Supporting Information for:

Controllable synthesis of 3-iodo-2*H*-quinolizin-2-ones and 1,3-diiodo-2*H*-quinolizin-2-ones via electrophilic cyclization of azacyclic ynones

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Table of contents:

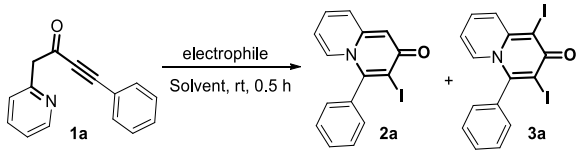
1. General information

NMR spectra were recorded with tetramethylsilane as the internal standard. NMR spectra were recorded on a BrukerAvanceII400M type (^{1}H NMR, 400 MHz; ^{13}C NMR, 100 MHz) spectrometer. High resolution mass spectra (HRMS) were recorded on a Q-TOF mass spectrometry (Micromass, Wythenshawe, UK) equipped with Z-spray ionization source. Infrared spectra (IR) was measured using a Nicolet NEXUS FT-IR spectrophotometer. Melting points were measured on a RY-I apparatus and are reported uncorrected. Substrates **1a-1b**, **1e-1g** and **1i-1w** were prepared according to the previous report.[1] Substrates **1c-1d** and **1h** were synthesized by a similar procedure.

1. (a) Natarajan, S. R.; Chen, M.-H.; Heller, S. T.; Tynebor, R. M.; Crawford, E. M.; Minxiang, C.; Kaizheng, H.; Dong, J.; Hu, B.; Hao, W.; Chen, S.-H. *Tetrahedron Lett.* **2006**, *47*, 5063. (b) James, M. J.; Grant, N. D.; O'Brien, P.; Taylor, R. J. K.; Unsworth, W. P. *Org. Lett.* **2016**, *18*, 6256. (c) Min, X.-L.; Sun, C.; He, Y. *Org. Lett.* **2019**, *21*, 724.

2. Optimization of reaction conditions

Table S1 Optimization of reaction conditions [a]



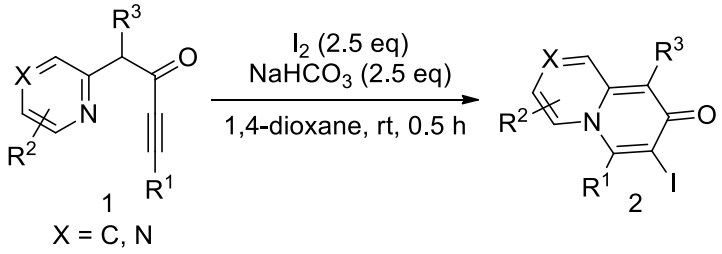
entry	electrophile (x eq)	additive	solvent	yield (%) [b] **2a/3a**
1	I_2 (1.2)	-	CH_2Cl_2	55/-
2	NIS (1.2)	-	CH_2Cl_2	35/21
3	ICl (1.2)	-	CH_2Cl_2	8/6
4	NIS (1.5)	-	CH_2Cl_2	44/38
5	NIS (2.0)	-	CH_2Cl_2	24/64
6	NIS (2.5)	-	CH_2Cl_2	Trace/74
7	I_2 (2.5)	-	CH_2Cl_2	63/-
8	I_2 (2.5)	$NaHCO_3$	CH_2Cl_2	76/-
9	I_2 (2.5)	$NaHCO_3$	DCE	74/-
10	I_2 (2.5)	$NaHCO_3$	CH_3CN	44/27
11	I_2 (2.5)	$NaHCO_3$	Toluene	56/-
12	I_2 (2.5)	$NaHCO_3$	THF	68/trace
13	**I_2 (2.5)**	**$NaHCO_3$**	**1,4-dioxane**	**87/trace**
14[c]	I_2 (2.5)	$NaHCO_3$	1,4-dioxane	82/trace
15	NIS (2.5)	**-**	DCE	trace/76
16	NIS (2.5)	-	CH_3CN	trace/61
17	NIS (2.5)	-	Toluene	trace/37
18	NIS (2.5)	-	THF	trace/46
19	NIS (2.5)	-	1,4-dioxane	trace/23
20[d]	**NIS (2.5)**	**-**	**DCE**	**-/90**

[a] Reaction conditions: **1a** (0.20 mmol, 1.0 equiv), electrophile, additive (2.5 eq), solvent (2.0 mL), rt, 0.5 h. [b] Isolated yields. [c] 1 h.

[d] 2 h.

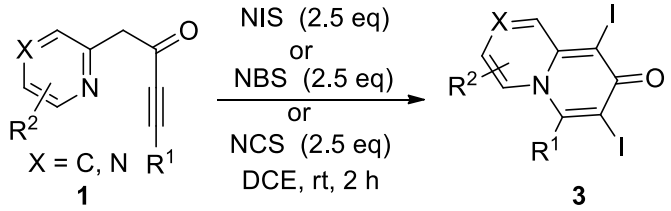
3. General experimental procedures

3.1 General procedure for the synthesis of products 2



A 10 mL reaction tube was successively charged with 0.2 mmol azacyclic ynones **1**, 0.5 mmol I_2, 0.5 mmol $NaHCO_3$ and 2.0 mL 1,4-dioxane. The tube was sealed and the reaction mixture was stirred at room temperature for 0.5 h. After completion of this reaction, the resulting mixture was quenched with saturated solution of NaS_2O_3 (15 ml) and then extracted with dichloromethane (15 mL×3). Then the combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered and concentrated in-vacuo. The crude reaction mixture was purified by column chromatography on silica gel (dichloromethane/methanol) to give products **2**.

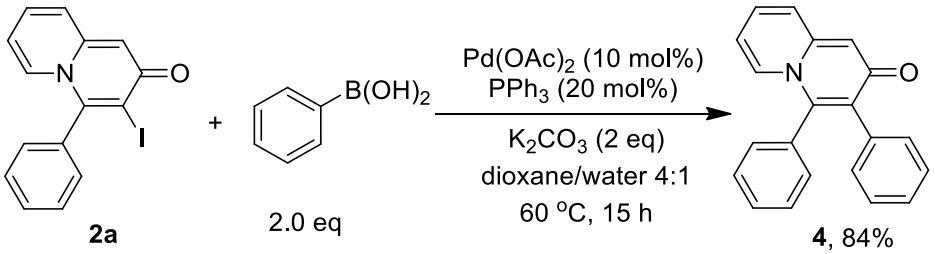
3.2 General procedure for the synthesis of products 3



A 10 mL reaction tube was successively charged with 0.20 mmol azacyclic ynones **1**, 0.5 mmol NIS and 2.0 mL DCE. The tube was sealed and the reaction mixture was stirred at room temperature for 2 h. After completion of this reaction, the resulting mixture was quenched with saturated solution of $NaHCO_3$ (15 ml) and then extracted with dichloromethane (15 mL×3). Then the combined organic layers were washed with brine,

dried over anhydrous Na_2SO_4, filtered and concentrated in-vacuo. The crude reaction mixture was purified by column chromatography on silica gel (dichloromethane/methanol) to give products **3**.

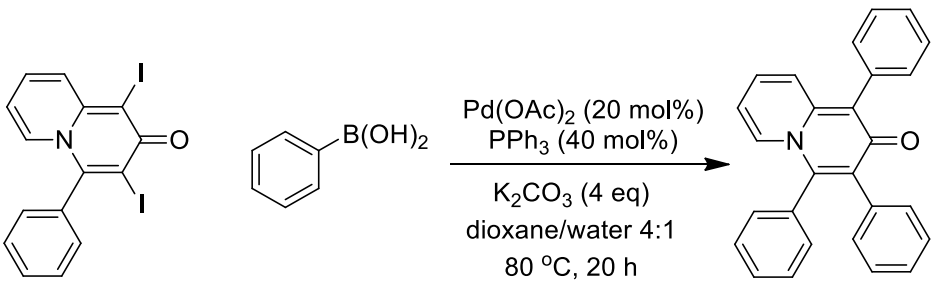
3.3 General procedure for the synthesis of product 4



2a 2.0 eq **4**, 84%

The 3-iodo-4-phenyl-2H-quinolizin-2-one **2a** (0.3 mmol), phenylboronic acid (0.6 mmol), palladium acetate (0.03 mmol), triphenylphosphine (0.06 mmol) and potassium carbonate (0.6 mmol) were dissolved in dioxane/water 4:1 (3 ml). The solution was degassed and flushed with nitrogen and subjected to stirring at 60ºC for 15 h. Then the reaction mixture was diluted with ethyl acetate (50 ml) and washed with water (50 ml) and brine (50 ml). Organic layer was dried under Na_2SO_4 and concentrated in vacuo. Purification was performed by column chromatography (dichloromethane/methanol = 25:1) affording **4** (74.6 mg, 84% yield).

3.4 General procedure for the synthesis of product 5

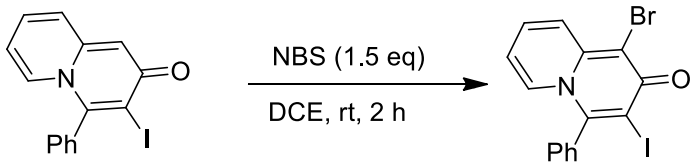


3a 4.0 eq **5**, 72%

The 1,3-diiodo-4-phenyl-2H-quinolizin-2-one **3a** (0.3 mmol), phenylboronic acid (1.2 mmol), palladium acetate (0.03 mmol), triphenylphosphine (0.06 mmol) and potassium

carbonate (1.2 mmol) were dissolved in dioxane/water 4:1 (4 ml). The solution was degassed and flushed with nitrogen and subjected to stirring at 80ºC for 20 h. Then the reaction mixture was diluted with ethyl acetate (50 ml) and washed with water (50 ml) and brine (50 ml). Organic layer was dried under Na_2SO_4 and concentrated in vacuo. Purification was performed by column chromatography (dichloromethane/methanol =100:1) affording **5** (80.7 mg, 72% yield).

3.5 General procedure for the synthesis of product 6

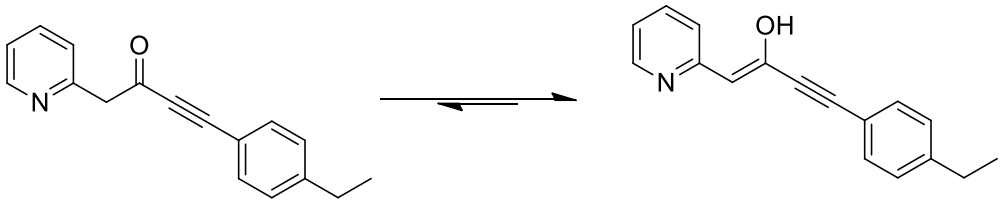


2a **6**, 94%

A 10 mL reaction tube was successively charged with 0.20 mmol **2a**, 0.3 mmol NBS and 2.0 mL DCE. The tube was sealed and the reaction mixture was stirred at room temperature for 2 h. After completion of this reaction, the resulting mixture was quenched with saturated solution of $NaHCO_3$ (15 ml) and then extracted with dichloromethane (15 mL×3). Then the combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered and concentrated in-vacuo. The crude reaction mixture was purified by column chromatography on silica gel (dichloromethane/methanol) to give product **6**.

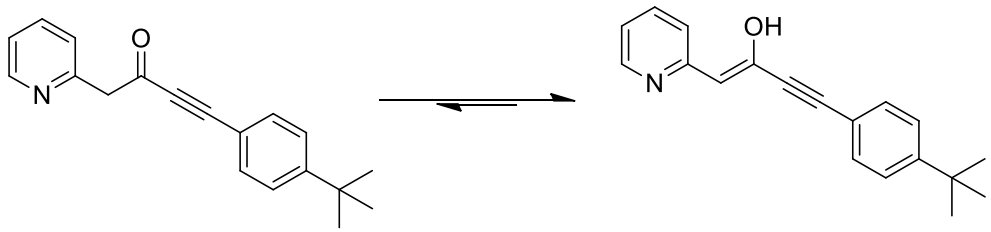
4. Characterization data

4-(4-Ethylphenyl)-1-(pyridin-2-yl)but-3-yn-2-one (1c):



Purified by column chromatography (petroleum ether/ethyl acetate = 10:1); yellow solid (544.6 mg, 71% yield for 3mmol 2-methylpyridine as material; mp 52.8–54.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 14.96 (s, 1H, *enol*), 8.61 (d, *J* = 4.2 Hz, 1H, *keto*), 8.27 (d, *J* = 4.5 Hz, 1H, *enol*), 7.69 (td, *J* = 7.7, 1.8 Hz, 1H, *keto*), 7.62 (td, *J* = 7.9, 1.7 Hz, 1H, *enol*), 7.46 (d, *J* = 8.2 Hz, 2H, *enol*), 7.39 (d, *J* = 8.2 Hz, 2H, *keto*), 7.32 (d, *J* = 7.8 Hz, 1H, *keto*), 7.22 (dd, *J* = 6.8, 5.0 Hz, 1H, *keto*), 7.18 (d, *J* = 8.1 Hz, 3H, *enol*), 7.03–6.93 (m, 3H, *keto*+*enol*), 5.87 (s, 1H, *enol*), 4.16 (s, 2H, *keto*), 2.66 (q, *J* = 7.6 Hz, 4H, *keto*+*enol*), 1.23 (td, *J* = 7.6, 5.3 Hz, 6H, *keto*+*enol*), (*enol*:*keto* = 76:24); ^{13}C NMR (75 MHz, $CDCl_3$) δ 184.0, 157.7, 154.0, 149.7, 149.7, 147.9, 145.6, 144.1, 137.5, 136.7, 133.3, 132.0, 128.2, 128.0, 124.5, 122.3, 121.4, 119.2, 119.1, 116.8, 103.6, 100.0, 93.7, 90.1, 87.8, 86.0, 77.6, 77.2, 76.8, 54.4, 29.0, 28.9, 15.3, 15.1; IR (KBr, cm^{-1}): 3434, 3076, 2966, 2927, 2877, 2193, 1607, 1542, 1460; HRMS (ESI-TOF) calcd for $C_{17}H_{16}NO^{+}$ ($[M+H]^{+}$): 250.1226, found: 250.1227.

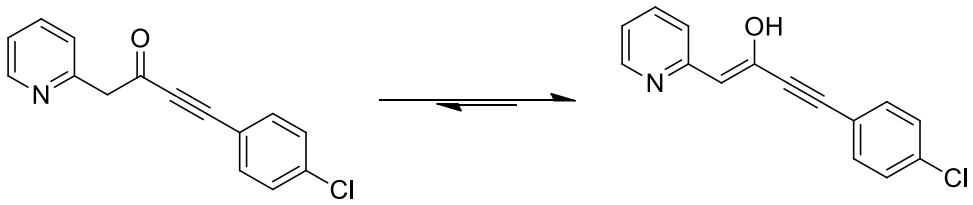
4-(4-Tert-butylphenyl)-1-(pyridin-2-yl)but-3-yn-2-one (1d):



Purified by column chromatography (petroleum ether/ethyl acetate = 10:1); yellow solid (657.3 mg, 79% yield for 3mmol 2-methylpyridine as material); mp 89.2–90.0 ℃; ^{1}H

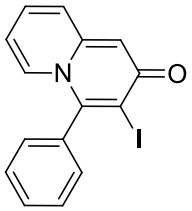
NMR (400 MHz, $CDCl_3$) δ 14.95 (s, 1H, *enol*), 8.61 (d, *J* = 4.7 Hz, 1H, *keto*), 8.28–8.24 (m, 1H, *enol*), 7.69 (td, *J* = 7.7, 1.7 Hz, 1H, *keto*), 7.64–7.58 (m, 1H, *enol*), 7.50–7.46 (m, 4H, *enol*), 7.41–7.30 (m, 5H, *keto*+*enol*), 7.22 (dd, *J* = 7.4, 5.1 Hz, 1H, *keto*), 7.03–6.96 (m, 4H, *keto*+*enol*), 5.87 (s, 1H, *enol*), 4.16 (s, 2H, *keto*), 1.31 (d, *J* = 6.1 Hz, 18H, *keto*+*enol*), (*enol*:*keto* = 80:20); ^{13}C NMR (75 MHz, $CDCl_3$) δ 184.0, 157.7, 154.7, 154.0, 152.4, 149.7, 149.7, 144.1, 137.5, 136.7, 133.1, 131.8, 125.7, 125.4, 124.5, 122.3, 121.4, 119.1, 119.0, 116.7, 103.7, 93.7, 90.0, 87.8, 85.9, 54.4, 35.1, 34.9, 31.2, 31.0; IR (KBr, cm^{-1}): 3431, 3082, 3046, 2961, 2866, 2194, 1607, 1545, 1509, 1464; HRMS (ESI-TOF) calcd for $C_{19}H_{20}NO^+$ $(M+H)^+$ 278.1539, found: 278.1540.

4-(4-Chlorophenyl)-1-(pyridin-2-yl)but-3-yn-2-one (1h):



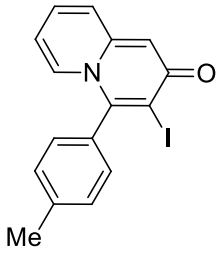
Purified by column chromatography (petroleum ether/ethyl acetate = 10:1); yellow solid (475.6 mg, 62% yield for 3mmol 2-methylpyridine as material); mp 85.6–87.4 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 14.97 (s, 1H, *enol*), 8.63 (s, 1H, *keto*), 8.29 (s, 1H, *enol*), 7.78–7.58 (m, 2H, *keto*+*enol*), 7.54–7.22 (m, 10H, *keto*+*enol*), 7.10–6.97 (m, 2H, *enol*), 5.89 (d, *J* = 8.1 Hz, 1H, *enol*), 4.20 (s, 2H, *keto*), (*enol*:*keto* = 86:14); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.5, 153.7, 149.6, 149.3, 144.0, 137.5, 136.8, 135.1, 134.3, 133.1, 129.1, 128.8, 124.6, 122.4, 121.5, 120.6, 119.2, 118.2, 103.9, 91.4, 88.4, 87.4, 54.2; IR (KBr, cm^{-1}): 3401, 2961, 1617, 1595, 1551, 1490, 1474; HRMS (ESI-TOF) calcd for $C_{15}H_{11}ClNO^+$ ($[M+H]^+$): 256.0524, found: 256.0525.

3-Iodo-4-phenyl-2*H*-quinolizin-2-one (2a):



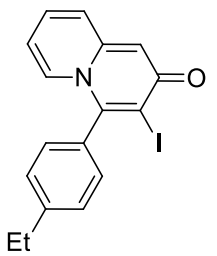
Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (60.3 mg, 87% yield); mp 257.9–259.6 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.68–7.57 (m, 3H), 7.36 (d, *J* = 7.5 Hz, 1H), 7.30 (dd, *J* = 7.9, 1.4 Hz, 2H), 7.21 (d, *J* = 9.0 Hz, 1H), 7.08 (dd, *J* = 8.8, 6.4 Hz, 1H), 6.69 (s, 1H), 6.39–6.32 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.8, 146.9, 144.3, 136.9, 130.6, 130.4, 130.2, 129.1, 128.5, 124.4, 112.3, 109.3, 106.9; IR (KBr, cm^{-1}): 3439, 3090, 2961, 1643, 1592, 1535, 1503; HRMS (ESI-TOF) calcd for $C_{15}H_{11}INO^{+}$ ($[M+H]^{+}$): 347.9880, found: 347.9884.

3-Iodo-4-(p-tolyl)-2*H*-quinolizin-2-one (2b):



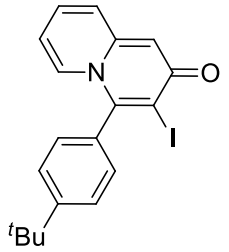
Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (68.1 mg, 94% yield); mp 200.0–201.7 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.44 (d, *J* = 7.9 Hz, 2H), 7.40–7.35 (m, 1H), 7.18 (dd, *J* = 8.3, 6.6 Hz, 3H), 7.10–7.03 (m, 1H), 6.67 (s, 1H), 6.38–6.32 (m, 1H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.9, 147.1, 144.3, 140.6, 134.0, 130.8, 130.7, 129.0, 128.6, 124.4, 112.3, 109.3, 106.8, 21.6; IR (KBr, cm^{-1}): 3439, 3132, 3050, 2920, 1645, 1589, 1526, 1482, 1407; HRMS (ESI-TOF) calcd for $C_{16}H_{13}INO^{+}$ ($[M+H]^{+}$): 362.0036, found: 362.0037.

4-(4-Ethylphenyl)-3-iodo-2*H*-quinolizin-2-one (2c):



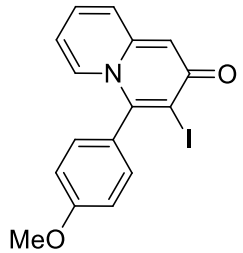
Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (70.7 mg, 94% yield); mp 164.1–165.8 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.46 (d, *J* = 8.1 Hz, 2H), 7.40 (d, *J* = 7.5 Hz, 1H), 7.20 (d, *J* = 8.2 Hz, 3H), 7.10–7.04 (m, 1H), 6.68 (s, 1H), 6.38–6.33 (m, 1H), 2.80 (q, *J* = 7.6 Hz, 2H), 1.34 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.8, 147.2, 146.7, 144.3, 134.2, 130.7, 129.6, 129.0, 128.7, 124.4, 112.4, 109.2, 106.8, 28.8, 15.2; IR (KBr, cm^{-1}): 3431, 3128, 3048, 2962, 2926, 2869, 1643, 1591, 1523, 1408; HRMS (ESI-TOF) calcd for $C_{17}H_{15}INO^{+}$ ($[M+H]^{+}$): 376.0193, found: 376.0194.

4-(4-(*Tert*-butyl)phenyl)-3-iodo-2*H*-quinolizin-2-one (2d):



Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (68.8 mg, 85% yield); mp 285.6–287.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.63 (d, *J* = 8.3 Hz, 2H), 7.39 (d, *J* = 7.5 Hz, 1H), 7.20 (t, *J* = 8.1 Hz, 3H), 7.07 (dd, *J* = 8.7, 6.7 Hz, 1H), 6.68 (s, 1H), 6.40–6.32 (m, 1H), 1.42 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.9, 153.7, 147.2, 144.3, 134.0, 130.8, 128.7, 128.5, 127.0, 124.4, 112.2, 109.3, 106.8, 35.0, 31.3; IR (KBr, cm^{-1}): 3431, 2957, 2865, 1644, 1599, 1527, 1478, 1454, 1401; HRMS (ESI-TOF) calcd for $C_{19}H_{19}INO^{+}$ ($[M+H]^{+}$): 404.0506, found: 404.0509.

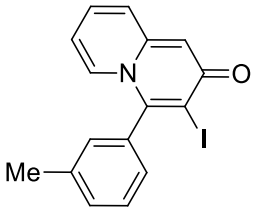
3-Iodo-4-(4-methoxyphenyl)-2*H*-quinolizin-2-one (2e):



Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (72.4 mg, 96% yield); mp 231.6–233.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.46–7.41 (m, 1H), 7.23–7.11 (m, 5H), 7.10–7.04 (m, 1H), 6.66 (s, 1H), 6.39–6.34 (m, 1H),

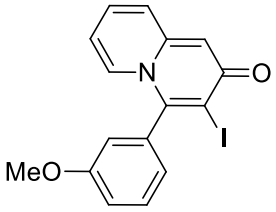
3.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.9, 160.8, 146.9, 144.3, 130.7, 130.6, 129.1, 128.6, 124.3, 115.5, 112.3, 109.9, 106.8, 55.5; IR (KBr, cm^{-1}): 3436, 3114, 3084. 2959, 2836, 1642, 1596, 1522, 1482, 1407; HRMS (ESI-TOF) calcd for $C_{16}H_{13}INO_2^+$ ($[M+H]^+$): 377.9986, found: 377.9993.

3-Iodo-4-(m-tolyl)-2*H*-quinolizin-2-one (2f):



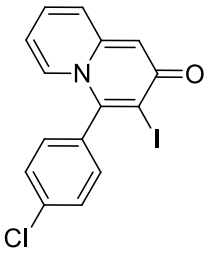
Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (62.1 mg, 86% yield); mp 101.7–103.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.52 (t, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 7.4 Hz, 2H), 7.21 (d, *J* = 9.0 Hz, 1H), 7.12–7.04 (m, 3H), 6.69 (s, 1H), 6.40–6.34 (m, 1H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.8, 147.2, 144.3, 140.2, 136.8, 131.1, 130.8, 130.0, 129.4, 128.8, 126.1, 124.4, 112.6, 108.7, 106.8, 21.5; IR (KBr, cm^{-1}): 3426, 3054, 2964, 2845, 2216, 1646, 1590, 1518, 1466; HRMS (ESI-TOF) calcd for $C_{16}H_{13}INO_2^+$ ($[M+H]^+$): 362.0036, found: 362.0039.

3-Iodo-4-(3-methoxyphenyl)-2*H*-quinolizin-2-one (2g):



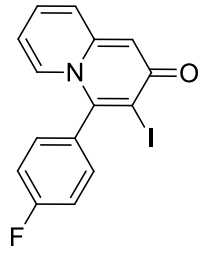
Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (70.4 mg, 93% yield); mp 127.3–129.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.55 (t, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 7.5 Hz, 1H), 7.20 (d, *J* = 9.0 Hz, 1H), 7.15–7.04 (m, 2H), 6.87 (d, *J* = 7.5 Hz, 1H), 6.82 (s, 1H), 6.68 (s, 1H), 6.37 (t, *J* = 6.9 Hz, 1H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.8, 160.8, 146.7, 144.3, 137.9, 131.4, 130.7, 128.7, 124.4, 121.0, 116.0, 114.5, 112.4, 108.7, 106.8, 55.6; IR (KBr, cm^{-1}): 3421, 3136, 3052, 2964, 2846, 2217, 1647, 1590, 1521, 1493; HRMS (ESI-TOF) calcd for $C_{16}H_{13}INO_2^+$ ($[M+H]^+$): 377.9986, found: 377.9984.

4-(4-Chlorophenyl)-3-iodo-2*H*-quinolizin-2-one (2h):



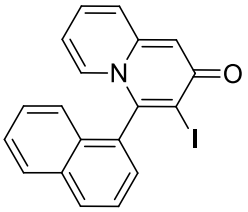
Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (56.0 mg, 73% yield); mp 227.1–229.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.64 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 7.5 Hz, 1H), 7.27 (d, *J* = 8.3 Hz, 2H), 7.22 (d, *J* = 9.1 Hz, 1H), 7.13–7.05 (m, 1H), 6.68 (s, 1H), 6.40 (t, *J* = 6.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.6, 145.7, 144.3, 136.7, 135.2, 130.7, 130.6, 130.3, 128.7, 124.5, 112.6, 109.5, 107.0; IR (KBr, cm^{-1}): 3434, 3116, 3088, 3042, 1646, 1594, 1534, 1497; HRMS (ESI-TOF) calcd for $C_{15}H_{10}ICINO^{+}$ ($[M+H]^{+}$): 381.9490, found: 381.9493.

4-(4-Fluorophenyl)-3-iodo-2*H*-quinolizin-2-one (2i):



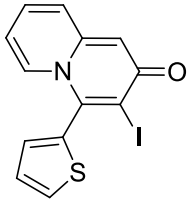
Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (67.2 mg, 92% yield); mp 273.0–274.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.43–7.28 (m, 5H), 7.20 (d, *J* = 9.1 Hz, 1H), 7.07 (ddd, *J* = 9.1, 6.5, 0.8 Hz, 1H), 6.67 (s, 1H), 6.40–6.33 (m, 1H); ^{13}C NMR (75 MHz, DMSO) δ (ppm): 170.8, 163.2 (d, $J_{C\text{-}F}$ = 245.9 Hz), 146.6, 144.6, 133.9 (d, $J_{C\text{-}F}$ = 3.4 Hz), 132.5 (d, $J_{C\text{-}F}$ = 8.6 Hz), 131.4, 129.8, 124.2, 117.5 (d, $J_{C\text{-}F}$ = 21.8 Hz), 113.1, 110.4, 106.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -108.8; IR (KBr, cm^{-1}): 3435, 3117, 3044, 1645, 1594, 1521, 1483, 1405; HRMS (ESI-TOF) calcd for $C_{15}H_{10}IFNO^{+}$ ($[M+H]^{+}$): 365.9786, found: 365.9786.

3-Iodo-4-(naphthalen-1-yl)-2*H*-quinolizin-2-one (2j):



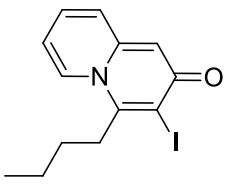
Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (77.4 mg, 97% yield); mp 272.0–274.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.10 (d, *J* = 8.3 Hz, 1H), 8.01 (d, *J* = 8.2 Hz, 1H), 7.68 (dd, *J* = 20.3, 12.2 Hz, 1H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.27 (dd, *J* = 8.5, 6.3 Hz, 2H), 7.13 (d, *J* = 7.4 Hz, 1H), 7.05 (dd, *J* = 25.9, 17.1 Hz, 1H), 6.78 (s, 1H), 6.25 (dd, *J* = 10.2, 3.7 Hz, 1H); ^{13}C NMR (75 MHz, DMSO) δ (ppm): 170.9, 145.9 144.8, 134.3, 134.1, 131.1, 131.0, 129.8, 129.8, 129.4, 129.0 128.4, 127.5, 126.9, 124.5, 123.8, 113.4, 111.1, 106.3; IR (KBr, cm^{-1}): 3431, 3043, 2928, 1643, 1591, 1526, 1494, 1449, 1403; HRMS (ESI-TOF) calcd for $C_{19}H_{13}INO^{+}$ ($[M+H]^{+}$): 398.0036, found: 398.0039.

3-Iodo-4-(thiophen-2-yl)-2*H*-quinolizin-2-one (2k):



Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (45.4 mg, 64% yield); mp 278.0–280.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.68 (dd, *J* = 5.1, 0.9 Hz, 1H), 7.53 (d, *J* = 7.5 Hz, 1H), 7.28 (dd, *J* = 5.1, 3.6 Hz, 1H), 7.18 (t, *J* = 5.1 Hz, 2H), 7.12–7.06 (m, 1H), 6.67 (s, 1H), 6.45–6.39 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.5, 144.6, 140.3, 136.7, 130.8, 130.4, 129.7, 129.0, 128.4, 124.2, 113.2, 112.7, 107.2; IR (KBr, cm^{-1}): 3437, 3126, 3068, 2925, 1640, 1591, 1530, 1481, 1421; HRMS (ESI-TOF) calcd for $C_{13}H_9INOS^{+}$ ($[M+H]^{+}$): 353.9444, found: 353.9443.

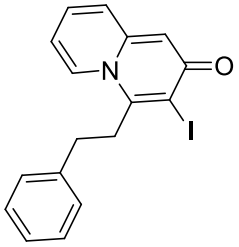
4-Butyl-3-iodo-2H-quinolizin-2-one (2m):



Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid

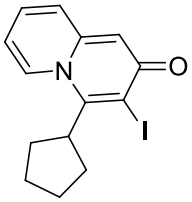
(29.2 mg, 45% yield); mp 111.6–112.9 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.89 (d, *J* = 7.5 Hz, 1H), 7.19 (d, *J* = 8.8 Hz, 1H), 7.11 (dd, *J* = 8.8, 6.5 Hz, 1H), 6.70–6.62 (m, 1H), 6.59 (s, 1H), 3.48–3.38 (m, 2H), 1.73–1.53 (m, 4H), 1.04 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.7, 146.3, 144.2, 128.2, 128.1, 125.2, 113.1, 109.9, 106.8, 37.9, 27.7, 22.6, 13.7; IR (KBr, cm^{-1}): 3359, 3157, 3095, 2925, 2863, 1648, 1587, 1515, 1474; HRMS (ESI-TOF) calcd for $C_{13}H_{15}INO^{+}$ ($[M+H]^{+}$): 328.0193, found: 328.0198.

3-Iodo-4-phenethyl-2*H*-quinolizin-2-one (2n):



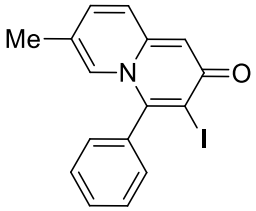
Purified by column chromatography (dichloromethane/methanol = 25:1); brown solid (56.6 mg, 67% yield); mp 205.2–207.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.88 (d, *J* = 7.5 Hz, 1H), 7.38–7.23 (m, 5H), 7.17 (d, *J* = 8.7 Hz, 1H), 7.07 (dd, *J* = 8.8, 6.3 Hz, 1H), 6.61–6.55 (m, 2H), 3.75–3.66 (m, 2H), 3.06–2.95 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 171.5, 145.2, 144.2, 139.0, 128.9, 128.3, 128.1, 127.0, 125.2, 113.3, 110.4, 106.9, 39.9, 31.8; IR (KBr, cm^{-1}): 3440, 3151, 2923 ,1645, 1594, 1534, 1476; HRMS (ESI-TOF) calcd for $C_{17}H_{15}INO^{+}$ ($[M+H]^{+}$): 376.0193, found 376.0190.

4-Cyclopentyl-3-iodo-2*H*-quinolizin-2-one (2o):



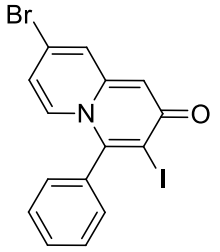
Purified by column chromatography (dichloromethane/methanol = 25:1); brown solid (38.7 mg, 57% yield); mp 192.5–194.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.71 (d, *J* = 7.6 Hz, 1H), 7.20 (d, *J* = 8.9 Hz, 1H), 7.07 (dd, *J* = 8.8, 6.6 Hz, 1H), 6.57 (s, 1H), 6.56–6.48 (m, 1H), 4.78–4.64 (m, 1H), 2.24–2.08 (m, 2H), 1.99 (ddd, *J* = 12.2, 10.2, 7.5 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 171.9, 147.5, 144.3, 129.2, 127.8, 125.7, 112.9, 111.5, 106.8, 50.4, 28.0, 27.0; IR (KBr, cm^{-1}): 3434, 2941, 2878, 1645, 1596, 1528, 1460, 1405; HRMS (ESI-TOF) calcd for $C_{14}H_{15}INO^{+}$ ($[M+H]^{+}$): 340.0193, found 340.0191.

3-Iodo-7-methyl-4-phenyl-2*H*-quinolizin-2-one (2p):



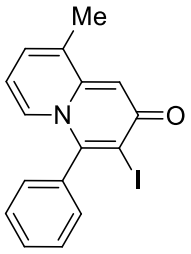
Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (57.6 mg, 80% yield); mp 242.3–244.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.69–7.54 (m, 3H), 7.29–7.26 (m, 2H), 7.14 (d, *J* = 9.2 Hz, 1H), 7.09 (s, 1H), 6.94 (d, *J* = 9.1 Hz,1H), 6.66 (s, 1H), 2.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.7, 146.5, 143.2, 137.1, 131.9, 130.3, 130.1, 129.1, 127.5, 124.0, 122.1, 108.9, 106.7, 18.2; IR (KBr, cm^{-1}): 3432, 3057, 2920, 2857, 1599, 1532, 1506, 1447; HRMS (ESI-TOF) calcd for $C_{16}H_{13}INO^+$ ($[M+H]^+$): 362.0036, found: 362.0036.

8-Bromo-3-iodo-4-phenyl-2H-quinolizin-2-one (2q):



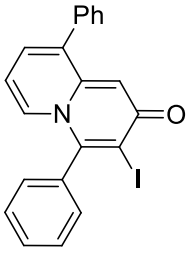
Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (57.5 mg, 68% yield); mp 277.2–279.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.69–7.58 (m, 3H), 7.37 (d, *J* = 2.1 Hz, 1H), 7.30–7.26 (m, 2H), 7.20 (d, *J* = 7.9 Hz, 1H), 6.57 (s, 1H), 6.38 (dd, *J* = 7.9, 2.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.9, 146.9, 144.1, 136.5, 131.3, 130.6, 130.3, 129.1, 125.4, 123.4, 116.0, 109.2, 106.2; IR (KBr, cm^{-1}): 3430, 3123, 3051, 2922, 1680, 1626, 1596, 1514, 1442; HRMS (ESI-TOF) calcd for $C_{15}H_{10}BrINO^+$ ($[M+H]^+$): 425.8985, found: 425.8988.

3-Iodo-9-methyl-4-phenyl-2*H*-quinolizin-2-one (2r):



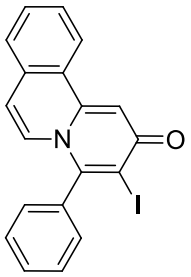
Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (61.5 mg, 85% yield); mp 212.2–214.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.72–7.55 (m, 3H), 7.28 (dd, *J* = 14.1, 5.9 Hz, 3H), 6.96 (d, *J* = 6.6 Hz, 1H), 6.80 (s, 1H), 6.29 (t, *J* = 7.1 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 172.0, 147.4, 144.7, 137.5, 130.8, 130.3, 130.1, 129.3, 129.1, 127.9, 111.8, 108.3, 104.4, 77.4, 77.1, 76.8, 19.6; IR (KBr, cm^{-1}): 3435, 3047, 1906, 1638, 1587, 1540, 1447; HRMS (ESI-TOF) calcd for $C_{16}H_{13}INO^{+}$ ($[M+H]^{+}$): 362.0036, found: 362.0034.

3-Iodo-4,9-diphenyl-2*H*-quinolizin-2-one (2s):



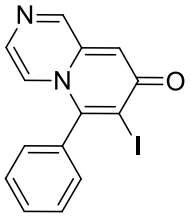
Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (76.4 mg, 90% yield); mp 224.5–225.8 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.70–7.59 (m, 3H), 7.50–7.41 (m, 4H), 7.38 (dd, *J* = 7.5, 1.7 Hz, 2H), 7.36–7.31 (m, 2H), 6.99 (d, *J* = 6.6 Hz, 1H), 6.74 (s, 1H), 6.44 (t, *J* = 7.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.9, 147.3, 144.5, 137.4, 136.8, 136.6, 130.4, 130.2, 130.2, 129.1, 129.0, 128.8, 128.7, 112.0, 108.5, 106.9; IR (KBr, cm^{-1}): 3440, 3122, 3048, 2924, 1766, 1593, 1541, 1506, 1443; HRMS (ESI-TOF) calcd for $C_{21}H_{15}INO^{+}$ ($[M+H]^{+}$): 424.0193, found: 424.0189.

3-Iodo-4-phenyl-2*H*-pyrido[2,1-*a*]isoquinolin-2-one (2t):



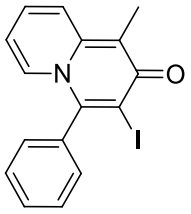
Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (49.7 mg, 63% yield); mp 281.9–282.8 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.29 (d, *J* = 7.7 Hz, 1H), 7.72–7.58 (m, 5H), 7.56 (s, 1H), 7.53–7.48 (m, 1H), 7.33 (dd, *J* = 7.8, 1.4 Hz, 2H), 7.20 (d, *J* = 7.8 Hz, 1H), 6.55 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 173.0, 148.7, 143.0, 137.5, 131.4, 130.3, 130.0, 129.5, 129.2, 129.2, 127.1, 127.0, 125.0, 124.2, 112.7, 105.3, 105.3; IR (KBr, cm^{-1}): 3441, 3023, 1648, 1589, 1481, 1452, 1433; HRMS (ESI-TOF) calcd for $C_{19}H_{13}INO^{+}$ ($[M+H]^{+}$): 398.0036, found: 398.0036.

7-Iodo-6-phenyl-8*H*-pyrido[1,2-*a*]pyrazin-8-one (2u):



Purified by column chromatography (dichloromethane/methanol =25:1); yellow solid (44.9 mg, 65% yield); mp 247.9–259.6 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.68 (s, 1H), 7.69–7.61 (m, 3H), 7.36–7.29 (m, 3H), 7.06 (d, *J* = 5.2 Hz, 1H), 6.84 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 172.8, 152.3, 147.1, 137.2, 135.3, 130.9, 130.2, 128.9, 127.9, 120.6, 111.2, 108.8; IR (KBr, cm^{-1}): 3439, 3132, 2922, 1592, 1495, 1404; HRMS (ESI-TOF) calcd for $C_{14}H_{10}IN_2O^{+}$ ($[M+H]^{+}$): 348.9832, found: 348.9831.

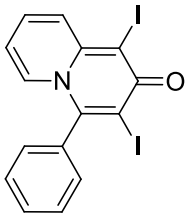
3-Iodo-1-methyl-4-phenyl-2*H*-quinolizin-2-one (2w):



Purified by column chromatography (dichloromethane/methanol =100:1); yellow solid (37.1 mg, 51% yield for I_2 as electrophile; 44.8 mg, 62% yield for NIS as electrophile); mp

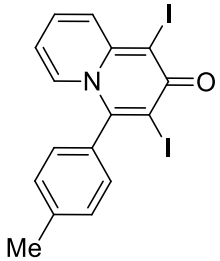
247.2–248.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.67–7.55 (m, 3H), 7.47 (d, *J* = 9.4 Hz, 1H), 7.40 (t, *J* = 12.1 Hz, 1H), 7.31–7.24 (m, 2H), 7.11 (ddd, *J* = 9.4, 6.4, 1.0 Hz, 1H), 6.32 (ddd, *J* = 7.7, 6.6, 1.4 Hz, 1H), 2.45–2.37 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 145.5, 141.0, 137.5, 131.3, 130.2, 130.1, 129.3, 127.8, 121.9, 114.0, 111.4, 107.2, 11.9; IR (KBr, cm^{-1}): 3434, 3143, 3046, 2915, 1640, 1559, 1503, 1449, 1413; HRMS (ESI-TOF) calcd for $C_{16}H_{13}INO^{+}$ ($[M+H]^{+}$): 362.0036, found: 362.0038.

1,3-Diiodo-4-phenyl-2*H*-quinolizin-2-one (3a):



Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (85.7 mg, 90% yield); mp 287.9–290.3 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.00 (d, *J* = 9.3 Hz, 1H), 7.72–7.58 (m, 3H), 7.43 (d, *J* = 7.4 Hz, 1H), 7.32–7.28 (m, 2H), 7.23–7.15 (m, 1H), 6.44–6.38 (m, 1H); ^{13}C NMR (100 MHz, DMSO) δ 168.4, 147.3, 143.4, 137.5, 133.1, 133.1, 130.6, 130.4 129.8, 128.3, 113.4, 103.3, 83.1; IR (KBr, cm^{-1}): 3439, 3084, 2925, 1639, 1573, 1477; HRMS (ESI-TOF) calcd for $C_{15}H_{10}I_2NO^{+}$ ($[M+H]^{+}$): 473.8846, found: 473.8847.

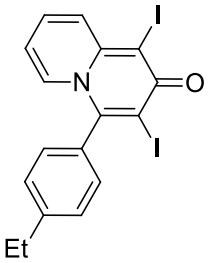
1,3-Diiodo-4-(p-tolyl)-2*H*-quinolizin-2-one (3b):



Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (93.5 mg, 96% yield); mp 229.0–231.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 7.99 (d, *J* = 9.3 Hz, 1H), 7.46 (dd, *J* = 10.4, 7.8 Hz, 3H), 7.24–7.13 (m, 3H), 6.45–6.37 (m, 1H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 168.7, 146.7, 143.2, 140.8, 133.9, 132.2, 131.3, 130.9, 129.3, 129.0, 112.6, 102.9, 83.2, 21.6; IR (KBr, cm^{-1}): 3437, 3043, 2921,

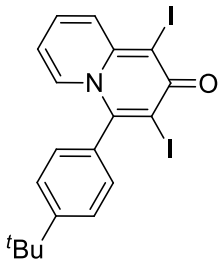
1638, 1573, 1519, 1469; HRMS (ESI-TOF) calcd for $C_{16}H_{12}I_2NO^+$ ([M+H]$^+$): 487.9003, found: 487.9000.

4-(4-Ethylphenyl)-1,3-diiodo-2H-quinolizin-2-one (3c):



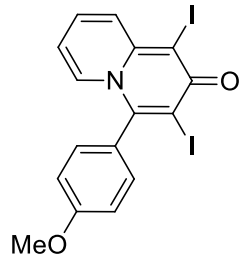
Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (95.9 mg, 96% yield); mp 238.9–240.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.99 (d, *J* = 9.3 Hz, 1H), 7.50–7.43 (m, 3H), 7.24–7.15 (m, 3H), 6.45–6.38 (m, 1H), 2.88–2.74 (m, 2H), 1.34 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 168.7, 146.9, 146.7, 143.2, 134.1, 132.2, 131.24, 129.7, 129.3, 129.0, 112.5, 102.9, 83.2, 28.8, 15.2; IR (KBr, cm^{-1}): 3444, 2963, 2926, 1638, 1572, 1517, 1469; HRMS (ESI-TOF) calcd for $C_{17}H_{14}I_2NO^+$ ([M+H]$^+$): 501.9159, found: 501.9158.

4-(4-(*Tert*-butyl)phenyl)-1,3-diiodo-2*H*-quinolizin-2-one (3d):



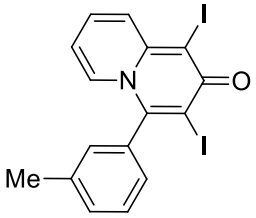
Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (97.3 mg, 92% yield); mp 301.8–303.6 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.98 (t, *J* = 9.5 Hz, 1H), 7.67–7.60 (m, 2H), 7.48 (d, *J* = 7.4 Hz, 1H), 7.24–7.16 (m, 3H), 6.45–6.39 (m, 1H), 1.42 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 168.8, 153.9, 146.8, 143.2, 133.9, 132.3, 131.2, 129.3, 128.8, 127.1, 112.5, 102.9, 83.1, 35.1, 31.3; IR (KBr, cm^{-1}): 3437, 3134, 3057, 2959, 2867, 1933, 1641, 1573, 1515, 1468; HRMS (ESI-TOF) calcd for $C_{19}H_{18}I_2NO^+$ ([M+H]$^+$): 529.9472, found: 529.9466.

1,3-Diiodo-4-(4-methoxyphenyl)-2*H*-quinolizin-2-one (3e):



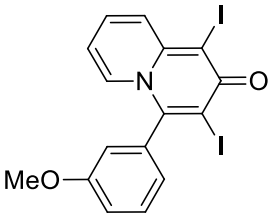
Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (95.9 mg, 95% yield); mp 272.5–274.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.98 (d, *J* = 9.4 Hz, 1H), 7.52 (d, *J* = 7.4 Hz, 1H), 7.24–7.17 (m, 3H), 7.17–7.11 (m, 2H), 6.45–6.40 (m, 1H), 3.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 168.8, 160.9, 146.5, 143.2, 132.2, 131.2, 130.6, 129.3, 129.0, 115.6, 112.5, 103.5, 83.2, 55.5; IR (KBr, cm^{-1}): 3437, 3130, 3066, 2943, 2832, 1572, 1513, 1468; HRMS (ESI-TOF) calcd for $C_{16}H_{12}I_2NO_2^+$ ($[M+H]^+$): 503.8952, found: 503.8947.

1,3-Diiodo-4-(m-tolyl)-2*H*-quinolizin-2-one (3f):



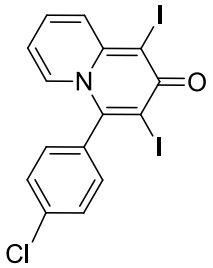
Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (93.6 mg, 96% yield); mp 220.8–222.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.99 (d, *J* = 9.3 Hz, 1H), 7.53 (t, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 7.4 Hz,1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.20 (ddd, *J* = 9.4, 6.5, 1.0 Hz, 1H), 7.08 (d, *J* = 7.1 Hz, 2H), 6.44–6.38 (m, 1H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 168.7, 146.7, 143.2, 140.3, 136.8, 132.2, 131.3, 131.2, 130.1, 129.5, 129.3, 126.1, 112.5, 102.6, 83.2, 21.6; IR (KBr, cm^{-1}): 3437, 3130, 3045, 2918, 2860, 1638, 1572, 1475; HRMS (ESI-TOF) calcd for $C_{16}H_{12}I_2NO^+$ ($[M+H]^+$): 487.9003, found: 487.9009.

1,3-Diiodo-4-(3-methoxyphenyl)-2*H*-quinolizin-2-one (3g):



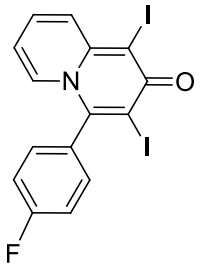
Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (95.2 mg, 95% yield); mp 235.5–236.8 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.99 (d, *J* = 9.4 Hz, 1H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.47 (d, *J* = 7.4 Hz, 1H), 7.25–7.18 (m, 1H), 7.12 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.85 (t, *J* = 7.4 Hz, 1H), 6.81 (d, *J* = 2.0 Hz, 1H), 6.46–6.40 (m, 1H), 3.87 (s, 3H); ^{13}C NMR (75 MHz, DMSO) δ (ppm): 168.3, 160.7, 147.1, 143.3, 138.6, 133.3, 133.1, 131.7, 128.2, 121.7, 116.2, 115.3, 113.4, 103.1, 83.0, 55.9; IR (KBr, cm^{-1}): 3439, 3140, 3056, 2928, 2842, 1638, 1575, 1467, 1429; HRMS (ESI-TOF) calcd for $C_{16}H_{12}I_2NO_2^+$ ($[M+H]^+$): 503.8952, found: 503.8958.

4-(4-Chlorophenyl)-1,3-diiodo-2*H*-quinolizin-2-one (3h):



Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (78.4 mg, 77% yield); mp 237.5–239.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.00 (d, *J* = 9.4 Hz, 1H), 7.67–7.60 (m, 2H), 7.41 (d, *J* = 7.4 Hz, 1H), 7.30–7.24 (m, 2H), 7.21 (ddd, *J* = 9.3, 6.6, 0.9 Hz, 1H), 6.48–6.41 (m, 1H); ^{13}C NMR (75 MHz, DMSO) δ (ppm): 168.3, 146.3, 143.4, 136.4, 135.5, 133.5, 133.2, 132.0, 130.6, 128.3, 113.5, 103.6, 83.2; IR (KBr, cm^{-1}): 3437, 3131, 3062, 1638, 1579, 1482; HRMS (ESI-TOF) calcd for $C_{15}H_9ClI_2NO^+$ ($[M+H]^+$): 507.8457, found: 507.8456.

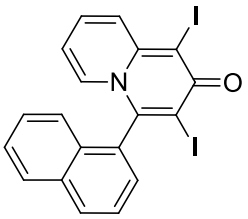
4-(4-Fluorophenyl)-1,3-diiodo-2*H*-quinolizin-2-one (3i):



Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (96.2 mg, 98% yield); mp 264.7–266.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.00 (d, *J* = 9.3 Hz, 1H), 7.43 (d, *J* = 7.4 Hz, 1H), 7.38–7.28 (m, 4H), 7.22 (ddd, *J* = 9.4, 6.6, 1.0 Hz,

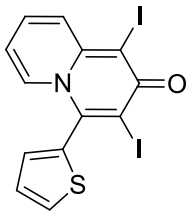
1H), 6.49–6.41 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 168.7, 163.7 (d, J_{C-F} = 250.8 Hz), 145.5, 143.3, 132.9 (d, J_{C-F} = 3.3 Hz), 131.9, 131.5 (d, J_{C-F} = 8.6 Hz), 131.2, 129.5, 117.6 (d, J_{C-F} = 21.9 Hz), 112.8, 103.3, 83.5; IR (KBr, cm^{-1}): 3438, 3068, 3046, 2030, 1927, 1799, 1639, 1571, 1512, 1468; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -108.4; HRMS (ESI-TOF) calcd for $C_{15}H_9FI_2NO^+$ ($[M+H]^+$): 491.8752, found: 491.8759.

1,3-Diiodo-4-(naphthalen-1-yl)-2*H*-quinolizin-2-one (3j):



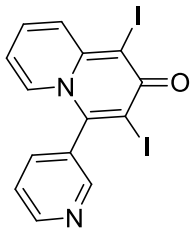
Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (94.2 mg, 90% yield); mp 271.0–272.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.11 (d, *J* = 8.3 Hz, 1H), 8.04 (dd, *J* = 15.8, 8.8 Hz, 2H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 6.6 Hz, 2H), 7.26–7.14 (m, 3H), 6.31 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, DMSO) δ 168.4, 145.7, 143.7, 134.4, 134.1, 133.1, 133.0, 131.1, 129.9, 129.4, 129.1, 128.6, 128.5, 127.5 126.9, 124.1, 113.8, 104.7, 83.6; IR (KBr, cm^{-1}): 3442, 3132, 3053, 1639, 1574,1474; HRMS (ESI-TOF) calcd for $C_{19}H_{12}I_2NO^+$ ($[M+H]^+$): 523.9003, found: 523.9006.

1,3-Diiodo-4-(thiophen-2-yl)-2*H*-quinolizin-2-one (3k):



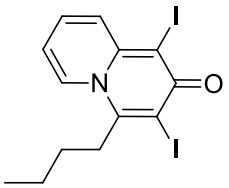
Purified by column chromatography (dichloromethane/methanol =100:1); yellow solid (64.0 mg, 67% yield); mp 258.0–260.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.00 (d, *J* = 9.3 Hz, 1H), 7.70 (d, *J* = 4.9 Hz, 1H), 7.63 (d, *J* = 7.3 Hz, 1H), 7.33–7.28 (m, 1H), 7.21 (dd, *J* = 13.2, 6.0 Hz, 2H), 6.50 (t, *J* = 6.7 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.5, 143.5, 139.8, 136.7, 132.2, 131.6, 130.7, 129.9, 129.3, 128.5, 112.8, 106.5, 83.8; IR (KBr, cm^{-1}): 3439, 3138, 3073, 1638, 1574, 1530, 1469, 1425; HRMS (ESI-TOF) calcd for $C_{13}H_8I_2NOS^+$ ($[M+H]^+$): 479.8411, found: 479.8414.

1,3-Diiodo-4-(pyridin-3-yl)-2*H*-quinolizin-2-one (3l):



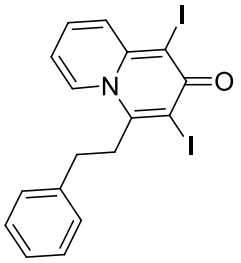
Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (35.1 mg, 37% yield); mp 274.0–276.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.88 (d, *J* = 3.5 Hz, 1H), 8.60 (d, *J* = 1.3 Hz, 1H), 8.02 (d, *J* = 9.3 Hz, 1H), 7.71 (dt, *J* = 7.8, 1.8 Hz, 1H), 7.62 (dd, *J* = 7.7, 4.9 Hz, 1H), 7.39 (d, *J* = 7.4 Hz, 1H), 7.24 (dd, *J* = 8.9, 7.0 Hz, 1H), 6.54–6.41 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$/CD_3OD = 20:1) δ (ppm): 168.8, 151.4, 149.7, 143.5, 143.3, 137.7, 133.3, 131.7, 131.6, 129.7, 124.9, 113.6, 103.6, 83.6; IR (KBr, cm^{-1}): 3452, 1638, 1569, 1475, 1408; HRMS (ESI-TOF) calcd for $C_{14}H_9I_2N_2O^+$ ($[M+H]^+$): 474.8799, found 474.8792.

4-Butyl-1,3-diiodo-2*H*-quinolizin-2-one (3m):



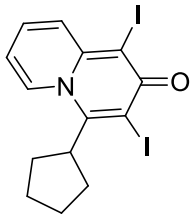
Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (45.8 mg, 51% yield); mp 175.6–177.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.99 (t, *J* = 10.2 Hz, 1H), 7.92 (t, *J* = 9.1 Hz, 1H), 7.22 (dd, *J* = 9.3, 6.5 Hz, 1H), 6.71–6.65 (m, 1H), 3.50–3.42 (m, 2H), 1.67 (dt, *J* = 15.9, 8.0 Hz, 2H), 1.57 (dt, *J* = 14.2, 7.1 Hz, 2H), 1.04 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 168.6, 146.0, 143.0, 130.9, 130.0, 129.7, 113.5, 103.5, 83.0, 38.3, 27.8, 22.6, 13.8; IR (KBr, cm^{-1}): 3433, 3135, 2953, 2861, 1640, 1577, 1466; HRMS (ESI-TOF) calcd for $C_{13}H_{14}I_2NO^+$ ($[M+H]^+$): 453.9159, found: 453.9161.

1,3-Diiodo-4-phenethyl-2*H*-quinolizin-2-one (3n):



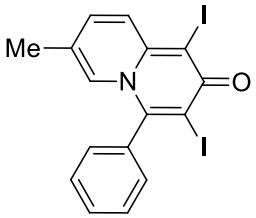
Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (72.2 mg, 72% yield); mp 222.8–224.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.01 (d, *J* = 9.6 Hz, 1H), 7.94 (d, *J* = 7.5 Hz, 1H), 7.38–7.26 (m, 5H), 7.21 (dd, *J* = 9.3, 6.5 Hz, 1H), 6.68–6.61 (m, 1H), 3.79–3.72 (m, 2H), 3.05–2.95 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$/CD_3OD = 20:1) δ (ppm): 168.8, 145.0, 143.1, 138.8, 131.2, 130.1, 129.5, 128.9, 128.2, 127.0, 113.8, 103.7, 83.2, 40.3, 31.8; IR (KBr, cm^{-1}): 3435, 1643, 1564, 1463; HRMS (ESI-TOF) calcd for $C_{17}H_{14}I_2NO^+$ ([M+H]$^+$): 501.9159, found 501.9151.

4-Cyclopentyl-1,3-diiodo-2*H*-quinolizin-2-one (3o):



Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (67.0 mg, 72% yield); mp 231.9–233.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.02 (t, *J* = 9.4 Hz, 1H), 7.74 (d, *J* = 7.5 Hz, 1H), 7.24–7.16 (m, 1H), 6.65–6.57 (m, 1H), 4.76–4.62 (m, 1H), 2.22–2.10 (m, 2H), 1.99 (ddd, *J* = 14.7, 13.8, 7.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 168.8, 147.2, 143.0, 130.6, 130.5, 130.4, 111.7, 106.4, 83.0, 50.5, 28.3, 27.1; IR (KBr, cm^{-1}): 3440, 3182, 2947, 1636, 1573, 1460; HRMS (ESI-TOF) calcd for $C_{14}H_{14}I_2NO^+$ ([M+H]$^+$): 465.9159, found 465.9155.

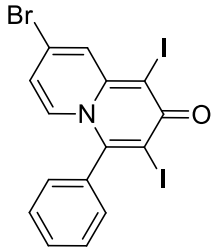
1,3-Diiodo-7-methyl-4-phenyl-2*H*-quinolizin-2-one (3p):



Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid

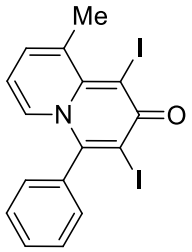
(89.2 mg, 92% yield); mp 250.7–252.7 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.71–7.59 (m, 3H), 7.28 (d, *J* = 6.9 Hz, 2H), 7.19 (s, 1H), 7.07 (d, *J* = 9.5 Hz, 1H), 2.08 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 168.5, 146.0, 142.2, 137.1, 134.4, 130.5, 130.2, 129.2, 129.0, 128.9, 122.4, 102.6, 83.0, 17.9; IR (KBr, cm^{-1}): 3432, 3041, 2973, 2918, 1650, 1575, 1489, 1436, 1417; HRMS (ESI-TOF) calcd for $C_{16}H_{12}I_2NO^+$ ($[M+H]^+$): 487.9003, found: 487.9006.

8-Bromo-1,3-diiodo-4-phenyl-2*H*-quinolizin-2-one (3q):



Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (80.8 mg, 73% yield); mp 250.0–252.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.20 (d, *J* = 2.0 Hz, 1H), 7.70–7.57 (m, 3H), 7.31–7.27 (m, 3H), 6.44 (dd, *J* = 7.8, 2.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 167.8, 145.5, 142.2, 135.4, 131.7, 129.8, 129.6, 129.4, 128.1, 125.7, 115.4, 101.6, 81.4; IR (KBr, cm^{-1}): 3434, 3067, 2923, 1709, 1626, 1577, 1522, 1503, 1462; HRMS (ESI-TOF) calcd for $C_{15}H_9BrI_2NO^+$ ($[M+H]^+$): 551.7951, found: 551.7947.

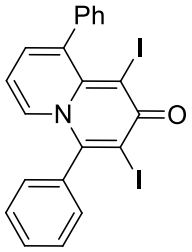
1,3-Diiodo-9-methyl-4-phenyl-2*H*-quinolizin-2-one (3r):



Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (77.2 mg, 79% yield); mp 207.2–209.0 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 7.67–7.55 (m, 3H), 7.48 (d, *J* = 7.4 Hz, 1H), 7.31–7.25 (m, 2H), 7.15 (d, *J* = 6.8 Hz, 2H), 6.33 (t, *J* = 7.1 Hz, 1H), 3.06 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 169.6, 147.4 145.2, 137.8, 132.5, 131.6, 131.3, 130.4, 130.2, 129.2, 111.8, 99.6, 80.2, 28.3; IR (KBr,

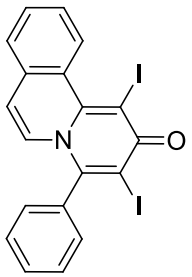
cm^{-1}): 3436, 3065, 1634, 1573, 1492, 1450; HRMS (ESI-TOF) calcd for $C_{16}H_{12}I_2NO^+$ ($[M+H]^+$): 487.9003, found: 487.9009.

1,3-Diiodo-4,9-diphenyl-2*H*-quinolizin-2-one (3s):



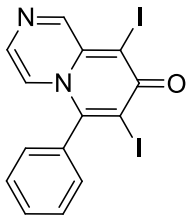
Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (34.9 mg, 32% yield); mp 190.0–192.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70–7.58 (m, 3H), 7.51 (d, *J* = 7.2 Hz, 1H), 7.42 (t, *J* = 7.2 Hz, 3H), 7.36 (d, *J* = 7.0 Hz, 2H), 7.32 (d, *J* = 7.3 Hz, 2H), 7.23 (d, *J* = 6.6 Hz, 1H), 6.46 (t, *J* = 7.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.0, 147.1, 143.3, 139.7, 137.4, 133.2, 131.4, 130.6, 130.2, 129.8, 129.4, 128.6, 128.2, 111.4, 100.3, 82.7; IR (KBr, cm^{-1}): 3737, 3125, 3063, 2923, 1631, 1574, 1489, 1451; HRMS (ESI-TOF) calcd for $C_{21}H_{14}I_2NO^+$ ($[M+H]^+$): 549.9159, found: 549.9161.

1,3-Diiodo-4-phenyl-2*H*-pyrido[2,1-*a*]isoquinolin-2-one (3t):



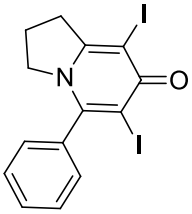
Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (74.4mg, 71% yield); mp 239.0–241.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 9.44 (d, *J* = 8.3 Hz, 1H), 7.69–7.53 (m, 5H), 7.45 (d, *J* = 7.5 Hz, 1H), 7.34 (dd, *J* = 7.2, 1.9 Hz, 2H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.54 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.6, 148.5, 144.6, 137.0, 131.9, 131.3, 131.1, 130.6, 129.9, 129.6, 127.4, 126.6, 125.8, 125.3, 112.5, 95.6, 84.7; IR (KBr, cm^{-1}): 3747, 3440, 3124, 3042, 2924, 1718, 1647, 1577, 1496, 1459; HRMS (ESI-TOF) calcd for $C_{19}H_{12}I_2NO^+$ ($[M+H]^+$): 523.9003, found: 523.9005.

7,9-Diiodo-6-phenyl-8*H*-pyrido[1,2-*a*]pyrazin-8-one (3u):



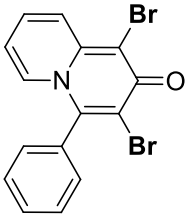
Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (51.1mg, 54% yield); mp 258.6–259.9 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 9.35 (s, 1H), 7.70–7.61 (m, 3H), 7.43 (d, *J* = 5.2 Hz, 1H), 7.30 (dd, *J* = 7.5, 1.6 Hz, 2H), 7.07 (d, *J* = 5.1 Hz, 1H); ^{13}C NMR (100 MHz, DMSO) δ 169.8, 155.6, 147.5, 136.2, 135.6, 130.9, 130.3, 129.7, 128.5, 122.4, 105.1, 86.0; IR (KBr, cm^{-1}): 3449, 2384, 2309, 1632, 1575, 1499, 1431; HRMS (ESI-TOF) calcd for $C_{14}H_9I_2N_2O^+$ ($[M+H]^+$): 474.8799, found: 474.8803.

6,8-Diiodo-5-phenyl-2,3-dihydroindolizin-7(1*H*)-one (3v):



Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (84.1mg, 91% yield); mp 253.6–255.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.59–7.47 (m, 3H), 7.27 (dd, *J* = 7.2, 2.1 Hz, 2H), 3.94 (t, *J* = 7.4 Hz, 2H), 3.23 (t, *J* = 7.8 Hz, 2H), 2.20 (p, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 171.0, 154.0, 149.2, 136.0, 129.0, 128.2, 127.1, 90.7, 81.4, 56.2, 36.2, 20.2; IR (KBr, cm^{-1}): 3442, 2958, 1642, 1580, 1480, 1434; HRMS (ESI-TOF) calcd for $C_{14}H_{12}I_2NO^+$ ($[M+H]^+$): 463.90028, found: 463.90051.

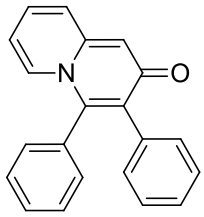
1,3-Dibromo-4-phenyl-2*H*-quinolizin-2-one (3x):



Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (71.3 mg, 94% yield); mp 264.2–266.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.98 (d, *J*

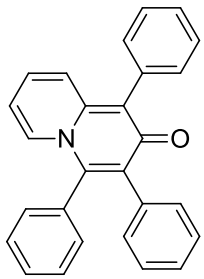
= 9.3 Hz, 1H), 7.68–7.57 (m, 3H), 7.47 (d, *J* = 7.4 Hz, 1H), 7.38–7.31 (m, 2H), 7.31–7.26 (m, 1H), 6.57–6.48 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3/CD_3OD$ = 20:1) δ (ppm): 165.8, 143.4, 141.4, 133.2, 131.0, 130.9, 130.6, 130.2, 129.0, 124.3, 122.4, 113.1, 106.3; IR (KBr, cm^{-1}): 3474, 2925, 1640, 1589, 1537, 1486; HRMS (ESI-TOF) calcd for $C_{15}H_{10}Br_2NO^+$ ($[M+H]^+$): 377.9124, found 377.9123.

3,4-Diphenyl-2*H*-quinolizin-2-one (4):



Purified by column chromatography (dichloromethane/methanol = 25:1); yellow solid (74.6 mg, 84% yield); mp 307.0–309.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.41 (d, *J* = 7.4 Hz, 1H), 7.36–7.29 (m, 3H), 7.20–7.11 (m, 5H), 7.10–6.96 (m, 4H), 6.76 (s, 1H), 6.36–6.29 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ174.4, 144.2, 143.4, 135.9, 134.9, 132.5, 130.4, 130.3, 130.0, 129.3, 129.1, 128.1, 127.6, 126.9, 124.3, 111.5; IR (KBr, cm^{-1}): 3432, 3088, 3061, 2963, 2924, 2857, 1969, 1612, 1524, 1441; HRMS (ESI-TOF) calcd for $C_{21}H_{16}NO^+$ ($[M+H]^+$): 298.1226, found: 298.1229.

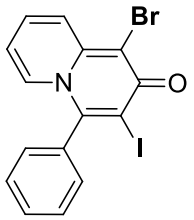
1,3,4-Triphenyl-2*H*-quinolizin-2-one (5):



Purified by column chromatography (dichloromethane/methanol =100:1); green solid (80.7 mg, 72% yield); mp 318.0–319.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.5 Hz, 1H), 7.46 (d, *J* = 4.4 Hz, 4H), 7.40–7.31 (m, 4H), 7.26 (t, *J* = 8.7 Hz, 3H), 7.15–7.08 (m, 4H), 7.08–7.01 (m, 1H), 6.90 (dd, *J* = 9.2, 6.4 Hz, 1H), 6.33 (t, *J* = 6.4 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.2, 142.8, 142.0, 135.3, 135.0, 135.0, 132.9, 131.3, 130.8, 130.4, 130.3, 129.2, 129.2, 128.4, 127.5, 127.3, 127.3, 126.6, 123.3, 123.0, 111.1; IR (KBr, cm^{-1}):

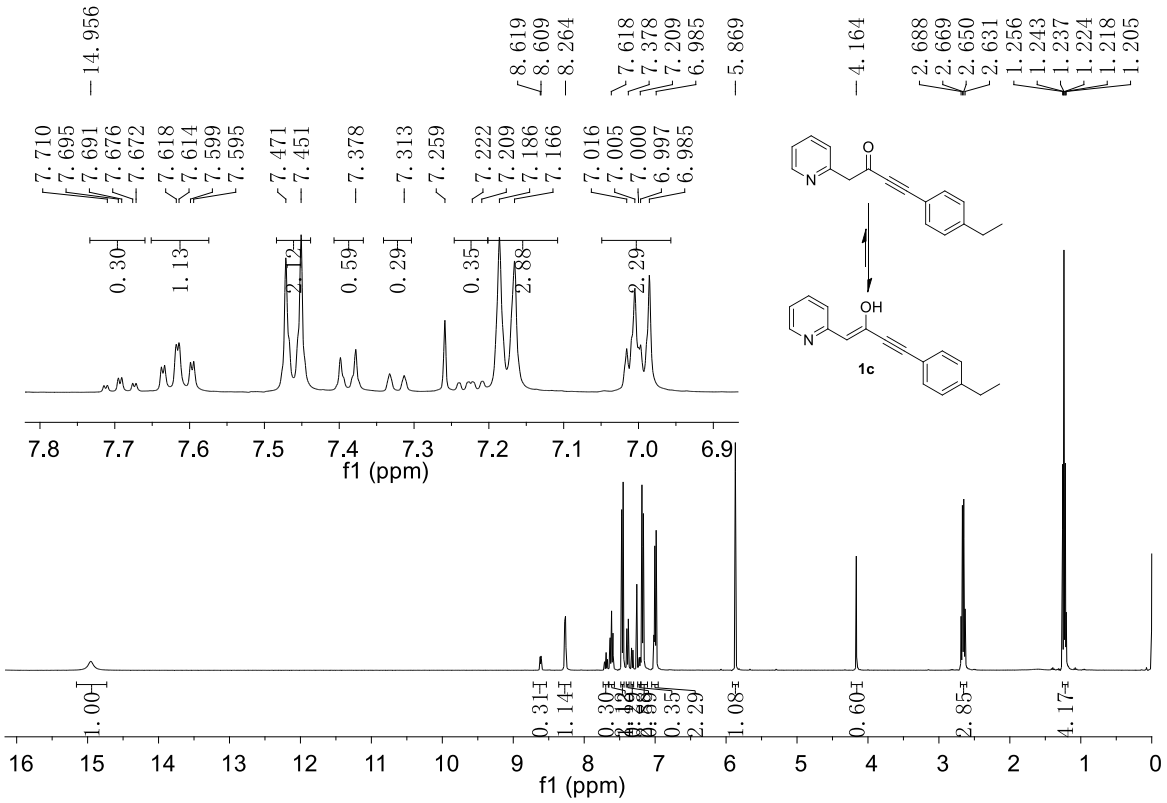
3388, 3062, 3028, 2928, 1726, 1607, 1563, 1519, 1481, 1438; HRMS (ESI-TOF) calcd for $C_{27}H_{20}NO^+$ ([M+H]$^+$): 374.1539, found: 374.1543.

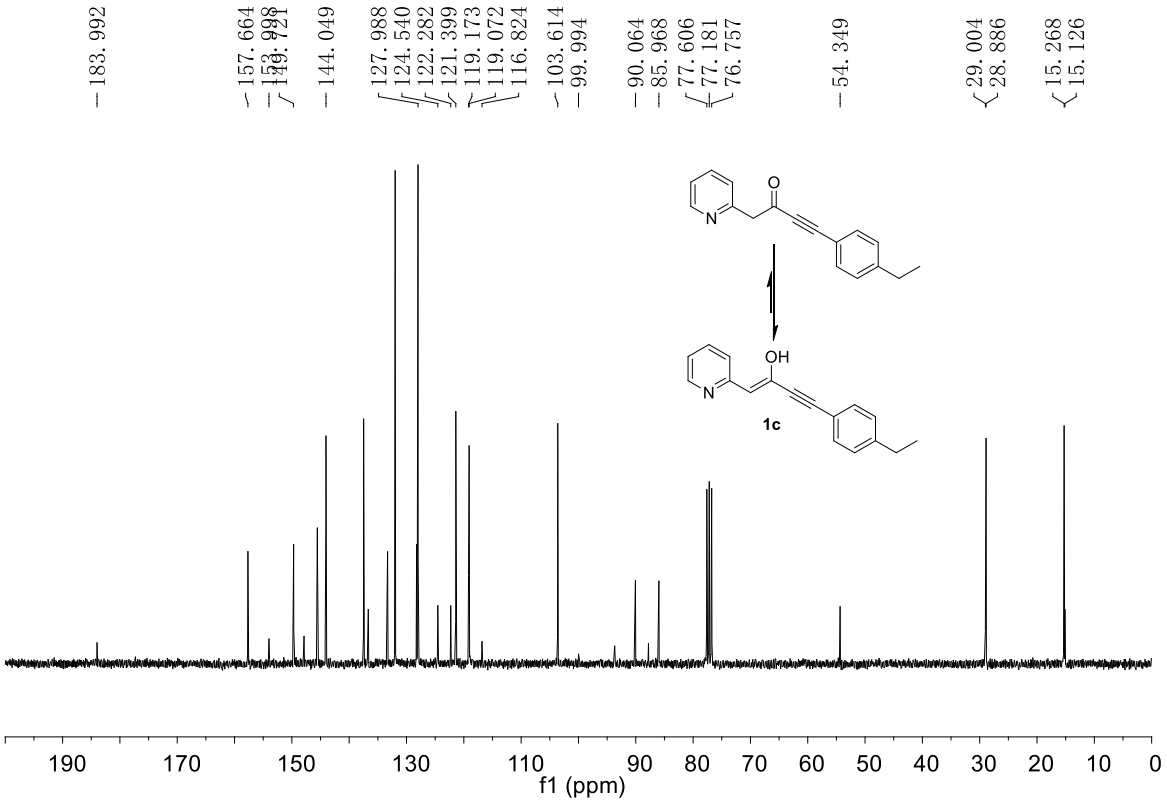
1-Bromo-3-iodo-4-phenyl-2*H*-quinolizin-2-one (6):

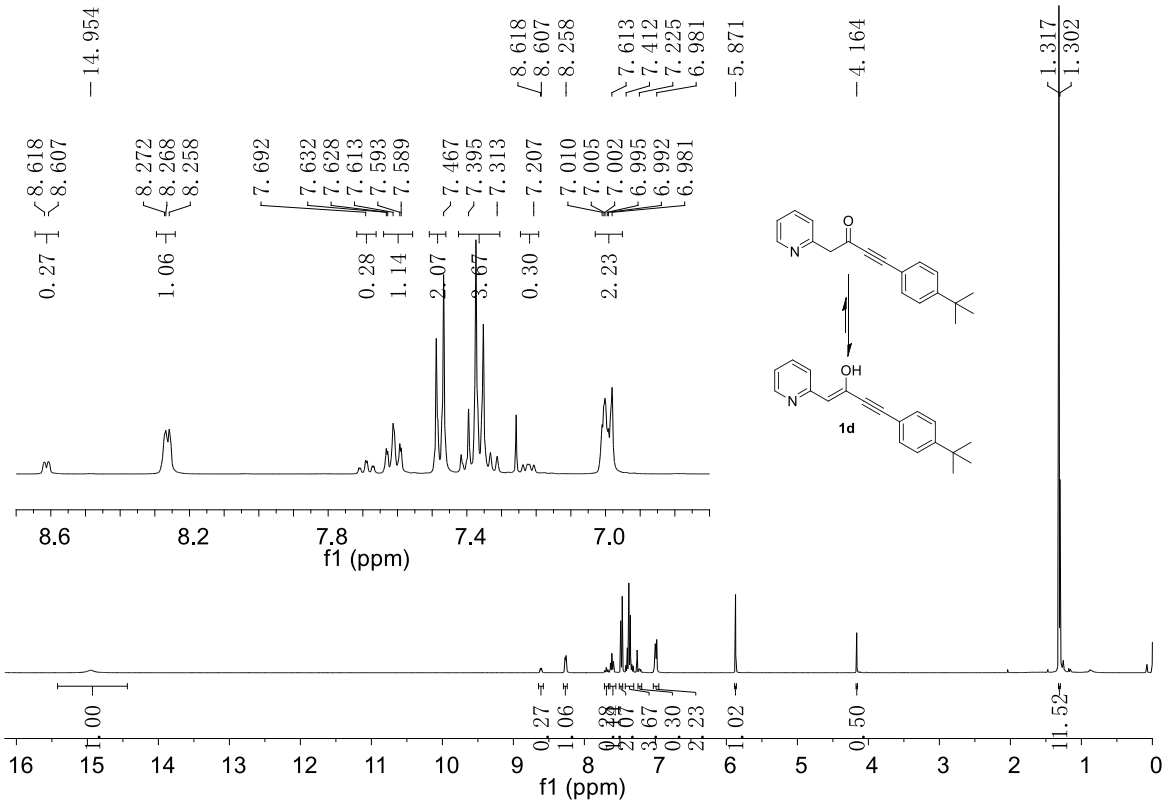


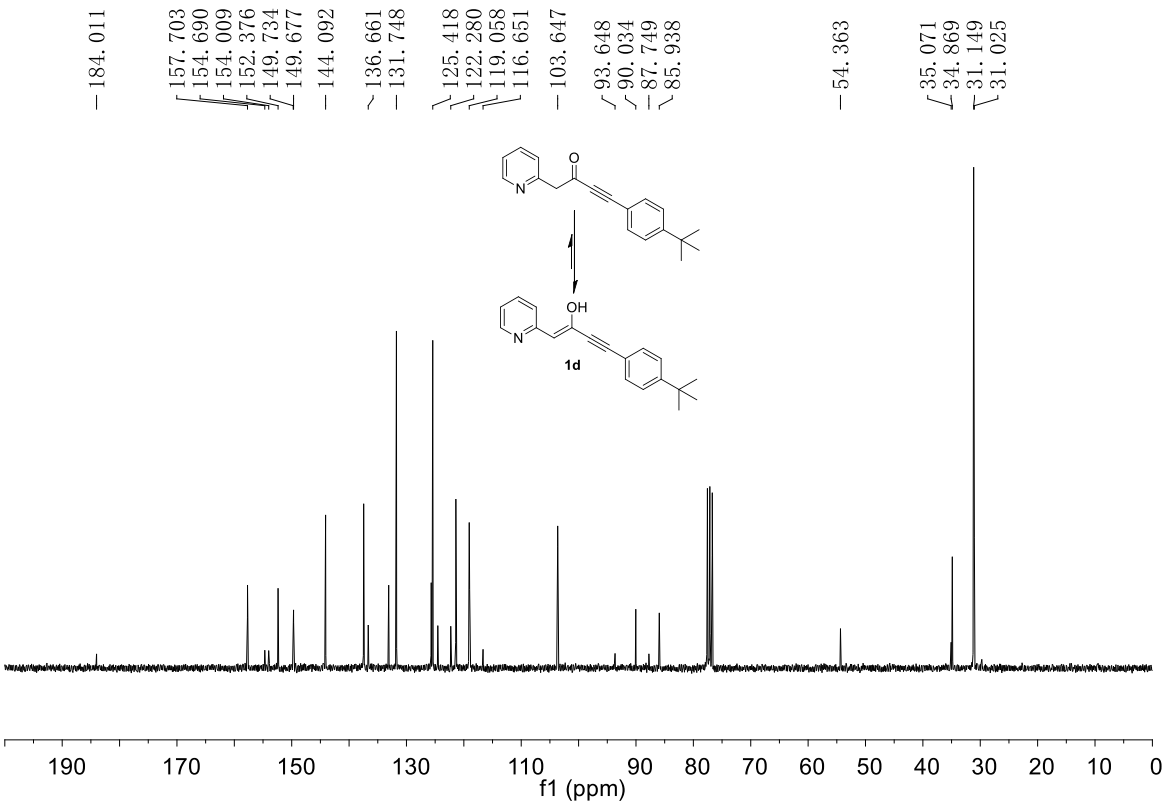
Purified by column chromatography (dichloromethane/methanol = 100:1); yellow solid (80.4 mg, 94% yield); mp 227.4–229.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.97 (d, *J* = 9.3 Hz, 1H), 7.71–7.57 (m, 3H), 7.47 (d, *J* = 7.4 Hz, 1H), 7.27 (dd, *J* = 14.7, 7.1 Hz, 3H), 6.48–6.39 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$/CD_3OD = 12:1) δ (ppm): 167.2, 146.3, 141.7, 136.6, 131.8, 131.0, 130.6, 130.3, 129.1, 124.3, 113.1, 105.6, 103.4; IR (KBr, cm^{-1}): 3441, 3062, 1637, 1577, 1485; HRMS (ESI-TOF) calcd for C15H9BrINO $C_{15}H_{10}BrINO^+$ ([M+H]$^+$): 425.8985, found 425.8984.

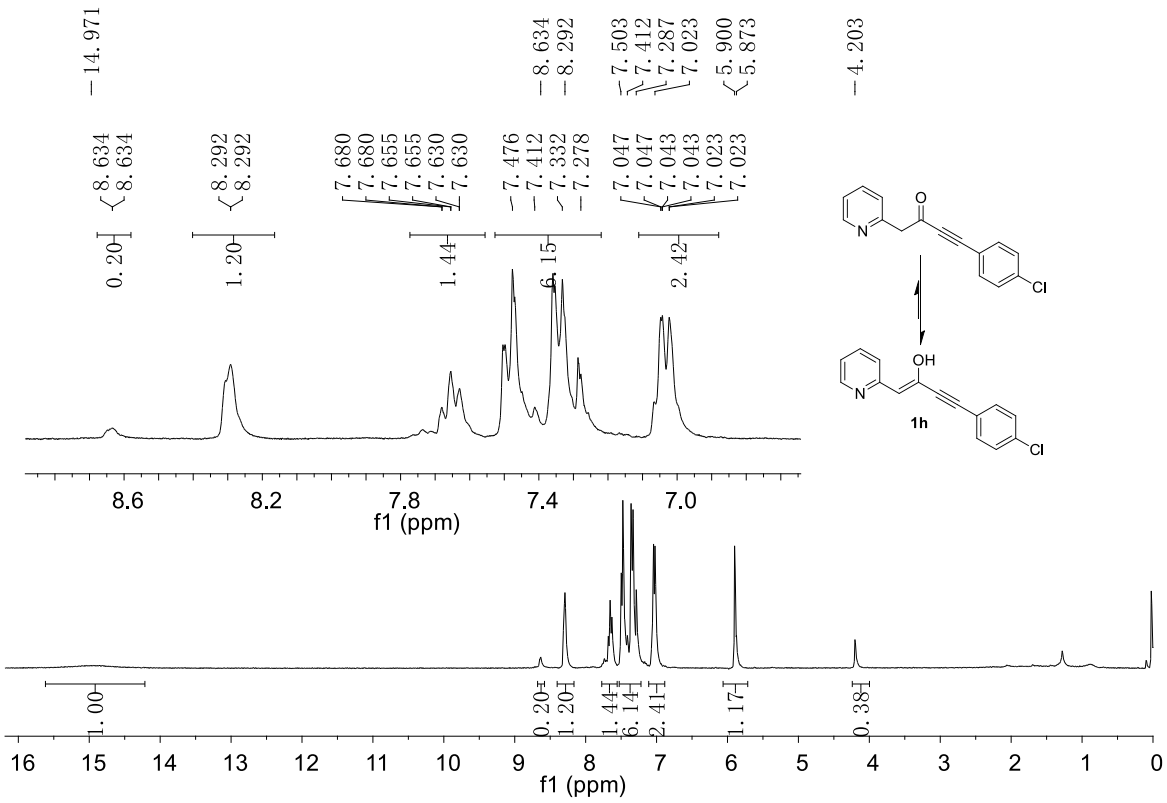
5. ^{1}H NMR and ^{13}C NMR Spectra






14.954
8.618
8.607
8.272
8.268
8.258
7.692
7.632
7.628
7.613
7.593
7.589
7.467
7.395
7.313
7.207
7.010
7.005
7.002
6.995
6.992
6.981
5.871
4.164
1.317
1.302
0.27
1.06
0.28
1.14
2.07
3.67
0.30
2.23
1.00
1.02
0.50
11.52
OH
1d
f1 (ppm)


184.011
157.703
154.690
154.009
152.376
149.734
149.677
144.092
136.661
131.748
125.418
122.280
119.058
116.651
103.647
93.648
90.034
87.749
85.938
54.363
35.071
34.869
31.149
31.025
OH
1d
f1 (ppm)


14.971
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8.634
8.292
8.292
7.680
7.680
7.655
7.655
7.630
7.630
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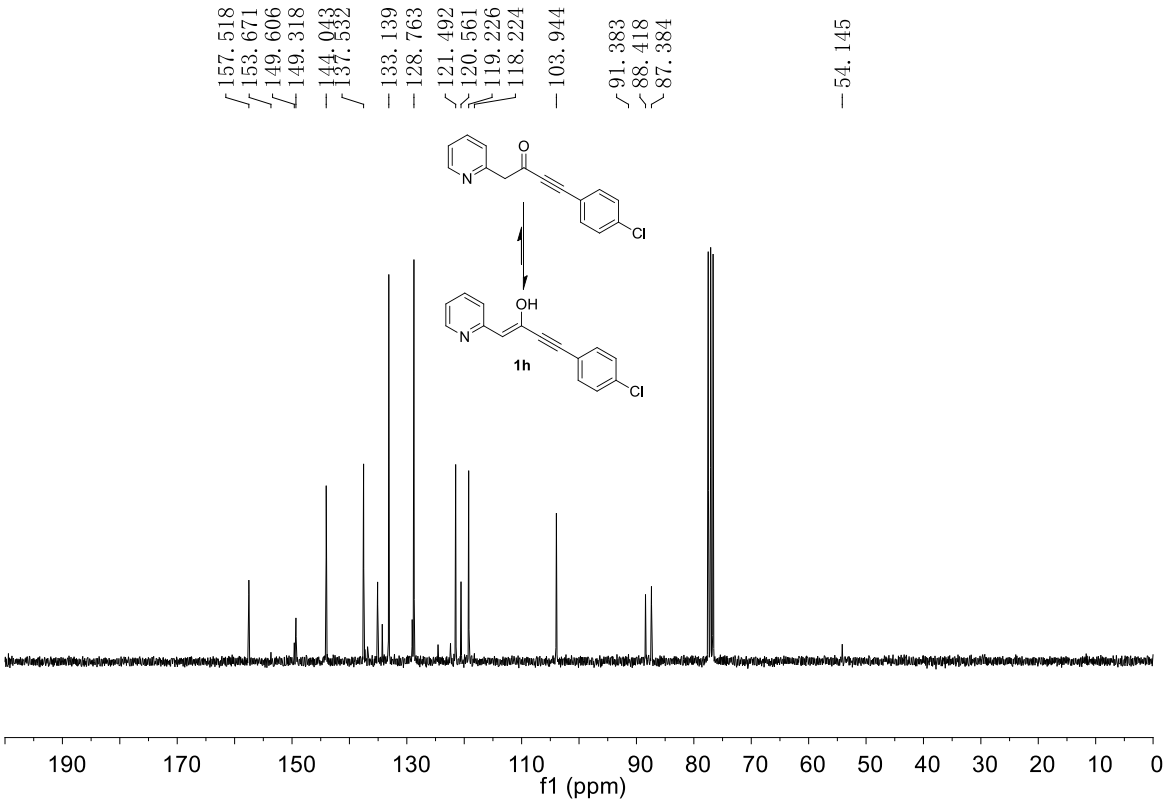
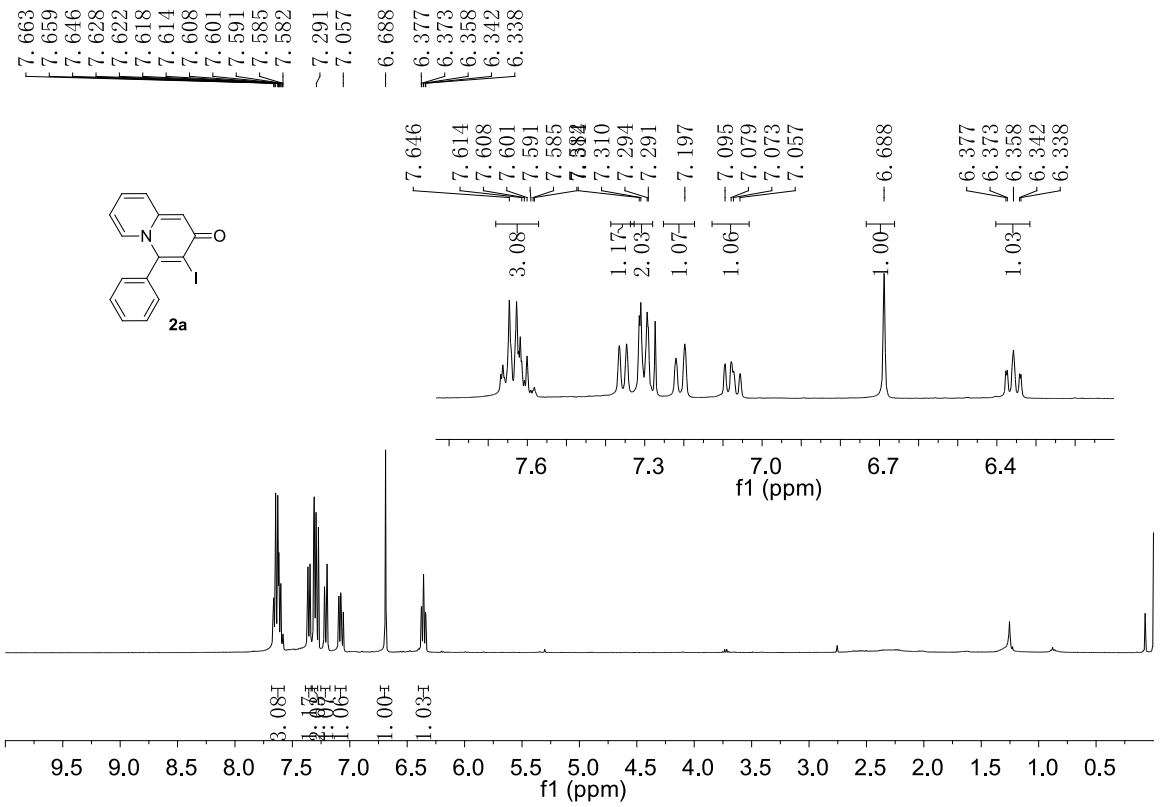
7.412
7.332
7.278
7.047
7.047
7.043
7.043
7.023
7.023
8.634
8.292
7.503
7.412
7.287
7.023
5.900
5.873
4.203
0.20
1.20
1.44
6.15
2.42
1h
f1 (ppm)
1.00
0.20
1.20
1.44
6.14
2.41
1.17
0.38
f1 (ppm)


157.518
153.671
149.606
149.318
144.043
137.532
133.139
128.763
121.492
120.561
119.226
118.224
103.944
91.383
88.418
87.384
54.145
1h
f1 (ppm)


7.663
7.659
7.646
7.628
7.622
7.618
7.614
7.608
7.601
7.591
7.585
7.582
7.291
7.057
6.688
6.377
6.373
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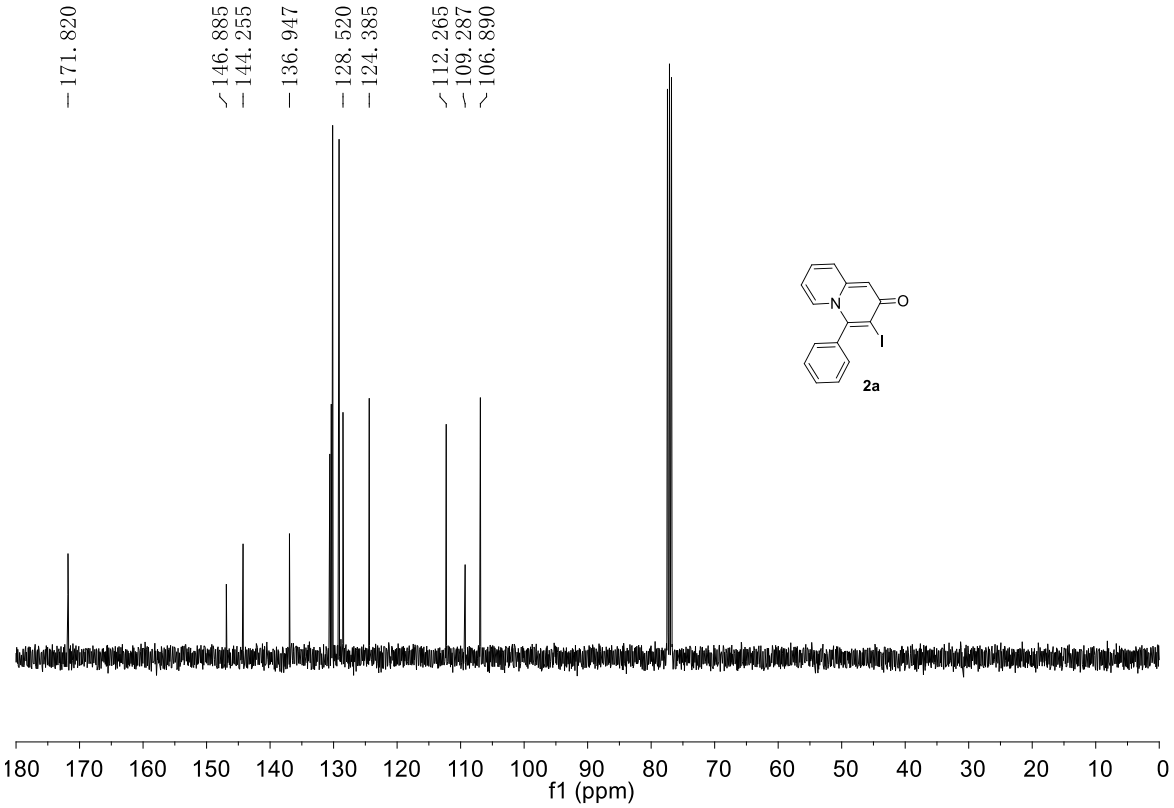
3.08
1.17
2.03
1.07
1.06
1.00
1.03
f1 (ppm)


171.820
146.885
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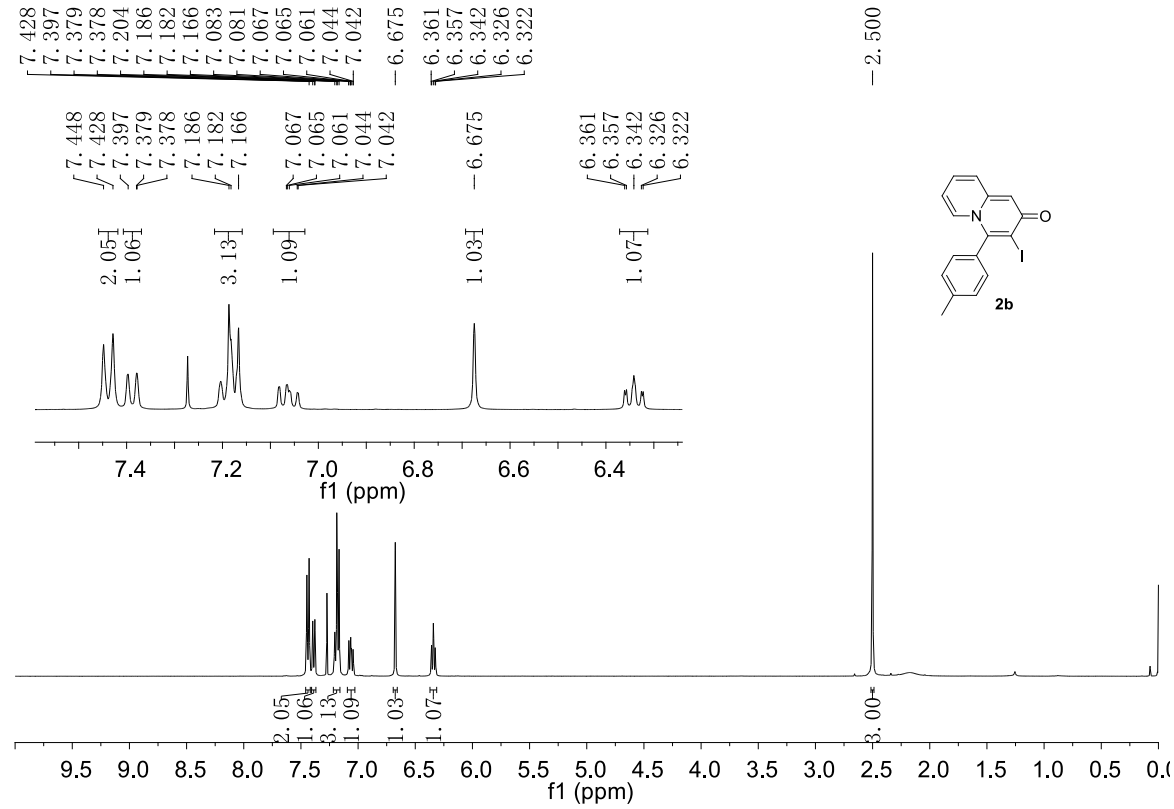
136.947
128.520
124.385
112.265
109.287
106.890
2a
f1 (ppm)


7.428
7.397
7.379
7.378
7.204
7.186
7.182
7.166
7.083
7.081
7.067
7.065
7.061
7.044
7.042
6.675
6.361
6.357
6.342
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6.322
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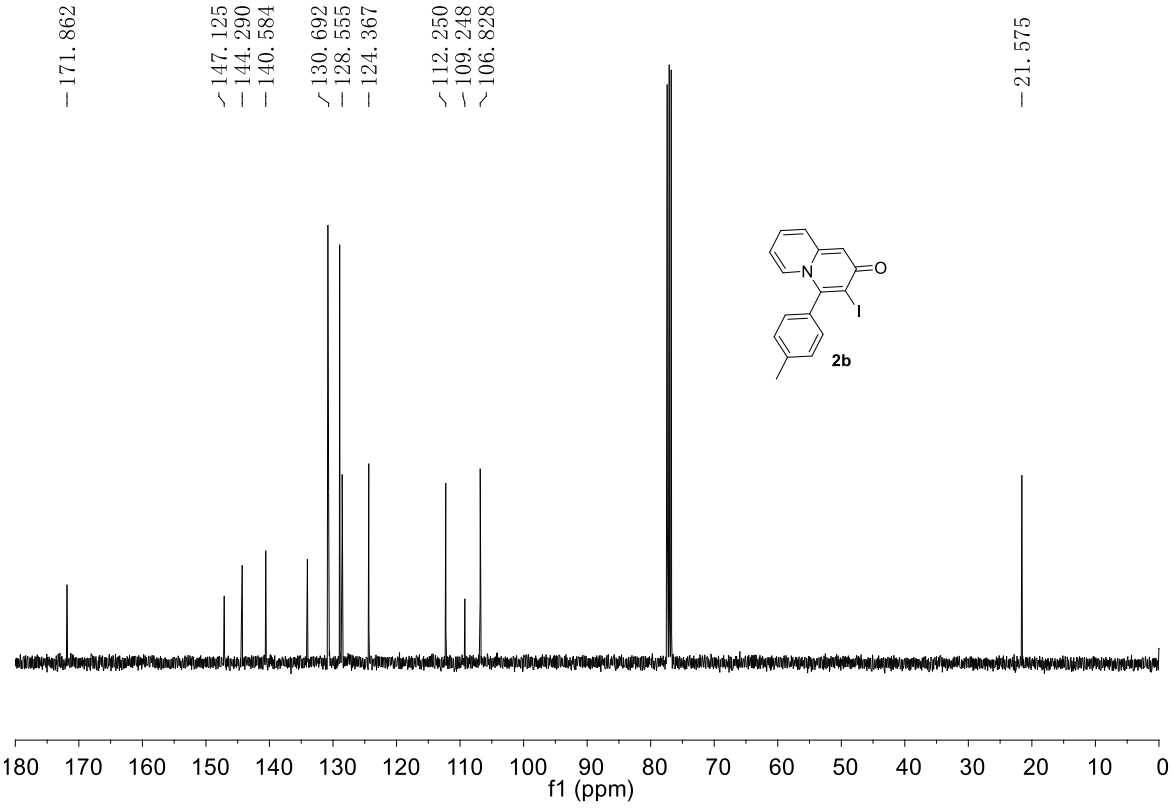
2.05
1.06
3.13
1.09
1.03
1.07
3.00
2b
f1 (ppm)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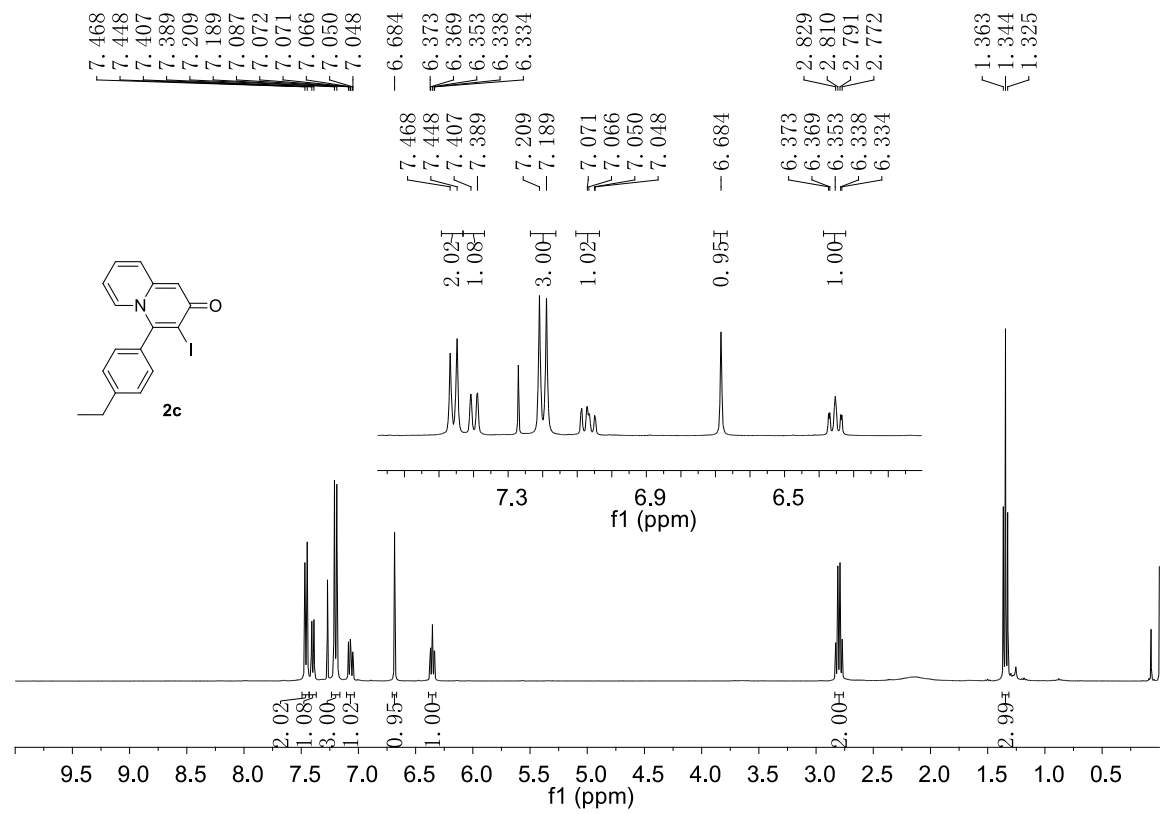
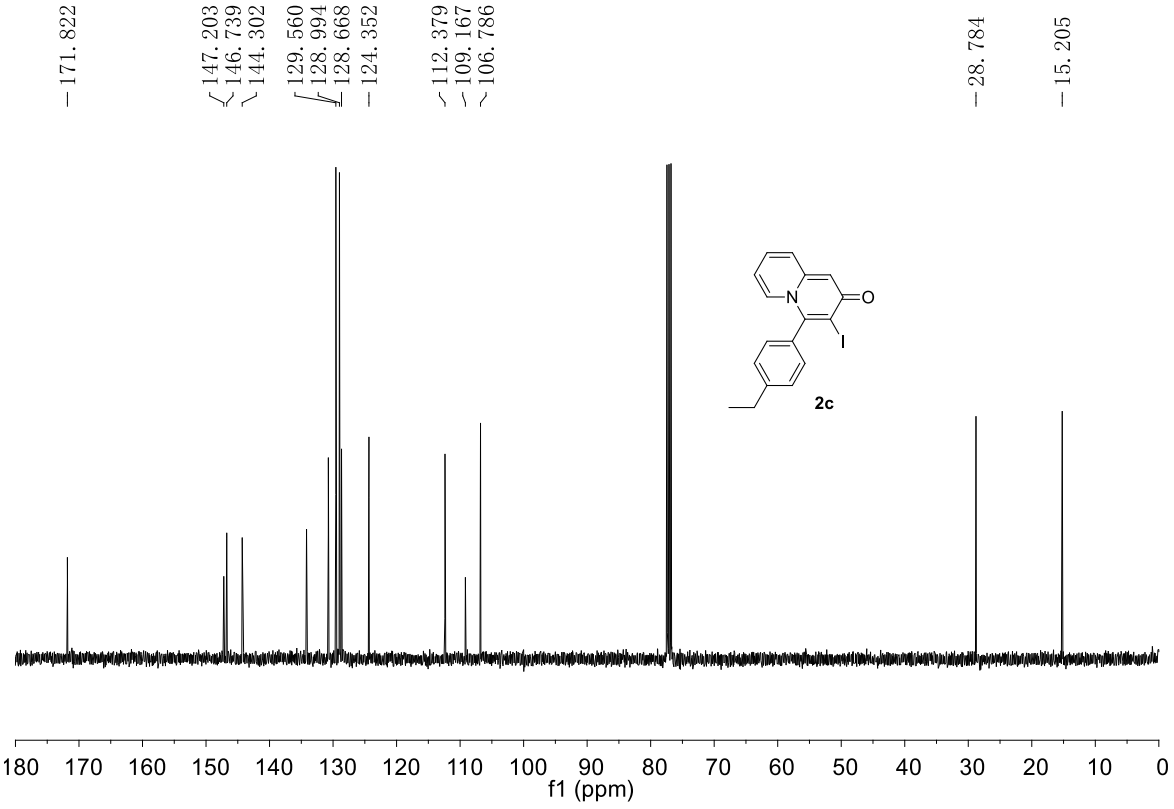
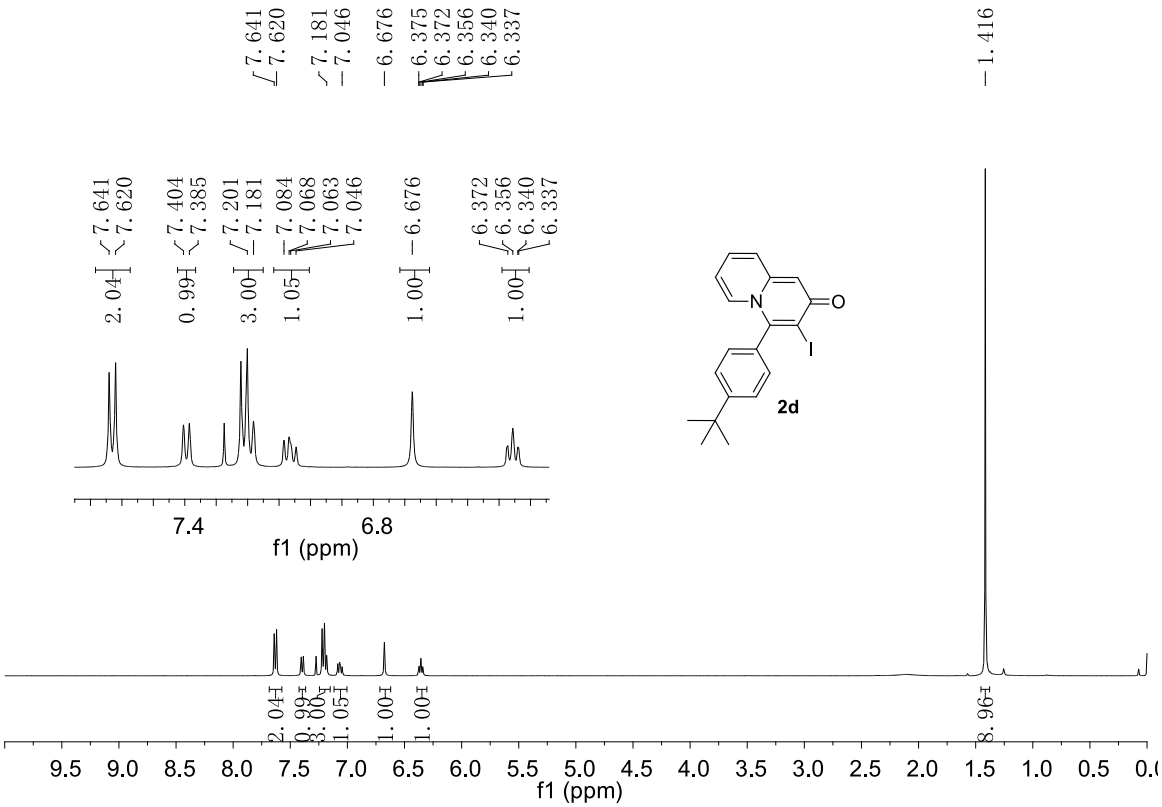
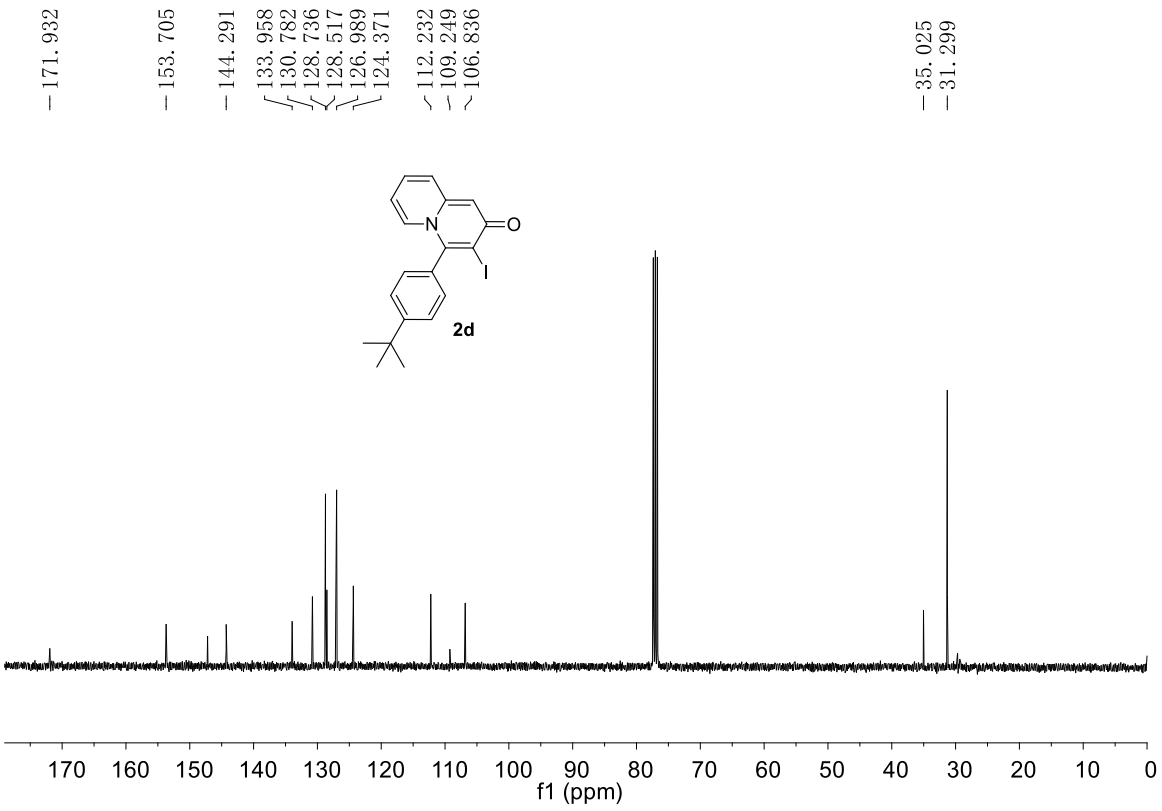
130.692
128.555
124.367
112.250
109.248
106.828
21.575
2b
f1 (ppm)


7.468
7.448
7.407
7.389
7.209
7.189
7.087
7.072
7.071
7.066
7.050
7.048
6.684
6.373
6.369
6.353
6.338
6.334
2.829
2.810
2.791
2.772
1.363
1.344
1.325
2.02
1.08
3.00
1.02
0.95
1.00
2.00
2.99
2c
7.3
6.9
6.5
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


171.822
147.203
146.739
144.302
129.560
128.994
128.668
124.352
112.379
109.167
106.786
28.784
15.205
2c
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.641
7.620
7.181
7.046
6.676
6.375
6.372
6.356
6.340
6.337
1.416
2.04
0.99
3.00
1.05
1.00
1.00
8.96
7.404
7.385
7.201
7.181
7.084
7.068
7.063
7.046
6.372
6.356
6.340
6.337
7.4
6.8
f1 (ppm)
N
O
I
2d
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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130.782
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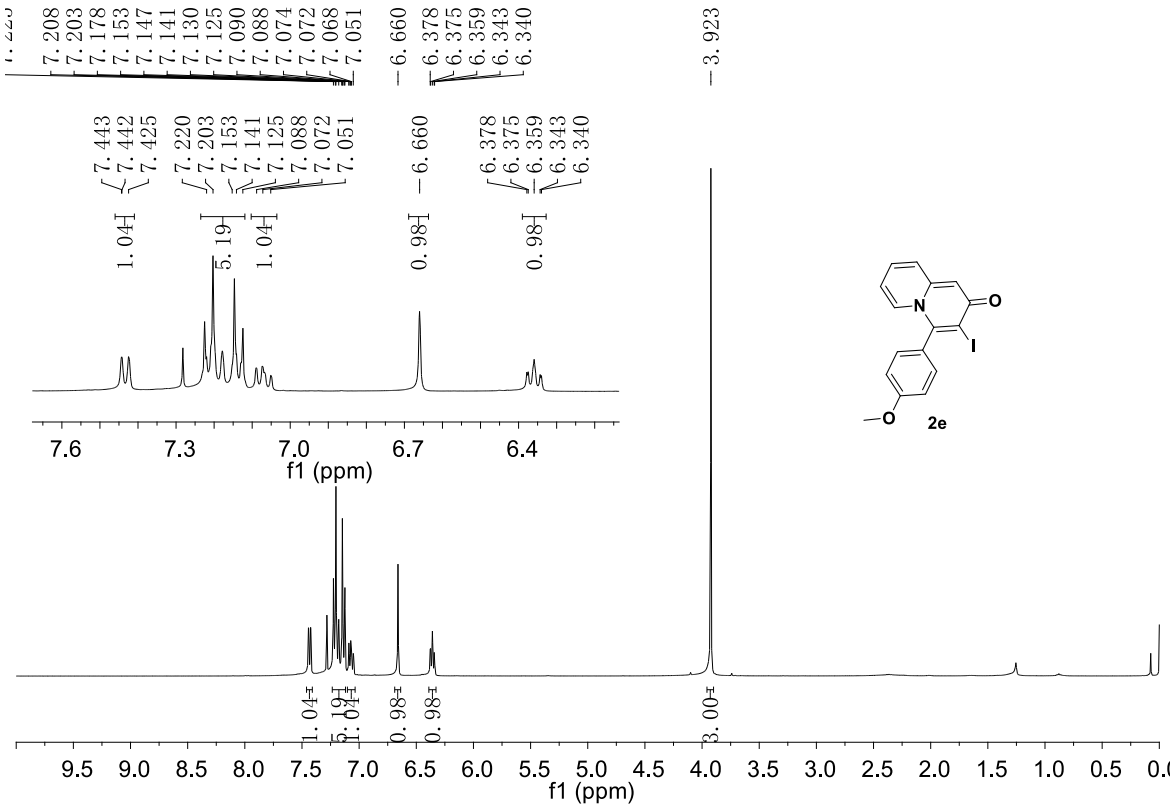
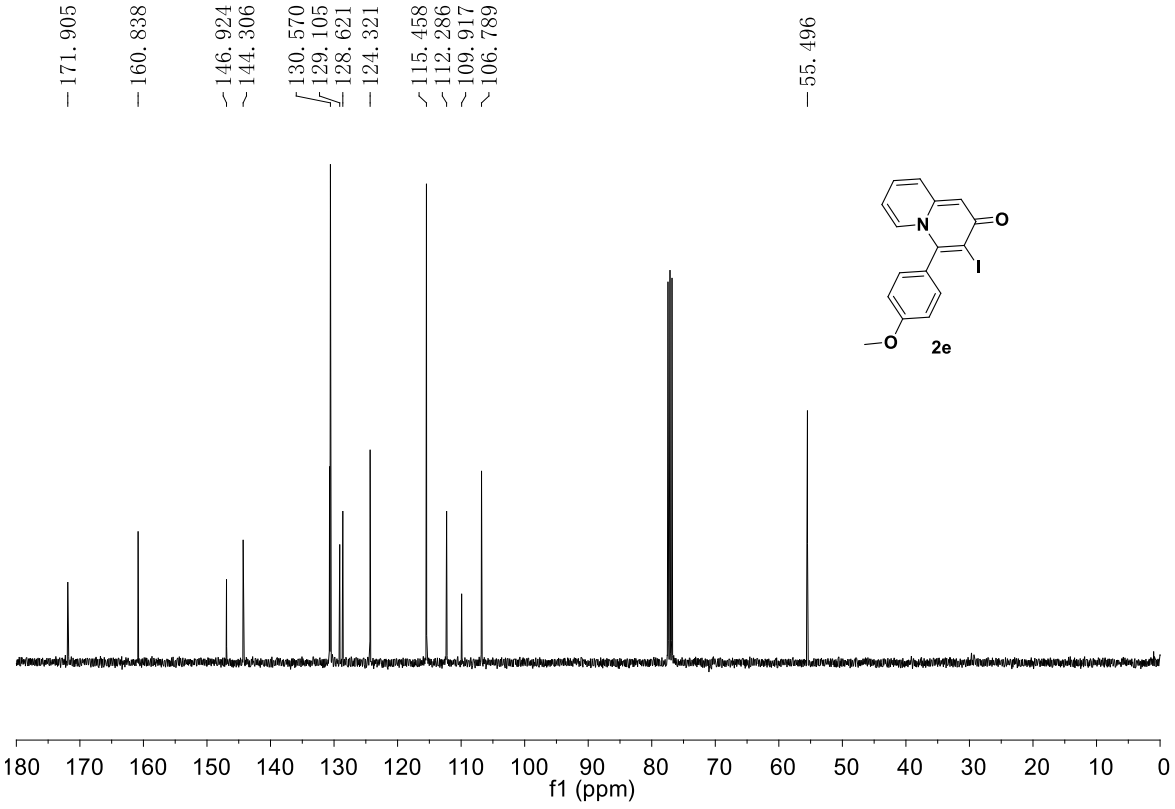
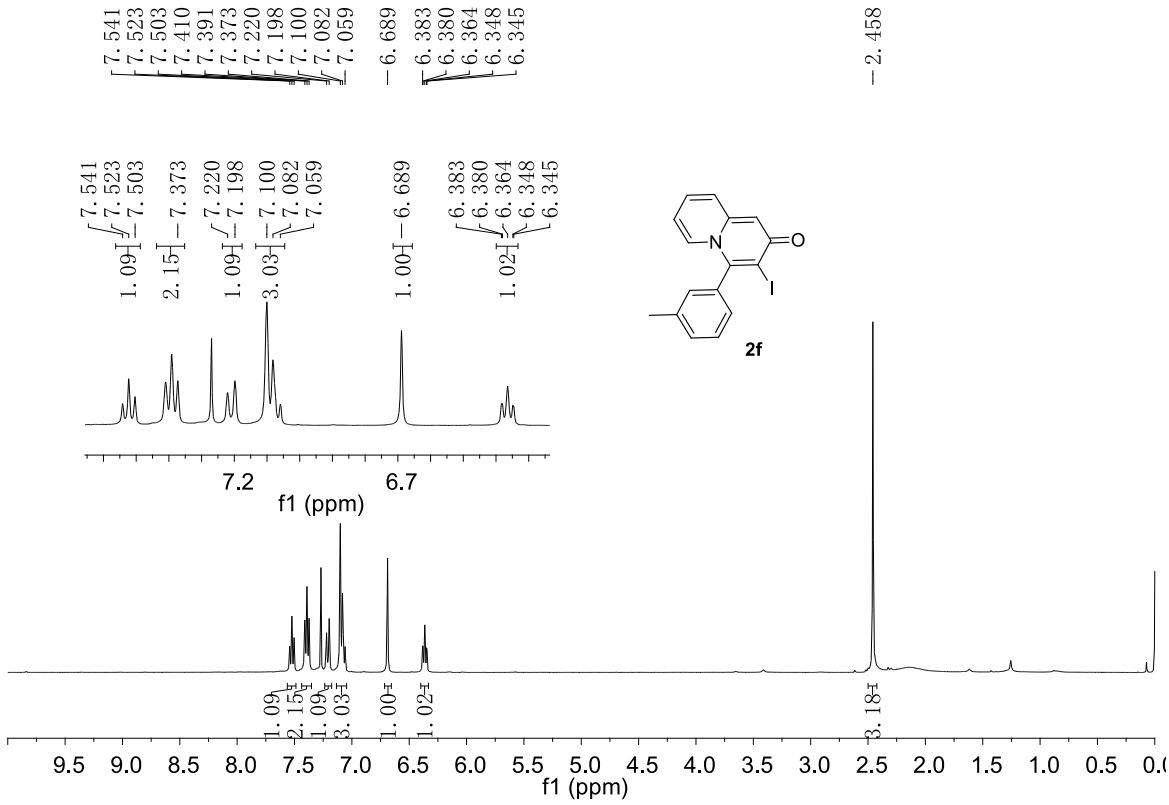
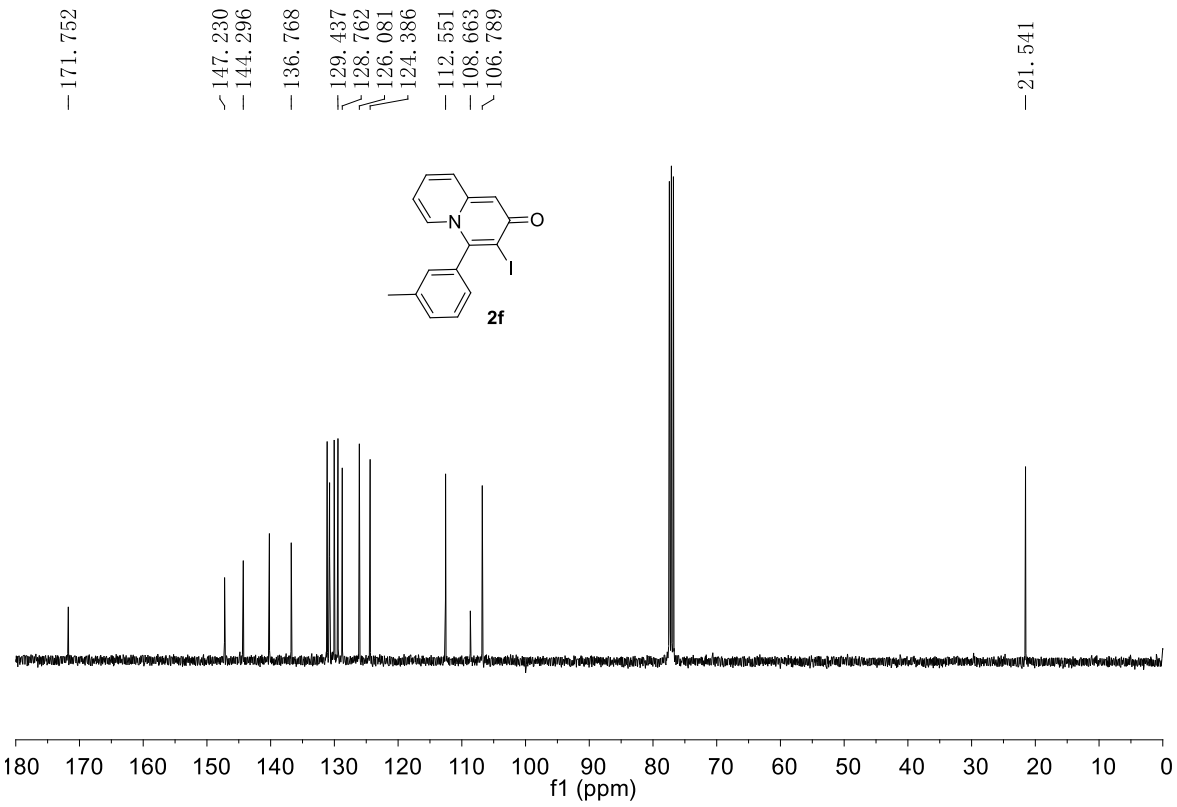
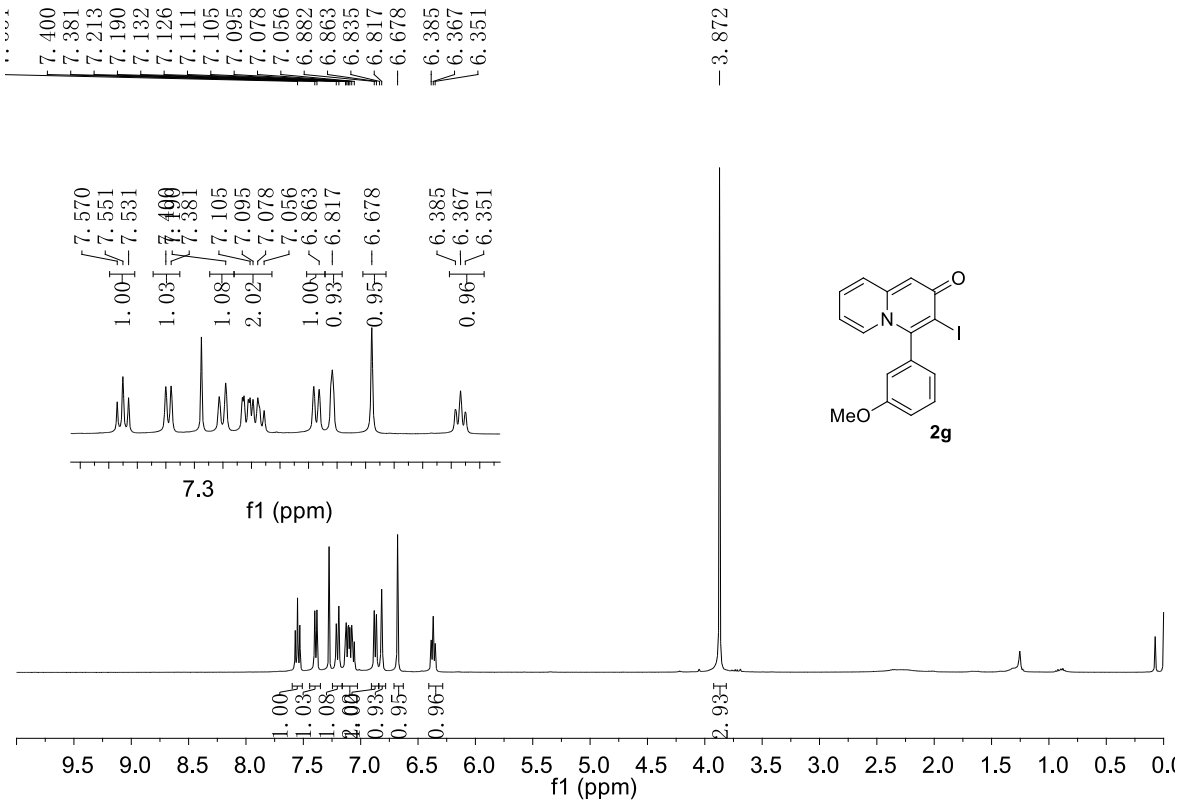
128.517
126.989
124.371
112.232
109.249
106.836
35.025
31.299
N
O
I
2d
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

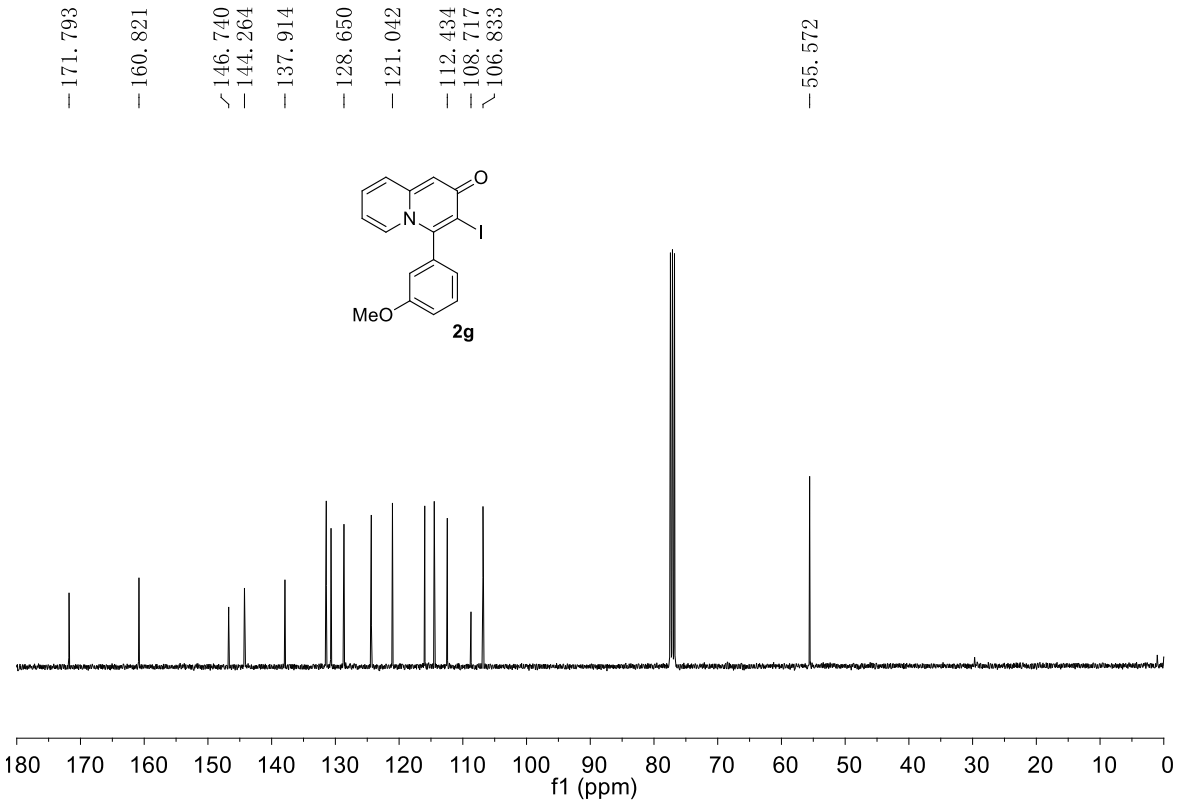

7.208
7.203
7.178
7.153
7.147
7.141
7.130
7.125
7.090
7.088
7.074
7.072
7.068
7.051
6.660
6.378
6.375
6.359
6.343
6.340
3.923
7.443
7.442
7.425
7.220
7.203
7.153
7.141
7.125
7.088
7.072
7.051
6.660
6.378
6.375
6.359
6.343
6.340
1.04
5.19
1.04
0.98
0.98
3.00
O
N
O
I
2e
f1 (ppm)

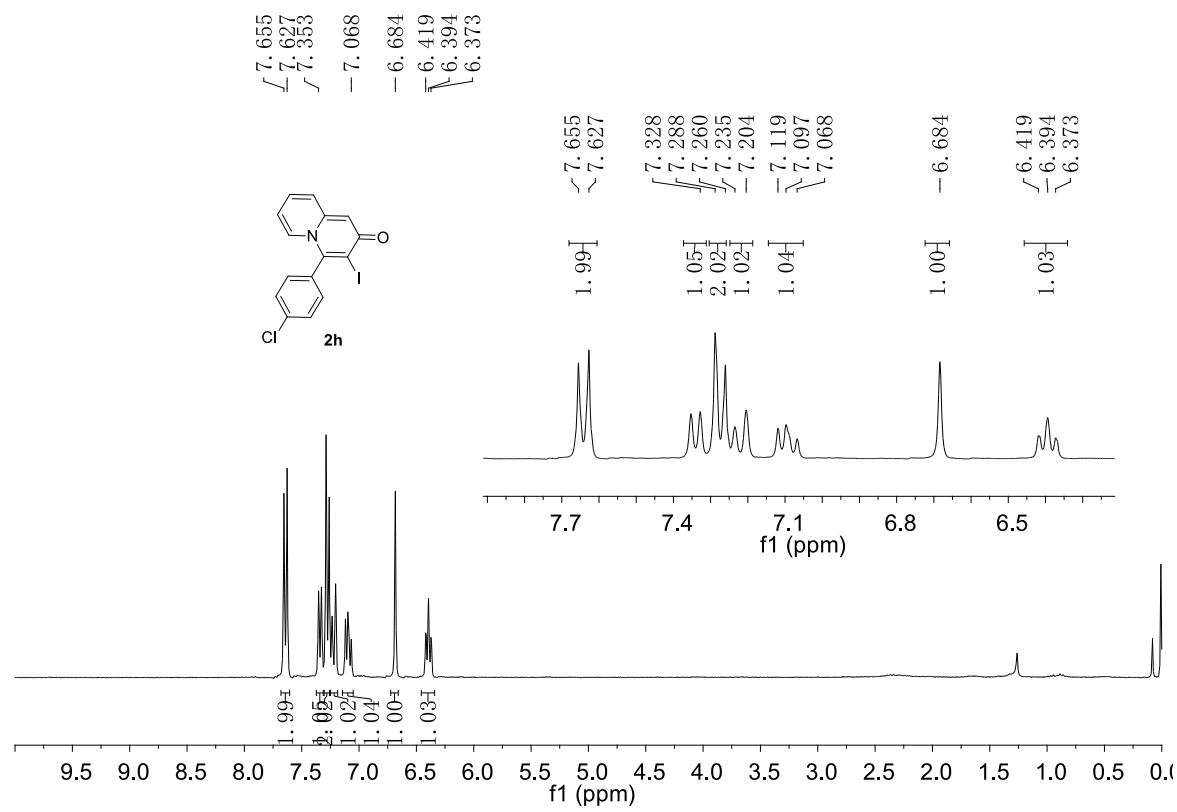

171.905
160.838
146.924
144.306
130.570
129.105
128.621
124.321
115.458
112.286
109.917
106.789
55.496
O
N
O
I
2e
f1 (ppm)

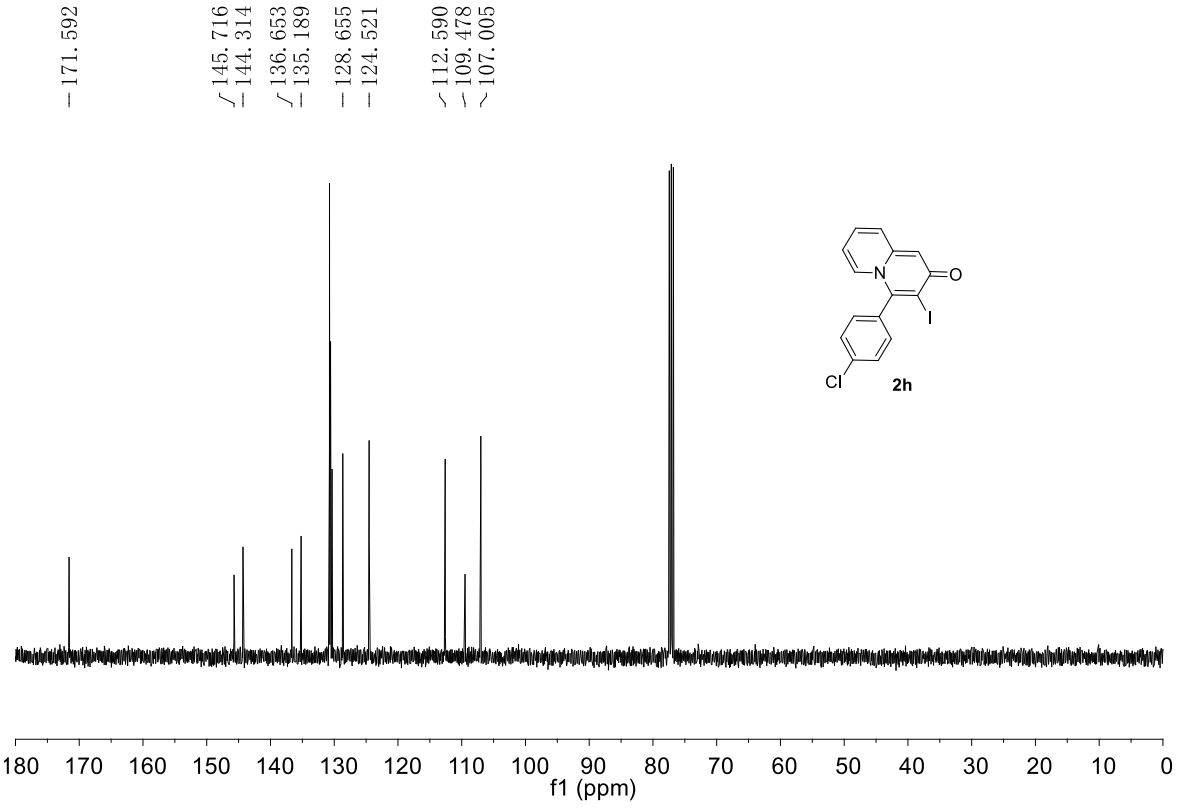

7.541
7.523
7.503
7.410
7.391
7.373
7.220
7.198
7.100
7.082
7.059
6.689
6.383
6.380
6.364
6.348
6.345
2.458
1.09
2.15
1.09
3.03
1.00
1.02
3.18
2f
7.2
6.7
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

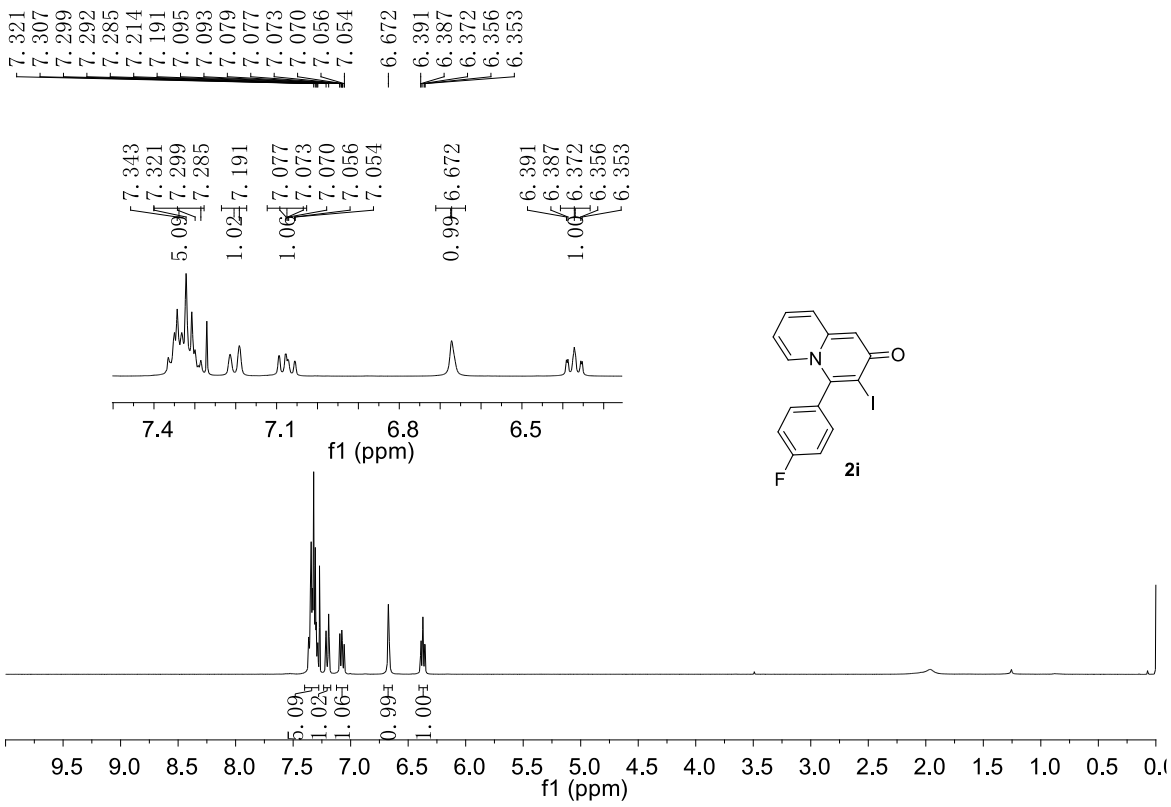

171.752
147.230
144.296
136.768
129.437
128.762
126.081
124.386
112.551
108.663
106.789
21.541
2f
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

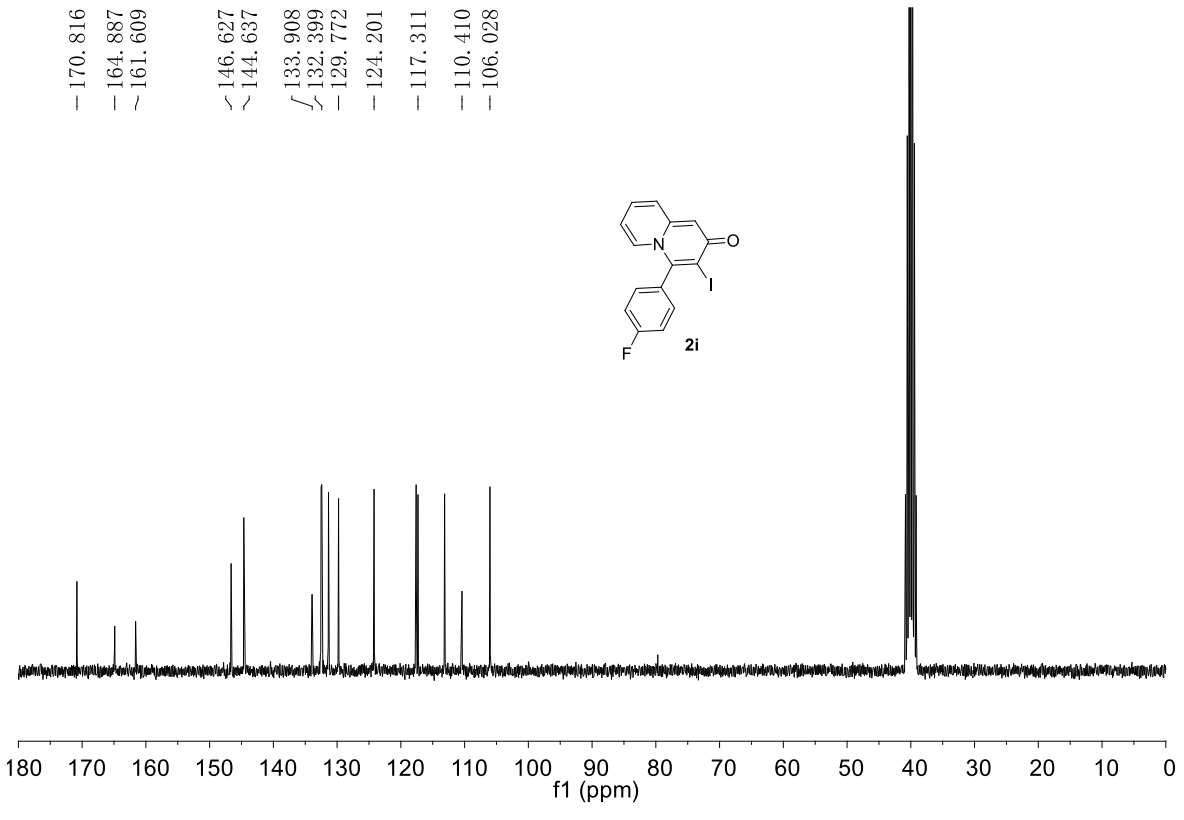

7.400
7.381
7.213
7.190
7.132
7.126
7.111
7.105
7.095
7.078
7.056
6.882
6.863
6.835
6.817
6.678
6.385
6.367
6.351
3.872
7.570
7.551
7.531
7.381
7.105
7.095
7.078
7.056
6.863
6.817
6.678
6.385
6.367
6.351
1.00
1.03
1.08
2.02
1.00
0.93
0.95
0.96
2.93
MeO
2g
7.3
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

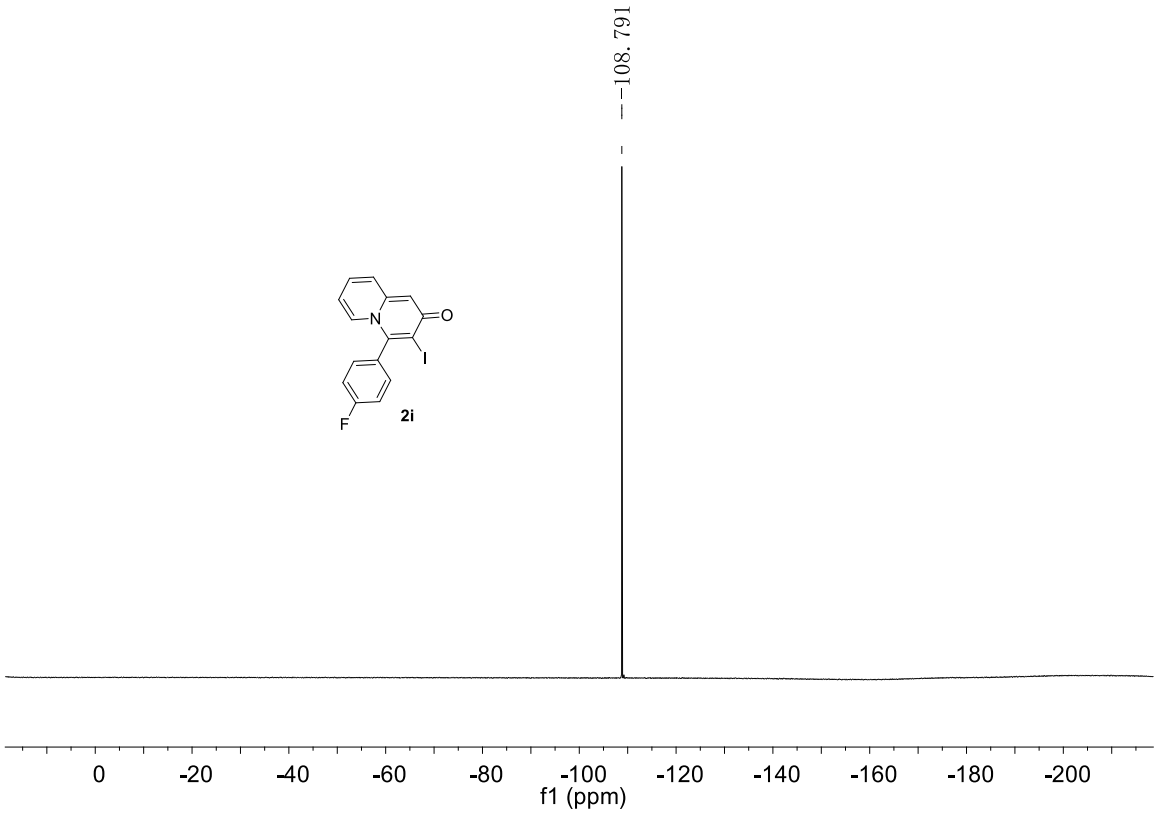

171.793
160.821
146.740
144.264
137.914
128.650
121.042
112.434
108.717
106.833
55.572
MeO
2g
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

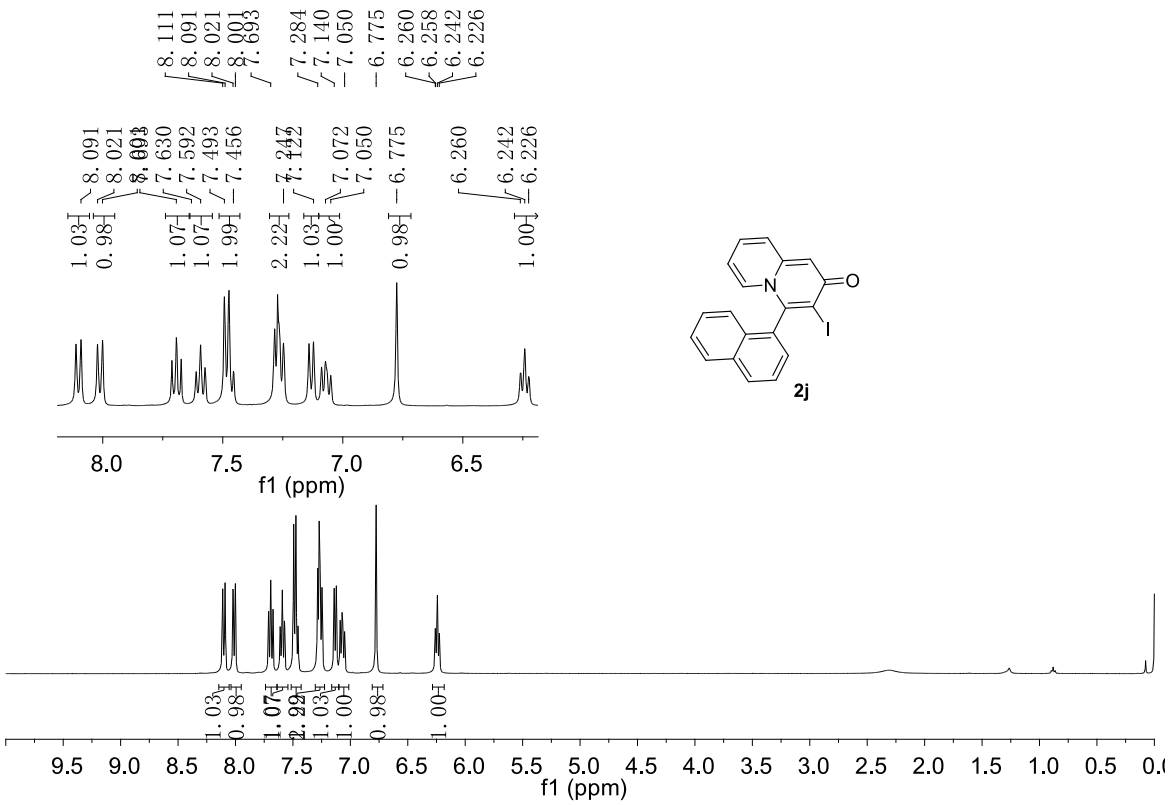

7.655
7.627
7.353
7.068
6.684
6.419
6.394
6.373
2h
f1 (ppm)

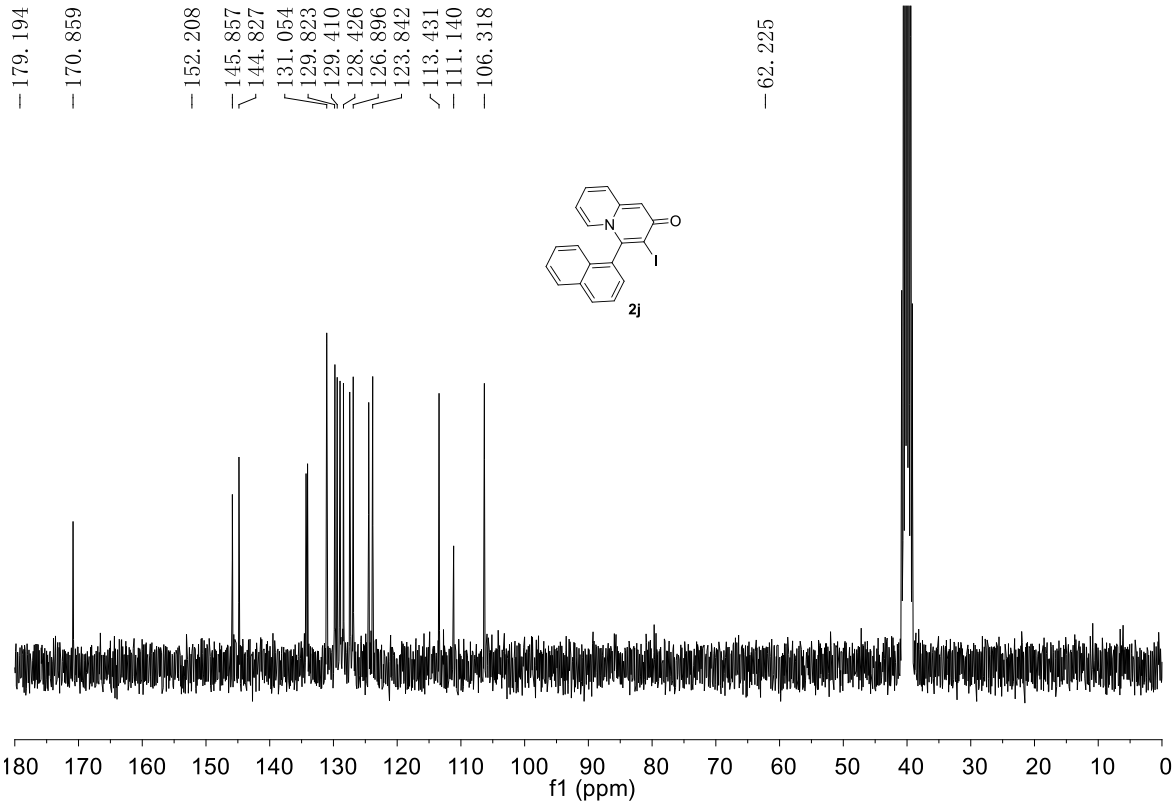

171.592
145.716
144.314
136.653
135.189
128.655
124.521
112.590
109.478
107.005
2h
f1 (ppm)

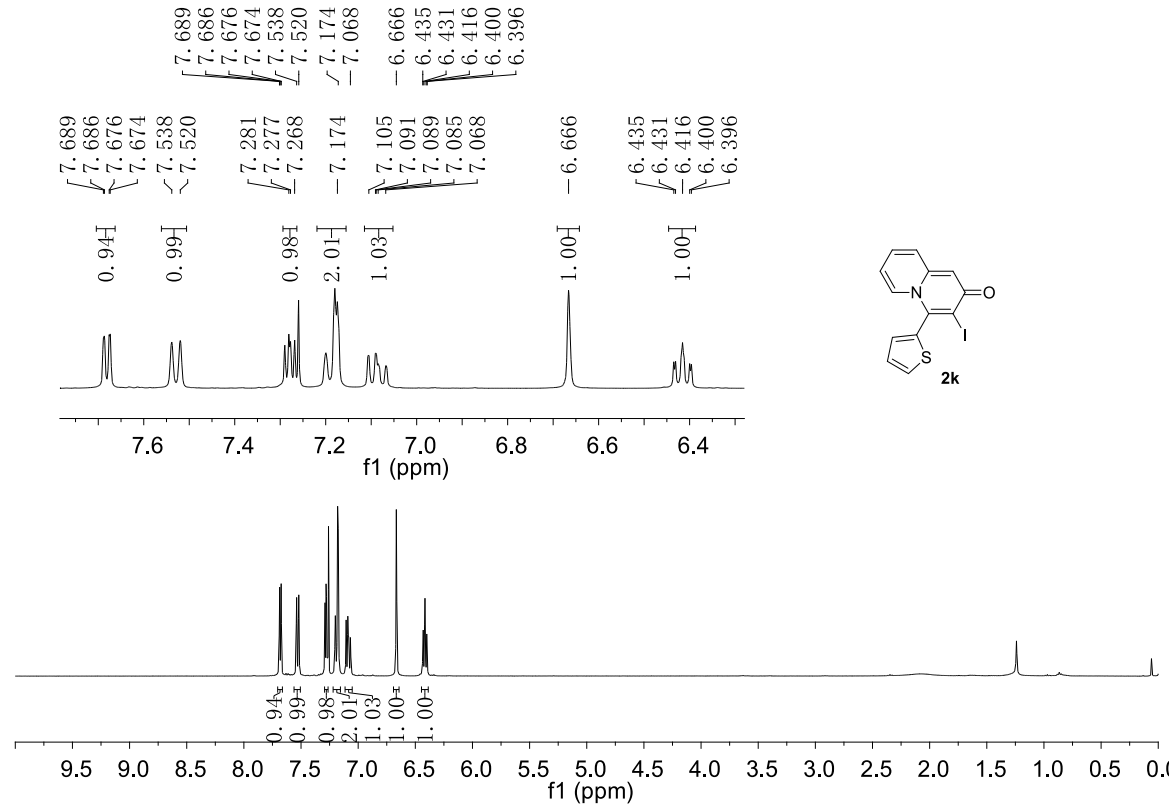

7.321
7.307
7.299
7.292
7.285
7.214
7.191
7.095
7.093
7.079
7.077
7.073
7.070
7.056
7.054
6.672
6.391
6.387
6.372
6.356
6.353
5.09
1.02
1.06
0.99
1.00
f1 (ppm)
O
N
I
F
2i

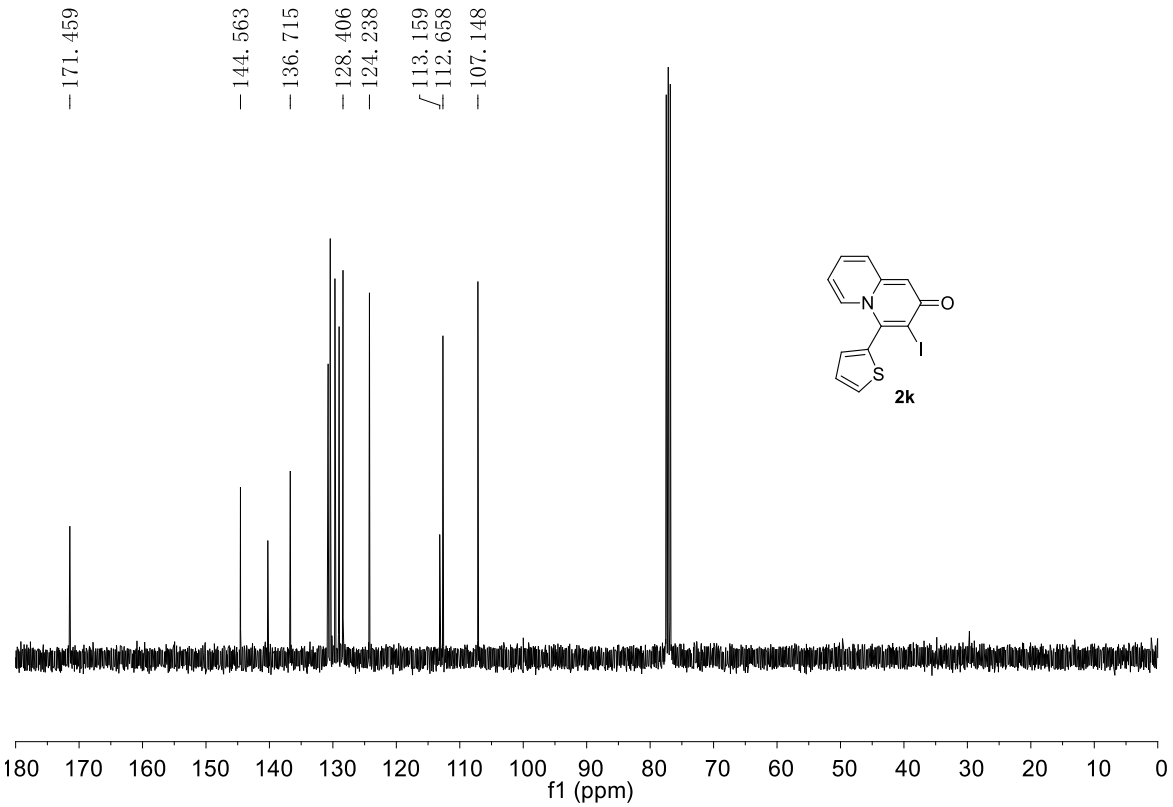

170.816
164.887
161.609
146.627
144.637
133.908
132.399
129.772
124.201
117.311
110.410
106.028
f1 (ppm)
O
N
I
F
2i

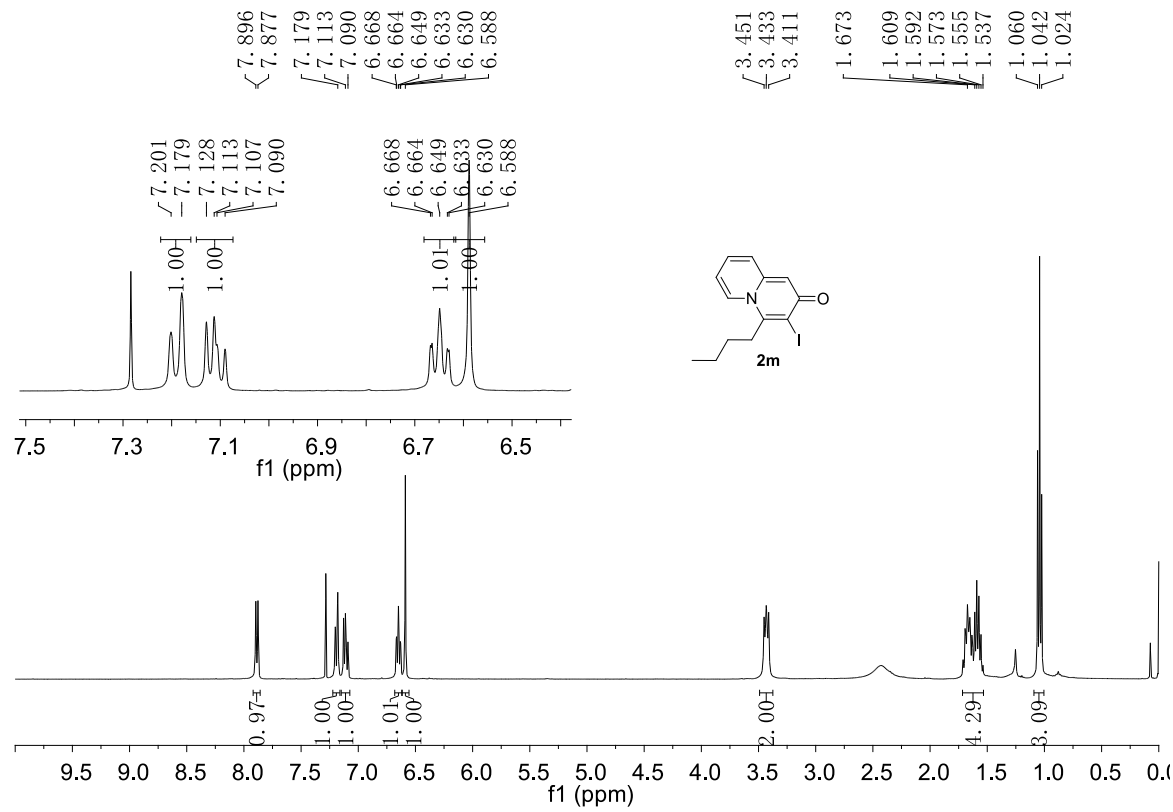

-108.791
O
N
I
F
2i
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

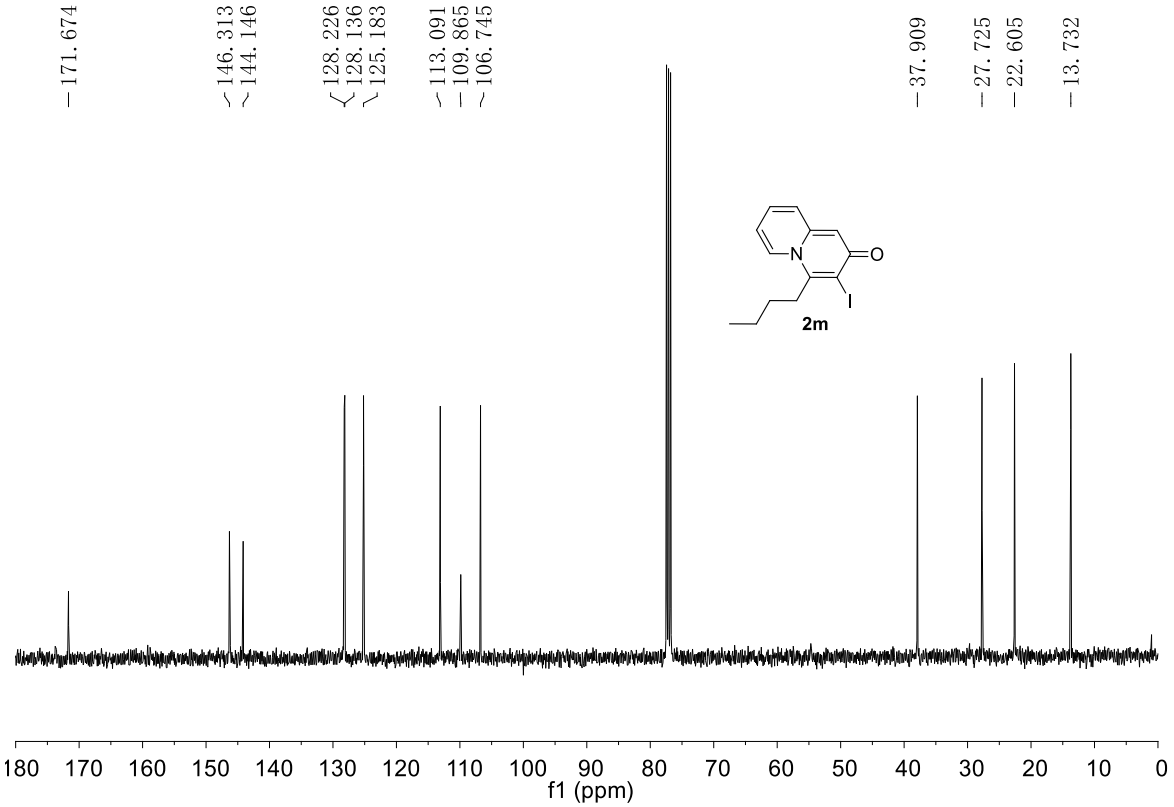

8.111
8.091
8.021
8.001
7.893
7.630
7.592
7.493
7.456
7.284
7.247
7.140
7.072
7.050
6.775
6.260
6.258
6.242
6.226
1.03
0.98
1.07
1.07
1.99
2.22
1.03
1.00
0.98
1.00
O
N
I
2j
8.0
7.5
7.0
6.5
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

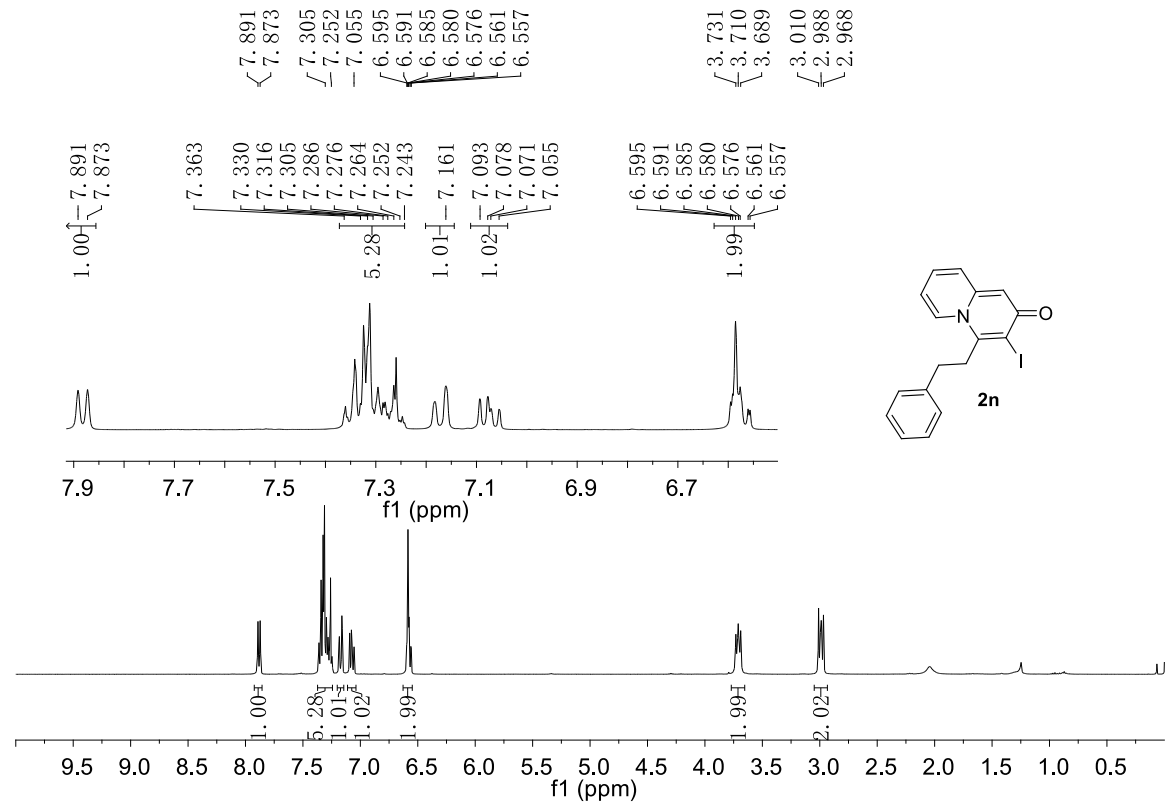

179.194
170.859
152.208
145.857
144.827
131.054
129.823
129.410
128.426
126.896
123.842
113.431
111.140
106.318
62.225
O
N
I
2j
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

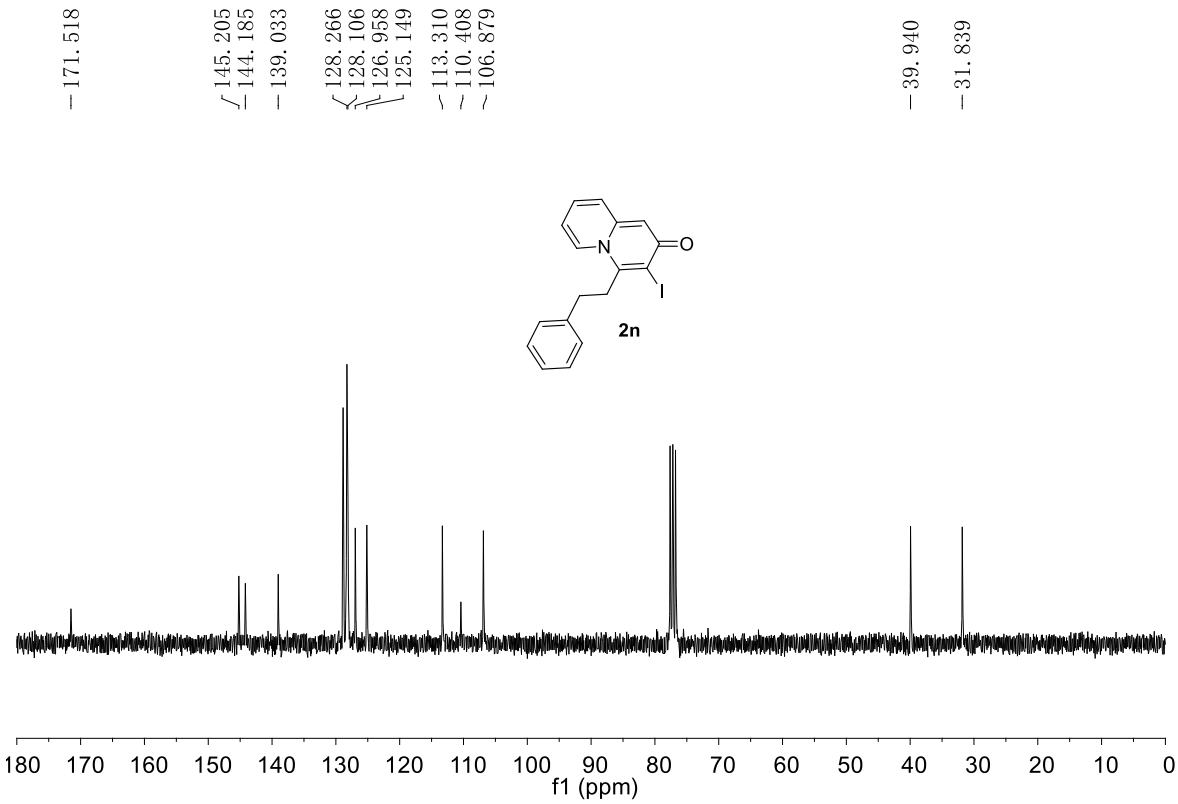

7.689
7.686
7.676
7.674
7.538
7.520
7.281
7.277
7.268
7.174
7.105
7.091
7.089
7.085
7.068
6.666
6.435
6.431
6.416
6.400
6.396
0.94
0.99
0.98
2.01
1.03
1.00
1.00
O
N
I
S
2k
7.6 7.4 7.2 7.0 6.8 6.6 6.4
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

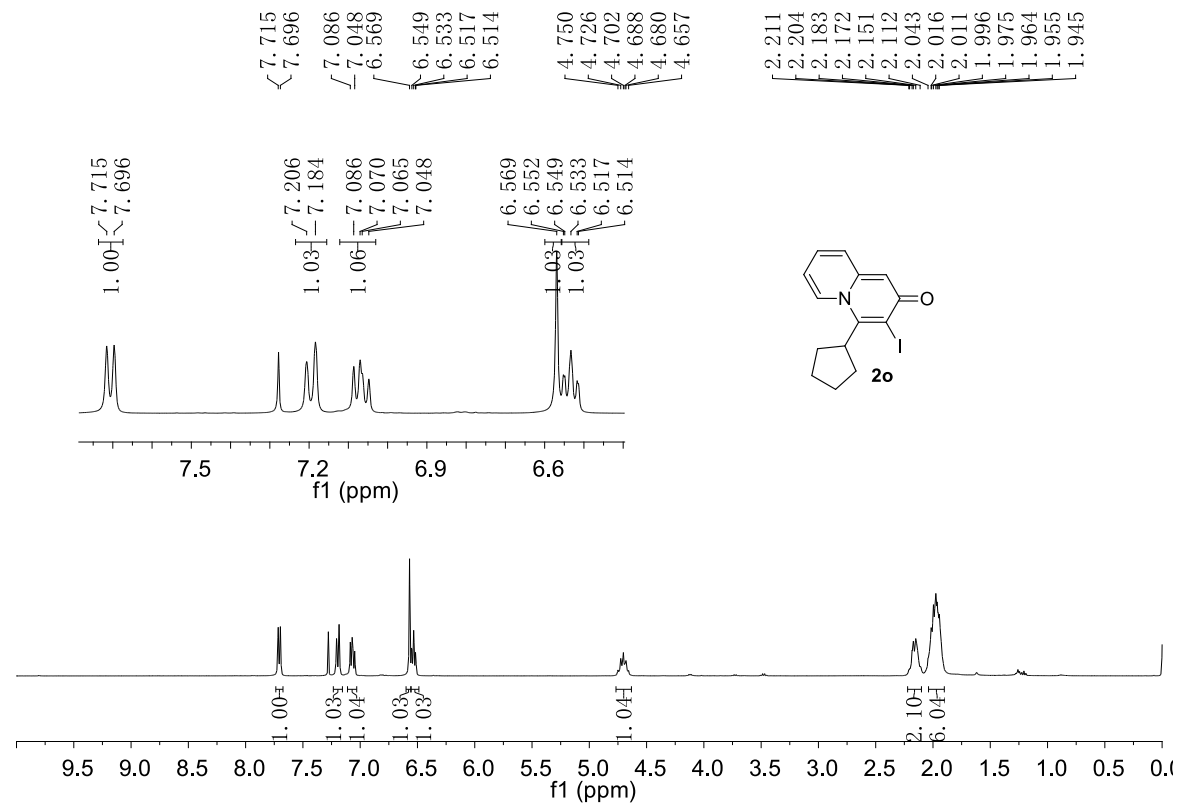

171.459
144.563
136.715
128.406
124.238
113.159
112.658
107.148
2k
f1 (ppm)

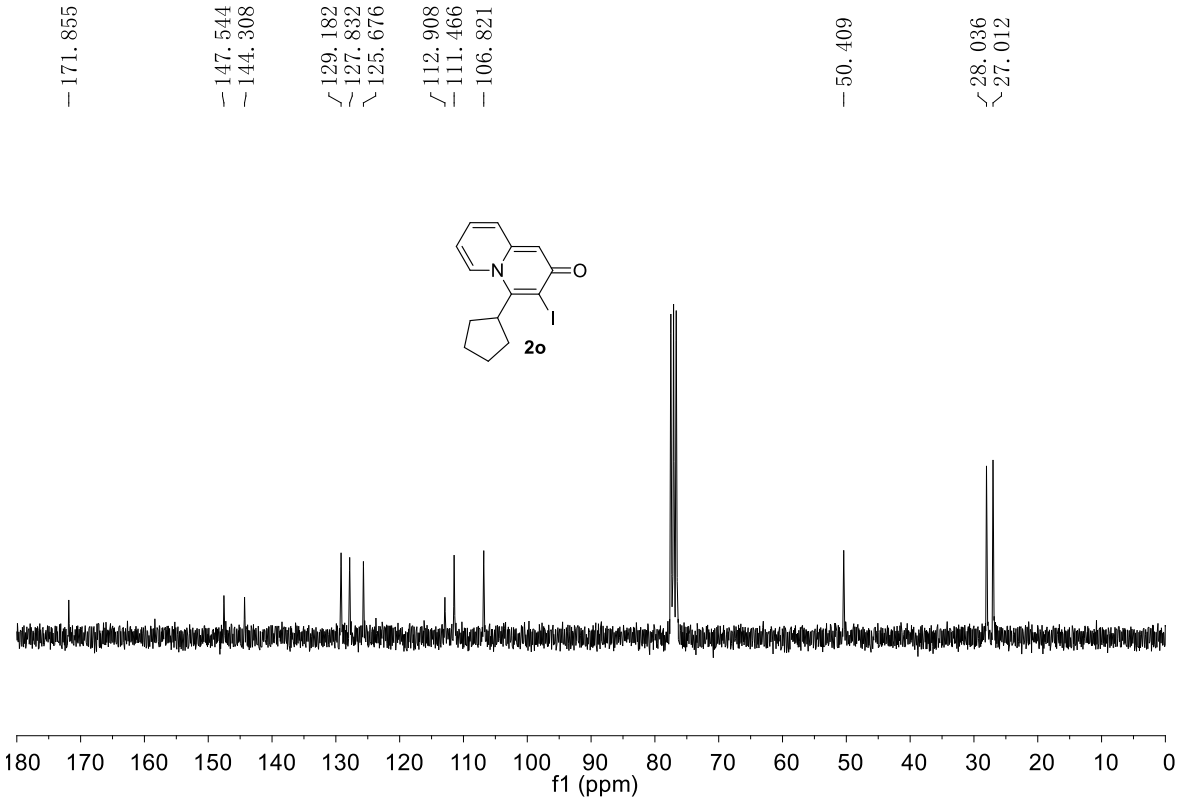

7.896
7.877
7.179
7.113
7.090
6.668
6.664
6.649
6.633
6.630
6.588
3.451
3.433
3.411
1.673
1.609
1.592
1.573
1.555
1.537
1.060
1.042
1.024
2m
f1 (ppm)

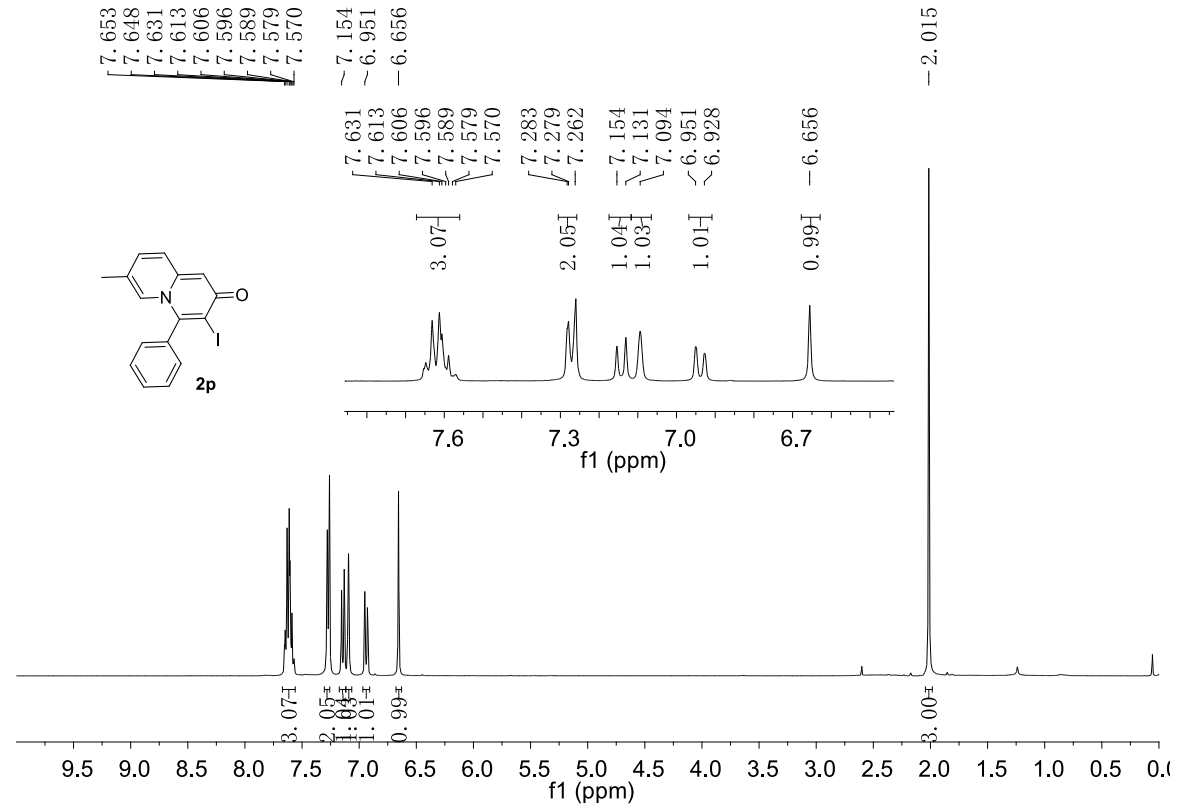

171.674
146.313
144.146
128.226
128.136
125.183
113.091
109.865
106.745
37.909
27.725
22.605
13.732
2m
f1 (ppm)


7.891
7.873
7.305
7.252
7.055
6.595
6.591
6.585
6.580
6.576
6.561
6.557
3.731
3.710
3.689
3.010
2.988
2.968
1.00
5.28
1.01
1.02
1.99
2n
f1 (ppm)


171.518
145.205
144.185
139.033
128.266
128.106
126.958
125.149
113.310
110.408
106.879
39.940
31.839
2n
f1 (ppm)


7.715
7.696
7.086
7.048
6.569
6.549
6.533
6.517
6.514
4.750
4.726
4.702
4.688
4.680
4.657
2.211
2.204
2.183
2.172
2.151
2.112
2.043
2.016
2.011
1.996
1.975
1.964
1.955
1.945
1.00
1.03
1.06
1.03
1.03
1.04
1.03
1.03
1.04
2.10
6.04
2o
f1 (ppm)


171.855
147.544
144.308
129.182
127.832
125.676
112.908
111.466
106.821
50.409
28.036
27.012
O
N
I
2o
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.648
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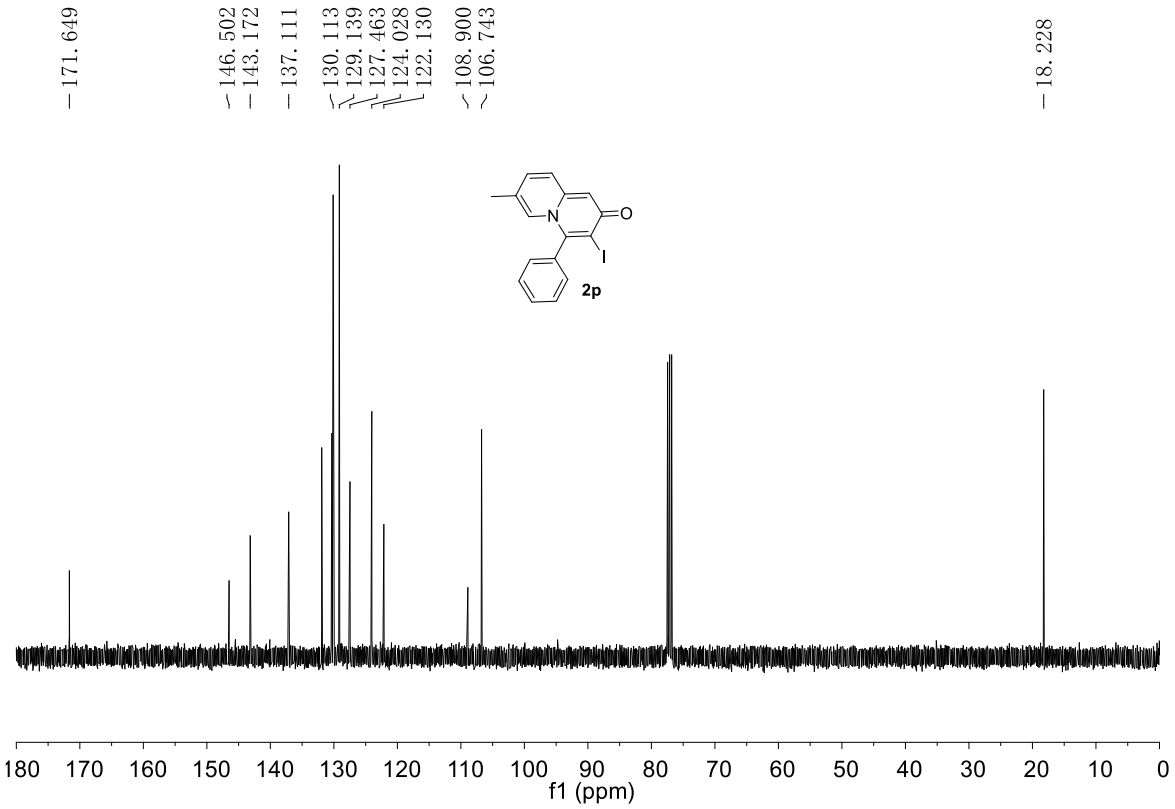
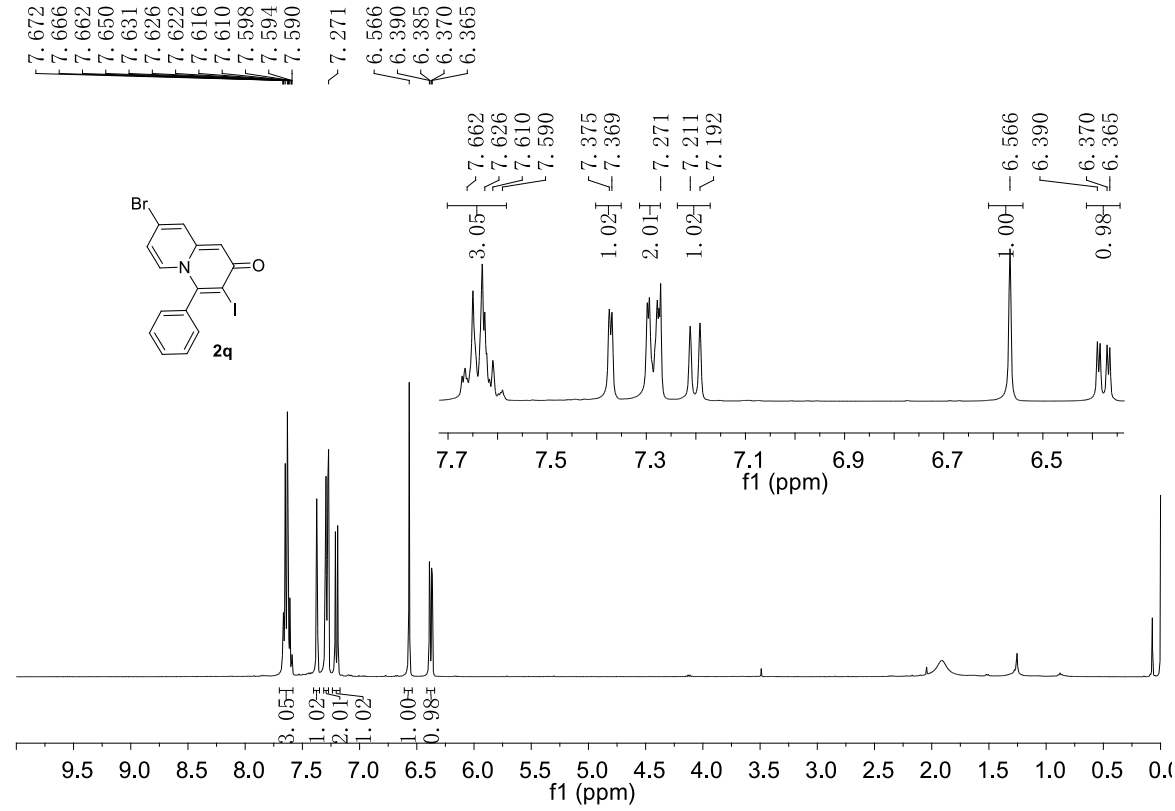
7.613
7.606
7.596
7.589
7.579
7.570
7.154
6.951
6.656
2.015
7.631
7.613
7.606
7.596
7.589
7.579
7.570
7.283
7.279
7.262
7.154
7.131
7.094
6.951
6.928
6.656
3.07
2.05
1.04
1.03
1.01
0.99
O
N
I
2p
7.6
7.3
7.0
6.7
f1 (ppm)
3.07
2.05
1.04
1.03
1.01
0.99
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


171.649
146.502
143.172
137.111
130.113
129.139
127.463
124.028
122.130
108.900
106.743
18.228
O
N
I
2p
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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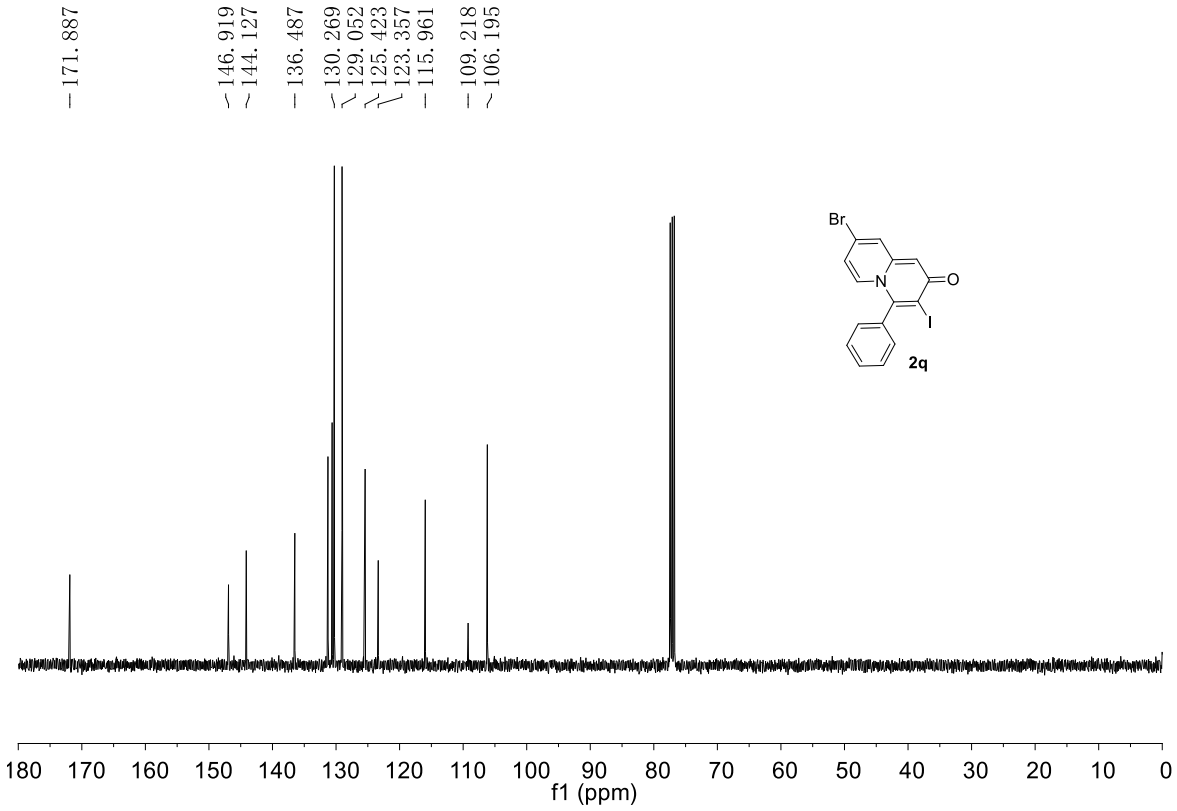
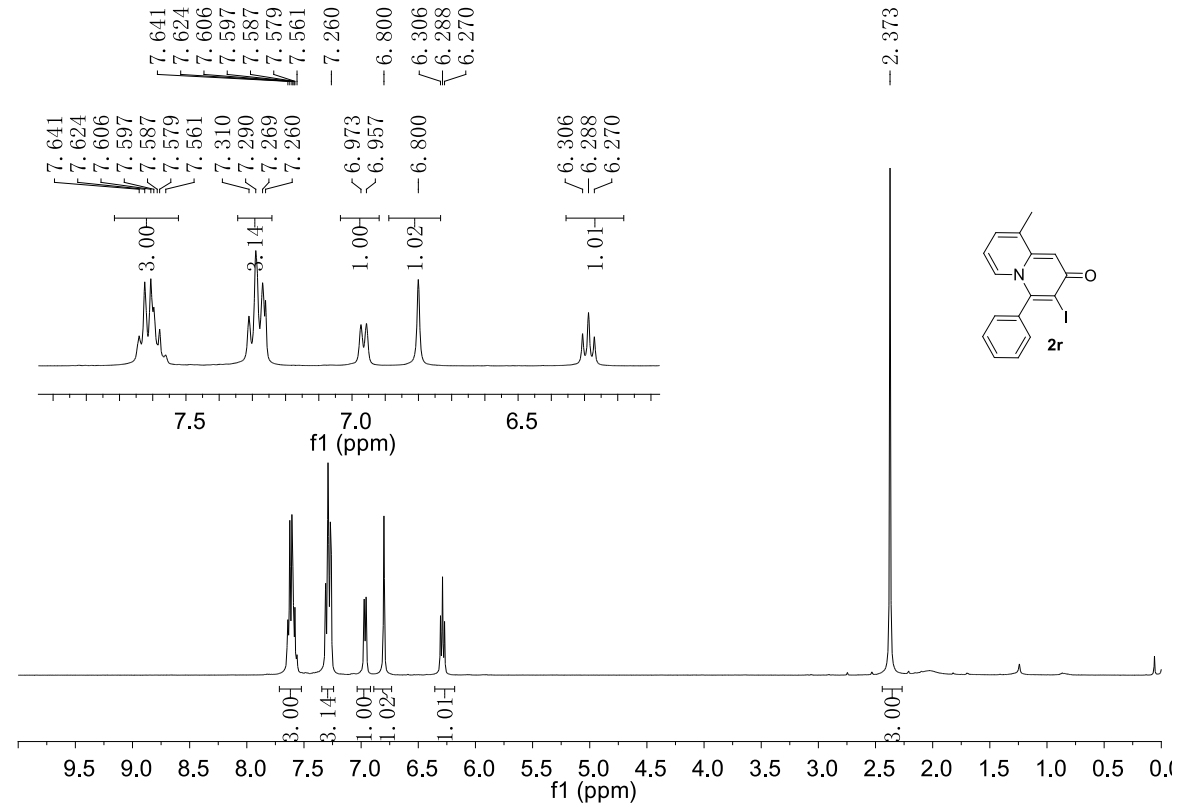
7.666
7.662
7.650
7.631
7.626
7.622
7.616
7.610
7.598
7.594
7.590
7.271
6.566
6.390
6.385
6.370
6.365
Br
O
N
I
2q
3.05
1.02
2.01
1.02
1.00
0.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)
7.662
7.626
7.610
7.590
7.375
7.369
7.271
7.211
7.192
6.566
6.390
6.370
6.365
3.05
1.02
2.01
1.02
1.00
0.98
7.7 7.5 7.3 7.1 6.9 6.7 6.5
f1 (ppm)


171.887
146.919
144.127
136.487
130.269
129.052
125.423
123.357
115.961
109.218
106.195
Br
N
O
I
2q
f1 (ppm)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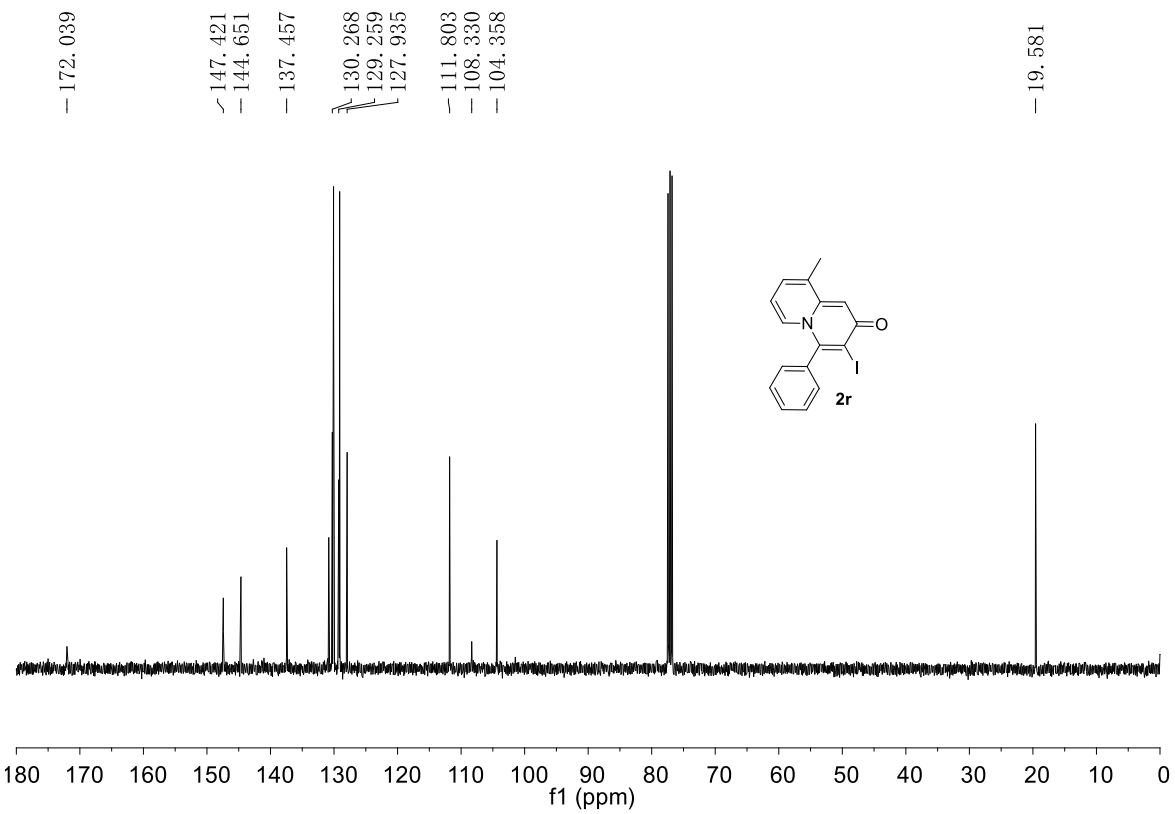
7.579
7.561
7.310
7.290
7.269
7.260
6.973
6.957
6.800
6.306
6.288
6.270
2.373
3.00
3.14
1.00
1.02
1.01
3.00
N
O
I
2r
f1 (ppm)


172.039
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129.259
127.935
111.803
108.330
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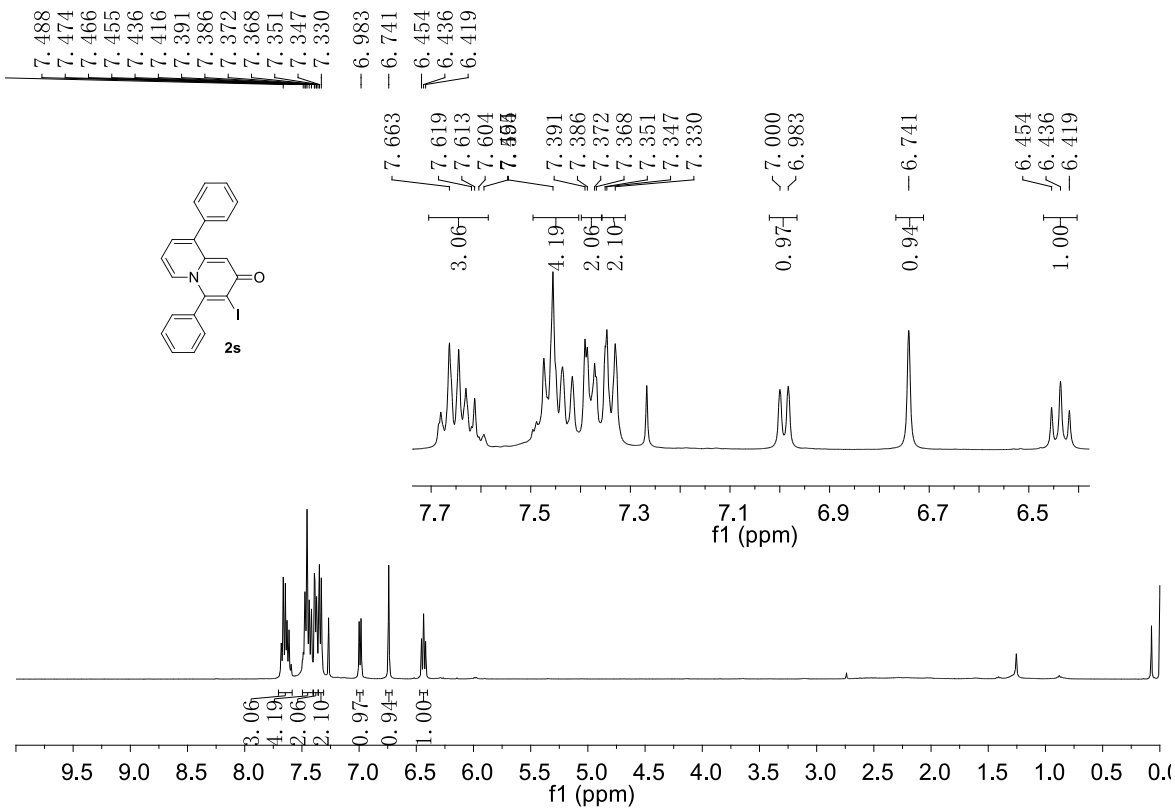
19.581
2r
f1 (ppm)


7.488
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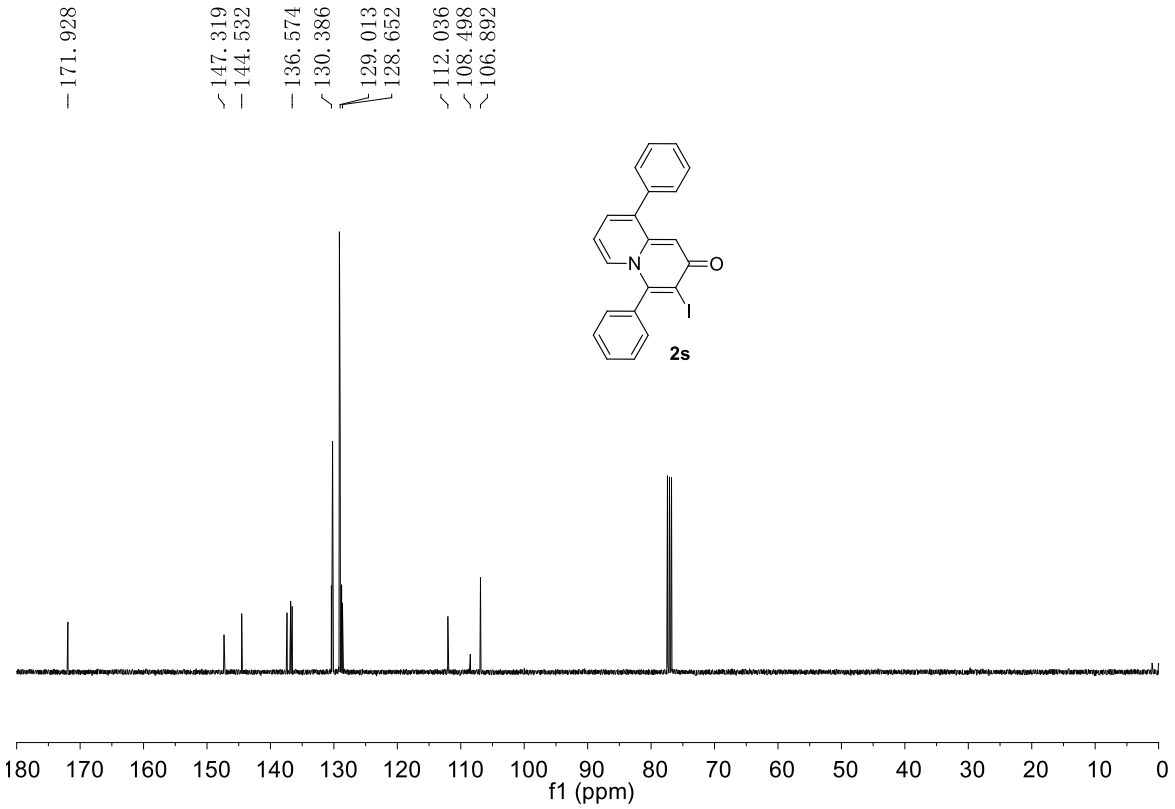
7.436
7.416
7.391
7.386
7.372
7.368
7.351
7.347
7.330
6.983
6.741
6.454
6.436
6.419
7.663
7.619
7.613
7.604
7.391
7.386
7.372
7.368
7.351
7.347
7.330
7.000
6.983
6.741
6.454
6.436
6.419
3.06
4.19
2.06
2.10
0.97
0.94
1.00
2s
f1 (ppm)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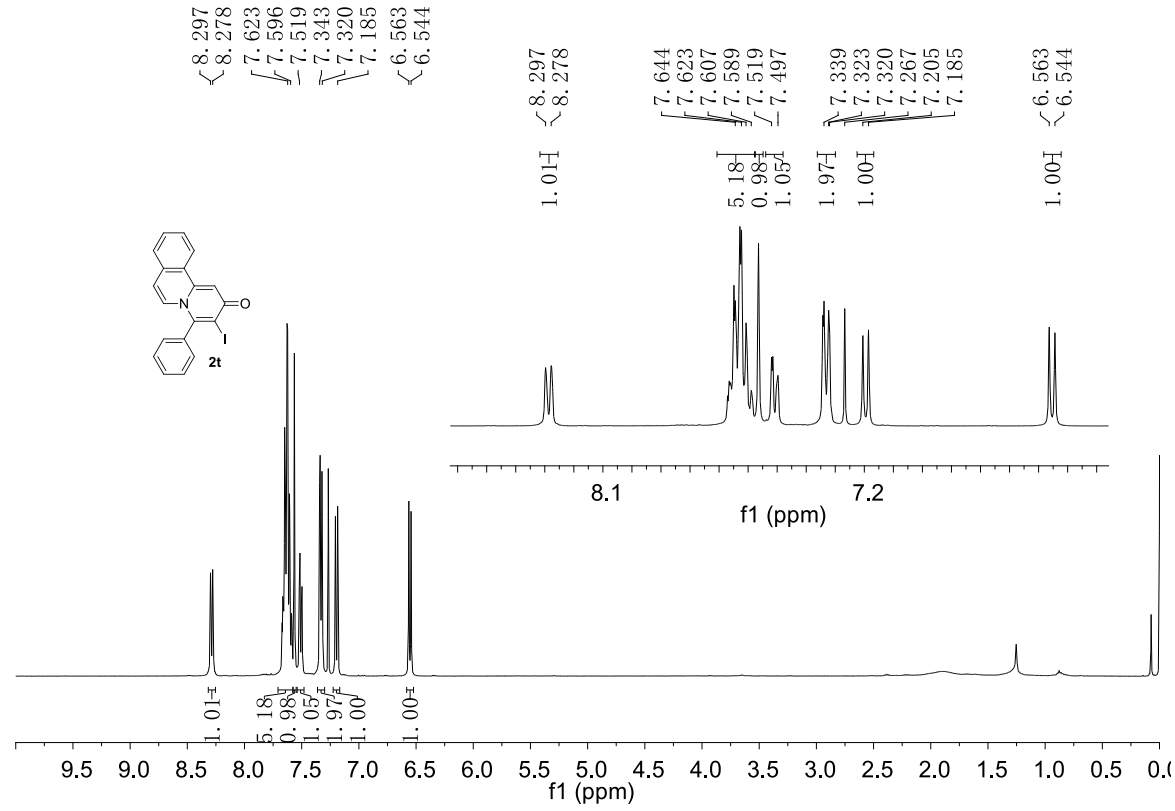
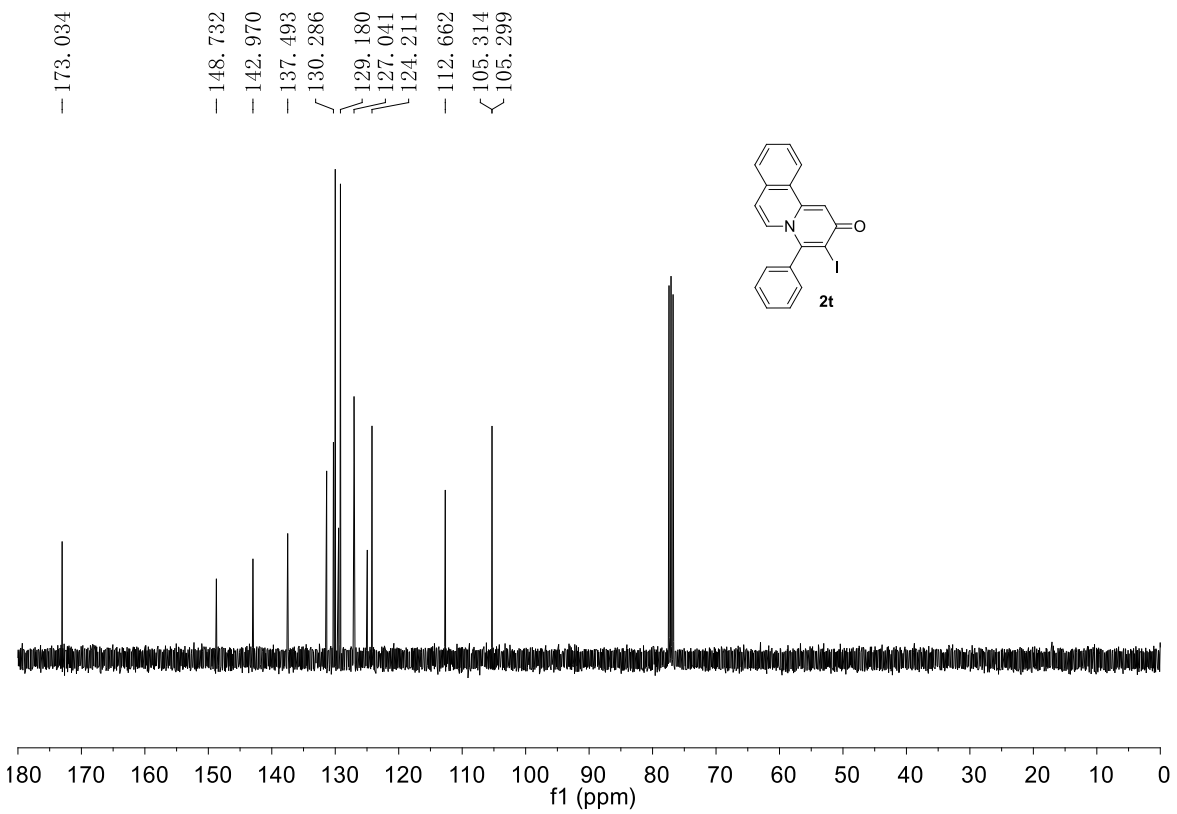
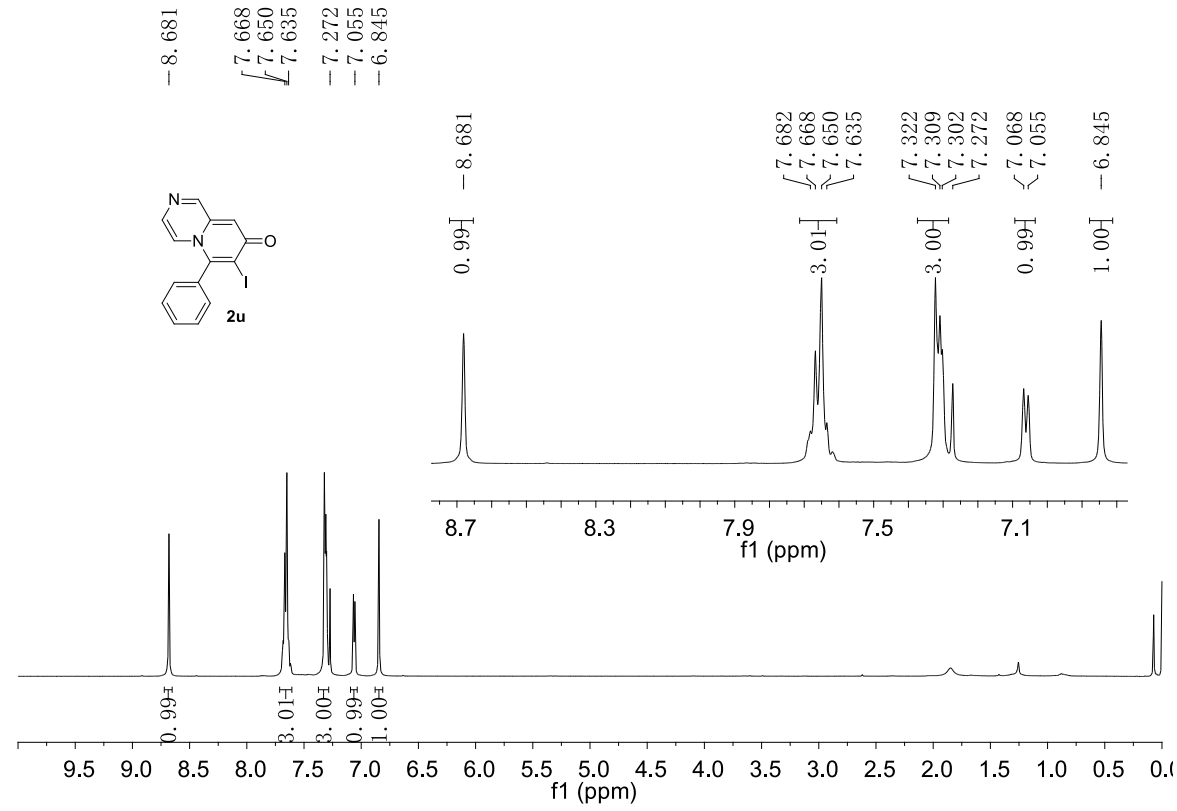
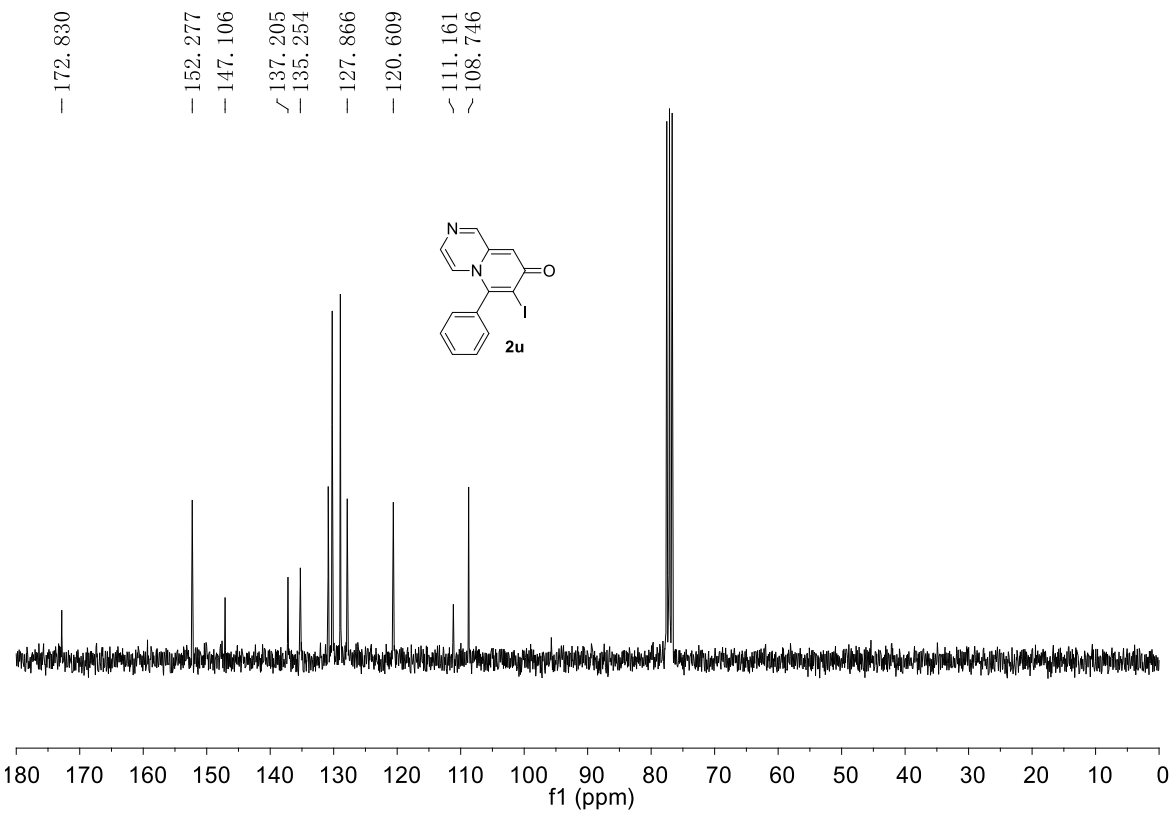
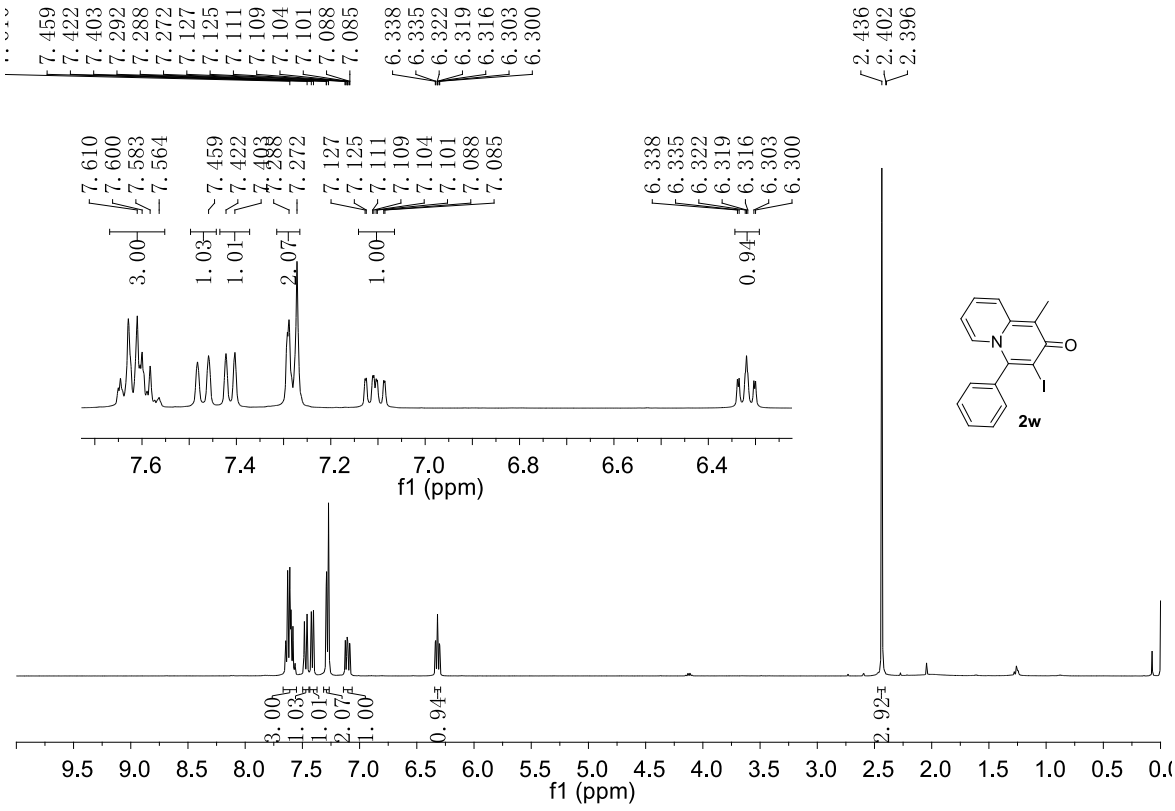
136.574
130.386
129.013
128.652
112.036
108.498
106.892
2s
f1 (ppm)

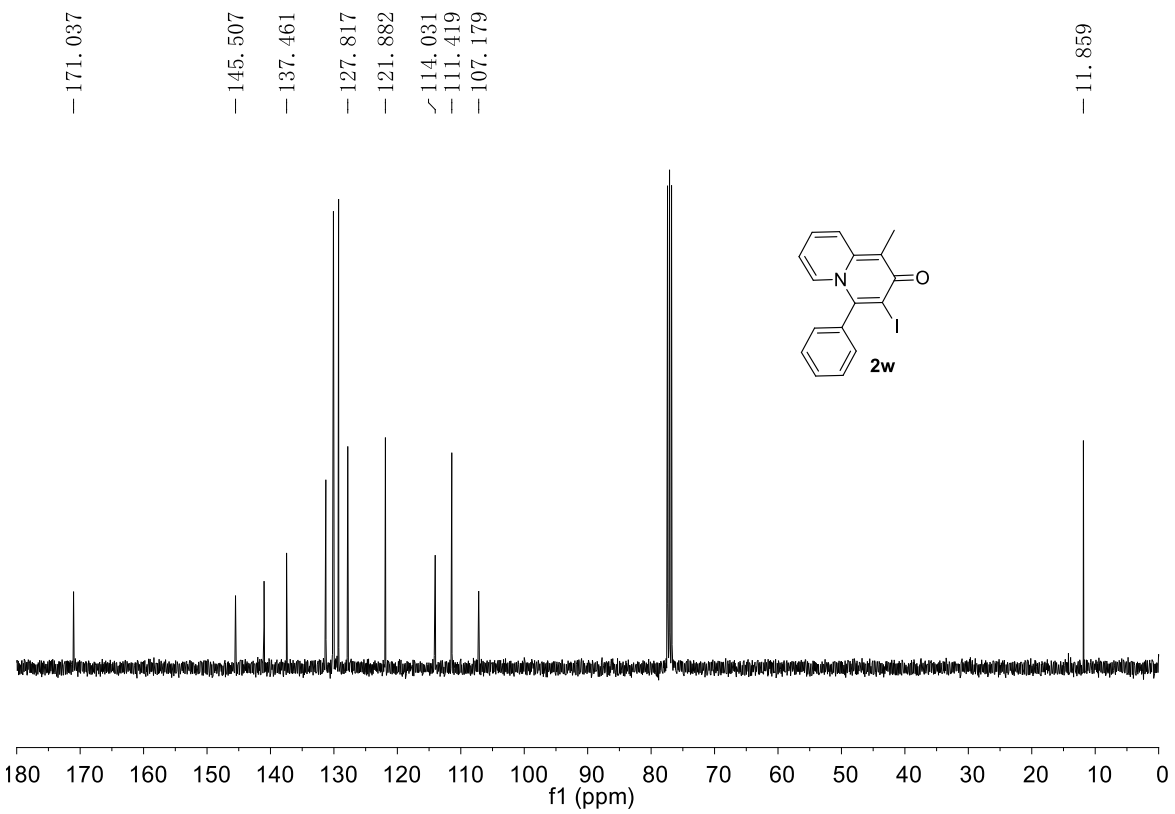

8.297
8.278
7.623
7.596
7.519
7.343
7.320
7.185
6.563
6.544
2t
f1 (ppm)

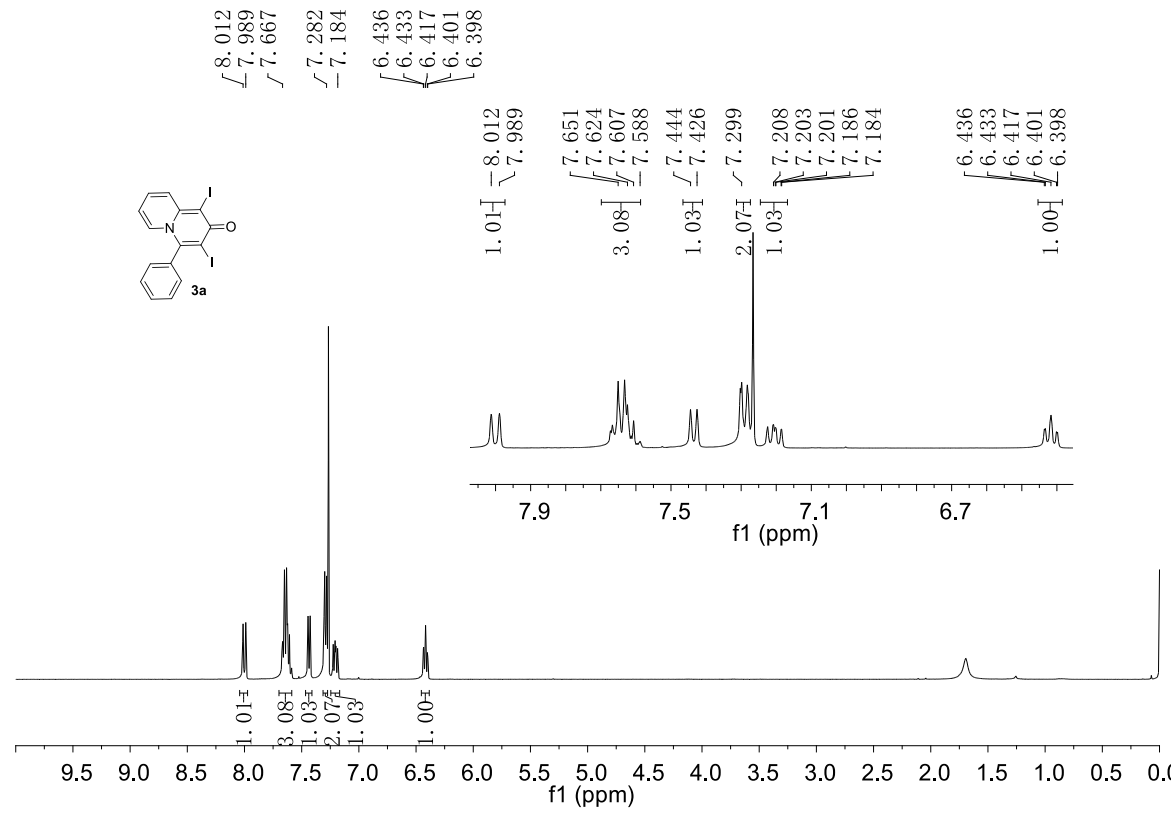

173.034
148.732
142.970
137.493
130.286
129.180
127.041
124.211
112.662
105.314
105.299
2t
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

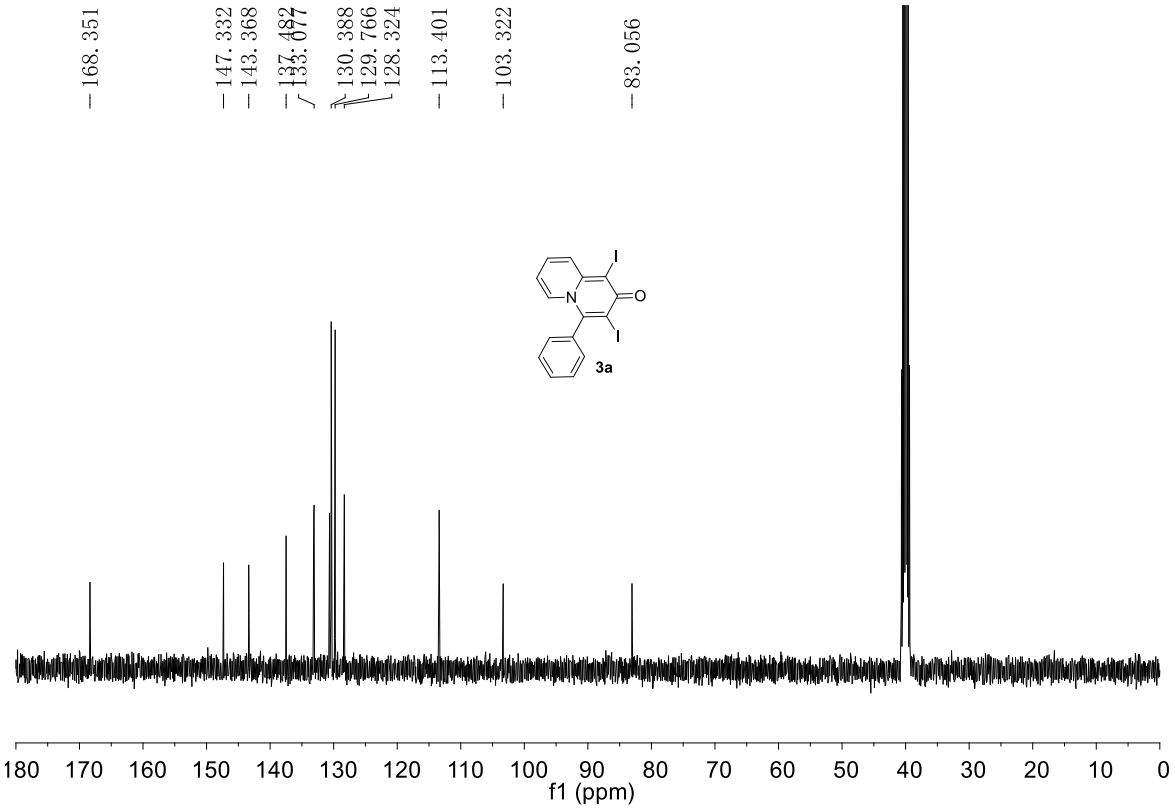

8.681
7.668
7.650
7.635
7.272
7.055
6.845
2u
0.99
3.01
3.00
0.99
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)
7.682
7.322
7.309
7.302
7.068
7.055
8.7 8.3 7.9 7.5 7.1
f1 (ppm)

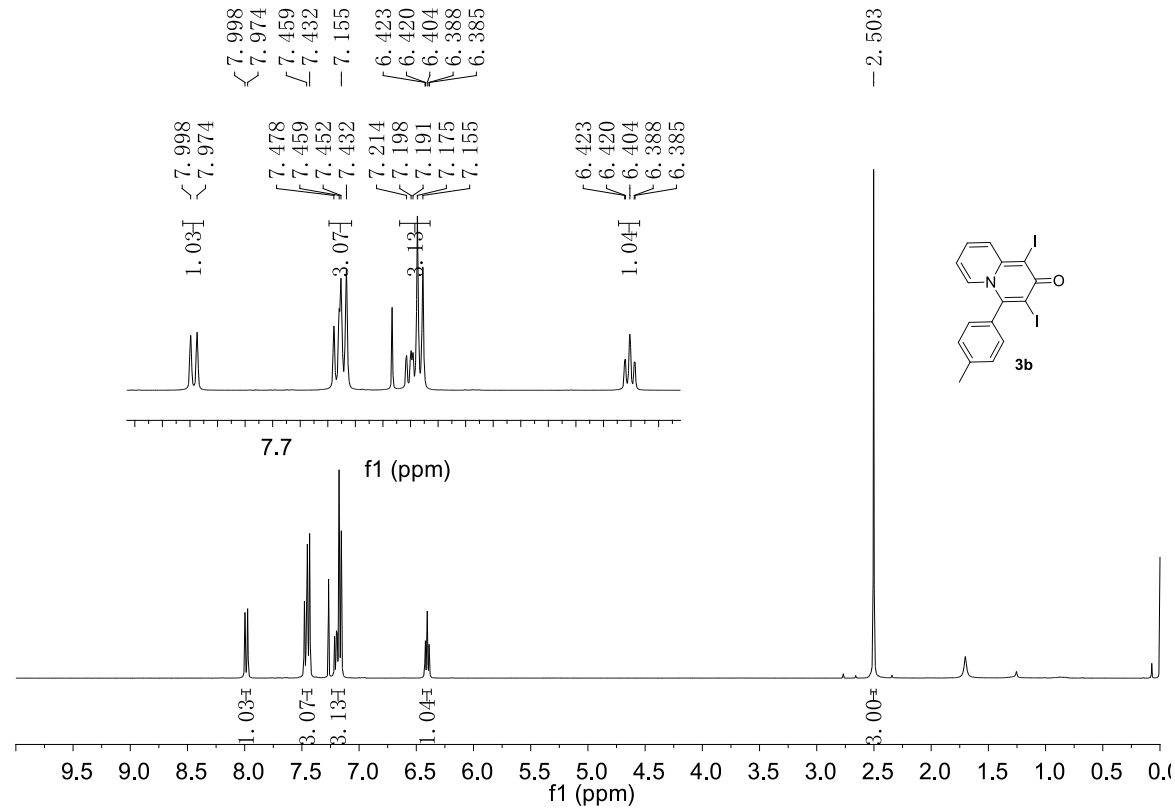

172.830
152.277
147.106
137.205
135.254
127.866
120.609
111.161
108.746
2u
f1 (ppm)

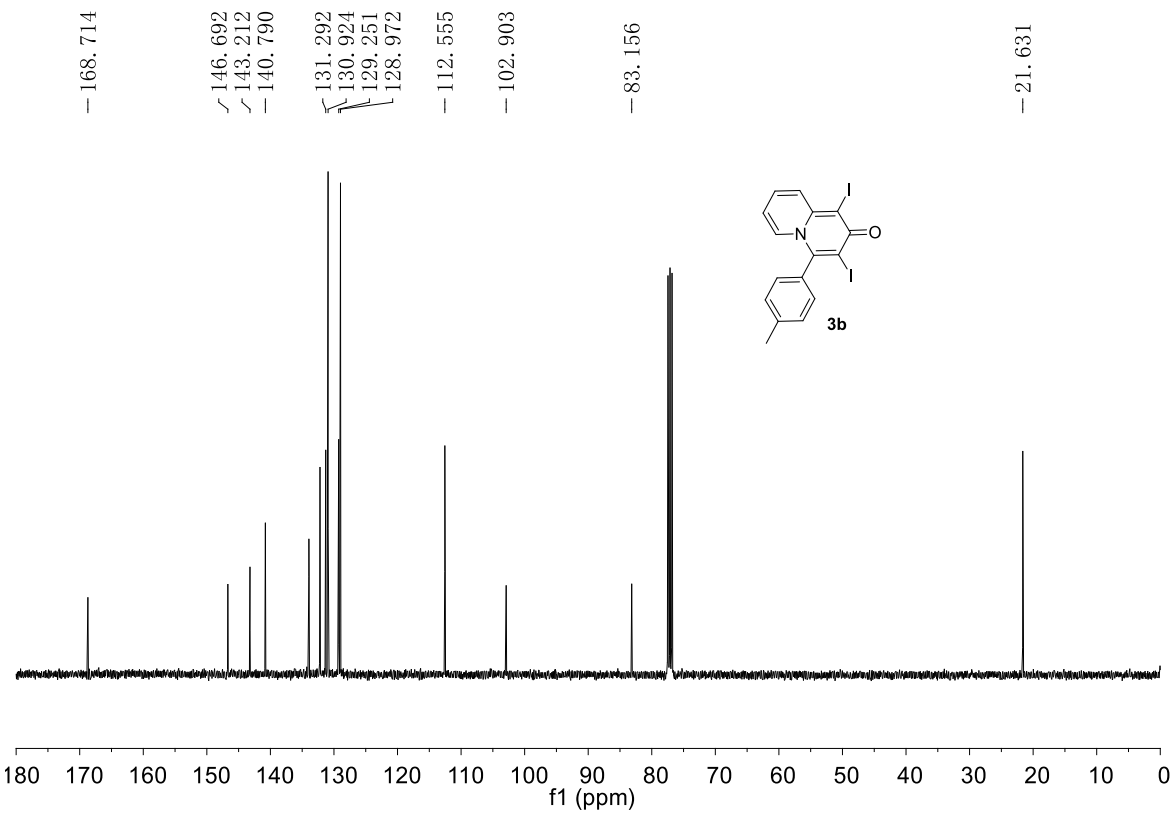

7.459
7.422
7.403
7.292
7.288
7.272
7.127
7.125
7.111
7.109
7.104
7.101
7.088
7.085
6.338
6.335
6.322
6.319
6.316
6.303
6.300
2.436
2.402
2.396
7.610
7.600
7.583
7.564
3.00
1.03
1.01
2.07
1.00
0.94
2w
f1 (ppm)

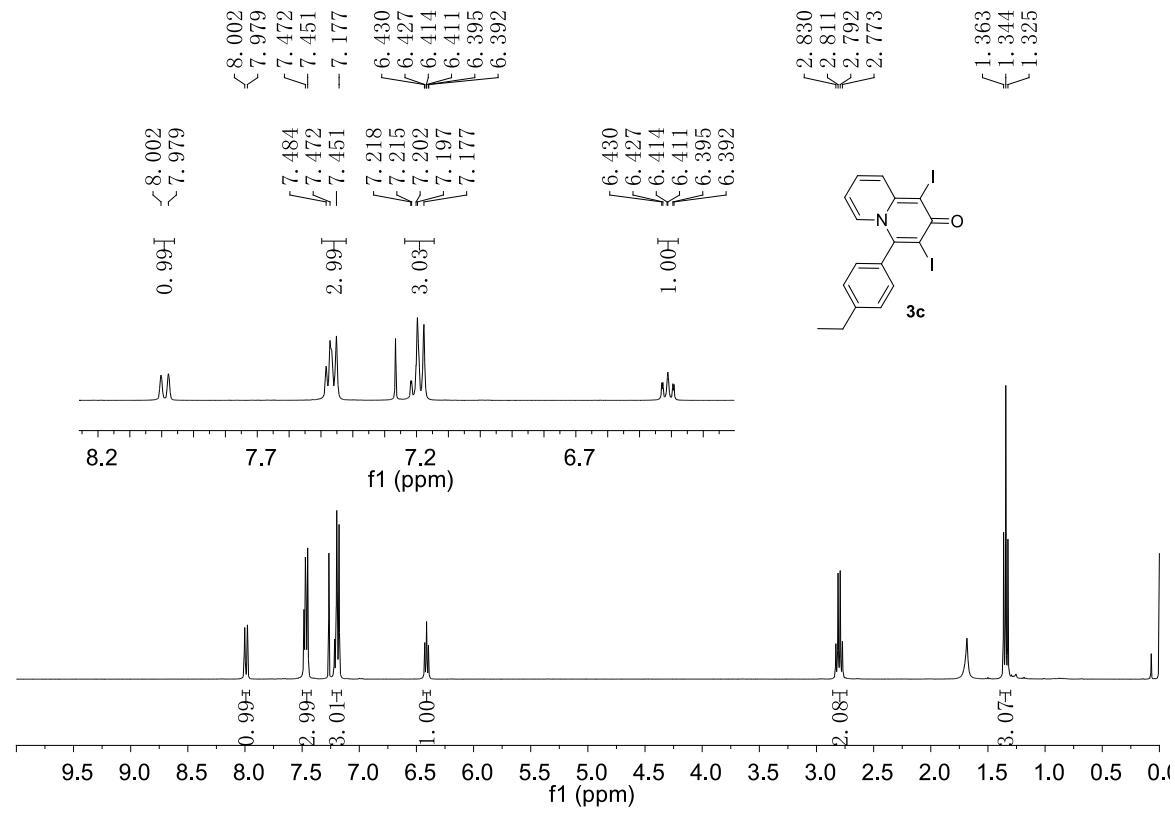

171.037
145.507
137.461
127.817
121.882
114.031
111.419
107.179
11.859
2w
f1 (ppm)

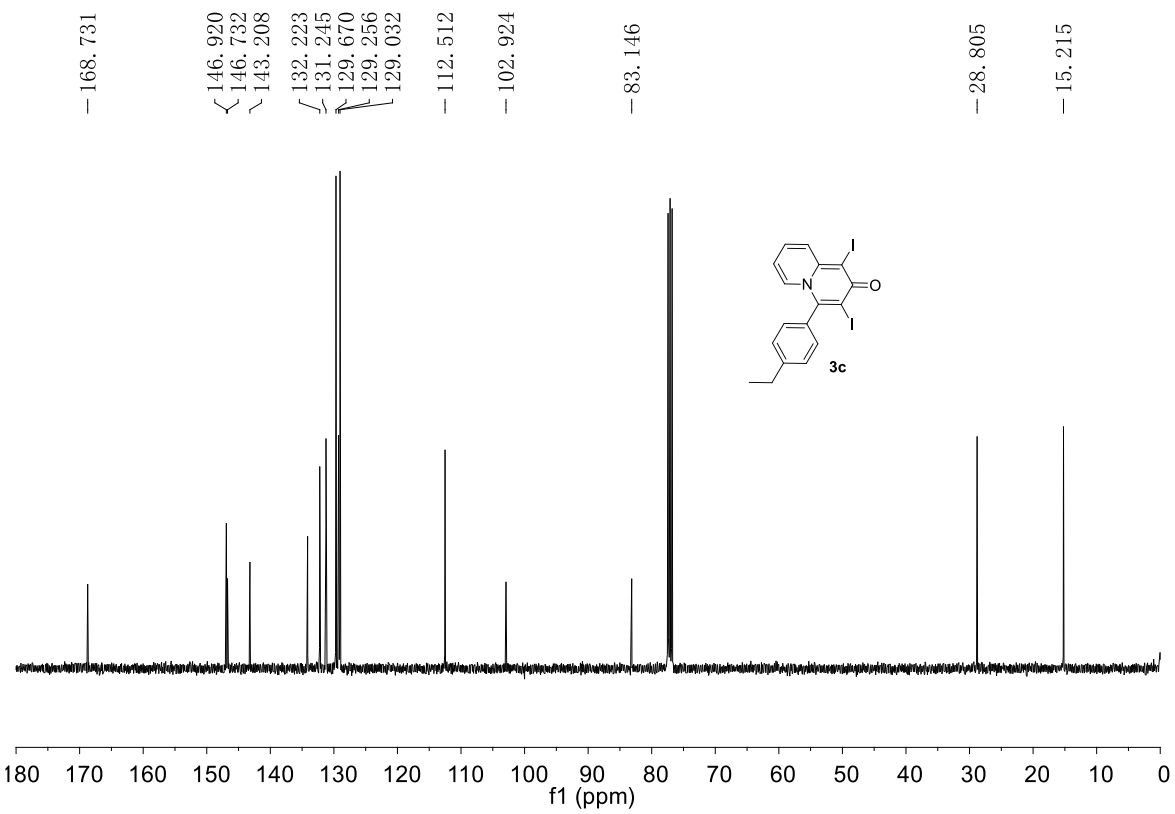

8.012
7.989
7.667
7.282
7.184
6.436
6.433
6.417
6.401
6.398
3a
1.01
3.08
1.03
2.07
1.03
1.00
f1 (ppm)

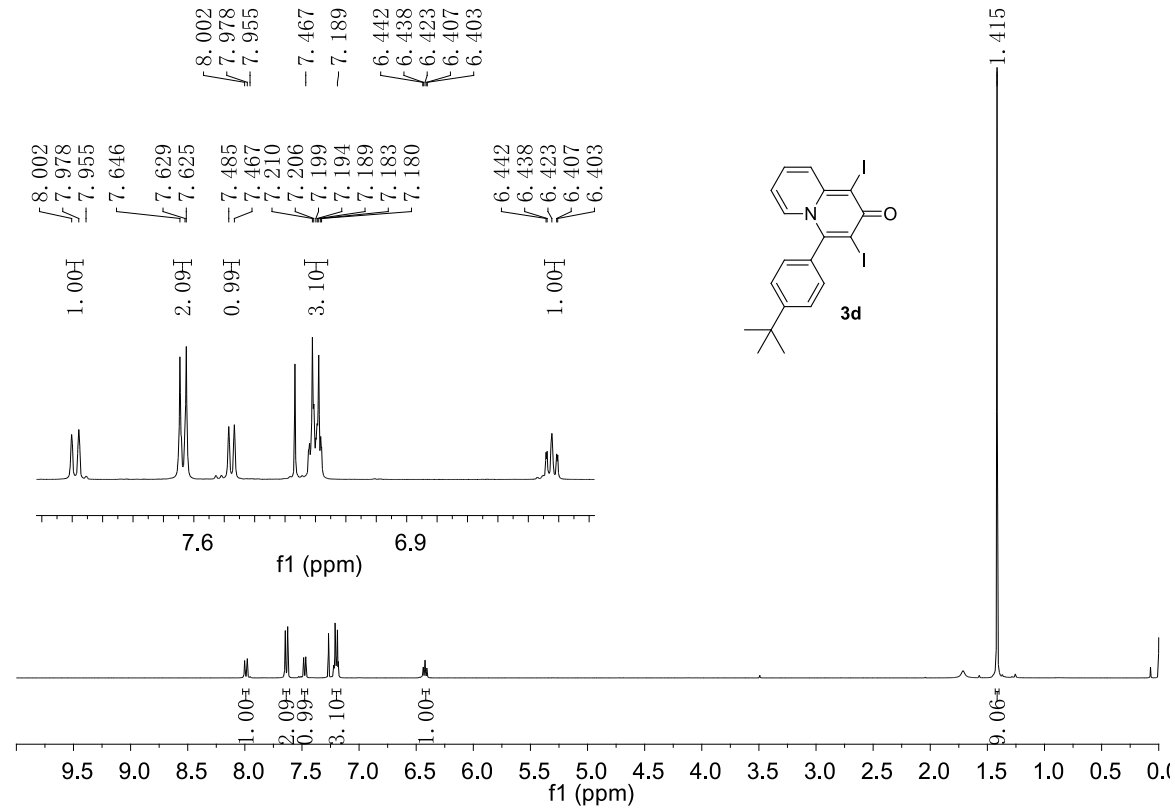

168.351
147.332
143.368
137.482
133.077
130.388
129.766
128.324
113.401
103.322
83.056
I
O
N
I
3a
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

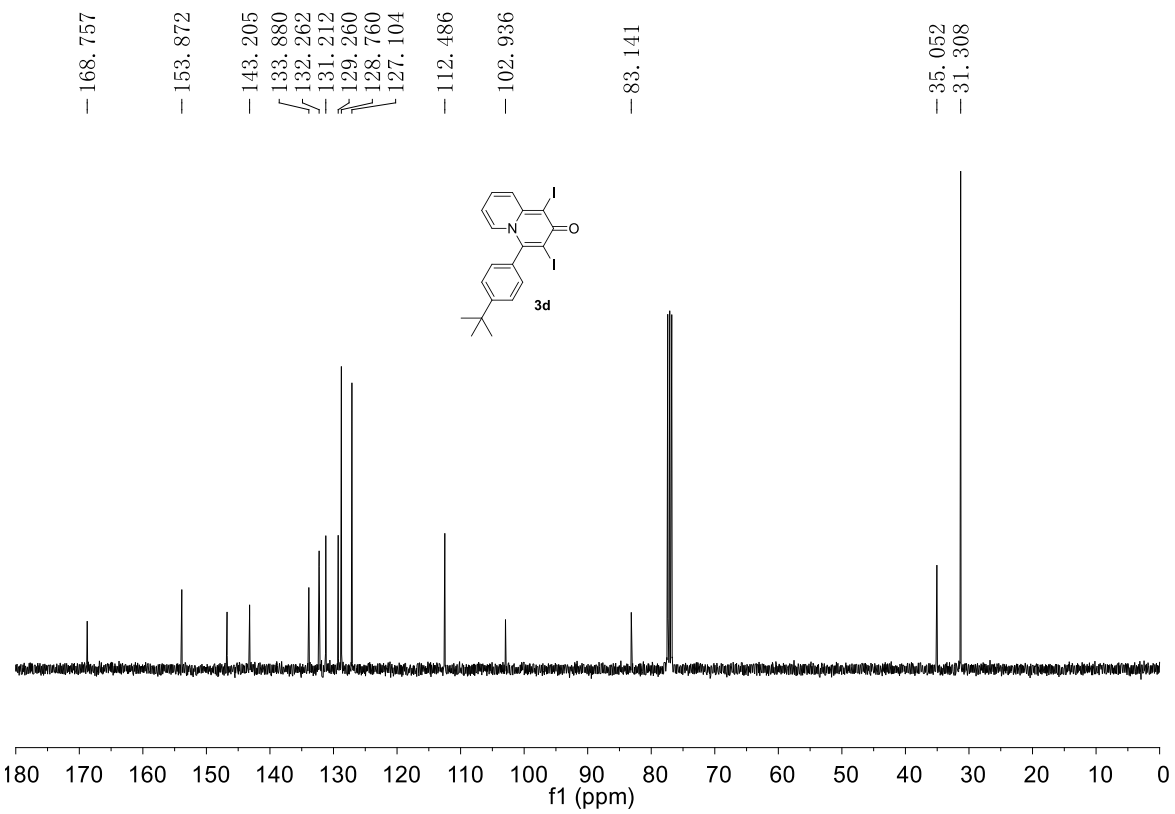

7.998
7.974
7.459
7.432
7.155
6.423
6.420
6.404
6.388
6.385
2.503
7.478
7.459
7.452
7.432
7.214
7.198
7.191
7.175
7.155
6.423
6.420
6.404
6.388
6.385
1.03
3.07
3.13
1.04
I
O
N
I
3b
7.7
f1 (ppm)
1.03
3.07
3.13
1.04
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

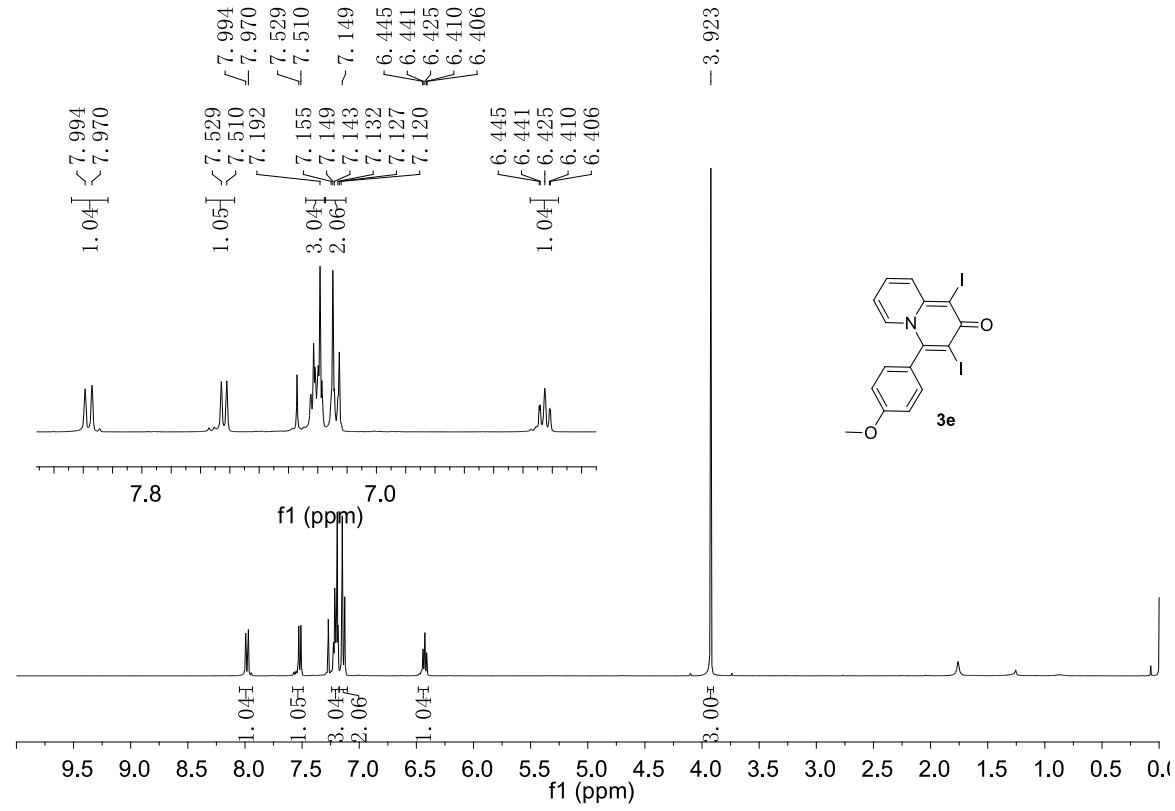

168.714
146.692
143.212
140.790
131.292
130.924
129.251
128.972
112.555
102.903
83.156
21.631
3b
f1 (ppm)

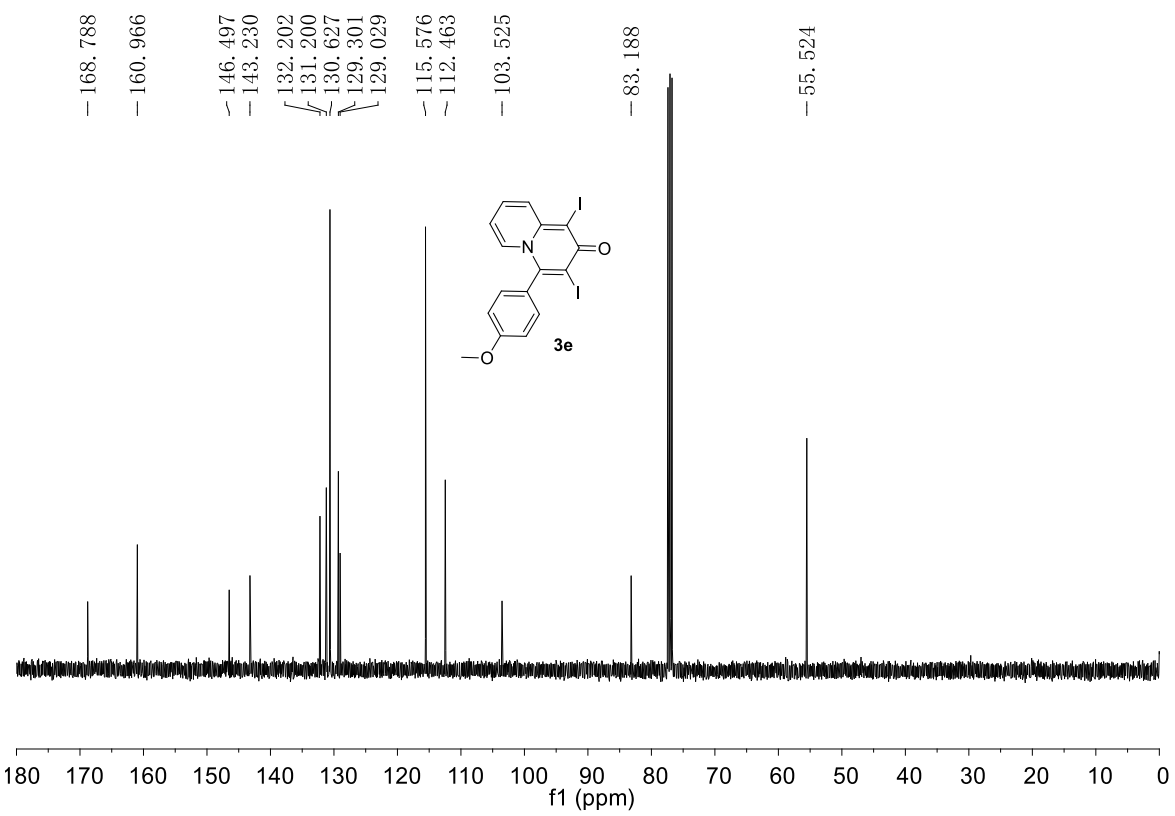

8.002
7.979
7.484
7.472
7.451
7.218
7.215
7.202
7.197
7.177
6.430
6.427
6.414
6.411
6.395
6.392
2.830
2.811
2.792
2.773
1.363
1.344
1.325
0.99
2.99
3.03
1.00
2.08
3.07
3c
f1 (ppm)

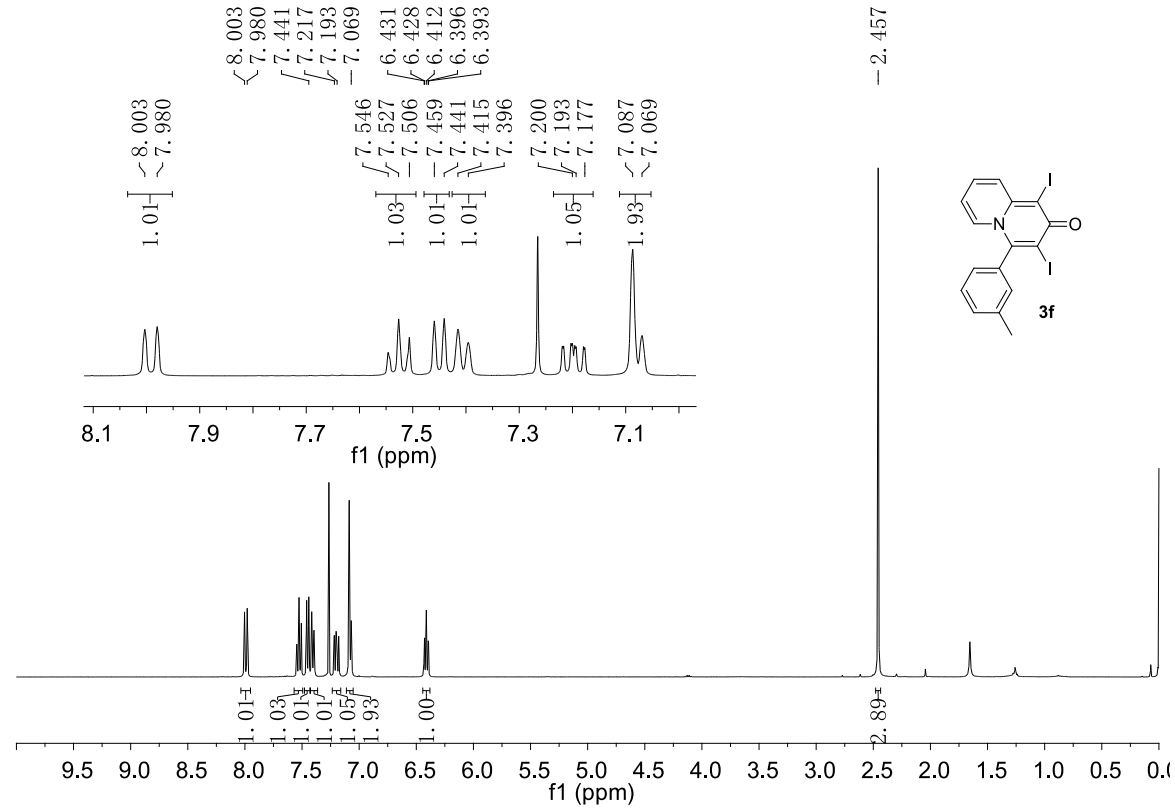

168.731
146.920
146.732
143.208
132.223
131.245
129.670
129.256
129.032
112.512
102.924
83.146
28.805
15.215
3c
f1 (ppm)

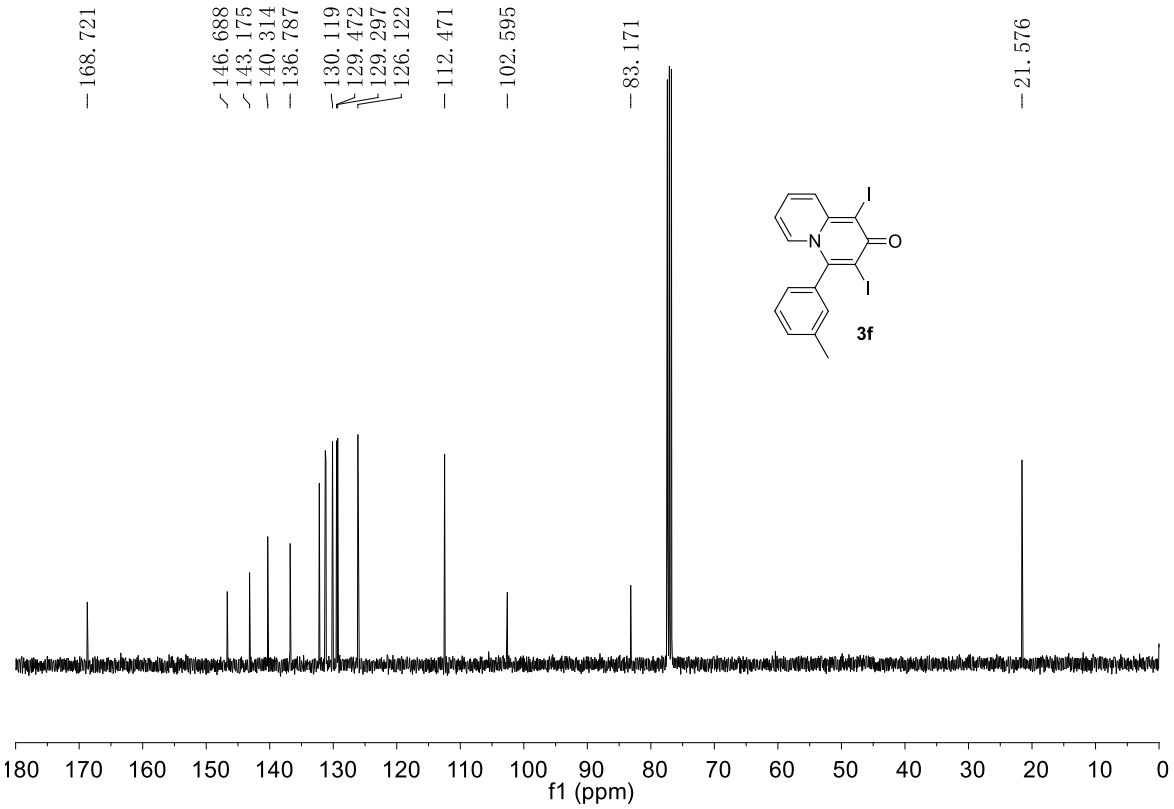

8.002
7.978
7.955
7.646
7.629
7.625
7.485
7.467
7.210
7.206
7.199
7.194
7.189
7.183
7.180
6.442
6.438
6.423
6.407
6.403
1.415
1.00
2.09
0.99
3.10
1.00
9.06
3d
7.6
6.9
f1 (ppm)

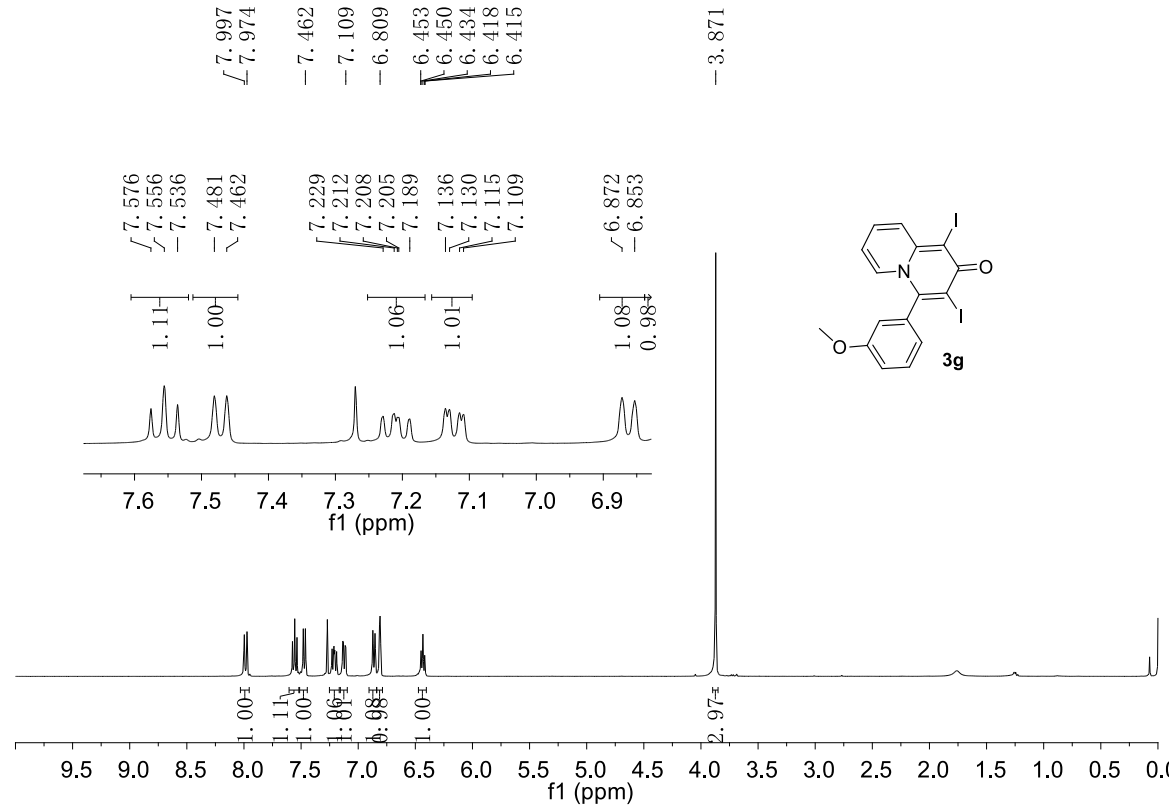

168.757
153.872
143.205
133.880
132.262
131.212
129.260
128.760
127.104
112.486
102.936
83.141
35.052
31.308
3d
f1 (ppm)

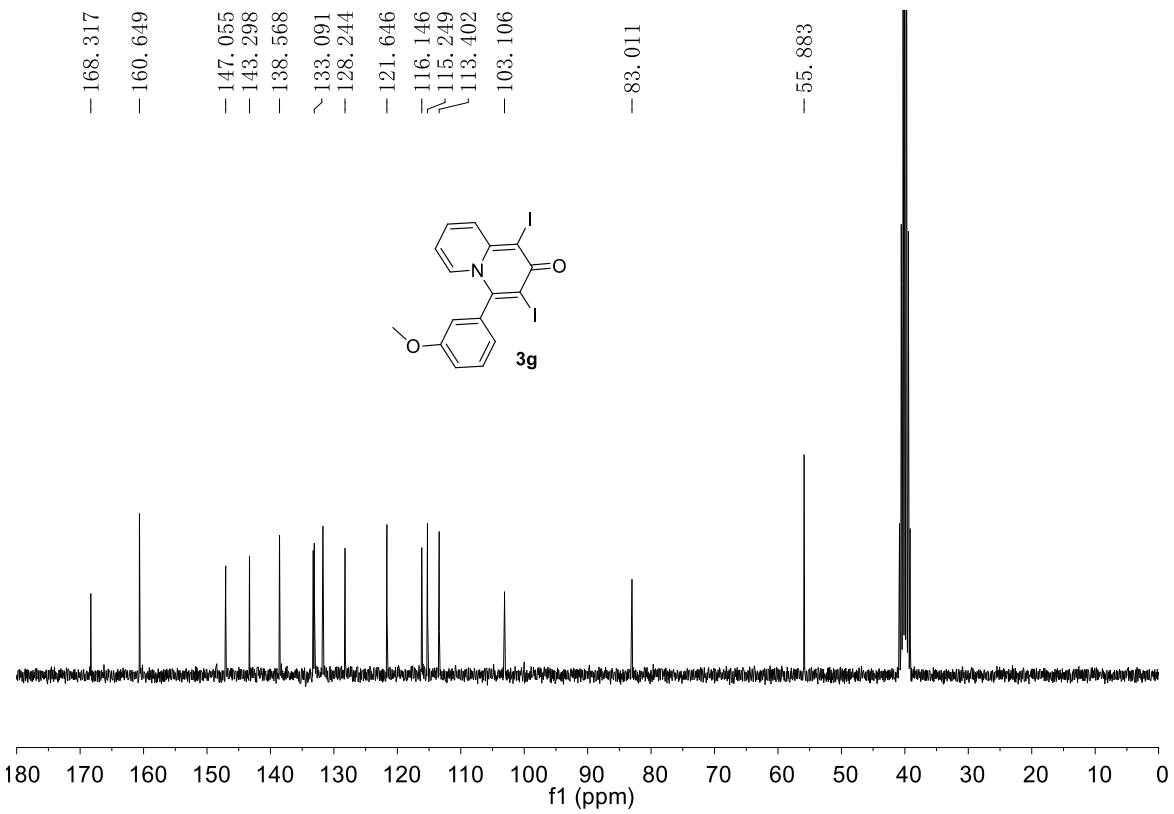

7.994
7.970
7.529
7.510
7.149
6.445
6.441
6.425
6.410
6.406
3.923
1.04
1.05
3.04
2.06
1.04
3.00
3e
f1 (ppm)

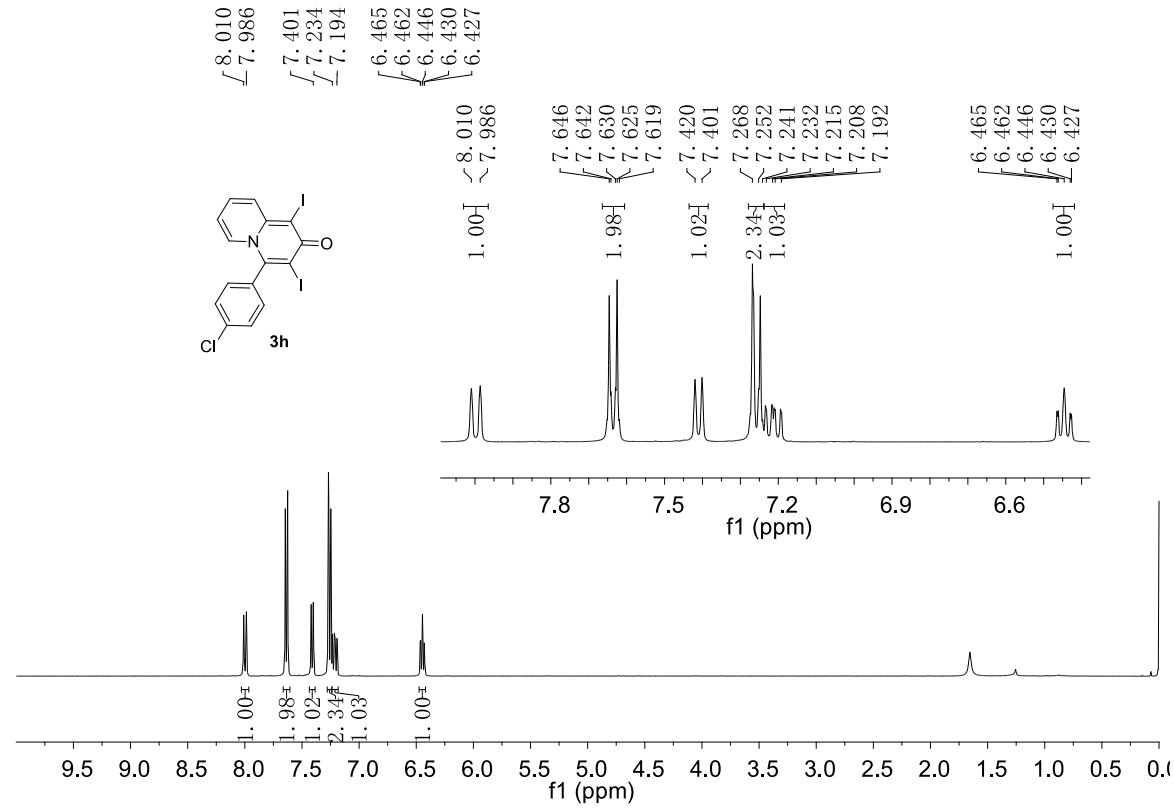

168.788
160.966
146.497
143.230
132.202
131.200
130.627
129.301
129.029
115.576
112.463
103.525
83.188
55.524
3e
f1 (ppm)

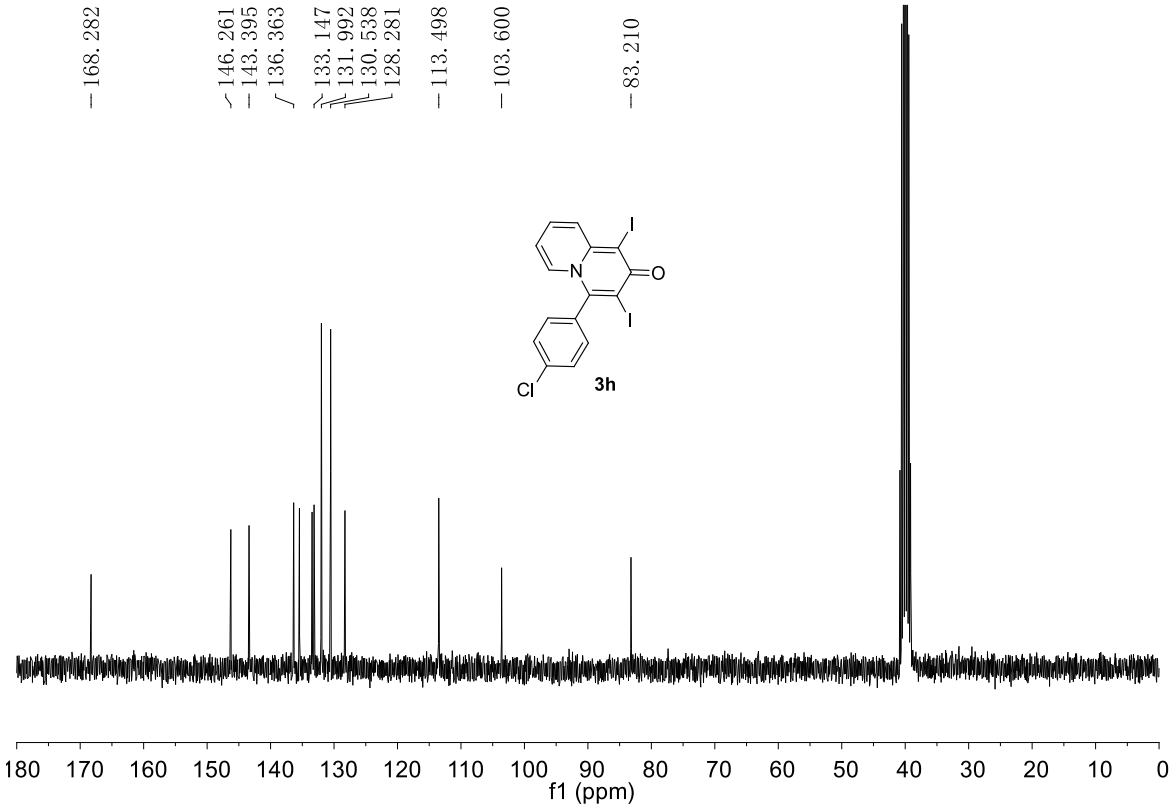

8.003
7.980
7.441
7.217
7.193
7.069
6.431
6.428
6.412
6.396
6.393
7.546
7.527
7.506
7.459
7.441
7.415
7.396
7.200
7.193
7.177
7.087
7.069
2.457
1.01
1.03
1.01
1.01
1.05
1.93
1.00
2.89
3f
f1 (ppm)

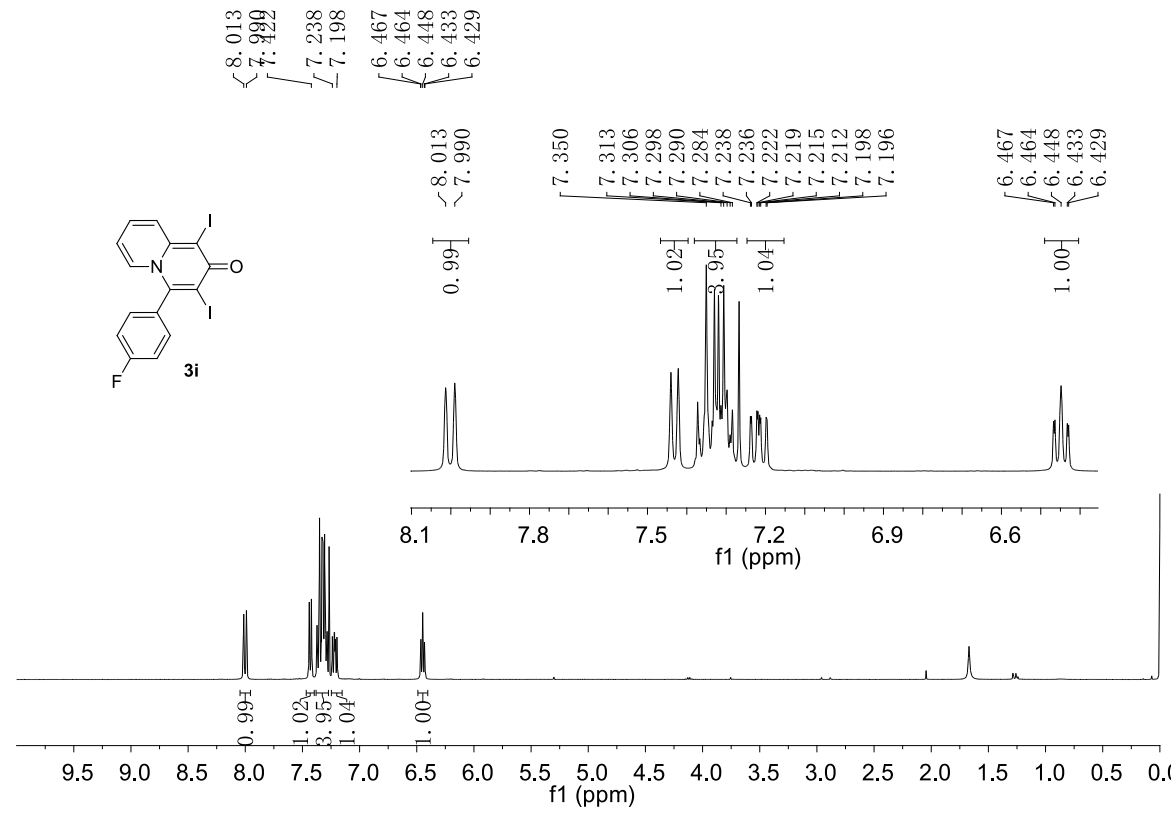

168.721
146.688
143.175
140.314
136.787
130.119
129.472
129.297
126.122
112.471
102.595
83.171
21.576
I
N
O
I
3f
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

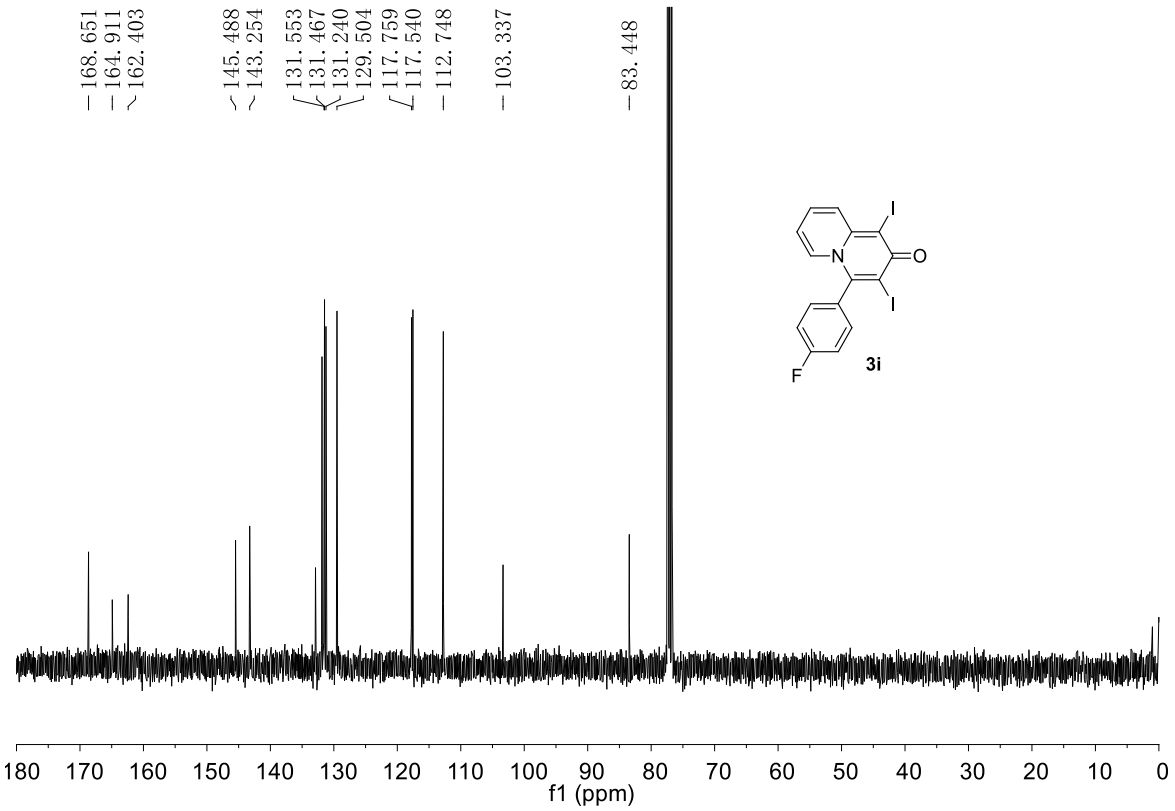

7.997
7.974
7.462
7.109
6.809
6.453
6.450
6.434
6.418
6.415
3.871
7.576
7.556
7.536
7.481
7.462
7.229
7.212
7.208
7.205
7.189
7.136
7.130
7.115
7.109
6.872
6.853
1.11
1.00
1.06
1.01
1.08
0.98
I
N
O
I
O
3g
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
1.00
1.11
1.00
1.06
1.01
0.98
1.00
2.97
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

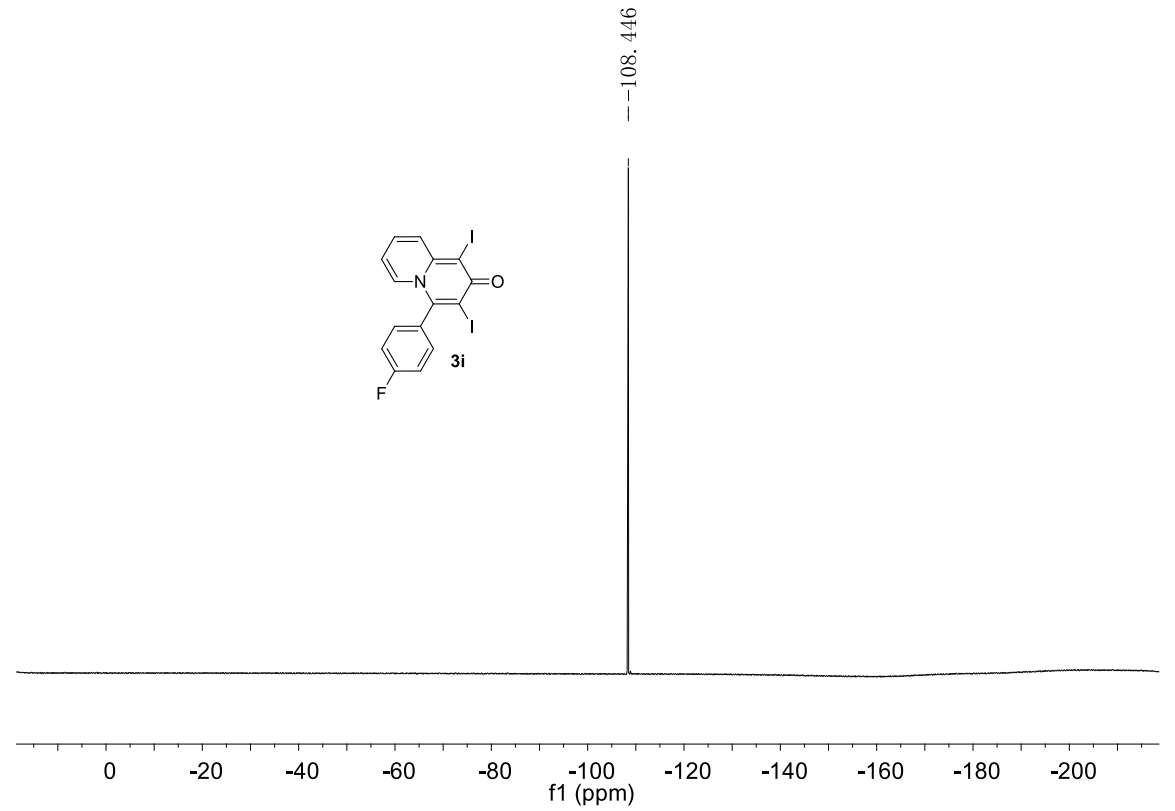

168.317
160.649
147.055
143.298
138.568
133.091
128.244
121.646
116.146
115.249
113.402
103.106
83.011
55.883
3g
f1 (ppm)

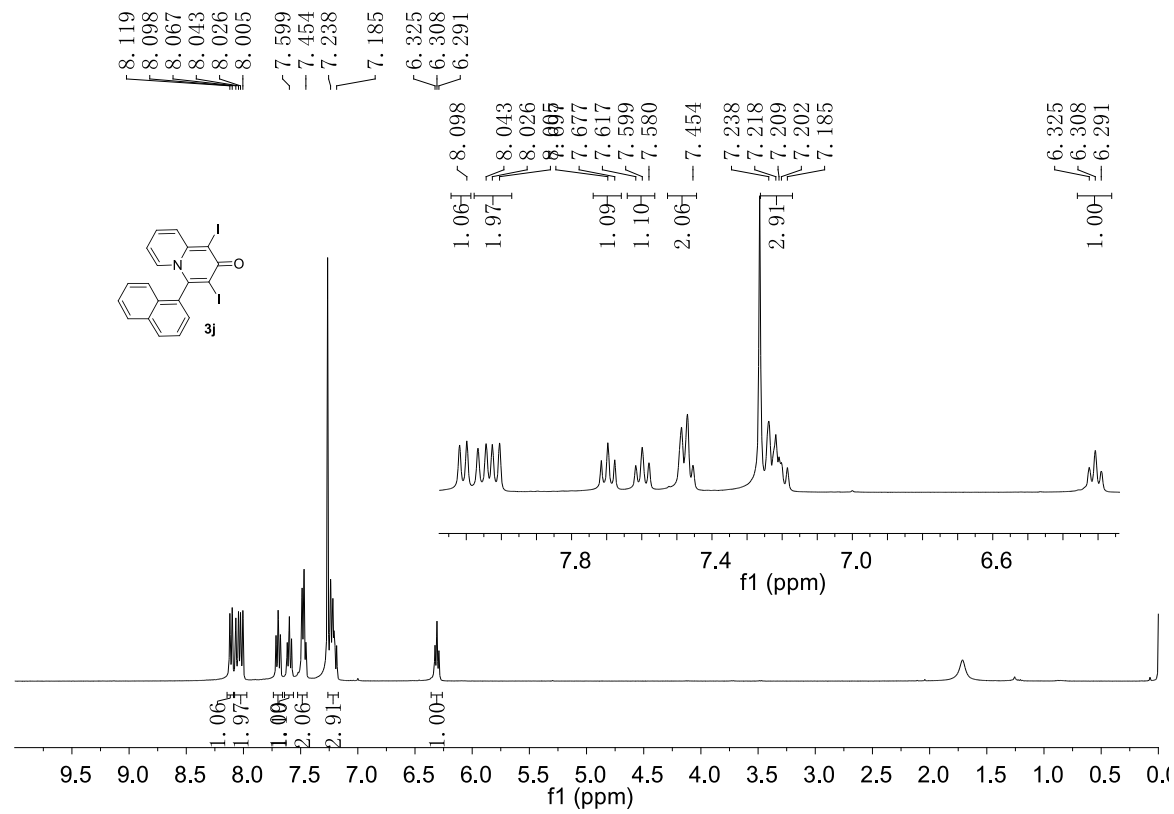

8.010
7.986
7.401
7.234
7.194
6.465
6.462
6.446
6.430
6.427
3h
1.00
1.98
1.02
2.34
1.03
1.00
f1 (ppm)


168.282
146.261
143.395
136.363
133.147
131.992
130.538
128.281
113.498
103.600
83.210
I
O
N
I
Cl
3h
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.013
7.990
7.422
7.238
7.198
6.467
6.464
6.448
6.433
6.429
I
O
N
I
F
3i
0.99
1.02
3.95
1.04
1.00
8.1 7.8 7.5 7.2 6.9 6.6
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


168.651
164.911
162.403
145.488
143.254
131.553
131.467
131.240
129.504
117.759
117.540
112.748
103.337
83.448
I
N
O
I
F
3i
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-108.446
I
N
O
I
F
3i
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200
f1 (ppm)


8.119
8.098
8.067
8.043
8.026
8.005
7.599
7.454
7.238
7.185
6.325
6.308
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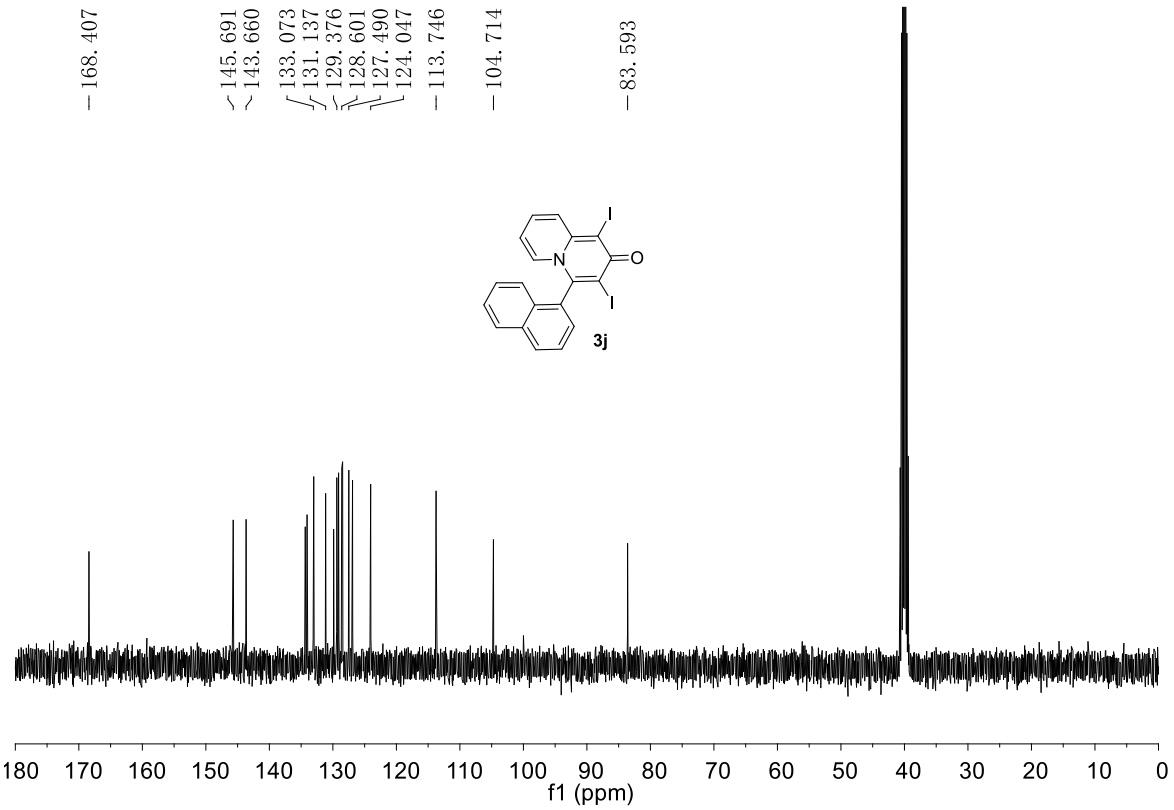
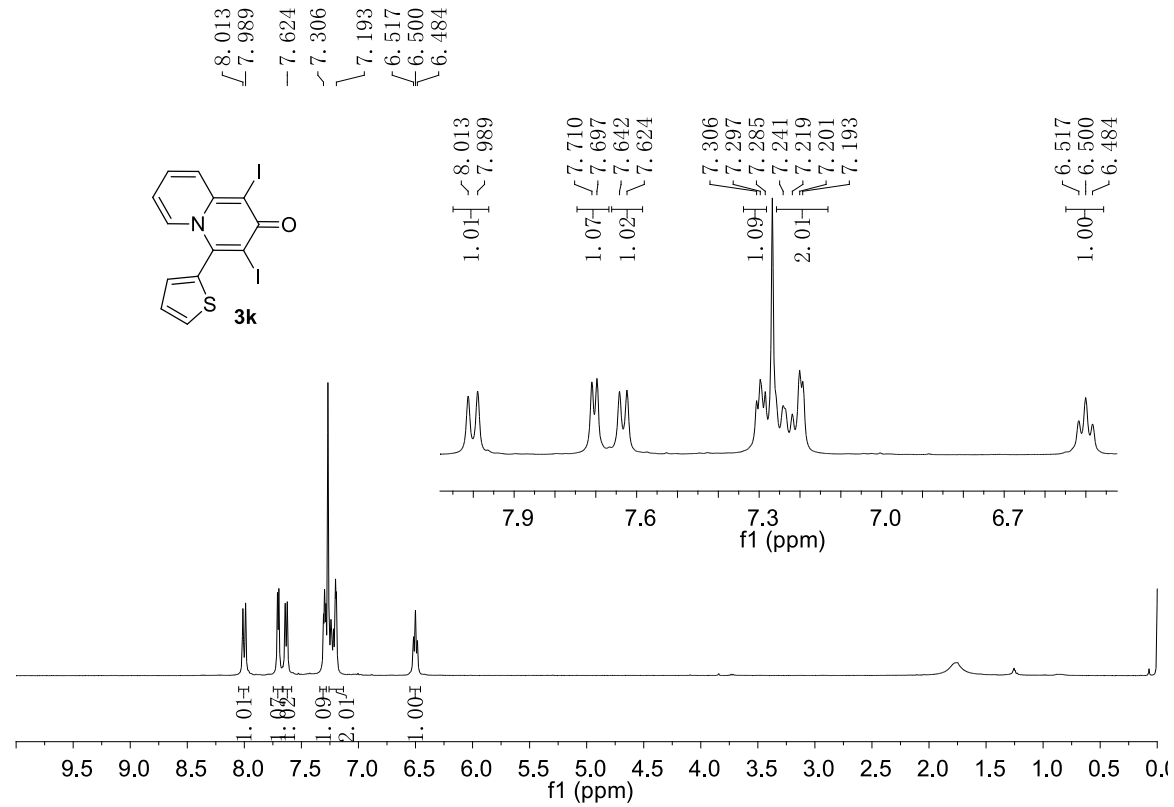
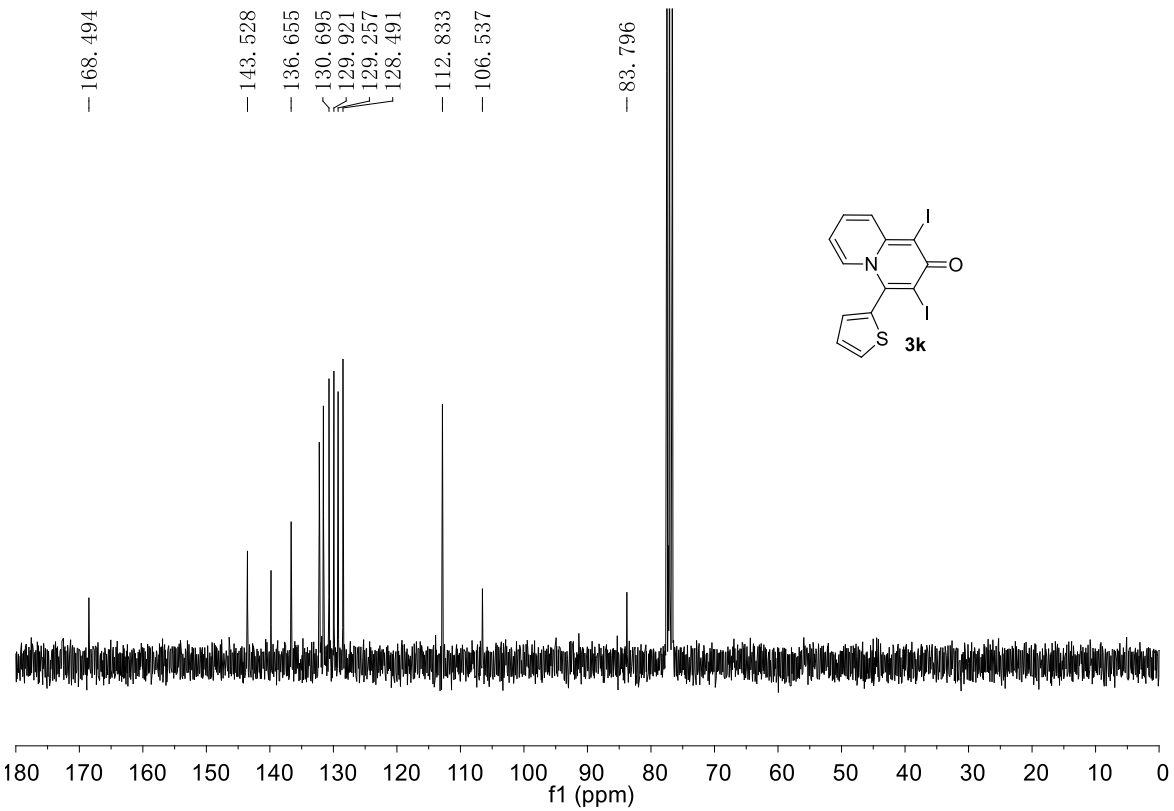
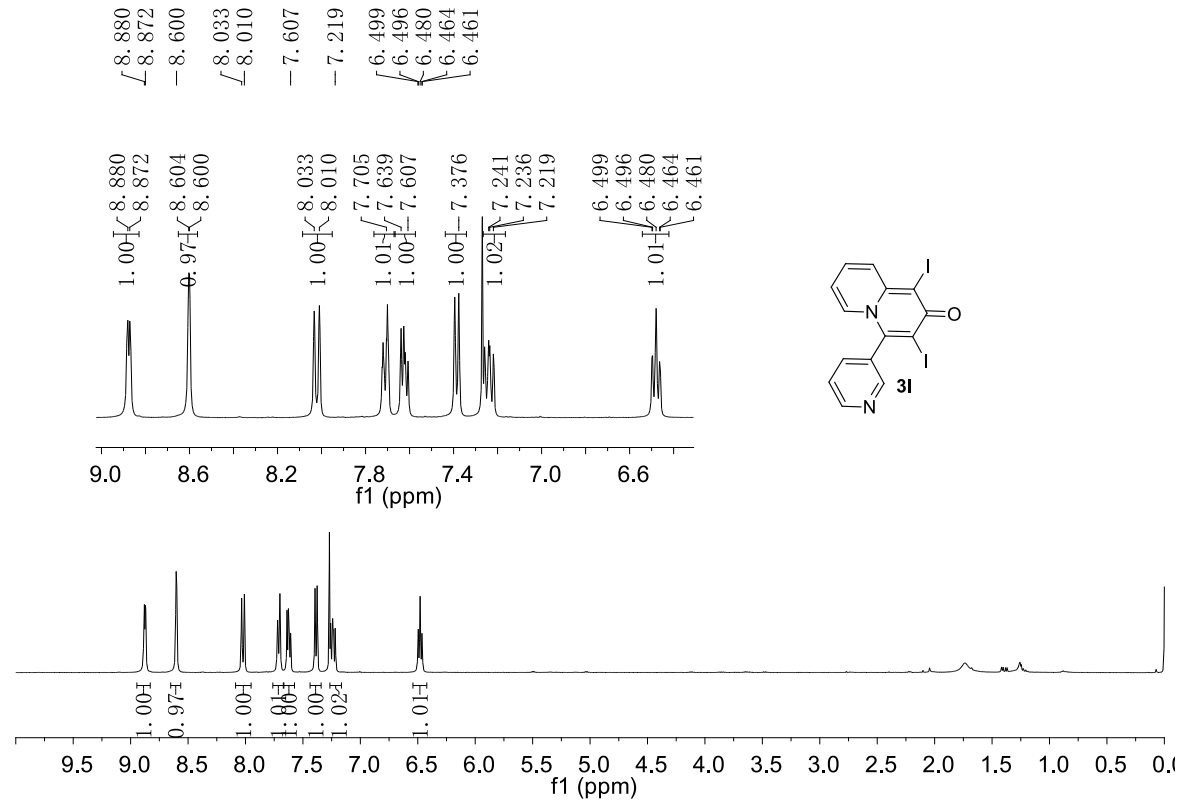
1.10
2.06
2.91
1.00
3j
f1 (ppm)

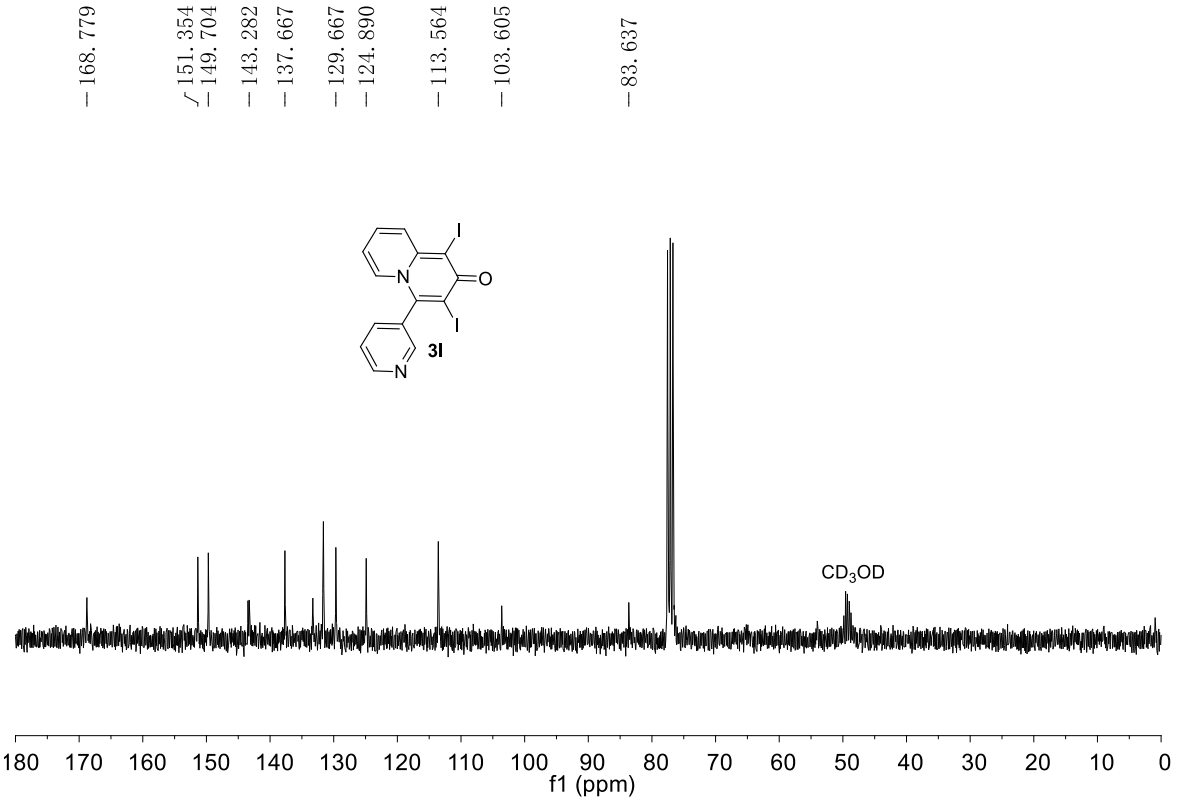

168.407
145.691
143.660
133.073
131.137
129.376
128.601
127.490
124.047
113.746
104.714
83.593
3j
f1 (ppm)

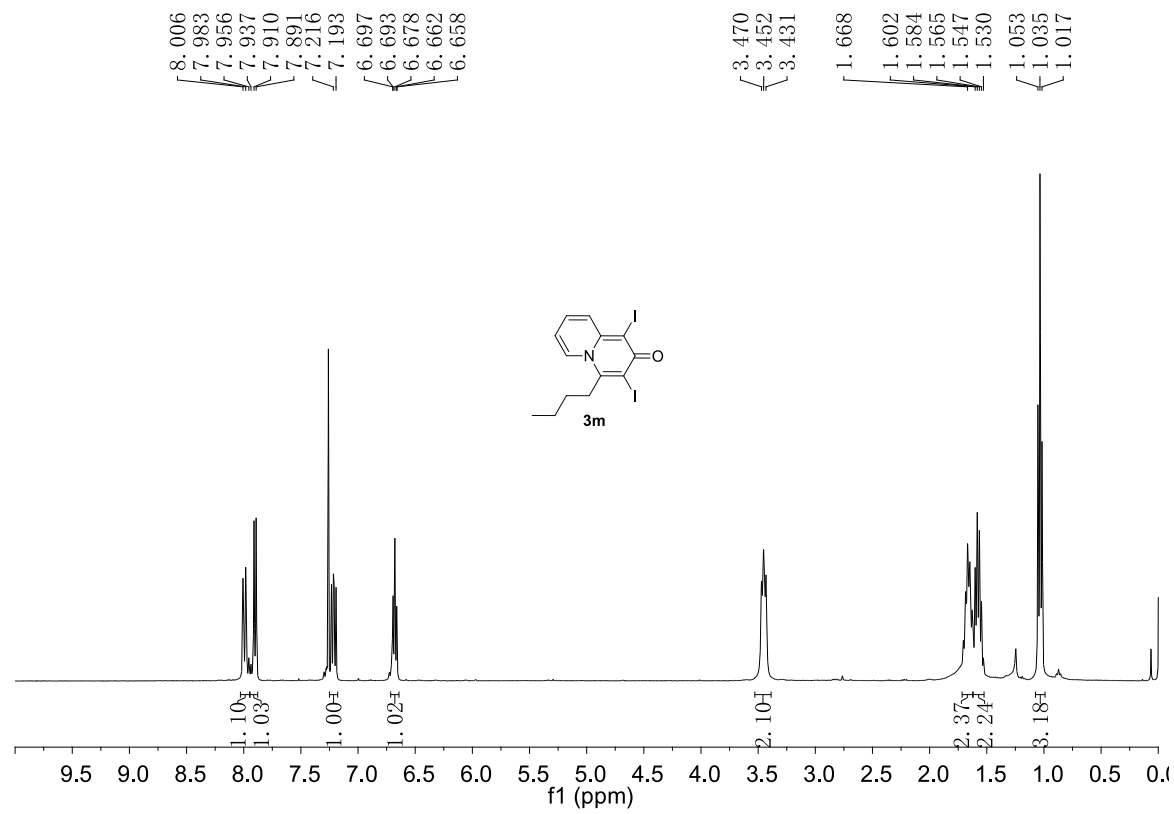

8.013
7.989
7.624
7.306
7.193
6.517
6.500
6.484
3k
1.01
1.07
1.02
1.09
2.01
1.00
7.710
7.697
7.642
7.624
7.306
7.297
7.285
7.241
7.219
7.201
7.193
6.517
6.500
6.484
7.9
7.6
7.3
7.0
6.7
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


168.494
143.528
136.655
130.695
129.921
129.257
128.491
112.833
106.537
83.796
3k
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.880
8.872
8.600
8.033
8.010
7.607
7.219
6.499
6.496
6.480
6.464
6.461
1.00
0.97
1.00
1.00
1.01
1.00
1.00
1.02
1.01
7.705
7.639
7.607
7.376
7.241
7.236
7.219
f1 (ppm)
3l

f1 (ppm)


168.779
151.354
149.704
143.282
137.667
129.667
124.890
113.564
103.605
83.637
CD3OD
3l
f1 (ppm)


8.006
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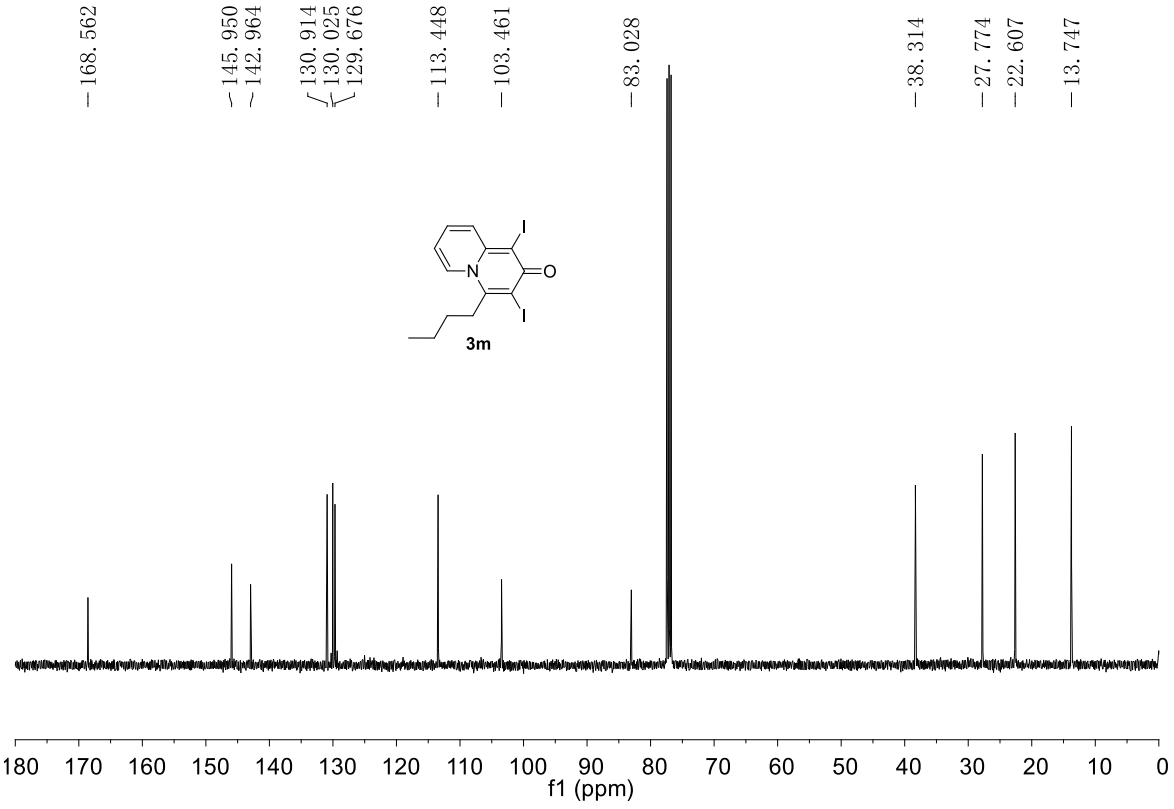
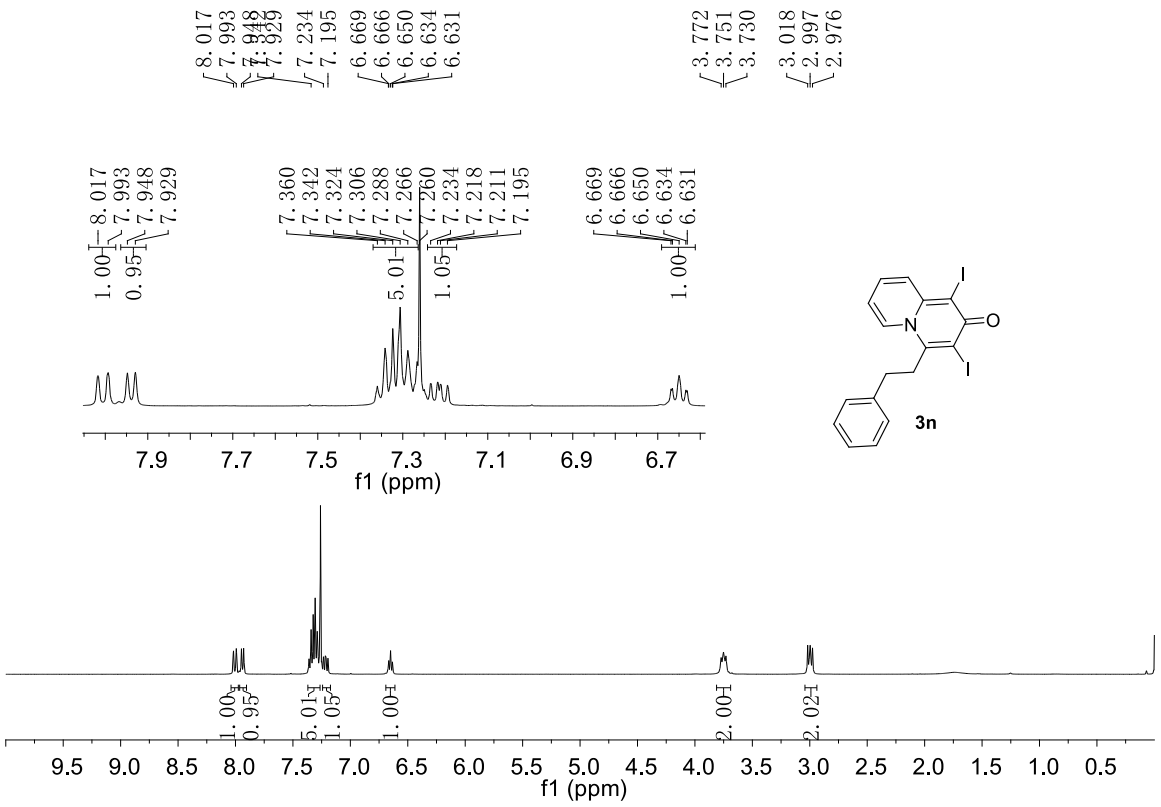
7.956
7.937
7.910
7.891
7.216
7.193
6.697
6.693
6.678
6.662
6.658
3.470
3.452
3.431
1.668
1.602
1.584
1.565
1.547
1.530
1.053
1.035
1.017
3m
1.10
1.03
1.00
1.02
2.10
2.37
2.24
3.18
f1 (ppm)


168.562
145.950
142.964
130.914
130.025
129.676
113.448
103.461
83.028
38.314
27.774
22.607
13.747
3m
f1 (ppm)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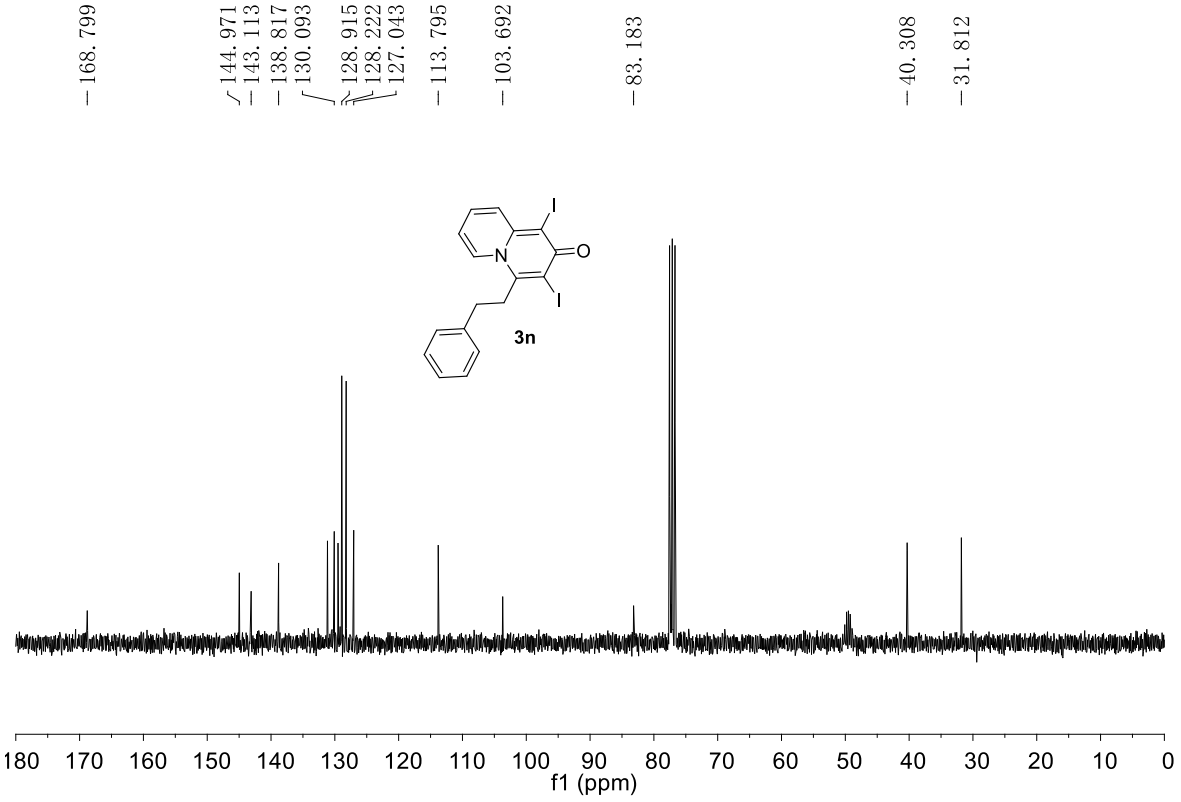
7.993
7.948
7.929
7.360
7.342
7.324
7.306
7.288
7.266
7.260
7.234
7.218
7.211
7.195
6.669
6.666
6.650
6.634
6.631
3.772
3.751
3.730
3.018
2.997
2.976
1.00
0.95
5.01
1.05
1.00
2.00
2.02
f1 (ppm)
3n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143.113
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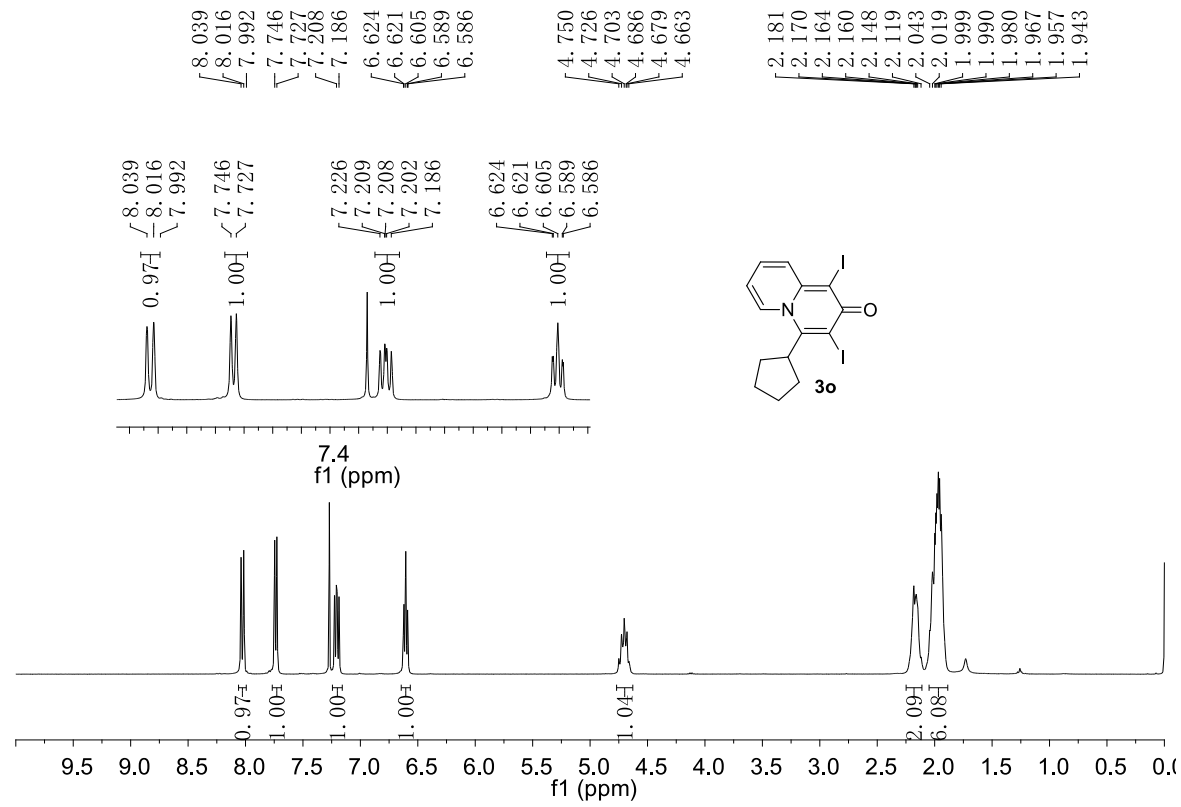
128.915
128.222
127.043
113.795
103.692
83.183
40.308
31.812
f1 (ppm)
3n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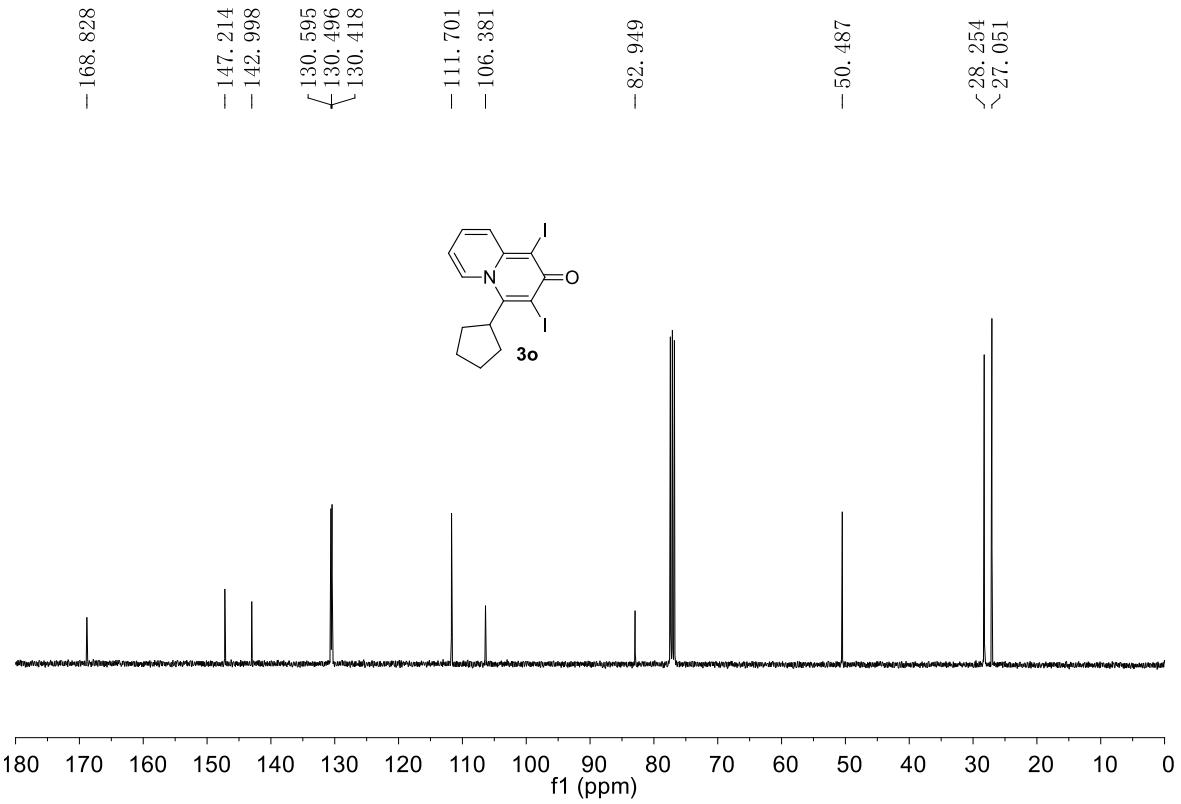
8.016
7.992
7.746
7.727
7.208
7.186
6.624
6.621
6.605
6.589
6.586
4.750
4.726
4.703
4.686
4.679
4.663
2.181
2.170
2.164
2.160
2.148
2.119
2.043
2.019
1.999
1.990
1.980
1.967
1.957
1.943
0.97
1.00
1.00
1.00
1.04
2.09
6.08
3o
7.4
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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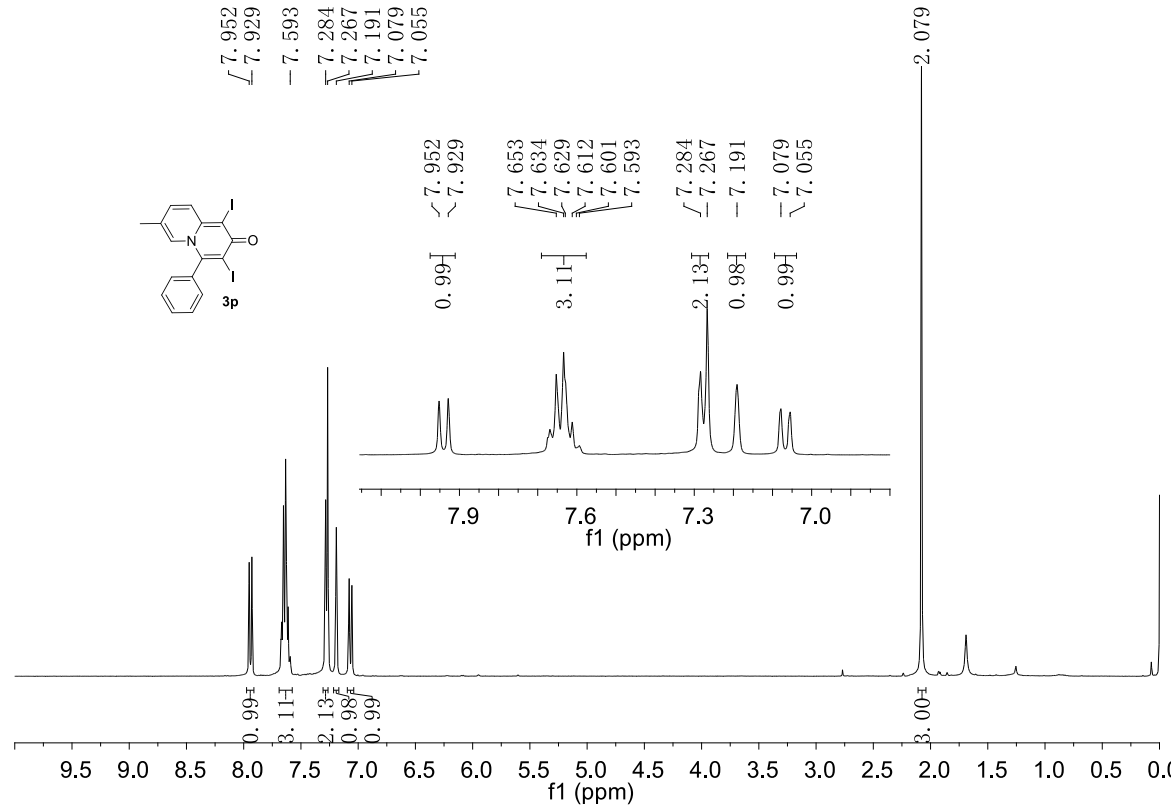
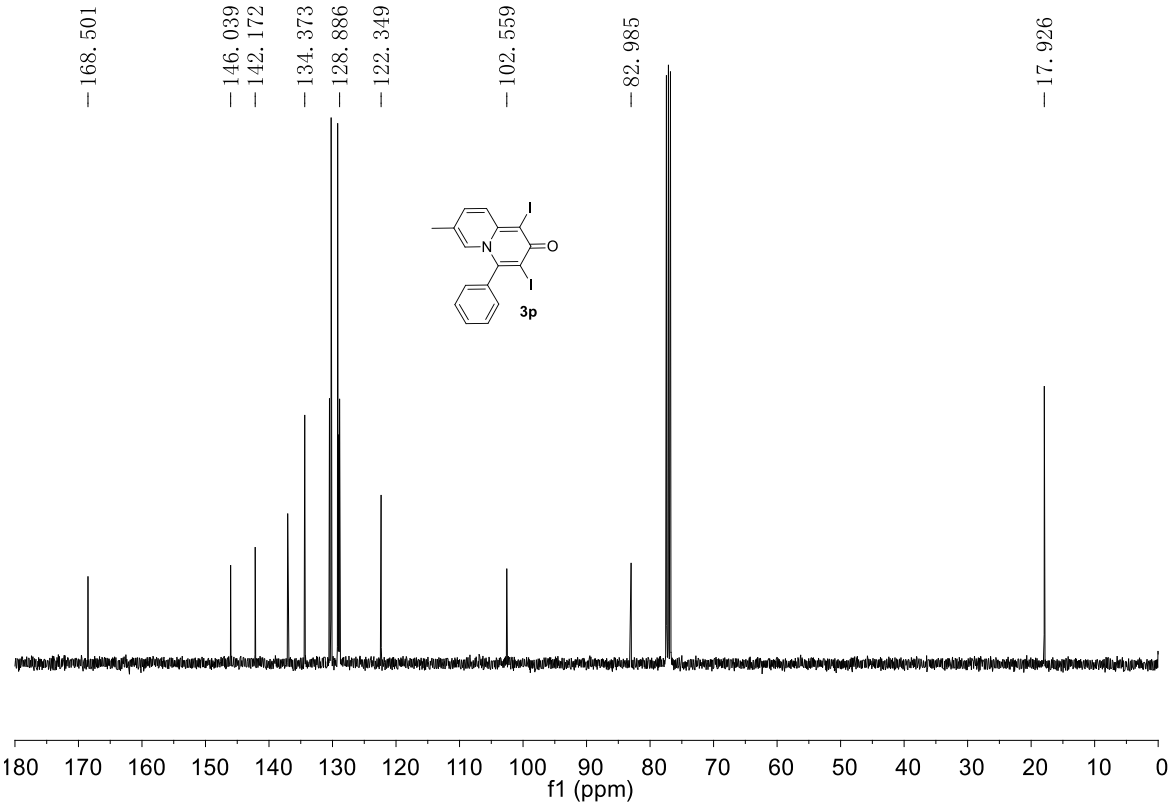
142.998
130.595
130.496
130.418
111.701
106.381
82.949
50.487
28.254
27.051
3o
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.952
7.929
7.593
7.284
7.267
7.191
7.079
7.055
2.079
7.653
7.634
7.629
7.612
7.601
7.593
0.99
3.11
2.13
0.98
0.99
3.00
3p
7.9
7.6
7.3
7.0
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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146.039
142.172
134.373
128.886
122.349
102.559
82.985
17.926
3p
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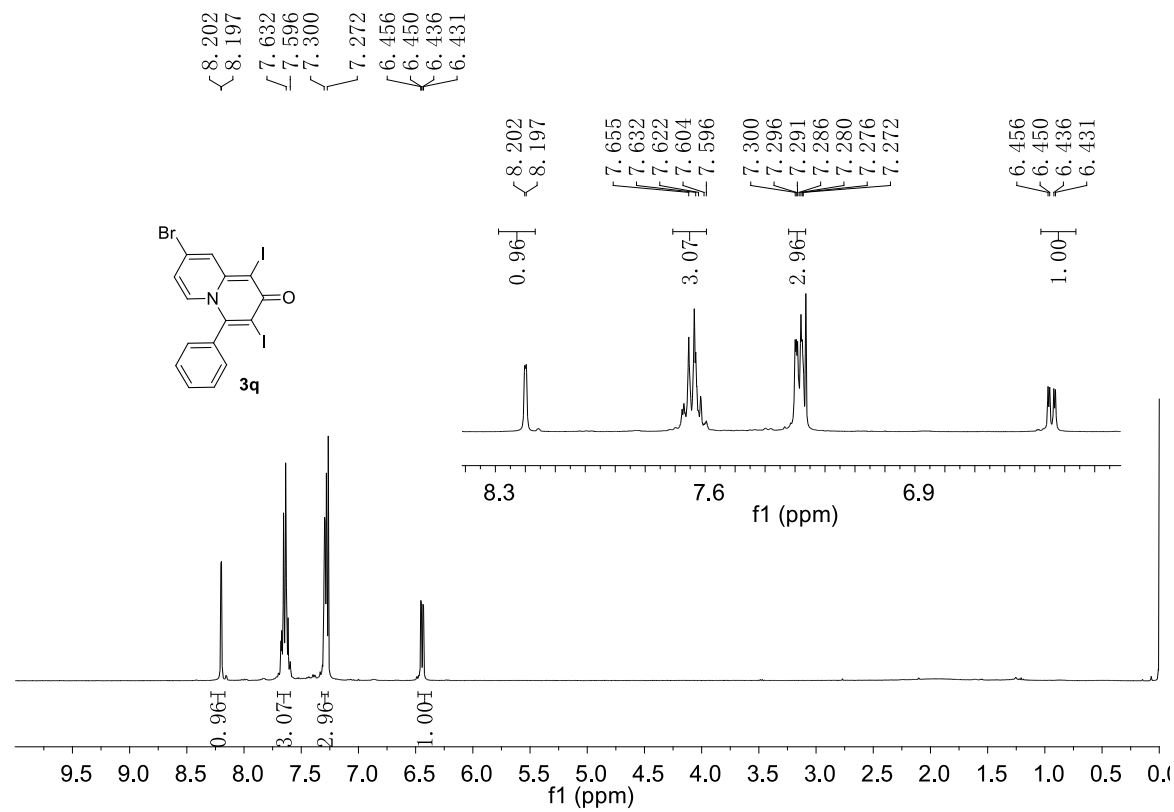
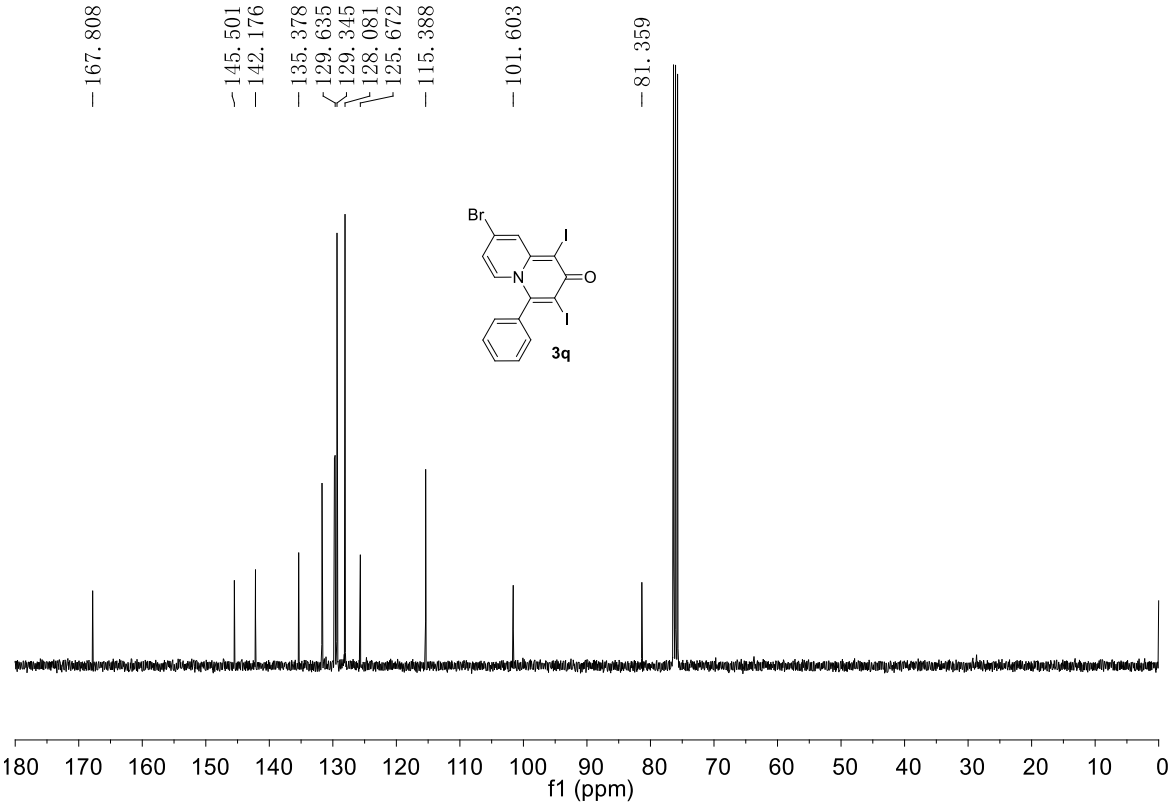
f1 (ppm)


8.202
8.197
7.632
7.596
7.300
7.272
6.456
6.450
6.436
6.431
0.96
3.07
2.96
1.00
Br
I
O
N
I
3q
8.3
7.6
6.9
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


167.808
145.501
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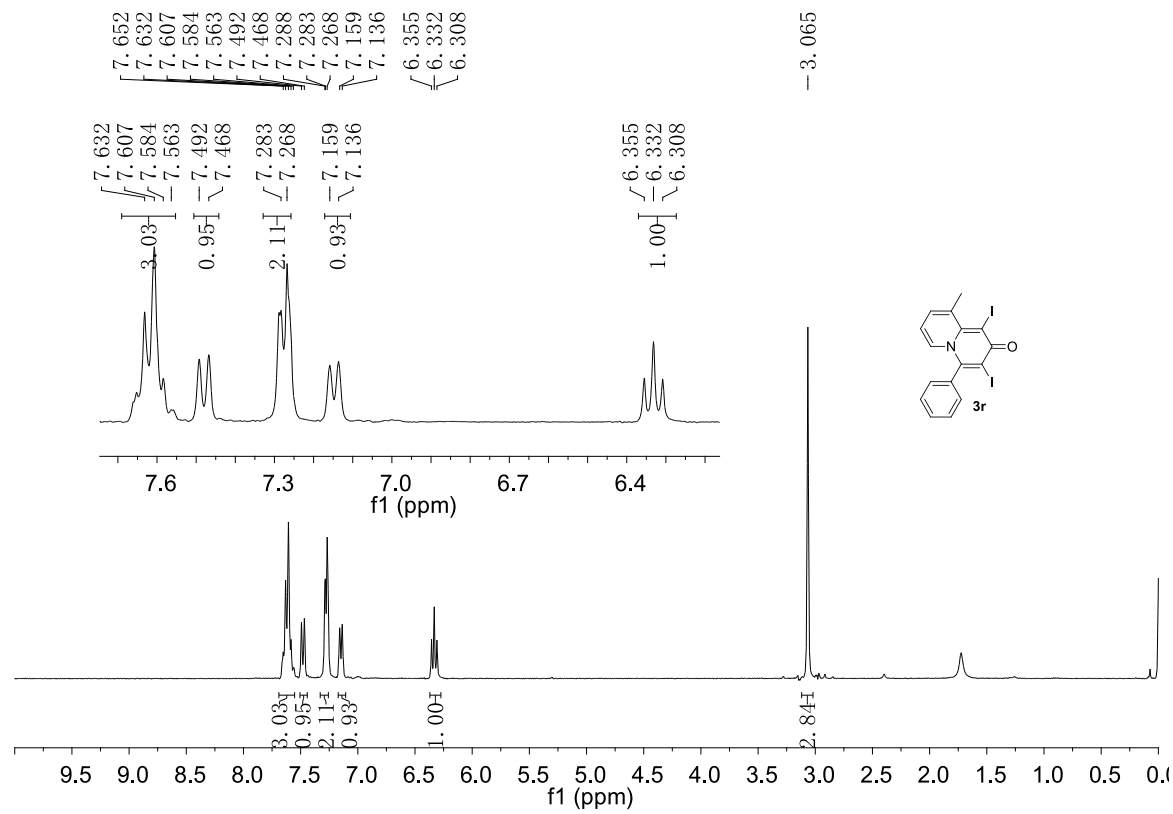
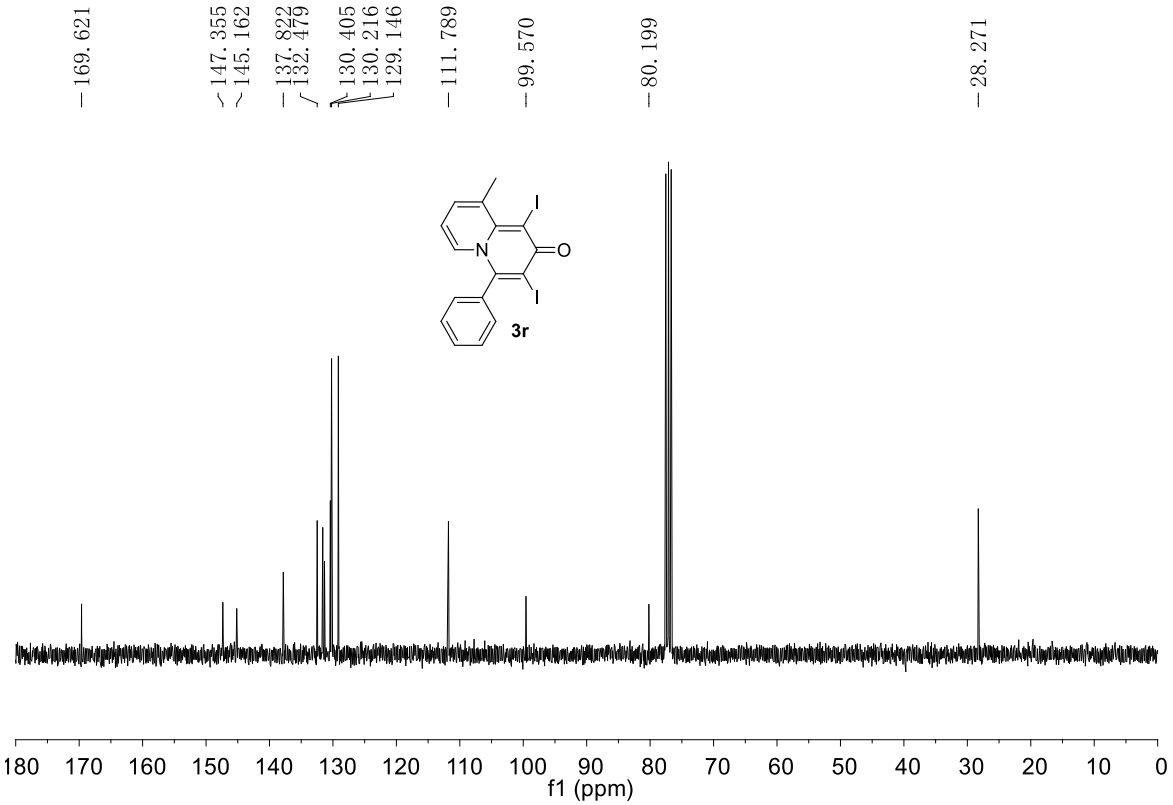
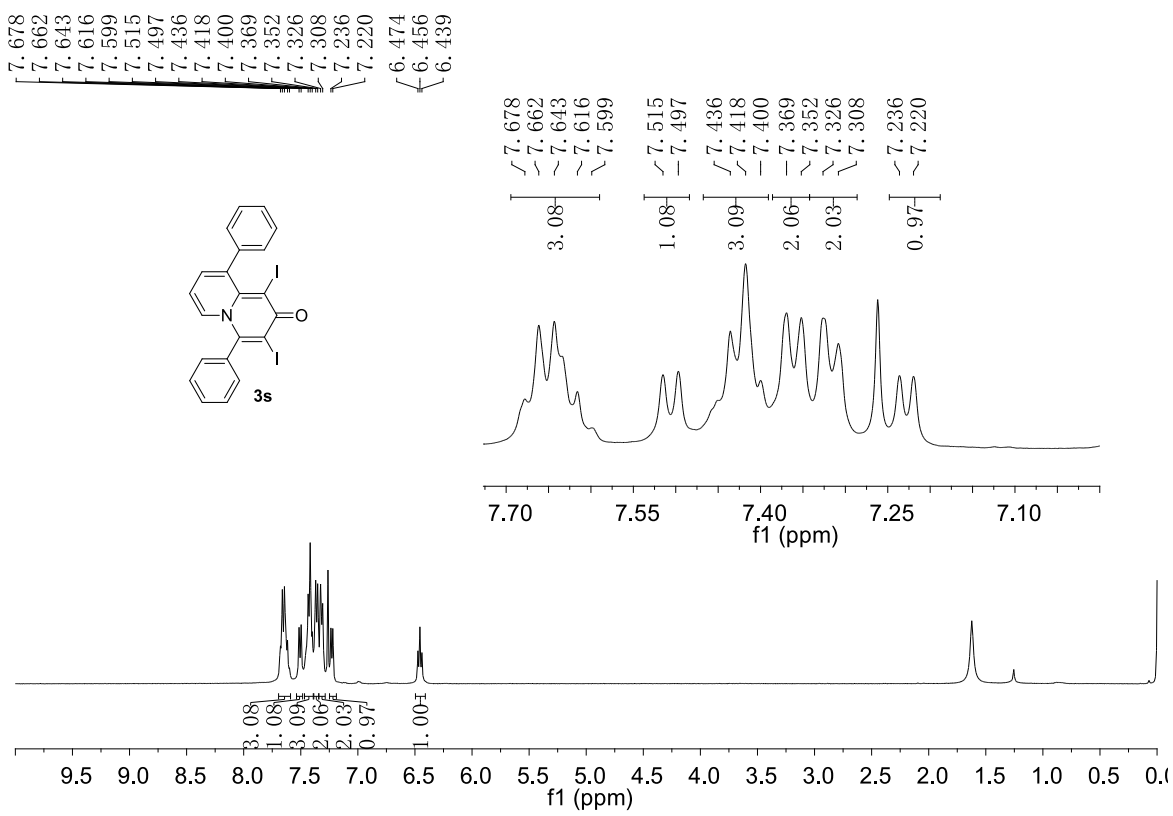
135.378
129.635
129.345
128.081
125.672
115.388
101.603
81.359
Br
I
O
N
I
3q
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.652
7.632
7.607
7.584
7.563
7.492
7.468
7.288
7.283
7.268
7.159
7.136
6.355
6.332
6.308
3.065
3.03
0.95
2.11
0.93
1.00
2.84
I
O
I
3r
f1 (ppm)


169.621
147.355
145.162
137.822
132.479
130.405
130.216
129.146
111.789
99.570
80.199
28.271
I
O
I
3r
f1 (ppm)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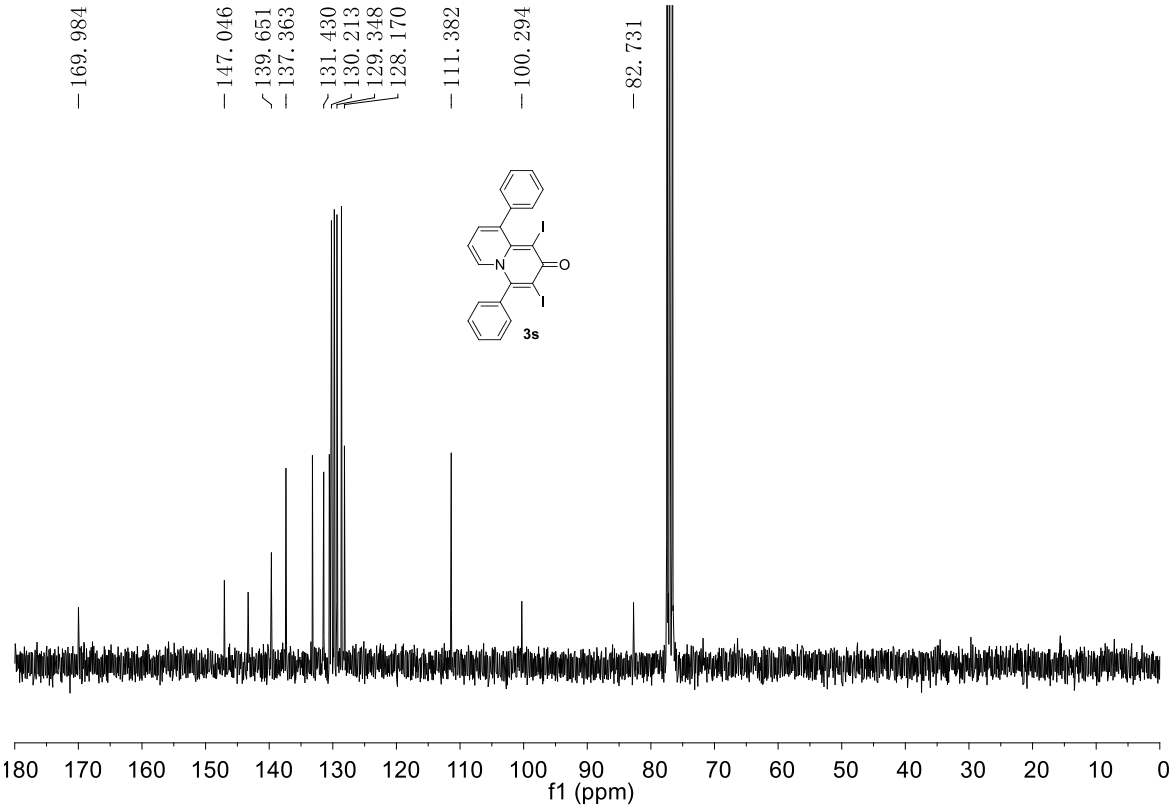
7.599
7.515
7.497
7.436
7.418
7.400
7.369
7.352
7.326
7.308
7.236
7.220
6.474
6.456
6.439
3.08
1.08
3.09
2.06
2.03
0.97
1.00
I
N
O
I
3s
f1 (ppm)


169.984
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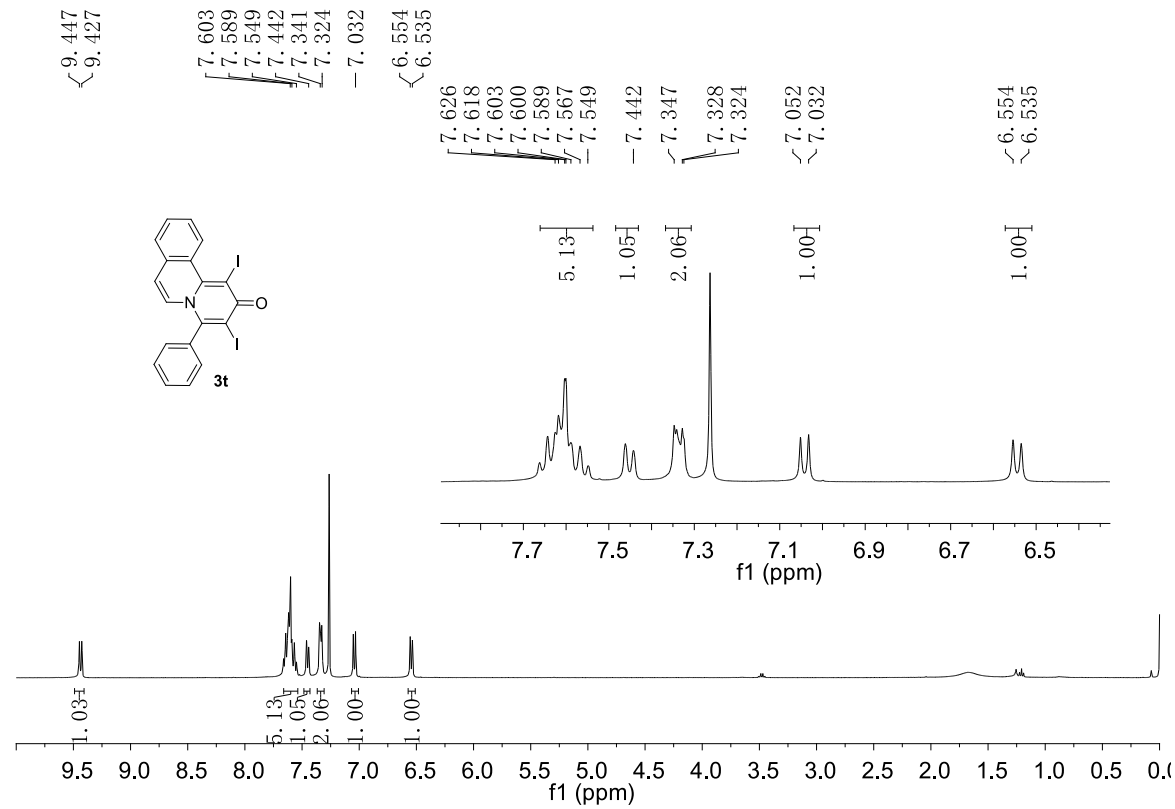
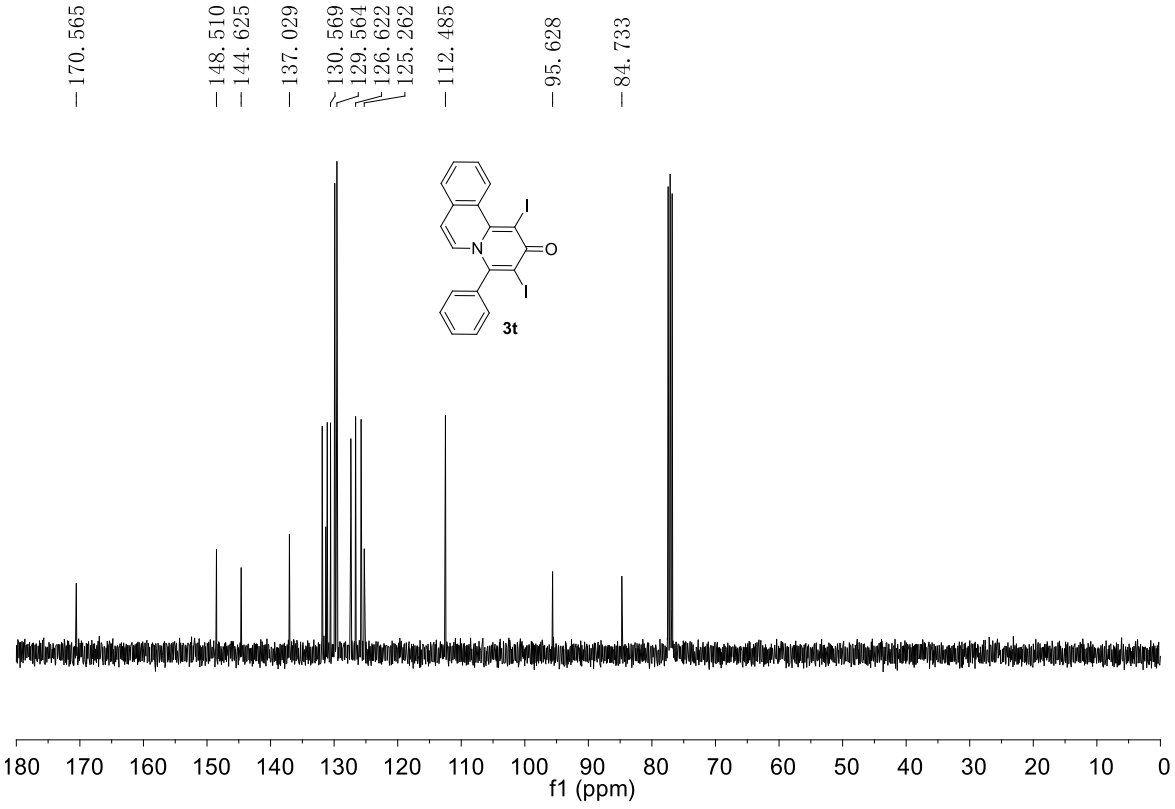
139.651
137.363
131.430
130.213
129.348
128.170
111.382
100.294
82.731
I
N
O
I
3s
f1 (ppm)


9.447
9.427
7.603
7.589
7.549
7.442
7.341
7.324
7.032
6.554
6.535
7.626
7.618
7.603
7.600
7.589
7.567
7.549
7.442
7.347
7.328
7.324
7.052
7.032
6.554
6.535
5.13
1.05
2.06
1.00
1.00
1.03
3t
f1 (ppm)


170.565
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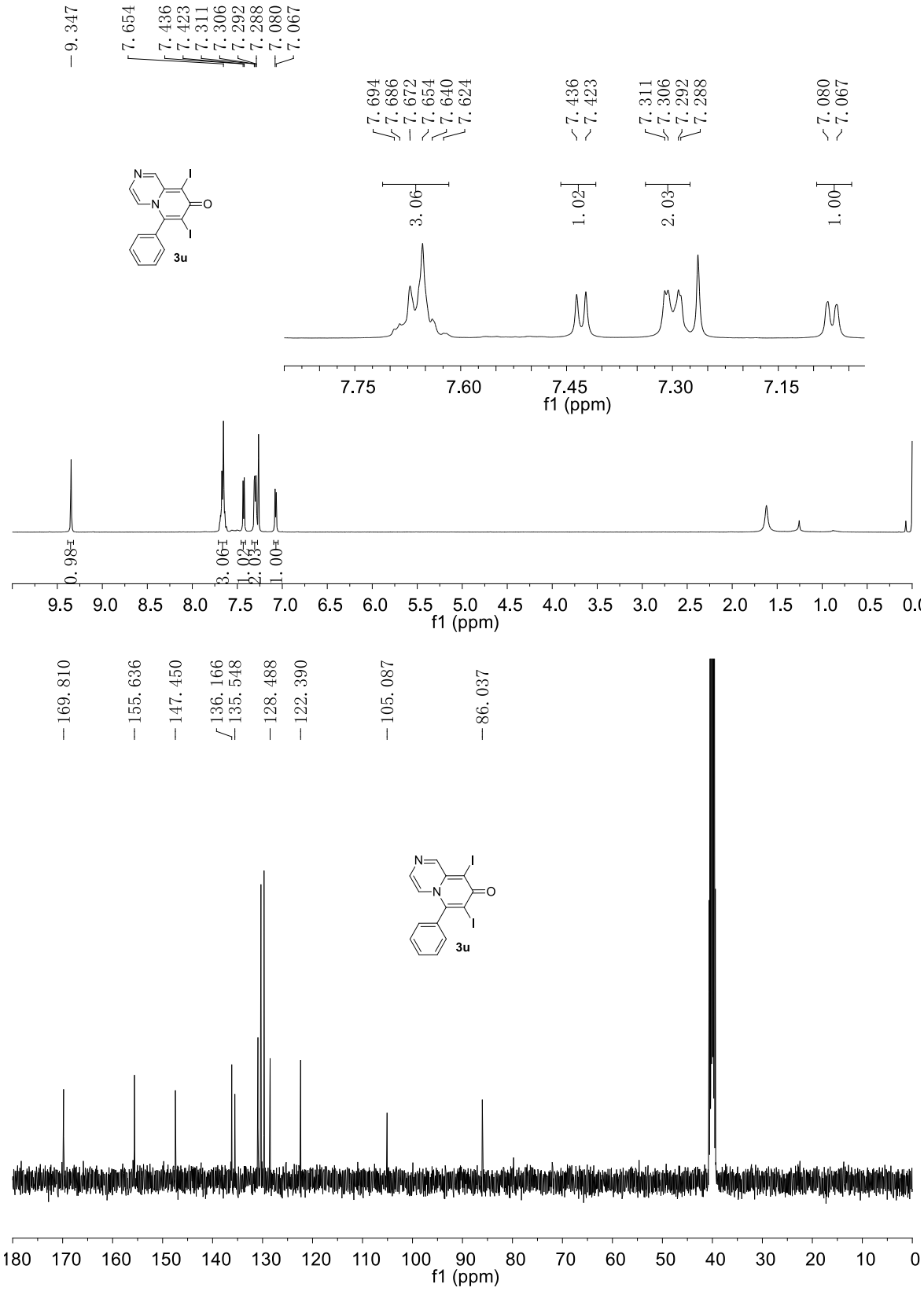
129.564
126.622
125.262
112.485
95.628
84.733
3t
f1 (ppm)


9.347
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7.436
7.423
7.311
7.306
7.292
7.288
7.080
7.067
7.694
7.686
7.672
7.654
7.640
7.624
3.06
1.02
2.03
1.00
3u
f1 (ppm)
0.98
3.06
1.02
2.03
1.00
f1 (ppm)
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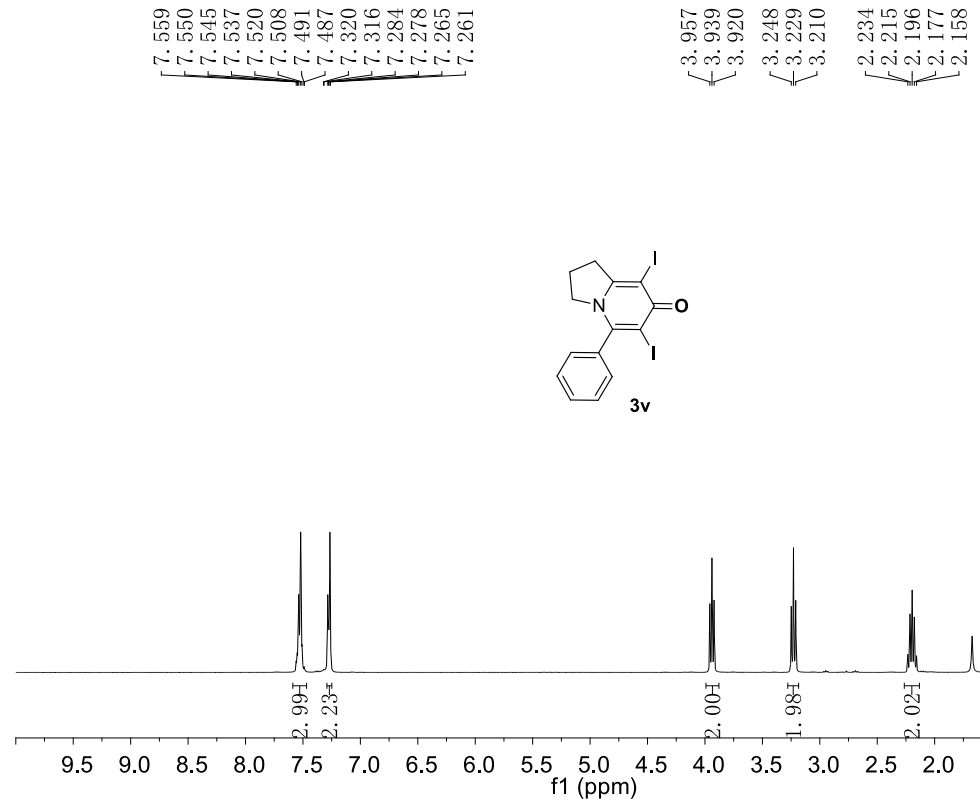
155.636
147.450
136.166
135.548
128.488
122.390
105.087
86.037
3u
f1 (ppm)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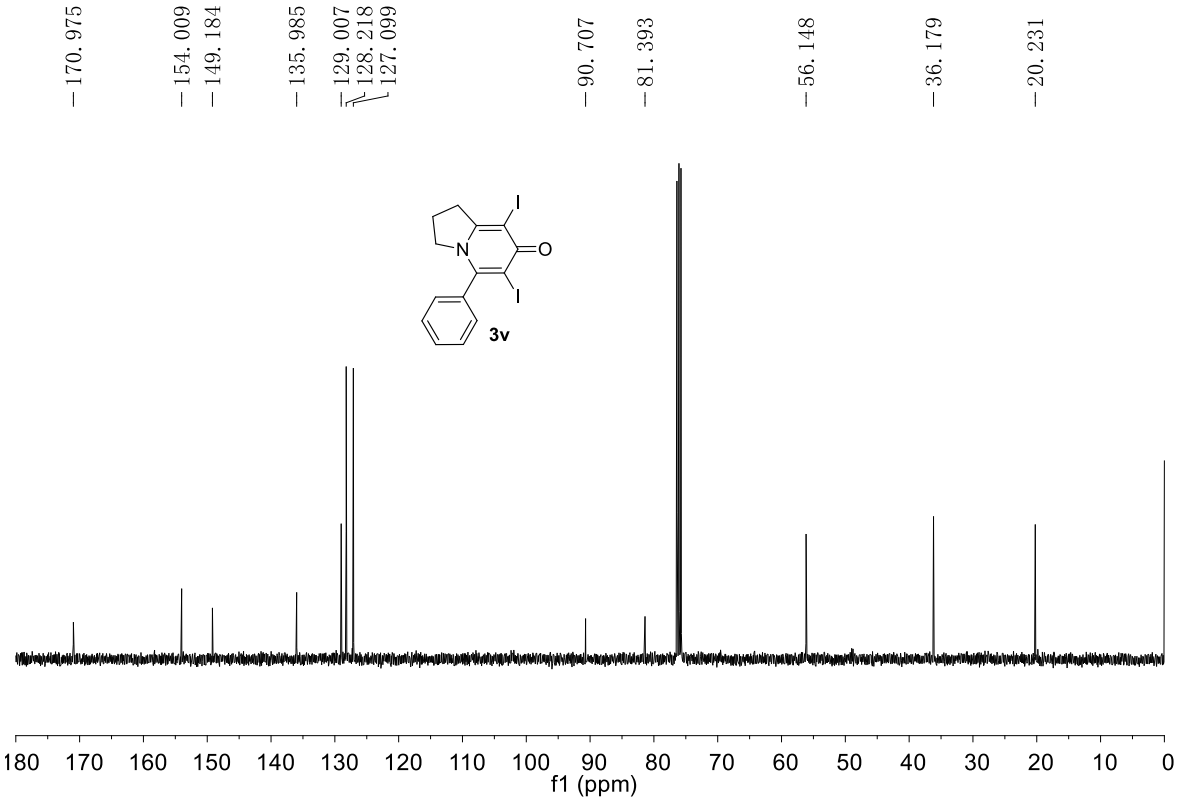
7.545
7.537
7.520
7.508
7.491
7.487
7.320
7.316
7.284
7.278
7.265
7.261
3.957
3.939
3.920
3.248
3.229
3.210
2.234
2.215
2.196
2.177
2.158
I
N
O
I
3v
2.99
2.23
2.00
1.98
2.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


170.975
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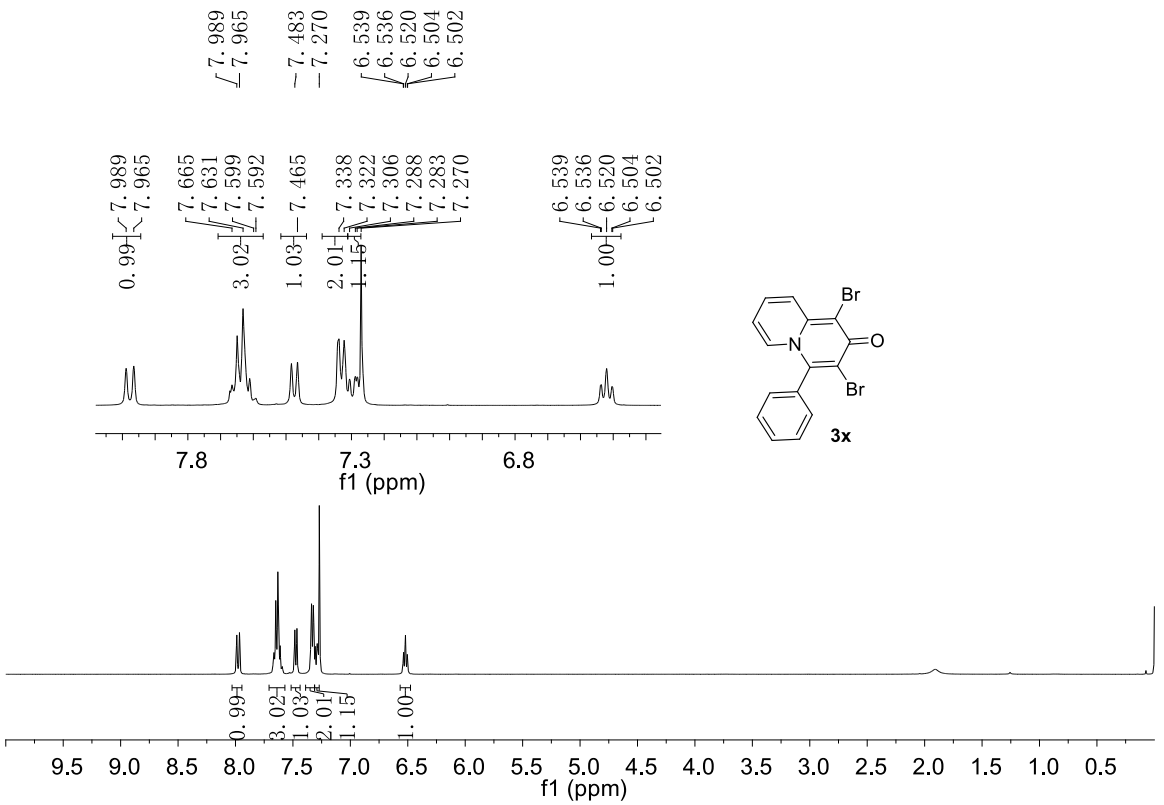
149.184
135.985
129.007
128.218
127.099
90.707
81.393
56.148
36.179
20.231
I
N
O
I
3v
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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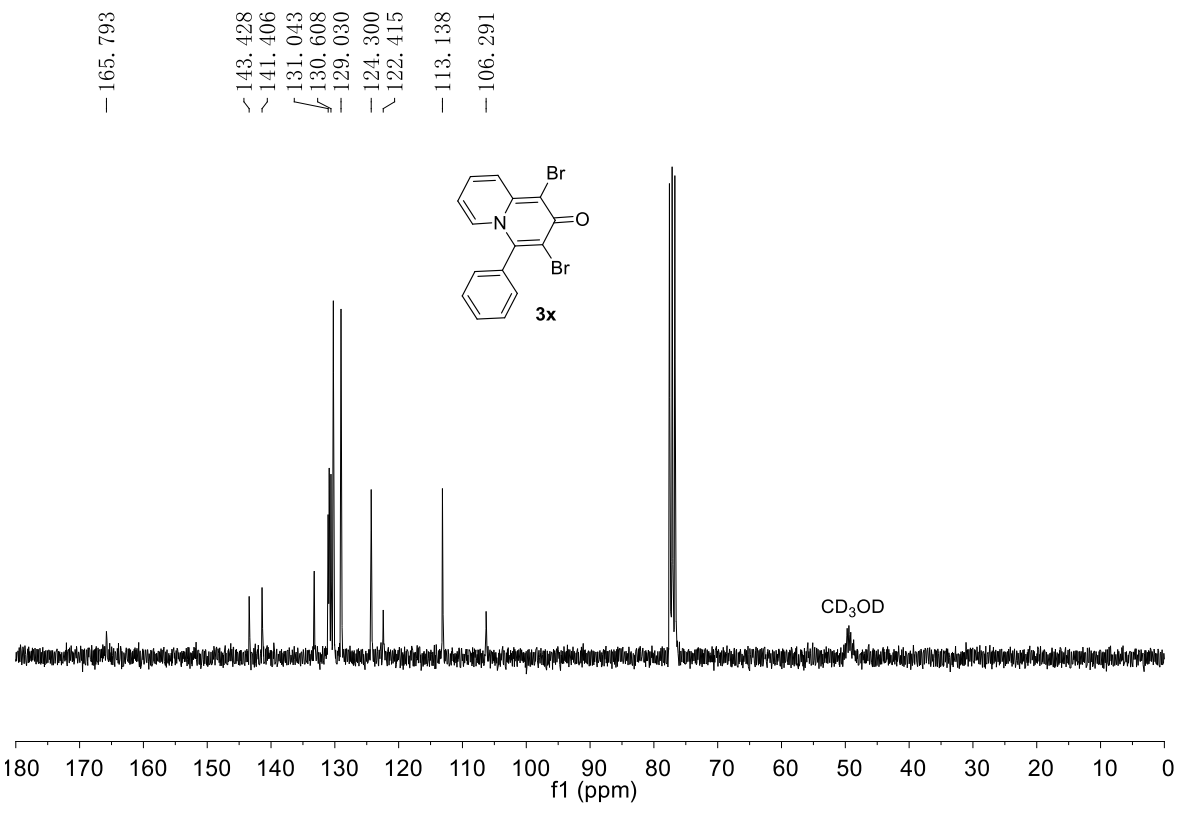
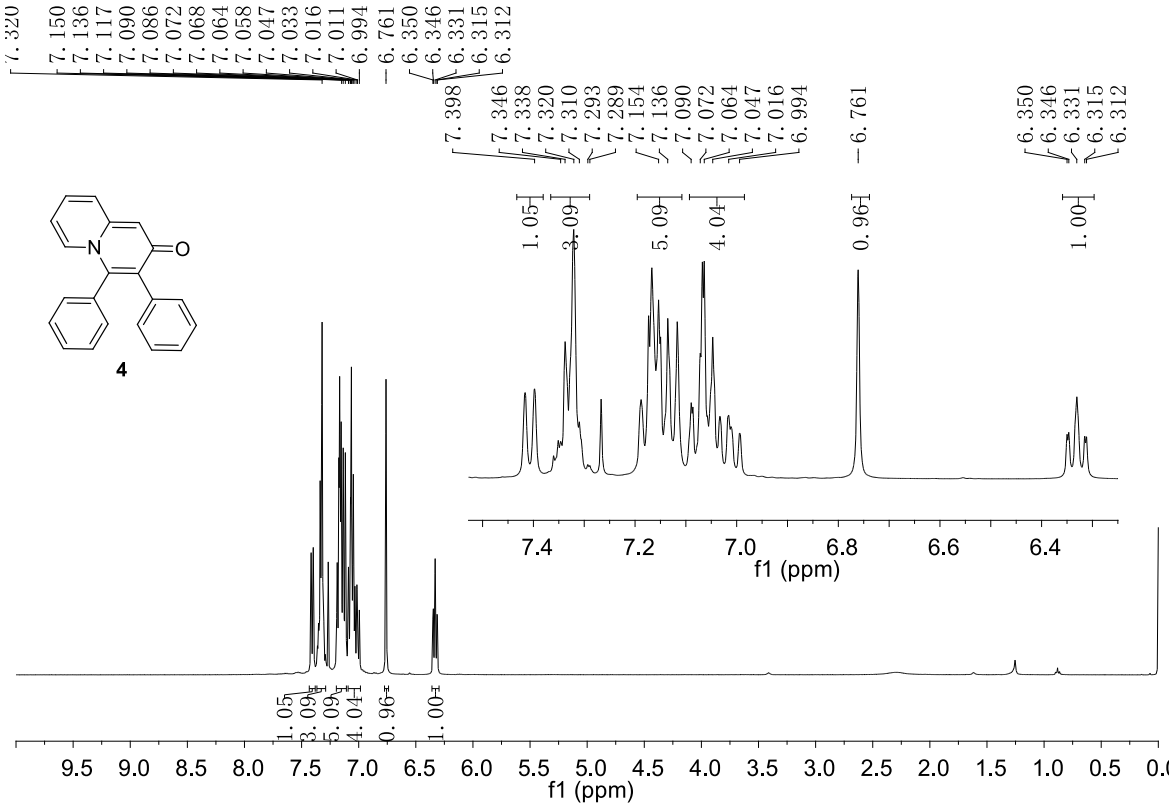
7.483
7.270
6.539
6.536
6.520
6.504
6.502
0.99
3.02
1.03
2.01
1.15
1.00
Br
O
Br
3x
f1 (ppm)


165.793
143.428
141.406
131.043
130.608
129.030
124.300
122.415
113.138
106.291
Br
O
Br
3x
CD3OD
f1 (ppm)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7.117
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7.086
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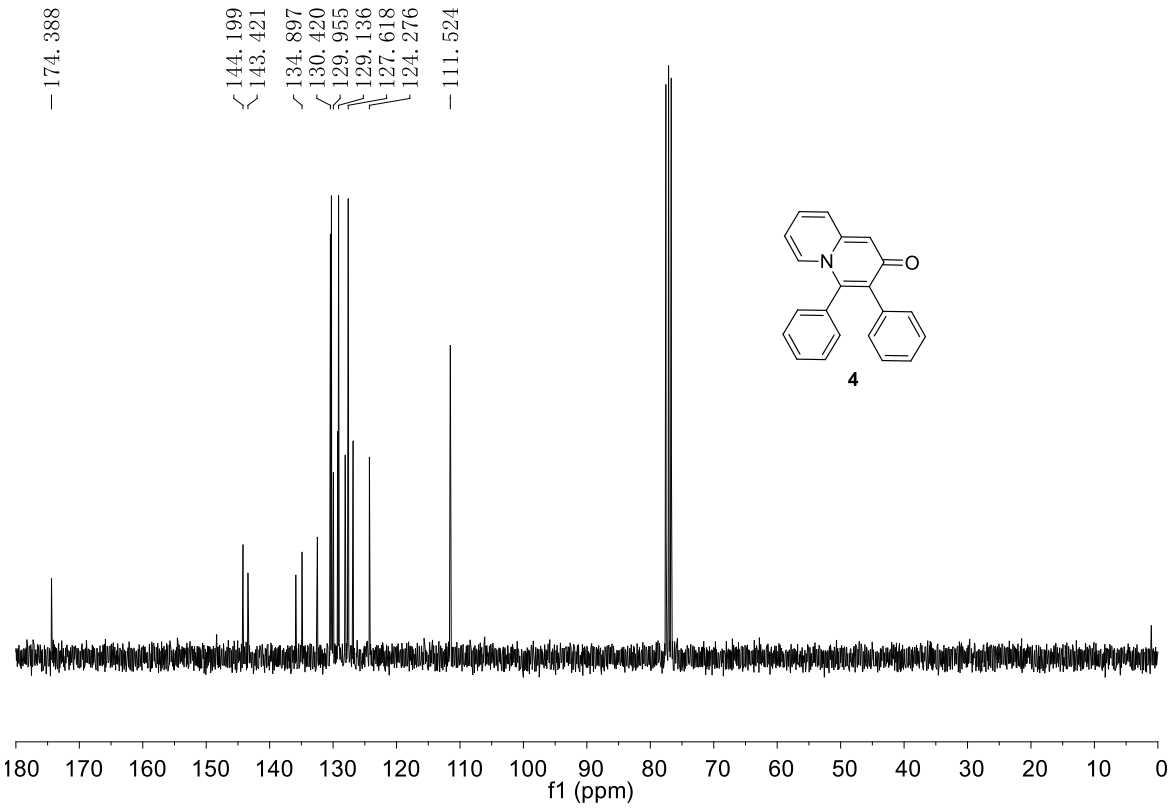
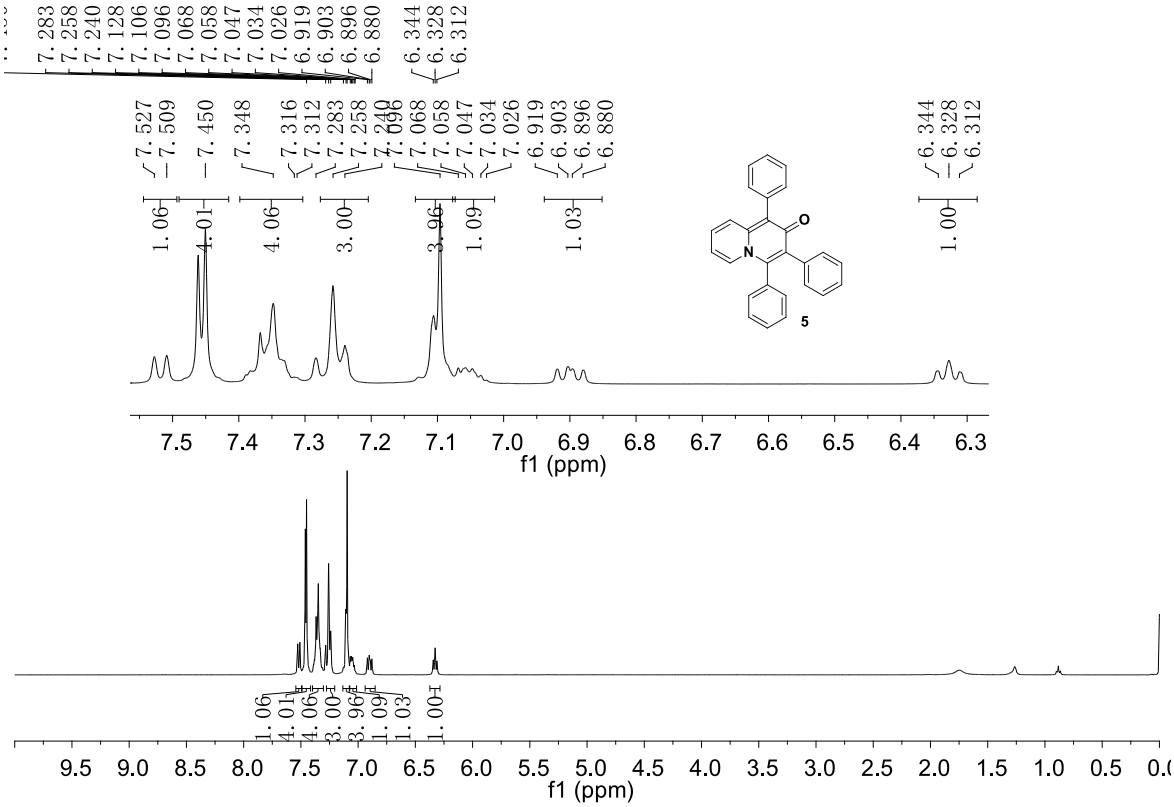
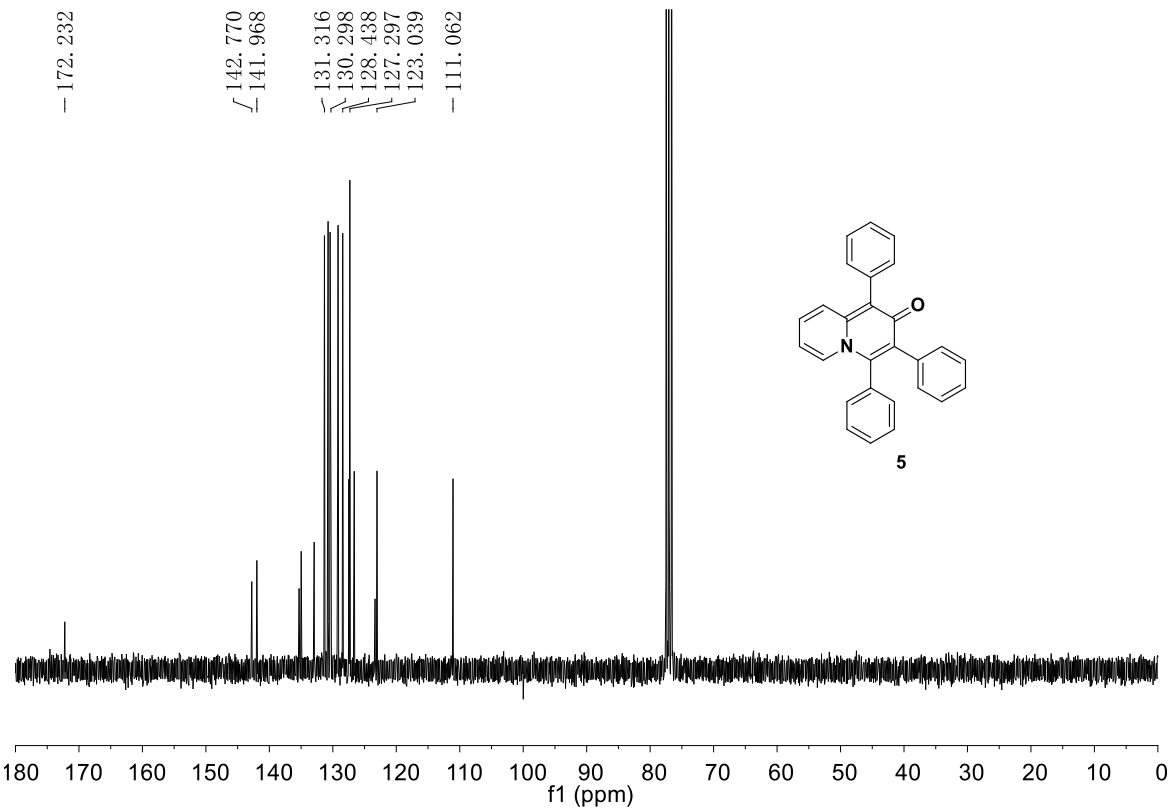
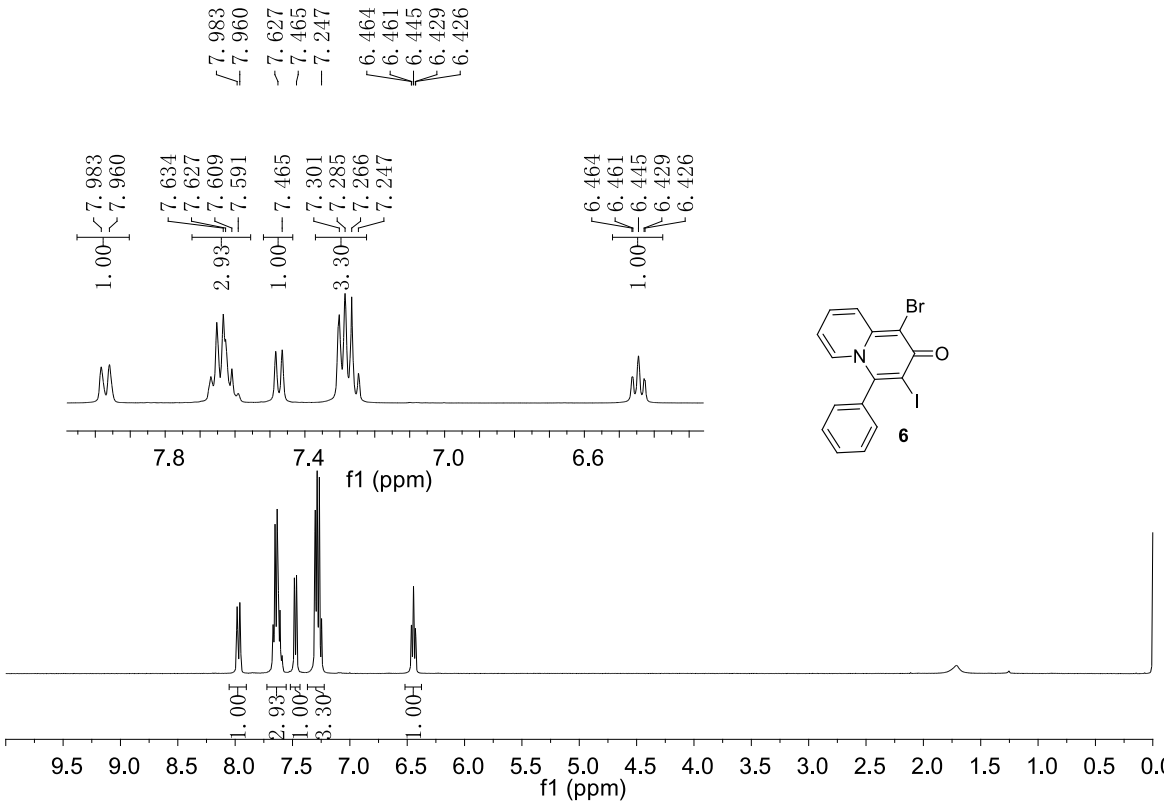
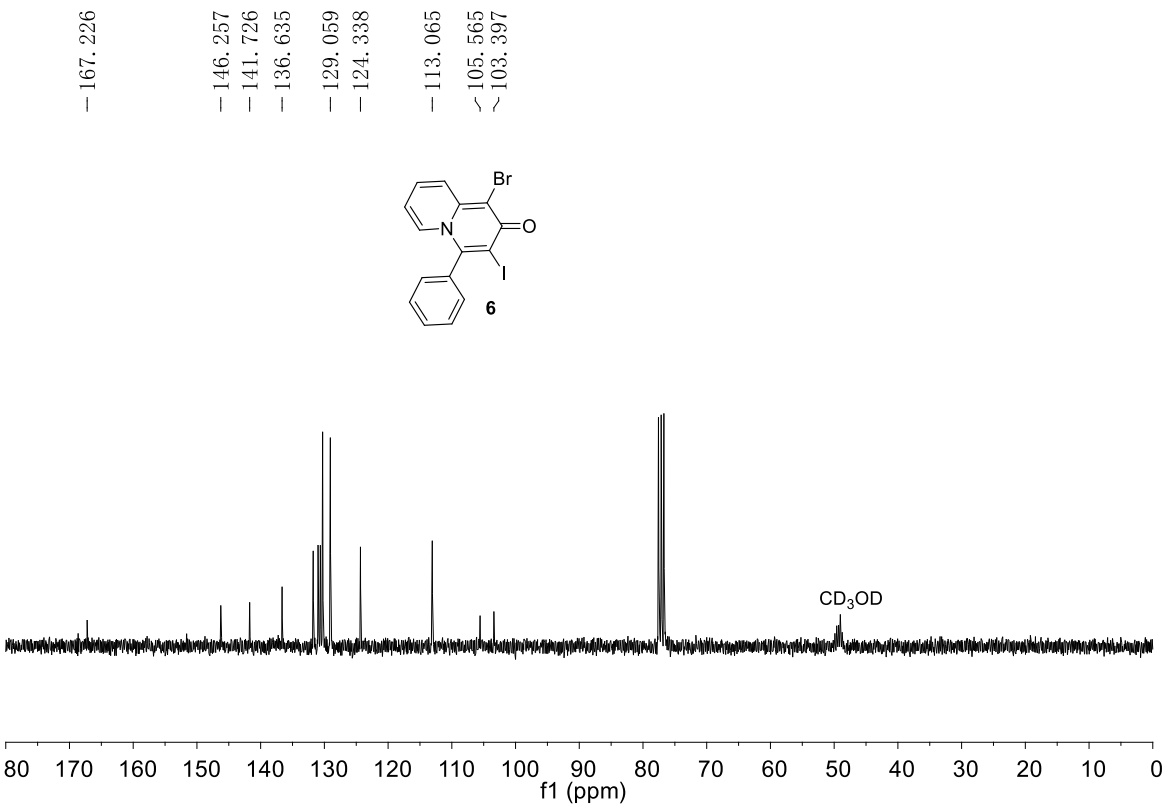
7.068
7.064
7.058
7.047
7.033
7.016
7.011
6.994
6.761
6.350
6.346
6.331
6.315
6.312
7.398
7.346
7.338
7.320
7.310
7.293
7.289
7.154
7.136
7.090
7.072
7.064
7.047
7.016
6.994
6.761
6.350
6.346
6.331
6.315
6.312
1.05
3.09
5.09
4.04
0.96
1.00
4
7.4
7.2
7.0
6.8
6.6
6.4
f1 (ppm)
1.05
3.09
5.09
4.04
0.96
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


174.388
144.199
143.421
134.897
130.420
129.955
129.136
127.618
124.276
111.524
4
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.283
7.258
7.240
7.128
7.106
7.096
7.068
7.058
7.047
7.034
7.026
6.919
6.903
6.896
6.880
6.344
6.328
6.312
7.527
7.509
7.450
7.348
7.316
7.312
7.283
7.258
7.240
7.096
7.068
7.058
7.047
7.034
7.026
6.919
6.903
6.896
6.880
6.344
6.328
6.312
1.06
4.01
4.06
3.00
3.96
1.09
1.03
1.00
O
N
5
7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3
f1 (ppm)
1.06
4.01
4.06
3.00
3.96
1.09
1.03
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


172.232
142.770
141.968
131.316
130.298
128.438
127.297
123.039
111.062
O
N
5
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.983
7.960
7.627
7.465
7.247
6.464
6.461
6.445
6.429
6.426
1.00
2.93
1.00
3.30
1.00
7.634
7.627
7.609
7.591
7.301
7.285
7.266
7.247
Br
N
O
I
6
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


167.226
146.257
141.726
136.635
129.059
124.338
113.065
105.565
103.397
Br
N
O
I
6
CD3OD
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

6. Crystallography

Diffraction datas were collected at 293 K on a Bruker SMART-CCD diffractometer using graphite-monochromated Mo Kα radiation. The structure was solved by direct methods and refined by full-matrix least squares on F^2. All nonhydrogen atoms were refined anisotropically, and the hydrogen atoms were included in idealized positions. All calculations were performed using the SHELXTL crystallographic software packages. CCDC-1940902 (**2a**) and CCDC-1940903 (**3a**) contain supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

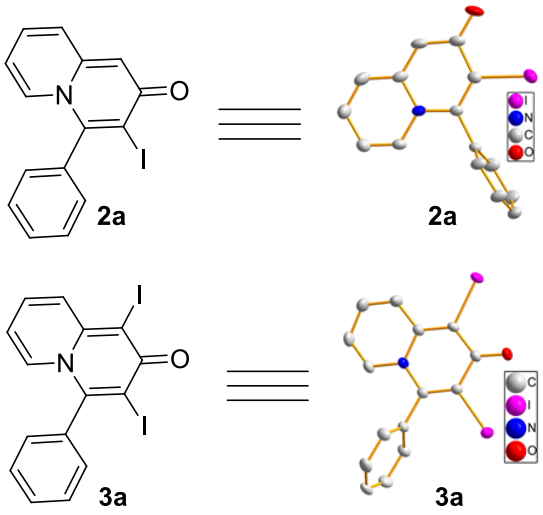
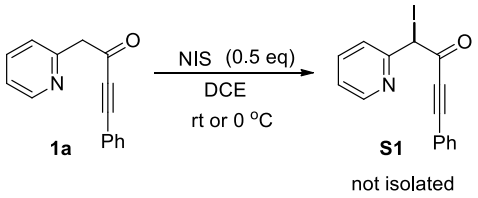


Figure S1 Molecular structures of **2a** and **3a** with thermal ellipsoids drawn at 30% probability. Hydrogen atoms have been omitted for clarity.

7. Mechanism Studies

To prove the alpha-iodination of substrate **1a** with NIS, we try our best to isolate the alpha-iodination product **S1**. Unfortunately, the compound **S1** can't be isolated possibly due to its instability.



Therefore, we attempt to capture the information of compound **S1** by monitoring the reaction course by ^{1}H NMR spectroscopy (Fig. S2). When substrate **1a** mixed with 0.5 eq NIS for 1 min, the characteristic peak of methyne (H5) in compound **S1** were observed at 6.13 ppm. Next, 2 eq NIS was added into the reaction mixture, and substrate **2a** and compound **S1** quickly disappeared. Meanwhile, the products **2a**, **3a** and succinimide were also observed. Expectedly, the diiodination product **3a** was almost only observed after 2 h. Base on the control experiments and ^{1}H NMR monitoring, two competitive reaction procedure for preparation of diiodination products **3** may occur during the cyclization process.

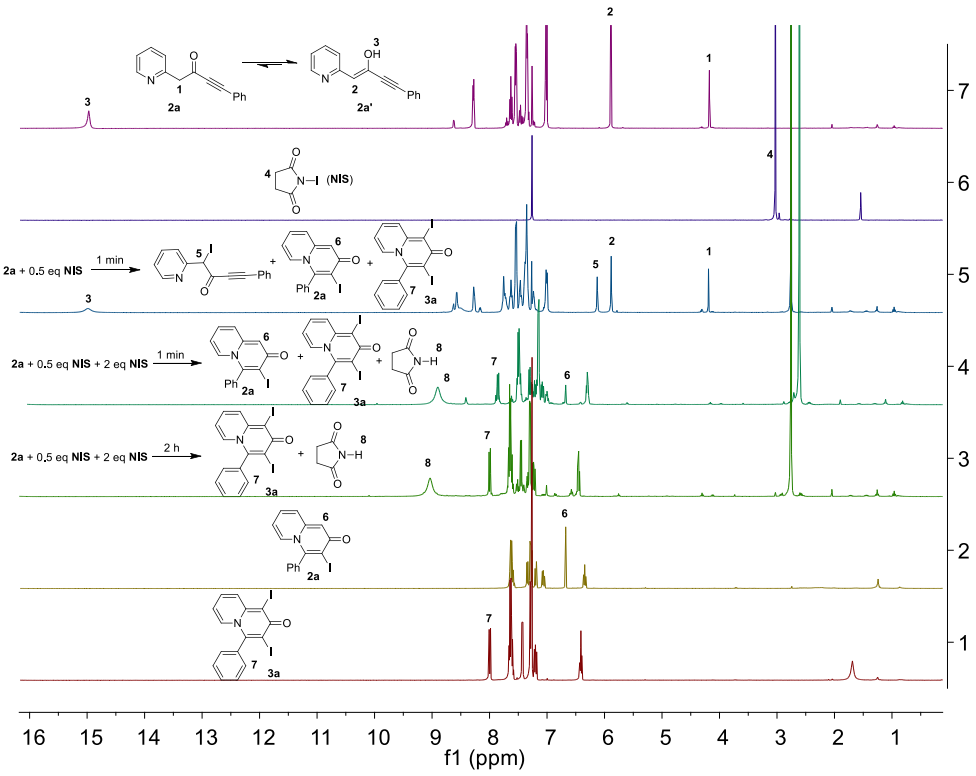


Fig. S2 Monitoring the reaction by ^{1}H NMR.