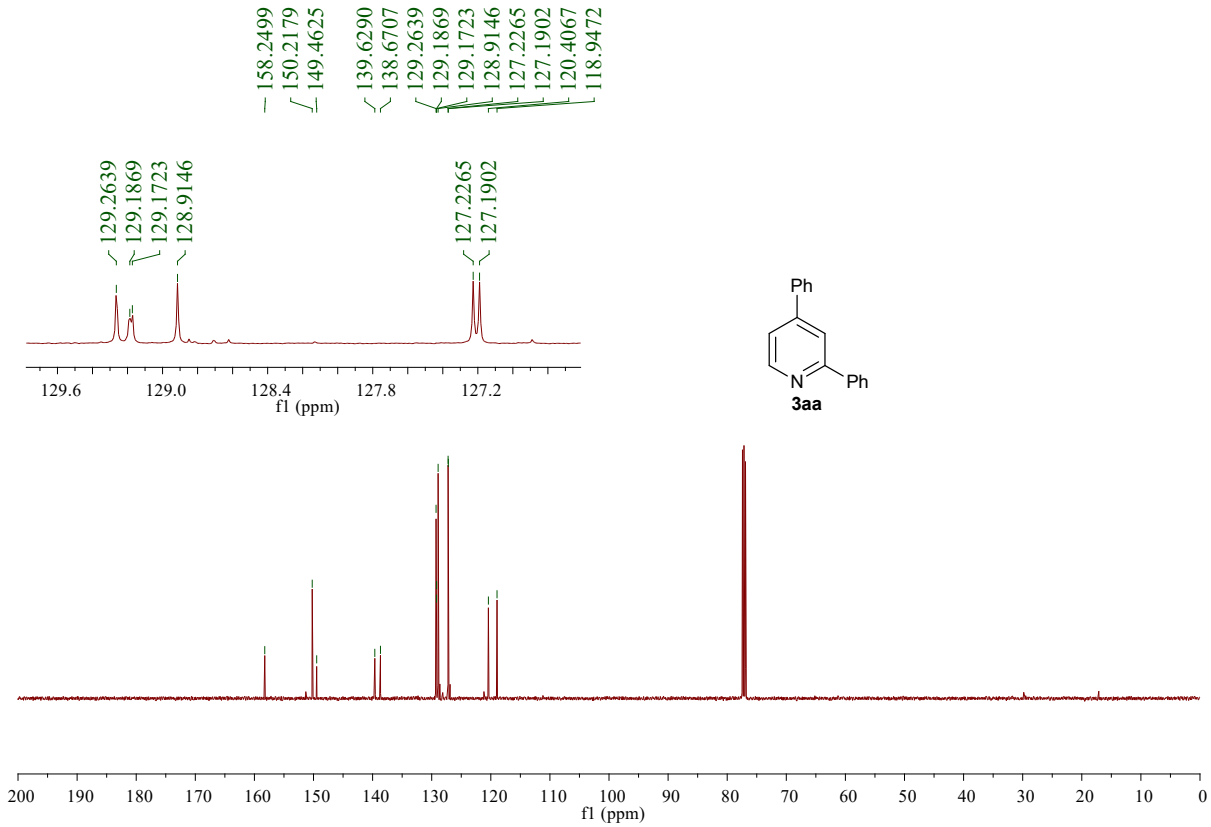
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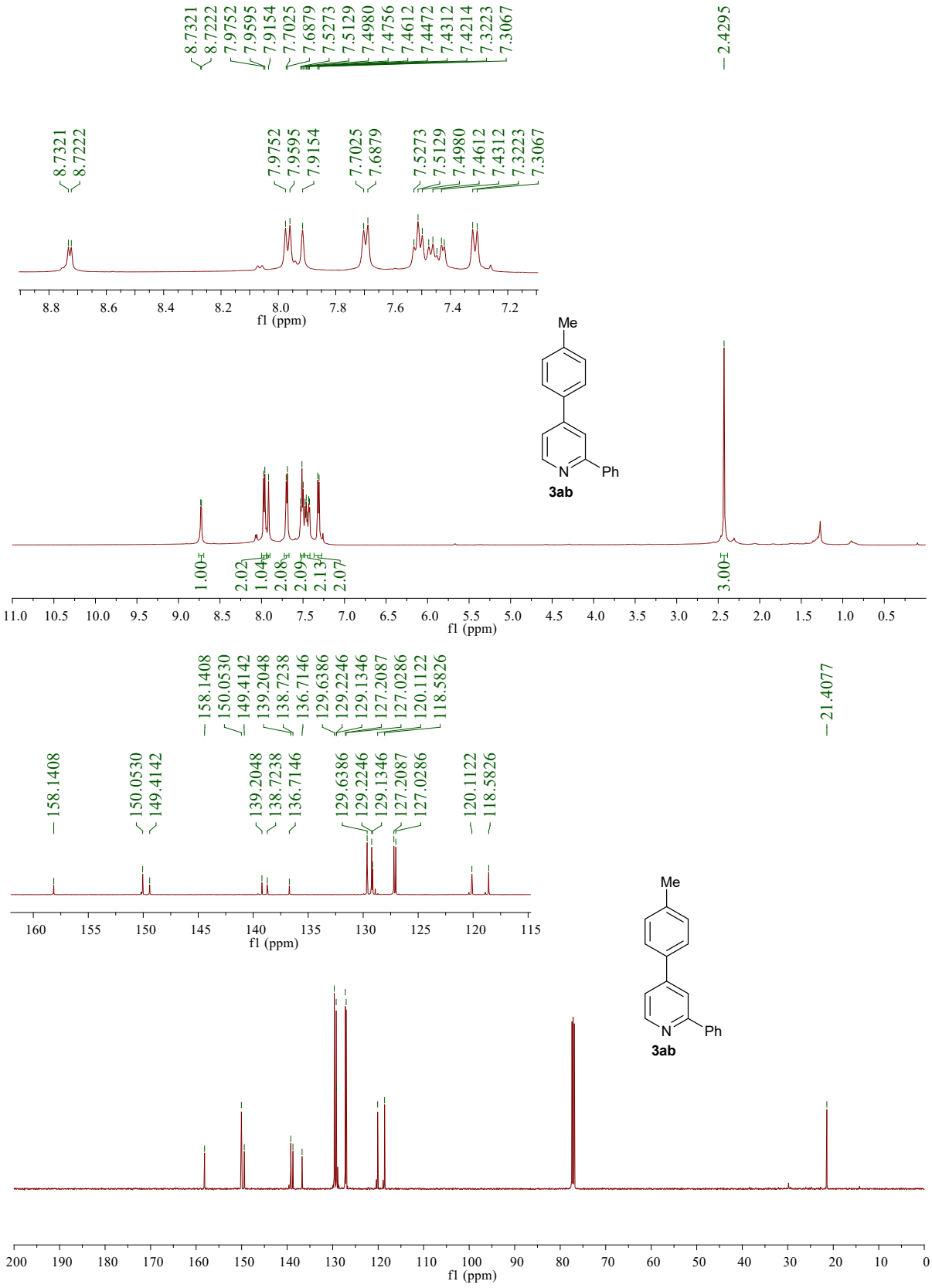
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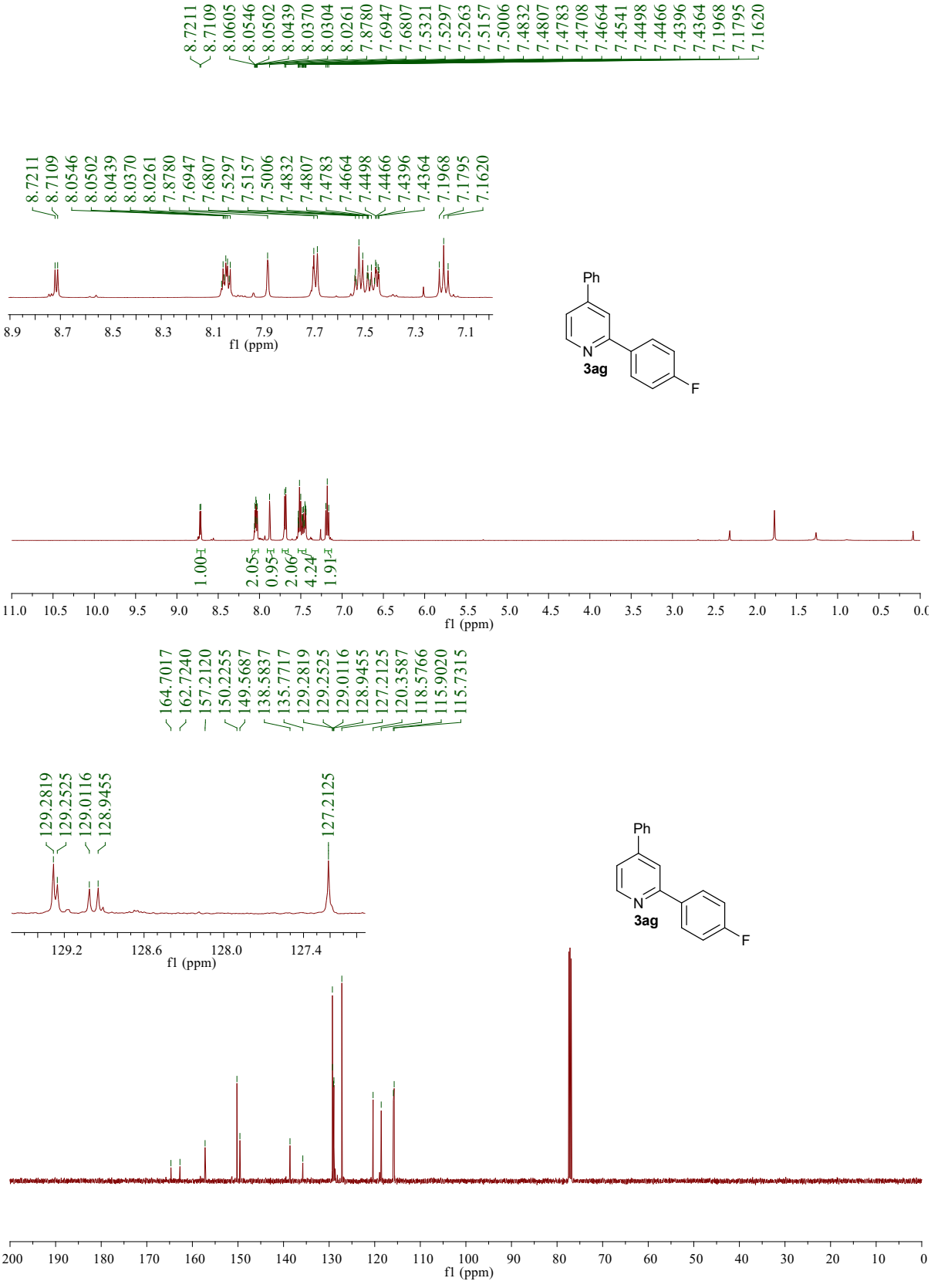
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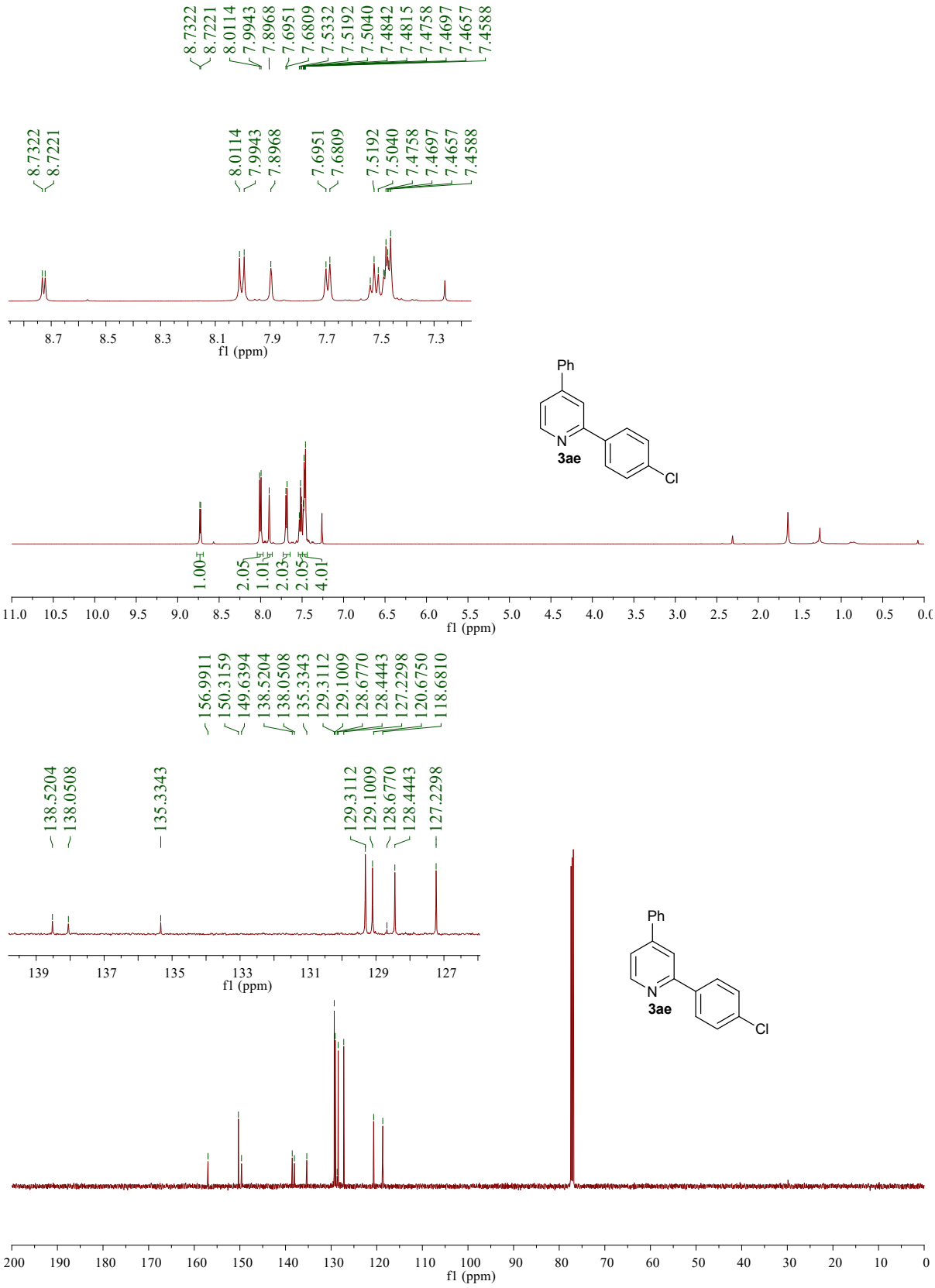
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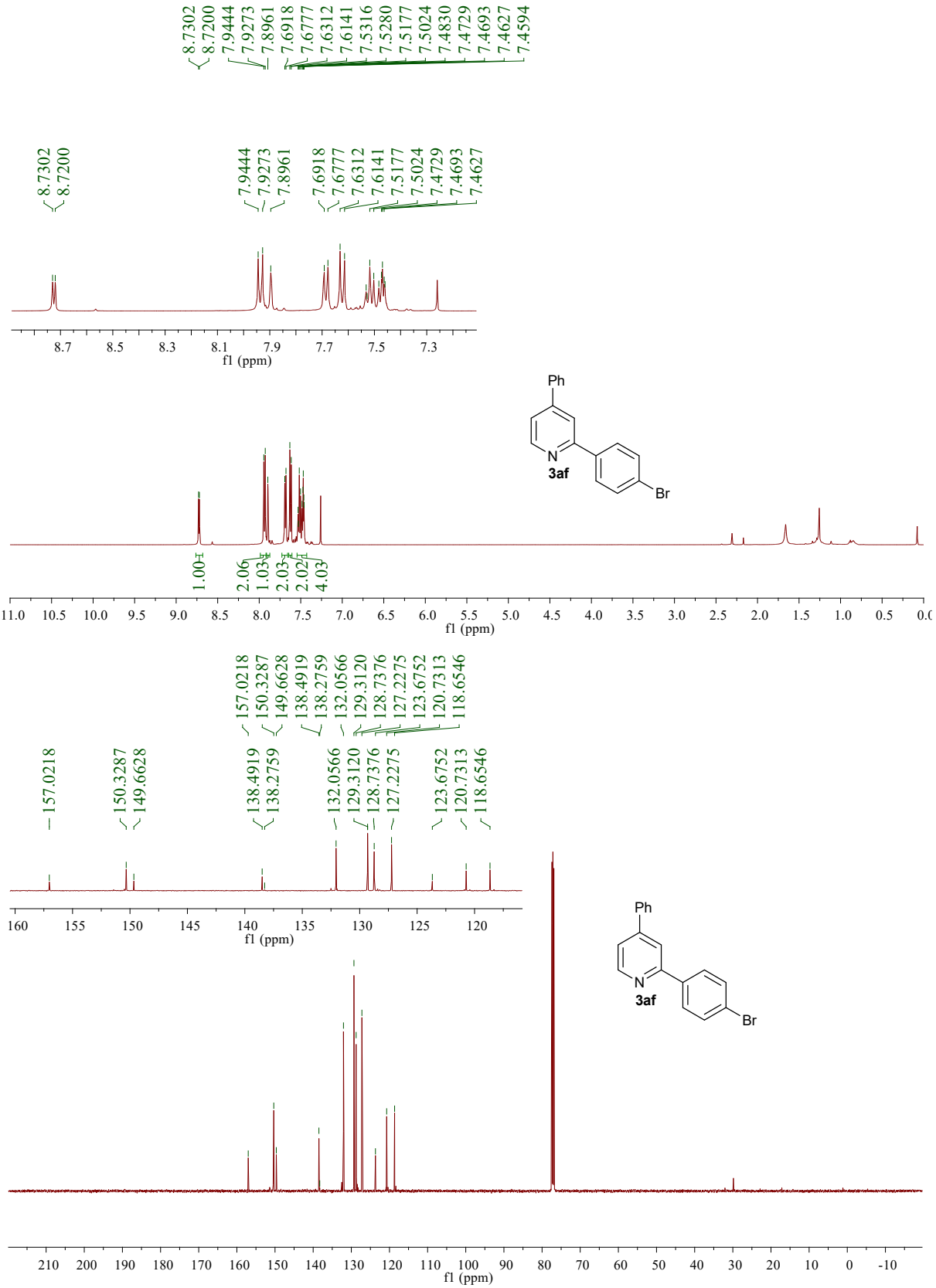
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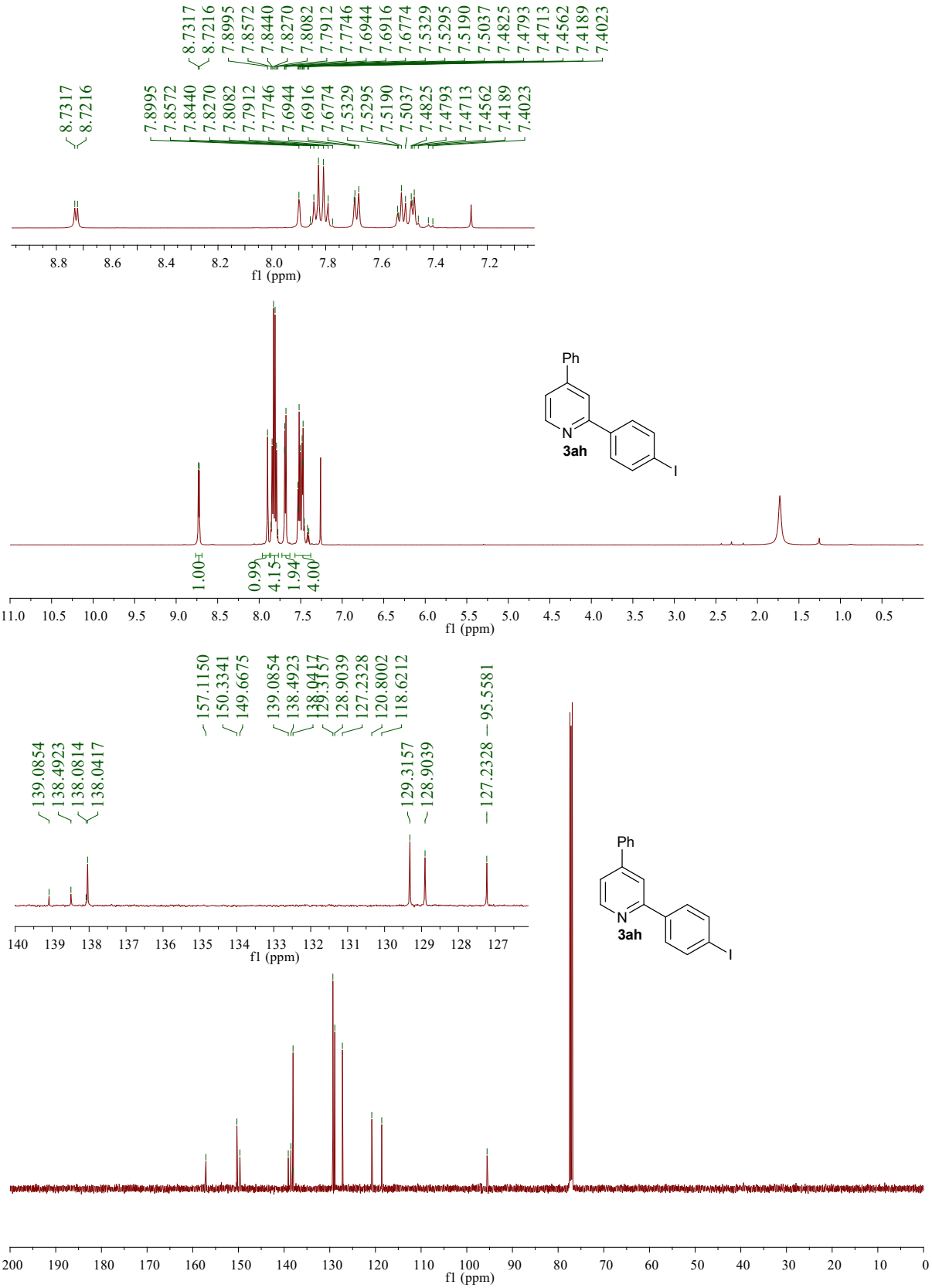
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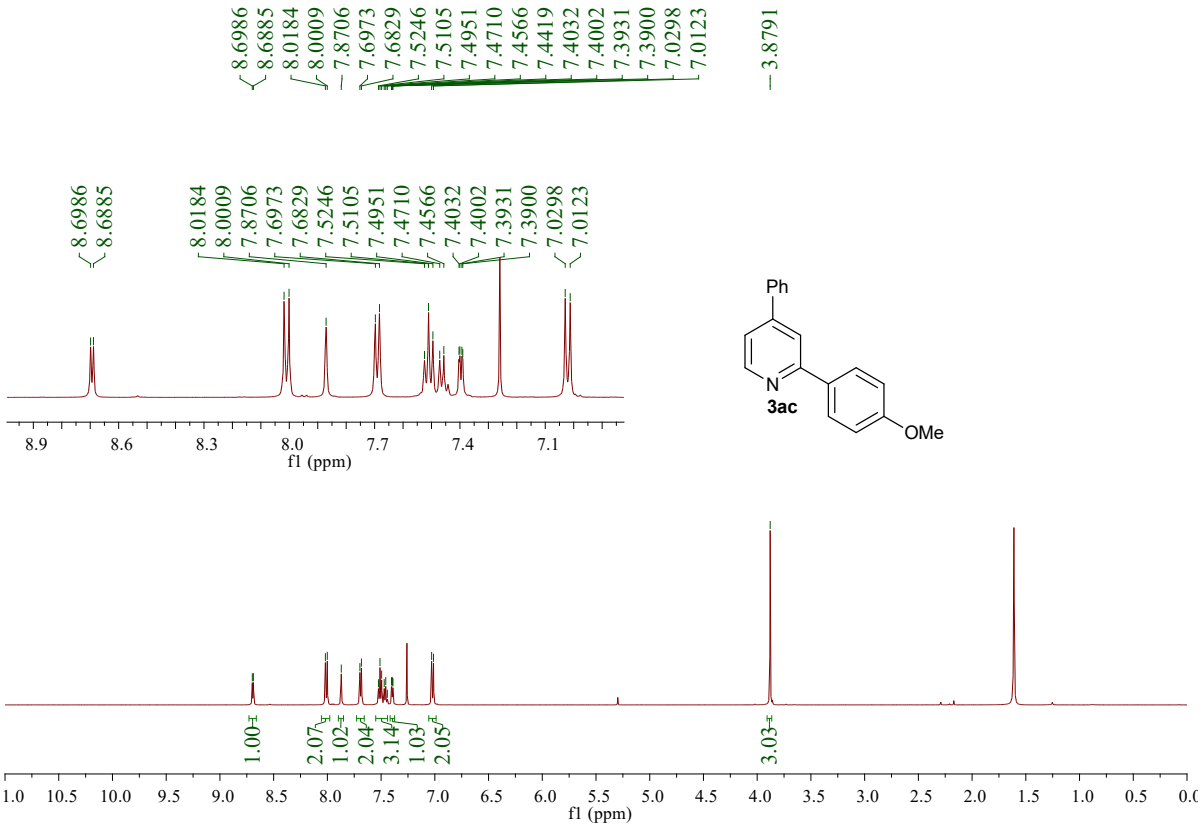
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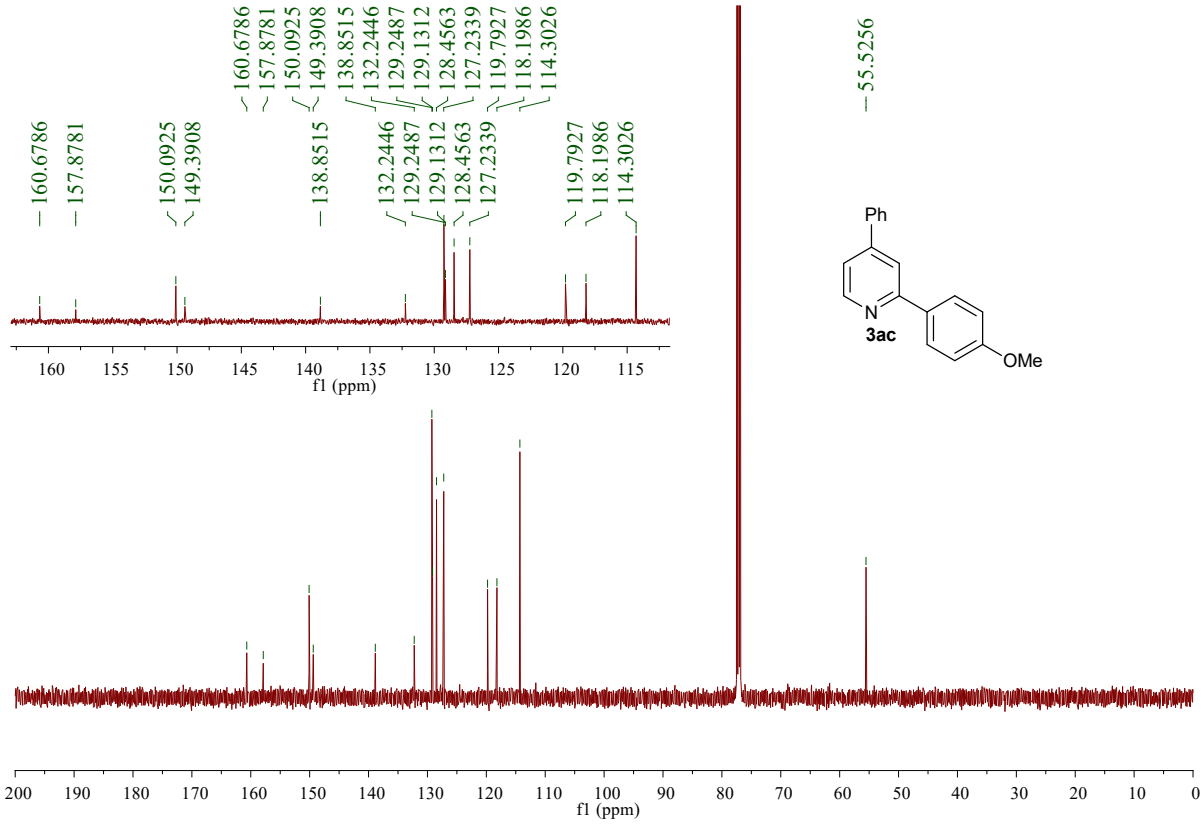
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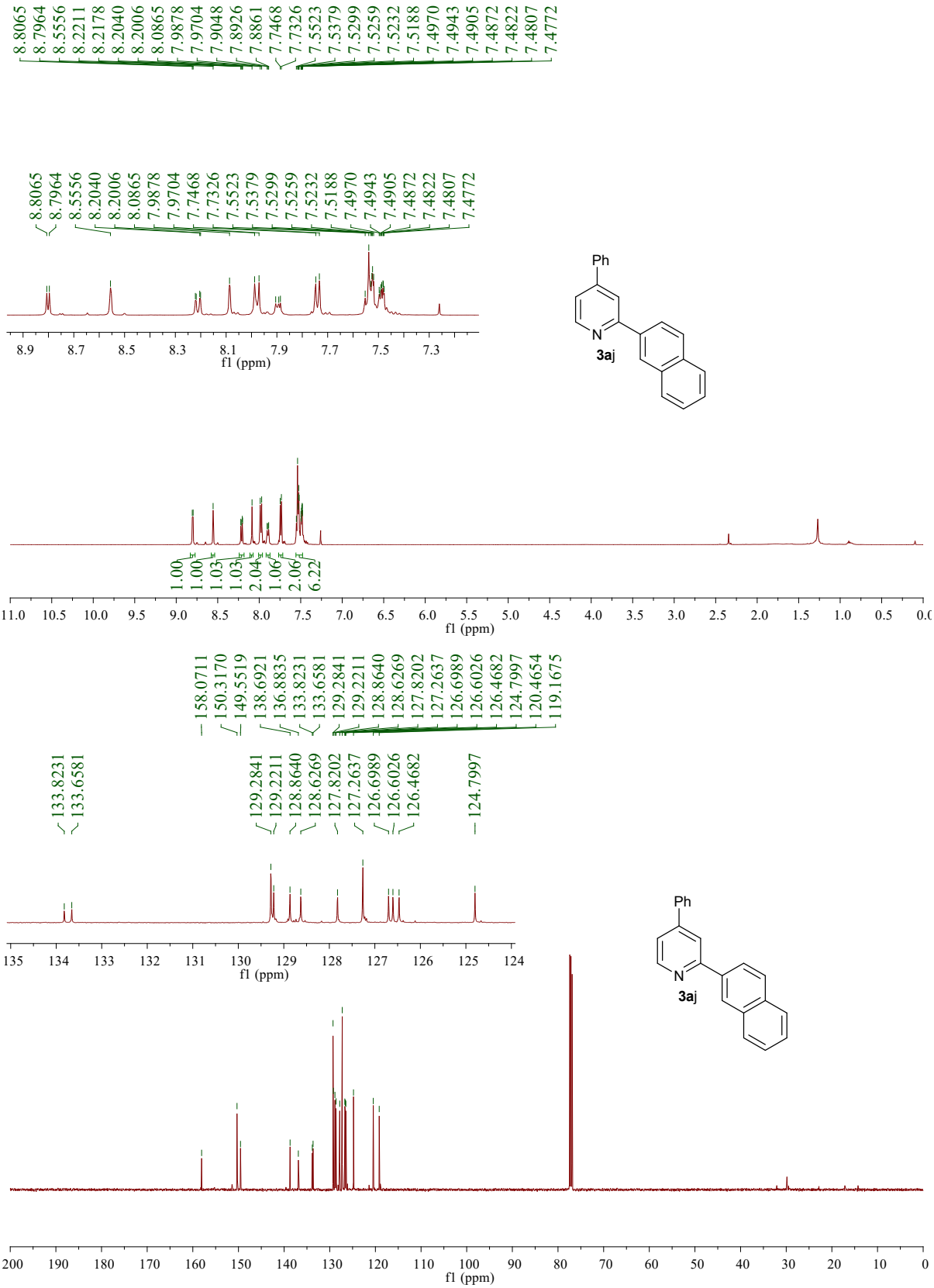
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8.2211
8.2178
8.2040
8.2006
8.0865
7.9878
7.9704
7.9048
7.8926
7.8861
7.7468
7.7326
7.5523
7.5379
7.5299
7.5259
7.5232
7.5188
7.4970
7.4943
7.4905
7.4872
7.4822
7.4807
7.4772
fl (ppm)
Ph
N
3aj
1.00
1.00
1.03
1.03
2.04
1.06
2.06
6.22
158.0711
150.3170
149.5519
138.6921
136.8835
133.8231
133.6581
129.2841
129.2211
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127.8202
127.2637
126.6989
126.6026
126.4682
124.7997
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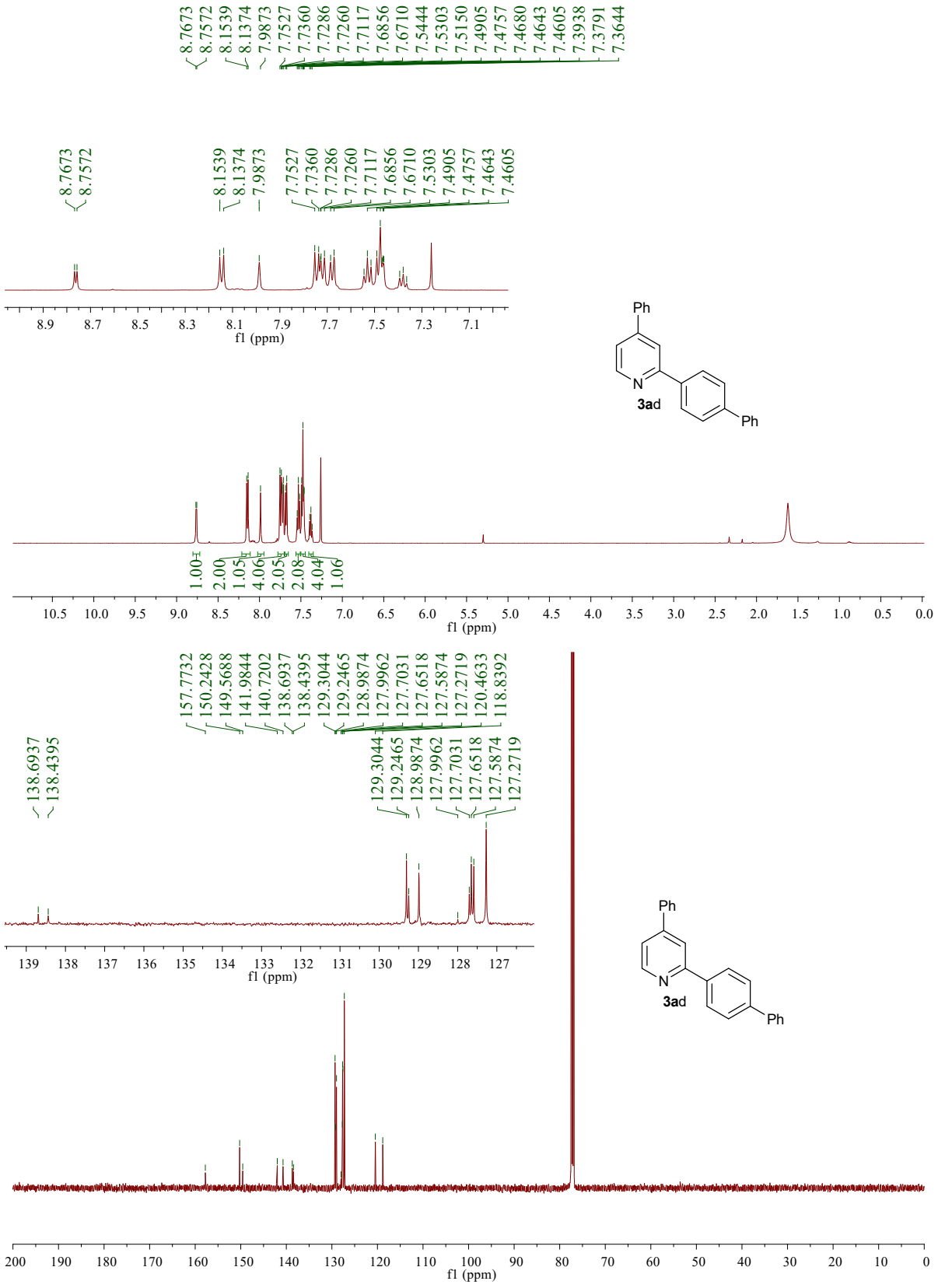
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8.1539
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7.9873
7.7527
7.7360
7.7286
7.7260
7.7117
7.6856
7.6710
7.5444
7.5303
7.5150
7.4905
7.4757
7.4680
7.4643
7.4605
7.3938
7.3791
7.3644
f1 (ppm)
Ph
N
3ad
Ph
1.00
2.00
1.05
4.06
2.05
2.08
4.04
1.06
157.7732
150.2428
149.5688
141.9844
140.7202
138.6937
138.4395
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127.5874
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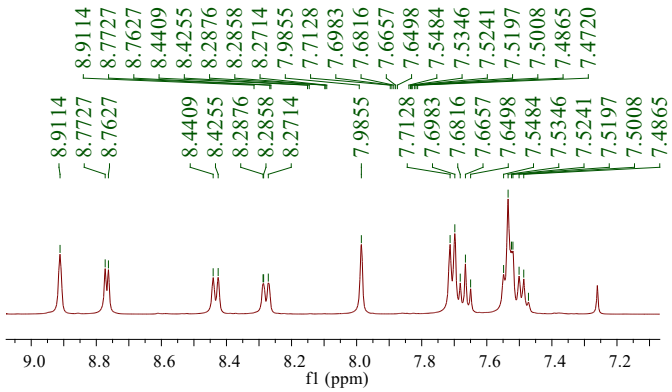
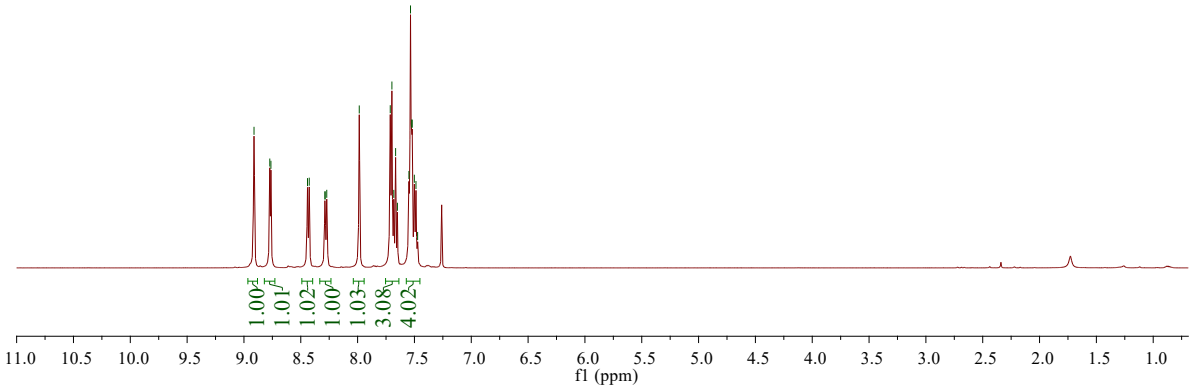
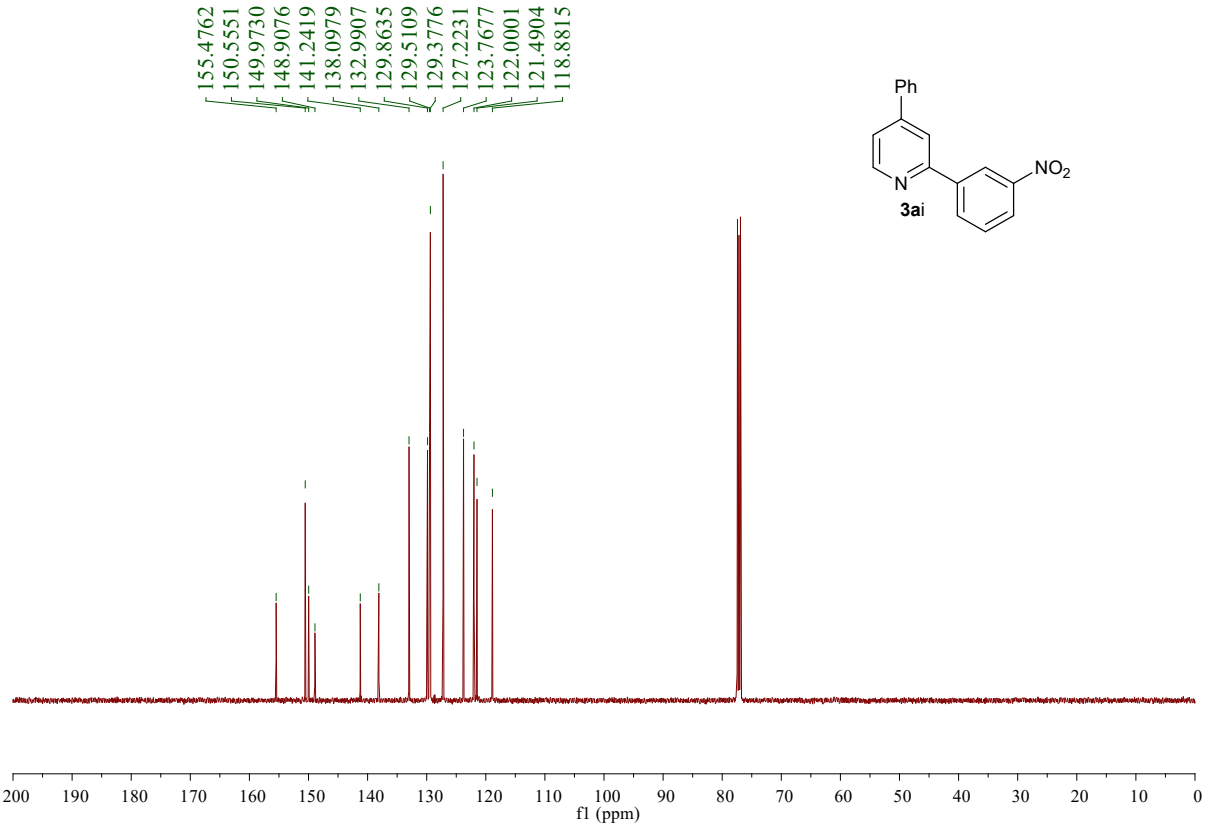
120.4633
118.8392

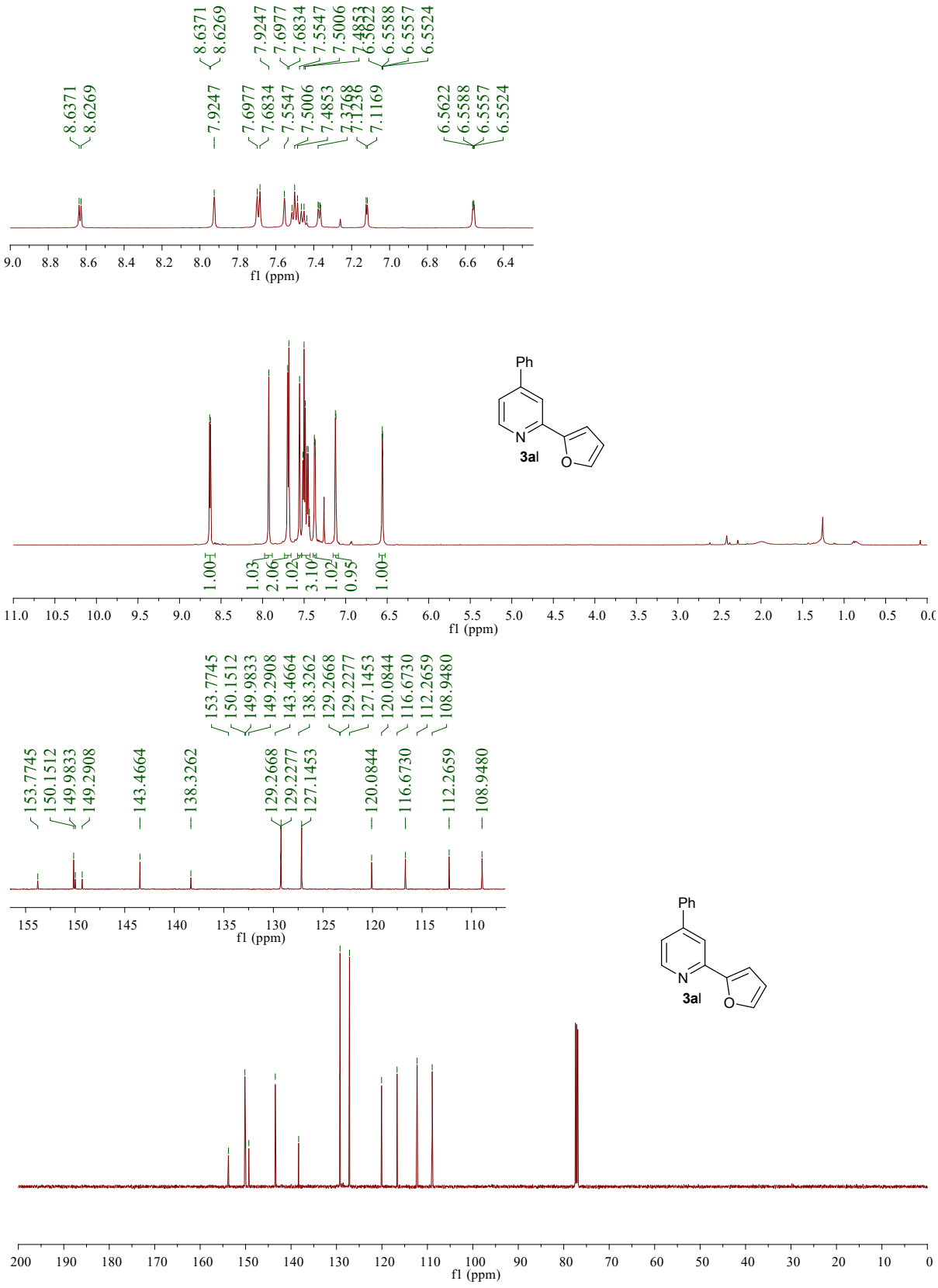

8.9114
8.7727
8.7627
8.4409
8.4255
8.2876
8.2858
8.2714
7.9855
7.7128
7.6983
7.6816
7.6657
7.6498
7.5484
7.5346
7.5241
7.5197
7.5008
7.4865
7.4720
9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2
f1 (ppm)

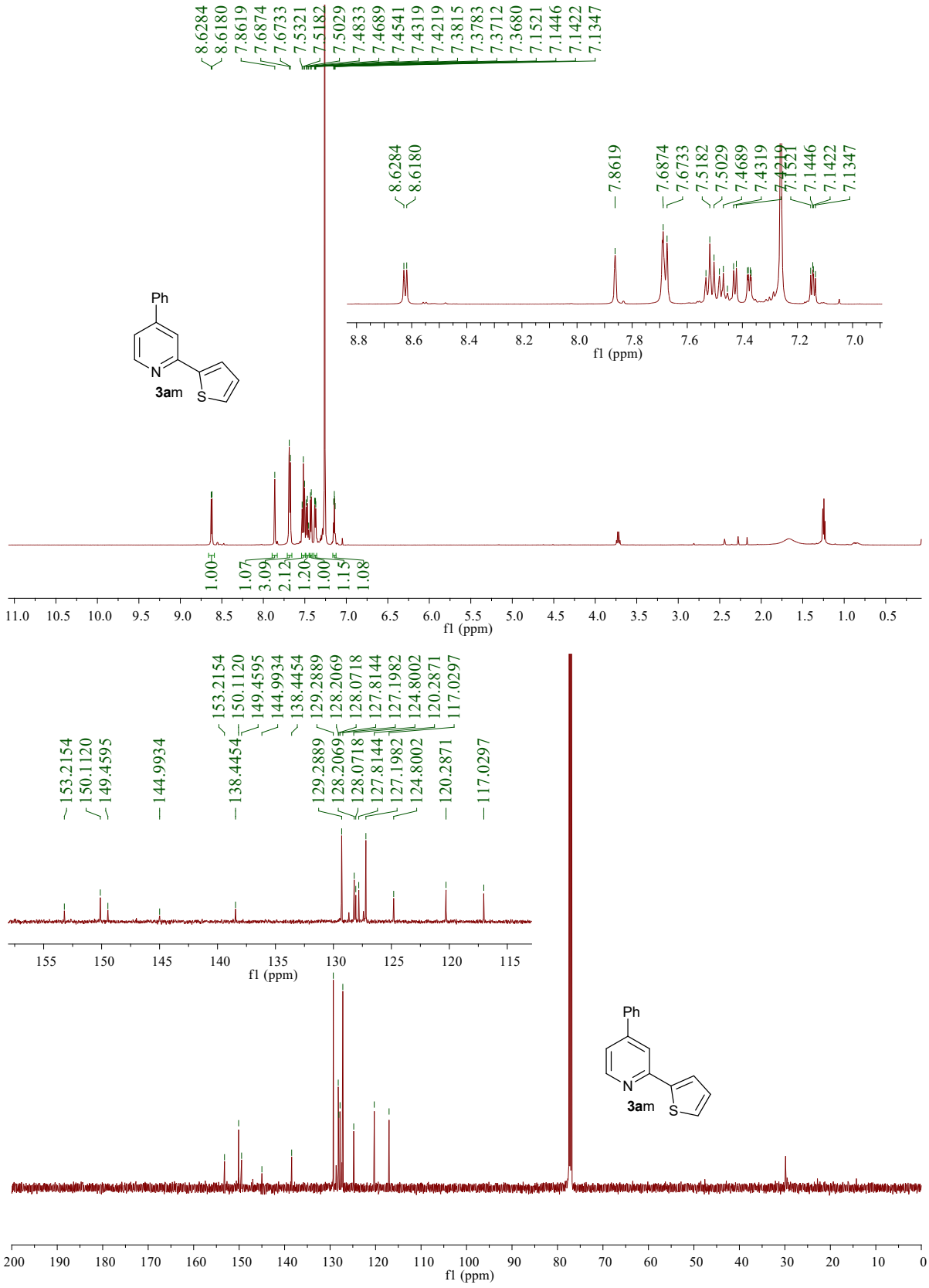

1.00
1.01
1.02
1.00
1.03
3.08
4.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)

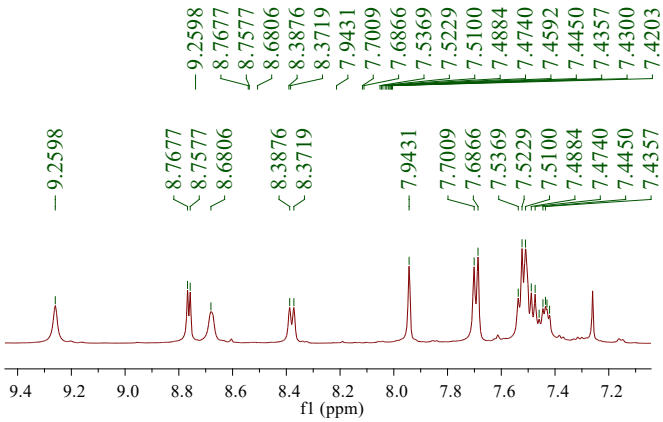

155.4762
150.5551
149.9730
148.9076
141.2419
138.0979
132.9907
129.8635
129.5109
129.3776
127.2231
123.7677
122.0001
121.4904
118.8815
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

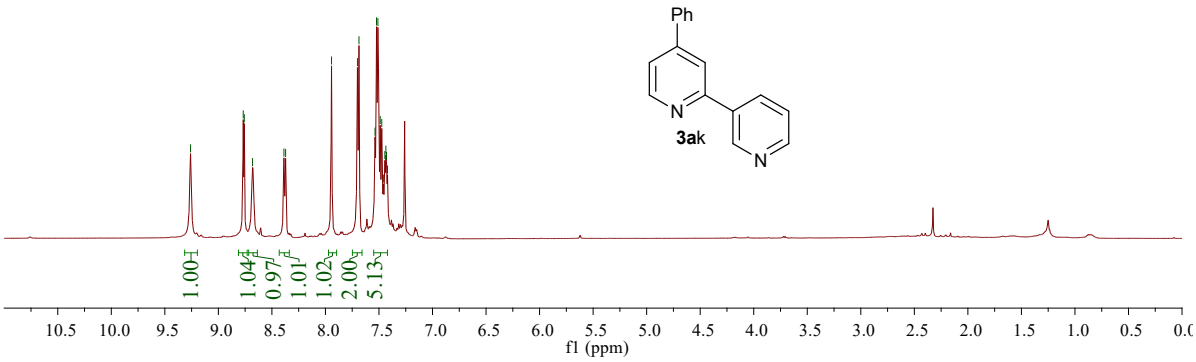
Ph
N
NO2

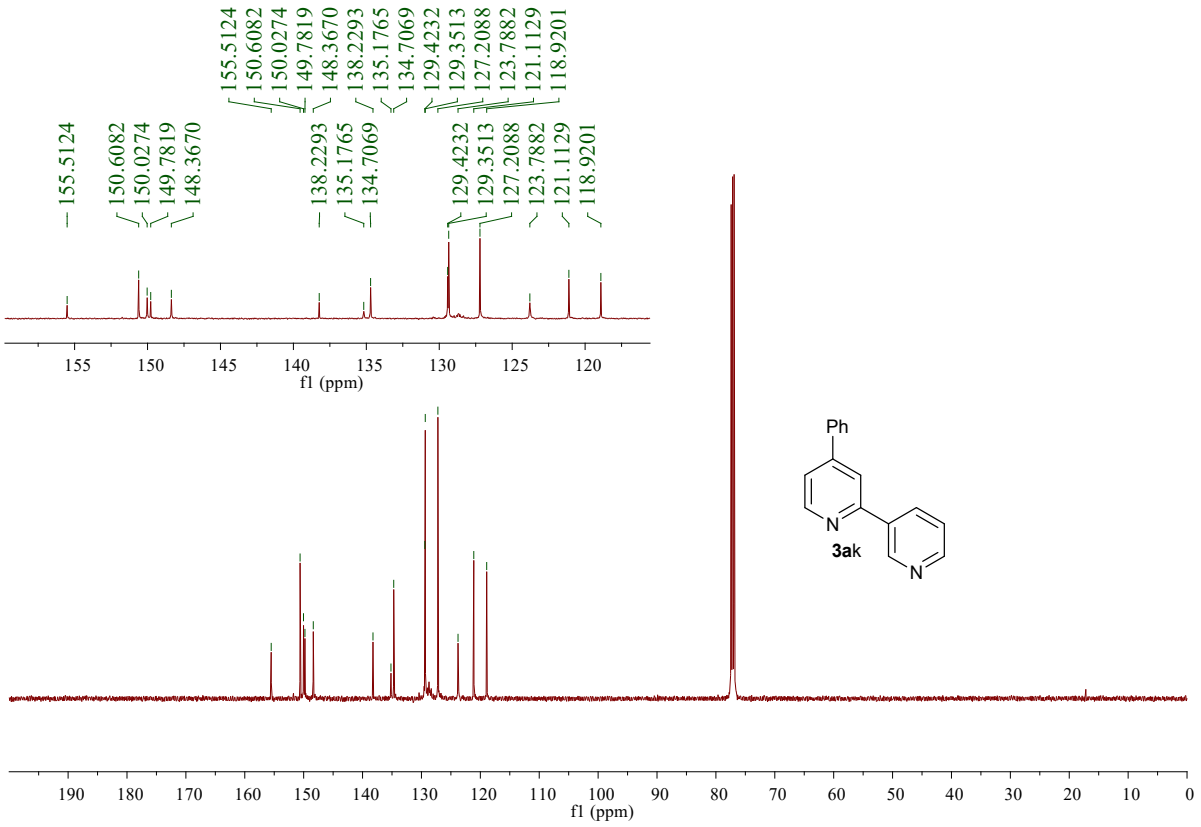
3ai

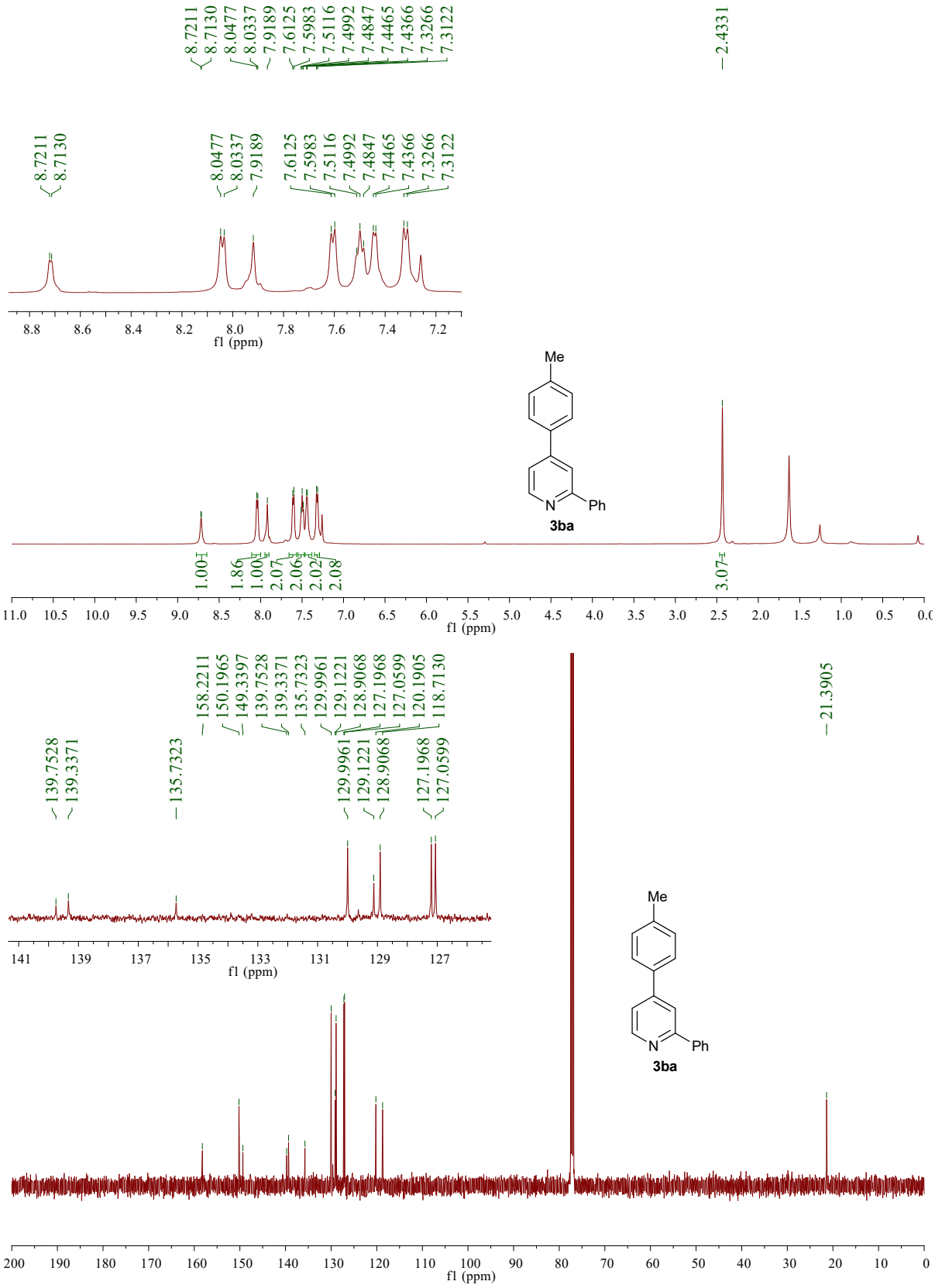

8.6371
8.6269
7.9247
7.6977
7.6834
7.5547
7.5006
7.4853
7.3768
7.3236
7.1169
6.5622
6.5588
6.5557
6.5524
f1 (ppm)
Ph
N
O
3al
1.00
1.03
2.06
1.02
3.10
1.02
0.95
1.00
f1 (ppm)
153.7745
150.1512
149.9833
149.2908
143.4664
138.3262
129.2668
129.2277
127.1453
120.0844
116.6730
112.2659
108.9480
f1 (ppm)
Ph
N
O
3al
f1 (ppm)


8.6284
8.6180
7.8619
7.6874
7.6733
7.5321
7.5182
7.5029
7.4833
7.4689
7.4541
7.4319
7.4219
7.3815
7.3783
7.3712
7.3680
7.1521
7.1446
7.1422
7.1347
Ph
N
S
3am
f1 (ppm)
153.2154
150.1120
149.4595
144.9934
138.4454
129.2889
128.2069
128.0718
127.8144
127.1982
124.8002
120.2871
117.0297
f1 (ppm)
Ph
N
S
3am
f1 (ppm)


9.2598
8.7677
8.7577
8.6806
8.3876
8.3719
7.9431
7.7009
7.6866
7.5369
7.5229
7.5100
7.4884
7.4740
7.4592
7.4450
7.4357
7.4300
7.4203
f1 (ppm)


Ph
N
3ak
N
1.00
1.04
0.97
1.01
1.02
2.00
5.13
f1 (ppm)


155.5124
150.6082
150.0274
149.7819
148.3670
138.2293
135.1765
134.7069
129.4232
129.3513
127.2088
123.7882
121.1129
118.9201
f1 (ppm)
Ph
N
3ak
N
f1 (ppm)


8.7211
8.7130
8.0477
8.0337
7.9189
7.6125
7.5983
7.5116
7.4992
7.4847
7.4465
7.4366
7.3266
7.3122
2.4331
fl (ppm)
Me
N
Ph
3ba
1.00
1.86
1.00
2.07
2.06
2.02
2.08
3.07
158.2211
150.1965
149.3397
139.7528
139.3371
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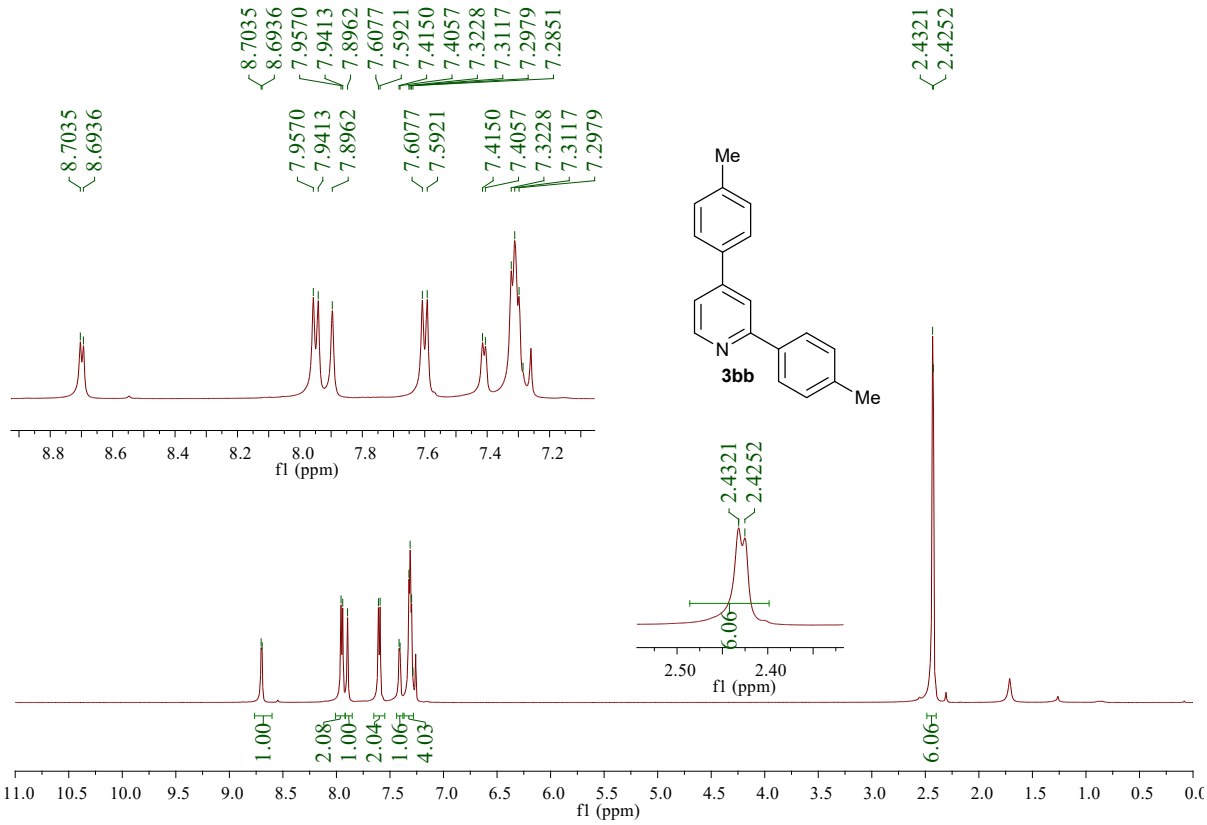
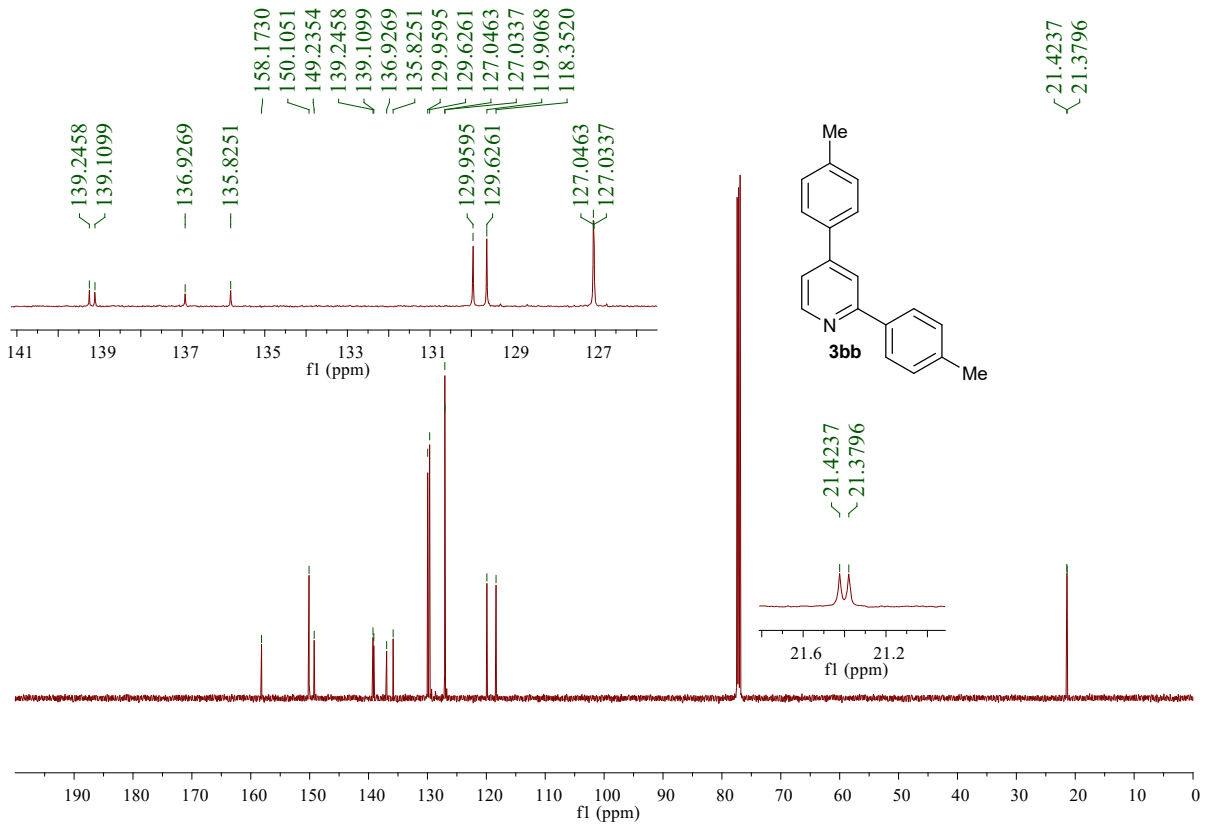
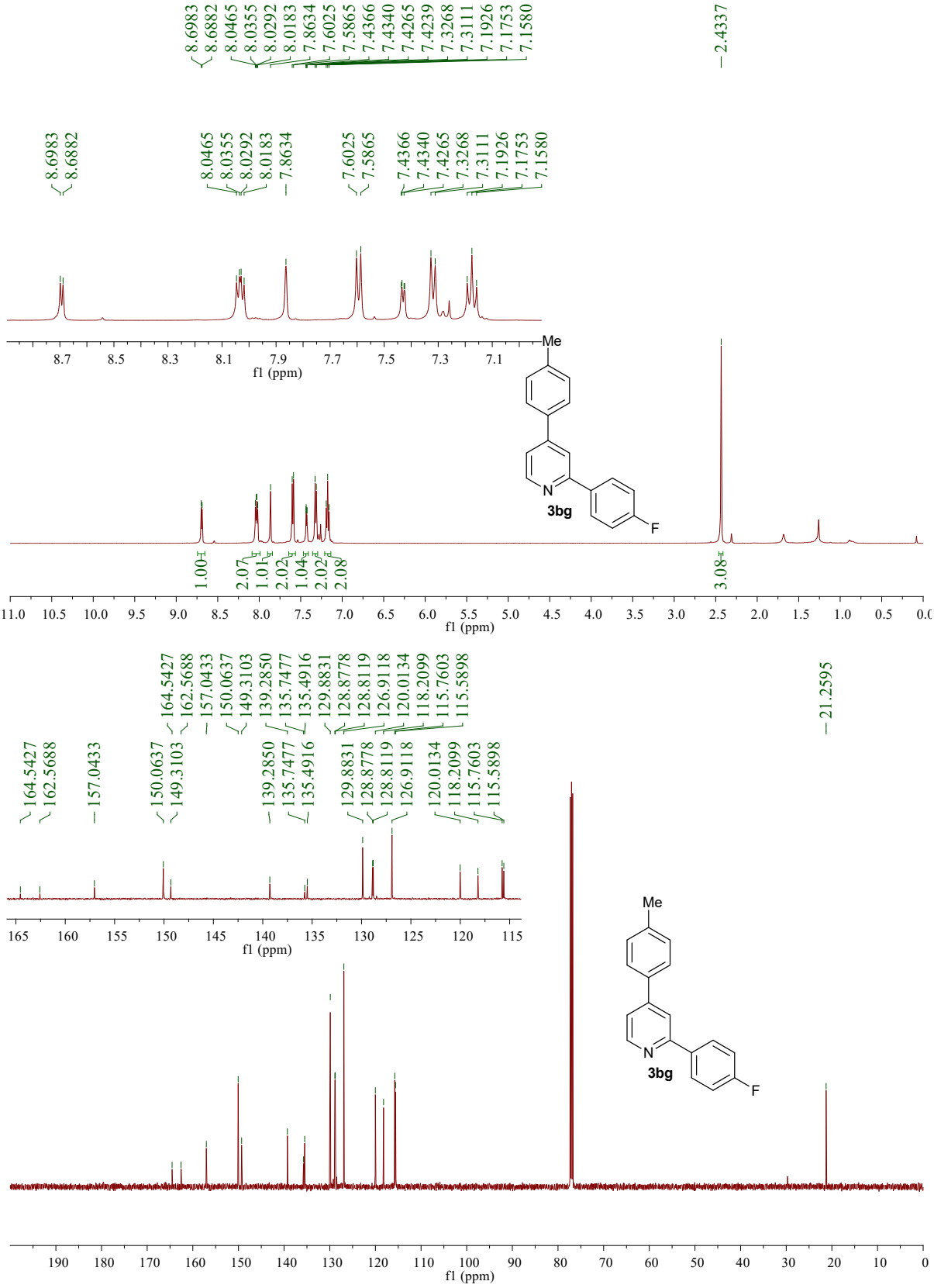
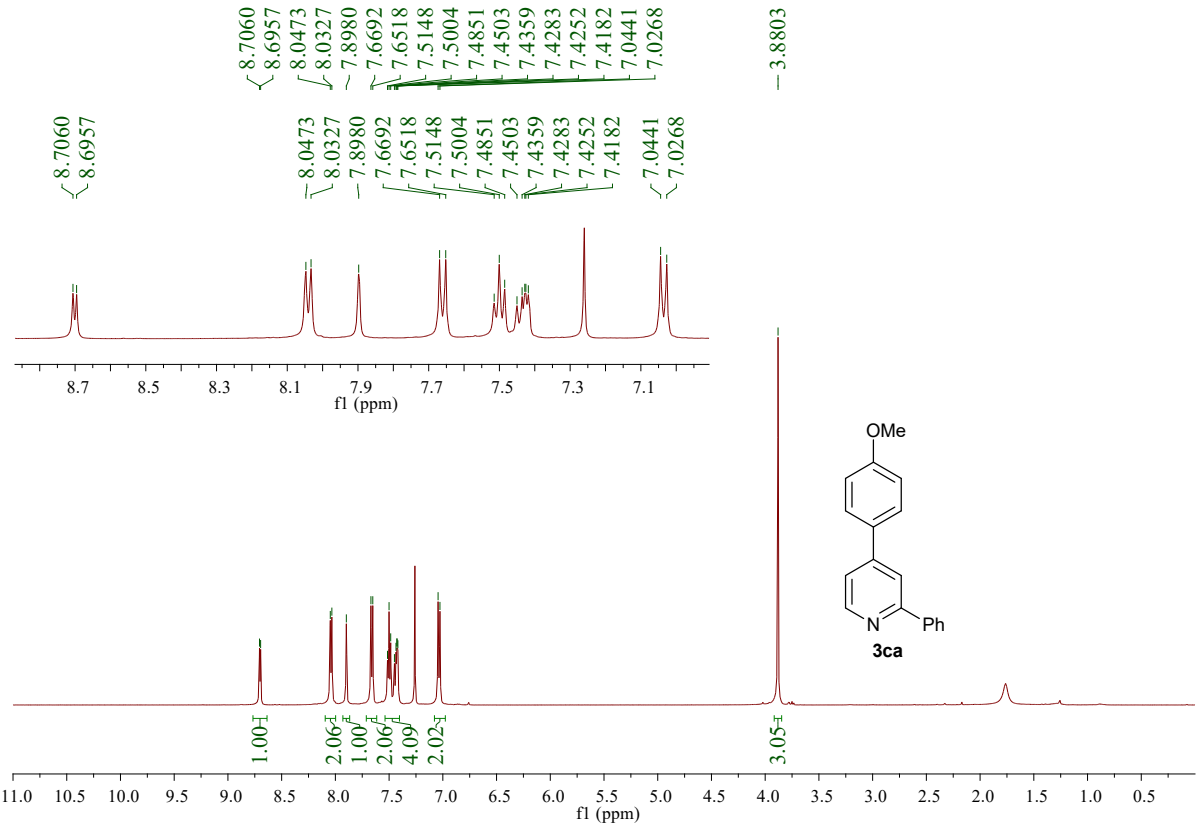
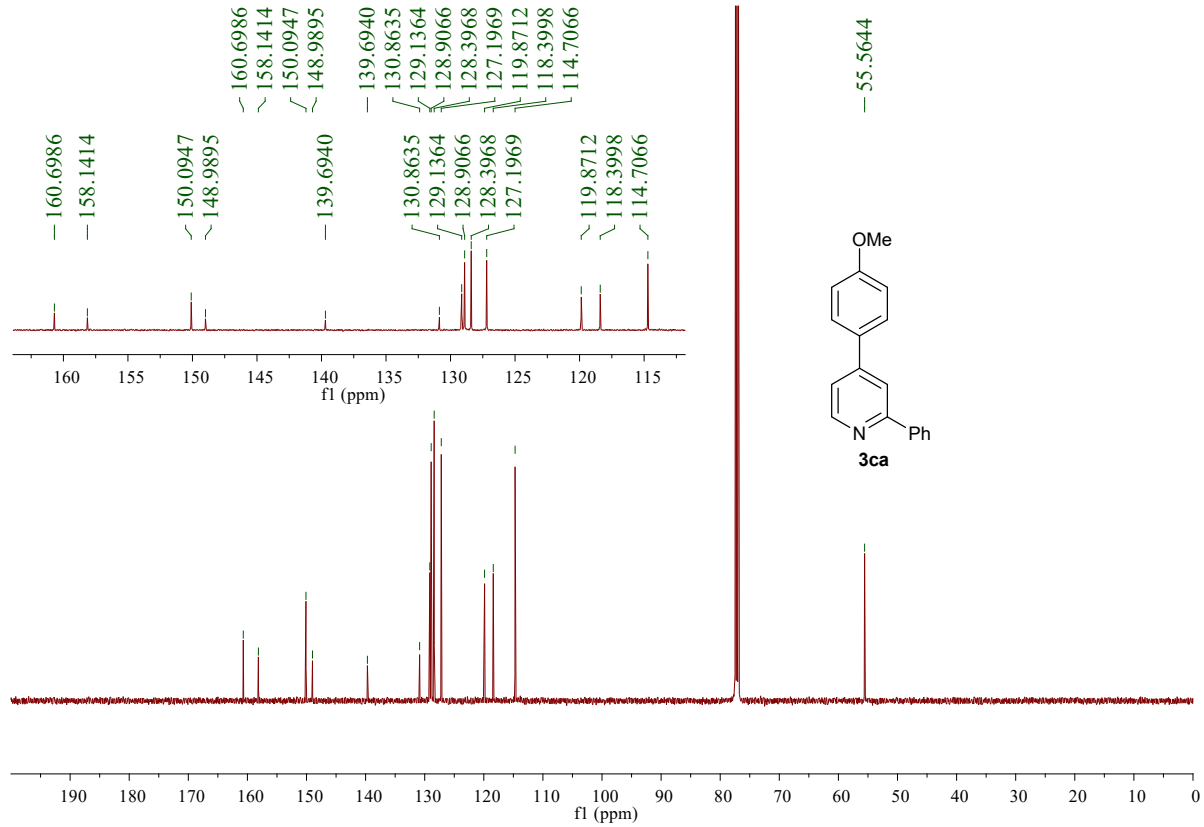
129.9961
129.1221
128.9068
127.1968
127.0599
120.1905
118.7130
21.3905

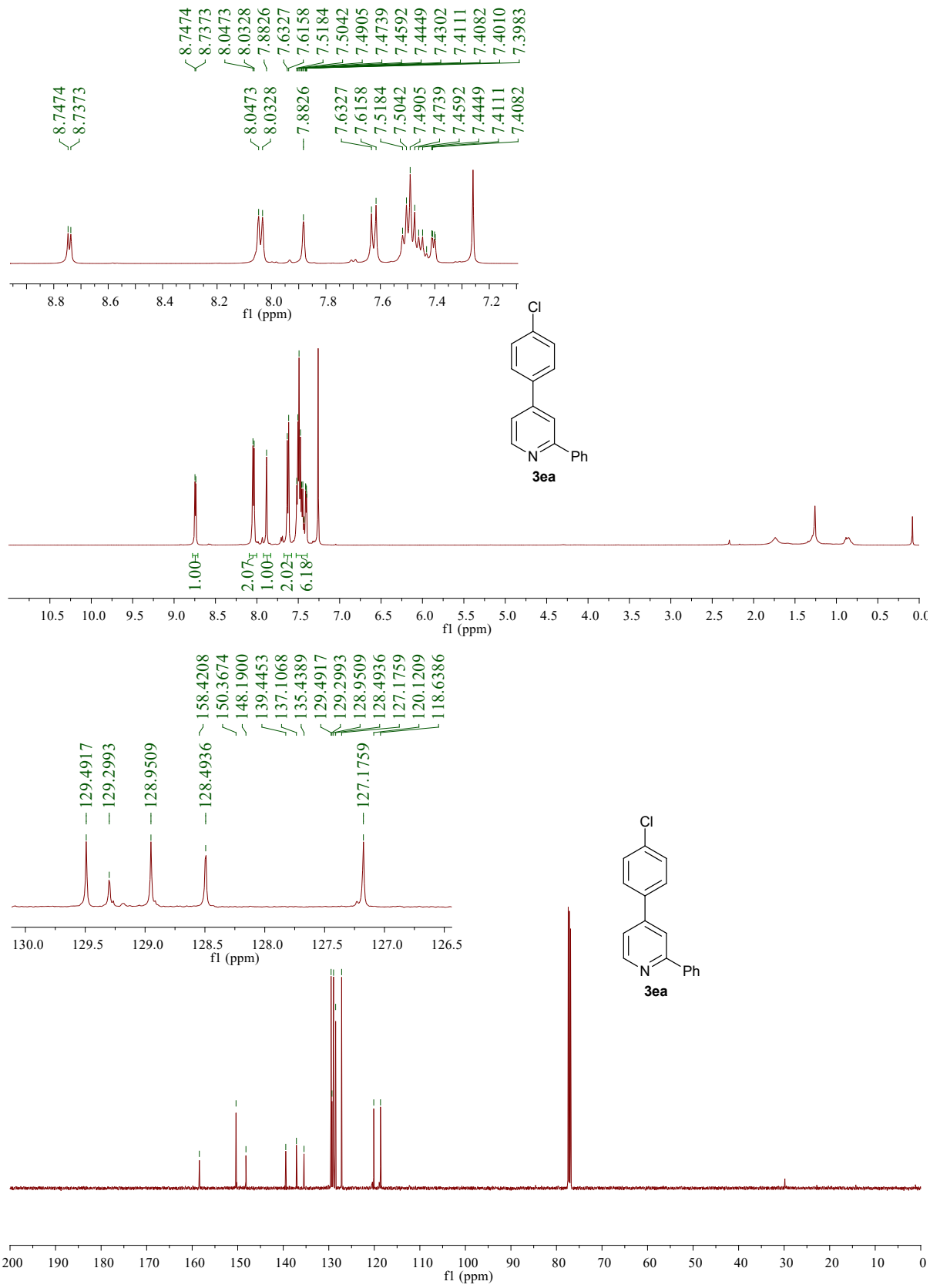

8.7035
8.6936
7.9570
7.9413
7.8962
7.6077
7.5921
7.4150
7.4057
7.3228
7.3117
7.2979
7.2851
2.4321
2.4252
Me
N
3bb
Me
f1 (ppm)
6.06
1.00
2.08
1.00
2.04
1.06
4.03
6.06

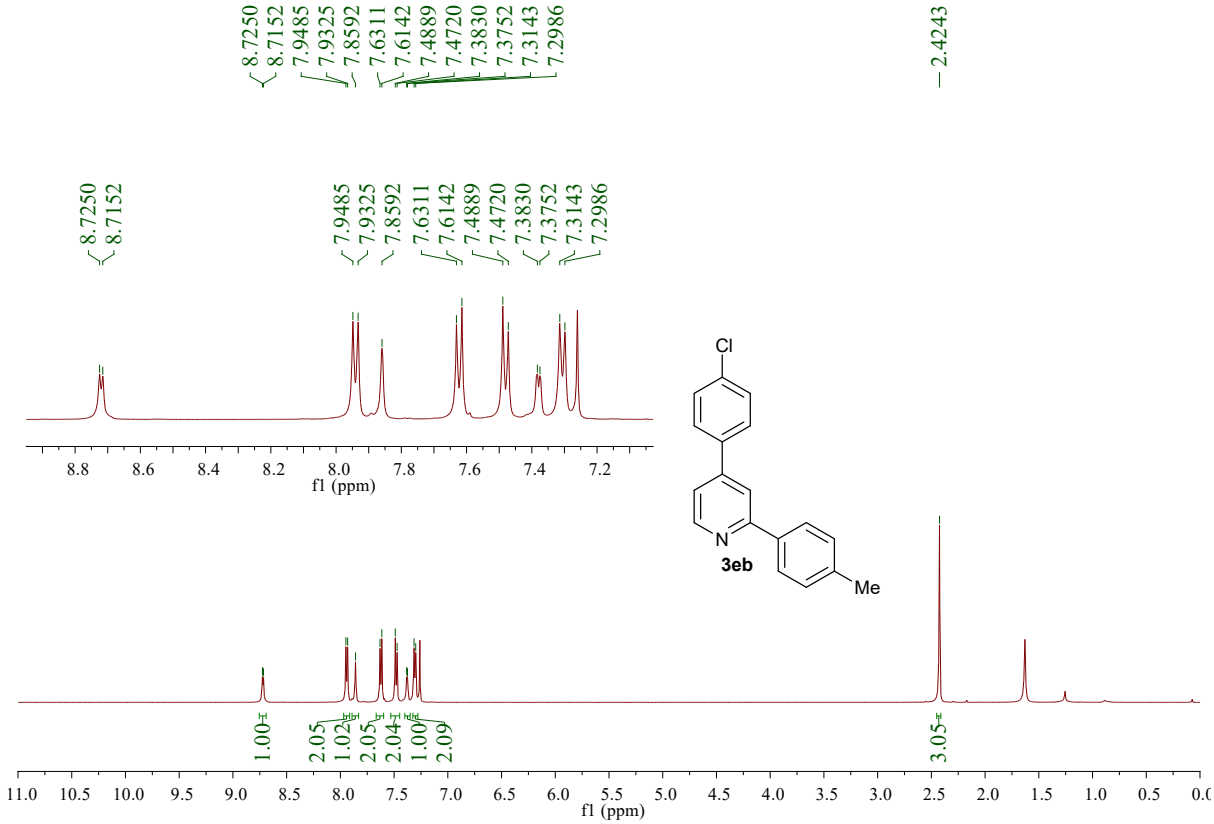

158.1730
150.1051
149.2354
139.2458
139.1099
136.9269
135.8251
129.9595
129.6261
127.0463
127.0337
119.9068
118.3520
21.4237
21.3796
Me
N
3bb
Me
f1 (ppm)


8.6983
8.6882
8.0465
8.0355
8.0292
8.0183
7.8634
7.6025
7.5865
7.4366
7.4340
7.4265
7.4239
7.3268
7.3111
7.1926
7.1753
7.1580
2.4337
f1 (ppm)
Me
N
F
3bg
1.00
2.07
1.01
2.02
1.04
2.02
2.08
3.08
164.5427
162.5688
157.0433
150.0637
149.3103
139.2850
135.7477
135.4916
129.8831
128.8778
128.8119
126.9118
120.0134
118.2099
115.7603
115.5898
21.2595


8.7060
8.6957
8.0473
8.0327
7.8980
7.6692
7.6518
7.5148
7.5004
7.4851
7.4503
7.4359
7.4283
7.4252
7.4182
7.0441
7.0268
3.8803
f1 (ppm)
OMe
N
Ph
3ca
1.00
2.06
1.00
2.06
4.09
2.02
3.05


160.6986
158.1414
150.0947
148.9895
139.6940
130.8635
129.1364
128.9066
128.3968
127.1969
119.8712
118.3998
114.7066
55.5644
f1 (ppm)
OMe
N
Ph
3ca


8.7474
8.7373
8.0473
8.0328
7.8826
7.6327
7.6158
7.5184
7.5042
7.4905
7.4739
7.4592
7.4449
7.4302
7.4111
7.4082
7.4010
7.3983
f1 (ppm)
Cl
N
Ph
3ea
1.00
2.07
1.00
2.02
6.18
f1 (ppm)
158.4208
150.3674
148.1900
139.4453
137.1068
135.4389
129.4917
129.2993
128.9509
128.4936
127.1759
120.1209
118.6386
f1 (ppm)
Cl
N
Ph
3ea
f1 (ppm)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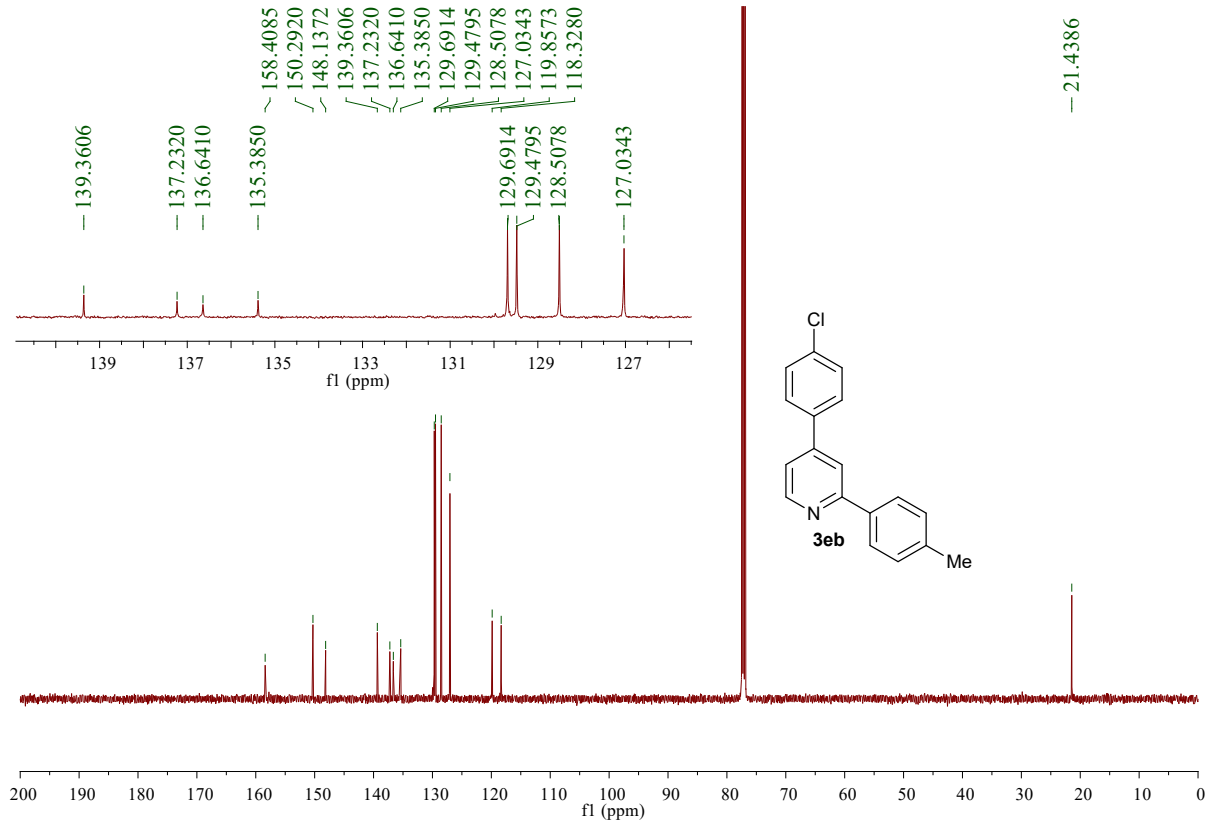
7.9485
7.9325
7.8592
7.6311
7.6142
7.4889
7.4720
7.3830
7.3752
7.3143
7.2986
2.4243
Cl
N
3eb
Me
1.00
2.05
1.02
2.05
2.04
1.00
2.09
3.05
f1 (ppm)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148.1372
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137.2320
136.6410
135.3850
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127.0343
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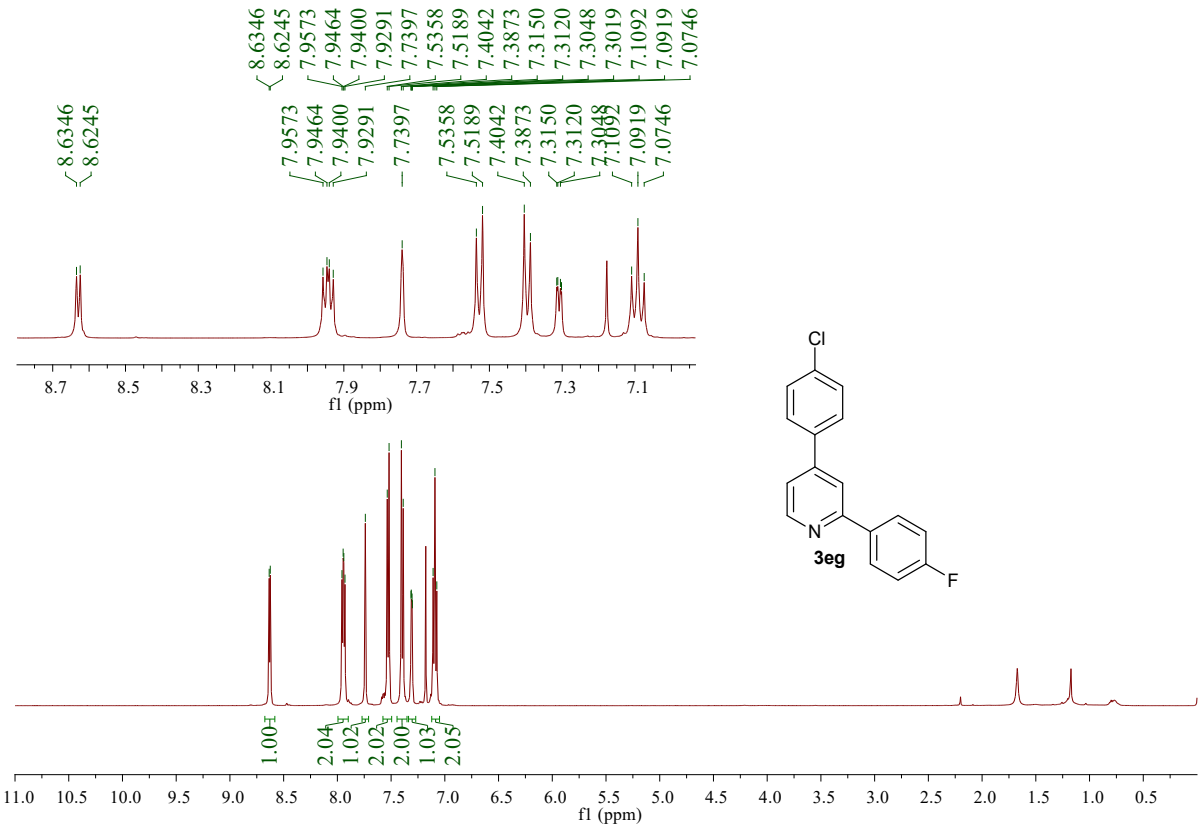
21.4386
Cl
N
3eb
Me
f1 (ppm)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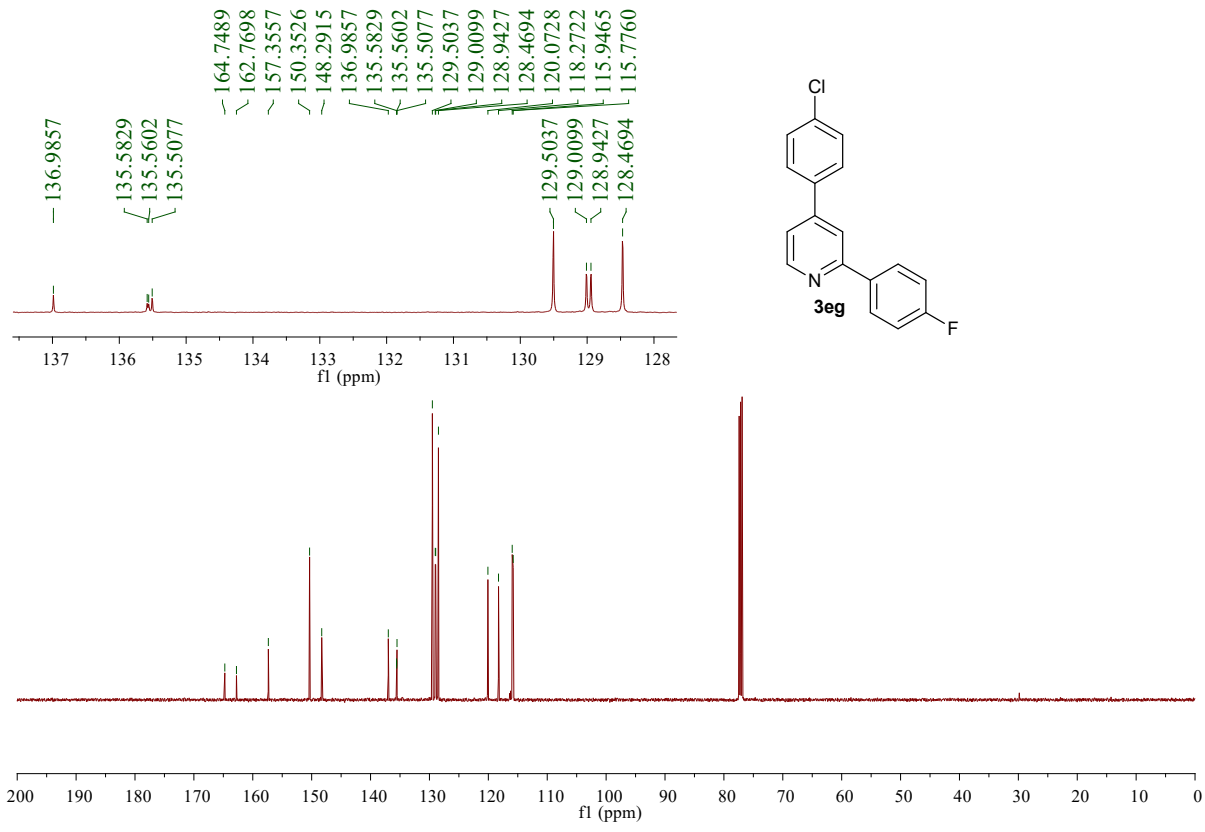
8.6245
7.9573
7.9464
7.9400
7.9291
7.7397
7.5358
7.5189
7.4042
7.3873
7.3150
7.3120
7.3048
7.3019
7.1092
7.0919
7.0746
f1 (ppm)
Cl
N
F
3eg
1.00
2.04
1.02
2.02
2.00
1.03
2.05
f1 (ppm)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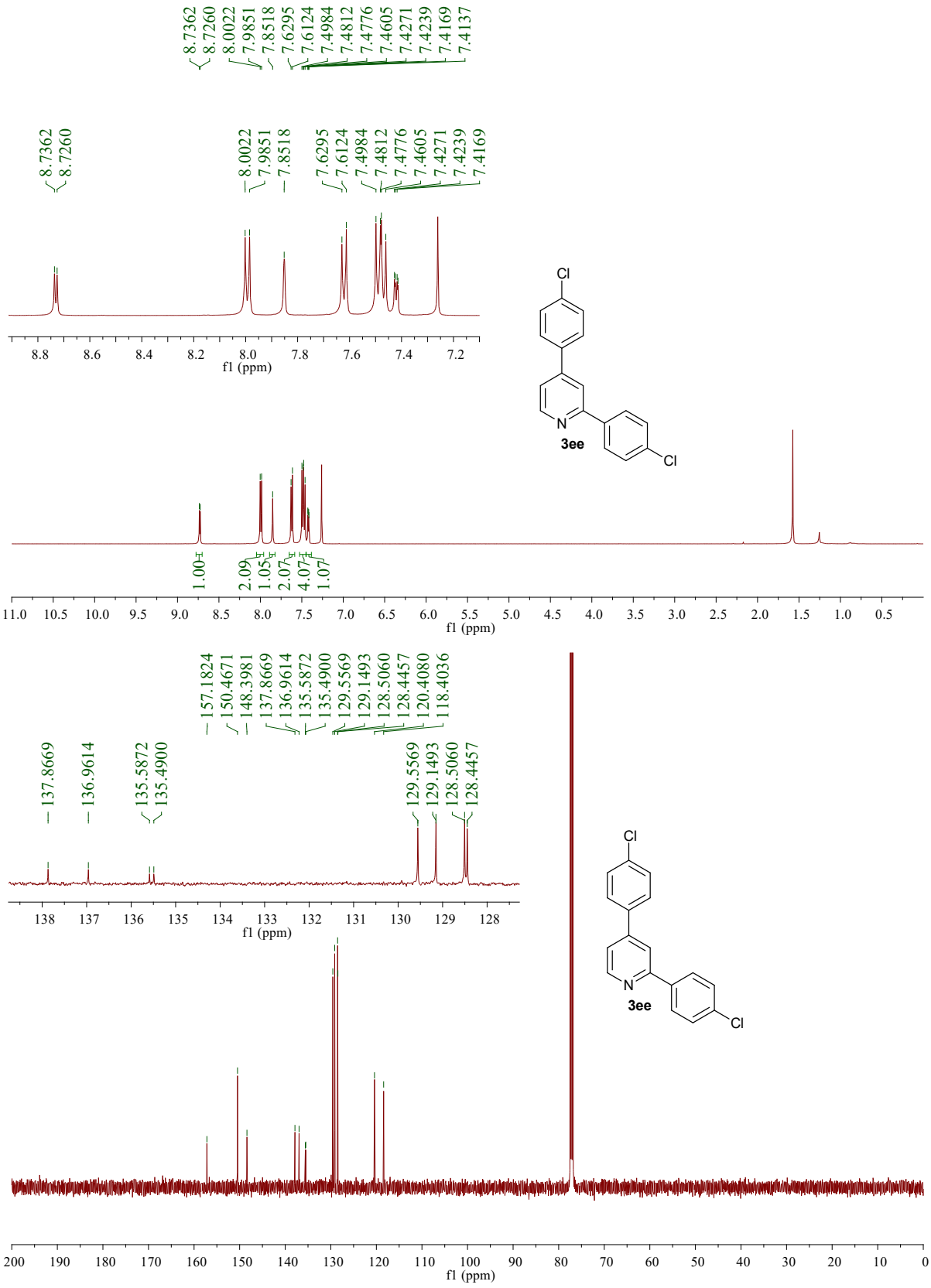
157.3557
150.3526
148.2915
136.9857
135.5829
135.5602
135.5077
129.5037
129.0099
128.9427
128.4694
120.0728
118.2722
115.9465
115.7760
f1 (ppm)
Cl
N
F
3eg
f1 (ppm)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7.8518
7.6295
7.6124
7.4984
7.4812
7.4776
7.4605
7.4271
7.4239
7.4169
7.4137
f1 (ppm)
Cl
N
3ee
Cl
1.00
2.09
1.05
2.07
4.07
1.07
f1 (ppm)
157.1824
150.4671
148.3981
137.8669
136.9614
135.5872
135.4900
129.5569
129.1493
128.5060
128.4457
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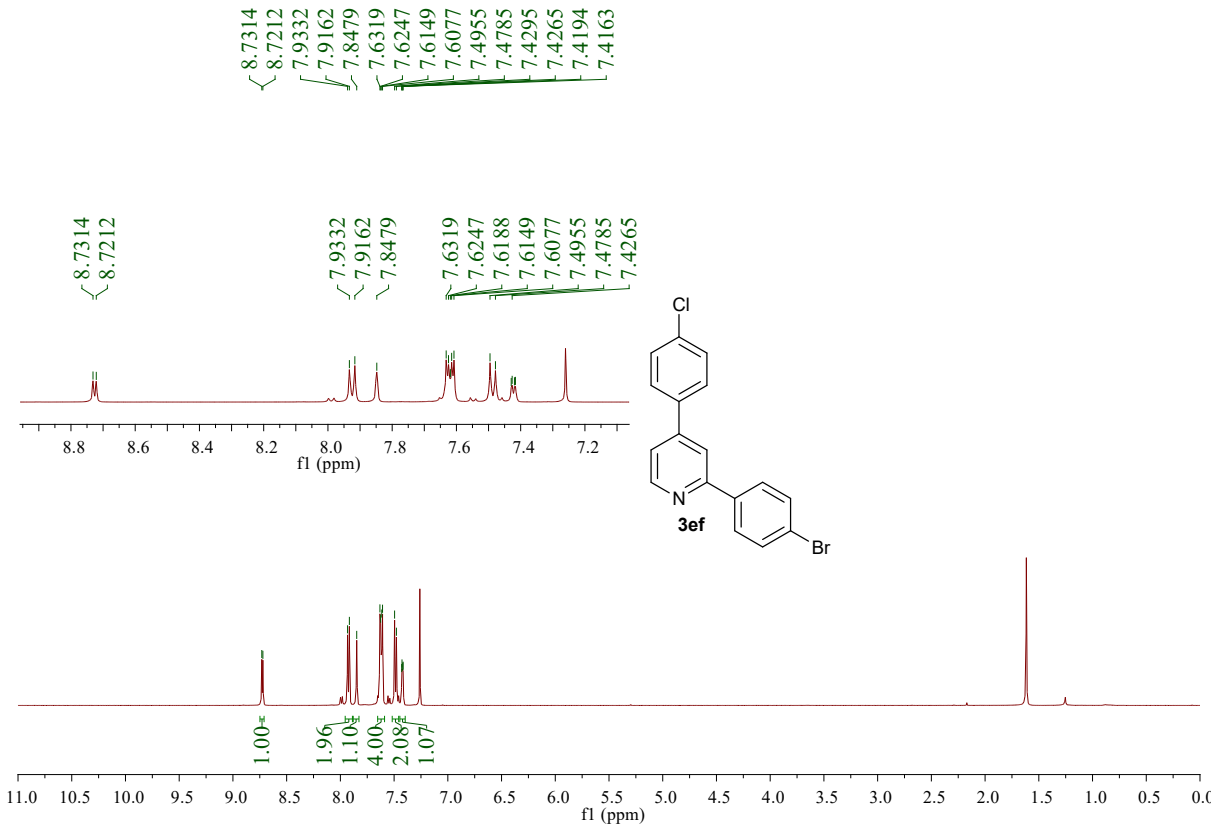
f1 (ppm)
Cl
N
3ee
Cl
f1 (ppm)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7.6247
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7.6077
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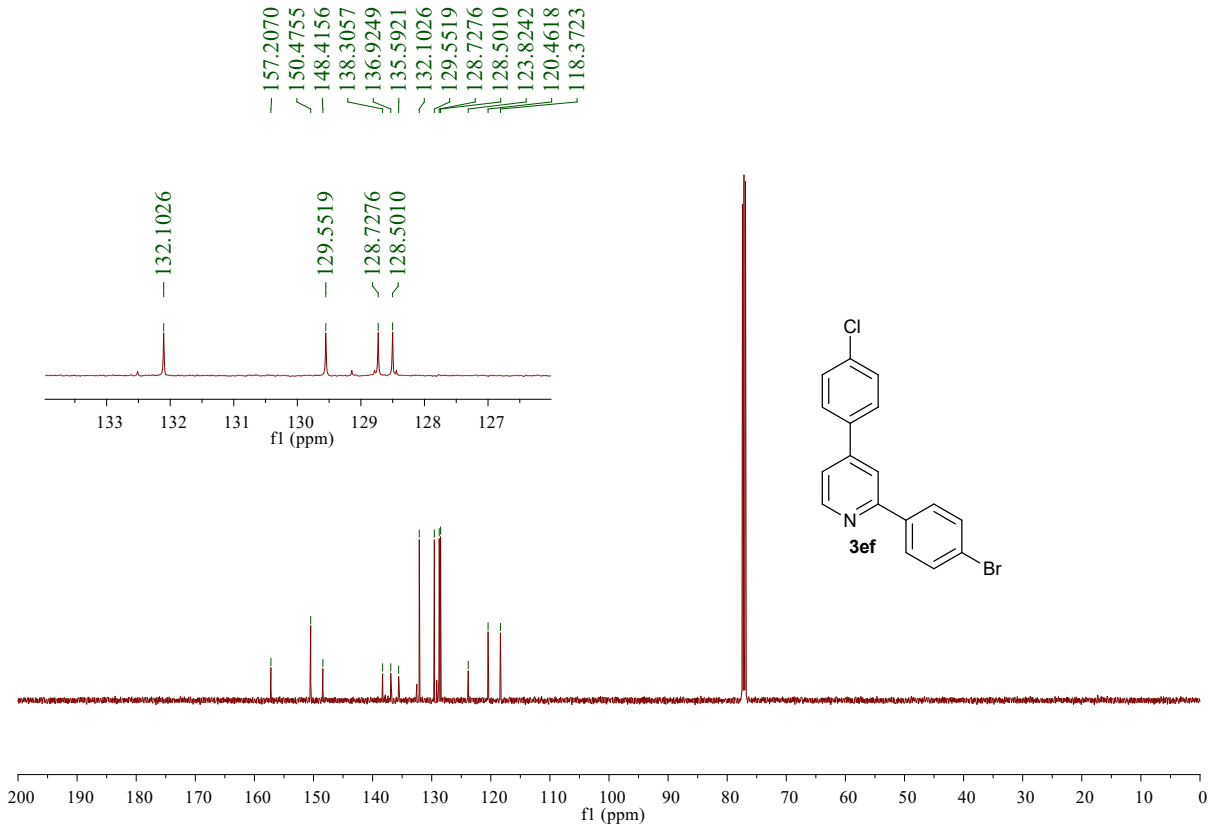
7.4785
7.4295
7.4265
7.4194
7.4163
8.7314
8.7212
7.9332
7.9162
7.8479
7.6319
7.6247
7.6188
7.6149
7.6077
7.4955
7.4785
7.4265
8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2
f1 (ppm)
Cl
N
3ef
Br
1.00
1.96
1.10
4.00
2.08
1.07
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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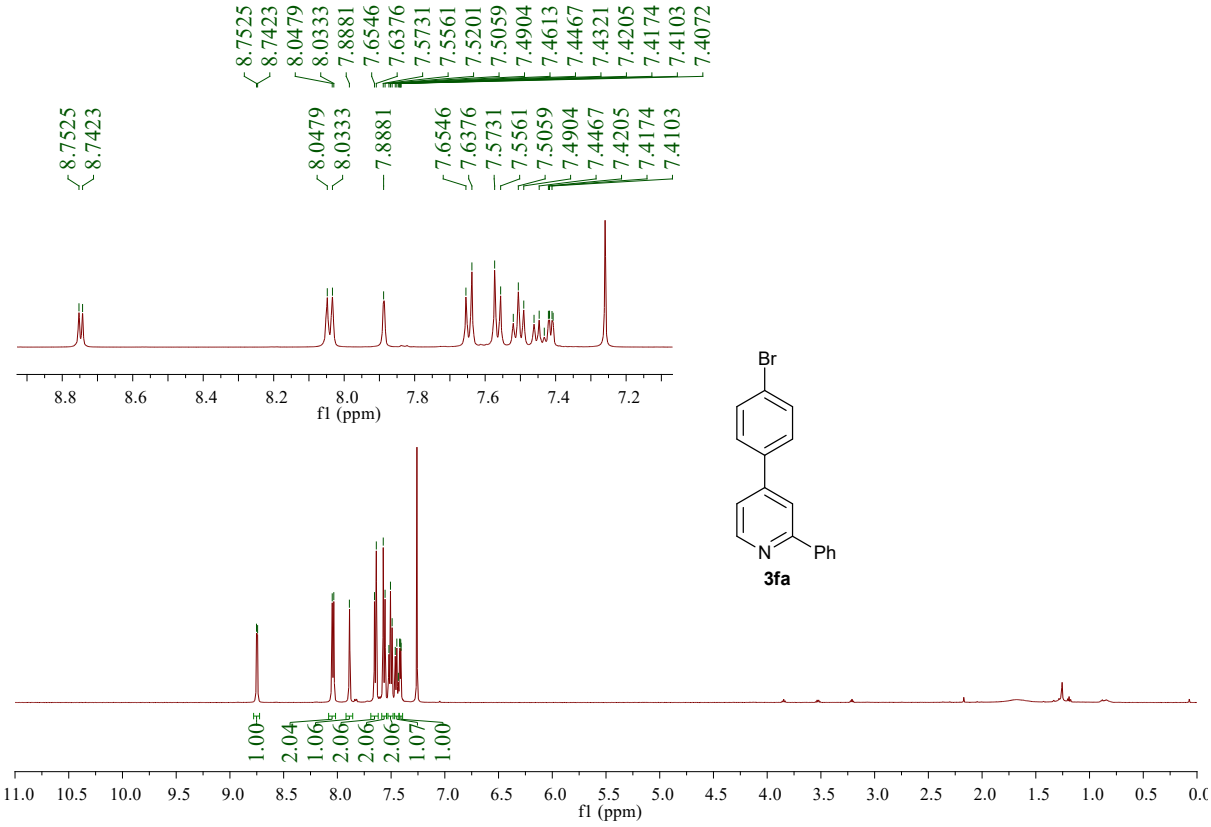
148.4156
138.3057
136.9249
135.5921
132.1026
129.5519
128.7276
128.5010
123.8242
120.4618
118.3723
132.1026
129.5519
128.7276
128.5010
133 132 131 130 129 128 127
f1 (ppm)
Cl
N
3ef
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.0333
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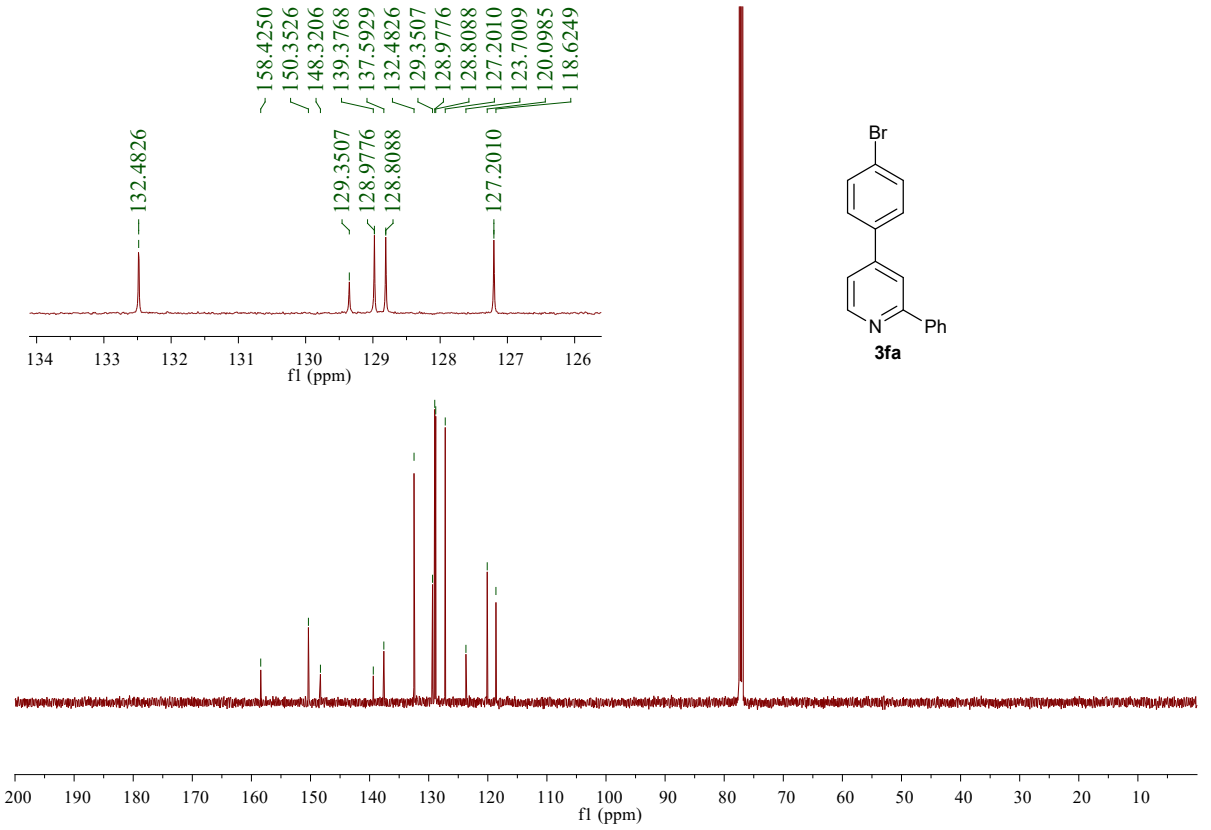
7.6376
7.5731
7.5561
7.5201
7.5059
7.4904
7.4613
7.4467
7.4321
7.4205
7.4174
7.4103
7.4072
f1 (ppm)
Br
N
Ph
3fa
1.00
2.04
1.06
2.06
2.06
2.06
1.07
1.00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148.3206
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137.5929
132.4826
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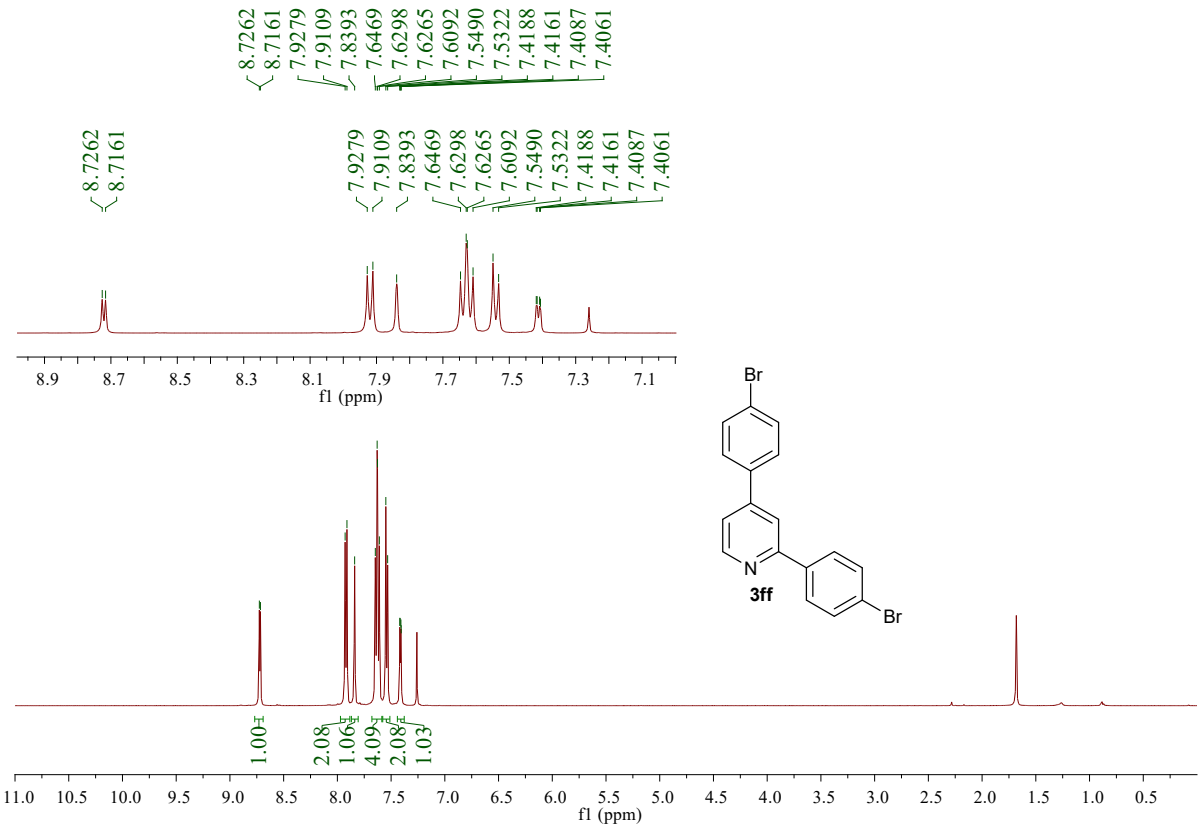
128.8088
127.2010
123.7009
120.0985
118.6249
f1 (ppm)
Br
N
Ph
3fa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7.6469
7.6298
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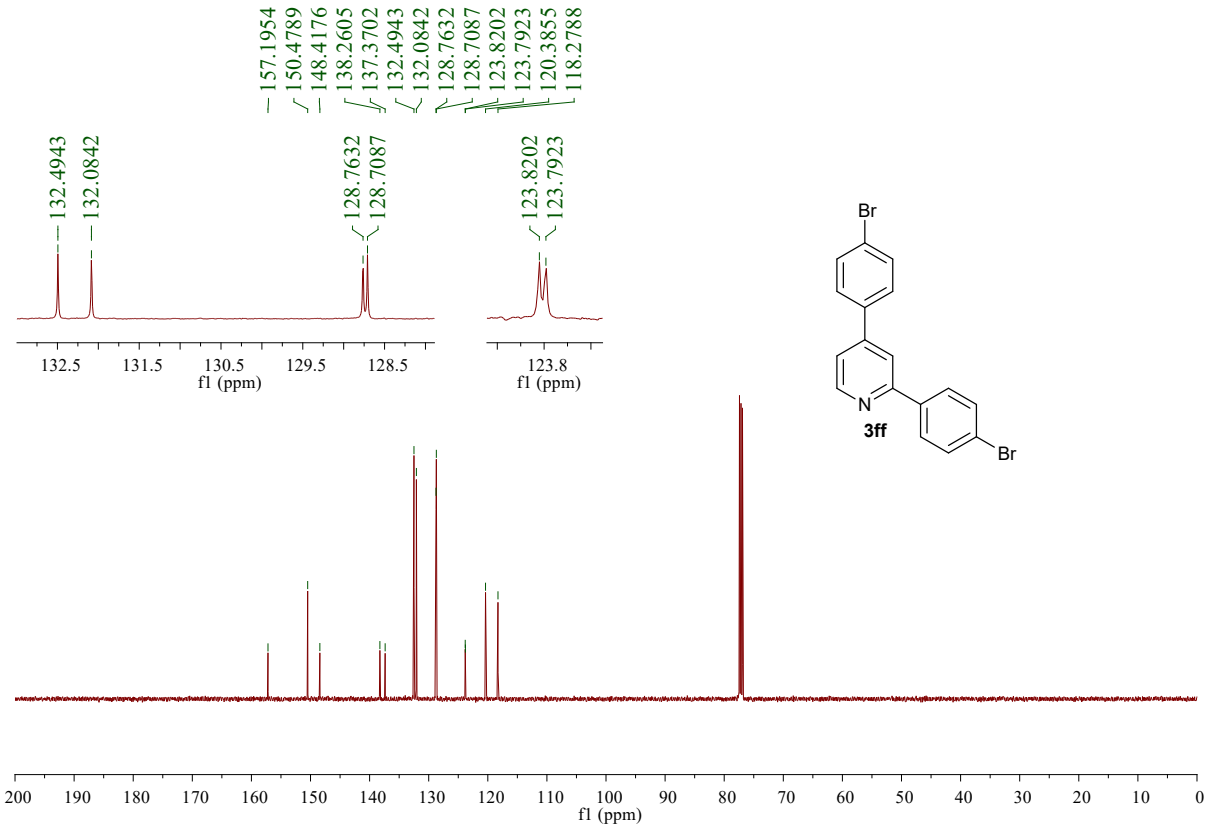
7.6092
7.5490
7.5322
7.4188
7.4161
7.4087
7.4061
f1 (ppm)
Br
N
3ff
Br
1.00
2.08
1.06
4.09
2.08
1.03
f1 (ppm)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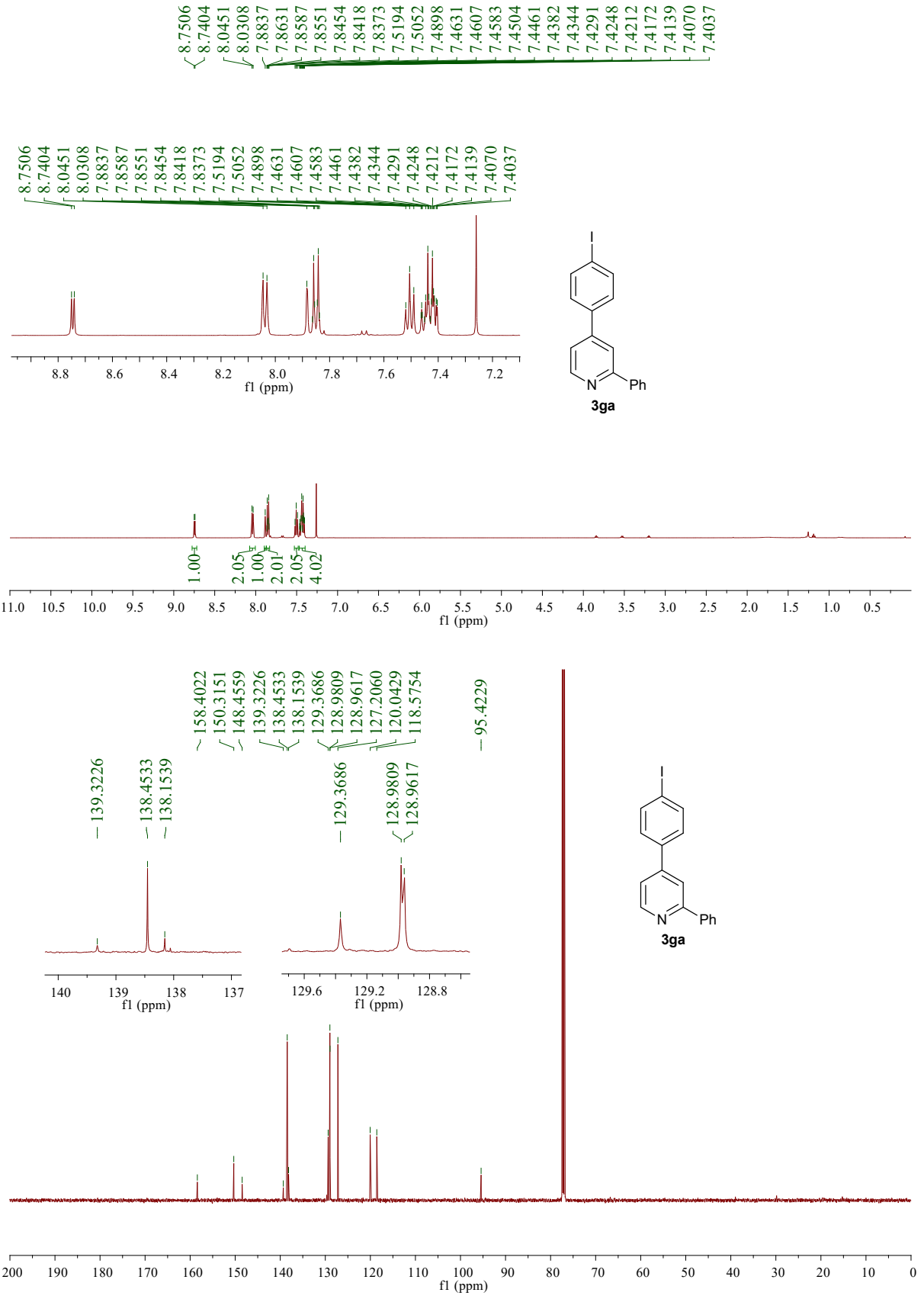
148.4176
138.2605
137.3702
132.4943
132.0842
128.7632
128.7087
123.8202
123.7923
120.3855
118.2788
f1 (ppm)
f1 (ppm)
Br
N
3ff
Br
f1 (ppm)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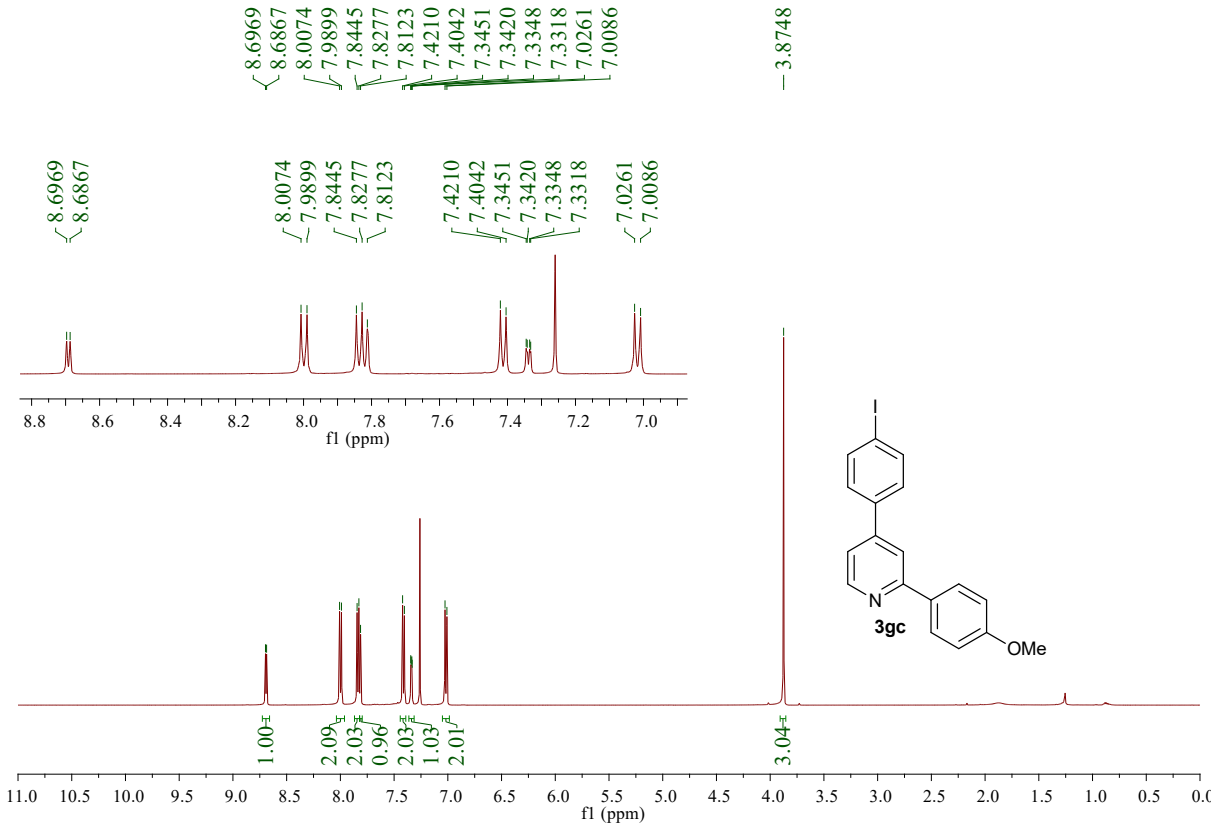
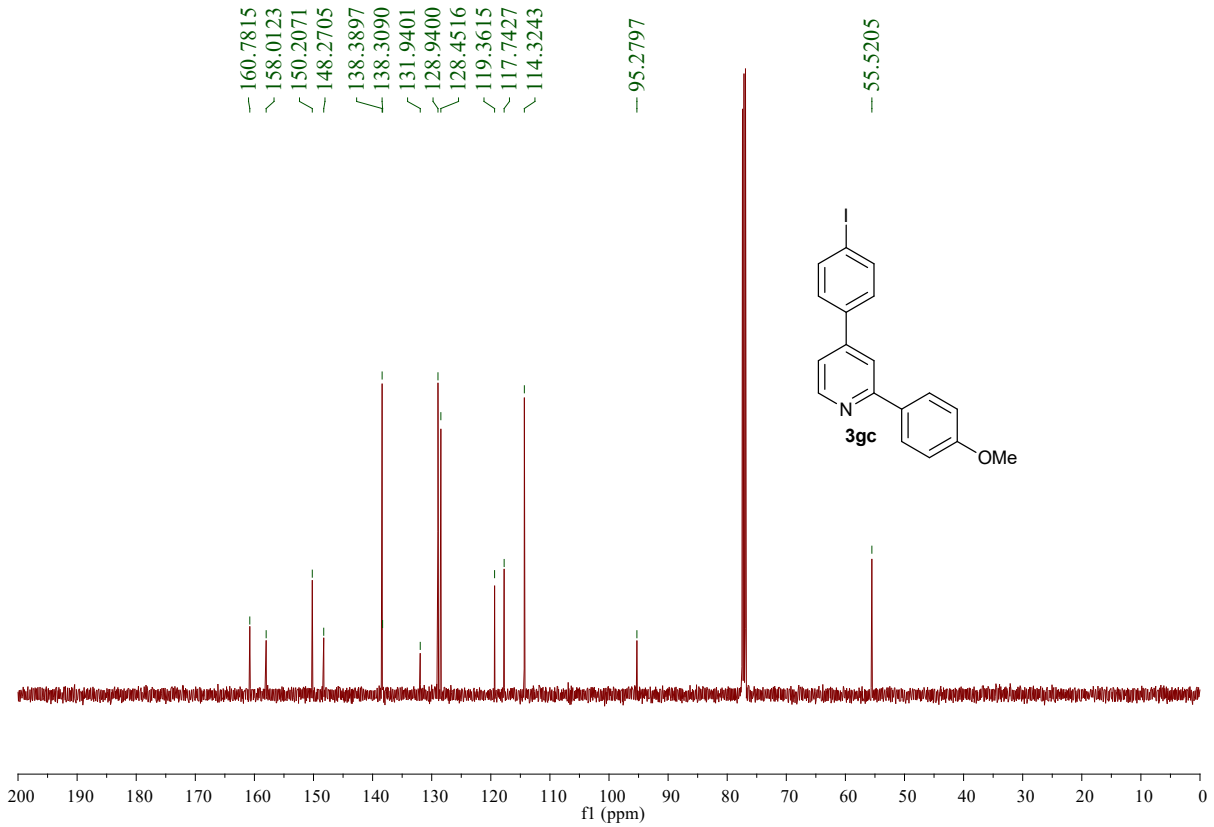
8.7404
8.0451
8.0308
7.8837
7.8631
7.8587
7.8551
7.8454
7.8418
7.8373
7.5194
7.5052
7.4898
7.4631
7.4607
7.4583
7.4504
7.4461
7.4382
7.4344
7.4291
7.4248
7.4212
7.4172
7.4139
7.4070
7.4037
f1 (ppm)
I
N
Ph
3ga
1.00
2.05
1.00
2.01
2.05
4.02
158.4022
150.3151
148.4559
139.3226
138.4533
138.1539
129.3686
128.9809
128.9617
127.2060
120.0429
118.5754
95.4229


8.6969
8.6867
8.0074
7.9899
7.8445
7.8277
7.8123
7.4210
7.4042
7.3451
7.3420
7.3348
7.3318
7.0261
7.0086
3.8748
f1 (ppm)
1.00
2.09
2.03
0.96
2.03
1.03
2.01
3.04
I
N
3gc
OMe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158.0123
150.2071
148.2705
138.3897
138.3090
131.9401
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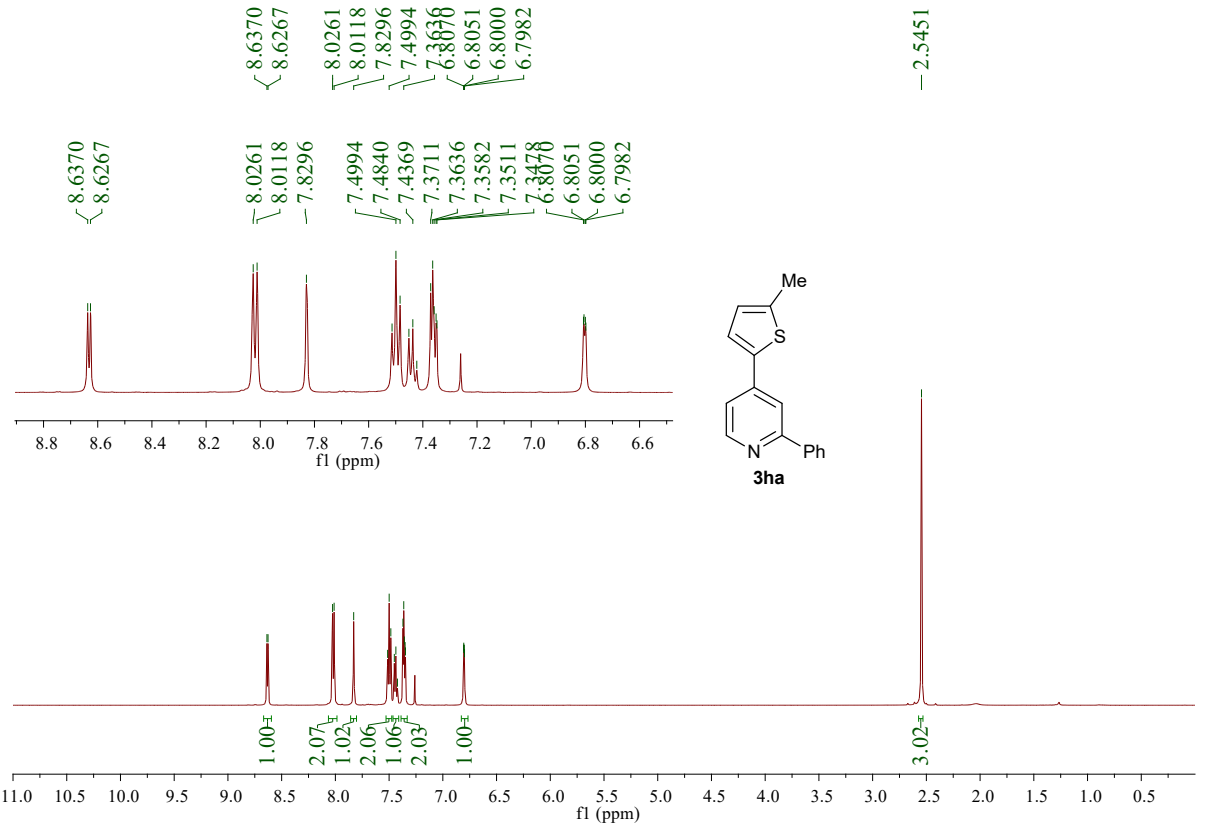
117.7427
114.3243
95.2797
55.5205
f1 (ppm)
I
N
3gc
OMe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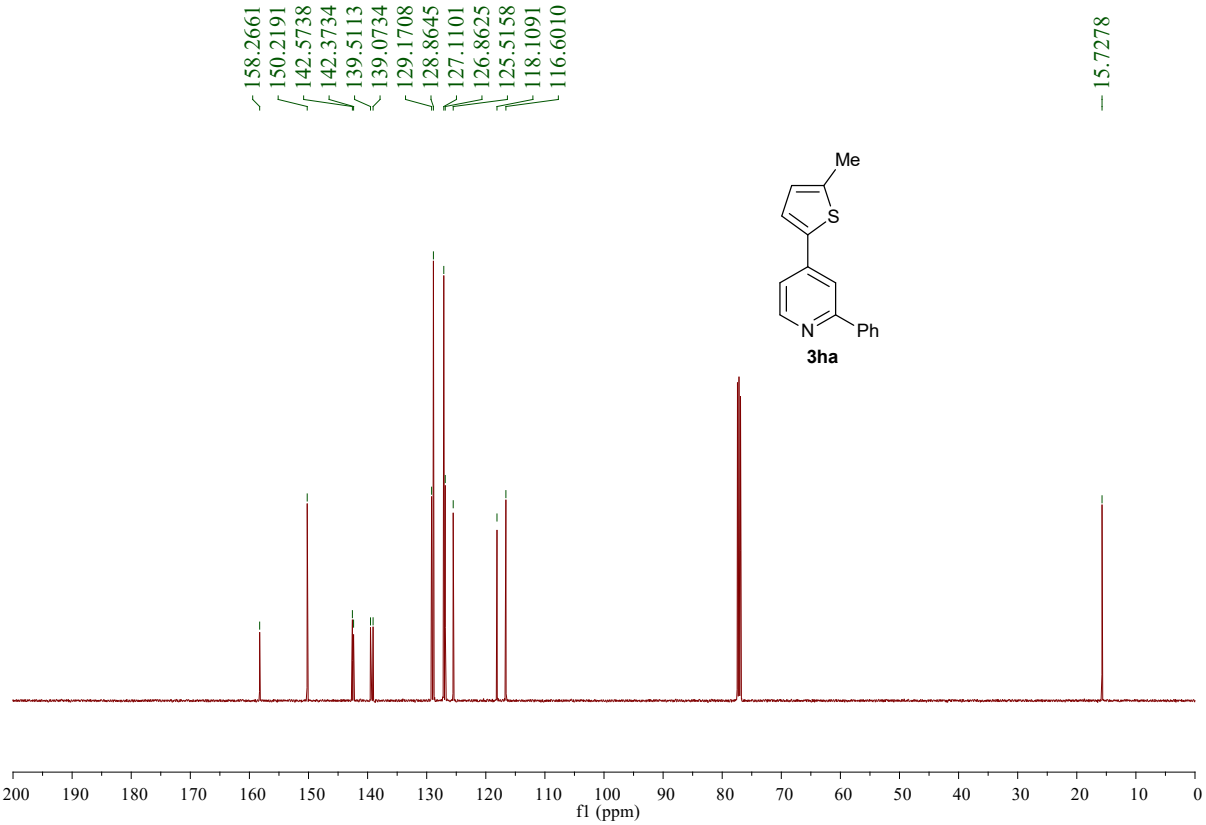
8.6267
8.0261
8.0118
7.8296
7.4994
7.4840
7.4369
7.3711
7.3636
7.3582
7.3511
6.8051
6.8000
6.7982
2.5451
Me
S
N
Ph
3ha
f1 (ppm)
1.00
2.07
1.02
2.06
1.06
2.03
1.00
3.02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150.2191
142.5738
142.3734
139.5113
139.0734
129.1708
128.8645
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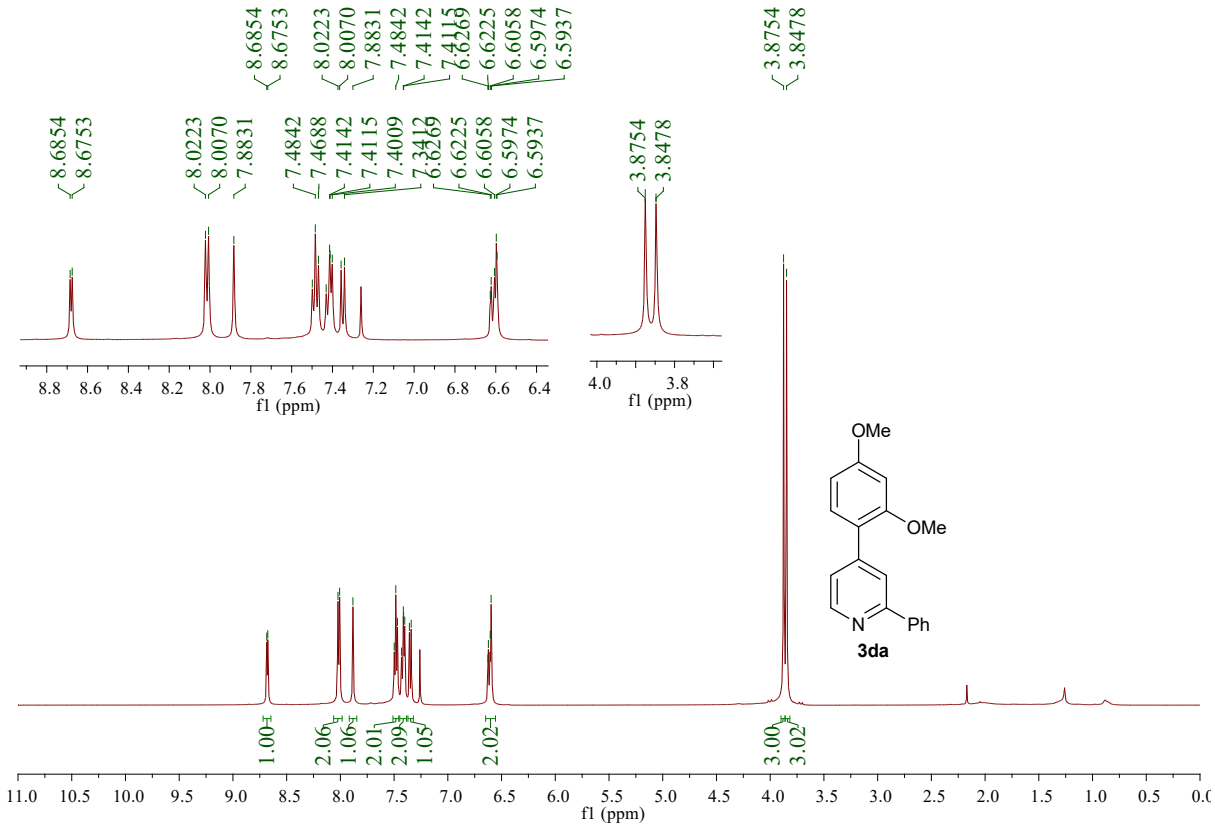
125.5158
118.1091
116.6010
15.7278
Me
S
N
Ph
3ha
f1 (ppm)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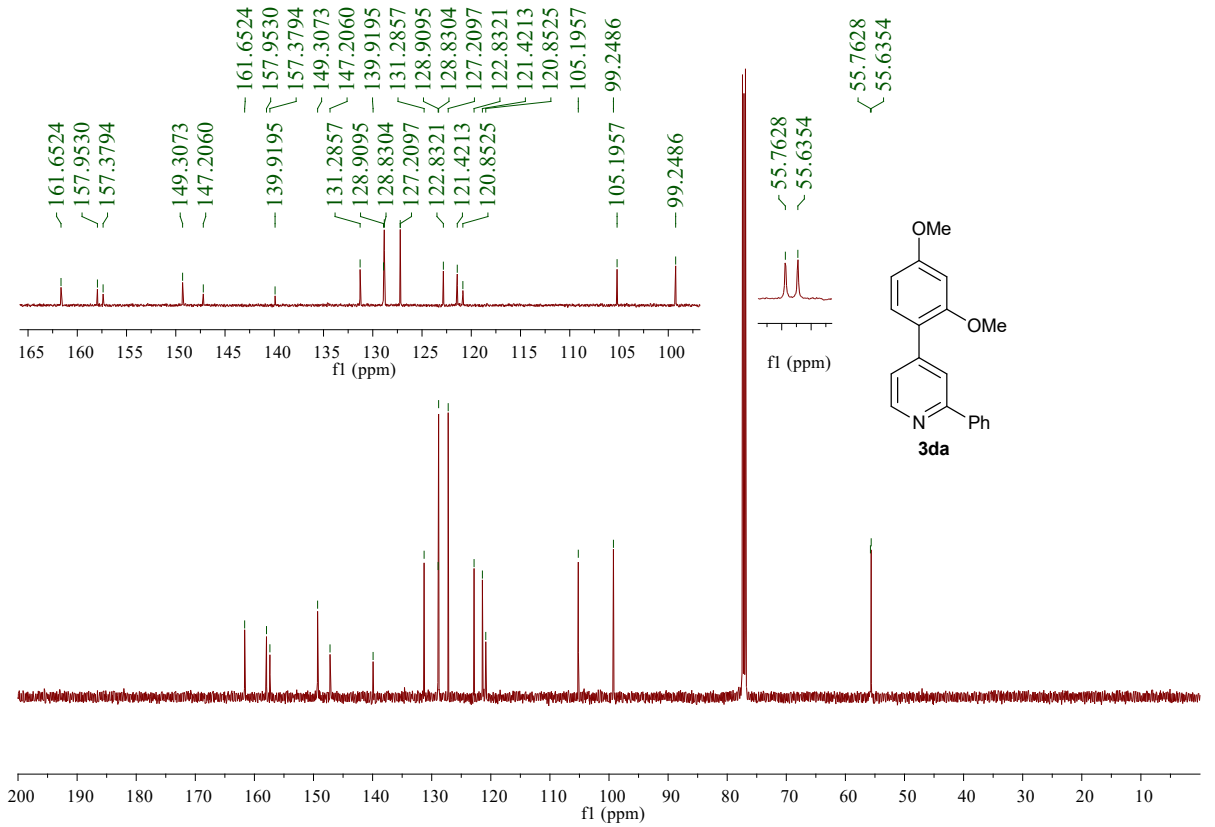
8.6753
8.0223
8.0070
7.8831
7.4842
7.4688
7.4142
7.4115
7.4009
7.3412
6.6269
6.6225
6.6058
6.5974
6.5937
3.8754
3.8478
OMe
OMe
N
Ph
3da
1.00
2.06
1.06
2.01
2.09
1.05
2.02
3.00
3.02
fl (ppm)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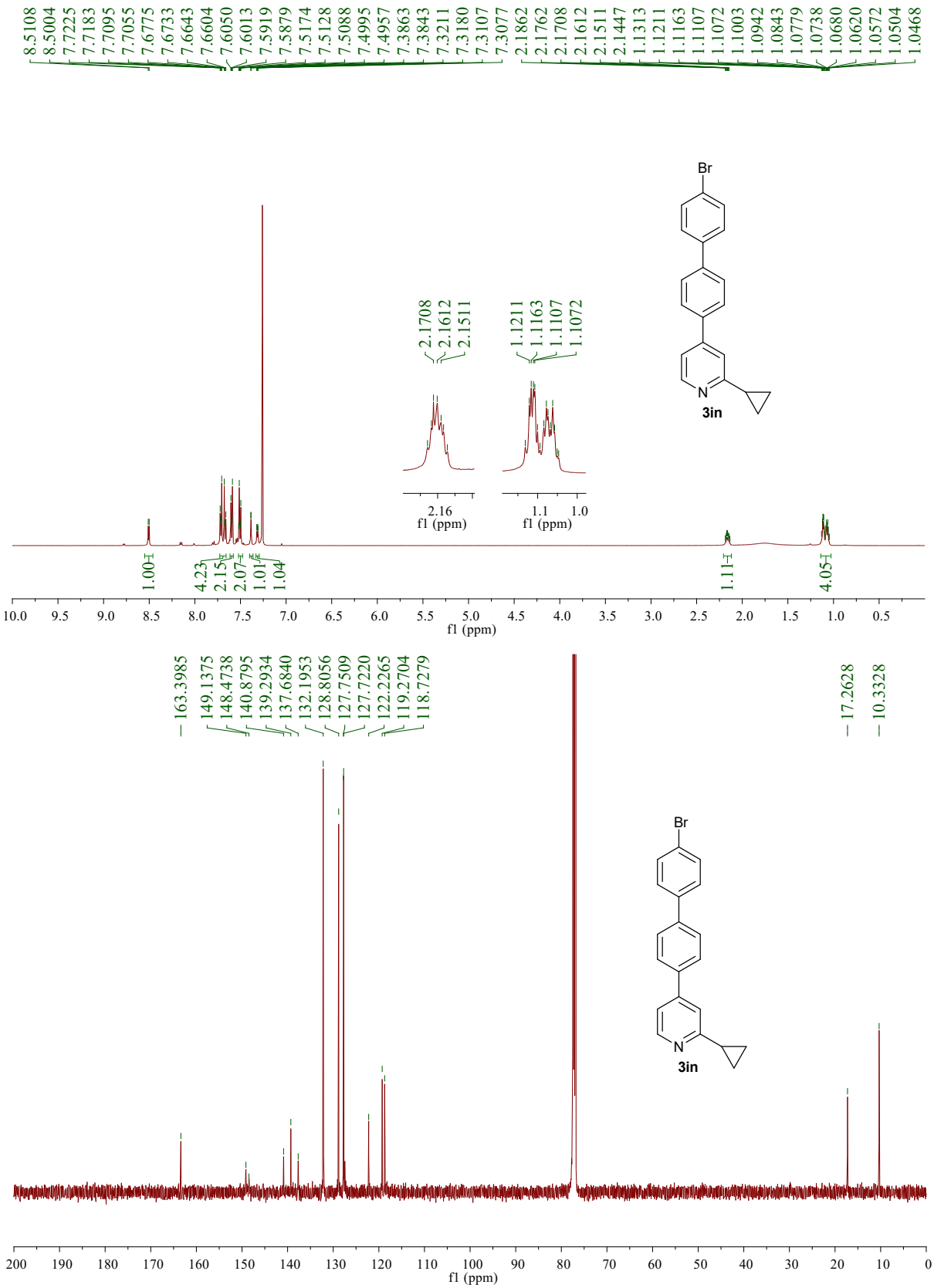
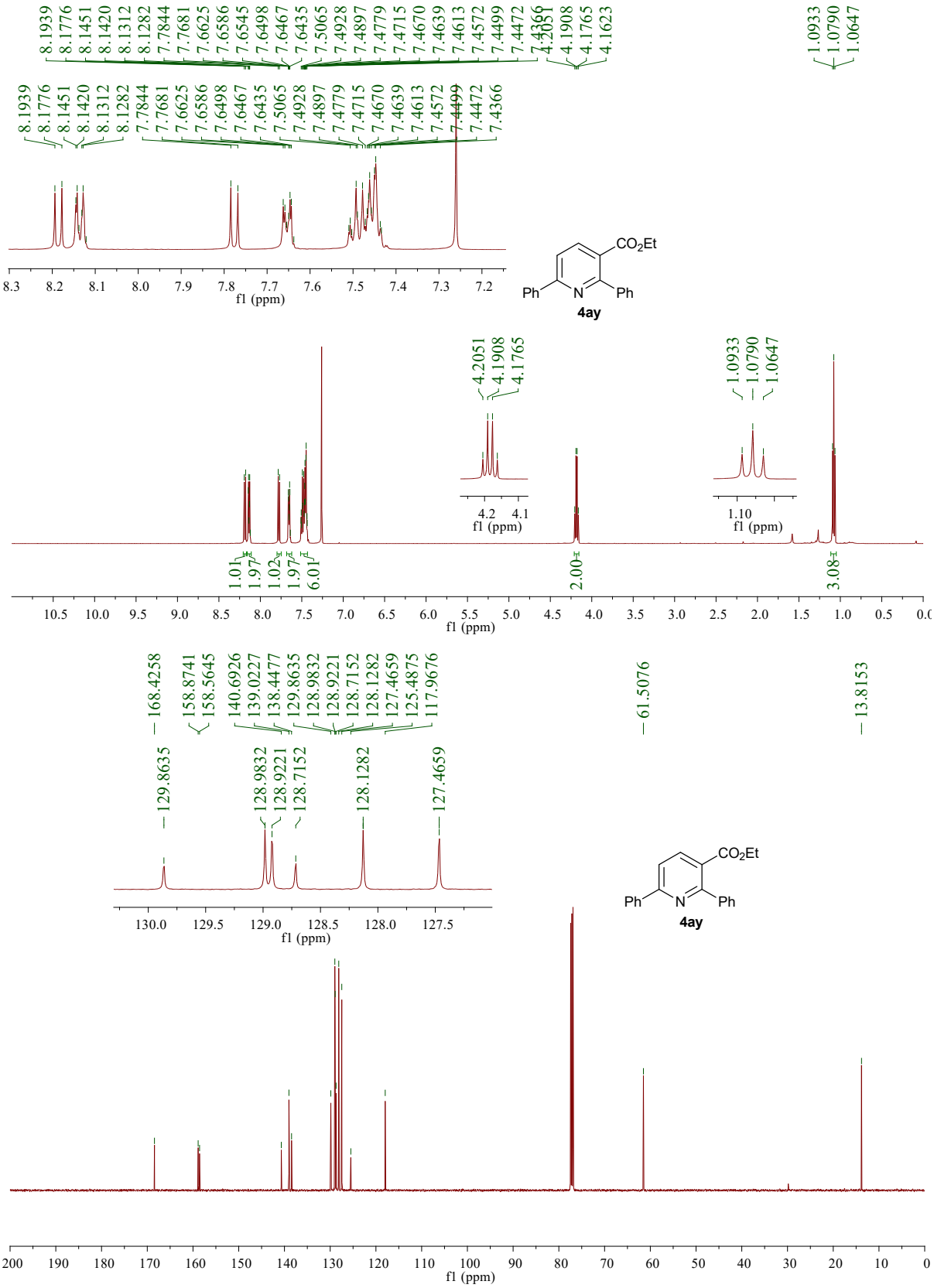
157.9530
157.3794
149.3073
147.2060
139.9195
131.2857
128.9095
128.8304
127.2097
122.8321
121.4213
120.8525
105.1957
99.2486
55.7628
55.6354
OMe
OMe
N
Ph
3da
fl (ppm)


8.5108
8.5004
7.7225
7.7183
7.7095
7.7055
7.6775
7.6733
7.6643
7.6604
7.6050
7.6013
7.5919
7.5879
7.5174
7.5128
7.5088
7.4995
7.4957
7.3863
7.3843
7.3211
7.3180
7.3107
7.3077
2.1862
2.1762
2.1708
2.1612
2.1511
2.1447
1.1313
1.1211
1.1163
1.1107
1.1072
1.1003
1.0942
1.0843
1.0779
1.0738
1.0680
1.0620
1.0572
1.0504
1.0468
Br
N
3in
2.1708
2.1612
2.1511
1.1211
1.1163
1.1107
1.1072
2.16
f1 (ppm)
1.1
1.0
f1 (ppm)
1.00
4.23
2.15
2.07
1.01
1.04
1.11
4.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)
163.3985
149.1375
148.4738
140.8795
139.2934
137.6840
132.1953
128.8056
127.7509
127.7220
122.2265
119.2704
118.7279
17.2628
10.3328
Br
N
3in
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.1776
8.1451
8.1420
8.1312
8.1282
7.7844
7.7681
7.6625
7.6586
7.6498
7.6467
7.6435
7.5065
7.4928
7.4897
7.4779
7.4715
7.4670
7.4639
7.4613
7.4572
7.4499
7.4472
7.4366
4.2051
4.1908
4.1765
4.1623
1.0933
1.0790
1.0647
f1 (ppm)
CO2Et
Ph
N
Ph
4ay
1.01
1.97
1.02
1.97
6.01
2.00
3.08
168.4258
158.8741
158.5645
140.6926
139.0227
138.4477
129.8635
128.9832
128.9221
128.7152
128.1282
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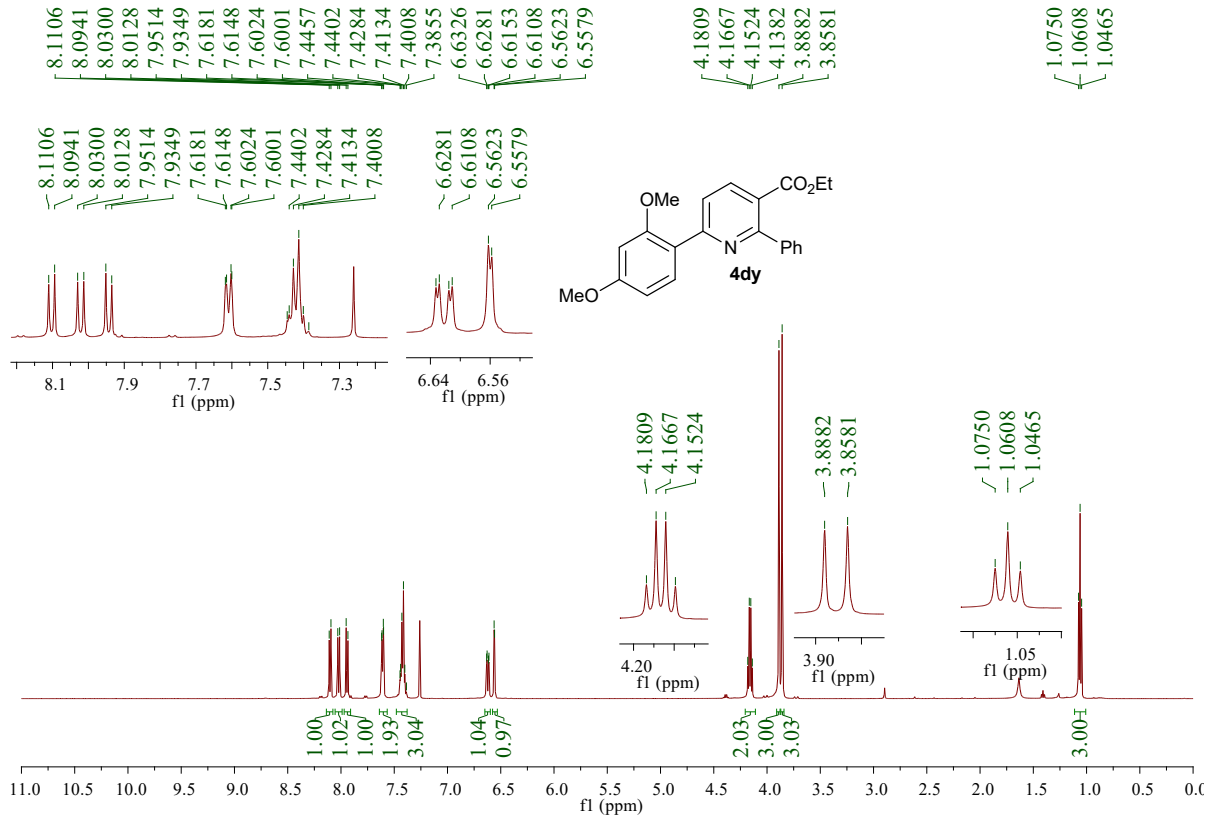
125.4875
117.9676
61.5076
13.8153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8.0300
8.0128
7.9514
7.9349
7.6181
7.6148
7.6024
7.6001
7.4457
7.4402
7.4284
7.4134
7.4008
7.3855
6.6326
6.6281
6.6153
6.6108
6.5623
6.5579
4.1809
4.1667
4.1524
4.1382
3.8882
3.8581
1.0750
1.0608
1.0465
OMe
CO2Et
N
Ph
MeO
4dy
f1 (ppm)
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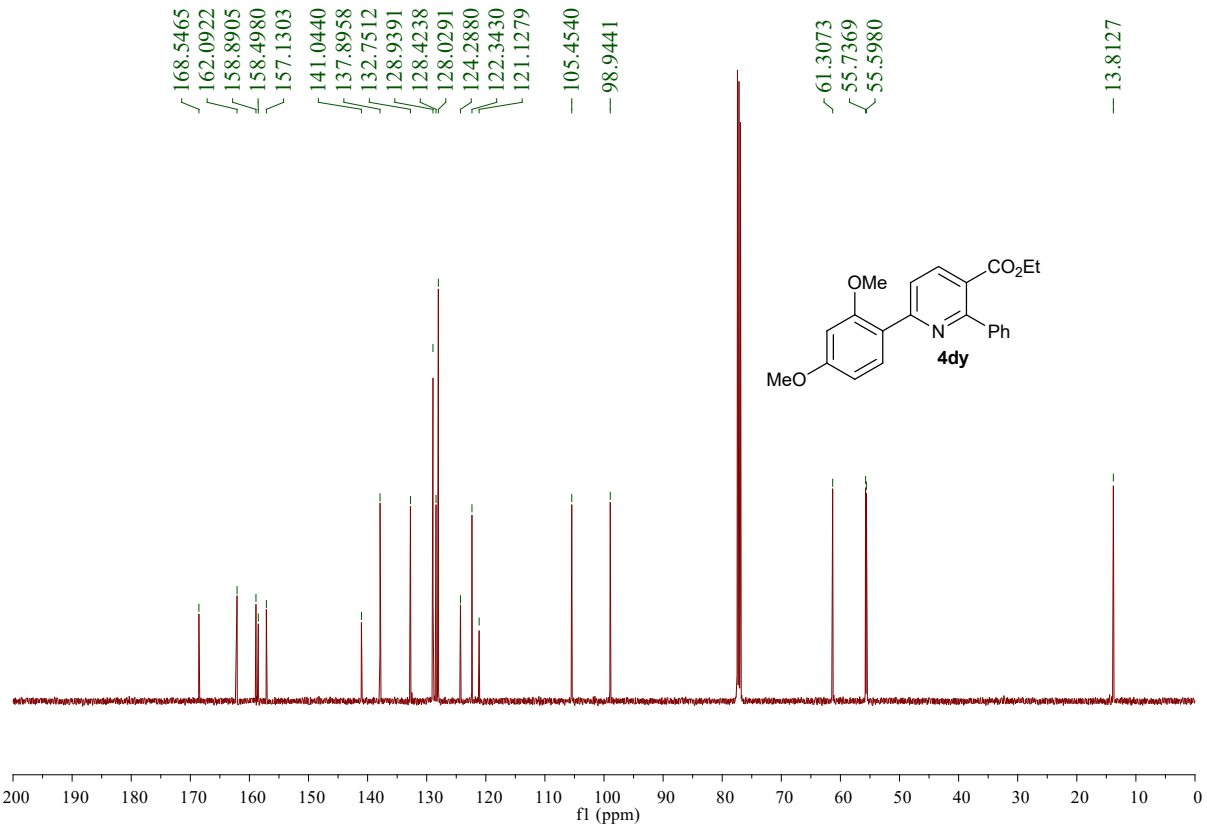
1.02
1.00
1.93
3.04
1.04
0.97
2.03
3.00
3.03
3.00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158.8905
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157.1303
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137.8958
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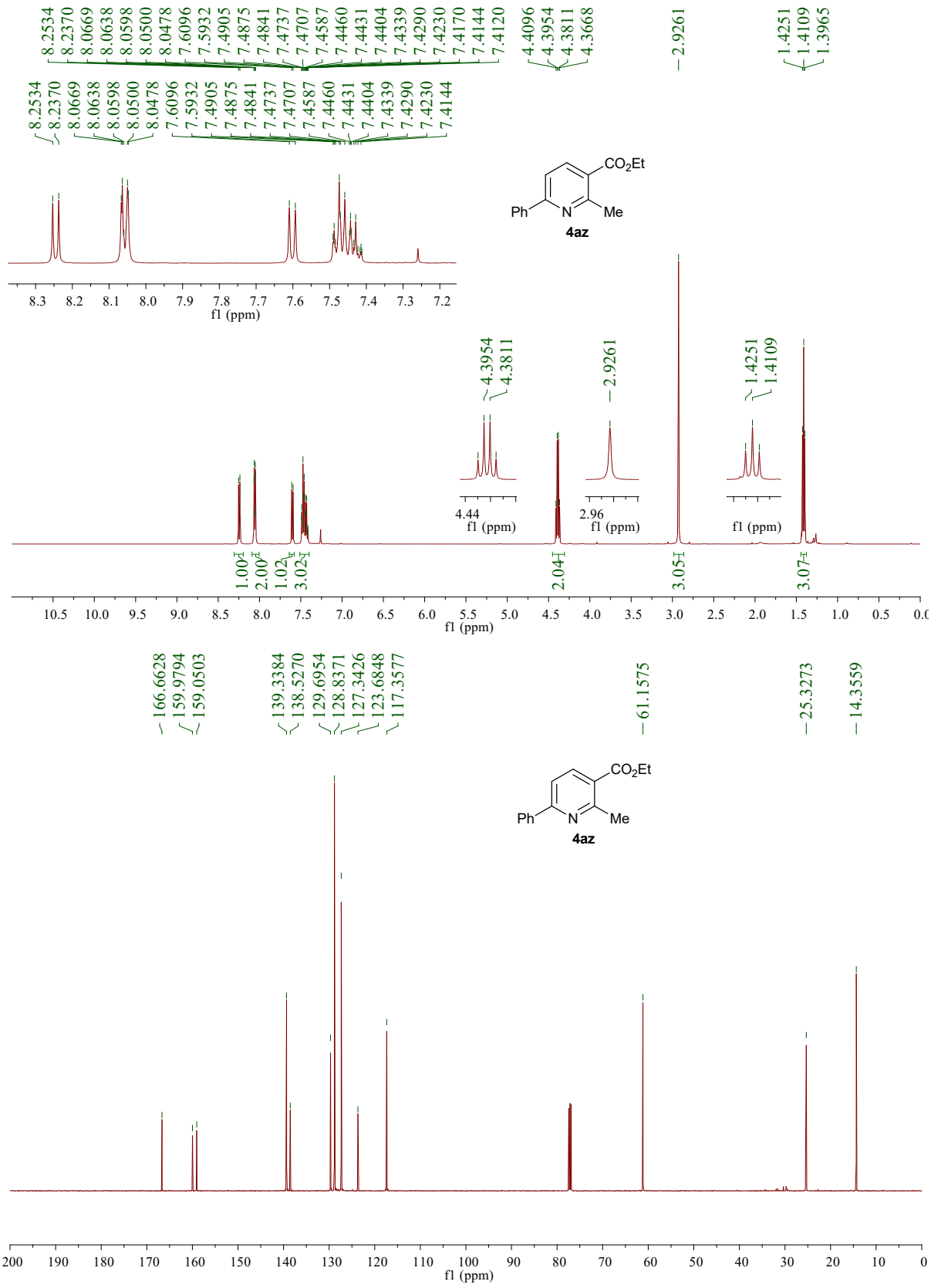
128.9391
128.4238
128.0291
124.2880
122.3430
121.1279
105.4540
98.9441
61.3073
55.7369
55.5980
13.8127
OMe
CO2Et
N
Ph
MeO
4dy
f1 (ppm)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8.0669
8.0638
8.0598
8.0500
8.0478
7.6096
7.5932
7.4905
7.4875
7.4841
7.4737
7.4707
7.4587
7.4460
7.4431
7.4404
7.4339
7.4290
7.4230
7.4170
7.4144
7.4120
4.4096
4.3954
4.3811
4.3668
2.9261
1.4251
1.4109
1.3965
CO2Et
Ph
N
Me
4az
f1 (ppm)
1.00
2.00
1.02
3.02
2.04
3.05
3.07
166.6628
159.9794
159.0503
139.3384
138.5270
129.6954
128.8371
127.3426
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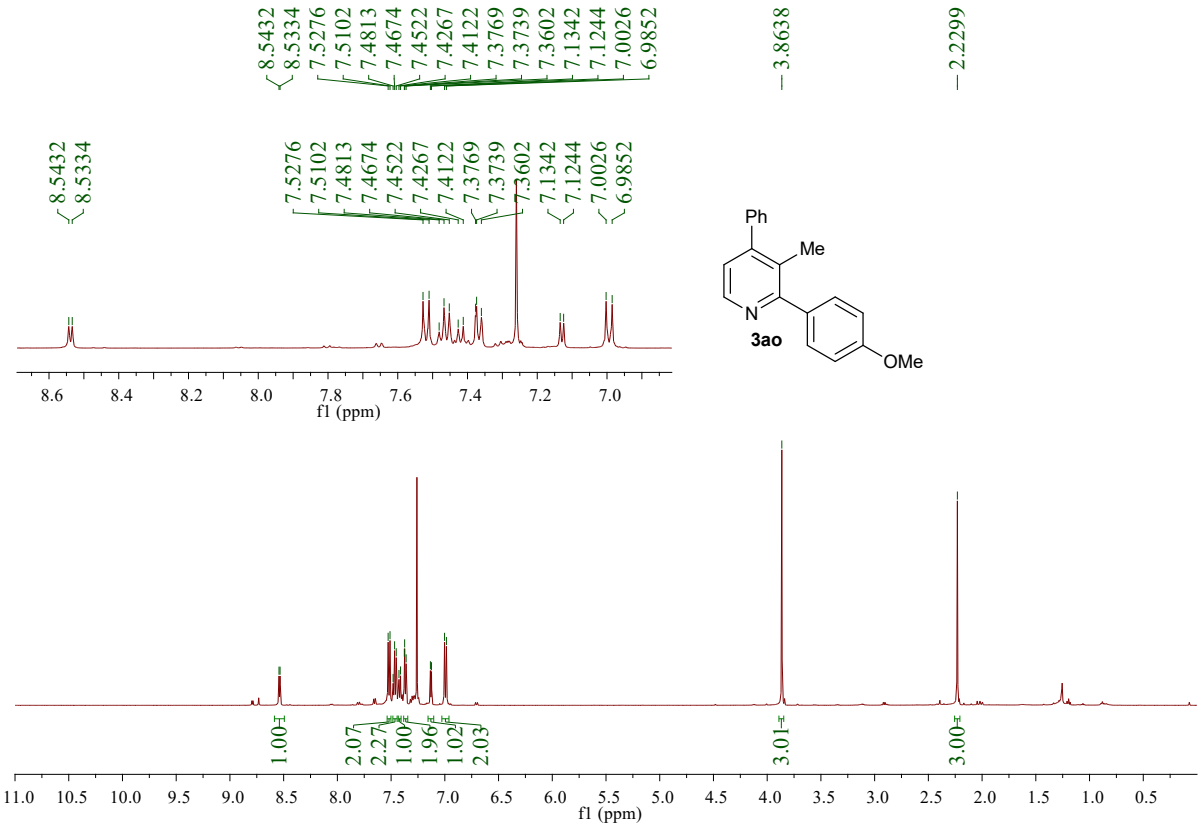
117.3577
61.1575
25.3273
14.3559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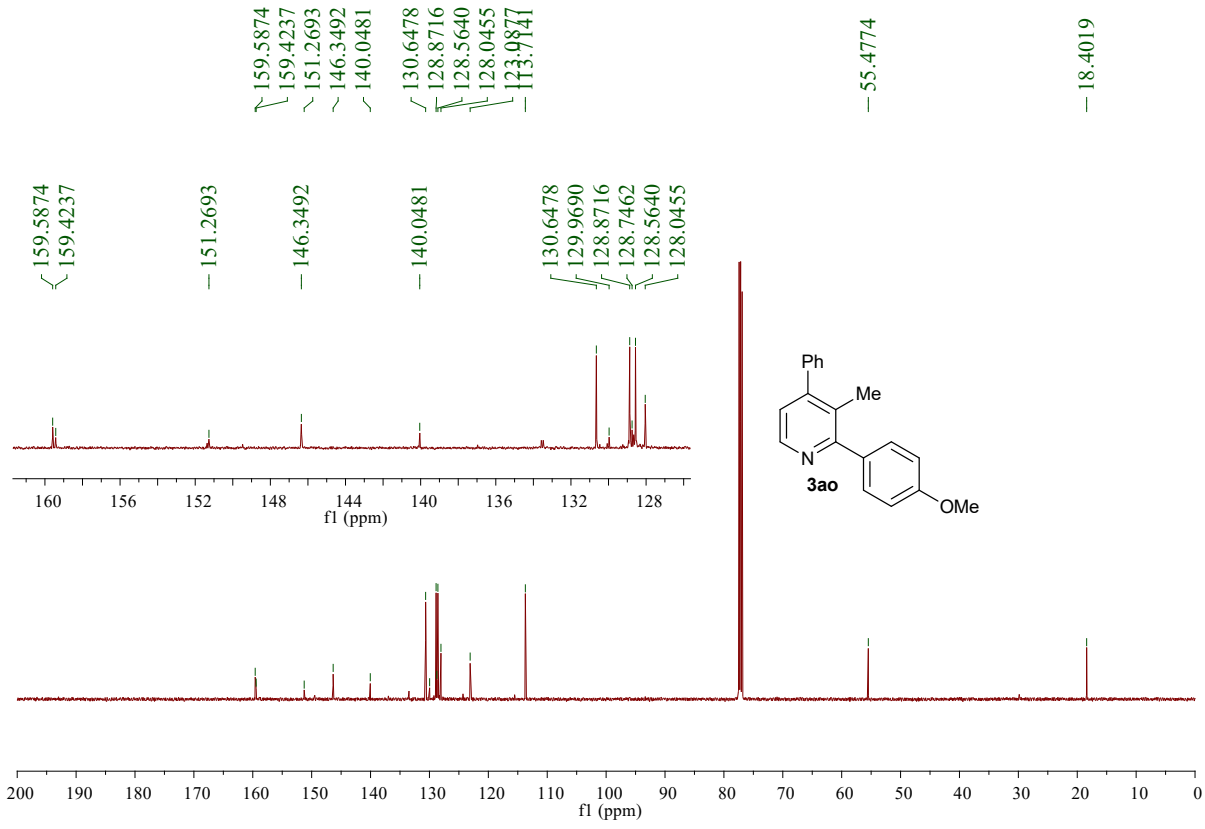
8.5334
7.5276
7.5102
7.4813
7.4674
7.4522
7.4267
7.4122
7.3769
7.3739
7.3602
7.1342
7.1244
7.0026
6.9852
3.8638
2.2299
Ph
Me
N
3ao
OMe
f1 (ppm)
1.00
2.07
2.27
1.00
1.96
1.02
2.03
3.01
3.00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146.3492
140.0481
130.6478
128.8716
128.5640
128.0455
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55.4774
18.4019
129.9690
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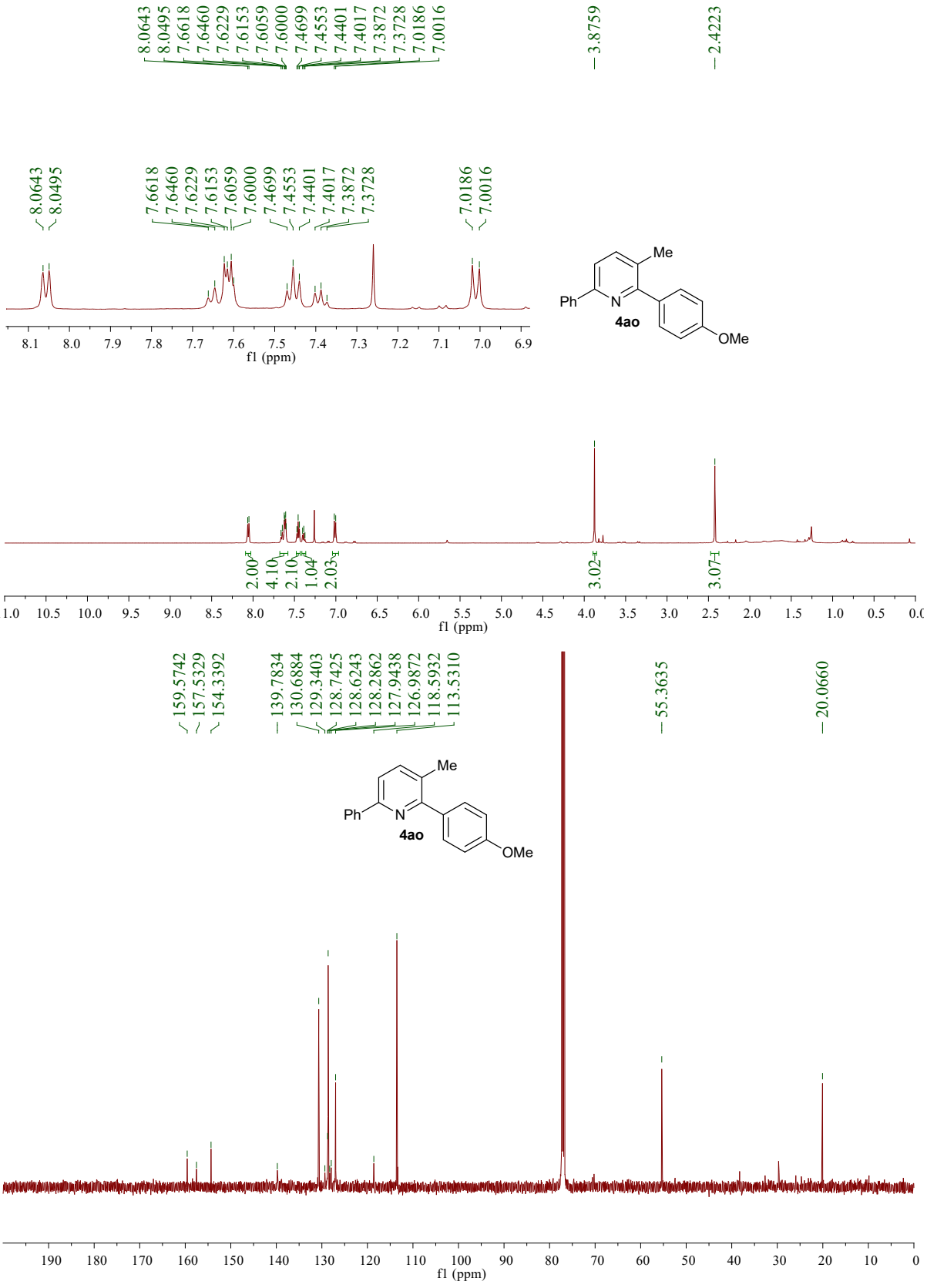
Ph
Me
N
3ao
OMe
f1 (ppm)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7.6229
7.6153
7.6059
7.6000
7.4699
7.4553
7.4401
7.4017
7.3872
7.3728
7.0186
7.0016
3.8759
2.4223
f1 (ppm)
Me
Ph
N
4ao
OMe
2.00
4.10
2.10
1.04
2.03
3.02
3.07
159.5742
157.5329
154.3392
139.7834
130.6884
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128.6243
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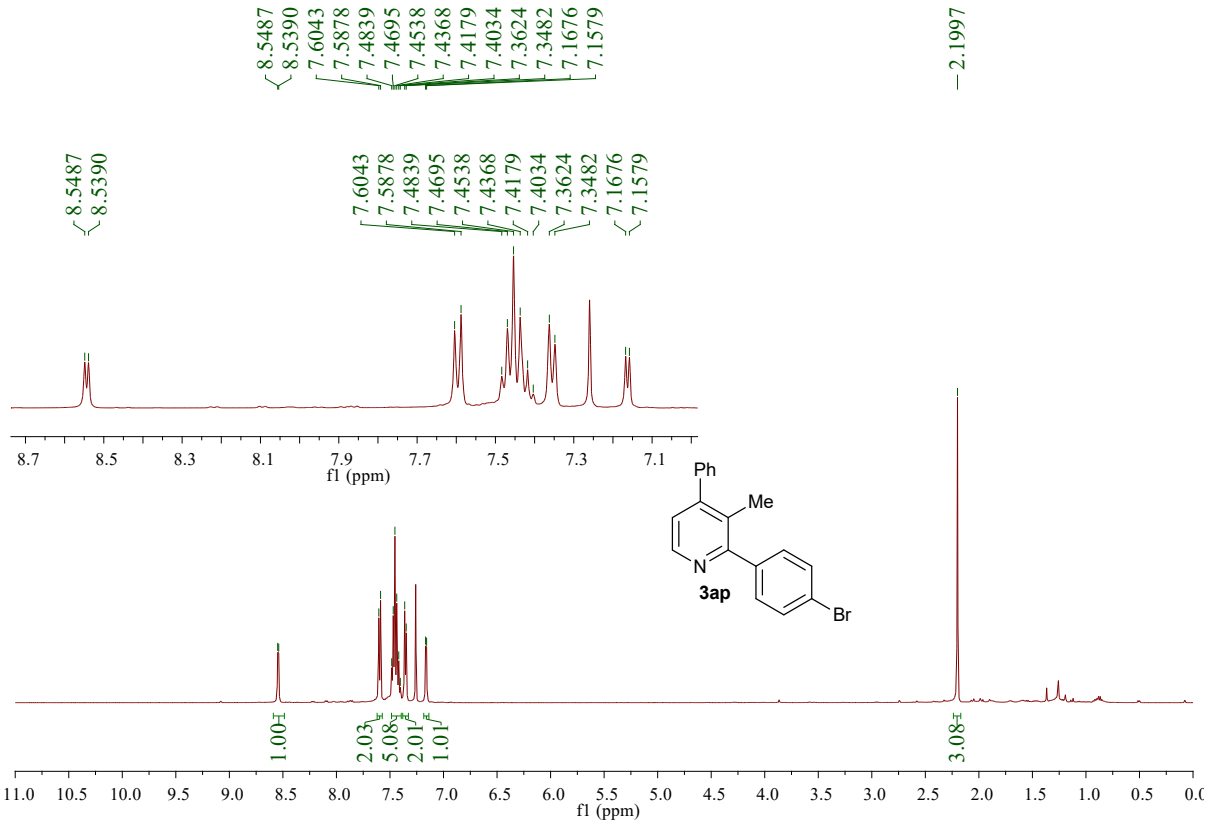
20.0660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7.4179
7.4034
7.3624
7.3482
7.1676
7.1579
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Ph
Me
N
3ap
Br
1.00
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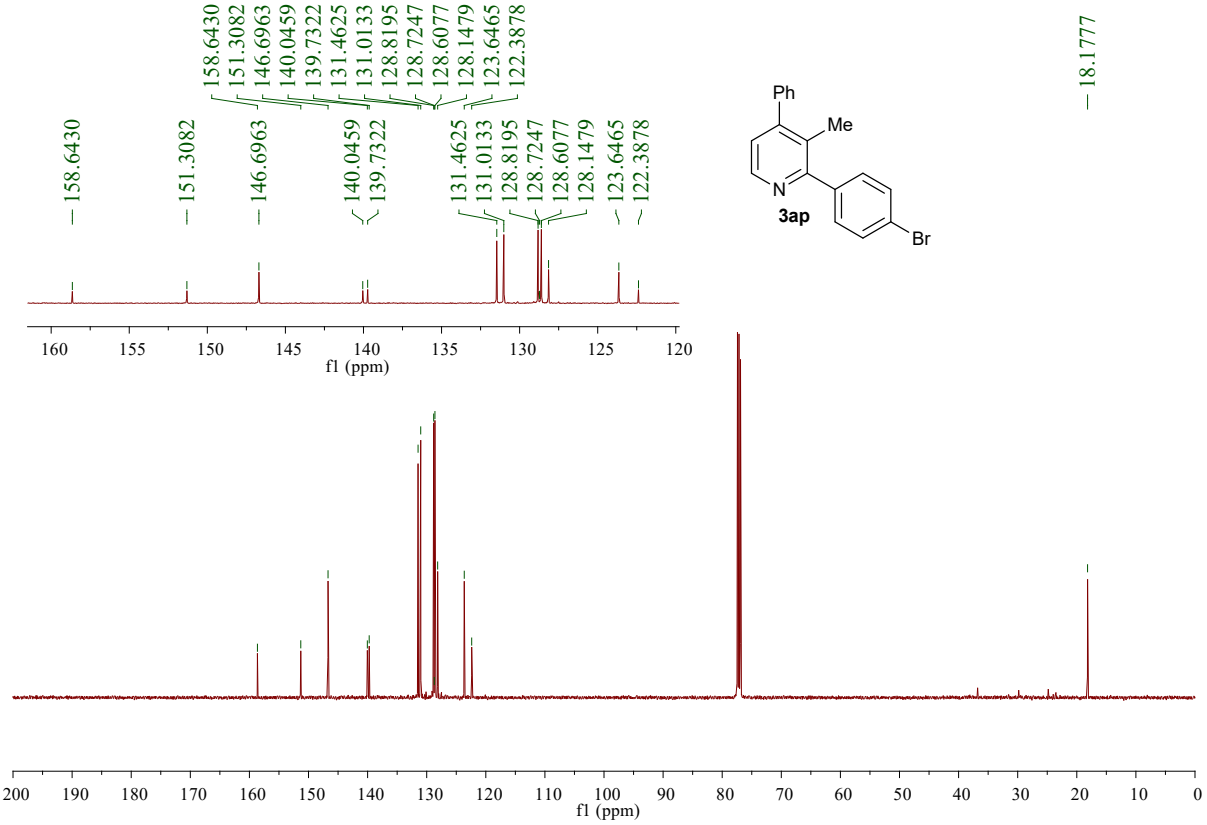
5.08
2.01
1.01
3.08
f1 (ppm)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131.0133
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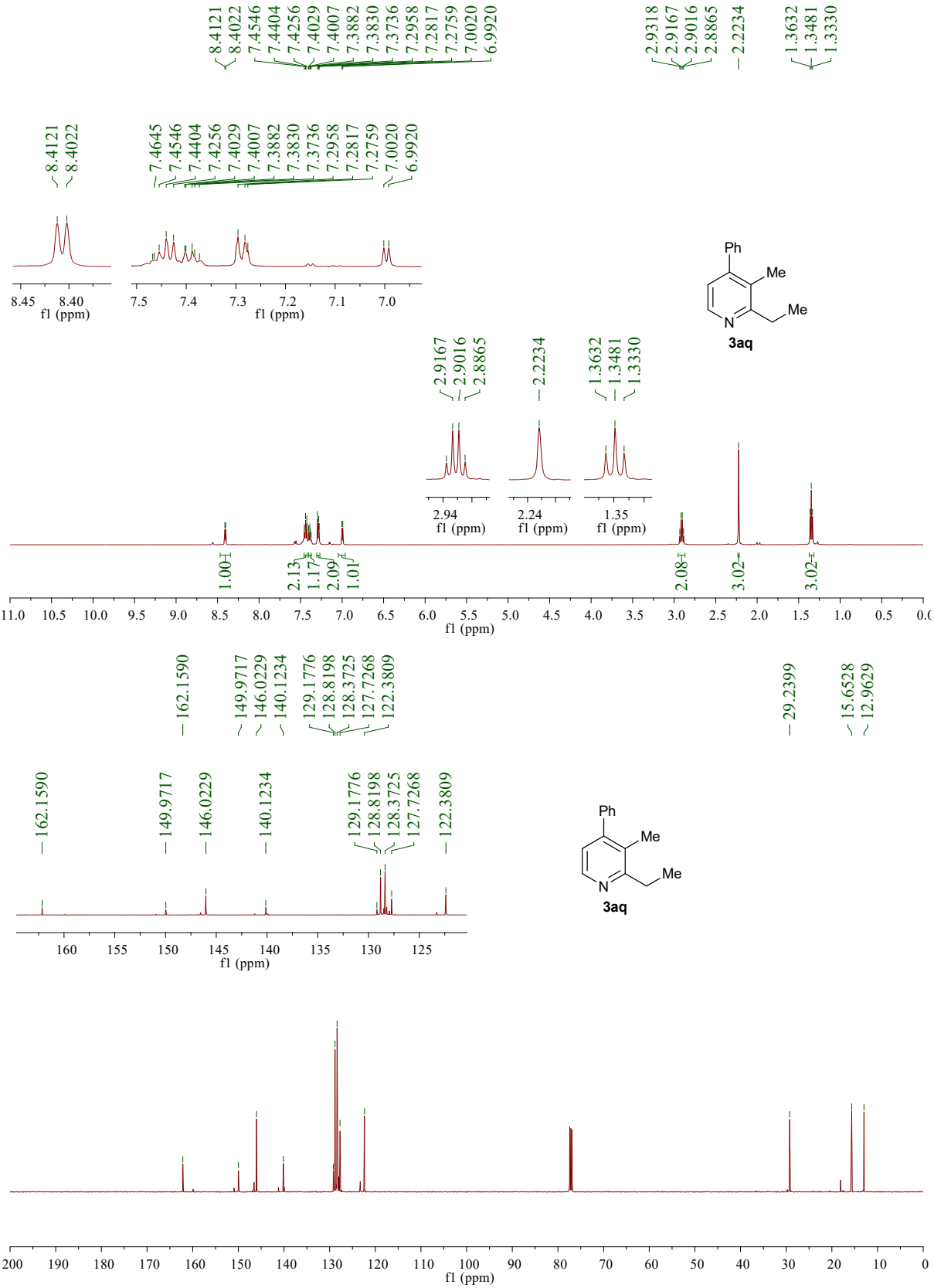
Ph
Me
N
3ap
Br
f1 (ppm)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7.3830
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7.2958
7.2817
7.2759
7.0020
6.9920
2.9318
2.9167
2.9016
2.8865
2.2234
1.3632
1.3481
1.3330
f1 (ppm)
Ph
Me
Me
N
3aq
1.00
2.13
1.17
2.09
1.01
2.08
3.02
3.02
162.1590
149.9717
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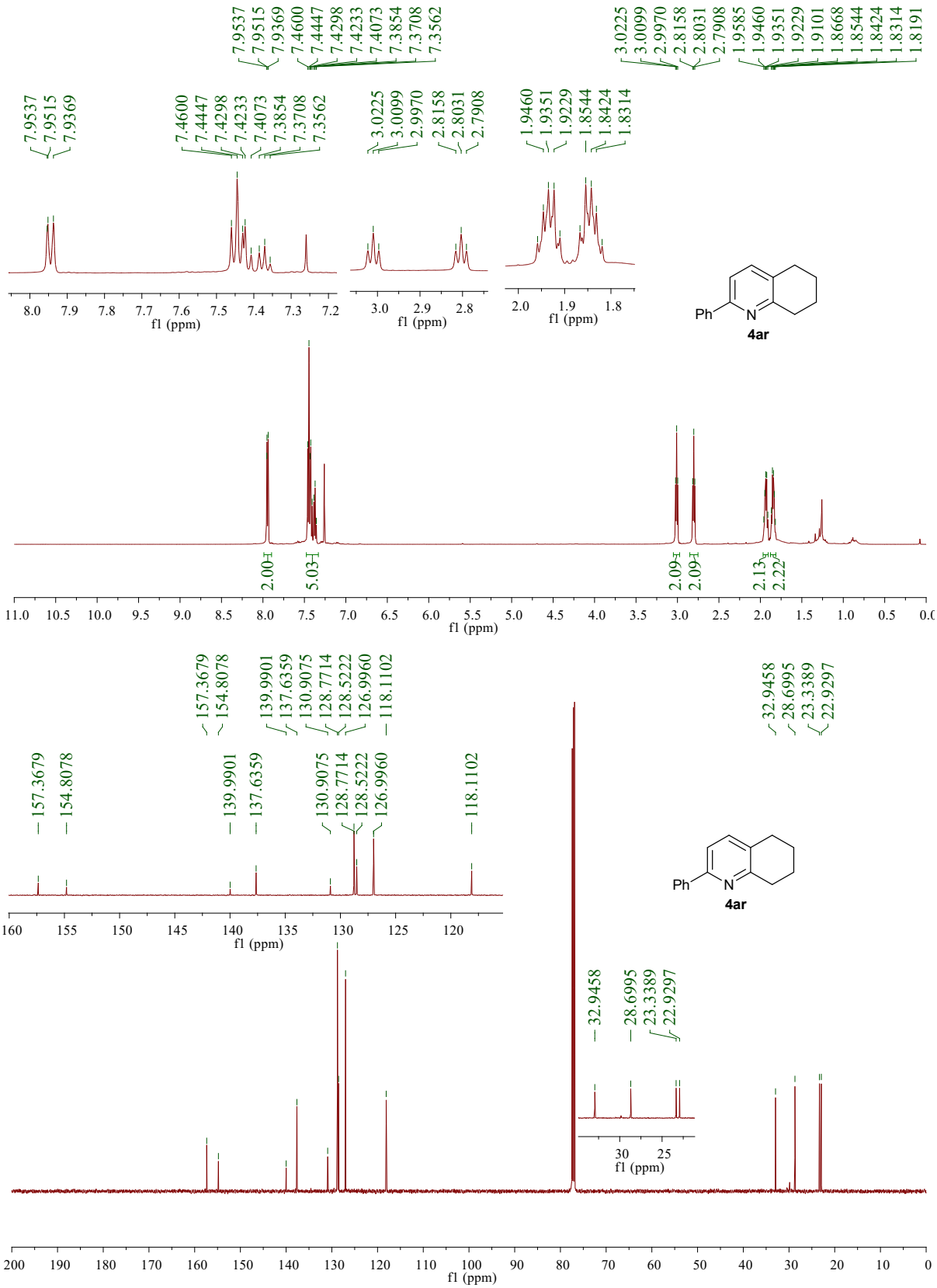
12.9629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7.4233
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7.3854
7.3708
7.3562
3.0225
3.0099
2.9970
2.8158
2.8031
2.7908
1.9585
1.9460
1.9351
1.9229
1.9101
1.8668
1.8544
1.8424
1.8314
1.8191
f1 (ppm)
Ph
N
4ar
2.00
5.03
2.09
2.09
2.13
2.22
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154.8078
139.9901
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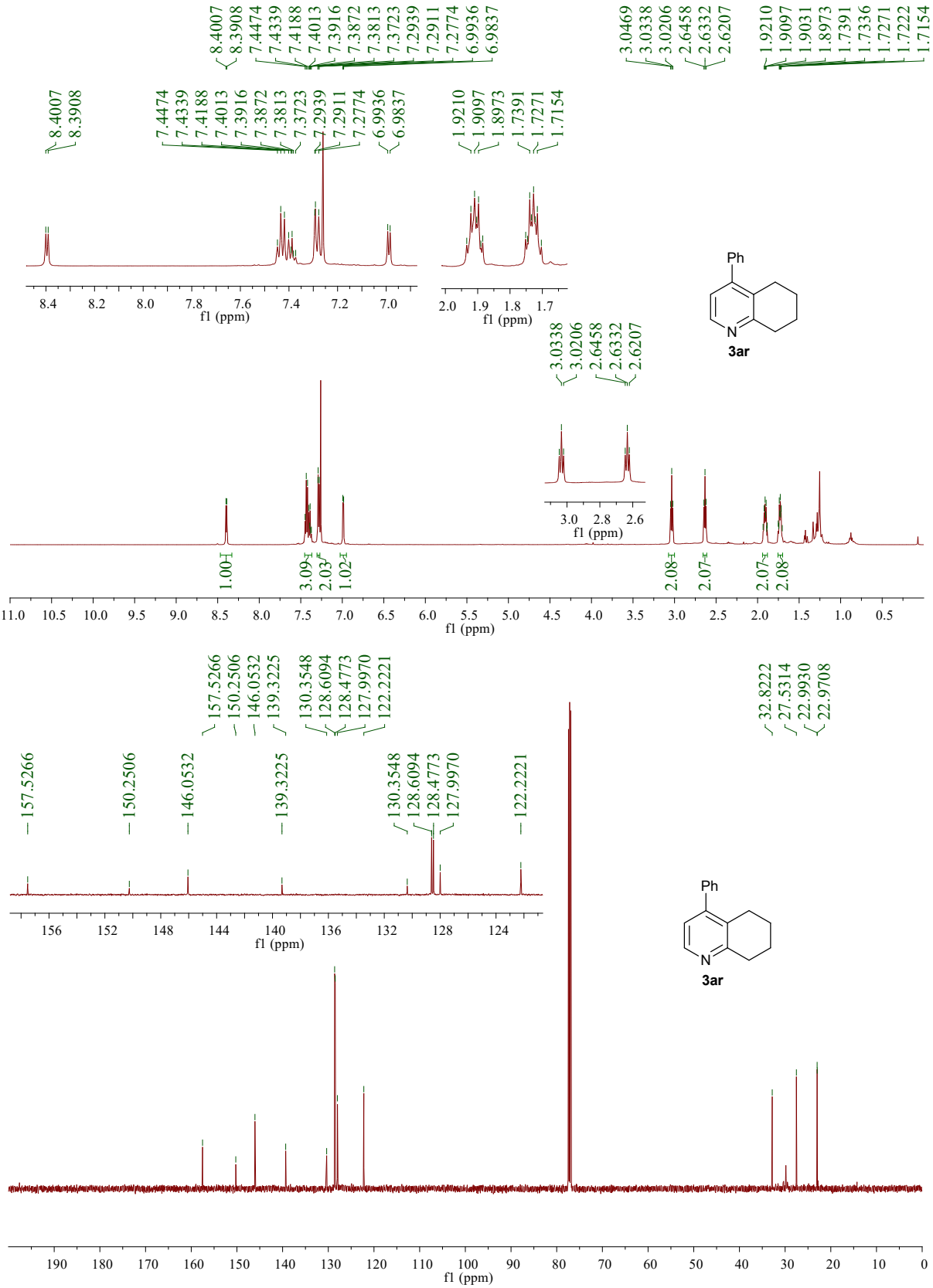
22.9297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7.3813
7.3723
7.2939
7.2911
7.2774
6.9936
6.9837
3.0469
3.0338
3.0206
2.6458
2.6332
2.6207
1.9210
1.9097
1.9031
1.8973
1.7391
1.7336
1.7271
1.7222
1.7154
f1 (ppm)
Ph
N
3ar
1.00
3.09
2.03
1.02
2.08
2.07
2.07
2.08
157.5266
150.2506
146.0532
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127.9970
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32.8222
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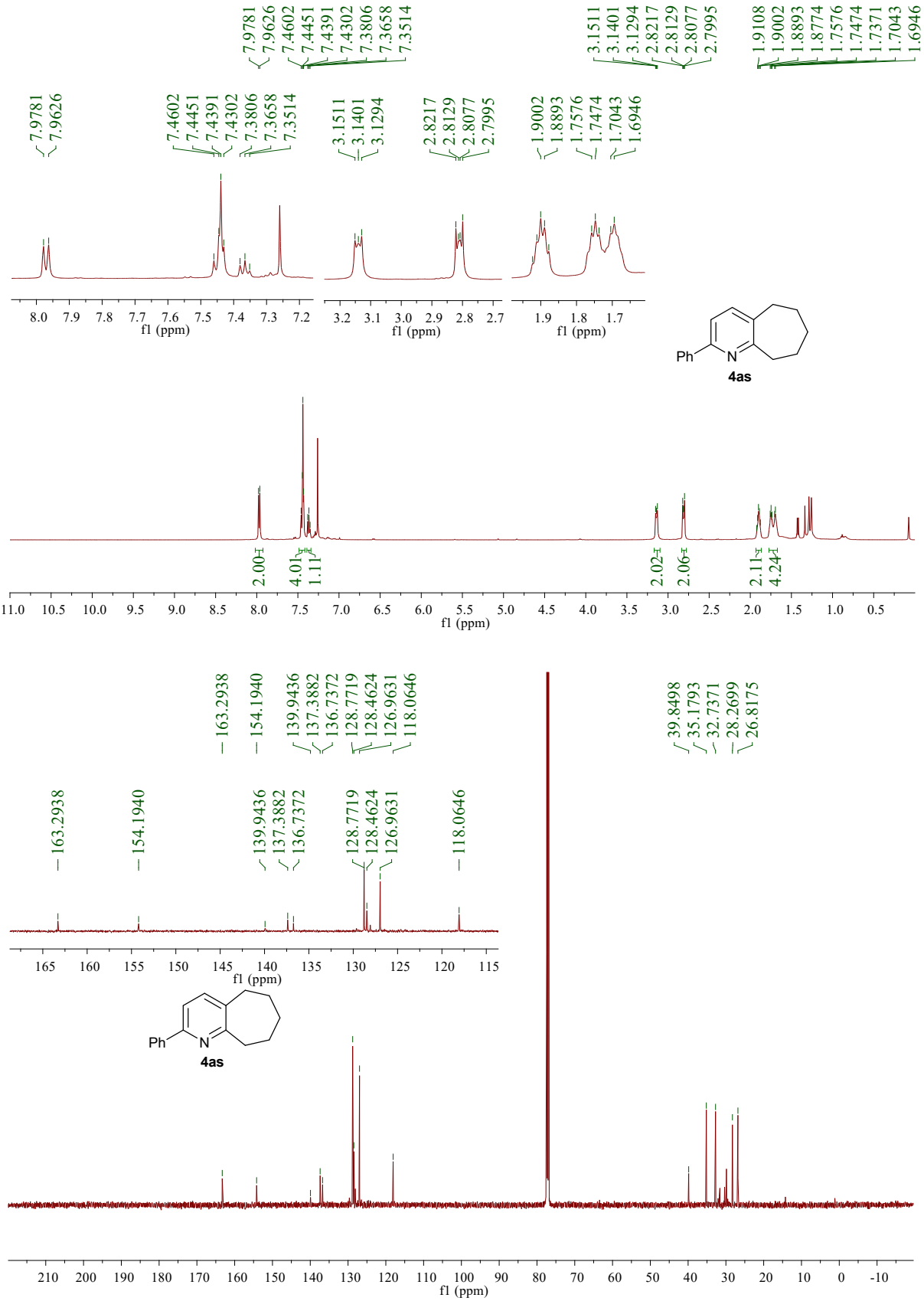
22.9708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3.1294
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2.8129
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1.9002
1.8893
1.8774
1.7576
1.7474
1.7371
1.7043
1.6946
f1 (ppm)
Ph
N
4as
2.00
4.01
1.11
2.02
2.06
2.11
4.24
163.2938
154.1940
139.9436
137.3882
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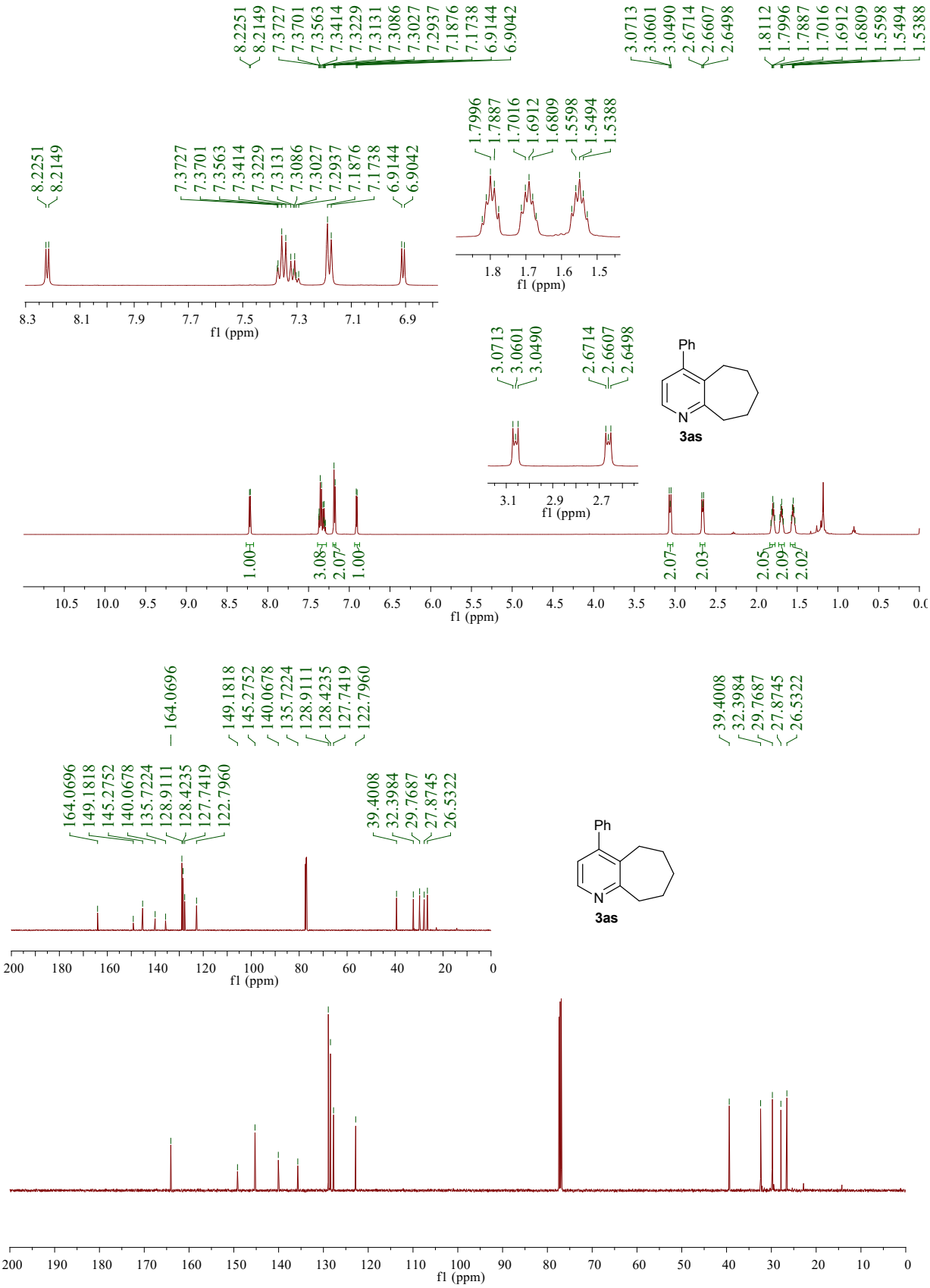
26.8175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7.1876
7.1738
6.9144
6.9042
3.0713
3.0601
3.0490
2.6714
2.6607
2.6498
1.8112
1.7996
1.7887
1.7016
1.6912
1.6809
1.5598
1.5494
1.5388
fl (ppm)
Ph
N
3as
1.00
3.08
2.07
1.00
2.07
2.03
2.05
2.09
2.02
164.0696
149.1818
145.2752
140.0678
135.7224
128.9111
128.4235
127.7419
122.7960
39.4008
32.3984
29.7687
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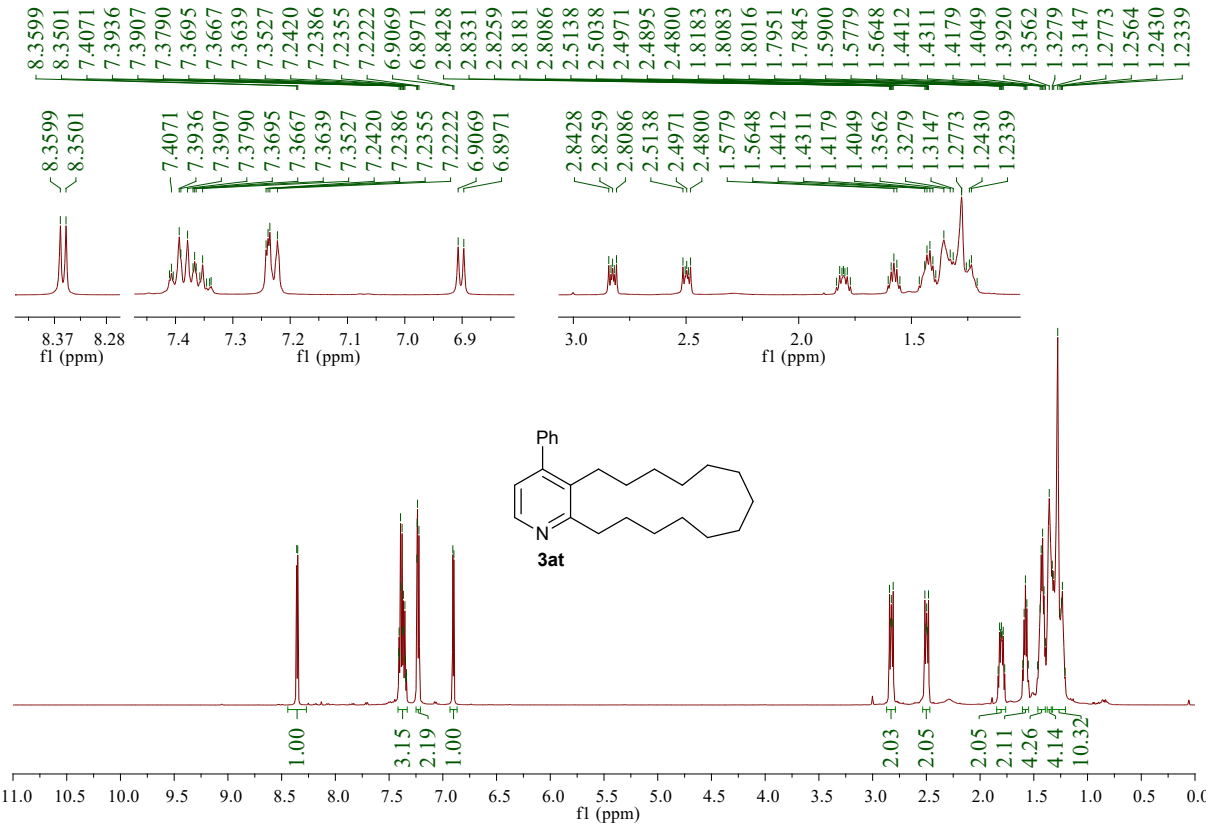
26.5322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7.3527
7.2420
7.2386
7.2355
7.2222
6.9069
6.8971
2.8428
2.8331
2.8259
2.8181
2.8086
2.5138
2.5038
2.4971
2.4895
2.4800
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1.8083
1.8016
1.7951
1.7845
1.5900
1.5779
1.5648
1.4412
1.4311
1.4179
1.4049
1.3920
1.3562
1.3279
1.3147
1.2773
1.2564
1.2430
1.2339
f1 (ppm)
Ph
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2.19
1.00
2.03
2.05
2.05
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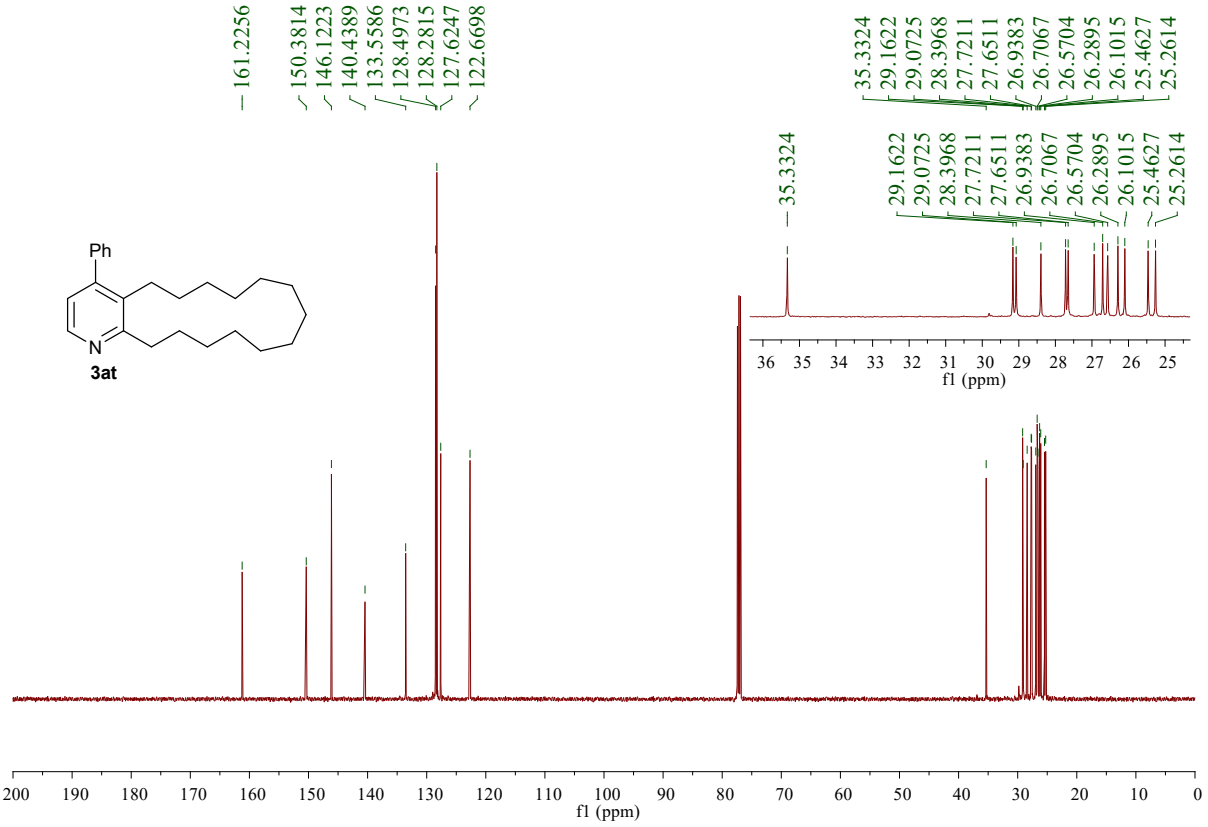
4.14
10.32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29.1622
29.0725
28.3968
27.7211
27.6511
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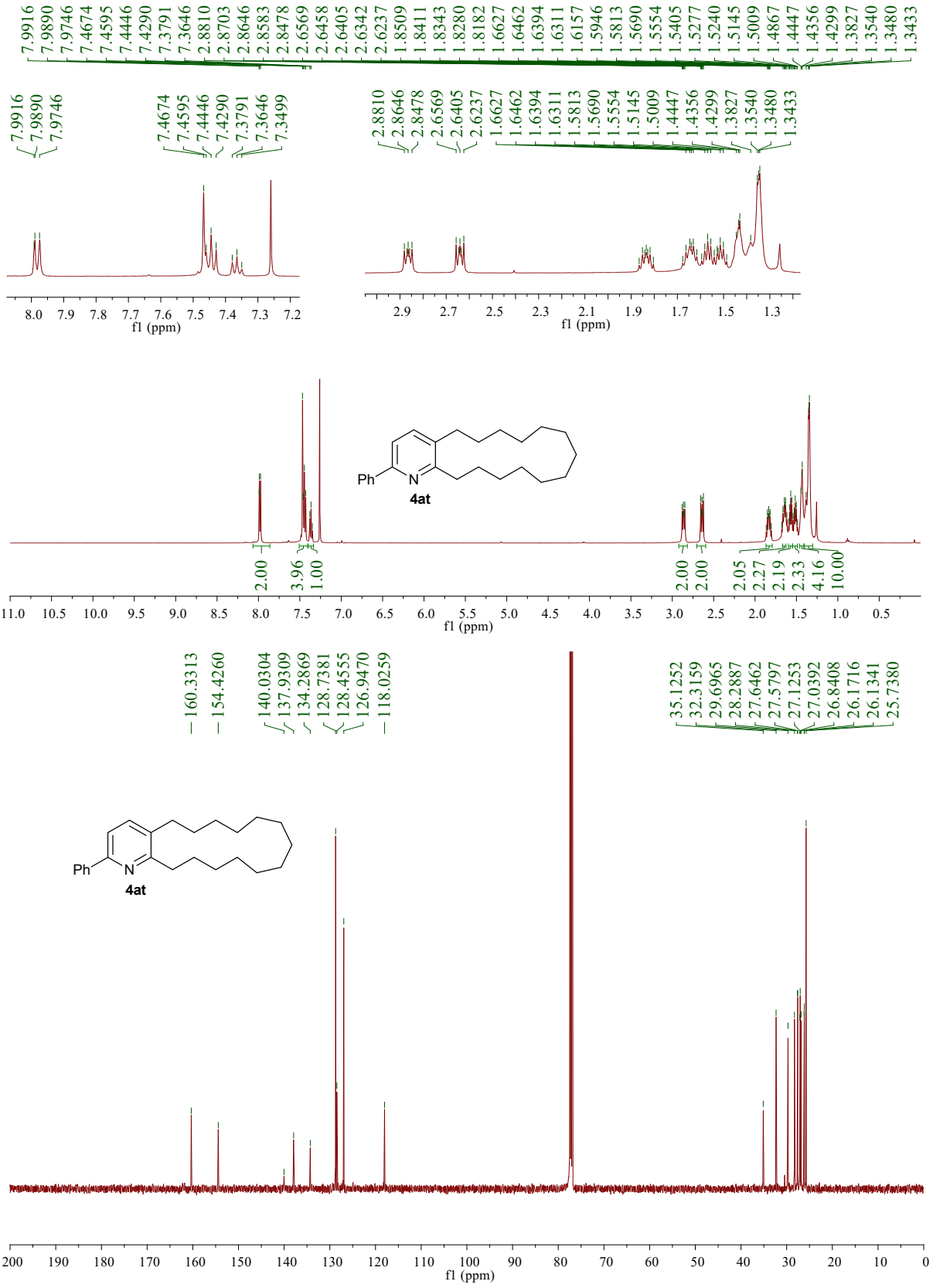
26.5704
26.2895
26.1015
25.4627
25.2614
f1 (ppm)
Ph
N
3at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2.8646
2.8583
2.8478
2.6569
2.6458
2.6405
2.6342
2.6237
1.8509
1.8411
1.8343
1.8280
1.8182
1.6627
1.6462
1.6394
1.6311
1.6157
1.5946
1.5813
1.5690
1.5554
1.5405
1.5277
1.5240
1.5145
1.5009
1.4867
1.4447
1.4356
1.4299
1.3827
1.3540
1.3480
1.3433
7.3499
fl (ppm)
Ph
N
4at
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3.96
1.00
2.05
2.27
2.19
2.33
4.16
10.00
160.3313
154.4260
140.0304
137.9309
134.2869
128.7381
128.4555
126.9470
118.0259
35.1252
32.3159
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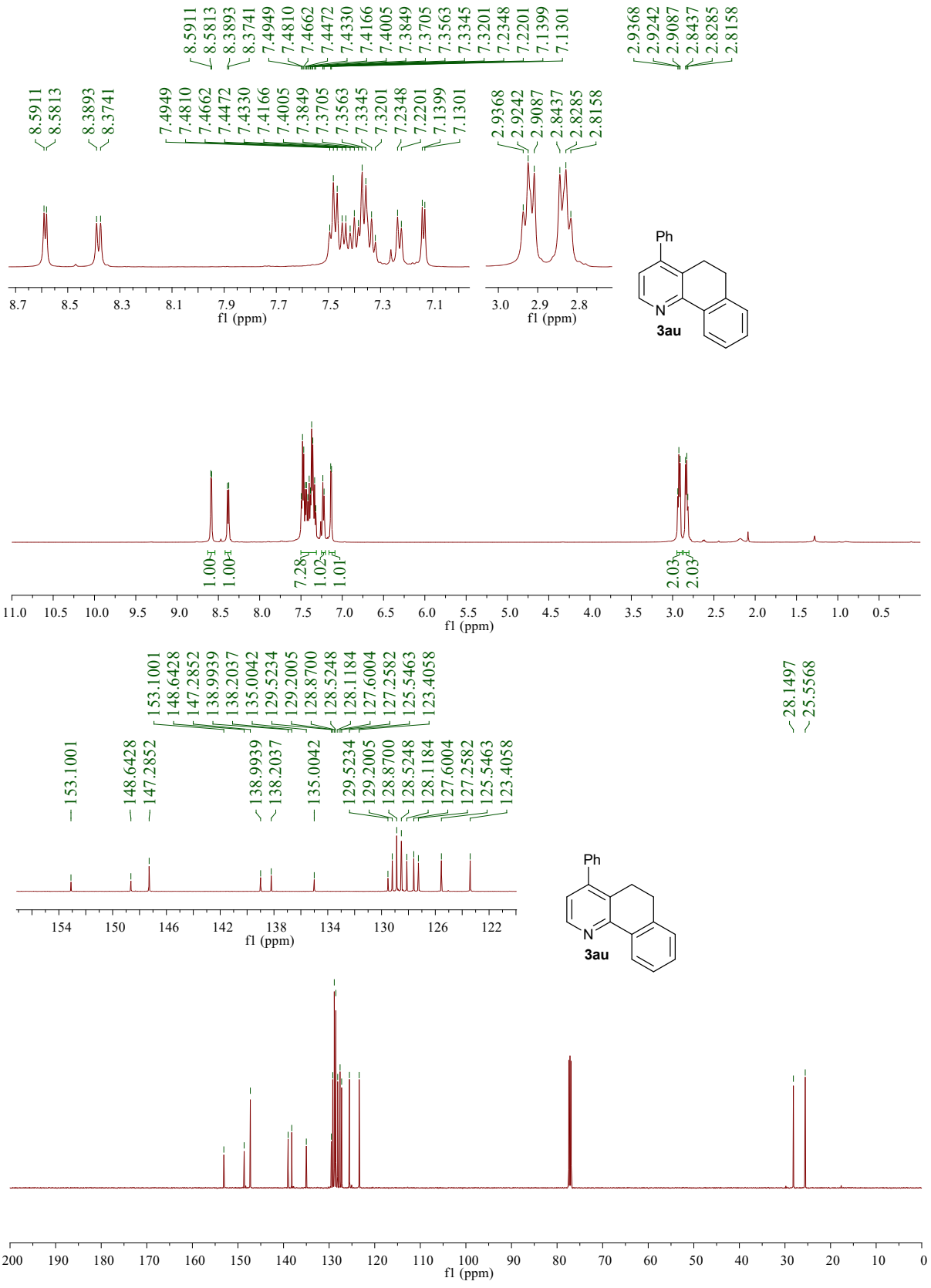
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7.4330
7.4166
7.4005
7.3849
7.3705
7.3563
7.3345
7.3201
7.2348
7.2201
7.1399
7.1301
2.9368
2.9242
2.9087
2.8437
2.8285
2.8158
f1 (ppm)
Ph
N
3au
1.00
1.00
7.28
1.02
1.01
2.03
2.03
153.1001
148.6428
147.2852
138.9939
138.2037
135.0042
129.5234
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127.6004
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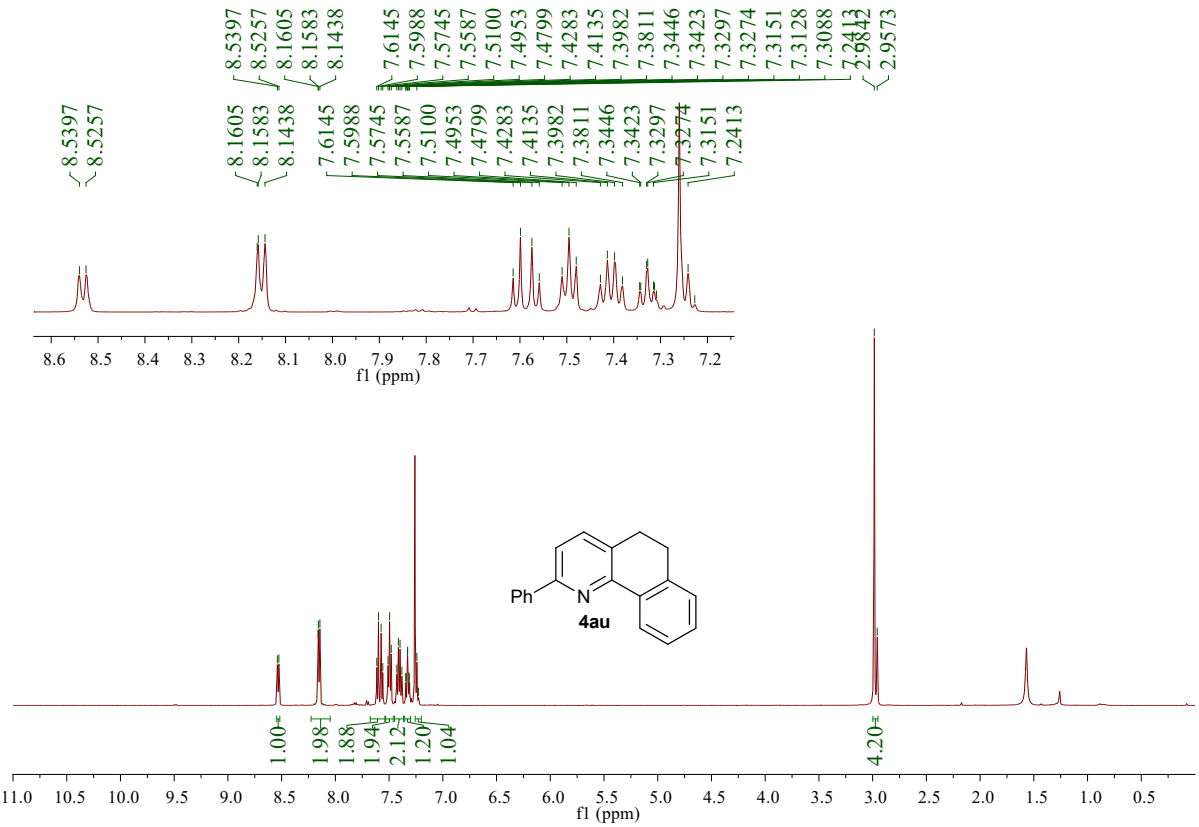
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7.5587
7.5100
7.4953
7.4799
7.4283
7.4135
7.3982
7.3811
7.3446
7.3423
7.3297
7.3274
7.3151
7.2413
2.9842
2.9573
f1 (ppm)
Ph
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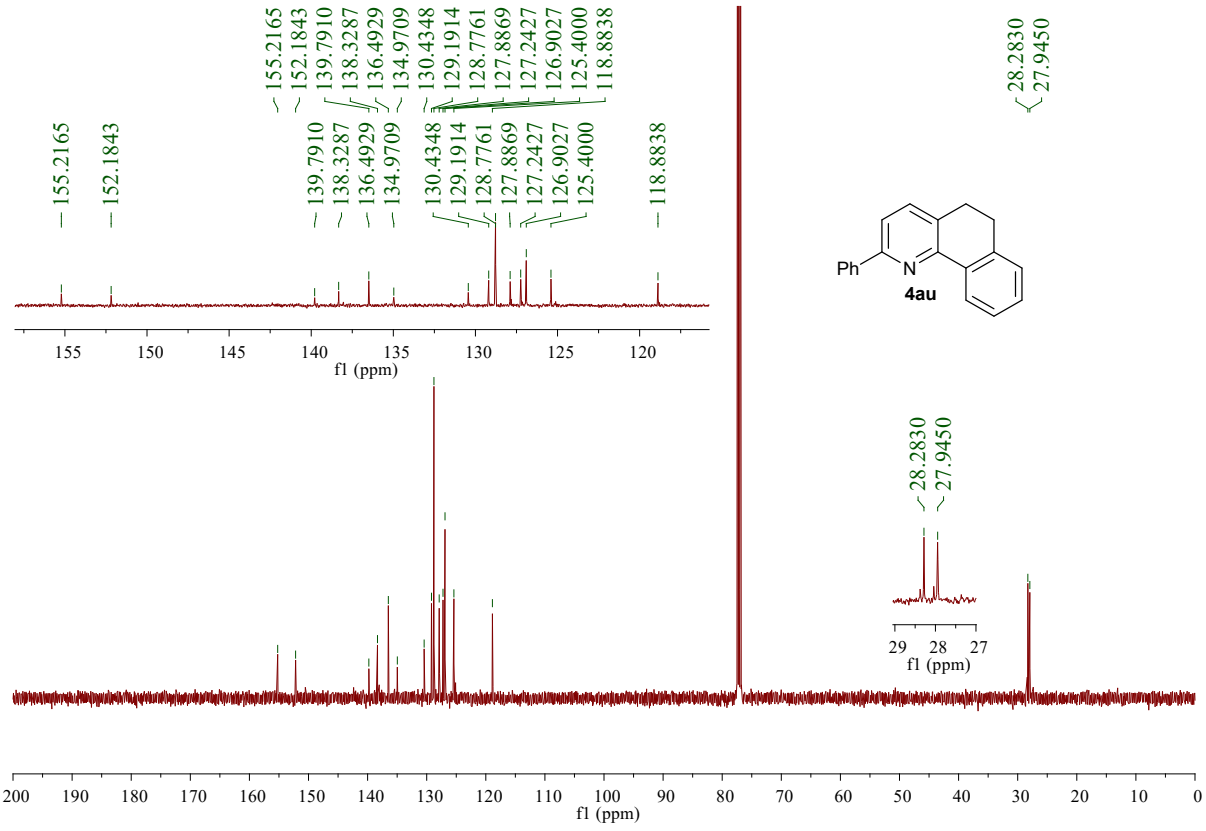
4au
1.00
1.98
1.88
1.94
2.12
1.20
1.04
4.20
f1 (ppm)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136.4929
134.9709
130.4348
129.1914
128.7761
127.8869
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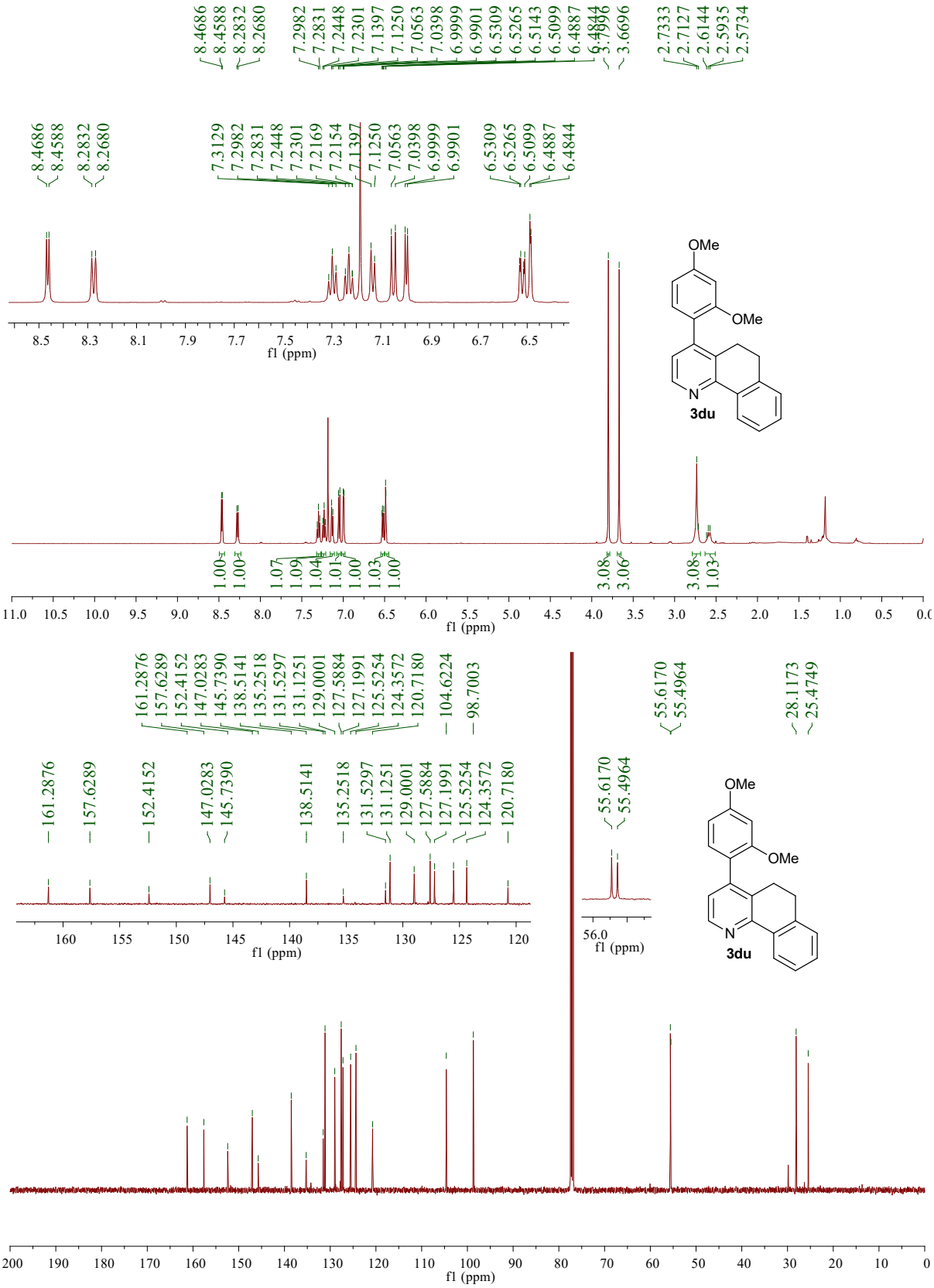
126.9027
125.4000
118.8838
28.2830
27.9450
f1 (ppm)
Ph
N
4au
f1 (ppm)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8.2832
8.2680
7.2982
7.2831
7.2448
7.2301
7.1397
7.1250
7.0563
7.0398
6.9999
6.9901
6.5309
6.5265
6.5143
6.5099
6.4887
6.4844
3.7996
3.6696
2.7333
2.7127
2.6144
2.5935
2.5734
7.3129
7.2169
7.2154
OMe
OMe
N
3du
1.00
1.00
1.07
1.09
1.04
1.01
1.00
1.03
1.00
3.08
3.06
3.08
1.03
f1 (ppm)
161.2876
157.6289
152.4152
147.0283
145.7390
138.5141
135.2518
131.5297
131.1251
129.0001
127.5884
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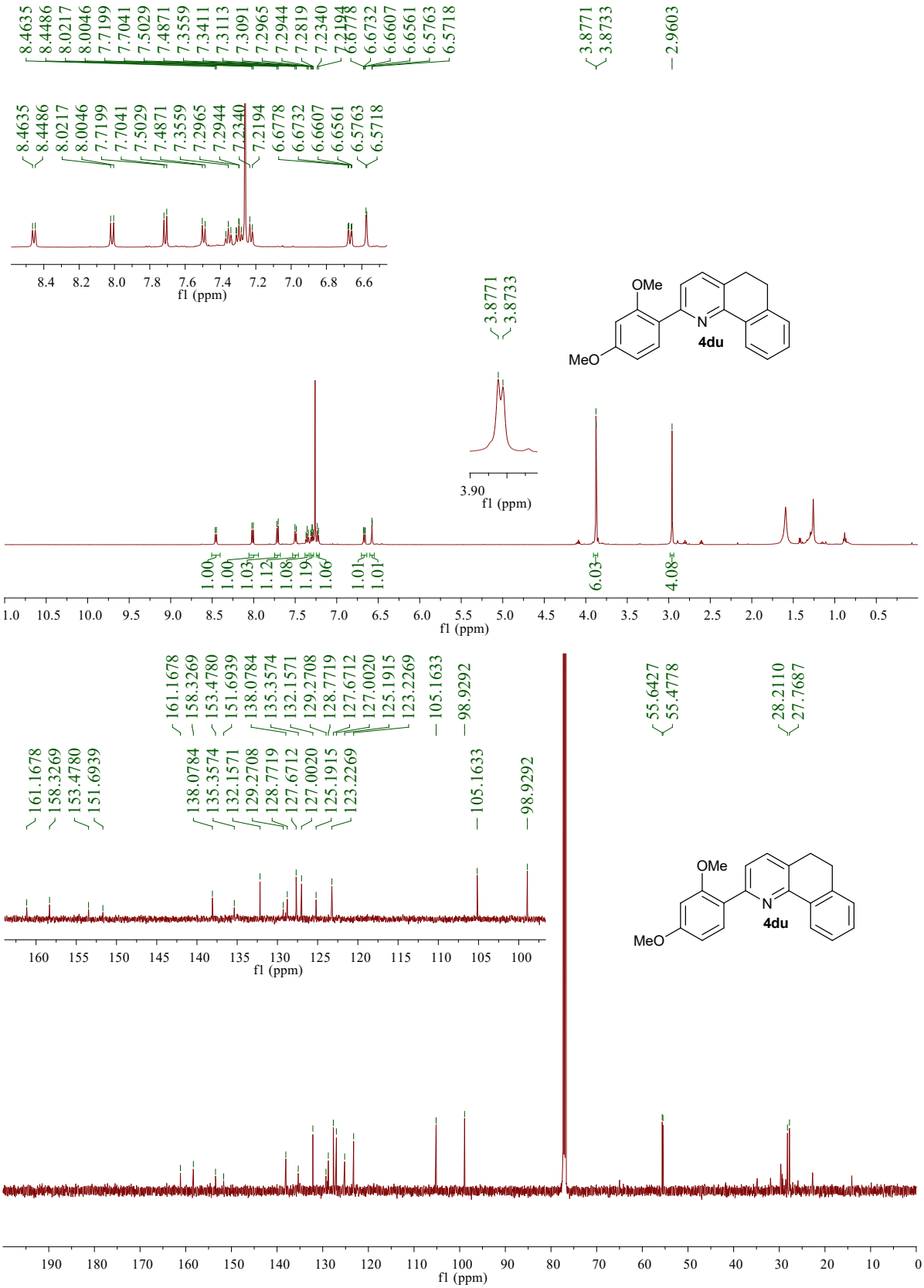
55.6170
55.4964
28.1173
25.4749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7.5029
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7.3559
7.3411
7.3113
7.3091
7.2965
7.2944
7.2819
7.2340
7.2194
6.6778
6.6732
6.6607
6.6561
6.5763
6.5718
3.8771
3.8733
2.9603
f1 (ppm)
OMe
MeO
N
4du
1.00
1.00
1.03
1.12
1.08
1.19
1.06
1.01
1.01
6.03
4.08
161.1678
158.3269
153.4780
151.6939
138.0784
135.3574
132.1571
129.2708
128.7719
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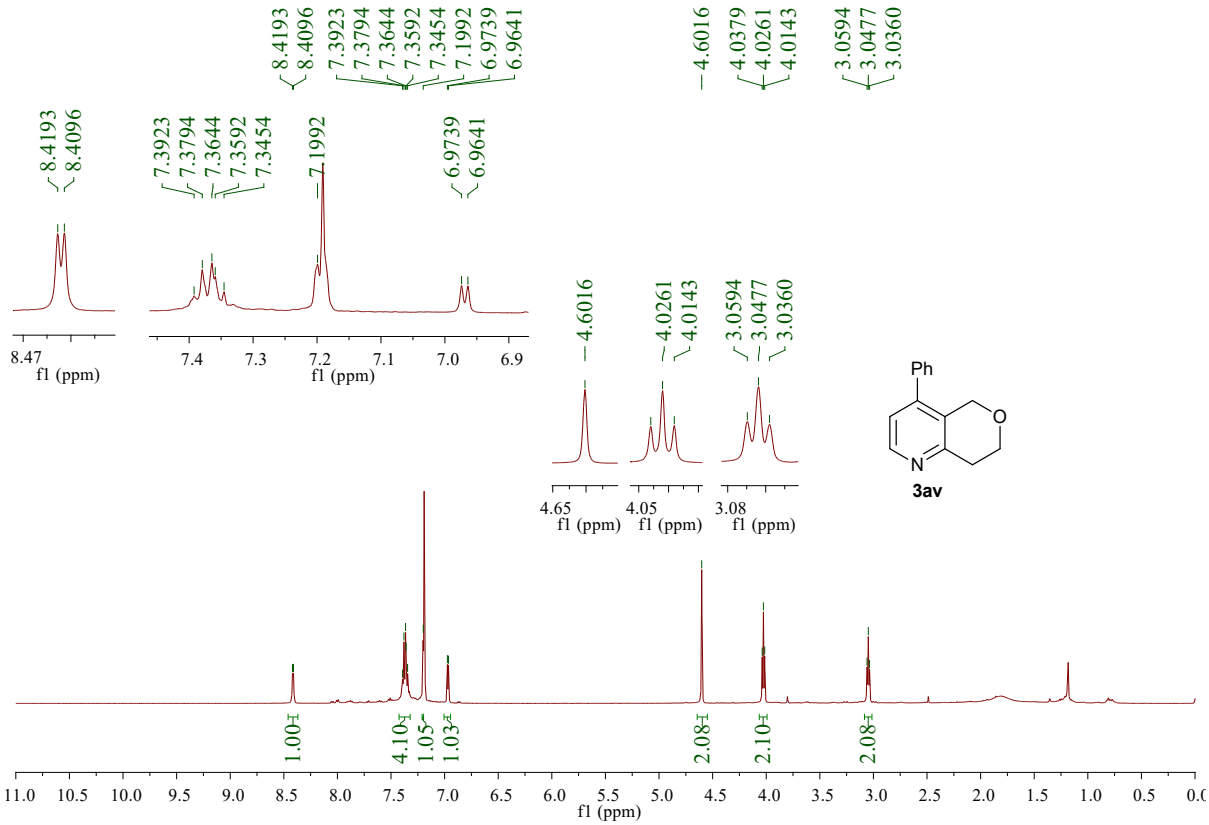
27.7687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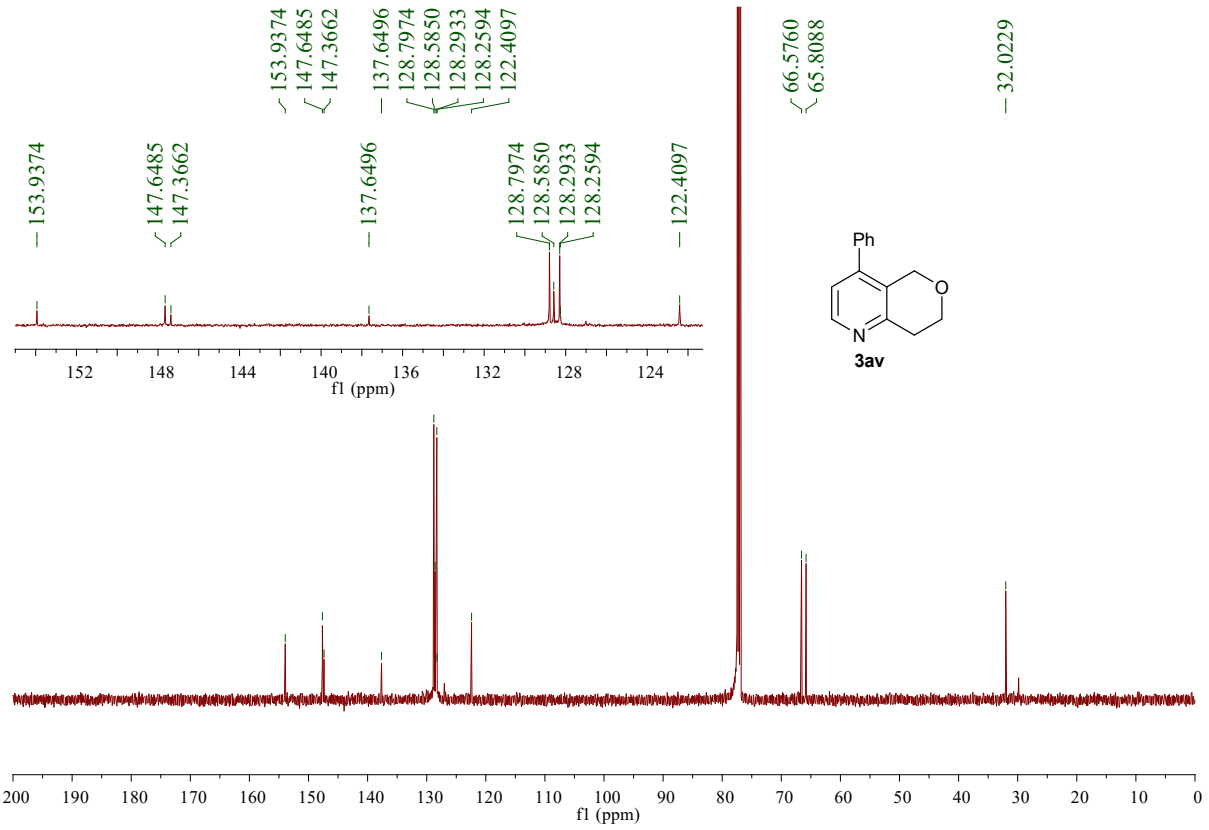
7.3644
7.3592
7.3454
7.1992
6.9739
6.9641
4.6016
4.0379
4.0261
4.0143
3.0594
3.0477
3.0360
Ph
O
N
3av
1.00
4.10
1.05
1.03
2.08
2.10
2.08
f1 (ppm)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122.4097
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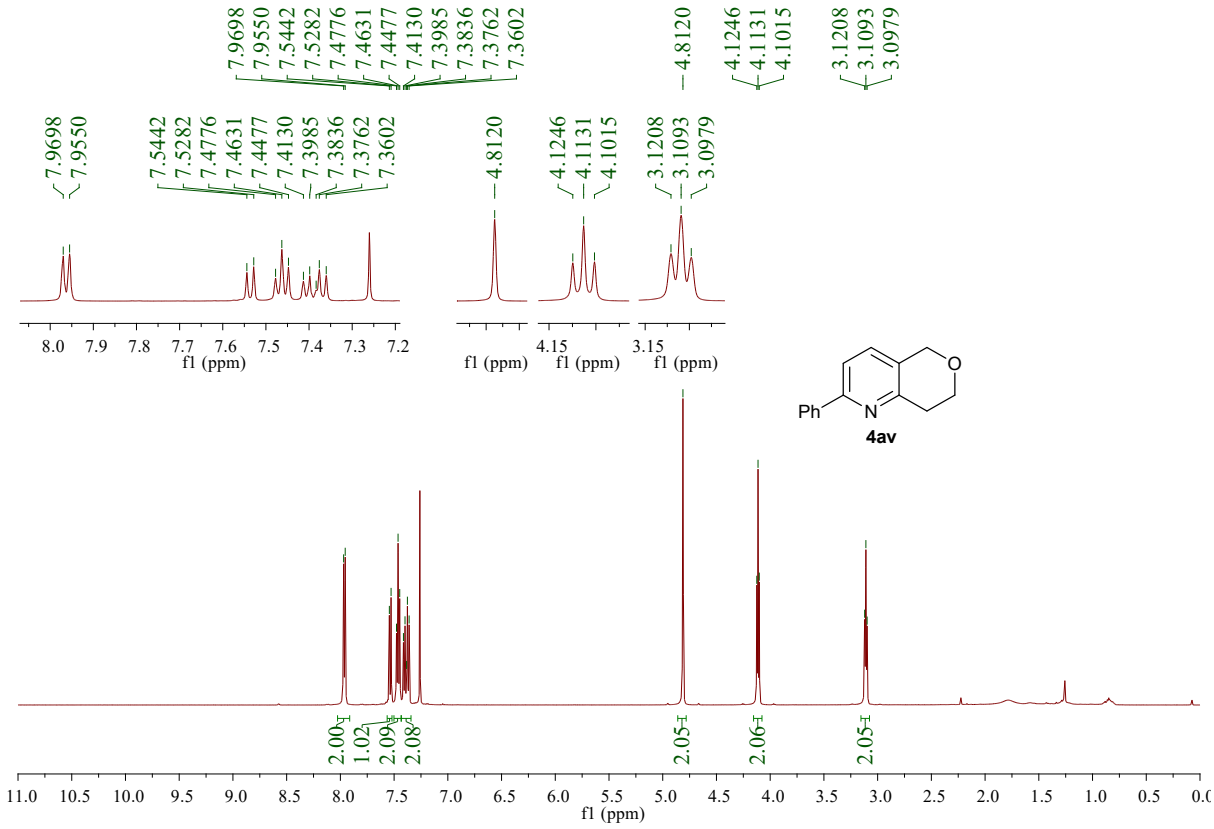
65.8088
32.0229
Ph
O
N
3av
f1 (ppm)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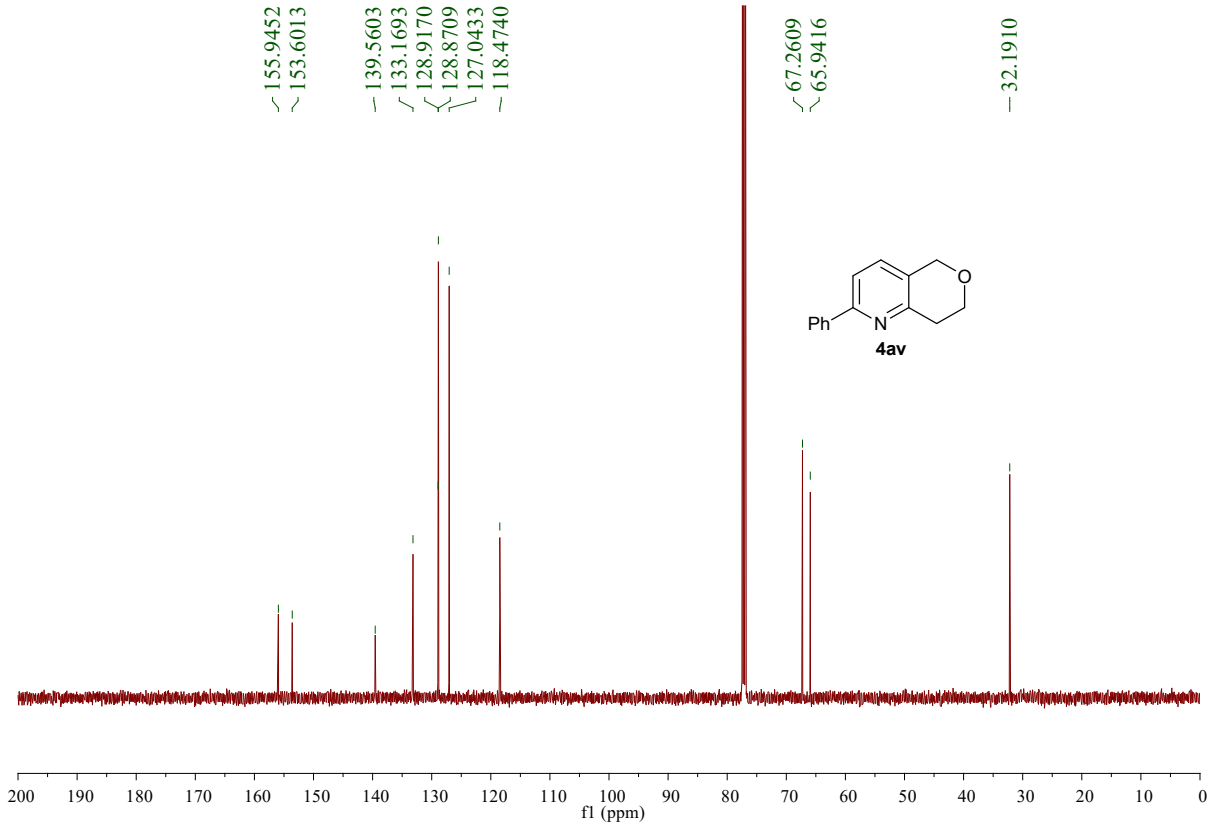
7.4477
7.4130
7.3985
7.3836
7.3762
7.3602
4.8120
4.1246
4.1131
4.1015
3.1208
3.1093
3.0979
f1 (ppm)
Ph
N
O
4av
2.00
1.02
2.09
2.08
2.05
2.06
2.05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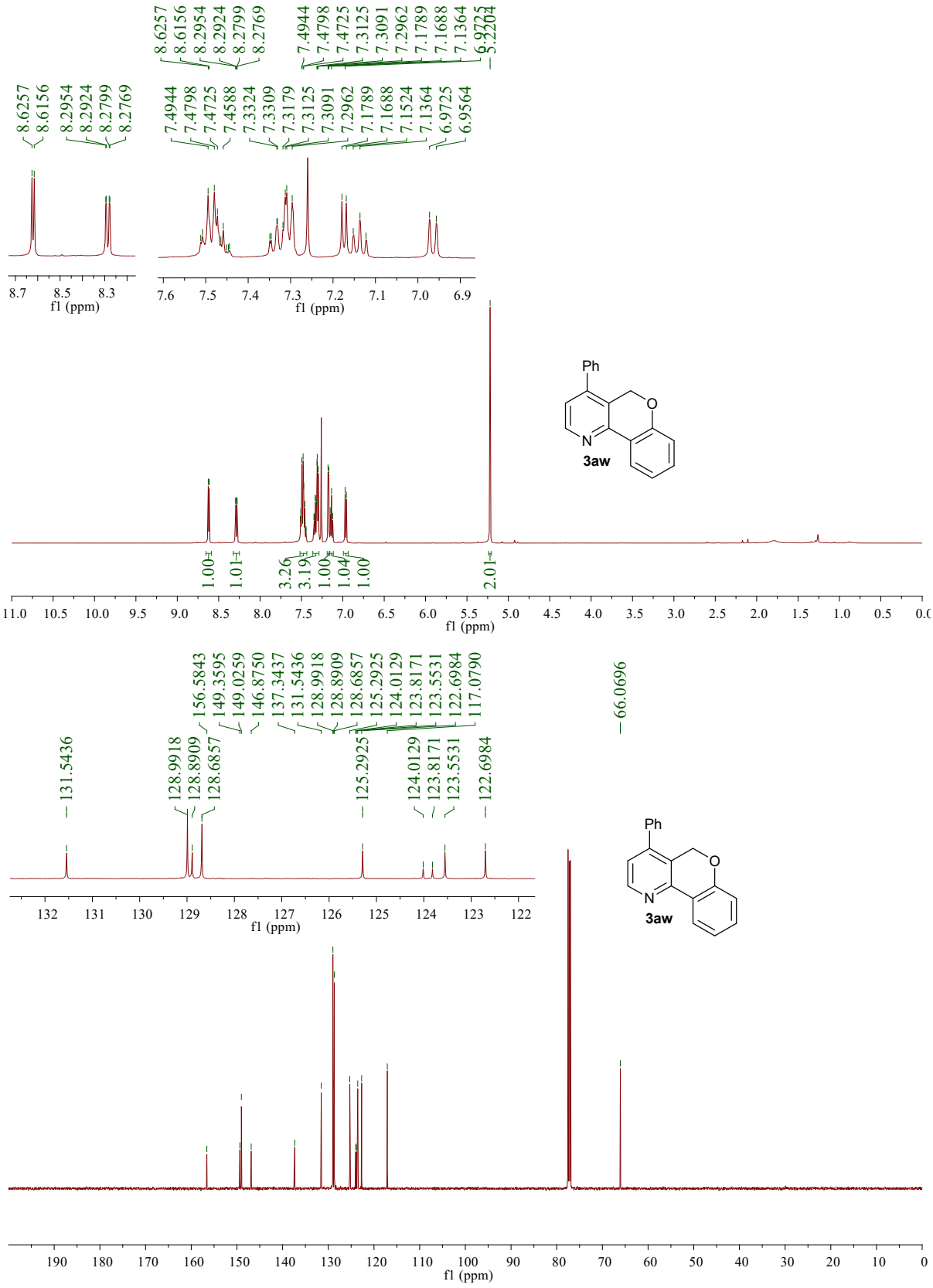
127.0433
118.4740
67.2609
65.9416
32.1910
f1 (ppm)
Ph
N
O
4av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8.2954
8.2924
8.2799
8.2769
7.4944
7.4798
7.4725
7.3125
7.3091
7.2962
7.1789
7.1688
7.1364
6.9725
5.2204
f1 (ppm)
Ph
O
N
3aw
1.00
1.01
3.26
3.19
1.00
1.04
1.00
2.01
f1 (ppm)
156.5843
149.3595
149.0259
146.8750
137.3437
131.5436
128.9918
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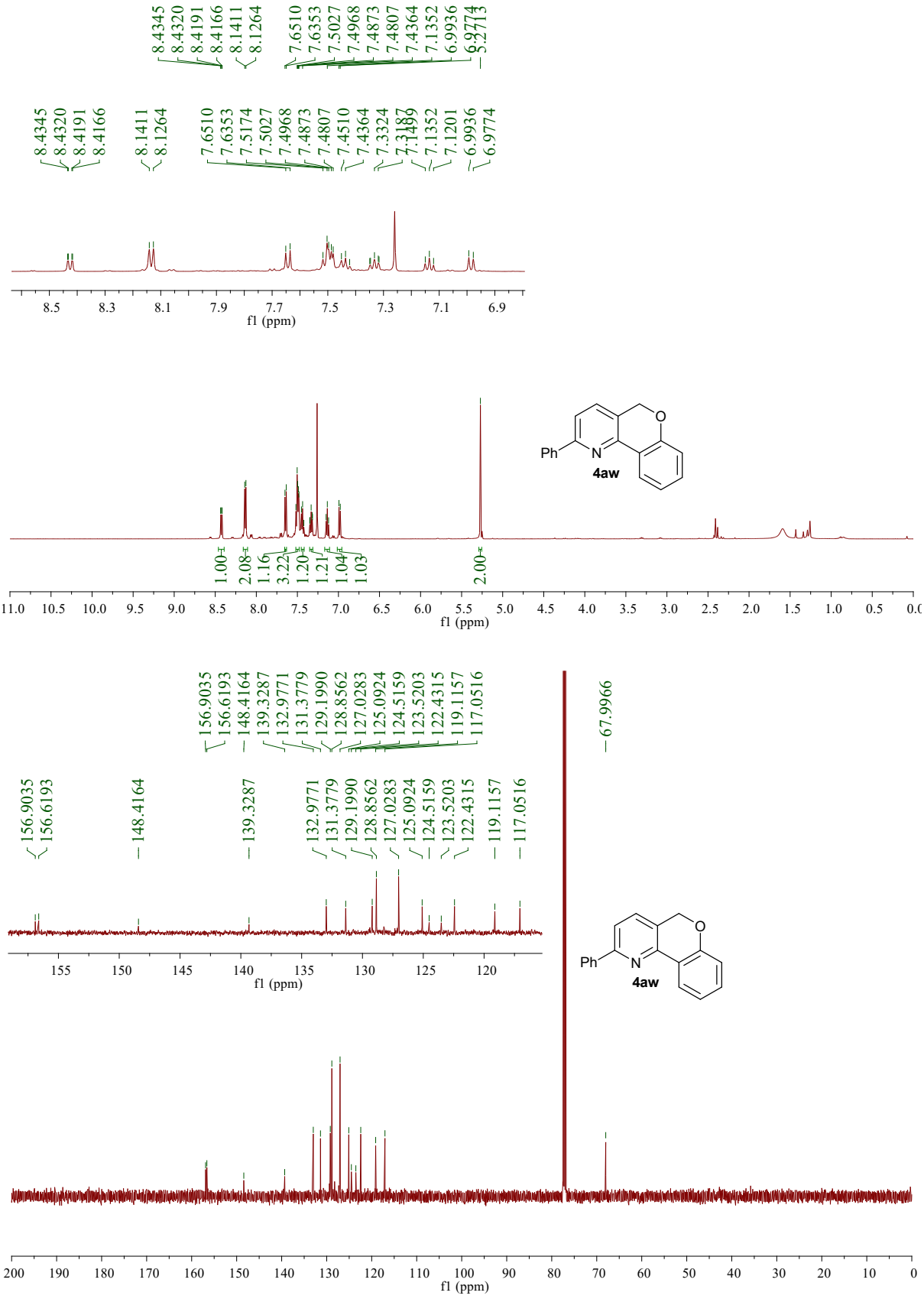
f1 (ppm)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7.4968
7.4873
7.4807
7.4510
7.4364
7.3324
7.3187
7.1499
7.1352
7.1201
6.9936
6.9774
5.2713
f1 (ppm)
Ph
N
O
4aw
1.00
2.08
1.16
3.22
1.20
1.21
1.04
1.03
2.00
156.9035
156.6193
148.4164
139.3287
132.9771
131.3779
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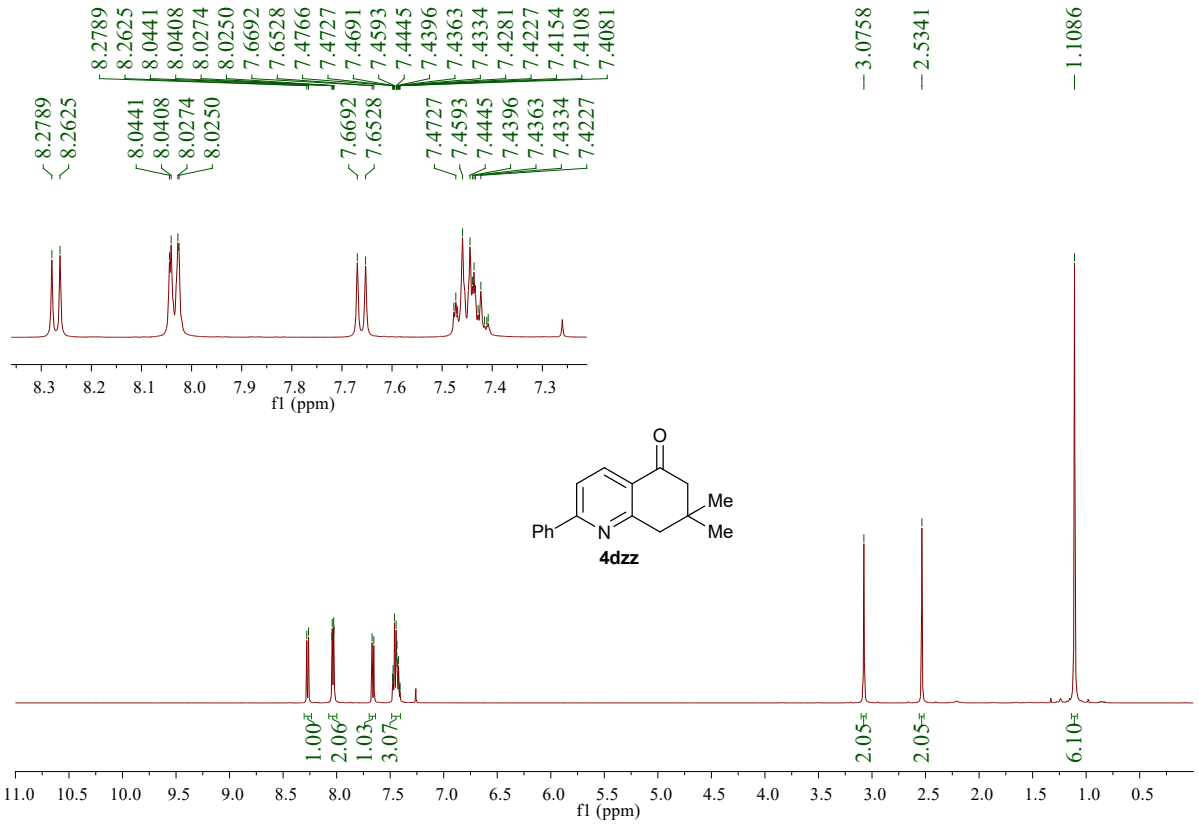
117.0516
67.9966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7.4727
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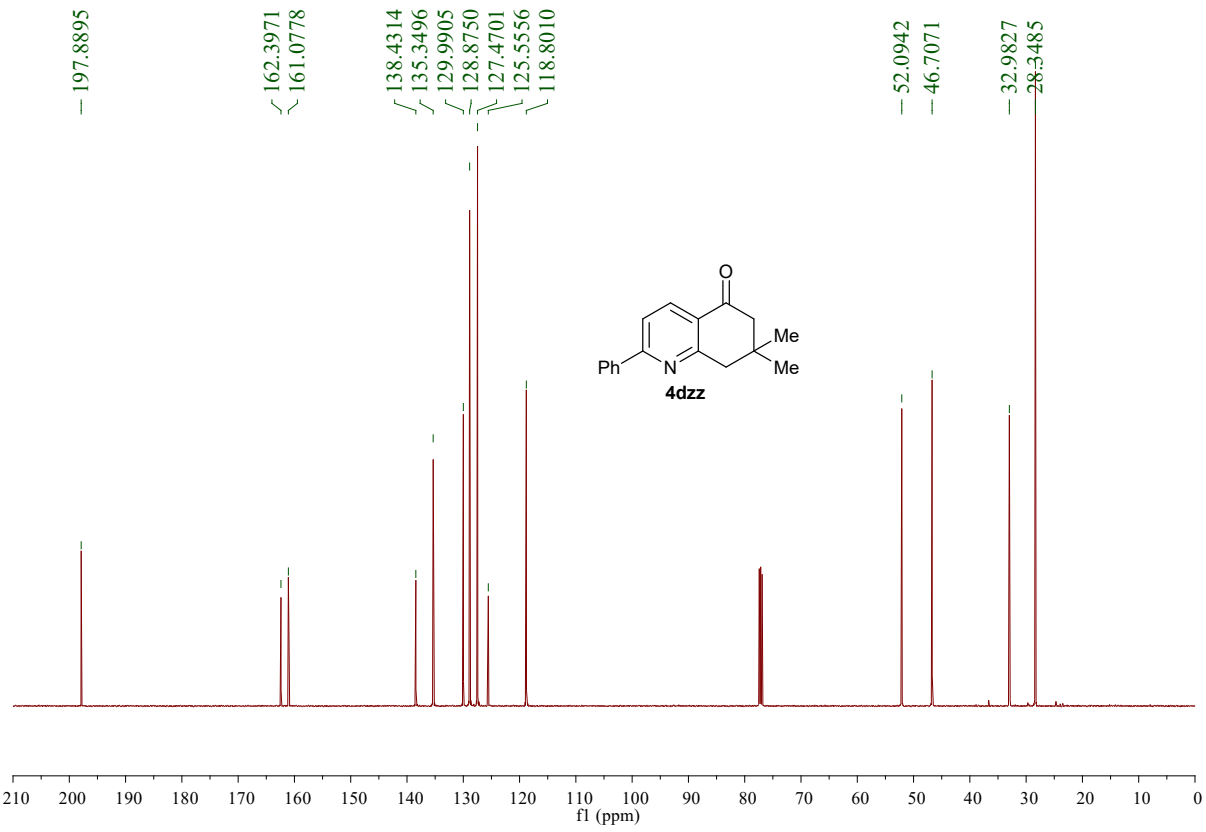
7.4593
7.4445
7.4396
7.4363
7.4334
7.4281
7.4227
7.4154
7.4108
7.4081
3.0758
2.5341
1.1086
f1 (ppm)
O
Me
Me
Ph
N
4dzz
1.00
2.06
1.03
3.07
2.05
2.05
6.10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127.4701
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46.7071
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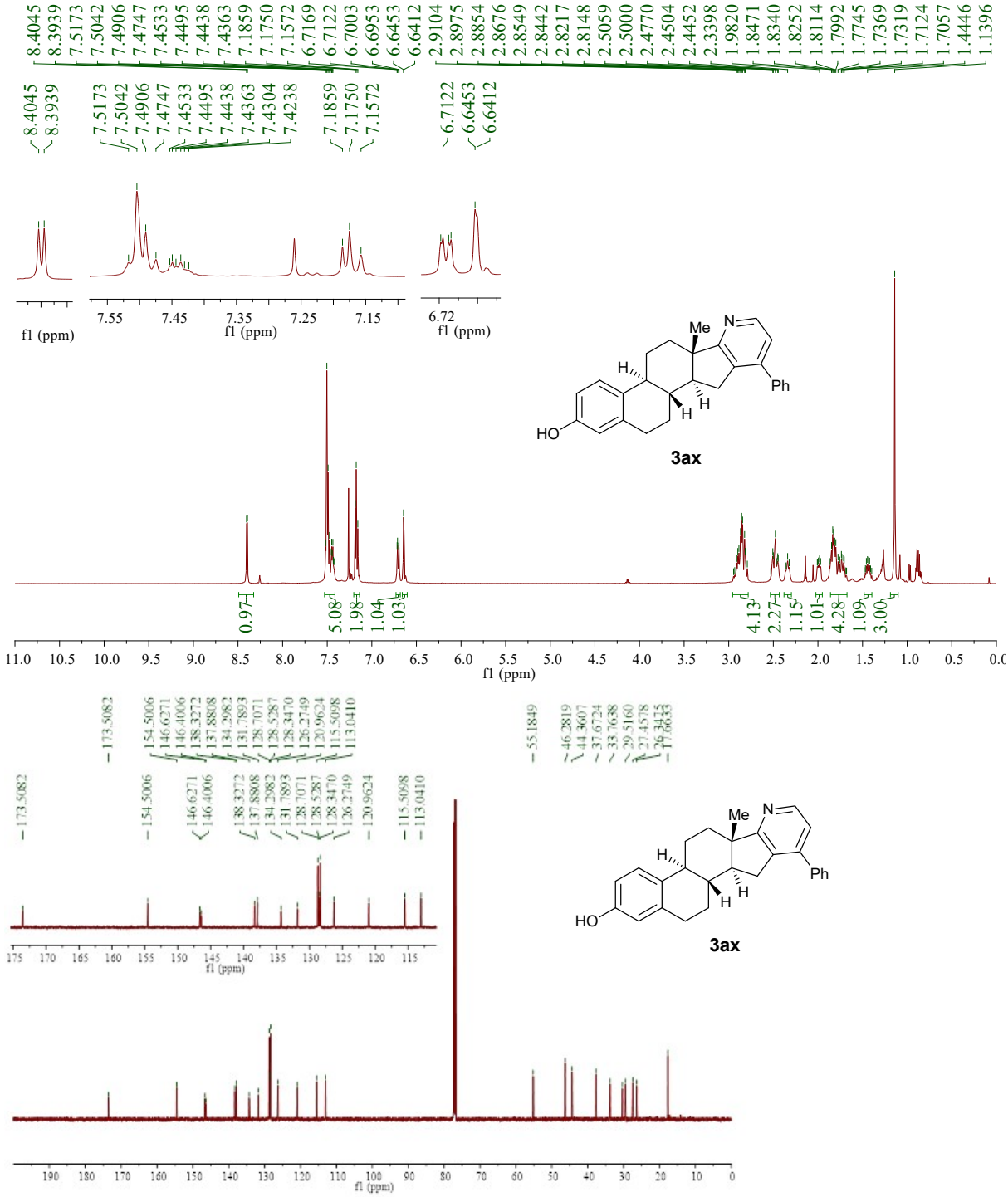
28.3485
f1 (ppm)
O
Me
Me
Ph
N
4dzz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7.4438
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7.1859
7.1750
7.1572
6.7169
6.7122
6.7003
6.6953
6.6453
6.6412
2.9104
2.8975
2.8854
2.8676
2.8549
2.8442
2.8217
2.8148
2.5059
2.5000
2.4770
2.4504
2.4452
2.3398
1.9820
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1.8340
1.8252
1.8114
1.7992
1.7745
1.7369
1.7319
1.7124
1.7057
1.4446
1.1396
f1 (ppm)
Me
N
H
Ph
H
HO
3ax
0.97
5.08
1.98
1.04
1.03
4.13
2.27
1.15
1.01
4.28
1.09
3.00
f1 (ppm)
173.5082
154.5006
146.6271
146.4006
138.3272
137.8808
134.2982
131.7893
128.7071
128.5287
128.3470
126.2749
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115.5098
113.0410
55.1849
46.2819
44.3607
37.6724
33.7638
29.5160
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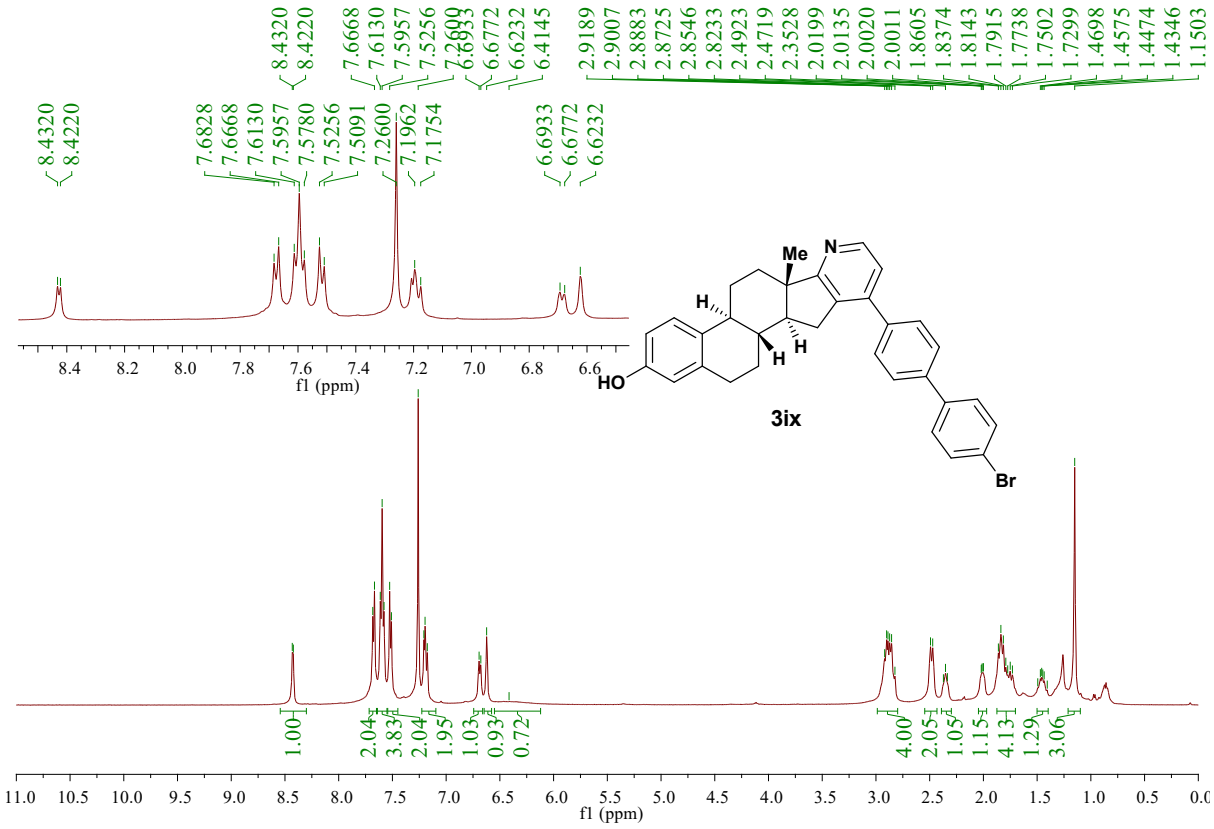
26.3415
17.6633
f1 (ppm)
Me
N
H
Ph
H
H
HO
3ax
f1 (ppm)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7.5780
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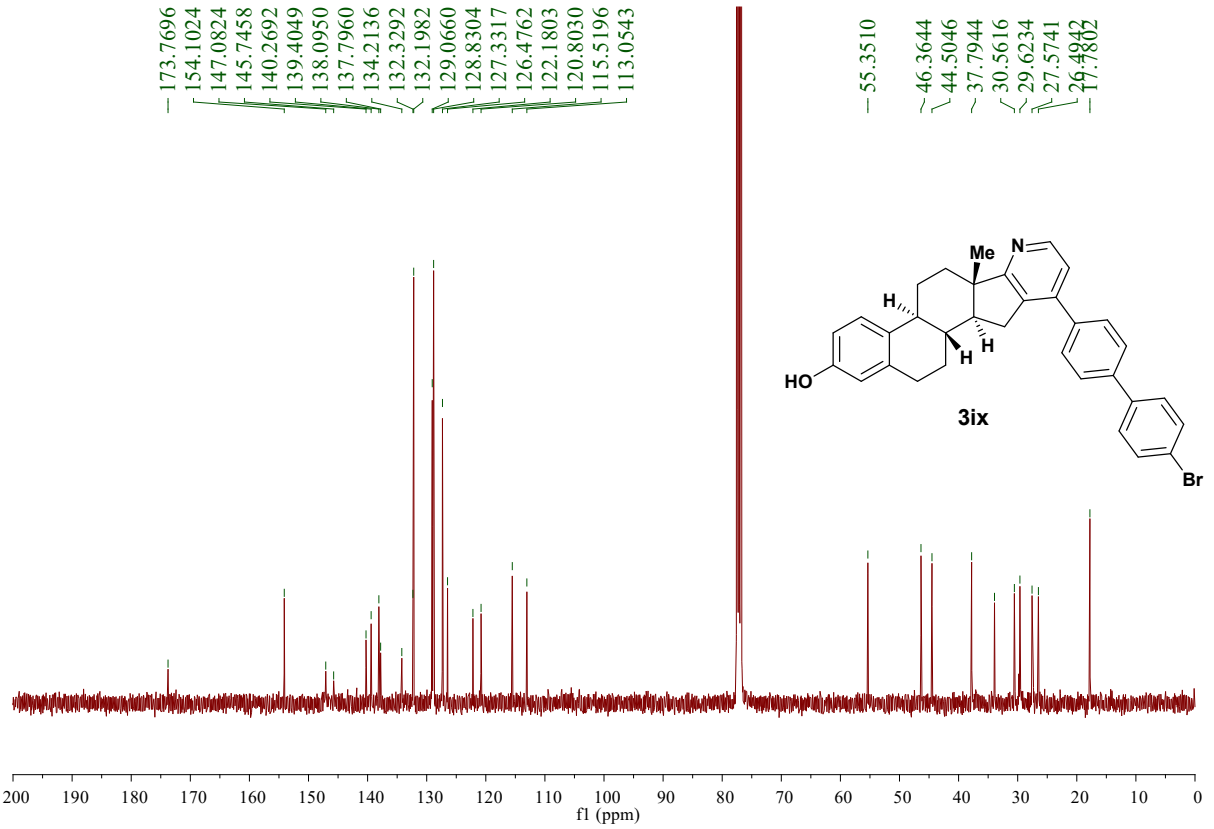
7.5091
7.2600
7.1962
7.1754
6.6933
6.6772
6.6232
f1 (ppm)
Me
N
H
H
H
HO
3ix
Br
1.00
2.04
3.83
2.04
1.95
1.03
0.93
0.72
4.00
2.05
1.05
1.15
4.13
1.29
3.06
f1 (ppm)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128.8304
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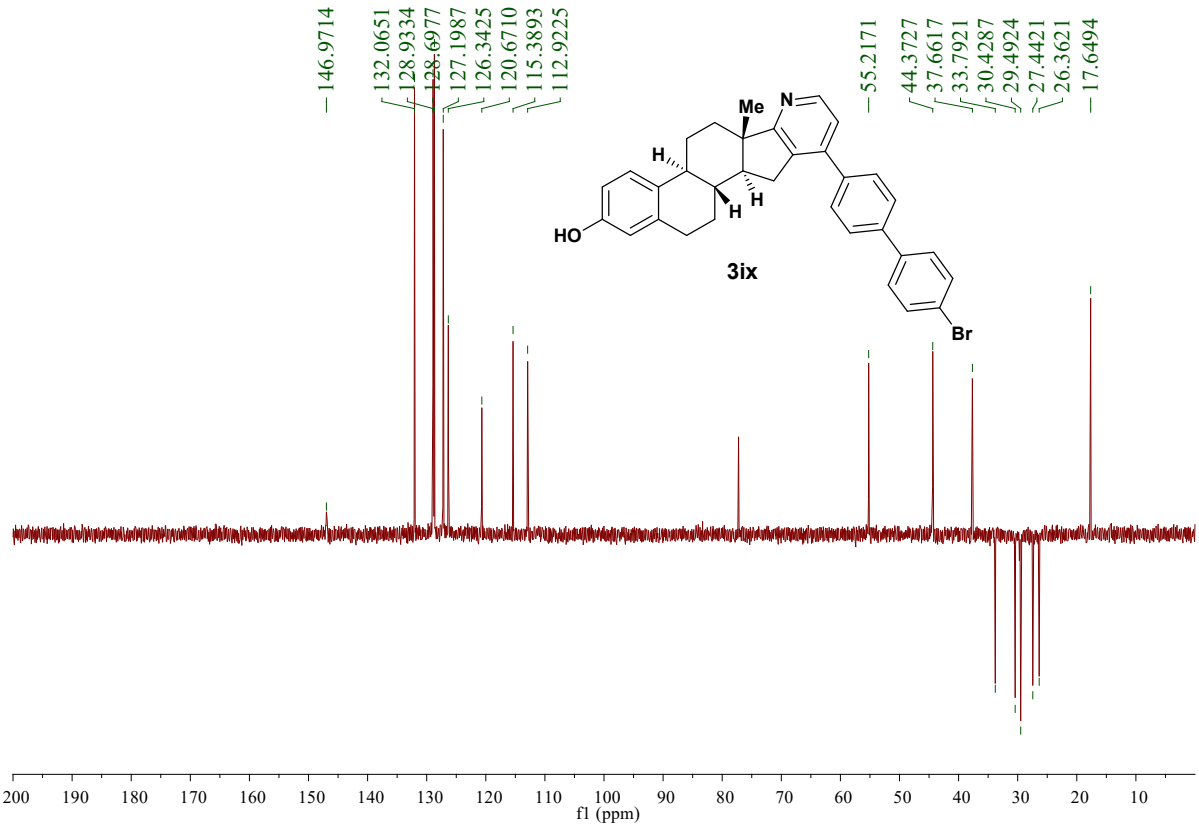
126.4762
122.1803
120.8030
115.5196
113.0543
55.3510
46.3644
44.5046
37.7944
30.5616
29.6234
27.5741
26.4842
17.7802
Me
N
H
H
H
HO
3ix
Br
f1 (ppm)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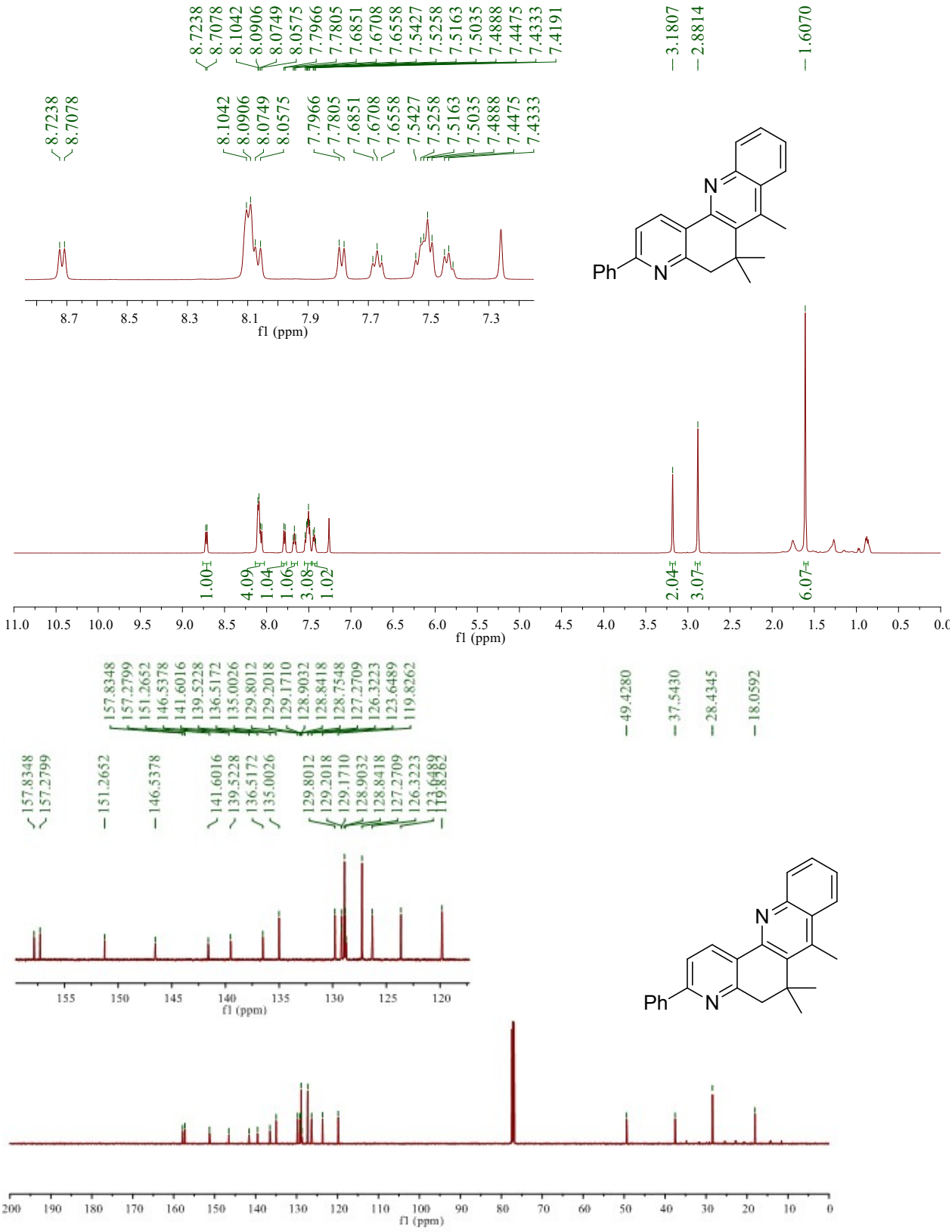
44.3727
37.6617
33.7921
30.4287
29.4924
27.4421
26.3621
17.6494
Me
N
H
H
H
HO
Br
3ix
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.6558
7.5427
7.5258
7.5163
7.5035
7.4888
7.4475
7.4333
7.4191
3.1807
2.8814
1.6070
N
Ph
N
f1 (ppm)
1.00
4.09
1.04
1.06
3.08
1.02
2.04
3.07
6.07
f1 (ppm)
157.8348
157.2799
151.2652
146.5378
141.6016
139.5228
136.5172
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129.1710
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126.3223
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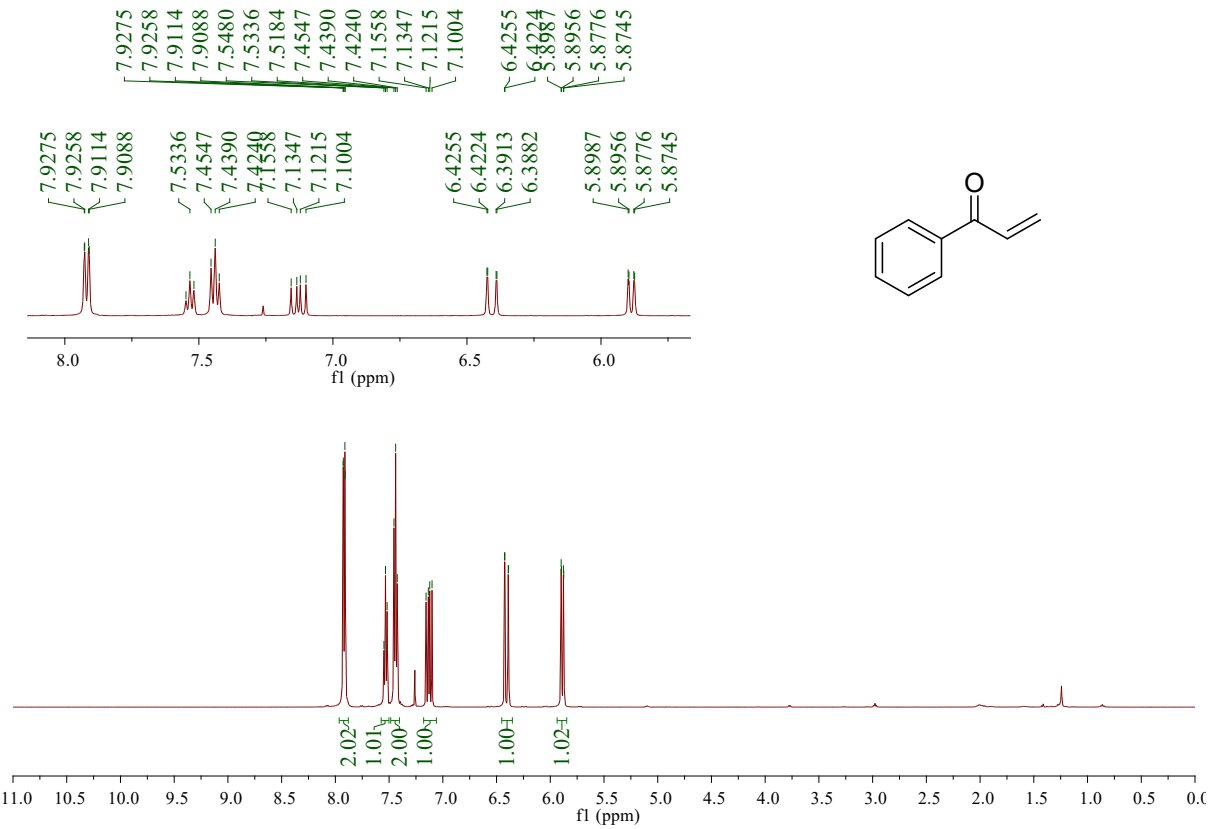
N
Ph
N
f1 (ppm)
f1 (ppm)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6.4255
6.4224
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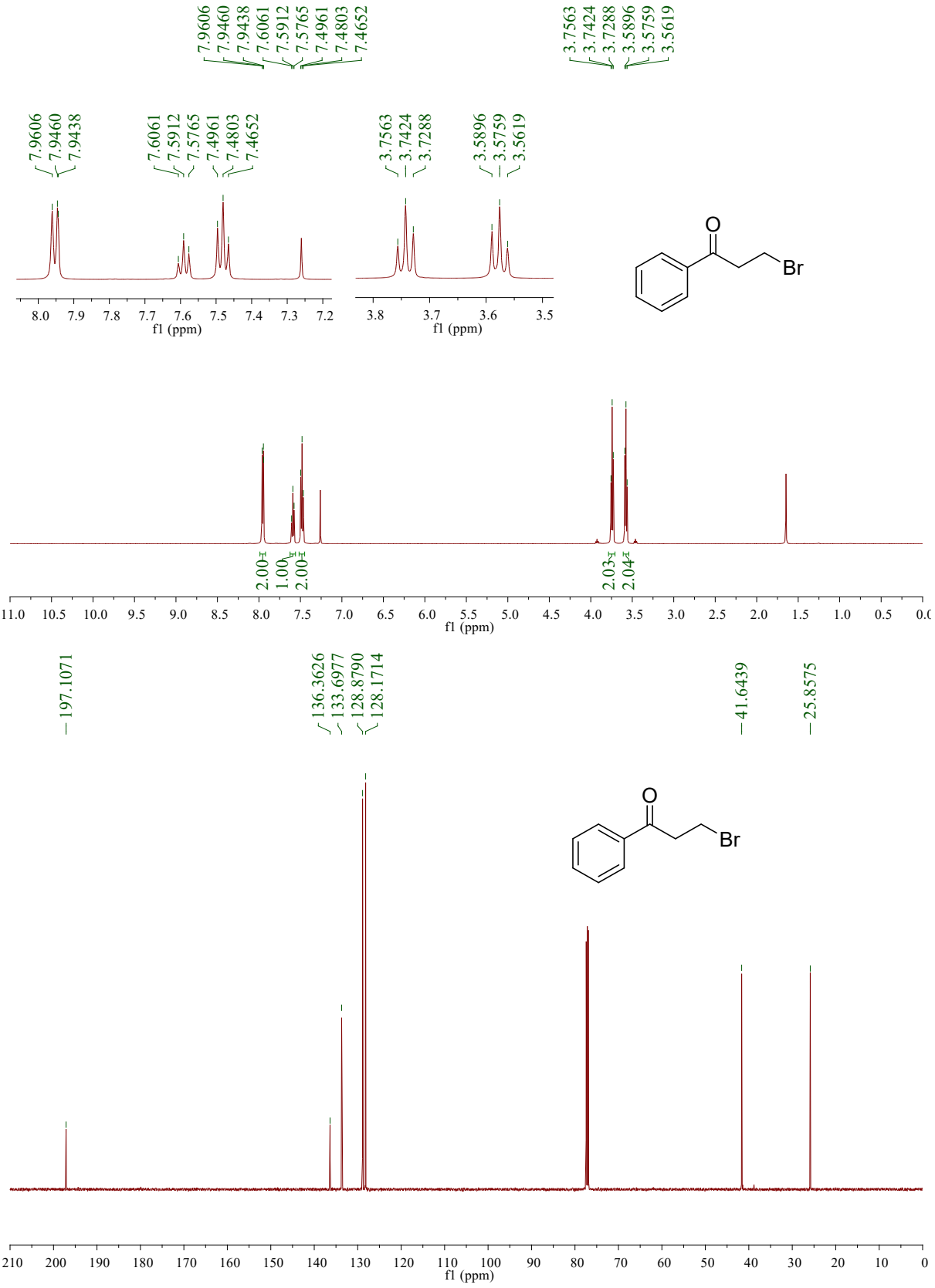
5.8956
5.8776
5.8745
f1 (ppm)
O
2.02
1.01
2.00
1.00
1.00
1.02
f1 (ppm)
190.9473
137.2802
132.9789
132.3891
130.0820
128.6779
128.6204
O
f1 (ppm)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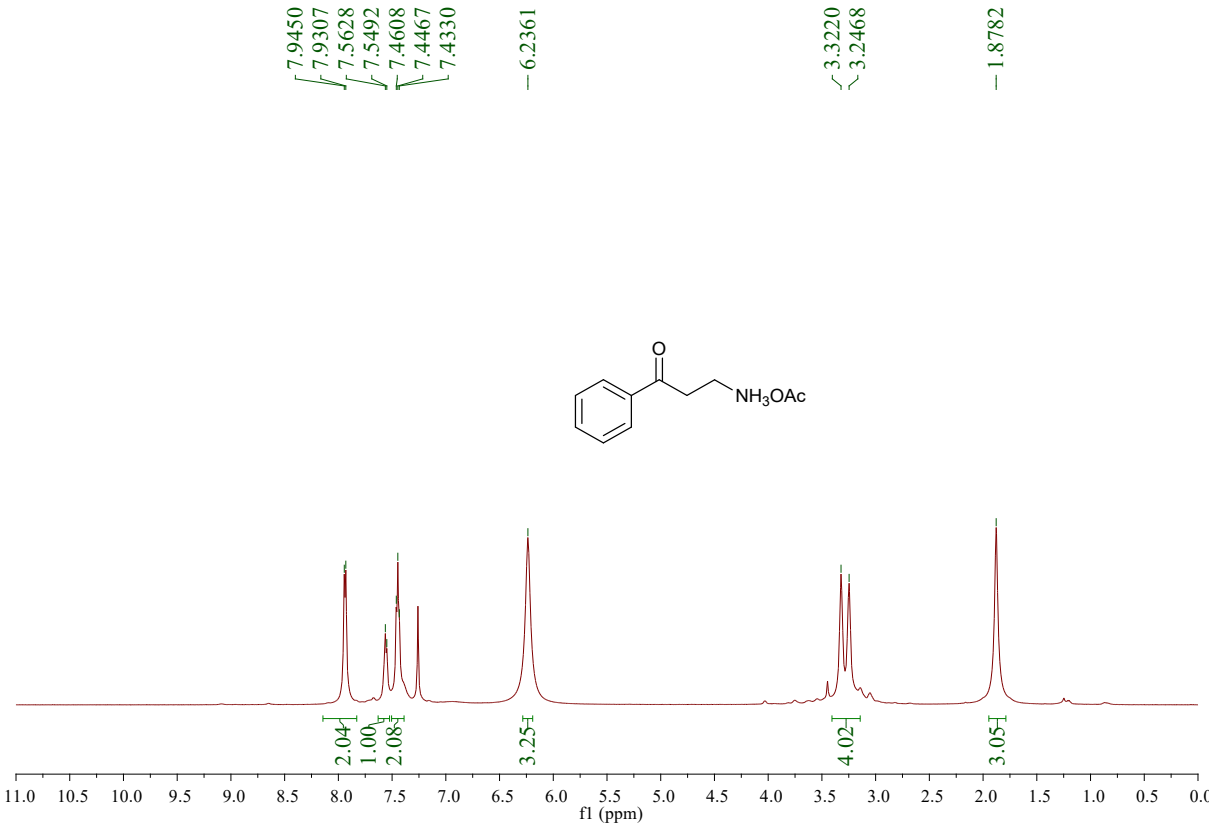
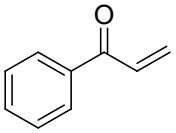
7.9460
7.9438
7.6061
7.5912
7.5765
7.4961
7.4803
7.4652
3.7563
3.7424
3.7288
3.5896
3.5759
3.5619
f1 (ppm)
O
Br
2.00
1.00
2.00
2.03
2.04
197.1071
136.3626
133.6977
128.8790
128.1714
41.6439
25.8575


7.9450
7.9307
7.5628
7.5492
7.4608
7.4467
7.4330
6.2361
3.3220
3.2468
1.8782
O
NH3OAc
2.04
1.00
2.08
3.25
4.02
3.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


O