Electronic Supplementary Information

Palladium-Catalyzed Selective Oxidative Olefination and Arylation of 2-Pyridones

Yuye Chen, Fen Wang, Aiqun Jia and Xingwei Li

Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023 China and School of Environmental and Biotechnology, Nanjing University of Science and Technology, Nanjing 210014, China

Email: xwli@dicp.ac.cn

Content

Ⅰ General Information.

All reagents were used as received unless otherwise noted. Reactions were monitored using thin-layer chromatography (TLC) on commercial silica gel plates. Visualization of the developed plates was performed under UV light (254 nm). Flash column chromatography was performed on silica gel. ^{1}H and ^{13}C NMR spectra were recorded on a 400 or 500 MHz spectrometer. Chemical shifts (δ) were reported in ppm referenced to an internal tetramethylsilane standard. ^{19}F NMR (470 MHz) spectra were recorded with CDCl3 as a solvent using hexafluorobenzene as an external standard. The following abbreviations were used to describe multiplicity when appropriate: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet，dd = doublets of doublet. Coupling constants *J* were reported in Hertz (Hz).

Ⅱ General Procedure of Catalysis

1 General Procedure for Mono-Olefination of Pyridones.

Pyridone (0.3 mmol), $Pd(OAc)_2$ (0.03 mmol, 0.1 equiv) and $Cu(OAc)_2$ (0.6 mmol, 2 equiv) were added to a Schlenk tube, to which was added PivOH (2 g) under N_2. The alkene (1.5 equiv) was added via syringe and the reaction mixture was heated at 110 °C for 16 h. The reaction was monitored by TLC using EtOAc and petroleum ether (1:1 v/v) as the mobile phase. All the volatiles were then removed under reduced pressure. The reaction mixture was diluted with CH_2Cl_2 (30 mL) and saturated aq $NaHCO_3$ (3×20 mL) was slowly added to neutralize the PivOH. After stirred for 20 min, the organic layer was separated and was dried over anhydrous Na_2SO_4. The solvent was removed and the residue obtained was purified by flash chromatography on silica gel to give the desired product (PE:EA=1:1).

2 General Procedure for Diolefination of Pyridones.

Pyridone (0.3 mmol), $Pd(OAc)_2$ (0.03 mmol, 0.1 equiv) and AgOAc (1.5 mmol, 5 equiv) were added to a Schlenk tube, to which was added PivOH (2 g) under N_2. Alkene (3 equiv) was slowly added via syringe and the reaction mixture was heated at 130 °C for 16 h. The reaction was monitored by TLC using EtOAc and petroleum ether as the mobile phase. The reaction mixture was cooled to room temperature and was diluted with CH_2Cl_2 (30 mL) and $NaHCO_3$ (3×20 mL) was added to neutralize PivOH. After stirred for 20 min, the organic layer was separated and was dried over Na_2SO_4. After removal of solvent, the residue was purified by flash chromatography on silica gel to give desired product (PE:EA=10:1).

3 General Procedure for Cross-Coupling of Polyfluoroarenes with Pyridones

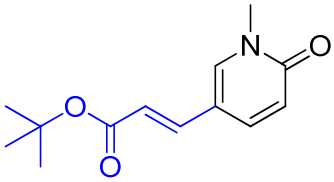
Pyridone (0.3 mmol), $Pd(OAc)_2$ (0.03 mmol, 0.1 equiv), AgOAc (0.9 mmol, 3 equiv), dioxane (2.0 mL), $(i\text{-}Pr)_2S$ (1.5 mmol, 5.0 equiv) and polyfluoroarene (0.9 mmol, 3.0 equiv) were added to a pressure tube. The tube was sealed and heated to 130 °C (oil bath). After

stirred for 16 h, the reaction mixture was cooled to room temperature and diluted with ethyl acetate and then concentrated under vacuum. The residue was purified by silica gel chromatography to provide the pure product (PE:EA=4:1).

H/D Exchange Studies

Under air atmosphere, $Pd(OAc)_2$ (0.03 mmol, 6.7 mg) was added into a Schlenk tube. The tube was purged with N_2 and was sealed. Then CD_3COOD (2 mL) and *N*-methyl-2-pyridone (**1a**, 0.30 mmol, 30 μL) were added via syringe. The mixture was stirred under N_2 atmosphere at 75 °C for 24 h. The resulting solution was analyzed by ^1H NMR spectroscopy.

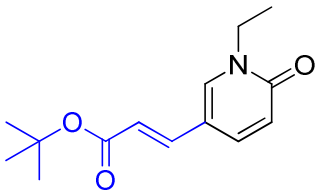
III Product Characterization



(2aa)

2aa, yellow solid (77% yield). ^1H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 9.5, 2.6 Hz, 1H), 7.42 (d, *J* = 2.4 Hz, 1H), 7.29 (d, *J* = 15.9 Hz, 1H), 6.60 (d, *J* = 9.5 Hz, 1H), 6.08 (d, *J* = 15.8 Hz, 1H), 3.57 (s, 3H), 1.52 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 162.4, 140.1, 138.2, 136.1, 121.0, 117.4, 114.5, 80.4, 37.7, 28.1. **IR**: 831, 1146, 1659, 1693 cm^{-1}

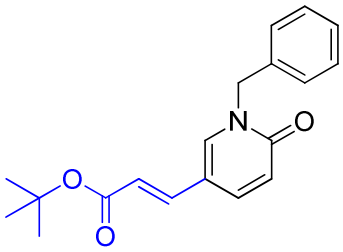
HRMS calculated for $(C_{13}H_{17}NO_3 + Na)^+$ 258.1106; Found: 258.1104.



(2ba)

2ba. yellow solid (71% yield). ^1H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 9.5 Hz, 1H), 7.44 (s, 1H), 7.31 (d, *J* = 15.4 Hz, 1H), 6.58 (d, *J* = 9.4 Hz, 1H), 6.08 (d, *J* = 15.8 Hz, 1H), 4.04 – 3.96 (m, 2H), 1.52 (s, 9H), 1.37 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 161.8, 139.0, 138.4, 135.9, 121.4, 117.3, 114.7, 80.4, 45.0, 28.1, 14.6. **IR**: 833, 1148, 1666, 1694 cm^{-1}

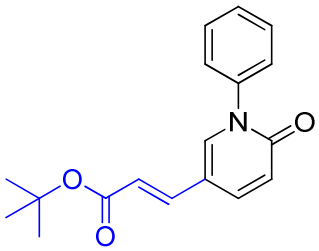
HRMS calculated for $(C_{14}H_{19}NO_3 + Na)^+$ 272.1263; Found: 272.1257.



(2ca)

2ca, yellow solid (65% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 9.6, 2.4 Hz, 1H), 7.39 (d, *J* = 2.3 Hz, 1H), 7.38 – 7.27 (m, 5H), 7.23 (d, *J* = 15.8 Hz, 1H), 6.63 (d, *J* = 9.5 Hz, 1H), 6.05 (d, *J* = 15.8 Hz, 1H), 5.12 (s, 2H), 1.50 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 162.1, 139.2, 138.4, 136.0, 135.6, 129.0, 128.4, 128.2, 121.6, 117.6, 114.8, 80.6, 52.1, 28.2. **IR**: 830, 1149, 1599, 1655, 1713 cm^{-1}

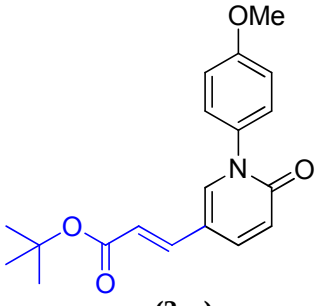
HRMS calculated for $(C_{19}H_{21}NO_3 + Na)^+$ 334.1419; Found: 334.1422.



(2da)

2da, yellow solid (19% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (dd, *J* = 9.6, 2.6 Hz, 1H), 7.53 – 7.48 (m, 3H), 7.45 (m, 1H), 7.37 (m, 2H), 7.31 (d, *J* = 15.8 Hz, 1H), 6.70 (d, *J* = 9.6 Hz, 1H), 6.13 (d, *J* = 15.8 Hz, 1H), 1.51 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.0, 161.8, 140.2, 139.8, 138.2, 136.5, 129.5, 128.9, 126.4, 122.2, 118.1, 114.7, 80.6, 28.2. **IR**: 1147, 1257, 1669, 1701 cm^{-1}

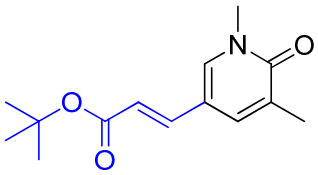
HRMS calculated for $(C_{18}H_{19}NO_3 + Na)^+$ 320.1263; Found: 320.1265.



(2ea)

2ea, yellow solid (65% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 9.5 Hz, 1H), 7.51 (s, 1H), 7.32 (m, 3H), 7.01 (d, *J* = 8.4 Hz, 2H), 6.69 (d, *J* = 9.5 Hz, 1H), 6.14 (d, *J* = 15.8 Hz, 1H), 3.86 (s, 3H), 1.53 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.9, 162.0, 159.6, 140.2, 138.2, 136.3, 132.9, 127.4, 122.0, 117.7, 114.6, 114.4, 80.5, 55.5, 28.1. **IR**: 979, 1144, 1243, 1283, 1665, 1699 cm^{-1}

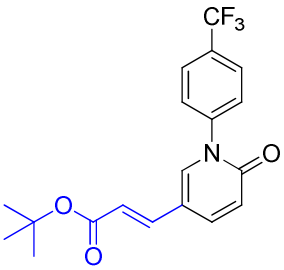
HRMS calculated for $(C_{19}H_{21}NO_4 + Na)^+$ 350.1368; Found: 320.1362.



(2fa)

2fa, yellow solid (74% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (s, 1H), 7.31 (s, 1H), 7.28 (d, *J* = 9.2 Hz, 1H), 6.08 (d, *J* = 15.8 Hz, 1H), 3.57 (s, 3H), 2.17 (s, 3H), 1.51 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 163.0, 138.8, 138.0, 133.1, 130.1, 117.1, 114.1, 80.4, 37.9, 28.2, 17.3. **IR**: 1149, 1257, 1653, 1706 cm^{-1}

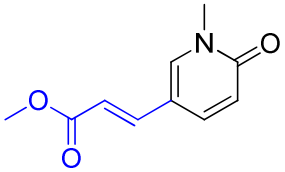
HRMS calculated for $(C_{14}H_{19}NO_3 + Na)^+$ 272.1263; Found: 272.1268.



2ga

2ga,yelow solid (72% yield) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.67 (dd, *J* = 9.7, 2.6 Hz, 1H), 7.54 (d, *J* = 8.3 Hz, 2H), 7.49 (d, *J* = 2.4 Hz, 1H), 7.31 (d, *J* = 15.9 Hz, 1H), 6.69 (d, *J* = 9.7 Hz, 1H), 6.15 (d, *J* = 15.8 Hz, 1H), 1.51 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.74, 161.31, 142.97, 138.81, 137.72, 136.87, 130.97 (q, *J* = 32.94 Hz), 127.01, 126.63 (q, *J* = 3.51 Hz), 123.72 (q, *J* = 271.08 Hz), 122.35, 118.64, 115.17, 80.67, 28.09. **IR**: 828, 987, 1159, 1329, 1669, 1707 cm^{-1}

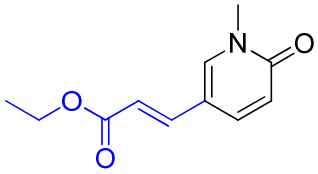
HRMS calculated for $(C_{19}H_{18}F_3NO_3 + Na)^+$ 388.1136; Found: 388.1135.



(2ab)

2ab, yellow solid (78% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 9.5, 2.6 Hz, 1H), 7.48 (d, *J* = 2.5 Hz, 1H), 7.41 (d, *J* = 15.9 Hz, 1H), 6.61 (d, *J* = 9.5 Hz, 1H), 6.15 (d, *J* = 15.8 Hz, 1H), 3.78 (s, 3H), 3.57 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 162.4, 140.8, 139.6, 136.0, 121.0, 114.8, 114.2, 51.5, 37.7. **IR**: 846, 1183, 1668,1707 cm^{-1}

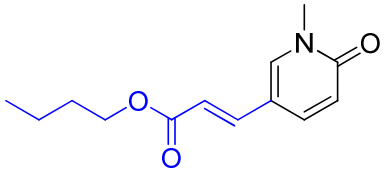
HRMS calculated for $(C_{10}H_{11}NO_3 + Na)^+$ 216.0637; Found: 216.0636.



(2ac)

2ac, yellow solid (83% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 9.5 Hz, 1H), 7.51 (s, 1H), 7.40 (d, *J* = 15.8 Hz, 1H), 6.61 (d, *J* = 9.5 Hz, 1H), 6.15 (d, *J* = 15.8 Hz, 1H), 4.24 (q, *J* = 6.7 Hz, 2H), 3.58 (s, 3H), 1.32 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 162.4, 140.7, 139.3, 136.0, 121.0, 115.3, 114.3, 60.4, 37.7, 14.2. **IR**: 840, 1171, 1639, 1698 cm^{-1}

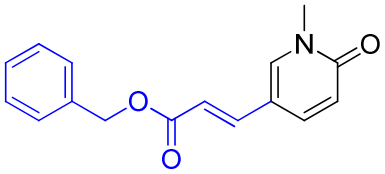
HRMS calculated for $(C_{11}H_{13}NO_3 + Na)^+$ 230.0793; Found: 230.0797.



(2ad)

2ad, yellow solid (80% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 9.5, 2.6 Hz, 1H), 7.47 (d, *J* = 2.5 Hz, 1H), 7.39 (d, *J* = 15.9 Hz, 1H), 6.61 (d, *J* = 9.5 Hz, 1H), 6.15 (d, *J* = 15.8 Hz, 1H), 4.19 (t, *J* = 6.7 Hz, 2H), 3.57 (s, 3H), 1.73 – 1.62 (m, 2H), 1.48 – 1.36 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 162.4, 140.6, 139.3, 136.0, 121.0, 115.4, 114.3, 64.3, 37.7, 30.7, 19.1, 13.6. **IR**: 837, 1185, 1668, 1695 cm^{-1}

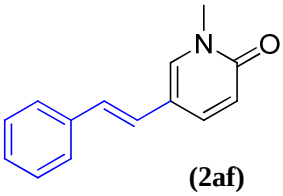
HRMS calculated for $(C_{13}H_{17}NO_3 + Na)^+$ 235.1106; Found: 258.1102.



(2ae)

2ae, yellow solid (64% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 9.6, 2.6 Hz, 1H), 7.45 (d, *J* = 2.5 Hz, 1H), 7.43 (d, *J* = 15.9 Hz, 1H), 7.40 – 7.31 (m, 5H), 6.59 (d, *J* = 9.5 Hz, 1H), 6.18 (d, *J* = 15.8 Hz, 1H), 5.22 (s, 2H), 3.55 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 162.3, 140.3, 139.9, 136.0, 128.5, 128.2, 128.1, 121.0, 121.0, 115.0, 114.2, 66.2, 37.7. **IR**: 835, 1171, 1669, 1699 cm^{-1}

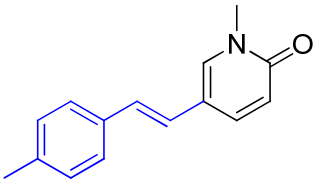
HRMS calculated for $(C_{16}H_{15}NO_3 + Na)^+$ 292.0950; Found: 292.0952.



(2af)

2af, yellow solid (83% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (dd, *J* = 9.5, 2.5 Hz, 1H), 7.43 (d, *J* = 7.6 Hz, 2H), 7.37 – 7.33 (m, 3H), 7.27 (d, *J* = 3.0 Hz, 1H), 6.80 (s, 2H), 6.63 (d, *J* = 9.5 Hz, 1H), 3.58 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.42, 136.84, 136.71, 136.46, 128.68, 127.54, 126.60, 126.08, 123.13, 120.81, 117.18, 37.63. **IR**: 1444, 1599, 1655 cm^{-1}

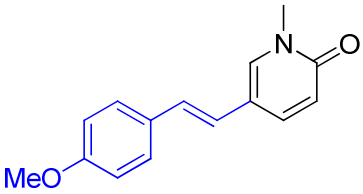
HRMS calculated for $(C_{14}H_{13}NO + Na)^+$ 234.0895; Found: 234.0891.



(2ag)

2ag, yellow soild (62% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 9.5, 2.4 Hz, 1H), 7.31 (m, *J* = 8.6, 5.3 Hz, 3H), 7.15 (d, *J* = 7.9 Hz, 2H), 6.81 – 6.69 (m, 2H), 6.61 (d, *J* = 9.5 Hz, 1H), 3.56 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 137.5, 136.5, 134.1, 129.4, 129.4, 126.6, 126.0, 122.2, 120.9, 117.3, 37.6, 21.2. **IR**: 837, 1601, 1677 cm^{-1}

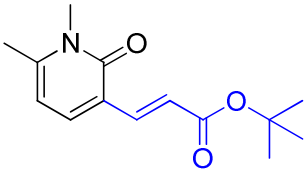
HRMS calculated for $(C_{15}H_{15}NO + Na)^+$ 248.1051; Found: 248.1057.



(2ah)

2ah, yellow solid (74% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 9.5, 2.3 Hz, 1H), 7.37 (d, *J* = 8.6 Hz, 2H), 7.29 (d, *J* = 2.1 Hz, 1H), 6.89 (d, *J* = 8.6 Hz, 2H), 6.75 (d, *J* = 16.3 Hz, 1H), 6.71 – 6.56 (m, 2H), 3.82 (s, 3H), 3.56 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 137.5, 136.5, 136.4, 134.1, 129.4, 126.5, 126.0, 122.2, 120.9, 117.3, 37.6, 21.2. **IR**: 835, 962, 1154, 1649 cm^{-1}

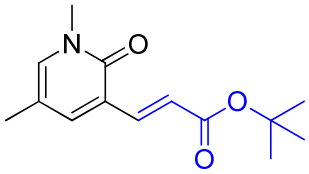
HRMS calculated for $(C_{15}H_{15}NO_2 + Na)^+$ 264.1000; Found: 264.1005.



(4ga)

4ga, yellow solid (70% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 15.9 Hz, 1H), 7.41 (d, *J* = 7.1 Hz, 1H), 6.95 (d, *J* = 15.9 Hz, 1H), 6.11 (d, *J* = 6.8 Hz, 1H), 3.57 (s, 3H), 2.40 (s, 3H), 1.50 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.2, 162.0, 147.9, 139.5, 139.3, 121.9, 121.4, 106.5, 79.9, 31.5, 28.2, 21.3. **IR**: 1146, 1303, 1654, 1697 cm^{-1}

HRMS calculated for $(C_{14}H_{19}NO_3 + Na)^+$ 272.1263; Found: 272.1259.

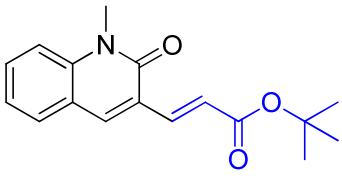


(4ha)

4ha, yellow solid (81% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 15.8 Hz, 1H), 7.32 (s, 1H), 7.10 (s, 1H), 6.94 (d, *J* = 15.7 Hz, 1H), 3.49 (s, 3H), 2.04 (s, 3H), 1.44 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.0, 160.6, 142.7, 138.8, 136.9, 124.8, 122.9, 114.5, 80.0, 37.8, 28.2, 16.9.

IR: 844, 1149, 1665, 1687 cm^{-1}

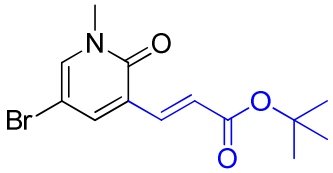
HRMS calculated for $(C_{14}H_{19}NO_3 + Na)^+$ 272.1263; Found: 272.1266.



(4ia)

4ia. yellow solid (69% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.68 (d, *J* = 16.0 Hz, 1H), 7.59 (m, 2H), 7.35 (d, *J* = 8.8 Hz, 1H), 7.26 (d, *J* = 7.7 Hz, 1H), 6.99 (d, *J* = 16.0 Hz, 1H), 3.75 (s, 3H), 1.53 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 160.9, 139.9, 138.7, 138.4, 129.4, 126.3, 124.1, 122.4, 120.1, 115.7, 114.1, 80.4, 29.7, 28.2.

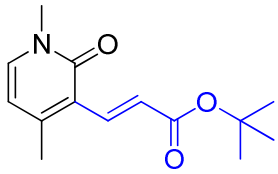
HRMS calculated for $(C_{17}H_{19}NO_3 + Na)^+$ 308.1263; Found: 308.1260.



(4ja)

4ja, yellow soild (74% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 2.5 Hz, 1H), 7.46 (m, 2H), 6.98 (d, *J* = 21.4 Hz, 1H), 3.58 (s, 3H), 1.51 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 159.9, 142.3, 138.5, 137.3, 126.8, 124.5, 97.2, 80.5, 38.0, 28.2. **IR**: 853, 987, 1154, 1659, 1686 cm^{-1}

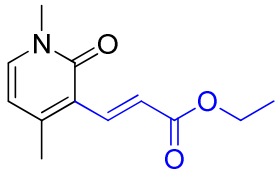
HRMS calculated for $(C_{13}H_{16}BrNO_3 + Na)^+$ 336.0211; Found: 336.0215.



(4ka)

4ka, yellow soild (77% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 15.7 Hz, 1H), 7.41 (d, *J* = 15.7 Hz, 1H), 7.29 (d, *J* = 6.8 Hz, 1H), 6.17 (d, *J* = 6.9 Hz 1H), 3.62 (s, 3H), 2.43 (s, 3H), 1.58 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9, 161.3, 151.2, 137.1, 135.5, 123.9, 122.1, 109.4, 79.8, 37.8, 28.1, 20.0. **IR**: 776, 982, 1143, 1292, 1650, 1687 cm^{-1}

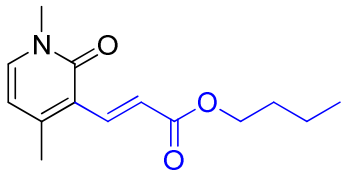
HRMS calculated for $(C_{14}H_{19}NO_3 + Na)^+$ 272.1263; Found: 272.1260.



(4kc)

4kc, yellow solid (71% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 15.7 Hz, 1H), 7.40 (d, *J* = 15.7 Hz, 1H), 7.25 (d, *J* = 6.8 Hz, 1H), 6.10 (d, *J* = 6.8 Hz, 1H), 4.24 (m, 2H), 3.55 (s, 3H), 2.37 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.5, 161.3, 151.6, 137.4, 136.6, 122.0, 121.9, 109.4, 60.1, 37.8, 20.1, 14.3. **IR**: 1165, 1285, 1649, 1709 cm^{-1}

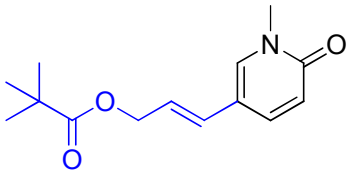
HRMS calculated for $(C_{12}H_{15}NO_3 + Na)^+$ 244.0950; Found: 244.047.



(4kd)

4kd, yellow soild (72% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 15.7 Hz, 1H), 7.42 (d, *J* = 15.7 Hz, 1H), 7.25 (d, *J* = 6.8 Hz, 1H), 6.11 (d, *J* = 6.8 Hz, 1H), 4.18 (t, *J* = 6.6 Hz, 2H), 3.56 (s, 3H), 2.37 (s, 3H), 1.73 – 1.55 (m, 2H), 1.49 – 1.33 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 161.3, 151.6, 137.4, 137.3, 136.5, 122.0, 109.5, 64.0, 37.8, 30.7, 20.1, 19.1, 13.7. **IR**: 1273, 1358, 1633, 1706 cm^{-1}

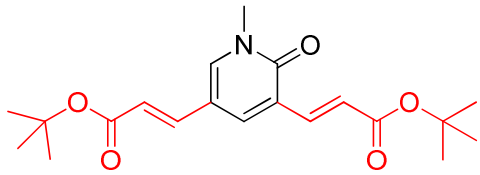
HRMS calculated for $(C_{14}H_{19}NO_3 + Na)^+$ 272.1263; Found: 272.1259.



(3)

3, yellow oil (78% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 9.5, 2.5 Hz, 1H), 7.24 (d, *J* = 2.4 Hz, 1H), 6.58 (d, *J* = 9.5 Hz, 1H), 6.34 (d, *J* = 15.8 Hz, 1H), 5.99 (m, 1H), 4.66 (dd, *J* = 6.3, 1.0 Hz, 2H), 3.55 (s, 3H), 1.22 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.2, 162.5, 137.0, 136.5, 128.5, 121.4, 120.8, 116.0, 64.6, 38.8, 37.6, 27.2. **IR**: 1497, 1522, 1633, 1699 cm^{-1}

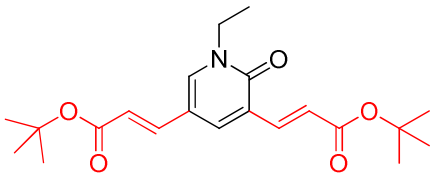
HRMS calculated for $(C_{14}H_{19}NO_3 + Na)^+$ 272.1263; Found: 272.1266.



(5aaa)

5aaa, yellow solid (70% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (s, 1H), 7.51 (d, *J* = 16.7 Hz, 2H), 7.29 (d, *J* = 16.5 Hz, 1H), 7.01 (d, *J* = 15.1 Hz, 1H), 6.13 (d, *J* = 16.0 Hz, 1H), 3.62 (s, 3H), 1.52 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 165.8, 160.8, 140.3, 137.9, 137.9, 136.4, 125.5, 124.0, 118.0, 114.1, 80.6, 80.3, 38.2, 28.0. **IR**: 851, 980, 1134, 1626, 1653, 1693 cm^{-1}

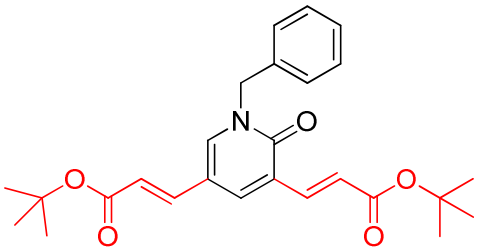
HRMS calculated for $(C_{20}H_{27}NO_5 + Na)^+$ 384.1787; Found: 384.1794.



(5baa)

5baa, yellow soild (77% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 2.4 Hz, 1H), 7.52 (d, *J* = 15.9 Hz, 1H), 7.48 (d, *J* = 2.4 Hz, 1H), 7.31 (d, *J* = 15.8 Hz, 1H), 7.01 (d, *J* = 15.9 Hz, 1H), 6.13 (d, *J* = 15.8 Hz, 1H), 4.06 (m, 2H), 1.52 (d, *J* = 3.9 Hz, 18H), 1.40 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 165.9, 160.2, 139.1, 138.1, 138.0, 136.3, 125.9, 124.1, 118.0, 114.4, 80.7, 80.4, 45.7, 28.2, 28.1, 14.6. **IR**: 1151, 1643, 1663,1709 cm^{-1}

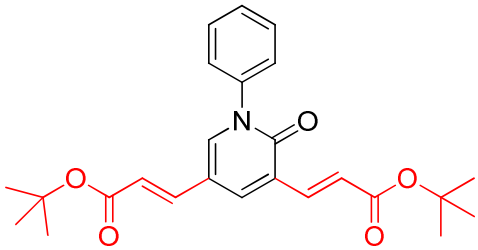
HRMS calculated for $(C_{21}H_{29}NO_5 + Na)^+$ 398.1943; Found: 398.1948.



(5caa)

5caa, yellow soild (62% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 2.4 Hz, 1H), 7.53 (d, *J* = 15.9 Hz, 1H), 7.47 (d, *J* = 2.4 Hz, 1H), 7.37 – 7.29 (m, 5H), 7.27 (d, *J* = 1.9 Hz, 1H), 7.03 (d, *J* = 15.9 Hz, 1H), 6.10 (d, *J* = 15.8 Hz, 1H), 5.19 (s, 2H), 1.51 (d, *J* = 1.9 Hz, 18H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 165.8, 160.5, 139.2, 138.0, 138.0, 136.4, 135.3, 129.1, 128.5, 128.2, 126.2, 124.4, 118.2, 114.4, 80.7, 80.4, 52.7, 28.1, 28.0. **IR**: 1148, 1632, 1659, 1705 cm^{-1}

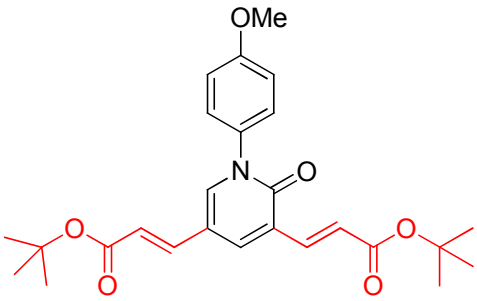
HRMS calculated for $(C_{16}H_{31}NO_5 + Na)^+$ 460.2100; Found: 460.2105.



(5daa)

5daa, yellow solid (51% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.59 – 7.44 (m, 5H), 7.37 (d, *J* = 7.7 Hz, 1H), 7.32 (d, *J* = 16.1 Hz, 1H), 6.18 (d, *J* = 17.1 Hz, 1H), 1.51 (d, *J* = 8.1 Hz, 18H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 165.8, 160.3, 140.1, 139.7, 137.9, 137.8, 137.1, 129.51, 129.1, 126.7, 126.5, 124.7, 118.7, 114.4, 80.7, 80.4, 28.2, 28.1.

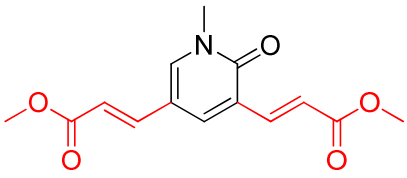
HRMS calculated for $(C_{25}H_{29}NO_5 + Na)^+$ 446.1943; Found: 446.1941.



(5eaa)

5eaa, yellow solid (53% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 2.5 Hz, 1H), 7.57 – 7.50 (m, 2H), 7.31 (d, *J* = 15.9 Hz, 1H), 7.29 – 7.26 (m, 2H), 7.06 – 6.99 (m, 3H), 6.17 (d, *J* = 15.8 Hz, 1H), 3.86 (s, 3H), 1.51 (d, *J* = 9.5 Hz, 18H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 165.8, 160.6, 159.8, 140.1, 138.0, 137.9, 137.0, 132.8, 127.5, 126.5, 124.6, 118.5, 114.7, 114.2, 80.8, 80.4, 55.6, 28.2, 28.1.

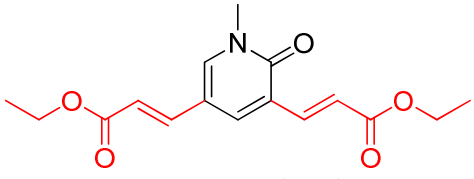
HRMS calculated for $(C_{26}H_{31}NO_6 + Na)^+$ 476.2049; Found: 476.2042.



(5abb)

5abb, yellow solid (72% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (d, *J* = 2.5 Hz, 1H), 7.62 (d, *J* = 15.9 Hz, 1H), 7.54 (d, *J* = 2.5 Hz, 1H), 7.42 (d, *J* = 15.9 Hz, 1H), 7.15 (d, *J* = 15.9 Hz, 1H), 6.21 (d, *J* = 15.9 Hz, 1H), 3.80 (s, 6H), 3.64 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.8, 167.0, 160.8, 140.9, 139.4, 139.2, 137.1, 125.3, 121.8, 115.7, 113.9, 51.72, 51.67, 38.3. **IR**: 1167, 1268, 1632, 1659, 1711 cm^{-1}.

HRMS calculated for $(C_{14}H_{15}NO_5 + Na)^+$ 300.0848; Found: 300.0843.

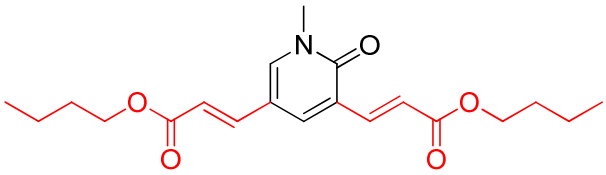


(5acc)

5acc yellow solid (87% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.65 – 7.54 (m, 2H), 7.41 (d, *J* = 15.9 Hz, 1H), 7.12 (d, *J* = 15.9 Hz, 1H), 6.21 (d, *J* = 16.0 Hz, 1H), 4.25 (m, 4H), 3.64 (s, 3H), 1.33 (t, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 166.6, 160.8, 140.8, 139.1,

138.9, 136.9, 125.4, 122.2, 116.1, 114.0, 60.6, 60.5, 38.3, 14.2. **IR**: 1036, 1159, 1633, 1656, 1706 cm^{-1}

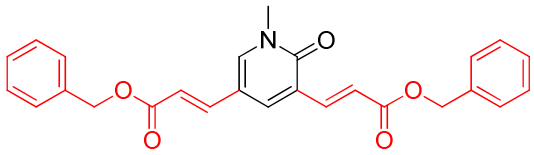
HRMS calculated for $(C_{16}H_{19}NO_5 + Na)^+$ 328.1161; Found: 328.1160.



(5add)

5add, yellow solid (73% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 2.4 Hz, 1H), 7.60 (d, *J* = 15.9 Hz, 1H), 7.55 (d, *J* = 2.3 Hz, 1H), 7.40 (d, *J* = 15.9 Hz, 1H), 7.13 (d, *J* = 14.6 Hz, 1H), 6.21 (d, *J* = 15.9 Hz, 1H), 4.20 (t, *J* = 6.6 Hz, 4H), 3.63 (s, 3H), 1.73 – 1.62 (m, 4H), 1.49 – 1.38 (m, 4H), 0.96 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.4, 166.7, 160.8, 140.7, 139.0, 138.8, 136.9, 125.5, 122.4, 116.3, 114.0, 64.5, 64.4, 38.3, 30.7, 19.2, 13.7.

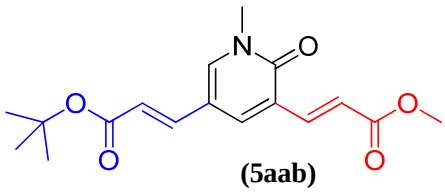
HRMS calculated for $(C_{20}H_{27}NO_5 + Na)^+$ 384.1787; Found: 384.1783.



(5aee)

5aee, yellow solid (52% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 2.5 Hz, 1H), 7.63 (d, *J* = 15.9 Hz, 1H), 7.52 (d, *J* = 2.5 Hz, 1H), 7.43 (d, *J* = 15.9 Hz, 1H), 7.41 – 7.30 (m, 10H), 7.19 (d, *J* = 15.9 Hz, 1H), 6.24 (d, *J* = 15.9 Hz, 1H), 5.24 (d, *J* = 4.2 Hz, 4H), 3.61 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.0, 166.3, 160.7, 141.0, 139.6, 139.4, 137.1, 136.1, 135.9, 128.6, 128.5, 128.3, 128.2, 128.1, 128.0, 125.4, 122.0, 115.9, 113.9, 66.4, 66.3, 38.3. **IR**: 1154, 1273, 1633, 1655, 1706 cm^{-1}

HRMS calculated for $(C_{26}H_{23}NO_5 + Na)^+$ 452.1474; Found: 452.1477.

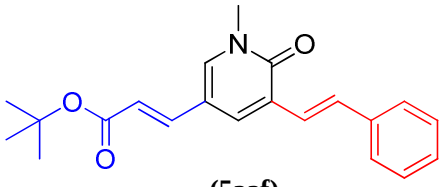


(5aab)

5aab, yellow solid (76% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 2.5 Hz, 1H), 7.61 (d, *J* = 15.9 Hz, 1H), 7.52 (d, *J* = 2.5 Hz, 1H), 7.29 (d, *J* = 15.9 Hz, 1H), 7.12 (d, *J* = 15.9 Hz, 1H), 6.14 (d, *J* = 15.8 Hz, 1H), 3.79 (s, 3H), 3.62 (s, 3H), 1.52 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.8,

165.8, 160.77, 140.5, 139.4, 137.7, 137.2, 125.3, 121.7, 118.3, 114.2, 80.7, 51.6, 38.3, 28.2. **IR**: 1156, 1285, 1635, 1667, 1698 cm^{-1}

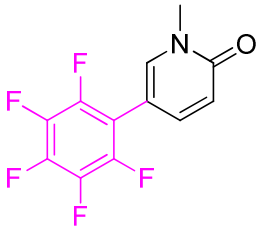
HRMS calculated for ($C_{17}H_{21}NO_5$ + Na) 342.1317; Found: 342,1315.



(5aaf)

5aaf, yellow solid (66% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.61 – 7.53 (m, 3H), 7.39 – 7.34 (m, 4H), 7.24 (d, *J* = 22.2 Hz, 2H), 6.19 (d, *J* = 16.5 Hz, 1H), 3.62 (s, 3H), 1.53 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 161.6, 138.6, 138.3, 132.3, 131.2, 128.7, 128.5 128.00, 126.9, 126.2, 123.2, 117.7, 114.5, 80.6, 38.2, 28.2. **IR**: 971, 1145, 1648, 1701 cm^{-1}

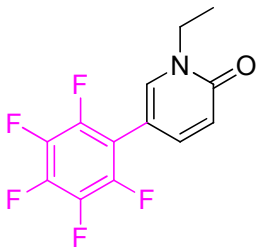
HRMS calculated for ($C_{21}H_{23}NO_3$ + Na)$^+$ 360.1575; Found: 360.1573.



(6aa)

6aa, yellow solid (72% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (s, 1H), 7.41 (m, 1H), 6.68 (d, *J* = 9.5 Hz, 1H), 3.63 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9, 144.1(dm, *J* = 247.4 Hz), 140.4(dm, *J* = 250.2 Hz), 140.4, 139.8, 137.9(dm, *J* = 248.9 Hz), 120.8, 111.4(m), 104.8, 38.0. ^{19}F NMR (470 MHz, $CDCl_3$) δ -146.0 (dd, *J* = 22.7, 8.0 Hz, 2F), -157.9 (t, *J* = 20.8 Hz, 1F), -164.5(td, *J* = 22.0, 8.0 Hz, 2F). **IR**: 976, 1082, 1494, 1665 cm^{-1}

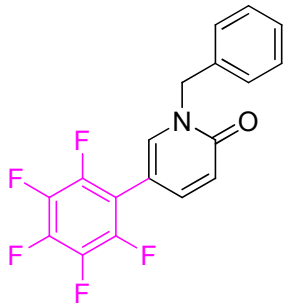
HRMS calculated for ($C_{12}H_6F_5NO$ + Na)$^+$ 298.0267; Found: 298.0269.



(6ba)

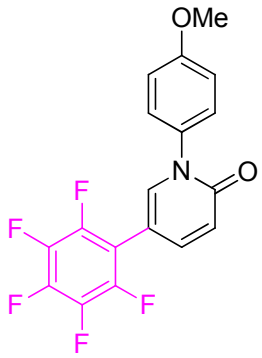
6ba, yellow solid (73% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.40 (m, 1H), 6.65 (d, *J* = 9.5 Hz, 1H), 4.07 (m, 2H), 1.42 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.1, 144.1 (dm, *J* = 243.1 Hz), 140.3 (dm, *J* = 254.9 Hz), 140.0, 138.6, 137.9 (dm, *J* = 251.8 Hz), 121.1, 111.6(m), 104.9, 45.2, 14.5. ^{19}F NMR (470 MHz, $CDCl_3$) δ -146.4 (dd, *J* = 22.8, 7.9 Hz,

2F), -158.0 (t, *J* = 20.9 Hz, 1F), -164.6 (td, *J* = 22.2, 8.0 Hz, 2F). **IR**: 992, 1084, 1493, 1658 cm^{-1}
HRMS calculated for $(C_{13}H_8F_5NO + Na)^+$ 312.0424; Found: 312.0422.



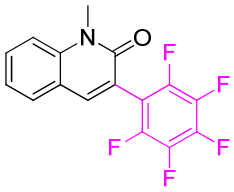
(6ca)

6ca, yellow solid (79% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (s, 1H), 7.44 – 7.03 (m, 7H), 6.70 (d, *J* = 9.4 Hz, 1H), 5.19 (s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.3, 144.1 (dm, *J* = 247.4 Hz), 140.3 (dm, *J* = 255.0 Hz,),140.1, 138.9, 137.9 (dm, *J* = 252.4 Hz). 135.6, 128.9, 128.8, 128.1, 121.2, 111.4(m), 105.0, 52.3. ^{19}F NMR (470 MHz, $CDCl_3$) δ -146.1 (dd, *J* = 22.8, 7.9 Hz, 2F), -157.9 (t, *J* = 21.0 Hz, 1F), -164.5 (td, *J* = 22.1, 8.0 Hz, 2F). **IR**: 990, 1064, 1494, 1669 cm^{-1}
HRMS calculated for $(C_{18}H_{10}F_5NO + Na)^+$ 374.0580; Found: 374.0589.



(6ea)

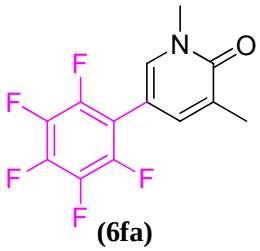
6da, yellow solid (68% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.46 (d, *J* = 9.4 Hz, 1H), 7.33 (d, *J* = 8.9 Hz, 2H), 7.01 (d, *J* = 8.9 Hz, 2H), 6.75 (d, *J* = 9.6 Hz, 1H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 159.7, 144.2 (dm, *J* = 246.3 Hz), 140.6, 140.5 (dm, *J* = 253.2 Hz), 139.9, 138.0 (dm, *J* = 258.9 Hz), 133.1, 127.5, 121.9, 114.7, 111.4(m) 104.9, 55.6. ^{19}F NMR (470 MHz, $CDCl_3$) δ 183.9 (dd, *J* = 22.8, 7.9 Hz, 2F), 172.1 (t, *J* = 21.0 Hz, 1F), 165.4 (td, *J* = 22.3, 8.0 Hz, 2F). **IR**: 845, 985, 1265, 1509, 1690 cm^{-1}
HRMS calculated for $(C_{18}H_{10}F_5NO_2 + Na)^+$ 390.0529; Found: 390.0523.



(6ia)

6ja, yellow solid (60% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (d, *J* = 9.5 Hz, 1H), 7.63 (m, 2H), 7.49 (d, *J* = 8.7 Hz, 1H), 6.77 (d, *J* = 9.5 Hz, 1H), 3.76 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.1, 144.3 (dm, *J* = 247.8 Hz), 140.6 (dm, *J* = 268.8 Hz), 140.5, , 138.6, 137.9 (dm, *J* = 238.8 Hz), 132.0, 130.4, 122.7, 120.8, 120.1, 114.6, 114.5(m), 29.5. ^{19}F NMR (470 MHz, $CDCl_3$) δ -146.48 (dd, *J* = 22.9, 8.0 Hz, 2F), -157.97 (t, *J* = 21.0 Hz, 1F), -164.83 (dd, *J* = 21.9, 7.8 Hz, 2F). **IR**: 976, 1084, 1156, 1473, 1659 cm^{-1}

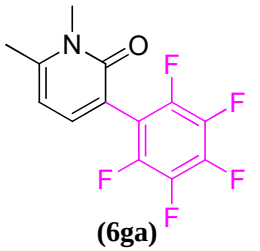
HRMS calculated for $(C_{16}H_8F_5NO + Na)^+$ 348.0424; Found: 348.0420.



(6fa)

6fa, yellow solid (82% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (s, 1H), 7.27 (s, 1H), 3.63 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 144.2 (dm, *J* = 243.1 Hz), 140.4 (dm, *J* = 232.9 Hz), 137.8 (dm, *J* = 235.7 Hz).137.4, 137.1, 130.1, 111.9 (m), 104.3, 37.8, 17.2. ^{19}F NMR (470 MHz, $CDCl_3$) δ -146.0 (dd, *J* = 22.9, 8.1 Hz, 2F), -158.2 (t, *J* = 20.8 Hz, 1F), -164.7 (td, *J* = 22.4, 7.9 Hz, 2F). **IR**: 992, 1159, 1493, 1658 cm^{-1}

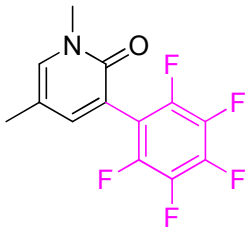
HRMS calculated for $(C_{13}H_8F_5NO + Na)^+$ 312.0424; Found: 312.0418.



(6ga)

6ga, yellow solid (48% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 6.8 Hz, 1H), 6.19 (d, *J* = 7.0 Hz, 1H), 3.61 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.9, 148.7, 144.7 (dm, *J* = 247.5 Hz), 140.7 (dm, *J* = 253.1 Hz), 140.9, 137.6 (dm, *J* = 251.8 Hz), 114.7, 112.0(m), 105.9, 31.7, 21.7. ^{19}F NMR (470 MHz, $CDCl_3$) δ -139.7 (dd, *J* = 22.9, 7.7 Hz, 2F), -155.8 (t, *J* = 20.8 Hz, 1F), -163.0 (dt, *J* = 22.5, 7.6 Hz, 2F). **IR**: 991, 1494, 1523, 1643 cm^{-1}

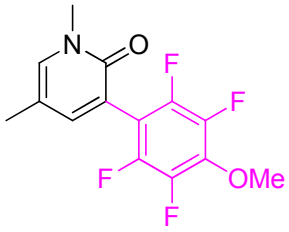
HRMS calculated for $(C_{13}H_8F_5NO + Na)^+$ 312.0424; Found: 312.0420.



(6ha)

6ha, yellow solid (75% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (s, 1H), 7.24 (s, 1H), 3.60 (s, 3H), 2.15 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.5, 144.7 (dm, *J* = 244.2 Hz), 144.3, 140.9 (dm, *J* = 263.9 Hz, 0H), 137.7, 137.7 (dm, *J* = 252.2 Hz), 118.0, 114.2, 111.5(m), 38.0, 16.9. ^{19}F NMR (470 MHz, $CDCl_3$) δ -142.65 (dd, *J* = 22.8, 7.6 Hz, 2F), -158.31 (t, *J* = 20.8 Hz, 1F), -165.84 (dt, *J* = 22.1, 7.5 Hz, 2F). **IR**: 999, 1105, 1496, 1523, 1664 cm^{-1}

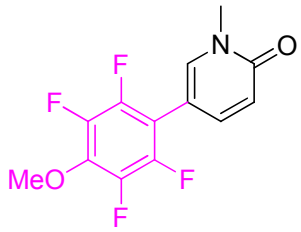
HRMS calculated for $(C_{13}H_8F_5NO + Na)^+$ 312.0424; Found: 312.0428.



(6hb)

6hb, yellow solid (75% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (s, 1H), 7.21 (s, 1H), 4.09 (s, 3H), 3.59 (s, 3H), 2.14 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.8, 144.8 (dm, *J* = 246.4 Hz), 144.2, 141.0 (dm, *J* = 242.7 Hz), 138.1(m), 137.3, 118.9, 114.2, 109.8 (t, *J* = 18.6 Hz), 62.1 (t, *J* = 3.4 Hz), 38.0, 17.0. ^{19}F NMR (470 MHz, $CDCl_3$) δ -144.4 (dd, *J* = 21.4, 7.9 Hz, 2F), -161.5 (dd, *J* = 21.8, 8.4 Hz, 2F). **IR**: 724, 984, 1488, 1667 cm^{-1}

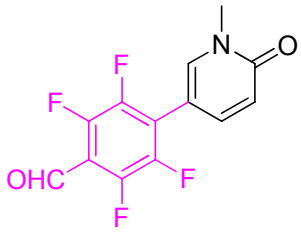
HRMS calculated for $(C_{14}H_{11}F_5NO_2 + Na)^+$ 324.0624; Found: 324.0620.



(6ab)

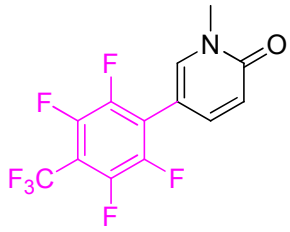
6ab, yellow solid (86% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (s, 1H), 7.41 (m, 1H), 6.65 (d, *J* = 9.5 Hz, 1H), 4.12 (t, *J* = 1.3 Hz, 3H), 3.62 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.9, 144.3 (dm, *J* = 245.1 Hz), 141.2 (dm, *J* = 247.7 Hz), 140.7, 139.6, 137.6(m), 120.5, 109.4 (t, *J* = 16.6 Hz), 105.7, 62.1 (t, *J* = 3.6 Hz), 37.9. ^{19}F NMR (470 MHz, $CDCl_3$) δ -148.1 (dd, *J* = 21.8, 8.4 Hz, 2F), -160.6 (dd, *J* = 21.8, 8.3 Hz, 2F). **IR**: 989, 1153, 1271, 1338, 1669 cm^{-1}

HRMS calculated for $(C_{13}H_9F_5NO_2 + Na)^+$ 310.0467; Found: 310.0468.



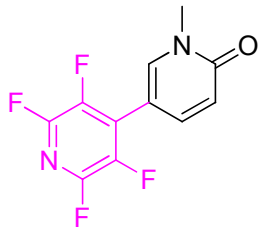
(6ac)

6ac, yellow solid (69% yield). ^{1}H NMR (500 MHz, acetone-d_6) δ 10.53 – 10.13 (m, 1H), 8.12 – 7.85 (m, 1H), 7.72 – 7.43 (m, 1H), 6.54 (d, *J* = 9.5 Hz, 1H), 3.61 (s, 3H). ^{13}C NMR (125 MHz, acetone-d_6) δ 183.5, 162.2, 148.0 (dm, *J* = 259.0 Hz), 144.9 (dm, *J* = 255.8 Hz), 143.0, 141.0, 123.4(m), 120.7, 115.0(t, *J* = 10.1 Hz), 104.9, 38.0. ^{19}F NMR (470 MHz, acetone-d_6) δ -145.1 (dd, *J* = 20.7, 13.0 Hz, 2F), -148.2 (dd, *J* = 20.0, 12.4 Hz, 2F). **IR**: 631, 1016, 1199, 1677, 1703 cm^{-1}
HRMS calculated for $(C_{13}H_7F_5NO_2 + Na)^+$ 308.0311; Found: 308.0301 .



(6ad)

6ad, yellow solid (77% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (s, 1H), 7.48 (d, *J* = 9.4 Hz, 1H), 6.70 (d, *J* = 9.1 Hz, 1H), 3.65 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.8, 144.5 (dm, J = 259.77Hz), 144.0 (dm, J = 251.74Hz), 140.5, 139.8, 120.9 ,120.7(dm, J = 251.74Hz), 120.4(m), 105.1, 104.6, 38.2. ^{19}F NMR (470 MHz, $CDCl_3$) δ -59.3 (t, *J* = 21.7 Hz, 3F), -143.0 – -143.2 (m, 2F), -144.6 (m, 2F). **IR**: 989, 1153, 1271, 1338, 1669 cm^{-1}
HRMS calculated for $(C_{13}H_6F_7NO + Na)^+$ 348.0235; Found: 348.0231.

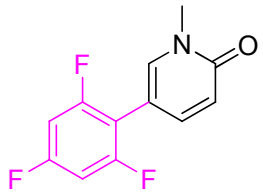


(6ae)

6ae, yellow soild (84% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 1.9 Hz, 1H), 7.56 (m,

1H), 6.73 (d, *J* = 9.6 Hz, 1H), 3.66 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.7, 144.1 (dm, *J* = 249.1 Hz), 141.1 (t, *J* = 3.8 Hz), 139.4, 138.9 (dm, *J* = 261.5 Hz), 128.8(m), 120.8, 104.9, 38.2. ^{19}F NMR (470 MHz, $CDCl_3$) δ -93.2 (m, 2F), -148.1 (m, 2F). **IR**: 969, 1184, 1462, 1662 cm^{-1}

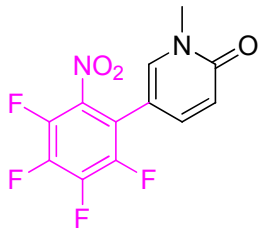
HRMS calculated for $(C_{11}H_6F_4N_2O + Na)^+$ 281.0314; Found: 281.0317.



(6af)

6af, yellow solid (62% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 12.9 Hz, 2H), 6.77 (t, *J* = 8.2 Hz, 2H), 6.65 (d, *J* = 9.3 Hz, 1H), 3.61 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1, 161.8 (dm, *J* = 250.9 Hz), 160.2 b(dm, *J* = 244.8 Hz,). 162.1, 141.2, 139.3, 120.4, 106.7, 100.8 (m), 38.0. ^{19}F NMR (470 MHz, $CDCl_3$) δ -111.0 – -111.2 (m, 1F), -114.3 (t, *J* = 6.8 Hz, 2F). **IR**: 826, 1021, 1126, 1674 cm^{-1}

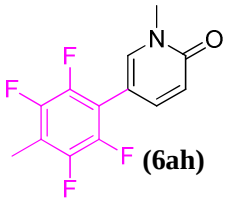
HRMS calculated for $(C_{12}H_8F_3NO + Na)^+$ 262.0456; Found: 262.0451.



(6ag)

6ag, yellow solid (76% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (d, *J* = 2.6 Hz, 1H), 7.23 (m, 1H), 6.64 (d, *J* = 9.5 Hz, 1H), 3.58 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.8, 145.0 (dm, *J* = 251.1 Hz), 143.6 (m), 141.9 (m), 141.4 (m), 139.9 (m), 139.2, 135.5 (m), 121.4, 116.2 (dd, *J* = 18.1, 4.2 Hz), 104.7, 38.1. ^{19}F NMR (377 MHz, $CDCl_3$) δ -137.29 (dd, *J* = 22.6, 10.5 Hz, 1F), -146.54 – -147.07 (m, 1F), -148.92 (t, *J* = 21.5 Hz, 1F), -151.26 (t, *J* = 21.0 Hz, 1F). **IR**: 840, 1074, 1359, 1546, 1663 cm^{-1}

HRMS calculated for $(C_{13}H_6F_4N_2O_3 + Na)^+$ 325.0212; Found: 325.0216.

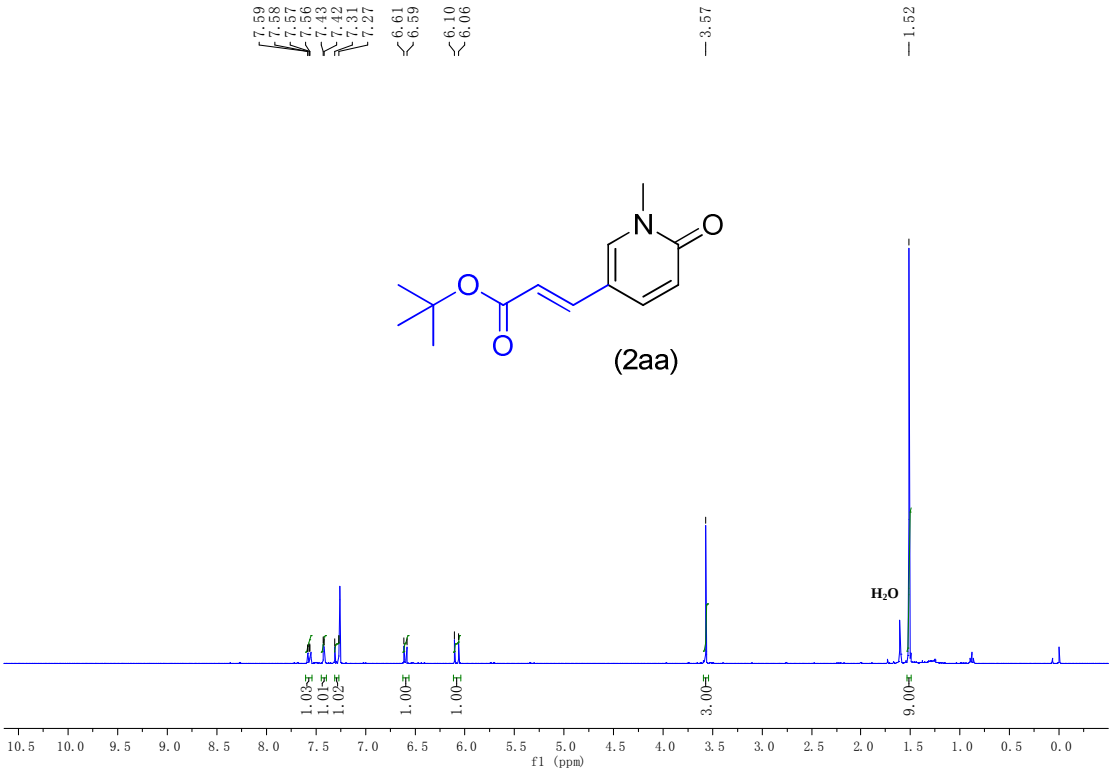


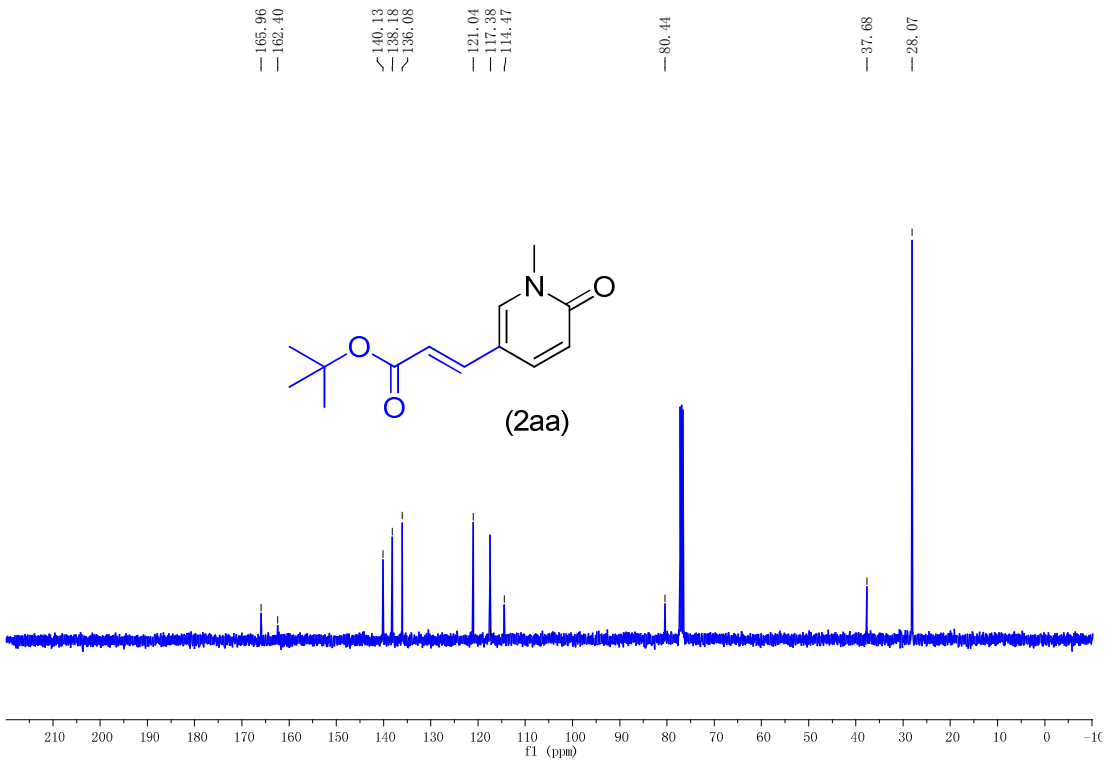
(6ah)

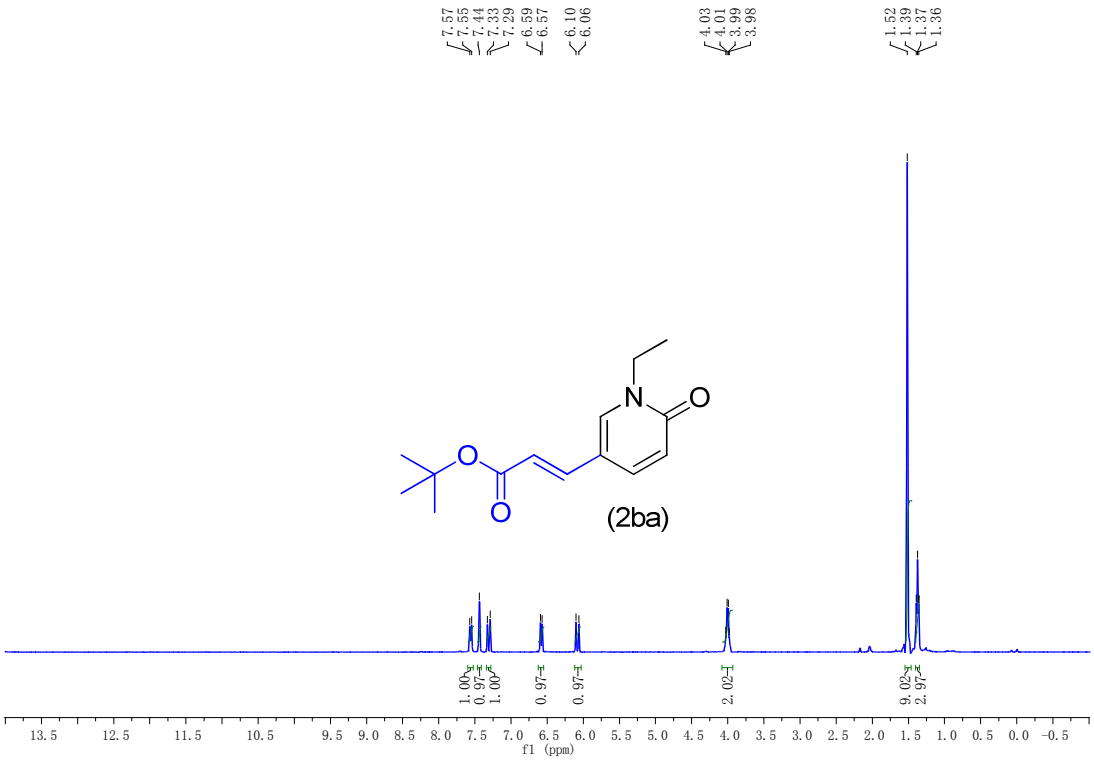
6ah, yellow solid (68% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (s, 1H), 7.45 (d, *J* = 9.3 Hz, 1H), 6.67 (d, *J* = 9.5 Hz, 1H), 3.63 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9, 145.2 (dm, *J* = 248.7 Hz), 143.5 (dm, *J* = 255.1 Hz),140.7, 139.6, 120.5, 115.4 (t, *J* = 19.3 Hz), 113.2 (t, *J* = 15.5 Hz),106.2, 38.0, 7.6. ^{19}F NMR (470 MHz, $CDCl_3$) δ -146.4 (dd, *J* = 22.0, 12.4 Hz, 2F), -148.5 (dd, *J* = 22.0, 12.5 Hz, 2F). **IR**: 826, 1486, 1677 cm^{-1}

HRMS calculated for $(C_{13}H_9F_4NO + Na)^+$ 294.0518; Found: 294.0512.

Ⅳ NMR Spectra



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7.29
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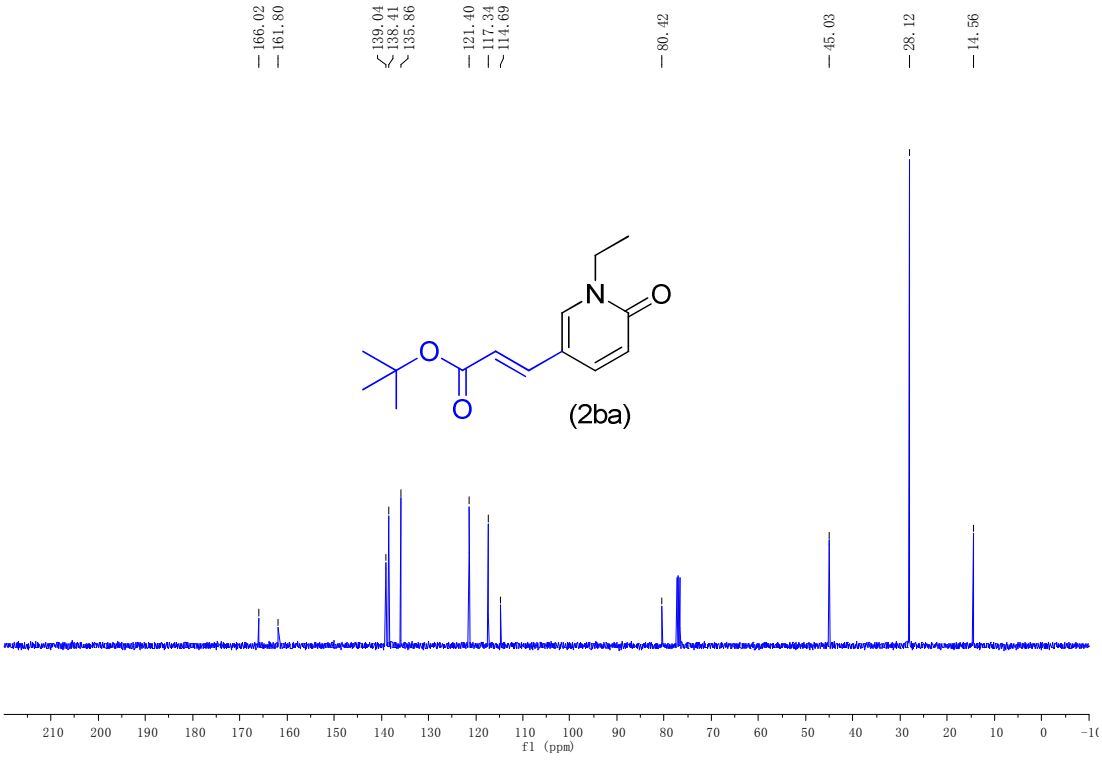
6.57
6.10
6.06
4.03
4.01
3.99
3.98
1.52
1.39
1.37
1.36
(2ba)
1.00
0.97
1.00
0.97
0.97
2.02
9.02
2.97
f1 (ppm)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114.69
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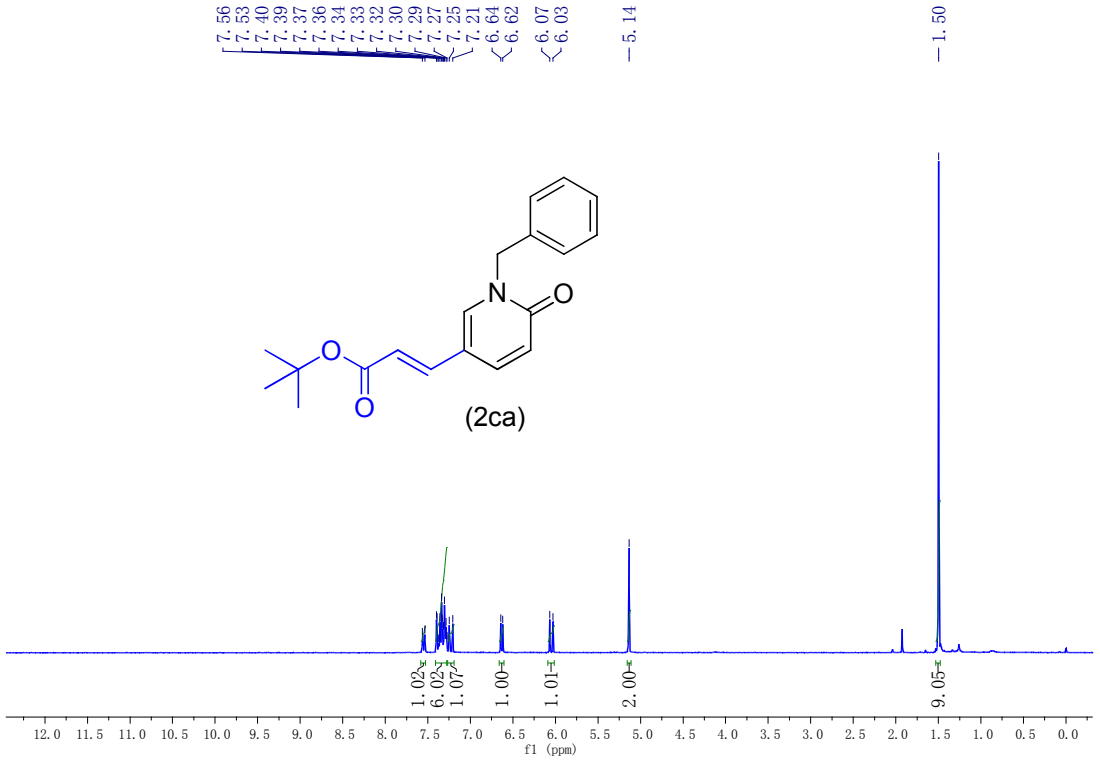
(2ba)
f1 (ppm)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6.07
6.03
5.14
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O
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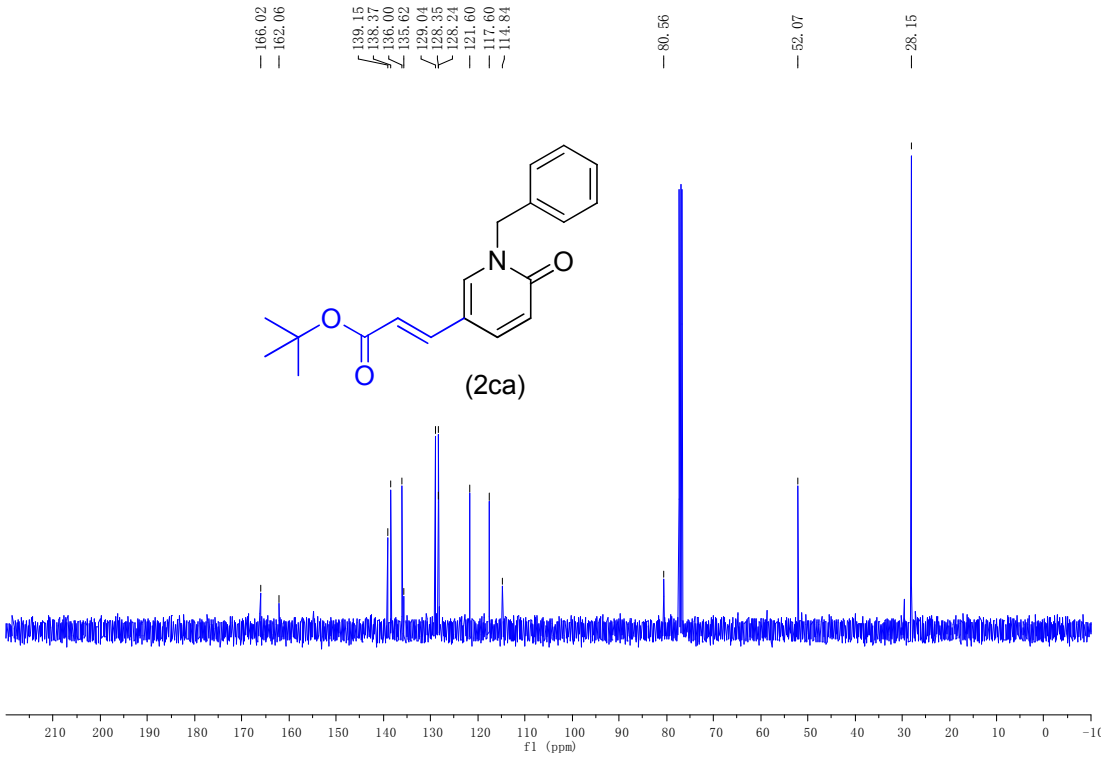
1.07
1.00
1.01
2.00
9.05
f1 (ppm)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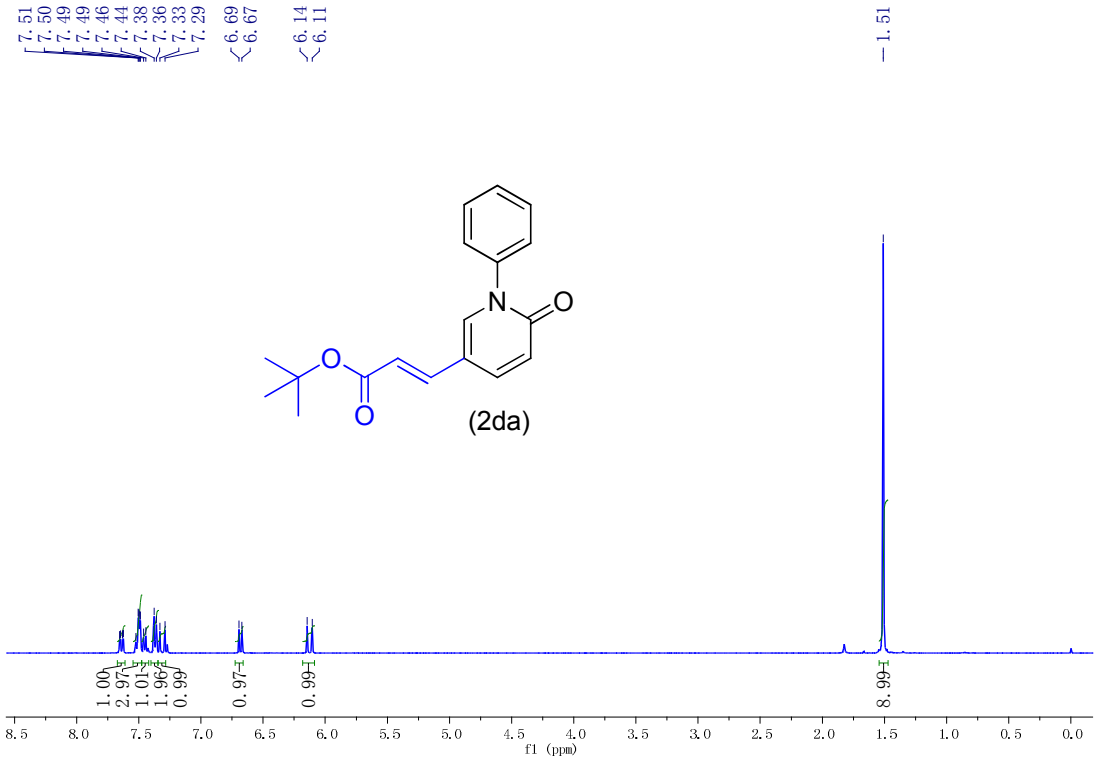
O
(2ca)
f1 (ppm)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6.11
1.51
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O
(2da)
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1.01
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0.97
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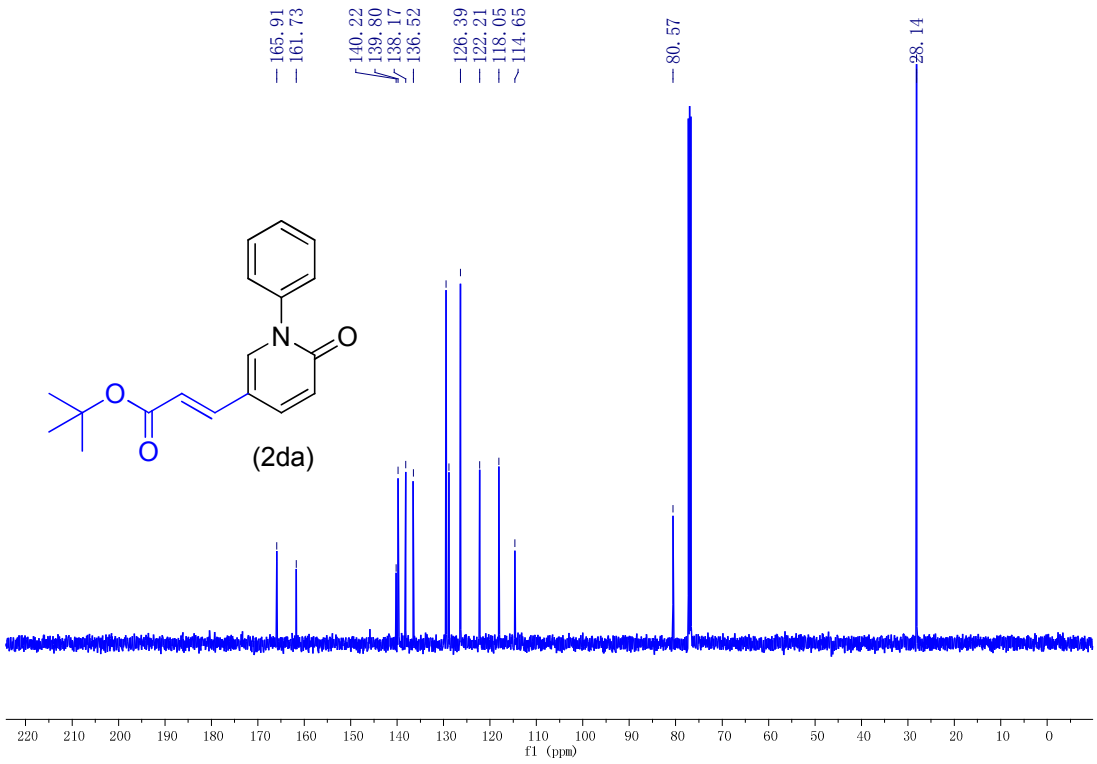
8.99
f1 (ppm)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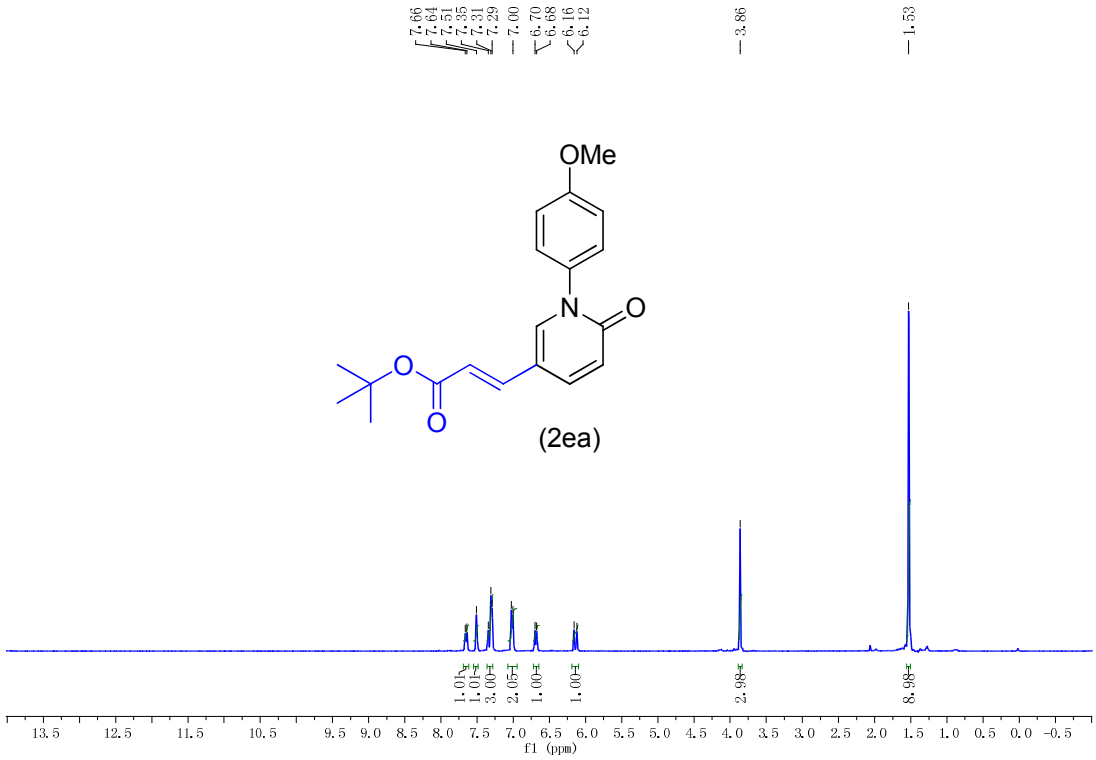
(2da)
f1 (ppm)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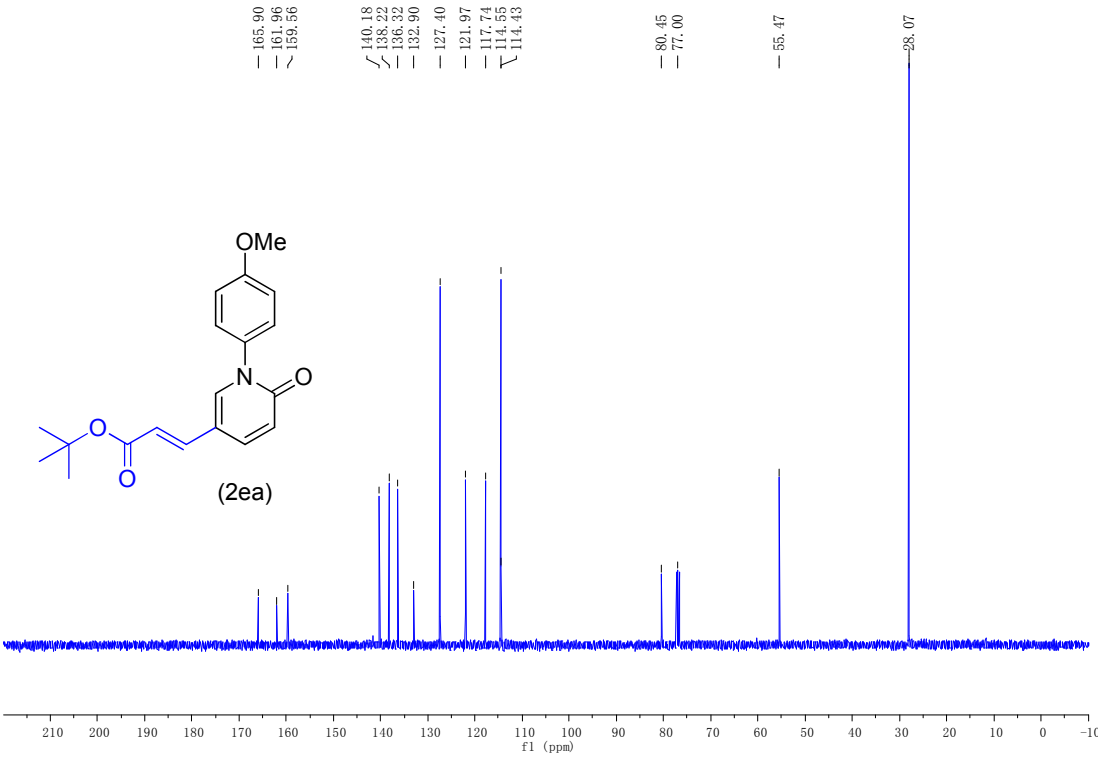
f1 (ppm)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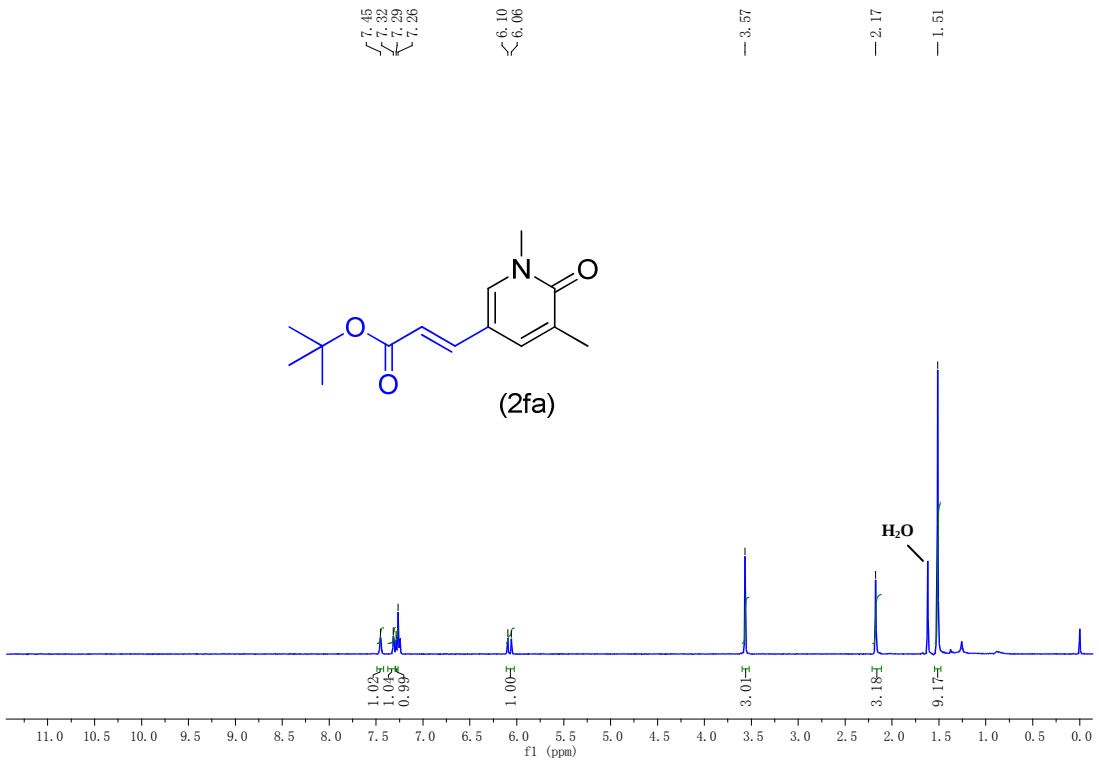
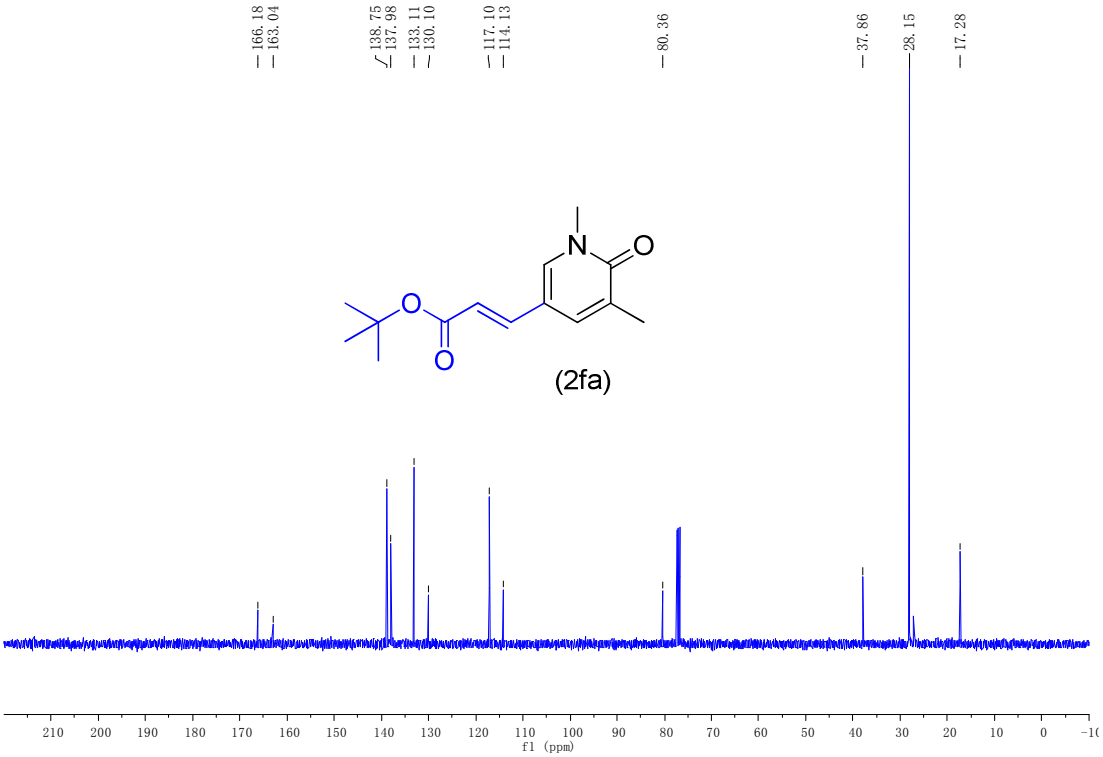
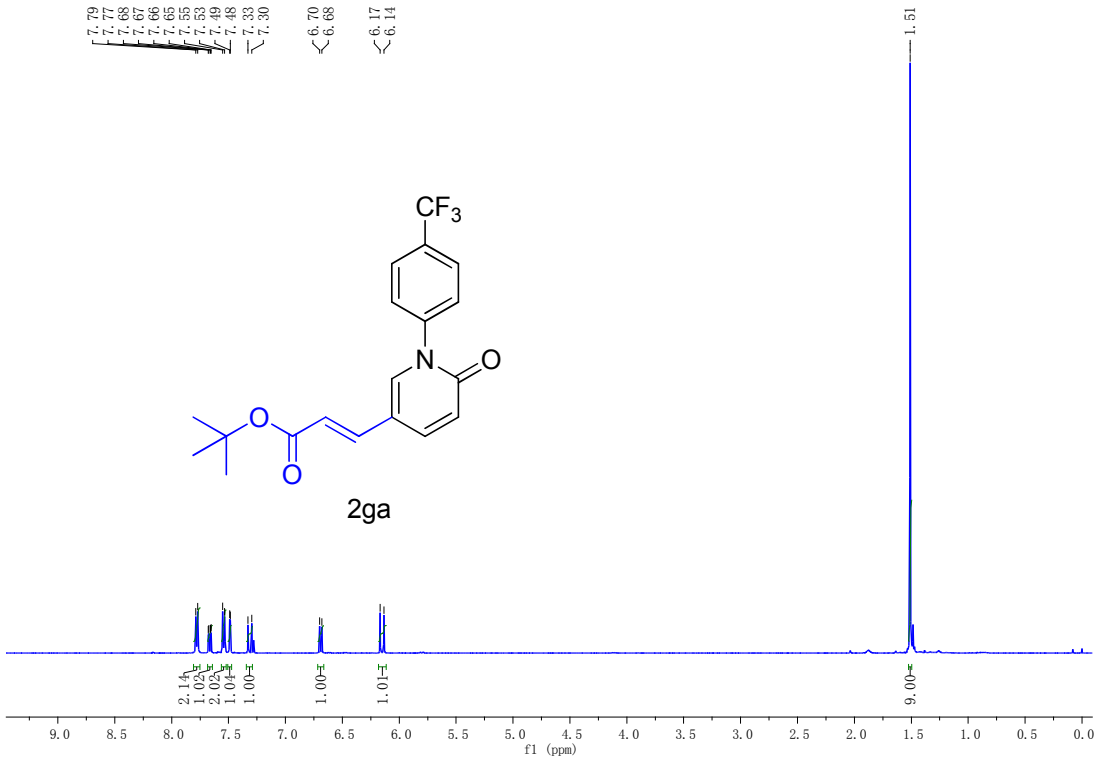
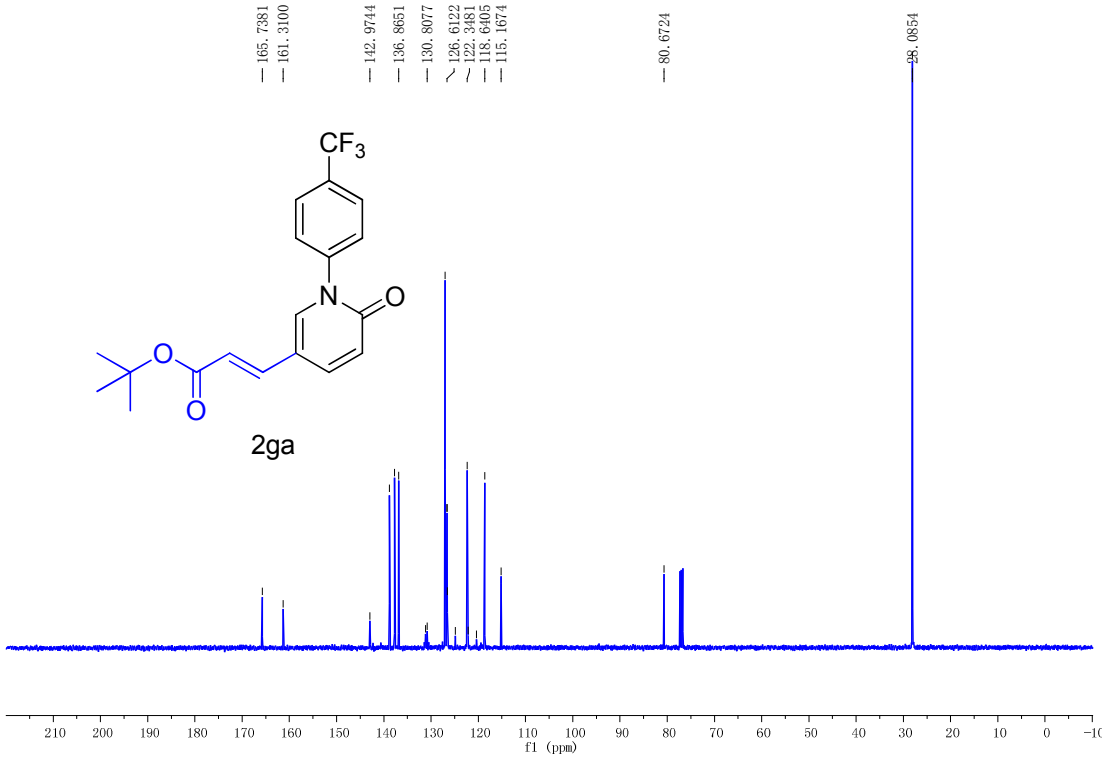
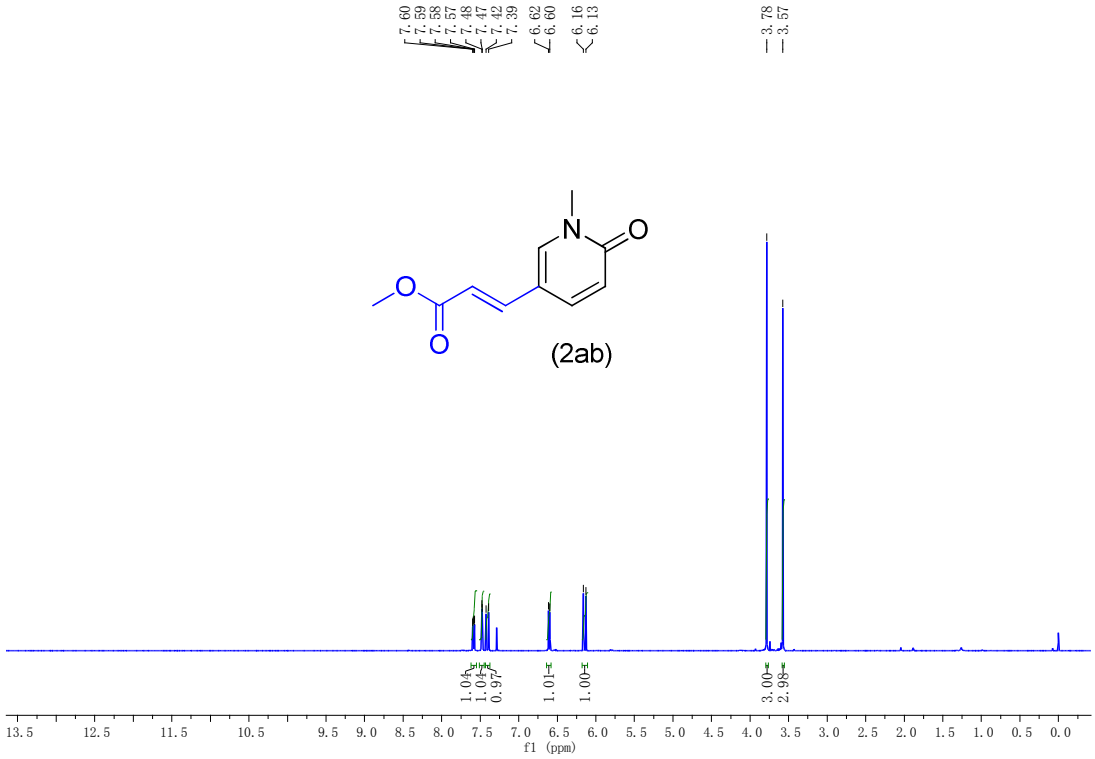
O
(2ea)
f1 (ppm)

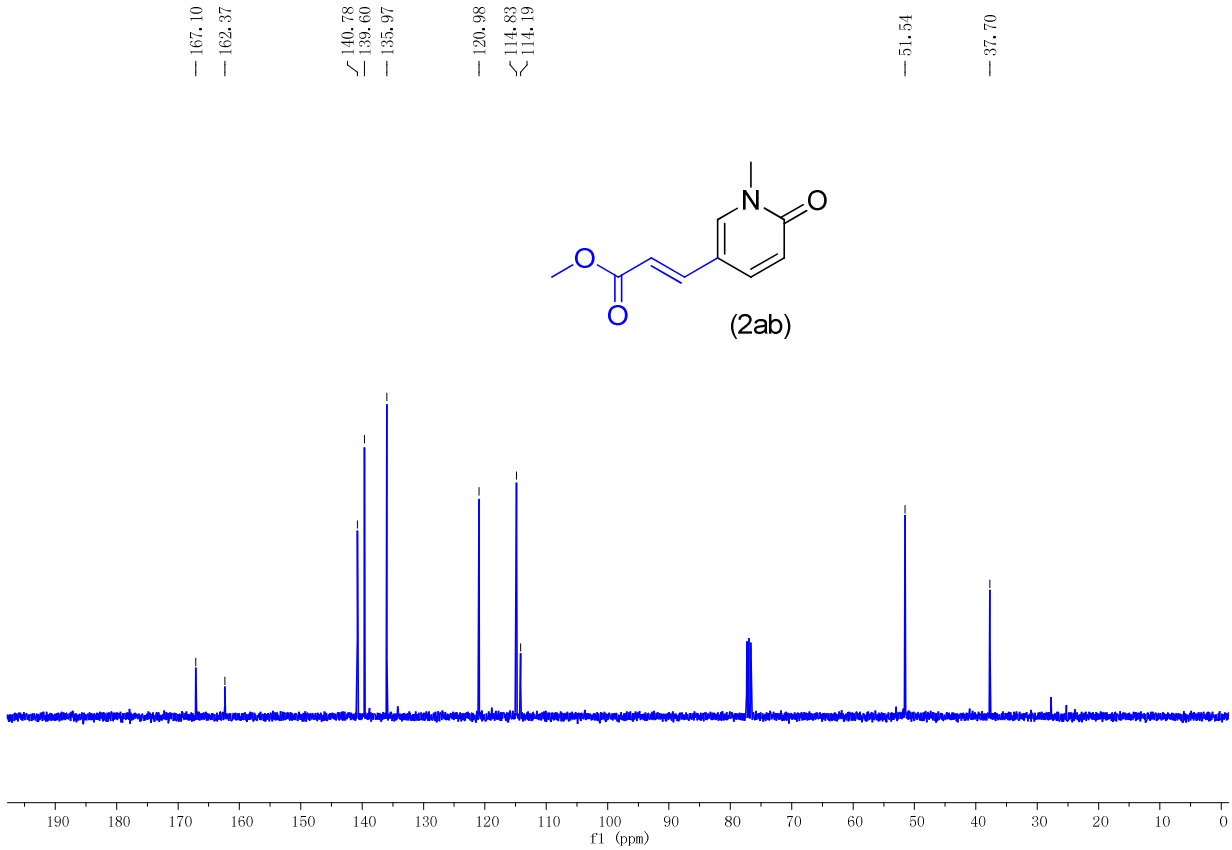

7.45
7.32
7.29
7.26
6.10
6.06
3.57
2.17
1.51
N
O
O
O
(2fa)
H2O
1.02
1.04
0.99
1.00
3.01
3.18
9.17
f1 (ppm)

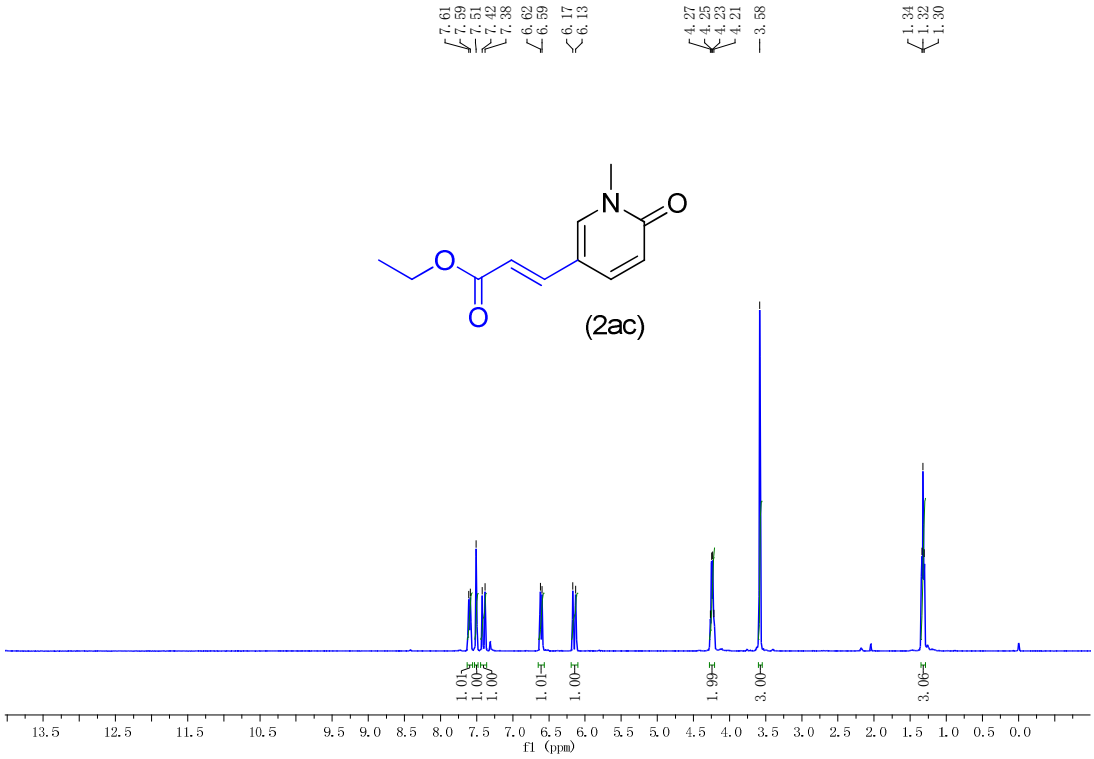

166.18
163.04
138.75
137.98
133.11
130.10
117.10
114.13
80.36
37.86
28.15
17.28
N
O
O
O
(2fa)
f1 (ppm)

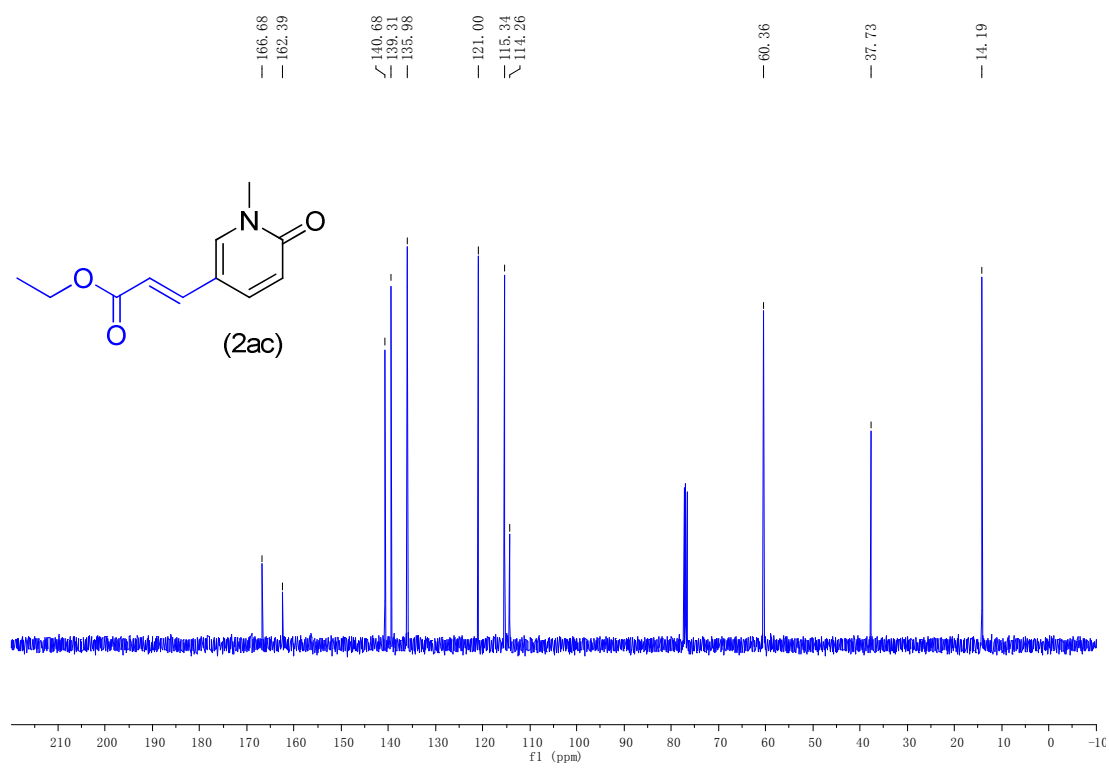

7.79
7.77
7.68
7.67
7.66
7.65
7.55
7.53
7.49
7.48
7.33
7.30
6.70
6.68
6.17
6.14
1.51
CF3
N
O
O
O
2ga
2.14
1.02
2.02
1.04
1.00
1.00
1.01
9.00
f1 (ppm)

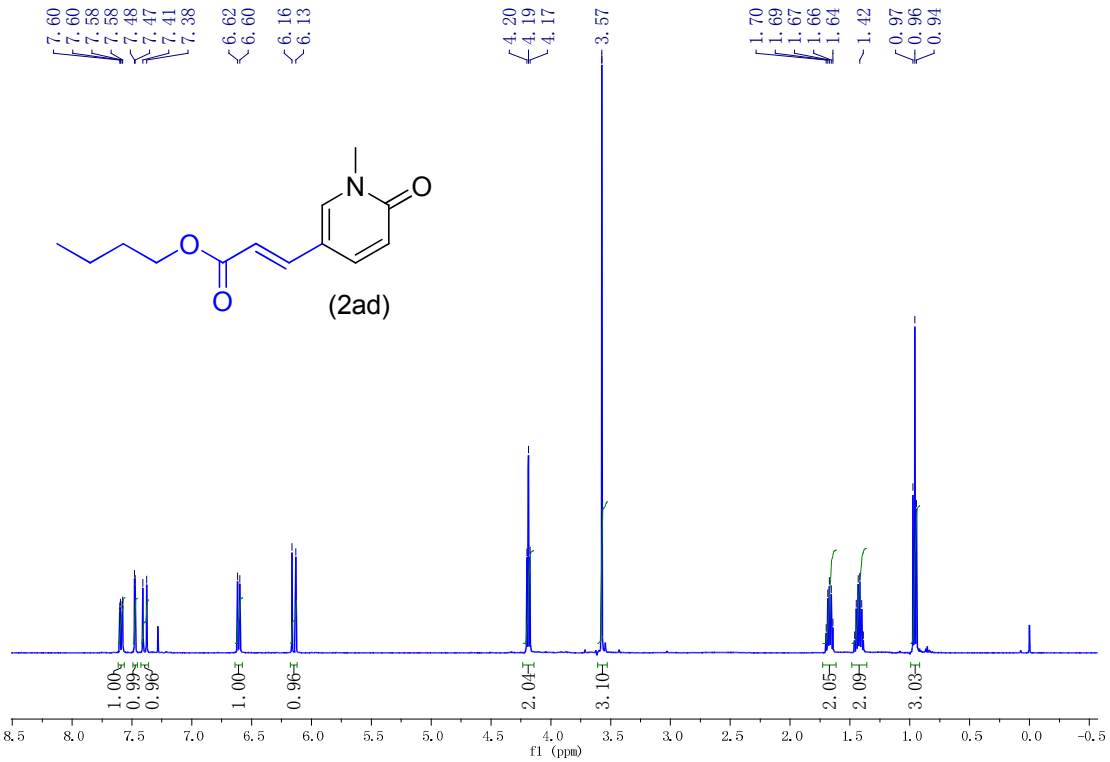

165.7381
161.3100
142.9744
136.8651
130.8077
126.6122
122.3481
118.6405
115.1674
80.6724
28.0854
CF3
N
O
O
O
2ga
f1 (ppm)

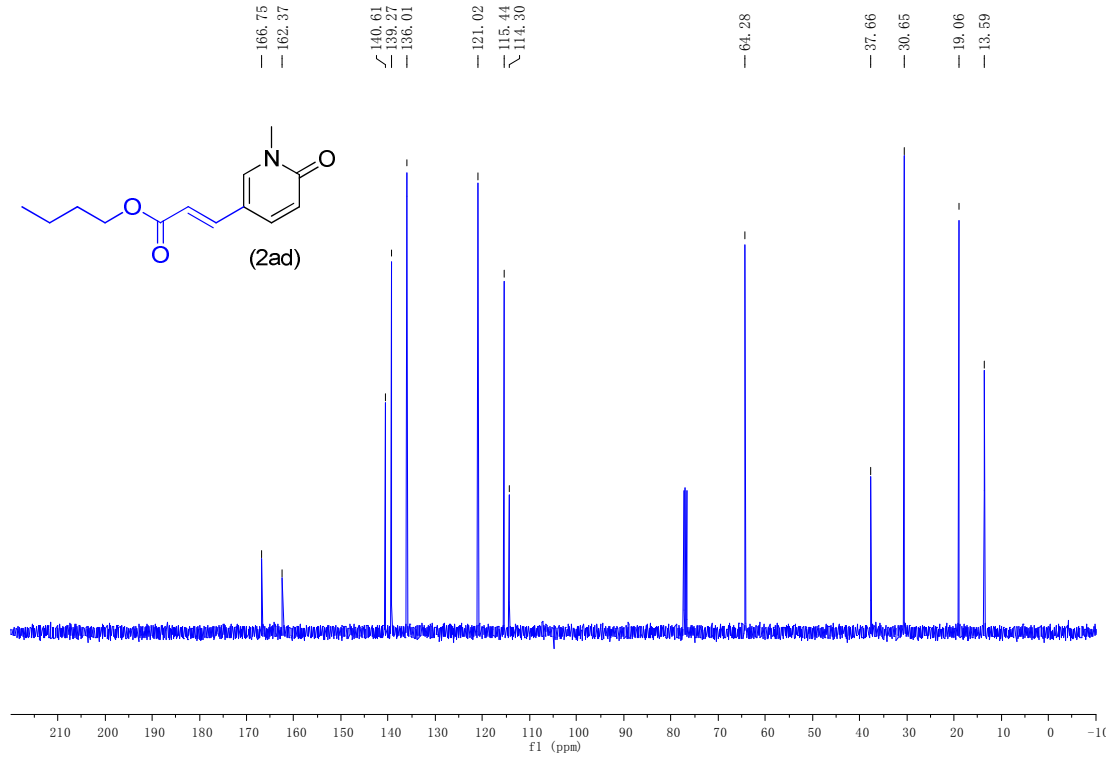

7.60
7.59
7.58
7.57
7.48
7.47
7.42
7.39
6.62
6.60
6.16
6.13
3.78
3.57
(2ab)
1.04
1.04
0.97
1.01
1.00
3.00
2.98
f1 (ppm)

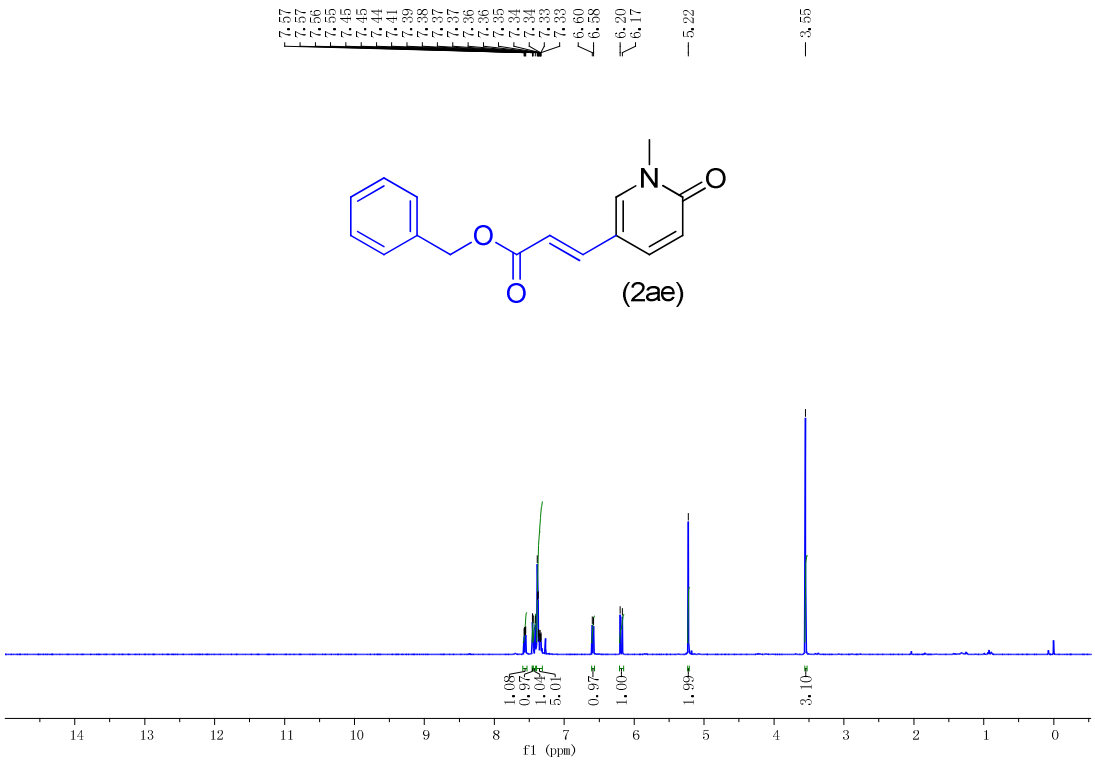

167.10
162.37
140.78
139.60
135.97
120.98
114.83
114.19
51.54
37.70
(2ab)
f1 (ppm)

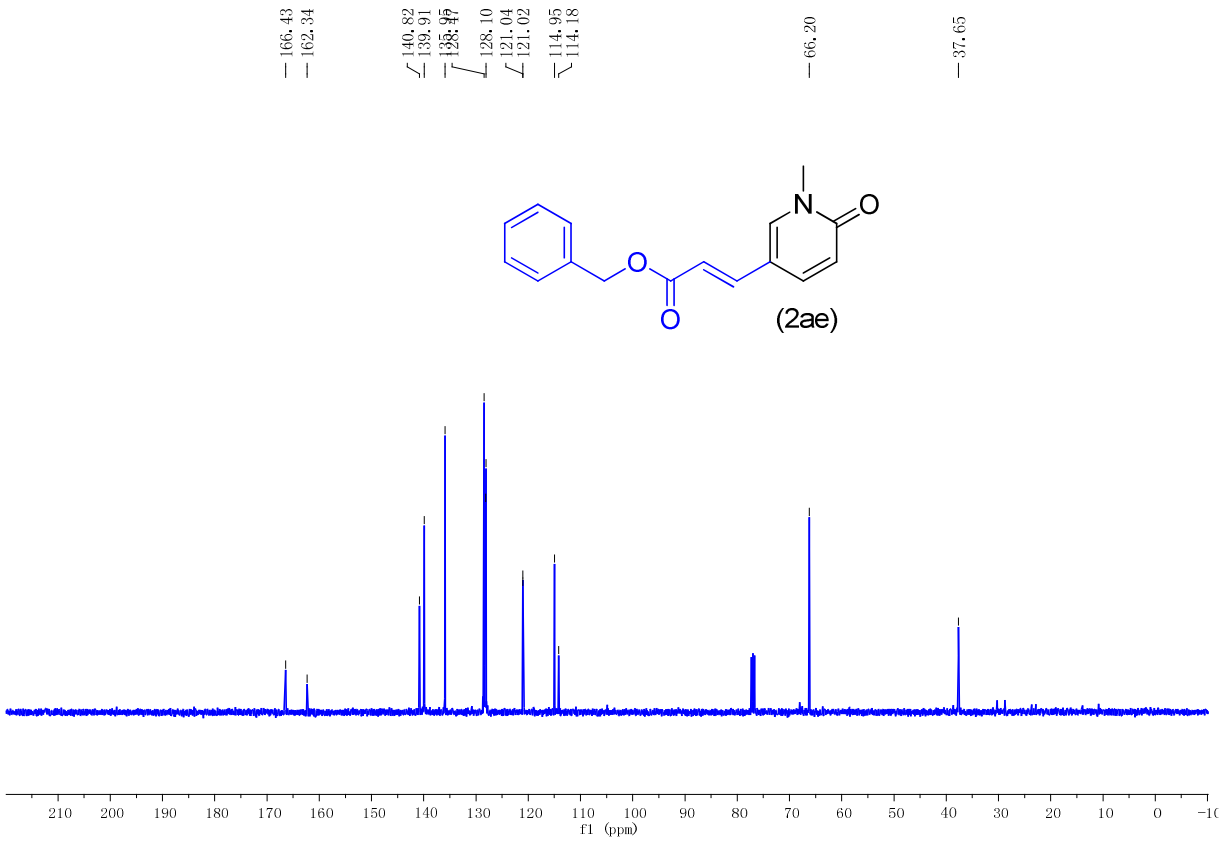

7.61
7.59
7.51
7.42
7.38
6.62
6.59
6.17
6.13
4.27
4.25
4.23
4.21
3.58
1.34
1.32
1.30
(2ac)
1.01
1.00
1.00
1.01
1.00
1.99
3.00
3.06
f1 (ppm)

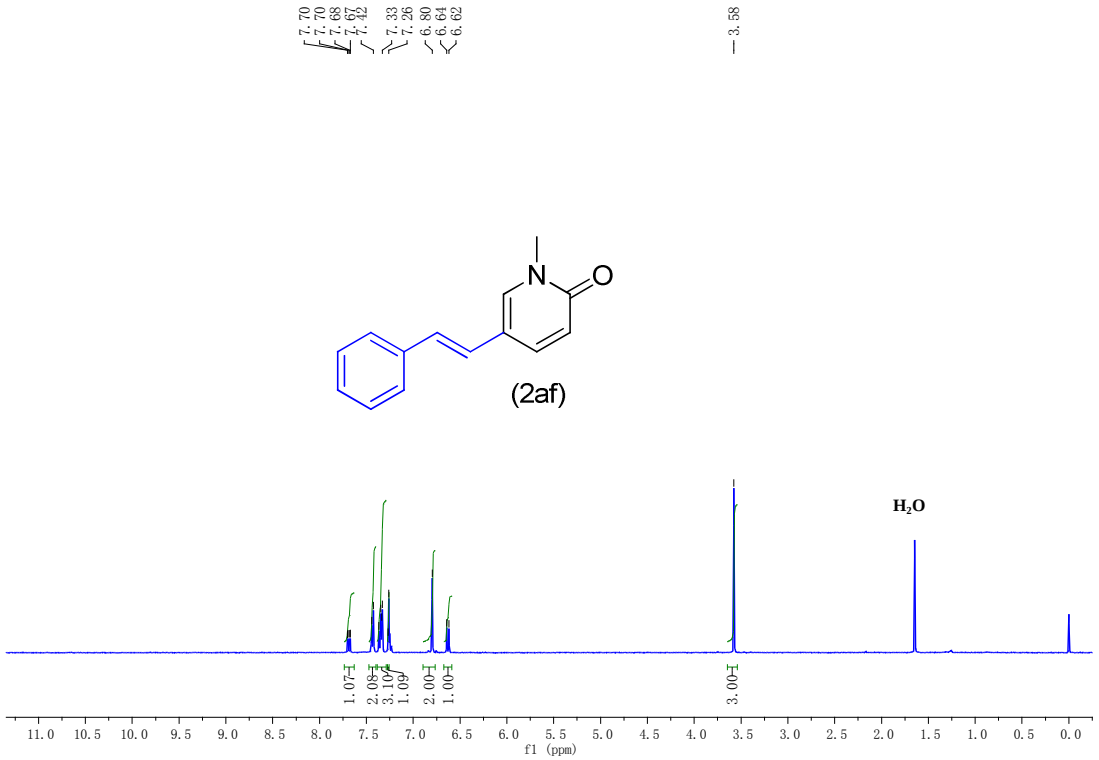

166.68
162.39
140.68
139.31
135.98
121.00
115.34
114.26
60.36
37.73
14.19
(2ac)
f1 (ppm)

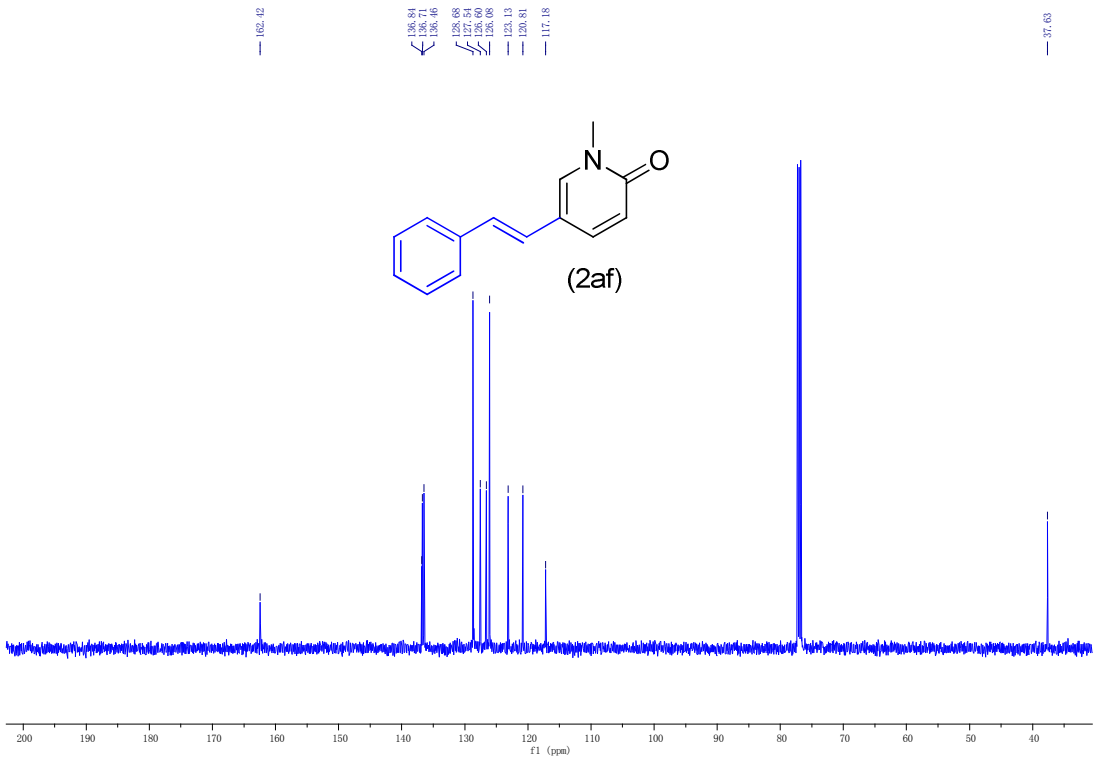

7.60
7.60
7.58
7.58
7.48
7.47
7.41
7.38
6.62
6.60
6.16
6.13
4.20
4.19
4.17
3.57
1.70
1.69
1.67
1.66
1.64
1.42
0.97
0.96
0.94
N
O
O
O
(2ad)
1.00
0.99
0.96
1.00
0.96
2.04
3.10
2.05
2.09
3.03
f1 (ppm)

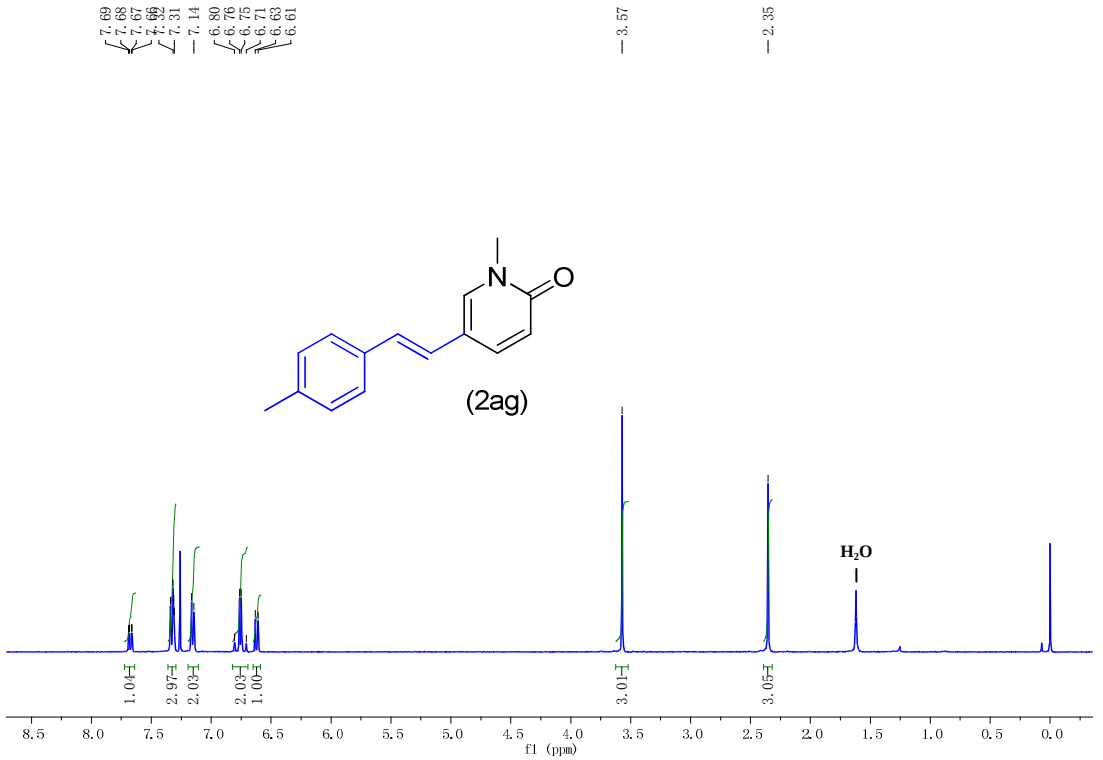

166.75
162.37
140.61
139.27
136.01
121.02
115.44
114.30
64.28
37.66
30.65
19.06
13.59
N
O
O
O
(2ad)
f1 (ppm)

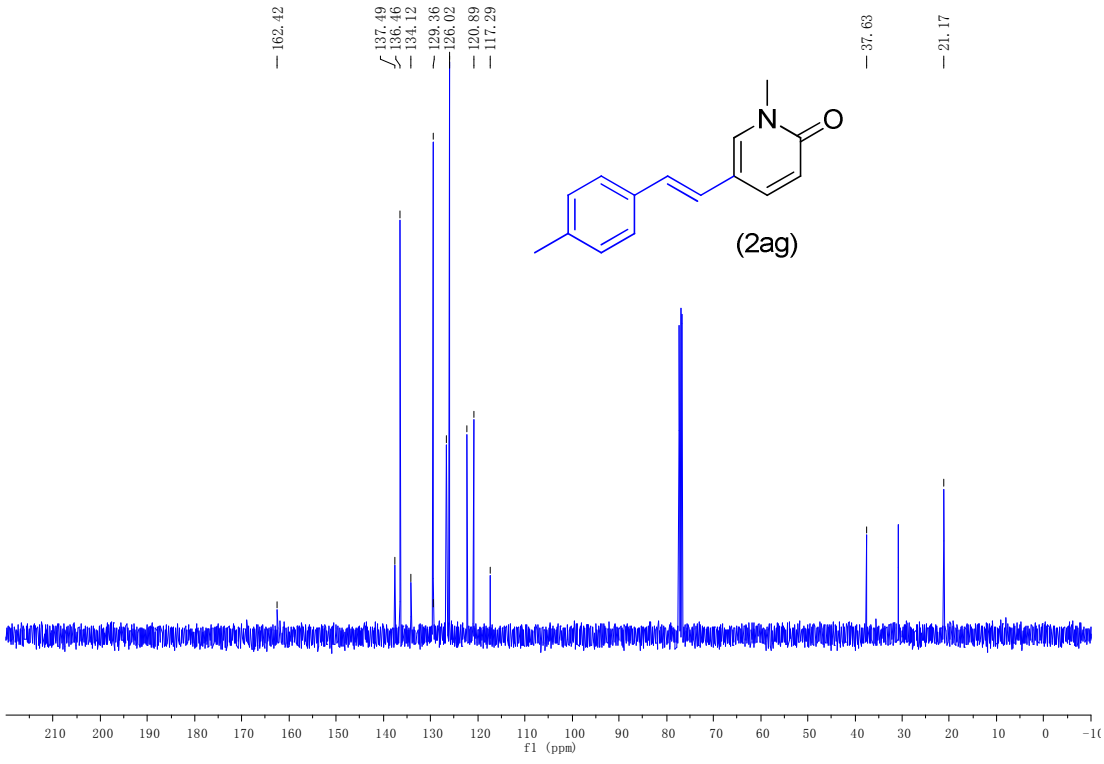

7.57
7.57
7.56
7.55
7.45
7.44
7.41
7.39
7.38
7.37
7.37
7.36
7.36
7.35
7.34
7.34
7.33
6.60
6.58
6.20
6.17
5.22
3.55
(2ae)
1.08
0.97
1.04
5.01
0.97
1.00
1.99
3.10
f1 (ppm)

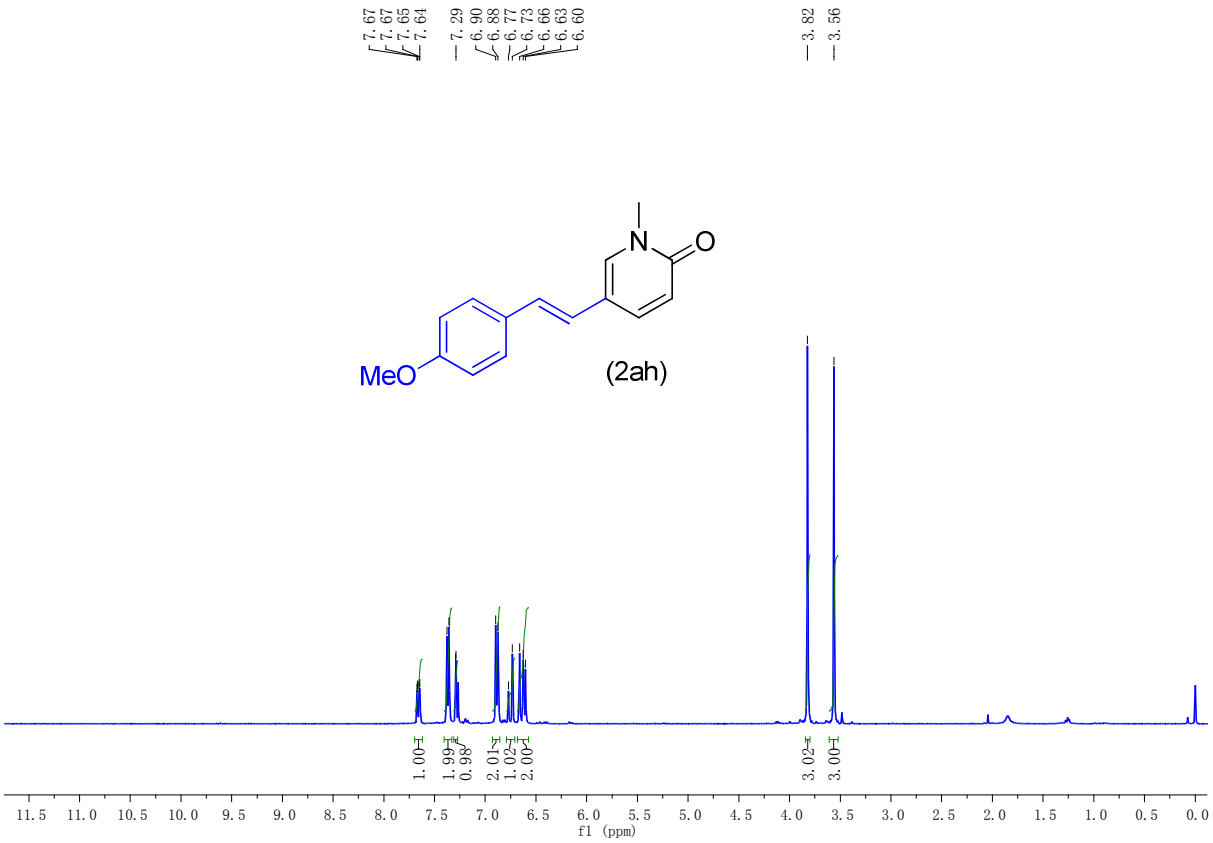

166.43
162.34
140.82
139.91
128.10
121.04
121.02
114.95
114.18
66.20
37.65
(2ae)
f1 (ppm)

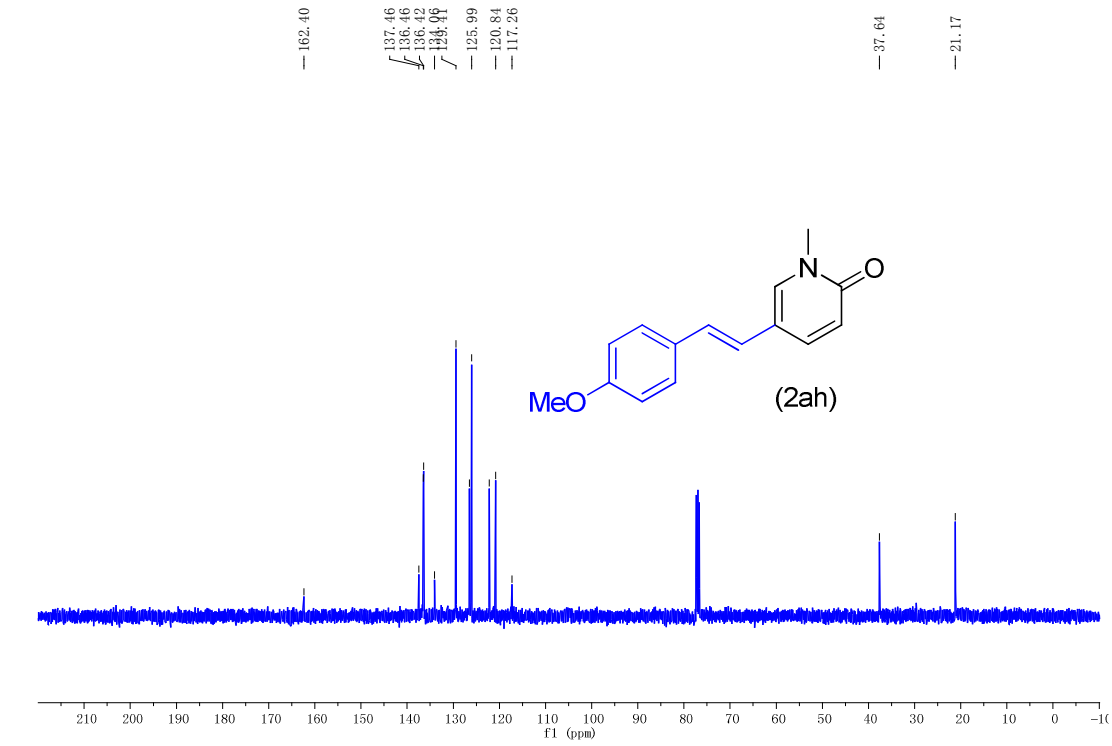

7.70
7.70
7.68
7.67
7.42
7.33
7.26
6.80
6.64
6.62
3.58
N
O
(2af)
H2O
1.07
2.08
3.10
1.09
2.00
1.00
3.00
f1 (ppm)

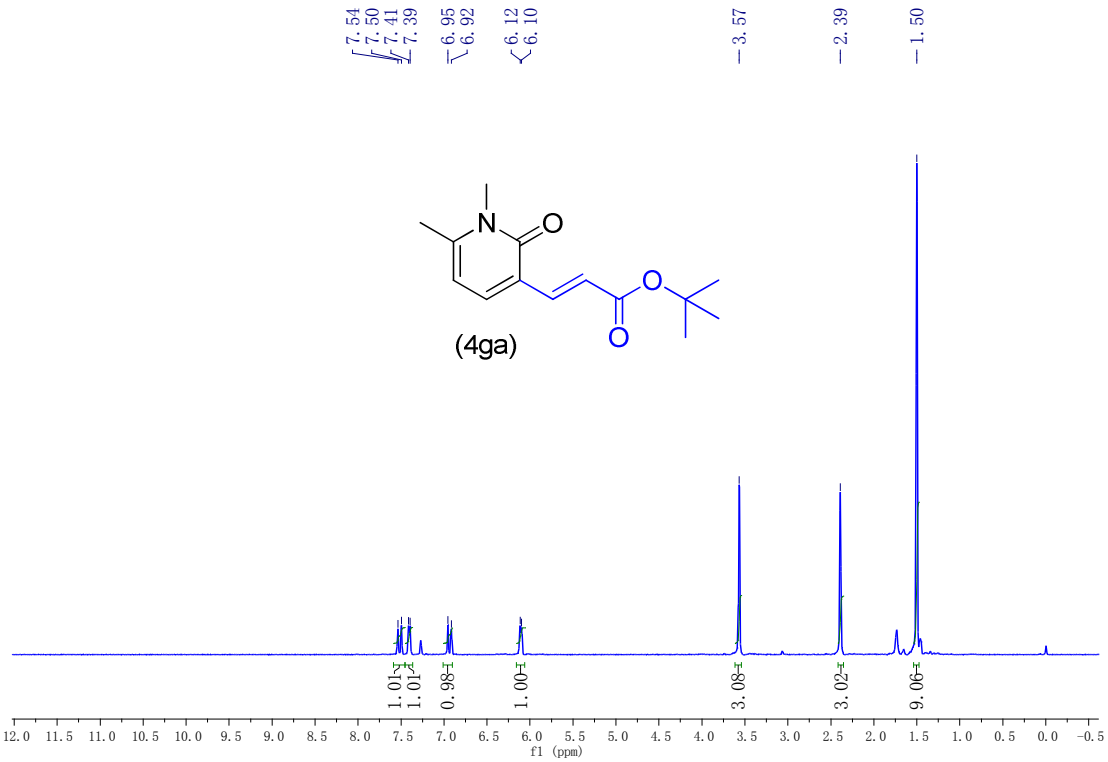

162.42
136.84
136.71
136.46
128.68
127.54
126.60
126.08
123.13
120.81
117.18
37.63
N
O
(2af)
f1 (ppm)

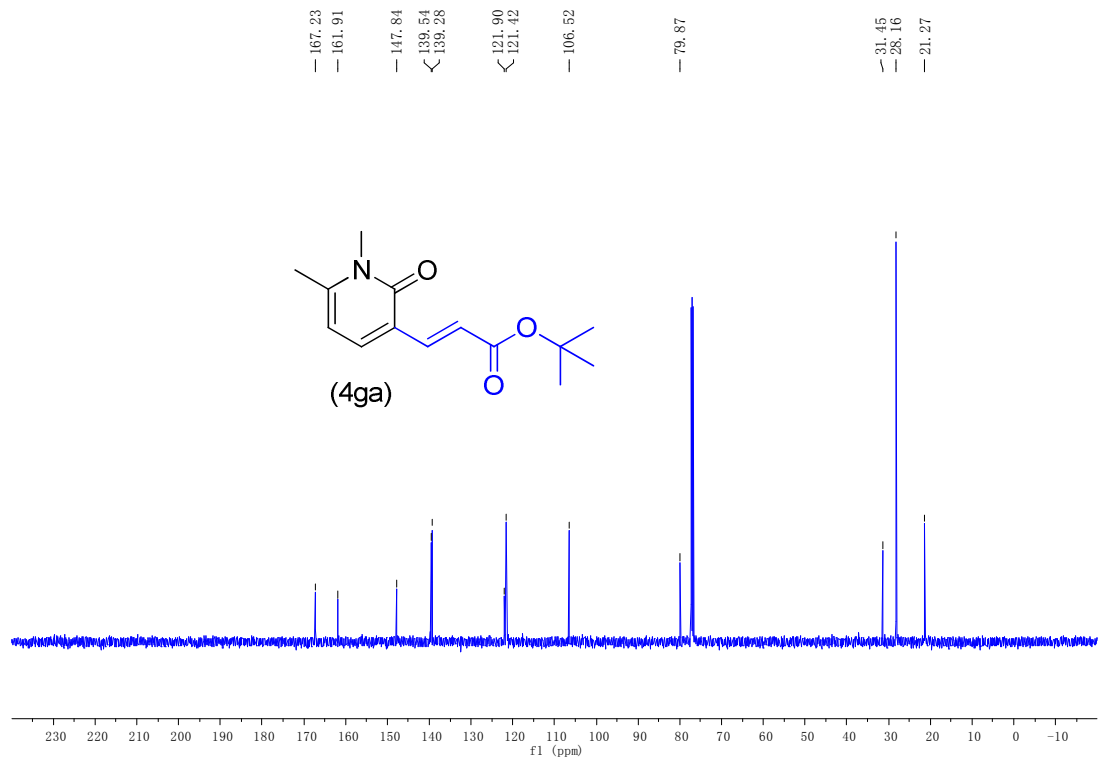

7.69
7.68
7.67
7.32
7.31
7.14
6.80
6.76
6.75
6.71
6.63
6.61
3.57
2.35
N
O
(2ag)
H2O
1.04
2.97
2.03
2.03
1.00
3.01
3.05
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

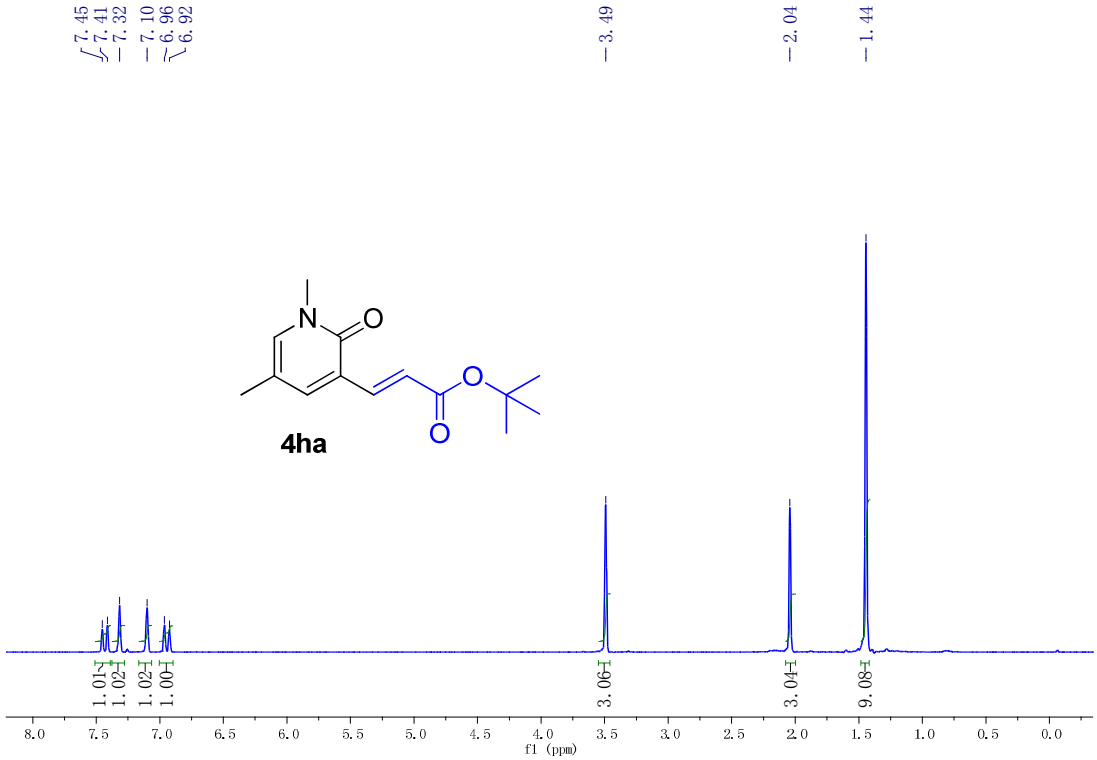

162.42
137.49
136.46
134.12
129.36
126.02
120.89
117.29
37.63
21.17
N
O
(2ag)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

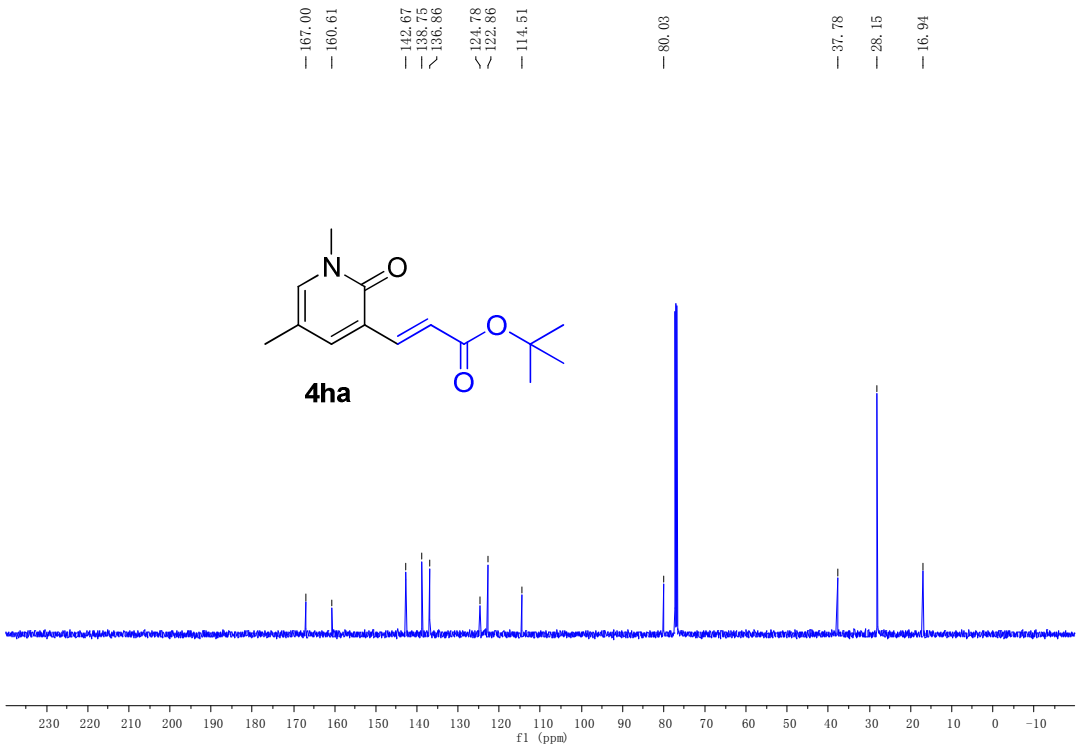

7.67
7.67
7.65
7.64
7.29
6.90
6.88
6.77
6.73
6.66
6.63
6.60
3.82
3.56
MeO
(2ah)
1.00
1.99
0.98
2.01
1.02
2.00
3.02
3.00
f1 (ppm)

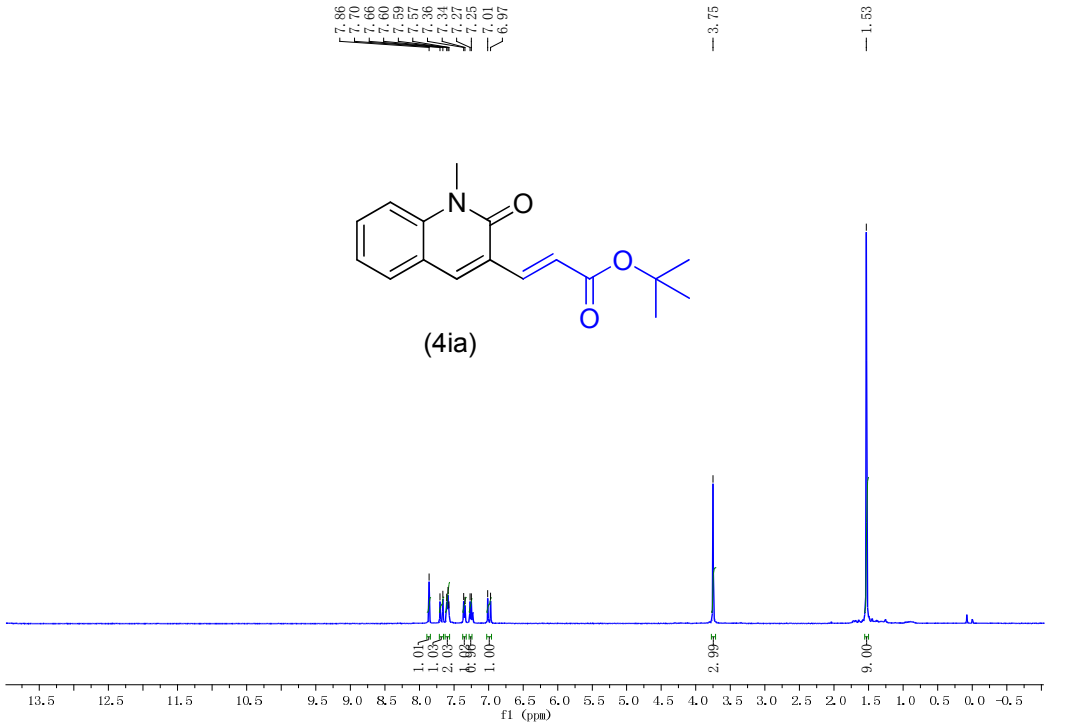

162.40
137.46
136.46
136.42
125.99
120.84
117.26
37.64
21.17
MeO
(2ah)
f1 (ppm)

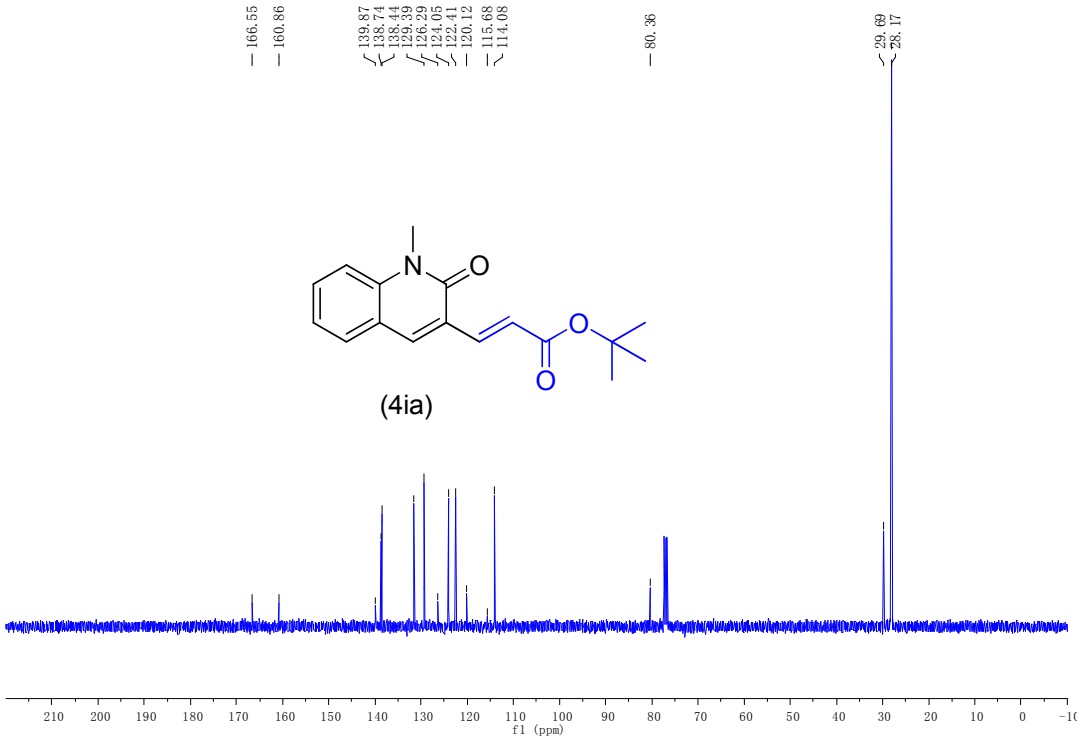

7.54
7.50
7.41
7.39
6.95
6.92
6.12
6.10
3.57
2.39
1.50
(4ga)
1.01
1.01
0.98
1.00
3.08
3.02
9.06
f1 (ppm)

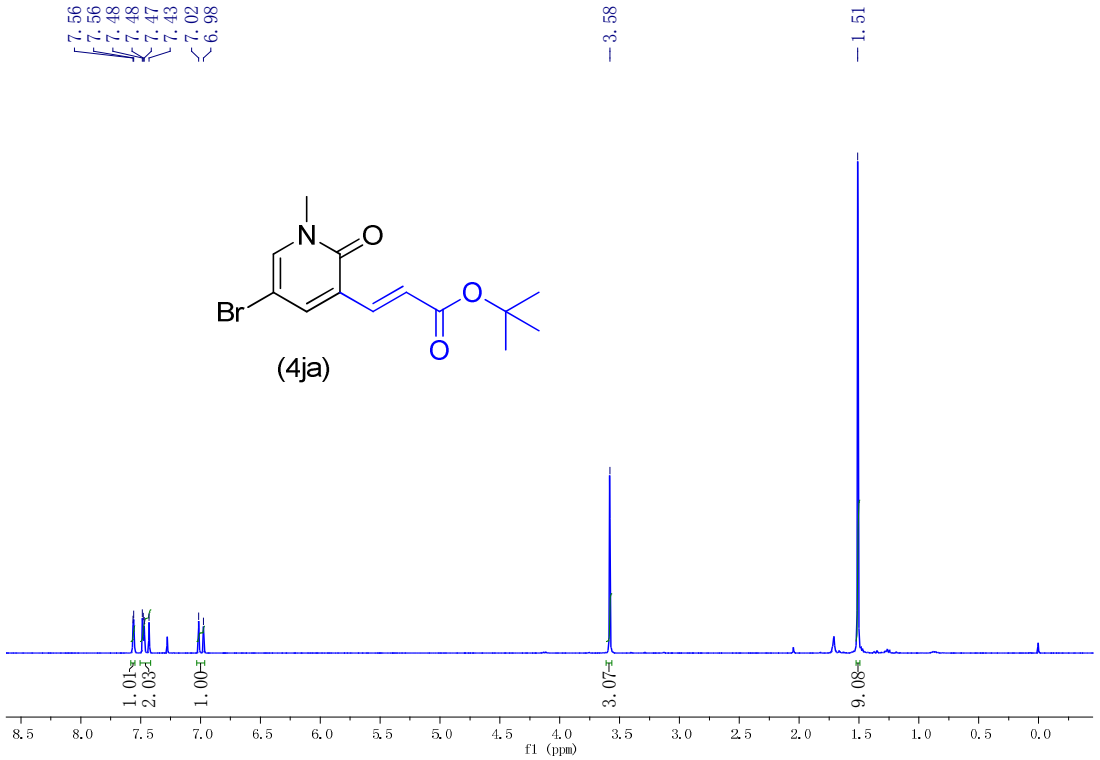

167.23
161.91
147.84
139.54
139.28
121.90
121.42
106.52
79.87
31.45
28.16
21.27
(4ga)
f1 (ppm)

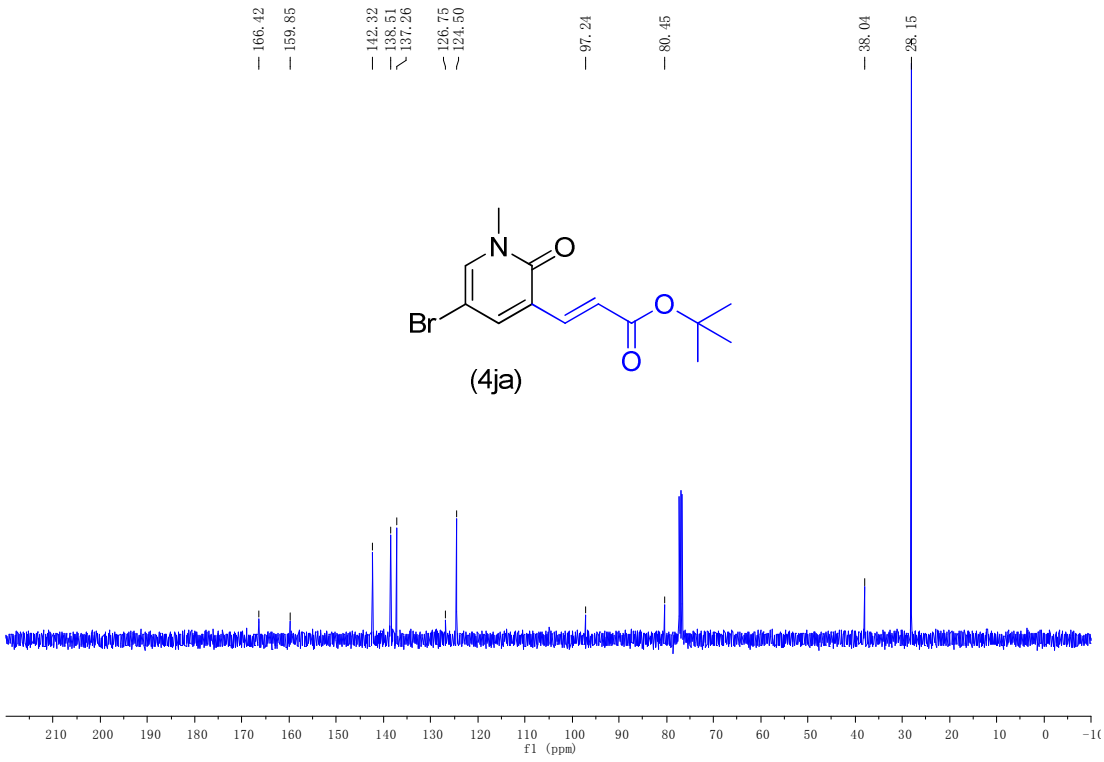

7.45
7.41
7.32
7.10
6.96
6.92
3.49
2.04
1.44
4ha
1.01
1.02
1.02
1.00
3.06
3.04
9.08
f1 (ppm)

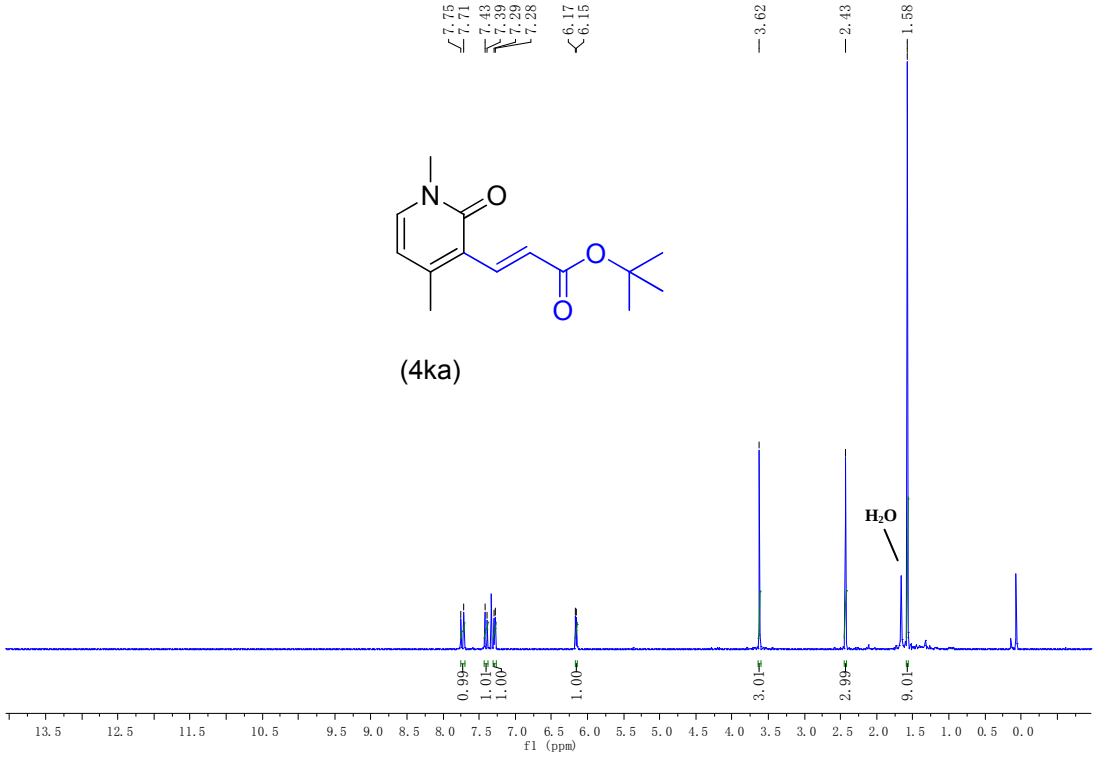

167.00
160.61
142.67
138.75
136.86
124.78
122.86
114.51
80.03
37.78
28.15
16.94
4ha
f1 (ppm)

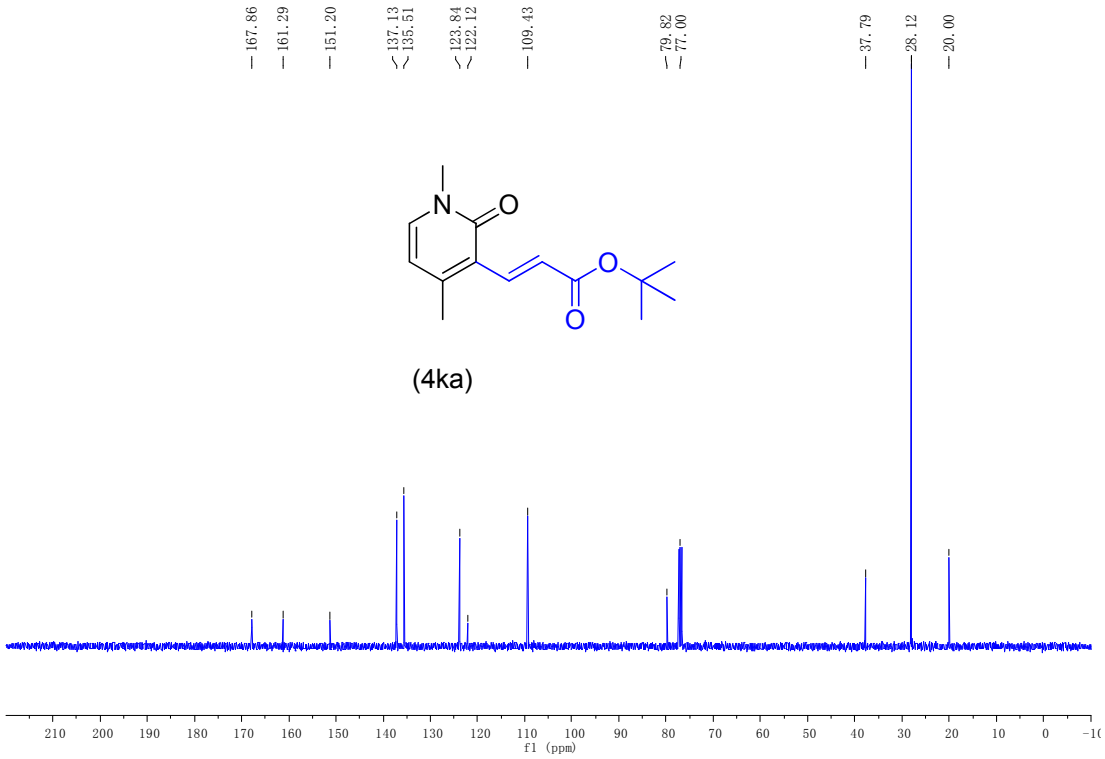

7.86
7.70
7.66
7.60
7.59
7.57
7.36
7.34
7.27
7.25
7.01
6.97
3.75
1.53
N
O
O
O
(4ia)
1.01
1.03
2.03
0.90
1.00
2.99
9.00
f1 (ppm)

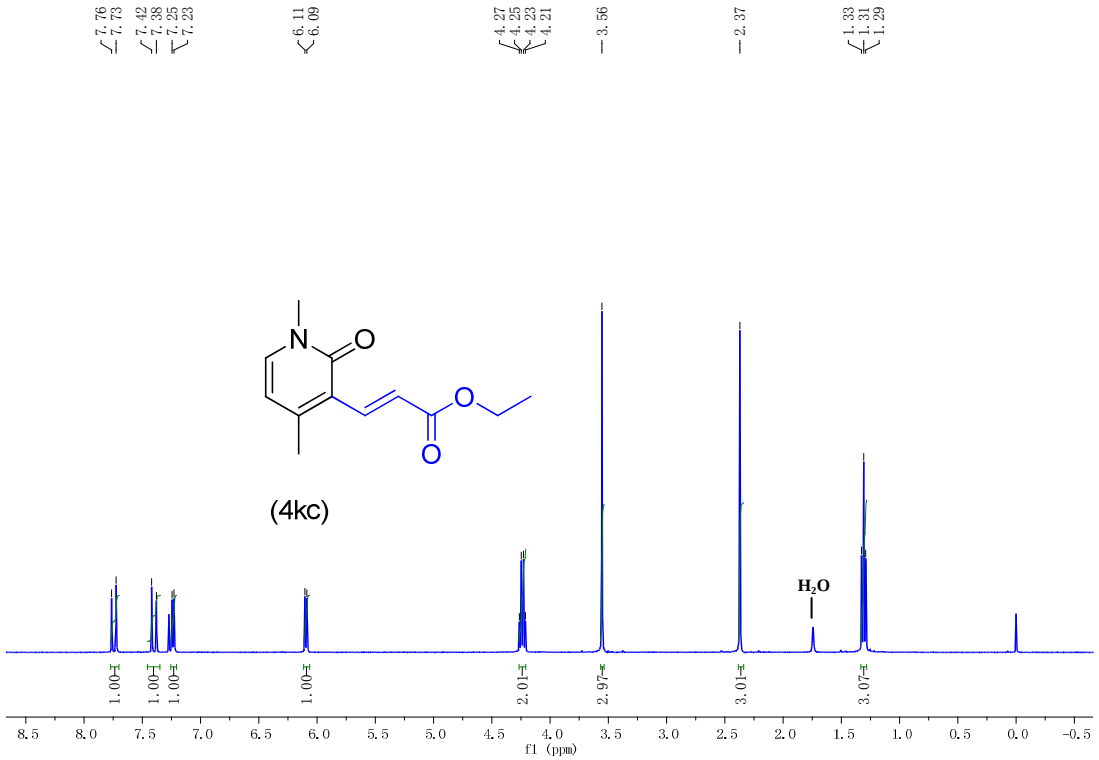

166.55
160.86
139.87
138.74
138.44
129.39
126.29
124.05
122.41
120.12
115.68
114.08
80.36
29.69
28.17
N
O
O
O
(4ia)
f1 (ppm)

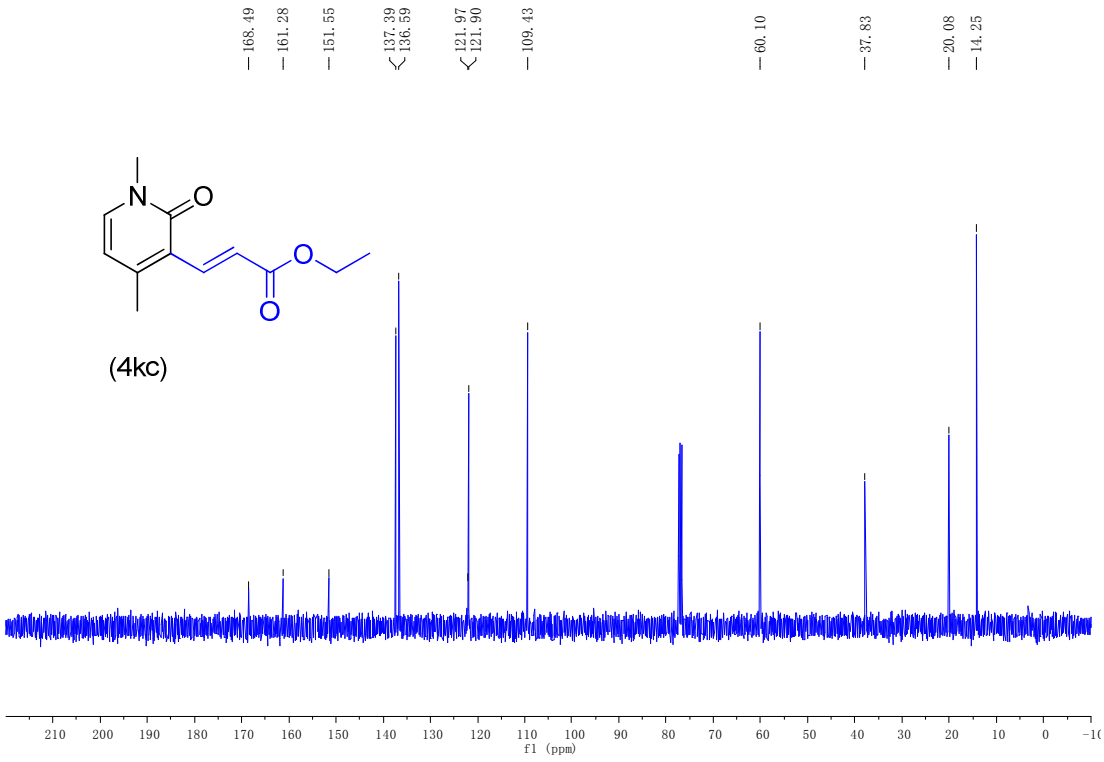

7.56
7.56
7.48
7.48
7.47
7.43
7.02
6.98
3.58
1.51
N
O
Br
O
O
(4ja)
1.01
2.03
1.00
3.07
9.08
f1 (ppm)

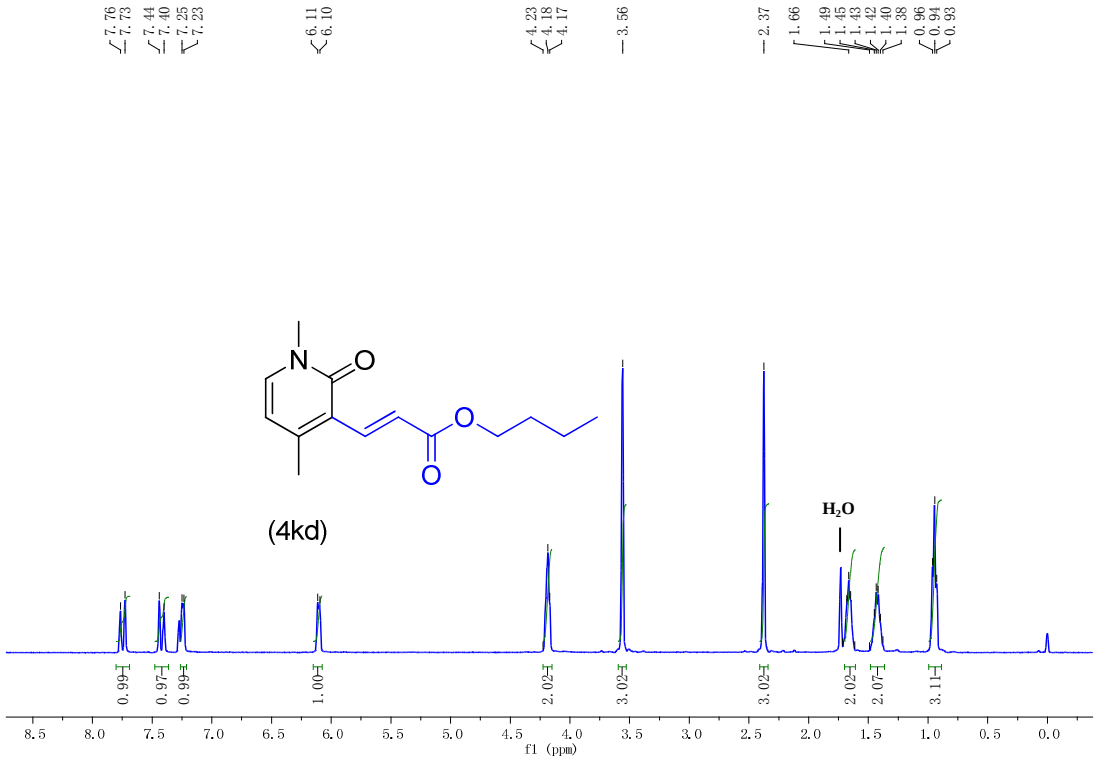

166.42
159.85
142.32
138.51
137.26
126.75
124.50
97.24
80.45
38.04
28.15
N
O
Br
O
O
(4ja)
f1 (ppm)

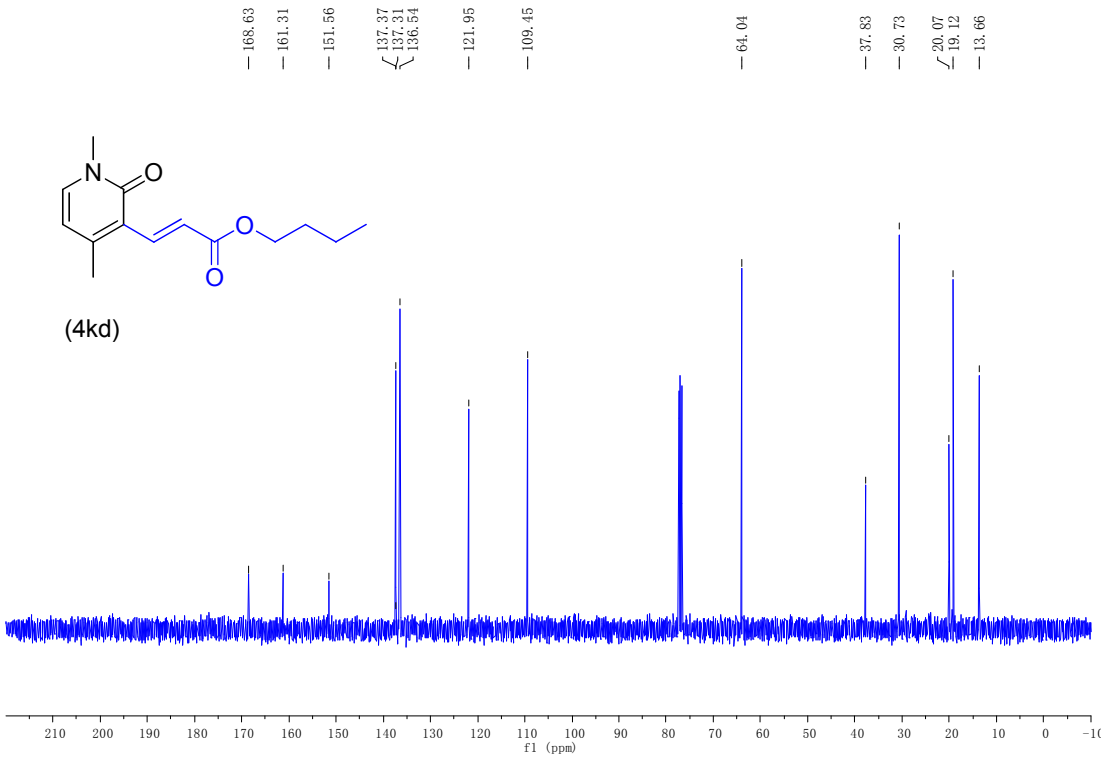

7.75
7.71
7.43
7.39
7.29
7.28
6.17
6.15
3.62
2.43
1.58
N
O
O
O
(4ka)
H2O
0.99
1.01
1.00
1.00
3.01
2.99
9.01
f1 (ppm)

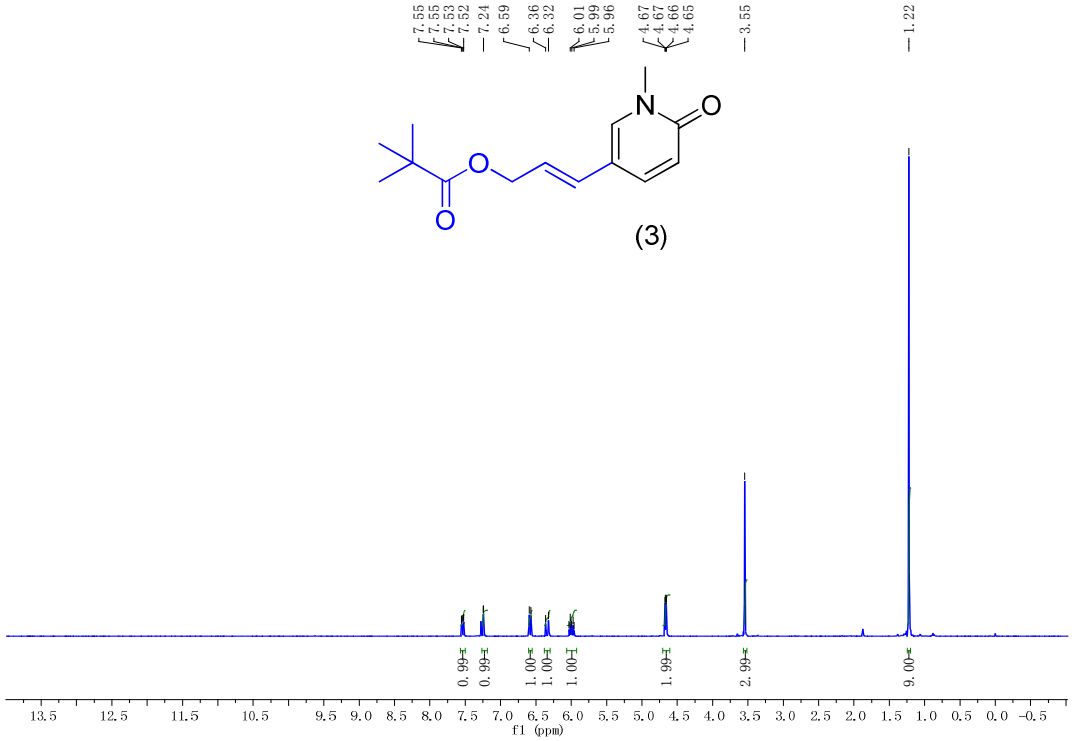

167.86
161.29
151.20
137.13
135.51
123.84
122.12
109.43
79.82
77.00
37.79
28.12
20.00
N
O
O
O
(4ka)
f1 (ppm)

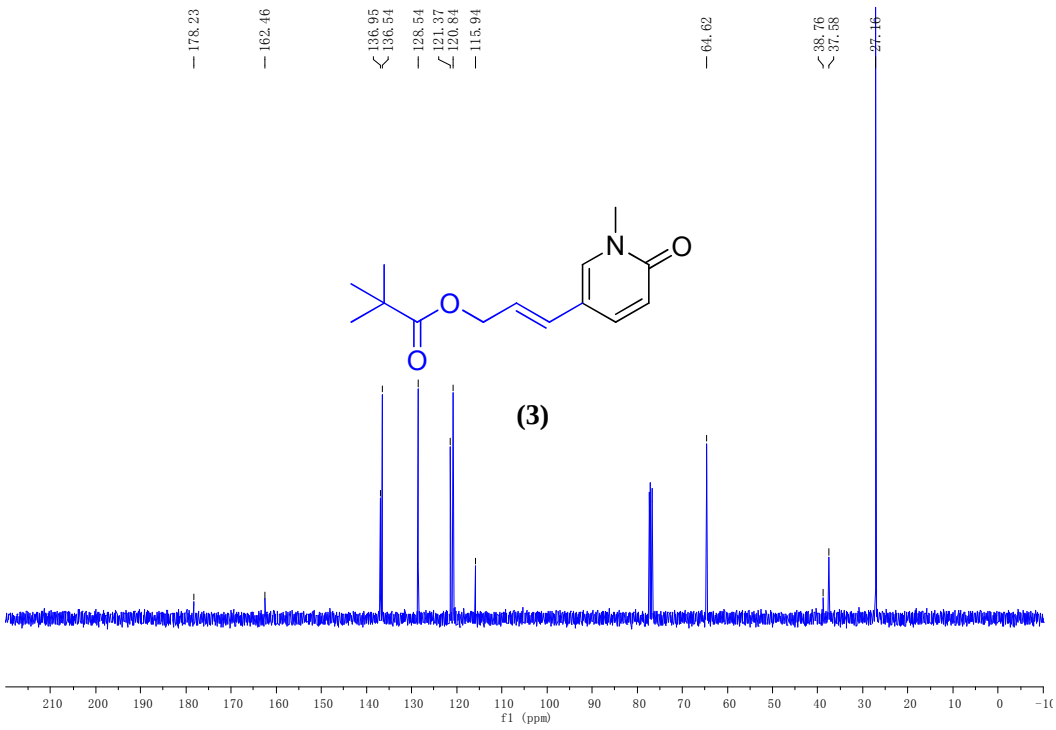

7.76
7.73
7.42
7.38
7.25
7.23
6.11
6.09
4.27
4.25
4.23
4.21
3.56
2.37
1.33
1.31
1.29
(4kc)
H2O
1.00
1.00
1.00
1.00
2.01
2.97
3.01
3.07
f1 (ppm)

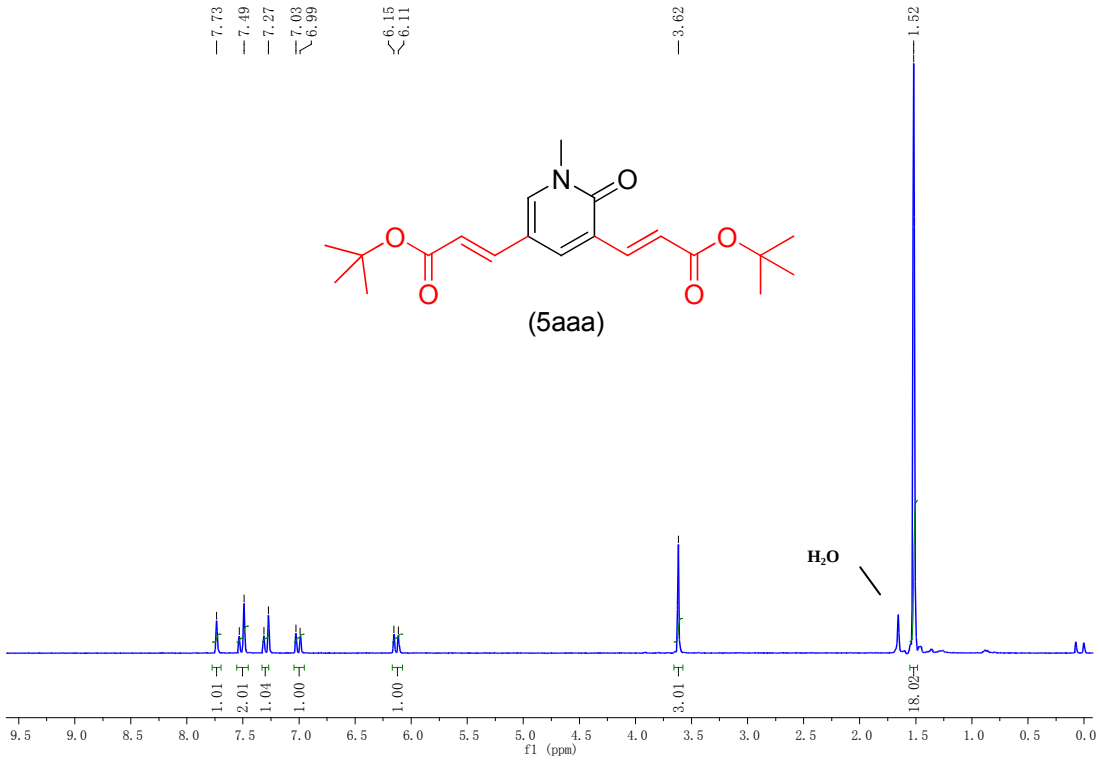

168.49
161.28
151.55
137.39
136.59
121.97
121.90
109.43
60.10
37.83
20.08
14.25
(4kc)
f1 (ppm)


7.76
7.73
7.44
7.40
7.25
7.23
6.11
6.10
4.23
4.18
4.17
3.56
2.37
1.66
1.49
1.45
1.43
1.42
1.40
1.38
0.96
0.94
0.93
(4kd)
H2O
0.99
0.97
0.99
1.00
2.02
3.02
3.02
2.02
2.07
3.11
f1 (ppm)

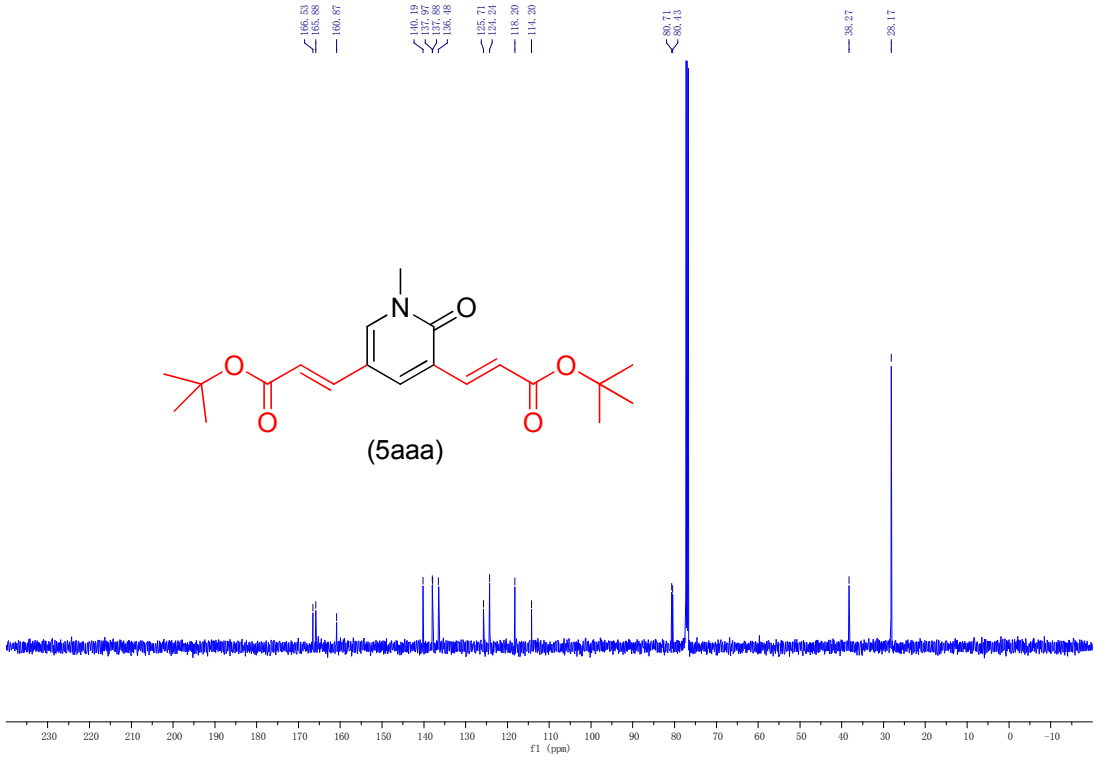

168.63
161.31
151.56
137.37
137.31
136.54
121.95
109.45
64.04
37.83
30.73
20.07
19.12
13.66
(4kd)
f1 (ppm)


7.55
7.55
7.53
7.52
7.24
6.59
6.36
6.32
6.01
5.99
5.96
4.67
4.67
4.66
4.65
3.55
1.22
N
O
O
O
(3)
0.99
0.99
1.00
1.00
1.00
1.99
2.99
9.00
f1 (ppm)


178.23
162.46
136.95
136.54
128.54
121.37
120.84
115.94
64.62
38.76
37.58
27.16
N
O
O
O
(3)
f1 (ppm)


7.73
7.49
7.27
7.03
6.99
6.15
6.11
3.62
1.52
(5aaa)
H2O
1.01
2.01
1.04
1.00
1.00
3.01
18.02
f1 (ppm)

\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165.98
160.87
140.19
137.97
137.88
136.48
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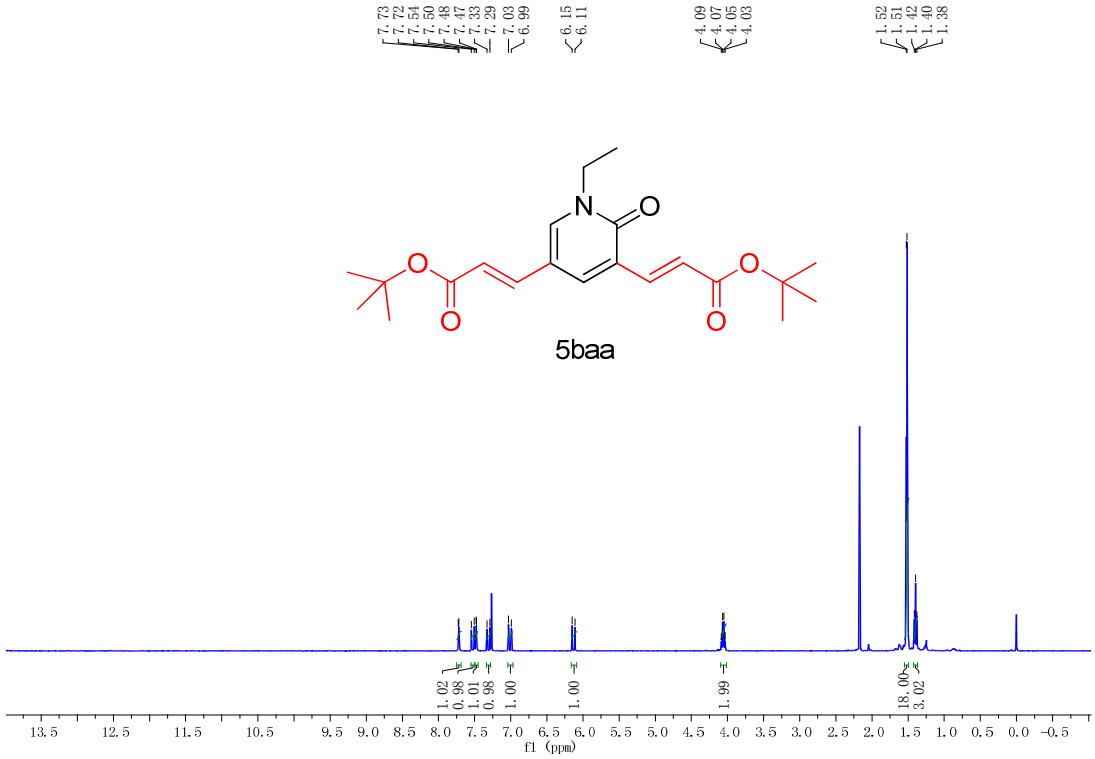
124.24
118.20
114.20
80.71
80.43
38.27
28.17
(5aaa)
f1 (ppm)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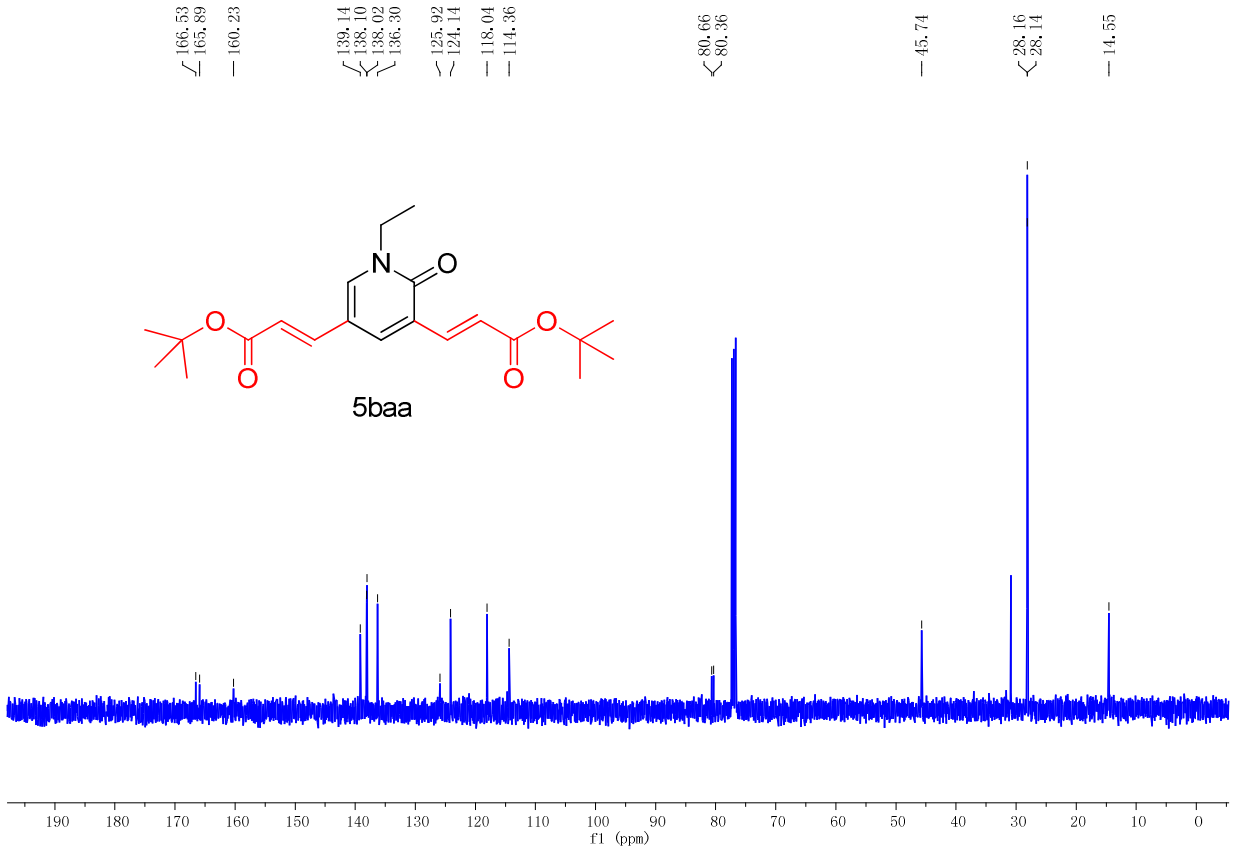
7.48
7.47
7.33
7.29
7.03
6.99
6.15
6.11
4.09
4.07
4.05
4.03
1.52
1.51
1.42
1.40
1.38
5baa
1.02
0.98
1.01
0.98
1.00
1.00
1.99
18.00
3.02
f1 (ppm)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139.14
138.10
138.02
136.30
125.92
124.14
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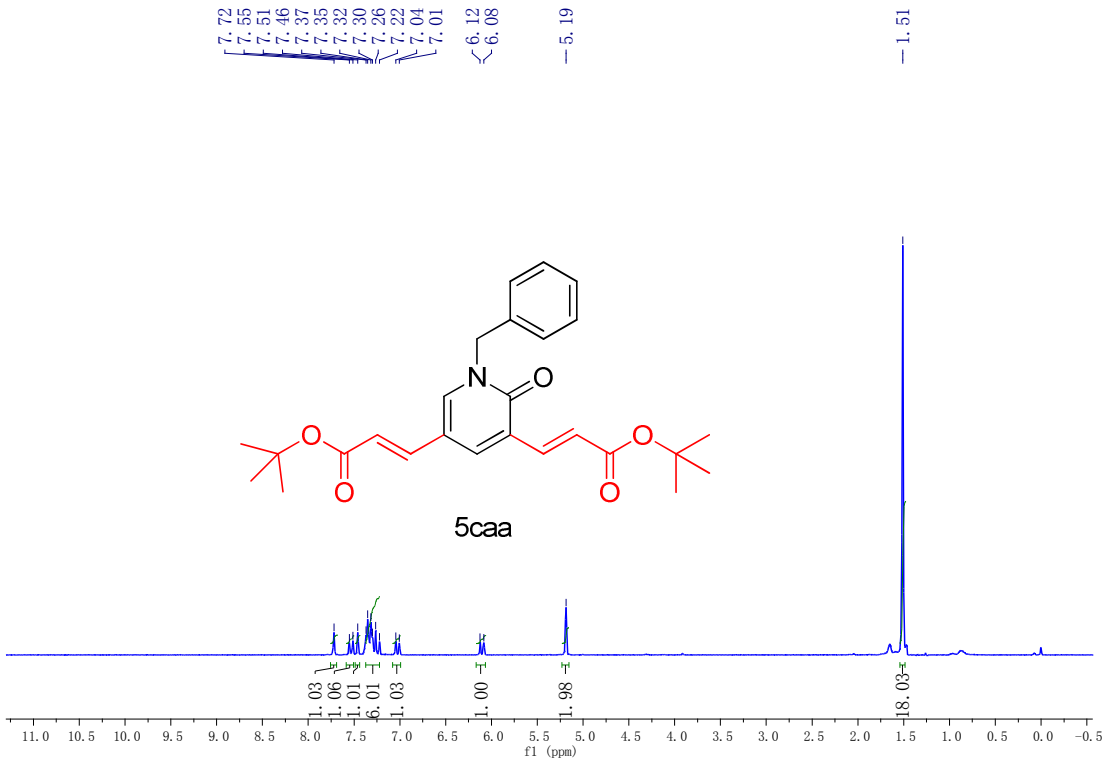
114.36
80.66
80.36
45.74
28.16
28.14
14.55
5baa
f1 (ppm)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7.55
7.51
7.46
7.37
7.35
7.32
7.30
7.26
7.22
7.04
7.01
6.12
6.08
5.19
1.51
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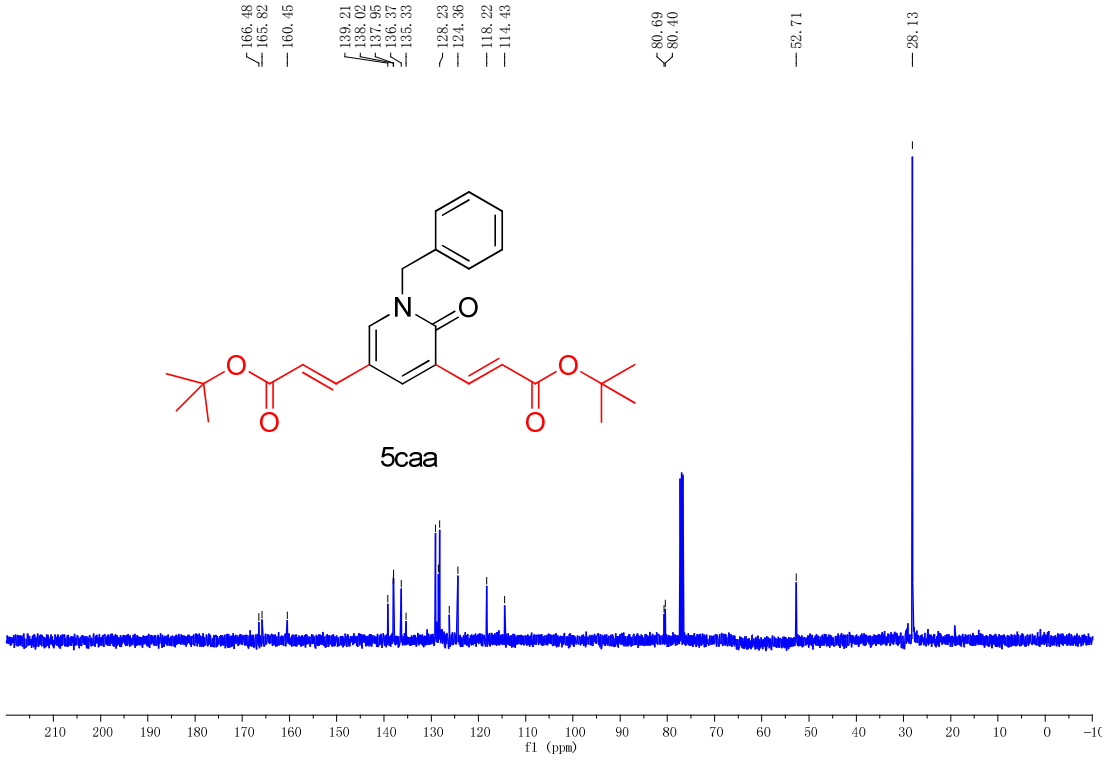
1.03
1.06
1.01
6.01
1.03
1.00
1.98
18.03
f1 (ppm)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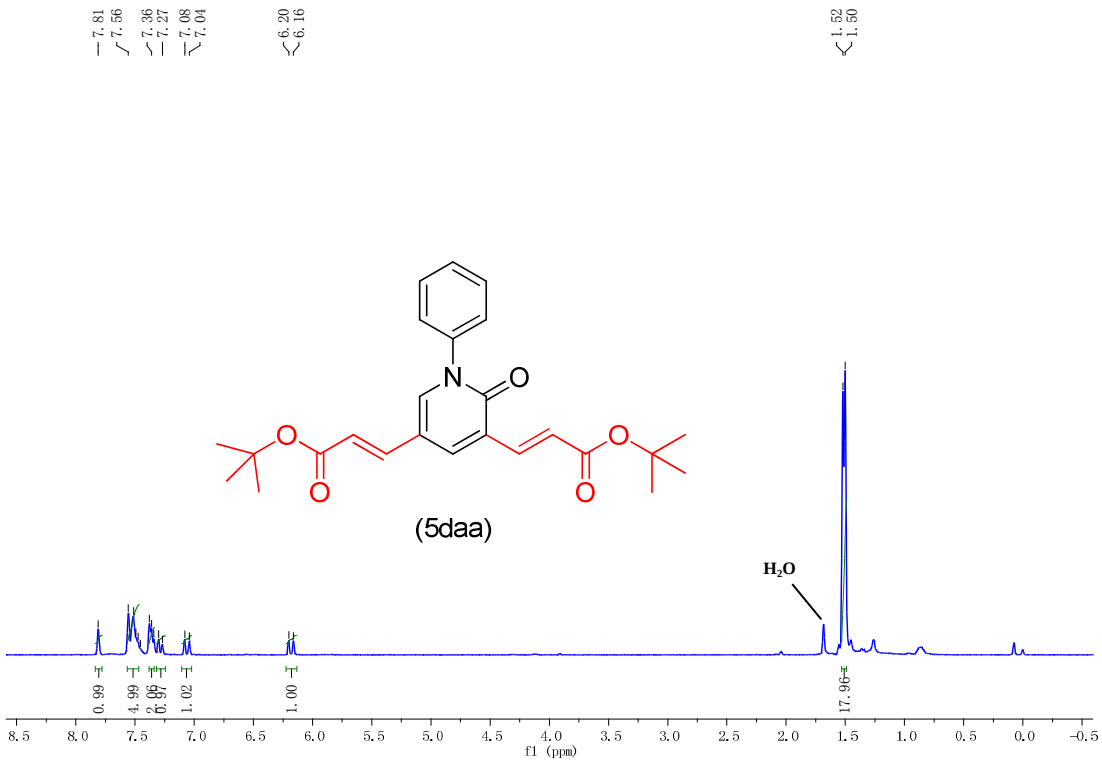
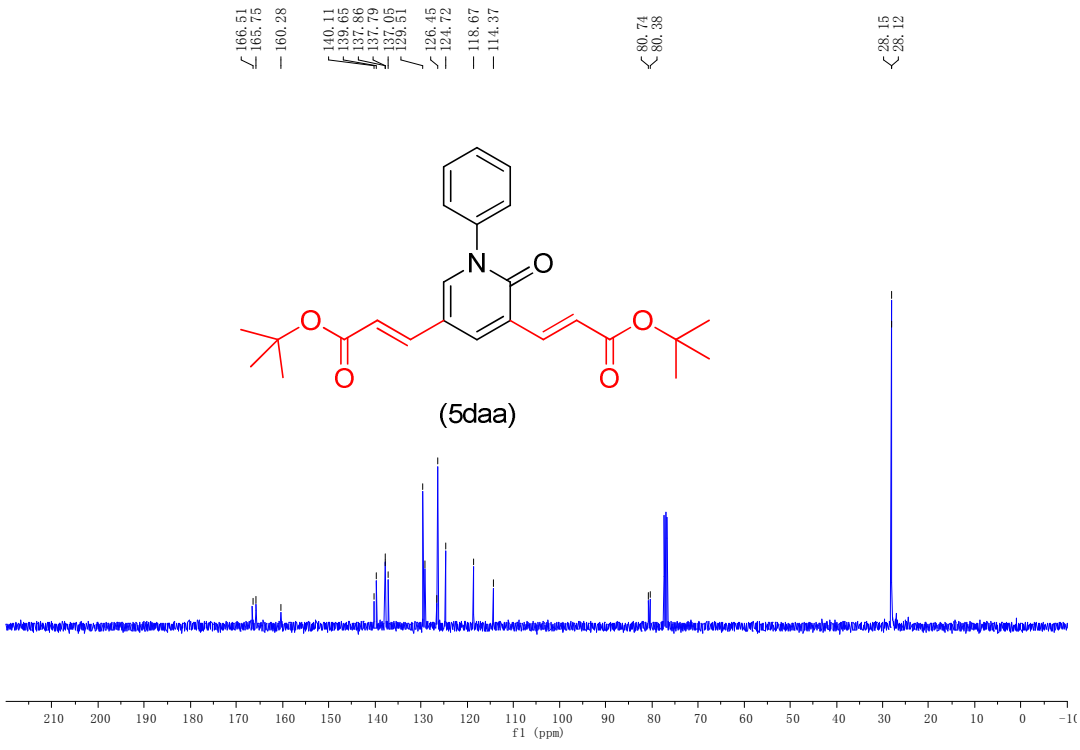
139.21
138.02
137.95
136.37
135.33
128.23
124.36
118.22
114.43
80.69
80.40
52.71
28.13
5caa
f1 (ppm)


7.81
7.56
7.36
7.27
7.08
7.04
6.20
6.16
1.52
1.50
(5daa)
H2O
0.99
4.99
2.06
0.97
1.02
1.00
17.96
f1 (ppm)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137.86
137.79
137.05
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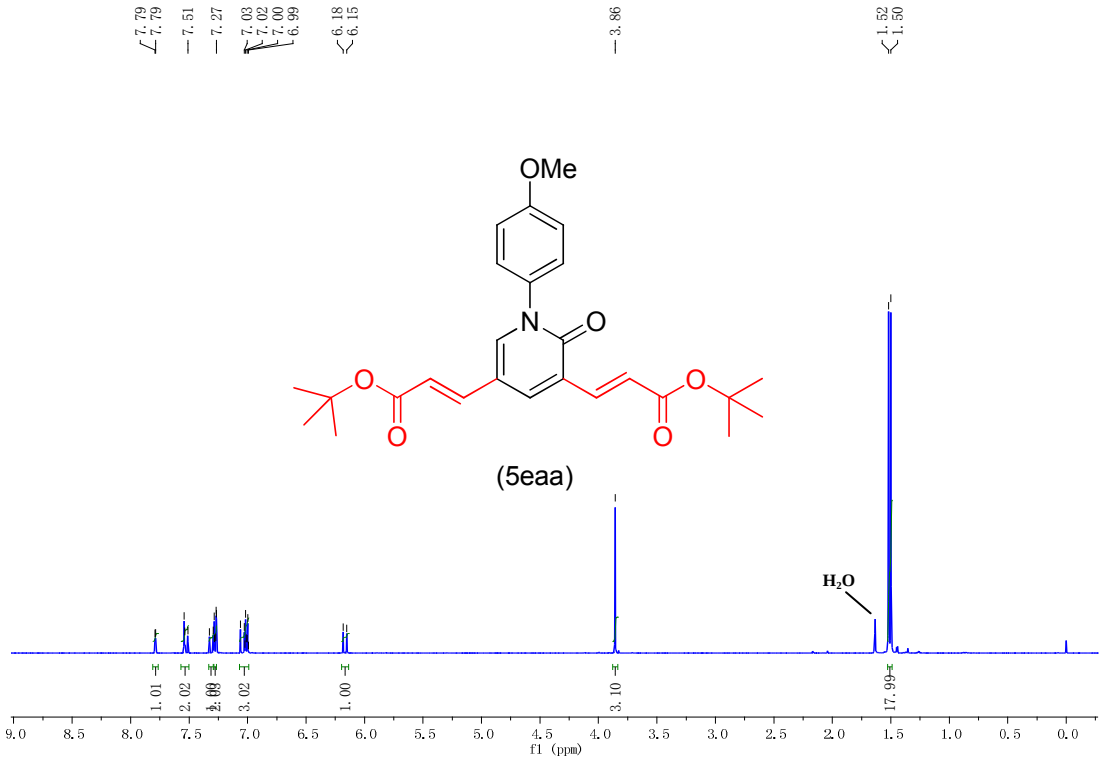
124.72
118.67
114.37
80.74
80.38
28.15
28.12
(5daa)
f1 (ppm)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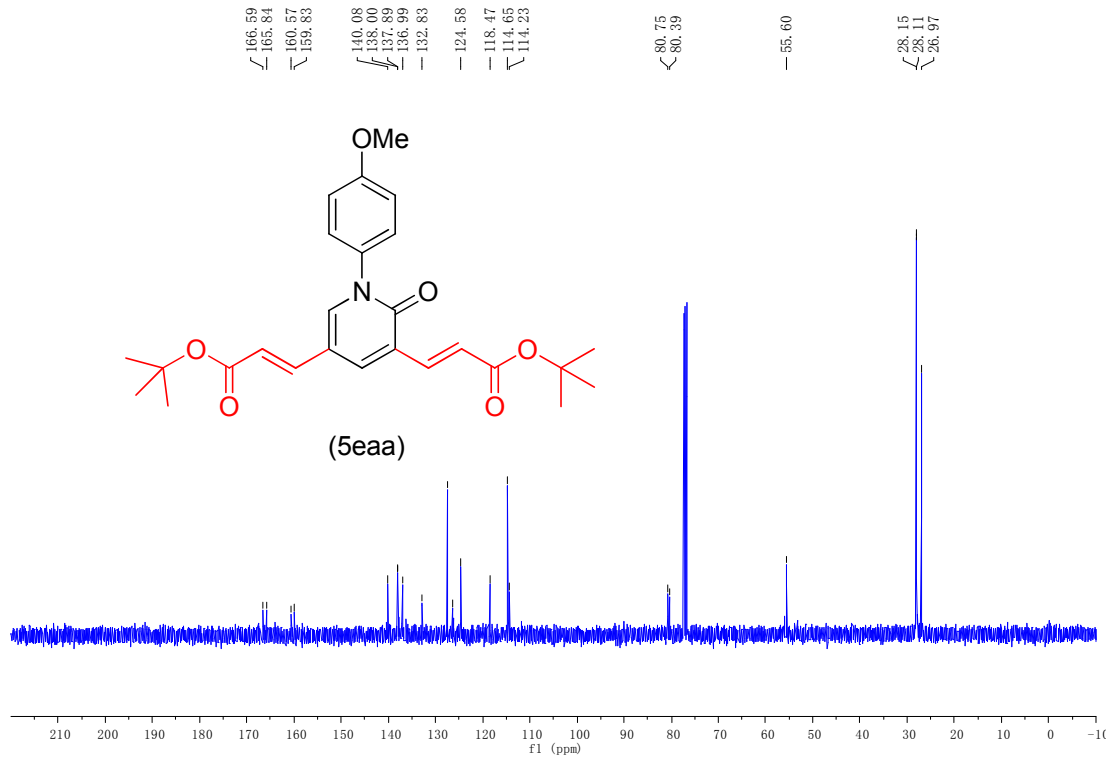
7.79
7.51
7.27
7.03
7.02
7.00
6.99
6.18
6.15
3.86
1.52
1.50
OMe
N
O
O
O
O
O
(5eaa)
H2O
1.01
2.02
3.02
1.00
3.10
17.99
f1 (ppm)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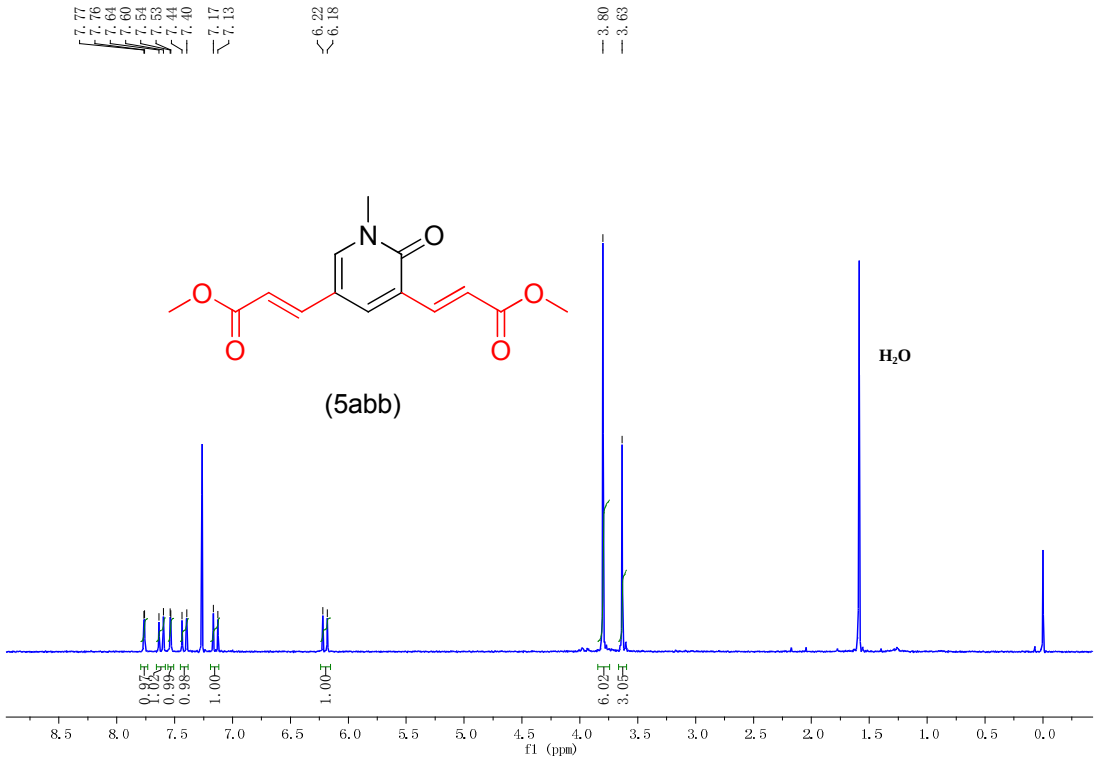
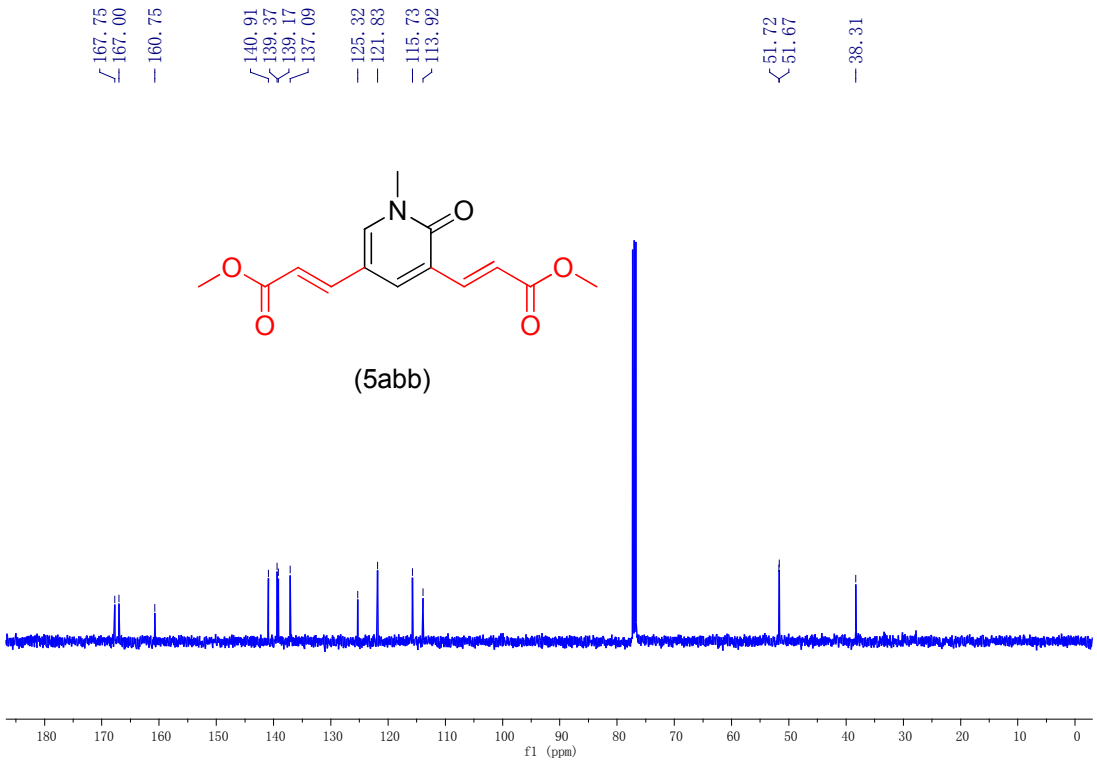
165.84
160.57
159.83
140.08
138.00
137.89
136.99
132.83
124.58
118.47
114.65
114.23
80.75
80.39
55.60
28.15
28.11
26.97
OMe
N
O
O
O
O
O
(5eaa)
f1 (ppm)


7.77
7.76
7.64
7.60
7.54
7.53
7.44
7.40
7.17
7.13
6.22
6.18
3.80
3.63
(5abb)
H2O
0.97
1.02
0.99
0.98
1.00
1.00
6.02
3.05
f1 (ppm)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167.00
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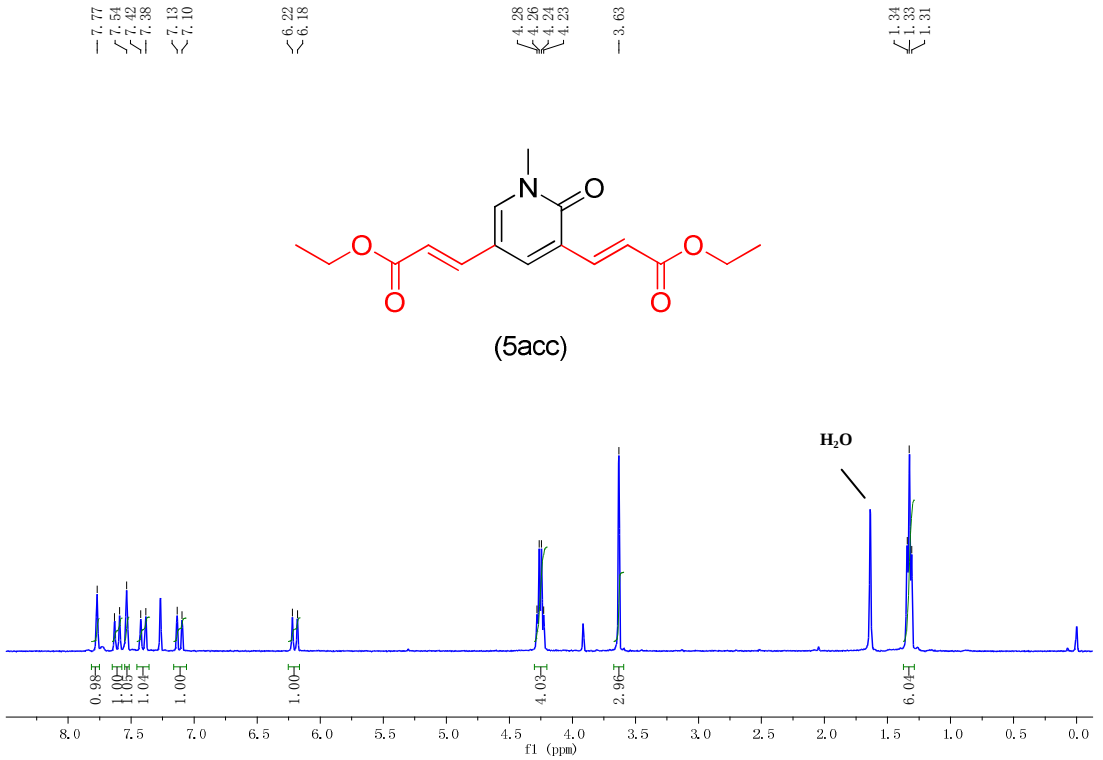
140.91
139.37
139.17
137.09
125.32
121.83
115.73
113.92
51.72
51.67
38.31
(5abb)
f1 (ppm)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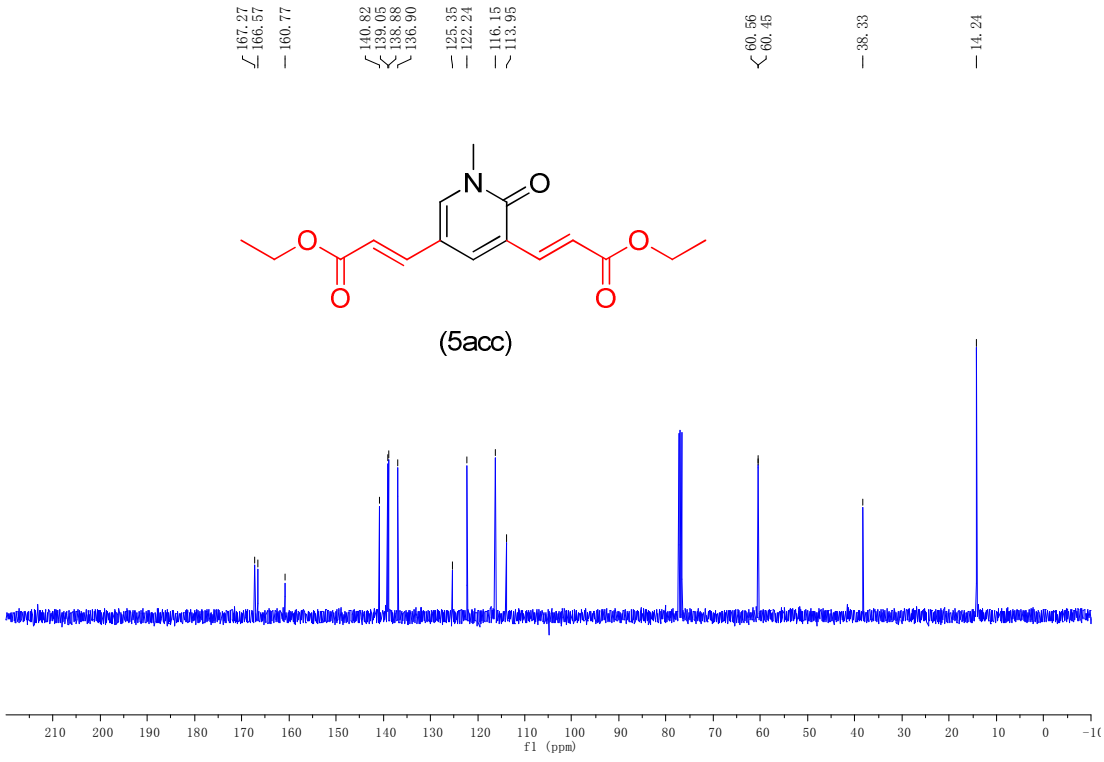
7.54
7.42
7.38
7.13
7.10
6.22
6.18
4.28
4.26
4.24
4.23
3.63
1.34
1.33
1.31
N
O
O
O
O
O
(5acc)
H2O
0.98
1.00
1.05
1.04
1.00
1.00
4.03
2.96
6.04
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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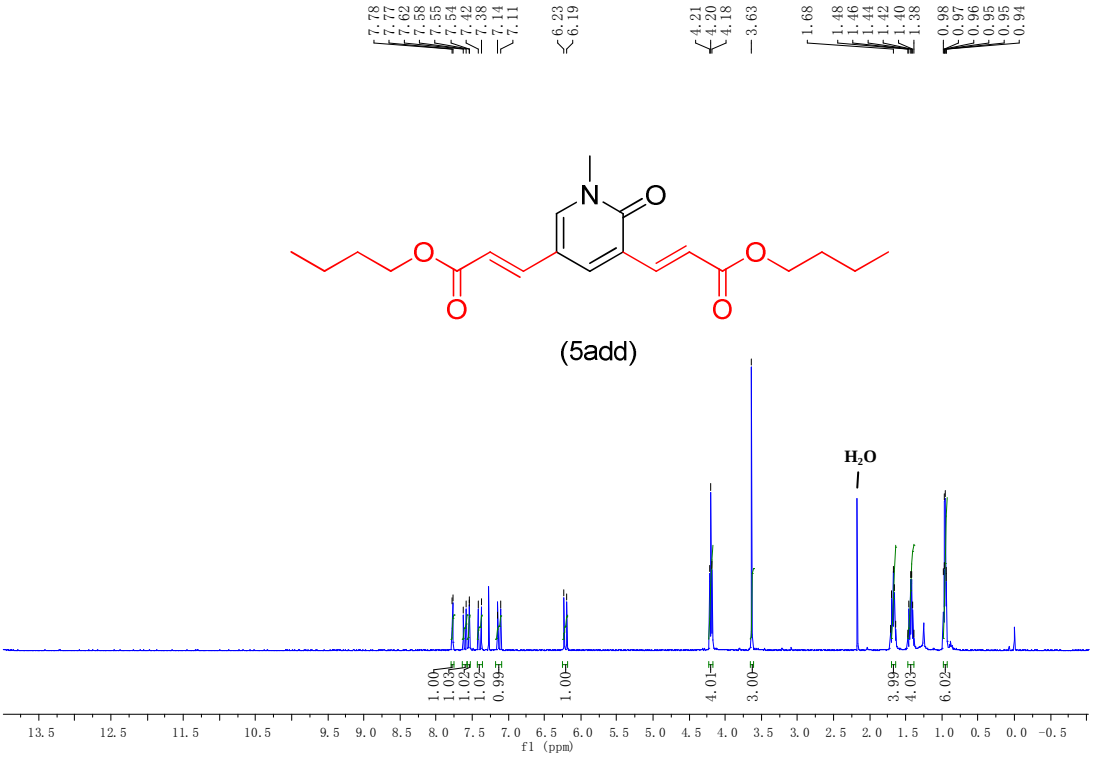
166.57
160.77
140.82
139.05
138.88
136.90
125.35
122.24
116.15
113.95
60.56
60.45
38.33
14.24
N
O
O
O
O
O
(5acc)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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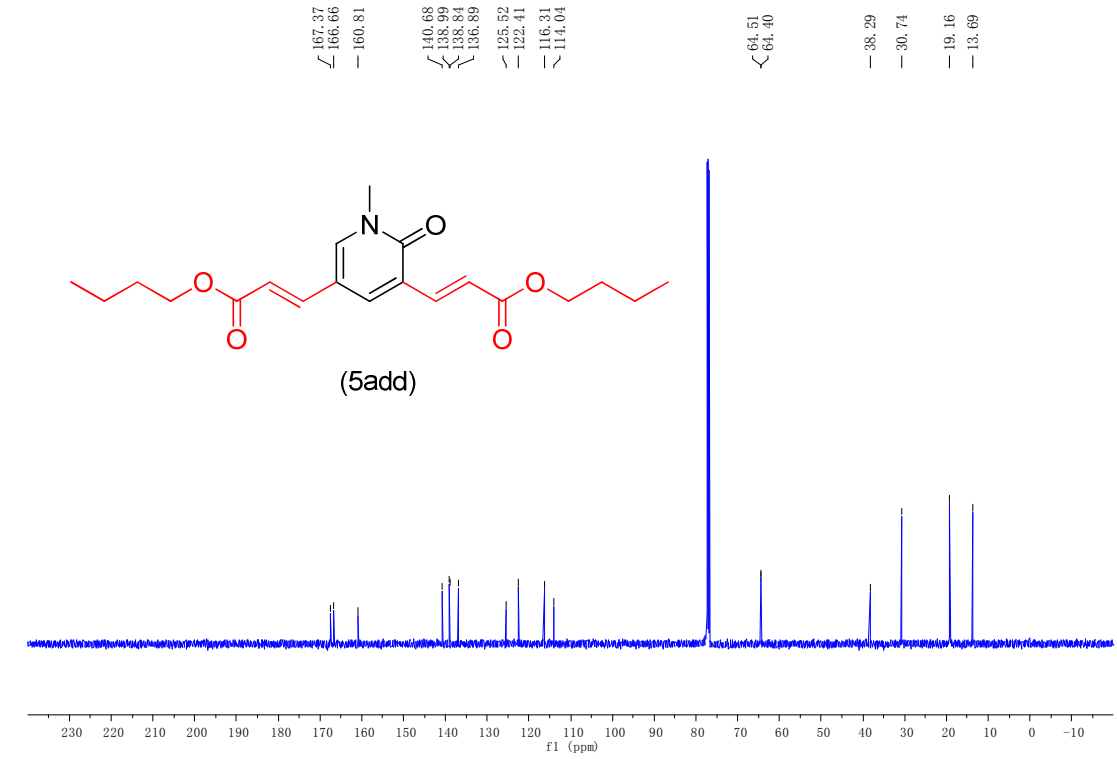
7.55
7.54
7.42
7.38
7.14
7.11
6.23
6.19
4.21
4.20
4.18
3.63
1.68
1.48
1.46
1.44
1.42
1.40
1.38
0.98
0.97
0.96
0.95
0.95
0.94
O
N
O
O
O
O
(5add)
H2O
1.00
1.03
1.02
1.02
0.99
1.00
4.01
3.00
3.99
4.03
6.02
f1 (ppm)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166.66
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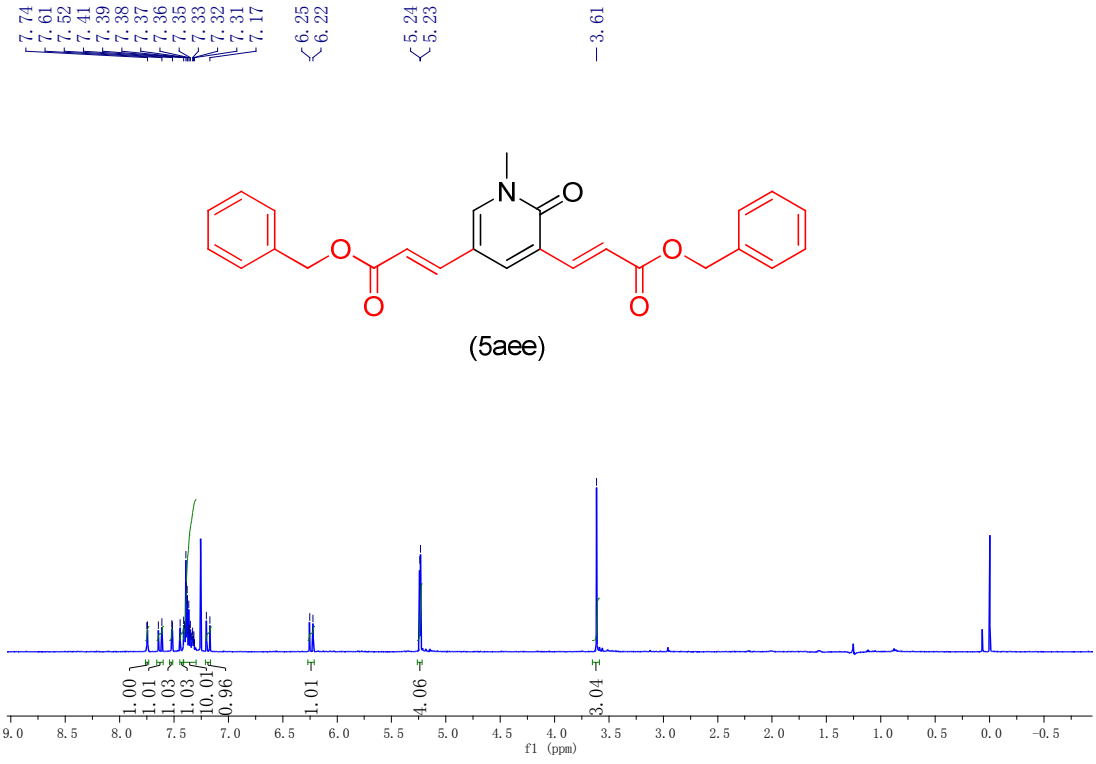
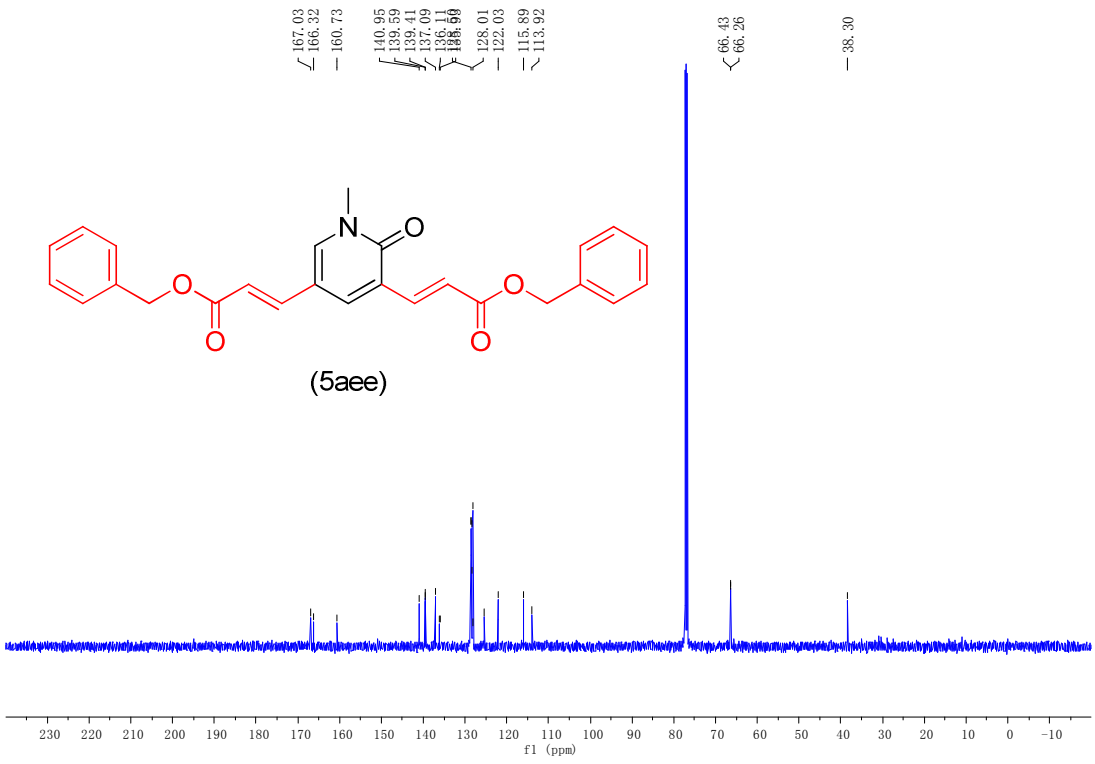
140.68
138.99
138.84
136.89
125.52
122.41
116.31
114.04
64.51
64.40
38.29
30.74
19.16
13.69
O
N
O
O
O
O
(5add)
f1 (ppm)


7.74
7.61
7.52
7.41
7.39
7.38
7.37
7.36
7.35
7.33
7.32
7.31
7.17
6.25
6.22
5.24
5.23
3.61
(5aee)
1.00
1.01
1.03
1.03
10.01
0.96
1.01
4.06
3.04
f1 (ppm)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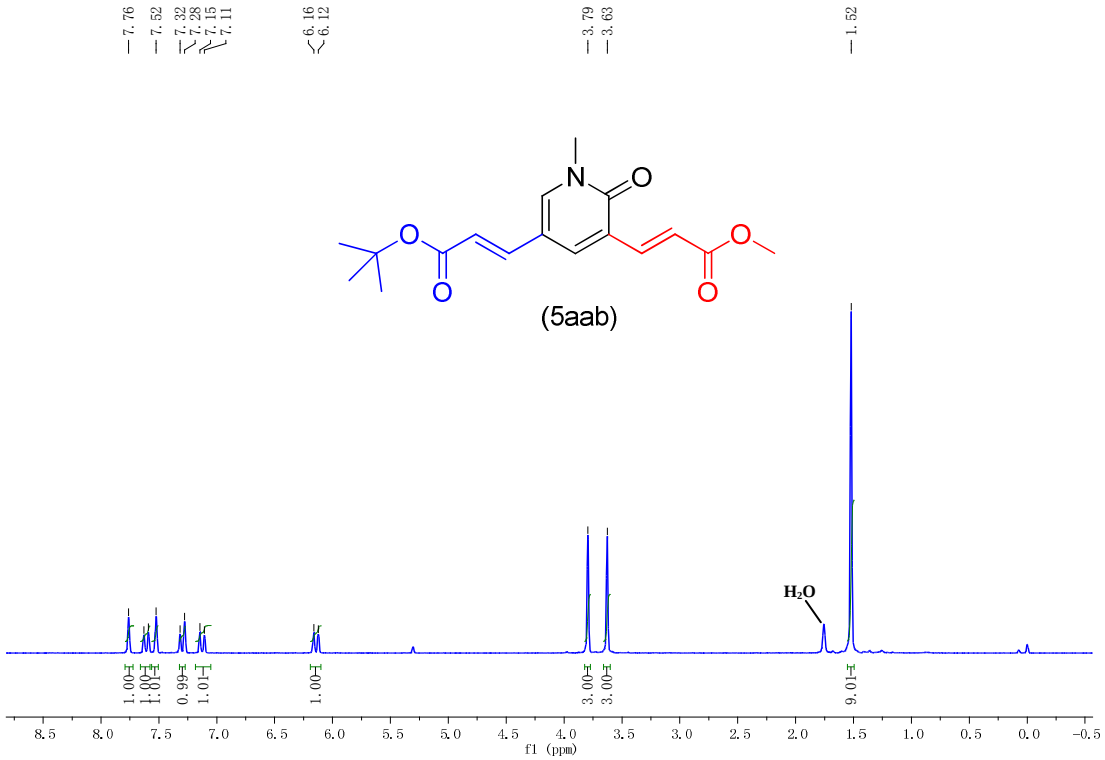
166.32
160.73
140.95
139.59
139.41
137.09
136.11
128.01
122.03
115.89
113.92
66.43
66.26
38.30
(5aee)
f1 (ppm)


7.76
7.52
7.32
7.28
7.15
7.11
6.16
6.12
3.79
3.63
1.52
(5aab)
H2O
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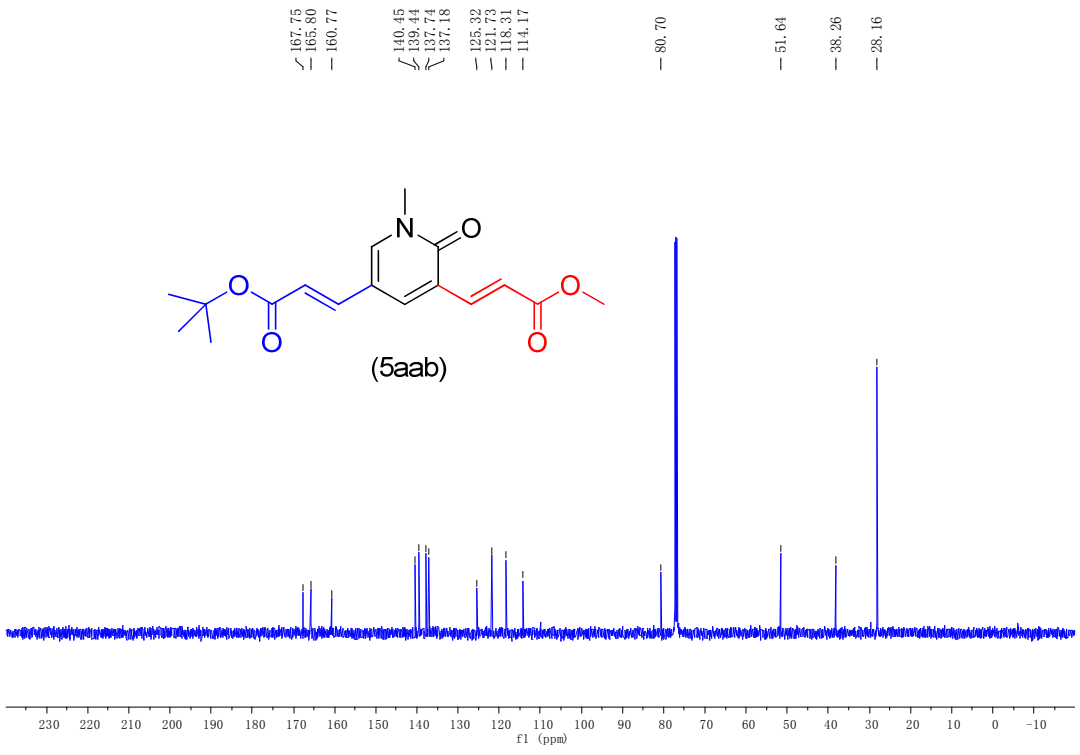
1.00
1.01
0.99
1.01
1.00
3.00
3.00
9.01
f1 (ppm)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140.45
139.44
137.74
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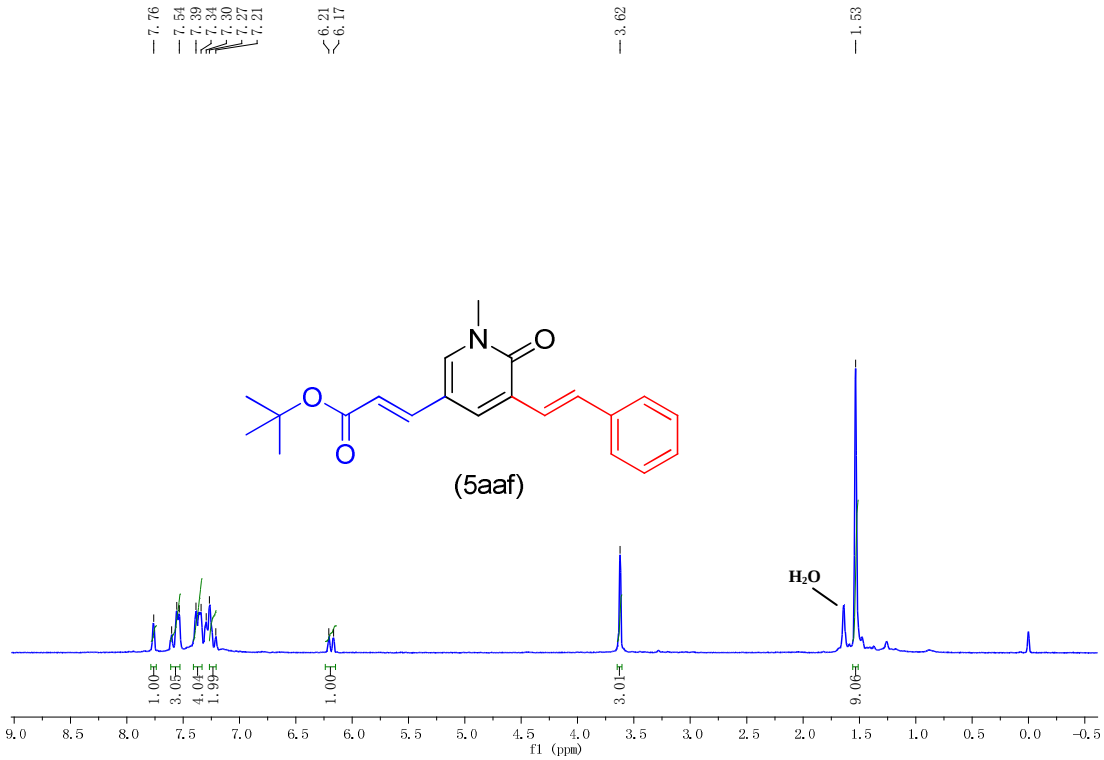
121.73
118.31
114.17
80.70
51.64
38.26
28.16
(5aab)
f1 (ppm)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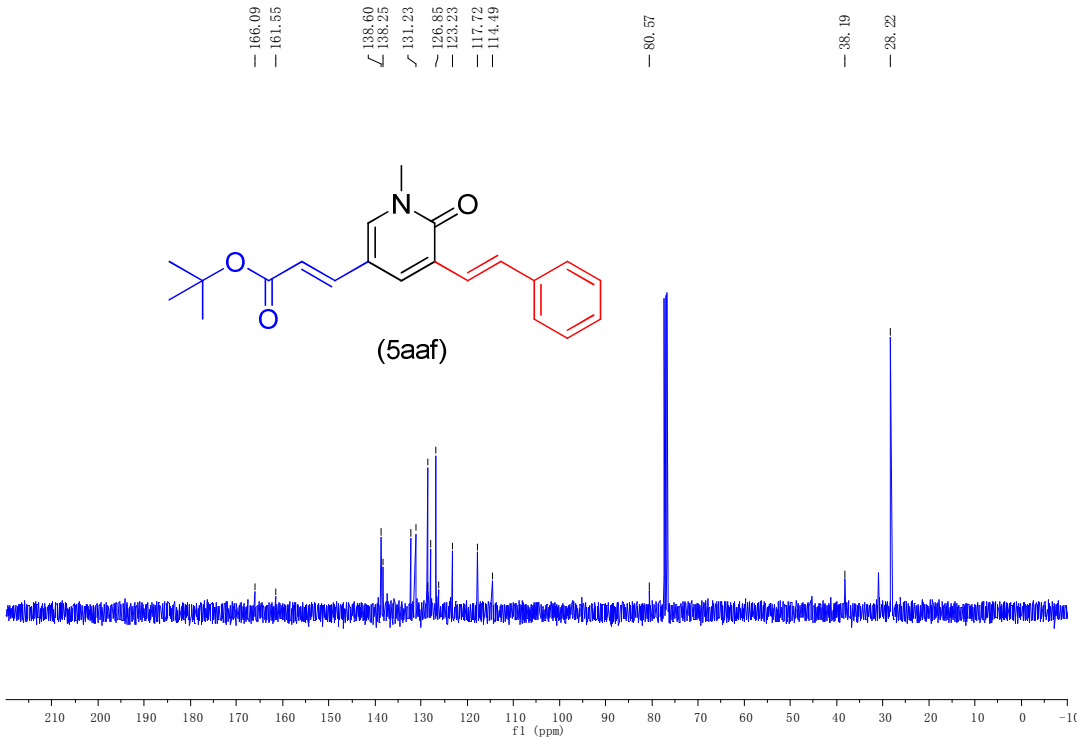
7.54
7.39
7.34
7.30
7.27
7.21
6.21
6.17
3.62
1.53
(5aaf)
H2O
1.00
3.05
4.04
1.99
1.00
3.01
9.06
f1 (ppm)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126.85
123.23
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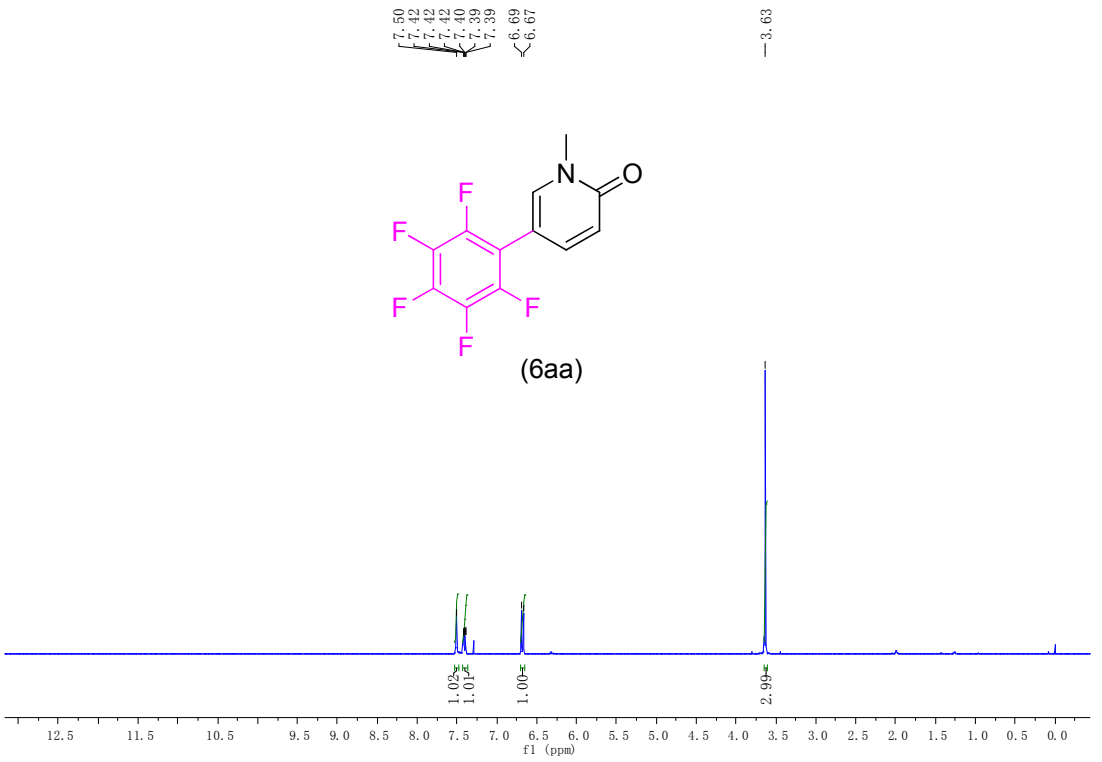
80.57
38.19
28.22
(5aaf)
f1 (ppm)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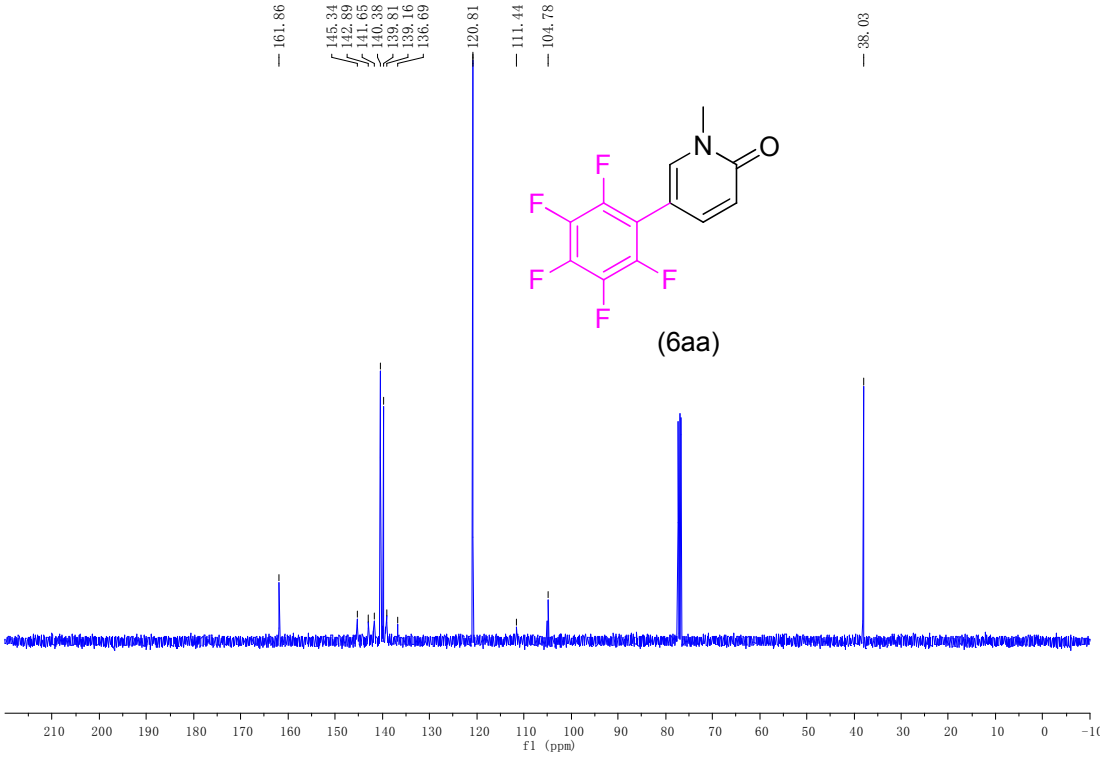
7.42
7.42
7.42
7.40
7.39
7.39
6.69
6.67
3.63
F
F
F
F
F
N
O
(6aa)
1.02
1.01
1.00
2.99
f1 (ppm)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141.65
140.38
139.81
139.16
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120.81
111.44
104.78
38.03
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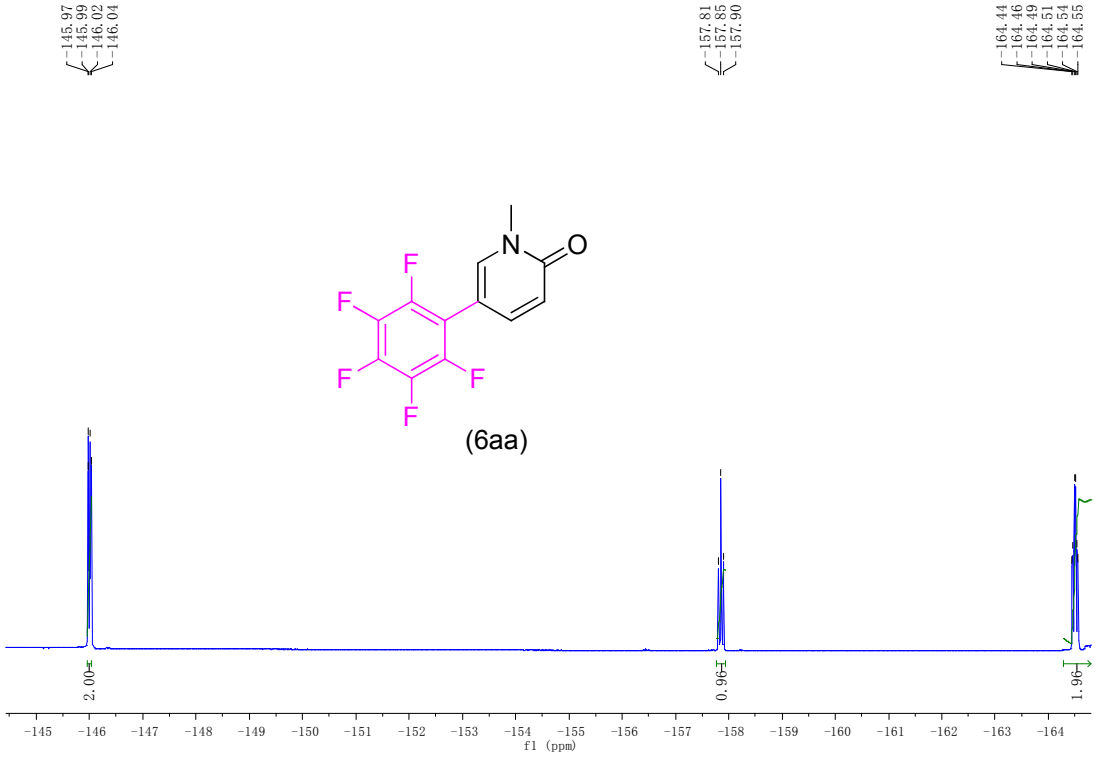
F
F
F
F
N
O
(6aa)
f1 (ppm)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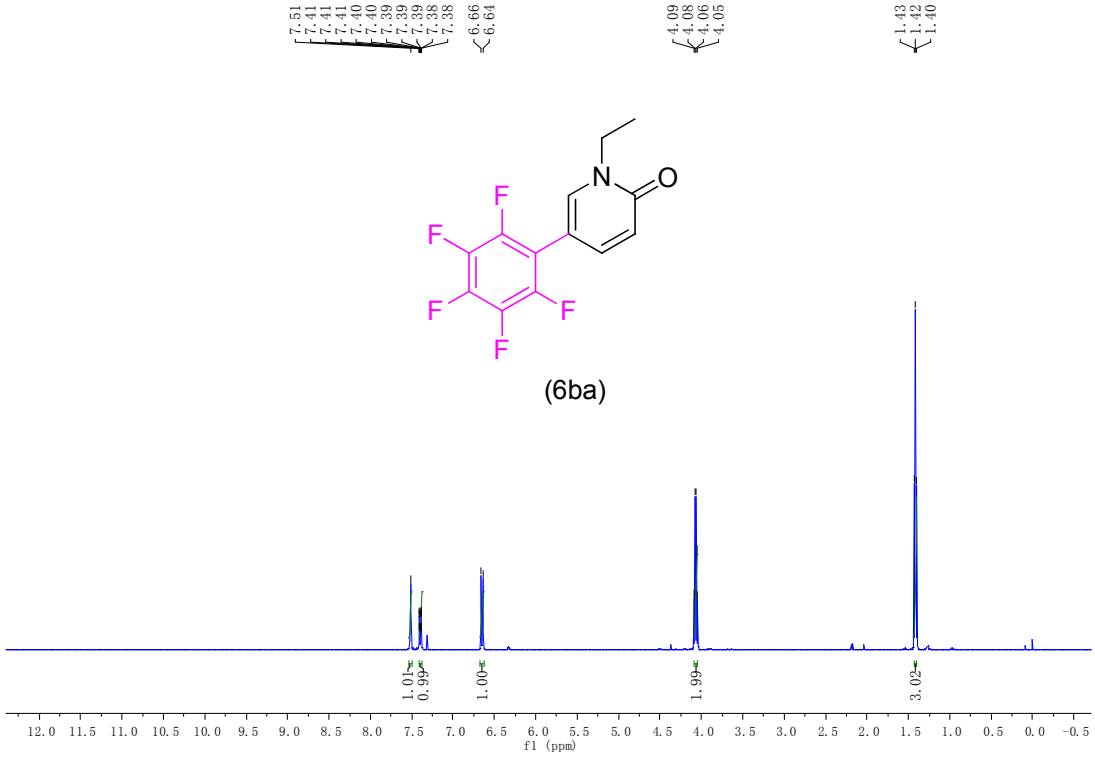
-145.99
-146.02
-146.04
-157.81
-157.85
-157.90
-164.44
-164.46
-164.49
-164.51
-164.54
-164.55
N
O
F
F
F
F
F
(6aa)
2.00
0.96
1.96
-145
-146
-147
-148
-149
-150
-151
-152
-153
-154
-155
-156
-157
-158
-159
-160
-161
-162
-163
-164
f1 (ppm)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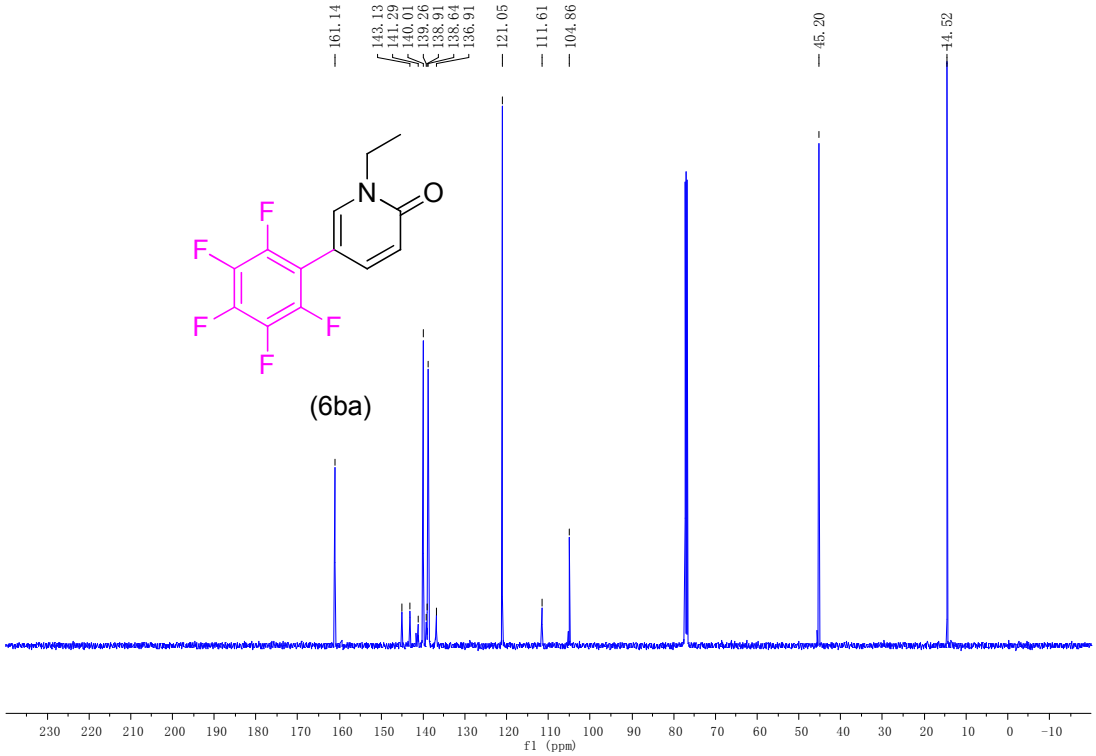
7.39
7.39
7.38
7.38
6.66
6.64
4.09
4.08
4.06
4.05
1.43
1.42
1.40
F
F
F
F
F
N
O
(6ba)
1.01
0.99
1.00
1.99
3.02
f1 (ppm)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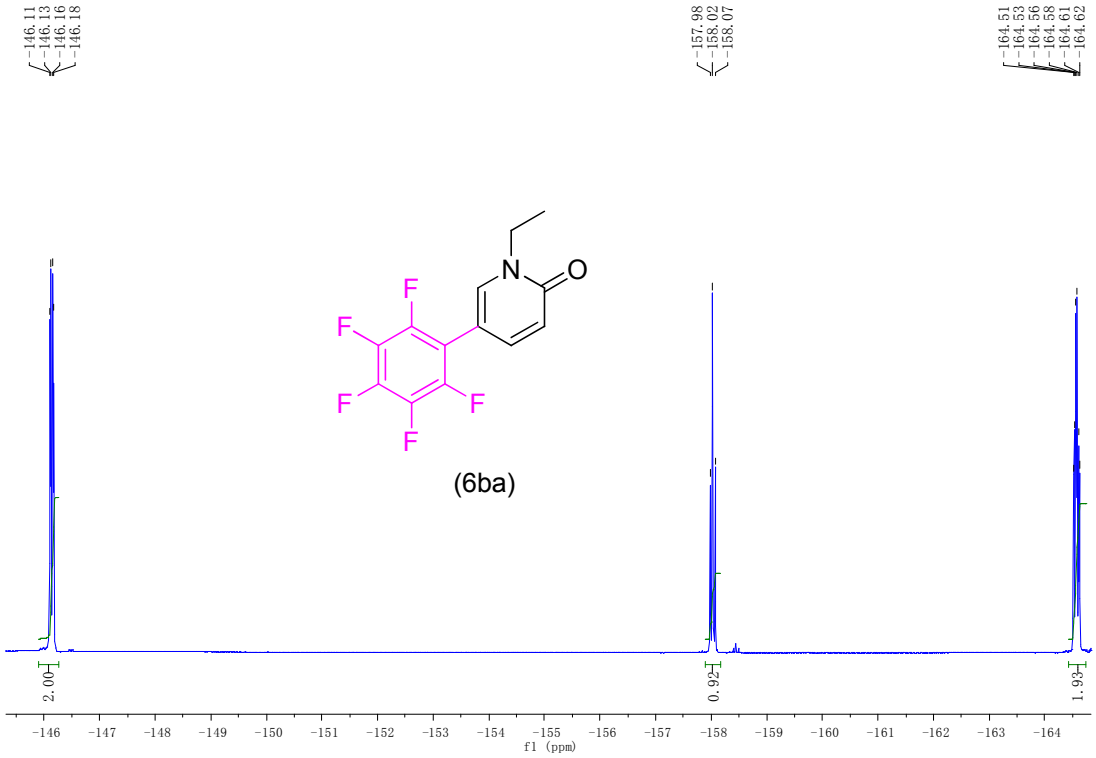
141.29
140.01
139.26
138.91
138.64
136.91
121.05
111.61
104.86
45.20
14.52
F
F
F
F
F
N
O
(6ba)
f1 (ppm)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-146.13
-146.16
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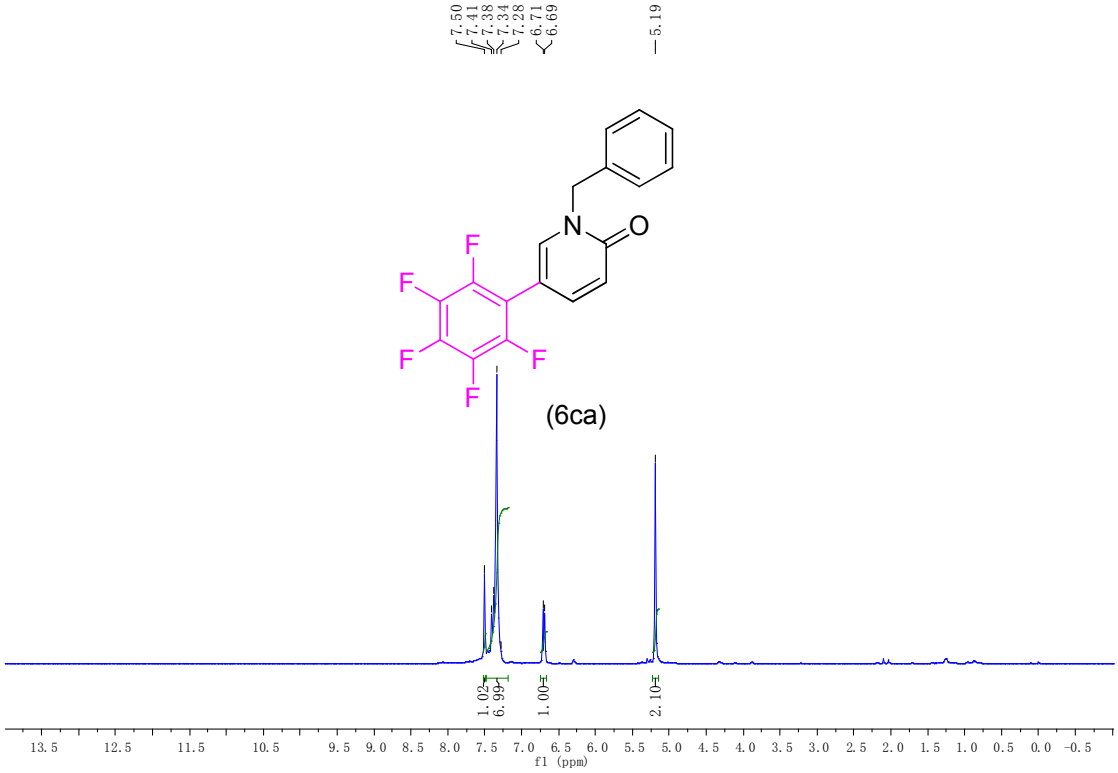
-157.98
-158.02
-158.07
-164.51
-164.53
-164.56
-164.58
-164.61
-164.62
F
F
F
F
F
N
O
(6ba)
2.00
0.92
1.93
-146
-147
-148
-149
-150
-151
-152
-153
-154
-155
-156
-157
-158
-159
-160
-161
-162
-163
-164
f1 (ppm)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7.41
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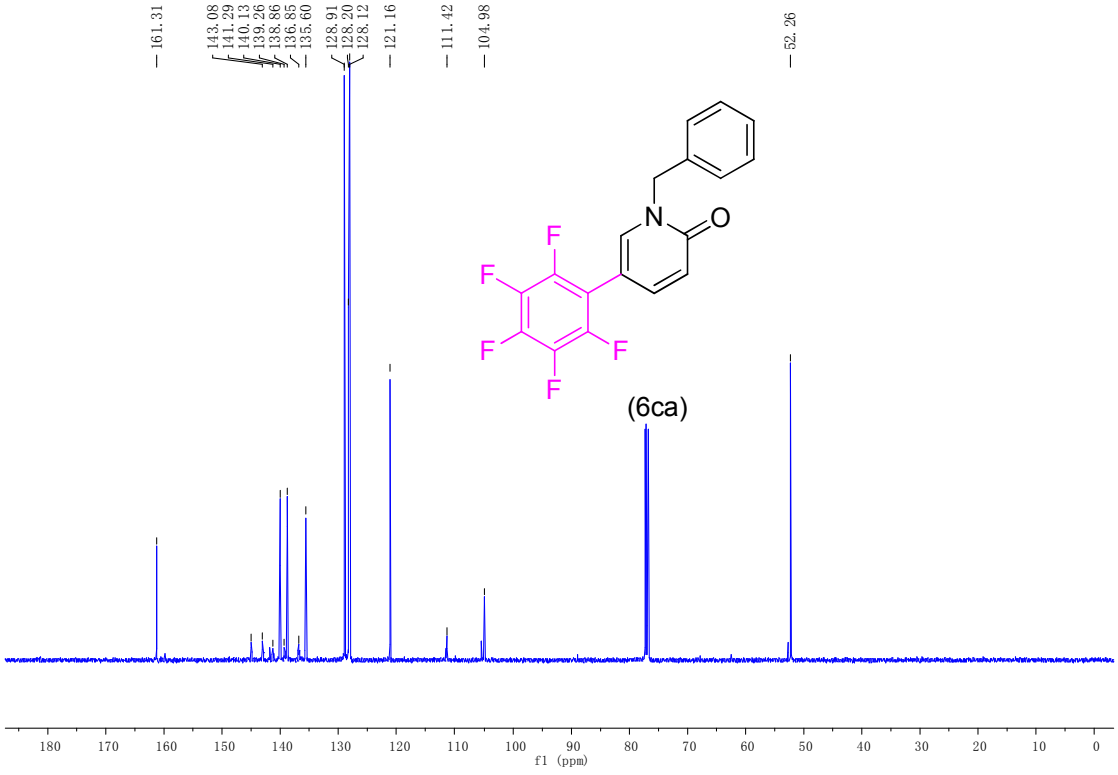
7.34
7.28
6.71
6.69
5.19
F
F
F
F
F
N
O
(6ca)
1.02
6.99
1.00
2.10
f1 (ppm)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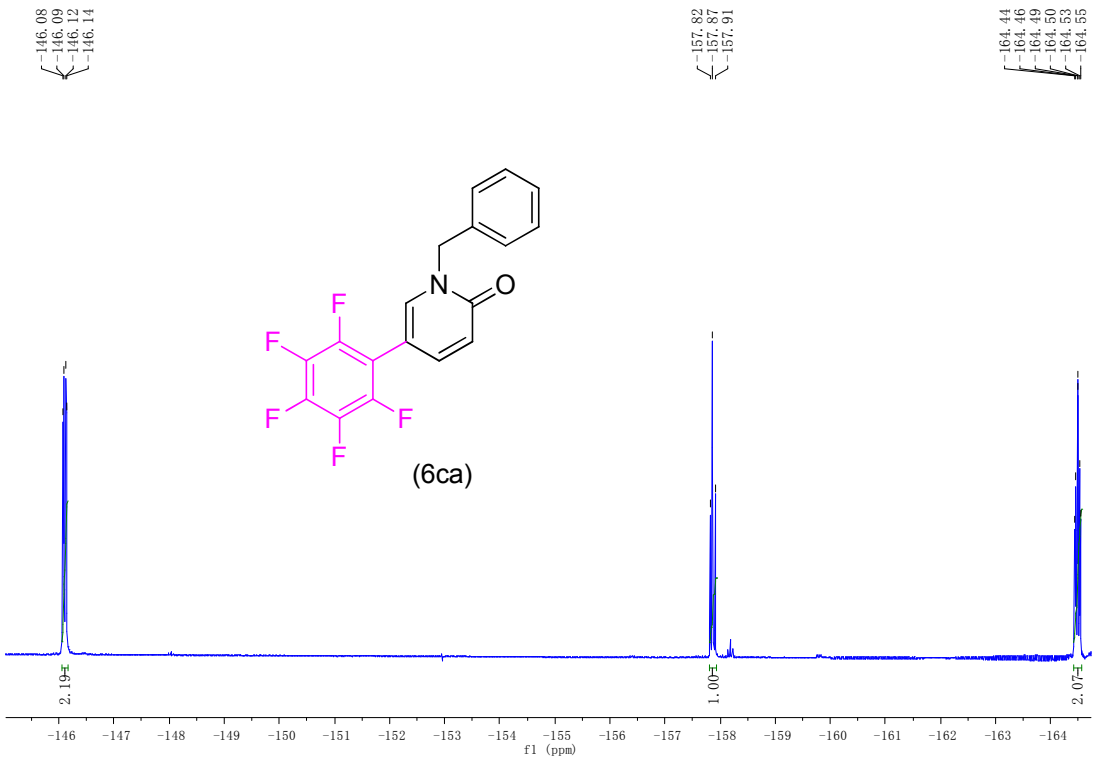
143.08
141.29
140.13
139.26
138.86
136.85
135.60
128.91
128.20
128.12
121.16
111.42
104.98
52.26
F
F
F
F
F
N
O
(6ca)
f1 (ppm)


146.08
146.09
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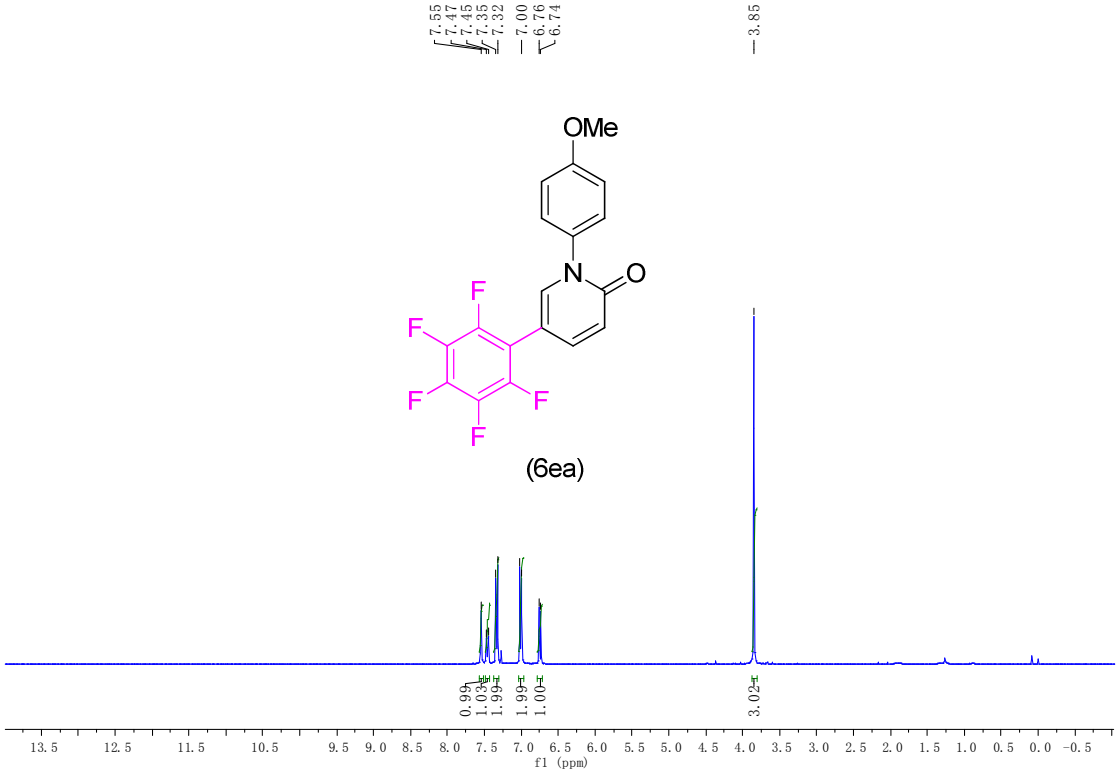
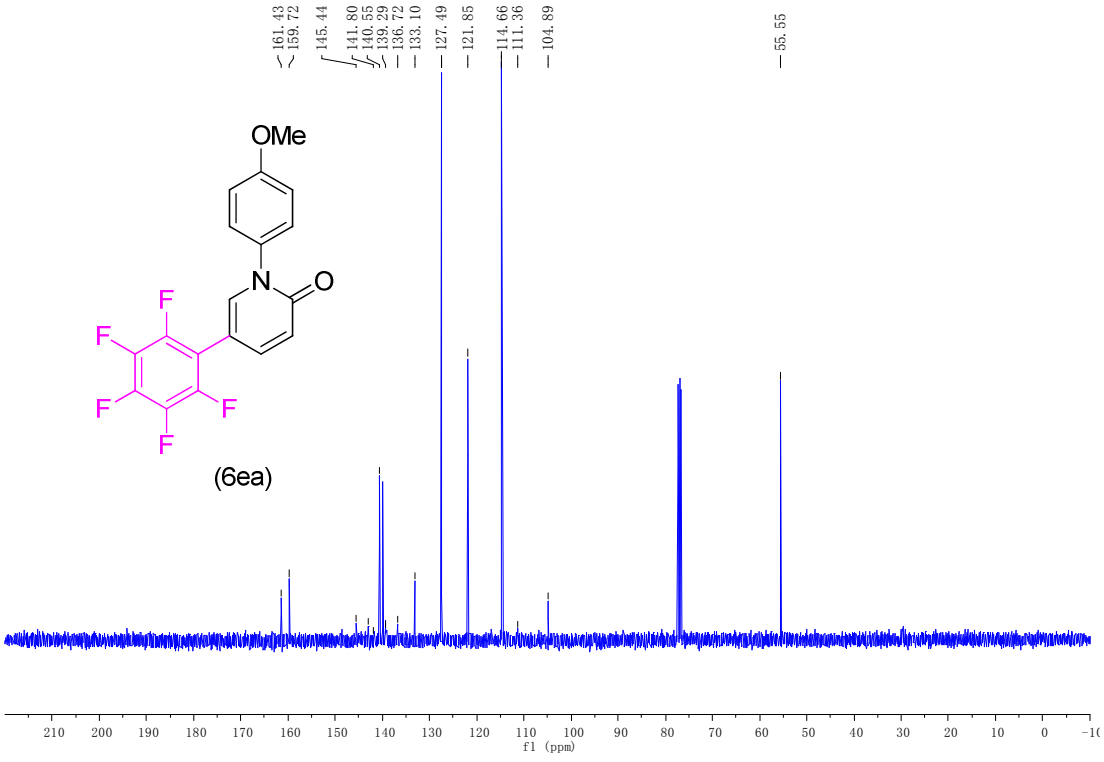
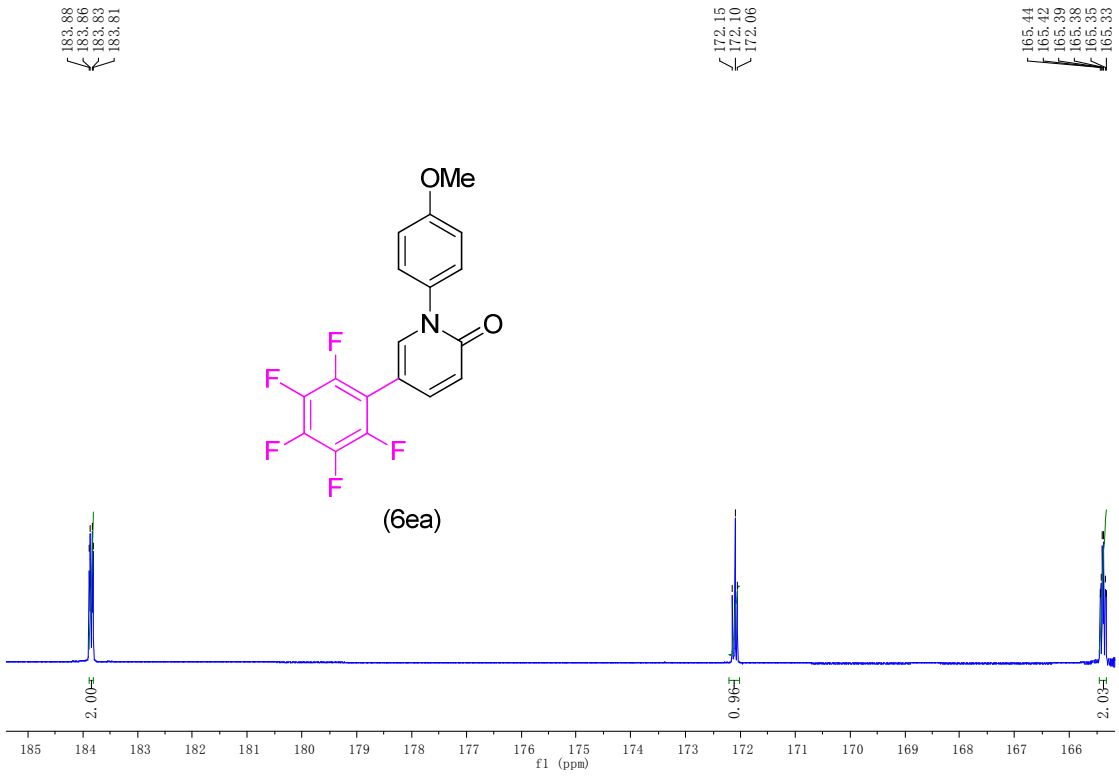
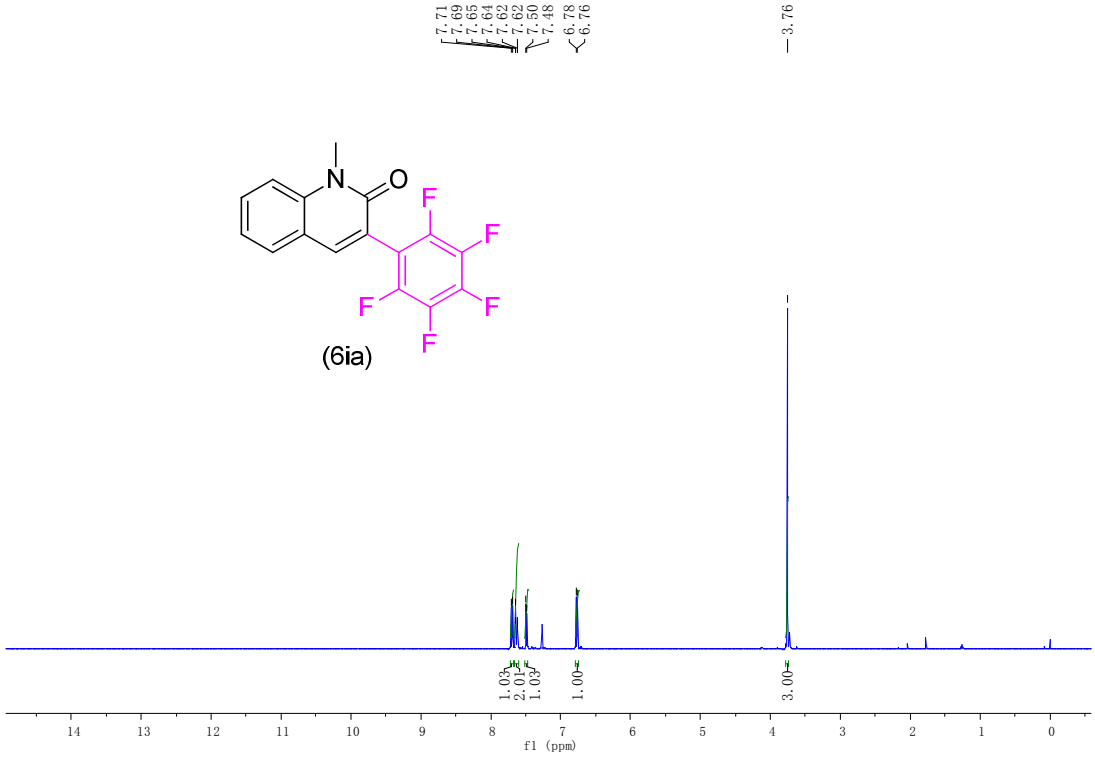
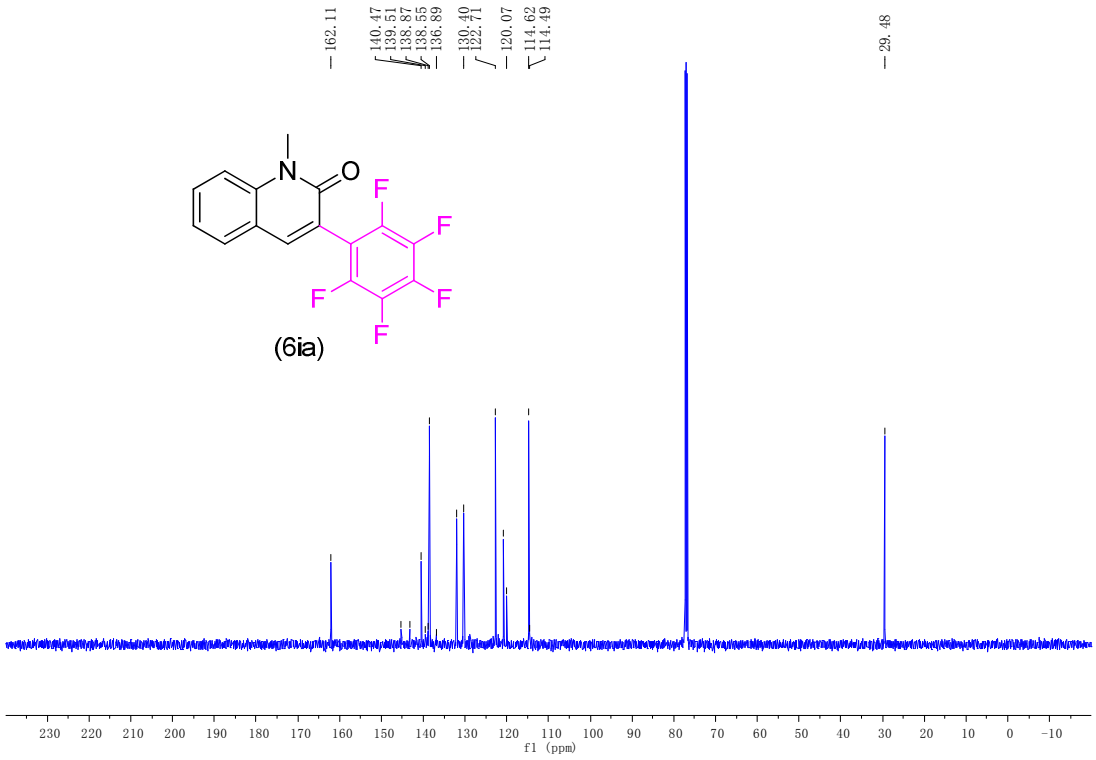
157.82
157.87
157.91
164.44
164.46
164.49
164.50
164.53
164.55
F
F
F
F
F
N
O
(6ca)
2.19
1.00
2.07
−146
−147
−148
−149
−150
−151
−152
−153
−154
−155
−156
−157
−158
−159
−160
−161
−162
−163
−164
f1 (ppm)

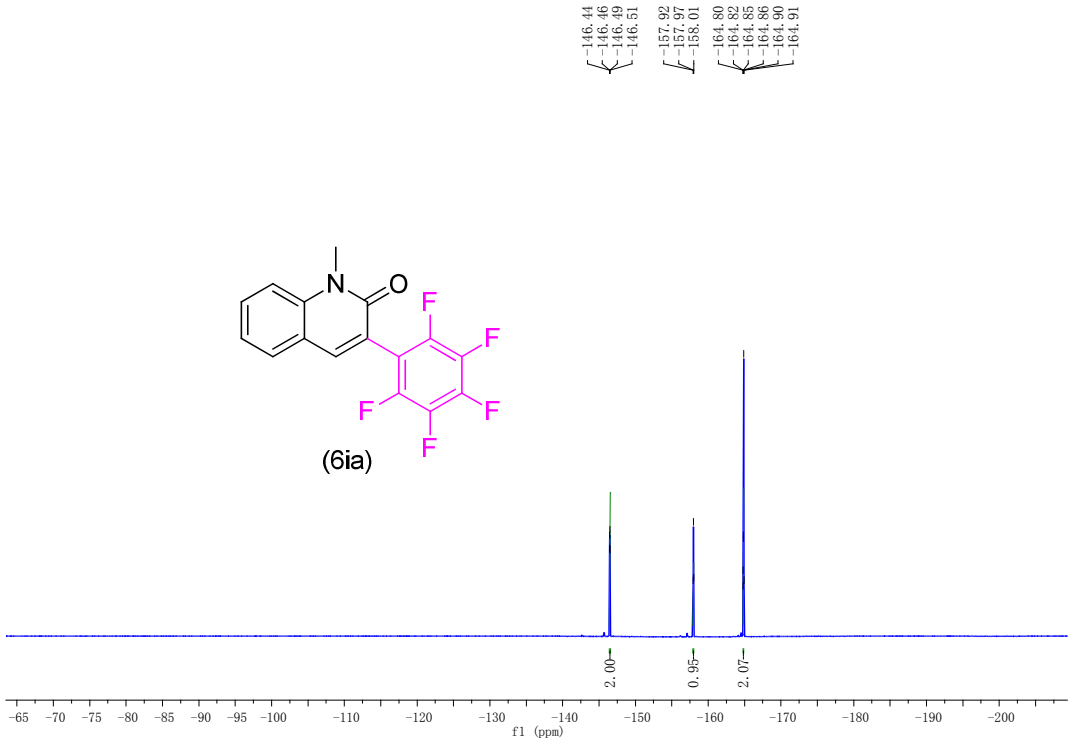

7.55
7.47
7.45
7.35
7.32
7.00
6.76
6.74
3.85
OMe
N
O
F
F
F
F
F
(6ea)
0.99
1.03
1.99
1.99
1.00
3.02
f1 (ppm)

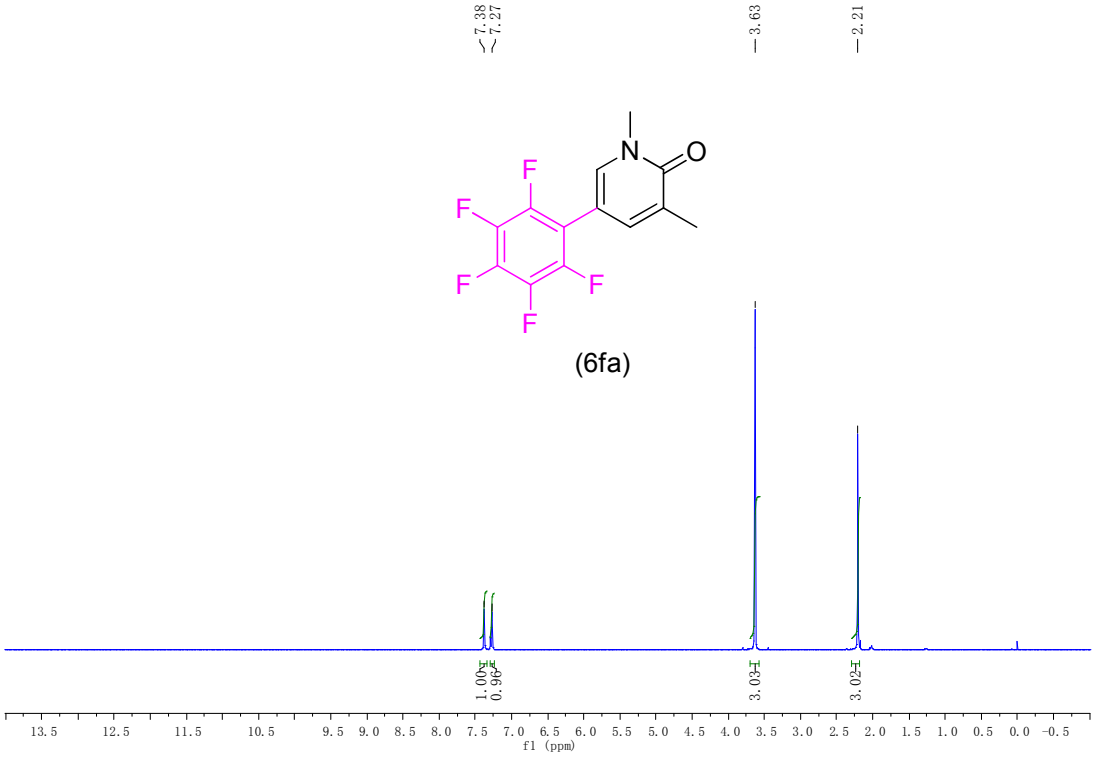

161.43
159.72
145.44
141.80
140.55
139.29
136.72
133.10
127.49
121.85
114.66
111.36
104.89
55.55
OMe
N
O
F
F
F
F
F
(6ea)
f1 (ppm)

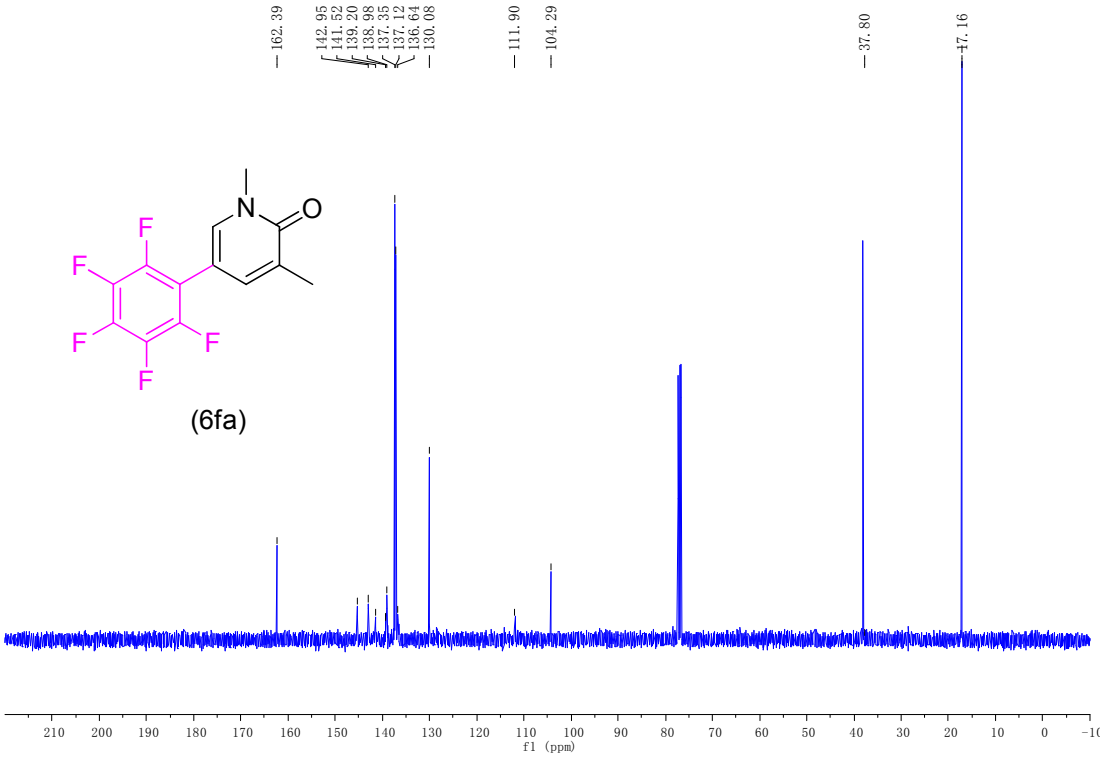

183.88
183.86
183.83
183.81
172.15
172.10
172.06
165.44
165.42
165.39
165.38
165.35
165.33
OMe
N
O
F
F
F
F
F
(6ea)
2.00
0.96
2.03
185
184
183
182
181
180
179
178
177
176
175
174
173
172
171
170
169
168
167
166
f1 (ppm)

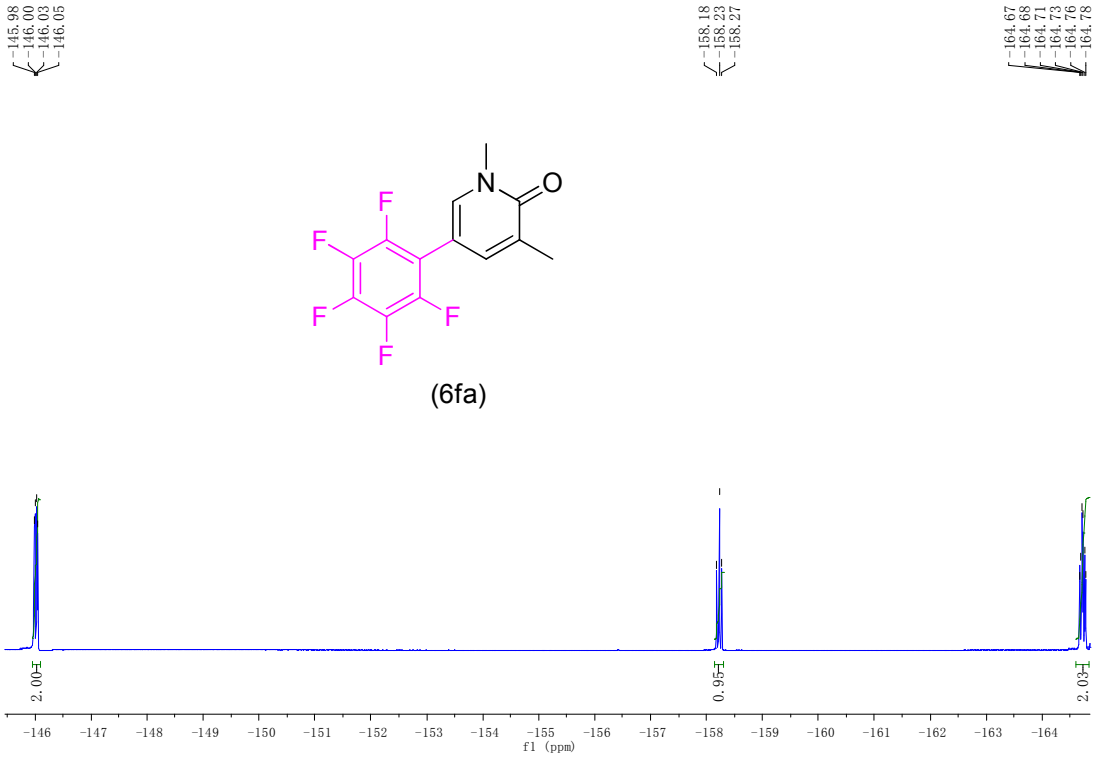

7.71
7.69
7.65
7.64
7.62
7.62
7.50
7.48
6.78
6.76
3.76
N
O
F
F
F
F
F
(6ia)
1.03
2.01
1.03
1.00
3.00
f1 (ppm)

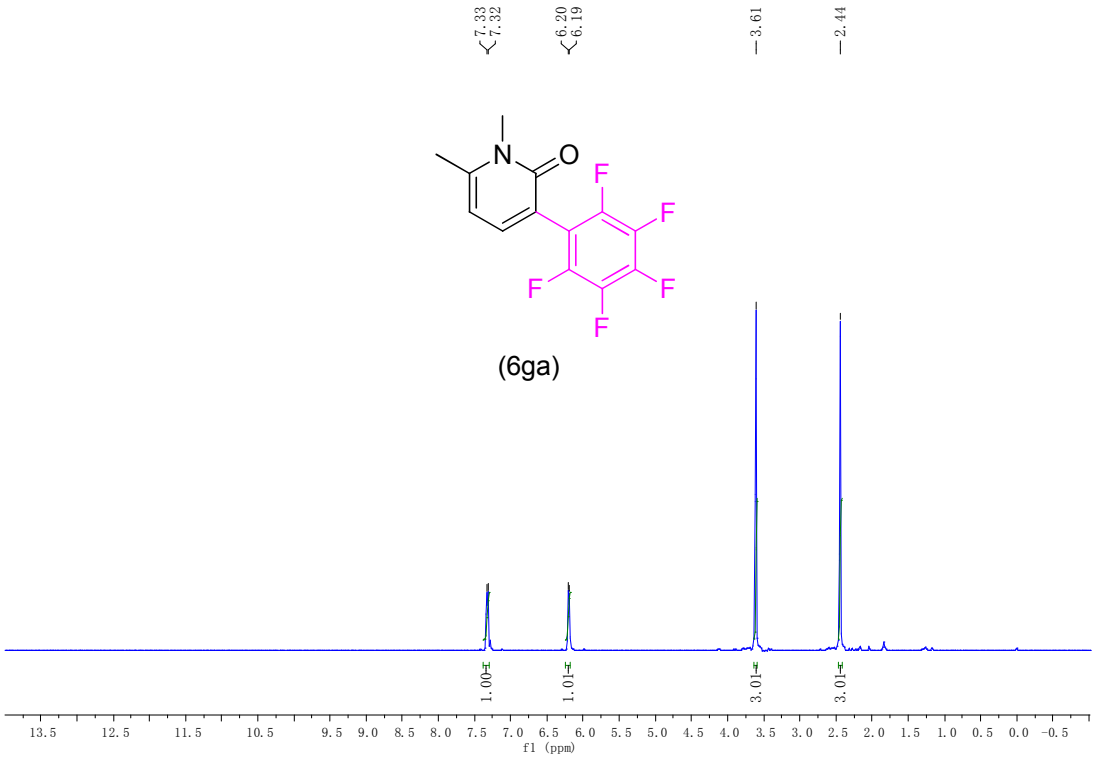

162.11
140.47
139.51
138.87
138.55
136.89
130.40
122.71
120.07
114.62
114.49
29.48
N
O
F
F
F
F
F
(6ia)
f1 (ppm)

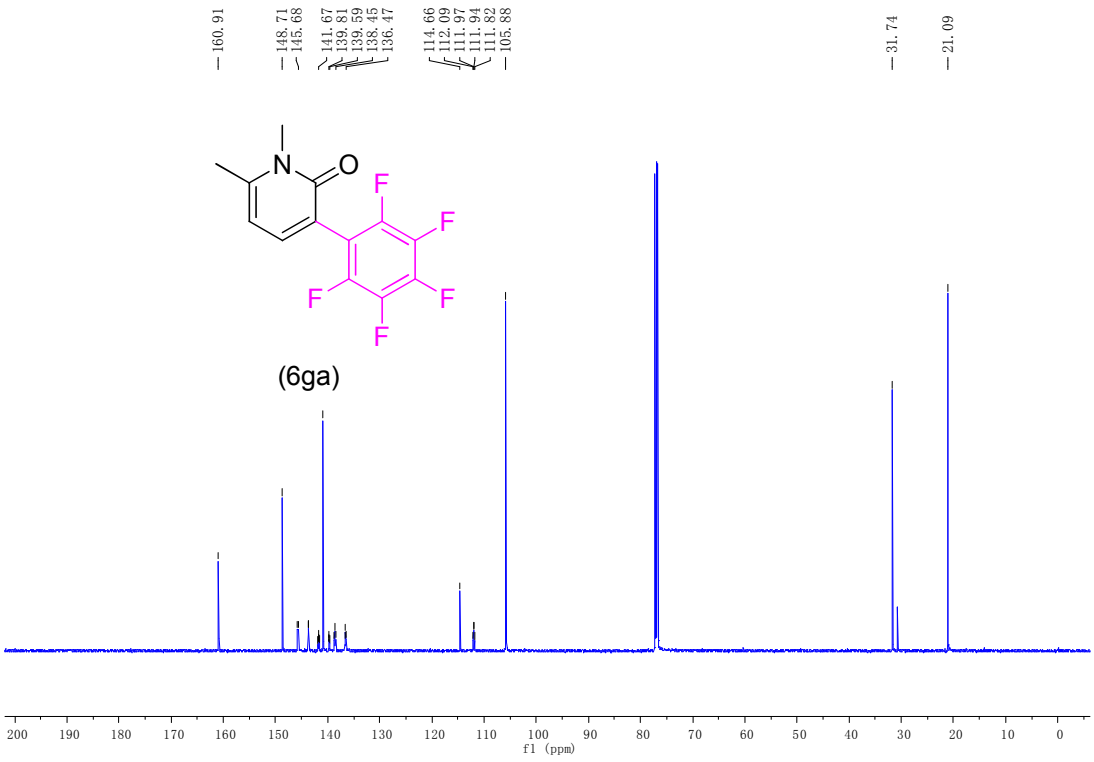

-146.44
-146.46
-146.49
-146.51
-157.92
-157.97
-158.01
-164.80
-164.82
-164.85
-164.86
-164.90
-164.91
N
O
F
F
F
F
F
(6ia)
2.00
0.95
2.07
-65 -70 -75 -80 -85 -90 -95 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

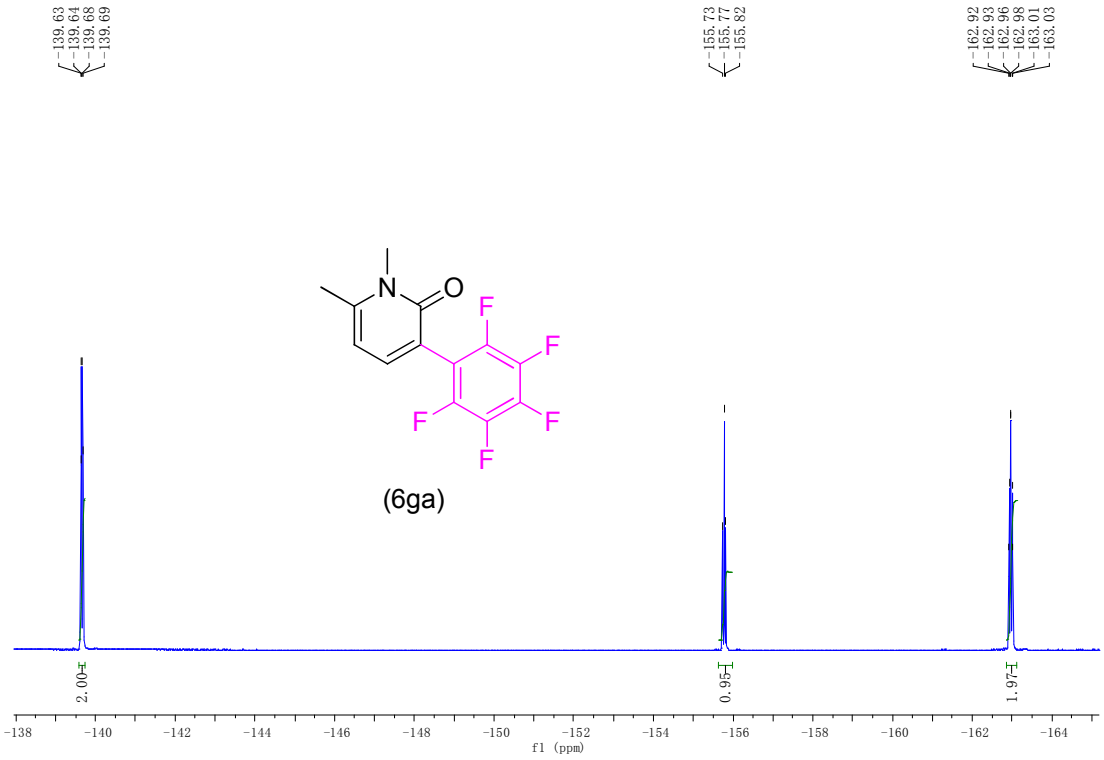

7.38
7.27
3.63
2.21
F
F
F
F
F
N
O
(6fa)
1.00
0.90
3.03
3.02
f1 (ppm)

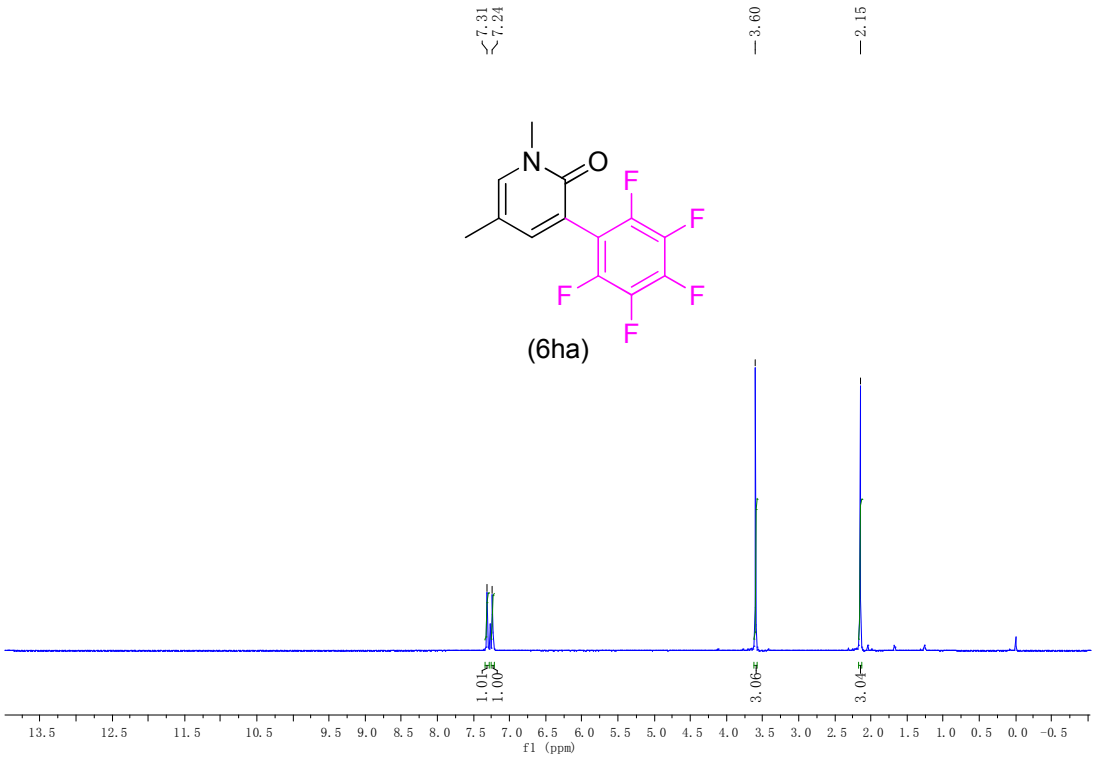

162.39
142.95
141.52
139.20
138.98
137.35
137.12
136.64
130.08
111.90
104.29
37.80
17.16
F
F
F
F
F
N
O
(6fa)
f1 (ppm)

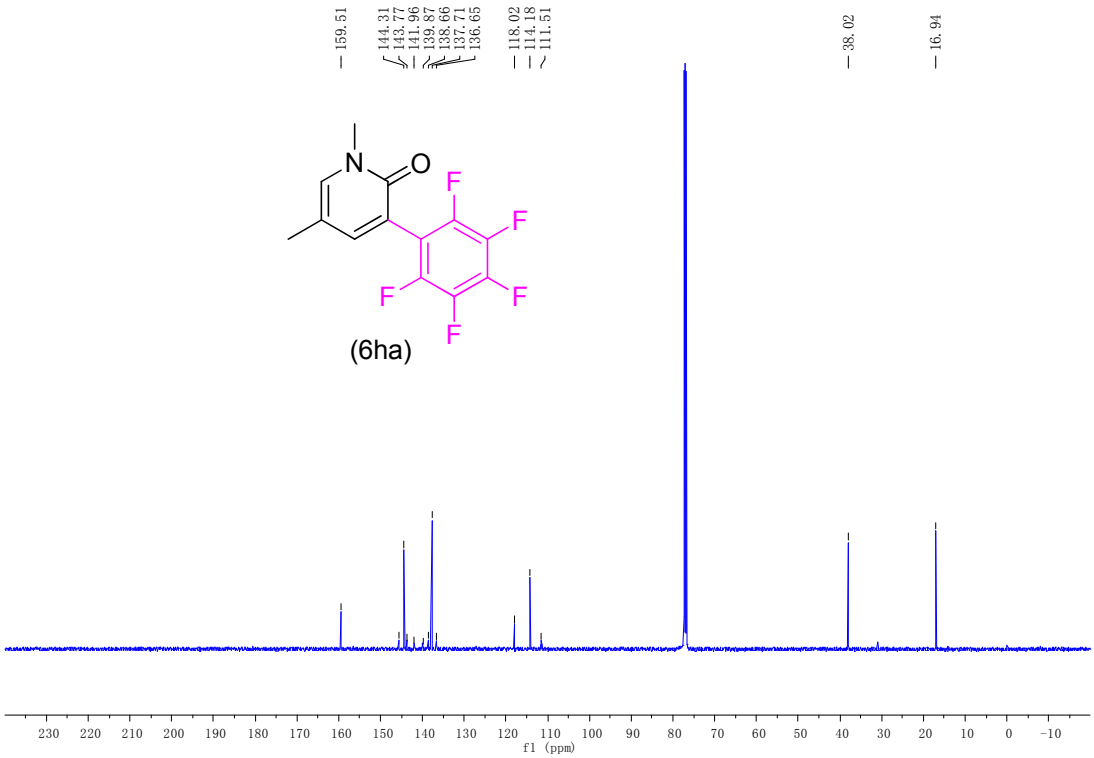

-145.98
-146.00
-146.03
-146.05
-158.18
-158.23
-158.27
-164.67
-164.68
-164.71
-164.73
-164.76
-164.78
N
O
F
F
F
F
F
(6fa)
2.00
0.95
2.03
-146
-147
-148
-149
-150
-151
-152
-153
-154
-155
-156
-157
-158
-159
-160
-161
-162
-163
-164
f1 (ppm)

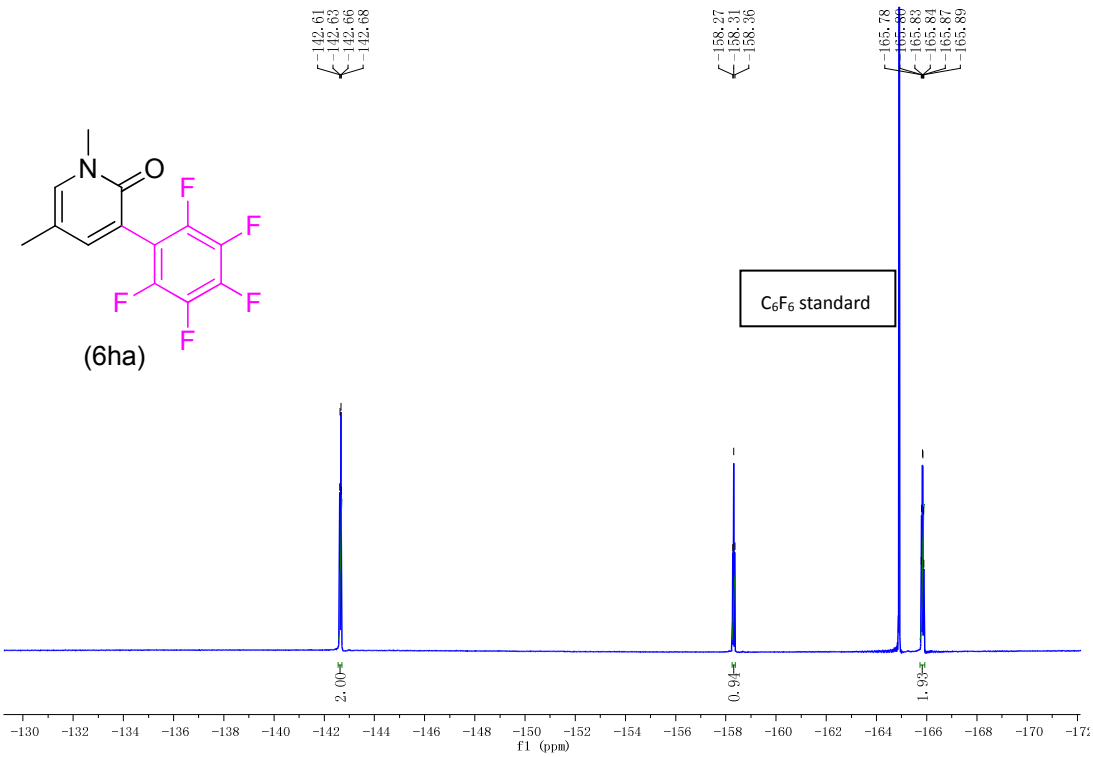

7.33
7.32
6.20
6.19
3.61
2.44
N
O
F
F
F
F
F
(6ga)
1.00
1.01
3.01
3.01
f1 (ppm)

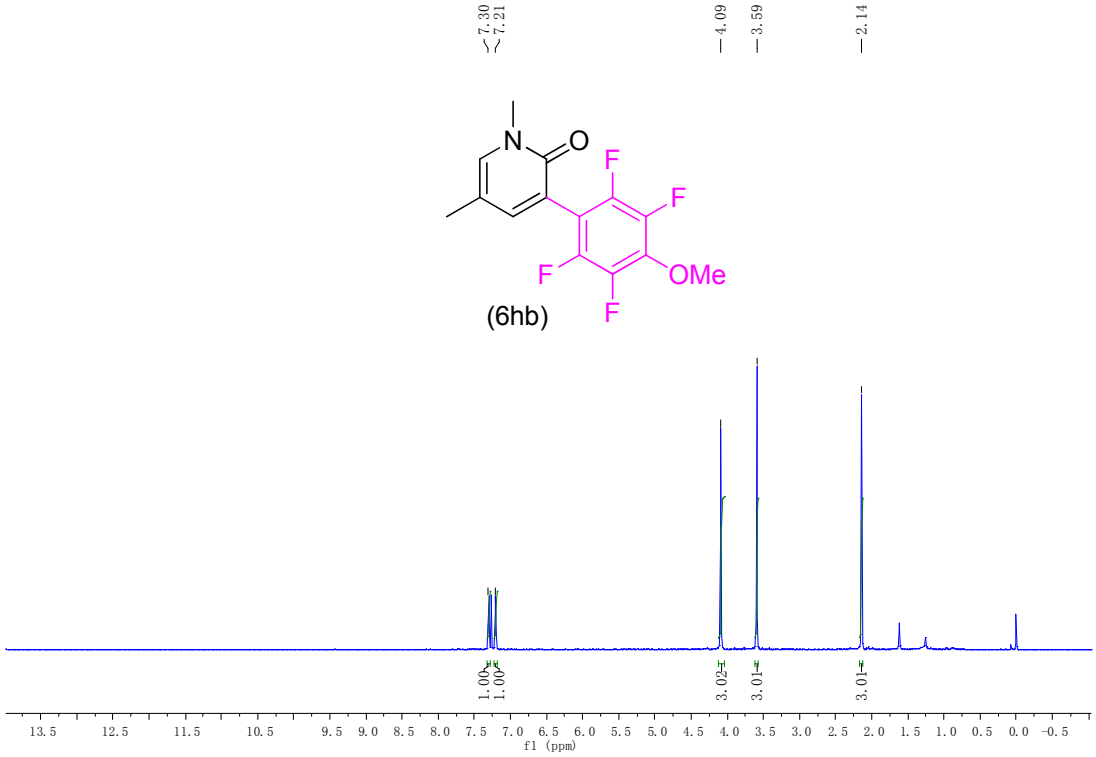

160.91
148.71
145.68
141.67
139.81
139.59
138.45
136.47
114.66
112.09
111.97
111.94
111.82
105.88
31.74
21.09
N
O
F
F
F
F
F
(6ga)
f1 (ppm)

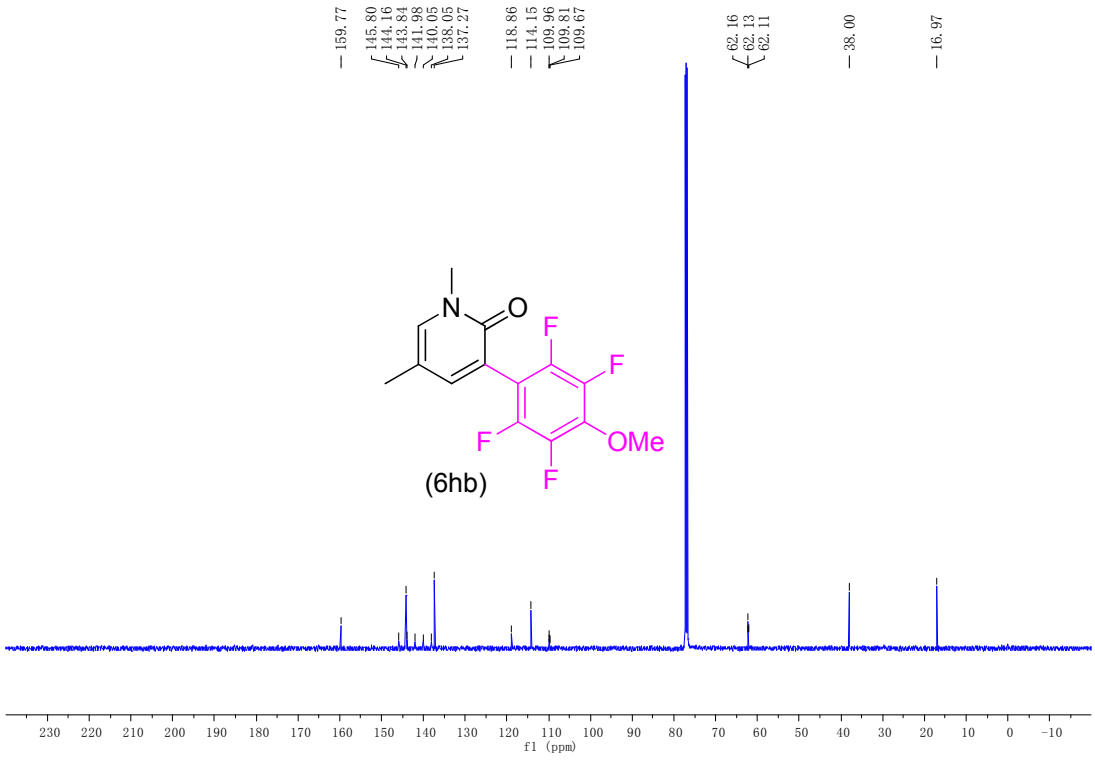

-139.63
-139.64
-139.68
-139.69
-155.73
-155.77
-155.82
-162.92
-162.93
-162.96
-162.98
-163.01
-163.03
N
O
F
F
F
F
F
(6ga)
2.00
0.95
1.97
-138
-140
-142
-144
-146
-148
-150
-152
-154
-156
-158
-160
-162
-164
f1 (ppm)

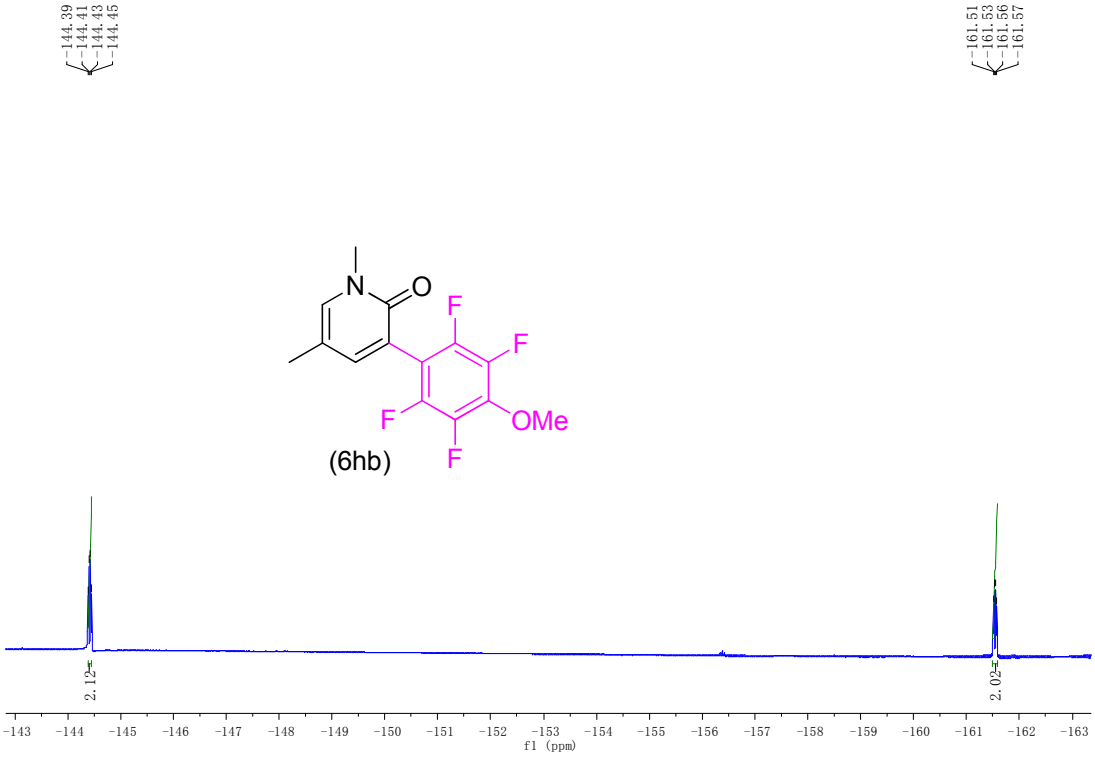


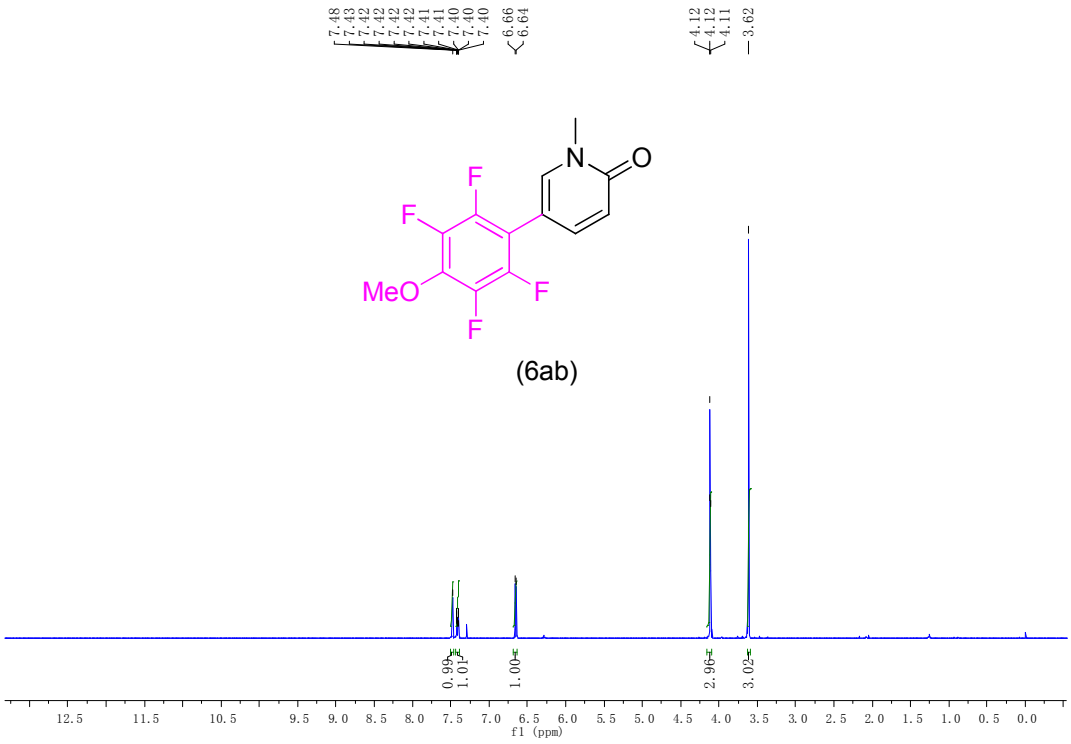


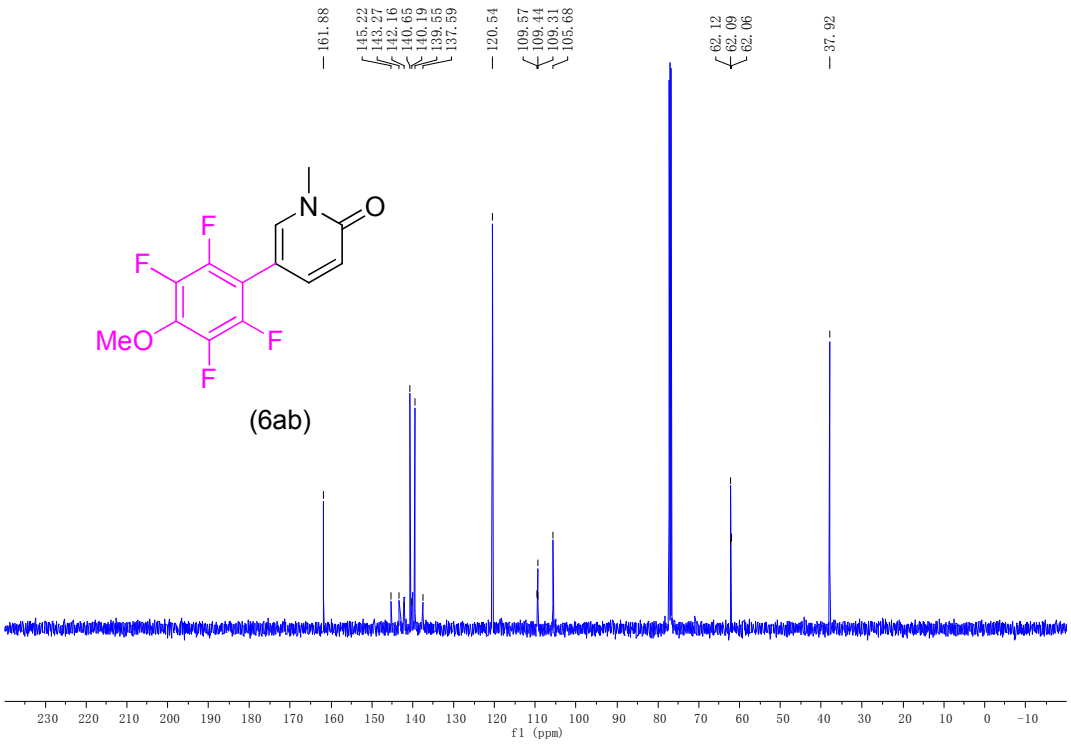

142.61
142.63
142.66
142.68
158.27
158.31
158.36
165.78
165.80
165.83
165.84
165.87
165.89
N
O
F
F
F
F
F
(6ha)
C6F6 standard
2.00
0.94
1.93
−130 −132 −134 −136 −138 −140 −142 −144 −146 −148 −150 −152 −154 −156 −158 −160 −162 −164 −166 −168 −170
f1 (ppm)

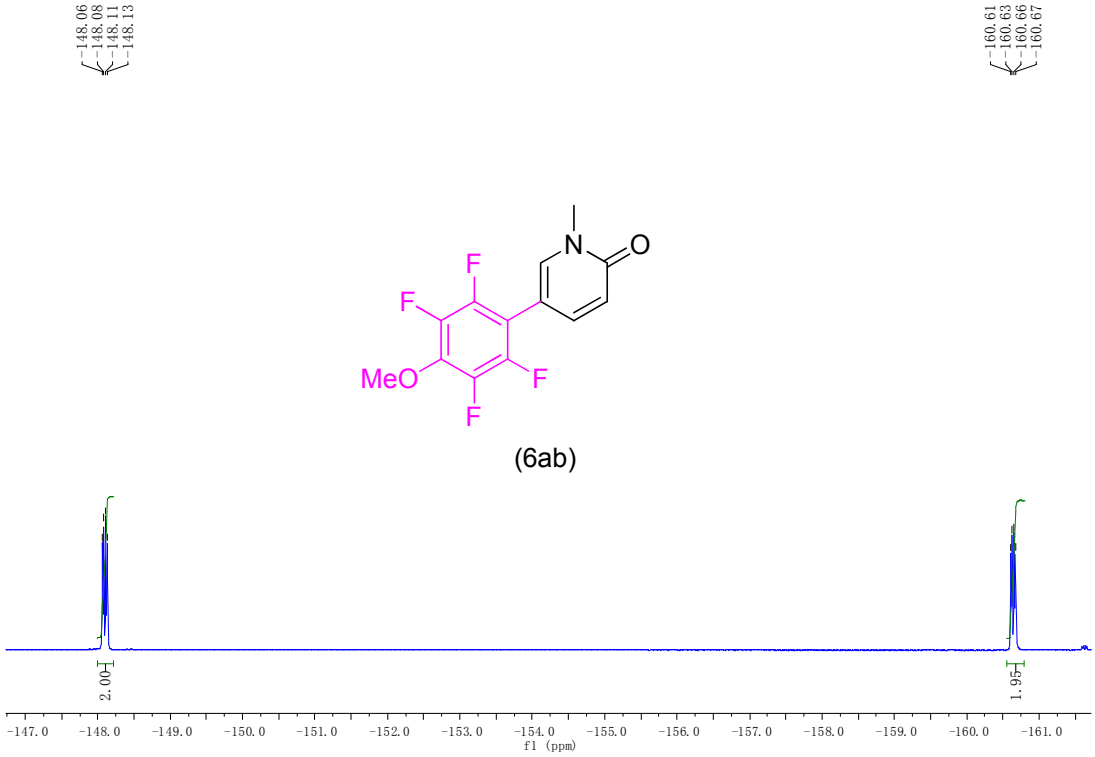

7.30
7.21
4.09
3.59
2.14
N
O
F
F
F
OMe
F
(6hb)
1.00
1.00
3.02
3.01
3.01
f1 (ppm)


159.77
145.80
144.16
143.84
141.98
140.05
138.05
137.27
118.86
114.15
109.96
109.81
109.67
62.16
62.13
62.11
38.00
16.97
N
O
F
F
F
OMe
F
(6hb)
f1 (ppm)

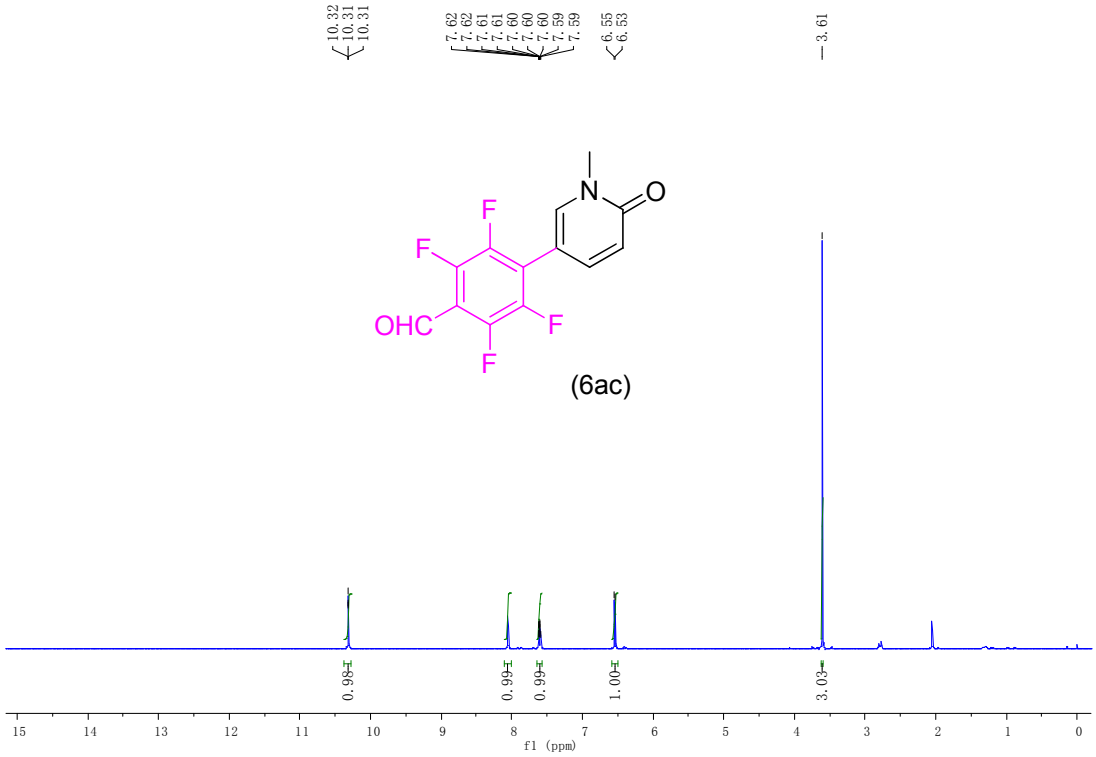

-144.39
-144.41
-144.43
-144.45
-161.51
-161.53
-161.56
-161.57
N
O
F
F
F
OMe
F
(6hb)
2.12
2.02
-143
-144
-145
-146
-147
-148
-149
-150
-151
-152
-153
-154
-155
-156
-157
-158
-159
-160
-161
-162
-163
f1 (ppm)

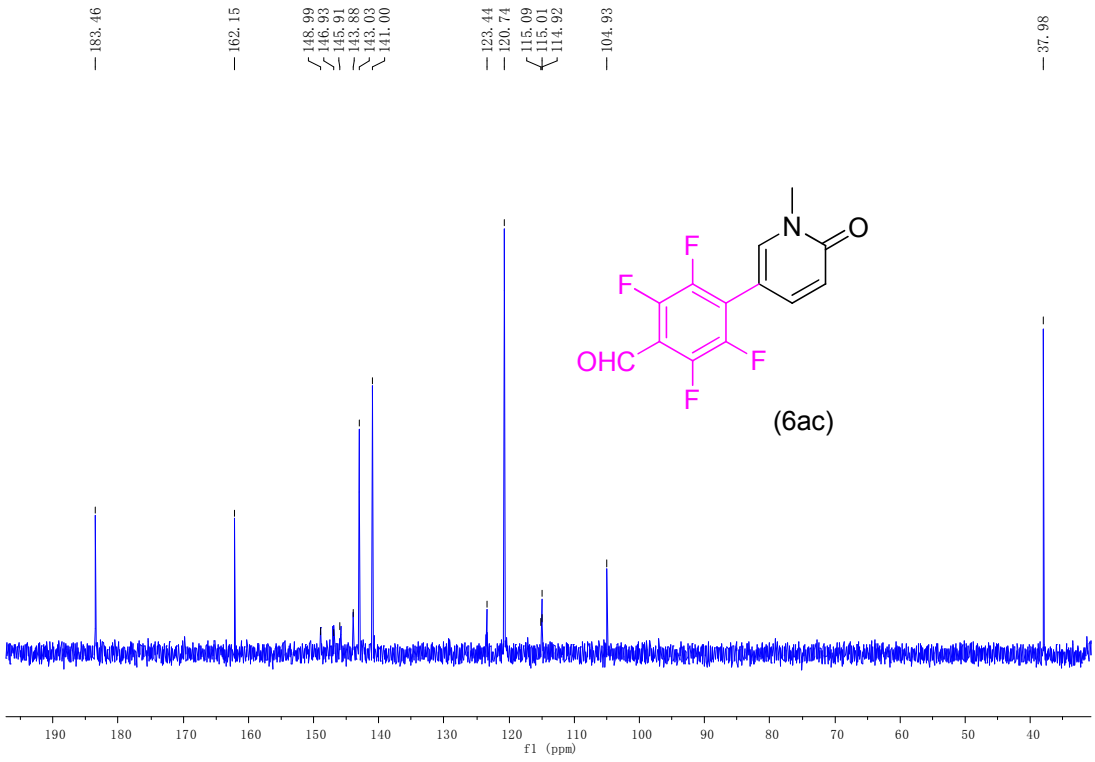

7.48
7.43
7.42
7.42
7.42
7.42
7.41
7.41
7.40
7.40
7.40
6.66
6.64
4.12
4.12
4.11
3.62
N
O
F
F
MeO
F
F
(6ab)
0.99
1.01
1.00
2.96
3.02
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

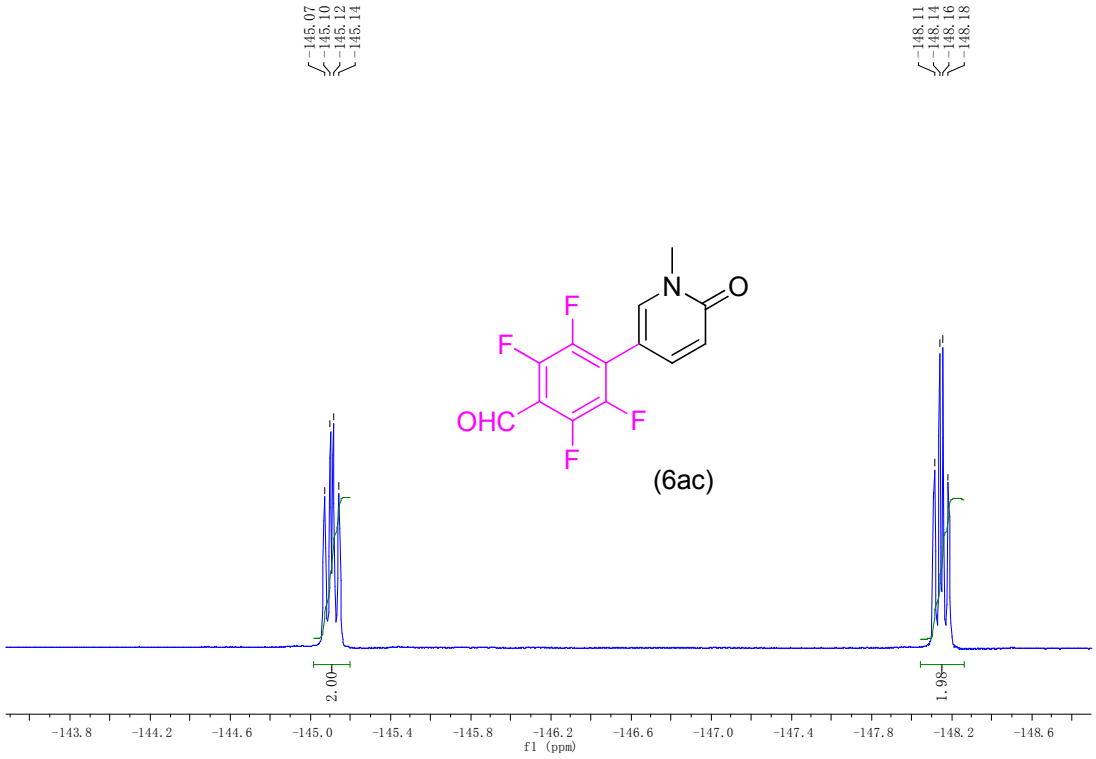

161.88
145.22
143.27
142.16
140.65
140.19
139.55
137.59
120.54
109.57
109.44
109.31
105.68
62.12
62.09
62.06
37.92
N
O
F
F
MeO
F
F
(6ab)
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

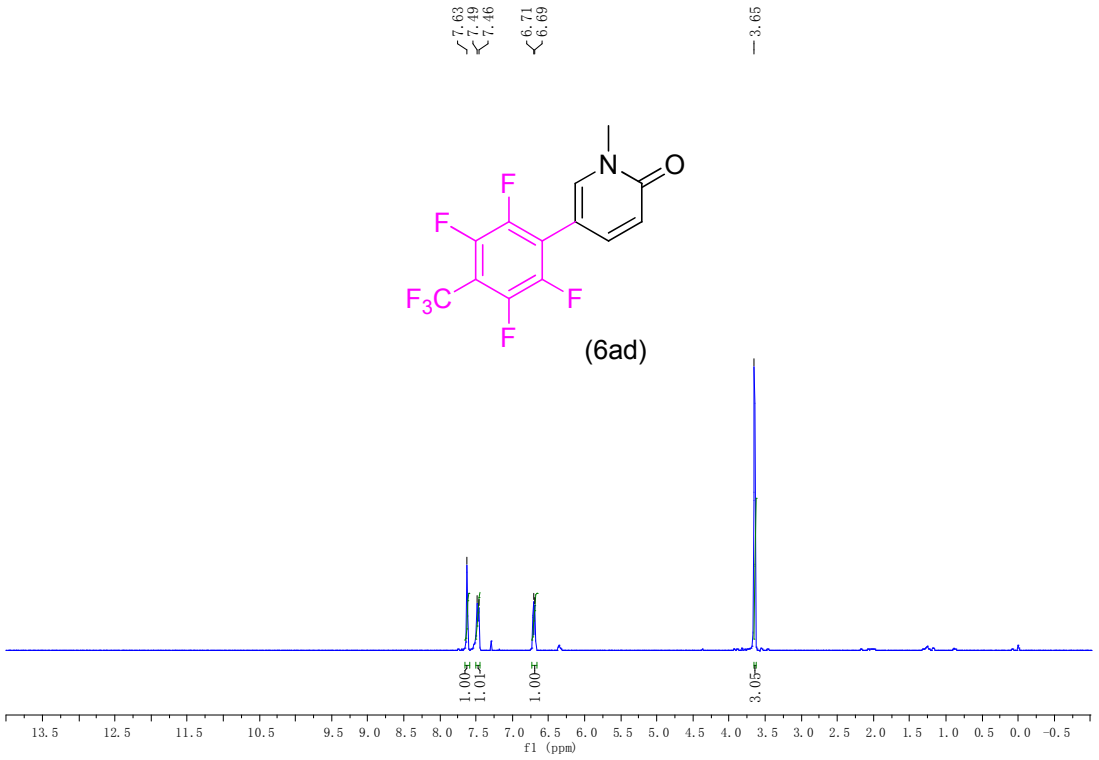

-148.06
-148.08
-148.11
-148.13
-160.61
-160.63
-160.66
-160.67
N
O
F
F
MeO
F
F
2.00
1.95
-147.0
-148.0
-149.0
-150.0
-151.0
-152.0
-153.0
-154.0
-155.0
-156.0
-157.0
-158.0
-159.0
-160.0
-161.0
f1 (ppm)

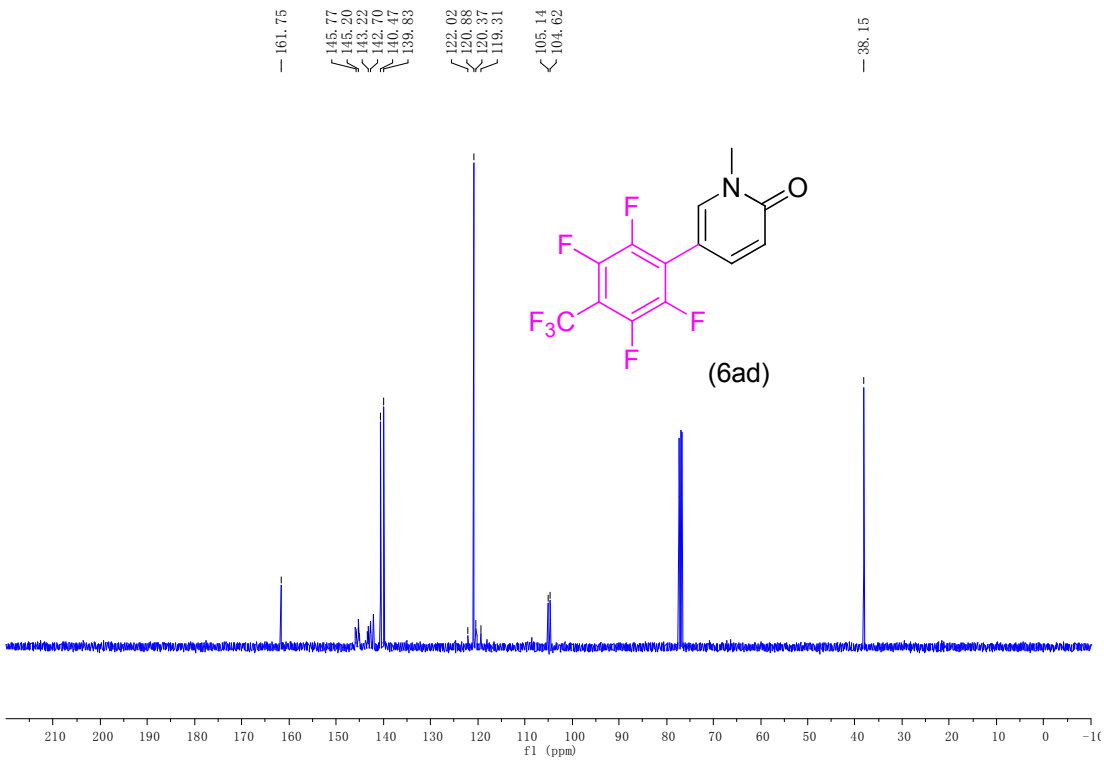
(6ab)

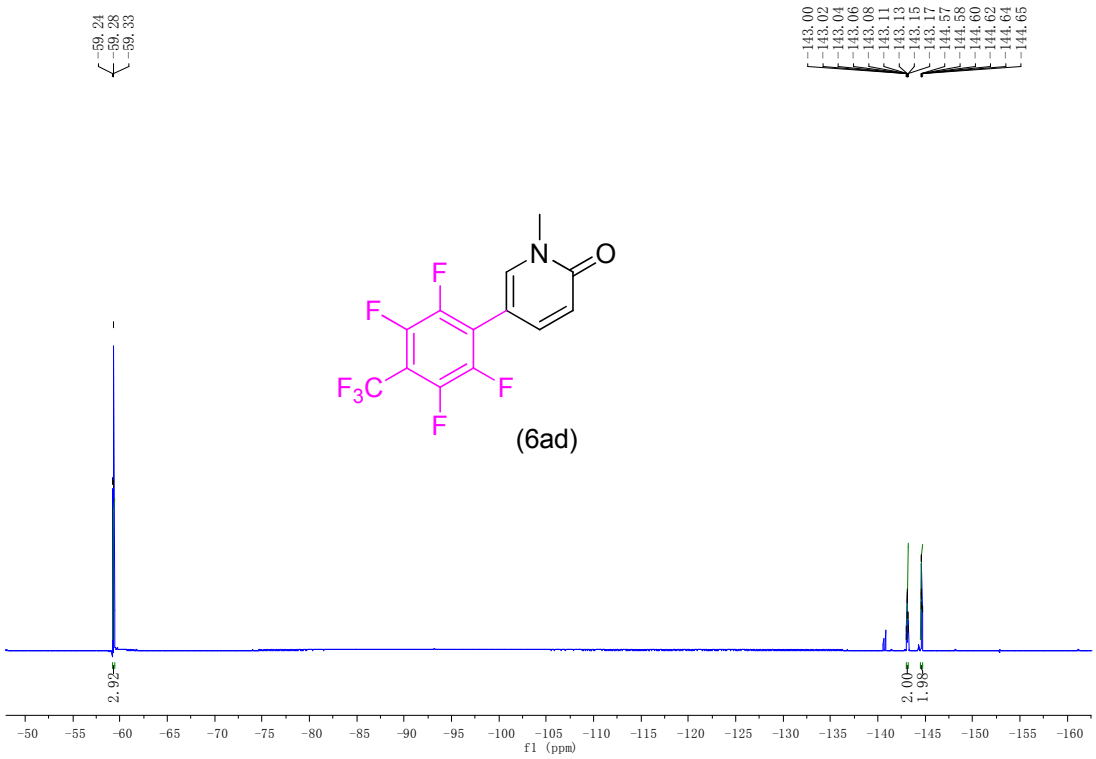

10.32
10.31
10.31
7.62
7.62
7.61
7.61
7.60
7.60
7.60
7.59
7.59
6.55
6.53
3.61
F
F
OHC
F
F
N
O
(6ac)
0.98
0.99
0.99
1.00
3.03
f1 (ppm)

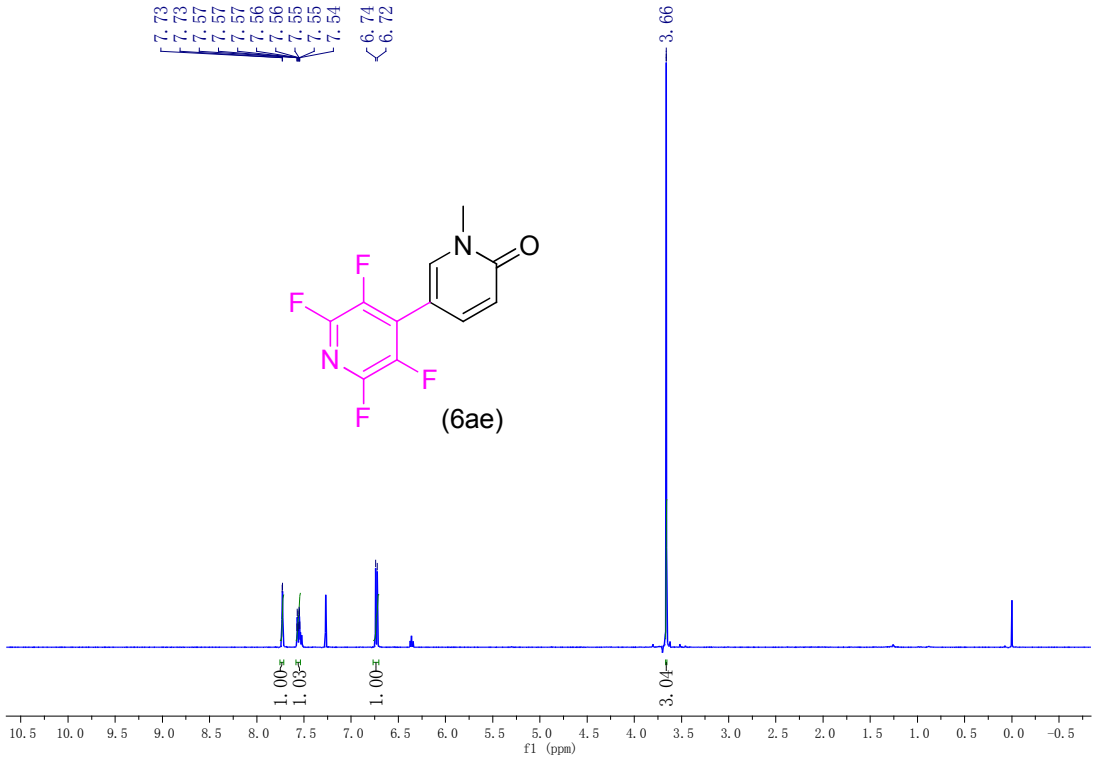

183.46
162.15
148.99
146.93
145.91
143.88
143.03
141.00
123.44
120.74
115.09
115.01
114.92
104.93
37.98
F
F
OHC
F
F
N
O
(6ac)
f1 (ppm)

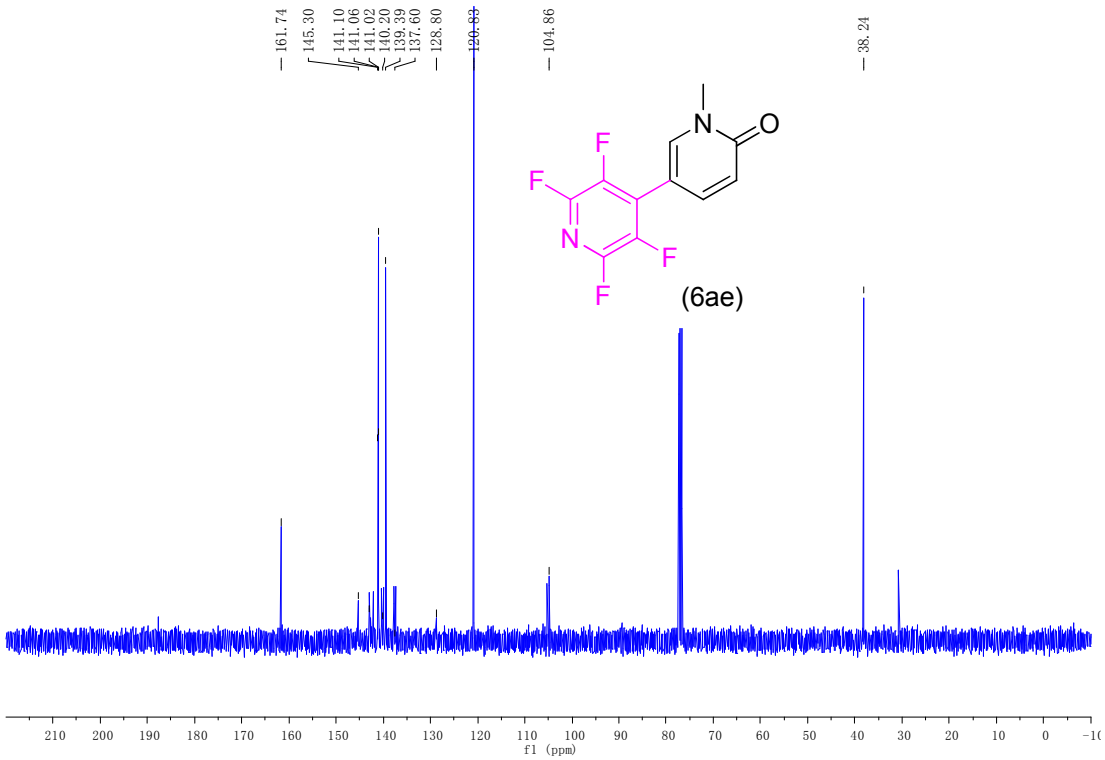

-145.07
-145.10
-145.12
-145.14
-148.11
-148.14
-148.16
-148.18
F
F
OHC
F
F
N
O
(6ac)
2.00
1.98
-143.8
-144.2
-144.6
-145.0
-145.4
-145.8
-146.2
-146.6
-147.0
-147.4
-147.8
-148.2
-148.6
f1 (ppm)

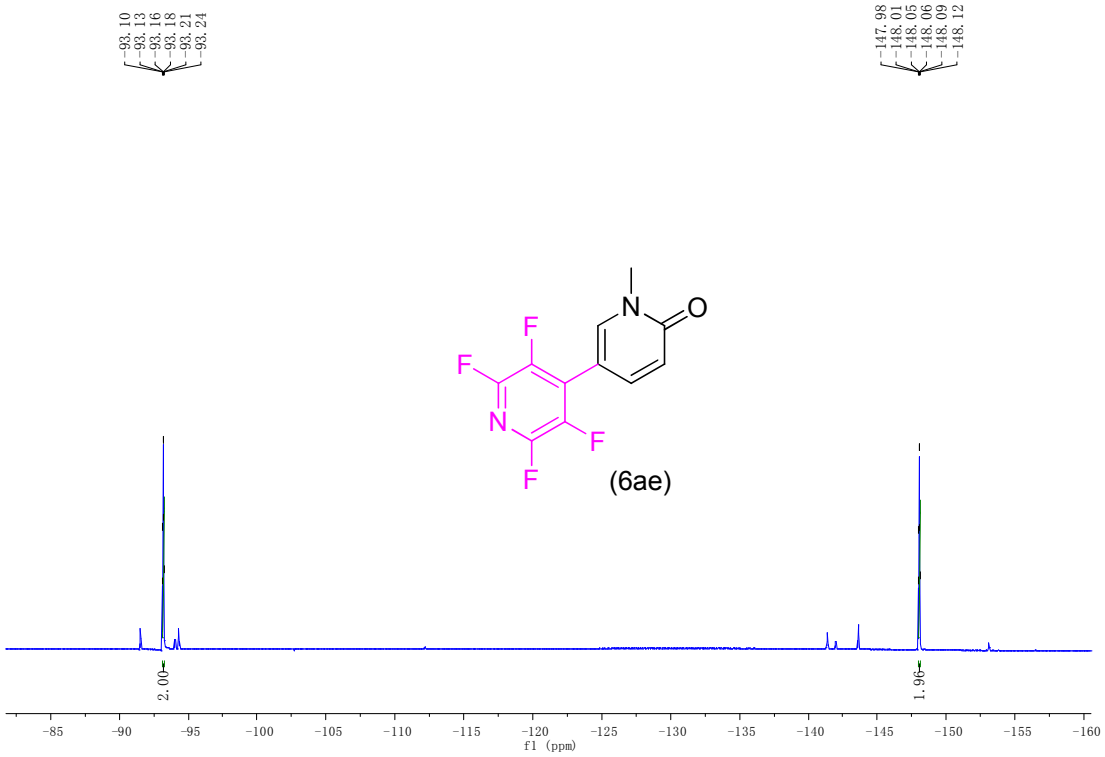

7.63
7.49
7.46
6.71
6.69
3.65
N
O
F
F
F3C
F
F
(6ad)
1.00
1.01
1.00
3.05
f1 (ppm)

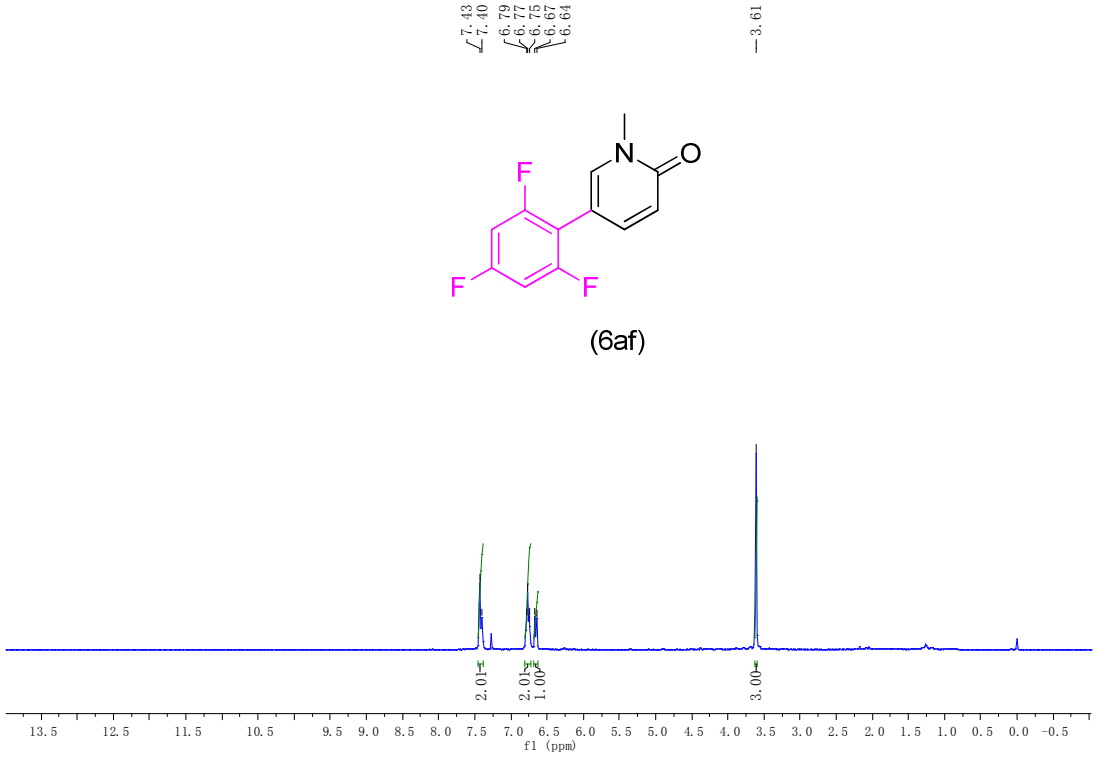

161.75
145.77
145.20
143.22
142.70
140.47
139.83
122.02
120.88
120.37
119.31
105.14
104.62
38.15
N
O
F
F
F3C
F
F
(6ad)
f1 (ppm)

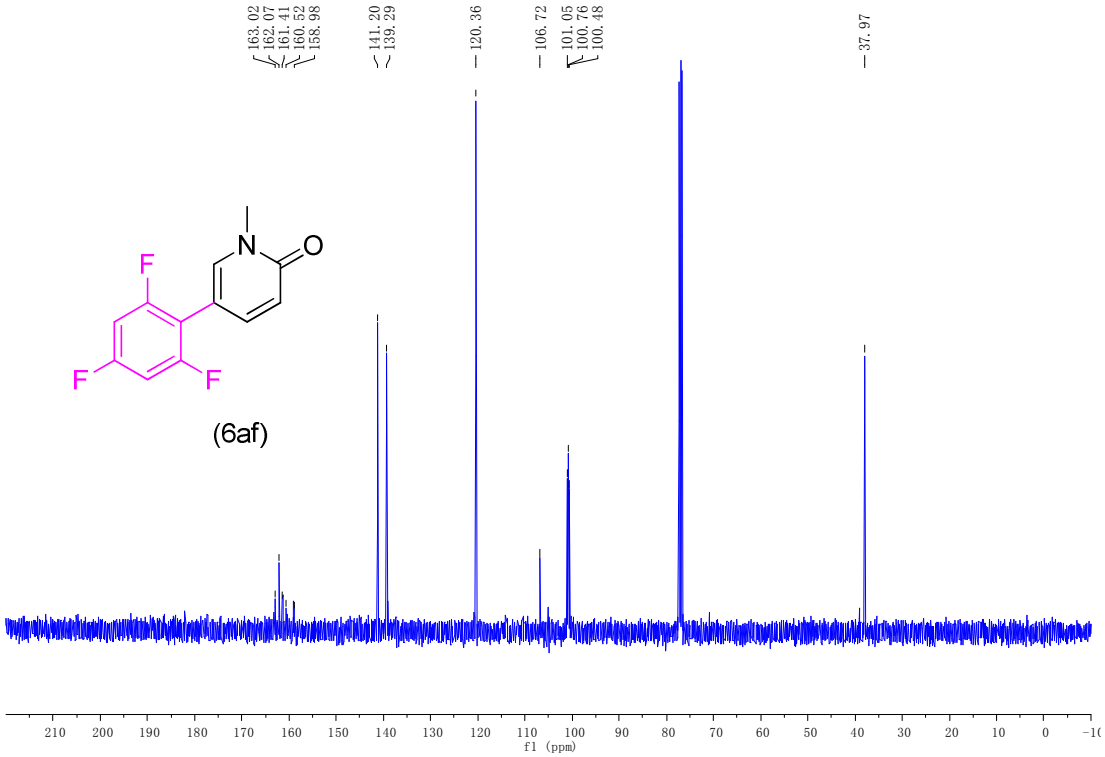

-59.24
-59.28
-59.33
-143.00
-143.02
-143.04
-143.06
-143.08
-143.11
-143.13
-143.15
-143.17
-144.57
-144.58
-144.60
-144.62
-144.64
-144.65
F
F
F3C
F
F
N
O
(6ad)
2.92
2.00
1.98
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
f1 (ppm)

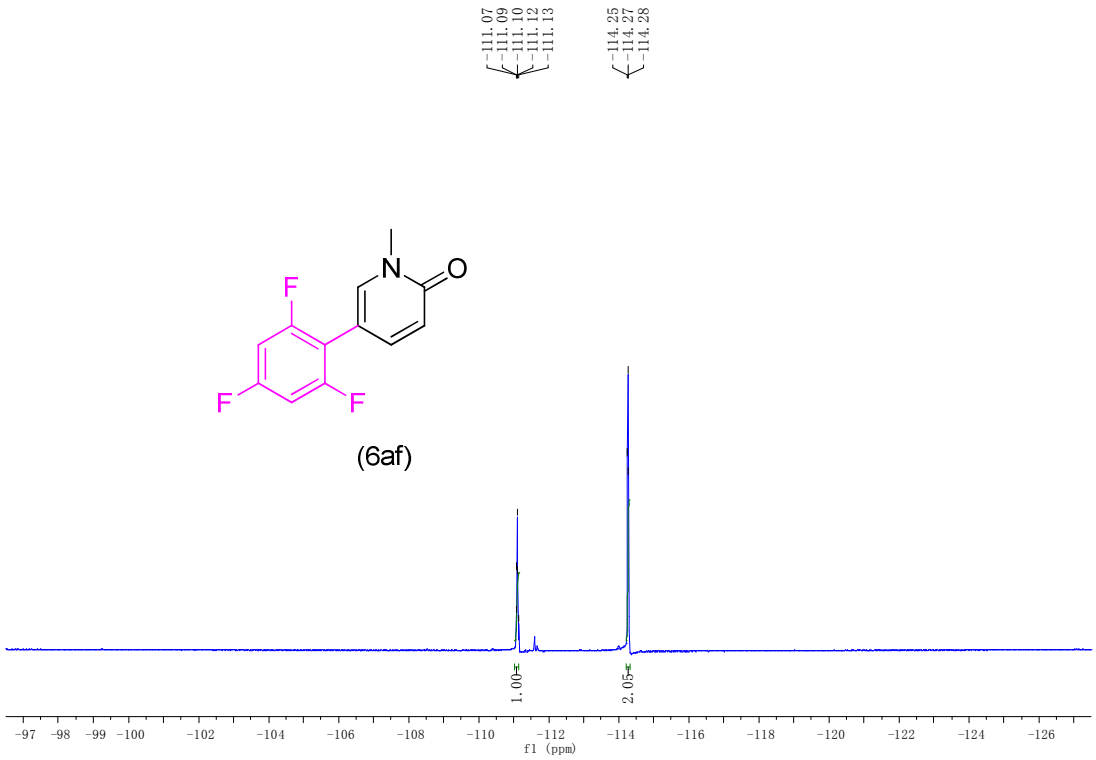

7.73
7.73
7.57
7.57
7.57
7.56
7.56
7.55
7.55
7.54
6.74
6.72
3.66
F
F
N
F
F
O
(6ae)
1.00
1.03
1.00
3.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

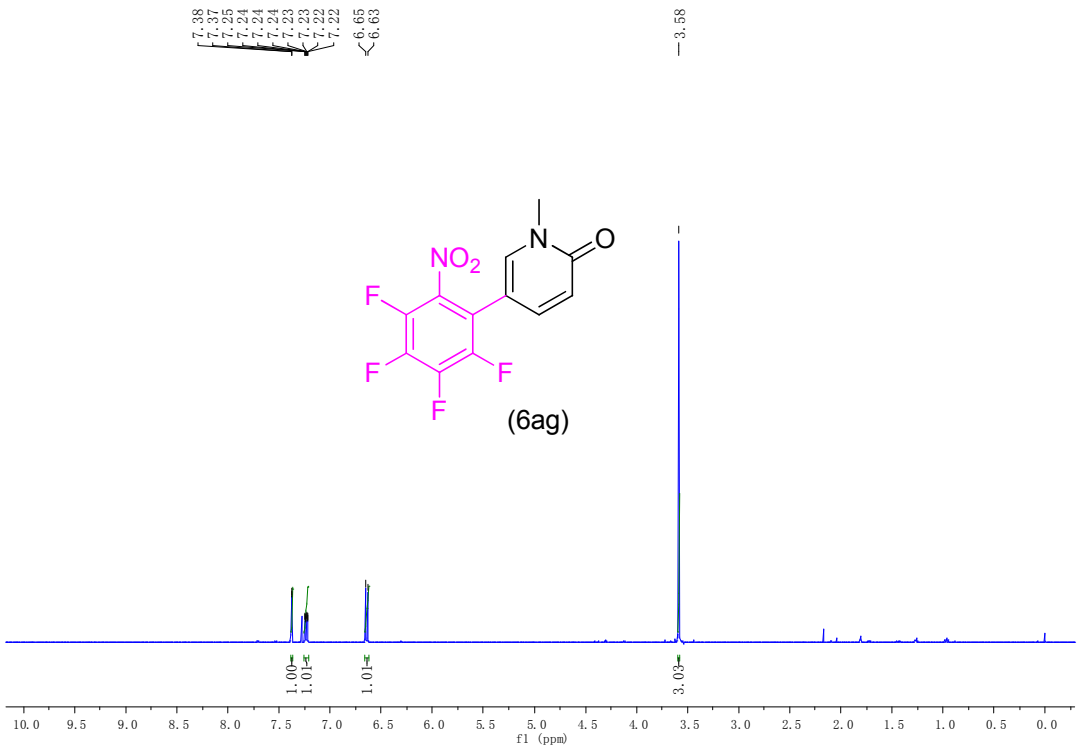

161.74
145.30
141.10
141.06
141.02
140.20
139.39
137.60
128.80
120.83
104.86
38.24
F
F
N
F
F
O
(6ae)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

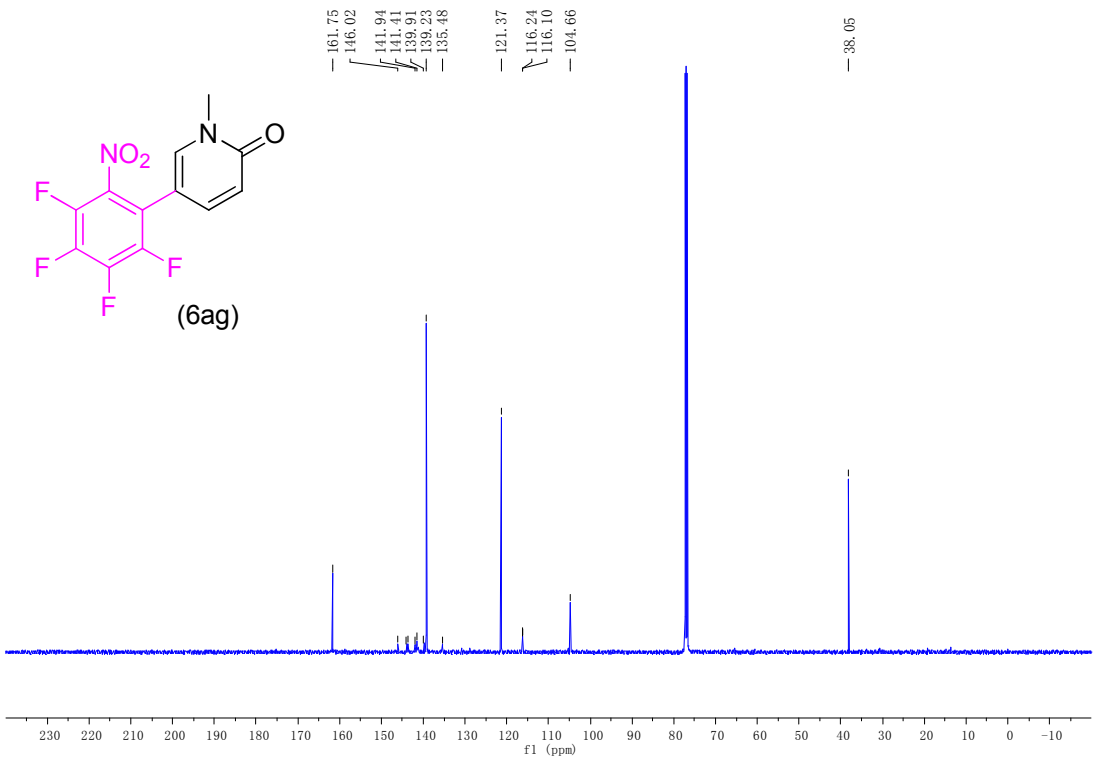

-93.10
-93.13
-93.16
-93.18
-93.21
-93.24
-147.98
-148.01
-148.05
-148.06
-148.09
-148.12
F
F
N
F
F
N
O
(6ae)
2.00
1.96
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
f1 (ppm)

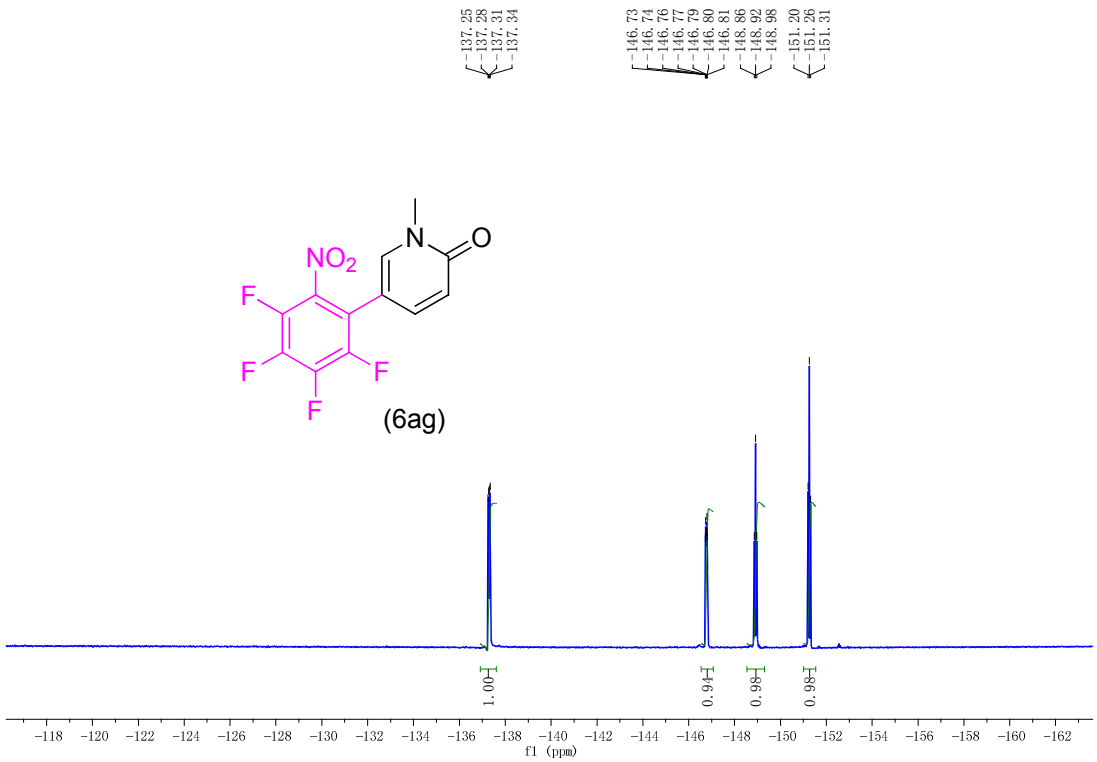

7.43
7.40
6.79
6.77
6.75
6.67
6.64
3.61
F
F
F
N
O
(6af)
2.01
2.01
1.00
3.00
f1 (ppm)

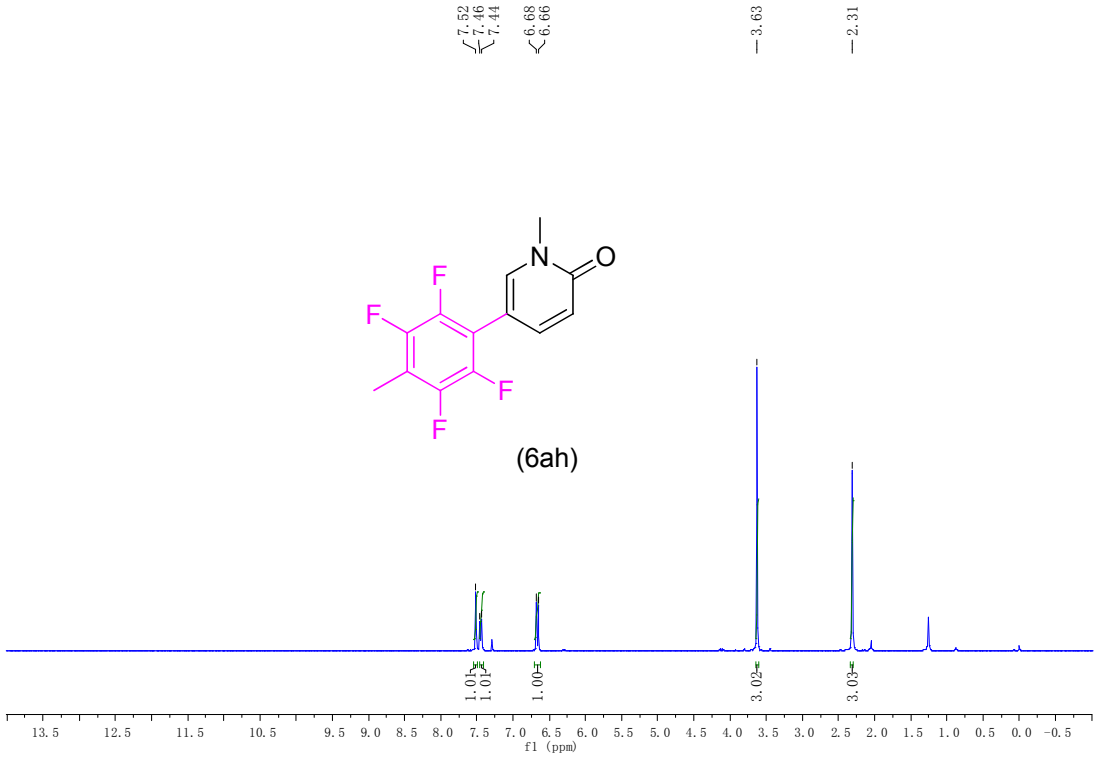

163.02
162.07
161.41
160.52
158.98
141.20
139.29
120.36
106.72
101.05
100.76
100.48
37.97
F
F
F
N
O
(6af)
f1 (ppm)

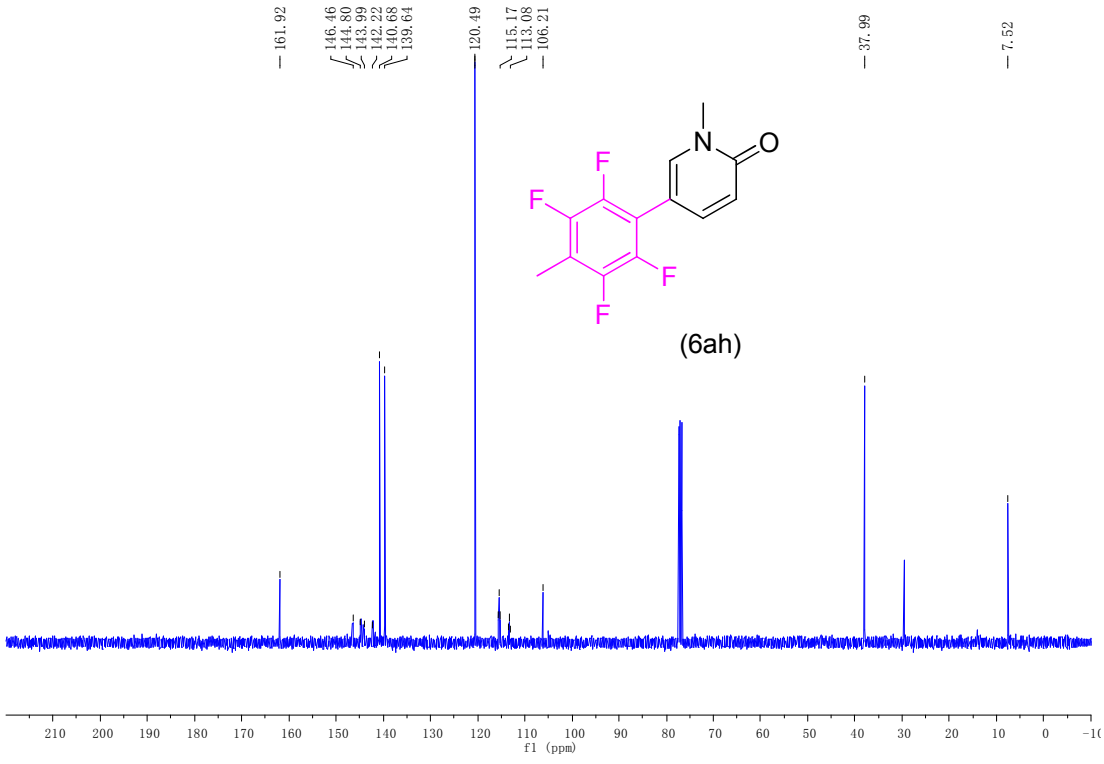

-111.07
-111.09
-111.10
-111.12
-111.13
-114.25
-114.27
-114.28
F
N
O
F
F
(6af)
1.00
2.05
-97 -98 -99 -100 -102 -104 -106 -108 -110 -112 -114 -116 -118 -120 -122 -124 -126
f1 (ppm)

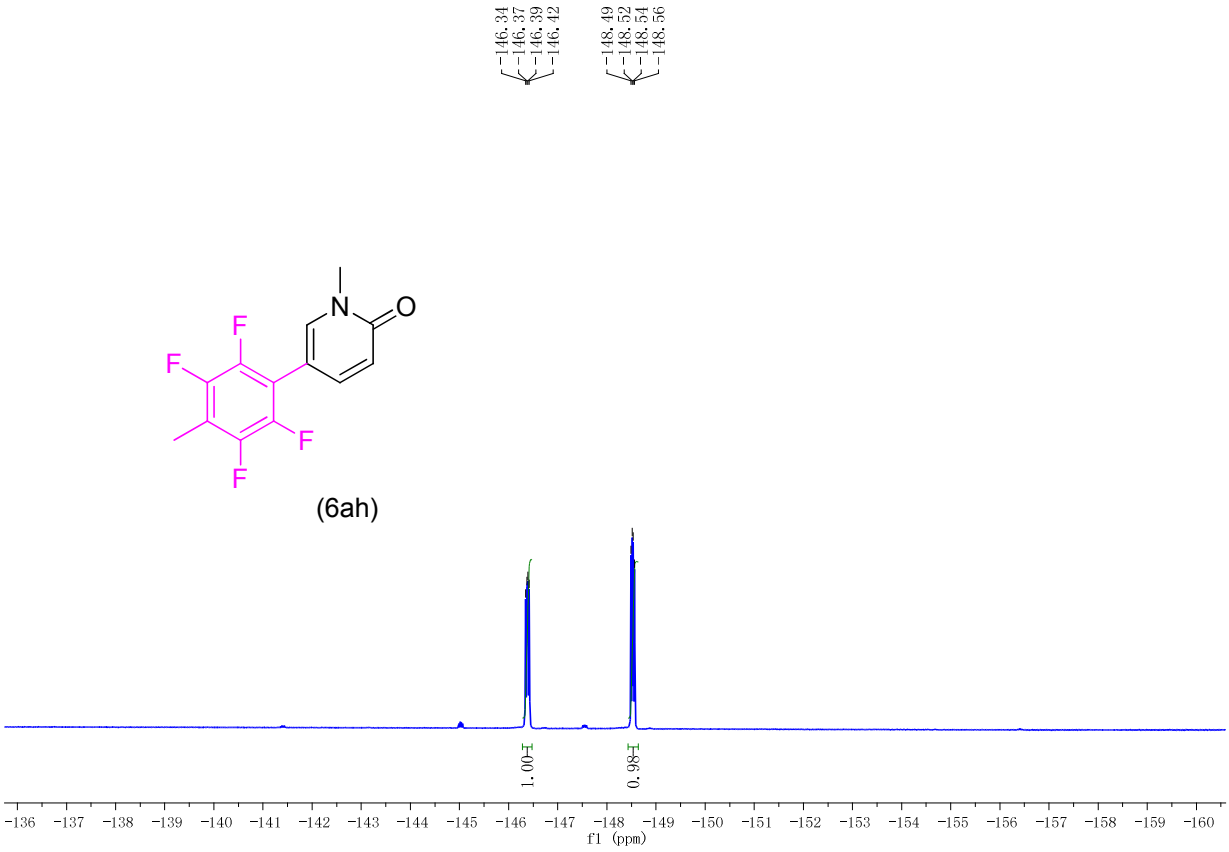

7.38
7.37
7.25
7.24
7.24
7.24
7.23
7.23
7.22
7.22
6.65
6.63
3.58
NO2
F
F
F
F
N
O
(6ag)
1.00
1.01
1.01
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


161.75
146.02
141.94
141.41
139.91
139.23
135.48
121.37
116.24
116.10
104.66
38.05
NO2
F
F
F
F
N
O
(6ag)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


137.25
137.28
137.31
137.34
146.73
146.74
146.76
146.77
146.79
146.80
146.81
148.86
148.92
148.98
151.20
151.26
151.31
NO2
F
F
F
F
N
O
(6ag)
1.00
0.94
0.98
0.98
−118 −120 −122 −124 −126 −128 −130 −132 −134 −136 −138 −140 −142 −144 −146 −148 −150 −152 −154 −156 −158 −160 −162
f1 (ppm)


7.52
7.46
7.44
6.68
6.66
3.63
2.31
F
F
F
F
N
O
(6ah)
1.01
1.01
1.00
3.02
3.03
f1 (ppm)


161.92
146.46
144.80
143.99
142.22
140.68
139.64
120.49
115.17
113.08
106.21
37.99
7.52
F
F
F
F
N
O
(6ah)
f1 (ppm)


146.34
146.37
146.39
146.42
148.49
148.52
148.54
148.56
N
O
F
F
F
F
(6ah)
1.00
0.98
−136 −137 −138 −139 −140 −141 −142 −143 −144 −145 −146 −147 −148 −149 −150 −151 −152 −153 −154 −155 −156 −157 −158 −159 −160
f1 (ppm)