Electronic Supplementary Material (ESI) for Chemical Science.


# Site-selective C–H Activation and Regiospecific Annulation Using Propargylic Carbonates

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# Supporting Information

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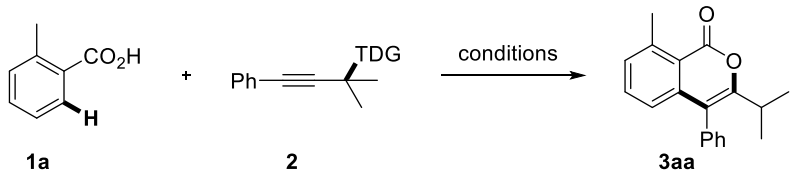
## General information

Unless otherwise noted, all reactions were carried out under an atmosphere of argon in oven-dried glassware cooled down under vacuum. Reaction temperatures are reported as the temperature of the heat transfer medium surrounding the vessel unless otherwise stated. Anhydrous solvents were purchased from ROTH and stored over molecular sieves under argon. Commercially available chemicals were obtained from Acros Organics, Aldrich Chemical Co., Alfa Aesar, ABCR, TCI Europe and used as received unless otherwise stated. $[Cp^*Rh(MeCN)_3](SbF_6)_2$[1], $[Cp^*Co(MeCN)_3](SbF_6)_2$[1-2], propargylic alcohol,[3] propargylic acetate,[4] (*S*)-methyl (3-methyl-1-phenylpent-1-yn-3-yl) carbonate (*S*)-**2e,**[5],[6] propargylic carbonate,[5, 7], 4-(Methylcarbamoyl)benzoic acid,[8] 4-(1*H*-pyrrolo[2,3-b]pyridin-1-yl)benzoic acid,[9] and 4-(pyridin-2-yloxy)benzoic acid[10] were prepared following literature procedures. Analytical thin layer chromatography was performed on Polygram SIL G/UV254 plates. TLC plates were visualized by exposure to short wave ultraviolet light (254 nm, 366 nm). Flash chromatography was performed on Merck silica gel (40-63 mesh) by standard techniques using appropriate mixtures of *n*-pentane and ethyl acetate. $^1H$ and $^{13}C$ NMR spectra were recorded on a Bruker AV 300 or AV 400, Varian 500 MHz INOVA or Varian Unity plus 600 in solvents as indicated. Chemical shifts (δ) for $^1H$ and $^{13}C$ NMR spectra are given in ppm relative to TMS. The residual solvent signals were used as references for $^1H$ and $^{13}C$ NMR spectra and the chemical shifts converted to the TMS scale (TMS: δH = 0.00 ppm; $CDCl_3$: δH = 7.26 ppm, δC = 77.16 ppm; $CD_3OD$: δH = 3.31 ppm, δC = 49.00 ppm; DMSO-$d_6$: δH = 2.50 ppm, δC = 39.52 ppm.). Exact ESI mass spectra were recorded on a Bruker Daltonics MicroTof. Mass Calibration was carried out directly before the measurement of the sample using clusters of sodium formate.

# Experimental section

## 1) Optimization of the reaction conditions.

Table S1 | Optimization of the reaction conditions.[a]

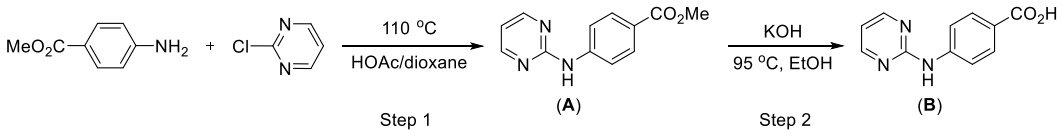



**1a** **2** **3aa**

| Entry | Catalyst | TDG | Additive | Time / h | Temp. / °C | **1a** / **2** | Yield / **3a** |
|---|---|---|---|---|---|---|---|
| 1 | $[Ru(p\text{-cymene})Cl_2]_2$ | OH | $K_3PO_4$ | 6 | 110 | 1 : 1.2 | 24 |
| 2 | $[Ru(p\text{-cymene})Cl_2]_2$ | OAc | $K_3PO_4$ | 6 | 110 | 1 : 1.2 | 58. |
| **3** | **$[Ru(p\text{-cymene})Cl_2]_2$** | **$OCO_2Me$** | **$K_3PO_4$** | **6** | **110** | **1 : 1.2** | **88** |
| 4 | $[Ru(p\text{-cymene})Cl_2]_2$ | OBoc | $K_3PO_4$ | 6 | 110 | 1 : 1.2 | 88 |
| 5 | - | $OCO_2Me$ | $K_3PO_4$ | 6 | 110 | 1 : 1.5 | n.d. |
| 6 | $[Ru(p\text{-cymene})Cl_2]_2$ | $OCO_2Me$ | $K_3PO_4$ | 15 | 100 | 1 : 1.5 | 91 |
| 7 | $[Ru(p\text{-cymene})Cl_2]_2$ | $OCO_2Me$ | $K_2CO_3$ | 15 | 100 | 1 : 1.5 | 78 |
| 8 | $[Ru(p\text{-cymene})Cl_2]_2$ | $OCO_2Me$ | $Cs_2CO_3$ | 15 | 100 | 1 : 1.5 | 84 |
| 9 | $[Ru(p\text{-cymene})Cl_2]_2$ | $OCO_2Me$ | KOAc | 15 | 100 | 1 : 1.5 | 60 |
| 10 | $[Ru(p\text{-cymene})Cl_2]_2$ | $OCO_2Me$ | $K_3PO_4$ | 15 | 100 | 1 : 1.2 | 92 |
| 11 | $[Ru(p\text{-cymene})Cl_2]_2$ | $OCO_2Me$ | - | 15 | 100 | 1 : 1.5 | n.d. |
| 12 | $[MnBr(CO)_5]$ | $OCO_2Me$ | $K_3PO_4$ | 6 | 110 | 1 : 1.2 | n.d. |
| 13 | $[Cp^*Rh(MeCN)_3](SbF_6)_2$ | $OCO_2Me$ | $K_3PO_4$ | 6 | 110 | 1 : 1.2 | 7 |
| 14 | $[Cp^*Co(MeCN)_3](SbF_6)_2$ | $OCO_2Me$ | $K_3PO_4$ | 6 | 110 | 1 : 1.2 | n.d. |
| 15 | $[(C_6H_5)_3P]_3RuCl_2$ | $OCO_2Me$ | $K_3PO_4$ | 6 | 110 | 1 : 1.2 | trace |
| 16 | $Ru(cod)Cl_2$ | $OCO_2Me$ | $K_3PO_4$ | 6 | 110 | 1 : 1.2 | 21 |
| 17 | $[Ru(C_6Me_6)Cl_2]_2$ | $OCO_2Me$ | $K_3PO_4$ | 6 | 110 | 1 : 1.2 | 77 |
| 18 | $[Cp^*IrCl_2]_2$ | $OCO_2Me$ | $K_3PO_4$, $Ag_2CO_3$ (10 mol%) | 6 | 110 | 1 : 1.2 | 29 |

[a] Unless otherwise specified, all reactions was carried out using **1a** (0.1 mmol), **2**, $[Ru(p\text{-cymene})Cl_2]_2$ (2.5 mol %), additives (0.5 equiv.) in DMA (1.0 mL) under different conditions. Yields was determined by $^1H$ NMR using 1,3,5-trimethoxybenzene as internal standard. TDG: traceless directing groups. n.d. = not detected.

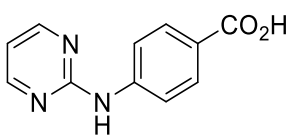
## 2) Synthesis of 4-(pyrimidin-2-ylamino)benzoic acid.




**General procedure**, Step 1:[11] To an oven-dried flask containing methyl 4-aminobenzoate (4.53 g, 30.0 mmol), a solution of 2-chloro-pyrimidine (2.29 g, 20.0 mmol) and acetic acid (20.0 mL) in 1,4-dioxane (50.0 mL) was added. The reaction mixture was stirred at 110 $^{o}$C for 24 h and monitored by TLC. Upon completion, the mixture was extracted with $CH_2Cl_2$ (3×100 mL). The combined organic phase was washed with brine and dried over $Na_2SO_4$. The solid was filtered off through a thin pad of Celite, and the filtrate was evaporated in vacuum to give the crude product which was purified by column chromatography on silica gel.

Step 2:[10] KOH (3.1 g, 55 mmol) was added to a solution of methyl 4-(pyrimidin-2-ylamino)benzoate (**A)** (2.29 g, 10 mmol) in EtOH (25 mL) and refluxed for 3 h. The volatiles were removed in vacuo, dissolved in $CH_2Cl_2$ (50 mL), and acidified by 1 M HCl (aq). The desired 4-(pyrimidin-2-ylamino)benzoic acid (**B**) was precipitated out from the solution. Then the solid was filtered and washed with EtOAc, giving the pure 4-(pyrimidin-2-ylamino)benzoic acid without further purification.

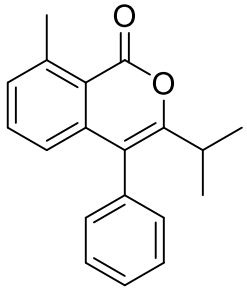
**4-(pyrimidin-2-ylamino)benzoic acid**: **$^{1}$H NMR** (**300 MHz**, DMSO-$d_6$) δ 11.12 (s, 1H), 10.09 (s, 1H), 8.56 (d, $J$ = 4.8 Hz, 2H), 7.94 – 7.80 (m, 4H), 6.94 (t, $J$ = 4.8 Hz, 1H); **$^{13}$C NMR (75 MHz,** DMSO-$d_6$**)** δ 167.17, 159.58, 158.17, 144.75, 130.31, 122.95, 117.59, 113.39; **HRMS** m/z (ESI): calcd. for $C_{11}H_9N3NaO_2$ (M + Na) 238.0587, found 238.0585.



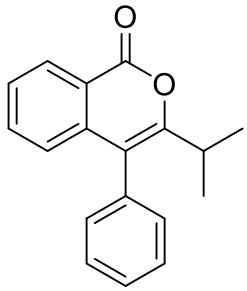

## 3) Procedure and analytical data of compounds 3-4.

**General procedure**: In a 10 mL dry Schlenk tube with a stirring bar, benzoic acid (**1**) (0.30 mmol) and $K_3PO_4$ (0.15 mmol) were added under air. Then the tube was transferred into the glove box. [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg) were added. After moving out, propargylic carbonate (**2**) (0.36 mmol) and *N*,*N*-dimethylacetamide (DMA) (1 mL) was added under argon atmosphere. The tube was sealed and the mixture was stirred at 110 ℃ for 6 h. Afterwards, the reaction mixture

was cooled to room temperature, brine and EtOAc were added (50 mL) each. The aqueous phase was extracted with EtOAc for 4 times. The combined organic phases were dried over $Na_2SO_4$. After rotary evaporation to remove solvent, the product was purified by flash chromatography ($SiO_2$, washed with 5 mL trimethylamine in 300 mL pentane) or basic Aluminum oxide using pentane/EtOAc as eluent.

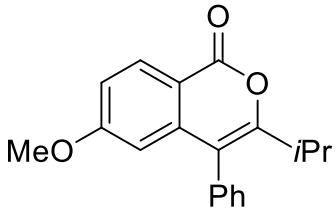


**3-isopropyl-8-methyl-4-phenyl-1*H*-isochromen-1-one**: Following the general procedure, the corresponding 2-methylbenzoic acid (**1**) (0.30 mmol, 40.8 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg), and the corresponding propargylic carbonate (**2c**) (0.36 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3aa** was isolated as colorless solid (86%, 71.6 mg); **$^1$H NMR (300 MHz, $CDCl_3$)** δ 7.44 – 7.26 (m, 4H), 7.19 – 7.11 (m, 3H), 6.65 (d, *J* = 8.0 Hz, 1H), 2.78 (s, 3H), 2.57 (hept, *J* = 6.9 Hz, 1H), 1.11 (d, *J* = 6.9 Hz, 6H); **$^{13}$C NMR (75 MHz, $CDCl_3$)** δ 162.23, 158.57, 143.42, 140.64, 135.25, 133.65, 130.67, 130.37, 129.07, 128.04, 123.26, 118.78, 114.72, 30.12, 23.66, 20.32; **HRMS** m/z (ESI): calcd. for $C_{19}H_{18}NaO_2$ (M + Na) 301,1199, found 301,1199.



**3-isopropyl-4-phenyl-1*H*-isochromen-1-one**: Following the general procedure, the corresponding benzoic acid (**1**) (0.30 mmol, 36.6 mg) , $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg) and the corresponding propargylic carbonate (**2c**) (0.36 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3ba** was isolated as colorless solid (76%, 60.0 mg); **$^1$H NMR (300 MHz, $CDCl_3$)** δ 8.36 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.62 – 7.55 (m, 1H), 7.55 – 7.42 (m, 4H), 7.33 – 7.26 (m, 1H), 6.96 (dd, *J* = 8.1, 1.2 Hz, 1H), 2.74 (hept, *J* = 6.9 Hz, 1H), 1.23 (d, *J* = 6.9 Hz, 6H); **$^{13}$C NMR (75 MHz, $CDCl_3$)** δ 162.94, 158.93, 139.04, 134.56, 134.53, 130.56, 129.50, 129.10, 128.19, 127.45, 125.02, 120.26, 114.72, 30.25, 20.39; **HRMS** m/z (ESI): calcd. for $C_{18}H_{16}NaO_2$ (M + Na) 287,1043, found 287,1045.

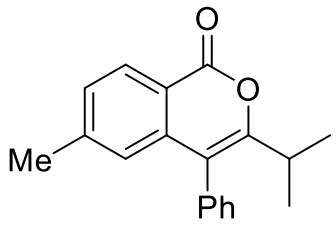
**3-isopropyl-6-methoxy-4-phenyl-1*H*-isochromen-1-one:** Following the general procedure, the




corresponding benzoic acid (**1**) (0.30 mmol, 45.6 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg) and the corresponding propargylic carbonate (**2c**) (0.36 mmol, 78.6 mg)

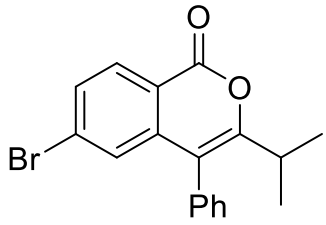
were used to react in DMA (1 mL) for 6 h, product **3ca** was isolated in 90% yield (79.5 mg) as a pale yellow solid; **$^1$H NMR (300 MHz, $CDCl_3$)** δ $^1$H NMR (300 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.8 Hz, 1H), 7.68 – 7.30 (m, 3H), 7.28– 7.26 (m, 2H), 6.99 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.31 (d, *J* = 2.4 Hz, 1H), 3.72 (s, 3H), 2.69 (hept, *J* = 6.9 Hz, 1H), 1.21 (d, *J* = 6.9 Hz, 6H). **$^{13}$C NMR (75 MHz, $CDCl_3$)** δ $^{13}$C NMR (75 MHz, $CDCl_3$) δ 164.62, 162.69, 159.53, 141.44, 134.62, 131.89, 130.53, 129.12, 128.21, 115.01, 114.64, 113.53, 108.12, 55.52, 30.35, 20.37. **HRMS** m/z (ESI): calcd. for $C_{19}H_{18}NaO_3$ (M + Na) 317.1148, found 317.1161.

**3-isopropyl-6-methyl-4-phenyl-1*H*-isochromen-1-one:** Following the general procedure, the



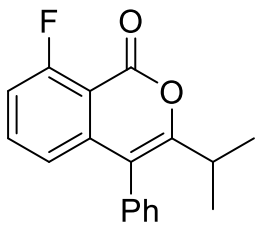

corresponding benzoic acid (**1**) (0.20 mmol, 27.2 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (5 mol%, 6.1 mg), and the corresponding propargylic carbonate (**2c**) (0.3 mmol) were used to react in DMA (1 mL) for 15 h, product **3da** was isolated in 75% yield (42.0 mg) as a pale yellow solid; **$^1$H NMR (300 MHz, $CDCl_3$):** δ 8.19 (d, *J* = 8.1 Hz, 1H), 7.51 – 7.39 (m, 3H), 7.26 – 7.18 (m, 3H), 6.66 (s, 1H), 2.65 (hept, *J* = 6.9 Hz, 1H), 2.29 (s, 3H), 1.16 (d, *J* = 6.9 Hz, 6H); **$^{13}$C NMR (75 MHz, $CD_3Cl_1$):** δ 163.03, 158.97, 145.68, 139.10, 134.69, 130.58, 129.54, 129.07, 128.84, 128.12, 124.97, 117.86, 114.63, 30.24, 22.23, 20.39; **HRMS**: m/z (ESI) calcd for $C_{19}H_{18}NaO_2$ $(M+Na)^+$: 301.1204, found 301.1204; **$R_f$** (Pentane/EtOAc = 20/1): 0.37.

**6-bromo-3-isopropyl-4-phenyl-1*H*-isochromen-1-one:** Following the general procedure, the



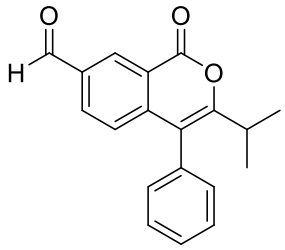

corresponding benzoic acid (**1**) (0.30 mmol), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (5.0 mol%, 6.12 mg), and the corresponding propargylic carbonate (**2c**) (0.45 mmol) were used to react in DMA (1 mL) for 15 h, product **3ea** was isolated in 65% yield (66.9 mg) as a white solid**; $^1$H NMR (300 MHz, $CDCl_3$):** δ 8.20 (d, *J* = 8.4 Hz, 1H), 7.61 – 7.46 (m, 4H), 7.31 – 7.25 (m, 2H), 7.08 (d, *J* = 1.8 Hz, 1H) 2.72 (hept, *J* = 6.8 Hz, 1H), 1.22 (d, *J* = 6.9 Hz, 6H); **$^{13}$C NMR (75 MHz, $CD_3Cl_1$):** δ 162.28, 160.43, 140.58, 133.72, 131.18, 130.87, 130.45, 130.37, 129.35, 128.55, 127.74, 118.94, 113.89, 30.40, 20.32; **HRMS**: m/z (ESI) calcd for $C_{18}H_{15}BrNaO_2$ $(M+Na)^+$: 365.0153, found 365. 0149; **$R_f$** (Pentane/EtOAc = 20/1): 0.39.

**8-fluoro-3-isopropyl-4-phenyl-1*H*-isochromen-1-one:** Following the general procedure, the

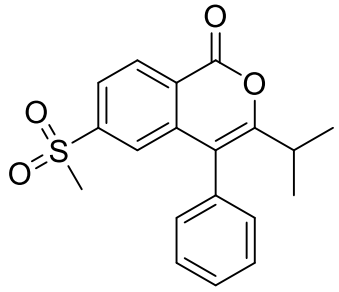


corresponding benzoic acid (**1**) (0.30 mmol), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg), and the corresponding propargylic carbonate (**2c**) (0.36 mmol) were used to react in DMA (1 mL) for 6 h, product **3fa** was isolated in 78% yield (66.4 mg) as a white solid**; $^1$H NMR (400 MHz, $CDCl_3$)** δ 7.46 – 7.35 (m, 4H), 7.20 – 7.14 (m, 2H), 7.02 (dd, *J* = 10.6, 8.2 Hz, 1H), 6.61 (d, *J* = 8.1 Hz, 1H), 2.60 (hept, *J* = 6.8 Hz, 1H), 1.12 (d, *J* = 6.9 Hz, 1H); **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 164.42, 161.78, 160.14, 158.33, 141.68, 135.73, 135.63, 134.42, 130.54, 129.23, 128.39, 120.98, 120.94, 114.69, 114.48, 114.10, 109.34, 109.27, 30.32, 20.25; **HRMS** m/z (ESI): calcd. for $C_{18}H_{15}FNaO_2$ (M + Na) 305.0948, found 305.0954.

**3-isopropyl-1-oxo-4-phenyl-1*H*-isochromene-7-carbaldehyde:** Following the general procedure,

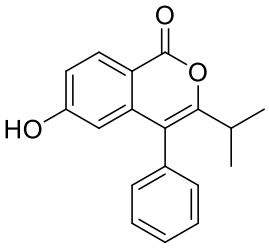


the corresponding 3-formylbenzoic acid (**1**) (0.30 mmol, 45.0 mg) $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg), and the corresponding propargylic carbonate (**2c**) (0.36 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3ga** was isolated in 49% yield (42.7 mg) as a solid; **$^1$H NMR (300 MHz, $CDCl_3$)** δ 10.01 (s, 1H), 8.71 (d, *J* = 1.8 Hz, 1H), 7.98 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.50 – 7.38 (m, 3H), 7.22 – 7.16 (m, 3H), 7.00 (d, *J* = 8.4 Hz, 1H), 2.68 (hept, *J* = 6.9 Hz, 1H), 1.16 (d, *J* = 6.9 Hz, 6H); **$^{13}$C NMR (75 MHz, $CDCl_3$)** δ 190.57, 162.41, 161.89, 143.80, 135.16, 133.69, 133.58, 132.78, 130.42, 129.40, 128.85, 128.65, 126.06, 120.45, 114.86, 30.61, 20.30; **HRMS** m/z (ESI): calcd. for $C_{19}H_{16}NaO_3$ (M + Na) 315.0992, found 315.0993.

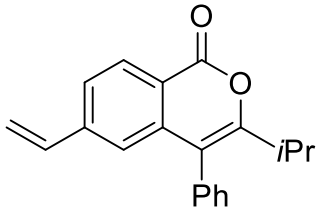


**3-isopropyl-6-(methylsulfonyl)-4-phenyl-1*H*-isochromen-1-one**: Following the general procedure, the corresponding benzoic acid (**1**) (0.20 mmol, 40.0 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (5 mol%, 6.1 mg), and the corresponding propargylic carbonate (**2c**) (0.30 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3ha** was isolated in 67% yield (46.1 mg) as colorless solid; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.45 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.88 (dt, *J* = 8.3, 1.6 Hz, 1H), 7.54 – 7.38 (m, 4H), 7.21 – 7.16 (m, 2H), 2.92 (d, *J* = 1.5 Hz, 3H), 2.67 (hept, *J* = 6.6 Hz, 1H), 1.19 – 1.11 (m, 6H); **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 161.42, 161.31, 146.03, 140.00, 133.01, 131.23, 130.33, 129.63, 128.97, 125.12, 124.27, 123.72, 114.38, 44.20, 30.47, 20.30; **HRMS** m/z (ESI):

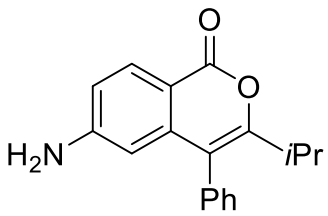
calcd. for $C_{19}H_{18}NaO_4S$ (M + Na) 365,0818, found 365,0824.



**6-hydroxy-3-isopropyl-4-phenyl-1H-isochromen-1-one:** Following the general procedure, the corresponding 4-hydroxybenzoic acid (**1**) (0.30 mmol, 41.4 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg), and the corresponding propargylic carbonate (**2c**) (0.36 mmol) were used to react in DMA (1.0 mL) for 6 h. Product **3ia** was isolated in 69% yield (58.3 mg) as white solid; **$^1$H NMR (400 MHz, DMSO-*d*$_6$)** δ 10.61 (s, 1H), 8.04 (d, *J* = 8.7 Hz, 1H), 7.54 (t, *J* = 7.7 Hz, 2H), 7.51 – 7.45 (m, 1H), 7.35 – 7.30 (m, 2H), 6.93 (dd, *J* = 8.8, 2.3 Hz, 1H), 6.19 (d, *J* = 2.3 Hz, 1H), 2.57 (hept, *J* = 6.9 Hz, 1H), 1.11 (d, *J* = 6.8 Hz, 6H); **$^{13}$C NMR (101 MHz, DMSO)** δ 163.84, 161.69, 158.65, 141.29, 134.63, 132.01, 130.71, 129.53, 128.57, 117.27, 114.41, 111.55, 109.77, 30.14, 20.43; **HRMS** m/z (ESI): calcd. for $C_{18}H_{16}NaO_3$ (M + Na) 303.0992, found 303.0995.

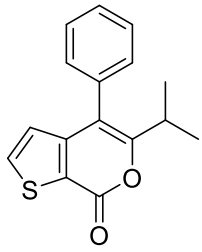


**3-isopropyl-4-phenyl-6-vinyl-1*H*-isochromen-1-one:** Following the general procedure, the corresponding benzoic acid (**1**) (0.30 mmol, 44.4 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg), and propargylic carbonate (**2c**) (0.36 mmol, 78.6 mg) were used to react in DMA (1 mL) for 6 h, product **3ja** was isolated in 42% yield (36.2 mg) as a pale yellow solid; **$^1$H NMR (300 MHz, CDCl$_3$)** δ 8.29 (d, *J* = 8.3 Hz, 1H), 7.59 – 7.40 (m, 4H), 7.33 – 7.19 (m, 2H), 6.85 (s, 1H), 6.64 (dd, *J* = 17.7, 11.0 Hz, 1H), 5.77 (d, *J* = 17.6 Hz, 1H), 5.36 (d, *J* = 11.0 Hz, 1H), 2.71 (hept, *J* = 6.9 Hz, 1H), 1.21 (d, *J* = 6.9 Hz, 6H). **$^{13}$C NMR (151 MHz, CDCl$_3$)** δ 162.77, 159.32, 143.56, 139.49, 136.06, 134.50, 130.62, 129.89, 129.15, 128.26, 124.71, 123.09, 119.41, 117.80, 114.72, 30.33, 20.41. **HRMS** m/z (ESI): calcd. for $C_{20}H_{18}NaO_2$ (M + Na) 313.1199, found 313,1197.



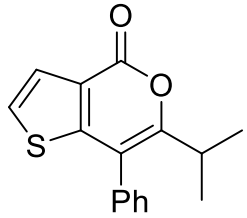
**6-amino-3-isopropyl-4-phenyl-1*H*-isochromen-1-one:** Following the general procedure, the corresponding benzoic acid (**1**) (0.30 mmol, 41.1 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg), and propargylic carbonate (**2c**) (0.36 mmol, 78.6 mg) were used to react in DMA (1 mL) for 6 h, product **3ka** was isolated in 44% yield (36.6 mg) as a pale yellow solid; **$^1$H NMR (300 MHz, CDCl$_3$)** δ 8.13 (d, *J* =

8.6 Hz, 1H), 7.51 – 7.41 (m, 3H), 7.26 (d, *J* = 8.2 Hz, 2H), 6.70 (d, *J* = 8.5 Hz, 1H), 5.99 (s, 1H), 4.11 (bs, 2H), 2.65 (hept, *J* = 6.7 Hz, 1H), 1.19 (d, *J* = 6.6 Hz, 6H). **$^{13}$C NMR (75 MHz, $CDCl_3$)** δ $^{13}$C NMR (75 MHz, $CDCl_3$) δ 162.97, 159.19, 152.26, 141.33, 135.08, 131.82, 130.66, 129.00, 127.99, 114.99, 114.38, 110.78, 107.74, 30.30, 20.36. **HRMS** m/z (ESI): calcd. for $C_{18}H_{17}NaO_2$ (M + Na) 302.1151, found 302.1165.



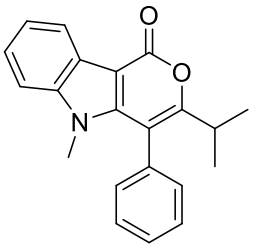
**5-isopropyl-4-phenyl-7*H*-thieno[2,3-c]pyran-7-one:** Following the general procedure, the corresponding thiophene-2-carboxylic acid (**1**) (0.30 mmol, 38.4 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg), and the corresponding propargylic carbonate (**2c**) (0.36 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3la** was isolated in 64% yield (52.1 mg) as yellow solid; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.63 (dd, *J* = 5.2, 1.7 Hz, 1H), 7.43 – 7.33 (m, 3H), 7.25 – 7.19 (m, 2H), 6.68 (dd, *J* = 5.2, 1.7 Hz, 1H), 2.78 (dh, *J* = 6.9, 1.6 Hz, 1H), 1.16 (dd, *J* = 6.9, 1.7 Hz, 6H); **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 161.54, 159.00, 149.45, 136.12, 134.78, 129.87, 129.04, 128.30, 124.85, 121.97, 114.12, 29.81, 20.76; **HRMS** m/z (ESI): calcd. for $C_{16}H_{14}NaO_2S$ (M + Na) 293.0607 , found 293.0614.

**6-isopropyl-7-phenyl-4*H*-thieno[3,2-c]pyran-4-one:** Following the general procedure, the



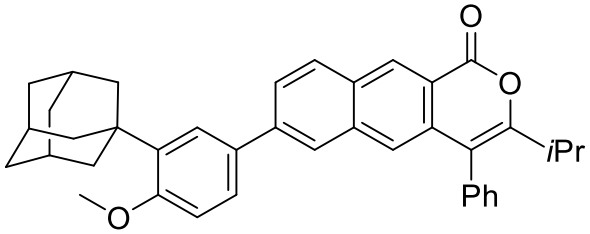
corresponding thiophene-3-carboxylic acid (**1**) (0.30 mmol, 38.4 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg), and the corresponding propargylic carbonate (**2c**) (0.36 mmol) were used to react in DMA (1.0 mL) for 15 h, product **3ma** was isolated in 75% yield (60.7 mg) as pale yellow solid; **$^1$H NMR (300 MHz, $CDCl_3$):** δ 7.59 (d, *J* = 5.3 Hz, 1H), 7.52 – 7.42 (m, 3H), 7.39 – 7.33 (m, 2H), 7.24 (d, *J* = 5.3 Hz, 1H), 2.85 (hept, *J* = 6.8 Hz, 1H), 1.24 (d, *J* = 6.8 Hz, 6H); **$^{13}$C NMR (75 MHz, $CD_3Cl_1$):** δ 160.26, 159.10, 154.46, 134.58, 129.52, 129.25, 128.84, 126.00, 125.55, 122.94, 113.39, 29.90, 20.74; **HRMS**: m/z (ESI) calcd for $C_{16}H_{14}NaO_2S$ $(M+Na)^+$: 293.0607, found 293.0619; **$R_f$** (Pentane/EtOAc = 20/1): 0.35.

**3-isopropyl-5-methyl-4-phenylpyrano[4,3-b]indol-1(5*H*)-one:** Following the general procedure,



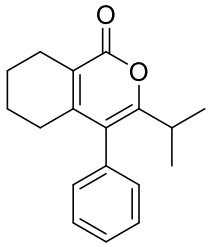
the corresponding 1-methyl-1*H*-indole-3-carboxylic acid (**1**) (0.30 mmol, 52.6 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg), and the corresponding propargylic carbonate (**2c**) (0.36 mmol) were used

to react in DMA (1.0 mL) for 6 h. Product **3na** was isolated in 92% yield (87.3 mg) as yellow solid; **$^1$H NMR (300 MHz, $CDCl_3$)** δ 8.20 – 8.14 (m, 1H), 7.47 – 7.39 (m, 3H), 7.31 – 7.26 (m, 2H), 7.25 – 7.20 (m, 2H), 7.16 – 7.10 (m, 1H), 2.97 (s, 3H), 2.62 (hept, *J* = 6.9 Hz, 1H), 1.13 (d, *J* = 6.9 Hz, 6H); **$^{13}$C NMR (75 MHz, $CDCl_3$)** δ 164.36, 160.00, 144.98, 139.45, 133.74, 130.86, 129.32, 128.88, 124.27, 123.94, 122.55, 121.18, 109.32, 108.20, 99.81, 31.63, 30.15, 20.60; **HRMS** m/z (ESI): calcd. for $C_{21}H_{19}NNaO_2$ (M + Na) 340.1308, found 340.1307.

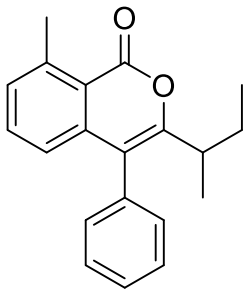



**7-(3-(-adamantan-1-yl)-4-methoxyphenyl )-3-isopropyl-4-phenyl-1*H*-benzo[g]isoch romen-1-one**: Following the general procedure, the corresponding adapalene (**1**) (0.20 mmol, 82.5 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (5 mol%, 6.1 mg) and the corresponding propargylic carbonate (**2c**) (0.30 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3oa** was isolated in 51% yield (56.4 mg) as colorless solid; **$^1$H NMR (300 MHz, $CDCl_3$)** δ 8.97 (s, 1H), 8.04 (d, *J* = 8.6 Hz, 1H), 7.84 (s, 1H), 7.77 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.62 – 7.45 (m, 5H), 7.37 (dd, *J* = 7.7, 1.5 Hz, 2H), 7.33 (s, 1H), 6.96 (d, *J* = 8.5 Hz, 1H), 3.88 (s, 3H), 2.73 (hept, *J* = 6.9 Hz, 1H), 2.23 – 2.04 (m, 9H), 1.79 (d, *J* = 3.1 Hz, 6H), 1.24 (d, *J* = 6.9 Hz, 6H); **$^{13}$C NMR (75 MHz, $CDCl_3$)** δ 163.33, 159.20, 157.27, 142.27, 139.16, 136.96, 135.19, 134.56, 132.30, 131.56, 130.76, 129.91, 129.19, 128.16, 126.64, 126.02, 125.89, 124.72, 123.71, 118.55, 114.61, 112.19, 55.28, 40.72, 37.34, 37.24, 30.28, 29.22, 20.38; **HRMS** m/z (ESI): calcd. for $C_{39}H_{38}NaO_3$ (M + Na) 577,2713, found 577,2703.

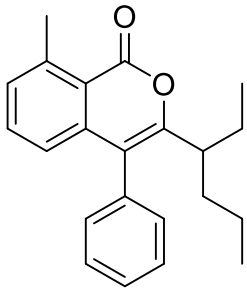
**3-isopropyl-4-phenyl-5,6,7,8-tetrahydro-1*H*-isochromen-1-one:** Following the general procedure, the corresponding cyclohex-1-ene-1-carboxylic acid (**1**) (0.30 mmol, 37.8 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg) and the corresponding propargylic carbonate (**2c**) (0.36 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3pa** was isolated in 40% yield (32.3 mg) as yellowish viscous; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.44 – 7.33 (m, 3H), 7.16 – 7.10 (m, 2H), 2.55 – 2.47 (m, 2H), 2.06 – 1.97 (m, 2H), 1.73 – 1.65 (m, 3H), 1.64 – 1.55 (m, 2H), 1.13 (d, *J* = 6.9 Hz, 6H); **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 163.65, 161.99, 151.76, 135.09, 130.12, 128.86, 127.95, 120.17, 117.81, 30.24, 28.68, 23.78, 21.85, 21.67, 20.39; **HRMS**



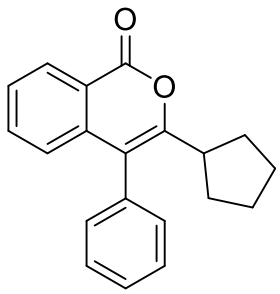
m/z (ESI): calcd. for $C_{18}H_{20}NaO_2$ (M + Na) 291.1356, found 291.1356.



**3-(sec-butyl)-8-methyl-4-phenyl-1*H*-isochromen-1-one**: Following the general procedure, the corresponding 2-methylbenzoic acid (**1**) (0.30 mmol, 40.8 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg) and the corresponding propargylic carbonate (**2**) (0.36 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3ab** was isolated in 78% yield (68.4 mg) as colorless solid; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.43 – 7.27 (m, 4H), 7.22 – 7.11 (m, 3H), 6.65 (d, *J* = 8.0 Hz, 1H), 2.79 (s, 3H), 2.39 – 2.39 (m, 1H), 1.78 – 1.63 (m, 1H), 1.44 – 131 (m, 1H), 1.10 (d, *J* = 6.9 Hz, 3H), 0.72 (t, *J* = 7.4 Hz, 3H); **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 162.25, 157.54, 143.45, 140.61, 135.30, 133.67, 131.09, 130.71, 130.41, 129.09, 128.95, 127.99, 123.28, 118.72, 116.22, 37.07, 27.28, 23.64, 19.00, 12.36; **HRMS** m/z (ESI): calcd. for $C_{20}H_{20}NaO_2$ (M + Na) 315,1356, found 315,1358.



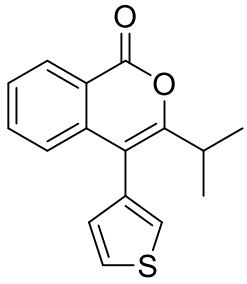
**3-(hexan-3-yl)-8-methyl-4-phenyl-1*H*-isochromen-1-one**: Following the general procedure, the corresponding 2-methylbenzoic acid (**1**) (0.30 mmol, 40.8 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg) and the corresponding propargylic carbonate (**2**) (0.36 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3ac** was isolated in 52% yield (50.0 mg) as colorless solid; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.43 – 7.27 (m, 4H), 7.18 – 7.09 (m, 3H), 6.63 (d, *J* = 8.0 Hz, 1H), 2.79 (s, 3H), 2.23 (tt, *J* = 9.9, 5.1 Hz, 1H), 1.74 – 1.60 (m, 2H), 1.48 – 1.26 (m, 2H), 1.25 – 1.04 (m, 2H), 0.78 – 0.66 (m, 6H); **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 162.30, 156.44, 143.44, 140.59, 135.23, 133.70, 131.31, 130.43, 128.87, 127.94, 123.34, 118.64, 117.54, 42.35, 35.56, 26.44, 23.65, 20.93, 14.32, 12.38; **HRMS** m/z (ESI): calcd. for $C_{22}H_{24}NaO_2$ (M + Na) 343,1669, found 343,1673.



**3-cyclopentyl-4-phenyl-1*H*-isochromen-1-one**: Following the general procedure, the corresponding sodium benzoate (**1**) (0.30 mmol, 43.2 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg) and the corresponding propargylic carbonate (**2**) (0.45 mmol) in DMA (1.0 mL) were used to react for 15 h. Product **3ad** was isolated in 75% yield (65.3 mg) as colorless solid; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.25 (d, *J* = 7.9 Hz, 1H), 7.47 (t, *J* =

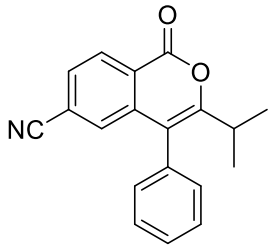
7.7 Hz, 1H), 7.44 – 7.32 (m, 4H), 7.22 – 7.16 (m, 2H), 6.86 (d, *J* = 8.1 Hz, 1H), 2.69 (p, *J* = 8.2 Hz, 1H), 1.91 – 1.63 (m, 6H), 1.51 – 1.33 (m, 2H); **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 162.99, 157.22, 138.98, 134.77, 134.56, 130.74, 129.51, 129.03, 128.13, 127.34, 124.91, 120.20, 115.64, 41.08, 31.42, 26.33; **HRMS** m/z (ESI): calcd. for $C_{20}H_{18}NaO_2$ (M + Na) 313,1199, found 313,1197.

**3-isopropyl-4-(thiophen-3-yl)-1*H*-isochromen-1-one**: Following the general procedure, the

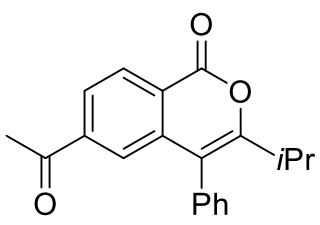


corresponding sodium benzoate (**1**) (0.20 mmol, 28.8 mg), $K_3PO_4$ (0.5 equiv.), $[Ru(p\text{-cymene})Cl_2]_2$ (5 mol%, 6.12 mg) and the corresponding propargylic carbonate (**2**) (0.30 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3ae** was isolated in 70% yield (37.6 mg) as solid; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.32 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.59 (td, *J* = 7.7, 1.5 Hz, 1H), 7.49 (dd, *J* = 4.9, 2.9 Hz, 1H), 7.45 (td, *J* = 7.8, 1.2 Hz, 1H), 7.25 – 7.19 (m, 1H), 7.11 – 6.93 (m, 2H), 2.81 (hept, *J* = 6.9 Hz, 1H), 1.22 (d, *J* = 6.8 Hz, 6H); **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 162.80, 159.61, 139.04, 134.69, 134.08, 129.58, 129.52, 127.55, 126.57, 125.16, 124.84, 120.20, 109.70, 30.33, 20.46; **HRMS** m/z (ESI): calcd. for $C_{16}H_{14}NaO_2S$ (M + Na) 293.0607, found 293.0618.

**3-isopropyl-1-oxo-4-phenyl-1*H*-isochromene-6-carbonitrile:** Following the general procedure,

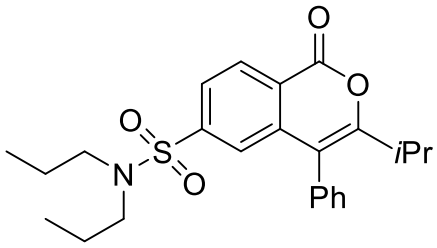


the corresponding 4-cyanobenzoic acid (**1**) (0.30 mmol, 44.1 mg), $K_3PO_4$ (0.5 equiv.), $[Ru(p\text{-cymene})Cl_2]_2$ (2.5 mol%, 4.6 mg) and the corresponding propargylic carbonate (**2c**) (0.36 mmol) were used to react in DMA (1.0 mL) for 6 h. Product **3qa** was isolated in 74% yield (64.6 mg) as yellow solid; **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.33 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.58 (dt, *J* = 8.1, 1.6 Hz, 1H), 7.50 – 7.41 (m, 3H), 7.17 (dq, *J* = 10.1, 2.3, 1.8 Hz, 3H), 2.66 (dh, *J* = 6.9, 1.4 Hz, 1H), 1.14 (dd, *J* = 6.9, 1.5 Hz, 6H); **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 161.31, 161.18, 139.55, 133.04, 130.46, 130.34, 129.60, 129.36, 128.91, 122.93, 118.07, 117.78, 113.74, 30.46, 20.25; **HRMS** m/z (ESI): calcd. for $C_{19}H_{15}NNaO_2$ (M + Na) 312.0995, found 312.1005.



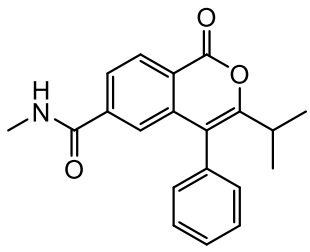
**6-acetyl-3-isopropyl-4-phenyl-1*H*-isochromen-1-one:** Following the general procedure, the corresponding benzoic acid (**1**) (0.30

mmol, 49.2 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg) and propargylic carbonate (**2c**) (0.36 mmol, 78.6 mg) were used to react in DMA (1.0 mL) for 6 h, product **3ra** was isolated in 54% yield (49.7 mg) as a pale yellow solid; **$^1$H NMR (300 MHz, $CDCl_3$)** δ 8.43 (d, *J* = 8.2 Hz, 1H), 7.97 (dd, *J* = 8.2, 1.6 Hz, 1H), 7.62 – 7.40 (m, 4H), 7.29 (dd, *J* = 6.1, 1.6 Hz, 2H), 2.75 (dt, *J* = 13.7, 6.8 Hz, 1H), 2.51 (s, 3H), 1.23 (d, *J* = 6.9 Hz, 6H). **$^{13}$C NMR (75 MHz, $CDCl_3$)** δ 197.55, 162.17, 159.94, 141.61, 139.33, 133.78, 130.45, 130.13, 129.36, 128.60, 126.33, 125.05, 123.11, 114.72, 30.34, 27.03, 20.36. **HRMS** m/z (ESI): calcd. for $C_{20}H_{18}NaO_3$ (M + Na) 329.1148, found 329.1157.



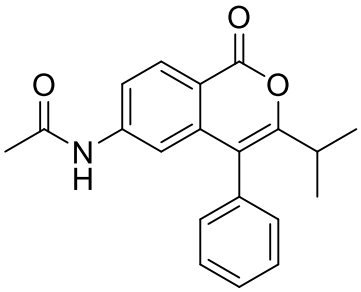

**3-isopropyl-1-oxo-4-phenyl-*N*,*N*-dipropyl-1*H*-isochromene-6-sulfonamide:** Following the general procedure, the corresponding benzoic acid (**1**) (0.30 mmol, 85.6 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg), and the corresponding propargylic carbonate (**2c**) (0.36 mmol, 78.6 mg) were used to react in DMA (1.0 mL) for 6 h, product **3sa** was isolated in 93% yield (119.1 mg) as a pale yellow solid; **$^1$H NMR (300 MHz, $CDCl_3$)** δ 8.21 (d, *J* = 8.3 Hz, 1H), 7.60 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.34 – 7.20 (m, 3H), 7.10 (d, *J* = 1.3 Hz, 1H), 7.06 – 6.96 (m, 2H), 2.83 – 2.70 (m, 4H), 2.52 (dt, *J* = 13.7, 6.8 Hz, 1H), 1.23 (dd, *J* = 15.2, 7.5 Hz, 4H), 0.99 (d, *J* = 6.9 Hz, 6H), 0.58 (t, *J* = 7.4 Hz, 6H).**$^{13}$C NMR (75 MHz, $CDCl_3$)** δ 161.66, 160.70, 146.16, 139.74, 133.41, 130.71, 130.30, 129.46, 128.80, 125.03, 123.49, 122.52, 114.41, 49.81, 30.43, 21.82, 20.31, 11.21. **HRMS** m/z (ESI): calcd. for $C_{24}H_{29}NNaO_4S$ (M + Na) 450.1710, found 450.1708.

**3-isopropyl-N-methyl-1-oxo-4-phenyl-1H-isochromene-6-carboxamide:**



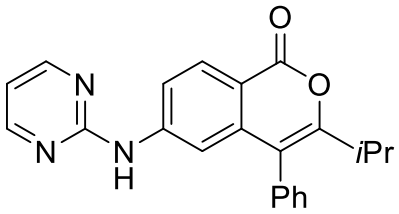

Following the general procedure, 4-(1*H*-pyrazol-1-yl)benzoic acid (**1**) (0.20 mmol, 35.8 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 3.1 mg), and the corresponding propargylic carbonate (**2c**) (0.30 mmol, 65.5 mg) in DMA (1.0 mL) were used to react for 15 h. Product **3ta** was isolated in 72% yield (46.2 mg) as yellowish white solid. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.3 (dd, *J* = 8.2, 1.6 Hz, 1H), 7.7 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.4 (qd, *J* = 8.4, 4.4 Hz, 3H), 7.2 – 7.2 (m, 2H), 6.2 (s, 1H), 2.9 (d, *J* = 4.7 Hz, 3H), 2.6 (hept,

*J* = 6.9 Hz, 1H), 1.1 (d, *J* = 6.9 Hz, 6H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** $^{13}$C NMR (101 MHz, $CDCl_3$) δ 167.24, 162.27, 159.97, 140.39, 139.29, 133.84, 130.50, 130.09, 129.37, 128.54, 125.39, 123.71, 122.02, 114.68, 30.32, 27.07, 20.35; **HRMS** m/z (ESI): calcd for $C_{20}H_{19}NNaO_3$ (M+Na) 344.1257 found 344.1252.

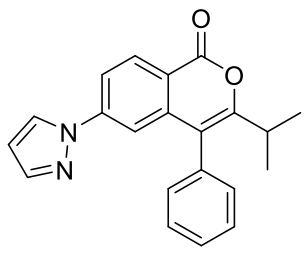


***N*-(3-isopropyl-1-oxo-4-phenyl-1H-isochromen-6-yl)acetamide**: Following the general procedure, the corresponding benzoic acid (**1**) (0.20 mmol, 35.8 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (5 mol%, 6.1 mg), and the corresponding propargylic carbonate (**2c**) (0.3 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3ua** was isolated in 80% yield (51.3 mg) as colorless solid; **$^1$H NMR (300 MHz, $CDCl_3$)** 8.20 (d, *J* = 8.6 Hz, 1H), 7.72 (d, *J* = 8.2 Hz, 1H), 7.57 – 7.29 (m, 4H), 7.25 – 7.10 (m, 2H), 6.86 (s, 1H), 2.62 (hept, *J* = 7.5 Hz, 1H), 2.06 (s, 3H), 1.12 (d, *J* = 6.9 Hz, 6H); **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 168.95, 162.66, 159.48, 144.06, 140.53, 134.37, 131.11, 130.48, 129.12, 128.29, 118.88, 115.70, 114.72, 113.91, 30.32, 24.80, 20.37; **HRMS** m/z (ESI): calcd. for $C_{20}H_{19}NNaO_3$ (M + Na) 344,1257, found 344,1258.

**3-isopropyl-4-phenyl-6-(pyrimidin-2-ylamino)-1*H*-isochromen-1-one:** Following the general procedure, the corresponding benzoic acid (**1**) (0.20 mmol, 43.0 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (10 mol%, 12.2 mg) and the corresponding propargylic carbonate (**2c**) (0.3 mmol, 65.5 mg) were used to react in DMA (1 mL) for 15 h, product **3va** was isolated in 40% yield (28.3 mg) as a pale yellow solid; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.40 – 8.34 (m, 2H), 8.30 (d, *J* = 8.7 Hz, 1H), 7.92 (dd, *J* = 8.8, 2.3 Hz, 1H), 7.57 (bs, 1H), 7.55 – 7.43 (m, 3H), 7.37 – 7.29 (m, 2H), 7.10 (d, *J* = 2.2 Hz, 1H), 6.79 (t, *J* = 4.9 Hz, 1H), 2.74 (hept, *J* = 6.9 Hz, 1H), 1.22 (d, *J* = 6.8 Hz, 6H); **$^{13}$C NMR (126 MHz, $CDCl_3$)** δ162.69, 159.43, 159.32, 157.99, 145.41, 140.65, 134.88, 131.12, 131.05, 130.72, 129.03, 128.82, 128.09, 128.07, 118.05, 114.68, 114.18, 113.94, 112.87, 30.39, 20.42. **HRMS** m/z (ESI): calcd. for $C_{22}H_{19}NaN_3O_2$ (M + Na) 380.1369, found 380.1370.

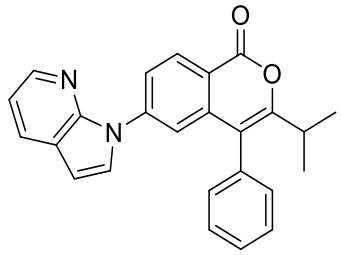


**3-isopropyl-4-phenyl-6-(1*H*-pyrazol-1-yl)-1*H*-isochromen-1-one**: Following the general procedure, the corresponding 4-(1*H*-pyrazol-1-yl)benzoic acid (**1**)

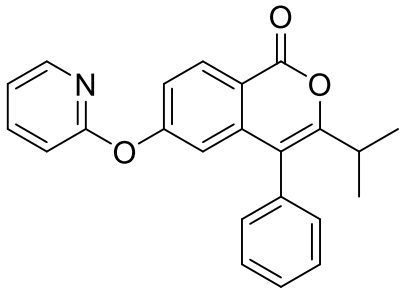


(0.20 mmol, 37.6 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 3.1 mg), and the corresponding propargylic carbonate (**2c**) (0.30 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3wa** was isolated in 50.0% yield (33.0 mg) as yellowish white solid; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.41 (d, *J* = 8.6 Hz, 1H), 7.86 – 7.79 (m, 2H), 7.69 (d, *J* = 1.9 Hz, 1H), 7.56 – 7.46 (m, 3H), 7.32 – 7.28 (m, 2H), 7.20 (d, *J* = 2.2 Hz, 1H), 6.44 (t, *J* = 2.2 Hz, 1H), 2.72 (p, *J* = 6.9 Hz, 1H), 1.22 (d, *J* = 6.9 Hz, 6H); **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 162.27, 160.19, 144.62, 142.37, 140.72, 134.08, 131.62, 130.53, 129.34, 128.51, 127.15, 118.13, 117.87, 114.63, 113.77, 108.84, 30.41, 20.36; **HRMS** m/z (ESI): calcd. for $C_{21}H_{18}N_2NaO_2$ (M + Na) 353.1260, found 353.1275.

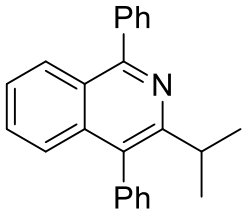
**3-isopropyl-4-phenyl-6-(1H-pyrrolo[2,3-b]pyridin-1-yl)-1*H*-isochromen-1-one**: Following the general procedure, the corresponding benzoic acid (**1**) (0.20 mmol, 47.7 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (5 mol%, 6.1 mg) and the corresponding propargylic carbonate (**2c**) (0.3 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3xa** was isolated in 59% yield (44.9 mg) as colorless solid; **$^1$H NMR (300 MHz, $CDCl_3$)** δ 8.47 (dd, *J* = 8.7, 0.5 Hz, 1H), 8.29 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.10 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.92 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.56 – 7.41 (m, 3H), 7.40 – 7.29 (m, 4H), 7.12 (dd, *J* = 7.9, 4.7 Hz, 1H), 6.60 (d, *J* = 3.7 Hz, 1H), 2.76 (hept, *J* = 6.9 Hz, 1H), 1.24 (d, *J* = 6.9 Hz, 6H); **$^{13}$C NMR (75 MHz, $CDCl_3$)**δ 162.44, 159.81, 147.57, 143.83, 143.81, 140.52, 134.26, 131.16, 130.61, 129.42, 129.15, 128.33, 126.82, 122.22, 122.15, 118.16, 117.54, 117.28, 114.68, 103.42, 30.39, 20.41; **HRMS** m/z (ESI): calcd. for $C_{25}H_{20}N_2NaO_2$ (M + Na) 403.1417, found 403.1404.



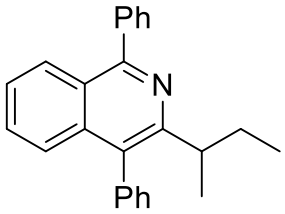

**3-isopropyl-4-phenyl-6-(pyridin-2-yloxy)-1*H*-isochromen-1-one**: Following the general procedure, the corresponding benzoic acid (**1**) (0.20 mmol, 43.0 mg), $K_3PO_4$ (0.5 equiv.), [Ru(*p*-cymene)$Cl_2$]$_2$ (5 mol%, 6.1 mg) and the corresponding propargylic carbonate (**2c**) (0.3 mmol) were used to react in DMA (1.0 mL) for 15 h. Product **3ya** was isolated in 72% yield (51.3 mg) as colorless solid; **$^1$H NMR (300 MHz, $CDCl_3$)** δ 8.28 (d, *J* = 8.7 Hz, 1H), 8.11 – 8.02 (m, 1H), 7.62 (ddd, *J* = 8.3, 7.2, 2.0 Hz, 1H), 7.42 – 7.29 (m, 3H), 7.22 – 7.16 (m, 2H), 7.09 (dd, *J* = 8.7, 2.3 Hz,



1H), 6.95 (ddd, *J* = 7.3, 5.0, 0.9 Hz, 1H), 6.83 (dt, *J* = 8.3, 0.9 Hz, 1H), 6.60 (d, *J* = 2.3 Hz, 1H), 2.63 (hept, *J* = 6.9 Hz, 1H), 1.13 (d, *J* = 6.9 Hz, 6H); **$^{13}$C NMR (75 MHz, $CDCl_3$)** δ 162.52, 162.42, 159.70, 159.63, 147.78, 141.37, 139.89, 134.24, 131.65, 130.52, 129.09, 128.22, 120.56, 119.59, 116.46, 116.15, 114.58, 112.41, 30.32, 20.36; **HRMS** m/z (ESI): calcd. for $C_{23}H_{19}NNaO_3$ (M + Na) 380,1257, found 380,1268.

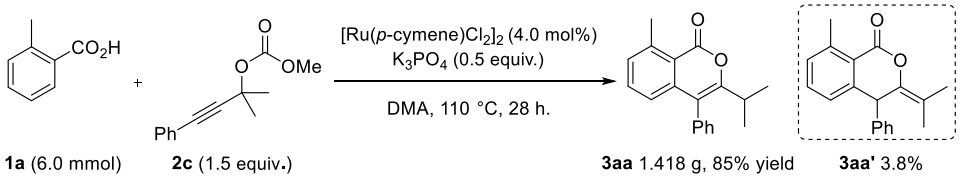



**3-isopropyl-1,4-diphenylisoquinoline**:[12] Following the general procedure, the corresponding benzophenone imine (**1**) (0.20 mmol), $K_3PO_4$ (0.5 equiv.), $[Ru(p\text{-cymene})Cl_2]_2$ (2.5 mol%, 3.1 mg) and the corresponding propargylic carbonate (**2c**) (0.30 mmol) were used to react in DMA (1.0 mL) for 17 h. Product **4a** was isolated in 53% yield (34.3 mg) as white solid; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.17 – 8.08 (m, 1H), 7.87 – 7.76 (m, 2H), 7.59 – 7.33 (m, 11H), 3.07 (p, *J* = 6.8 Hz, 1H), 1.29 (d, *J* = 6.7 Hz, 6H); **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 159.51, 156.62, 140.48, 138.22, 137.04, 130.46, 129.44, 128.62, 128.49, 128.46, 128.33, 127.51, 127.31, 126.01, 125.77, 124.77, 32.29, 22.75; **HRMS** m/z (ESI): calcd. for $C_{24}H_{22}N$ (M + H) 324.1747, found 324.1749.



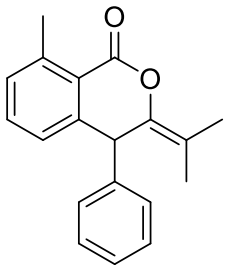

**3-(sec-butyl)-1,4-diphenylisoquinoline**: Following the general procedure, the corresponding benzophenone imine (**1**) (0.20 mmol), $K_3PO_4$ (0.5 equiv.), $[Ru(p\text{-cymene})Cl_2]_2$ (2.5 mol%, 3.1 mg) and the corresponding propargylic carbonate (**2**) (0.30 mmol) were used to react in DMA (1.0 mL) for 17 h. Product **4b** was isolated in 54% yield (36.5 mg) as white solid; **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.16 (d, *J* = 8.4 Hz, 1H), 7.89 – 7.77 (m, 2H), 7.62 – 7.36 (m, 11H), 2.93 – 2.75 (m, 1H), 2.11 – 1.98 (m, 1H), 1.64 – 1.54 (m, 1H), 1.29 (d, *J* = 6.7 Hz, 3H), 0.75 (t, *J* = 7.3 Hz, 3H); **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 159.58, 155.66, 140.50, 138.24, 136.97, 130.81, 130.45, 130.42, 129.62, 129.44, 128.62, 128.50, 128.43, 128.32, 127.44, 127.30, 126.04, 125.78, 124.66, 39.29, 29.47, 21.40, 12.66; **HRMS** m/z (ESI): calcd. for $C_{25}H_{23}NNa$ (M + Na) 360,1723, found 360,1718.

## 4) Gram-scale synthesis of 3aa.

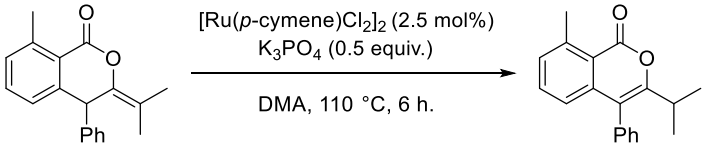



**1a** (6.0 mmol) **2c** (1.5 equiv.) **3aa** 1.418 g, 85% yield **3aa'** 3.8%

Following the standard procedure, **1a** (6.0 mmol, 816.9 mg), **2a** (1.5 equiv., 9.0 mmol), [Ru(*p*-cymene)$Cl_2$]$_2$ (4.0 mol%, 146.9 mg) and $K_3PO_4$ (0.5 equiv., 636.9 mg) were dissolved in DMA (20 mL) and heated to 110 ℃ for 28 h. Afterwards, the reaction mixture was cooled to room temperature, brine and EtOAc were added (100 mL) each. The aqueous phase was extracted with EtOAc for 4 times. The combined organic phases were dried over $Na_2SO_4$. The product was purified by flash chromatography ($SiO_2$, washed with 10 mL trimethylamine in 500 mL pentane) using pentane/EtOAc (100:1 to 50:1) as eluent. Product **3aa** was isolated in 85%, (1.418 g), **3aa´** was observed in 3.8% yield by NMR analysis using 1,3,5-trimethoxybenzene as internal standard.




**8-methyl-4-phenyl-3-(propan-2-ylidene)isochroman-1-one**: **$^1$H NMR (300 MHz, $CDCl_3$)** δ 7.37 (t, *J* = 7.6 Hz, 1H), 7.21 – 7.08 (m, 5H), 7.06 – 6.97 (m, 2H), 5.09 (s, 1H), 2.63 (s, 3H), 1.82 (s, 3H), 1.75 (s, 3H); **$^{13}$C NMR (75 MHz, $CDCl_3$)** δ 162.76, 142.99, 141.71, 141.53, 140.45, 133.22, 131.43, 128.82, 127.30, 127.21, 125.96, 123.20, 114.46, 44.25, 22.21, 18.62, 17.14; **HRMS** m/z (ESI): calcd. for $C_{19}H_{18}NaO_2$ (M + Na) 301,1199, found 301,1199.

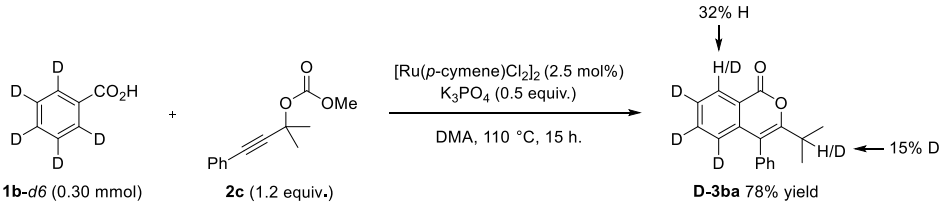



**3aa'** (0.1 mmol) **3aa** 100% yield

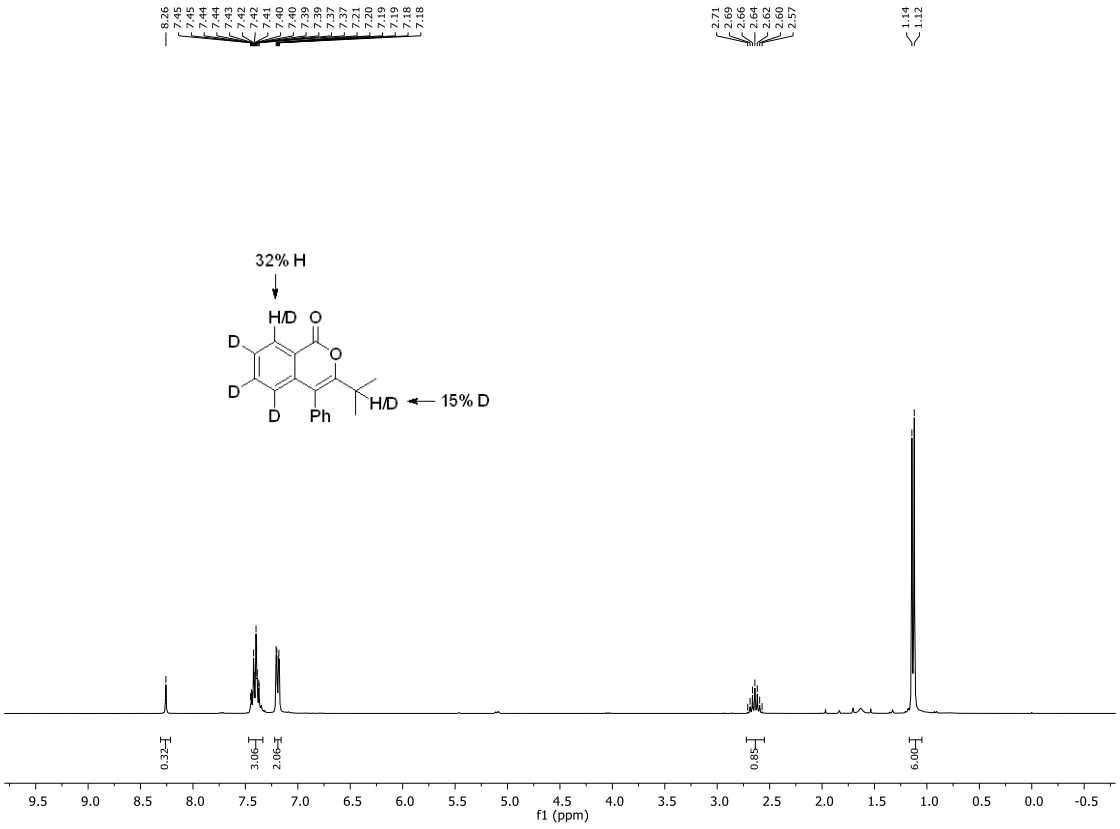
Following the standard procedure, **3aa´** (0.1 mmol, 27.8 mg), $K_3PO_4$ (0.5 equiv.) and [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 1.5 mg) were dissolved in DMA (1.0 mL) and heated to 110 ℃ for 6 h. Afterwards, the reaction mixture was cooled to room temperature and analyzed by NMR analysis using 1,3,5-trimethoxybenzene as internal standard. **3aa´** was stoichiometrically transformed into product **3aa**.

## 5) Isotope labeling experiment.

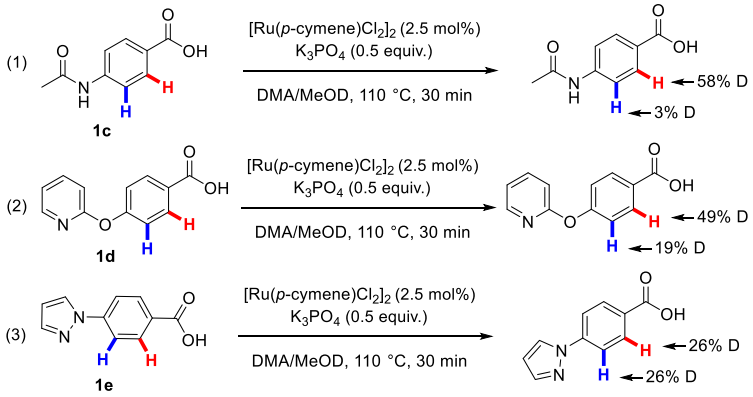
### 5.1) The reaction of isotopically-labeled [$D_5$]-benzoic acid with 2c.



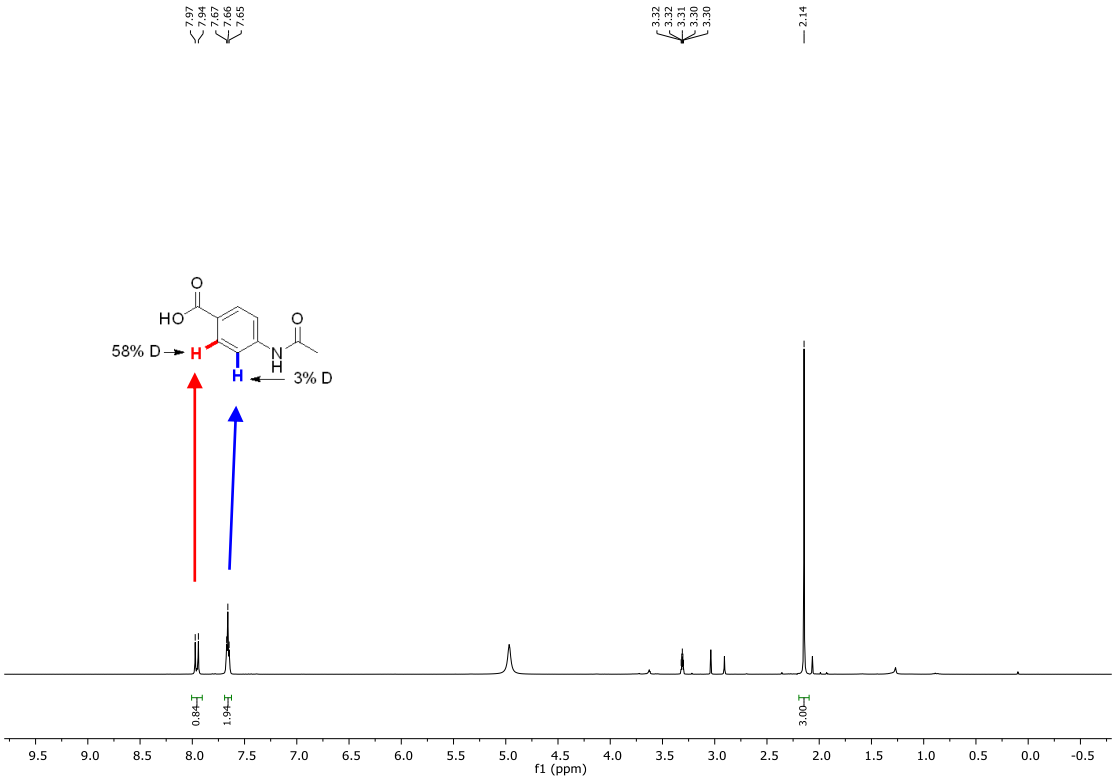

Following the standard procedure, **1b**-*d6* (0.30 mmol, 38.1 mg), **2c** (1.2 equiv., 0.36 mmol), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg) and $K_3PO_4$ (0.5 equiv., 31.8 mg) were dissolved in DMA (1 mL) and heated to 110 ℃ for 15 h. Afterwards, the reaction mixture was cooled to room temperature, brine and EtOAc were added (50 mL) each. The aqueous phase was extracted with EtOAc for 4 times. The combined organic phases were dried over $Na_2SO_4$. The product was purified by flash chromatography ($SiO_2$, washed with 5 mL trimethylamine in 300 mL pentane) using pentane/EtOAc (100:1 to 50:1) as eluent. Product **D-3ba** was isolated in 78% yield (63.0 mg).

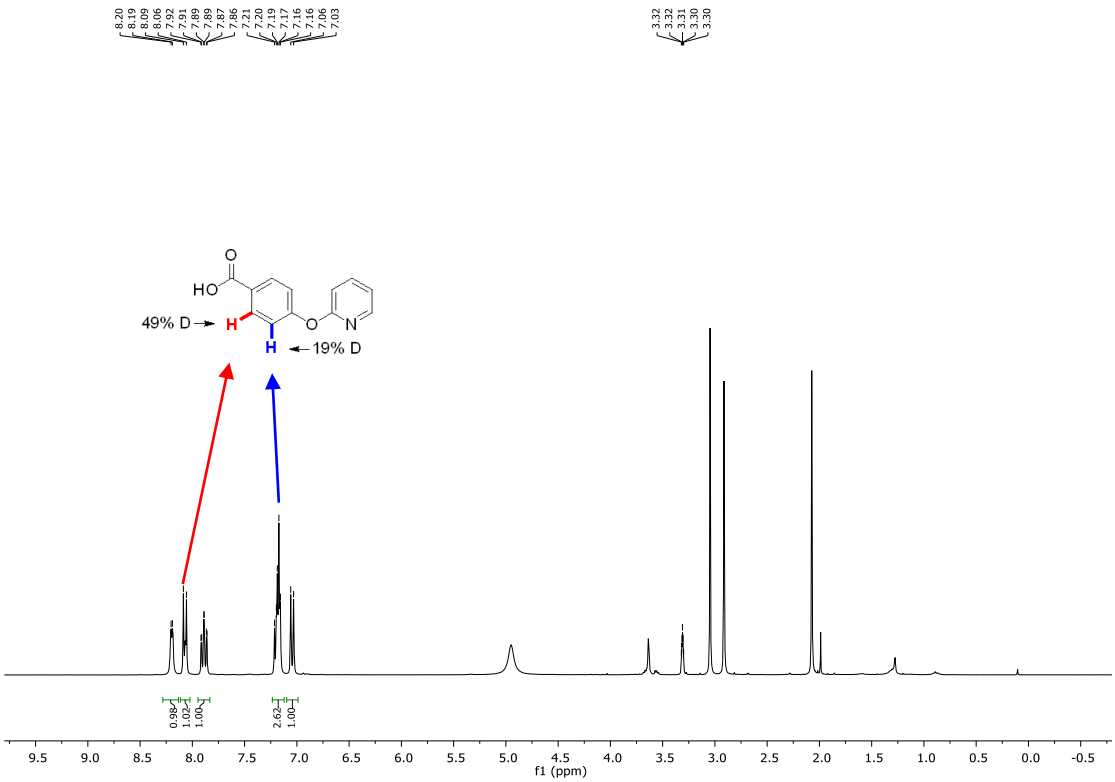


## 5.2) H/D scrambling experiments.




Following the standard procedure, the corresponding starting material **1** (0.20 mmol), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 3.1 mg) and $K_3PO_4$ (0.5 equiv.) were dissolved in DMA (0.9 mL) and $CD_3OD$ (0.1 mL). The reaction mixture was heated to 110 ℃ for 30 min. Afterwards, the reaction mixture was cooled to room temperature, brine and EtOAc were added (50 mL) each. The aqueous phase was extracted with EtOAc for 4 times. The combined organic phases were dried over $Na_2SO_4$. After rotary evaporation to remove solvent, the reaction mixture was analyzed by $^1$H NMR.




8.20
8.19
8.09
8.06
7.92
7.91
7.89
7.89
7.87
7.86
7.21
7.20
7.19
7.17
7.16
7.15
7.06
7.03
3.32
3.32
3.31
3.30
3.30
O
HO
49% D
H
O
N
H
19% D
0.98
1.02
1.00
2.62
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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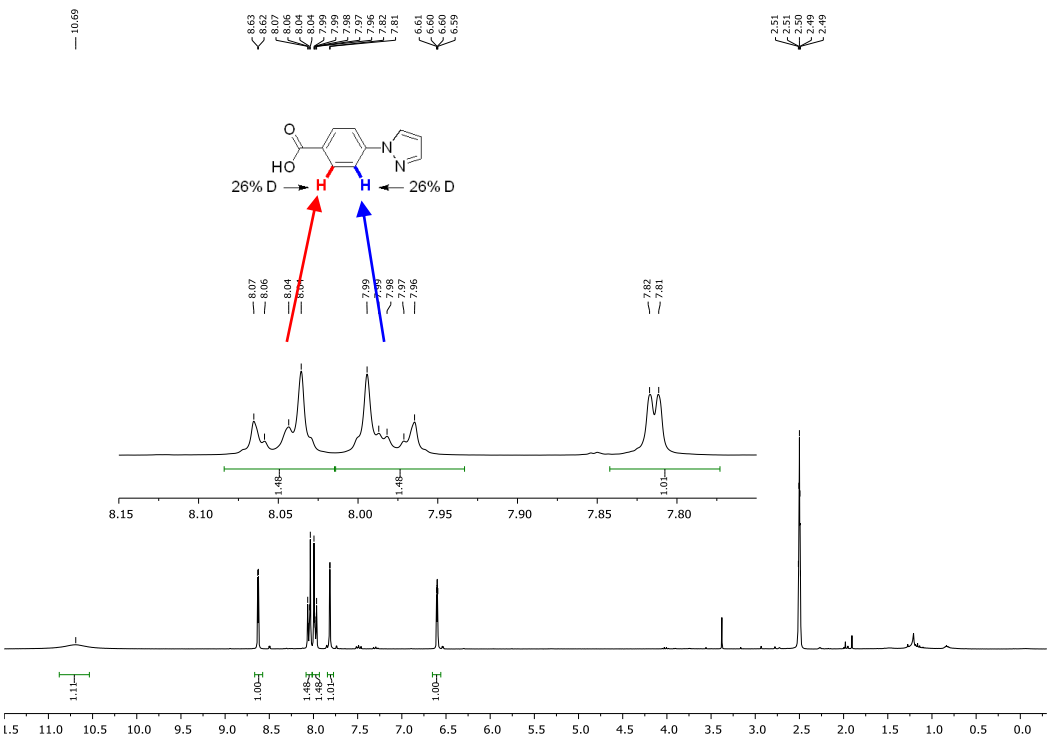
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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8.62
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8.04
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7.96
7.82
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6.60
6.60
6.59
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2.51
2.50
2.49
2.49
O
HO
N
N
26% D
H
H
26% D
8.07
8.06
8.04
8.04
7.99
7.98
7.98
7.97
7.96
7.82
7.81
1.48
1.48
1.01
8.15
8.10
8.05
8.00
7.95
7.90
7.85
7.80
1.11
1.00
1.48
1.48
1.01
1.00
11.5
11.0
10.5
10.0
9.5
9.0
8.5
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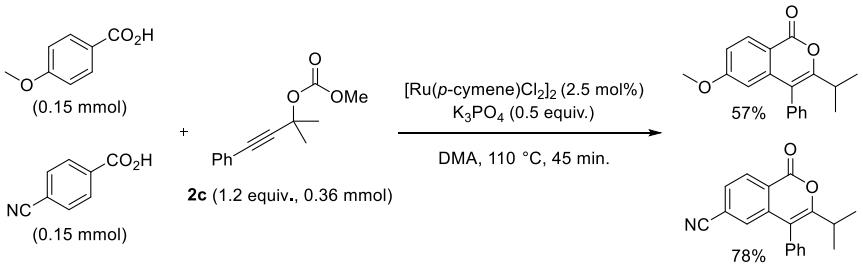
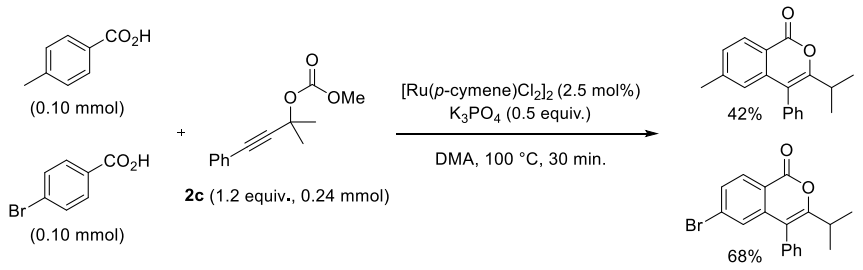
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

## 6) Intermolecular competition experiments.

### 6.1) Competition experiments between different compounds 1.

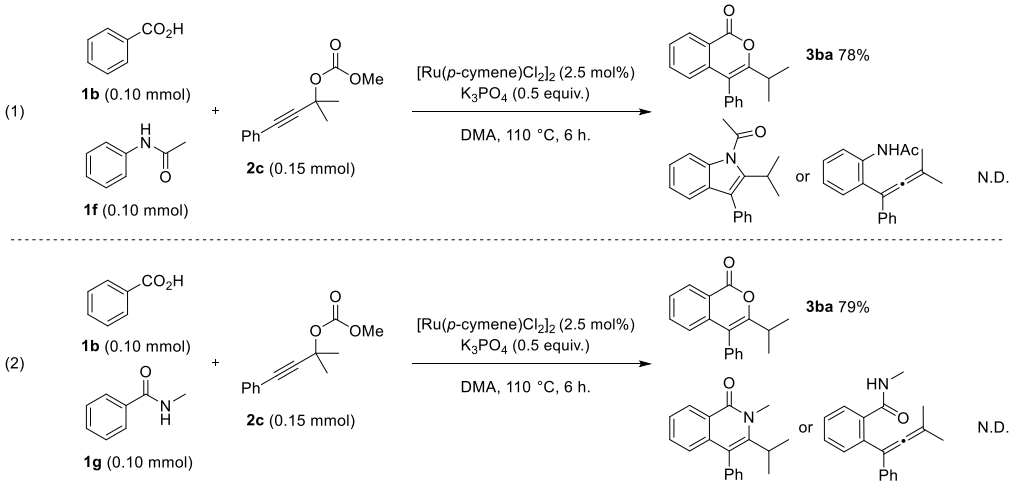



Following the standard procedure, 4-methoxybenzoic acid (0.15 mmol, 22.8 mg), 4-cyanobenzoic acid (0.15 mmol, 22.1 mg), **2c** (1.2 equiv., 0.36 mmol), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg) and $K_3PO_4$ (0.5 equiv., 31.8 mg) were dissolved in DMA (1 mL) and heated to 110 ℃ for 45 minutes. Afterwards, the reaction mixture was cooled to room temperature, brine and EtOAc were added (50 mL) each. The aqueous phase was extracted with EtOAc for 4 times. The combined organic phases were dried over $Na_2SO_4$. After rotary evaporation to remove solvent, the reaction mixture was analyzed by $^1$H NMR using 1,3,5-trimethoxybenzene as internal standard (the yield was based on the corresponding benzoic acid).



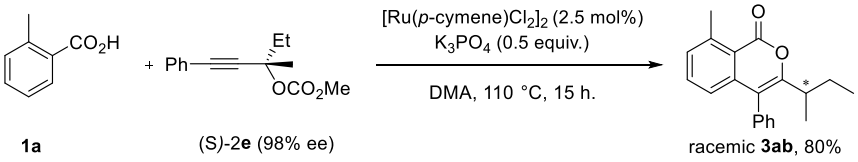

Following the standard procedure, 4-methylbenzoic acid (0.10 mmol, 13.6 mg), 4-bromobenzoic acid (0.10 mmol, 20.1 mg), **2c** (1.2 equiv., 0.24 mmol), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 3.06 mg) and $K_3PO_4$ (0.5 equiv., 21.2 mg) were dissolved in DMA (1 mL) and heated to 100 ℃ for 30 minutes. Afterwards, the reaction mixture was cooled to room temperature, brine and EtOAc were added (50 mL) each. The aqueous phase was extracted with EtOAc for 4 times. The combined organic phases were dried over $Na_2SO_4$. After rotary evaporation to remove solvent, the reaction mixture was analyzed by $^1$H NMR using 1,3,5-trimethoxybenzene as internal standard (the yield was based on the corresponding benzoic acid).

## 6.2) Competition experiments between compounds 1 with different directing groups.




Following the standard procedure, benzoic acid (**1b**, 0.10 mmol, 13.6 mg), *N*-phenylacetamide **1f** or *N*-methylbenzamide **1g** (0.10 mmol), **2c** (0.15 mmol), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 3.06 mg) and $K_3PO_4$ (0.10 mmol, 21.2 mg) were dissolved in DMA (0.5 mL) and heated to 110 ℃ for 6 h. Afterwards, the reaction mixture was cooled to room temperature, brine and EtOAc were added (50 mL) each. The aqueous phase was extracted with EtOAc for 4 times. The combined organic phases were dried over $Na_2SO_4$. After rotary evaporation to remove solvent, the reaction mixture was analyzed by GC-MS and the yield was determined by $^1$H NMR using 1,3,5-trimethoxybenzene as internal standard (the yield was based on the corresponding benzoic acid).

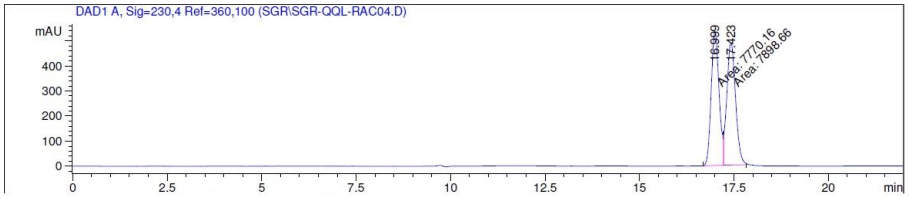
## 7) Chirality transfer experiment.




Following the standard procedure, **1a** (0.20 mmol, 27.2 mg), (***S*)-2e** (98% ee, 1.2 equiv., 0.24 mmol), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 3.1 mg) and $K_3PO_4$ (0.5 equiv., 21.2 mg) were dissolved in DMA (1 mL) and heated to 110 ℃ for 15 h. Afterwards, the reaction mixture was cooled to room temperature, brine and EtOAc were added (50 mL) each. The aqueous phase was extracted with EtOAc for 4 times. The combined organic phases were dried over $Na_2SO_4$. The product was purified by flash chromatography ($SiO_2$, washed with 5 mL trimethylamine in 300 mL pentane)

using pentane/EtOAc (100:1 to 50:1) as eluent. Product **3ac** was isolated in 80% yield (47.1 mg), which is racemic.

Conditions: OD-H column, 99/1 *n*-hexane/*i*-PrOH, 0.3 mL/min flow rate, 18 bar pressure.
For standard racemic product **3ab**:

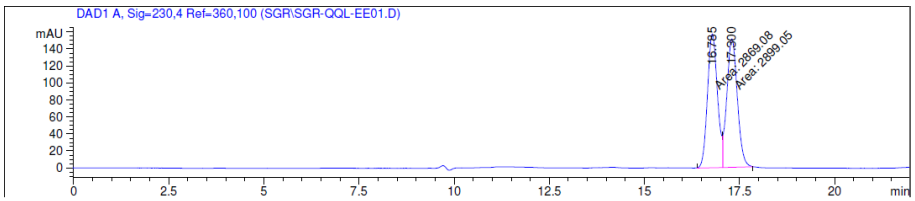



Signal 1: DAD1 A, Sig=230,4 Ref=360,100

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|---|---|---|---|---|---|---|
| 1 | 16.999 | MF | 0.2420 | 7770.15967 | 535.19635 | 49.5899 |
| 2 | 17.423 | FM | 0.2692 | 7898.66309 | 489.09302 | 50.4101 |

Totals : 1.56688e4 1024.28937

Racemic product **3ab** isolated from chirality transfer experiment:



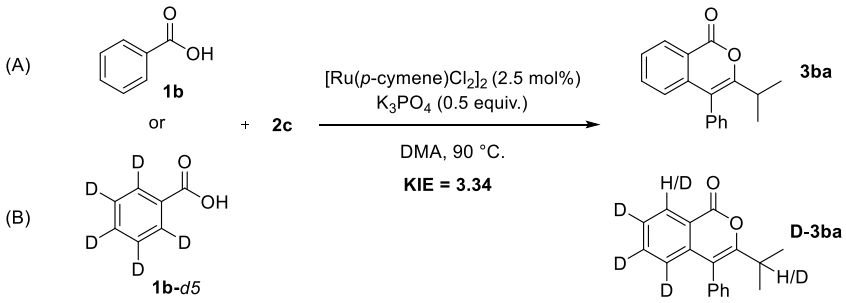

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|---|---|---|---|---|---|---|
| 1 | 16.785 | MF | 0.3038 | 2869.08374 | 157.38620 | 49.7402 |
| 2 | 17.300 | FM | 0.3200 | 2899.05273 | 151.01228 | 50.2598 |

Totals : 5768.13647 308.39848

## 8) KIE experiments.

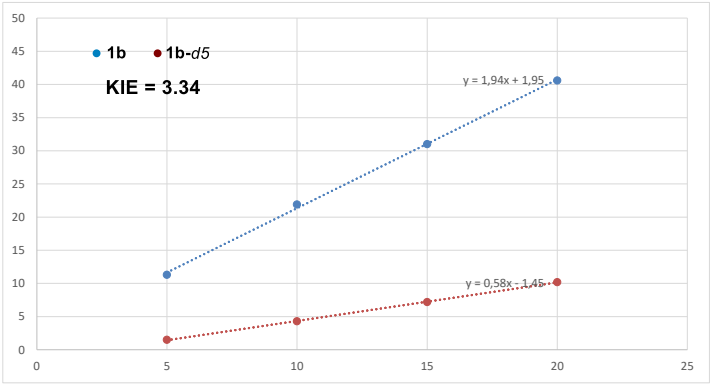
## Parallel experiments for the synthesis of 3ba.



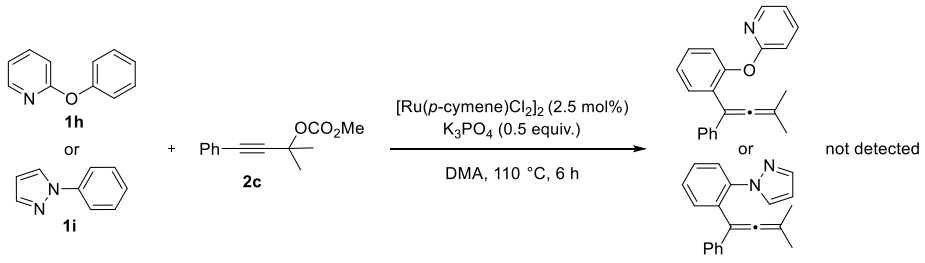

Following the standard procedure, **1a** (0.30 mmol, 38.1 mg), **1a**-*d6* (0.30 mmol, 38.1 mg), **2c** (1.2 equiv., 0.36 mmol), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 4.6 mg), $K_3PO_4$ (0.5 equiv., 31.8 mg) and 1,3,5-trimethoxybenzene (11.2 mg) as internal standard were dissolved in DMA (2.0 mL) and heated to 90 ℃. After 5, 10, 20 and 30 minutes 75 μL of the reaction mixture were filtered over

silica gel and submitted to GC-FID analysis.

| Time (min) | Yield of **3ba** (%) | Yield of **D-3ba** (%) |
|---|---|---|
| 5 | 11.3 | 1.5 |
| 10 | 21.9 | 4.3 |
| 15 | 31.0 | 7.2 |
| 20 | 40.6 | 10.2 |




## 9) Failed N-directing C–H functionalization.




Following the standard procedure, 1-phenyl-1H-pyrazole **1h** or 2-phenoxypyridine **1i** (0.20 mmol), **2c** (0.30 mmol), [Ru(*p*-cymene)$Cl_2$]$_2$ (2.5 mol%, 3.06 mg) and $K_3PO_4$ (0.10 mmol, 21.2 mg) were dissolved in DMA (1.0 mL) and heated to 110 ℃ for 6 h. Afterwards, the reaction mixture was cooled to room temperature, brine and EtOAc were added (50 mL) each. The aqueous phase was extracted with EtOAc for 4 times. The combined organic phases were dried over $Na_2SO_4$. After rotary evaporation to remove solvent, the reaction mixture was analyzed by GC-MS and $^1$H NMR using 1,3,5-trimethoxybenzene as internal standard. Propargylic carbonate **2c** was fully decomposed, and the recovery for **1h** and **1i** is 34% and 13% respectively (they might be stable under present basic condition).

## 10) X-ray data.

**X-Ray diffraction:** Data sets for compound **3aa** were collected with a Bruker APEX II CCD diffractometer. Programs used: data collection: APEX3 V2016.1-0 (Bruker AXS Inc., **2016**); cell refinement: SAINT V8.37A (Bruker AXS Inc., **2015**); data reduction: SAINT V8.37A (Bruker AXS Inc., **2015**); absorption correction, SADABS V2014/7 (Bruker AXS Inc., **2014**); structure solution SHELXT-2015 (Sheldrick, **2015**); structure refinement SHELXL-2015 (Sheldrick, **2015**). *R*-values are given for observed reflections, and $wR^2$ values are given for all reflections.

**X-ray crystal structure analysis of 3aa (glo9287):** A colorless plate-like specimen of $C_{19}H_{18}O_2$, approximate dimensions 0.030 mm x 0.140 mm x 0.140 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. A total of 1554 frames were collected. The total exposure time was 30.29 hours. The frames were integrated with the Bruker SAINT software package using a wide-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 10704 reflections to a maximum θ angle of 66.64 ° (0.84 Å resolution), of which 2564 were independent (average redundancy 4.175, completeness = 97.9%, $R_{int}$ = 3.91%, $R_{sig}$ = 3.33%) and 2025 (78.98%) were greater than $2\sigma(F^2)$. The final cell constants of a = 8.2948(3) Å, b = 9.5359(3) Å, c = 10.0158(3) Å, α = 75.291(2)°, β = 74.899(2)°, γ = 86.594(2) °, volume = 739.79(4) $Å^3$, are based upon the refinement of the XYZ-centroids of 4486 reflections above 20 σ(I) with 9.439° < 2θ < 133.1 °. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.828. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9170 and 0.9810. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group *P*-1, with Z = 2 for the formula unit, $C_{19}H_{18}O_2$. The final anisotropic full-matrix least-squares refinement on $F^2$ with 193 variables converged at R1 = 4.12%, for the observed data and wR2 = 11.13% for all data. The goodness-of-fit was 1.065. The largest peak in the final difference electron density synthesis was 0.173 $e^-/Å^3$ and the largest hole was -0.207 $e^-/Å^3$ with an RMS deviation of 0.043 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.249 $g/cm^3$ and F(000), 296 $e^-$. CCDC Nr.: 1866187.

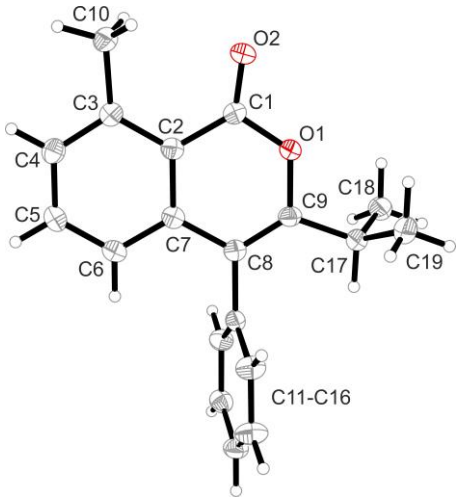



Figure S1. Crystal structure of compound **3aa**.
(Thermals ellipsoids are shown with 50% probability.)

*1.* *APEX3* (**2016**), *SAINT* (**2015**) and *SADABS* (**2014**), Bruker AXS Inc., Madison, Wisconsin, USA.

***2.*** *SHELX* software: Sheldrick, G. M. *Acta Cryst.*, **2015**, *A71*, 3-8.

## References

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[6] Q. Lu, S. Greßies, F. J. R. Klauck, F. Glorius, *Angew. Chem. Int. Ed.* **2017**, *56*, 6660 – 6664.

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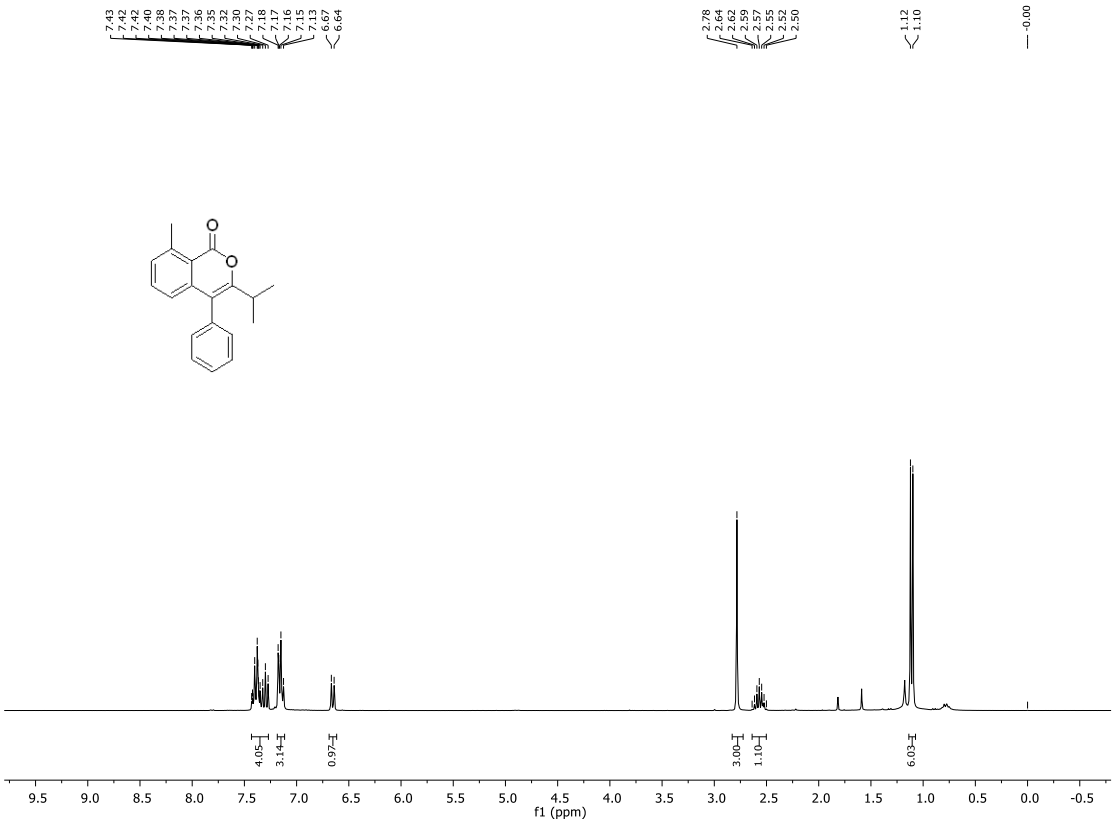
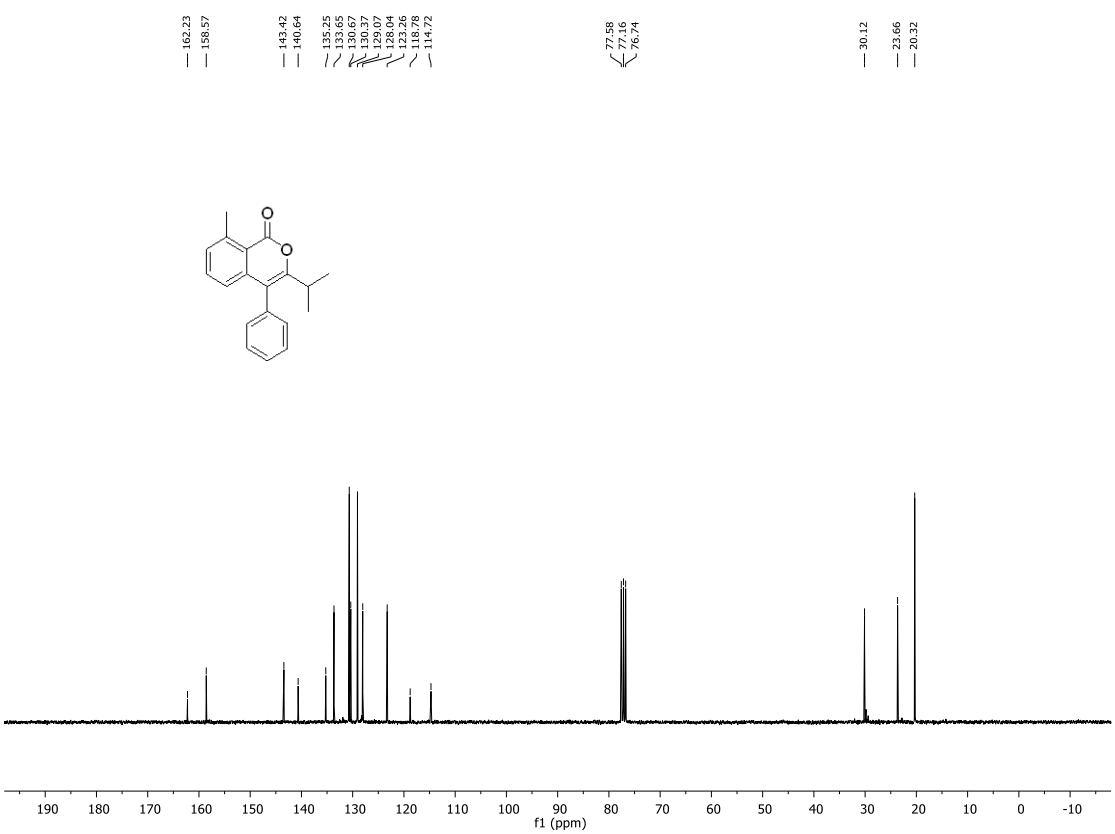
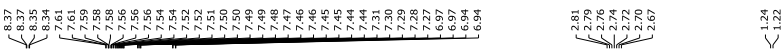
[12] Q. Lu, S. Greßies, S. Cembellín, F. J. R. Klauck, C. G. Daniliuc, F. Glorius, *Angew. Chem. Int. Ed.* **2017**, *56*, 12778 – 12782.

# NMR Spectra of Products

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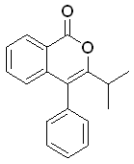
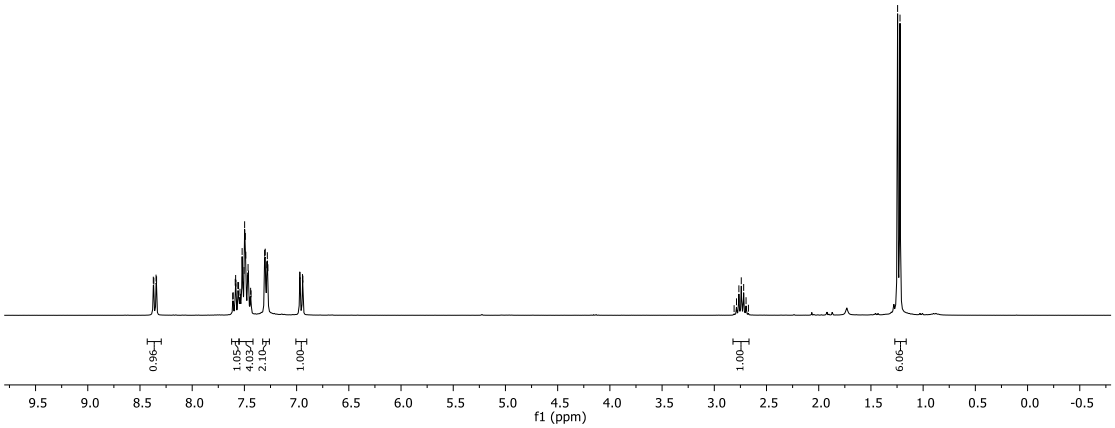
1.22

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1.00
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f1 (ppm)


162.94
158.93
139.04
134.56
134.53
130.56
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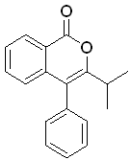
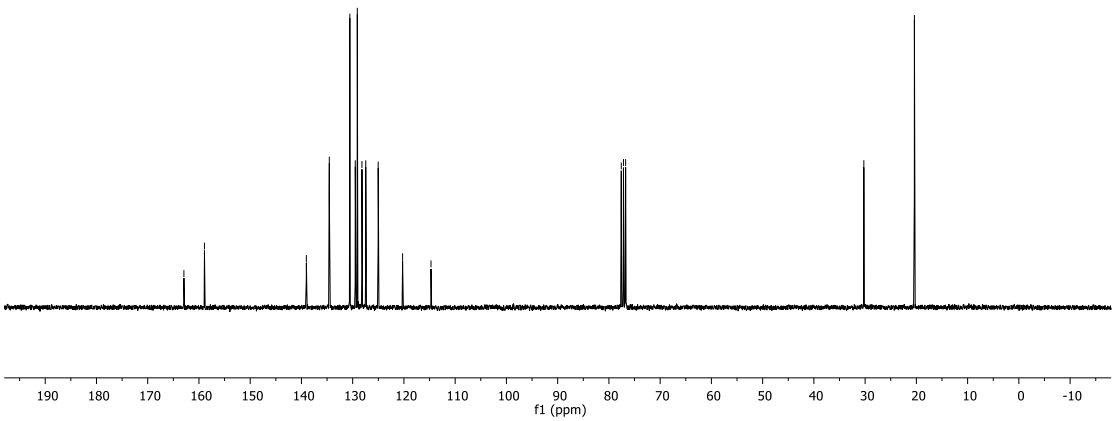
20.39

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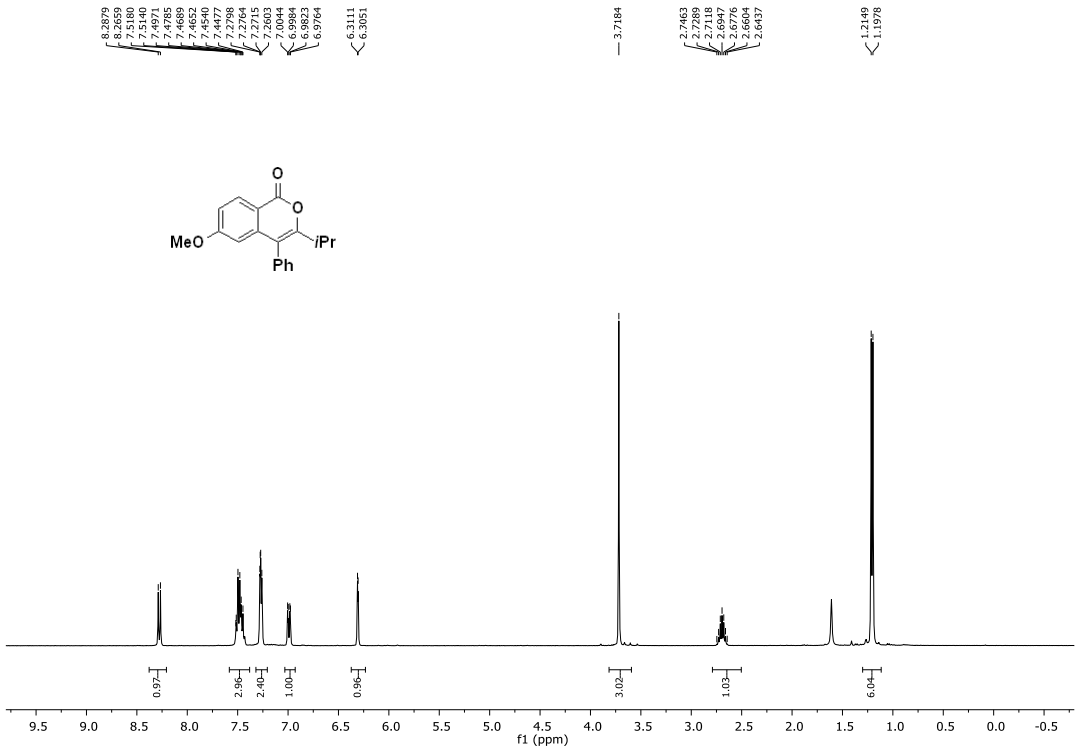
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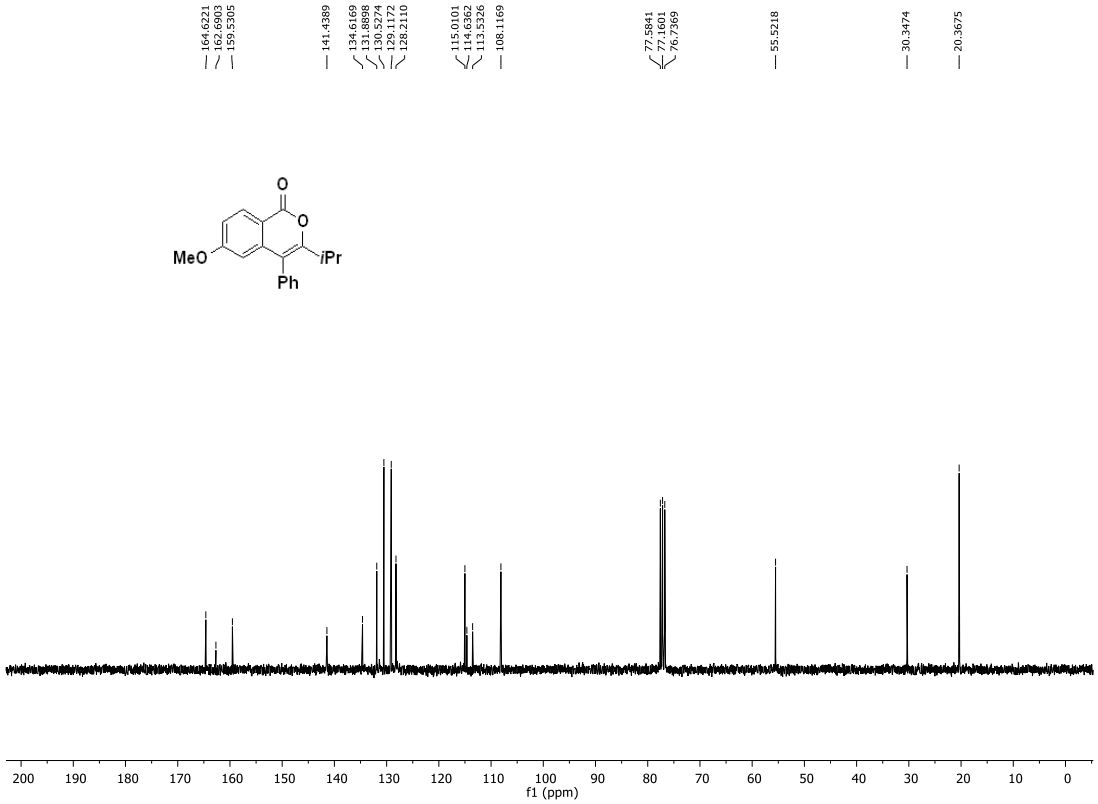
f1 (ppm)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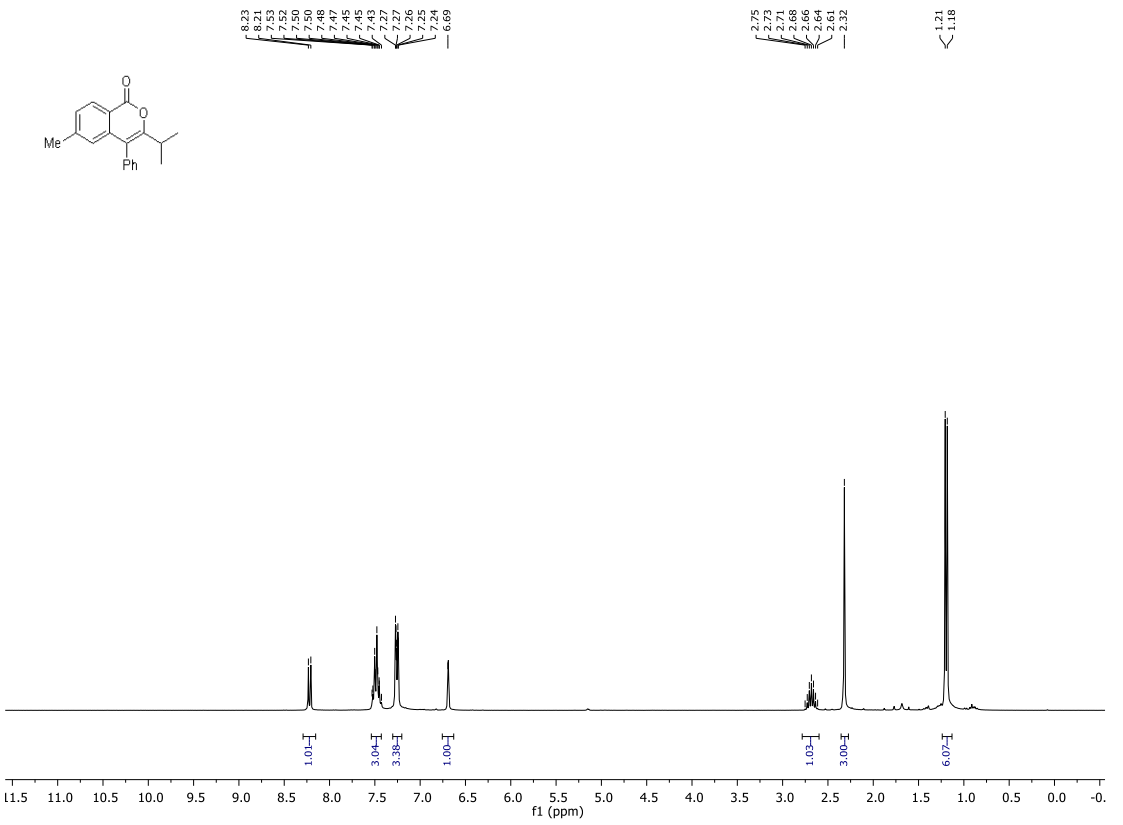
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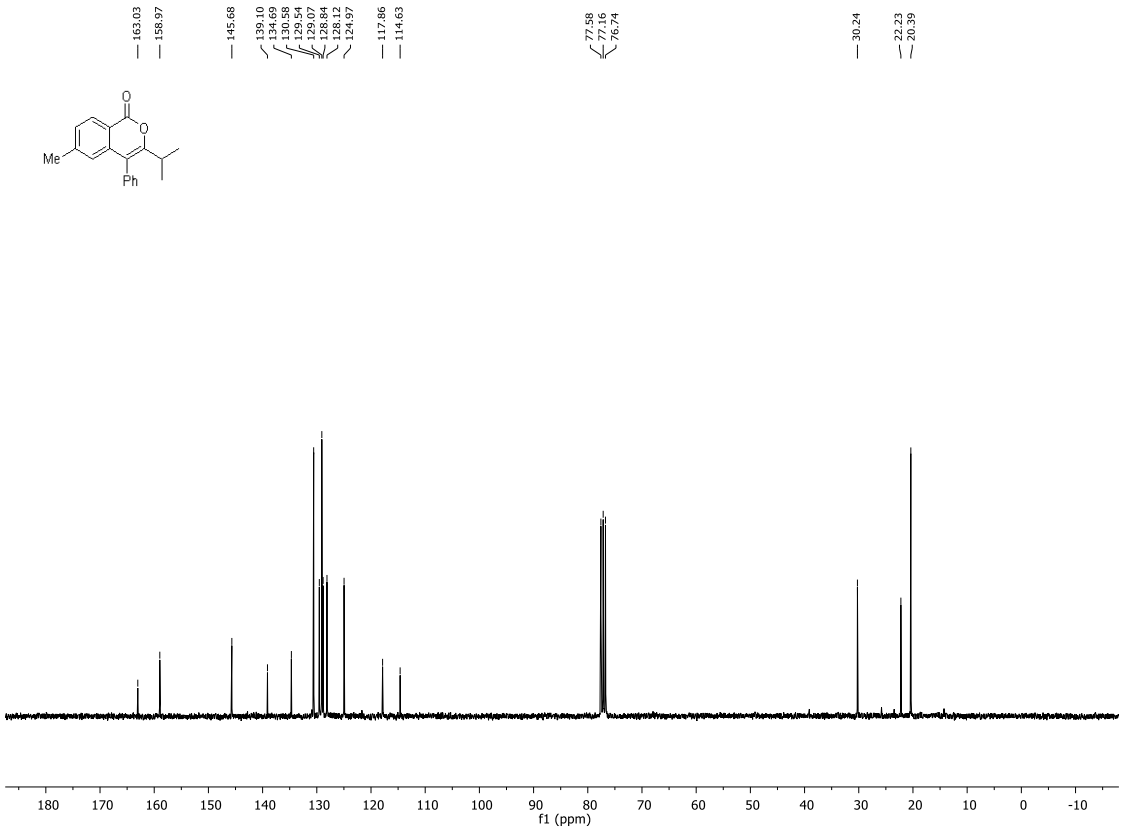
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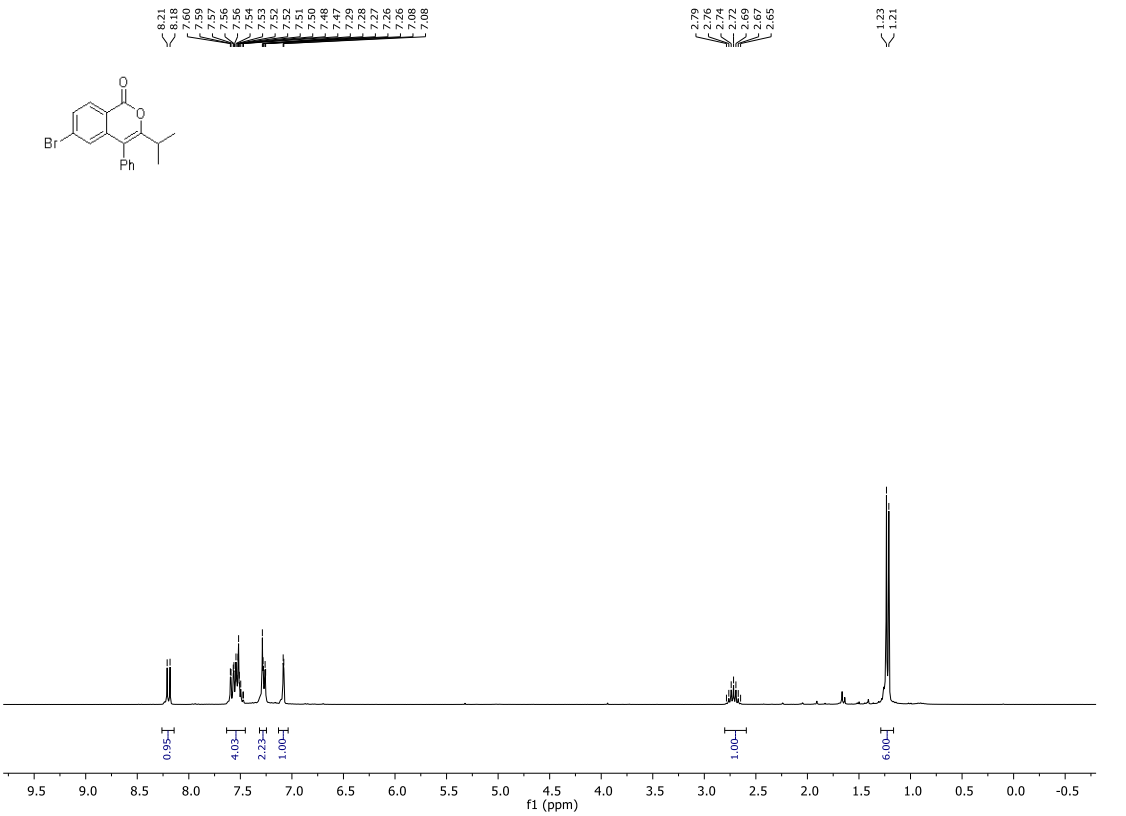
77.58
77.16
76.74
30.24
22.23
20.39
O
O
Me
Ph
f1 (ppm)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7.52
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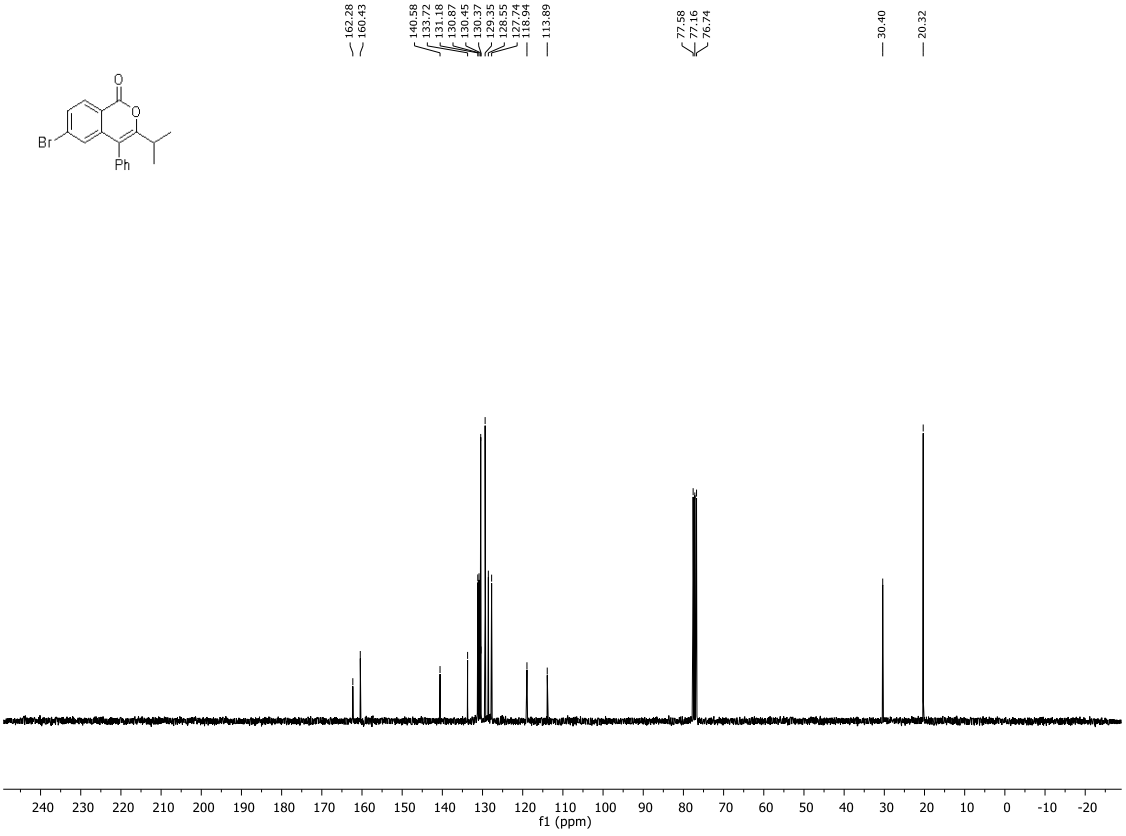
7.50
7.48
7.47
7.29
7.28
7.27
7.26
7.26
7.08
7.08
2.79
2.76
2.74
2.72
2.69
2.67
2.65
1.23
1.21
O
O
Br
Ph
0.95
4.03
2.23
1.00
1.00
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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133.72
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130.37
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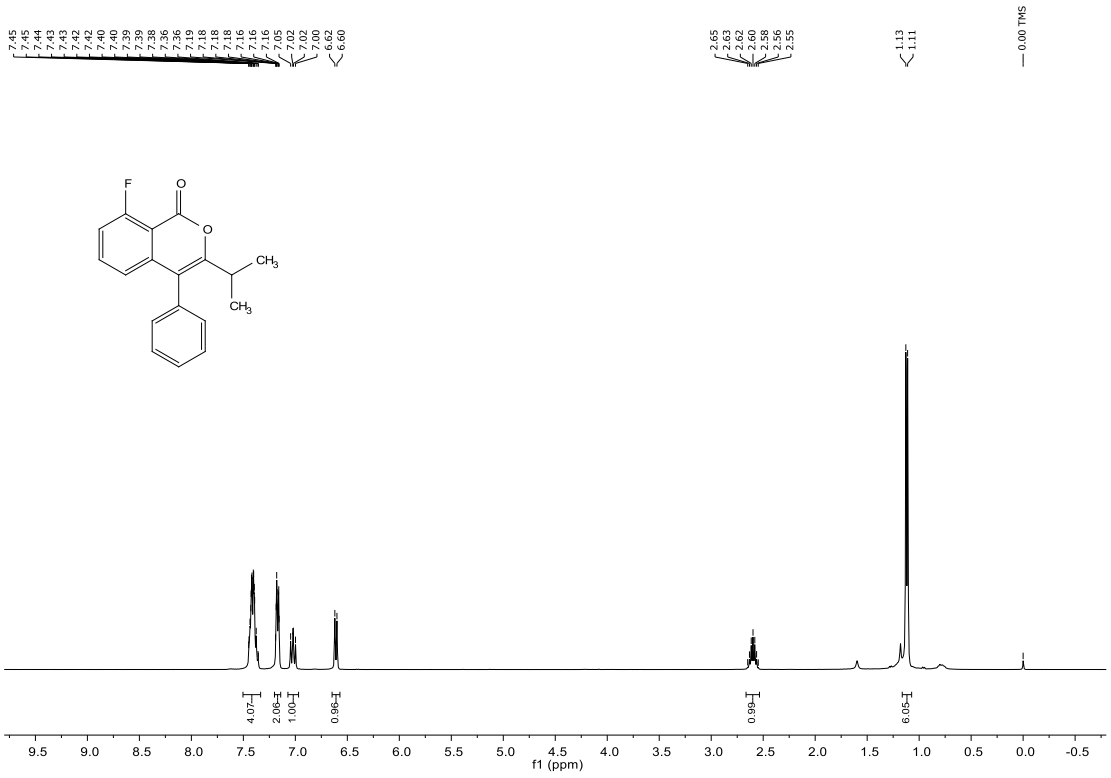
128.55
127.74
118.94
113.89
77.58
77.16
76.74
30.40
20.32
O
O
Br
Ph
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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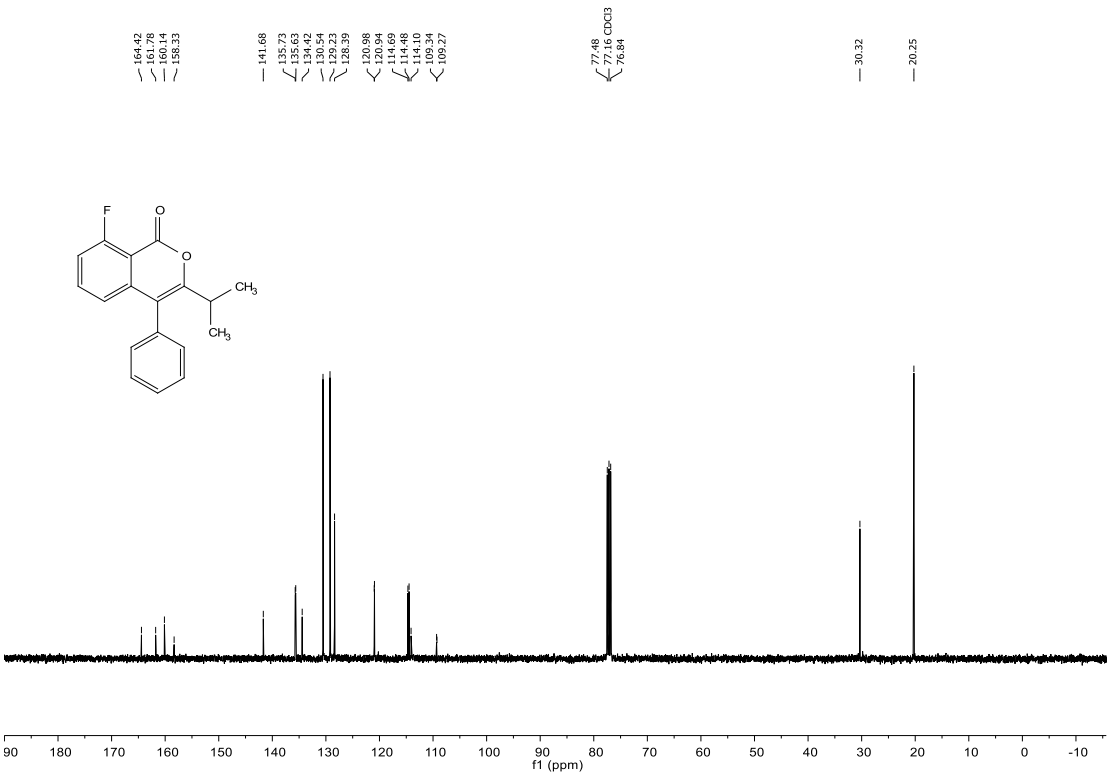
7.36
7.19
7.18
7.18
7.18
7.16
7.16
7.05
7.02
7.02
7.00
6.62
6.60
2.65
2.63
2.62
2.60
2.58
2.56
2.55
1.13
1.11
0.00 TMS
F
O
O
CH3
CH3
4.07
2.06
1.00
0.98
0.99
6.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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158.33
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134.42
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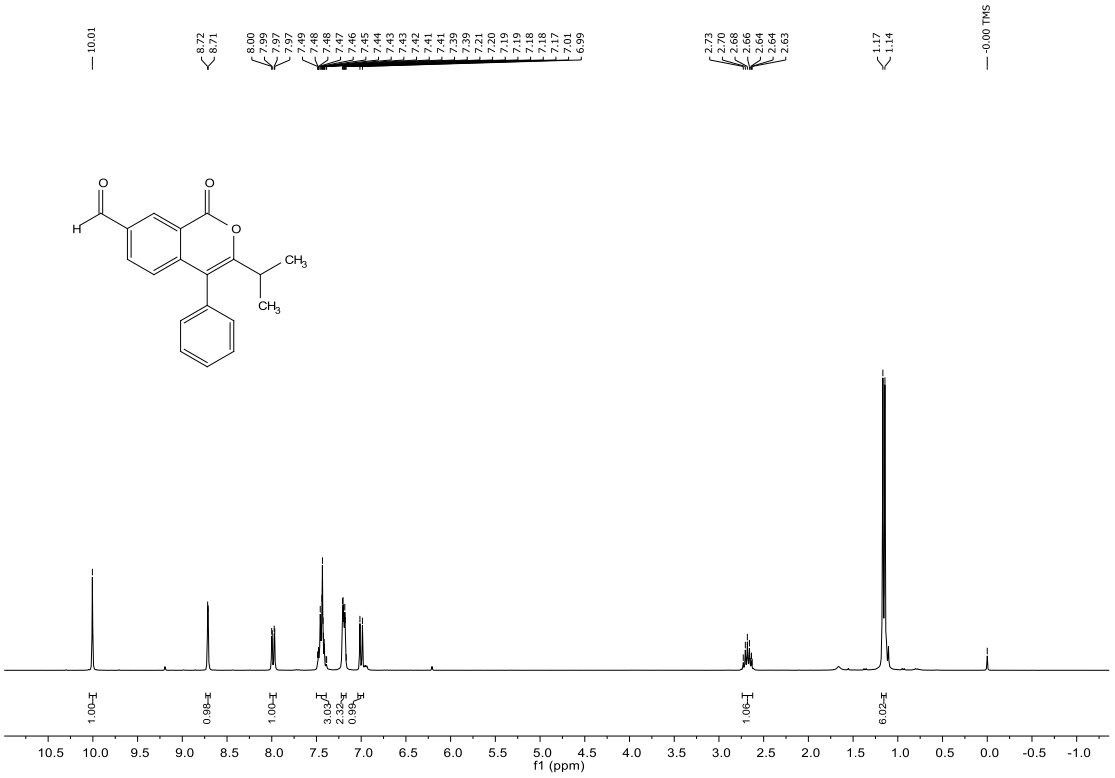
129.23
128.39
120.98
120.94
114.69
114.48
114.10
109.34
109.27
77.48
77.16 CDCl3
76.84
30.32
20.25
F
O
O
CH3
CH3
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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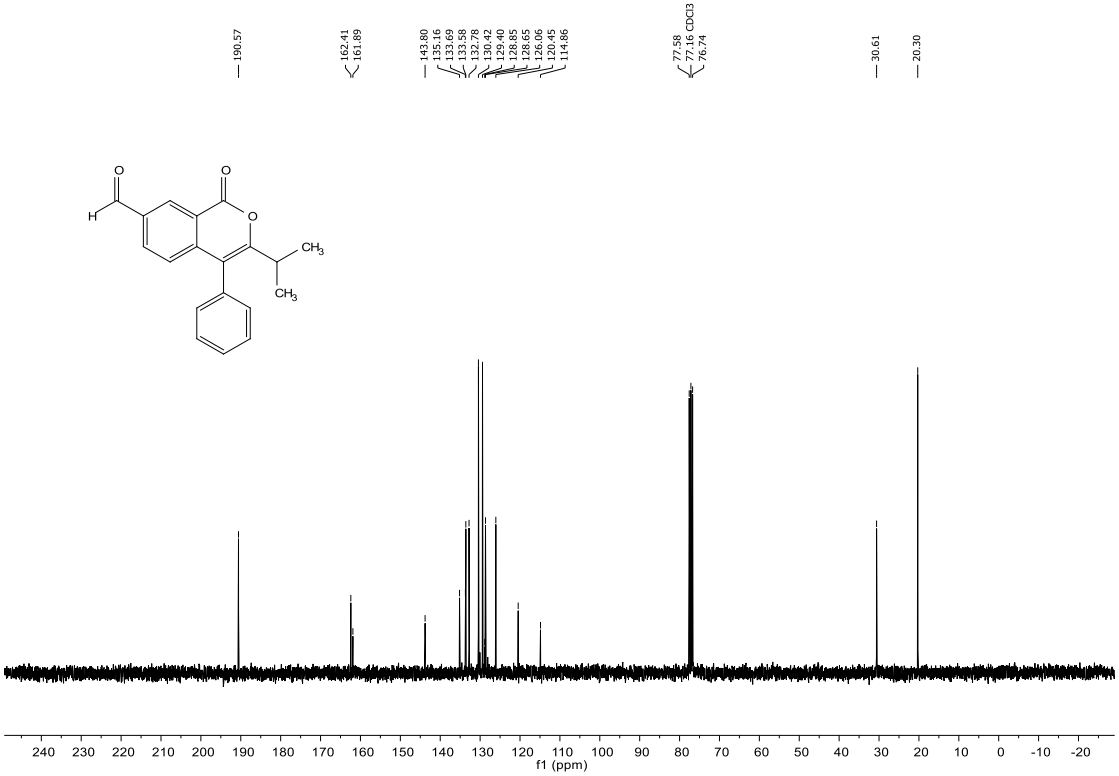
8.72
8.71
8.00
7.99
7.97
7.97
7.49
7.48
7.48
7.47
7.46
7.45
7.44
7.43
7.43
7.42
7.41
7.41
7.39
7.39
7.21
7.20
7.19
7.19
7.18
7.18
7.17
7.01
6.99
2.73
2.70
2.68
2.66
2.64
2.64
2.63
1.17
1.14
-0.00 TMS
O
O
H
O
CH3
CH3
1.00
0.98
1.00
3.03
2.32
0.99
1.06
6.02
f1 (ppm)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161.89
143.80
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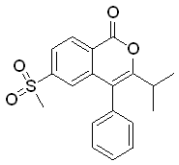
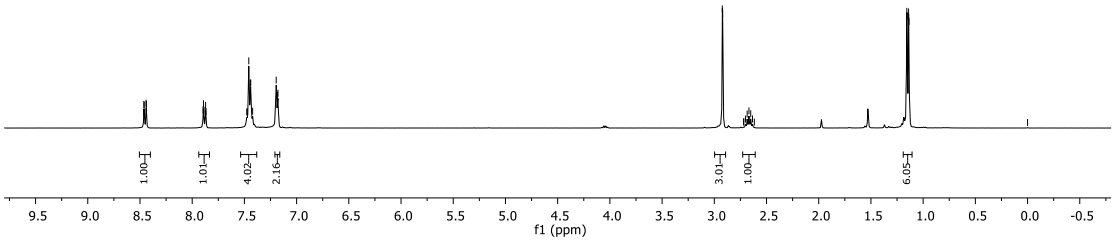
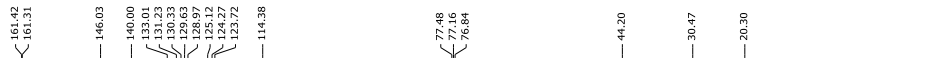
133.69
133.58
132.78
130.42
129.40
128.85
128.65
126.06
120.45
114.86
77.58
77.16 CDCl3
76.74
30.61
20.30
O
O
H
O
CH3
CH3
f1 (ppm)


8.46
8.46
8.44
8.44
7.90
7.89
7.89
7.88
7.87
7.87
7.48
7.47
7.46
7.44
7.44
7.20
7.18
7.18
2.92
2.92
2.72
2.72
2.70
2.69
2.67
2.65
2.63
2.62
1.16
1.15
1.14
1.14
0.00




1.00
1.01
4.02
2.16
3.01
1.00
6.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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161.31
146.03
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133.01
131.23
130.33
129.63
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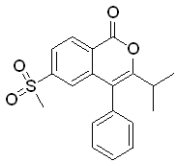
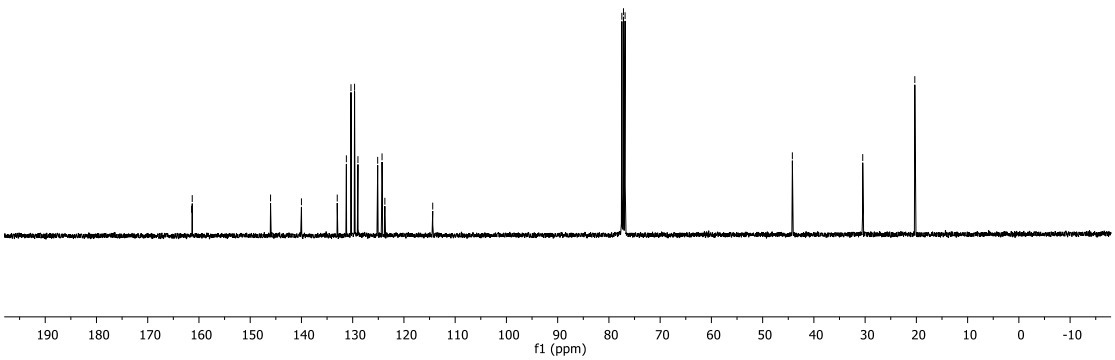
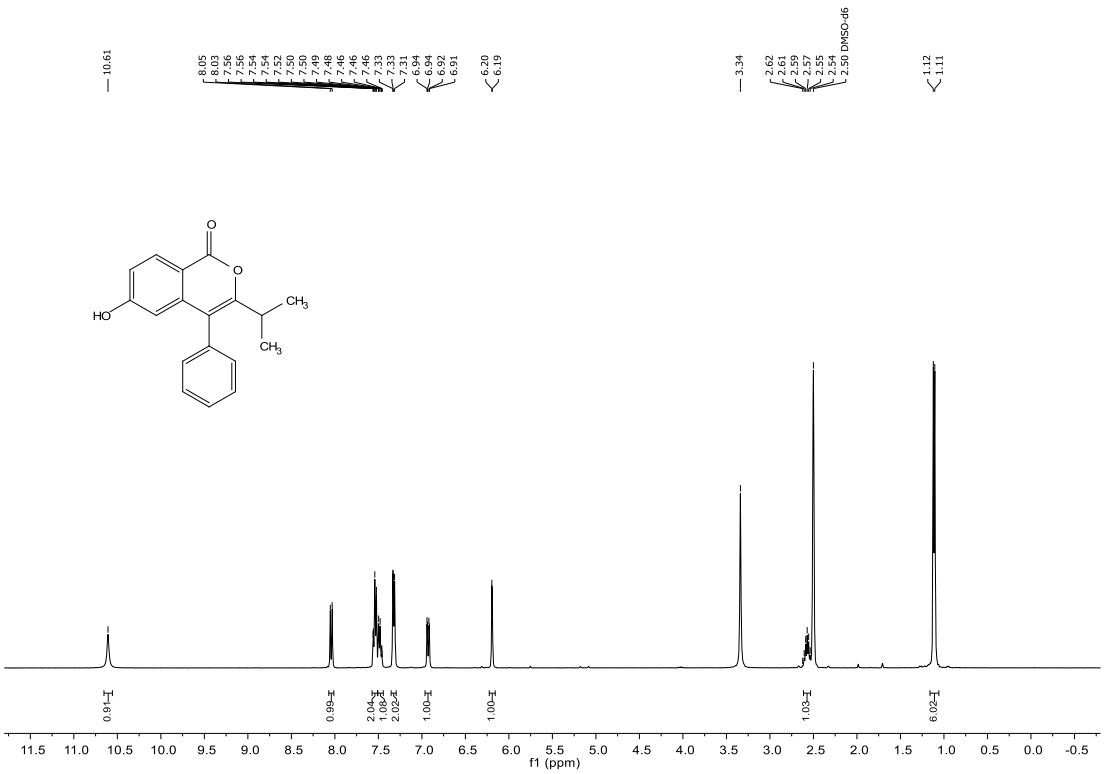
125.12
124.22
123.72
114.38
77.48
77.16
76.84
44.20
30.47
20.30




190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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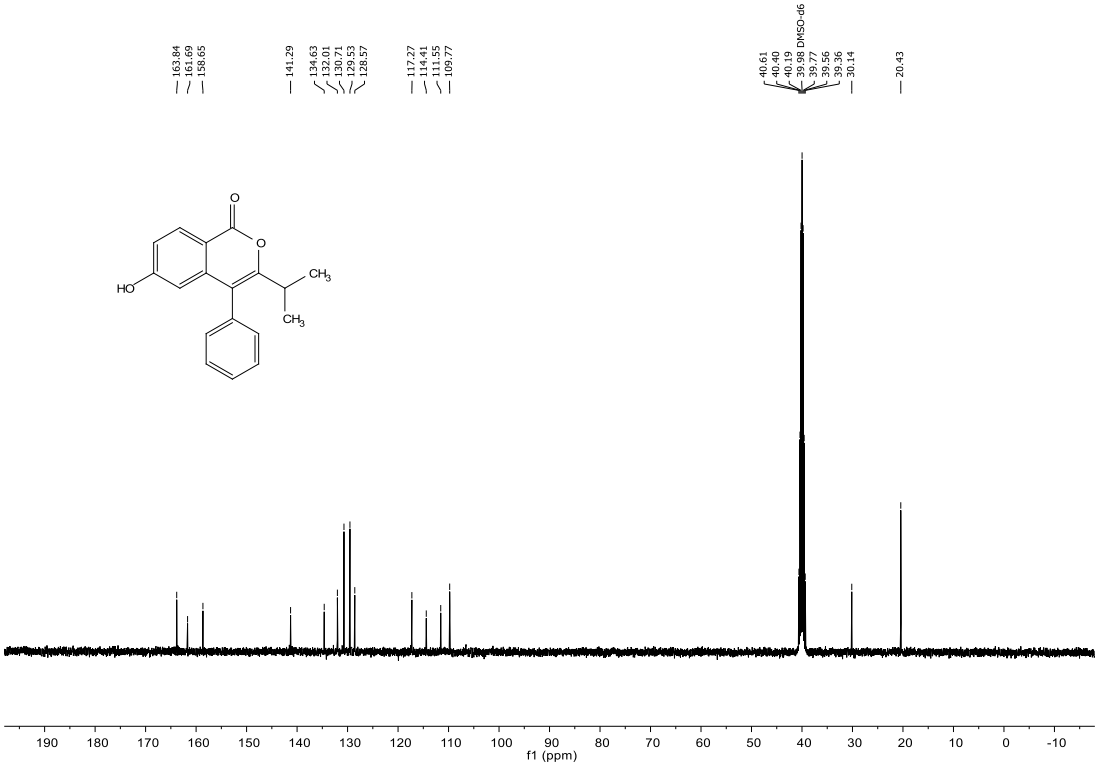
8.03
7.56
7.55
7.54
7.52
7.50
7.49
7.48
7.46
7.46
7.46
7.33
7.31
6.94
6.94
6.92
6.91
6.20
6.19
3.34
2.62
2.61
2.59
2.57
2.55
2.54
2.50 DMSO-d6
1.12
1.11
O
O
HO
CH3
CH3
0.91
0.99
2.04
1.08
2.02
1.00
1.00
1.03
6.02
f1 (ppm)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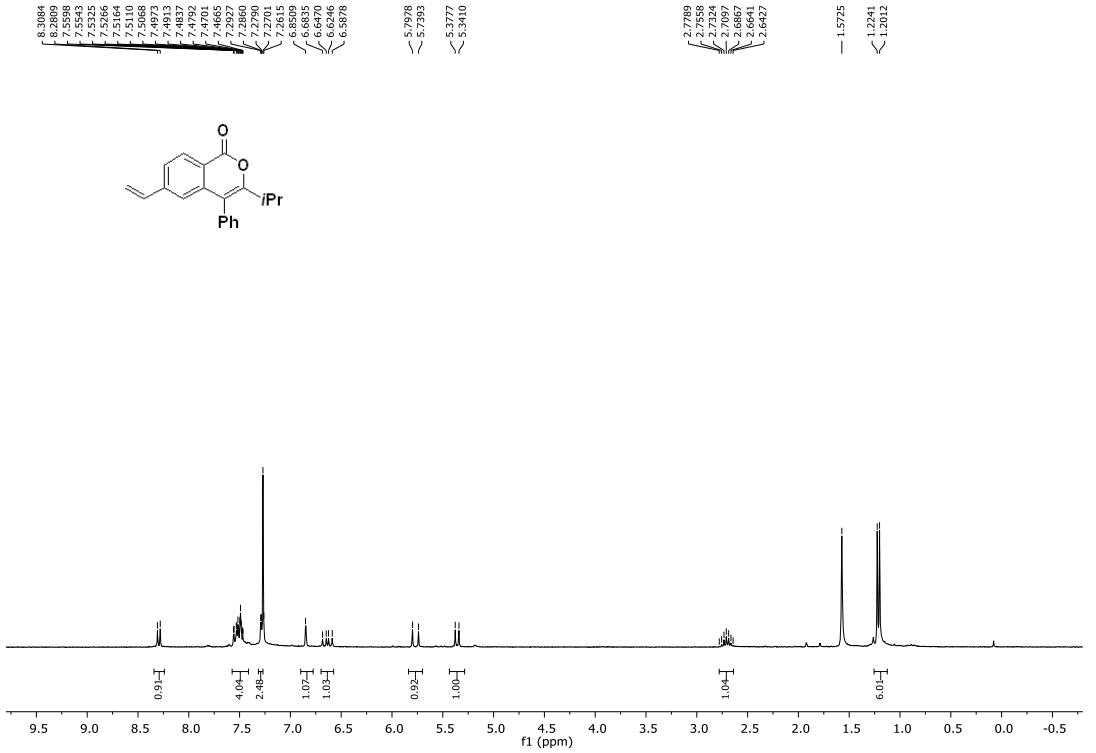
132.01
130.71
129.53
128.57
117.27
114.41
111.55
109.77
40.61
40.40
40.19
39.99 DMSO-d6
39.77
39.56
39.36
30.14
20.43
O
O
HO
CH3
CH3
f1 (ppm)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7.5598
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7.5315
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7.5164
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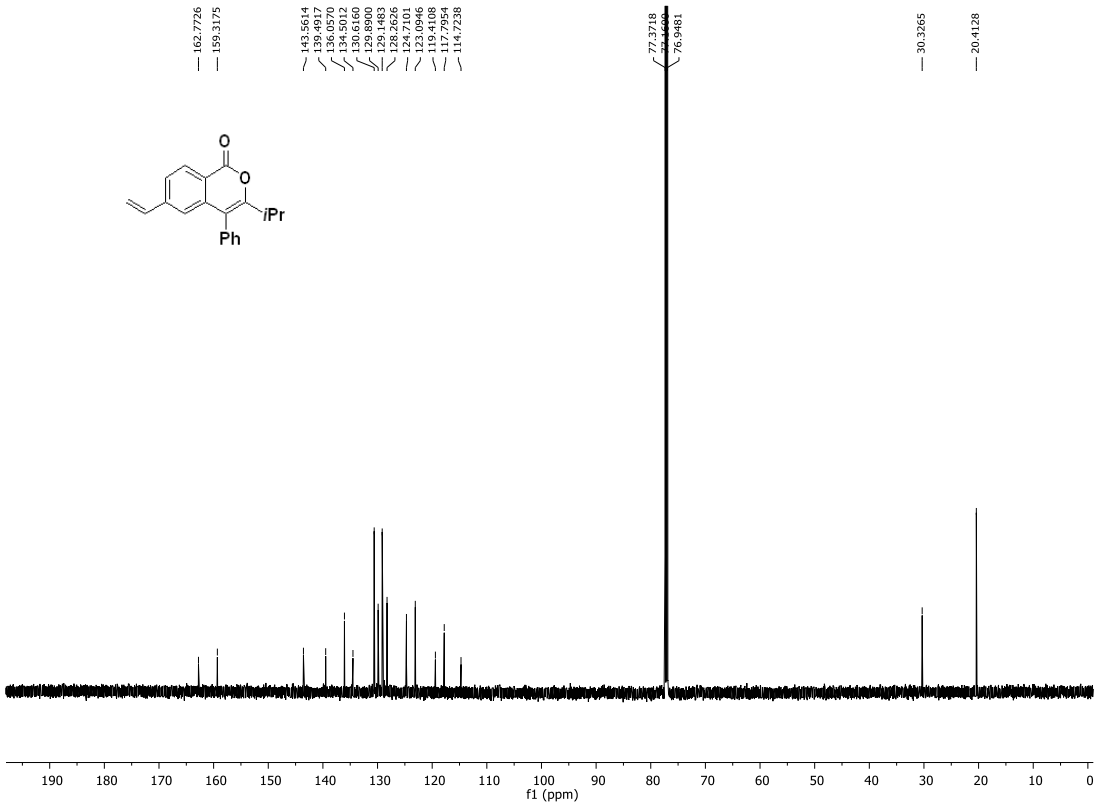
7.5068
7.4973
7.4913
7.4837
7.4792
7.4701
7.4665
7.2927
7.2860
7.2790
7.2701
7.2615
6.8509
6.6835
6.6470
6.6246
6.5878
5.7978
5.7393
5.3777
5.3410
2.7789
2.7558
2.7324
2.7097
2.6867
2.6641
2.6427
1.5725
1.2241
1.2012
O
O
iPr
Ph
0.91
4.04
2.48
1.07
1.03
0.92
1.00
1.04
6.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.8900
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128.2626
124.7101
123.0946
119.4108
117.7954
114.7238
77.3718
77.1600
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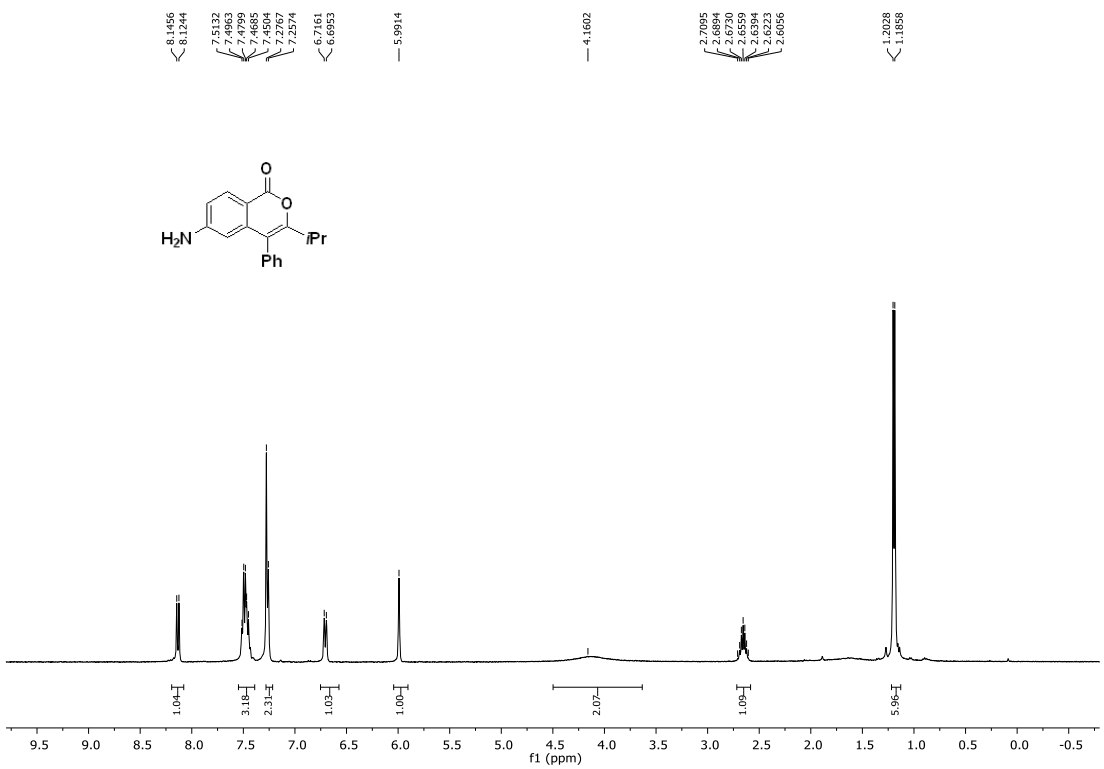
20.4128
O
O
iPr
Ph
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.2574
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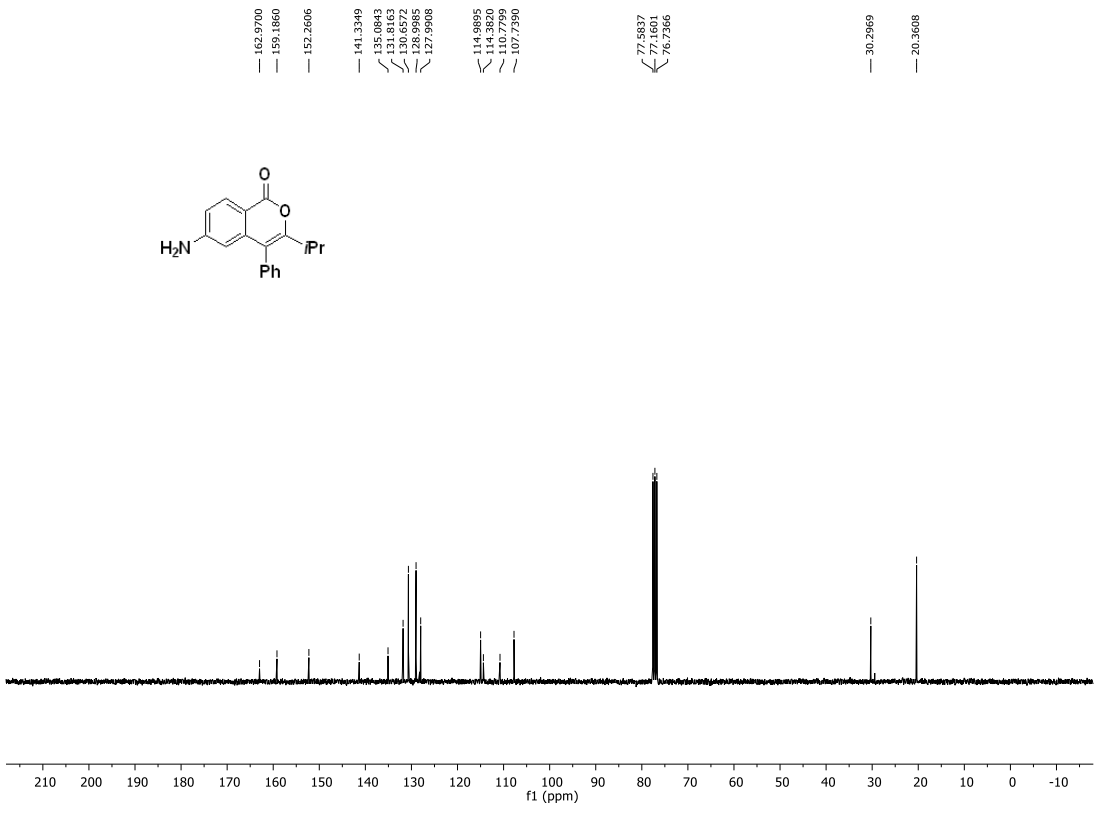
6.6953
5.9914
4.1602
2.7095
2.6894
2.6730
2.6559
2.6394
2.6223
2.6056
1.2028
1.1858
O
O
H2N
iPr
Ph
1.04
3.18
2.31
1.03
1.00
2.07
1.09
5.96
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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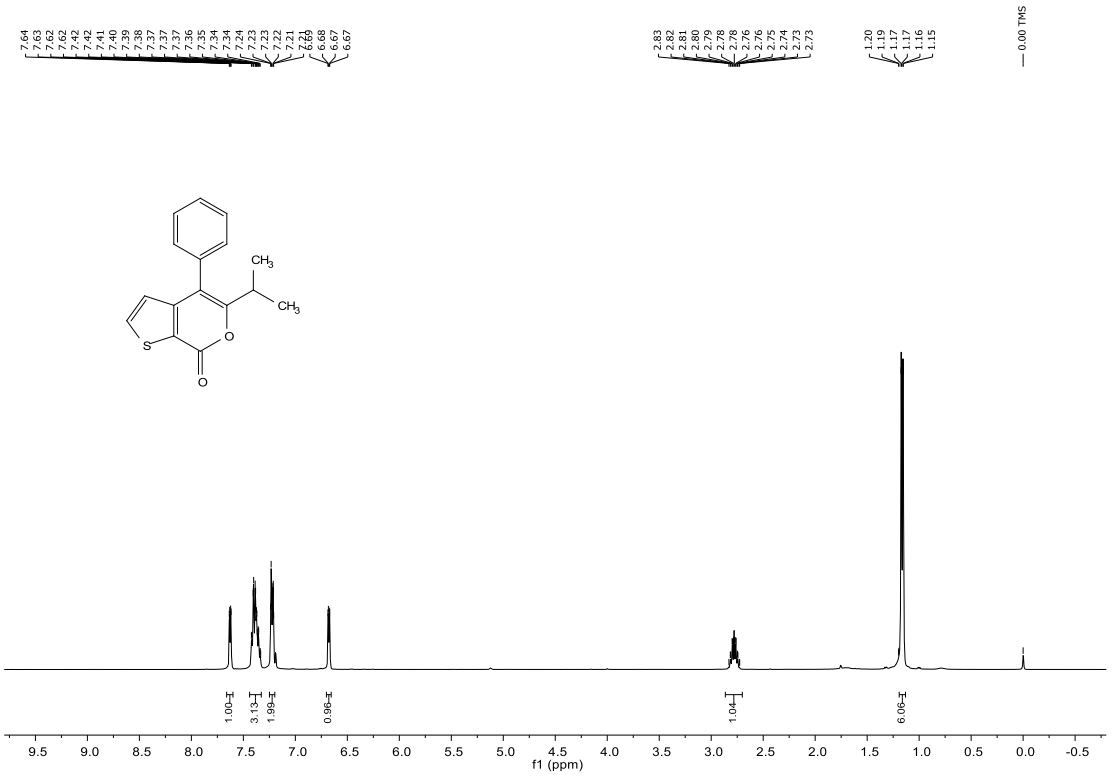
127.9908
114.9895
114.3820
110.7799
107.7390
77.5837
77.1601
76.7366
30.2969
20.3608
O
O
H2N
iPr
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.62
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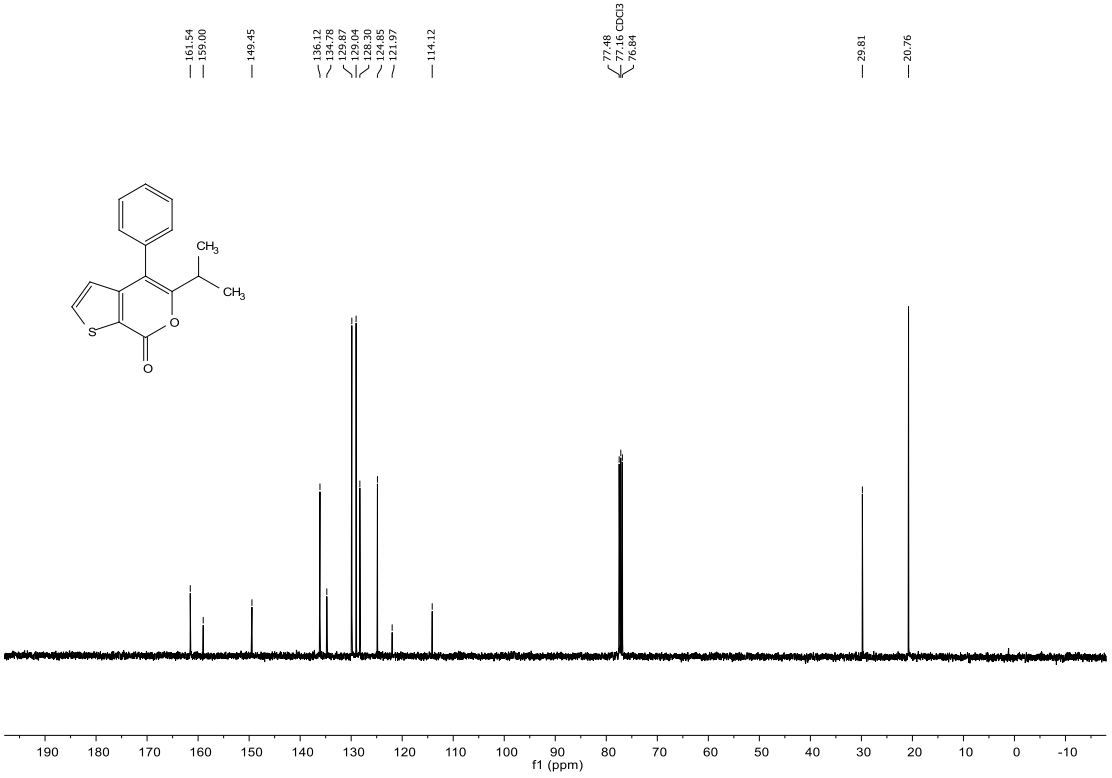
7.41
7.40
7.39
7.38
7.37
7.37
7.37
7.36
7.35
7.34
7.34
7.24
7.23
7.23
7.22
7.21
6.68
6.68
6.67
6.67
2.83
2.82
2.81
2.80
2.79
2.78
2.78
2.76
2.76
2.75
2.74
2.73
2.73
1.20
1.19
1.17
1.17
1.16
1.15
0.00 TMS
CH3
CH3
S
O
O
1.00
3.13
1.99
0.96
1.04
6.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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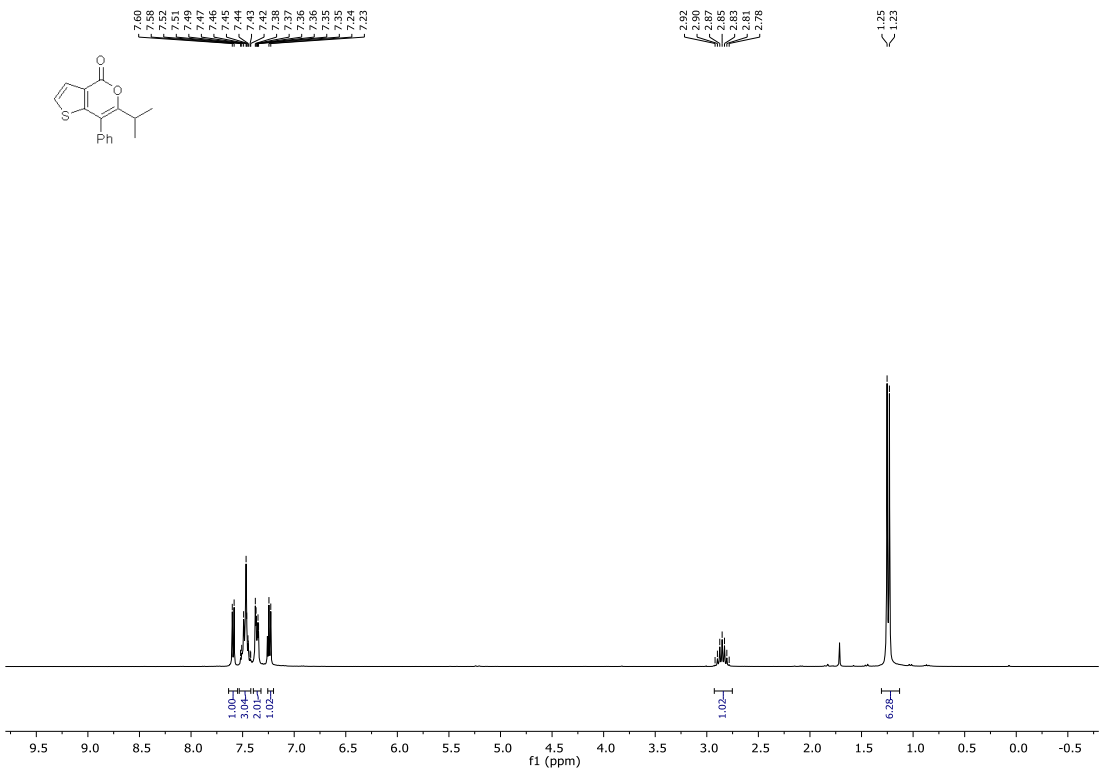
129.87
129.04
128.30
124.85
121.97
114.12
77.48
77.16 CDCl3
76.84
29.81
20.76
CH3
CH3
S
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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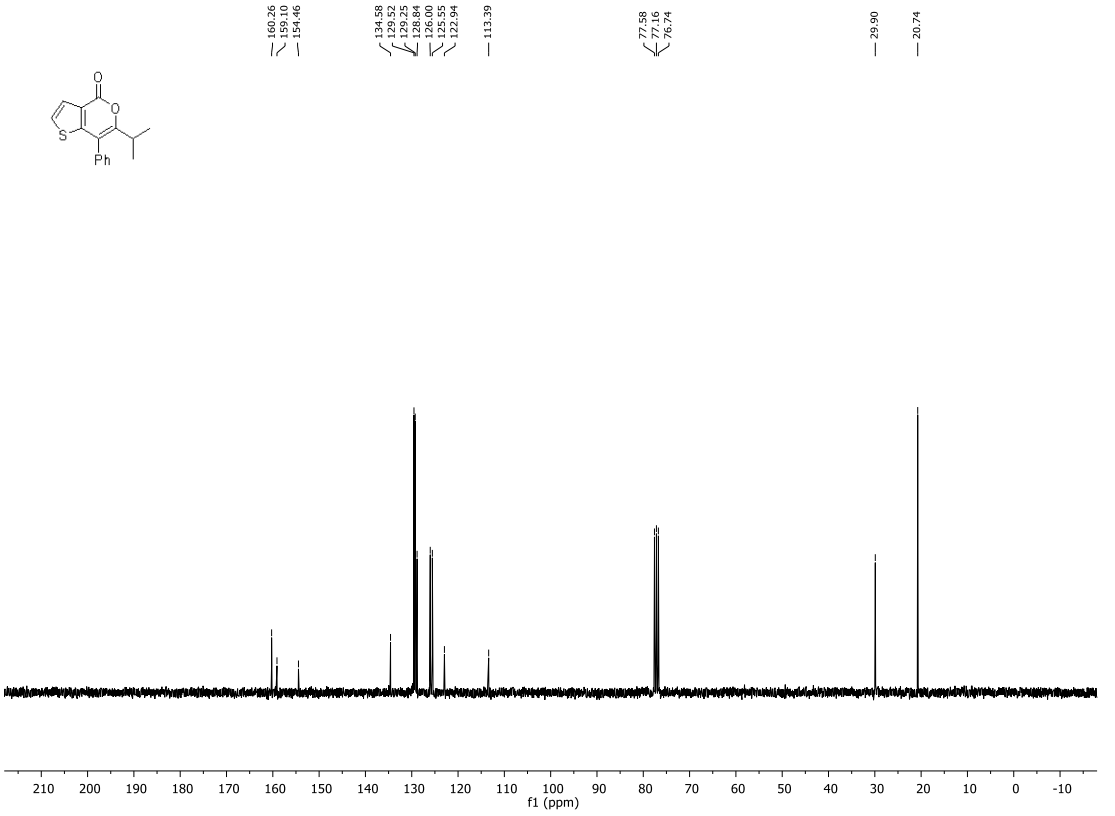
7.37
7.36
7.36
7.35
7.35
7.24
7.23
2.92
2.90
2.87
2.85
2.83
2.81
2.78
1.25
1.23
O
O
S
Ph
1.00
3.04
2.01
1.02
1.02
6.28
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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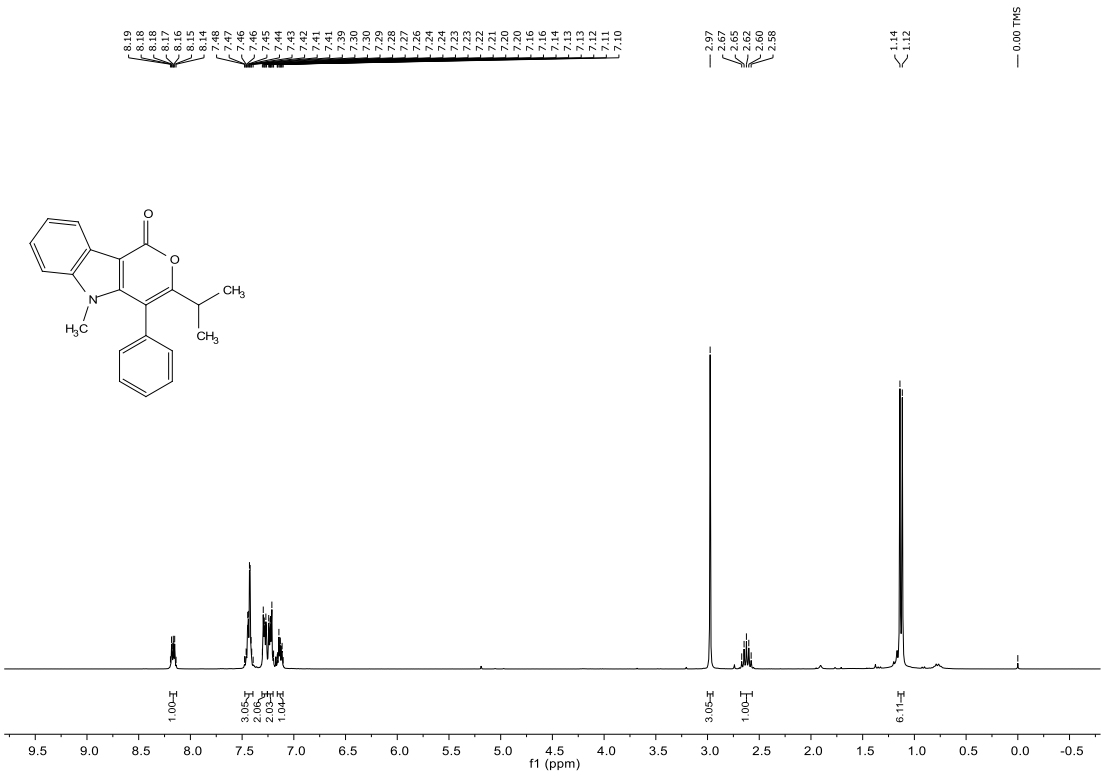
126.00
125.55
122.94
113.39
77.58
77.16
76.74
29.90
20.74
O
O
S
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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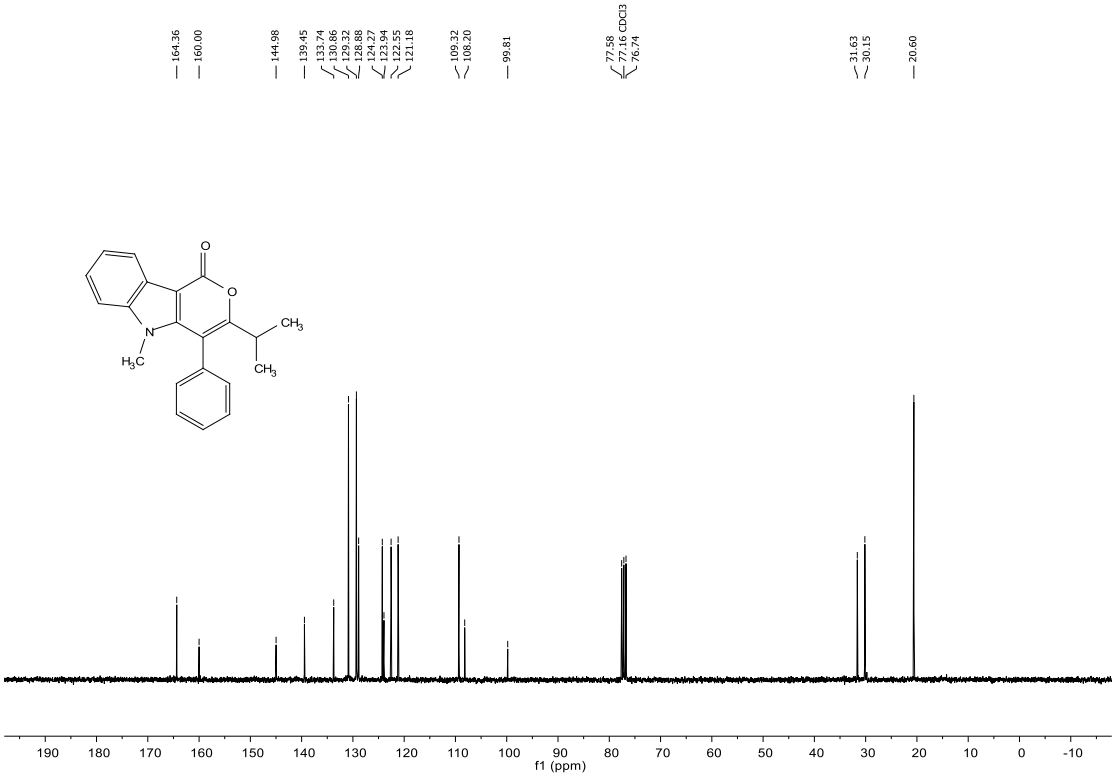
8.14
7.48
7.47
7.46
7.46
7.45
7.44
7.43
7.42
7.41
7.41
7.39
7.30
7.30
7.29
7.28
7.27
7.26
7.24
7.24
7.23
7.23
7.22
7.21
7.20
7.16
7.16
7.14
7.13
7.13
7.12
7.11
7.10
2.97
2.67
2.65
2.62
2.60
2.58
1.14
1.12
0.00 TMS
O
O
N
CH3
H3C
CH3
1.00
3.05
2.06
2.03
1.04
3.05
1.00
6.11
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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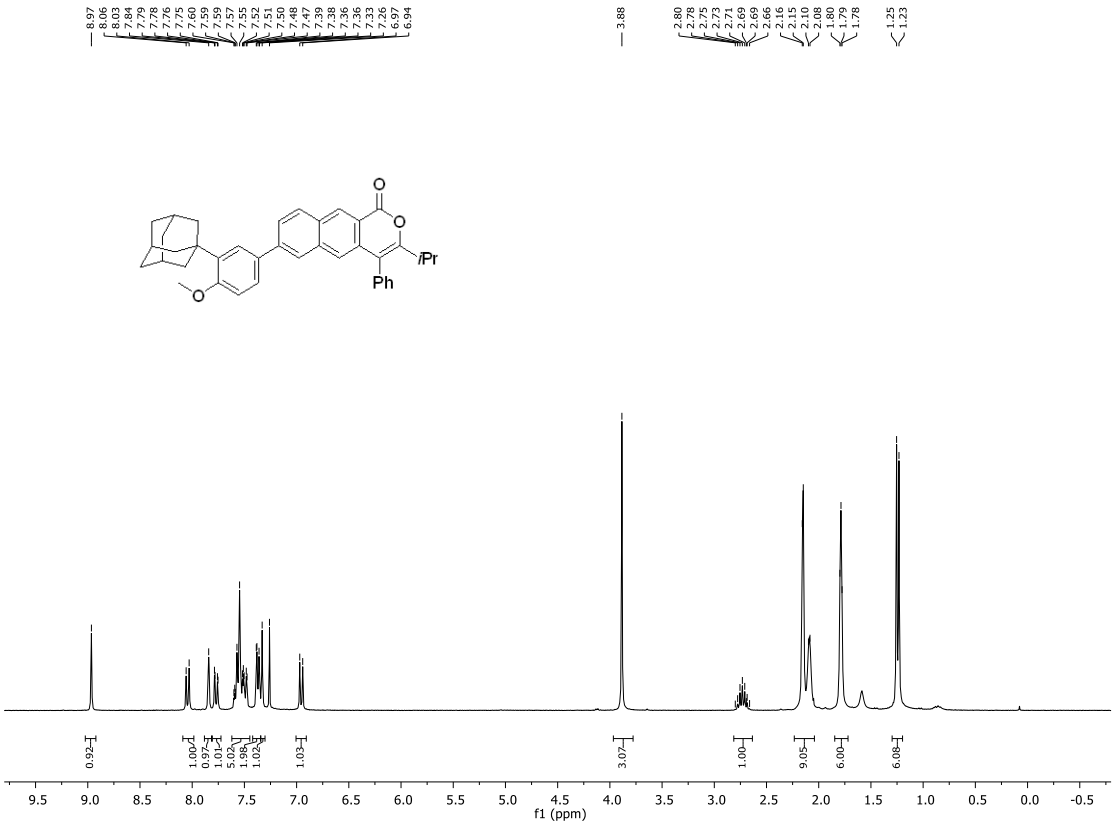
139.45
133.74
130.86
129.32
128.88
124.27
123.94
122.55
121.18
109.32
108.20
99.81
77.58
77.16 CDCl3
76.74
31.63
30.15
20.60
O
O
N
CH3
H3C
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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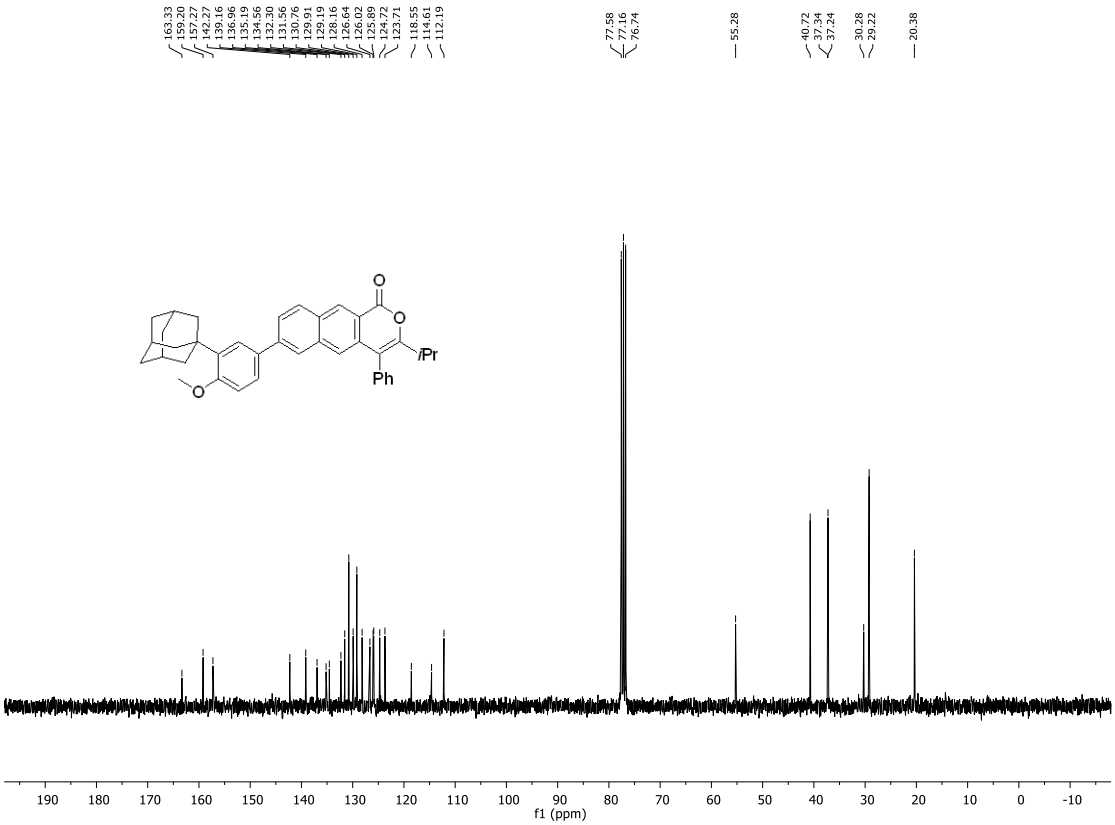
7.75
7.60
7.59
7.59
7.57
7.55
7.52
7.51
7.50
7.48
7.47
7.39
7.38
7.36
7.36
7.33
7.26
6.97
6.94
3.88
2.80
2.78
2.75
2.73
2.71
2.69
2.69
2.66
2.16
2.15
2.10
2.08
1.80
1.79
1.78
1.25
1.23
O
O
iPr
Ph
O
0.92
1.00
0.97
1.01
5.02
1.98
1.02
1.03
3.07
1.00
9.05
6.00
6.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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135.19
134.56
132.30
131.56
130.76
129.91
129.19
128.16
126.64
126.02
125.89
124.72
123.71
118.55
114.61
112.19
77.58
77.16
76.74
55.28
40.72
37.34
37.24
30.28
29.22
20.38
O
O
iPr
Ph
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.43
7.42
7.42
7.41
7.40
7.39
7.39
7.38
7.37
7.35
7.35
7.26 CDCl3
7.14
7.13
7.12
7.12
7.12
7.11
2.56
2.54
2.52
2.50
2.50
2.49
2.48
2.05
2.04
2.03
2.02
2.02
2.01
2.01
2.00
1.99
1.99
1.99
1.72
1.71
1.70
1.69
1.68
1.68
1.67
1.66
1.62
1.62
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1.60
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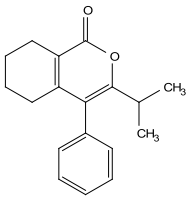
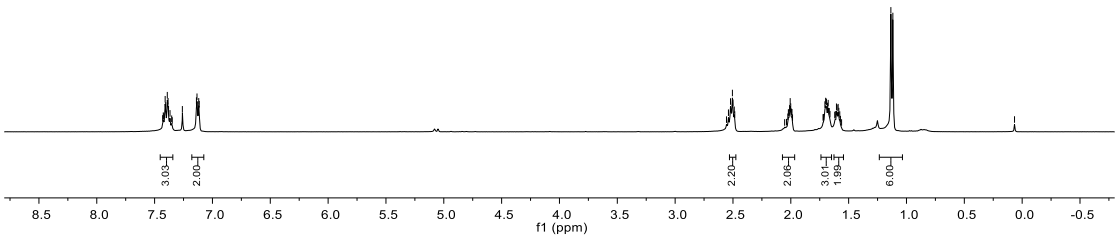
1.58
1.58
1.57
1.56
1.14
1.12
0.07


O
O
CH3
CH3


3.03
2.00
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2.06
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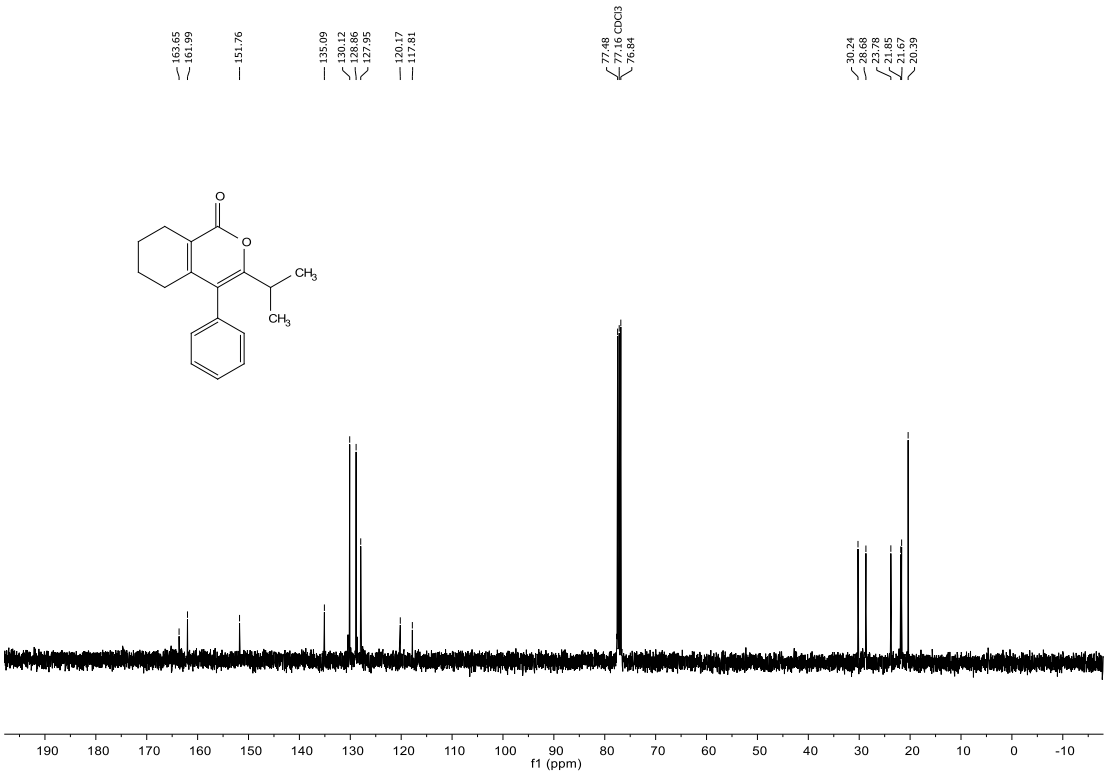
1.99
6.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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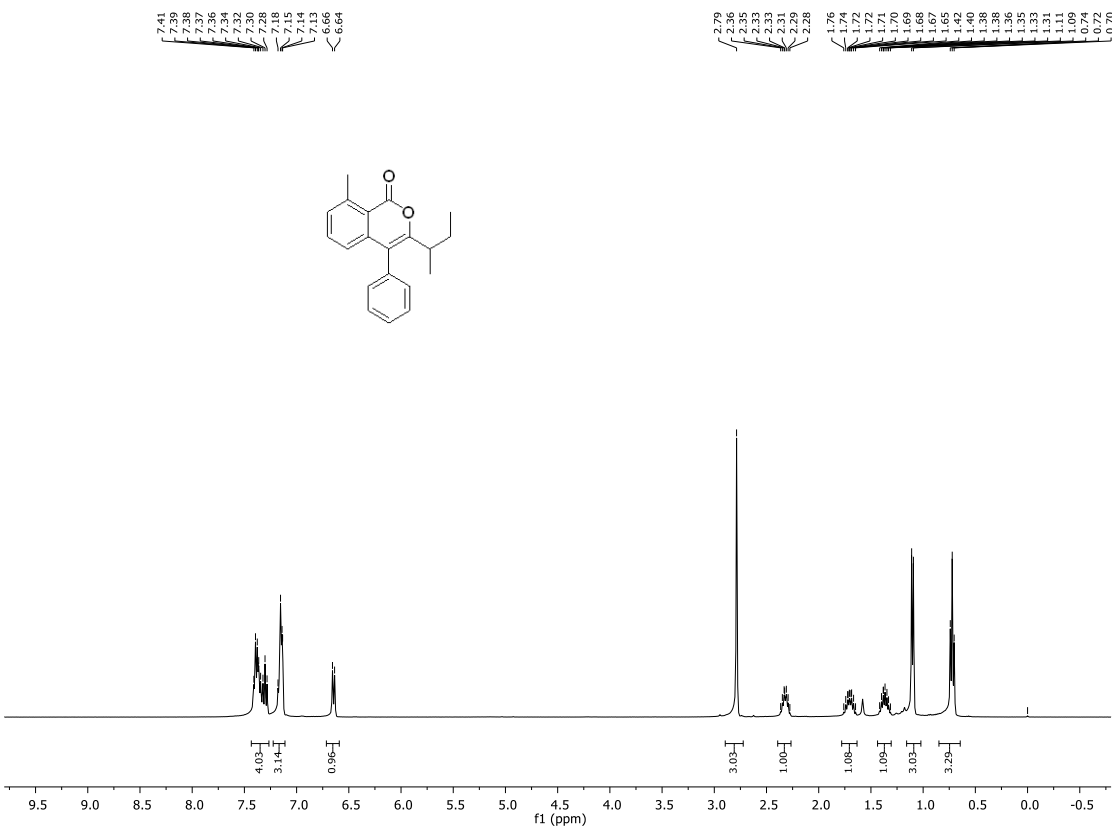
151.76
135.09
130.12
128.86
127.95
120.17
117.81
77.48
77.16 CDCl3
76.84
30.24
28.68
23.78
21.85
21.67
20.39
O
O
CH3
CH3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.14
7.13
6.66
6.64
2.29
2.36
2.35
2.33
2.33
2.31
2.29
2.28
1.76
1.74
1.72
1.72
1.71
1.70
1.69
1.68
1.67
1.65
1.42
1.40
1.38
1.38
1.36
1.35
1.33
1.31
1.11
1.09
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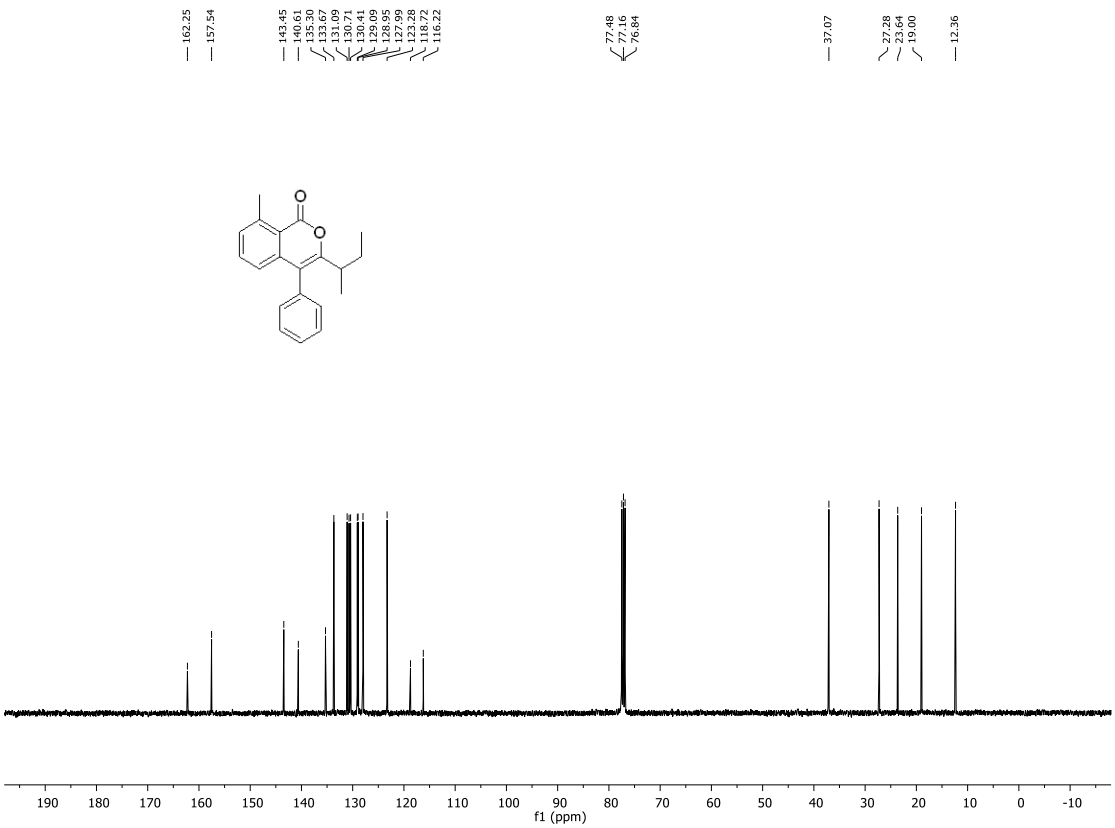
0.72
4.03
3.14
0.96
3.03
1.00
1.08
1.09
3.03
3.29
f1 (ppm)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140.61
135.20
133.67
131.09
130.71
130.41
129.09
128.95
127.99
123.28
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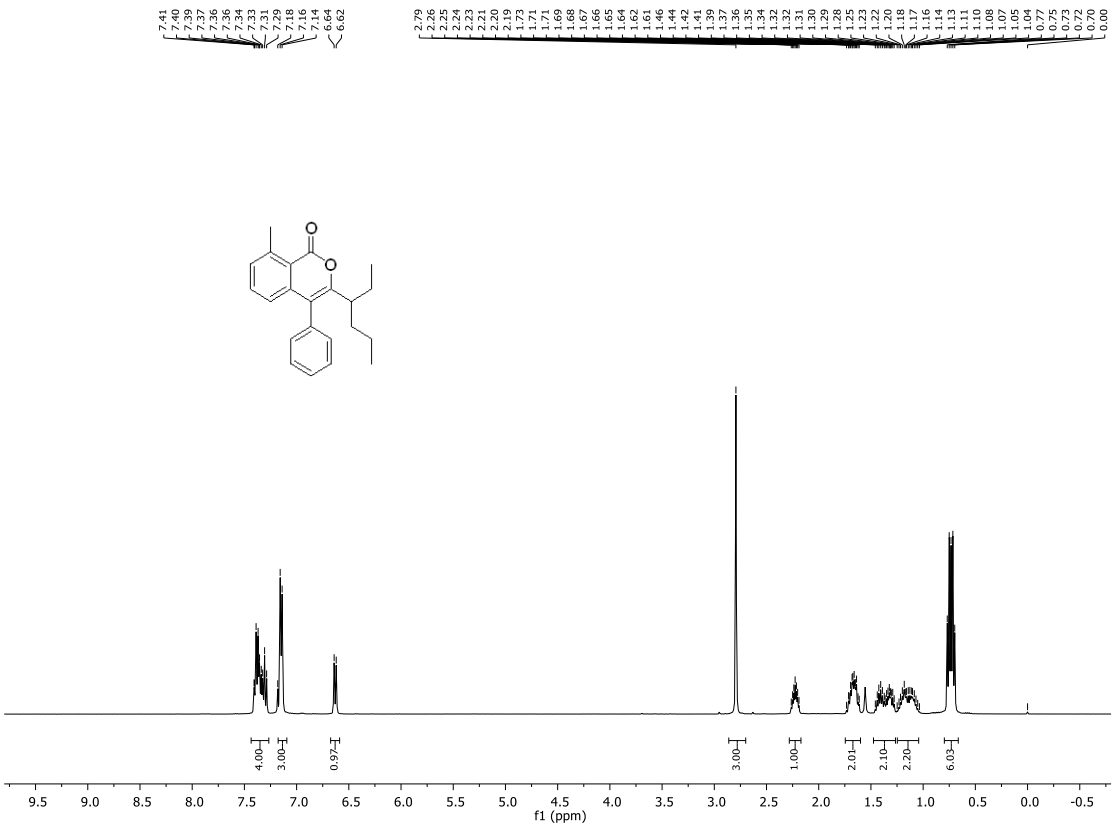
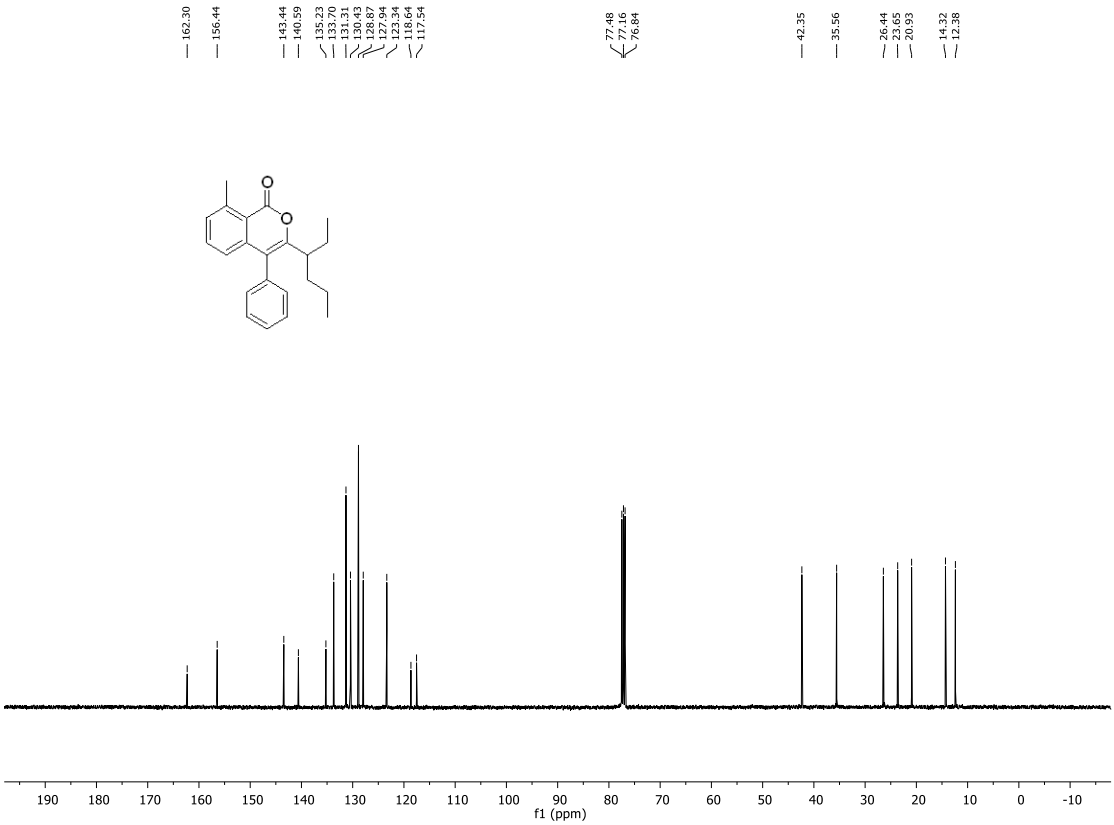
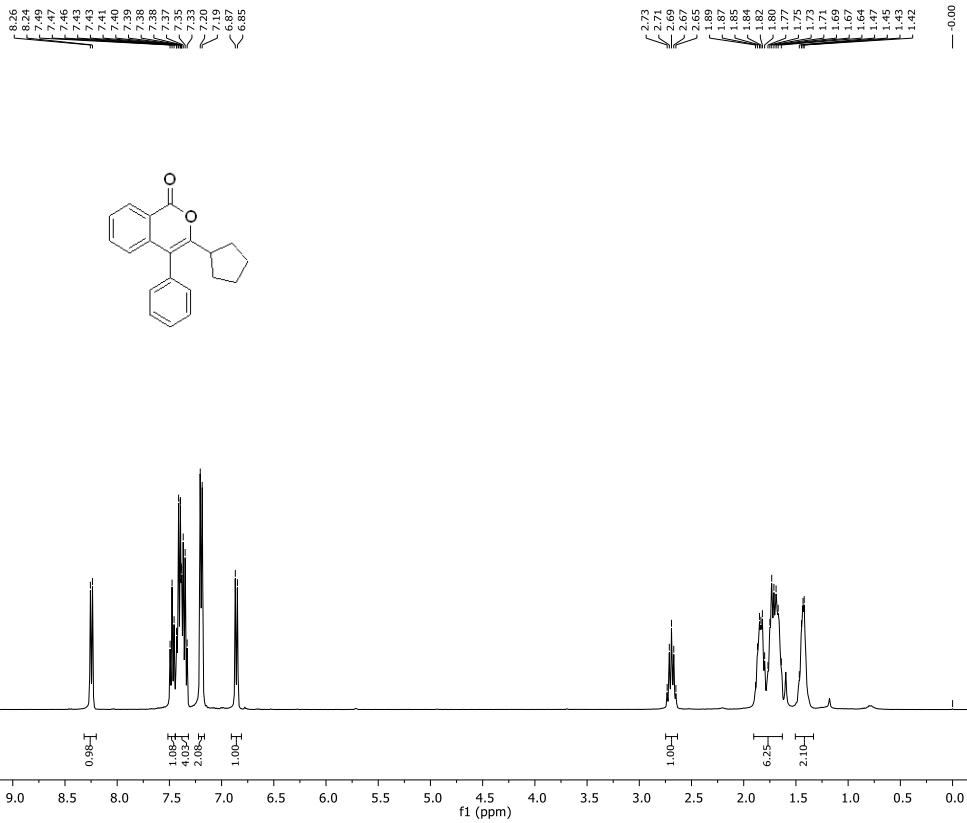
116.22
77.48
77.16
76.84
37.07
27.28
23.64
19.00
12.36
f1 (ppm)


7.41 7.40 7.39 7.37 7.36 7.36 7.34 7.33 7.31 7.29 7.18 7.16 7.14 6.64 6.62
2.79 2.26 2.25 2.24 2.23 2.21 2.20 2.19 1.73 1.71 1.71 1.69 1.68 1.67 1.66 1.65 1.64 1.62 1.61 1.46 1.44 1.42 1.41 1.39 1.37 1.36 1.35 1.34 1.32 1.32 1.31 1.30 1.29 1.28 1.25 1.23 1.22 1.20 1.18 1.17 1.16 1.14 1.13 1.11 1.10 1.08 1.07 1.05 1.04 0.77 0.75 0.73 0.72 0.70 0.00
4.00 3.00 0.97 3.00 1.00 2.01 2.10 2.20 6.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


162.30 156.44 143.44 140.59 135.23 133.70 131.31 130.43 128.87 127.94 123.34 118.64 117.54
77.48 77.16 76.84
42.35 35.56 26.44 23.65 20.93 14.32 12.38
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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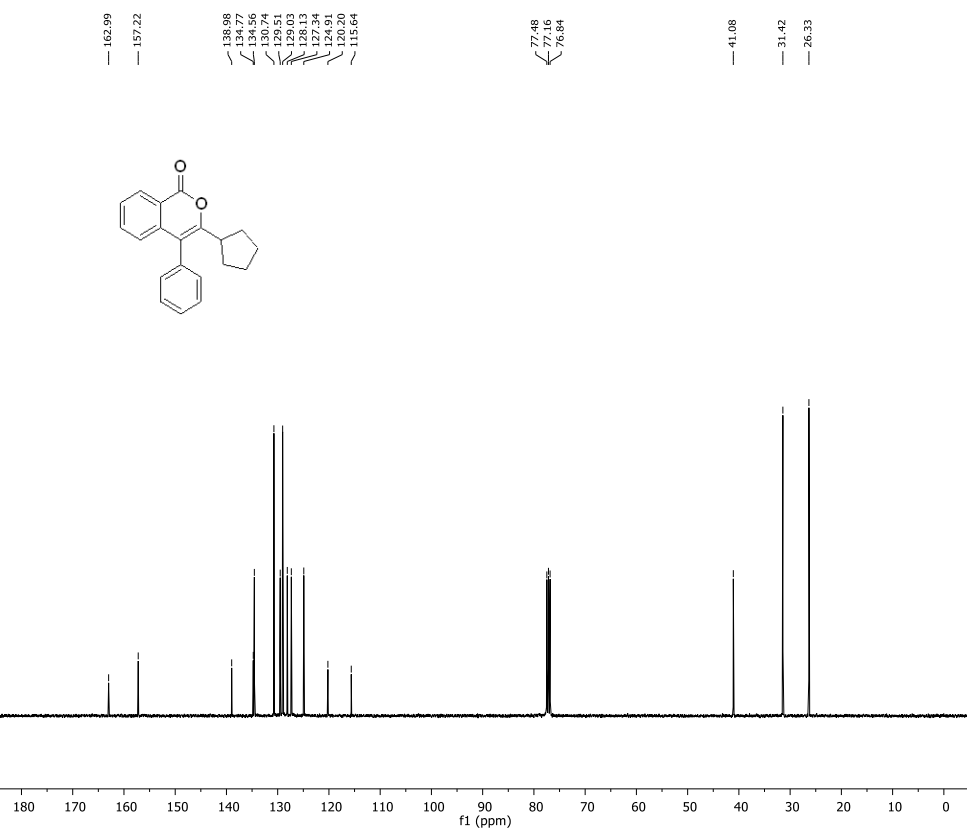
8.24
7.49
7.47
7.46
7.43
7.41
7.40
7.39
7.38
7.38
7.37
7.35
7.33
7.20
7.19
6.87
6.85
2.73
2.71
2.69
2.67
2.65
1.89
1.87
1.85
1.84
1.82
1.80
1.77
1.75
1.73
1.71
1.69
1.67
1.64
1.47
1.45
1.43
1.42
0.00
0.98
1.08
4.03
2.08
1.00
1.00
6.25
2.10
f1 (ppm)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157.22
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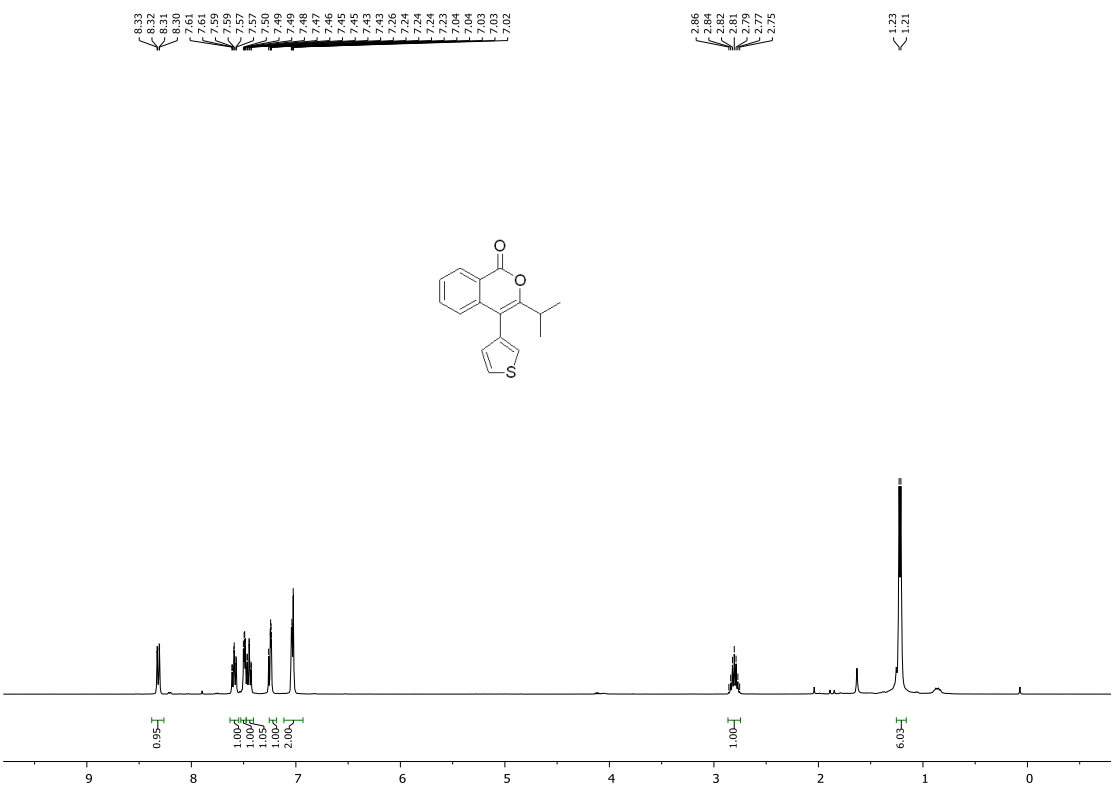
134.77
134.56
130.74
129.51
129.03
128.13
127.34
124.91
120.20
115.64
77.48
77.16
76.84
41.08
31.42
26.33
f1 (ppm)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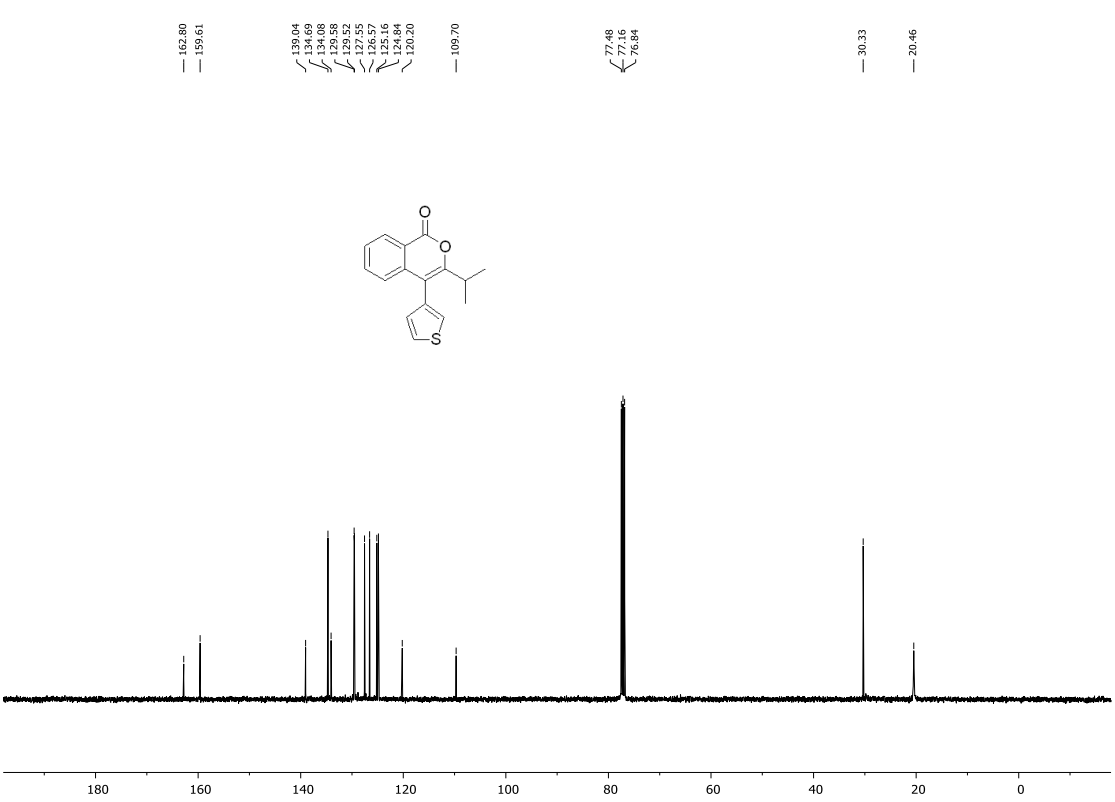
8.32
8.31
8.30
7.61
7.61
7.59
7.59
7.57
7.57
7.50
7.49
7.49
7.48
7.47
7.46
7.45
7.45
7.43
7.43
7.26
7.24
7.24
7.24
7.23
7.04
7.04
7.03
7.03
7.02
2.86
2.84
2.82
2.81
2.79
2.77
2.75
1.23
1.21
O
O
S
0.95
1.00
1.00
1.05
1.00
2.00
1.00
6.03
9
8
7
6
5
4
3
2
1
0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134.08
129.58
129.52
127.55
126.57
125.16
124.84
120.20
109.70
77.48
77.16
76.84
30.33
20.46
O
O
S
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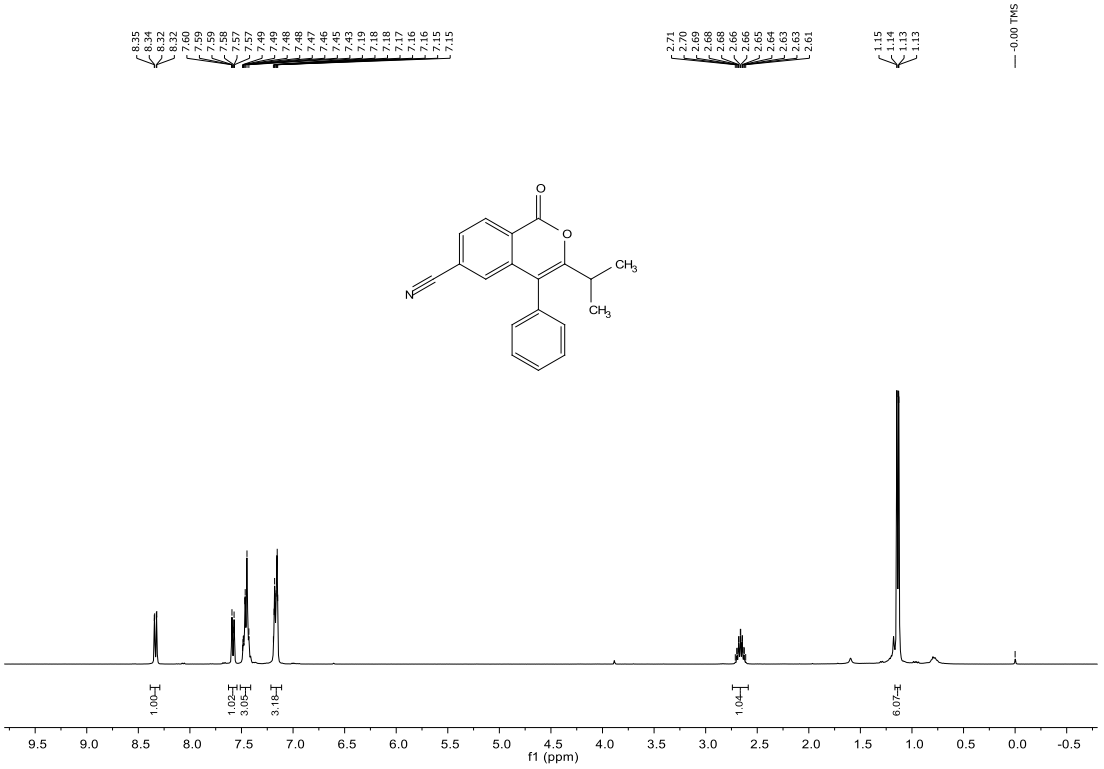
160
140
120
100
80
60
40
20
0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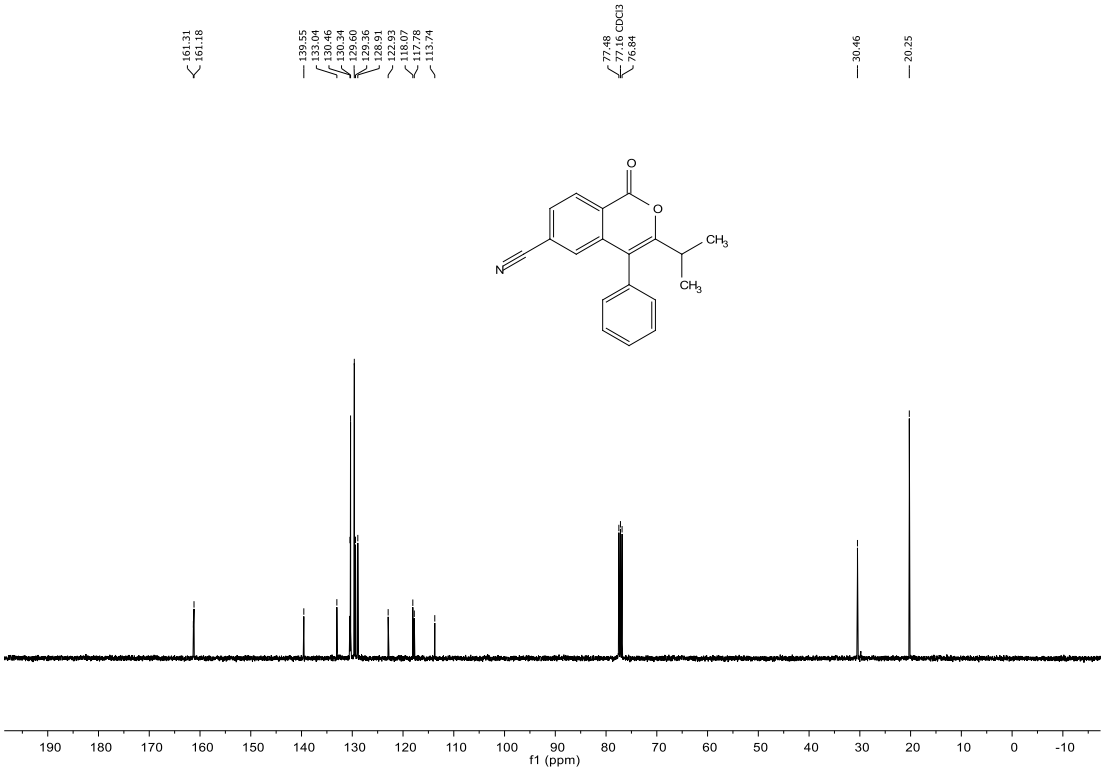
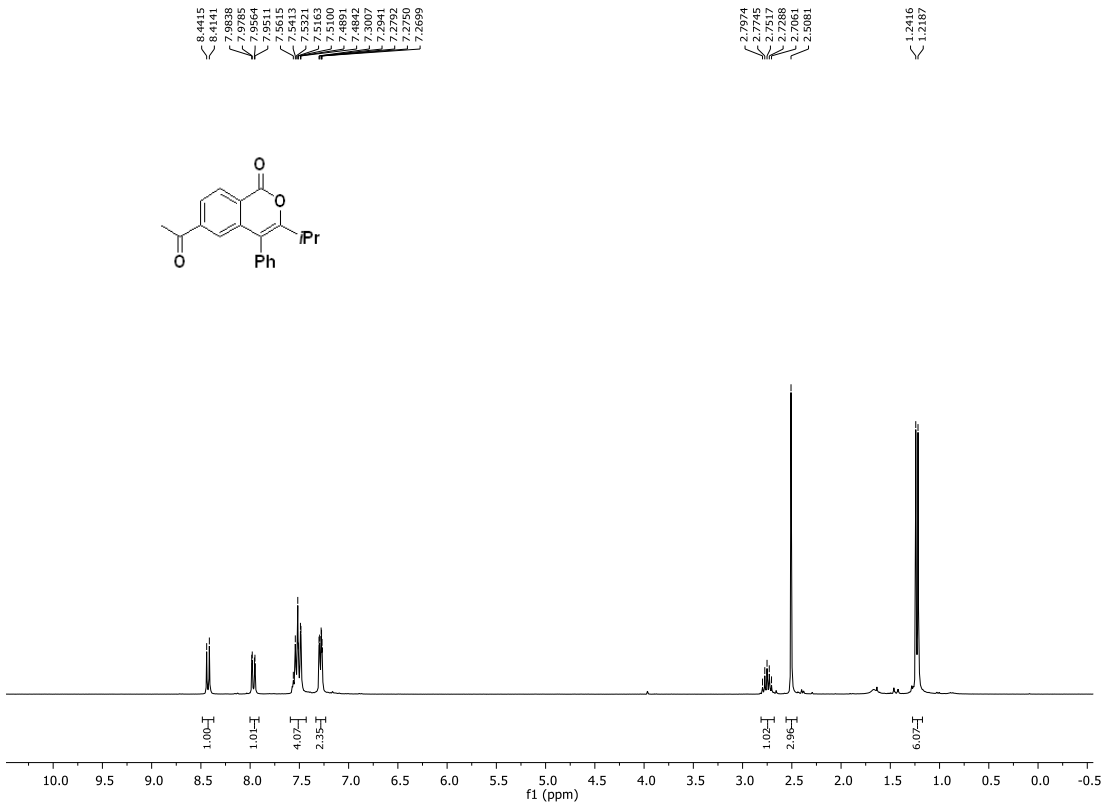
8.32
7.60
7.59
7.59
7.58
7.57
7.57
7.49
7.49
7.48
7.48
7.47
7.46
7.45
7.43
7.19
7.18
7.18
7.17
7.16
7.16
7.15
7.15
2.71
2.70
2.69
2.68
2.68
2.66
2.66
2.65
2.64
2.63
2.63
2.61
1.15
1.14
1.13
1.13
0.00 TMS
O
O
N
CH3
CH3
1.00
1.02
3.05
3.18
1.04
6.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


161.31
161.18
139.55
133.04
130.46
130.34
129.60
129.36
128.91
122.93
118.07
117.78
113.74
77.48
77.16 CDCl3
76.84
30.46
20.25
O
O
N
CH3
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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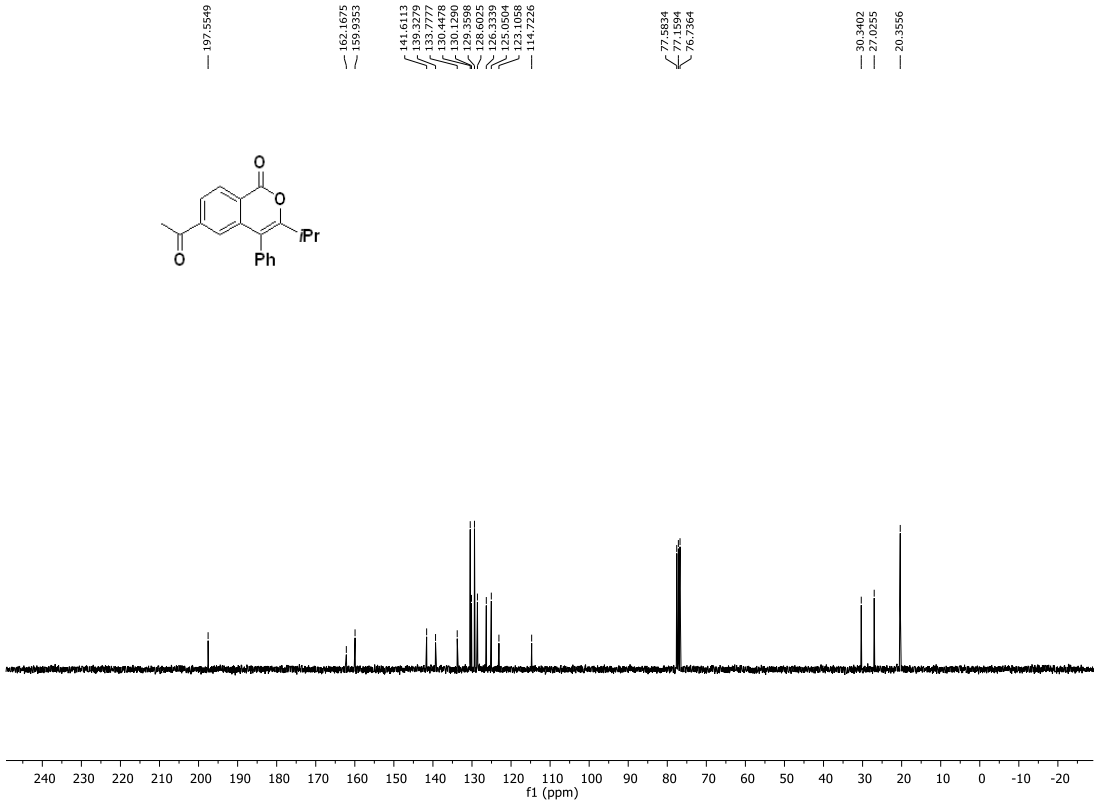
8.4141
7.9838
7.9785
7.9564
7.9511
7.5615
7.5413
7.5321
7.5163
7.5100
7.4891
7.4842
7.3007
7.2941
7.2792
7.2750
7.2699
2.7974
2.7745
2.7517
2.7288
2.7061
2.5081
1.2416
1.2187
O
O
O
iPr
Ph
1.00
1.01
4.07
2.35
1.02
2.96
6.07
f1 (ppm)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159.9353
141.6113
139.3279
133.7777
130.4748
130.1290
129.3598
128.6025
126.3339
125.0504
123.1058
114.7226
77.5834
77.1594
76.7364
30.3402
27.0255
20.3556
O
O
O
iPr
Ph
f1 (ppm)


8.2246
8.1971
7.6154
7.6098
7.5879
7.5822
7.3049
7.2931
7.2702
7.2569
7.1024
7.0979
7.0945
7.0361
7.0282
7.0165
7.0104
7.0050
2.7846
2.7591
2.7330
2.5659
2.5431
2.5202
2.4974
2.4746
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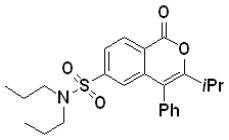
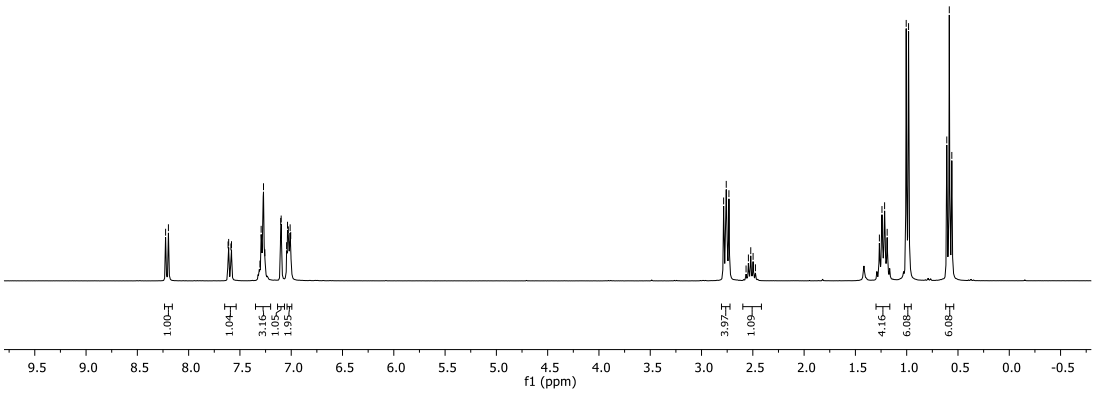
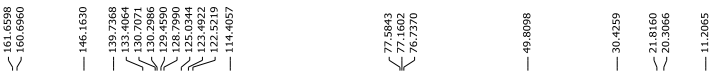
1.2409
1.2153
1.1903
1.0048
0.9819
0.6092
0.5848
0.5601


O
O
O
S
N
O
iPr
Ph


1.00
1.04
3.16
1.05
1.95
3.97
1.09
4.16
6.08
6.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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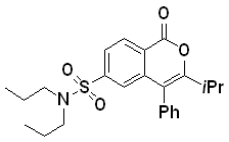
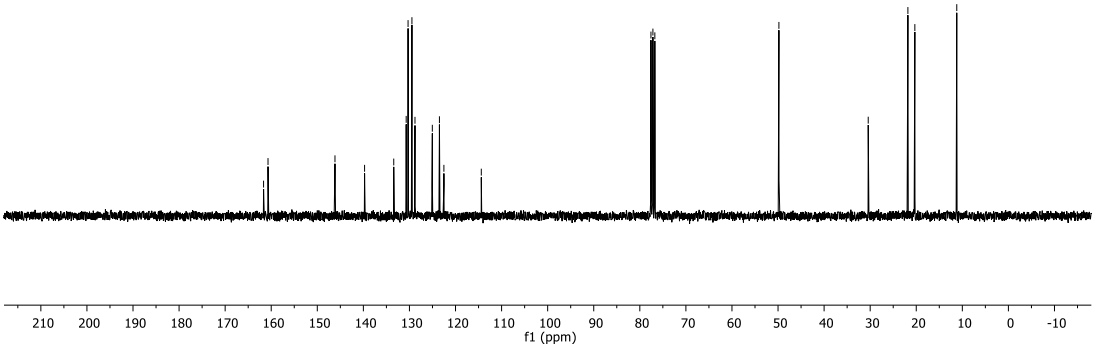
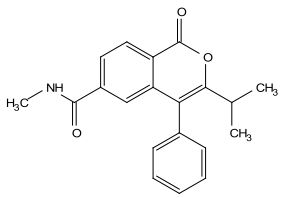
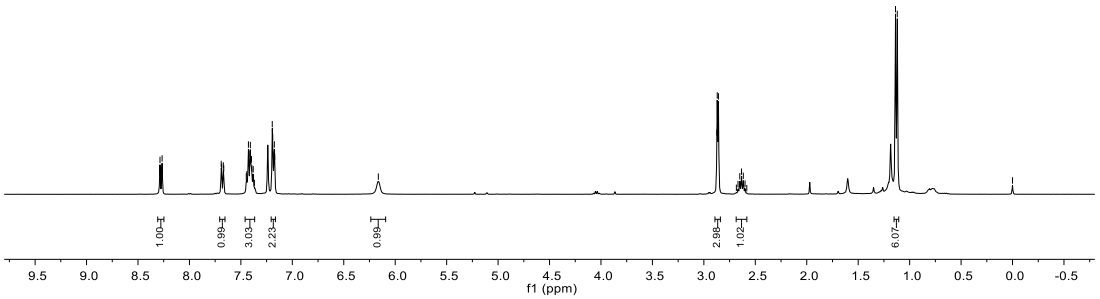
146.1630
139.7368
133.4064
130.7071
130.2986
129.4590
128.7990
128.6944
123.4922
122.5219
114.4057
77.5843
77.1602
76.7370
49.8098
30.4259
21.8160
20.3066
11.2065

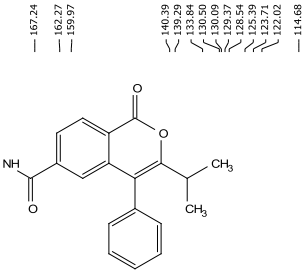

O
O
O
S
N
O
iPr
Ph


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.29
8.29
8.27
8.27
7.69
7.69
7.67
7.67
7.45
7.44
7.43
7.41
7.41
7.40
7.40
7.39
7.38
7.37
7.19
7.18
7.17
7.17
6.16
2.87
2.87
2.86
2.68
2.67
2.65
2.63
2.62
2.60
2.58
1.14
1.12
0.00


O
O
NH
H3C
O
CH3
CH3


1.00
0.99
3.03
2.23
0.89
2.98
1.02
6.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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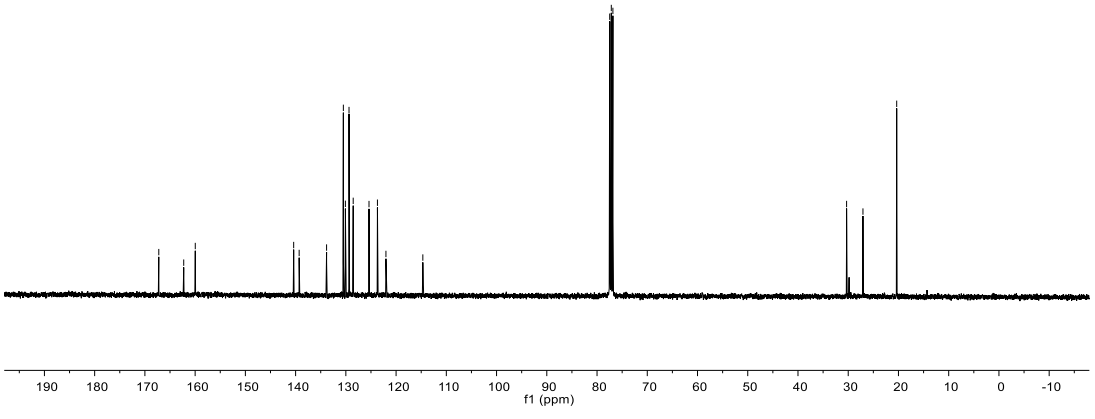
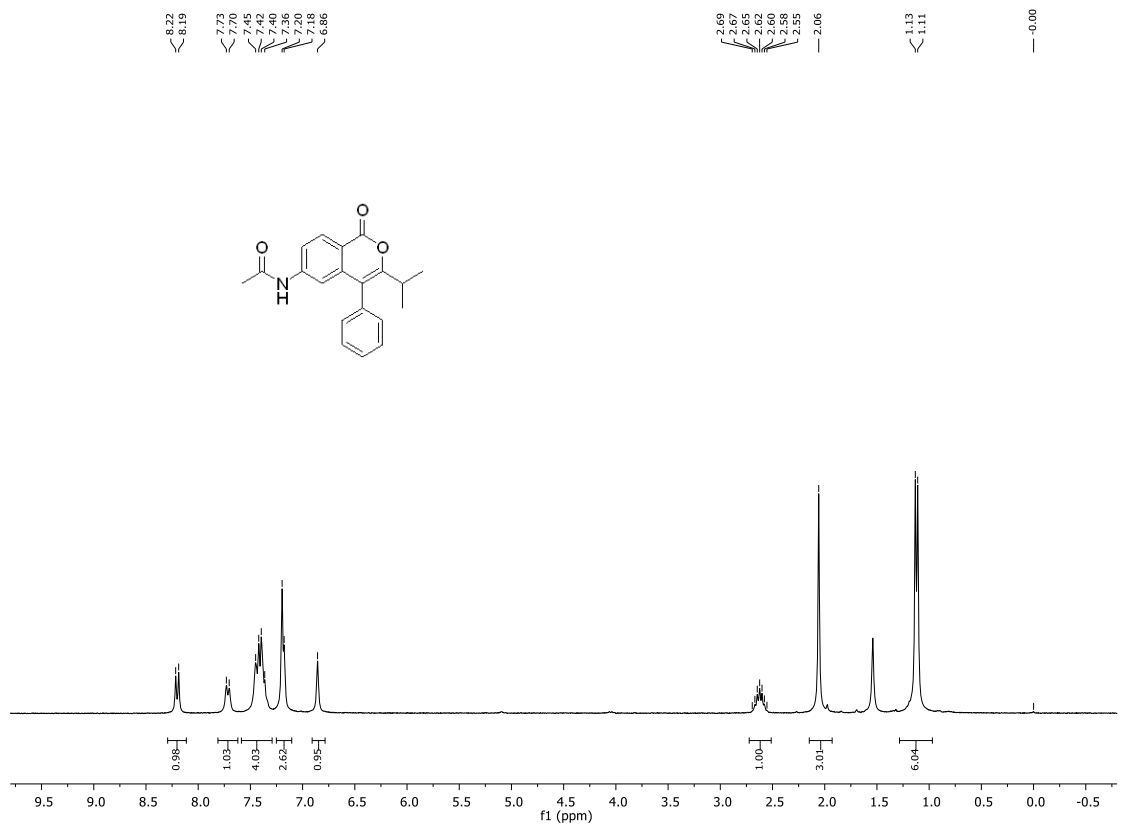
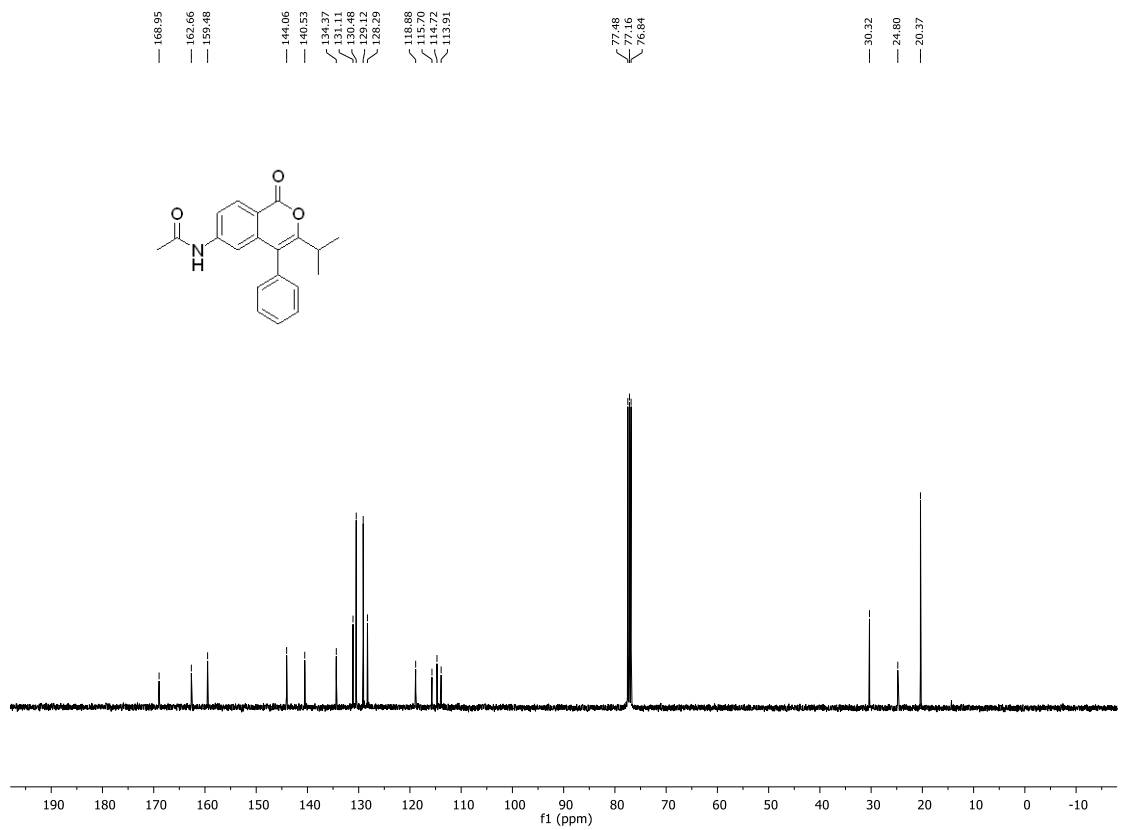
140.39
139.29
133.84
130.50
130.09
128.77
128.54
125.39
123.71
122.02
114.68
77.48
77.16
76.84
30.32
27.07
20.35


O
O
NH
H3C
O
CH3
CH3


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.22
8.19
7.73
7.70
7.45
7.42
7.40
7.36
7.20
7.18
6.86
2.69
2.67
2.65
2.62
2.60
2.58
2.55
2.06
1.13
1.11
0.00
O
O
O
N
H
0.98
1.03
4.03
2.62
0.95
1.00
3.01
6.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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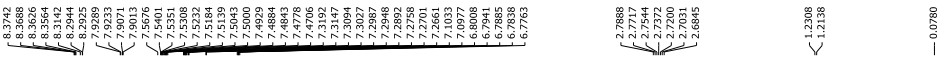
144.06
140.53
134.37
131.11
130.48
129.12
128.29
118.88
115.70
114.72
113.91
77.48
77.16
76.84
30.32
24.80
20.37
O
O
O
N
H
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.3626
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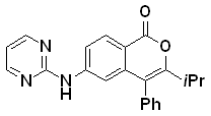
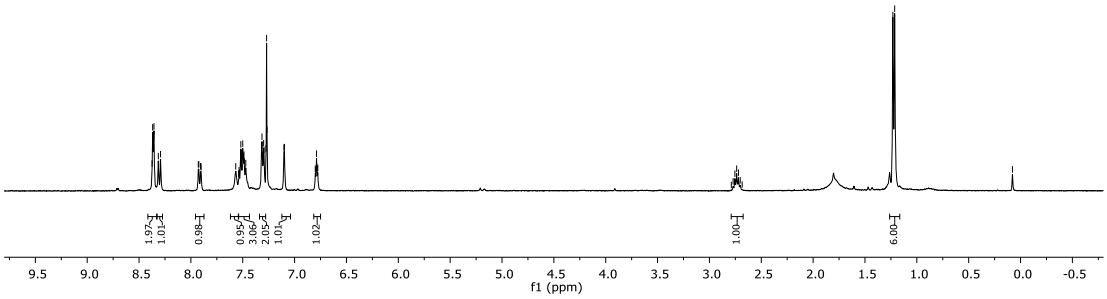
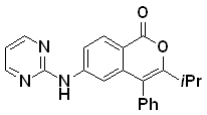
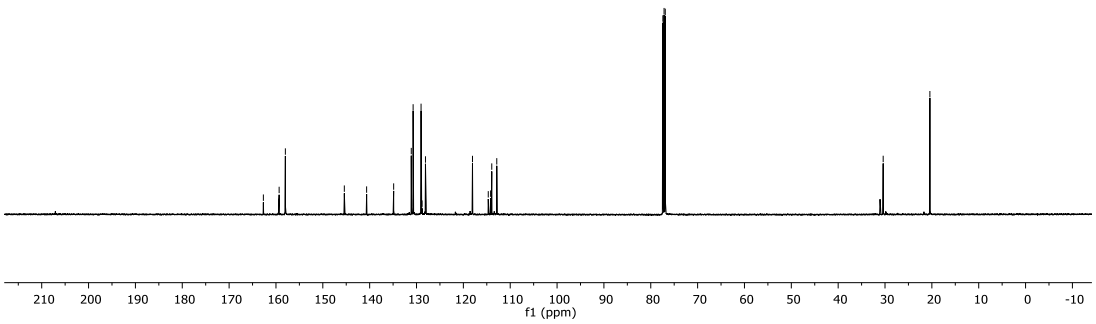
8.3142
8.2944
8.2925
7.9289
7.9233
7.9071
7.9013
7.5676
7.5401
7.5351
7.5308
7.5232
7.5184
7.5139
7.5043
7.5000
7.4909
7.4884
7.4843
7.4778
7.4706
7.3192
7.3147
7.3094
7.3027
7.2987
7.2948
7.2892
7.2758
7.2701
7.2661
7.1033
7.0977
6.8008
6.7941
6.7885
6.7838
6.7763
2.7888
2.7717
2.7544
2.7372
2.7200
2.7031
2.6845
1.2308
1.2138
0.0780


O
N
N
H
O
iPr
Ph

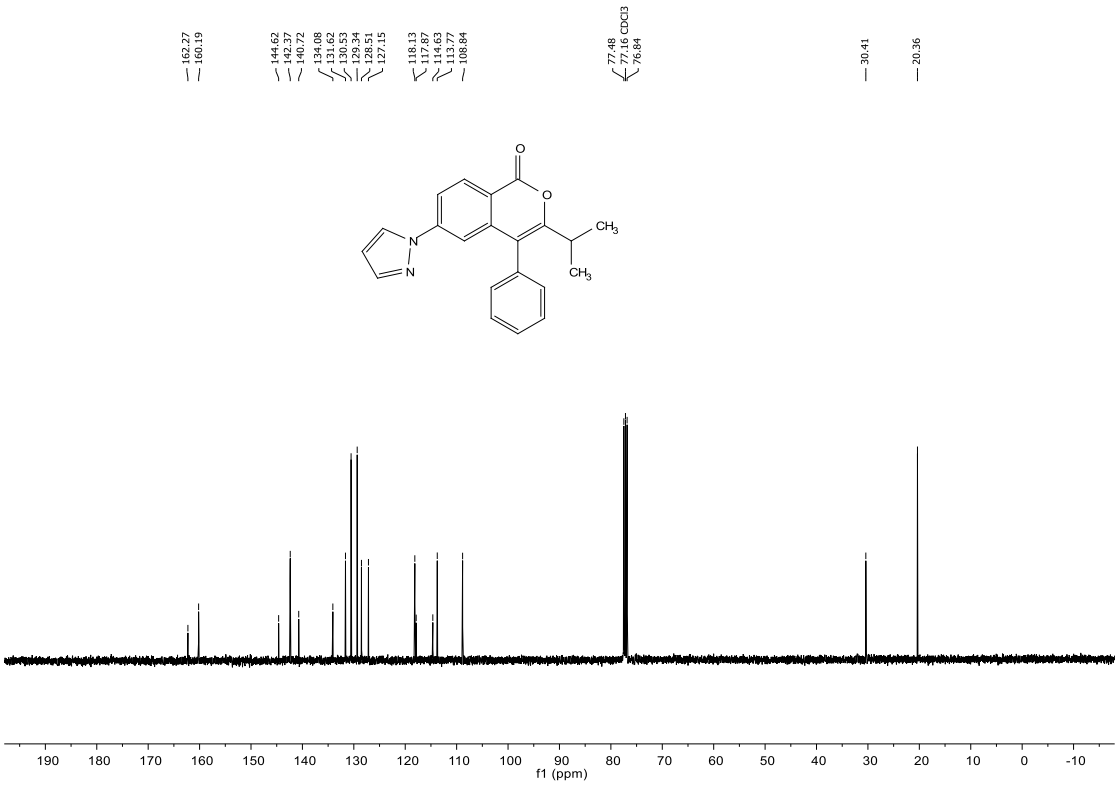

1.97
1.01
0.98
0.95
3.06
2.05
1.01
1.02
1.00
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

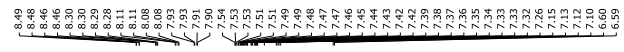

162.6885
159.4288
159.3249
157.9940
145.4090
140.6487
134.8761
131.1765
131.0495
130.7245
129.0286
128.8174
128.0887
128.0663
118.0517
114.6848
114.1836
113.9375
112.8681
77.4143
77.1599
76.9058
30.3922
20.4212

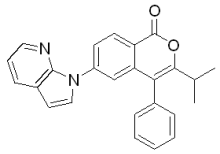

O
N
N
H
O
iPr
Ph

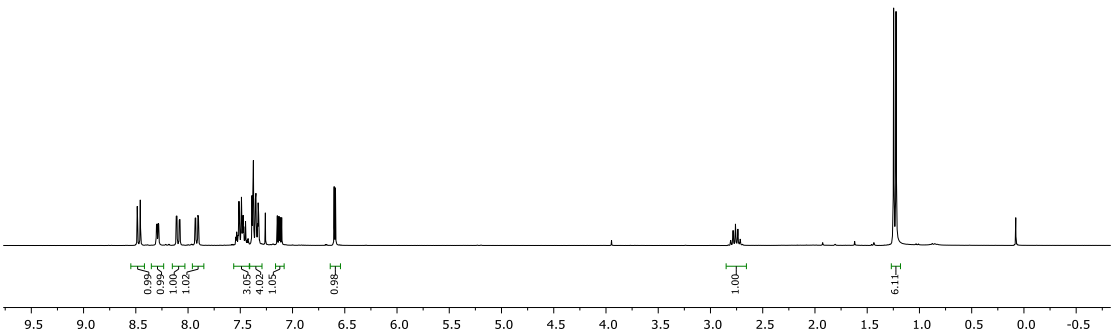

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.43
8.42
8.40
7.85
7.84
7.84
7.82
7.82
7.81
7.80
7.69
7.68
7.55
7.54
7.54
7.53
7.52
7.52
7.51
7.51
7.50
7.50
7.49
7.48
7.48
7.47
7.46
7.31
7.30
7.29
7.29
7.29
7.26 CDCl3
7.20
7.19
6.44
6.43
2.77
2.75
2.74
2.72
2.70
2.69
2.67
1.23
1.21
O
O
N
N
CH3
CH3
0.98
2.01
0.97
3.01
2.01
1.00
0.86
1.00
6.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

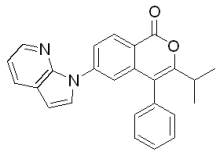

162.27
160.19
144.62
142.37
140.72
134.08
131.62
130.53
129.34
128.51
127.15
118.13
117.87
114.63
113.77
108.84
77.48
77.16 CDCl3
76.84
30.41
20.36
O
O
N
N
CH3
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

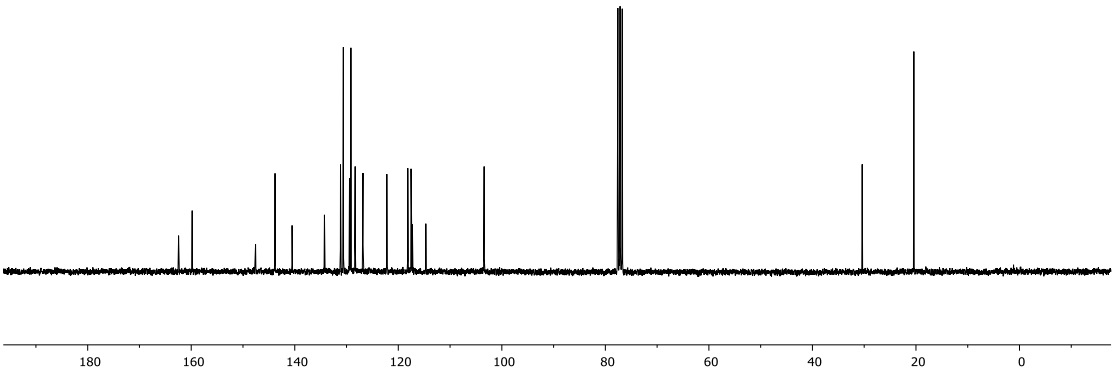

8.49
8.48
8.46
8.46
8.30
8.30
8.29
8.28
8.11
8.11
8.08
8.08
7.93
7.93
7.91
7.90
7.54
7.53
7.53
7.51
7.51
7.49
7.49
7.48
7.47
7.47
7.46
7.45
7.44
7.43
7.42
7.42
7.39
7.38
7.37
7.36
7.35
7.34
7.33
7.33
7.32
7.26
7.15
7.13
7.12
7.10
6.60
6.59
2.83
2.81
2.78
2.76
2.74
2.72
2.69
1.25
1.22


O
O
N
N

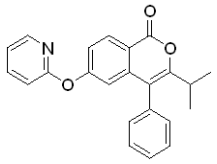

0.99
0.99
1.00
1.02
3.05
4.02
1.05
0.98
1.00
6.11
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

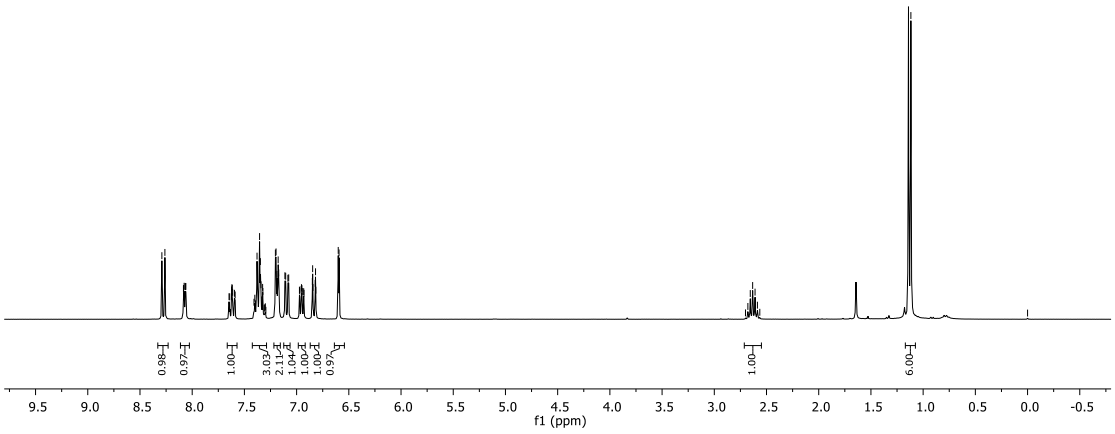

162.44
159.81
147.57
143.83
143.81
140.52
134.26
131.16
130.61
129.42
129.15
128.33
126.82
122.22
121.15
118.16
117.54
117.28
114.68
103.42
77.58
77.16
76.74
30.39
20.41

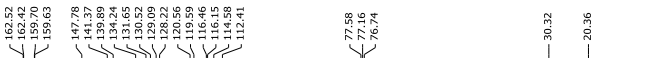

O
O
N
N

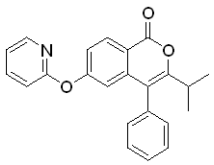

180
160
140
120
100
80
60
40
20
0

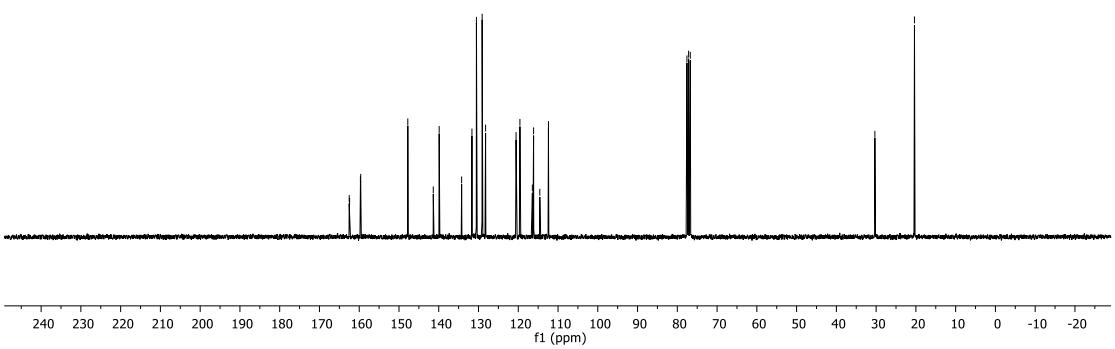

8.29
8.26
8.08
8.08
8.08
8.08
8.07
8.07
8.06
7.65
7.64
7.62
7.62
7.62
7.61
7.60
7.59
7.41
7.40
7.39
7.38
7.35
7.35
7.34
7.33
7.33
7.32
7.31
7.30
7.30
7.29
7.20
7.20
7.19
7.18
7.18
7.17
7.11
7.10
7.08
7.08
6.97
6.97
6.96
6.95
6.95
6.95
6.93
6.93
6.85
6.85
6.84
6.82
6.82
6.82
6.60
6.59
2.70
2.68
2.66
2.63
2.61
2.59
2.56
1.14
1.12
0.00


O
N
O
O

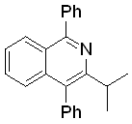

0.98
0.97
1.00
3.03
2.11
1.04
1.00
1.00
0.97
1.00
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

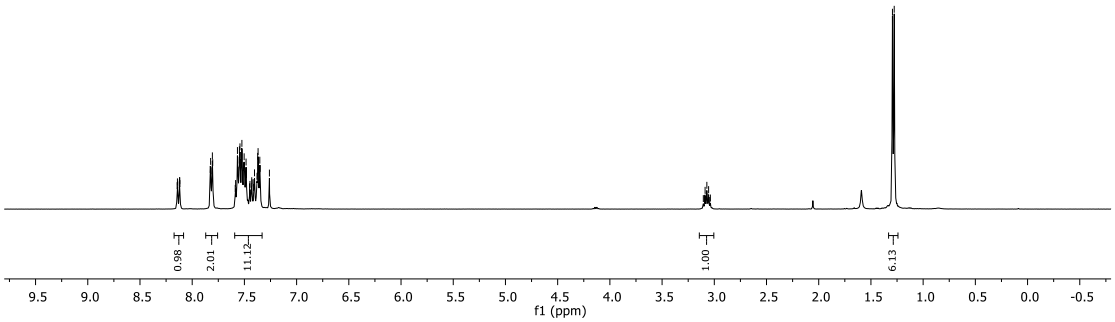

162.52
162.42
159.70
159.63
147.78
141.37
139.89
134.24
131.65
130.52
130.09
128.22
120.56
119.59
116.46
116.15
114.58
112.41
77.58
77.16
76.74
30.32
20.36

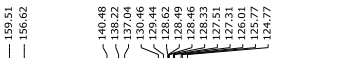

O
N
O
O

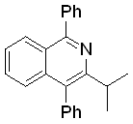

240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

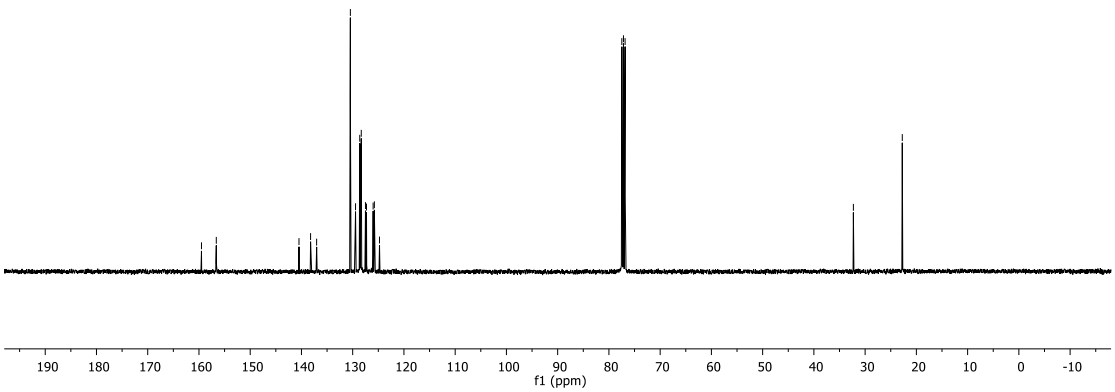

8.14
8.14
8.14
8.12
8.12
8.12
8.12
8.12
7.83
7.82
7.81
7.81
7.80
7.59
7.58
7.58
7.57
7.56
7.56
7.55
7.55
7.54
7.54
7.53
7.52
7.51
7.50
7.49
7.48
7.48
7.45
7.45
7.43
7.43
7.43
7.41
7.41
7.40
7.38
7.37
7.37
7.36
7.35
7.35
7.26
3.11
3.09
3.09
3.08
3.07
3.06
3.05
3.04
3.04
1.29
1.28


Ph
N
Ph

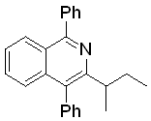

0.98
2.01
11.12
1.00
6.13
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

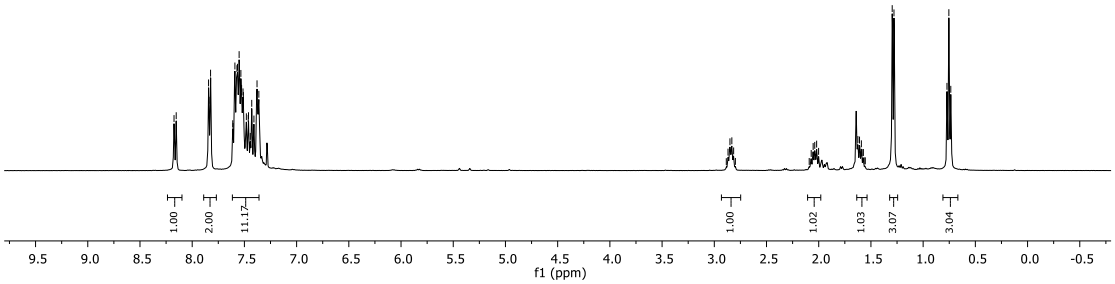

159.51
156.62
140.48
138.22
137.04
130.46
129.44
128.62
128.49
128.46
128.33
127.51
127.31
126.01
125.77
124.77
77.48
77.16
76.84
32.29
22.75

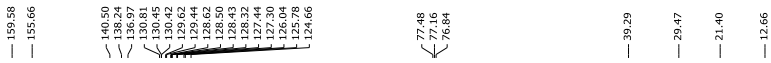

Ph
N
Ph

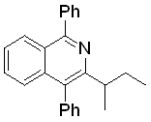

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

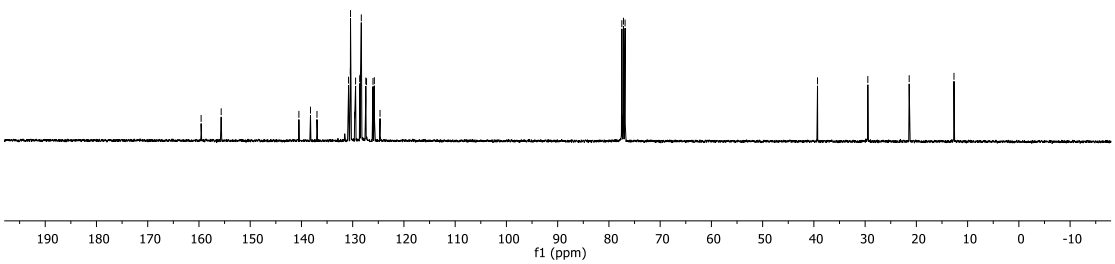

8.17
8.15
7.84
7.84
7.82
7.61
7.61
7.59
7.57
7.57
7.55
7.53
7.53
7.51
7.51
7.48
7.46
7.46
7.44
7.43
7.41
7.38
7.36
2.89
2.87
2.85
2.83
2.81
2.80
2.09
2.07
2.05
2.04
2.02
2.00
1.63
1.61
1.59
1.58
1.57
1.56
1.56
1.30
1.28
0.77
0.75
0.74


Ph
N
Ph

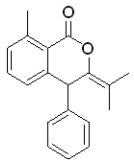

1.00
2.00
11.17
1.00
1.02
1.03
3.07
3.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

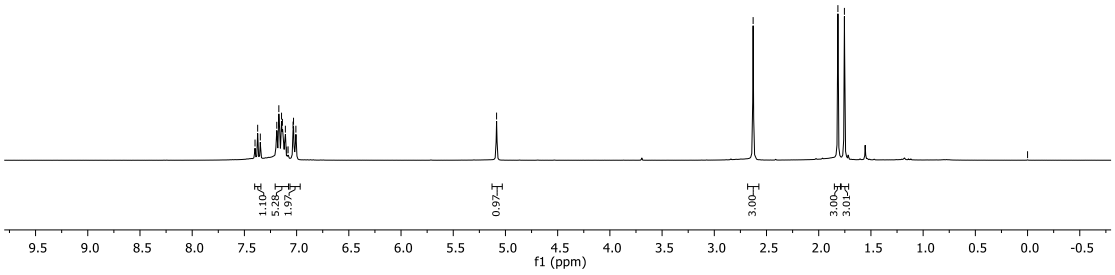

159.58
155.66
140.50
138.24
136.97
130.81
130.45
130.42
129.62
129.44
128.62
128.50
128.43
128.32
127.44
127.30
126.04
125.78
124.66
77.48
77.16
76.84
39.29
29.47
21.40
12.66


Ph
N
Ph

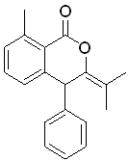

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

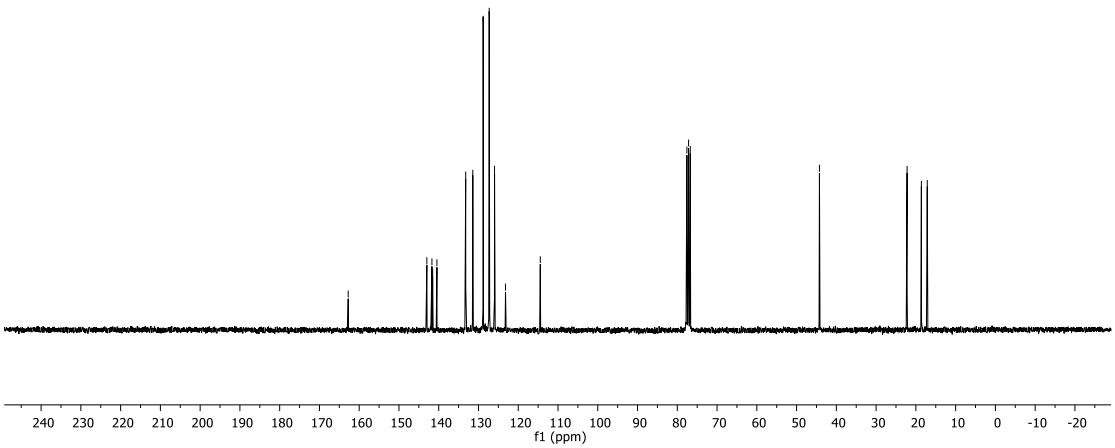

7.40
7.37
7.35
7.19
7.17
7.14
7.14
7.11
7.09
7.08
7.03
7.03
7.01
5.09
2.63
1.82
1.75
0.00




1.10
5.28
1.97
0.97
3.00
3.00
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


162.76
142.99
141.71
141.53
140.45
133.22
131.43
128.82
127.30
127.21
125.96
123.20
114.46
77.59
77.16
76.74
44.25
22.21
18.62
17.14




240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)