Rhodium(III)-Catalyzed C-H Activation/Annulation of N-Iminopyridinium Ylides with Alkynes and Diazo Compounds

Xiang Li,*[a,b] Ruihong Zhang,[a] Yaoting Qi,[a] Qing Zhao,[a] Tuanli Yao[a,b]

[a] College of Chemistry and Chemical Engineering, Shaanxi University of Science and Technology, Xi'an, Shaanxi 710021, China

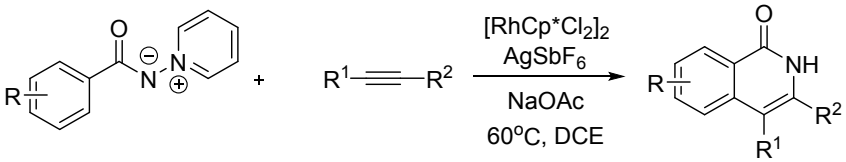
[b] Shaanxi Key Laboratory of Chemical Additives for Industry, Shaanxi University of Science and Technology, Xi'an, Shaanxi 710021, China

Contents

General Information: Unless otherwise noted, all reactions were performed in air, all reagents and solvents were obtained from commercial suppliers and used without any purification. Purifications of reaction products were carried out by chromatography using silica gel (200-300 mesh). NMR spectra were recorded for ^{1}H NMR at 400 MHz and for ^{13}C NMR at 100 MHz. For ^{1}H NMR, tetramethylsilane (TMS) served as internal standard (δ=0) and data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), and coupling constant(s) in Hz. For ^{13}C NMR, TMS (δ=0) was used as internal standard and spectra were obtained with complete proton decoupling.

N-iminopyridinium ylides,[1] alkynes[2] and diazo compounds[3] were prepared according to the reported literatures.

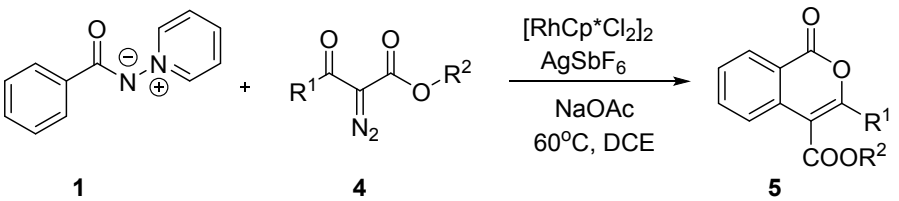
General Procedure for Rhodium(III)-Catalyzed C-H Activation/Annulation of N-Iminopyridinium Ylides with Alkynes



1 **2** **3**

An oven-dried 25 mL Schlenk tube was charged with the N-iminopyridinium ylides **1** (0.2 mmol), alkynes **2** (0.4 mmol), $[Cp^*RhCl_2]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), NaOAc (0.4 mmol) and DCE (2.0 mL) was added under air. The reaction mixture was stirred at 60℃ for 12 h. After the reaction was complete, the mixture was evaporated in vacuum. The crude product was purified by flash chromatography on silica gel using hexane/ethyl acetate or DCM/MeOH as the eluent to give the pure product **3**.

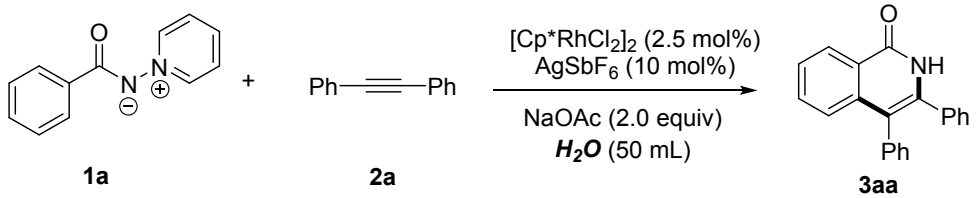
General Procedure for Rhodium(III)-Catalyzed C-H Activation/Annulation of N-Iminopyridinium Ylides with Diazo Compounds



1 **4** **5**

An oven-dried 25 mL Schlenk tube was charged with the N-iminopyridinium ylides **1** (0.2 mmol), diazo compounds **4** (0.4 mmol), $[Cp^*RhCl_2]_2$ (2.5 mol%), $AgSbF_6$ (2.5 mol%), NaOAc or HOAc (0.4 mmol) and DCE (2.0 mL) was added under air. The reaction mixture was stirred at 60℃ for 12 h. After the reaction was complete, the mixture was evaporated in vacuum. The crude product was purified by flash chromatography on silica gel using hexane/ethyl acetate as the eluent to give the pure product **5**.

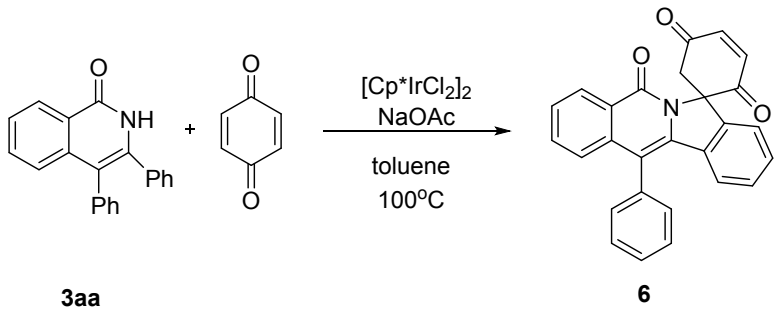
Procedure for Scale-up Experiment



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

An oven-dried 250 mL Schlenk tube was charged with the N-iminopyridinium ylides **1** (5.0 mmol), diphenylacetylene **2a** (10.0 mmol), $[Cp^*RhCl_2]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), NaOAc (10.0 mmol) and H_2O (50 mL) was added under air. The reaction mixture was stirred at 60℃ for 24 h. After the reaction was complete, the mixture was extracted with ethyl acetate (50 mL) three times, the combined organic layer was evaporated in vacuum. The crude product was purified by flash chromatography on silica gel using hexane/ethyl acetate or DCM/MeOH as the eluent to give the pure product **3aa** in 78% yield.

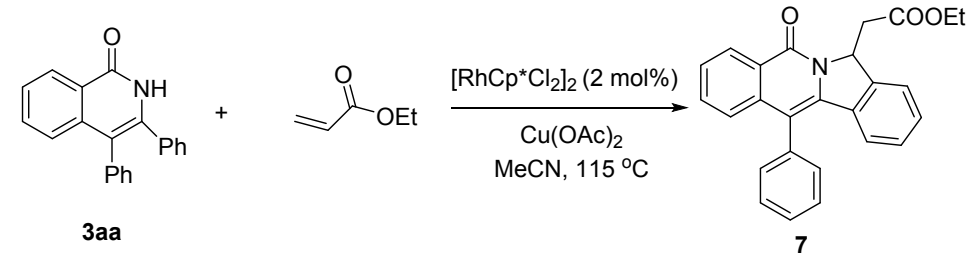
Iridium(III)-Catalyzed C-H Annulation of 3aa with benzoquinone[4]



3aa **6**

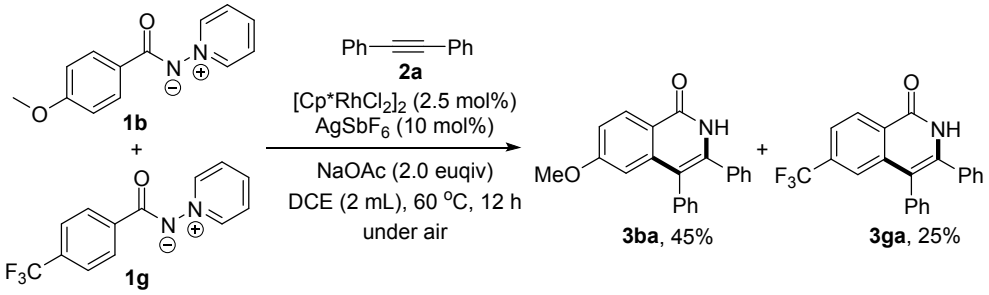
An oven-dried 25 mL Schlenk tube was charged with **3aa** (0.2 mmol), benzoquinone(0.44 mmol), $[IrCp^*Cl_2]_2$ (3.0 mol%), NaOAc (0.1 mmol) and toluene (1.0 mL) was added under N_2. The reaction mixture was stirred at 100℃ for 12 h. After the reaction was complete, the mixture was evaporated in vacuum. The crude product was purified by flash chromatography on silica gel using hexane/ethyl acetate as the eluent to give the pure product **6**.

Rhodium(III)-Catalyzed C-H Annulation of 3aa with Ethyl Acrylate[5]



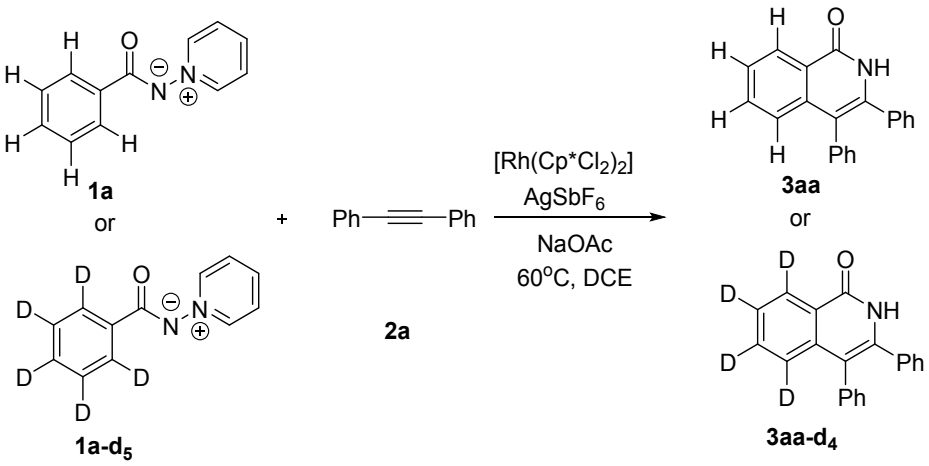
An oven-dried 25 mL Schlenk tube was charged with **3aa** (0.2 mmol), ethyl acrylate (0.4 mmol), $[RhCp^*Cl_2]_2$ (2.0 mol%), $Cu(OAc)_2$ (2.0 equiv) and MeCN (2.0 mL) was added under N_2. The reaction mixture was stirred at 115℃ for 12 h. After the reaction was complete, the mixture was evaporated in vacuum. The crude product was purified by flash chromatography on silica gel using hexane/ethyl acetate as the eluent to give the pure product **7**.

Competitive Experiment



An oven-dried 25 mL Schlenk tube was charged with the N-iminopyridinium ylides **1b** (0.1 mmol) and **1g** (0.1 mmol), diphenylacetylene **2a** (0.2 mmol), $[Cp^*RhCl_2]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), NaOAc (0.4 mmol) and DCE (2.0 mL) was added under air. The reaction mixture was stirred at 60℃ for 24 h. After the reaction was complete, the mixture was evaporated in vacuum. The crude product was purified by flash chromatography on silica gel using DCM/MeOH as the eluent to give the product **3ba** and **3ga** in 45% and 25% yield, respectively.

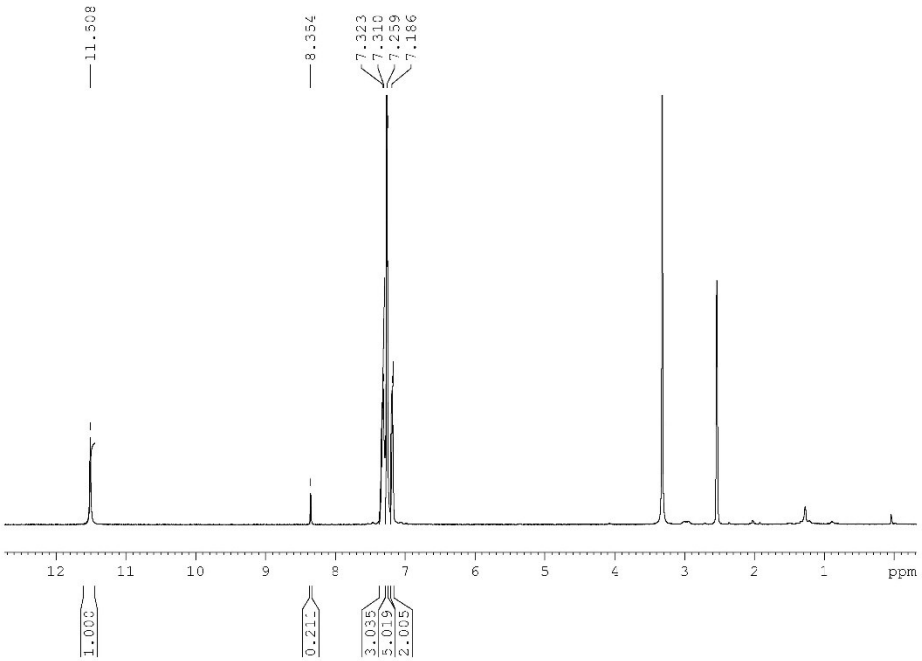
KIE Experiments

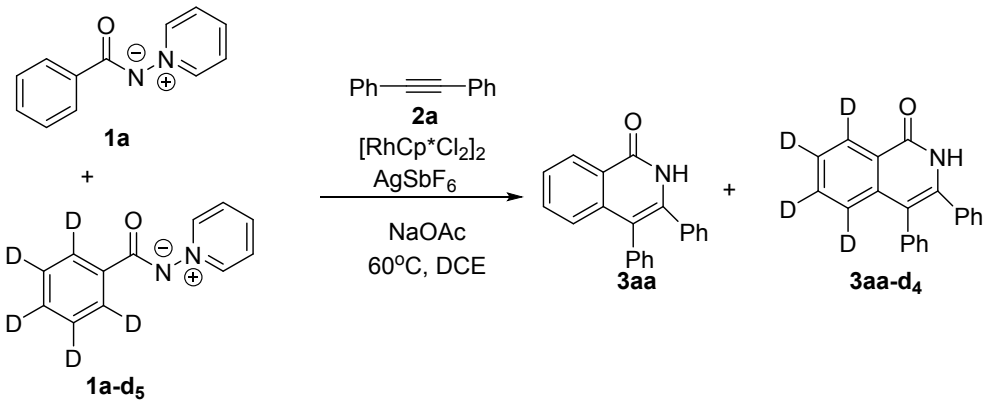


An oven-dried 25 mL Schlenk tube was charged with the N-iminopyridinium ylides **1a** (0.1 mmol), diphenylacetylene **2a** (0.2 mmol), $[RhCp^*Cl_2]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), NaOAc (0.2 mmol) and DCE (2.0 mL) was added into above under air. The reaction mixture was stirred at 60℃ for 12 h. After the reaction was complete, the mixture was evaporated in vacuum. The crude product was purified by flash chromatography on silica gel using DCM/MeOH as the eluent to give the pure product **3aa** in 95% yield.

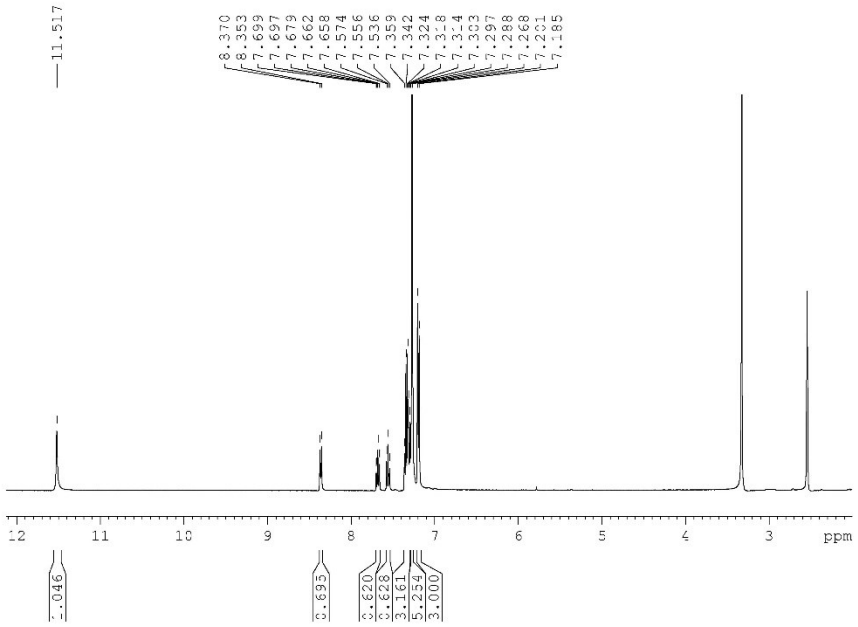
An oven-dried 25 mL Schlenk tube was charged with the N-iminopyridinium ylides **1a-d_5** (0.1 mmol), diphenylacetylene **2a** (0.2 mmol), $[RhCp^*Cl_2]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), NaOAc (0.2 mmol) and DCE (2.0 mL) was added into above under air. The reaction mixture was stirred at 60℃ for 12 h. After the reaction was complete, the mixture was evaporated in vacuum. The crude product was purified by flash chromatography on silica gel using DCM/MeOH as the eluent to give the pure product **3aa-d_4** in 59% yield.

The KIE value was determined to be 1.6 based on the isolated yield.

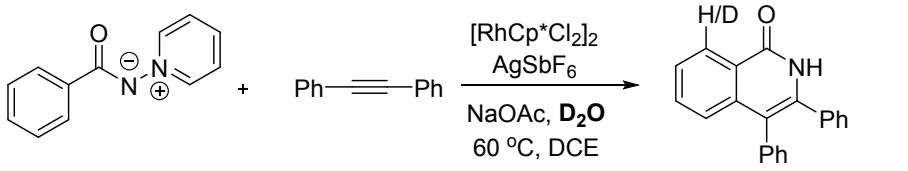




An oven-dried 25 mL Schlenk tube was charged with the N-iminopyridinium ylides **1a** (0.1 mmol) and N-iminopyridinium ylides **1a-d$_5$** (0.1 mmol), diphenylacetylene **2a** (0.2 mmol), $[RhCp^*Cl_2]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), NaOAc (0.4 mmol) and DCE (2.0 mL) was added under air. The reaction mixture was stirred at 60℃ for 12 h. After the reaction was complete, the mixture was evaporated in vacuum. The crude product was purified by flash chromatography on silica gel using DCM/MeOH as the eluent to give the product **3aa** and **3aa-d$_4$** as a mixture. The KIE value was determined to be 1.6 based on ^{1}H NMR analysis.

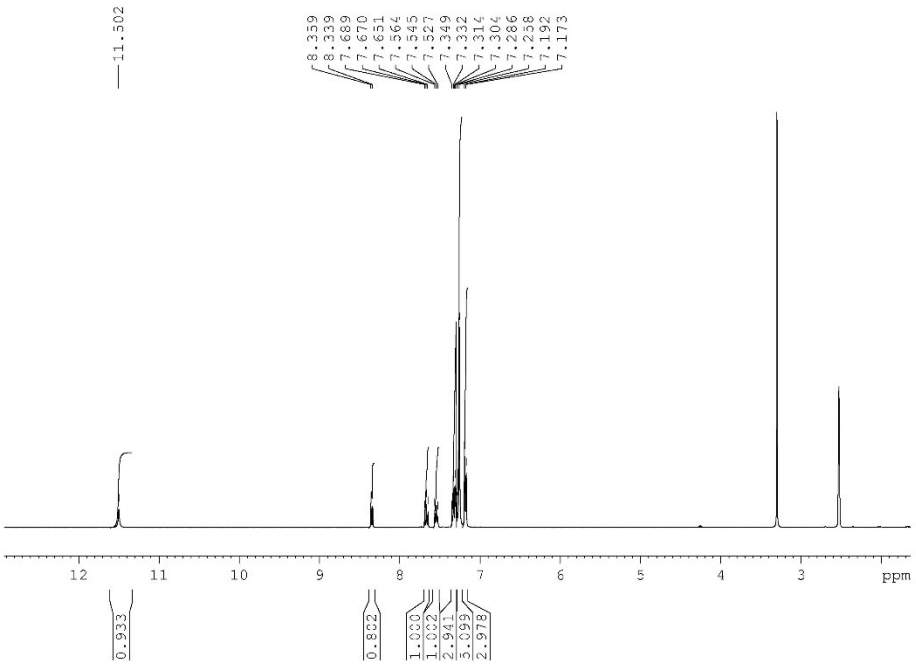


H/D Exchange Experiment



1a **2a** **3aa-d$_1$**, 56% yield, 21% **D**

An oven-dried 25 mL Schlenk tube was charged with the N-iminopyridinium ylides (0.1 mmol), diphenylacetylene **2a** (0.2 mmol), $[RhCp^*Cl_2]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), NaOAc (0.2 mmol), D_2O (10 mmol) and DCE (2.0 mL) was added under air. The reaction mixture was stirred at 60℃ for 12 h. After the reaction was complete, the mixture was evaporated in vacuum. The crude product was purified by flash chromatography on silica gel using DCM/MeOH as the eluent to give the pure product **3aa-d$_1$** in 56% yield. The deuterium incorporation was calculated to be 20% based on ^{1}H NMR spectroscopy.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10
9
8
7
6
5
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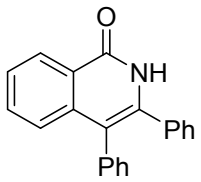
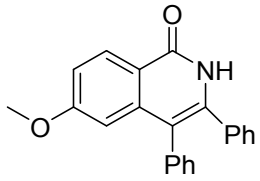
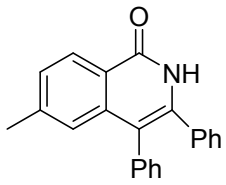
^{1}H NMR and ^{13}C NMR of All Products



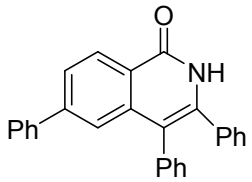
3,4-diphenylisoquinolin-1(2H)-one (3aa): white solid, yield: 95% (This compound is known[6]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.52 (s, 1H), 8.35 (d, *J*=7.9 Hz, 1H), 7.67 (t, *J*=8.3 Hz, 1H), 7.54 (t, *J*=7.5 Hz, 1H), 7.34-7.28 (m, 3H), 7.26 (s, 5H), 7.18 (d, *J*=6.8 Hz, 3H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 162.1, 139.0, 138.6, 136.3, 135.1, 132.9, 132.2, 130.3, 128.7, 128.6, 128.1, 127.5, 127.3, 126.7, 125.5, 125.4.



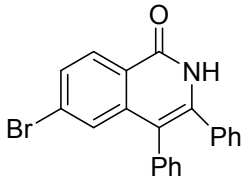
6-methoxy-3,4-diphenylisoquinolin-1(2H)-one (3ba): white solid, yield: 97% (This compound is known[6]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.34 (s, 1H), 8.28 (d, *J*= 8.80 Hz, 1H), 7.34-7.28 (m, 3H), 7.24 (s, 5H),7.18-7.15 (m, 3H), 6.53 (s, 1H), 3.70 (s, 3H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 162.8, 161.8, 140.6, 139.7, 136.4, 135.1, 132.1, 130.2, 129.6, 128.7, 128.6, 128.1, 127.5, 119.4, 115.6, 114.9, 107.7, 55.6.



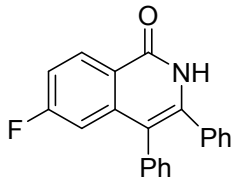
6-methyl-3,4-diphenylisoquinolin-1(2H)-one (3ca) : white solid, yield: 98% (This compound is known[6]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.43(s,1H), 8.26 (d, *J*=8.11 Hz, 1H), 7.38 (d, *J*=8.12 Hz, 1H), 7.36-7.30 (m, 3H),7.26 (s, 5H), 7.18 (d, *J*=6.44 Hz, 2H), 6.97 (s, 1H), 2.35 (s, 3H). **^{13}CNMR (100 MHz, DMSO- d6)** δ 162.1, 142.9, 139.1, 138.7, 136.4, 135.1, 132.2, 130.3, 128.7, 128.6, 128.2, 128.1, 127.5, 127.4, 124.9, 123.4, 115.7, 22.1.



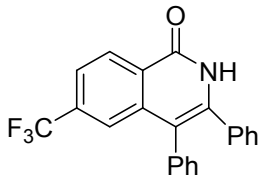
3,4,6-triphenylisoquinolin-1(2H)-one (3da): white solid, yield: 93% (This compound is known[7]). **^{1} HNMR (400 MHz, DMSO-d6)** δ 11.55 (s, 1H), 8.41 (d, *J*=8.28 Hz, 1H), 7.80 (dd, *J*=1.65 Hz、8.33Hz, 1H), 7.51 (d, *J*=7.16 Hz, 2H), 7.45 (t, *J*=7.38 Hz, 2H), 7.40-7.27 (m, 5H), 7.25-7.21 (m, 7H). ^{13}CNMR (100 MHz, DMSO-d6) δ 162.0, 144.5, 140.0, 139.6, 136.2, 135.0, 132.2, 130.4, 130.3, 129.6, 128.7, 128.1, 127.6, 127.4, 125.5, 124.5, 123.2, 116.0.



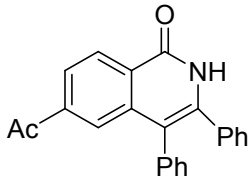
6-bromo-3,4-diphenylisoquinolin-1(2H)-one (3ea): white solid, yield: 86% (This compound is known[6]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.64 (s, 1H), 8.26 (d, *J*=8.28 Hz, 1H), 7.69 (d, *J*=8.00 Hz, 1H), 7.34 (d, *J*=6.92 Hz, 3H), 7.26 (s, 6H), 7.19 (d, *J*=6.08 Hz, 2H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 161.7, 140.8, 140.4, 135.6, 134.7, 132.1, 130.2, 129.8, 129.6, 128.9, 128.2, 127.8, 127.4, 127.2, 124.4, 114.9.



6-fluoro-3,4-diphenylisoquinolin-1(2H)-one (3fa): white solid, yield: 84% (This compound is known[6]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.64 (s, 1H), 8.42 (t, *J*=7.61 Hz, 1H), 7.42-7.31(m, 4H), 7.27 (s, 5H), 7.19 (d, *J*=6.83 Hz ,2H), 6.77 (d, *J*=10.88 Hz, 1H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 166.3, 163.8, 161.5, 141.2, 141.1, 140.7, 135.8, 134.7, 132.0, 131.0, 130.9, 130.2, 128.9, 128.2, 127.8, 122.4, 115.4, 115.2, 115.0, 110.2, 110.0. **^{19}FNMR (376 MHz, DMSO-d6)** δ -106.30.

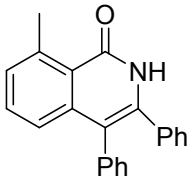


3,4-diphenyl-6-(trifluoromethyl)isoquinolin-1(2H)-one (3ga): white solid, yield: 66% (This compound is known[8]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.90 (s, 1H), 8.56 (d, *J*=8.36 Hz, 1H), 7.85 (d, *J*=8.33 Hz, 1H), 7.43(s, 1H), 7.39-7.34 (m, 3H), 7.29 (s, 5H), 7.23 (d, *J*=7.28 Hz, 2H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 161.4, 141.0, 138.8, 135.4, 134.5, 132.8 (d, *J*=31.5 Hz), 132.1, 130.2, 129.1, 128.9, 128.2, 128.0, 125.6, 122.9, 122.4, 122.1, 120.1, 115.6. **^{19}FNMR (376 MHz, DMSO-d6)** δ -61.74.

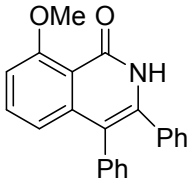


6-acetyl-3,4-diphenylisoquinolin-1(2H)-one (3ha): white solid, yield: 74% (This compound is known[6]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.69 (s, 1H), 8.45 (d, *J*=8.30 Hz, 1H), 8.06 (dd, *J*=8.3 Hz, 1H), 7.74 (s, 1H), 7.37-7.32 (m, 3H), 7.27 (s, 5H), 7.20 (d, *J*= 6.24 Hz, 2H), 2.54 (s, 3H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 198.2, 161.7, 140.0, 139.9, 138.5, 135.8, 134.8, 132.2, 130.3,

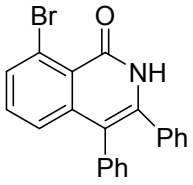
128.8, 128.2, 128.1, 128.0, 127.8, 125.7, 125.3, 116.2, 27.4.



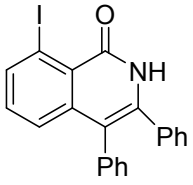
8-methyl-3,4-diphenylisoquinolin-1(2H)-one (3ia): white solid, yield: 93% (This compound is known[7]). **^{1}HNMR (400 MHz, DMSO-d$_6$)** δ 11.26 (s, 1H), 7.47 (t, *J*=7.76 Hz, 1H), 7.34-7.24 (m, 9H), 7.15 (d, *J*=6.76 Hz, 2H), 6.97 (d, *J*=8.12 Hz, 1H), 2.92 (s, 3H). **^{13}CNMR (100 MHz, DMSO-d$_6$)** δ 163.2, 141.1, 140.4, 138.9, 137.0, 135.0, 132.3, 131.9, 130.2, 129.5, 128.7, 128.5, 128.1, 127.4, 123.8, 123.7, 115.9.



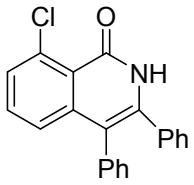
8-methoxy-3,4-diphenylisoquinolin-1(2H)-one (3ja): white solid, yield: 65% (This compound is known[6]). **^{1}HNMR (400 MHz, DMSO-d$_6$)** δ 11.11 (s, 1H), 7.51 (t, *J*=8.22 Hz, 1H), 7.32-7.22 (m, 8H), 7.14 (d, *J*=6.49 Hz, 2H), 7.03 (d, *J*=8.04 Hz, 1H), 6.65 (d, *J*=8.00 Hz, 1H), 3.91 (s, 3H). **^{13}CNMR (100 MHz, DMSO-d$_6$)** δ 161.1, 160.6, 141.7, 139.7, 137.0, 134.9, 133.4, 132.3, 130.1, 128.6, 128.5, 128.0, 127.4, 117.5, 115.2, 115.0, 109.0, 56.5.



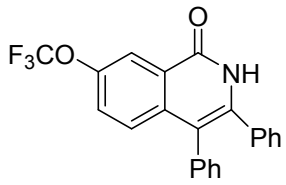
8-bromo-3,4-diphenylisoquinolin-1(2H)-one (3ka): white solid, yield: 66% (This compound is known[9]) **^{1}HNMR (400 MHz, DMSO-d$_6$)** δ 11.55 (s, 1H), 7.75 (d, *J*=7.52 Hz, 1H), 7.45 (t, *J*=8.04 Hz, 1H), 7.34-7.28 (m, 3H), 7.24 (s, 5H), 7.16 (d, *J*=6.44Hz, 2H), 7.12 (d, *J*=8.11 Hz, 1H). **^{13}CNMR (100 MHz, DMSO-d$_6$)** δ 160.4, 141.9, 140.2, 136.4, 134.6, 133.3, 132.2, 130.1, 128.8, 127.6, 125.6, 122.5, 122.3, 115.5.



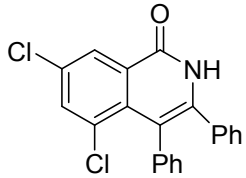
8-iodo-3,4-diphenylisoquinolin-1(2H)-one (3la): white solid, yield: 62% (This compound is known[10]) **^{1}HNMR (400 MHz, DMSO-d$_6$)** δ 11.55 (s, 1H), 8.12 (d, *J*=6.67 Hz, 1H), 7.34-7.28 (m, 3H), 7.26-7.22 (m, 6H), 7.17-7.12 (m, 3H). **^{13}CNMR (100 MHz, DMSO-d$_6$)** δ 160.3, 140.9, 140.8, 139.7, 136.4, 134.6, 133.3, 132.2, 130.1, 128.8, 128.1, 127.6, 126.3, 123.7.



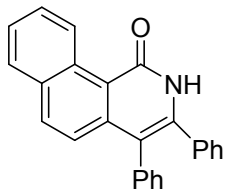
8-chloro-3,4-diphenylisoquinolin-1(2H)-one (3ma): white solid, yield: 81% (This compound is known[7]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.52 (s, 1H), 7.54 (q, *J*=7.29 Hz, 2H), 7.34-7.28 (m, 3H),7.24 (s, 5H), 7.16 (dd, *J*=6.37 Hz, 2H), 7.07 (dd, *J*=5.05 Hz, 1H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 160.4, 141.9, 140.3, 136.4, 134.5, 134.4, 132.8, 132.2, 130.1, 129.5, 128.8, 128.1, 127.6, 124.9, 121.7, 115.4.



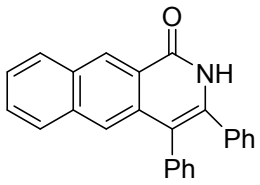
3,4-diphenyl-7-(trifluoromethoxy)isoquinolin-1(2H)-one (3na): white solid, yield: 63%. **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.82 (s, 1H), 8.19 (s, 1H), 7.70 (d, *J*=8.91 Hz, 1H), 7.37-7.33 (m, 3H), 7.32-7.28 (m, 6H), 7.23-7.21 (m, 2H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 161.3, 146.8, 139.9, 137.6, 135.8, 134.7, 132.1, 130.3, 128.8, 128.3, 128.2, 127.7, 126.5, 126.3, 121.9, 119.3, 118.1, 115.4. $[M+H]^{+}$: 382.1049, found: 382.1042. **^{19}FNMR (376 MHz, DMSO-d6)** δ -56.87.



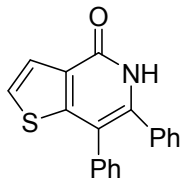
5,7-dichloro-3,4-diphenylisoquinolin-1(2H)-one (3oa): white solid, yield: 50%. **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.96 (s, 1H), 8.34 (d, *J*=2.44 Hz, 1H), 7.86 (d, *J*=2.40 Hz, 1H), 7.23-7.19 (m,5H), 7.16-7.11 (m, 5H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 160.2, 142.3, 137.3, 135.6, 135.0, 133.6, 132.7, 131.6, 131.1, 130.2, 129.2, 128.6, 127.9, 127.6, 127.3, 126.4, 113.8. $[M+H]^{+}$: 366.0447, found: 366.0441.



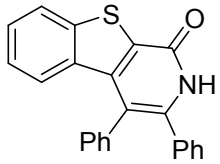
3,4-diphenylbenzo[h]isoquinolin-1(2H)-one (3pa): white solid, yield: 96% (This compound is known [7]) **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.34 (s, 1H), 9.05 (s, 1H), 8.24 (dd, *J*=8.77 Hz, 1H), 7.88 (dd, *J*=8.64 Hz, 1H), 7.66 (s, 1H), 7.59 (m, 2H), 7.39-7.33 (m, 3H), 7.27 (m, 7H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 162.6, 137.9, 136.6, 135.3, 135.2, 135.1, 132.3, 131.2, 130.3, 129.5, 128.8, 128.7, 128.5, 128.2, 128.1, 127.6, 126.6, 124.4, 123.8.115.7.



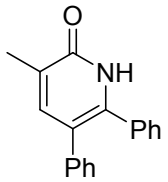
3,4-diphenylbenzo[g]isoquinolin-1(2H)-one (3qa): white solid, yield: 95% (This compound is known[11]) **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.35 (s, 1H), 9.05 (s, 1H), 8.24 (d, *J*=9.12 Hz, 1H), 7.88 (d, *J*=8.92 Hz, 1H), 7.66 (s, 1H), 7.59 (m,2H), 7.39-7.33 (m,3H), 7.31-7.25 (m, 7H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 162.6, 137.9, 136.6, 135.3, 135.2,135.1, 132.3, 131.2, 130.3, 129.6, 128.8, 128.7, 128.5, 128.2, 128.1, 127.6, 126.6, 125.8, 124.4, 123.8, 115.7.



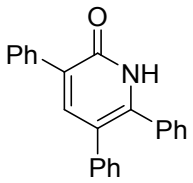
6,7-diphenylthieno[3,2-c]pyridin-4(5H)-one (3ra) : white solid, yield: 91% (This compound is known[6]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.70 (s, 1H), 7.99 (d, *J*=5.25 Hz, 1H), 7.27-7.22 (m, 8H), 7.12 (d, *J*=6.40 Hz, 2H), 6.90 (d, *J*=5.24 Hz, 1H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 158.5, 147.2, 140.3, 136.8, 134.5, 134.4, 131.2, 130.5, 128.8, 128.7, 128.5, 128.2, 127.4, 125.0, 115.2.



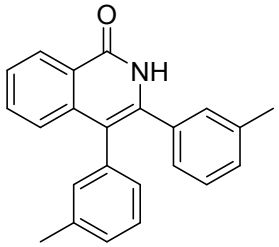
3,4-diphenylbenzo[4,5]thieno[2,3-c]pyridin-1(2H)-one (3sa): white solid, yield: 52%. **^{1}HNMR (400 MHz, DMSO-d6)** δ 12.14 (s, 1H), 8.15 (d, *J*=8.11 Hz, 1H), 7.51 (t, *J*=7.32 Hz, 1H), 7.41 (m, 3H), 7.33 (m, 4H), 7.29 (m, 3H), 7.15 (t, *J*=7.94 Hz, 1H), 6.58 (d, *J*=8.32 Hz, 1H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 158.8, 142.1, 141.6, 141.0, 136.4, 135.9, 134.4, 131.9, 130.4, 128.9, 128.7, 128.3, 128.1, 127.9, 125.5, 124.8, 124.2, 116.1. $[M+H]^+$: 354.0947, found: 354.0941.



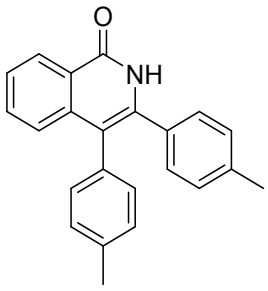
3-methyl-5,6-diphenylpyridin-2(1H)-one (3ta): white solid, yield: 94% (This compound is known[12]) **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.67 (s, 1H), 7.45 (s, 1H), 7.33-7.27 (m, 3H), 7.22-7.18 (m, 5H), 7.05 (d, *J*=6.40 Hz, 2H), 2.10 (s, 3H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 162.9, 142.3, 138.7, 134.5, 130.2, 129.9, 129.0, 128.5, 128.4, 127.4, 126.8, 117.9, 16.5.



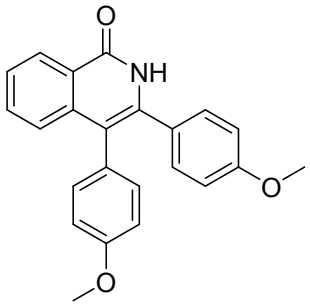
3,5,6-triphenylpyridin-2(1H)-one (3ua): white solid, yield: 65% (This compound is known[13]) **^{1}HNMR (400 MHz, DMSO-d6)** δ 12.00 (s, 1H), 7.86 (d, *J*=7.20 Hz, 2H), 7.72 (s, 1H), 7.44 (t, *J*=7.42 Hz, 2H), 7.39-7.32 (m, 4H), 7.30-7.28 (m, 2H), 7.26-7.21 (m, 3H), 7.16-7.15 (m, 2H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 161.4, 141.5, 138.4, 136.8, 130.2, 130.0, 129.3, 128.8, 128.6, 128.5, 128.4, 127.8, 127.0.



3,4-di-m-tolylisoquinolin-1(2H)-one (3ab): white solid, yield: 58%. (This compound is known[15]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.44 (s, 1H), 8.34 (d, *J*=7.9 Hz, 1H), 7.66 (t, *J*=7.6 Hz, 1H), 7.53 (t, *J*=7.5 Hz, 1H), 7.23-7.07 (m, 6H), 7.03 (s, 2H), 6.96 (d, *J*=3.7 Hz, 1H), 2.27 (s, 3H), 2.23 (s, 3H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 162.1, 138.9, 138.7, 137.6, 137.1, 136.3, 134.9, 132.9, 132.7, 130.9, 129.2, 128.5, 128.1, 127.9, 127.4, 127.2, 126.6, 125.5, 125.4, 115.9, 21.4, 21.3.

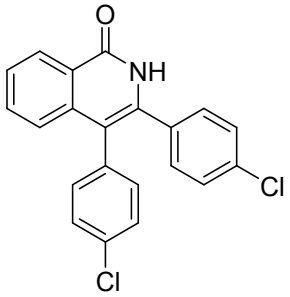


3,4-di-p-tolylisoquinolin-1(2H)-one (3ac): white solid, yield: 61%. (This compound is known[14]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.43 (s, 1H), 8.34 (d, *J*=7.9 Hz, 1H), 7.65 (t, *J*=7.6 Hz, 1H), 7.53 (t, *J*=7.5 Hz, 1H), 7.18-7.15 (m, 5H), 7.07-7.06 (m, 4H), 2.33 (s, 3H), 2.28 (s, 3H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 162.2, 138.9, 138.8, 137.9, 136.5, 133.4, 132.8, 132.3, 132.0, 130.1, 129.4, 128.8, 127.2, 126.5, 125.4, 115.6, 21.23, 21.22.

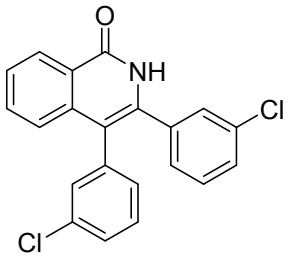


3,4-bis(4-methoxyphenyl)isoquinolin-1(2H)-one (3ad): white solid, yield: 42%. (This compound

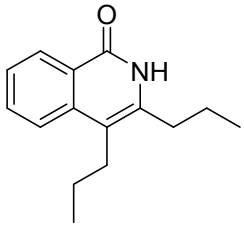
is known[16]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.40 (s, 1H), 8.33 (d, *J*=7.9 Hz, 1H), 7.65 (t, *J*=7.6 Hz, 1H), 7.52 (t, *J*=7.5 Hz, 1H), 7.19 (d, *J*=8.3 Hz, 3H), 7.09 (d, *J*=8.4 Hz, 2H), 6.91 (d, *J*=8.4 Hz, 2H), 6.82 (d, *J*=8.5 Hz, 2H), 3.78 (s, 3H), 3.75 (s, 3H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 162.2, 159.3, 158.5, 139.1, 138.8, 133.2, 132.8, 131.6, 128.5, 127.5, 127.2, 126.4, 125.4, 125.3, 115.2, 114.2, 113.6, 55.5, 55.4.



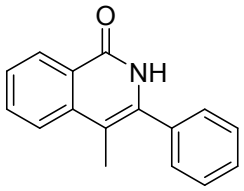
3,4-bis(4-chlorophenyl)isoquinolin-1(2H)-one (3ae): white solid, yield: 85% (This compound is known[14]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.63 (s, 1H), 8.35 (d, *J*=7.84 Hz, 1H), 7.69 (t, *J*=8.13 Hz, 1H), 7.57 (t, *J*=7.85 Hz, 1H), 7.41 (d, *J*=8.36 Hz, 2H), 7.36 (d, *J*=8.51 Hz, 2H), 7.29 (d, *J*=8.50 Hz, 2H), 7.22 (d, *J*=8.31 Hz, 2H), 7.16 (d, *J*=8.09 Hz, 1H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 162.1, 138.2, 135.0, 134.0, 133.7, 133.6, 133.1, 132.5, 132.2, 128.9, 128.3, 127.4, 127.0, 125.6, 125.2, 114.9.



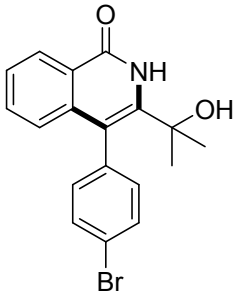
3,4-bis(3-chlorophenyl)isoquinolin-1(2H)-one (3af): white solid, yield: 96%. **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.66 (s, 1H), 8.35 (d, *J*=7.08 Hz, 1H), 7.71 (t, *J*=7.00 Hz, 1H), 7.58 (t, *J*=7.21 Hz, 1H), 7.40-7.36 (m, 4H), 7.31 (t, *J*=7.62 Hz, 2H), 7.23-7.20 (m, 2H), 7.16 (d, *J*=8.08 Hz, 1H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 162.0, 138.3, 138.0, 136.7, 133.3, 133.2, 132.8, 131.8, 131.0, 130.6, 130.2, 130.0, 129.1, 128.8, 127.8, 127.4, 127.1, 125.6, 125.2, 115.0. $[M+H]^{+}$: 366.0447, found: 366.0447.



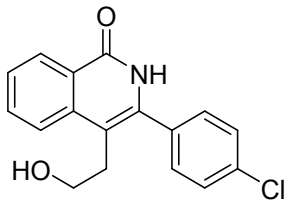
3,4-dipropylisoquinolin-1(2H)-one (3ag): white solid, yield: 55%. (This compound is known[16]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.06 (s, 1H), 8.22 (d, *J*=7.8 Hz, 1H), 7.73-7.72 (m, 2H), 7.458-7.43 (m, 1H), 2.66 (t, *J*=7.9 Hz, 2H), 2.56 (t, *J*=7.9 Hz, 2H),1.66-1.58 (m, 2H), 1.56-1.48 (m. 2H), 1.02 (t, *J*=7.3 Hz, 3H), 0.97 (t, *J*=7.3 Hz, 3H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 162.2, 139.2, 138.3, 132.7, 127.4, 125.5, 123.5, 111.3, 32.2, 28.2, 23.7, 22.9, 14.5, 14.1.



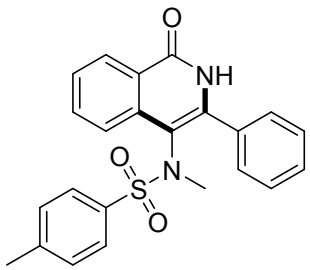
4-methyl-3-phenylisoquinolin-1(2H)-one (3ah): white solid, yield: 70%. (This compound is known[14]). **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.23 (s, 1H), 8.31 (d, *J*=7.8 Hz, 1H), 7.82-7.80 (m, 2H), 7.58-7.47 (m, 6H), 2.15 (s, 3H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 161.9, 138.7, 138.3, 135.3, 133.0, 130.1, 129.1, 128.7, 127.4, 126.5, 125.9, 124.2, 107.6, 14.0.



3-(4-bromophenyl)-4-(2-hydroxypropan-2-yl)isoquinolin-1(2H)-one (3ai): white solid, yield: 43%. **^{1}HNMR (400 MHz, DMSO-d6)** δ 9.96 (s, 1H), 8.26 (d, *J*=7.89 Hz, 1H), 7.71 (d, *J*=8.33 Hz, 2H), 7.60 (t, *J*=8.37 Hz, 1H), 7.49 (t, *J*=7.96 Hz, 1H), 7.27 (d, *J*=8.33 Hz, 2 H), 6.75 (d, *J*=8.08 Hz, 1H), 5.98 (s, 1H), 1.24 (s, 6H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 161.0, 144.2, 139.9, 136.4, 134.6, 133.0, 131.9, 126.9, 126.5, 125.5, 124.8, 121.7, 111.6, 70.76, 30.97. $[M+H]^+$: 358.0437, found: 358.0430.

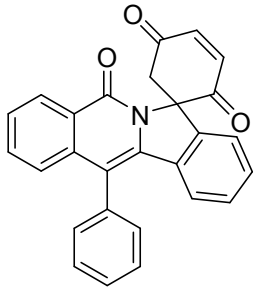


3-(4-chlorophenyl)-4-(2-hydroxyethyl)isoquinolin-1(2H)-one (3aj): white solid, yield: 67%. **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.28 (s, 1H), 8.30 (d, *J*=7.68 Hz, 1H), 7.87 (d, *J*=8.12 Hz, 1H), 7.81 (t, *J*=7.32 Hz, 1H), 7.55 (m, 5H), 4.66 (t, *J*=5.38 Hz, 1H), 3.52 (q, *J*=6.75 Hz, 2H), 2.71 (t, *J*=7.44 Hz, 2H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 161.7, 138.6, 137.9, 134.2, 134.0, 132.9, 131.9, 128.7, 127.5, 126.6, 126.3, 124.2, 109.5, 61.1, 30.9. $[M+H]^+$: 300.0786, found: 300.0780.

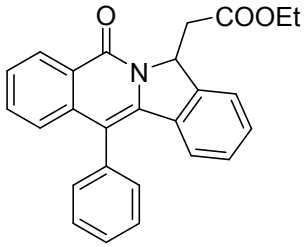


N,4-dimethyl-N-(1-oxo-4-phenyl-1,2-dihydroisoquinolin-3-yl)benzenesulfonamide (3ak): white solid, yield: 99%. **^{1}HNMR (400 MHz, DMSO-d6)** δ 11.60 (s, 1H), 8.29 (d, *J*=7.32 Hz,

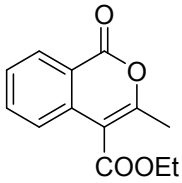
1H), 7.74 (t, *J*=6.99 Hz, 1H), 7.59-7.38 (m, 7H), 7.17 (d, *J*=8.17 Hz, 2H), 7.11 (d, *J*=8.23 Hz, 2H), 3.17 (s, 3H), 2.38 (s, 3H). **^{13}CNMR (100 MHz, DMSO-d6)** δ 161.6, 143.6, 143.5, 137.3, 136.5, 133.6, 133.2, 129.8, 129.2, 128.6, 127.7, 127.5, 127.1, 125.9, 123.6, 116.0, 21.4. $[M+H]^+$: 405.1267, found: 405.1263.



5-phenylspiro[benzo[b]fluorene-11,1'-cyclohexan]-3'-ene-2',5',10(10aH)-trione (6): yellow solid, yield: 72% (This compound is known[4]) **^{1}HNMR (400 MHz, $CDCl_3$)** δ 8.51 (d, *J*=7.93 Hz, 1H), 7.67-7.62 (m, 4H), 7.56 (t, *J*=7.93 Hz, 1H),7,51-7.47 (m, 2H), 7.34-7.28 (m, 3H),7.21-7.15(m, 3H), 6.47 (d, *J*=7.96 Hz, 1H), 4.95 (d, *J*=16.08 Hz, 1H), 3.02 (d, *J*=16.09 Hz, 1H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 195.1, 189.1, 160.3, 142.8, 141.4, 140.1, 138.9, 137.0, 134.6, 133.3, 132.7, 131.0, 130.9, 129.8, 129.7, 129.6, 129.5, 128.7, 127.6, 126.9, 125.6, 125.2, 125.0, 121.0, 115.3, 74.5, 46.0.

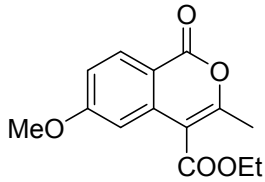


Ethyl 2-(5-oxo-12-phenyl-5,7-dihydroisoindolo[2,1-b]isoquinolin-7-yl)acetate (7): white solid, yield: 83% (This compound is known[5]) **^{1}HNMR (400 MHz, $CDCl_3$)** δ 8.58 (d, *J*=7.79 Hz, 1H), 7.65-7.48 (m,7H), 7.40-7.34 (m, 2H), 7.24 (d, *J*=8.12 Hz, 1H), 7.13 (t, *J*=7.64 Hz, 1H), 6.43 (d, *J*=7.96 Hz, 1H), 6.05 (dd, *J*=7.65,3.54Hz, 1H), 4.15 (q, *J*=7.14 Hz, 2H), 3.76 (dd, *J*=12.41, 3.65Hz, 1H), 3.10 (q, *J*=8.29 Hz, 1H), 1.19 (t, *J*=7.13 Hz, 3H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 170.3, 160.9, 141.7, 138.7, 138.0, 135.3, 133.6, 132.1, 131.1, 131.0, 129.5, 128.5, 128.4, 127.4, 126.3, 125.2, 124.9, 124.0, 122.9, 114.5.

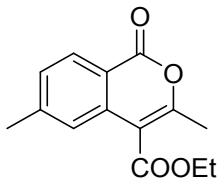


Ethyl 3-methyl-1-oxo-1H-isochromene-4-carboxylate (5aa): yellow solid, yield 75% (This compound is known[17]). **^{1}HNMR (400 MHz, $CDCl_3$)** δ 8.30 (d, *J*=7.44Hz, 1H), 7.80-7.73 (m, 2H), 7.53 (t, *J*=8.09 Hz, 1H), 4.48 (q, *J*=7.12 Hz, 2H), 2.48 (s, 3H), 1.46 (t, *J*=7.12 Hz, 3H). **^{13}CNMR**

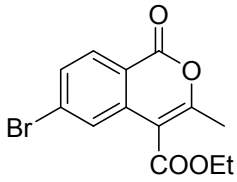
(100 MHz, $CDCl_3$) δ 165.7, 161.1, 157.7, 135.0, 134.6, 129.6, 128.1, 124.1, 119.5, 110.2, 61.6, 19.2, 14.2.



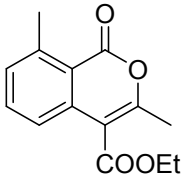
Ethyl 6-methoxy-3-methyl-1-oxo-1H-isochromene-4-carboxylate (5ba): white solid, yield: 31% (This compound is known[17]). **^{1}HNMR (400 MHz, $CDCl_3$)** δ 8.25 (d, *J*=8.84 Hz, 1H), 7.29 (d, *J*=2.40 Hz, 1H), 7.08 (dd, *J*=8.85 Hz, 2.40 Hz, 1H), 4.49 (q, *J*=7.16 Hz, 2H), 3.95 (s, 3H), 2.50 (s, 3H), 1.48 (t, *J*=7.14 Hz, 3H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 165.9, 165.0, 160.9, 158.8, 136.9, 131.9, 116.2, 112.6, 109.9, 107.0, 61.5, 55.6, 19.5, 14.2.



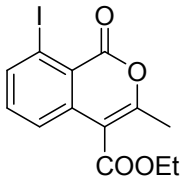
Ethyl 3,6-dimethyl-1-oxo-1H-isochromene-4-carboxylate (5ca): white solid, yield: 55% (This compound is known[17]) **^{1}HNMR (400 MHz, $CDCl_3$)** δ 8.21 (d, *J*=8.12 Hz, 1H), 7.58 (s, 1H), 7.36 (d, *J*=8.11 Hz, 1H), 4.50 (q, *J*=7.13 Hz, 2H), 2.52 (s, 3H), 2.48 (s, 1H), 1.48 (t, *J*=7.12 Hz, 3H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 165.9, 161.2, 157.5, 146.2, 134.7, 129.7, 129.5, 124.0, 117.1, 110.2, 61.6, 22.3, 19.2, 14.2.



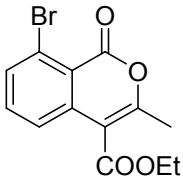
Ethyl 6-bromo-3-methyl-1-oxo-1H-isochromene-4-carboxylate (5da): white solid, yield: 76% (This compound is known[17]) **^{1}HNMR (400 MHz, $CDCl_3$)** δ 8.17 (d, *J*=8.45 Hz, 1H), 8.06 (s, 1H), 7.67 (dd, *J*=8.49 Hz, 1.76 Hz, 1H), 4.50 (q, *J*=7.12 Hz, 2H), 2.53 (s, 3H), 1.48 (t, *J*=7.13 Hz, 3H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 165.2, 160.5, 159.6, 136.1, 131.5, 131.2, 130.9, 127.2, 118.2, 109.1, 61.8, 19.6, 14.2.



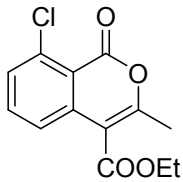
Ethyl 3,8-dimethyl-1-oxo-1H-isochromene-4-carboxylate (5ea): white solid, yield: 72%. **^{1}HNMR (400 MHz, $CDCl_3$)** δ 7.61-7.33(m, 3H), 4.47 (q, *J*=7.17 Hz, 2H), 2.84 (s, 3H), 2.43 (s, 3H), 1.45 (t, *J*=7.16 Hz, 3H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 166.3, 160.4, 156.4, 143.6, 136.1, 134.2, 131.1, 121.8, 118.0, 110.7, 61.6, 23.4, 18.8, 14.2. $[M+H]^+$: 247.0965, found: 247.0961.



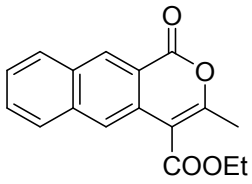
Ethyl 8-iodo-3-methyl-1-oxo-1H-isochromene-4-carboxylate (5fa): white solid, yield: 55%. **^{1}HNMR (400 MHz, $CDCl_3$)** δ 8.23 (d, *J*=7.76 Hz, 1H), 7.75 (d, *J*=8.24 Hz, 1H), 7.35 (s, 1H), 4.49 (q, *J*=7.12 Hz, 2H), 2.47 (s, 3H), 1.48 (t, *J*=7.10 Hz, 3H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 165.7, 158.1, 157.3, 142.5, 136.8, 134.7, 124.3, 119.8, 110.5, 96.2, 61.8, 29.6, 19.0, 14.2. $[M+H]^+$: 358.9775, found: 358.9771.



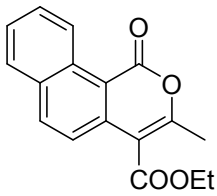
Ethyl 8-bromo-3-methyl-1-oxo-1H-isochromene-4-carboxylate (5ga): white solid, yield: 53%. **^{1}HNMR (400 MHz, $CDCl_3$)** δ 7.83 (d, *J*=7.82 Hz, 1H), 7.71 (d, *J*=8.14 Hz, 1H), 7.53 (t, *J*=7.97 Hz, 1H), 4.49 (q, *J*=7.15 Hz, 2H), 2.47 (s, 3H), 1.47 (t, *J*=7.14 Hz, 3H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 165.7, 157.7, 137.6, 134.9, 124.9, 123.5, 117.9, 110.2, 61.8, 19.1, 14.1. $[M+H]^+$: 310.9913, found: 310.9907.



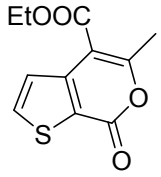
Ethyl 8-chloro-3-methyl-1-oxo-1H-isochromene-4-carboxylate (5ha): white solid, yield: 60% (This compound is known[17]). **^{1}HNMR (400 MHz, $CDCl_3$)** δ 7.68-7.56 (m, 3H), 4.49 (q, *J*=7.17 Hz, 2H), 2.46 (s, 3H), 1.47 (t, *J*=7.17 Hz, 3H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 165.7, 157.9, 157.5, 137.6, 137.2, 134.6, 131.1, 122.7, 116.7, 110.2, 61.8, 19.1, 14.1.



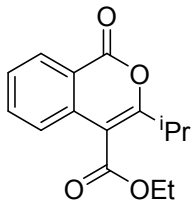
Ethyl 3-methyl-1-oxo-1H-benzo[g]isochromene-4-carboxylate (5ia): white solid, yield: 65% (This compound is known[17]). **^{1}HNMR (400 MHz, $CDCl_3$)** δ 8.92 (S, 1H), 8.21 (s, 1H), 8.02 (d, *J*=8.24 Hz, 1H), 7.94 (d, *J*=8.32 Hz, 1H), 7.67 (t, *J*=7.36 Hz, 1H), 7.58 (t, *J*=7.34 Hz, 1H), 4.55 (q, *J*=7.14 Hz, 2H), 2.50 (s, 3H), 1.51 (t, *J*=7.15 Hz, 3H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 166.1, 161.3, 156.0, 136.5, 132.0, 131.9, 129.5, 129.3, 129.1, 128.3, 127.0, 123.0, 117.8, 110.1, 61.6, 19.2, 14.3.



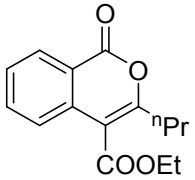
Ethyl 3-methyl-1-oxo-1H-benzo[h]isochromene-4-carboxylate (5ja): white solid, yield: 83%. **^{1}HNMR (400 MHz, $CDCl_3$)** δ 8.96 (s, 1H), 8.24 (s, 1H), 8.05 (d, *J*=8.24 Hz, 1H), 7.96 (d, *J*=8.34 Hz, 1H), 7.69 (t, *J*=7.70 Hz, 1H), 7.60 (t, *J*=7.48 Hz, 1H), 4.56 (q, *J*=7.16 Hz, 2H), 2.52 (s, 3H), 1.52 (t, *J*=7.16 Hz, 3H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 166.1, 161.4, 156.0, 136.5, 132.1, 131.9, 129.5, 129.4, 129.1, 128.3, 127.0, 123.0, 117.8, 110.2, 61.6, 19.3, 14.3. $[M+H]^+$: 283.0965, found: 283.0961.



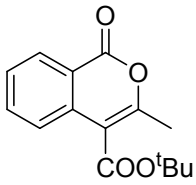
Ethyl 5-methyl-7-oxo-7H-thieno[2,3-c]pyran-4-carboxylate (5ka): white solid, yield: 73% (This compound is known[17]). **^{1}HNMR (400 MHz, $CDCl_3$)** δ 7.86 (d, *J*=5.24 Hz, 1H), 7.75 (d, *J*=5.24 Hz, 1H), 4.45 (q, *J*=7.15 Hz, 2H), 2.68 (s, 3H), 1.46 (t, *J*=7.15 Hz, 3H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 164.8, 164.4, 156.9, 145.2, 136.5, 126.2, 122.3, 108.1, 61.5, 20.0, 14.2.



Ethyl 3-isopropyl-1-oxo-1H-isochromene-4-carboxylate (5ab): white solid, yield: 65% (This compound is known[17]). **^{1}HNMR (400 MHz, $CDCl_3$)** δ 8.34 (d, *J*=7.97 Hz, 1H), 7.77 (t, *J*=8.33 Hz, 1H), 7.64 (d, *J*=8.04 Hz, 1H), 7.55 (t, *J*=8.02 Hz, 1H), 4.49 (q, *J*=7.16 Hz,2H), 3.19 (m, 1H), 1.47 (t, *J*=7.16 Hz, 3H), 1.37 (d, *J*=6.81 Hz, 6H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 166.0, 163.1, 161.4, 134.9, 134.7, 129.7, 128.1, 123.9, 119.7, 109.1, 61.7, 31.5, 20.0, 14.2.



Ethyl 3-butyl-1-oxo-1H-isochromene-4-carboxylate (5ac): white solid, yield: 55% (This compound is known[17]). **^{1}HNMR (400 MHz, $CDCl_3$)** δ 8.33 (d, *J*=7.96 Hz, 1H), 7.75 (m, 2H), 7.55 (t, *J*=7.95 Hz, 1H), 4.49 (q, *J*=7.12 Hz, 2H), 2.72 (t, *J*=7.44 Hz, 2H), 1.84 (m, 2H), 1.47 (t, *J*=7.12 Hz, 3H), 1.05 (t, *J*=7.42 Hz, 3H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 165.9, 161.4, 160.3, 135.0, 134.7, 129.6, 128.1, 124.1, 119.6, 110.4, 61.7, 34.5, 21.1, 14.2, 13.6.



tert-Butyl 3-methyl-1-oxo-1H-isochromene-4-carboxylate (5ad): white solid, yield: 74% (This compound is known[17]). **^{1}HNMR (400 MHz, $CDCl_3$)** δ 8.33 (d, *J*=7.87 Hz, 1H), 7.78 (m, 2H), 7.56 (m, 1H), 2.49 (s, 3H), 1.70 (s, 9H). **^{13}CNMR (100 MHz, $CDCl_3$)** δ 165.0, 161.3, 156.2, 135.0, 129.6, 128.0, 123.8, 119.6, 116.7, 83.0, 28.2, 18.9.

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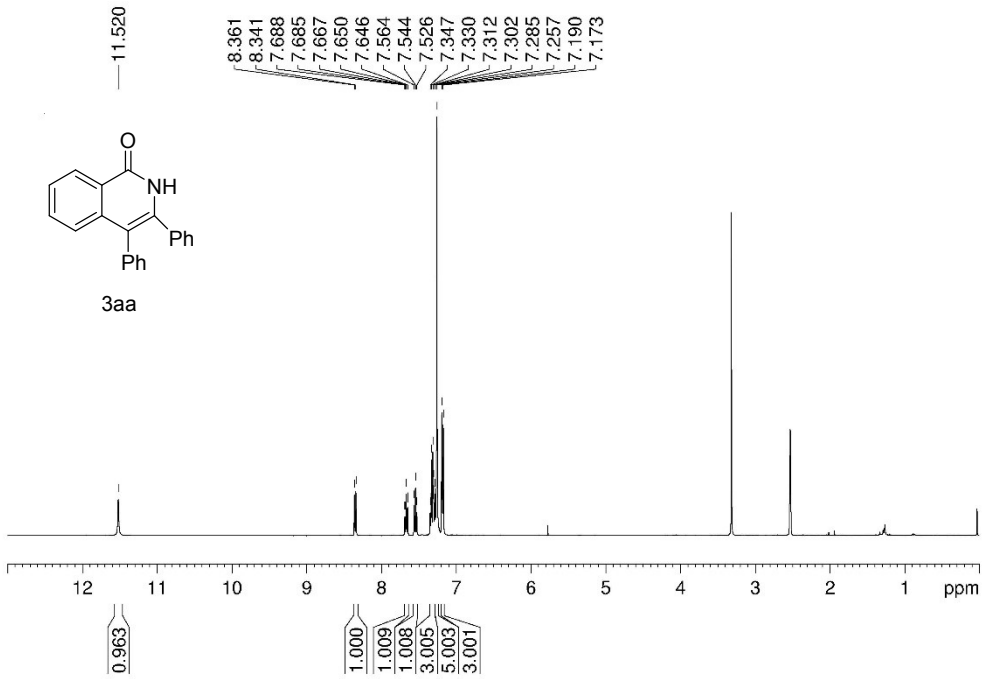
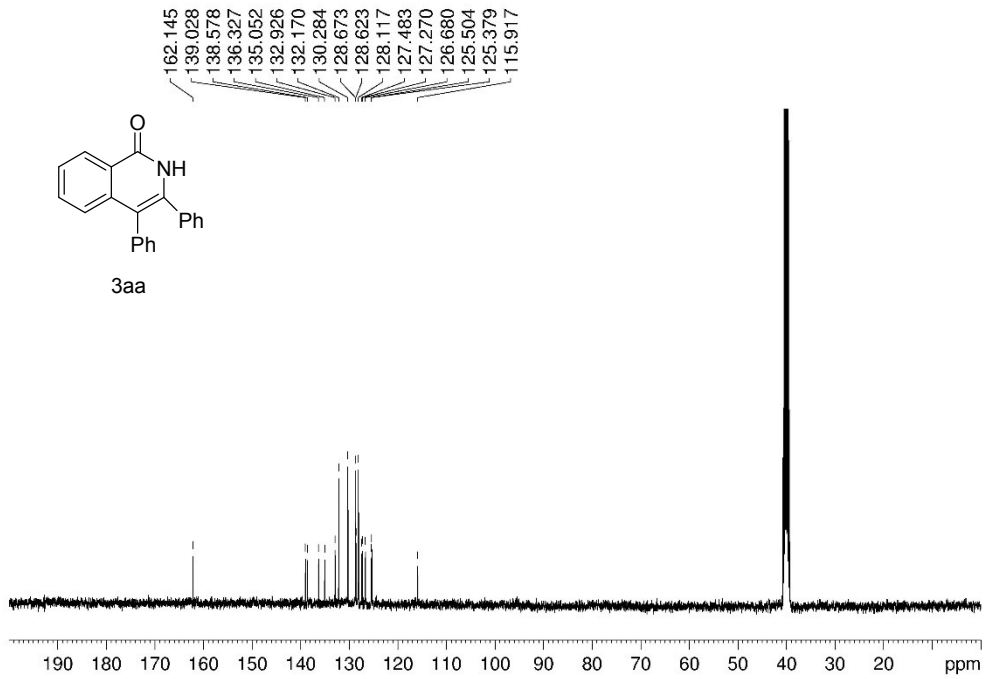
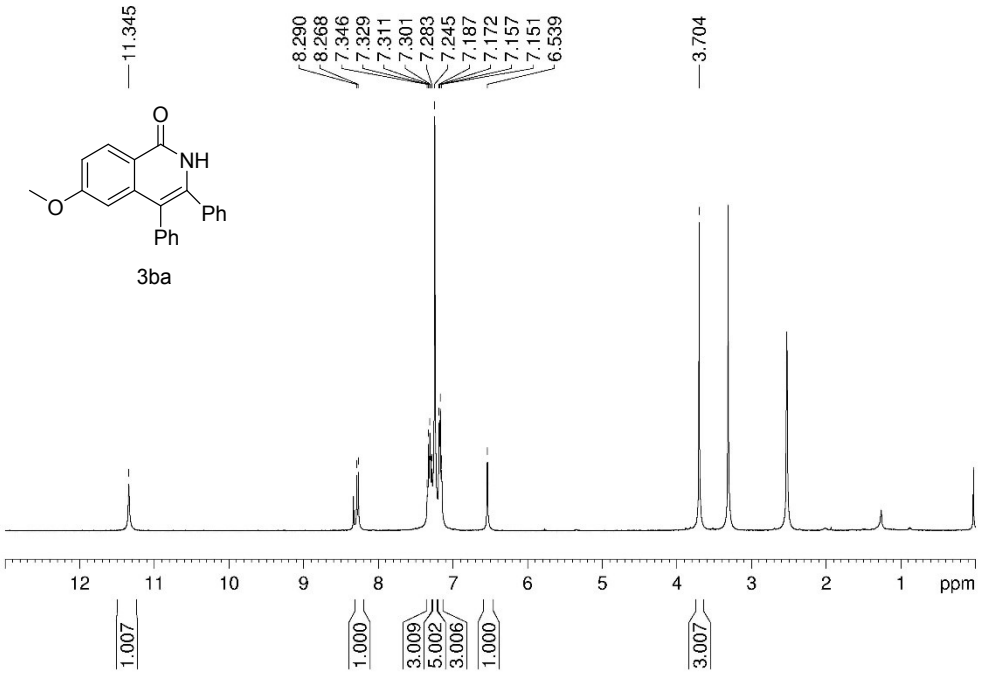
Copies of ^{1}H NMR and ^{13}C NMR Spectra of All Products



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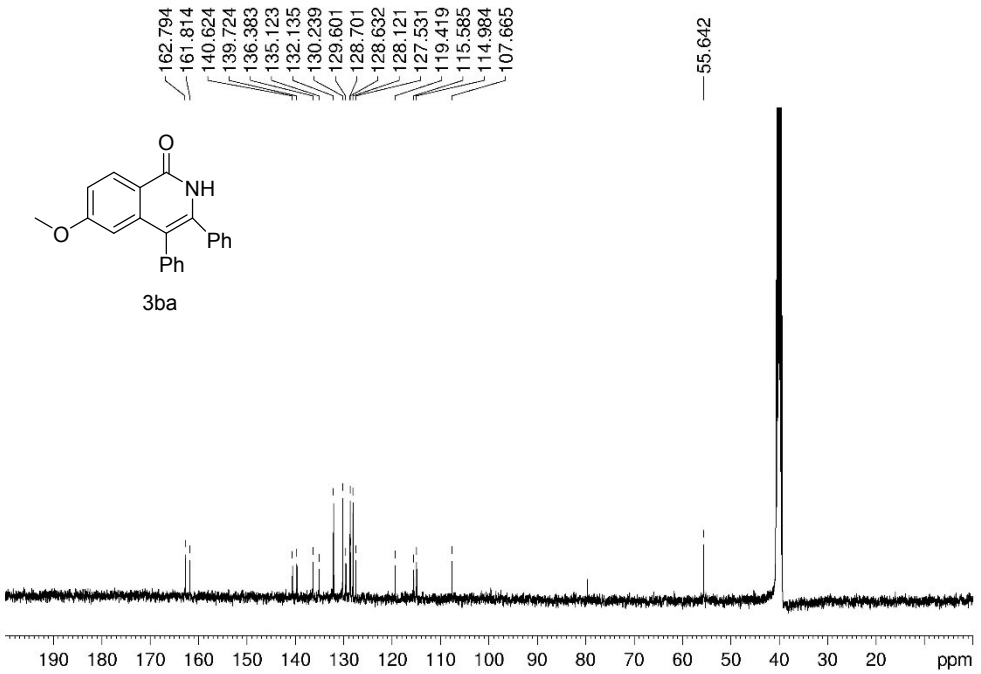
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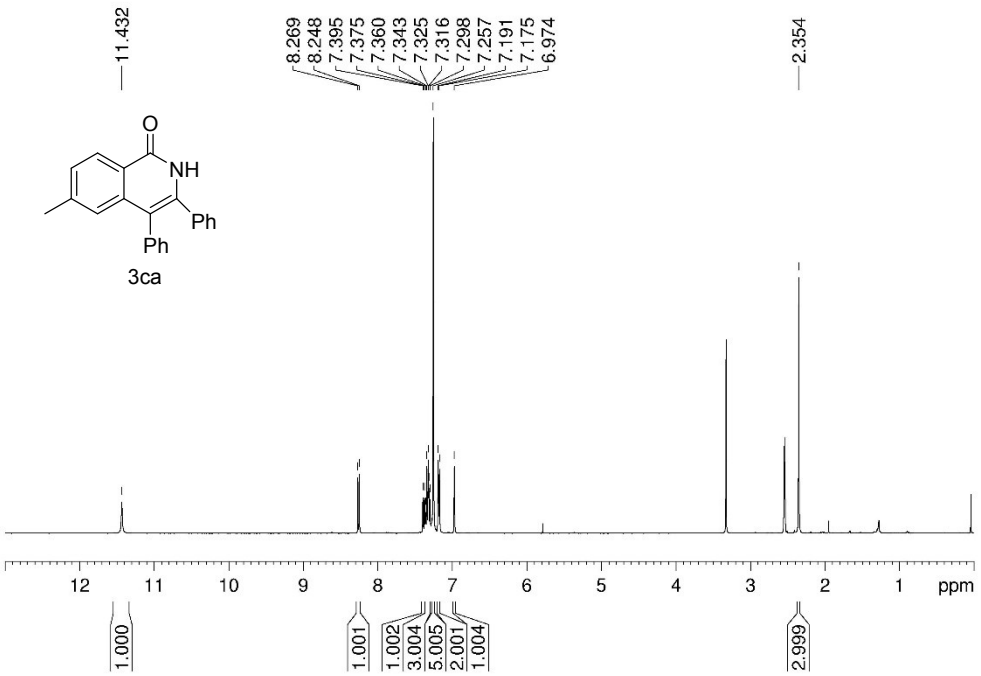
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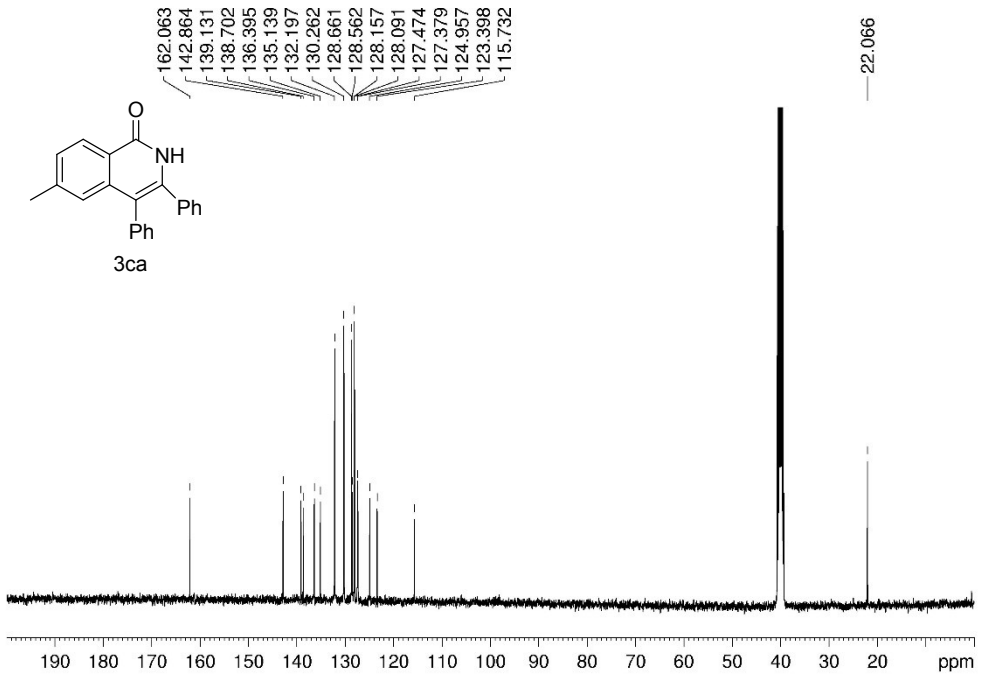
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136.395
135.139
132.197
130.262
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128.562
128.157
128.091
127.474
127.379
124.957
123.398
115.732
22.066
O
NH
Ph
Ph
3ca
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180
170
160
150
140
130
120
110
100
90
80
70
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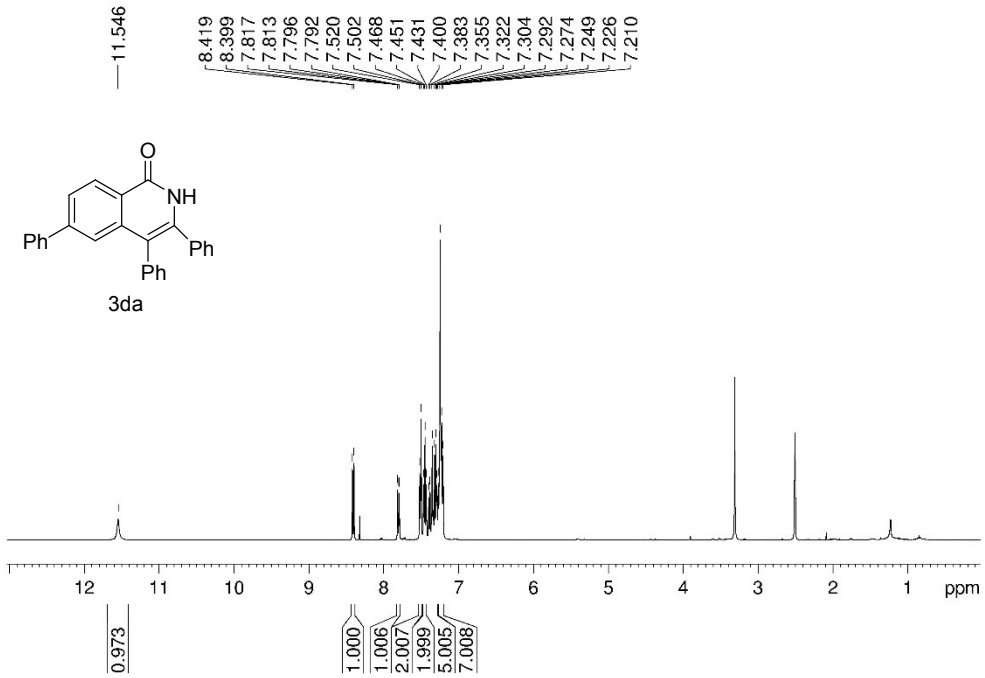
50
40
30
20
ppm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8.399
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7.792
7.520
7.502
7.468
7.451
7.431
7.400
7.383
7.355
7.322
7.304
7.292
7.274
7.249
7.226
7.210
O
NH
Ph
Ph
Ph
3da
12
11
10
9
8
7
6
5
4
3
2
1
ppm
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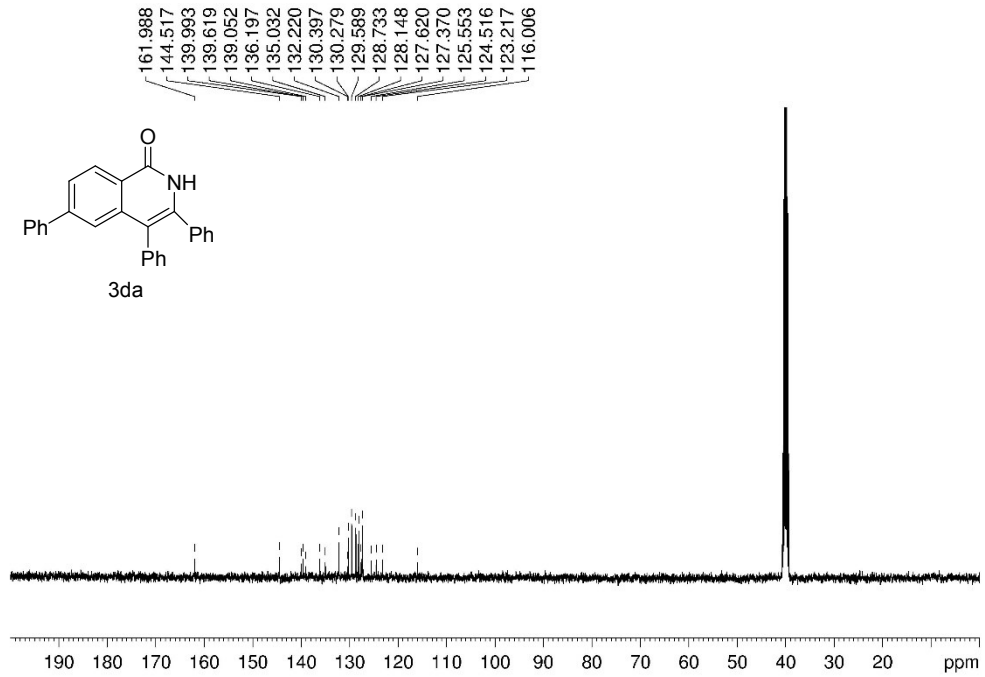
1.006
2.007
1.999
5.005
7.008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132.220
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130.279
129.589
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128.148
127.620
127.370
125.553
124.516
123.217
116.006
O
NH
Ph
Ph
Ph
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160
150
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130
120
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100
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80
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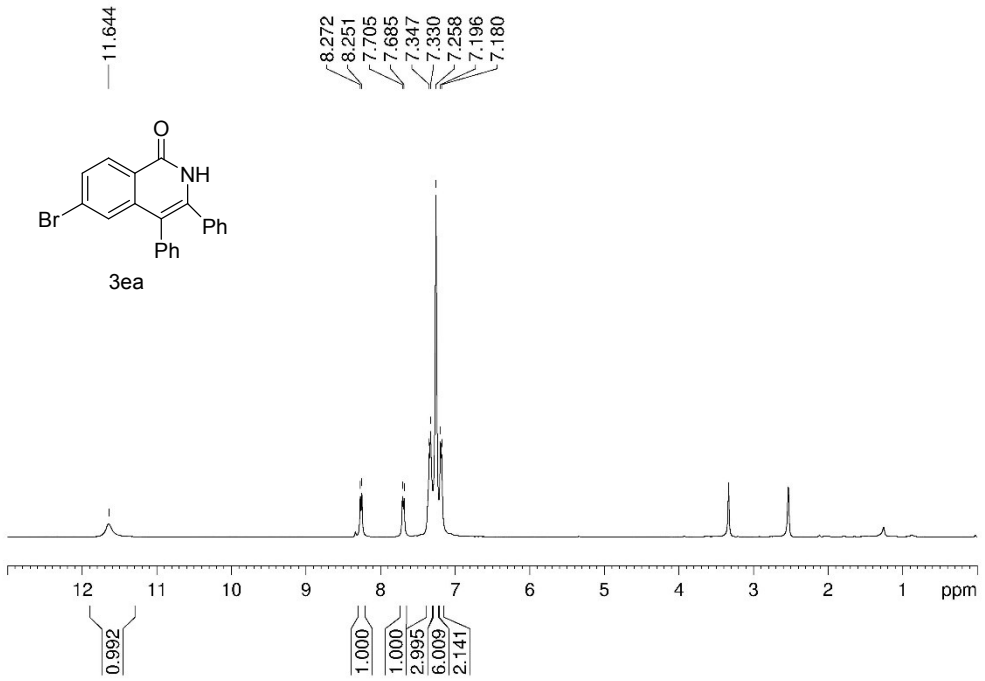
40
30
20
ppm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8.251
7.705
7.685
7.347
7.330
7.258
7.196
7.180
O
NH
Br
Ph
Ph
3ea
12
11
10
9
8
7
6
5
4
3
2
1
ppm
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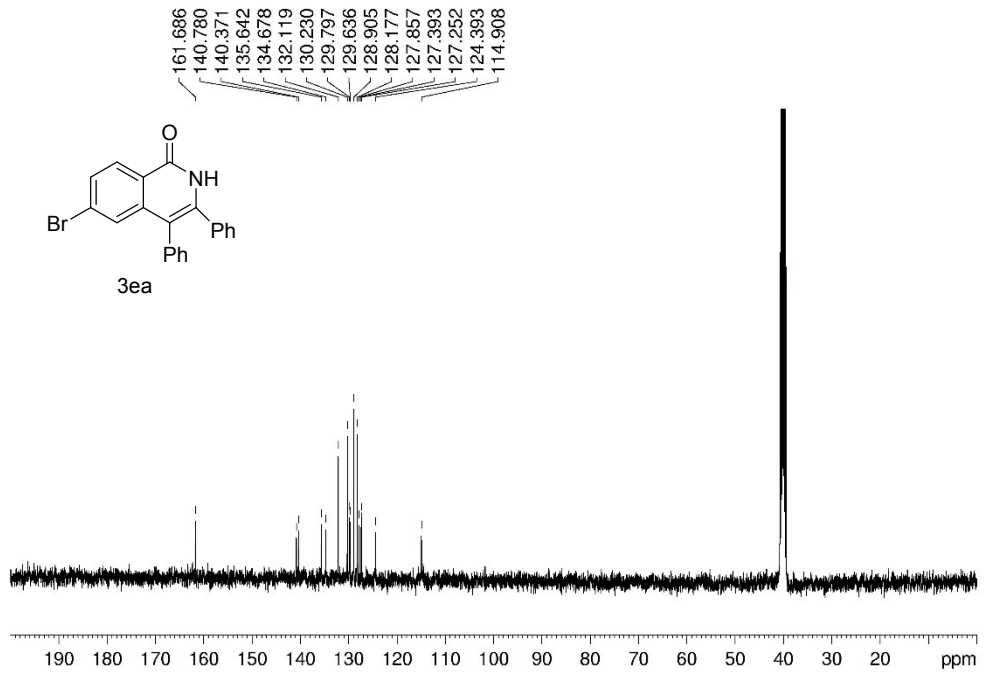
1.000
1.000
2.995
6.009
2.141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129.797
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128.177
127.857
127.393
127.252
124.393
114.908
O
NH
Br
Ph
Ph
3ea
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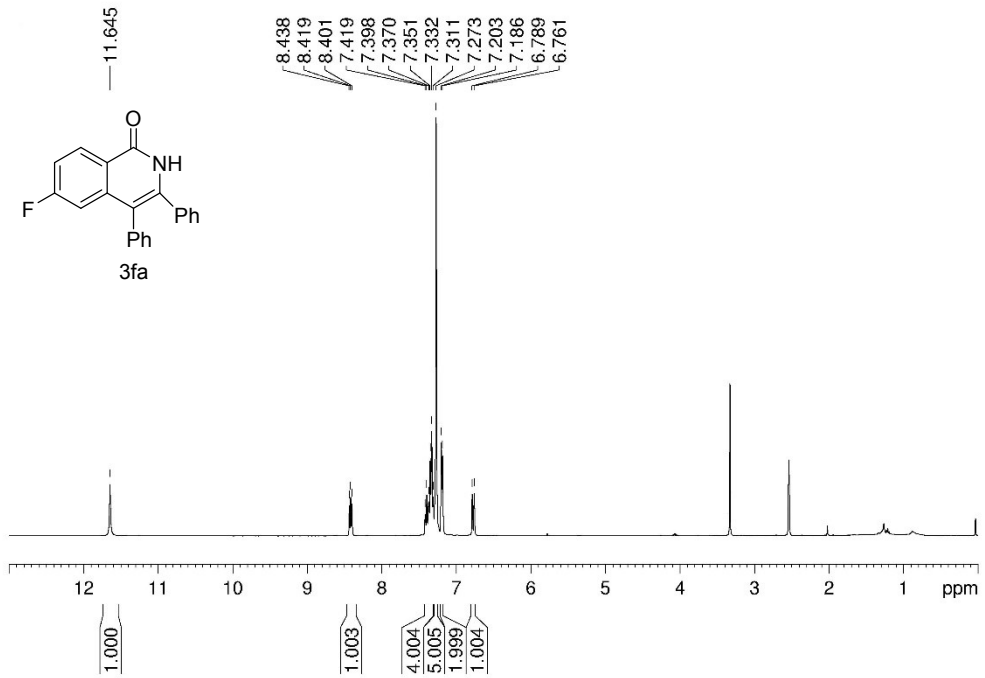
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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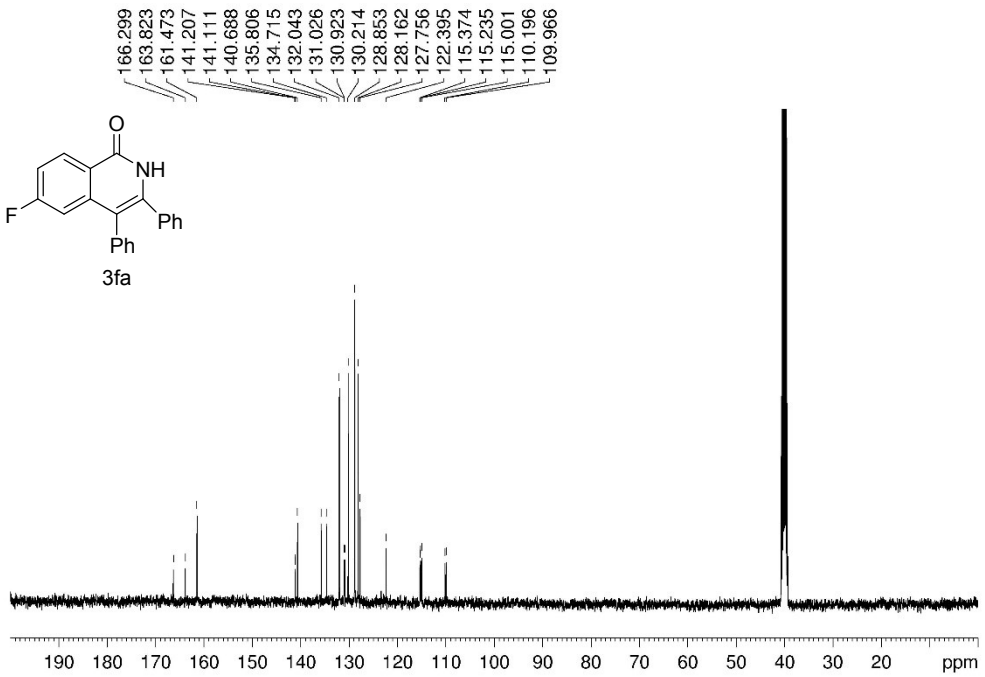
8.438
8.419
8.401
7.419
7.398
7.370
7.351
7.332
7.311
7.273
7.203
7.186
6.789
6.761
O
NH
F
Ph
Ph
3fa
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.003
4.004
5.005
1.999
1.004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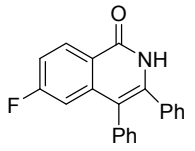
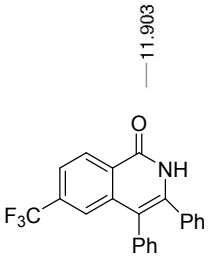
161.473
141.207
141.111
140.688
135.806
134.715
132.043
131.026
130.923
130.214
128.853
128.162
127.756
122.395
115.374
115.235
115.001
110.196
109.966
O
NH
F
Ph
Ph
3fa
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


O
NH
F
Ph
Ph

3fa

-106.298
0
-20
-40
-60
-80
-100
-120
-140
ppm


O
NH
F3C
Ph
Ph

3ga

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8.571
8.550
7.865
7.844
7.431
7.395
7.377
7.360
7.337
7.292
7.241
7.223
13
12
11
10
9
8
7
6
5
4
3
2
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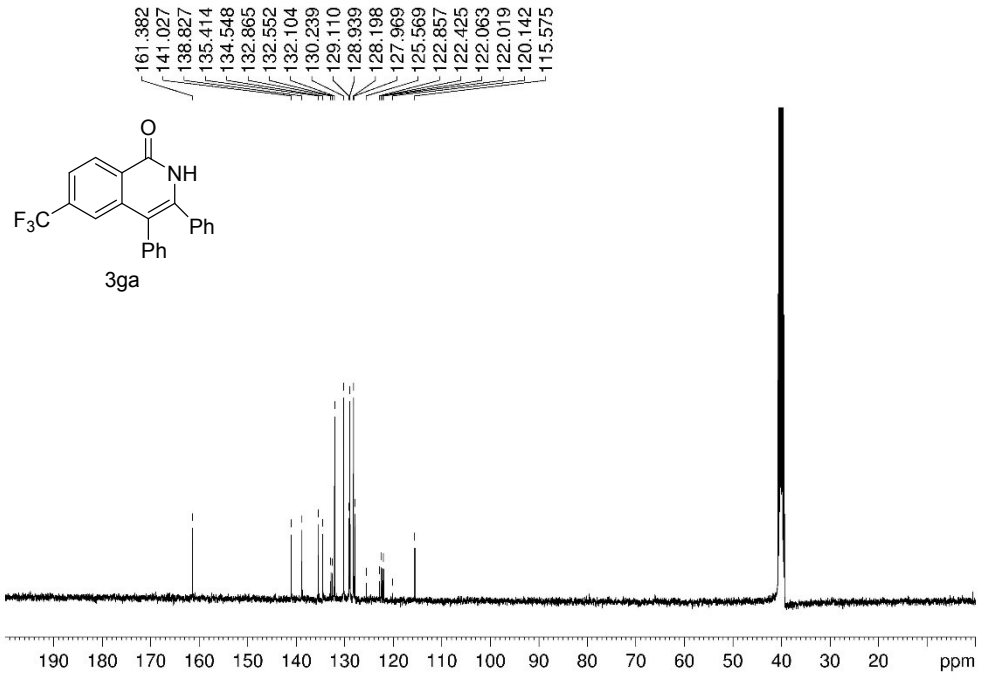
1.000
1.005
1.004
3.007
5.008
2.005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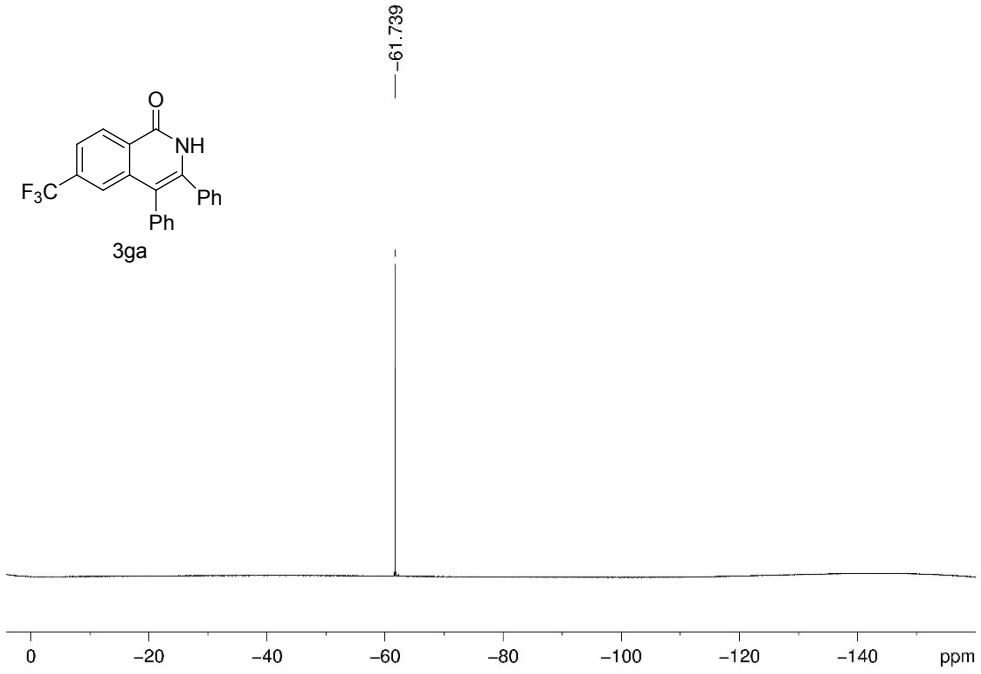
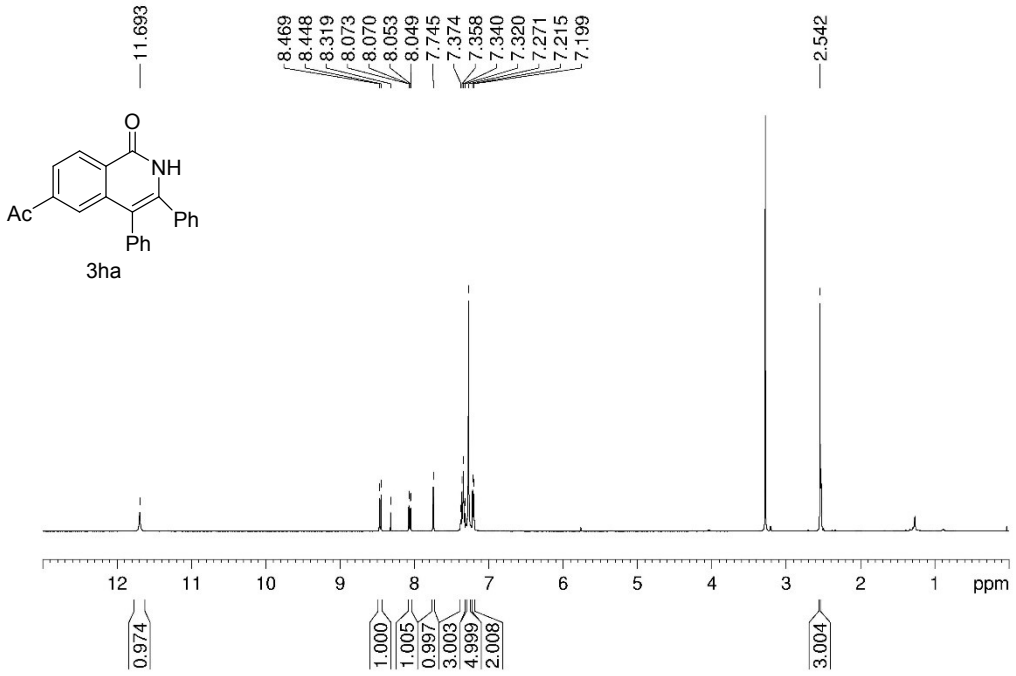
141.027
138.827
135.414
134.548
132.865
132.552
132.104
130.239
129.110
128.939
128.198
127.969
125.569
122.857
122.425
122.063
122.019
120.142
115.575
O
NH
F3C
Ph
Ph
3ga
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


-61.739
O
NH
F3C
Ph
Ph
3ga
0 −20 −40 −60 −80 −100 −120 −140 ppm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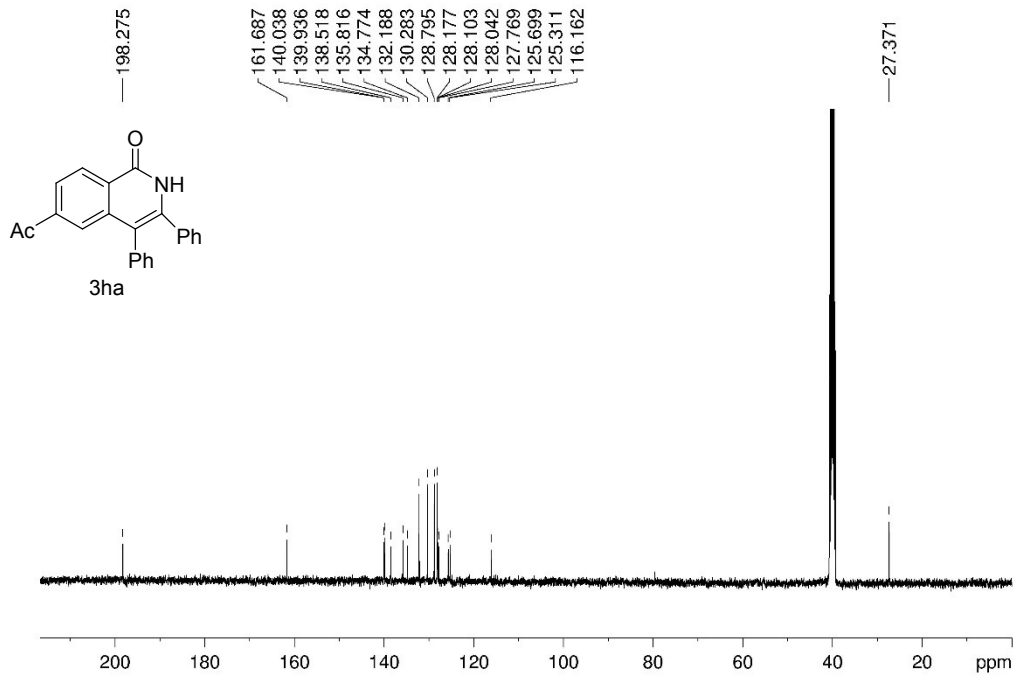
8.469
8.448
8.319
8.073
8.070
8.053
8.049
7.745
7.374
7.358
7.340
7.320
7.271
7.215
7.199
2.542
O
NH
Ac
Ph
Ph
3ha
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.974
1.000
1.005
0.997
3.003
4.999
2.008
3.004


198.275
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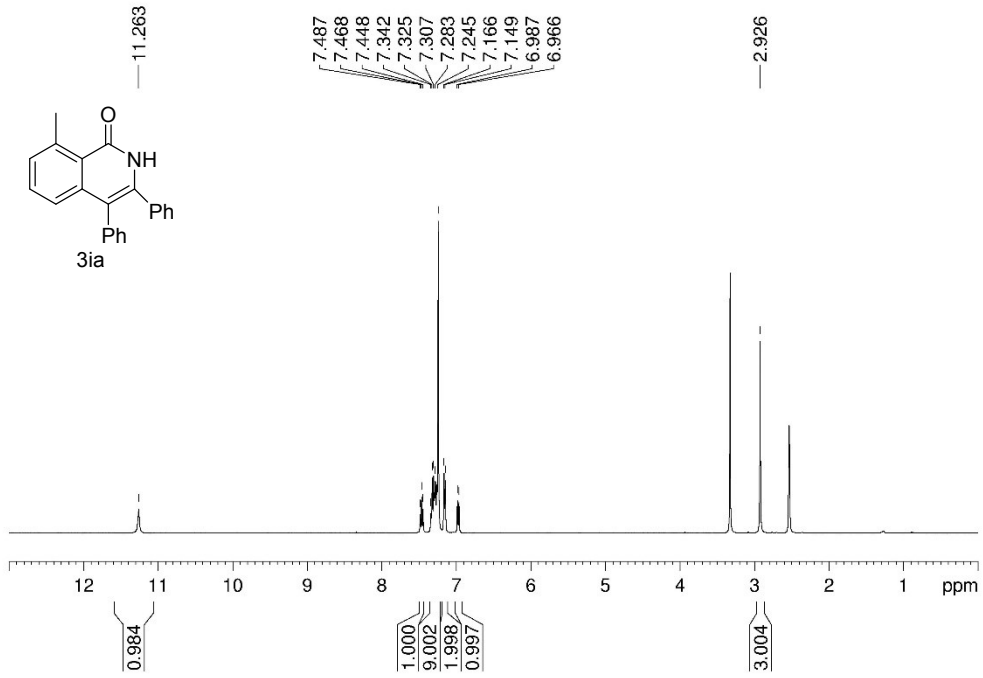
138.518
135.816
134.774
132.188
130.283
128.795
128.177
128.103
128.042
127.769
125.699
125.311
116.162
27.371
O
NH
Ac
Ph
Ph
3ha
200
180
160
140
120
100
80
60
40
20
ppm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7.487
7.468
7.448
7.342
7.325
7.307
7.283
7.245
7.166
7.149
6.987
6.966
2.926
O
NH
Ph
Ph
3ia
12
11
10
9
8
7
6
5
4
3
2
1
ppm
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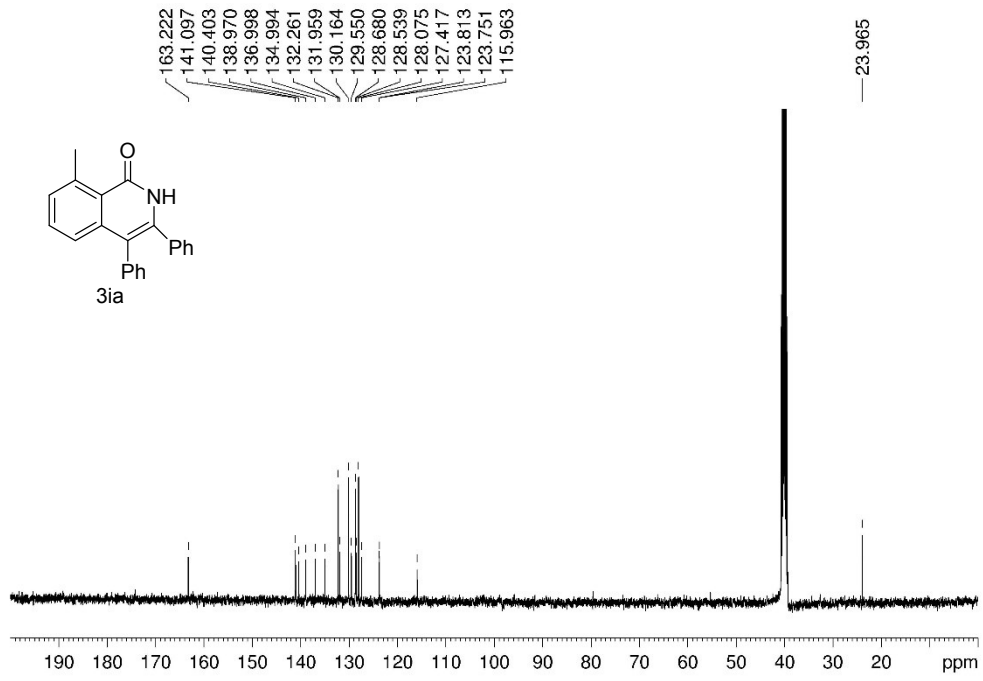
1.000
9.002
1.998
0.997
3.004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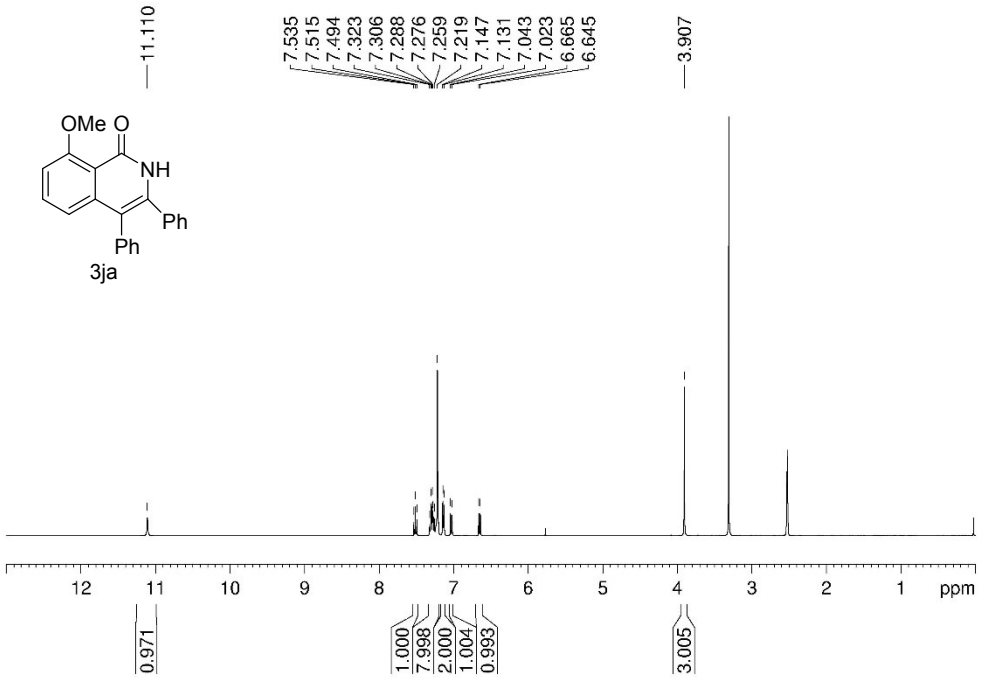
140.403
138.970
136.998
134.994
132.261
131.959
130.164
129.550
128.680
128.539
128.075
127.417
123.813
123.751
115.963
23.965
O
NH
Ph
Ph
3ia
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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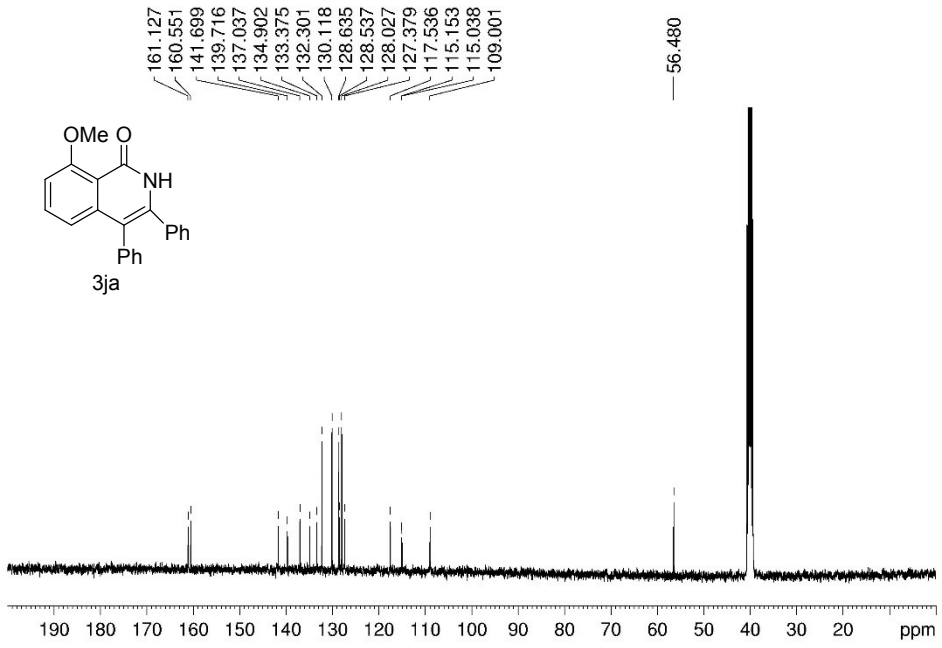
7.535
7.515
7.494
7.323
7.306
7.288
7.276
7.259
7.219
7.147
7.131
7.043
7.023
6.665
6.645
3.907
OMe O
NH
Ph
Ph
3ja
12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.971
1.000
7.998
2.000
1.004
0.993
3.005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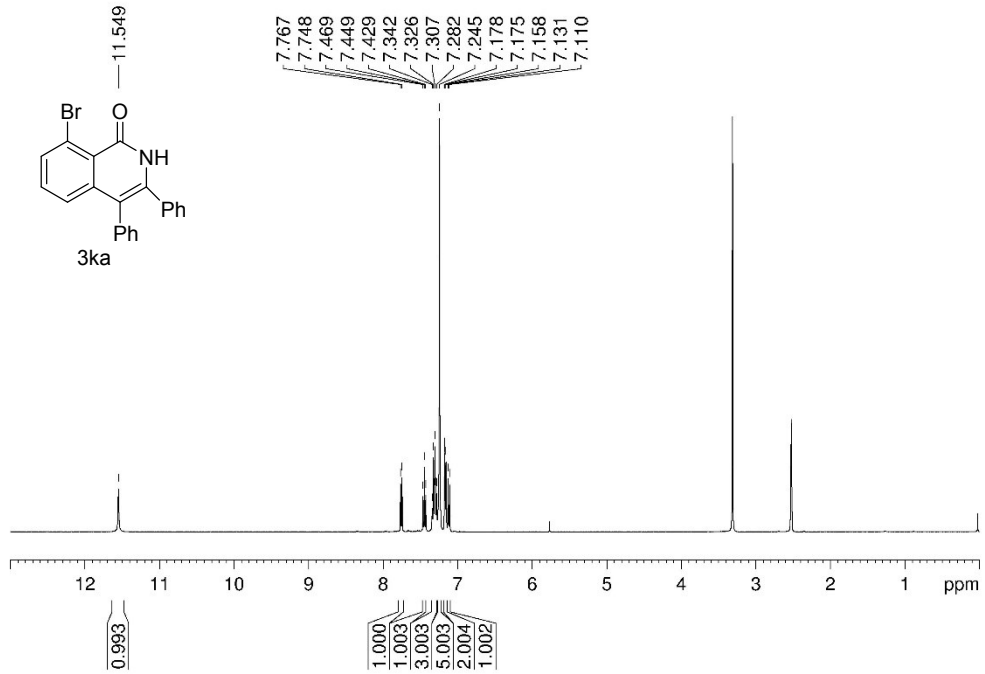
160.551
141.699
139.716
137.037
134.902
133.375
132.301
130.118
128.635
128.537
128.027
127.379
117.536
115.153
115.038
109.001
56.480
OMe O
NH
Ph
Ph
3ja
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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7.748
7.469
7.449
7.429
7.342
7.326
7.307
7.282
7.245
7.178
7.175
7.158
7.131
7.110
Br
O
NH
Ph
Ph
3ka
12
11
10
9
8
7
6
5
4
3
2
1
ppm
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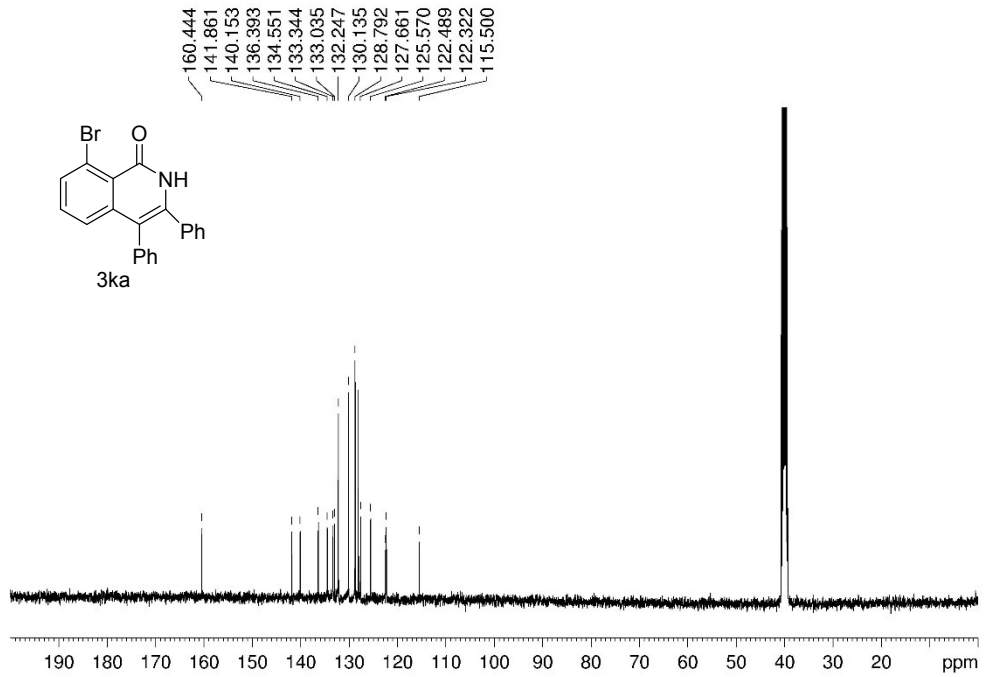
1.000
1.003
3.003
5.003
2.004
1.002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140.153
136.393
134.551
133.344
133.035
132.247
130.135
128.792
127.661
125.570
122.489
122.322
115.500
Br
O
NH
Ph
Ph
3ka
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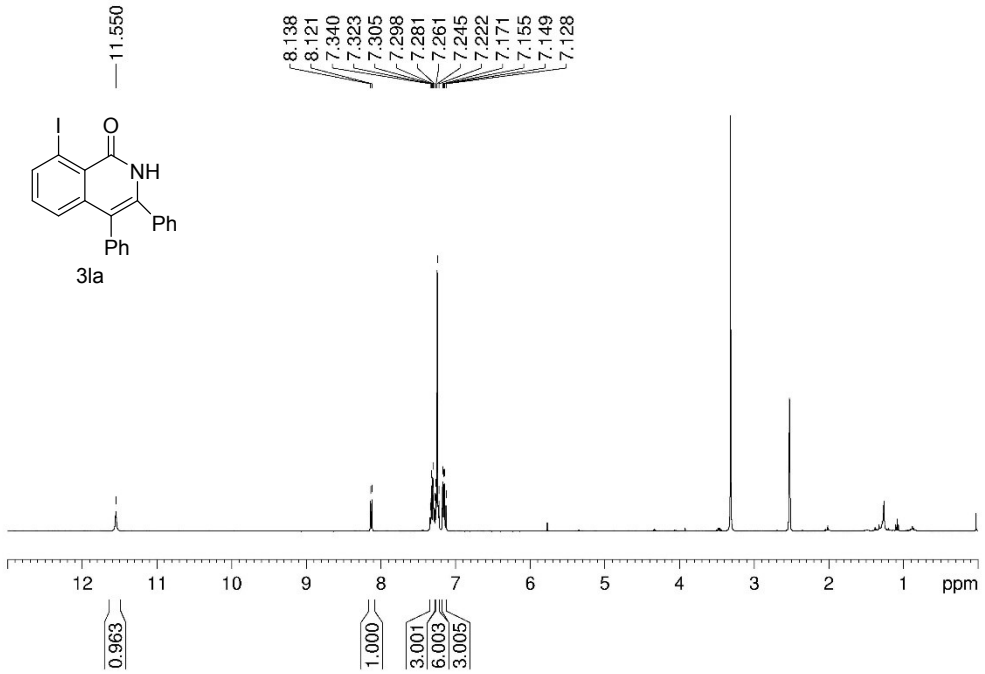
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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8.121
7.340
7.323
7.305
7.298
7.281
7.261
7.245
7.222
7.171
7.155
7.149
7.128
I
O
NH
Ph
Ph
3la
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.963
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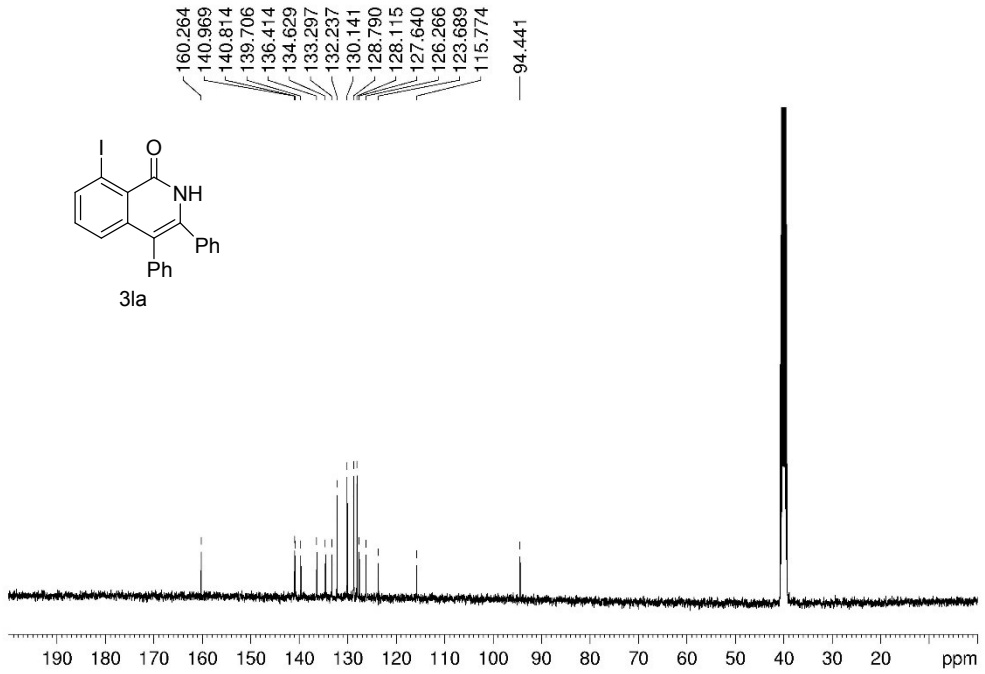
3.001
6.003
3.005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140.814
139.706
136.414
134.629
133.297
132.237
130.141
128.790
128.115
127.640
126.266
123.689
115.774
94.441
I
O
NH
Ph
Ph
3la
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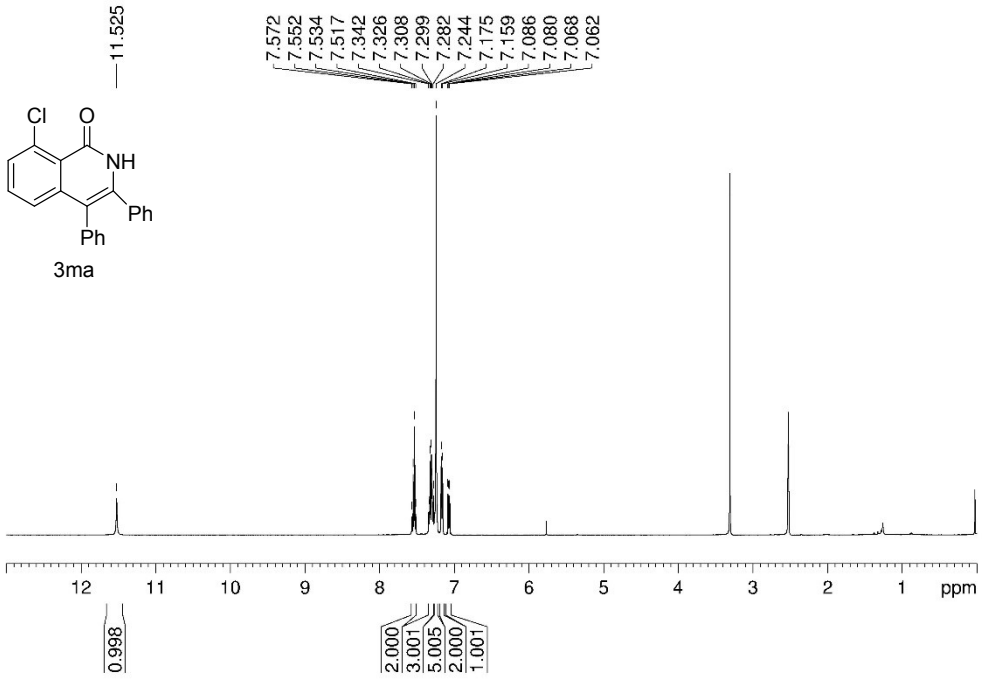
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.552
7.534
7.517
7.342
7.326
7.308
7.299
7.282
7.244
7.175
7.159
7.086
7.080
7.068
7.062
Cl
O
NH
Ph
Ph
3ma
12
11
10
9
8
7
6
5
4
3
2
1
ppm
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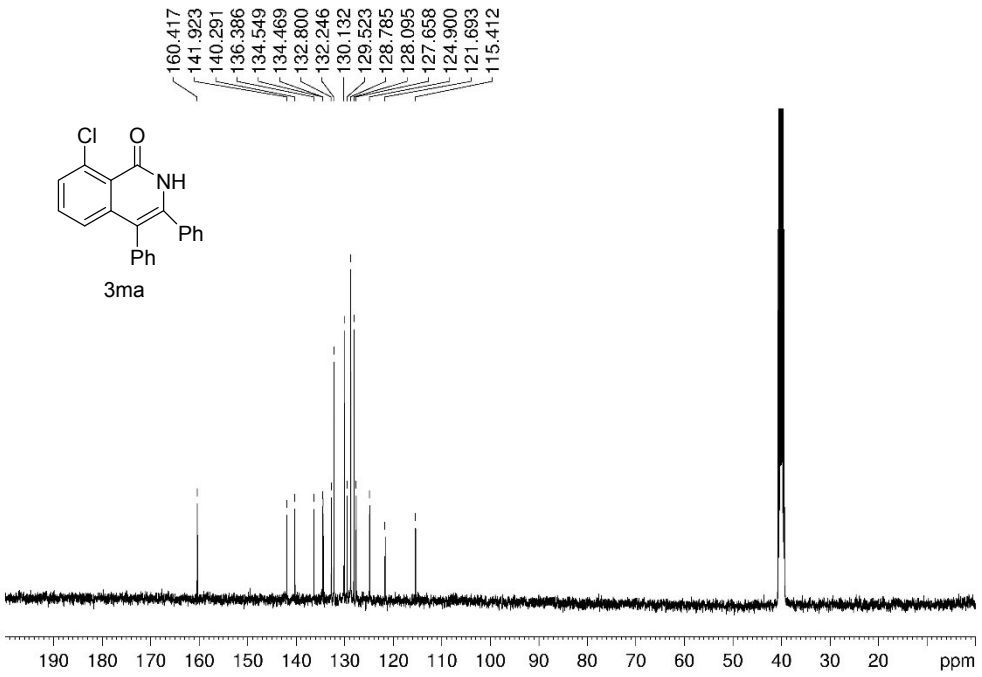
2.000
3.001
5.005
2.000
1.001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140.291
136.386
134.549
134.469
132.800
132.246
130.132
129.523
128.785
128.095
127.658
124.900
121.693
115.412
Cl
O
NH
Ph
Ph
3ma
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180
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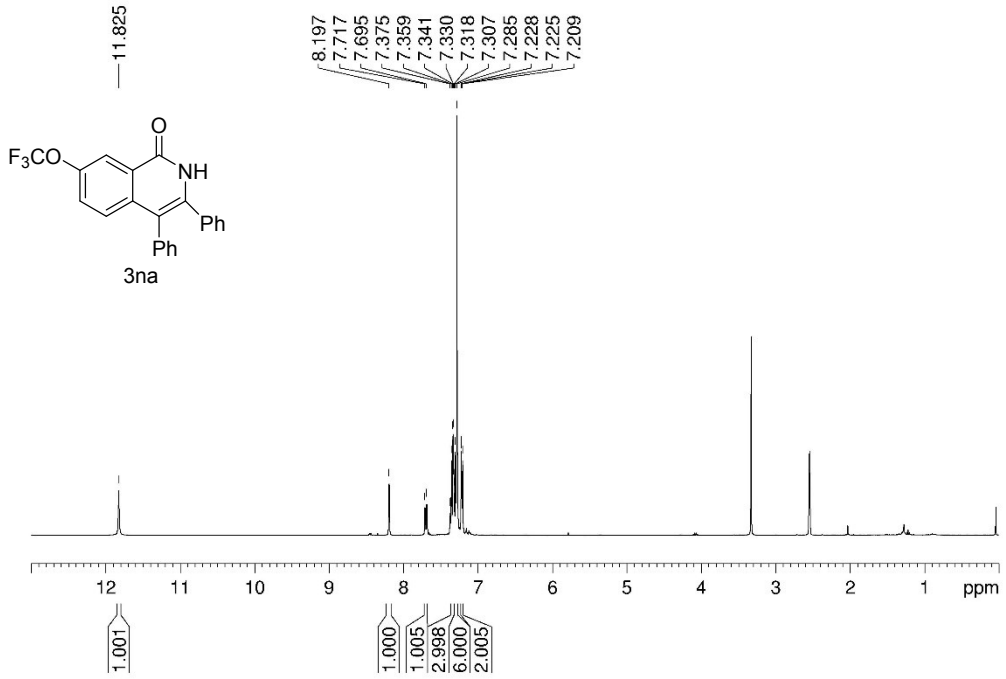
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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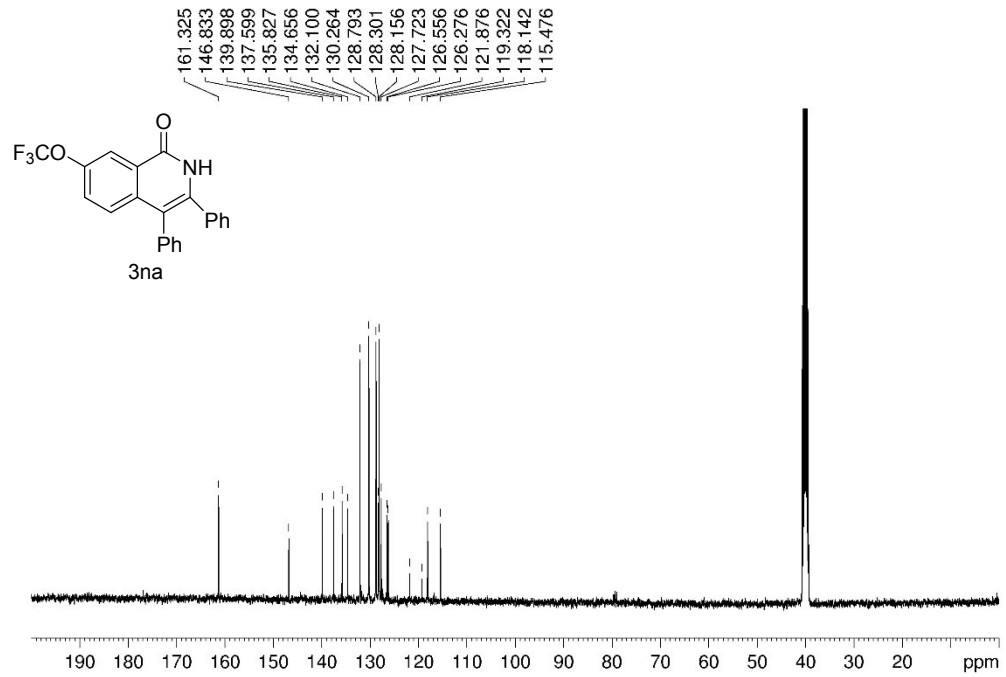
7.717
7.695
7.375
7.359
7.341
7.330
7.318
7.307
7.285
7.228
7.225
7.209
O
F3CO
NH
Ph
Ph
3na
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.001
1.000
1.005
2.998
6.000
2.005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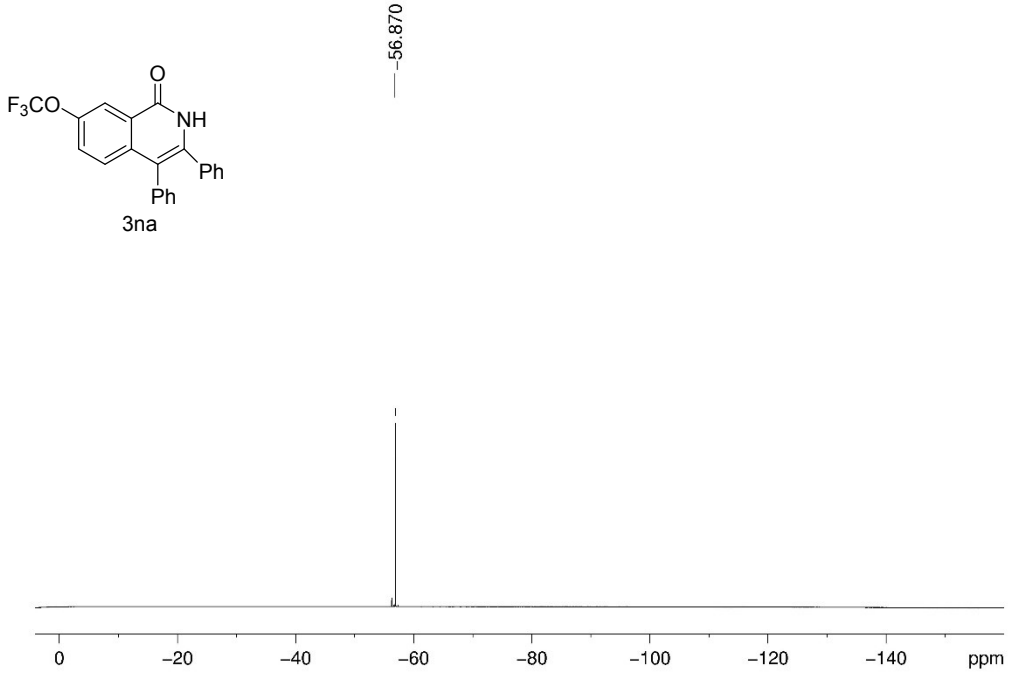
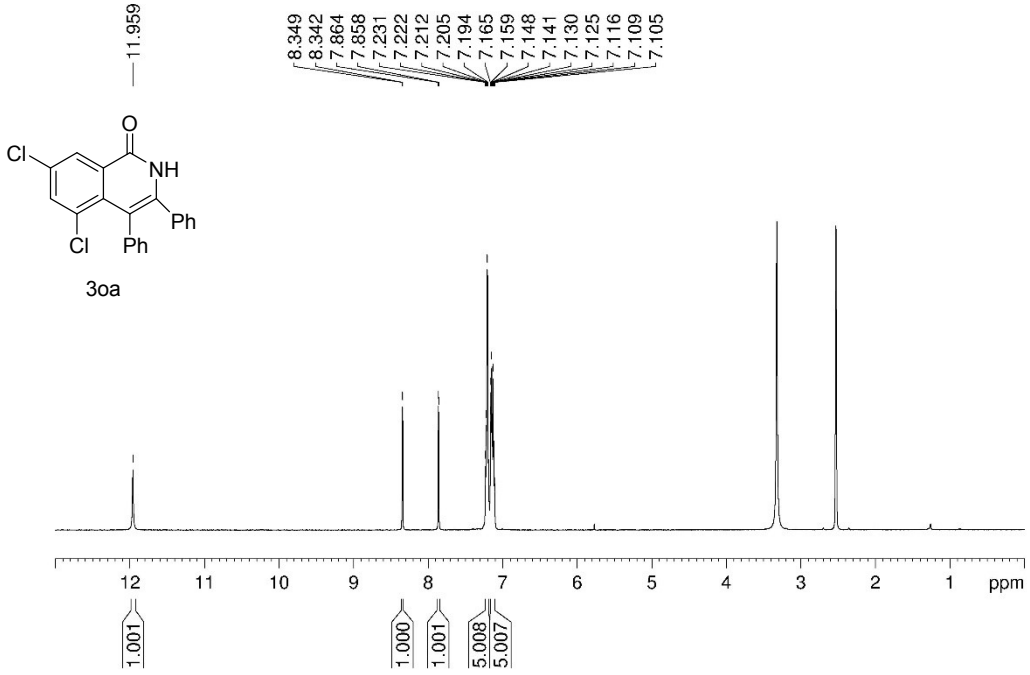
139.898
137.599
135.827
134.656
132.100
130.264
128.793
128.301
128.156
127.723
126.556
126.276
121.876
119.322
118.142
115.476
O
F3CO
NH
Ph
Ph
3na
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


F3CO
O
NH
Ph
Ph
3na
−56.870
0
−20
−40
−60
−80
−100
−120
−140
ppm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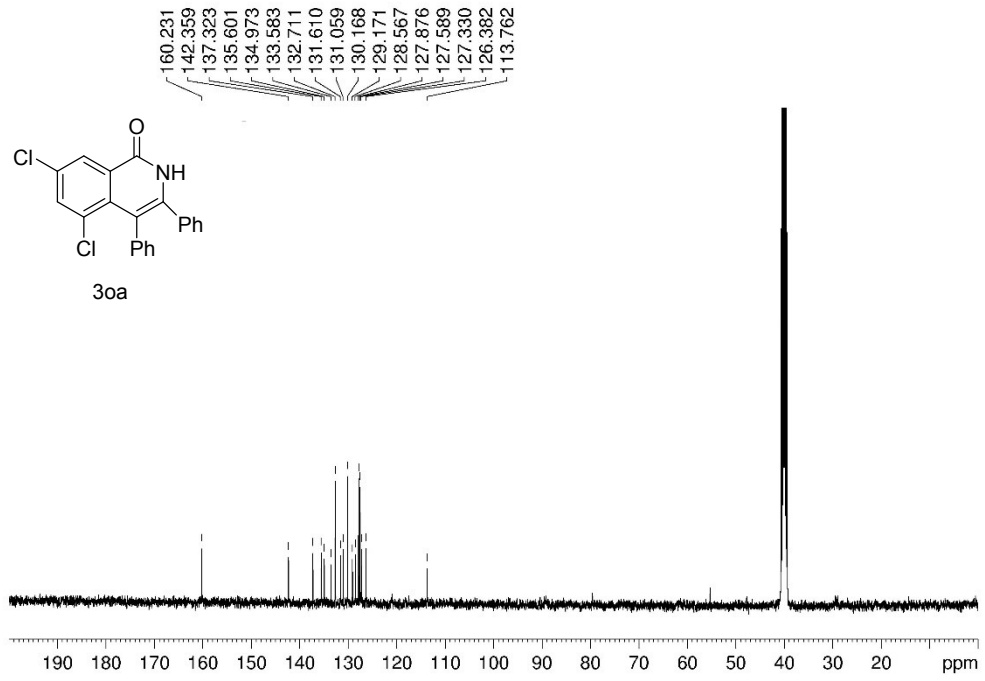
8.342
7.864
7.858
7.231
7.222
7.212
7.205
7.194
7.165
7.159
7.148
7.141
7.130
7.125
7.116
7.109
7.105
Cl
O
NH
Ph
Cl
Ph
3oa
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.001
1.000
1.001
5.008
5.007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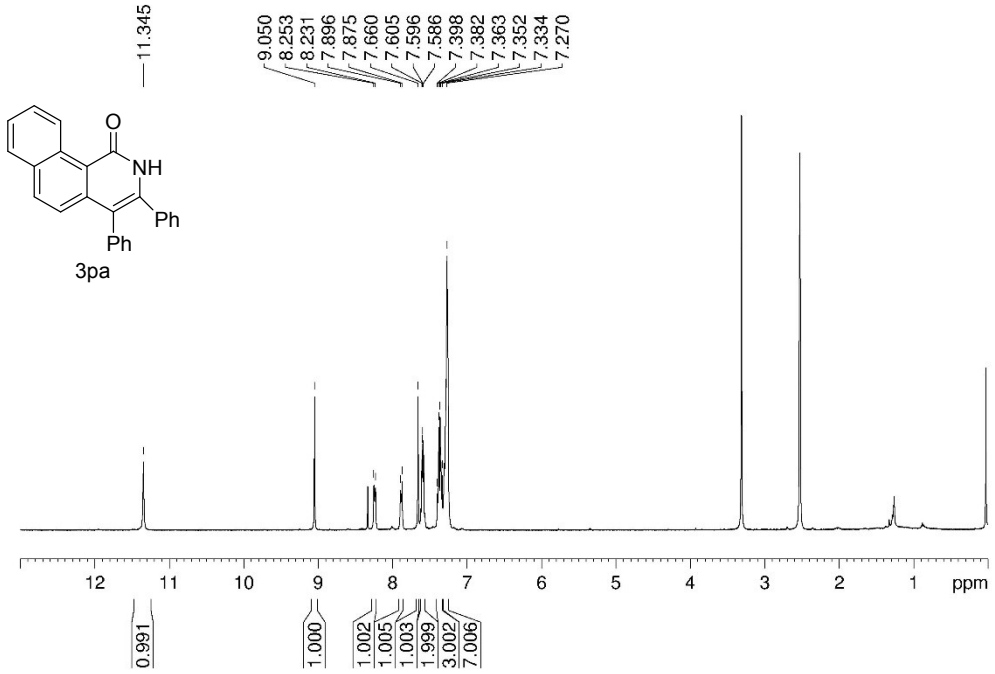
142.359
137.323
135.601
134.973
133.583
132.711
131.610
131.059
130.168
129.171
128.567
127.876
127.589
127.330
126.382
113.762
O
NH
Cl
Cl
Ph
Ph
3oa
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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9.050
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8.231
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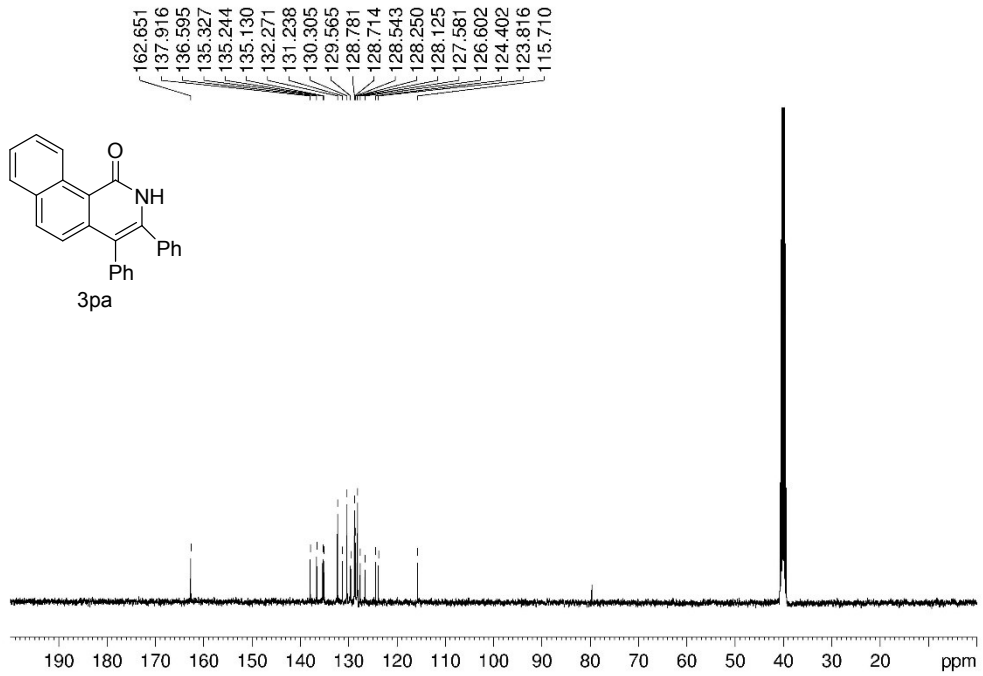
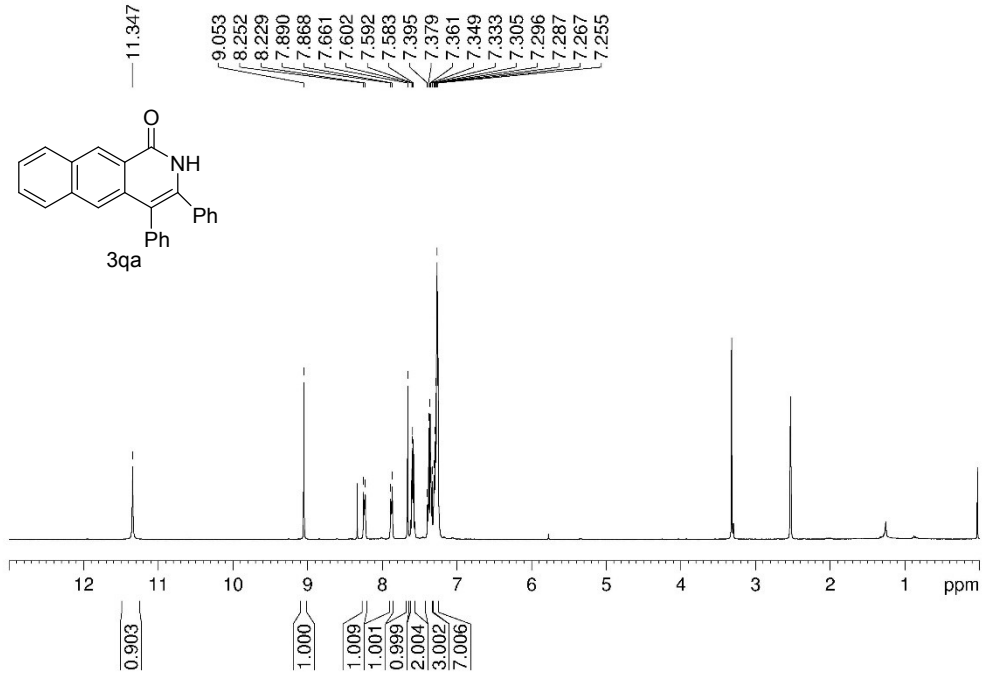
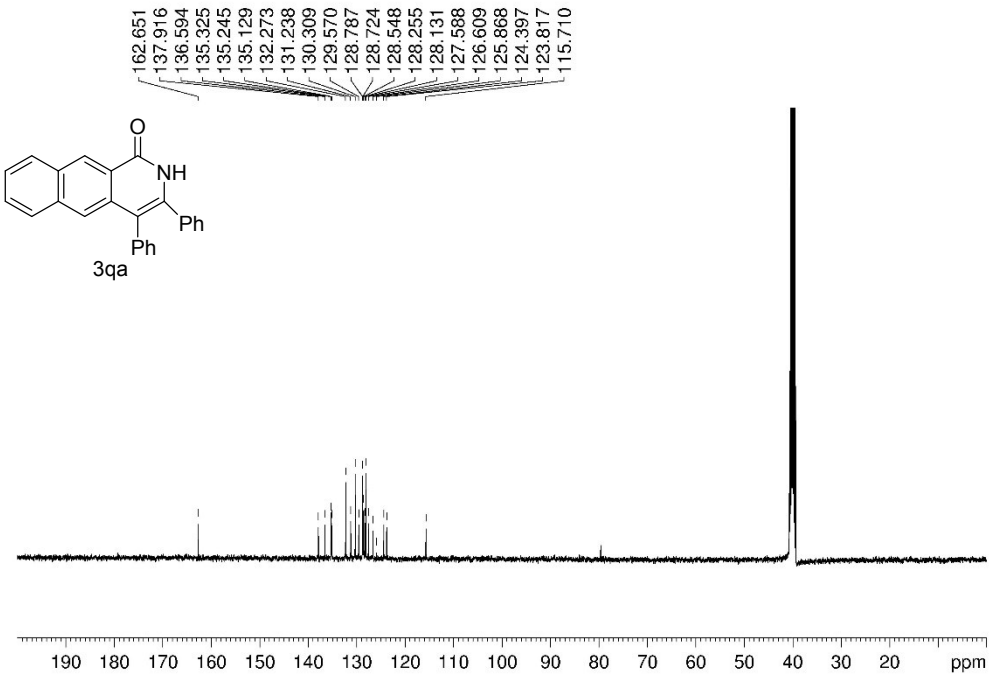
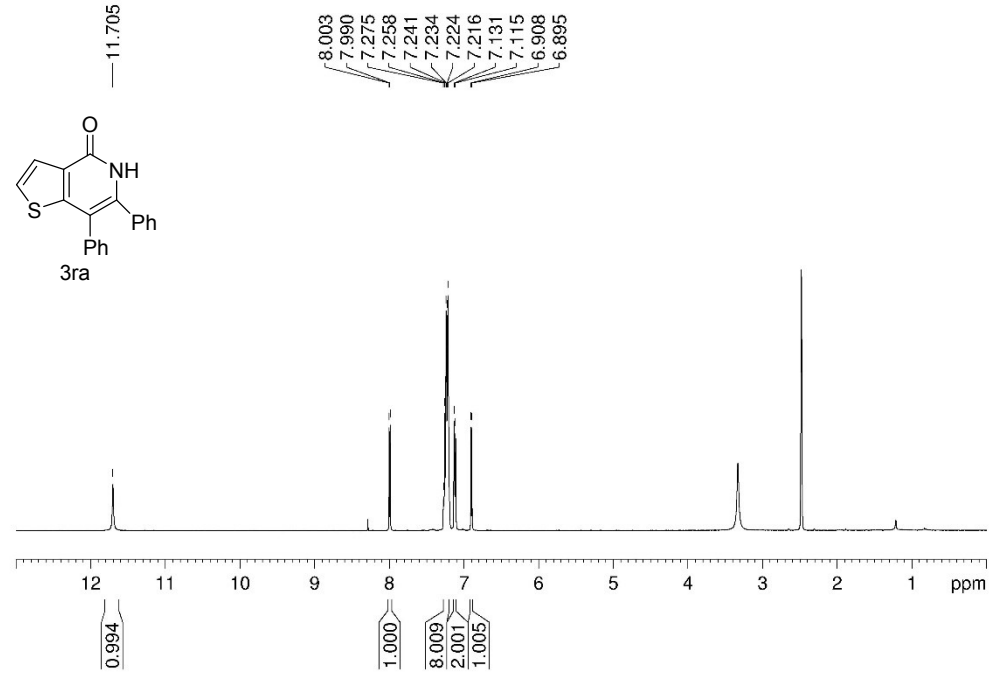
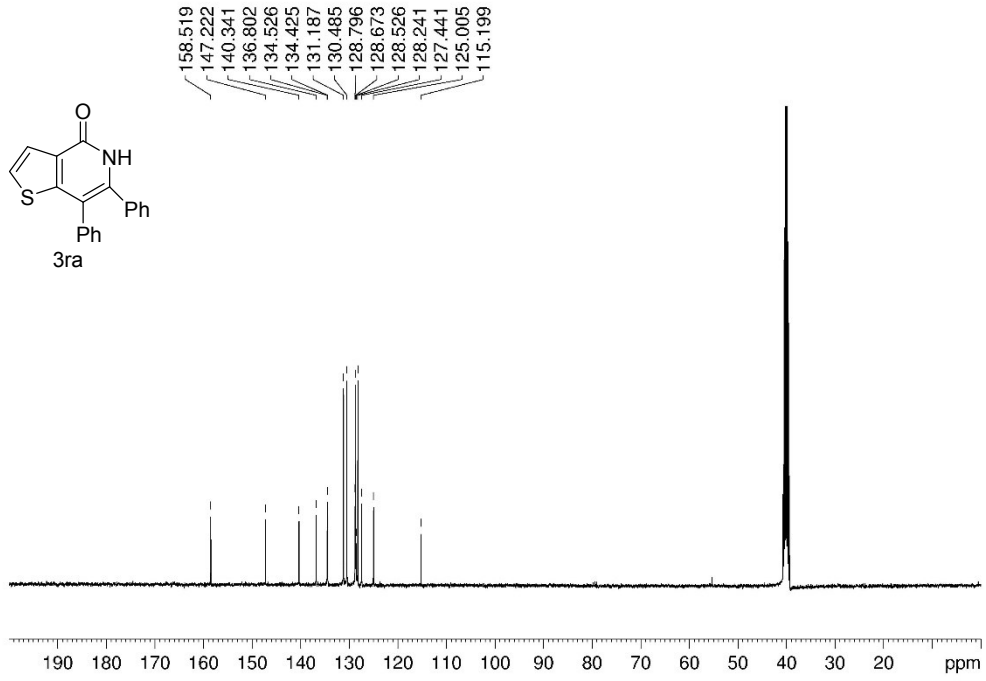
7.660
7.605
7.596
7.586
7.398
7.382
7.363
7.352
7.334
7.270
O
NH
Ph
Ph
3pa
12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.991
1.000
1.002
1.005
1.003
1.999
3.002
7.006

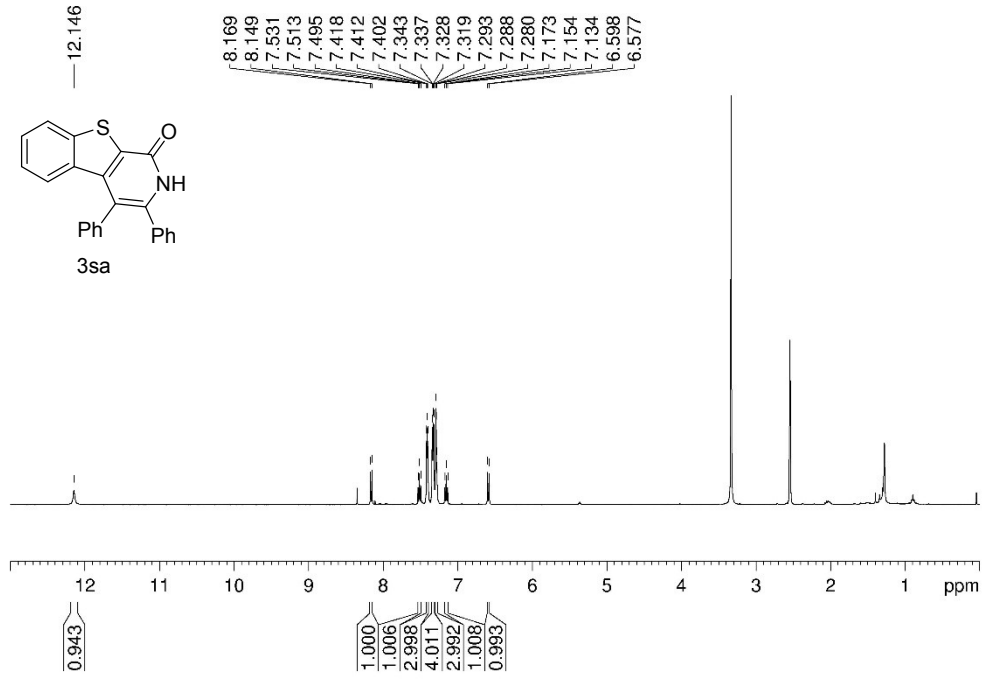

162.651
137.916
136.595
135.327
135.244
135.130
132.271
131.238
130.305
129.565
128.781
128.714
128.543
128.250
128.125
127.581
126.602
124.402
123.816
115.710
O
NH
Ph
Ph
3pa
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

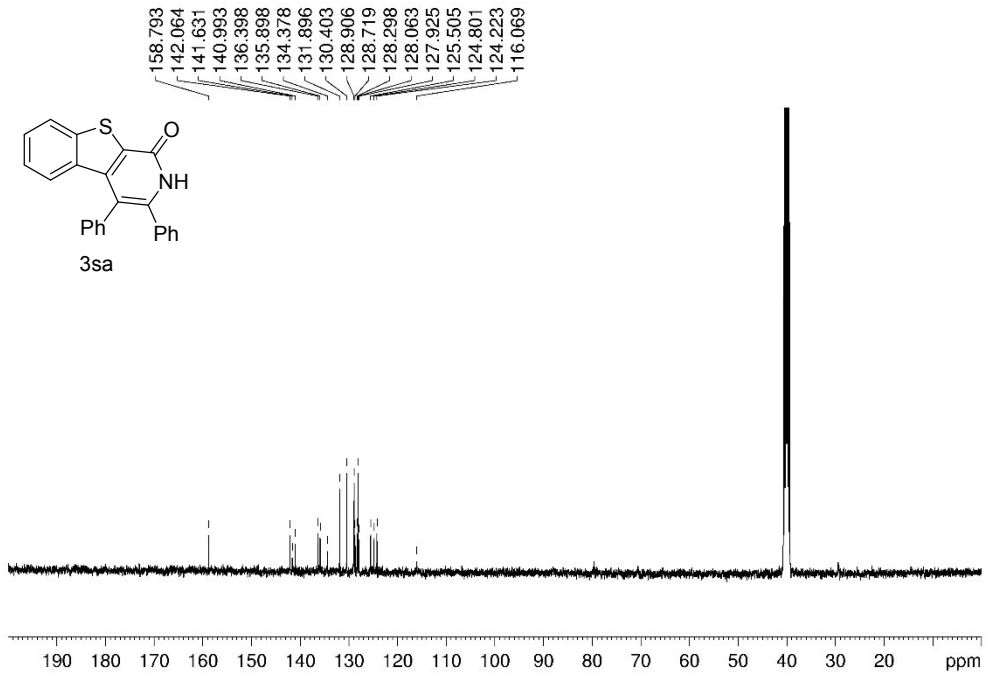

11.347
9.053
8.252
8.229
7.890
7.868
7.661
7.602
7.592
7.583
7.395
7.379
7.361
7.349
7.333
7.305
7.296
7.287
7.267
7.255
O
NH
Ph
Ph
3qa
12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.903
1.000
1.009
1.001
0.999
2.004
3.002
7.006

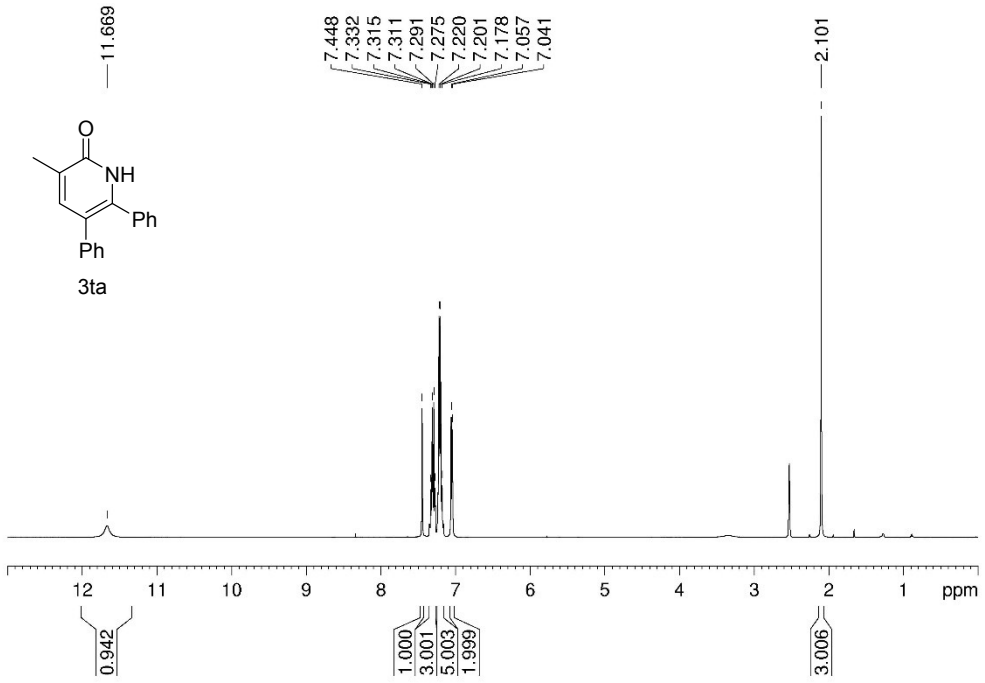

162.651
137.916
136.594
135.325
135.245
135.129
132.273
131.238
130.309
129.570
128.787
128.724
128.548
128.255
128.131
127.588
126.609
125.868
124.397
123.817
115.710
O
NH
Ph
Ph
3qa
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

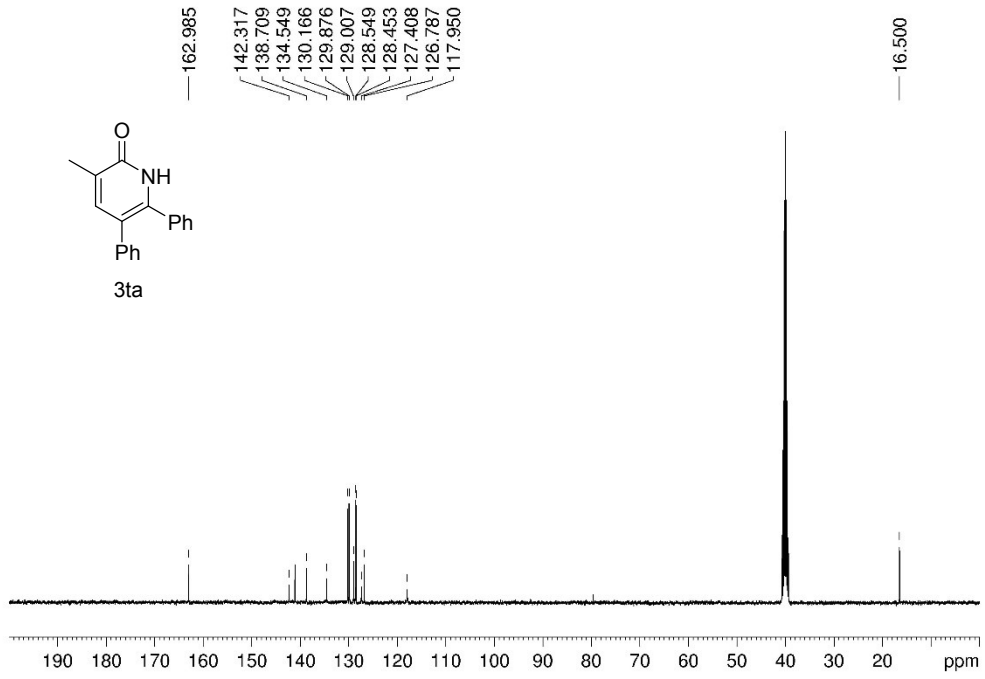

11.705
8.003
7.990
7.275
7.258
7.241
7.234
7.224
7.216
7.131
7.115
6.908
6.895
O
NH
S
Ph
Ph
3ra
12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.994
1.000
8.009
2.001
1.005

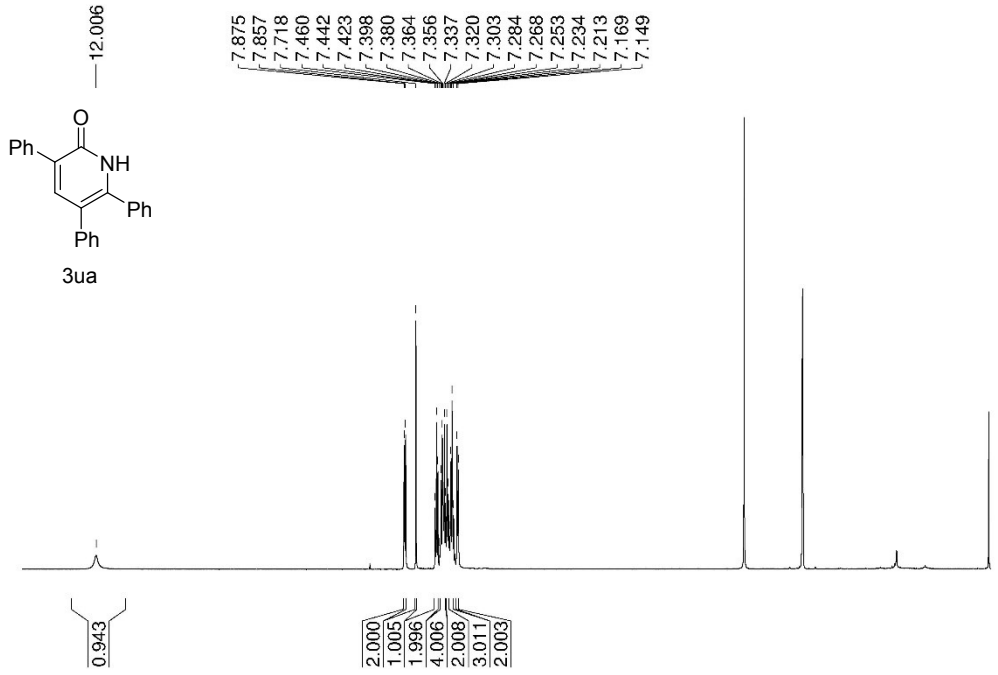

158.519
147.222
140.341
136.802
134.526
134.425
131.187
130.485
128.796
128.673
128.526
128.241
127.441
125.005
115.199
O
NH
S
Ph
Ph
3ra
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

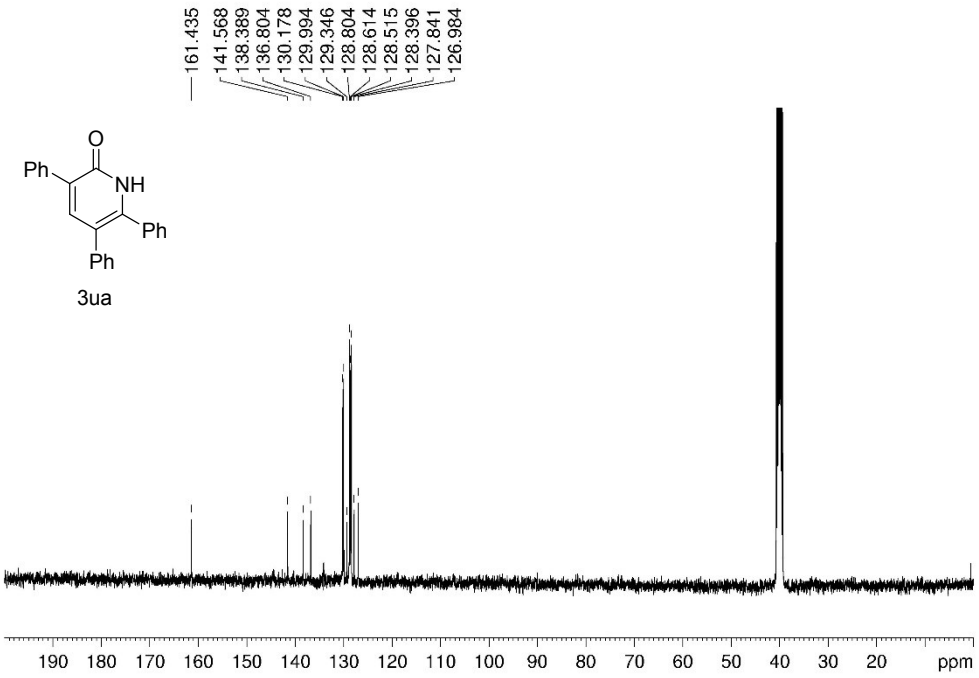

12.146
8.169
8.149
7.531
7.513
7.495
7.418
7.412
7.402
7.343
7.337
7.328
7.319
7.293
7.288
7.280
7.173
7.154
7.134
6.598
6.577
S
O
NH
Ph
Ph
3sa
12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.943
1.000
1.006
2.998
4.011
2.992
1.008
0.993

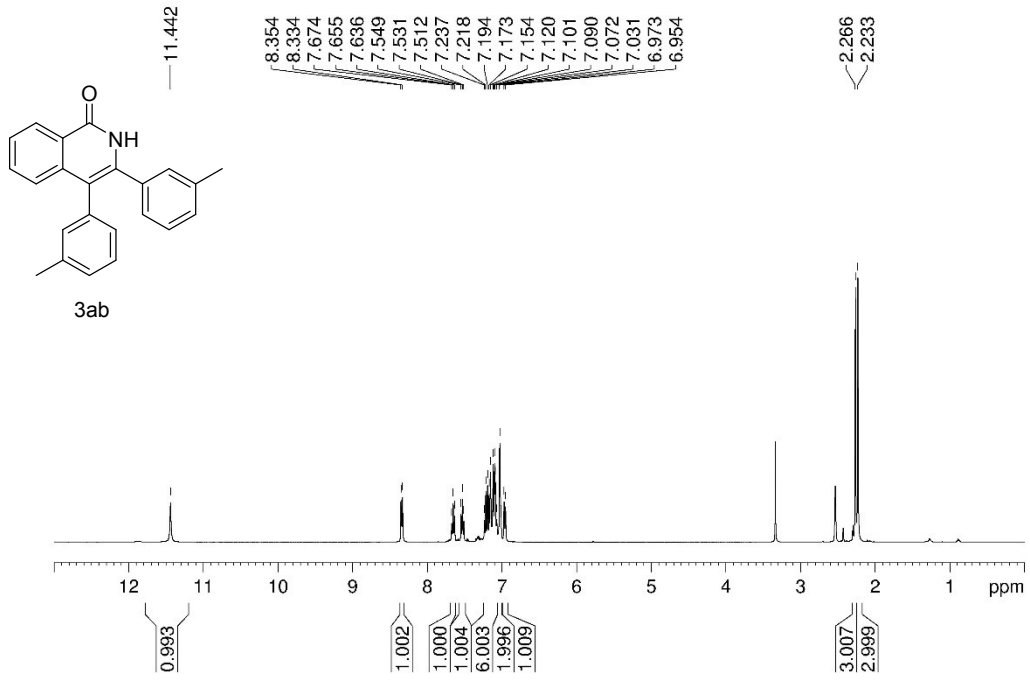

158.793
142.064
141.631
140.993
136.398
135.898
134.378
131.896
130.403
128.906
128.719
128.298
128.063
127.925
125.505
124.801
124.223
116.069
S
O
NH
Ph
Ph
3sa
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

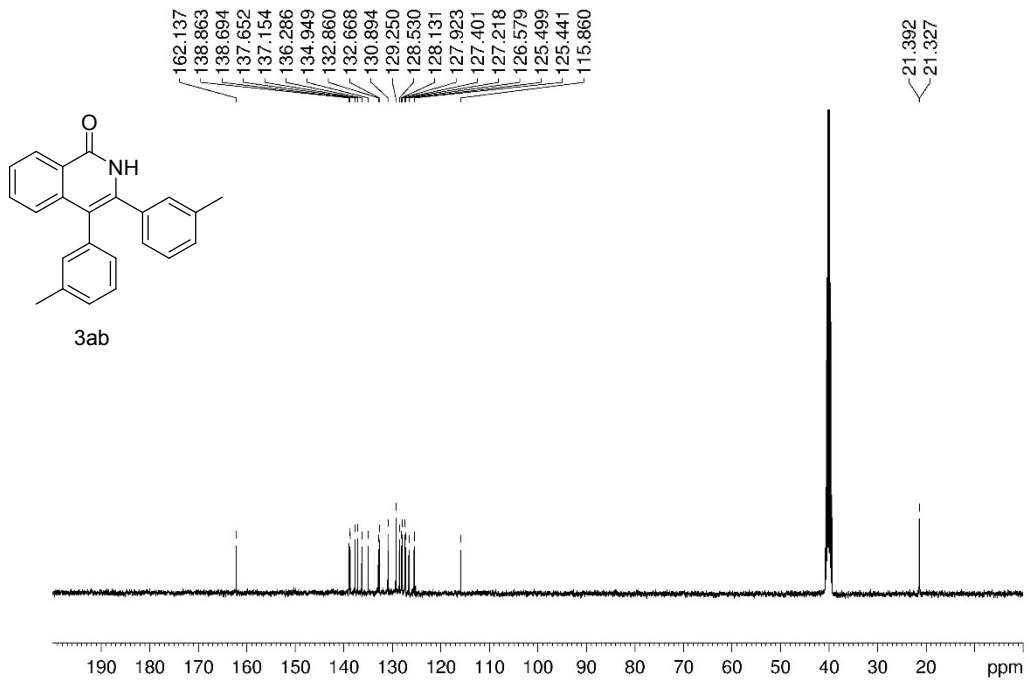

11.669
7.448
7.332
7.315
7.311
7.291
7.275
7.220
7.201
7.178
7.057
7.041
2.101
O
NH
Ph
Ph
3ta
12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.942
1.000
3.001
5.003
1.999
3.006

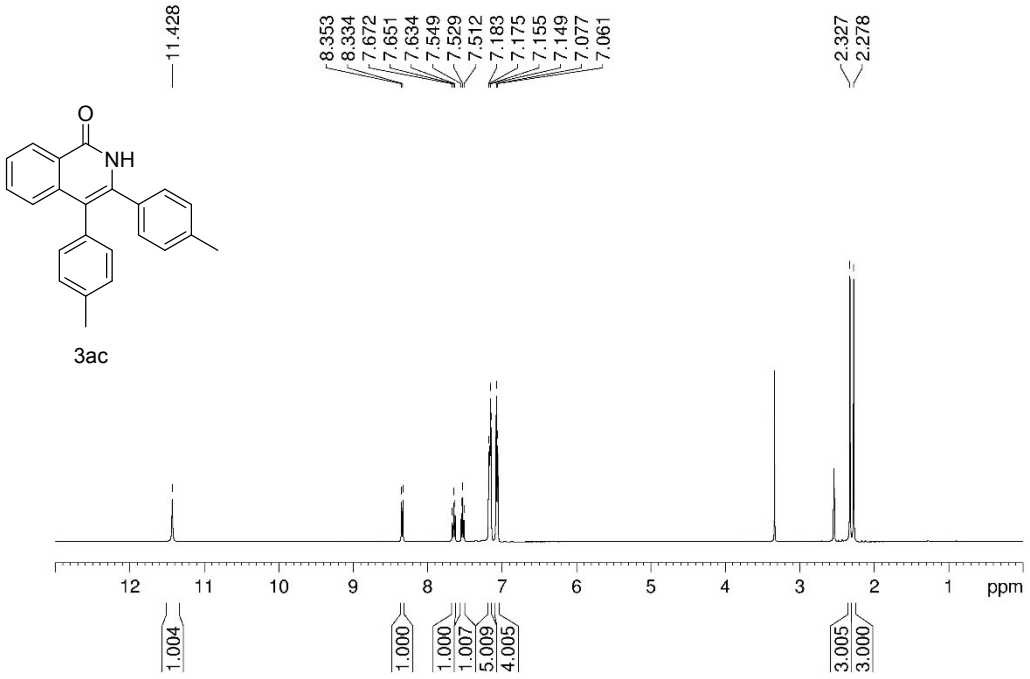

162.985
142.317
138.709
134.549
130.166
129.876
129.007
128.549
128.453
127.408
126.787
117.950
16.500
O
NH
Ph
Ph
3ta
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

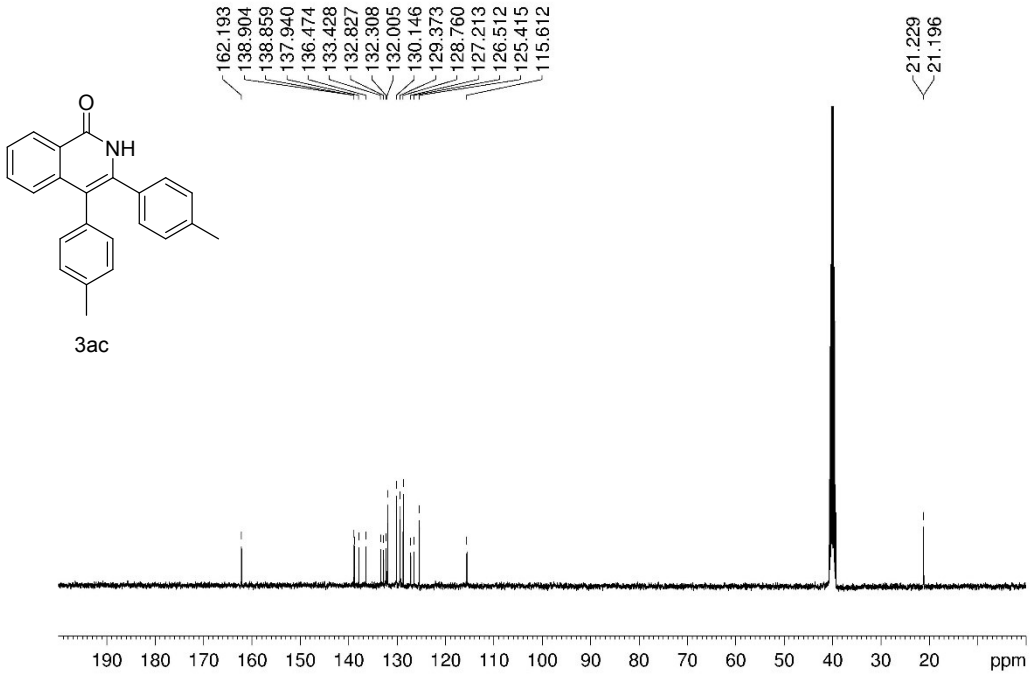

12.006
7.875
7.857
7.718
7.460
7.442
7.423
7.398
7.380
7.364
7.356
7.337
7.320
7.303
7.284
7.268
7.253
7.234
7.213
7.169
7.149
O
Ph
NH
Ph
Ph
3ua
0.943
2.000
1.005
1.996
4.006
2.008
3.011
2.003


161.435
141.568
138.389
136.804
130.178
129.994
129.346
128.804
128.614
128.515
128.396
127.841
126.984
O
NH
Ph
Ph
Ph
3ua
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

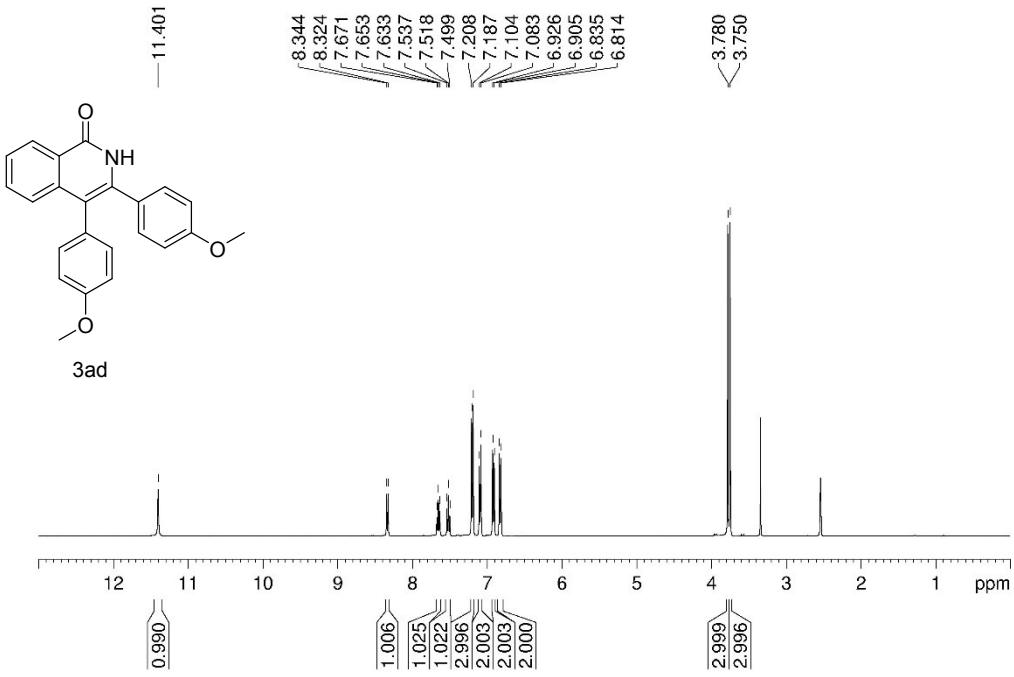

11.442
8.354
8.334
7.674
7.655
7.636
7.549
7.531
7.512
7.237
7.218
7.194
7.173
7.154
7.120
7.101
7.090
7.072
7.031
6.973
6.954
2.266
2.233
O
NH
3ab
12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.993
1.002
1.000
1.004
6.003
1.996
1.009
3.007
2.999


162.137
138.863
138.694
137.652
137.154
136.286
134.949
132.860
132.668
130.894
129.250
128.530
128.131
127.923
127.401
127.218
126.579
125.499
125.441
115.860
21.392
21.327
O
NH
3ab
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

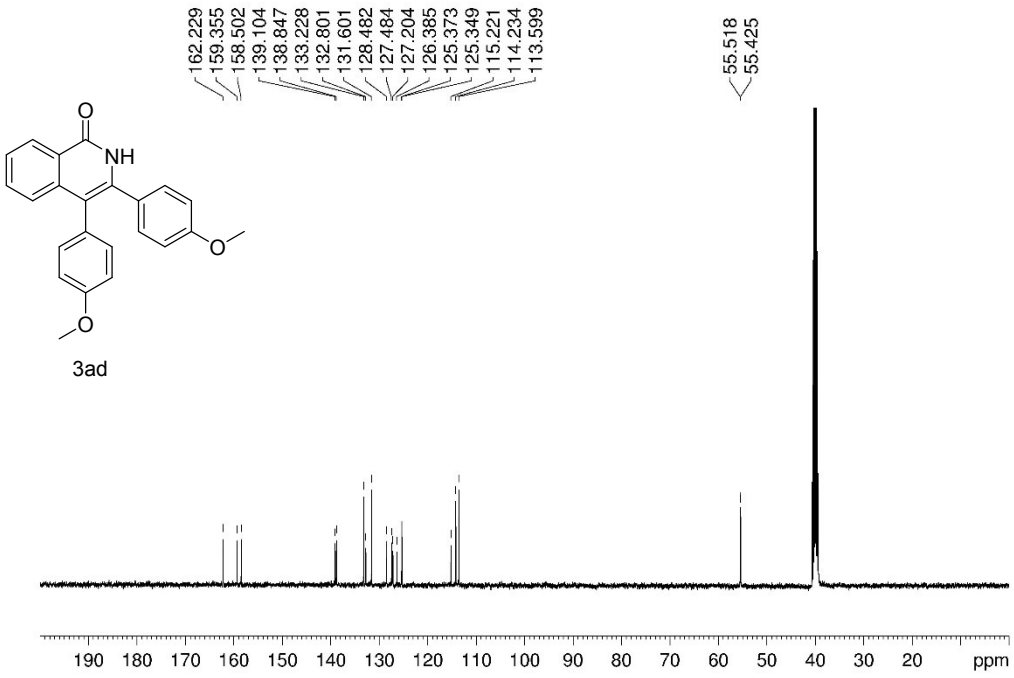

11.428
8.353
8.334
7.672
7.651
7.634
7.549
7.529
7.512
7.183
7.175
7.155
7.149
7.077
7.061
2.327
2.278
O
NH
3ac
12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.004
1.000
1.000
1.007
5.009
4.005
3.005
3.000

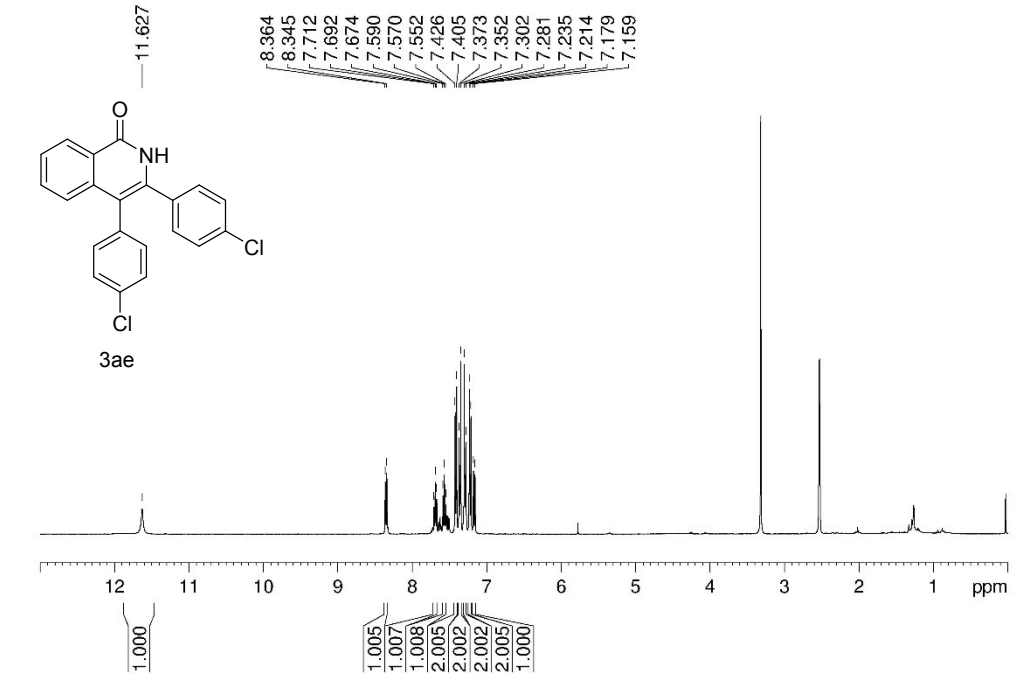

162.193
138.904
138.859
137.940
136.474
133.428
132.827
132.308
132.005
130.146
129.373
128.760
127.213
126.512
125.415
115.612
21.229
21.196
O
NH
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

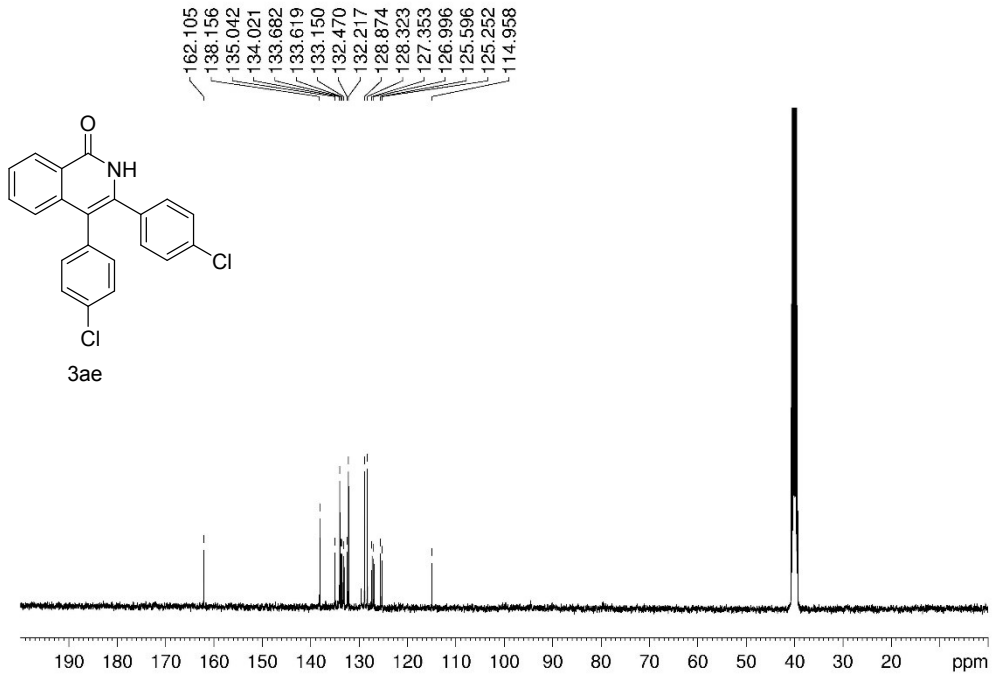
3ac

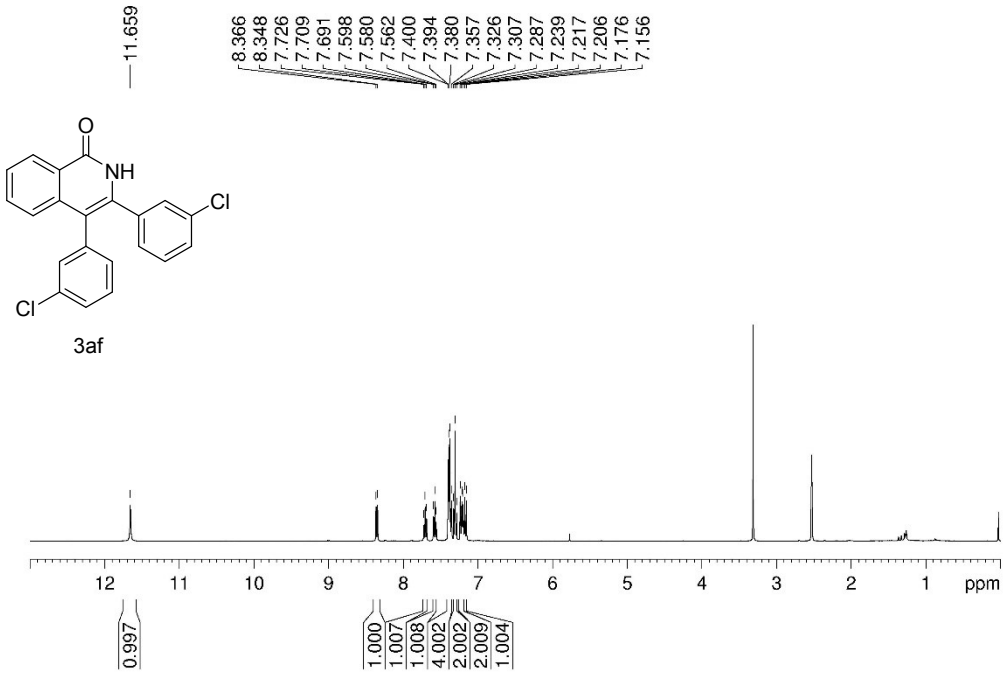

11.401
8.344
8.324
7.671
7.653
7.633
7.537
7.518
7.499
7.208
7.187
7.104
7.083
6.926
6.905
6.835
6.814
3.780
3.750
O
NH
O
O
12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.990
1.006
1.025
1.022
2.996
2.003
2.003
2.000
2.999
2.996

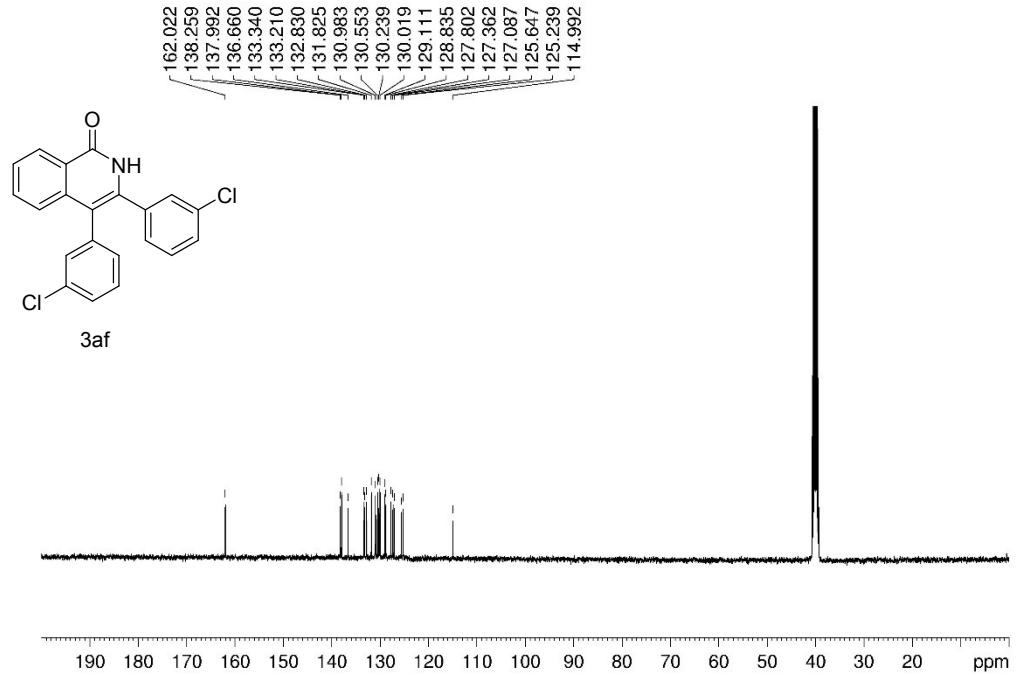
3ad

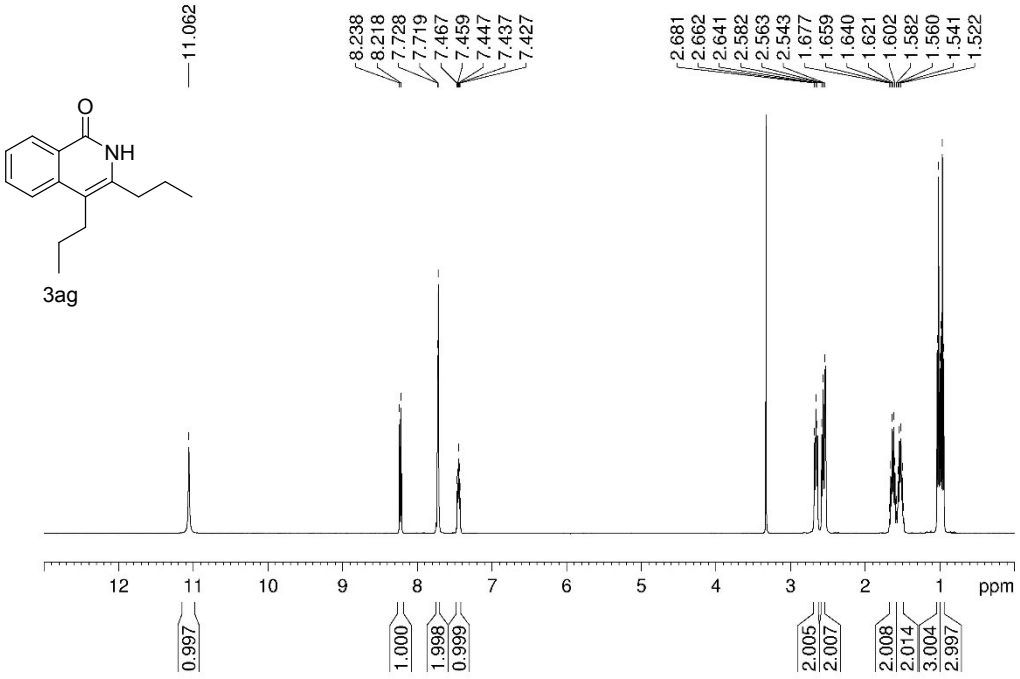

162.229
159.355
158.502
139.104
138.847
133.228
132.801
131.601
128.482
127.484
127.204
126.385
125.373
125.349
115.221
114.234
113.599
55.518
55.425
O
NH
O
O
3ad
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

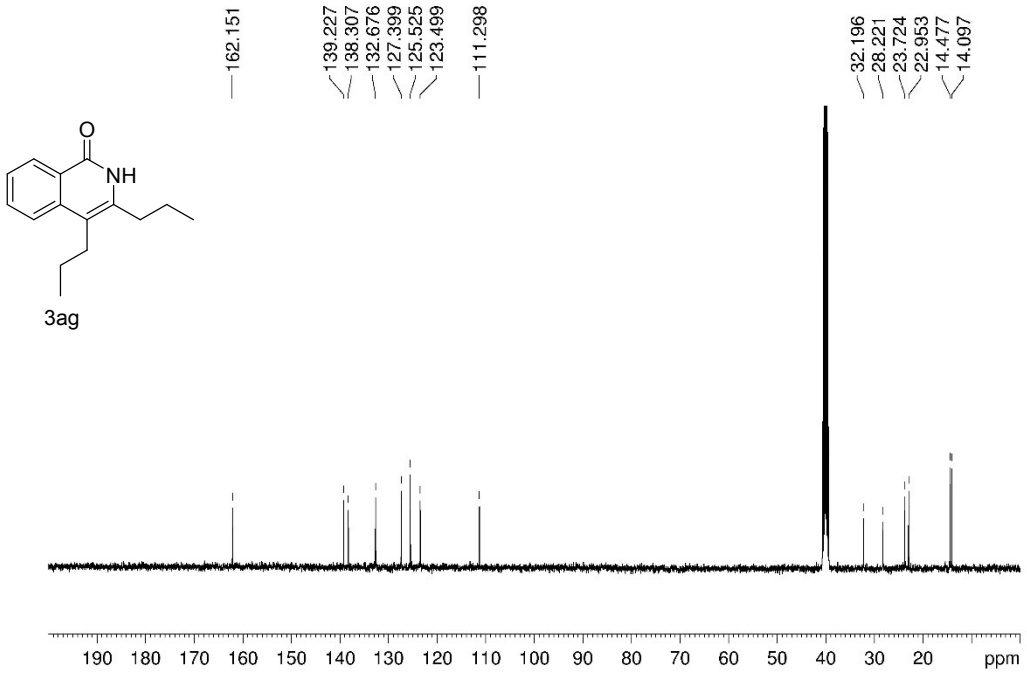

11.627
8.364
8.345
7.712
7.692
7.674
7.590
7.570
7.552
7.426
7.405
7.373
7.352
7.302
7.281
7.235
7.214
7.179
7.159
O
NH
Cl
Cl
3ae
12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.000
1.005
1.007
1.008
2.005
2.002
2.002
2.005
1.000

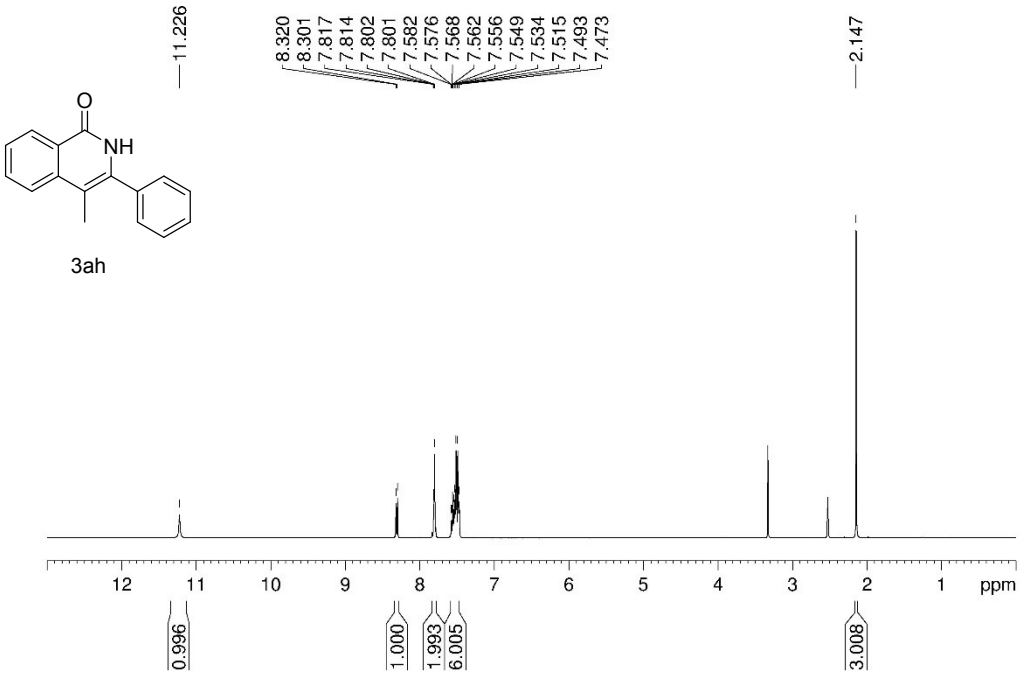

162.105
138.156
135.042
134.021
133.682
133.619
133.150
132.470
132.217
128.874
128.323
127.353
126.996
125.596
125.252
114.958
O
NH
Cl
Cl
3ae
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

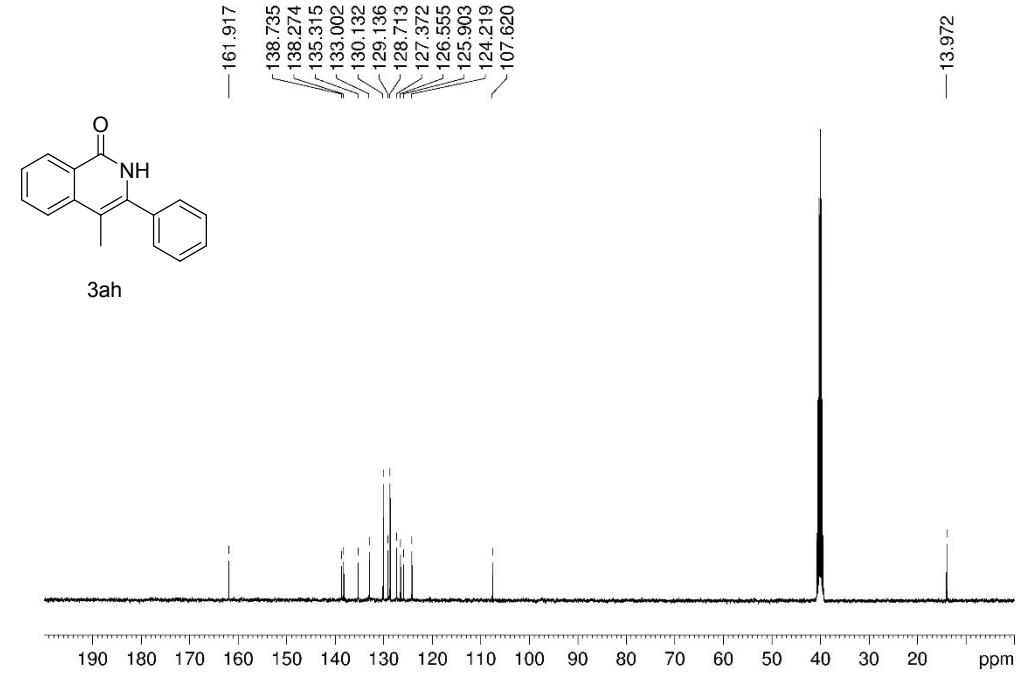

11.659
8.366
8.348
7.726
7.709
7.691
7.598
7.580
7.562
7.400
7.394
7.380
7.357
7.326
7.307
7.287
7.239
7.217
7.206
7.176
7.156
O
NH
Cl
Cl
3af
12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.997
1.000
1.007
1.008
4.002
2.002
2.009
1.004

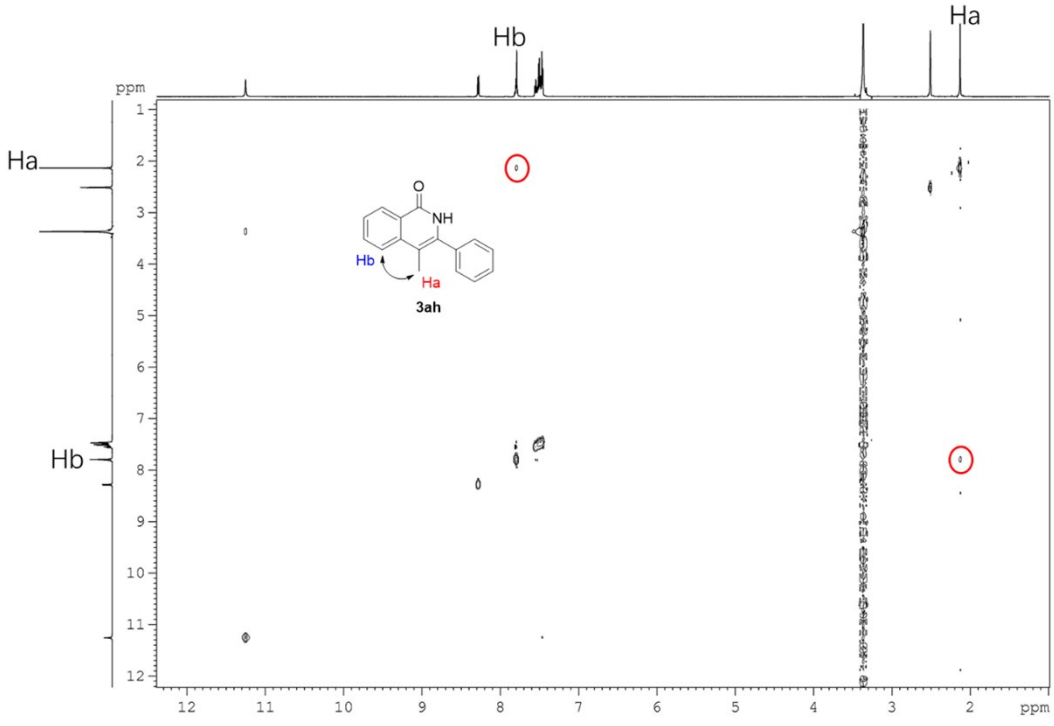

162.022
138.259
137.992
136.660
133.340
133.210
132.830
131.825
130.983
130.553
130.239
130.019
129.111
128.835
127.802
127.362
127.087
125.647
125.239
114.992
O
NH
Cl
Cl
3af
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

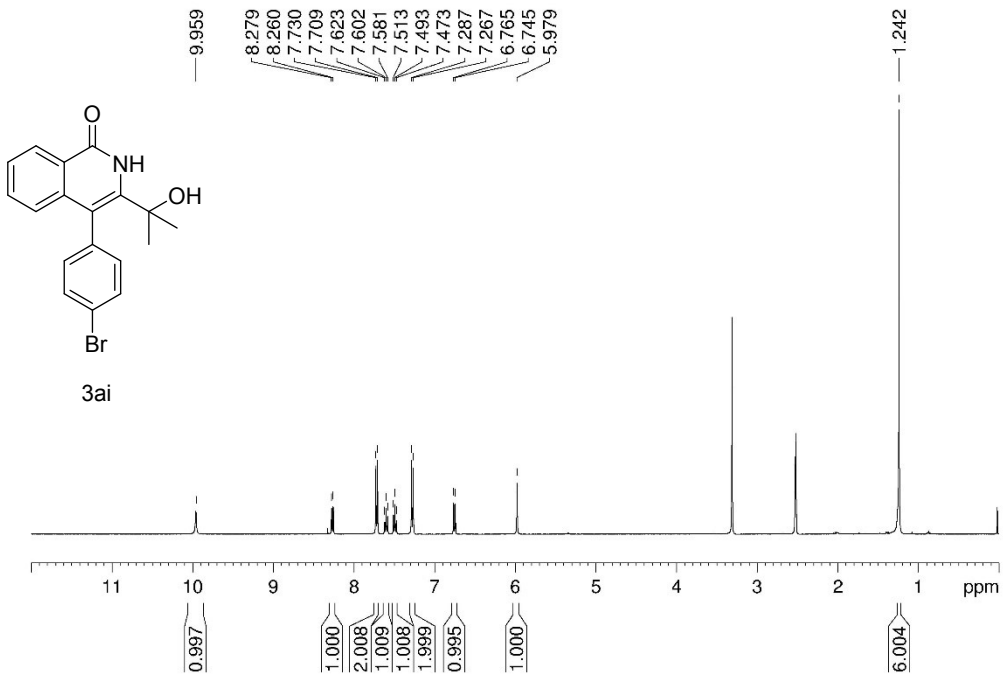

11.062
8.238
8.218
7.728
7.719
7.467
7.459
7.447
7.437
7.427
2.681
2.662
2.641
2.582
2.563
2.543
1.677
1.659
1.640
1.621
1.602
1.582
1.560
1.541
1.522
O
NH
3ag
12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.997
1.000
1.998
0.999
2.005
2.007
2.008
2.014
3.004
2.997

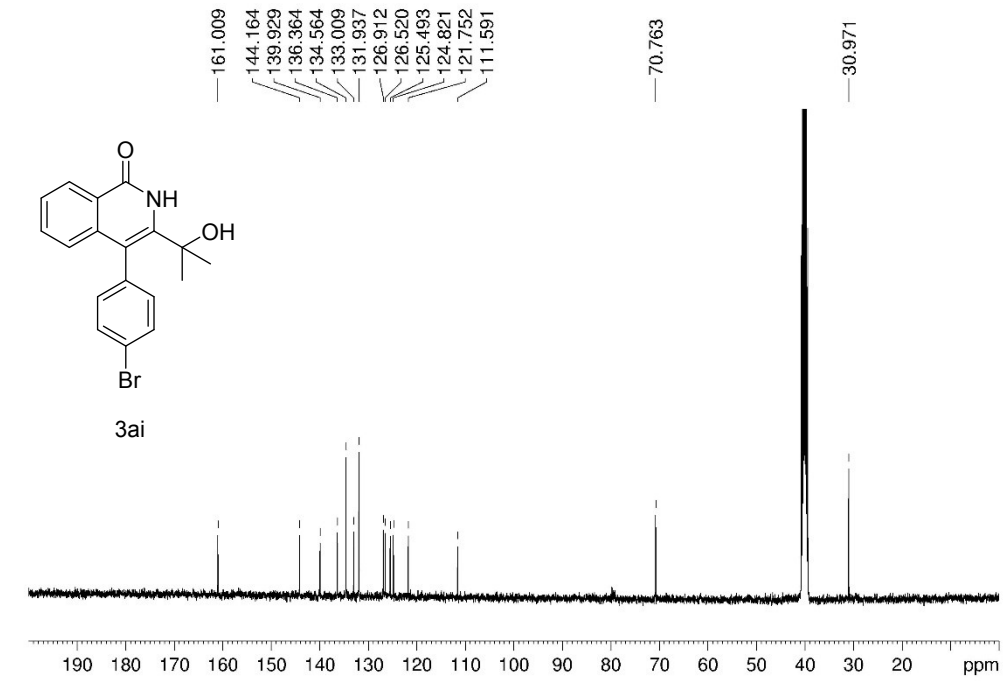

162.151
139.227
138.307
132.676
127.399
125.525
123.499
111.298
32.196
28.221
23.724
22.953
14.477
14.097
O
NH
3ag
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

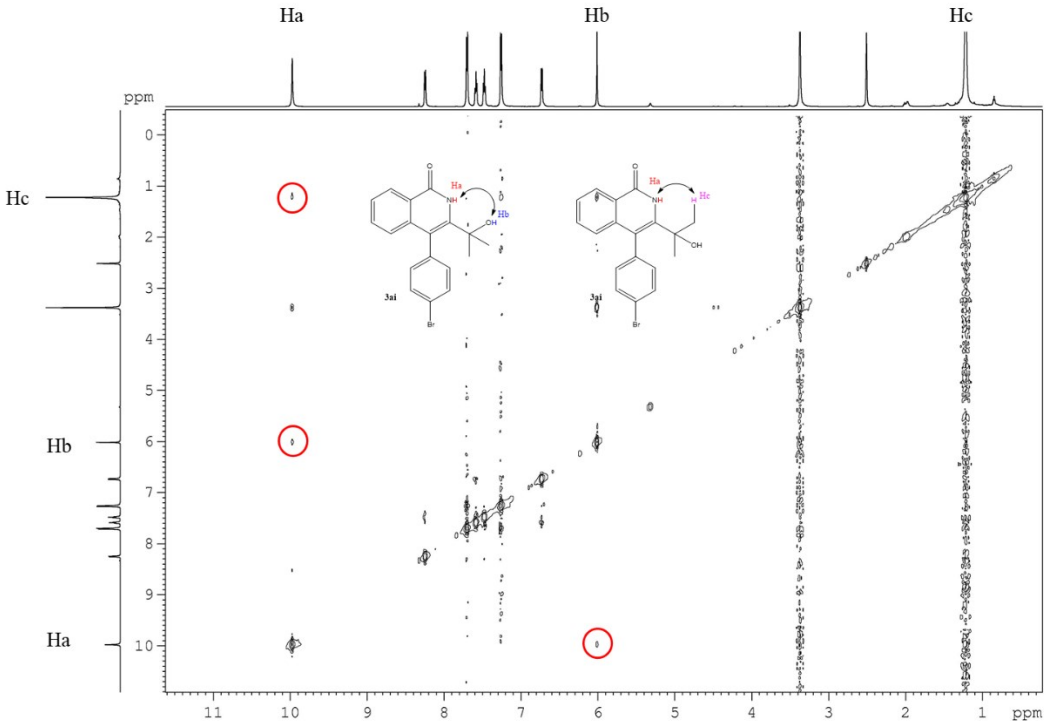

11.226
8.320
8.301
7.817
7.814
7.802
7.801
7.582
7.576
7.568
7.562
7.556
7.549
7.534
7.515
7.493
7.473
2.147
O
NH
3ah
12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.996
1.000
1.993
6.005
3.008

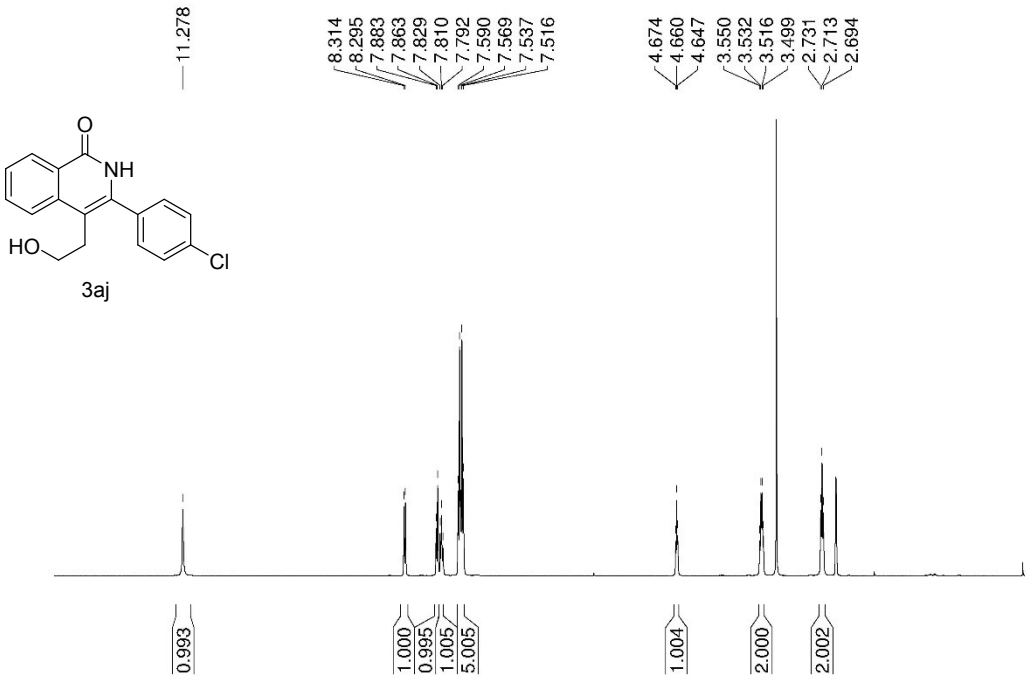

161.917
138.735
138.274
135.315
133.002
130.132
129.136
128.713
127.372
126.555
125.903
124.219
107.620
13.972
O
NH
3ah
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

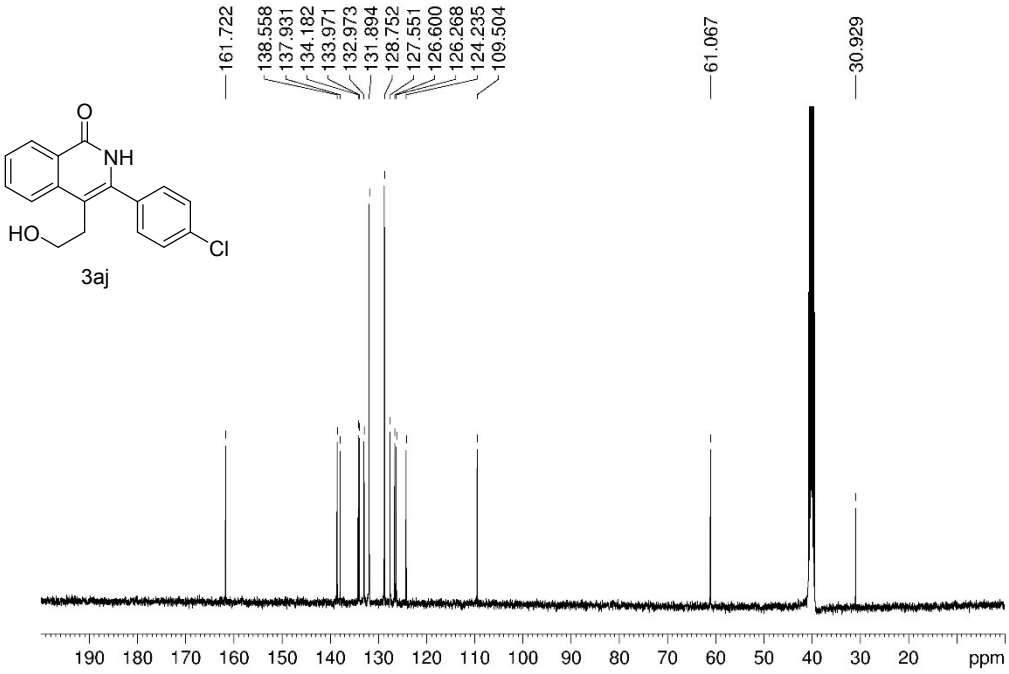

Hb
Ha
ppm
Ha
Hb
O
NH
Hb
Ha
3ah
1 2 3 4 5 6 7 8 9 10 11 12
12 11 10 9 8 7 6 5 4 3 2 ppm

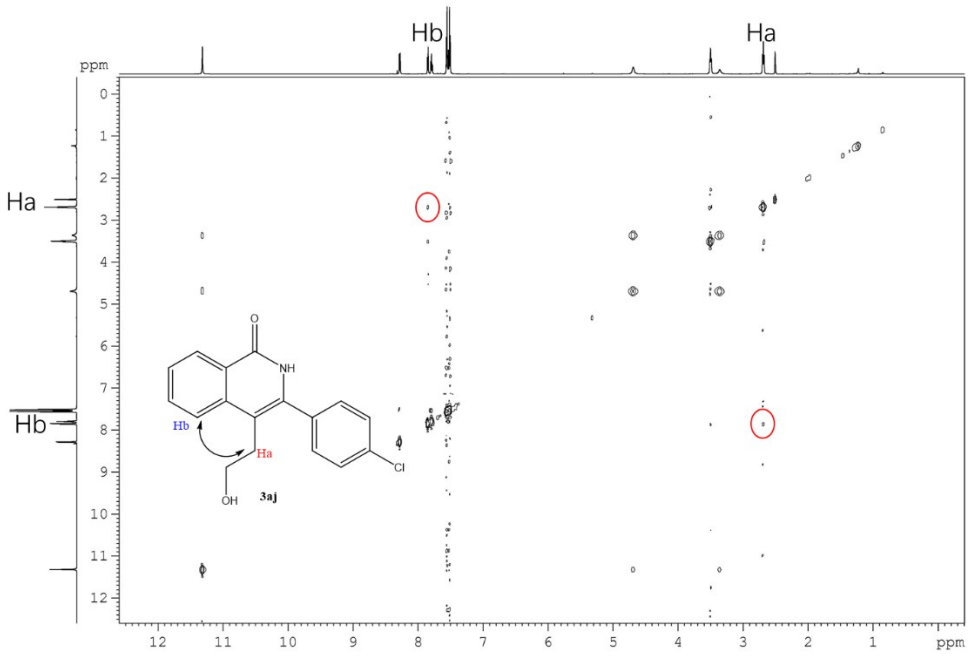

9.959
8.279
8.260
7.730
7.709
7.623
7.602
7.581
7.513
7.493
7.473
7.287
7.267
6.765
6.745
5.979
1.242
O
NH
OH
Br
3ai
11
10
9
8
7
6
5
4
3
2
1
ppm
0.997
1.000
2.008
1.009
1.008
1.999
0.995
1.000
6.004

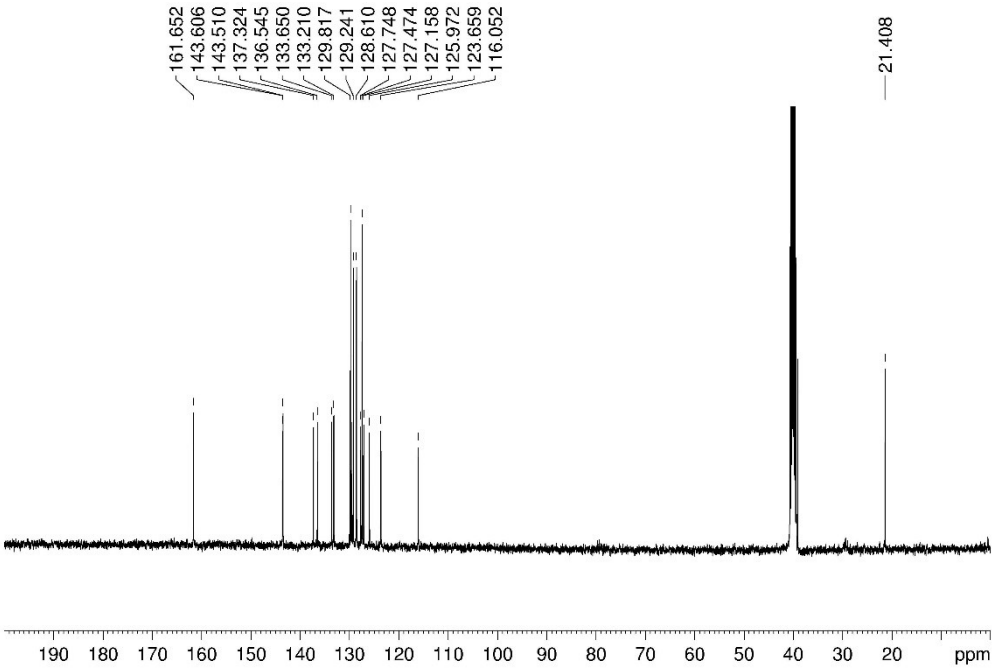

161.009
144.164
139.929
136.364
134.564
133.009
131.937
126.912
126.520
125.493
124.821
121.752
111.591
70.763
30.971
O
NH
OH
Br
3ai
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

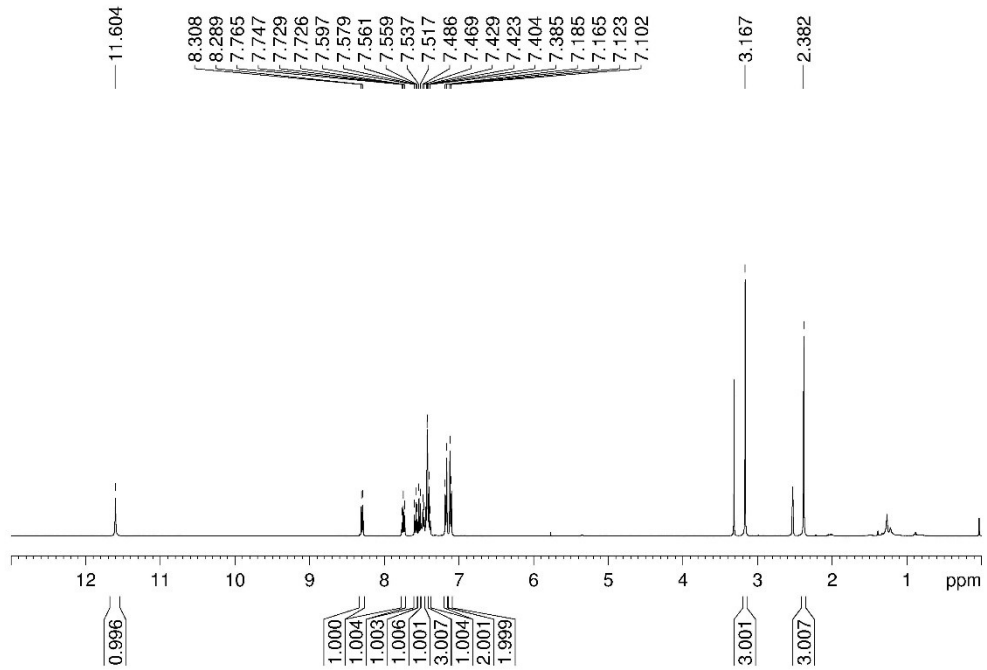

Ha
Hb
Hc
ppm
Hc
Hb
Ha
11
10
9
8
7
6
5
4
3
2
1
ppm

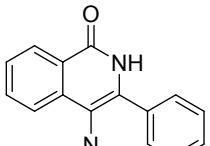

11.278
8.314
8.295
7.883
7.863
7.829
7.810
7.792
7.590
7.569
7.537
7.516
4.674
4.660
4.647
3.550
3.532
3.516
3.499
2.731
2.713
2.694
O
NH
HO
Cl
3aj
0.993
1.000
0.995
1.005
5.005
1.004
2.000
2.002

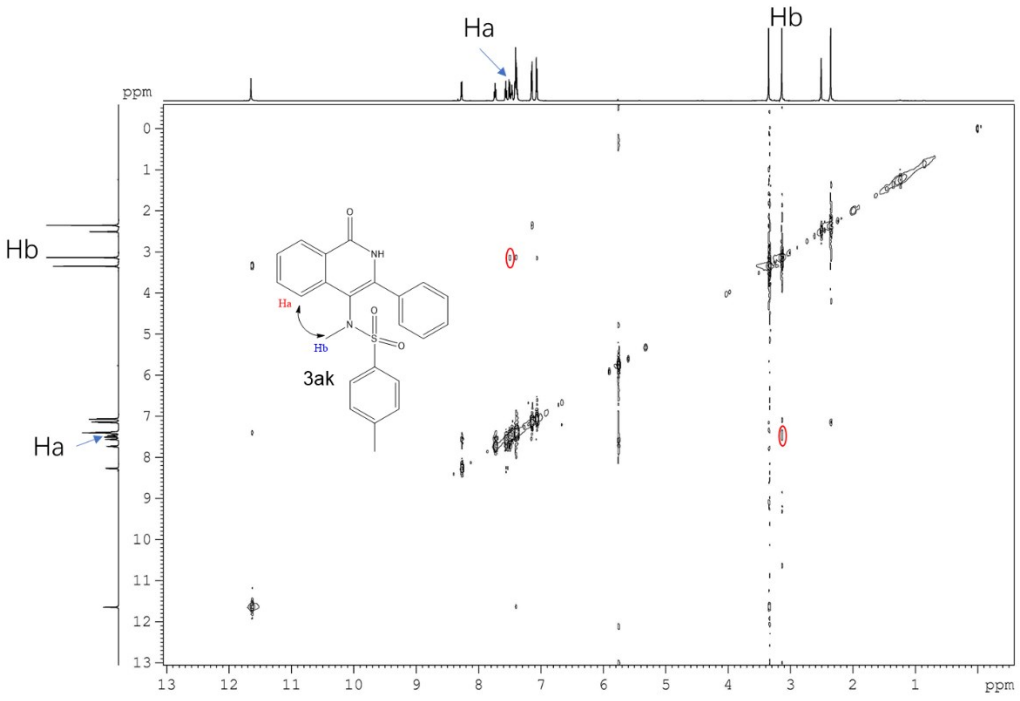

161.722
138.558
137.931
134.182
133.971
132.973
131.894
128.752
127.551
126.600
126.268
124.235
109.504
61.067
30.929
O
NH
HO
Cl
3aj
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

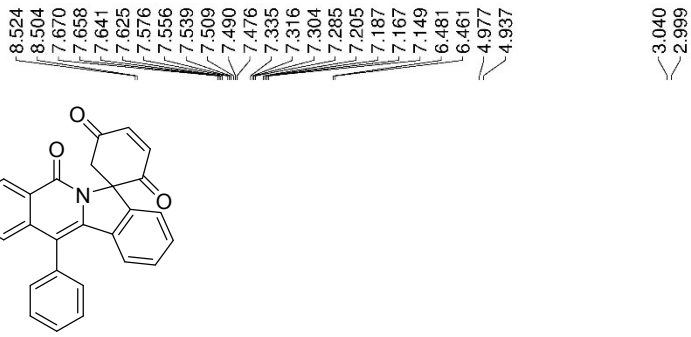

Hb
Ha
ppm
Ha
Hb
O
NH
Hb
Ha
Cl
OH
3aj
12 11 10 9 8 7 6 5 4 3 2 1 ppm


161.652
143.606
143.510
137.324
136.545
133.650
133.210
129.817
129.241
128.610
127.748
127.474
127.158
125.972
123.659
116.052
21.408
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

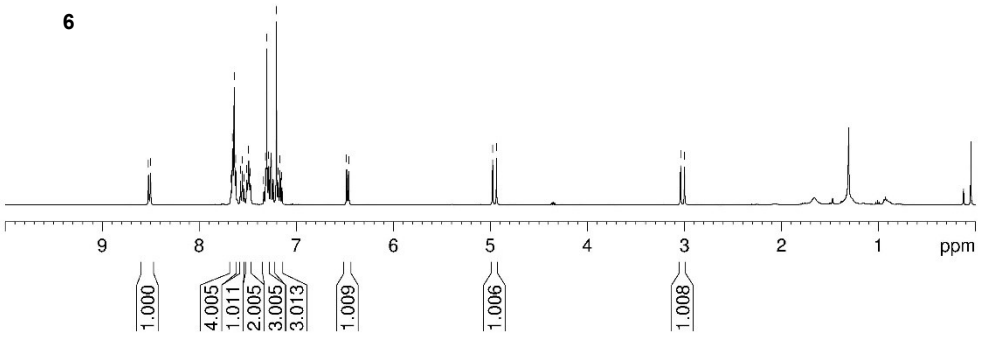

11.604
8.308
8.289
7.765
7.747
7.729
7.726
7.597
7.579
7.561
7.559
7.537
7.517
7.486
7.469
7.429
7.423
7.404
7.385
7.185
7.165
7.123
7.102
3.167
2.382
12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.996
1.000
1.004
1.003
1.006
1.001
3.007
1.004
2.001
1.999
3.001
3.007

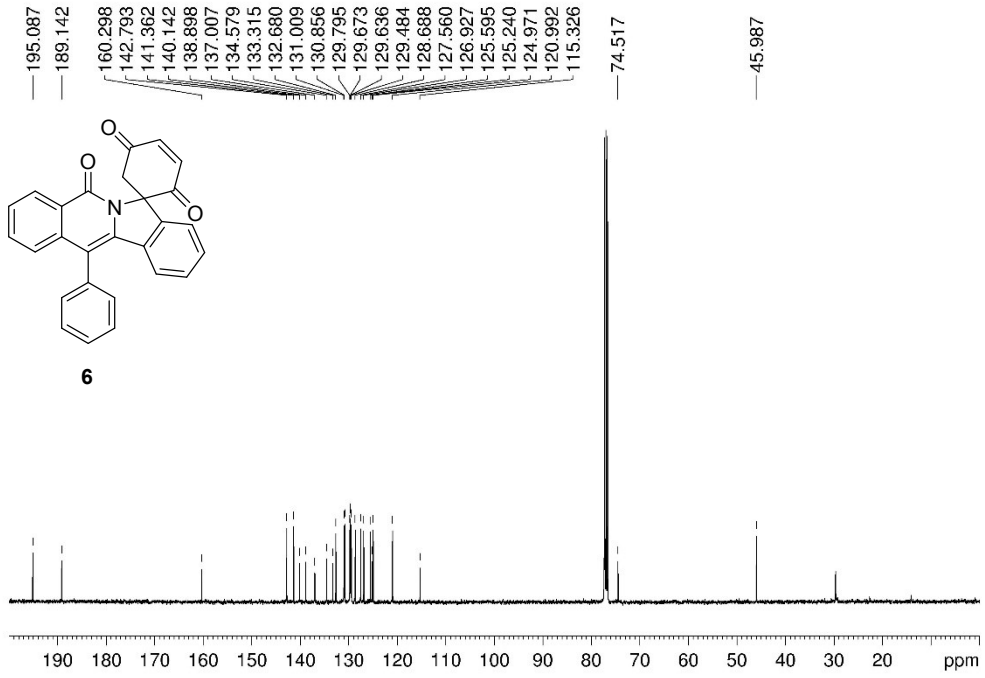

O
NH
N


Ha
Hb
ppm
Hb
Ha
3ak

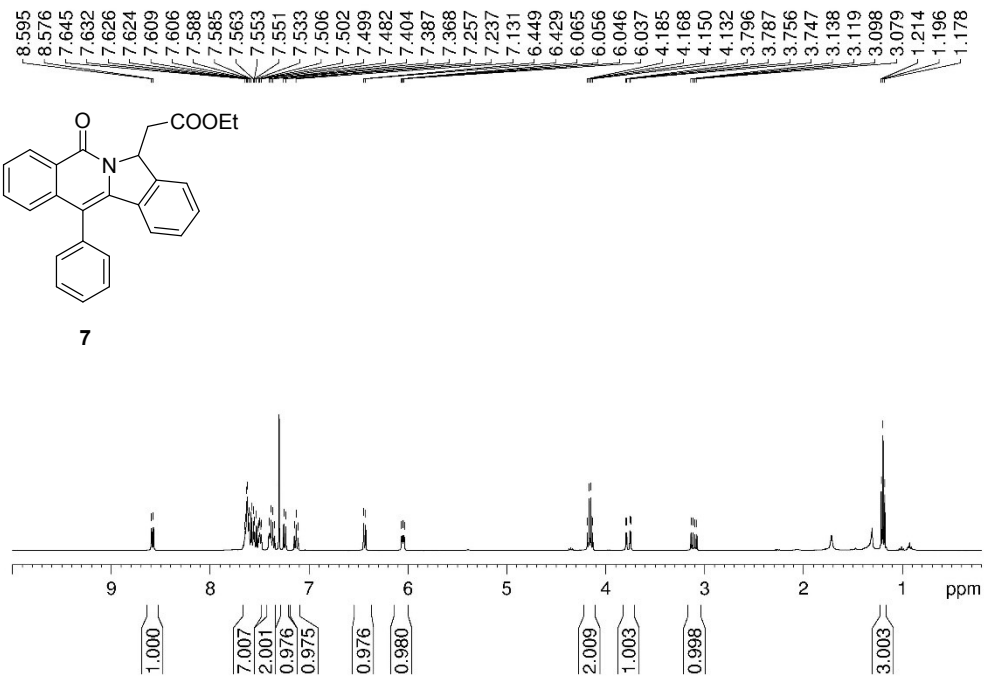

8.524
8.504
7.670
7.658
7.641
7.625
7.576
7.556
7.539
7.509
7.490
7.476
7.335
7.316
7.304
7.285
7.205
7.187
7.167
7.149
6.481
6.461
4.977
4.937
3.040
2.999

6

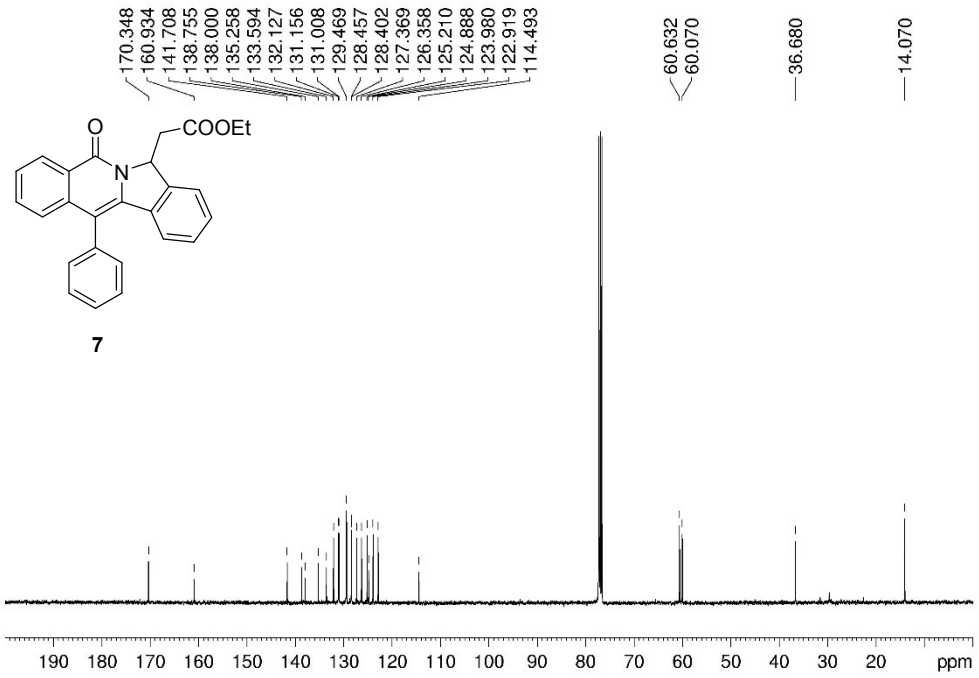

ppm
1.000
4.005
1.011
2.005
3.005
3.013
1.009
1.006
1.008


195.087
189.142
160.298
142.793
141.362
140.142
138.898
137.007
134.579
133.315
132.680
131.009
130.856
129.795
129.673
129.636
129.484
128.688
127.560
126.927
125.595
125.240
124.971
120.992
115.326
74.517
45.987
O
O
N
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

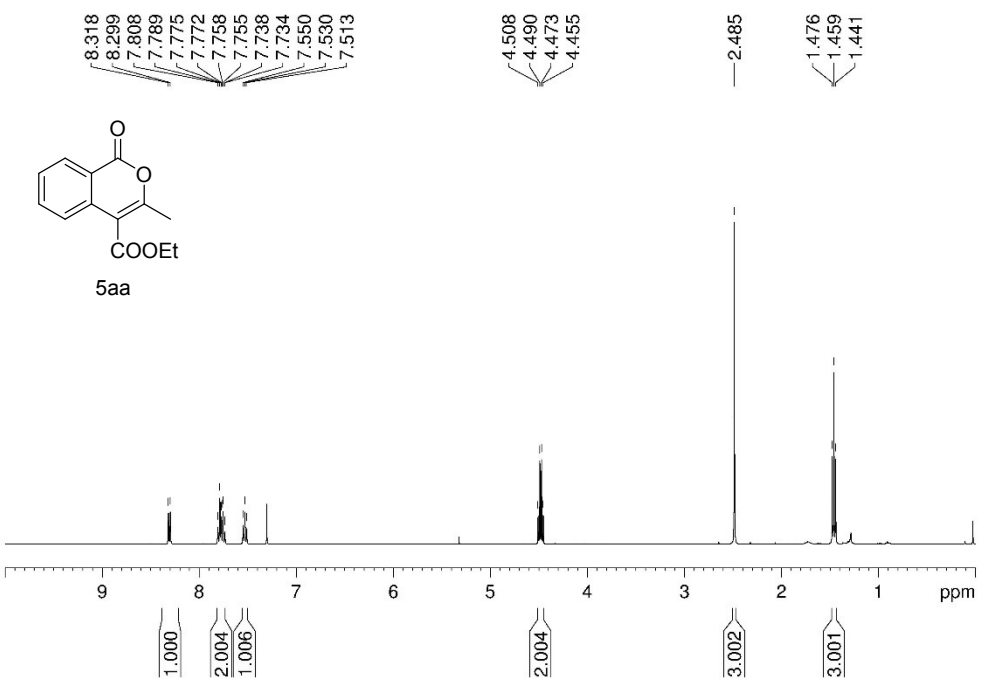
6


8.595
8.576
7.645
7.632
7.626
7.624
7.609
7.606
7.588
7.585
7.563
7.553
7.551
7.533
7.506
7.502
7.499
7.482
7.404
7.387
7.368
7.257
7.237
7.131
6.449
6.429
6.065
6.056
6.046
6.037
4.185
4.168
4.150
4.132
3.796
3.787
3.756
3.747
3.138
3.119
3.098
3.079
1.214
1.196
1.178
O
COOEt
N
9 8 7 6 5 4 3 2 1 ppm
1.000
7.007
2.001
0.976
0.975
0.976
0.980
2.009
1.003
0.998
3.003

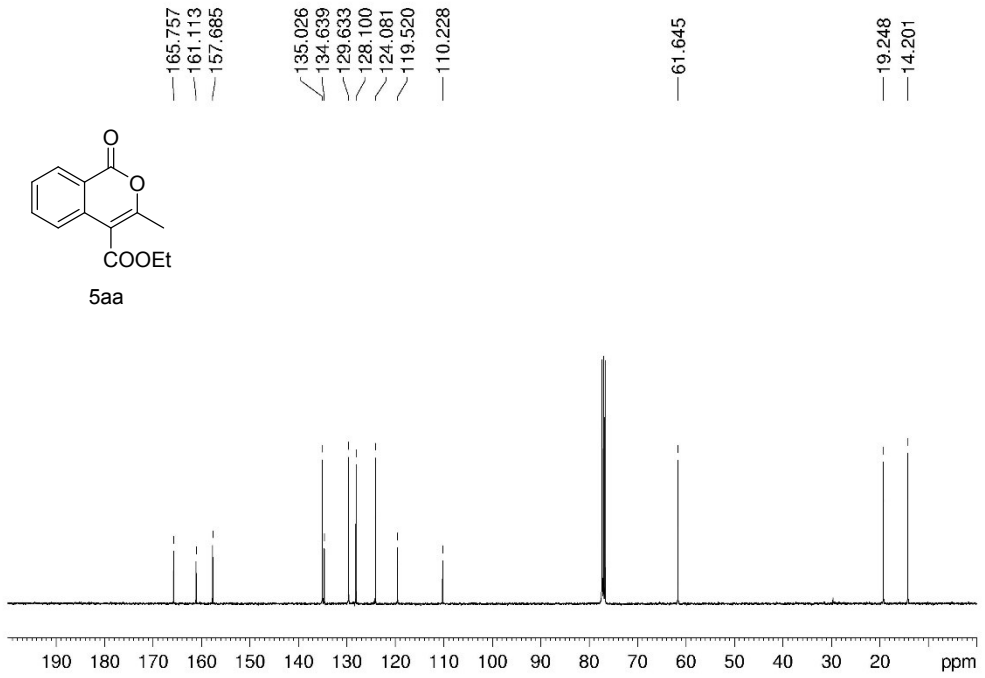
7


170.348
160.934
141.708
138.755
138.000
135.258
133.594
132.127
131.156
131.008
129.469
128.457
128.402
127.369
126.358
125.210
124.888
123.980
122.919
114.493
60.632
60.070
36.680
14.070
O
N
COOEt
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

7


8.318
8.299
7.808
7.789
7.775
7.772
7.758
7.755
7.738
7.734
7.550
7.530
7.513
4.508
4.490
4.473
4.455
2.485
1.476
1.459
1.441
O
O
COOEt
9 8 7 6 5 4 3 2 1 ppm
1.000
2.004
1.006
2.004
3.002
3.001

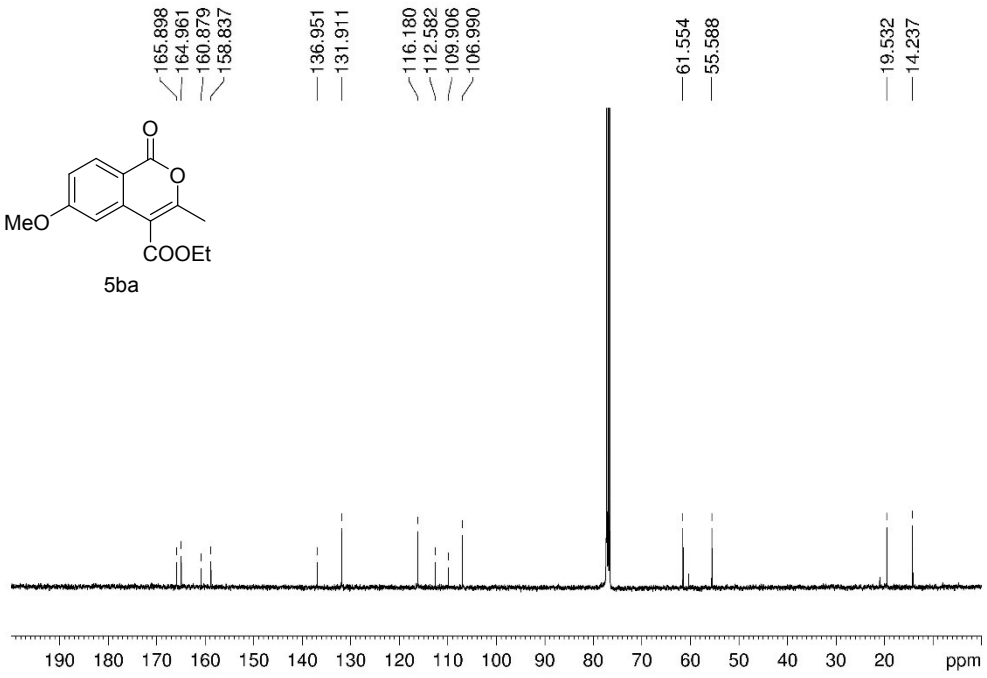
5aa

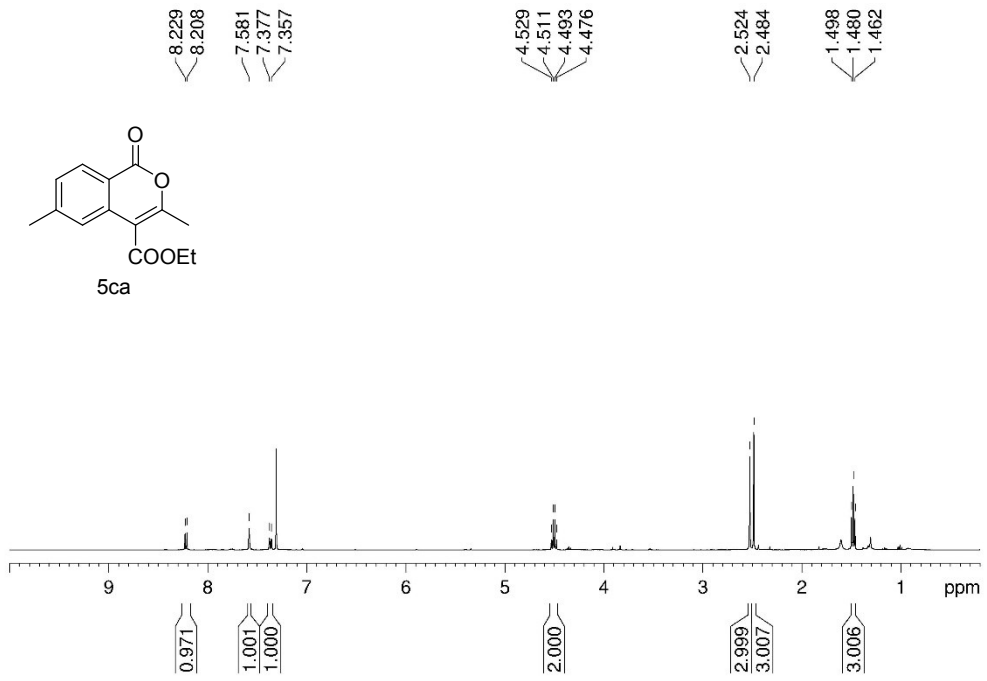

165.757
161.113
157.685
135.026
134.639
129.633
128.100
124.081
119.520
110.228
61.645
19.248
14.201
O
O
COOEt
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

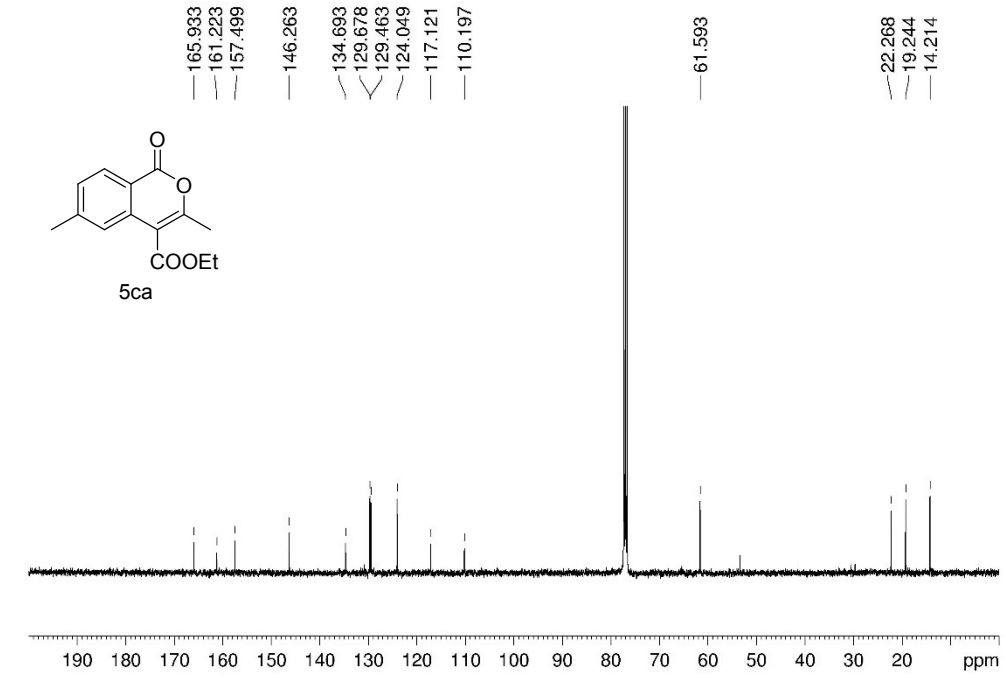
5aa

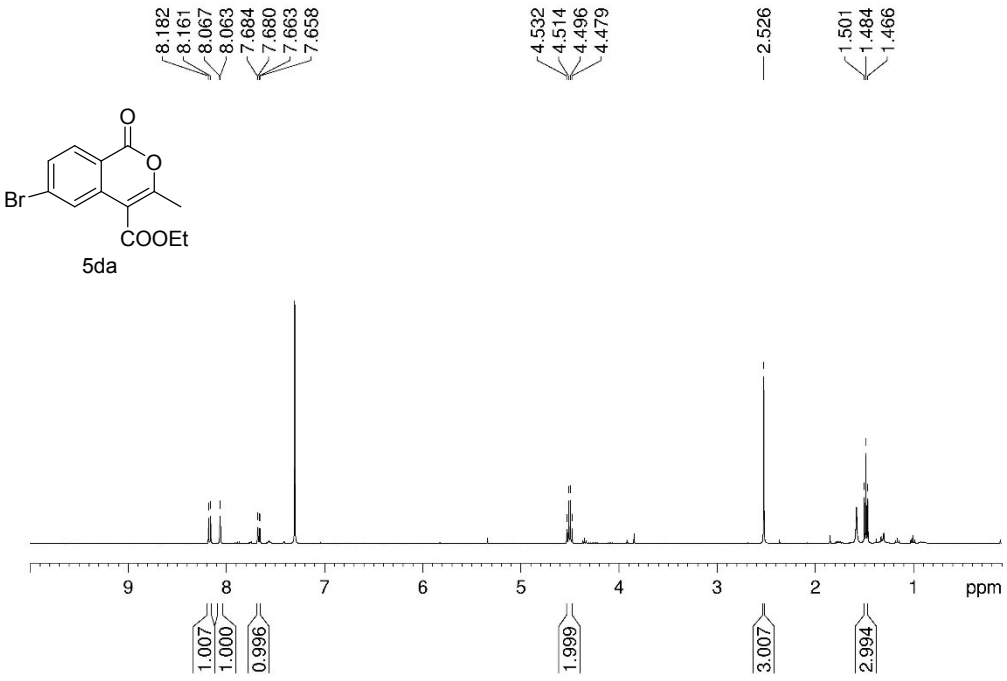

8.265
8.243
7.292
7.286
7.097
7.091
7.075
7.069
4.520
4.502
4.484
4.466
3.952
2.500
1.496
1.478
1.460
O
O
MeO
COOEt
9 8 7 6 5 4 3 2 1 ppm
1.000
0.999
1.003
2.006
3.004
3.009
3.012

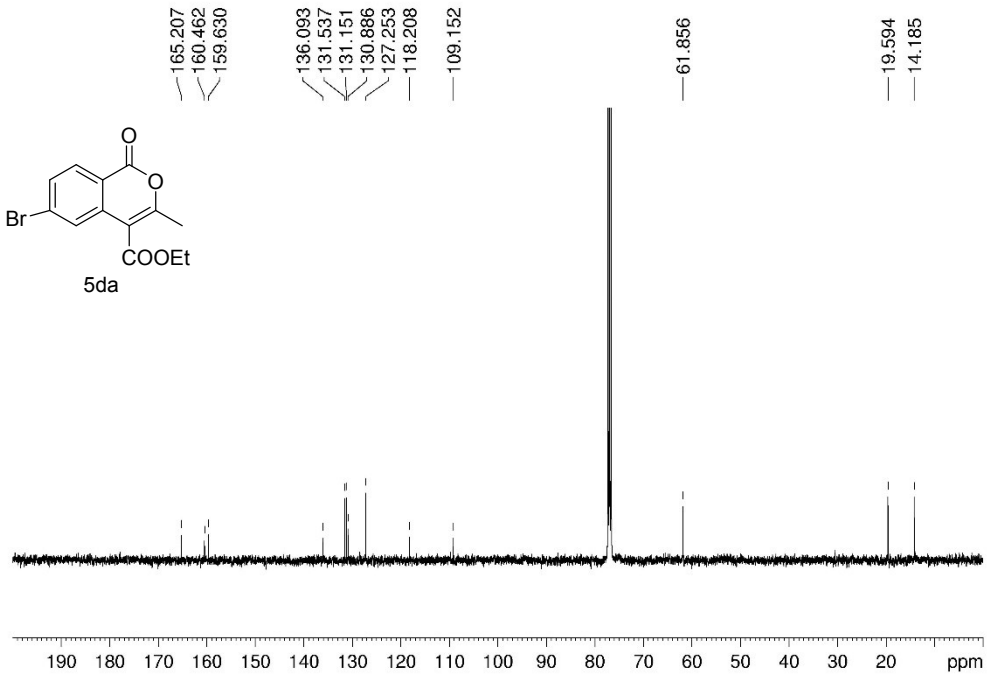
5ba

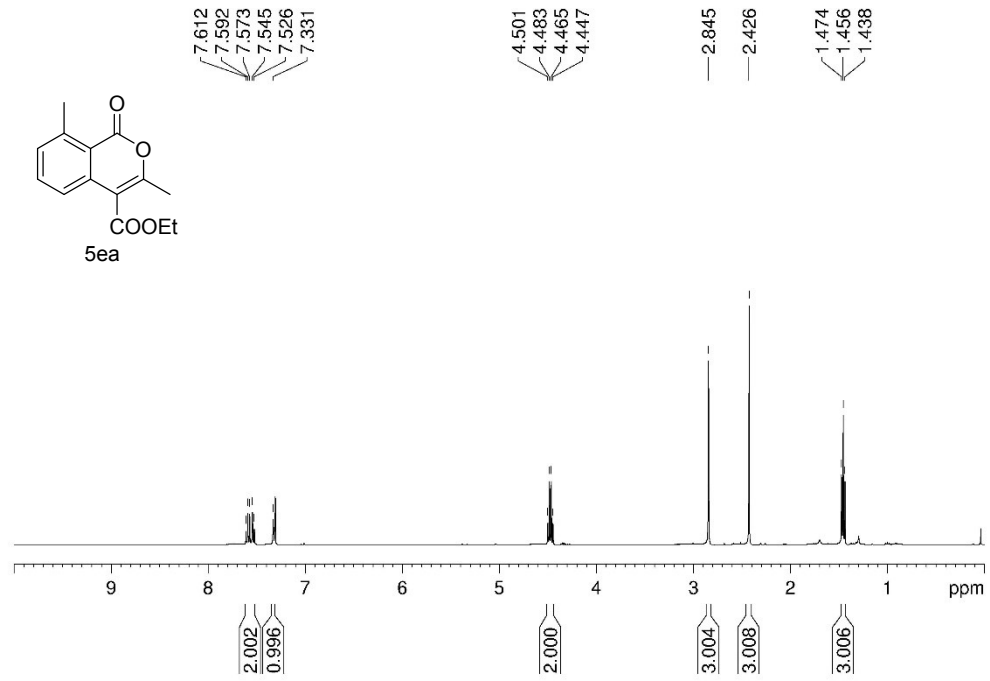

165.898
164.961
160.879
158.837
136.951
131.911
116.180
112.582
109.906
106.990
61.554
55.588
19.532
14.237
O
O
MeO
COOEt
5ba
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

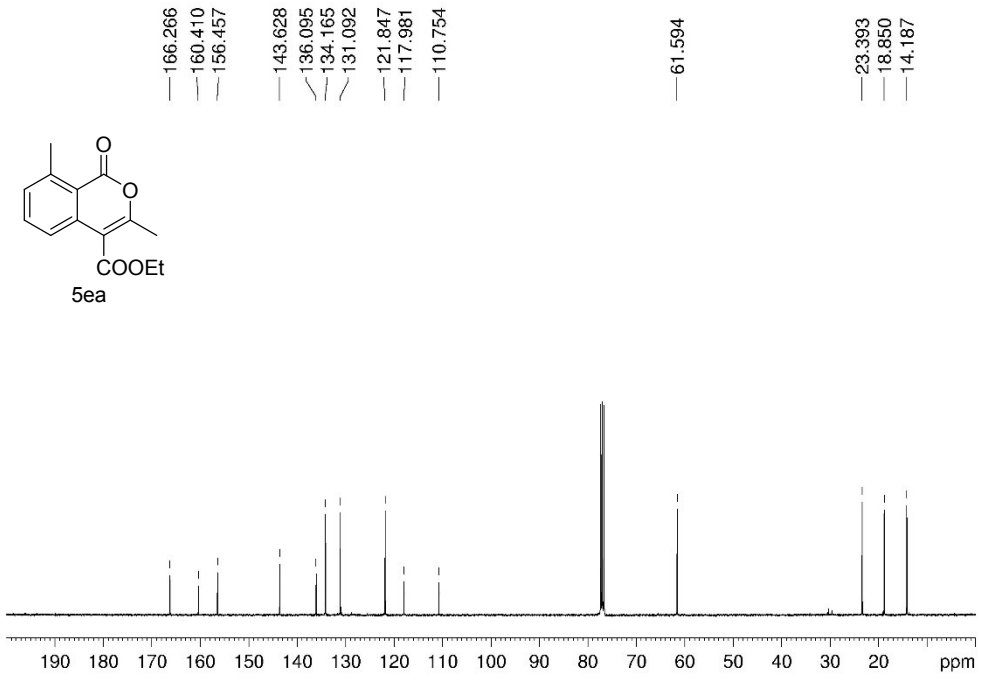

8.229
8.208
7.581
7.377
7.357
4.529
4.511
4.493
4.476
2.524
2.484
1.498
1.480
1.462
O
O
COOEt
5ca
9 8 7 6 5 4 3 2 1 ppm
0.971
1.001
1.000
2.000
2.999
3.007
3.006


165.933
161.223
157.499
146.263
134.693
129.678
129.463
124.049
117.121
110.197
61.593
22.268
19.244
14.214
O
O
COOEt
5ca
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

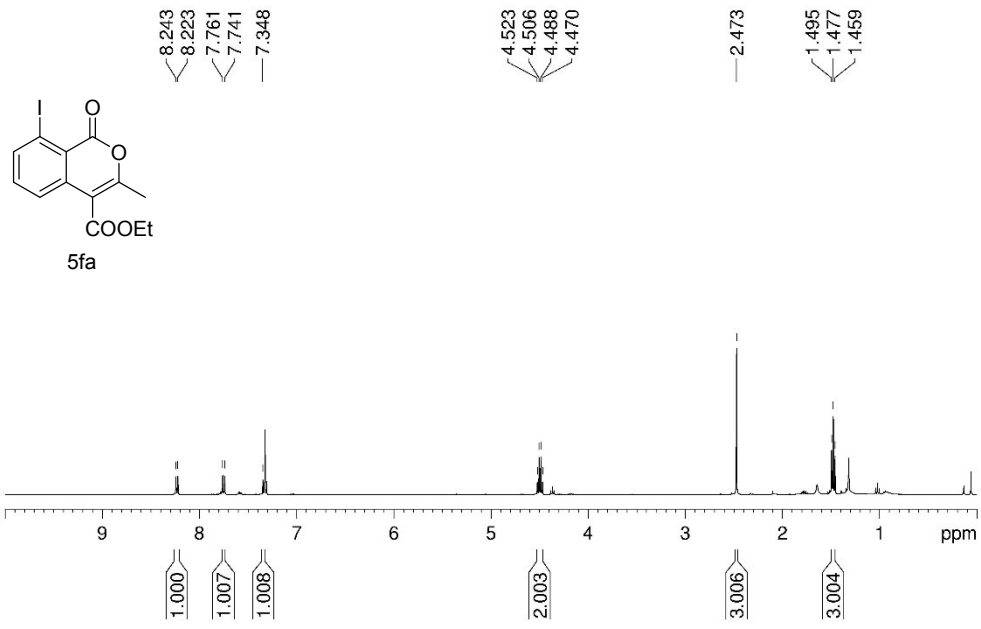

8.182
8.161
8.067
8.063
7.684
7.680
7.663
7.658
4.532
4.514
4.496
4.479
2.526
1.501
1.484
1.466
O
O
Br
COOEt
5da
9 8 7 6 5 4 3 2 1 ppm
1.007
1.000
0.996
1.999
3.007
2.994


165.207
160.462
159.630
136.093
131.537
131.151
130.886
127.253
118.208
109.152
61.856
19.594
14.185
O
O
Br
COOEt
5da
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

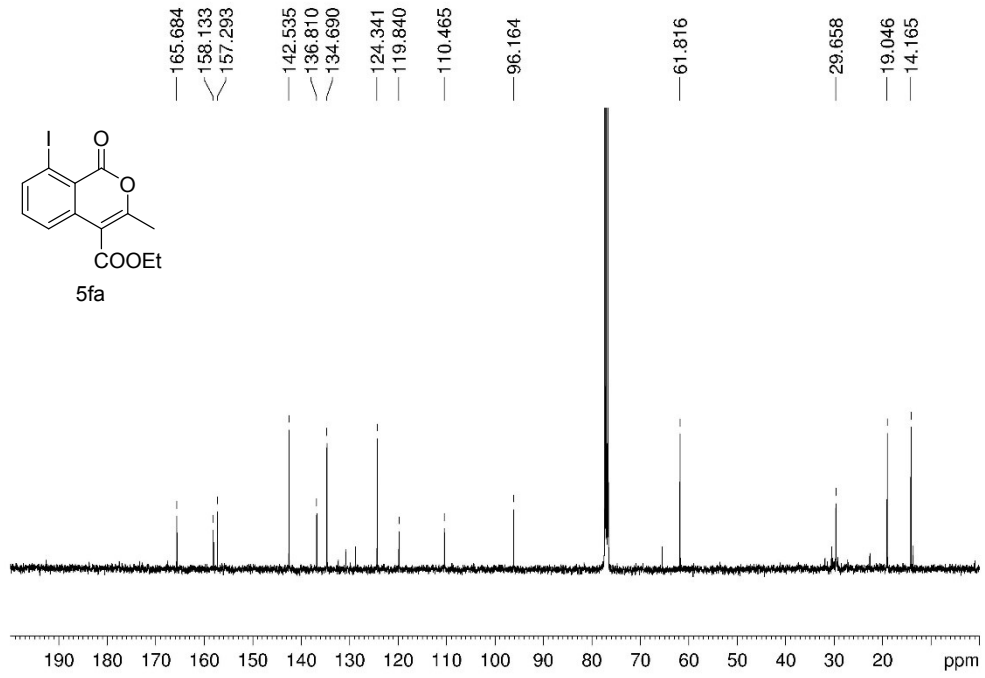

7.612
7.592
7.573
7.545
7.526
7.331
4.501
4.483
4.465
4.447
2.845
2.426
1.474
1.456
1.438
O
O
COOEt
5ea
9 8 7 6 5 4 3 2 1 ppm
2.002
0.996
2.000
3.004
3.008
3.006


166.266
160.410
156.457
143.628
136.095
134.165
131.092
121.847
117.981
110.754
61.594
23.393
18.850
14.187
O
O
COOEt
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

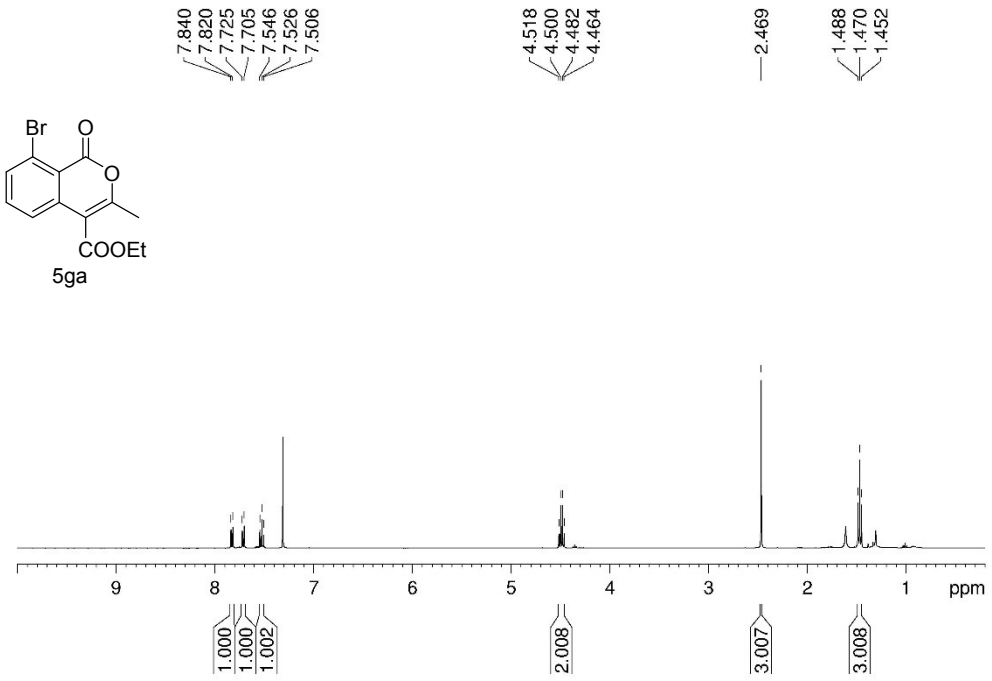
5ea


8.243
8.223
7.761
7.741
7.348
4.523
4.506
4.488
4.470
2.473
1.495
1.477
1.459
I
O
O
COOEt
9 8 7 6 5 4 3 2 1 ppm
1.000
1.007
1.008
2.003
3.006
3.004

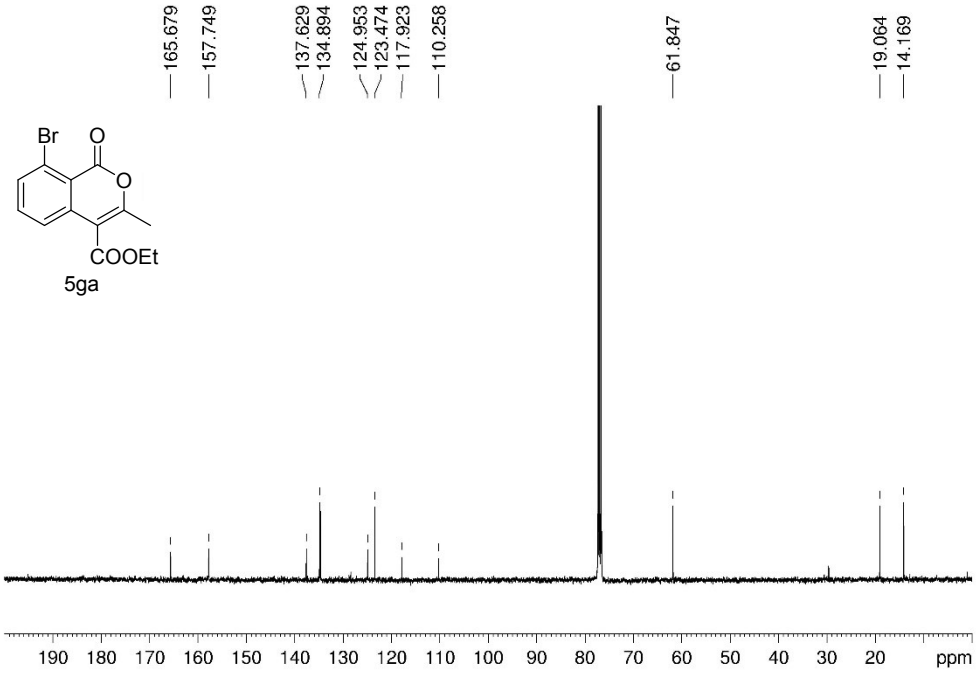
5fa

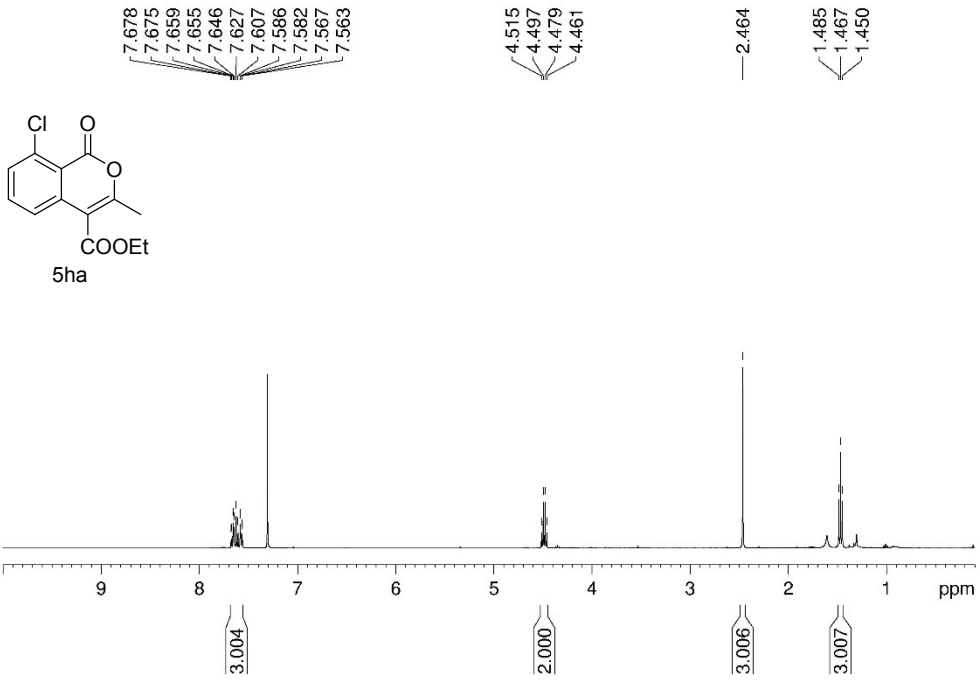

165.684
158.133
157.293
142.535
136.810
134.690
124.341
119.840
110.465
96.164
61.816
29.658
19.046
14.165
I
O
O
COOEt
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

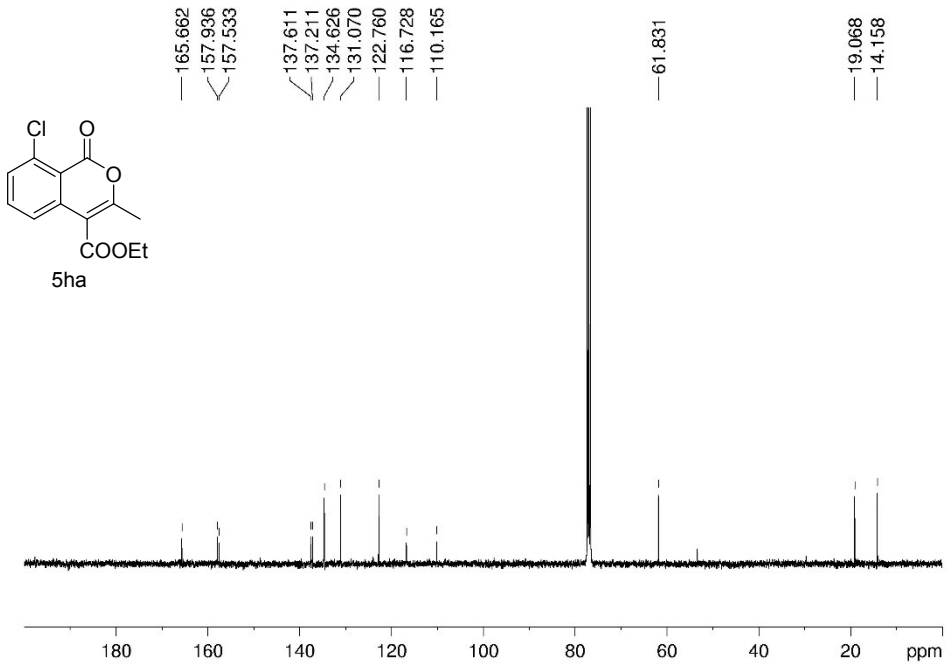
5fa


7.840
7.820
7.725
7.705
7.546
7.526
7.506
4.518
4.500
4.482
4.464
2.469
1.488
1.470
1.452
Br
O
O
COOEt
9 8 7 6 5 4 3 2 1 ppm
1.000
1.000
1.002
2.008
3.007
3.008

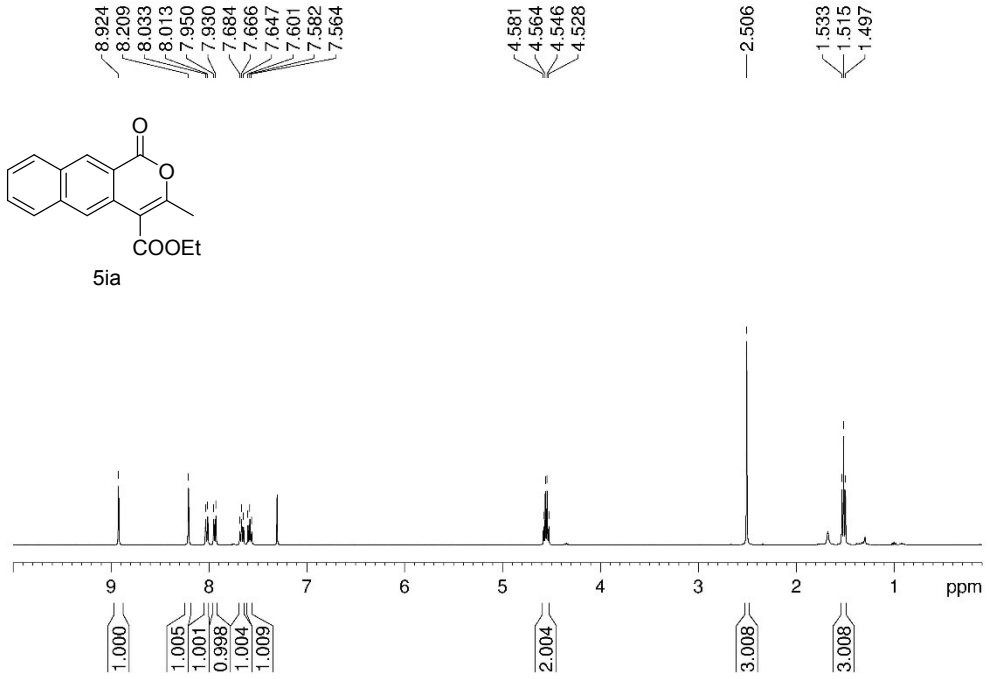
5ga


165.679
157.749
137.629
134.894
124.953
123.474
117.923
110.258
61.847
19.064
14.169
Br
O
O
COOEt
5ga
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

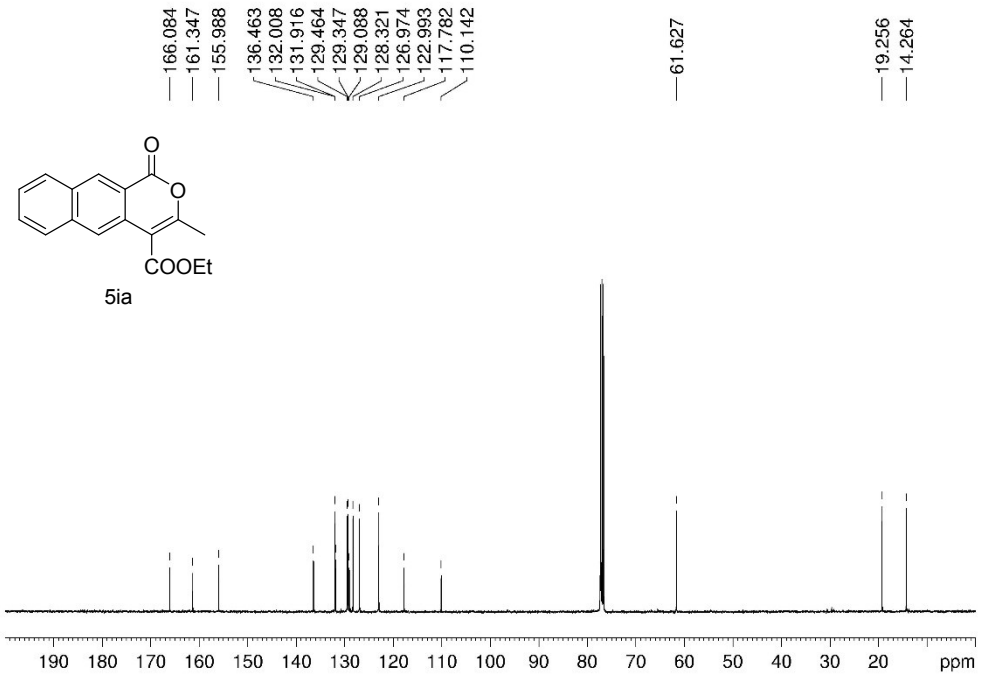

7.678
7.675
7.659
7.655
7.646
7.627
7.607
7.586
7.582
7.567
7.563
4.515
4.497
4.479
4.461
2.464
1.485
1.467
1.450
Cl
O
O
COOEt
5ha
9 8 7 6 5 4 3 2 1 ppm
3.004
2.000
3.006
3.007


165.662
157.936
157.533
137.611
137.211
134.626
131.070
122.760
116.728
110.165
61.831
19.068
14.158
Cl
O
O
COOEt
180
160
140
120
100
80
60
40
20
ppm

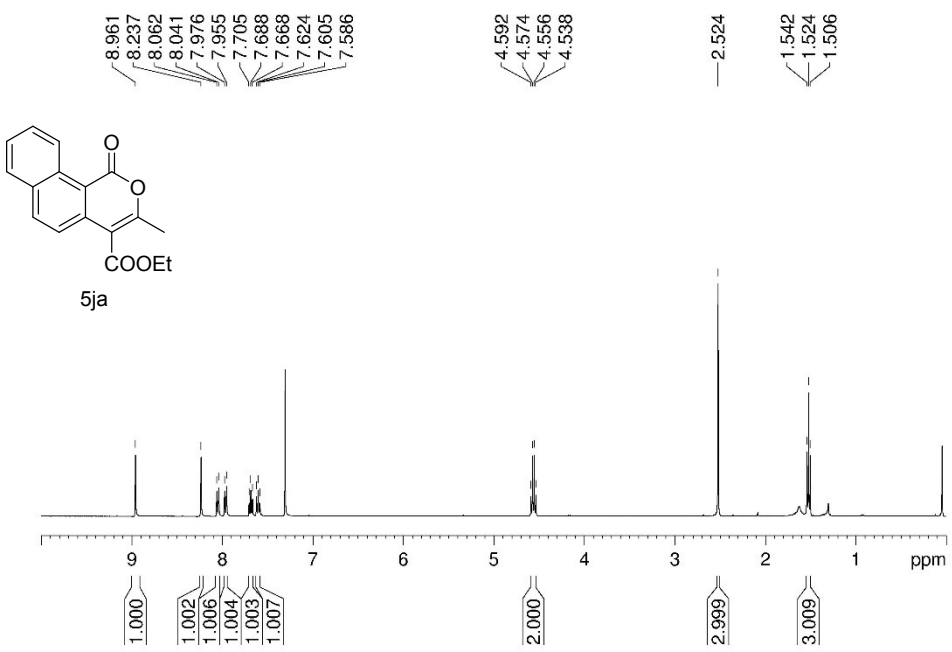
5ha


8.924
8.209
8.033
8.013
7.950
7.930
7.684
7.666
7.647
7.601
7.582
7.564
4.581
4.564
4.546
4.528
2.506
1.533
1.515
1.497
O
O
COOEt
9
8
7
6
5
4
3
2
1
ppm
1.000
1.005
1.001
0.998
1.004
1.009
2.004
3.008
3.008

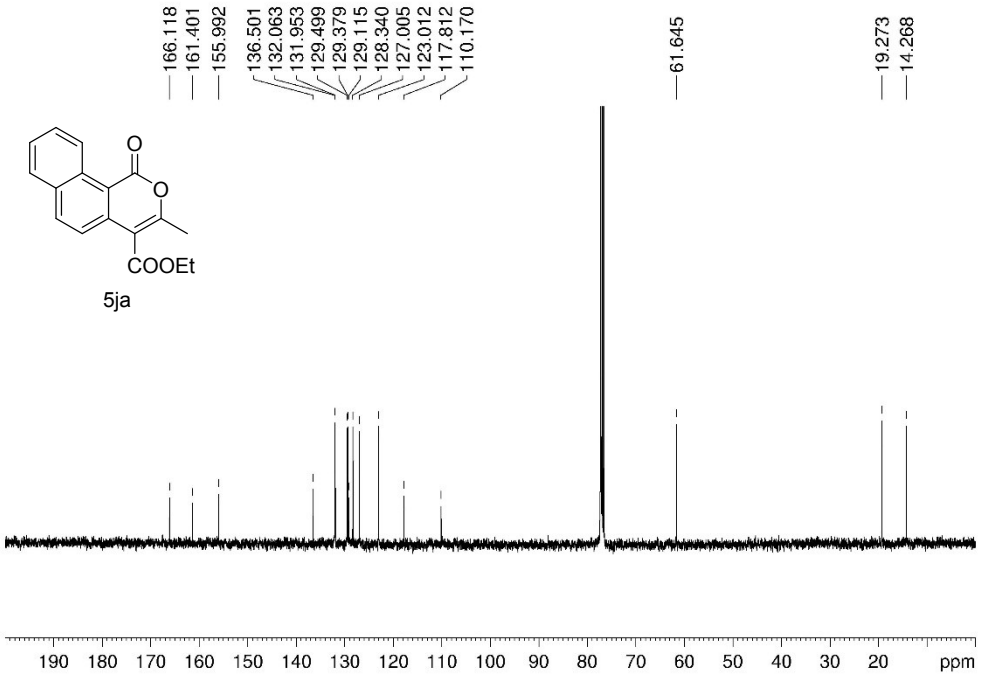
5ia


166.084
161.347
155.988
136.463
132.008
131.916
129.464
129.347
129.088
128.321
126.974
122.993
117.782
110.142
61.627
19.256
14.264
O
O
COOEt
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

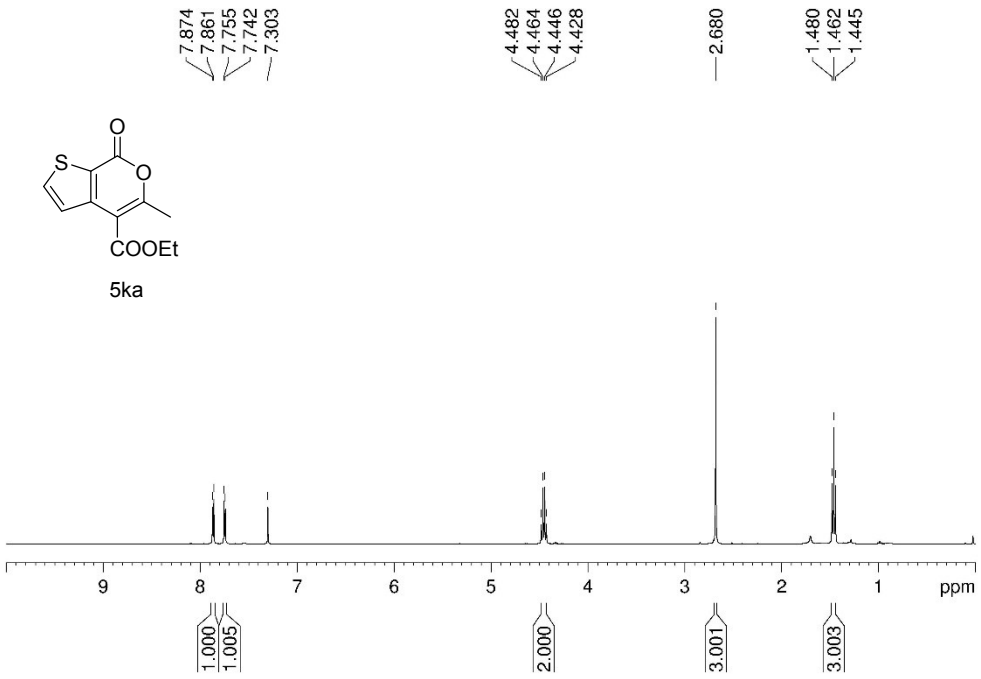
5ia


8.961
8.237
8.062
8.041
7.976
7.955
7.705
7.688
7.668
7.624
7.605
7.586
4.592
4.574
4.556
4.538
2.524
1.542
1.524
1.506
O
O
COOEt
9 8 7 6 5 4 3 2 1 ppm
1.000
1.002
1.006
1.004
1.003
1.007
2.000
2.999
3.009

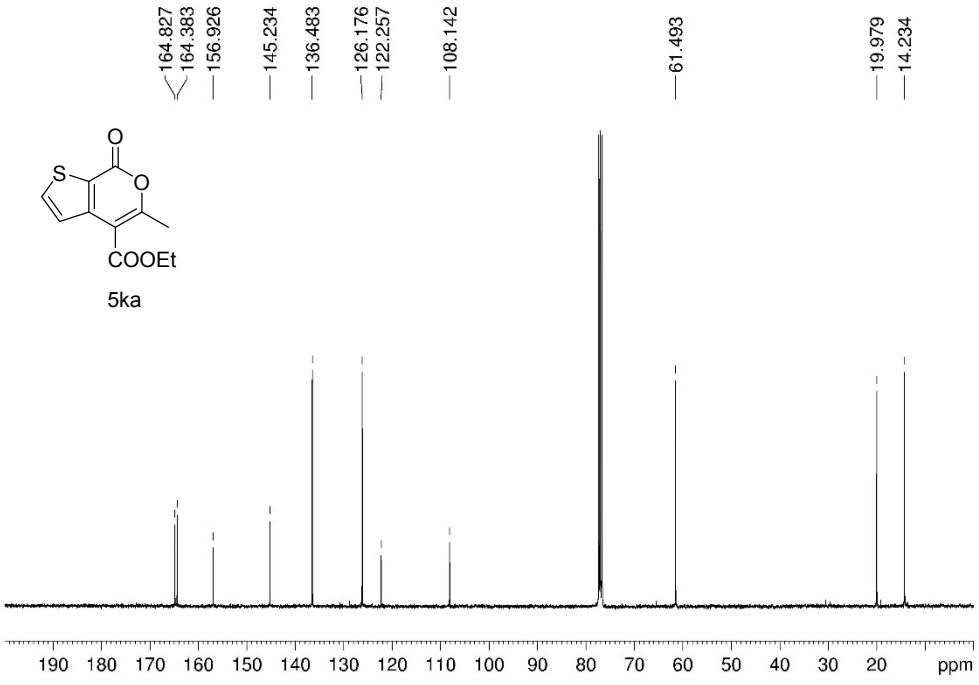
5ja

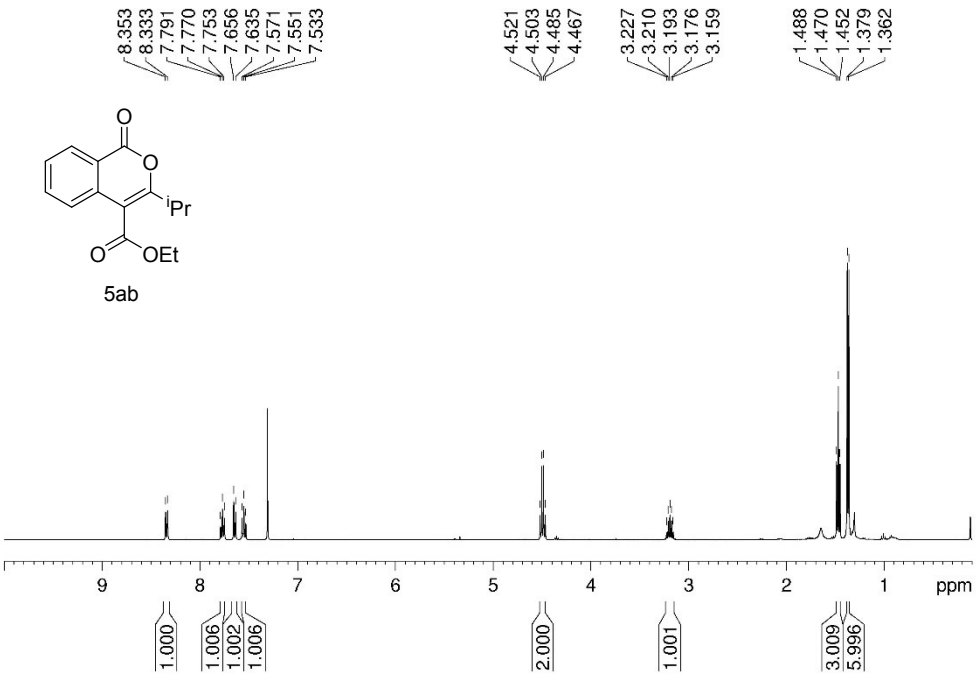

166.118
161.401
155.992
136.501
132.063
131.953
129.499
129.379
129.115
128.340
127.005
123.012
117.812
110.170
61.645
19.273
14.268
O
O
COOEt
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

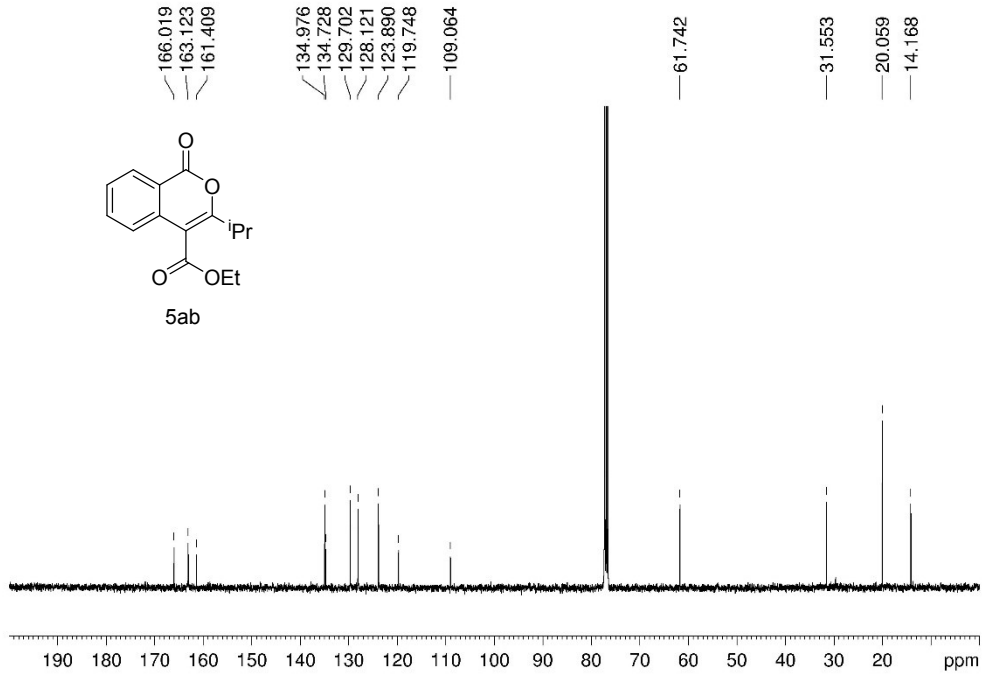
5ja

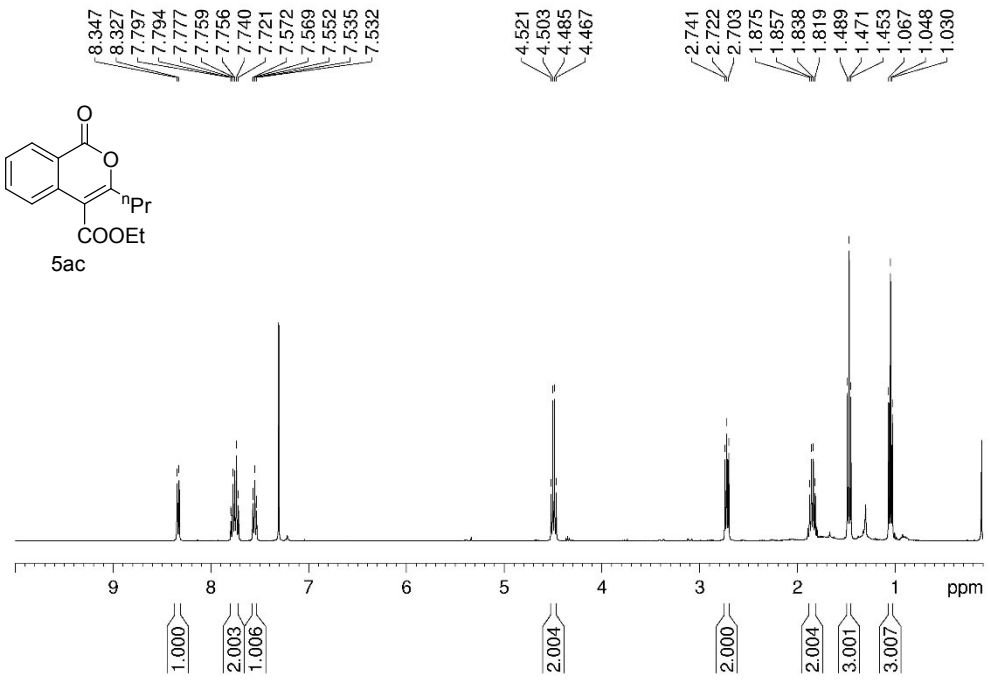

7.874
7.861
7.755
7.742
7.303
4.482
4.464
4.446
4.428
2.680
1.480
1.462
1.445
O
S
O
COOEt
9 8 7 6 5 4 3 2 1 ppm
1.000
1.005
2.000
3.001
3.003

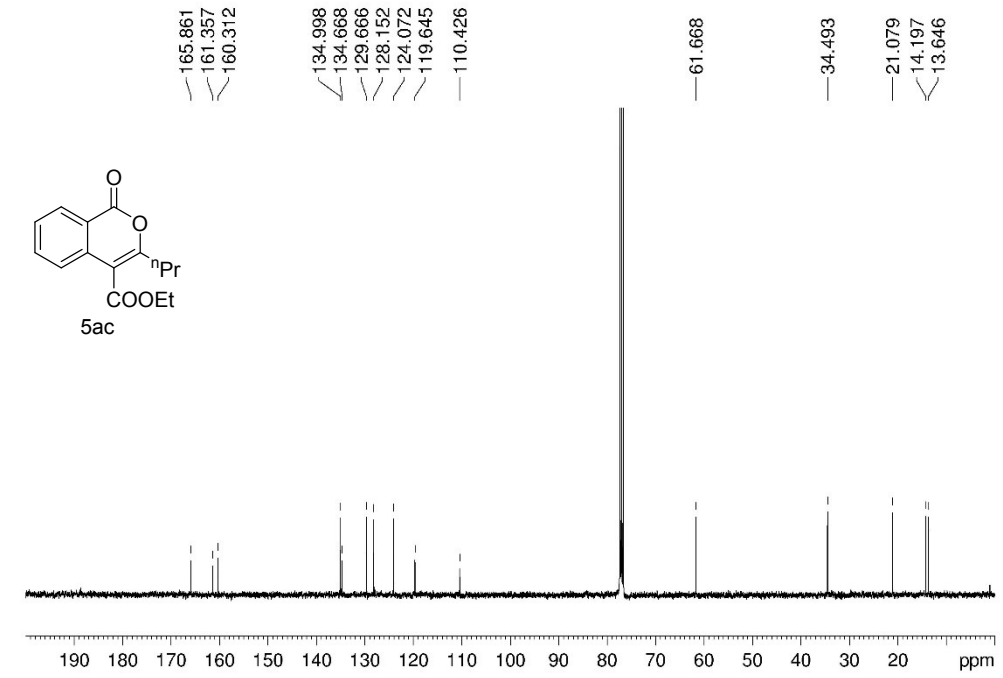
5ka

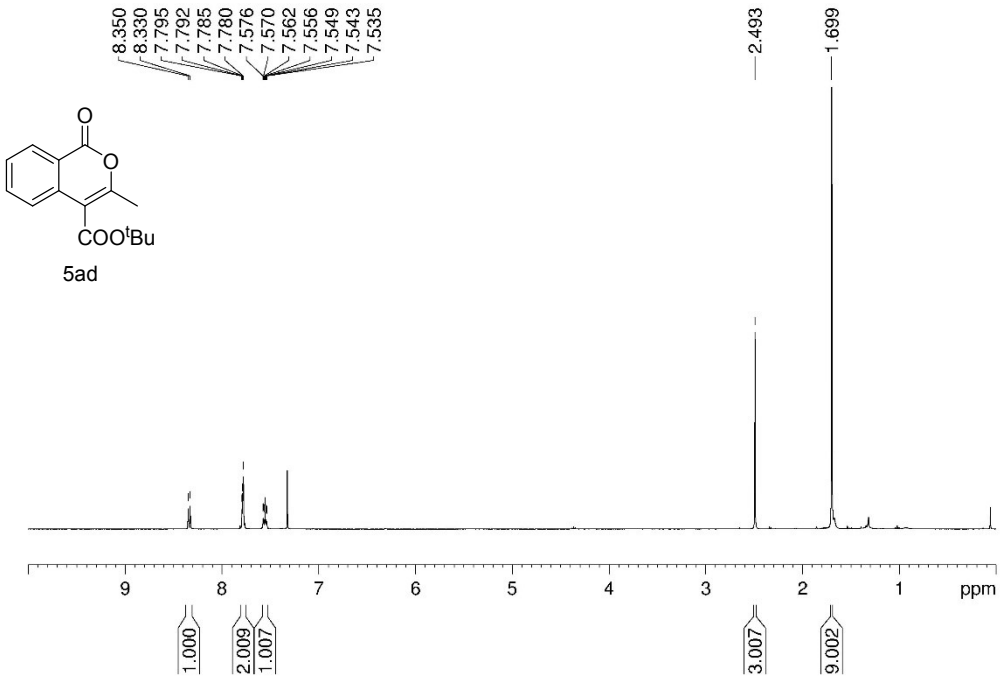

164.827
164.383
156.926
145.234
136.483
126.176
122.257
108.142
61.493
19.979
14.234
O
S
O
COOEt
5ka
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

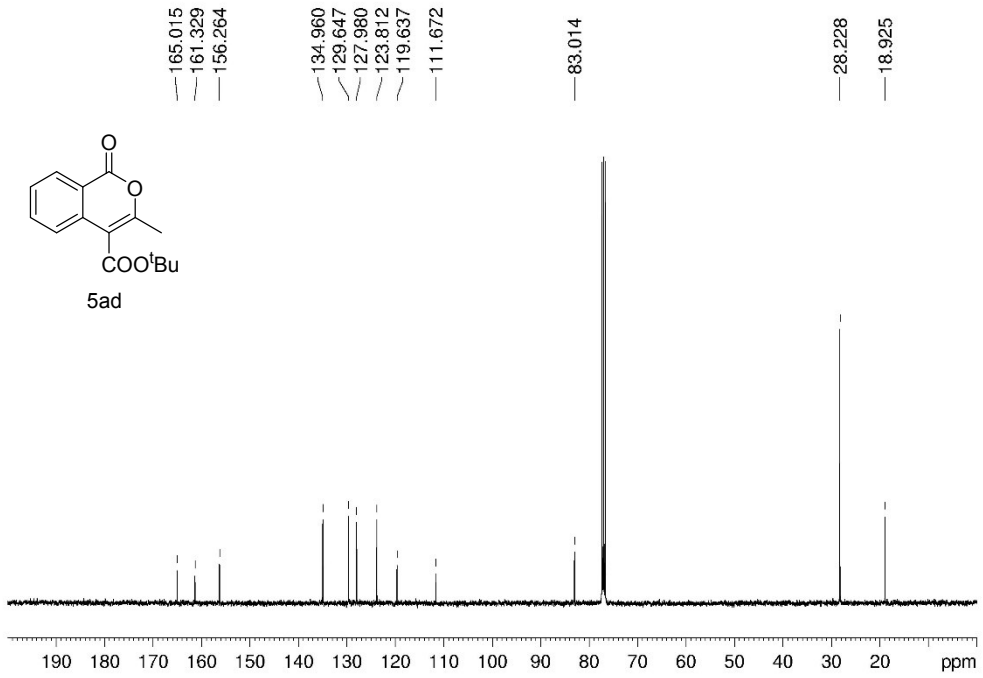

8.353
8.333
7.791
7.770
7.753
7.656
7.635
7.571
7.551
7.533
4.521
4.503
4.485
4.467
3.227
3.210
3.193
3.176
3.159
1.488
1.470
1.452
1.379
1.362
O
O
iPr
O
OEt
5ab
9 8 7 6 5 4 3 2 1 ppm
1.000
1.006
1.002
1.006
2.000
1.001
3.009
5.996

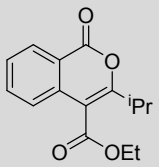

166.019
163.123
161.409
134.976
134.728
129.702
128.121
123.890
119.748
109.064
61.742
31.553
20.059
14.168
O
O
iPr
O
OEt
5ab
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


8.347
8.327
7.797
7.794
7.777
7.759
7.756
7.740
7.721
7.572
7.569
7.552
7.535
7.532
4.521
4.503
4.485
4.467
2.741
2.722
2.703
1.875
1.857
1.838
1.819
1.489
1.471
1.453
1.067
1.048
1.030
O
O
nPr
COOEt
5ac
9 8 7 6 5 4 3 2 1 ppm
1.000
2.003
1.006
2.004
2.000
2.004
3.001
3.007


165.861
161.357
160.312
134.998
134.668
129.666
128.152
124.072
119.645
110.426
61.668
34.493
21.079
14.197
13.646
O
O
nPr
COOEt
5ac
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


8.350
8.330
7.795
7.792
7.785
7.780
7.576
7.570
7.562
7.556
7.549
7.543
7.535
2.493
1.699
O
O
COOtBu
5ad
9 8 7 6 5 4 3 2 1 ppm
1.000
2.009
1.007
3.007
9.002


165.015
161.329
156.264
134.960
129.647
127.980
123.812
119.637
111.672
83.014
28.228
18.925
O
O
COO^{t}Bu
5ad
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm



5ab