Supporting Information for:

Solvent-controlled divergent annulation of ynones and (iso)quinoline *N*-oxides: synthesis of 3-((iso)quinolin-1-yl)-4*H*-chromen-4-ones and 13*H*-isoquinolino[2,1-*a*]quinolin-13-ones

Wan-Wan Yang, [†] Lu-Lu Chen, [†] Pei Chen, [†] Ya-Fang Ye, [†] Yan-Bo Wang[*, †] and Xiao Zhang[*, ‡]

[†] *Institute of Functional Organic Molecular Engineering, Henan Engineering Laboratory of Flame-Retardant and Functional Materials, College of Chemistry and Chemical Engineering, Henan University, Kaifeng, 475004, China.*

[‡] *College of Science, State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Changping, Beijing, 102249, China.*

E-mail: wangyanokf@henu.edu.cn

Email: zhangxiao@cup.edu.cn

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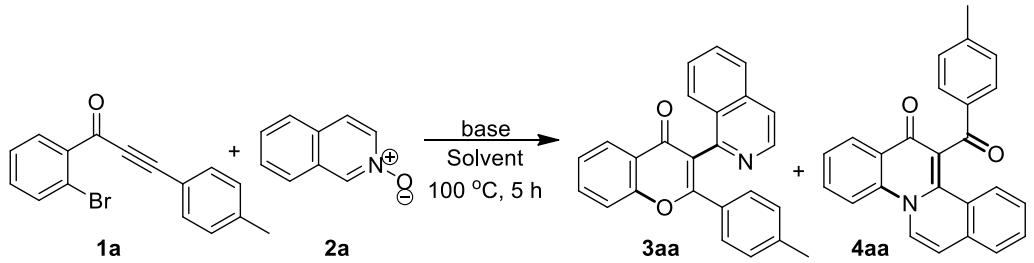
1. General information

Unless otherwise statement, all manipulations were performed using standard Schlenk techniques under a dry nitrogen atmosphere. 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. Acetonitrile was distilled from phosphorus pentoxide under N_2 atmosphere. Et_3N, NMP, DMSO and DMF were distilled from calcium hydride under N_2 atmosphere. Substrates **1** and **2** were prepared by the by previous report.[1, 2]

1. (a) Ji, K.; Yang, F.; Gao, S.; Tang, J.; Gao, J. *Chem. – Eur. J.*, **2016**, *22*, 10225; (b) Cheng, X.; Zhou, Y.; Zhang, F.; Zhu, K.; Liu, Y.; Li, Y. *Chem. – Eur. J.*, **2016**, *22*, 12655. (c) Liu, X.; Hong, D.; She, Z.; Hersh, W. H.; Yoo, B.; Chen, Y. *Tetrahedron*, **2018**, *74*, 6593; (d) Zheng, Z.; Tao, Q.; Ao, Y.; Xu, M.; Li, Y. *Org. Lett.,* **2018**, *20*, 3907; (e) Singh, S.; Samineni, R.; Pabbaraja, S.; Mehta, G. *Angew. Chem., Int. Ed.,* **2018**, *57*,16847.

2. (a) Chen, Z.-S.; Yang, F.; Ling, H.; Li, M.; Gao, J.-M.; Ji, K. *Org. Lett.* **2016**, *18*, 5828. (b) Ji, K.; Yang, F.; Gao, S.; Tang, J.; Gao, J. *Chem. Eur. J.* **2016**, *22*, 10225. (c) Biswas, A.; Karmakar, U.; Pal, A.; Samanta, R. *Chem. Eur. J.* **2016**, *22*, 13826. (d) Zhang, B.; Huang, L.; Yin, S.; Li, X.; Xu, T.; Zhuang, B.; Wang, T.; Zhang, Z.; Hashmi, A. S. K. *Org. Lett*. **2017**, *19*, 4327. (e) Roudesly, F.; Veiros, L. F.; Oble, J.; Poli, G. *Org. Lett.* **2018***, 20,* 2346. (f) Li, X.; Wang, T.; Zhang, Z. *Adv. Synth. Catal.* **2019**, *361*, 696. (g) Li, X.; Zhou, G.; Du, X.; Wang, T.; Zhang Z. *Org. Lett.* **2019**, *21*, 5630.

2. Optimization of reaction conditions



1a **2a** **3aa** **4aa**

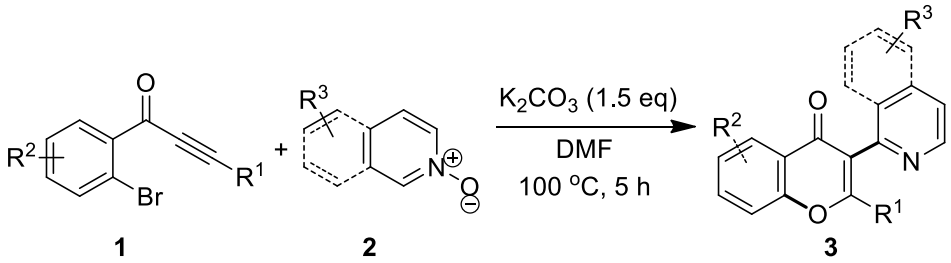
entry	base	**1a**/**2a**/base	solvent	yield (%) [b] **3aa/4aa**
1	**K_2CO_3**	**1.2/1/1.5**	**DMF**	**91/trace**
2	Na_2CO_3	1.2/1/1.5	DMF	58/18
3	Cs_2CO_3	1.2/1/1.5	DMF	89/trace
4	NaOH	1.2/1/1.5	DMF	35/10
5	KOH	1.2/1/1.5	DMF	38/-
3	DBU	1.2/1/1.5	DMF	-/-
7	DABCO	1.2/1/1.5	DMF	48/30
8	K_2CO_3	1.2/1/1.2	DMF	86/trace
9	K_2CO_3	1.2/1/1.5	DMSO	82/trace
10	K_2CO_3	1.2/1/1.5	NMP	81/trace
11	K_2CO_3	1.2/1/1.5	CH_3CN	34/trace
12	K_2CO_3	1.2/1/1.5	DCE	19/23
13	K_2CO_3	1.2/1/1.5	1,4-dioxane	trace/67
14	K_2CO_3	1.2/1/1.5	toluene	trace /70
15	Cs_2CO_3	1.2/1/1.5	toluene	trace/62
16	Na_2CO_3	1.2/1/1.5	toluene	15/43
17	NaOH	1.2/1/1.5	toluene	trace/15
18	KOH	1.2/1/1.5	toluene	34/40
19	DBU	1.2/1/1.5	toluene	-/-
20	DABCO	1.2/1/1.5	toluene	trace/37
21	**K_2CO_3**	**1.5/1/1.5**	**toluene**	**trace /78**

[a]Reaction conditions: ynone **1a**, **2a** (0.20 mmol, 1.0 equiv.), base and 2.0 mL solvent.

[b]Isolated yields.

3. General experimental procedures

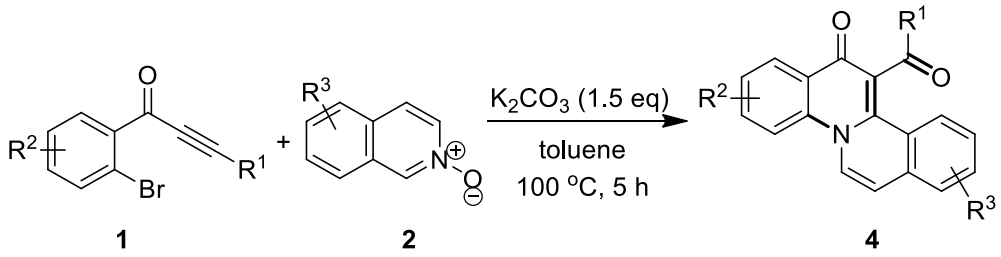
3.1 General procedure for the synthesis of products 3



1 2 3

A 10 mL oven-dried Schlenck tube was successively charged with 0.24 mmol ynones **1**, 0.20 mmol (iso)quinoline N-oxides **2**, 2.0 mL DMF and 0.3 mmol K_2CO_3. The tube was sealed and the reaction mixture was stirred at 100 ℃ for 5 h. After completion of this reaction, the resulting mixture was diluted with ethyl acetate (10 mL) and washed with brine (10 mL). The aqueous phase was extracted with ethyl acetate (2×10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated in-vacuo. The crude reaction mixture was purified by column chromatography on silica gel (petroleum ether/ethyl acetate) to give products **3**.

3.2 General procedure for the synthesis of products 4

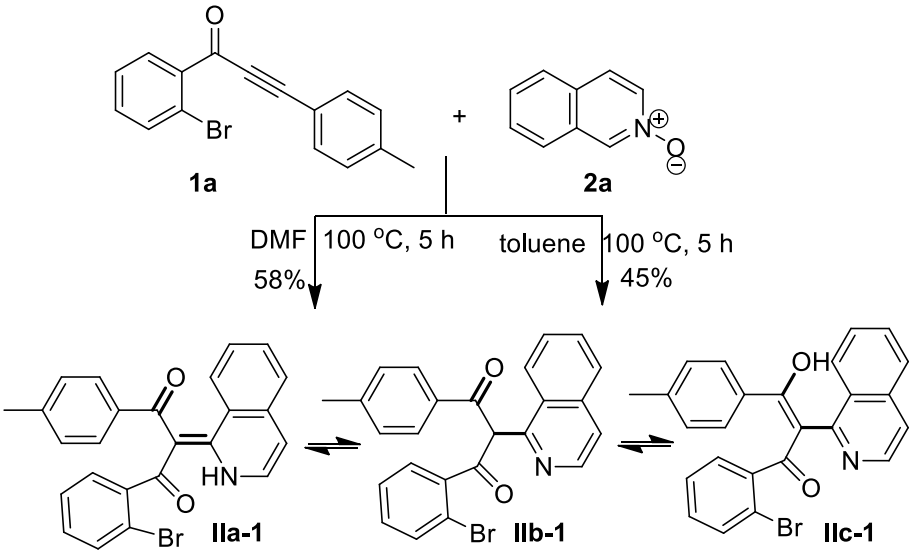


1 2 4

A 10 mL oven-dried Schlenck tube was successively charged with 0.30 mmol ynones **1**, 0.20 mmol isoquinoline N-oxides **2**, 2.0 mL toluene and 0.30 mmol K_2CO_3. The tube was sealed and the reaction mixture was stirred at 100 ℃ for 5 h. After completion of this reaction, the resulting mixture was diluted with ethyl acetate (10 mL) and washed with

brine (10 mL). The aqueous phase was extracted with ethyl acetate (2×10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated in-vacuo. The crude reaction mixture was purified by column chromatography on silica gel (petroleum ether/ethyl acetate) to give products **4**.

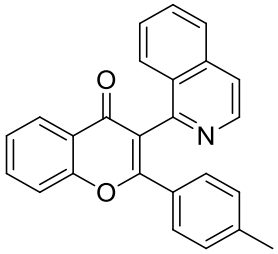
3.3 General procedure for the synthesis of the intermediates



A 10 mL oven-dried Schlenck tube was successively charged with 0.24 mmol ynones **1**, 0.20 mmol isoquinoline N-oxides **2** and 2.0 mL DMF. The tube was sealed and the reaction mixture was stirred at 100 ℃ for 5 h. After completion of this reaction, the resulting mixture was diluted with ethyl acetate (10 mL) and washed with brine (10 mL). The aqueous phase was extracted with ethyl acetate (2×10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated in-vacuo. The crude reaction mixture was purified by column chromatography on silica gel (petroleum ether/ethyl acetate) to give the mixed intermediates (**IIa-1**, **IIb-1** and **IIc-1**) in 58% yield. The mixed intermediates (**IIa-1**, **IIb-1** and **IIc-1**) could be also obtained in 45% yield using 0.3 mmol ynone **1a** and 0.20 mmol isoquinoline N-oxide **2a** as materials with the similar procedure.

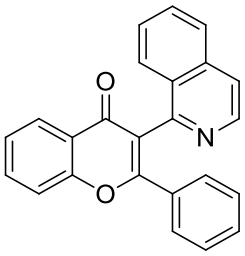
4. Characterization data

3-(Isoquinolin-1-yl)-2-p-tolyl-4*H*-chromen-4-one (3aa):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (66.1 mg, 91% yield); mp 178.5–179.3 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.54 (d, *J* = 5.6 Hz, 1H), 8.30 (d, *J* = 7.6 Hz, 1H), 7.96–7.81 (m, 2H), 7.76 (t, *J* = 7.7 Hz, 1H), 7.64 (dd, *J* = 9.8, 7.2 Hz, 3H), 7.48 (dd, *J* = 16.9, 8.6 Hz, 2H), 7.23 (d, *J* = 7.9 Hz, 2H), 6.96 (d, *J* = 7.9 Hz, 2H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.4, 163.4, 156.3, 155.0, 142.7, 140.9, 136.3, 133.9, 130.2, 129.9, 129.0, 128.8, 128.6, 127.7, 127.1, 126.6, 126.3, 125.3, 123.6, 121.3, 120.8, 118.1, 21.4; IR (KBr, cm^{-1}): 3053, 2917, 1633, 1616, 1575, 1560, 1511, 1499, 1465, 1401; HRMS (ESI-TOF) calcd for $C_{25}H_{18}NO_2^+$ ($[M+H]^+$): 364.1332, found: 364.1336.

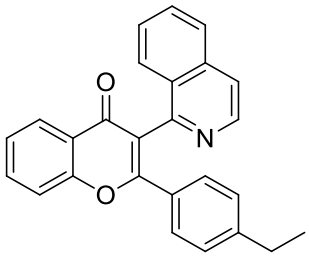
3-(Isoquinolin-1-yl)-2-phenyl-4*H*-chromen-4-one (3ba):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (65.7 mg, 94% yield); mp 225.2–227.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.52 (d, *J* = 5.7 Hz, 1H), 8.30 (d, *J* = 7.8 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.83 (d, *J* = 8.2 Hz, 1H), 7.78–7.70 (m, 1H), 7.63 (t, *J* = 5.9 Hz, 3H), 7.47 (dd, *J* = 16.3, 8.1 Hz, 2H), 7.33 (d, *J* = 7.8 Hz, 2H), 7.23 (d, *J* = 7.3 Hz, 1H), 7.14 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.4, 163.3, 156.3, 154.7, 142.6, 136.3, 134.1, 132.8, 1305, 130.2, 128.8, 128.7, 128.2, 127.7, 127.2, 126.5, 126.3, 125.4, 123.6, 121.7, 120.9, 118.1; IR (KBr, cm^{-1}): 3049, 2925, 1629, 1627, 1572, 1556, 1497, 1463, 1447, 1405; HRMS (ESI-TOF) calcd for

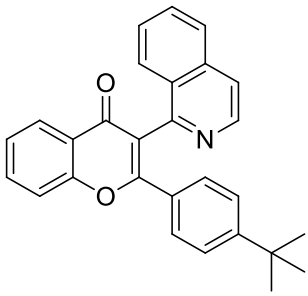
$C_{24}H_{16}NO_2^+$ ([M+H]$^+$): 350.1176, found: 350.1174.

2-(4-Ethylphenyl)-3-(isoquinolin-1-yl)-4*H*-chromen-4-one (3ca):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (61.1 mg, 81% yield); mp 193.4–194.9 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.53 (d, *J* = 5.7 Hz, 1H), 8.29 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.87 (dd, *J* = 12.0, 8.4 Hz, 2H), 7.80–7.71 (m, 1H), 7.63 (dd, *J* = 11.3, 6.9 Hz, 3H), 7.47 (dt, *J* = 10.5, 7.6 Hz, 2H), 7.25 (d, *J* = 7.8 Hz, 2H), 6.97 (d, *J* = 8.2 Hz, 2H), 2.52 (q, *J* = 7.6 Hz, 2H), 1.12 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.4, 163.4, 156.3, 155.0, 147.1, 142.6, 136.3, 133.9, 130.2, 130.1, 128.8, 128.7, 127.8, 127.7, 127.1, 126.6, 126.3, 125.3, 123.6, 121.3, 120.8, 118.1, 28.6, 15.0; IR (KBr, cm^{-1}): 3060, 2963, 2925, 1974, 1637, 1621, 1610, 1576, 1557, 1499, 1466, 1400; HRMS (ESI-TOF) calcd for $C_{26}H_{20}NO_2^+$ ([M+H]$^+$): 378.1489, found: 378.1487.

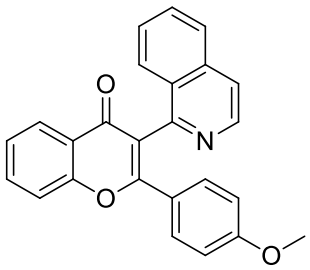
2-(4-Tert-butylphenyl)-3-(isoquinolin-1-yl)-4*H*-chromen-4-one (3da):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); yellow solid (76.6 mg, 85% yield); mp 199.2–200.5 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.54 (d, *J* = 5.7 Hz, 1H), 8.28 (d, *J* = 7.9 Hz, 1H), 7.87 (t, *J* = 8.4 Hz, 2H), 7.74 (dd, *J* = 11.3, 4.2 Hz, 1H), 7.64 (dd, *J* = 14.9, 7.0 Hz, 3H), 7.56–7.38 (m, 2H), 7.29–7.25 (m, 2H), 7.16 (d, *J* = 8.6 Hz, 2H), 1.19 (d, *J* = 4.6 Hz, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 177.5, 163.1, 156.3, 155.0, 154.0, 142.7, 136.3, 133.9, 130.2, 129.8, 128.9, 128.5, 127.7, 127.1, 126.6, 126.3, 125.3, 125.2, 123.6, 121.3, 120.9, 118.1, 34.8, 31.0; IR (KBr, cm^{-1}): 3054, 2959, 1638, 1623, 1574, 1558, 1501, 1465, 1402; HRMS (ESI-TOF) calcd for $C_{28}H_{24}NO_2^+$

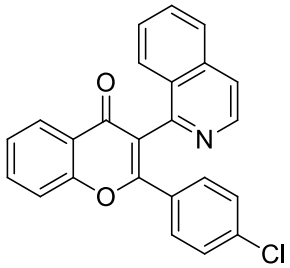
([M+H]$^+$): 406.1802, found: 406.1800.

3-(Isoquinolin-1-yl)-2-(4-methoxyphenyl)-4*H*-chromen-4-one (3ea):



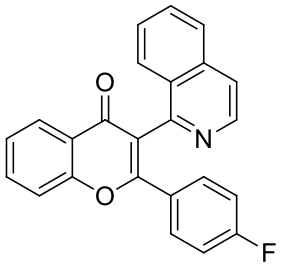
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (60.7 mg, 80% yield); mp 175.2–176.7 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.55 (d, *J* = 5.7 Hz, 1H), 8.31–8.22 (m, 1H), 7.86 (t, *J* = 8.6 Hz, 2H), 7.74 (t, *J* = 7.1 Hz, 1H), 7.63 (dd, *J* = 14.5, 7.0 Hz, 3H), 7.47 (dt, *J* = 12.0, 7.8 Hz, 2H), 7.27 (d, *J* = 7.2 Hz, 2H), 6.64 (d, *J* = 8.8 Hz, 2H), 3.69 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.4, 163.0, 161.2, 156.3, 155.2, 142.7, 136.3, 133.9, 130.4, 130.3, 128.8, 127.7, 127.1, 126.6, 126.3, 125.3, 124.9, 123.6, 120.8, 120.7, 118.0, 113.7, 55.2; IR (KBr, cm^{-1}): 3046, 3010, 2935, 2839, 1649, 1620, 1603, 1579, 1570, 1555, 1512, 1496, 1465, 1416; HRMS (ESI-TOF) calcd for $C_{25}H_{18}NO_3^+$ ([M+H]$^+$): 380.1281, found: 380.1280.

2-(4-Chlorophenyl)-3-(isoquinolin-1-yl)-4*H*-chromen-4-one (3fa):



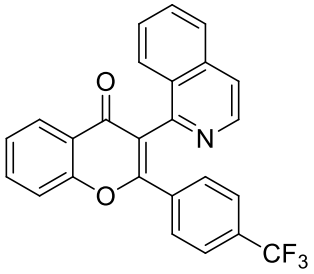
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (62.9 mg, 82% yield); mp 206.5–207.5 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.53 (d, *J* = 5.7 Hz, 1H), 8.34–8.21 (m, 1H), 7.86 (d, *J* = 8.3 Hz, 2H), 7.81–7.71 (m, 1H), 7.64 (dd, *J* = 16.0, 6.9 Hz, 3H), 7.56–7.38 (m, 2H), 7.26 (t, *J* = 4.3 Hz, 2H), 7.12 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.2, 162.0, 156.2, 154.3, 142.6, 136.7, 136.3, 134.2, 131.2, 130.4, 130.0, 128.7, 128.6, 127.9, 127.2, 126.4, 125.6, 123.5, 121.9, 121.1, 118.1; IR (KBr, cm^{-1}): 3056, 3011, 1651, 1640, 1622, 1585, 1576, 1556, 1492, 1465, 1402; HRMS (ESI-TOF) calcd for $C_{24}H_{15}ClNO_2^+$ ([M+H]$^+$): 384.0786, found: 384.0784.

2-(4-Fluorophenyl)-3-(isoquinolin-1-yl)-4*H*-chromen-4-one (3ga):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (69.1 mg, 94% yield); mp 182.7–184.6 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.53 (d, J = 5.7 Hz, 1H), 8.30 (dd, J = 7.9, 1.0 Hz, 1H), 7.86 (d, J = 8.8 Hz, 2H), 7.78 (dd, J = 11.3, 4.2 Hz, 1H), 7.64 (dd, J = 14.6, 7.0 Hz, 3H), 7.49 (dd, J = 15.6, 7.8 Hz, 2H), 7.33 (dd, J = 8.8, 5.3 Hz, 2H), 6.84 (t, J = 8.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.3, 163.7 (d, $J_{C\text{-}F}$ = 252.5 Hz), 162.2, 156.2, 154.5, 142.6, 136.3, 134.1, 131.0, 130.9, 130.3, 128.9 (d, $J_{C\text{-}F}$ = 3.4 Hz), 128.7, 127.8, 127.2, 126.4 (d, $J_{C\text{-}F}$ = 3.8 Hz), 125.5, 123.5, 121.6, 121.0, 118.1, 115.5 (d, $J_{C\text{-}F}$ = 21.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -108.6; IR (KBr, cm^{-1}): 3050, 2925, 1927, 1637, 1625, 1606, 1574, 1555, 1510, 1466, 1405; HRMS (ESI-TOF) calcd for $C_{24}H_{15}FNO_2^+$ ($[M+H]^+$): 368.1081, found: 368.1080.

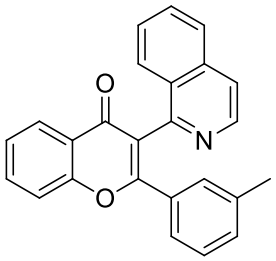
3-(Isoquinolin-1-yl)-2-(4-(trifluoromethyl)phenyl)-4*H*-chromen-4-one (3ha):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (66.8 mg, 80% yield); mp 201.9–203.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.51 (d, J = 5.7 Hz, 1H), 8.31 (d, J = 7.9 Hz, 1H), 7.87 (d, J = 8.6 Hz, 2H), 7.79 (t, J = 7.8 Hz, 1H), 7.72–7.58 (m, 3H), 7.57–7.37 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.2, 161.6, 156.3, 154.0, 142.6, 136.3, 136.2, 134.4, 132.0 (q, $J_{C\text{-}F}$ = 32.8 Hz), 130.5, 129.1, 128.8, 128.0, 127.3, 126.4, 126.3, 125.7, 125.2 (q, $J_{C\text{-}F}$ = 3.7 Hz), 123.5, 123.5 (q, $J_{C\text{-}F}$ = 271.1 Hz), 122.6, 121.2, 118.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -63.1; IR (KBr, cm^{-1}): 3060, 2933, 1645, 1615, 1583, 1568, 1560, 1513, 1500, 1466, 1410; HRMS (ESI-TOF)

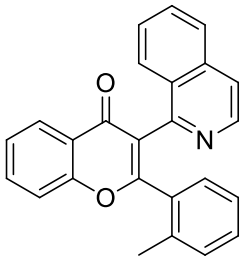
calcd for $C_{25}H_{15}F_3NO_2^+$ ([M+H]$^+$): 418.1049, found: 418.1048.

3-(Isoquinolin-1-yl)-2-m-tolyl-4*H*-chromen-4-one (3ia):



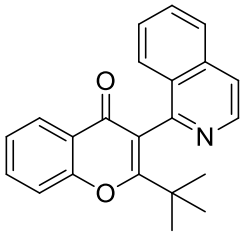
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (64.7 mg, 89% yield); mp 153.3–155.1 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.52 (d, *J* = 5.7 Hz, 1H), 8.35–8.25 (m, 1H), 7.84 (dt, *J* = 17.0, 8.6 Hz, 2H), 7.79 (s, 1H), 7.64 (dd, *J* = 9.5, 4.6 Hz, 3H), 7.48 (q, *J* = 7.6 Hz, 2H), 7.26 (s, 1H), 7.11–6.92 (m, 3H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.4, 163.5, 156.4, 154.9, 142.5, 138.0, 136.2, 134.0, 132.6, 131.3, 130.2, 129.3, 128.8, 128.0, 127.7, 127.1, 126.6, 126.3, 125.9, 125.4, 123.6, 121.7, 120.8, 118.1, 21.3; IR (KBr, cm^{-1}): 3055, 2920, 1952, 1638, 1625, 1611, 1585, 1571, 1560, 1500, 1462, 1400; HRMS (ESI-TOF) calcd for $C_{25}H_{18}NO_2^+$ ([M+H]$^+$): 364.1332, found: 364.1330.

3-(Isoquinolin-1-yl)-2-(o-tolyl)-4*H*-chromen-4-one (3ja):



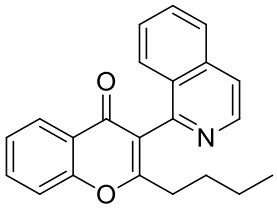
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); yellow solid (38.4 mg, 53% yield); mp 237.2–238.3 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.50 (d, *J* = 5.7 Hz, 1H), 8.39 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.93 (d, *J* = 8.5 Hz, 1H), 7.85–7.76 (m, 2H), 7.70–7.46 (m, 5H), 7.24–7.13 (m, 3H), 6.95–6.84 (m, 1H), 2.48 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 177.2, 165.3, 156.4, 154.1, 142.4, 137.0, 136.1, 134.1, 132.3, 130.3, 130.0, 130.0, 129.6, 128.5, 127.3, 127.1, 126.4, 125.5, 125.1, 123.9, 123.4, 120.6, 118.1, 20.1; IR (KBr, cm^{-1}): 3052, 2926, 2861, 1636, 1464, 1402; HRMS (ESI-TOF) calcd for $C_{25}H_{18}NO_2^+$ ([M+H]$^+$): 364.1332, found: 364.1330.

2-Tert-butyl-3-(isoquinolin-1-yl)-4*H*-chromen-4-one (3ka):



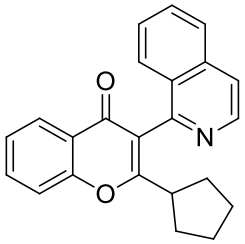
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); yellow solid (19.1 mg, 29% yield); mp 122.7–124.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.59 (d, *J* = 5.7 Hz, 1H), 8.17 (d, *J* = 7.3 Hz, 1H), 7.86 (d, *J* = 8.2 Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.74–7.68 (m, 2H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.51 (dd, *J* = 14.2, 7.8 Hz, 2H), 7.39 (t, *J* = 7.5 Hz, 1H), 1.11 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 178.4, 172.3, 156.1, 156.0, 142.0, 136.0, 133.7, 130.1, 129.5, 127.6, 127.1, 126.7, 126.0, 125.0, 122.9, 120.9, 120.8, 117.7, 39.2, 29.0; IR (KBr, cm^{-1}): 3057, 2959, 2867, 1648, 1638, 1618, 1604, 1583, 1571, 1556, 1495, 1485, 1466, 1401; HRMS (ESI-TOF) calcd for $C_{22}H_{20}NO_2^+$ ($[M+H]^+$): 330.1489, found: 330.1487.

2-Butyl-3-(isoquinolin-1-yl)-4*H*-chromen-4-one (3la):



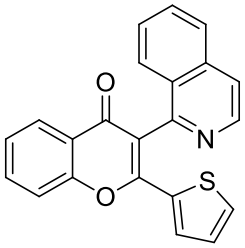
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); yellow oil (18.7 mg, 28% yield); ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.63 (d, *J* = 5.7 Hz, 1H), 8.27–8.23 (m, 1H), 7.89 (d, *J* = 8.3 Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.76–7.64 (m, 3H), 7.52 (t, *J* = 8.3 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 1H), 2.44 (ddd, *J* = 14.3, 9.3, 5.1 Hz, 2H), 1.77–1.46 (m, 2H), 1.30–1.12 (m, 2H), 0.71 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 176.8, 168.8, 156.3, 154.6, 142.6, 136.4, 133.6, 130.3, 128.5, 127.6, 127.1, 126.8, 126.3, 125.1, 123.7, 121.9, 121.0, 117.9, 32.5, 29.1, 22.3, 13.6; IR (KBr, cm^{-1}): 3054, 2957, 2866, 1636, 1568, 1463; HRMS (ESI-TOF) calcd for $C_{22}H_{20}NO_2^+$ ($[M+H]^+$): 330.1489, found: 330.1488.

2-Cyclopentyl-3-(isoquinolin-1-yl)-4*H*-chromen-4-one (3ma):



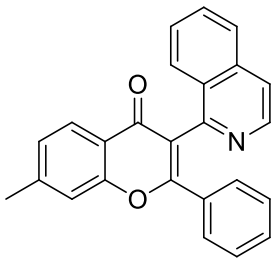
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); yellow oil (16.4 mg, 24% yield); ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.64 (d, *J* = 5.7 Hz, 1H), 8.24 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.77–7.63 (m, 3H), 7.51 (dd, *J* = 10.5, 4.6 Hz, 2H), 7.47–7.38 (m, 1H), 2.68 (p, *J* = 8.4 Hz, 1H), 2.03 (dtd, *J* = 11.9, 8.1, 4.1 Hz, 2H), 1.83 (dddd, *J* = 15.5, 12.2, 8.5, 4.0 Hz, 3H), 1.63–1.38 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 176.8, 170.8, 156.3, 154.9, 142.6, 136.4, 133.6, 130.3, 128.6, 127.6, 127.1, 126.8, 126.3, 125.0, 123.7, 121.1, 120.9, 117.8, 42.4, 31.4, 26.4; IR (KBr, cm^{-1}): 3055, 2954, 2929, 2864, 1635, 1570, 1464, 1403; HRMS (ESI-TOF) calcd for $C_{23}H_{20}NO_2^+$ ($[M+H]^+$): 342.1489, found: 342.1487.

3-(Isoquinolin-1-yl)-2-(thiophen-2-yl)-4*H*-chromen-4-one (3oa):



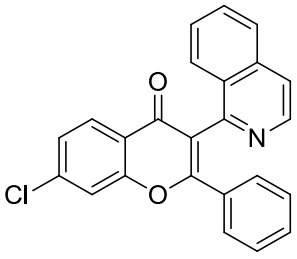
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (59.7 mg, 84% yield); mp 213.6–214.9 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.70 (d, *J* = 5.7 Hz, 1H), 8.26 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.89 (dd, *J* = 15.2, 8.4 Hz, 2H), 7.82–7.58 (m, 4H), 7.53–7.41 (m, 2H), 7.31 (d, *J* = 5.0 Hz, 1H), 7.02 (d, *J* = 2.8 Hz, 1H), 6.90–6.81 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 177.2, 157.0, 156.0, 154.2, 143.2, 136.7, 134.3, 134.0, 131.4, 131.2, 130.6, 128.8, 127.9, 127.5, 127.2, 126.2, 126.0, 125.3, 123.5, 121.6, 119.0, 117.9; IR (KBr, cm^{-1}): 3095, 3074, 1629, 1618, 1596, 1552, 1521, 1497, 1467, 1425, 1404; HRMS (ESI-TOF) calcd for $C_{22}H_{14}NO_2S^+$ $(M+H)^+$ 356.0740, found 356.0738.

3-(Isoquinolin-1-yl)-7-methyl-2-phenyl-4*H*-chromen-4-one (3pa):



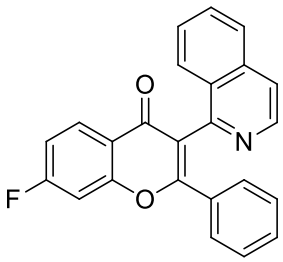
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (62.5 mg, 86% yield); mp 166.4–167.8 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.50 (d, *J* = 5.7 Hz, 1H), 8.17 (d, *J* = 8.1 Hz, 1H), 7.85 (dd, *J* = 15.4, 8.3 Hz, 2H), 7.63 (t, *J* = 5.0 Hz, 2H), 7.47 (dd, *J* = 13.8, 6.5 Hz, 1H), 7.42 (s, 1H), 7.29 (dd, *J* = 11.0, 6.5 Hz, 3H), 7.22 (d, *J* = 7.2 Hz, 1H), 7.12 (t, *J* = 7.5 Hz, 2H), 2.54 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.3, 163.0, 156.5, 154.9, 145.4, 142.6, 136.3, 132.9, 130.4, 130.2, 128.8, 128.7, 128.2, 127.6, 127.1, 126.9, 126.6, 126.1, 121.6, 121.4, 120.8, 117.8, 22.0; IR (KBr, cm^{-1}): 3057, 1651, 1628, 1583, 1567, 1553, 1494, 1459, 1448, 1421; HRMS (ESI-TOF) calcd for $C_{25}H_{18}NO_2^+$ ($[M+H]^+$): 364.1332, found: 364.1331.

7-Chloro-3-(isoquinolin-1-yl)-2-phenyl-4*H*-chromen-4-one (3qa):



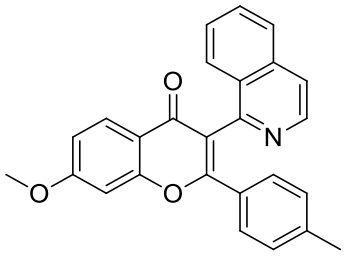
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (62.9 mg, 82% yield); mp 176.2–178.4 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.50 (t, *J* = 8.8 Hz, 1H), 8.23 (d, *J* = 8.5 Hz, 1H), 7.85 (d, *J* = 8.7 Hz, 2H), 7.69–7.61 (m, 3H), 7.55–7.40 (m, 2H), 7.27 (q, *J* = 7.5 Hz, 3H), 7.14 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 176.6, 163.4, 156.4, 154.3, 142.6, 140.0, 136.3, 132.4, 130.7, 130.3, 128.7, 128.6, 128.3, 127.8, 127.7, 127.2, 126.3, 126.3, 122.1, 122.0, 121.0, 118.2; IR (KBr, cm^{-1}): 3049, 2924, 1918, 1630, 1623, 1609, 1557, 1496, 1447, 1430; HRMS (ESI-TOF) calcd for $C_{24}H_{15}ClNO_2^+$ ($[M+H]^+$): 384.0786, found: 384.0784.

7-Fluoro-3-(isoquinolin-1-yl)-2-phenyl-4*H*-chromen-4-one (3ra):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); yellow solid (78.6 mg, 93% yield); mp 177.7–179.2 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.51 (d, *J* = 5.7 Hz, 1H), 8.31 (dd, *J* = 8.6, 6.5 Hz, 1H), 7.88–7.79 (m, 2H), 7.63 (t, *J* = 5.2 Hz, 2H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.29 (t, *J* = 7.9 Hz, 3H), 7.27 (s, 1H), 7.15 (dd, *J* = 16.2, 8.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 176.5, 165.9 (d, $J_{C\text{-}F}$ = 255.3 Hz, 1H), 163.5, 157.3 (d, $J_{C\text{-}F}$ = 13.4 Hz), 154.3, 142.6, 136.3, 132.4, 130.6, 130.3, 128.9 (d, $J_{C\text{-}F}$ = 10.7 Hz), 128.7, 128.6, 128.3, 127.8, 127.2, 126.4, 121.8, 121.0, 120.4 (d, $J_{C\text{-}F}$ = 2.2 Hz), 114.2 (d, $J_{C\text{-}F}$ = 22.8 Hz), 104.8 (d, $J_{C\text{-}F}$ = 25.3 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -102.5; IR (KBr, cm^{-1}): 3057, 3042, 1911, 1853, 1642, 1627, 1616, 1583, 1576, 1556, 1493, 1466, 1446, 1402; HRMS (ESI-TOF) calcd for $C_{24}H_{15}FNO_2^+$ ($[M+H]^+$): 368.1081, found: 368.1080.

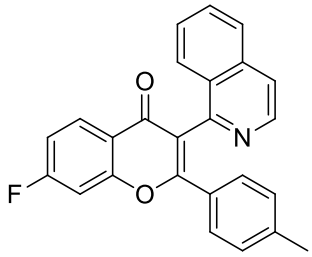
3-(Isoquinolin-1-yl)-7-methoxy-2-p-tolyl-4*H*-chromen-4-one (3sa):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); yellow solid (45.6 mg, 58% yield); mp 201.1–203.1 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.52 (d, *J* = 5.7 Hz, 1H), 8.18 (d, *J* = 9.0 Hz, 1H), 7.86 (dd, *J* = 15.0, 8.3 Hz, 2H), 7.73–7.60 (m, 2H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.20 (d, *J* = 8.2 Hz, 2H), 7.08–6.98 (m, 2H), 6.93 (d, *J* = 8.1 Hz, 2H), 3.95 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 164.3, 162.9, 158.1, 155.1, 142.6, 140.7, 136.3, 130.2, 129.9, 128.9, 128.9, 128.5, 127.7, 127.6, 127.1, 126.7, 121.1, 120.8, 117.4, 114.7, 100.2, 55.9, 21.4; IR (KBr, cm^{-1}): 3671, 3059, 2965, 1626, 1619,

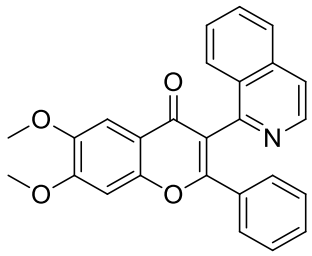
1598, 1560, 1499, 1438; HRMS (ESI-TOF) calcd for $C_{26}H_{20}NO_3^+$ ([M+H]$^+$): 394.1438, found: 394.1436.

7-Fluoro-3-(isoquinolin-1-yl)-2-p-tolyl-4*H*-chromen-4-one (3ta):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); yellow solid (65.6 mg, 86% yield); mp 215.5–216.7 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.53 (d, J = 5.7 Hz, 1H), 8.29 (dd, J = 8.7, 6.5 Hz, 1H), 7.85 (dd, J = 7.8, 5.1 Hz, 2H), 7.64 (t, J = 6.4 Hz, 2H), 7.49 (t, J = 7.6 Hz, 1H), 7.36–7.26 (m, 1H), 7.18 (t, J = 7.4 Hz, 3H), 6.94 (d, J = 8.0 Hz, 2H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 175.5, 164.8 (d, $J_{C\text{-}F}$ = 255.1 Hz), 163.5, 162.6, 156.2 (d, $J_{C\text{-}F}$ = 13.4 Hz), 156.1, 153.5, 141.5, 140.1, 135.2, 129.2, 128.4, 127.9, 127.8 (d, $J_{C\text{-}F}$ = 10.6 Hz), 127.7, 127.5, 126.7, 126.1, 125.4, 120.2, 119.9, 119.4 (d, $J_{C\text{-}F}$ = 2.3 Hz), 113.1 (d, $J_{C\text{-}F}$ = 22.8 Hz), 103.7 (d, $J_{C\text{-}F}$ = 25.3 Hz), 20.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -102.7; IR (KBr, cm^{-1}): 3050, 2925, 2854, 1654, 1619, 1582, 1568, 1557, 1492, 1439; HRMS (ESI-TOF) calcd for $C_{25}H_{17}FNO_2^+$ ([M+H]$^+$): 382.1238, found: 382.1236.

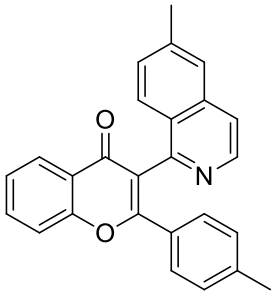
3-(Isoquinolin-1-yl)-6,7-dimethoxy-2-phenyl-4*H*-chromen-4-one (3ua):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (63.9 mg, 78% yield); mp 236.5–238.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.48 (d, J = 5.7 Hz, 1H), 7.88 (d, J = 8.4 Hz, 1H), 7.80 (d, J = 8.2 Hz, 1H), 7.67–7.56 (m, 3H), 7.47 (t, J = 7.6 Hz, 1H), 7.28 (d, J = 7.8 Hz, 2H), 7.20 (t, J = 7.3 Hz, 1H), 7.10 (t, J = 7.7 Hz, 2H), 7.01 (d, J = 12.6 Hz, 1H), 4.00 (s, 3H), 3.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm):

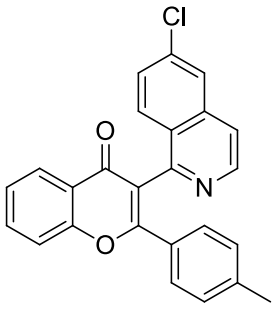
176.4, 162.6, 155.0, 154.7, 152.4, 147.9, 142.5, 136.2, 132.9, 130.2, 130.2, 128.9, 128.6, 128.1, 127.7, 127.1, 126.6, 121.1, 120.8, 116.9, 104.9, 99.8, 56.5, 56.4; IR (KBr, cm^{-1}): 3012, 2928, 1736, 1627, 1608, 1585, 1560, 1508, 1476, 1455,1431, 1402; HRMS (ESI-TOF) calcd for $C_{26}H_{20}NO_4^+$ ($[M+H]^+$): 410.1387, found: 410.1385

3-(6-Methylisoquinolin-1-yl)-2-p-tolyl-4*H*-chromen-4-one (3ab):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); yellow solid (63.2 mg, 87% yield); mp 166.2–167.7 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.46 (d, *J* = 5.7 Hz, 1H), 8.27 (d, *J* = 7.6 Hz, 1H), 7.75 (d, *J* = 8.6 Hz, 1H), 7.68 (t, *J* = 7.7 Hz, 1H), 7.57 (d, *J* = 11.8 Hz, 2H), 7.51 (d, *J* = 5.7 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.28 (d, *J* = 8.5 Hz, 1H), 7.25–7.16 (m, 2H), 6.91 (d, *J* = 8.0 Hz, 2H), 2.45 (s, 3H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.4, 163.3, 156.3, 154.5, 142.7, 140.9, 140.6, 136.6, 133.9, 130.0, 129.9, 129.0, 128.6, 127.3, 126.4, 126.2, 126.0, 125.3, 123.6, 121.3, 120.4, 118.1, 21.9, 21.4; IR (KBr, cm^{-1}): 3044, 2921, 1635, 1617, 1575, 1563, 1510, 1496, 1461, 1407; HRMS (ESI-TOF) calcd for $C_{26}H_{20}NO_2^+$ ($[M+H]^+$): 378.1489, found: 378.1487.

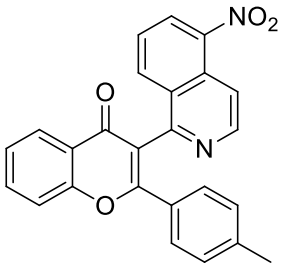
3-(6-Chloroisoquinolin-1-yl)-2-p-tolyl-4*H*-chromen-4-one (3ac):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (62.9 mg, 79% yield); mp 220.5–221.6 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.55 (d, *J* = 5.7 Hz, 1H), 8.28 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.82 (d, *J* = 8.9 Hz, 2H), 7.79–7.69 (m, 1H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.56 (d, *J* = 5.7 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.41 (dd, *J* = 8.9, 2.0

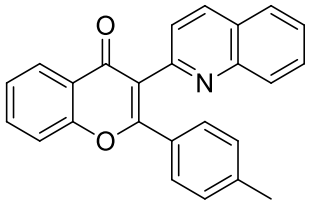
Hz, 1H), 7.20 (d, J = 8.2 Hz, 2H), 6.96 (d, J = 8.1 Hz, 2H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.3, 163.6, 156.3, 155.1, 143.8, 141.1, 137.1, 136.4, 134.1, 129.7, 129.1, 128.7, 128.6, 128.5, 127.0, 126.3, 125.9, 125.4, 123.5, 120.9, 119.9, 118.1, 21.4; IR (KBr, cm^{-1}): 3066, 3005, 2918, 1636, 1620, 1567, 1554, 1510, 1485, 1465, 1402; HRMS (ESI-TOF) calcd for $C_{25}H_{17}ClNO_2^+$ ([M+H]$^+$): 398.0942, found: 398.0942.

3-(5-Nitroisoquinolin-1-yl)-2-p-tolyl-4*H*-chromen-4-one (3ad):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); yellow solid (68.6 mg, 84% yield); mp 234.2–236.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.73 (d, J = 6.2 Hz, 1H), 8.45 (t, J = 6.6 Hz, 2H), 8.26 (d, J = 8.2 Hz, 2H), 7.76 (t, J = 7.7 Hz, 1H), 7.66–7.54 (m, 2H), 7.46 (t, J = 7.5 Hz, 1H), 7.18 (d, J = 8.1 Hz, 2H), 6.98 (d, J = 8.0 Hz, 2H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.2, 164.0, 156.3, 156.1, 145.9, 145.3, 141.5, 134.3, 133.9, 129.4, 129.2, 129.2, 128.8, 128.6, 128.3, 126.2, 126.1, 125.6, 123.4, 120.7, 118.2, 115.8, 21.4; IR (KBr, cm^{-1}): 3093, 3066, 3035, 2857, 1640, 1616, 1584, 1565, 1556, 1524, 1493, 1462, 1412; HRMS (ESI-TOF) calcd for $C_{25}H_{17}N_2O_4^+$ ([M+H]$^+$): 409.1183, found: 409.1182.

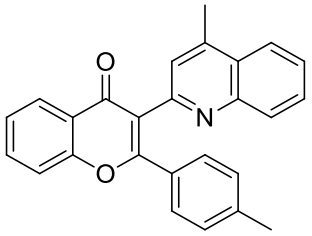
3-(Quinolin-2-yl)-2-p-tolyl-4*H*-chromen-4-one (3ae):



Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); yellow solid (43.6 mg, 60% yield); mp 161.3–163.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.30 (dd, J = 7.9, 1.2 Hz, 1H), 8.15 (d, J = 8.4 Hz, 1H), 7.99 (d, J = 8.4 Hz, 1H), 7.82 (d, J = 8.0 Hz, 1H), 7.75–7.69 (m, 1H), 7.67 (t, J = 7.7 Hz, 1H), 7.55 (dd, J = 14.7, 7.7 Hz, 2H), 7.45 (dd, J = 14.9, 7.9 Hz, 2H), 7.30 (t, J = 9.1 Hz, 2H), 7.00 (d, J = 8.1 Hz, 2H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.4, 163.3, 156.2, 154.0, 148.2, 140.8, 136.2, 133.8,

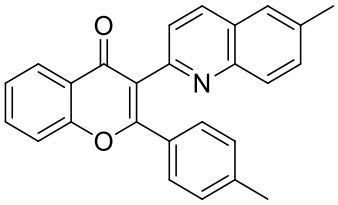
129.9, 129.6, 129.3, 129.3, 128.9, 127.6, 127.2, 126.7, 126.3, 125.2, 124.3, 123.8, 122.8, 118.0, 21.4; IR (KBr, cm^{-1}): 3039, 2924, 1642, 1611, 1599, 1553, 1501, 1465, 1424, 1411; HRMS (ESI-TOF) calcd for $C_{25}H_{18}NO_2^+$ ($[M+H]^+$): 364.1332, found: 364.1331.

3-(4-Methylquinolin-2-yl)-2-p-tolyl-4*H*-chromen-4-one (3af):



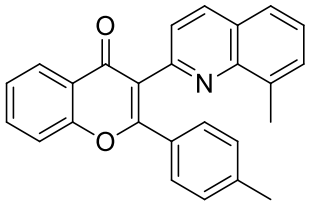
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); yellow solid (50.6 mg, 67% yield); mp 213.8–215.5 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.29 (d, *J* = 7.9 Hz, 0H), 8.05–7.92 (m, 1H), 7.75–7.60 (m, 1H), 7.59–7.49 (m, 1H), 7.42 (t, *J* = 7.5 Hz, 0H), 7.34 (d, *J* = 8.9 Hz, 1H), 6.99 (d, *J* = 8.0 Hz, 1H), 2.69 (s, 1H), 2.24 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.6, 163.2, 156.1, 153.6, 147.9, 144.5, 140.7, 133.8, 130.1, 130.0, 129.3, 129.0, 128.9, 127.4, 126.5, 126.2, 125.2, 124.8, 123.8, 123.7, 122.8, 118.0, 21.4, 18.9; IR (KBr, cm^{-1}): 2923, 1939, 1822, 1631, 1598, 1561, 1503, 1455, 1407; HRMS (ESI-TOF) calcd for $C_{26}H_{20}NO_2^+$ ($[M+H]^+$): 378.1489, found: 378.1487.

3-(6-Methylquinolin-2-yl)-2-p-tolyl-4*H*-chromen-4-one (3ag):



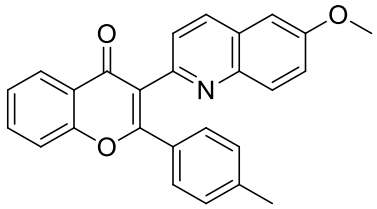
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (67.2 mg, 89% yield); mp 172.8–174.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.29 (d, *J* = 7.7 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.6 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.63–7.53 (m, 2H), 7.49 (d, *J* = 8.6 Hz, 1H), 7.43 (dd, *J* = 7.8, 5.2 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 6.99 (d, *J* = 8.0 Hz, 2H), 2.53 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ (ppm): 176.9, 162.8, 156.1, 153.4, 146.6, 141.0, 136.8, 135.8, 135.0, 132.2, 130.1, 129.4, 129.3, 129.1, 127.2, 127.0, 126.1, 125.7, 124.9, 123.4, 123.1, 119.0, 21.6, 21.3; IR (KBr, cm^{-1}): 2962, 2924, 1641, 1618, 1602, 1559, 1494, 1464; HRMS (ESI-TOF) calcd for $C_{26}H_{20}NO_2^+$ ($[M+H]^+$): 378.1489, found: 378.1487.

3-(8-Methylquinolin-2-yl)-2-p-tolyl-4*H*-chromen-4-one (3ah):



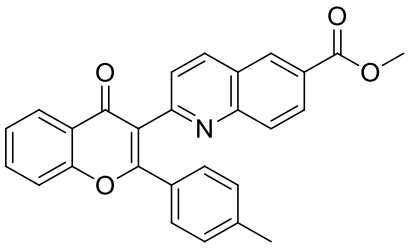
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); white solid (58.1 mg, 77% yield); mp 166.0–167.8 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.32 (d, *J* = 7.8 Hz, 1H), 8.13 (d, *J* = 8.4 Hz, 1H), 7.77–7.67 (m, 1H), 7.67–7.60 (m, 2H), 7.56 (d, *J* = 8.3 Hz, 1H), 7.41 (dt, *J* = 15.0, 7.3 Hz, 3H), 7.25 (t, *J* = 6.7 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 177.5, 164.3, 156.2, 152.3, 147.1, 140.4, 137.5, 136.0, 133.8, 130.8, 129.3, 129.2, 128.7, 127.2, 126.3, 126.2, 125.5, 125.2, 124.1, 124.0, 123.1, 118.1, 21.4, 17.8; IR (KBr, cm^{-1}): 2924, 1639, 1615, 1561, 1510, 1498, 1465, 1409; HRMS (ESI-TOF) calcd for $C_{26}H_{20}NO_2^+$ ($[M+H]^+$): 378.1489, found: 378.1487.

3-(6-Methoxyquinolin-2-yl)-2-p-tolyl-4*H*-chromen-4-one (3ai):



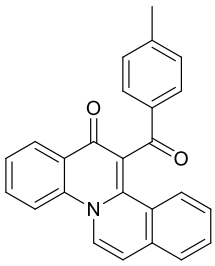
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); ywllow solid (52.7 mg, 67% yield); mp 151.2–152.9 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.34–8.24 (m, 1H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.88 (d, *J* = 9.2 Hz, 1H), 7.73–7.64 (m, 1H), 7.54 (d, *J* = 8.3 Hz, 1H), 7.40 (dd, *J* = 7.8, 4.3 Hz, 2H), 7.30 (dd, *J* = 7.3, 2.8 Hz, 2H), 7.26 (s, 1H), 7.06 (d, *J* = 2.5 Hz, 1H), 6.98 (d, *J* = 8.1 Hz, 2H), 3.89 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 177.5, 163.2, 158.0, 156.1, 151.2, 144.3, 140.7, 135.1, 133.8, 130.9, 130.0, 129.3, 128.9, 128.2, 126.2, 125.2, 124.5, 123.8, 122.7, 122.1, 118.0, 105.0, 55.5, 21.4; IR (KBr, cm^{-1}): 2963, 2842, 1637, 1620, 1575, 1563, 1499, 1467, 1442, 1405; HRMS (ESI-TOF) calcd for $C_{26}H_{20}NO_3^+$ ($[M+H]^+$): 394.1438, found: 394.1436.

Methyl 2-(4-oxo-2-p-tolyl-4*H*-chromen-3-yl)quinoline-6-carboxylate (3aj):



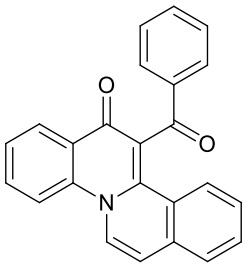
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1); yellow solid (55.6 mg, 66% yield); mp 196.6–198.2 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.48 (d, *J* = 1.3 Hz, 1H), 8.19 (dd, *J* = 7.9, 1.2 Hz, 1H), 8.14 (d, *J* = 8.6 Hz, 2H), 7.91 (d, *J* = 8.8 Hz, 1H), 7.65–7.57 (m, 1H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 1H), 7.22–7.17 (m, 1H), 6.89 (d, *J* = 8.1 Hz, 2H), 3.87 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 177.2, 166.6, 163.7, 156.5, 156.1, 150.0, 141.1, 137.3, 134.0, 130.7, 129.8, 129.7, 129.3, 129.0, 128.9, 128.2, 126.3, 126.2, 125.4, 125.2, 123.7, 122.5, 118.1, 52.4, 21.4; IR (KBr, cm^{-1}): 2925, 1720, 1638, 1619, 1577, 1466, 1423; HRMS (ESI-TOF) calcd for $C_{27}H_{20}NO_4^+$ ($[M+H]^+$): 422.1387, found: 422.1386.

12-(4-Methylbenzoyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4aa):



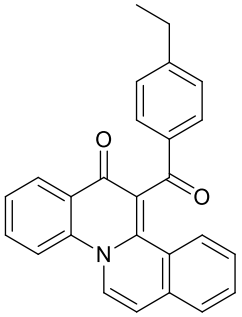
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (56.7 mg, 78% yield); mp 221.3–223.0 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.47 (d, *J* = 7.9 Hz, 1H), 8.13 (d, *J* = 7.7 Hz, 1H), 7.99 (d, *J* = 7.9 Hz, 2H), 7.94–7.86 (m, 2H), 7.75 (t, *J* = 7.7 Hz, 1H), 7.56–7.41 (m, 3H), 7.23 (dd, *J* = 13.4, 7.1 Hz, 3H), 6.83 (d, *J* = 7.7 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 198.2, 174.5, 144.4, 143.7, 138.1, 135.5, 132.6, 132.1, 131.5, 129.7, 129.5, 129.3, 127.8, 126.9, 126.6, 126.4, 126.0, 125.0, 124.4, 119.4, 116.4, 112.3, 21.8; IR (KBr, cm^{-1}): 3041, 1659, 1596, 1573, 1557, 1524, 1478, 1424, 1407; HRMS (ESI-TOF) calcd for $C_{25}H_{18}NO_2^+$ ($[M+H]^+$): 364.1332, found: 364.1333.

12-Benzoyl-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ba):



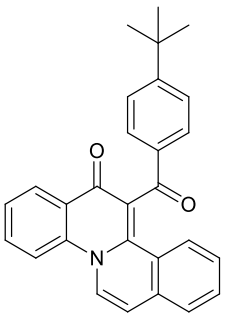
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (51.7 mg, 74% yield); mp 238.8–240.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.50–8.43 (m, 1H), 8.15 (d, *J* = 7.7 Hz, 1H), 8.10 (d, *J* = 7.3 Hz, 2H), 7.91 (t, *J* = 9.4 Hz, 1H), 7.88 (s, 1H), 7.75 (dd, *J* = 11.5, 4.2 Hz, 1H), 7.60–7.37 (m, 6H), 7.25–7.16 (m, 1H), 6.85 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 198.5, 174.5, 143.8, 138.1, 137.9, 133.5, 132.7, 132.1, 131.6, 129.4, 129.3, 129.0, 127.9, 126.9, 126.7, 126.4, 126.1, 125.1, 124.3, 119.2, 116.3, 112.4; IR (KBr, cm^{-1}): 1655, 1599, 1575, 1552, 1520, 1483, 1469, 1421; HRMS (ESI-TOF) calcd for $C_{24}H_{16}NO_2^+$ ($[M+H]^+$): 350.1176, found: 350.1175.

12-(4-Ethylbenzoyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ca):



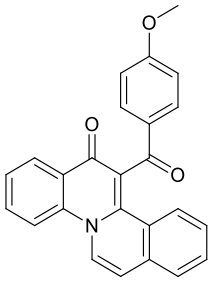
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (64.9 mg, 86% yield); mp 224.5–226.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.48 (d, *J* = 7.9 Hz, 1H), 8.14 (d, *J* = 7.7 Hz, 1H), 8.02 (d, *J* = 7.9 Hz, 2H), 7.91 (t, *J* = 7.6 Hz, 2H), 7.75 (d, *J* = 6.6 Hz, 1H), 7.58–7.42 (m, 3H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.23 (t, *J* = 7.5 Hz, 1H), 6.85 (dd, *J* = 7.2, 3.7 Hz, 1H), 2.70 (q, *J* = 7.6 Hz, 2H), 1.25 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 198.1, 174.5, 150.4, 143.7, 138.1, 135.7, 132.6, 132.1, 131.5, 129.6, 129.4, 128.5, 127.9, 126.9, 126.7, 126.4, 126.0, 125.1, 124.4, 119.5, 116.3, 112.3, 29.1, 15.0; IR (KBr, cm^{-1}): 2965, 2926, 1661, 1596, 1572, 1553, 1522, 1471, 1422; HRMS (ESI-TOF) calcd for $C_{26}H_{20}NO_2^+$ ($[M+H]^+$): 378.1489, found: 378.1488.

12-(4-Tert-butylbenzoyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4da):



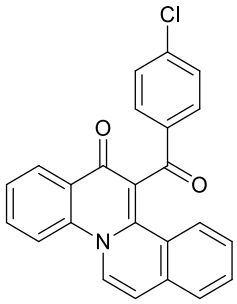
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (61.6 mg, 76% yield); mp 251.3–252.6 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.49 (dd, *J* = 7.9, 1.2 Hz, 1H), 8.16 (d, *J* = 7.7 Hz, 1H), 8.03 (d, *J* = 8.4 Hz, 2H), 7.93 (dd, *J* = 8.5, 5.5 Hz, 2H), 7.84–7.74 (m, 1H), 7.59–7.43 (m, 5H), 7.29–7.22 (m, 1H), 6.88 (d, *J* = 7.7 Hz, 1H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 198.1, 174.5, 157.1, 143.6, 138.1, 135.3, 132.6, 132.1, 131.4, 129.4, 129.3, 127.9, 126.9, 126.7, 126.4, 126.0, 126.0, 125.1, 124.4, 119.5, 116.3, 112.3, 35.2, 31.1; IR (KBr, cm^{-1}): 2959, 2868, 1665, 1651, 1604, 1593, 1573, 1554, 1521, 1485, 1473, 1422, 1408; HRMS (ESI-TOF) calcd for $C_{28}H_{24}NO_2^+$ ($[M+H]^+$): 406.1802, found: 406.1800.

12-(4-Methoxybenzoyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ea):



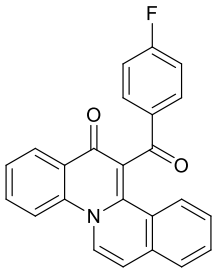
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (49.3 mg, 65% yield); mp 147.7–148.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.45 (dd, *J* = 8.0, 1.5 Hz, 1H), 8.12 (d, *J* = 7.8 Hz, 1H), 8.08–8.01 (m, 2H), 7.96–7.85 (m, 2H), 7.72 (ddd, *J* = 8.7, 7.1, 1.6 Hz, 1H), 7.51–7.37 (m, 3H), 7.20 (ddd, *J* = 8.5, 7.0, 1.6 Hz, 1H), 6.95–6.87 (m, 2H), 6.80 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 196.9, 174.4, 163.9, 143.6, 138.1, 132.6, 132.1, 131.8, 131.5, 131.1, 129.3, 127.8, 126.9, 126.7, 126.4, 126.0, 125.1, 124.5, 119.5, 116.3, 114.2, 112.3, 55.5; IR (KBr, cm^{-1}): 2927, 1662, 1596, 1569, 1552, 1523,1509, 1470, 1442; HRMS (ESI-TOF) calcd for $C_{25}H_{18}NO_3^+$ ($[M+H]^+$): 380.1281, found: 380.1280.

12-(4-Chlorobenzoyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4fa):



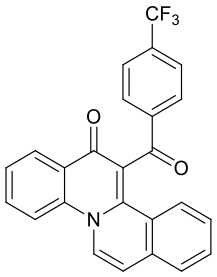
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (62.2 mg, 81% yield); mp 209.2–210.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.46 (dd, *J* = 7.9, 1.1 Hz, 1H), 8.16 (d, *J* = 7.7 Hz, 1H), 8.07–8.00 (m, 2H), 7.92 (d, *J* = 8.7 Hz, 1H), 7.81–7.72 (m, 2H), 7.58–7.46 (m, 3H), 7.45–7.40 (m, 2H), 7.24 (ddd, *J* = 8.5, 6.7, 1.8 Hz, 1H), 6.88 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 197.3, 174.4, 144.0, 139.8, 138.0, 136.4, 132.8, 132.2, 131.7, 130.8, 129.3, 129.2, 127.9, 126.8, 126.5, 126.2, 125.0, 124.1, 118.4, 116.4, 112.5; IR (KBr, cm^{-1}): 1664, 1595, 1571, 1553, 1520, 1470, 1421; HRMS (ESI-TOF) calcd for $C_{24}H_{15}ClNO_2^+$ ($[M+H]^+$): 384.0786, found: 384.0785.

12-(4-Fluorobenzoyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ga):



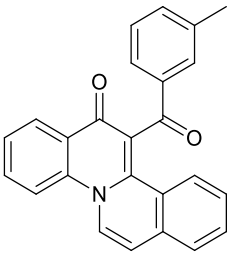
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (58.0 mg, 79% yield); mp 221.0–222.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.48 (dd, *J* = 7.9, 1.1 Hz, 1H), 8.17 (d, *J* = 7.7 Hz, 1H), 8.12 (dd, *J* = 8.6, 5.5 Hz, 2H), 7.93 (d, *J* = 8.7 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.82–7.73 (m, 1H), 7.59–7.47 (m, 3H), 7.29–7.21 (m, 1H), 7.12 (t, *J* = 8.6 Hz, 2H), 6.89 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 196.9, 174.4, 166.1 (d, $J_{C\text{-}F}$ = 255.1 Hz), 143.9, 138.1, 134.4 (d, $J_{C\text{-}F}$ = 2.8 Hz), 132.7, 132.1 (d, $J_{C\text{-}F}$ = 9.5 Hz), 132.0, 131.7, 129.2, 127.9, 126.9, 126.7, 126.5, 126.2, 125.1, 124.2, 118.8, 116.3, 116.1 (d, $J_{C\text{-}F}$ = 22.0 Hz), 112.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -104.9; IR (KBr, cm^{-1}): 1665, 1595, 1571, 1554, 1522, 1500, 1470, 1423, 1406; HRMS (ESI-TOF) calcd for $C_{24}H_{15}FNO_2^+$ ($[M+H]^+$): 368.1081, found: 368.1080.

12-(4-(Trifluoromethyl)benzoyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ha):



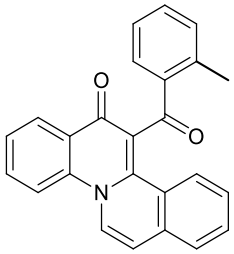
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (66.8 mg, 80% yield); mp 255.7–257.5 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.45 (dd, *J* = 7.9, 1.0 Hz, 1H), 8.20 (t, *J* = 7.3 Hz, 3H), 7.94 (d, *J* = 8.7 Hz, 1H), 7.82–7.76 (m, 1H), 7.74 (d, *J* = 8.3 Hz, 3H), 7.54 (q, *J* = 7.8 Hz, 3H), 7.30–7.19 (m, 1H), 6.91 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 197.6, 174.5, 144.5, 140.7, 138.1, 134.5 (q, $J_{C\text{-}F}$ = 32.7 Hz), 132.9, 132.2, 131.9, 129.6, 129.2, 128.0, 126.9, 126.6, 126.3, 126.1 (q, $J_{C\text{-}F}$ = 3.7 Hz), 125.0, 124.0, 123.7 (q, $J_{C\text{-}F}$ = 270.8 Hz), 118.1, 116.3, 112.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -63.0; IR (KBr, cm^{-1}): 1676, 1652, 1596, 1568, 1555, 1522, 1476, 1422, 1405; HRMS (ESI-TOF) calcd for $C_{25}H_{15}F_3NO_2^+$ ($[M+H]^+$): 418.1049, found: 418.1049.

12-(3-Methylbenzoyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ia):



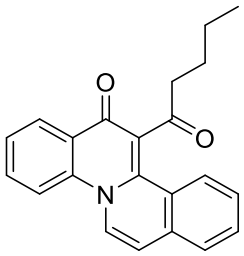
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (58.1 mg, 80% yield); mp 222.3–224.0 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.48 (d, *J* = 7.9 Hz, 1H), 8.15 (d, *J* = 7.6 Hz, 1H), 7.90 (dd, *J* = 11.4, 7.3 Hz, 4H), 7.82–7.67 (m, 1H), 7.52 (dd, *J* = 14.8, 7.0 Hz, 3H), 7.41–7.28 (m, 2H), 7.28–7.16 (m, 1H), 6.86 (d, *J* = 7.6 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 198.8, 174.5, 143.6, 138.7, 138.1, 138.0, 134.4, 132.6, 132.1, 131.5, 129.7, 129.3, 128.9, 127.8, 126.9, 126.7, 126.6, 126.4, 126.0, 125.1, 124.3, 119.4, 116.4, 112.3, 21.4; IR (KBr, cm^{-1}): 2925, 1664, 1595, 1550, 1520, 1470, 1442; HRMS (ESI-TOF) calcd for $C_{25}H_{18}NO_2^+$ ($[M+H]^+$): 364.1332, found: 364.1331.

12-(2-Methylbenzoyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ja):



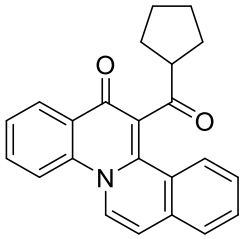
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (44.1 mg, 61% yield); mp 293.9–294.5 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.48 (d, *J* = 8.0 Hz, 1H), 8.16 (d, *J* = 7.7 Hz, 1H), 8.01 (d, *J* = 8.5 Hz, 1H), 7.93 (d, *J* = 8.8 Hz, 1H), 7.88–7.72 (m, 2H), 7.61–7.48 (m, 3H), 7.46–7.26 (m, 3H), 7.15 (t, *J* = 7.4 Hz, 1H), 6.89 (d, *J* = 7.7 Hz, 1H), 2.83 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3/CD_3OD$ = 12:1) δ (ppm): 200.1, 174.7, 143.8, 140.6, 138.1, 137.2, 132.8, 132.4, 132.4, 132.2, 131.7, 131.3, 129.4, 127.9, 126.9, 126.5, 126.5, 126.3, 126.0, 125.0, 124.3, 120.9, 116.4, 112.7, 21.9; IR (KBr, cm^{-1}): 2924, 1662, 1601, 1519, 1471, 1417; HRMS (ESI-TOF) calcd for $C_{25}H_{18}NO_2^+$ ($[M+H]^+$): 364.1332, found: 364.1331.

12-pentanoyl-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4la):



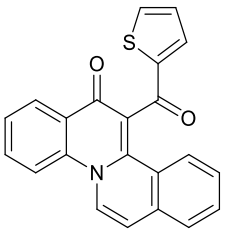
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (31.3 mg, 48% yield); mp 115.6–116.8 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.56 (dd, *J* = 8.0, 1.5 Hz, 1H), 8.14 (d, *J* = 7.7 Hz, 1H), 7.98 (d, *J* = 8.3 Hz, 1H), 7.92 (d, *J* = 8.6 Hz, 1H), 7.87–7.74 (m, 1H), 7.72–7.62 (m, 1H), 7.59 (dd, *J* = 9.0, 4.4 Hz, 2H), 7.53–7.43 (m, 1H), 6.91 (d, *J* = 7.6 Hz, 1H), 3.00–2.86 (m, 2H), 1.86 (dt, *J* = 15.1, 7.5 Hz, 2H), 1.52–1.35 (m, 2H), 0.96 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 208.1, 173.8, 142.2, 137.8, 132.6, 132.1, 131.7, 128.7, 127.9, 127.0, 126.6, 126.5, 126.0, 125.2, 124.4, 122.0, 116.2, 112.0, 44.8, 25.9, 22.3, 14.1; IR (KBr, cm^{-1}): 2945, 1694, 1600, 1562, 1519, 1472; HRMS (ESI-TOF) calcd for $C_{22}H_{20}NO_2^+$ ($[M+H]^+$): 330.1489, found: 330.1486.

12-(Cyclopentanecarbonyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ma):



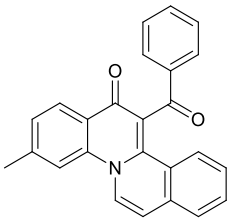
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (12.2 mg, 18% yield); mp 178.0–179.9 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.55 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.12 (d, *J* = 7.6 Hz, 1H), 7.99 (d, *J* = 8.3 Hz, 1H), 7.88 (d, *J* = 8.6 Hz, 1H), 7.78 (t, *J* = 7.2 Hz, 1H), 7.64 (t, *J* = 7.1 Hz, 1H), 7.60–7.52 (m, 2H), 7.49–7.39 (m, 1H), 6.89 (d, *J* = 7.6 Hz, 1H), 3.16–3.02 (m, 1H), 2.09 (dd, *J* = 12.5, 7.5 Hz, 2H), 1.83–1.63 (m, 4H), 1.58–1.42 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 209.8, 173.5, 142.7, 137.8, 132.6, 132.1, 131.8, 129.4, 127.8, 127.1, 127.1, 126.3, 126.0, 125.3, 124.6, 122.3, 116.1, 111.9, 53.8, 29.5, 26.2; IR (KBr, cm^{-1}): 2948, 2864, 1687, 1643, 1598, 1523, 1475, 1421; HRMS (ESI-TOF) calcd for $C_{23}H_{20}NO_2^+$ ($[M+H]^+$): 342.1489, found: 342.1487.

12-(Thiophene-2-carbonyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4oa):



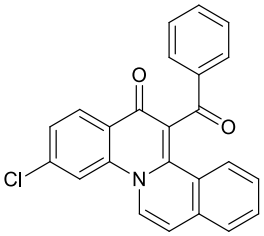
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (54.0 mg, 76% yield); mp 254.1–255.0 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.51 (d, *J* = 7.8 Hz, 1H), 8.13 (t, *J* = 7.0 Hz, 2H), 7.92 (d, *J* = 8.6 Hz, 1H), 7.78 (t, *J* = 7.8 Hz, 1H), 7.63 (d, *J* = 4.8 Hz, 2H), 7.53 (dd, *J* = 15.2, 7.7 Hz, 3H), 7.34–7.17 (m, 1H), 7.08–6.94 (m, 1H), 6.88 (d, *J* = 7.4 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$/CD_3OD = 20:1) δ (ppm): 190.2, 174.3, 145.4, 143.7, 138.0, 134.7, 134.1, 132.9, 132.0, 131.7, 129.2, 128.4, 128.0, 126.9, 126.6, 126.4, 126.3, 125.1, 124.2, 119.1, 116.5, 112.6; IR (KBr, cm^{-1}): 3037, 1647, 1594, 1567, 1551, 1515, 1467, 1426, 1407; HRMS (ESI-TOF) calcd for $C_{22}H_{14}NO_2S^+$ ($[M+H]^+$): 356.0740, found: 356.0738.

12-Benzoyl-3-methyl-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4pa):



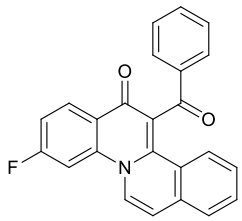
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (53.1 mg, 73% yield); mp 296.7–298.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.37 (d, *J* = 8.1 Hz, 1H), 8.15 (d, *J* = 7.8 Hz, 1H), 8.12–8.07 (m, 2H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.71 (s, 1H), 7.61–7.53 (m, 1H), 7.53–7.48 (m, 2H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.22 (ddd, *J* = 8.5, 6.0, 2.6 Hz, 1H), 6.86 (d, *J* = 7.7 Hz, 1H), 2.59 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 198.5, 174.5, 143.7, 143.6, 138.4, 137.9, 133.4, 132.1, 131.4, 129.4, 129.4, 128.9, 127.9, 127.7, 126.8, 126.3, 125.1, 125.0, 124.5, 119.2, 116.0, 112.1, 22.4; IR (KBr, cm^{-1}): 1654, 1644, 1613, 1591, 1571, 1552, 1523, 1486, 1476, 1450, 1413; HRMS (ESI-TOF) calcd for $C_{25}H_{18}NO_2^+$ ($[M+H]^+$): 364.1332, found: 364.1333.

12-Benzoyl-3-chloro-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4qa):



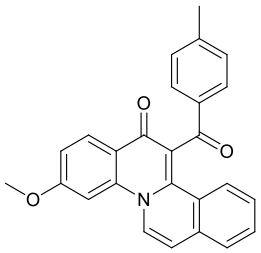
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (67.6 mg, 88% yield); mp 306.6–308.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.44 (d, *J* = 8.5 Hz, 1H), 8.06 (dd, *J* = 14.1, 7.7 Hz, 3H), 7.94 (s, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.61–7.41 (m, 6H), 7.23 (d, *J* = 6.6 Hz, 1H), 6.89 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (75 MHz, DMSO) δ (ppm): 198.0, 173.2, 143.7, 139.4, 138.4, 137.8, 134.2, 132.7, 132.5, 129.6, 129.4, 128.8, 128.2, 127.9, 127.3, 127.2, 127.1, 125.3, 123.9, 119.2, 118.3, 112.4; IR (KBr, cm^{-1}): 2924, 1662, 1653, 1587, 1567, 1552, 1519, 1486, 1475, 1448, 1416; HRMS (ESI-TOF) calcd for $C_{24}H_{15}ClNO_2^+$ ($[M+H]^+$): 384.0786, found: 384.0785.

12-Fenzoyl-3-fluoro-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ra):



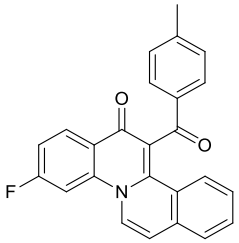
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (68.3 mg, 93% yield); mp 280.7–282.6 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.50 (dd, *J* = 8.5, 6.9 Hz, 1H), 8.08 (d, *J* = 7.5 Hz, 2H), 7.98 (d, *J* = 7.7 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.61 (d, *J* = 10.5 Hz, 1H), 7.56 (dd, *J* = 14.3, 7.0 Hz, 1H), 7.52–7.41 (m, 4H), 7.25 (dt, *J* = 18.3, 7.4 Hz, 2H), 6.88 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 197.0, 172.8, 164.3 (d, $J_{C\text{-}F}$ = 253.0 Hz), 143.2, 138.5 (d, *J* = 11.0 Hz), 136.6, 132.6, 130.9, 130.7, 128.9 (d, *J* = 10.5 Hz), 128.3, 127.9, 127.1, 125.5, 123.7, 123.3, 122.6 (d, *J* = 1.7 Hz), 118.4, 113.8 (d, *J* = 22.6 Hz), 111.7, 101.9 (d, *J* = 27.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -103.8; IR (KBr, cm^{-1}): 1671, 1623, 1600, 1577, 1553, 1525, 1483, 1466, 1449, 1419; HRMS (ESI-TOF) calcd for $C_{24}H_{15}FNO_2^+$ ($[M+H]^+$): 368.1081, found: 368.1082.

3-Methoxy-12-(4-methylbenzoyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4sa):



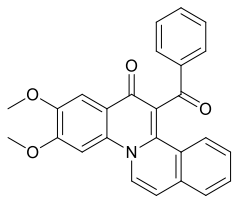
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (52.7 mg, 67% yield); mp 255.9–257.5 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.28 (d, *J* = 8.9 Hz, 1H), 7.91 (dd, *J* = 7.9, 4.1 Hz, 3H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.36 (t, *J* = 7.2 Hz, 1H), 7.30 (d, *J* = 6.9 Hz, 1H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.14–7.07 (m, 2H), 7.00 (dd, *J* = 8.9, 2.0 Hz, 1H), 6.67 (d, *J* = 7.7 Hz, 1H), 3.88 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 198.3, 174.1, 163.2, 144.3, 143.6, 139.7, 135.6, 131.9, 131.3, 129.7, 129.5, 129.2, 128.5, 127.7, 126.3, 125.0, 124.5, 121.0, 119.2, 114.6, 112.1, 99.3, 55.9, 21.8; IR (KBr, cm^{-1}): 1665, 1611, 1591, 1564, 1552, 1531, 1492, 1468, 1444, 1418; HRMS (ESI-TOF) calcd for $C_{26}H_{20}NO_3^+$($[M+H]^+$): 394.1438, found: 394.1438.

3-Fluoro-12-(4-methylbenzoyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ta):



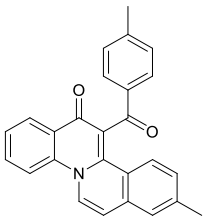
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (49.6 mg, 65% yield); mp 316.7–318.5 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.49 (dd, *J* = 8.8, 6.6 Hz, 1H), 7.99 (dd, *J* = 12.4, 8.0 Hz, 3H), 7.90 (d, *J* = 8.4 Hz, 1H), 7.63 (dd, *J* = 10.9, 1.8 Hz, 1H), 7.56–7.43 (m, 2H), 7.31–7.20 (m, 4H), 6.89 (d, *J* = 7.7 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$/CD_3OD = 60:1) δ (ppm): 197.7, 173.9, 165.3 (d, *J* = 252.8 Hz), 144.6, 144.2, 139.5 (d, *J* = 11.0 Hz), 135.3, 131.9, 131.8, 129.9 (d, *J* = 10.5 Hz), 129.7, 129.5, 129.4, 128.1, 126.5, 124.8, 124.4, 123.6 (d, *J* = 1.6 Hz), 119.7, 114.8 (d, *J* = 22.7 Hz, 0H), 112.8, 103.0 (d, *J* = 27.6 Hz), 21.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm): -103.8; IR (KBr, cm^{-1}): 2924, 2853, 1653, 1619, 1581, 1557, 1491, 1454, 1438; HRMS (ESI-TOF) calcd for $C_{25}H_{17}FNO_2^+$ ($[M+H]^+$): 382.1238, found: 382.1237. .

12-Benzoyl-2,3-dimethoxy-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ua):



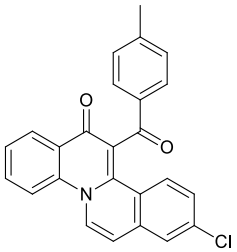
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (67.1 mg, 82% yield); mp 325.1–326.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.11 (d, *J* = 7.3 Hz, 2H), 8.06 (d, *J* = 7.7 Hz, 1H), 7.82 (t, *J* = 8.9 Hz, 1H), 7.74 (s, 1H), 7.58 (t, *J* = 7.3 Hz, 1H), 7.51–7.41 (m, 3H), 7.33 (d, *J* = 7.4 Hz, 1H), 7.21 (dd, *J* = 10.4, 3.0 Hz, 2H), 6.74 (d, *J* = 7.7 Hz, 1H), 4.07 (s, 3H), 3.98 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 199.0, 173.2, 153.6, 148.6, 142.5, 138.1, 133.4, 133.0, 131.6, 130.9, 129.3, 129.0, 128.8, 127.6, 126.3, 124.7, 124.3, 121.2, 118.3, 112.4, 105.4, 97.9, 56.5, 56.2; IR (KBr, cm^{-1}): 1660, 1614, 1597, 1552, 1527, 1505, 1421; HRMS (ESI-TOF) calcd for $C_{26}H_{20}NO_4^+$ ($[M+H]^+$): 410.1387, found: 410.1386.

9-Methyl-12-(4-methylbenzoyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ab):



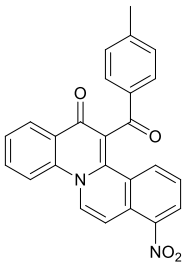
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (54.4 mg, 72% yield); mp 256.6–258.5 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.48 (d, *J* = 7.9 Hz, 1H), 8.13 (d, *J* = 7.7 Hz, 1H), 7.99 (d, *J* = 8.1 Hz, 2H), 7.90 (d, *J* = 8.7 Hz, 1H), 7.82–7.71 (m, 2H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.30–7.21 (m, 3H), 7.05 (d, *J* = 8.4 Hz, 1H), 6.80 (d, *J* = 7.7 Hz, 1H), 2.39 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 98.3, 174.3, 144.3, 143.8, 142.3, 138.0, 135.6, 132.5, 132.2, 129.7, 129.5, 129.3, 129.3, 126.8, 126.7, 126.3, 125.9, 125.0, 122.0, 118.8, 116.2, 112.3, 21.8, 21.3; IR (KBr, cm^{-1}): 1657, 1598, 1574, 1555, 1520, 1477, 1400; HRMS (ESI-TOF) calcd for $C_{26}H_{20}NO_2^+$ ($[M+H]^+$): 378.1489, found: 378.1487.

9-Chloro-12-(4-methylbenzoyl)-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ac):



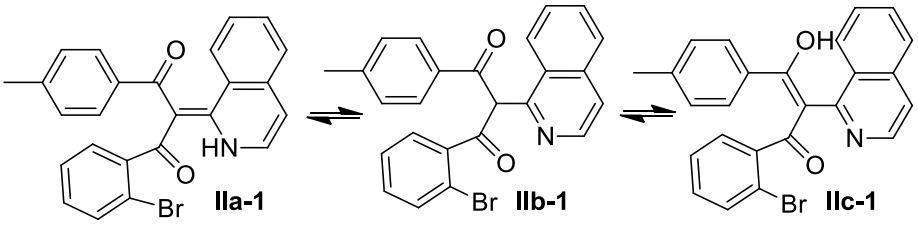
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (51.7 mg, 65% yield); mp 253.2–255.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.43 (d, *J* = 7.9 Hz, 1H), 8.14 (d, *J* = 7.8 Hz, 1H), 7.96 (d, *J* = 8.1 Hz, 2H), 7.88 (d, *J* = 8.7 Hz, 1H), 7.77 (t, *J* = 7.0 Hz, 1H), 7.75 (s, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.37 (s, 1H), 7.25 (d, *J* = 8.1 Hz, 2H), 7.14 (dd, *J* = 8.9, 2.0 Hz, 1H), 6.71 (d, *J* = 7.7 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 97.8, 174.5, 144.7, 142.9, 138.0, 137.8, 135.2, 133.5, 132.8, 130.7, 129.8, 129.5, 128.1, 126.9, 126.7, 126.3, 126.2, 125.6, 122.7, 119.6, 116.2, 111.0, 21.8; IR (KBr, cm^{-1}): 2233, 1652, 1602, 1594, 1573, 1546, 1518, 1480, 1450; HRMS (ESI-TOF) calcd for $C_{25}H_{17}ClNO_2^+$ ($[M+H]^+$): 398.0942, found: 398.0942.

12-(4-Methylbenzoyl)-8-nitro-13*H*-isoquinolino[2,1-*a*]quinolin-13-one (4ad):



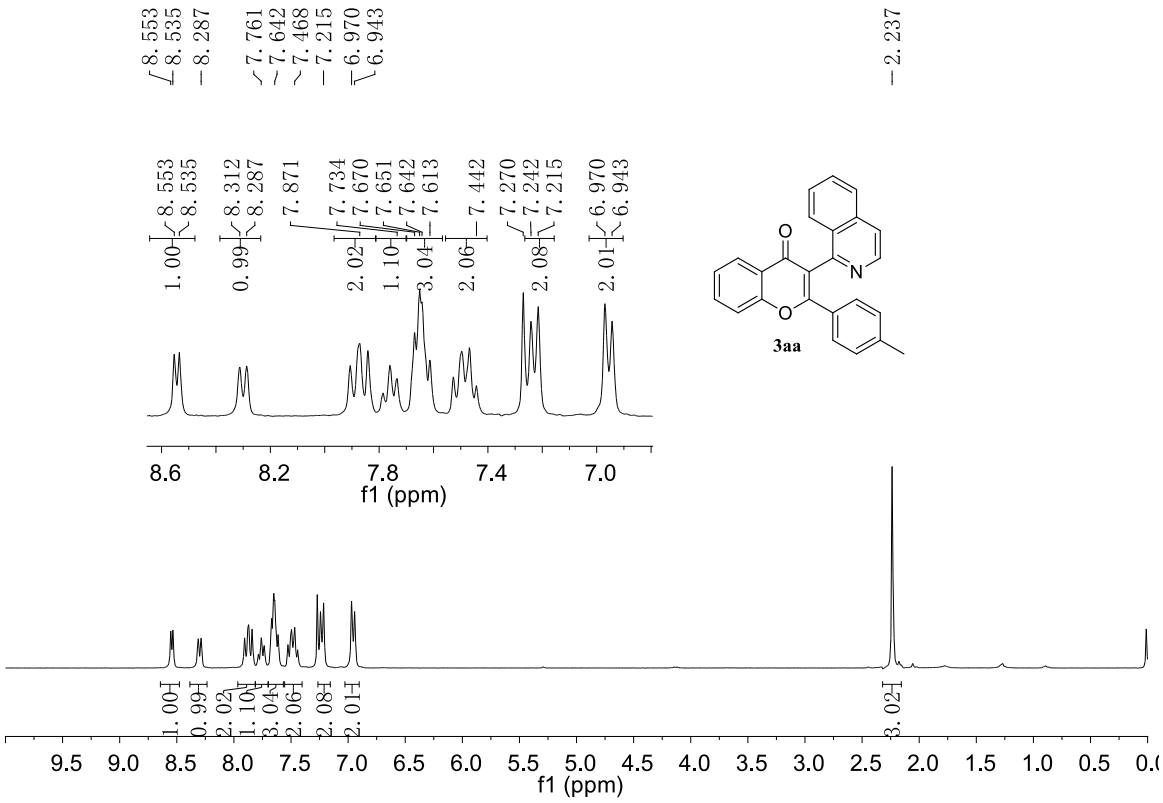
Purified by column chromatography (petroleum ether/ethyl acetate = 2:1–1:1); yellow solid (70.2 mg, 86% yield); mp 265.2–266.9 ℃; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm): 8.49 (d, *J* = 7.8 Hz, 1H), 8.29 (d, *J* = 8.2 Hz, 1H), 8.19 (dd, *J* = 15.1, 8.2 Hz, 2H), 7.96 (d, *J* = 8.2 Hz, 3H), 7.88 (t, *J* = 7.7 Hz, 1H), 7.63 (t, *J* = 8.6 Hz, 2H), 7.34 (t, *J* = 8.2 Hz, 1H), 7.29 (d, *J* = 3.2 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3/CD_3OD$ = 12:1) δ (ppm): 197.1, 174.8, 145.1, 144.8, 142.4, 137.7, 134.8, 134.5, 133.4, 129.8, 129.5, 128.9, 128.0, 126.9, 126.9, 126.8, 126.6, 126.3, 126.3, 120.9, 116.4, 105.7, 21.7; IR (KBr, cm^{-1}): 1655, 1598, 1579, 1551, 1525, 1474, 1409; HRMS (ESI-TOF) calcd for $C_{25}H_{17}N_2O_4^+$ ($[M+H]^+$): 409.1183, found: 409.1182.

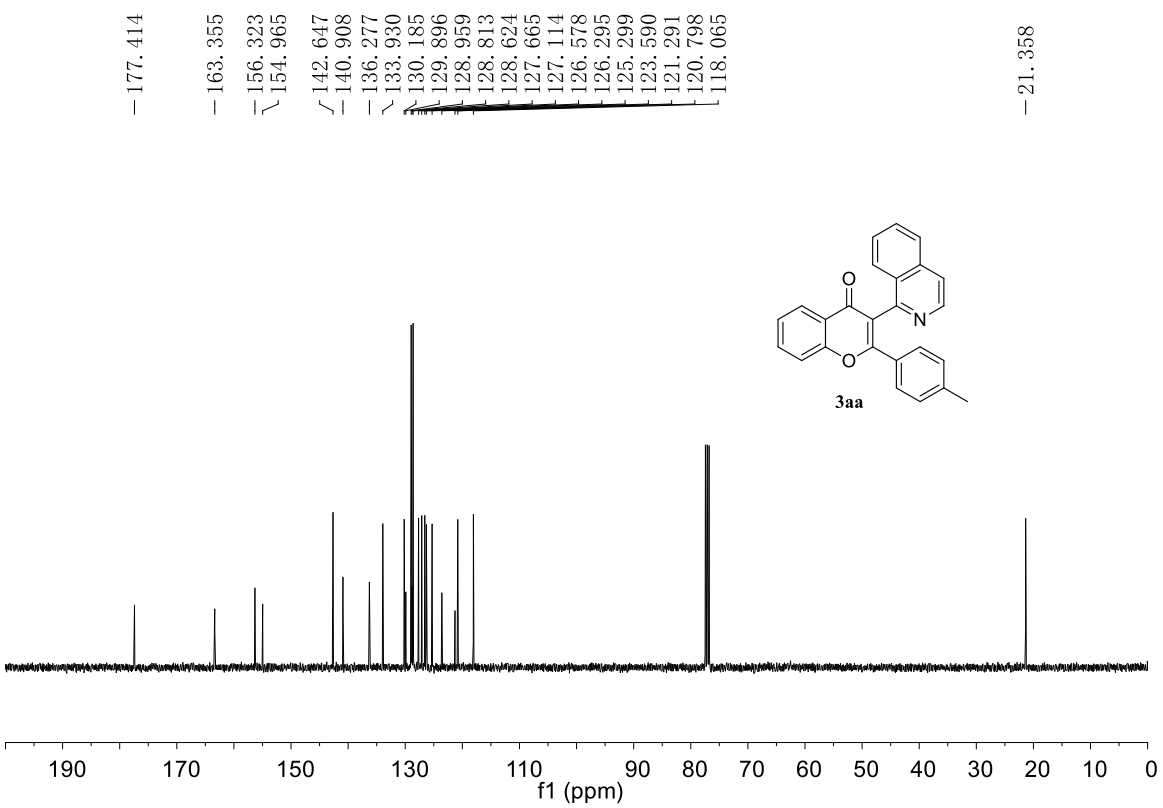
Enamine (IIa-1), Keto (IIb-1), Enol (IIc-1):

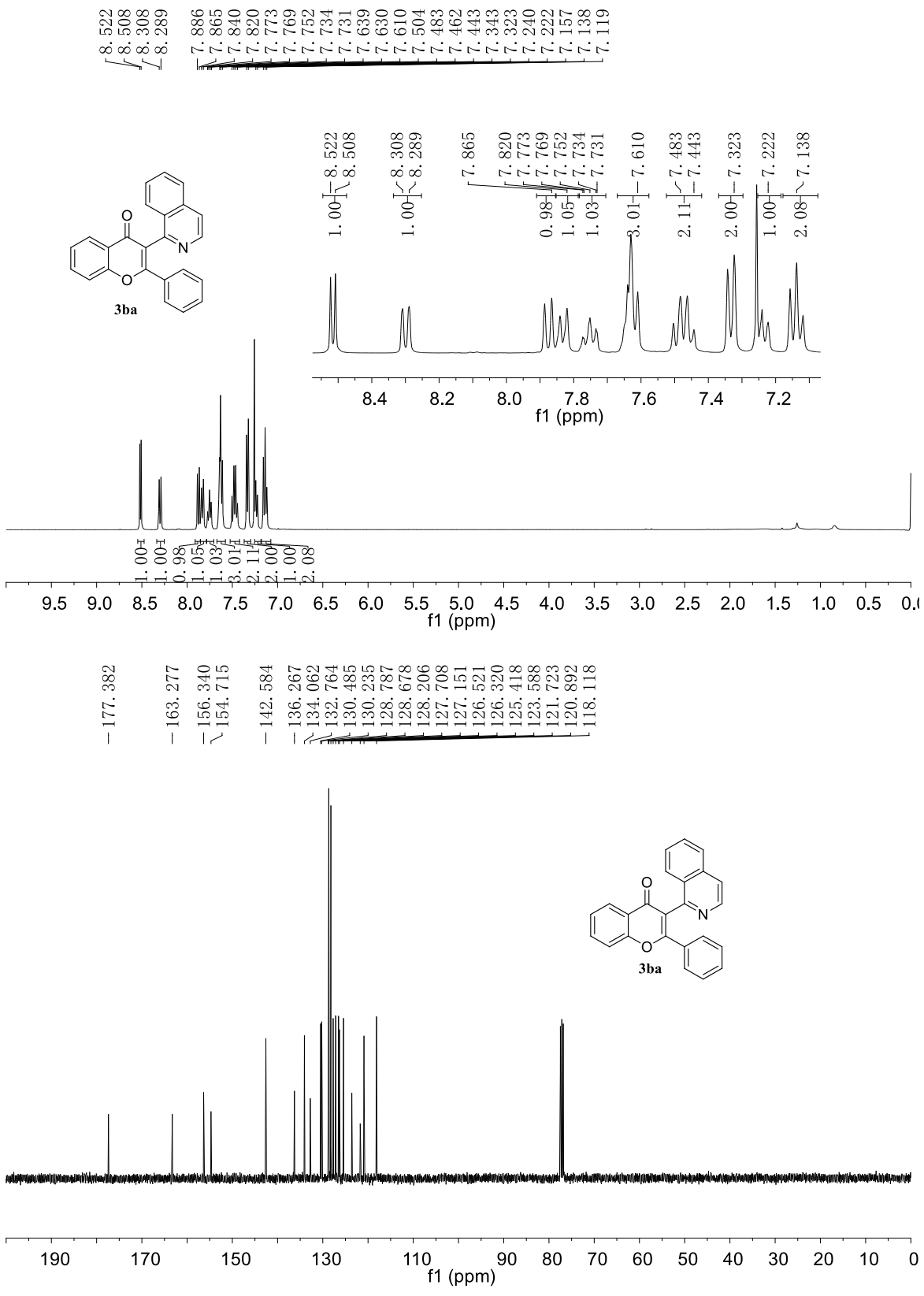


yellow solid (51.5 mg, 58% yield for DMF as solvent; 40.0 mg, 45% yield for toluene as solvent;); ^{1}H NMR (400 MHz, $CDCl_3$) δ 17.66 (s, 1H, *Enamine*), 17.59 (s, 1H, *Enol*), 8.45 (d, *J* = 5.7 Hz, 1H, *Keto*), 8.36 (d, *J* = 5.3 Hz, 1H, *Enol*), 8.17 (d, *J* = 8.2 Hz, 1H, *Keto*), 8.11 (d, *J* = 8.2 Hz, 1H, *Enol*), 7.86-7.28 (m, 6H, *Enol*+*Keto*+*Enamine*), 7.23-6.83 (m, 6H, *Enol*+*Keto*+*Enamine*), 2.34 (s, 3H, *Keto*), 2.27 (s, 3H, *Enamine*), 2.18 (s, 3H, *Enol*) (*Enol**(**IIa-1**)*:*Keto**(**IIb-1**)*:*Enamine**(**IIc-1**)* ≈ 1:8:10); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 13C NMR (101 MHz, CDCl3) δ 196.26, 192.89, 155.24, 143.26, 140.99, 139.12, 135.66, 132.76, 131.59, 130.93, 130.10, 129.15, 128.34, 128.03, 127.95, 127.66, 126.93, 126.60, 126.31, 125.27, 123.93, 119.77, 119.08, 114.76, 20.58, 20.43; IR (KBr, cm^{-1}): 3422, 3052, 1627, 1579, 1513, 1460, 1421; HRMS (ESI-TOF) calcd for $C_{25}H_{19}BrNO_2^+$ ($[M+H]^+$): 444.0594, found: 444.0592.

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



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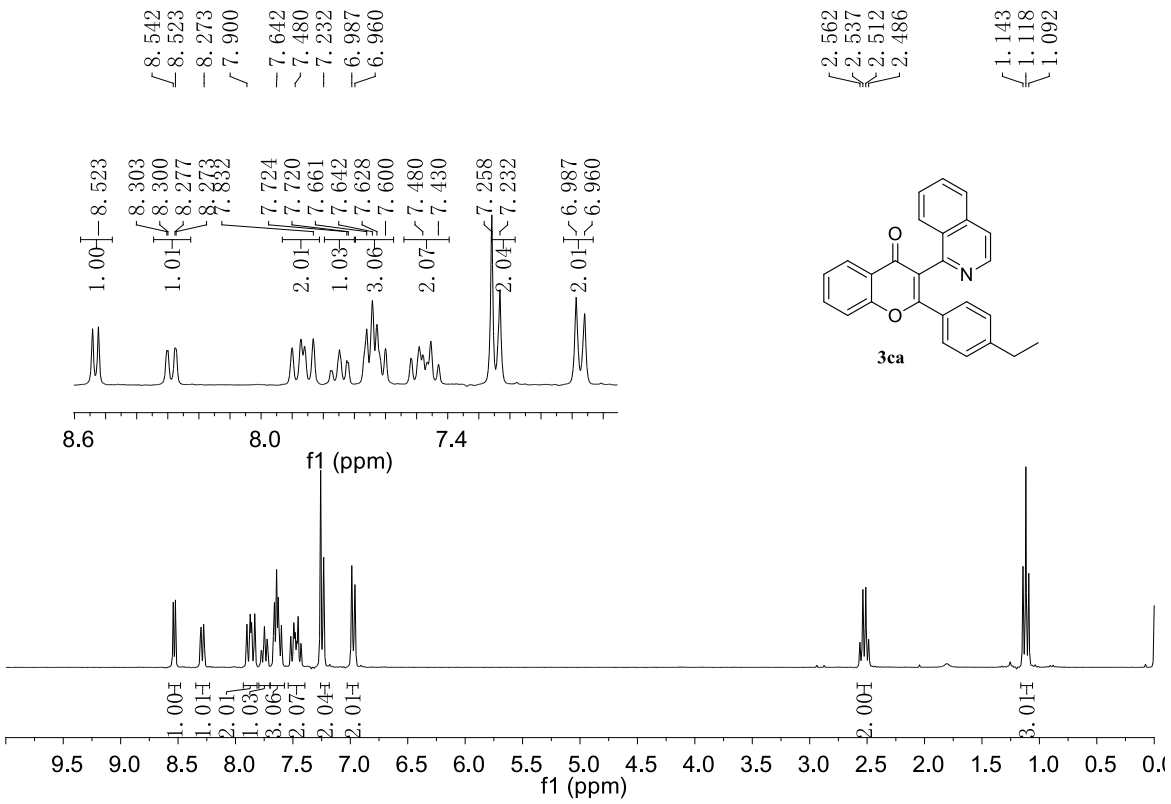
8.289
7.886
7.865
7.840
7.820
7.773
7.769
7.752
7.734
7.731
7.639
7.630
7.610
7.504
7.483
7.462
7.443
7.343
7.323
7.240
7.222
7.157
7.138
7.119
3ba
f1 (ppm)
177.382
163.277
156.340
154.715
142.584
136.267
134.062
132.764
130.485
130.235
128.787
128.678
128.206
127.708
127.151
126.521
126.320
125.418
123.588
121.723
120.892
118.118
3ba
f1 (ppm)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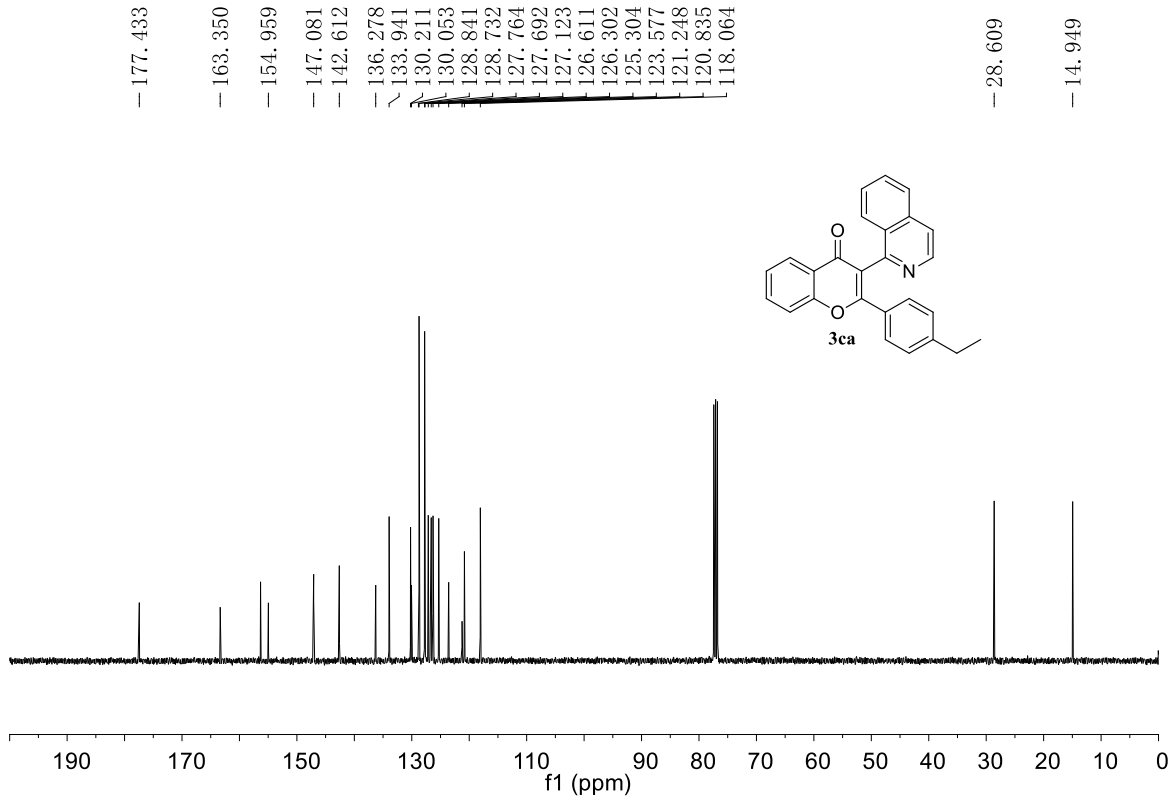
8.523
8.273
7.900
7.642
7.480
7.232
6.987
6.960
2.562
2.537
2.512
2.486
1.143
1.118
1.092
8.523
8.303
8.300
8.277
8.273
7.832
7.724
7.720
7.661
7.642
7.628
7.600
7.480
7.430
7.258
7.232
6.987
6.960
1.00
1.01
2.01
1.03
3.06
2.07
2.04
2.01
8.6
8.0
7.4
f1 (ppm)
O
N
O
3ca
1.00
1.01
2.01
1.03
3.06
2.07
2.04
2.01
2.00
3.01
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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147.081
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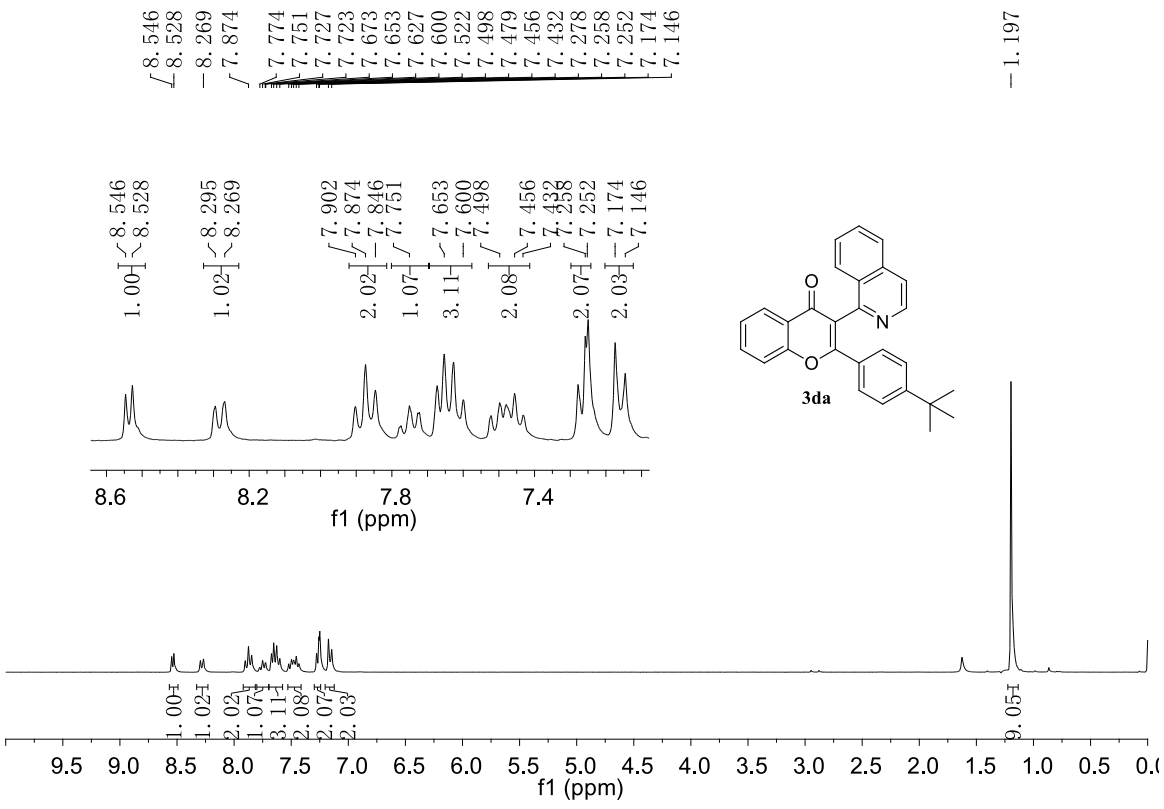
136.278
133.941
130.211
130.053
128.841
128.732
127.764
127.692
127.123
126.611
126.302
125.304
123.577
121.248
120.835
118.064
28.609
14.949
O
N
O
3ca
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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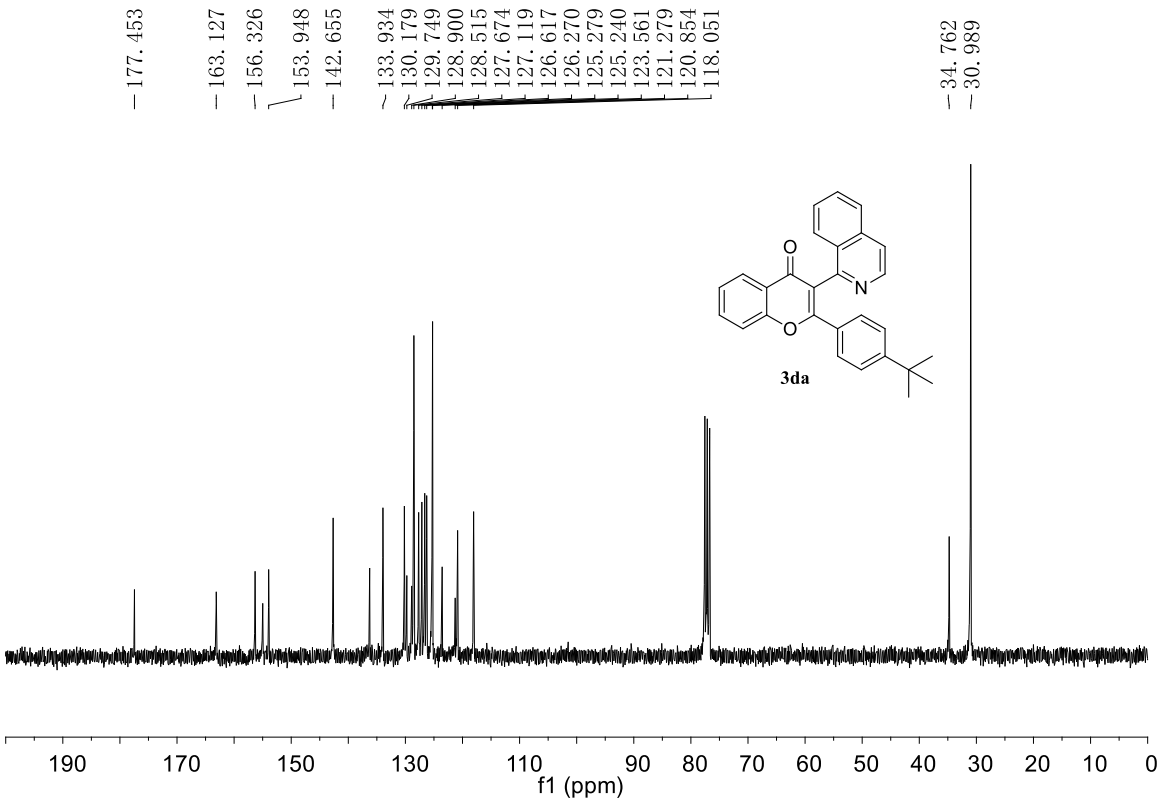
8.528
8.269
7.874
7.774
7.751
7.727
7.723
7.673
7.653
7.627
7.600
7.522
7.498
7.479
7.456
7.432
7.278
7.258
7.252
7.174
7.146
1.197
1.00
1.02
2.02
1.07
3.11
2.08
2.07
2.03
9.05
3da
f1 (ppm)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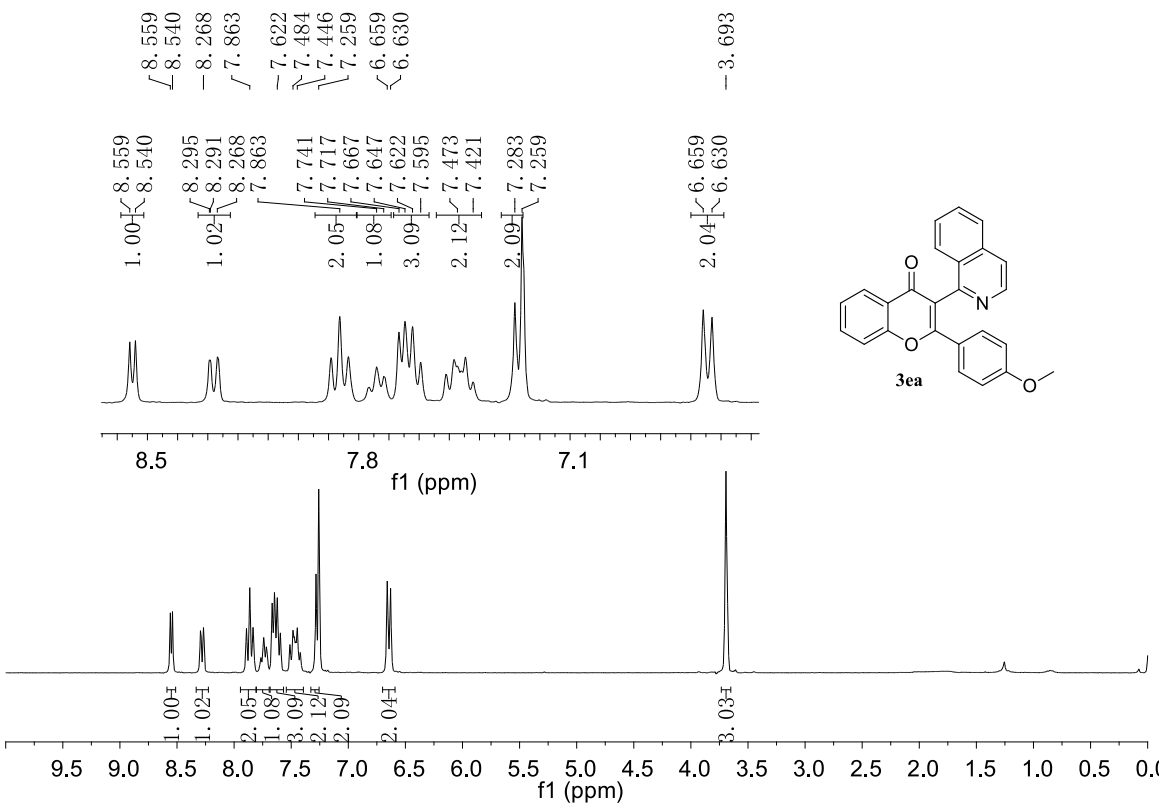
153.948
142.655
133.934
130.179
129.749
128.900
128.515
127.674
127.119
126.617
126.270
125.279
125.240
123.561
121.279
120.854
118.051
34.762
30.989
3da
f1 (ppm)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7.622
7.484
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7.259
6.659
6.630
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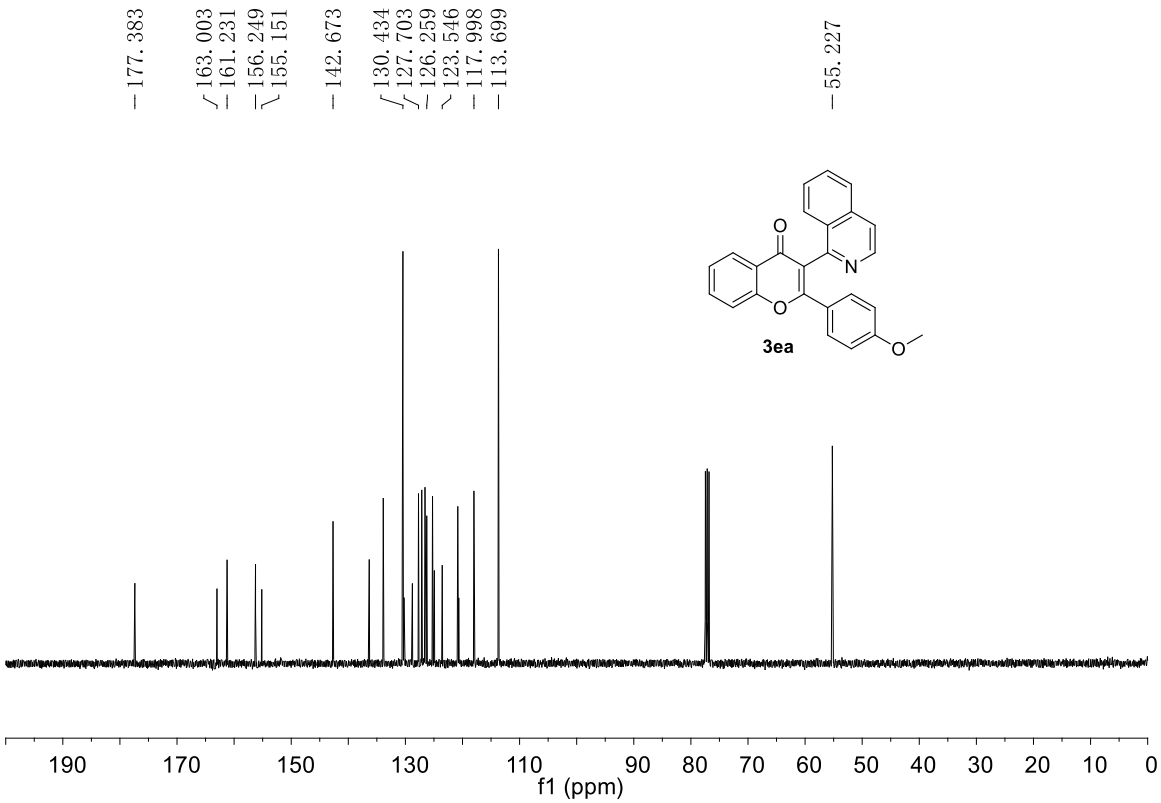
2.05
1.08
3.09
2.12
2.09
2.04
3.03
3ea
f1 (ppm)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161.231
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155.151
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127.703
126.259
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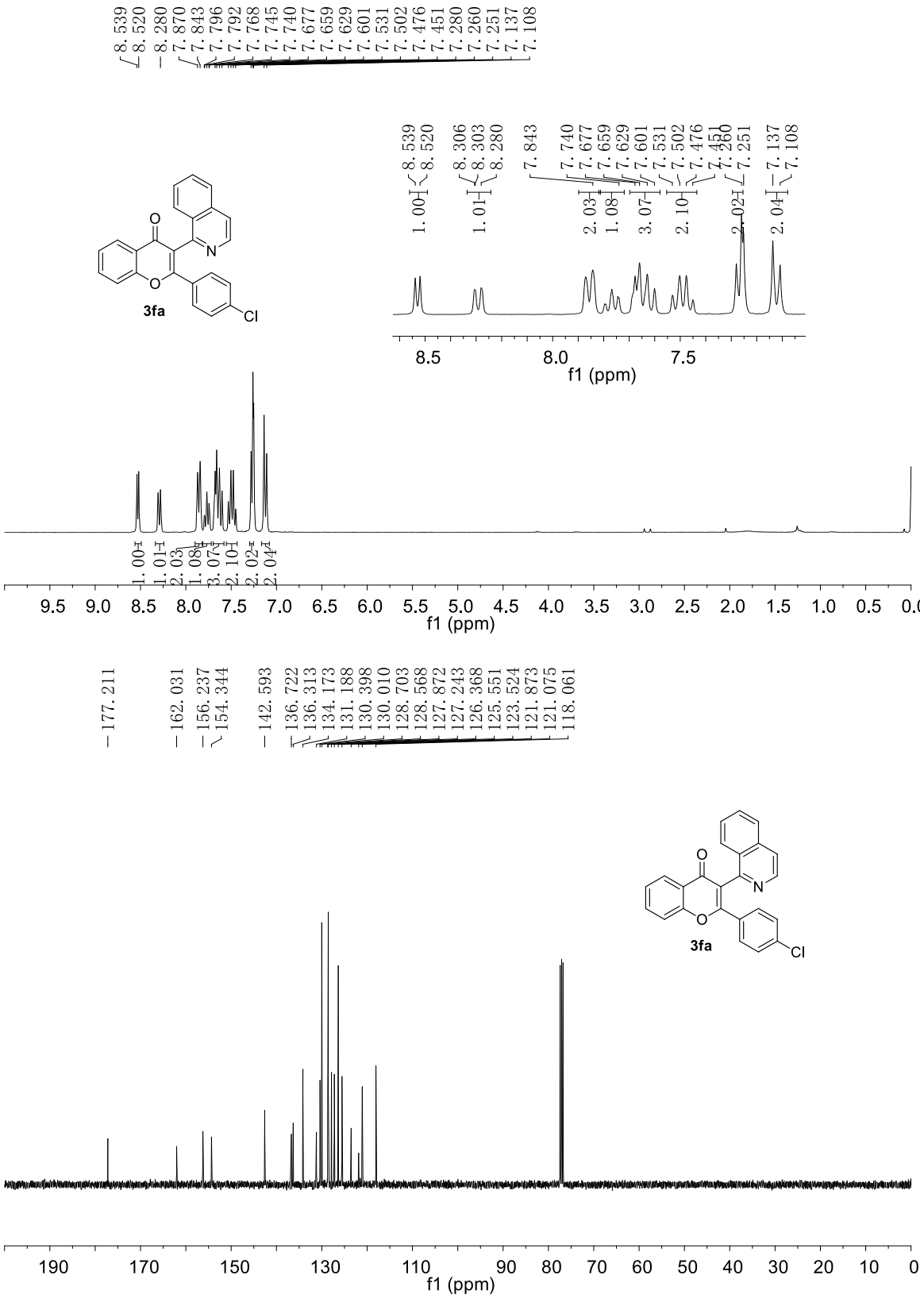
113.699
55.227
3ea
f1 (ppm)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7.796
7.792
7.768
7.745
7.740
7.677
7.659
7.629
7.601
7.531
7.502
7.476
7.451
7.280
7.260
7.251
7.137
7.108
3fa
Cl
O
N
O
1.00
1.01
2.03
1.08
3.07
2.10
2.02
2.04
f1 (ppm)

177.211
162.031
156.237
154.344
142.593
136.722
136.313
134.173
131.188
130.398
130.010
128.703
128.568
127.872
127.243
126.368
125.551
123.524
121.873
121.075
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3fa
Cl
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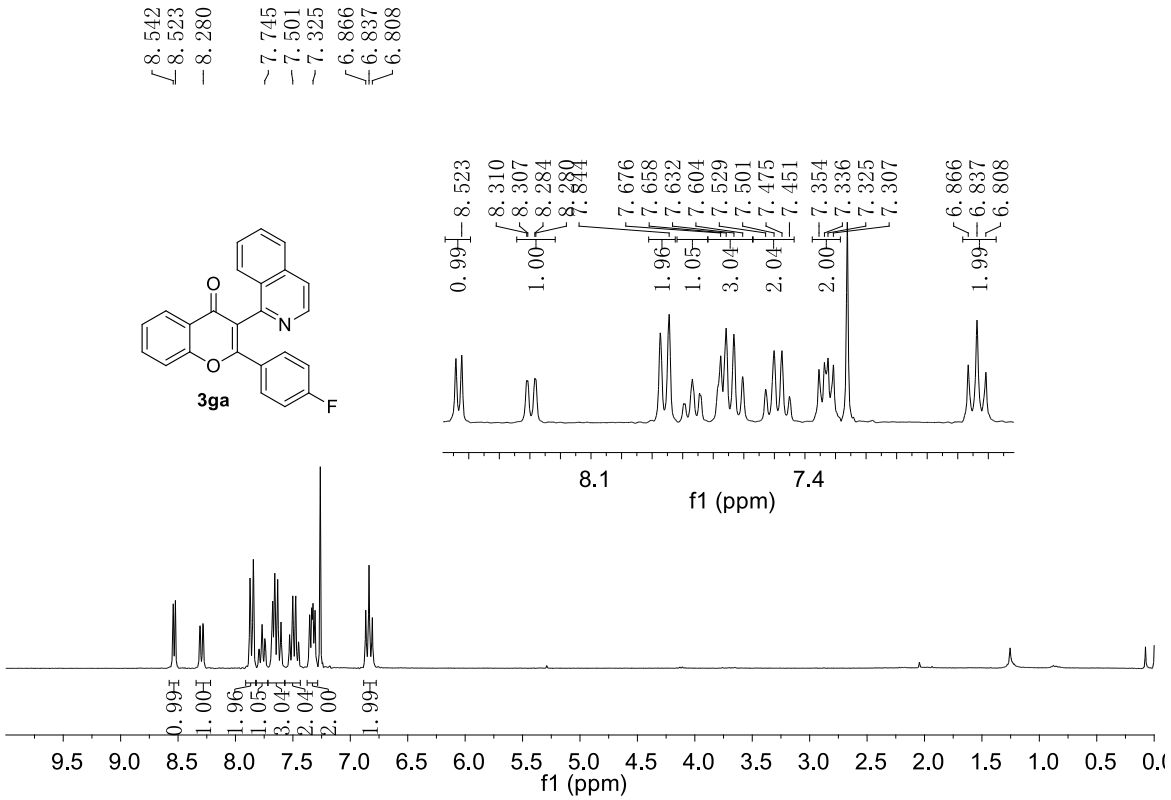
N
O
f1 (ppm)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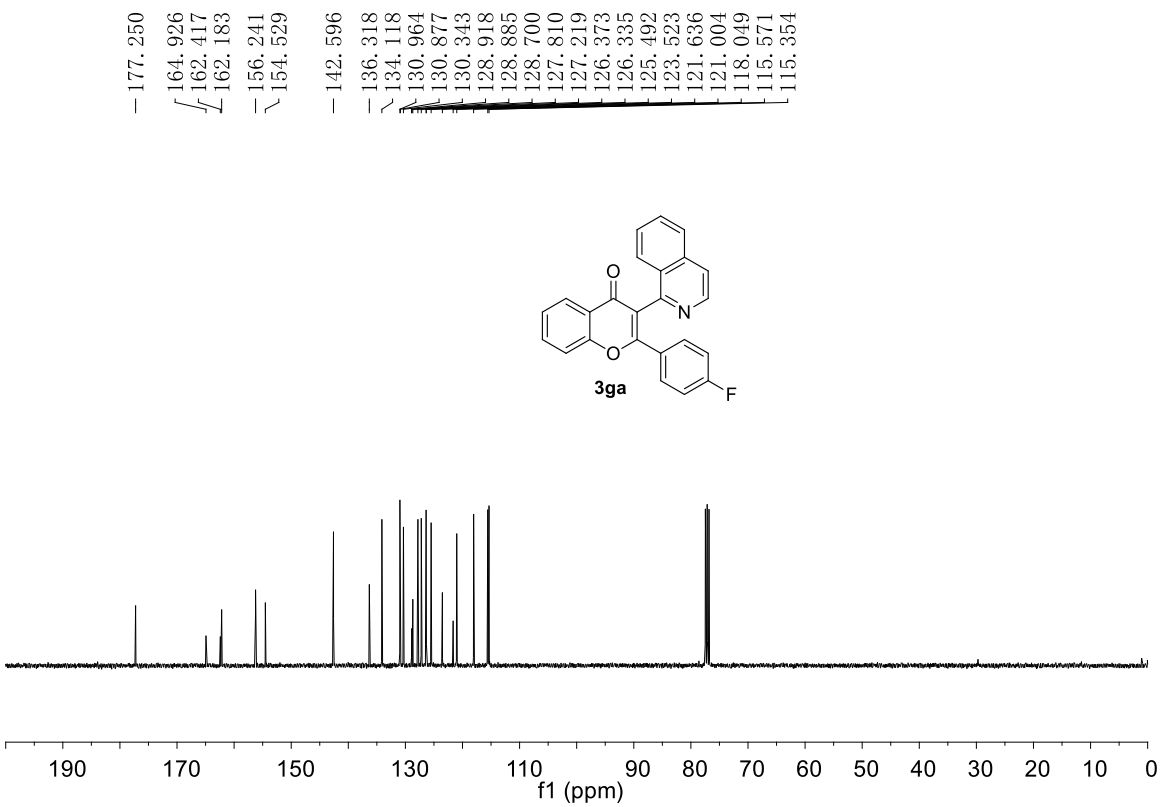
8.280
7.745
7.501
7.325
6.866
6.837
6.808
3ga
O
N
O
F
0.99
1.00
1.96
1.05
3.04
2.04
2.00
1.99
8.523
8.310
8.307
8.284
8.280
8.277
7.676
7.658
7.632
7.604
7.529
7.501
7.475
7.451
7.354
7.336
7.325
7.307
6.866
6.837
6.808
8.1
7.4
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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156.241
154.529
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136.318
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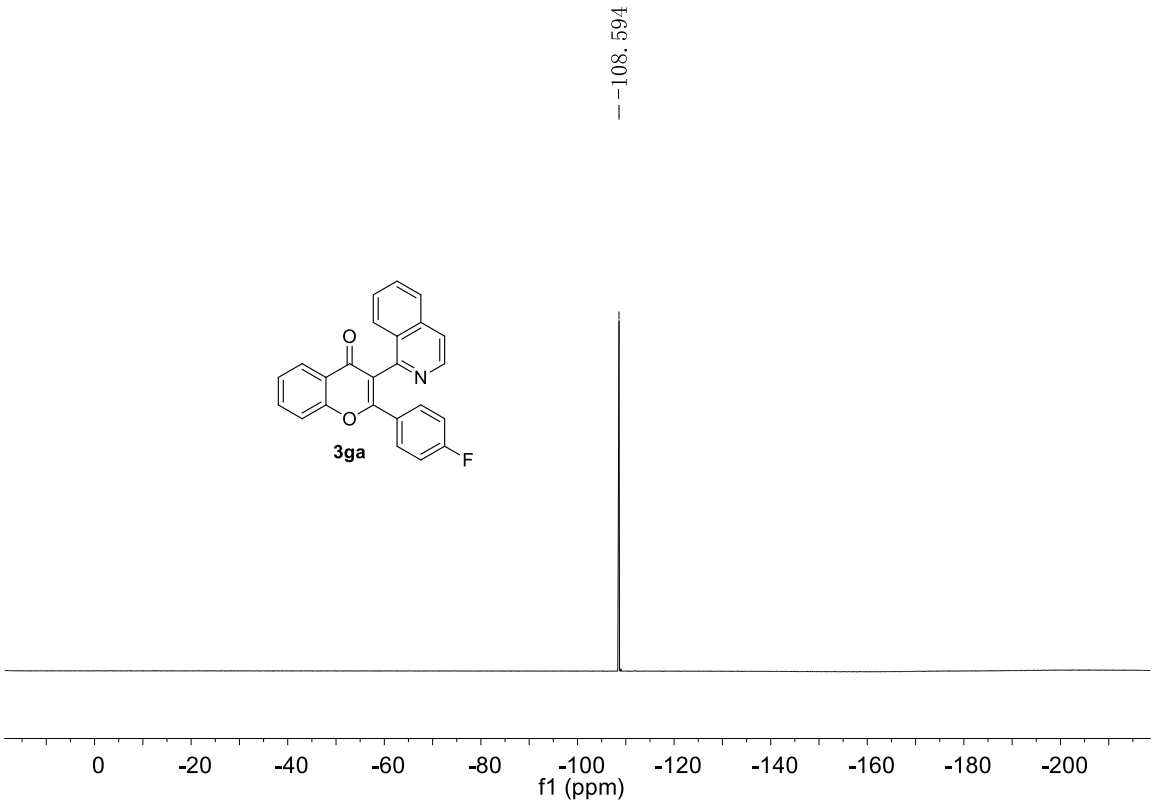
128.885
128.700
127.810
127.219
126.373
126.335
125.492
123.523
121.636
121.004
118.049
115.571
115.354
3ga
O
N
O
F
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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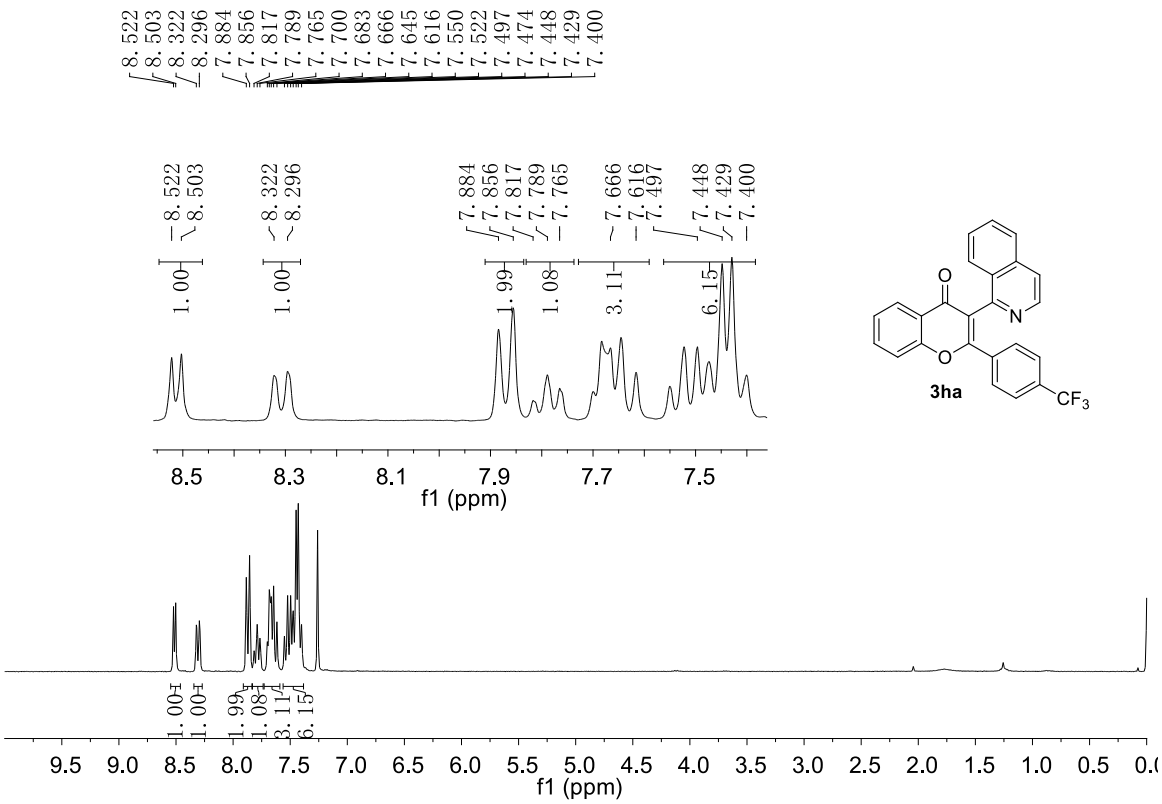
3ga
F
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)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7.683
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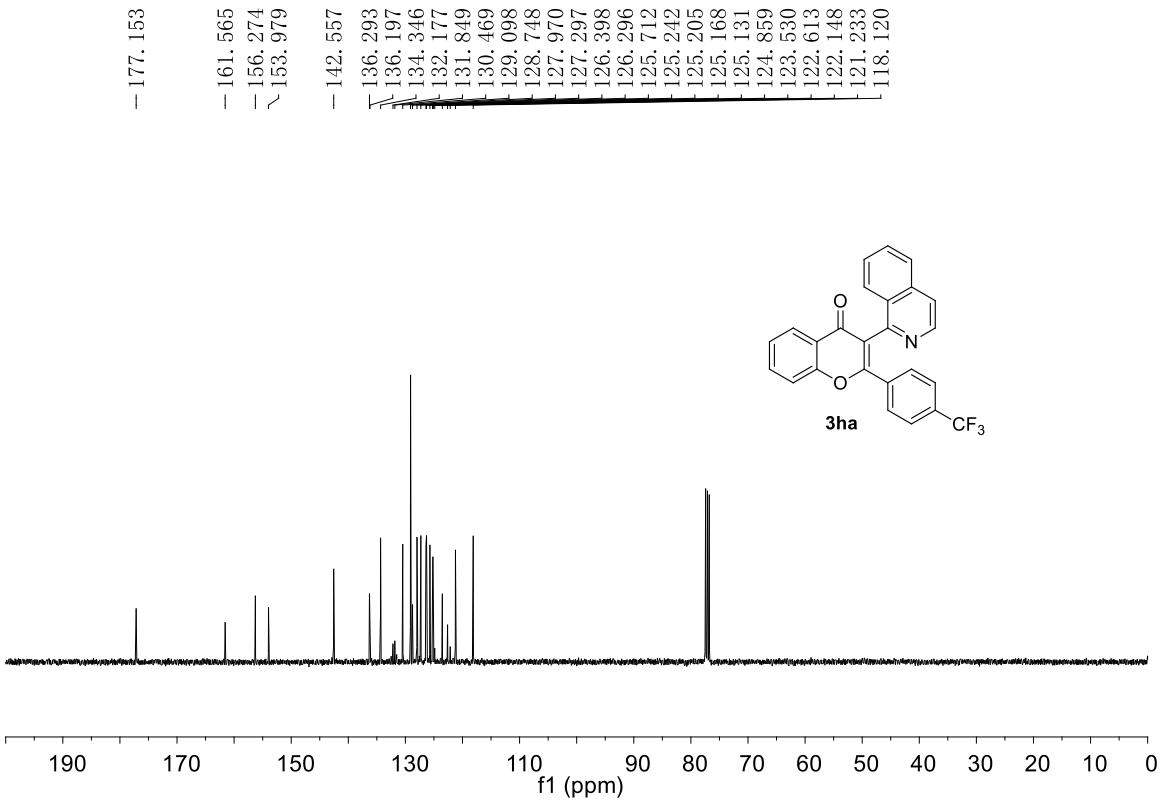
7.616
7.550
7.522
7.497
7.474
7.448
7.429
7.400
1.00
1.00
1.99
1.08
3.11
6.15
3ha
CF3
8.5
8.3
8.1
7.9
7.7
7.5
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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153.979
142.557
136.293
136.197
134.346
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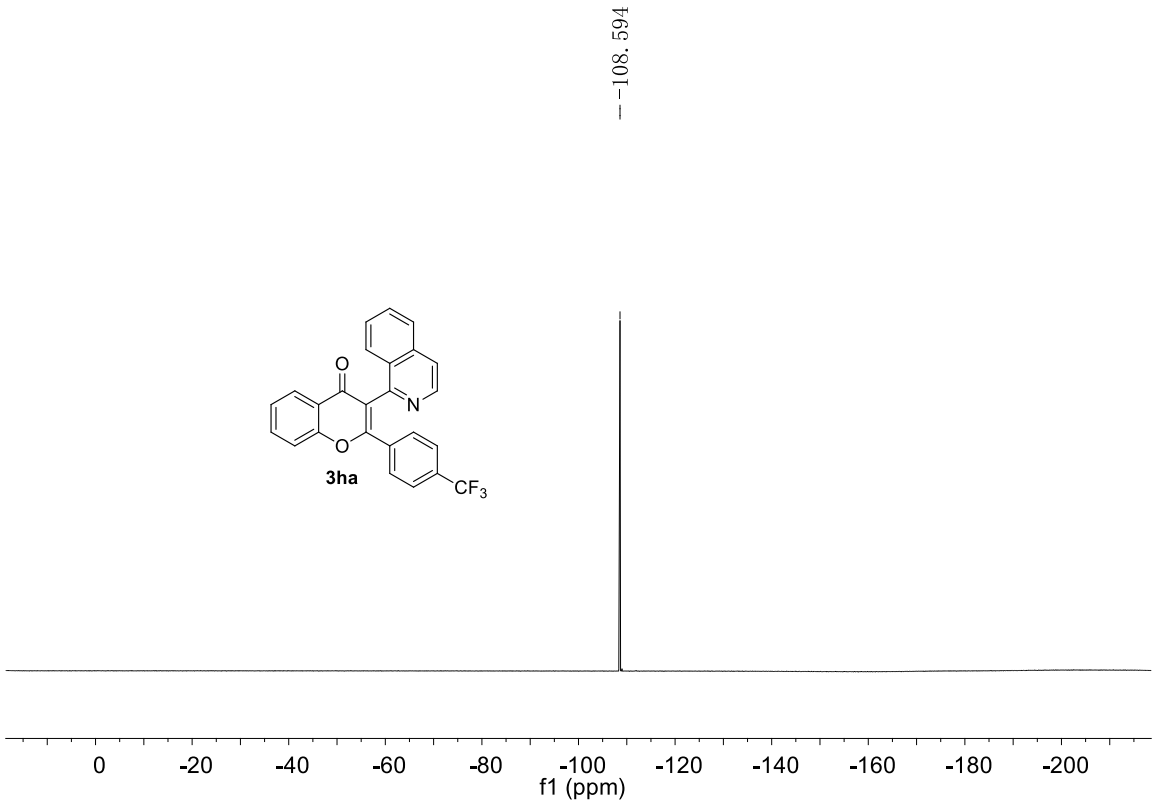
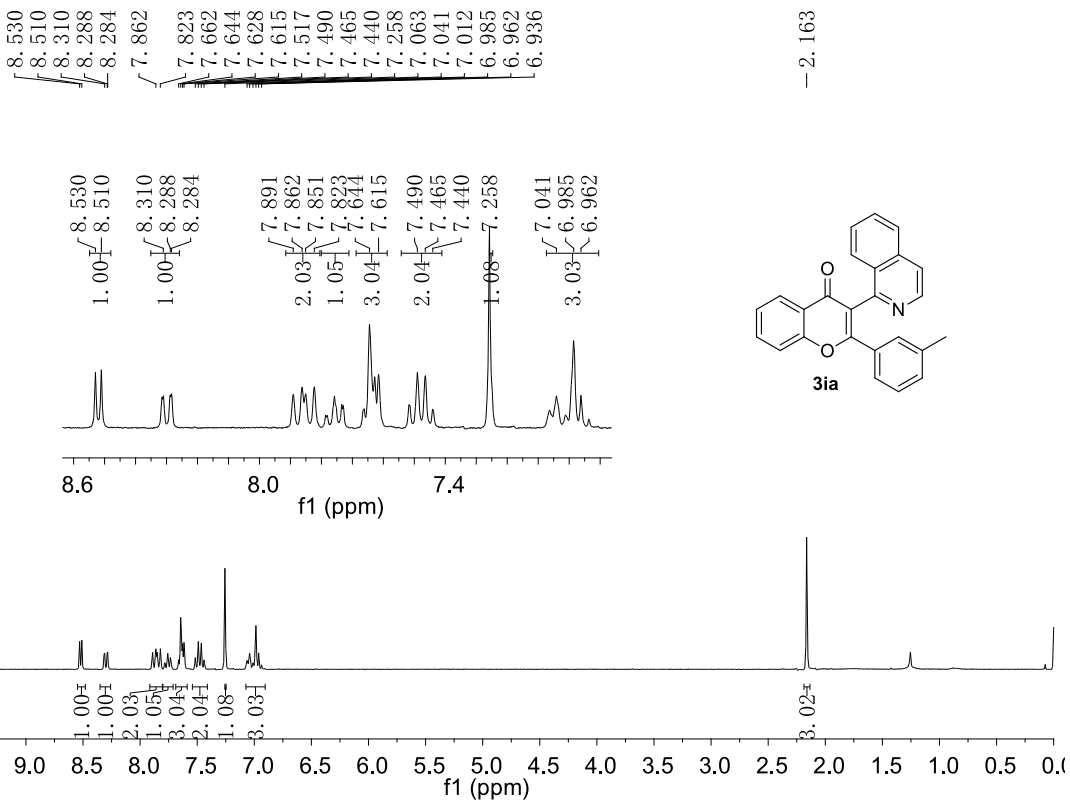
131.849
130.469
129.098
128.748
127.970
127.297
126.398
126.296
125.712
125.242
125.205
125.168
125.131
124.859
123.530
122.613
122.148
121.233
118.120
O
N
O
3ha
CF3
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-108.594
O
N
O
3ha
CF3
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)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7.662
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7.628
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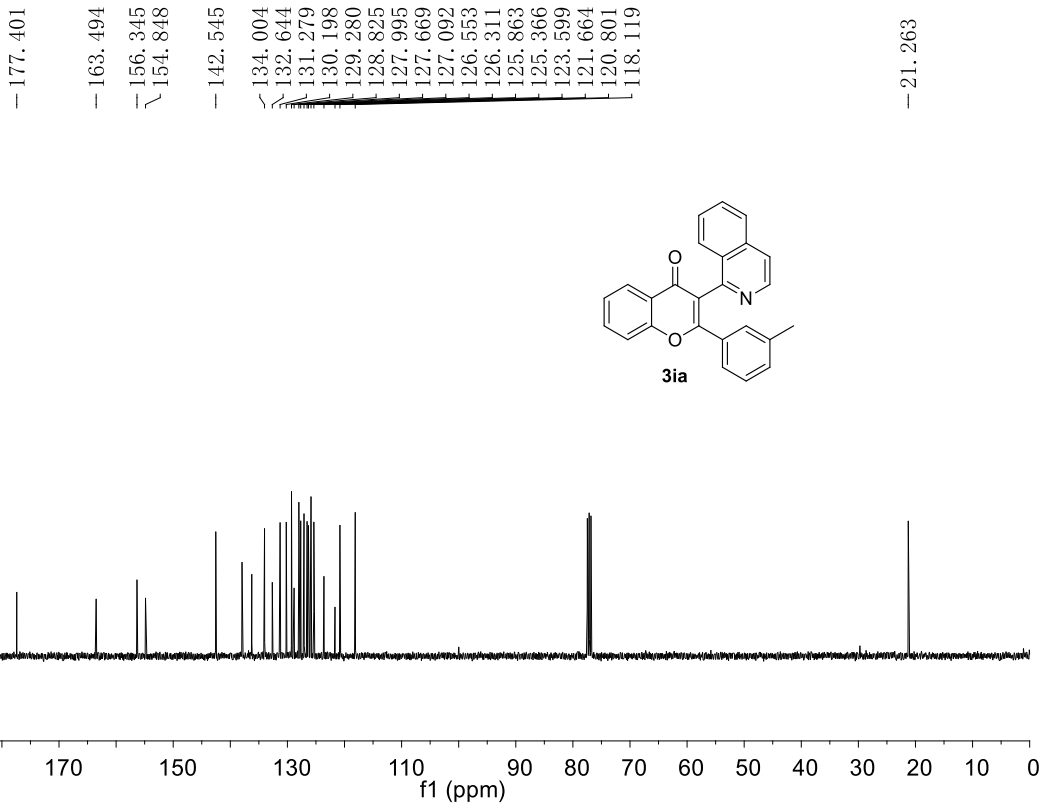
7.465
7.440
7.258
7.063
7.041
7.012
6.985
6.962
6.936
2.163
1.00
1.00
2.03
1.05
3.04
2.04
1.08
3.03
3.02
f1 (ppm)

O
N
O

3ia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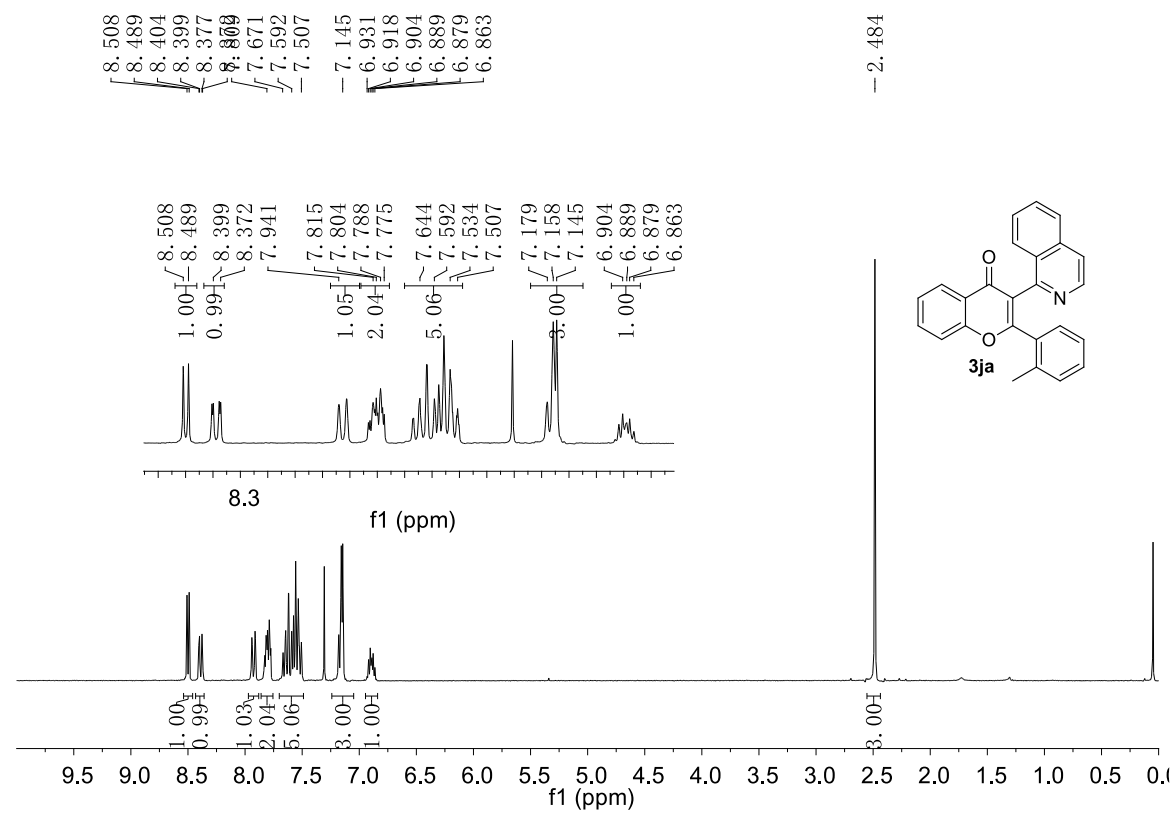
127.092
126.553
126.311
125.863
125.366
123.599
121.664
120.801
118.119
21.263
f1 (ppm)

O
N
O

3ia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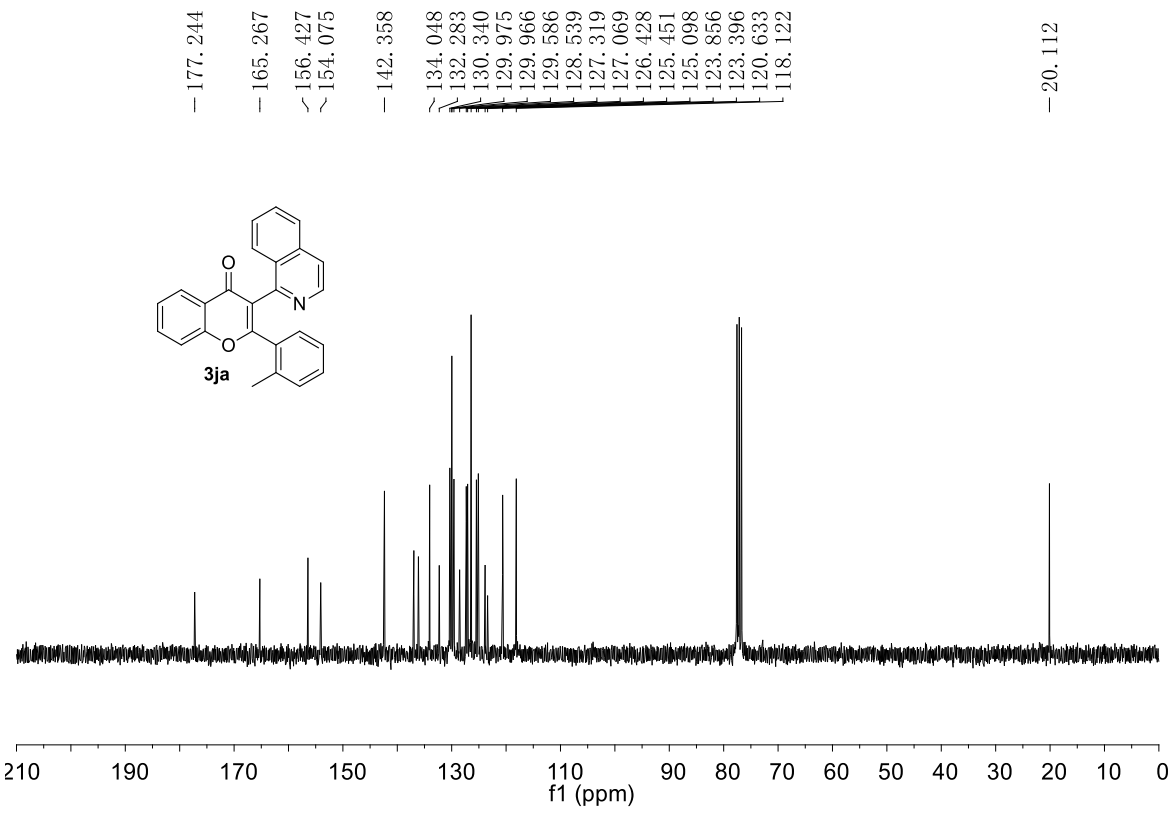
8.489
8.404
8.399
8.377
7.671
7.592
7.507
7.145
6.931
6.918
6.904
6.889
6.879
6.863
2.484
1.00
0.99
1.03
2.04
5.06
3.00
1.00
3.00
8.3
f1 (ppm)
3ja
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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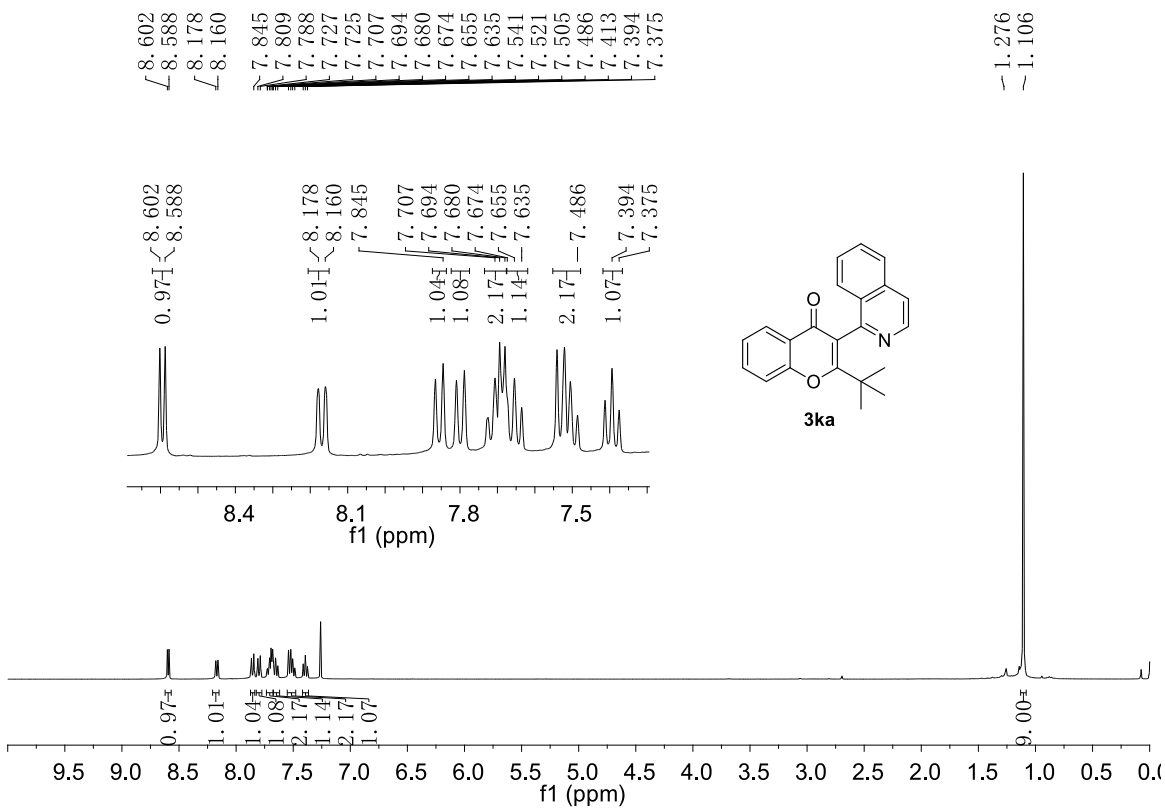
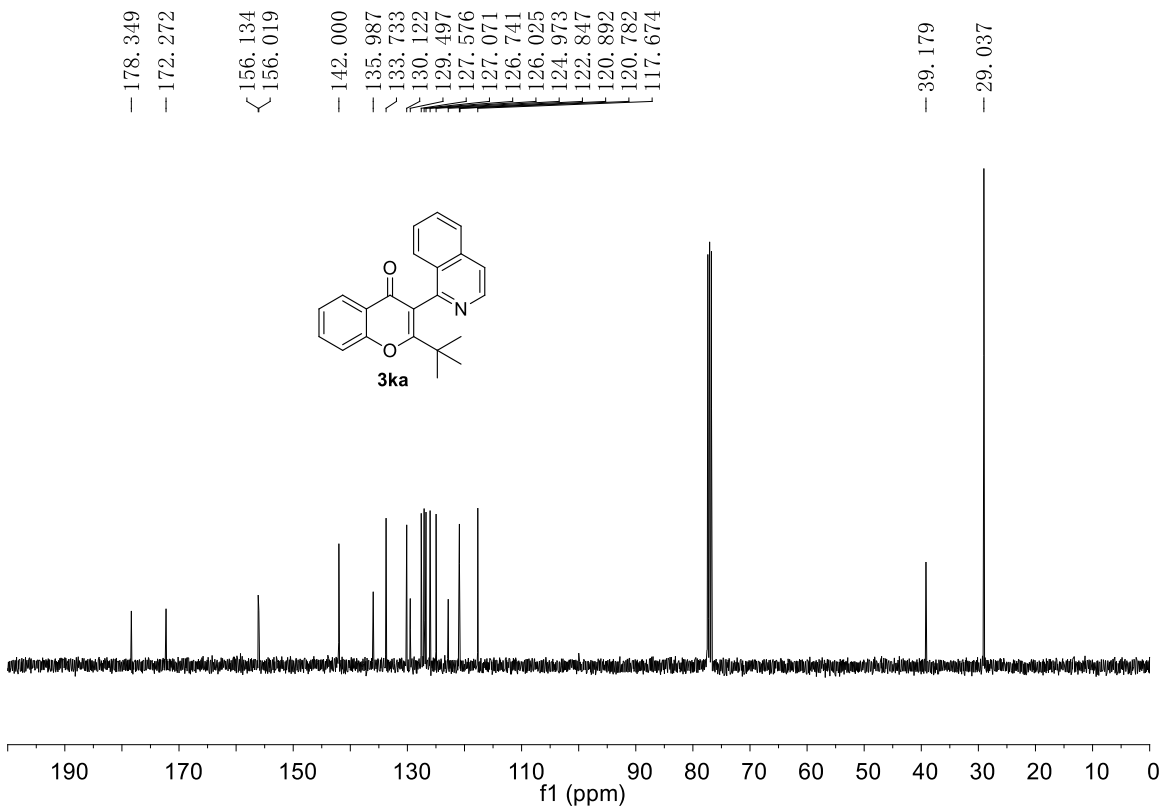
165.267
156.427
154.075
142.358
134.048
132.283
130.340
129.975
129.966
129.586
128.539
127.319
127.069
126.428
125.451
125.098
123.856
123.396
120.633
118.122
20.112
3ja
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.602
8.588
8.178
8.160
7.845
7.809
7.788
7.727
7.725
7.707
7.694
7.680
7.674
7.655
7.635
7.541
7.521
7.505
7.486
7.413
7.394
7.375
1.276
1.106
0.97
1.01
1.04
1.08
2.17
1.14
2.17
1.07
9.00
3ka
f1 (ppm)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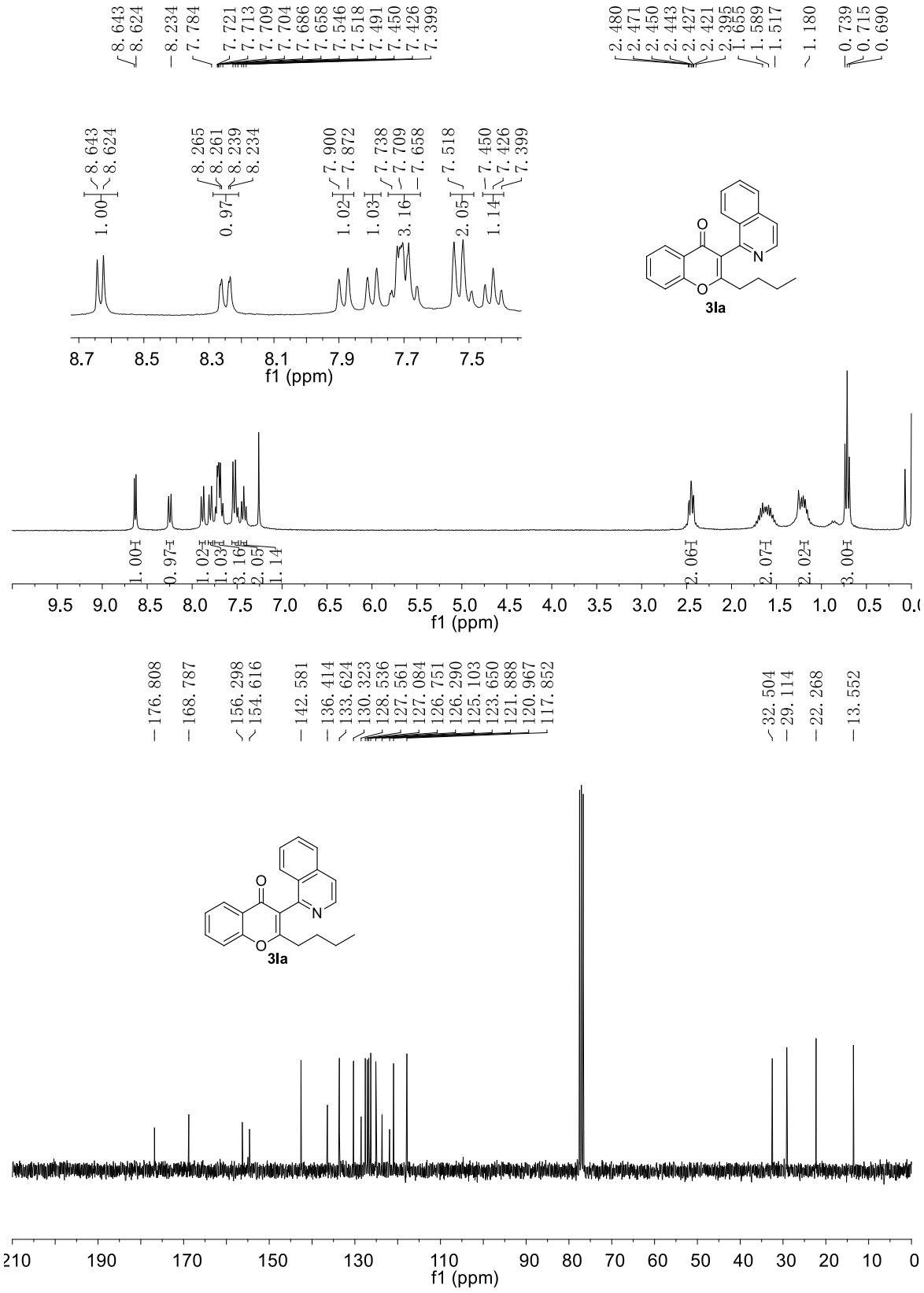
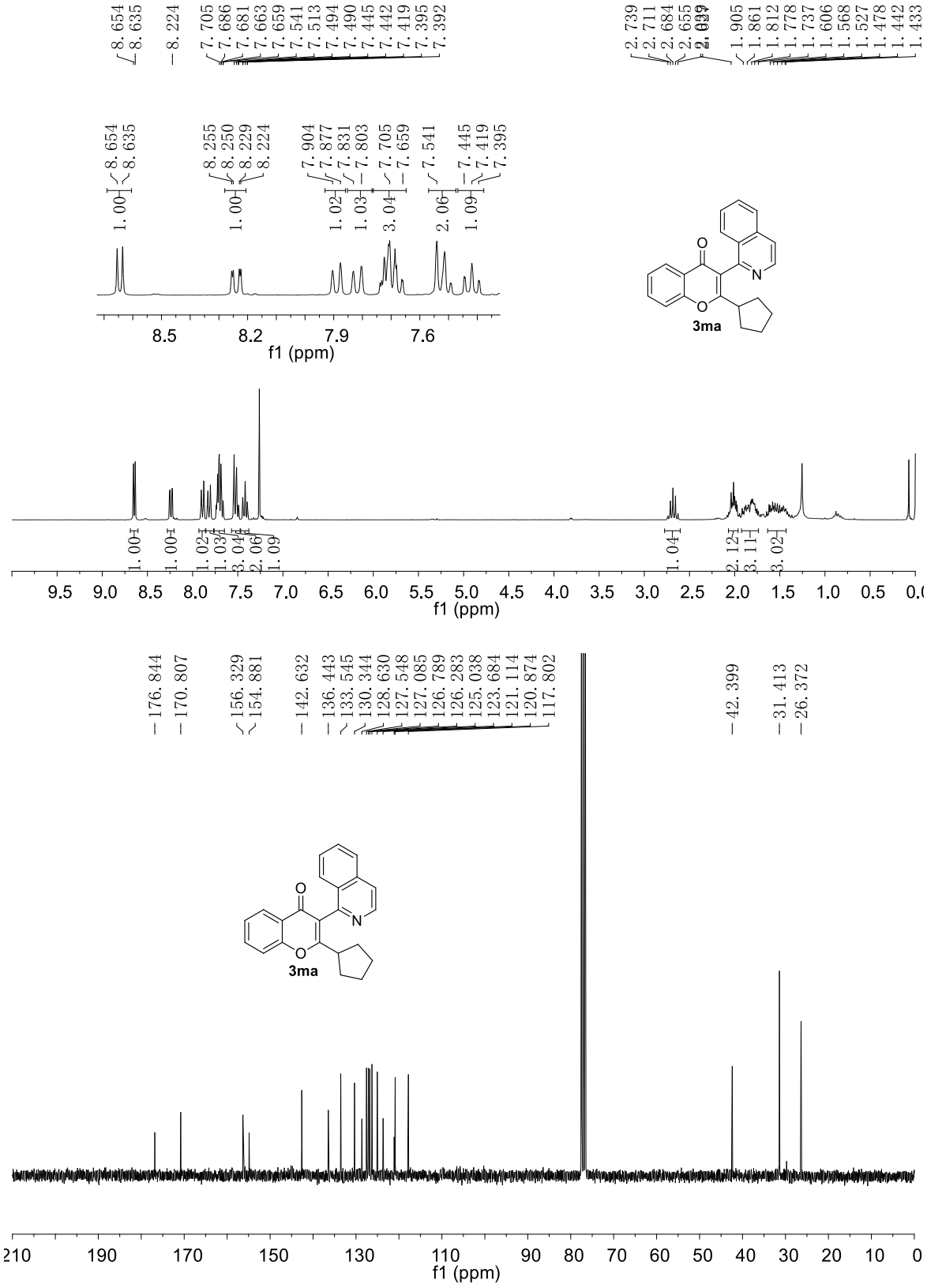
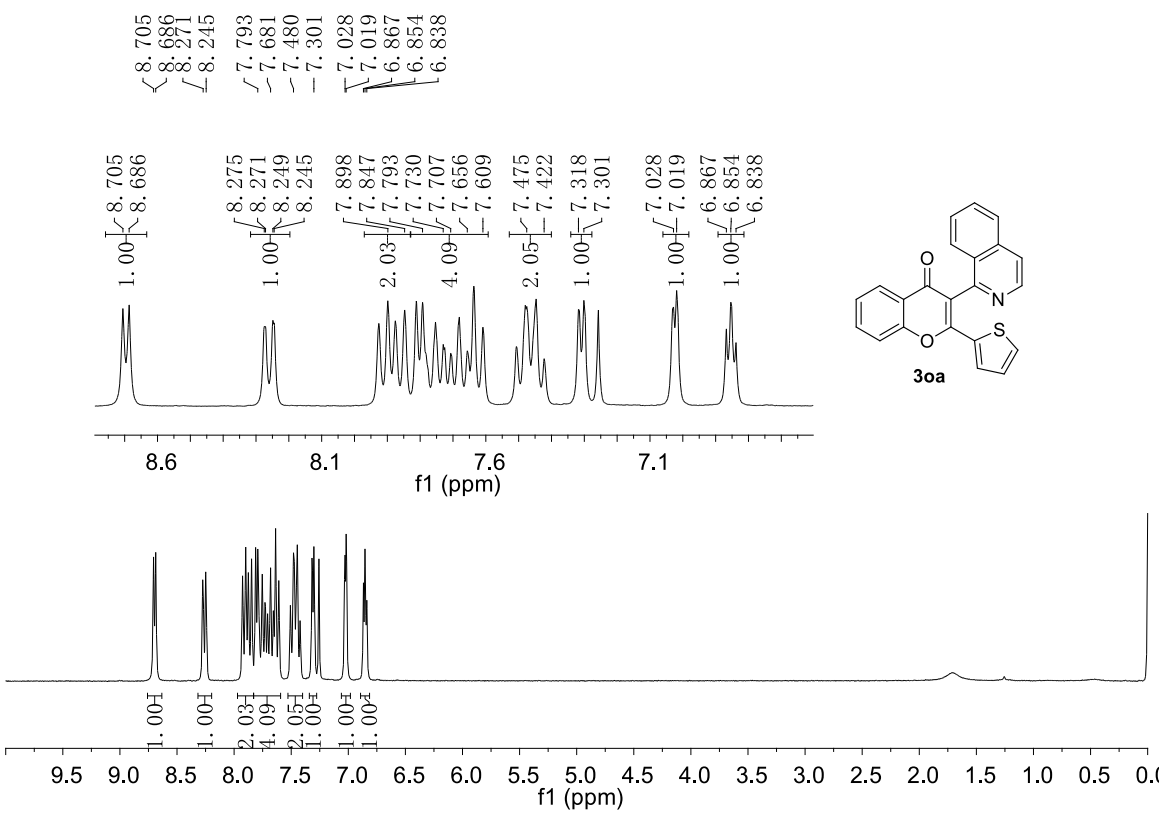
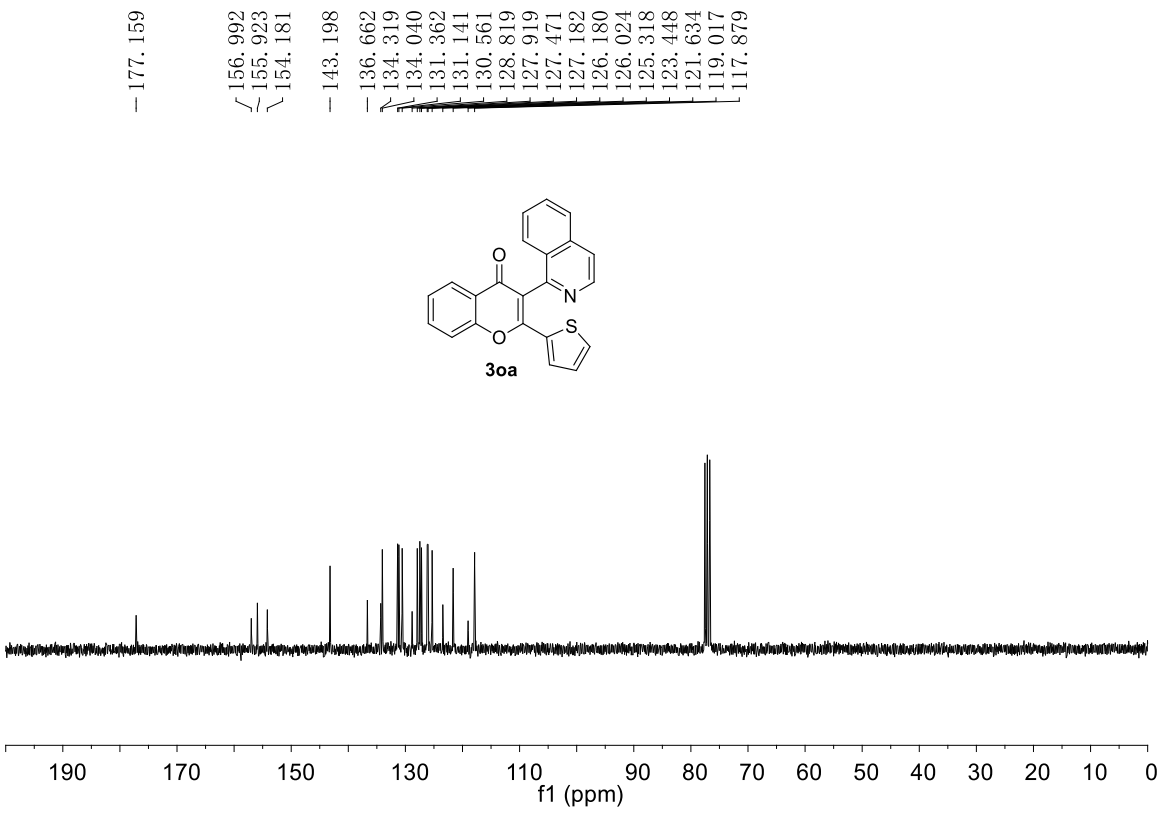
172.272
156.134
156.019
142.000
135.987
133.733
130.122
129.497
127.576
127.071
126.741
126.025
124.973
122.847
120.892
120.782
117.674
39.179
29.037
3ka
f1 (ppm)

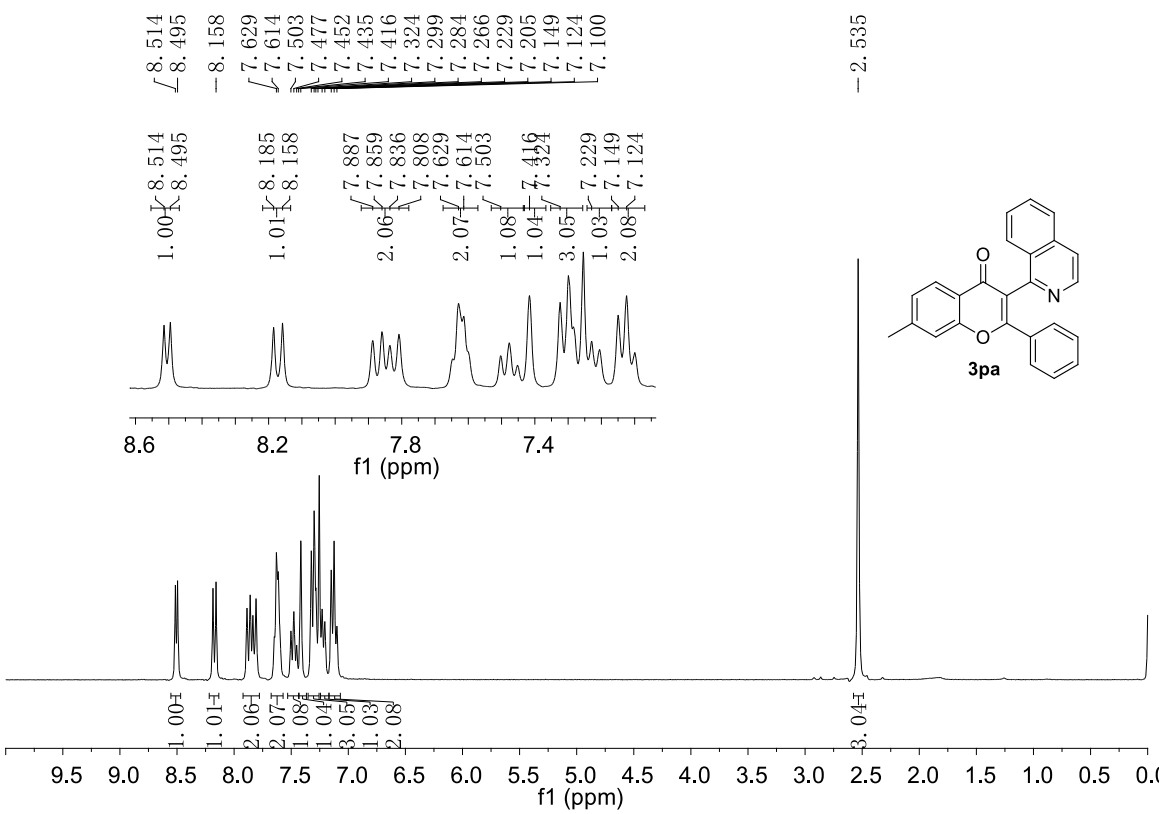

8.643
8.624
8.234
7.784
7.721
7.713
7.709
7.704
7.686
7.658
7.546
7.518
7.491
7.450
7.426
7.399
2.480
2.471
2.450
2.443
2.427
2.421
2.395
1.655
1.589
1.517
1.180
0.739
0.715
0.690
1.00
0.97
1.02
1.03
3.16
2.05
1.14
2.06
2.07
2.02
3.00
8.265
8.261
8.239
8.234
7.900
7.872
7.738
7.709
7.658
7.518
7.450
7.426
7.399
O
N
O
3la
f1 (ppm)
176.808
168.787
156.298
154.616
142.581
136.414
133.624
130.323
128.536
127.561
127.084
126.751
126.290
125.103
123.650
121.888
120.967
117.852
32.504
29.114
22.268
13.552
O
N
O
3la
f1 (ppm)

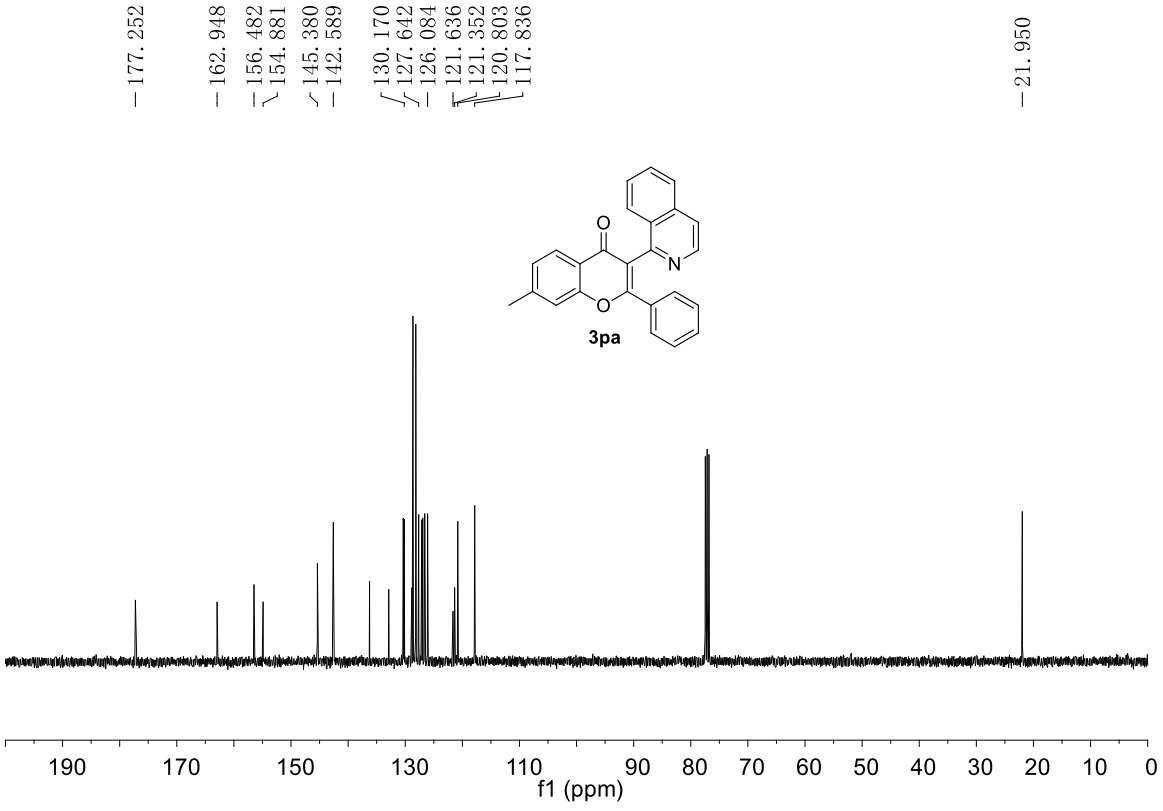

8.654
8.635
8.224
7.705
7.686
7.681
7.663
7.659
7.541
7.513
7.494
7.490
7.445
7.442
7.419
7.395
7.392
2.739
2.711
2.684
2.655
1.905
1.861
1.812
1.778
1.737
1.606
1.568
1.527
1.478
1.442
1.433
1.00
1.00
1.02
1.03
3.04
2.06
1.09
8.255
8.250
8.229
8.224
7.904
7.877
7.831
7.803
7.705
7.659
7.541
7.445
7.419
7.395
8.5
8.2
7.9
7.6
f1 (ppm)
O
N
O
3ma
1.00
1.00
1.02
1.03
3.04
2.06
1.09
1.04
2.12
3.11
3.02
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)
176.844
170.807
156.329
154.881
142.632
136.443
133.545
130.344
128.630
127.548
127.085
126.789
126.283
125.038
123.684
121.114
120.874
117.802
42.399
31.413
26.372
O
N
O
3ma
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

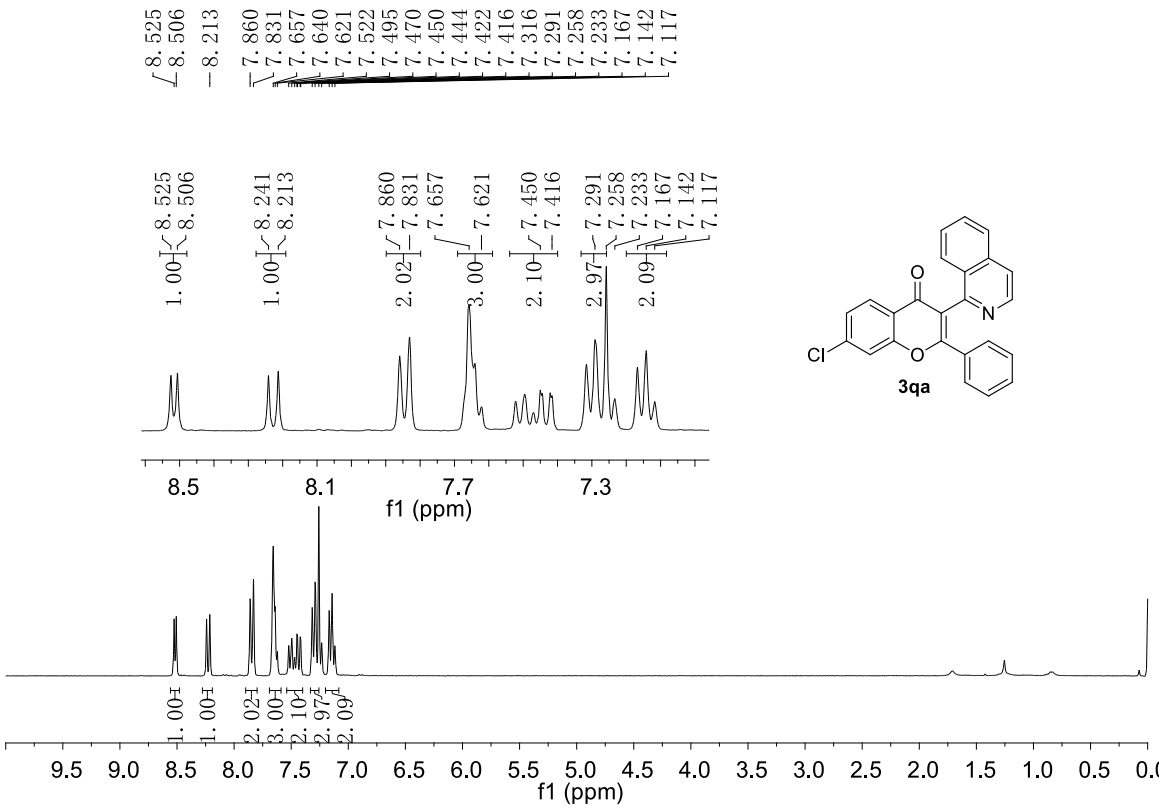

8.705
8.686
8.271
8.245
7.793
7.681
7.480
7.301
7.028
7.019
6.867
6.854
6.838
1.00
1.00
2.03
4.09
2.05
1.00
1.00
1.00
f1 (ppm)
O
N
S
O
3oa

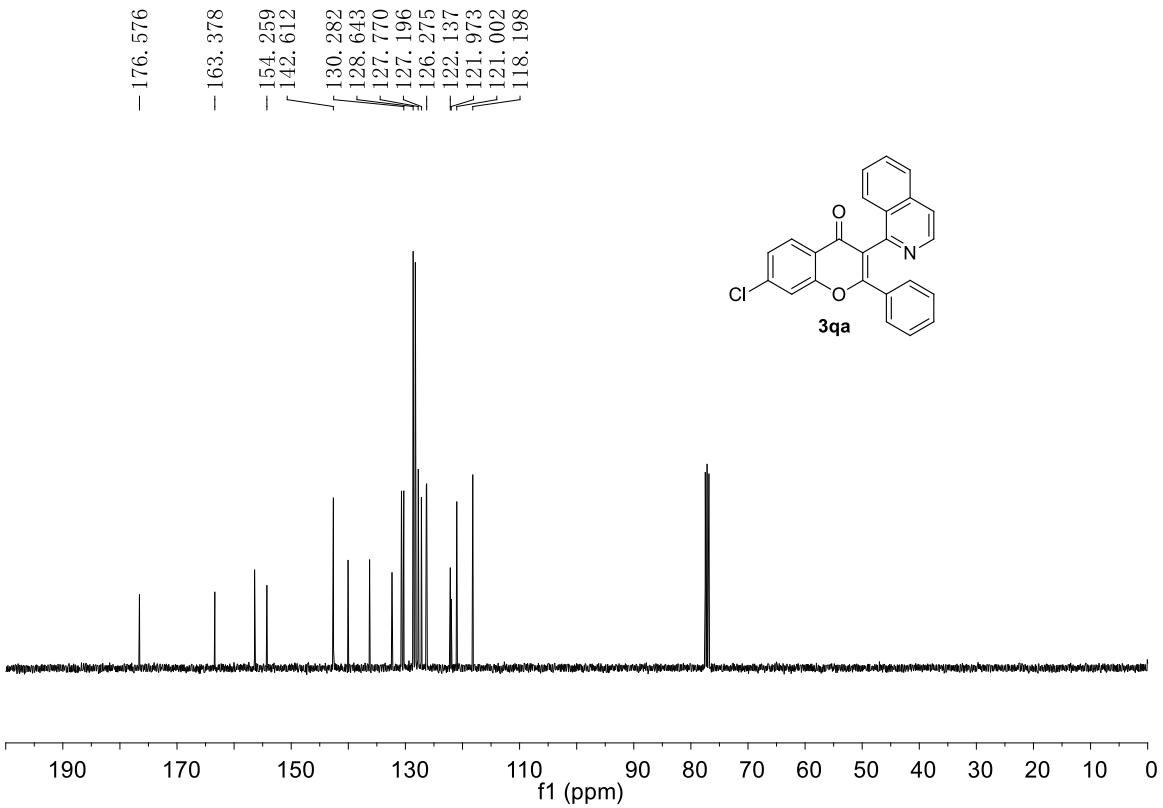
1.00
1.00
2.03
4.09
2.05
1.00
1.00
1.00
f1 (ppm)

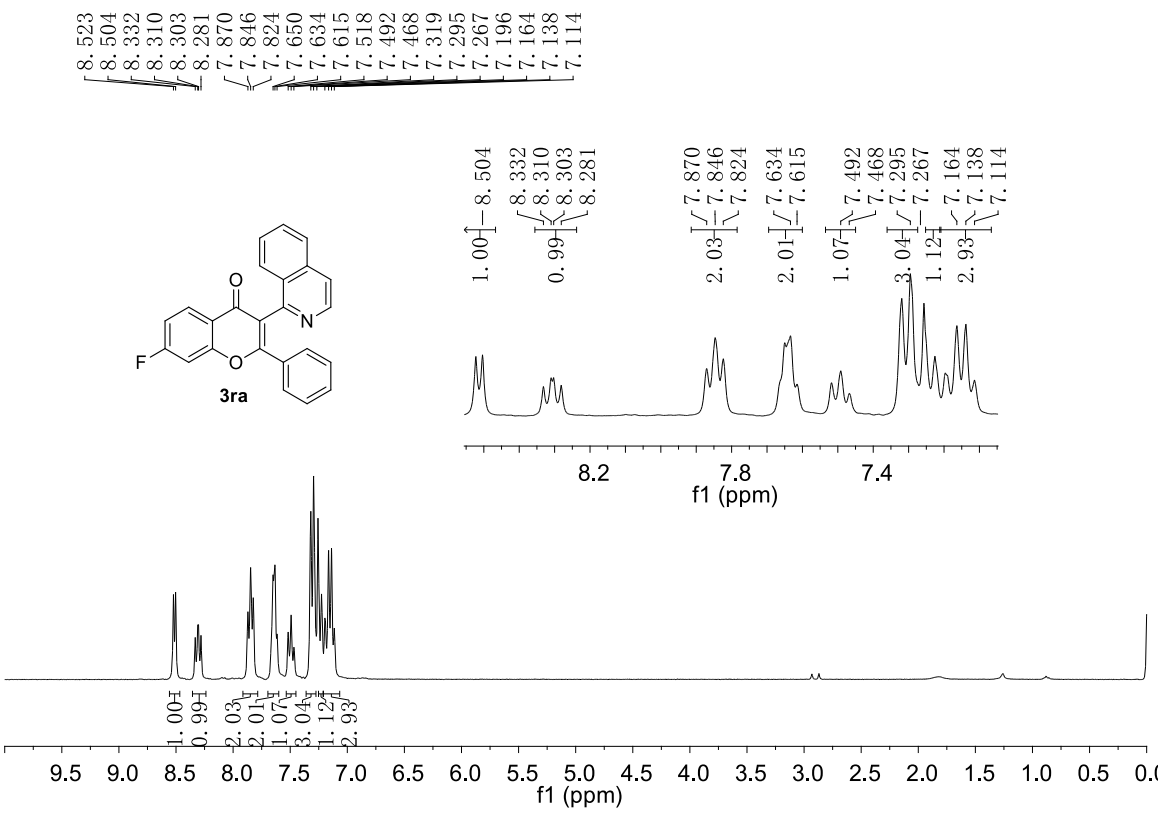

177.159
156.992
155.923
154.181
143.198
136.662
134.319
134.040
131.362
131.141
130.561
128.819
127.919
127.471
127.182
126.180
126.024
125.318
123.448
121.634
119.017
117.879
O
N
S
O
3oa
f1 (ppm)

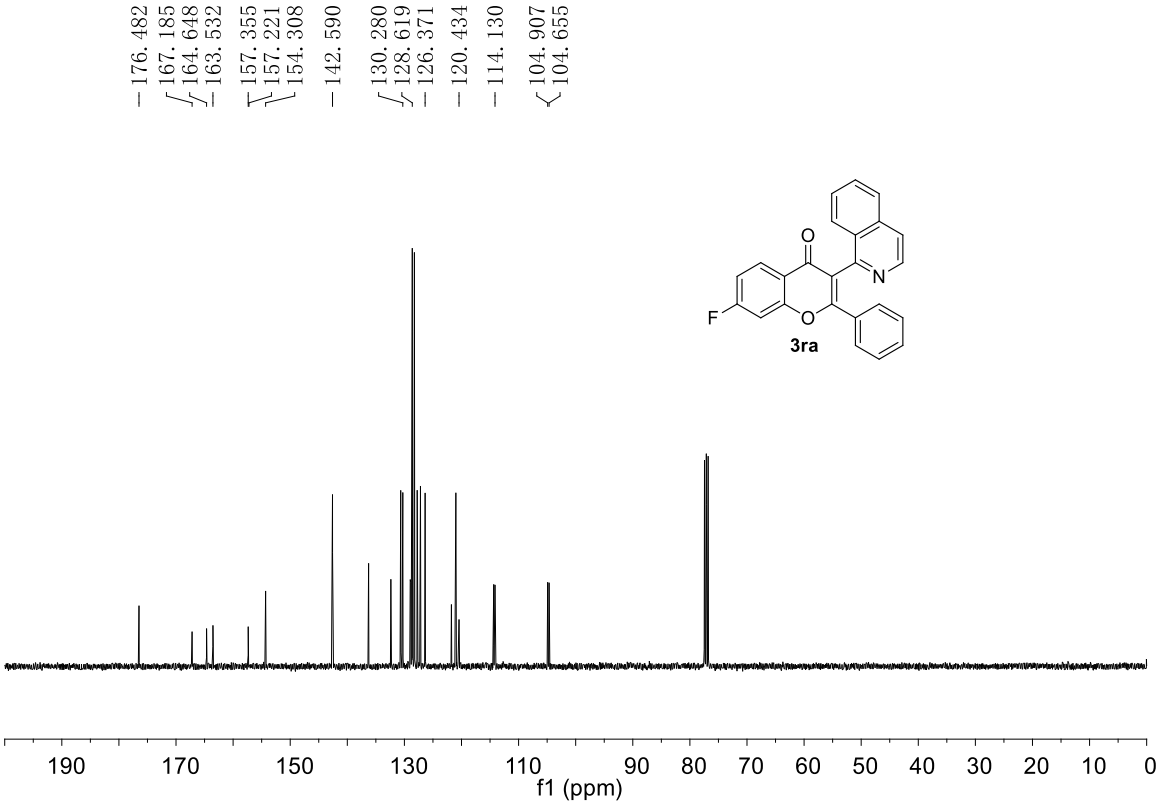

8.514
8.495
8.158
7.629
7.614
7.503
7.477
7.452
7.435
7.416
7.324
7.299
7.284
7.266
7.229
7.205
7.149
7.124
7.100
2.535
1.00
1.01
2.06
2.07
1.08
1.04
3.05
1.03
2.08
3.04
3pa
f1 (ppm)

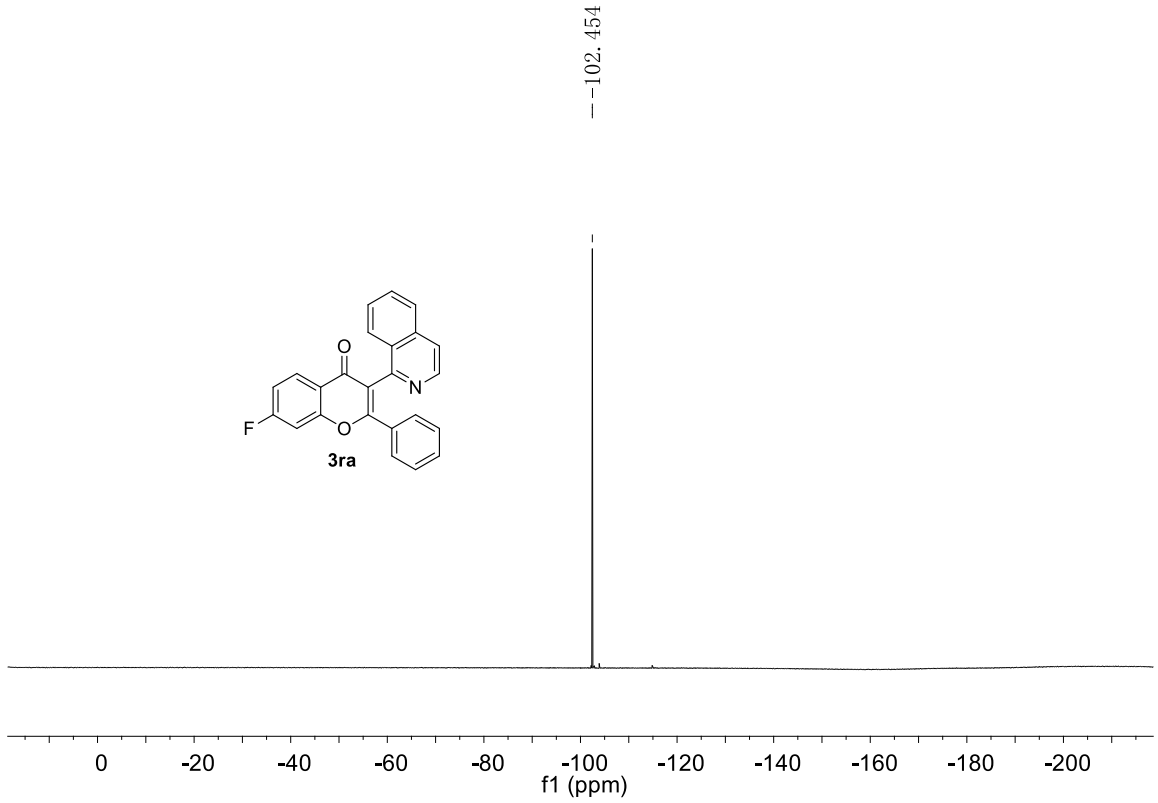

177.252
162.948
156.482
154.881
145.380
142.589
130.170
127.642
126.084
121.636
121.352
120.803
117.836
21.950
3pa
f1 (ppm)

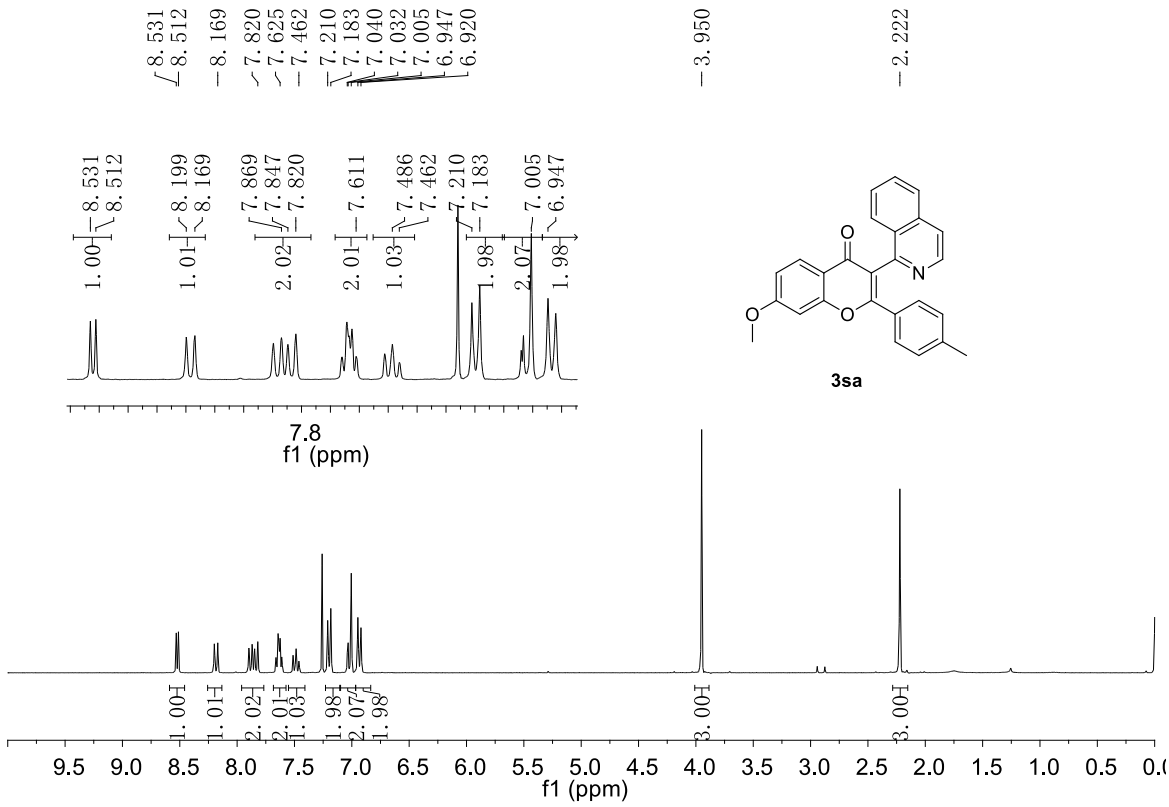

8.525
8.506
8.213
7.860
7.831
7.657
7.640
7.621
7.522
7.495
7.470
7.450
7.444
7.422
7.416
7.316
7.291
7.258
7.233
7.167
7.142
7.117
1.00
1.00
2.02
3.00
2.10
2.97
2.09
f1 (ppm)
Cl
O
N
3qa

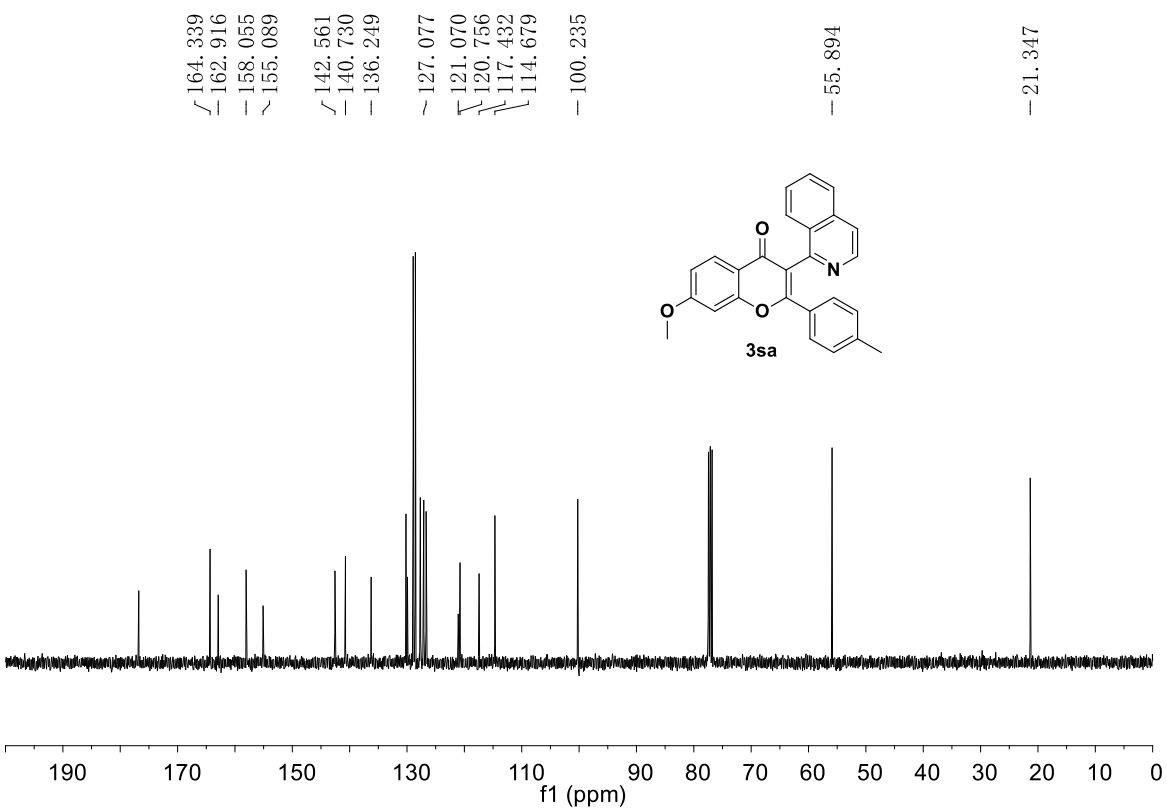

176.576
163.378
154.259
142.612
130.282
128.643
127.770
127.196
126.275
122.137
121.973
121.002
118.198
f1 (ppm)
Cl
O
N
3qa

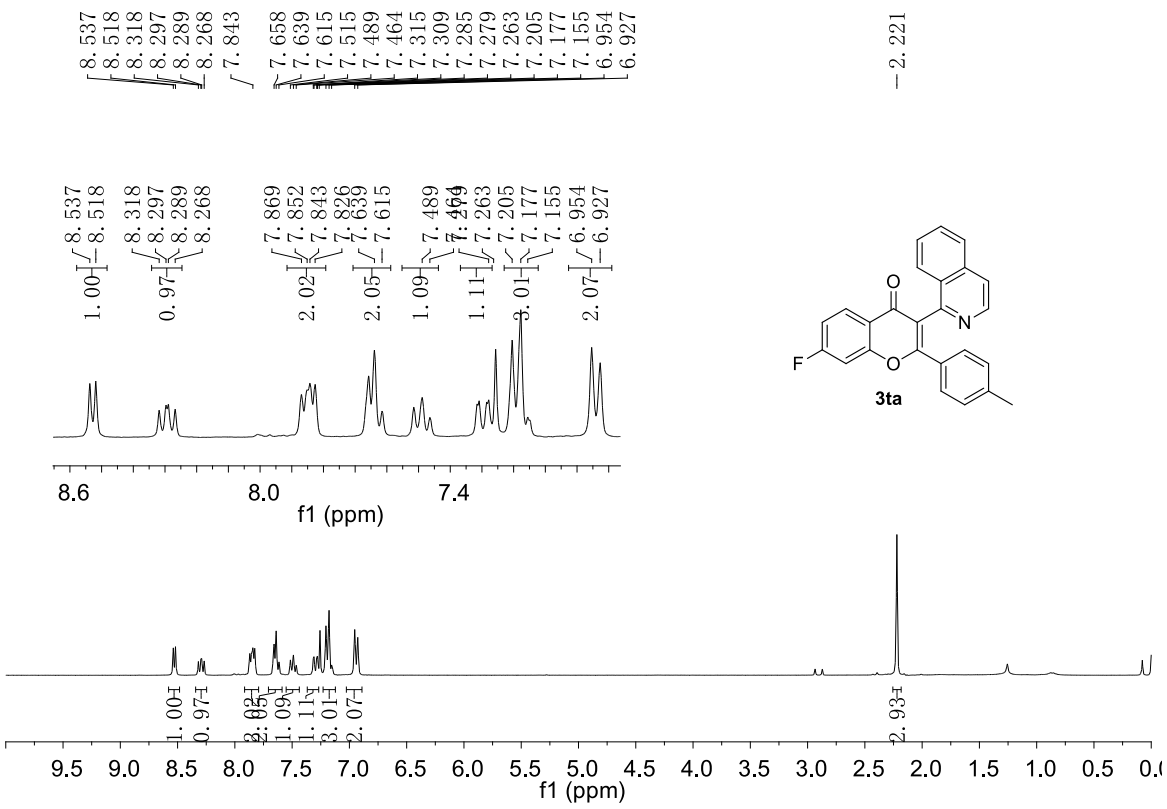

8.523
8.504
8.332
8.310
8.303
8.281
7.870
7.846
7.824
7.650
7.634
7.615
7.518
7.492
7.468
7.319
7.295
7.267
7.196
7.164
7.138
7.114
1.00
0.99
2.03
2.01
1.07
3.04
1.12
2.93
F
O
N
O
3ra
8.2
7.8
7.4
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

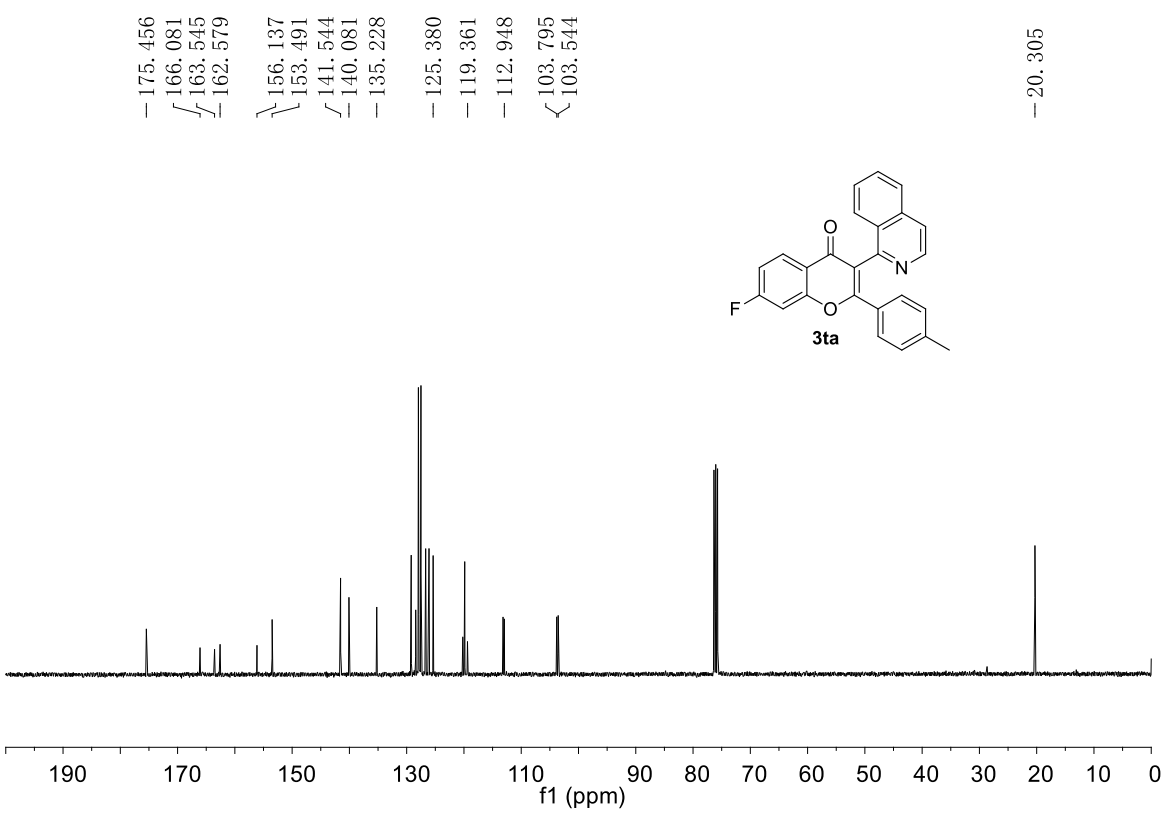

176.482
167.185
164.648
163.532
157.355
157.221
154.308
142.590
130.280
128.619
126.371
120.434
114.130
104.907
104.655
F
O
N
O
3ra
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

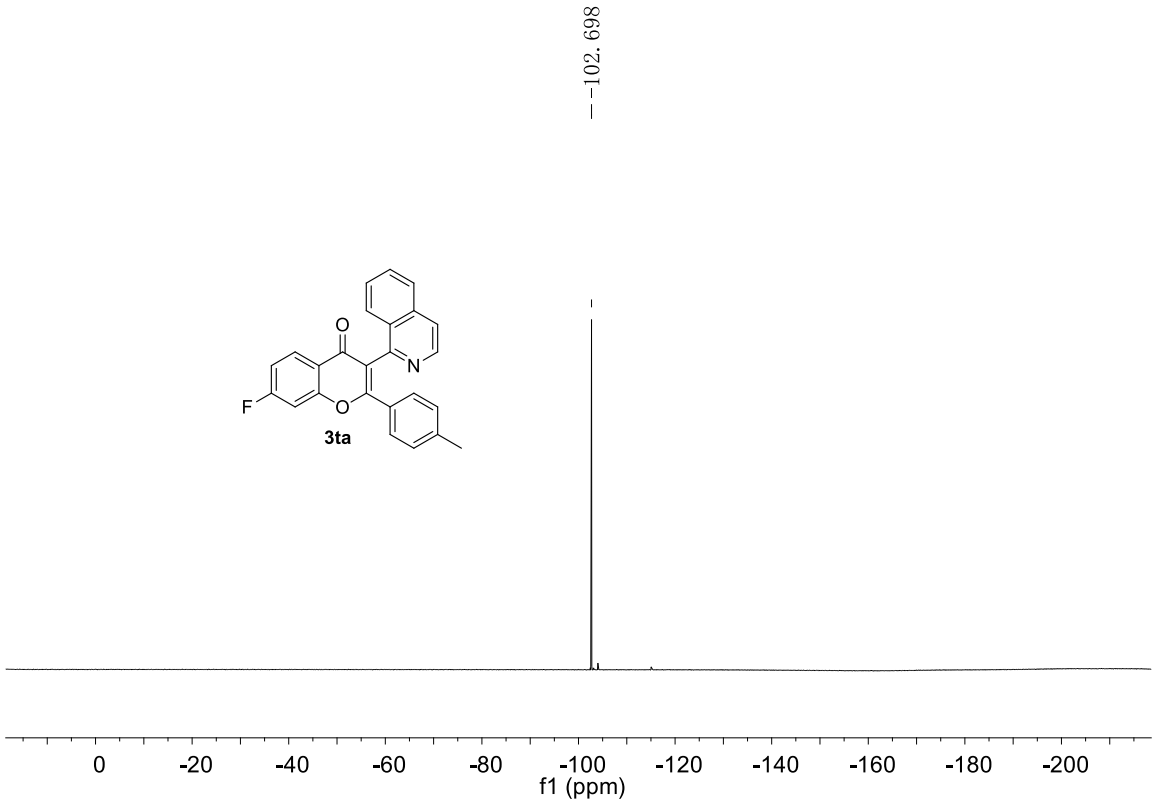

-102.454
O
N
F
O
3ra
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

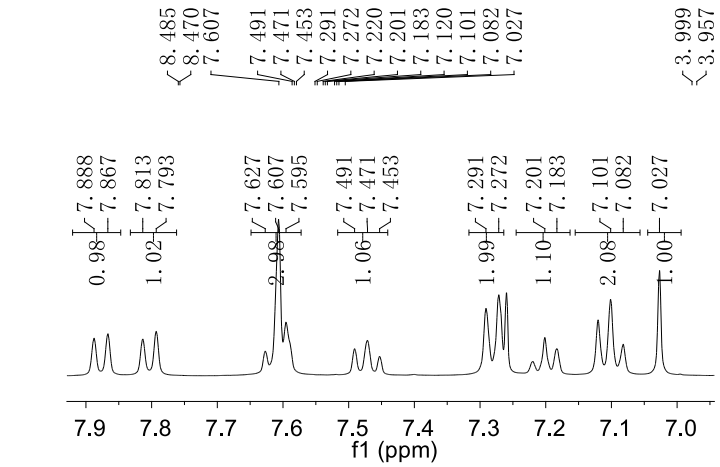

8.531
8.512
8.169
7.820
7.625
7.462
7.210
7.183
7.040
7.032
7.005
6.947
6.920
3.950
2.222
1.00
1.01
2.02
2.01
1.03
1.98
2.07
1.98
O
N
O
O
3sa
7.8
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


164.339
162.916
158.055
155.089
142.561
140.730
136.249
127.077
121.070
120.756
117.432
114.679
100.235
55.894
21.347
O
N
O
O
3sa
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.537
8.518
8.318
8.297
8.289
8.268
7.843
7.658
7.639
7.615
7.515
7.489
7.464
7.315
7.309
7.285
7.279
7.263
7.205
7.177
7.155
6.954
6.927
2.221
1.00
0.97
2.02
2.05
1.09
1.11
3.01
2.07
2.93
O
N
F
O
3ta
8.6
8.0
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)


175.456
166.081
163.545
162.579
156.137
153.491
141.544
140.081
135.228
125.380
119.361
112.948
103.795
103.544
20.305
O
N
F
O
3ta
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-102.698
O
N
F
O
3ta
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)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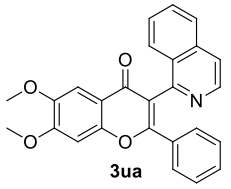
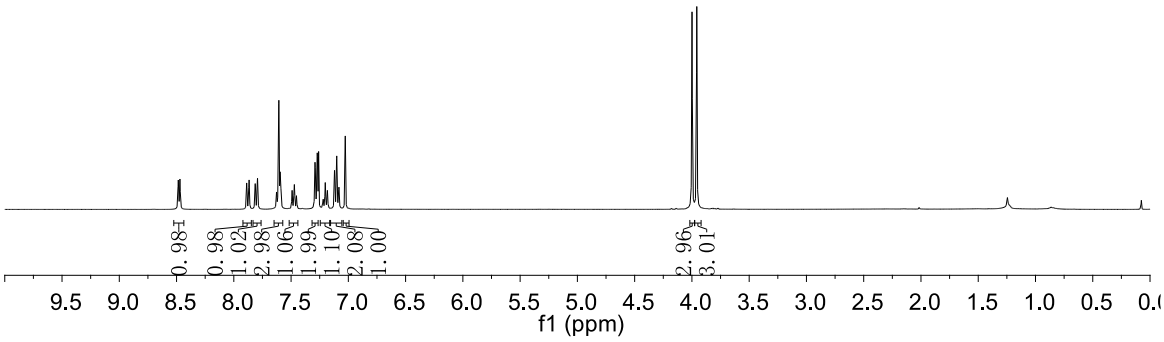
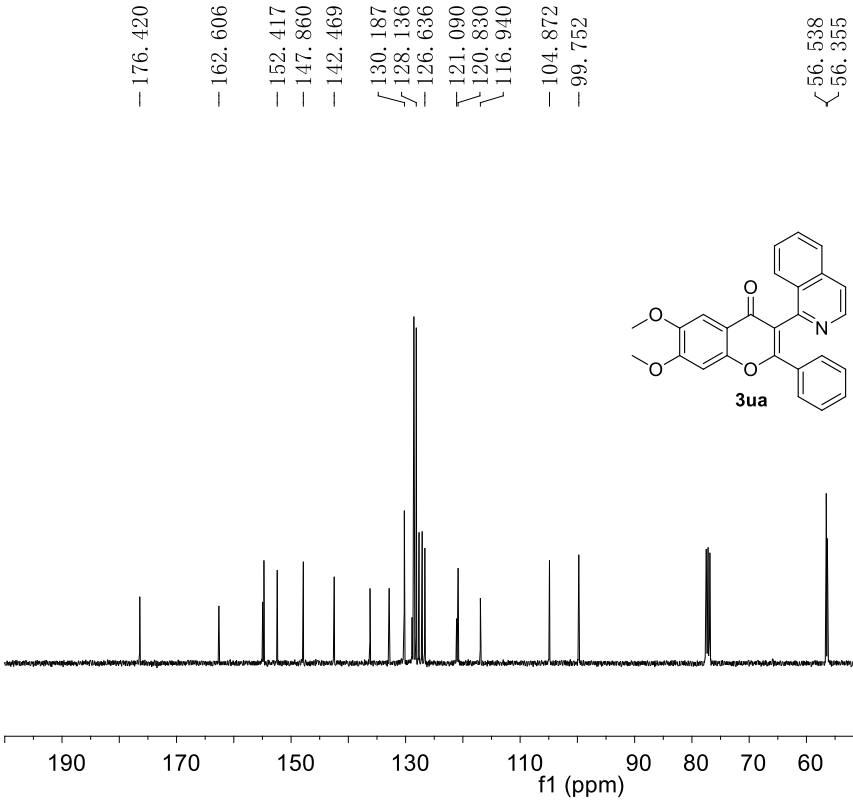
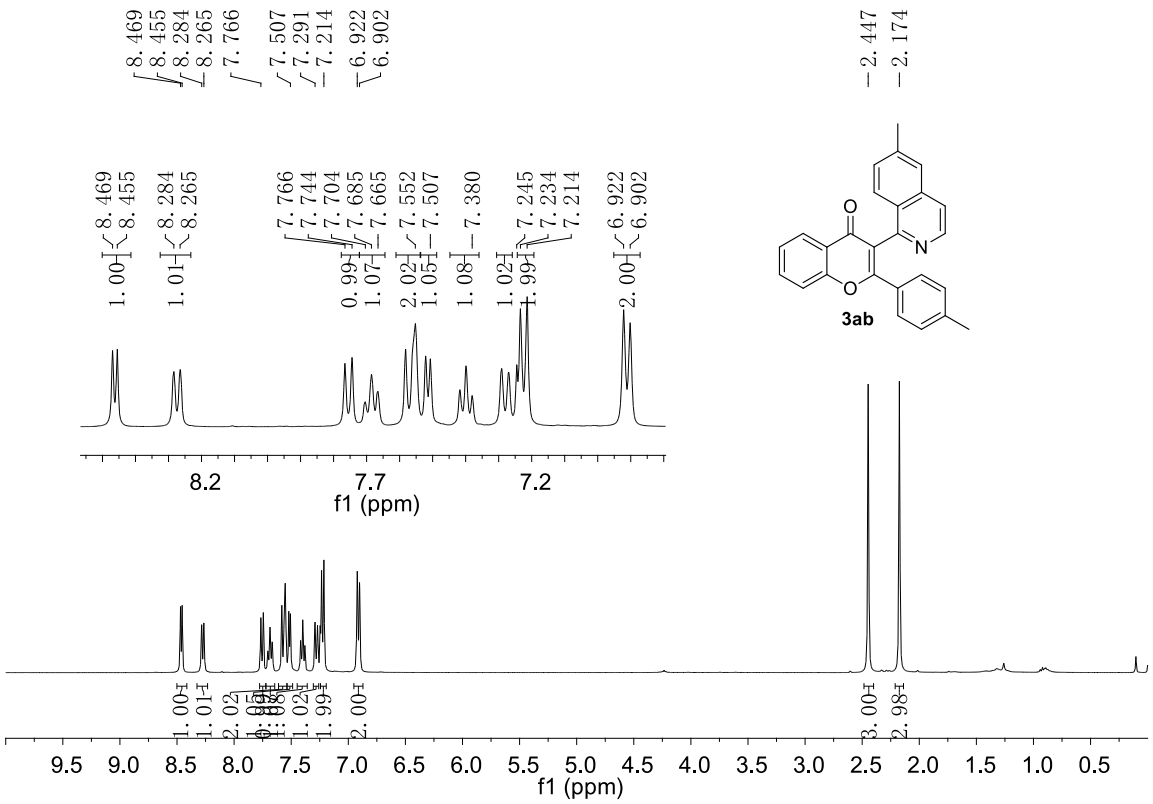
8.470
7.607
7.491
7.471
7.453
7.291
7.272
7.220
7.201
7.183
7.120
7.101
7.082
7.027
3.999
3.957
7.888
7.867
7.813
7.793
7.627
7.607
7.595
7.491
7.471
7.453
7.291
7.272
7.201
7.183
7.101
7.082
7.027
0.98
1.02
2.98
1.06
1.99
1.10
2.08
1.00
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)

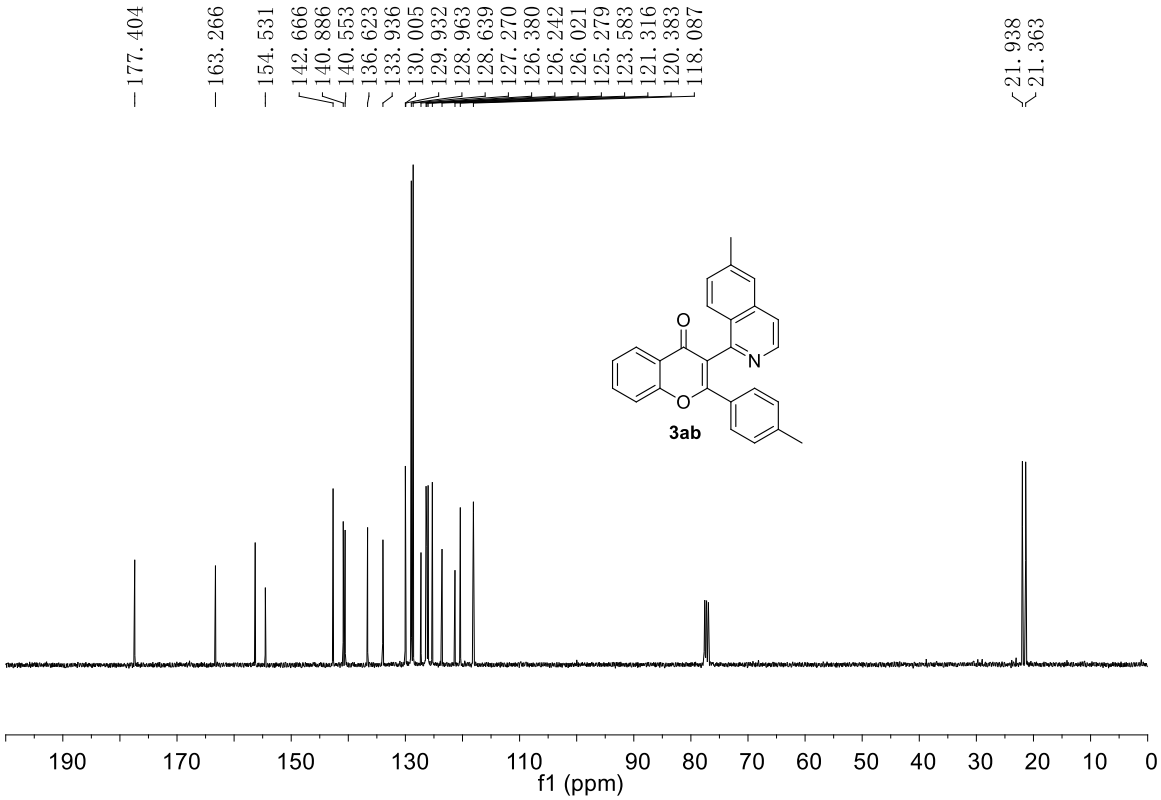

O
O
O
N
O
3ua

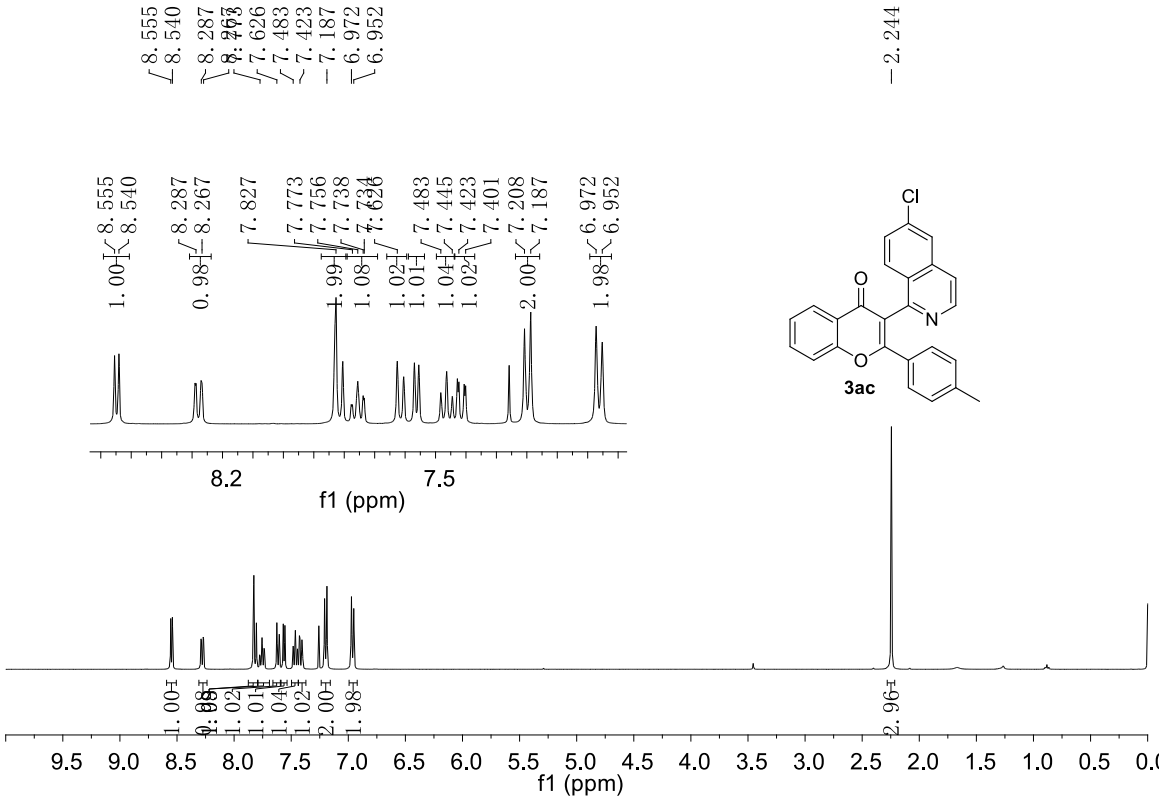

0.98
0.98
1.02
2.98
1.06
1.99
1.10
2.08
1.00
2.96
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


176.420
162.606
152.417
147.860
142.469
130.187
128.136
126.636
121.090
120.830
116.940
104.872
99.752
56.538
56.355
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

O
O
O
N
O
3ua


8.469
8.455
8.284
8.265
7.766
7.507
7.291
7.214
6.922
6.902
2.447
2.174
3ab
8.2
7.7
7.2
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)


177.404
163.266
154.531
142.666
140.886
140.553
136.623
133.936
130.005
129.932
128.963
128.639
127.270
126.380
126.242
126.021
125.279
123.583
121.316
120.383
118.087
21.938
21.363
3ab
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.555
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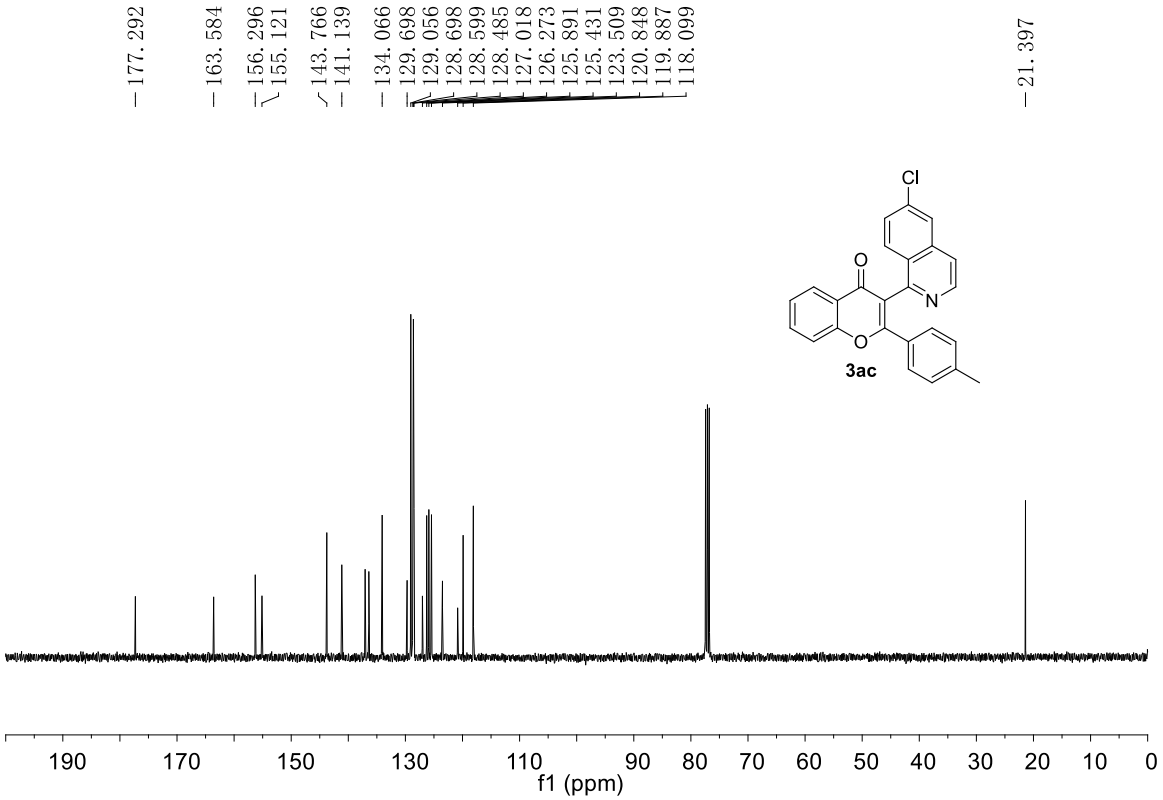
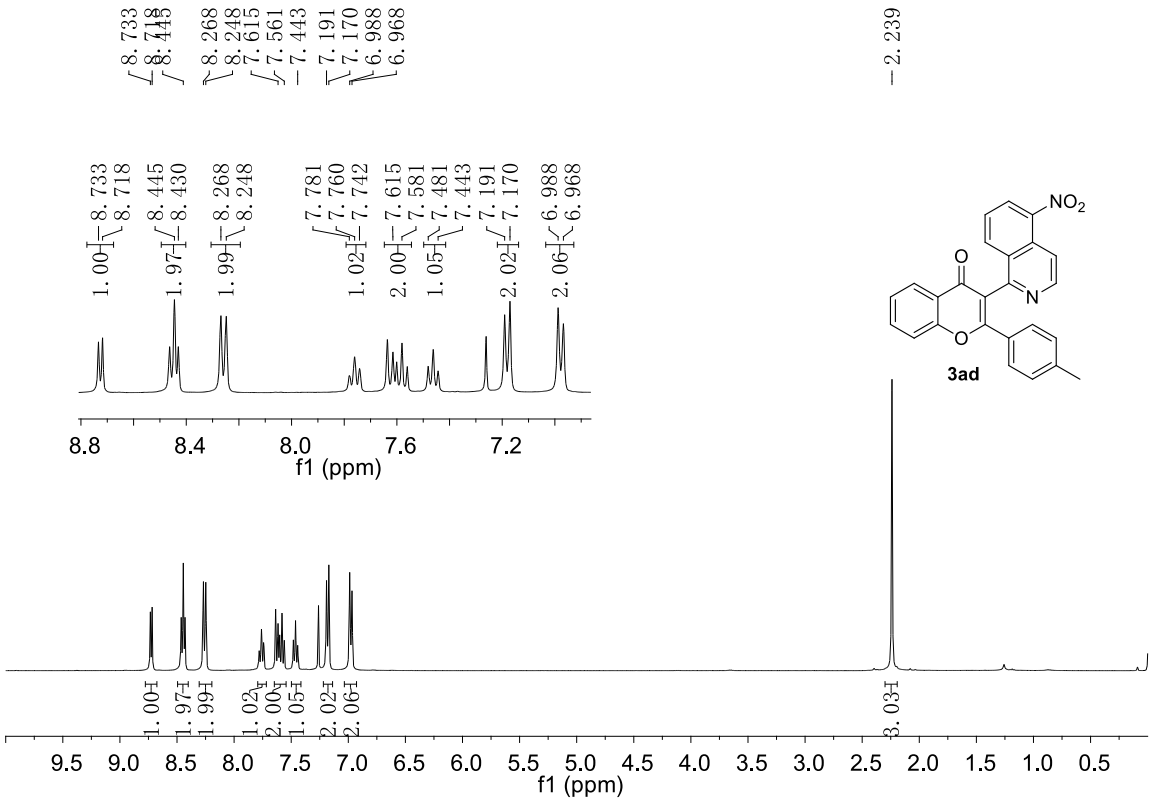
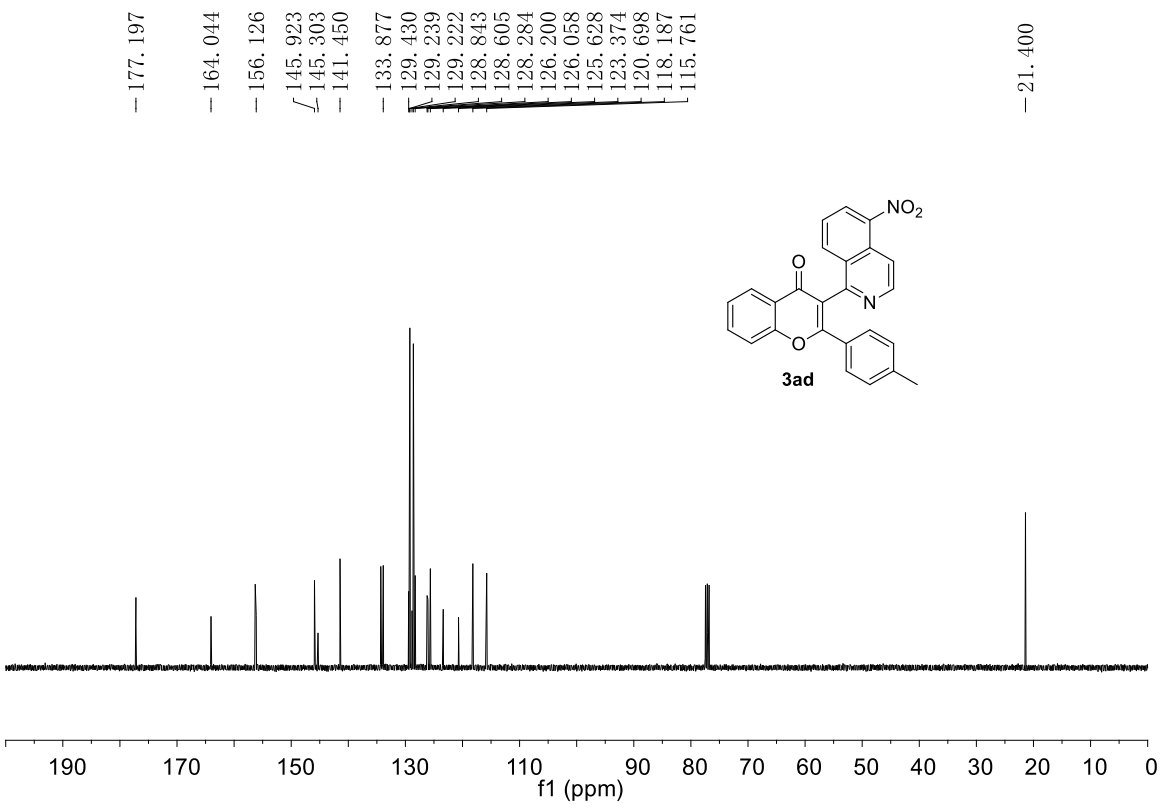
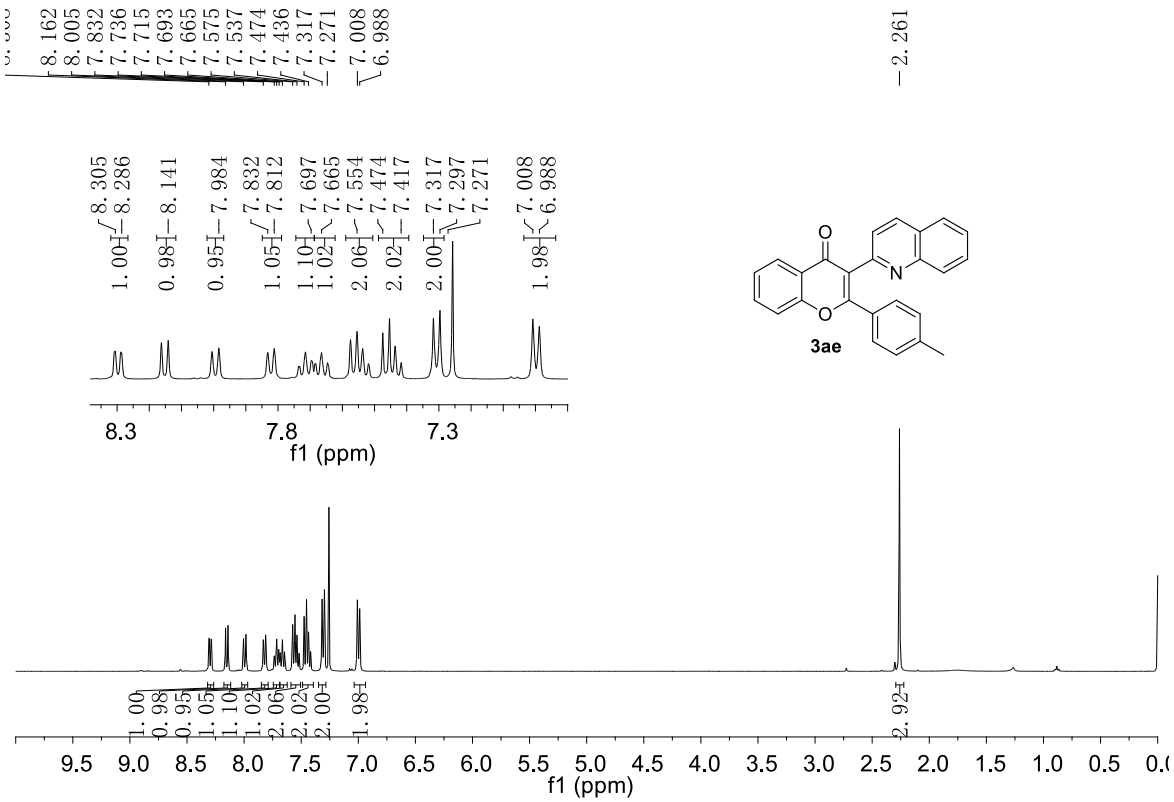
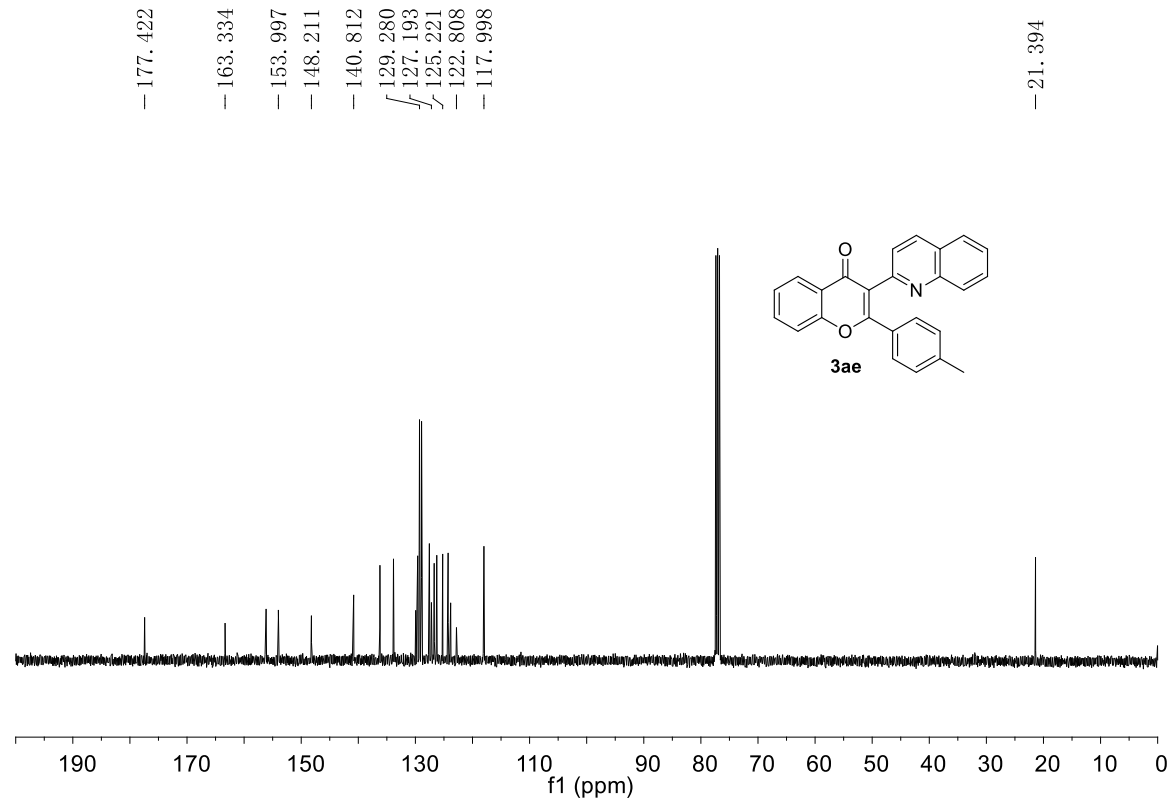
8.287
8.267
7.827
7.773
7.756
7.738
7.626
7.483
7.445
7.423
7.401
7.208
7.187
6.972
6.952
2.244
1.00
0.98
1.99
1.08
1.02
1.01
1.04
1.02
2.00
1.98
2.96
Cl
O
N
O
3ac
8.2
7.5
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

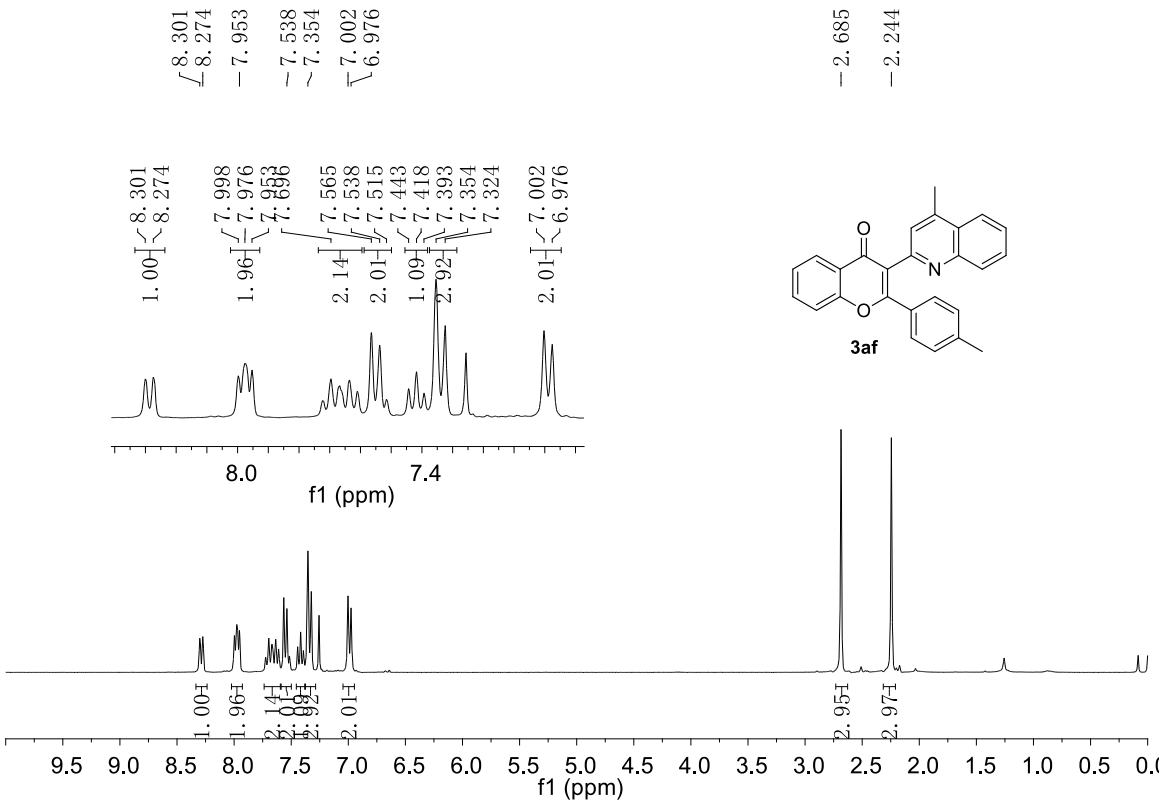

177.292
163.584
156.296
155.121
143.766
141.139
134.066
129.698
129.056
128.698
128.599
128.485
127.018
126.273
125.891
125.431
123.509
120.848
119.887
118.099
21.397
Cl
O
N
O
3ac
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

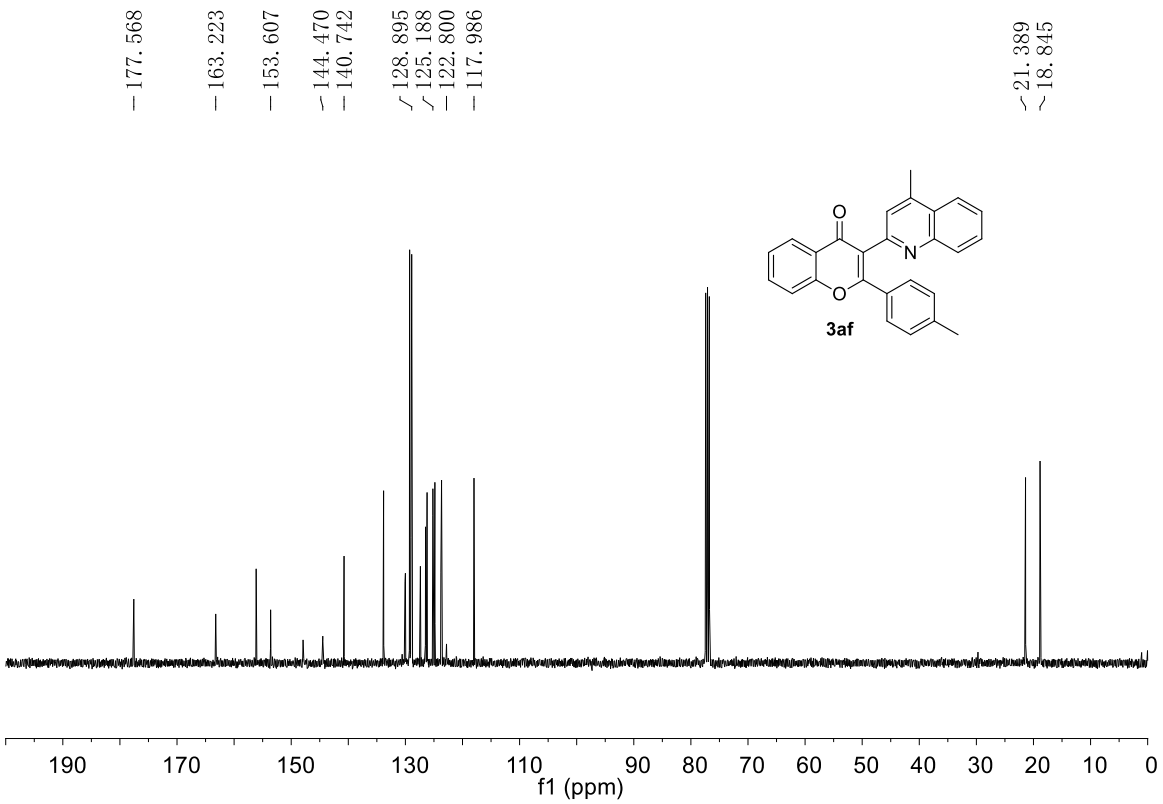

8.733
8.718
8.445
8.430
8.268
8.248
7.615
7.561
7.443
7.191
7.170
6.988
6.968
2.239
1.00
1.97
1.99
2.00
1.05
2.02
2.06
3.03
NO2
O
N
O
3ad
f1 (ppm)

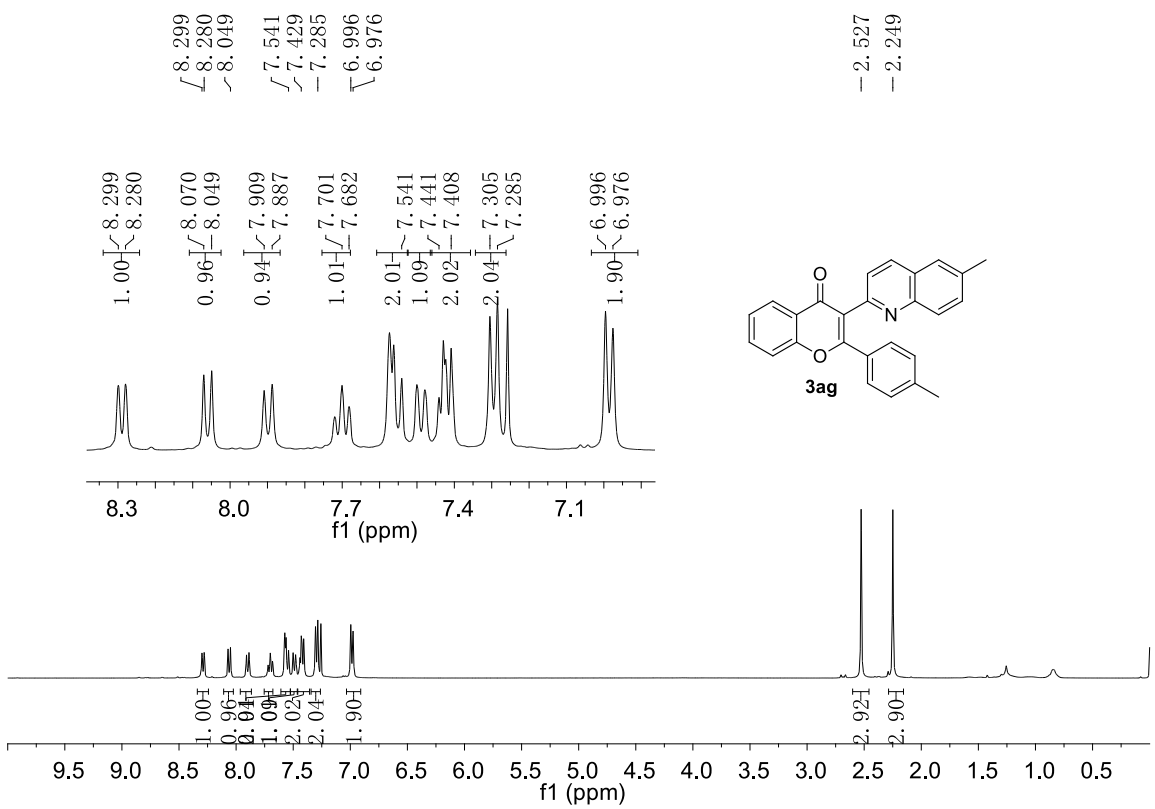

177.197
164.044
156.126
145.923
145.303
141.450
133.877
129.430
129.239
129.222
128.843
128.605
128.284
126.200
126.058
125.628
123.374
120.698
118.187
115.761
21.400
NO2
O
N
O
3ad
f1 (ppm)

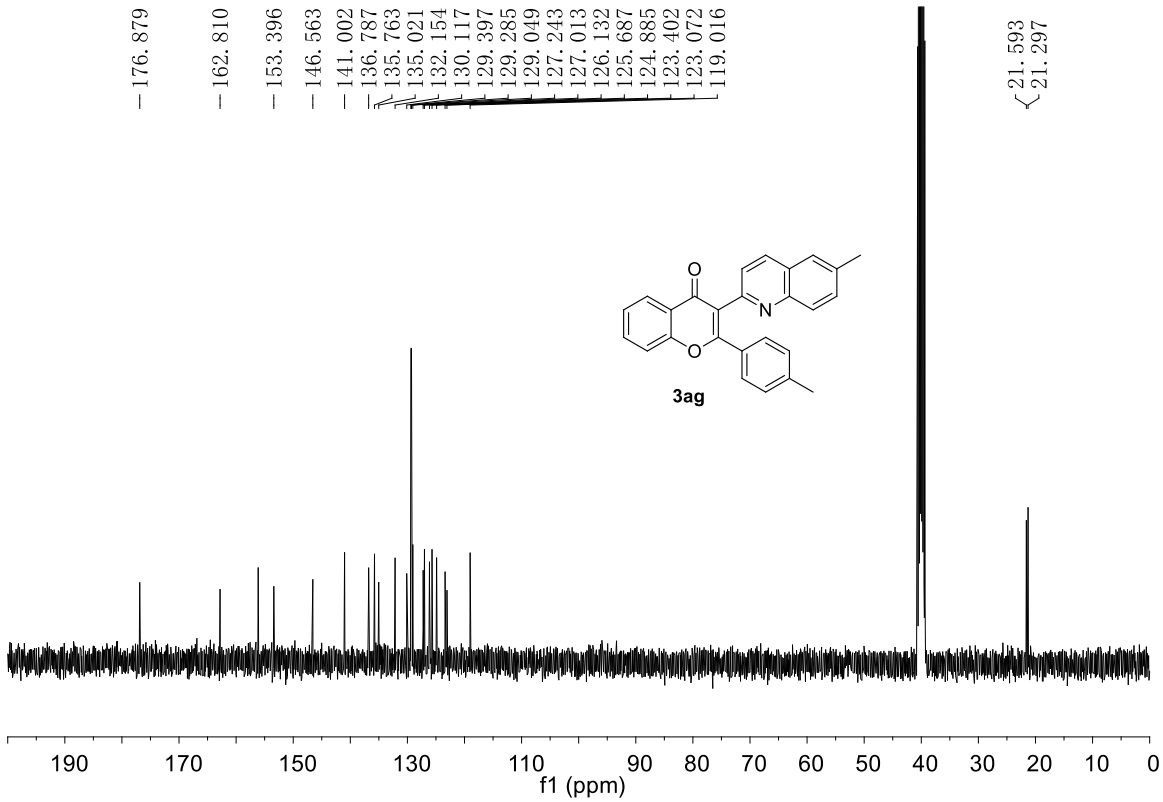

8.162
8.005
7.832
7.736
7.715
7.693
7.665
7.575
7.537
7.474
7.436
7.317
7.271
7.008
6.988
2.261
8.305
8.286
8.141
7.984
7.832
7.812
7.697
7.665
7.554
7.474
7.417
7.317
7.297
7.271
7.008
6.988
1.00
0.98
0.95
1.05
1.10
1.02
2.06
2.02
2.00
1.98
2.92
3ae
f1 (ppm)

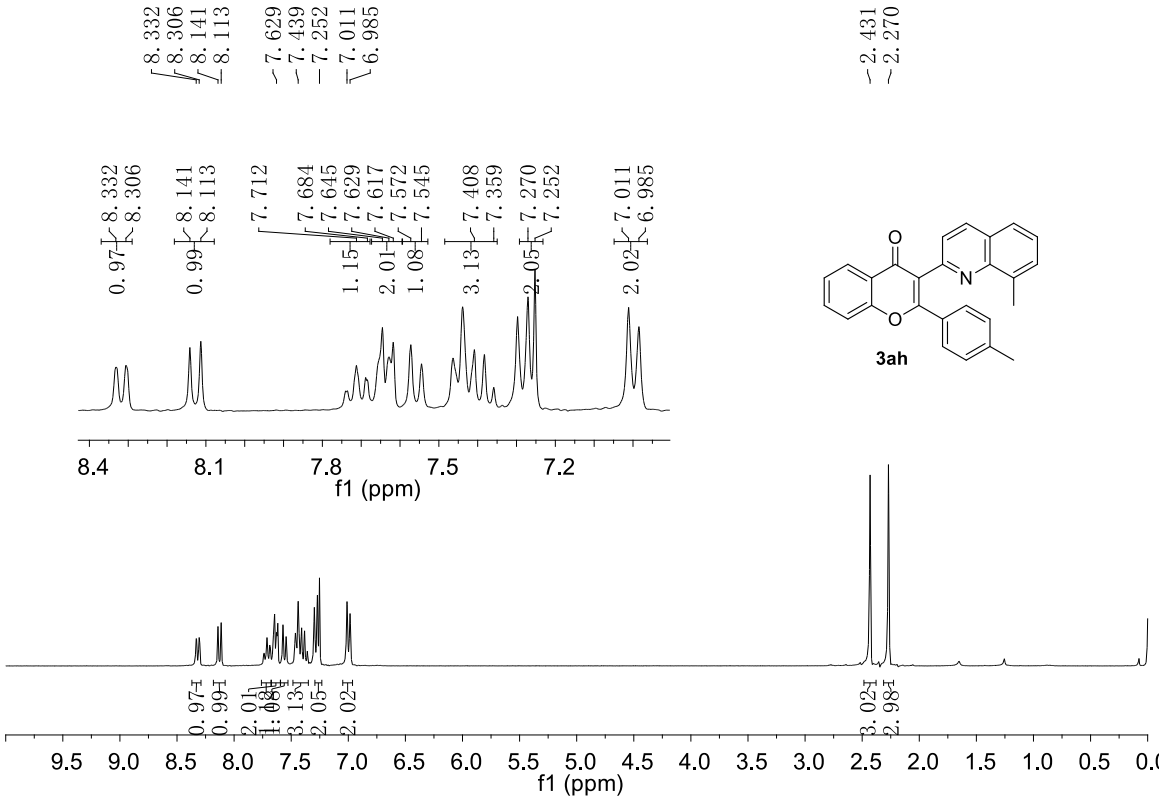

177.422
163.334
153.997
148.211
140.812
129.280
127.193
125.221
122.808
117.998
21.394
3ae
f1 (ppm)

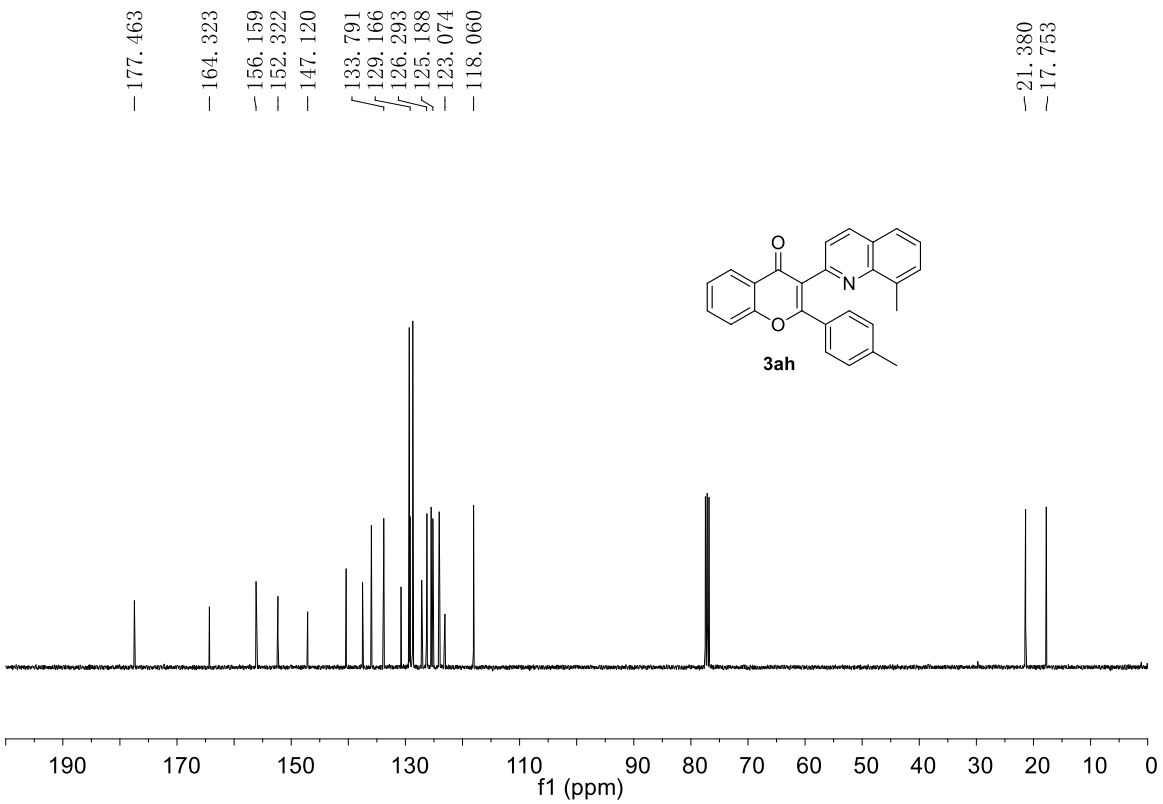

8.301
8.274
7.953
7.538
7.354
7.002
6.976
2.685
2.244
7.998
7.976
7.565
7.538
7.515
7.443
7.418
7.393
7.354
7.324
1.00
1.96
2.14
2.01
1.09
2.92
2.01
2.95
2.97
3af
8.0
7.4
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

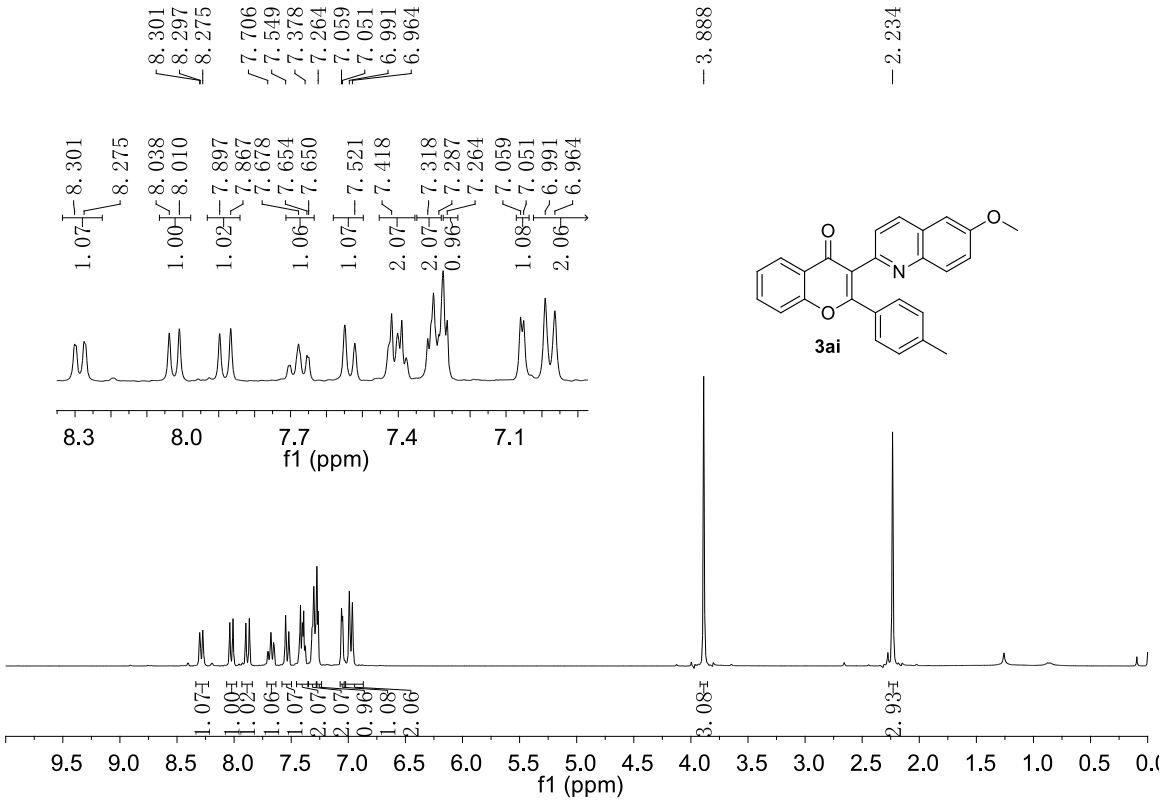

177.568
163.223
153.607
144.470
140.742
128.895
125.188
122.800
117.986
21.389
18.845
3af
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

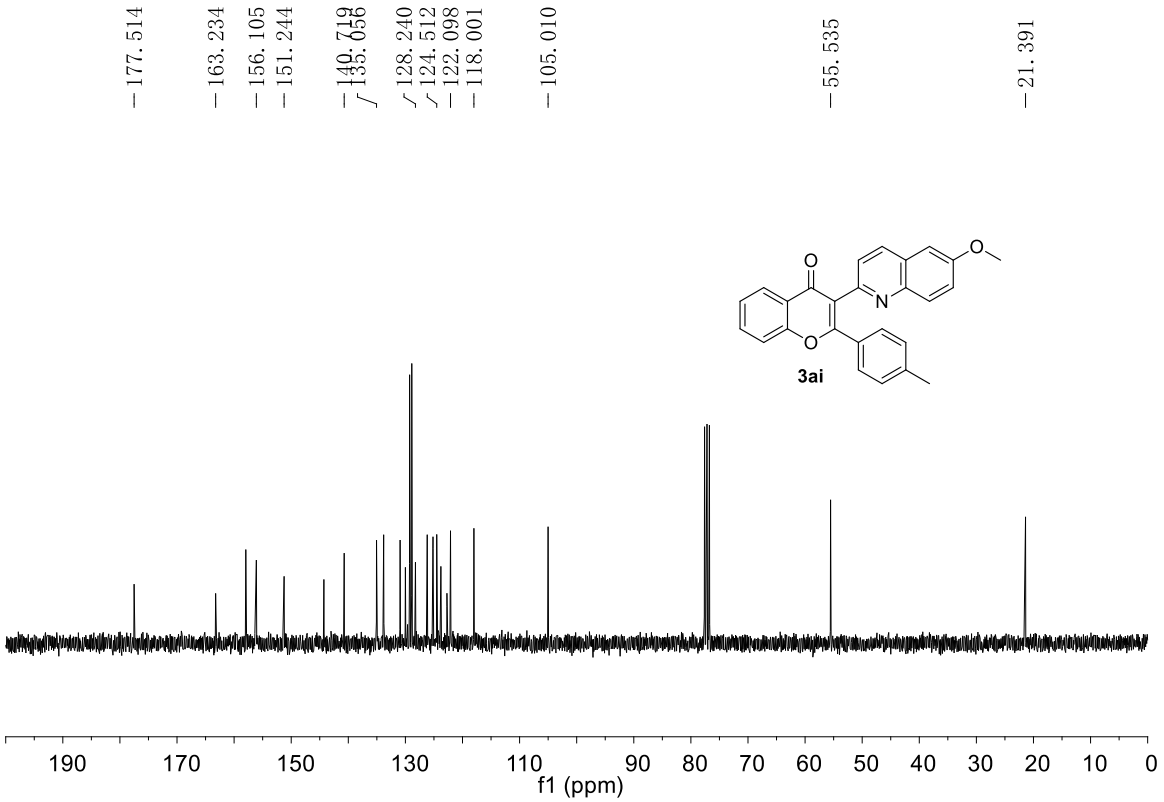

8.299
8.280
8.049
7.541
7.429
7.285
6.996
6.976
2.527
2.249
1.00
0.96
0.94
1.01
2.01
1.09
2.02
2.04
1.90
2.92
2.90
3ag
f1 (ppm)

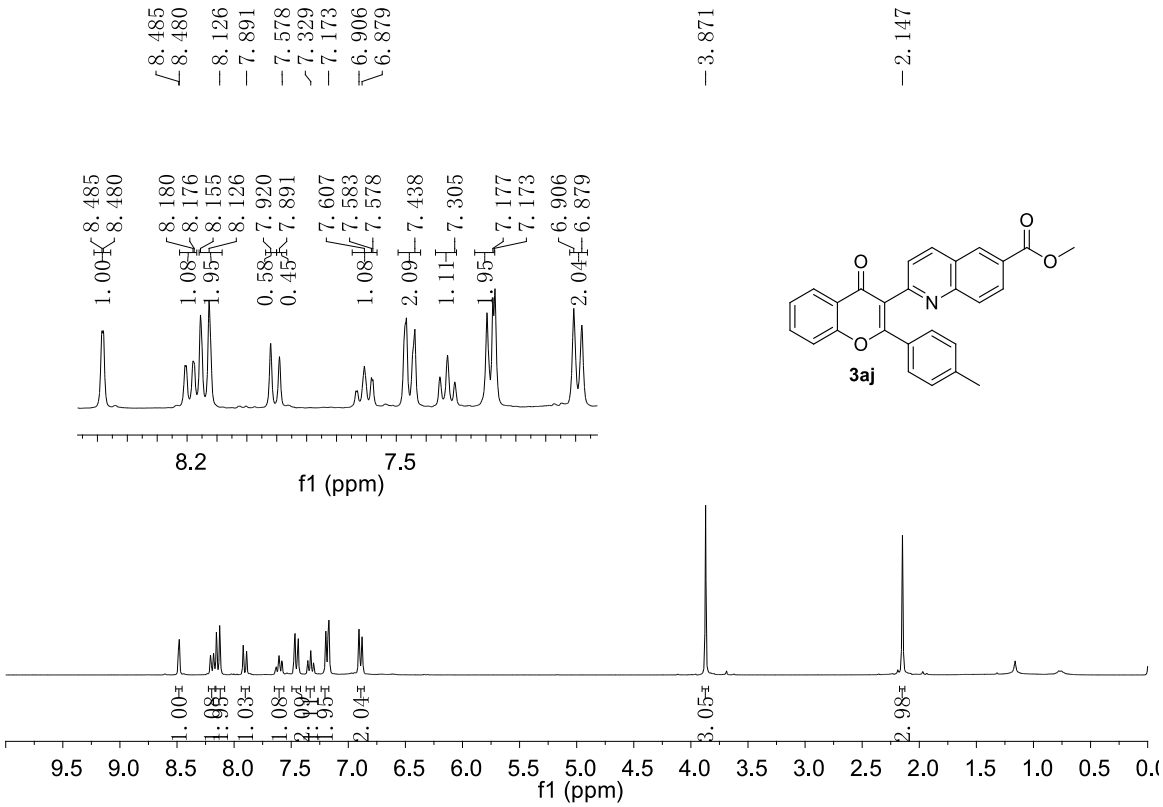

176.879
162.810
153.396
146.563
141.002
136.787
135.763
135.021
132.154
130.117
129.397
129.285
129.049
127.243
127.013
126.132
125.687
124.885
123.402
123.072
119.016
21.593
21.297
3ag
f1 (ppm)

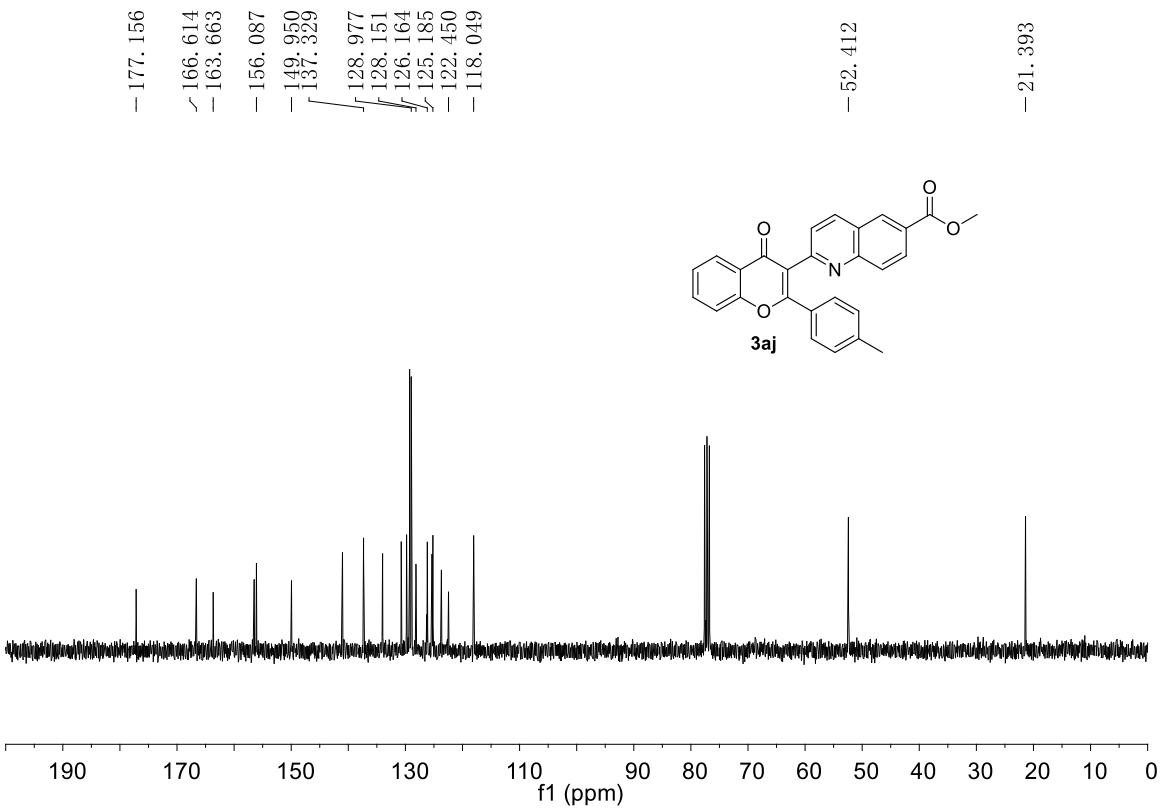

8.332
8.306
8.141
8.113
7.629
7.439
7.252
7.011
6.985
2.431
2.270
0.97
0.99
2.01
1.08
3.13
2.05
2.02
3.02
2.98
3ah
f1 (ppm)

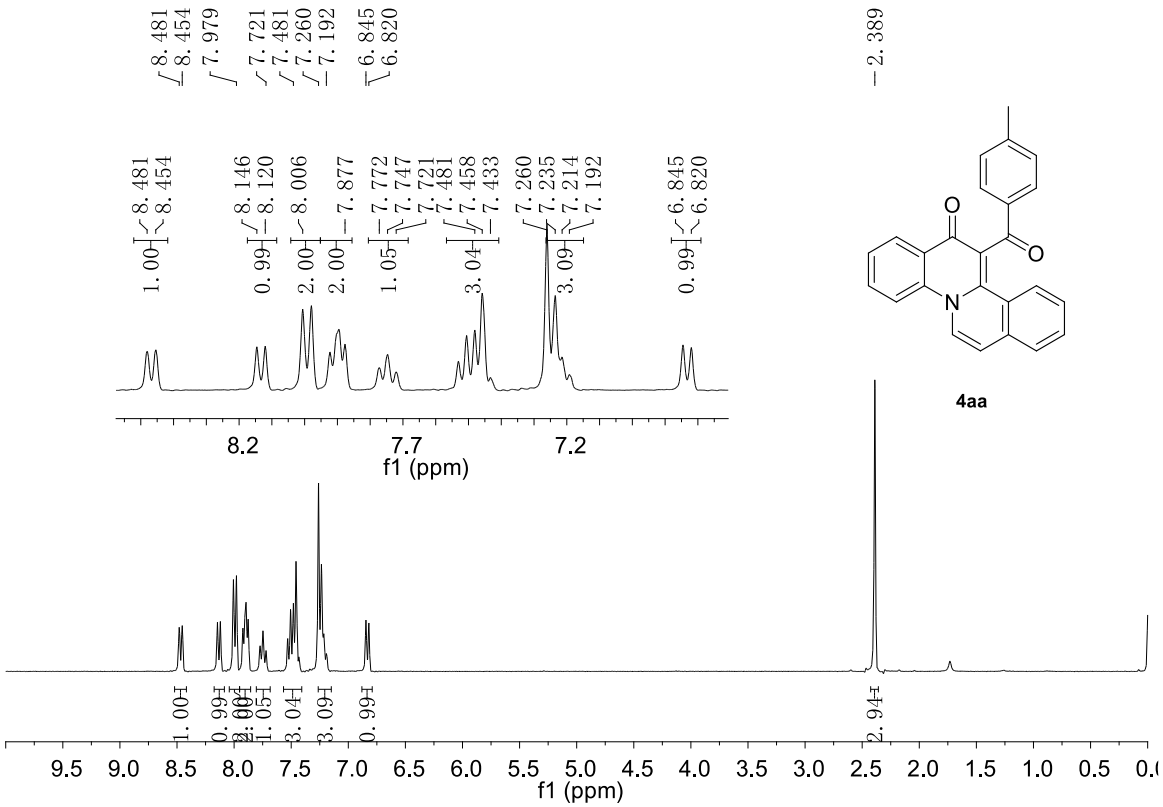

177.463
164.323
156.159
152.322
147.120
133.791
129.166
126.293
125.188
123.074
118.060
21.380
17.753
3ah
f1 (ppm)

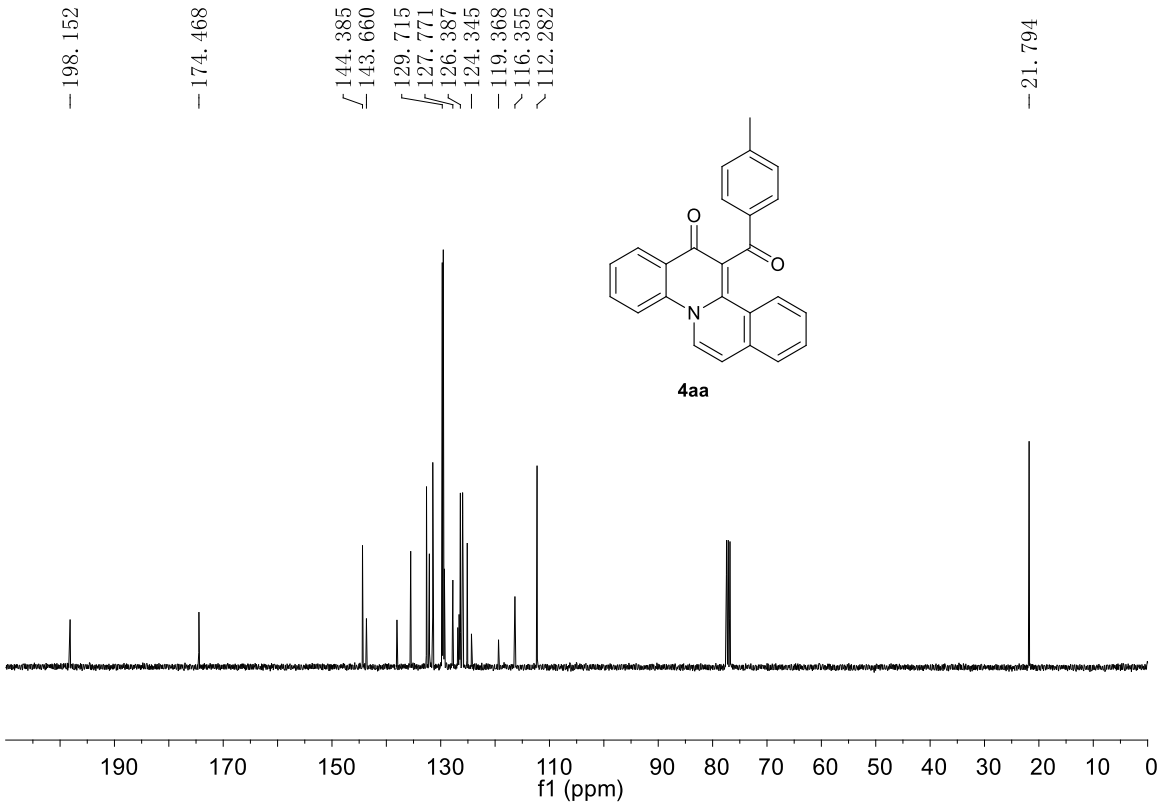

8.301
8.297
8.275
7.706
7.549
7.378
7.264
7.059
7.051
6.991
6.964
3.888
2.234
1.07
1.00
1.02
1.06
1.07
2.07
0.96
1.08
2.06
3.08
2.93
3ai
f1 (ppm)

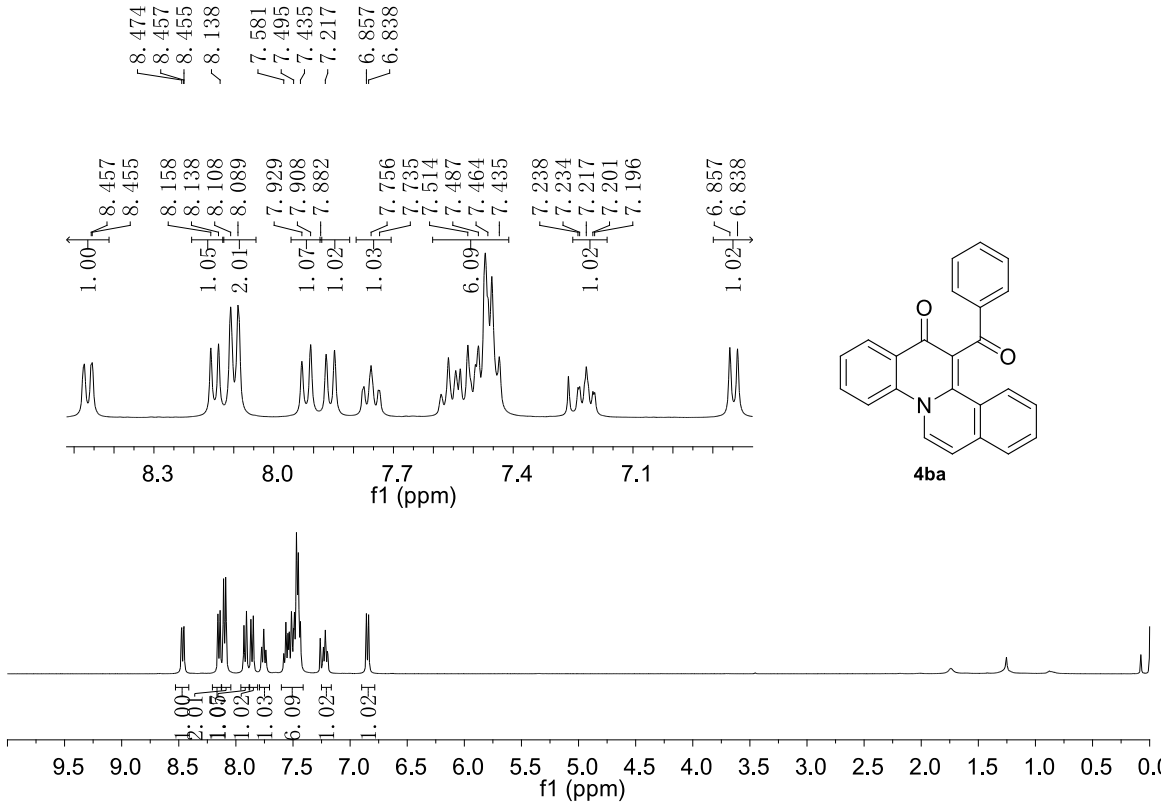

177.514
163.234
156.105
151.244
140.719
135.056
128.240
124.512
122.098
118.001
105.010
55.535
21.391
3ai
f1 (ppm)


8.485
8.480
8.126
7.891
7.578
7.329
7.173
6.906
6.879
3.871
2.147
1.00
1.08
1.95
1.03
1.08
2.09
1.95
2.04
3.05
2.98
f1 (ppm)
3aj

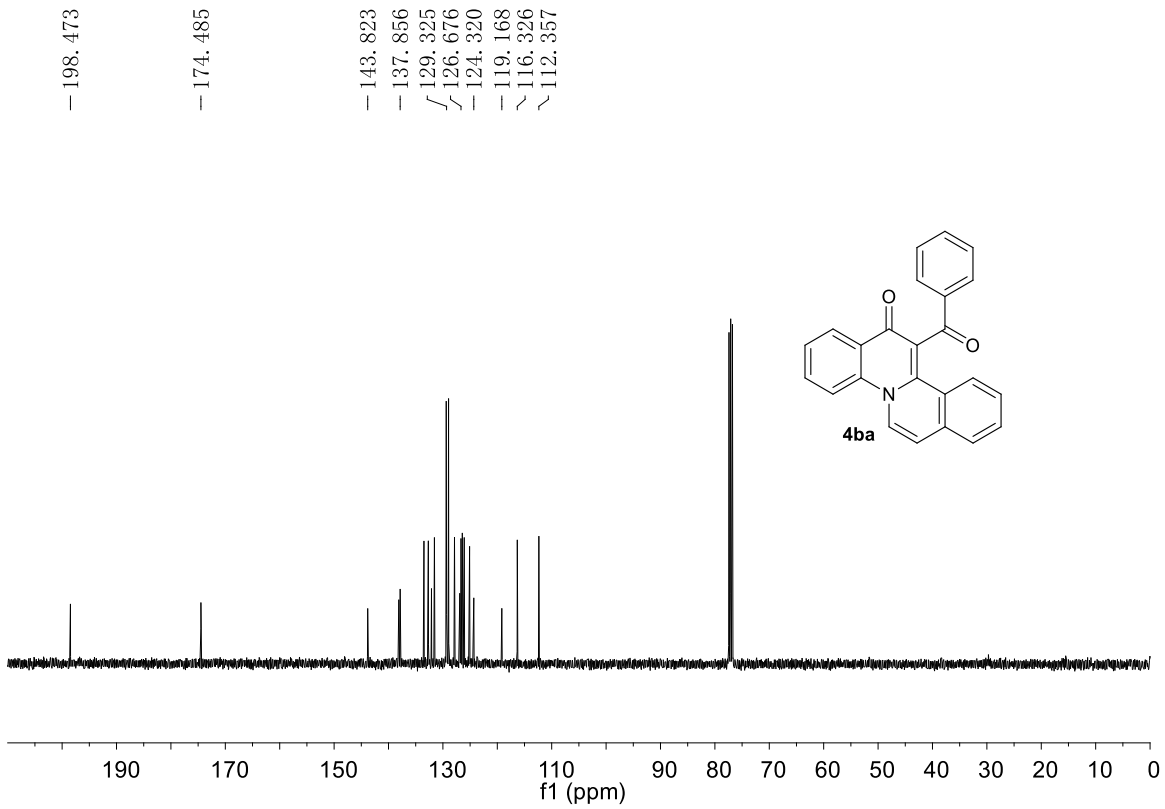

177.156
166.614
163.663
156.087
149.950
137.329
128.977
128.151
126.164
125.185
122.450
118.049
52.412
21.393
f1 (ppm)
3aj

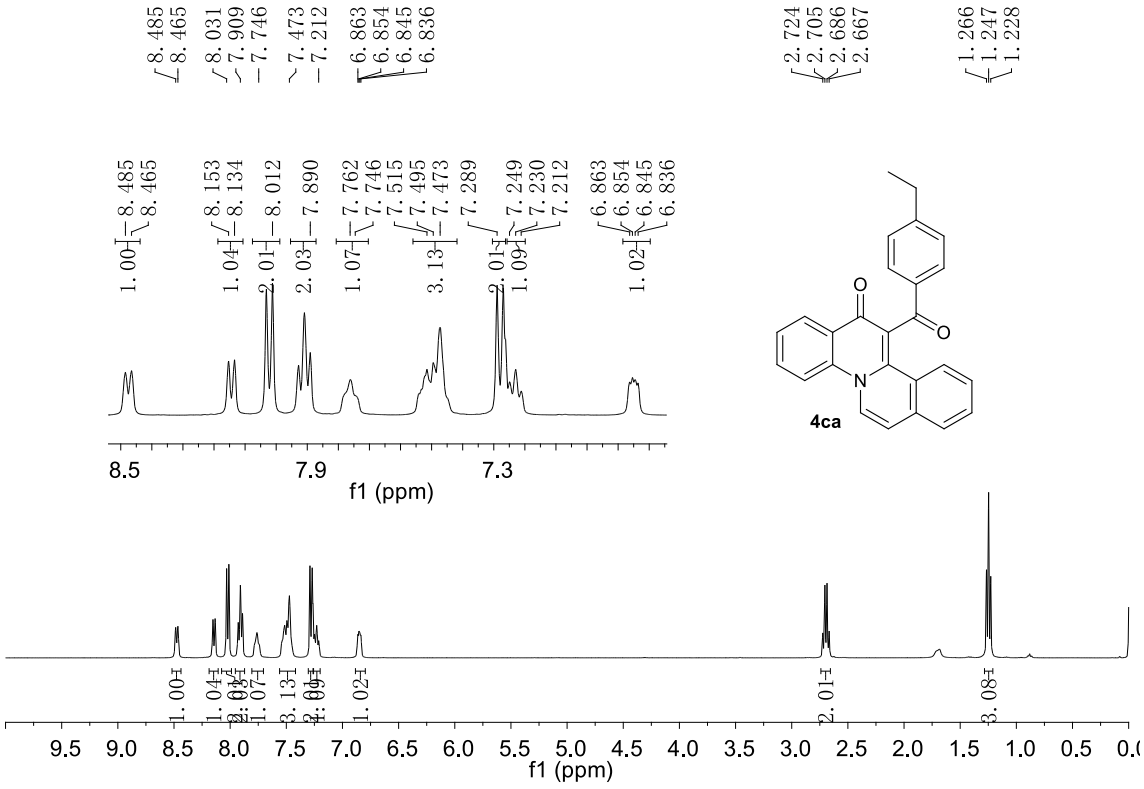

8.481
8.454
7.979
7.721
7.481
7.260
7.192
6.845
6.820
2.389
1.00
0.99
2.00
2.00
1.05
3.04
3.09
0.99
2.94
4aa
f1 (ppm)

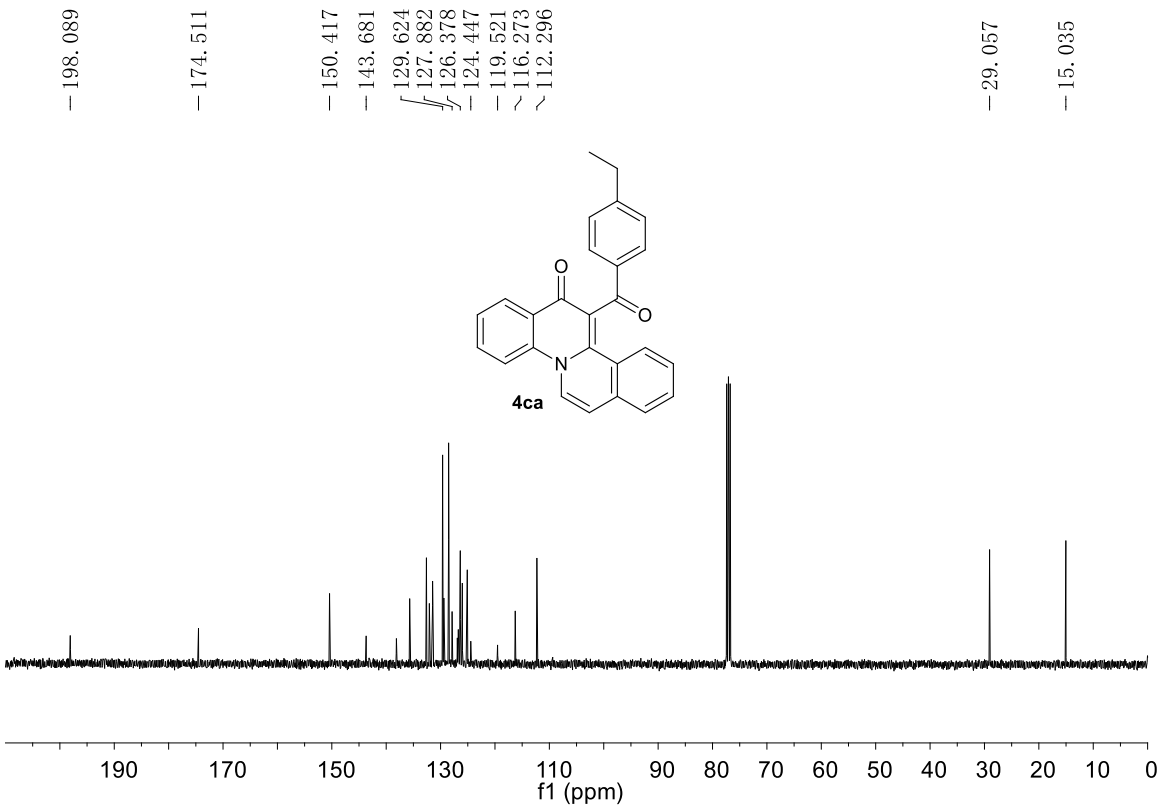

198.152
174.468
144.385
143.660
129.715
127.771
126.387
124.345
119.368
116.355
112.282
21.794
4aa
f1 (ppm)

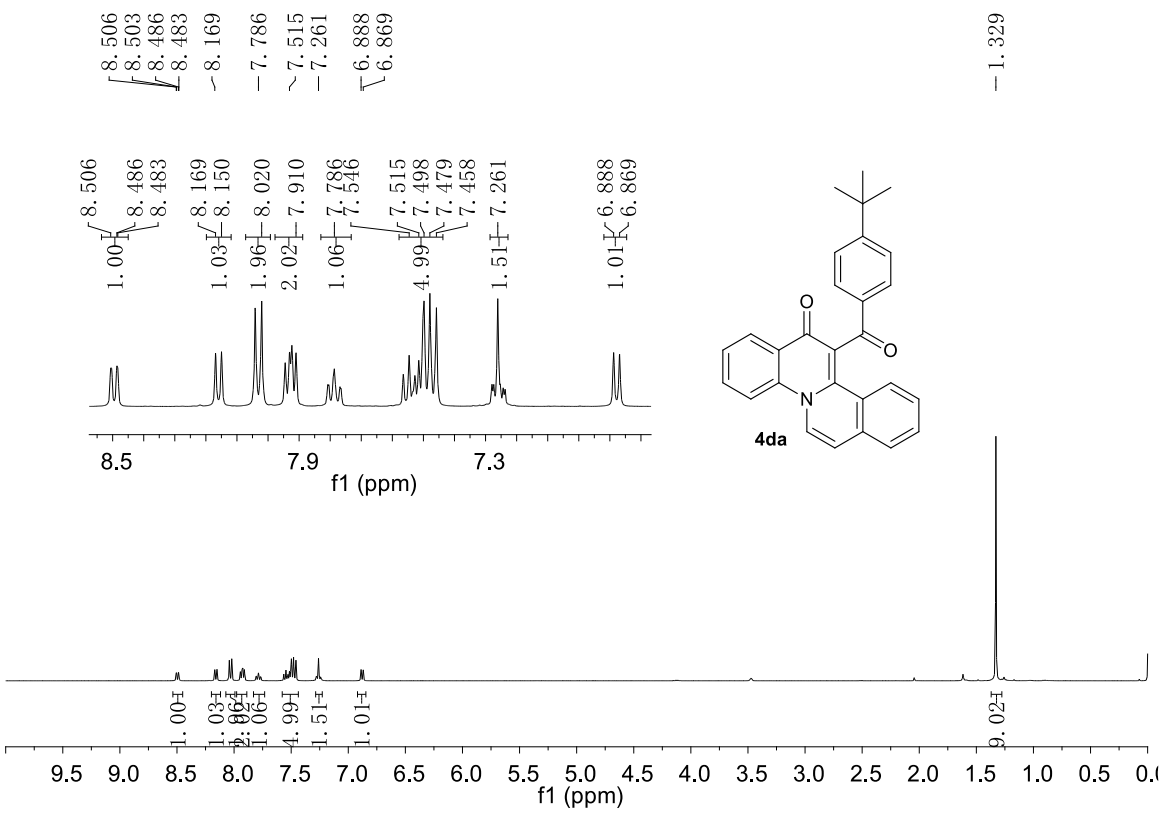

8.474
8.457
8.455
8.138
7.581
7.495
7.435
7.217
6.857
6.838
8.457
8.455
8.158
8.138
8.108
8.089
7.929
7.908
7.882
7.756
7.735
7.514
7.487
7.464
7.435
7.238
7.234
7.217
7.201
7.196
6.857
6.838
1.00
1.05
2.01
1.07
1.02
1.03
6.09
1.02
1.02
8.3
8.0
7.7
7.4
7.1
f1 (ppm)
O
O
N
4ba

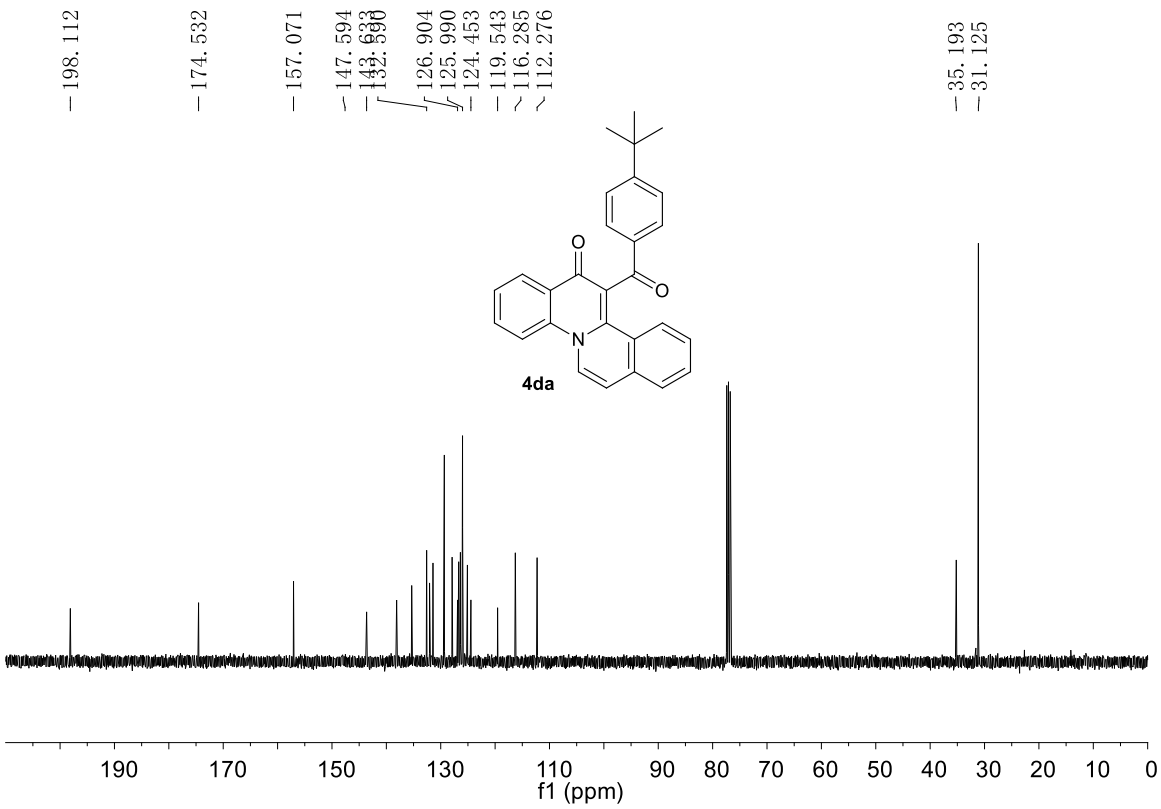
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

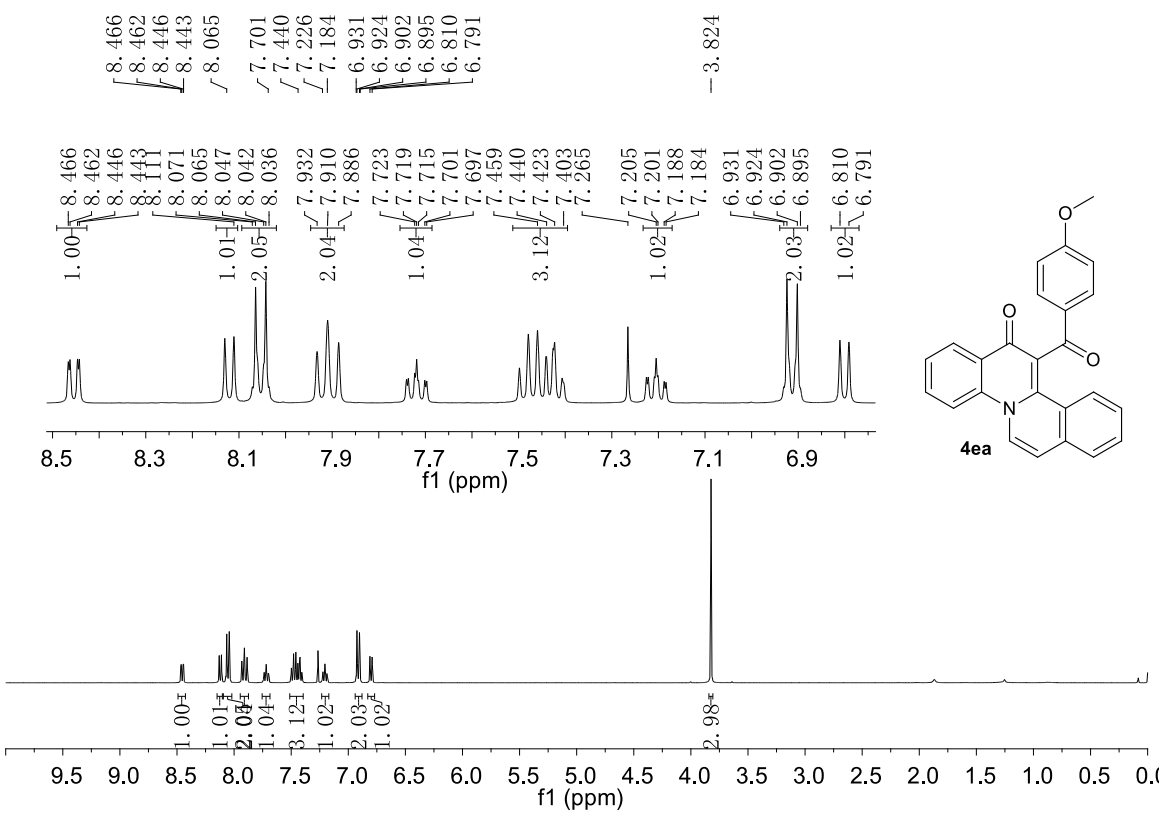

198.473
174.485
143.823
137.856
129.325
126.676
124.320
119.168
116.326
112.357
O
O
N
4ba
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

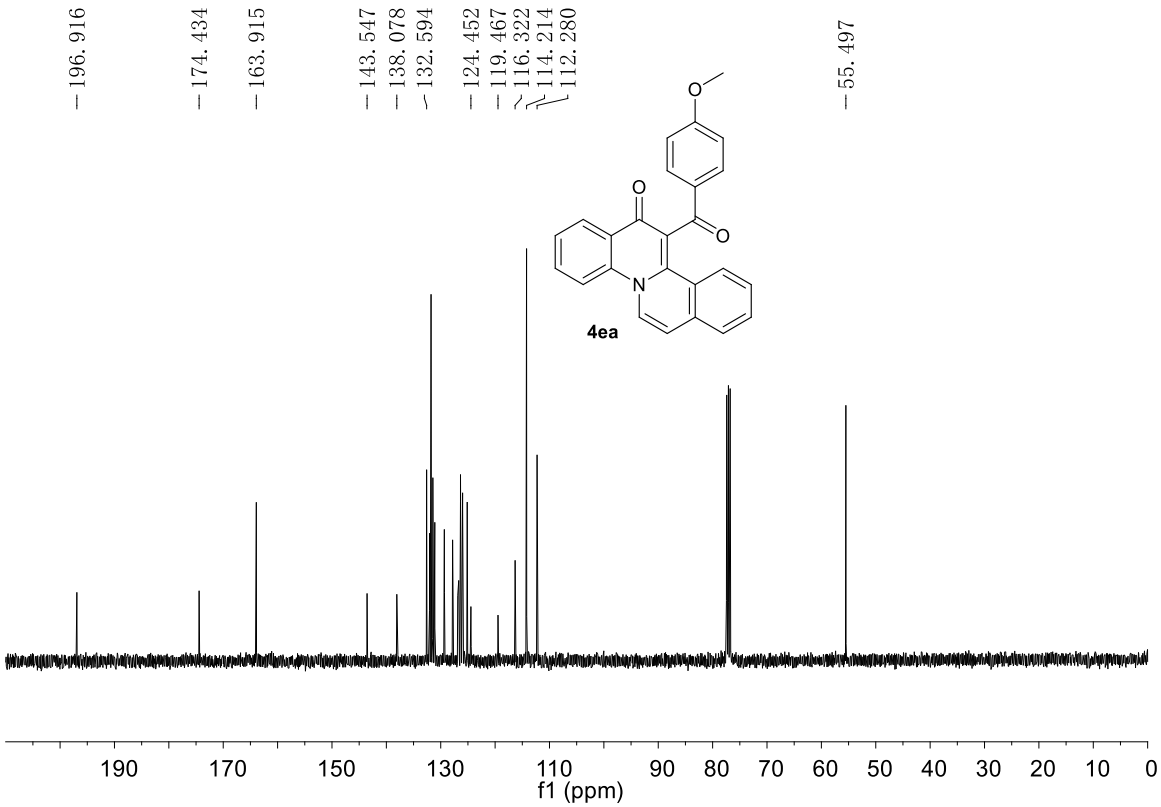

8.485
8.465
8.031
7.909
7.746
7.473
7.212
6.863
6.854
6.845
6.836
2.724
2.705
2.686
2.667
1.266
1.247
1.228
1.00
1.04
2.01
2.03
1.07
3.13
2.01
1.09
1.02
8.153
8.134
8.012
7.890
7.762
7.746
7.515
7.495
7.473
7.289
7.249
7.230
7.212
6.863
6.854
6.845
6.836
8.5
7.9
7.3
f1 (ppm)
4ca
1.00
1.04
3.13
1.07
1.02
2.01
3.08
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)

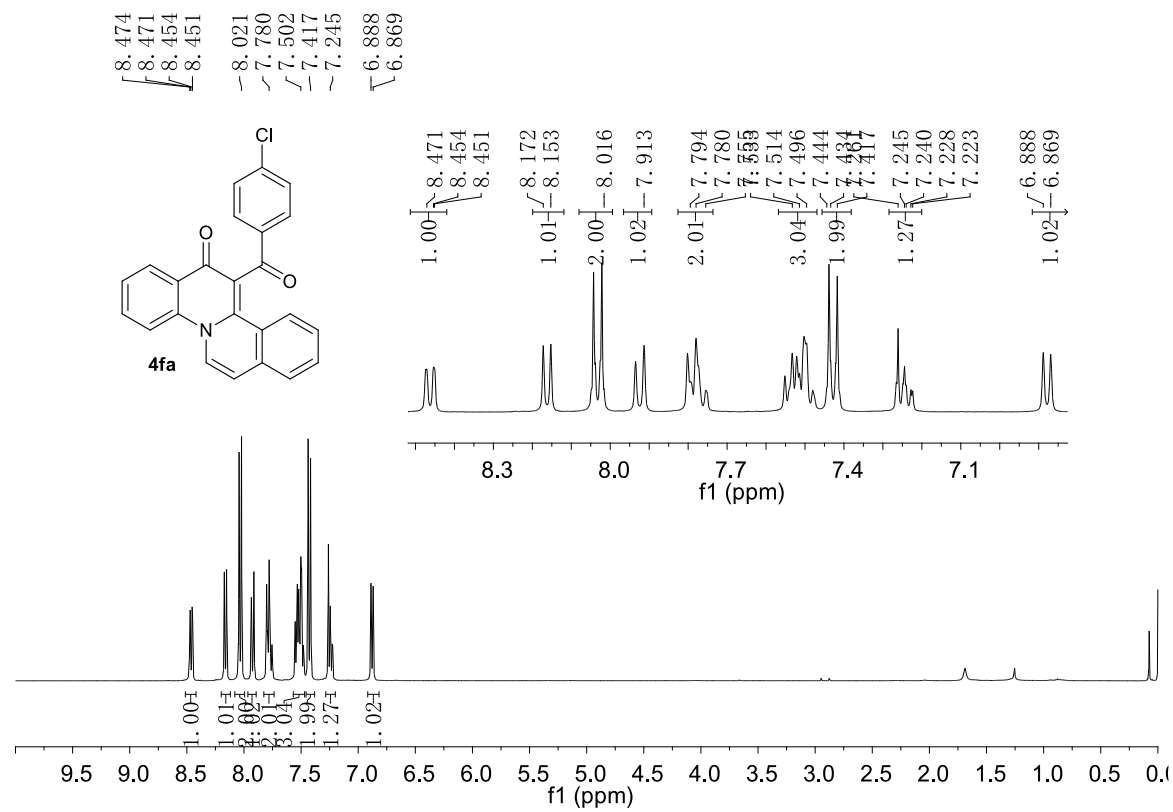

198.089
174.511
150.417
143.681
129.624
127.882
126.378
124.447
119.521
116.273
112.296
29.057
15.035
4ca
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

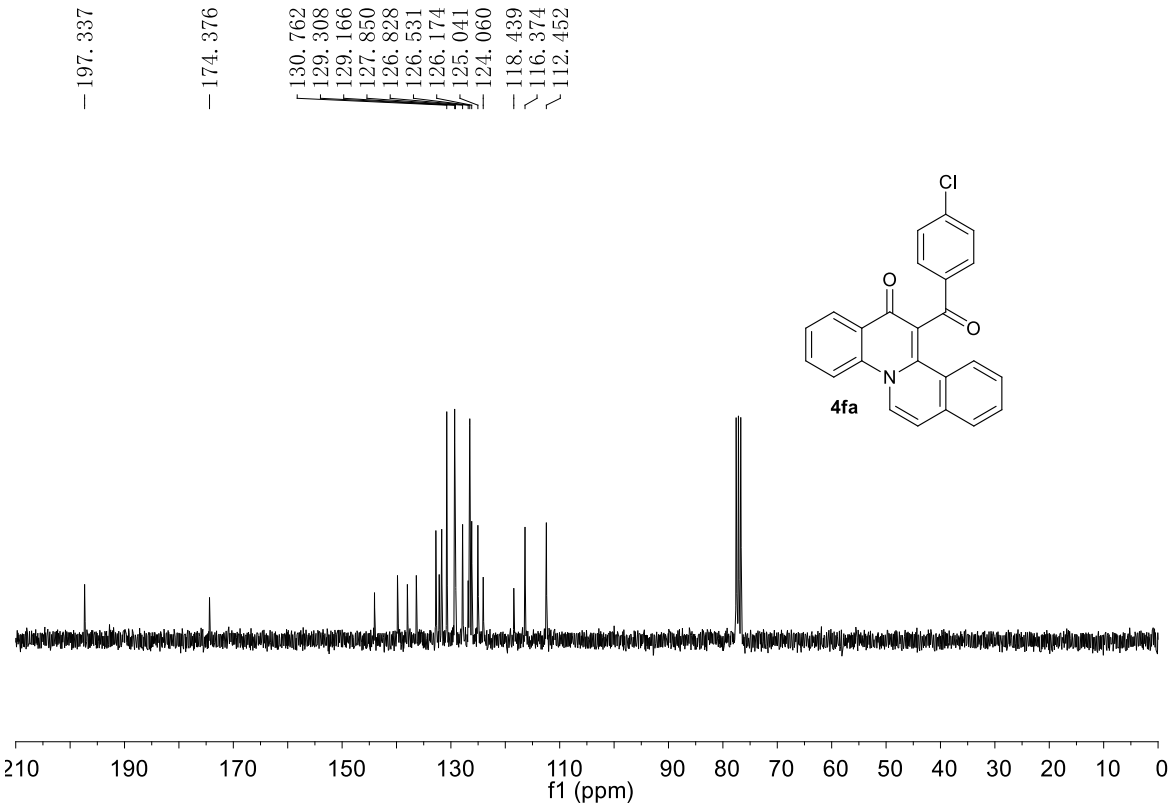

8.506
8.503
8.486
8.483
8.169
7.786
7.515
7.261
6.888
6.869
1.329
1.00
1.03
2.06
1.06
4.99
1.51
1.01
9.02
8.5
7.9
7.3
f1 (ppm)
4da

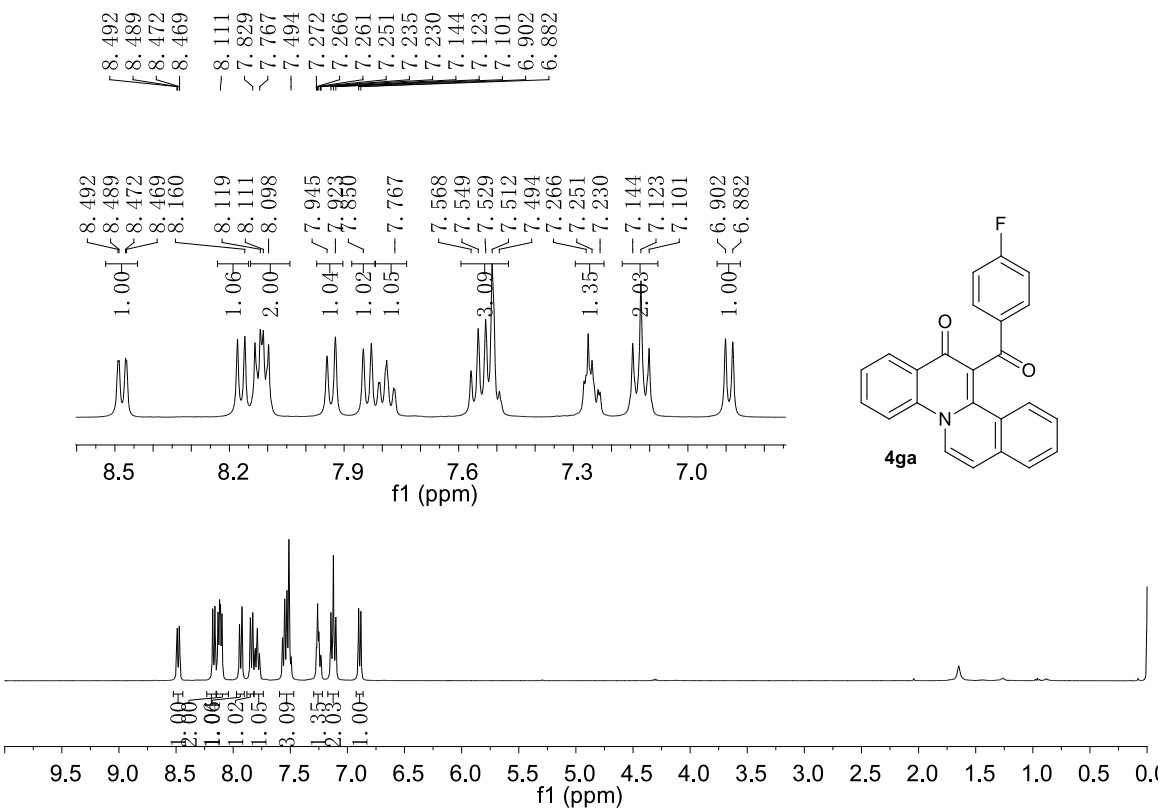

198.112
174.532
157.071
147.594
143.633
132.590
126.904
125.990
124.453
119.543
116.285
112.276
35.193
31.125
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
4da

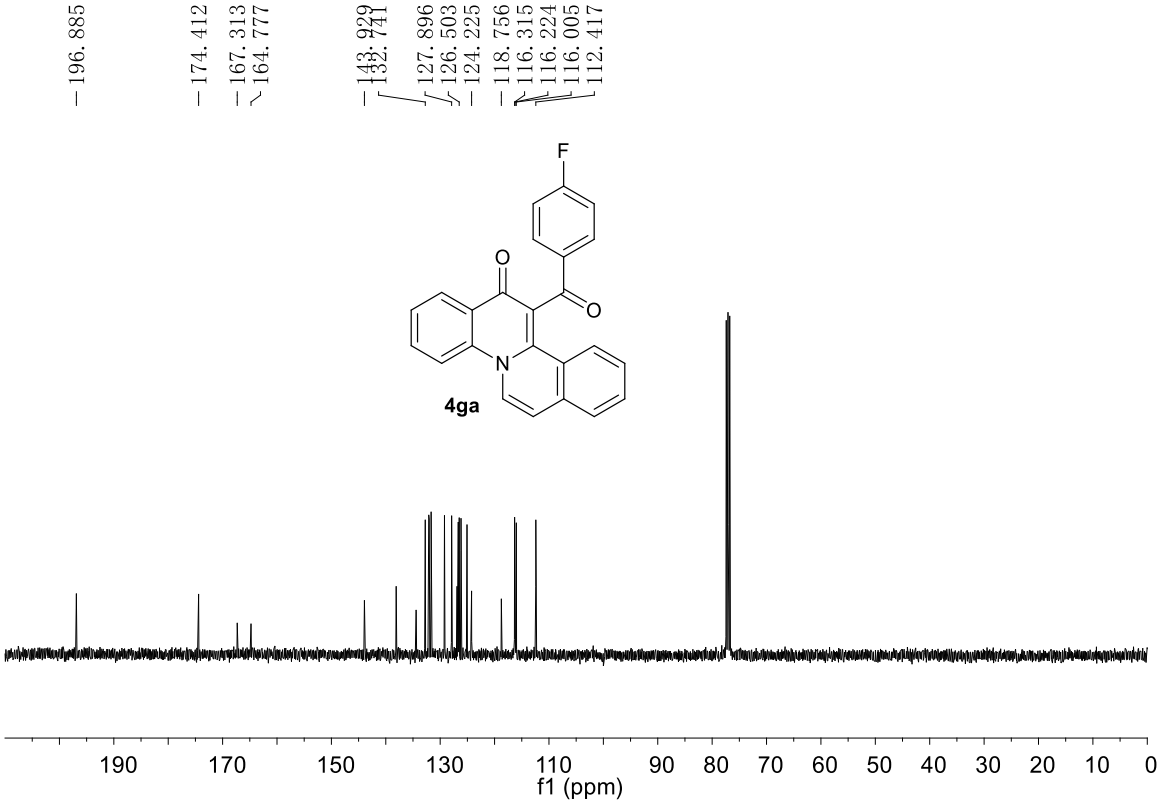

8.466
8.462
8.446
8.443
8.065
7.701
7.440
7.226
7.184
6.931
6.924
6.902
6.895
6.810
6.791
3.824
1.00
1.01
2.05
2.04
1.04
3.12
1.02
2.03
1.02
2.98
f1 (ppm)
4ea

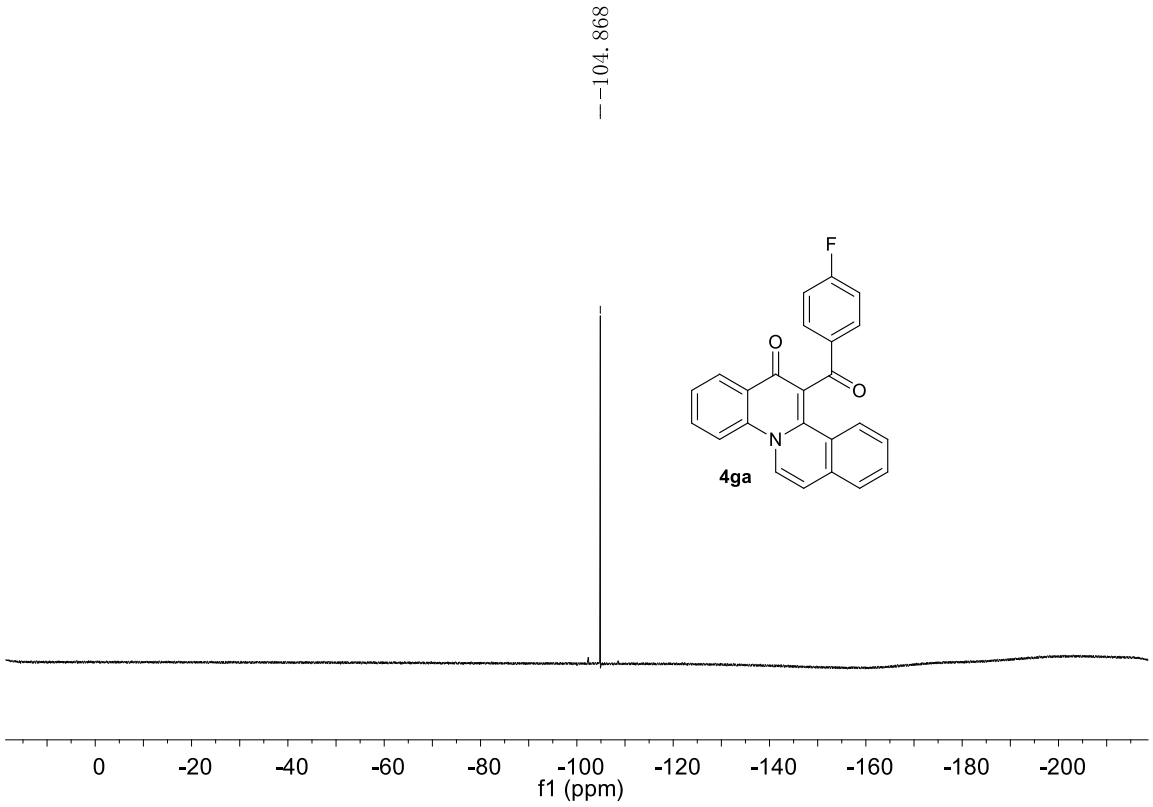

196.916
174.434
163.915
143.547
138.078
132.594
124.452
119.467
116.322
114.214
112.280
55.497
f1 (ppm)
4ea

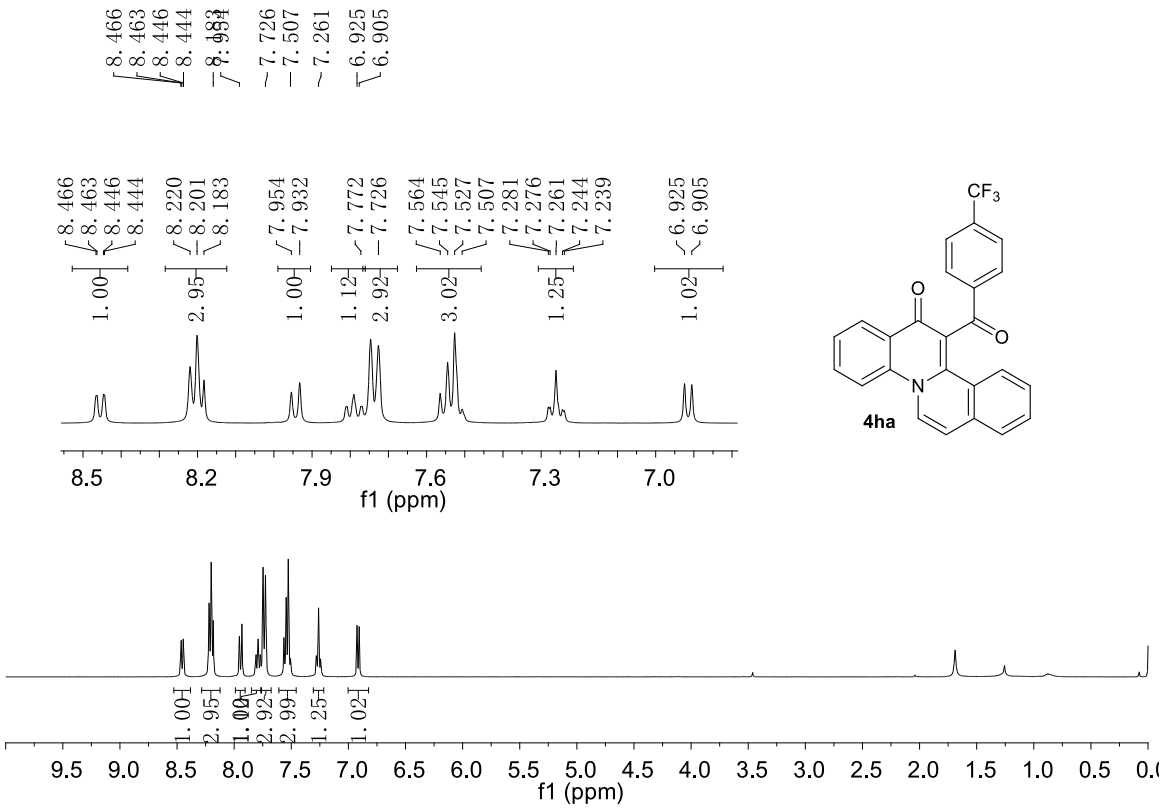

8.474
8.471
8.454
8.451
8.021
7.780
7.502
7.417
7.245
6.888
6.869
Cl
O
O
N
4fa
1.00
1.01
2.00
1.02
2.01
3.04
1.99
1.27
1.02
8.3
8.0
7.7
7.4
7.1
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

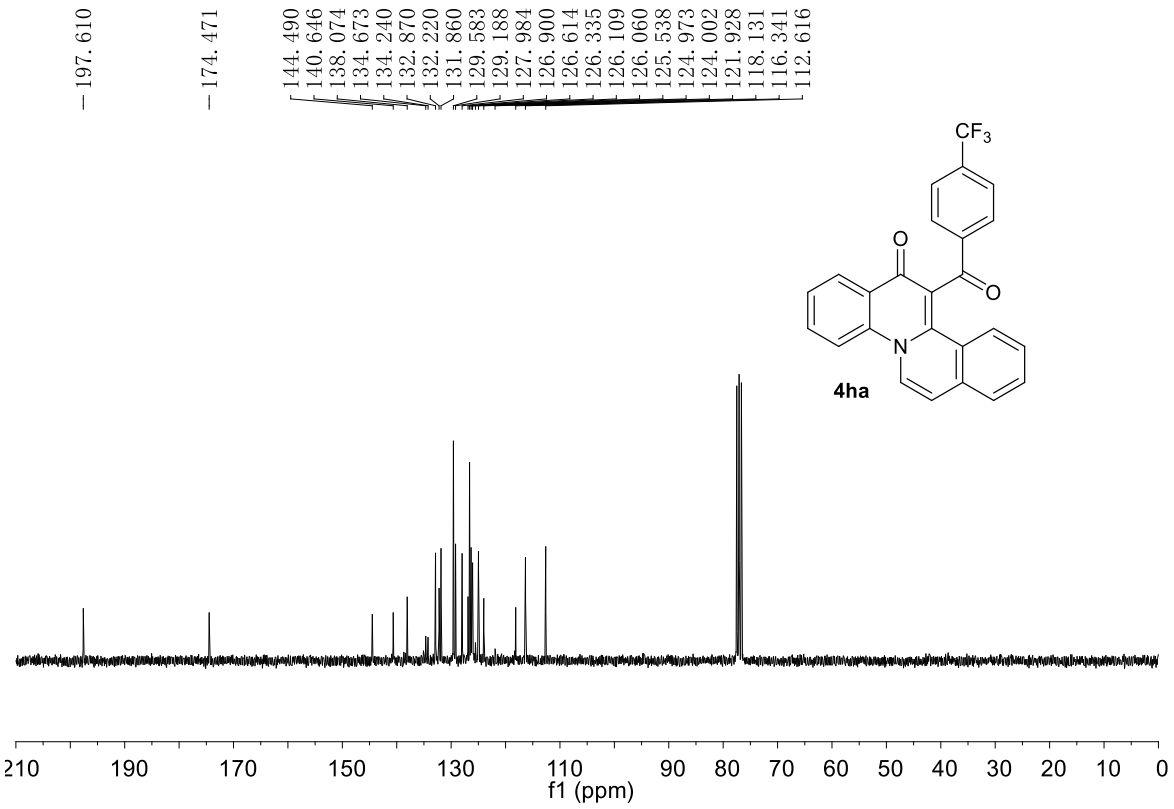

197.337
174.376
130.762
129.308
129.166
127.850
126.828
126.531
126.174
125.041
124.060
118.439
116.374
112.452
Cl
O
O
N
4fa
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

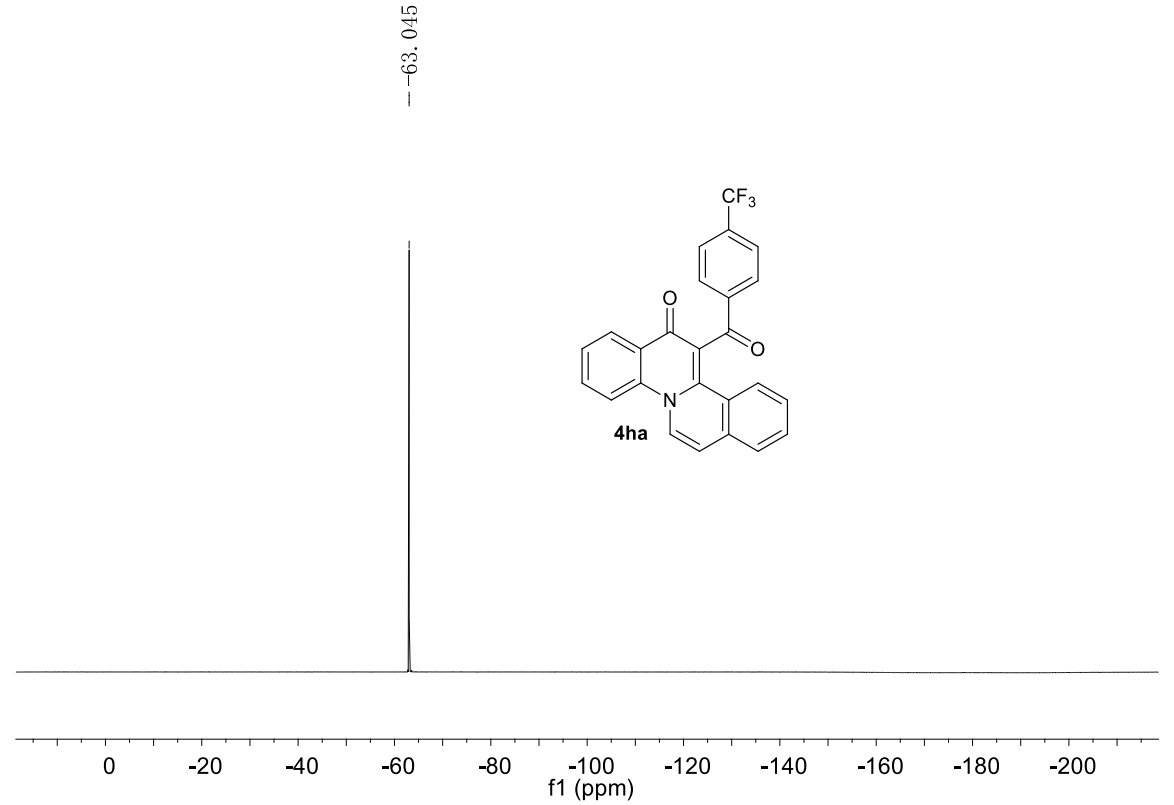

8.492
8.489
8.472
8.469
8.160
8.119
8.111
8.098
7.945
7.923
7.850
7.767
7.568
7.549
7.529
7.512
7.494
7.266
7.251
7.230
7.144
7.123
7.101
6.902
6.882
1.00
1.06
2.00
1.04
1.02
1.05
3.09
1.35
2.03
1.00
F
O
O
N
4ga
8.5
8.2
7.9
7.6
7.3
7.0
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

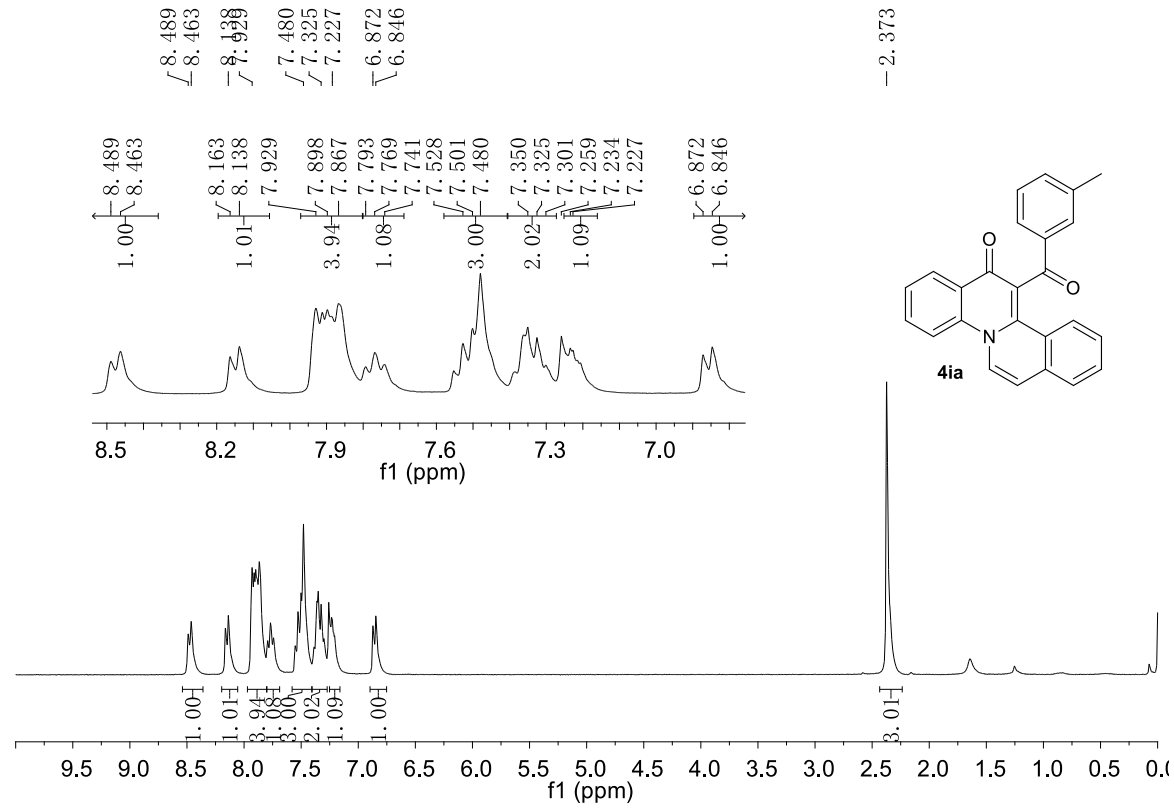

196.885
174.412
167.313
164.777
143.929
132.741
127.896
126.503
124.225
118.756
116.315
116.224
116.005
112.417
F
O
O
N
4ga
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

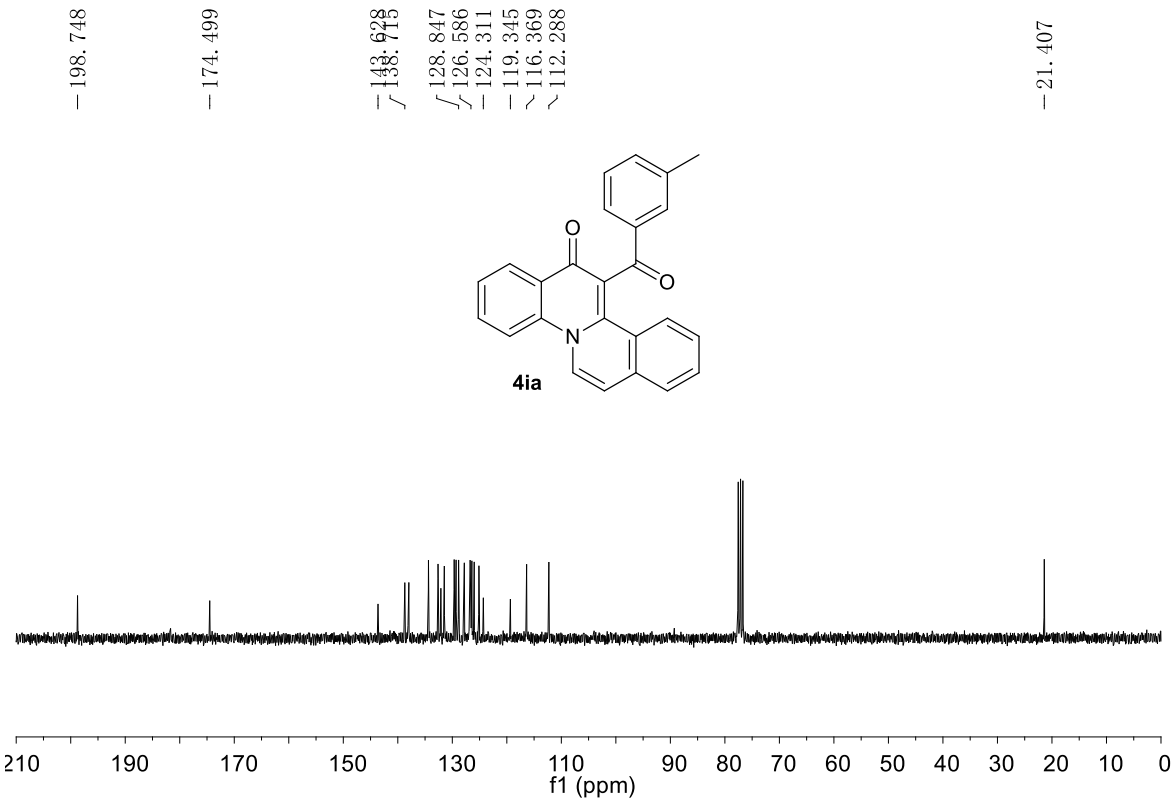

-104.868
F
O
O
N
4ga
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

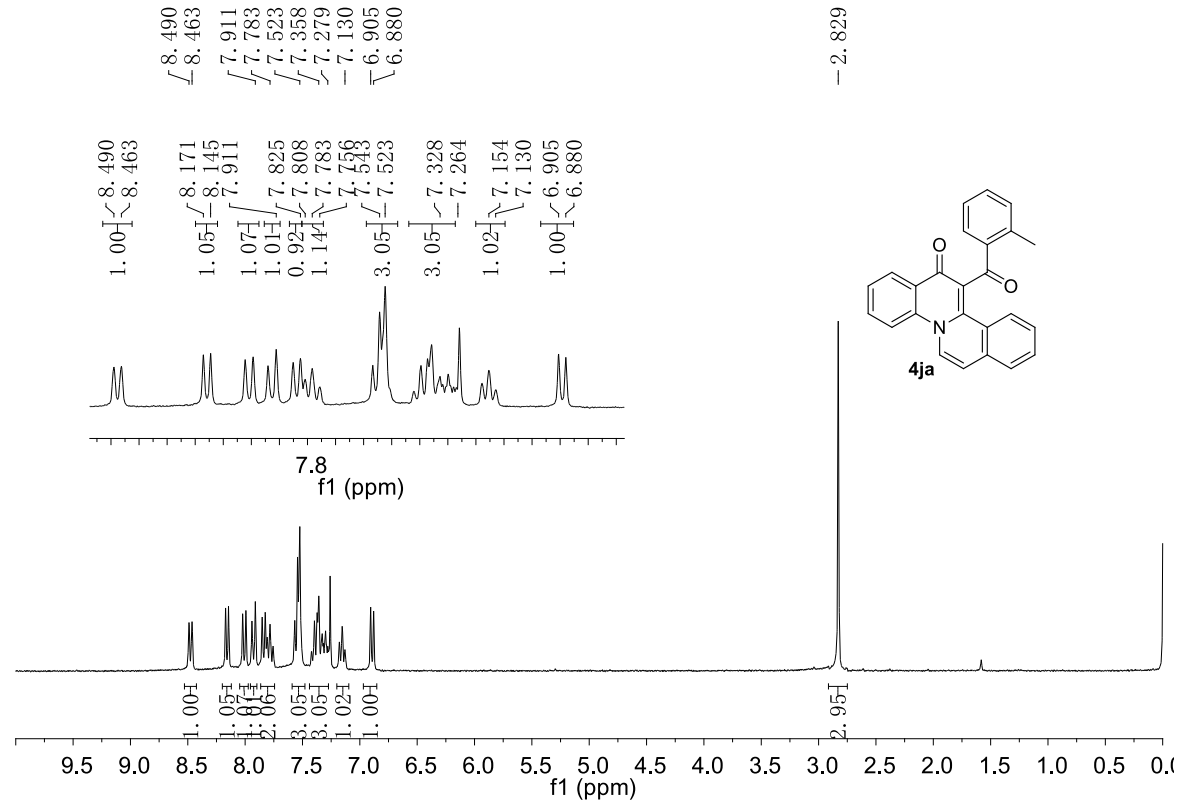

8.466
8.463
8.446
8.444
7.726
7.507
7.261
6.925
6.905
1.00
2.95
1.00
1.12
2.92
3.02
1.25
1.02
CF3
O
O
N
4ha
8.5
8.2
7.9
7.6
7.3
7.0
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

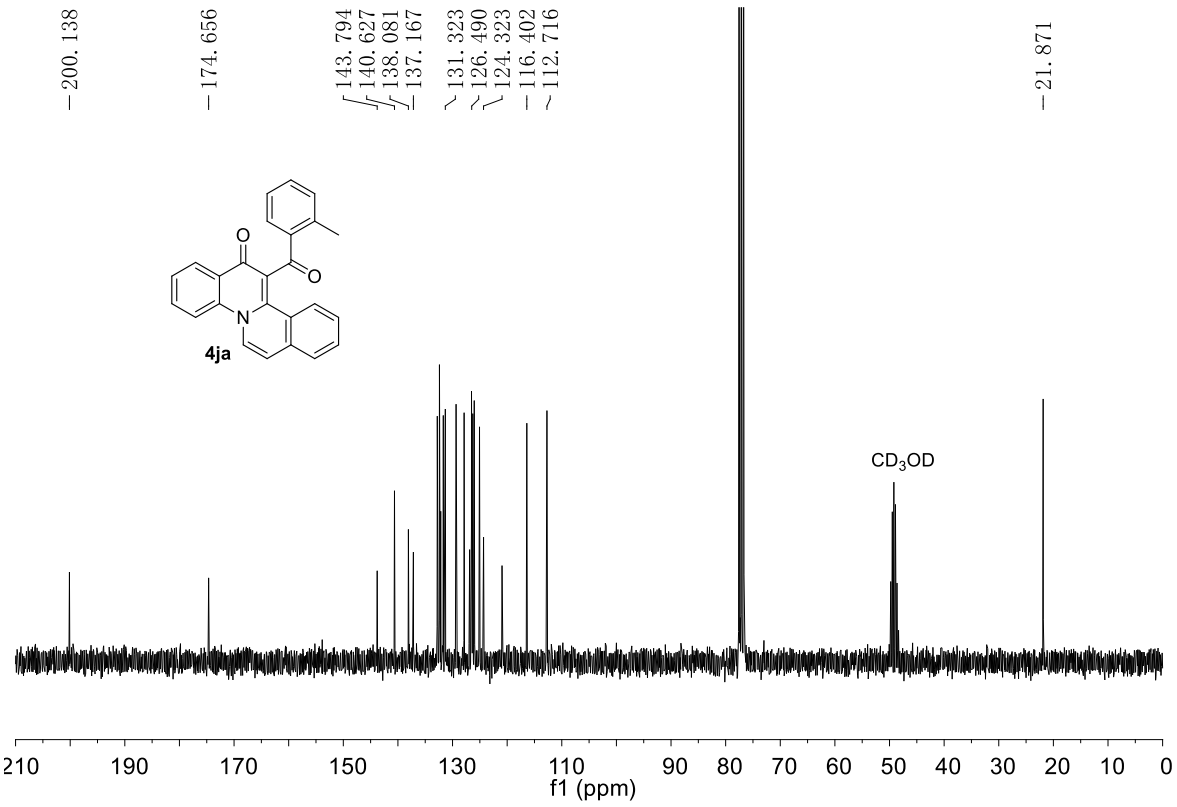

197.610
174.471
144.490
140.646
138.074
134.673
134.240
132.870
132.220
131.860
129.583
129.188
127.984
126.900
126.614
126.335
126.109
126.060
125.538
124.973
124.002
121.928
118.131
116.341
112.616
CF3
O
O
N
4ha
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

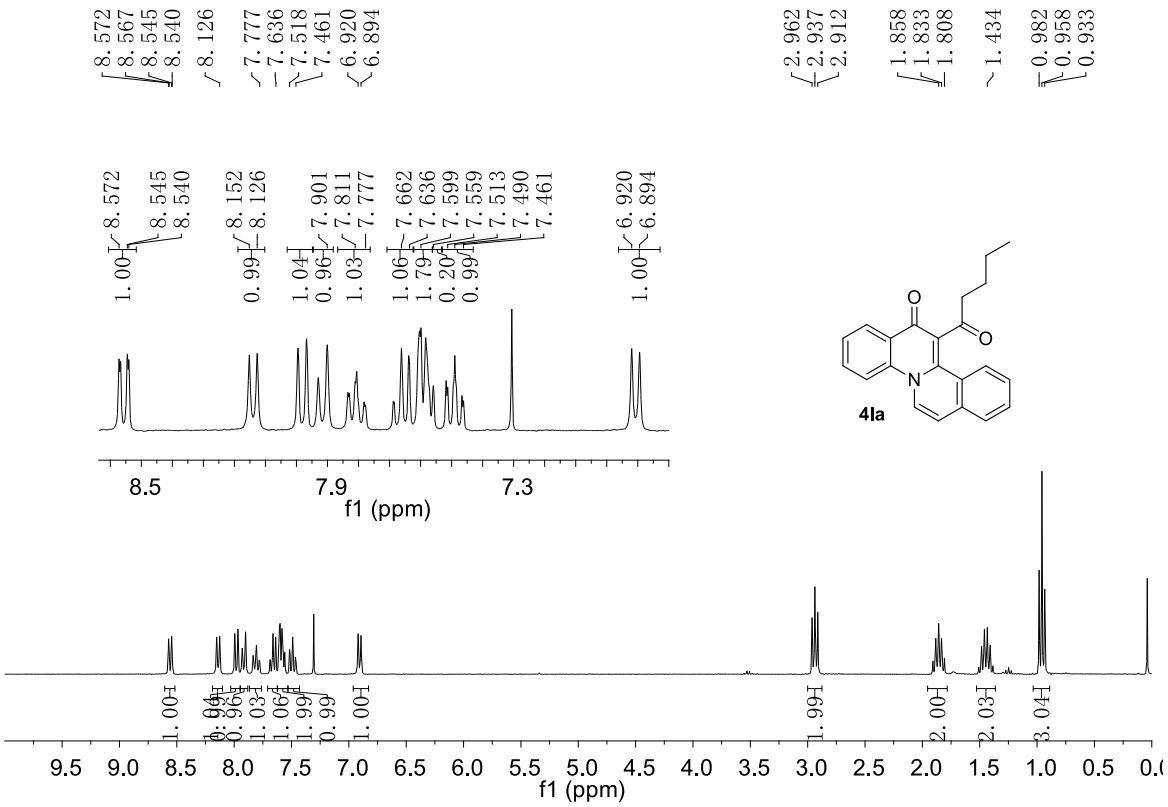

-63.045
CF3
O
O
N
4ha
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

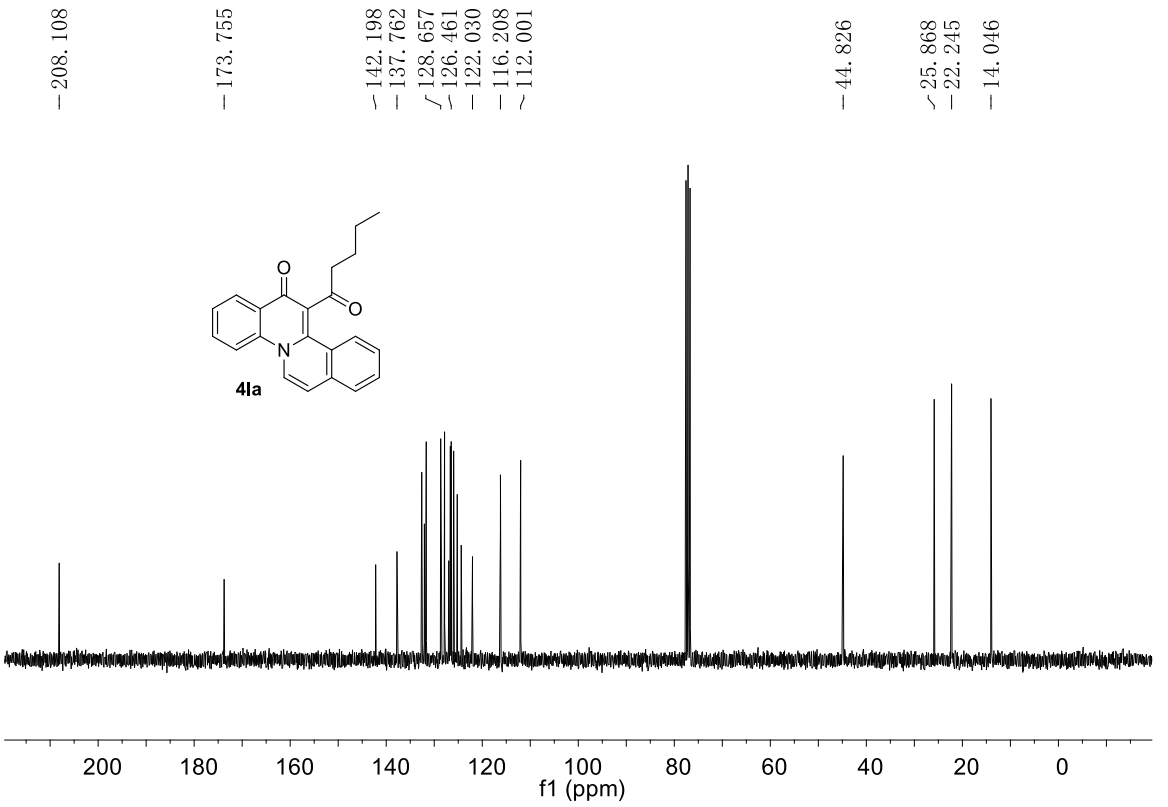

8.489
8.463
8.163
8.138
7.929
7.898
7.867
7.793
7.769
7.741
7.528
7.501
7.480
7.350
7.325
7.301
7.259
7.234
7.227
6.872
6.846
2.373
1.00
1.01
3.94
1.08
3.00
2.02
1.09
1.00
3.01
4ia
f1 (ppm)

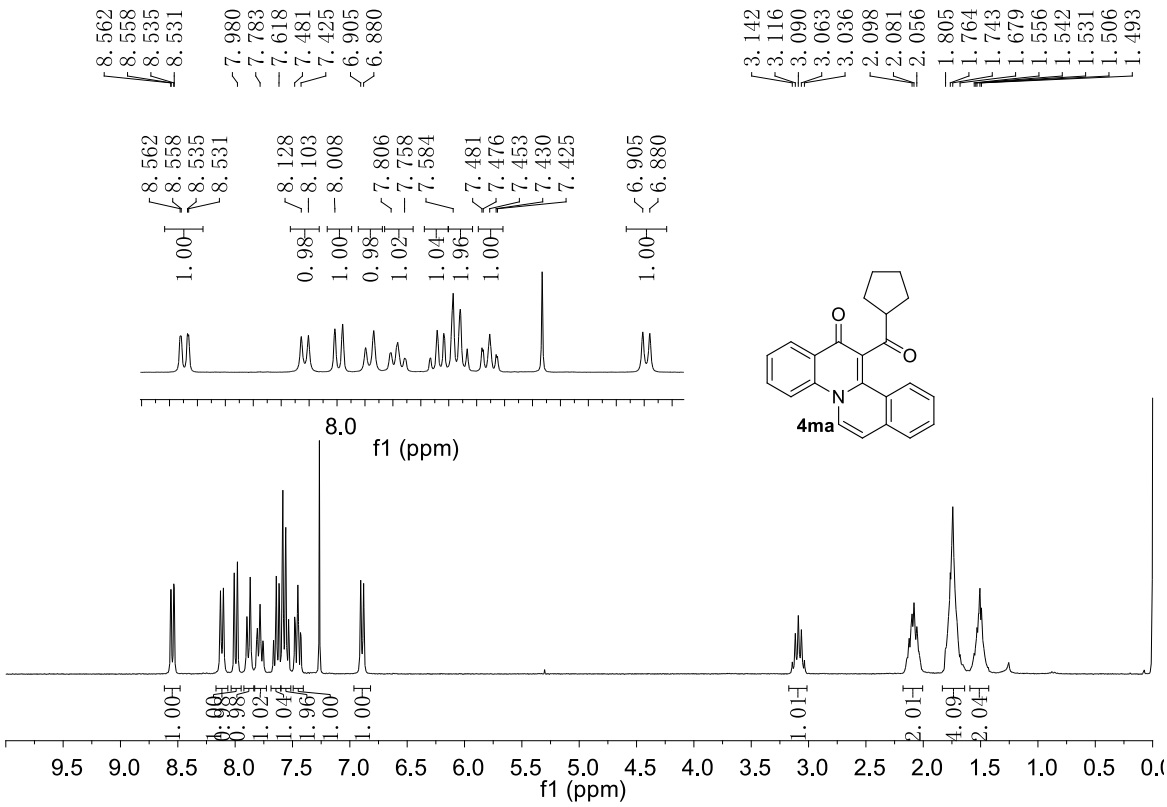

198.748
174.499
143.628
138.715
128.847
126.586
124.311
119.345
116.369
112.288
21.407
4ia
f1 (ppm)

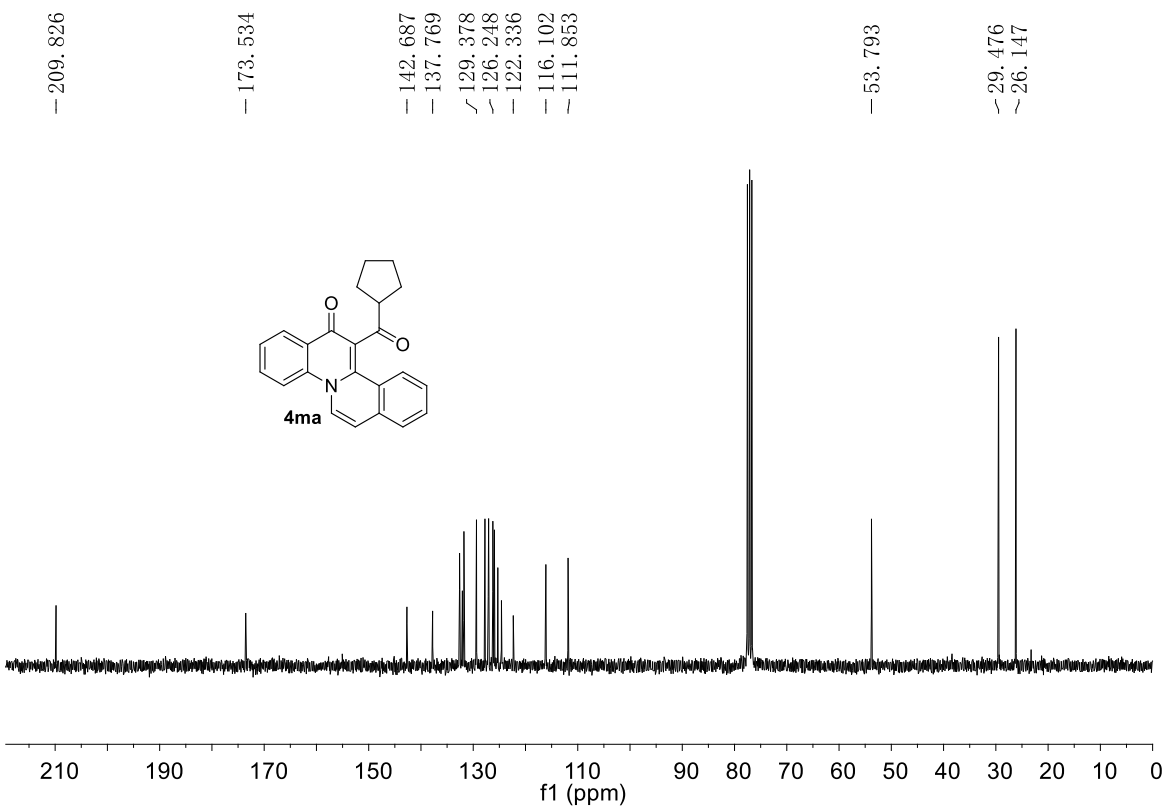

8.490
8.463
7.911
7.783
7.523
7.358
7.279
7.130
6.905
6.880
2.829
1.00
1.05
1.07
1.01
0.92
1.14
3.05
3.05
1.02
1.00
2.95
4ja
7.8
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

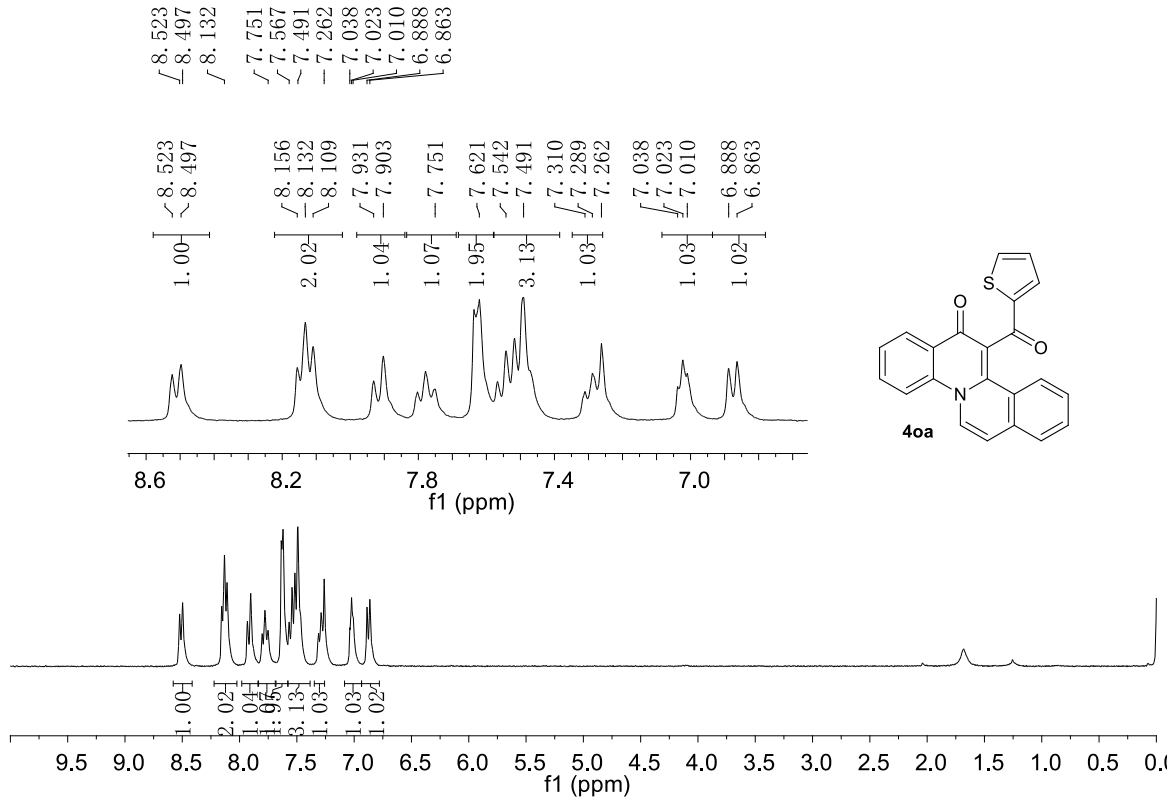

200.138
174.656
143.794
140.627
138.081
137.167
131.323
126.490
124.323
116.402
112.716
21.871
4ja
CD3OD
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

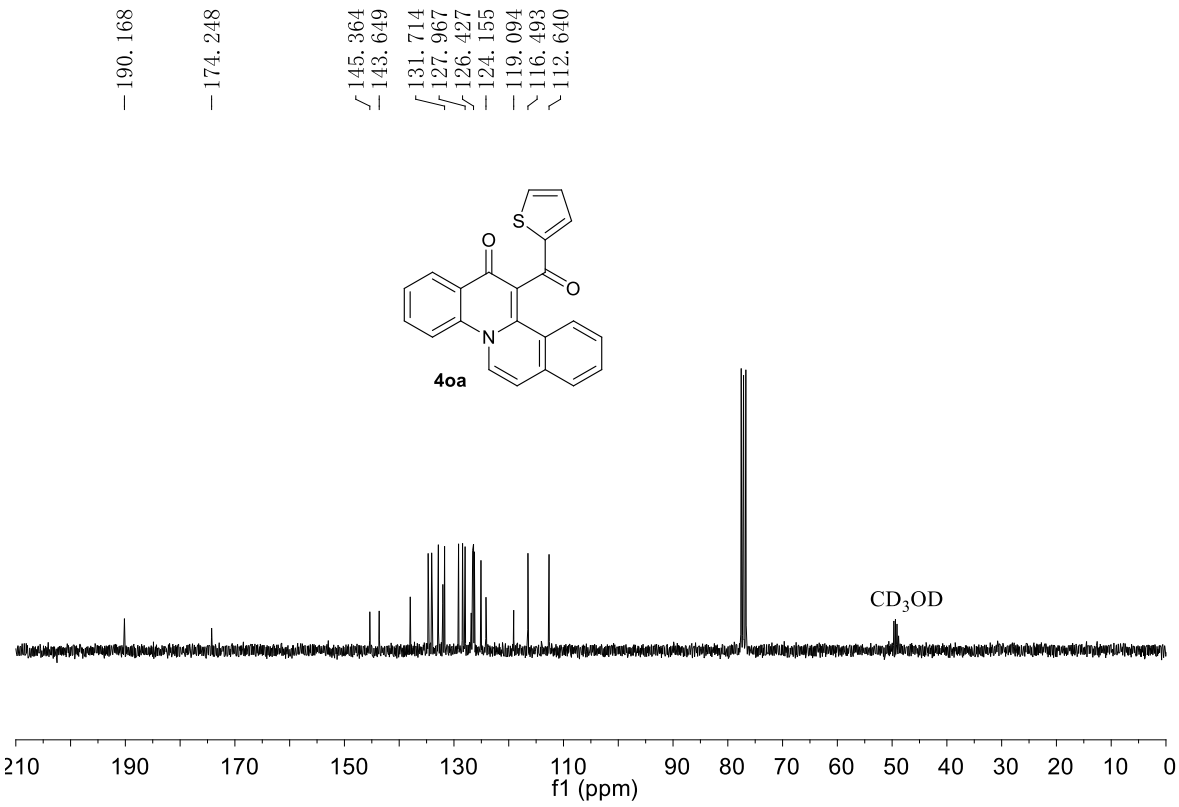

8.572
8.567
8.545
8.540
8.126
7.777
7.636
7.518
7.461
6.920
6.894
2.962
2.937
2.912
1.858
1.833
1.808
1.434
0.982
0.958
0.933
1.00
0.99
1.04
0.96
1.03
1.06
1.79
0.20
0.99
1.00
1.99
2.00
2.03
3.04
4la
f1 (ppm)

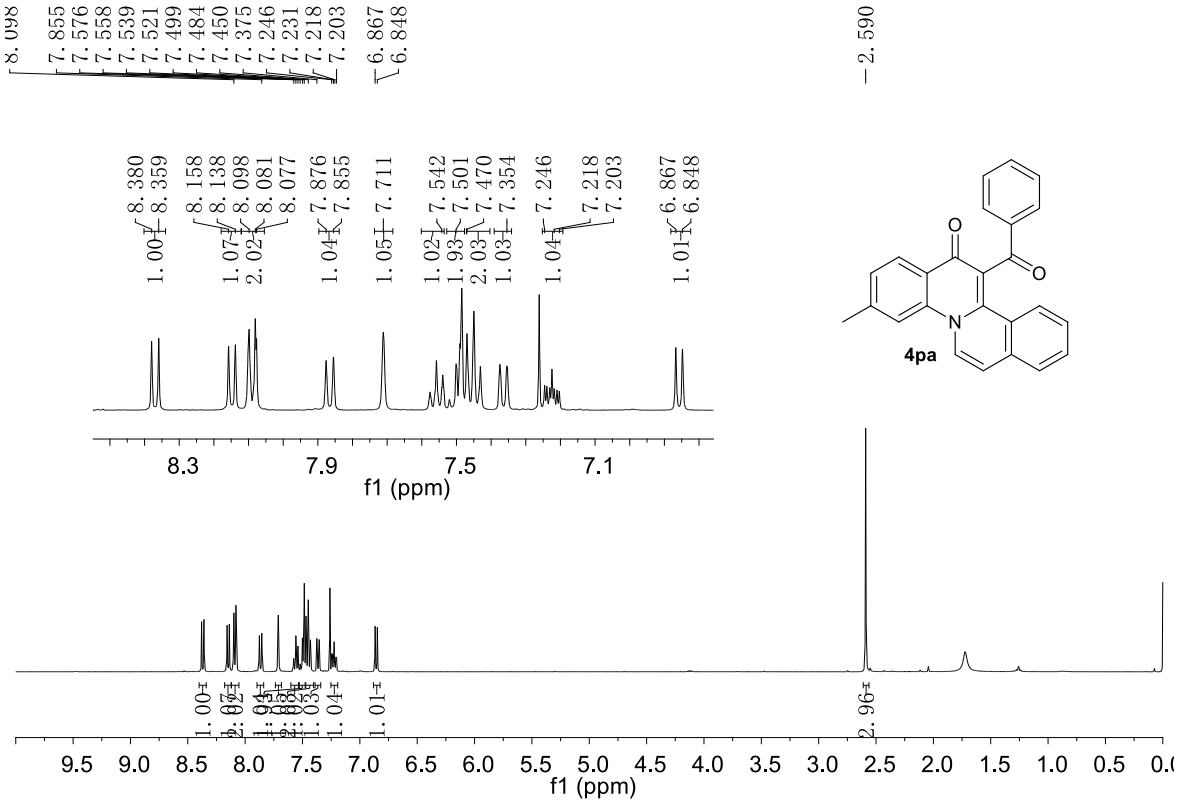

208.108
173.755
142.198
137.762
128.657
126.461
122.030
116.208
112.001
44.826
25.868
22.245
14.046
4la
f1 (ppm)

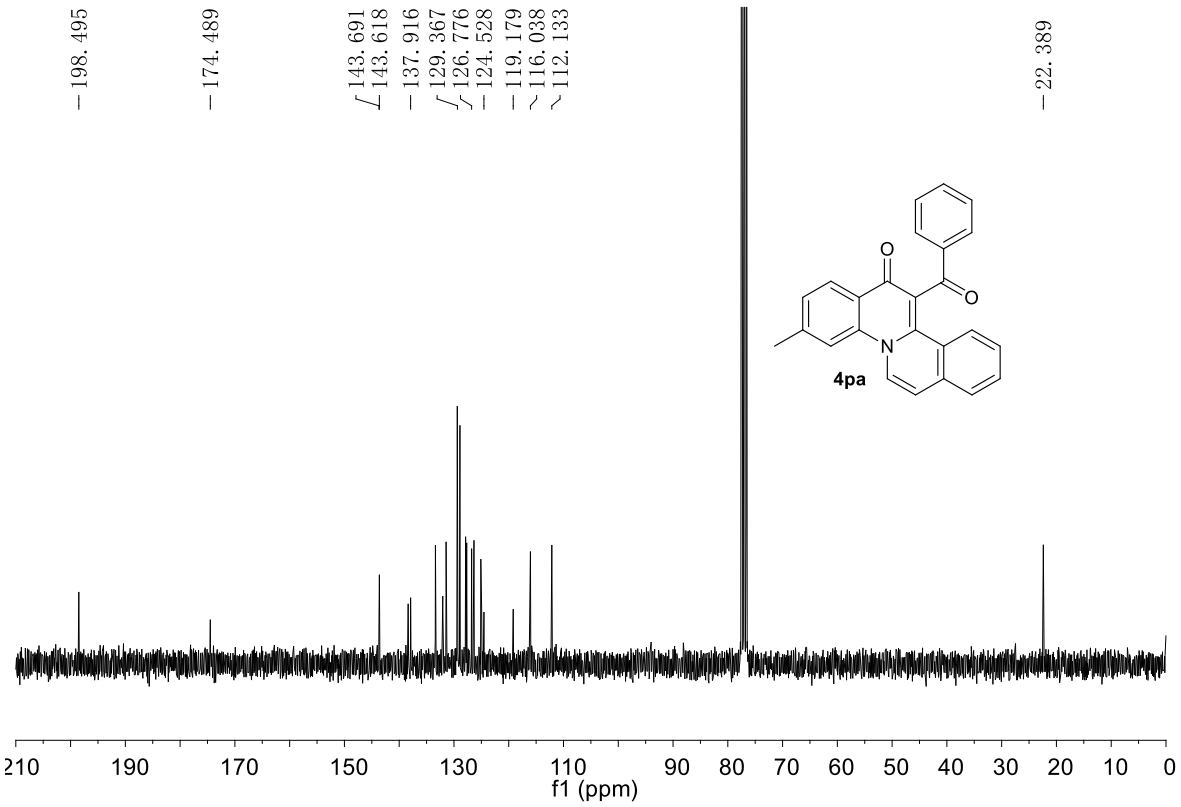

8.562
8.558
8.535
8.531
7.980
7.783
7.618
7.481
7.425
6.905
6.880
3.142
3.116
3.090
3.063
3.036
2.098
2.081
2.056
1.805
1.764
1.743
1.679
1.556
1.542
1.531
1.506
1.493
8.128
8.103
8.008
7.806
7.758
7.584
7.481
7.476
7.453
7.430
7.425
1.00
0.98
1.00
0.98
1.02
1.04
1.96
1.00
1.00
8.0
f1 (ppm)
4ma
1.00
1.01
2.01
4.09
2.04
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)

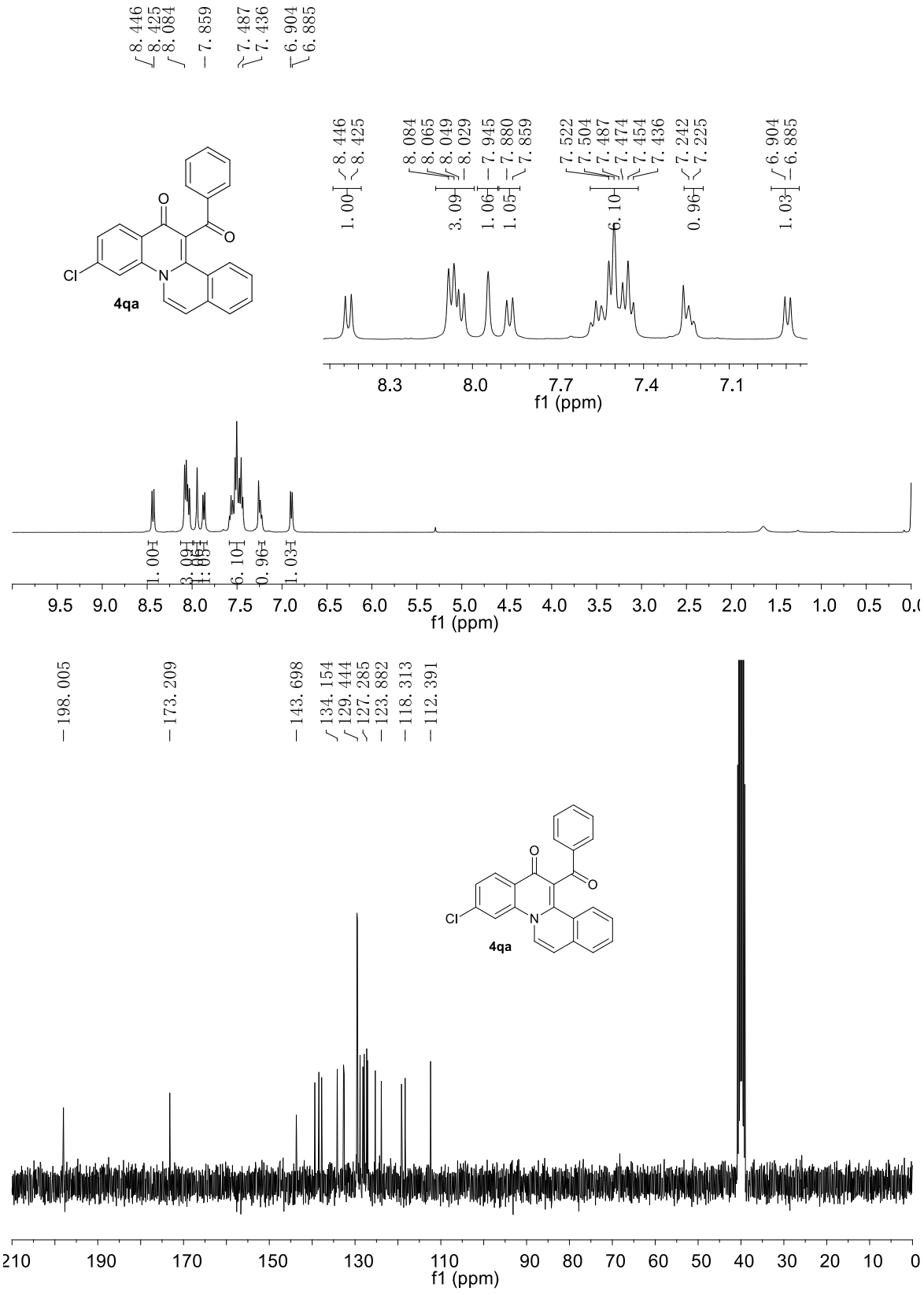

209.826
173.534
142.687
137.769
129.378
126.248
122.336
116.102
111.853
53.793
29.476
26.147
4ma
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

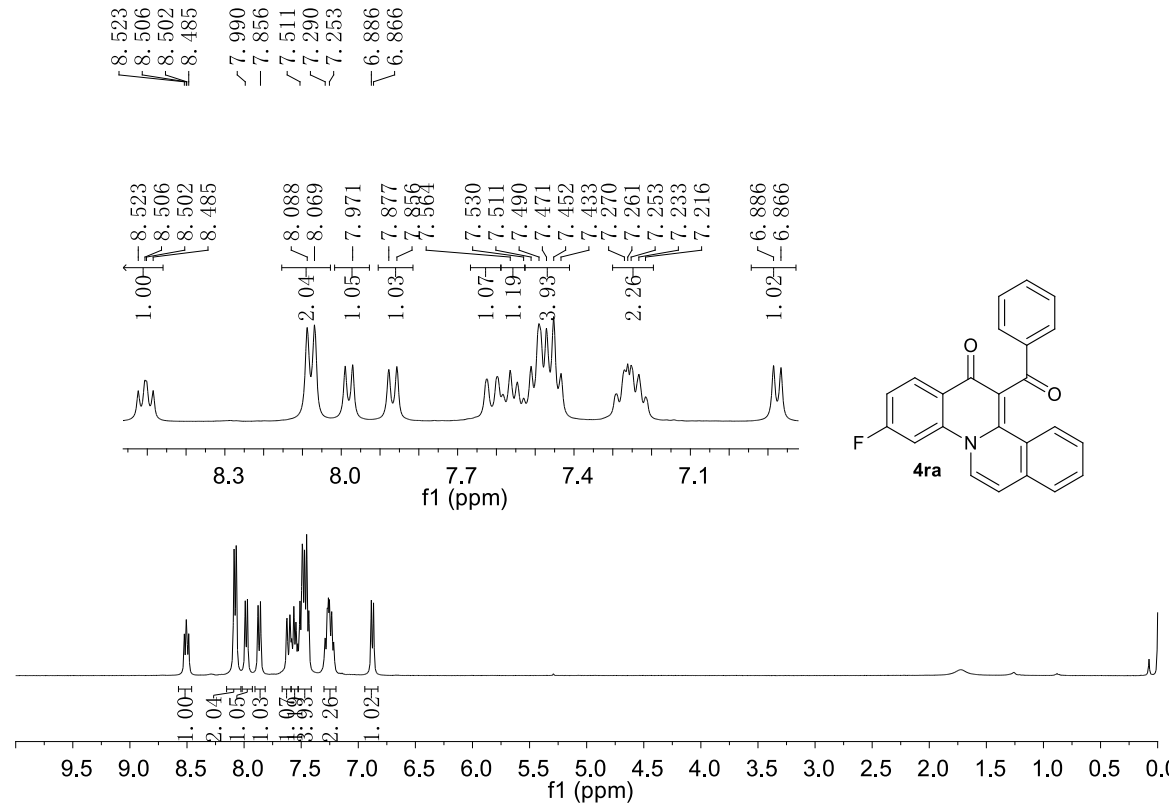

8.523
8.497
8.132
7.751
7.567
7.491
7.262
7.038
7.023
7.010
6.888
6.863
1.00
2.02
1.04
1.07
1.95
3.13
1.03
1.03
1.02
8.6
8.2
7.8
7.4
7.0
f1 (ppm)
4oa
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

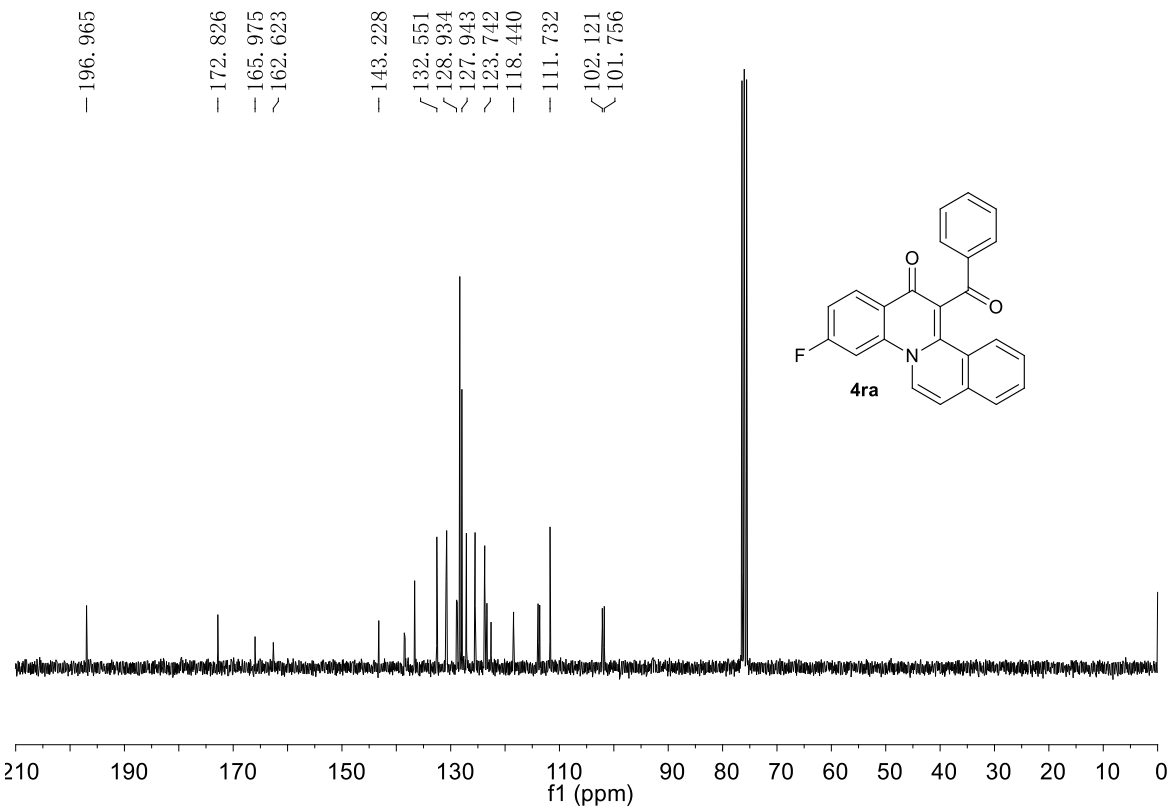

190.168
174.248
145.364
143.649
131.714
127.967
126.427
124.155
119.094
116.493
112.640
4oa
CD3OD
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

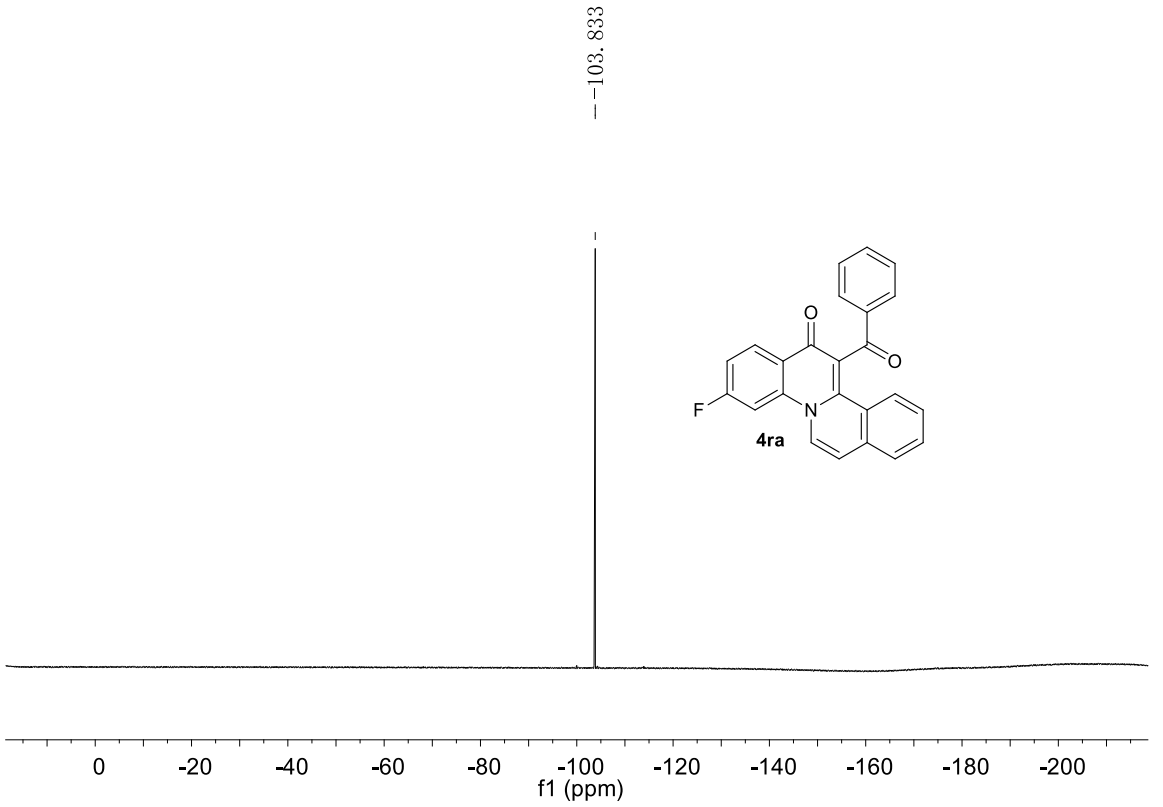

8.098
7.855
7.576
7.558
7.539
7.521
7.499
7.484
7.450
7.375
7.246
7.231
7.218
7.203
6.867
6.848
2.590
8.380
8.359
8.158
8.138
8.098
8.081
8.077
7.876
7.855
7.711
7.542
7.501
7.470
7.354
7.246
7.218
7.203
6.867
6.848
1.00
1.07
2.02
1.04
1.05
1.02
1.93
2.03
1.03
1.04
1.01
2.96
4pa
8.3
7.9
7.5
7.1
f1 (ppm)
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)

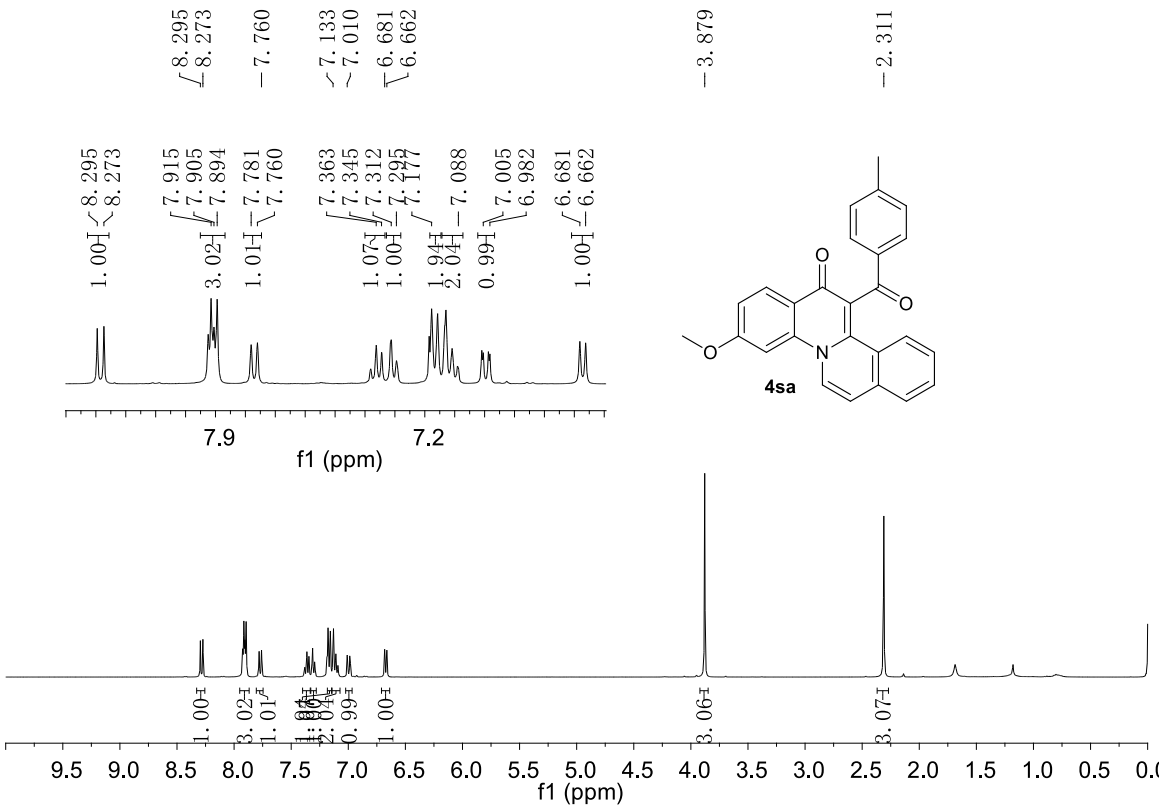

198.495
174.489
143.691
143.618
137.916
129.367
126.776
124.528
119.179
116.038
112.133
22.389
4pa
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

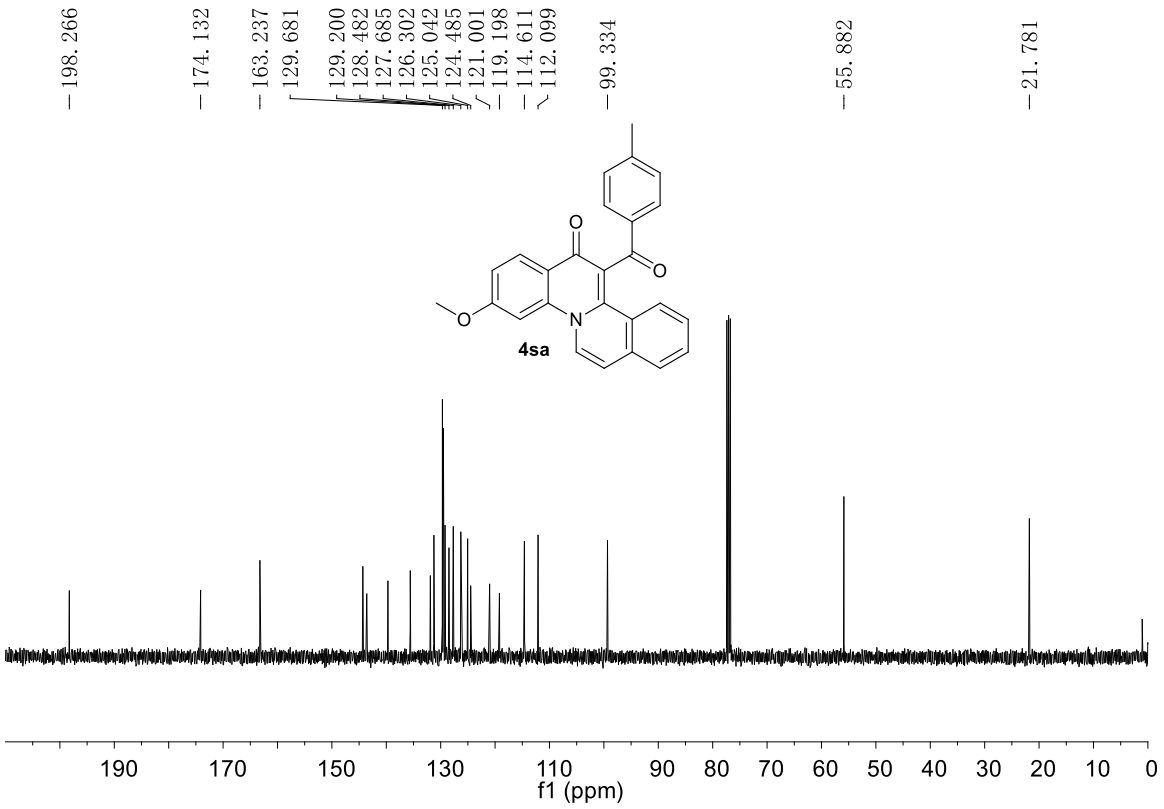

8.446
8.425
8.084
7.859
7.487
7.436
6.904
6.885
4qa
1.00
3.09
1.06
1.05
6.10
0.96
1.03
f1 (ppm)
198.005
173.209
143.698
134.154
129.444
127.285
123.882
118.313
112.391
4qa
f1 (ppm)

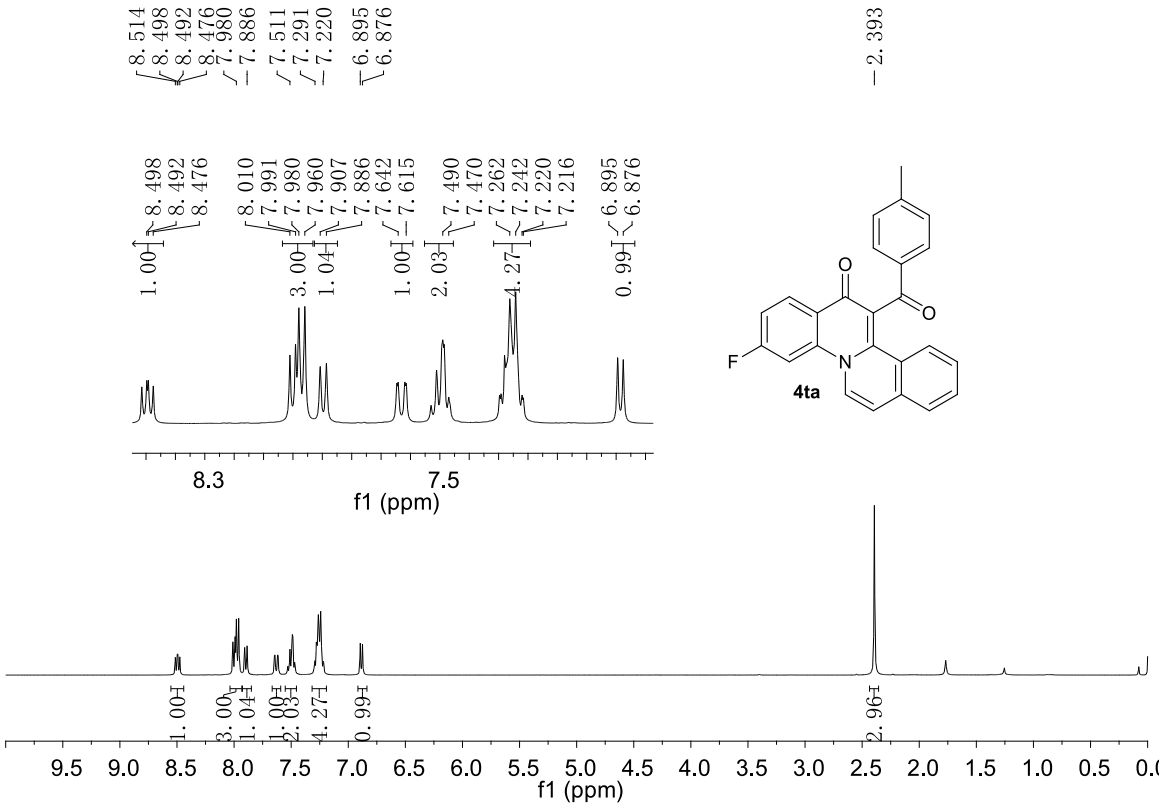

8.523
8.506
8.502
8.485
7.990
7.856
7.511
7.290
7.253
6.886
6.866
1.00
2.04
1.05
1.03
1.07
1.19
3.93
2.26
1.02
8.088
8.069
7.971
7.877
7.856
7.564
7.530
7.511
7.490
7.471
7.452
7.433
7.270
7.261
7.253
7.233
7.216
8.3
8.0
7.7
7.4
7.1
f1 (ppm)
O
O
F
N
4ra
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

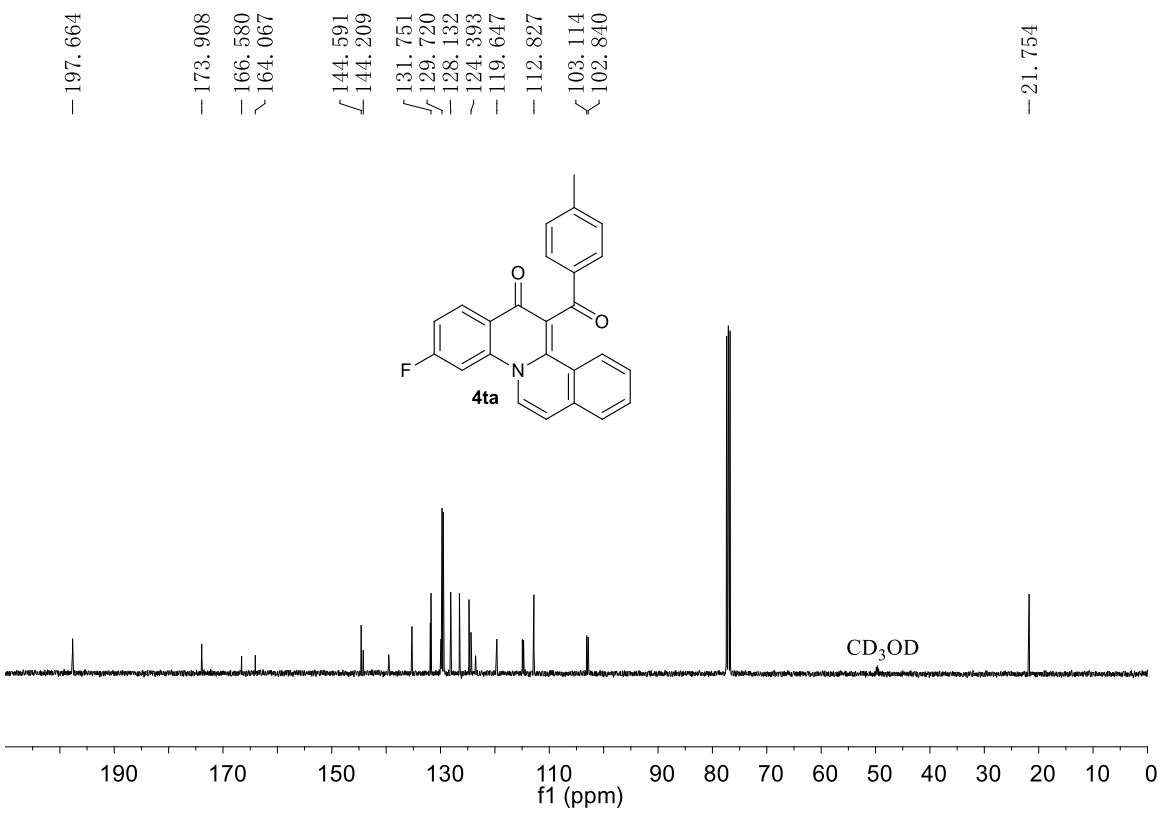

196.965
172.826
165.975
162.623
143.228
132.551
128.934
127.943
123.742
118.440
111.732
102.121
101.756
O
O
F
N
4ra
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

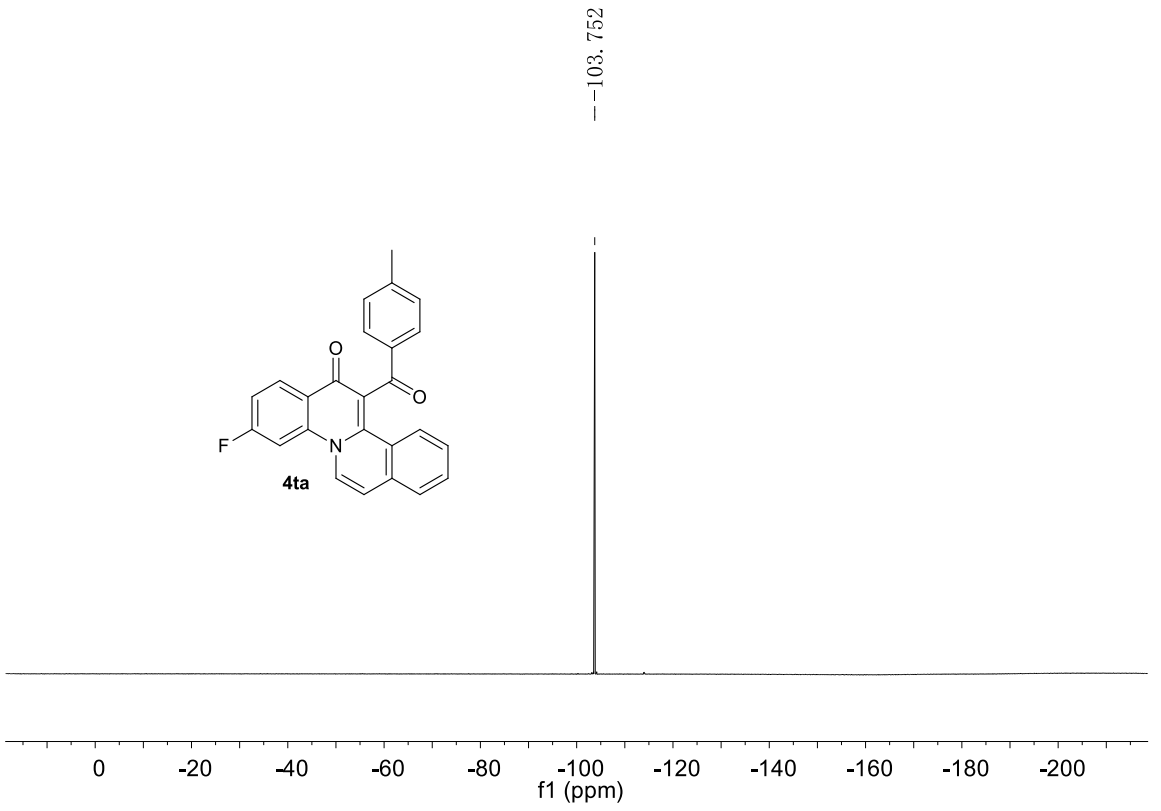

-103.833
4ra
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

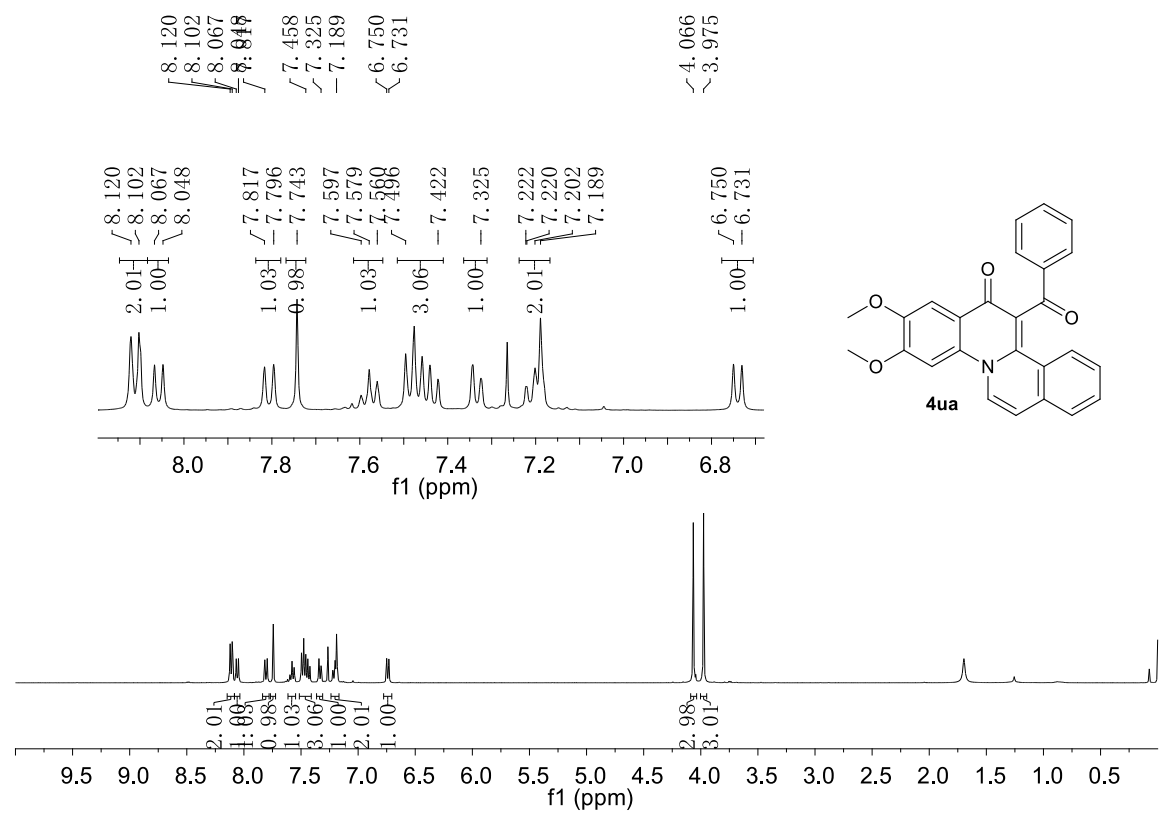

8.295
8.273
7.760
7.133
7.010
6.681
6.662
3.879
2.311
4sa
7.9
7.2
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

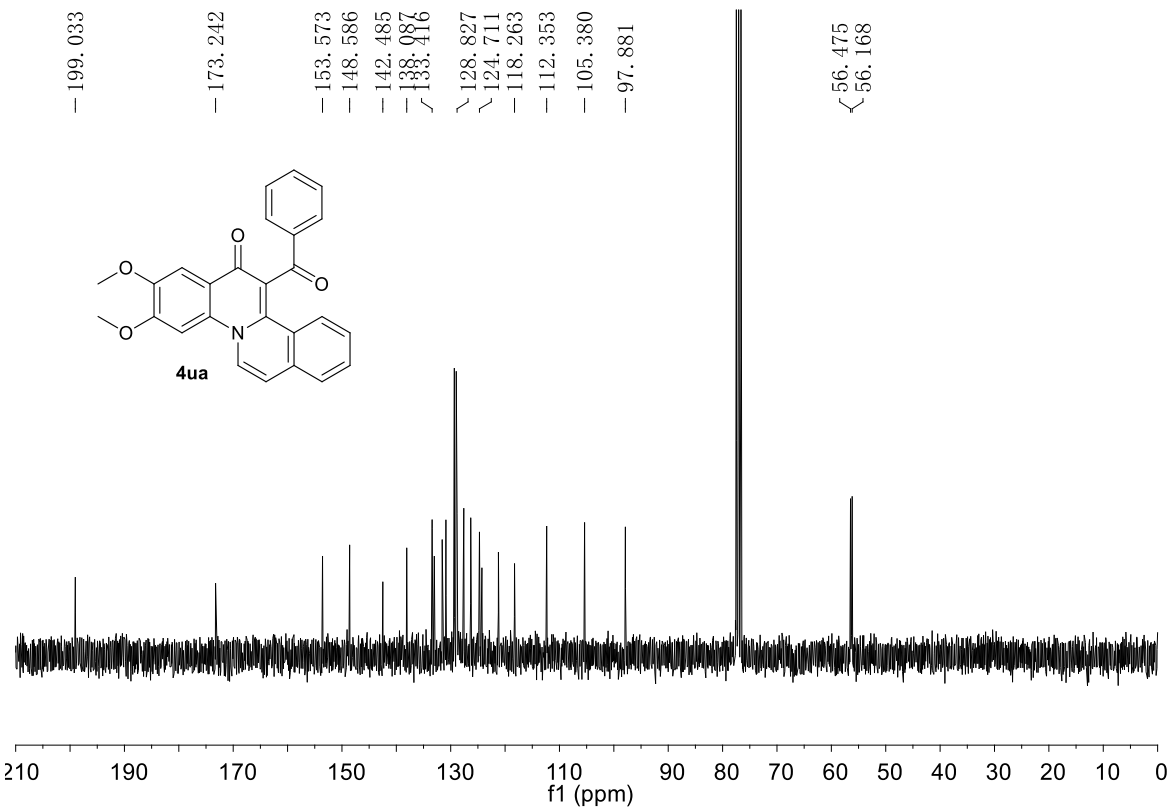

198.266
174.132
163.237
129.681
129.200
128.482
127.685
126.302
125.042
124.485
121.001
119.198
114.611
112.099
99.334
55.882
21.781
4sa
f1 (ppm)

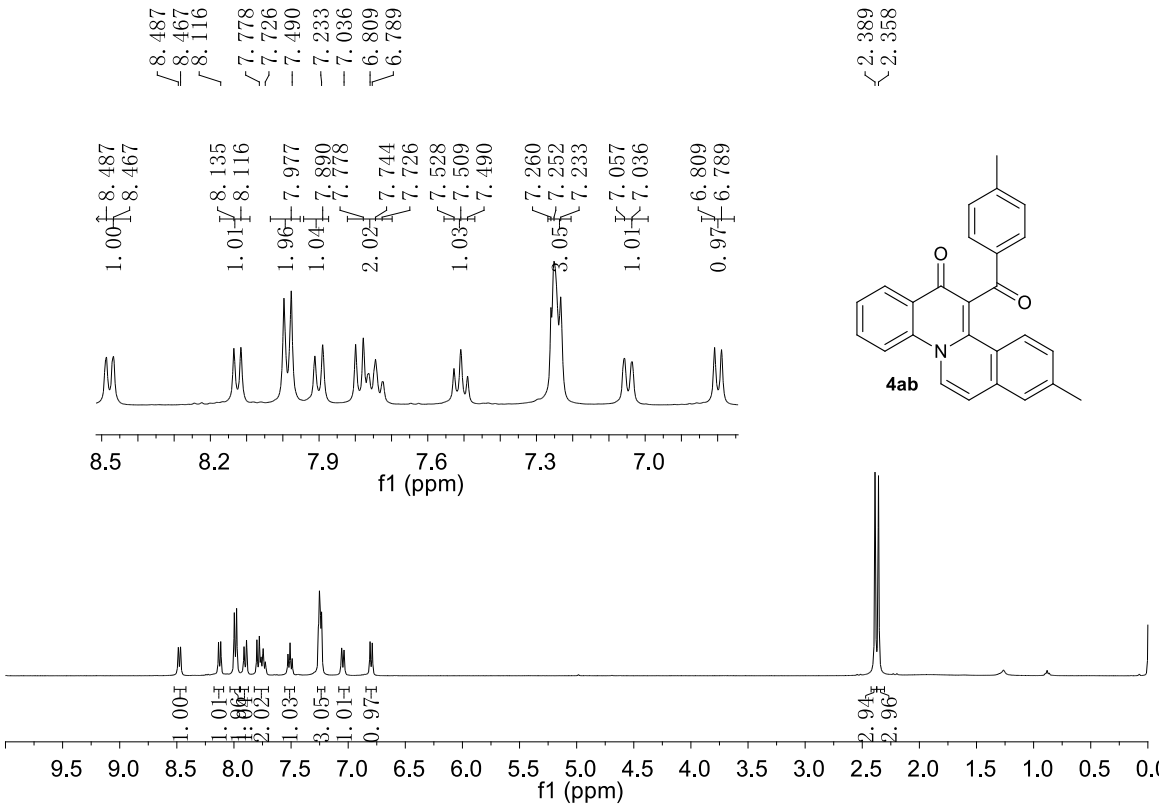

8.514
8.498
8.492
8.476
7.980
7.886
7.511
7.291
7.220
6.895
6.876
2.393
1.00
3.00
1.04
1.00
2.03
4.27
0.99
2.96
4ta
f1 (ppm)

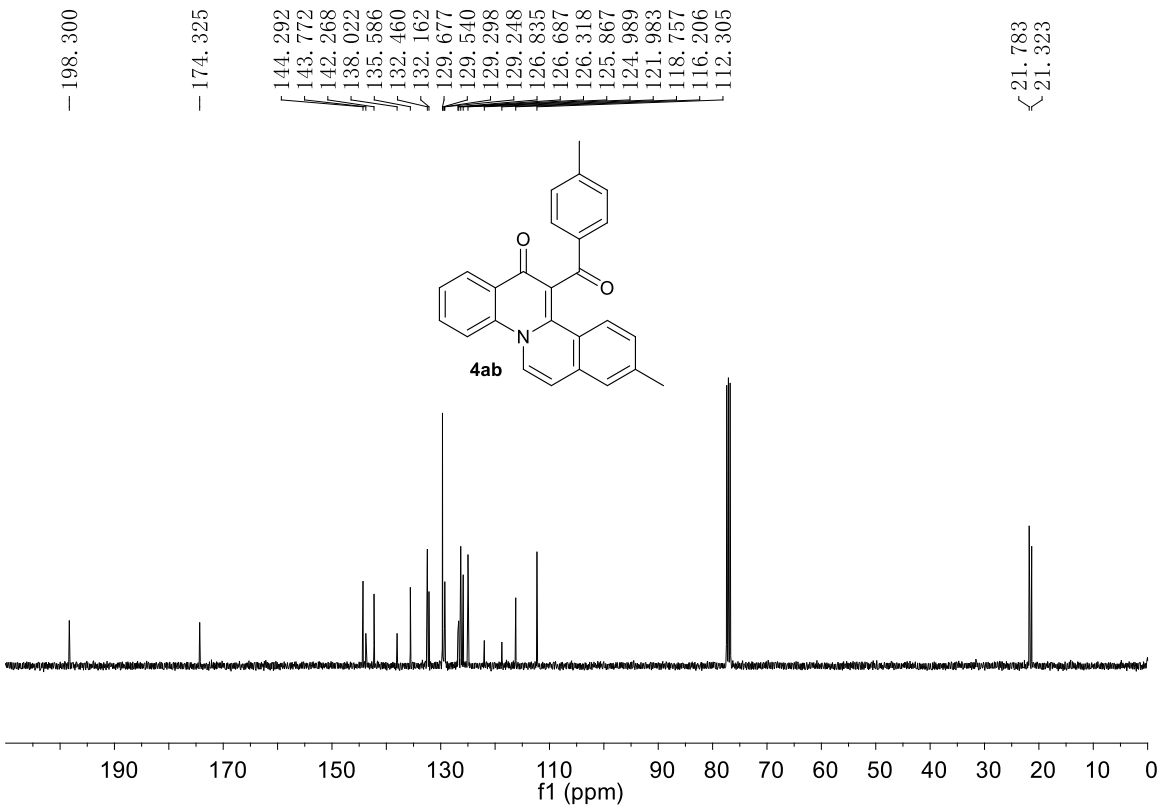

197.664
173.908
166.580
164.067
144.591
144.209
131.751
129.720
128.132
124.393
119.647
112.827
103.114
102.840
21.754
O
O
F
N
4ta
CD3OD
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


103.752
O
O
F
N
4ta
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)


8.120
8.102
8.067
8.048
7.817
7.796
7.743
7.597
7.579
7.560
7.496
7.422
7.325
7.222
7.220
7.202
7.189
6.750
6.731
4.066
3.975
2.01
1.00
1.03
0.98
3.06
1.00
2.01
1.00
2.98
3.01
f1 (ppm)
4ua


199.033
173.242
153.573
148.586
142.485
138.087
133.416
128.827
124.711
118.263
112.353
105.380
97.881
56.475
56.168
f1 (ppm)
4ua


8.487
8.467
8.116
7.778
7.726
7.490
7.233
7.036
6.809
6.789
2.389
2.358
1.00
1.01
1.96
1.04
2.02
1.03
3.05
1.01
0.97
2.94
2.96
8.5
8.2
7.9
7.6
7.3
7.0
f1 (ppm)
4ab
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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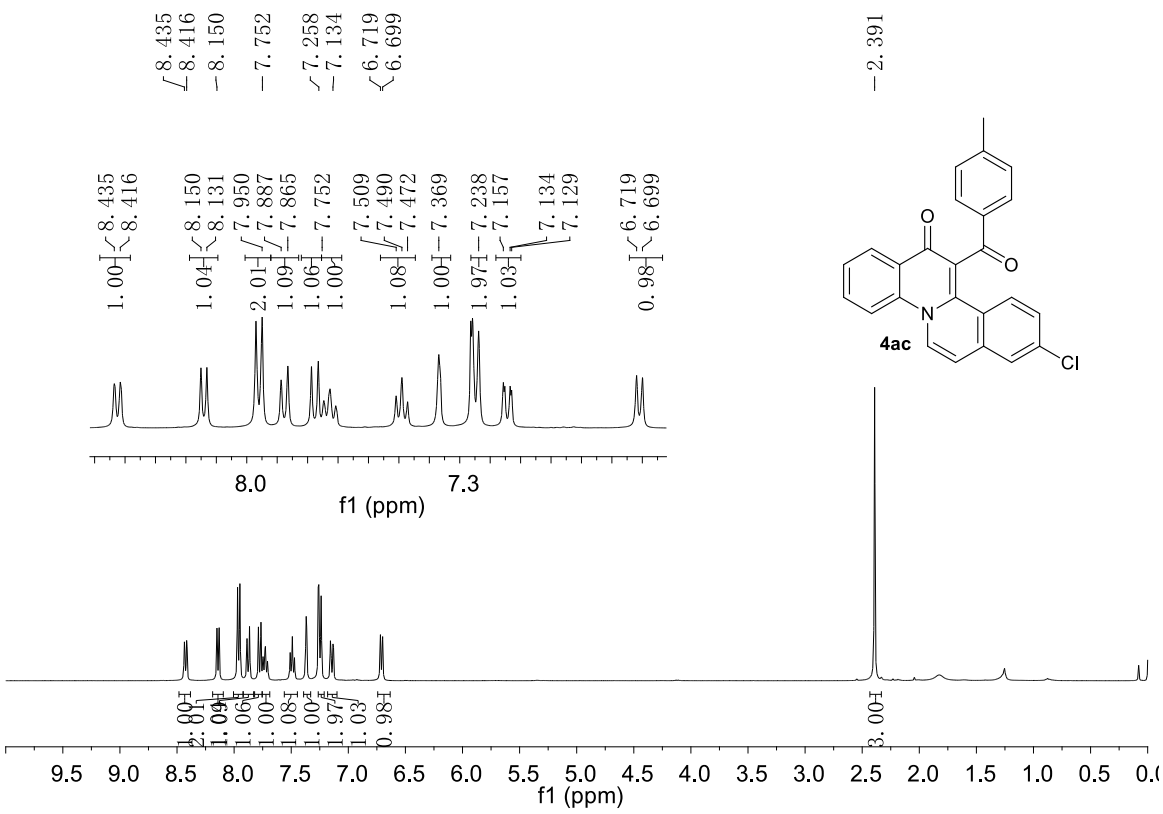
174.325
144.292
143.772
142.268
138.022
135.586
132.460
132.162
129.677
129.540
129.298
129.248
126.835
126.687
126.318
125.867
124.989
121.983
118.757
116.206
112.305
21.783
21.323
4ab
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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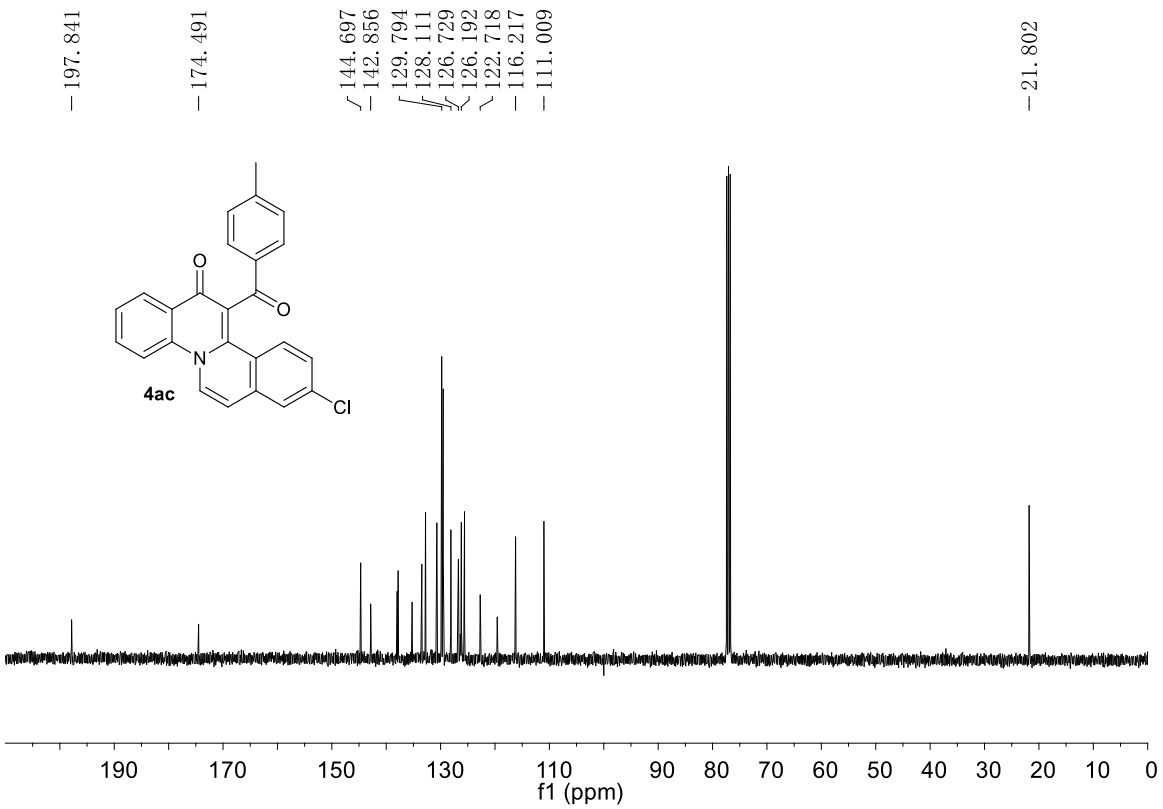
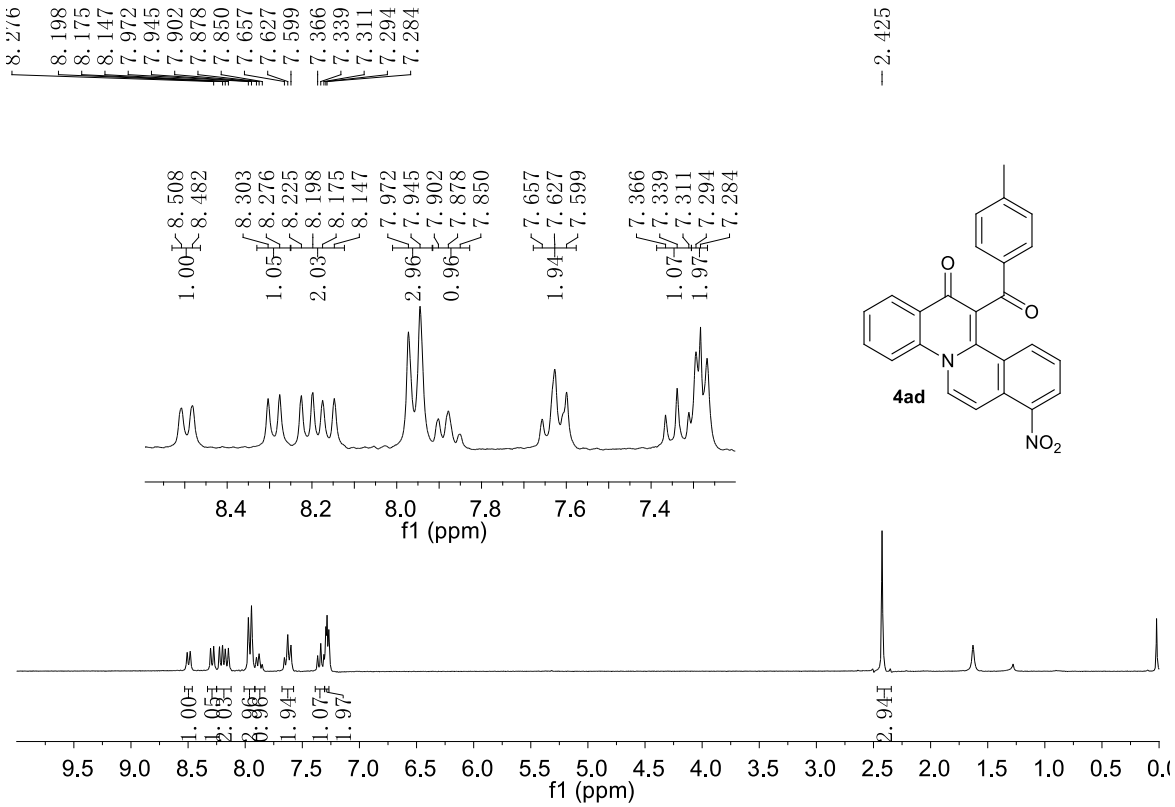
8.416
8.150
7.752
7.258
7.134
6.719
6.699
2.391
1.00
1.04
2.01
1.09
1.06
1.00
1.08
1.00
1.97
1.03
0.98
3.00
4ac
Cl
8.0
7.3
f1 (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


197.841
174.491
144.697
142.856
129.794
128.111
126.729
126.192
122.718
116.217
111.009
21.802
4ac
Cl
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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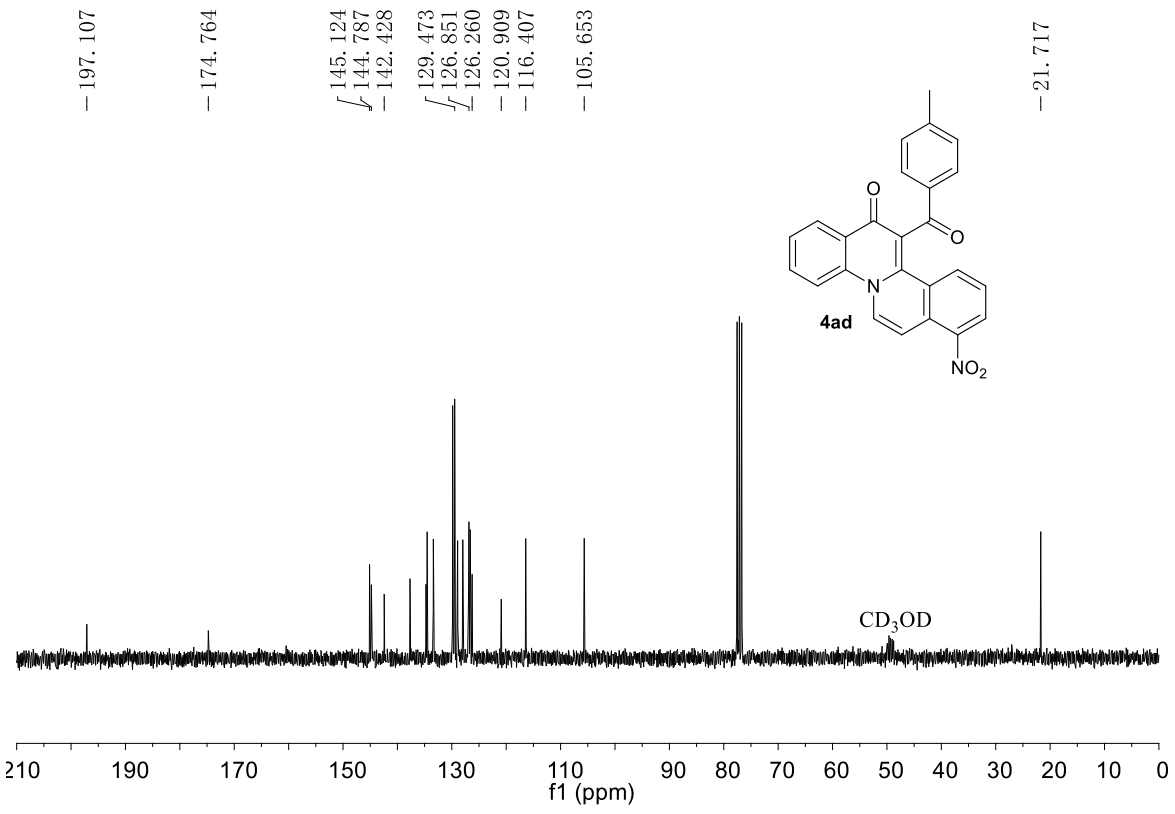
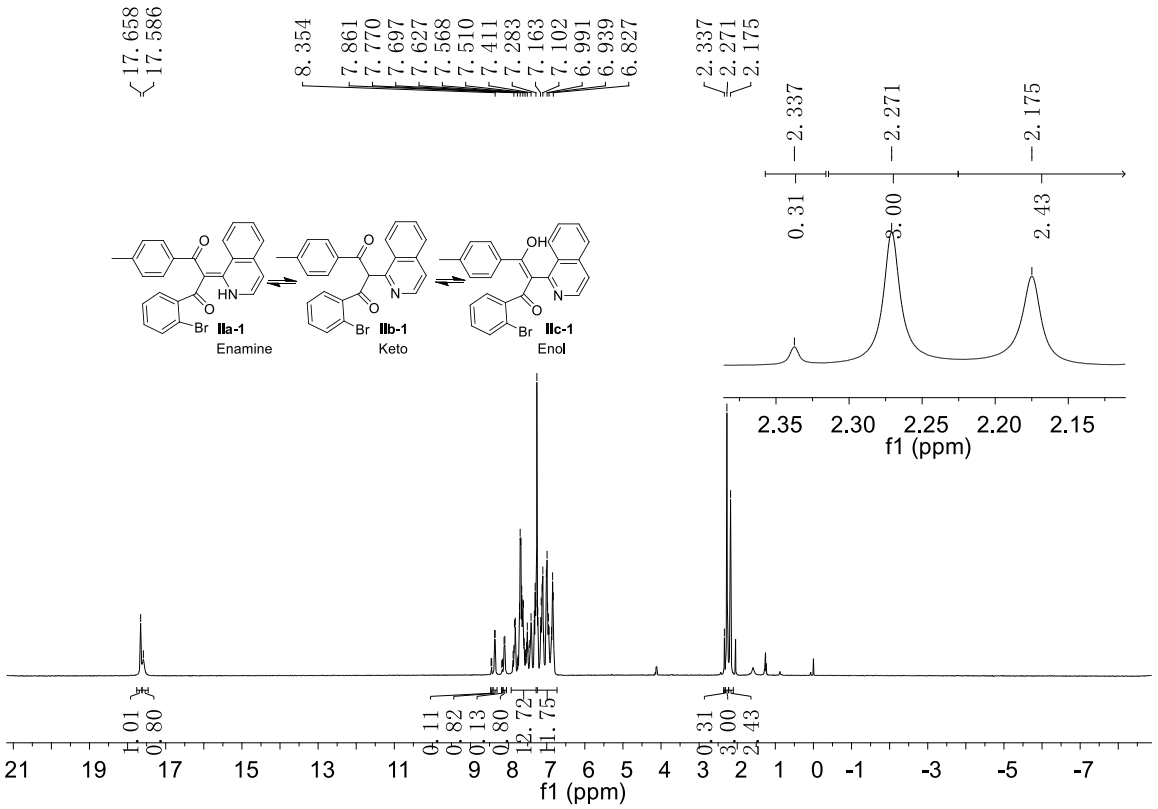
8.198
8.175
8.147
7.972
7.945
7.902
7.878
7.850
7.657
7.627
7.599
7.366
7.339
7.311
7.294
7.284
2.425
8.508
8.482
8.303
8.276
8.225
8.198
8.175
8.147
7.972
7.945
7.902
7.878
7.850
7.657
7.627
7.599
7.366
7.339
7.311
7.294
7.284
1.00
1.05
2.03
2.96
0.96
1.94
1.07
1.97
2.94
4ad
NO2
f1 (ppm)


197.107
174.764
145.124
144.787
142.428
129.473
126.851
126.260
120.909
116.407
105.653
21.717
4ad
NO2
CD3OD
f1 (ppm)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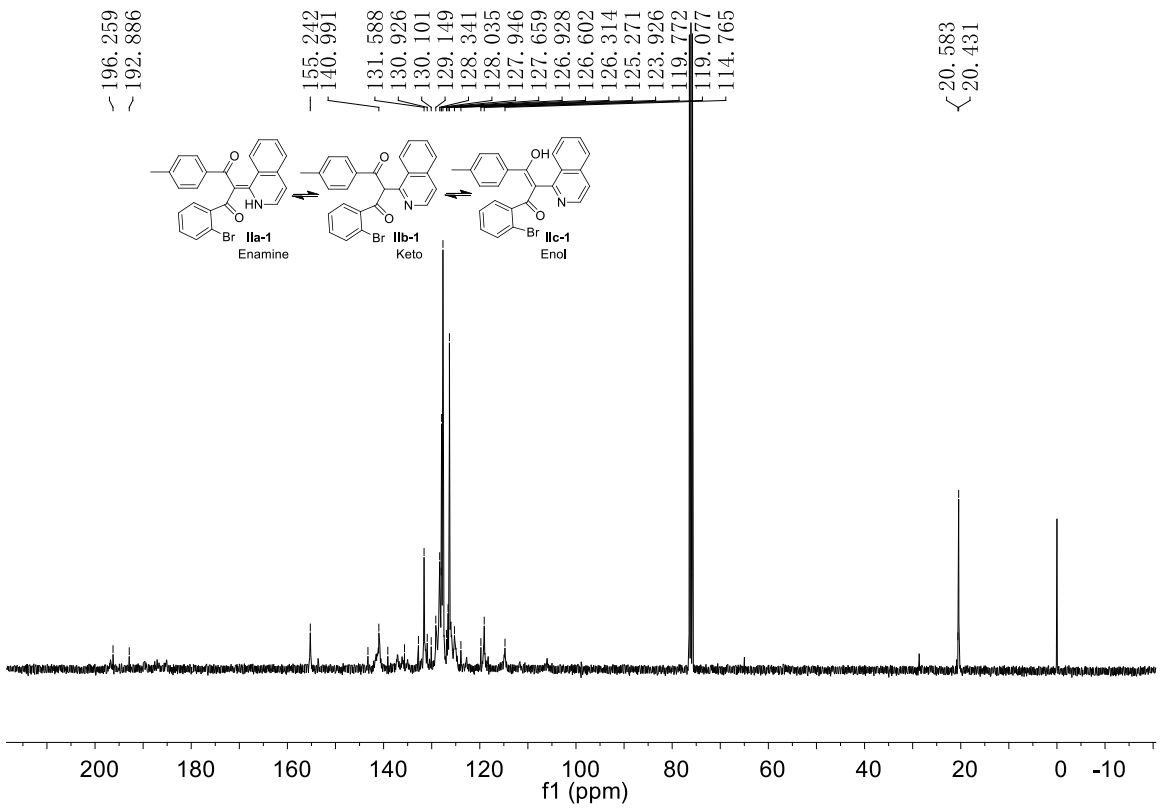
17.586
8.354
7.861
7.770
7.697
7.627
7.568
7.510
7.411
7.283
7.163
7.102
6.991
6.939
6.827
2.337
2.271
2.175
IIa-1
Enamine
IIb-1
Keto
IIc-1
Enol
1.01
0.80
0.11
0.82
0.13
0.80
12.72
11.75
0.31
3.00
2.43
f1 (ppm)


196.259
192.886
155.242
140.991
131.588
130.926
130.101
129.149
128.341
128.035
127.946
127.659
126.928
126.602
126.314
125.271
123.926
119.772
119.077
114.765
20.583
20.431
IIa-1
Enamine
IIb-1
Keto
IIc-1
Enol
f1 (ppm)

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-1956830 (**3ra**), CCDC-1956831 (**4ga**) and CCDC-1959692 (**IIa-1**) 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.

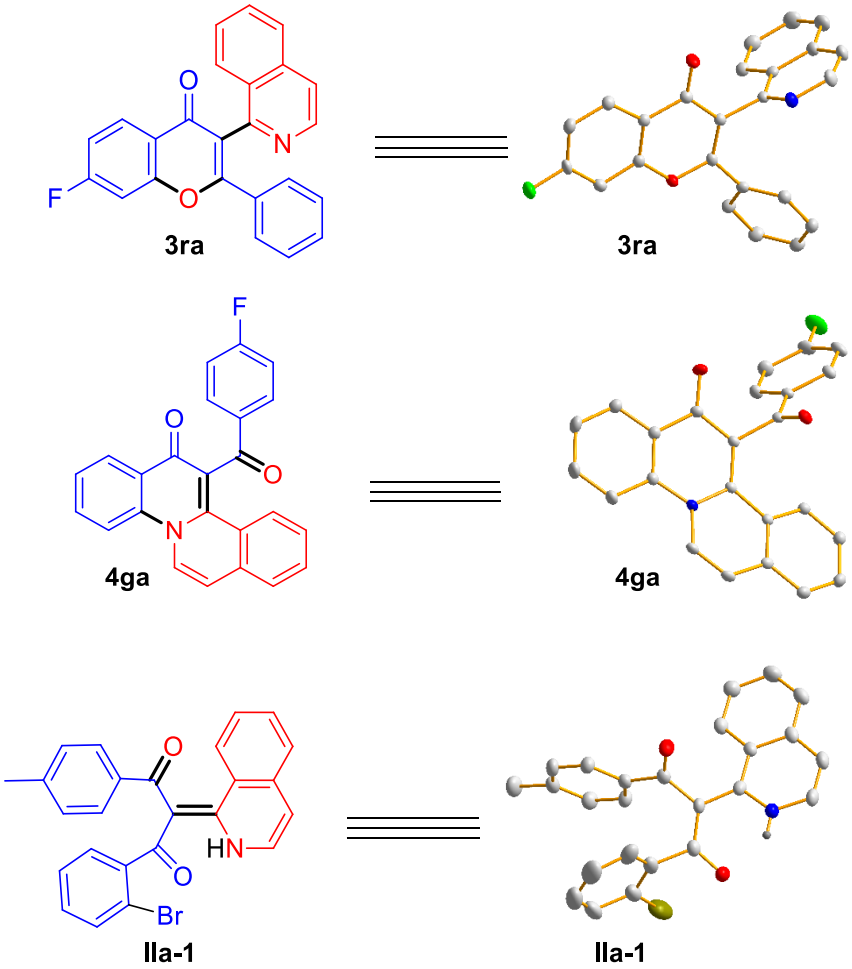


Figure S1 Molecular structures of **3na 4ga** and **IIa-1** with thermal ellipsoids drawn at 30% probability. Hydrogen atoms have been omitted for clarity.

7. Monitoring the process of reaction

We monitored the reaction of ynone **1a** with isoquinoline N-oxide **2a** by ^{1}H NMR (Fig. S2 and S3). Form the characteristic peak changes, the starting material **1a** and isoquinoline N-oxide **2a** were continuously consumed. In the meanwhile, the products **3aa** and **4aa** were divergently obtained using d^{7}-DMF and d^{8}-toluene as solvent, respectively.

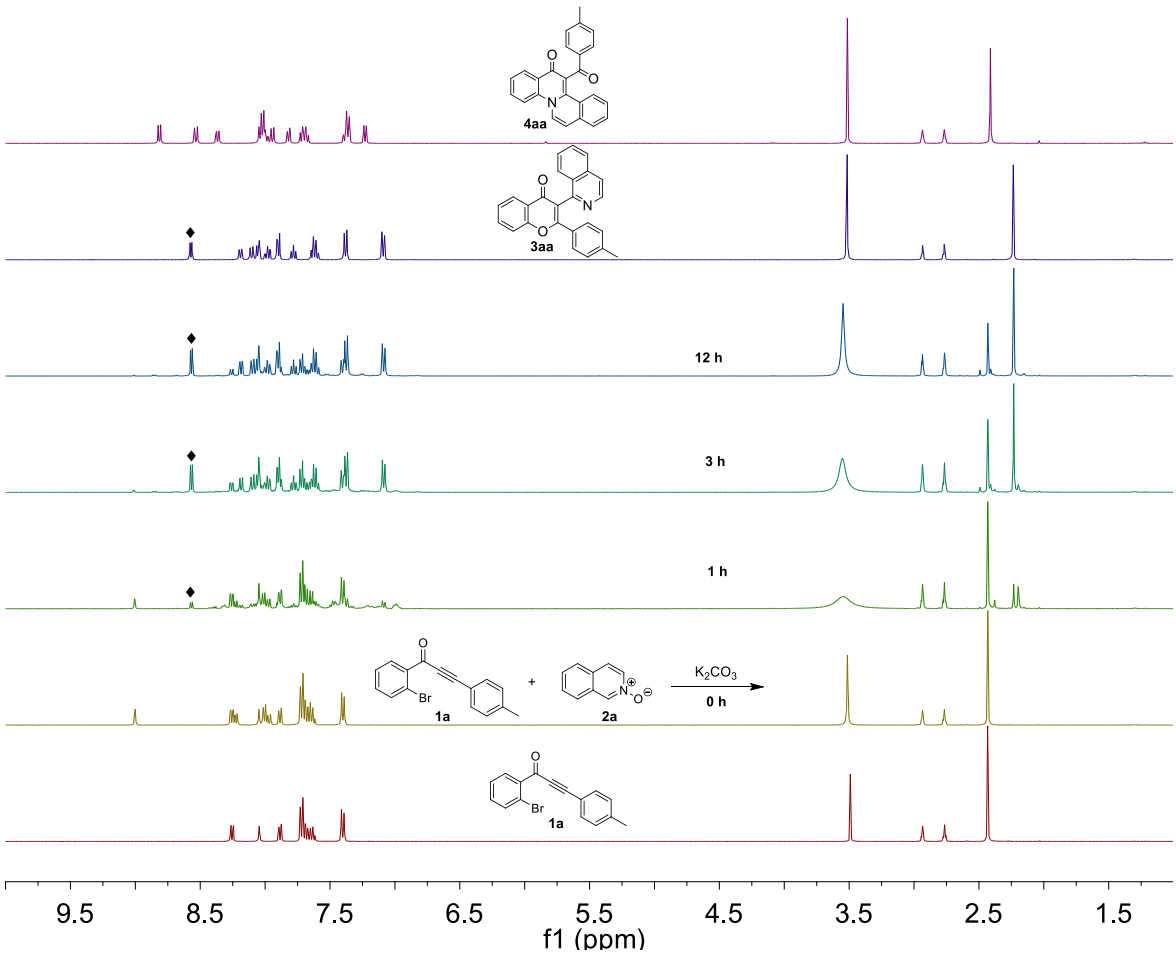


Fig. S2 Monitoring the reaction by ^{1}H NMR using d^{7}-DMF as solvent.

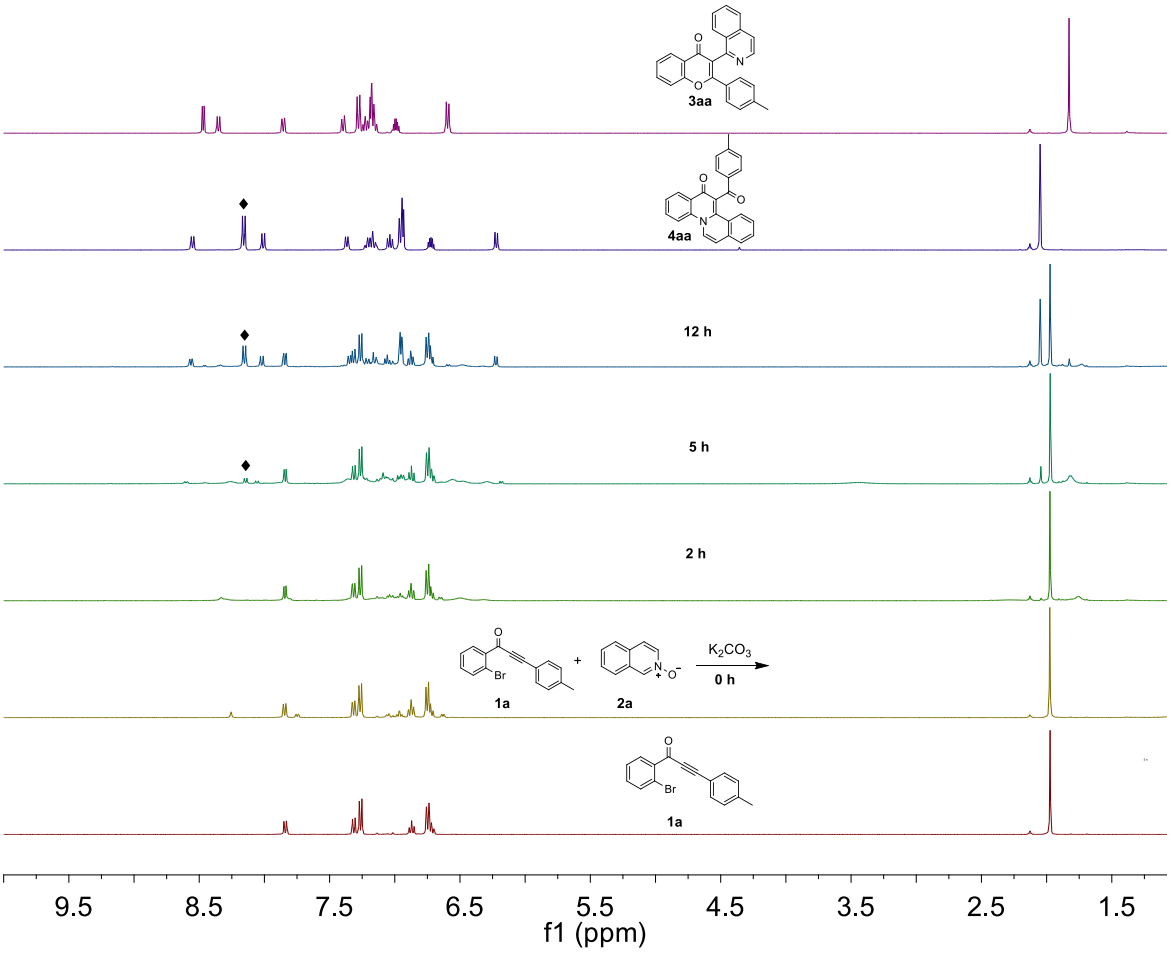


Fig. S3 Monitoring the reaction by ^{1}H NMR using d^{8}-toluene as solvent.