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Supporting Information

Access to π-conjugated azaindole derivatives via rhodium (III)-catalyzed cascade reaction of azaindoles and diazo compounds

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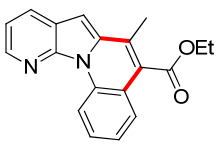
1. General Methods

NMR data were obtained for ^{1}H at 400 MHz or 600 MHz, and for ^{13}C at 100 MHz or 151 MHz. Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard in $CDCl_3$ solution. ESI HRMS was recorded on a Waters SYNAPT G2 and Water XEVO G2 Q-ToF. UV detection was monitored at 220 nm. TLC was performed on glass-backed silica plates. Column chromatography was performed on silica gel (200-300 mesh), eluting with ethyl acetate and petroleum ether. *N*-substituted 7-azaindoles were prepared according to the literature procedures. [1]

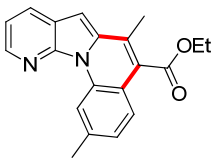
2. General Procedure for Synthesis of 7-azaindole Derived Fused Compounds and Characterization Data

1-phenyl-1H-pyrrolo[2,3-b]pyridine **1a** (9.7 mg, 0.05 mmol), ethyl α-diazoacetoacetate **2a** (23.4 mg, 0.15 mmol) and $[Cp^*RhCl_2]_2$ (1.6 mg, 5 mol %) were stirred in *t*-BuOH (0.5 mL) at 80 °C for 10 h. After completion, the reaction mixture was purified by flash chromatography eluting with ethyl acetate and petroleum ether (1:100) to give the product **3a** as a green solid (11.0 mg, 73%).



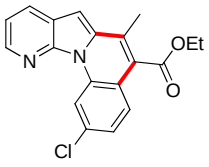
3a

ethyl 6-methylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3a**). 10 h, 11.1 mg, 73% yield (12:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.21 (d, J = 8.4 Hz, 1H), 8.59 (d, J = 4.4 Hz, 1H), 8.14 (d, J = 8.0 Hz, 1H), 7.66 (t, J = 8.0 Hz, 1H), 7.61 (d, J = 7.6 Hz, 1H), 7.38-7.32 (m, 2H), 6.84 (s, 1H), 4.55 (q, J = 7.2 Hz, 2H), 2.50 (s, 3H), 1.48 (t, J = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 146.5, 142.5, 135.6,134.8, 128.9, 128.6, 127.0, 125.3, 125.1, 123.6, 122.0, 120.3, 118.2, 117.9, 94.5, 61.6, 15.7, 14.4, ppm. ESI HRMS: calcd. for $C_{19}H_{16}N_2O2$+H 305.1290, found 305.1293.



3b

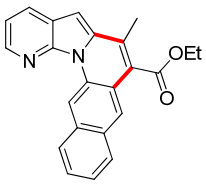
ethyl 2,6-dimethylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3b**). 10 h, 11.4 mg, 72% yield (30:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.05 (s, 1H), 8.59 (dd, J_1 = 1.6 Hz, J_2 = 4.8 Hz, 1H), 8.12 (dd, J_1 = 1.6 Hz, J_2 = 8 Hz, 1H), 7.49 (d, J = 8 Hz, 1H), 7.34-7.31 (m, 1H), 7.18 (d, J = 8.0 Hz, 1H), 6.80 (s, 1H), 4.53 (q, J = 7.2 Hz, 2H), 2.62 (s, 3H), 2.48 (s, 3H), 1.47 (t, J = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.4, 146.5, 142.2, 139.4, 135.8, 134.8, 128.4, 126.9, 125.0, 124.8, 124.1, 122.0, 118.3, 117.9, 117.9, 94.2, 61.6, 22.1, 15.6, 14.4, ppm. ESI HRMS: calcd. for $C_{20}H_{18}N_2O_2$+H 319.1447, found 319.1440.



3c

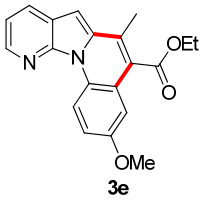
ethyl 2-chloro-6-methylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3c**). 10 h, 12.7 mg, 75% yield (11:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.30 (s, 1H), 8.59 (d, J = 4.4 Hz, 1H), 8.12 (d, J = 8.0 Hz, 1H), 7.53 (d, J = 8.8 Hz 1H), 7.36-7.30 (m, 2H), 6.82 (s, 1H), 4.54 (q, J = 7.2 Hz, 2H), 2.48 (s, 3H), 1.47 (t, J = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.9, 146.4, 142.8, 135.3, 135.2, 134.5, 128.7, 126.2, 126.1, 125.8, 123.9, 122.0, 118.8, 118.3, 118.2, 95.1, 61.7, 15.7, 14.3 ppm. ESI HRMS: calcd. for $C_{19}H_{15}ClN_2$+H 339.0900, found 339.0895.

ethyl 6-methylbenzo[g]pyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-7-carboxylate (**3d**). 10 h, 13.9 mg,



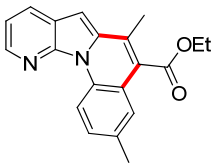
3d

74% yield (9:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.54 (s, 1H), 8.64-8.63 (m, 1H), 8.12-8.07 (m, 2H), 8.01 (s, 1H), 7.88 (d, *J* = 8 Hz, 1H), 7.54 (t, *J* = 8 Hz, 1H), 7.46 (t, *J* = 8 Hz, 1H), 7.32-7.29 (m, 1H), 6.84-6.82 (m, 1H), 4.61 (q, *J* = 7.2 Hz, 2H), 2.47 (s, 3H), 1.52 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.4, 147.5, 143.1, 135.4, 133.4, 132.4, 129.6, 128.6, 128.1, 127.9, 127.2, 126.7, 125.5, 125.2, 124.4, 122.0, 120.8, 117.8, 115.1, 96.5, 61.7, 15.8, 14.4 ppm. ESI HRMS: calcd. for $C_{23}H_{18}N_2O_2$+Na 377.1266, found 377.1266.



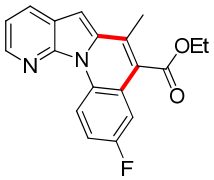
3e

ethyl 3-methoxy-6-methylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3e**). 10 h, 11.4 mg, 68% yield (17:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.13 (d, *J* = 9.2 Hz, 1H), 8.51 (d, *J* = 4.4 Hz, 1H), 8.13 (d, *J* = 7.8 Hz, 1H), 7.33-7.30 (m, 1H), 7.26-7.23 (m, 1H), 7.11 (d, *J* = 2.4 Hz, 1H), 6.82 (s, 1H), 4.55 (q, *J* = 7.2 Hz, 2H), 3.89 (s, 3H), 2.50 (s, 3H), 1.48 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 155.4, 146.0, 142.4, 135.2, 129.3, 128.6, 126.5, 126.1, 121.7, 121.4, 119.5, 117.7, 115.8, 108.7, 94.0, 61.6, 55.5, 15.8, 14.4, ppm. ESI HRMS: calcd. for $C_{20}H_{18}N_2O_3$+H 335.1396, found 335.1396.



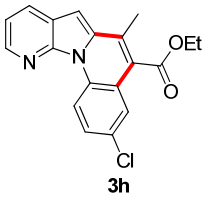
3f

ethyl 3,6-dimethylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3f**). 10 h, 12.4 mg, 78% yield (9:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.05 (d, *J* = 8.8 Hz, 1H), 8.57 (dd, J_1 = 1.6 Hz, J_2 = 4.8Hz, 1H), 8.12 (dd, J_1 = 1.6 Hz, J_2 = 8 Hz,1H), 7.46 (dd, J_1 = 1.6 Hz, J_2 = 8.4 Hz, 1H), 7.38 (s, 1H), 7.33-7.30 (m, 1H), 6.80 (s, 1H), 4.55 (q, *J* = 7.2 Hz, 2H), 2.48 (s, 3H), 2.47 (s, 3H), 1.48 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.5, 146.3, 142.3, 135.5, 133.0, 132.7, 129.9, 128.5, 126.9, 125.1, 125.0, 121.9, 120.2, 118.0, 117.8, 94.1, 61.6, 21.2, 15.7, 14.4 ppm. ESI HRMS: calcd. for $C_{20}H_{18}N_2O_2$+H 319.1447, found 319.1447.



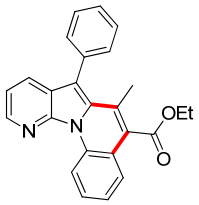
3g

ethyl 3-fluoro-6-methylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3g**). 10 h, 12.7 mg, 79% yield (7:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.44 10.23-10.20 (m, 1H), 8.58 (d, *J* = 3.6 Hz,1H), 8.15 (d, *J* = 8 Hz, 1H), 7.38-7.32 (m, 3H), 6.85 (s, 1H), 4.55 (q, *J* = 7.2 Hz, 2H), 2.51 (s, 3H), 1.48 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$): δ 167.7, 158.5 (d, *J* = 241.3 Hz), 146.1, 142.7, 135.1, 131.2, 128.8, 127.2, 125.9,121.8 (d, *J* = 8.2 Hz), 119.9 (d, *J* = 7.8 Hz), 121.7, 118.0, 115.9 (d, *J* = 22.8 Hz), 110.0 (d, *J* = 24.3 Hz), 94.9, 61.8, 15.8, 14.3 ppm. ESI HRMS: calcd. for $C_{19}H_{15}FN_2O_2$+H 323.1196, found 323.1191.



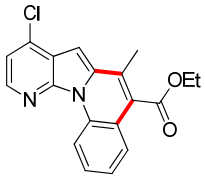
3h

ethyl 3-chloro-6-methylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3h**). 10 h, 12.3 mg, 73% yield (3:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.16 (d, *J* = 8.8 Hz, 1H), 8.58 (d, *J* = 4 Hz, 1H), 8.14 (d, *J* = 7.6 Hz, 1H), 7.59-7.57 (m, 2H), 7.36-7.33 (m, 1H), 6.85 (s, 1H), 4.55 (q, *J* = 7.2 HZ, 2H), 2.50 (s, 3H), 1.49 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 146.3, 142.8, 136.1, 133.1, 128.8, 128.6, 127.0, 125.7, 124.6, 121.9, 121.7, 119.6, 118.1, 96.1, 61.8, 15.8, 14.3 ppm. ESI HRMS: calcd. for $C_{19}H_{15}ClN_2O_2$+H 339.0900, found 339.0901.



3i

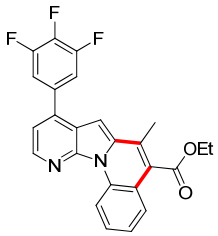
ethyl 6-methyl-7-phenylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3i**). 22 h, 8.5 mg, 46% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.31 (d, *J* = 8.4 Hz, 1H), 8.62 (d, *J* = 4.4 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.67 (t, *J* = 8.4 Hz, 1H), 7.52 (d, *J* = 8.8 Hz, 1H), 7.48-7.41 (m, 5H), 7.35 (t, *J* = 8.0 Hz, 1H), 7.31-7.28 (m, 1H), 4.49 (q, *J* = 7.2 Hz, 2H), 2.09 (s, 3H), 1.42 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$):δ 168.7, 145.1, 143.1, 135.0, 131.5, 130.6, 129.0, 128.3, 127 9, 127.7, 127.4, 125.9, 124.8, 123.6, 123.3, 120.2, 118.5, 118.0, 111.7, 61.6, 18.5, 14.3 ppm. ESI HRMS: calcd. for $C_{25}H_{20}N_2O_2$+H 381.1603, found 381.1608.



3j

ethyl 8-chloro-6-methylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate **(3j)**. 10 h, 10.6 mg, 63% yield (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.10 (d, *J* = 8.8 Hz, 1H), 8.43 (d, *J* = 5.2 Hz, 1H), 7.67-7.60 (m, 2H), 7.39-7.34 (m, 2H), 6.89 (s, 1H), 4.56 (q, *J* = 7.2 Hz, 2H), 2.50 (s, 3H), 1.49 (t, *J* = 3.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.0, 146.6, 142.3, 135.9, 135.5, 134.4, 129.0, 127.6, 125.2, 125.0, 124.0, 121.3, 120.3, 118.2, 117.8, 92.8, 61.7, 15.6, 14.3 ppm. ESI HRMS: calcd. for $C_{19}H_{15}N_2O_2$+H 339.0900, found 339.0898.

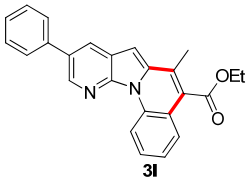
ethyl 6-methyl-8-(3,4,5-trifluorophenyl)pyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate



3k

(**3k**). 10 h, 15.8 mg, 73% yield (5:2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.20 (d, *J* = 8.4 Hz, 1H), 8.60 (d, *J* = 4.4 Hz, 1H), 7.68-7.60 (m, 2H), 7.43-7.36 (m, 3H), 7.29 (d, *J* = 4.8 Hz, 1H), 6.88 (s, 1H), 4.56 (q, *J* = 7.2Hz, 2H), 2.48 (s, 3H), 1.48 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.1, 151.5 (ddd, J_1 = 249.2 Hz, J_2 = 10 Hz, J_3 = 4 Hz), 147.0, 142.5, 138.2, 135.5 (d, *J* = 195 Hz), 134.9-134.7 (m), 129.1, 127.7, 126.3 (d, *J* = 268 Hz), 125.3, 124.0, 120.4, 119.6, 118.4, 116.7, 112.9 (dd, J_1 = 15.8 Hz, J_2 = 6 Hz), 92.8, 61.7, 15.7,14.4 ppm. ESI HRMS: calcd. for $C_{25}H_{17}F_3N_2O_2$+H 435.1320, found 435.1320.

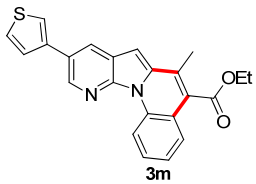
ethyl 6-methyl-9-phenylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3l**). 10 h, 11.7 mg,



3l

58% yield (32:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.19 (d, *J* = 8.4 Hz, 1H), 8.82 (d, *J* = 2.0 Hz, 1H), 8.28 (d, *J* = 2.0 Hz 1H), 7.71-7.61 (m, 4H), 7.51 (t, *J* = 8.0 Hz, 2H), 7.42-7.35 (m, 2H), 6.85 (s, 1H), 4.55 (q, *J* = 7.2 Hz, 2H), 2.50 (s, 3H), 1.48 (t, *J* = 8 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 145.9, 141.8, 139.2, 136.3, 134.9-134.6 (m), 131.4, 129.0, 129.0, 127.6, 127.4, 127.0, 126.6, 125.2, 125.2, 123.7, 121.9, 120.3, 118.1, 94.6, 61.7, 15.7, 14.4 ppm. ESI HRMS: calcd. for $C_{25}H_{20}N_2O_2$+Na 403.1422, found 403.1424.

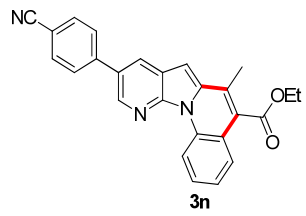
ethyl 6-methyl-9-(thiophen-3-yl)pyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3m**). 10 h,



3m

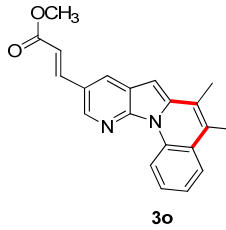
13.9 mg, 68% yield (14:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.16 (d, *J* = 8.8 Hz, 1H), 8.84 (s, 1H), 8.27 (s, 1H), 7.66 (t, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.56 (s, 1H), 7.51-7.46 (m, 2H), 7.36 (t, *J* = 7.6 Hz 1H), 6.82 (s, 1H), 4.55 (q, *J* = 6.8 Hz, 2H), 2.49 (s, 3H), 1.48 (t, *J* = 3.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 145.6, 141.3, 140.1, 136.3, 134.6, 128.9, 127.0, 126.7, 126.4, 126.3, 125.7, 125.2, 123.7, 121.9, 120.4, 120.2, 118.1, 94.6, 61.6, 15.4, 14.4 ppm. ESI HRMS: calcd. for $C_{23}H_{18}N_2O_2S$+Na 409.0987, found 409.0993.

ethyl 9-(4-cyanophenyl)-6-methylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3n**). 22 h, 12.7 mg, 63% yield (6:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.18 (d, *J* = 8.4 Hz, 1H), 8.80 (d, *J* = 2.0 Hz, 1H), 8.30 (d, *J* = 2.4 Hz, 1H), 7.80 (s, 4H), 7.68 (t, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 8 Hz,1H), 7.39 (t, *J* = 7.2 Hz, 1H), 6.89 (s, 1H), 4.56 (q, *J* = 7.2 Hz, 2H), 2.51 (s, 3H), 1.49 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.1, 146.3, 143.8, 141.3, 136.8, 134.5, 132.8, 129.3, 129.1, 128.0, 126.8, 125.3, 125.1, 124.0, 121.9, 120.3, 118.8, 118.2, 111.0, 94.7, 61.8, 15.7, 14.4 ppm. ESI HRMS: calcd. for $C_{26}H_{19}N_3O_2$+H 406.1556, found 406.1555.



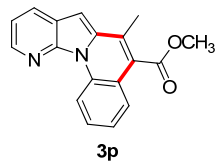
3n

ethyl 9-(3-methoxy-3-oxoprop-1-en-1-yl)-6-methylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3o**). 10 h, 15.2 mg, 74% yield (11:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.07 (d, *J* = 8.4 Hz, 1H), 8.68 (s, 1H), 8.21 (s, 1H), 7.88 (d, *J* = 16 Hz, 1H), 7.64 (t, *J* = 8.4 Hz, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 6.78 (s, 1H), 6.57 (d, *J* = 16 Hz, 1H), 4.55 (q, *J* = 7.2 Hz, 2H), 3.85 (s, 3H), 2.46 (s, 3H), 1.48 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.1, 167.3, 146.8, 142.8, 136.8, 134.4, 129.0, 127.5, 127.1, 125.3, 125.0, 124.5, 124.0, 121.7, 120.3, 118.3, 117.5, 94.8, 61.7, 51.8, 15.7, 14.4 ppm. ESIHRMS: calcd. for $C_{23}H_{20}N_2O_4$+Na 411.1321, found 411.1326.



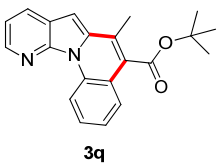
3o

methyl 6-methylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3p**). 10 h, 10.7 mg, 74% yield (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.20 (d, *J* = 8.8 Hz, 1H), 8.58 (dd, J_1 = 4.4 Hz, J_2 = 1.2 Hz, 1H), 8.12 (dd, J_1 = 8 Hz, J_2 = 1.2 Hz, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.57 (d, *J* = 8 Hz, 1H), 7.37-7.31 (m, 2H), 6.82 (s, 1H), 4.05 (s, 3H), 2.48 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.8, 146.5, 142.5, 135.5, 134.8, 128.9, 128.6, 126.7, 125.6, 125.2, 123.6, 121.9, 120.2, 118.2, 118.0, 94.6, 52.4, 15.8 ppm. ESI HRMS: calcd. for $C_{18}H_{14}N_2O_2$+H 291.1134, found 291.1131.



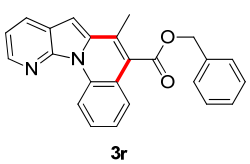
3p

tert-butyl 6-methylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3q**). 10 h, 7.5 mg, 45% yield (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.19 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 8.57 (dd, J_1 = 4.8 Hz, J_2 = 1.6 Hz, 1H), 8.11 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.67-7.63 (m, 2H), 7.36 (td, J_1 = 7.8 Hz, *J* = 1.2 Hz, 1H), 7.33-7.30 (m, 1H), 6.79 (s, 1H), 2.49 (s, 3H), 1.70 (s, 9H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 146.5, 142.2, 135.6, 134.8, 128.7, 128.4, 128.2, 125.0, 124.0, 123.5, 122.0, 120.4, 118.2, 117.9, 94.1, 82.9, 28.3, 15.4 ppm. ESI HRMS: calcd. for $C_{21}H_{20}N_2O_2$+H 333.1603, found 333.1603.



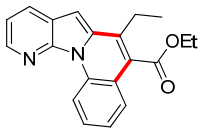
3q

benzyl 6-methylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3r**). 10 h, 15.3 mg, 70% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.19 (d, *J* = 8.4 Hz, 1H),8.58 (dd, J_1 = 4.8 Hz, J_2 = 1.6 Hz, 1H), 8.13 (dd, J_1 = 8 Hz, J_2 = 1.6 Hz, 1H), 7.64 (td, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.54 (dd, J_1 = 8 Hz, J_2 = 1.2 Hz, 1H), 7.51-7.49 (m, 2H), 7.43-7.37 (m, 3H), 7.34-7.28 (m, 2H), 6.81 (s, 1H), 5.51 (s, 2H), 2.44 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.2, 146.5,



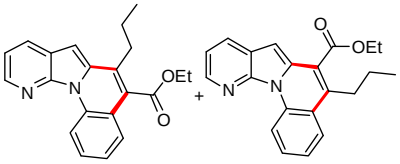
3r

142.5, 135.5, 135.3, 134.8, 128.9, 128.7, 128.7, 128.6, 128.6, 126.6, 125.6, 125.2, 123.6, 121.9, 120.2, 118.2, 118.0, 94.6, 67.4, 15.7 ppm. ESI HRMS: calcd. for $C_{24}H_{18}N_2O_2$+H 367.1447, found 367.1449.



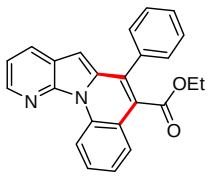
3s

ethyl 6-ethylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3s**). 10 h, 12.0 mg, 71% yield (7:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.22 (d, *J* = 8.4 Hz, 1H), 8.59 (d, *J* = 4.4 Hz, 1H), 8.14 (d, *J* = 8 Hz, 1H), 7.66 (t, *J* = 8 Hz, 1H), 7.59 (d, *J* = 8 Hz, 1H), 7.37-7.32 (m, 2H), 6.88 (s, 1H), 4.54 (q, *J* = 7.2 Hz, 2H), 2.89 (q, *J* = 7.6 Hz, 2H), 1.47 (t, *J* = 7.2 Hz, 3H), 1.41 (t, *J* = 9.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 146.4, 142.4, 134.9, 134.7, 131.1, 128.9, 128.5, 126.4, 125.2, 123.6, 122.0, 120.4, 118.2, 117.9, 94.3, 61.6, 24.1, 14.3, 14.1ppm. ESI HRMS: calcd. for $C_{20}H_{18}N_2O_2$+Na 341.1266, found 341.1263.



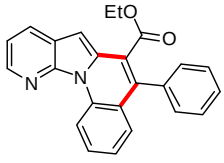
3t **4t** **(5:1)**

ethyl 6-propylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline -5-carboxylate (**3t**). ethyl 5-propylpyrido[3',2':4,5] pyrrolo[1,2-a]quinoline-6-carboxylate (**4t**). 10 h, 7.6 mg, 46% yield. ^{1}H NMR (mixture of **3t** and **4t**) (400 MHz, $CDCl_3$): δ 10.26 (d, *J* = 8.4 Hz, 1H), 10.22 (d, *J* = 8.0 Hz, 1H), 8.59 (dd, J_1 = 4.4 Hz, J_2 = 1.6 Hz, 1H), 8.54 (dd, J_1 = 4.4 Hz, J_2 = 1.6 Hz, 1H), 8.14 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 8.09 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.71 (t, *J* = 7.2 Hz, 1H), 7.65 (t, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.41-7.37 (m, 2H), 7.35-7.32 (m, 2H), 6.86 (s, 1H), 6.69 (s, 1H), 4.54 (q, *J* = 7.2 Hz, 2H), 4.54 (q, *J* = 7.2 Hz, 2H), 2.95 (t, *J* = 8.0 Hz, 2H), 2.84 (t, *J* = 8.0 Hz, 2H), 1.91-1.87 (m, 2H), 1.86-1.77 (m, 2H), 1.47 (t, *J* = 7.2 Hz, 3H), 1.47 (t, *J* = 7.2 Hz, 3H), 1.09 (t, *J* = 7.2 Hz, 3H) 1.08 (t, *J* = 7.2 Hz, 3H) ppm. ESI HRMS: calcd. for $C_{21}H_{20}N_2O_2$+H 333.1603, found 333.1609.



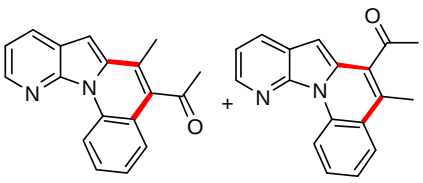
3u

ethyl 6-phenylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-5-carboxylate (**3u**). 10 h, 14.3 mg, 78% yield (3:2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.27 (d, *J* = 8.8 Hz, 1H), 8.61 (d, *J* = 4.4 Hz, 1H), 8.05 (d, *J* = 8 Hz, 1H), 7.77 (d, *J* = 8 Hz, 1H) 7.72 (t, *J* = 7.2 Hz, 1H), 7.55-7.45 (m, 5H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.34-7.30 (m, 1H), 6.51 (s, 1H), 4.12 (q, *J* = 7.2 Hz, 2H), 0.95 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 1.67.6, 146.5, 142.6, 136.2, 135.4, 135.3, 131.0, 129.6, 129.1, 128.7, 128.5, 128.5, 127.2, 125.9, 123.8, 122.0, 120.3, 118.4, 118.0, 97.1, 61.3, 13.6 ppm. ESI HRMS: calcd. for $C_{24}H_{18}N_2O_2$+H 367.1447, found 367.1440.



4u

ethyl 5-phenylpyrido[3',2':4,5]pyrrolo[1,2-a]quinoline-6-carboxylate (**4u**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.28 (d, *J* = 8.4 Hz, 1H), 8.59 (dd, J_1 = 4.8 Hz, J_2 = 1.6 Hz, 1H), 8.15 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.71 (t, *J* = 8.4 Hz, 1H) 7.51-7.46 (m, 3H), 7.41-7.34 (m, 4H), 7.27-7.23 (m, 1H), 6.90 (s, 1H), 4.09 (q, *J* = 7.2 Hz, 2H), 0.93 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 1.66.5, 146.1, 142.1, 136.9, 136.6, 136.2, 132.5, 130.4, 129.6, 128.6, 128.4, 128.2, 128.0, 123.4, 123.0, 122.2, 118.1, 118.1, 94.5, 61.2, 13.5 ppm. ESI HRMS: calcd. for $C_{24}H_{18}N_2O_2$+H 367.1447, found 367.1443.



3v **4v**

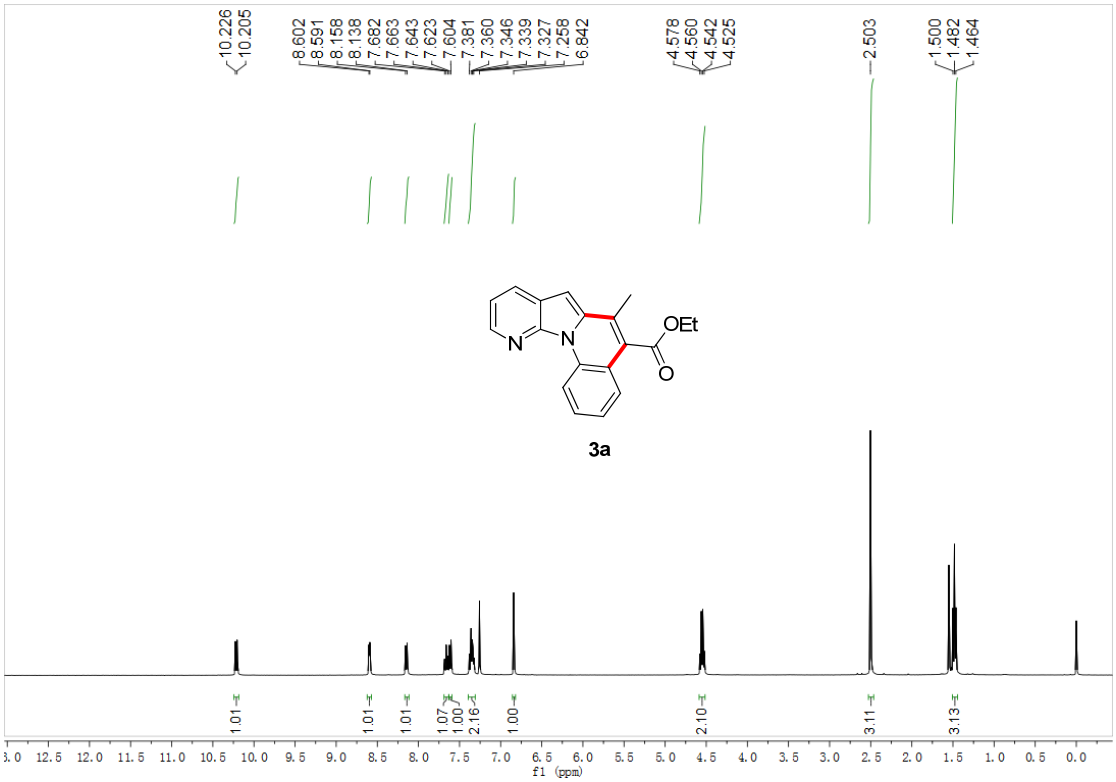
(**1:1**)

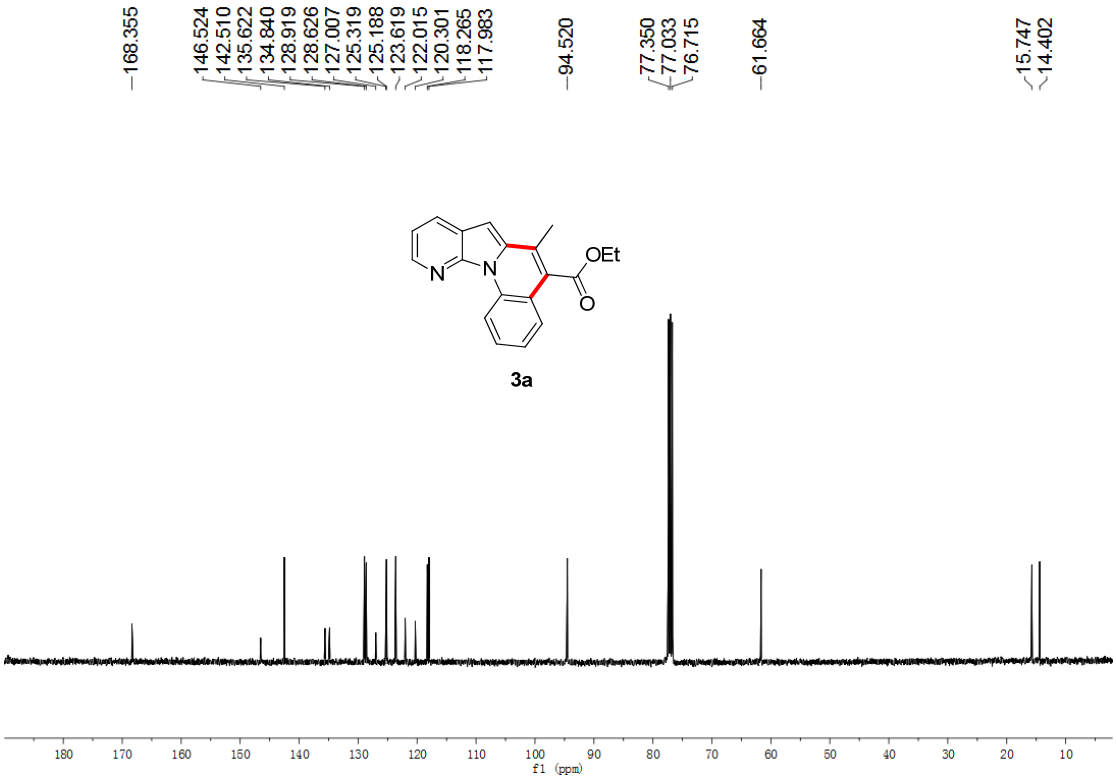
1-(6-methylpyrido[3',2':4,5]pyrrolo[1,2-a]quinolin-5-yl)ethanone (**3v**). 1-(5-methylpyrido[3',2':4,5]pyrrolo[1,2-a]quinolin-6-yl)ethanone (**4v**). 10 h, 38% yield (5.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.22 (d, J = 8.4 Hz, 2H), 8.56 (dd, J_1 = 14.4 Hz, J_2 = 4.4 Hz, 2H), 8.13 (d, J = 7.6 Hz, 1H), 8.08 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 7.6 Hz, 1H), 7.73-7.64 (m, 2H), 7.42-7.30 (m, 5H), 6.79 (s, 1H), 6.46 (s, 1H), 2.69 (s, 3H), 2.64 (s, 3H), 2.48 (s, 3H), 2.41 (s, 3H) ppm. ESI HRMS: calcd. for $C_{18}H_{14}N_2O$+H 275.1184, found 275.1187.

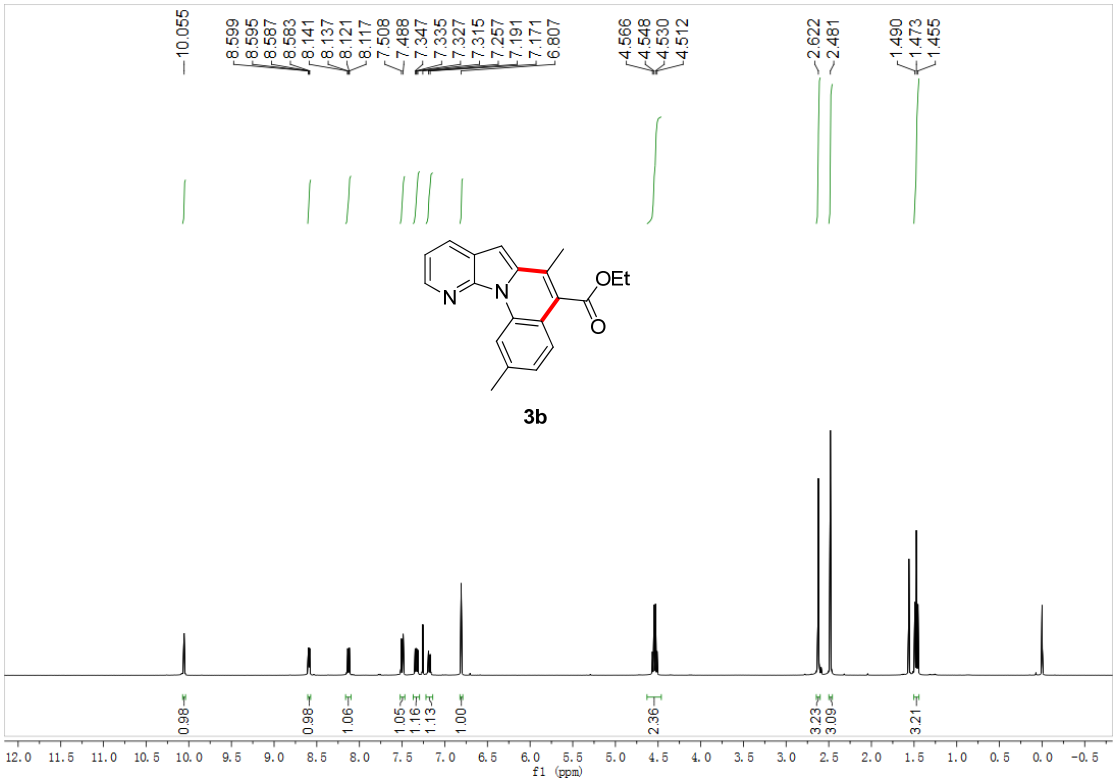
Reference

[1] Qian, G.; Hong, X.; Liu, B.; Mao, H.; Xu, B. *Org. Lett.* **2014,** *16* (20), 5294-5297.

3. NMR Spectra of 7-azaindole Derived Fused Compounds and Structure Determination



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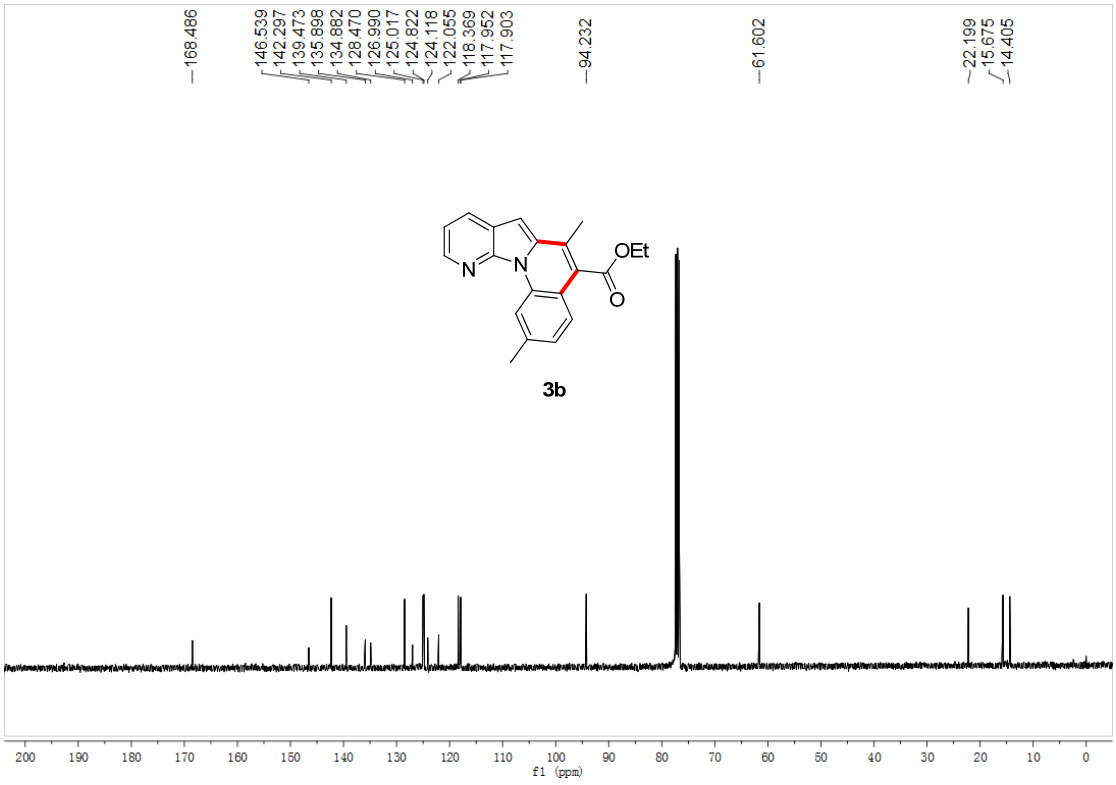
8.595
8.587
8.583
8.141
8.137
8.121
8.117
7.508
7.488
7.347
7.335
7.327
7.315
7.257
7.191
7.171
6.807
4.566
4.548
4.530
4.512
2.622
2.481
1.490
1.473
1.455
OEt
O
N
N
3b
0.98
0.98
1.06
1.05
1.16
1.13
1.00
2.36
3.23
3.09
3.21
f1 (ppm)


168.486
146.539
142.297
139.473
135.898
134.882
128.470
126.990
125.017
124.822
124.118
122.055
118.369
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117.903
94.232
61.602
22.199
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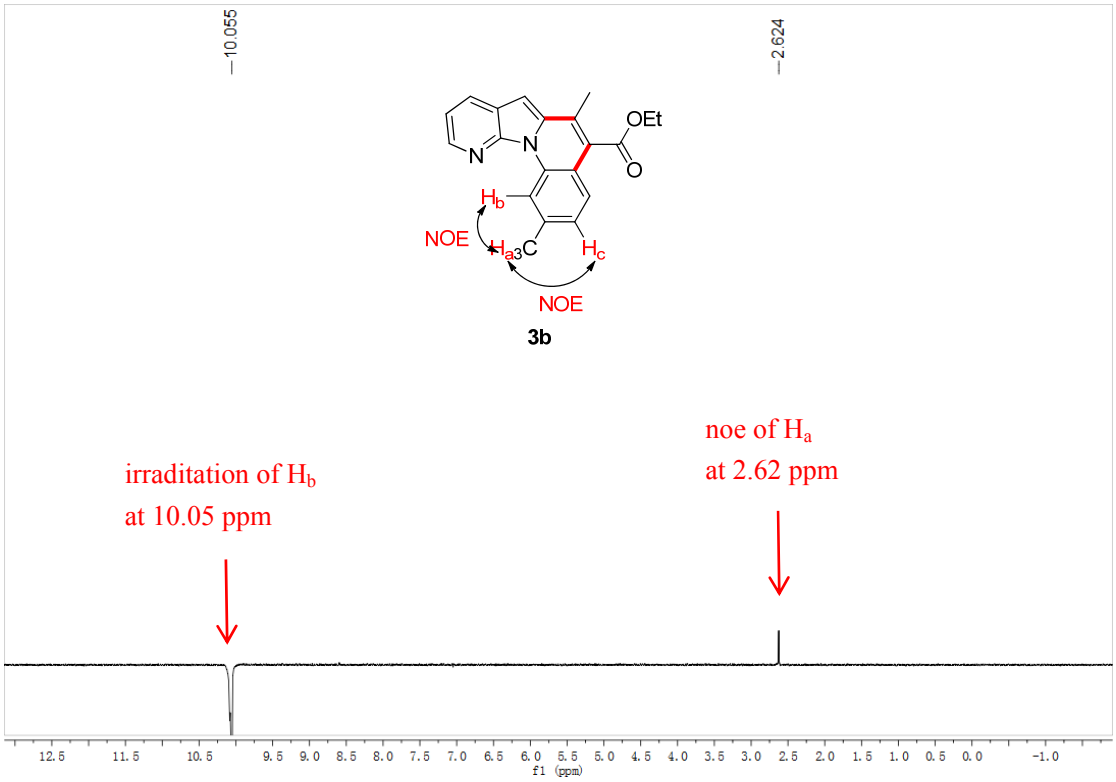
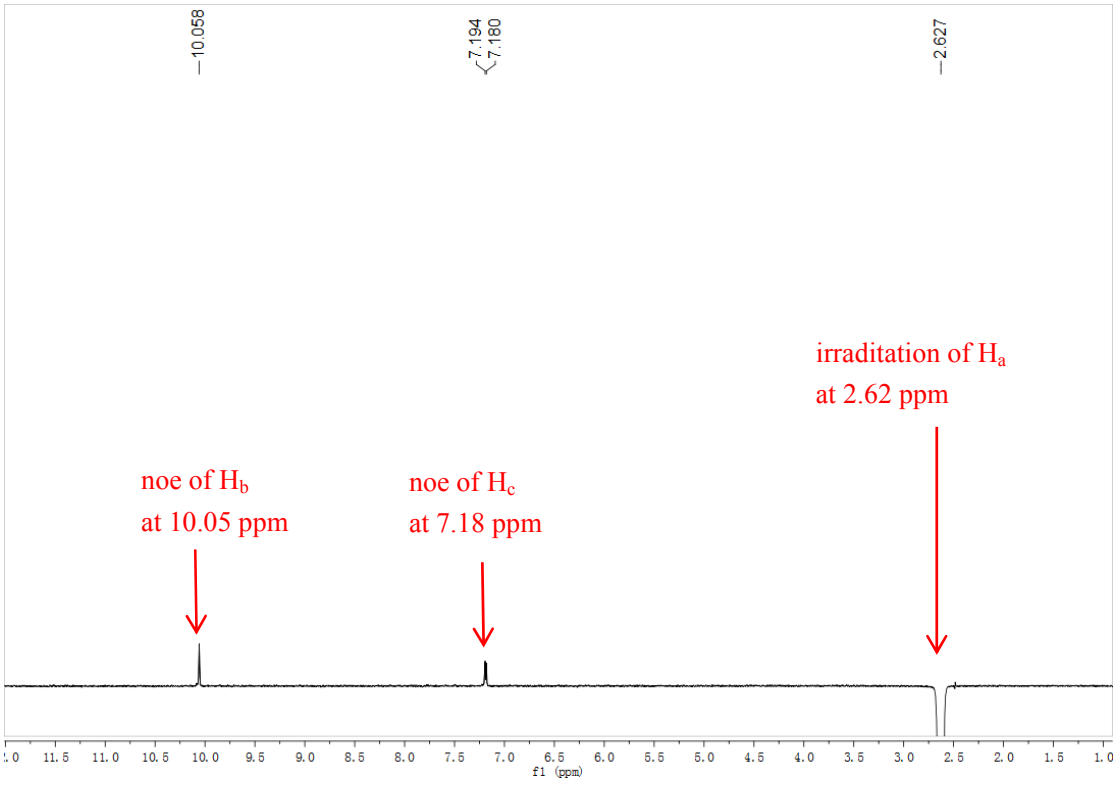
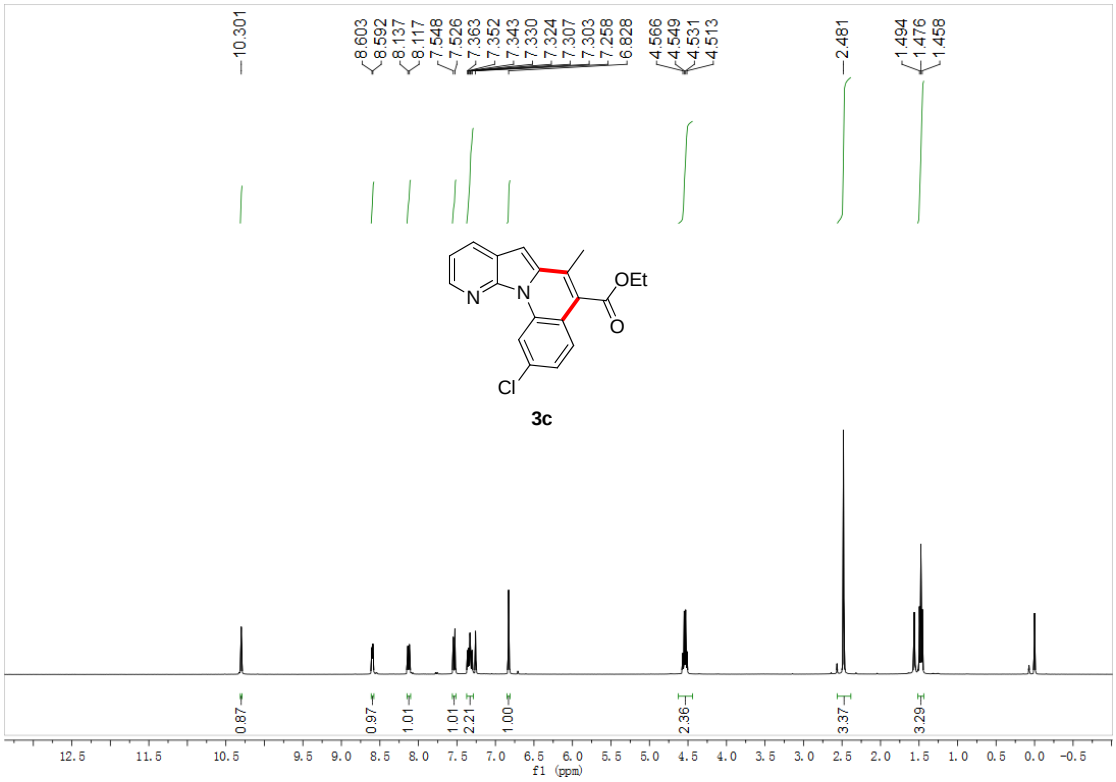
14.405
OEt
O
N
N
3b
f1 (ppm)





The single peak at about 10.40 ppm on **3c** and **3d** illustrate the same regioseletivty as **3b**.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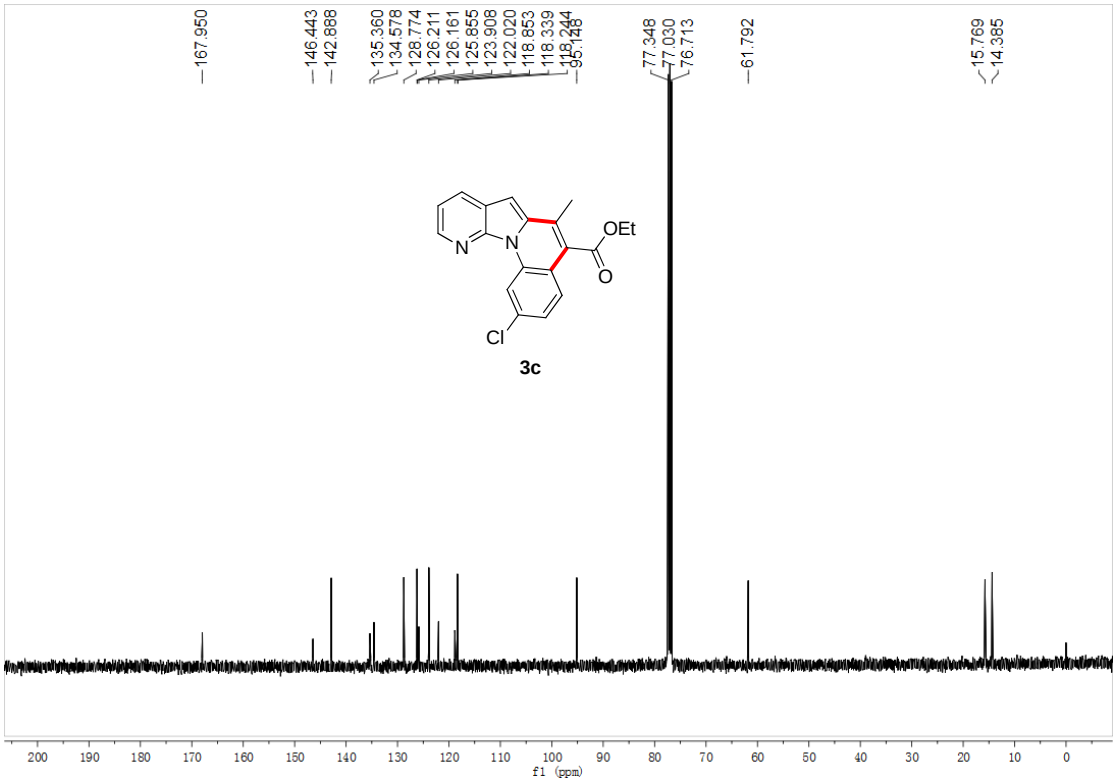
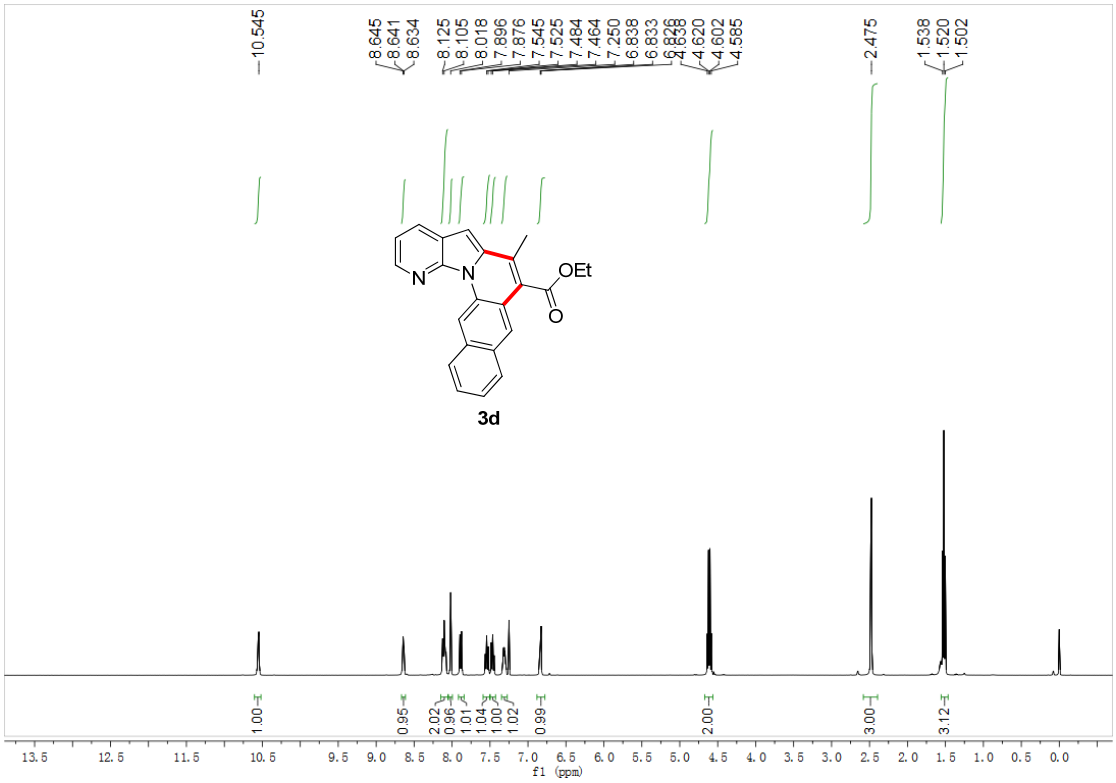
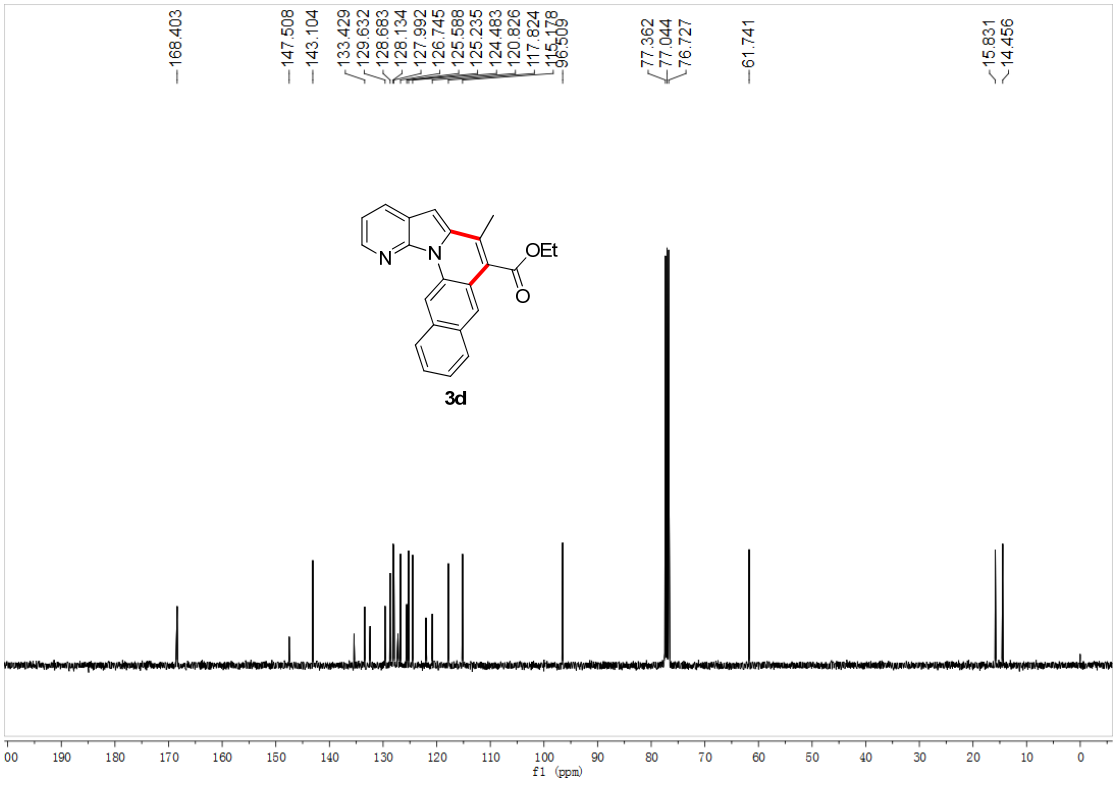
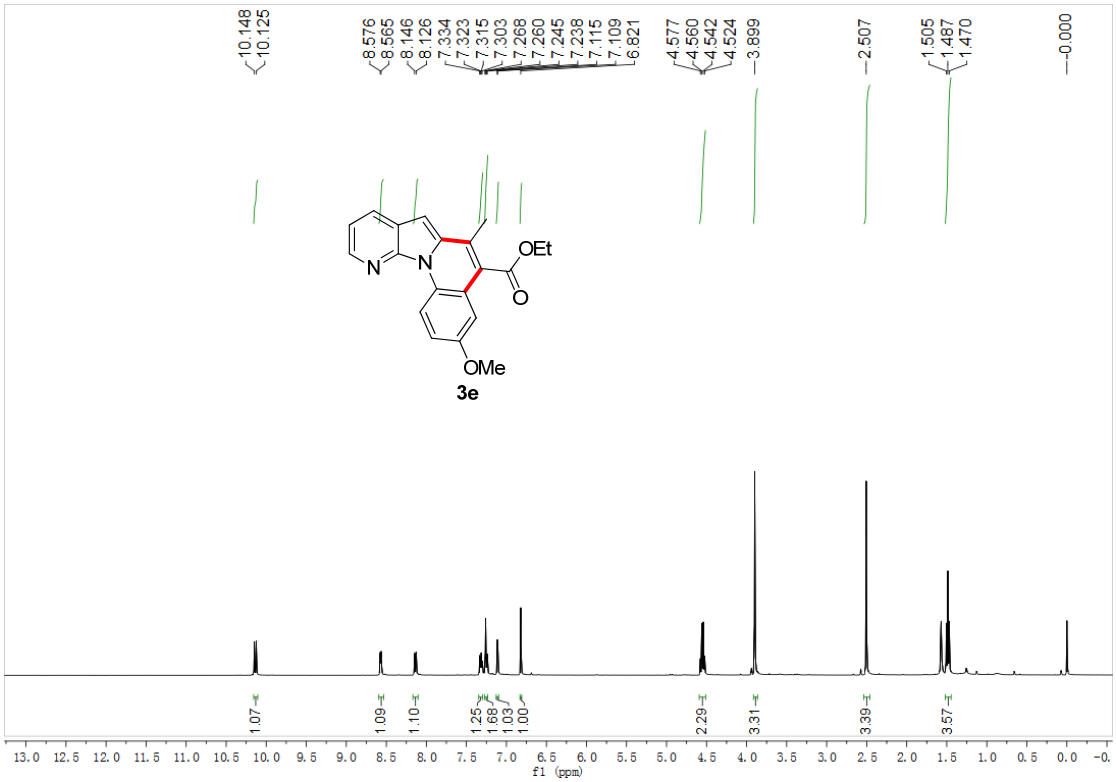
8.592
8.137
8.117
7.548
7.526
7.363
7.352
7.343
7.330
7.324
7.307
7.303
7.258
6.828
4.566
4.549
4.531
4.513
2.481
1.494
1.476
1.458
OEt
O
N
N
Cl
3c
0.87
0.97
1.01
1.01
2.21
1.00
2.36
3.37
3.29
f1 (ppm)


167.950
146.443
142.888
135.360
134.578
128.774
126.211
126.161
125.855
123.908
122.020
118.853
118.339
95.148
77.348
77.030
76.713
61.792
15.769
14.385
OEt
O
N
N
Cl
3c
f1 (ppm)


10.545
8.645
8.641
8.634
8.125
8.105
8.018
7.896
7.876
7.545
7.525
7.484
7.464
7.250
6.838
6.833
6.826
6.638
4.620
4.602
4.585
2.475
1.538
1.520
1.502
OEt
O
N
N
3d
1.00
0.95
2.02
0.96
1.01
1.04
1.00
1.02
0.99
2.00
3.00
3.12
f1 (ppm)


168.403
147.508
143.104
133.429
129.632
128.683
128.134
127.992
126.745
125.588
125.235
124.483
120.826
117.824
115.178
96.509
77.362
77.044
76.727
61.741
15.831
14.456
OEt
O
N
N
3d
f1 (ppm)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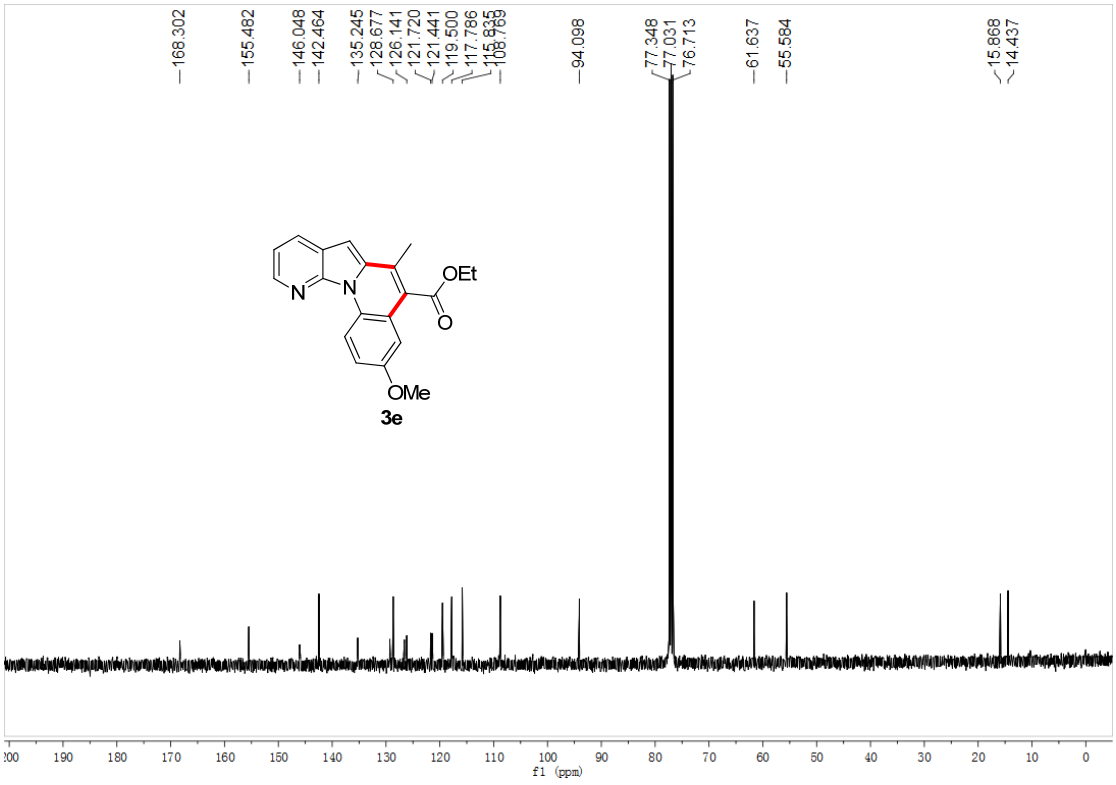
8.576
8.565
8.146
8.126
7.334
7.323
7.315
7.303
7.268
7.260
7.245
7.238
7.115
7.109
6.821
4.577
4.560
4.542
4.524
3.899
2.507
1.505
1.487
1.470
0.000
OEt
O
N
N
OMe
3e
1.07
1.09
1.10
1.25
1.68
1.03
1.00
2.29
3.31
3.39
3.57
f1 (ppm)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146.048
142.464
135.245
128.677
126.141
121.720
121.441
119.500
117.786
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108.769
94.098
77.348
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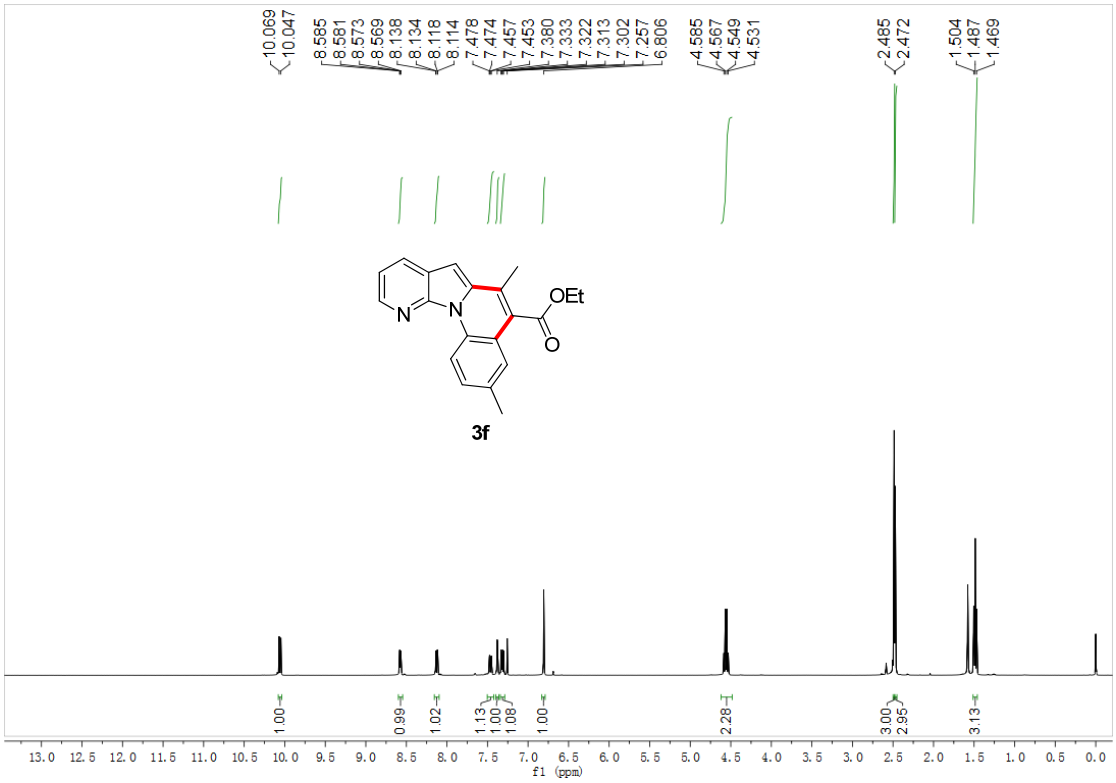
OEt
O
N
N
OMe
3e
f1 (ppm)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10.047
8.585
8.581
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8.569
8.138
8.134
8.118
8.114
7.478
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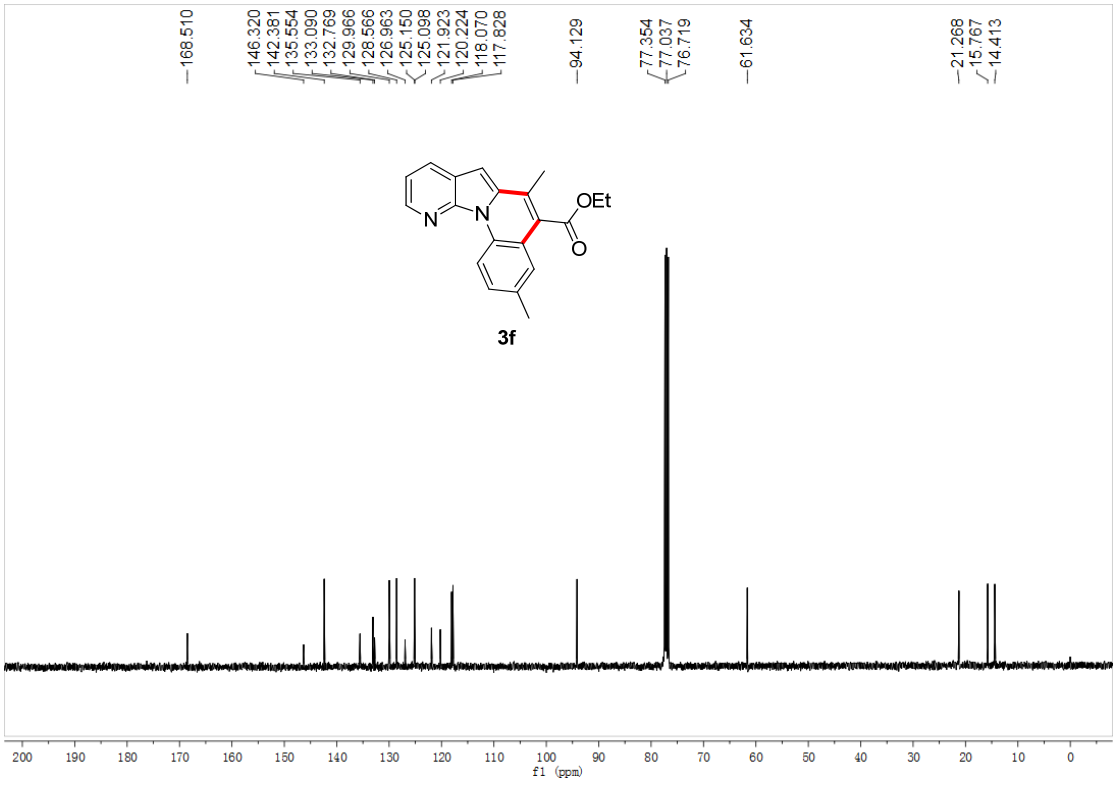
7.453
7.380
7.333
7.322
7.313
7.302
7.257
6.806
4.585
4.567
4.549
4.531
2.485
2.472
1.504
1.487
1.469
OEt
O
N
N
3f
1.00
0.99
1.02
1.13
1.00
1.08
1.00
2.28
3.00
2.95
3.13
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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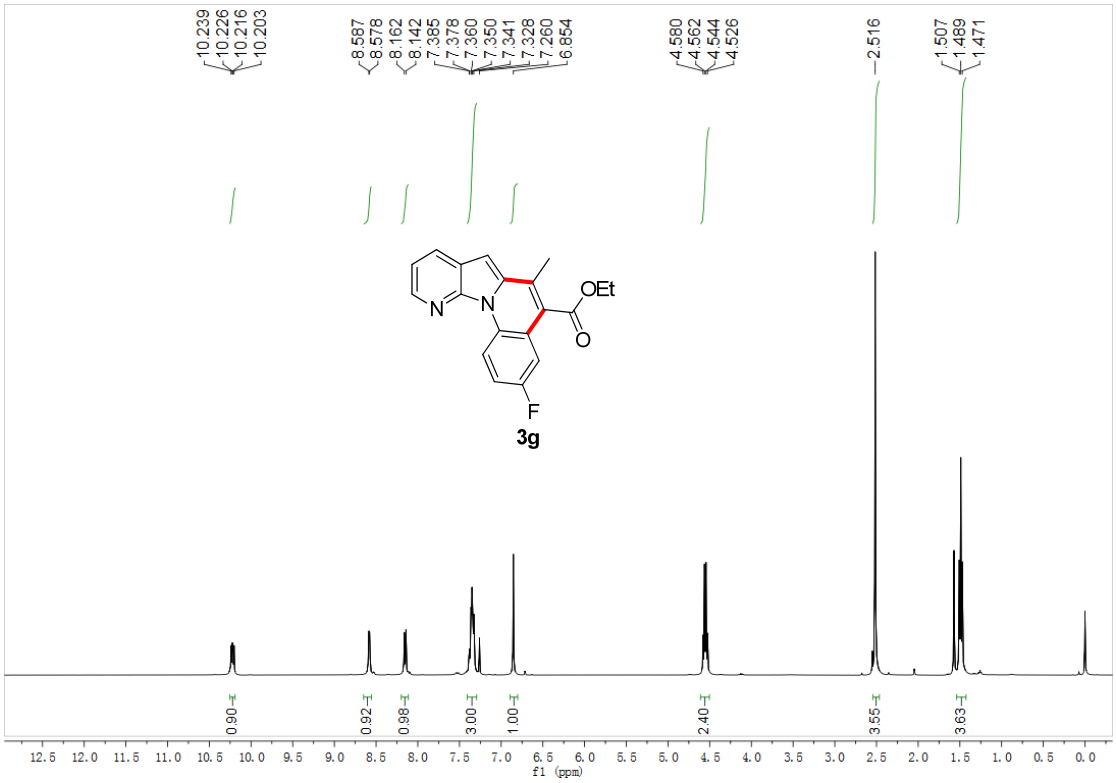
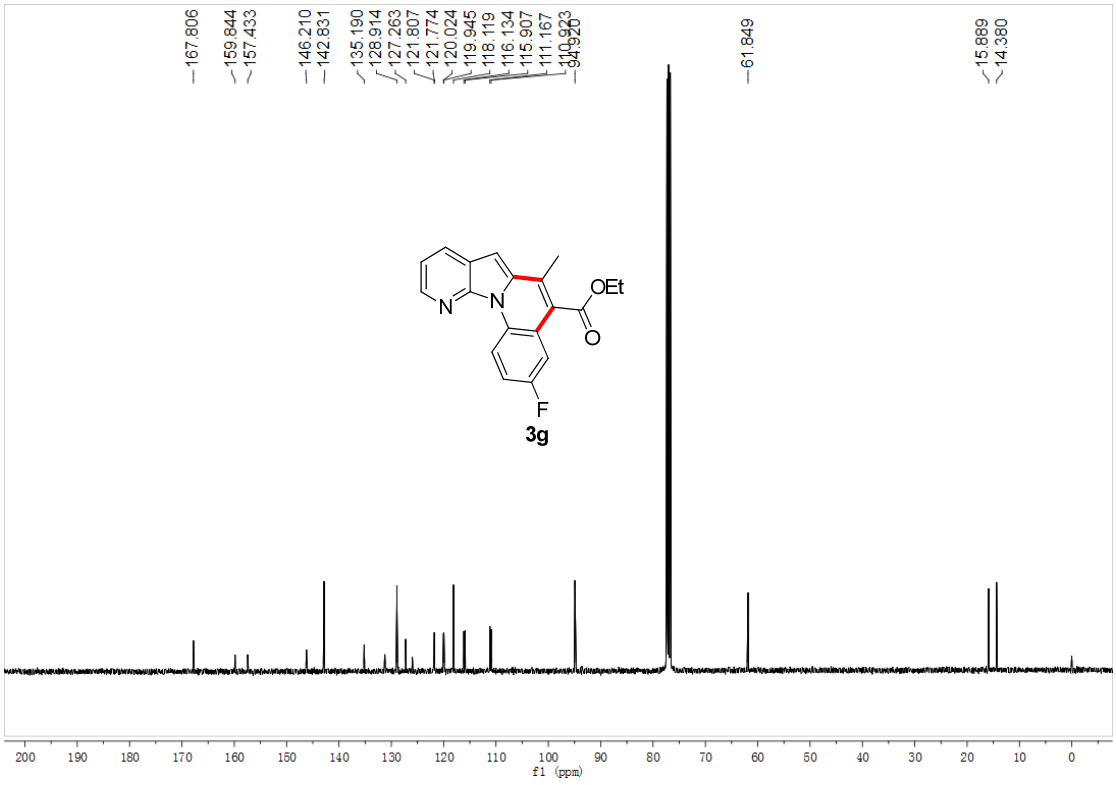
133.090
132.769
129.966
128.566
126.963
125.150
125.098
121.923
120.224
118.070
117.828
94.129
77.354
77.037
76.719
61.634
21.268
15.767
14.413
OEt
O
N
N
3f
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


10.239
10.226
10.216
10.203
8.587
8.578
8.162
8.142
7.385
7.378
7.360
7.350
7.341
7.328
7.260
6.854
4.580
4.562
4.544
4.526
2.516
1.507
1.489
1.471
OEt
O
N
N
F
3g
0.90
0.92
0.98
3.00
1.00
2.40
3.55
3.63
f1 (ppm)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157.433
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142.831
135.190
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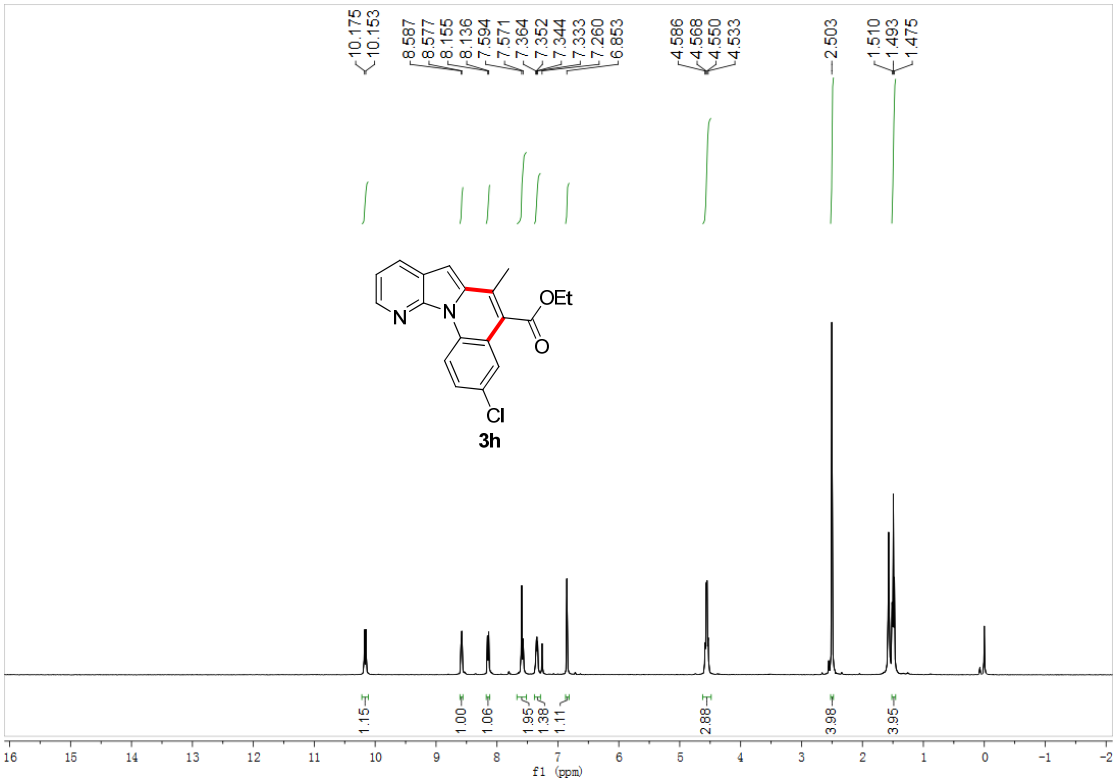
127.263
121.807
121.774
120.024
119.945
118.119
116.134
115.907
111.167
110.923
94.920
61.849
15.889
14.380
OEt
O
N
N
F
3g
f1 (ppm)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8.577
8.155
8.136
7.594
7.571
7.364
7.352
7.344
7.333
7.260
6.853
4.586
4.568
4.550
4.533
2.503
1.510
1.493
1.475
OEt
O
N
Cl
3h
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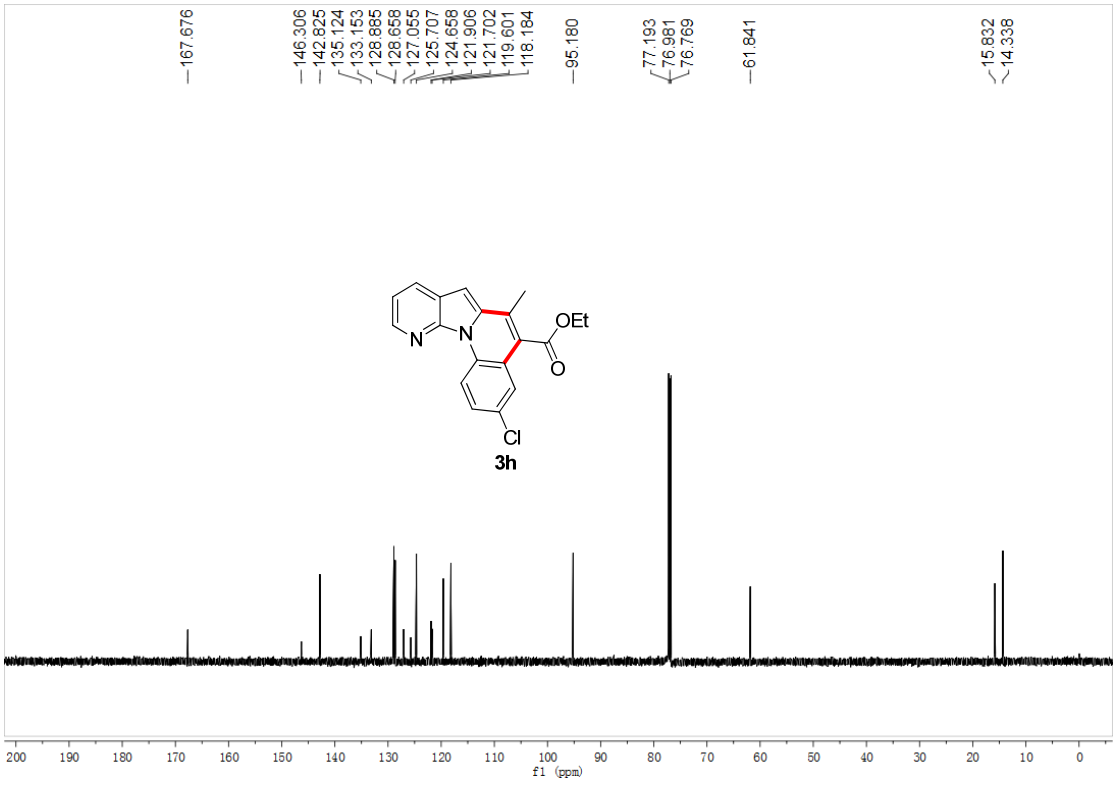
1.00
1.06
1.95
1.38
1.11
2.88
3.98
3.95
f1 (ppm)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127.055
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124.658
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121.702
119.601
118.184
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76.769
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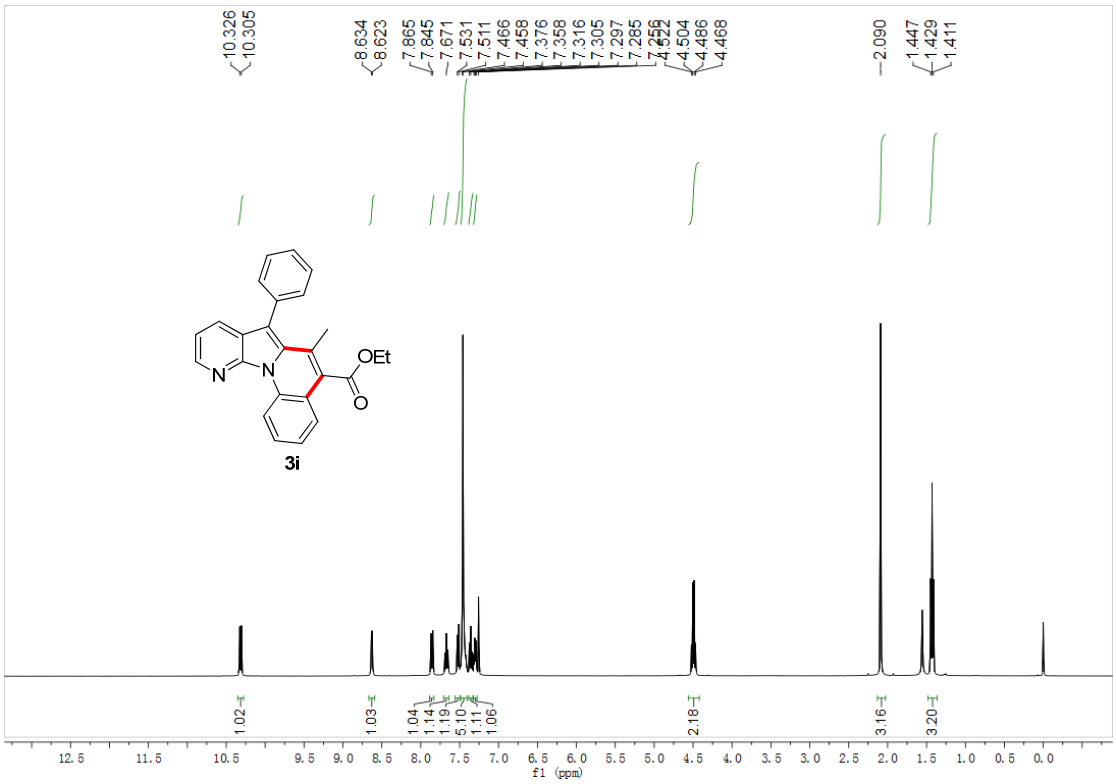
14.338
OEt
O
N
Cl
3h
f1 (ppm)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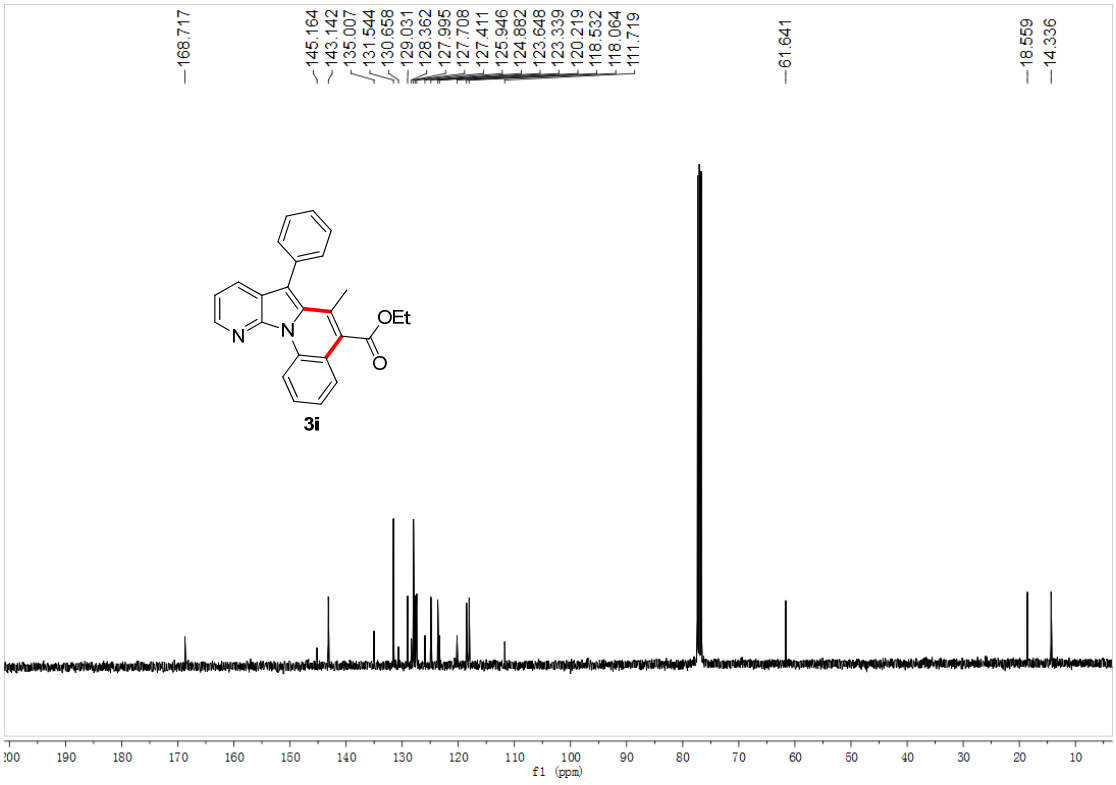
10.305
8.634
8.623
7.865
7.845
7.671
7.531
7.511
7.466
7.458
7.376
7.358
7.316
7.305
7.297
7.285
4.504
4.486
4.468
2.090
1.447
1.429
1.411
OEt
O
N
N
3i
1.02
1.03
1.04
1.14
1.19
5.10
1.11
1.06
2.18
3.16
3.20
f1 (ppm)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128.362
127.995
127.708
127.411
125.946
124.882
123.648
123.339
120.219
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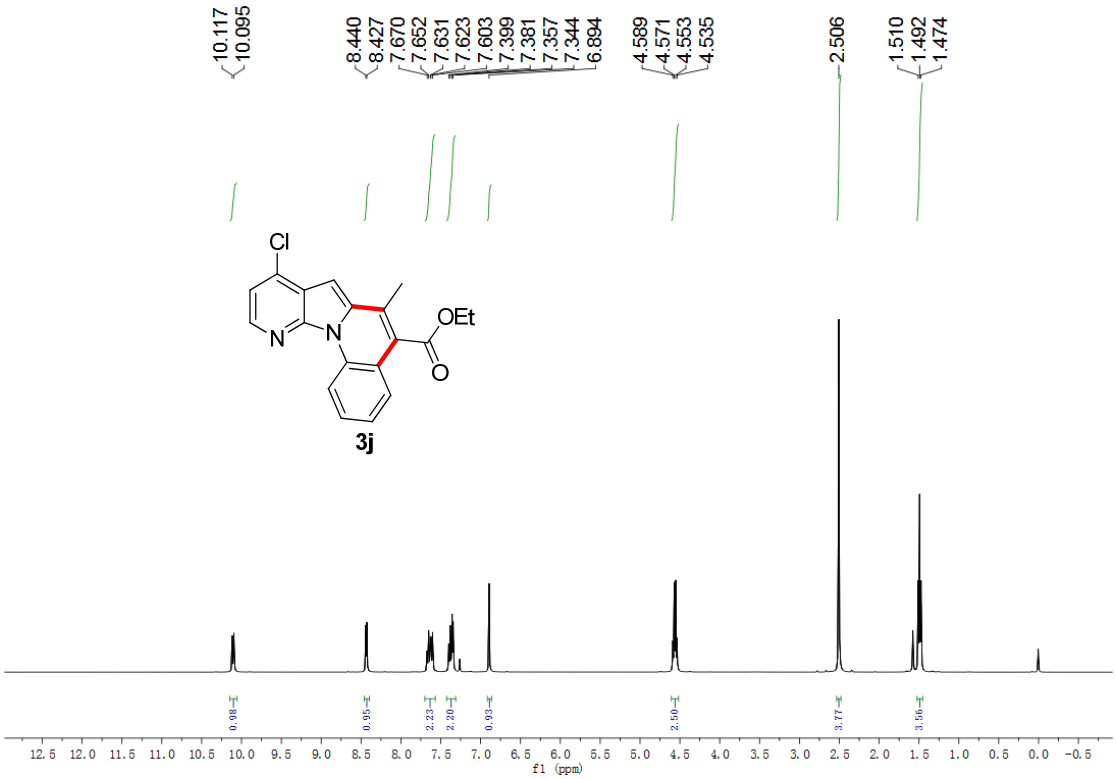
118.064
111.719
61.641
18.559
14.336
OEt
O
N
N
3i
f1 (ppm)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10.095
8.440
8.427
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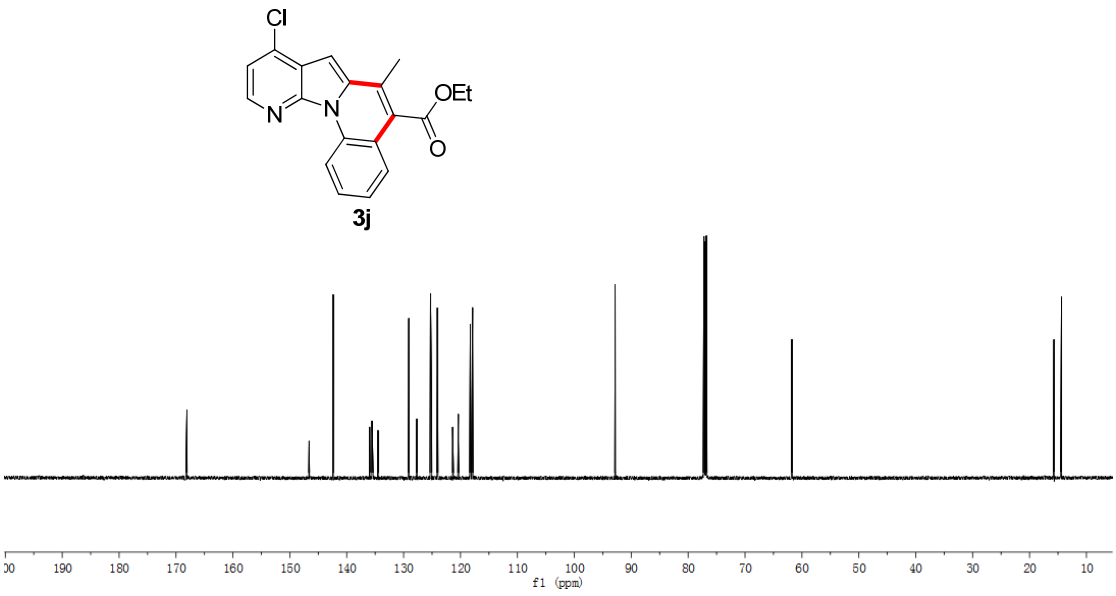
7.652
7.631
7.623
7.603
7.399
7.381
7.357
7.344
6.894
4.589
4.571
4.553
4.535
2.506
1.510
1.492
1.474
Cl
N
N
OEt
O
0.98
0.95
2.23
2.20
0.93
2.50
3.77
3.56
f1 (ppm)

3j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142.396
142.385
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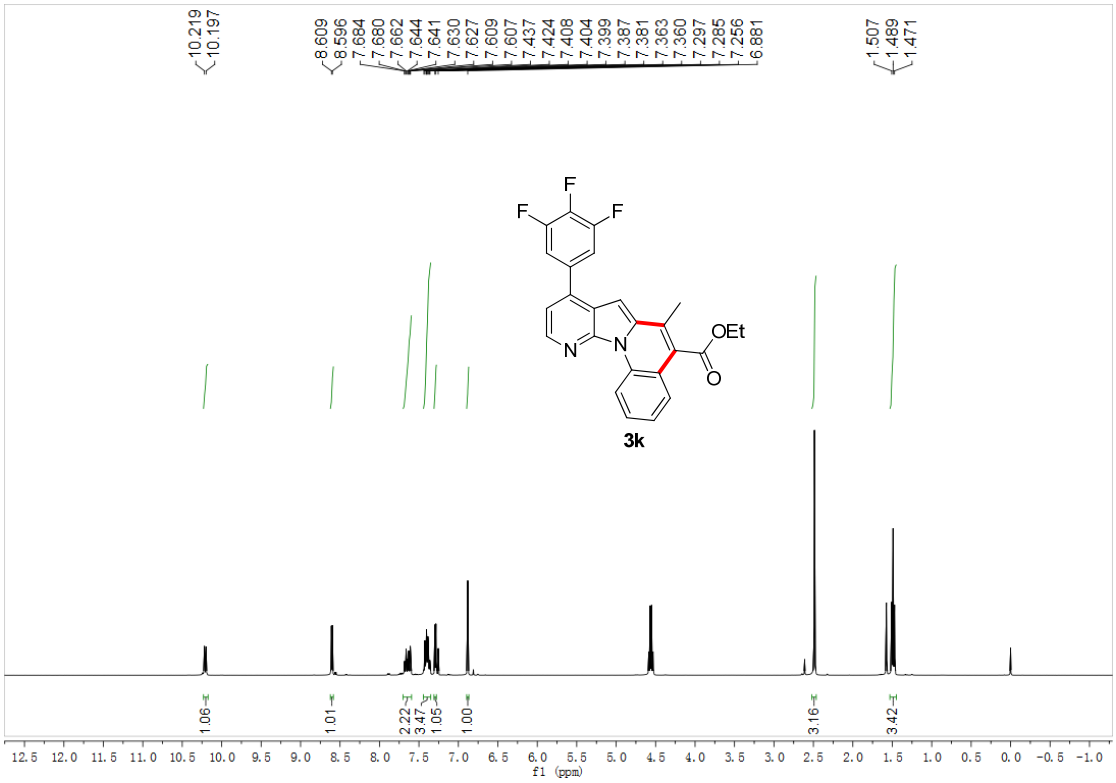
135.550
134.499
129.074
127.663
125.277
125.083
124.076
124.065
121.377
120.387
118.282
117.879
92.823
77.222
77.010
76.798
61.758
15.703
15.693
14.396
14.385
Cl
N
N
OEt
O
f1 (ppm)

3j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10.197
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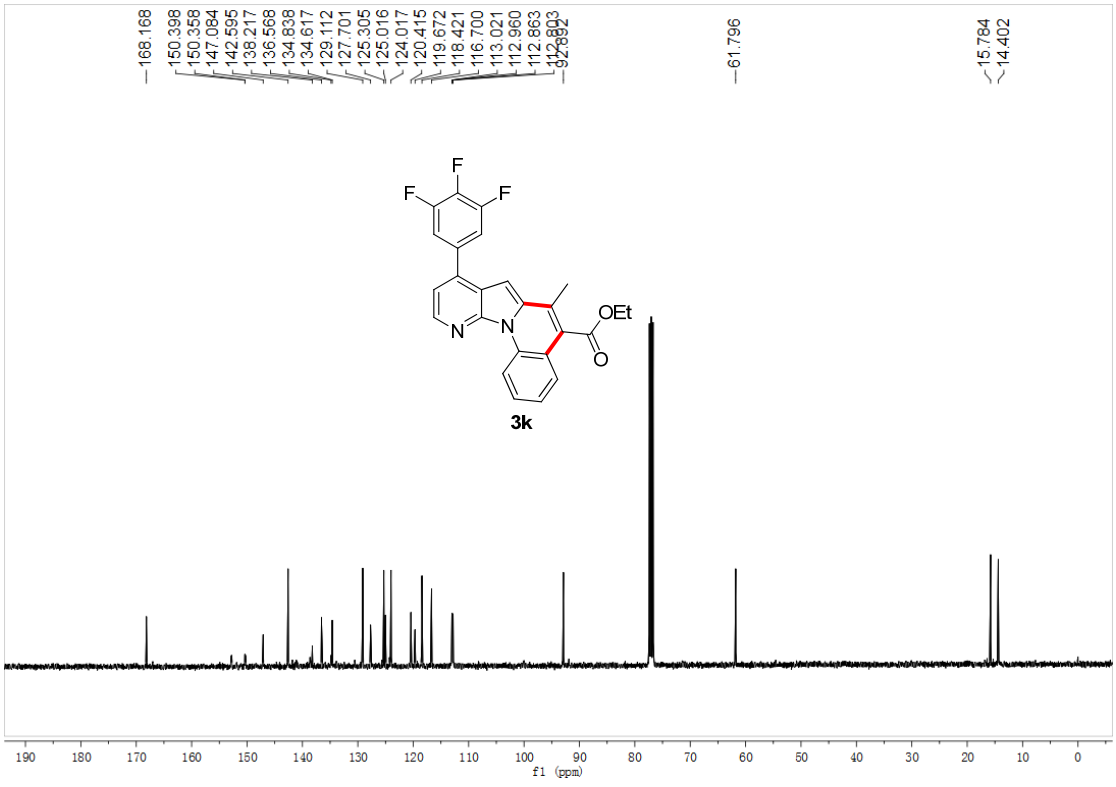
8.596
7.684
7.680
7.662
7.644
7.641
7.630
7.627
7.609
7.607
7.437
7.424
7.408
7.404
7.399
7.387
7.381
7.363
7.360
7.297
7.285
7.256
6.881
1.507
1.489
1.471
F
F
F
N
N
OEt
O
3k
1.06
1.01
2.22
3.47
1.05
1.00
3.16
3.42
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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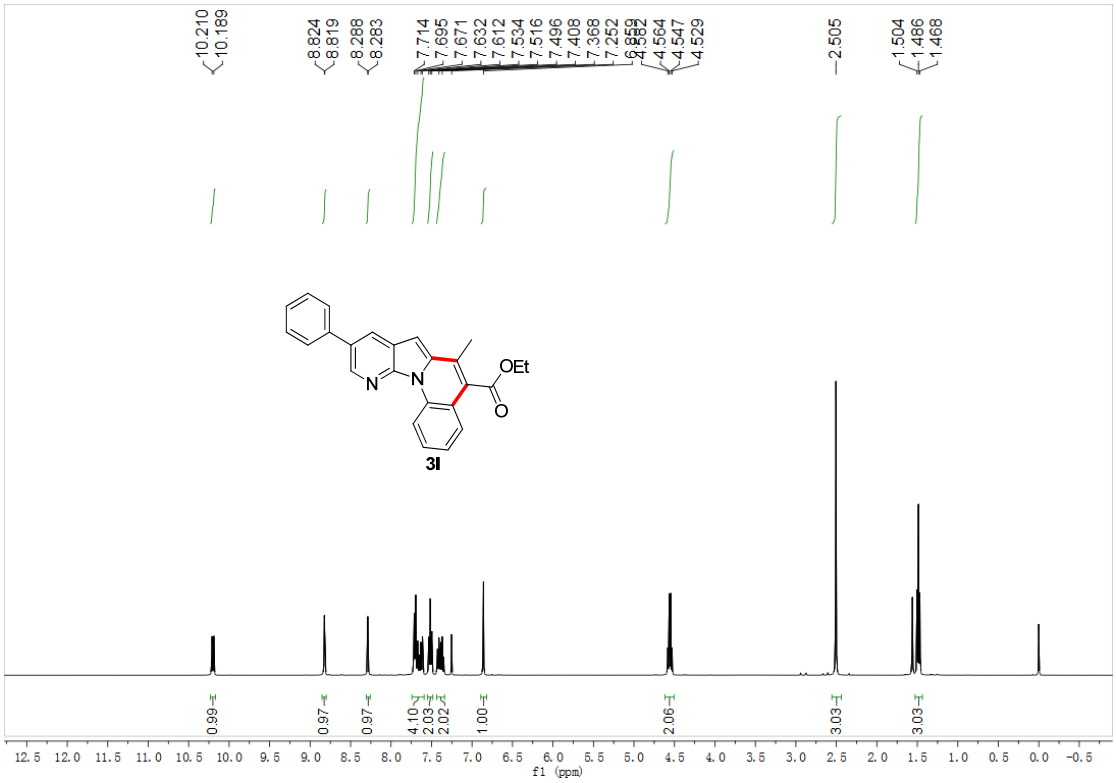
150.398
150.358
147.084
142.595
138.217
136.568
134.838
134.617
129.112
127.701
125.305
125.016
124.017
120.415
119.672
118.421
116.700
113.021
112.960
112.863
112.803
92.892
61.796
15.784
14.402
F
F
F
N
N
OEt
O
3k
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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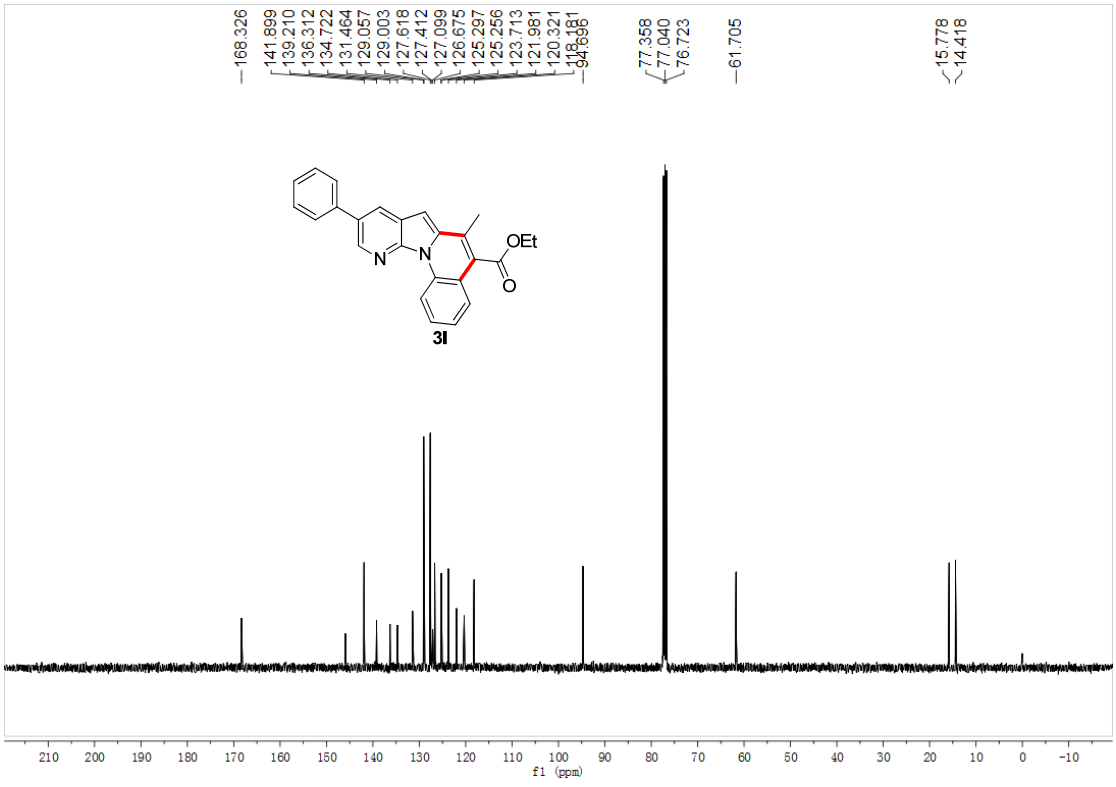
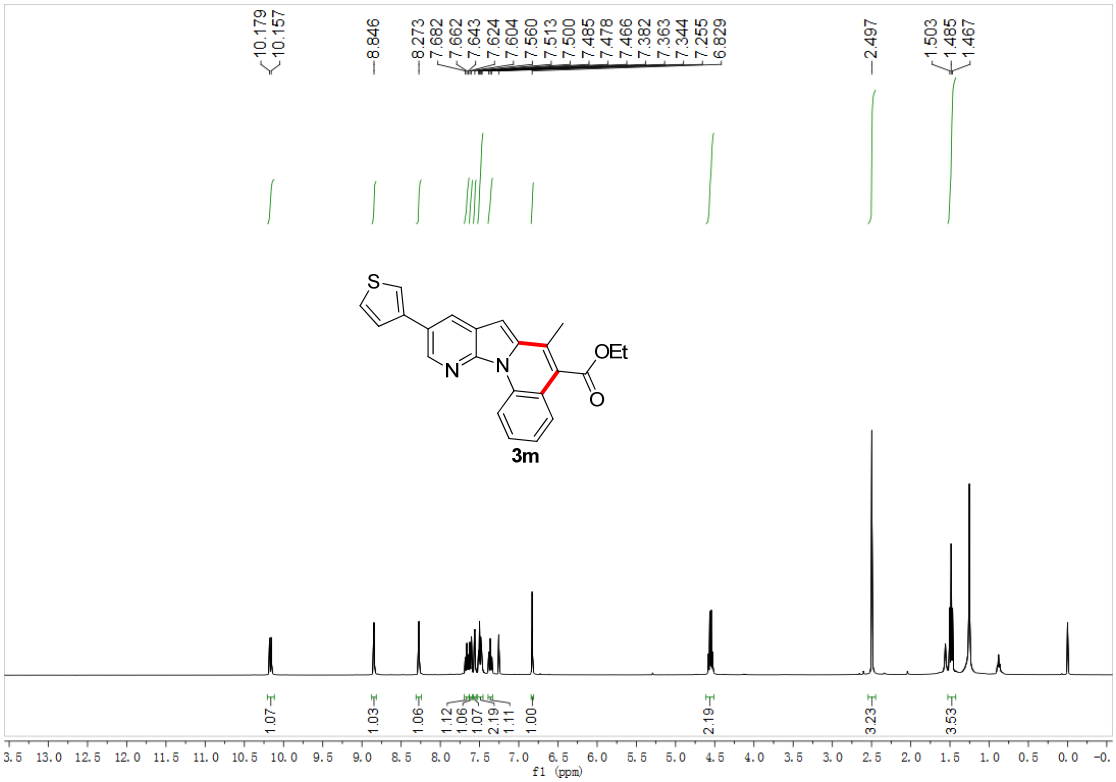
10.189
8.824
8.819
8.288
8.283
7.714
7.695
7.671
7.632
7.612
7.534
7.516
7.496
7.408
7.368
7.252
4.564
4.547
4.529
2.505
1.504
1.486
1.468
OEt
O
N
N
3l
0.99
0.97
0.97
4.10
2.03
2.02
1.00
2.06
3.03
3.03
f1 (ppm)


168.326
141.899
139.210
136.312
134.722
131.464
129.057
129.003
127.618
127.412
127.099
126.675
125.297
125.256
123.713
121.981
120.321
118.181
94.696
77.358
77.040
76.723
61.705
15.778
14.418
OEt
O
N
N
3l
f1 (ppm)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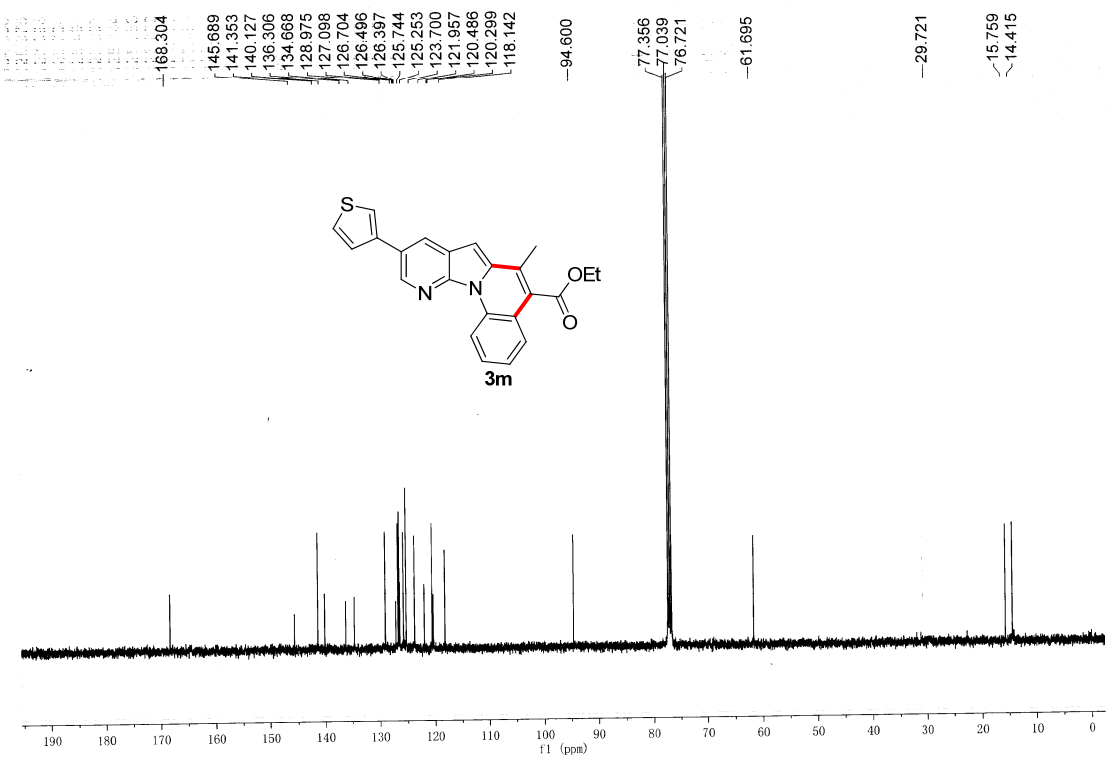
10.157
8.846
8.273
7.682
7.662
7.643
7.624
7.604
7.560
7.513
7.500
7.485
7.478
7.466
7.382
7.363
7.344
7.255
6.829
2.497
1.503
1.485
1.467
S
N
N
OEt
O
3m
1.07
1.03
1.06
1.12
1.06
1.07
2.19
1.11
1.00
2.19
3.23
3.53
f1 (ppm)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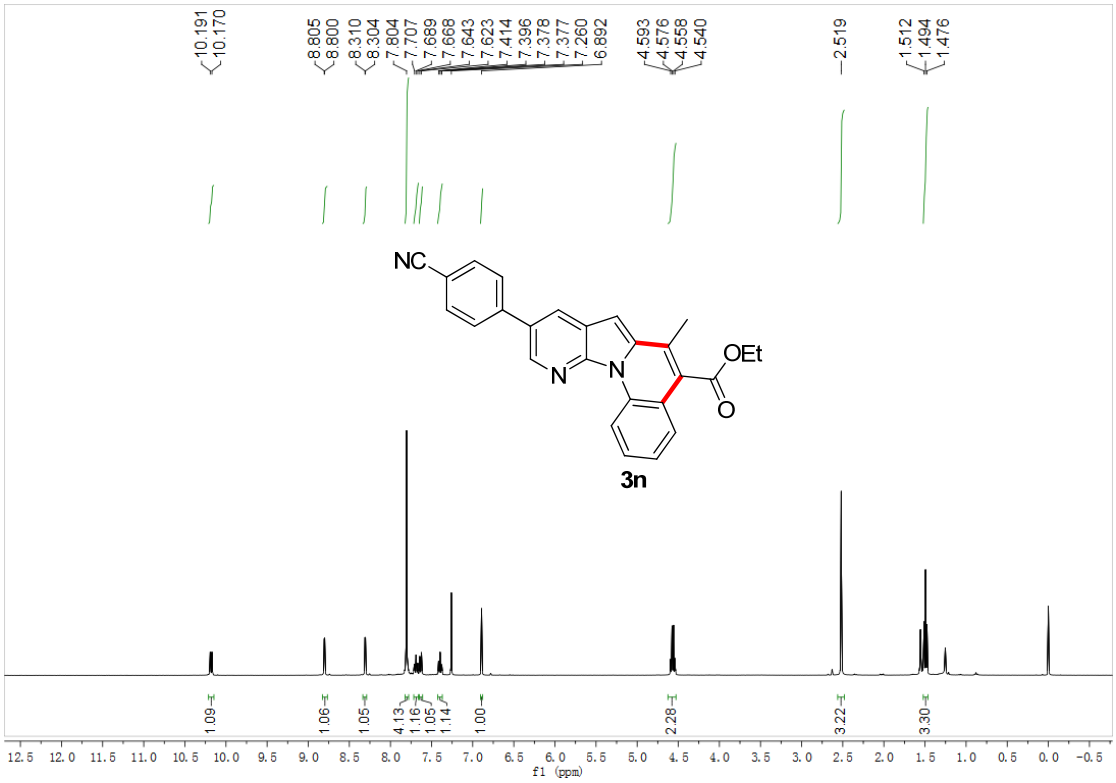
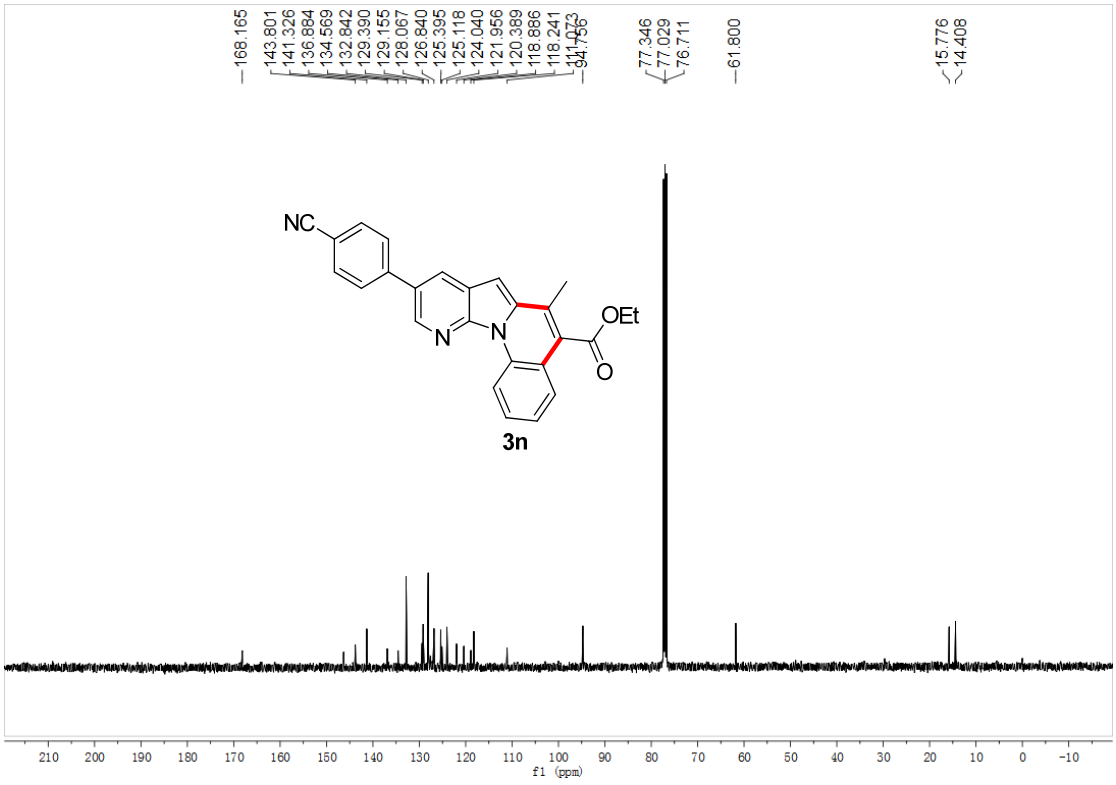
141.353
140.127
136.306
134.668
128.975
127.098
126.704
126.496
126.397
125.744
125.253
123.700
121.957
120.486
120.299
118.142
94.600
77.356
77.039
76.721
61.695
29.721
15.759
14.415
S
N
N
OEt
O
3m
f1 (ppm)


10.191
10.170
8.805
8.800
8.310
8.304
7.804
7.707
7.689
7.668
7.643
7.623
7.414
7.396
7.378
7.377
7.260
6.892
4.593
4.576
4.558
4.540
2.519
1.512
1.494
1.476
NC
OEt
N
N
O
3n
1.09
1.06
1.05
4.13
1.16
1.05
1.14
1.00
2.28
3.22
3.30
f1 (ppm)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129.390
129.155
128.067
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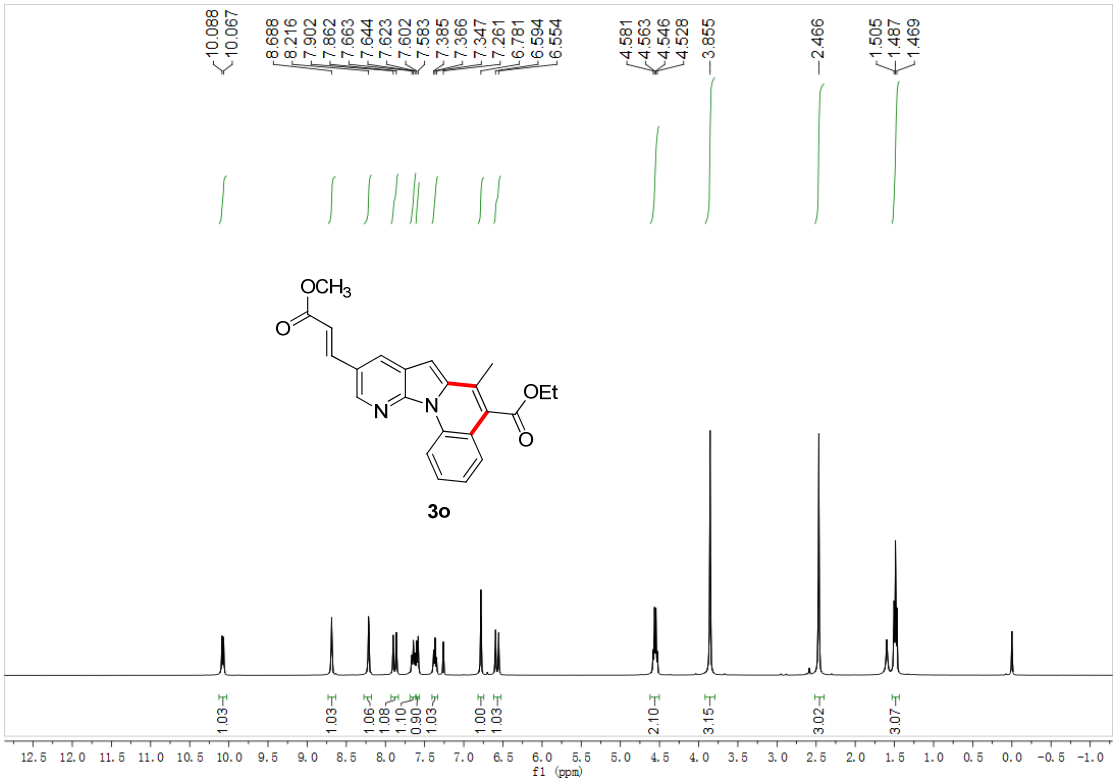
125.395
125.118
124.040
121.956
120.389
118.886
118.241
111.073
94.756
77.346
77.029
76.711
61.800
15.776
14.408
NC
OEt
N
N
O
3n
f1 (ppm)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7.644
7.623
7.602
7.583
7.385
7.366
7.347
7.261
6.781
6.594
6.554
4.581
4.563
4.546
4.528
3.855
2.466
1.505
1.487
1.469
OCH3
O
N
N
OEt
O
1.03
1.03
1.06
1.08
1.10
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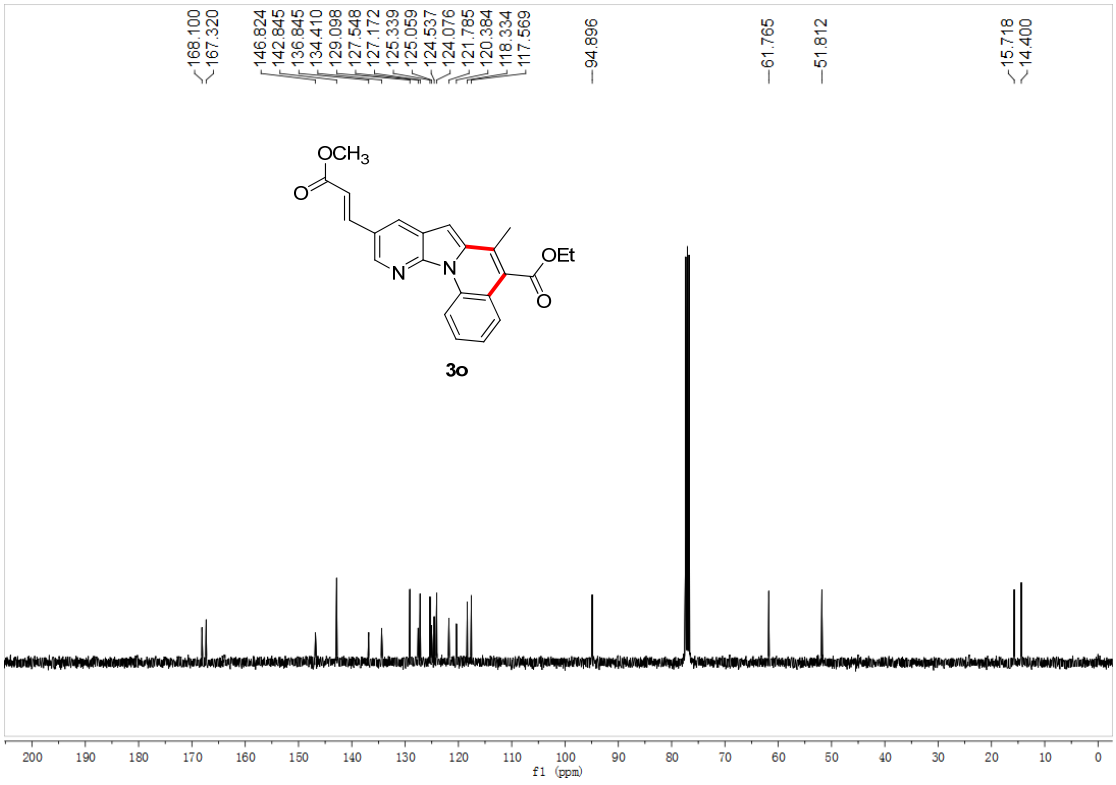
1.03
1.00
1.03
2.10
3.15
3.02
3.07
f1 (ppm)

3o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127.548
127.172
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125.059
124.537
124.076
121.785
120.384
118.334
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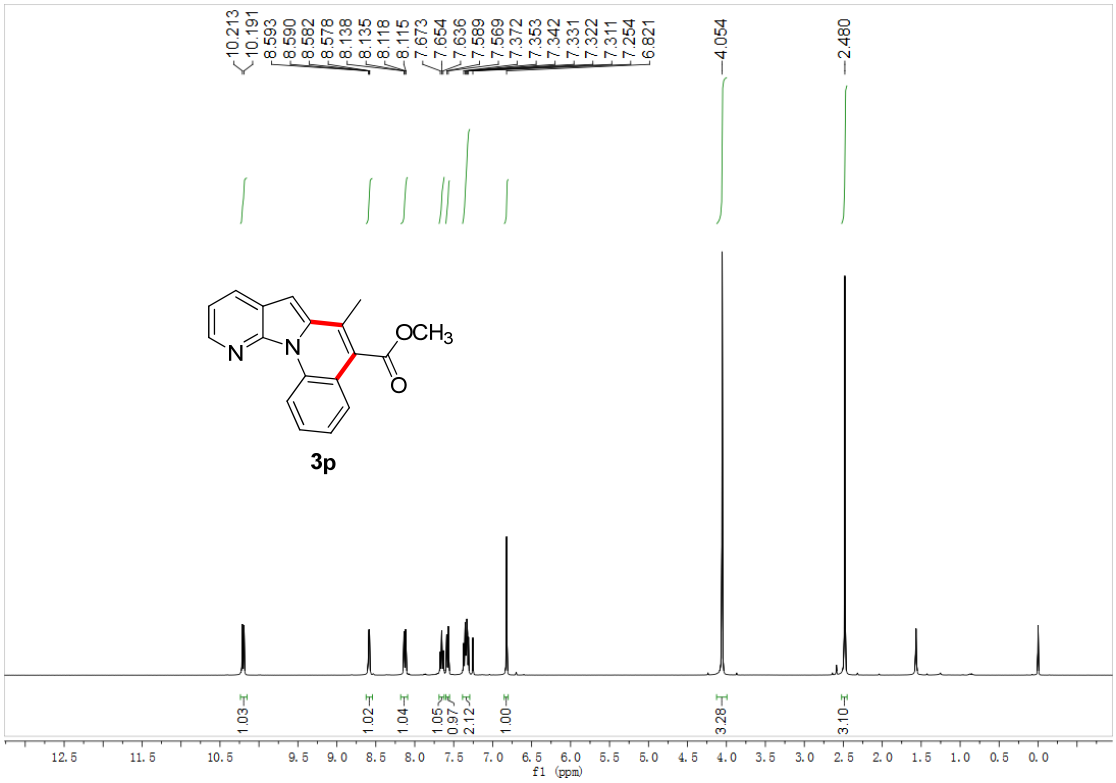
51.812
15.718
14.400
OCH3
O
N
N
OEt
O
f1 (ppm)

3o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8.590
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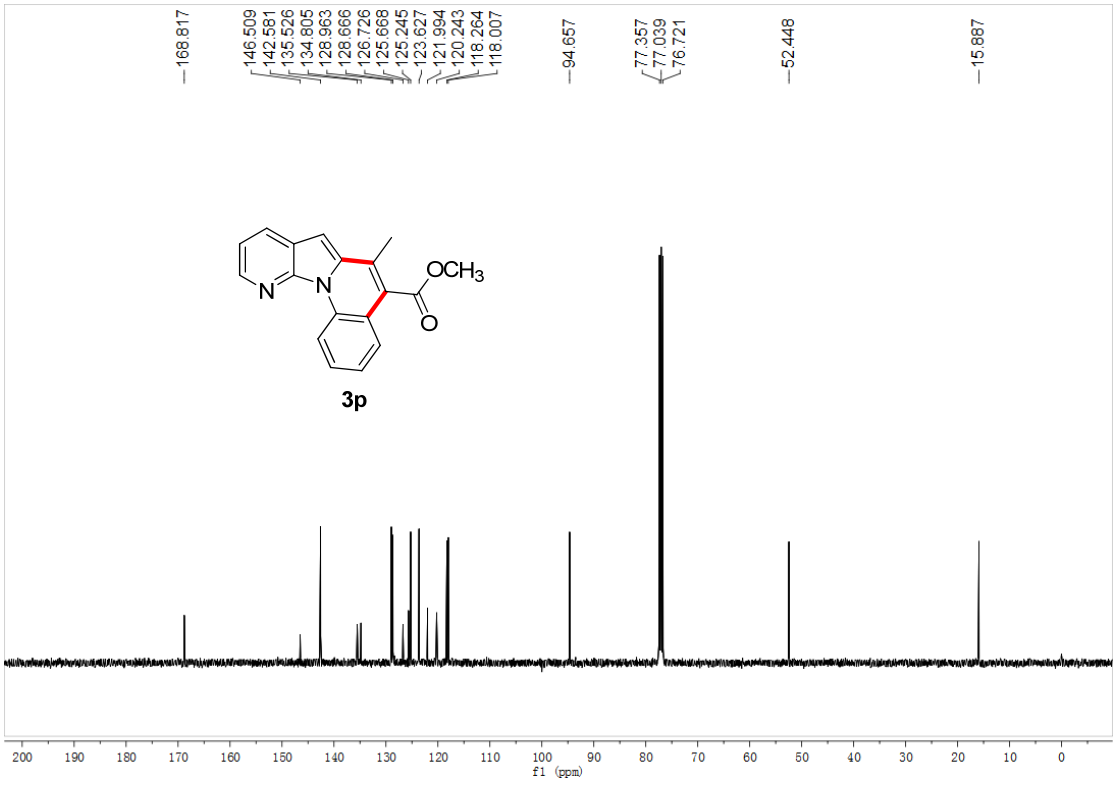
8.578
8.138
8.135
8.118
8.115
7.673
7.654
7.636
7.589
7.569
7.372
7.353
7.342
7.331
7.322
7.311
7.254
6.821
4.054
2.480
OCH3
O
N
N
1.03
1.02
1.04
1.05
0.97
2.12
1.00
3.28
3.10
f1 (ppm)

3p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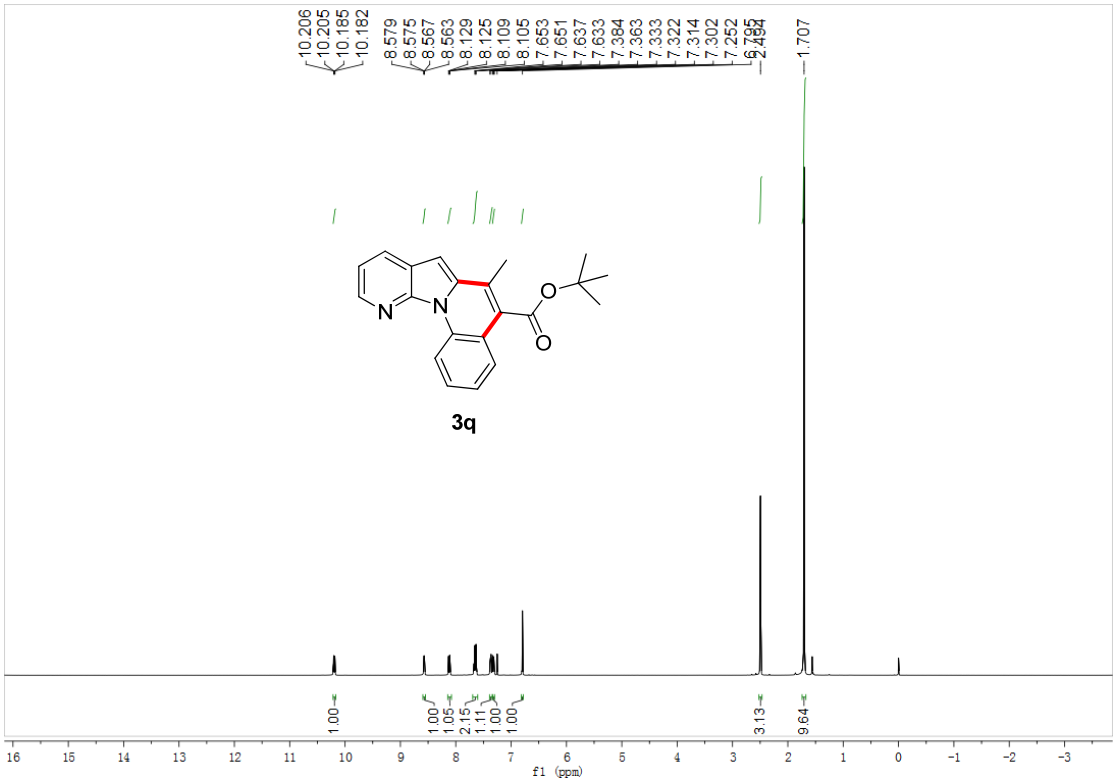
126.726
125.668
125.245
123.627
121.994
120.243
118.264
118.007
94.657
77.357
77.039
76.721
52.448
15.887
OCH3
O
N
N
f1 (ppm)

3p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10.205
10.185
10.182
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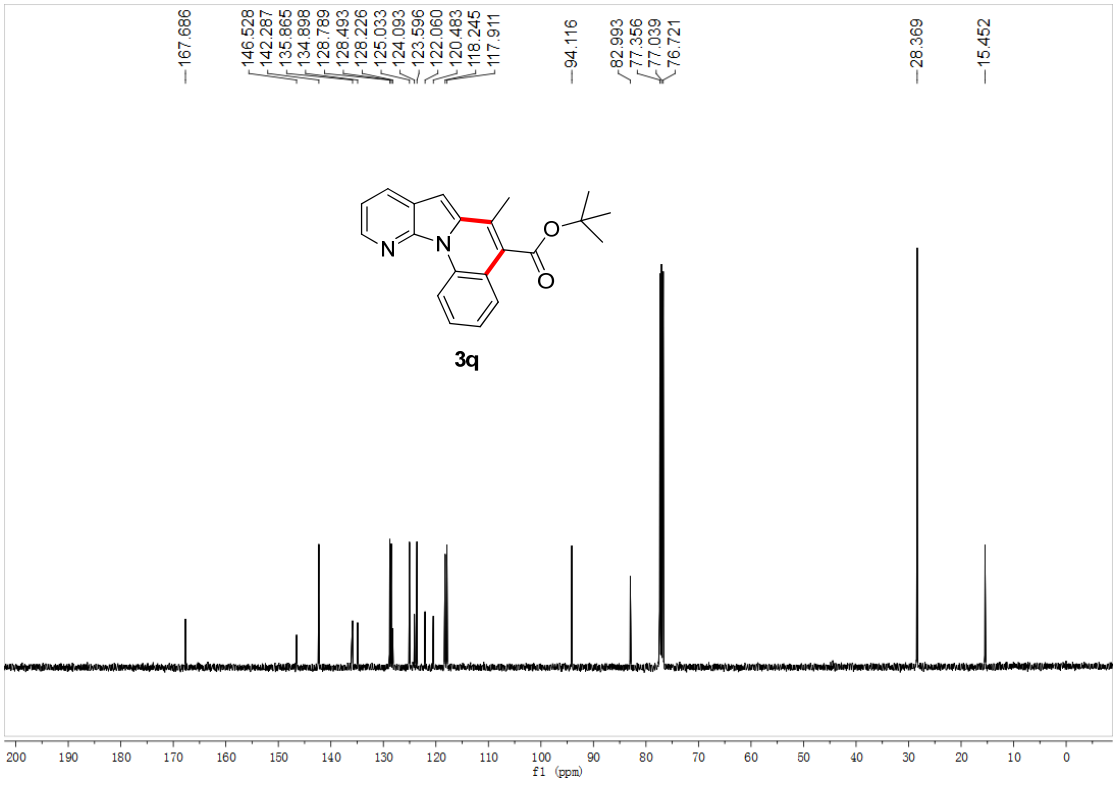
8.575
8.567
8.563
8.129
8.125
8.109
8.105
7.653
7.651
7.637
7.633
7.384
7.363
7.333
7.322
7.314
7.302
7.252
2.494
1.707
1.00
1.00
1.05
2.15
1.11
1.00
1.00
3.13
9.64
f1 (ppm)

3q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128.226
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124.093
123.596
122.060
120.483
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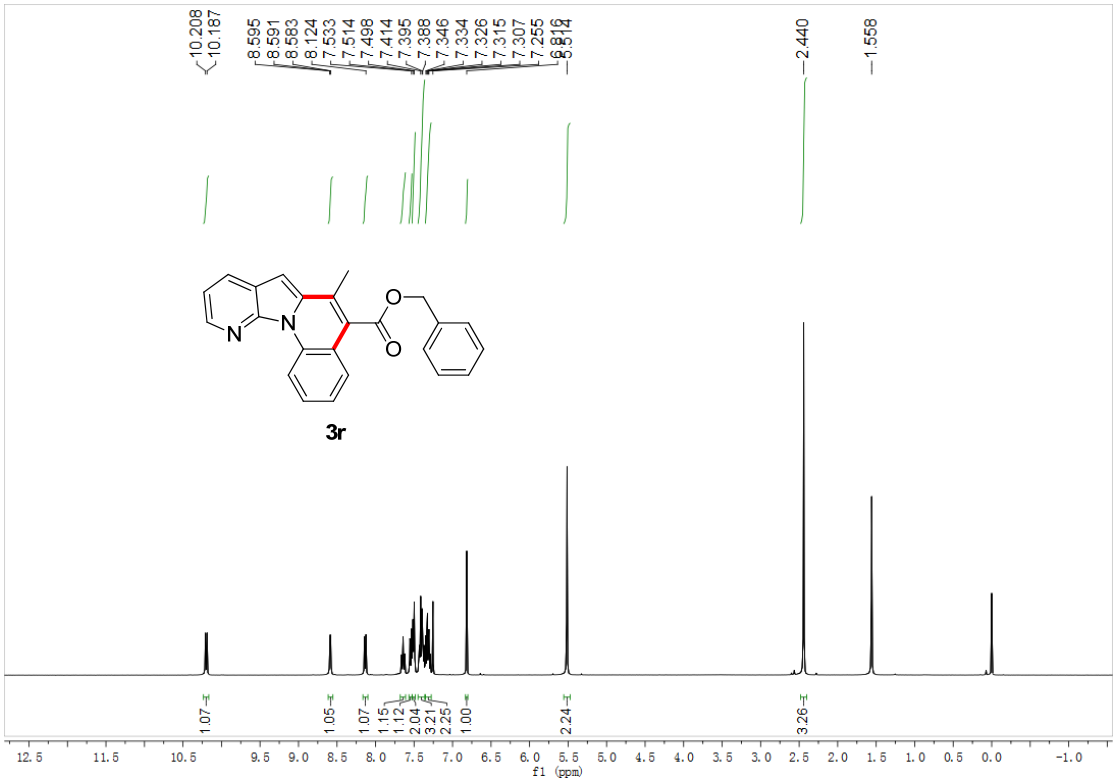
117.911
94.116
82.993
77.356
77.039
76.721
28.369
15.452
f1 (ppm)

3q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8.591
8.583
8.124
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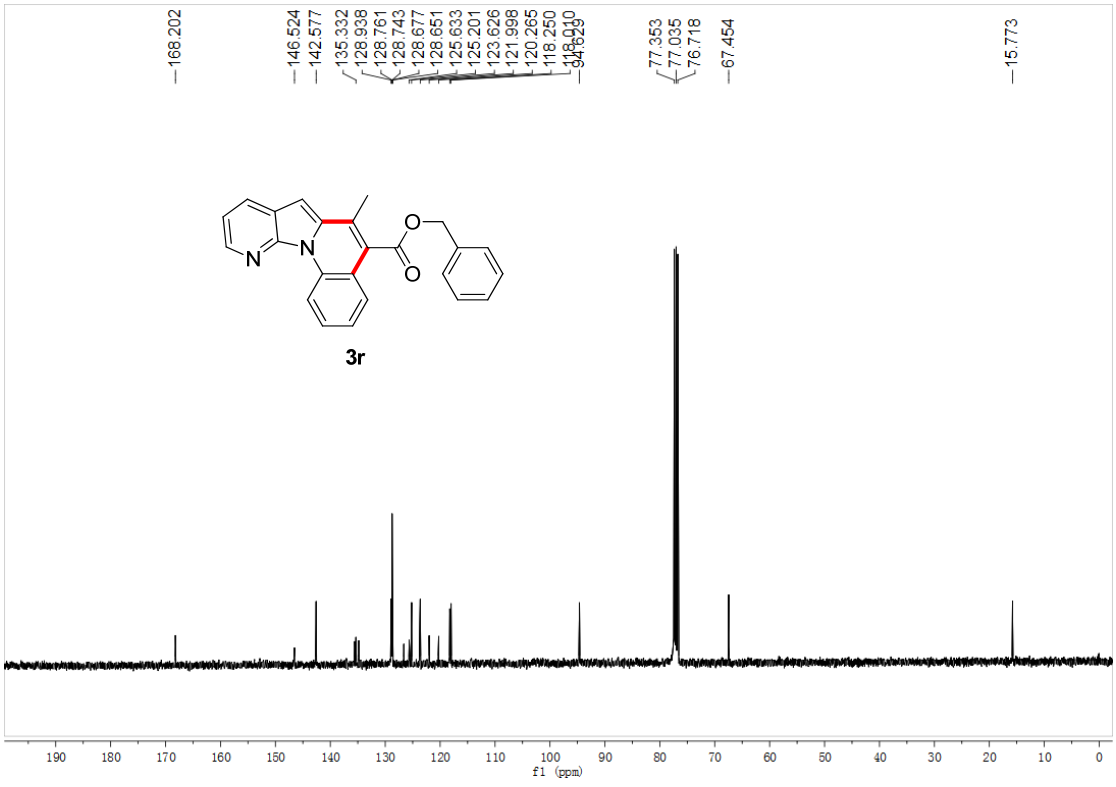
7.514
7.498
7.414
7.395
7.388
7.346
7.334
7.326
7.315
7.307
7.255
6.816
6.814
2.440
1.558
1.07
1.05
1.07
1.15
1.12
2.04
3.21
2.25
1.00
2.24
3.26
f1 (ppm)

3r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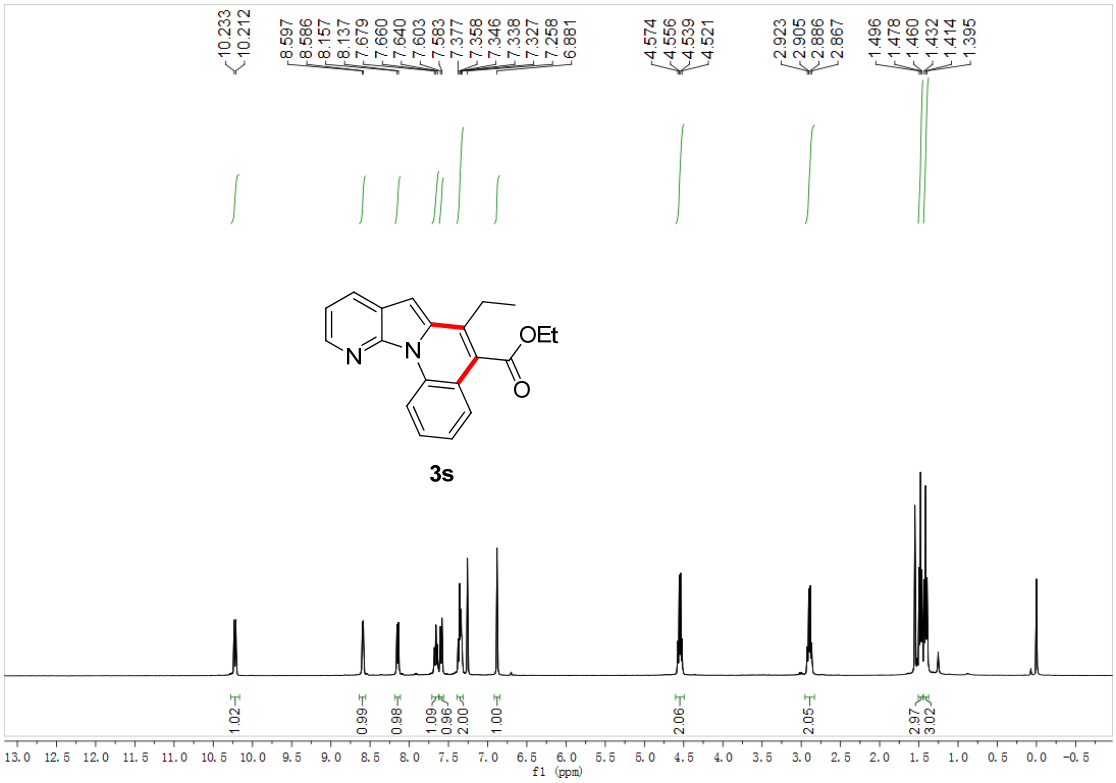
128.743
128.677
128.651
125.633
125.201
123.626
121.998
120.265
118.250
94.629
77.353
77.035
76.718
67.454
15.773
f1 (ppm)

3r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8.586
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8.137
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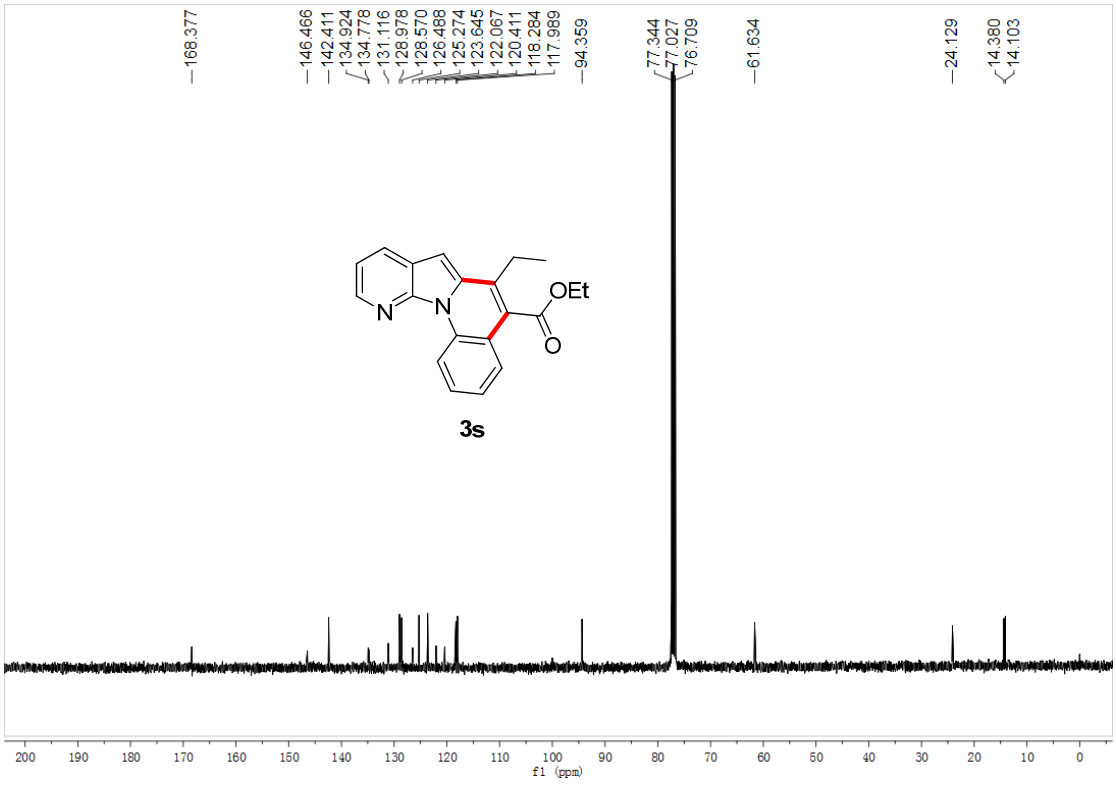
7.660
7.640
7.603
7.583
7.377
7.358
7.346
7.338
7.327
7.258
6.881
4.574
4.556
4.539
4.521
2.923
2.905
2.886
2.867
1.496
1.478
1.460
1.432
1.414
1.395
OEt
O
N
N
3s
1.02
0.99
0.98
1.09
0.96
2.00
1.00
2.06
2.05
2.97
3.02
f1 (ppm)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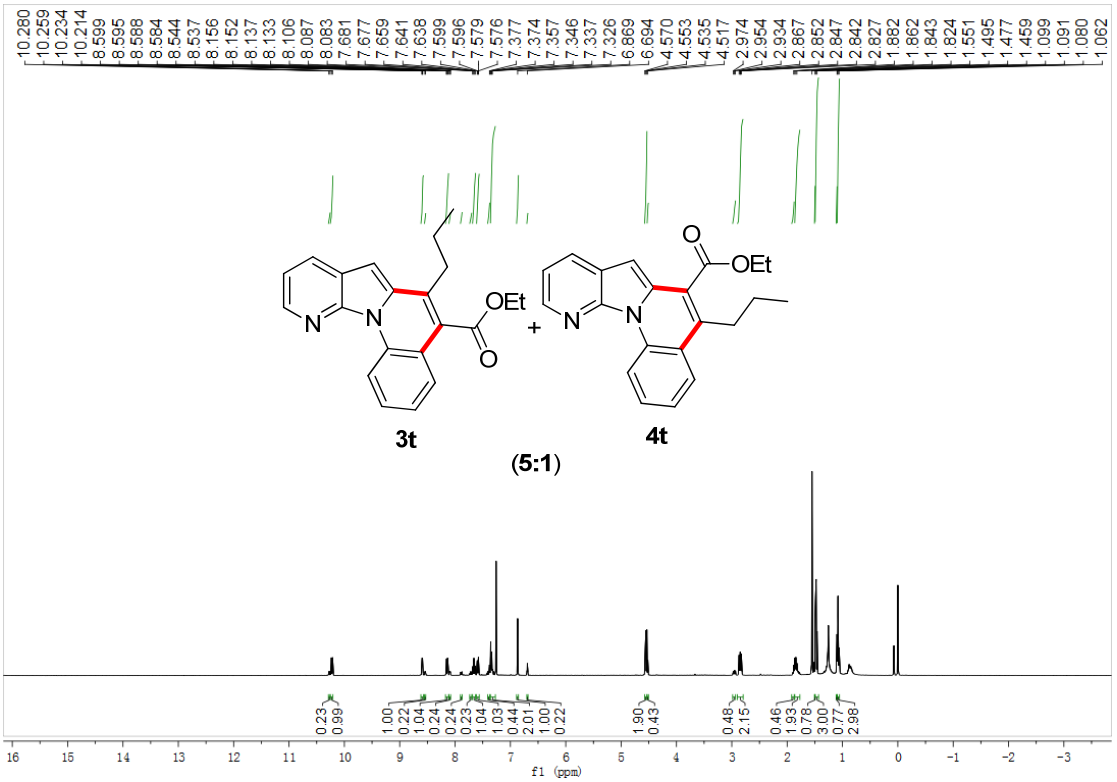
125.274
123.645
122.067
120.411
118.284
117.989
94.359
77.344
77.027
76.709
61.634
24.129
14.380
14.103
OEt
O
N
N
3s
f1 (ppm)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8.137
8.133
8.106
8.087
8.083
7.681
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7.659
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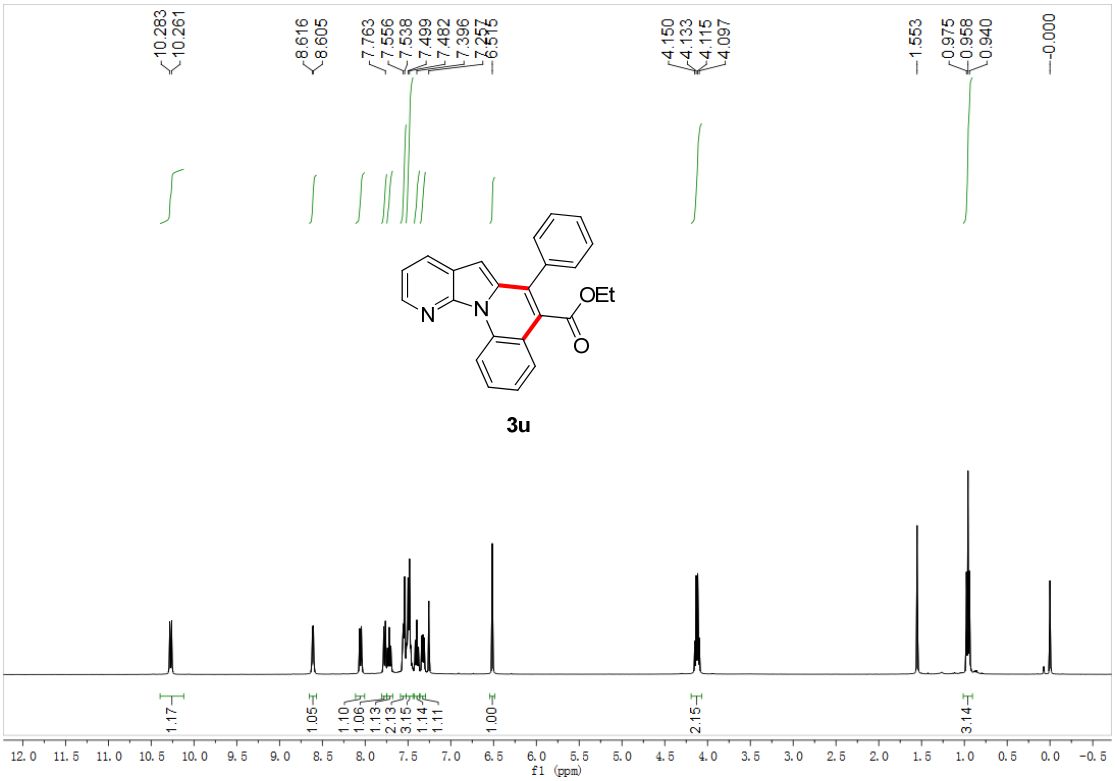
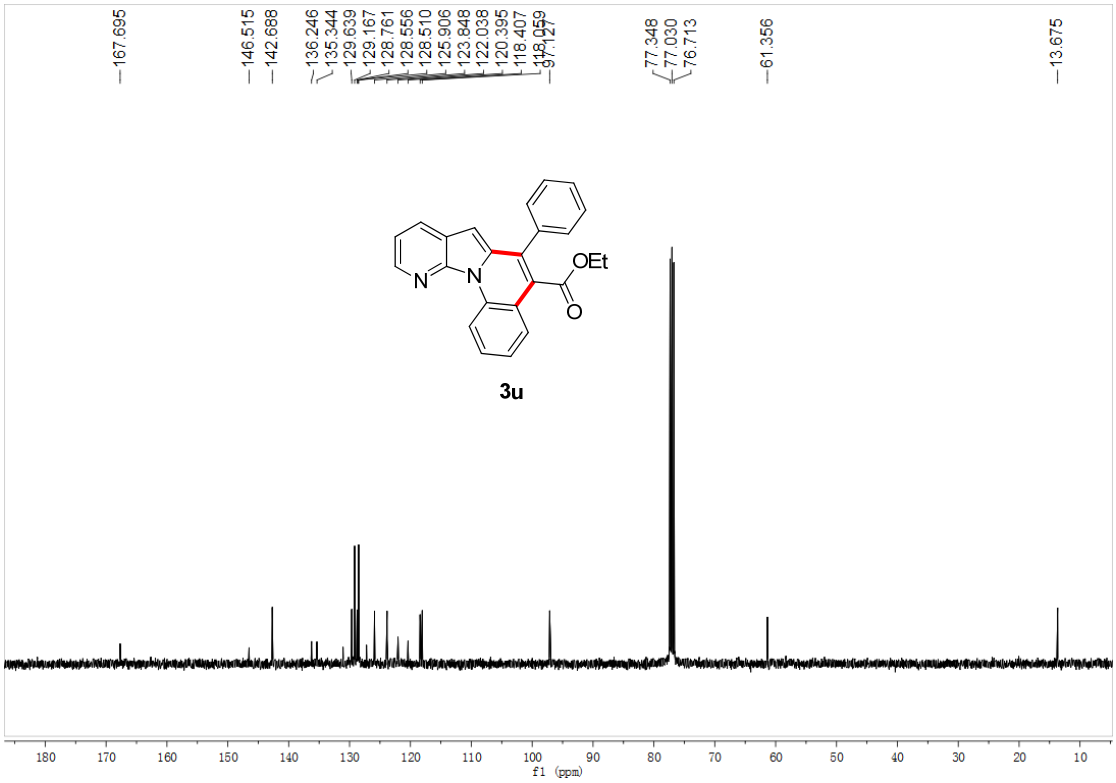
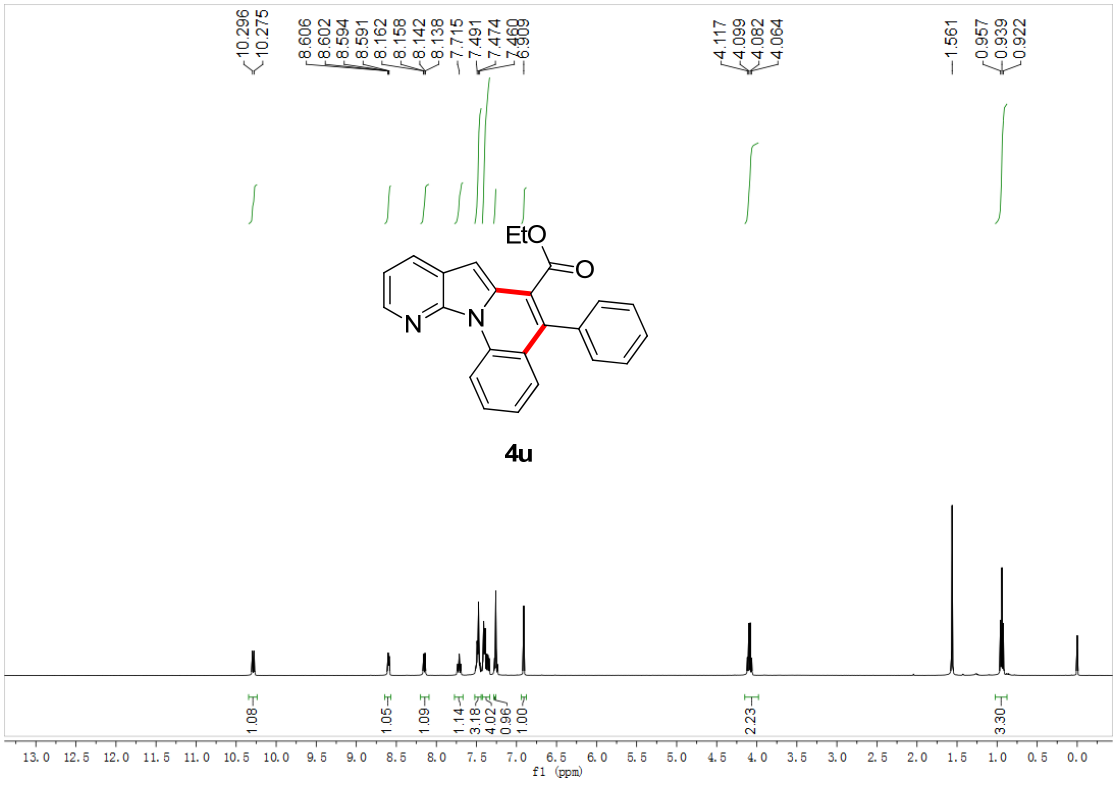
7.638
7.599
7.596
7.579
7.576
7.377
7.374
7.357
7.346
7.337
7.326
6.869
6.694
4.570
4.553
4.535
4.517
2.974
2.954
2.934
2.867
2.852
2.847
2.842
2.827
1.882
1.862
1.843
1.824
1.551
1.495
1.477
1.459
1.099
1.091
1.080
1.062
OEt
O
N
N
+
OEt
O
N
N
3t
4t
(5:1)
0.23
0.99
1.00
0.22
1.04
0.24
0.24
0.23
1.04
1.03
0.44
2.01
1.00
0.22
1.90
0.43
0.48
2.15
0.46
1.93
0.78
3.00
0.77
2.98
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

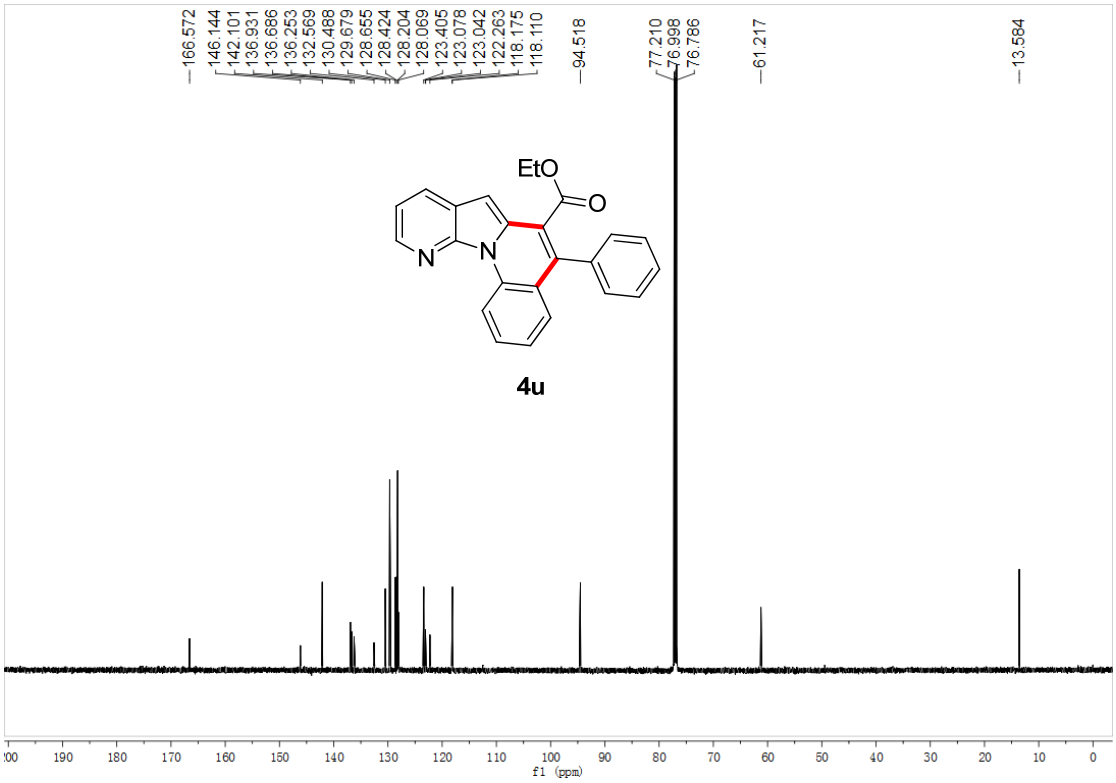

10.283
10.261
8.616
8.605
7.763
7.556
7.538
7.499
7.482
7.396
7.257
6.515
4.150
4.133
4.115
4.097
1.553
0.975
0.958
0.940
0.000
OEt
O
N
N
3u
1.17
1.05
1.10
1.06
1.13
2.13
3.15
1.14
1.11
1.00
2.15
3.14
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

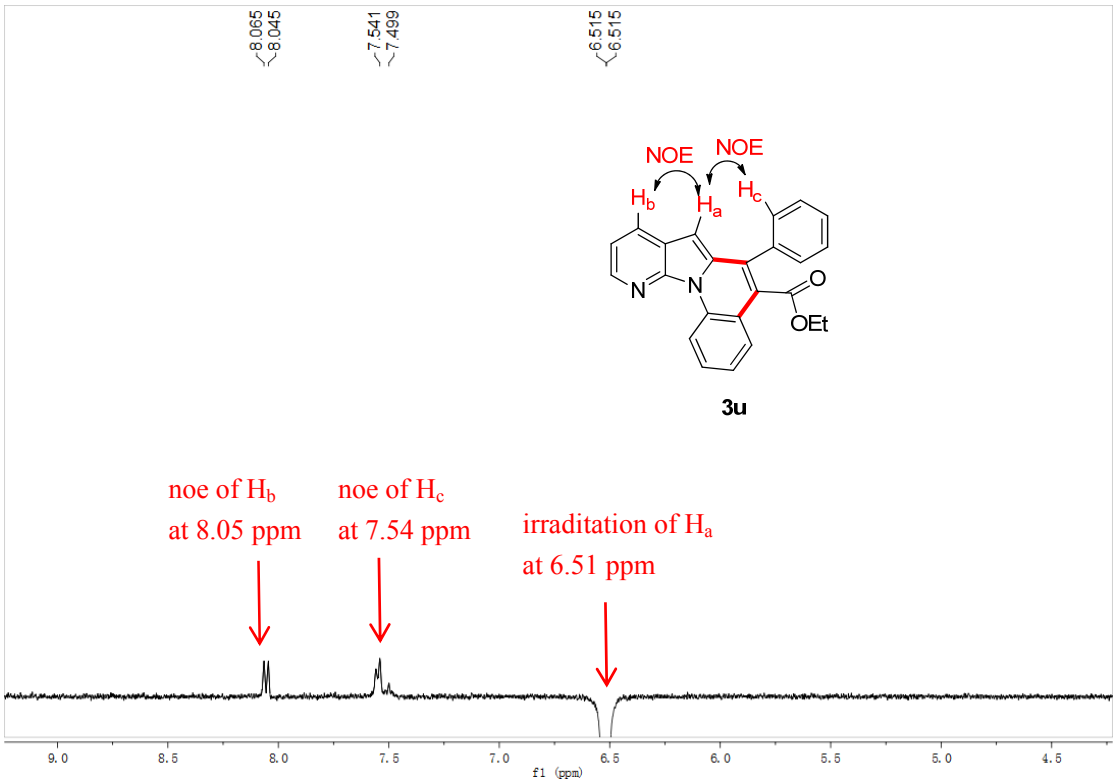

167.695
146.515
142.688
136.246
135.344
129.639
129.167
128.761
128.556
128.510
125.906
123.848
122.038
120.395
118.407
118.059
97.127
77.348
77.030
76.713
61.356
13.675
OEt
O
N
N
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

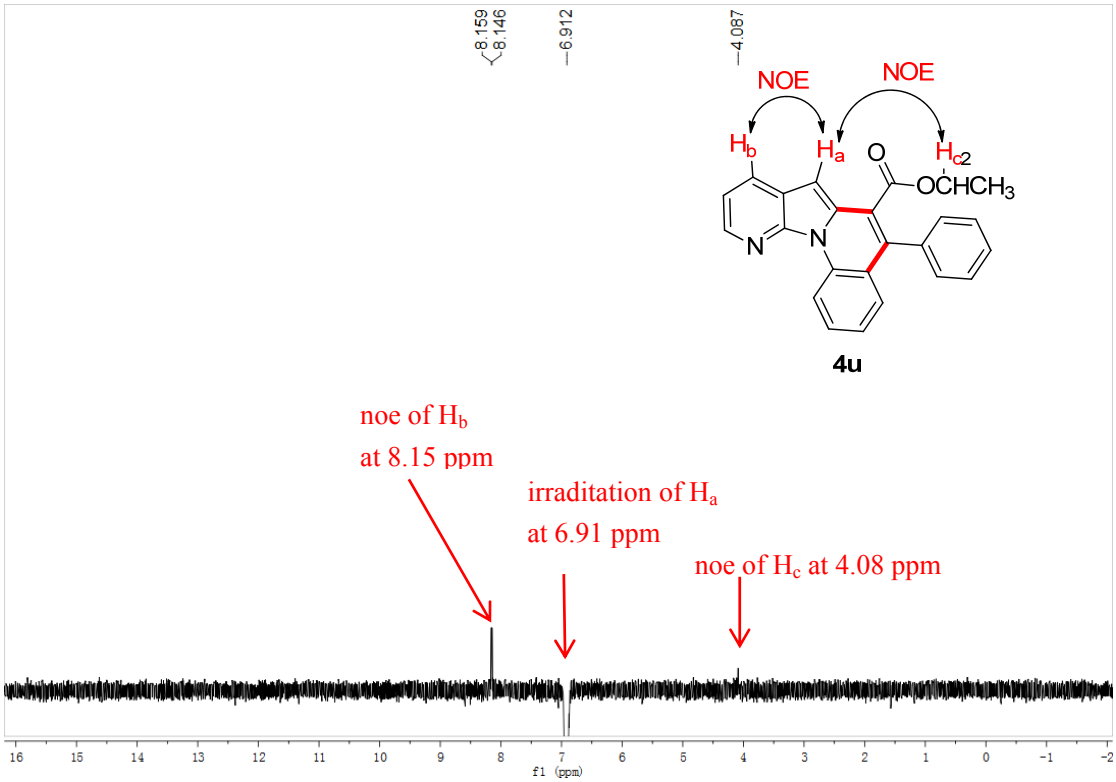
3u

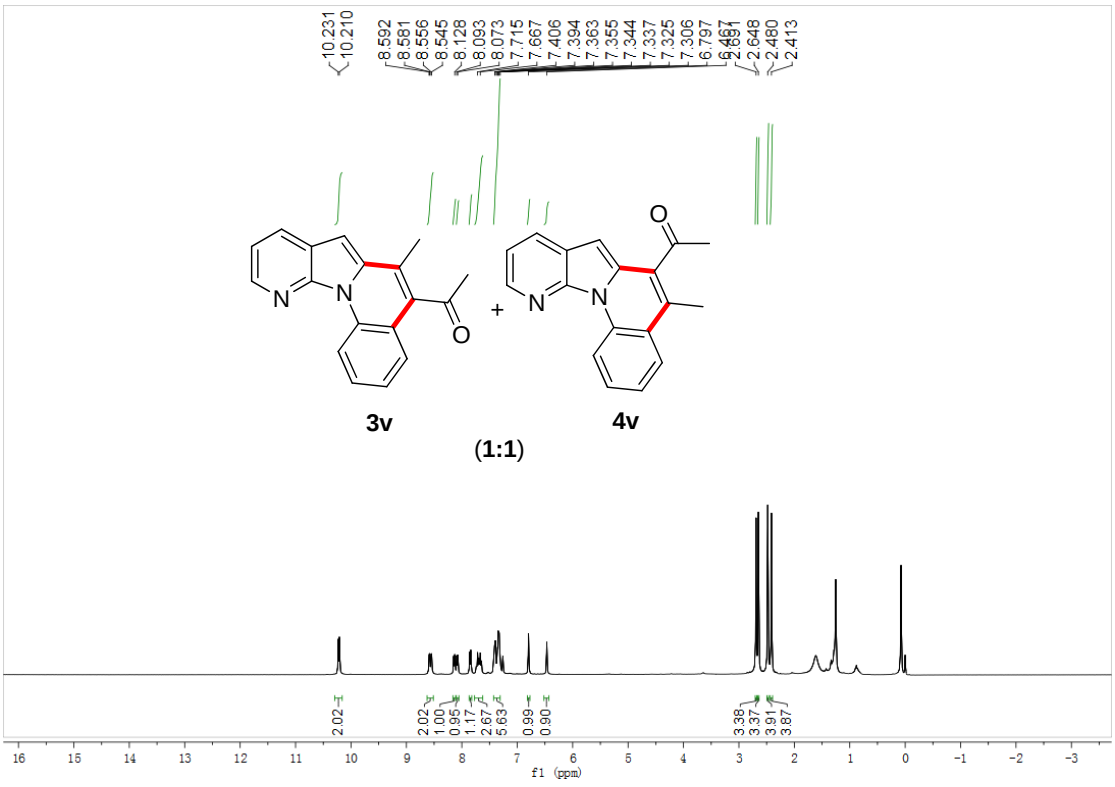

10.296
10.275
8.606
8.602
8.594
8.591
8.162
8.158
8.142
8.138
7.715
7.491
7.474
7.460
6.909
4.117
4.099
4.082
4.064
1.561
0.957
0.939
0.922
EtO
O
N
N
1.08
1.05
1.09
1.14
3.18
4.02
0.96
1.00
2.23
3.30
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

4u

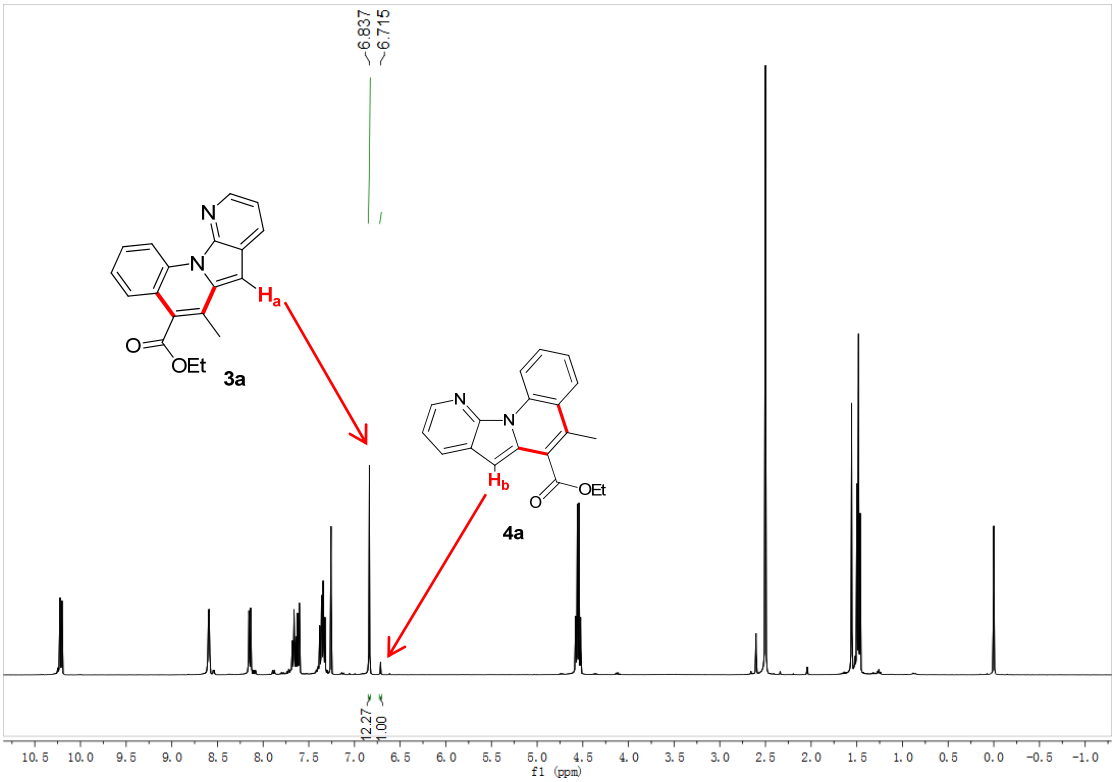

166.572
146.144
142.101
136.931
136.686
136.253
132.569
130.488
129.679
128.655
128.424
128.204
128.069
123.405
123.078
123.042
122.263
118.175
118.110
94.518
77.210
76.998
76.786
61.217
13.584
EtO
O
N
N
4u
f1 (ppm)

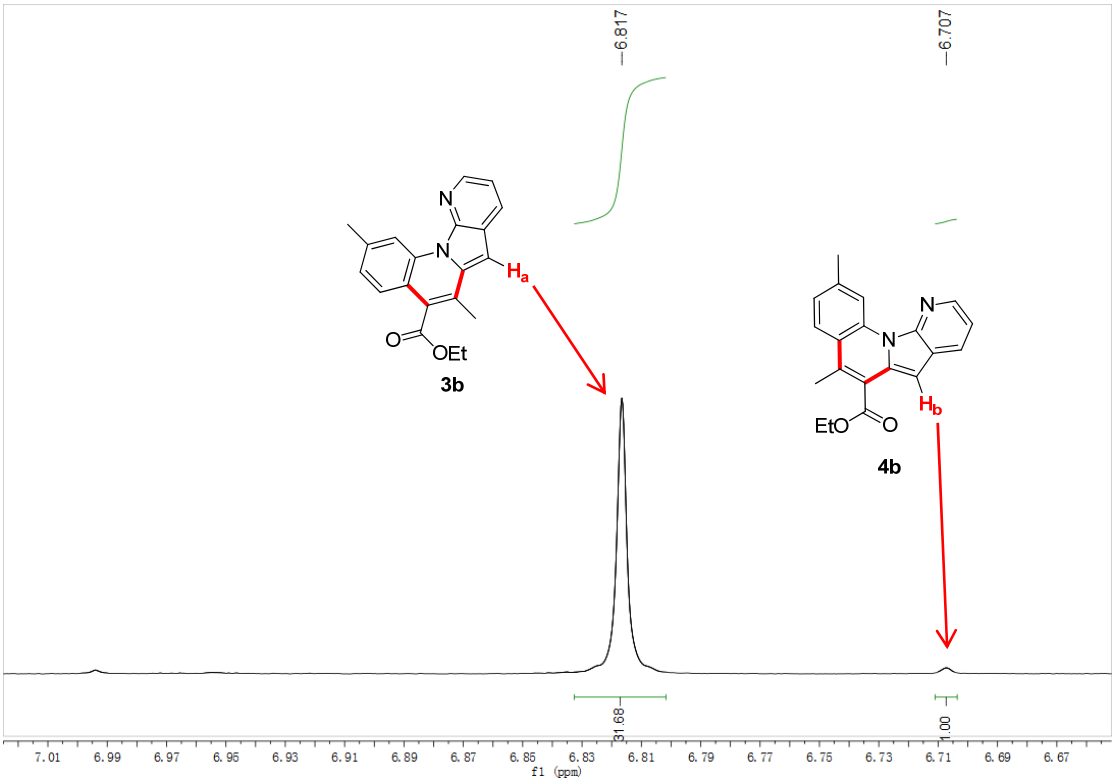

8.065
8.045
7.541
7.499
6.515
6.515
NOE
NOE
Hb
Ha
Hc
N
N
O
OEt
3u
noe of Hb
at 8.05 ppm
noe of Hc
at 7.54 ppm
irraditation of Ha
at 6.51 ppm
f1 (ppm)

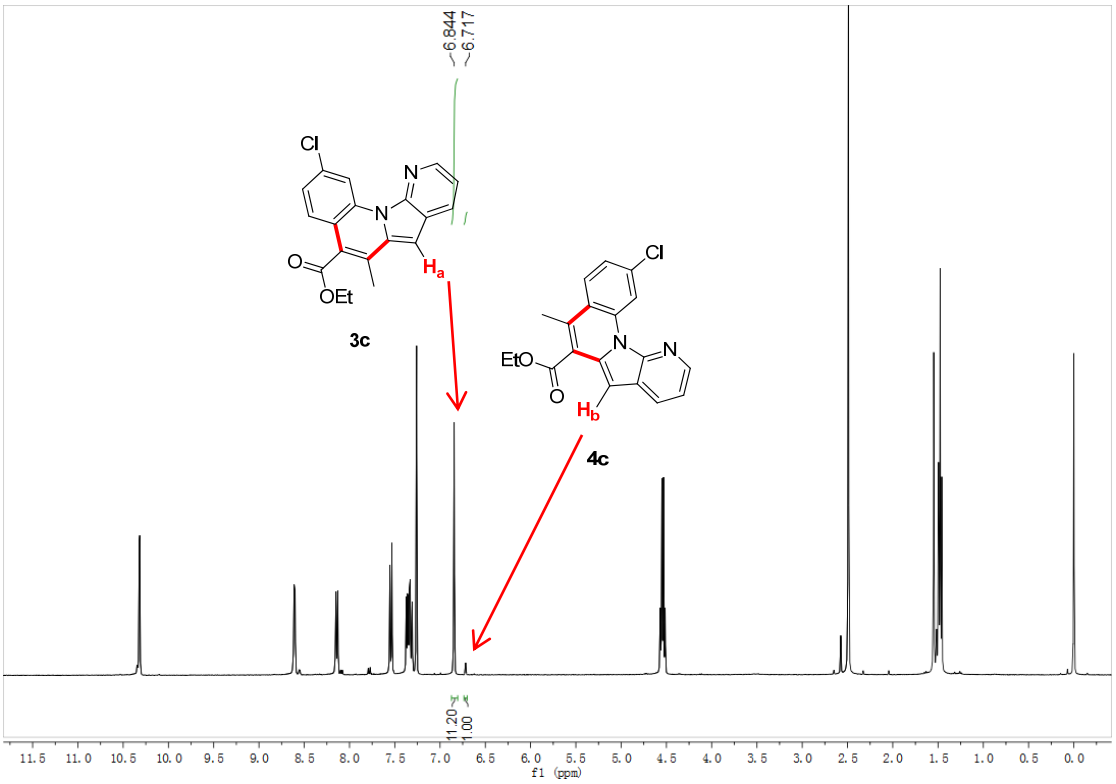

8.159
8.146
6.912
4.087
NOE
NOE
H_b
H_a
O
H_{c2}
$OCHCH_3$
N
N
4u
noe of H_b
at 8.15 ppm
irraditation of H_a
at 6.91 ppm
noe of H_c at 4.08 ppm
f1 (ppm)

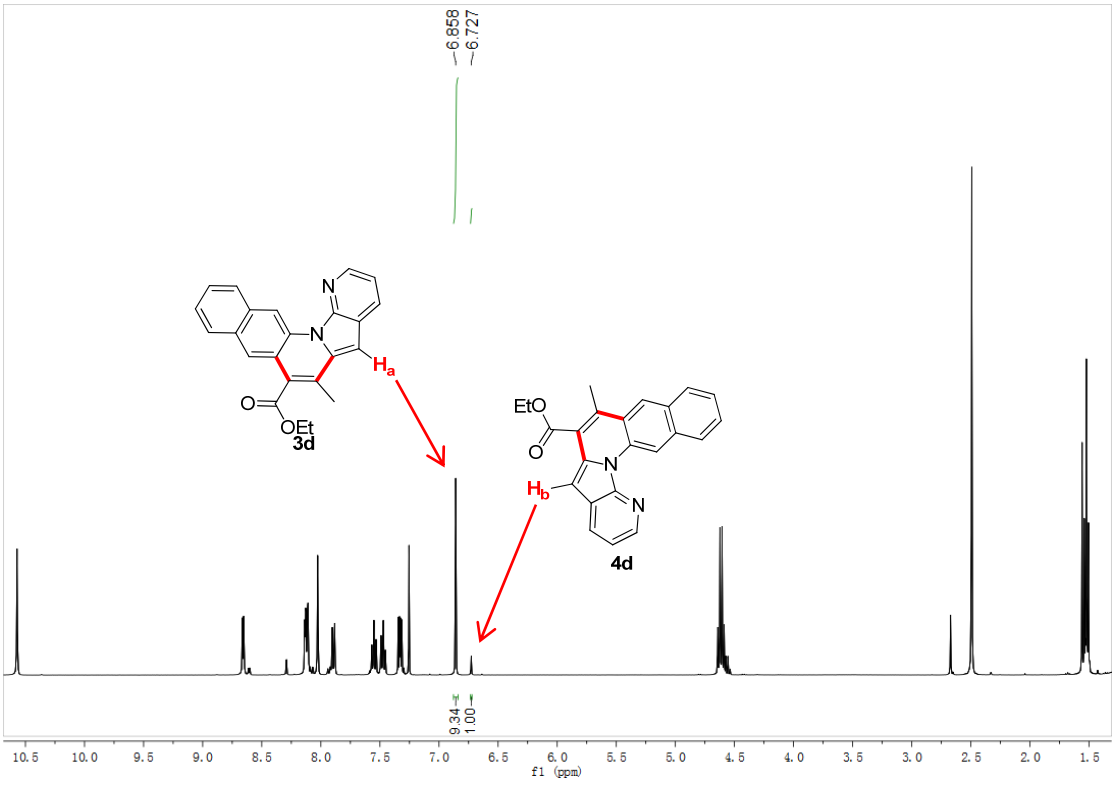

10.231
10.210
8.592
8.581
8.556
8.545
8.128
8.093
8.073
7.715
7.667
7.406
7.394
7.363
7.355
7.344
7.337
7.325
7.306
6.797
2.648
2.480
2.413
N
N
O
+
N
N
O
3v
4v
(1:1)
2.02
2.02
1.00
0.95
1.17
2.67
5.63
0.99
0.90
3.38
3.37
3.91
3.87
f1 (ppm)

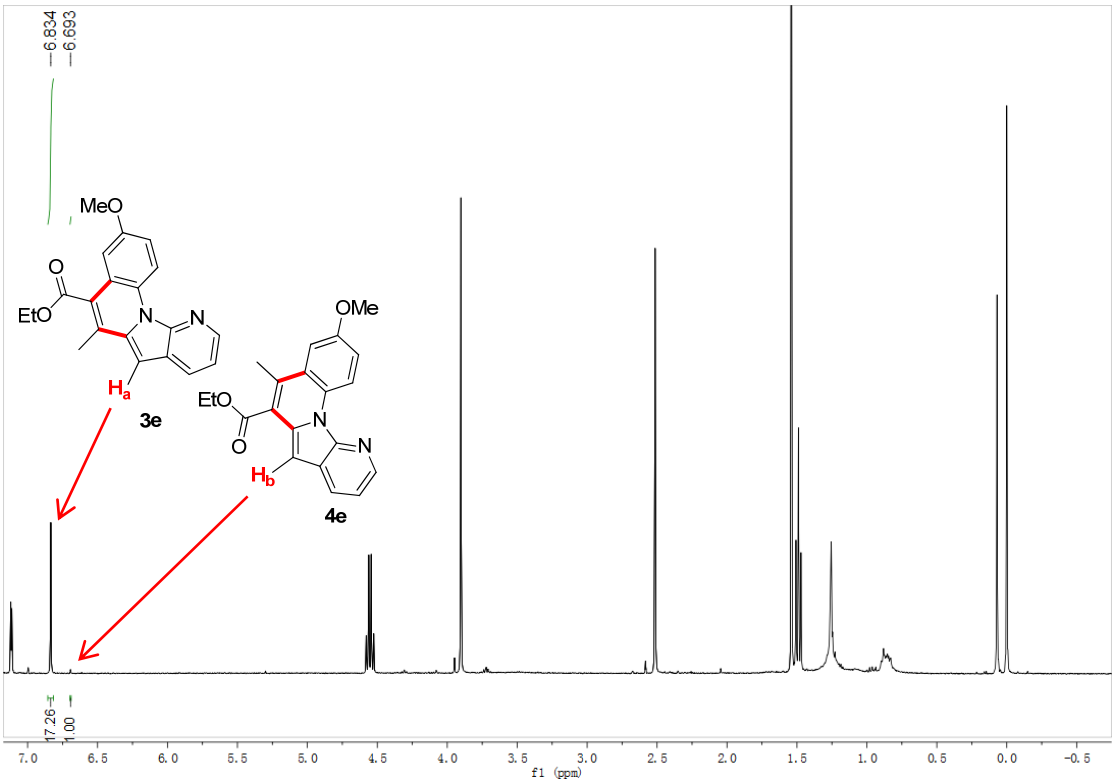
4. NMR Spectra of Ratio of 3 and 4.

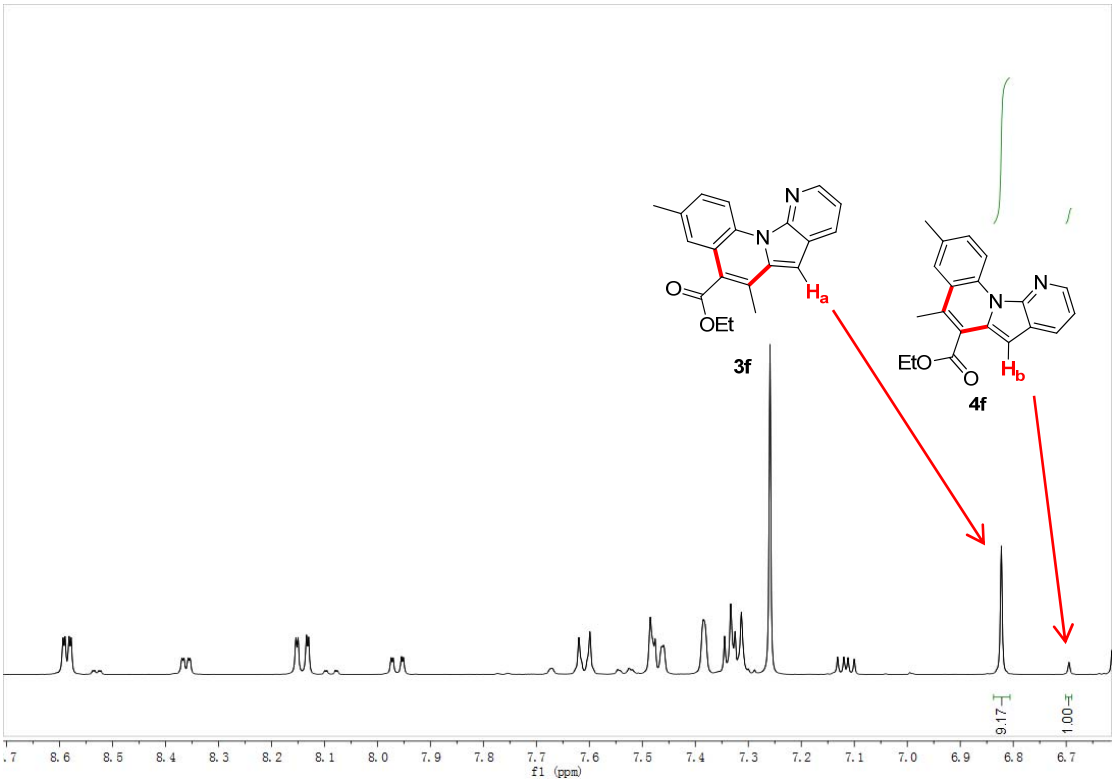


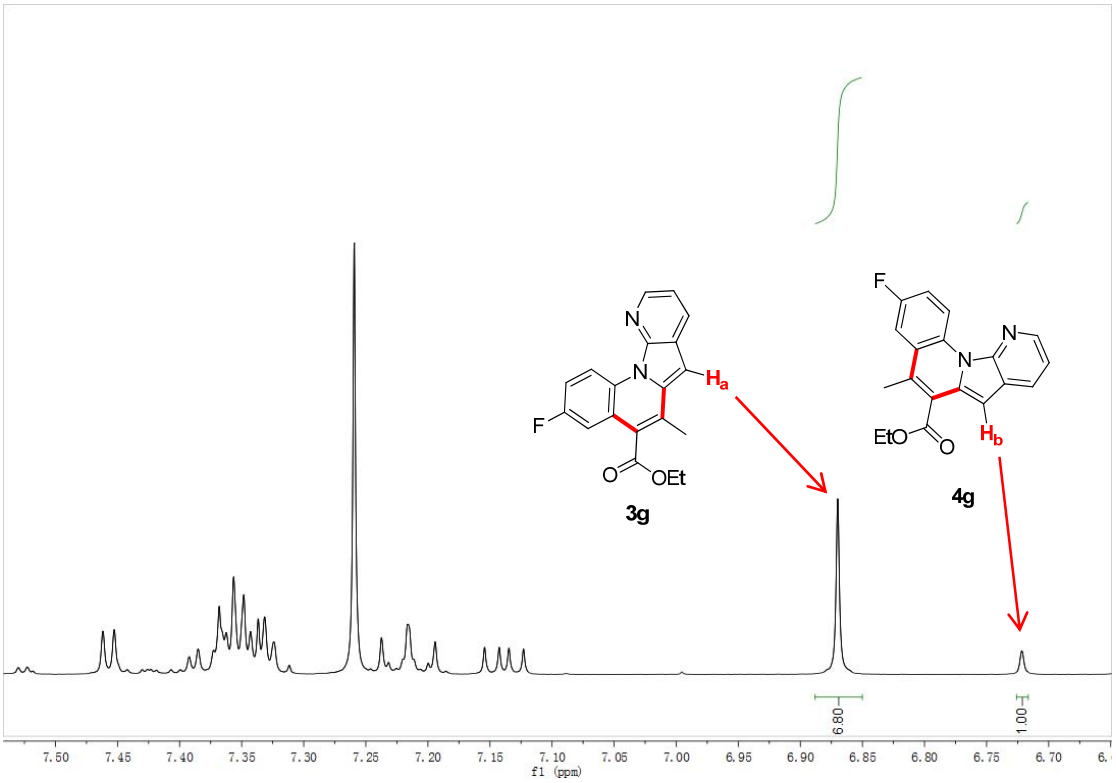


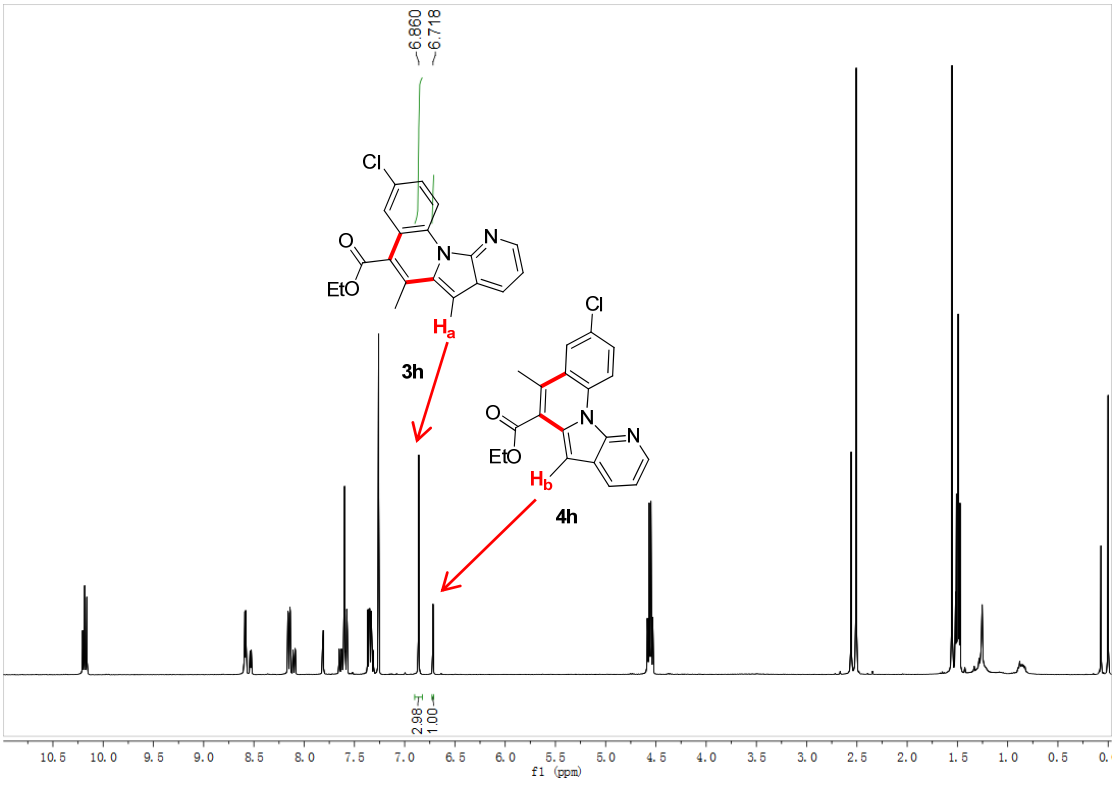

6.844
6.717
Cl
N
N
O
OEt
Ha
3c
Cl
EtO
O
N
N
Hb
4c
11.20
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

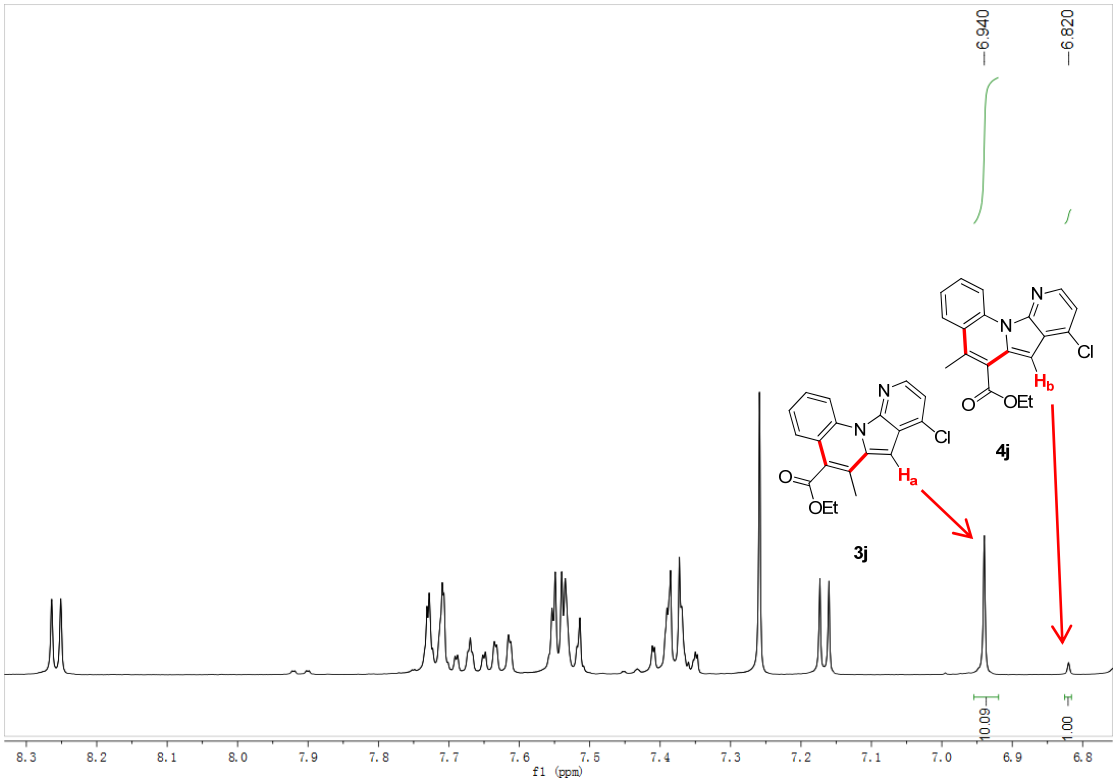

6.858
6.727
N
N
Ha
O
OEt
3d
EtO
O
N
Hb
N
4d
9.34
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)

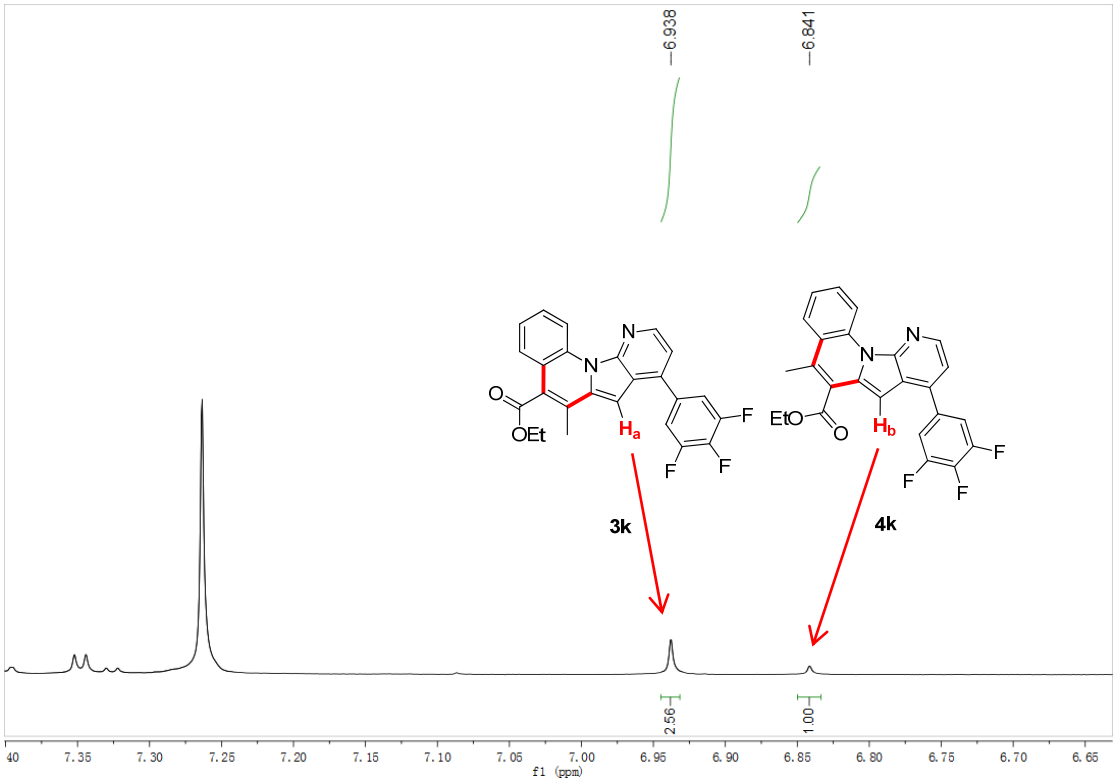

6.834
6.693
MeO
O
EtO
N
N
Ha
3e
OMe
EtO
O
N
N
Hb
4e
17.26
1.00
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

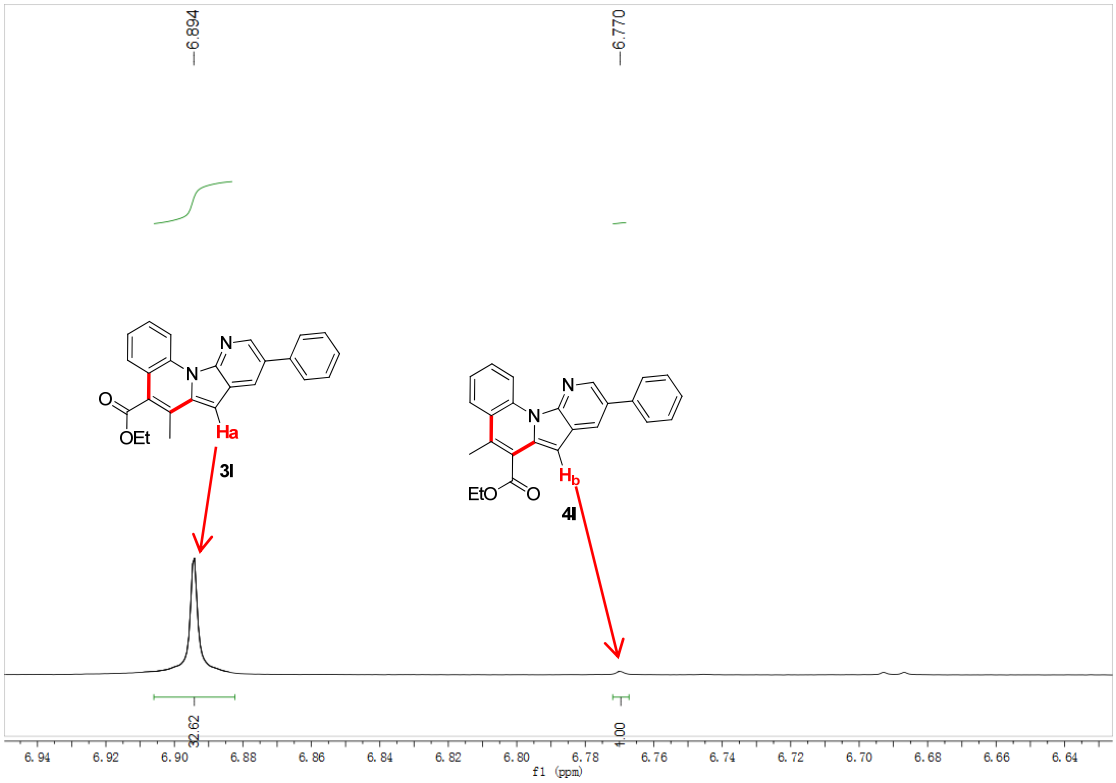

N
N
O
OEt
Ha
3f
N
N
EtO
O
Hb
4f
9.17
1.00
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
f1 (ppm)

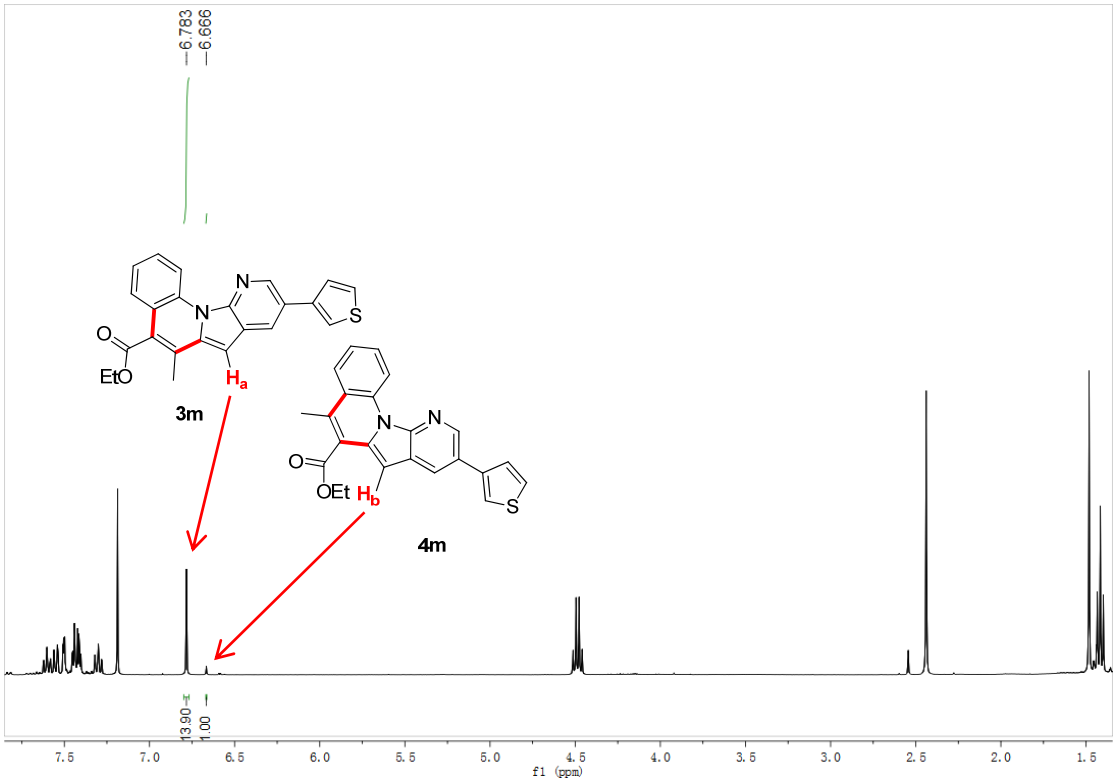

F
N
N
Ha
F
O
OEt
3g
F
N
N
EtO
O
Hb
4g
6.80
1.00
7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85 6.80 6.75 6.70
f1 (ppm)

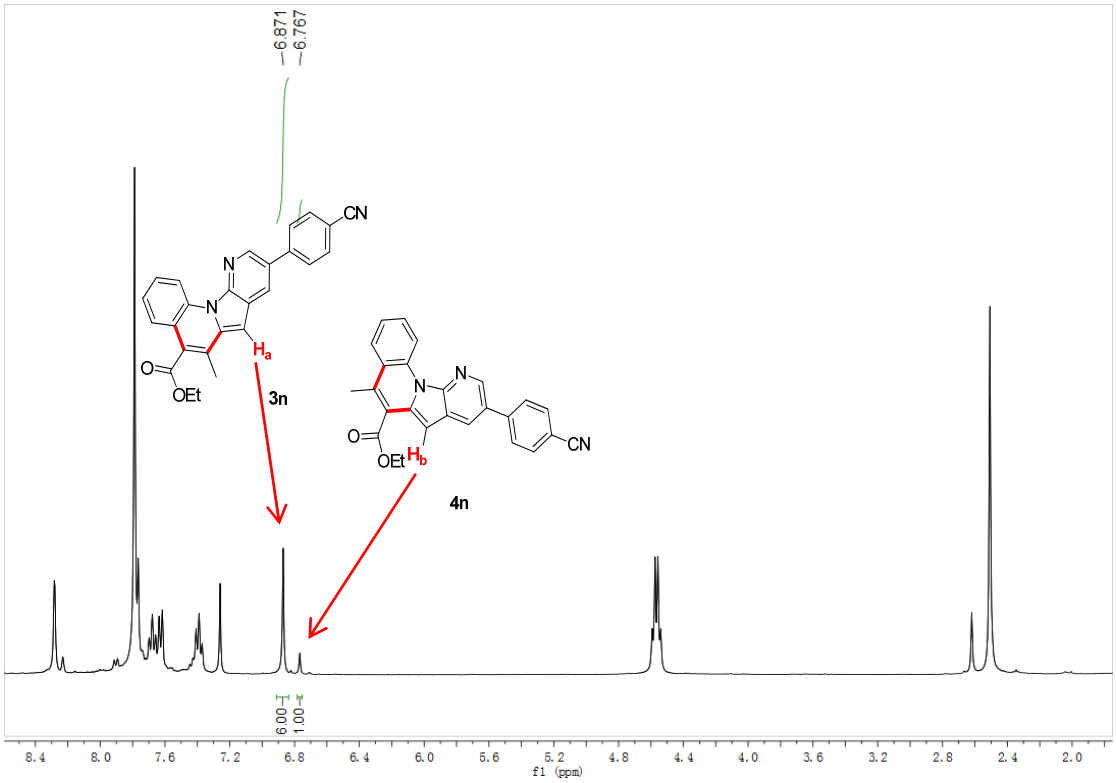

6.660
6.718
Cl
O
EtO
N
N
Ha
3h
Cl
O
EtO
N
N
Hb
4h
2.98
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

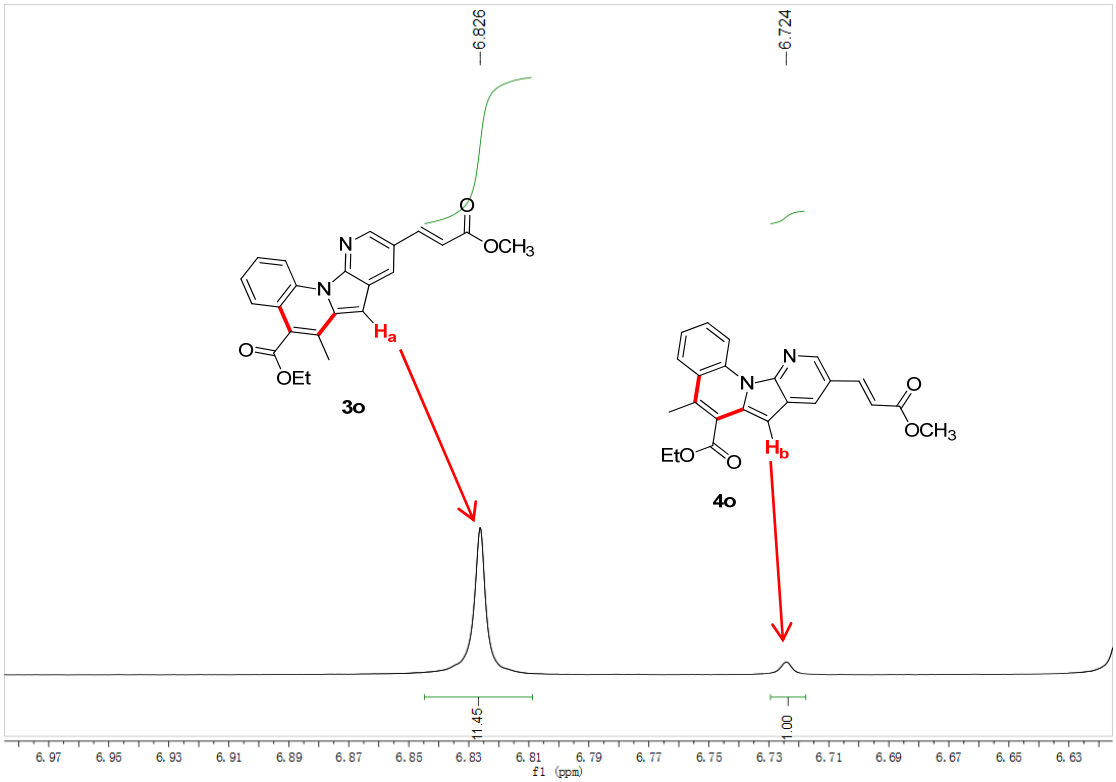

6.940
6.820
N
N
Cl
Hb
O
OEt
4j
N
N
Cl
O
OEt
Ha
3j
10.09
1.00
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
f1 (ppm)

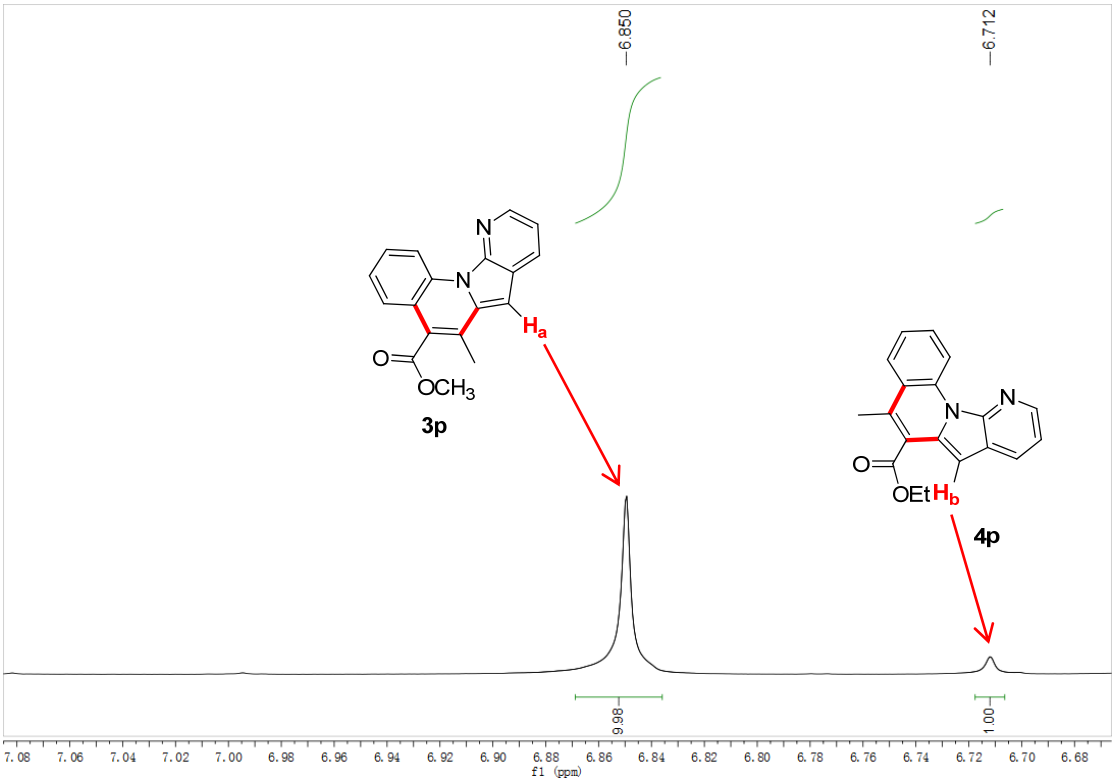

6.938
6.841
N
N
O
OEt
Ha
F
F
F
3k
EtO
O
N
N
Hb
F
F
F
4k
2.56
1.00
40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
6.85
6.80
6.75
6.70
6.65
f1 (ppm)

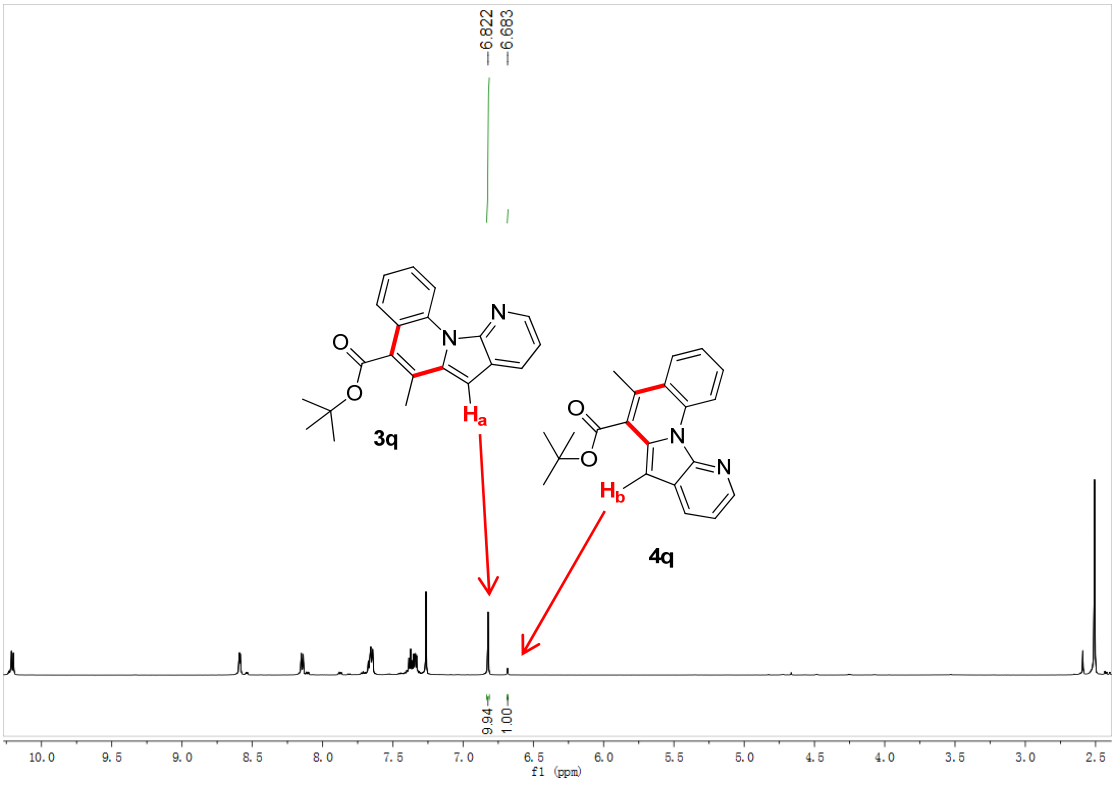

6.894
6.770
N
N
O
OEt
Ha
3l
N
N
EtO
O
Hb
4l
32.62
1.00
6.94
6.92
6.90
6.88
6.86
6.84
6.82
6.80
6.78
6.76
6.74
6.72
6.70
6.68
6.66
6.64
f1 (ppm)

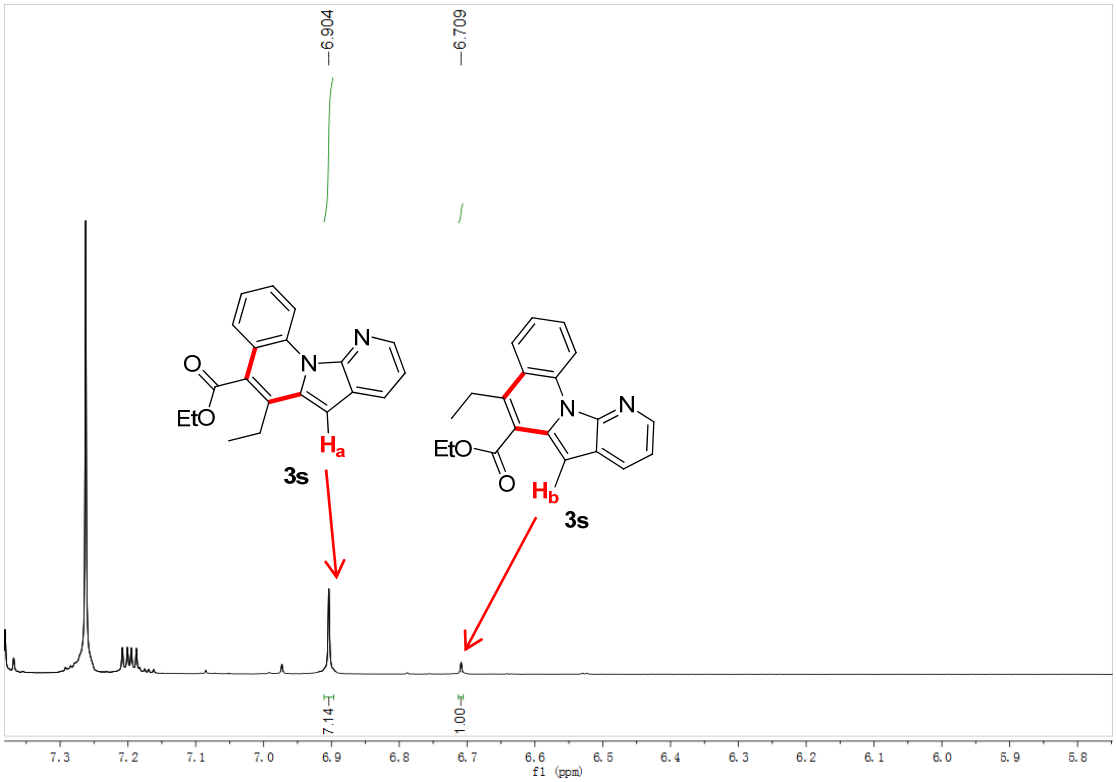

6.783
6.666
N
S
O
EtO
Ha
3m
N
N
O
OEt
Hb
S
4m
13.90
1.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)

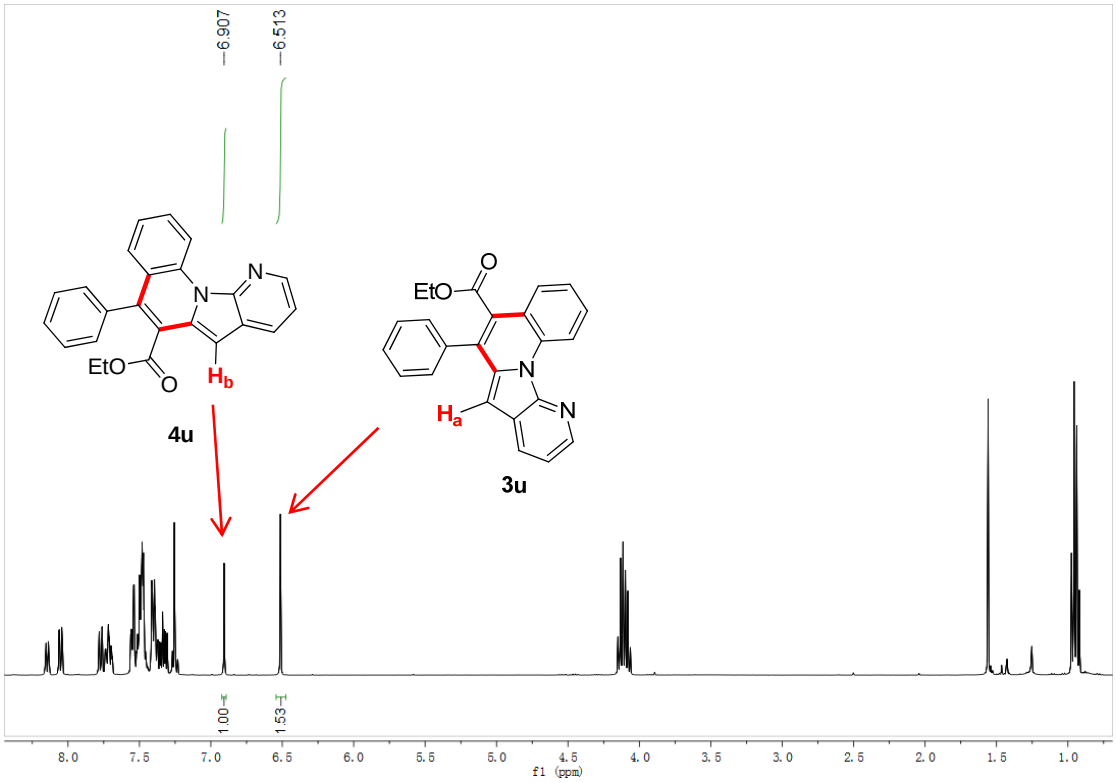

6.871
6.767
CN
N
N
O
OEt
Ha
3n
N
N
O
OEt
Hb
CN
4n
6.00
1.00
8.4
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
f1 (ppm)


6.826
6.724
O
OCH3
N
N
O
OEt
Ha
3o
N
N
O
OCH3
EtO
O
Hb
4o
11.45
1.00
6.97
6.95
6.93
6.91
6.89
6.87
6.85
6.83
6.81
6.79
6.77
6.75
6.73
6.71
6.69
6.67
6.65
6.63
f1 (ppm)


6.850
6.712
N
N
Ha
O
OCH3
3p
N
N
O
OEt
Hb
4p
9.98
1.00
7.08 7.06 7.04 7.02 7.00 6.98 6.96 6.94 6.92 6.90 6.88 6.86 6.84 6.82 6.80 6.78 6.76 6.74 6.72 6.70 6.68
f1 (ppm)


6.822
6.683
N
N
O
O
Ha
3q
O
O
N
N
Hb
4q
9.94
1.00
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
f1 (ppm)


6.904
6.709
O
EtO
N
N
Ha
3s
EtO
O
N
N
Hb
3s
7.14
1.00
7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 5.9 5.8
f1 (ppm)


6.907
6.513
N
N
EtO
O
Hb
4u
O
EtO
N
Ha
N
3u
1.00
1.53
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)