Electronic Supplementary Information

Gold-catalyzed oxidation of terminal alkynes to glyoxals and their reactions with 2-phenylimidazo[1,2-*a*]pyridines: one-pot synthesis of 1,2-diones

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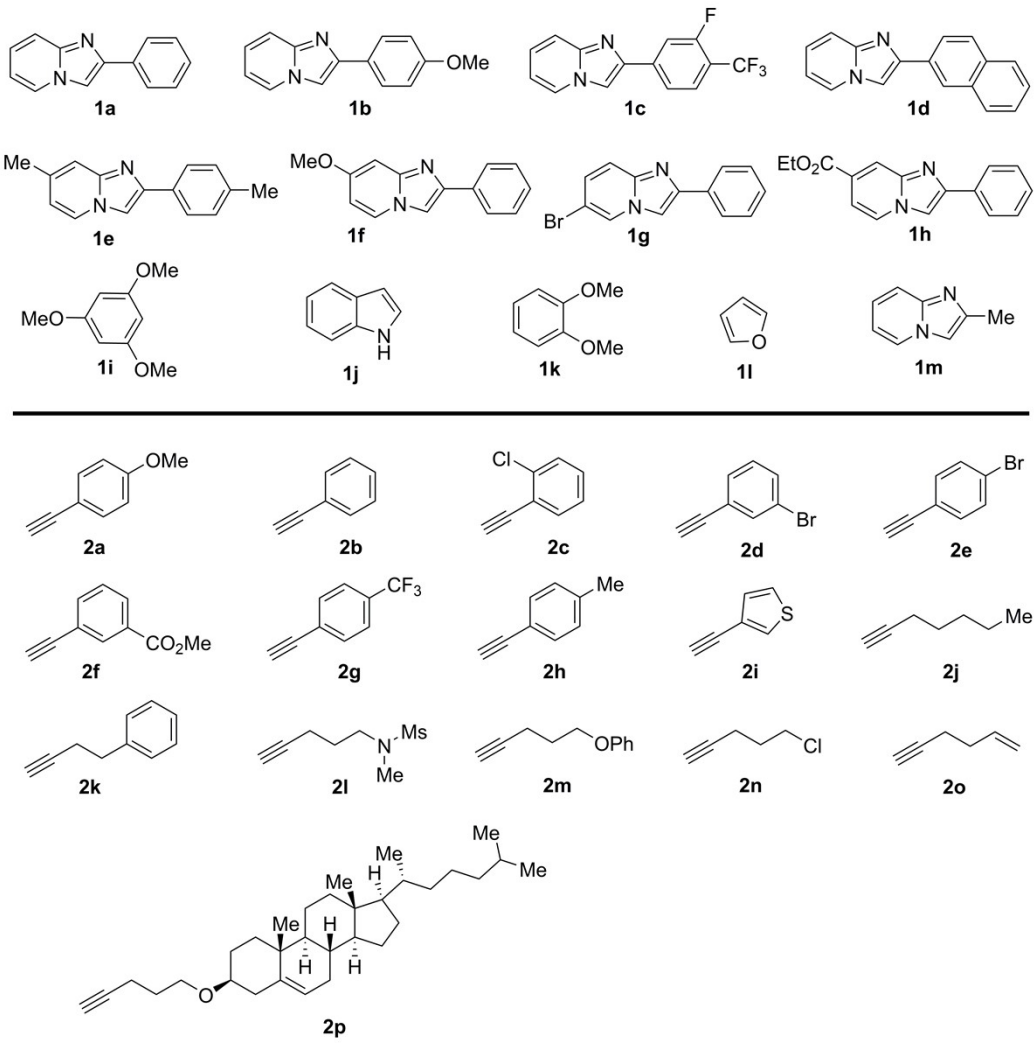
1. General Experimental Remarks

Chemicals obtained from commercial suppliers were used without further purification. Solvents were dried under CaH_2 and distilled. Analytical thin layer chromatography was performed on HSGF254 plates. Visualization was accomplished with UV light (254 nm) or $KMnO_4$ staining. Melting points (m.p.) were determined without correction. Flash column chromatography was performed using silica gel (200-300 mesh). Mass spectrometry data were collected with a Bruker maXis/Q-TOF instrument for high-resolution or a Bruker amaZon SL instrument for low-resolution with both by ESI ionization. The NMR spectra were recorded on Bruker AC 500 or 700 NMR spectrometer with TMS as an internal standard. The residual solvent peaks were used for the chemical shifts as an internal references (ppm): ^1H ($CDCl_3$: δ 7.26, MeOD: δ 3.34, $(CD_3)_2CO$: δ 2.05); ^{13}C ($CDCl_3$: δ 77.0, MeOD: δ 49.0, $(CD_3)_2CO$: δ 30). The substrates **1a**, **1i-m**, **2a-k**, **2n-o** are commercial available and **1b**[1], **1d**[1], **1e**[2], **1f**[l], **1g**[3], **2m**[4] are known and synthesized by following the previous procedure (Table S1).

Table S1. Substrates used in this study

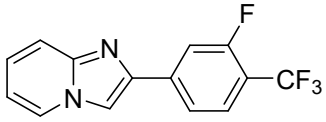


2. Synthesis of the compounds

2.1 General procedure for the synthesis of 2-phenylimidazo[1,2-a]pyridines

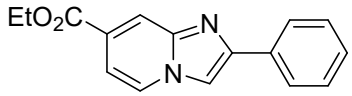
To a 50 mL flask, 2-aminopyridines (2.0 mmol, 1.0 equiv.), 2-bromoacetophenones (2.4 mmol, 1.2 equiv.) and $NaHCO_3$ (4 mmol, 2.0 equiv.) were added, and the mixture was dissolved in ethanol (10 mL) and stirred at room temperature for 24 h. After the reaction was completed, the solvent was removed, and the residue was dissolved in AcOEt (40 mL), washed with H_2O (3 × 10 mL), and dried over Na_2SO_4. The organic layer was filtered and removed under the reduced pressure. The residue was purified with silico gel column chromatograph (PE/EA = 6:1 to 2:1 as eluent) to afford the products.

2-(3-fluoro-4-(trifluoromethyl)phenyl)imidazo[1,2-a]pyridine (1c)



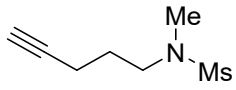
Following the general procedure, 2-aminopyridine (188 mg) and 2-bromo-1-(4-fluoro-3-(trifluoromethyl)phenyl)ethan-1-one (475 mg) were used, and the product **1c** was obtained as a gray solid (465 mg). Yield 83%, M.P. 142-144 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 (d, *J* = 6.5 Hz, 1H), 8.14 (d, *J* = 6.4 Hz, 2H), 7.87 (s, 1H), 7.66 (d, *J* = 9.1 Hz, 1H), 7.25 (dd, *J* = 20.3, 8.3 Hz, 2H), 6.84 (t, *J* = 6.6 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.38 (d, *J* = 257.3 Hz), 145.65, 143.24, 131.25 (d, *J* = 8.5 Hz), 130.15 (d, *J* = 3.7 Hz), 125.73, 125.52, 124.71 (d, *J* = 3.8 Hz), 123.66, 121.50, 118.73 (dd, *J* = 33.0, 12.8 Hz), 117.50, 117.29 (d, *J* = 21.0 Hz), 113.02, 108.29. HRMS (ESI): calcd for $C_{14}H_9F_4N_2$ $[M + H]^+$ 281.0696, found: 281.0704.

ethyl 2-phenylimidazo[1,2-a]pyridine-7-carboxylate (1h)



Following the general procedure, ethyl 2-aminoisonicotinate (322 mg) and 2-bromoacetophenone (682 mg) were used, and the product **1h** was obtained as a slight yellow solid (356 mg). Yield 67%, M.P.116-118 ˚C. ^{1}H NMR (700 MHz, $CDCl_3$) δ 8.39 (s, 1H), 8.14 (d, *J* = 7.0 Hz, 1H), 7.97 (d, *J* = 7.8 Hz, 2H), 7.96 (s, 1H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.40 (d, *J* = 7.0 Hz, 1H), 7.36 (t, *J* = 7.4 Hz, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 1.42 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 165.13, 148.06, 144.55, 133.08, 128.83, 128.49, 126.44, 126.16, 124.97, 119.99, 111.86, 109.56, 61.51, 14.23. HRMS (ESI): calcd for $C_{16}H_{15}N_2O_2$ $[M + H]^+$ 267.1128, found: 267.1132.

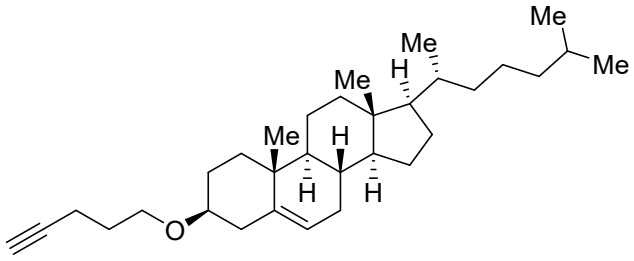
2.2 Synthesis of N-methyl-N-(pent-4-yn-1-yl)methanesulfonamide (**2l**)



To a 50 mL flask, 5-chloropent-1-yne (2.0 mmol, 200 mg, 1.0 equiv.), N-methylmethanesulfonamide (2.4 mmol, 260 mg, 1.2 equiv.), Cs_2CO_3 (3 mmol, 980 mg, 1.5 equiv.) and KI (0.2 mmol, 33 mg, 0.1 equiv.) were added, and the reaction mixture was dissolved in DMF (6 mL) and stirred at room temperature for about 12 h. After the reaction was completed, the solvent was removed, and the residue was dissolved in AcOEt (50 mL), washed with H_2O (3 × 15 mL), and dried over Na_2SO_4. The organic layer was filtered and removed under the reduced pressure. The residue was purified with silico gel column chromatograph (PE/EA = 10:1 to 2:1 as eluent) to afford the product **2l** as colorless oil (280 mg). Yield 80%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.23 (t, *J* = 7.0 Hz, 2H), 2.86 (s, 3H), 2.80 (s, 3H), 2.27 (td, *J* = 7.0, 2.5 Hz, 2H), 1.98 (t, *J* = 2.6 Hz, 1H), 1.82 (p, *J* = 7.0 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 83.02, 69.15, 48.97, 35.40, 34.88, 26.94, 15.59. HRMS (ESI): calcd for $C_7H_{14}NO_2S$ $[M + H]^+$ 176.0740, found: 176.0740.

2.3 Synthesis of (3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-((R)-6-

methylheptan-2-yl)-3-(pent-4-yn-1-yloxy)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthrene (**2p**)

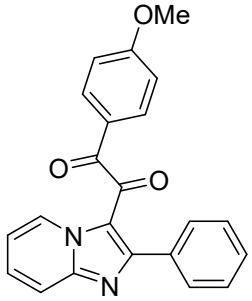


To a 50 mL flame-dried Schlenk tube backfilled with N_2, NaH (4 mmol, 160 mg, 2 equiv., 56-60% in mineral oil) and anhydrous DMF (12 mL) were added. The reaction mixture was cooled down and stirred at 0 °C, and then cholesterol (2 mmol, 770 mg, 1 equiv.) was added in portions. After 10 min, 5-chloropent-1-yne (4 mmol, 410 mg, 2.0 equiv.), KI (0.4 mmol, 66 mg, 0.2 equiv.) were added, and the mixture was stirred at this temperature for about 20 min. The reaction was then heated at 60 °C overnight. After completion, the reaction was quenched with ice-water, and the solvent was removed. The residue was dissolved in AcOEt (60 mL), washed with H_2O (3 × 15 mL), and dried over Na_2SO_4. The organic layer was filtered and removed under the reduced pressure. The residue was purified with silico gel column chromatograph (PE as eluent) to afford the product **2p** as colorless solid (300 mg). Yield 33%, M.P. 69-72 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.35 (s, 1H), 3.55 (t, *J* = 6.0 Hz, 2H), 3.14 (dt, *J* = 15.5, 5.5 Hz, 1H), 2.36 (dd, *J* = 13.1, 2.3 Hz, 1H), 2.29 (td, *J* = 7.0, 2.4 Hz, 2H), 2.18 (t, *J* = 11.3 Hz, 1H), 2.01 (t, *J* = 13.0 Hz, 2H), 1.97 – 1.91 (m, 1H), 1.91 – 1.81 (m, 3H), 1.80 – 1.73 (m, 2H), 1.56 – 1.39 (m, 6H), 1.40 – 1.28 (m, 3H), 1.29 (s, 2H), 1.18 – 1.05 (m, 6H), 1.04 – 0.97 (m, 6H), 0.91 (d, *J* = 6.5 Hz, 4H), 0.86 (dd, *J* = 6.5, 1.8 Hz, 6H), 0.67 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.03, 121.50, 84.10, 79.11, 68.33, 66.21, 56.78, 56.16, 50.20, 42.32, 39.79, 39.51, 39.15, 37.25, 36.89, 36.18, 35.78, 31.95, 31.89, 28.99, 28.44, 28.23, 28.00, 24.28, 23.82, 22.81, 22.55, 21.06, 19.38, 18.71, 15.26, 11.85. HRMS (ESI): calcd for $C_{32}H_{53}O$ $[M + H]^+$ 353.4091, found: 353.4087.

2.4 General procedure for the synthesis of 1,2-diones

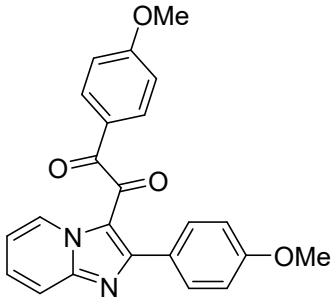
To a 10 mL vial, 2-phenylimidazo[1,2-a]pyridines (0.24 mmol, 1.2 equiv.) or other electron-rich arenes (0.4 mmol, 2.0 equiv.), alkynes (0.2 mmol, 1.0 equiv.), 8-methylquinoline N-oxide (0.6 mmol, 96 mg, 3.0 equiv.) and PiDalPhosAuCl (0.01 mmol, 7.0 mg, 0.05 equiv.) dissolved in DCE (2 mL) were added. $AgNTf_2$ (0.02 mmol, 8.0 mg, 0.1 equiv.) was then added and the mixture was stirred at 60 °C in air for 24 h. After completion, the solvent was removed, and the residue was purified directly with silico gel column chromatograph (PE/EA =15:1 to 2:1 as eluent) to afford the product **3**.

1-(4-methoxyphenyl)-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)ethane-1,2-dione (3a)



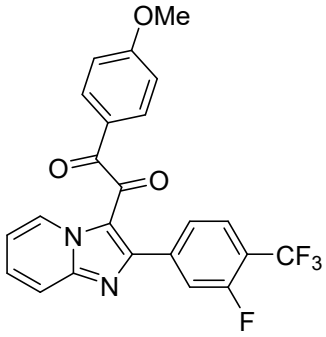
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and 4-ethynylanisole **2a** (26.4 mg) were used, and the product **3a** was obtained as a gray solid (59 mg). Yield 83%, M.P. 163-166 ˚C (lit: 166-168 ˚C)[5]. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.84 (d, *J* = 6.8 Hz, 1H), 7.93 (d, *J* = 8.8 Hz, 1H), 7.70 (t, *J* = 9.2 Hz, 3H), 7.34 (d, *J* = 7.7 Hz, 2H), 7.31 – 7.26 (m, 2H), 7.13 (t, *J* = 7.5 Hz, 2H), 6.88 (d, *J* = 8.5 Hz, 2H), 3.89 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.03, 184.99, 164.35, 158.26, 148.11, 132.83, 132.01, 130.89, 129.99, 129.40, 129.30, 127.84, 126.61, 118.92, 117.55, 115.76, 113.91, 55.55. HRMS (ESI): calcd for $C_{22}H_{17}N_2O_3$ $[M + H]^+$ 357.1234, found: 357.1228.

1-(4-methoxyphenyl)-2-(2-(4-methoxyphenyl)imidazo[1,2-a]pyridin-3-yl)ethane-1,2-dione (3b)



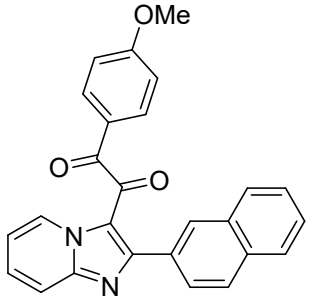
Following the general procedure, 2-(4-methoxyphenyl)imidazo[1,2-a]pyridine **1b** (54 mg) and 4-ethynylanisole **2a** (26.4 mg) were used, and the product **3b** was obtained as a slight yellow solid (60 mg). Yield 77%, M.P. 122-125 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.82 (d, *J* = 6.8 Hz, 1H), 7.81 (d, *J* = 8.9 Hz, 1H), 7.73 (d, *J* = 8.8 Hz, 2H), 7.63 (dd, *J* = 11.7, 4.2 Hz, 1H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.19 (dd, *J* = 9.9, 3.9 Hz, 1H), 6.87 (d, *J* = 8.9 Hz, 2H), 6.64 (d, *J* = 8.6 Hz, 2H), 3.88 (s, 3H), 3.75 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.24, 184.97, 164.32, 160.57, 158.39, 148.32, 132.00, 131.39, 130.76, 129.29, 126.69, 125.39, 118.88, 117.44, 115.49, 113.87, 113.36, 55.55, 55.25. HRMS (ESI): calcd for $C_{23}H_{19}N_2O_4$ $[M + H]^+$ 387.1339, found: 387.1347.

1-(2-(4-fluoro-3-(trifluoromethyl)phenyl)imidazo[1,2-a]pyridin-3-yl)-2-(4-methoxyphenyl)ethane-1,2-dione (3c)



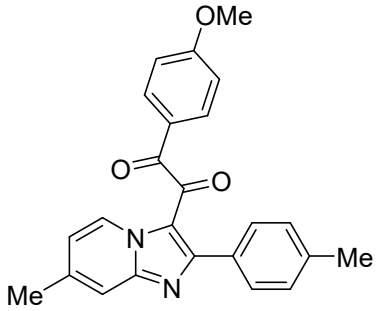
Following the general procedure, 2-(4-fluoro-3-(trifluoromethyl)phenyl)imidazo[1,2-a]pyridine **1c** (67.2 mg) and 4-ethynylanisole **2a** (26.4 mg) were used, and the product **3c** was obtained as a slight yellow solid (69 mg). Yield 78%, M.P. 145-147 ˚C. ^{1}H NMR (500 MHz, MeOD) δ 9.86 (d, J = 6.9 Hz, 1H), 7.95 – 7.84 (m, 2H), 7.69 (d, J = 8.8 Hz, 2H), 7.67 – 7.62 (m, 1H), 7.53 (d, J = 6.7 Hz, 1H), 7.47 (td, J = 6.5, 2.2 Hz, 1H), 7.27 – 7.20 (t, J = 9.12 Hz, 1H), 6.98 (d, J = 8.8 Hz, 2H), 4.10 – 3.73 (s, 3H). ^{13}C NMR (176 MHz, MeOD) δ 192.06, 186.23, 166.77, 161.56 (d, $J_{C\text{-}F}$ = 258.2 Hz), 156.17, 149.40, 137.57 (d, $J_{C\text{-}F}$ = 9.0 Hz), 133.49, 133.17, 130.81, 130.60 (d, $J_{C\text{-}F}$ = 6.8 Hz), 130.25, 127.13, 125.78, 123.47 (q, $J_{C\text{-}F}$ = 271.7 Hz), 121.15, 120.53, 118.69, 118.56 (dd, $J_{C\text{-}F}$ = 33.2, 13.0 Hz), 118.42, 118.06 (d, $J_{C\text{-}F}$ = 13.7 Hz), 117.81 (d, $J_{C\text{-}F}$ = 21.3 Hz) 115.47, 56.28. HRMS (ESI): calcd for $C_{23}H_{15}F_4N_2O_3$ $[M + H]^+$ 443.1013, found: 443.1029.

1-(4-methoxyphenyl)-2-(2-(naphthalen-2-yl)imidazo[1,2-a]pyridin-3-yl)ethane-1,2-dione (3d)



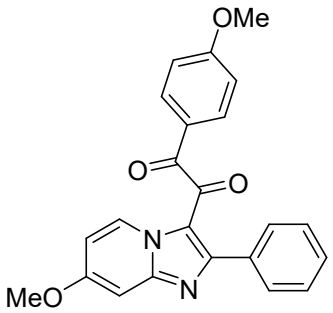
Following the general procedure, 2-(naphthalen-2-yl)imidazo[1,2-a]pyridine **1d** (58 mg) and 4-ethynylanisole **2a** (26.4 mg) were used, and the product **3d** was obtained as a gray solid (65 mg). Yield 80%, M.P. 179-182 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.86 (d, J = 5.8 Hz, 1H), 7.99 (s, 1H), 7.77 (d, J = 8.2 Hz, 1H), 7.71 (d, J = 7.9 Hz, 3H), 7.62 – 7.55 (m, 3H), 7.46 (t, J = 7.4 Hz, 1H), 7.34 (t, J = 7.2 Hz, 1H), 7.30 (d, J = 19.4 Hz, 2H), 6.77 (d, J = 6.9 Hz, 2H), 3.86 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 189.99, 185.12, 164.25, 158.32, 148.40, 133.50, 132.23, 131.94, 130.82, 130.66, 130.37, 129.29, 128.09, 127.99, 127.58, 126.75, 126.66, 126.58, 126.08, 119.23, 117.64, 115.68, 113.83, 55.55. HRMS (ESI): calcd for $C_{26}H_{19}N_2O_3$ $[M + H]^+$ 407.1390, found: 407.1388.

1-(4-methoxyphenyl)-2-(7-methyl-2-(p-tolyl)imidazo[1,2-a]pyridin-3-yl)ethane-1,2-dione (3e)



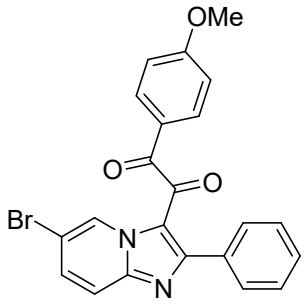
Following the general procedure, 7-methyl-2-(p-tolyl)imidazo[1,2-a]pyridine **1e** (53.3 mg) and 4-ethynylanisole **2a** (26.4 mg) were used, and the product **3e** was obtained as a white solid (59 mg). Yield 77%, M.P. 177-179 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.68 (d, *J* = 7.0 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 2H), 7.59 (s, 1H), 7.19 (d, *J* = 7.9 Hz, 2H), 7.03 (d, *J* = 7.0 Hz, 1H), 6.91 (d, *J* = 7.8 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 3.88 (s, 3H), 2.54 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.32, 184.54, 164.25, 158.88, 148.70, 142.68, 139.30, 132.01, 130.12, 129.86, 128.50, 128.46, 126.82, 118.68, 117.94, 116.28, 113.75, 55.54, 21.71, 21.30. HRMS (ESI): calcd for $C_{24}H_{21}N_2O_3$ $[M + H]^+$ 385.1547, found: 385.1548.

1-(7-methoxy-2-phenylimidazo[1,2-a]pyridin-3-yl)-2-(4-methoxyphenyl)ethane-1,2-dione (3f)



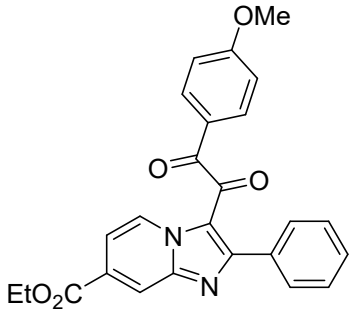
Following the general procedure, 7-methoxy-2-phenylimidazo[1,2-a]pyridine **1f** (53.7 mg) and 4-ethynylanisole **2a** (26.4 mg) were used, and the product **3f** was obtained as a gray solid (54 mg). Yield 71%, M.P. 182-184 ˚C. ^{1}H NMR (500 MHz, MeOD) δ 9.67 (d, *J* = 7.6 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 2H), 7.32 (t, *J* = 7.5 Hz, 1H), 7.28 (d, *J* = 7.5 Hz, 2H), 7.22 (d, *J* = 2.5 Hz, 1H), 7.15 (t, *J* = 7.7 Hz, 2H), 7.09 (dd, *J* = 7.6, 2.5 Hz, 1H), 6.96 (d, *J* = 8.8 Hz, 2H), 4.05 (s, 3H), 3.91 (s, 3H). ^{13}C NMR (126 MHz, MeOD) δ 192.17, 185.82, 166.29, 164.39, 159.95, 151.88, 133.89, 133.19, 131.24, 131.20, 130.62, 128.83, 127.69, 119.61, 115.13, 110.93, 96.43, 56.87, 56.22. HRMS (ESI): calcd for $C_{23}H_{19}N_2O_4$ $[M + H]^+$ 387.1339, found: 387.1344.

1-(6-bromo-2-phenylimidazo[1,2-a]pyridin-3-yl)-2-(4-methoxyphenyl)ethane-1,2-dione (3g)



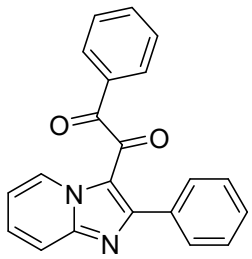
Following the general procedure, 6-bromo-2-phenylimidazo[1,2-a]pyridine **1g** (65.3 mg) and 4-ethynylanisole **2a** (26.4 mg) were used, and the product **3g** was obtained as a slight yellow solid (64 mg). Yield 74%, M.P. 169-172 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.01 (s, 1H), 7.76 – 7.64 (m, 4H), 7.29 (t, *J* = 7.9 Hz, 3H), 7.12 (t, *J* = 7.7 Hz, 2H), 6.88 (d, *J* = 8.8 Hz, 2H), 3.89 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 189.60, 185.14, 164.49, 158.25, 146.53, 134.10, 132.50, 132.04, 129.92, 129.58, 129.33, 127.93, 126.42, 118.95, 118.06, 113.99, 110.48, 55.58. HRMS (ESI): calcd for $C_{22}H_{16}BrN_2O_3$ $[M + H]^+$ 435.0339, found: 435.0342.

ethyl 3-(2-(4-methoxyphenyl)-2-oxoacetyl)-2-phenylimidazo[1,2-a]pyridine-7-carboxylate (3h)



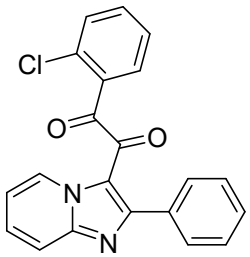
Following the general procedure, ethyl 2-phenylimidazo[1,2-a]pyridine-7-carboxylate **1h** (64 mg) and 4-ethynylanisole **2a** (26.4 mg) were used, and the product **3h** was obtained as a white solid (60.8 mg). Yield 71%, M.P. 174-177 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.82 (d, *J* = 7.1 Hz, 1H), 8.51 (s, 1H), 7.78 (dd, *J* = 7.1, 1.0 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 2H), 7.34 (d, *J* = 7.4 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 2H), 6.88 (d, *J* = 8.8 Hz, 2H), 4.48 (q, *J* = 7.1 Hz, 2H), 3.89 (s, 3H), 1.46 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 189.59, 185.40, 164.54, 164.18, 158.90, 147.33, 132.54, 132.09, 129.98, 129.62, 128.78, 127.96, 126.39, 119.61, 119.31, 114.83, 114.02, 62.18, 55.59, 14.22. HRMS (ESI): calcd for $C_{25}H_{21}N_2O_5$ $[M + H]^+$ 429.1445, found: 429.1447.

1-phenyl-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)ethane-1,2-dione (3i)



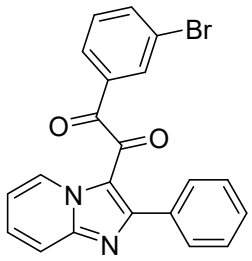
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and ethynylbenzene **2b** (20.4 mg) were used, and the product **3i** was obtained as a slight yellow solid (40 mg). Yield 61%, M.P. 121-123 ˚C (lit: 122-123 ˚C) [5-6]. ^{1}H NMR (500 MHz, MeOD) δ 9.87 (d, *J* = 6.9 Hz, 1H), 7.94 – 7.85 (m, 2H), 7.71 (d, *J* = 7.3 Hz, 2H), 7.65 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 3H), 7.31 (dd, *J* = 16.4, 7.7 Hz, 3H), 7.13 (t, *J* = 7.7 Hz, 2H). ^{13}C NMR (126 MHz, MeOD) δ 192.97, 186.24, 159.29, 149.49, 135.58, 134.54, 133.77, 133.36, 131.36, 130.69, 130.54, 129.82, 128.99, 120.13, 117.90, 117.75. HRMS (ESI): calcd for $C_{21}H_{15}N_2O_2$ $[M + H]^+$ 327.1128, found: 327.1127.

1-(2-chlorophenyl)-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)ethane-1,2-dione (3j)



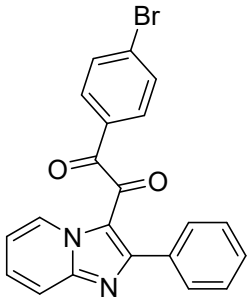
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and 1-chloro-2-ethynylbenzene **2c** (27.2 mg) were used, and the product **3j** was obtained as a slight yellow gel (30.2 mg). Yield 42%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.81 (d, *J* = 5.9 Hz, 1H), 8.02 (s, 1H), 7.73 (s, 1H), 7.62 (d, *J* = 7.3 Hz, 1H), 7.53 (d, *J* = 6.4 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.30 (dd, *J* = 15.0, 8.6 Hz, 2H), 7.29 – 7.19 (m, 4H). ^{13}C NMR (126 MHz, MeOD) δ 191.00, 184.80, 158.37, 149.40, 136.03, 135.36, 134.13, 133.87, 133.37, 133.20, 132.13, 131.13, 130.80, 130.29, 129.23, 128.48, 119.89, 117.89, 117.72. HRMS (ESI): calcd for $C_{21}H_{14}ClN_2O_2$ $[M + H]^+$ 361.0738, found: 361.0746.

1-(3-bromophenyl)-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)ethane-1,2-dione (3k)



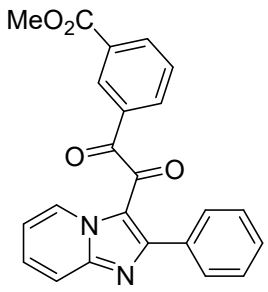
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and 1-bromo-3-ethynylbenzene **2d** (36 mg) were used, and the product **3k** was obtained as a yellow solid (38.8 mg). Yield 48%, M.P. 130-133 ˚C. ^{1}H NMR (500 MHz, MeOD) δ 9.83 (d, *J* = 6.8 Hz, 1H), 7.90 – 7.85 (m, 2H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.71 (d, *J* = 6.4 Hz, 1H), 7.68 (d, *J* = 7.8 Hz, 1H), 7.47 – 7.40 (m, 1H), 7.37 (td, *J* = 7.6, 3.0 Hz, 2H), 7.28 (d, *J* = 7.3 Hz, 2H), 7.18 (t, *J* = 7.7 Hz, 2H). ^{13}C NMR (126 MHz, MeOD) δ 191.54, 185.15, 159.42, 149.57, 138.22, 136.35, 133.73, 133.50, 132.72, 131.66, 131.41, 130.78, 130.55, 129.56, 129.07, 123.82, 120.12, 117.94, 117.82. HRMS (ESI): calcd for $C_{21}H_{14}BrN_2O_2$ $[M + H]^+$ 405.0233, found: 405.0232, 407.0213.

1-(4-bromophenyl)-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)ethane-1,2-dione (3l)



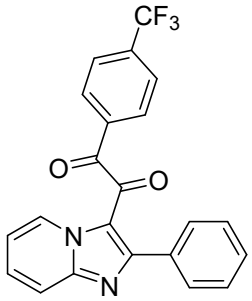
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and 1-bromo-4-ethynylbenzene **2e** (36 mg) were used, and the product **3l** was obtained as a slight yellow solid (45.2 mg). Yield 56%, M.P. 135-138 ˚C (138-140 ˚C)[5a, 5b, 6b]. ^{1}H NMR (700 MHz, $CDCl_3$) δ 9.82 (s, 1H), 7.92 (s, 1H), 7.71 (s, 1H), 7.57 (d, *J* = 25.2 Hz, 4H), 7.33 – 7.24 (m, 4H), 7.15 (s, 2H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 190.12, 183.90, 158.13, 148.06, 132.32, 132.12, 132.05, 131.58, 131.05, 130.21, 129.80, 129.68, 129.39, 128.13, 118.82, 117.77, 116.24. HRMS (ESI): calcd for $C_{21}H_{14}BrN_2O_2$ $[M + H]^+$ 405.0233, found: 405.0232, 407.0211.

methyl 3-(2-oxo-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)acetyl)benzoate (3m)



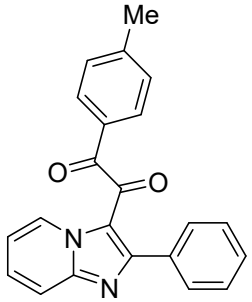
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and methyl 3-ethynylbenzoate **2f** (32 mg) were used, and the product **3m** was obtained as a yellow solid (38.4 mg). Yield 50%, M.P. 173-175 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.88 (d, *J* = 6.7 Hz, 1H), 8.41 (s, 1H), 8.28 (d, *J* = 7.6 Hz, 1H), 7.93 (t, *J* = 7.7 Hz, 2H), 7.75 (t, *J* = 7.8 Hz, 1H), 7.53 (t, *J* = 7.7 Hz, 1H), 7.38 – 7.26 (m, 4H), 7.13 (t, *J* = 7.5 Hz, 2H), 3.97 (s, 3H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 190.20, 183.87, 165.84, 157.73, 147.81, 134.92, 133.57, 133.46, 131.98, 131.80, 130.77, 130.19, 129.89, 129.58, 129.44, 128.96, 128.13, 118.76, 117.59, 116.40, 52.48. HRMS (ESI): calcd for $C_{23}H_{17}N_2O_4$ $[M + H]^+$ 385.1183, found: 385.1184.

1-(2-phenylimidazo[1,2-a]pyridin-3-yl)-2-(4-(trifluoromethyl)phenyl)ethane-1,2-dione (3n)



Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and 1-ethynyl-4-(trifluoromethyl)benzene **2g** (34 mg) were used, and the product **3n** was obtained as a slight yellow solid (25.2 mg). Yield 32%, M.P. 159-162 ˚C (lit: 164 ˚C) **5c**. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.83 (s, 1H), 7.94 (s, 1H), 7.84 (d, *J* = 5.5 Hz, 2H), 7.74 (s, 1H), 7.66 (d, *J* = 5.6 Hz, 2H), 7.30 (d, *J* = 6.8 Hz, 4H), 7.13 (s, 2H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 189.92, 183.50, 158.24, 148.18, 135.93, 135.21 (q, $J_{C\text{-}F}$ = 32.4 Hz), 132.24, 131.86, 130.39, 130.15, 129.91, 129.50, 128.20, 125.69, 123.37 (d, $J_{C\text{-}F}$ = 272.9 Hz), 118.88, 118.00, 116.44. HRMS (ESI): calcd for $C_{22}H_{14}F_3N_2O_2$ $[M + H]^+$ 395.1002, found: 395.1007.

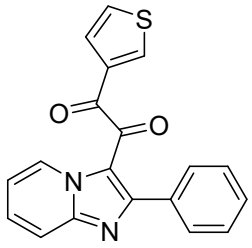
1-(2-phenylimidazo[1,2-a]pyridin-3-yl)-2-(p-tolyl)ethane-1,2-dione (3o)



Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and 1-ethynyl-4-methylbenzene **2h** (23.2 mg) were used, and the product **3o** was obtained as a slight yellow solid (56.4 mg). Yield 83%, M.P. 152-155 ˚C (lit: 151-154 ˚C)**5**. ^{1}H

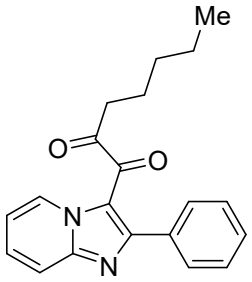
NMR (500 MHz, $CDCl_3$) δ 9.88 – 9.79 (m, 1H), 7.89 – 7.79 (m, 1H), 7.70 – 7.57 (m, 3H), 7.35 – 7.29 (m, 2H), 7.29 – 7.21 (m, 2H), 7.20 (t, *J* = 7.1 Hz, 2H), 7.11 (dd, *J* = 7.4, 4.0 Hz, 2H), 2.41 (s, 3H).^{13}C NMR (126 MHz, $CDCl_3$) δ 191.01, 184.81, 158.42, 148.20, 145.27, 132.84, 130.99, 130.91, 130.00, 129.72, 129.40, 129.30, 127.89, 118.88, 117.58, 115.76, 21.87. HRMS (ESI): calcd for $C_{22}H_{17}N_2O_2$ $[M + H]^+$ 341.1285, found: 341.1287.

1-(2-phenylimidazo[1,2-a]pyridin-3-yl)-2-(thiophen-3-yl)ethane-1,2-dione (3p)



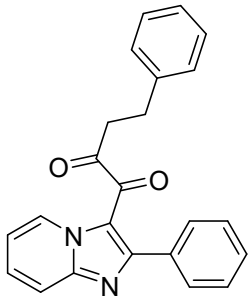
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and 3-ethynylthiophene **2i** (21.6 mg) were used, and the product **3p** was obtained as a slight yellow solid (58.4 mg). Yield 88%, M.P. 129-132 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.78 (d, *J* = 4.9 Hz, 1H), 8.11 (s, 1H), 7.94 (s, 1H), 7.70 (s, 1H), 7.38 (d, *J* = 5.0 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.30 (s, 3H), 7.20 (d, *J* = 5.9 Hz, 2H).^{13}C NMR (126 MHz, $CDCl_3$) δ 184.67, 184.11, 157.41, 147.64, 138.43, 135.90, 132.26, 131.50, 130.05, 129.76, 129.23, 128.13, 127.19, 126.77, 118.34, 117.51, 116.20. HRMS (ESI): calcd for $C_{19}H_{13}N_2O_2S$ $[M + H]^+$ 333.0692, found: 333.0694.

1-(2-phenylimidazo[1,2-a]pyridin-3-yl)heptane-1,2-dione (3q)



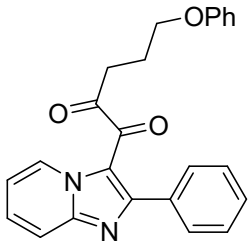
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and hept-1-yne **2j** (19.2 mg) were used, and the product **3q** was obtained as a slight yellow oil (36.5 mg). Yield 57%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.62 (d, *J* = 6.4 Hz, 1H), 7.88 (d, *J* = 7.4 Hz, 1H), 7.65 (s, 1H), 7.53 (d, *J* = 5.6 Hz, 2H), 7.45 (d, *J* = 6.5 Hz, 3H), 7.21 (d, *J* = 5.9 Hz, 1H), 2.62 (t, *J* = 7.2 Hz, 2H), 1.37 – 1.28 (m, 2H), 1.23 (dt, *J* = 14.0, 7.0 Hz, 2H), 1.18 – 1.10 (m, 2H), 0.85 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.68, 185.31, 157.25, 147.80, 133.13, 131.08, 129.91, 129.83, 128.96, 128.54, 117.52, 115.87, 38.75, 31.05, 22.28, 22.08, 13.82. HRMS (ESI): calcd for $C_{20}H_{21}N_2O_2$ $[M + H]^+$ 321.1598, found: 321.1600.

4-phenyl-1-(2-phenylimidazo[1,2-a]pyridin-3-yl)butane-1,2-dione (3r)



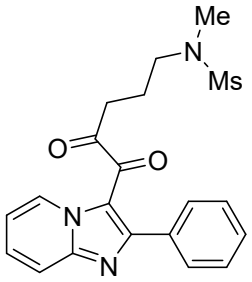
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and but-3-yn-1-ylbenzene **2k** (26 mg) were used, and the product **3r** was obtained as a yellow solid (46.7 mg). Yield 83%, M.P. 113-116 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.62 (d, *J* = 5.2 Hz, 1H), 7.94 (s, 1H), 7.68 (s, 1H), 7.56 (s, 2H), 7.55 – 7.44 (m, 3H), 7.31 – 7.22 (m, 3H), 7.19 (t, *J* = 7.3 Hz, 1H), 7.08 (d, *J* = 7.4 Hz, 2H), 2.97 (d, *J* = 7.8 Hz, 2H), 2.59 (d, *J* = 7.1 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.50, 184.86, 157.19, 147.78, 140.24, 132.99, 131.29, 130.03, 129.97, 128.98, 128.64, 128.50, 128.18, 126.20, 117.51, 116.02, 40.70, 28.57. HRMS (ESI): calcd for $C_{23}H_{19}N_2O_2$ $[M + H]^+$ 355.1441, found: 355.1448.

5-phenoxy-1-(2-phenylimidazo[1,2-a]pyridin-3-yl)pentane-1,2-dione (3s)



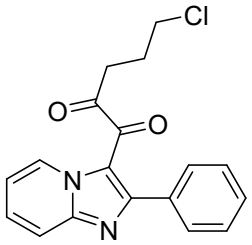
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and (pent-4-yn-1-yloxy)benzene **2l** (32 mg) were used, and the product **3s** was obtained as a slight yellow solid (49 mg). Yield 83%, M.P. 75-78 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.61 (d, *J* = 6.2 Hz, 1H), 7.88 (s, 1H), 7.65 (s, 1H), 7.54 (s, 2H), 7.40 (s, 3H), 7.28 (t, *J* = 7.9 Hz, 2H), 7.20 (s, 1H), 6.95 (t, *J* = 7.3 Hz, 1H), 6.85 (d, *J* = 8.1 Hz, 2H), 3.82 (t, *J* = 5.9 Hz, 2H), 2.93 (t, *J* = 6.8 Hz, 2H), 1.81 – 1.78 (m, 2H).^{13}C NMR (126 MHz, $CDCl_3$) δ 200.97, 184.70, 158.62, 157.58, 147.97, 133.33, 131.00, 129.79, 129.75, 129.37, 128.87, 128.57, 120.67, 117.50, 117.39, 115.80, 114.39, 66.08, 35.18, 22.28. HRMS (ESI): calcd for $C_{24}H_{21}N_2O_3$ $[M + H]^+$ 385.1547, found: 385.1557.

N-(4,5-dioxo-5-(2-phenylimidazo[1,2-a]pyridin-3-yl)pentyl)-N-methylmethanesulfonamide (3t)



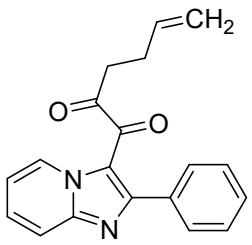
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and N-methyl-N-(pent-4-yn-1-yl)methanesulfonamide **2m** (35 mg) were used, and the product **3t** was obtained as a slight yellow gel (56.7 mg). Yield 71%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.61 (d, *J* = 6.8 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.65 (t, *J* = 7.9 Hz, 1H), 7.54 – 7.49 (m, 2H), 7.46 (d, *J* = 3.3 Hz, 3H), 7.21 (t, *J* = 6.9 Hz, 1H), 2.98 (t, *J* = 6.9 Hz, 2H), 2.75 (t, *J* = 4.2 Hz, 6H), 2.72 (d, *J* = 7.2 Hz, 2H), 1.57 (p, *J* = 7.1 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.87, 184.51, 157.60, 148.05, 133.40, 131.17, 129.90, 129.76, 128.99, 128.55, 117.46, 115.91, 48.86, 35.61, 35.27, 34.48, 20.73. HRMS (ESI): calcd for $C_{20}H_{22}N_3O_4S$ $[M + H]^+$ 400.1326, found: 400.1332.

5-chloro-1-(2-phenylimidazo[1,2-a]pyridin-3-yl)pentane-1,2-dione (3u)



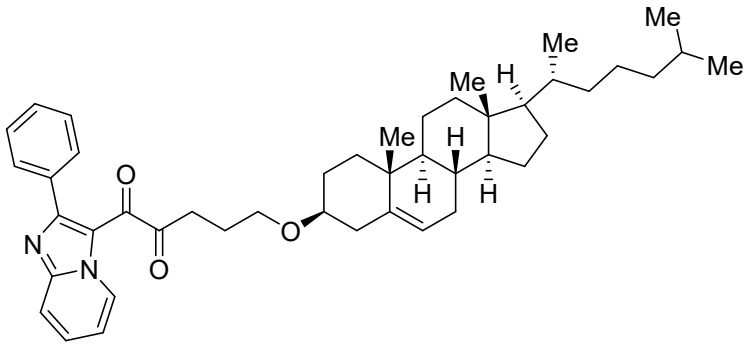
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and 5-chloropent-1-yne **2n** (20 mg) were used, and the product **3u** was obtained as a slight white solid (45.6 mg). Yield 70%, M.P. 113-116 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.61 (d, *J* = 6.3 Hz, 1H), 7.88 (d, *J* = 7.6 Hz, 1H), 7.66 (s, 1H), 7.53 (s, 2H), 7.48 (s, 3H), 7.21 (t, *J* = 5.5 Hz, 1H), 3.40 (t, *J* = 6.1 Hz, 2H), 2.91 (t, *J* = 6.7 Hz, 2H), 1.82 – 1.75 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.32, 184.40, 157.65, 148.03, 133.36, 131.18, 129.88, 129.82, 128.95, 128.68, 117.61, 117.37, 115.95, 43.96, 35.64, 25.37. HRMS (ESI): calcd for $C_{18}H_{16}ClN_2O_2$ $[M + H]^+$ 327.0895, found: 327.0901.

1-(2-phenylimidazo[1,2-a]pyridin-3-yl)hex-5-ene-1,2-dione (3v)



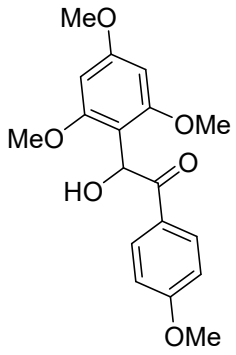
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and hex-1-en-5-yne **2o** (16 mg) were used, and the product **3v** was obtained as a slight yellow solid (35 mg). Yield 58%, M.P. 89-92 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.60 (d, *J* = 6.4 Hz, 1H), 7.87 (d, *J* = 7.9 Hz, 1H), 7.64 (s, 1H), 7.52 (d, *J* = 6.1 Hz, 2H), 7.47 (dd, *J* = 14.8, 7.1 Hz, 3H), 7.19 (t, *J* = 6.2 Hz, 1H), 5.66 (ddt, *J* = 13.1, 10.2, 6.5 Hz, 1H), 4.95 (t, *J* = 14.2 Hz, 2H), 2.75 (t, *J* = 7.4 Hz, 2H), 2.04 (dd, *J* = 13.3, 6.5 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.59, 184.85, 157.41, 147.88, 136.37, 133.18, 131.10, 129.84, 128.91, 128.56, 117.51, 117.43, 115.88, 115.39, 37.97, 26.46. HRMS (ESI): calcd for $C_{19}H_{17}N_2O_2$ $[M + H]^+$ 305.1285, found: 305.1291.

5-(((3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl)oxy)-1-(2-phenylimidazo[1,2-a]pyridin-3-yl)pentane-1,2-dione (3w)



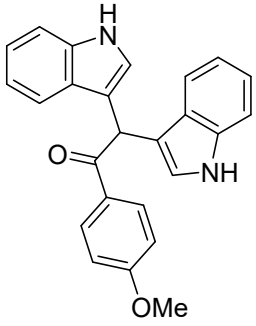
Following the general procedure, 2-phenylimidazo[1,2-a]pyridine **1a** (46.6 mg) and (3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)-3-(pent-4-yn-1-yloxy)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthrene **2p** (90.2 mg) were used, and the product **3w** was obtained as a yellow solid (100 mg). Yield 74%, M.P. 72-75 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.63 (d, *J* = 5.6 Hz, 1H), 7.93 (s, 1H), 7.68 (s, 1H), 7.55 (s, 2H), 7.47 (s, 3H), 7.23 (s, 1H), 5.34 (d, *J* = 4.7 Hz, 1H), 3.33 (t, *J* = 5.7 Hz, 2H), 3.12 – 3.03 (m, 1H), 2.78 (t, *J* = 6.0 Hz, 2H), 2.30 (d, *J* = 9.9 Hz, 1H), 2.15 (t, *J* = 11.8 Hz, 1H), 1.99 (t, *J* = 15.6 Hz, 2H), 1.82 (dd, *J* = 22.9, 9.8 Hz, 3H), 1.57 (d, *J* = 6.6 Hz, 3H), 1.54 – 1.47 (m, 3H), 1.43 (dd, *J* = 18.7, 14.1 Hz, 2H), 1.39 – 1.28 (m, 4H), 1.12 (tdd, *J* = 23.8, 13.2, 5.2 Hz, 7H), 1.00 (d, *J* = 11.9 Hz, 6H), 0.94 – 0.88 (m, 4H), 0.87 (d, *J* = 2.1 Hz, 3H), 0.85 (d, *J* = 2.1 Hz, 3H), 0.67 (s, 3H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 201.22, 185.03, 156.88, 147.57, 140.94, 132.85, 131.37, 129.98, 129.01, 128.69, 121.55, 117.54, 117.41, 116.09, 78.93, 66.49, 56.76, 56.13, 50.18, 42.30, 39.76, 39.50, 39.14, 37.21, 36.87, 36.17, 35.77, 31.93, 31.87, 29.69, 28.43, 28.22, 28.00, 24.27, 23.80, 23.17, 22.80, 22.54, 21.05, 19.38, 18.70, 11.84. HRMS (ESI): calcd for $C_{45}H_{61}N_2O_3$ $[M + H]^+$ 677.4677, found: 677.4662.

2-hydroxy-1-(4-methoxyphenyl)-2-(2,4,6-trimethoxyphenyl)ethan-1-one (3x)



Following the general procedure, 1,3,5-trimethoxybenzene **1i** (67 mg) and 4-ethynylanisole **2a** (26.4 mg) were used, and the product **3x** was obtained as a white solid (43 mg). Yield 65%, M.P. 100-103 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.2 Hz, 2H), 6.79 (d, *J* = 7.3 Hz, 2H), 6.12 (d, *J* = 1.5 Hz, 1H), 6.05 (d, *J* = 1.4 Hz, 2H), 3.79 (s, 3H), 3.76 (s, 3H), 3.74 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 198.60, 163.22, 161.59, 158.80, 130.30, 127.01, 113.40, 109.98, 91.05, 67.66, 55.71, 55.28, 55.23. HRMS (ESI): calcd for $C_{18}H_{20}O_6$ $[M + Na]^+$ 355.1152, found: 355.1154.

2,2-di(1H-indol-3-yl)-1-(4-methoxyphenyl)ethan-1-one (3y)



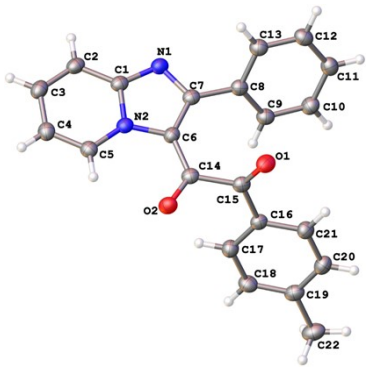
Following the general procedure, indole **1j** (23.4 mg) and 4-ethynylanisole **2a** (26.4 mg) were used, and the product **3y** was obtained as a gray solid (51 mg). Yield 67%, M.P. 220-223 ^{1}H NMR (500 MHz, $(CD_3)_2CO$) δ 10.10 (s, 2H), 8.21 (d, *J* = 8.8 Hz, 2H), 7.63 (d, *J* = 7.9 Hz, 2H), 7.38 (d, *J* = 8.1 Hz, 2H), 7.19 (d, *J* = 2.0 Hz, 2H), 7.07 (t, *J* = 7.5 Hz, 2H), 6.97 (dd, *J* = 7.8, 5.0 Hz, 4H), 6.65 (s, 1H), 3.84 (s, 3H). ^{13}C NMR (126 MHz, $(CD_3)_2CO$) δ 196.25, 163.34, 136.98, 130.91, 130.14, 127.15, 124.30, 121.30, 119.15, 118.72, 114.26, 113.70, 111.39, 55.01, 41.67. HRMS (ESI): calcd for $C_{25}H_{21}N_2NaO_2$ $[M + Na]^+$ 403.1417, found: 403.1413.

References:

1. H. Su, L. Wang, H. Rao and H. Xu, Orga. lett., 2017, **19**, 2226.
2. K. Godugu and C. G. R. Nallagondu, J. Heterocyclic. Chem., 2021, **58**, 250.
3. J. Gerencser, G. Panka, T. Nagy, O. Egyed, G. Dorman, L. Urge and F. Darvas, J. comb. chem., 2005, **7**, 530..

4. M. Rivara, M. K. Patel, L. Amori and V. Zuliani, Bioorg. med. chem. lett., 2012, **22**, 6401.
5. (a) M. Chennapuram, N. R. Emmadi, C. Bingi and K. Atmakur, RSC Adv., 2015, **5**, 19418; (b) S. M. A. Shakoor, D. S. Agarwal, A. Kumar and R. Sakhuja, Tetrahedron, 2016, *72*, 645; (c) N. K. Nandwana, O. P. S. Patel, M. R. Srivathsa and A. Kumar, ACS omega, 2019, **4**, 10140.
6. (a) Y. Liu, H. Zhan, K. Yao, Y. Mai, E. Wang, J. He and P. Guo, Euro. J. Org. Chem., 2016, **2016**, 4991; (b) T. Guo, X. H. Fu, M. Zhang, Y. L. Li and Y. C. Ma, Org. biomol. chem., 2019, **17**, 3150.

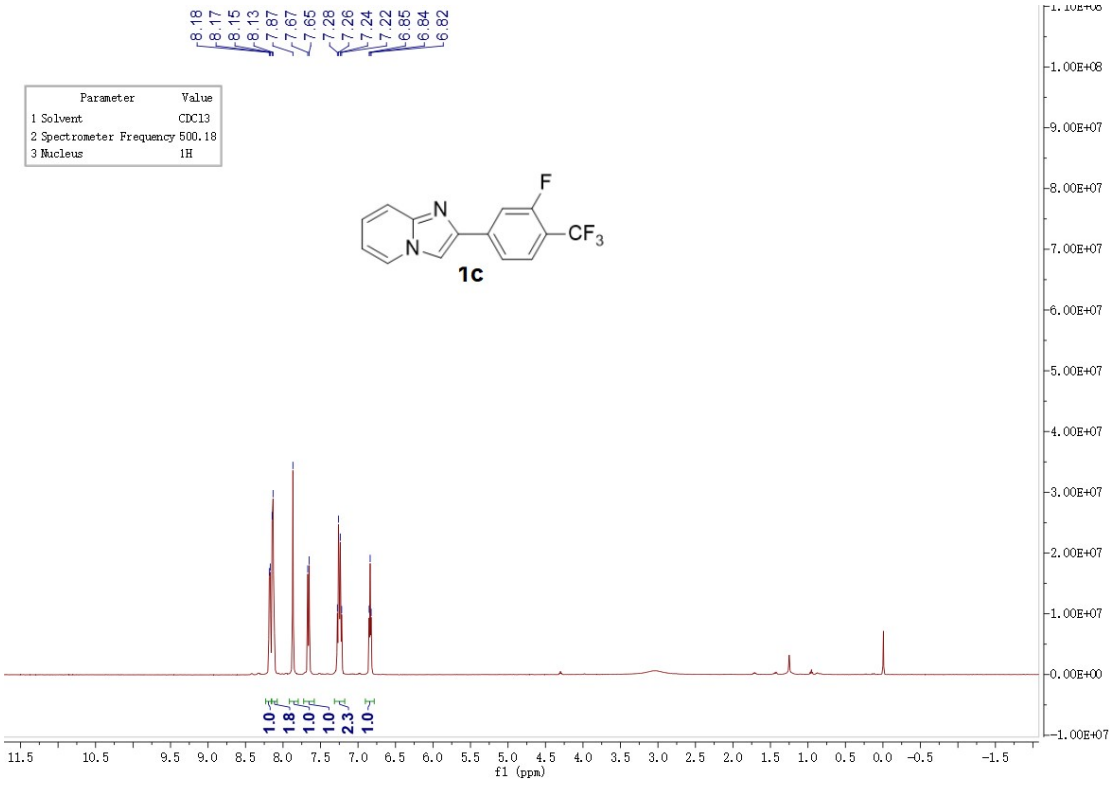
Table S2. Crystal data and structure refinement for **3o** (CCDC 2097492). Its thermal ellipsoid at 50% probability level

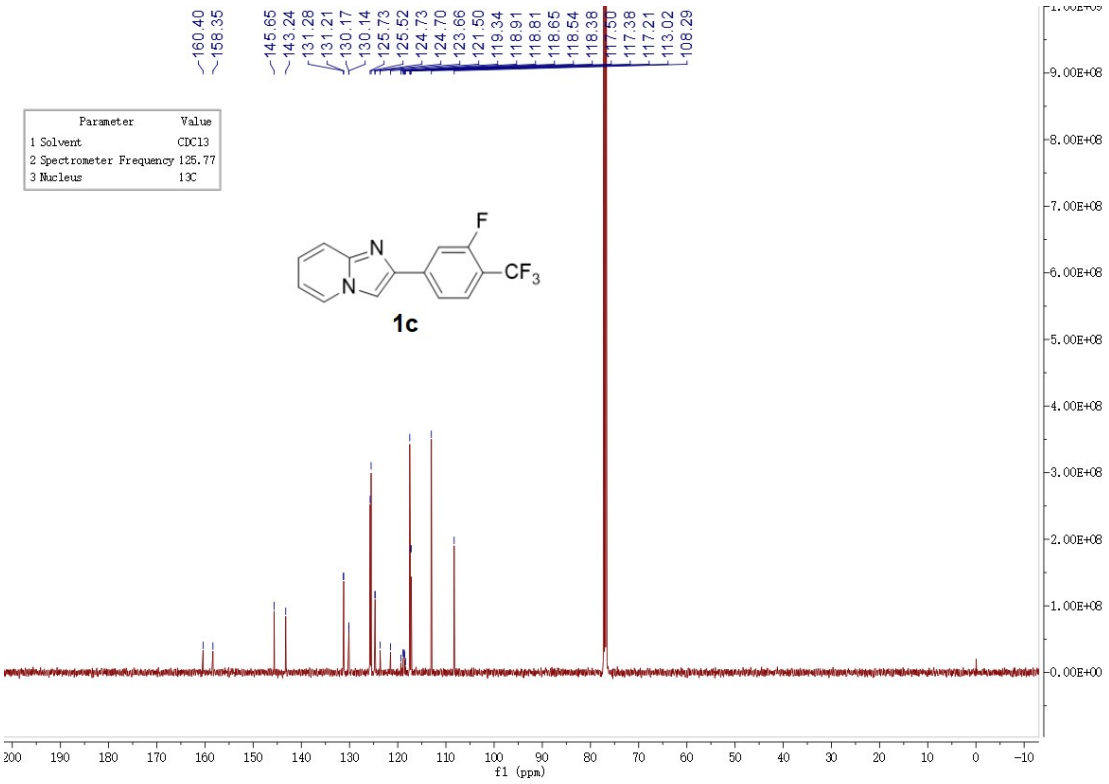


Identification code	**3o**
Empirical formula	$C_{22}H_{16}N_2O_2$
Formula weight	340.37
Temperature/K	110(15)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	19.2136(2)
b/Å	10.69070(10)
c/Å	8.13480(10)
α/°	90
β/°	98.4000(10)
γ/°	90
Volume/Å^3	1653.02(3)
Z	4

ρ_{calc}/g/cm^3	1.368
μ/mm^{-1}	0.712
F(000)	712.0
Crystal size/mm^3	0.07 × 0.06 × 0.04
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.306 to 148.784
Index ranges	-23 ≤ h ≤ 23, -7 ≤ k ≤ 13, -5 ≤ l ≤ 9
Reflections collected	8977
Independent reflections	3264 [R_{int} = 0.0282, R_{sigma} = 0.0326]
Data/restraints/parameters	3264/0/236
Goodness-of-fit on F^2	1.068
Final R indexes [I>=2σ (I)]	R_1 = 0.0392, wR_2 = 0.1096
Final R indexes [all data]	R_1 = 0.0421, wR_2 = 0.1121
Largest diff. peak/hole / e Å^{-3}	0.17/-0.24

Copies of spectra

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125.52
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123.66
121.50
119.34
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118.81
118.65
118.54
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117.38
117.21
113.02
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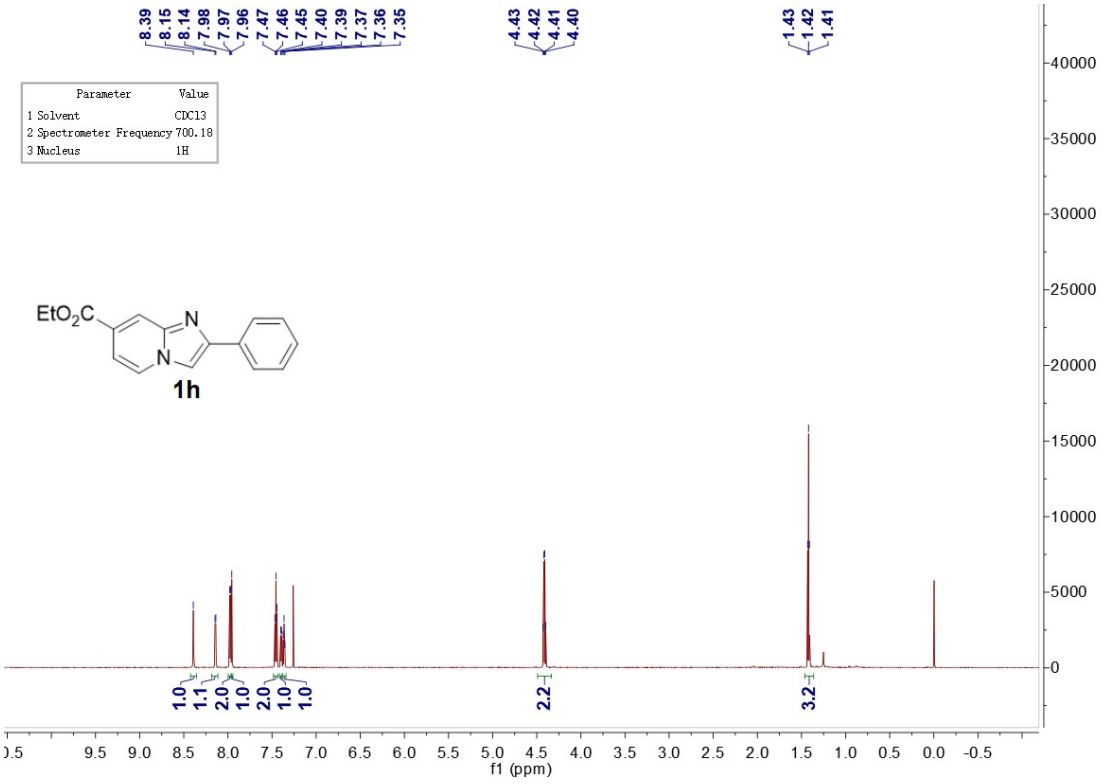
N
CF3
1c
f1 (ppm)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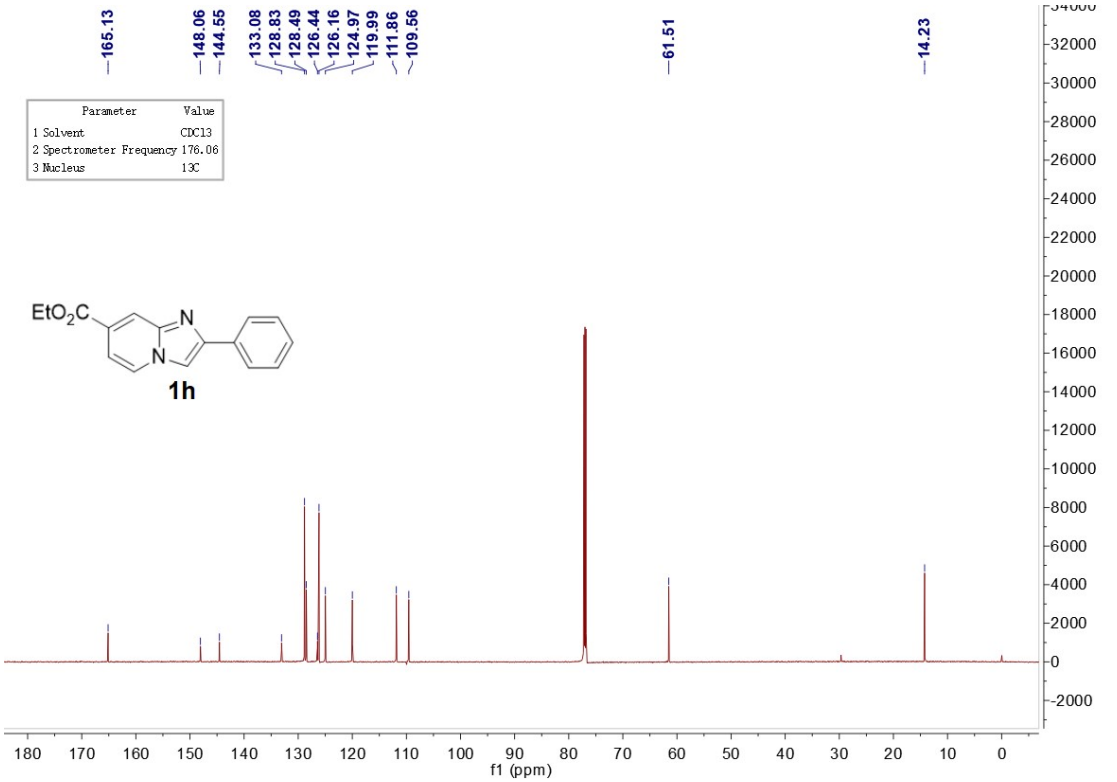
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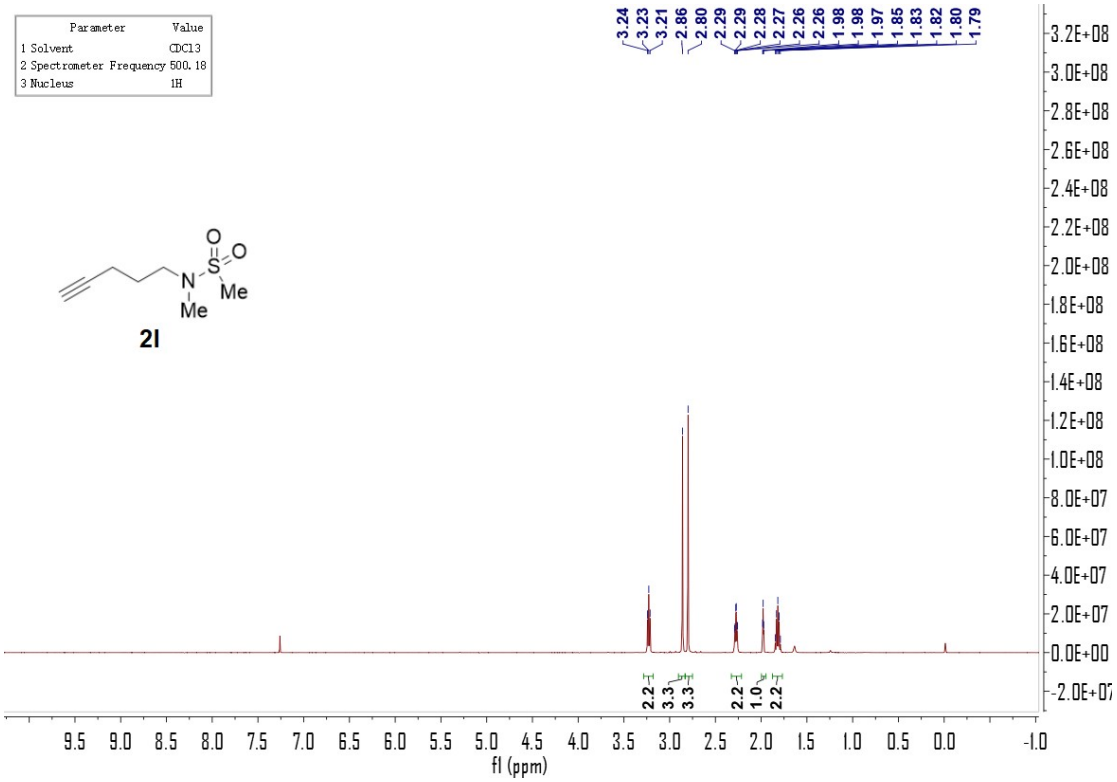
f1 (ppm)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1.82
1.80
1.79
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Me
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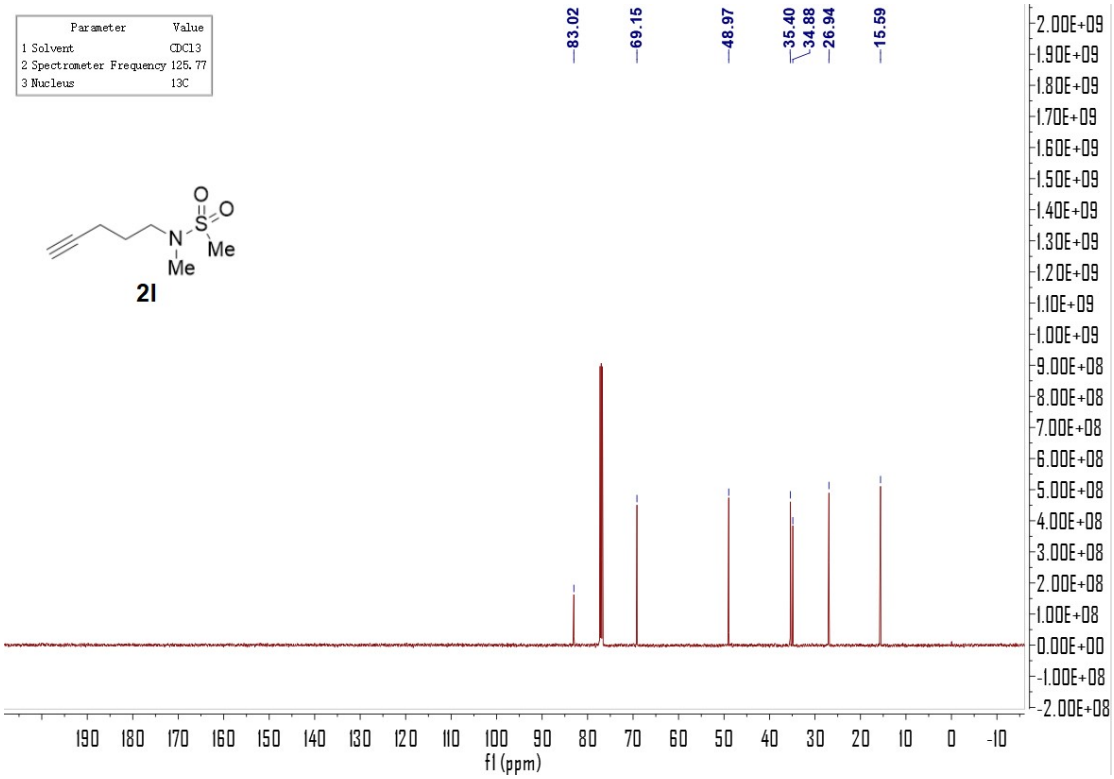
2.2
f1 (ppm)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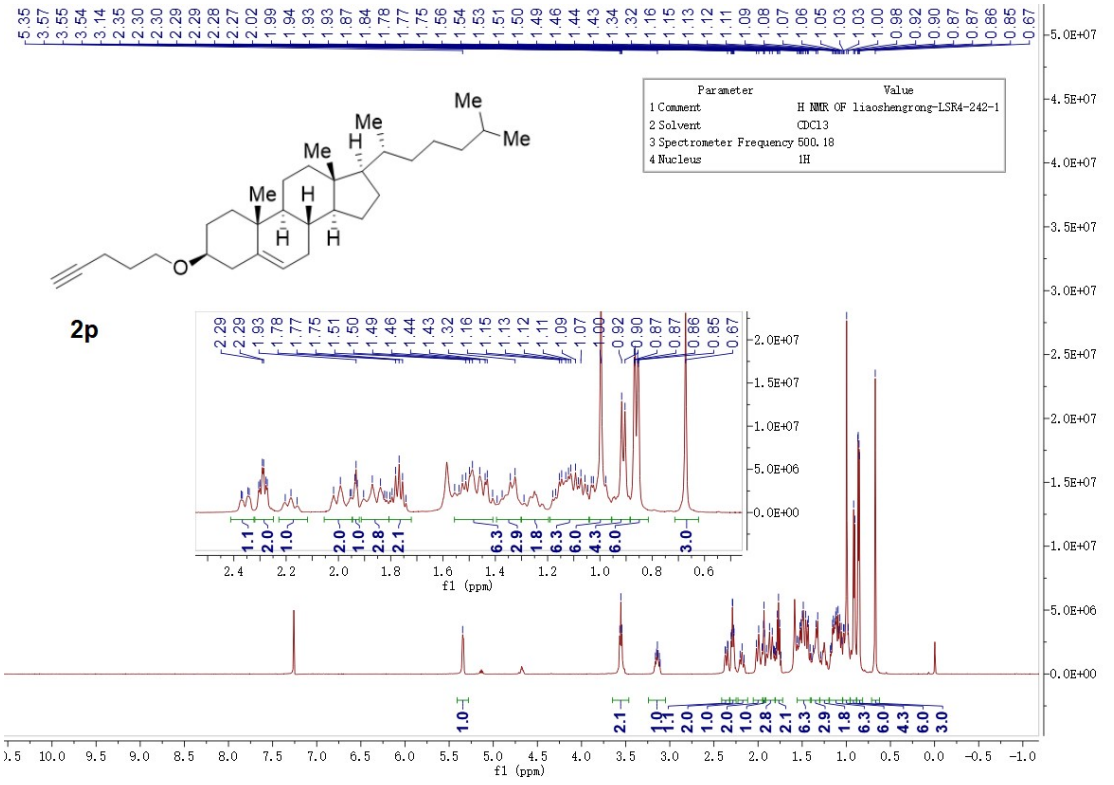
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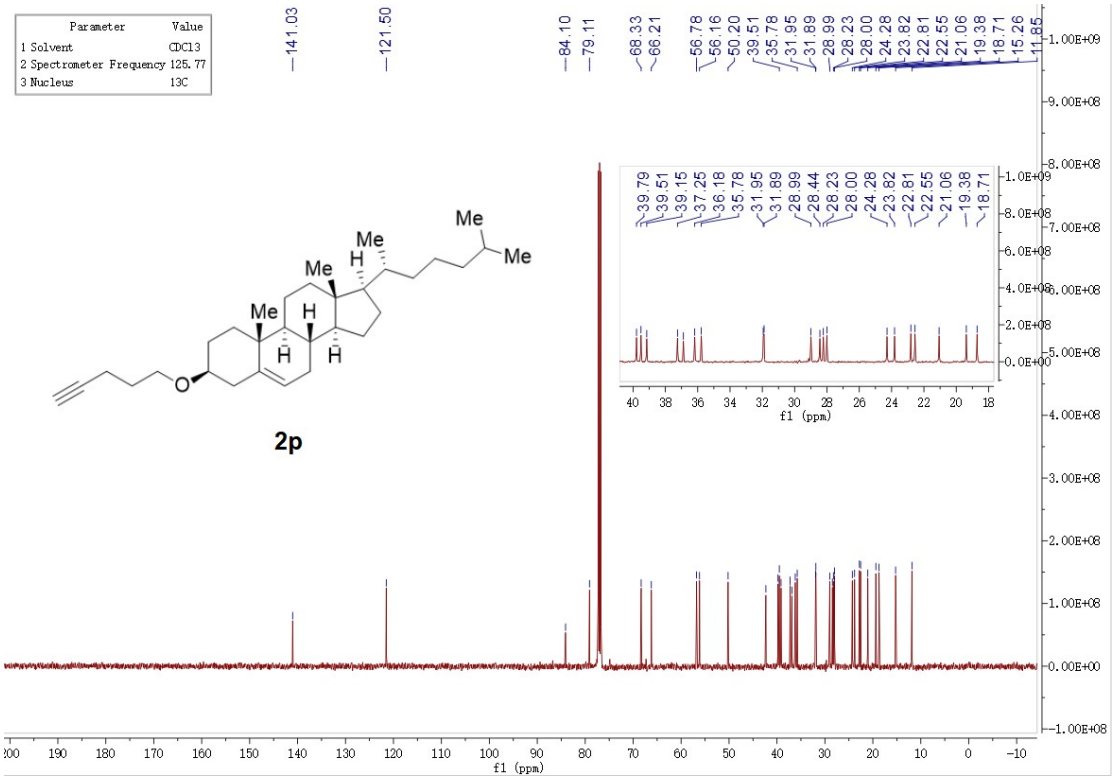
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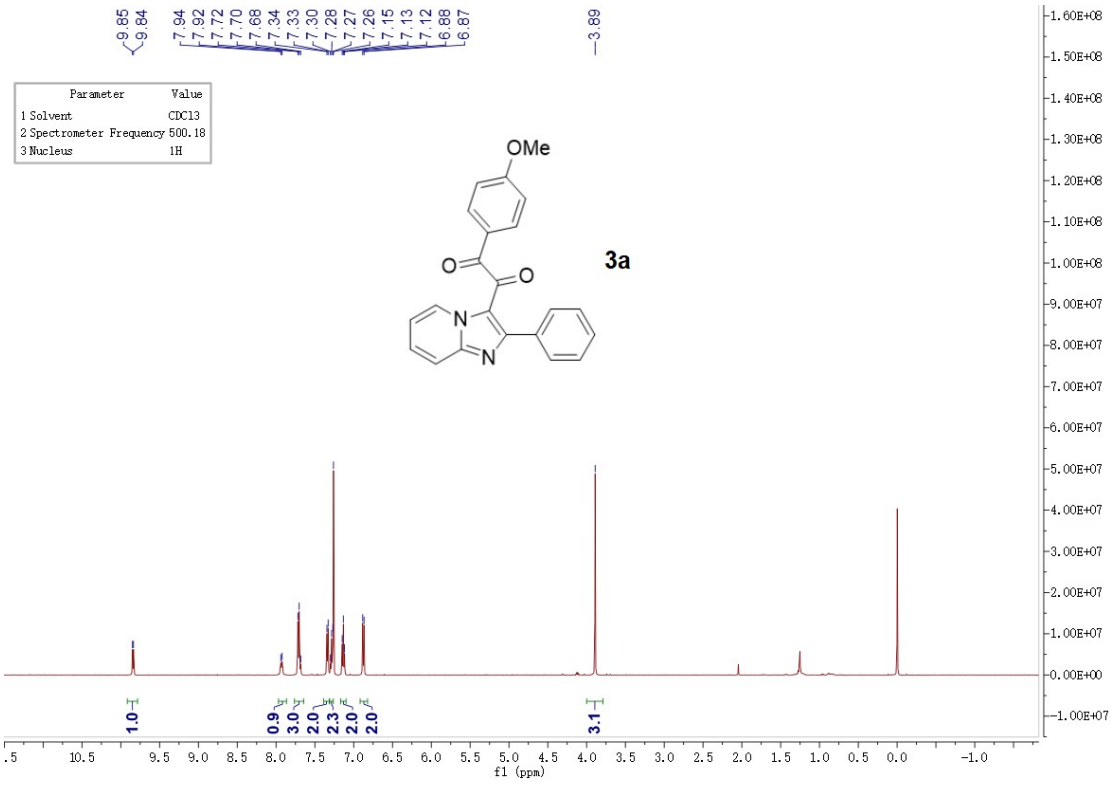
f1 (ppm)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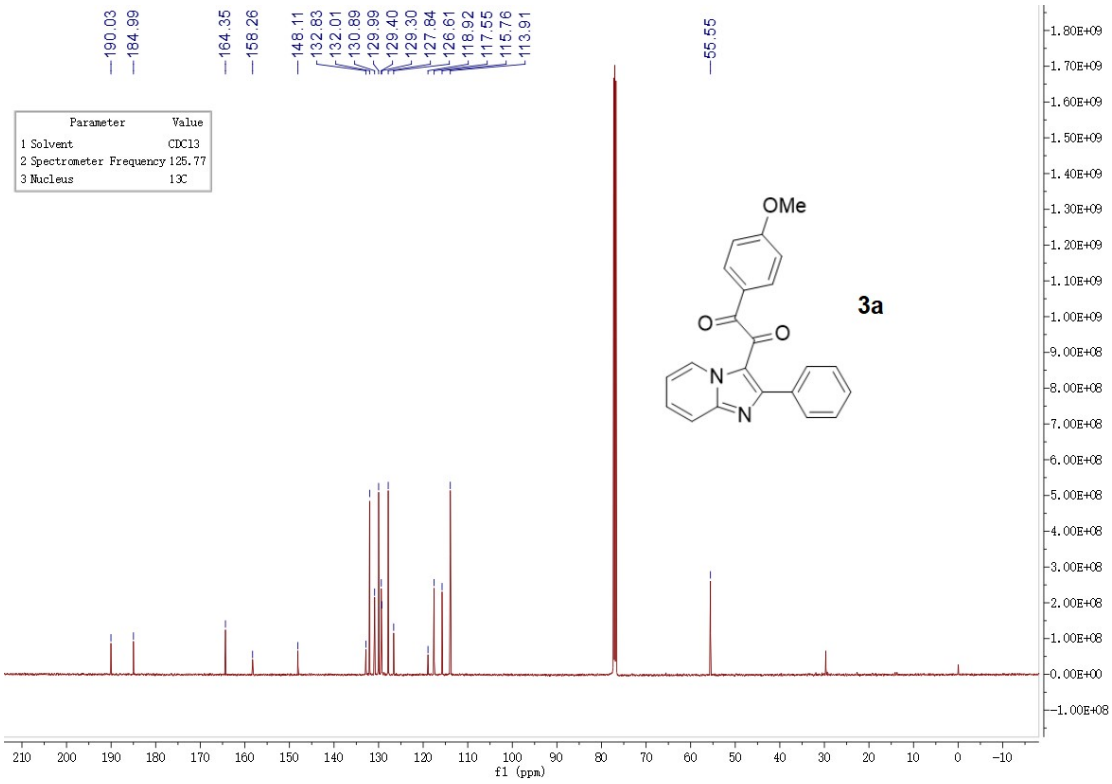
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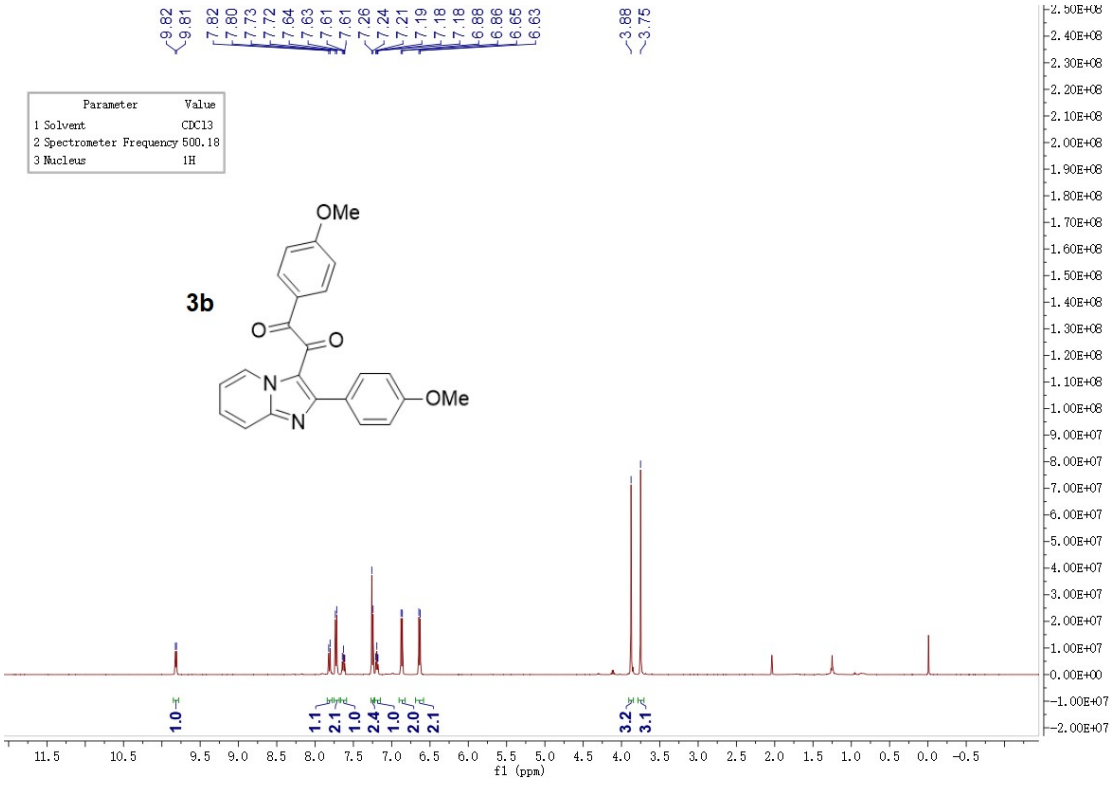
f1 (ppm)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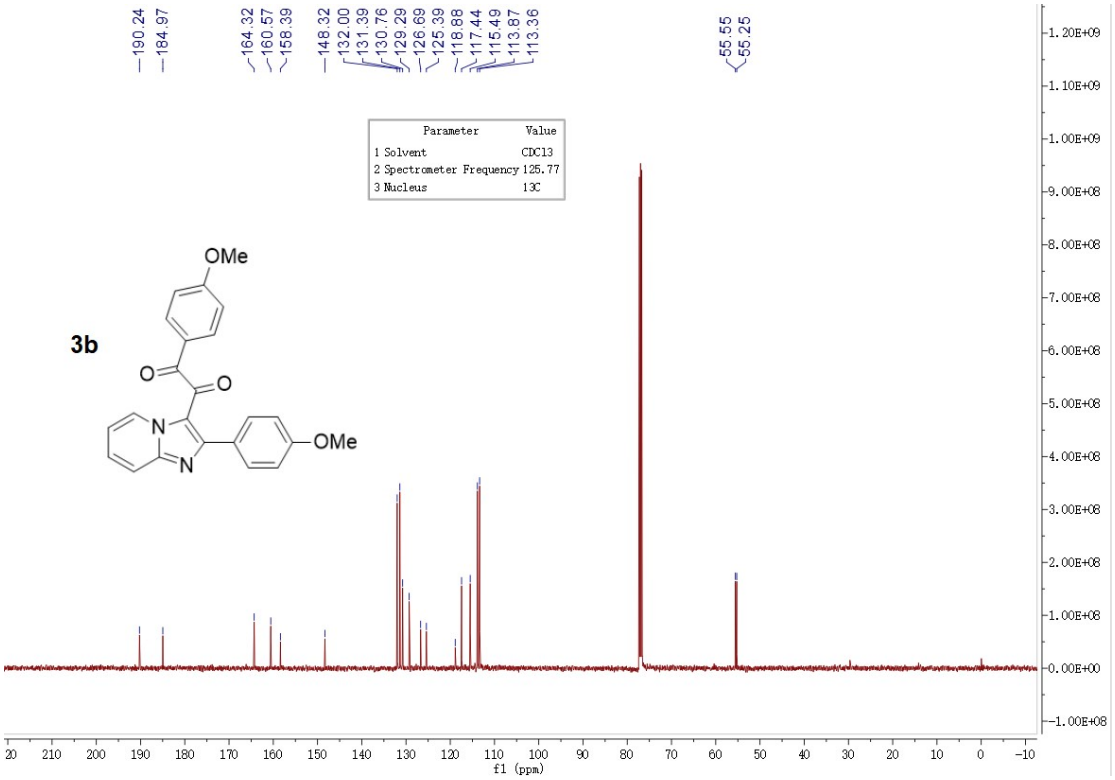
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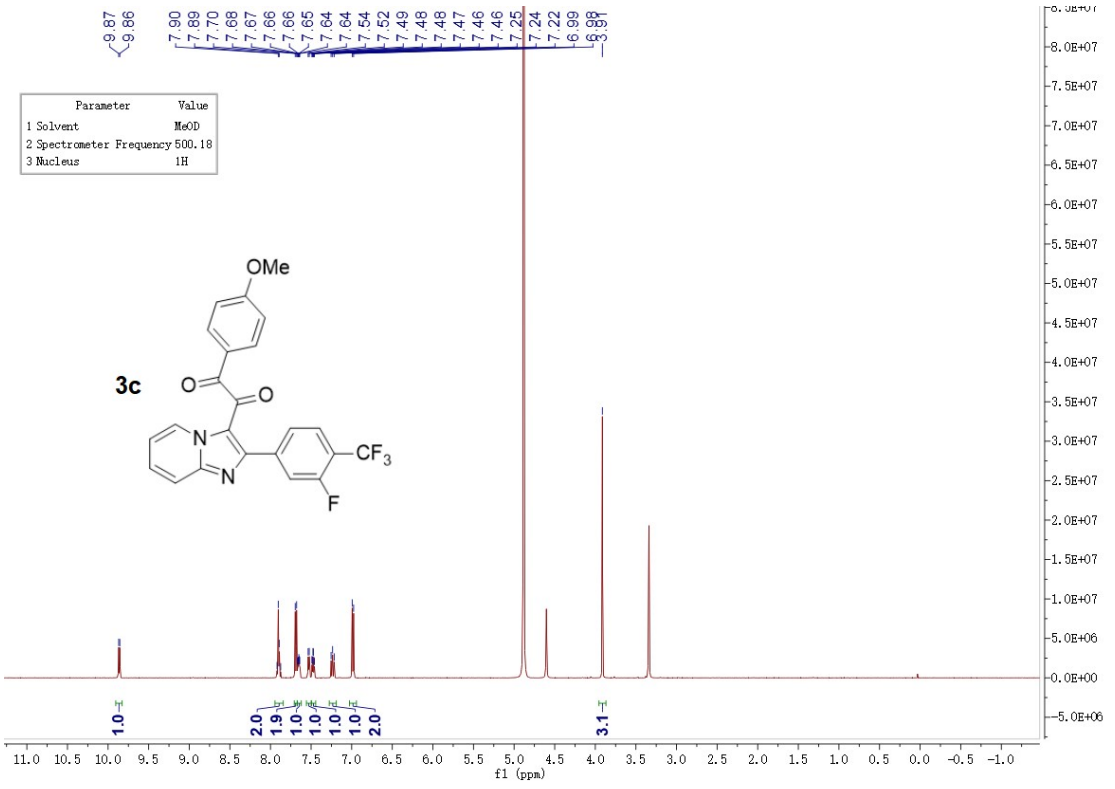
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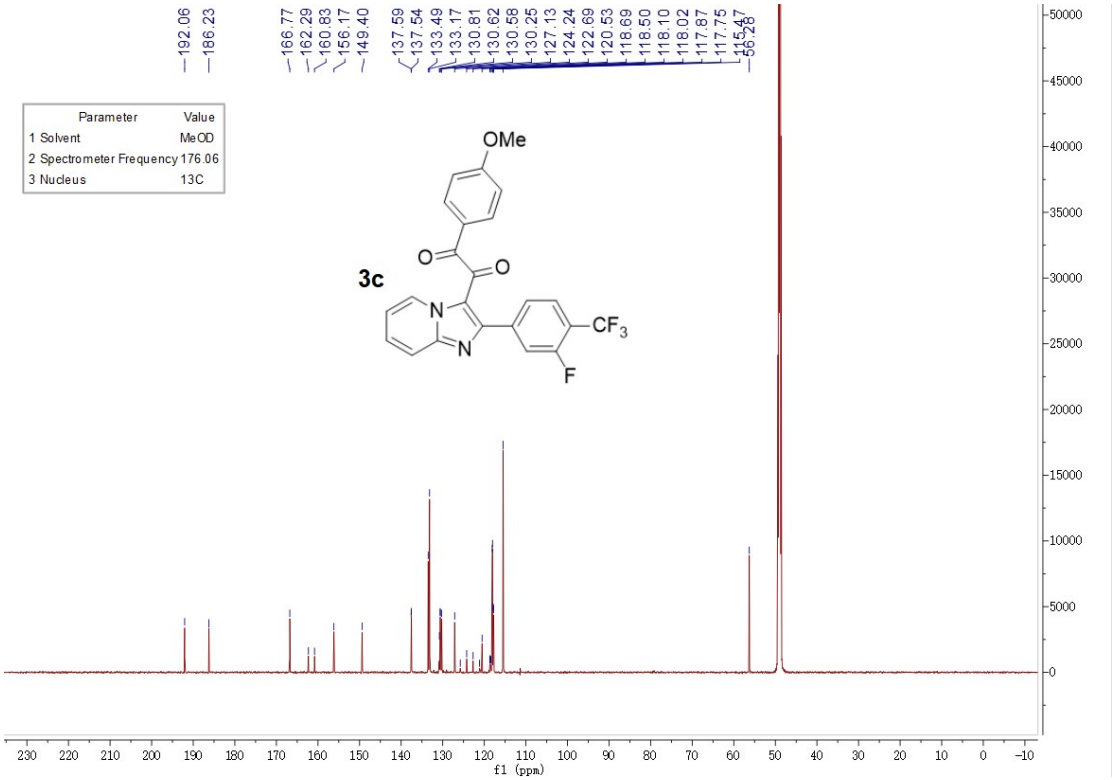
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3c
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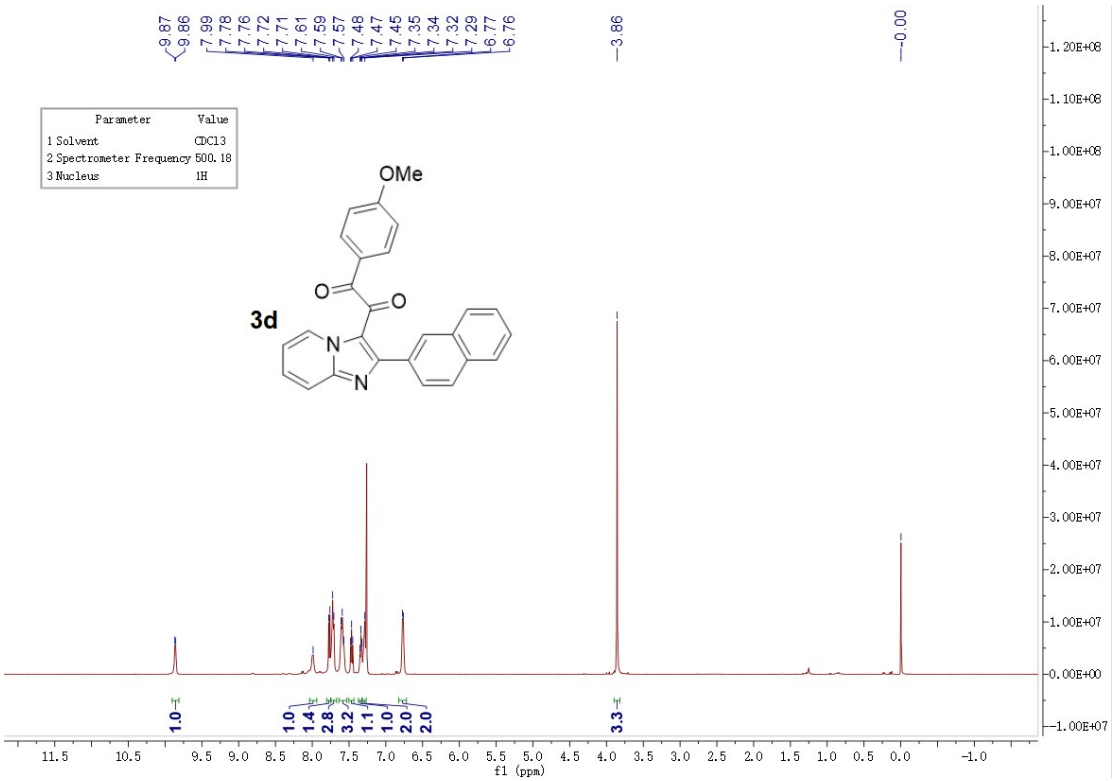
f1 (ppm)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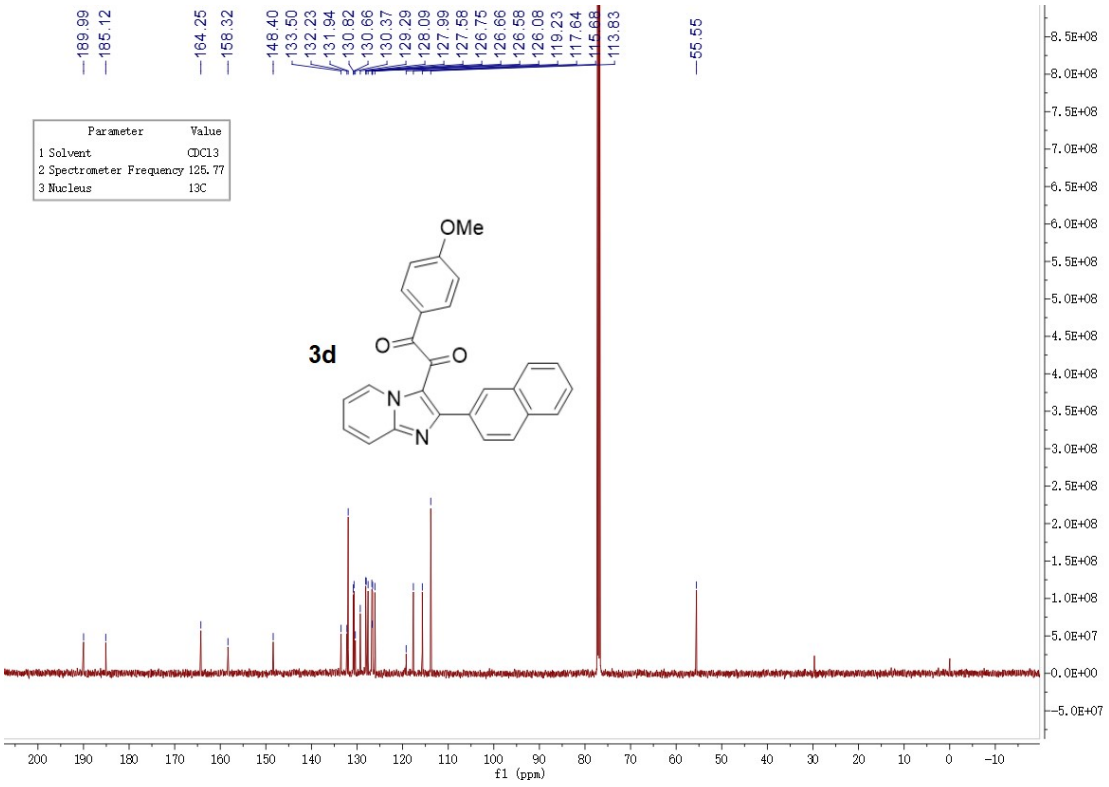
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130.66
130.37
129.29
128.09
127.99
127.58
126.75
126.66
126.58
126.08
119.23
117.64
115.68
113.83
55.55
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2 Spectrometer Frequency 125.77
3 Nucleus 13C
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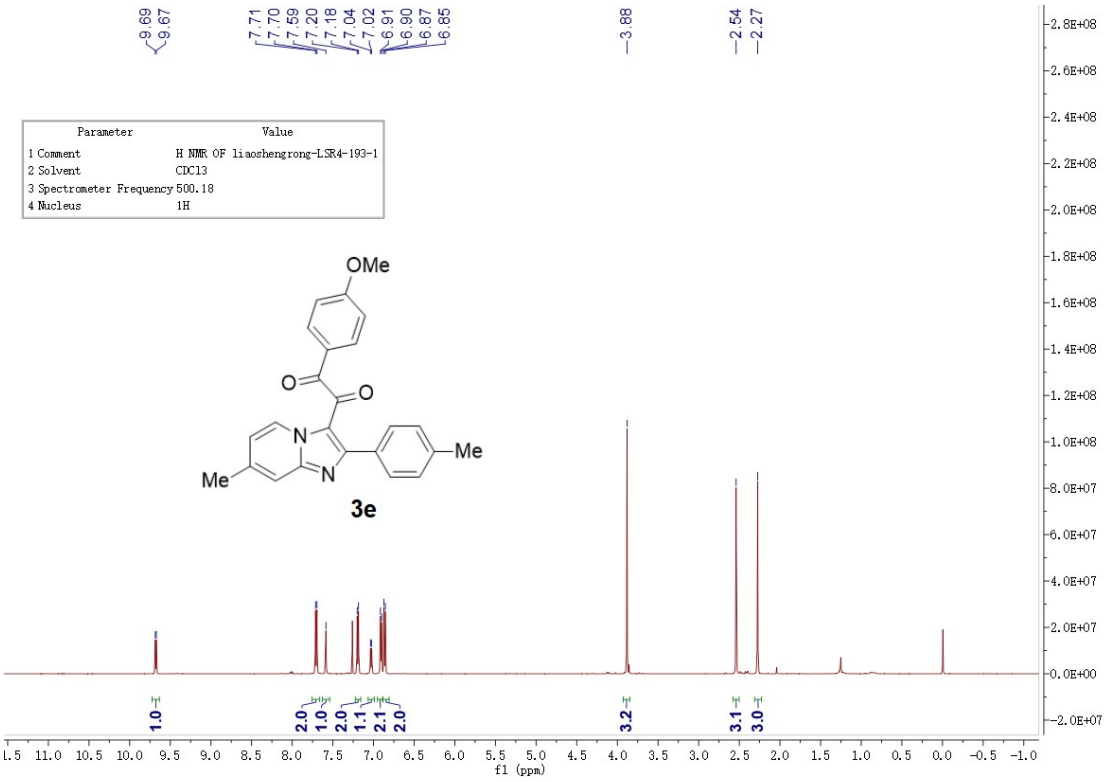
N
3d
f1 (ppm)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6.85
3.88
2.54
2.27
Parameter Value
1 Comment H NMR OF liaoshengrong-LSR4-193-1
2 Solvent CDCl3
3 Spectrometer Frequency 500.18
4 Nucleus 1H
OMe
O
O
N
N
Me
Me
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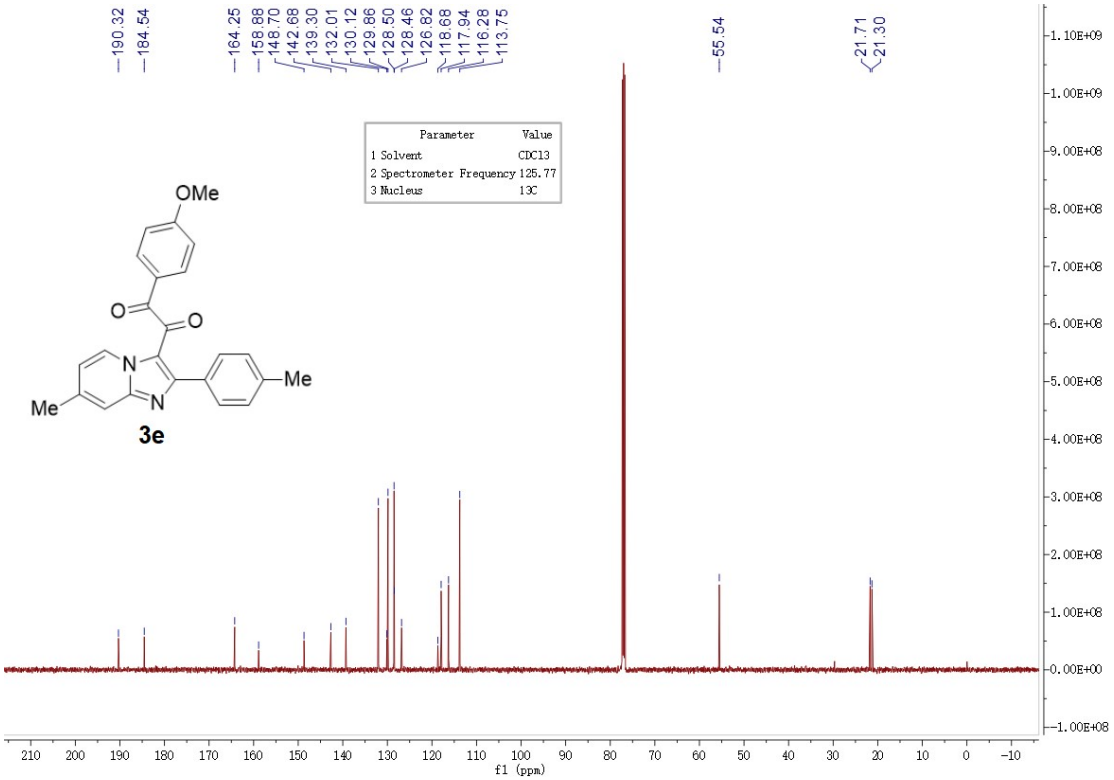
3.0
f1 (ppm)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128.46
126.82
118.68
117.94
116.28
113.75
55.54
21.71
21.30
Parameter Value
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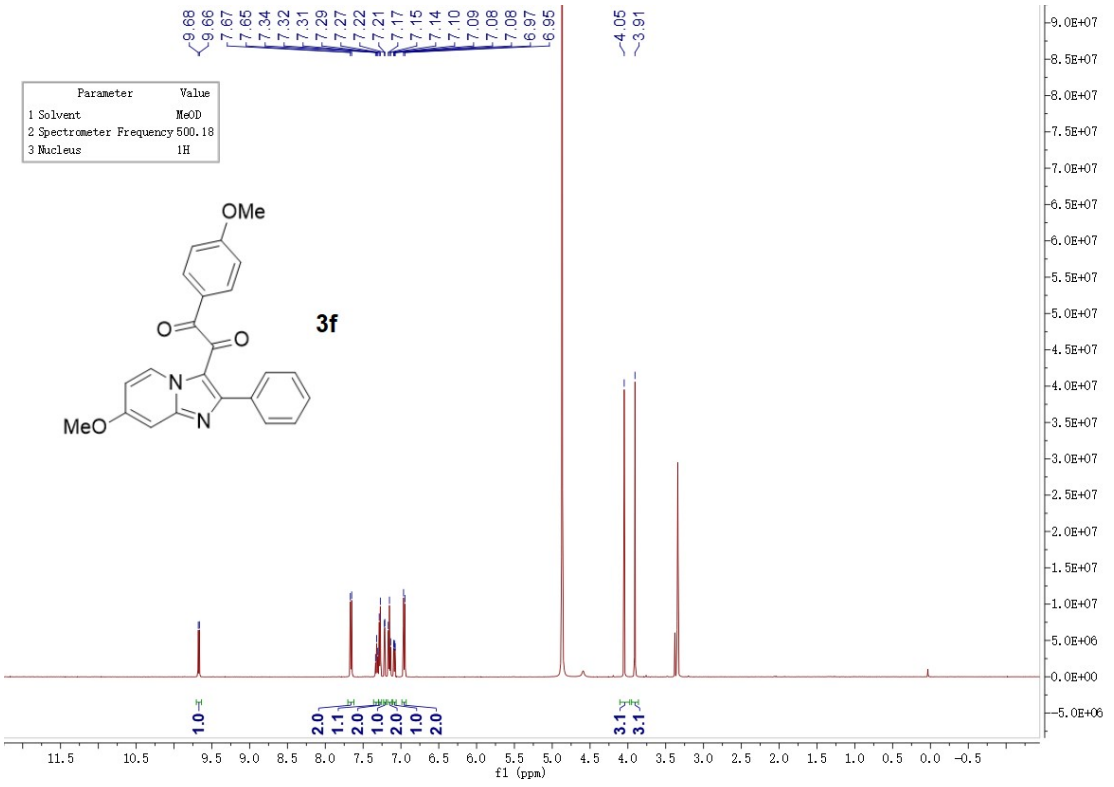
2 Spectrometer Frequency 125.77
3 Nucleus 13C
OMe
O
O
N
N
Me
Me
3e
f1 (ppm)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7.22
7.21
7.17
7.15
7.14
7.10
7.09
7.08
7.08
6.97
6.95
4.05
3.91
Parameter Value
1 Solvent MeOD
2 Spectrometer Frequency 500.18
3 Nucleus 1H
OMe
O
O
N
N
MeO
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2.0
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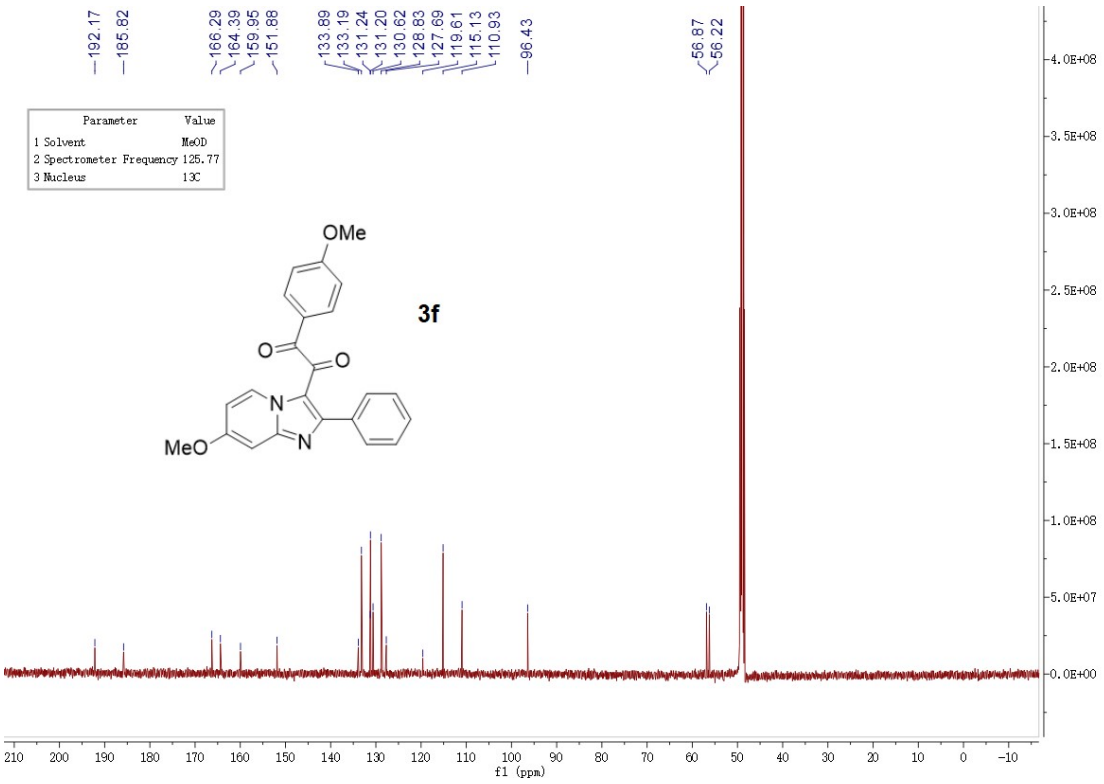
3.1
f1 (ppm)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133.19
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128.83
127.69
119.61
115.13
110.93
96.43
56.87
56.22
Parameter Value
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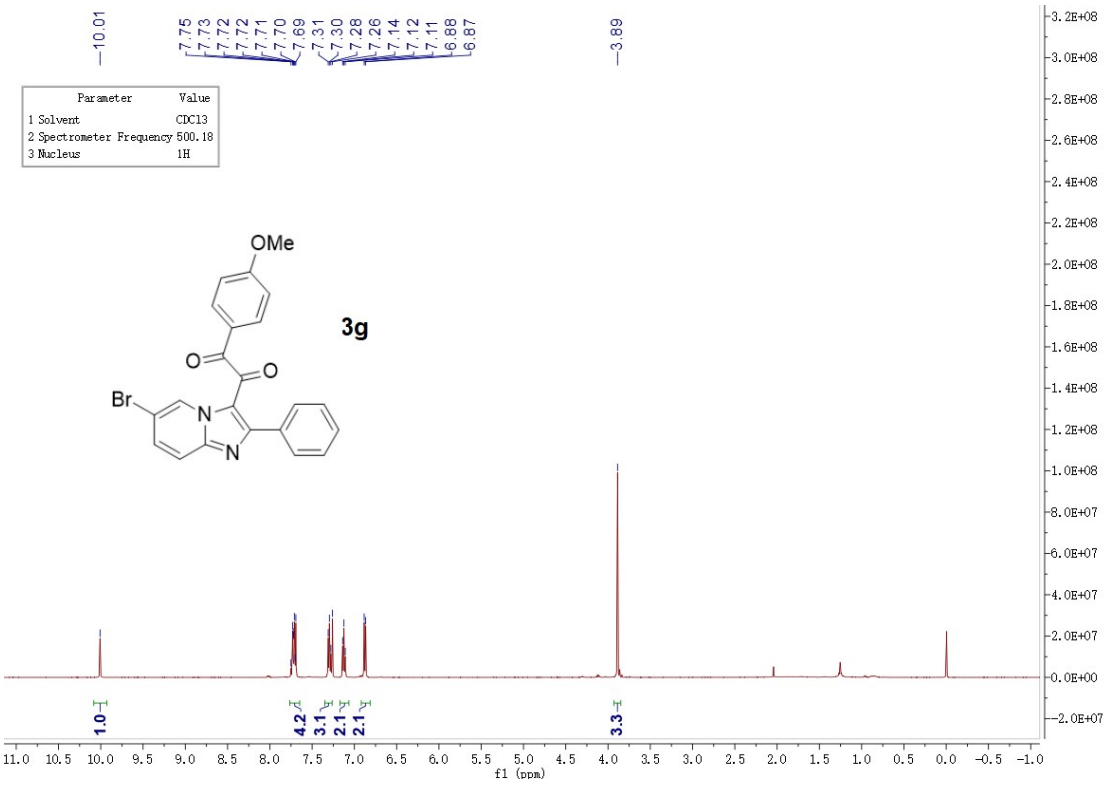
2 Spectrometer Frequency 125.77
3 Nucleus 13C
OMe
O
O
N
N
MeO
3f
f1 (ppm)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7.30
7.28
7.26
7.14
7.12
7.11
6.88
6.87
3.89
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
OMe
O
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Br
N
N
3g
1.0
4.2
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2.1
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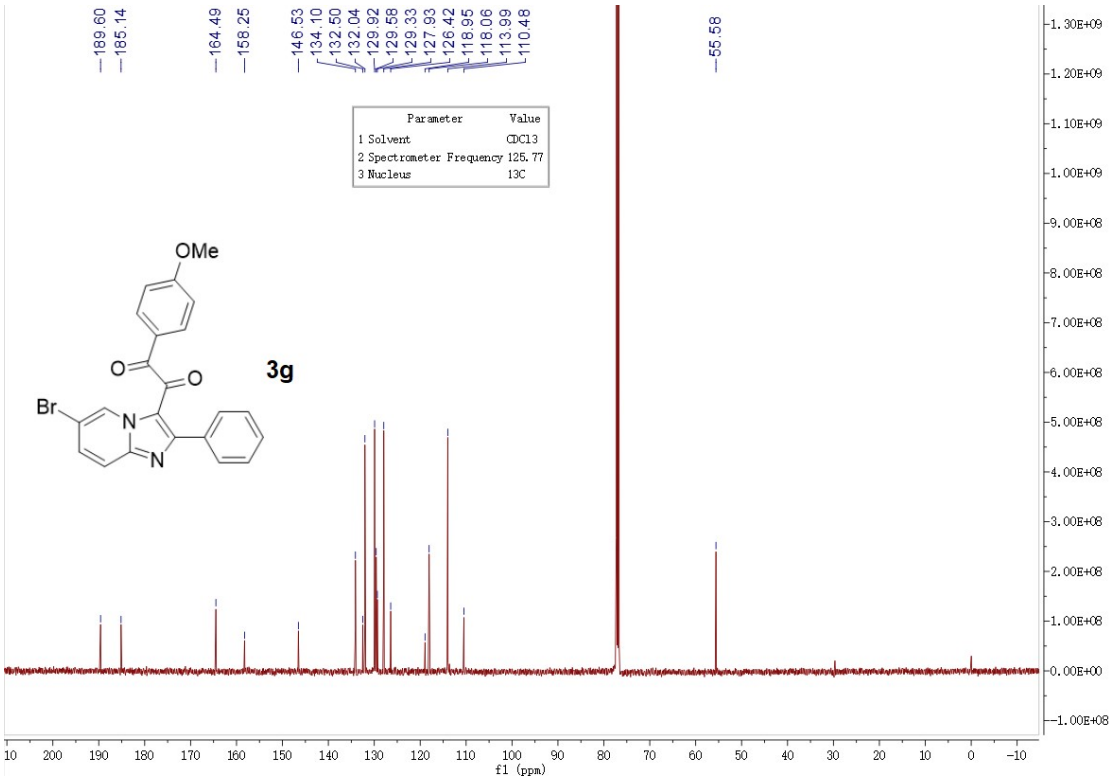
3.3
f1 (ppm)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127.93
126.42
118.95
118.06
113.99
110.48
55.58
Parameter Value
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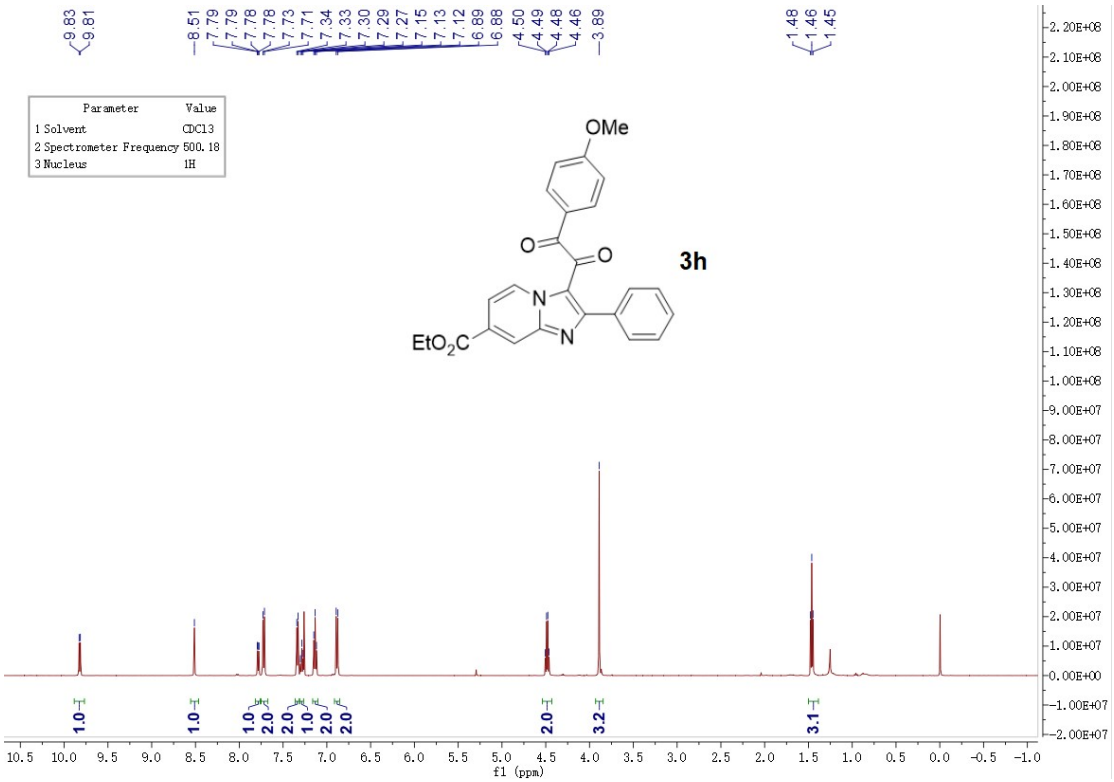
2 Spectrometer Frequency 125.77
3 Nucleus 13C
OMe
O
O
Br
N
N
3g
f1 (ppm)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7.29
7.27
7.15
7.13
7.12
6.89
6.88
4.50
4.49
4.48
4.46
3.89
1.48
1.46
1.45
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
OMe
O
O
N
N
EtO2C
3h
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2.0
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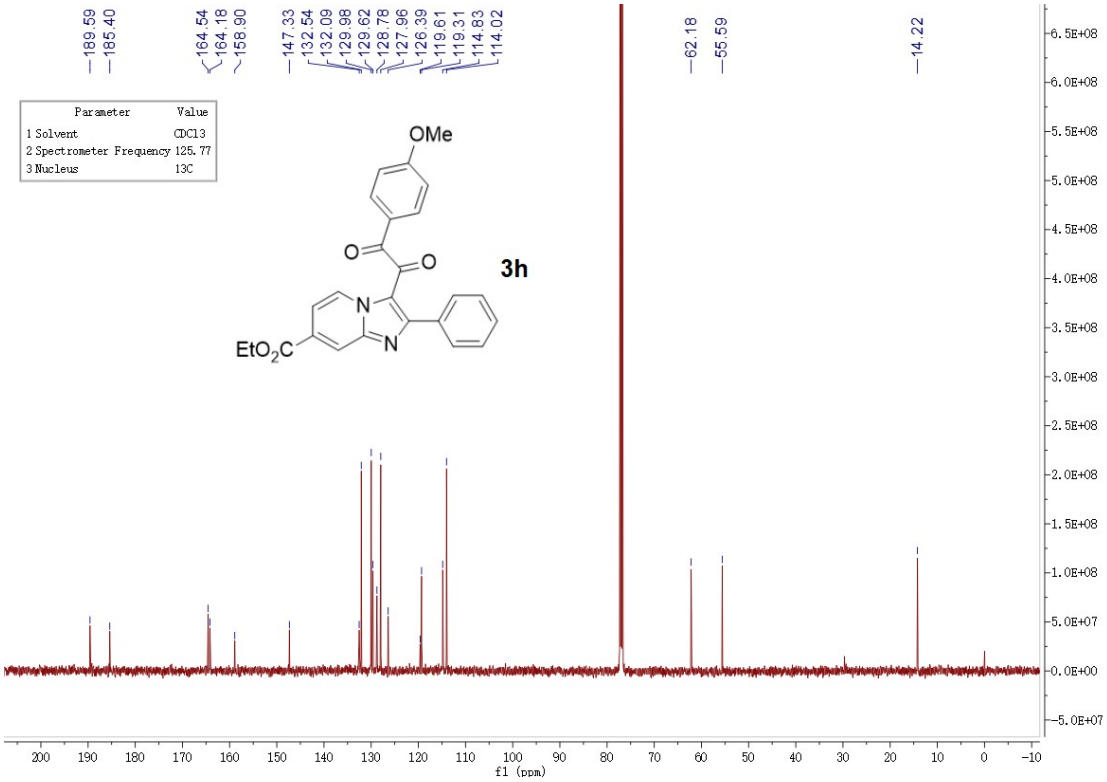
3.1
f1 (ppm)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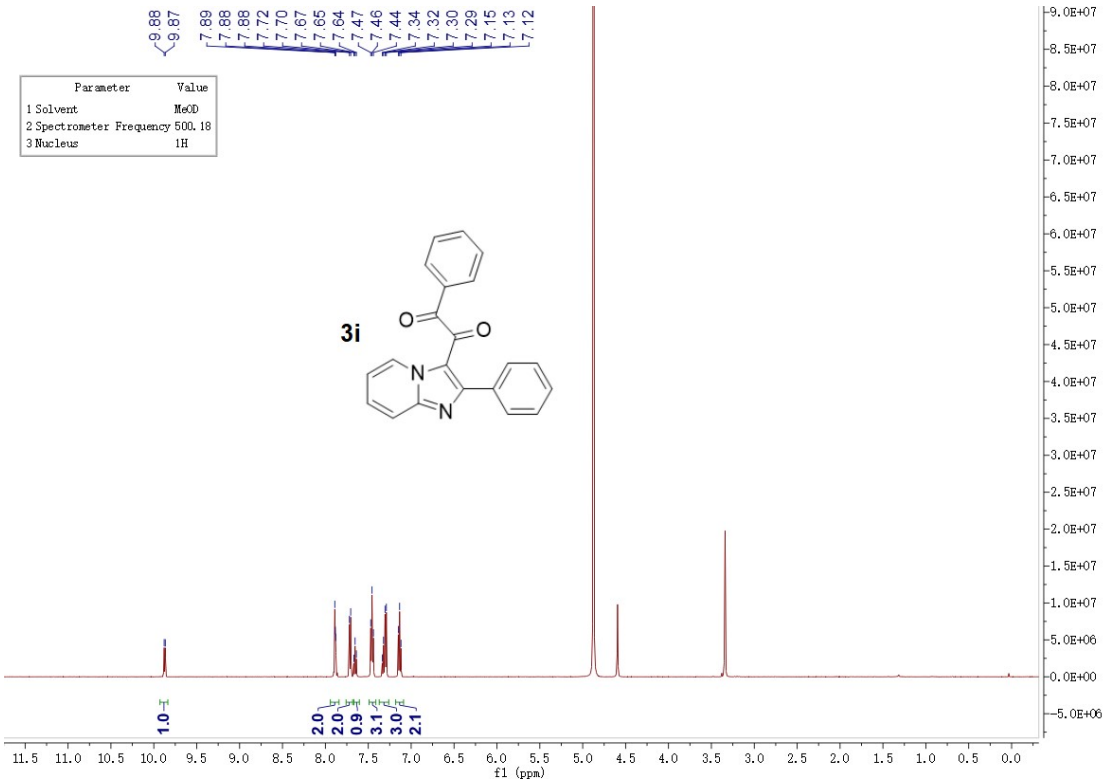
126.39
119.61
119.31
114.83
114.02
62.18
55.59
14.22
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 125.77
3 Nucleus 13C
OMe
O
O
N
N
EtO2C
3h
f1 (ppm)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7.47
7.46
7.44
7.34
7.32
7.30
7.29
7.15
7.13
7.12
Parameter Value
1 Solvent MeOD
2 Spectrometer Frequency 500.18
3 Nucleus 1H
3i
O
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N
N
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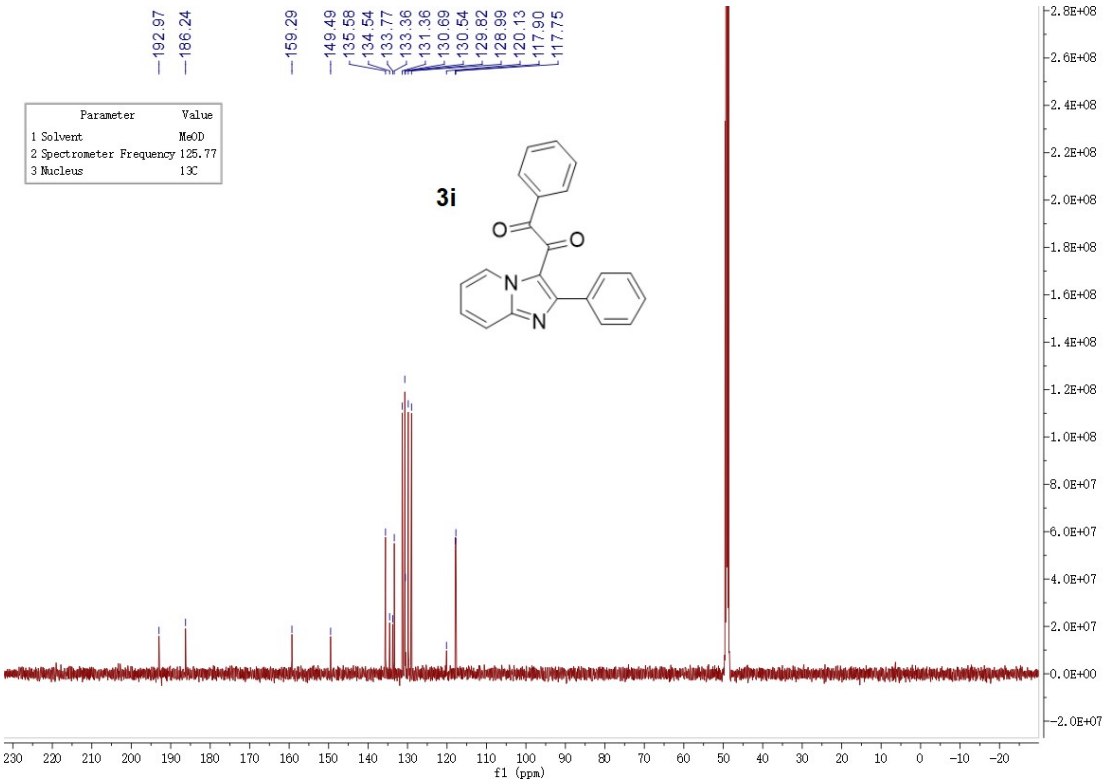
3.1
3.0
2.1
f1 (ppm)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117.75
Parameter Value
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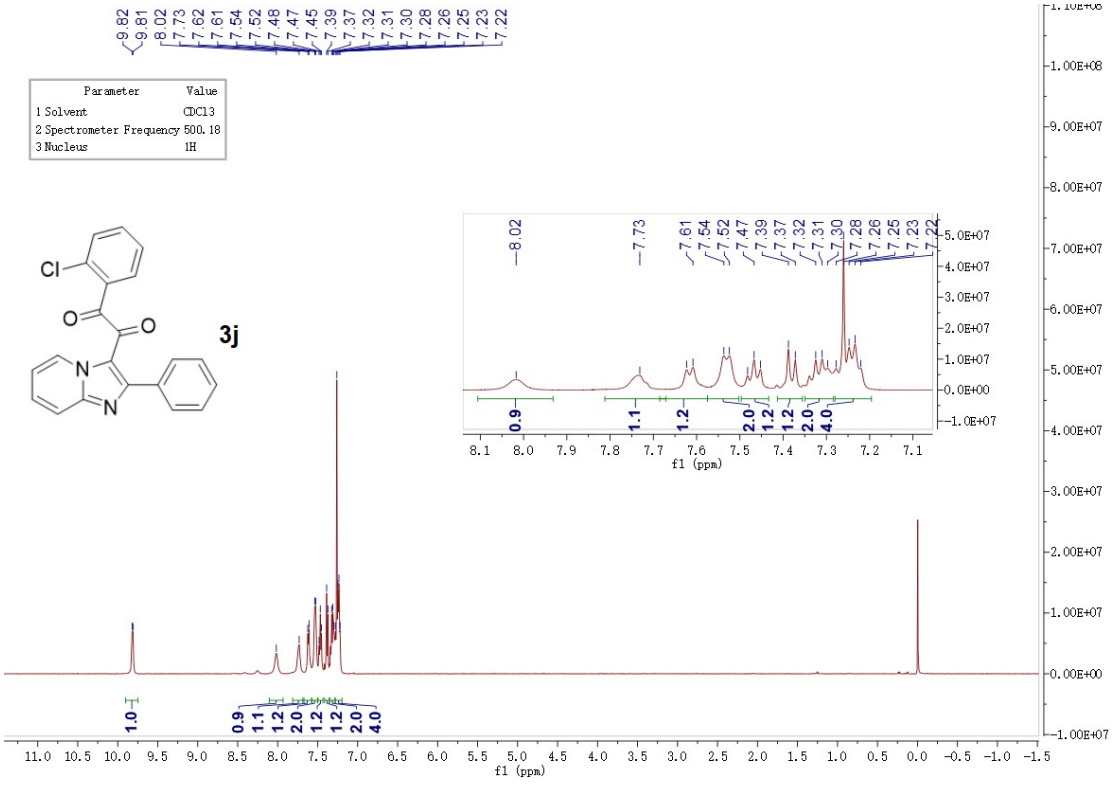
2 Spectrometer Frequency 125.77
3 Nucleus 13C
3i
f1 (ppm)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7.32
7.31
7.30
7.28
7.26
7.25
7.23
7.22
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
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1.1
1.2
2.0
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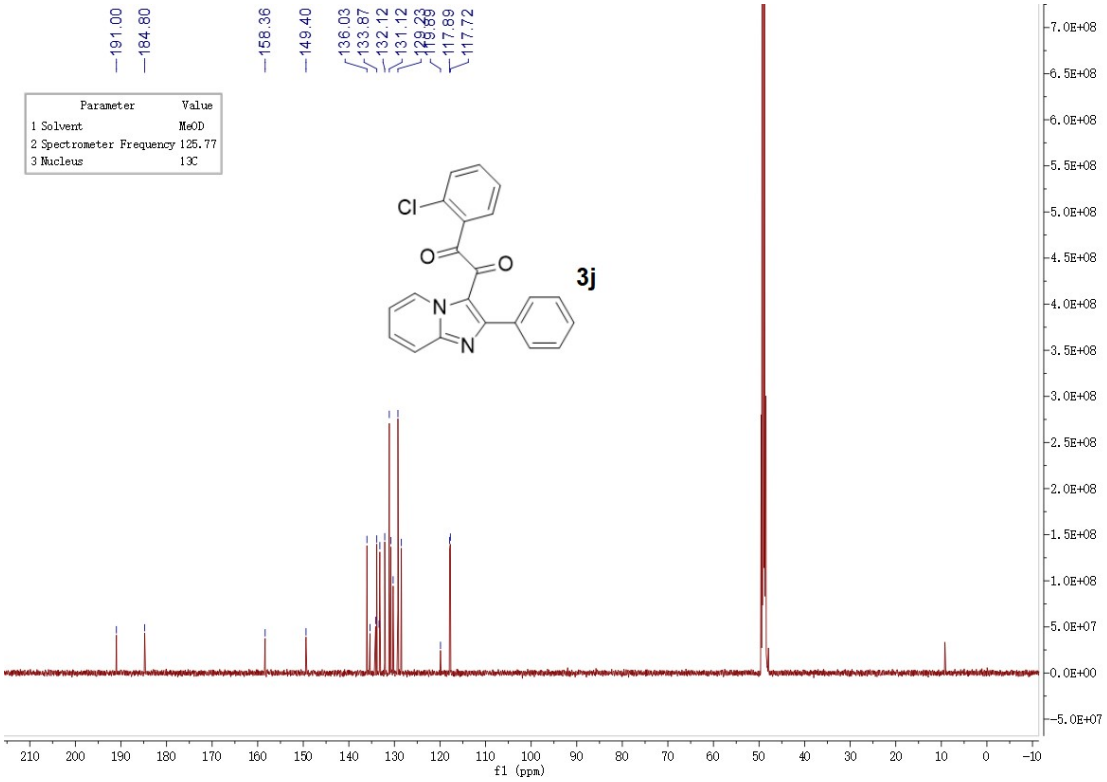
4.0
f1 (ppm)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119.89
117.89
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Parameter Value
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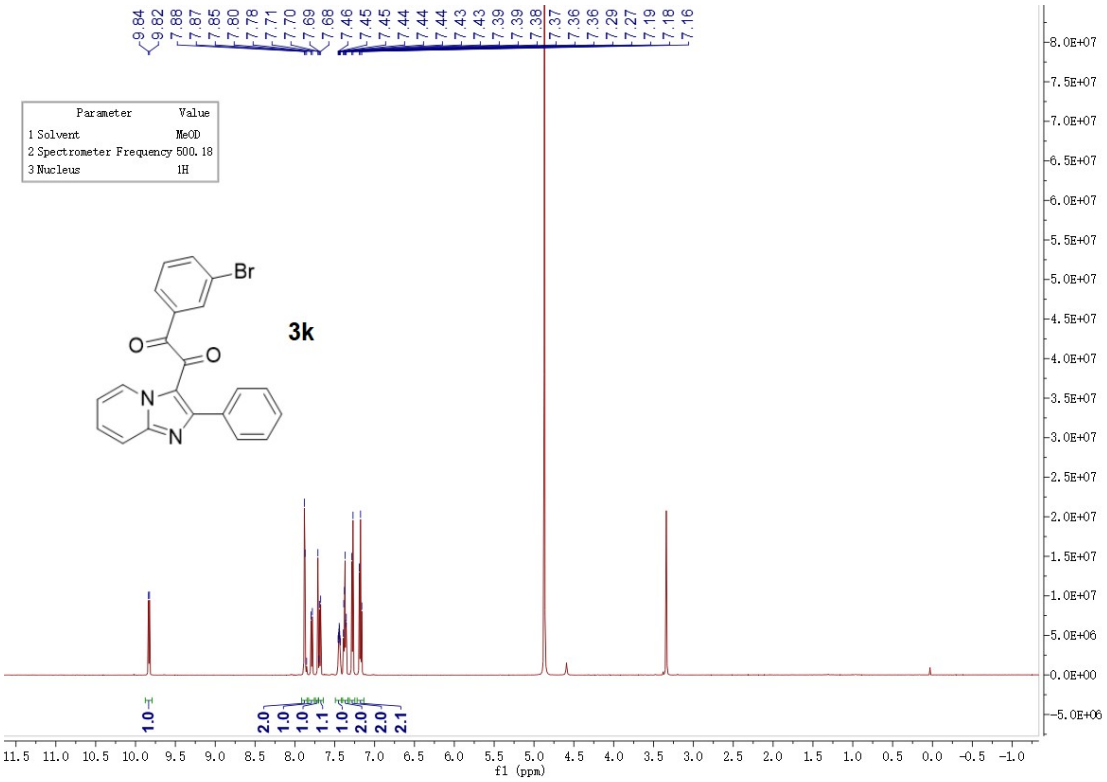
2 Spectrometer Frequency 125.77
3 Nucleus 13C
Cl
O
O
N
N
3j
f1 (ppm)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7.45
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7.44
7.43
7.43
7.39
7.39
7.38
7.37
7.36
7.36
7.29
7.27
7.19
7.18
7.16
Parameter Value
1 Solvent MeOD
2 Spectrometer Frequency 500.18
3 Nucleus 1H
Br
O
O
N
N
3k
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2.0
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1.0
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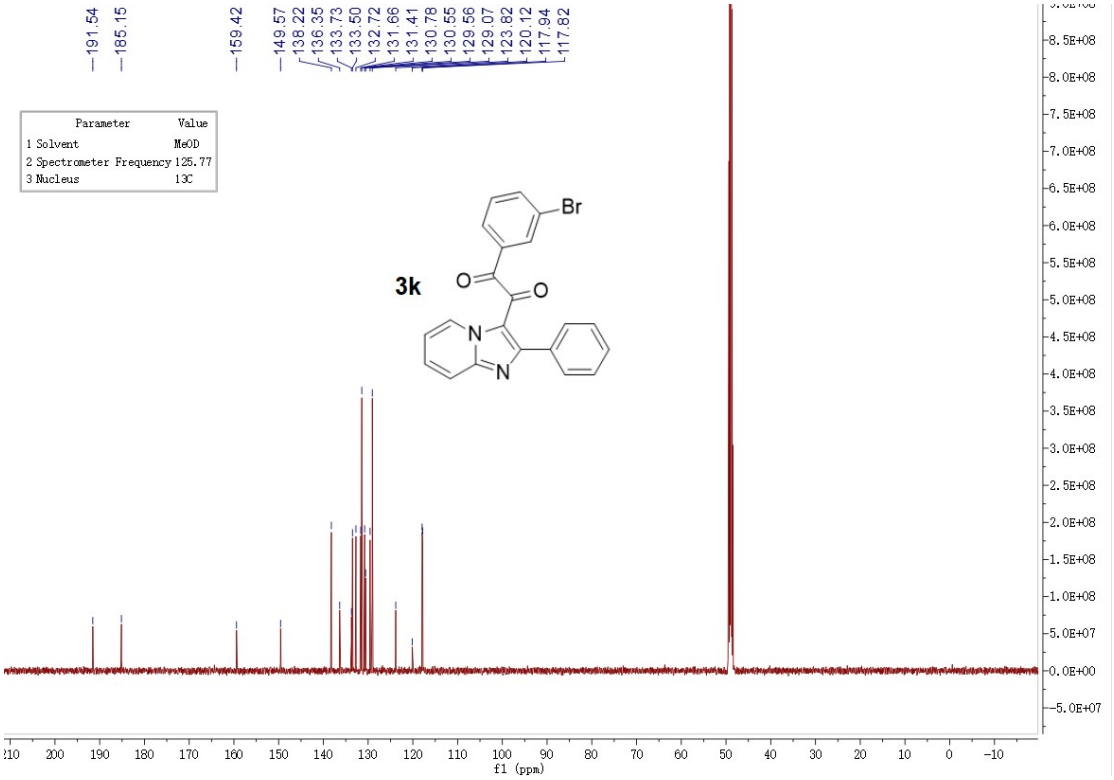
2.1
f1 (ppm)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129.56
129.07
123.82
120.12
117.94
117.82
Parameter Value
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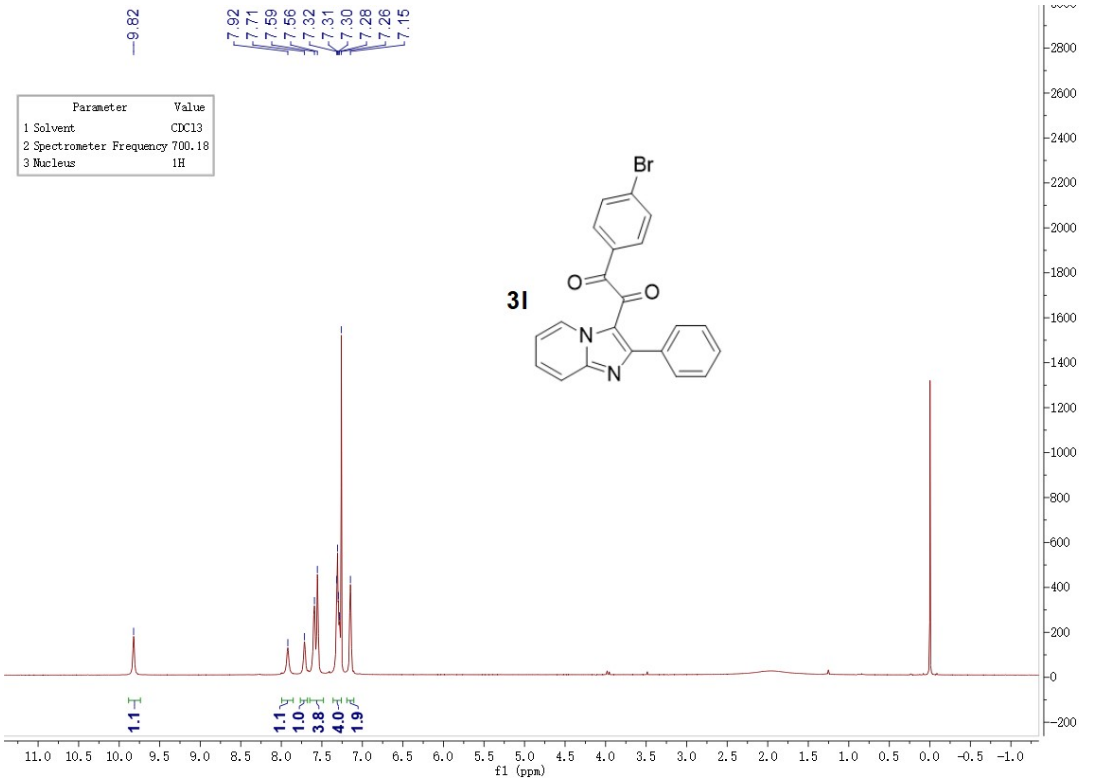
2 Spectrometer Frequency 125.77
3 Nucleus 13C
Br
O
O
N
N
3k
f1 (ppm)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7.30
7.28
7.26
7.15
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 700.18
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N
N
3l
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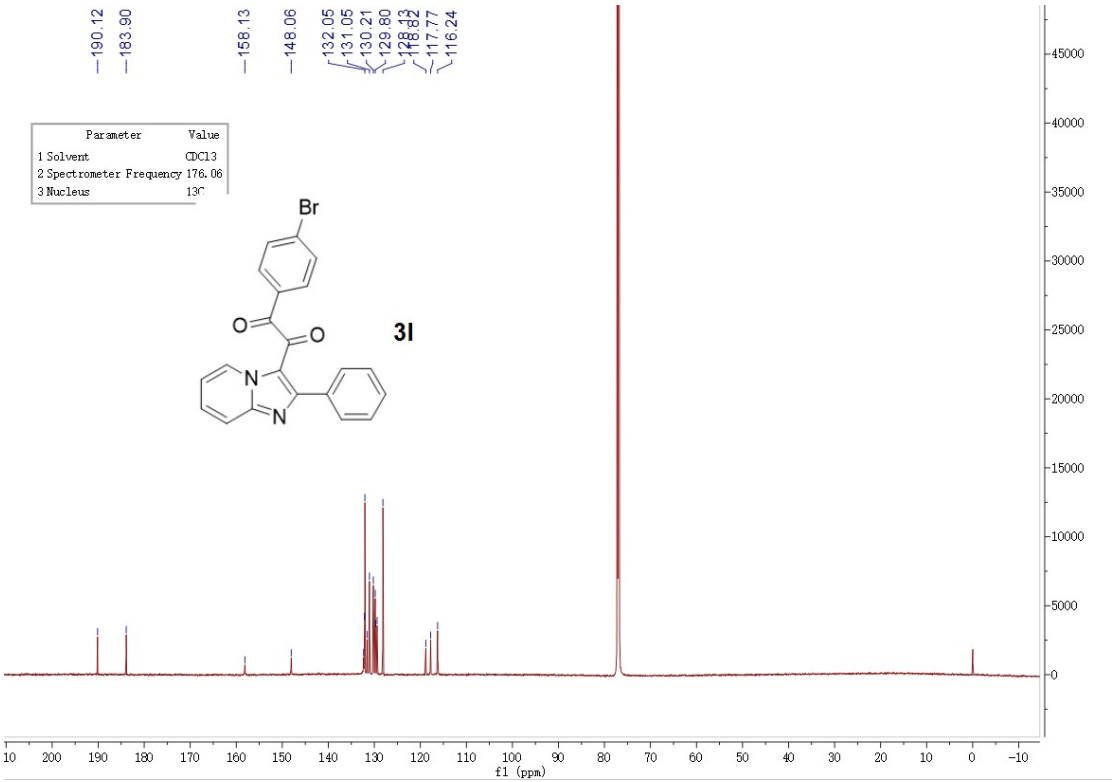
3.8
4.0
1.9
f1 (ppm)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117.77
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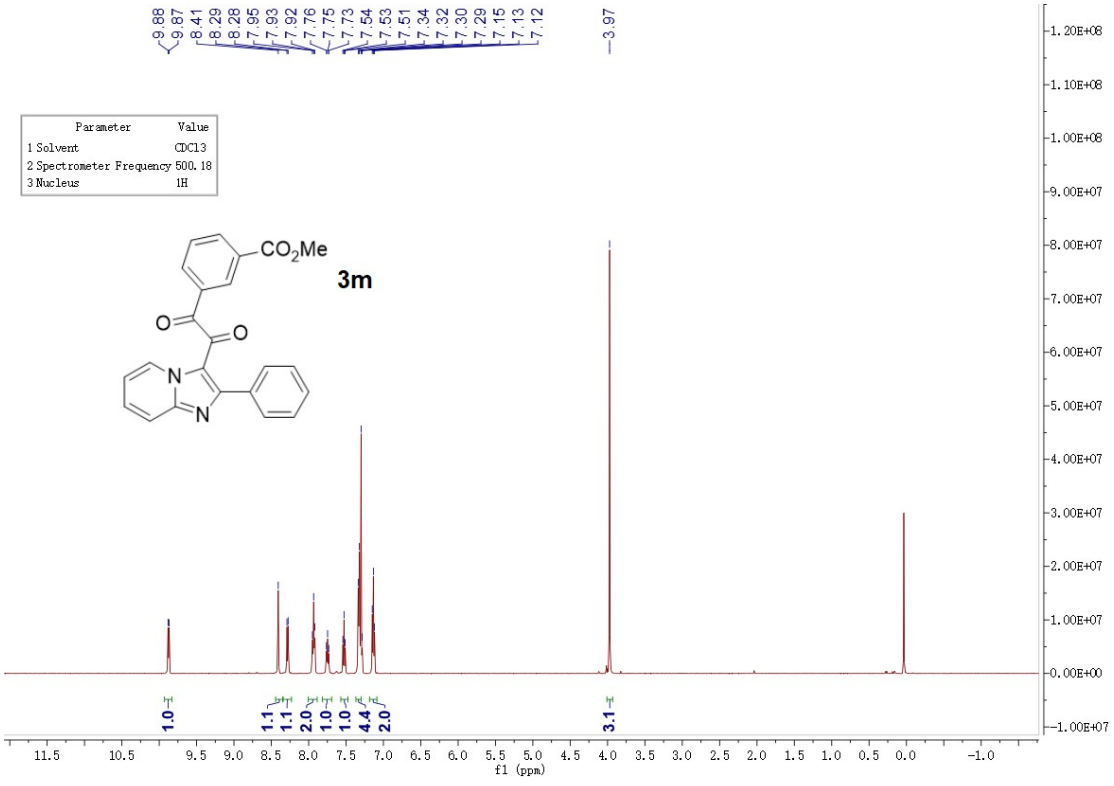
2 Spectrometer Frequency 176.06
3 Nucleus 13C
Br
O
O
N
N
3l
f1 (ppm)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7.73
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7.53
7.51
7.34
7.32
7.30
7.29
7.15
7.13
7.12
3.97
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
CO2Me
O
O
N
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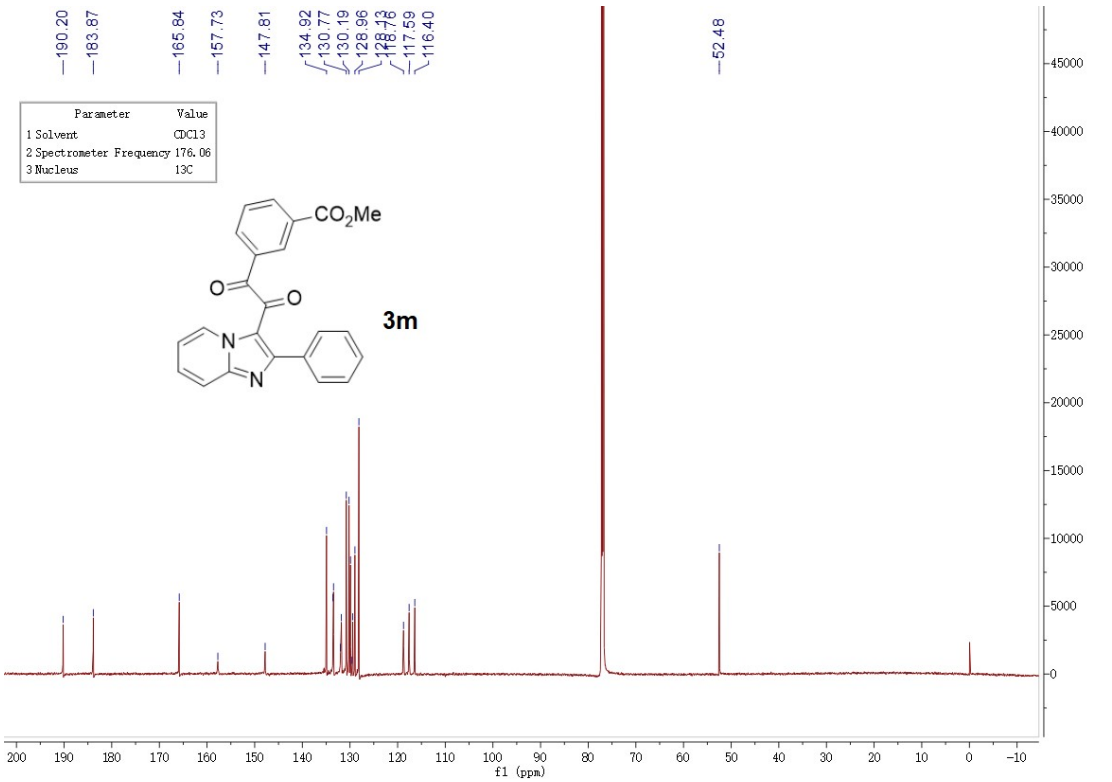
3.1
f1 (ppm)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117.59
116.40
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Parameter Value
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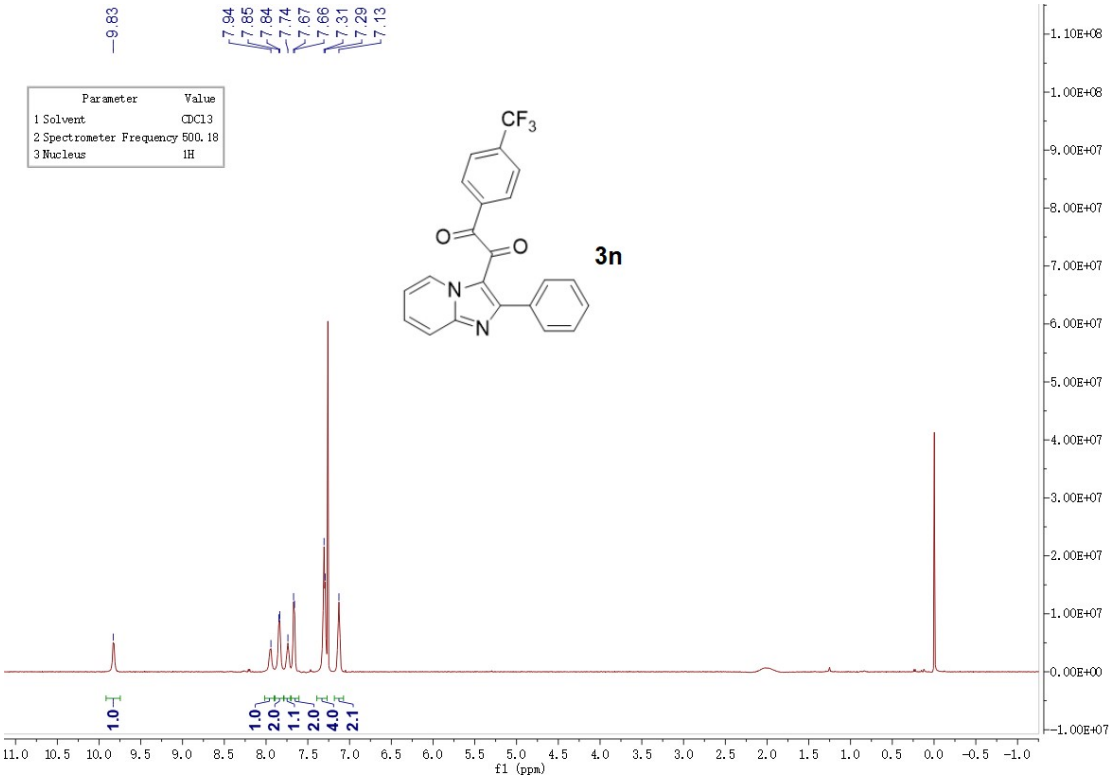
2 Spectrometer Frequency 176.06
3 Nucleus 13C
CO2Me
O
O
N
N
3m
f1 (ppm)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7.31
7.29
7.13
Parameter Value
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2 Spectrometer Frequency 500.18
3 Nucleus 1H
CF3
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N
3n
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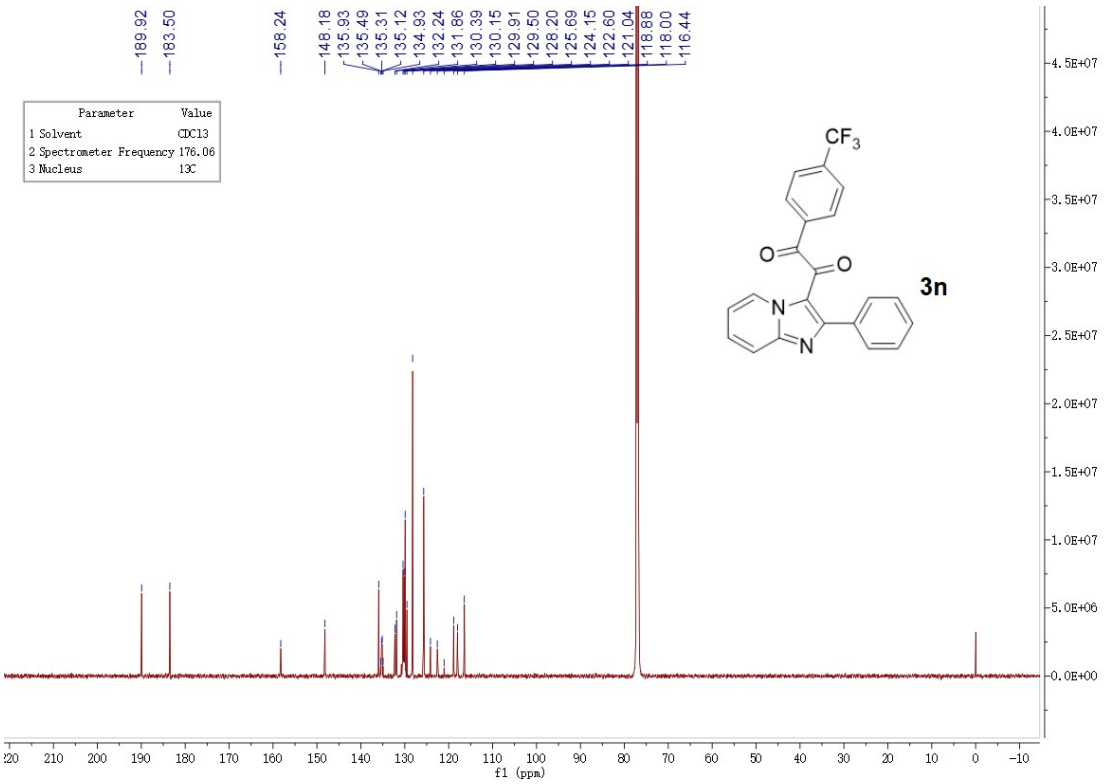
1.0
2.0
1.1
2.0
4.0
2.1
f1 (ppm)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129.91
129.50
128.20
125.69
124.15
122.60
121.04
118.88
118.00
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Parameter Value
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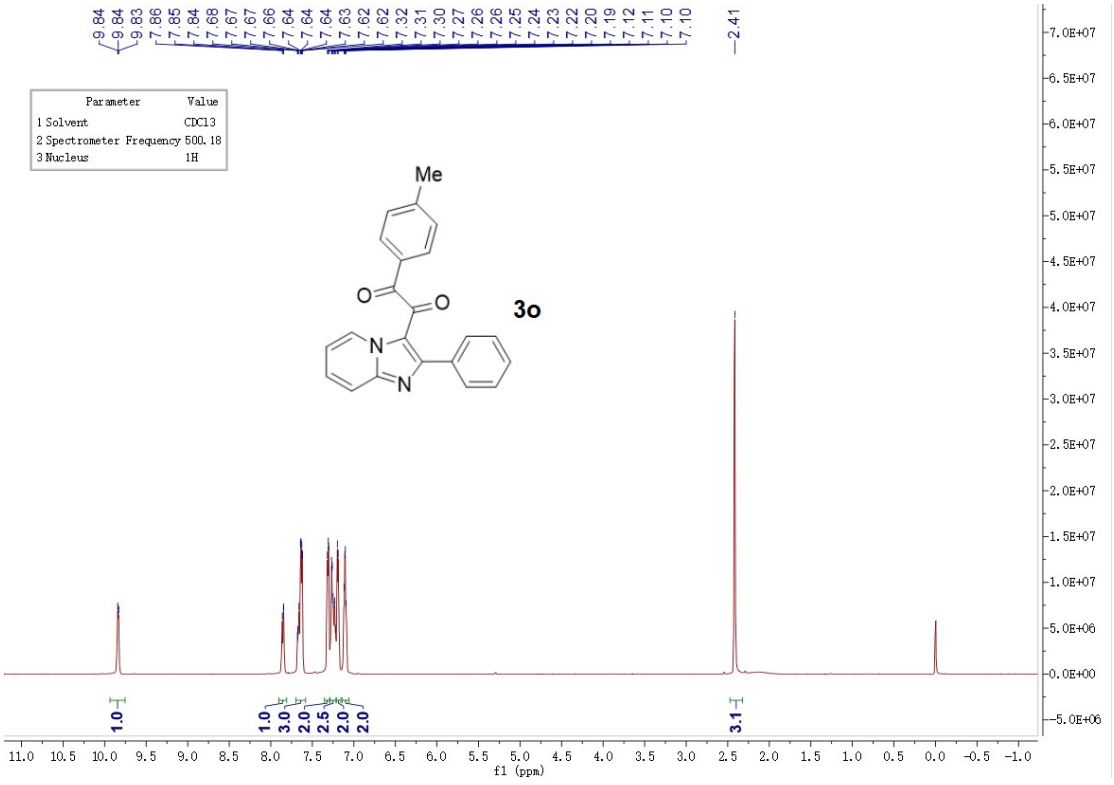
3 Nucleus 13C
CF3
O
O
N
N
3n
f1 (ppm)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7.26
7.25
7.24
7.23
7.22
7.20
7.19
7.12
7.11
7.10
7.10
2.41
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
Me
O
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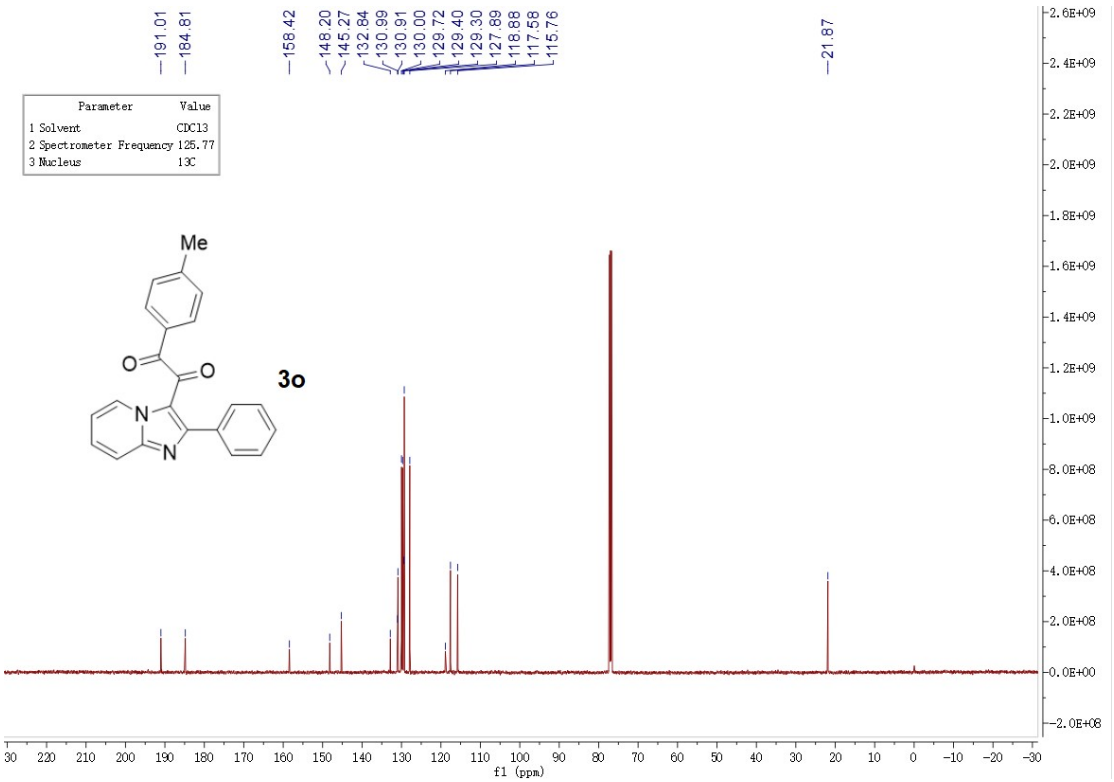
3.1
f1 (ppm)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129.40
129.30
127.89
118.88
117.58
115.76
21.87
Parameter Value
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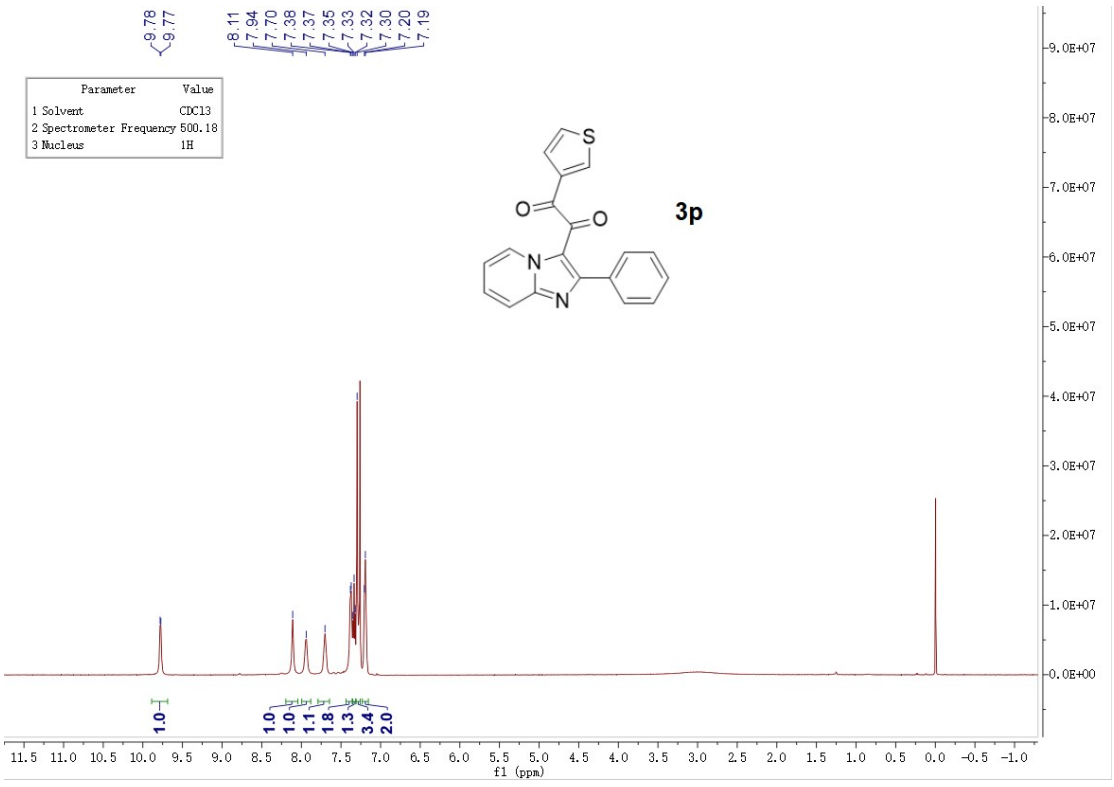
2 Spectrometer Frequency 125.77
3 Nucleus 13C
Me
O
O
N
N
3o
f1 (ppm)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7.38
7.37
7.35
7.33
7.32
7.30
7.20
7.19
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
S
O
O
N
N
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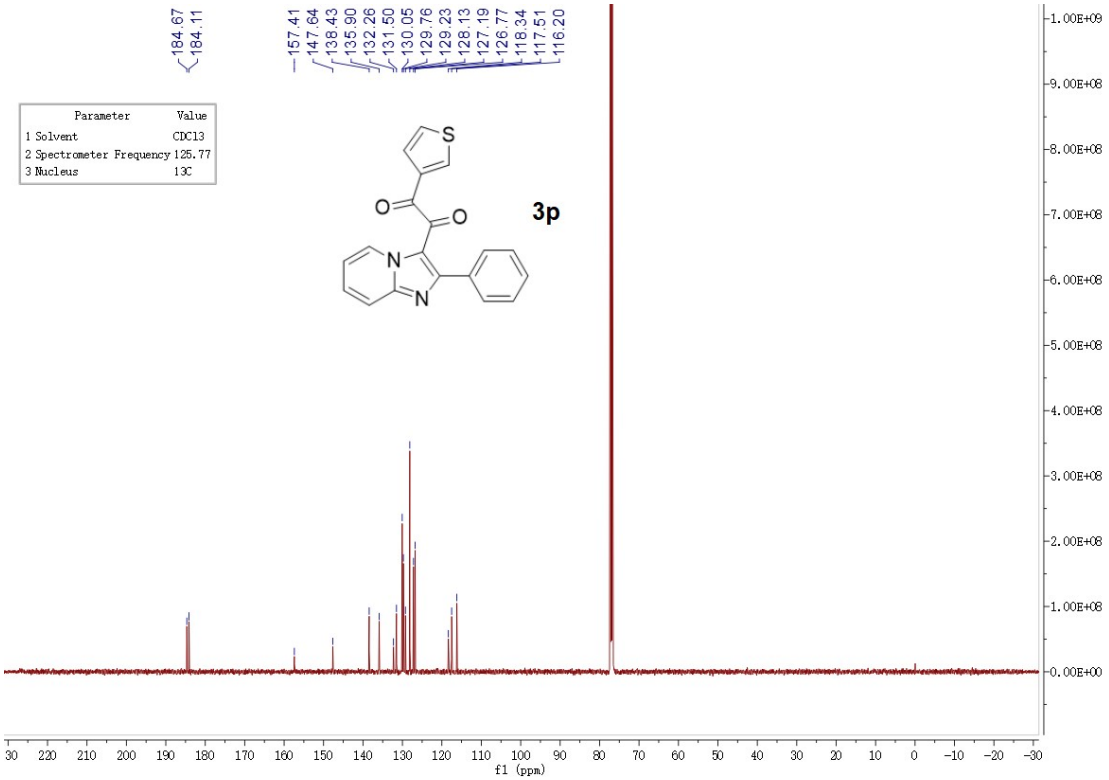
1.0
1.0
1.1
1.8
1.3
3.4
2.0
f1 (ppm)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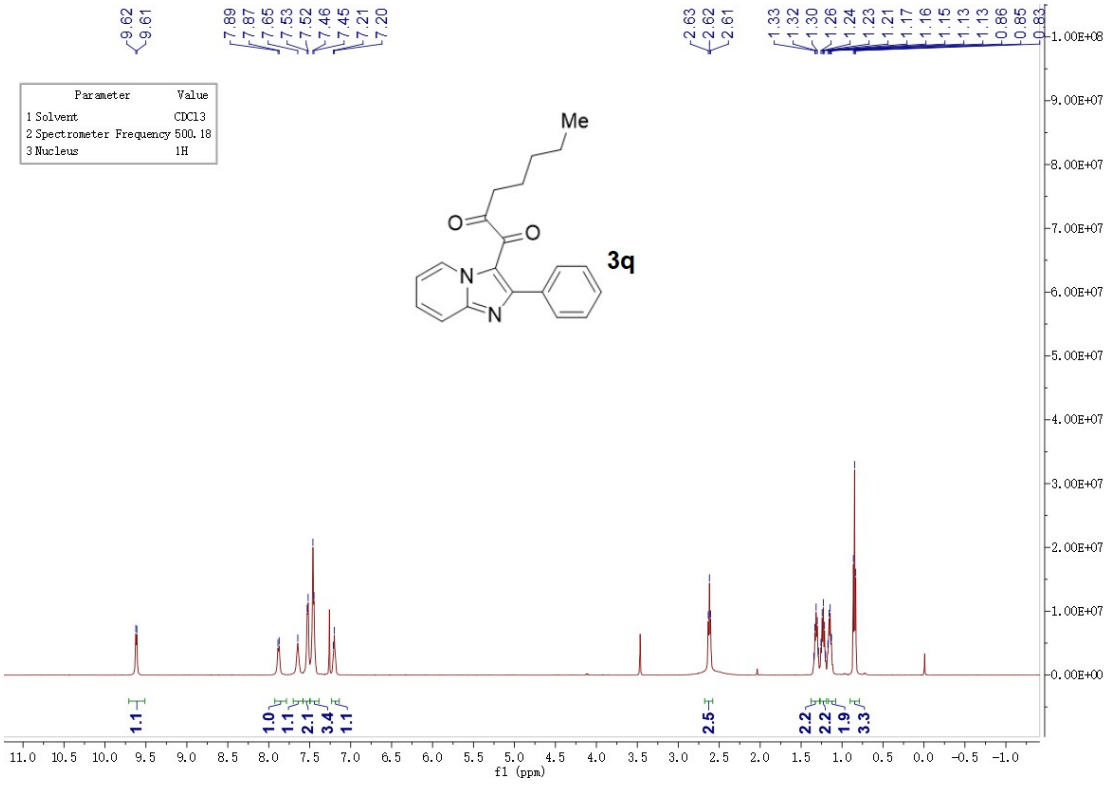
129.76
129.23
128.13
127.19
126.77
118.34
117.51
116.20
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 125.77
3 Nucleus 13C
S
O
O
N
N
3p
f1 (ppm)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7.52
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7.21
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2.62
2.61
1.33
1.32
1.30
1.26
1.24
1.23
1.21
1.17
1.16
1.15
1.13
1.13
0.86
0.85
0.83
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
Me
O
O
N
N
3q
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2.5
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2.2
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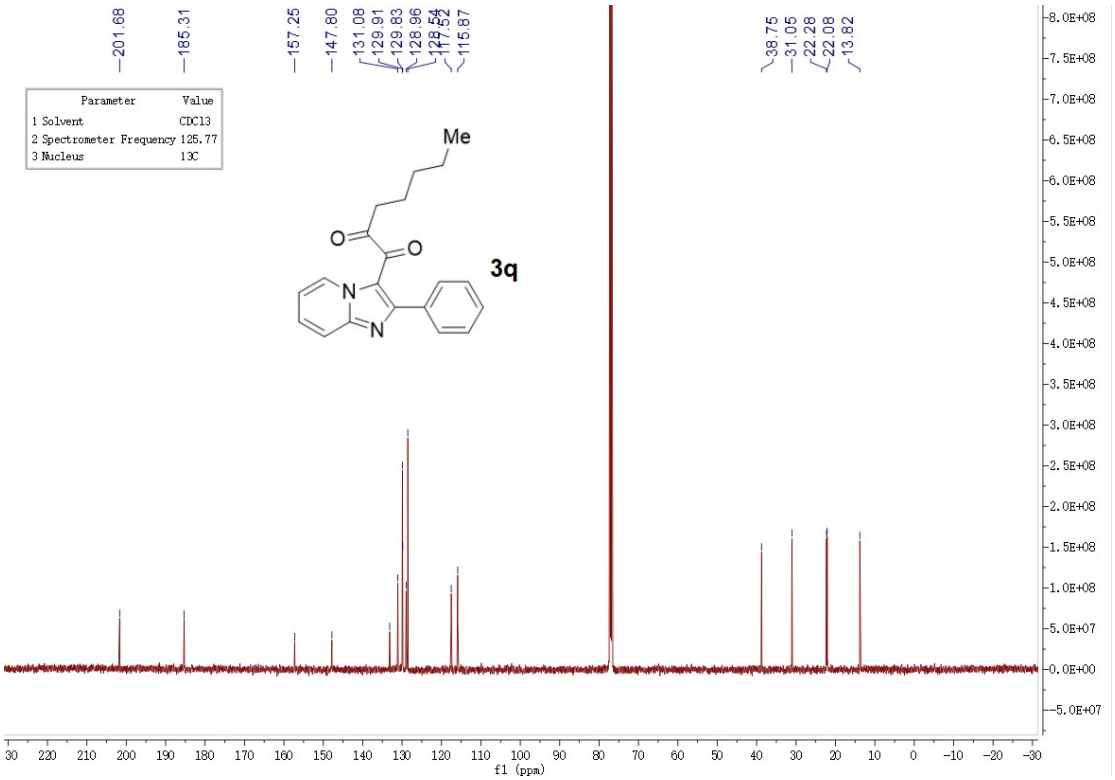
3.3
f1 (ppm)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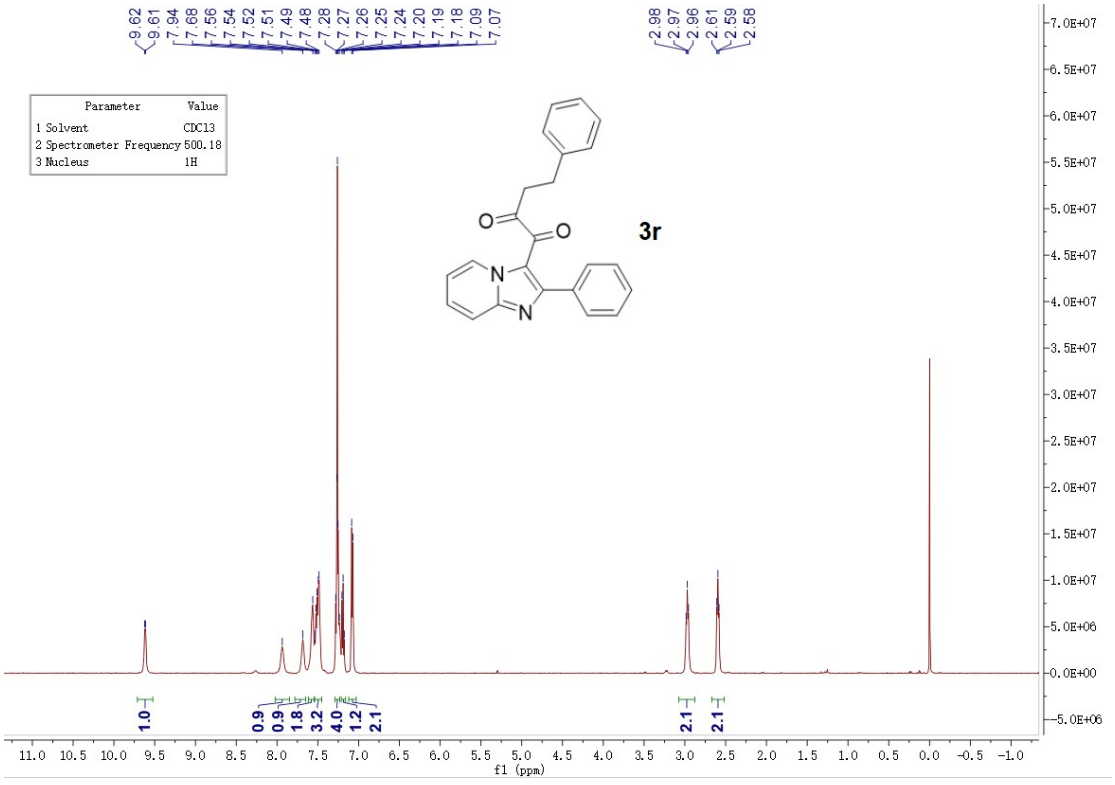
117.52
115.87
38.75
31.05
22.28
22.08
13.82
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 125.77
3 Nucleus 13C
Me
O
O
N
N
3q
f1 (ppm)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9.61
7.94
7.68
7.56
7.54
7.52
7.51
7.49
7.48
7.28
7.27
7.26
7.25
7.24
7.20
7.19
7.18
7.09
7.07
2.98
2.97
2.96
2.61
2.59
2.58
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
O
O
N
N
3r
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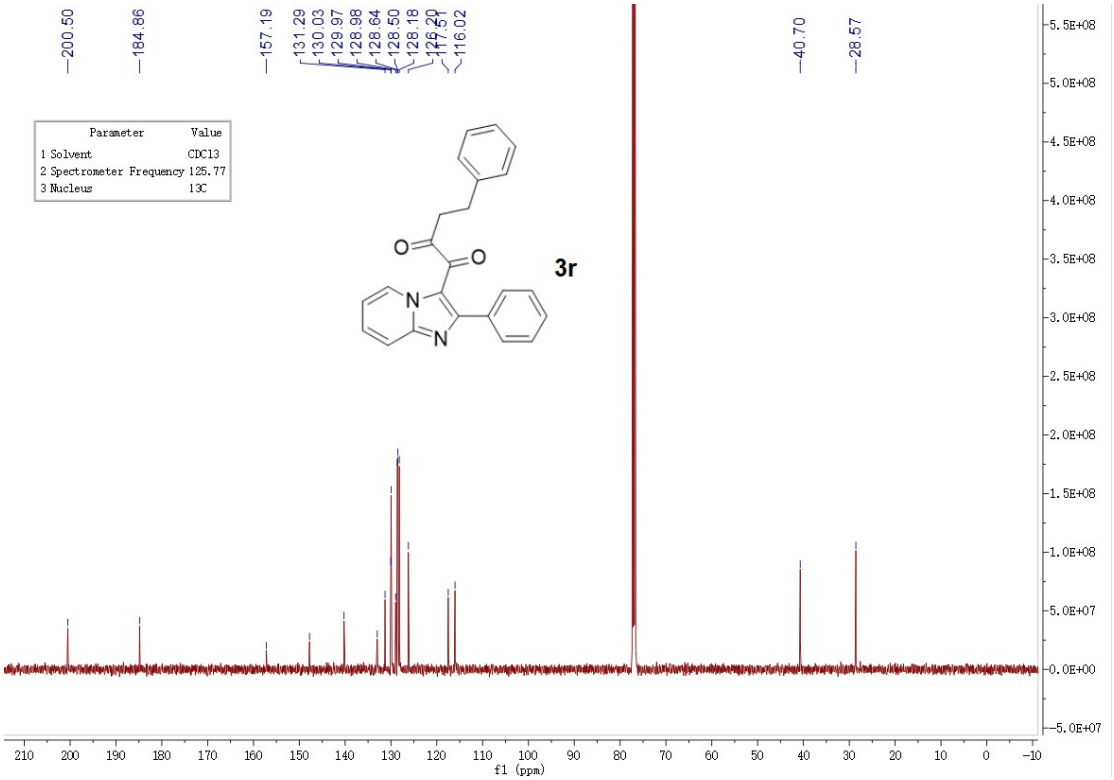
0.9
1.8
3.2
4.0
1.2
2.1
2.1
2.1
f1 (ppm)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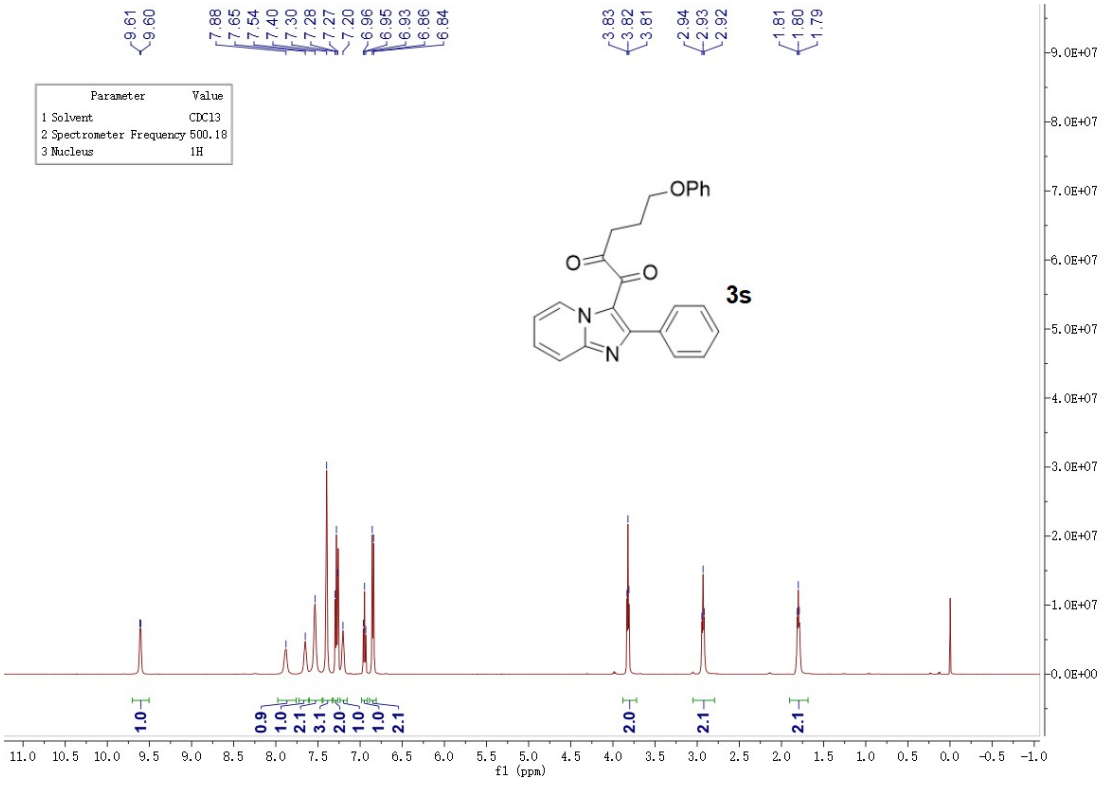
184.86
157.19
131.29
130.03
129.97
128.98
128.64
128.50
128.18
126.20
117.51
116.02
40.70
28.57
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 125.77
3 Nucleus 13C
3r
f1 (ppm)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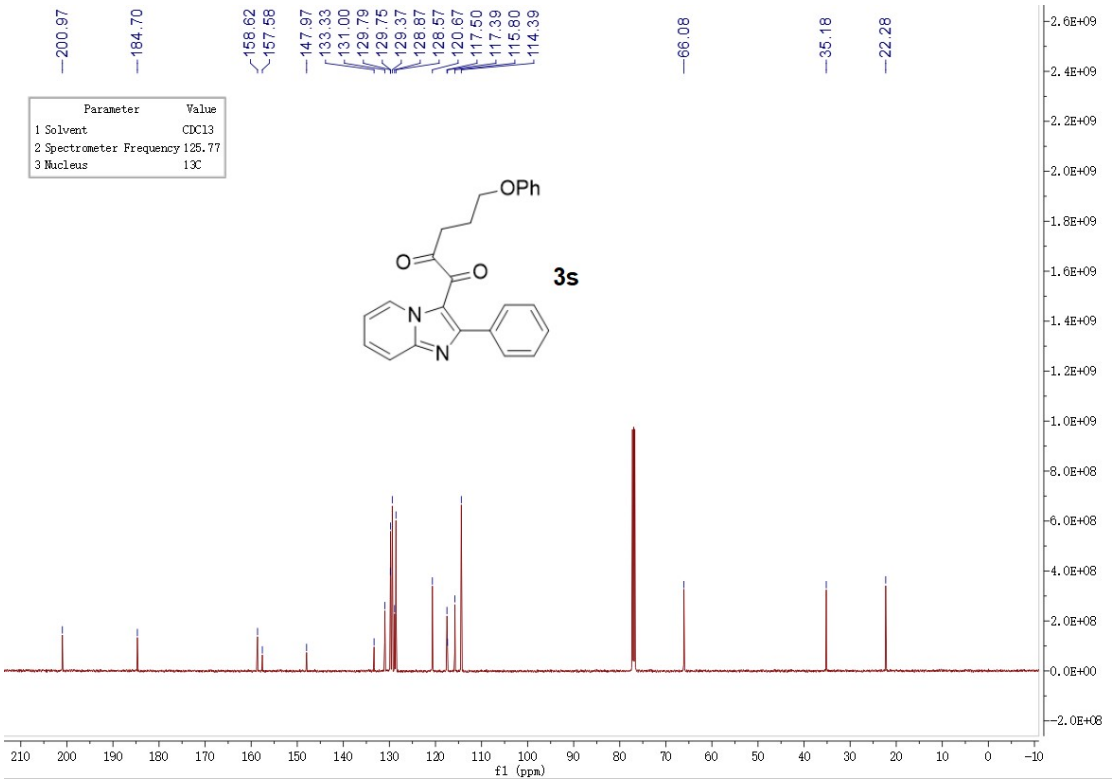
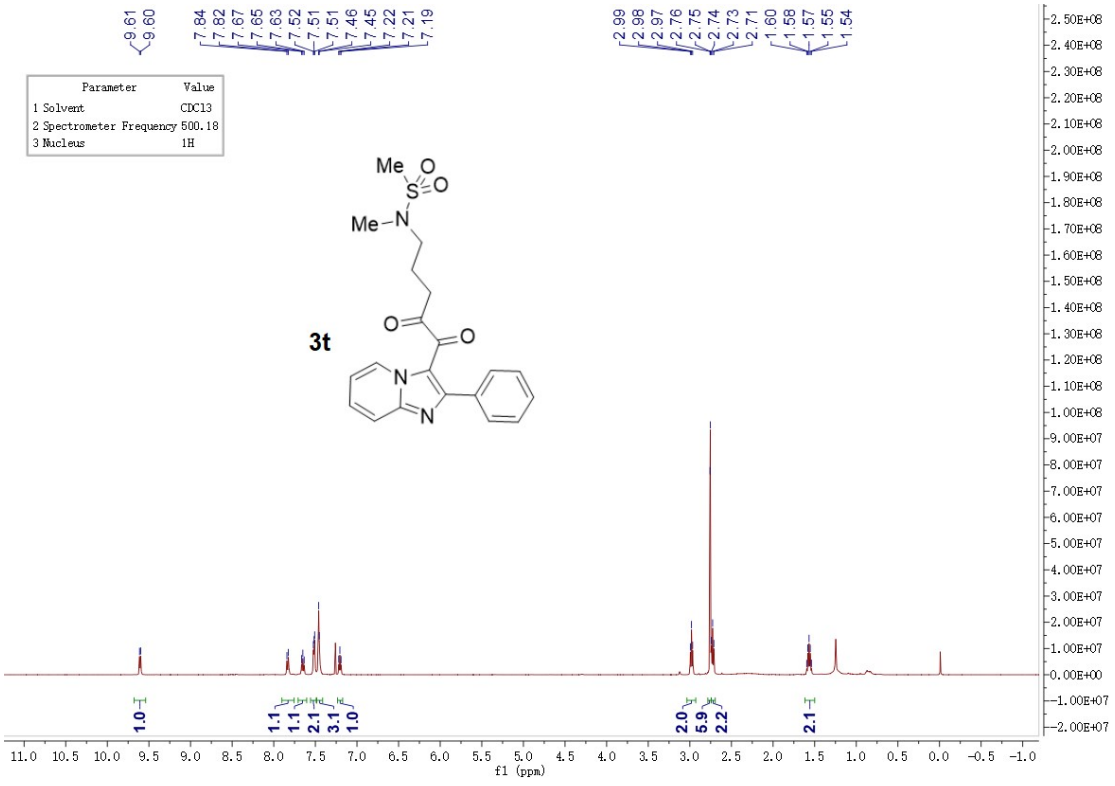
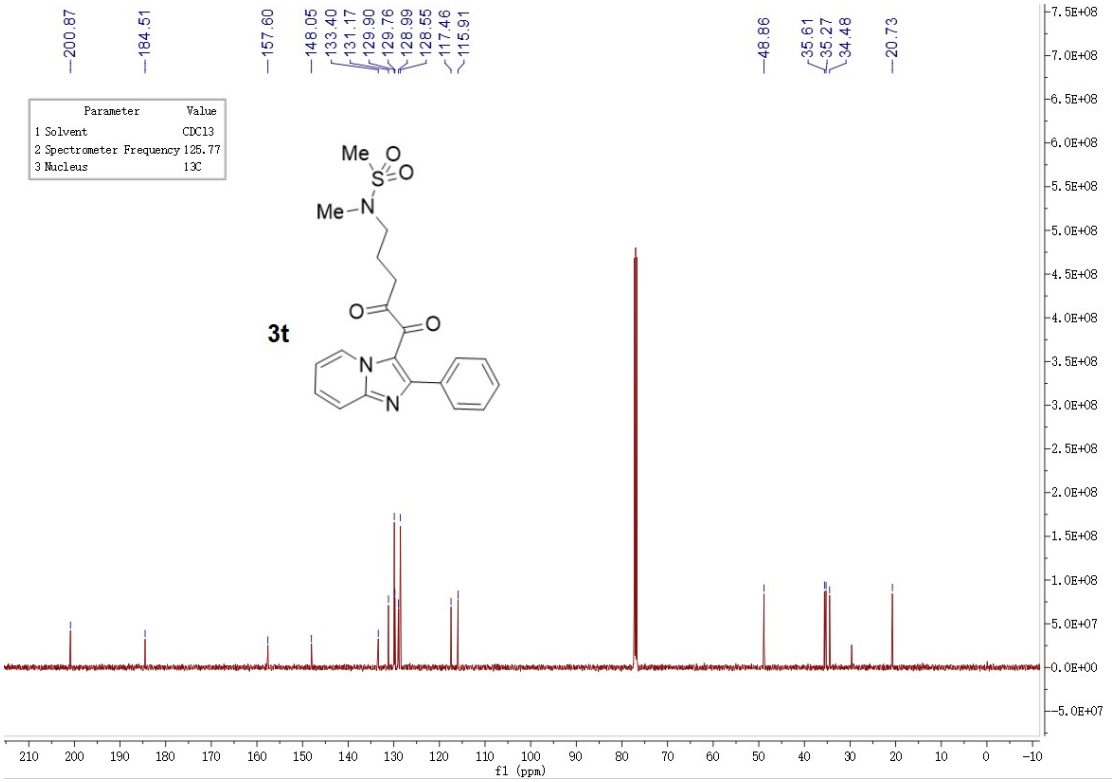
7.65
7.54
7.40
7.30
7.28
7.27
7.20
6.96
6.95
6.93
6.86
6.84
3.83
3.82
3.81
2.94
2.93
2.92
1.81
1.80
1.79
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
OPh
3s
1.0
0.9
1.0
2.1
3.1
2.0
1.0
1.0
2.1
2.0
2.1
2.1
f1 (ppm)


200.97
184.70
158.62
157.58
147.97
133.33
131.00
129.79
129.75
129.37
128.87
128.57
120.67
117.50
117.39
115.80
114.39
66.08
35.18
22.28
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 125.77
3 Nucleus 13C
OPh
O
O
N
N
3s
f1 (ppm)


9.61
9.60
7.84
7.82
7.67
7.65
7.63
7.52
7.51
7.51
7.46
7.45
7.22
7.21
7.19
2.99
2.98
2.97
2.76
2.75
2.74
2.73
2.71
1.60
1.58
1.57
1.55
1.54
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
Me
O
S
O
Me
N
O
O
N
N
3t
1.0
1.1
1.1
2.1
3.1
1.0
2.0
5.9
2.2
2.1
f1 (ppm)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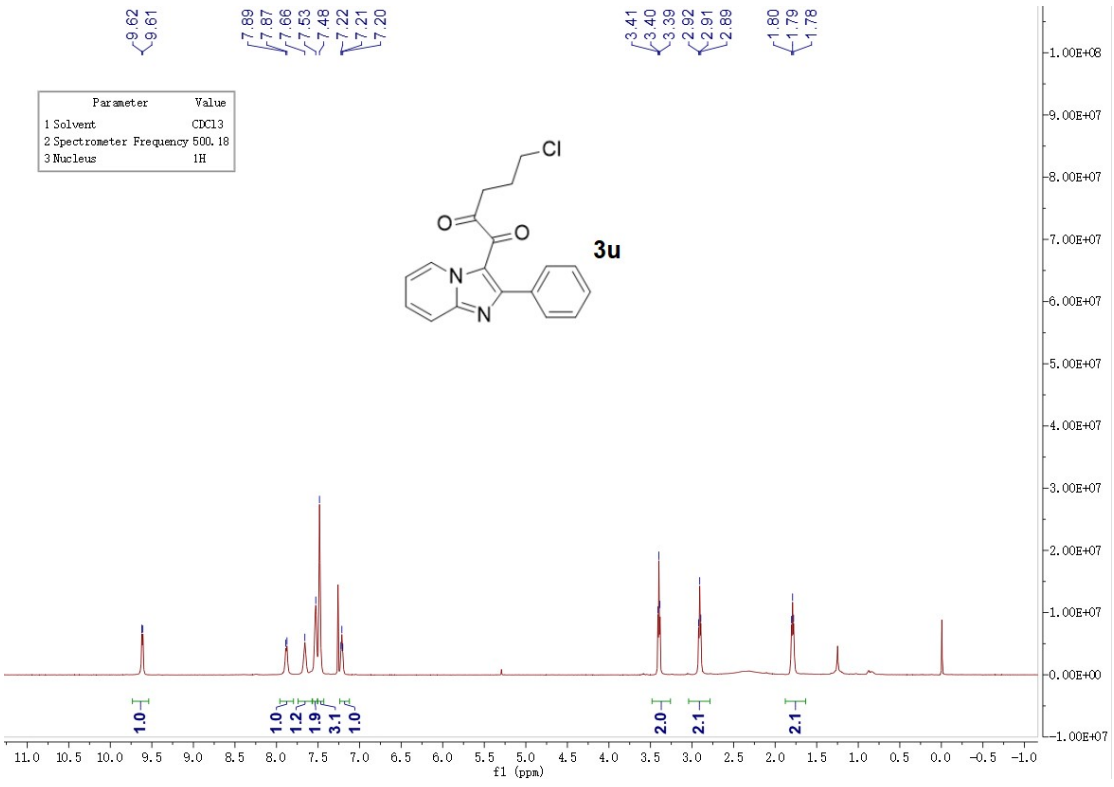
157.60
148.05
133.40
131.17
129.90
129.76
128.99
128.55
117.46
115.91
48.86
35.61
35.27
34.48
20.73
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 125.77
3 Nucleus 13C
Me
O
S
O
Me
N
O
O
N
N
3t
f1 (ppm)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9.61
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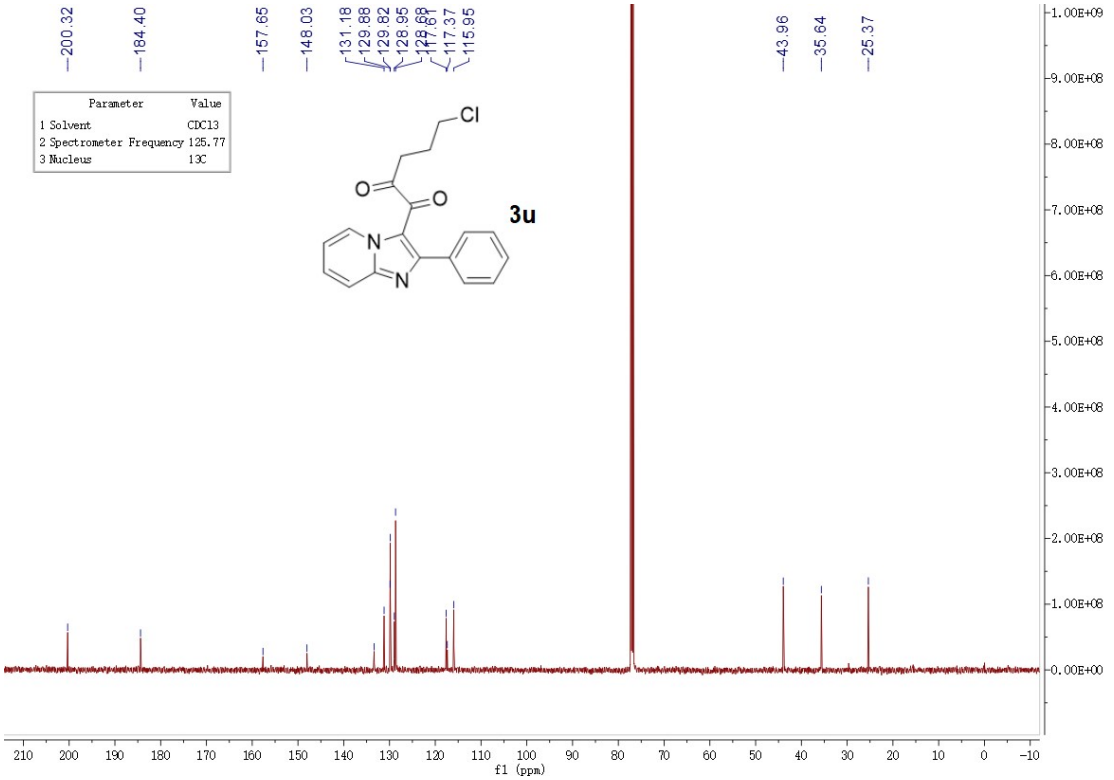
7.66
7.53
7.48
7.22
7.21
7.20
3.41
3.40
3.39
2.92
2.91
2.89
1.80
1.79
1.78
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
Cl
O
O
N
N
3u
1.0
1.0
1.2
1.9
3.1
1.0
2.0
2.1
2.1
f1 (ppm)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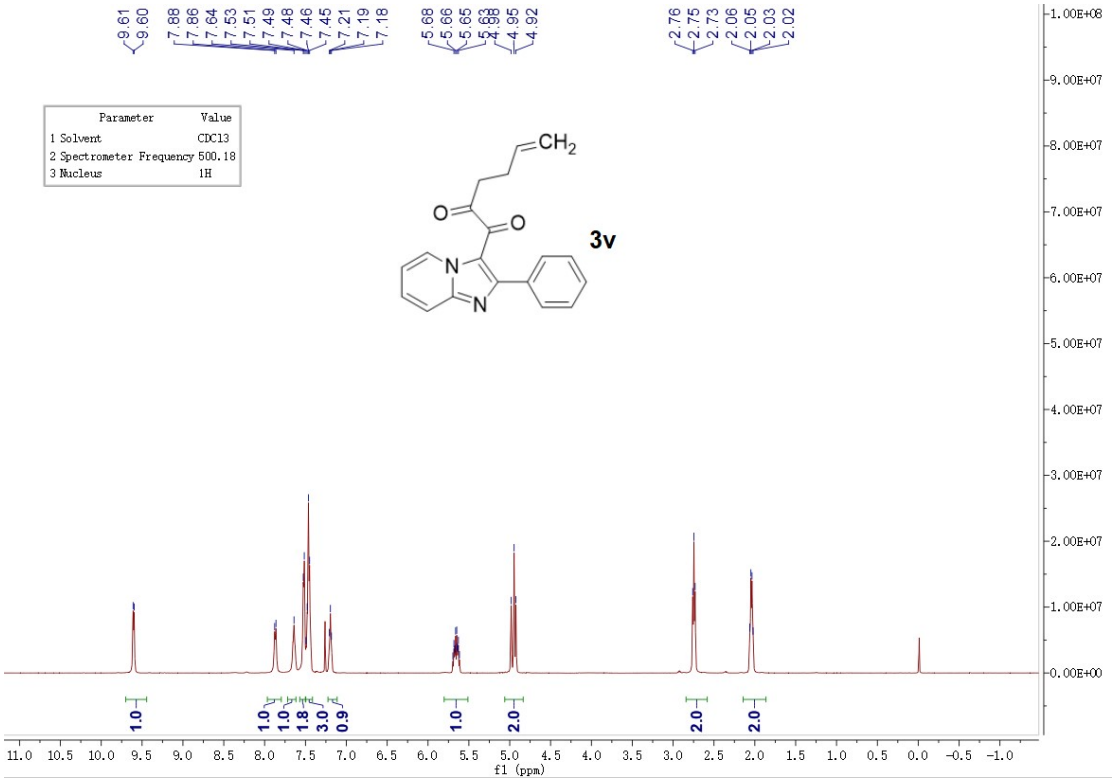
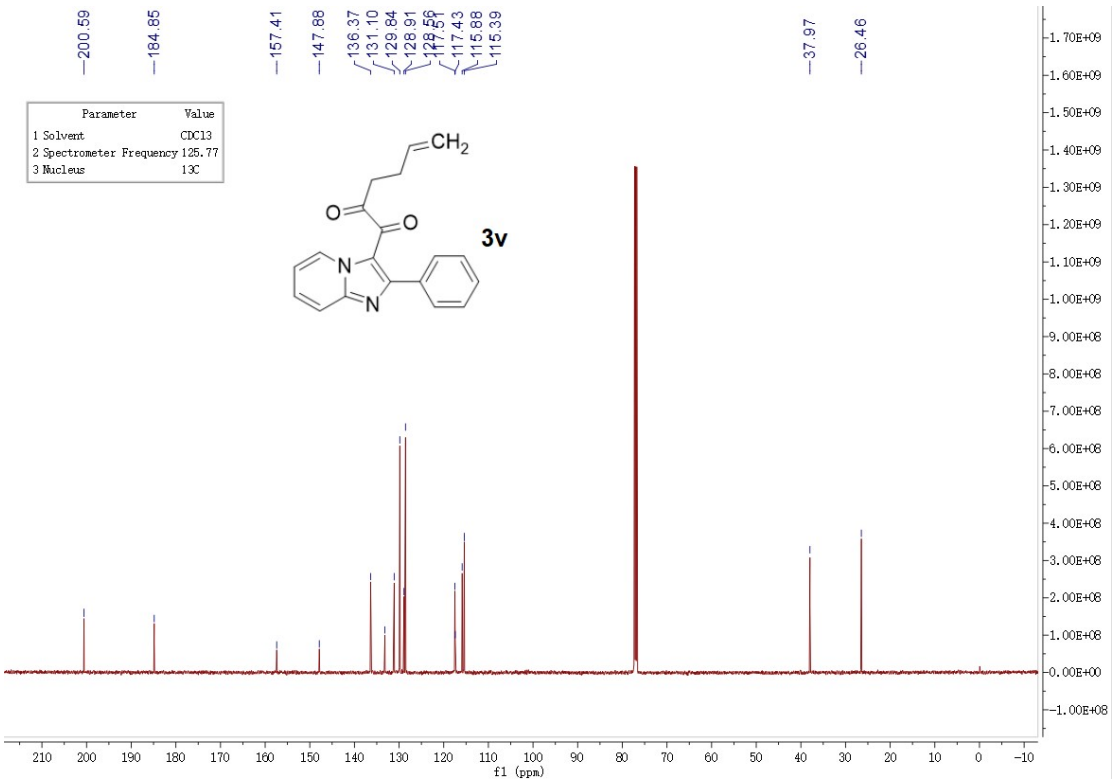
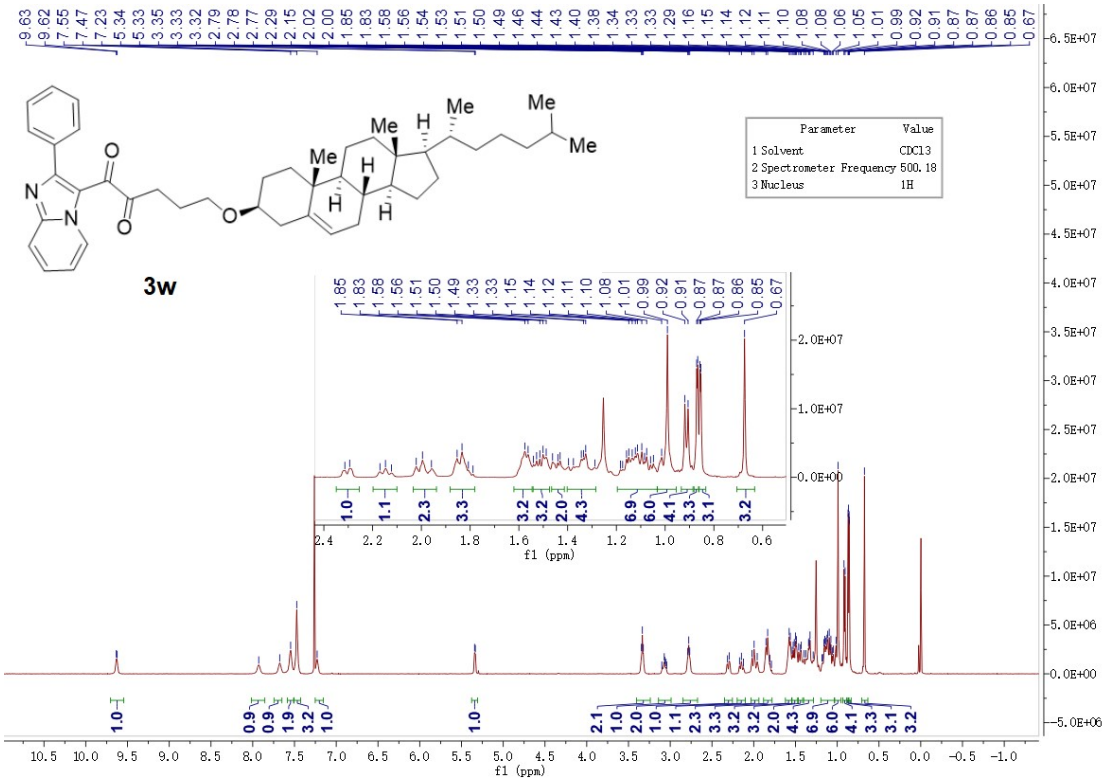
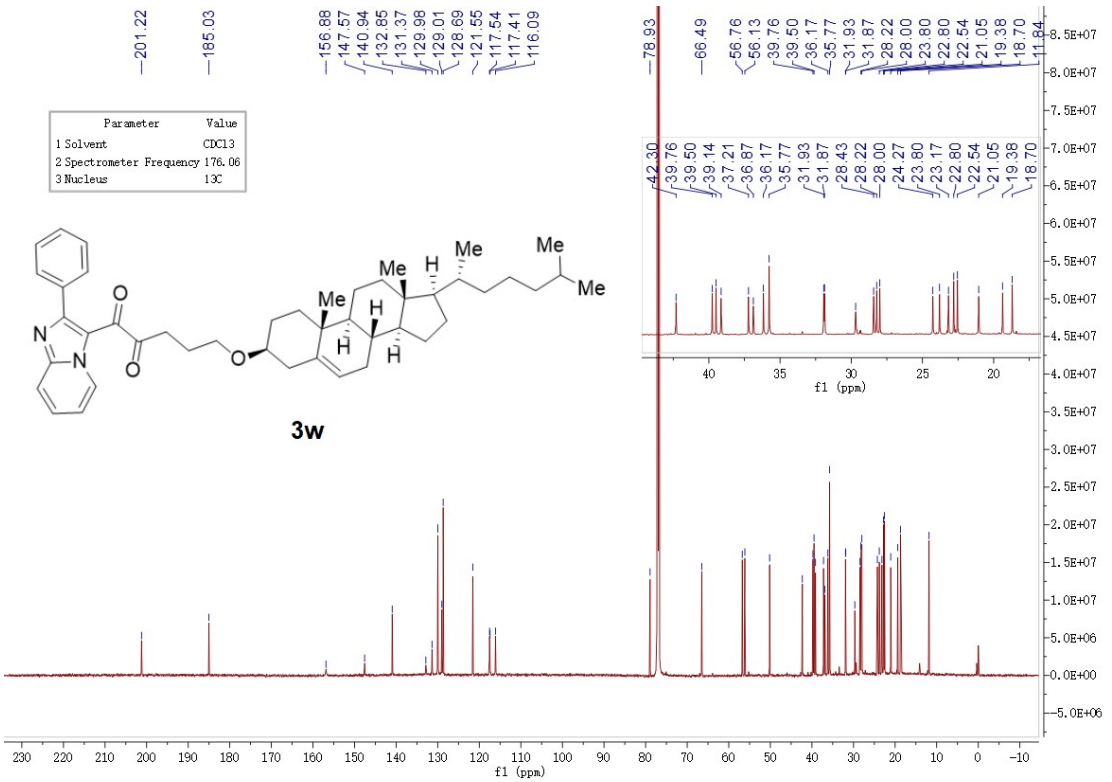
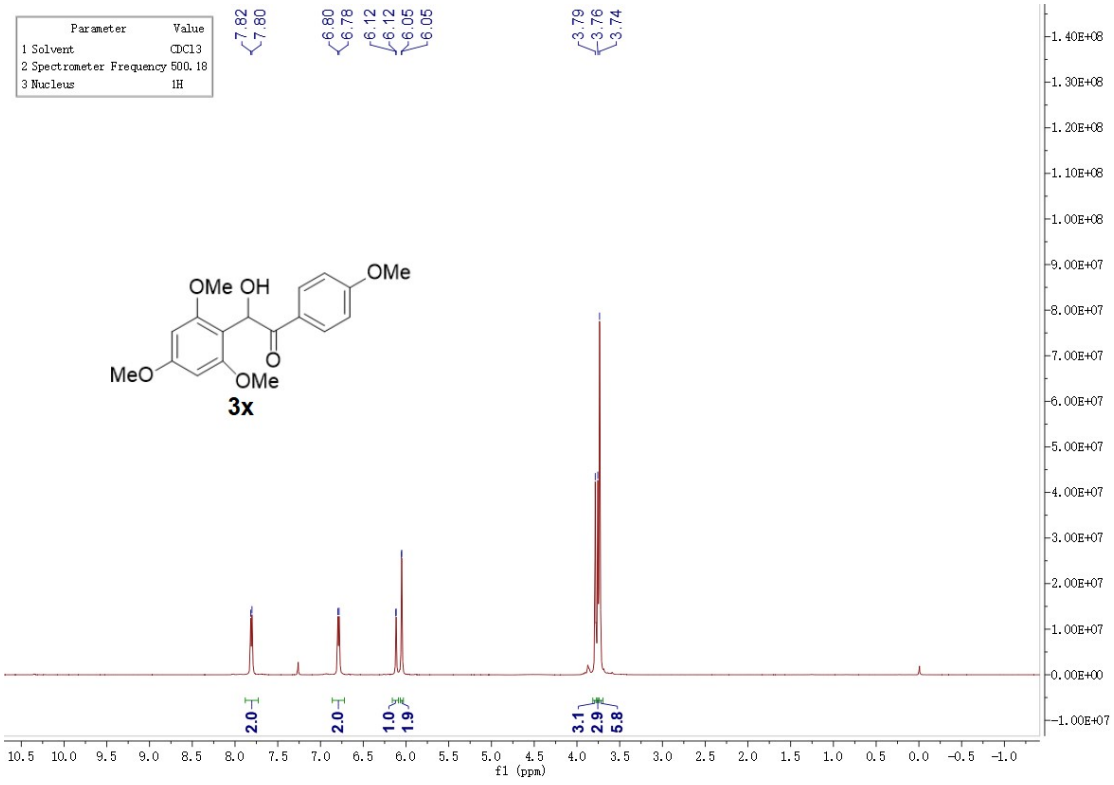
184.40
157.65
148.03
131.18
129.88
129.82
128.95
128.68
117.37
115.95
43.96
35.64
25.37
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 125.77
3 Nucleus 13C
Cl
O
O
N
N
3u
f1 (ppm)

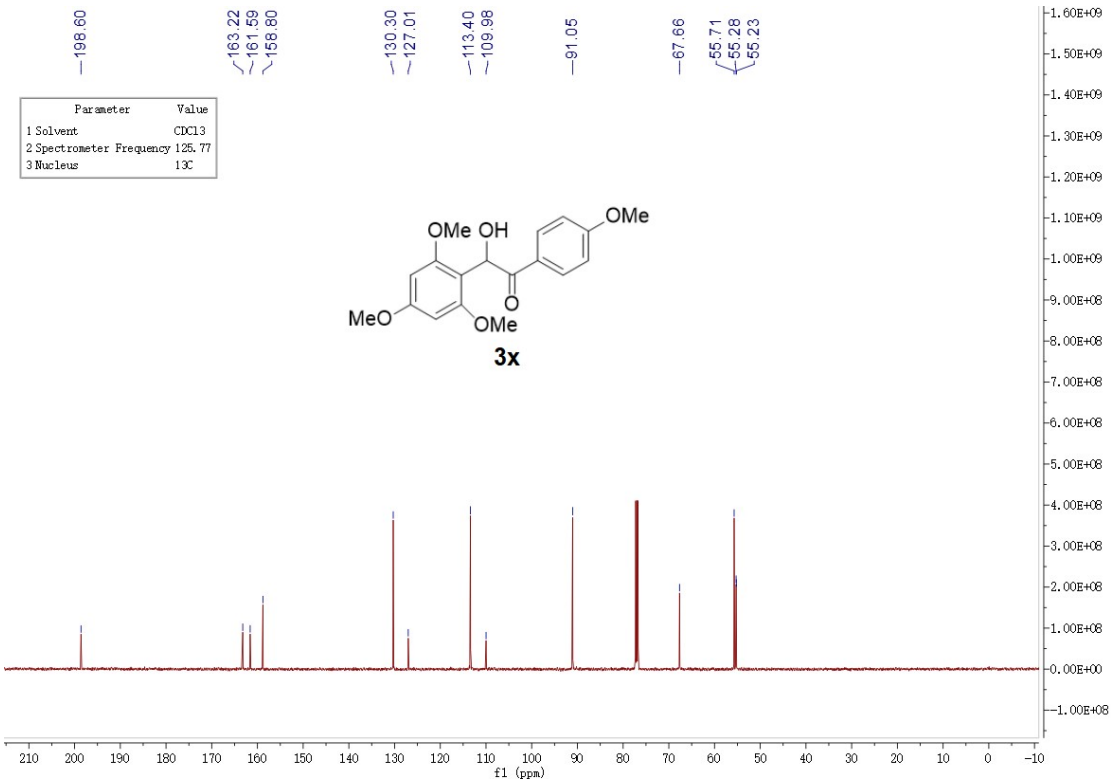

9.61
9.60
7.88
7.86
7.64
7.53
7.51
7.49
7.48
7.46
7.45
7.21
7.19
7.18
5.68
5.66
5.65
5.63
4.98
4.95
4.92
2.76
2.75
2.73
2.06
2.05
2.03
2.02
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
CH2
O
O
N
N
3v
1.0
1.0
1.0
1.8
3.0
0.9
1.0
2.0
2.0
2.0
f1 (ppm)

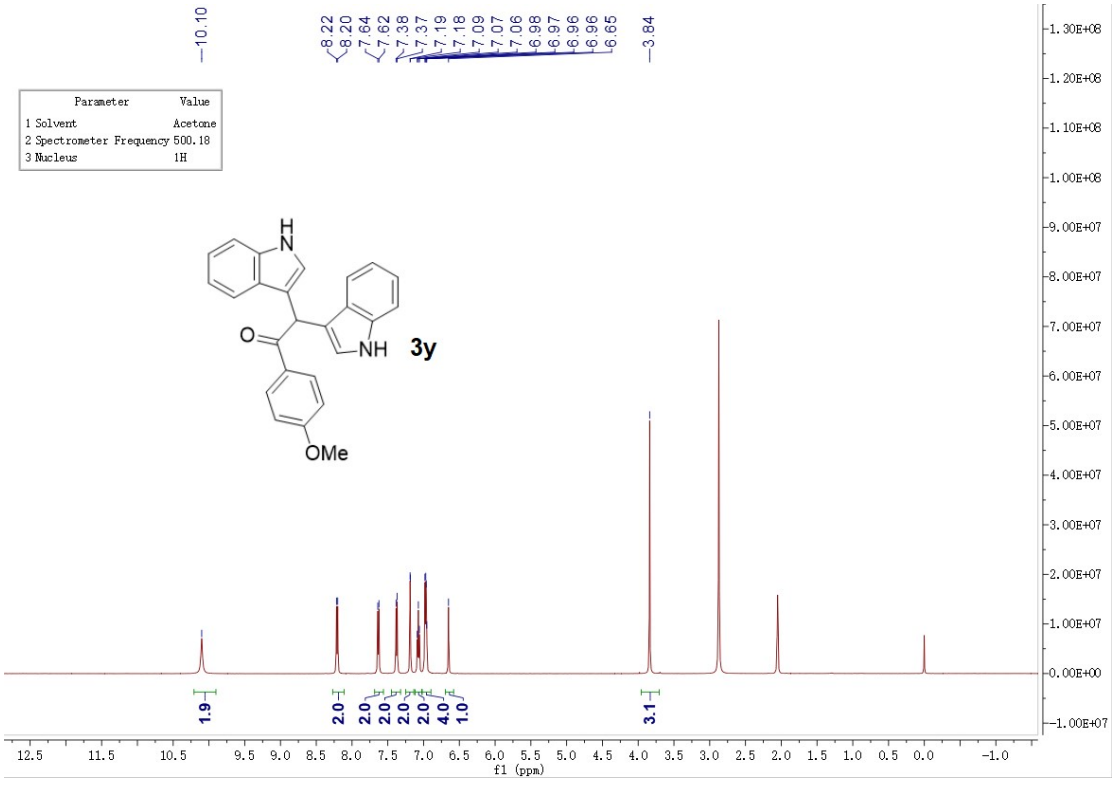

200.59
184.85
157.41
147.88
136.37
131.10
129.84
128.91
128.56
117.51
117.43
115.88
115.39
37.97
26.46
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 125.77
3 Nucleus 13C
3v
f1 (ppm)

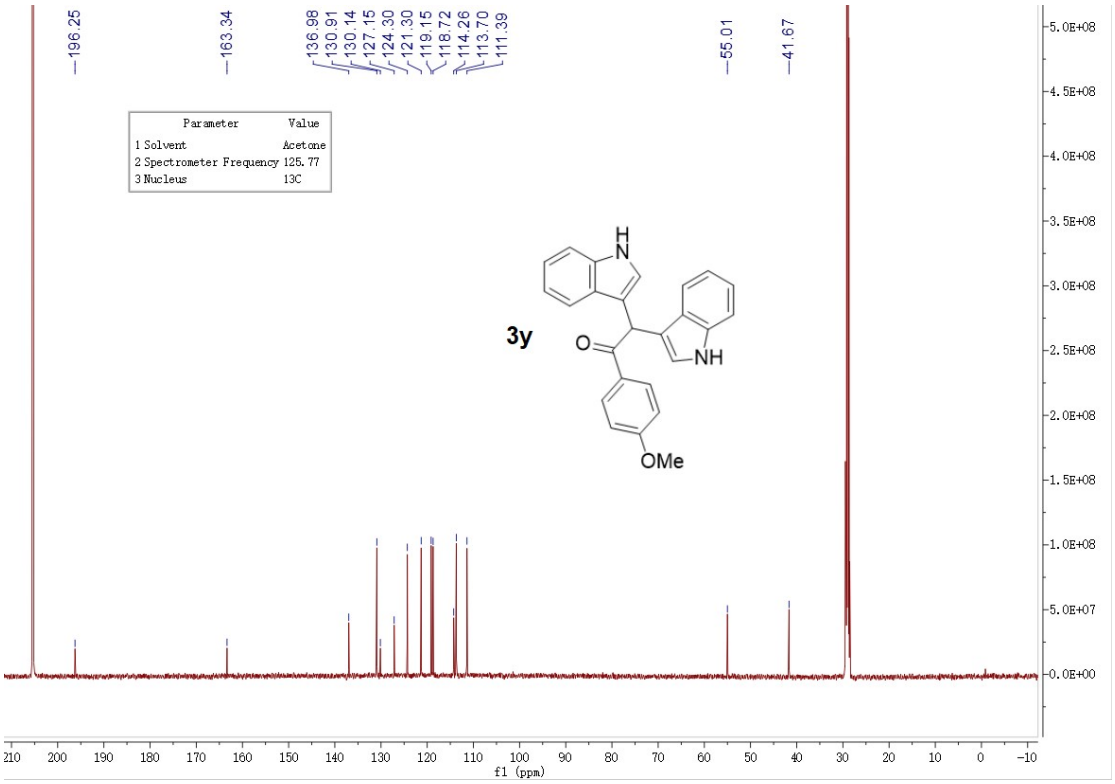

Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
3w
f1 (ppm)


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 176.06
3 Nucleus 13C
3w
f1 (ppm)


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 500.18
3 Nucleus 1H
3x
f1 (ppm)


198.60
163.22
161.59
158.80
130.30
127.01
113.40
109.98
91.05
67.66
55.71
55.28
55.23
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 125.77
3 Nucleus 13C
OMe OH
OMe
MeO
OMe
O
3x
f1 (ppm)


10.10
8.22
8.20
7.64
7.62
7.38
7.37
7.19
7.18
7.09
7.07
7.06
6.98
6.97
6.96
6.96
6.65
3.84
Parameter Value
1 Solvent Acetone
2 Spectrometer Frequency 500.18
3 Nucleus 1H
H
N
O
NH
3y
OMe
1.9
2.0
2.0
2.0
2.0
4.0
1.0
3.1
f1 (ppm)


196.25
163.34
136.98
130.91
130.14
127.15
124.30
121.30
119.15
118.72
114.26
113.70
111.39
55.01
41.67
Parameter Value
1 Solvent Acetone
2 Spectrometer Frequency 125.77
3 Nucleus 13C
3y
H
N
O
NH
OMe
f1 (ppm)