Electronic Supplementary Information

Diversity-oriented Synthesis of Imidazo[2,1-*a*]isoquinolines

Shaoyu Mai,[a] Yixin Luo,[b] Xianyun Huang,[a] Zhenghao Shu,[a] Bingnan Li,[a] Yu Lan,[b] and Qiuling Song[a,*]

[a] Institute of Next Generation Matter Transformation, College of Chemical Engineering at Huaqiao University, 668 Jimei Blvd, Xiamen, Fujian, 361021, P. R. China

[b] School of Chemistry and Chemical Engineering, Chongqing University, Chongqing, 400030, P. R. China

*E-mail: qsong@hqu.edu.cn

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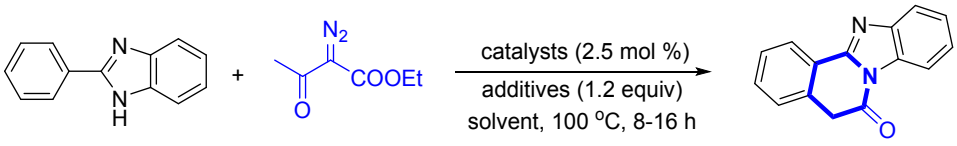
1. General Information

Unless specified, all metal complexes, reagents, and starting materials were purchased from commercial sources and used as received. Metal salts were stored in a nitrogen atmosphere dry box. Acetonitrile, methanol, toluene, THF, Et_2O, and CH_2Cl_2 were dried by filtration through alumina according to the procedure of Grubbs.[S1] Analytical thin layer chromatography was performed on 0.25 mm extra hard silica gel plates with UV254 fluorescent indicator. ^1H NMR and ^{13}C NMR spectra were recorded at ambient temperature using Bruker Avance III 500MHz NMR spectrometer. The data are reported as follows: chemical shift in ppm from internal tetramethylsilane on the δ scale, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integrations. High-resolution mass spectra (HRMS) were recorded with a Waters Micromass GCT Premier using an Agilent 1290 with electrospray ionization (ESI) technique.

2. Optimization of the Reaction Conditions

Table S1. Optimization of the reaction conditions



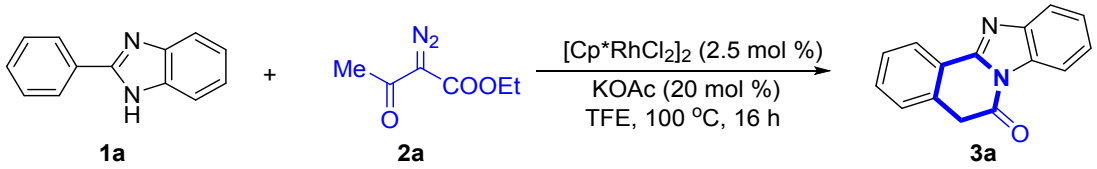
1a **2a** **3a**

entry	catalysts	additives	solvent	yield (%)[b]
1	$[Cp^*RhCl_2]_2$	-	DCE	0
2	$[Cp^*RhCl_2]_2$	-	Toluene	0
3	$[Cp^*RhCl_2]_2$	-	EtOH	trace
4	$[Cp^*RhCl_2]_2$	-	TFE	20
5	$[Cp^*RhCl_2]_2$	NaOAc	TFE	46
6	$[Cp^*RhCl_2]_2$	CsOAc	TFE	22
7	$[Cp^*RhCl_2]_2$	KOAc	TFE	54
8	$[Cp^*RhCl_2]_2$	HOAc	TFE	0
9[c]	$[Cp^*RhCl_2]_2$	KOAc	TFE	88
10[c, d]	$[Cp^*RhCl_2]_2$	KOAc	TFE	**99 (90)**[e]
11[c, d]	$[Ru(p\text{-cymene})Cl_2]$	KOAc	TFE	55
12[c, d]	$[Cp^*IrCl_2]_2$	KOAc	TFE	0
13[c, d]	$[Cp^*Co(CO)I_2]$	KOAc	TFE	0

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.24 mmol) in solvent (1.0 mL) at 100 °C for 8 h. [b]GC yields use *n*-Dodecane as an internal standard. [c]20 mol% KOAc was used for 16 h (entries 9-13). [d]1.5 mL TFE was used. [e]Isolated yield. TFE = 2,2,2-Trifluoroethanol.

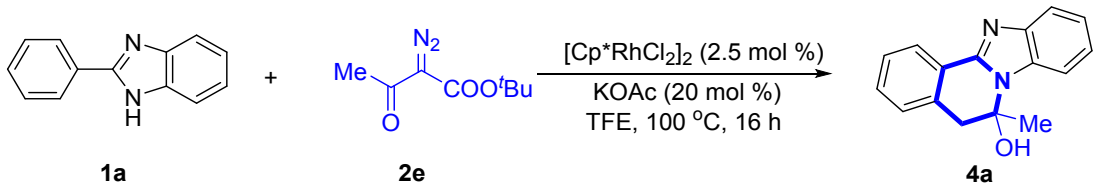
3. General Procedure for Cp*Rh^{III}-Catalyzed [4+2] Annulation

3.1 Synthesis of Imidazo[2,1-*a*]isoquinolin-6(5*H*)-ones by [Cp*RhCl$_2$]$_2$/KOAc System



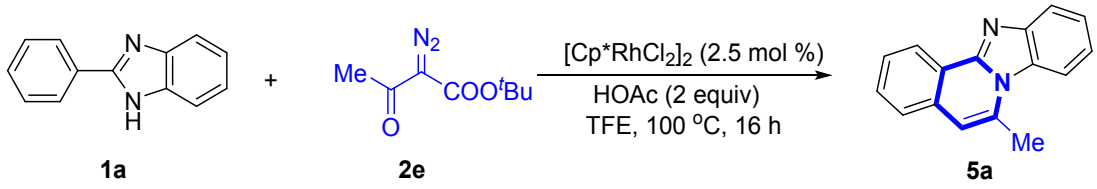
A 25 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **1a** (38.8 mg, 0.2 mmol), ethyl 2-diazo-3-oxobutanoate **2a** (37.4 mg, 0.24 mmol), [Cp*RhCl$_2$]$_2$ (3.1 mg, 0.005 mmol), KOAc (3.9 mg, 0.04 mmol), and TFE (1.5 mL). The reaction mixture was stirred at 100 °C under nitrogen atmosphere for 16 h. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc: 10/1), giving the expected product **3a** (42.1 mg, 90%) as a yellow solid.

3.2 Synthesis of 5,6-Dihydroimidazo[2,1-*a*]isoquinolin-5-ols by [Cp*RhCl$_2$]$_2$/KOAc System



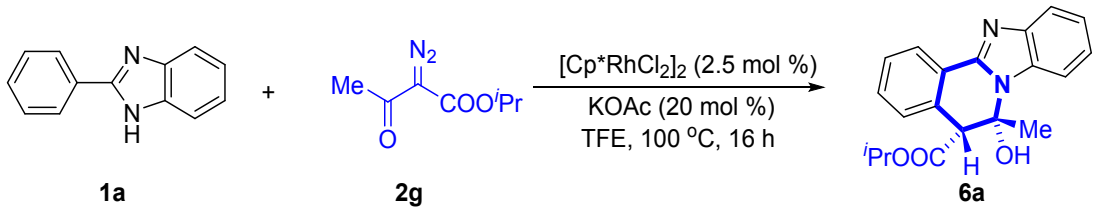
A 25 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **1a** (38.8 mg, 0.2 mmol), *tert*-butyl 2-diazo-3-oxobutanoate **2e** (44.1 mg, 0.24 mmol), [Cp*RhCl$_2$]$_2$ (3.1 mg, 0.005 mmol), KOAc (3.9 mg, 0.04 mmol), and TFE (1.5 mL). The reaction mixture was stirred at 100 °C under nitrogen atmosphere for 16 h. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc: 5/1), giving the expected product **4a** (36.0 mg, 72%) as a white solid.

3.3 Synthesis of Imidazo[2,1-*a*]isoquinolines by [Cp*RhCl$_2$]$_2$/HOAc System



A 25 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **1a** (38.8 mg, 0.2 mmol), *tert*-butyl 2-diazo-3-oxobutanoate **2e** (44.1 mg, 0.24 mmol), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol), HOAc (24 μL, 0.4 mmol), and TFE (1.5 mL). The reaction mixture was stirred at 100 °C under nitrogen atmosphere for 16 h. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc: 15/1), giving the expected product **5a** (45.9 mg, 99%) as a yellow solid.

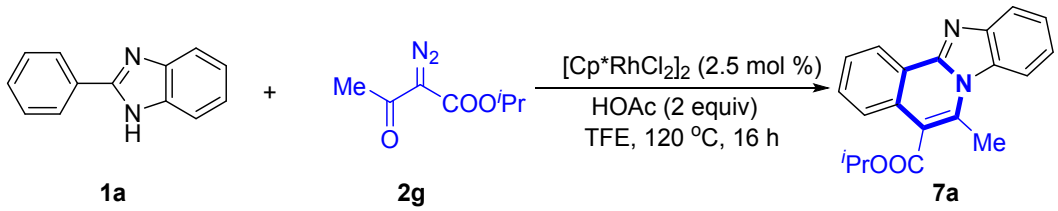
3.4 Synthesis of Isopropyl 5-hydroxy-imidazo[2,1-*a*]isoquinoline-6-carboxylates by $[Cp^*RhCl_2]_2$/KOAc System



1a **2g** **6a**

A 25 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **1a** (38.8 mg, 0.2 mmol), isopropyl 2-diazo-3-oxobutanoate **2g** (40.8 mg, 0.24 mmol), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol), KOAc (3.9 mg, 0.04 mmol), and TFE (1.5 mL). The reaction mixture was stirred at 100 °C under nitrogen atmosphere for 16 h. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc: 5/1), giving the expected product **6a** (61.8 mg, 92%) as a white solid.

3.5 Synthesis of Isopropyl imidazo[2,1-*a*]isoquinoline-6-carboxylates by $[Cp^*RhCl_2]_2$/HOAc System

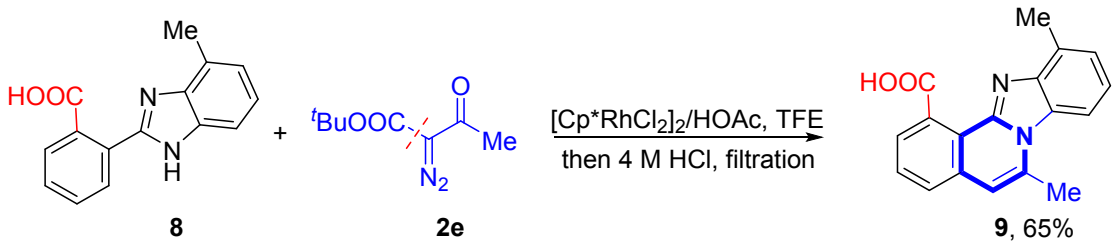


1a **2g** **7a**

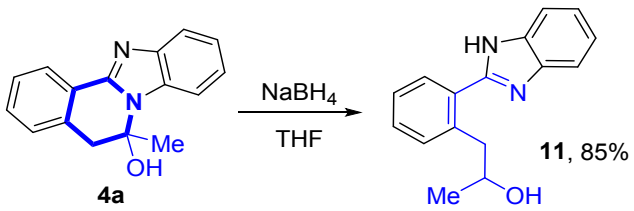
A 25 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **1a** (38.8 mg, 0.2 mmol), isopropyl 2-diazo-3-oxobutanoate **2g** (40.8 mg, 0.24 mmol), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol), KOAc (3.9 mg, 0.04 mmol), and TFE (1.5 mL). The reaction mixture was stirred at 100 °C under nitrogen atmosphere for 16 h. After the reaction was completed, the solvent was evaporated and the

organic product purified by column chromatography (petroleum ether/EtOAc: 5/1), giving the expected product **7a** (31.8 mg, 50%) as a yellow solid.

4. Synthetic Applications

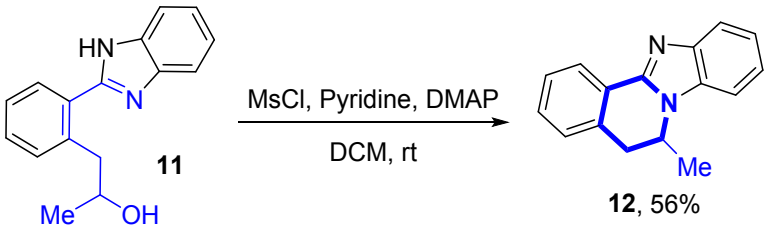


A 100 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **8** (252 mg, 1.0 mmol), *tert*-butyl 2-diazo-3-oxobutanoate **2e** (220.5 mg, 1.2 mmol), $[Cp^*RhCl_2]_2$ (15.5 mg, 0.025 mmol), HOAc (120 μL, 2 mmol), and TFE (7.5 mL). The reaction mixture was stirred at 100 °C under nitrogen atmosphere for 16 h. After the reaction was completed, 4 M HCl in MeOH (0.5 mL) was added. After further stirring at 100 °C for 1 h, the reaction came to end and solid was precipitated out as the desired product. The precipitate was colleted by filtration and washed by petroleum ether, and then kept in desiccator under vacuum to afford the **6,11-dimethylbenzo[4,5]imidazo[2,1-*a*]isoquinoline-1-carboxylic acid 9** (188.5 mg, 65%) as a gray solid, m. p. = 117–118; **^{1}H NMR (500 MHz, CF_3COOD)** δ 9.11 (d, J = 7.5 Hz, 1H), 8.42 (d, J = 7.1 Hz, 2H), 8.19 (t, J = 7.7 Hz, 1H), 7.78 (d, J = 3.5 Hz, 2H), 7.69 (s, 1H), 3.39 (s, 3H), 2.89 (s, 3H); **^{13}C NMR (126 MHz, CF_3COOD)** δ 174.4, 143.1, 139.5, 139.3, 138.4, 137.0, 134.9, 132.0, 131.9, 130.7, 129.0, 127.4, 127.2, 119.7, 116.9, 115.7, 20.0, 16.7. **HRMS (ESI) calcd for** $C_{18}H_{15}N_2O_2^+$ $[M + H]^+$: 291.1128; Found: 291.1123.

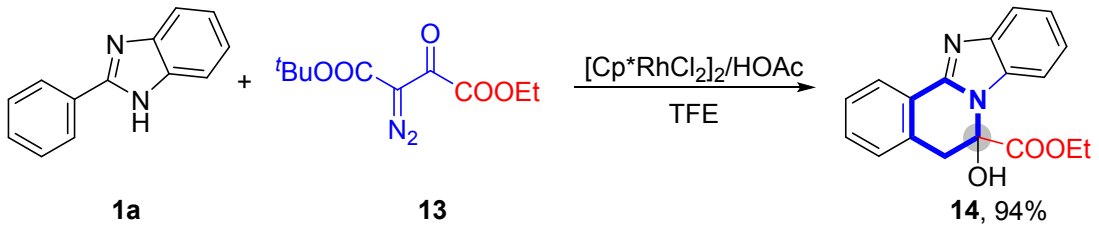


A 50 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **4a** (250 mg, 1 mmol), Sodium borohydride (76 mg, 2 mmol), and THF (10 mL). The reaction mixture was stirred at room temperature for 3 h. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc: 1/1), giving the **1-(2-(1*H*-benzo[*d*]imidazol-2-yl)phenyl)propan-2-ol 11** (214 mg, 85%) as a white solid, m. p. = 193–194; **^{1}H NMR (500 MHz, DMSO)** δ 7.77–7.72 (m, 1H), 7.65 (dt, J = 6.6, 3.3 Hz, 2H), 7.54–7.46 (m, 2H), 7.46–7.40 (m, 1H), 7.31–7.25 (m, 2H), 3.95–3.85 (m,

1H), 3.07 (ddd, J = 21.0, 13.3, 6.2 Hz, 2H), 1.12 (d, J = 6.2 Hz, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 153.0, 140.0, 132.6, 131.0, 130.6, 130.4, 127.2, 126.4, 123.2, 116.0, 68.7, 43.0, 25.0; **HRMS (ESI) calcd for** $C_{16}H_{17}N_2O^+$ $[M + H]^+$: 253.1335; Found: 253.1338.

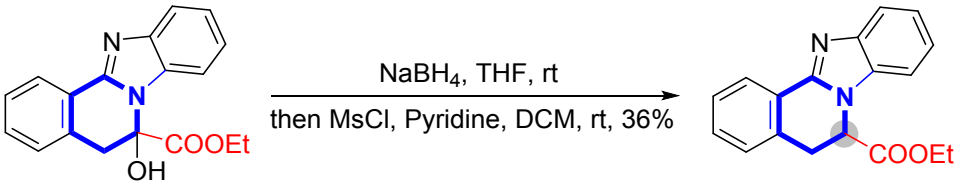


A 25 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **11** (50.4, 0.5 mmol), MsCl (286 mg, 2.5 mmol), Pyridine (198 mg, 5 mmol), DMAP (30.5 mg, 0.25 mmol) and DCM (5 mL). The reaction mixture was stirred at room temperature for 12 h. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc: 3/1), giving the **6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline 12** (65.5 mg, 56%) as a white solid, m. p. = 100–101; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.31 (dd, J = 5.7, 3.2 Hz, 1H), 7.88–7.80 (m, 1H), 7.45–7.36 (m, 3H), 7.34–7.27 (m, 3H), 4.94–4.82 (m, 1H), 3.58 (dd, J = 15.7, 6.6 Hz, 1H), 2.98 (d, J = 15.1 Hz, 1H), 1.33 (d, J = 6.7 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 147.9, 143.7, 133.6, 132.6, 130.4, 129.0, 127.7, 125.9, 125.6, 122.7, 122.5, 119.7, 109.0, 47.4, 34.7, 19.4; **HRMS (ESI) calcd for** $C_{16}H_{15}N_2^+$ $[M + H]^+$: 235.1230; Found: 235.1232.



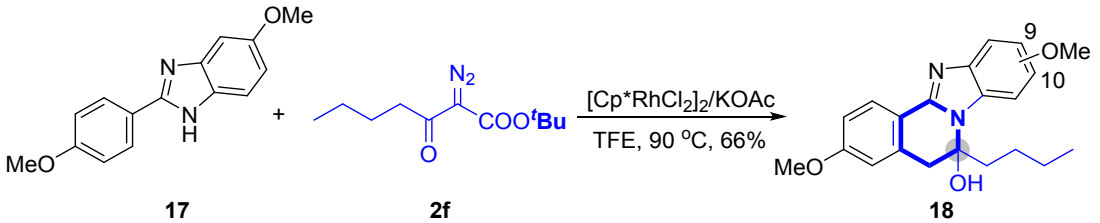
A 100 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **1a** (194 mg, 1.0 mmol), **13** (290 mg, 1.2 mmol), $[Cp^*RhCl_2]_2$ (15.5 mg, 0.025 mmol), HOAc (120 µL, 2 mmol), and TFE (7.5 mL). The reaction mixture was stirred at 100 °C under nitrogen atmosphere for 16 h. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc: 5/1), giving the **ethyl 6-hydroxy-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-6-carboxylate 14** (31.8 mg, 94%) as a white solid, m. p. = 120–114; **^{1}H NMR (500 MHz, DMSO)** δ 8.24–8.16 (m, 1H), 8.14 (s, 1H), 7.73 (d, J = 5.6 Hz, 2H), 7.52–7.41 (m, 3H), 7.31–7.22 (m, 2H), 4.18–

4.02 (m, 2H), 3.68 (dd, J = 65.7, 16.1 Hz, 2H), 1.03 (t, J = 7.0 Hz, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 170.0, 149.7, 144.6, 134.8, 133.1, 131.3, 129.3, 128.7, 126.2, 125.8, 123.7, 123.3, 120.1, 114.0, 86.6, 62.9, 14.7; **HRMS (ESI) calcd for** $C_{18}H_{17}N_2O_3^+$ $[M + H]^+$: 309.1234; Found: 309.1233.



14 **15**, 36%

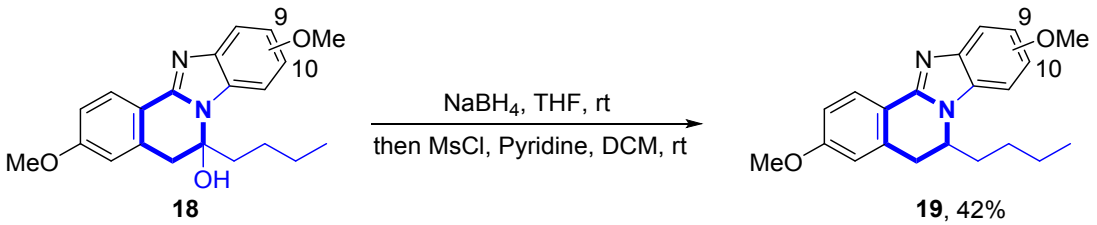
A 25 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **14** (154 mg, 0.5 mmol), Sodium borohydride (9.5 mg, 0.25 mmol), and THF (4 mL). The reaction mixture was stirred at room temperature for 3 h. After the reaction was completed, the solvent was evaporated and the MsCl (286 mg, 2.5 mmol), Pyridine (198 mg, 5 mmol), DMAP (30.5 mg, 0.25 mmol) and DCM (5 mL) were added. The reaction mixture was stirred at room temperature for 12 h. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc: 5/1), giving the **ethyl 5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-6-carboxylate 15** (52.6 mg, 36%) as slight yellow oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.31 (d, J = 7.2 Hz, 1H), 7.85 (dd, J = 5.4, 2.6 Hz, 1H), 7.47–7.35 (m, 2H), 7.35–7.27 (m, 4H), 5.27 (d, J = 5.9 Hz, 1H), 4.02 (q, J = 7.1 Hz, 2H), 3.63 (dt, J = 36.6, 11.3 Hz, 2H), 1.01 (t, J = 7.1 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 169.1, 148.6, 143.6, 134.5, 131.5, 130.4, 128.2, 128.1, 126.1, 125.7, 123.1, 122.9, 119.9, 108.9, 62.0, 53.4, 31.4, 13.9; **HRMS (ESI) calcd for** $C_{18}H_{17}N_2O_2^+$ $[M + H]^+$: 293.1285; Found: 293.1287.



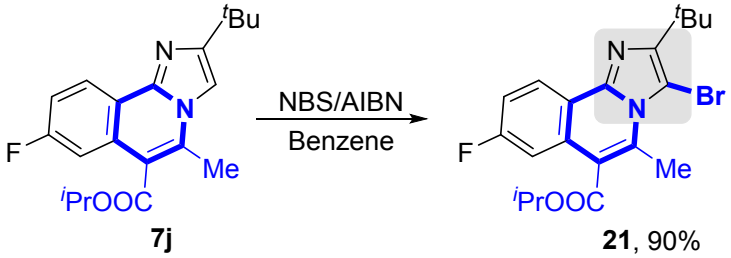
17 **2f** **18**

A 100 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **17** (254 mg, 1.0 mmol), **2f** (271 mg, 1.2 mmol), $[Cp^*RhCl_2]_2$ (15.5 mg, 0.025 mmol), HOAc (120 μL, 2 mmol), and TFE (7.5 mL). The reaction mixture was stirred at 90 °C under nitrogen atmosphere for 12 h. After the reaction was completed,

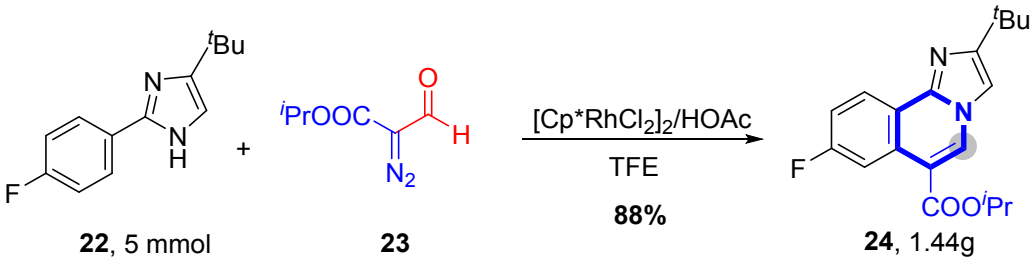
the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc: 2/1), giving the mixture **18** (232 mg, 66%) as a yellow oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.85 (d, J = 8.5 Hz, 1H), 7.75 (t, J = 8.4 Hz, 2H), 7.36 (dd, J = 23.6, 5.3 Hz, 6.81 (d, J = 1.5 Hz), 6.70 (td, J = 9.1, 2.1 Hz), 6.57–6.42 (m), 3.76 (s), 3.74 (s), 3.73 (s), 3.64 (s), 3.27 (dd, J = 99.4, 15.6 Hz), 1.28–1.19 (m), 1.18–1.04 (m), 0.73 (t, J = 6.7 Hz); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 161.0, 160.8, 156.0, 148.6, 148.1, 143.4, 137.4, 135.4, 135.0, 134.1, 127.9, 126.9, 126.7, 118.4, 118.0, 117.7, 114.2, 113.3, 112.7, 112.6, 112.4, 111.5, 99.9, 97.5, 88.9, 82.5, 60.5, 55.8, 55.3, 55.2, 42.1, 39.1, 39.0, 31.6, 26.0, 24.7, 22.6, 13.9; **HRMS (ESI) calcd for** $C_{21}H_{25}N_2O_3^+$ $[M + H]^+$: 353.1860; Found: 353.1860.



A 25 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **18** (176 mg, 0.5 mmol), Sodium borohydride (38 mg, 1 mmol), and THF (4 mL). The reaction mixture was stirred at room temperature for 3 h. After the reaction was completed, the solvent was evaporated and the MsCl (286 mg, 2.5 mmol), Pyridine (198 mg, 5 mmol), DMAP (30.5 mg, 0.25 mmol) and DCM (5 mL) were added. The reaction mixture was stirred at room temperature for 12 h. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc: 5/1), giving the expected mixture **19** (70.5 mg, 42%, 2:1) as yellow oil. Major isomer was isolated: **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.37 (dd, J = 10.4, 4.3 Hz, 2H), 6.96 (s, 1H), 6.83 (dd, J = 8.7, 2.3 Hz, 1H), 6.73 (d, J = 2.5 Hz, 1H), 6.44 (dd, J = 8.5, 2.5 Hz, 1H), 4.07–3.90 (m, 1H), 3.79 (s, 3H), 3.65 (s, 3H), 3.04 (dd, J = 13.7, 9.7 Hz, 1H), 2.77 (dd, J = 13.7, 2.9 Hz, 1H), 1.68 (qt, J = 13.4, 6.8 Hz, 2H), 1.59–1.32 (m, 3H), 0.93 (t, J = 7.2 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 160.3, 156.2, 151.9, 140.2, 133.2, 131.0, 123.2, 116.6, 115.4, 113.2, 111.9, 111.6, 99.9, 74.1, 55.7, 55.1, 40.1, 38.3, 27.9, 22.9, 14.2; **HRMS (ESI) calcd for** $C_{21}H_{25}N_2O_2^+$ $[M + H]^+$: 337.1911; Found: 337.1912.



A 25 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **7j** (68.4 mg, 0.2 mmol), NBS (78.3 mg, 0.44 mmol), AIBN (1.6 mg, 0.02 mmol) and Benzene (2.5 mL). The reaction mixture was stirred at 90 °C for 4 h. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc: 20/1), giving the **isopropyl 3-bromo-2-(*tert*-butyl)-8-fluoro-5-methylimidazo[2,1-*a*]isoquinoline-6-carboxylate 21** (76 mg, 90%) as a yellow solid, m. p. = 150–152;. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.62 (dd, J = 8.9, 5.7 Hz, 1H), 7.31–7.26 (m, 1H), 7.21 (dd, J = 10.1, 2.4 Hz, 1H), 5.41 (dt, J = 12.6, 6.3 Hz, 1H), 3.08 (s, 3H), 1.53 (s, 9H), 1.45 (d, J = 6.3 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 167.0, 162.5 (d, J = 248.1 Hz), 152.0, 142.0, 134.0, 127.8 (d, J = 9.6 Hz), 126.0 (d, J = 9.1 Hz), 119.6 (d, J = 2.0 Hz), 118.8 (d, J = 3.6 Hz), 116.5 (d, J = 23.8 Hz), 109.0 (d, J = 23.8 Hz), 70.0, 33.4, 29.4, 21.8, 19.7; **HRMS (ESI) calcd for** $C_{20}H_{23}BrFN_2O_2^+$ $[M + H]^+$: 310.1350; Found: 310.1346.

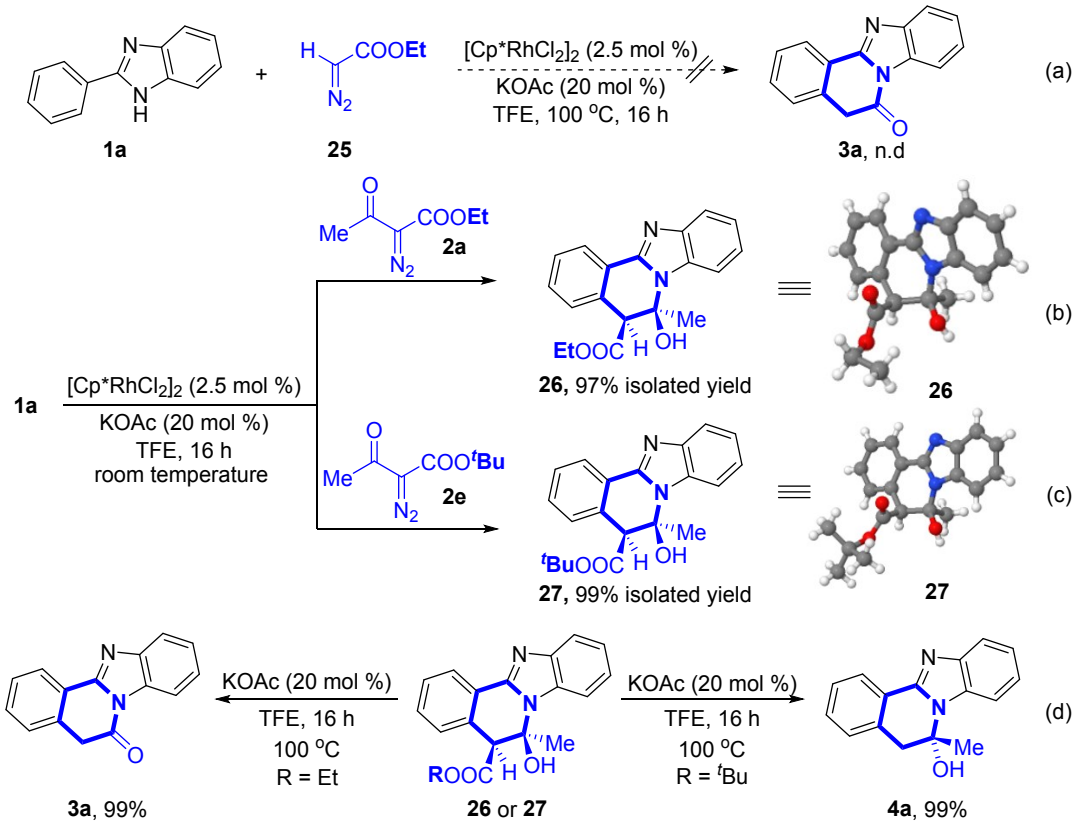


22, 5 mmol **23** **24**, 1.44g

A 100 mL round bottom Schlenk flask equipped with a magnetic stirring bar was charged with **22** (1.09 g, 5.0 mmol), **23** (936 mg, 6 mmol), $[Cp^*RhCl_2]_2$ (77.5 mg, 0.025 mmol), HOAc (600 μL, 2 mmol), and TFE (37.5 mL). The reaction mixture was stirred at 120 °C under nitrogen atmosphere for 16 h. After the reaction was completed, the solvent was evaporated and the organic product purified by column chromatography (petroleum ether/EtOAc: 20/1), giving the **isopropyl 2-(*tert*-butyl)-8-fluoroimidazo[2,1-*a*]isoquinoline-6-carboxylate 24** (1.44g, 88%) as a white solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.75 (s, 1H), 8.69–8.60 (m, 2H), 7.35–7.30 (m, 1H), 7.32 (s, 1H), 5.33 (hept, J = 6.3 Hz, 1H), 1.43 (d, J = 6.3 Hz, 6H), 1.42 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 164.8, 162.7 (d, J = 246.6 Hz), 157.1, 143.0, 130.8, 128.8 (d, J = 10.4 Hz), 126.1 (d, J = 9.1 Hz), 120.0, 116.5 (d, J = 23.9 Hz), 112.4 (d, J = 3.7 Hz), 111. 6 (d, J = 25.4 Hz), 108.7, 68.9, 32.4, 30.1, 22.0; **HRMS (ESI) calcd for** $C_{19}H_{22}FN_2O_2^+$ $[M + H]^+$: 329.1660; Found: 329.1664.

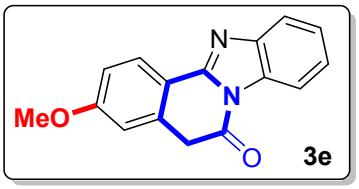
5. Mechanistic Studies

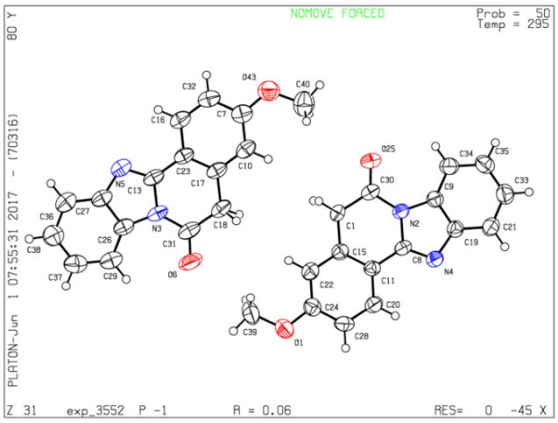
To shed light on the mechanism of the reaction that generates these unexpected products, we conducted a series of control experiments (Scheme S1). Firstly, treatment of **1a** and ethyl diazoacetate **25** under the standard conditions did not lead to any desired products (Scheme S1, a). Furthermore, when the reaction of **1a** with **2a** or **2e** were carried out at room temperature, the direct 1,2-addition products (**26** and **27**) were both isolated in high yields (Scheme S1, b and c). In addition, exposure of **26** or **27** at 100 °C without Rh-catalyst provided the desired products **3a** and **4a** in high yield, which suggested that the Rh-catalyst only play the role in C-H activation process and the different types of ester group are crucial factors for the formation of diverse products (Scheme S1, d).



Scheme S1. Mechanistic Studies

6. Crystal Structure of Products





Bond precision: C-C = 0.0042 A Wavelength=0.71073

Cell: a=7.0483(8) b=12.6910(13) c=14.4533(15)
alpha=103.668(9) beta=90.921(9) gamma=102.650(9)
Temperature: 295 K

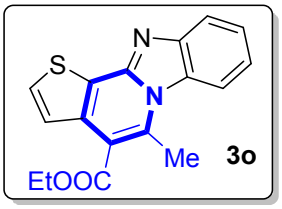
	Calculated	Reported
Volume	1222.6(2)	1222.6(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H12 N2 O2	C16 H12 N2 O2
Sum formula	C16 H12 N2 O2	C16 H12 N2 O2
Mr	264.28	264.29
Dx,g cm-3	1.436	1.436
Z	4	4
Mu (mm-1)	0.097	0.097
F000	552.0	552.3
F000'	552.24	
h,k,lmax	8,15,17	8,15,17
Nref	4298	4294
Tmin,Tmax		
Tmin'		

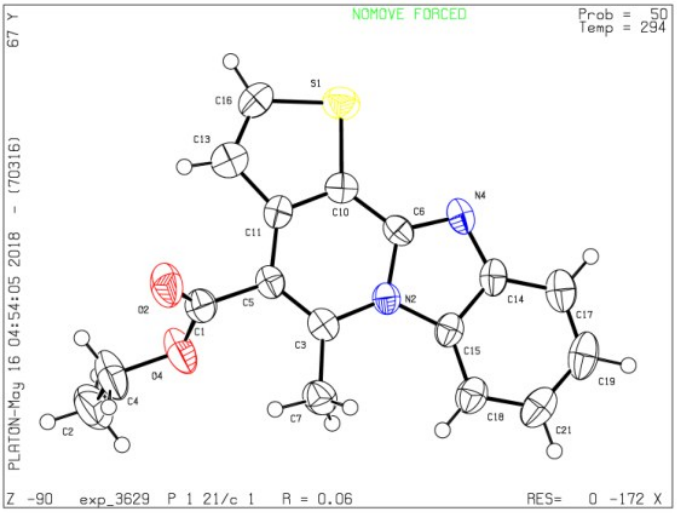
Correction method= Not given

Data completeness= 0.999 Theta(max)= 25.000

R(reflections)= 0.0624(2521) wR2(reflections)= 0.1270(4294)

S = 1.054 Npar= 379





Bond precision: C-C = 0.0051 A Wavelength=0.71073

Cell: a=7.1819(13) b=12.909(3) c=16.108(3)
alpha=90 beta=99.316(18) gamma=90
Temperature: 294 K

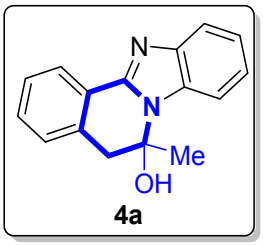
	Calculated	Reported
Volume	1473.7(5)	1473.7(5)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C17 H14 N2 O2 S	C17 H14 N2 O2 S
Sum formula	C17 H14 N2 O2 S	C17 H14 N2 O2 S
Mr	310.36	310.38
Dx,g cm-3	1.399	1.399
Z	4	4
Mu (mm-1)	0.228	0.228
F000	648.0	648.8
F000'	648.75	
h,k,lmax	8,15,19	8,15,19
Nref	2601	2600
Tmin,Tmax		
Tmin'		

Correction method= Not given

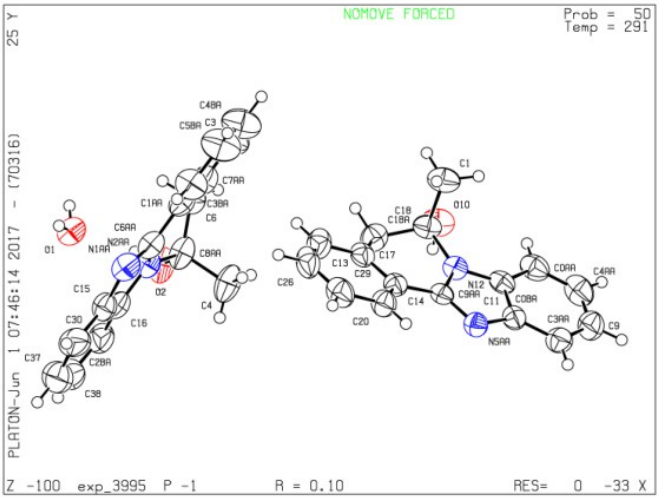
Data completeness= 1.000 Theta(max)= 25.000

R(reflections)= 0.0643(1572) wR2(reflections)= 0.1486(2600)

S = 1.002 Npar= 201



4a



Bond precision: C-C = 0.0081 A Wavelength=0.71073

Cell: a=10.711(3) b=11.136(2) c=13.512(3)
alpha=100.641(16) beta=104.19(2) gamma=113.52(2)
Temperature: 291 K

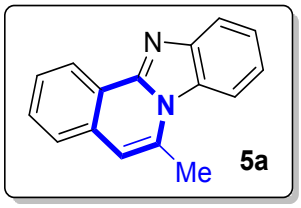
	Calculated	Reported
Volume	1358.4(7)	1358.4(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C16 H14 N2 O), H2 O	2(C16 H14 N2 O), H2 O
Sum formula	C32 H30 N4 O3	C32 H30 N4 O3
Mr	518.60	518.62
Dx,g cm-3	1.268	1.268
Z	2	2
Mu (mm-1)	0.083	0.083
F000	548.0	548.2
F000'	548.22	
h,k,lmax	12,13,16	12,13,16
Nref	4787	4779
Tmin,Tmax		
Tmin'		

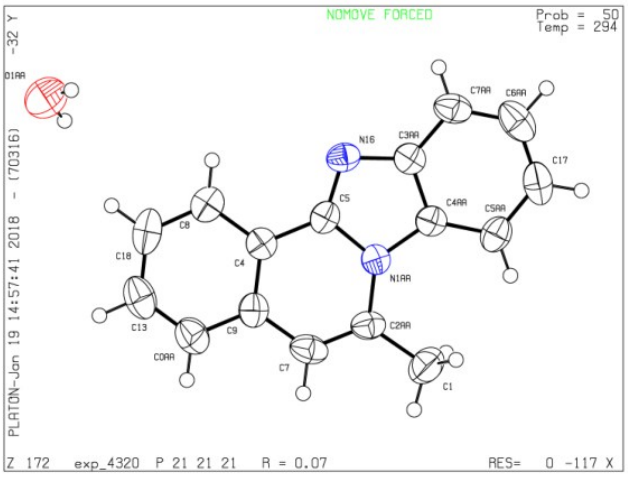
Correction method= Not given

Data completeness= 0.998 Theta(max)= 24.990

R(reflections)= 0.0960(2716) wR2(reflections)= 0.1936(4779)

S = 1.111 Npar= 359





Bond precision: C-C = 0.0063 A Wavelength=0.71073

Cell: a=5.7290(15) b=14.295(5) c=15.456(4)
alpha=90 beta=90 gamma=90
Temperature: 294 K

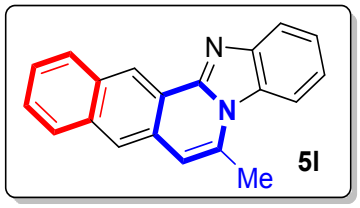
	Calculated	Reported
Volume	1265.8(6)	1265.9(6)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C16 H12 N2, H2 O	C16 H12 N2, H2 O
Sum formula	C16 H14 N2 O	C16 H14 N2 O
Mr	250.29	250.30
Dx,g cm-3	1.313	1.313
Z	4	4
Mu (mm-1)	0.084	0.084
F000	528.0	528.2
F000'	528.20	
h,k,lmax	6,17,18	6,16,18
Nref	2228[1320]	2039
Tmin,Tmax		
Tmin'		

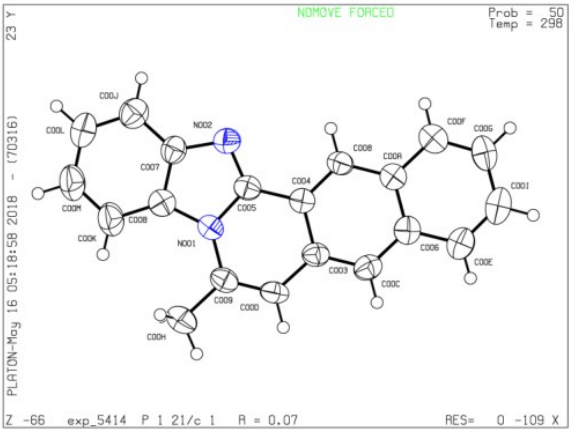
Correction method= Not given

Data completeness= 1.54/0.92 Theta(max)= 25.000

R(reflections)= 0.0744(1289) wR2(reflections)= 0.1071(2039)

S = 1.059 Npar= 176





Bond precision: C-C = 0.0045 A Wavelength=0.71073

Cell: a=7.0181(4) b=7.9004(5) c=25.5706(16)
alpha=90 beta=92.661(6) gamma=90
Temperature: 298 K

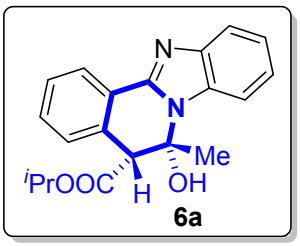
	Calculated	Reported
Volume	1416.25(15)	1416.25(15)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C20 H14 N2	C20 H14 N2
Sum formula	C20 H14 N2	C20 H14 N2
Mr	282.33	282.35
Dx,g cm-3	1.324	1.324
Z	4	4
Mu (mm-1)	0.078	0.078
F000	592.0	592.2
F000'	592.20	
h,k,lmax	8,9,30	8,9,30
Nref	2508	2485
Tmin,Tmax		0.501,1.000
Tmin'		

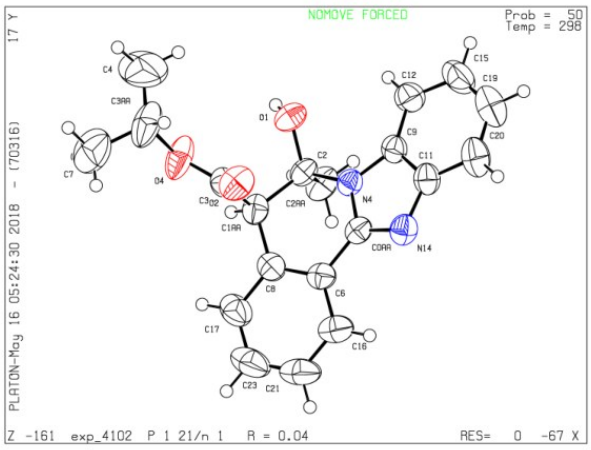
Correction method= # Reported T Limits: Tmin=0.501 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 25.000

R(reflections)= 0.0701(1323) wR2(reflections)= 0.2151(2485)

S = 0.962 Npar= 200





Bond precision: C-C = 0.0033 A Wavelength=0.71073

Cell: a=9.8482(6) b=12.1953(6) c=15.5327(10)
alpha=90 beta=106.980(7) gamma=90
Temperature: 298 K

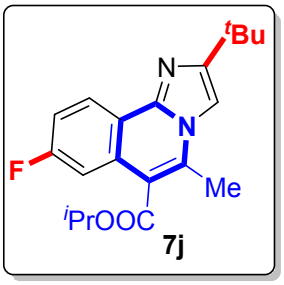
	Calculated	Reported
Volume	1784.18(19)	1784.18(18)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2ybc (x-
Moiety formula	C20 H20 N2 O3	C20 H20 N2 O3
Sum formula	C20 H20 N2 O3	C20 H20 N2 O3
Mr	336.38	336.39
Dx,g cm-3	1.252	1.252
Z	4	4
Mu (mm-1)	0.085	0.085
F000	712.0	712.4
F000'	712.32	
h,k,lmax	11,14,18	11,14,18
Nref	3152	3147
Tmin,Tmax		
Tmin'		

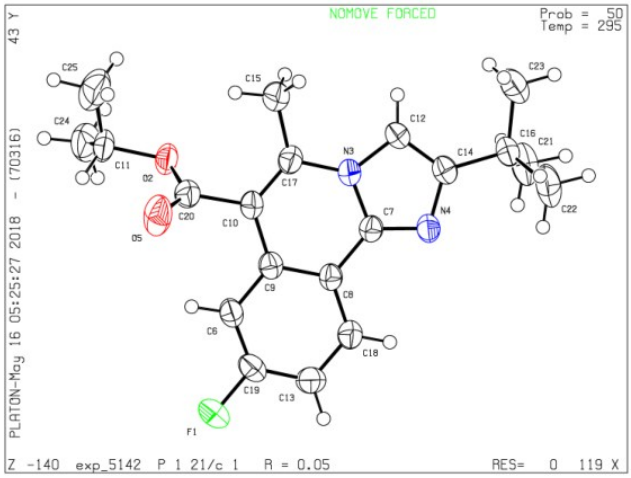
Correction method= Not given

Data completeness= 0.998 Theta(max)= 25.000

R(reflections)= 0.0445(2422) wR2(reflections)= 0.1153(3147)

S = 1.069 Npar= 230





Bond precision: C-C = 0.0031 A Wavelength=0.71073

Cell: a=11.9347(6) b=13.0246(5) c=12.4263(6)
alpha=90 beta=112.805(5) gamma=90
Temperature: 295 K

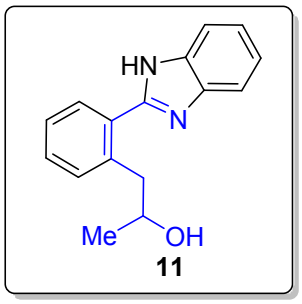
	Calculated	Reported
Volume	1780.61(16)	1780.61(15)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C20 H23 F N2 O2	C20 H23 F N2 O2
Sum formula	C20 H23 F N2 O2	C20 H23 F N2 O2
Mr	342.40	342.42
Dx,g cm-3	1.277	1.277
Z	4	4
Mu (mm-1)	0.090	0.090
F000	728.0	728.4
F000'	728.35	
h,k,lmax	14,15,14	14,15,14
Nref	3137	3129
Tmin,Tmax		0.766,1.000
Tmin'		

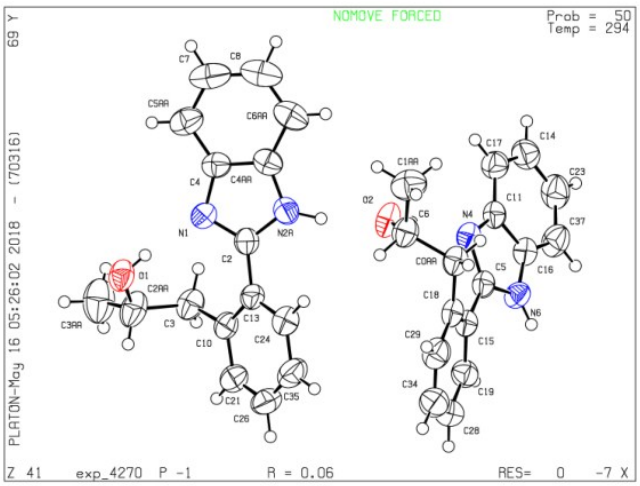
Correction method= # Reported T Limits: Tmin=0.766 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 25.000

R(reflections)= 0.0494(2174) wR2(reflections)= 0.1239(3129)

S = 1.053 Npar= 231





Bond precision: C-C = 0.0040 A Wavelength=0.71073

Cell: a=11.1136(8) b=11.2993(9) c=12.7113(6)
alpha=105.175(5) beta=101.292(5) gamma=114.625(8)
Temperature: 294 K

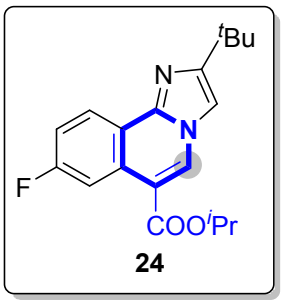
	Calculated	Reported
Volume	1313.2(2)	1313.2(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H16 N2 O	C16 H16 N2 O
Sum formula	C16 H16 N2 O	C16 H16 N2 O
Mr	252.31	252.32
Dx,g cm-3	1.276	1.276
Z	4	4
Mu (mm-1)	0.081	0.081
F000	536.0	536.2
F000'	536.20	
h,k,lmax	13,13,15	13,13,15
Nref	4639	4631
Tmin,Tmax		
Tmin'		

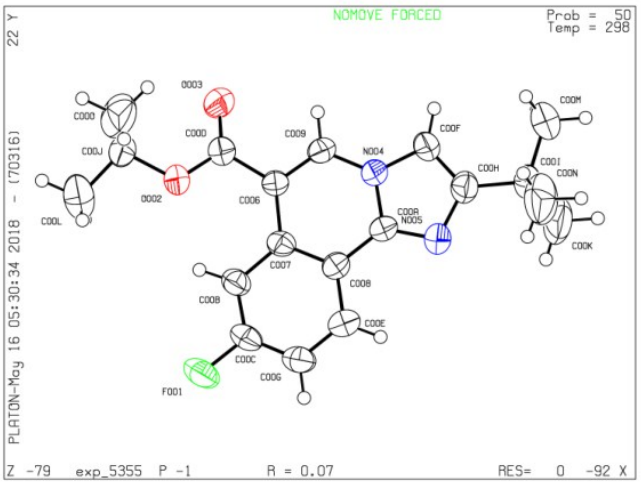
Correction method= Not given

Data completeness= 0.998 Theta(max)= 25.000

R(reflections)= 0.0554(3348) wR2(reflections)= 0.1550(4631)

S = 1.065 Npar= 351





Bond precision: C-C = 0.0051 A Wavelength=0.71073

Cell: a=6.3592(9) b=9.7262(14) c=15.058(2)
alpha=92.739(11) beta=99.147(11) gamma=106.484(12)
Temperature: 298 K

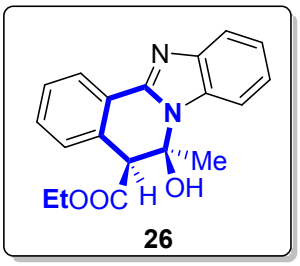
	Calculated	Reported
Volume	877.5(2)	877.4(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C19 H21 F N2 O2	C19 H21 F N2 O2
Sum formula	C19 H21 F N2 O2	C19 H21 F N2 O2
Mr	328.38	328.39
Dx,g cm-3	1.243	1.243
Z	2	2
Mu (mm-1)	0.088	0.088
F000	348.0	348.2
F000'	348.17	
h,k,lmax	7,11,17	7,11,17
Nref	3094	3088
Tmin,Tmax		0.392,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.392 Tmax=1.000
AbsCorr = MULTI-SCAN

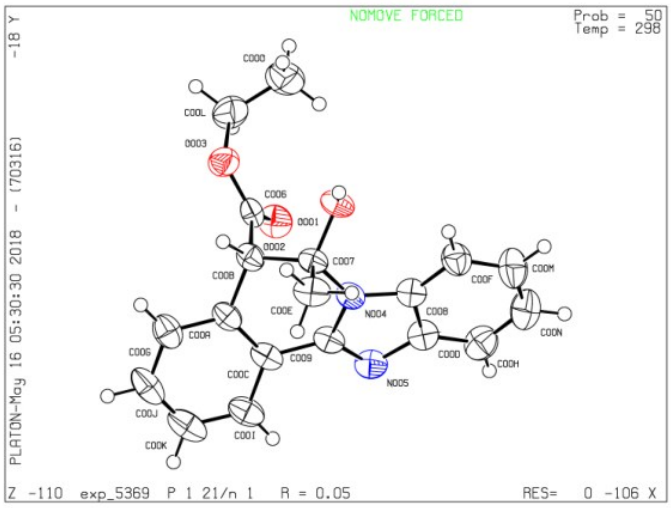
Data completeness= 0.998 Theta(max)= 25.000

R(reflections)= 0.0664(1559) wR2(reflections)= 0.2011(3088)

S = 1.041 Npar= 221



26



Bond precision: C-C = 0.0038 A Wavelength=0.71073

Cell: a=9.0284(9) b=12.6694(8) c=14.2980(11)
alpha=90 beta=96.266(8) gamma=90
Temperature: 298 K

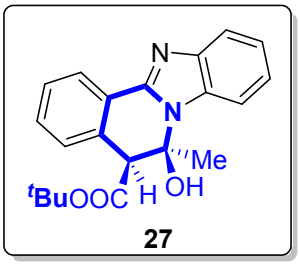
	Calculated	Reported
Volume	1625.7(2)	1625.7(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2ybc (x-
Moiety formula	C19 H18 N2 O3	C19 H18 N2 O3
Sum formula	C19 H18 N2 O3	C19 H18 N2 O3
Mr	322.35	322.37
Dx,g cm-3	1.317	1.317
Z	4	4
Mu (mm-1)	0.090	0.090
F000	680.0	680.3
F000'	680.31	
h,k,lmax	10,15,17	10,15,17
Nref	2859	2850
Tmin,Tmax		0.580,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.580 Tmax=1.000
AbsCorr = MULTI-SCAN

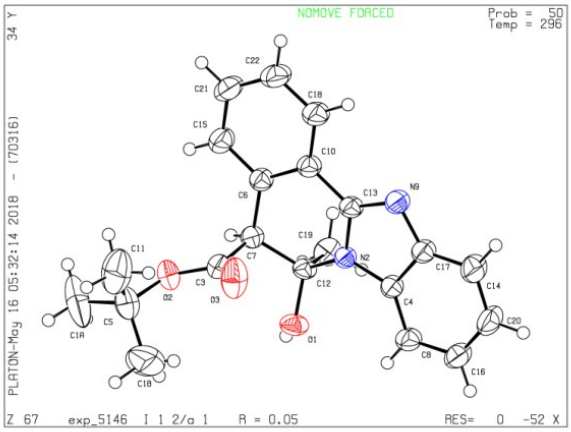
Data completeness= 0.997 Theta(max)= 25.000

R(reflections)= 0.0527(1893) wR2(reflections)= 0.1359(2850)

S = 1.065 Npar= 220



27



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Bond precision:  C-C = 0.0027 A          Wavelength=0.71073

Cell:            a=13.1564(5)     b=14.1743(6)      c=20.5373(10)
                 alpha=90         beta=93.892(5)    gamma=90
Temperature:     296 K

                 Calculated                 Reported
Volume           3821.0(3)                  3821.0(3)
Space group      I 2/a                      I 1 2/a 1
Hall group       -I 2ya                     -I 2ya
Moiety formula   C21 H22 N2 O3              C21 H22 N2 O3
Sum formula      C21 H22 N2 O3              C21 H22 N2 O3
Mr               350.41                     350.42
Dx,g cm-3        1.218                      1.218
Z                8                          8
Mu (mm-1)        0.082                      0.082
F000             1488.0                     1488.7
F000'            1488.66
h,k,lmax         15,16,24                   15,16,24
Nref             3361                       3352
Tmin,Tmax                                   0.606,1.000
Tmin'

Correction method= # Reported T Limits: Tmin=0.606 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 24.990

R(reflections)= 0.0474( 2619)     wR2(reflections)= 0.1528( 3352)

S = 1.067                 Npar= 239
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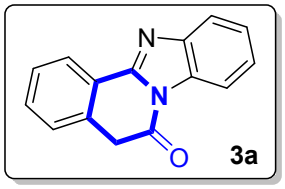
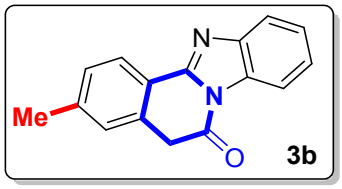
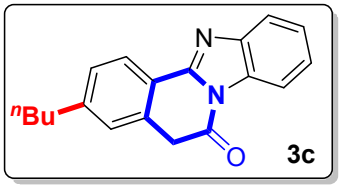
6. Characterization of Products



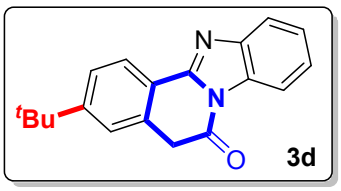
Benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3a) was obtained as a yellow solid (42 mg, 90%), m.p. = 147–150 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.44–8.37 (m, 1H), 8.29 (dd, J = 6.7, 2.4 Hz, 1H), 7.79 (dd, J = 6.6, 2.2 Hz, 1H), 7.52–7.36 (m, 4H), 7.35–7.27 (m, 1H), 4.19 (s, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.5, 150.6, 143.8, 132.3, 131.3, 131.1, 128.1, 127.7, 126.1, 125.8, 125.6, 123.2, 119.8, 115.4, 37.5; **HRMS (ESI) calcd for** $C_{15}H_{11}N_2O^+$ $[M + H]^+$: 235.0866; Found: 235.0864.



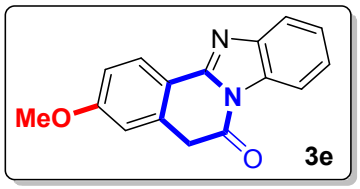
3-Methylbenzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3b) was obtained as a yellow solid (39 mg, 78%), m.p. = 164–166 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.41–8.26 (m, 2H), 7.86–7.73 (m, 1H), 7.51–7.37 (m, 2H), 7.32 (d, J = 8.0 Hz, 1H), 7.17 (s, 1H), 4.20 (s, 2H), 2.45 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.6, 150.8, 143.8, 141.9, 132.3, 131.0, 129.0, 128.1, 125.9, 125.7, 125.3, 120.5, 119.5, 115.3, 37.4, 21.5; **HRMS (ESI) calcd for** $C_{16}H_{13}N_2O^+$ $[M + H]^+$: 249.1022; Found: 249.1023.



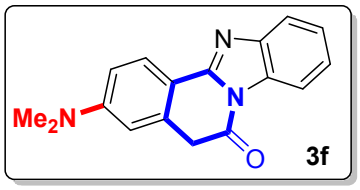
3-Butylbenzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3c) was obtained as a yellow solid (42 mg, 73%), m.p. = 149–151 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.51–8.16 (m, 2H), 7.91–7.63 (m, 1H), 7.43–7.36 (m, 2H), 7.28 (d, J = 8.1 Hz, 1H), 7.11 (s, 1H), 4.16 (s, 2H), 2.72–2.58 (m, 2H), 1.63 (dt, J = 15.4, 7.6 Hz, 2H), 1.38 (dt, J = 14.9, 7.4 Hz, 2H), 0.95 (t, J = 7.4 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.7 150.9, 147.0, 143.9, 132.4, 131.1, 128.5, 127.5, 126.0, 125.7, 125.3, 120.8, 119.6, 115.4, 37.5, 35.6, 33.2, 22.3, 13.9; **HRMS (ESI) calcd for** $C_{19}H_{19}N_2O^+$ $[M + H]^+$: 291.1492; Found: 291.1495.



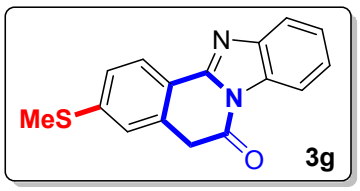
3-(*tert*-Butyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3d) was obtained as a yellow solid (41 mg, 70%), m.p. = 136–137 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.37–8.25 (m, 2H), 7.78 (dd, J = 8.0, 1.0 Hz, 1H), 7.51 (dd, J = 8.3, 1.3 Hz, 1H), 7.44–7.35 (m, 2H), 7.32 (s, 1H), 4.20 (s, 2H), 1.37 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.8, 155.2, 150.8, 143.9, 132.2, 131.1, 125.8, 125.7, 125.5, 125.3, 124.5, 120.6, 119.6, 115.4, 37.8, 35.1, 31.1. **HRMS (ESI) calcd for** $C_{19}H_{19}N_2O^+$ $[M + H]^+$: 291.1492; Found: 291.1494.



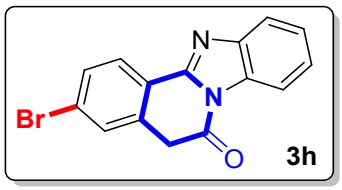
3-Methoxybenzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3e) was obtained as a yellow solid (52 mg, 98%), m.p. = 154–155 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** 8.32–8.15 (m, 2H), 7.72 (dd, J = 7.0, 0.8 Hz, 1H), 7.44–7.30 (m, 2H), 6.95 (dd, J = 8.7, 2.4 Hz, 1H), 6.76–6.65 (m, 1H), 4.11 (s, 2H), 3.83 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.4, 162.0, 150.7, 143.9, 134.4, 131.0, 127.7, 125.6, 125.0, 119.3, 115.9, 115.2, 114.6, 112.2, 55.5, 37.6; **HRMS (ESI) calcd for** $C_{16}H_{13}N_2O_2^+$ $[M + H]^+$: 265.0972; Found: 265.0973.



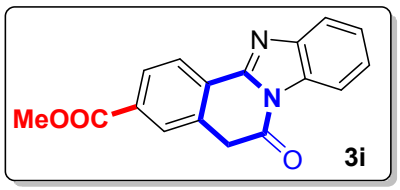
3-(Dimethylamino)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3f) was obtained as a mazarine solid (44 mg, 80%), m.p. = 156–158 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.23 (d, J = 7.9 Hz, 1H), 8.16 (d, J = 8.9 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.34 (ddd, J = 25.9, 11.3, 4.2 Hz, 2H), 6.69 (dd, J = 8.9, 2.3 Hz, 1H), 6.33 (d, J = 1.3 Hz, 1H), 4.04 (s, 2H), 2.95 (d, J = 6.7 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 167.0, 151.9, 151.8, 144.4, 134.2, 131.1, 127.2, 125.4, 124.3, 118.8, 115.1, 111.7, 110.5, 108.9, 39.9, 37.9; **HRMS (ESI) calcd for** $C_{17}H_{16}N_3O^+$ $[M + H]^+$: 278.1288; Found: 278.1290.



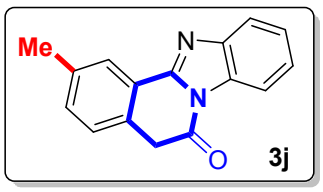
3-(Methylthio)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3g) was obtained as a mazarine solid (42 mg, 75%), m.p. = 108–110 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.36–8.24 (m, 2H), 7.83–7.70 (m, 1H), 7.48–7.35 (m, 2H), 7.29 (dd, J = 8.4, 1.5 Hz, 1H), 7.12 (s, 1H), 4.16 (s, 2H), 2.54 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.2, 150.5, 143.9, 143.8, 132.6, 131.1, 126.3, 125.8, 125.4, 125.1, 123.9, 119.7, 119.6, 115.4, 37.4, 14.9; **HRMS (ESI) calcd for** $C_{16}H_{13}N_2OS^+$ $[M + H]^+$: 281.0743; Found: 281.0746.



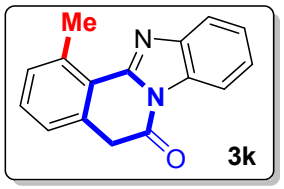
3-Bromobenzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3h) was obtained as a yellow solid (41 mg, 65%), m.p. = 157–160 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.30–8.20 (m, 2H), 7.76 (dd, J = 5.9, 2.7 Hz, 1H), 7.58 (d, J = 8.4 Hz, 1H), 7.47 (s, 1H), 7.45–7.36 (m, 2H), 4.16 (s, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 165.5, 149.7, 143.7, 134.0, 131.5, 131.0, 130.7, 127.4, 126.0, 125.9, 125.8, 122.2, 119.8, 115.4, 37.1; **HRMS (ESI) calcd for** $C_{15}H_{10}BrN_2O^+$ $[M + H]^+$: 312.9971; Found: 312.9973.



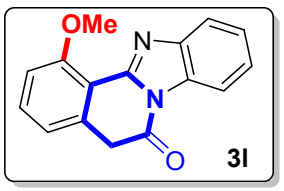
6-Oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-3-yl acetate (3i) was obtained as a yellow solid (23 mg, 40%), m.p. = 208–210 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.50 (d, J = 8.2 Hz, 1H), 8.43–8.27 (m, 1H), 8.12 (d, J = 8.2 Hz, 1H), 8.02 (s, 1H), 7.92–7.75 (m, 1H), 7.54–7.38 (m, 2H), 4.28 (s, 2H), 3.97 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.0, 165.9, 149.5, 143.8, 132.32, 132.28, 131.1, 129.1, 129.0, 127.1, 126.24, 126.14, 126.13, 120.2, 115.6, 52.6, 37.4; **HRMS (ESI) calcd for** $C_{17}H_{13}N_2O_3^+$ $[M + H]^+$: 293.0921; Found: 293.0923.



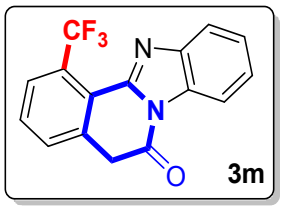
2-Methylbenzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3j) was obtained as a yellow solid (37 mg, 75%), m.p. = 142–144 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.35–8.28 (m, 1H), 8.25 (s, 1H), 7.90–7.74 (m, 1H), 7.48–7.37 (m, 2H), 7.31 (dd, J = 7.8, 1.1 Hz, 1H), 7.22 (d, J = 7.9 Hz, 1H), 4.18 (s, 2H), 2.45 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.8, 150.9, 143.8, 138.1, 132.4, 131.1, 129.4, 127.6, 126.2, 125.8, 125.5, 123.0, 119.7, 115.5, 37.2, 21.01; **HRMS (ESI) calcd for** $C_{16}H_{13}N_2O^+$ [M + H]$^+$: 249.1022; Found: 249.1024.



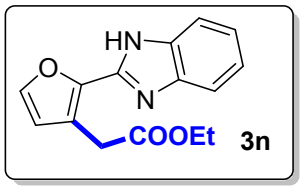
1-Methylbenzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3k) was obtained as a yellow solid (26 mg, 53%), m.p. = 155–156 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.37–8.26 (m, 1H), 7.83–7.74 (m, 1H), 7.43–7.34 (m, 2H), 7.30 (t, J = 7.4 Hz, 1H), 7.26–7.22 (m, 1H), 7.11 (d, J = 7.4 Hz, 1H), 4.14 (s, 2H), 2.97 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.6, 150.8, 143.9, 139.9, 133.2, 131.1, 130.2, 130.0, 125.53, 125.50, 125.42 (s), 121.7, 120.0, 115.3, 38.1 24.0; **HRMS (ESI) calcd for** $C_{16}H_{13}N_2O^+$ [M + H]$^+$: 249.1022; Found: 249.1023.



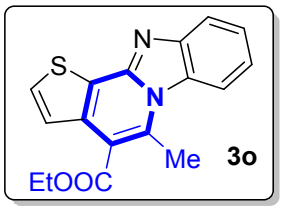
1-Methoxybenzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3l) was obtained as a yellow solid (25 mg, 48%), m.p. = 158–159 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.34 (dd, J = 6.2, 2.8 Hz, 1H), 8.14–7.93 (m, 1H), 7.80 (dd, J = 5.9, 2.2 Hz, 1H), 7.52–7.32 (m, 3H), 7.09–6.87 (m, 1H), 4.07 (s, 2H), 3.91 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.8, 156.1, 150.7, 143.8, 131.1, 128.8, 125.8, 125.6, 124.1, 121.3, 119.8, 117.8, 115.5, 112.0, 55.6, 32.9; **HRMS (ESI) calcd for** $C_{16}H_{13}N_2O^+$ [M + H]$^+$: 265.0972; Found: 265.0975.



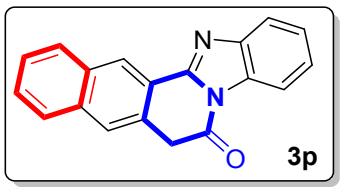
1-(Trifluoromethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3m) was obtained as a yellow solid (27 mg, 45%), m.p. = 142–144 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.37–8.28 (m, 1H), 7.95–7.85 (m, 2H), 7.61–7.50 (m, 2H), 7.48–7.41 (m, 2H), 4.27 (s, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 165.4, 146.6, 143.7, 134.9, 131.8, 130.4, 130.1, 128.4 (d, J = 33.1 Hz), 127.5 (q, J = 7.2 Hz), 126.5, 125.9, 123.3 (q, J = 273.4 Hz), 122.1, 120.9, 115.4, 38.2; **HRMS (ESI) calcd for** $C_{16}H_{10}F_3N_2O^+$ $[M + H]^+$: 303.0740; Found: 303.0741.



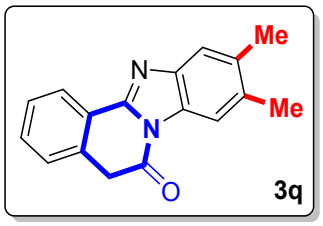
Ethyl 2-(2-(1H-benzo[*d*]imidazol-2-yl)furan-3-yl)acetate (3n) was obtained as a mazarine oil (27 mg, 50%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.40 (s, 1H), 7.63 (s, 2H), 7.45 (d, J = 1.6 Hz, 1H), 7.28–7.23 (m, 2H), 6.58 (d, J = 1.6 Hz, 1H), 4.22 (q, J = 7.1 Hz, 2H), 4.08 (s, 2H), 1.30 (t, J = 7.1 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 171.9, 143.8, 143.1, 142.2, 123.0, 122.89, 122.85, 118.9, 114.4, 61.4, 31.3, 14.1; **HRMS (ESI) calcd for** $C_{15}H_{15}N_2O_3^+$ $[M + H]^+$: 271.1077; Found: 271.1076.



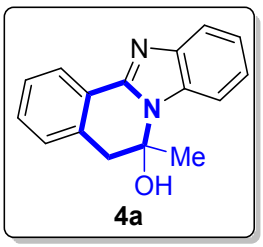
Ethyl 5-methylbenzo[4,5]imidazo[1,2-*a*]thieno[2,3-*c*]pyridine-4-carboxylate (3o) was obtained as a yellow solid (40 mg, 64%), m.p. = 127–128 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.17 (d, J = 8.5 Hz, 1H), 7.98 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 5.3 Hz, 1H), 7.61 (d, J = 5.3 Hz, 1H), 7.56–7.49 (m, 1H), 7.39–7.30 (m, 1H), 4.54 (q, J = 7.2 Hz, 2H), 3.25 (s, 3H), 1.50 (t, J = 7.2 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 167.0, 145.2, 145.2, 138.6, 136.6, 131.2, 129.8, 125.4, 125.1, 124.9, 121.7, 119.9, 115.2, 112.8, 61.8, 19.0, 14.4; **HRMS (ESI) calcd for** $C_{17}H_{15}N_2O_2S^+$ $[M + H]^+$: 311.0849; Found: 311.0846.



Benzo[*g*]benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(7*H*)-one (3p) was obtained as a yellow solid (24 mg, 42%), m.p. = 140–142 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.96 (s, 1H), 8.32 (dd, J = 7.0, 1.5 Hz, 1H), 7.96 (d, J = 7.5 Hz, 1H), 7.89–7.77 (m, 1H), 7.74 (s, 2H), 7.53 (pd, J = 6.8, 1.4 Hz, 2H), 7.49–7.33 (m, 2H), 4.36 (s, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.5, 150.7, 143.9, 134.4, 132.4, 131.3, 128.9, 128.2, 128.1, 127.4, 126.9, 126.7, 126.5, 125.9, 125.6, 120.9, 119.7, 115.5, 37.6; **HRMS (ESI) calcd for** $C_{19}H_{13}N_2O^+$ $[M + H]^+$: 285.1022; Found: 285.1021.

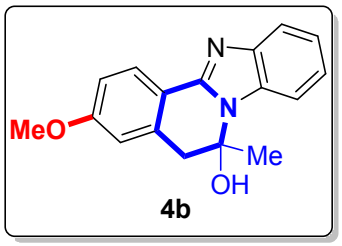


9,10-Dimethylbenzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3q) was obtained as a yellow solid (21 mg, 41%), m.p. = 148–151 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.39 (dd, J = 6.1, 2.9 Hz, 1H), 8.07 (s, 1H), 7.54 (s, 1H), 7.51–7.42 (m, 2H), 7.36–7.28 (m, 1H), 4.18 (s, 2H), 2.40 (s, 3H), 2.38 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.5, 149.9, 142.3, 134.9, 134.8, 132.2, 130.9, 129.4, 128.0, 127.7, 125.9, 123.6, 120.0, 115.7, 37.5, 20.5, 20.5; **HRMS (ESI) calcd for** $C_{17}H_{15}N_2O^+$ $[M + H]^+$: 263.1179; Found: 263.1176.



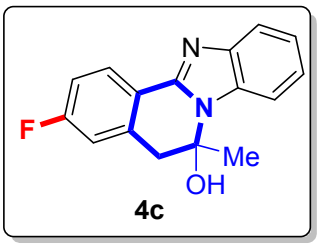
6-Methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-a]isoquinolin-6-ol (4a) was obtained as a white solid (36 mg, 72%), m.p. = 95–98 ºC; **^{1}H NMR (500 MHz, DMSO)** δ 8.25–8.11 (m, 1H), 8.09–7.95 (m, 1H), 7.79–7.65 (m, 1H), 7.50 (m, 2H), 7.49 (s, 1H), 7.36–7.21 (m, 3H), 3.46 (dd, J = 85.1, 15.3 Hz, 1H), 1.56 (s, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 149.0, 144.2, 135.2, 134.2, 131.4, 129.7, 128.5, 126.0, 123.6, 123.1,

119.8, 114.6, 87.3, 44.2, 27.2; **HRMS (ESI) calcd for** $C_{16}H_{15}N_2O^+$ [M + H]$^+$: 251.1179; Found: 251.1180.



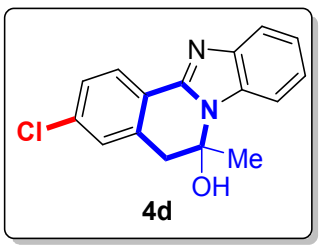
4b

3-Methoxy-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-6-ol (4b) was obtained as a white solid (39 mg, 69%), m.p. = 100–101 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.93–7.76 (m, 2H), 7.54 (dd, J = 6.6, 2.1 Hz, 1H), 7.16–7.05 (m, 2H), 6.66–6.54 (m, 1H), 6.51 (dd, *J* = 8.6, 2.4 Hz, 1H), 3.76 (s, 3H), 3.27 (dd, *J* = 108.2, 15.6 Hz, 2H), 1.62 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 161.1, 148.7, 143.5, 134.9, 133.2, 127.3, 122.5, 122.3, 118.5, 117.7, 113.6, 113.3, 112.9, 86.6, 55.3, 44.8, 26.2; **HRMS (ESI) calcd for** $C_{17}H_{17}N_2O_2^+$ [M + H]$^+$: 281.1285; Found: 281.1283.



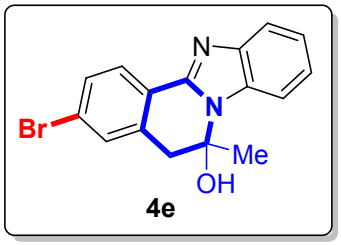
4c

3-Fluoro-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-6-ol (4c) was obtained as a white solid (35 mg, 65%), m.p. = 121–124 ºC; **^{1}H NMR (500 MHz, DMSO)** δ 8.21 (dd, J = 8.6, 5.8 Hz, 1H), 8.03–7.93 (m, 1H), 7.74–7.65 (m, 1H), 7.38 (dd, *J* = 9.4, 2.4 Hz, 1H), 7.35–7.28 (m, 1H), 7.26 (s, 1H), 7.28–7.25 (m, 2H), 3.47 (dd, J = 58.0, 16.0 Hz, 2H), 1.57 (s, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 163.9 (d, *J* = 247.9 Hz), 148.4, 144.8, 138.0 (d, *J* = 8.9 Hz), 134.3, 128.3 (d, *J* = 9.1 Hz), 123.3, 123.0 (d, *J* = 2.7 Hz), 122.9, 120.0, 116.4 (d, *J* = 22.4 Hz), 115.7 (d, *J* = 22.1 Hz), 114.4, 86.9, 44.1, 27.3; **HRMS (ESI) calcd for** $C_{16}H_{14}FN_2O^+$ [M + H]$^+$: 269.1085; Found: 269.1087.



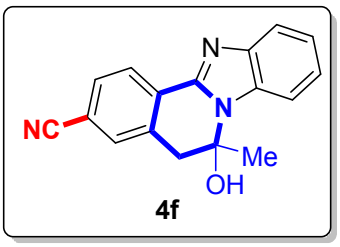
4d

3-Chloro-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-6-ol (4d) was obtained as a white solid (45 mg, 79%), m.p. = 130–131 ºC; **^{1}H NMR (500 MHz, DMSO)** δ 8.16 (d, J = 8.3 Hz, 1H), 8.03–7.96 (m, 1H), 7.76–7.68 (m, 1H), 7.60 (d, J = 1.6 Hz, 1H), 7.52 (dd, J = 8.3, 2.0 Hz, 1H), 7.31–7.24 (m, 3H), 3.46 (dd, J = 49.3, 16.0 Hz, 2H), 1.57 (s, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 148.2, 144.8, 137.3, 135.5, 134.4, 129.5, 128.6, 127.6, 125.3, 123.6, 123.1, 120.1, 114.5, 87.0, 43.8, 27.3; **HRMS (ESI) calcd for** $C_{16}H_{14}ClN_2O^+$ $[M + H]^+$: 285.0789; Found: 285.0787.



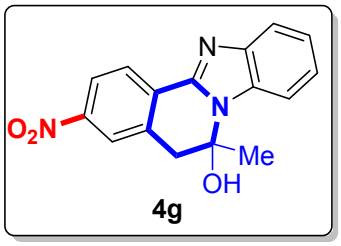
4e

3-Bromo-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-6-ol (4e) was obtained as a white solid (42 mg, 64%), m.p. = 143–145 ºC; **^{1}H NMR (500 MHz, DMSO)** δ 8.09 (d, J = 8.3 Hz, 1H), 8.05–7.96 (m, 1H), 7.75 (d, J = 0.9 Hz, 1H), 7.74–7.69 (m, 1H), 7.66 (dd, J = 8.3, 1.7 Hz, 1H), 7.34–7.23 (m, 3H), 3.47 (dd, J = 51.4, 16.0 Hz, 2H), 1.57 (s, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 148.3, 144.8, 137.5, 134.3, 132.3, 131.4, 127.8, 125.6, 124.2, 123.6, 123.1, 120.1, 114.5, 87.0, 43.7, 27.3; **HRMS (ESI) calcd for** $C_{16}H_{14}BrN_2O^+$ $[M + H]^+$: 329.0284; Found: 329.0288.



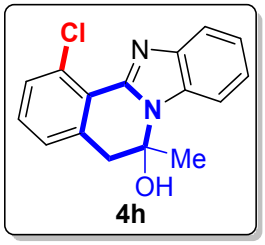
4f

6-Hydroxy-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-3-carbonitrile (4f) was obtained as a white solid (31 mg, 56%), m.p. = 185–186 ºC; **^{1}H NMR (500 MHz, DMSO)** δ 8.31 (d, J = 8.0 Hz, 1H), 8.06–7.96 (m, 2H), 7.92 (dd, J = 8.0, 1.2 Hz, 1H), 7.77 (dd, J = 6.9, 1.8 Hz, 1H), 7.35 (s, 1H), 7.31 (ddd, J = 14.2, 7.1, 1.4 Hz, 2H), 3.51 (q, J = 16.0 Hz, 2H), 1.60 (s, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 147.4, 144.8, 136.1, 134.4, 133.5, 132.2, 130.5, 126.4, 124.3, 123.4, 120.6, 119.5, 114.7, 112.9, 87.0, 43.6, 27.4; **HRMS (ESI) calcd for** $C_{17}H_{14}N_3O^+$ $[M + H]^+$: 276.1131; Found: 276.1134.



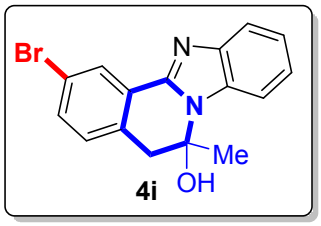
4g

6-Methyl-3-nitro-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-6-ol (4g) was obtained as a white solid (42 mg, 77%), m.p. = 160–162 ºC; **^{1}H NMR (500 MHz, DMSO)** δ 8.45–8.34 (m, 2H), 8.28 (d, J = 8.2 Hz, 1H), 8.04 (d, J = 7.7 Hz, 1H), 7.78 (d, J = 7.6 Hz, 1H), 7.40 (s, 1H), 7.37–7.23 (m, 2H), 3.62 (q, J = 16.1 Hz, 2H), 1.62 (s, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 148.8, 147.1, 144.9, 136.6, 134.5, 132.2, 127.0, 124.9, 124.5, 123.7, 123.6, 120.7, 114.8, 87.1, 43.7, 27.4; **HRMS (ESI) calcd for** $C_{16}H_{14}N_3O_3^+$ $[M + H]^+$: 296.1030; Found: 296.1031.



4h

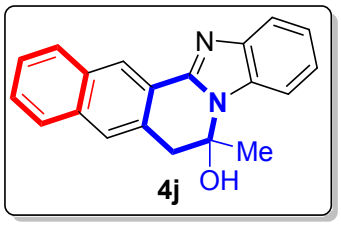
1-Chloro-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-6-ol (4h) was obtained as a white solid (44 mg, 78%), m.p. = 133–135 ºC; **^{1}H NMR (500 MHz, DMSO)** δ 8.04 (dd, J = 7.2, 1.1 Hz, 1H), 7.78 (dd, J = 7.1, 1.3 Hz, 1H), 7.59–7.52 (m, 1H), 7.49–7.43 (m, 2H), 7.34–7.26 (m, 2H), 7.26 (s, 1H), 3.45 (dd, J = 61.7, 15.5 Hz, 2H), 1.58 (s, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 146.3, 144.4, 138.3, 133.4, 132.2, 131.6, 131.5, 128.8, 124.0, 122.9, 120.6, 114.5, 86.2, 45.2, 26.9; **HRMS (ESI) calcd for** $C_{16}H_{14}ClN_2O^+$ $[M + H]^+$: 285.0789; Found: 285.0787.



4i

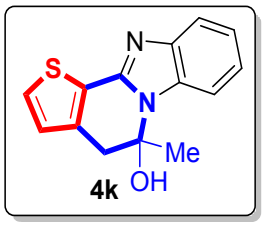
2-Bromo-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-6-ol (4i) was obtained as a white solid (36 mg, 55%), m.p. = 148–151 ºC; **^{1}H NMR (500 MHz, DMSO)** δ 8.26 (m, 1H), 8.00 (d, J = 4.1 Hz, 1H), 7.72 (dd, J = 41.8, 19.7 Hz, 2H), 7.45 (d, J = 7.0 Hz, 1H), 7.28 (m, 3H), 3.49–3.32 (m, 2H), 1.57 (s, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 147.6, 144.7, 134.4, 134.3, 133.6, 132.0, 128.4, 128.0, 123.8,

123.2, 121.3, 120.3, 114.6, 87.1, 43.7, 27.3; **HRMS (ESI) calcd for** $C_{16}H_{14}BrN_2O^+$ $[M + H]^+$: 329.0284; Found: 329.0282.



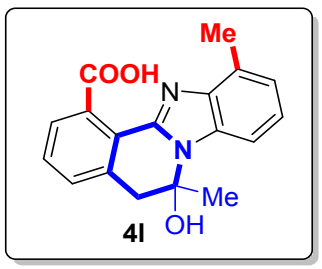
4j

6-Methyl-6,7-dihydrobenzo[*g*]benzo[4,5]imidazo[2,1-*a*]isoquinolin-6-ol (4j) was obtained as a white solid (35 mg, 58%), m.p. = 117–119 ºC; **^{1}H NMR (500 MHz, DMSO)** δ 8.80 (s, 1H), 8.13 (d, J = 7.7 Hz, 1H), 8.07–8.01 (m, 1H), 7.99 (s, 1H), 7.97 (d, J = 7.8 Hz, 1H), 7.78–7.71 (m, 1H), 7.67–7.55 (m, 1H), 7.31 (s, 1H), 7.29 (dd, J = 6.1, 3.2 Hz, 2H), 3.61 (dd, J = 64.5, 15.4 Hz, 2H), 1.59 (s, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 149.0, 145.0, 134.6, 134.5, 133.1, 132.0, 129.5, 128.3, 128.3, 127.9, 127.3, 125.7, 124.6, 123.4, 123.0, 120.0, 114.6, 87.1, 44.7, 27.4; **HRMS (ESI) calcd for** $C_{20}H_{17}N_2O^+$ $[M + H]^+$: 301.1335; Found: 301.1334.



4k

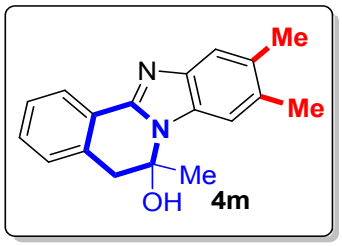
5-Methyl-4,5-dihydrobenzo[4,5]imidazo[1,2-*a*]thieno[2,3-*c*]pyridin-5-ol (4k) was obtained as a white solid (16 mg, 32%), m.p. = 128–131 ºC; **^{1}H NMR (500 MHz, DMSO)** δ 7.95 (dd, J = 6.8, 1.9 Hz, 1H), 7.78 (d, J = 4.9 Hz, 1H), 7.66–7.58 (m, 1H), 7.27 (s, 1H), 7.27–7.21 (m, 2H), 7.20 (d, J = 4.9 Hz, 1H), 3.46–3.35 (m, 2H), 1.57 (s, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 146.4, 144.9, 139.8, 134.2, 129.9, 128.9, 125.9, 123.4, 122.8, 119.7, 114.0, 88.8, 41.2, 27.2; **HRMS (ESI) calcd for** $C_{14}H_{13}SN_2O^+$ $[M + H]^+$: 257.0743; Found: 257.0746.



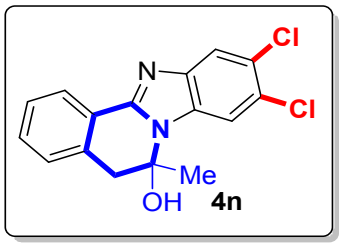
4l

6-Hydroxy-6,11-dimethyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-1-carboxylic acid (4l) was obtained as a white solid (46 mg, 75%), m.p. = 180–183 ºC;

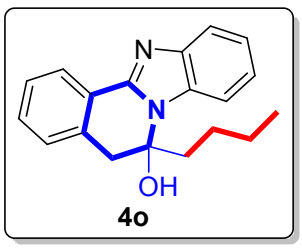
^{1}H NMR (500 MHz, DMSO) δ 8.01 (d, J = 7.5 Hz, 1H), 7.91 (d, J = 8.2 Hz, 1H), 7.66 (d, J = 7.3 Hz, 1H), 7.61 (t, J = 7.6 Hz, 1H), 7.40 (s, 1H), 7.33–7.25 (m, 1H), 7.18 (d, J = 7.3 Hz, 1H), 3.54 (dd, J = 59.6, 15.8 Hz, 2H), 2.61 (s, 3H), 1.61 (s, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 168.9, 146.4, 140.4, 136.6, 133.3, 132.6, 132.5, 131.7, 131.2, 128.7, 124.8, 124.1, 122.5, 112.5, 86.8, 44.9, 26.8, 17.2.



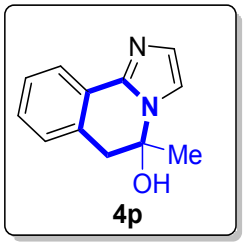
6,9,10-Trimethyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-6-ol (4m) was obtained as a white solid (32 mg, 58%), m.p. = 111–112 ºC; **^{1}H NMR (500 MHz, DMSO)** δ 8.16–8.09 (m, 1H), 7.78 (s, 1H), 7.47 (s, 1H), 7.46–7.39 (m, 3H), 7.13 (s, 1H), 3.41 (dd, J = 78.6, 15.7 Hz, 2H), 2.38 (s, 3H), 2.35 (s, 3H), 1.53 (s, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 148.3, 143.5, 134.8, 132.9, 131.9, 131.2, 130.7, 129.5, 128.3, 126.6, 125.6, 120.0, 114.5, 86.9, 44.3, 27.2, 21.3, 20.9; **HRMS (ESI) calcd for** $C_{18}H_{19}N_2O^+$ $[M + H]^+$: 279.1492; Found: 279.1495.



9,10-Dichloro-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-6-ol (4n) was obtained as a white solid (45 mg, 70%), m.p. = 119–120 ºC; **^{1}H NMR (500 MHz, DMSO)** δ 8.17 (s, 1H), 8.17–8.13 (m, 1H), 7.99 (s, 1H), 7.57–7.46 (m, 3H), 7.46 (s, 1H), 3.46 (dd, J = 72.5, 15.8 Hz, 2H), 1.54 (s, 3H). **^{13}C NMR (126 MHz, DMSO)** δ 151.5, 144.5, 135.4, 133.7, 132.0, 129.8, 128.7, 126.2, 125.5, 125.5, 121.1, 115.4, 87.7, 43.9, 27.1; **HRMS (ESI) calcd for** $C_{16}H_{13}Cl_2N_2O^+$ $[M + H]^+$: 319.0399; Found: 319.0398.

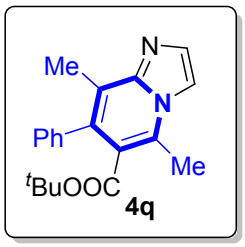


6-Butyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-6-ol (4o) was obtained as a white solid (46 mg, 78%), m.p. = 111–112 ºC; **^{1}H NMR (500 MHz, $CHCl_3$)** δ 8.02–7.86 (m, 2H), 7.59 (dd, J = 6.2, 2.3 Hz, 1H), 7.22–7.11 (m, 3H), 7.10–6.98 (m, 2H), 3.35 (q, J = 15.7 Hz, 2H), 1.98–1.69 (m, 2H), 1.36–1.22 (m, 2H), 1.14 (ddd, J = 14.4, 9.7, 5.0 Hz, 2H), 0.75 (t, J = 7.3 Hz, 3H); **^{13}C NMR (126 MHz, $CHCl_3$)** δ 148.5, 143.4, 133.6, 133.1, 130.1, 127.8, 127.5, 125.5, 125.3, 122.8, 122.4, 118.9, 113.9, 89.1, 42.3, 38.9, 26.0, 22.6, 13.8; **HRMS (ESI) calcd for** $C_{19}H_{21}N_2O^+$ [M + H]$^+$: 293.1648; Found: 293.1648.



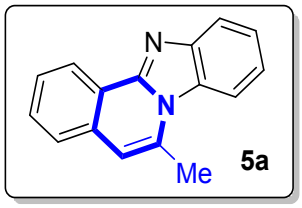
4p

5-Methyl-5,6-dihydroimidazo[2,1-*a*]isoquinolin-5-ol (4p) was obtained as a white solid (25 mg, 62%), m.p. = 200–201 ºC; **^{1}H NMR (500 MHz, DMSO)** δ 7.95–7.79 (m, 1H), 7.44 (d, J = 1.0 Hz, 1H), 7.40–7.26 (m, 3H), 7.06 (d, J = 0.8 Hz, 1H), 6.72 (s, 1H), 3.23 (s, 2H), 1.63 (s, 3H); **^{13}C NMR (126 MHz, DMSO)** δ 143.4, 133.0, 129.7, 129.5, 129.1, 128.0, 127.1, 123.6, 116.6, 83.9, 43.1, 28.6; **HRMS (ESI) calcd for** $C_{12}H_{13}N_2O^+$ [M + H]$^+$: 201.1022; Found: 201.1024.



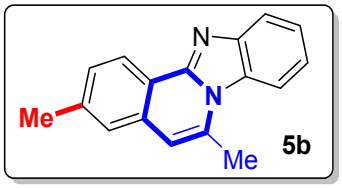
4q

***tert*-Butyl 5,8-dimethyl-7-phenylimidazo[1,2-*a*]pyridine-6-carboxylate (4q)** was obtained as a yellow solid (49 mg, 76%), m.p. = 103–106 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.74 (s, 1H), 7.55 (s, 1H), 7.46–7.34 (m, 3H), 7.26 (m, 2H), 2.63 (s, 3H), 2.39 (s, 3H), 1.15 (s, 9H); **^{13}C NMR (126 MHz, DMSO)** δ 166.8, 145.4, 138.0, 134.1, 129.7, 129.6, 128.1, 127.5, 126.4, 122.9, 121.8, 110.6, 82.2, 27.4, 16.2, 14.3; **HRMS (ESI) calcd for** $C_{20}H_{23}N_2O_2^+$ [M + H]$^+$: 323.1754; Found: 323.1756.

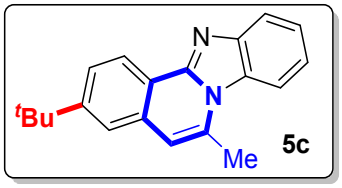


5a

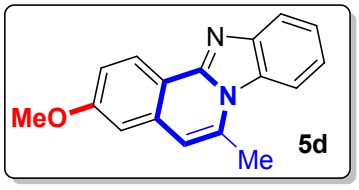
6-Methylbenzo[4,5]imidazo[2,1-*a*]isoquinoline (5a) was obtained as a yellow solid (46 mg, 99%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.88–8.74 (m, 1H), 8.05 (dd, J = 16.5, 8.3 Hz, 2H), 7.68–7.56 (m, 3H), 7.49 (dd, J = 11.3, 4.0 Hz, 1H), 7.37–7.29 (m, 1H), 6.73 (s, 1H), 2.98 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 148.3, 144.2, 134.7, 131.7, 131.3, 129.9, 127.1, 125.7, 124.9, 124.2, 122.1, 121.6, 119.8, 113.9, 110.8, 21.2; **HRMS (ESI) calcd for** $C_{16}H_{13}N_2^+$ $[M + H]^+$: 233.1073; Found: 233.1075.



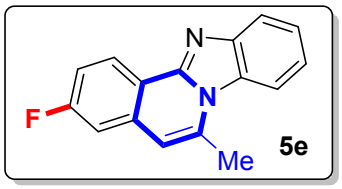
3,6-Dimethylbenzo[4,5]imidazo[2,1-*a*]isoquinoline (5b) was obtained as a yellow solid (47 mg, 95%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.64 (d, J = 8.2 Hz, 1H), 7.99 (d, J = 8.1 Hz, 1H), 7.94 (d, J = 8.4 Hz, 1H), 7.45 (t, J = 7.6 Hz, 1H), 7.38 (d, J = 8.1 Hz, 1H), 7.31–7.22 (m, 2H), 6.52 (s, 1H), 2.85 (s, 3H), 2.46 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 148.3, 144.1, 140.0, 134.5, 131.7, 131.1, 128.5, 125.4, 124.6, 123.9, 121.2, 119.6, 119.5, 113.7, 110.5, 21.7, 21.1. **HRMS (ESI) calcd for** $C_{17}H_{15}N_2^+$ $[M + H]^+$: 247.1230; Found: 247.1231.



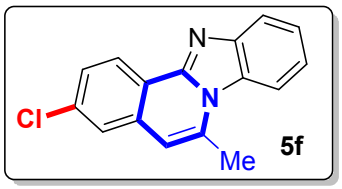
3-(*tert*-butyl)-6-Methylbenzo[4,5]imidazo[2,1-a]isoquinoline (5c) was obtained as a yellow solid (53 mg, 92%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.74 (d, J = 8.5 Hz, 1H), 8.00 (d, J = 8.3 Hz, 2H), 7.69 (dd, J = 8.5, 1.9 Hz, 1H), 7.58 (d, J = 1.7 Hz, 1H), 7.45 (dd, J = 11.3, 4.1 Hz, 1H), 7.33–7.17 (m, 1H), 6.71 (s, 1H), 2.93 (s, 3H), 1.43 (s, 9H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 153.6, 147.9, 143.3, 134.5, 131.8, 130.9, 125.6, 124.8, 124.3, 121.8, 121.6, 119.3, 119.2, 113.9, 111.6, 35.2, 31.3, 21.2. **HRMS (ESI) calcd for** $C_{20}H_{21}N_2^+$ $[M + H]^+$: 289.1699; Found: 289.1698.



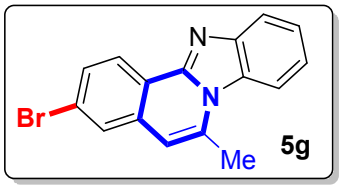
3-Methoxy-6-methylbenzo[4,5]imidazo[2,1-*a*]isoquinoline (5d) was obtained as a yellow solid (52 mg, 99%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.60 (d, J = 8.8 Hz, 1H), 7.94 (d, J = 8.1 Hz, 1H), 7.85 (d, J = 8.4 Hz, 1H), 7.41 (dd, J = 11.3, 3.9 Hz, 1H), 7.24–7.17 (m, 1H), 7.10 (dd, J = 8.8, 2.4 Hz, 1H), 6.76 (d, J = 2.4 Hz, 1H), 6.44 (s, 1H), 3.79 (s, 3H), 2.77 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 160.8, 148.2, 143.9, 135.0, 133.4, 130.9, 126.5, 124.0, 121.0, 119.1, 116.5, 115.5, 113.6, 110.5, 106.7, 55.2, 21.0. **HRMS (ESI) calcd for** $C_{17}H_{15}N_2O^+$ [M + H]$^+$: 263.1179; Found: 263.1178.



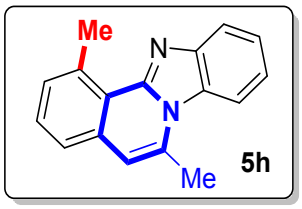
3-Fluoro-6-methylbenzo[4,5]imidazo[2,1-*a*]isoquinoline (5e) was obtained as a yellow solid (44 mg, 88%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.74 (dd, J = 8.8, 5.6 Hz, 1H), 7.97 (d, J = 8.7 Hz, 2H), 7.47 (t, J = 7.8 Hz, 1H), 7.28 (m, 2H), 7.19 (dd, J = 9.3, 2.4 Hz, 1H), 6.59 (s, 1H), 2.91 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 163.5 (d, J = 250.0 Hz), 147.7, 144.0, 136.0, 133.5 (d, J = 9.8 Hz), 131.1, 127.5 (d, J = 9.4 Hz), 124.3, 121.7, 119.7, 118.6, 115.7 (d, J = 23.7 Hz), 113.8, 110.6 (d, J = 22.0 Hz), 109.9 (d, J = 3.3 Hz), 21.1. **HRMS (ESI) calcd for** $C_{17}H_{15}N_2F^+$ [M + H]$^+$: 251.0979; Found: 251.0977.



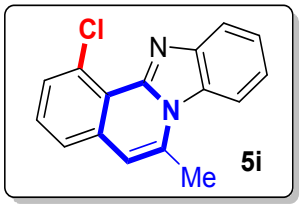
3-Chloro-6-methylbenzo[4,5]imidazo[2,1-*a*]isoquinoline (5f) was obtained as a yellow solid (51 mg, 95%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.64 (d, J = 9.2 Hz, 1H), 7.96 (dd, J = 12.6, 8.3 Hz, 2H), 7.52–7.44 (m, 3H), 7.30 (t, J = 7.8 Hz, 1H), 6.52 (s, 1H), 2.88 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 147.4, 144.0, 136.0, 135.9, 132.7, 131.0, 127.5, 126.4, 124.9, 124.4, 121.9, 120.2, 119.8, 113.8, 109.5, 21.2. **HRMS (ESI) calcd for** $C_{17}H_{15}N_2Cl^+$ [M + H]$^+$: 267.0684; Found: 267.0682.



3-Bromo-6-methylbenzo[4,5]imidazo[2,1-*a*]isoquinoline (5g) was obtained as a yellow solid (56 mg, 91%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.55 (d, J = 8.5 Hz, 1H), 7.94 (dd, J = 20.1, 8.3 Hz, 2H), 7.65–7.59 (m, 2H), 7.51–7.43 (m, 1H), 7.32–7.26 (m, 1H), 6.47 (d, J = 7.5 Hz, 1H), 2.85 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 147.3, 143.9, 135.9, 132.8, 130.9, 130.1, 127.9, 126.3, 124.3, 124.2, 121.8, 120.4, 119.7, 113.8, 109.3, 21.1. $C_{17}H_{15}N_2Br^+$ $[M + H]^+$: 311.0178; Found: 311.0179.

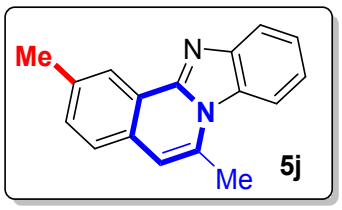


1,6-Dimethylbenzo[4,5]imidazo[2,1-*a*]isoquinoline (5h) was obtained as a yellow solid (44 mg, 90%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.05 (t, J = 8.0 Hz, 2H), 7.51–7.42 (m, 2H), 7.43–7.36 (m, 2H), 7.33 (dd, J = 11.8, 4.4 Hz, 1H), 6.63 (s, 1H), 3.27 (s, 3H), 2.91 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 148.8, 144.1, 138.4, 134.2, 132.9, 130.3, 129.6, 128.8, 123.6, 123.6, 121.5, 121.05, 120.11, 113.7, 111.5, 24.5, 21.2. **HRMS (ESI) calcd for** $C_{17}H_{15}N_2O^+$ $[M + H]^+$: 247.1230; Found: 247.1233.

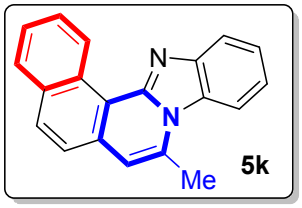


1-Chloro-6-methylbenzo[4,5]imidazo[2,1-*a*]isoquinoline (5i) was obtained as a yellow solid (52 mg, 98%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.13 (d, J = 8.2 Hz, 1H), 8.01 (d, J = 8.4 Hz, 1H), 7.60 (dd, J = 7.0, 1.8 Hz, 1H), 7.48 (t, J = 7.6 Hz, 1H), 7.45–7.38 (m, 2H), 7.33 (t, J = 7.7 Hz, 1H), 6.64 (s, 1H), 2.93 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 145.9, 143.8, 135.5, 134.1, 132.1, 130.1, 129.8, 129.3,

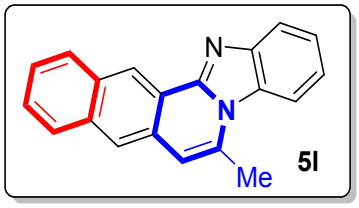
124.6, 124.1, 122.3, 120.8, 119.5, 113.7, 110.9, 21.3. **HRMS (ESI) calcd for** $C_{16}H_{12}ClN_2^+$ $[M + H]^+$: 267.0684; Found: 267.0686.



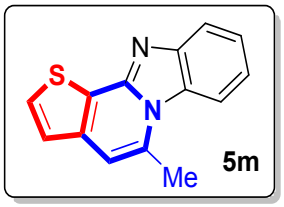
2,6-Dimethylbenzo[4,5]imidazo[2,1-*a*]isoquinoline (5j) was obtained as a yellow solid (42 mg, 85%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.57 (s, 1H), 7.99 (dd, J = 15.2, 8.3 Hz, 2H), 7.48–7.43 (m, 2H), 7.37 (dd, J = 8.1, 1.3 Hz, 1H), 7.27 (ddd, J = 7.2, 4.5, 1.2 Hz, 1H), 6.59 (s, 1H), 2.87 (s, 3H), 2.53 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 148.1, 143.9, 137.1, 133.6, 131.4, 131.2, 129.4, 125.5, 124.5, 124.0, 121.8, 121.4, 119.6, 113.8, 110.6, 21.5, 21.0. **HRMS (ESI) calcd for** $C_{17}H_{15}N_2^+$ $[M + H]^+$: 247.1230; Found: 247.1235.



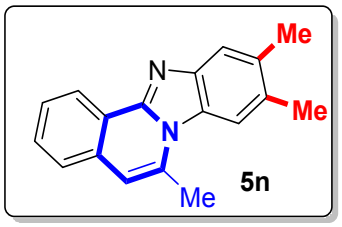
8-methylbenzo[*h*]benzo[4,5]imidazo[2,1-*a*]isoquinoline (5k) was obtained as a white solid (42 mg, 75%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.91 (d, J = 8.5 Hz, 1H), 8.15 (dd, J = 16.4, 8.2 Hz, 2H), 8.01–7.87 (m, 3H), 7.68 (ddd, J = 8.0, 6.9, 1.1 Hz, 1H), 7.59–7.51 (m, 2H), 7.36 (ddd, J = 8.3, 7.1, 1.2 Hz, 1H), 6.84 (s, 1H), 3.03 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 148.4, 144.6, 135.6, 132.4, 131.9, 131.0, 130.1, 130.0, 128.5, 128.3, 128.1, 126.3, 124.4, 124.3, 121.4, 120.1, 116.8, 114.1, 111.8, 21.4. **HRMS (ESI) calcd for** $C_{20}H_{15}N_2^+$ $[M + H]^+$: 283.1230; Found: 283.1228.



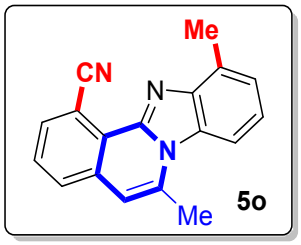
6-Methylbenzo[*g*]benzo[4,5]imidazo[2,1-*a*]isoquinoline (5l) was obtained as a yellow solid (30 mg, 54%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.29 (s, 1H), 8.07 (dd, J = 6.0, 3.4 Hz, 1H), 8.02 (*d*, J = 8.1 Hz, 1H), 7.97–7.91 (m, 2H), 7.85 (dd, J = 5.9, 3.5 Hz, 1H), 7.54–7.48 (m, 2H), 7.46 (t, J = 7.6 Hz, 1H), 7.34–7.28 (m, 1H), 6.69 (s, 1H), 2.89 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 148.3, 143.8, 133.9, 133.9, 132.0, 131.7, 128.9, 128.7, 127.6, 127.0, 126.0, 124.7, 123.9, 123.8, 122.2, 120.6, 119.8, 113.6, 110.8, 21.2; **HRMS (ESI) calcd for** $C_{20}H_{15}N_2^+$ $[M + H]^+$: 283.1230; Found: 283.1235.



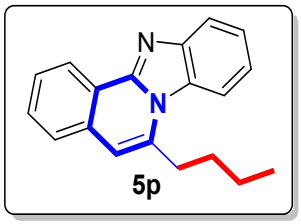
5-Methylbenzo[4,5]imidazo[1,2-*a*]thieno[2,3-*c*]pyridinee (5m) was obtained as a yellow solid (39 mg, 81%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.02 (d, J = 8.4 Hz, 1H), 7.96 (d, J = 8.2 Hz, 1H), 7.59 (d, J = 5.1 Hz, 1H), 7.46 (t, J = 7.6 Hz, 1H), 7.30–7.20 (m, 2H), 6.84 (s, 1H), 2.95 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 145.7, 144.5, 139.0, 135.0, 130.7, 129.7, 124.6, 124.3, 123.9, 121.0, 119.3, 114.1, 107.2, 21.2; **HRMS (ESI) calcd for** $C_{14}H_{11}SN_2^+$ $[M + H]^+$: 239.0637; Found: 239.0638.



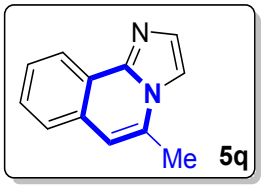
6,9,10-Trimethylbenzo[4,5]imidazo[2,1-*a*]isoquinoline (5n) was obtained as a yellow solid (28 mg, 54%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.77 (d, J = 3.5 Hz, 1H), 7.74 (d, J = 8.0 Hz, 2H), 7.63–7.48 (m, 3H), 6.64 (s, 1H), 2.91 (s, 3H), 2.42 (s, 3H), 2.39 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 142.7, 134.7, 133.2, 131.5, 130.7, 129.4, 126.9, 125.6, 124.7, 122.2, 119.6, 113.9, 110.2, 21.2, 20.8, 20.4; **HRMS (ESI) calcd for** $C_{18}H_{17}N_2^+$ $[M + H]^+$: 261.1386; Found: 261.1389.



6,11-Dimethylbenzo[4,5]imidazo[2,1-*a*]isoquinoline-1-carbonitrile (5o) was obtained as a yellow solid (54 mg, 99%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, Acetone)** δ 8.14–8.03 (m, 3H), 7.83 (t, J = 7.7 Hz, 1H), 7.42–7.27 (m, 2H), 7.08 (d, J = 0.9 Hz, 1H), 3.12 (s, 3H), 2.81 (s, 3H); **^{13}C NMR (126 MHz, Acetone)** δ 145.1, 139.3, 136.1, 134.5, 132.2, 131.8, 130.8, 126.0, 124.3, 123.3, 119.8, 113.7, 111.3, 110.3, 21.9, 17.6; **HRMS (ESI) calcd for** $C_{18}H_{14}N_2^+$ $[M + H]^+$: 272.1182; Found: 272.1185.

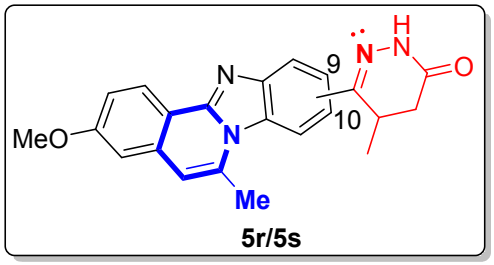


6-Butylbenzo[4,5]imidazo[2,1-*a*]isoquinoline (5p) was obtained as a white solid (43 mg, 79%), m.p. = 166–168 ºC; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.87–8.74 (m, 1H), 8.03 (d, J = 8.1 Hz, 1H), 7.92 (d, J = 8.4 Hz, 1H), 7.59 (dd, J = 6.7, 2.4 Hz, 3H), 7.48 (t, J = 7.6 Hz, 1H), 7.34 (t, J = 7.5 Hz, 1H), 6.71 (s, 1H), 3.53–2.93 (m, 2H), 1.96–1.76 (m, 2H), 1.64–1.52 (m, 2H), 1.02 (t, J = 7.4 Hz, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 148.2, 143.7, 138.9, 131.6, 130.5, 130.0, 127.1, 125.8, 125.0, 124.2, 121.9, 121.8, 119.7, 114.2, 109.7, 33.0, 29.3, 22.3, 13.9. **HRMS (ESI) calcd for** $C_{19}H_{19}N_2^+$ $[M + H]^+$: 275.1543; Found: 275.1544.



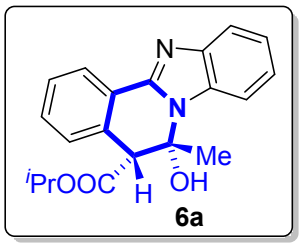
5-Methylimidazo[2,1-*a*]isoquinoline (5q) was obtained as a white solid (21 mg, 58%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.64 (d, J = 7.9 Hz, 1H), 7.64 (dd, J = 8.4, 0.9 Hz, 2H), 7.61–7.51 (m, 3H), 6.87 (s, 1H), 2.60 (s, 3H). **^{13}C NMR (126 MHz,**

$CDCl_3$) δ 143.3, 131.5, 131.1, 129.9, 128.2, 127.3, 126.1, 123.2, 122.3, 111.6, 111.4, 18.6. **HRMS (ESI) calcd for** $C_{12}H_{11}N_2^+$ $[M + H]^+$: 183.0917; Found: 183.0919.



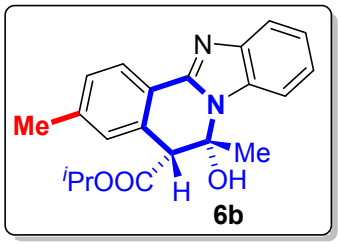
5r/5s

6-(3-Methoxy-6-methylbenzo[4,5]imidazo[2,1-*a*]isoquinolin-10-yl)-5-methyl-4,5-dihydropyridazin-3(2*H*)-one (5r) and 6-(3-Methoxy-6-methylbenzo[4,5]imidazo[2,1-*a*]isoquinolin-9-yl)-5-methyl-4,5-dihydropyridazin-3(2*H*)-one (5s) was Yellow solid (49 mg, 66%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ [9.06 (s) + 9.01 (s), 1H], 8.76, (t, 1H), [8.55 (s) + 8.29 (s), 1H], 8.03 (dd, J = 29.8, 8.7 Hz, 1H), 7.87 (dd, J = 37.6, 8.7 Hz, 1H), 7.27–7.12 (m, 1H), 7.01 (dd, J = 11.0, 2.2 Hz, 1H), 6.76 (d, J = 15.1 Hz, 1H), [3.95 (s) + 3.94 (s), 3H], 3.61–3.45 (m, 1H), [3.03 (s) + 3.02 (s), 3H], 2.82 (ddd, J = 16.8, 6.7, 3.0 Hz, 1H), 2.56 (d, J = 15 Hz, 1H), 1.38–1.31 (m, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.9, 166.8, 161.6, 161.5, 154.6, 154.1, 149.6, 148.9, 135.2, 135.0, 134.0, 133.8, 131.6, 127.78, 127.0, 122.4, 119.5, 118.8, 117.2, 117.2, 116.8, 114.2, 111.7, 111.6, 111.5, 107.2, 107.0, 55.5, 34.0 28.6, 28.3, 22.6, 21.3, 21.2, 16.5, 14.1. **HRMS (ESI) calcd for** $C_{22}H_{21}N_4O_2^+$ $[M + H]^+$: 373.1659; Found: 373.1658.

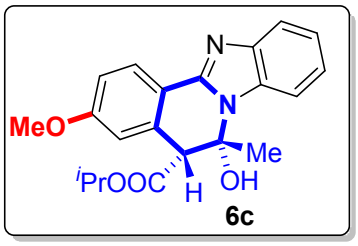


6a

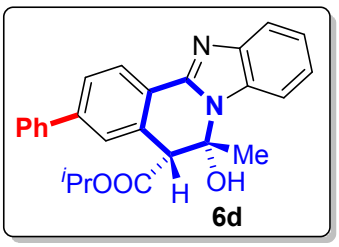
Isopropyl 6-hydroxy-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (6a) was obtained as a white solid (62 mg, 92%), m. p. = 140–142; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.31–8.23 (m, 1H), 8.09–7.96 (m, 1H), 7.78 (dt, J = 4.6, 2.8 Hz, 1H), 7.51–7.36 (m, 3H), 7.31–7.23 (m, 2H), 6.13 (s, 1H), 4.88 (hept, J = 6.2 Hz, 1H), 4.04 (s, 1H), 1.62 (s, 3H), 1.17 (d, J = 6.2 Hz, 3H), 0.91 (d, J = 6.2 Hz, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.8, 147.7, 144.2, 133.7, 131.0, 130.2, 130.1, 129.1, 128.9, 126.7, 125.9, 125.2, 123.2, 122.6, 119.6, 113.4, 87.2, 70.2, 55.5, 26.6, 21.4, 21.1. **HRMS (ESI) calcd for** $C_{20}H_{21}N_2O_3^+$ $[M + H]^+$: 337.1547; Found: 337.1548.



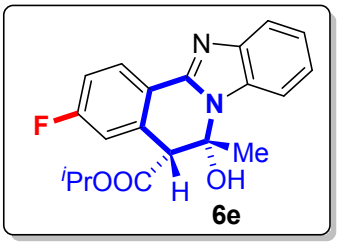
Isopropyl 6-hydroxy-3,6-dimethyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (6b) was obtained as white solid (48 mg, 68%), m. p. = 144–145; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.14 (d, J = 8.3 Hz, 1H), 8.01 (dd, J = 6.6, 2.3 Hz, 1H), 7.77 (dd, J = 6.5, 2.2 Hz, 1H), 7.31–7.20 (m, 4H), 6.14 (s, 1H), 4.92–4.80 (m, 1H), 3.98 (s, 1H), 2.42 (s, 3H), 1.59 (s, 3H), 1.16 (d, J = 6.2 Hz, 3H), 0.91 (d, J = 6.2 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.8, 148.0, 144.1, 140.5, 133.6, 131.0, 130.6, 129.9, 125.8, 122.9, 122.5, 122.4, 119.4, 113.2, 87.1, 70.0, 55.6, 26.6, 21.5, 21.4, 21.1. **HRMS (ESI) calcd for** $C_{21}H_{23}N_2O_3^+$ [M + H]$^+$: 351.1703; Found: 351.1709.



Isopropyl 6-hydroxy-3-methoxy-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (6c) was obtained as white solid (53 mg, 73%), m. p. = 159–162; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.21 (d, J = 8.2 Hz, 1H), 7.99 (d, J = 7.3 Hz, 1H), 7.76 (d, J = 7.3 Hz, 1H), 7.23 (m, J = 13.4, 6.3 Hz, 2H), 7.04–6.93 (m, 2H), 5.94 (s, 1H), 4.96–4.72 (m, 1H), 3.97 (s, 1H), 3.88 (s, 3H), 1.59 (s, 3H), 1.17 (d, J = 6.2 Hz, 3H), 0.94 (d, J = 6.2 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.6, 161.0, 147.9, 143.9, 133.5, 132.8, 127.8, 122.8, 122.4, 119.1, 117.9, 115.6, 114.5, 113.1, 87.1, 70.1, 55.8, 55.5, 26.5, 21.5, 21.2.. **HRMS (ESI) calcd for** $C_{21}H_{23}N_2O_4^+$ [M + H]$^+$: 367.1652; Found: 367.1657.

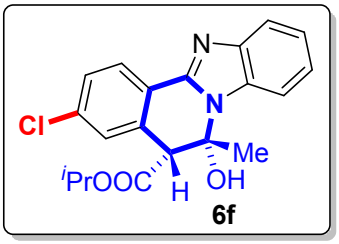


Isopropyl 6-hydroxy-6-methyl-3-phenyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (6d) was obtained as a white solid (73 mg, 88%), m. p. = 150–152; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.34 (d, J = 8.6 Hz, 1H), 8.05 (dd, *J* = 6.2, 2.6 Hz, 1H), 7.81 (dd, *J* = 6.1, 2.5 Hz, 1H), 7.68 (dd, *J* = 21.1, 7.1 Hz, 4H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.42 (t, *J* = 7.3 Hz, 1H), 7.29 (dd, J = 9.3, 5.7 Hz, 2H), 6.20 (s, 1H), 4.97–4.81 (m, 1H), 4.12 (s, 1H), 1.66 (s, 3H), 1.19 (d, *J* = 6.2 Hz, 3H), 0.94 (d, *J* = 6.2 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.7, 147.6, 144.2, 142.9, 139.7, 133.7, 131.5, 129.0, 128.7, 128.0, 127.8, 127.0, 126.4, 124.0, 123.2, 122.6, 119.5, 113.3, 87.2, 70.2, 55.7, 26.7, 21.5, 21.2. **HRMS (ESI) calcd for** $C_{26}H_{25}N_2O_3^+$ [M + H]$^+$: 413.1860; Found: 413.1864.



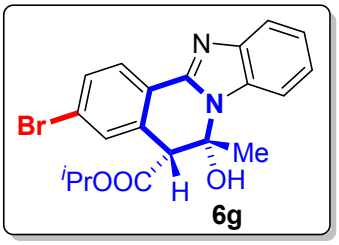
6e

Isopropyl 3-fluoro-6-hydroxy-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (6e) was obtained as a white solid (46 mg, 65%), m. p. = 126–128; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.26 (dd, *J* = 8.5, 5.6 Hz, 1H), 8.11–7.89 (m, 1H), 7.84–7.72 (m, 1H), 7.32–7.22 (m, 2H), 7.17 (ddd, *J* = 17.0, 8.6, 2.5 Hz, 2H), 6.22 (s, 1H), 5.00–4.76 (m, 1H), 4.00 (s, 1H), 1.60 (s, 3H), 1.18 (d, *J* = 6.2 Hz, 3H), 0.94 (d, *J* = 6.2 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.2, 163.4 (d, *J* = 251.6 Hz), 146.9, 144.0, 133.6, 133.4 (d, *J* = 8.6 Hz), 128.2 (d, *J* = 8.8 Hz), 123.3, 122.7, 121.7 (d, J = 3.0 Hz), 119.5, 117.1 (d, *J* = 23.1 Hz), 116.5 (d, *J* = 22.0 Hz), 113.3, 87.1, 70.5, 55.3, 26.7, 21.4, 21.1. **HRMS (ESI) calcd for** $C_{20}H_{20}N_2FO_3^+$ [M + H]$^+$: 355.1452; Found: 355.1456.



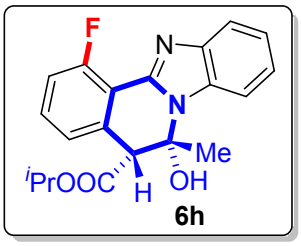
6f

Isopropyl 3-chloro-6-hydroxy-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (6f) was obtained as a white solid (55 mg, 74%), m. p. = 111–112; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.20 (d, J = 8.3 Hz, 1H), 8.04–7.97 (m, 1H), 7.81–7.74 (m, 1H), 7.46 (d, J = 1.9 Hz, 1H), 7.43 (dd, J = 8.3, 2.0 Hz, 1H), 7.32–7.23 (m, 2H), 6.21 (s, 1H), 4.94–4.83 (m, 1H), 3.99 (s, 1H), 1.60 (s, 3H), 1.18 (d, J = 6.2 Hz, 3H), 0.94 (d, J = 6.2 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.3, 146.8, 144.0, 135.8, 133.6, 132.6, 130.1, 129.4, 127.2, 123.8, 123.5, 122.8, 119.6, 113.4, 87.2, 70.6, 55.1, 26.7, 21.4, 21.1; **HRMS (ESI) calcd for** $C_{20}H_{20}N_2ClO_3^+$ $[M + H]^+$: 371.1157; Found: 371.1157.



6g

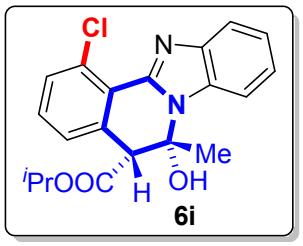
Isopropyl 3-bromo-6-hydroxy-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (6g) was obtained as a white solid (46 mg, 56%), m. p. = 108–109; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.11 (d, J = 8.3 Hz, 1H), 8.04–7.99 (m, 1H), 7.80–7.73 (m, 1H), 7.62 (d, J = 1.6 Hz, 1H), 7.57 (dd, J = 8.3, 1.8 Hz, 1H), 7.31–7.23 (m, 2H), 6.25 (s, 1H), 4.93–4.83 (m, 1H), 3.98 (s, 1H), 1.60 (s, 3H), 1.18 (d, J = 6.2 Hz, 3H), 0.94 (d, J = 6.2 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.2, 146.8, 144.0, 133.6, 133.0, 132.8, 132.3, 127.3, 124.2, 124.0, 123.5, 122.8, 119.6, 113.4, 87.1, 70.5, 55.1, 26.7, 21.4, 21.1. $C_{20}H_{20}N_2BrO_3^+$ $[M + H]^+$: 415.0652; Found: 415.0658.



6h

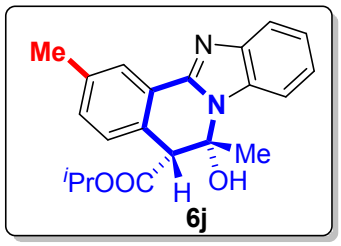
Isopropyl 1-fluoro-6-hydroxy-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (6h) was as a white solid (45 mg, 63%), m. p. = 156–157; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.03 (dd, J = 5.8, 3.1 Hz, 1H), 7.87 (dd, J = 5.7, 3.1 Hz, 1H), 7.39 (dd, J = 12.8, 7.8 Hz, 1H), 7.31–7.14 (m, 4H), 6.24 (s, 1H), 4.92–4.77 (m, 1H), 4.03 (s, 1H), 1.60 (s, 3H), 1.13 (d, J = 6.2 Hz, 3H), 0.87 (d, J = 6.2 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.5, 159.7 (d, J = 260.2 Hz), 144.4, 143.7 (d,

J = 7.3 Hz), 133.6, 132.7, 130.9 (d, J = 9.1 Hz), 126.1 (d, J = 3.5 Hz), 123.6, 122.5, 120.3, 117.2 (d, J = 21.6 Hz), 113.9 (d, J = 10.8 Hz), 113.2, 87.0, 70.5, 55.6, 26.6, 21.3, 21.1. **HRMS (ESI) calcd for** $C_{20}H_{20}N_2FO_3^+$ [M + H]$^+$: 355.1452; Found: 355.1454.



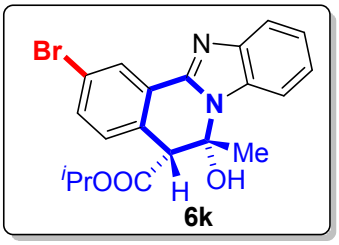
6i

Isopropyl 1-chloro-6-hydroxy-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (6i) was obtain as a white solid (52 mg, 70%), m. p. = 263–265; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 8.07–8.00 (m, 1H), 7.92–7.86 (m, 1H), 7.55 (dd, J = 7.7, 1.4 Hz, 1H), 7.39–7.29 (m, 2H), 7.30–7.26 (m, 2H), 6.28 (s, 1H), 4.89–4.68 (m, 1H), 3.98 (s, 1H), 1.62 (s, 3H), 1.10 (d, J = 6.2 Hz, 3H), 0.84 (d, J = 6.2 Hz, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)** δ 170.6, 144.9, 143.8, 134.1, 132.9, 132.7, 132.3, 129.8, 129.0, 123.8, 123.3, 122.4, 120.5, 113.1, 86.5, 70.6, 56.1, 26.6, 21.3, 21.1; **HRMS (ESI) calcd for** $C_{20}H_{20}N_2ClO_3^+$ [M + H]$^+$: 371.1157; Found: 371.1157.



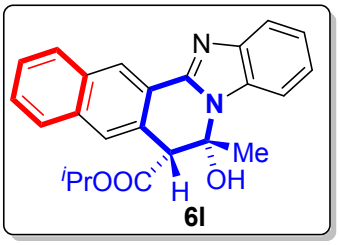
6j

Isopropyl 6-hydroxy-2,6-dimethyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (6j) was obtained as a white solid (39 mg, 55%), m. p. = 163–165; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 8.12 (s, 1H), 8.05–7.98 (m, 1H), 7.83–7.74 (m, 1H), 7.35 (d, J = 7.7 Hz, 1H), 7.31–7.16 (m, 3H), 6.07 (s, 1H), 4.95–4.78 (m, 1H), 4.00 (s, 1H), 2.42 (s, 3H), 1.60 (s, 3H), 1.17 (d, J = 6.2 Hz, 3H), 0.92 (d, J = 6.2 Hz, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)** δ 171.0, 147.9, 144.2, 139.1, 133.7, 131.0, 130.1, 128.0, 126.3, 124.9, 123.1, 122.5, 119.5, 113.3, 87.2, 70.0, 55.1, 26.6, 21.5, 21.17, 21.09; **HRMS (ESI) calcd for** $C_{21}H_{23}N_2O_3^+$ [M + H]$^+$: 351.1703; Found: 351.1704.



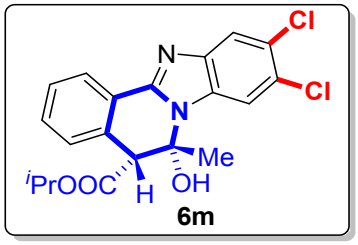
6k

Isopropyl 2-bromo-6-hydroxy-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (6k) was obtained as a white solid (52 mg, 63%), m. p. = 166–167; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.46 (s, 1H), 8.08–7.97 (m, 1H), 7.83–7.74 (m, 1H), 7.54 (d, J = 7.7 Hz, 1H), 7.34 (d, J = 8.1 Hz, 1H), 7.31–7.27 (m, 2H), 6.15 (s, 1H), 5.01–4.73 (m, 1H), 4.00 (s, 1H), 1.60 (s, 3H), 1.18 (d, J = 6.1 Hz, 3H), 0.94 (d, J = 6.1 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.4, 146.3, 144.1, 133.7, 132.9, 131.8, 129.8, 128.7, 127.0, 123.7, 123.2, 122.9, 119.8, 113.4, 87.2, 70.5, 54.9, 26.7, 21.5, 21.2; **HRMS (ESI) calcd for** $C_{20}H_{20}N_2BrO_3^+$ $[M + H]^+$: 415.0652; Found: 415.0651.

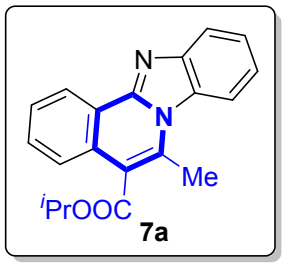


6l

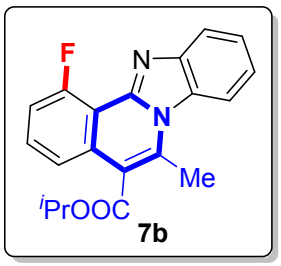
Isopropyl 6-hydroxy-6-methyl-6,7-dihydrobenzo[*g*]benzo[4,5]imidazo[2,1-*a*]isoquinoline-7-carboxylate (6l) was obtained as a yellow solid (31 mg, 40%), m. p. = 118–120; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.84 (s, 1H), 8.06 (dd, J = 7.0, 1.7 Hz, 1H), 8.00–7.94 (m, 1H), 7.93 (s, 1H), 7.89–7.85 (m, 1H), 7.83 (dd, J = 7.0, 1.8 Hz, 1H), 7.60–7.51 (m, 2H), 7.30 (dt, J = 7.5, 5.7 Hz, 2H), 6.15 (s, 1H), 4.91–4.82 (m, 1H), 4.23 (s, 1H), 1.64 (s, 3H), 1.14 (d, J = 6.2 Hz, 3H), 0.84 (d, J = 6.2 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 171.1, 147.9, 144.4, 133.9, 133.8, 133.3, 129.5, 128.8, 128.2, 127.6, 127.5, 127.1, 126.1, 123.2, 122.7, 122.6, 119.6, 113.5, 87.3, 70.3, 56.1, 27.0, 21.4, 21.1; **HRMS (ESI) calcd for** $C_{24}H_{23}N_2O_3^+$ $[M + H]^+$: 387.1703; Found: 387.1704.



Isopropyl 9,10-dichloro-6-hydroxy-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (6m) was obtained as a white solid (69 mg, 85%), m. p. = 155–157; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.25–8.17 (m, 1H), 8.14 (s, 1H), 7.82 (s, 1H), 7.52–7.42 (m, 3H), 6.29 (s, 1H), 4.88 (hept, J = 6.2 Hz, 1H), 4.04 (s, 1H), 1.59 (s, 3H), 1.17 (d, J = 6.2 Hz, 3H), 0.90 (d, J = 6.2 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.7, 149.6, 143.5, 132.7, 131.2, 130.8, 130.4, 129.3, 127.0, 126.7, 126.1, 124.4, 120.4, 114.5, 87.4, 70.5, 55.2, 26.6, 21.4, 21.1. **HRMS (ESI) calcd for** $C_{20}H_{19}N_2Cl_2O_2^+$ $[M + H]^+$: 405.0767; Found: 405.0766.

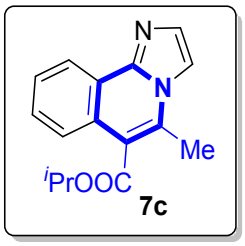


Isopropyl 6-methylbenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (7a) was obtained as a yellow solid (32 mg, 50%), m. p. = 139–140; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.94–8.79 (m, 1H), 8.12 (d, J = 8.4 Hz, 1H), 8.04 (d, J = 8.1 Hz, 1H), 7.76–7.62 (m, 3H), 7.56–7.49 (m, 1H), 7.38 (ddd, J = 8.4, 7.2, 1.2 Hz, 1H), 5.48 (hept, J = 6.3 Hz, 1H), 3.09 (s, 3H), 1.49 (d, J = 6.3 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 167.3, 147.6, 144.5, 134.3, 131.6, 130.4, 128.7, 127.7, 125.3, 124.7, 123.9, 122.1, 122.1, 120.2, 116.6, 114.4, 69.9, 21.9, 19.0. **HRMS (ESI) calcd for** $C_{20}H_{19}N_2O_2^+$ $[M + H]^+$: 319.1441; Found: 319.1442.



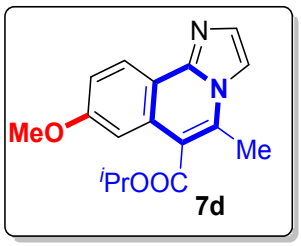
Isopropyl 1-fluoro-6-methylbenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (7b) was obtained as a yellow solid (28 mg, 41%), m. p. = 135–139; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.10 (dd, J = 18.1, 8.3 Hz, 2H), 7.62 (m, 1H), 7.49 (m, 2H), 7.41–

7.31 (m, 2H), 5.55–5.40 (m, 1H), 3.06 (s, 3H), 1.48 (d, J = 6.3 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 167.0, 156.0 (d, J = 260.9 Hz), 144.6, 143.8 (d, J = 8.3 Hz), 135.2, 130.9, 130.8 (d, J = 9.2 Hz), 130.4, 124.8, 122.7, 120.8, 119.6 (d, J = 4.2 Hz), 116.3 (d, J = 2.4 Hz), 114.4 (d, J = 21.0 Hz), 114.2, 111.5 (d, J = 11.0 Hz), 70.1, 21.8, 19.1; **HRMS (ESI) calcd for** $C_{20}H_{18}FN_2O_2^+$ [M + H]$^+$: 337.1347; Found: 337.1346.



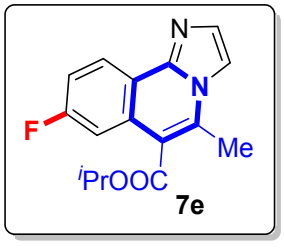
7c

Isopropyl 5-methylimidazo[2,1-*a*]isoquinoline-6-carboxylate (7c) was obtained as a green oil (17 mg, 32%); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.69–8.60 (m, 1H), 7.78–7.72 (m, 1H), 7.66 (d, J = 1.2 Hz, 1H), 7.64–7.55 (m, 3H), 5.51–5.38 (m, 1H), 2.67 (s, 3H), 1.46 (d, J = 6.3 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 167.1, 143.0, 132.2, 131.0, 128.5, 127.8, 126.7, 124.1, 123.4, 122.4, 117.4, 112.1, 69.8, 21.9, 16.7; **HRMS (ESI) calcd for** $C_{16}H_{17}N_2O_2^+$ [M + H]$^+$: 269.1285; Found: 269.1285.



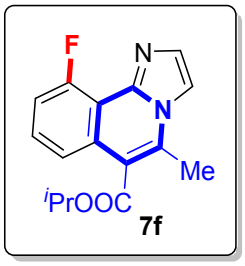
7d

Isopropyl 8-methoxy-5-methylimidazo[2,1-*a*]isoquinoline-6-carboxylate (7d) was obtained as a yellow solid (24 mg, 40%), m. p. = 127–1128; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.56 (d, J = 8.9 Hz, 1H), 7.61 (d, J = 1.4 Hz, 1H), 7.52 (d, J = 1.4 Hz, 1H), 7.24 (dd, J = 8.9, 2.4 Hz, 1H), 7.17 (d, J = 2.4 Hz, 1H), 5.45 (hept, J = 6.3 Hz, 1H), 3.90 (s, 3H), 2.66 (s, 3H), 1.46 (d, J = 6.3 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 167.1, 159.8, 143.2, 132.0, 131.9, 128.4, 125.1, 117.4, 116.9, 116.6, 111.5, 105.8, 69.6, 55.3, 21.9, 16.9; **HRMS (ESI) calcd for** $C_{17}H_{19}N_2O_3^+$ [M + H]$^+$: 299.1390; Found: 299.1389.

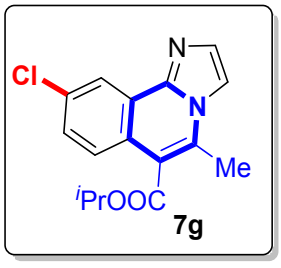


7e

Isopropyl 8-fluoro-5-methylimidazo[2,1-*a*]isoquinoline-6-carboxylate (7e) was obtained as a yellow solid (36 mg, 62%), m. p. = 129–130; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.65 (dd, J = 8.9, 5.8 Hz, 1H), 7.64 (d, J = 1.1 Hz, 1H), 7.57 (d, J = 1.2 Hz, 1H), 7.46 (dd, J = 10.5, 2.4 Hz, 1H), 7.35 (td, J = 8.5, 2.4 Hz, 1H), 5.49–5.39 (m, 1H), 2.69 (s, 3H), 1.46 (d, J = 6.3 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.6, 162.5 (d, J = 247.6 Hz), 142.7, 132.9, 132.4, 128.5 (d, J = 9.5 Hz), 125.9 (d, J = 9.1 Hz), 119.0 (d, J = 1.8 Hz), 116.7, 116.7 (d, J = 3.6 Hz), 116.5, 112.1, 109.8 (d, J = 24.1 Hz), 70.1, 21.9, 16.9; **HRMS (ESI) calcd for** $C_{16}H_{16}FN_2O_2^+$ $[M + H]^+$: 287.1190; Found: 287.1188.

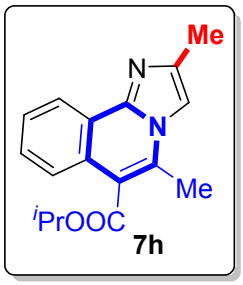


Isopropyl 10-fluoro-5-methylimidazo[2,1-*a*]isoquinoline-6-carboxylate (7f) was obtained as a yellow solid (33 mg, 58%), m. p. = 142–143; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.76 (d, J = 1.3 Hz, 1H), 7.60 (d, J = 1.0 Hz, 1H), 7.51 (dd, J = 5.6, 3.4 Hz, 2H), 7.38–7.30 (m, 1H), 5.52– 5.31 (m, 1H), 2.66 (s, 3H), 1.44 (d, J = 6.3 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.7, 158.8 (d, J = 258.1 Hz), 139.3 (d, J = 7.6 Hz), 133.0 (d, J = 2.4 Hz), 131.9 (s), 129.0 (d, J = 3.1 Hz), 128.7 (d, J = 8.9 Hz), 119.8 (d, J = 4.2 Hz), 117.1 (d, J = 2.6 Hz), 114.1 (d, J = 20.3 Hz), 112.0, 111.9, 70.0, 21.8, 16.9; **HRMS (ESI) calcd for** $C_{16}H_{16}FN_2O_2^+$ $[M + H]^+$: 287.1190; Found: 287.1193.



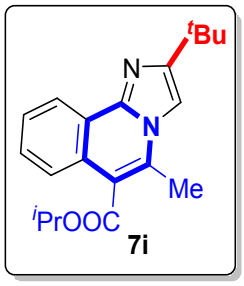
Isopropyl 9-chloro-5-methylimidazo[2,1-*a*]isoquinoline-6-carboxylate (7f) was obtained as a yellow solid (18 mg, 30%), m. p. = 139–140; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.65 (d, J = 2.2 Hz, 1H), 7.70 (dd, J = 9.4, 5.0 Hz, 2H), 7.60 (d, J = 1.3 Hz, 1H), 7.53 (dd, J = 8.8, 2.2 Hz, 1H), 5.75–5.18 (m, 1H), 2.69 (s, 3H), 1.46 (d, J = 6.3 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.7, 141.8, 133.9, 132.5, 131.6, 129.1,

125.9, 125.1, 123.3, 122.9, 117.0, 112.6, 70.1, 21.9, 16.8; **HRMS (ESI) calcd for** $C_{16}H_{16}ClN_2O_2^+$ $[M + H]^+$: 303.0895; Found: 303.0896.



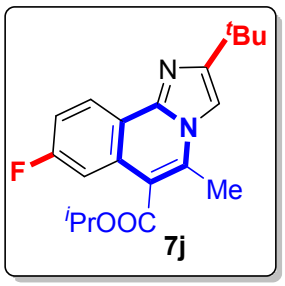
7h

Isopropyl 2,5-dimethylimidazo[2,1-*a*]isoquinoline-6-carboxylate (7h) was obtained as a yellow solid (20 mg, 35%), m. p. = 117–118; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.83–8.54 (m, 1H), 7.88–7.70 (m, 1H), 7.66–7.45 (m, 2H), 7.32 (d, J = 0.8 Hz, 1H), 5.44 (hept, J = 6.3 Hz, 1H), 2.64 (s, 3H), 2.52 (s, 3H), 1.45 (d, J = 6.3 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 167.2, 142.5, 142.0, 130.9, 128.3, 127.5, 126.7, 124.1, 123.3, 121.8, 116.7, 109.1, 69.7, 21.9, 16.8, 14.4; **HRMS (ESI) calcd for** $C_{17}H_{18}N_2O_2^+$ $[M + H]^+$: 283.1441; Found: 283.1443.



7i

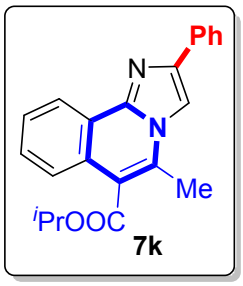
Isopropyl 2-(*tert*-butyl)-5-methylimidazo[2,1-*a*]isoquinoline-6-carboxylate (7i) was obtained as a yellow solid (34 mg, 53%), m. p. = 161–163; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.69 (d, J = 7.6 Hz, 1H), 7.74 (d, J = 7.8 Hz, 1H), 7.62–7.50 (m, 2H), 7.29 (s, 1H), 5.49–5.38 (m, 1H), 2.66 (s, 3H), 1.46 (d, J = 6.0 Hz, 6H), 1.45 (s, 9H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 167.4, 156.1, 142.4, 131.2, 128.0, 127.2, 126.6, 124.0, 123.7, 122.2, 116.4, 106.1, 69.6, 32.4, 30.3, 21.9, 16.8; **HRMS (ESI) calcd for** $C_{20}H_{25}N_2O_2^+$ $[M + H]^+$: 325.1911; Found: 325.1913.



7j

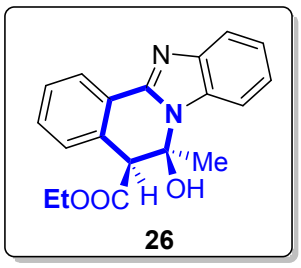
Isopropyl 2-(*tert*-butyl)-8-fluoro-5-methylimidazo[2,1-*a*]isoquinoline-6-carboxylate (7j) was obtained as a yellow solid (57 mg, 84%), m. p. = 151–152; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.68 (dd, J = 8.7, 5.9 Hz, 1H), 7.46 (dd, J = 10.6, 1.7 Hz,

1H), 7.30 (dd, J = 8.5, 1.8 Hz, 1H), 7.28 (s, 1H), 5.42 (m, 1H), 2.67 (s, 3H), 1.46 (d, J = 6.3 Hz, 6H), 1.44 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.8, 162.3 (d, J = 246.7 Hz), 156.2, 142.1, 133.1, 128.3 (d, J = 9.5 Hz), 126.2 (d, J = 9.2 Hz), 118.8, 116.0 (d, J = 23.8 Hz), 115.6 (d, J = 3.6 Hz), 109.5 (d, J = 24.0 Hz), 106.0, 69.8, 32.4, 30.2, 21.9, 17.0; **HRMS (ESI) calcd for** $C_{20}H_{24}N_2FO_2^+$ $[M + H]^+$: 343.1816; Found: 343.1816.



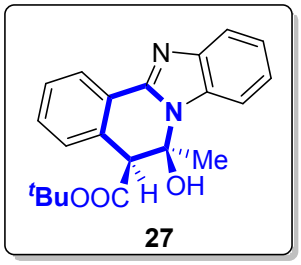
7k

Isopropyl 5-methyl-2-phenylimidazo[2,1-*a*]isoquinoline-6-carboxylate (7k) was obtained as a yellow solid (32 mg, 46%), m. p. = 125–127; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.76 (dd, J = 7.8, 0.9 Hz, 1H), 8.08–7.99 (m, 2H), 7.82 (s, 1H), 7.76 (d, J = 7.7 Hz, 1H), 7.65–7.55 (m, 2H), 7.45 (t, J = 7.7 Hz, 2H), 7.33 (t, J = 7.4 Hz, 1H), 5.53–5.40 (m, 1H), 2.69 (s, 3H), 1.48 (d, J = 6.3 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 167.1, 144.7, 143.2, 133.7, 131.0, 128.7, 128.5, 127.8, 127.6, 126.8, 125.9, 124.1, 123.7, 122.2, 117.3, 107.6 69.8, 21.9, 16.8; **HRMS (ESI) calcd for** $C_{22}H_{21}N_2O_2^+$ $[M + H]^+$: 345.1598; Found: 345.1599.



26

Ethyl 6-hydroxy-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate (**26**) was obtained as a white solid (62 mg, 97%), m. p. = 150–152; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.33–8.22 (m, 1H), 8.03 (dd, J = 6.1, 3.0 Hz, 1H), 7.84–7.74 (m, 1H), 7.53–7.38 (m, 3H), 7.31–7.22 (m, 2H), 6.17 (s, 1H), 4.07 (s, 1H), 4.14–3.94 (m, 2H), 1.61 (s, 3H), 1.07 (t, J = 7.1 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 171.4, 147.7, 144.2, 133.7, 130.9, 1303, 130.2, 129.1, 126.0, 125.3, 123.3, 122.6, 119.6, 113.4, 87.3, 62.2, 55.3, 26.6, 13.7; **HRMS (ESI) calcd for** $C_{19}H_{19}N_2O_3^+$ $[M + H]^+$: 323.1390; Found: 323.1394.



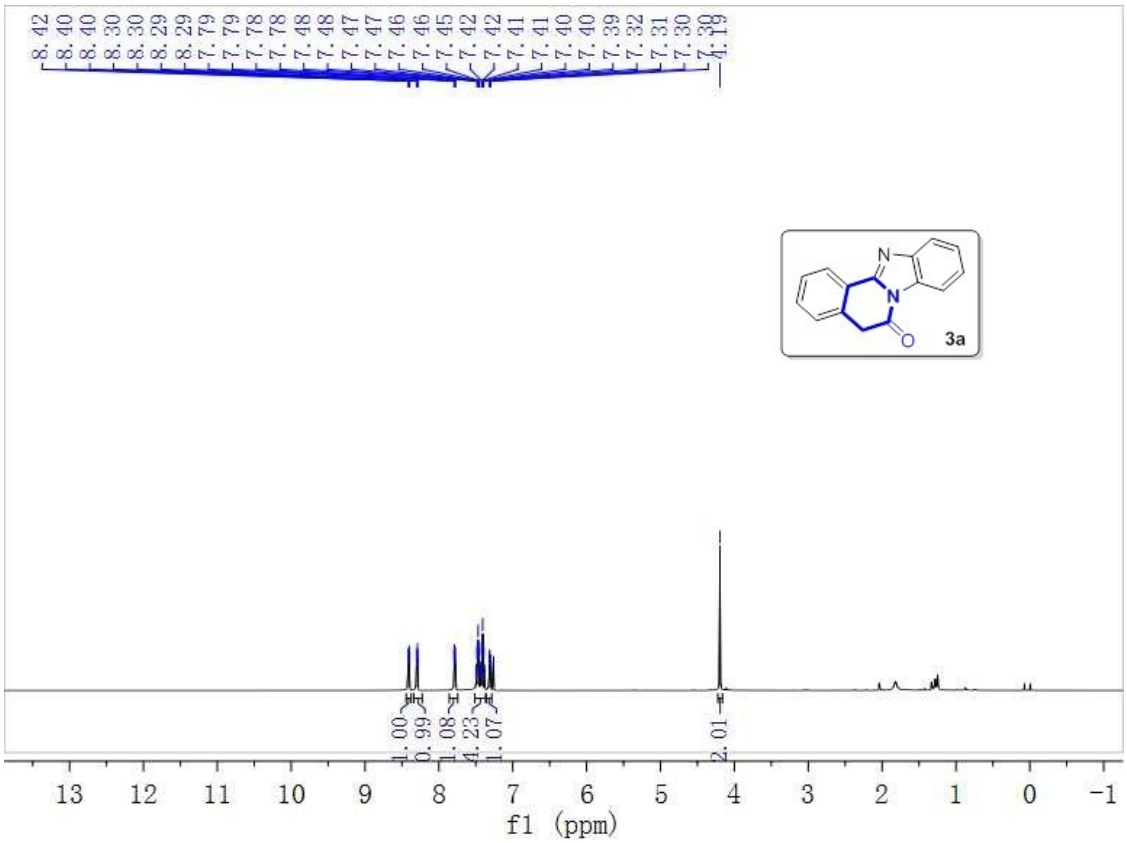
27

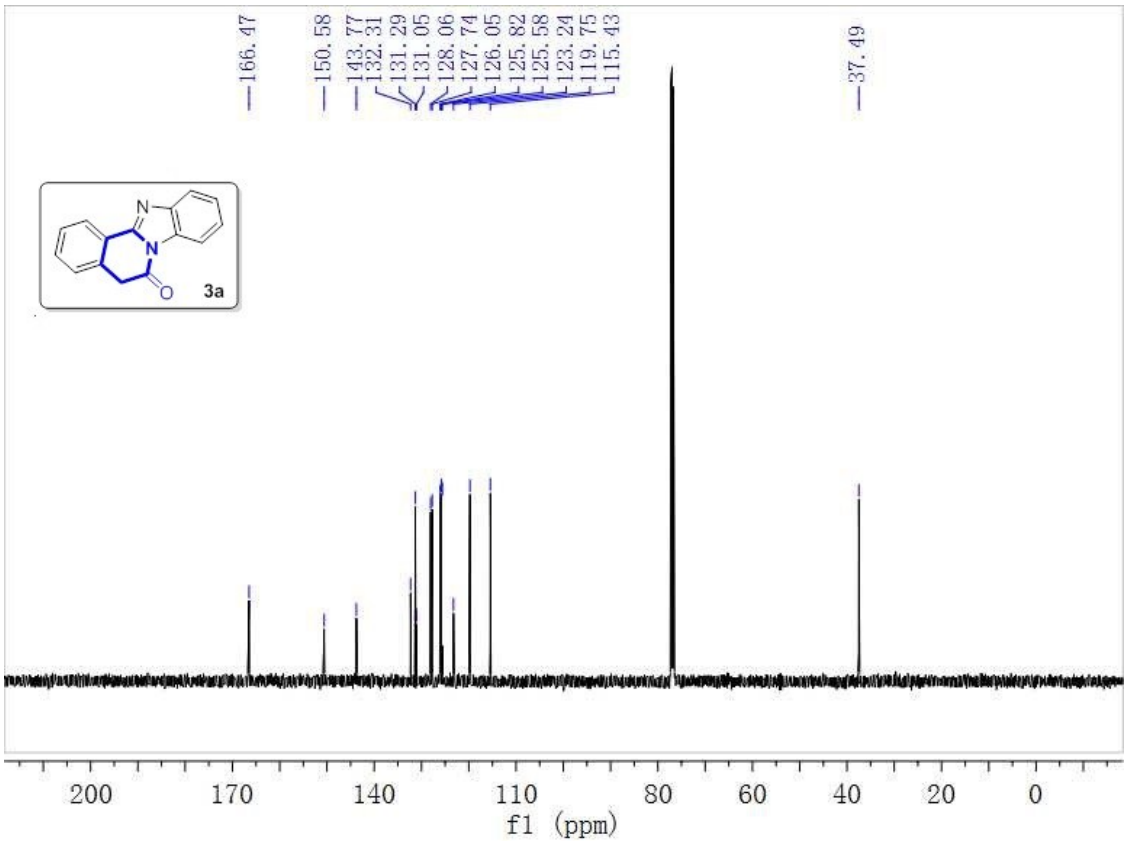
***tert*-Butyl 6-hydroxy-6-methyl-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-5-carboxylate** (**27**) was obtained as a white solid (69 mg, 99%), m. p. = 162–165; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.29 (d, J = 7.6 Hz, 1H), 8.09–7.95 (m, 1H), 7.85–7.72 (m, 1H), 7.51–7.36 (m, 3H), 7.33–7.14 (m, 2H), 6.11 (s, 1H), 3.98 (s, 1H), 1.60 (s, 3H), 1.23 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 170.7, 147.8, 144.2, 133.7, 131.6, 130.2, 130.0, 128.9, 125.9, 125.2, 123.2, 122.5, 119.6, 113.4, 87.3, 83.8, 56.1, 27.6, 26.7; **HRMS (ESI) calcd for** $C_{21}H_{23}N_2O_3^+$ $[M + H]^+$: 351.1703; Found: 315.1705.

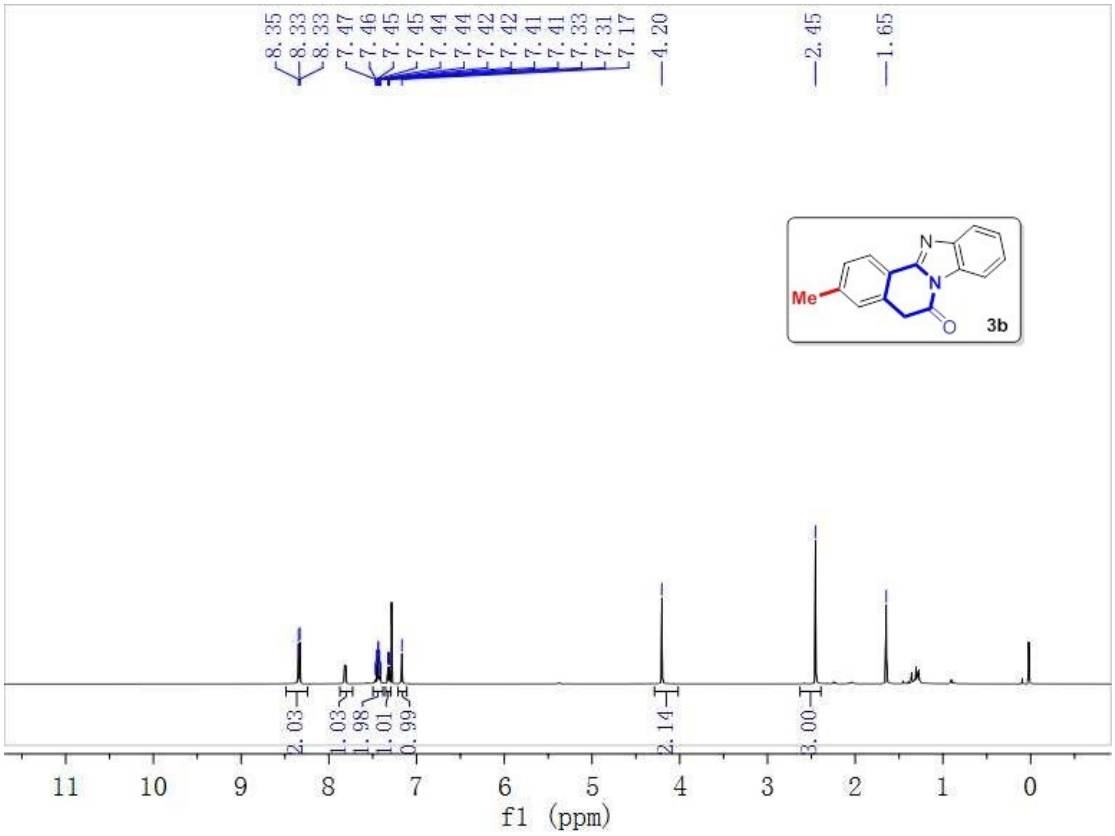
9. References

[S1] Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996***, 15*, 1518.

10. NMR Spectra



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7.31
7.17
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2.45
1.65
Me
N
N
O
3b
2.03
1.03
1.98
1.01
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9
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5
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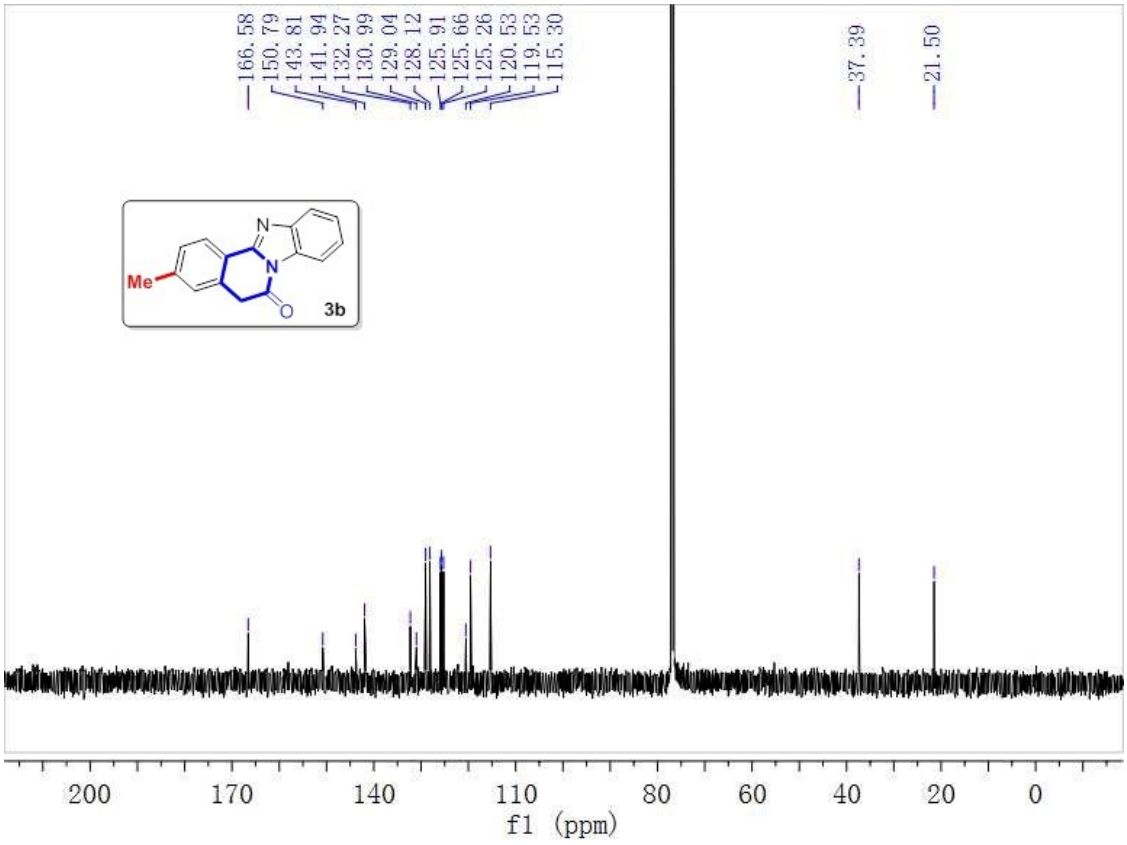
f1 (ppm)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N
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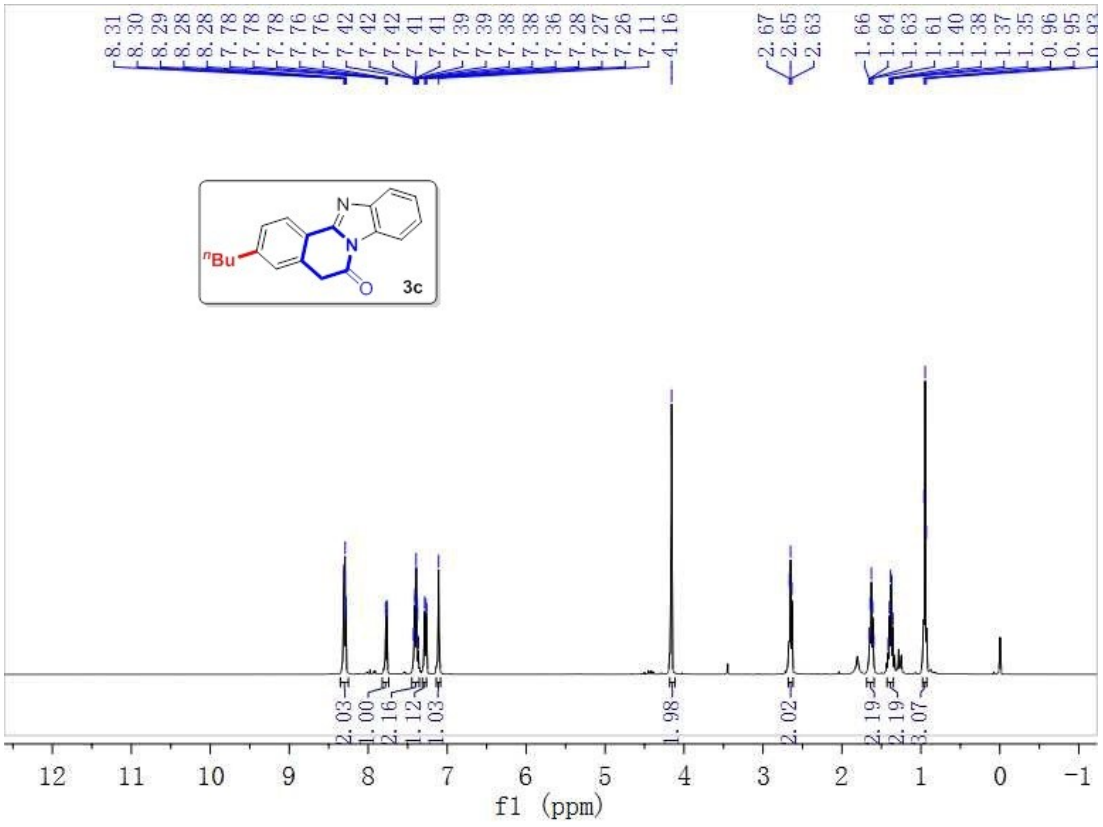
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2.02
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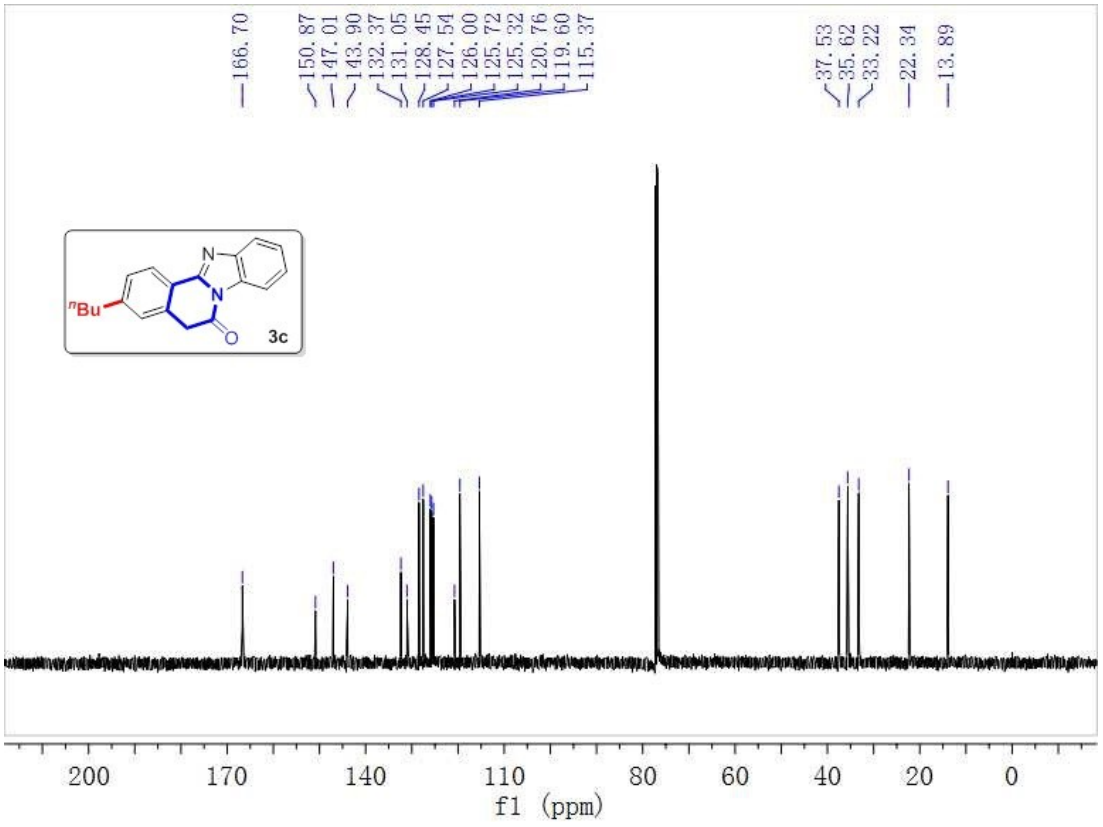
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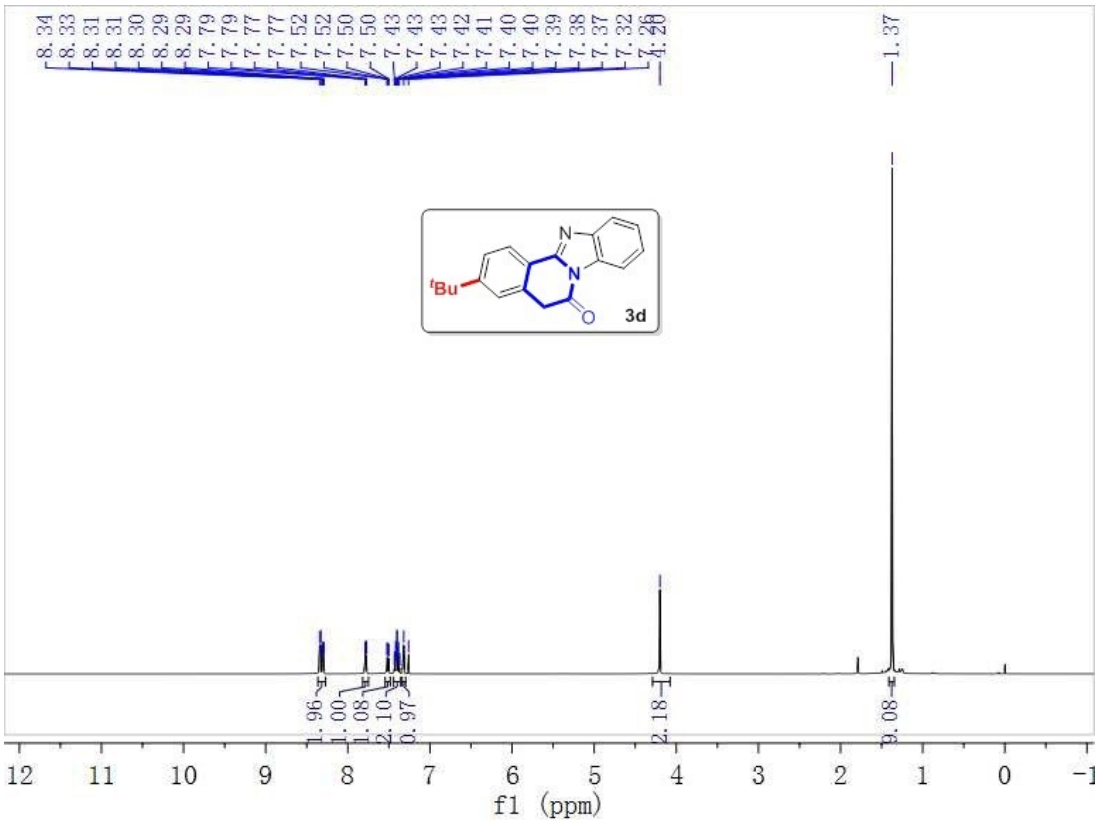
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4
3
2
1
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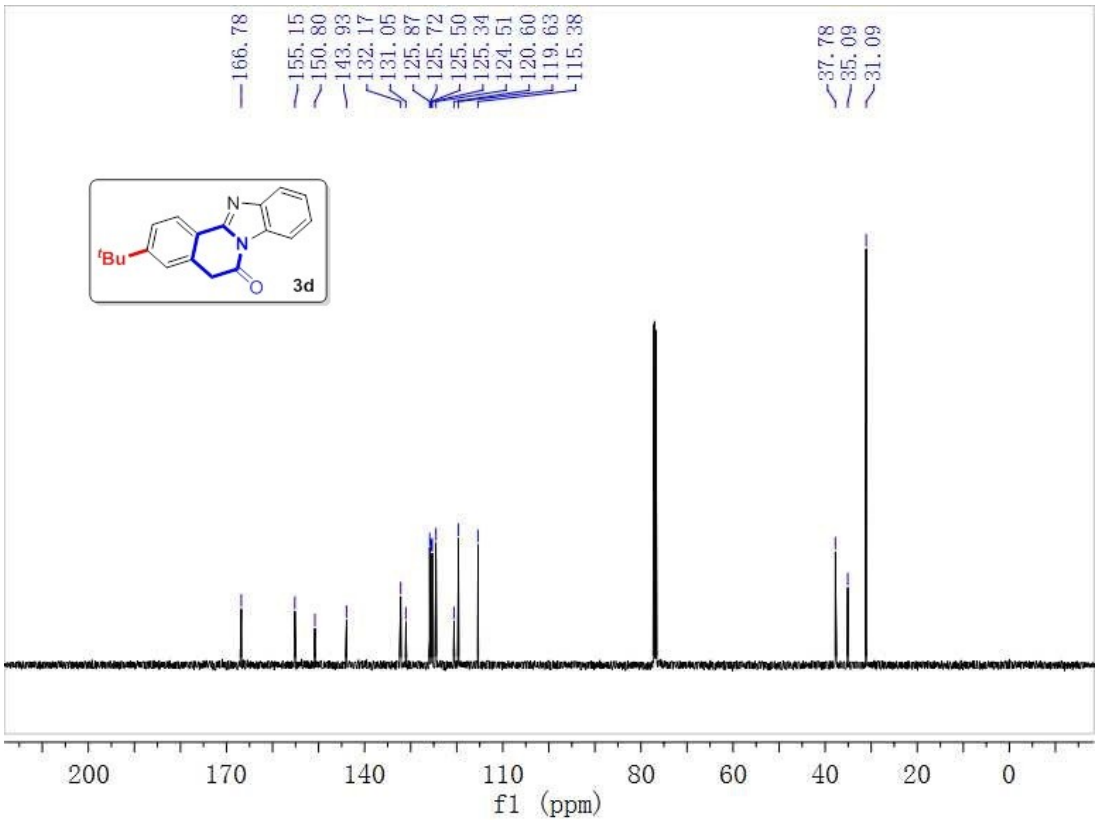
f1 (ppm)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37.78
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N
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3d
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20
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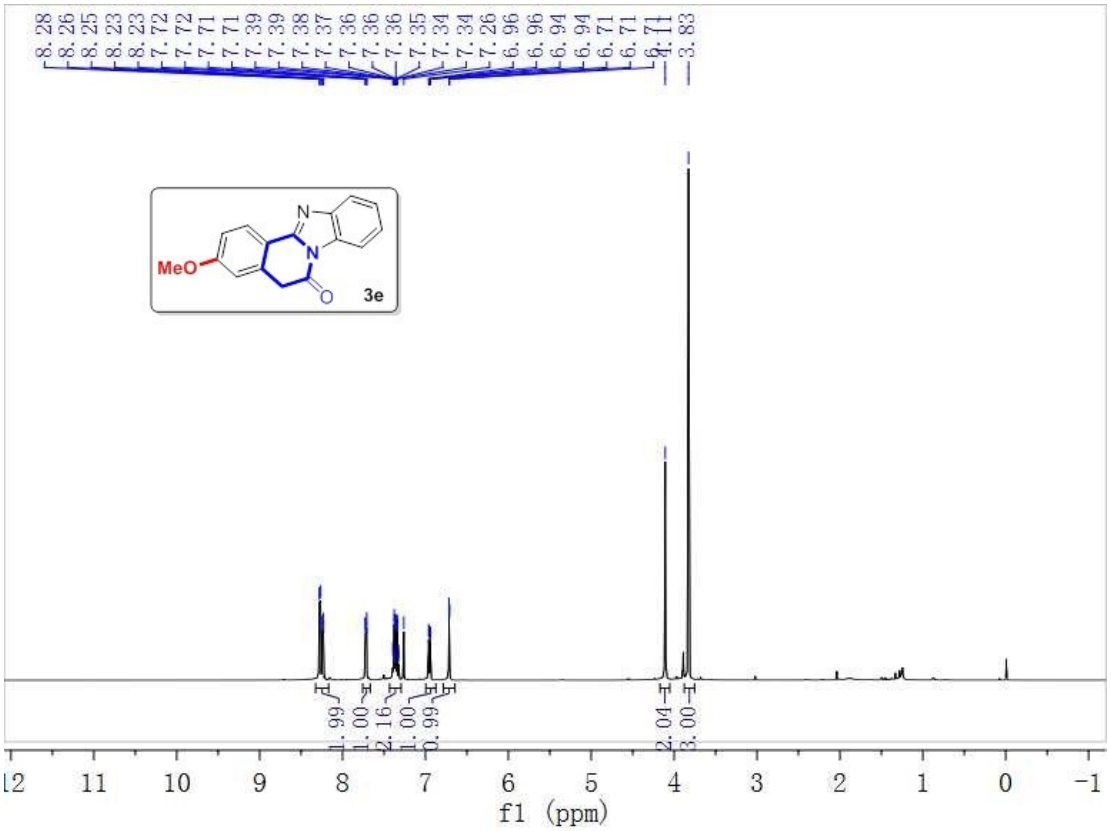
f1 (ppm)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7.36
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7.35
7.34
7.34
7.26
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6.96
6.94
6.94
6.71
6.71
4.11
3.83
MeO
3e
1.99
1.00
2.16
1.00
0.99
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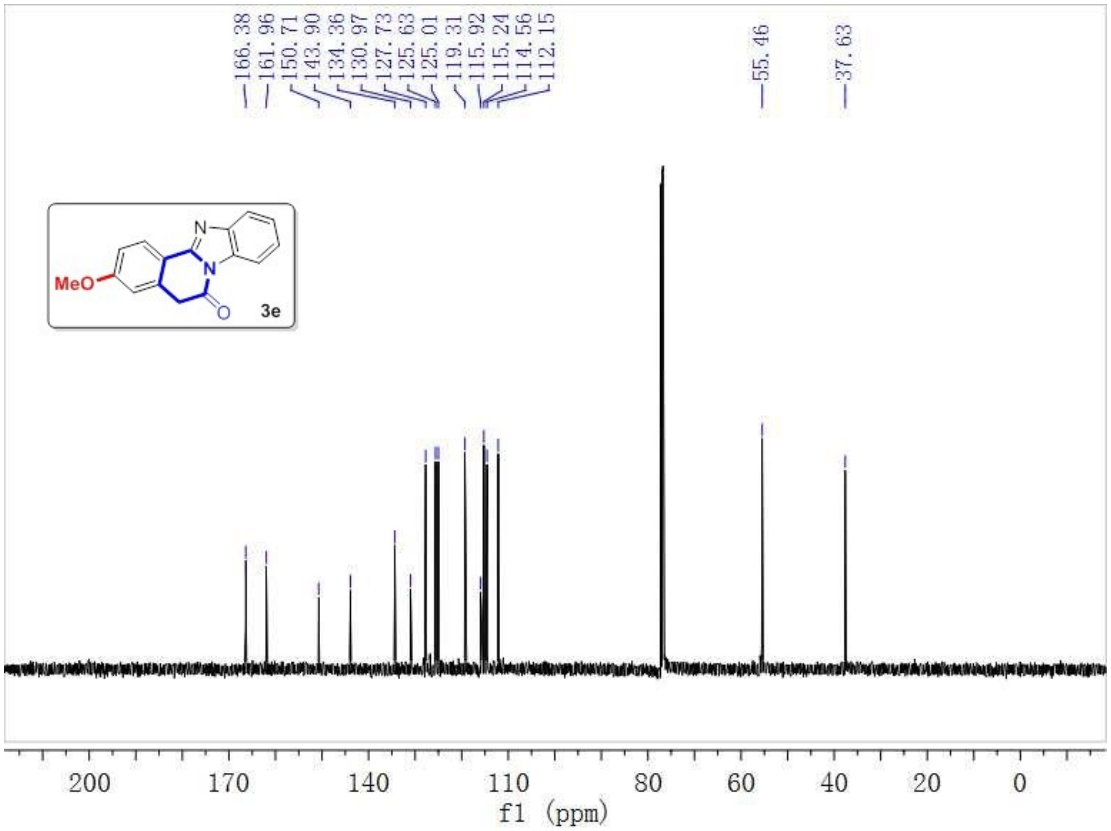
-1
f1 (ppm)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3e
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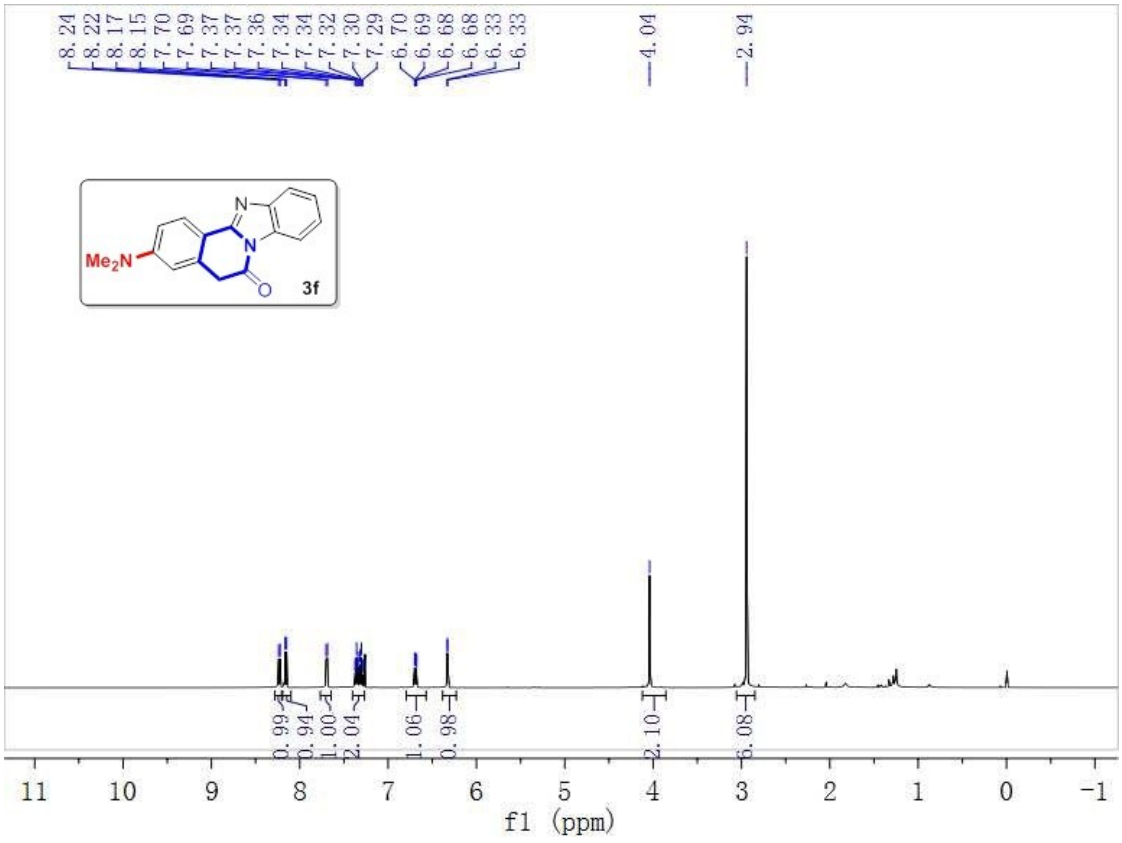
f1 (ppm)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6.70
6.69
6.68
6.68
6.33
6.33
4.04
2.94
Me2N
3f
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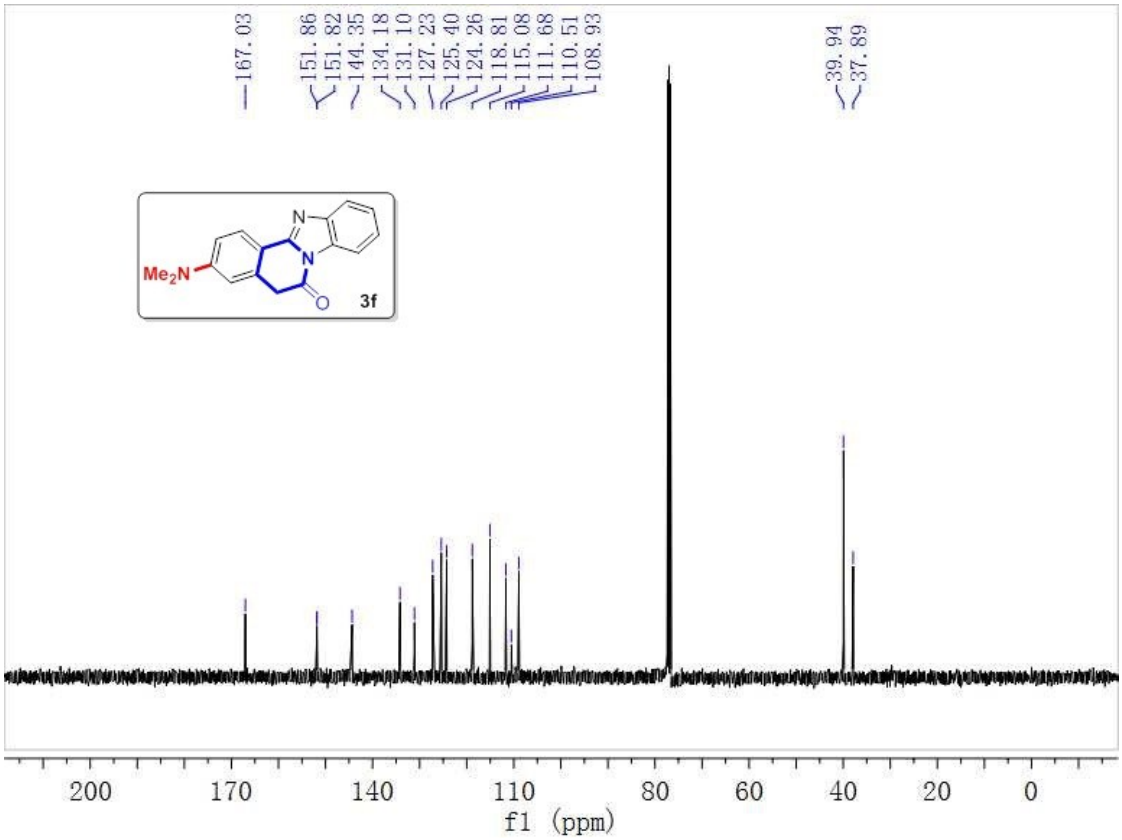
1.06
0.98
2.10
6.08
11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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37.89
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3f
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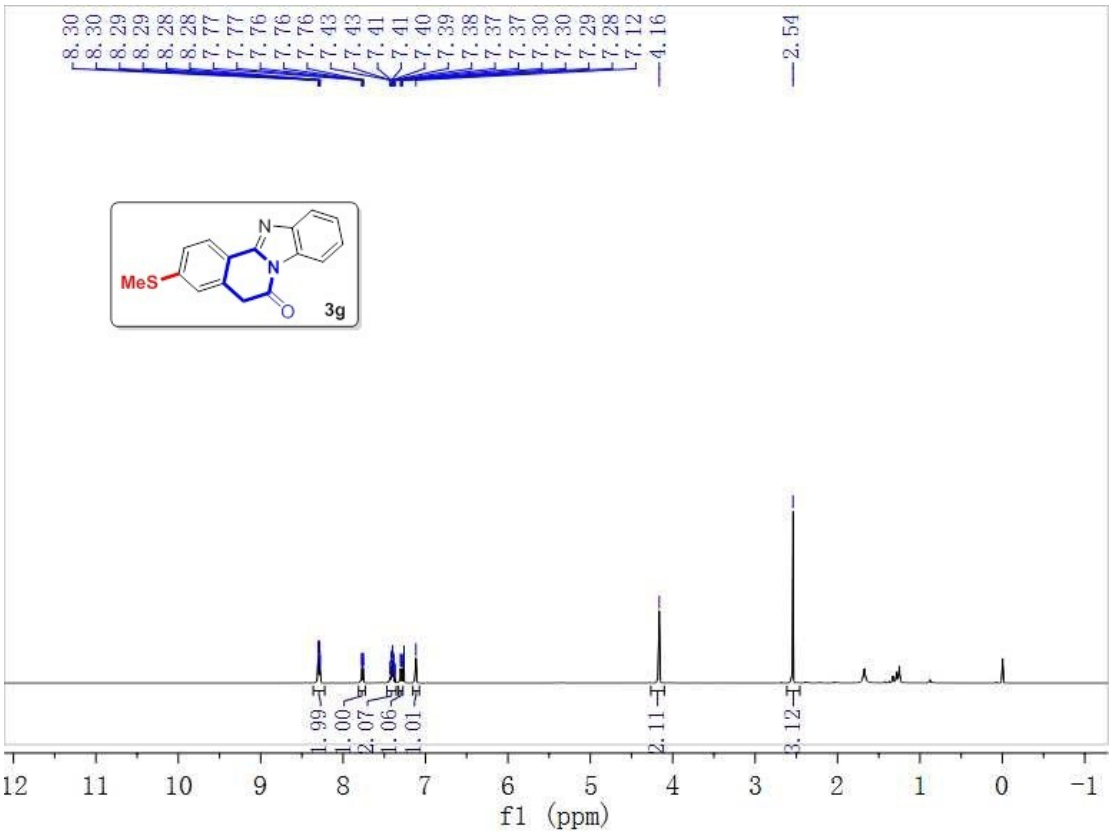
f1 (ppm)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7.41
7.40
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7.38
7.37
7.37
7.30
7.30
7.29
7.28
7.12
4.16
2.54
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1.00
2.07
1.06
1.01
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12
11
10
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8
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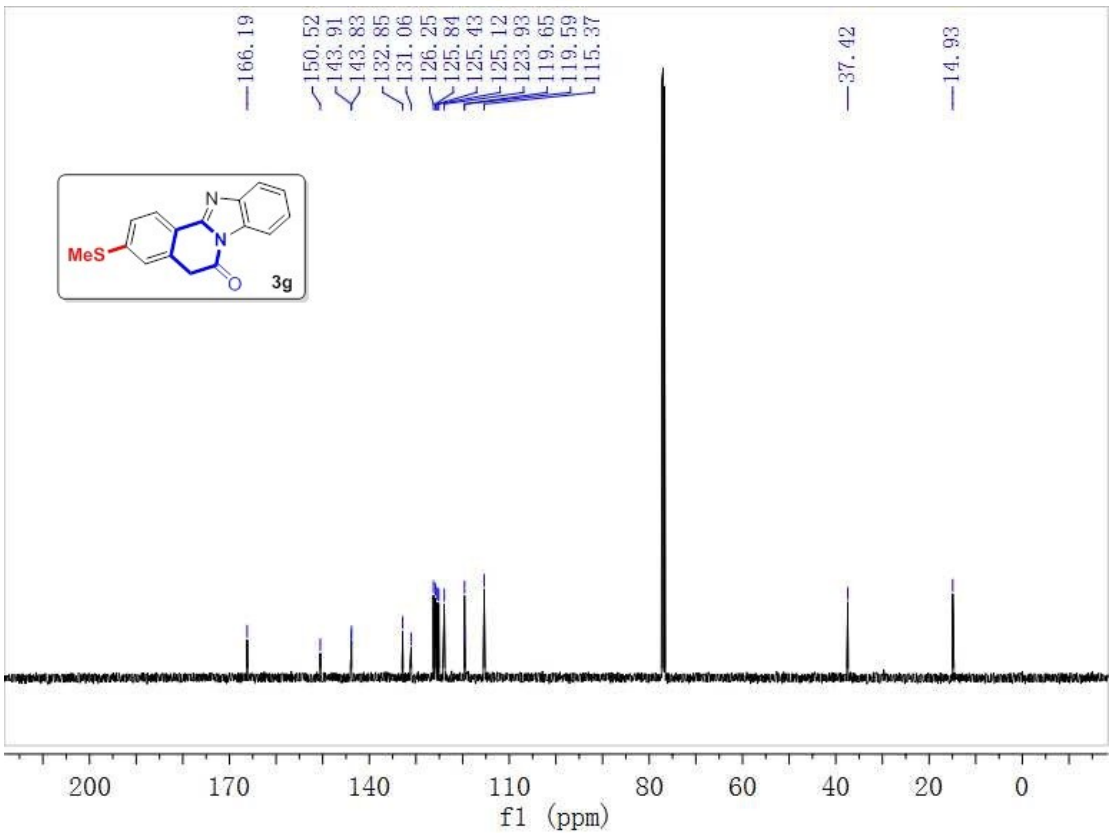
f1 (ppm)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125.12
123.93
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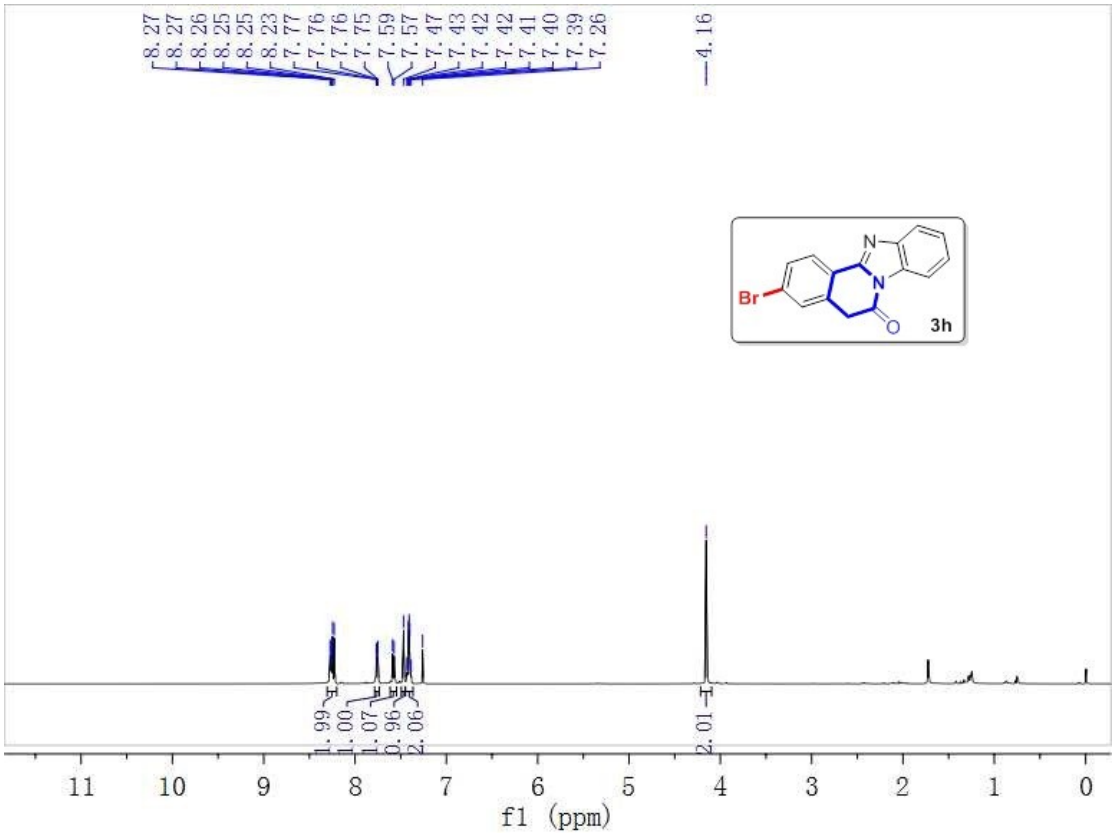
14.93
MeS
3g
200
170
140
110
80
60
40
20
0
f1 (ppm)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7.75
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7.47
7.43
7.42
7.42
7.41
7.40
7.39
7.26
4.16
Br
N
N
O
3h
1.99
1.00
1.07
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2.06
2.01
11
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9
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7
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5
4
3
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1
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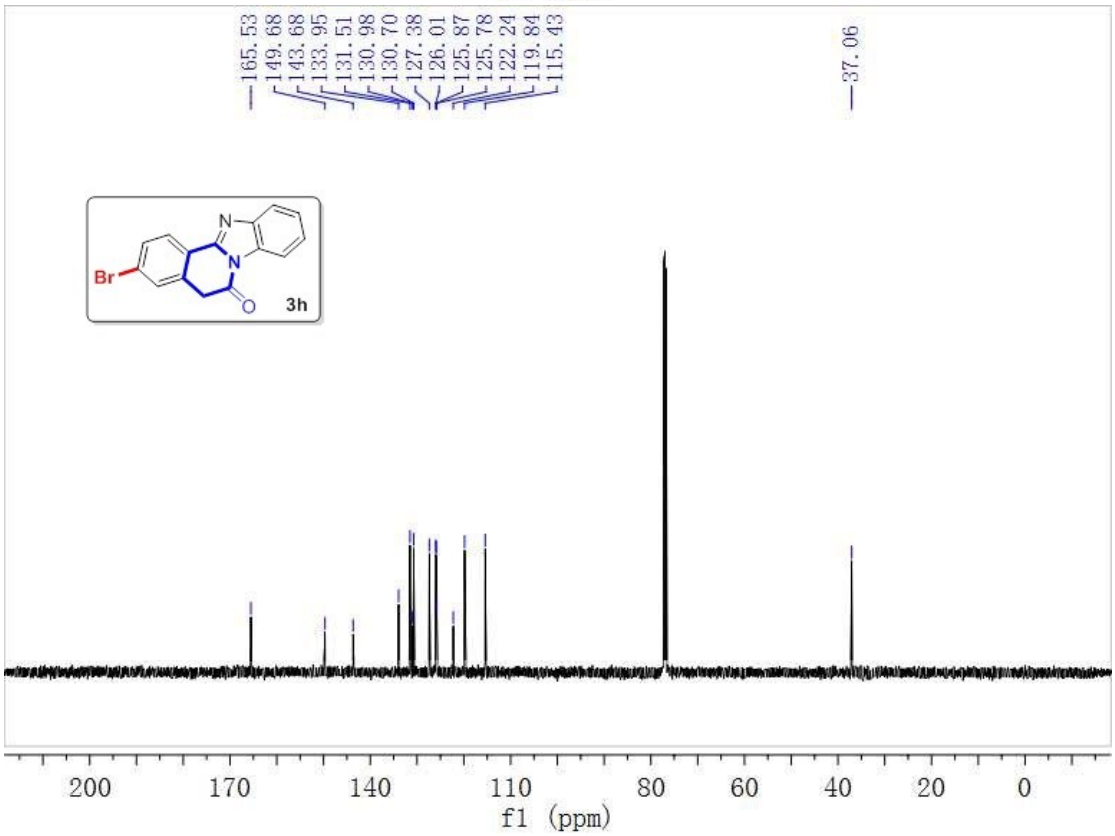
f1 (ppm)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126.01
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125.78
122.24
119.84
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37.06
Br
N
N
O
3h
200
170
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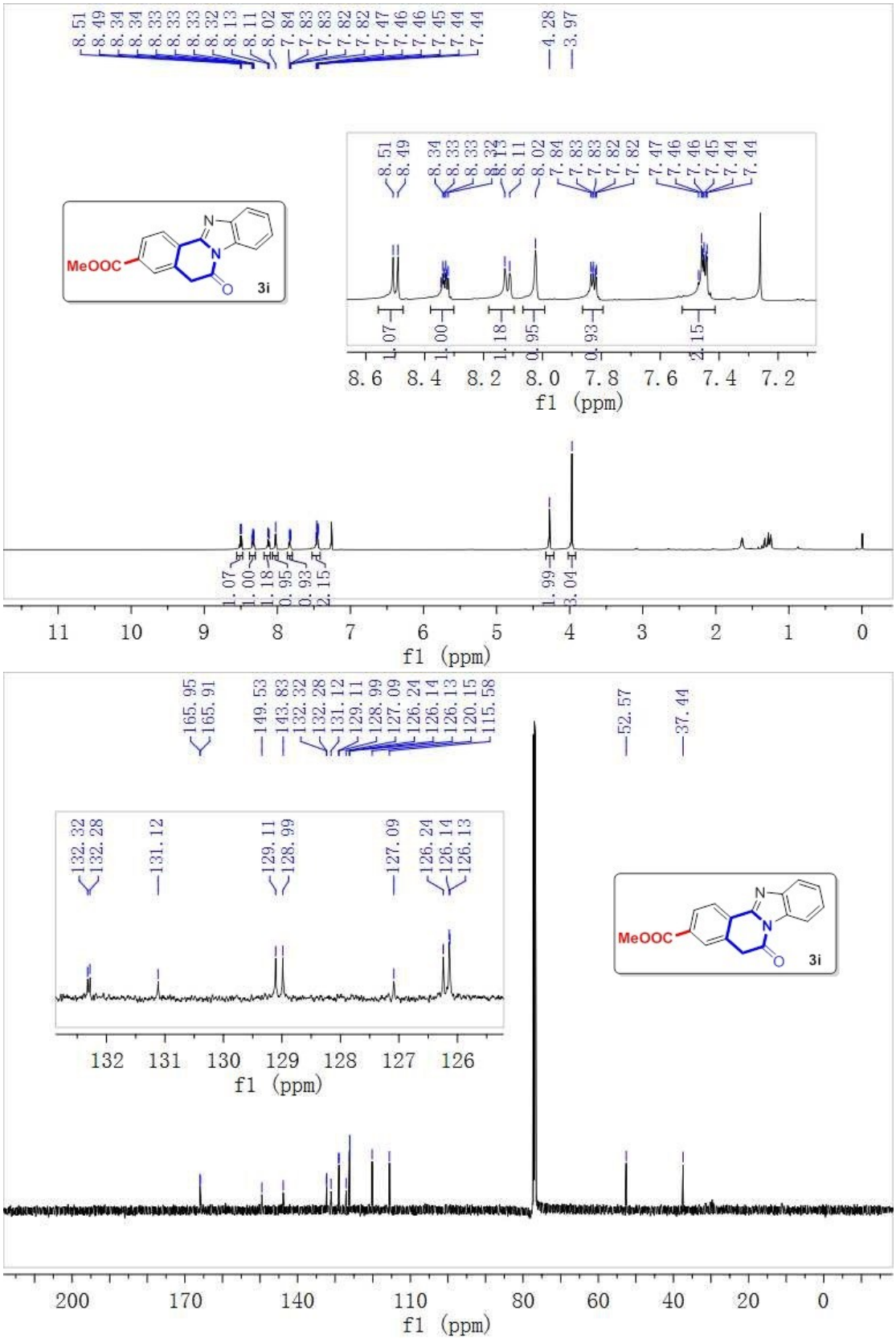
110
80
60
40
20
0
f1 (ppm)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8.32
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7.82
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7.46
7.46
7.45
7.44
7.44
4.28
3.97
MeOOC
3i
1.07
1.00
1.18
0.95
0.93
2.15
1.99
3.04
f1 (ppm)
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165.91
149.53
143.83
132.32
132.28
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126.13
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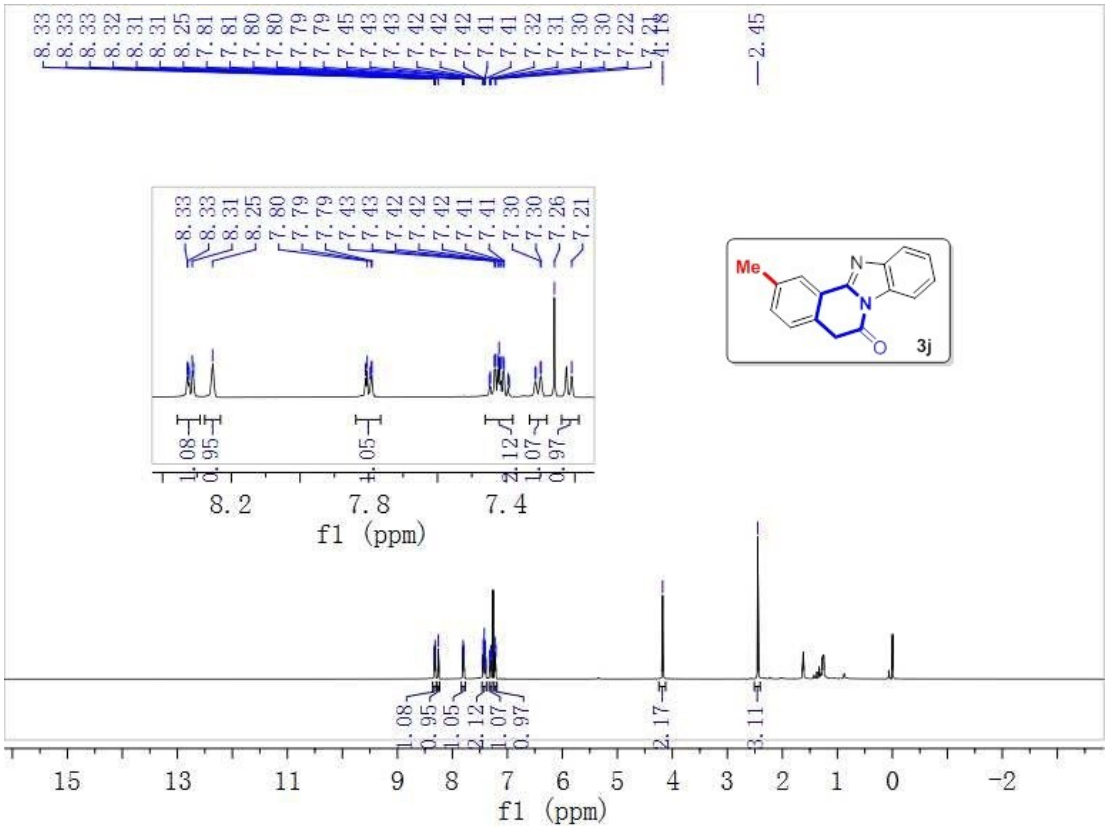
52.57
37.44
f1 (ppm)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7.42
7.42
7.41
7.41
7.32
7.31
7.30
7.30
7.22
7.21
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8.25
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7.43
7.42
7.42
7.42
7.41
7.41
7.30
7.30
7.26
7.21
1.08
0.95
1.05
2.12
1.07
0.97
8.2
7.8
7.4
f1 (ppm)
Me
N
N
O
3j
1.08
0.95
1.05
2.12
1.07
0.97
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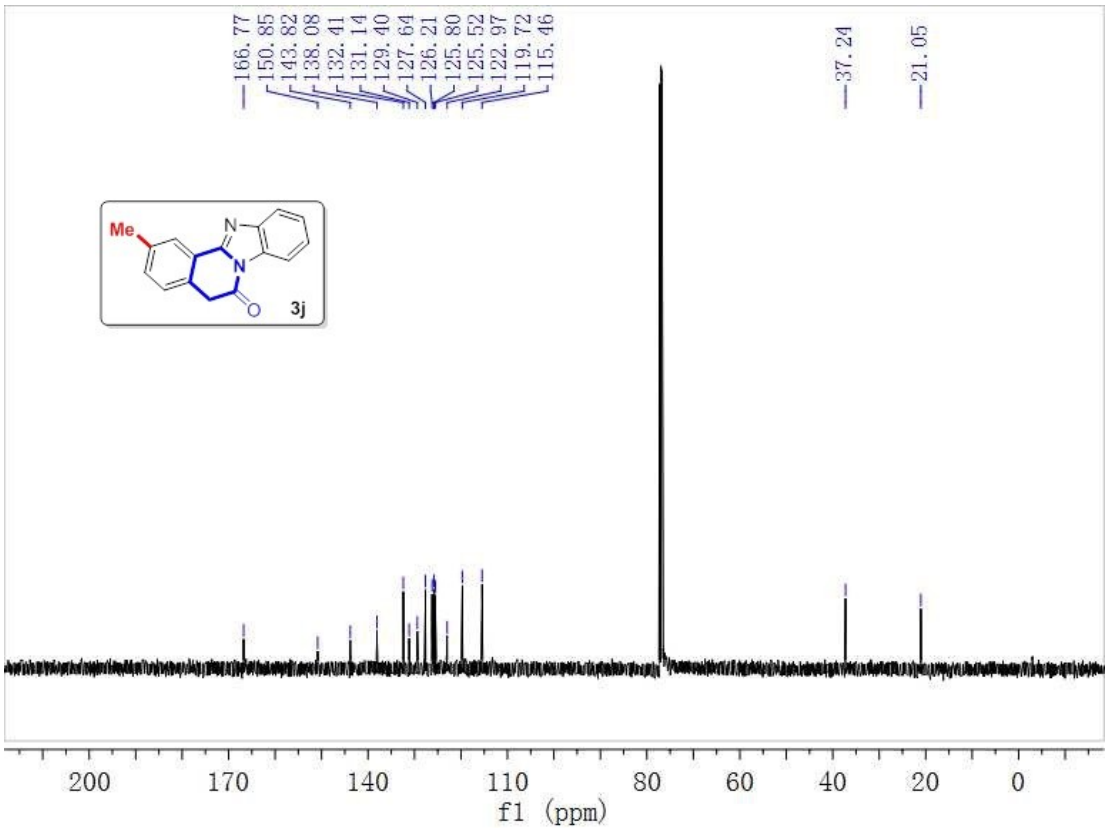
15
13
11
9
8
7
6
5
4
3
2
1
0
-2
f1 (ppm)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122.97
119.72
115.46
37.24
21.05
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N
O
3j
200
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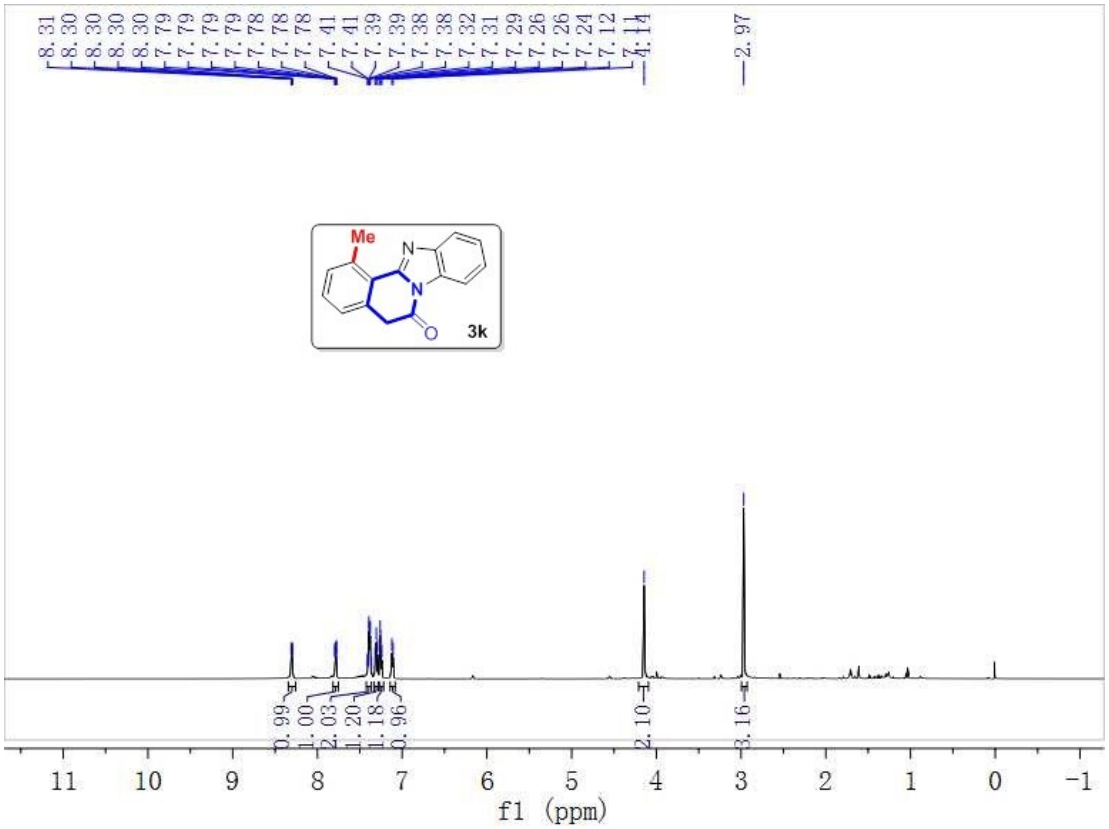
110
80
60
40
20
0
f1 (ppm)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7.38
7.32
7.31
7.29
7.26
7.26
7.24
7.12
7.11
2.97
Me
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N
O
3k
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1.00
2.03
1.20
1.18
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10
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8
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6
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4
3
2
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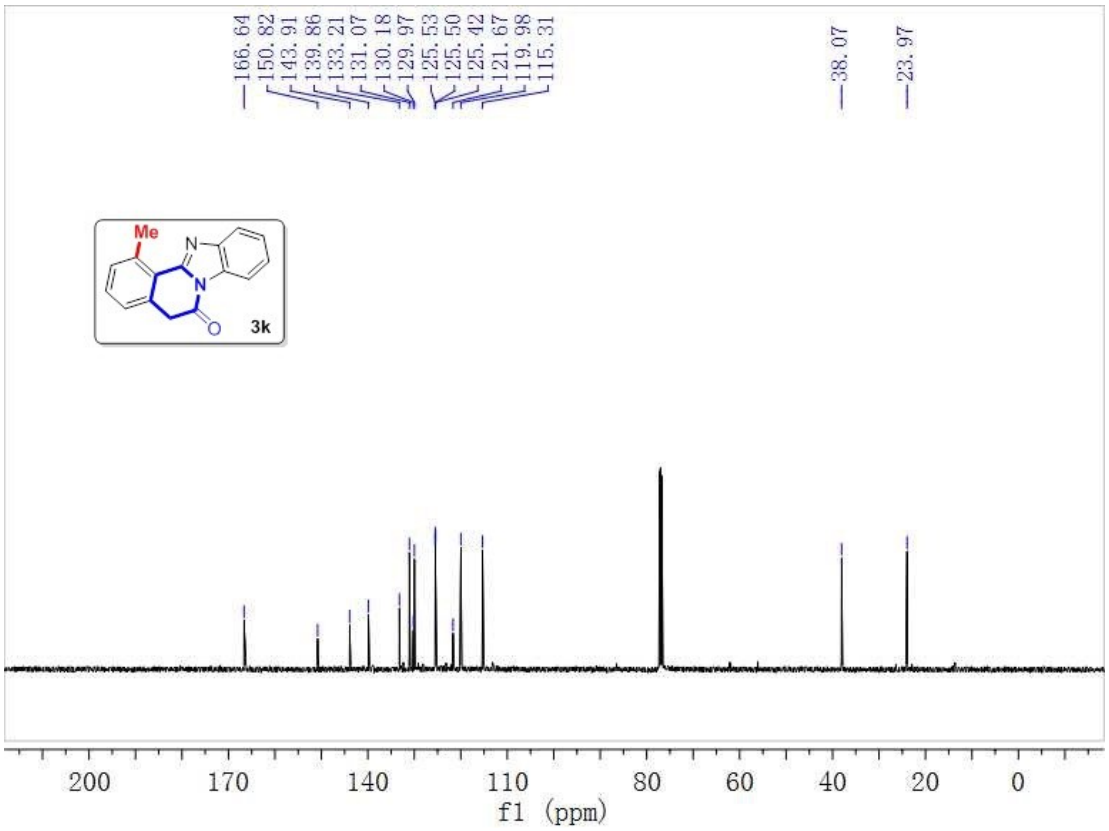
0
-1
f1 (ppm)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119.98
115.31
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N
O
3k
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110
80
60
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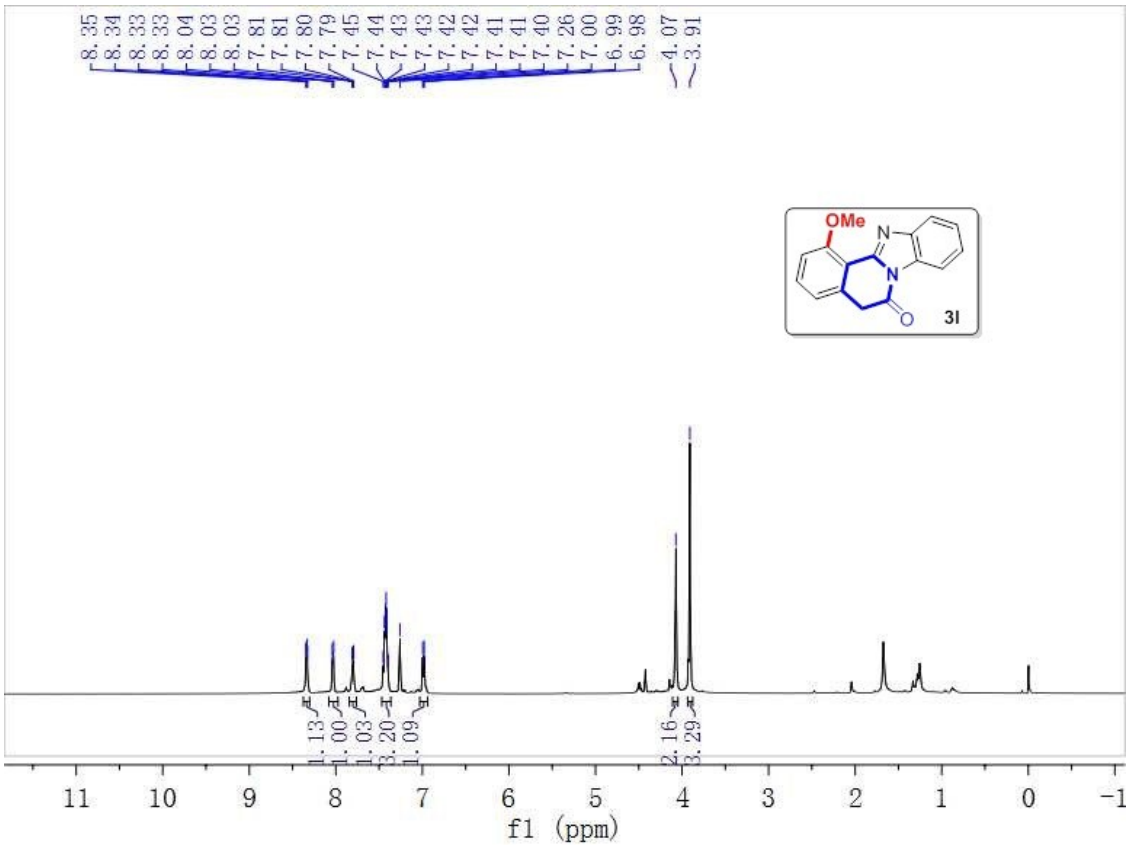
20
0
f1 (ppm)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7.43
7.43
7.42
7.42
7.41
7.41
7.40
7.26
7.00
6.99
6.98
4.07
3.91
OMe
N
N
O
3l
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1.03
3.20
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6
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3
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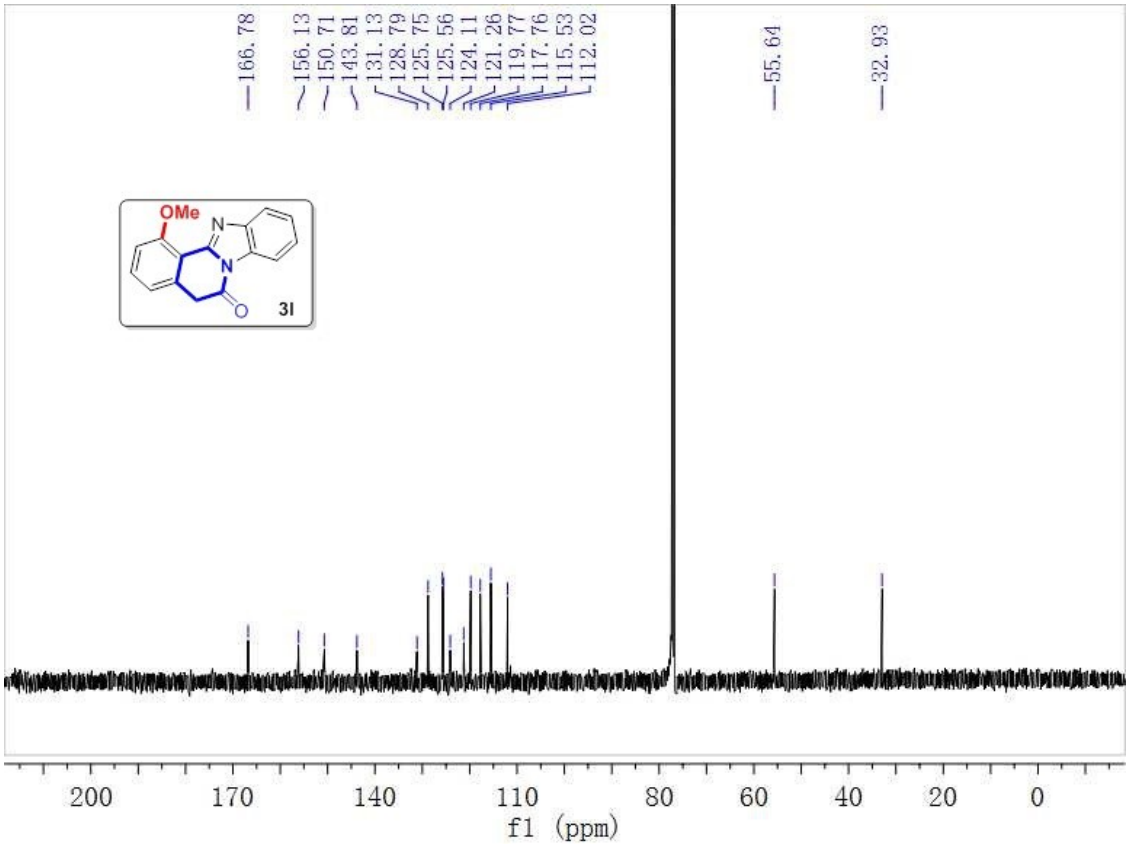
0
-1
f1 (ppm)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117.76
115.53
112.02
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N
O
3l
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110
80
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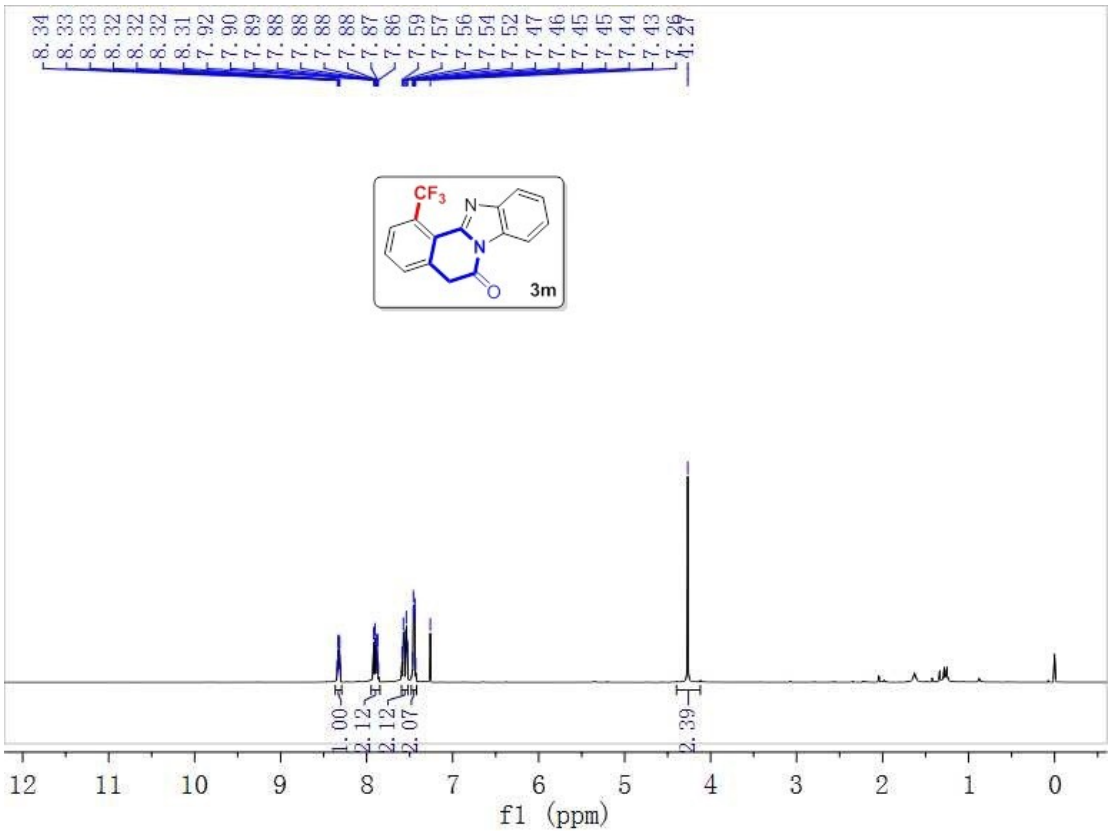
f1 (ppm)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7.54
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7.47
7.46
7.45
7.45
7.44
7.43
7.26
4.27
CF3
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N
O
3m
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5
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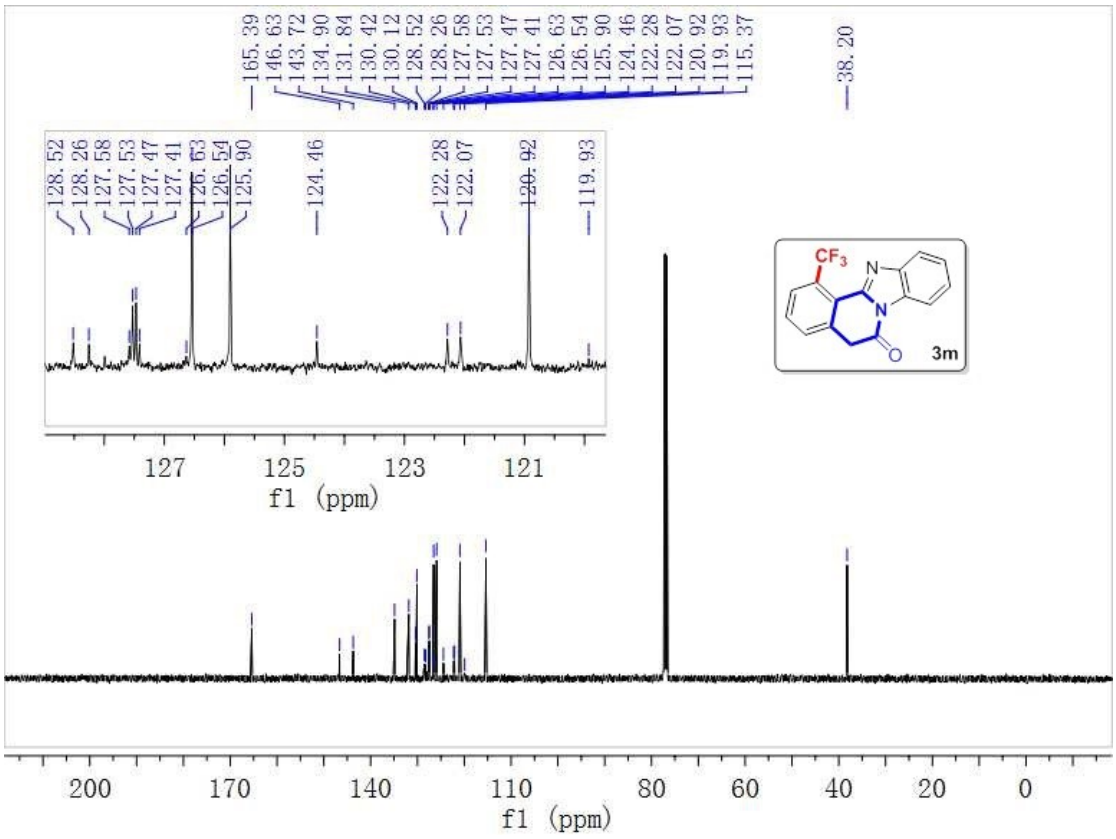
f1 (ppm)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127.41
126.63
126.54
125.90
124.46
122.28
122.07
120.92
119.93
115.37
38.20
CF3
N
N
O
3m
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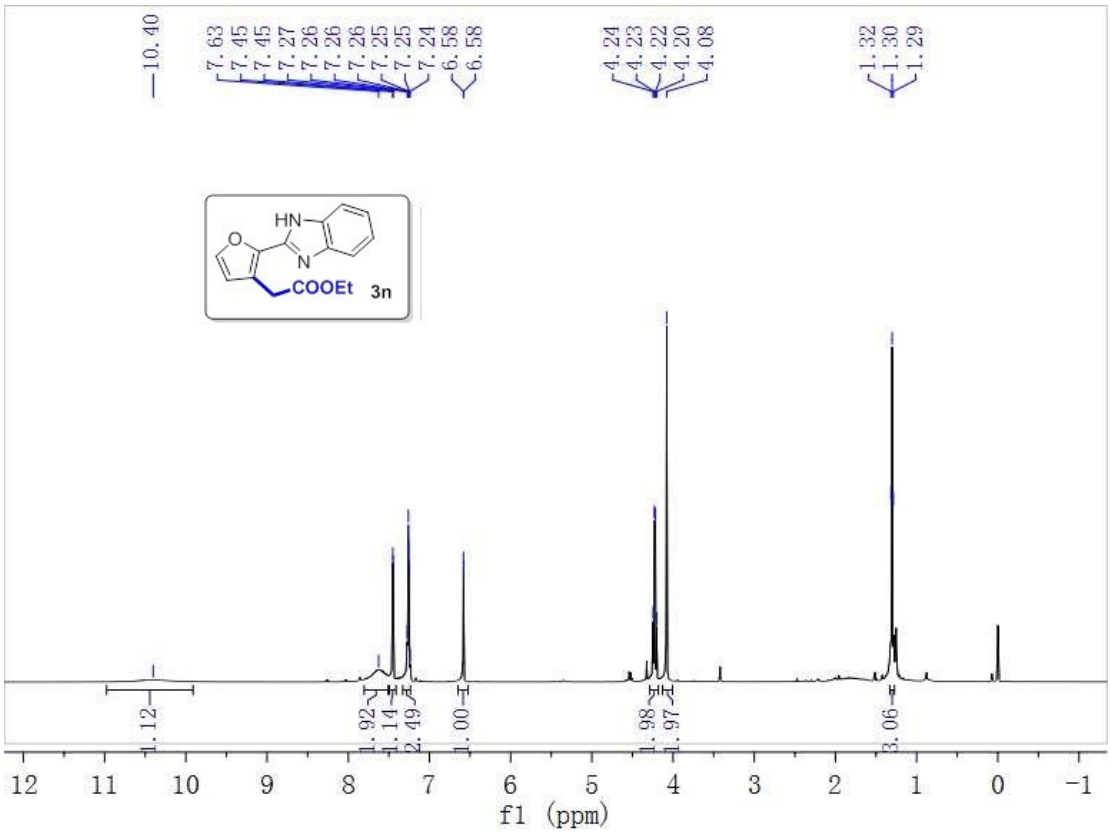
125
123
121
f1 (ppm)
200
170
140
110
80
60
40
20
0
f1 (ppm)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7.26
7.26
7.25
7.25
7.24
6.58
6.58
4.24
4.23
4.22
4.20
4.08
1.32
1.30
1.29
HN
O
N
COOEt
3n
1.12
1.92
1.14
2.49
1.00
1.98
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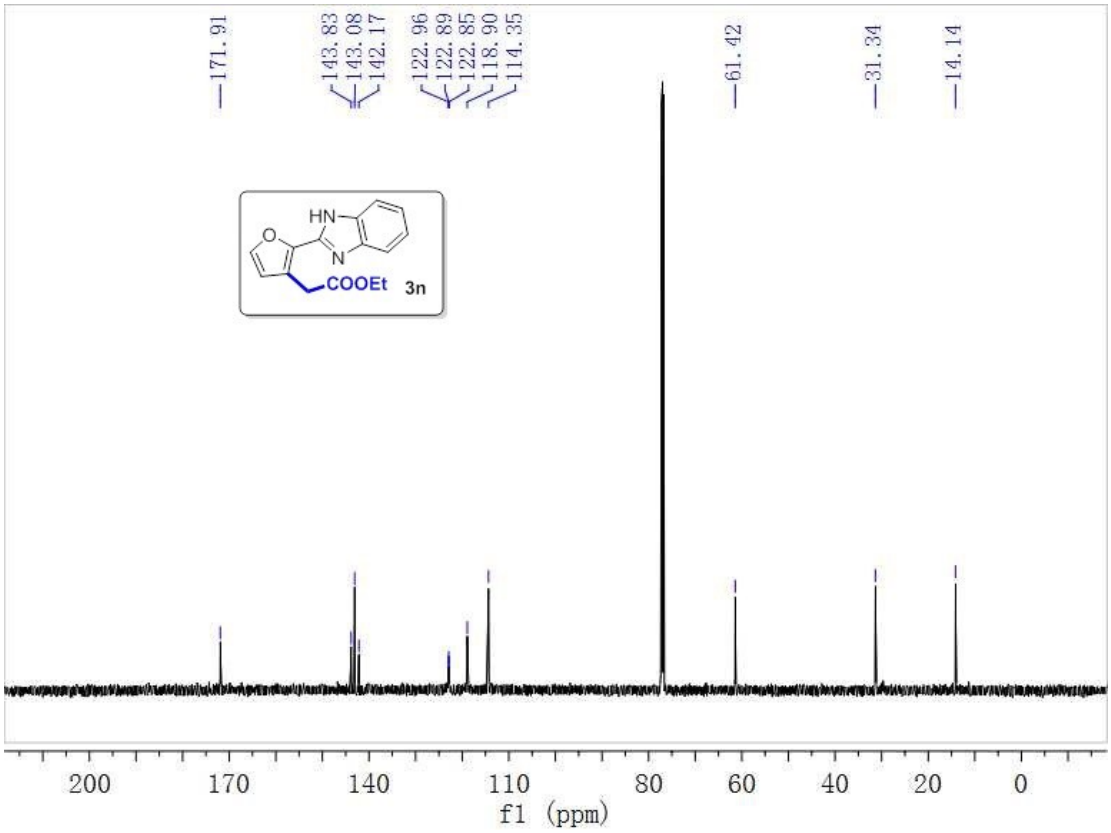
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)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114.35
61.42
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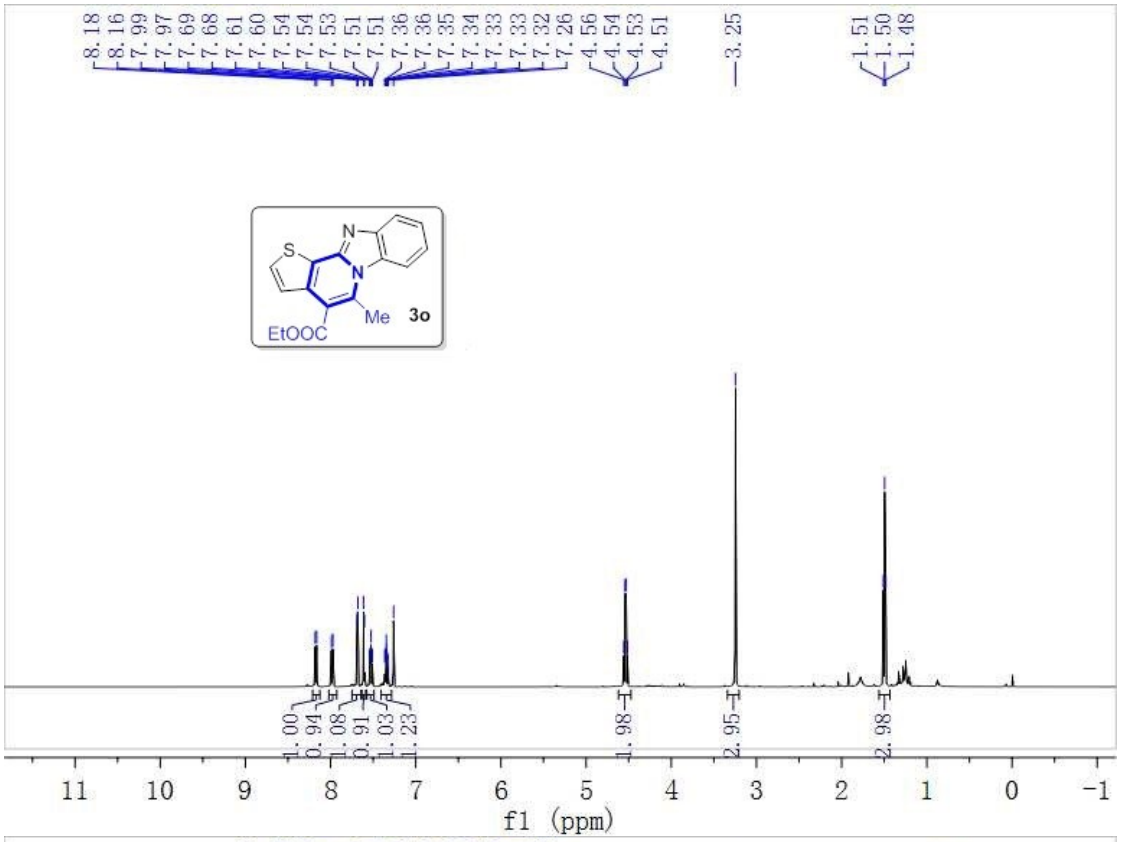
O
N
COOEt
3n
200
170
140
110
80
60
40
20
0
f1 (ppm)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7.36
7.35
7.34
7.33
7.33
7.32
7.26
4.56
4.54
4.53
4.51
3.25
1.51
1.50
1.48
N
S
N
Me
EtOOC
3o
1.00
0.94
1.08
0.91
1.03
1.23
1.98
2.95
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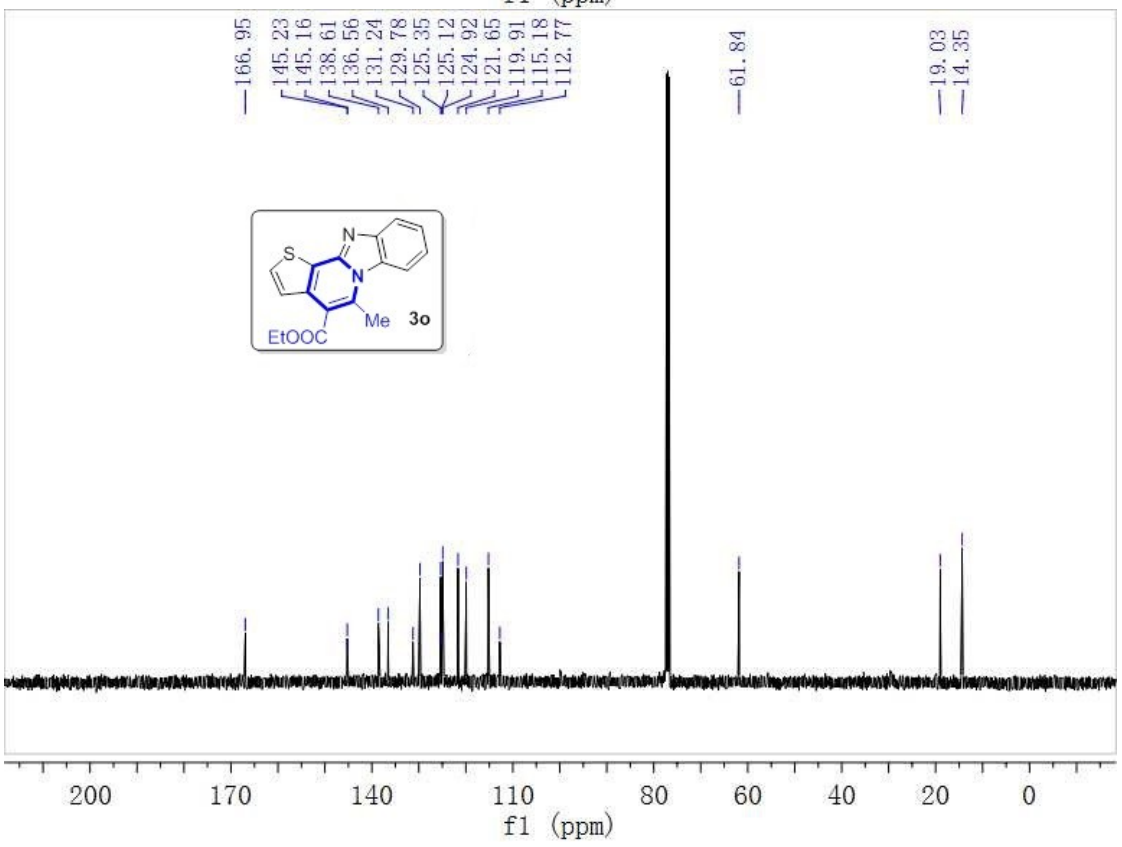
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)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112.77
61.84
19.03
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N
Me
EtOOC
3o
200
170
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110
80
60
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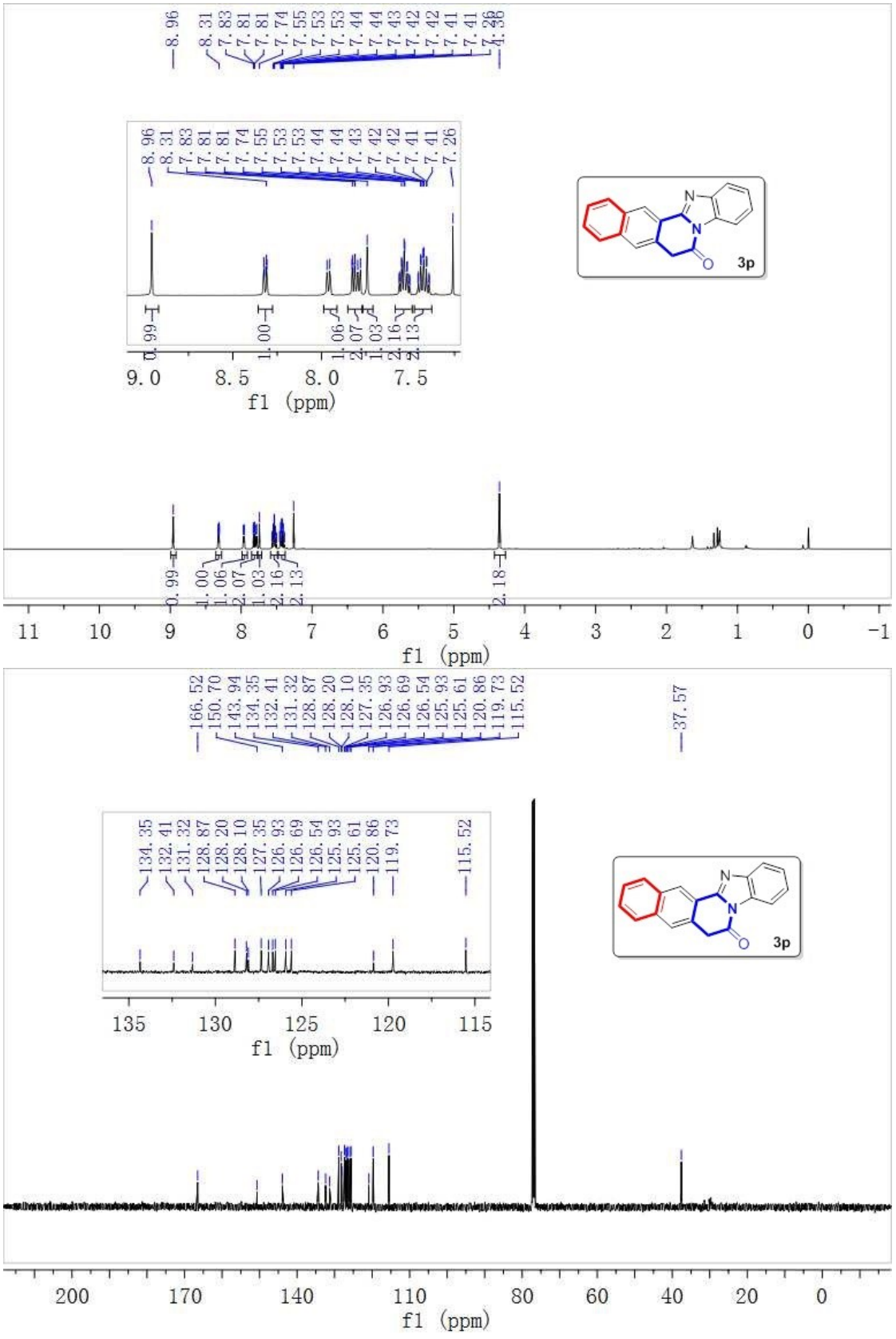
20
0
f1 (ppm)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7.42
7.42
7.41
7.41
7.26
0.99
1.00
1.06
2.07
1.03
2.16
2.13
9.0
8.5
8.0
7.5
f1 (ppm)
3p
2.18
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)
166.52
150.70
143.94
134.35
132.41
131.32
128.87
128.20
128.10
127.35
126.93
126.69
126.54
125.93
125.61
120.86
119.73
115.52
37.57
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120
115
f1 (ppm)
3p
200
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110
80
60
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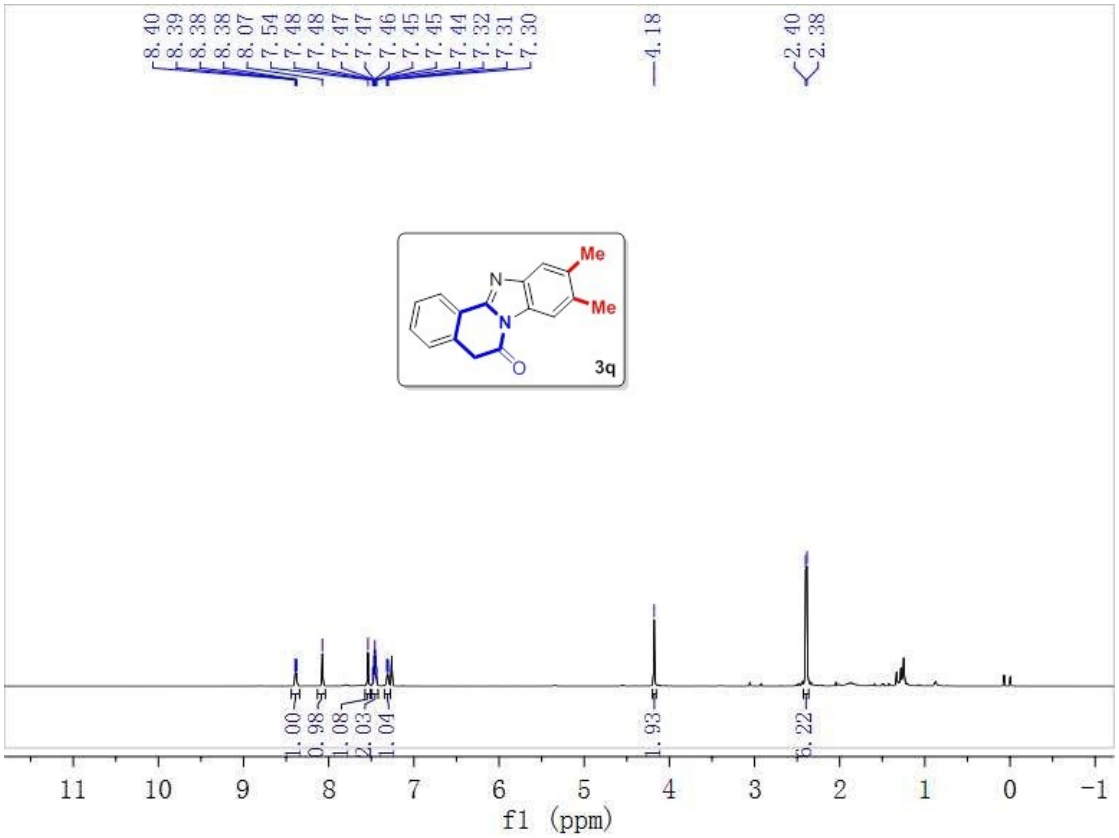
20
0
f1 (ppm)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7.48
7.48
7.47
7.47
7.46
7.45
7.45
7.44
7.32
7.31
7.30
4.18
2.40
2.38
Me
Me
N
N
O
3q
1.00
0.98
1.08
2.03
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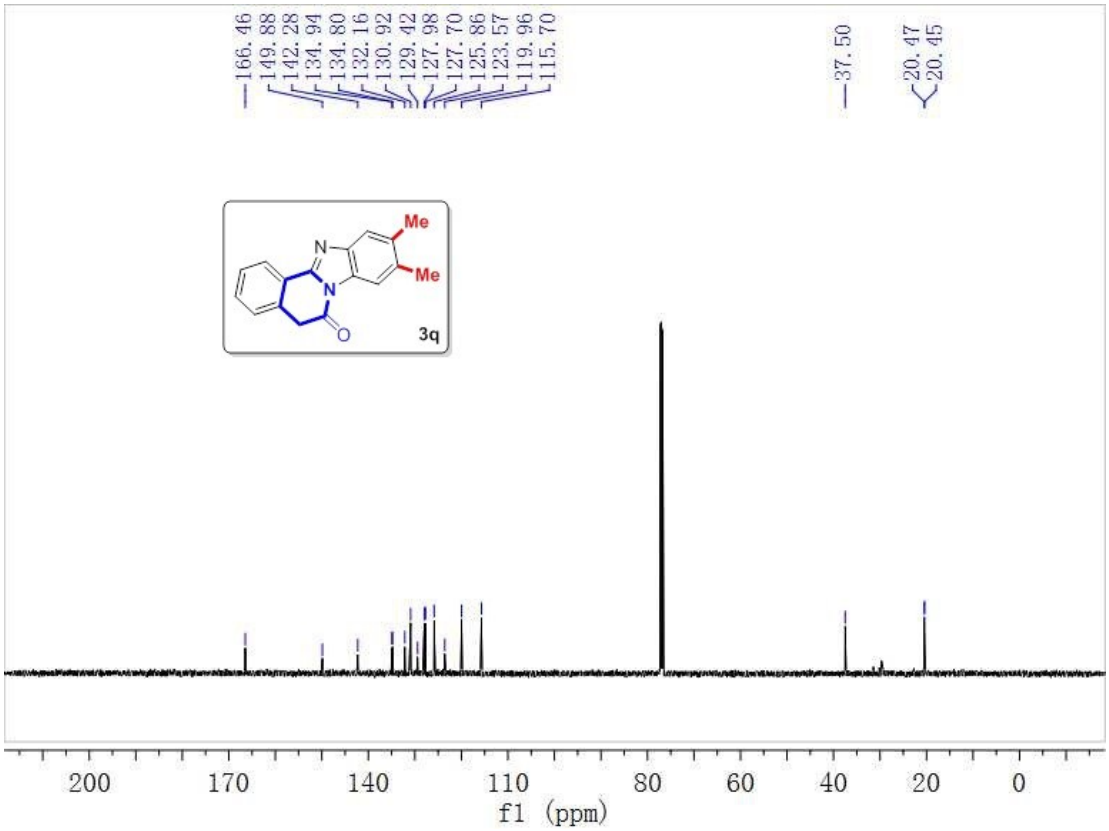
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)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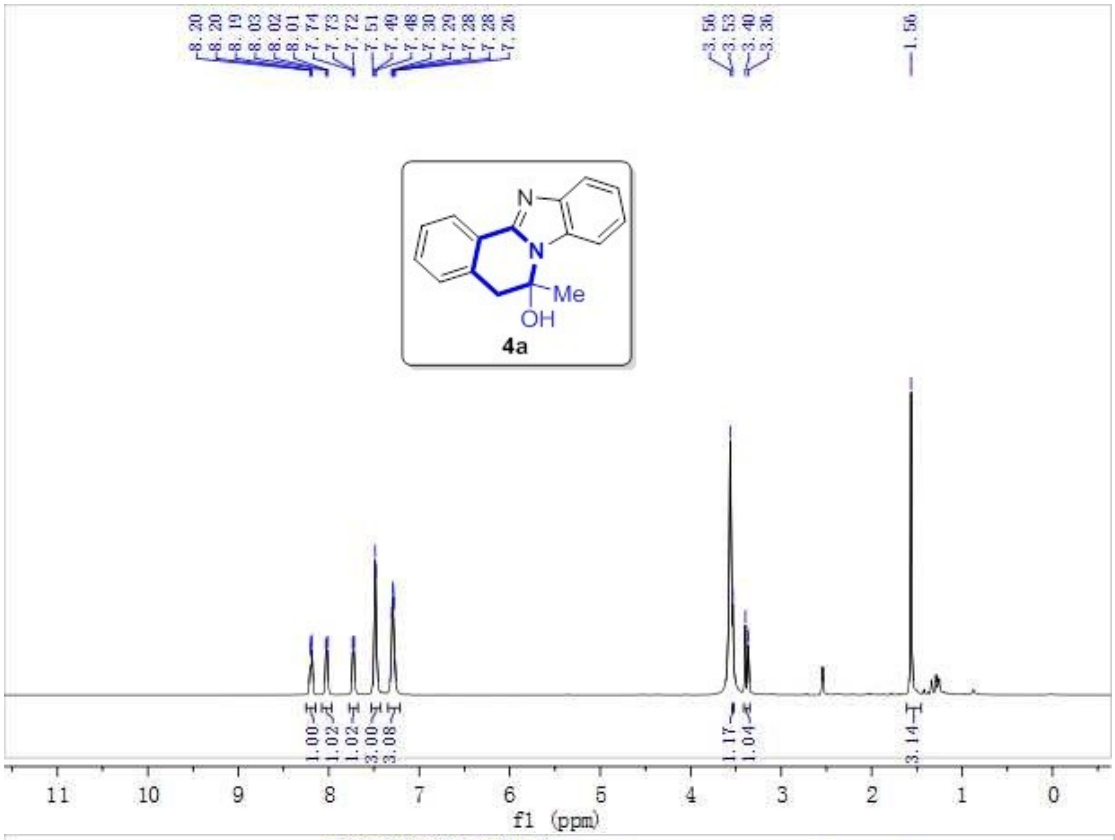
127.70
125.86
123.57
119.96
115.70
37.50
20.47
20.45
Me
Me
N
N
O
3q
200
170
140
110
80
60
40
20
0
f1 (ppm)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7.29
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7.28
7.26
3.56
3.53
3.40
3.36
1.56
N
N
Me
OH
4a
1.00
1.02
1.02
3.00
3.08
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3.14
11
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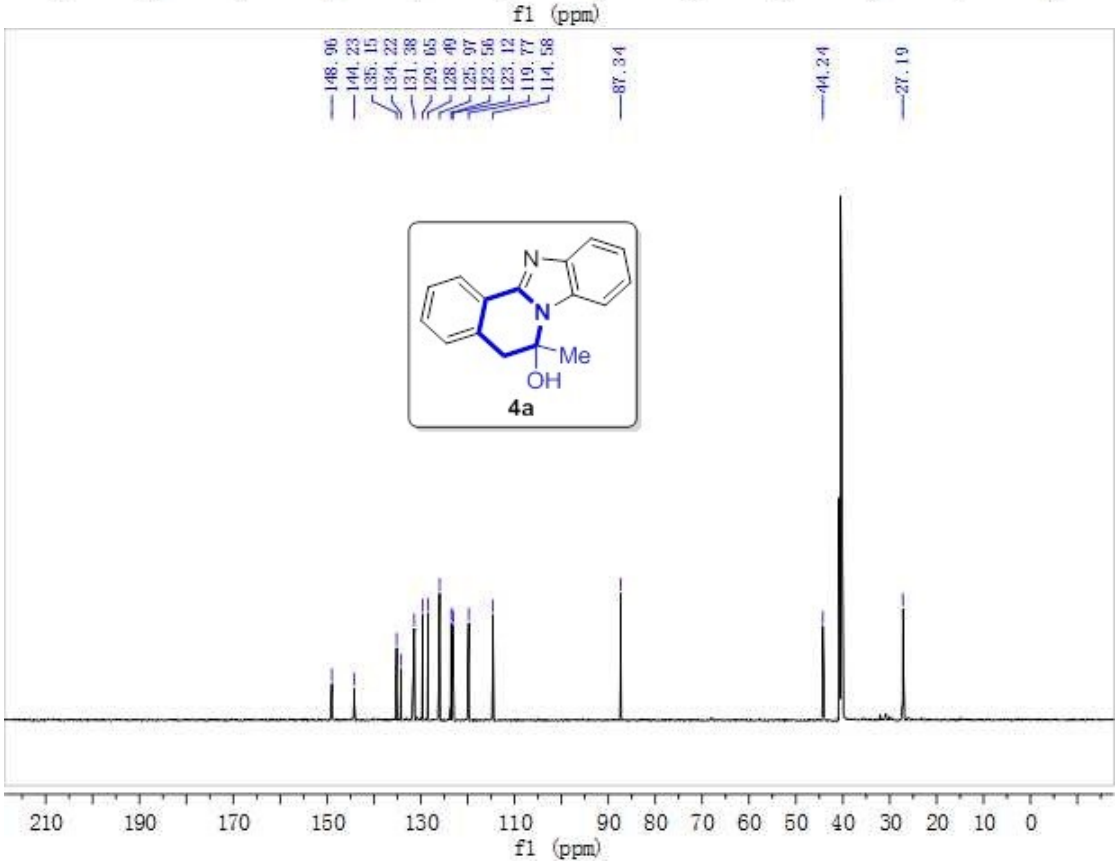
f1 (ppm)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128.49
125.97
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123.12
119.77
114.58
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44.24
27.19
N
N
Me
OH
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130
110
90
80
70
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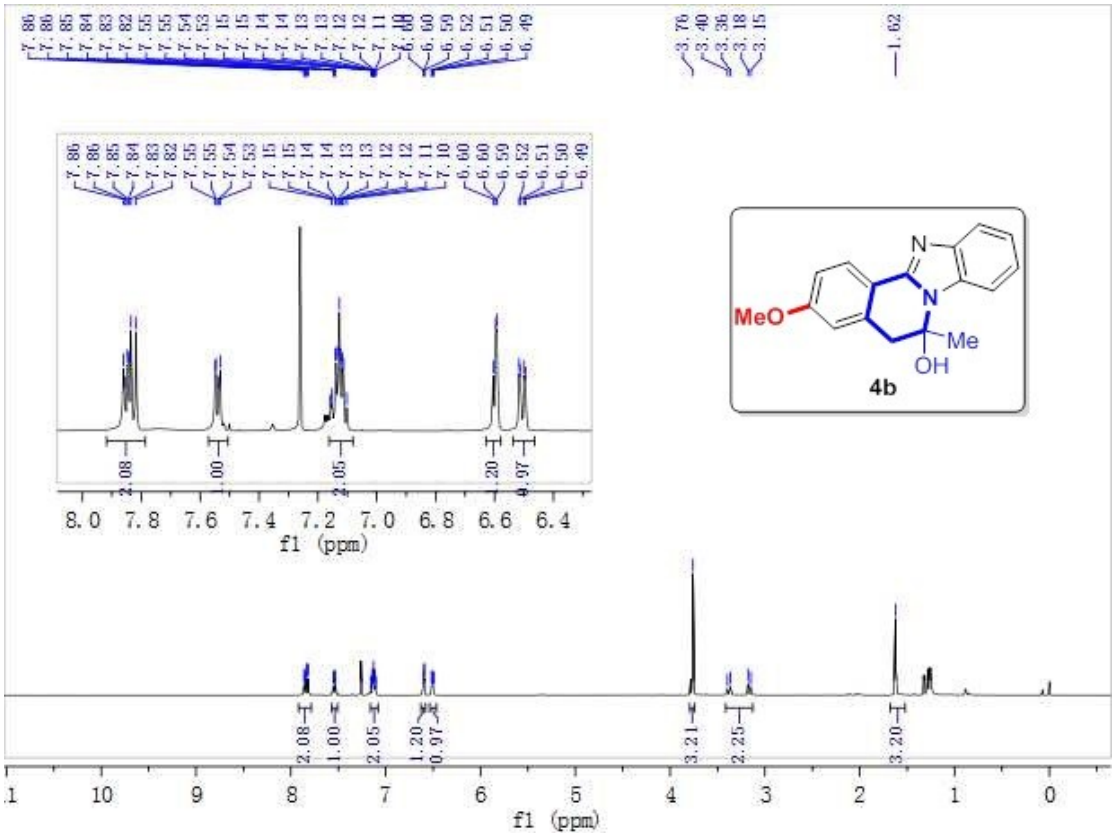
50
40
30
20
10
0
f1 (ppm)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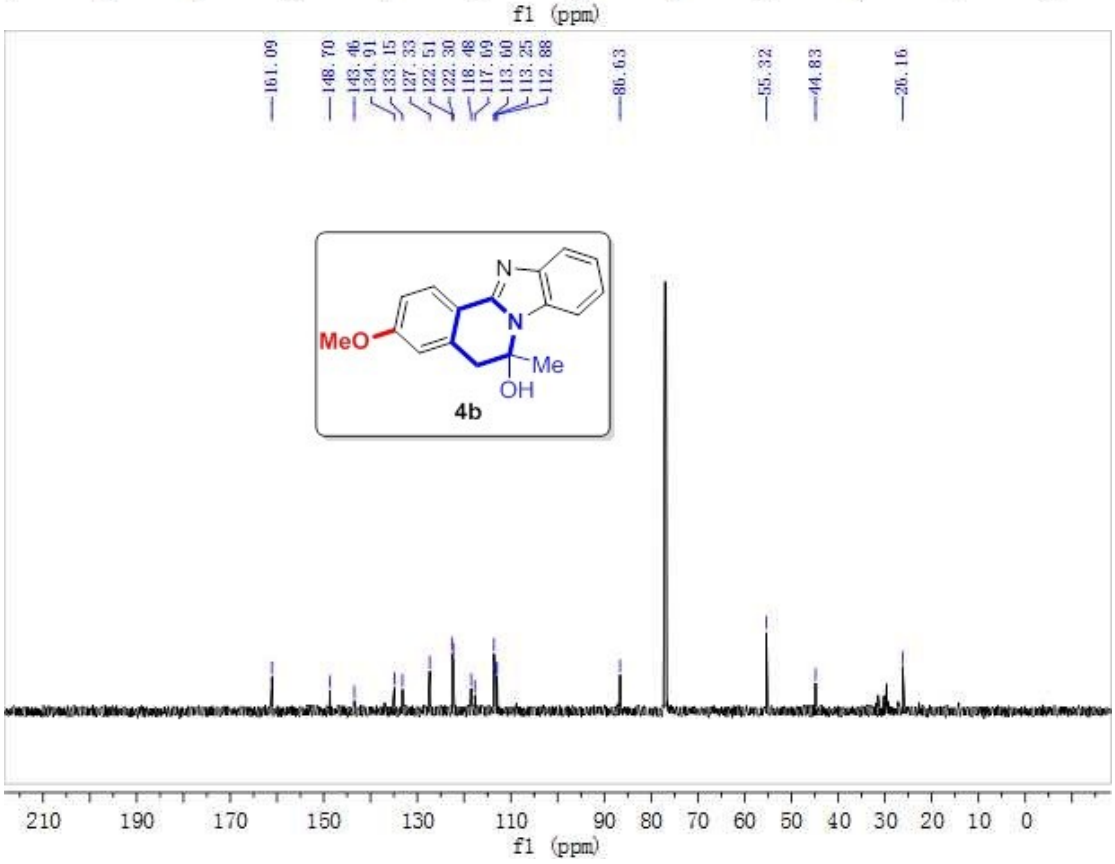
Me
OH
4b
f1 (ppm)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OH
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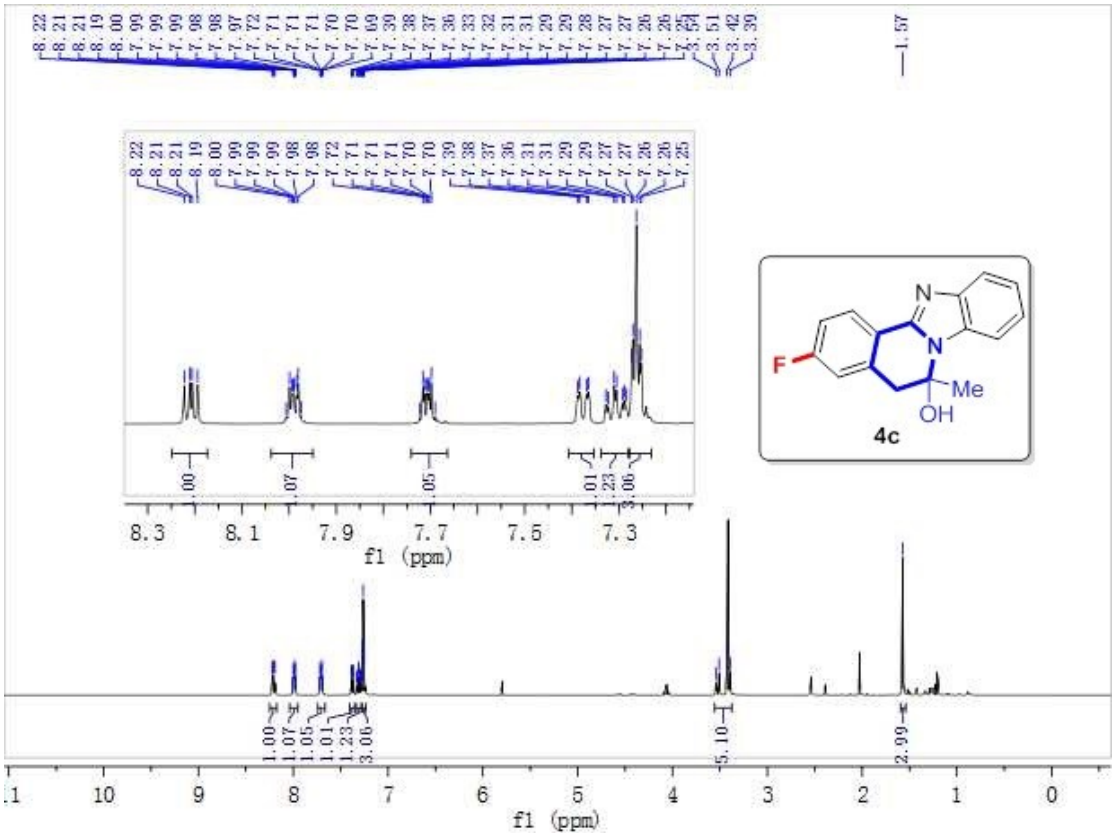
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7.71
7.71
7.70
7.70
7.69
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7.38
7.37
7.36
7.33
7.32
7.31
7.31
7.29
7.29
7.28
7.27
7.27
7.26
7.26
7.25
3.51
3.42
3.39
1.57
1.00
1.07
1.05
1.01
1.23
3.06
5.10
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8.1
7.9
7.7
7.5
7.3
f1 (ppm)
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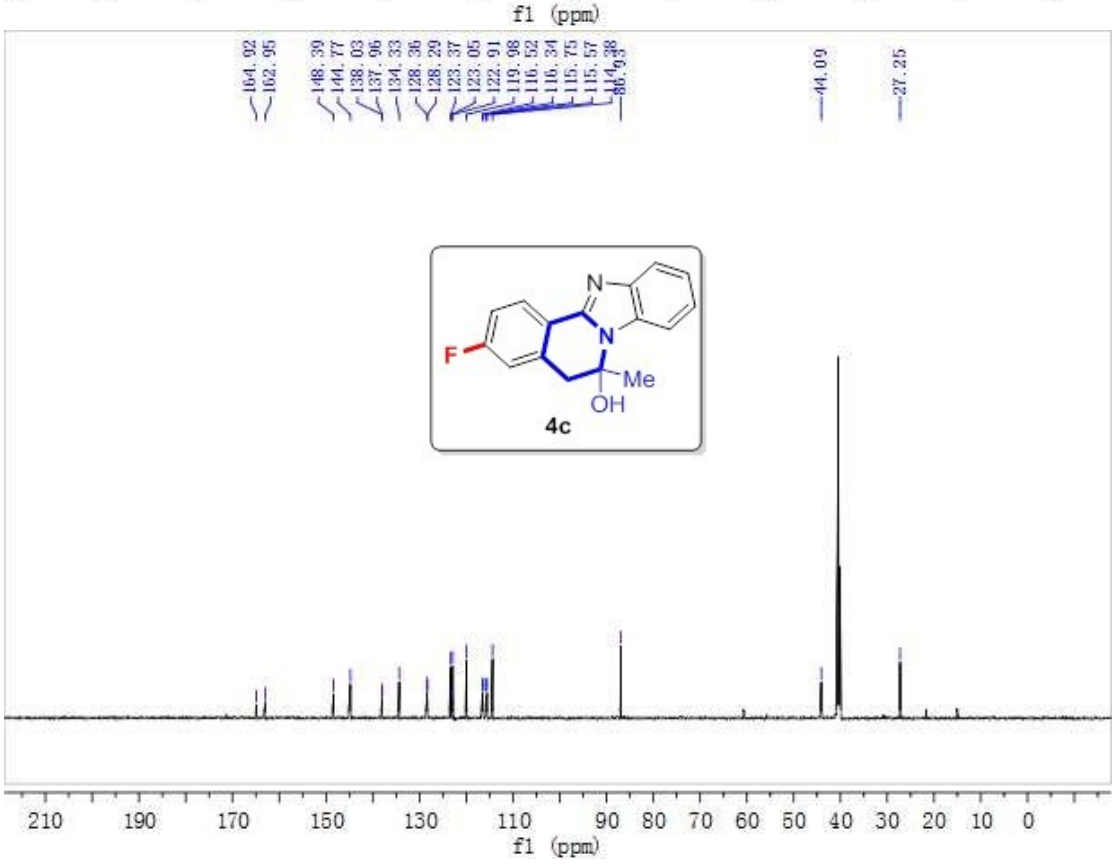
N
Me
OH
4c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123.37
123.05
122.91
119.98
116.52
116.34
115.75
115.57
114.38
86.93
44.09
27.25
F
N
N
Me
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150
130
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90
80
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50
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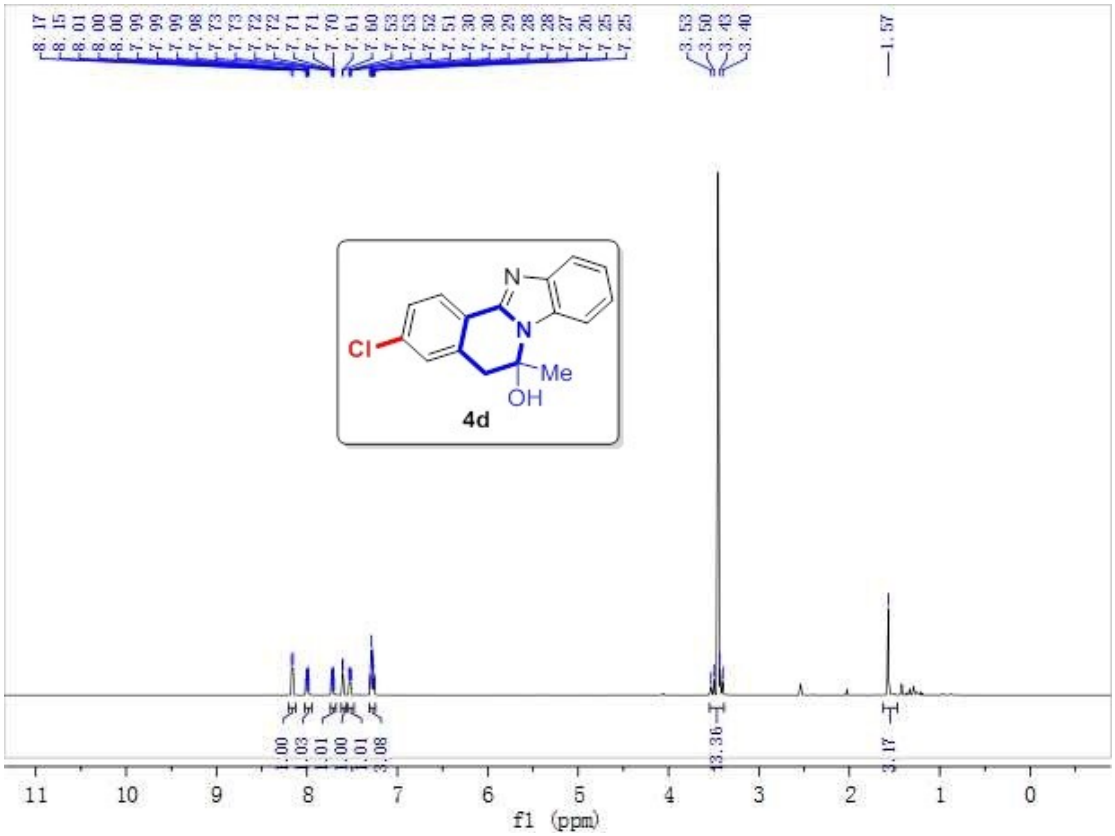
0
f1 (ppm)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7.72
7.71
7.71
7.70
7.61
7.60
7.53
7.53
7.52
7.51
7.30
7.30
7.29
7.28
7.28
7.27
7.26
7.25
7.25
3.53
3.50
3.43
3.40
1.57
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N
Cl
Me
OH
4d
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1.03
1.01
1.00
1.01
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3.17
11
10
9
8
7
6
5
4
3
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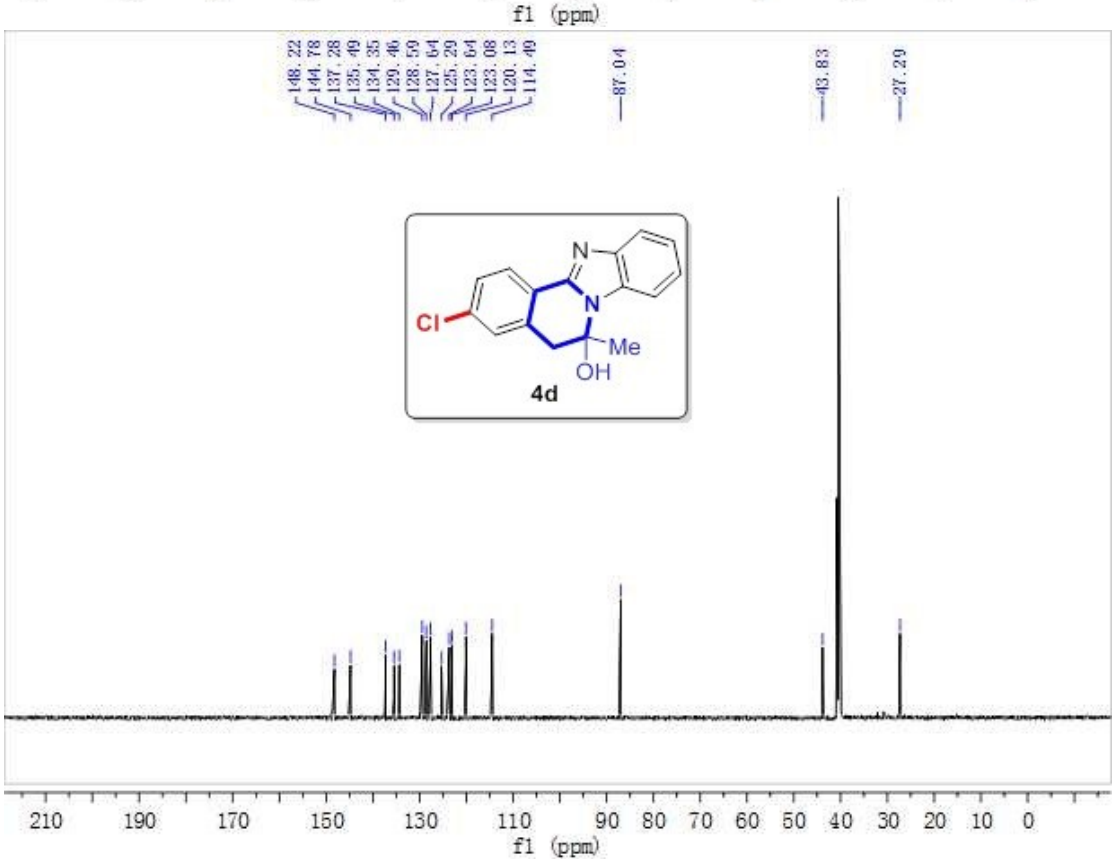
1
0
f1 (ppm)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129.46
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127.64
125.29
123.64
123.08
120.13
114.49
87.04
43.83
27.29
N
N
Cl
Me
OH
4d
210
190
170
150
130
110
90
80
70
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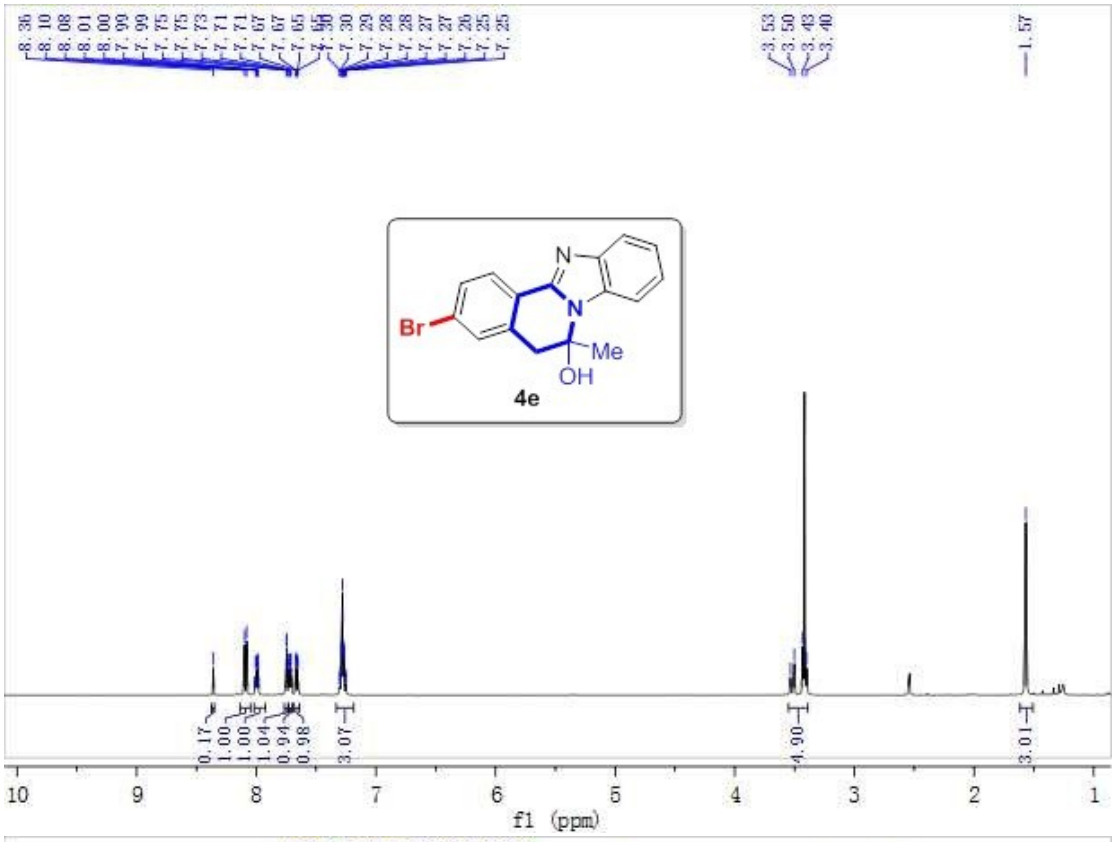
50
40
30
20
10
0
f1 (ppm)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7.30
7.29
7.28
7.27
7.27
7.26
7.25
7.25
3.53
3.50
3.43
3.40
1.57
N
N
Br
Me
OH
4e
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1.00
1.00
1.04
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6
5
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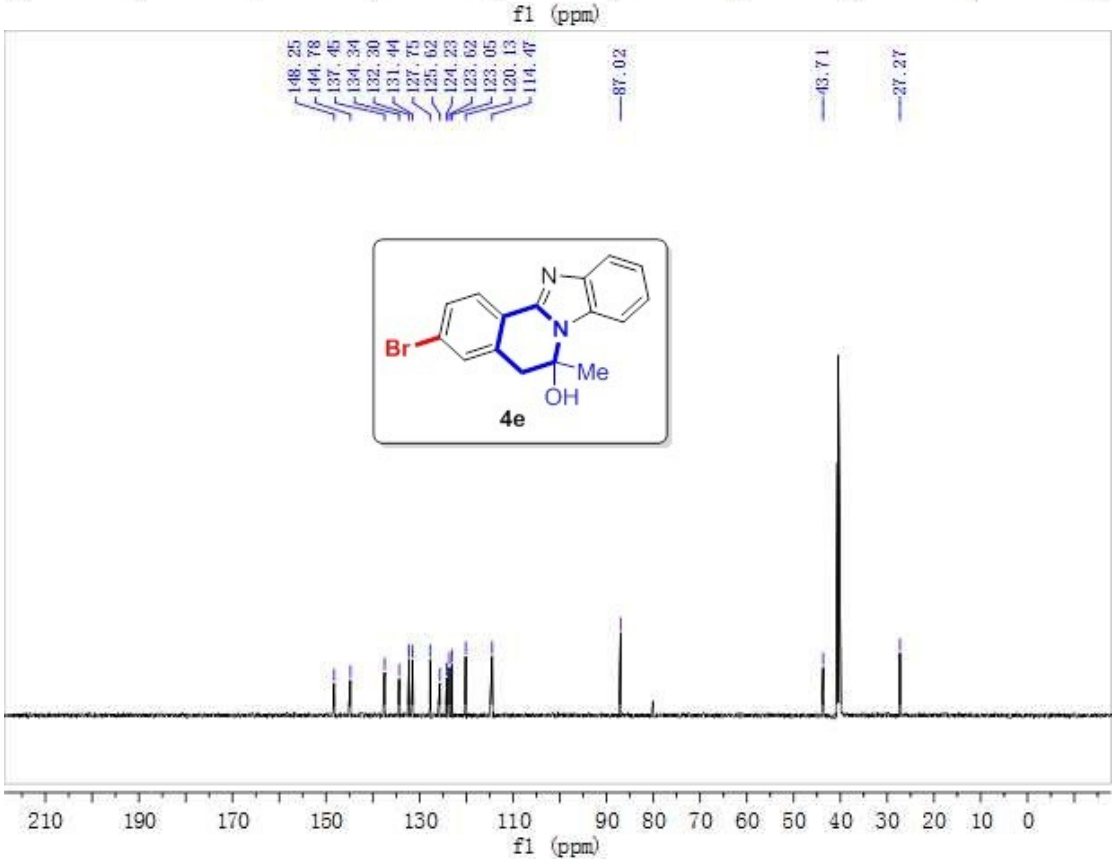
2
1
f1 (ppm)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123.62
123.05
120.13
114.47
87.02
43.71
27.27
N
N
Br
Me
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150
130
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90
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70
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50
40
30
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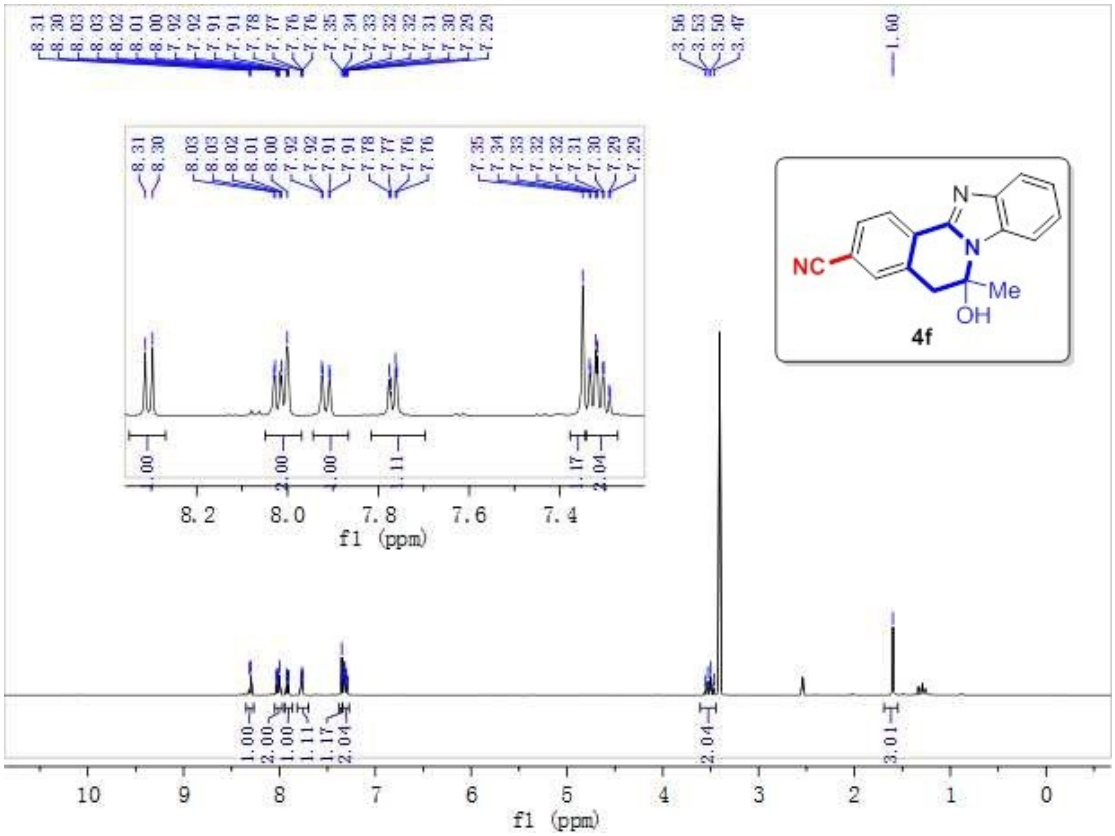
10
0
f1 (ppm)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8.03
8.02
8.01
8.00
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7.91
7.91
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7.77
7.76
7.76
7.35
7.34
7.33
7.32
7.32
7.31
7.30
7.29
7.29
3.56
3.53
3.50
3.47
1.60
1.00
2.00
1.00
1.11
1.17
2.04
8.2
8.0
7.8
7.6
7.4
f1 (ppm)
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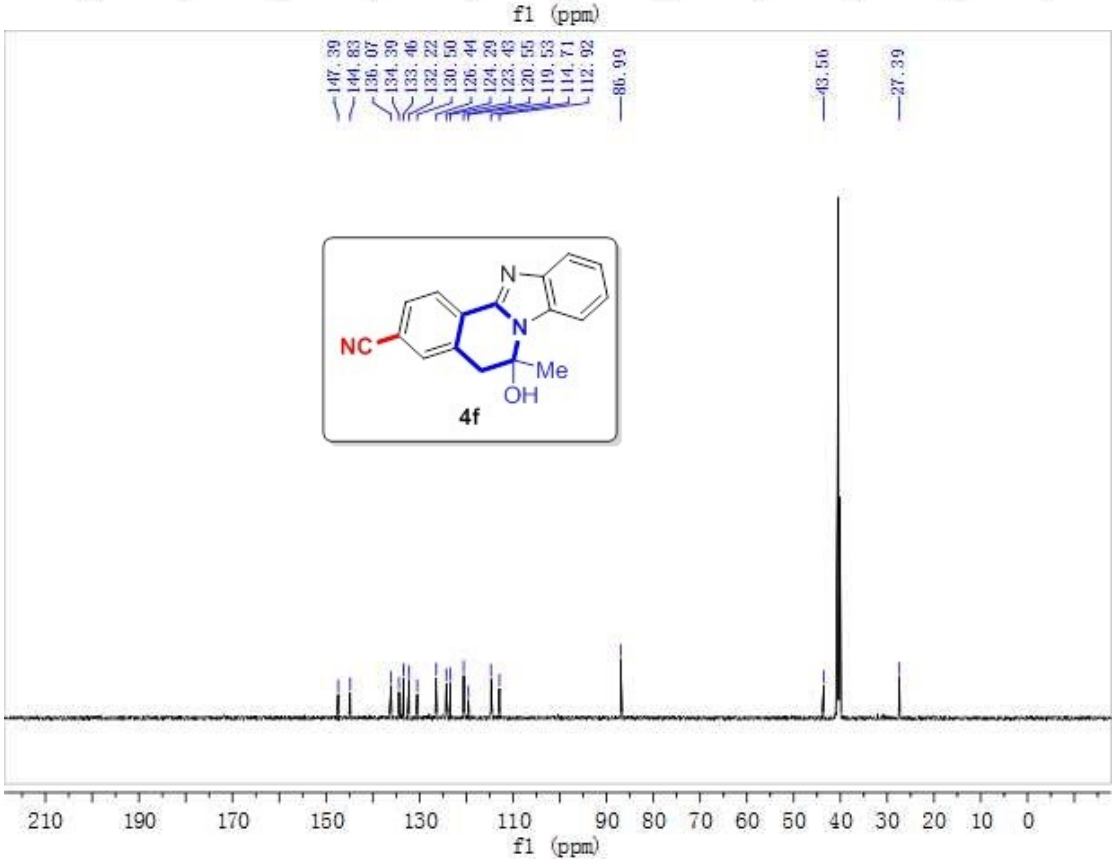
NC
N
Me
OH
4f
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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132.22
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126.44
124.29
123.43
120.55
119.53
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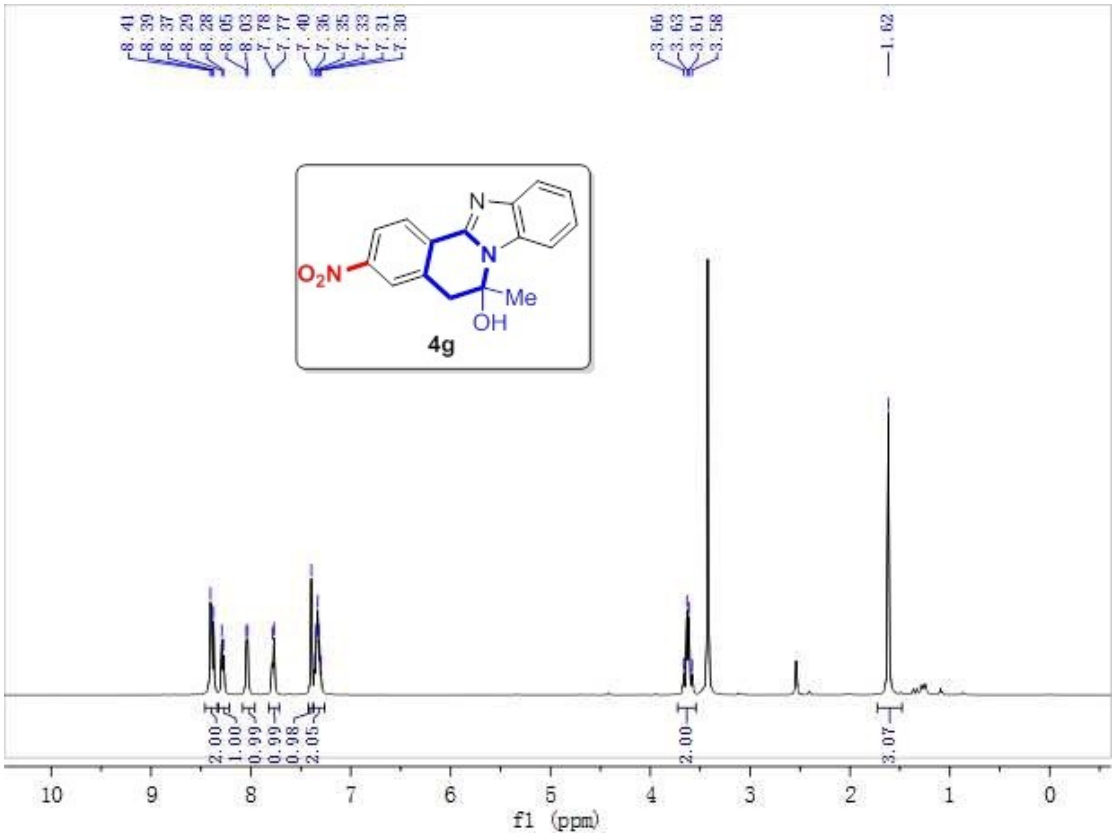
86.99
43.56
27.39
N
NC
N
Me
OH
4f
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.77
7.40
7.36
7.35
7.33
7.31
7.30
3.66
3.63
3.61
3.58
1.62
N
N
O2N
Me
OH
4g
2.00
1.00
0.99
0.99
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2.00
3.07
10
9
8
7
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5
4
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2
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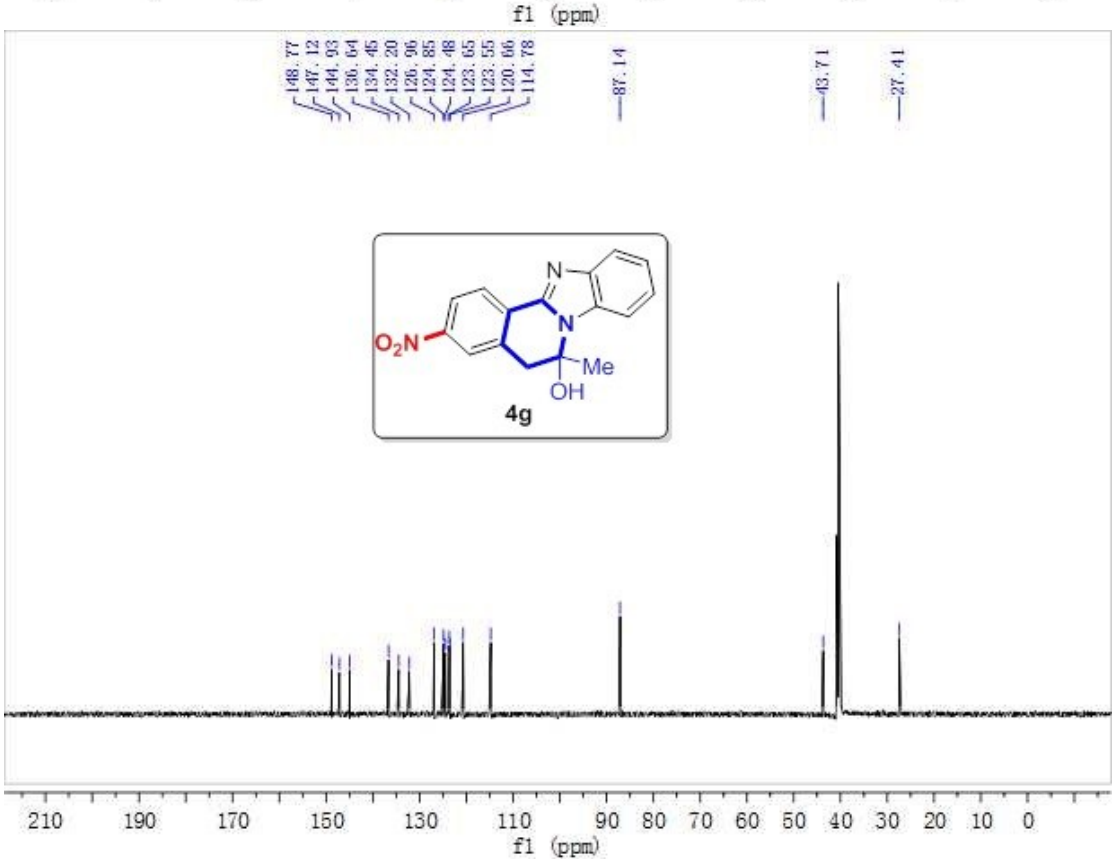
0
f1 (ppm)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124.85
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123.65
123.55
120.66
114.78
87.14
43.71
27.41
N
N
O2N
Me
OH
4g
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170
150
130
110
90
80
70
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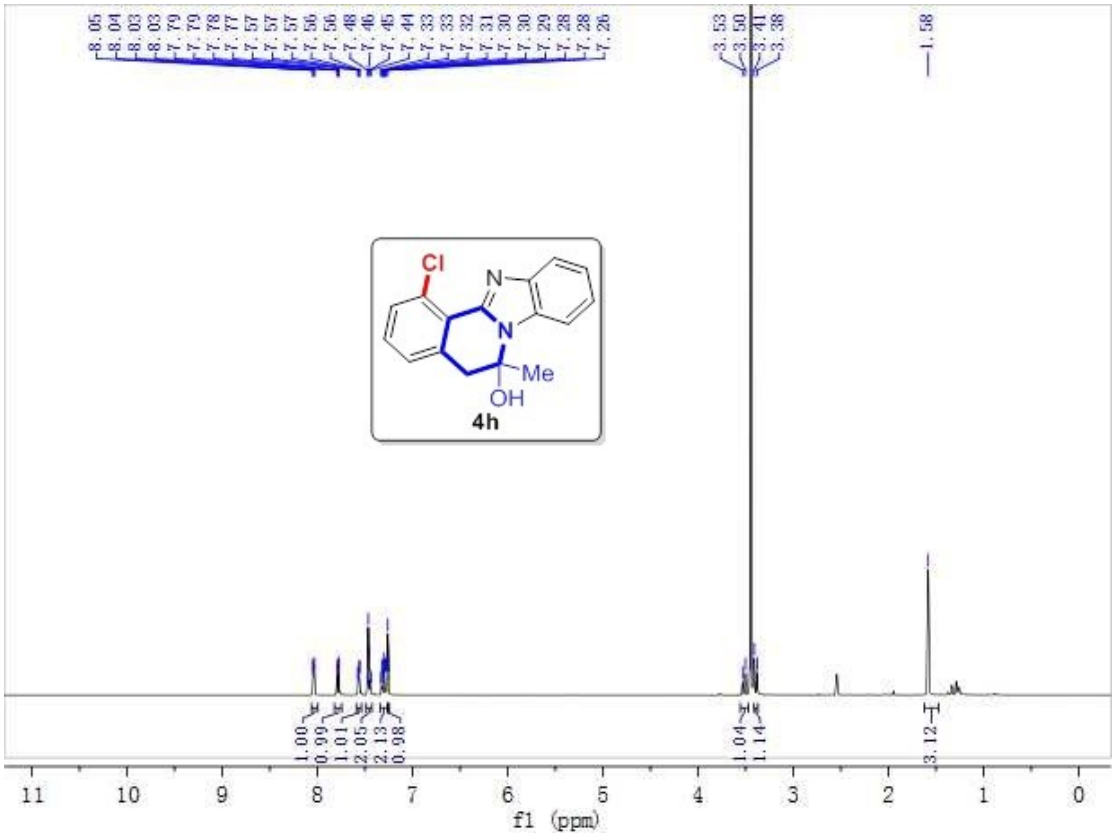
50
40
30
20
10
0
f1 (ppm)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7.77
7.57
7.57
7.57
7.56
7.56
7.48
7.46
7.45
7.44
7.33
7.32
7.31
7.30
7.30
7.29
7.28
7.28
7.26
3.53
3.50
3.41
3.38
1.58
Cl
N
N
Me
OH
4h
1.00
0.99
1.01
2.05
2.13
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1.04
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3.12
11
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9
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7
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5
4
3
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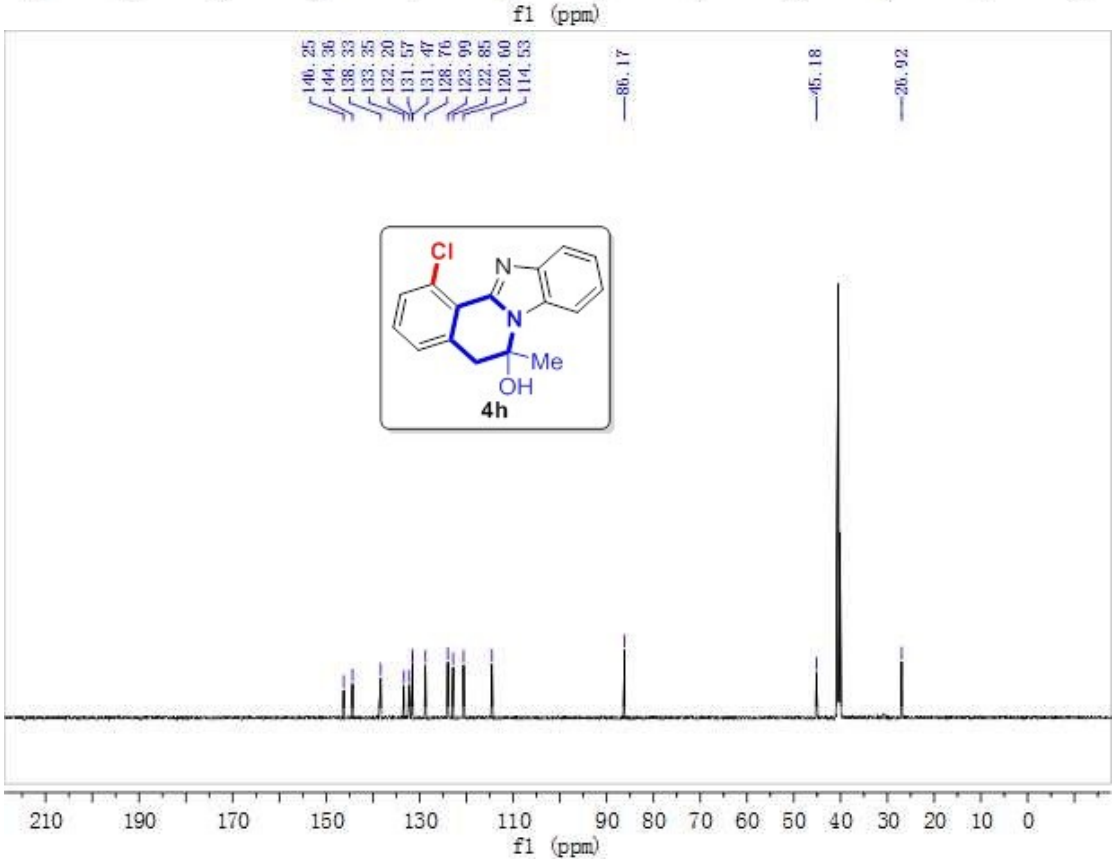
1
0
f1 (ppm)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128.76
123.99
122.85
120.60
114.53
86.17
45.18
26.92
Cl
N
N
Me
OH
4h
210
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170
150
130
110
90
80
70
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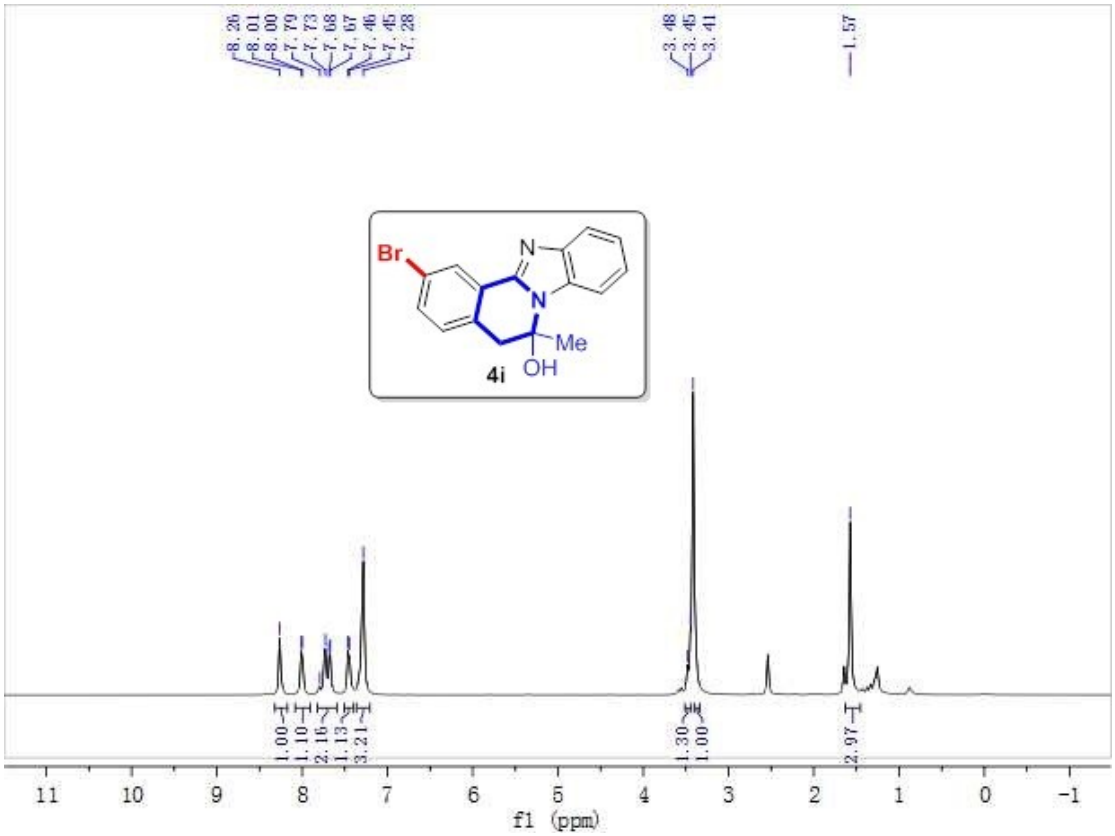
50
40
30
20
10
0
f1 (ppm)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7.28
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3.45
3.41
1.57
Br
N
N
Me
OH
4i
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1.10
2.16
1.13
3.21
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11
10
9
8
7
6
5
4
3
2
1
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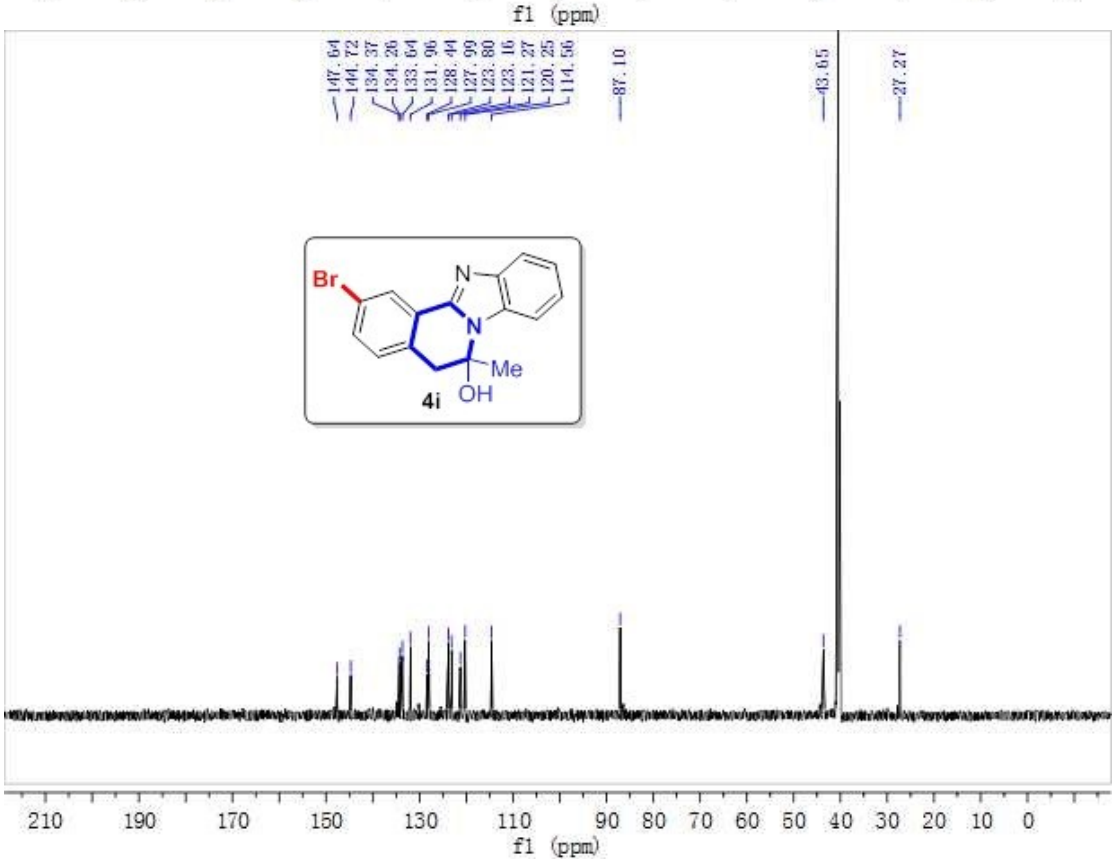
-1
f1 (ppm)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123.16
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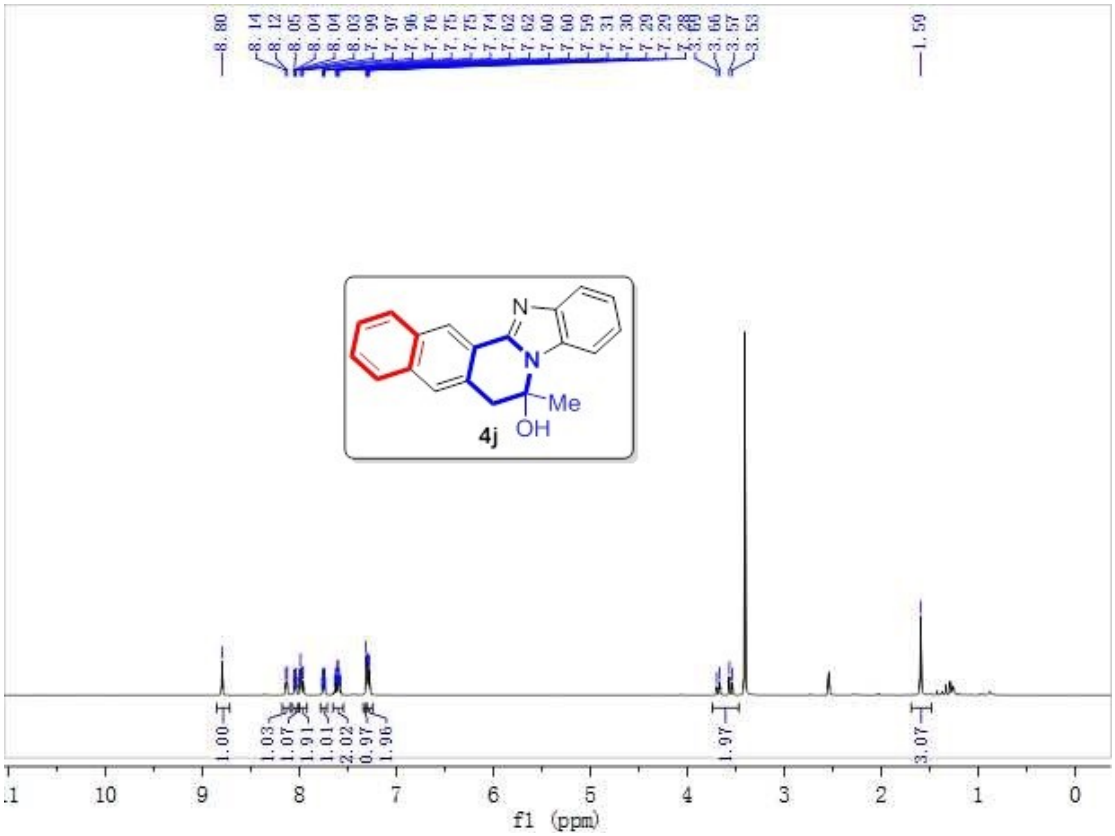
114.56
87.10
43.65
27.27
Br
N
N
Me
OH
4i
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.75
7.74
7.62
7.62
7.60
7.60
7.59
7.31
7.30
7.29
7.29
3.66
3.57
3.53
1.59
N
N
Me
OH
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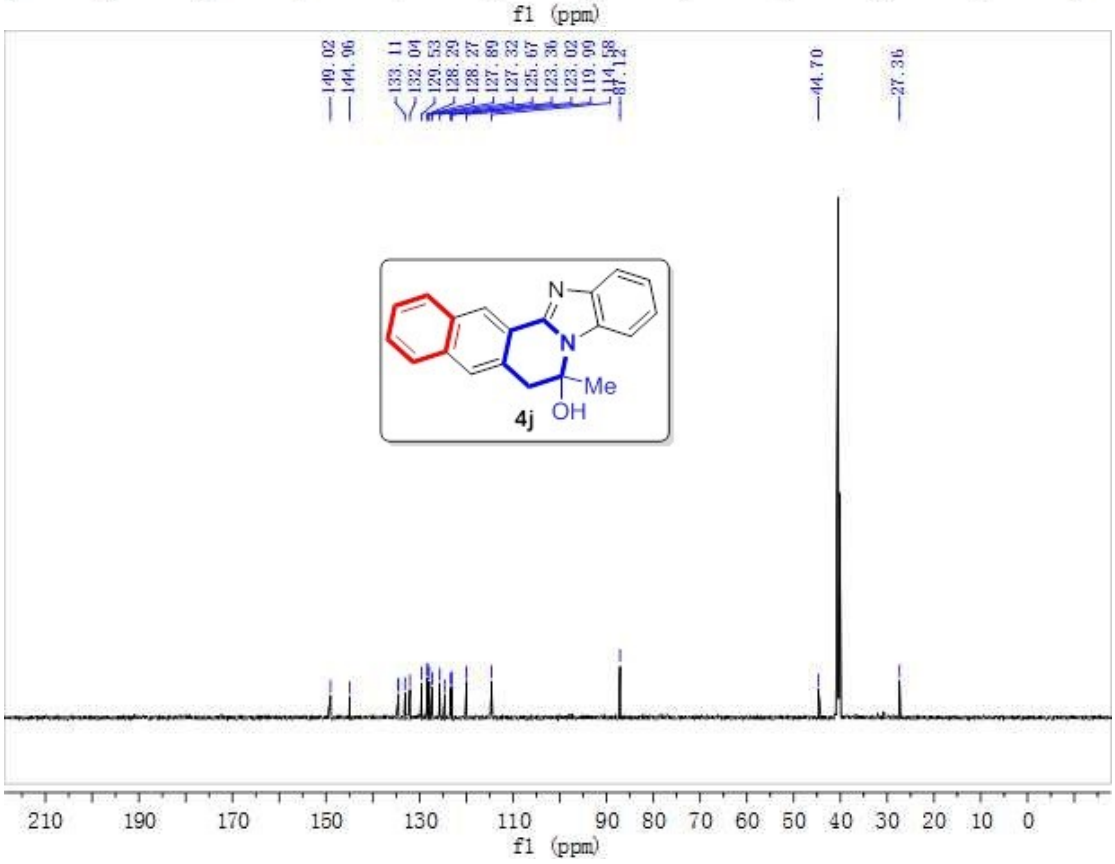
1.96
1.97
3.07
f1 (ppm)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N
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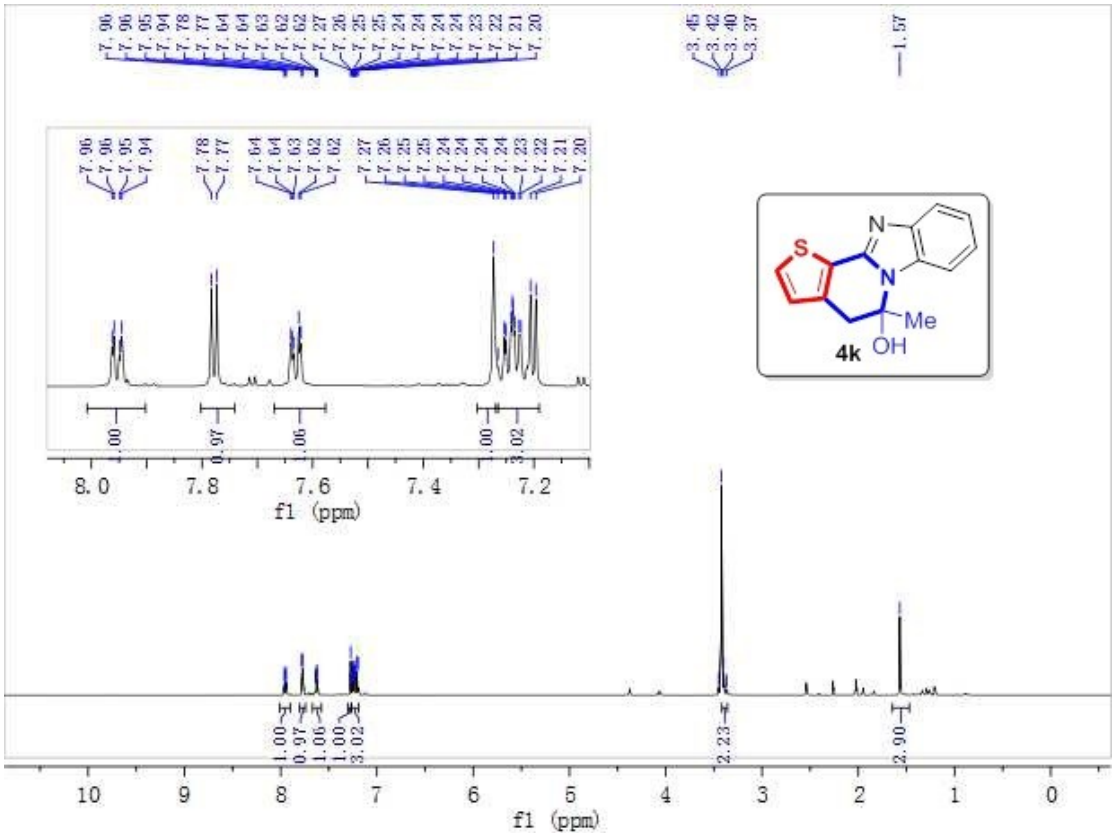
Me
OH
4j
f1 (ppm)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7.62
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7.26
7.25
7.25
7.24
7.24
7.24
7.24
7.23
7.22
7.21
7.20
3.45
3.42
3.40
3.37
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1.00
0.97
1.06
1.00
3.02
2.23
2.90
8.0
7.8
7.6
7.4
7.2
f1 (ppm)
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6
5
4
3
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f1 (ppm)
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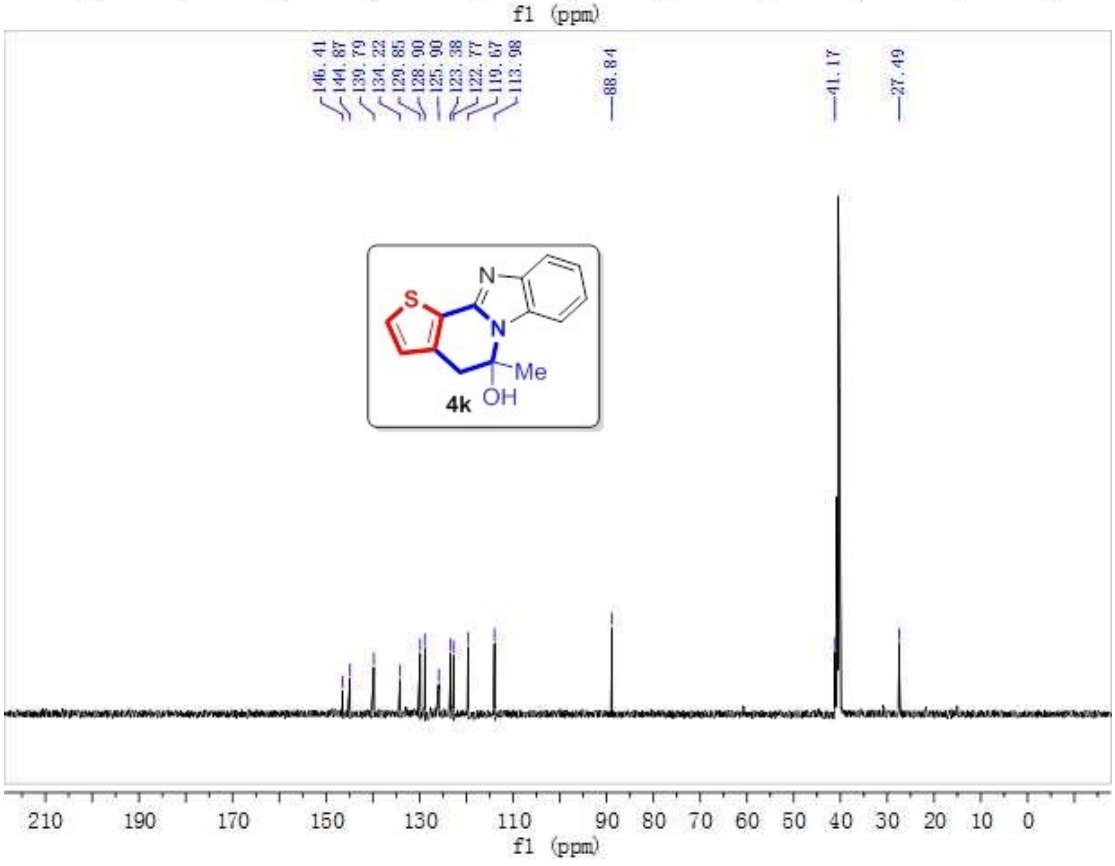
S
N
Me
OH
4k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113.98
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41.17
27.49
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
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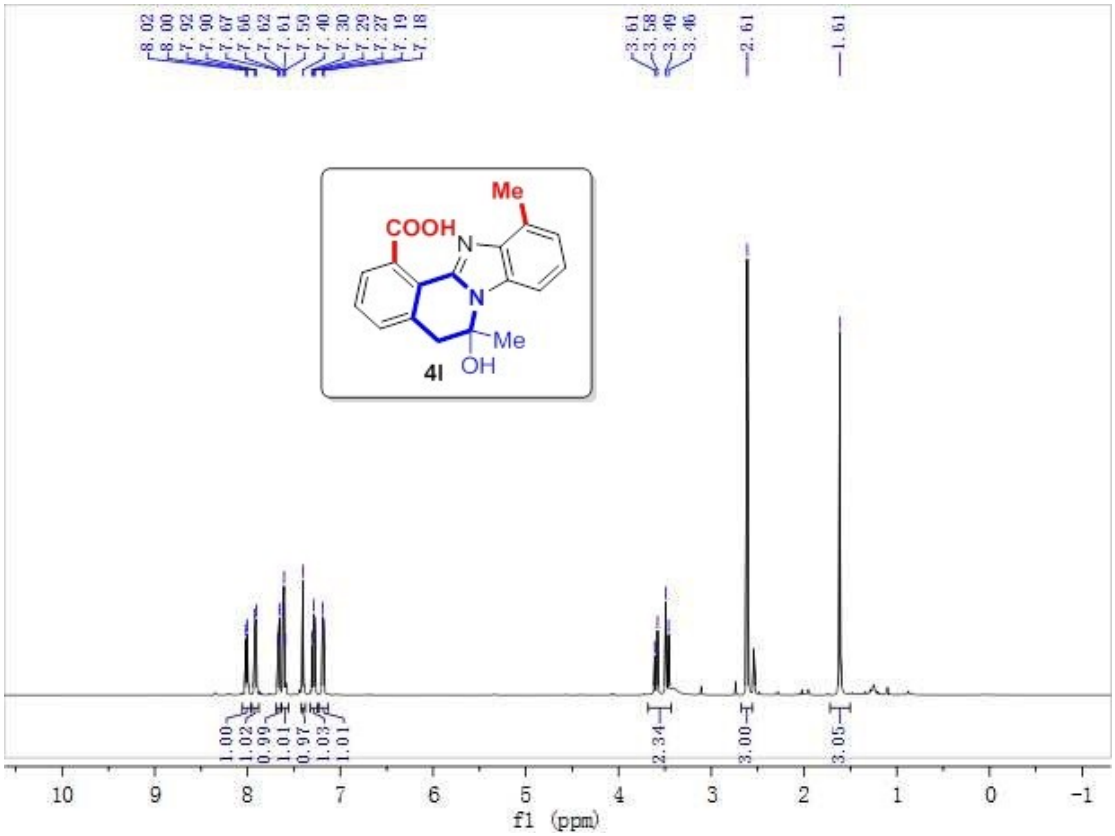
S
N
Me
OH
4k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7.59
7.40
7.30
7.29
7.27
7.19
7.18
3.61
3.58
3.49
3.46
2.61
1.61
Me
COOH
N
N
Me
OH
4l
1.00
1.02
0.99
1.01
0.97
1.03
1.01
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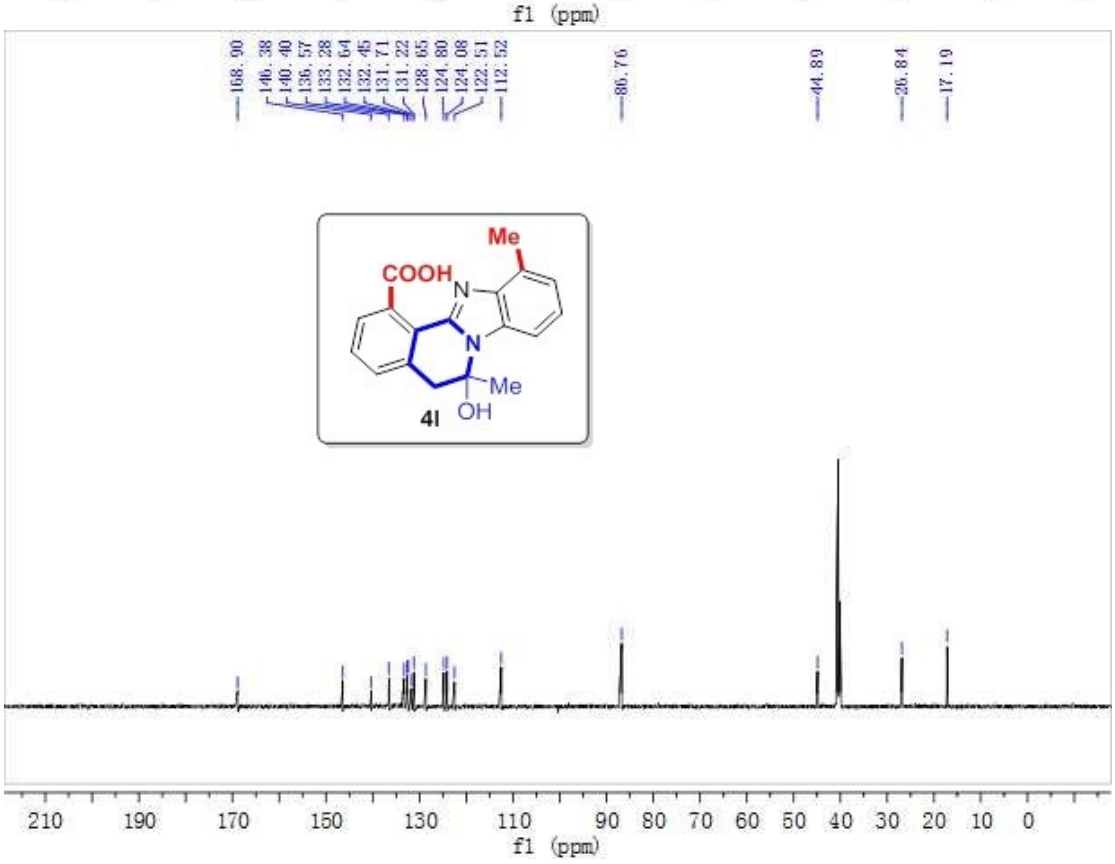
3.05
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)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131.71
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124.08
122.51
112.52
80.76
44.89
26.84
17.19
Me
COOH
N
N
Me
OH
4l
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170
150
130
110
90
80
70
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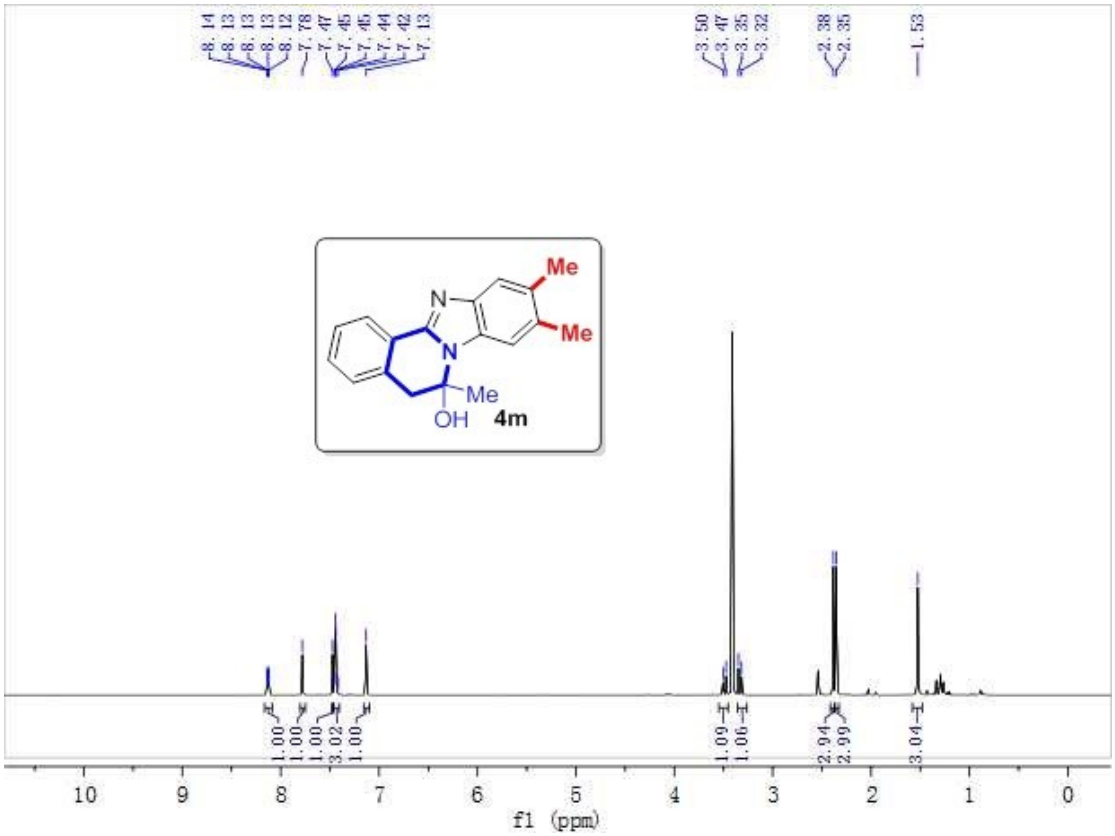
50
40
30
20
10
0
f1 (ppm)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7.45
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7.42
7.13
3.50
3.47
3.35
3.32
2.38
2.35
1.53
Me
Me
N
N
Me
OH
4m
1.00
1.00
1.00
3.02
1.00
1.09
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3.04
10
9
8
7
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5
4
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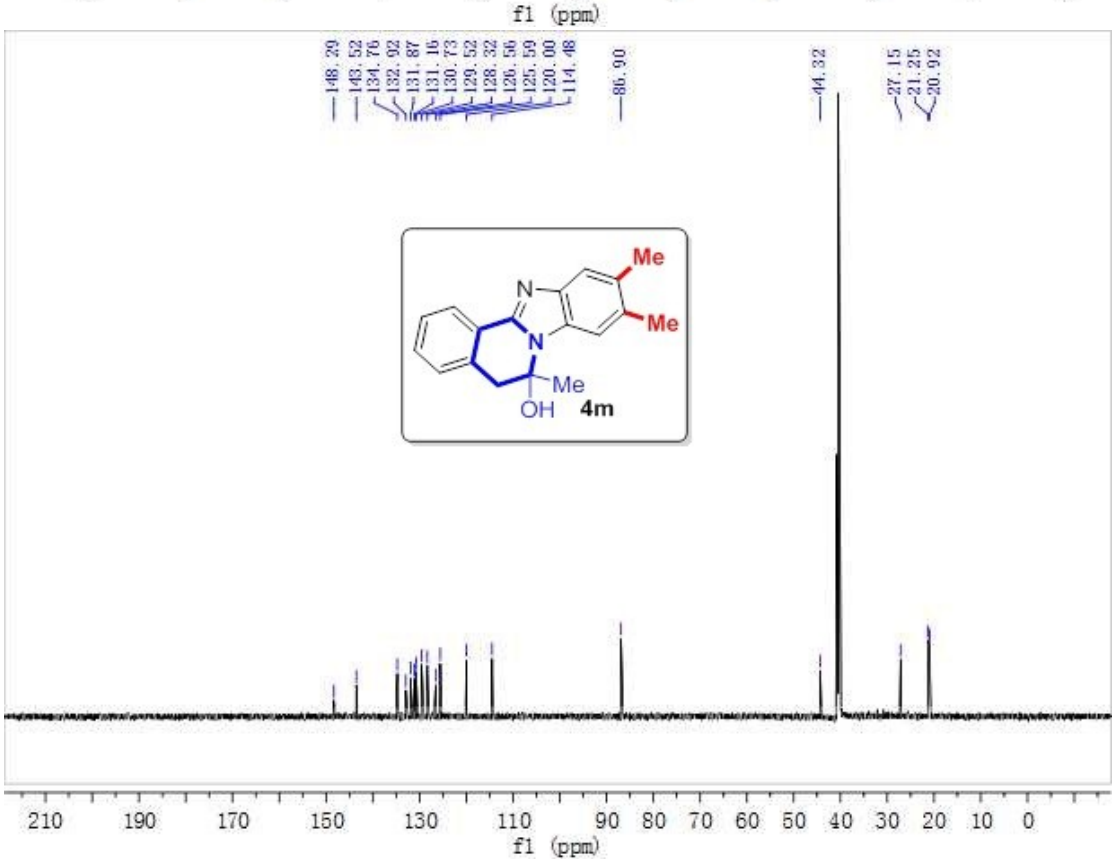
2
1
0
f1 (ppm)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131.16
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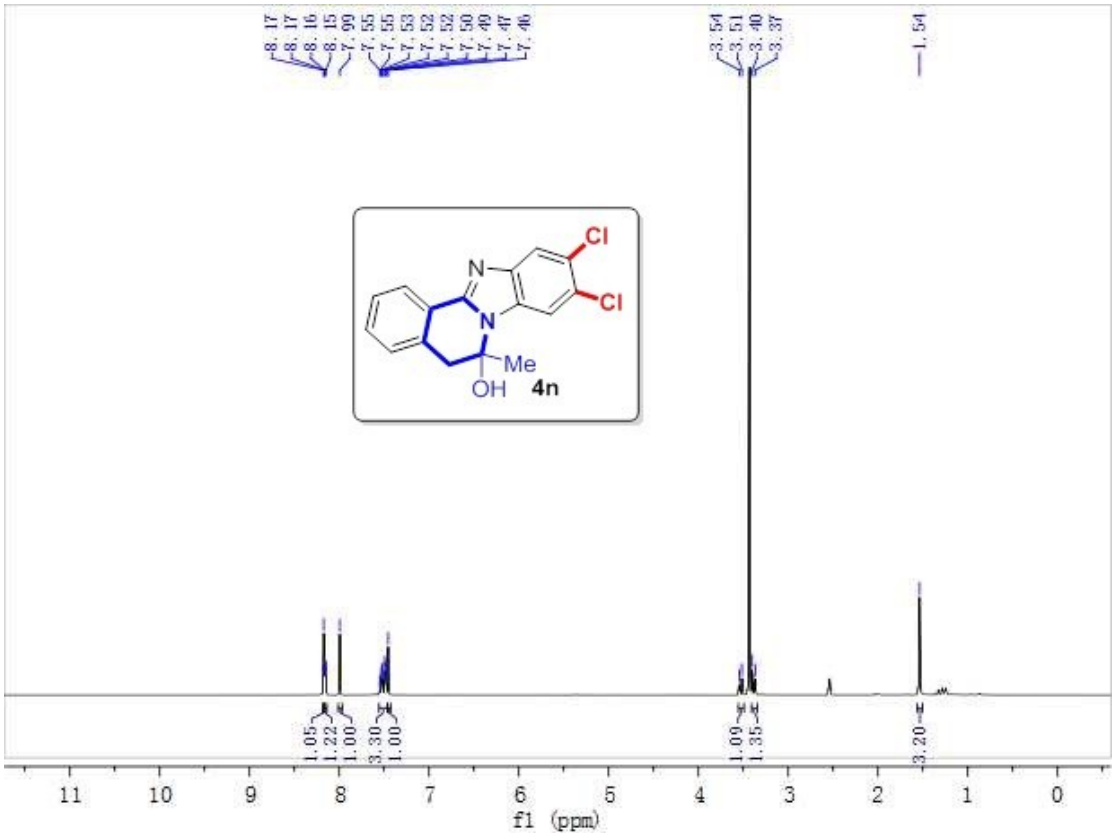
126.56
125.59
120.00
114.48
86.90
44.32
27.15
21.25
20.92
Me
Me
N
N
Me
OH
4m
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.16
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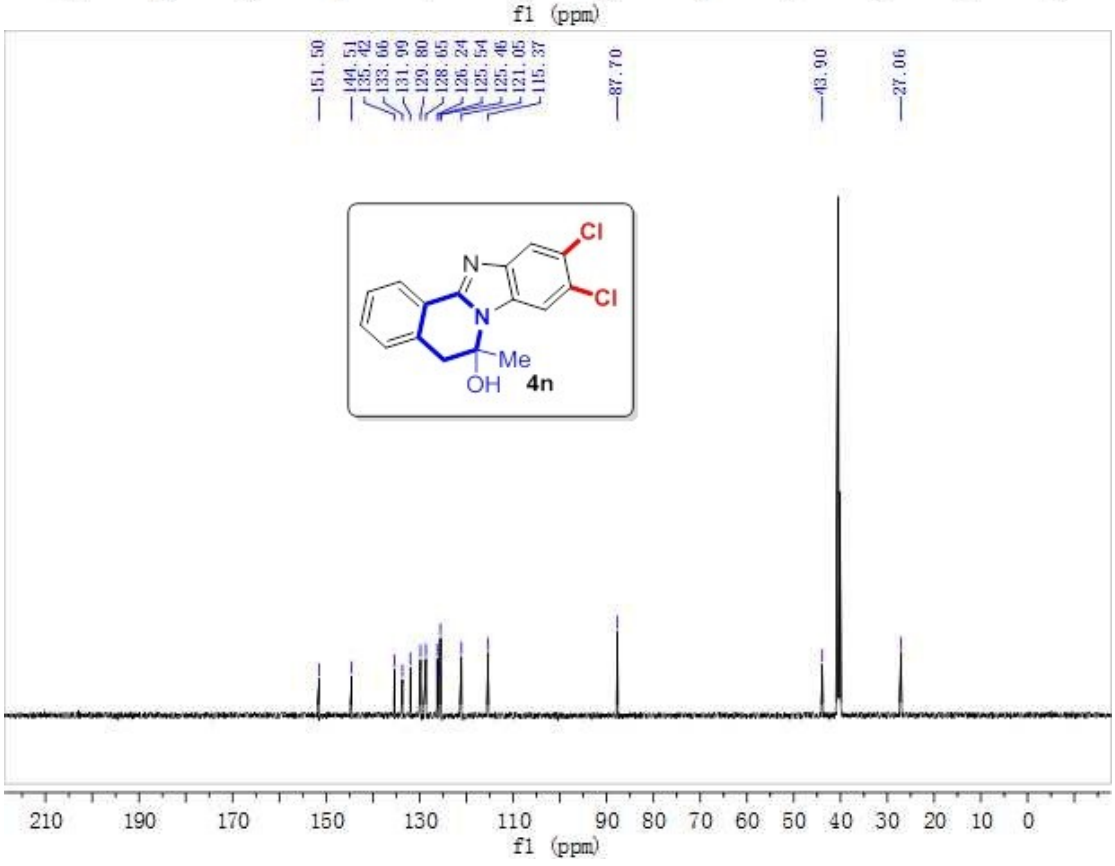
7.55
7.55
7.53
7.52
7.52
7.50
7.49
7.47
7.46
3.54
3.51
3.40
3.37
1.54
Cl
Cl
N
N
Me
OH
4n
1.05
1.22
1.00
3.30
1.00
1.09
1.35
3.20
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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135.42
133.66
131.99
129.80
128.65
126.24
125.54
125.46
121.05
115.37
87.70
43.90
27.06
Cl
Cl
N
N
Me
OH
4n
210
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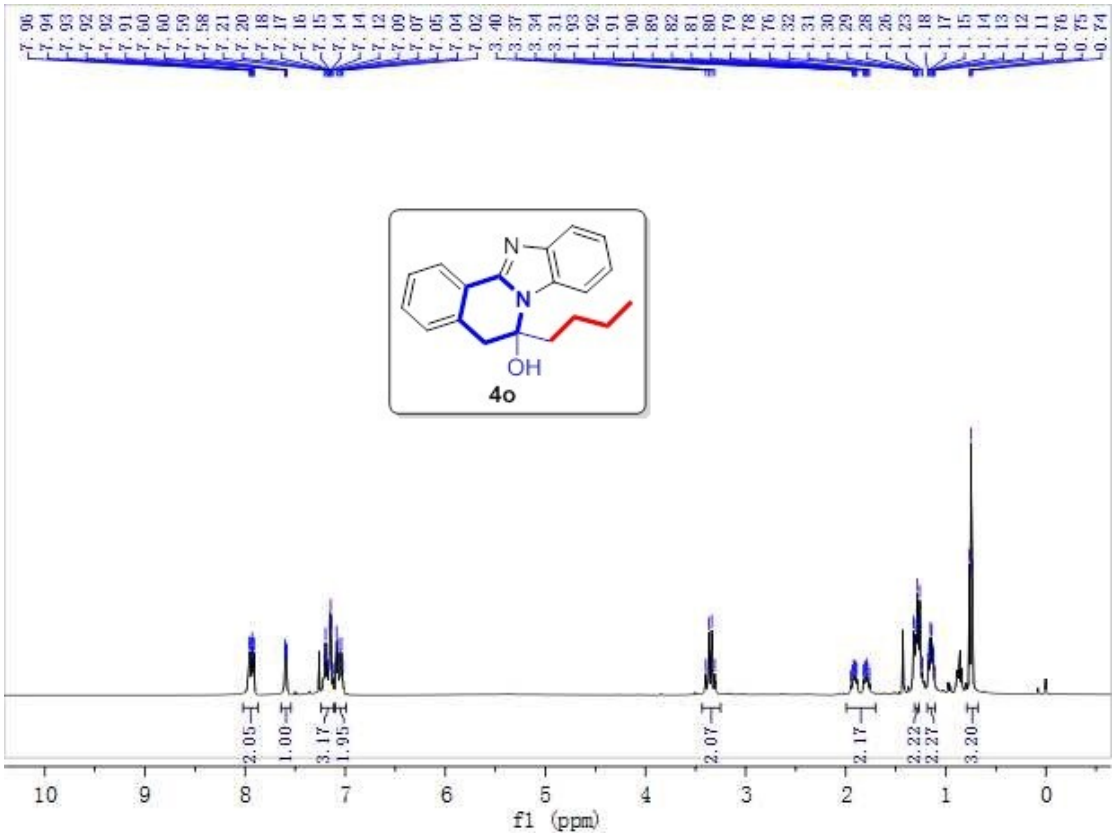
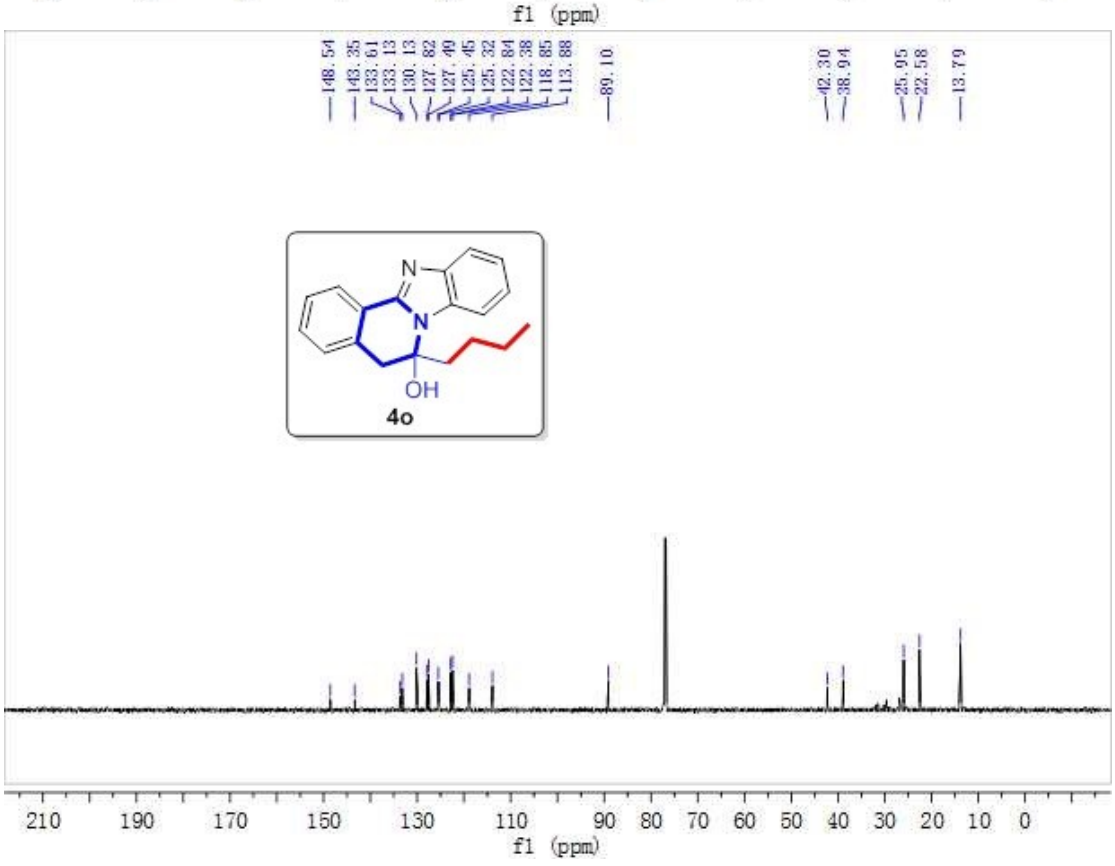
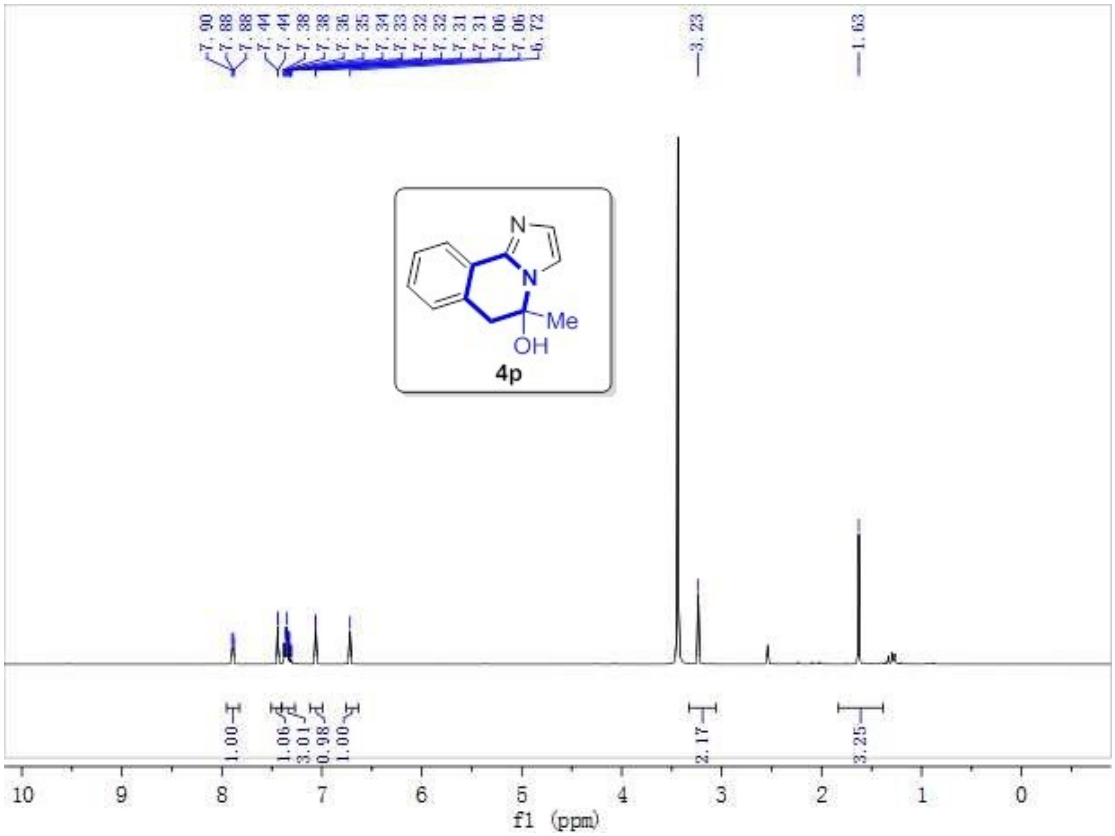
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.96 7.94 7.93 7.92 7.92 7.91 7.60 7.60 7.59 7.58 7.21 7.20 7.18 7.17 7.16 7.15 7.14 7.14 7.12 7.09 7.07 7.05 7.04 7.02 3.40 3.37 3.34 3.31 1.93 1.92 1.91 1.90 1.80 1.82 1.81 1.80 1.79 1.78 1.76 1.32 1.31 1.30 1.29 1.28 1.26 1.23 1.18 1.17 1.15 1.14 1.13 1.12 1.11 0.76 0.75 0.74
N
N
OH
4o
2.05 1.00 3.17 1.95 2.07 2.17 2.22 2.27 3.20
10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


148.54 143.35 133.61 133.13 130.13 127.82 127.49 125.45 125.32 122.84 122.38 118.85 113.88 89.10 42.30 38.94 25.95 22.58 13.79
N
N
OH
4o
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.88
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7.36
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7.34
7.33
7.32
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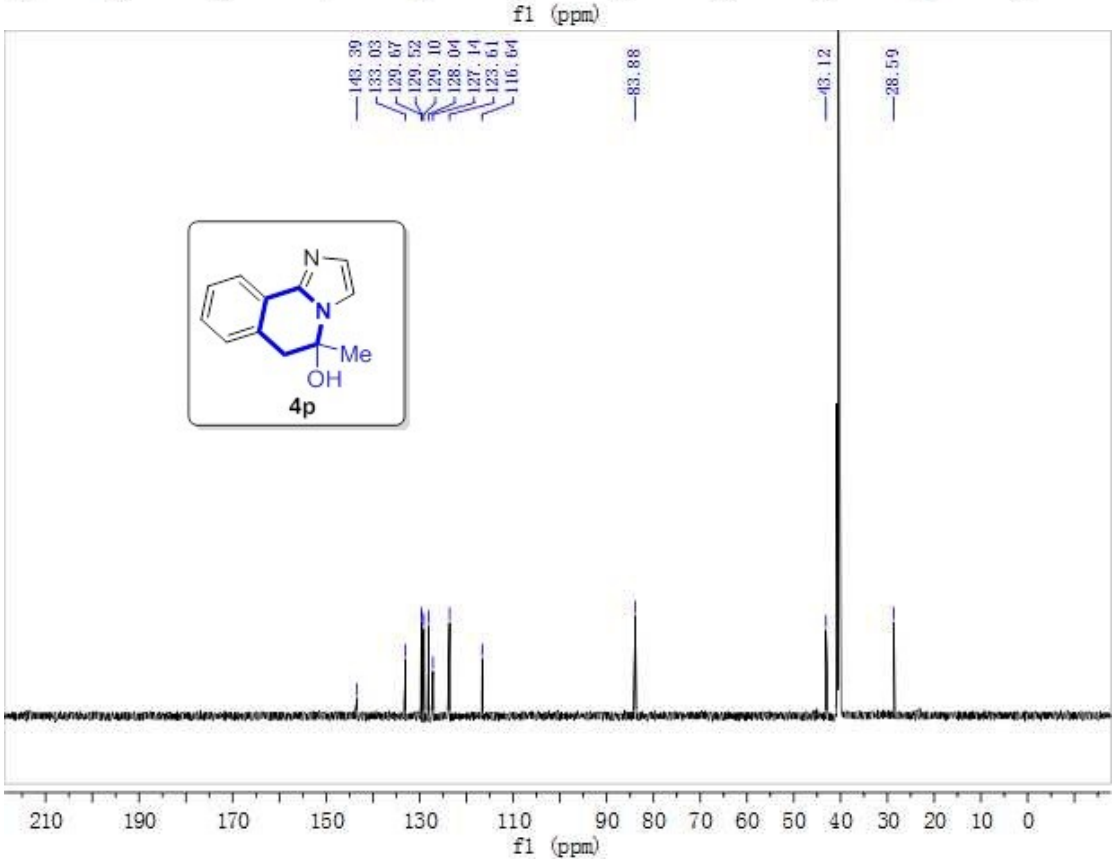
7.31
7.31
7.06
7.06
6.72
3.23
1.63
N
N
Me
OH
4p
1.00
1.06
3.01
0.98
1.00
2.17
3.25
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


143.39
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123.61
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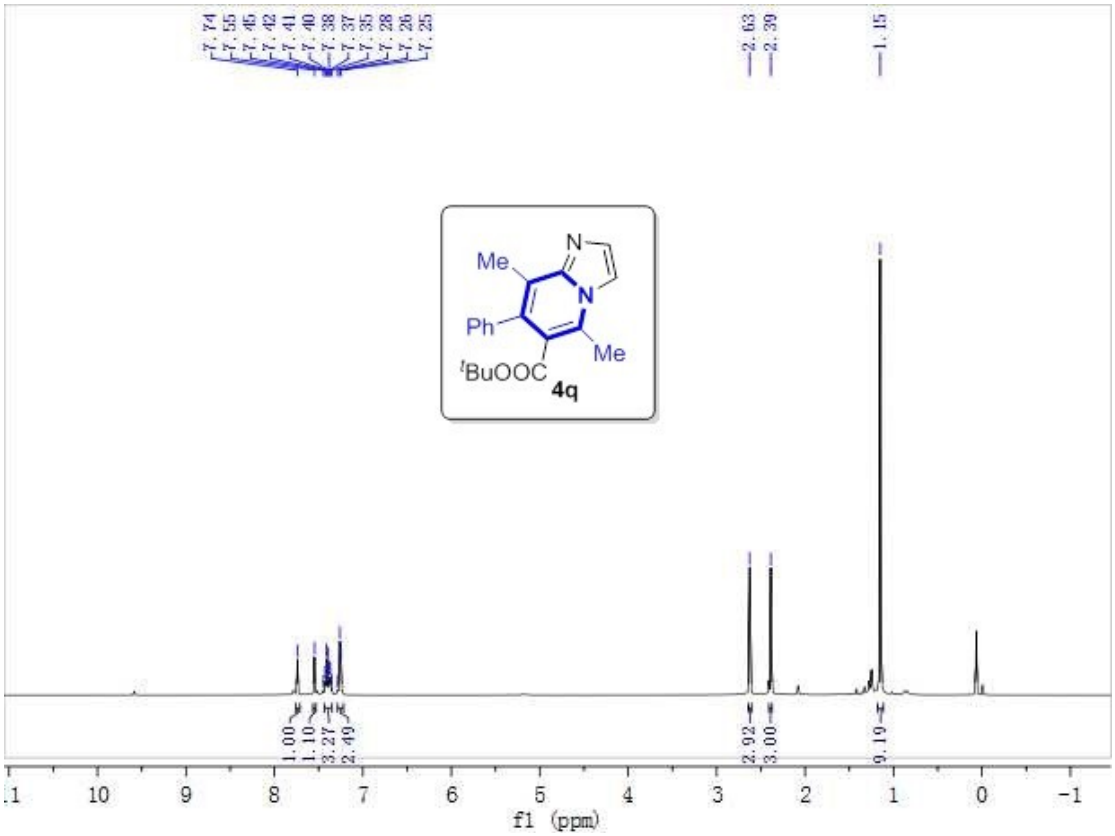
83.88
43.12
28.59
N
N
Me
OH
4p
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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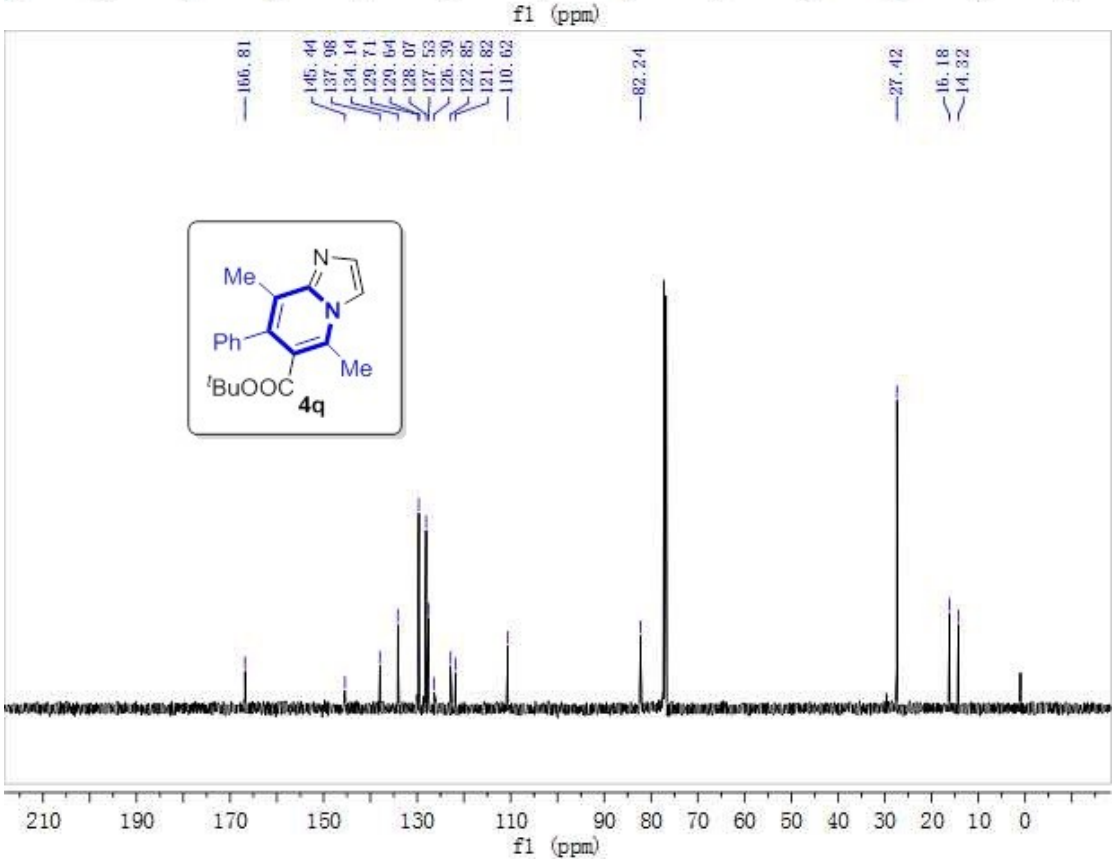
7.40
7.38
7.37
7.35
7.28
7.26
7.25
2.63
2.39
1.15
Me
N
Ph
Me
tBuOOC
4q
1.00
1.10
3.27
2.49
2.92
3.00
9.19
f1 (ppm)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129.71
129.64
128.07
127.53
126.39
122.85
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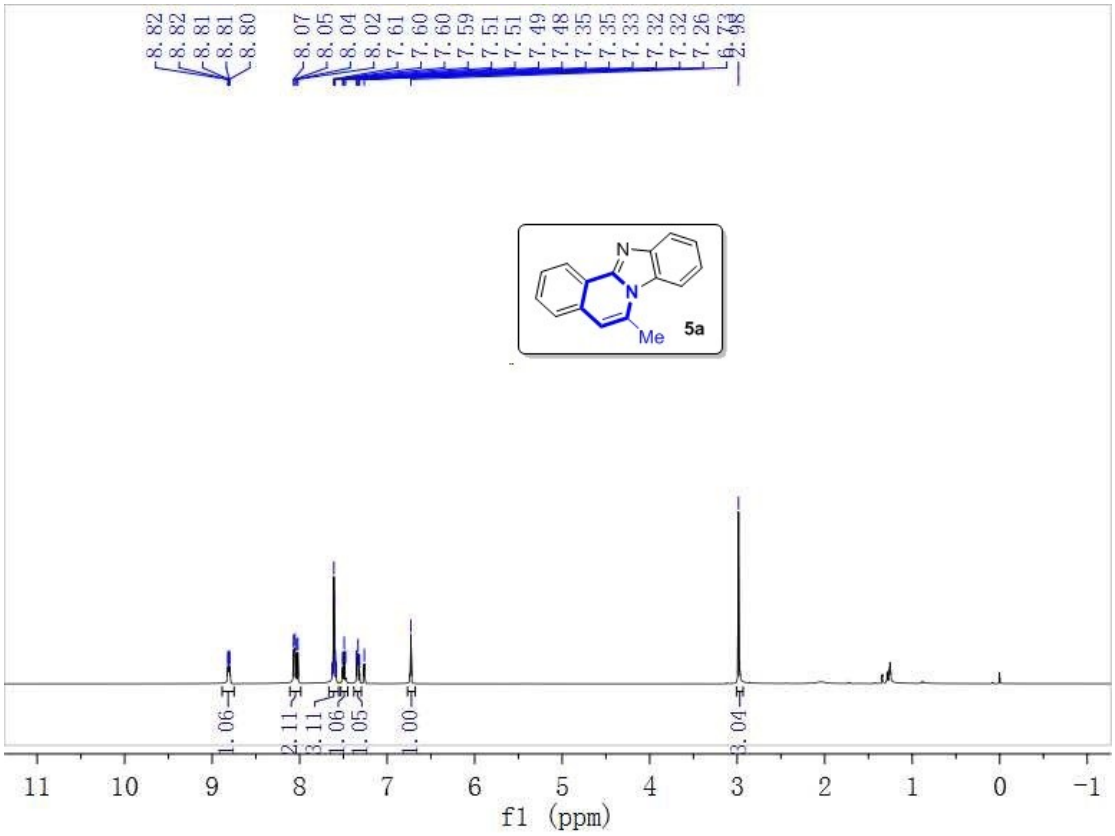
82.24
27.42
16.18
14.32
Me
N
Ph
Me
tBuOOC
4q
f1 (ppm)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8.81
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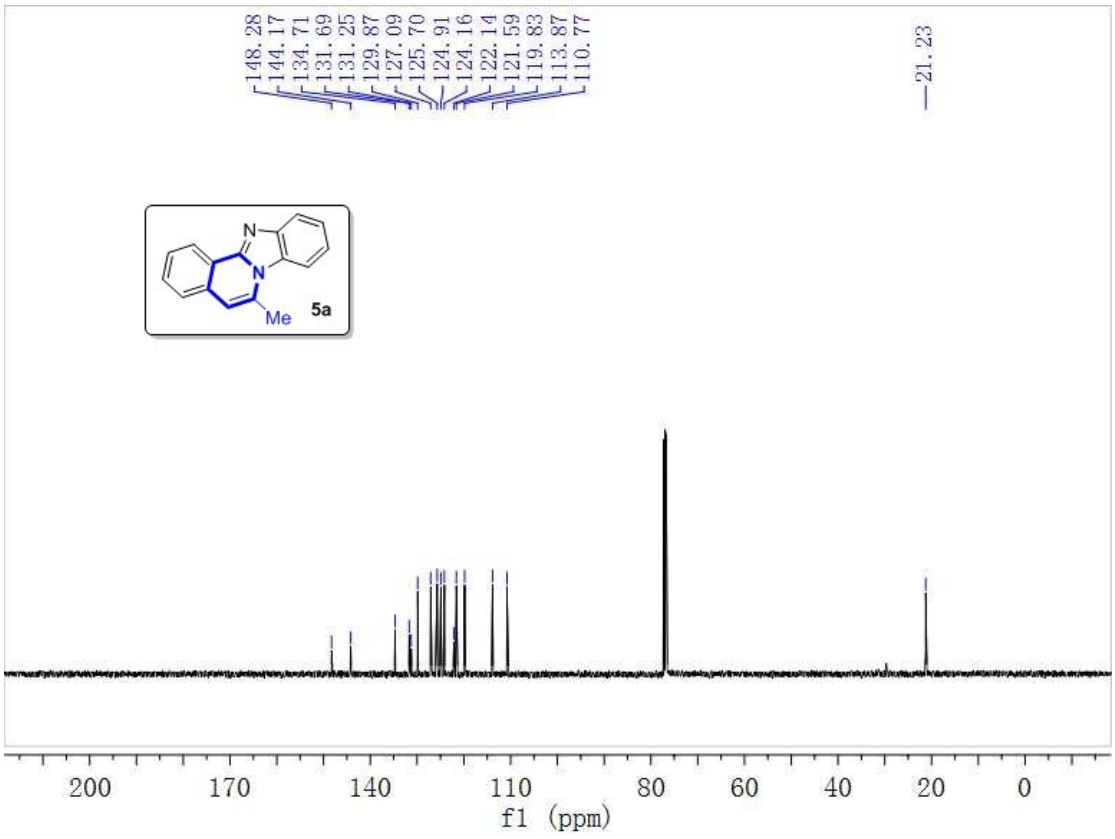
8.07
8.05
8.04
8.02
7.61
7.60
7.60
7.59
7.51
7.51
7.49
7.48
7.35
7.35
7.33
7.32
7.32
7.26
6.73
2.98
N
N
Me
5a
1.06
2.11
3.11
1.06
1.05
1.00
3.04
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)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129.87
127.09
125.70
124.91
124.16
122.14
121.59
119.83
113.87
110.77
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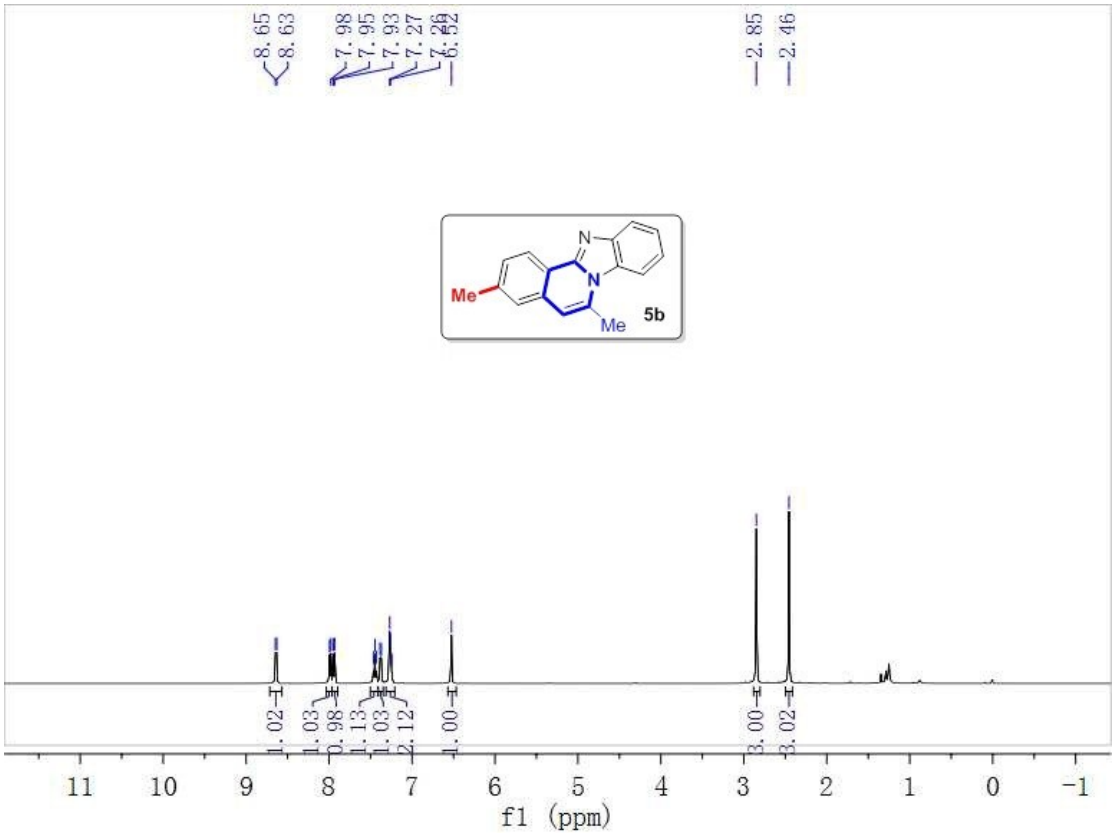
N
N
Me
5a
200
170
140
110
80
60
40
20
0
f1 (ppm)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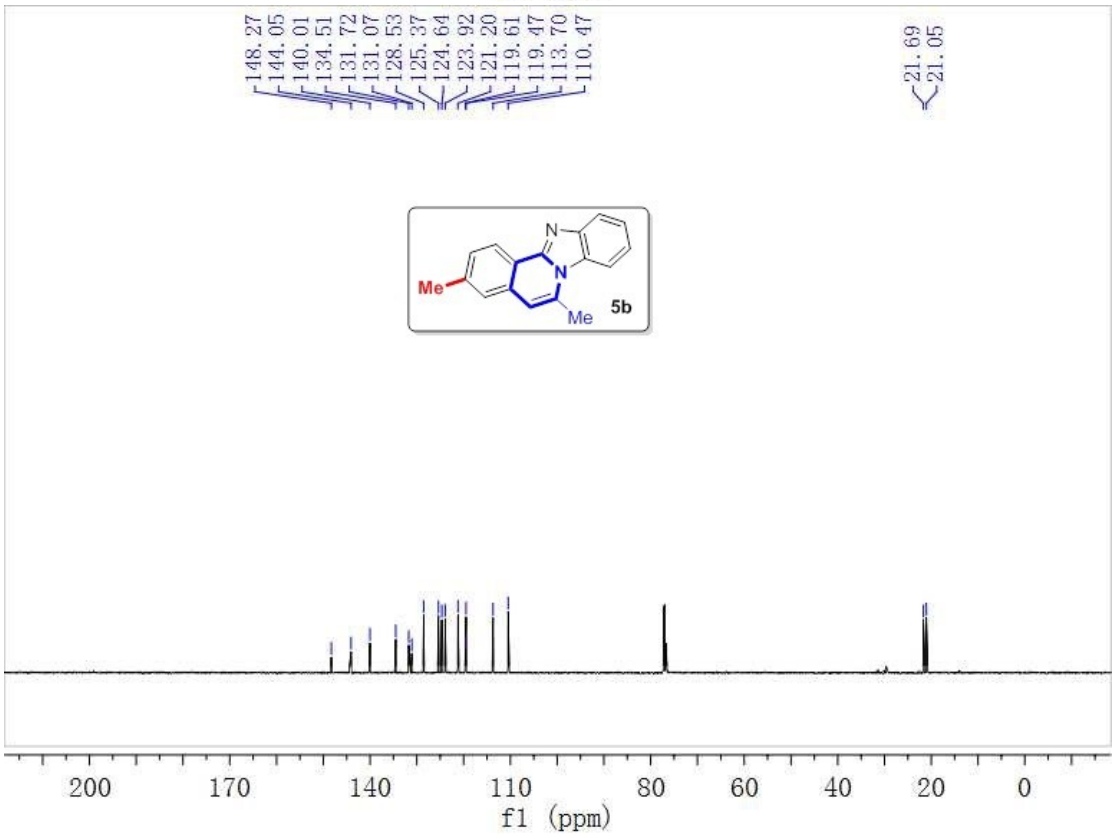
7.95
7.93
7.27
2.85
2.46
Me
N
N
Me
5b
1.02
1.03
0.98
1.13
1.03
2.12
1.00
3.00
3.02
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)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131.07
128.53
125.37
124.64
123.92
121.20
119.61
119.47
113.70
110.47
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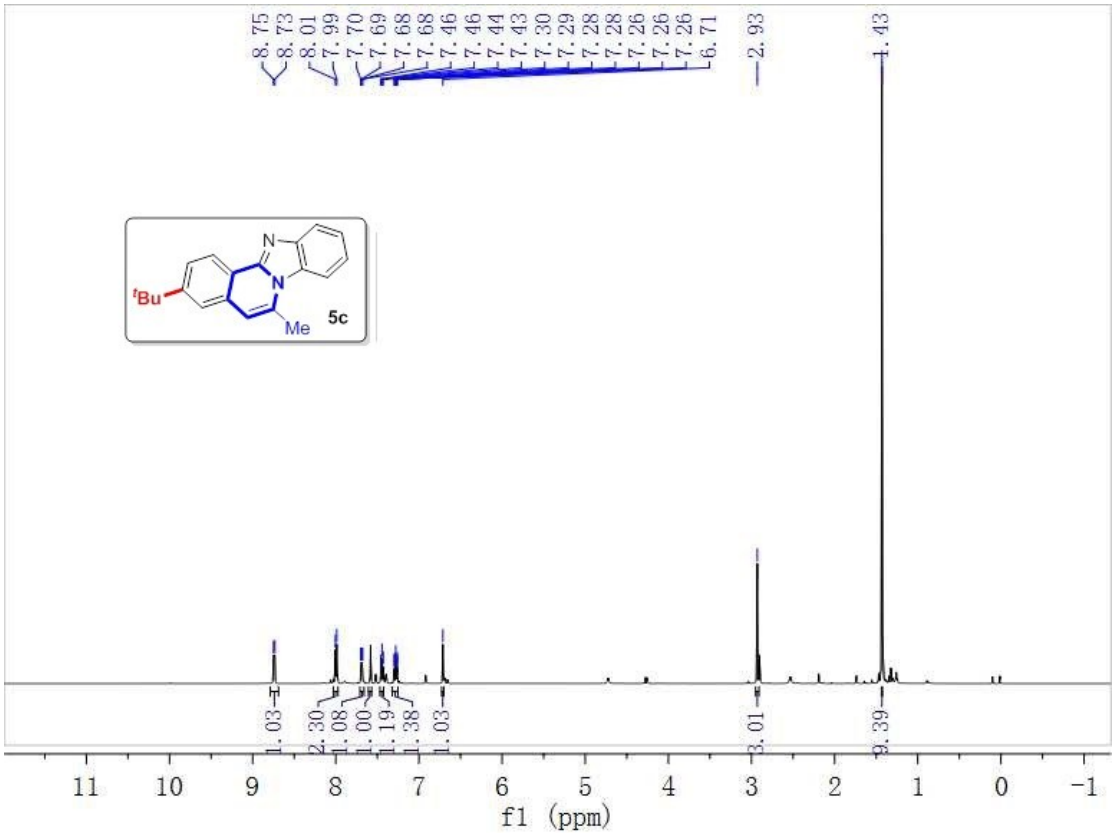
21.05
Me
N
N
Me
5b
200
170
140
110
80
60
40
20
0
f1 (ppm)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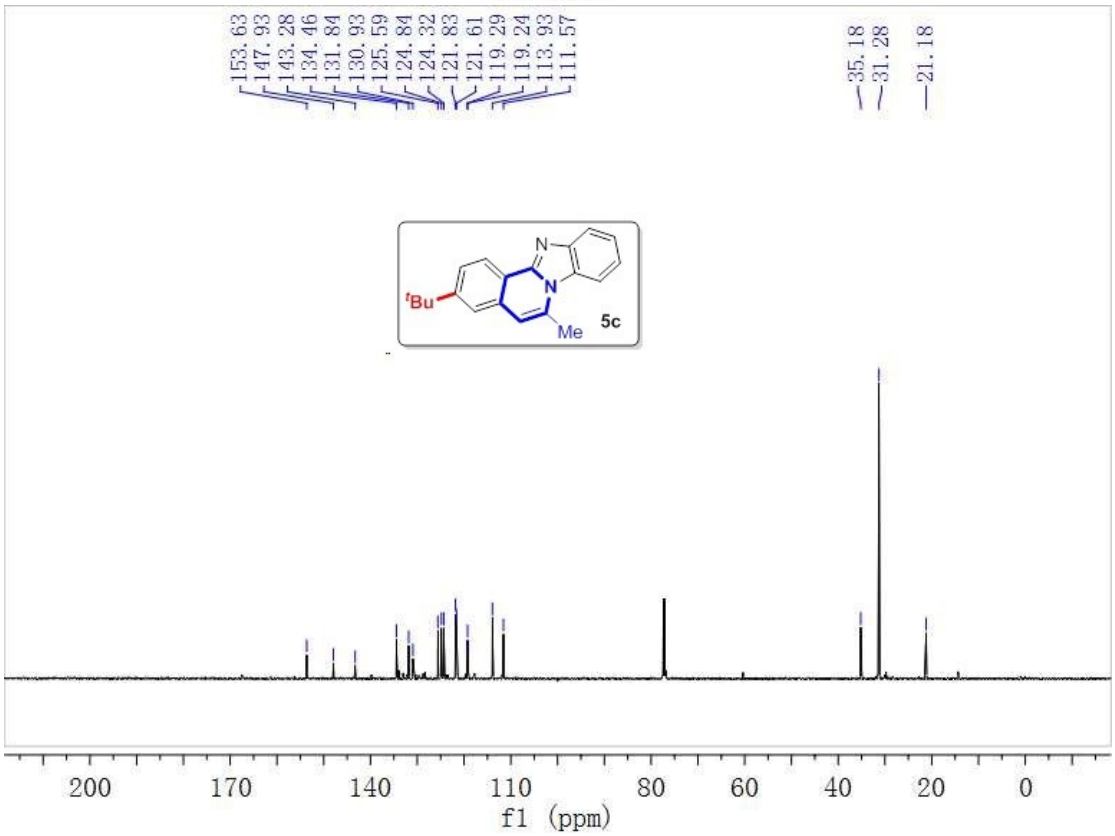
7.30
7.29
7.28
7.28
7.26
7.26
7.26
6.71
2.93
1.43
1.03
2.30
1.08
1.00
1.19
1.38
1.03
3.01
9.39
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)
tBu
Me
5c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124.84
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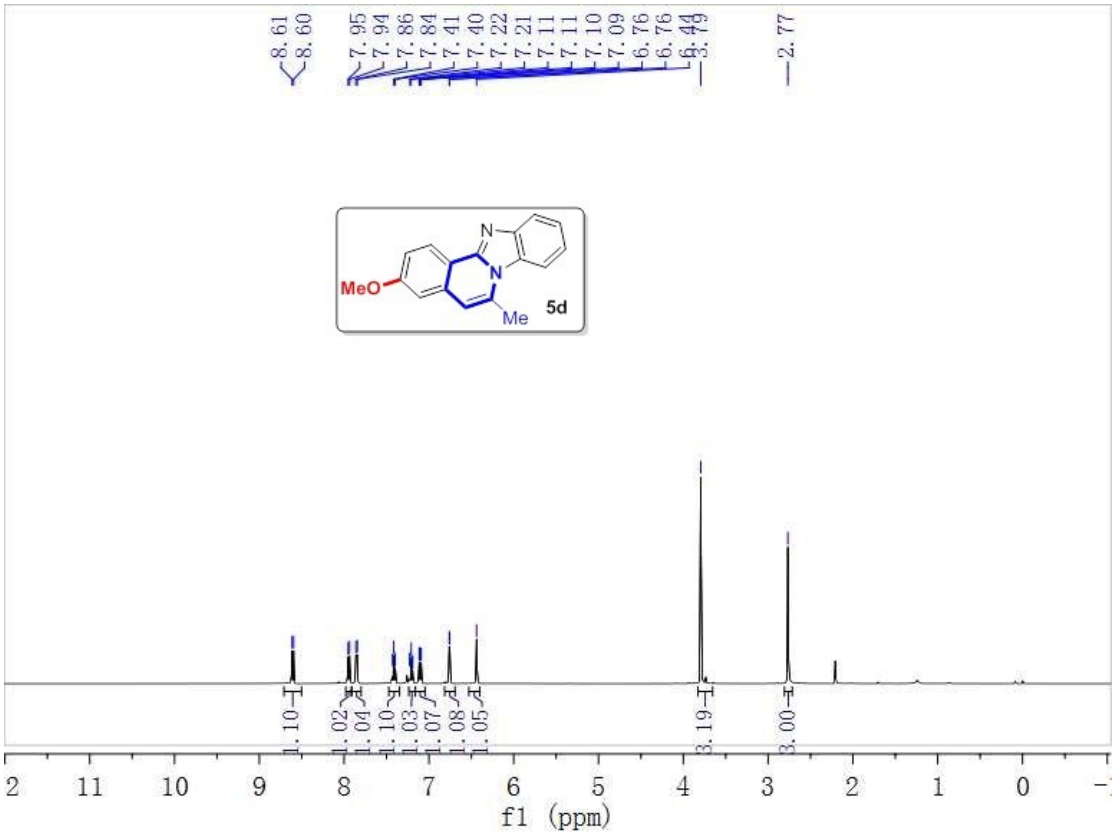
121.83
121.61
119.29
119.24
113.93
111.57
35.18
31.28
21.18
200
170
140
110
80
60
40
20
0
f1 (ppm)
tBu
Me
5c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7.84
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7.40
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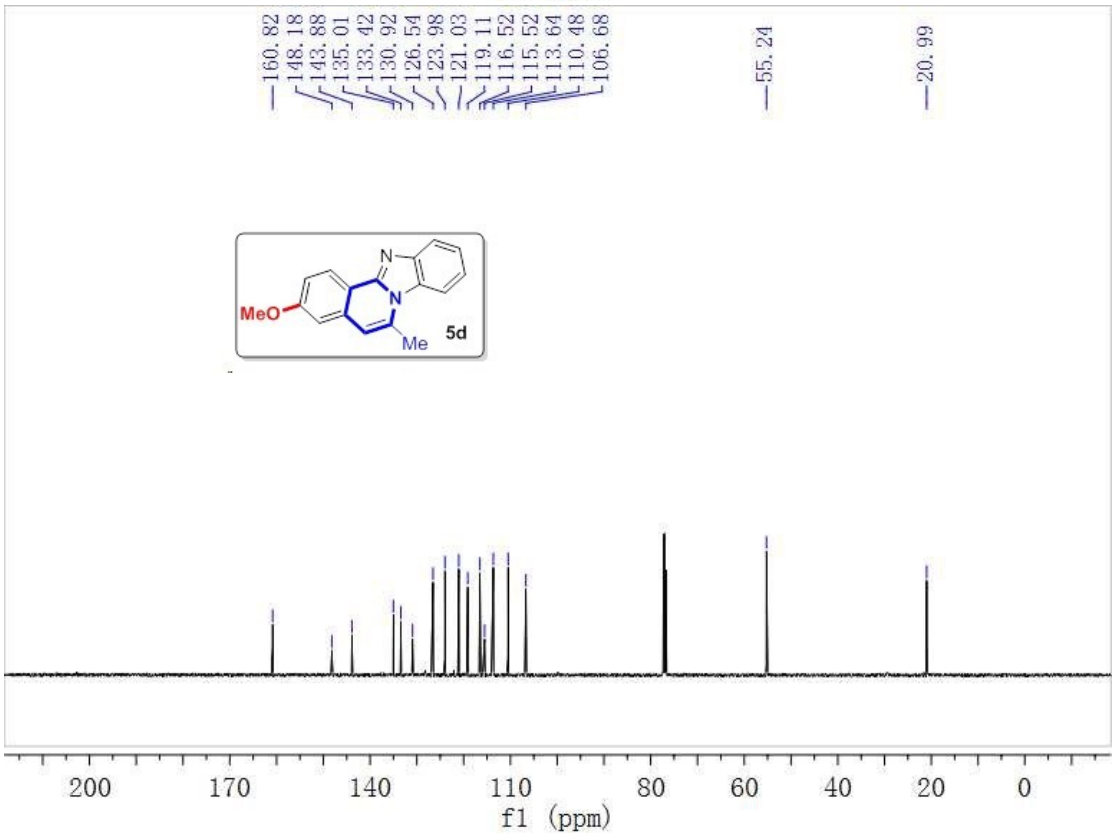
7.21
7.11
7.11
7.10
7.09
6.76
6.76
6.44
3.19
2.77
MeO
N
N
Me
5d
1.10
1.02
1.04
1.10
1.03
1.07
1.08
1.05
3.19
3.00
f1 (ppm)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119.11
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110.48
106.68
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20.99
MeO
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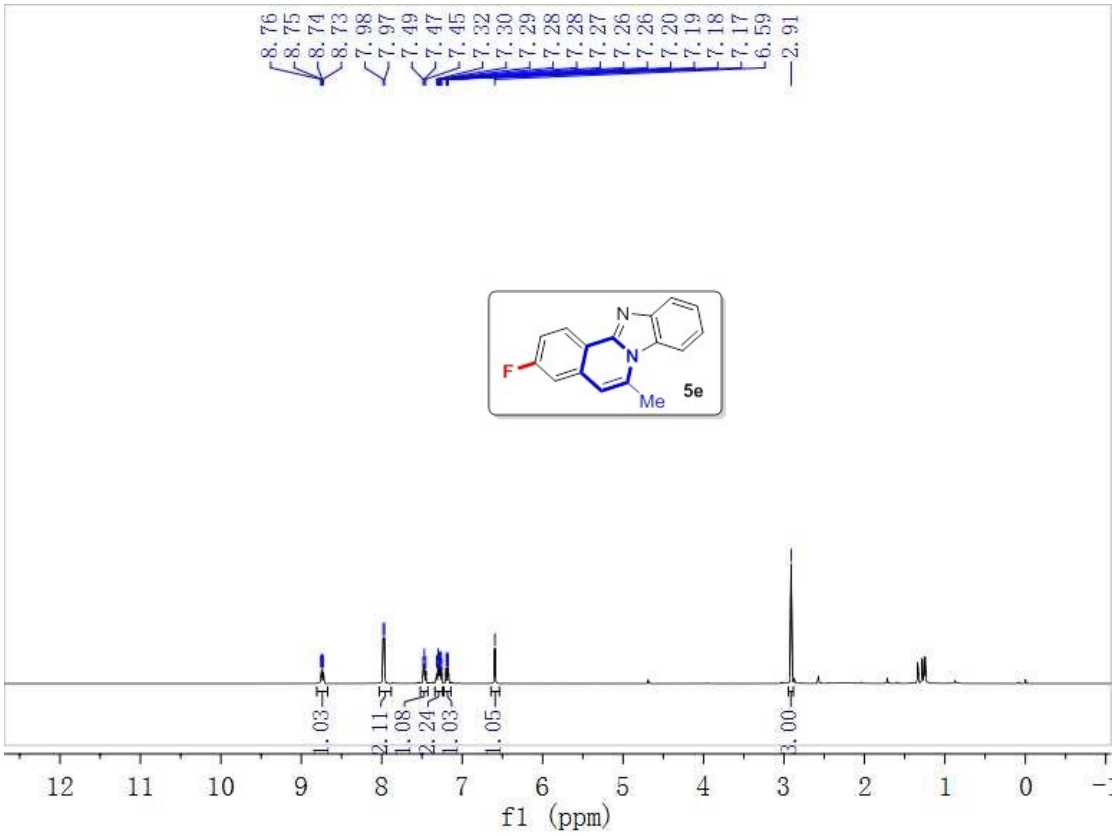
N
Me
5d
f1 (ppm)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7.30
7.29
7.28
7.28
7.27
7.26
7.26
7.20
7.19
7.18
7.17
6.59
2.91
N
F
N
Me
5e
1.03
2.11
1.08
2.24
1.03
1.05
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12
11
10
9
8
7
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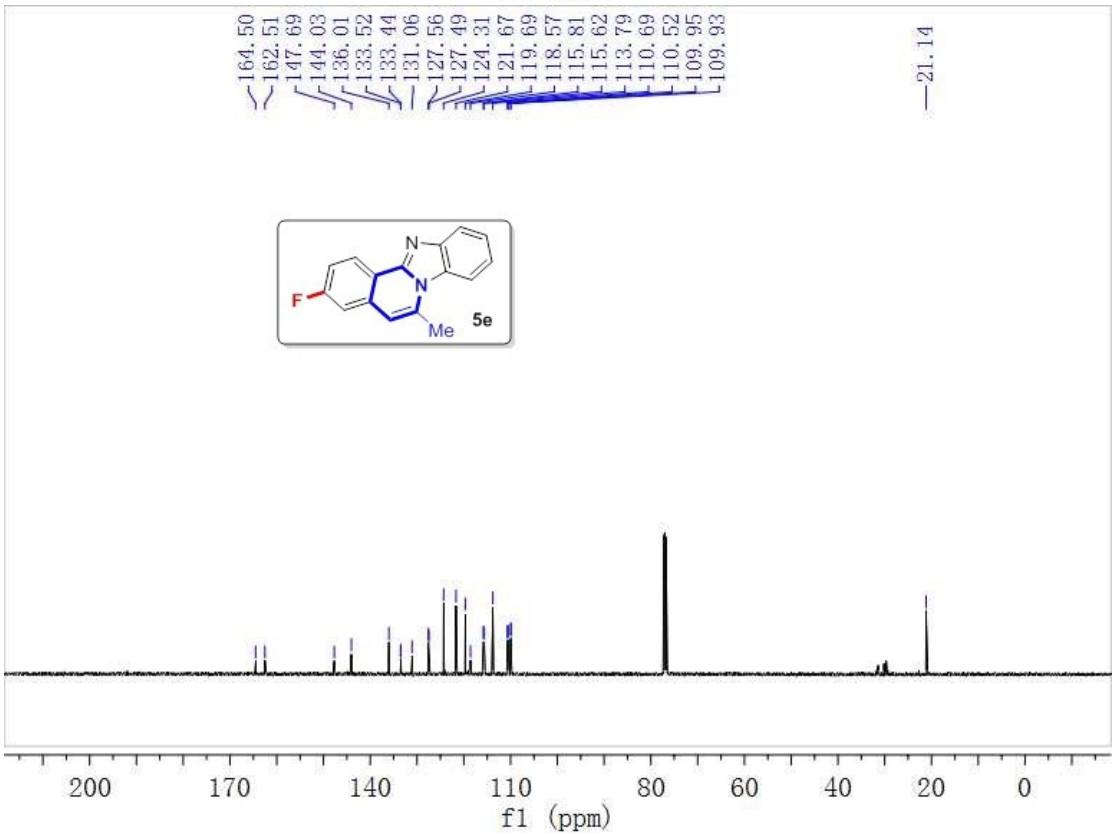
5
4
3
2
1
0
f1 (ppm)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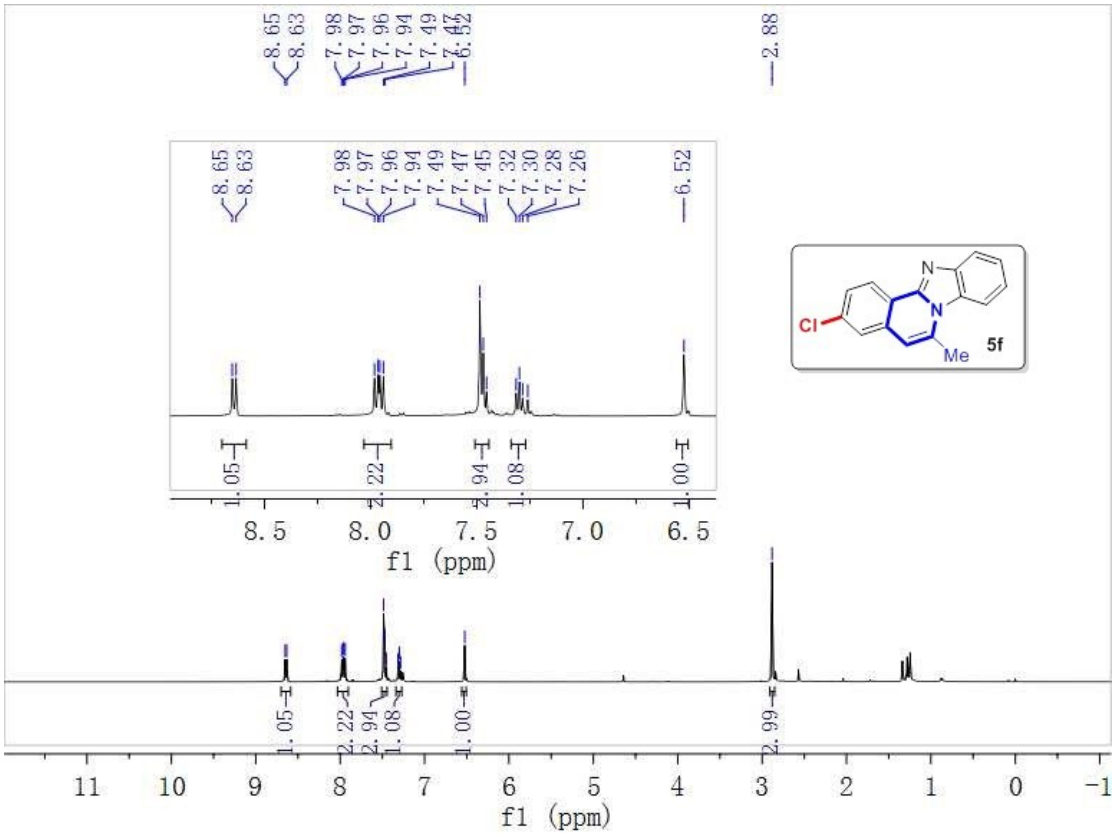
127.49
124.31
121.67
119.69
118.57
115.81
115.62
113.79
110.69
110.52
109.95
109.93
21.14
N
F
N
Me
5e
200
170
140
110
80
60
40
20
0
f1 (ppm)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7.47
6.52
2.88
7.45
7.32
7.30
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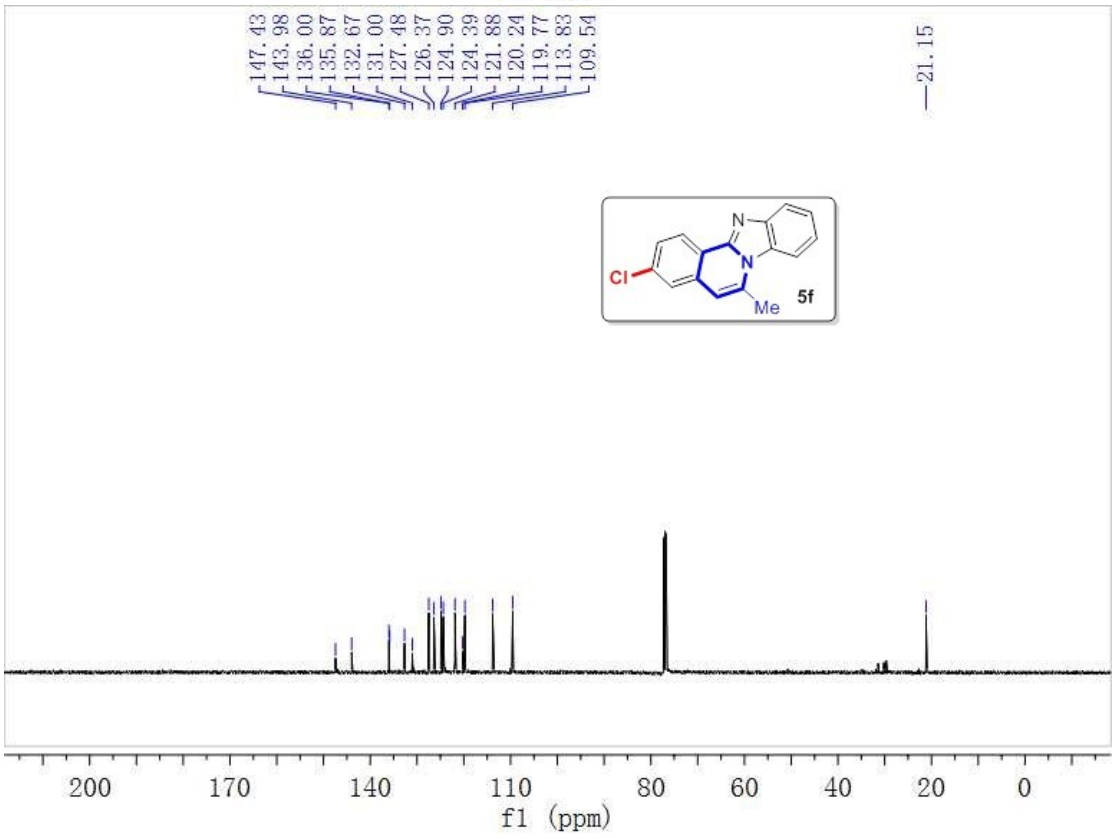
2.22
4.94
1.08
1.00
2.99
Cl
N
Me
5f
f1 (ppm)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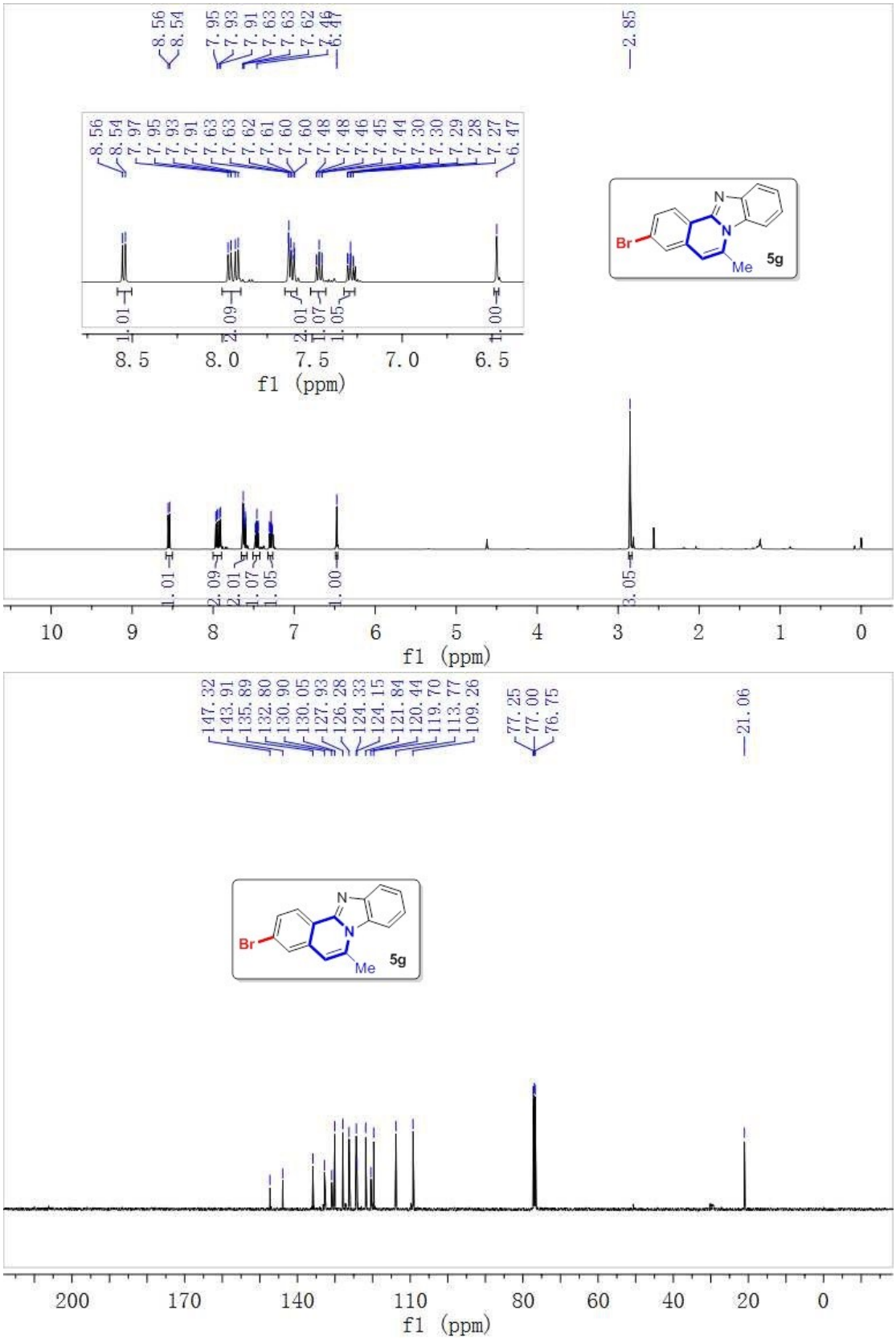
109.54
21.15
Cl
N
Me
5f
f1 (ppm)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6.47
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Br
N
N
Me
5g
f1 (ppm)
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143.91
135.89
132.80
130.90
130.05
127.93
126.28
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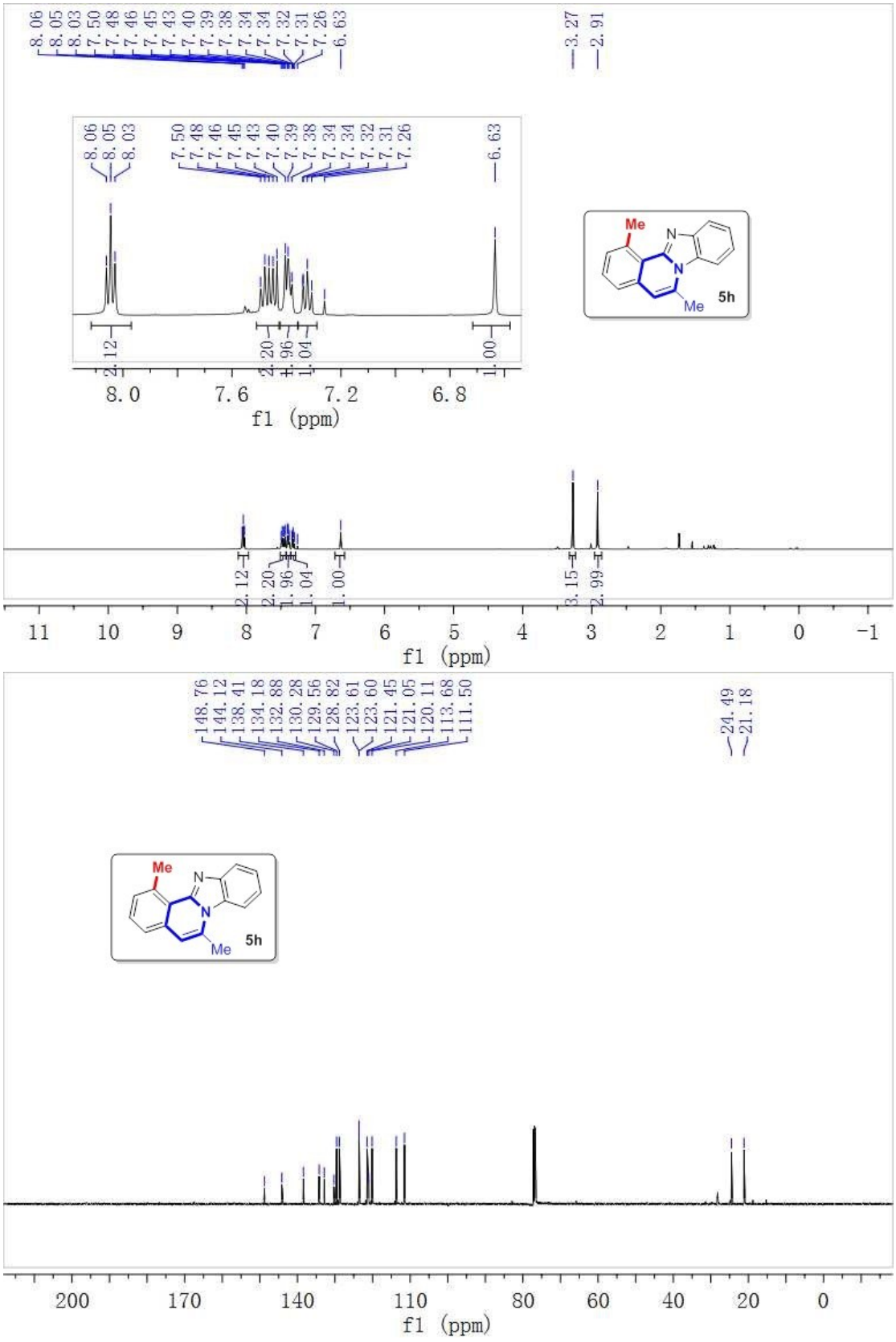
109.26
77.25
77.00
76.75
21.06
f1 (ppm)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7.38
7.34
7.34
7.32
7.31
7.26
6.63
3.27
2.91
Me
N
N
Me
5h
2.12
2.20
1.96
1.04
1.00
3.15
2.99
f1 (ppm)
148.76
144.12
138.41
134.18
132.88
130.28
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111.50
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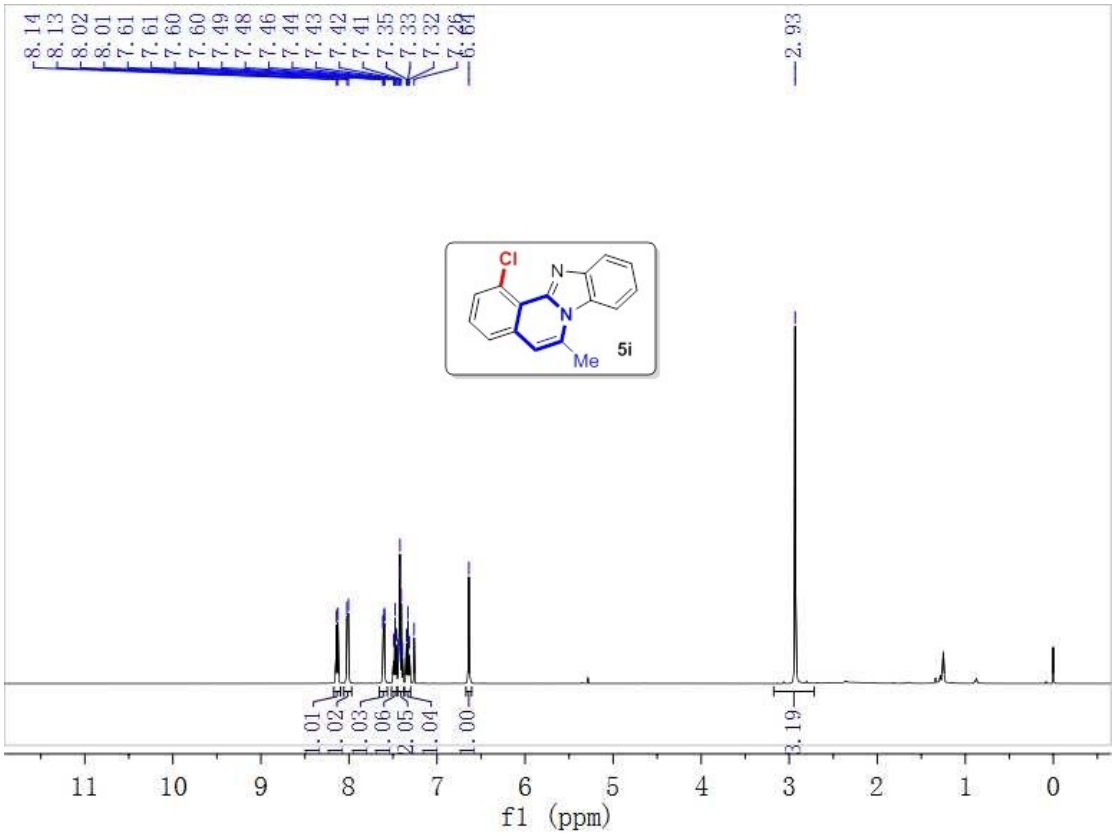
21.18
f1 (ppm)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7.43
7.42
7.41
7.35
7.33
7.32
2.93
Cl
N
N
Me
5i
1.01
1.02
1.03
1.06
2.05
1.04
1.00
3.19
11
10
9
8
7
6
5
4
3
2
1
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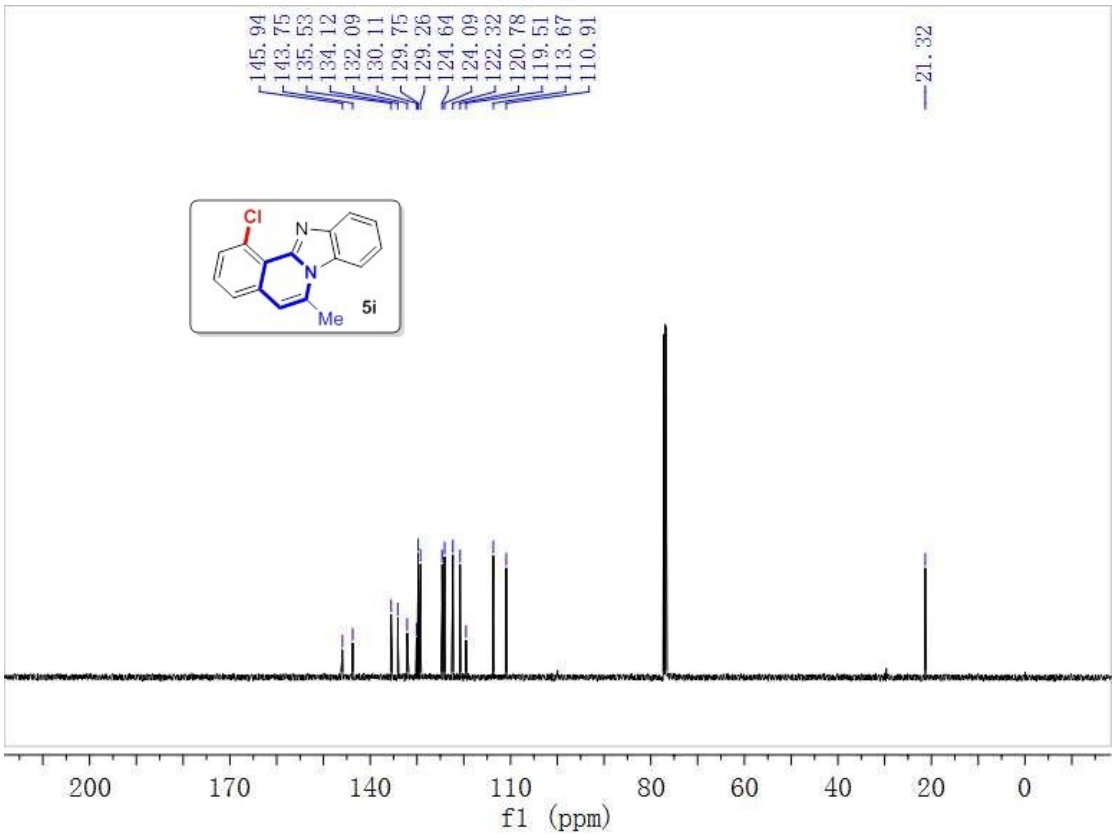
f1 (ppm)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124.64
124.09
122.32
120.78
119.51
113.67
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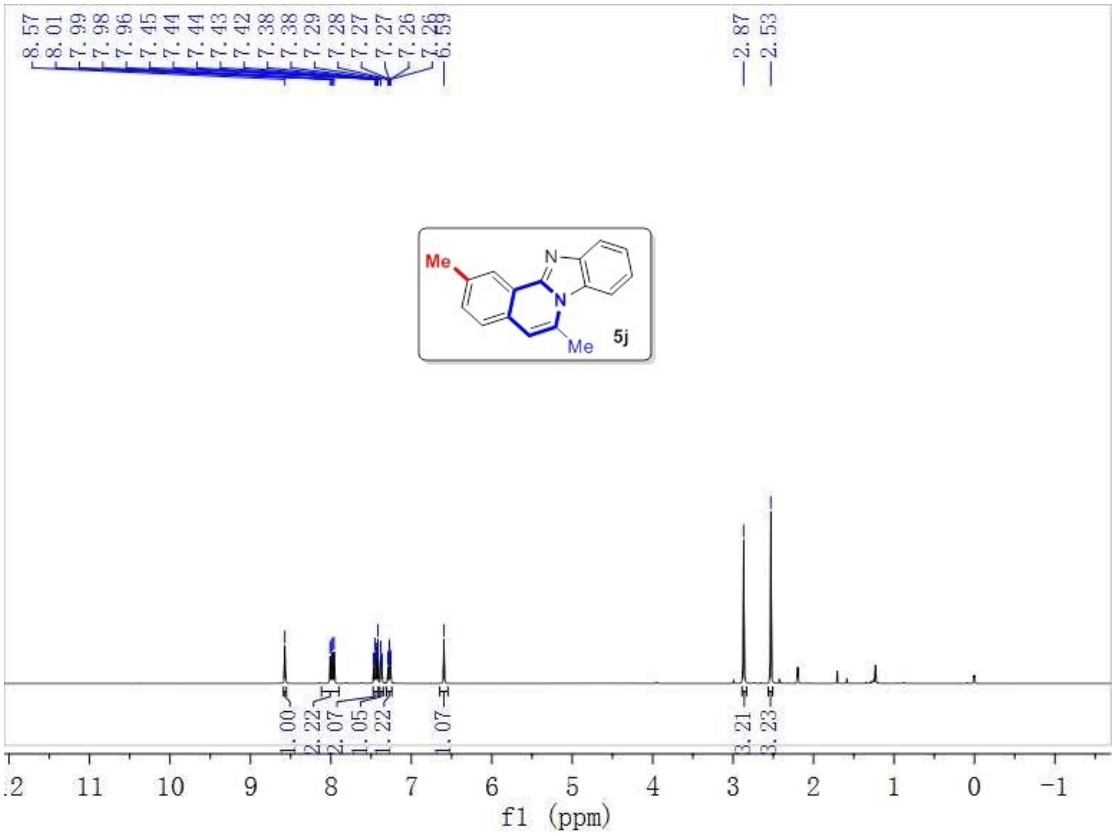
21.32
Cl
N
N
Me
5i
200
170
140
110
80
60
40
20
0
f1 (ppm)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7.38
7.29
7.28
7.27
7.27
7.26
7.26
6.59
2.87
2.53
Me
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N
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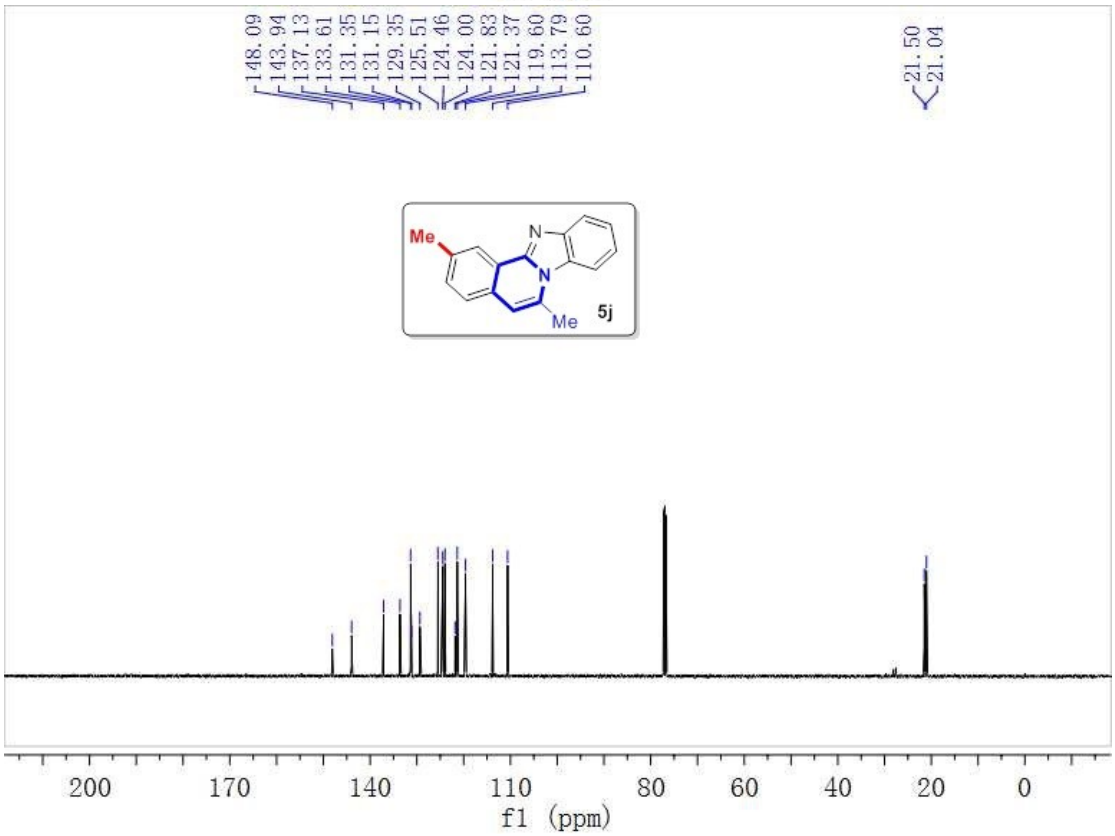
2.22
2.07
1.05
1.22
1.07
3.21
3.23
f1 (ppm)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129.35
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124.46
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113.79
110.60
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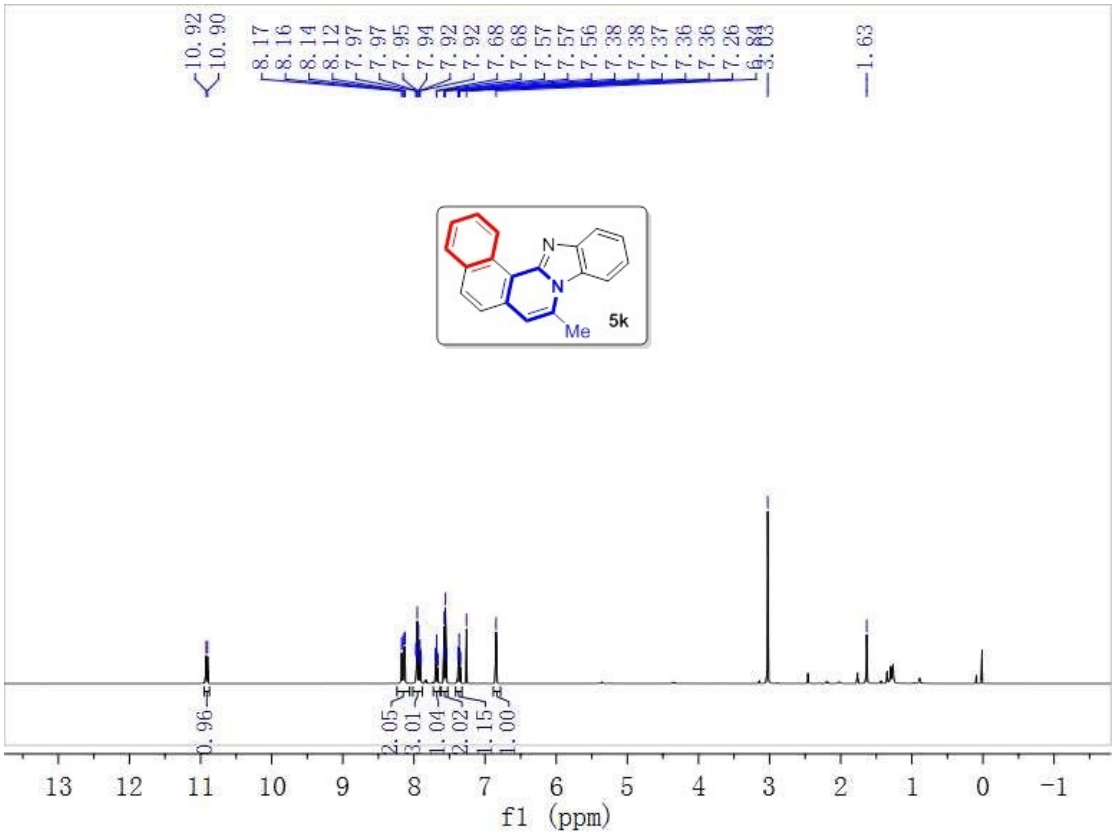
21.04
Me
N
N
Me
5j
f1 (ppm)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7.97
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7.68
7.57
7.57
7.56
7.38
7.38
7.37
7.36
7.36
7.26
1.63
N
N
Me
5k
0.96
2.05
3.01
1.04
2.02
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1.00
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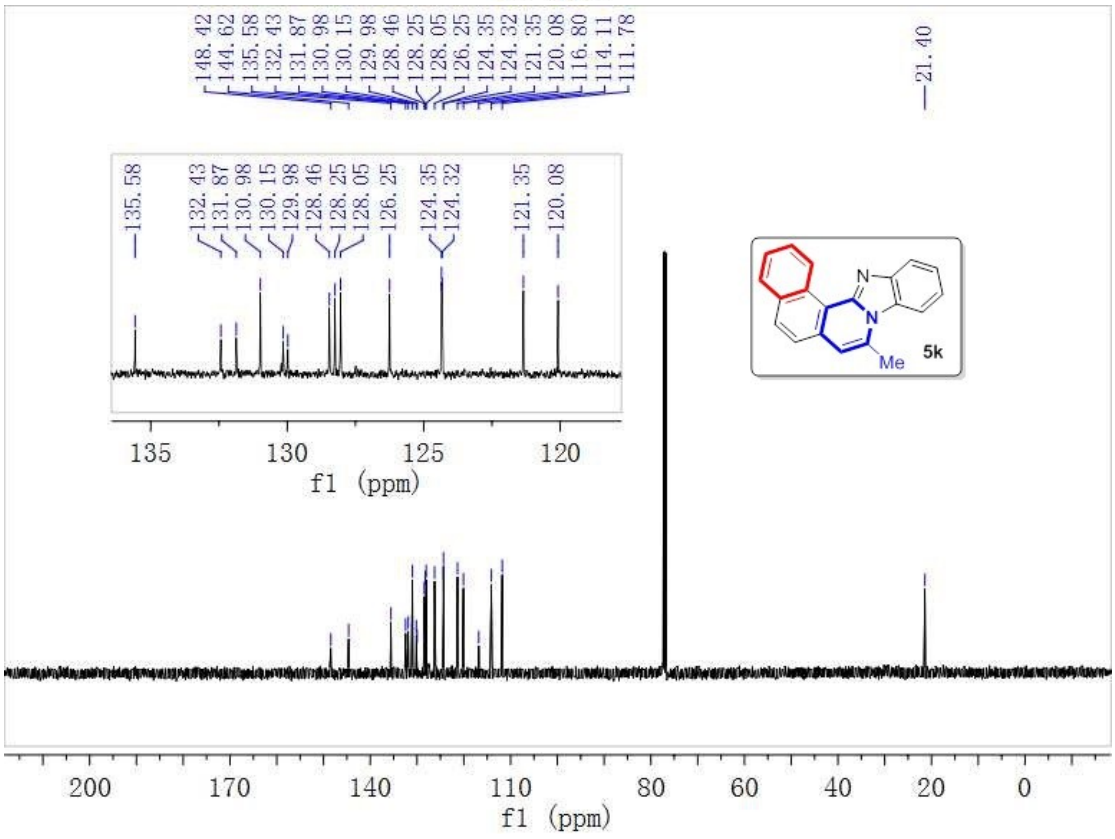
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)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124.32
121.35
120.08
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114.11
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132.43
131.87
130.98
130.15
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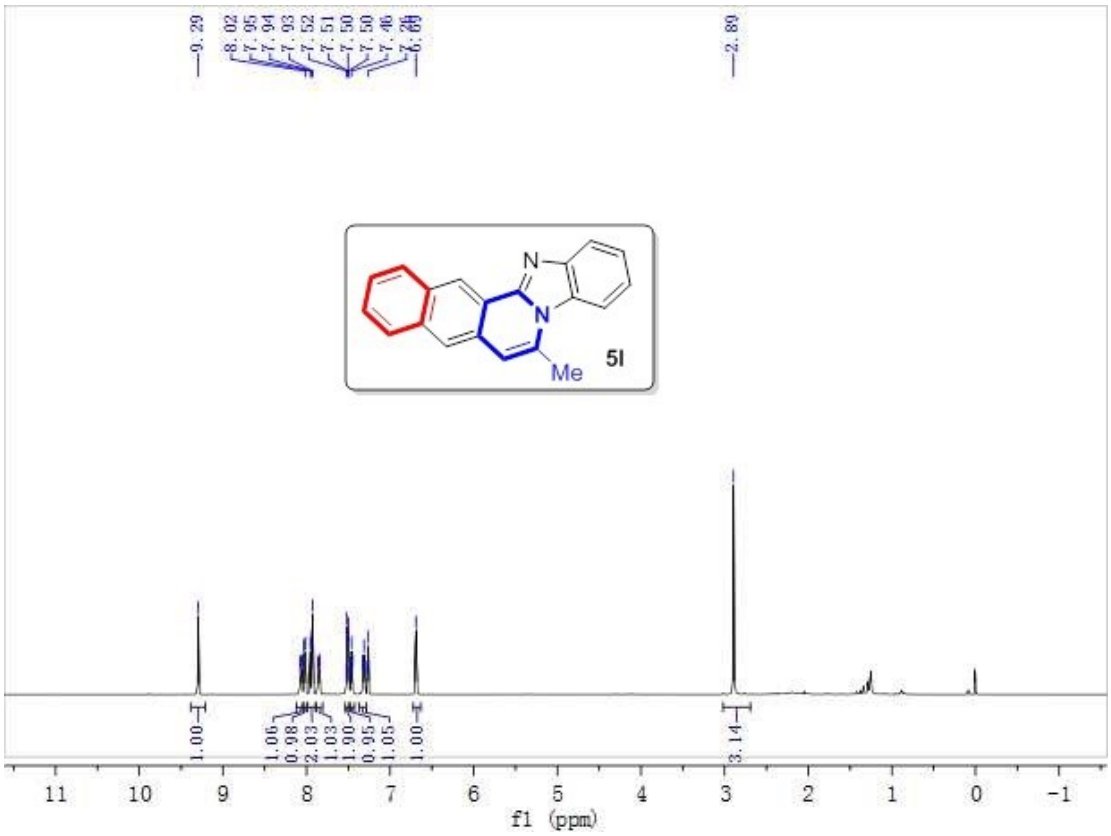
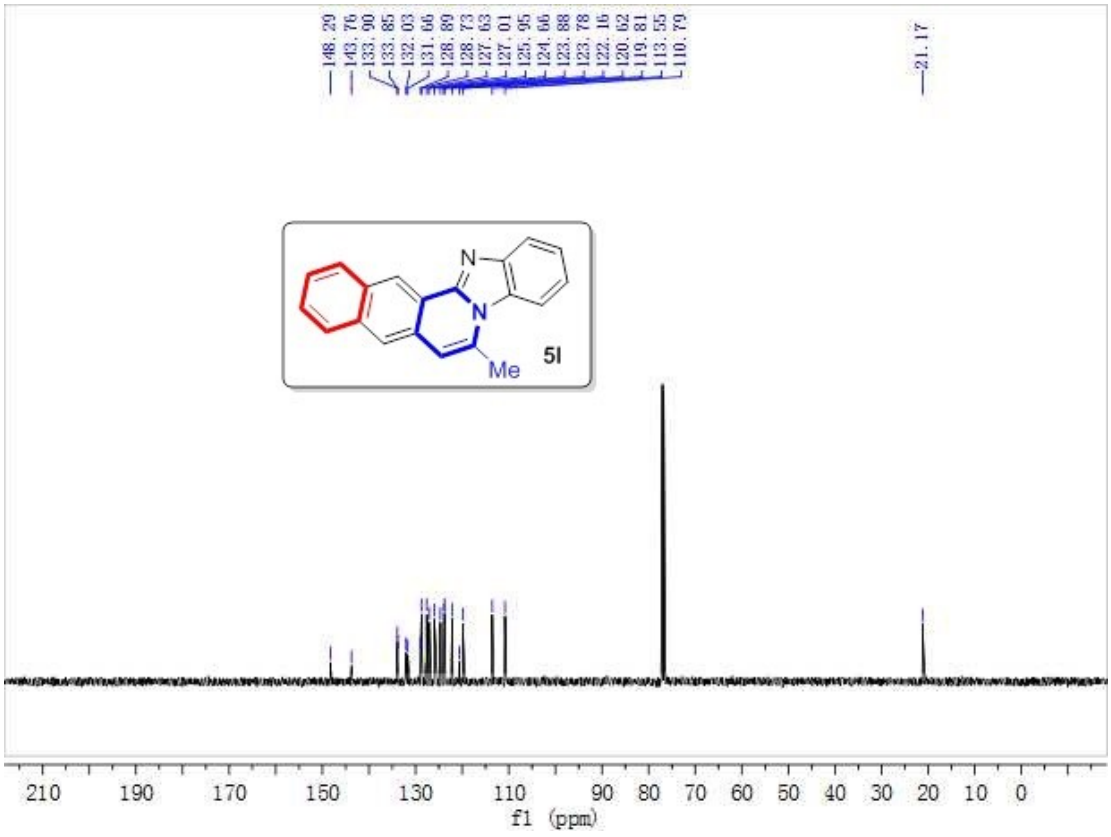
128.46
128.25
128.05
126.25
124.35
124.32
121.35
120.08
N
N
Me
5k
135
130
125
120
f1 (ppm)
200
170
140
110
80
60
40
20
0
f1 (ppm)


9.29
8.02
7.95
7.94
7.93
7.52
7.51
7.50
7.50
7.46
2.89
N
N
Me
5l
1.00
1.06
0.98
2.03
1.03
1.90
0.95
1.05
1.00
3.14
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)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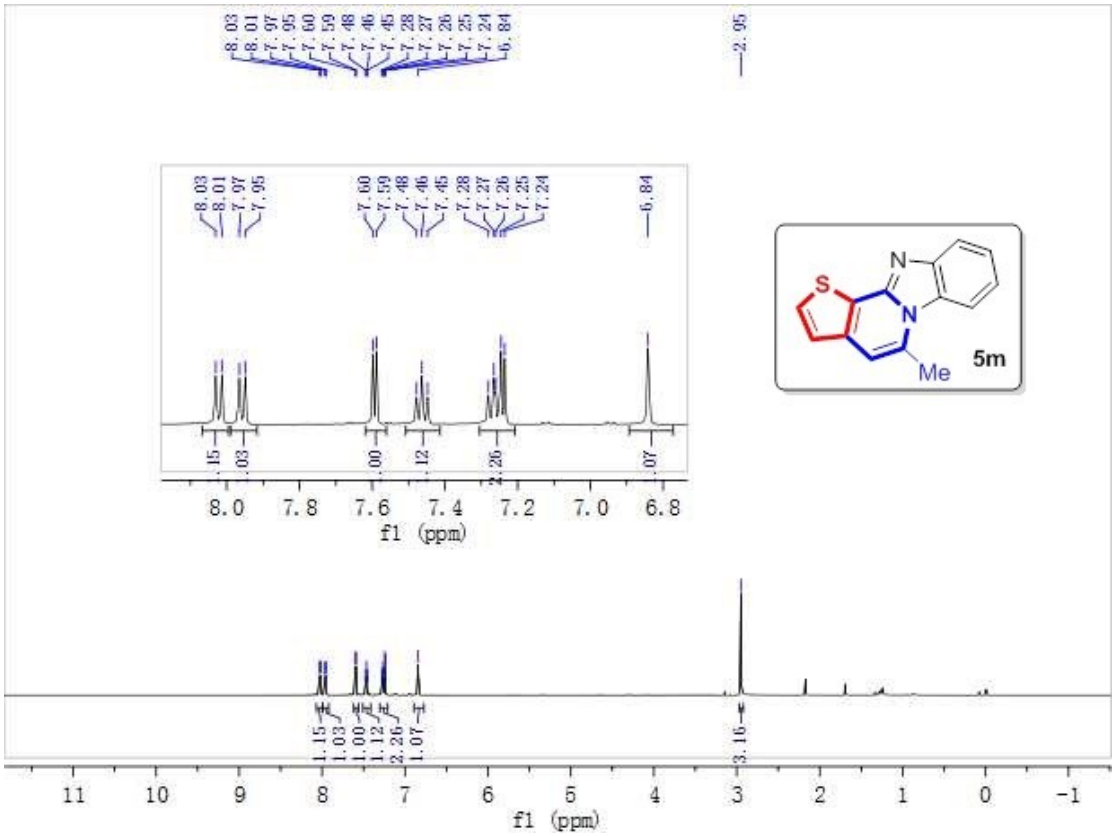
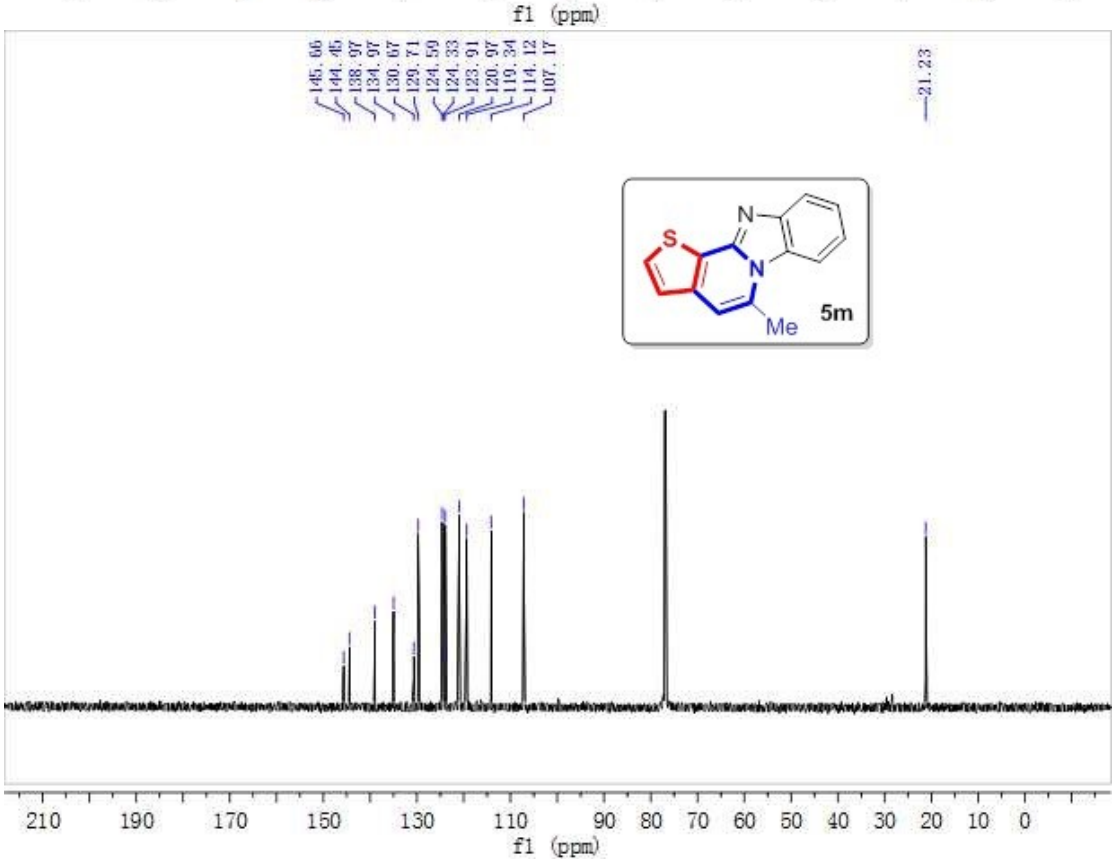
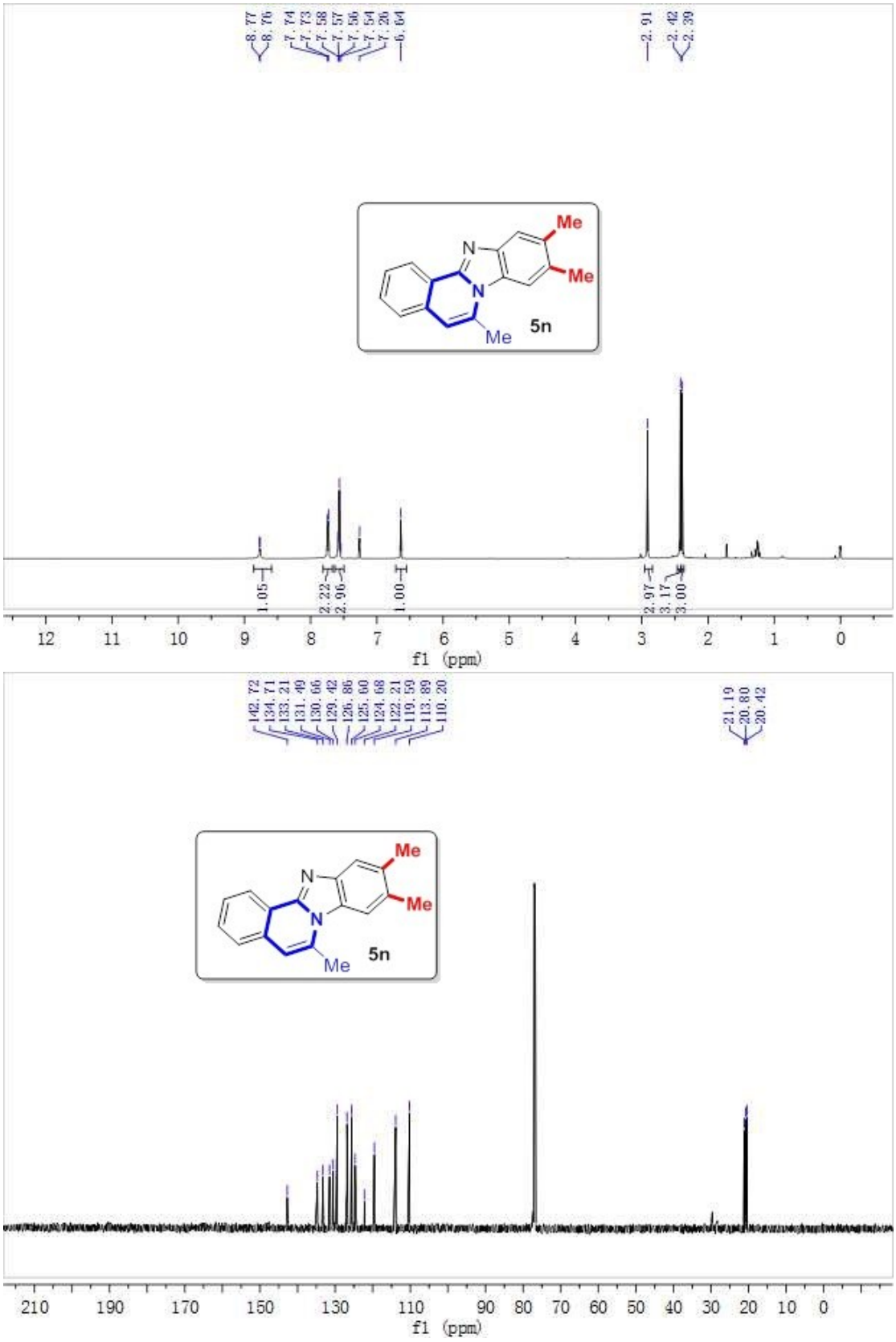
143.76
133.90
133.85
132.03
131.66
128.89
128.73
127.63
127.01
125.95
124.66
123.88
123.78
122.16
120.62
119.81
113.55
110.79
21.17
N
N
Me
5l
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.03
8.01
7.97
7.95
7.60
7.59
7.48
7.46
7.45
7.28
7.27
7.26
7.25
7.24
6.84
2.95
5m
Me
f1 (ppm)
1.15
1.03
1.00
1.12
2.26
1.07
3.16


145.66
144.45
138.97
134.97
130.67
129.71
124.59
124.33
123.91
120.97
119.34
114.12
107.17
21.23
5m
Me
f1 (ppm)


8.77
8.76
7.74
7.73
7.58
7.57
7.56
7.54
7.26
6.64
2.91
2.42
2.39
Me
Me
N
N
Me
5n
1.05
2.22
2.96
1.00
2.97
3.17
3.00
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)
142.72
134.71
133.21
131.49
130.66
129.42
126.86
125.60
124.68
122.21
119.59
113.89
110.20
21.19
20.80
20.42
Me
Me
N
N
Me
5n
210
190
170
150
130
110
90
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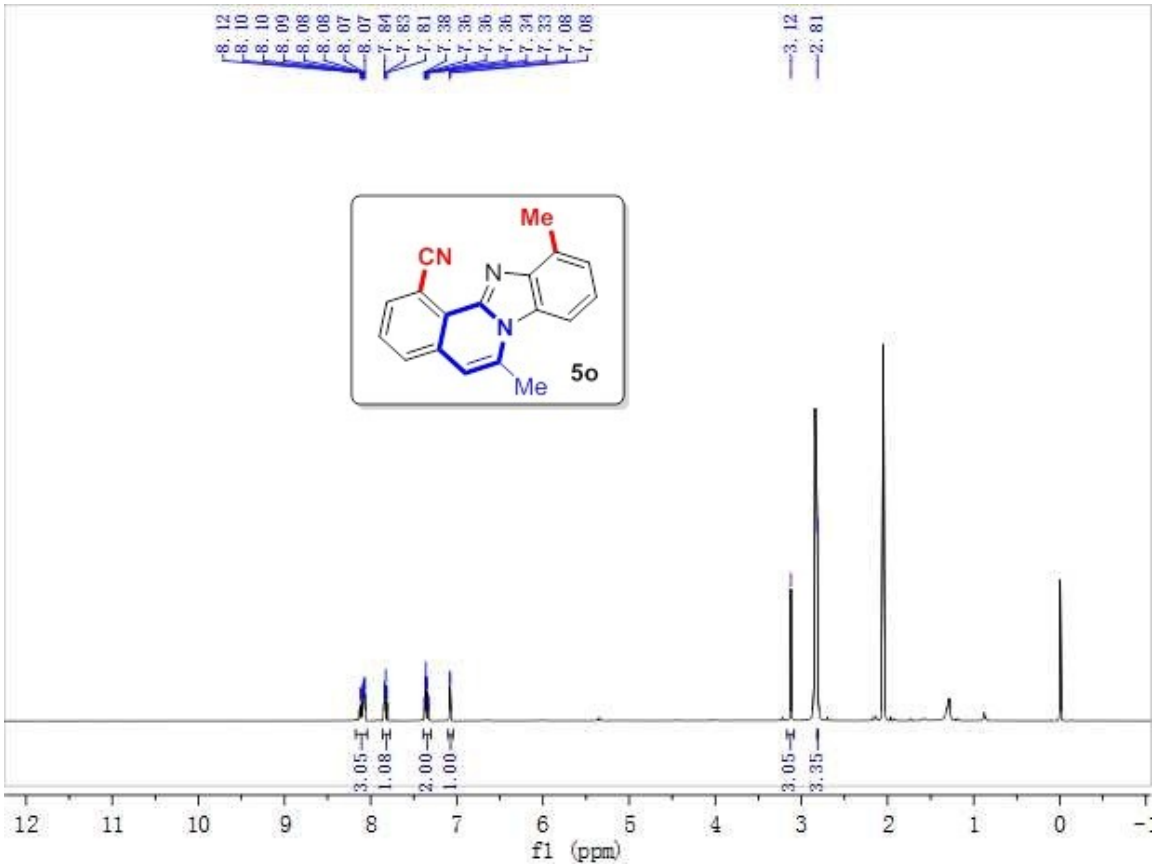
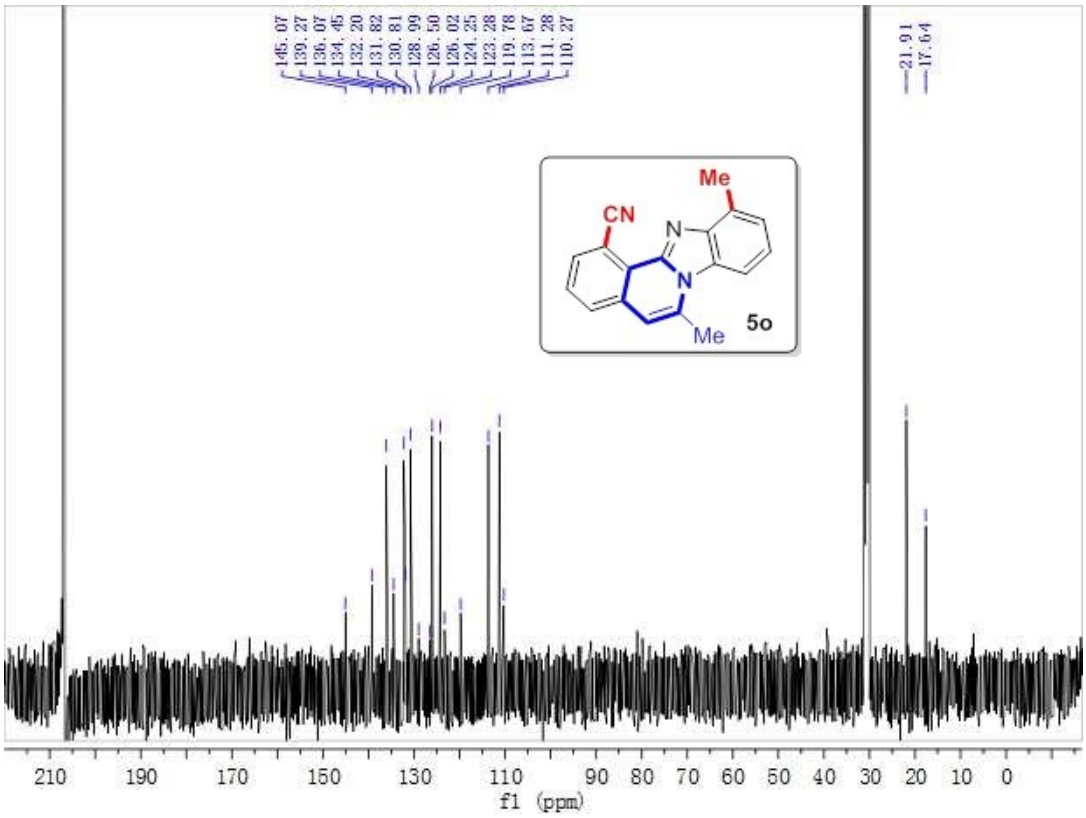
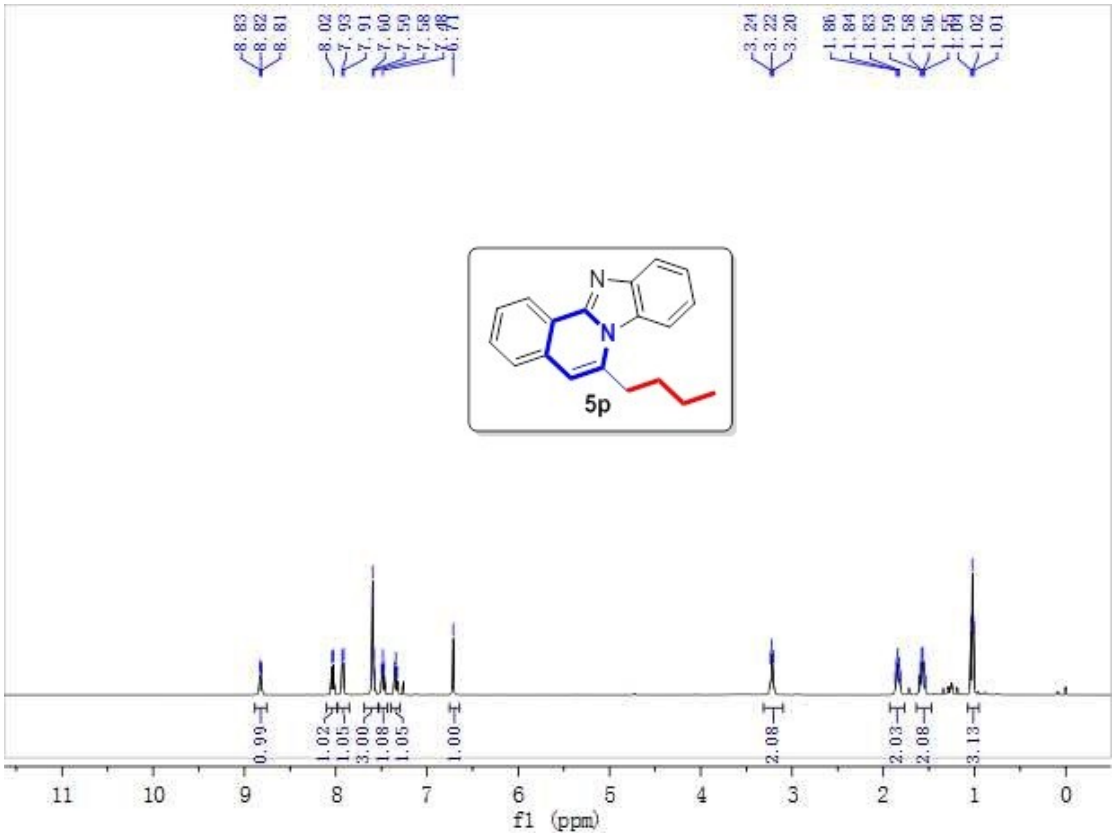
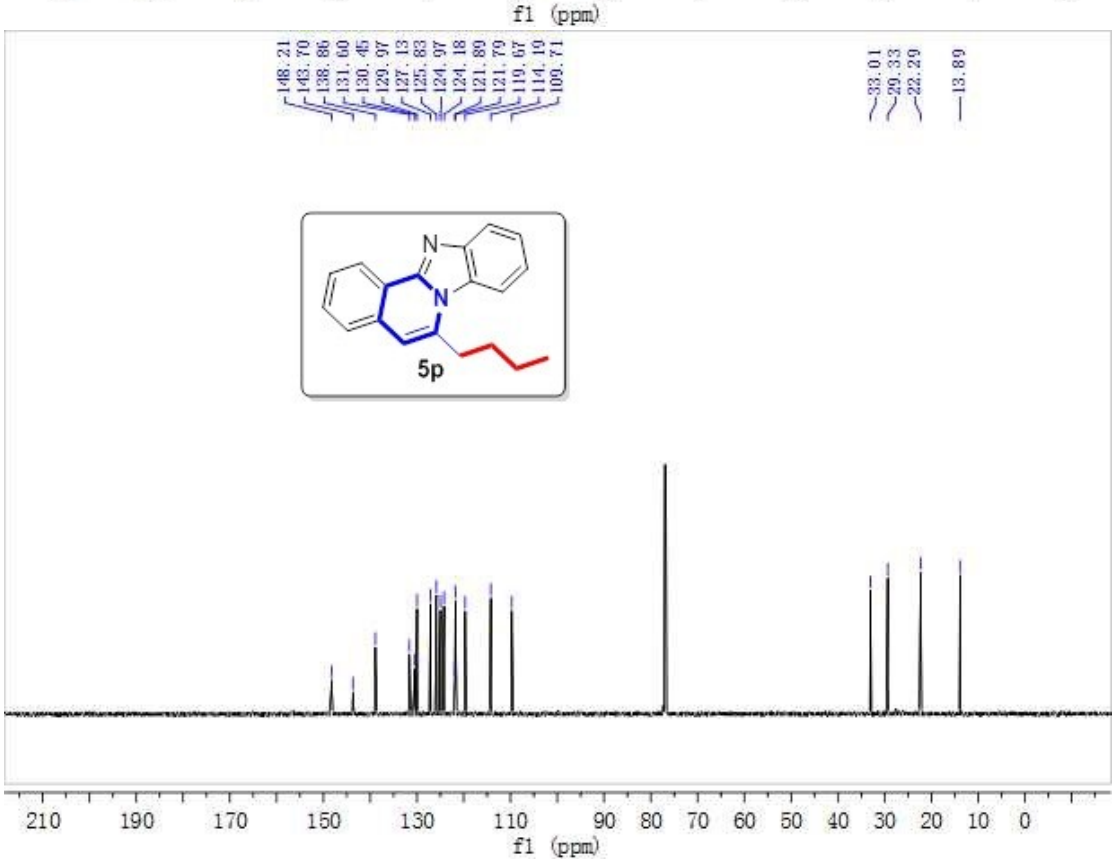
70
60
50
40
30
20
10
0
f1 (ppm)


8.12
8.10
8.10
8.09
8.08
8.08
8.07
8.07
7.84
7.83
7.81
7.38
7.36
7.36
7.36
7.34
7.33
7.08
7.08
3.12
2.81
Me
CN
N
N
Me
5o
3.05
1.08
2.00
1.00
3.05
3.35
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


145.07
139.27
136.07
134.45
132.20
131.82
130.81
128.99
126.50
126.02
124.25
123.28
119.78
113.67
111.28
110.27
21.91
17.64
Me
CN
N
N
Me
5o
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.83
8.82
8.81
8.02
7.93
7.91
7.60
7.59
7.58
3.24
3.22
3.20
1.86
1.84
1.83
1.59
1.58
1.56
1.02
1.01
N
N
5p
0.99
1.02
1.05
3.00
1.08
1.05
1.00
2.08
2.03
2.08
3.13
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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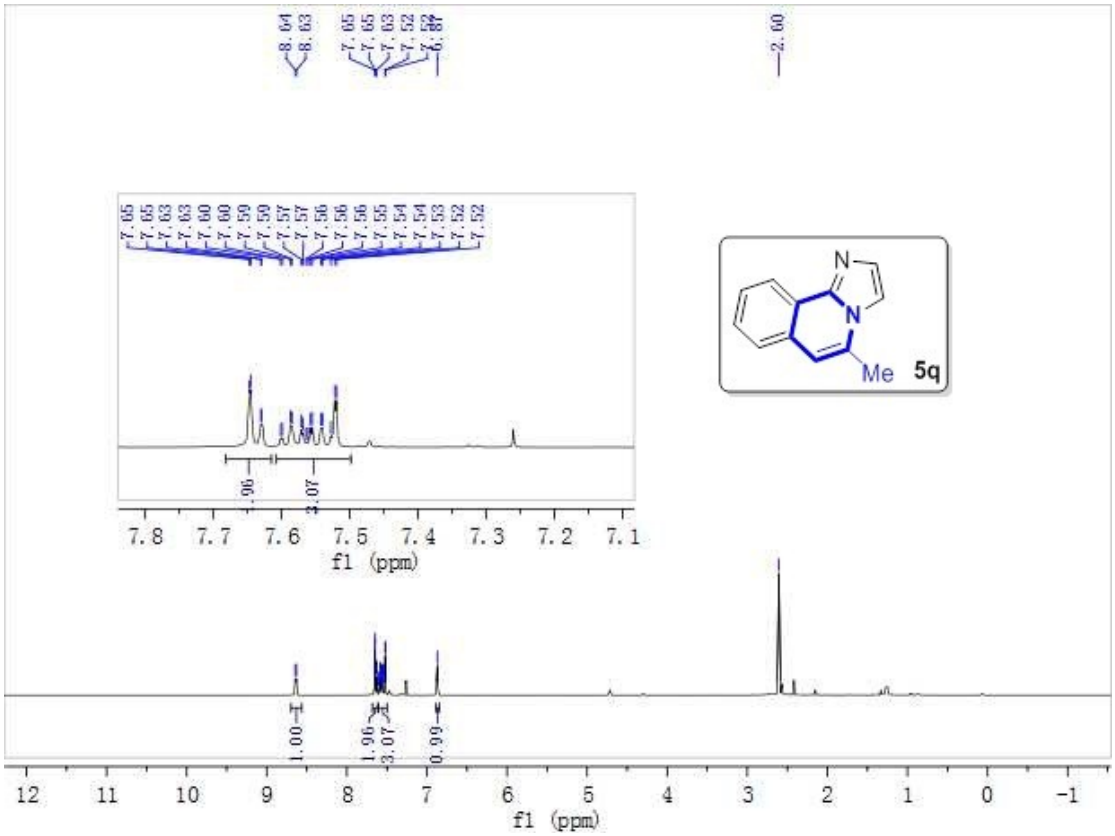
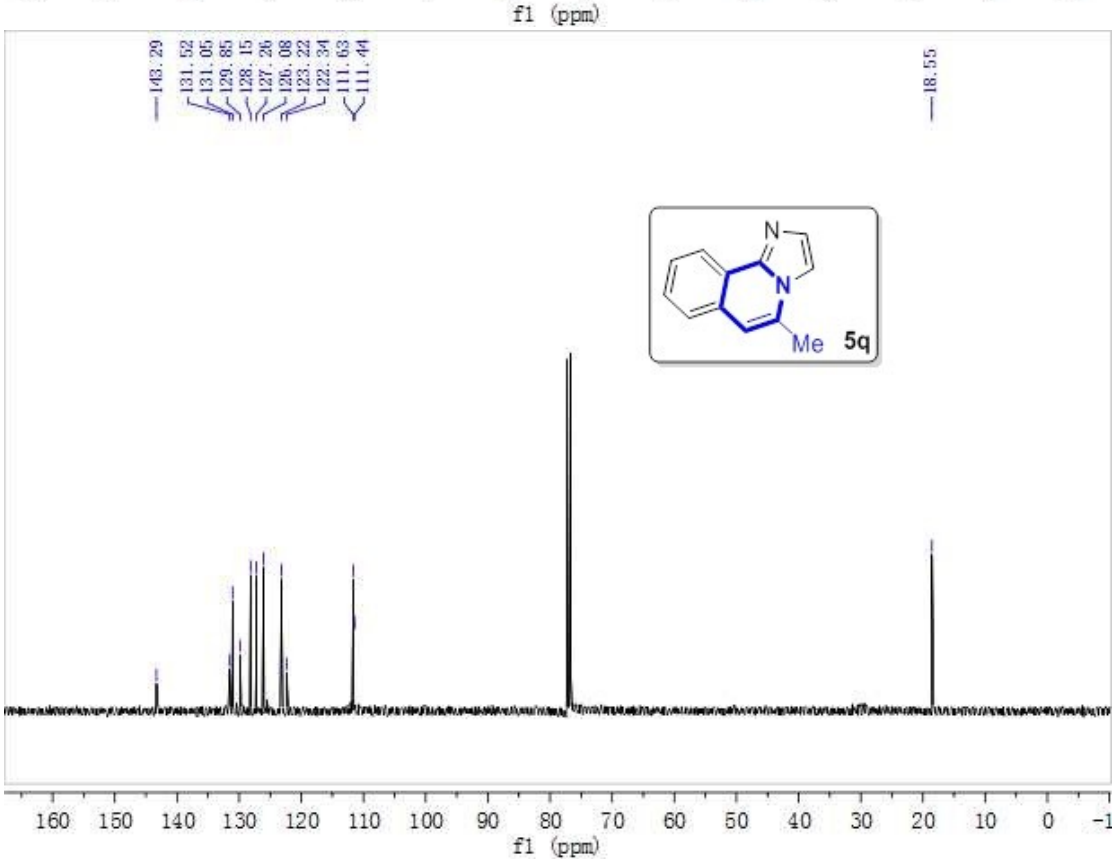
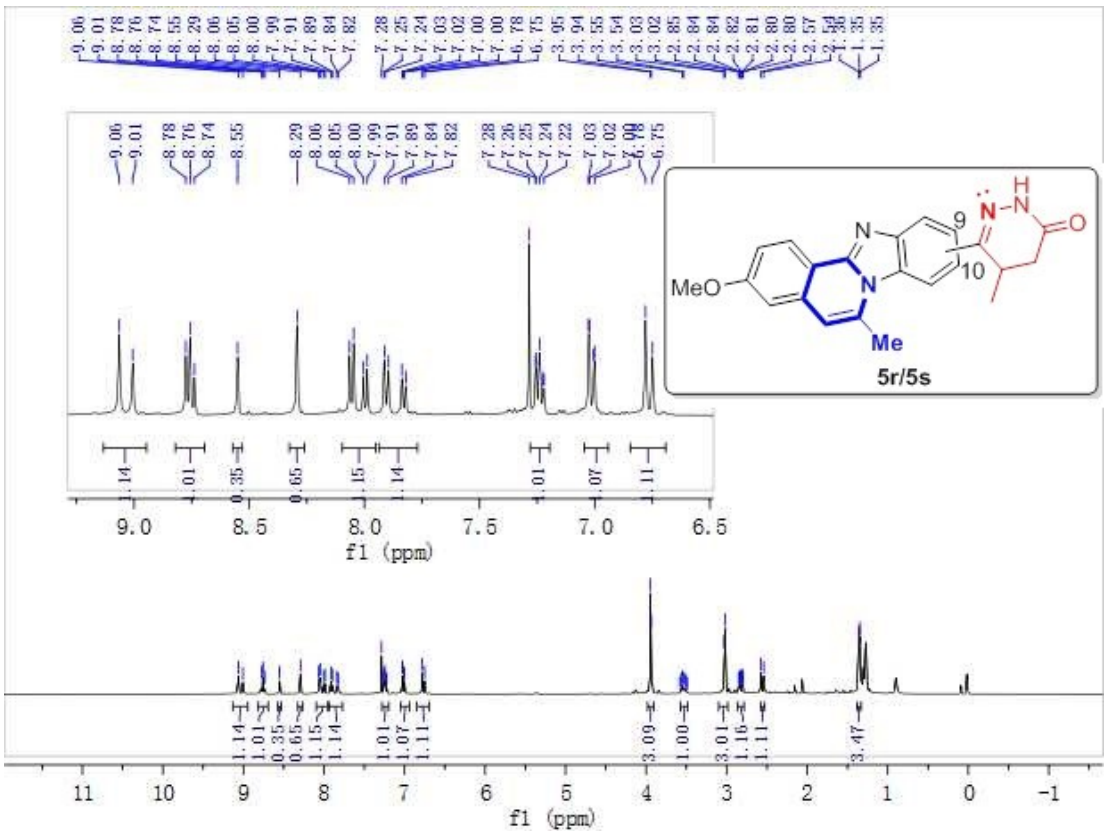
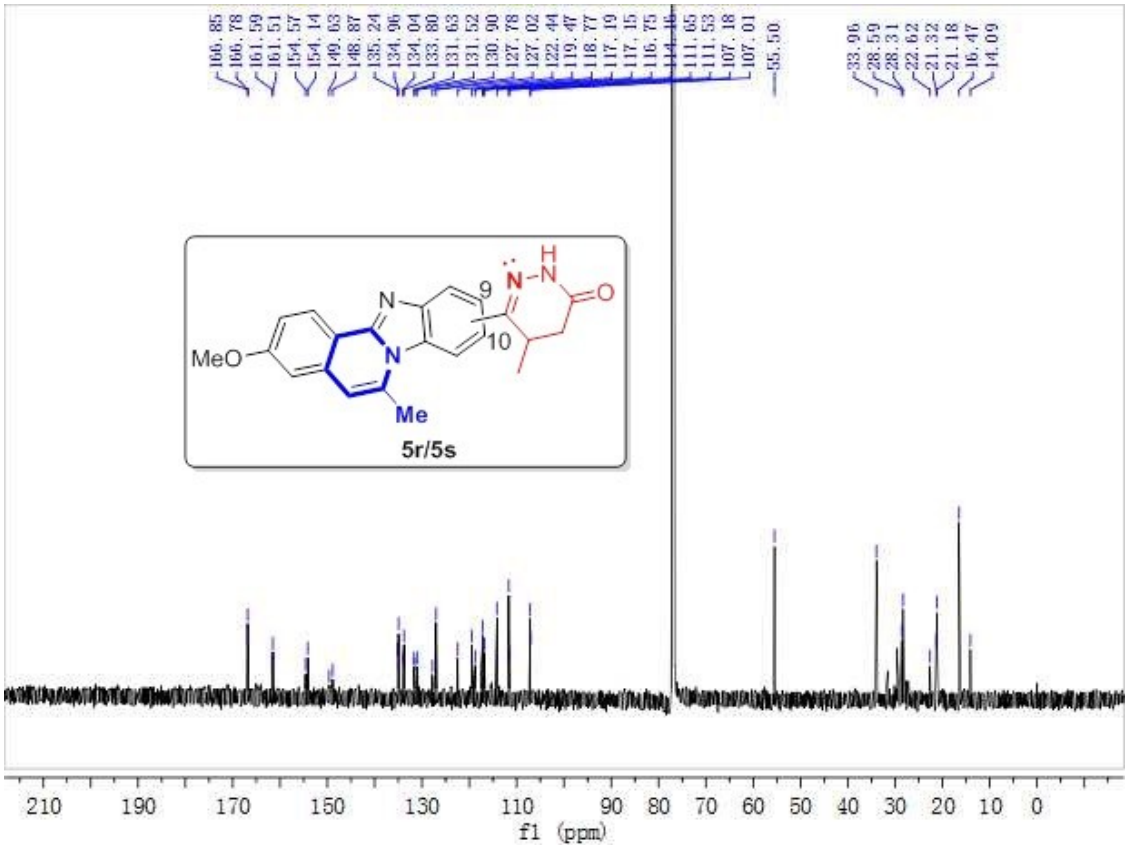
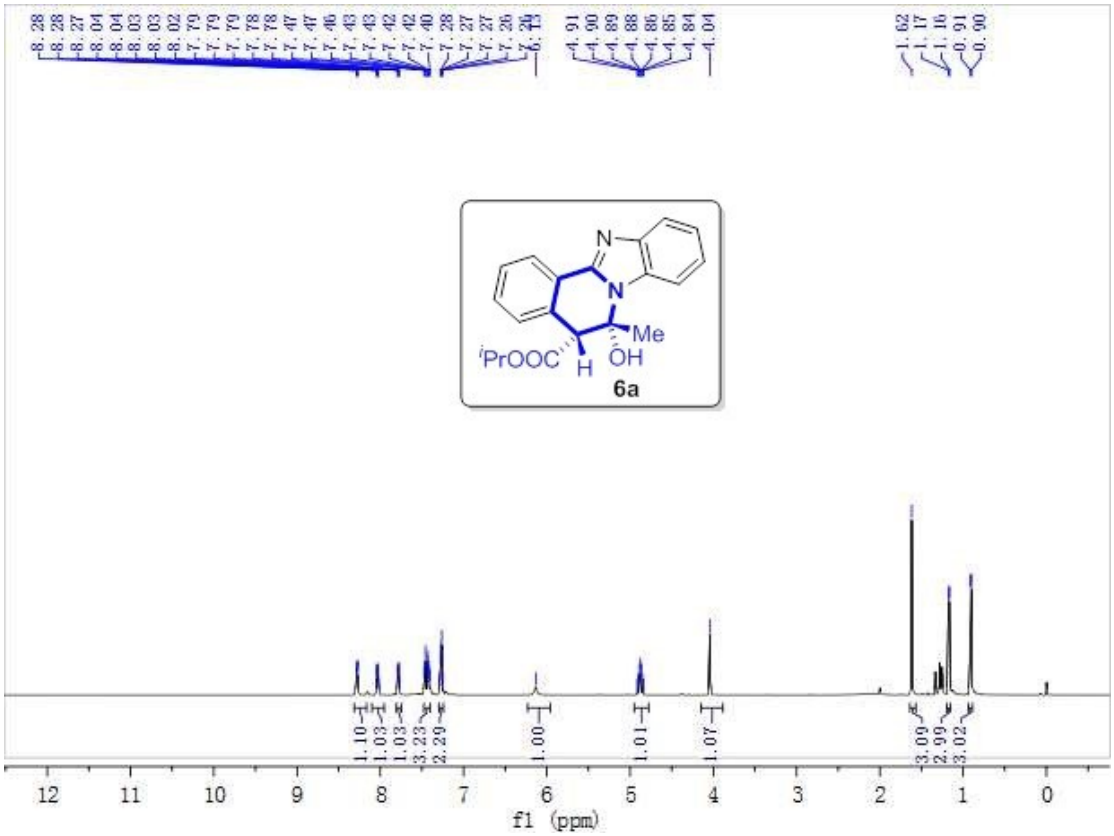
143.70
138.86
131.60
130.45
129.97
127.13
125.83
124.97
124.18
121.89
121.79
119.67
114.19
109.71
33.01
29.33
22.29
13.89
N
N
5p
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.64
8.63
7.65
7.65
7.63
7.52
2.60
7.65
7.65
7.63
7.63
7.60
7.60
7.59
7.59
7.57
7.57
7.56
7.56
7.56
7.55
7.54
7.54
7.53
7.52
7.52
.96
3.07
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
N
N
Me
5q
1.00
1.96
3.07
0.99
12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


143.29
131.52
131.05
129.85
128.15
127.26
126.08
123.22
122.34
111.63
111.44
18.55
N
N
Me
5q
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


MeO
Me
5r/5s
f1 (ppm)


MeO
Me
5r/5s
f1 (ppm)


8.28
8.28
8.27
8.04
8.04
8.03
8.03
8.02
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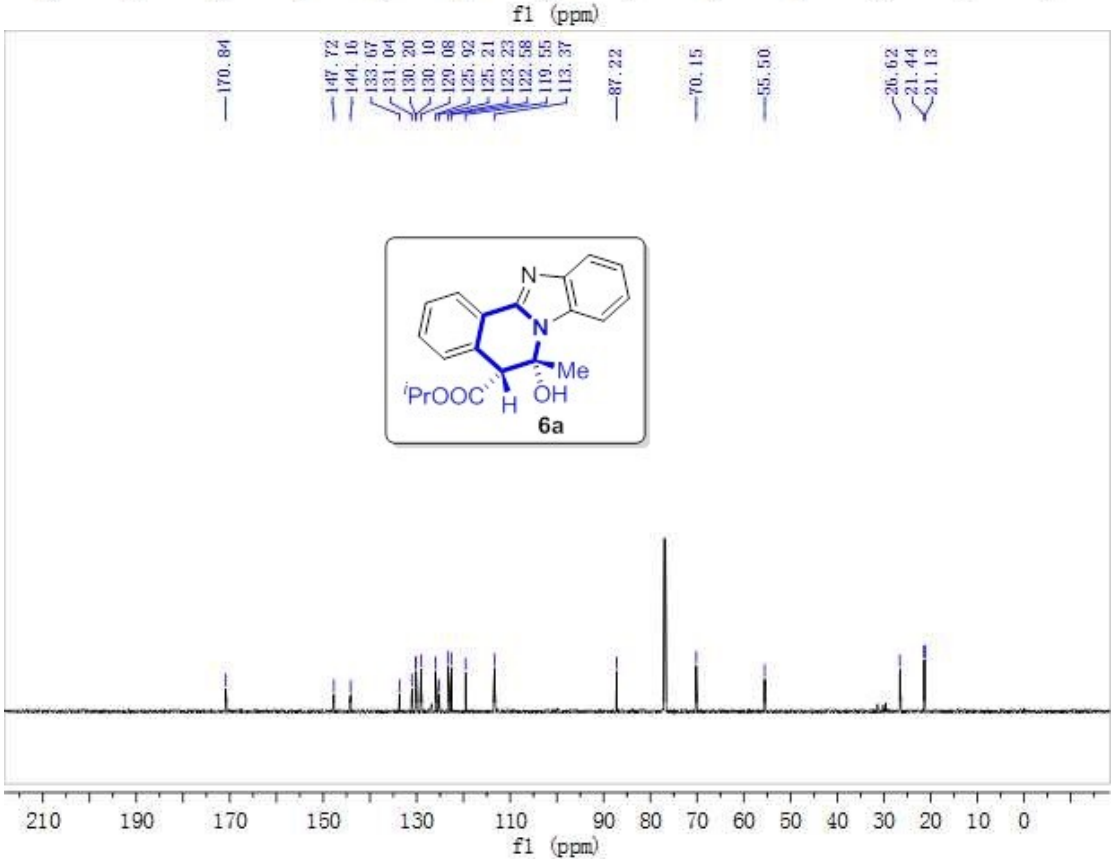
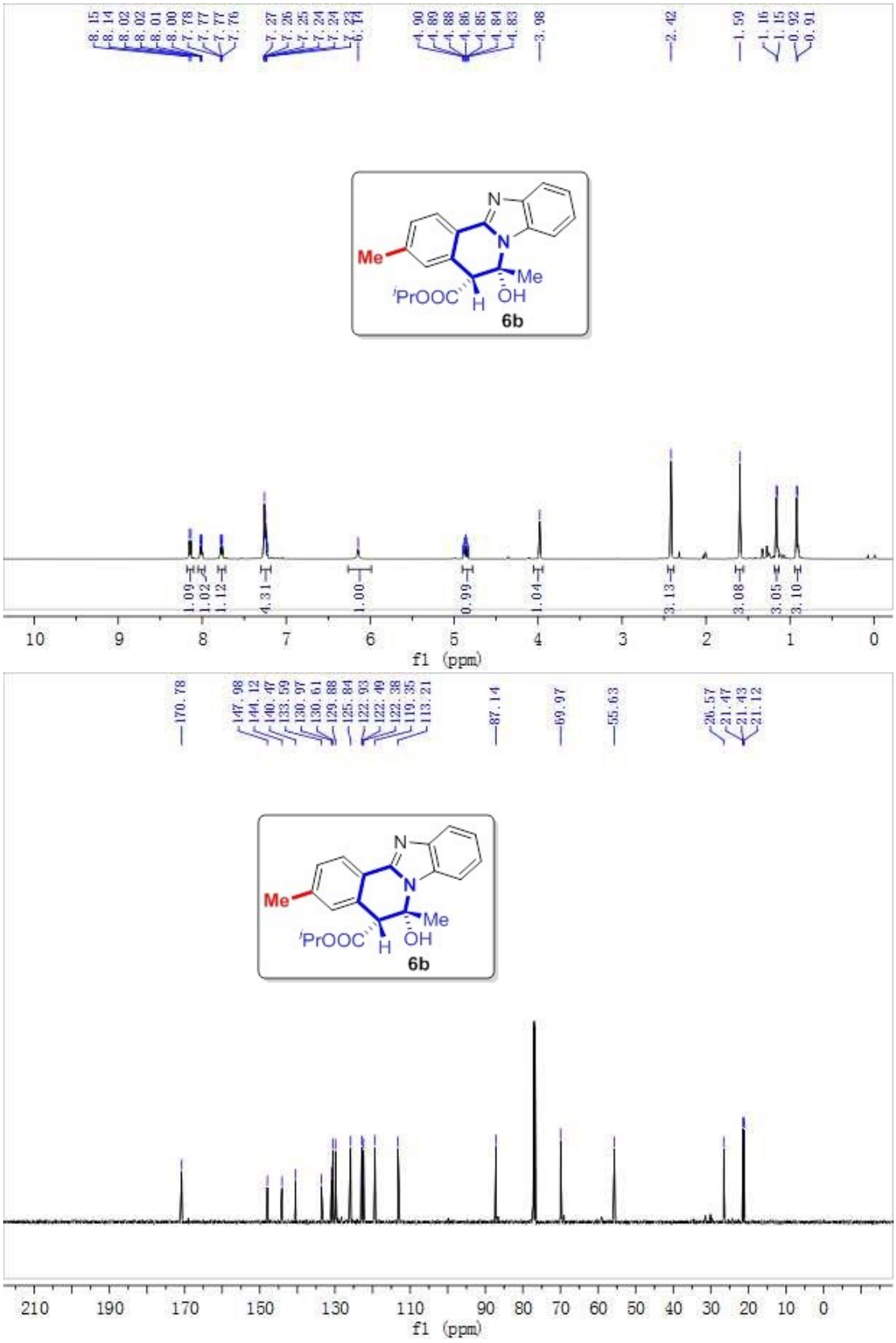
7.79
7.79
7.78
7.78
7.47
7.47
7.46
7.43
7.43
7.42
7.42
7.40
7.28
7.27
7.27
7.26
7.25
6.13
4.91
4.90
4.89
4.88
4.86
4.85
4.84
4.04
1.62
1.17
1.16
0.91
0.90
N
N
Me
iPrOOC
H
OH
6a
1.10
1.03
1.03
3.23
2.29
1.00
1.01
1.07
3.09
2.99
3.02
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


170.84
147.72
144.16
133.67
131.04
130.20
130.10
129.08
125.92
125.21
123.23
122.58
119.55
113.37
87.22
70.15
55.50
26.62
21.44
21.13
N
N
Me
iPrOOC
H
OH
6a
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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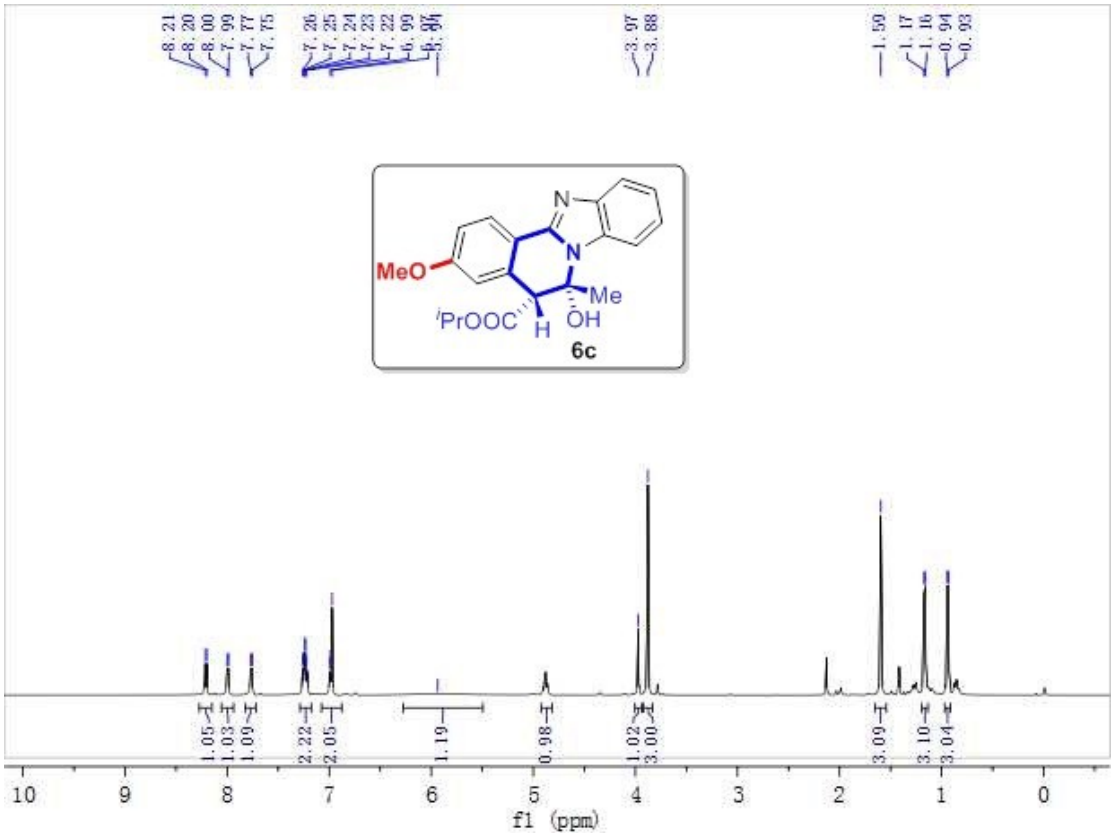
8.14
8.02
8.02
8.01
8.00
7.78
7.77
7.77
7.76
7.27
7.26
7.25
7.24
7.24
7.23
6.14
4.90
4.89
4.88
4.86
4.85
4.84
4.83
3.98
2.42
1.59
1.16
1.15
0.92
0.91
N
N
Me
Me
iPrOOC
H
OH
6b
1.09
1.02
1.12
4.31
1.00
0.99
1.04
3.13
3.08
3.05
3.10
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)
170.78
147.98
144.12
140.47
133.59
130.97
130.61
129.88
125.84
122.93
122.49
122.38
119.35
113.21
87.14
69.97
55.63
26.57
21.47
21.43
21.12
N
N
Me
Me
iPrOOC
H
OH
6b
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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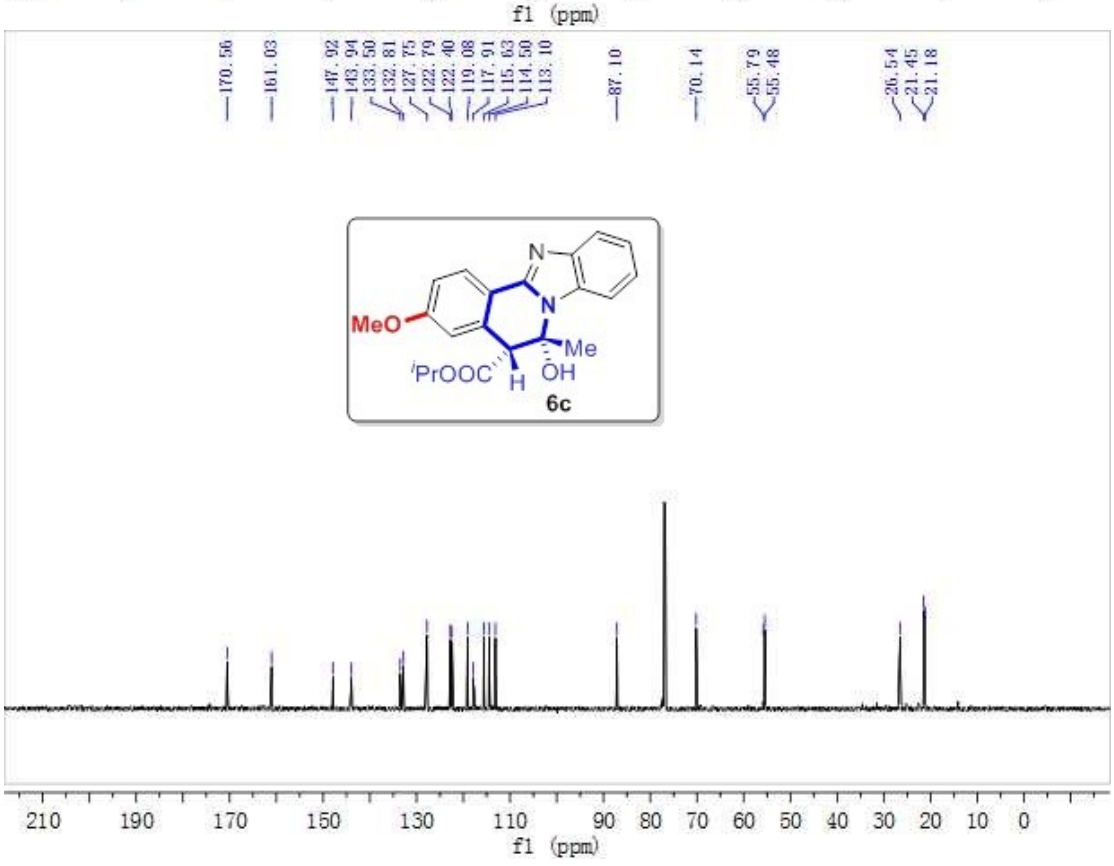
7.75
7.26
7.25
7.24
7.23
7.22
6.99
3.97
3.88
1.59
1.17
1.16
0.94
0.93
MeO
N
N
Me
OH
H
iPrOOC
6c
1.05
1.03
1.09
2.22
2.05
1.19
0.98
1.02
3.00
3.09
3.10
3.04
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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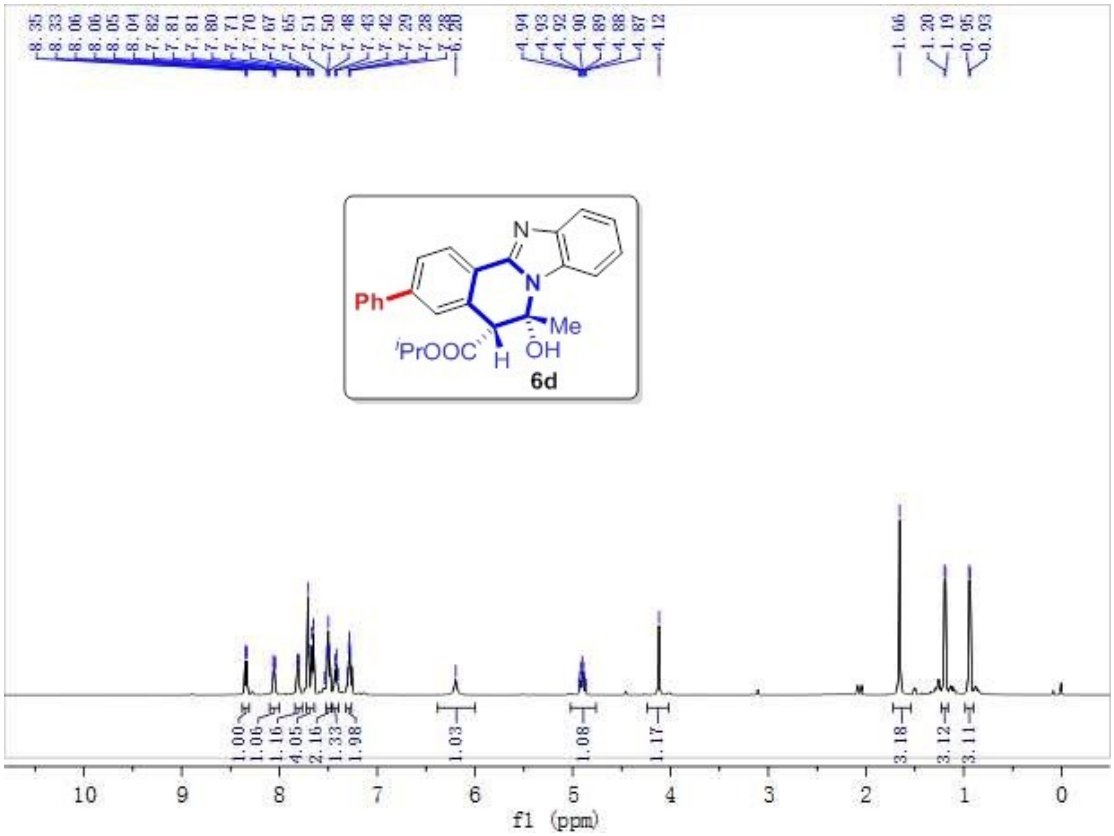
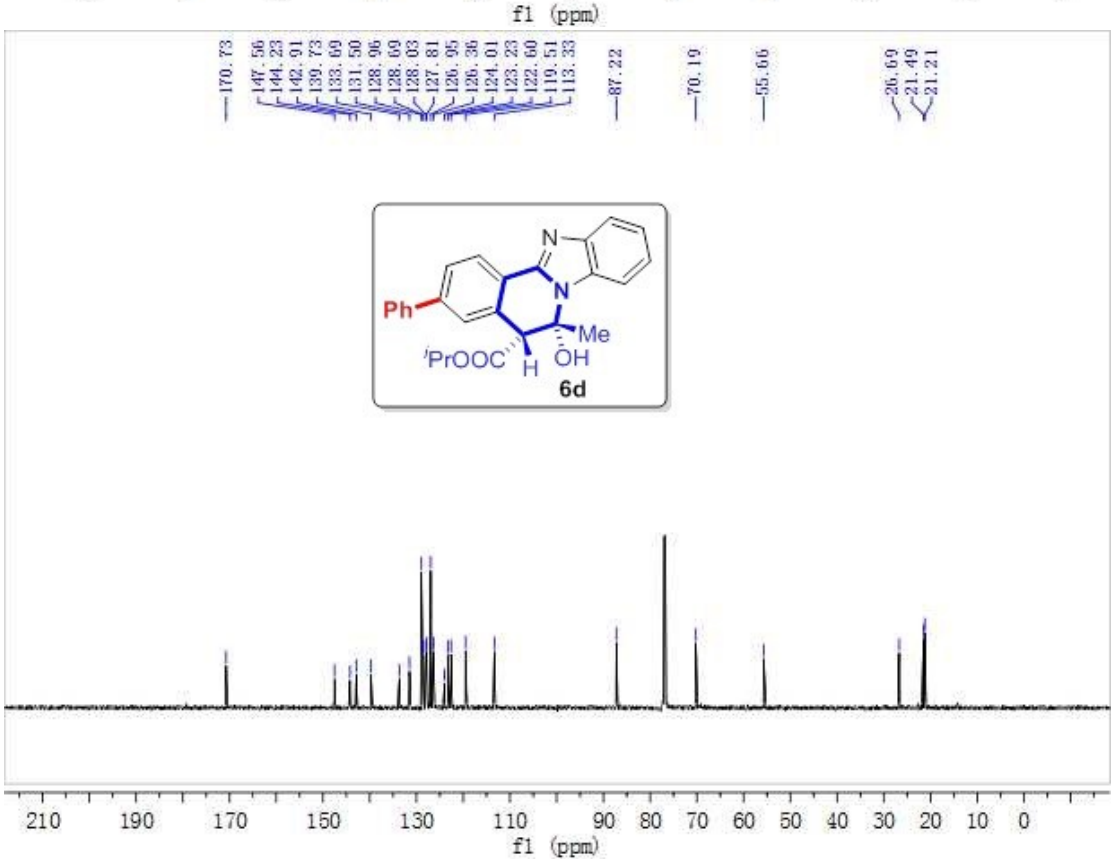
122.79
122.40
119.08
117.91
115.63
114.50
113.10
87.10
70.14
55.79
55.48
26.54
21.45
21.18
MeO
N
N
Me
OH
H
iPrOOC
6c
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.35
8.33
8.06
8.06
8.05
8.04
7.82
7.81
7.81
7.80
7.71
7.70
7.67
7.65
7.51
7.50
7.48
7.43
7.42
7.29
7.28
7.28
7.20
4.94
4.93
4.92
4.90
4.89
4.88
4.87
4.12
1.66
1.20
1.19
0.95
0.93
N
N
Ph
Me
iPrOOC
H
OH
6d
1.00
1.06
1.16
4.05
2.16
1.33
1.98
1.03
1.08
1.17
3.18
3.12
3.11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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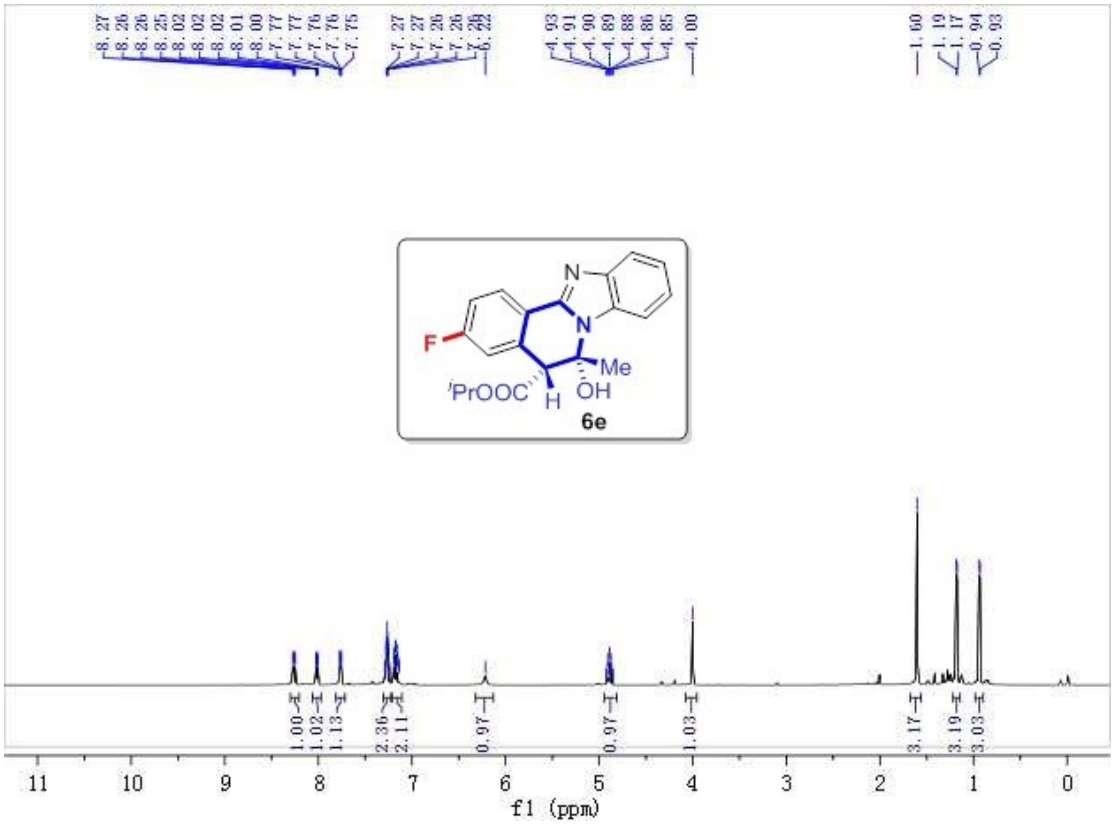
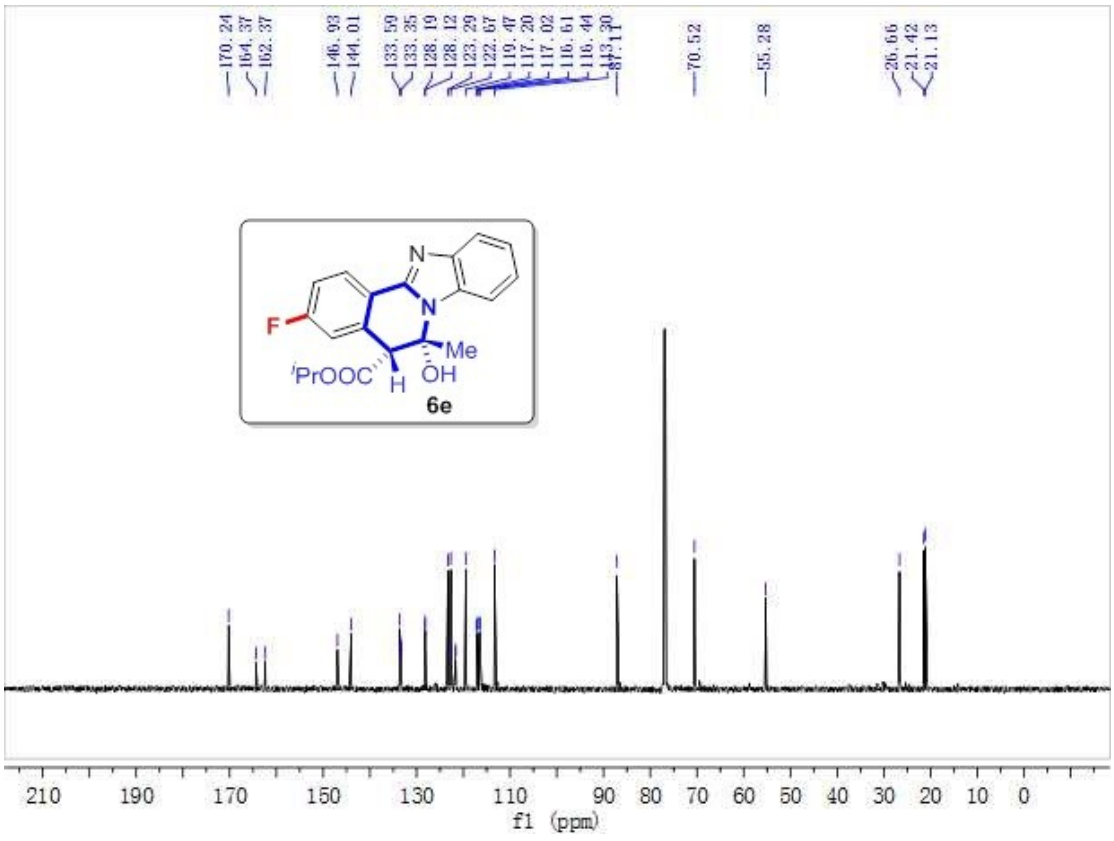
142.91
139.73
133.69
131.50
128.96
128.69
128.03
127.81
126.95
126.36
124.01
123.23
122.60
119.51
113.33
87.22
70.19
55.66
26.69
21.49
21.21
N
N
Ph
Me
iPrOOC
H
OH
6d
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.27
8.26
8.26
8.25
8.02
8.02
8.02
8.01
8.00
7.77
7.77
7.76
7.76
7.75
7.27
7.27
7.26
7.26
6.24
4.93
4.91
4.90
4.89
4.88
4.86
4.85
4.00
1.60
1.19
1.17
0.94
0.93
N
F
N
Me
iPrOOC
H
OH
6e
1.00
1.02
1.13
2.36
2.11
0.97
0.97
1.03
3.17
3.19
3.03
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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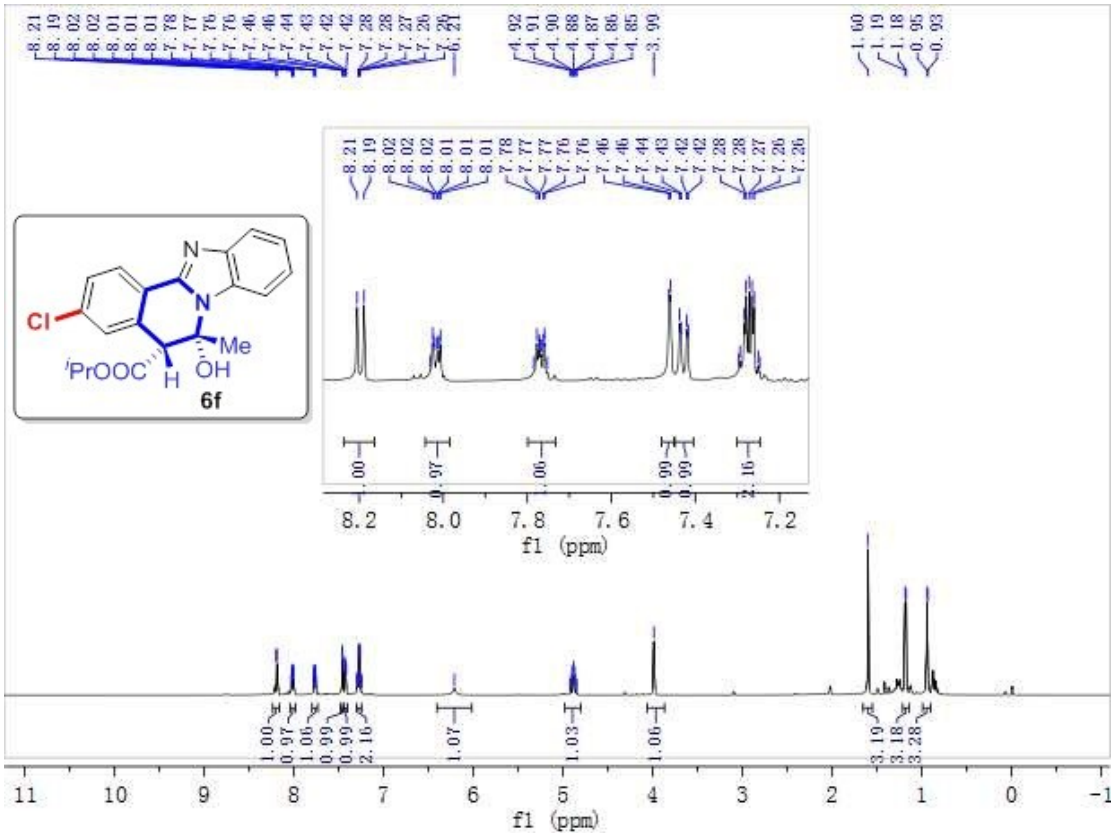
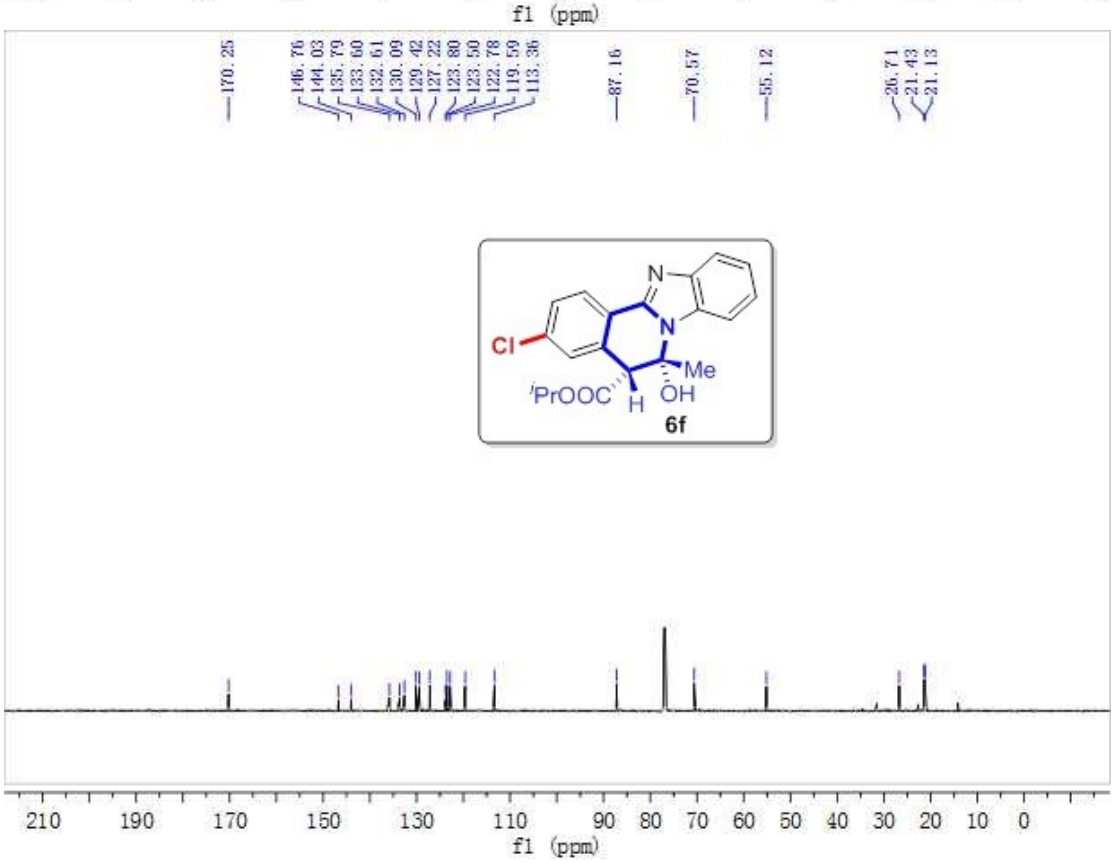
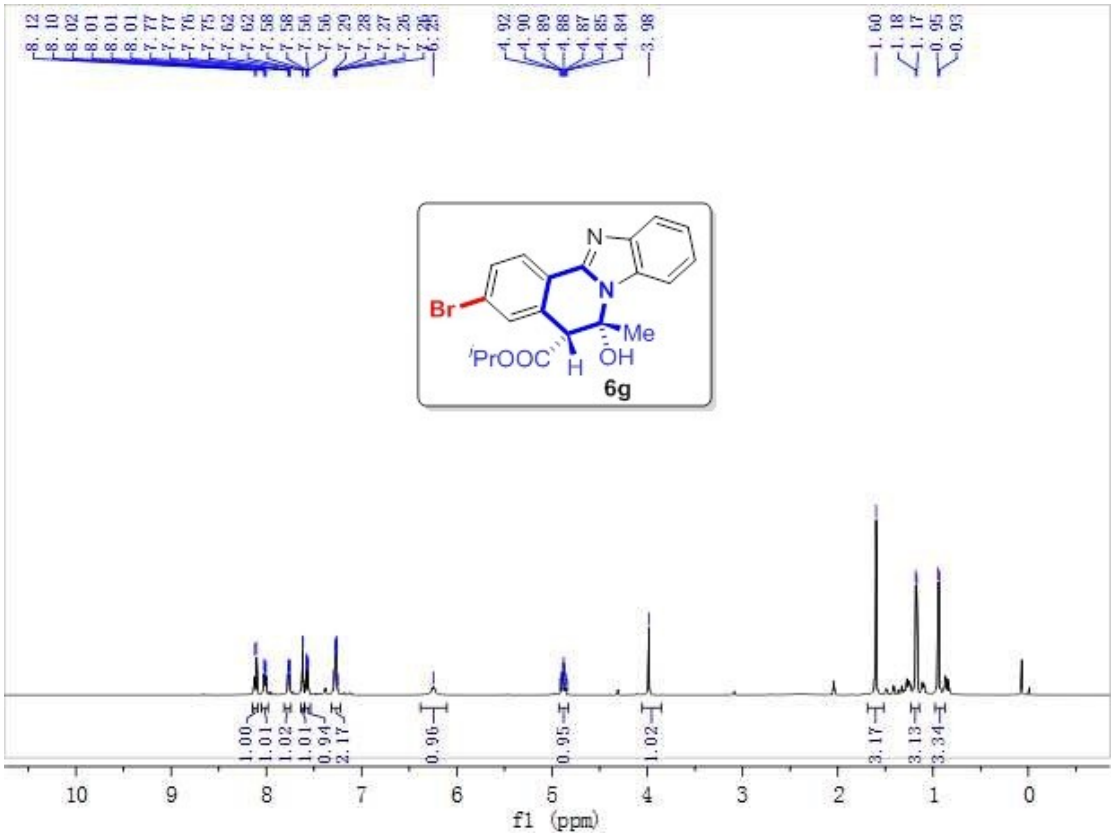
164.37
162.37
146.93
144.01
133.59
133.35
128.19
128.12
123.29
122.67
119.47
117.20
117.02
116.61
116.44
87.11
70.52
55.28
26.66
21.42
21.13
N
F
N
Me
iPrOOC
H
OH
6e
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.21 8.19 8.02 8.02 8.01 8.01 7.78 7.77 7.76 7.46 7.44 7.43 7.42 7.42 7.28 7.27 7.26 7.21
4.92 4.91 4.90 4.88 4.87 4.86 4.85 3.99
1.60 1.19 1.18 0.95 0.93
Cl
N
N
Me
OH
H
iPrOOC
6f
1.00 0.97 1.06 0.99 0.99 2.16
8.2 8.0 7.8 7.6 7.4 7.2
f1 (ppm)
1.00 0.97 1.06 0.99 0.99 2.16 1.07 1.03 1.06 3.19 3.18 3.28
11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


170.25
146.76 144.03 135.79 133.60 132.61 130.09 129.42 127.22 123.80 123.50 122.78 119.59 113.36
87.16
70.57
55.12
26.71 21.43 21.13
Cl
N
N
Me
OH
H
iPrOOC
6f
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.12
8.10
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8.01
8.01
7.77
7.77
7.76
7.75
7.62
7.62
7.58
7.58
7.56
7.56
7.29
7.28
7.27
7.26
4.92
4.90
4.89
4.88
4.87
4.85
4.84
3.98
1.60
1.18
1.17
0.95
0.93
Br
N
N
Me
OH
H
iPrOOC
6g
1.00
1.01
1.02
1.01
0.94
2.17
0.96
0.95
1.02
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3.34
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7
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5
4
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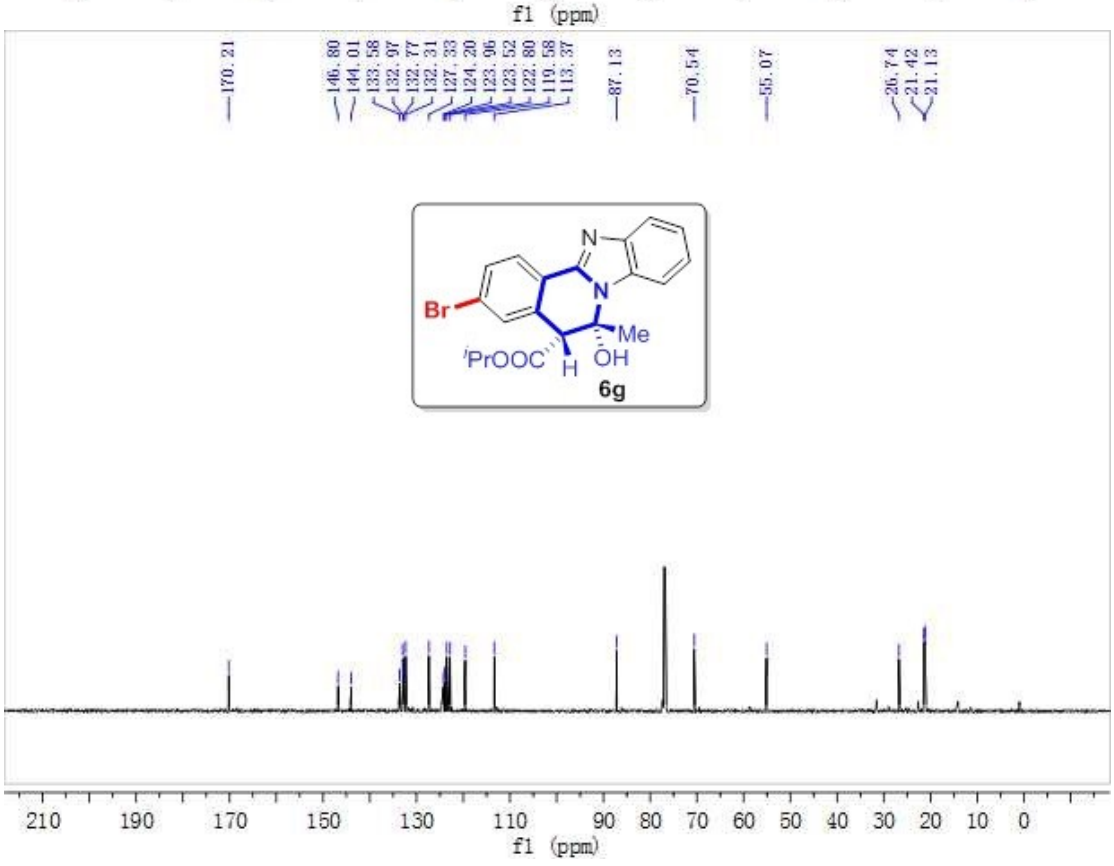
0
f1 (ppm)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146.80
144.01
133.58
132.97
132.77
132.31
127.33
124.20
123.96
123.52
122.80
119.58
113.37
87.13
70.54
55.07
26.74
21.42
21.13
Br
N
N
Me
OH
H
iPrOOC
6g
210
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170
150
130
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90
80
70
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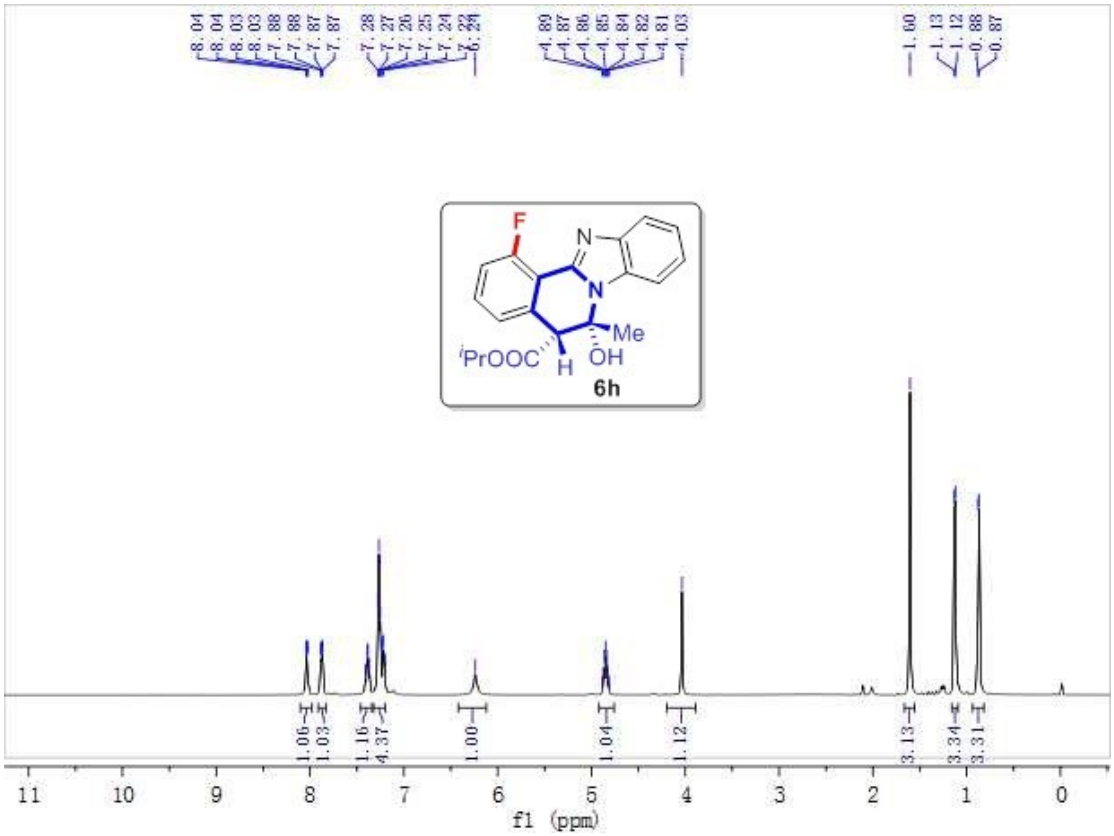
50
40
30
20
10
0
f1 (ppm)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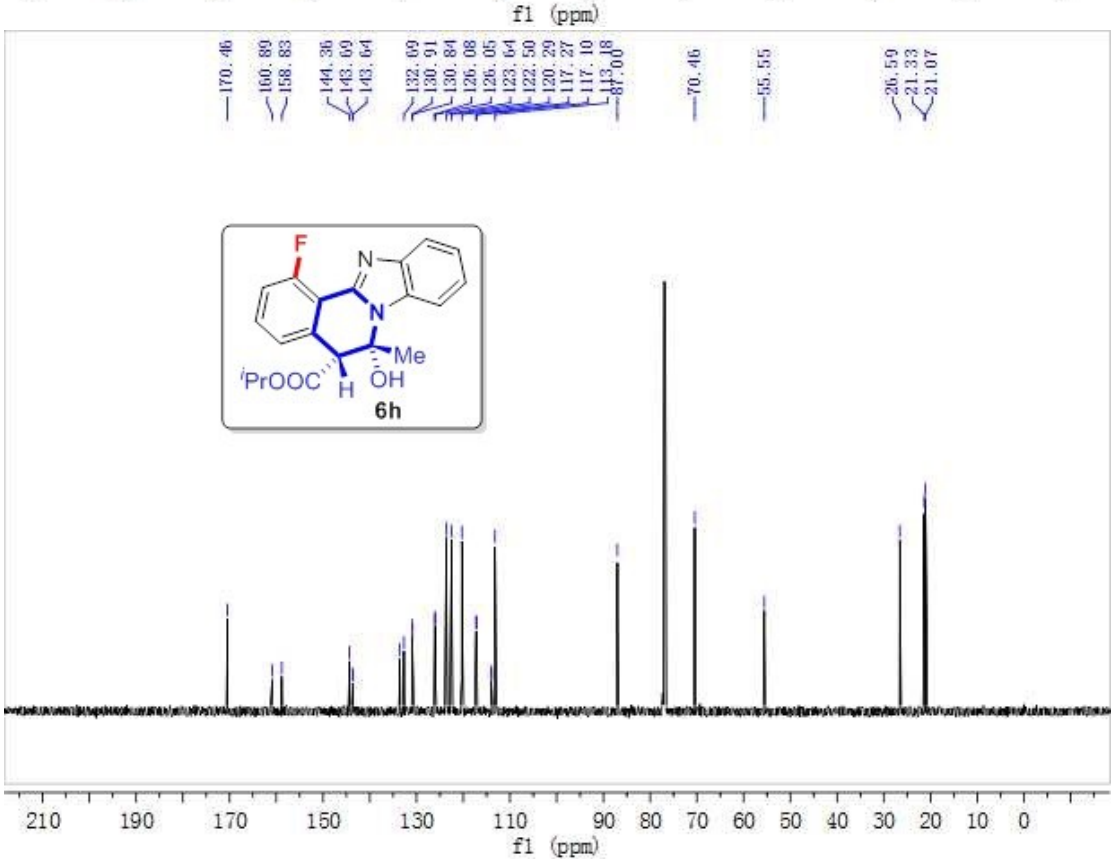
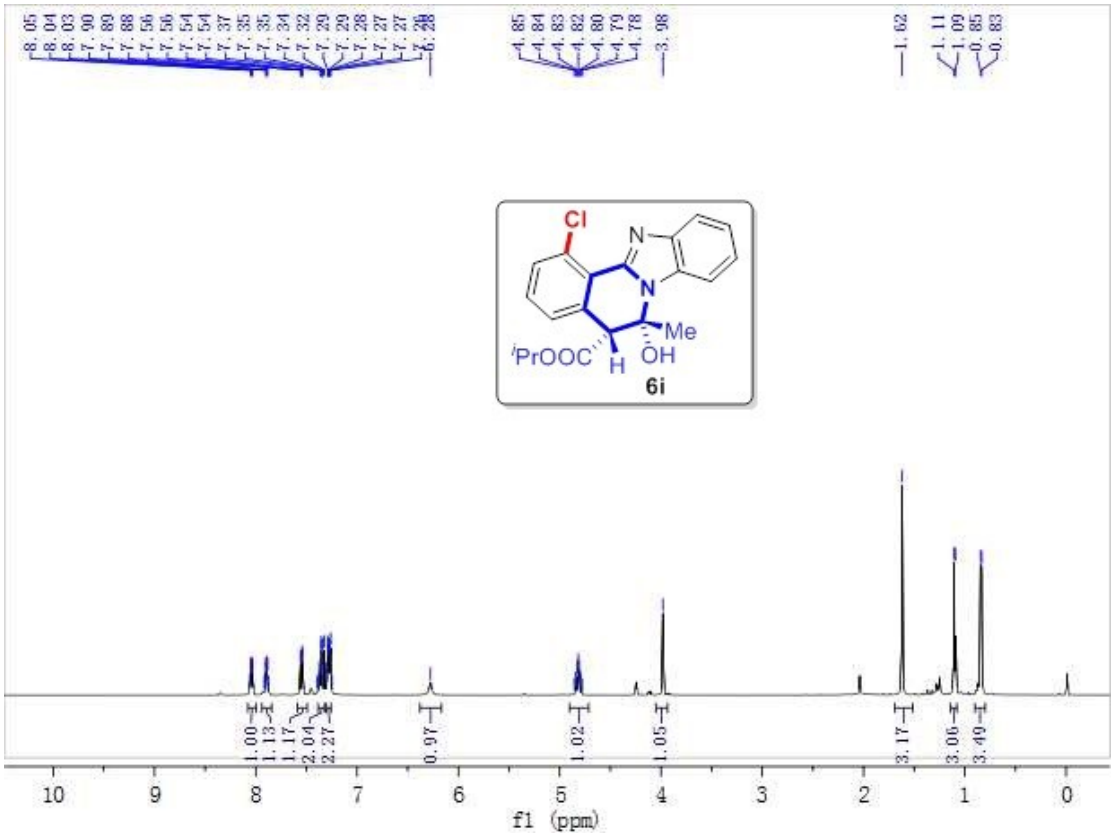
Me
iPrOOC
H
OH
6h
f1 (ppm)


F
N
N
Me
iPrOOC
H
OH
6h
f1 (ppm)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8.04
8.03
7.90
7.89
7.88
7.56
7.56
7.54
7.54
7.37
7.35
7.35
7.34
7.32
7.29
7.29
7.28
7.27
7.27
6.28
4.85
4.84
4.83
4.82
4.80
4.79
4.78
3.98
1.62
1.11
1.09
0.85
0.83
Cl
N
N
Me
iPrOOC
H
OH
6i
1.00
1.13
1.17
2.04
2.27
0.97
1.02
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3.06
3.49
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9
8
7
6
5
4
3
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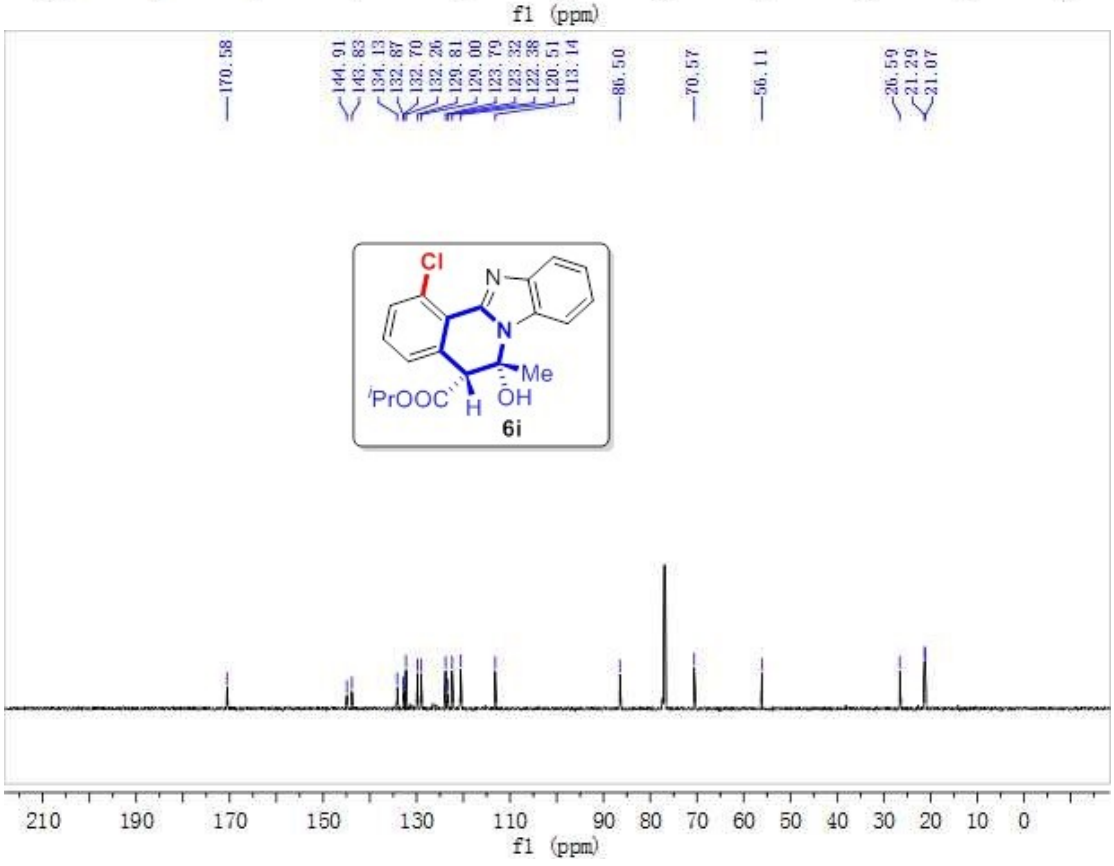
1
0
f1 (ppm)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132.70
132.26
129.81
129.00
123.79
123.32
122.38
120.51
113.14
86.50
70.57
56.11
26.59
21.29
21.07
Cl
N
N
Me
iPrOOC
H
OH
6i
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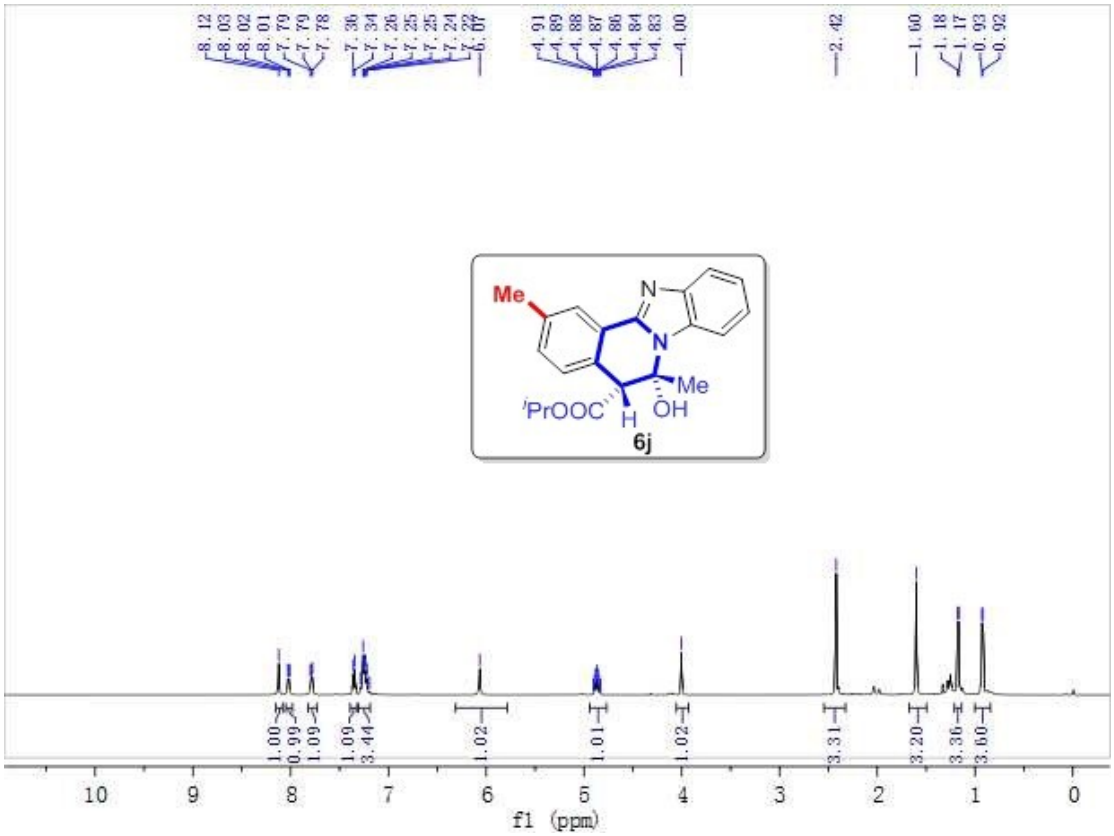
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.12
8.03
8.02
8.01
7.79
7.79
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7.36
7.34
7.26
7.25
7.25
7.24
6.07
4.91
4.89
4.88
4.87
4.86
4.84
4.83
4.00
2.42
1.60
1.18
1.17
0.93
0.92
Me
N
N
Me
iPrOOC
H
OH
6j
1.00
0.99
1.09
1.09
3.44
1.02
1.01
1.02
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3.60
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7
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5
4
3
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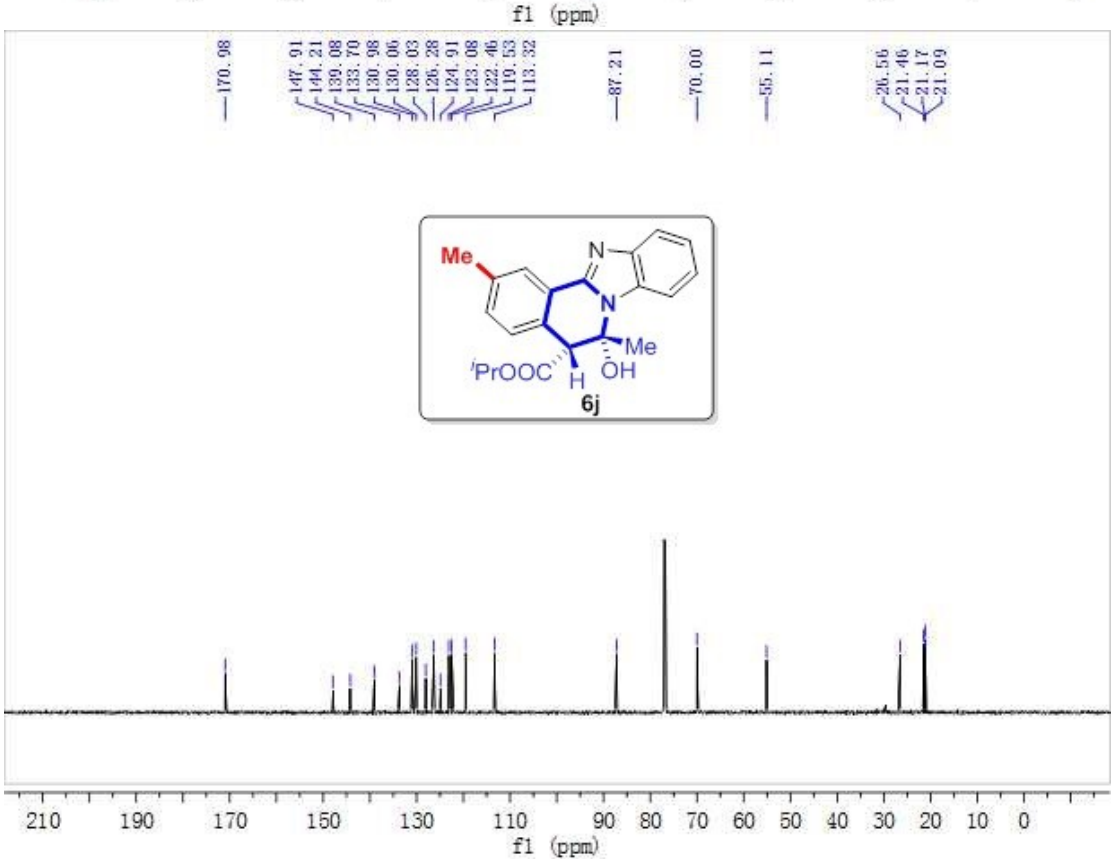
1
0
f1 (ppm)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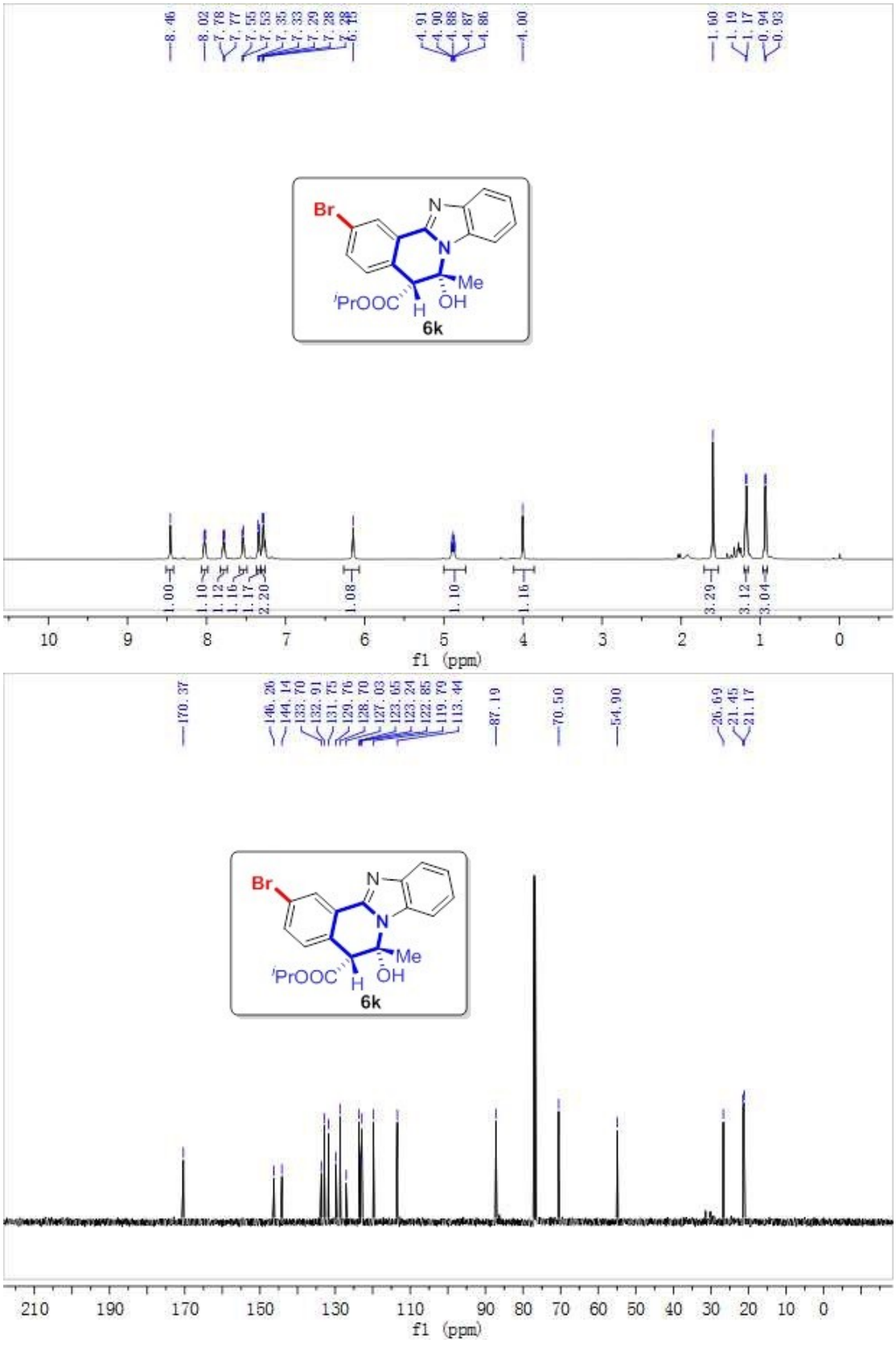
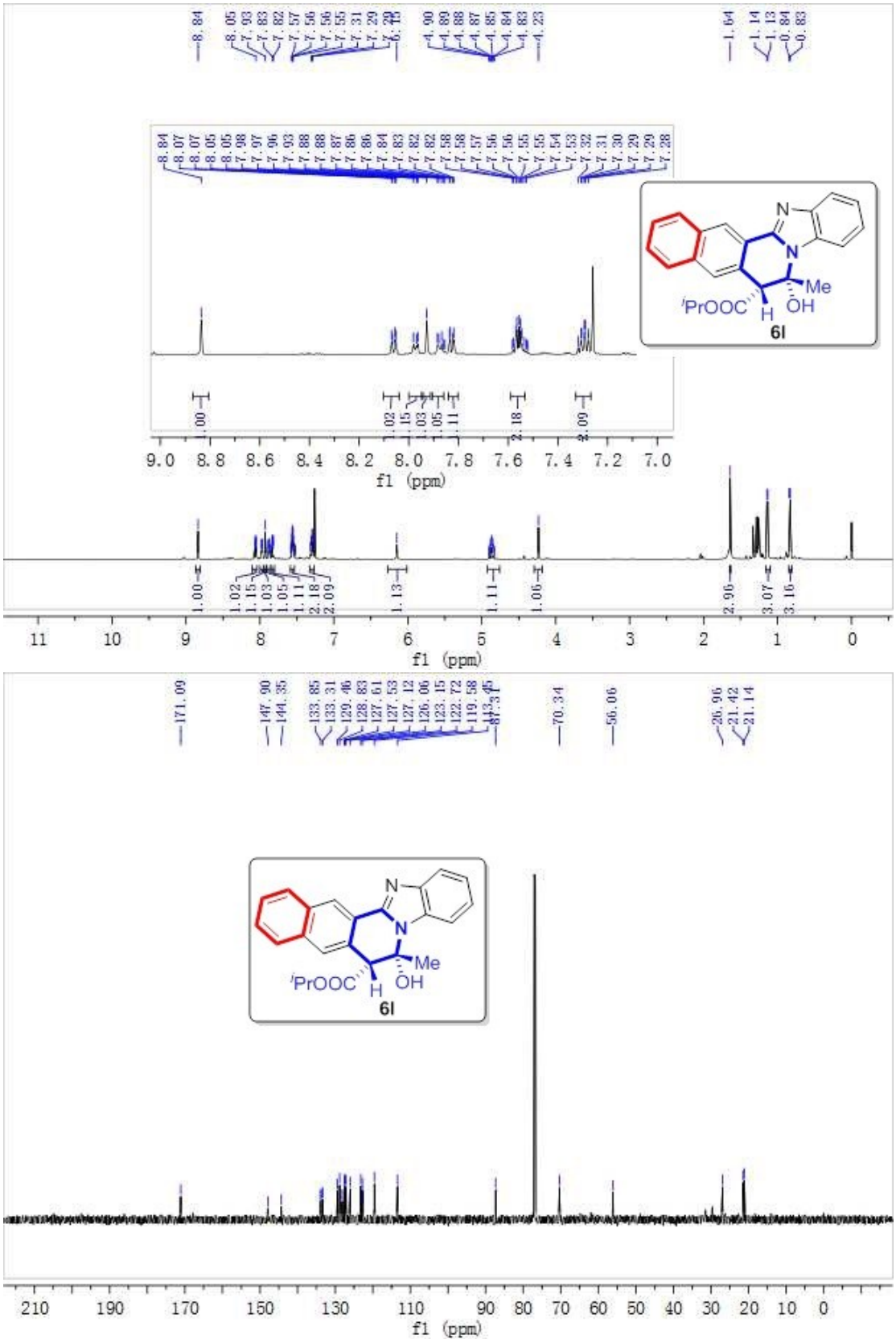
130.98
130.06
128.03
126.28
124.91
123.08
122.46
119.53
113.32
87.21
70.00
55.11
26.56
21.46
21.17
21.09
Me
N
N
Me
iPrOOC
H
OH
6j
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Br
N
N
Me
iPrOOC
H
OH
6k
f1 (ppm)
Br
N
N
Me
iPrOOC
H
OH
6k
f1 (ppm)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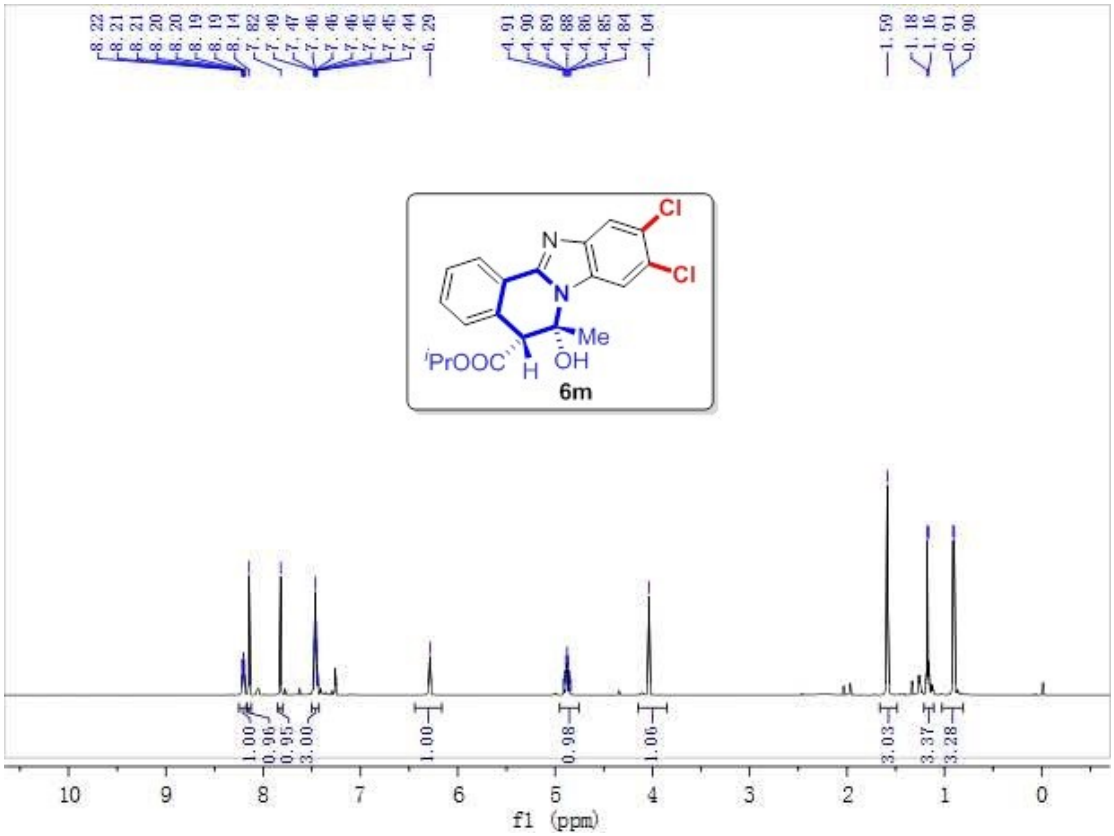
7.82
7.57
7.56
7.56
7.55
7.31
7.29
4.90
4.89
4.88
4.87
4.85
4.84
4.83
4.23
1.64
1.14
1.13
0.84
0.83
N
N
Me
'PrOOC
H
OH
6l
f1 (ppm)
f1 (ppm)

171.09
147.90
144.35
133.85
133.31
129.46
128.83
127.61
127.53
127.12
126.06
123.15
122.72
119.58
70.34
56.06
26.96
21.42
21.14
N
N
Me
'PrOOC
H
OH
6l
f1 (ppm)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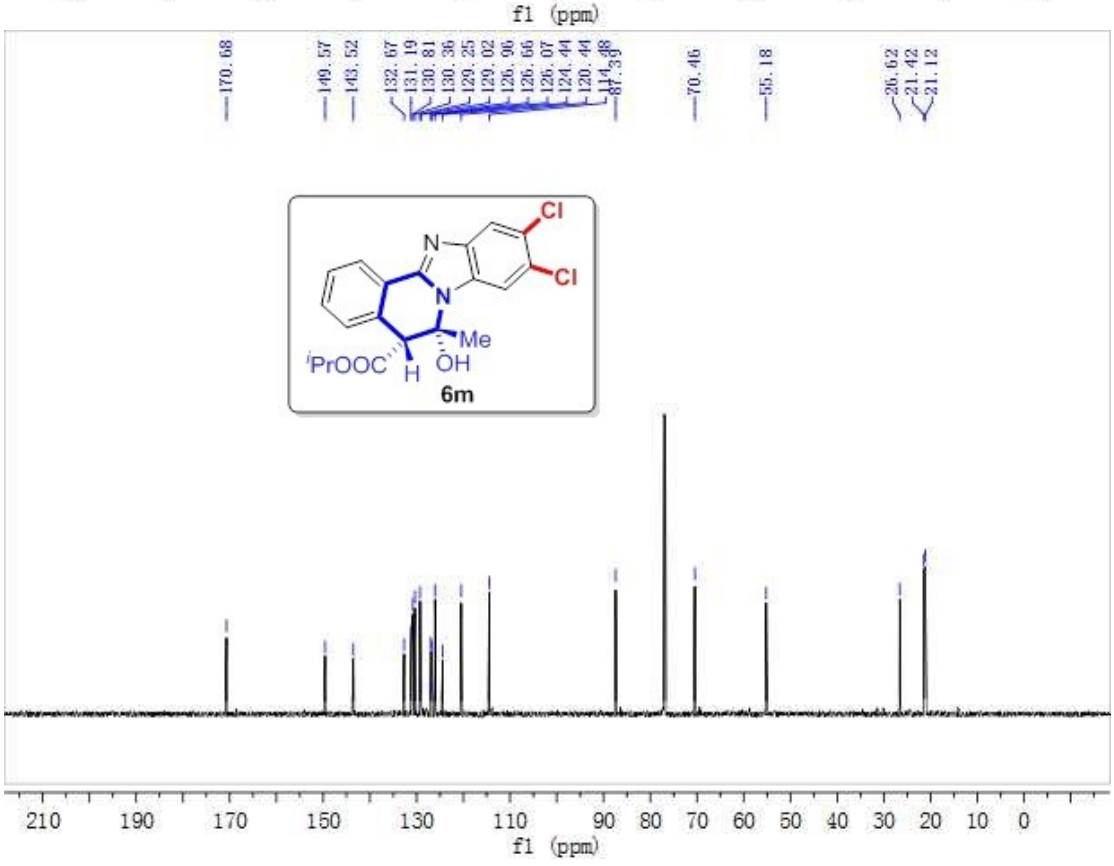
8.21
8.21
8.20
8.20
8.19
8.19
8.14
7.82
7.49
7.47
7.46
7.46
7.46
7.45
7.45
7.44
6.29
4.91
4.90
4.89
4.88
4.86
4.85
4.84
4.04
1.59
1.18
1.16
0.91
0.90
Cl
Cl
N
N
Me
OH
iPrOOC
H
6m
1.00
0.96
0.95
3.00
1.00
0.98
1.06
3.03
3.37
3.28
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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129.25
129.02
126.90
126.66
126.07
124.44
120.44
114.48
87.33
70.46
55.18
26.62
21.42
21.12
Cl
Cl
N
N
Me
OH
iPrOOC
H
6m
210
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170
150
130
110
90
80
70
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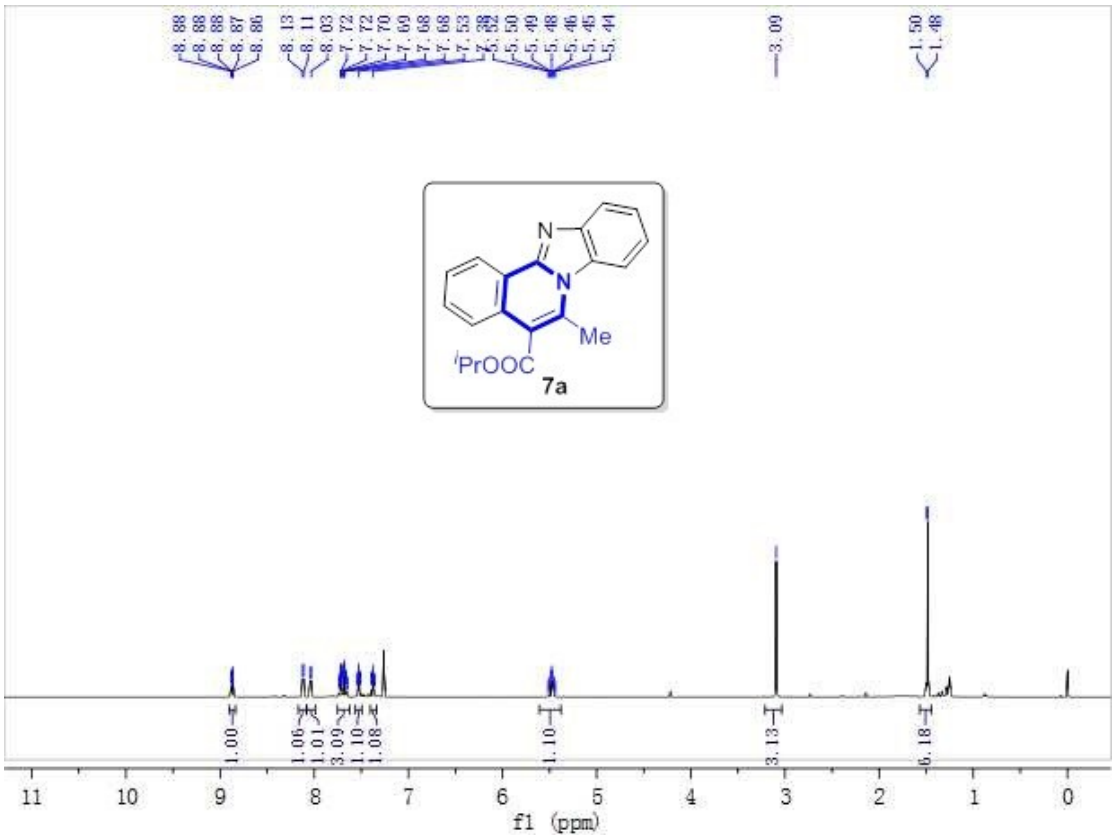
50
40
30
20
10
0
f1 (ppm)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8.88
8.88
8.87
8.86
8.13
8.11
8.03
7.72
7.72
7.70
7.69
7.68
7.68
7.53
5.50
5.49
5.48
5.46
5.45
5.44
3.00
1.50
1.48
N
N
Me
iPrOOC
7a
1.00
1.06
1.01
3.09
1.10
1.08
1.10
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6.18
11
10
9
8
7
6
5
4
3
2
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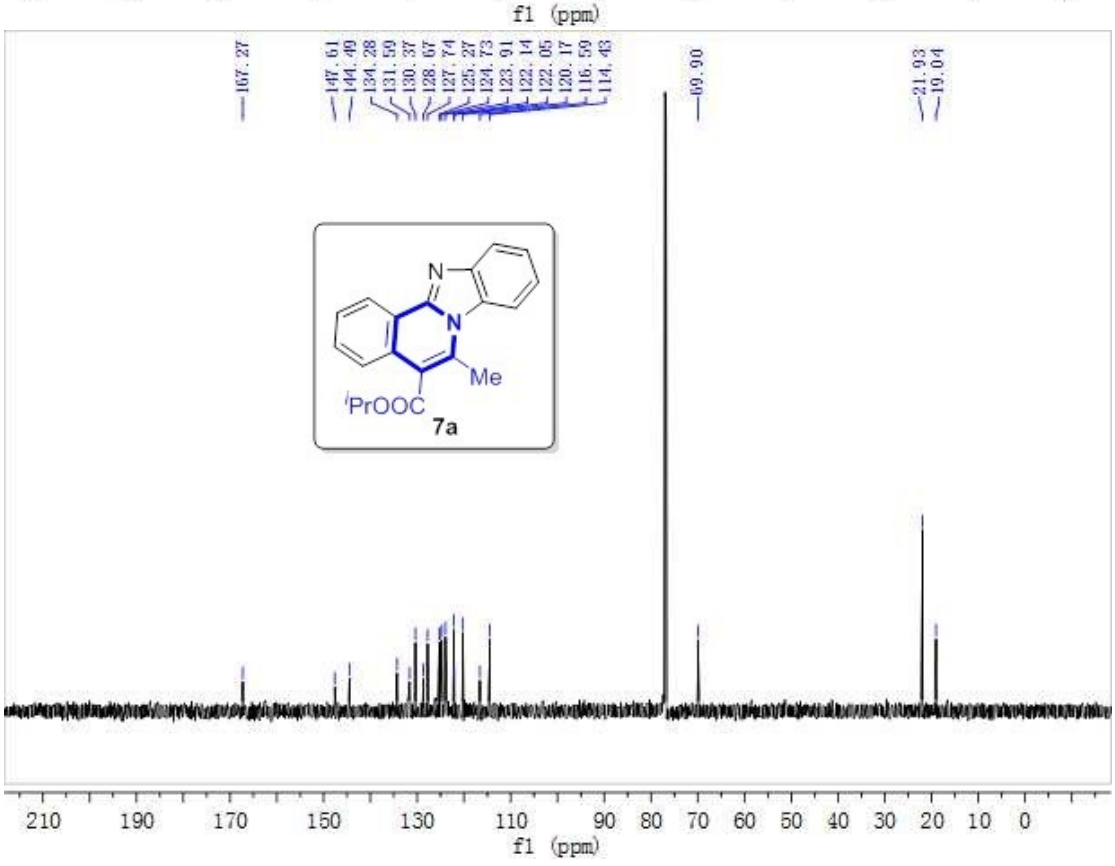
0
f1 (ppm)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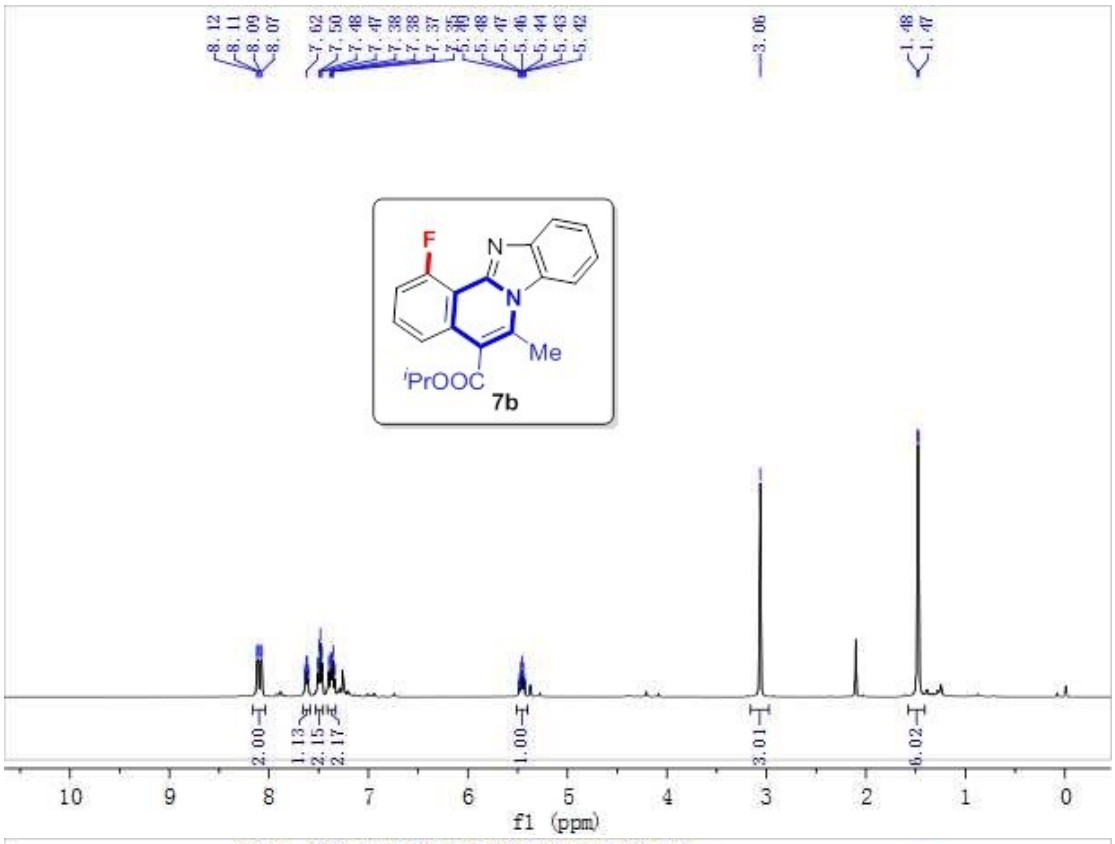
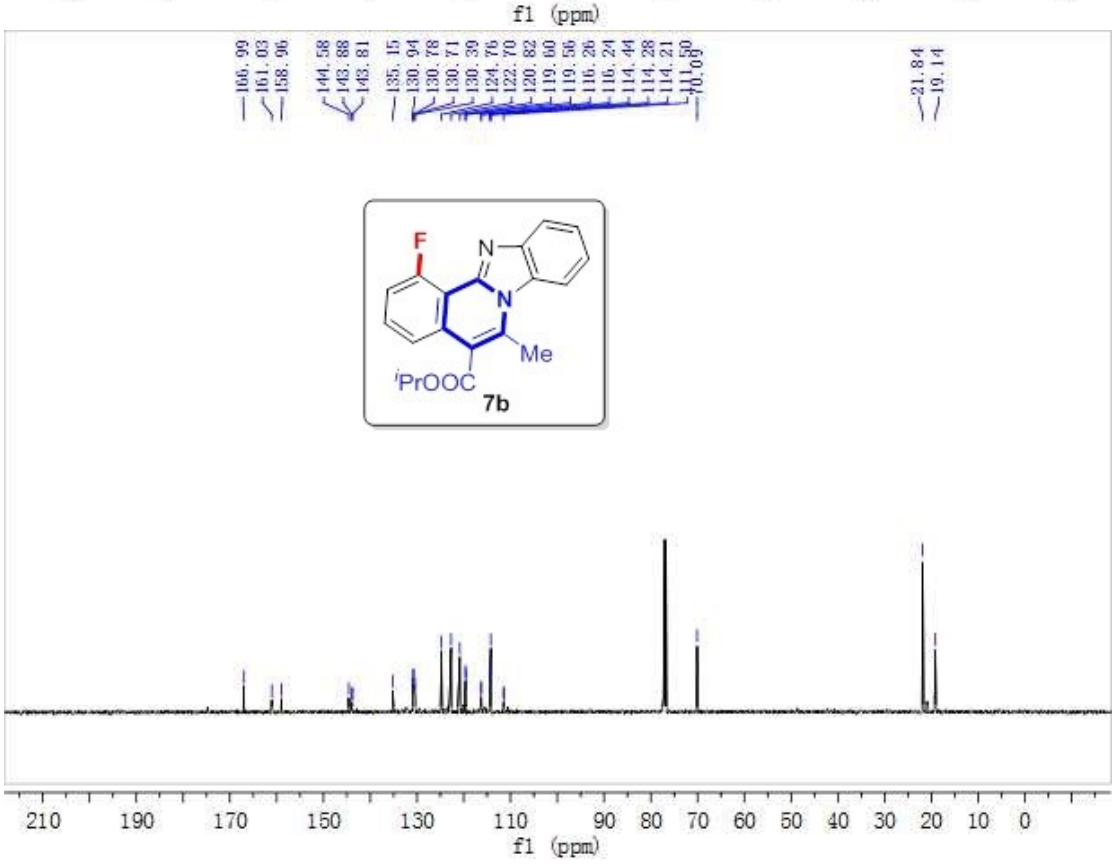
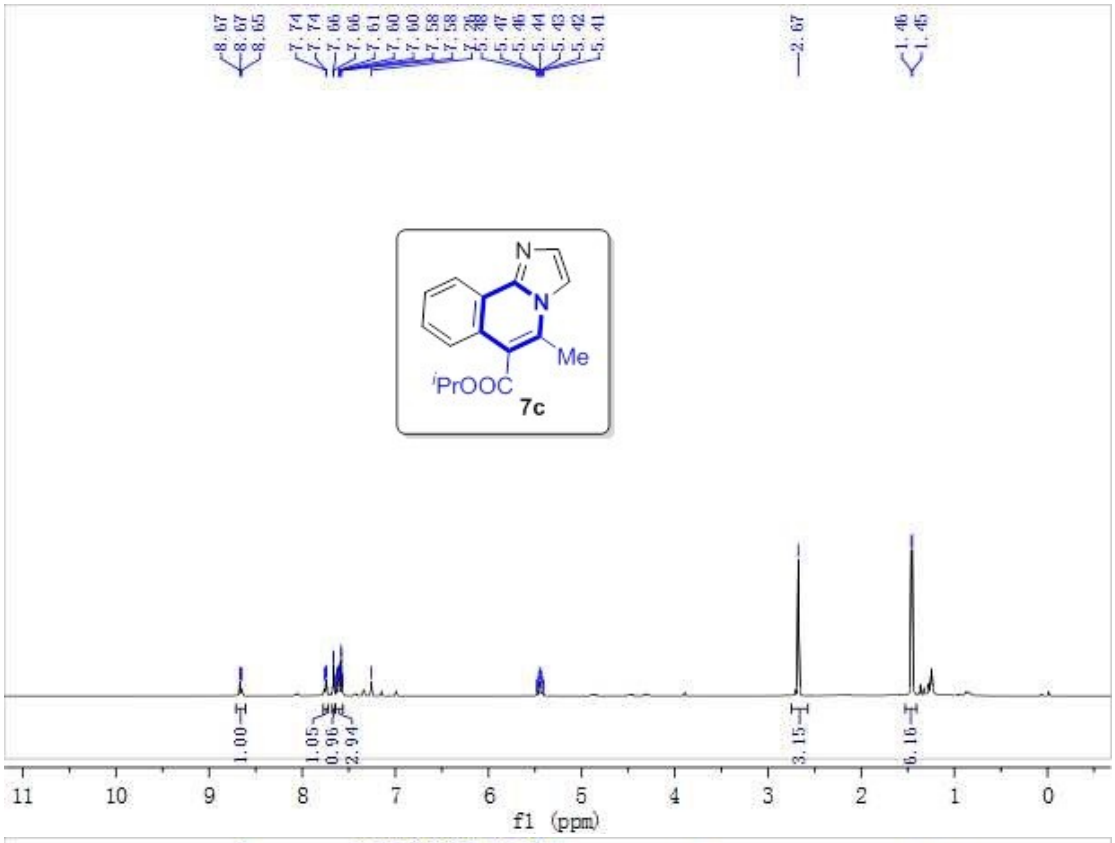
130.37
128.67
127.74
125.27
124.73
123.91
122.14
122.05
120.17
116.59
114.43
69.90
21.93
19.04
N
N
Me
iPrOOC
7a
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


F
N
N
Me
iPrOOC
7b
f1 (ppm)


F
N
N
Me
iPrOOC
7b
f1 (ppm)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8.67
8.65
7.74
7.74
7.66
7.66
7.61
7.60
7.60
7.58
7.58
5.47
5.46
5.44
5.43
5.42
5.41
2.67
1.46
1.45
N
N
Me
iPrOOC
7c
1.00
1.05
0.96
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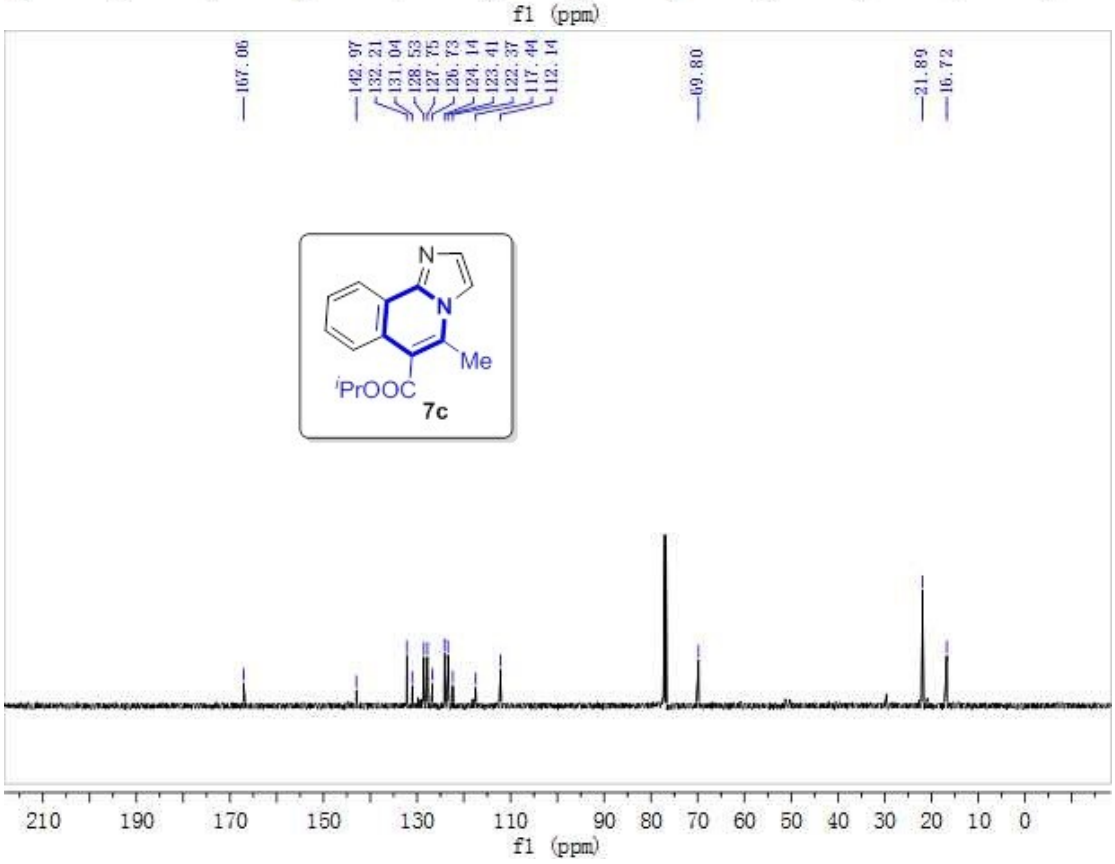
6.16
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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124.14
123.41
122.37
117.44
112.14
69.80
21.89
16.72
N
N
Me
iPrOOC
7c
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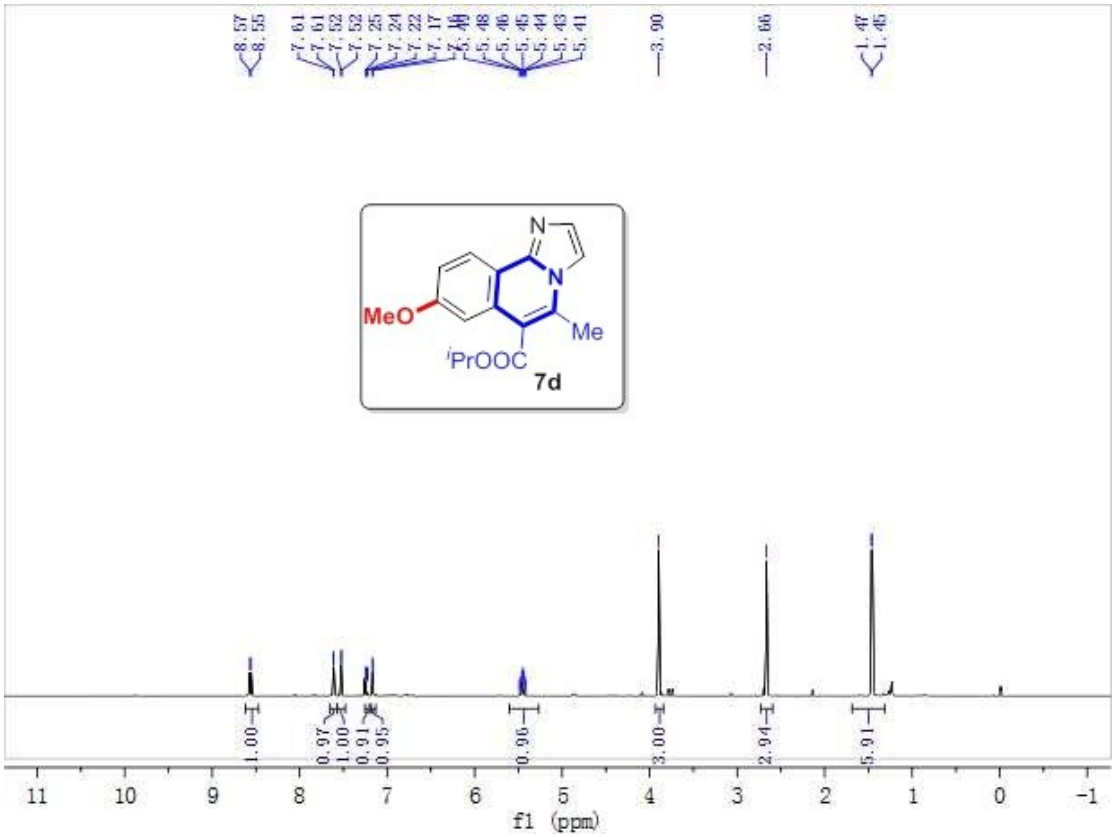
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.25
7.24
7.22
7.17
5.48
5.46
5.45
5.44
5.43
5.41
3.90
2.66
1.47
1.45
MeO
Me
iPrOOC
7d
1.00
0.97
1.00
0.91
0.95
0.96
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2.94
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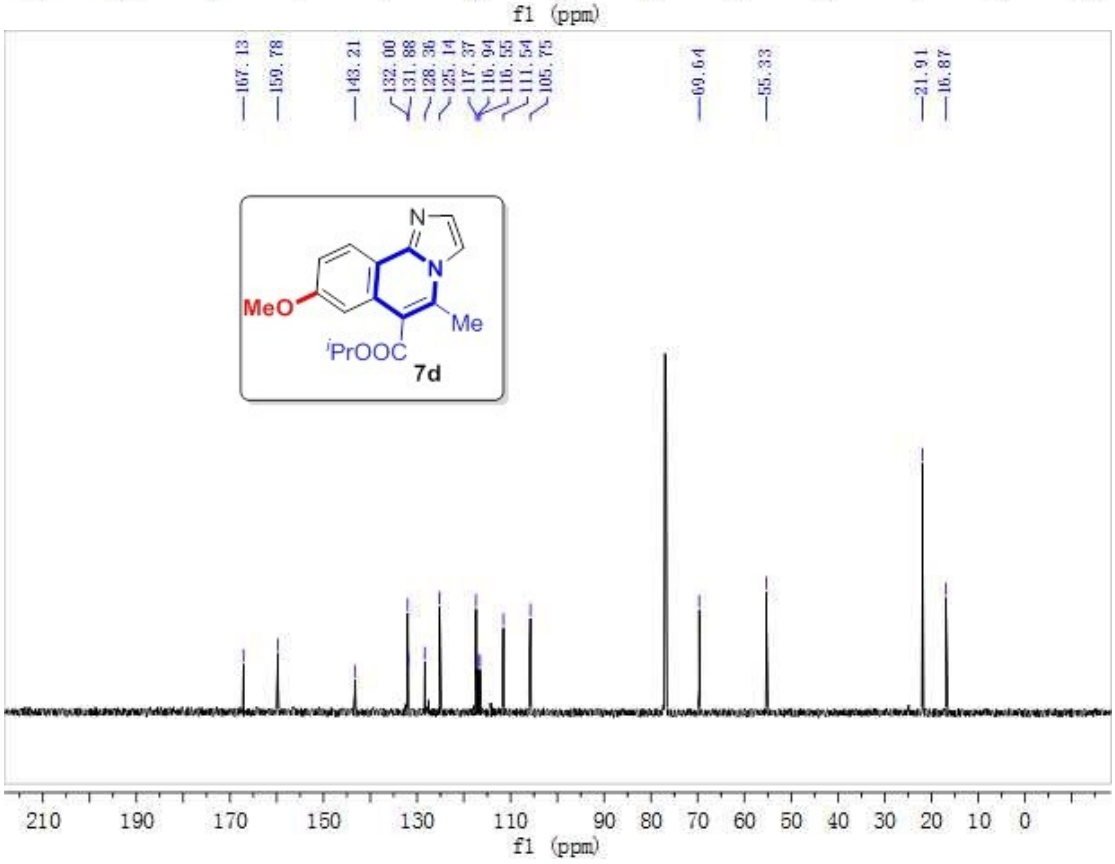
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)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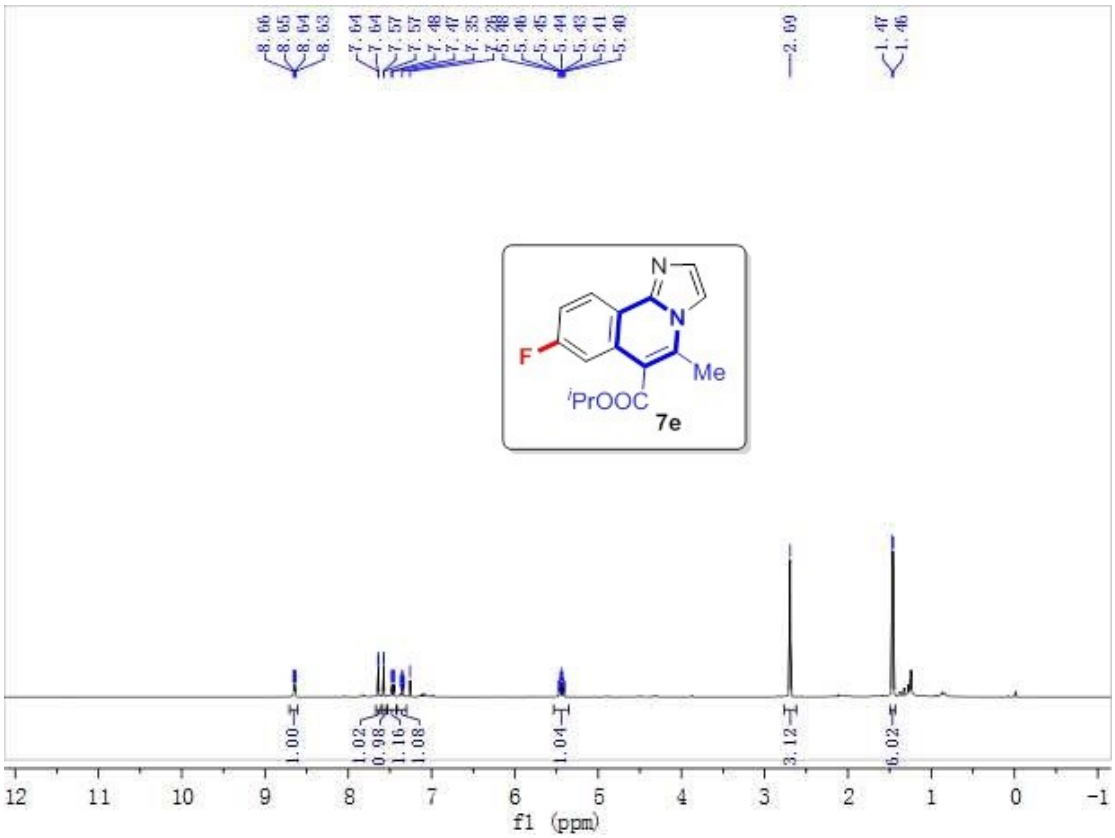
125.14
117.37
116.94
116.55
111.54
105.75
69.64
55.33
21.91
16.87
MeO
Me
iPrOOC
7d
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.57
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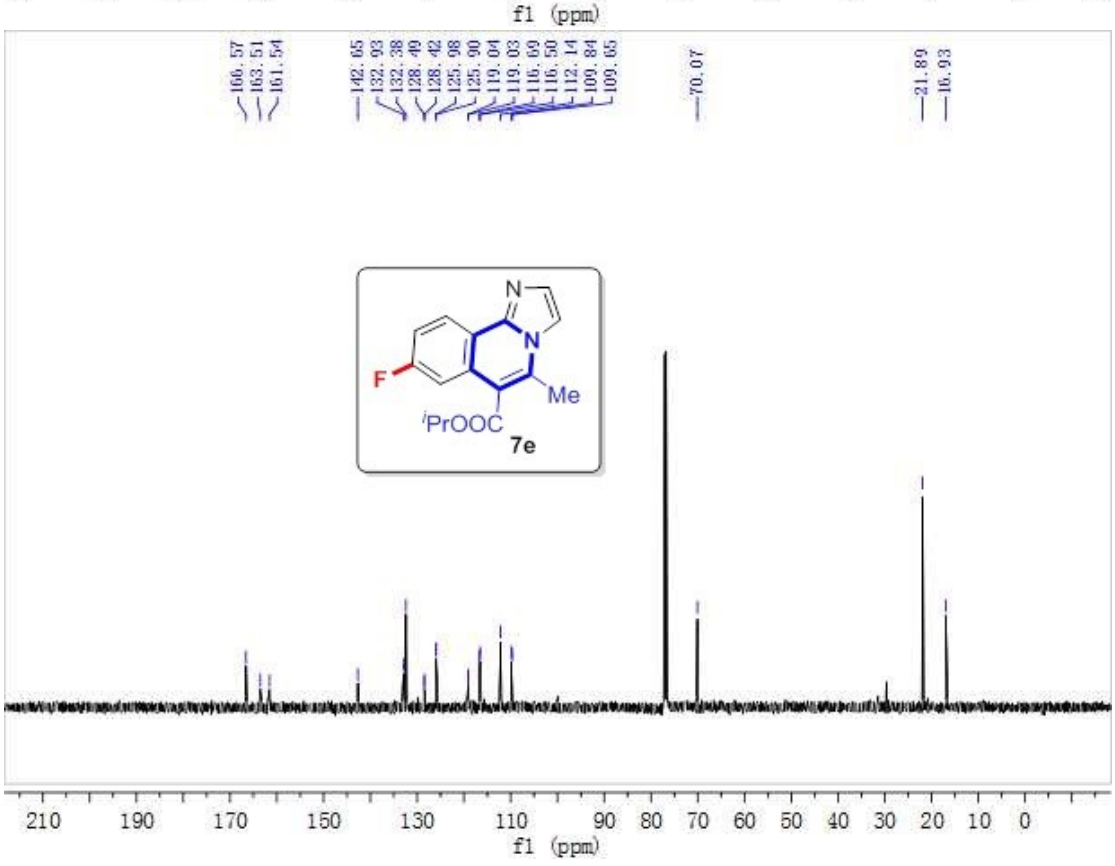
7.47
7.35
5.46
5.45
5.44
5.43
5.41
5.40
2.69
1.47
1.46
N
N
F
Me
iPrOOC
7e
1.00
1.02
0.98
1.16
1.08
1.04
3.12
6.02
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)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125.90
119.04
119.03
116.69
116.50
112.14
109.84
109.65
70.07
21.89
16.93
N
N
F
Me
iPrOOC
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170
150
130
110
90
80
70
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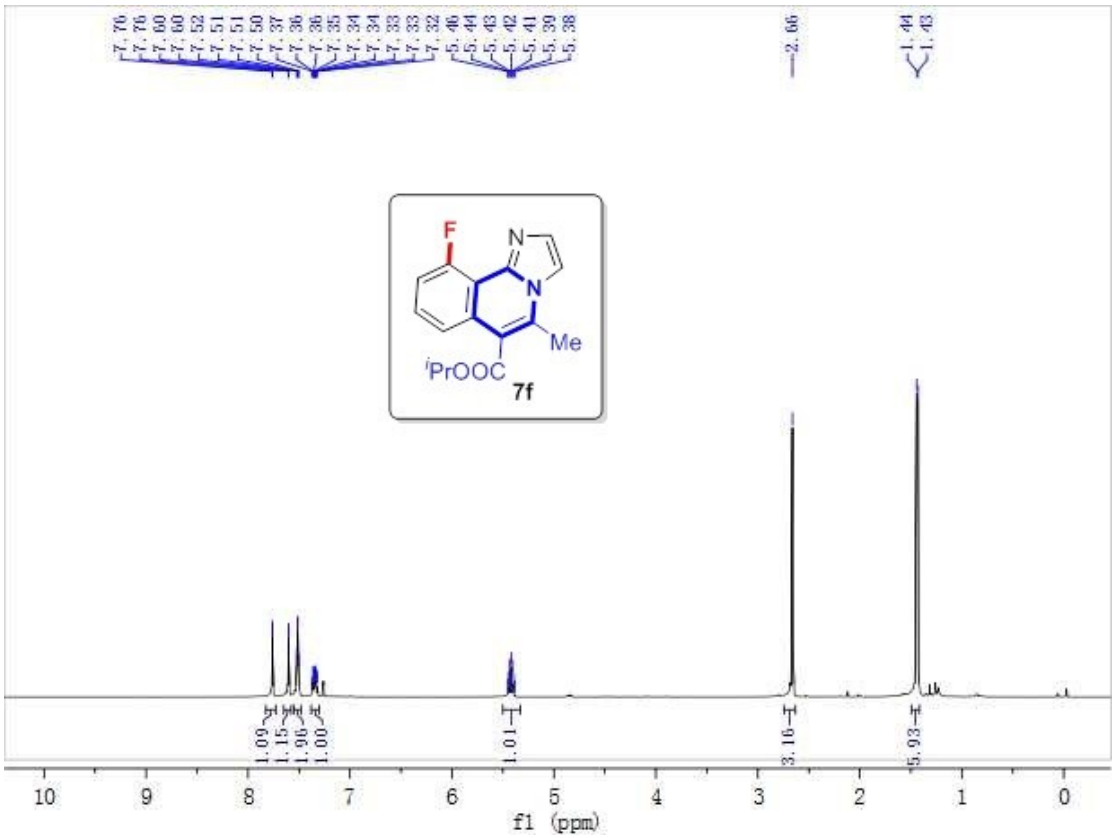
50
40
30
20
10
0
f1 (ppm)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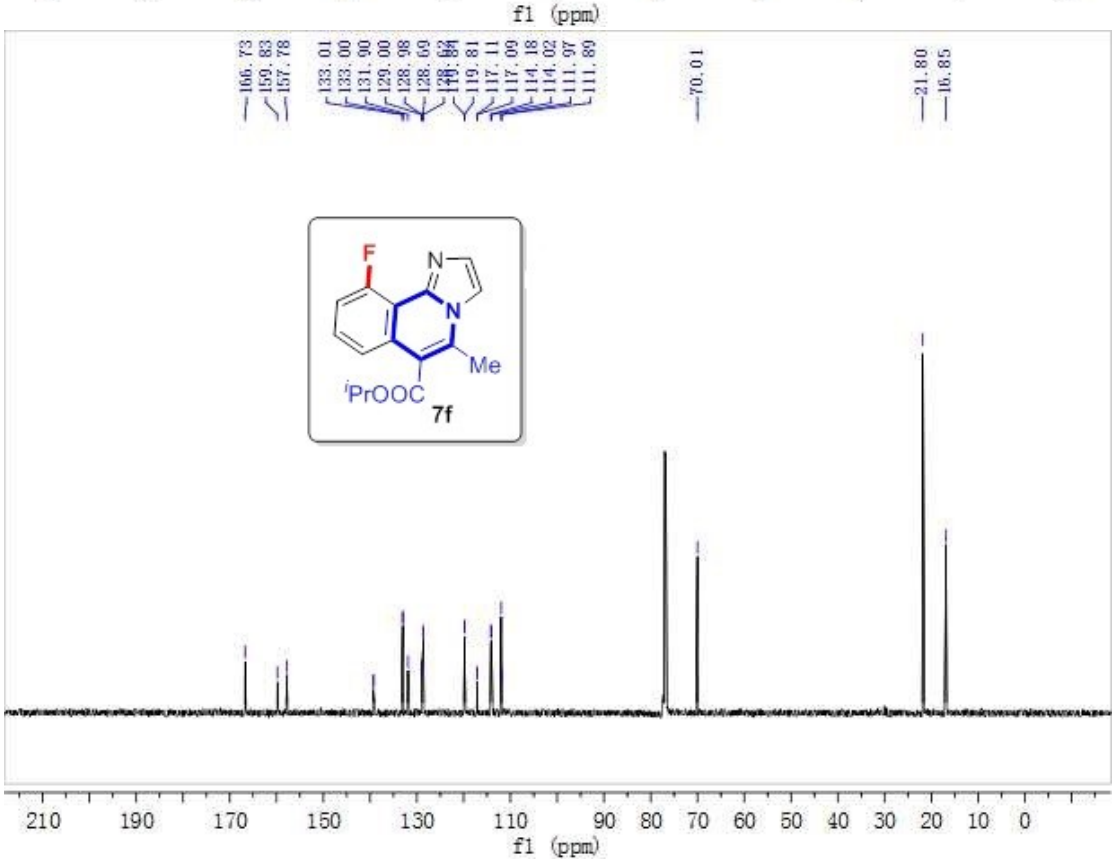
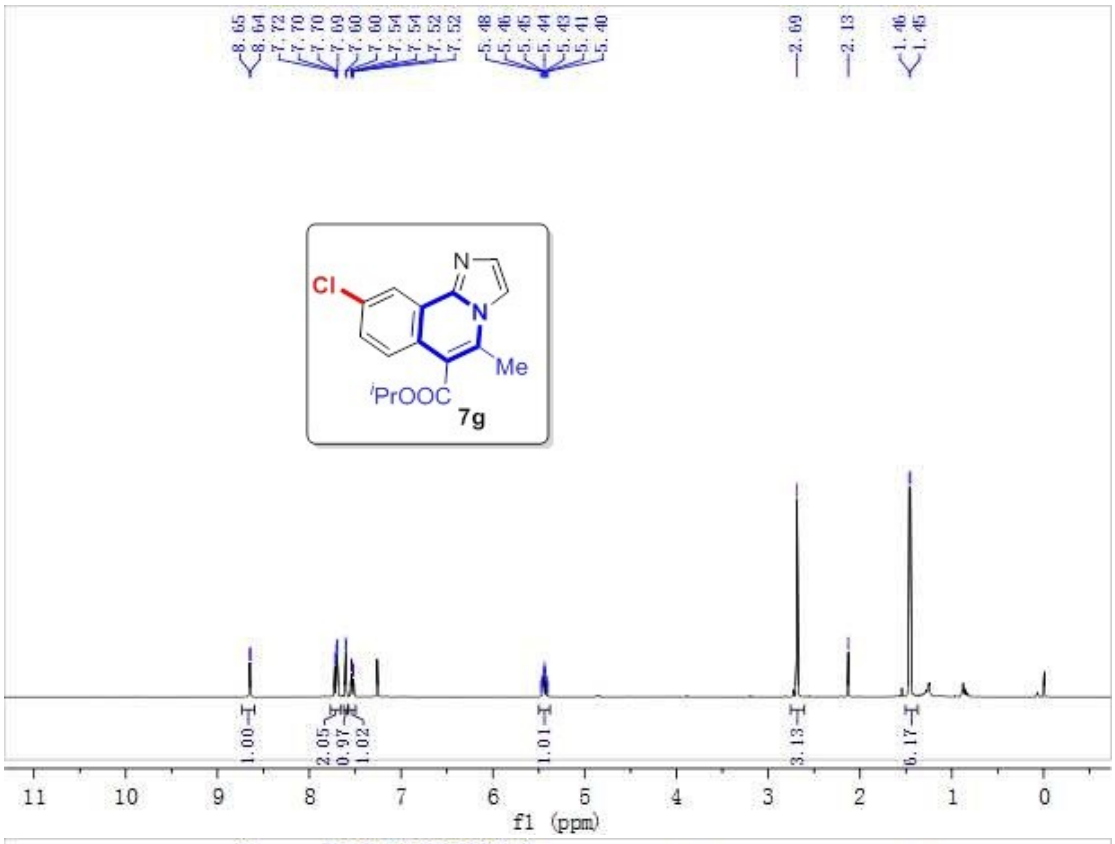
N
N
Me
iPrOOC
7f
f1 (ppm)


F
N
N
Me
iPrOOC
7f
f1 (ppm)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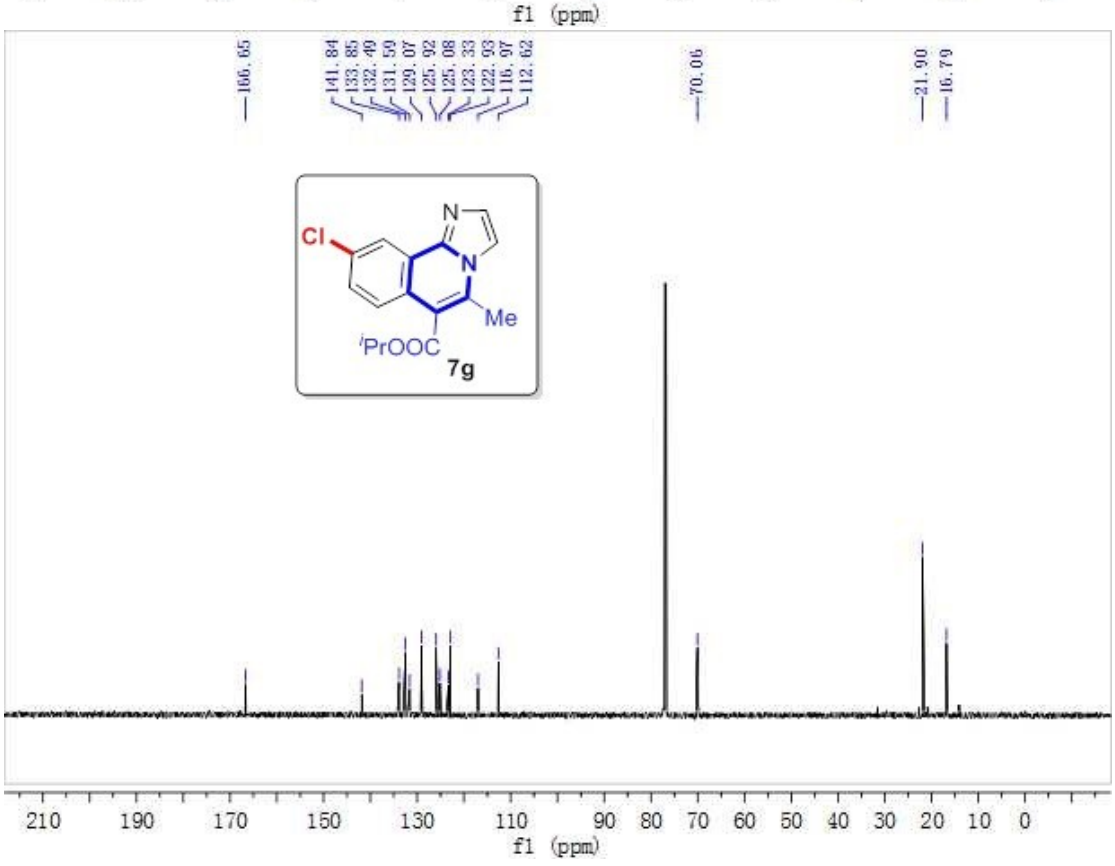
7.60
7.54
7.54
7.52
7.52
5.48
5.46
5.45
5.44
5.43
5.41
5.40
2.69
2.13
1.46
1.45
Cl
N
N
Me
iPrOOC
7g
1.00
2.05
0.97
1.02
1.01
3.13
6.17
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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129.07
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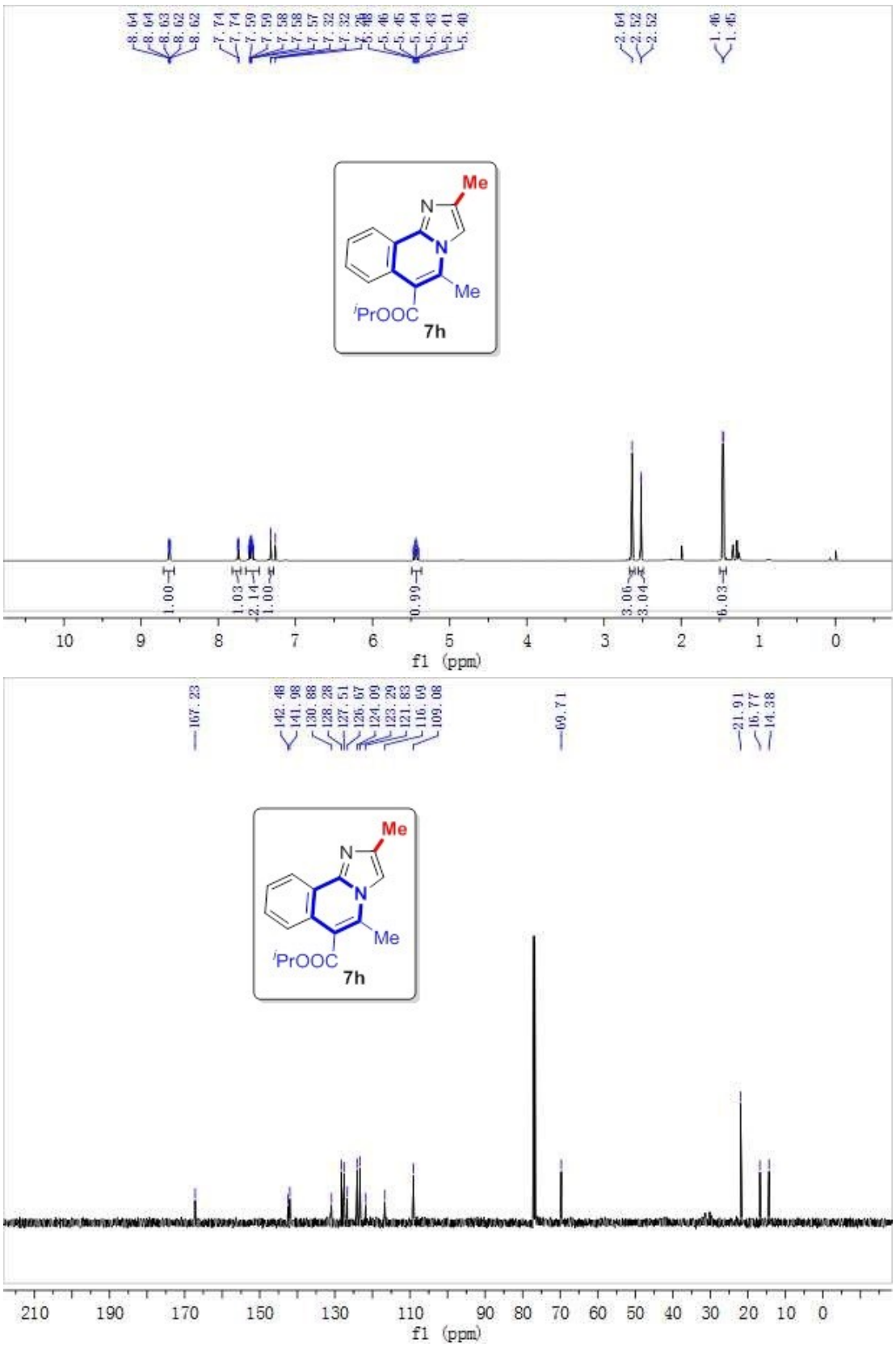
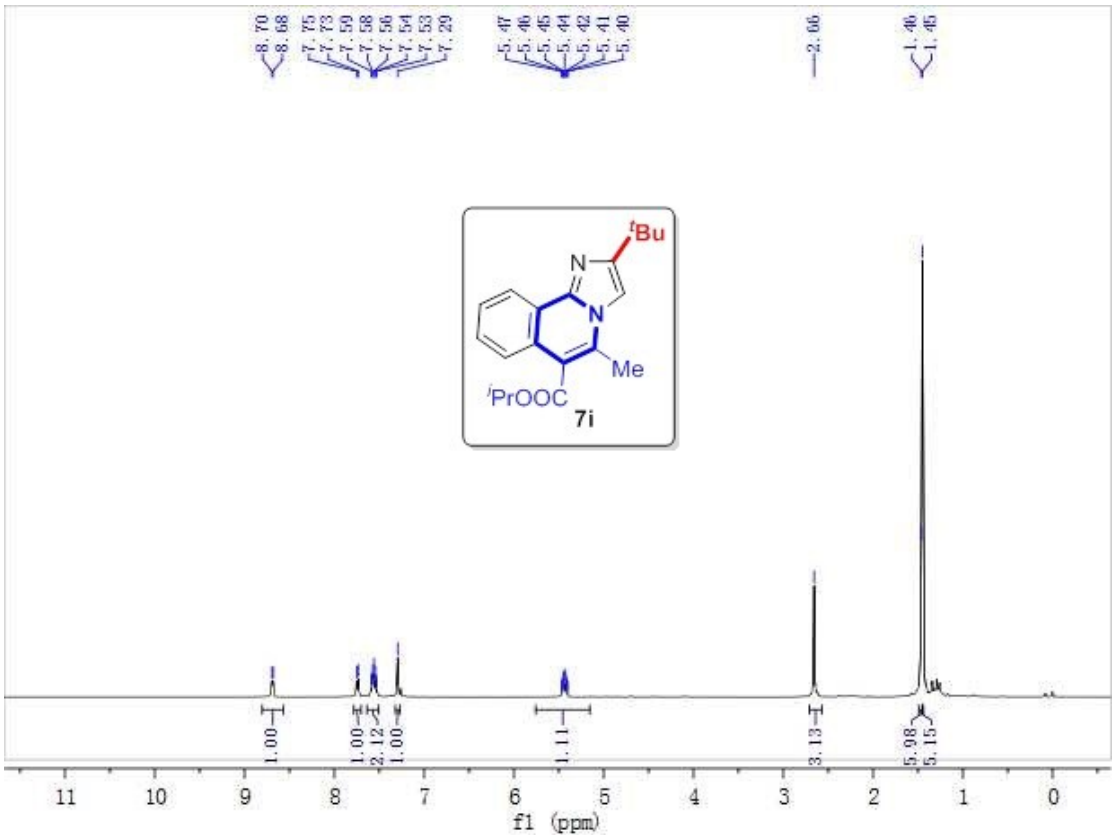
125.08
123.33
122.93
116.97
112.62
70.06
21.90
16.79
Cl
N
N
Me
iPrOOC
7g
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Me
N
N
Me
iPrOOC
7h
f1 (ppm)
f1 (ppm)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7.58
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7.54
7.53
7.29
5.47
5.46
5.45
5.44
5.42
5.41
5.40
2.66
1.46
1.45
tBu
N
N
Me
iPrOOC
7i
1.00
1.00
2.12
1.00
1.11
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5.15
11
10
9
8
7
6
5
4
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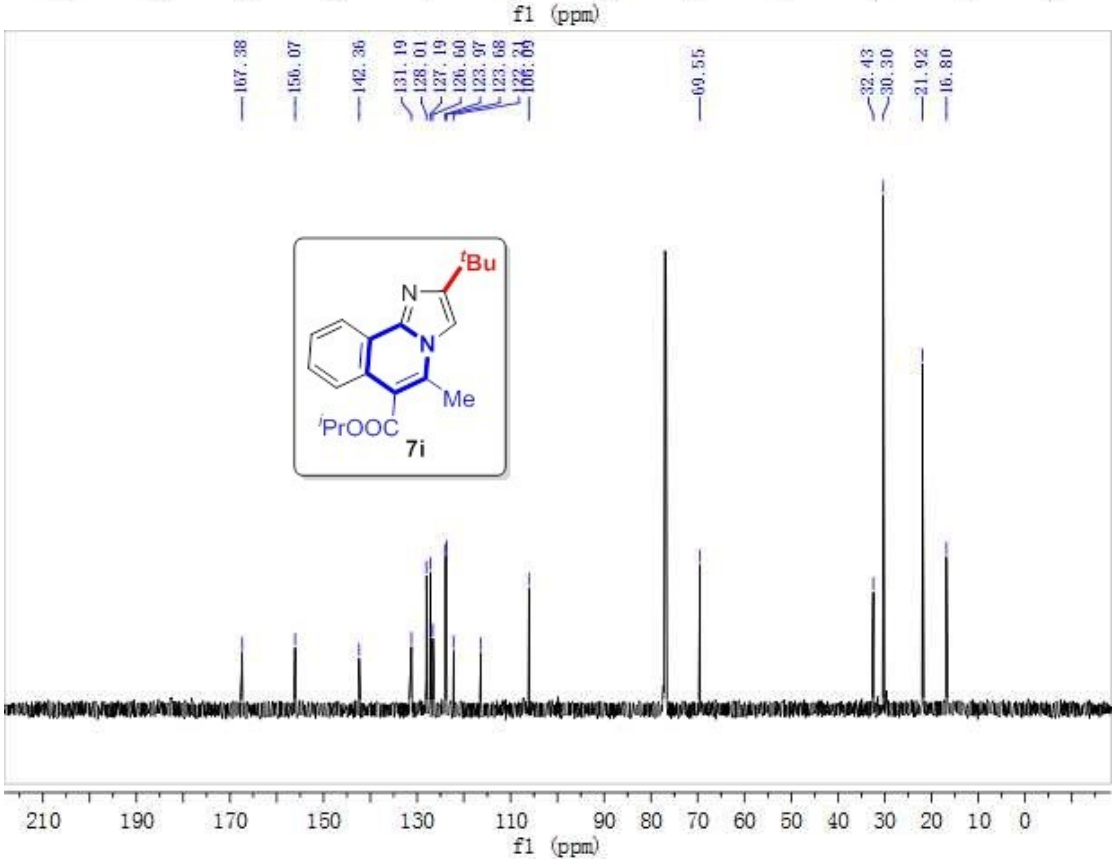
2
1
0
f1 (ppm)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128.01
127.19
126.60
123.97
123.68
122.21
106.09
69.55
32.43
30.30
21.92
16.80
tBu
N
N
Me
iPrOOC
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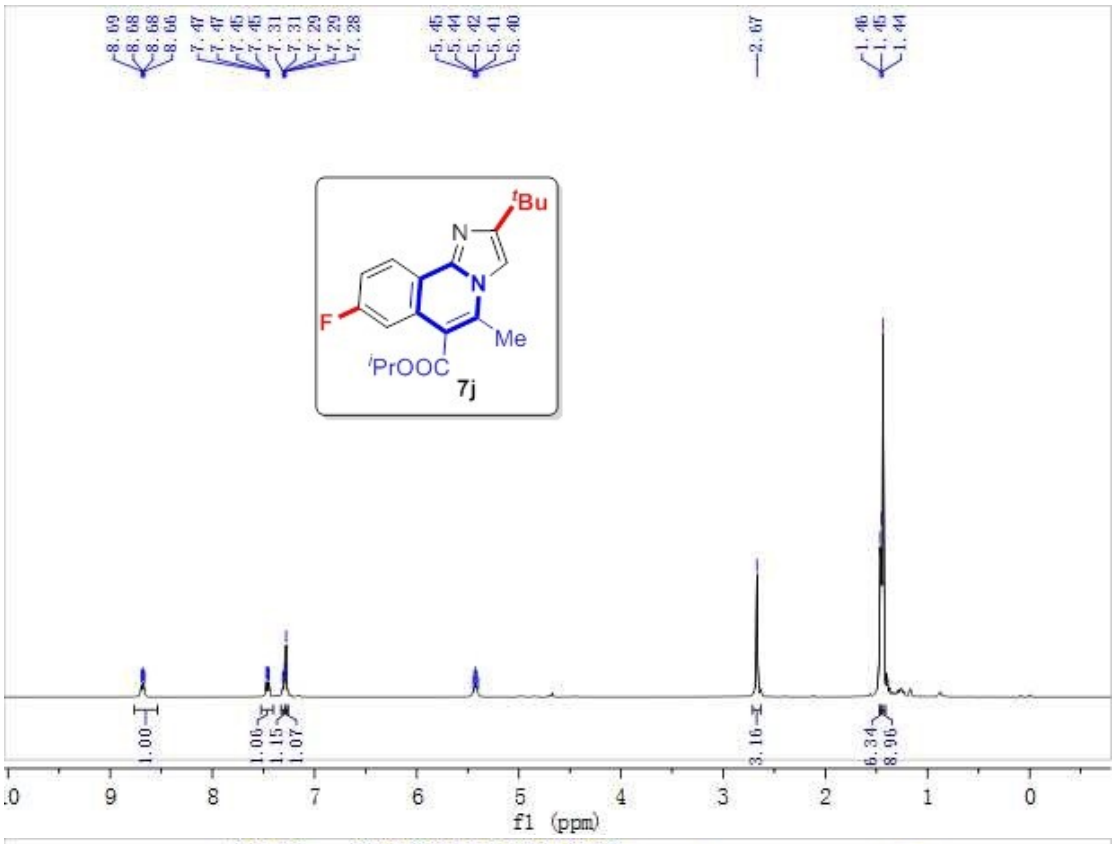
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7.45
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7.28
5.45
5.44
5.42
5.41
5.40
2.67
1.46
1.45
1.44
tBu
N
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F
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7j
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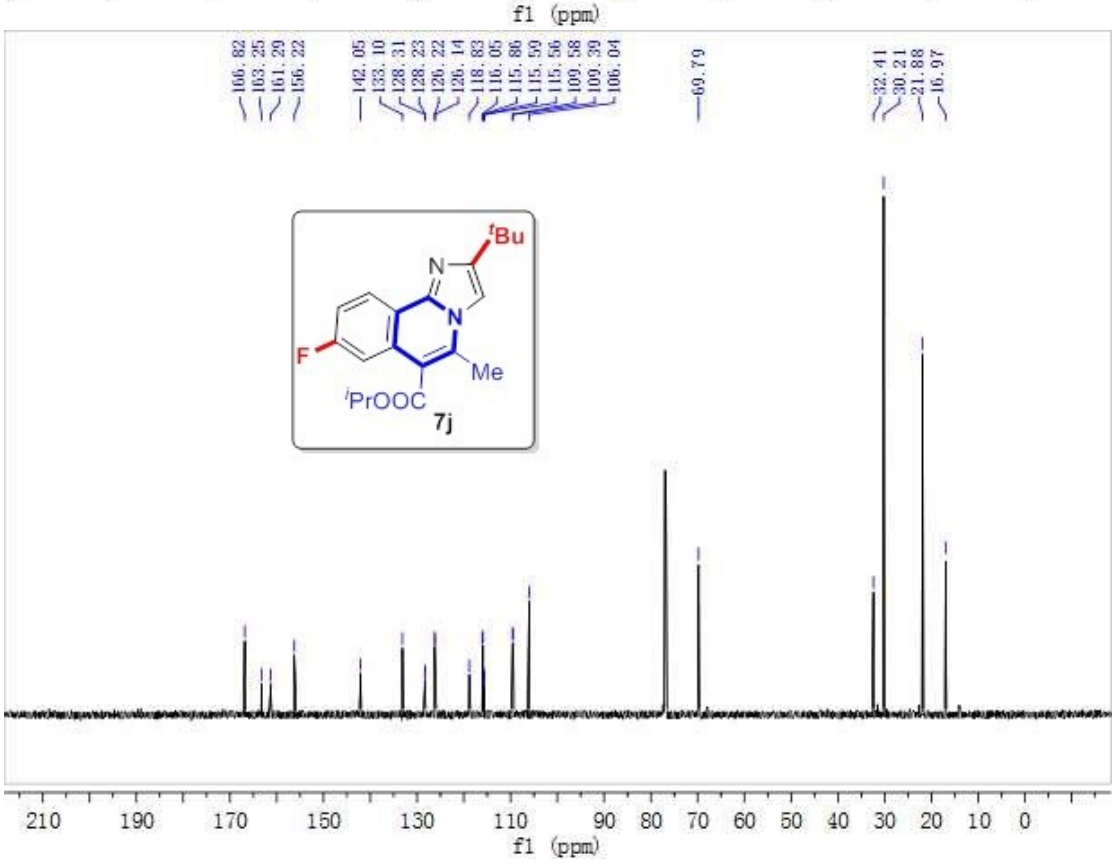
f1 (ppm)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115.56
109.58
109.39
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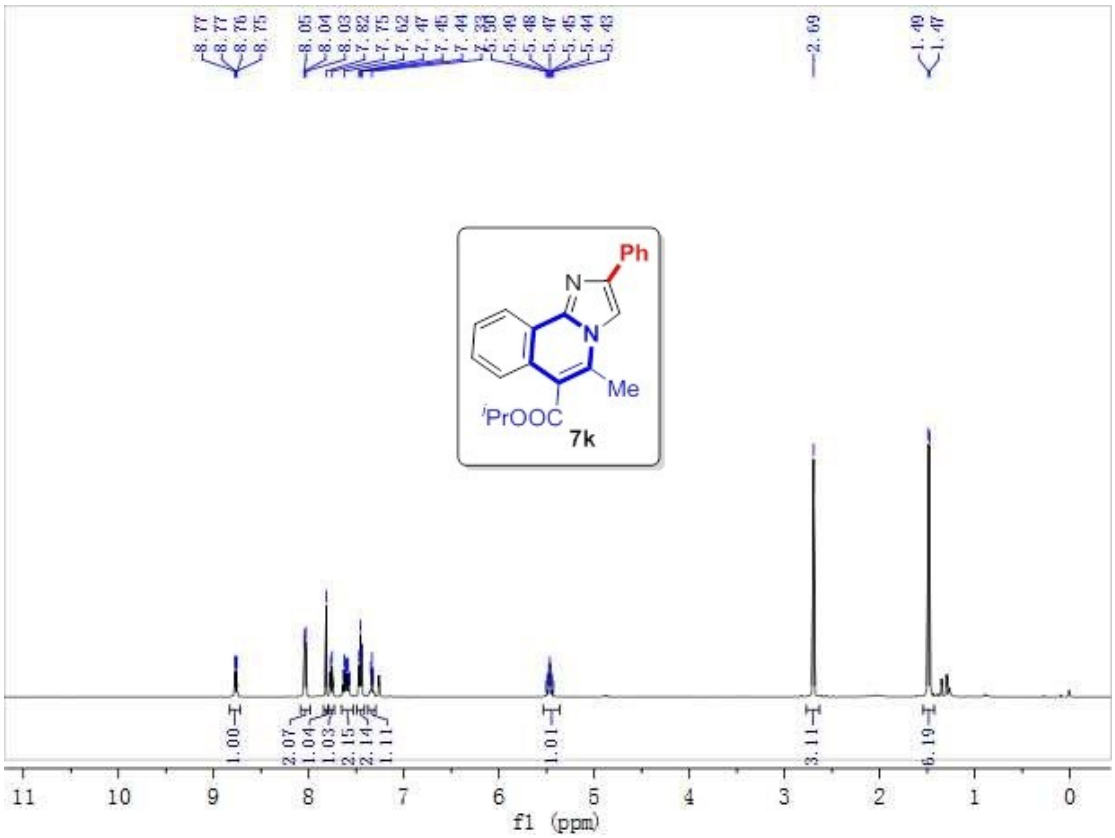
16.97
tBu
N
N
F
Me
iPrOOC
7j
f1 (ppm)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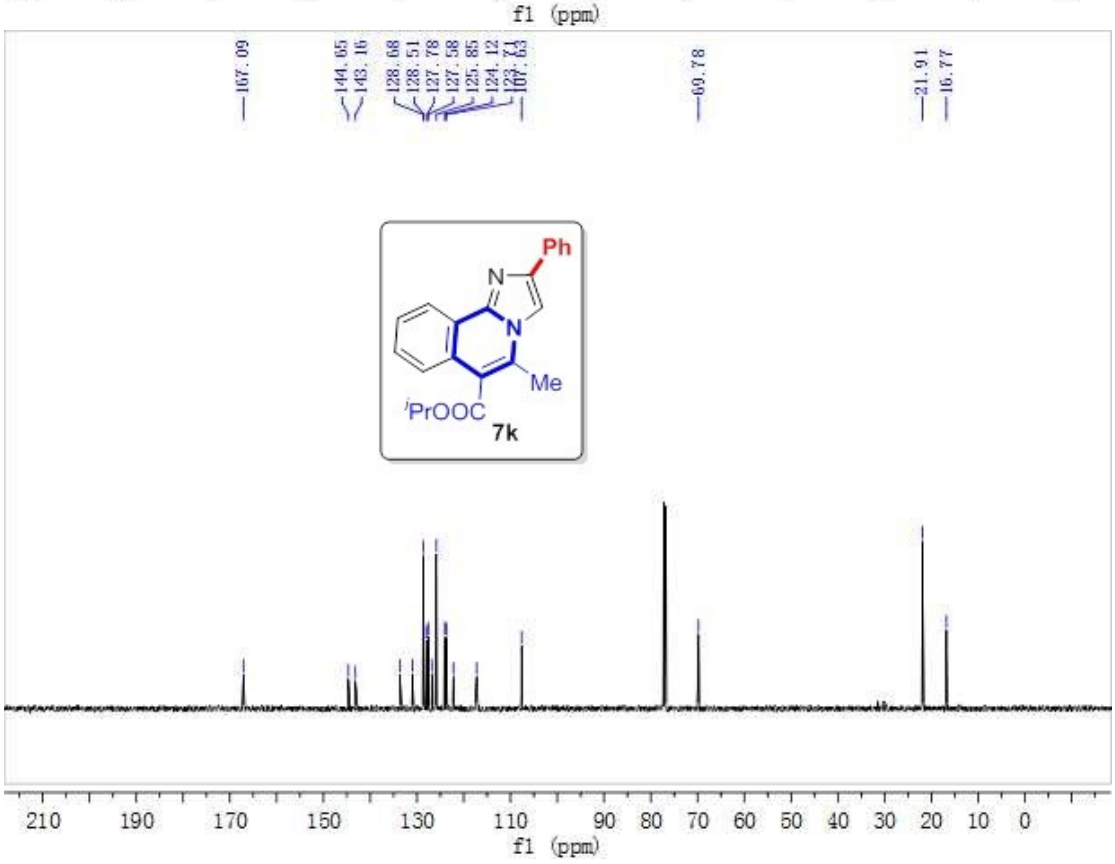
Me
iPrOOC
7k
f1 (ppm)


Ph
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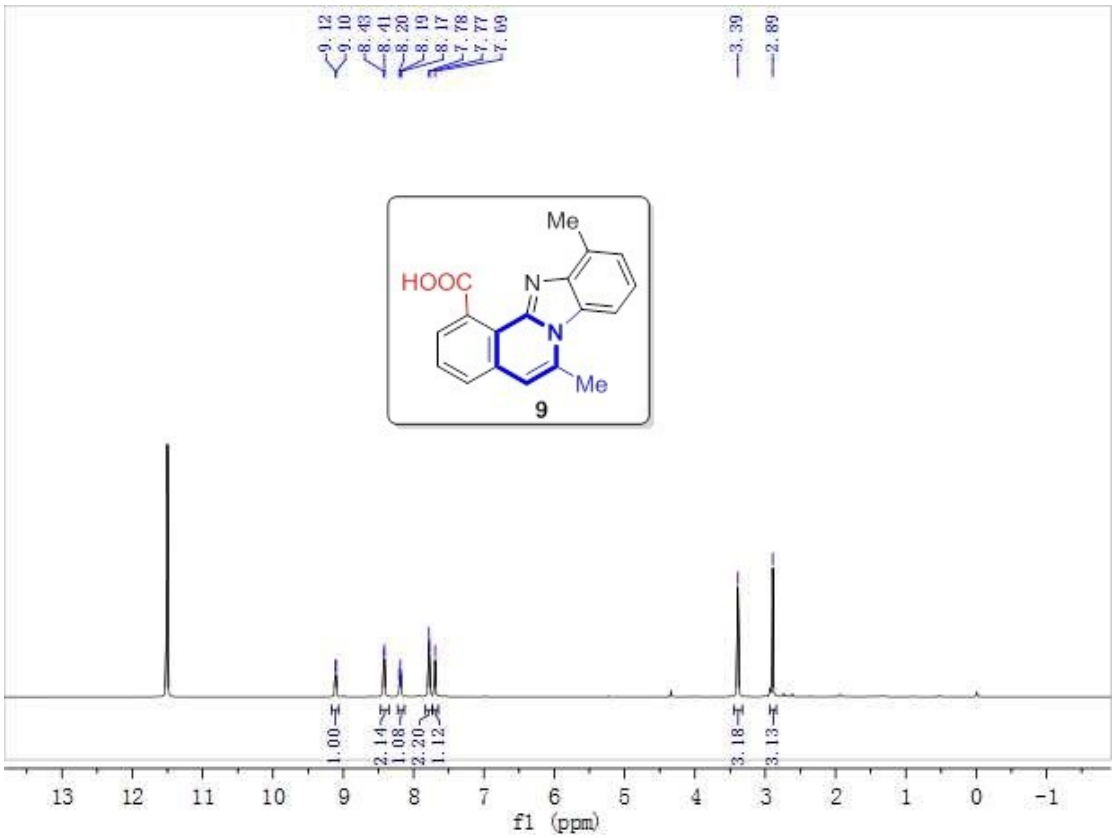
N
Me
iPrOOC
7k
f1 (ppm)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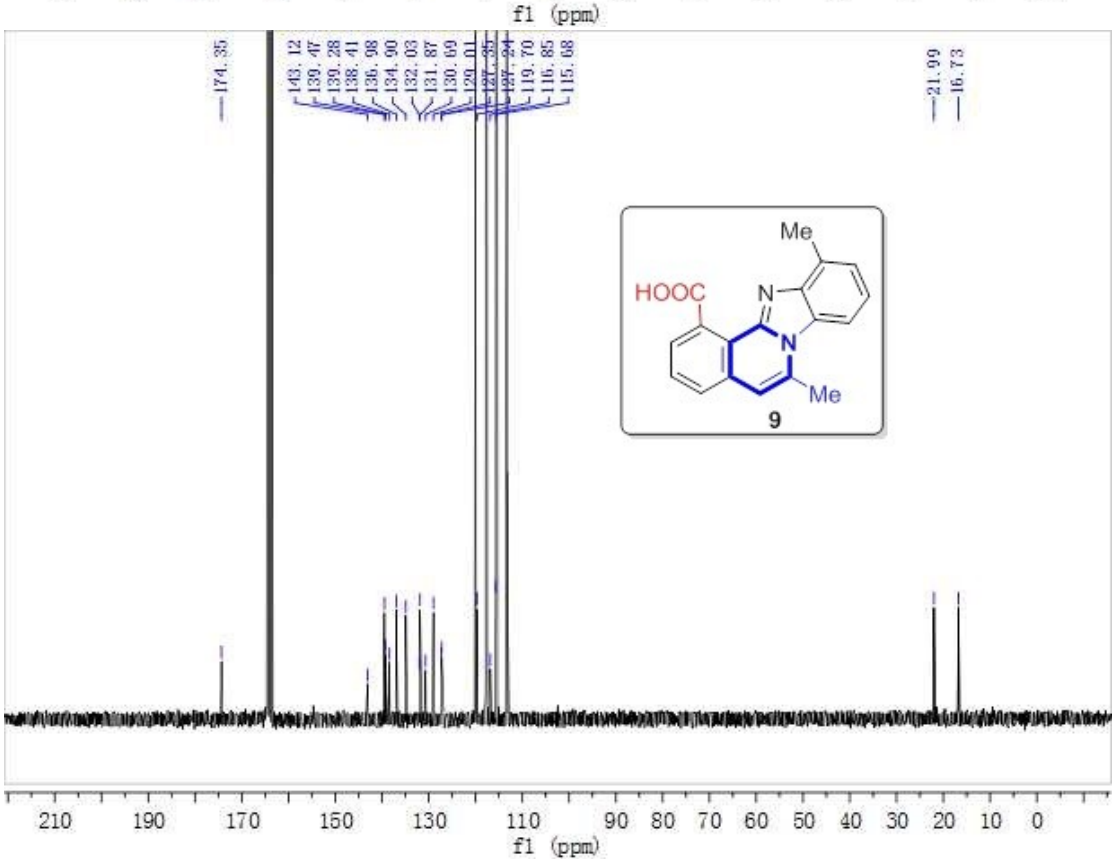
8.41
8.20
8.19
8.17
7.78
7.77
7.69
3.39
2.89
Me
HOOC
N
N
Me
9
1.00
2.14
1.08
2.20
1.12
3.18
3.13
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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139.28
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136.98
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132.03
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130.69
129.01
119.70
116.85
115.68
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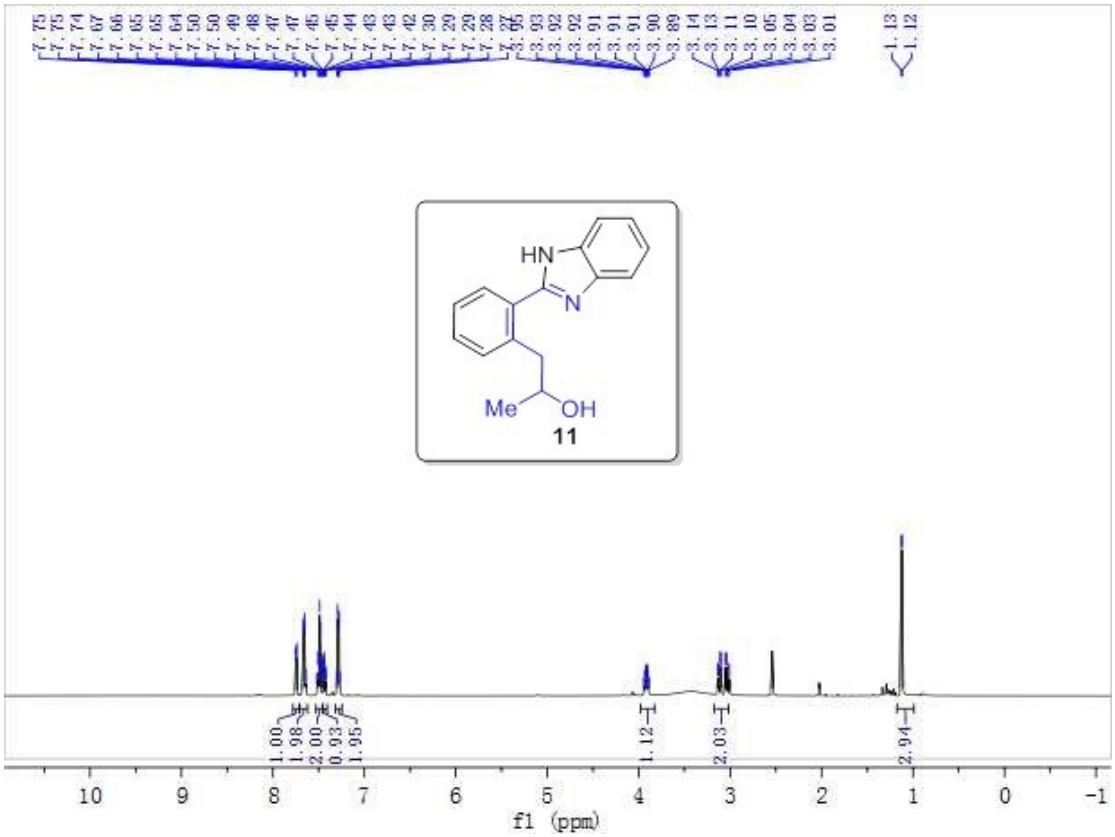
16.73
Me
HOOC
N
N
Me
9
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


HN
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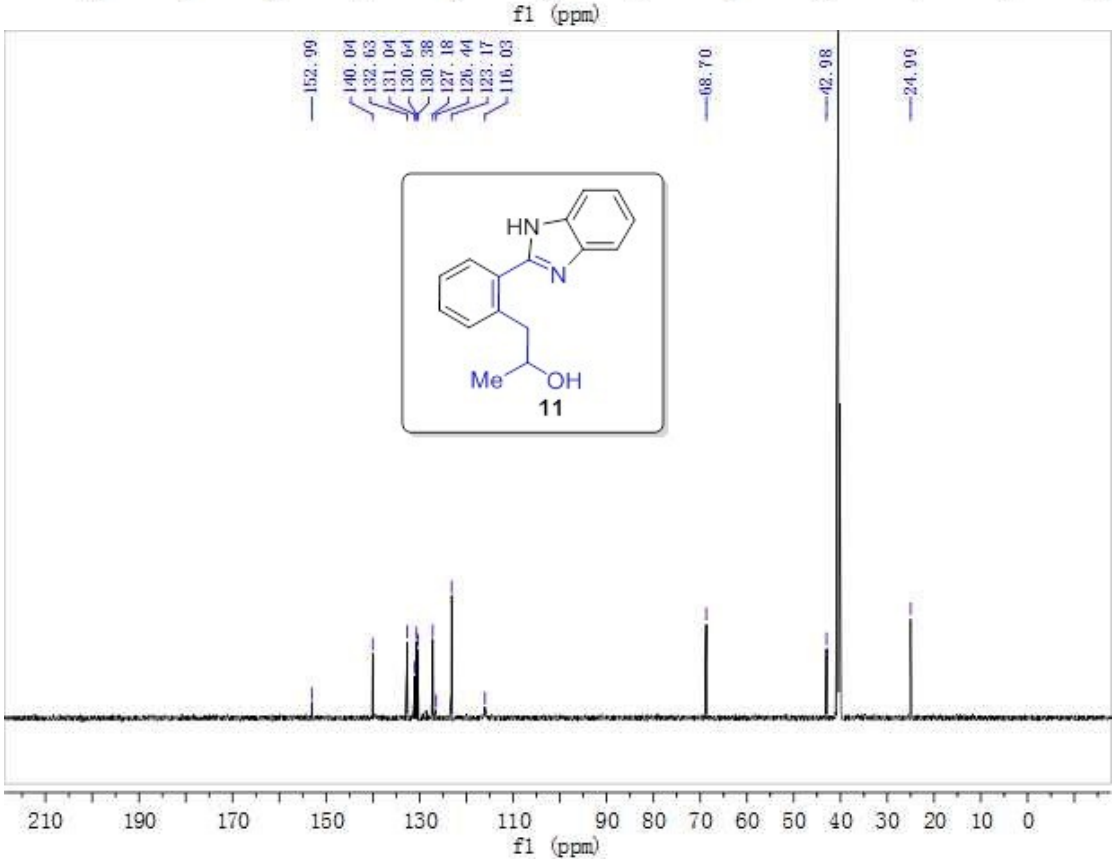
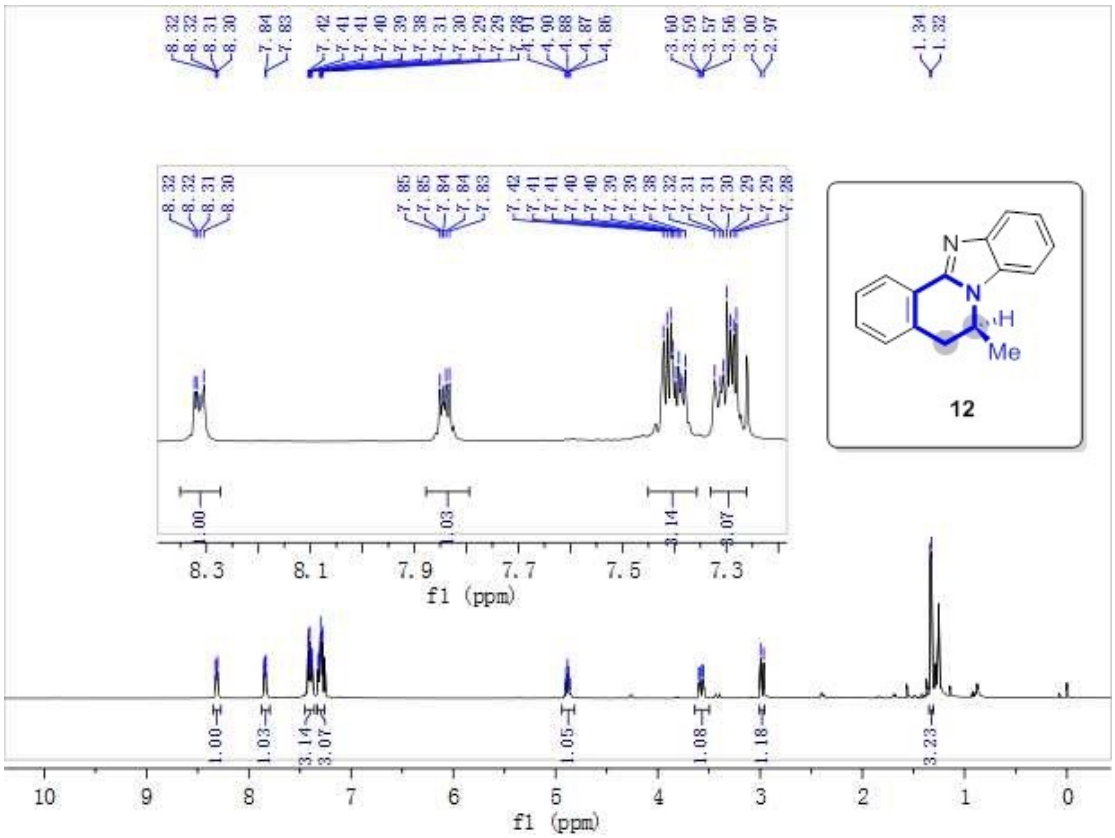
Me
OH
11
f1 (ppm)


HN
N
Me
OH
11
f1 (ppm)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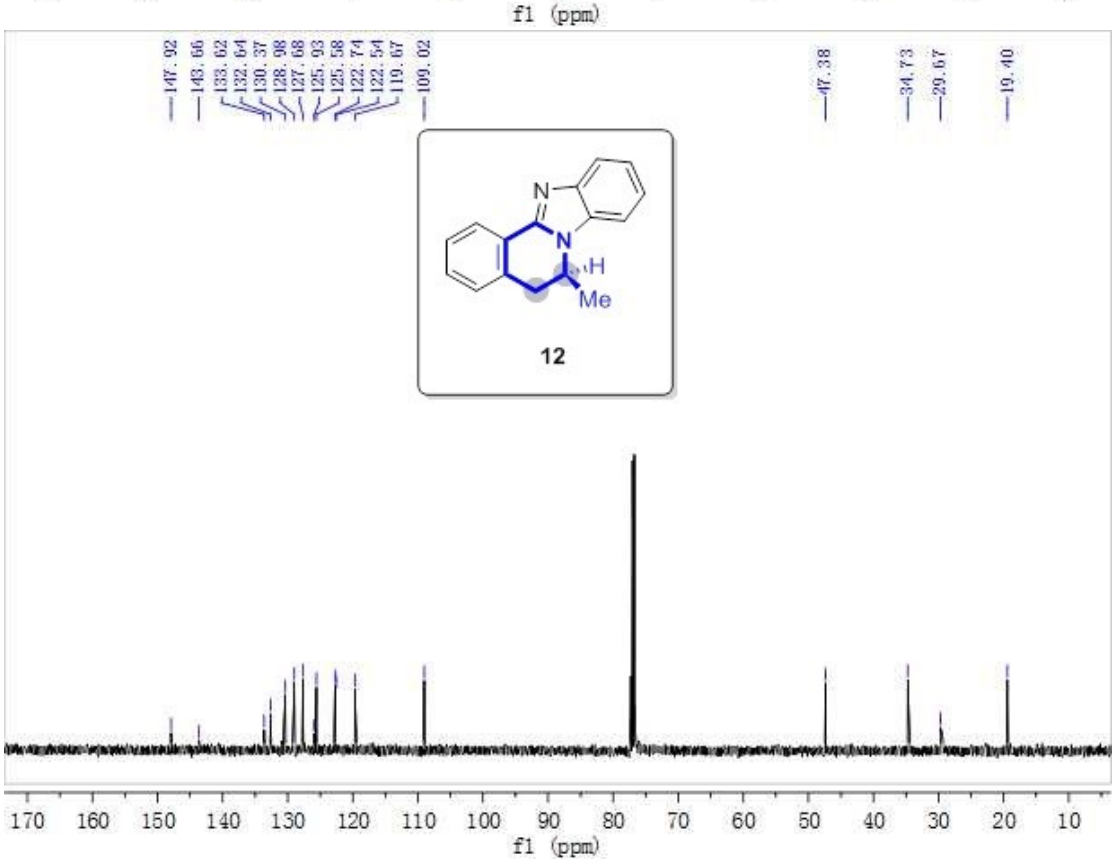
7.40
7.39
7.38
7.31
7.30
7.29
7.29
7.28
4.90
4.88
4.87
4.86
3.60
3.59
3.57
3.56
3.00
2.97
1.34
1.32
1.00
1.03
3.14
3.07
8.3
8.1
7.9
7.7
7.5
7.3
f1 (ppm)
N
N
H
Me
12
1.00
1.03
3.14
3.07
1.05
1.08
1.18
3.23
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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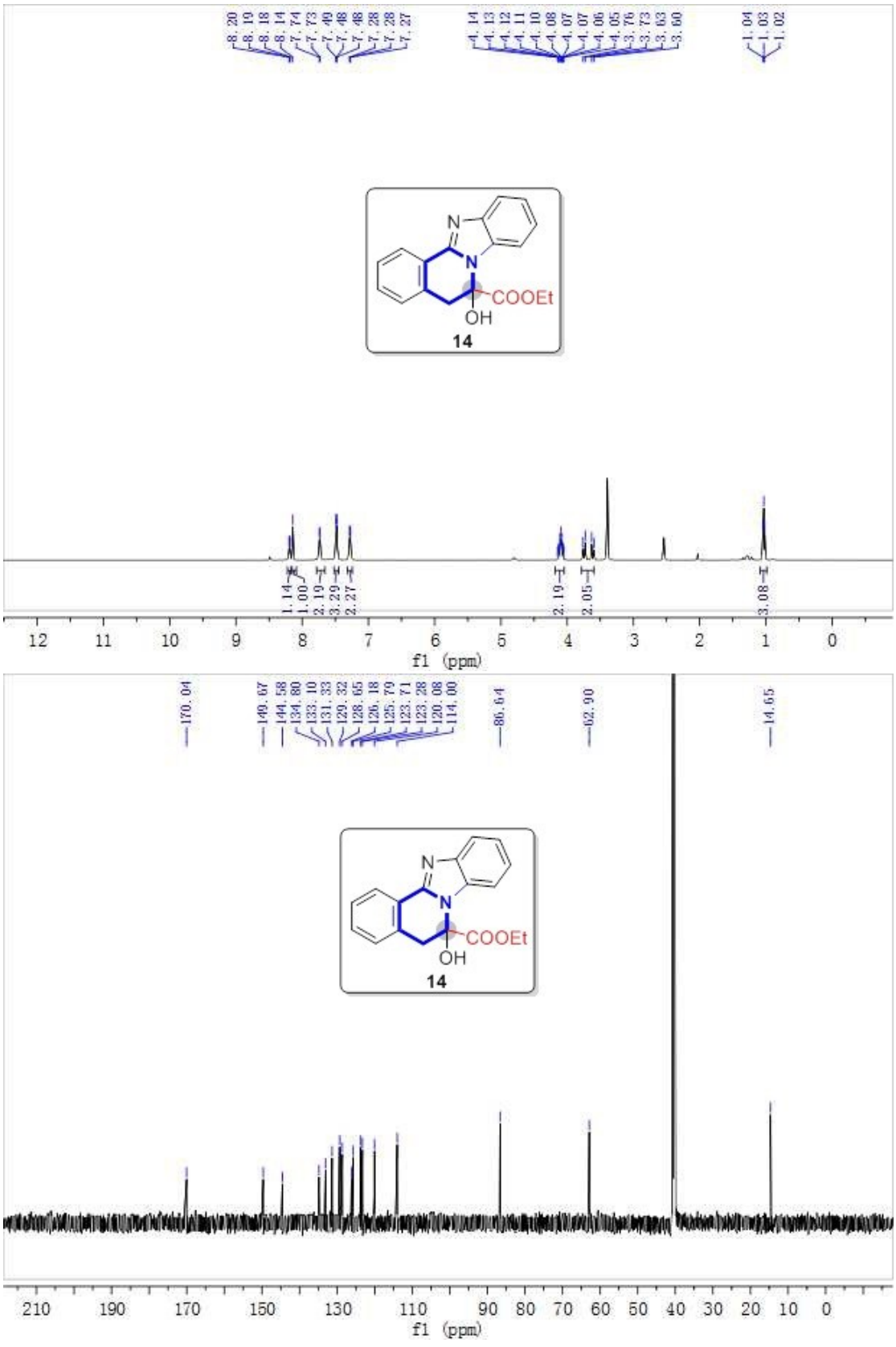
128.98
127.68
125.93
125.58
122.74
122.54
119.67
109.02
47.38
34.73
29.67
19.40
N
N
H
Me
12
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.73
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7.48
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7.28
7.28
7.27
4.14
4.13
4.12
4.11
4.10
4.08
4.07
4.07
4.06
4.05
3.76
3.73
3.63
3.60
1.04
1.03
1.02
N
N
COOEt
OH
14
1.14
1.00
2.19
3.29
2.27
2.19
2.05
3.08
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)
170.04
149.67
144.58
134.80
133.10
131.33
129.32
128.65
126.18
125.79
123.71
123.28
120.08
114.00
86.64
62.90
14.65
N
N
COOEt
OH
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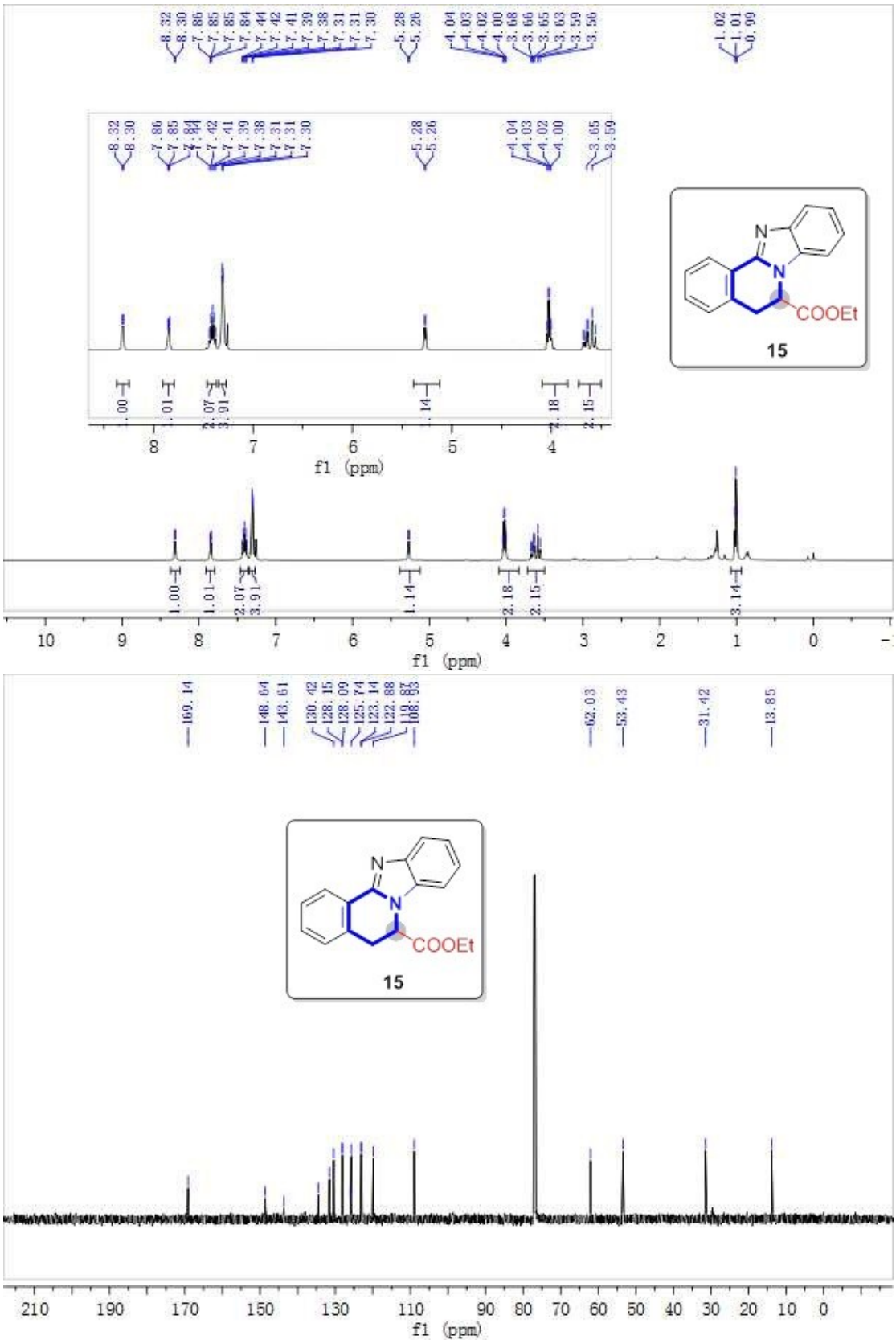
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.85
7.85
7.84
7.44
7.42
7.41
7.39
7.38
7.31
7.31
7.30
5.28
5.26
4.04
4.03
4.02
4.00
3.68
3.65
3.63
3.59
3.56
1.02
1.01
0.99
1.00
1.01
2.07
3.91
1.14
2.18
2.15
3.14
f1 (ppm)
N
N
COOEt
15
169.14
148.64
143.61
130.42
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125.74
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122.88
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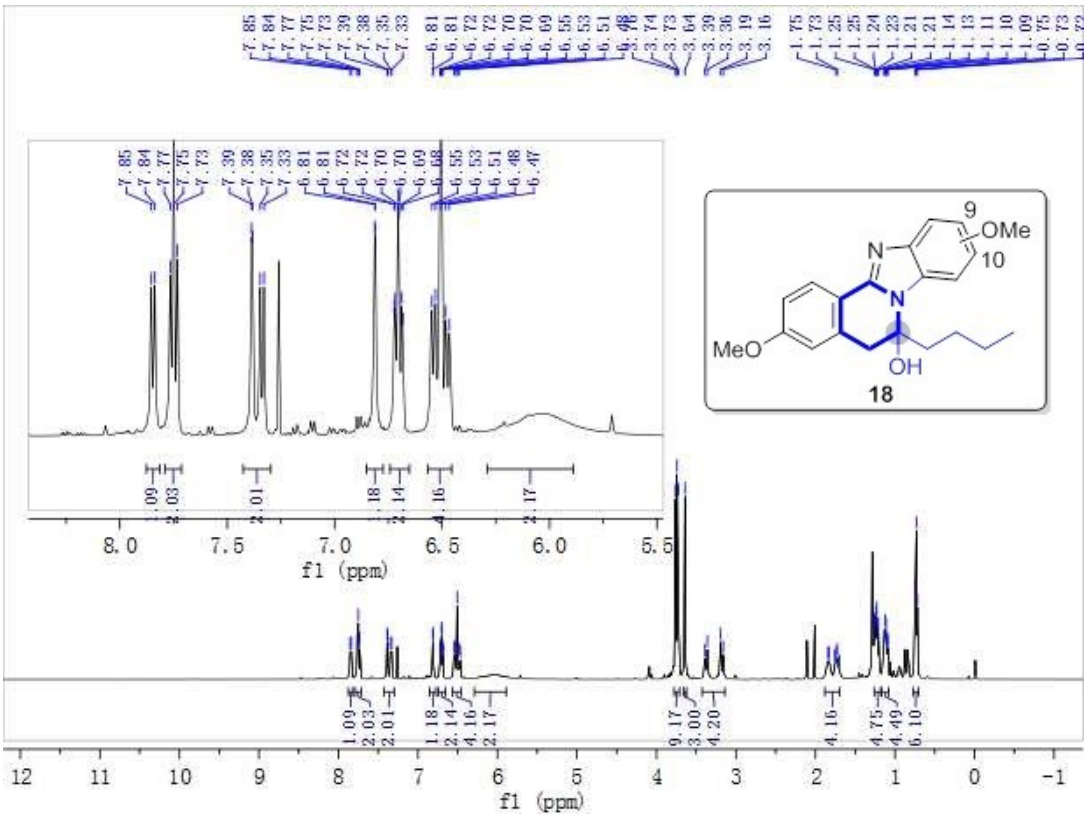
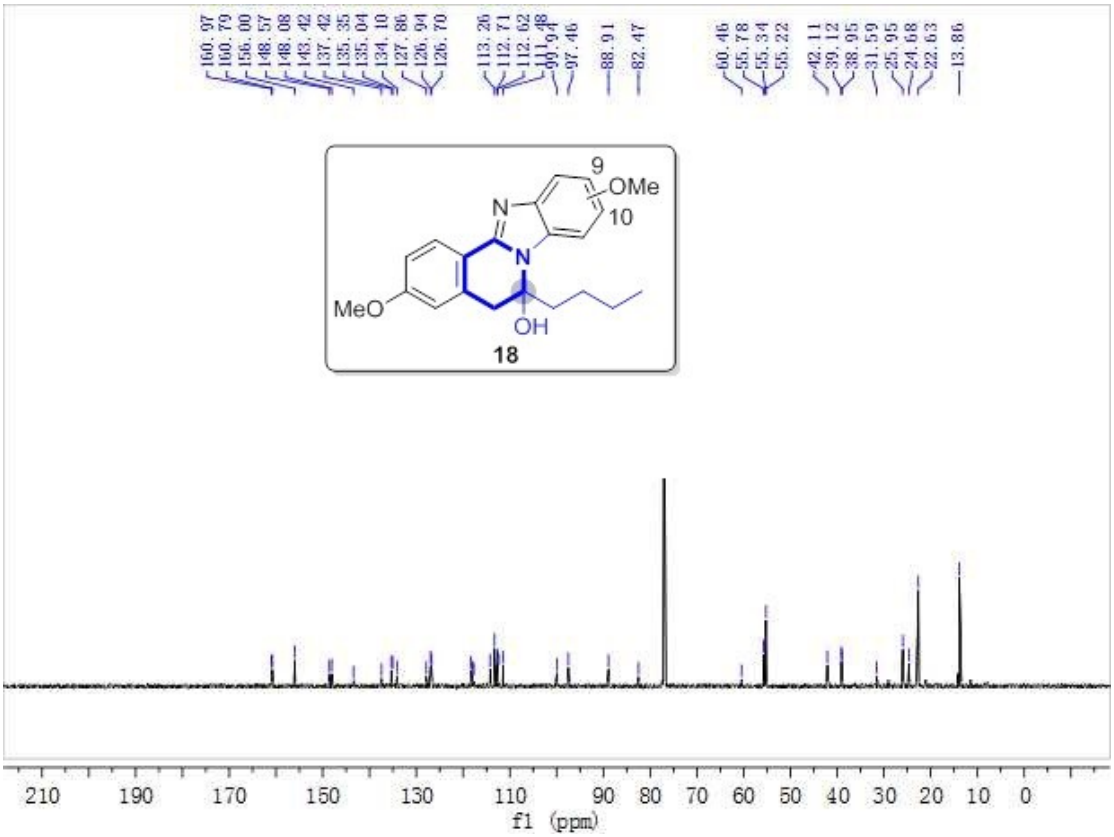
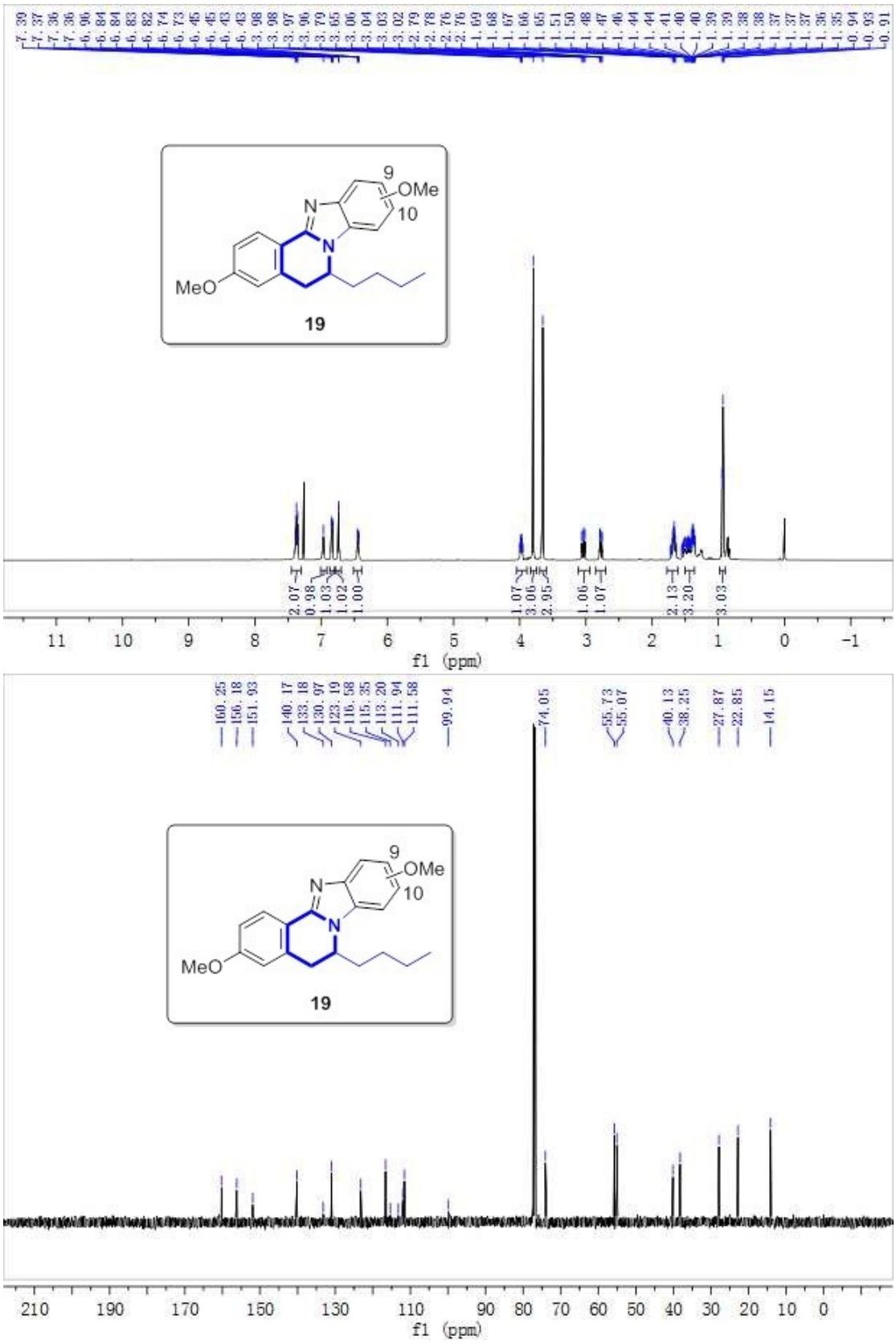
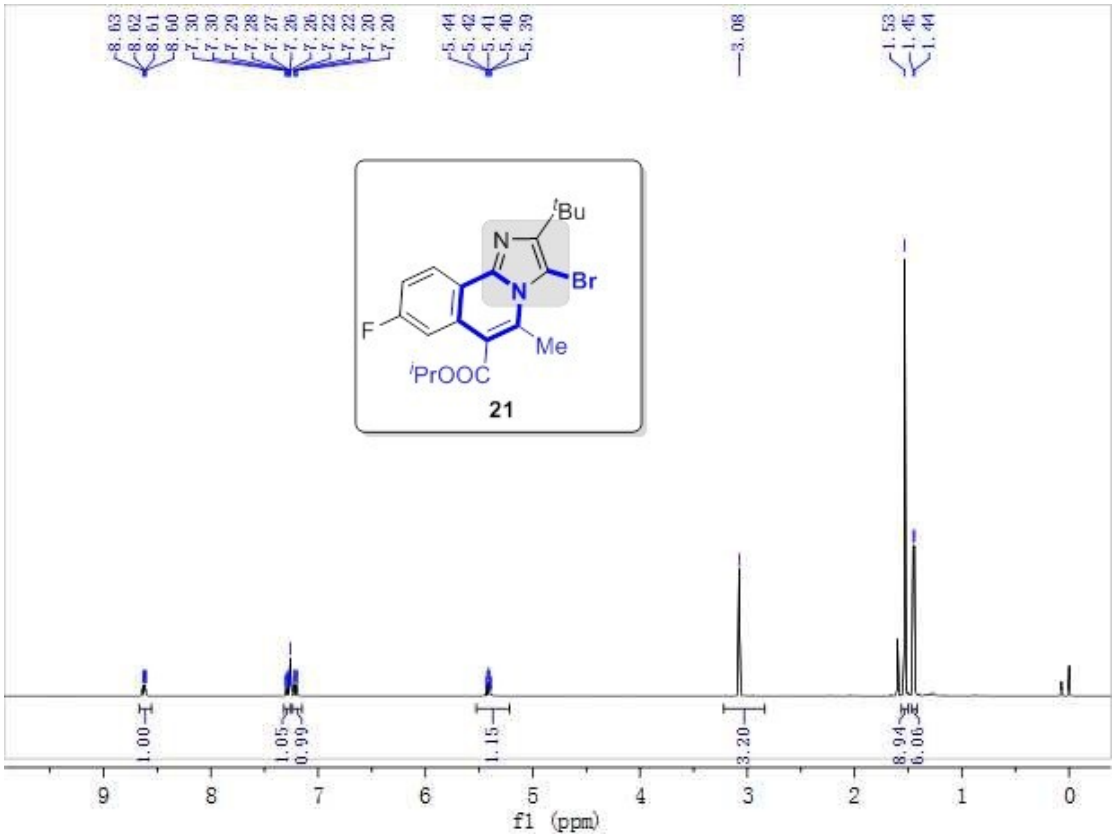
108.83
62.03
53.43
31.42
13.85


9
OMe
10
N
N
MeO
OH
18
f1 (ppm)


9
OMe
10
N
N
MeO
OH
18
f1 (ppm)


9
OMe
10
N
N
MeO
19
f1 (ppm)
9
OMe
10
N
N
MeO
19
f1 (ppm)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8.61
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7.29
7.28
7.27
7.26
7.26
7.22
7.22
7.20
7.20
5.44
5.42
5.41
5.40
5.39
3.08
1.53
1.45
1.44
tBu
N
Br
F
Me
iPrOOC
21
1.00
1.05
0.99
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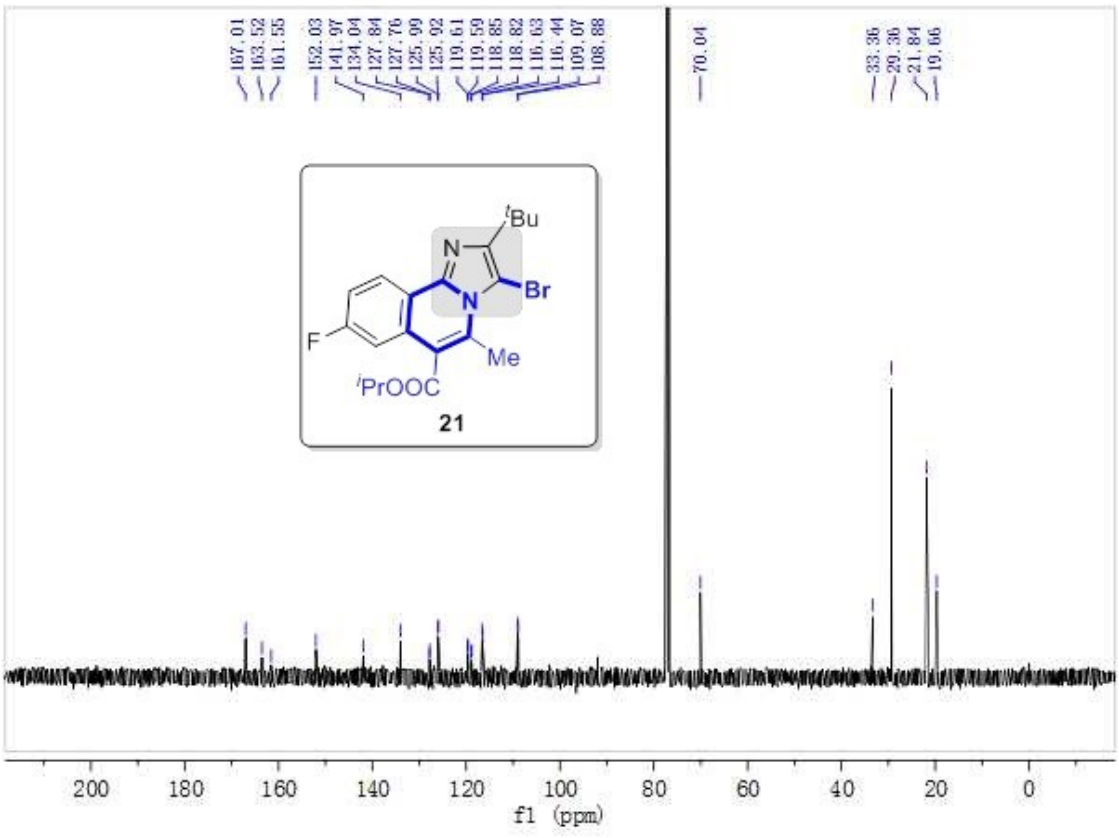
8.94
6.06
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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125.92
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119.59
118.85
118.82
116.63
116.44
109.07
108.88
70.04
33.36
29.30
21.84
19.66
tBu
N
Br
F
Me
iPrOOC
21
200
180
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140
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100
80
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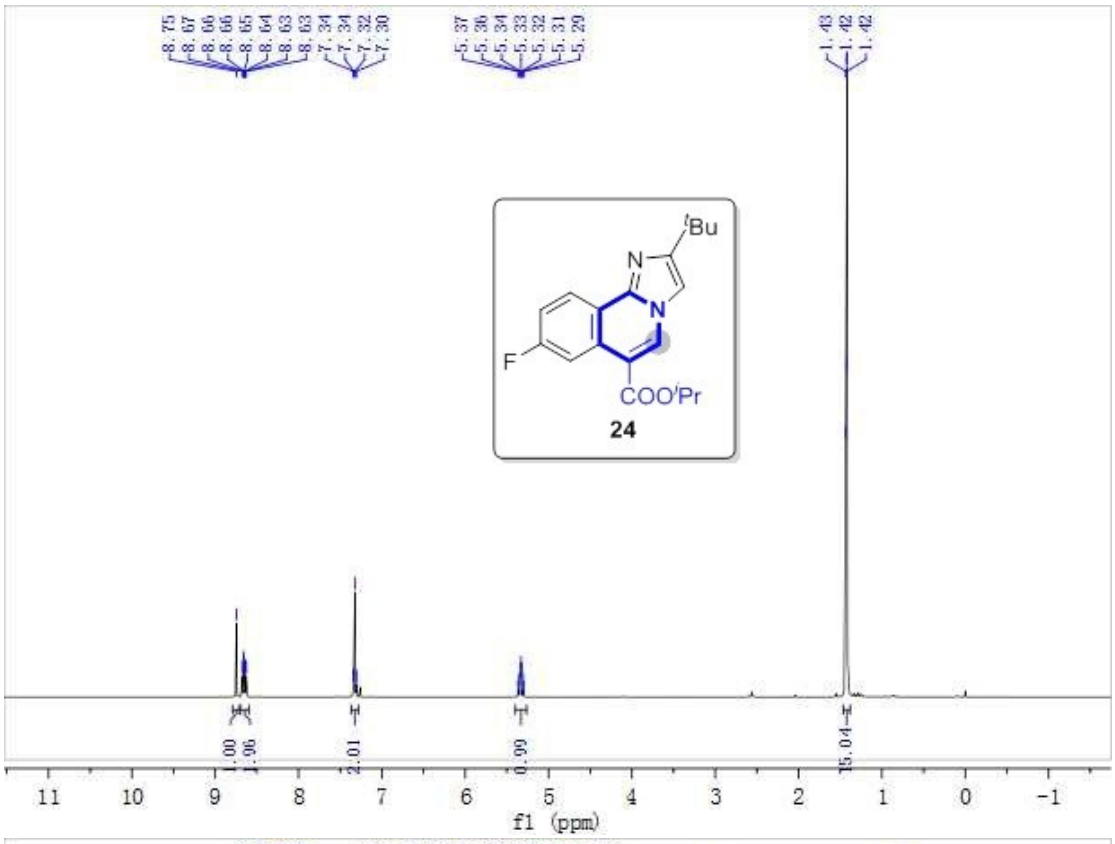
20
0
f1 (ppm)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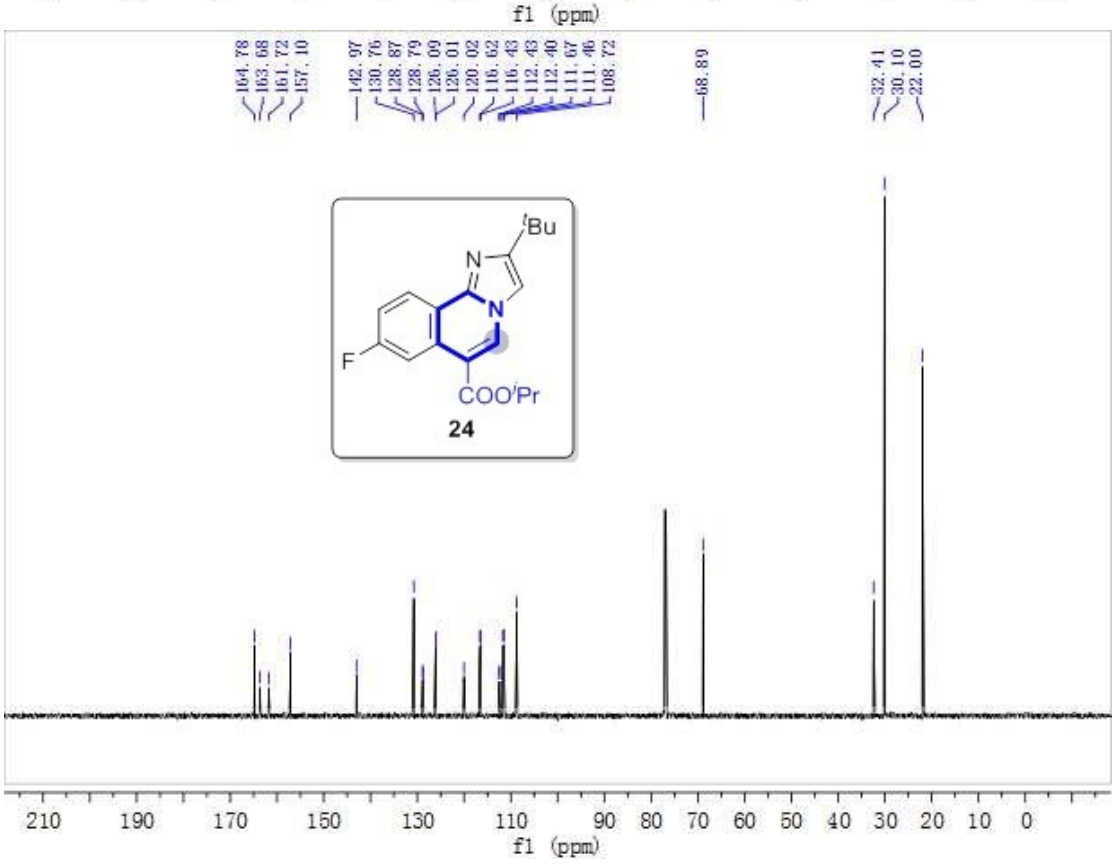
5.37
5.36
5.34
5.33
5.32
5.31
5.29
1.43
1.42
1.42
tBu
N
N
F
COO'Pr
24
1.00
1.96
2.01
0.99
15.04
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)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120.02
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116.43
112.43
112.40
111.67
111.46
108.72
68.89
32.41
30.10
22.00
tBu
N
N
F
COO'Pr
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90
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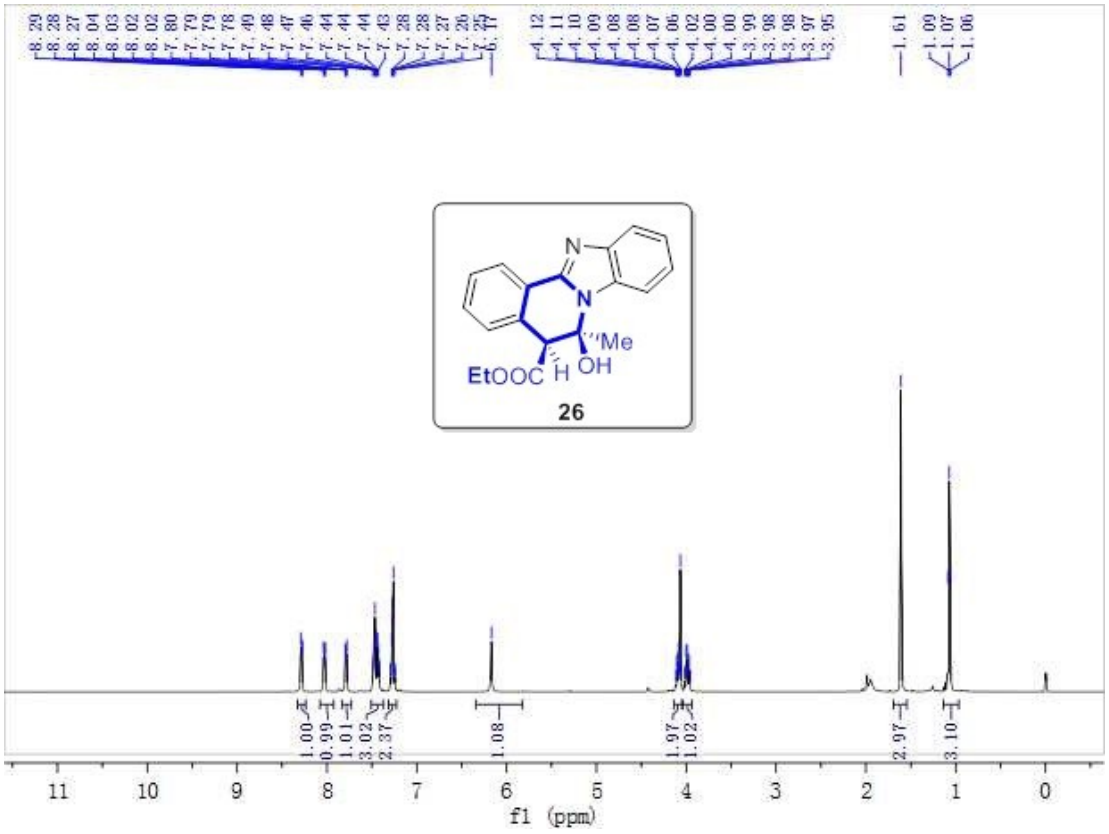
f1 (ppm)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7.46
7.44
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7.44
7.43
7.28
7.28
7.27
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7.25
6.17
4.12
4.11
4.10
4.09
4.08
4.08
4.07
4.06
4.02
4.00
4.00
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3.98
3.98
3.97
3.95
1.61
1.09
1.07
1.06
N
N
Me
EtOOC H OH
26
1.00
0.99
1.01
3.02
2.37
1.08
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3.10
11
10
9
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5
4
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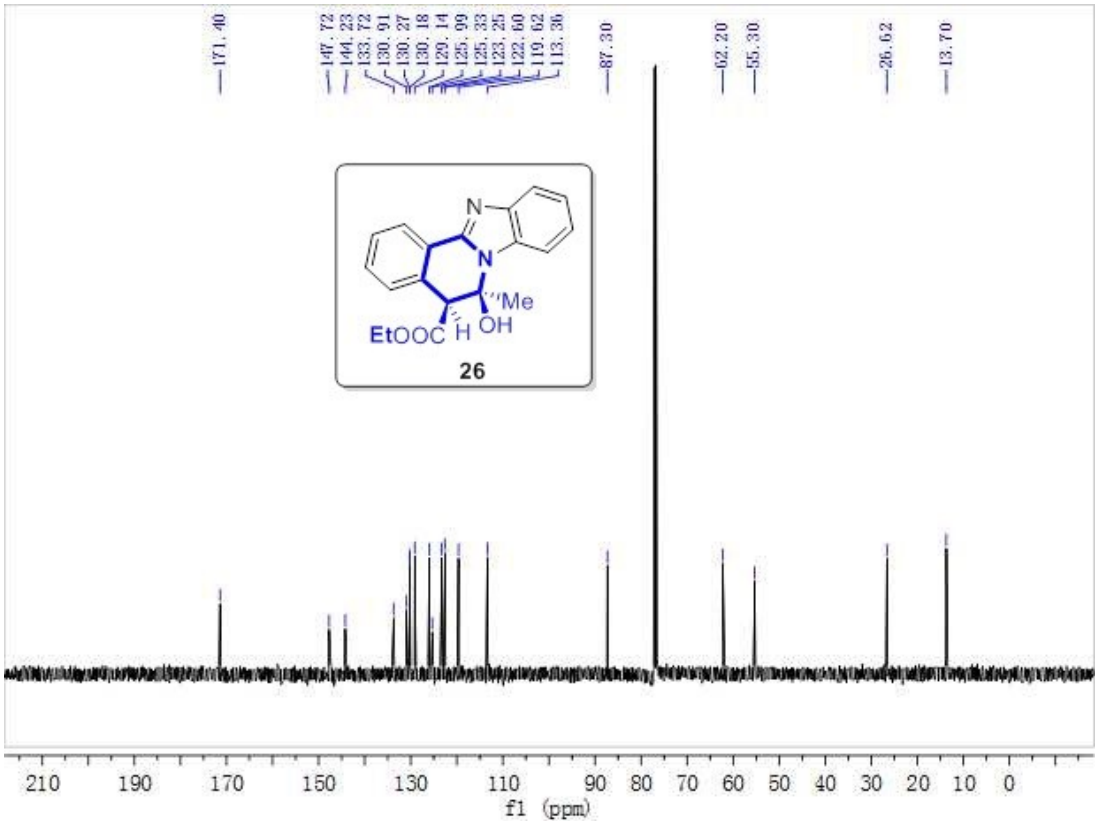
2
1
0
f1 (ppm)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119.62
113.36
87.30
62.20
55.30
26.62
13.70
N
N
Me
EtOOC H OH
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170
150
130
110
90
80
70
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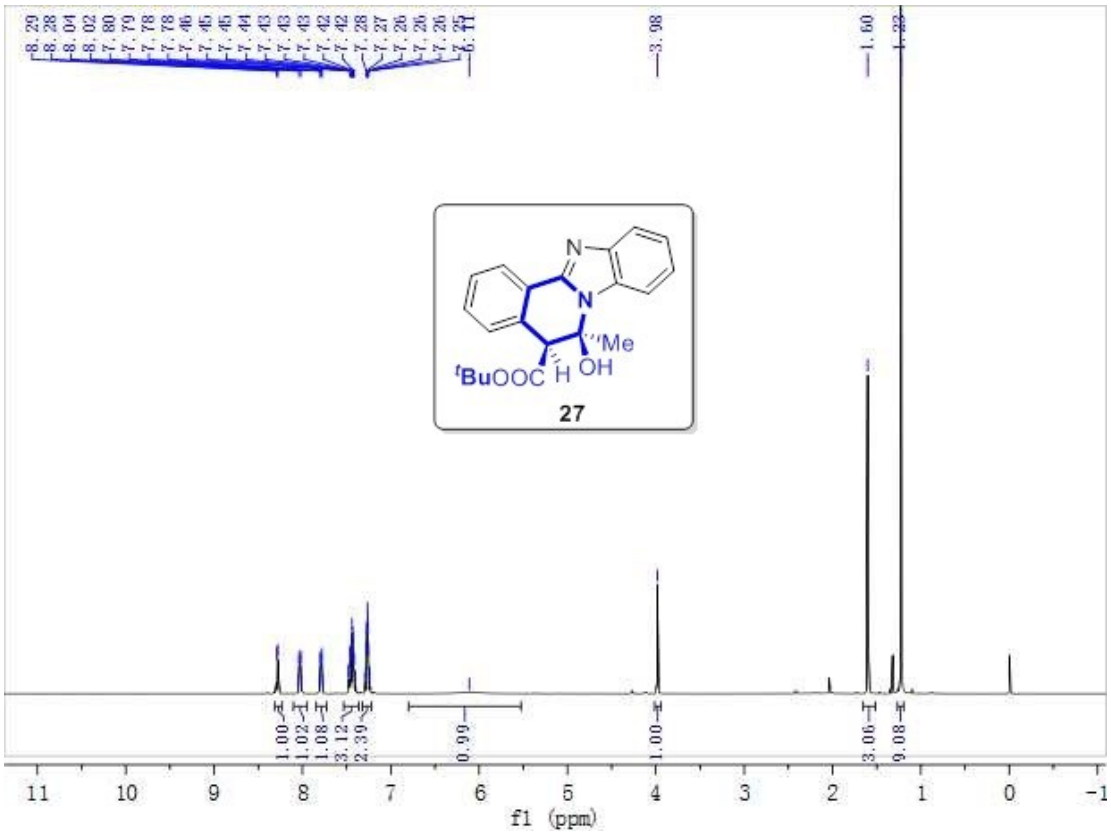
50
40
30
20
10
0
f1 (ppm)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7.46
7.45
7.45
7.44
7.43
7.43
7.43
7.42
7.42
7.28
7.27
7.26
7.26
7.26
7.25
6.71
3.98
1.60
1.23
N
N
Me
tBuOOC H OH
27
1.00
1.02
1.08
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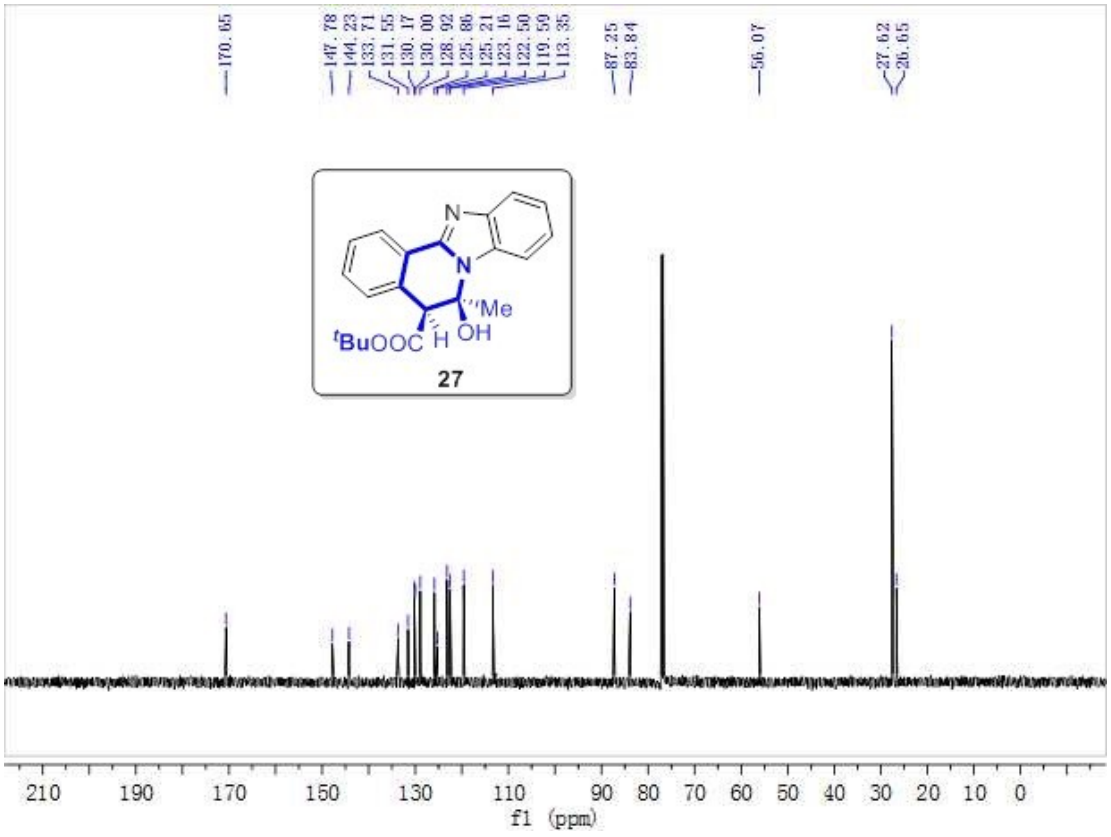
2.39
0.99
1.00
3.06
9.08
11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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119.59
113.35
87.25
83.84
56.07
27.62
26.65
N
N
Me
tBuOOC H OH
27
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)