A Metal-Free Aromative Cascade for the Synthesis of Diverse Heterocycles

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Supplementary Information

A. Materials and Methods

Reagents

Reagents and solvents were obtained from Sigma-Aldrich (www.sigma-aldrich.com), Chem-Impex (www.chemimpex.com) or Acros Organics (www.fishersci.com) and used without further purification unless otherwise indicated. Dry solvents (acetonitrile) were obtained from Acros Organics (www.fishersci.com), and dichloromethane was distilled over CaH_2 under N_2 unless otherwise indicated. THF purchased from Sigma-Aldrich was distilled over Na metal with benzophenone indicator. Toluene was obtained from Sigma-Aldrich.

Reactions

All reactions were performed in flame-dried glassware under positive N_2 pressure with magnetic stirring unless otherwise noted. Liquid reagents and solutions were transferred thru rubber septa via syringes flushed with N_2 prior to use. Cold baths were generated as follows: 0 °C with wet ice/water and −78 °C with dry ice/acetone.

Chromatography

TLC was performed on 0.25 mm E. Merck silica gel 60 F254 plates and visualized under UV light (254 nm) or by staining with potassium permanganate ($KMnO_4$), cerium ammonium molybdenate (CAM), phosphomolybdic acid (PMA), and ninhydrin. Silica flash chromatography was performed on Sorbtech 230–400 mesh silica gel 60.

Analytical Instrumentation

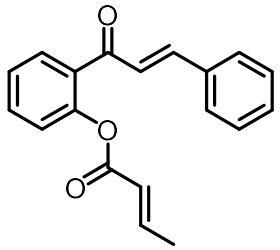
IR spectra were recorded on a Shimadzu IRAffinity-1 FTIR or a Nicolet 6700 FTIR spectrometer with peaks reported in cm^{-1}. NMR spectra were recorded on a Varian VNMRS 300, 400, 500 and 600 MHz NMR spectrometer in $CDCl_3$ unless otherwise indicated. Chemical shifts are expressed in ppm relative to solvent signals: $CDCl_3$ ((^1H, 7.26 ppm, ^{13}C, 77.0 ppm); coupling constants are expressed in Hz. NMR spectra were processed using Mnova (www.mestrelab.com/software/mnova-nmr). Mass spectra were obtained at the OU Analytical Core Facility on an Agilent 6538 High-Mass-Resolution QTOF Mass Spectrometer and an Agilent 1290 UPLC.

Nomenclature

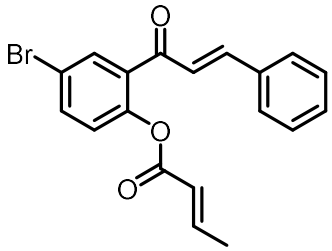
N.B.: Atom numbers shown in chemical structures herein correspond to IUPAC nomenclature, which was used to name each compound.

B. General Procedure 1 for the Synthesis of Crotonylhydroxychalcones (1)

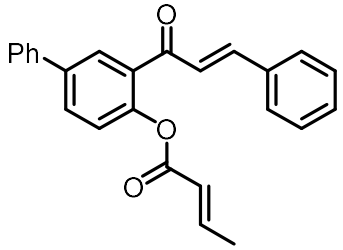
To a round bottom flask was measured 2'-hydroxyacetophenones (**1**) (1.0 equiv.), which was then dissolved in dichloromethane (0.2 M). This solution was cooled in an ice/water bath then crotonic acid (1.2 equiv.) and DMAP (0.1 equiv.) were added, followed by the addition of 1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride (EDCI, 1.5 equiv.). The reaction vessel was allowed to warm naturally to room temperature with stirring over 16 hours. The reaction mixture was then diluted with excess dichloromethane and washed sequentially with 1N HCl (2x) and sat. $NaHCO_3$ (2x). Organics were dried over anhydrous Na_2SO_4, concentrated in vacuo, then purified by flash chromatography eluting with 1:20 ethyl acetate:hexanes gradient to 2:5 ethyl acetate:hexanes to furnish crotonylhydroxychalcones **1a**-**1h**.



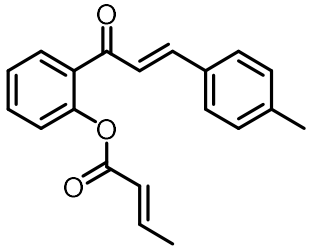
2-cinnamoylphenyl (*E*)-but-2-enoate (1a). Synthesized using general procedure 1. Yellow oil (272 mg, 79% yield). **TLC**: R_f 0.23 (ethyl acetate/hexanes = 1: 4). **IR** (neat): 3032, 1733, 1604, 1448, 1331, 1194, 1146, 1098, 964, 748. **^{1}H NMR** (600 MHz) δ 7.70 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.60–7.51 (m, 4H), 7.41–7.31 (m, 4H), 7.20 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.17–7.08 (m, 2H), 5.97 (dd, *J* = 15.5, 1.8 Hz, 1H), 1.82 (dd, *J* = 6.9, 1.7 Hz, 3H). **^{13}C NMR** (151 MHz) δ 191.6, 164.4, 148.7, 147.7, 145.1, 134.6, 132.6, 132.3, 130.5, 129.8, 128.9, 128.39, 125.9, 125.7, 123.4, 121.6, 18.1. **HRMS** (ESI) *m/z* calcd for $C_{19}H_{16}O_3Na$ ([M + Na]$^+$) 315.0997; found 315.0995.



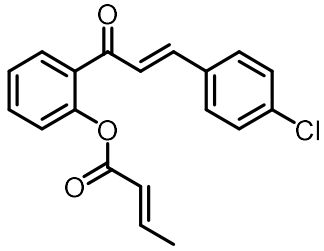
4-bromo-2-cinnamoylphenyl (*E*)-but-2-enoate (1b). Synthesized using general procedure 1. Yellow oil (103 mg, 74% yield). **TLC**: R_f 0.29 (ethyl acetate/hexanes = 3: 7). **IR** (neat): 3060, 3026, 2973, 1736, 1651, 1598, 1448, 1189, 1144, 966, 863, 741, 691. **^{1}H NMR** (600 MHz) δ 7.79 (d, *J* = 2.4 Hz, 1H), 7.63 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.59–7.50 (m, 3H), 7.39 (m, 3H), 7.16–7.06 (m, 4H), 5.94 (dd, *J* = 15.6, 1.7 Hz, 1H), 1.82 (dd, *J* = 7.0, 1.7 Hz, 3H). **^{13}C NMR** (151 MHz) δ 190.1, 164.1, 148.4, 147.6, 145.9, 135.07, 134.3, 134.2, 132.4, 130.8, 128.9, 128.5, 125.2, 125.0, 121.2, 119.1, 18.2. **HRMS** (ESI) *m/z* calcd for $C_{19}H_{15}BrO_3Na$ ([M + Na]$^+$) 393.0102; found 393.0102.



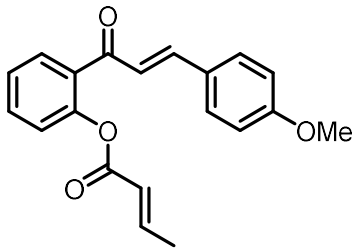
3-cinnamoyl-[1,1'-biphenyl]-4-yl (*E*)-but-2-enoate (1c). Synthesized using general procedure 1. Yellow oil (154 mg, 35% yield). **TLC**: R_f 0.27 (ethyl acetate/hexanes = 3: 7). **IR** (neat): 3029, 1734, 1652, 1596, 1477, 1330, 1189, 1097, 964, 789. **^{1}H NMR** (600 MHz) δ 7.89 (d, *J* = 2.3 Hz, 1H), 7.75 (dd, *J* = 8.4, 2.3 Hz, 1H), 7.65–7.59 (m, 3H), 7.59–7.53 (m, 2H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.42–7.35 (m, 4H), 7.28 (d, *J* = 8.4 Hz, 1H), 7.18 (m, 2H), 5.99 (dd, *J* = 15.5, 1.8 Hz, 1H), 1.84 (dd, *J* = 6.9, 1.7 Hz, 3H). **^{13}C NMR** (75 MHz) δ 191.7, 164.6, 148.0, 145.4, 139.5, 139.2, 134.6, 132.8, 130.9, 130.7, 129.0, 128.9, 128.5, 128.4, 127.8, 127.2, 125.6, 123.8, 121.5, 18.3. **HRMS** (ESI) *m/z* calcd for $C_{25}H_{20}O_3Na$ ($[M + Na]^+$) 391.1310; found 391.1316.



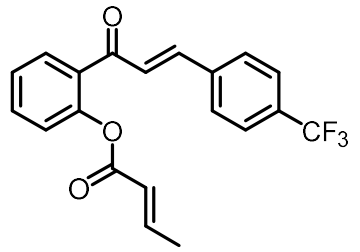
2-((*E*)-3-(p-tolyl)acryloyl)phenyl (*E*)-but-2-enoate (1d). Synthesized using general procedure 1. Yellow oil (328 mg, 12% yield). **TLC**: R_f 0.39 (ethyl acetate/hexanes = 1: 4). **IR** (neat): 2916, 1713, 1605, 1443, 1395, 1271, 1076, 887, 811, 781. **^{1}H NMR** (600 MHz) δ 7.68 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.55 (d, *J* = 16.0 Hz, 1H), 7.51 (ddd, *J* = 8.2, 7.4, 1.7 Hz, 1H), 7.43 (d, *J* = 7.9 Hz, 2H), 7.32 (td, *J* = 7.5, 1.2 Hz, 1H), 7.19 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.17 (d, *J* = 7.8 Hz, 2H), 7.15–7.07 (m, 2H), 5.96 (dd, *J* = 15.5, 1.7 Hz, 1H), 2.35 (s, 3H), 1.82 (dd, *J* = 6.9, 1.7 Hz, 3H). **^{13}C NMR** (151 MHz) δ 191.7, 164.4, 148.7, 147.7, 145.4, 141.1, 132.7, 132.3, 131.8, 129.8, 129.7, 128.5, 125.9, 124.6, 123.5, 121.6, 21.5, 18.2. **HRMS** (ESI) *m/z* calcd for $C_{20}H_{19}O_3$ ($[M + H]^+$) 307.1334; found 307.1325.



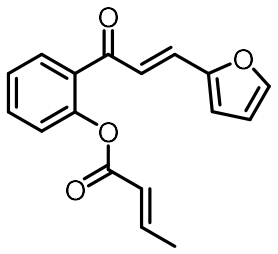
2-((*E*)-3-(4-chlorophenyl)acryloyl)phenyl (*E*)-but-2-enoate (1e). Synthesized using general procedure 1. Yellow oil (525 mg, 52% yield). **TLC**: R_f 0.25 (ethyl acetate/hexanes = 3: 7). **IR** (neat): 2915, 1732, 1603, 1489, 1293, 1192, 1092, 964, 820, 730. **^{1}H NMR** (600 MHz) δ 7.68 (dd, *J* = 7.6, 1.9 Hz, 1H), 7.53 (m, 1H), 7.52–7.47 (d, *J* = 18 Hz, 1H), 7.45 (m, 2H), 7.33 (m, 3H), 7.19 (dd, *J* = 8.3, 1.9 Hz, 1H), 7.15–7.07 (m, 2H), 5.96 (d, *J* = 15.6 Hz, 1H), 1.85–1.81 (d, *J* = 6 Hz, 3H). **^{13}C NMR** (151 MHz) δ 191.4, 164.4, 148.7, 147.9, 143.6, 136.4, 133.1, 132.5, 129.8, 129.5, 129.2, 126.0, 123.5, 121.5, 18.2. **HRMS** (ESI) *m/z* calcd for $C_{19}H_{15}ClO_3Na$ ($[M + Na]^+$) 349.0607; found 349.0612.



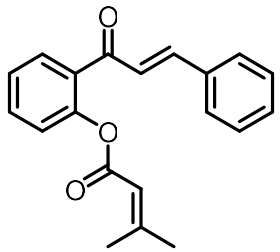
2-((*E*)-3-(4-methoxyphenyl)acryloyl)phenyl (*E*)-but-2-enoate (1f). Synthesized using general procedure 1. Yellow oil (146 mg, 45% yield). **TLC**: R_f 0.13 (ethyl acetate/hexanes = 3: 7). **IR** (neat): 2936, 1733, 1589, 1509, 1194, 1171, 1098, 1021, 966, 826, 730. **^{1}H NMR** (600 MHz) δ 7.67 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.55–7.47 (m, 4H), 7.33 (td, *J* = 7.6, 1.1 Hz, 1H), 7.19 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.11 (dq, *J* = 15.5, 6.9 Hz, 1H), 7.01 (d, *J* = 15.8 Hz, 1H), 6.89 (d, *J* = 8.8 Hz, 2H), 5.97 (dd, *J* = 15.5, 1.8 Hz, 1H), 3.83 (s, 3H), 1.84 (dd, *J* = 7.0, 1.7 Hz, 3H). **^{13}C NMR** (151 MHz) δ 191.8, 164.5, 161.7, 148.6, 147.7, 145.2, 132.8, 132.1, 130.2, 129.7, 127.3, 125.8, 123.4, 121.6, 114.4, 113.5, 55.4, 18.2. **HRMS** (ESI) *m/z* calcd for $C_{20}H_{18}O_4Na$ ($[M + Na]^+$) 345.1103; found 345.1109.



2-((*E*)-3-(4-(trifluoromethyl)phenyl)acryloyl)phenyl (*E*)-but-2-enoate (1g). Synthesized using general procedure 1. Yellow solid (565 mg, 68% yield, m.p. 55–56 ºC). **TLC**: R_f 0.47 (ethyl acetate/hexanes = 1:4). **IR** (neat): 3014, 1734, 1655, 1597, 1442, 1321, 1289, 1211, 1145, 1066, 963, 836, 771. **^{1}H NMR** (400 MHz) δ 7.70 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.58 (d, *J* = 14.9 Hz, 4H), 7.54–7.43 (m, 2H), 7.31 (td, *J* = 7.6, 1.2 Hz, 1H), 7.24–7.17 (m, 2H), 7.09 (m, *J* = 15.6, 1H), 5.95 (dd, *J* = 15.5, 1.7 Hz, 1H), 1.79 (dd, *J* = 7.0, 1.8 Hz, 3H). **^{13}C NMR** (151 MHz) δ 191.0, 164.4, 148.8, 148.0, 142.7, 138.0, 132.8, 131.7, 132.1, 129.9, 128.5, 127.6, 126.0, 125.7 (q, $J_{C\text{-}F}$ = 3.4 Hz), 123.5, 121.44, 18.1 [Note : While peaks corresponding to the CF_3 were observed, some portion of the peaks were lost in signal noise]. **HRMS** (ESI) *m/z* calcd for $C_{20}H_{15}F_3O_3Na$ ($[M + Na]^+$) 383.0871; found 383.0869.

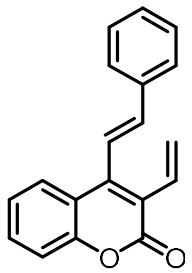


2-((*E*)-3-(furan-2-yl)acryloyl)phenyl (*E*)-but-2-enoate (1h). Synthesized using general procedure 1. Yellow oil (190 mg, 42% yield). **TLC**: R_f 0.30 (ethyl acetate/hexanes = 3: 7). **IR** (neat): 3057, 1732, 1655, 1598, 1550, 1477, 1037, 1217, 1194, 1098, 1012, 934, 750. **^{1}H NMR** (300 MHz) δ 7.71–7.65 (m, 1H), 7.53–7.48 (m, 1H), 7.47 (td, *J* = 1.4, 0.8 Hz, 1H), 7.37–7.25 (m, 2H), 7.20–7.01 (m, 3H), 6.63 (dd, *J* = 3.4, 0.6 Hz, 1H), 6.45 (dd, *J* = 3.4, 1.8 Hz, 1H), 5.98 (dd, *J* = 15.5, 1.8 Hz, 1H), 1.85 (dd, *J* = 6.9, 1.7 Hz, 3H). **^{13}C NMR** (75 MHz) δ 190.8, 164.4, 151.3, 148.8, 147.6, 145.1, 132.4, 131.0, 129.8, 125.9, 123.5, 122.9, 121.6, 116.4, 112.7, 18.2. **HRMS** (ESI) *m/z* calcd for $C_{17}H_{14}O_4Na$ ($[M + Na]^+$) 305.0790; found 305.0790.



2-cinnamoylphenyl 3-methylbut-2-enoate (1i). Synthesized using general procedure 1. Yellow oil (350 mg, 88% yield). **TLC**: R_f 0.48 (ethyl acetate/hexanes = 1: 4). **IR** (neat): 3061, 2917, 2359, 1738, 1605, 1448, 1332, 1200, 1119, 1063, 749. **^{1}H NMR** (600 MHz) δ 7.70 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.59–7.51 (m, 4H), 7.37 (m, 3H), 7.35–7.31 (t, 2H), 7.19–7.13 (m, 2H), 5.85 (d, *J* = 1.4 Hz, 1H), 2.11 (s, 3H), 1.83 (s, 3H). **^{13}C NMR** (151 MHz) δ 191.8, 164.5, 161.0, 148.8, 144.9, 134.7, 132.6, 132.4, 130.5, 129.8, 128.8, 128.4, 125.8, 125.7, 123.6, 114.7, 27.6, 20.5. **HRMS** (ESI) *m/z* calcd for $C_{20}H_{18}O_3Na$ ($[M + Na]^+$) 329.1154; found 329.1153.

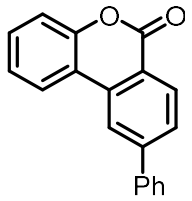
C. Synthesis of (*E*)-4-styryl-3-vinyl-2*H*-chromen-2-one (2)



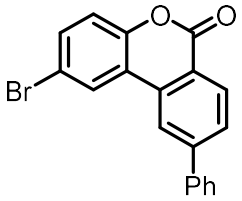
(*E*)-4-styryl-3-vinyl-2*H*-chromen-2-one (2). To a 4.0 mL vial was measured crotonylhydroxychalcone (**1**) (1.0 equiv.). DMSO (0.15M) was then added, followed by the addition of DBU (3.0 equiv.). The reaction vessel was equipped with a magnetic stir bar, sealed, and stirred at room temperature for 90 minutes. The reaction mixture was then diluted into ethyl acetate. Organics were washed sequentially with sat. NH_4Cl (2x) and water (2x) then dried over anhydrous Na_2SO_4. Organics were concentrated in vacuo and purified by flash chromatography to furnish (E)-4-styryl-3-vinyl-2H-chromen-2-one (2). Yellow oil (375 mg, 60% yield). **TLC**: R_f 0.53 (ethyl acetate/hexanes = 1:1). **IR** (neat): 3025, 1709, 1603, 1449, 1320, 1100, 984, 712. **^{1}H NMR** (400 MHz) δ 7.72 (d, *J* = 8.0 Hz, 1H), 7.57 (d, *J* = 7.5 Hz, 2H), 7.42 (tq, *J* = 14.3, 7.5 Hz, 4H), 7.30–7.20 (m, 2H), 7.15–7.06 (m, 1H), 6.91–6.76 (m, 2H), 6.41 (dd, *J* = 17.6, 1.9 Hz, 1H), 5.60 (dd, *J* = 11.9, 1.9 Hz, 1H). **^{13}C NMR** (101 MHz) δ 159.8, 152.4, 146.5, 139.6, 135.6, 131.3, 129.6, 129.3, 129.0, 128.6, 127.0, 126.3, 124.1, 122.9, 120.8, 119.4, 116.7. **HRMS** (ESI) *m/z* calcd for $C_{19}H_{15}O_2$ ($[M + H]^+$) 275.1072; found 275.1081.

D. General Procedure 2 for the Synthesis of Benzo[*c*]coumarins (3)

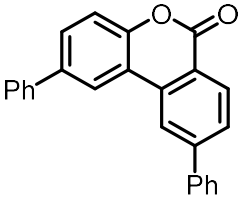
To a 15 mL round bottom flask was measured crotonylhydroxychalcone (**1**) (1.0 equiv.). DMSO (0.15M) was then added, followed by the addition of DBU (3.0 equiv.). The reaction vessel was equipped with a magnetic stir bar and stirred open to air at room temperature for 90 minutes. The reaction mixture was then heated to 80 ºC and stirred at this temperature for 16 hours. The reaction mixture was then cooled to room temperature and diluted into ethyl acetate. Organics were washed sequentially with sat. NH_4Cl (2x) and water (2x) then dried over anhydrous Na_2SO_4. Organics were concentrated in vacuo and purified by flash chromatography 1:20 ethyl acetate:hexanes gradient to 2:5 ethyl acetate:hexanes to furnish benzo[c]coumarins **3a**-**3h**.



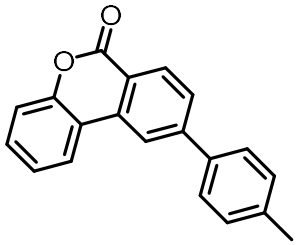
9-phenyl-6*H*-benzo[*c*]chromen-6-one (3a). Synthesized using general procedure 2. (223 mg, 82% yield). Characterization data was in accordance with previous reports.[1]



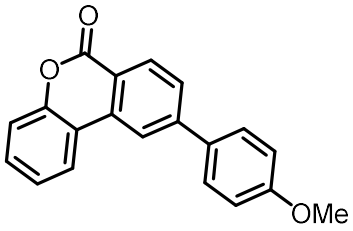
2-bromo-9-phenyl-6*H*-benzo[*c*]chromen-6-one (3b). Synthesized using general procedure 2. (46 mg, 88% yield). Characterization data was in accordance with previous reports. [2]



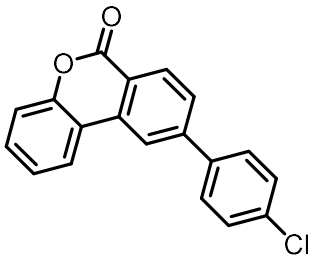
2,9-diphenyl-6*H*-benzo[*c*]chromen-6-one (3c). Synthesized using general procedure 2. Gray solid (35 mg, 67% yield, m.p. 184–185 ºC). **TLC**: R_f 0.54 (ethyl acetate/hexanes = 1:4). **IR** (neat): 3057, 2925, 1723, 1611, 1484, 1270, 1076, 883, 761. **^{1}H NMR** (600 MHz) δ 8.44 (dd, *J* = 8.1, 1.5 Hz, 1H), 8.31 (s, 1H), 8.26 (s, 1H), 7.78 (s, 1H), 7.71 (d, *J* = 7.3 Hz, 2H), 7.68 (d, *J* = 8.6, 1H), 7.64 (d, *J* = 7.4 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 2H), 7.51–7.45 (m, 3H), 7.44–7.37 (m, 2H). **^{13}C NMR** (151 MHz) δ 161.0, 150.9, 147.8, 140.1, 139.6, 137.9, 135.0, 131.2, 129.5, 129.1, 129.0, 128.8, 128.0, 127.7, 127.5, 127.2, 121.2, 120.1, 120.0, 118.2. **HRMS** (ESI) *m/z* calcd for $C_{25}H_{16}O_2Na$ ($[M + Na]^+$) 371.1048; found 371.1047.



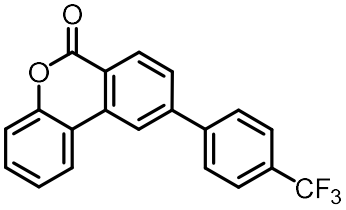
9-(p-tolyl)-6*H*-benzo[*c*]chromen-6-one (3d). Synthesized using general procedure 2. (33 mg, 77% yield). Characterization data was in accordance with previous reports. [1]



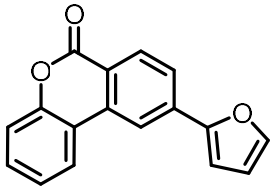
9-(4-methoxyphenyl)-6*H*-benzo[*c*]chromen-6-one (3e). Synthesized using general procedure 2. (37 mg, 82% yield). Characterization data was in accordance with previous reports. [2]



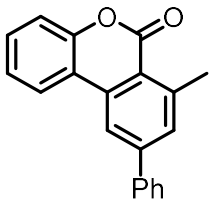
9-(4-chlorophenyl)-6*H*-benzo[*c*]chromen-6-one (3f). Synthesized using general procedure 2. (42 mg, 92% yield). Characterization data was in accordance with previous reports. [2]



9-(4-(trifluoromethyl)phenyl)-6*H*-benzo[*c*]chromen-6-one (3g). Synthesized using general procedure 2. Beige solid (24 mg, 46% yield, m.p. 172–174 ºC). **TLC**: R_f 0.27 (ethyl acetate/hexanes = 1:5). **IR** (neat): 3021, 2160, 1977, 1712, 1611, 1449, 1322, 1165, 1107, 1087, 826, 871. **^{1}H NMR** (400 MHz) δ 8.51 (d, *J* = 8.2 Hz, 1H), 8.30 (d, *J* = 1.8 Hz, 1H), 8.16 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.85–7.76 (m, 5H), 7.53 (m, *J* = 8.5 Hz, 1H), 7.44–7.35 (m, 2H). **^{13}C NMR** (101 MHz) δ 160.9, 151.5, 146.2, 143.2, 135.3, 131.4, 130.8, 127.9, 126.1 (d, *J* = 3.8 Hz), 124.7, 122.7, 120.7, 120.4, 119.1 (q, $J_{C\text{-}F}$ = 272.1 Hz, 1C), 117.8 [Note : While peaks corresponding to the CF_3 were observed, some portion of the peaks were lost in signal noise]. **HRMS** (ESI) *m/z* calcd for $C_{20}H_{12}F_3O_2$ ($[M + H]^+$) 341.0789; found 341.0794.



9-(furan-2-yl)-6*H*-benzo[*c*]chromen-6-one (3h). Synthesized using general procedure 2. Yellow oil (24 mg, 62% yield). **TLC**: R_f 0.40 (ethyl acetate/hexanes = 1:4). **IR** (neat): 2922, 2852, 1716, 1612, 1476, 1275, 1208, 1105, 916, 898, 734. **^{1}H NMR** (400 MHz) δ 8.39 (dd, *J* = 5.0, 3.3 Hz, 2H), 8.19–8.11 (m, 1H), 7.83 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.60 (d, *J* = 1.8 Hz, 1H), 7.50 (ddd, *J* = 8.4, 7.0, 1.6 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 2H), 6.95 (d, *J* = 3.4 Hz, 1H), 6.58 (dd, *J* = 3.5, 1.8 Hz, 1H). **^{13}C NMR** (101 MHz) δ 161.0, 152.3, 151.5, 143.9, 136.4, 135.4, 131.1, 130.6, 124.5, 124.1, 122.9, 119.5, 118.0, 117.8, 116.0, 112.4, 108.7. **HRMS** (ESI) *m/z* calcd for $C_{17}H_{11}O_3$ ($[M + H]^+$) 263.0708; found 263.0710.



7-methyl-9-phenyl-6*H*-benzo[*c*]chromen-6-one (3i). Synthesized using general procedure 2. (25 mg, 59% yield). Characterization data was in accordance with previous reports. [2]

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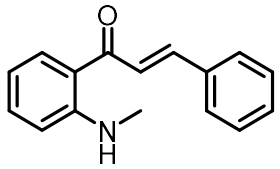
1. Xiao, J.; Chen, Y.; Zhu, S.; Wang, L.; Xu, L.; Wei, H. *Adv. Synth. Catal.* **2014,** *356*, 1835-1845.

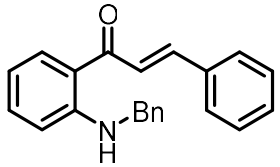
2. Mou, C.; Zhu, T.; Zheng, P.; Yang, S.; Song, B. *Adv. Synth. Catal.* **2016,** *358*, 707-712.

E. General Procedure 3 for the Synthesis of *N*-Alkylaminochalcones

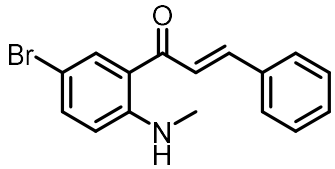
To a solution of *N*-methylacetophenones (1.0 equiv.) in ethanol (2.5 M) was added solid NaOH (3.0 equiv.). After the solid was fully dissolved, the appropriate benzaldehyde (1.2 equiv.) was added, and the mixture was stirred at room temperature overnight. The reaction mixture was then cooled to 0 ºC in an ice/water bath and the mixture was carefully neutralized using 1N HCl. The crude mixture was extracted with dichloromethane (3x) then washed with water (2x) and brine (2x). Organics were dried over Na_2SO_4 and concentrated to furnish chalcones which were purified by flash chromatography 1:20 ethyl acetate:hexanes gradient to 2:5 ethyl acetate:hexanes to furnish *N*-alkylaminochalcones.



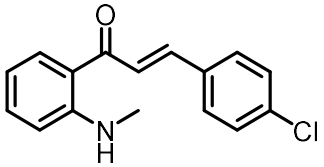
(*E*)-1-(2-(methylamino)phenyl)-3-phenylprop-2-en-1-one. Synthesized using general procedure 3. (1.17 g, 66% yield). Characterization data was in accordance with previous reports.[3]



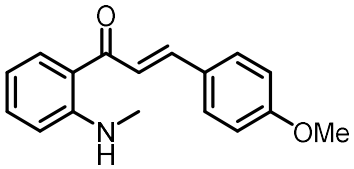
(*E*)-1-(2-(benzylamino)phenyl)-3-phenylprop-2-en-1-one. Synthesized using general procedure 3. (55 mg, 35% yield). Characterization data was in accordance with previous reports. [4]



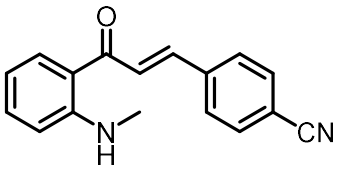
(*E*)-1-(5-bromo-2-(methylamino)phenyl)-3-phenylprop-2-en-1-one. Synthesized using general procedure 3. Orange solid (270 mg, 28% yield, mp 73 – 75 ºC). **TLC**: R_f 0.70 (ethyl acetate/hexanes = 1:4). **IR** (neat): 3309, 3924, 2907, 1642, 1585, 1447, 1187, 1165, 984, 813. **^{1}H NMR** (400 MHz) δ 8.98 (bs, 1H), 7.96 (s, 1H), 7.72 (d, J = 15.5 Hz, 1H), 7.64 (m, J = 9.1 Hz, 2H), 7.55 (d, J = 15.5 Hz, 1H), 7.41 (s, 4H), 6.62 (d, J = 9.1 Hz, 1H), 2.92 (s, 3H). **^{13}C NMR** (101 MHz) δ 190.5, 151.5, 143.4, 137.5, 135.0, 133.5, 130.3, 128.9, 128.4, 122.4, 119.5, 113.3, 105.2, 29.5. **HRMS** (ESI) *m/z* calcd for $C_{16}H_{15}BrNO$ ($[M+H]^+$) 316.0337; found 316.0338.



(*E*)-3-(4-chlorophenyl)-1-(2-(methylamino)phenyl)prop-2-en-1-one. Synthesized using general procedure 3. (273 mg, 88% yield). Characterization data was in accordance with previous reports.[5]



(*E*)-3-(4-methoxyphenyl)-1-(2-(methylamino)phenyl)prop-2-en-1-one. Synthesized using general procedure 3. (315 mg, quant. yield). Characterization data was in accordance with previous reports. [6]



(*E*)-4-(3-(2-(methylamino)phenyl)-3-oxoprop-1-en-1-yl)benzonitrile. Synthesized using general procedure 3. (251 mg, 83% yield). Characterization data was in accordance with previous reports. [7]

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3. Castaing, M.; Wason, S. L.; Estepa, B.; Hooper, J. F.; Willis, M. C. *Angew. Chem. Int. Ed.* **2013** *52*, 13280-13283.

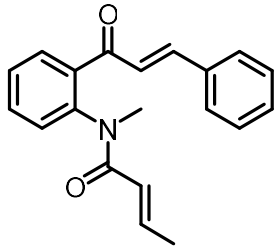
4. Litkei, G.; Totildekes, A. L. *Synth. Comm.* **2006**, *21*, 1597-1609.

5. Li, L.; Chen, J.; Kan, X.; Zhang, L.; Zhao, Y. *Eur. J. Org. Chem.* **2015,** *22*, 4892-4899.

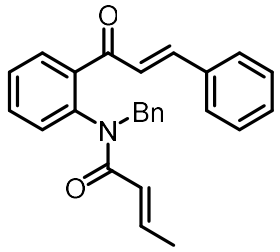
6. Tang, E.; Chen, B.; Zhang, L.; Li, W.; Lin, J. *Synlett* **2011**, *5*, 707-711.

F. General Procedure 4 for the Synthesis of *N*-Alkyl-*N*-Crotonylaminochalcones (4)

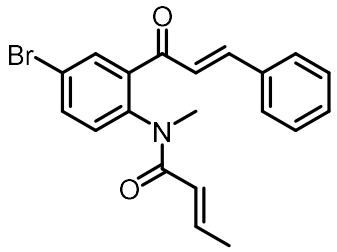
To a solution of *N*-alkylaminochalcone (1.0 equiv.) in dichloromethane (0.2M) at 0 ºC was added solid $NaHCO_3$ (1.5 equiv.). The mixture was stirred at this temperature for 10 minutes before crotonyl chloride (1.2 equiv.) was added slowly by syringe. The reaction mixture was allowed to warm naturally to room temperature and stirred at this temperature overnight. The reaction mixture was diluted with dichloromethane, then washed with water (2x). The organic layer was then dried over Na_2SO_4 and concentrated to give crude *N*-alkyl-*N*-crotonylaminochalcones (**5**) as a separable mixture of E/Z isomers, which were then purified via column chromatography 1:10 ethyl acetate:hexanes gradient to 1:1 ethyl acetate:hexanes to furnish pure *N*-alkyl-*N*-crotonylaminochalcones **4a**-**4i**.



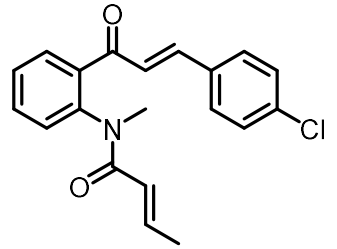
(*E*)-*N*-(2-cinnamoylphenyl)-*N*-methylbut-2-enamide (4a). Synthesized using general procedure 4. Orange oil (970 mg, 81% yield). **TLC**: R_f 0.23 (ethyl acetate/hexanes = 2:5). **IR** (neat): 3033, 1664, 1631, 1595, 1478, 1367, 1288, 1206, 1095, 963, 771. **^{1}H NMR** (500 MHz) δ 7.68 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.59 (td, *J* = 7.7, 1.7 Hz, 1H), 7.56–7.47 (m, 6H), 7.40 (m, 4H), 7.28 (d, *J* = 6.1 Hz, 1H), 7.01 (d, *J* = 16.0 Hz, 1H), 6.90 (dq, *J* = 15.0, 6.9 Hz, 1H), 5.74 (dd, *J* = 15.0, 1.7 Hz, 1H), 3.28 (s, 3H). **^{13}C NMR** (75 MHz) δ 192.9, 165.8, 145.8, 141.8, 138.1, 134.2, 132.1, 130.8, 129.9, 129.6, 129.3, 128.9, 128.4, 128.1, 125.1, 122.5, 37.7, 18.0. HRMS (ESI) *m/z* calcd for $C_{20}H_{10}NO_2$ ($[M + H]^+$) 306.1494; found 306.1486.



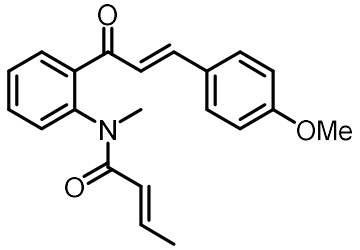
(*E*)-*N*-benzyl-*N*-(2-cinnamoylphenyl)but-2-enamide (4b). Synthesized using general procedure 4. Yellow oil (44 mg, 47% yield). **TLC**: R_f 0.43 (ethyl acetate/hexanes = 3:7). **IR** (neat): 3028, 2245, 1662, 1595, 1446, 1386, 1354, 1288, 1203, 907, 725. **^{1}H NMR** (300 MHz) δ 7.66–7.61 (m, 1H), 7.52–7.45 (m, 2H), 7.40 (m, *J* = 8.5 Hz, 5H), 7.21–7.14 (m, 4H), 7.03–6.92 (m, 2H), 6.90–6.85 (m, 1H), 5.74 (dq, *J* = 15.0, 1.6 Hz, 1H), 5.48 (d, *J* = 14.3 Hz, 1H), 4.24 (d, *J* = 14.4 Hz, 1H), 1.70 (dd, *J* = 6.9, 1.7 Hz, 3H). **^{13}C NMR** (75 MHz) δ 192.9, 165.9, 145.9, 142.4, 139.8, 138.4, 137.1, 134.3, 131.6, 131.0, 130.9, 129.5, 129.3, 129.0, 128.5, 128.3, 128.1, 127.4, 125.1, 122.9, 53.3, 18.1. **HRMS** (ESI) *m/z* calcd for $C_{26}H_{24}NO_2$ ($[M+H]^+$ 382.1807; found 382.1806.



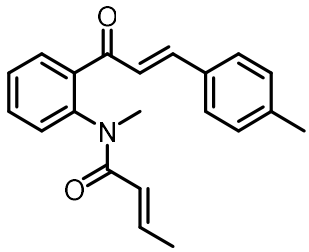
(*E*)-*N*-(4-bromo-2-cinnamoylphenyl)-*N*-methylbut-2-enamide (4d). Synthesized using general procedure 4. Yellow oil (347 mg, 90% yield). **TLC**: R_f 0.26 (ethyl acetate/hexanes = 3:7). **IR** (neat): 3055, 2631, 1597, 1447, 1393, 1293, 1198, 1102, 962, 823, 774. **^{1}H NMR** (400 MHz) δ 7.77 (d, J = 2.4 Hz, 1H), 7.68 (dd, J = 8.3, 2.5 Hz, 1H), 7.56–7.48 (m, 3H), 7.39 (d, J = 6.7 Hz, 3H), 7.14 (d, J = 8.4 Hz, 1H), 6.99–6.83 (m, 2H), 5.75–5.66 (m, 1H), 3.23 (s, 3H), 1.71 (dd, J = 7.0, 1.7 Hz, 3H). **^{13}C NMR** (101 MHz) δ 191.3, 165.7, 146.6, 142.8, 140.7, 139.8, 135.1, 134.0, 132.5, 131.2, 131.0, 129.1, 128.6, 124.4, 122.1, 121.8, 37.7, 18.1. **HRMS** (ESI) *m/z* calcd for $C_{20}H_{19}BrNO_2$ ($[M + H]^+$) 384.0599; found 384.0601.



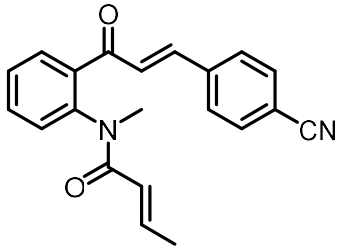
(*E*)-*N*-(2-((*E*)-3-(4-chlorophenyl)acryloyl)phenyl)-*N*-methylbut-2-enamide (4f). Synthesized using general procedure 4. Yellow oil (337 mg, 99% yield). **IR** (neat): 2911, 1663, 1590, 1488, 1367, 1290, 1204, 1089, 962, 768. **TLC**: R_f 0.30 (ethyl acetate/hexanes = 2:5). **^{1}H NMR** (300 MHz) δ 7.65 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.57 (td, *J* = 7.6, 1.7 Hz, 1H), 7.45 (m, *J* = 16.3, 4H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.25 (dd, *J* = 7.9, 1.2 Hz, 1H), 6.94 (d, *J* = 15.9 Hz, 1H), 6.89–6.79 (m, 1H), 5.75–5.64 (m, 1H), 3.24 (s, 3H), 1.67 (dd, *J* = 7.0, 1.7 Hz, 3H). **^{13}C NMR** (75 MHz) δ 192.5, 165.8, 144.1, 142.2, 141.7, 138.0, 136.7, 132.8, 132.3, 129.7, 129.6, 129.3, 129.3, 128.1, 125.4, 122.4, 37.8, 18.1. **HRMS** (ESI) *m/z* calcd for $C_{20}H_{18}ClNO_2Na$ ($[M + Na]^+$) 362.0924 ; found 362.0920.



(*E*)-*N*-(2-((*E*)-3-(4-methoxyphenyl)acryloyl)phenyl)-*N*-methylbut-2-enamide (4g). Synthesized using general procedure 4. Yellow oil (295 mg, 75% yield). **IR** (neat): 2933, 1663, 1592, 1444, 1329, 1303, 1171, 1020, 962, 826, 730. **TLC**: R_f 0.18 (ethyl acetate/hexanes = 2:5). **^{1}H NMR** (300 MHz) δ 7.61 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.52 (td, *J* = 7.6, 1.8 Hz, 1H), 7.48–7.39 (m, 4H), 7.21 (dd, *J* = 7.8, 1.3 Hz, 1H), 6.92–6.78 (m, 4H), 5.70 (dd, *J* = 15.0, 1.7 Hz, 1H), 3.79 (s, 3H), 3.22 (s, 3H), 1.65 (dd, *J* = 6.9, 1.7 Hz, 3H). **^{13}C NMR** (75 MHz) δ 193.1, 165.9, 161.9, 145.9, 141.8, 141.5, 138.49, 131.9, 130.3, 129.5, 129.3, 128., 126.9, 122.9, 122.5, 114.5, 55.4, 37.7, 18.0. **HRMS** (ESI) *m/z* calcd for $C_{21}H_{21}NO_3Na$ ($[M + Na]^+$) 358.1419 ; found 358.1418.



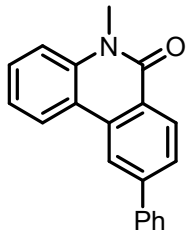
(E)-N-methyl-N-(2-((E)-3-(p-tolyl)acryloyl)phenyl)but-2-enamide (4h). Synthesized using general procedure 4. Yellow oil (495 mg, 77% yield). **IR** (neat): 3050, 2915, 1664, 1628, 1596, 1445, 1370, 1297, 1205, 1040, 963, 813, 731. **TLC**: R_f 0.48 (ethyl acetate/hexanes = 1:1). **^{1}H NMR** (300 MHz) δ 7.61 (d, *J* = 9.1 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.48 – 7.40 (m, 2H), 7.36 (d, *J* = 8.1 Hz, 2H), 7.22 (d, *J* = 8.8 Hz, 1H), 7.14 (d, *J* = 7.9 Hz, 2H), 6.92 (d, *J* = 15.9 Hz, 1H), 6.88 – 6.77 (m, 1H), 5.70 (d, *J* = 16.7 Hz, 1H), 3.23 (s, 3H), 2.32 (s, 3H), 1.67 – 1.59 (m, 3H). **^{13}C NMR** (75 MHz) δ. **HRMS** (ESI) *m/z* calcd for $C_{21}H_{22}NO_2$ ($[M + H]^+$) 320.1651; found 320.1649.



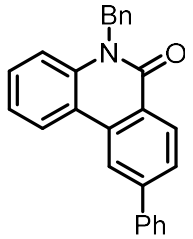
(*E*)-*N*-(2-((*E*)-3-(4-cyanophenyl)acryloyl)phenyl)-*N*-methylbut-2-enamide (4i). Synthesized using general procedure 4. Yellow oil (102 mg, 32% yield). **IR** (neat): 3462, 3054, 2226, 1661, 1445, 1295, 1096, 963, 827, 770. **TLC**: R_f 0.18 (ethyl acetate/hexanes = 2:5). **^{1}H NMR** (300 MHz) δ 7.72–7.52 (m, 9H), 7.50–7.43 (m, 2H), 7.29–7.21 (m, 1H), 7.03 (d, *J* = 15.9 Hz, 1H), 6.95–6.79 (m, 1H), 5.68 (dd, *J* = 15.0, 1.7 Hz, 1H), 3.24 (s, 3H), 1.67 (dd, *J* = 7.0, 1.6 Hz, 3H). **^{13}C NMR** (75 MHz) δ 191.8, 165.8, 142.5, 142.4, 141.9, 138.7, 137.5, 132.9, 132.7, 129.9, 129.3, 128.7, 128.2, 127.8, 122.2, 118.3, 113.6, 37.8, 18.1. **HRMS** (ESI) *m/z* calcd for $C_{21}H_{18}N_2O_2Na$ ($[M + Na]^+$) 352.1266; found 352.1266.

G. General Procedure 5 for the Synthesis of Phenanthradin-6(5*H*)-ones (5) :

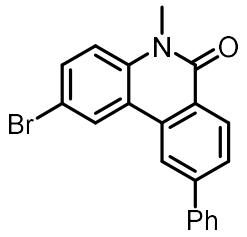
To a 15 mL round bottom flask was measured *N*-aklyl-*N*-crotonylaminochalcone (**4**) (1.0 equiv.). DMSO (0.15M) was then added, followed by the addition of DBU (3.0 equiv.). The reaction vessel was equipped with a magnetic stir bar and stirred open to air at room temperature for 90 minutes. The reaction mixture was then heated to 80 °C and stirred at this temperature for 16 hours. The reaction mixture was then cooled to room temperature and diluted with ethyl acetate. Organics were washed sequentially with sat. NH_4Cl (2x) and water (2x) then dried over anhydrous Na_2SO_4. Organics were concentrated in vacuo and purified by flash chromatography using a 1:10 ethyl acetate:hexanes gradient to 1:1 ethyl acetate:hexanes to furnish phenanthradinones **5a-5i**.



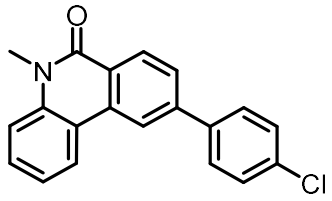
5-methyl-9-phenylphenanthridin-6(5*H*)-one (5a). Synthesized using general procedure 5. Yellow oil (259 mg, 91% yield). **TLC**: R_f 0.43 (ethyl acetate/hexanes = 3:10). **IR** (neat): 3029, 2252, 1625, 1584, 1466, 1417, 1277, 1158, 1075, 866, 744. **^{1}H NMR** (500 MHz) δ 8.63 (d, *J* = 8.2 Hz, 1H), 8.47 (d, *J* = 1.7 Hz, 1H), 7.82 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.75 (dd, *J* = 8.2, 1.3 Hz, 2H), 7.59 (ddd, *J* = 8.6, 7.1, 1.5 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 2H), 7.48–7.44 (m, 2H), 7.36 (ddd, *J* = 8.1, 7.2, 1.1 Hz, 1H), 3.85 (s, 3H). **^{13}C NMR** (75 MHz) δ 161.5, 145.1, 140.4, 138.2, 133.8, 129.7, 129.5, 129.0, 128.3, 127.5, 127.1, 124.4, 123.2, 122.5, 120.1, 119.3, 115.1, 30.0. **HRMS** (ESI) *m/z* calcd for $C_{20}H_{16}NO$ ($[M + H]^+$) 286.1232; found 286.1237.



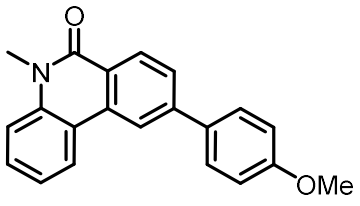
5-benzyl-9-phenylphenanthridin-6(5*H*)-one (5b). Synthesized using general procedure 5. (36 mg, 86% yield). Characterization data was in accordance with previous reports.[7]



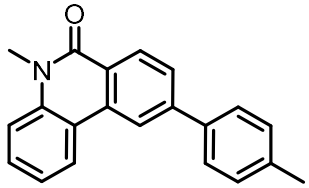
2-bromo-5-methyl-9-phenylphenanthridin-6(5*H*)-one (5e). Synthesized using general procedure 5. Yellow oil (29 mg, 70% yield). **TLC**: R_f 0.45 (ethyl acetate/hexanes = 3:10). **IR** (neat): 3085, 2920, 2120, 1639, 1582, 1361, 1187, 1033, 853, 625. **^{1}H NMR** (600 MHz) δ 8.59 (d, J = 8.3 Hz, 1H), 8.44 (s, 1H), 8.35 (d, J = 1.7 Hz, 1H), 7.84 (dd, J = 8.3, 1.7 Hz, 1H), 7.76–7.70 (m, 2H), 7.65 (dd, J = 8.8, 2.2 Hz, 1H), 7.54 (t, J = 7.5 Hz, 2H), 7.46 (t, J = 7.5 Hz, 1H), 7.31 (d, J = 8.9 Hz, 1H), 3.81 (s, 3H). **^{13}C NMR** (151 MHz) δ 161.2, 145.6, 140.1, 137.3, 132.6, 132.3, 129.6, 129.0, 128.4, 127.8, 127.5, 126.0, 124.6, 121.1, 120.2, 116.8, 115.7, 30.1. **HRMS** (ESI) *m/z* calcd for $C_{20}H_{15}BrNO$ ($[M + H]^+$) 364.0337; found 364.0342.



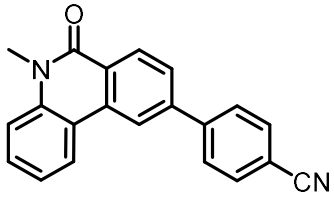
9-(4-chlorophenyl)-5-methylphenanthridin-6(5*H*)-one (5f). Synthesized using general procedure 5. Yellow Oil (38 mg, 80% yield). **TLC**: R_f 0.28 (ethyl acetate/hexanes = 1:4). **IR** (neat): 2923, 1644, 1585, 1444, 1389, 1343, 1092, 1005, 814, 689. **^{1}H NMR** (300 MHz) δ 8.61 (dd, *J* = 8.3, 0.5 Hz, 1H), 8.42–8.39 (m, 1H), 8.36 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.78–7.73 (m, 1H), 7.70–7.63 (m, 2H), 7.58 (ddd, *J* = 8.5, 7.1, 1.5 Hz, 1H), 7.52–7.47 (m, 2H), 7.47–7.42 (m, 1H), 7.35 (ddd, *J* = 8.3, 7.3, 1.2 Hz, 1H), 3.84 (s, 3H). **^{13}C NMR** (75 MHz) δ 161.4, 143.9, 138.8, 138.3, 134.5, 133.9, 129.8, 129.7, 129.2, 128.8, 126.9, 124.7, 123.2, 122.5, 120.0, 119.1, 115.2, 30.0. **HRMS** (ESI) *m/z* calcd for $C_{20}H_{15}ClNO$ ($[M + H]^+$) 320.0842; found 320.0851.



9-(4-methoxyphenyl)-5-methylphenanthridin-6(5*H*)-one (5g). Synthesized using general procedure 5. Yellow oil (45 mg, 81% yield). **TLC**: R_f 0.21 (ethyl acetate/hexanes = 1:4). **IR** (neat): 2927, 1643, 1585, 1520, 1444, 1298, 1246, 1178, 1032, 826, 750. **^{1}H NMR** (300 MHz) δ 8.58 (d, *J* = 8.3 Hz, 1H), 8.41 (d, *J* = 1.7 Hz, 1H), 8.38 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.78 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.72–7.65 (m, 2H), 7.57 (ddd, *J* = 8.5, 7.1, 1.5 Hz, 1H), 7.44 (dd, *J* = 8.5, 1.2 Hz, 1H), 7.35 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H), 7.05 (d, *J* = 8.7 Hz, 2H), 3.89 (s, 3H), 3.84 (s, 3H). **^{13}C NMR** (75 MHz) δ 159.9, 144.8, 138.3, 133.9, 129.6, 129.5, 128.6, 126.8, 124.0, 123.2, 122.4, 121.8, 119.4, 115.1, 114.4, 55.4, 30.0. **HRMS** (ESI) *m/z* calcd for $C_{21}H_{18}NO_2$ ($[M + H]^+$) 316.1338; found 316.1345.



5-methyl-9-(p-tolyl)phenanthridin-6(5H)-one (5h). Synthesized using general procedure 5. Yellow solid (269 mg, 89% yield, m.p. 136–138 ºC). **TLC**: R_f 0.33 (ethyl acetate/hexanes = 1:3). **IR** (neat): 2914, 1920, 1642, 1614, 1584, 1445, 1338, 1306, 1101, 1044, 814, 781, 684. **^{1}H NMR** (300 MHz) δ 8.51 (d, *J* = 8.3 Hz, 1H), 8.30 (s, 1H), 8.23 (d, *J* = 7.8 Hz, 2H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.29 (q, *J* = 7.2 Hz, 4H), 3.73 (s, 3H), 2.42 (s, 3H). **^{13}C NMR** (75 MHz). δ 161.4, 144.9, 138.2, 137.3, 133.7, 129.7, 129.5, 129.4, 127.3, 126.8, 124.1, 123.1, 122.3, 119.6, 119.2, 115.0, 29.9, 21.2. **HRMS** (ESI) *m/z* calcd for $C_{21}H_{18}NO$ ($[M + H]^+$) 300.1388; found 300.1389.



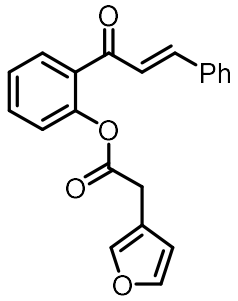
4-(5-methyl-6-oxo-5,6-dihydrophenanthridin-9-yl)benzonitrile (5i). Synthesized using general procedure 5. Yellow oil (31 mg, 68% yield,). **TLC**: R_f 0.14 (ethyl acetate/hexanes = 1:4). **IR** (neat): 3090, 3035, 2219, 1645, 1604, 1478, 1347, 1035, 824. **^{1}H NMR** (300 MHz) δ 8.64 (dd, *J* = 8.3, 0.5 Hz, 1H), 8.43 (d, *J* = 1.8 Hz, 1H), 8.35 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.82 (d, *J* = 1.5 Hz, 4H), 7.77 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.60 (ddd, *J* = 8.5, 7.1, 1.5 Hz, 1H), 7.45 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.36 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H), 3.83 (s, 3H). **^{13}C NMR** (75 MHz) δ 161.2, 144.8, 143.0, 138.3, 134.1, 132.8, 130.1, 129.9, 128.2, 126.8, 125.4, 123.2, 122.6, 120.5, 118.9, 118.7, 115.3, 111.9, 30.1. **HRMS** (ESI) *m/z* calcd for $C_{21}H_{15}N_2O$ ($[M + H]^+$) 311.1184; found 311.1191.

7. Bernini, R.; Cacchi, S.; Fabrizi, G.; Sferrazza, A. *Synthesis,* **2008,** *5*, 729-738.

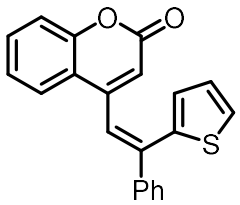
H. General Procedure 6 for the Synthesis of Arylaceticchalcones (6)

a.) To a round bottom flask was measured 2'-hydroxyacetophenones (**1**) (1.0 equiv.), which was then dissolved in dichloromethane (0.2 M). This solution was cooled in an ice/water bath then arylacetic acid (1.2 equiv.) and DMAP (0.1 equiv.) were added, followed by the addition of 1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride (EDCI, 1.5 equiv.). The reaction vessel was allowed to warm naturally to room temperature and stirred for 4 hours. The reaction mixture was then diluted with excess dichloromethane and washed sequentially with 1N HCl (2x) and sat. $NaHCO_3$ (2x). Organics were dried over anhydrous Na_2SO_4, concentrated in vacuo, then purified by flash chromatography eluting with 1:20 ethyl acetate:hexanes gradient to 2:5 ethyl acetate:hexanes to furnish arylacetichydroxychalcones **6a-6d**.

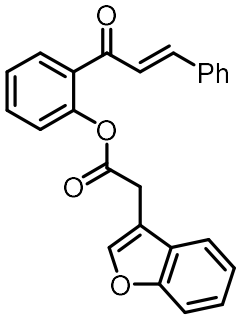
b.) To a stirred solution of corresponding arylacetic acid (1.2 equiv.) was added one drop of DMF. The reaction vessel was equipped with a reflux condenser and a 2M solution of $(COCl)_2$ (1.5 equiv.) was slowly added by syringe. The mixture was heated to reflux with stirring for 90 minutes, then cooled to room temperature. Solvent was removed by rotary evaporation and the crude acyl chloride was carried forward without further purification. To a solution of *N*-methylaminochalcone (1.0 equiv.) in dichloromethane (0.2M) at 0 °C was added solid $NaHCO_3$ (1.5 equiv.). The mixture was stirred at this temperature for 10 minutes before crude acyl chloride (1.2 equiv.) was added slowly by syringe. The reaction mixture was allowed to warm naturally to room temperature and stirred at this temperature overnight. The reaction mixture was diluted with dichloromethane, then washed with water (2x). The organic layer was then dried over Na_2SO_4 and concentrated to give crude *N*-alkyl-*N*-arylaceticaminochalcones (**6**), which were then purified via column chromatography 3:10 ethyl acetate:hexanes gradient to 1:1 ethyl acetate:hexanes to furnish pure *N*-alkyl-*N*-arylaminochalcones **6f-6h**.



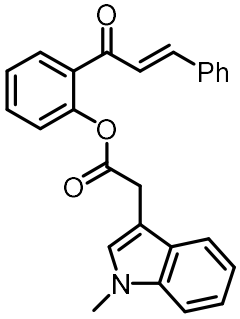
2-cinnamoylphenyl 2-(furan-3-yl)acetate (6a). Synthesized using general procedure 6a. Yellow oil (467 mg, 80% yield). **TLC**: R_f 0.33 (ethyl acetate/hexanes = 1:4). **IR** (neat): 3058, 2915, 1761, 1666, 1604, 1448, 1303, 1194, 1112, 1020, 998, 872, 731. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.70 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.60 – 7.50 (m, 4H), 7.44 – 7.31 (m, 6H), 7.21 – 7.10 (m, 2H), 6.38 (s, 1H), 3.68 (s, 3H). **^{13}C NMR** (75 MHz, Chloroform-*d*) δ 191.7, 169.6, 148.6, 145.7, 143.0, 140.7, 134.4, 132.5, 132.2, 130.9, 129.9, 129.0, 128.5, 126.2, 125.3, 123.4, 116.4, 111.4, 30.7. **HRMS** (ESI) *m/z* calcd for $C_{21}H_{16}O_4Na$ ([M + Na]$^+$) 355.0946; found 355.0948.



(*Z*)-4-(2-phenyl-2-(thiophen-2-yl)vinyl)-2*H*-chromen-2-one (6b). Synthesized using general procedure 6a. Yellow oil (690 mg, 77% yield). **TLC**: R_f 0.32 (ethyl acetate/hexanes = 1:4). **IR** (neat): 3028, 2923, 2854, 1703, 1603, 1450, 1282, 1110, 1051, 970. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 8.1 Hz, 1H), 7.55 (d, *J* = 7.0 Hz, 1H), 7.54 – 7.47 (m, 3H), 7.43 (t, *J* = 7.0 Hz, 4H), 7.38 (d, *J* = 7.0 Hz, 1H), 7.32 (d, *J* = 9.2 Hz, 1H), 7.12 – 7.09 (m, 1H), 7.04 (d, *J* = 4.7 Hz, 2H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 160.3, 153.0, 146.5, 138.6, 135.8, 134.7, 131.5, 131.26, 129.2, 129.0, 128.2, 127.1, 126.6, 124.3, 122.5, 119.0, 118.7, 117.2. **HRMS** (ESI) *m/z* calcd for $C_{21}H_{15}O_2S$ ($[M + H]^+$) 331.0793; found 331.0788.

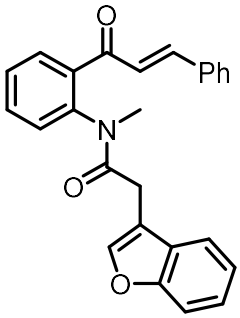


2-cinnamoylphenyl 2-(benzofuran-3-yl)acetate (6c). Synthesized using general procedure 6a. Yellow oil (260 mg, 76% yield). **TLC**: R_f 0.25 (ethyl acetate/hexanes = 1:4). **IR** (neat): 3060, 2954, 1760, 1604, 1449, 1331, 1303, 1196, 1097, 731. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.69 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.59 – 7.49 (m, 6H), 7.45 (d, *J* = 8.1 Hz, 1H), 7.43 – 7.33 (m, 4H), 7.32 – 7.25 (m, 1H), 7.21 (d, *J* = 7.5 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 1H), 7.09 (d, *J* = 16.1 Hz, 1H), 3.92 (s, 2H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 191.7, 169.2, 155.1, 148.6, 145.8, 143.2, 134.3, 132.5, 132.2, 130.9, 129.8, 129.0, 128.5, 127.5, 126.3, 125.2, 124.5, 123.5, 122.7, 119.8, 112.3, 111.5, 29.6. **HRMS** (ESI) *m/z* calcd for $C_{25}H_{19}O_4$ ($[M + H]^+$) 383.1283; found 383.1289.

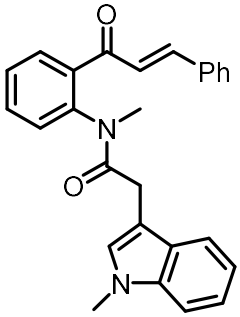


2-cinnamoylphenyl 2-(1-methyl-1*H*-indol-3-yl)acetate (6d). Synthesized using general procedure 6b. Yellow oil (140 mg, 19% yield). **TLC**: R_f 0.22 (ethyl acetate/hexanes = 1:4). **IR** (neat): 3057, 2929, 1756, 1603, 1474, 1447, 1330, 1193, 1104, 1013, 916, 775. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.66 (d, *J* = 7.6 Hz, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.54 – 7.45 (m, 4H), 7.41 – 7.29 (m, 4H), 7.24 (t, *J* = 6.7 Hz, 2H), 7.20 – 7.10 (m, 2H), 7.07 (m, 1H), 6.99 (d, *J* = 19.7 Hz, 1H), 3.96 (s, 2H), 3.66 (s, 3H). **^{13}C NMR** (151 MHz, Chloroform-*d*) δ 192.1, 170.3, 148.7, 145.5, 136.8, 134.5, 132.5, 132.2, 130.6, 129.7, 128.9,

128.5, 128.0, 127.7, 126.0, 125.6, 123.4, 121.8, 119.3, 118.9, 109.3, 105.6, 32.6, 31.2. **HRMS** (ESI) *m/z* calcd for $C_{26}H_{21}NO_3Na$ ($[M + Na]^+$) 418.1419; found 418.1411.



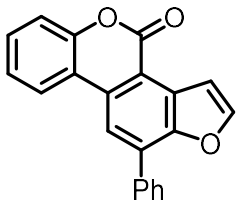
2-(benzofuran-3-yl)-N-(2-cinnamoylphenyl)-N-methylacetamide (6e). Synthesized using general procedure 6b. Yellow oil (184 mg, 93% yield). **TLC**: R_f 0.53 (ethyl acetate/hexanes = 1:1). **IR** (neat): 3060, 2924, 2247, 1731, 1644, 1596, 1449, 1330, 1207, 1095, 906, 856, 725. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.73 – 7.68 (m, 1H), 7.57 – 7.53 (m, 2H), 7.52 – 7.48 (m, 2H), 7.47 – 7.43 (m, 2H), 7.42 – 7.32 (m, 5H), 7.28 – 7.22 (m, 1H), 7.22 – 7.19 (m, 1H), 7.19 – 7.12 (m, 1H), 7.00 (d, *J* = 16.0 Hz, 1H), 3.25 (s, 3H). **^{13}C NMR** (75 MHz, Chloroform-*d*) δ 192.5, 170.2, 155.0, 146.5, 142.9, 141.8, 137.6, 134.1, 132.4, 131.1, 129.7, 129.6, 129.0, 128.6, 128.6, 127.9, 124.8, 124.2, 122.5, 119.9, 114.08, 111.3, 29.9. **HRMS** (ESI) *m/z* calcd for $C_{26}H_{21}NO_2$ ($[M + H]^+$) 396.1600; found 396.1604.



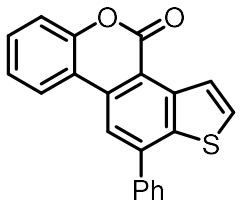
N-(2-cinnamoylphenyl)-N-methyl-2-(1-methyl-1H-indol-3-yl)acetamide (6f). Synthesized using general procedure 6b. Yellow oil (117 mg, 65% yield). **TLC**: R_f 0.40 (ethyl acetate/hexanes = 1:1). **IR** (neat): 3055, 2928, 2240, 1644, 1596, 1484, 1447, 1371, 1329, 1206, 1109, 1012, 908, 728. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.65 (d, *J* = 8.9 Hz, 1H), 7.50 (dd, *J* = 15.8, 9.0 Hz, 3H), 7.36 (s, 5H), 7.23 (d, *J* = 7.6 Hz, 2H), 7.12 (s, 2H), 7.01 (s, 1H), 6.84 (s, 1H), 6.72 (d, *J* = 15.9 Hz, 1H), 3.61 (d, *J* = 5.2 Hz, 2H), 3.55 (s, 3H), 3.29 (s, 3H). **^{13}C NMR** (75 MHz, Chloroform-*d*) δ 192.3, 171.5, 145.6, 142.3, 137.8, 136.6, 134.1, 132.4, 130.9, 129.7, 128.9, 128.6, 128.3, 127.9, 127.7, 124.5, 121.4, 118.9, 118.7, 109.2, 107.3, 38.1, 32.6, 31.1. **HRMS** (ESI) *m/z* calcd for $C_{27}H_{25}N_2O_2$ ($[M + H]^+$) 409.1916; found 409.1922.

I. General Procedure 7 for the Synthesis of Heteroarylbenzo[*c*]coumarins and Heteroarylphenanthradin-6(5H)-ones (7)

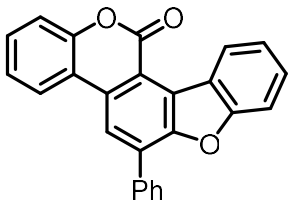
To a 15 mL round bottom flask was measured arylaceticchalcone (**6**) (1.0 equiv.). DMSO (0.15M) was then added, followed by the addition of DBU (3.0 equiv.). The reaction vessel was equipped with a magnetic stir bar, and stirred open to air at room temperature for 90 minutes. The reaction mixture was then heated to 120 ºC and stirred at this temperature for 16 hours. The reaction mixture was then cooled to room temperature and diluted into ethyl acetate. Organics were washed sequentially with sat. NH_4Cl (2x) and water (2x) then dried over anhydrous Na_2SO_4. Organics were concentrated in vacuo and purified by flash chromatography 1:20 ethyl acetate:hexanes gradient to 2:5 ethyl acetate:hexanes to furnish heteroarylbenzo[c]coumarins **7a**-**7d**.



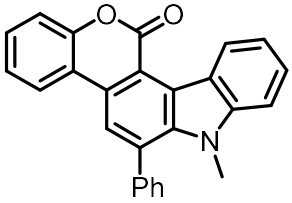
11-phenyl-4*H*-benzofuro[4,5-c]chromen-4-one (7a). Synthesized using general procedure 7. Beige solid (61 mg, 90% yield, m.p. 204–206 ºC). **TLC**: R_f 0.50 (ethyl acetate/hexanes = 1:4). **IR** (neat): 3027, 2921, 1726, 1607, 1482, 1350, 1251, 1200, 1109, 1025, 873, 684. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 8.15 (d, *J* = 9.1 Hz, 2H), 7.94 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.86 (dd, *J* = 24.4, 2.1 Hz, 2H), 7.63 – 7.50 (m, 3H), 7.50 – 7.38 (m, 2H), 7.36 (d, *J* = 7.8 Hz, 1H). **^{13}C NMR** (75 MHz, Chloroform-*d*) δ 160.3, 152.2, 151.3, 148.0, 135.0, 132.6, 132.1, 129.9, 129.2, 129.2, 129.1, 128.9, 124.5, 122.9, 118.4, 117.8, 117.1, 112.7, 108.8. **HRMS** (ESI) *m/z* calcd for $C_{21}H_{13}O_3$ ($[M + H]^+$) 313.0865; found 313.0867.



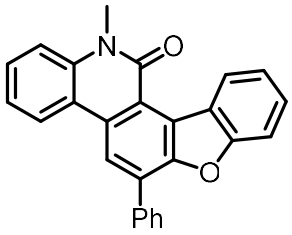
11-phenyl-4*H*-thieno[2',3':5,6]benzo[1,2-c]chromen-4-one (7b). Synthesized using general procedure 7. Beige solid (19 mg, 83% yield, m.p. 206–208 ºC). **TLC**: R_f 0.50 (ethyl acetate/hexanes = 1:4). **IR** (neat): 2923, 2359, 1702, 1583, 1498, 1332, 1280, 1199, 967, 746. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.22 (d, *J* = 8.0 Hz, 1H), 8.12 (s, 1H), 7.74 (d, *J* = 5.6 Hz, 1H), 7.68 (d, *J* = 6.8 Hz, 2H), 7.62 – 7.47 (m, 6H), 7.40 (t, *J* = 7.4 Hz, 1H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 160.6, 151.2, 144.4, 139.8, 139.1, 132.8, 131.0, 130.4, 129.2, 128.9, 128.7, 124.7, 123.3, 123.0, 118.3, 117.9. **HRMS** (ESI) *m/z* calcd for $C_{21}H_{14}O_2S$ ($[M + H]^+$) 329.0636; found 329.0643.



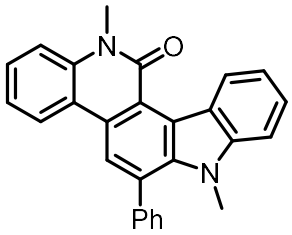
6-phenyl-12*H*-benzo[2,3]benzofuro[4,5-c]chromen-12-one (7c). Synthesized using general procedure 7. Beige solid (12 mg, 89% yield, m.p. 247–249 ºC). **TLC**: R_f 0.42 (ethyl acetate/hexanes = 1:4). **IR** (neat): 2919, 2849, 1723, 1599, 1451, 1364, 1252, 1195, 1142, 966, 874, 767. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 9.41 (d, *J* = 9.3 Hz, 1H), 8.30 (s, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.97 (d, *J* = 6.8 Hz, 2H), 7.67 – 7.51 (m, 5H), 7.51 – 7.45 (m, 2H), 7.45 – 7.38 (m, 1H), 7.37 – 7.29 (m, 1H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 160.2, 157.5, 153.6, 151.1, 135.2, 132.8, 132.1, 130.0, 129.4, 129.2, 129.0, 128.3, 125.7, 124.5, 123.4, 123.1, 123.0, 120.4, 118.3, 117.6, 115.2, 111.4. **HRMS** (ESI) *m/z* calcd for $C_{25}H_{15}O_3$ ([M + H]$^+$) 363.1021; found 363.1029.



7-methyl-6-phenylchromeno[4,3-c]carbazol-12(7*H*)-one (7d). Synthesized using general procedure 7. Yellow solid (19 mg, 71% yield, m.p. 251–253 ºC). **TLC**: R_f 0.40 (ethyl acetate/hexanes = 1:4). **IR** (neat): 2919, 2850, 1712, 1594, 1400, 1321, 1143, 1005, 873, 738. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 9.66 (d, *J* = 8.7 Hz, 1H), 8.09 – 8.01 (m, 2H), 7.56 (s, 6H), 7.41 – 7.32 (m, 4H), 7.27 (d, *J* = 4.6 Hz, 1H), 3.40 (s, 3H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 160.8, 150.8, 143.4, 139.5, 139.1, 133.2, 129.5, 129.0, 128.4, 128.4, 128.2, 127.4, 124.1, 123.4, 122.7, 121.9, 120.1, 118.9, 117.2, 115.1, 108.7, 33.4. **HRMS** (ESI) *m/z* calcd for $C_{26}H_{18}NO_2$ ([M + H]$^+$) 376.1338; found 376.1340.

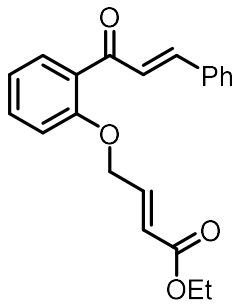


13-methyl-6-phenylbenzofuro[3,2-i]phenanthridin-12(13H)-one (7e). Synthesized using general procedure 7. Beige solid (58 mg, 86% yield, m.p. 234–236 ºC). **TLC**: R_f 0.38 (ethyl acetate/hexanes = 1:1). **IR** (neat): 3032, 2921, 1915, 1642, 1604, 1486, 1328, 1219, 1047, 866, 743. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 9.60 (d, *J* = 8.1 Hz, 1H), 8.38 (s, 1H), 8.27 (d, *J* = 9.4 Hz, 1H), 7.94 (d, *J* = 6.9 Hz, 2H), 7.60 (t, *J* = 7.2 Hz, 3H), 7.54 (d, *J* = 7.0 Hz, 1H), 7.46 (q, *J* = 8.3 Hz, 3H), 7.36 (d, *J* = 9.3 Hz, 1H), 7.26 (t, 1H), 3.85 (s, 3H). **^{13}C NMR** (75 MHz, Chloroform-*d*) δ 161.3, 157.2, 153.4, 137.6, 135.8, 130.7, 130.5, 129.3, 129.2, 129.0, 128.8, 128.7, 128.0, 124.3, 124.1, 123.4, 123.0, 122.3, 120.86, 120.7, 119.5, 114.8, 111.1, 30.0. **HRMS** (ESI) *m/z* calcd for $C_{25}H_{18}NO_2$ ([M + H]$^+$) 376.1338; found 376.1338.

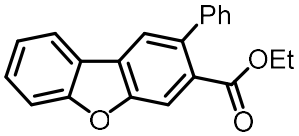


7,13-dimethyl-6-phenyl-7,13-dihydro-12H-indolo[3,2-i]phenanthridin-12-one (7f). Synthesized using general procedure 7. Yellow oil (48 mg, 63% yield). **TLC**: R_f 0.46 (ethyl acetate/hexanes = 1:1). **IR** (neat): 3050, 2925, 2241, 1629, 1598, 1448, 1307, 1246, 1078, 907, 729. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 8.13 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.59 (ddd, *J* = 8.5, 7.1, 1.5 Hz, 1H), 7.45 (dd, *J* = 8.1, 1.1 Hz, 2H), 7.37 – 7.30 (m, 1H), 7.30 – 7.25 (m, 4H), 7.24 (d, *J* = 8.7 Hz, 1H), 7.22 – 7.17 (m, 1H), 7.10 – 7.03 (m, 2H), 6.86 (d, *J* = 16.8 Hz, 1H), 3.84 (s, 3H), 3.79 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 161.7, 142.7, 139.6, 136.9, 136.7, 136.2, 131.3, 129.7, 128.7, 128.1, 127.6, 127.4, 126.6, 125.0, 124.6, 121.8, 121.5, 121.3, 120.4, 119.6, 114.4, 109.5, 109.3, 33.0, 30.3. **HRMS** (ESI) *m/z* calcd for $C_{27}H_{21}N_2O$ ($[M + H]^+$) 389.1654; found 389.1654.

J. Synthesis of Ethyl 2-phenyldibenzo[b,d]furan-3-carboxylate (8)

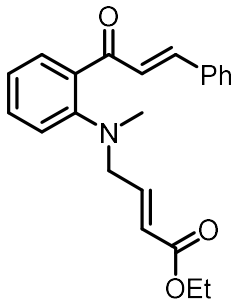


ethyl (*E*)-4-(2-cinnamoylphenoxy)but-2-enoate (8). To a suspension of anhydrous potassium carbonate (6.0 mmol, 829 mg, 3.0 equiv.) in DMSO (2 mL) was added hydroxychalcone (448 mg, 2.0 mmol, 1.0 equiv.). Ethyl 4-bromocrotonate (0.736 mL, 4.0 mmol, 2.0 equiv.) was then added dropwise via syringe. The mixture was then stirred at room temperature for 6 hours. The inorganic solids were removed via filtration and organics were quenched via addition of cold water. The aqueous solution was extracted with dichloromethane (3x 20 mL) and the organics were washed with water (3x 15 mL). Organics were dried over dried over anhydrous Na_2SO_4, concentrated, and purified by flash chromatography to furnish Ethyl (E)-4-(2-cinnamoylphenoxy)but-2-enoate **8**. Yellow oil (362 mg, 54% yield). **TLC**: R_f = 0.21 (ethyl acetate/hexanes = 1:4). **IR** (neat): 2980, 1715, 1660, 1599, 1448, 1303, 1271, 1177, 1021, 970, 753. **^{1}H NMR** (300 MHz) δ 7.67–7.59 (m, 2H), 7.58–7.51 (m, 2H), 7.47–7.38 (m, 2H), 7.38–7.30 (m, 3H), 7.09–6.97 (m, 2H), 6.92 (dd, *J* = 8.4, 0.9 Hz, 1H), 6.15 (dt, *J* = 15.8, 2.1 Hz, 1H), 4.75 (dd, *J* = 3.9, 2.1 Hz, 2H), 4.05 (q, *J* = 7.1 Hz, 2H), 1.13 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (75 MHz) δ 192.6, 165.9, 156.4, 143.4, 141.4, 134.8, 132.9, 130.6, 130.3, 129.7, 128.8, 128.5, 126.9, 122.2, 121.5, 112.7, 67.1, 60.4, 14.1. **HRMS** (ESI) *m/z* calcd for $C_{21}H_{21}O_4$ ($[M + H]^+$) 337.1440; found 337.1431.

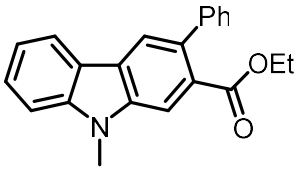


ethyl 2-phenyldibenzo[b,d]furan-3-carboxylate (10). To a 15 mL round bottom flask was measured ethyl (*E*)-4-(2-cinnamoylphenoxy)but-2-enoate (**8**) (1.0 equiv.). DMSO (0.15M) was then added, followed by the addition of DBU (3.0 equiv.). The reaction vessel was equipped with a magnetic stir bar, and stirred open to air at room temperature for 90 minutes. The reaction mixture was then heated to 120 ºC and stirred at this temperature for 16 hours. The reaction mixture was then cooled to room temperature and diluted into ethyl acetate. Organics were washed sequentially with sat. NH_4Cl (2x) and water (2x) then dried over anhydrous Na_2SO_4. Organics were concentrated in vacuo and purified by flash chromatography to furnish dibenzofuran **10**. Yellow oil (26 mg, 55% yield). **TLC**: R_f 0.57 (ethyl acetate/hexanes = 1:4). **IR** (neat): 3057, 2979, 2358, 1707, 1458, 1217, 1106, 1017,786. **^{1}H NMR** (600 MHz) δ 8.07 (d, *J* = 2.2 Hz, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 2.2 Hz, 1H), 7.62 (d, *J* = 8.3 Hz, 1H), 7.53 (t, *J* = 7.9 Hz, 1H), 7.45–7.33 (m, 6H), 4.13 (q, *J* = 7.0 Hz, 2H), 1.02 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (151 MHz) δ 168.3, 157.5, 154.7, 141.9, 137.8, 130.0, 128.7, 128.4, 128.0, 127.0, 126.8, 126.5, 123.4, 123.1, 122.6, 121.2, 118.7, 117.5, 113.2, 112.0, 61.12 13.6. **HRMS** (ESI) *m/z* calcd for $C_{21}H_{16}O_3Na$ ($[M + Na]^+$) 339.0997; found 339.0986.

K. Synthesis of Ethyl 9-methyl-3-phenyl-9H-carbazole-2-carboxylate (11)

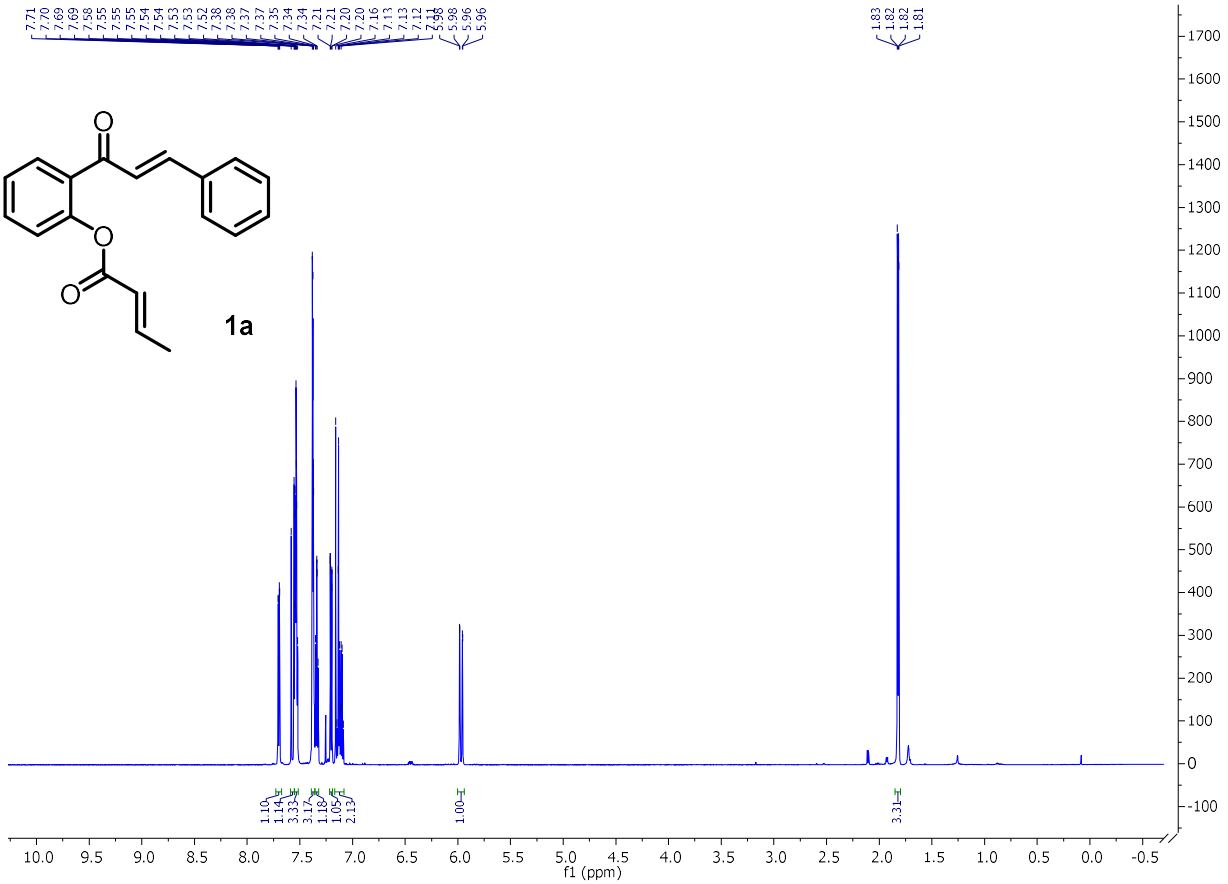


ethyl (*E*)-4-((2-cinnamoylphenyl)(methyl)amino)but-2-enoate (9). To a solution of N-methylaminochalcone (356 mg, 1.50 mmol, 1.0 equiv.) and ethyl 4-bromocrotonate (0.310 mL, 1.80 mmol, 1.2 equiv.) in MeCN (3 mL) was added anhydrous potassium carbonate (207 mg, 1.50 mmol, 1.0 equiv.). The reaction vessel was sealed and heated to reflux with stirring for 16 hours. The reaction mixture was cooled to room temperature and inorganic salts were removed via filtration. Organics were then concentrated and purified by flash chromatography to furnish Ethyl (E)-4-((2-cinnamoylphenyl)(methyl)amino)but-2-enoate **9**. Yellow oil (468 mg, 89% yield). **TLC**: R_f 0.32 (ethyl acetate/hexanes = 1:4). **IR** (neat): 2980, 1715, 1658, 1597, 1485, 1448, 1367, 1265, 1173, 1030, 974, 704. **^{1}H NMR** (400 MHz) δ 7.65 (d, *J* = 16.0 Hz, 1H), 7.59–7.54 (m, 2H), 7.50 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.44–7.34 (m, 3H), 7.30 (d, *J* = 16.0 Hz, 1H), 7.03 (qd, *J* = 7.8, 7.4, 1.0 Hz, 2H), 6.87 (dt, *J* = 15.7, 5.7 Hz, 1H), 5.93 (dt, *J* = 15.7, 1.7 Hz, 1H), 4.09 (q, *J* = 7.1 Hz, 2H), 3.80 (dd, *J* = 5.7, 1.6 Hz, 2H), 2.79 (s, 3H), 1.18 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz) δ 195.2, 165.9, 150.8, 143.8, 143.2, 134.9, 132.8, 131.8, 130.3 (d, *J* = 2.3 Hz), 128.9, 128.4, 126.3, 123.5, 121.4, 118.5, 60.4, 57.9, 41.3, 14.1. **HRMS** (ESI) *m/z* calcd for $C_{22}H_{24}NO_3$ ($[M + H]^+$) 350.1756; found 350.1758.



ethyl 9-methyl-3-phenyl-9H-carbazole-2-carboxylate (11). To a 15 mL round bottom flask was measured ethyl (*E*)-4-((2-cinnamoylphenyl)(methyl)amino)but-2-enoate (**9**) (1.0 equiv.). DMSO (0.15M) was then added, followed by the addition of DBU (3.0 equiv.). The reaction vessel was equipped with a magnetic stir bar, and stirred open to air at room temperature for 90 minutes. The reaction mixture was then heated to 120 °C and stirred at this temperature for 16 hours. The reaction mixture was then cooled to room temperature and diluted into ethyl acetate. Organics were washed sequentially with sat. NH_4Cl (2x) and water (2x) then dried over anhydrous Na_2SO_4. Organics were concentrated in vacuo and purified by flash chromatography to furnish carbazole **9**. Orange oil (64 mg, 69% yield). **TLC**: R_f 0.36 (ethyl acetate/hexanes = 1:4). **IR** (neat): 2978, 1701, 1493, 1460, 1368, 1234, 1095, 1018, 908, 785, 699. **^{1}H NMR** (500 MHz) δ 8.11 (d, *J* = 7.8 Hz, 1H), 8.07 (d, *J* = 1.5 Hz, 1H), 7.95 (d, *J* = 1.5 Hz, 1H), 7.56 (t, *J* = 7.9 Hz, 1H), 7.46 (d, *J* = 8.3 Hz, 1H), 7.45–7.34 (m, 4H), 7.30–7.26 (m, 2H), 4.14 (qd, *J* = 7.1, 1.4 Hz, 2H), 3.94 (d, *J* = 1.6 Hz, 3H), 1.01 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz) δ 169.6, 142.8, 142.4, 139.5, 133.6, 128.9, 128.5, 127.9, 126.9, 126.5, 125.o, 122.2 (d, *J* = 12.1 Hz), 121.0, 119.4, 110.4, 108.8, 61.0, 29.3, 13.6. **LRMS*** (ESI) *m/z* calcd for $C_{22}H_{22}NO_3$ ($[M + H + H_2O]^+$) 348.2; found 348.5.

*We were unable to obtain an accurate HRMS in ESI for this compound.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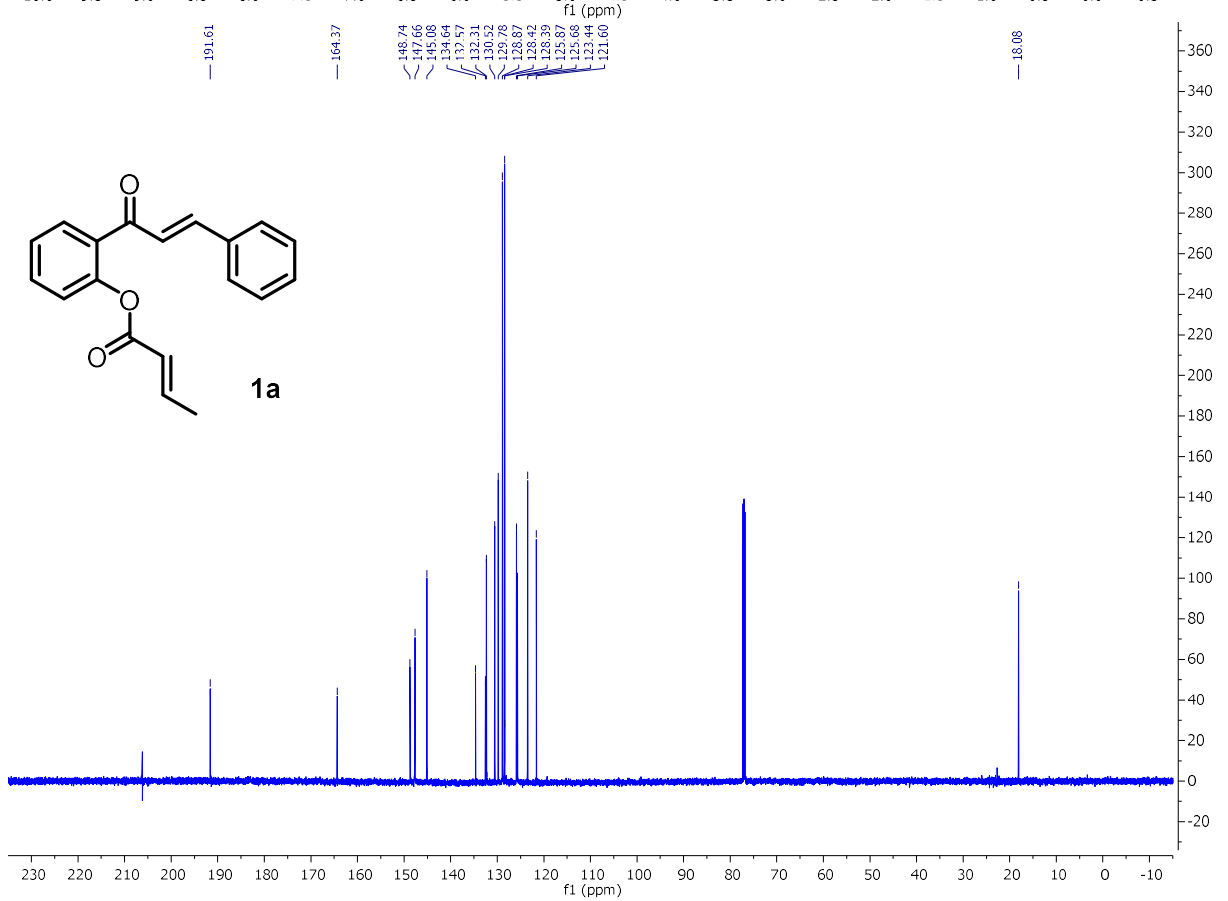
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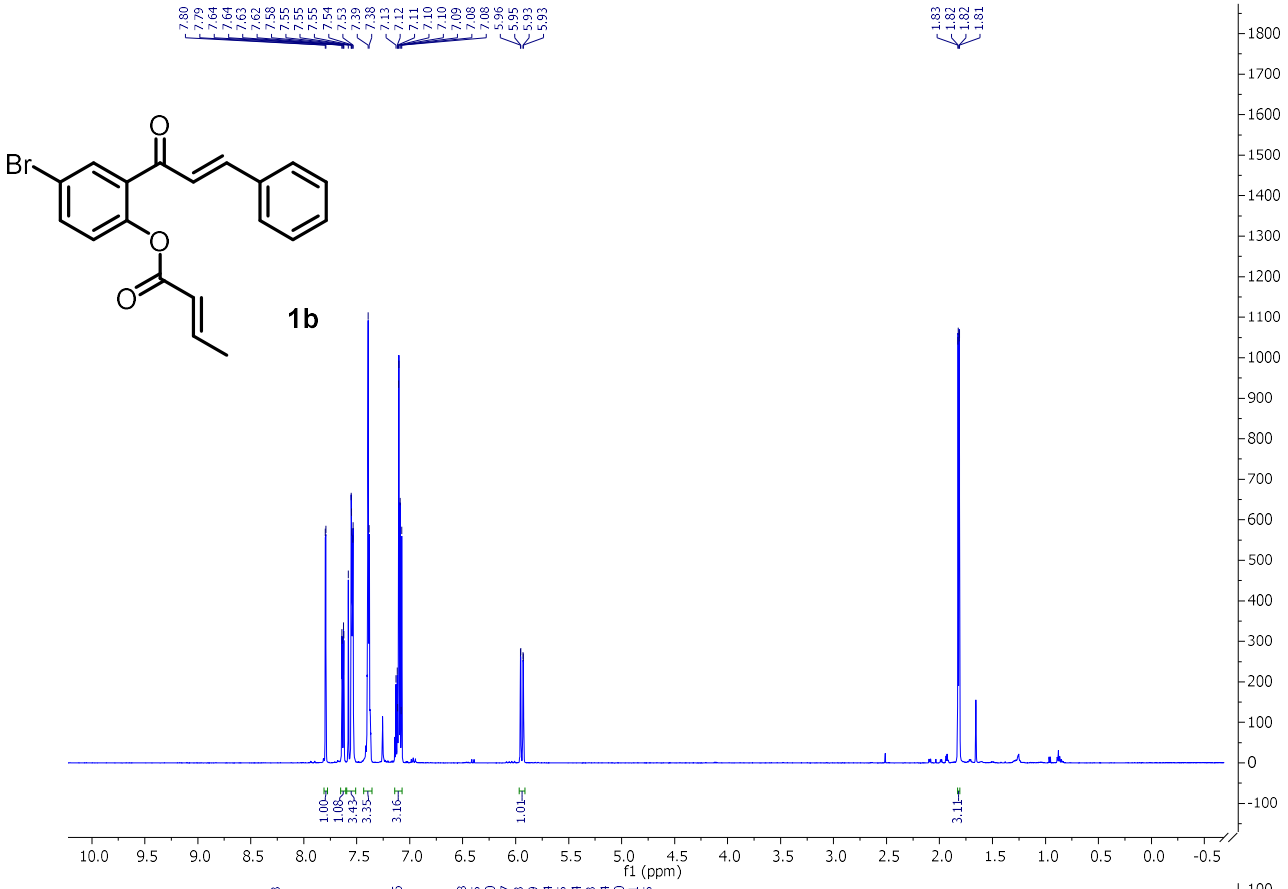
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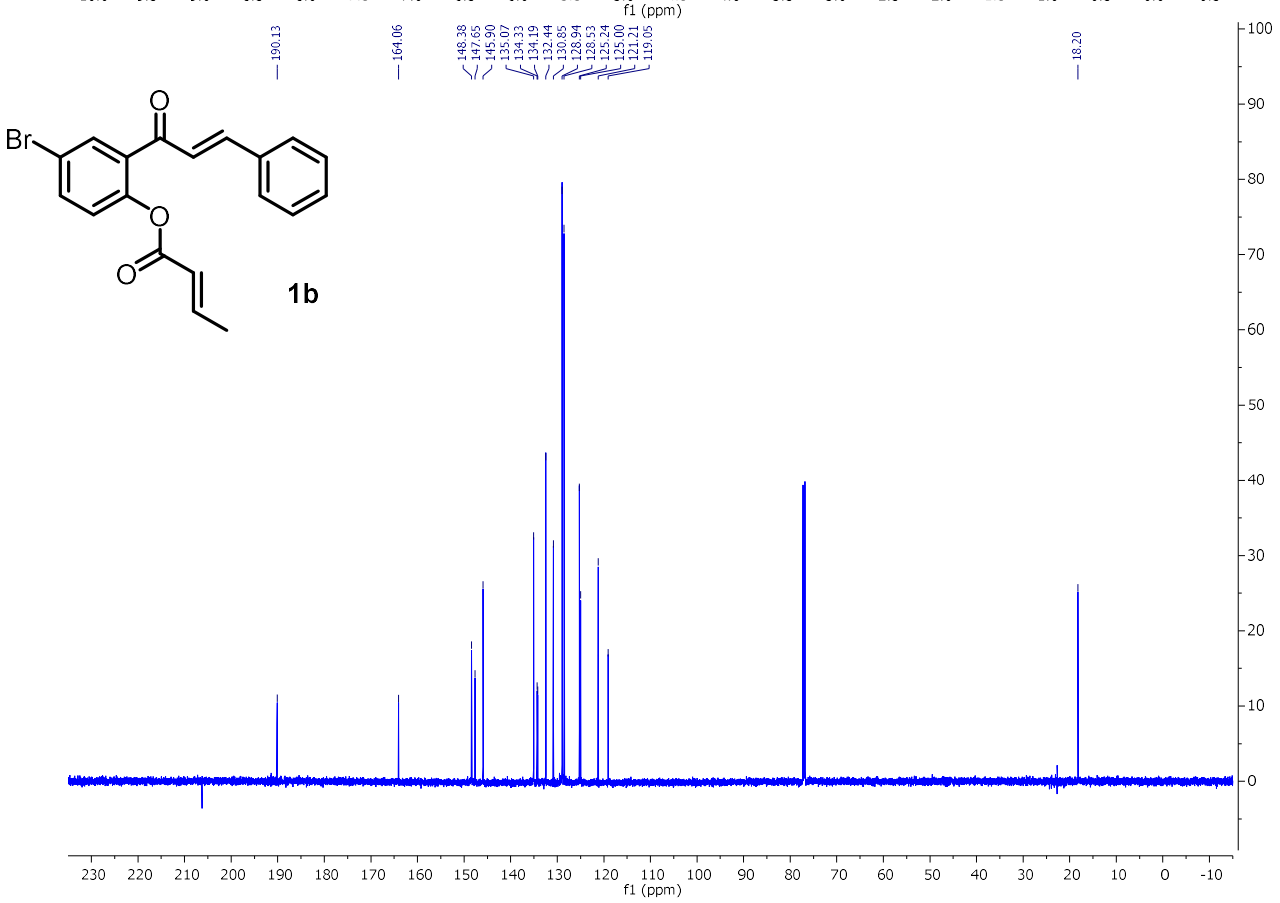
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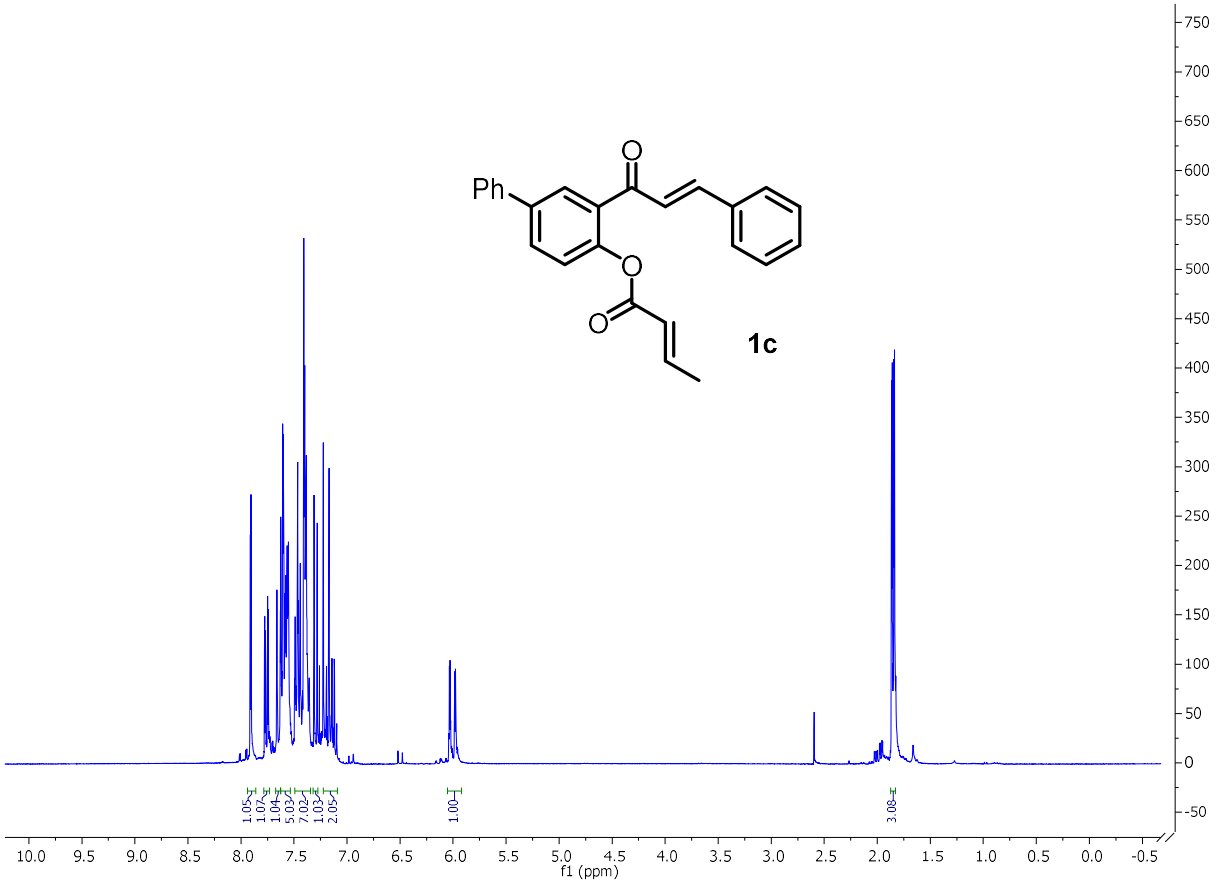
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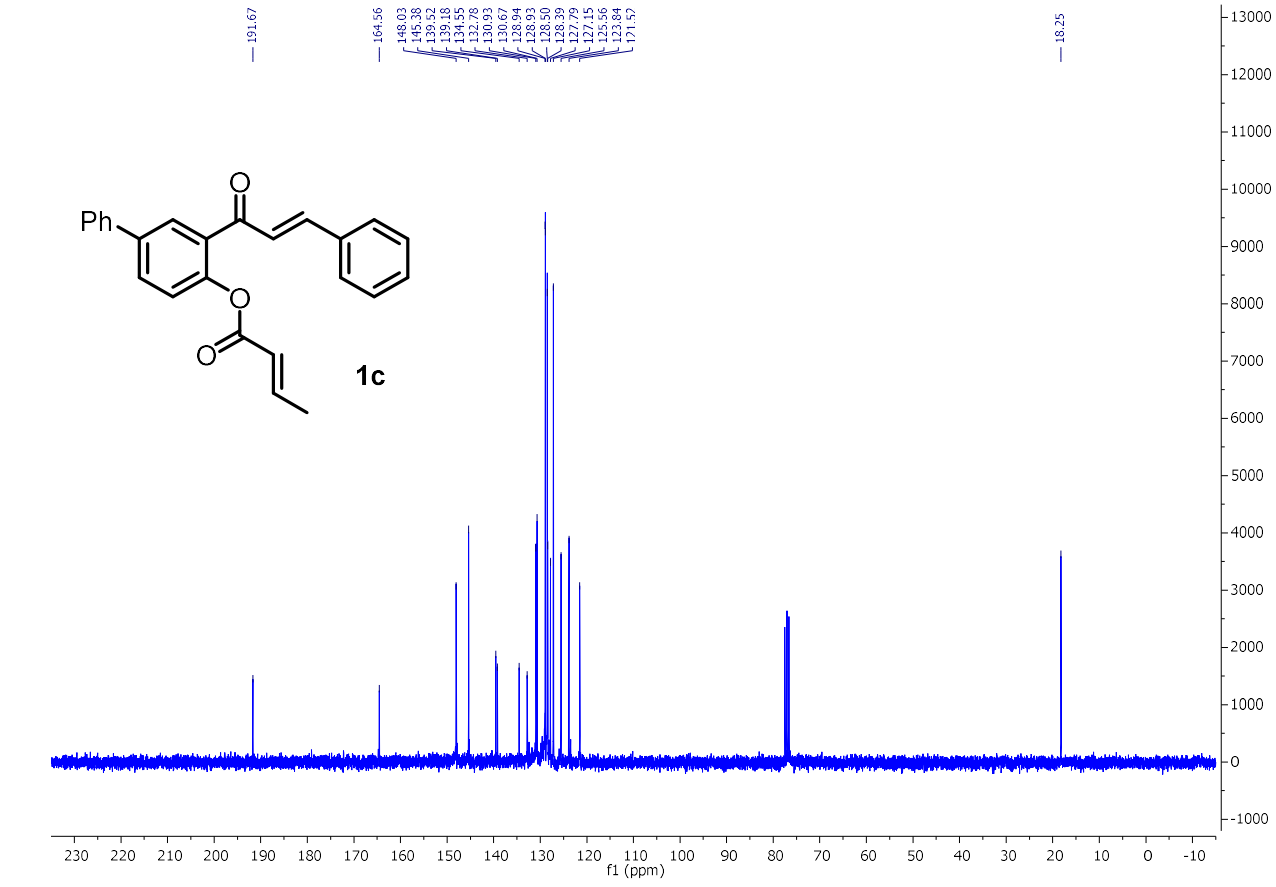
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Ph
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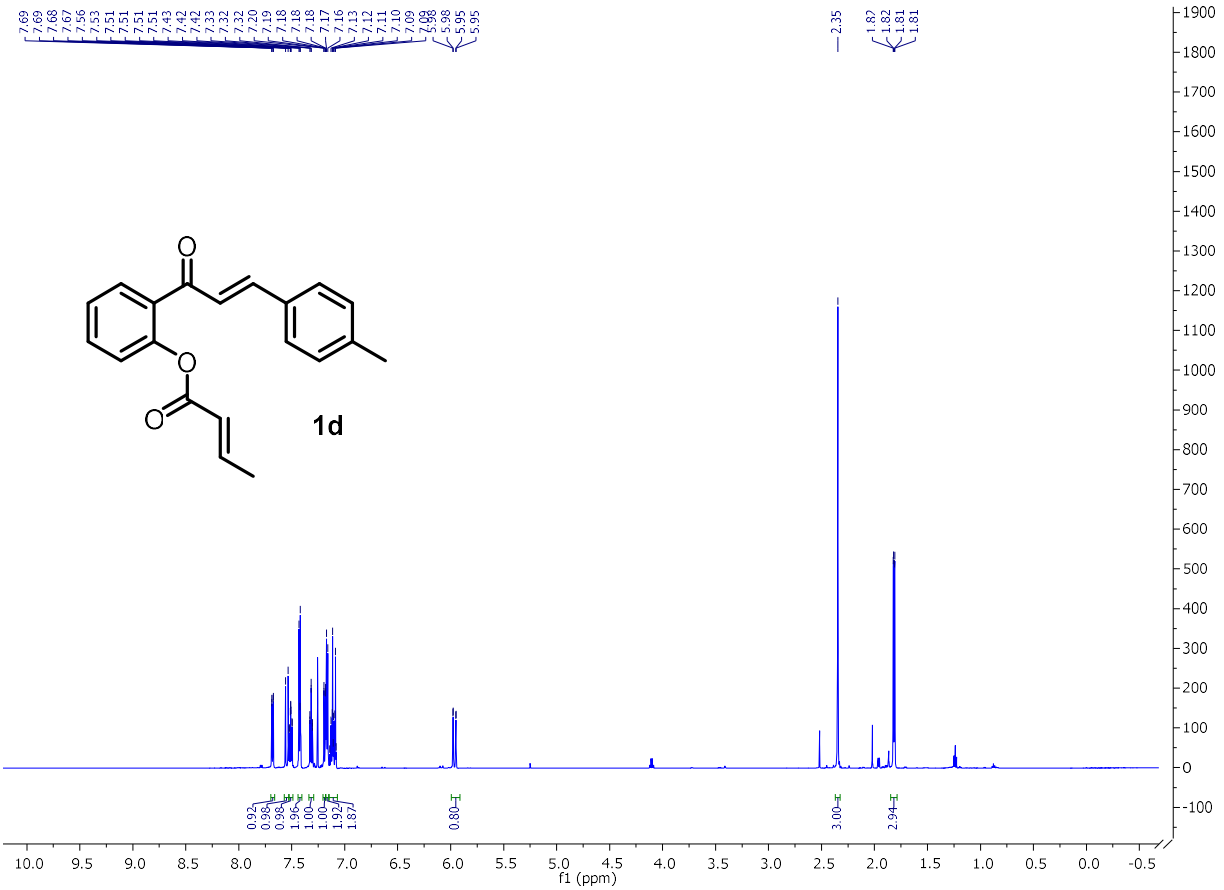
1c
f1 (ppm)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7.42
7.33
7.32
7.32
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7.19
7.18
7.18
7.18
7.17
7.16
7.13
7.12
7.11
7.10
7.09
7.09
5.98
5.98
5.95
5.95
2.35
1.82
1.82
1.81
1.81
1d
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1.00
1.92
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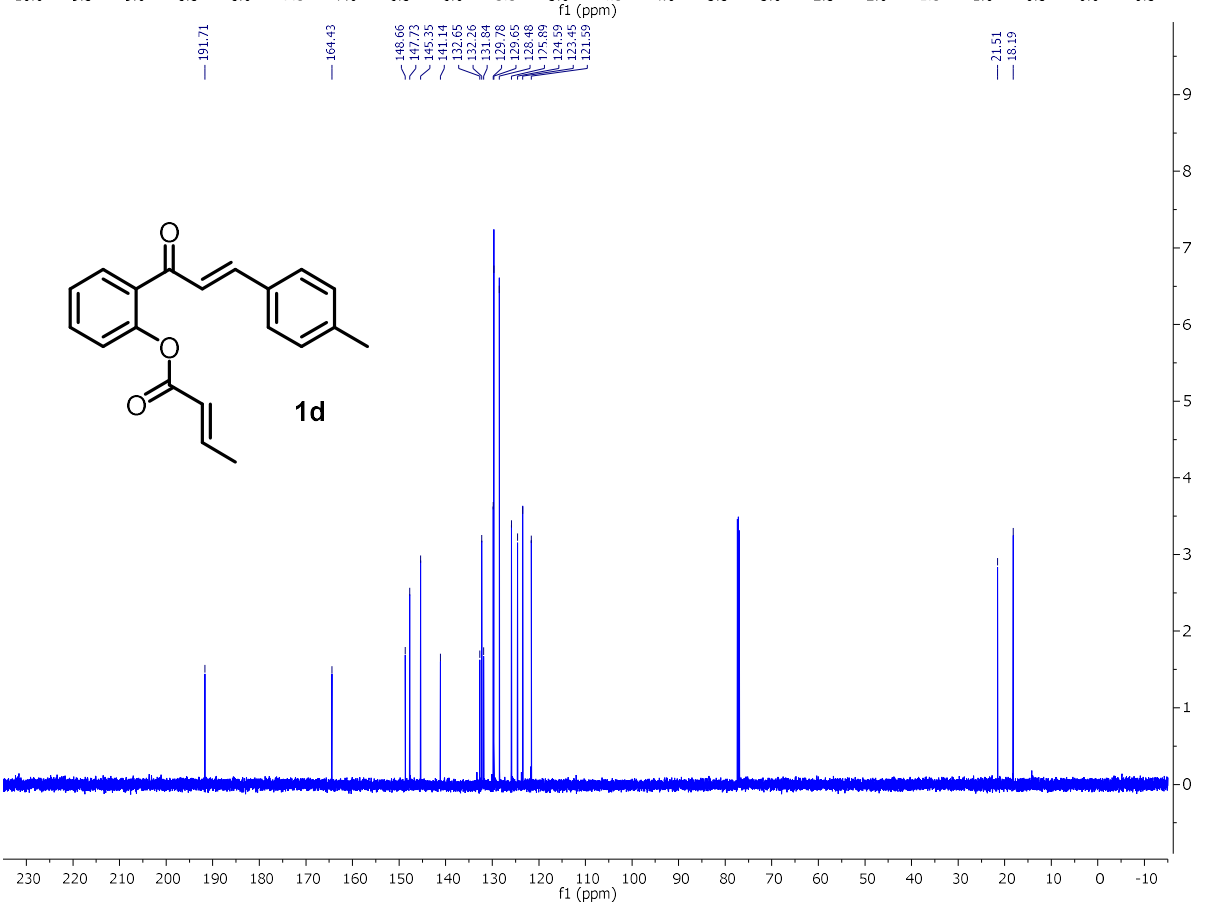
0.80
3.00
2.94
f1 (ppm)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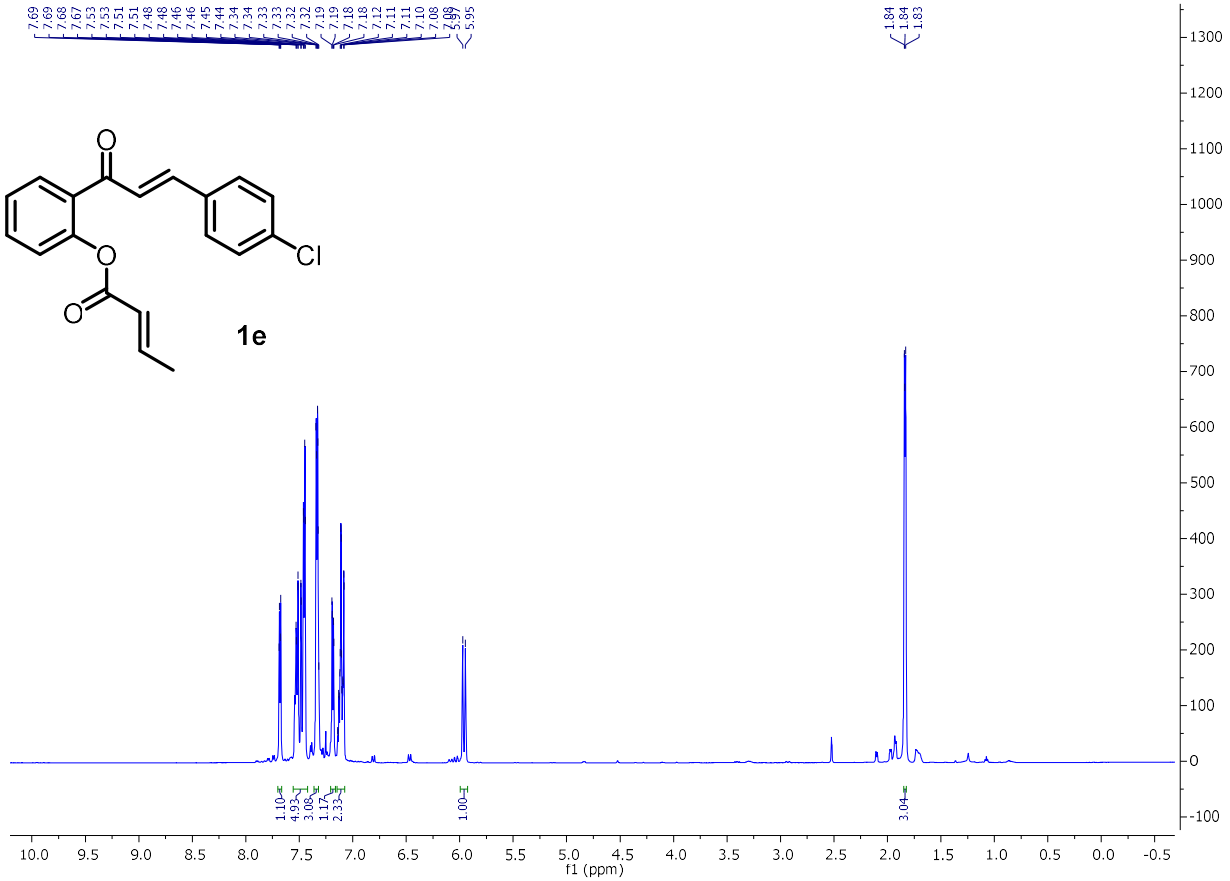
121.59
21.51
18.19
1d
f1 (ppm)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7.34
7.33
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7.32
7.32
7.19
7.19
7.18
7.18
7.12
7.11
7.11
7.10
7.08
5.99
5.95
1.84
1.84
1.83
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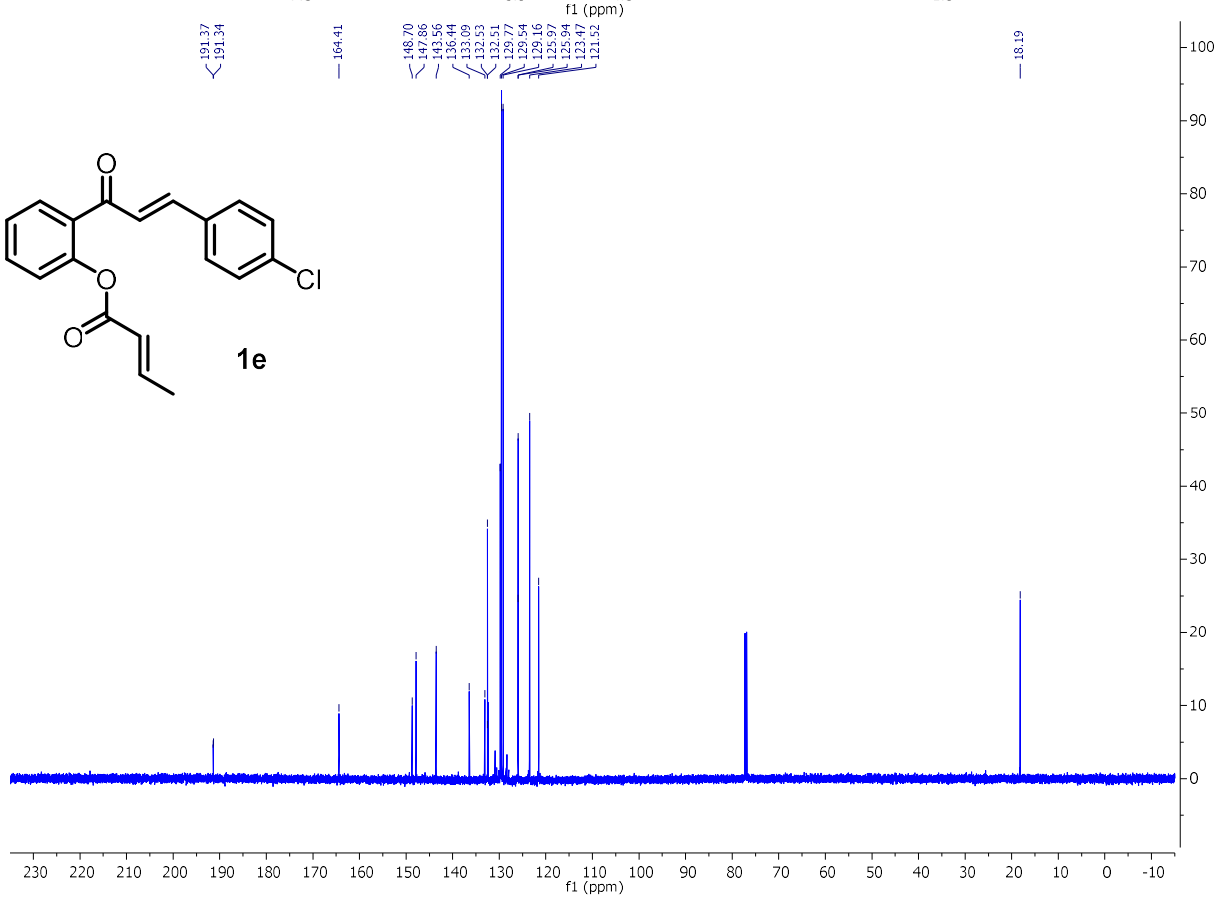
1.10
4.93
3.08
1.17
2.33
1.00
3.04
f1 (ppm)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125.94
123.47
121.52
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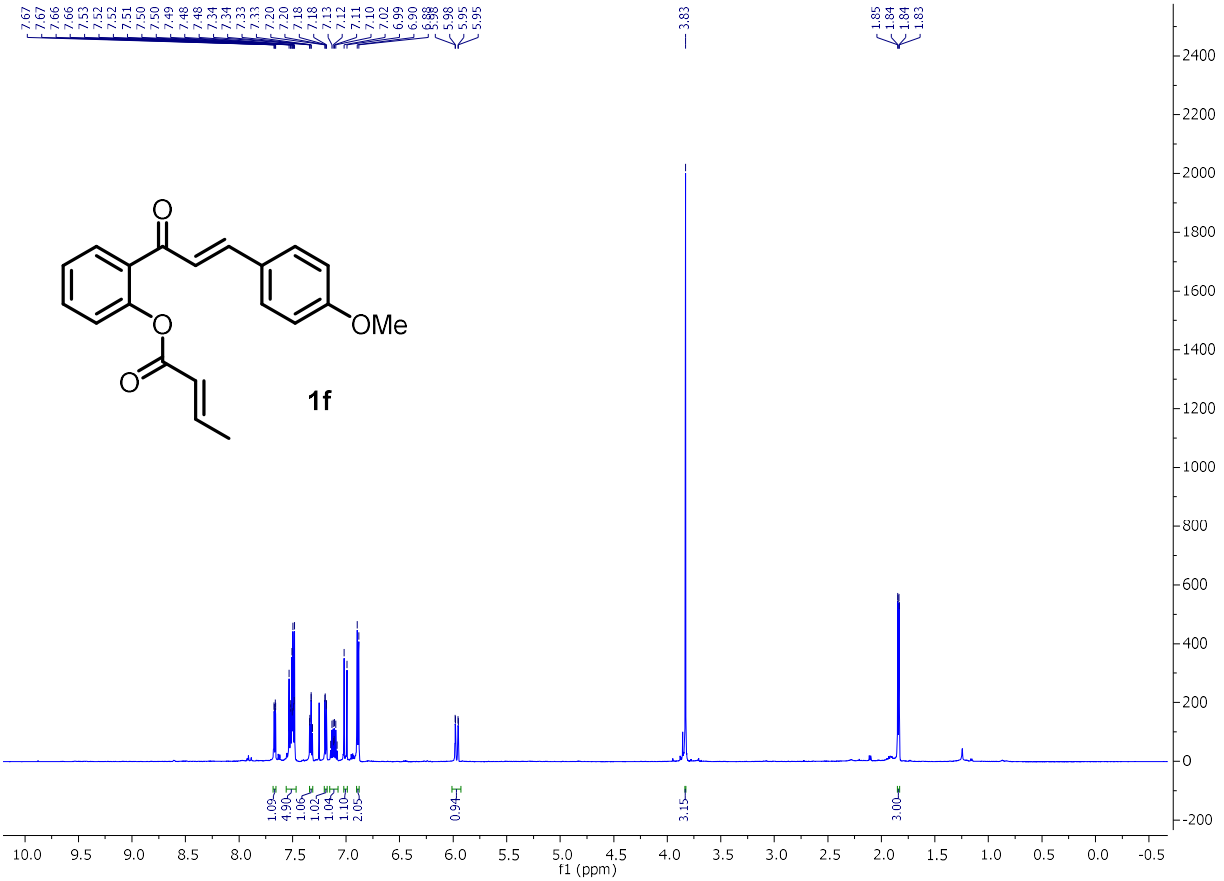
O
O
O
Cl
1e
f1 (ppm)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7.34
7.34
7.33
7.33
7.20
7.20
7.18
7.18
7.13
7.12
7.11
7.10
7.02
6.99
6.90
6.88
5.98
5.95
5.95
3.83
1.85
1.84
1.84
1.83
OMe
1f
1.09
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1.06
1.02
1.04
1.10
2.05
0.94
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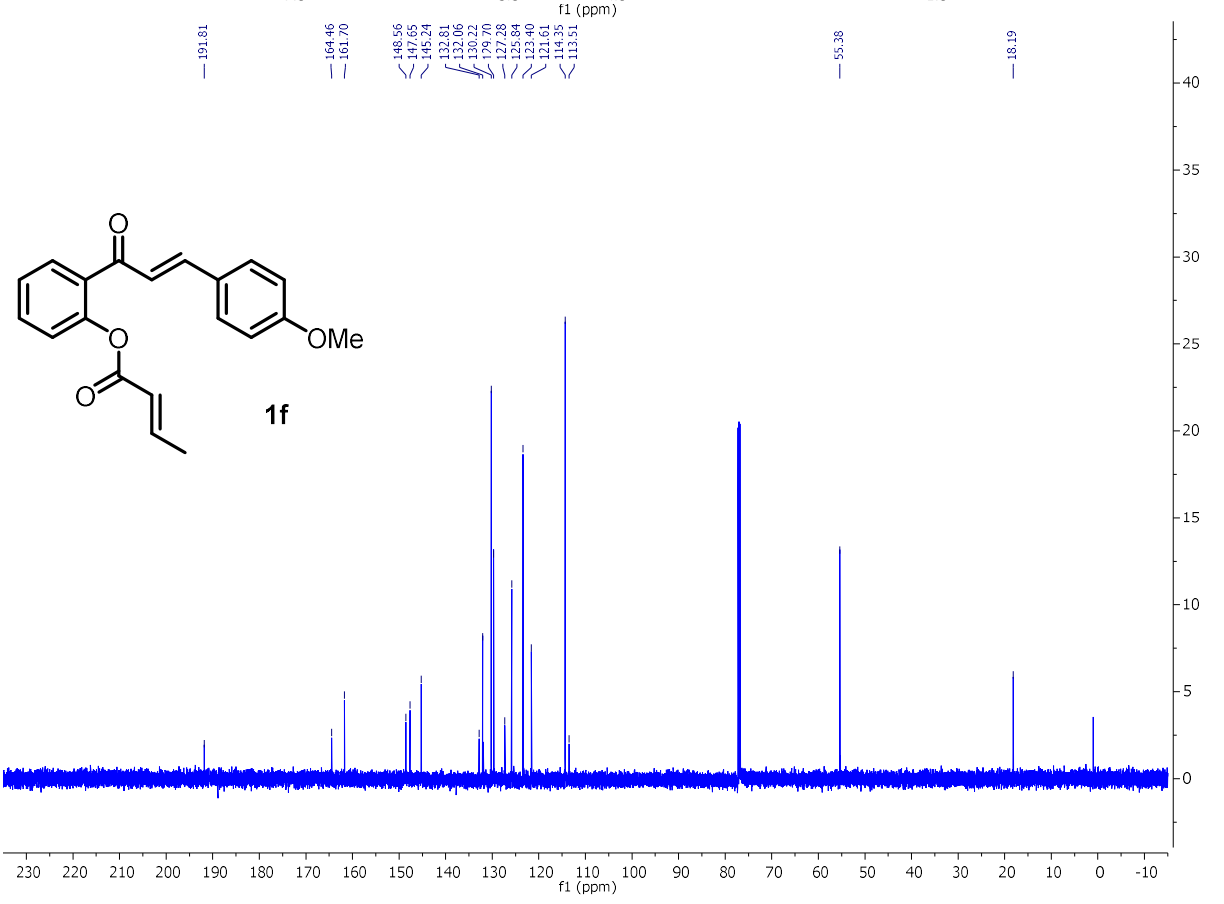
3.00
f1 (ppm)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123.40
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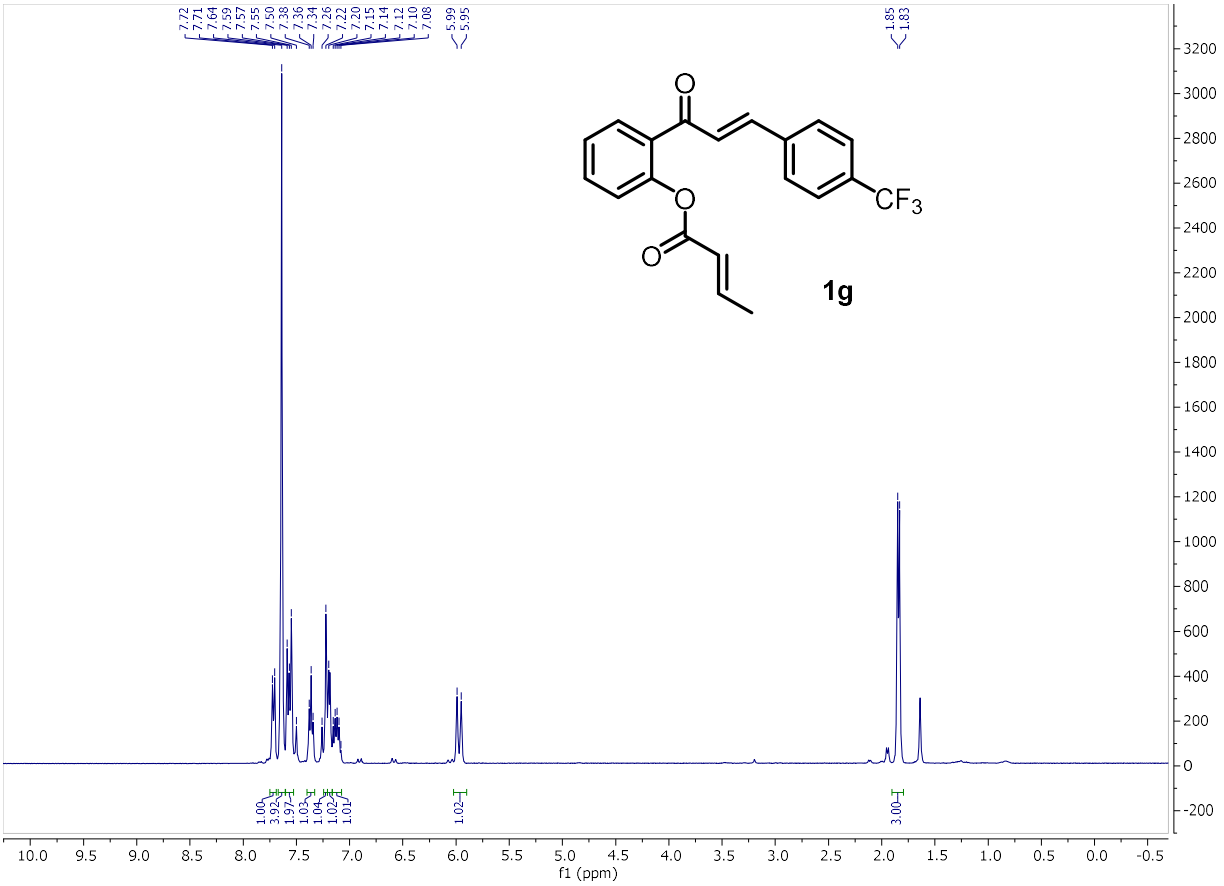
114.35
113.51
55.38
18.19
OMe
1f
f1 (ppm)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7.14
7.12
7.10
7.08
5.99
5.95
1.85
1.83
1.00
3.92
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1.02
1.01
1.02
3.00
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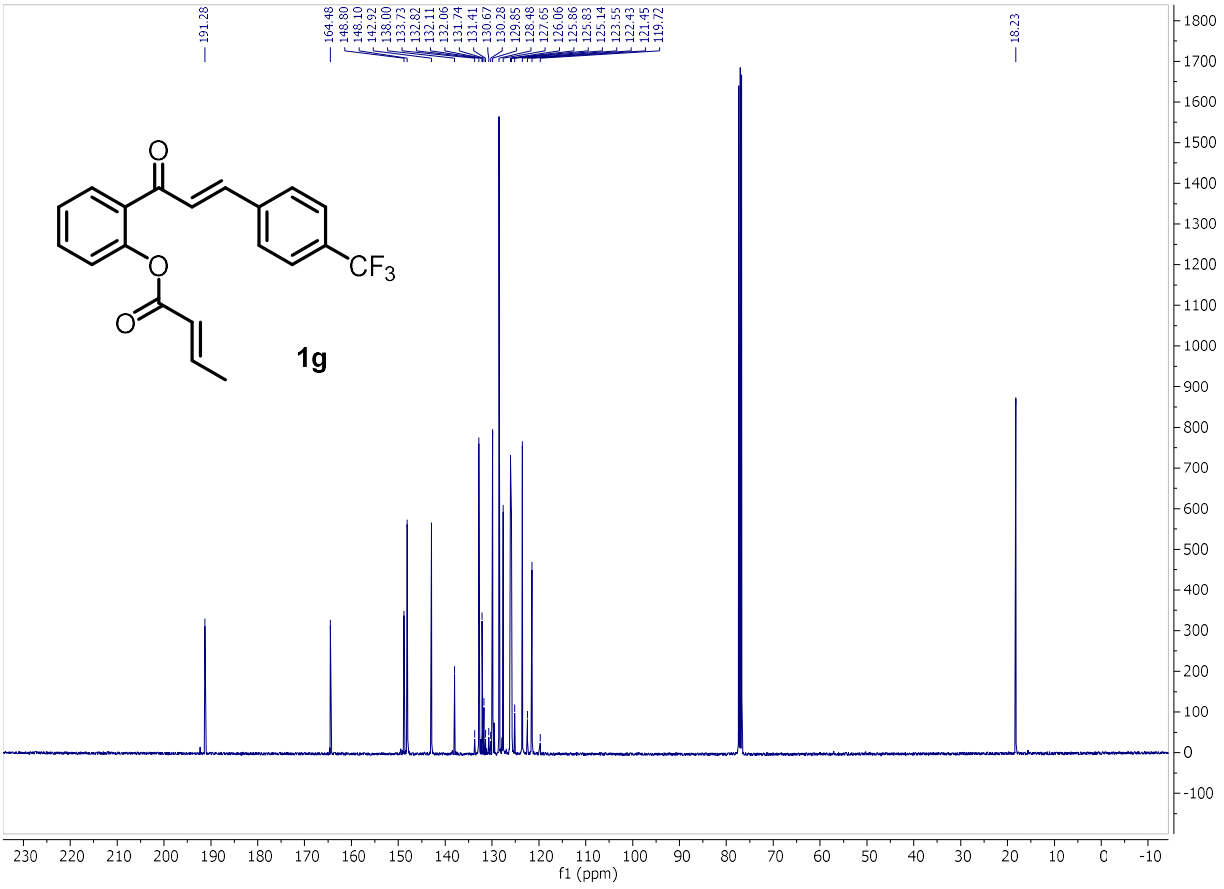
O
O
CF3
1g
f1 (ppm)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129.85
128.48
127.65
126.06
125.86
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122.43
121.45
119.72
18.23
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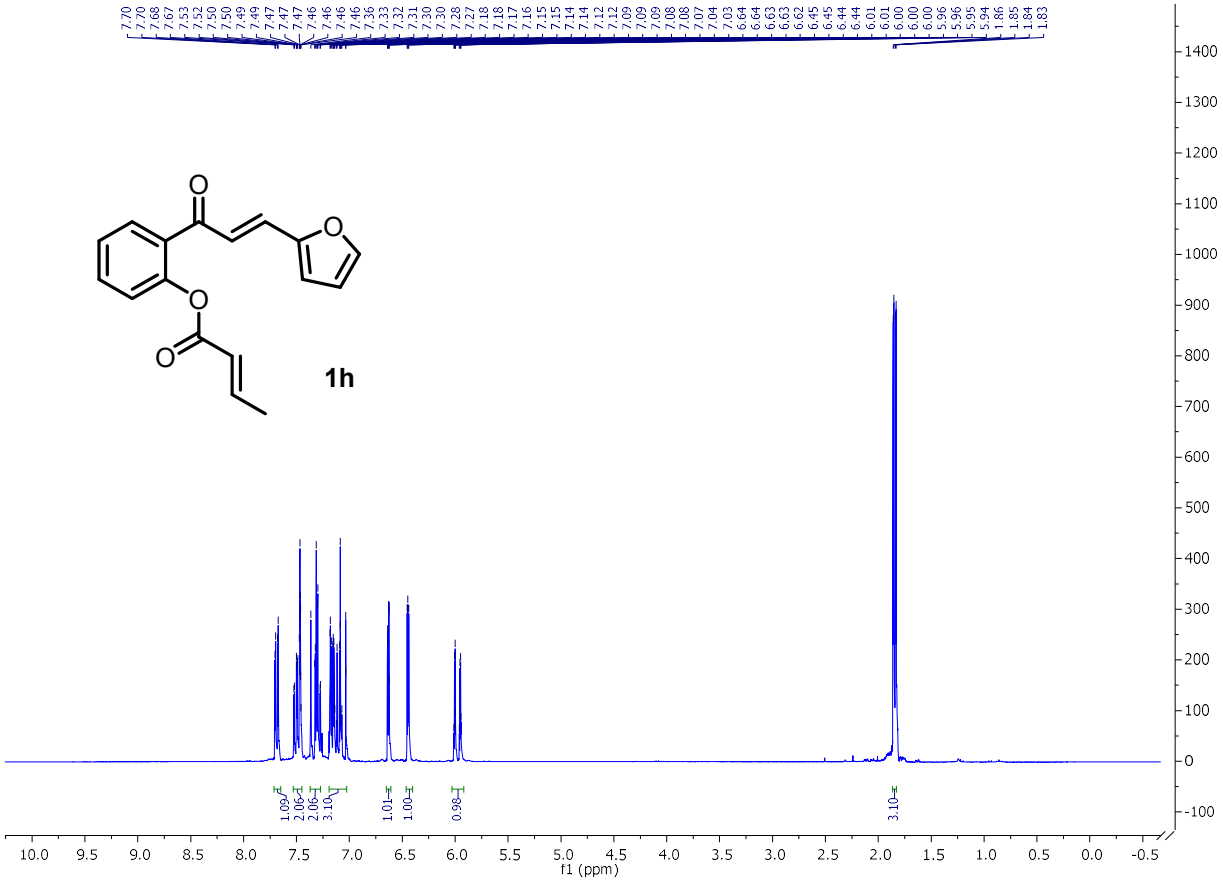
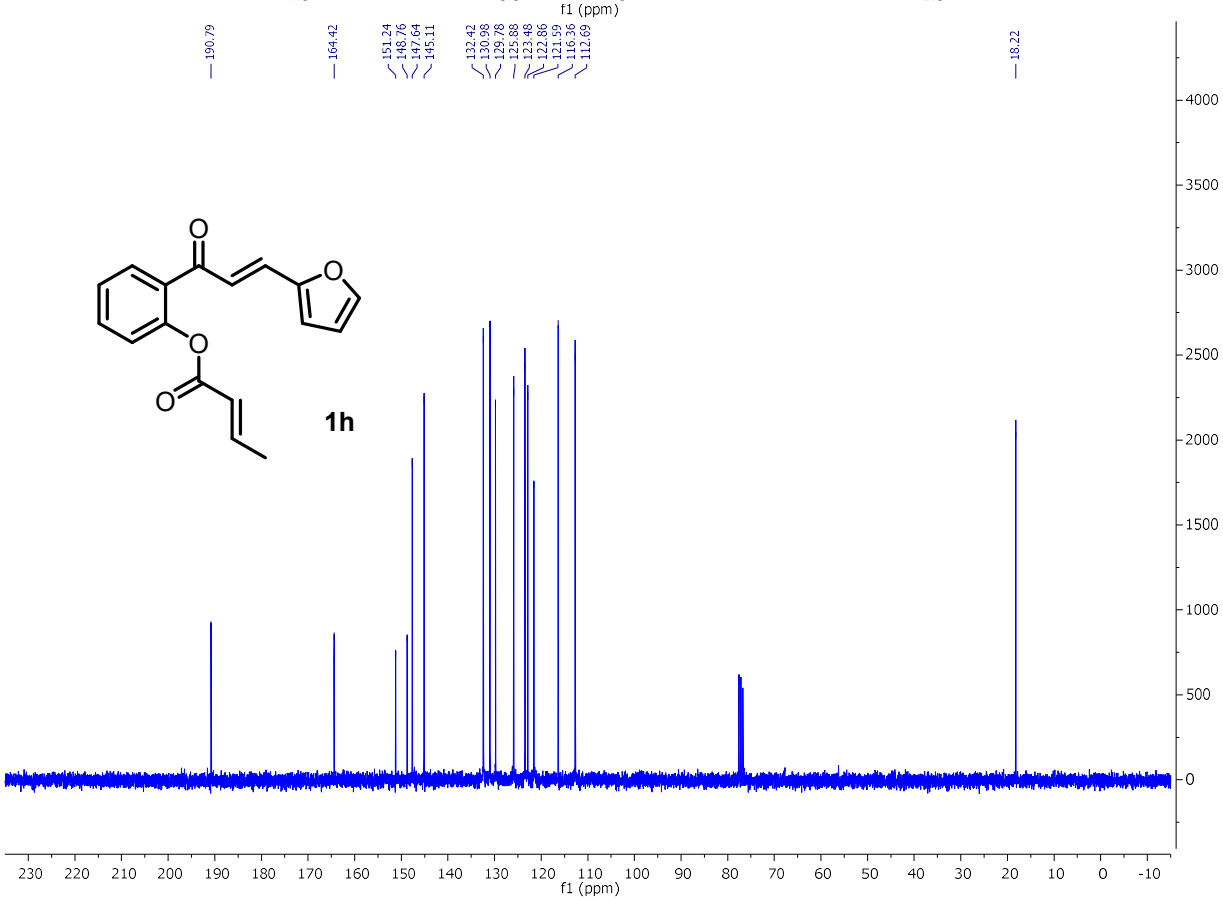
O
O
CF3
1g
f1 (ppm)


1h
f1 (ppm)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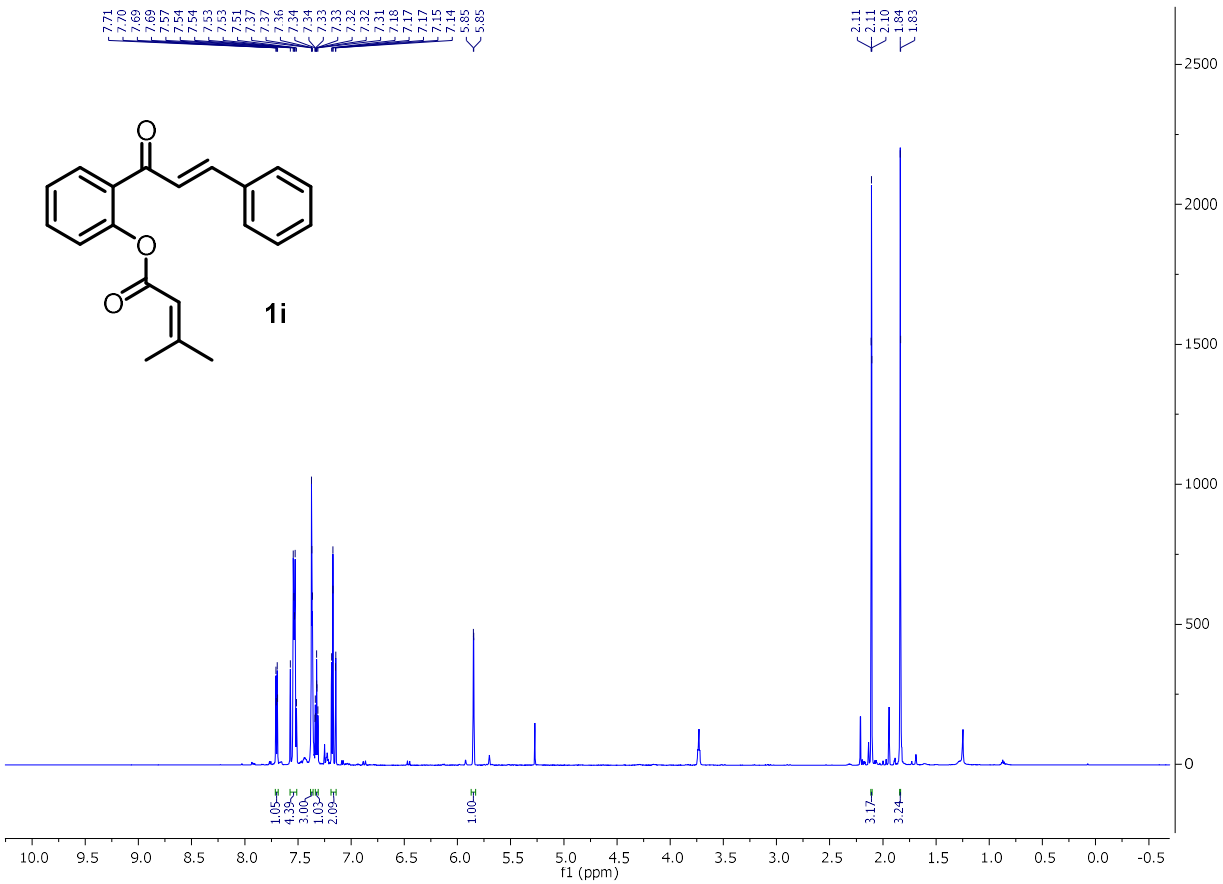
116.36
112.69
18.22
1h
f1 (ppm)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7.31
7.18
7.17
7.17
7.15
7.14
5.85
5.85
2.11
2.11
2.10
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2.09
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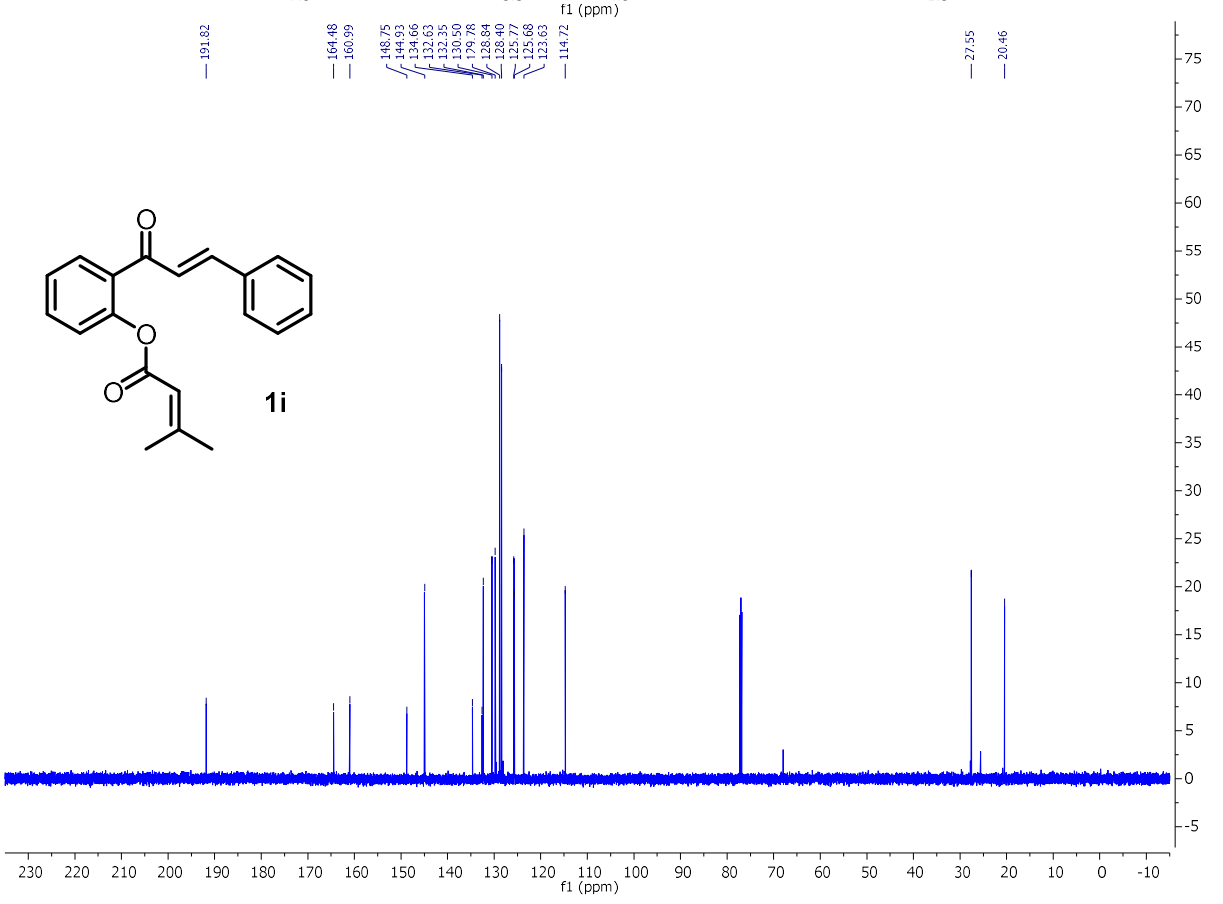
3.17
3.24
1i
f1 (ppm)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114.72
27.55
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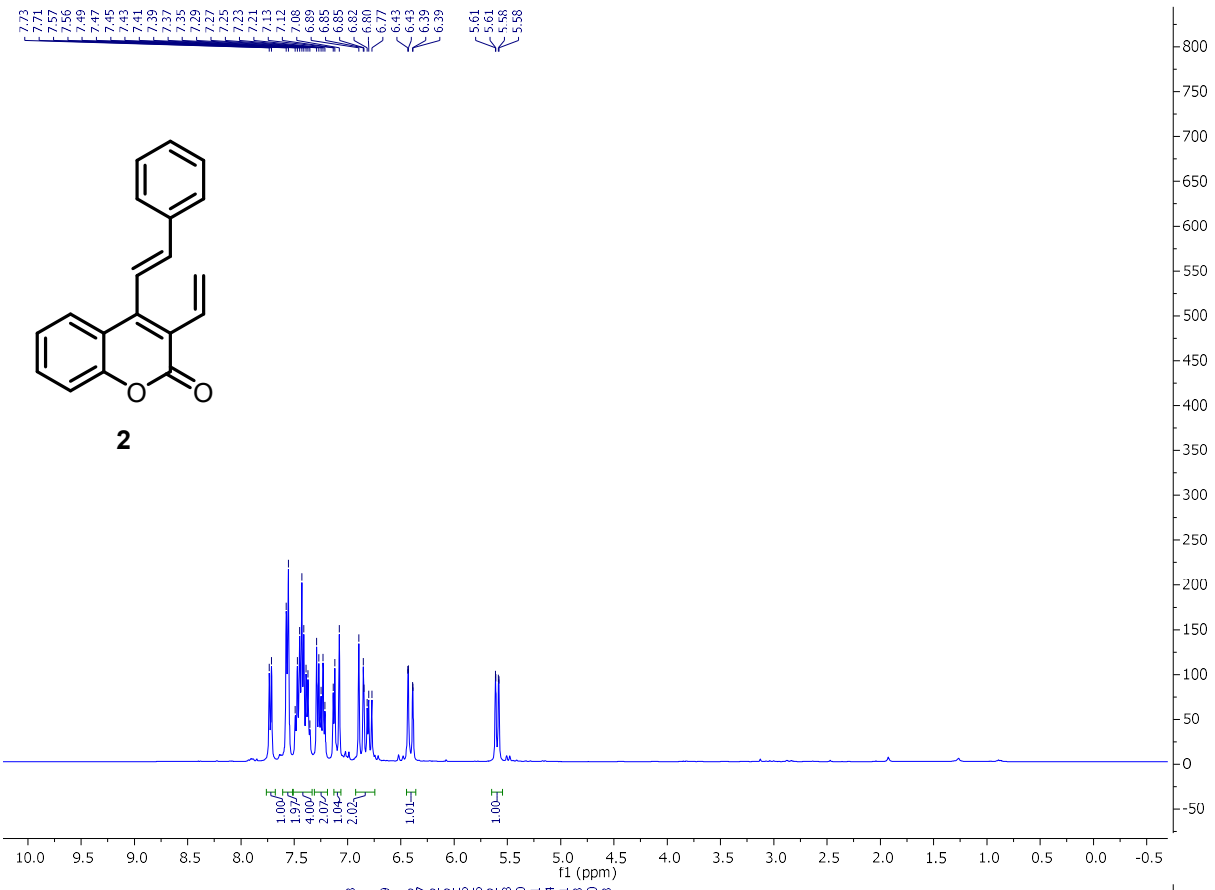
1i
f1 (ppm)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7.25
7.23
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7.13
7.12
7.08
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6.85
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6.82
6.80
6.77
6.43
6.43
6.39
6.39
5.61
5.61
5.58
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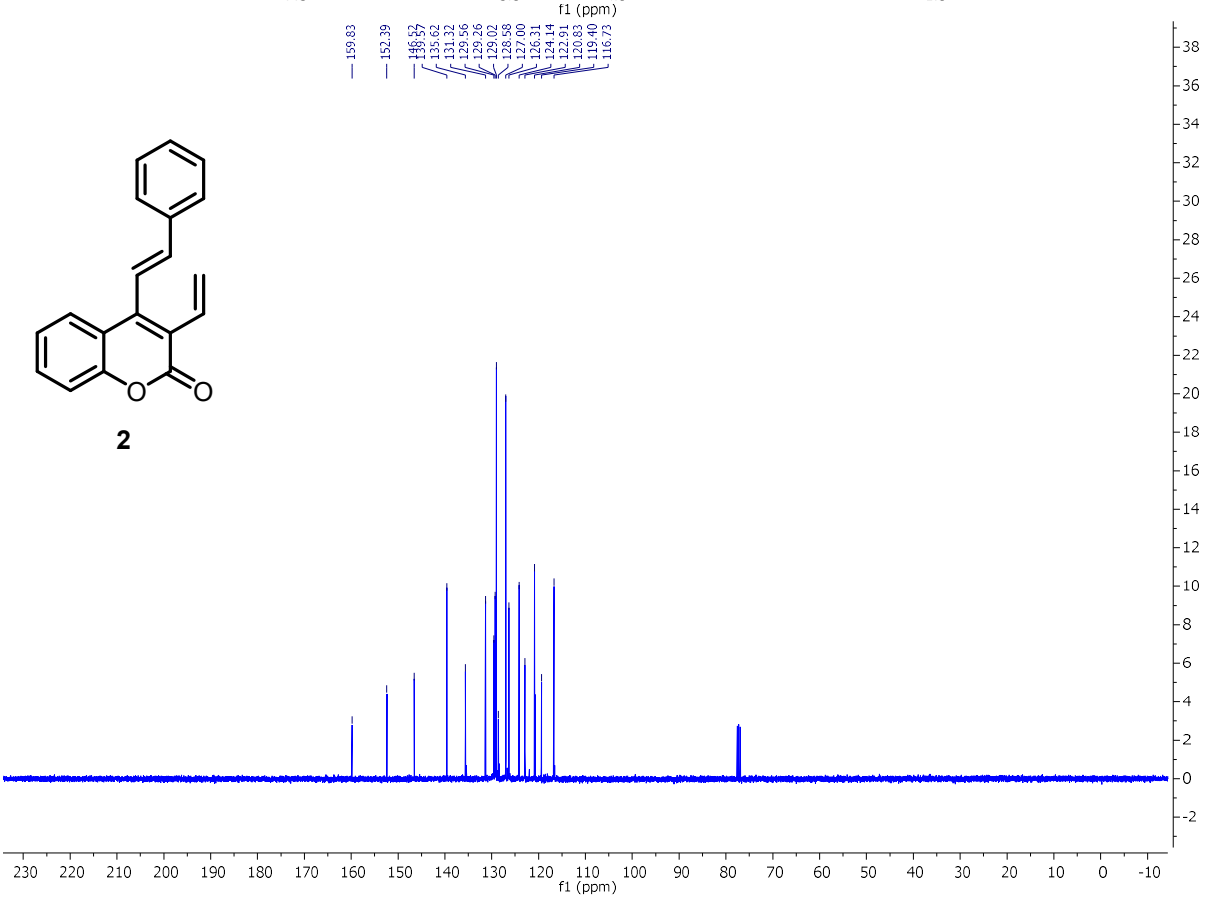
1.97
4.00
2.07
1.04
2.02
1.01
1.00
f1 (ppm)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122.91
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119.40
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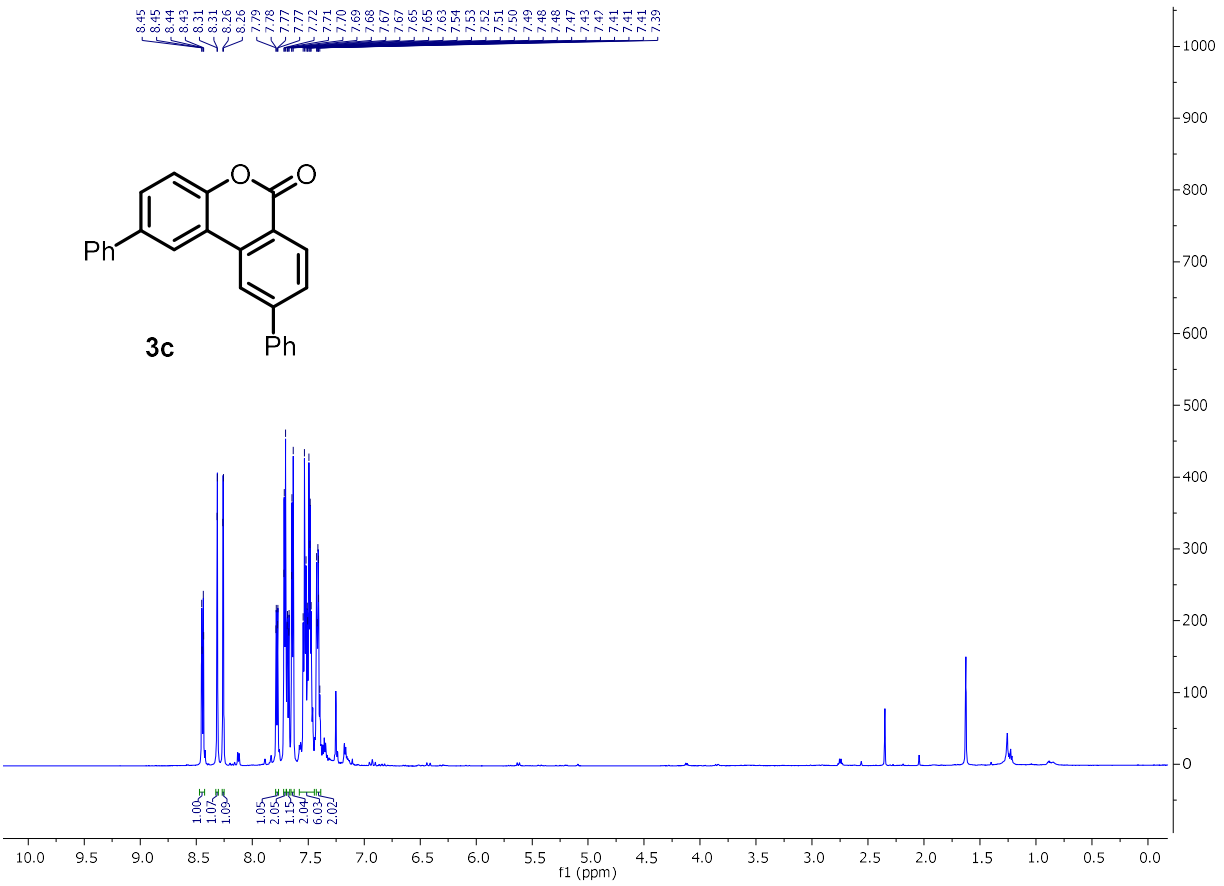
O
O
2
f1 (ppm)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7.68
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7.51
7.50
7.49
7.48
7.48
7.47
7.43
7.42
7.41
7.41
7.41
7.39
O
O
Ph
Ph
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1.07
1.09
1.05
2.05
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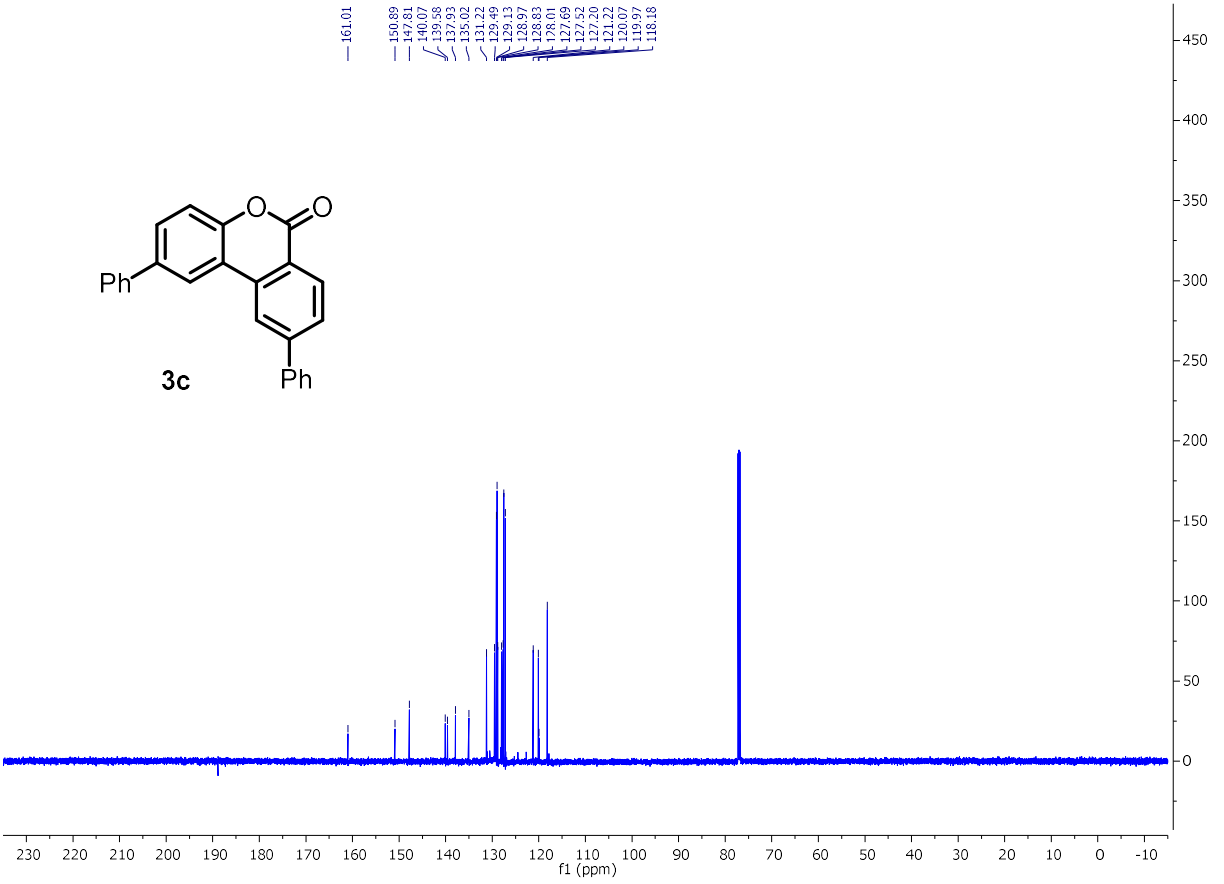
2.04
6.03
2.02
f1 (ppm)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121.22
120.07
119.97
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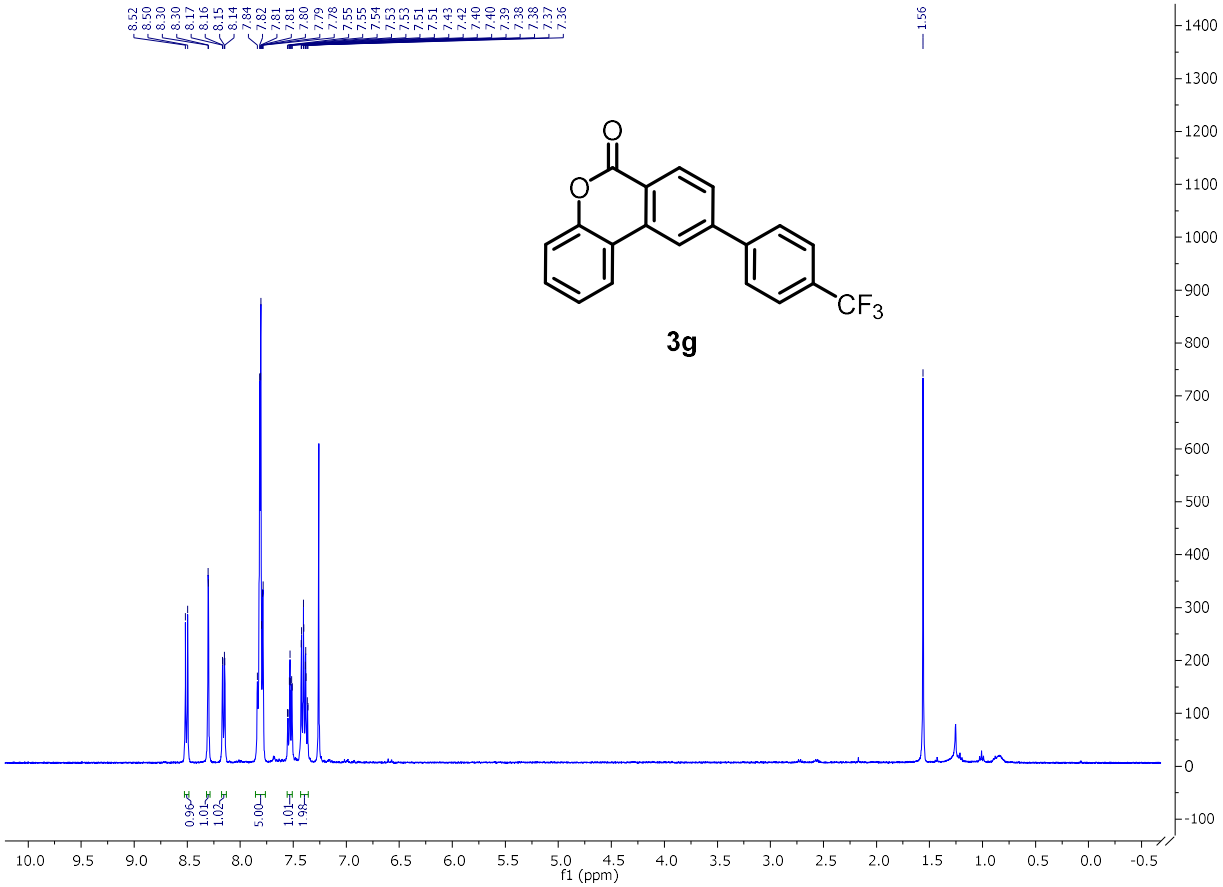
O
O
Ph
Ph
3c
f1 (ppm)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7.40
7.40
7.39
7.38
7.38
7.37
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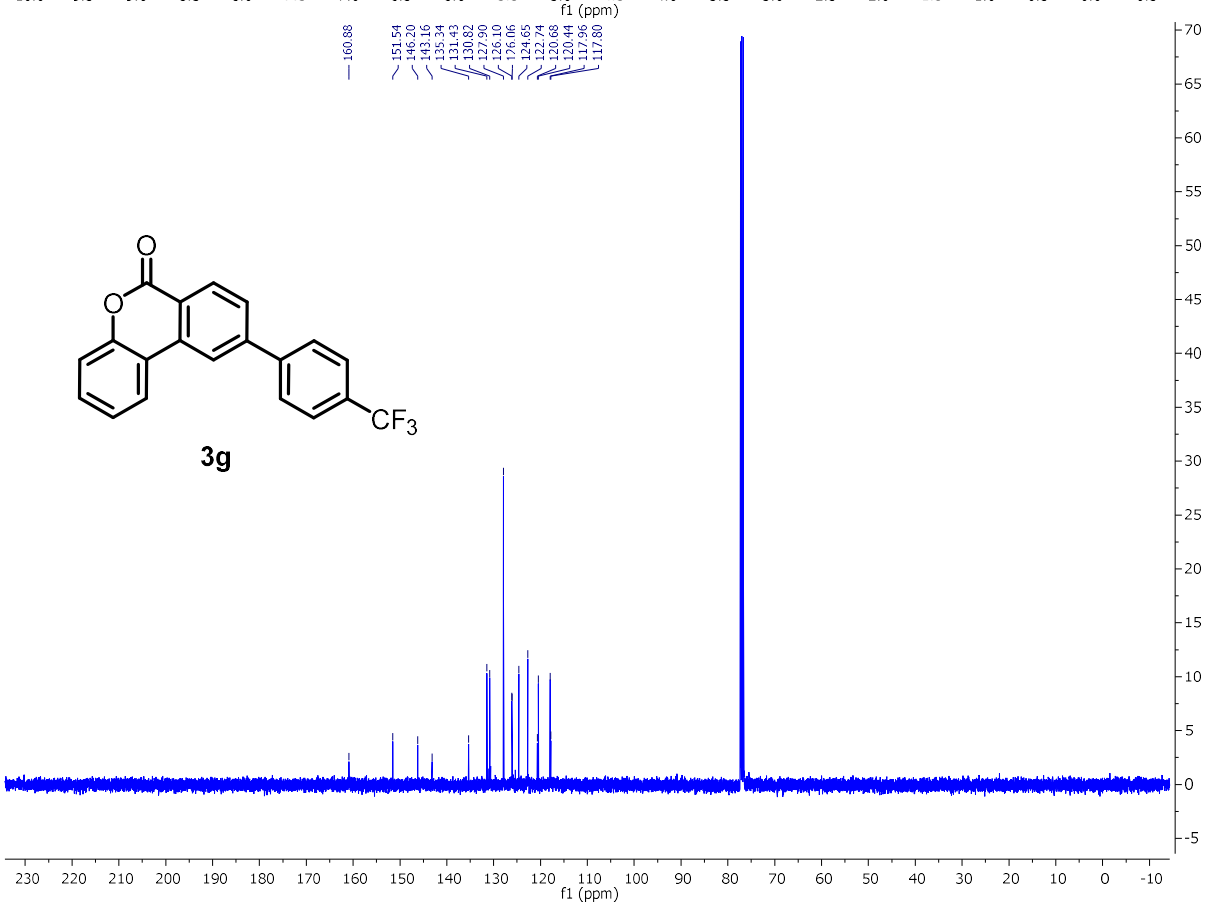
f1 (ppm)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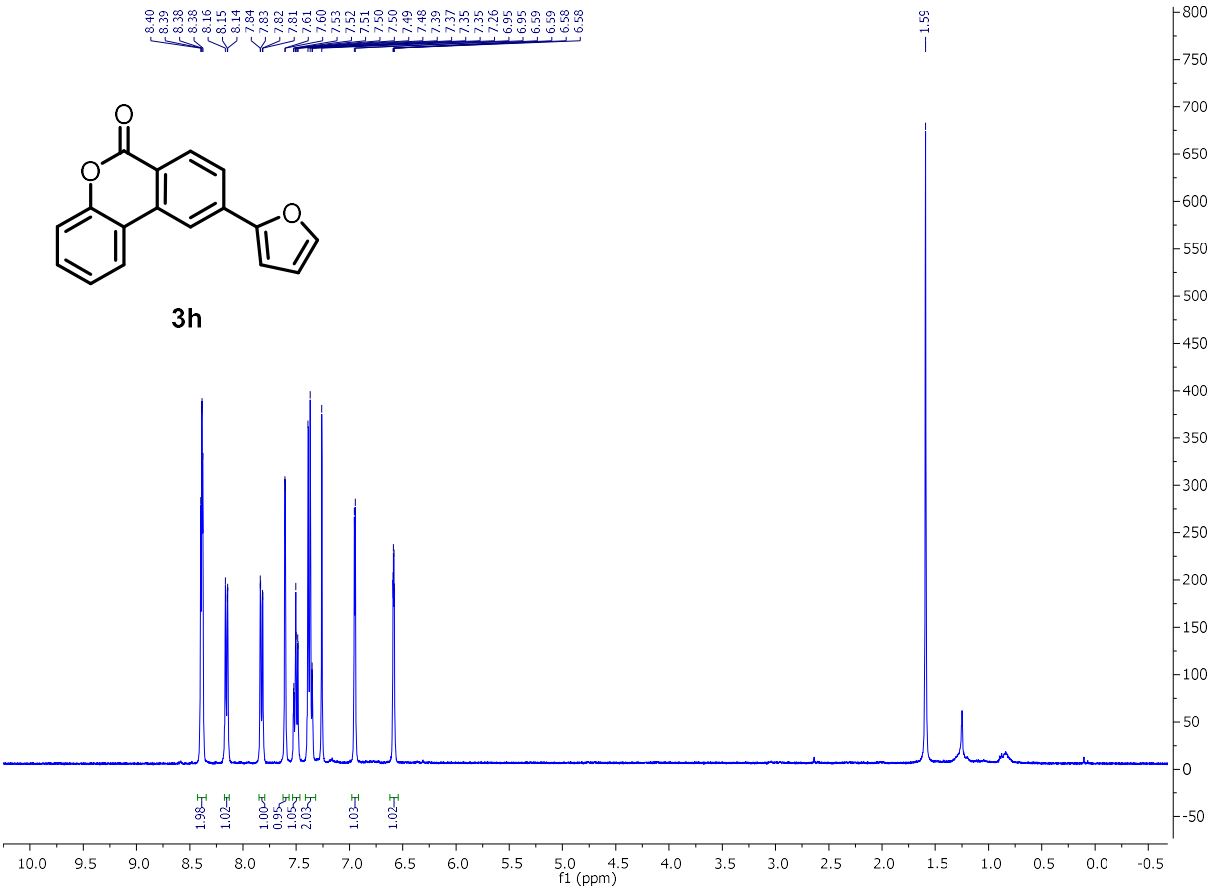
CF3
3g
f1 (ppm)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6.59
6.58
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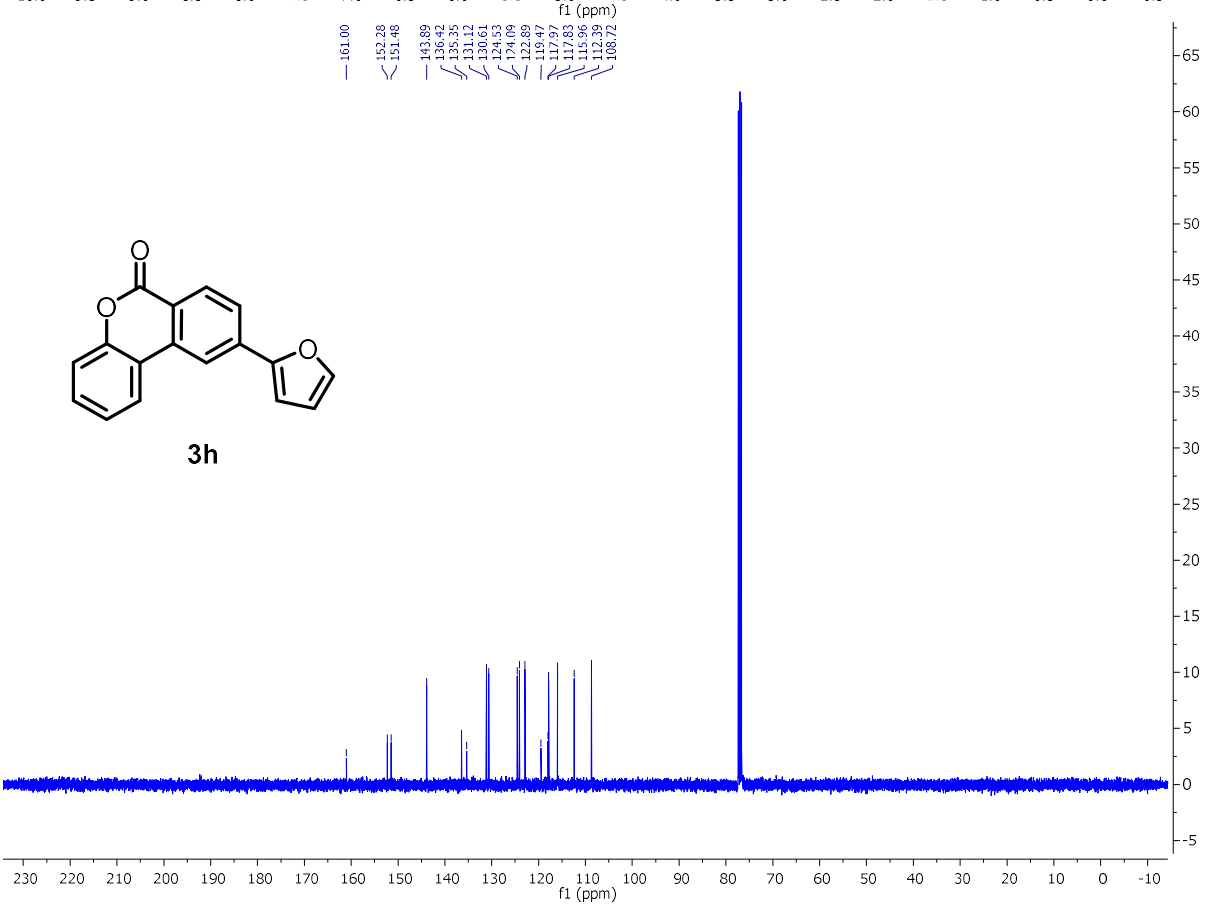
1.02
f1 (ppm)

3h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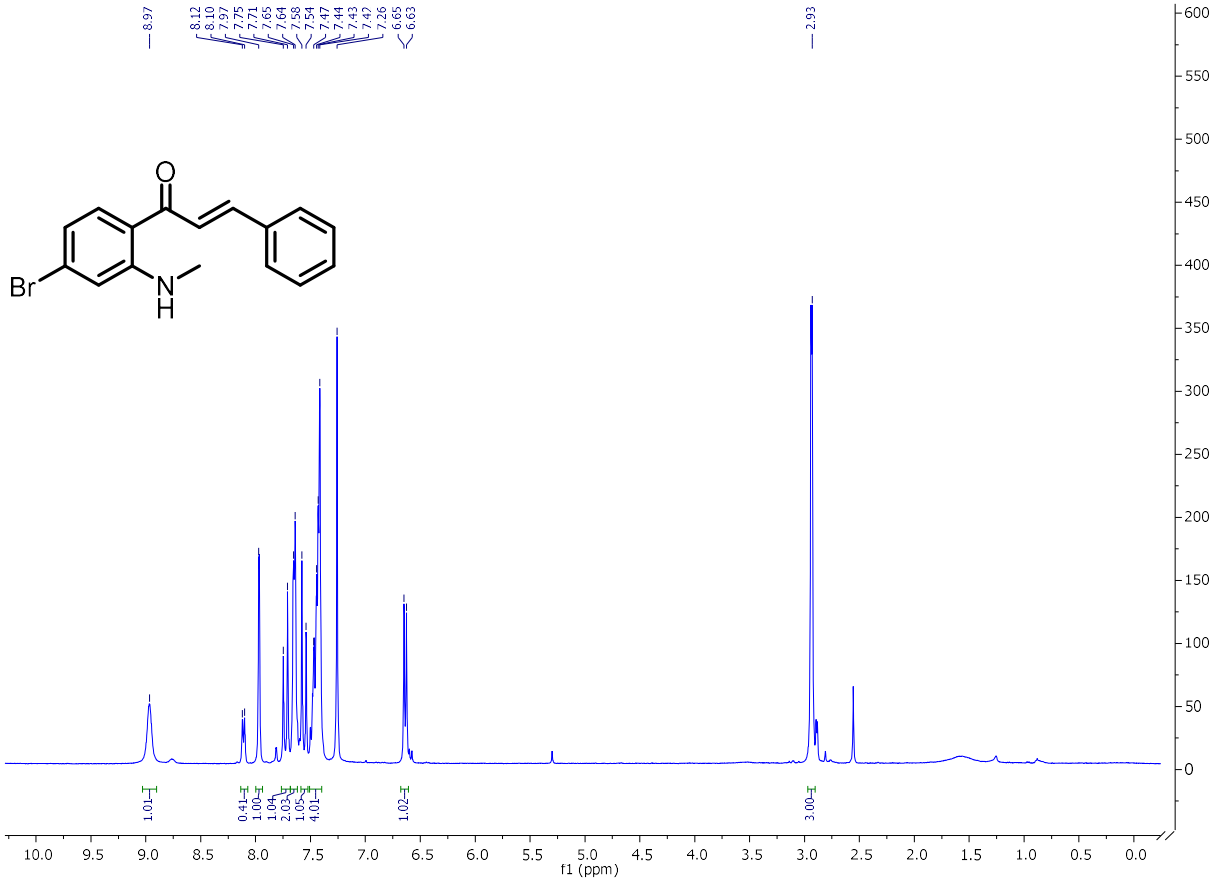
117.97
117.83
115.96
112.39
108.72
f1 (ppm)

3h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7.43
7.42
7.26
6.65
6.63
2.93
Br
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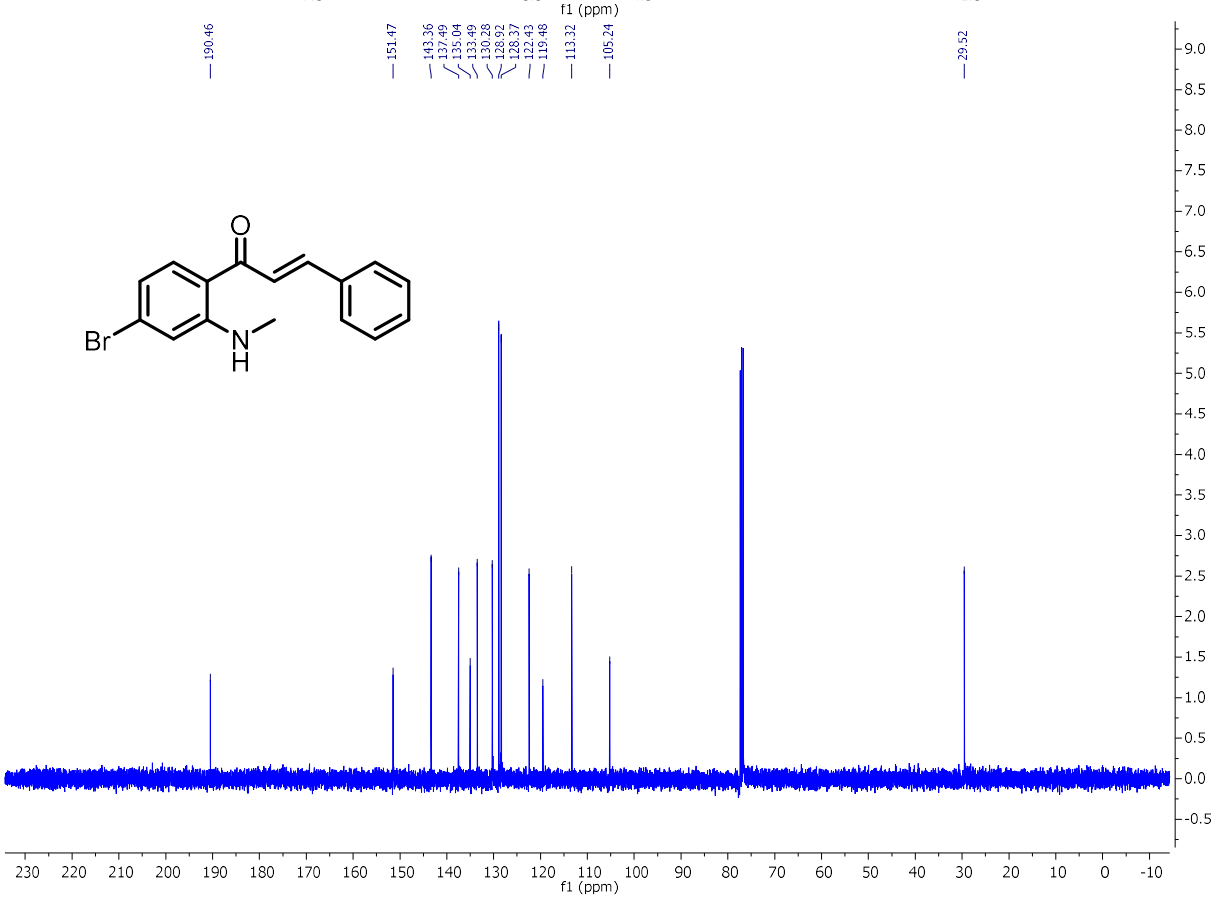
0.41
1.00
1.04
2.03
1.05
4.01
1.02
3.00
f1 (ppm)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113.32
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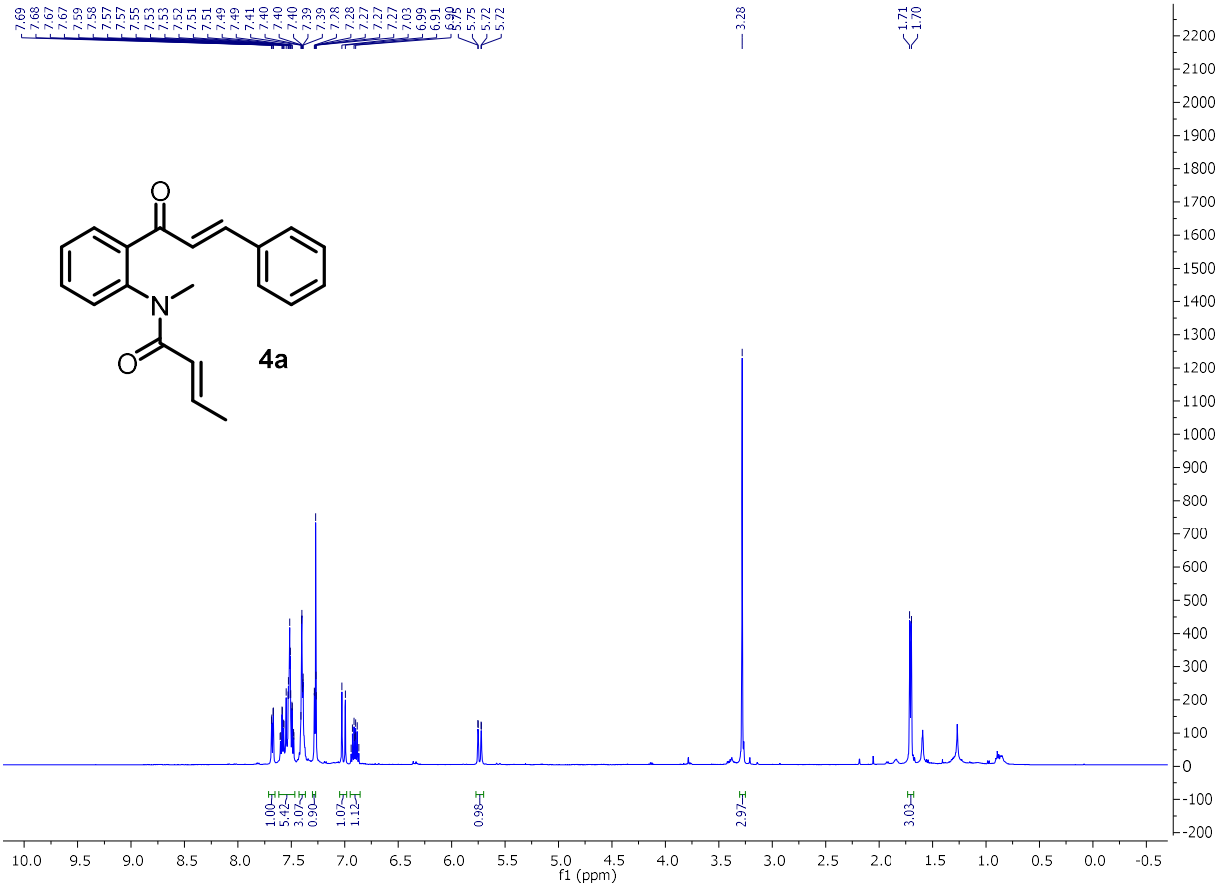
29.52
Br
N
H
O
f1 (ppm)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6.90
5.75
5.72
5.72
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1.71
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1.07
1.12
0.98
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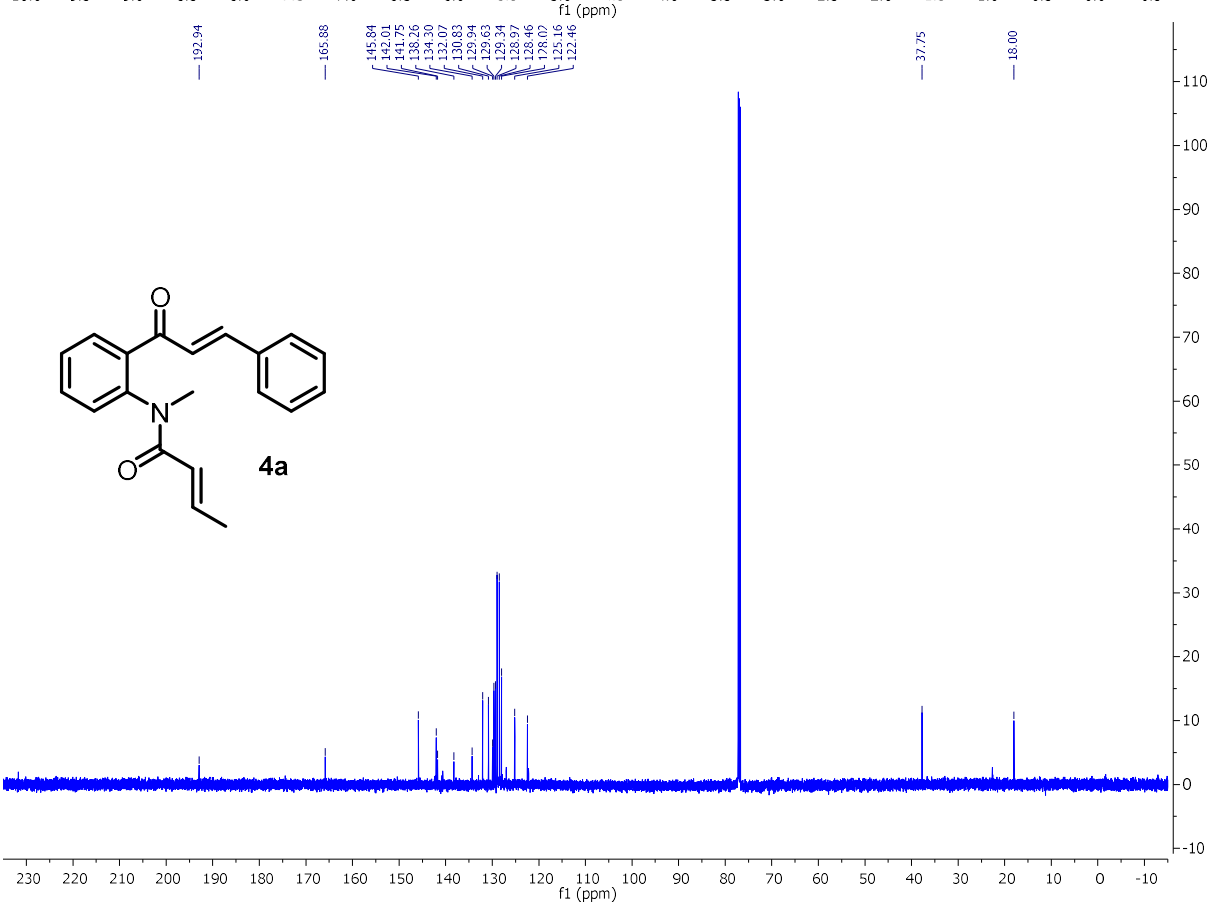
3.03
f1 (ppm)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128.07
125.16
122.46
37.75
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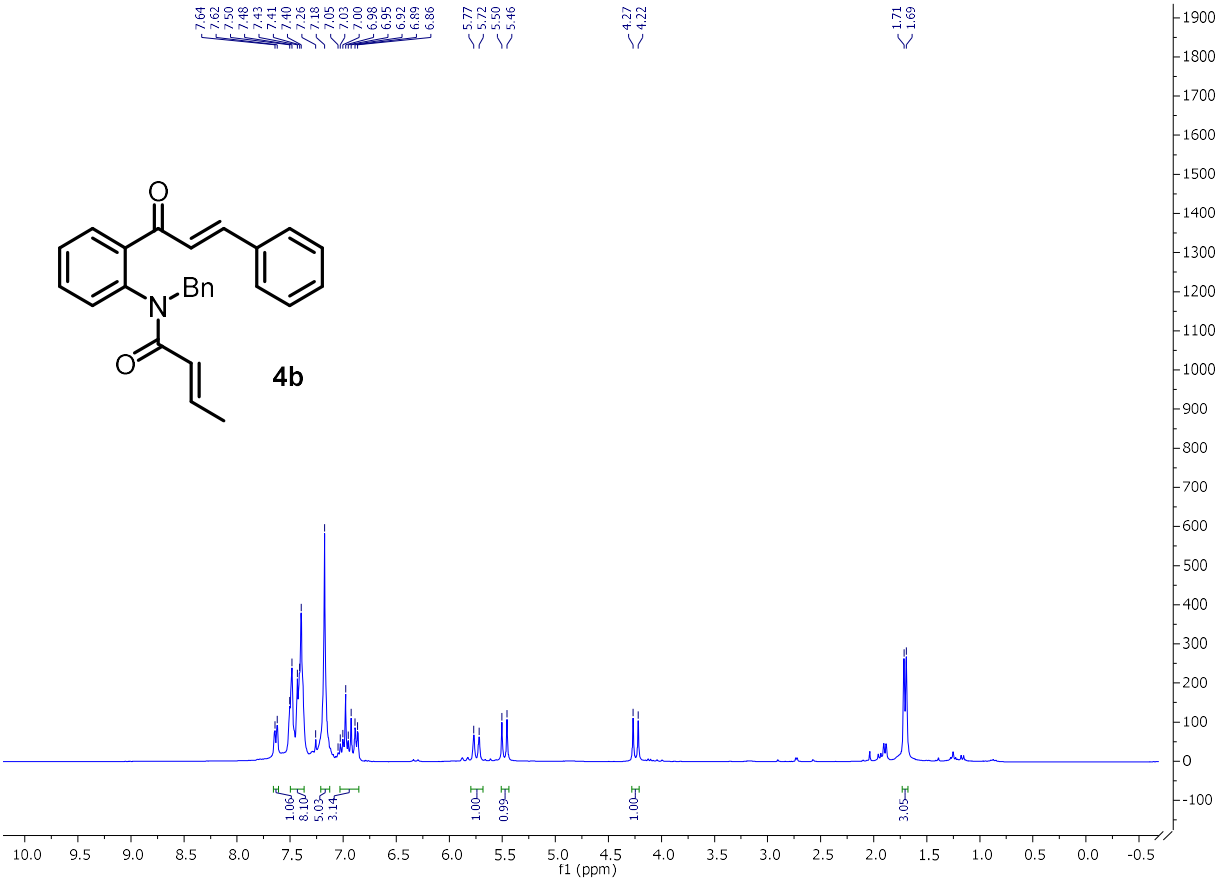
4a
f1 (ppm)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6.95
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6.89
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5.72
5.50
5.46
4.27
4.22
1.71
1.69
Bn
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8.10
5.03
3.14
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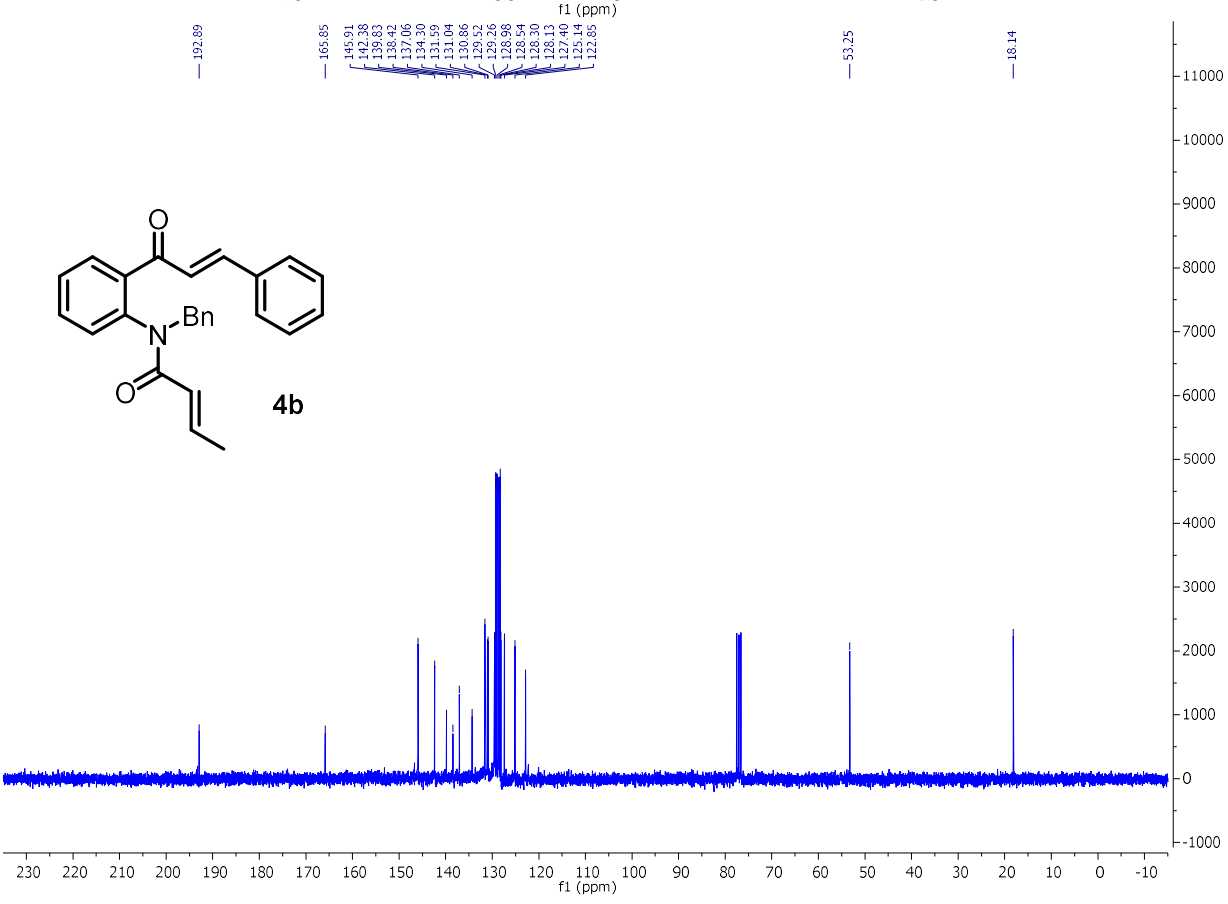
0.99
1.00
3.05
f1 (ppm)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129.26
128.98
128.54
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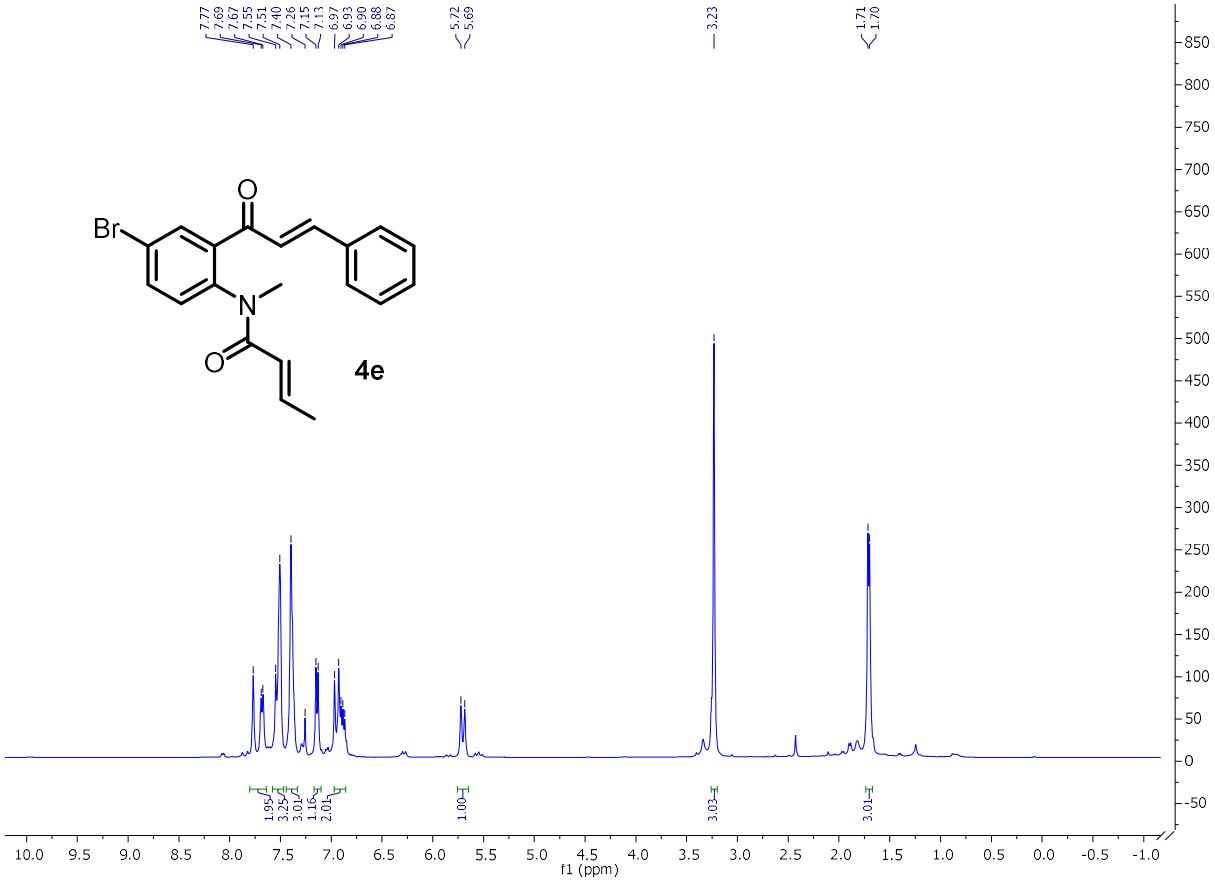
127.40
125.14
122.85
53.25
18.14
Bn
N
O
O
4b
f1 (ppm)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6.97
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6.90
6.88
6.87
5.72
5.69
3.23
1.71
1.70
Br
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N
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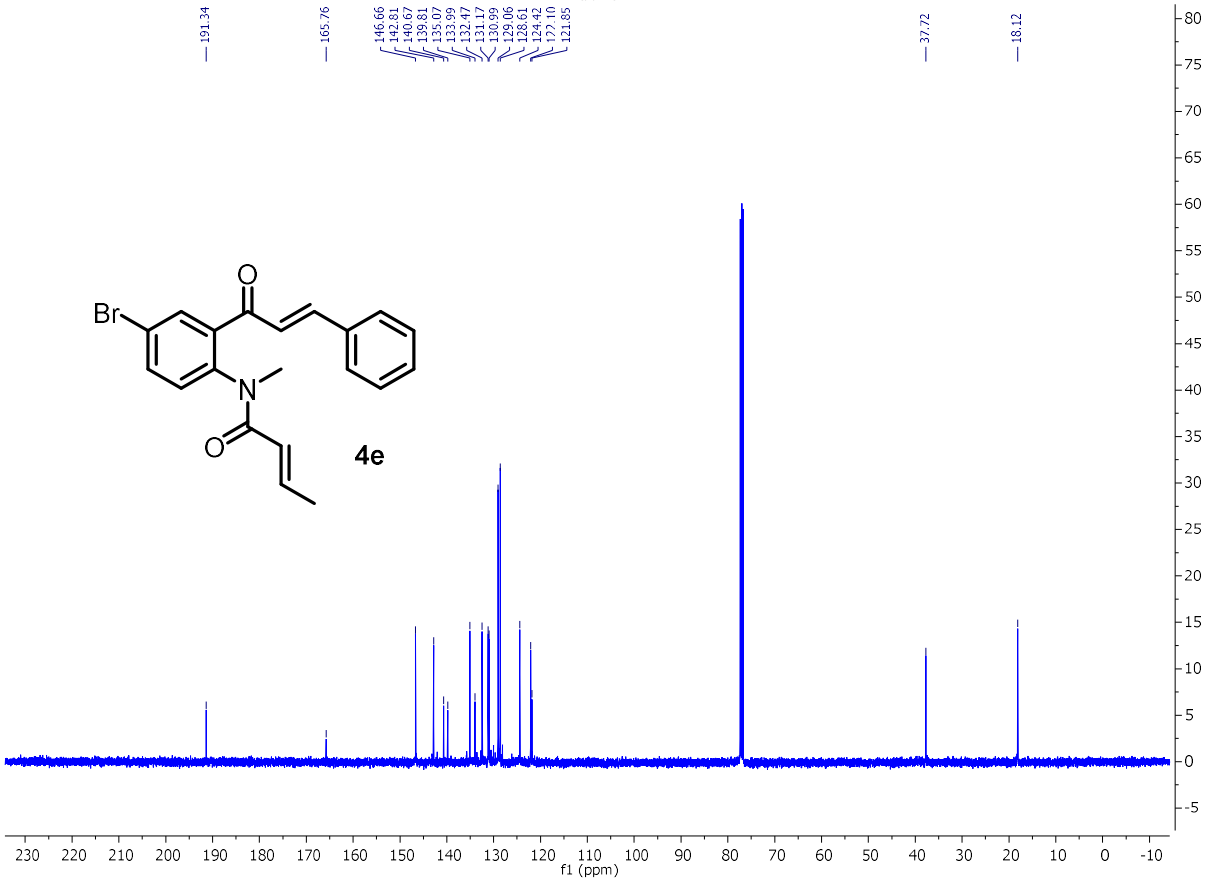
4e
1.95
3.25
3.01
1.16
2.01
1.00
3.03
3.01
f1 (ppm)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Br
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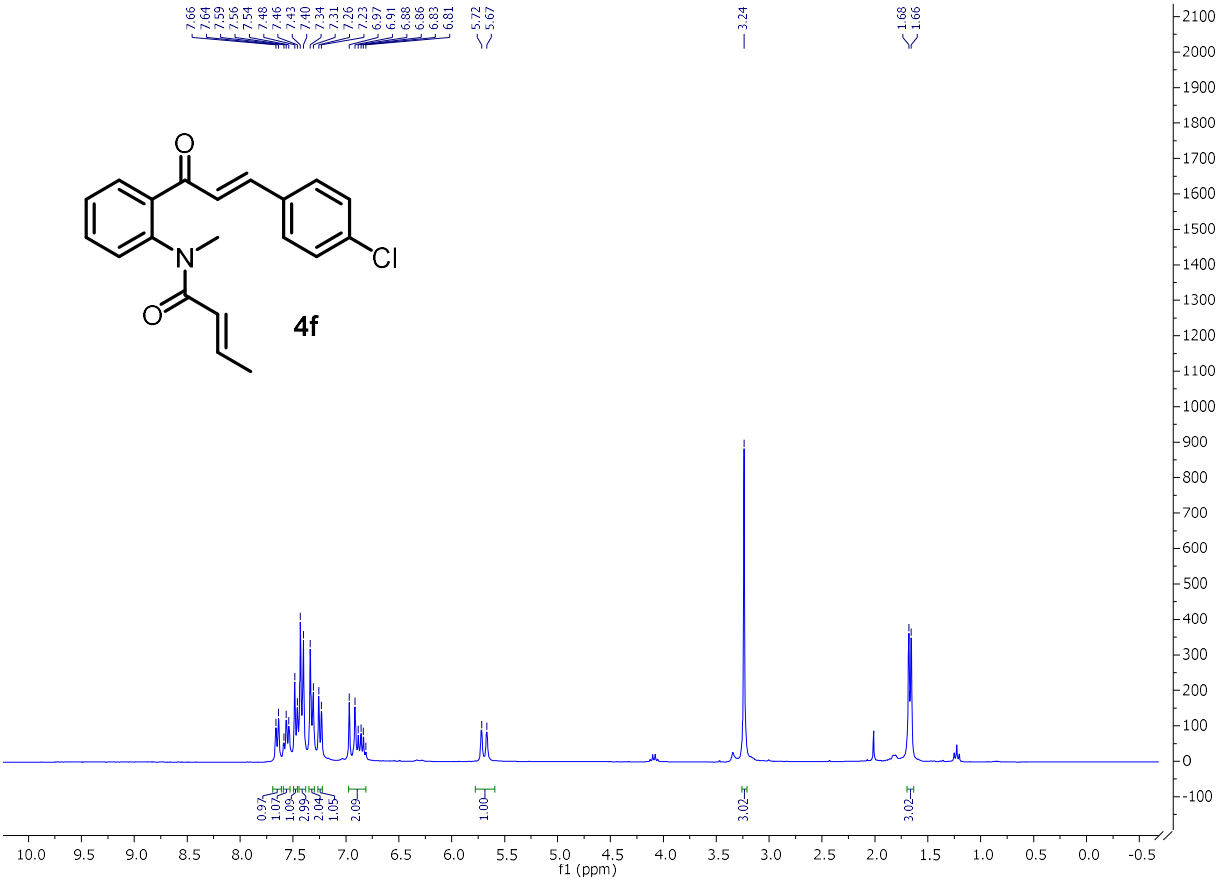
N
O
4e
f1 (ppm)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7.34
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7.26
7.23
6.97
6.91
6.88
6.86
6.83
6.81
5.72
5.67
3.24
1.68
1.66
O
N
O
Cl
4f
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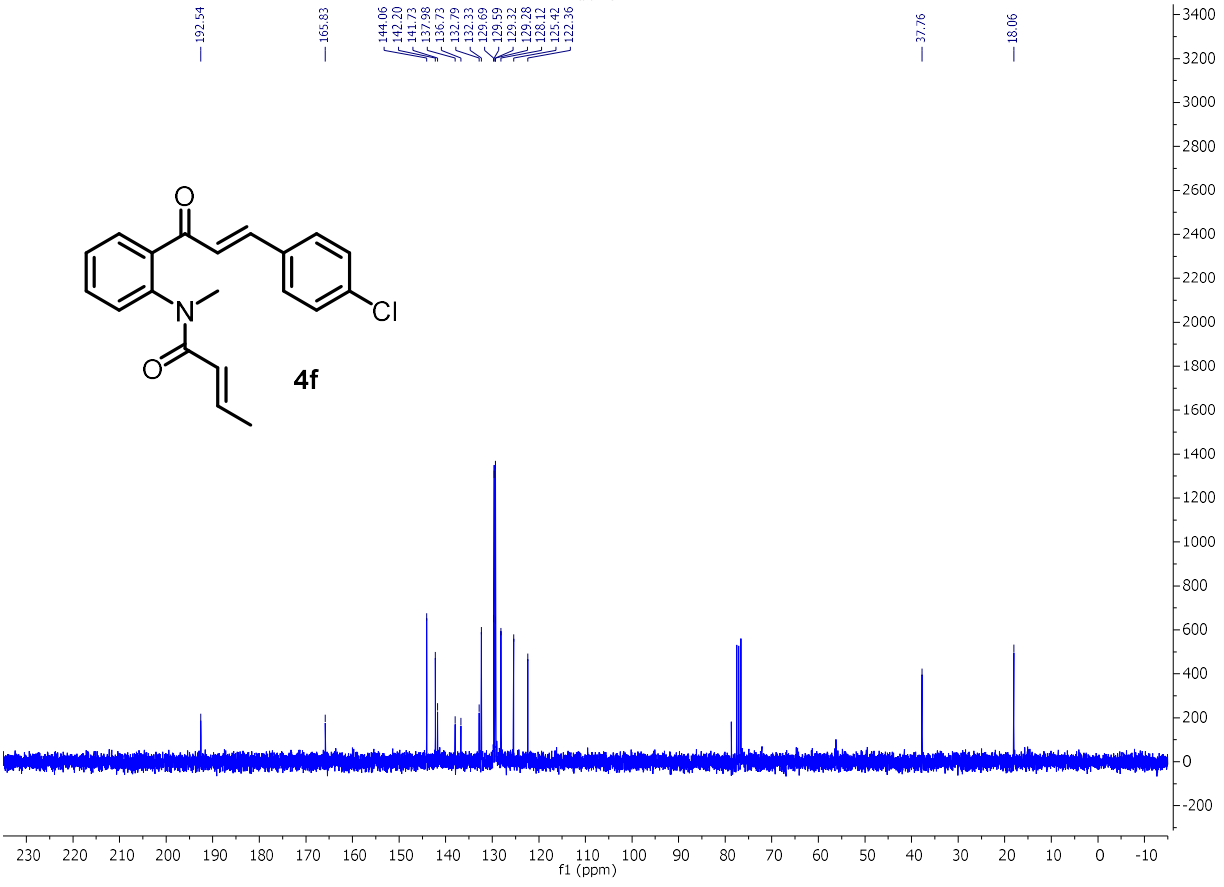
1.09
2.99
2.04
1.05
2.09
1.00
3.02
3.02
f1 (ppm)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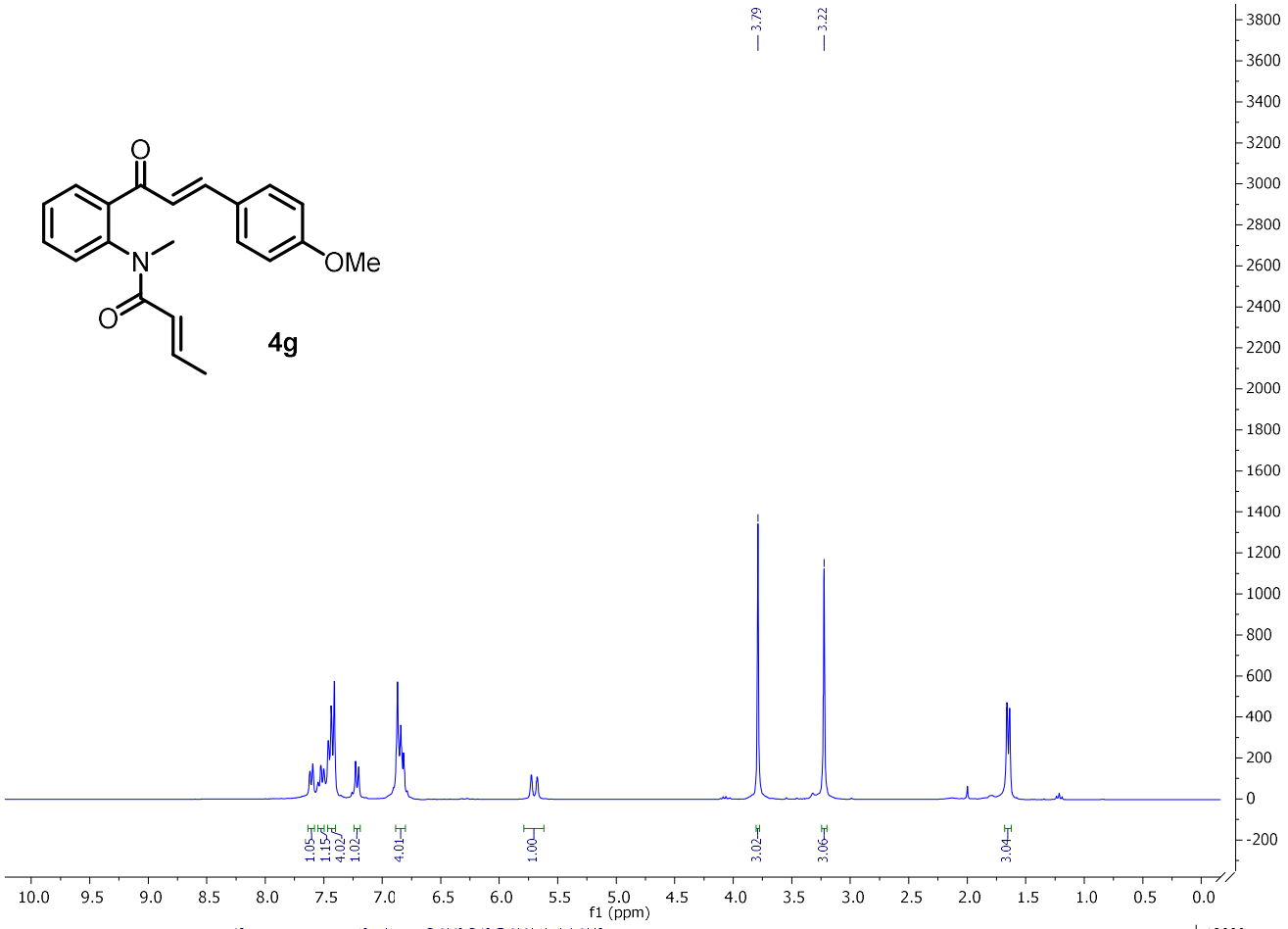
125.42
122.36
37.76
18.06
O
N
O
Cl
4f
f1 (ppm)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1.02
4.01
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3.02
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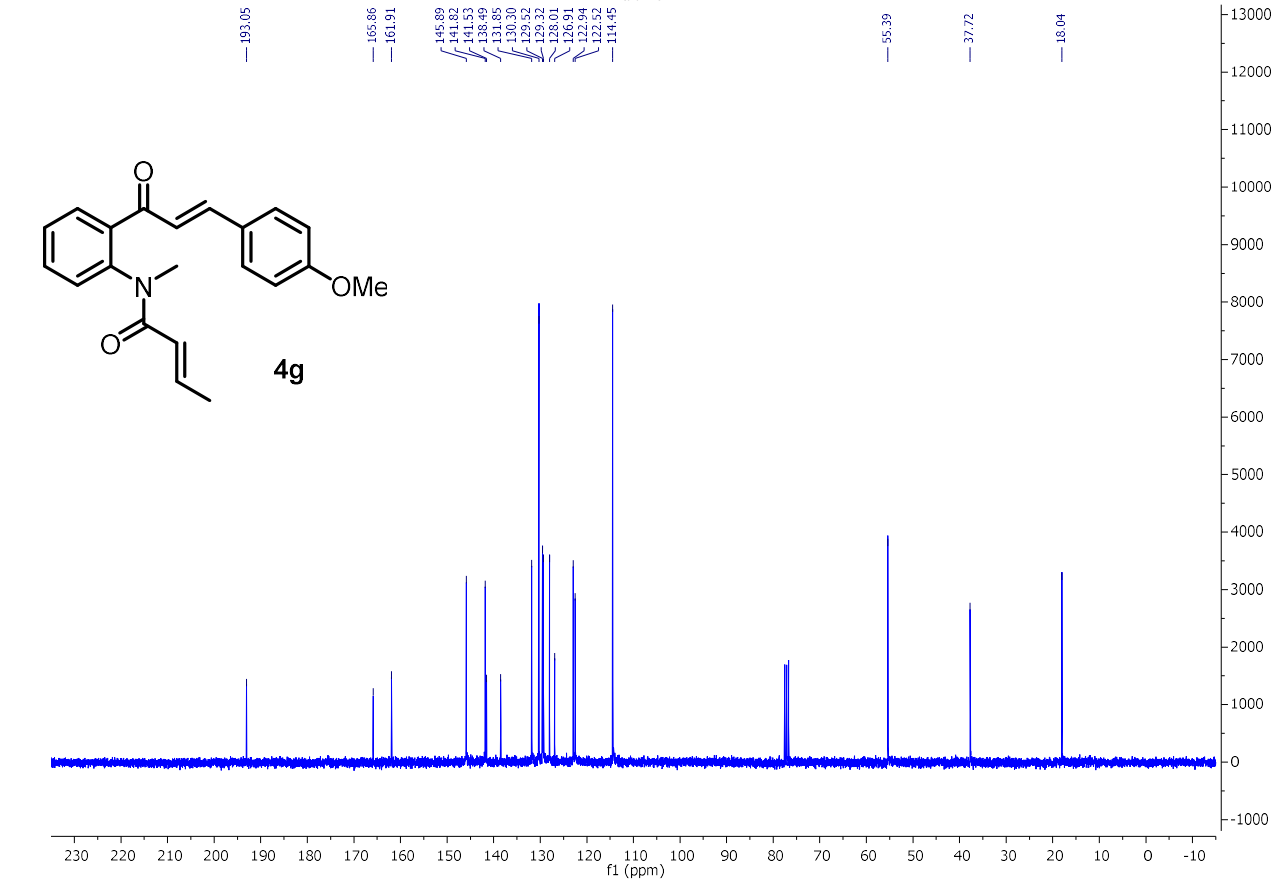
3.04
f1 (ppm)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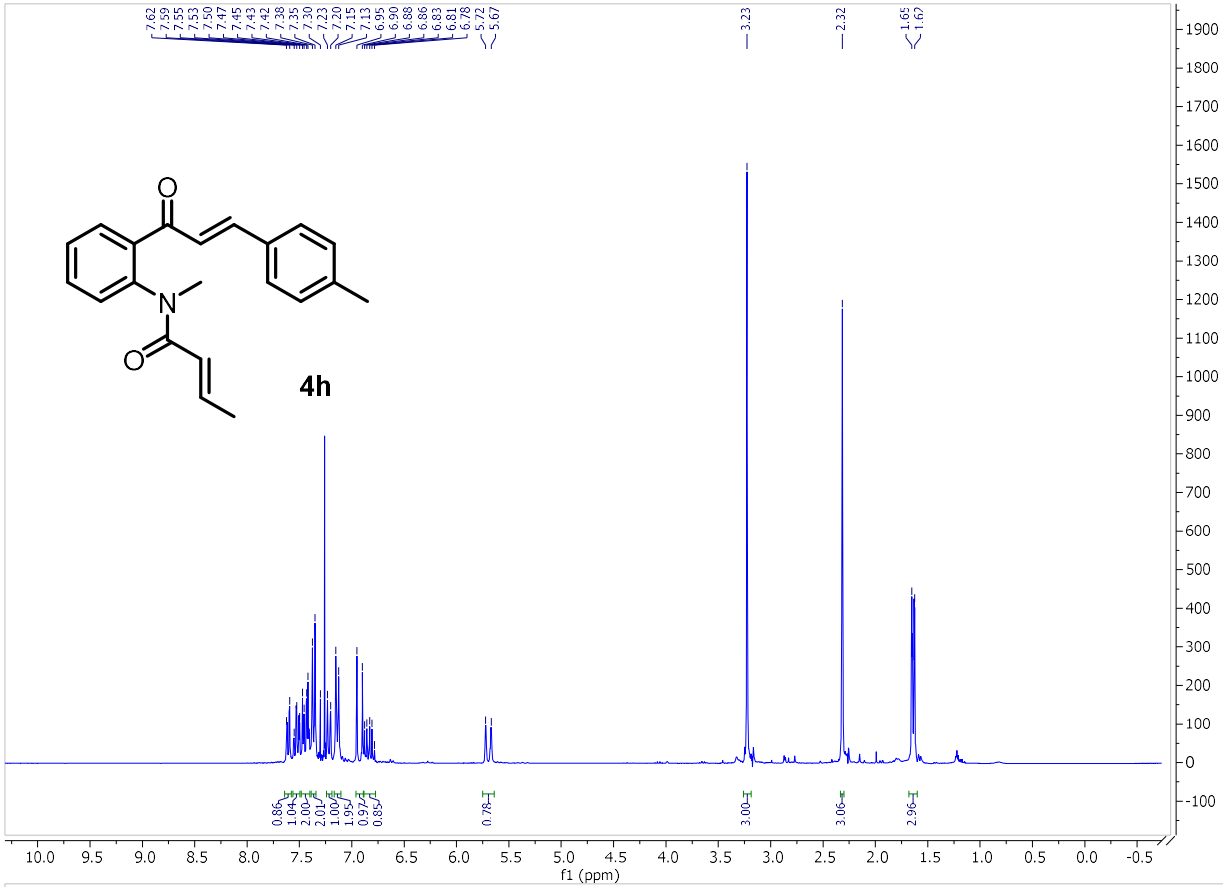
122.94
122.52
114.45
55.39
37.72
18.04
OMe
4g
f1 (ppm)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7.15
7.13
6.95
6.90
6.88
6.86
6.83
6.81
6.78
5.72
5.67
3.23
2.32
1.65
1.62
4h
0.86
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2.00
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0.78
3.00
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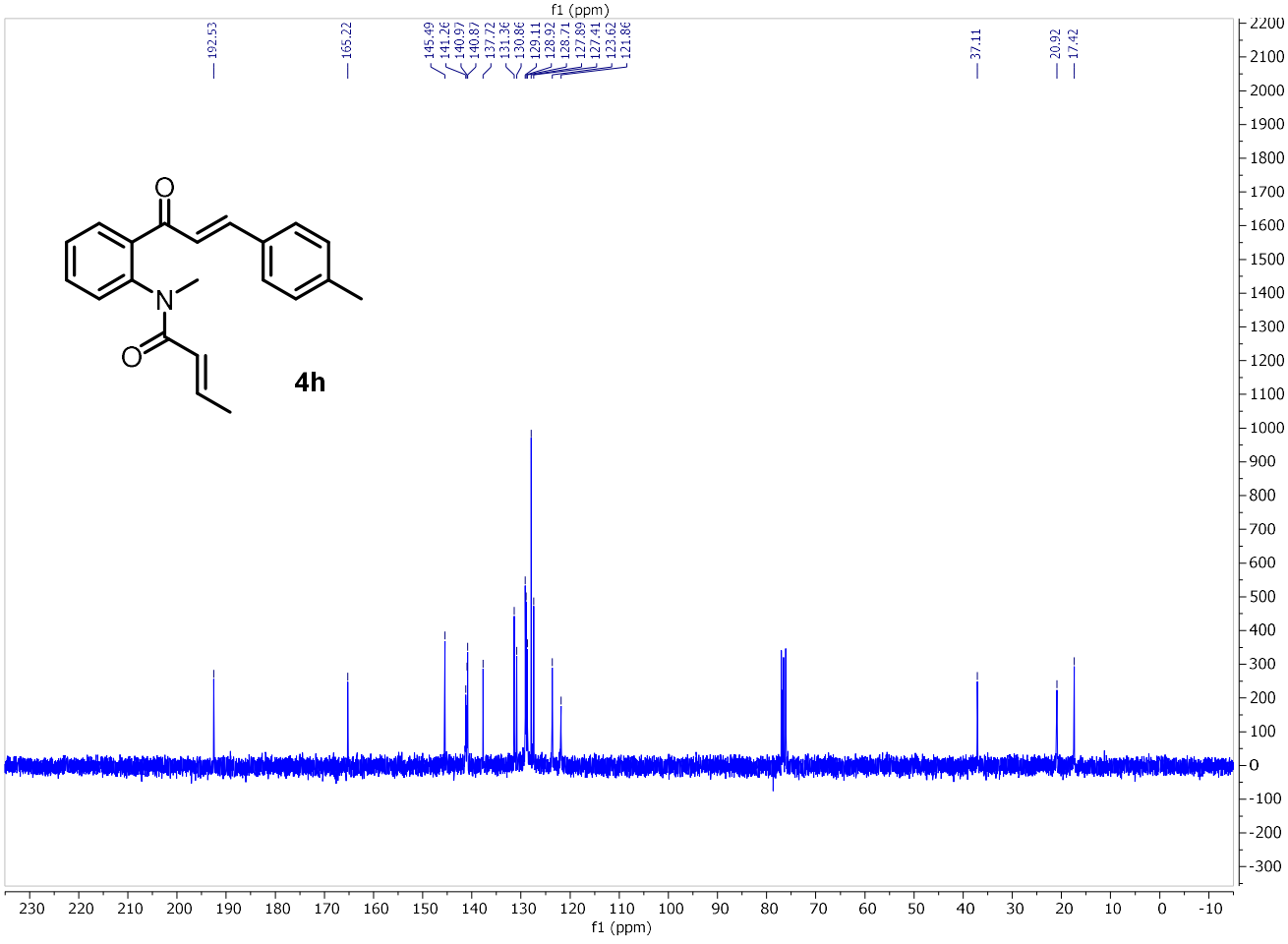
2.96
f1 (ppm)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121.86
37.11
20.92
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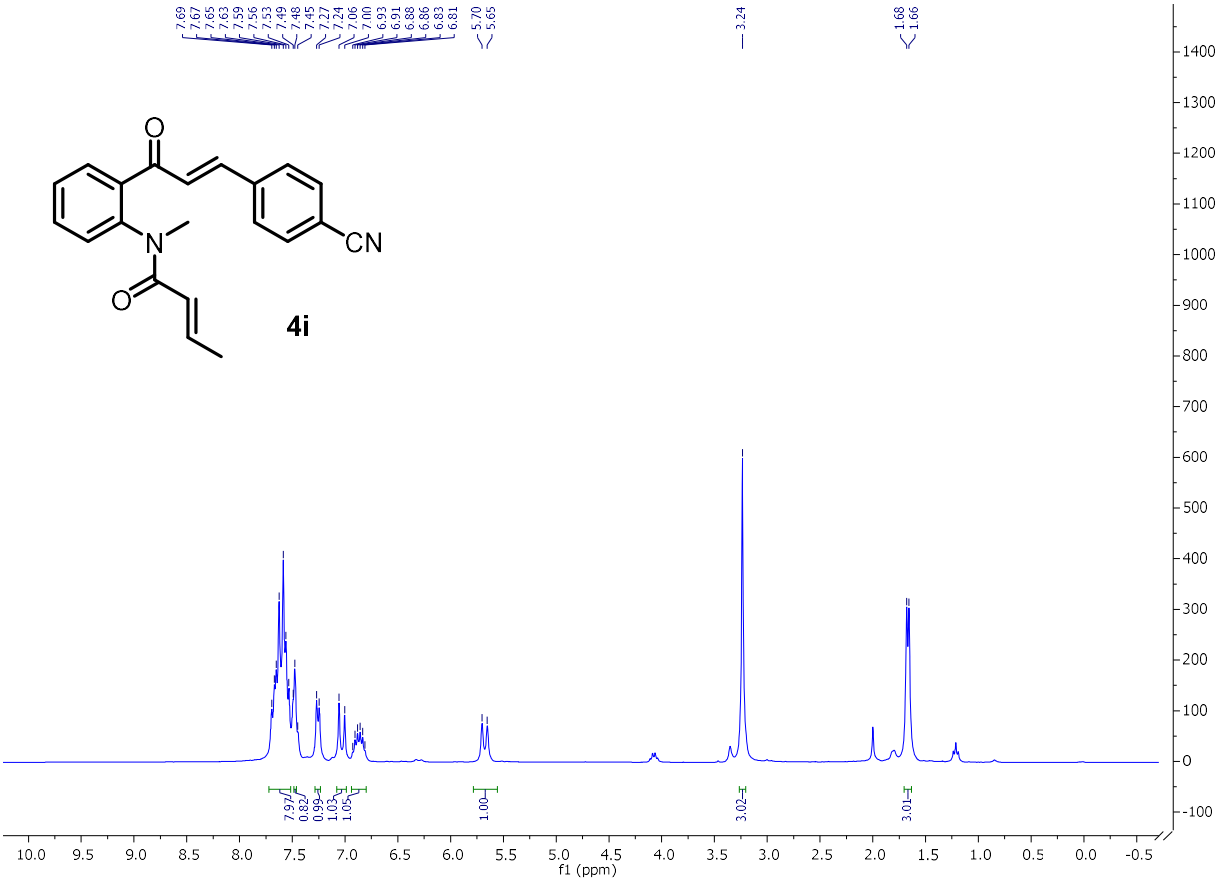
4h
f1 (ppm)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6.91
6.88
6.86
6.83
6.81
5.70
5.65
3.24
1.68
1.66
O
N
O
CN
4i
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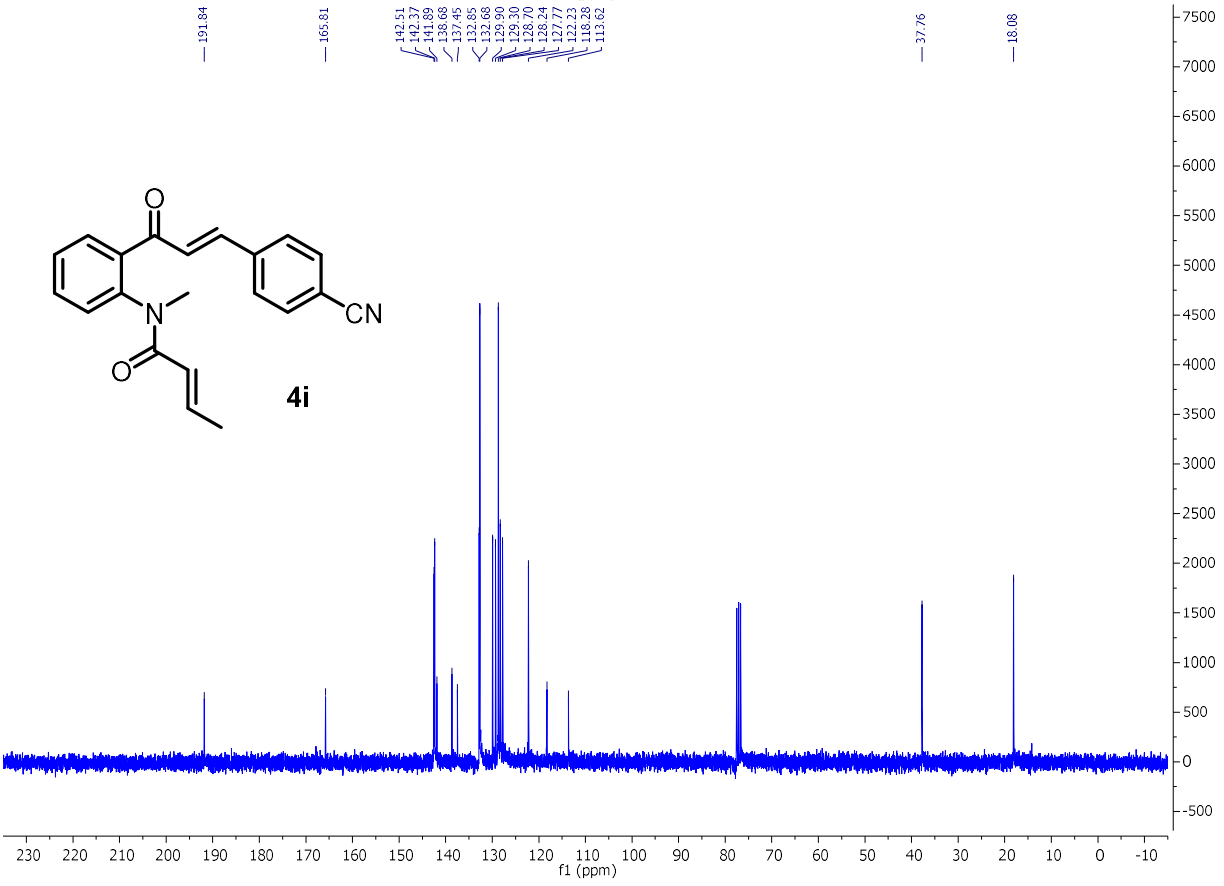
0.99
1.03
1.05
1.00
3.02
3.01
f1 (ppm)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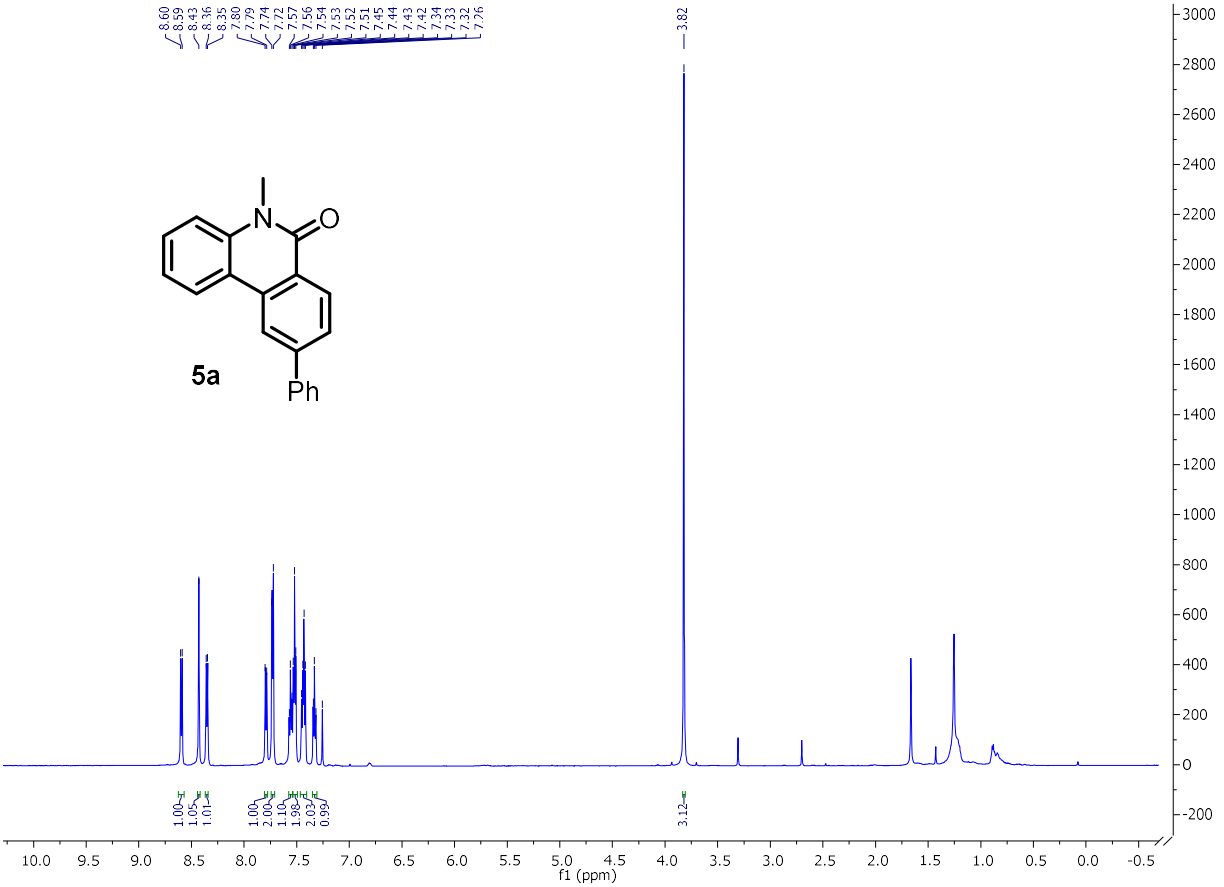
O
N
O
CN
4i
f1 (ppm)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7.53
7.52
7.51
7.45
7.44
7.43
7.42
7.34
7.33
7.32
7.26
3.82
N
O
5a
Ph
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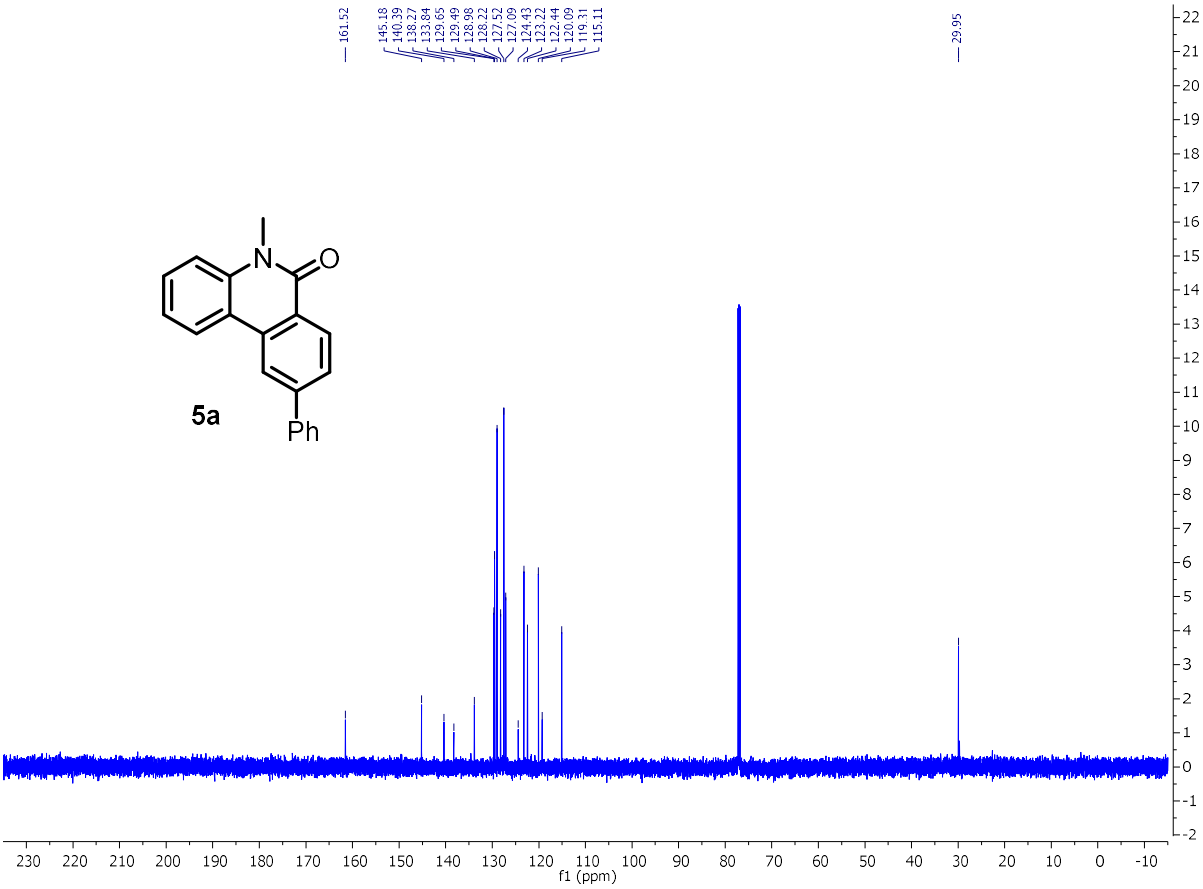
1.01
1.00
2.00
1.10
1.98
2.03
0.99
3.12
f1 (ppm)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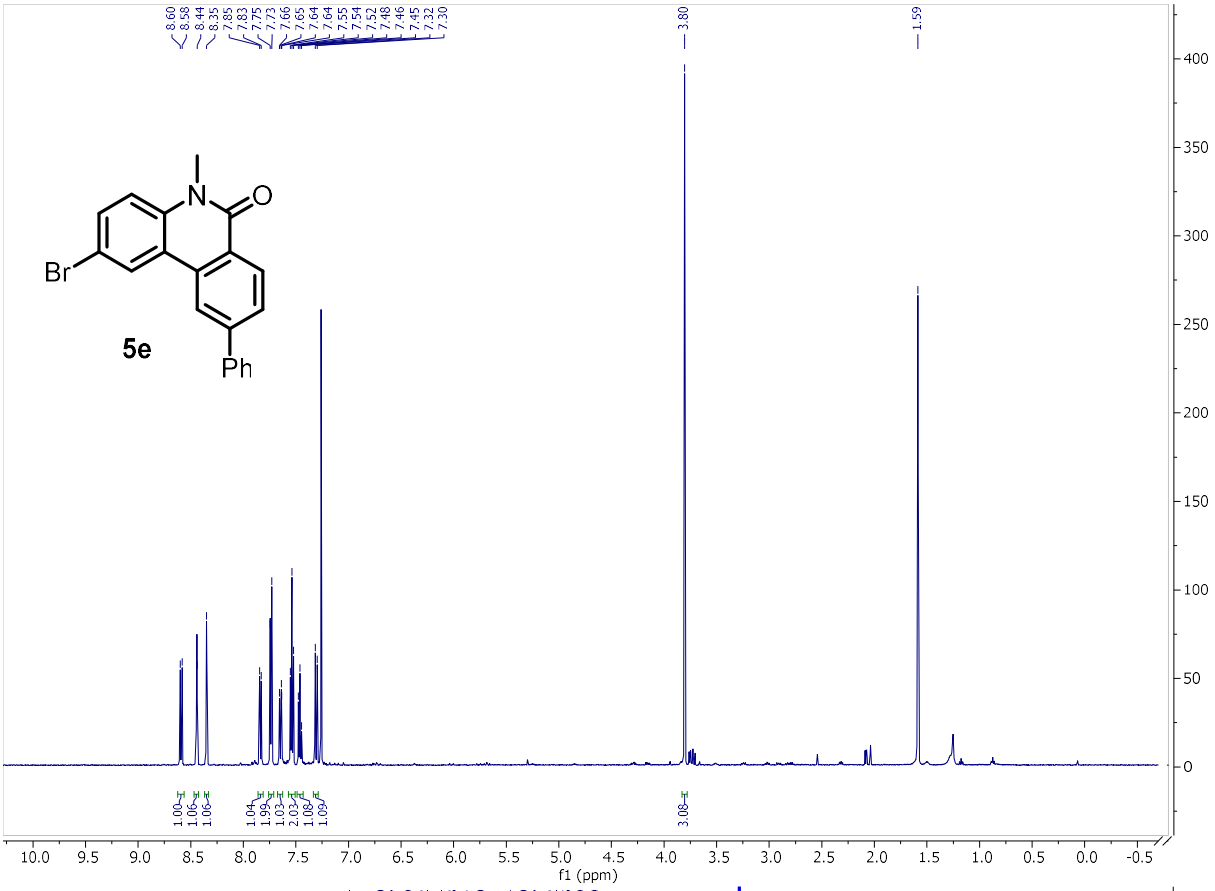
122.44
120.09
119.31
115.11
29.95
N
O
5a
Ph
f1 (ppm)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1.59
1.00
1.06
1.06
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1.03
2.03
1.08
1.09
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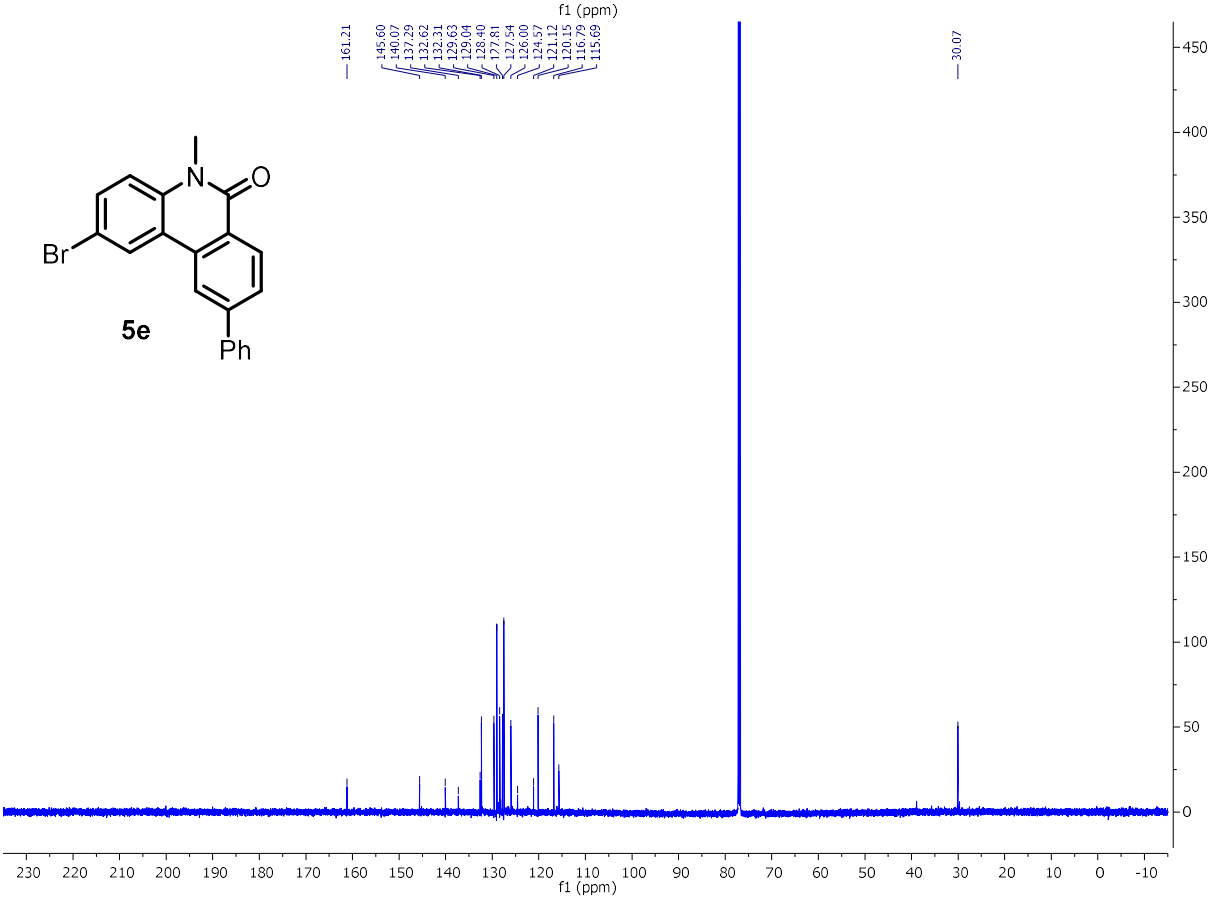
Br
N
O
Ph
5e
f1 (ppm)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129.04
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121.12
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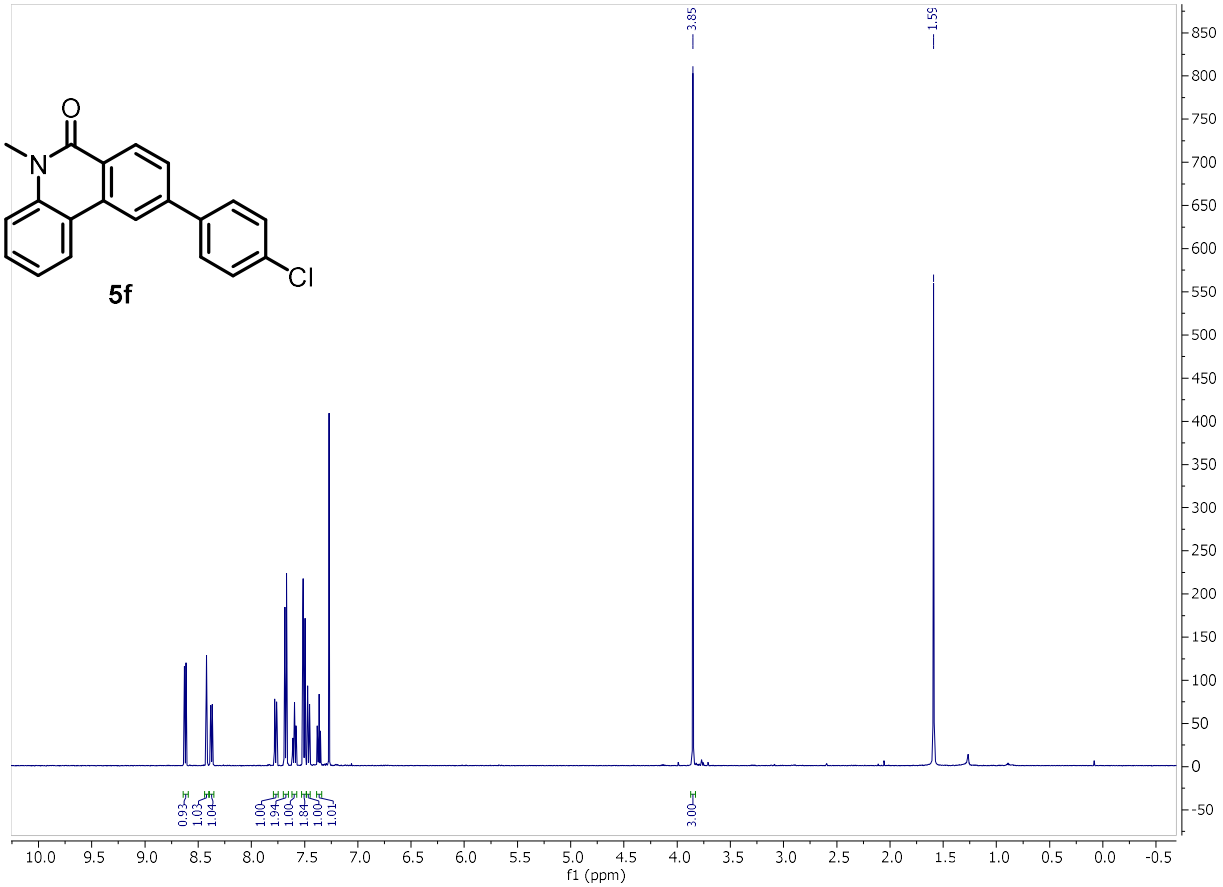
115.69
30.07
Br
N
O
Ph
5e
f1 (ppm)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1.59
5f
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1.04
1.00
1.94
1.00
1.84
1.00
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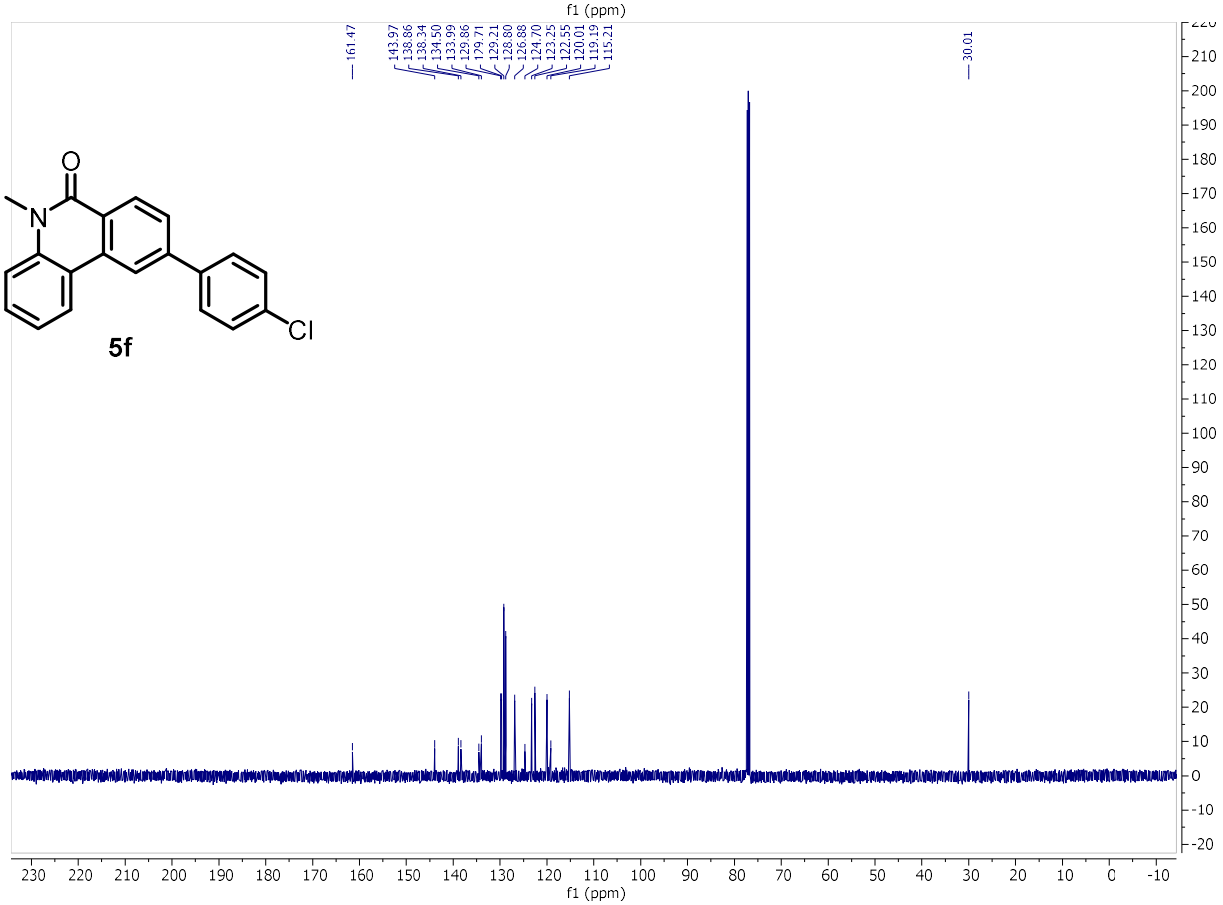
3.00
f1 (ppm)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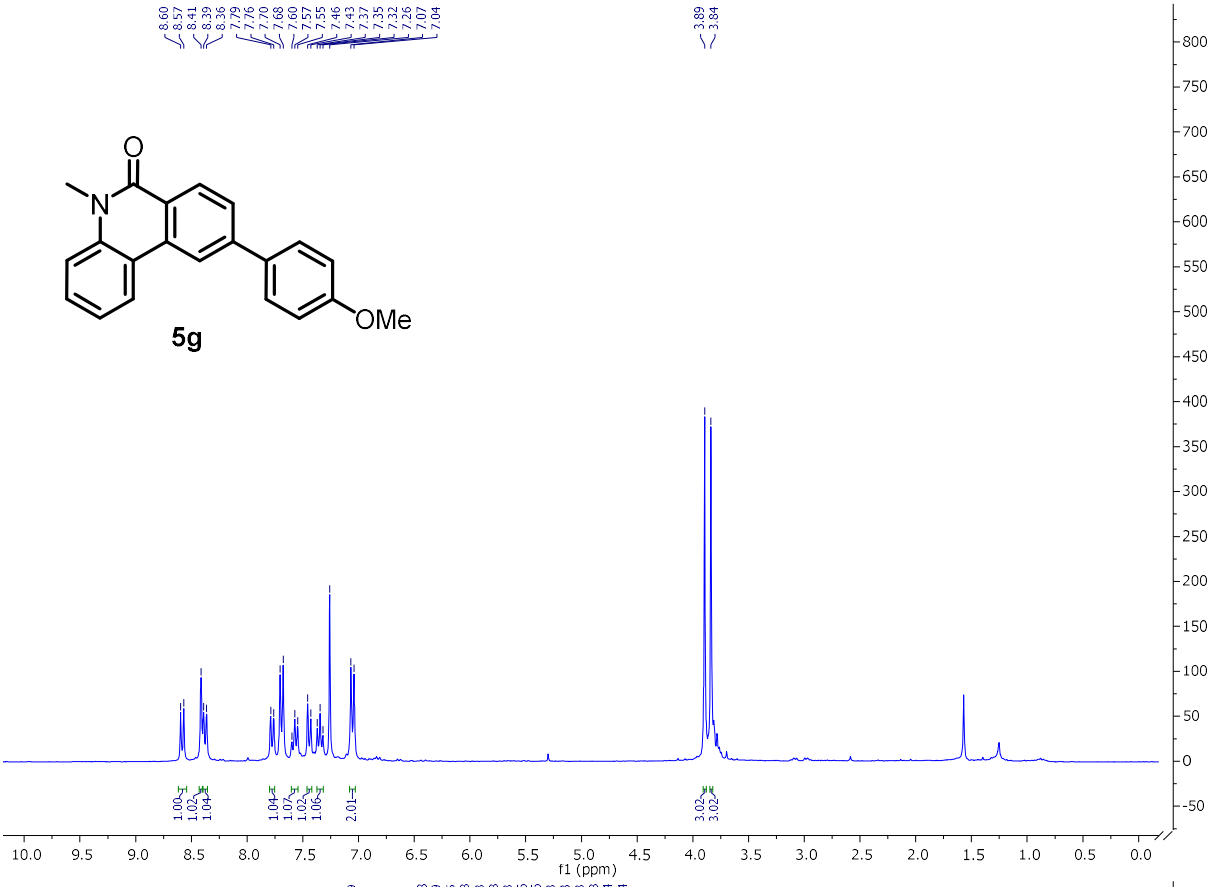
5f
f1 (ppm)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7.46
7.43
7.37
7.35
7.32
7.26
7.07
7.04
3.89
3.84
O
N
OMe
5g
1.00
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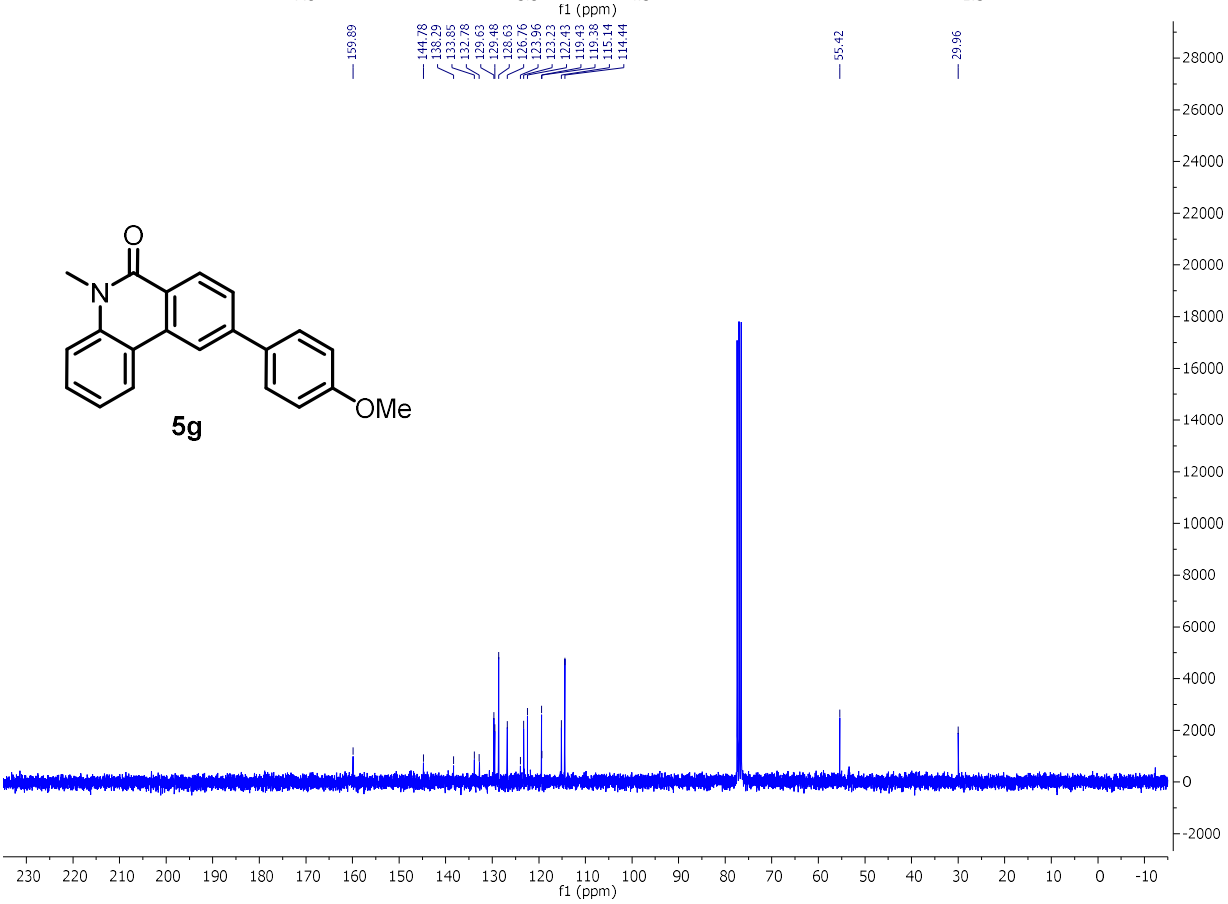
1.04
1.04
1.07
1.02
1.06
2.01
3.02
3.02
f1 (ppm)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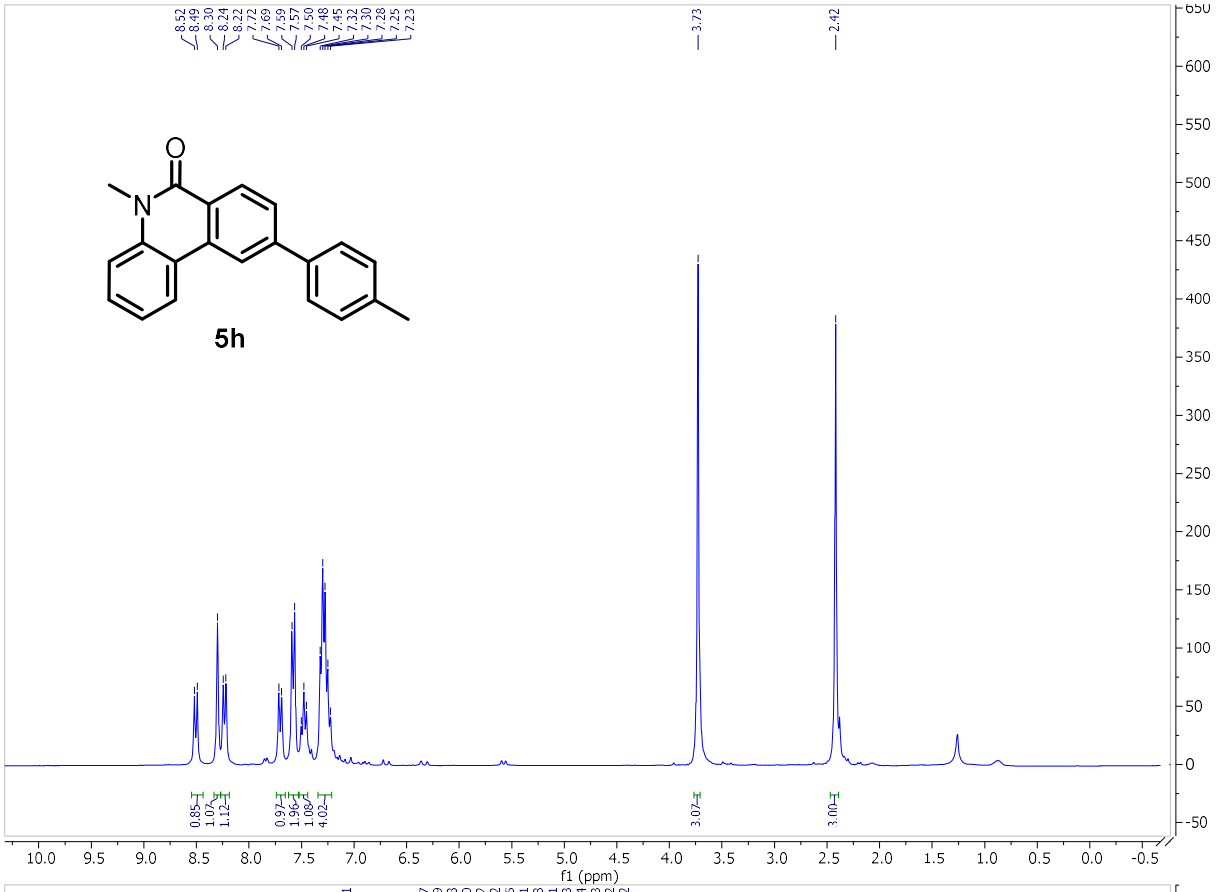
29.96
O
N
OMe
5g
f1 (ppm)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7.48
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7.32
7.30
7.28
7.25
7.23
3.73
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1.07
1.12
0.97
1.96
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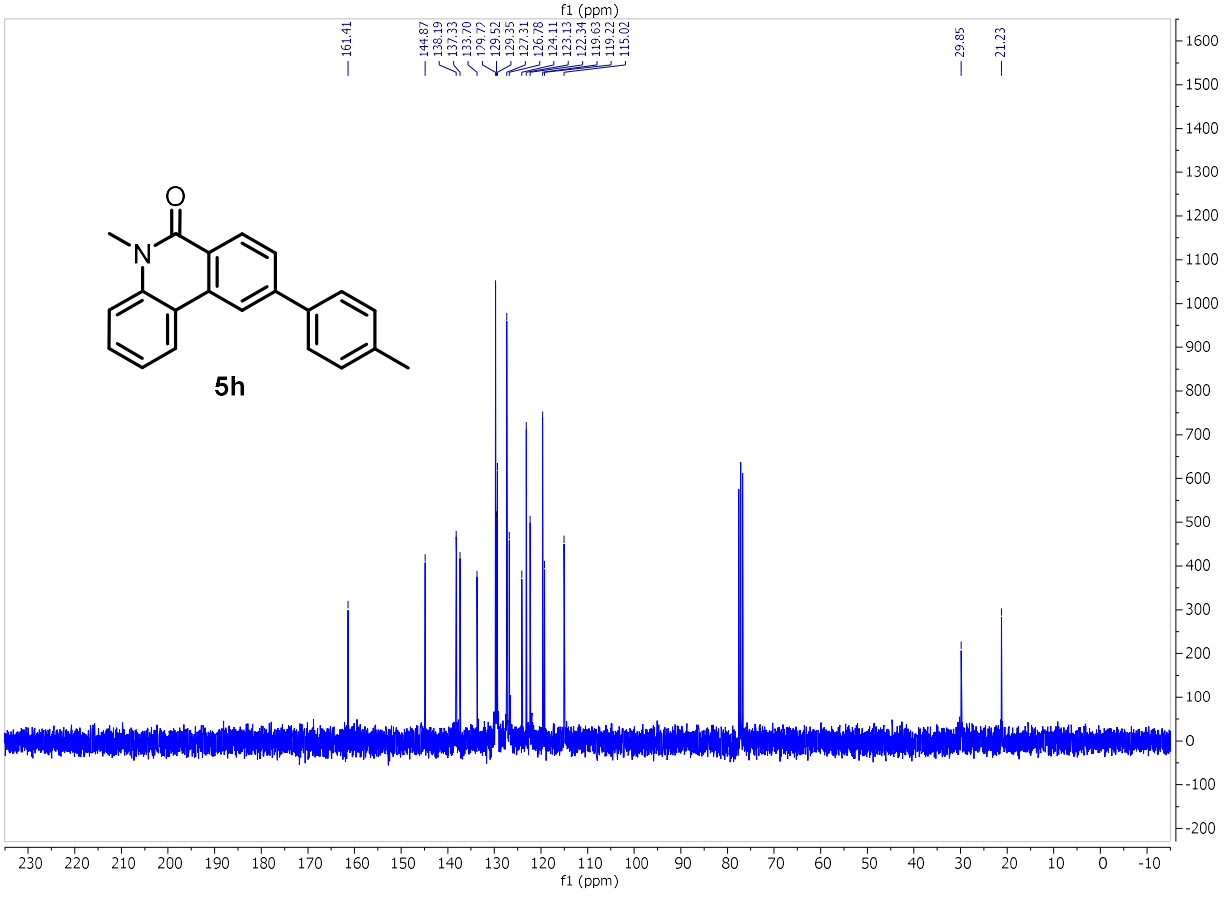
4.02
3.07
3.00
f1 (ppm)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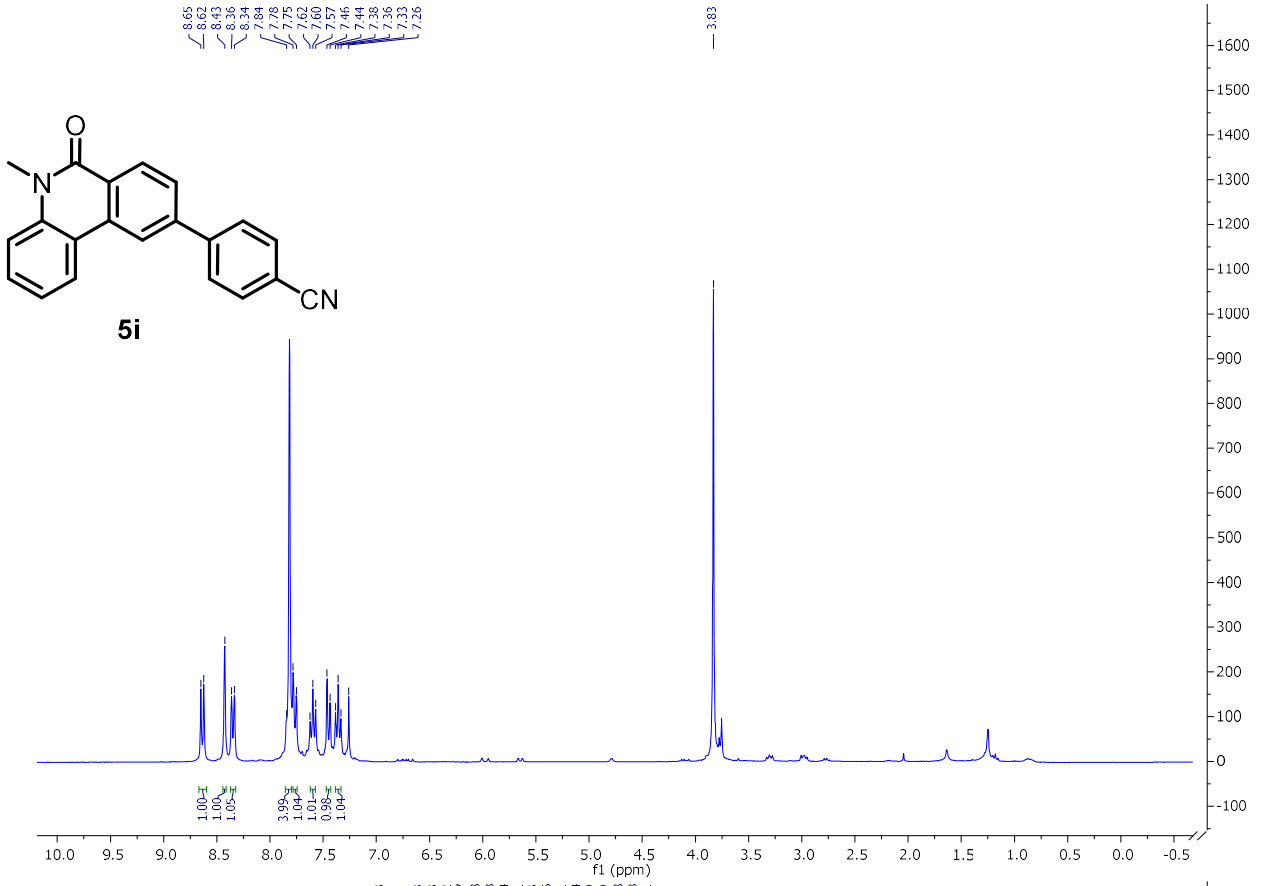
5h
f1 (ppm)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7.26
3.83
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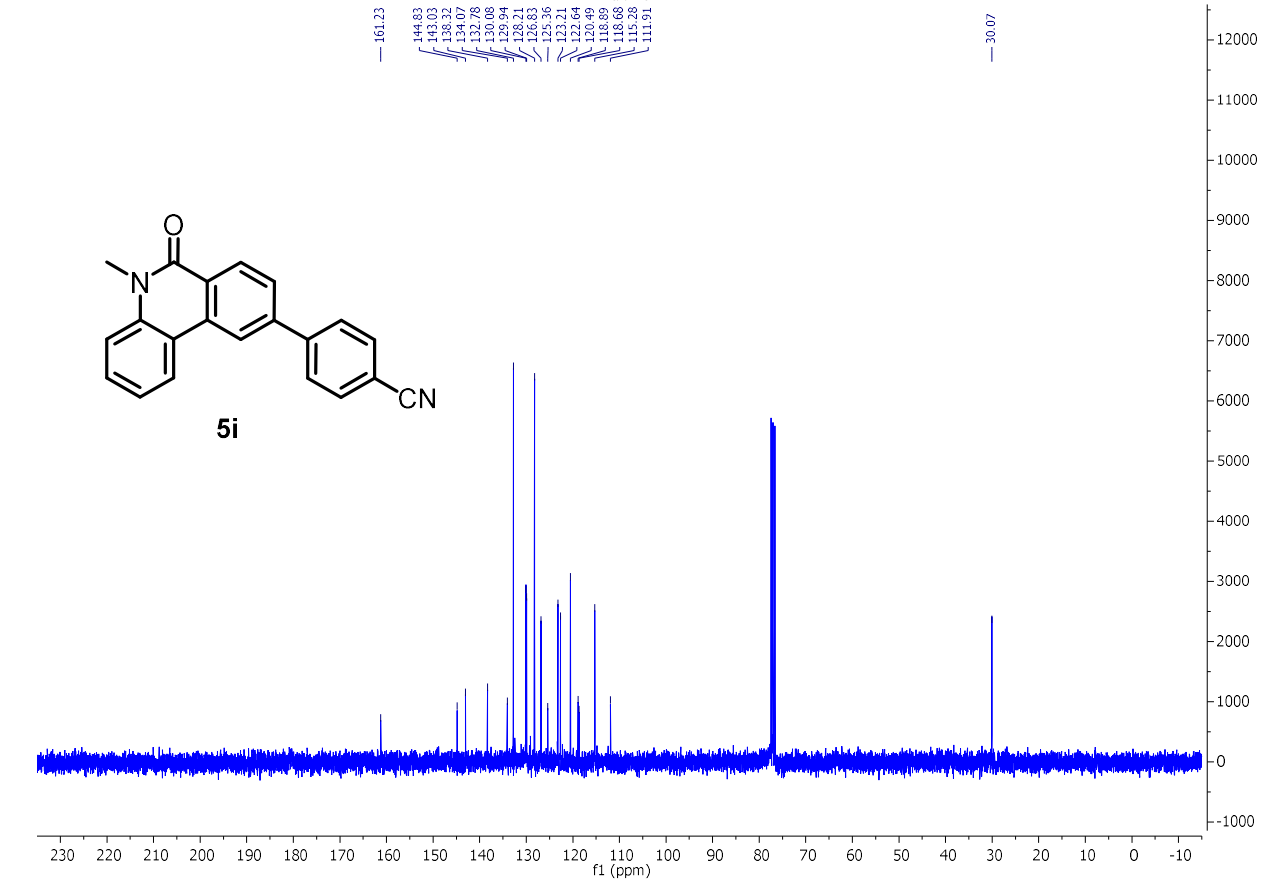
1.04
f1 (ppm)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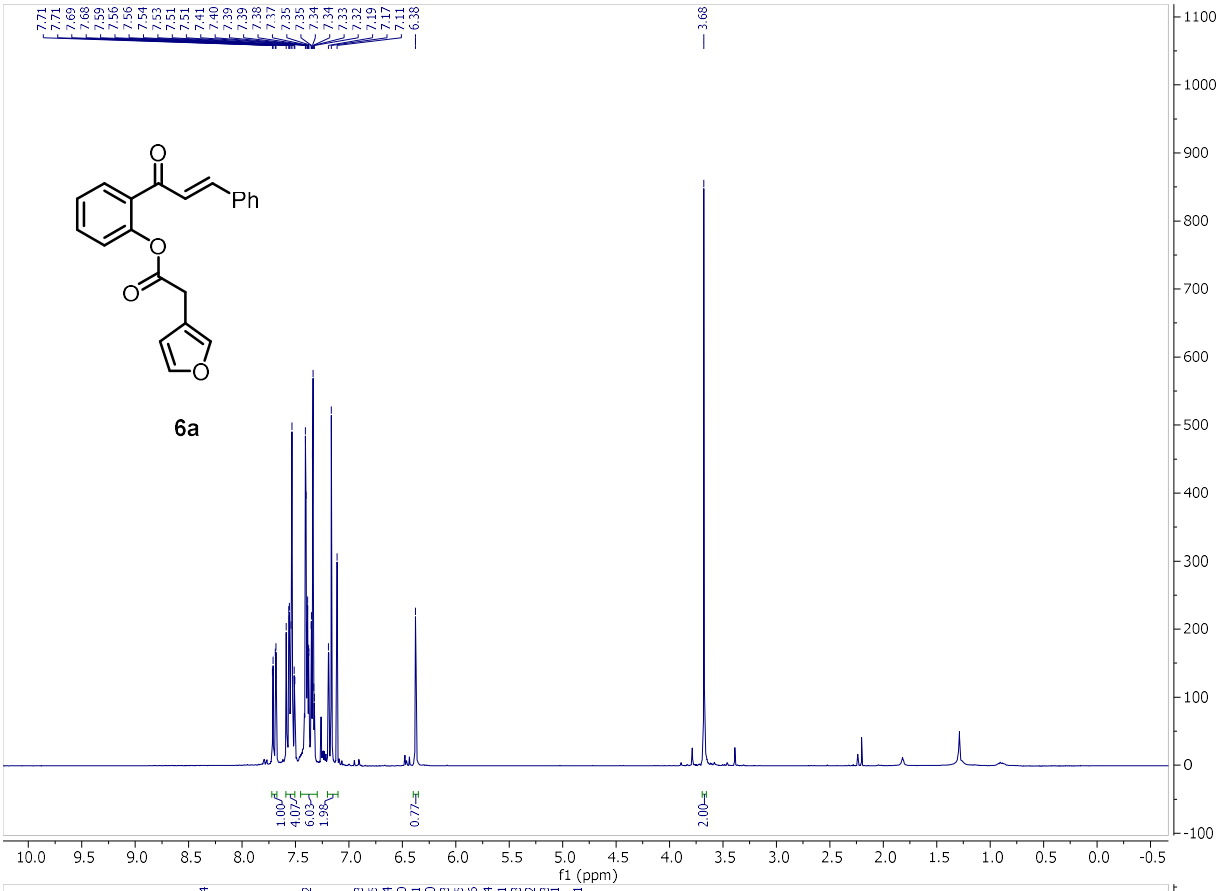
30.07
O
N
CN
5i
f1 (ppm)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7.17
7.11
6.38
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O
O
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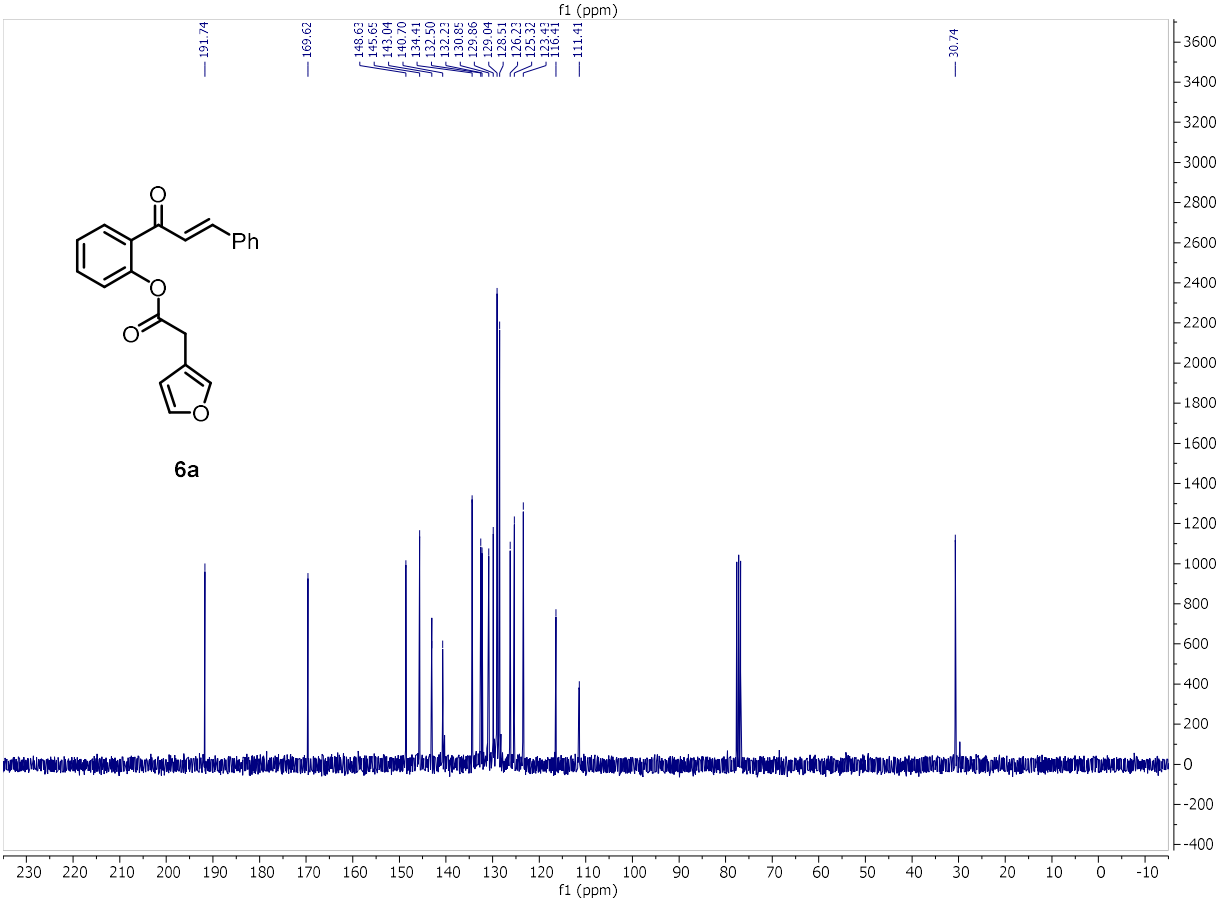
f1 (ppm)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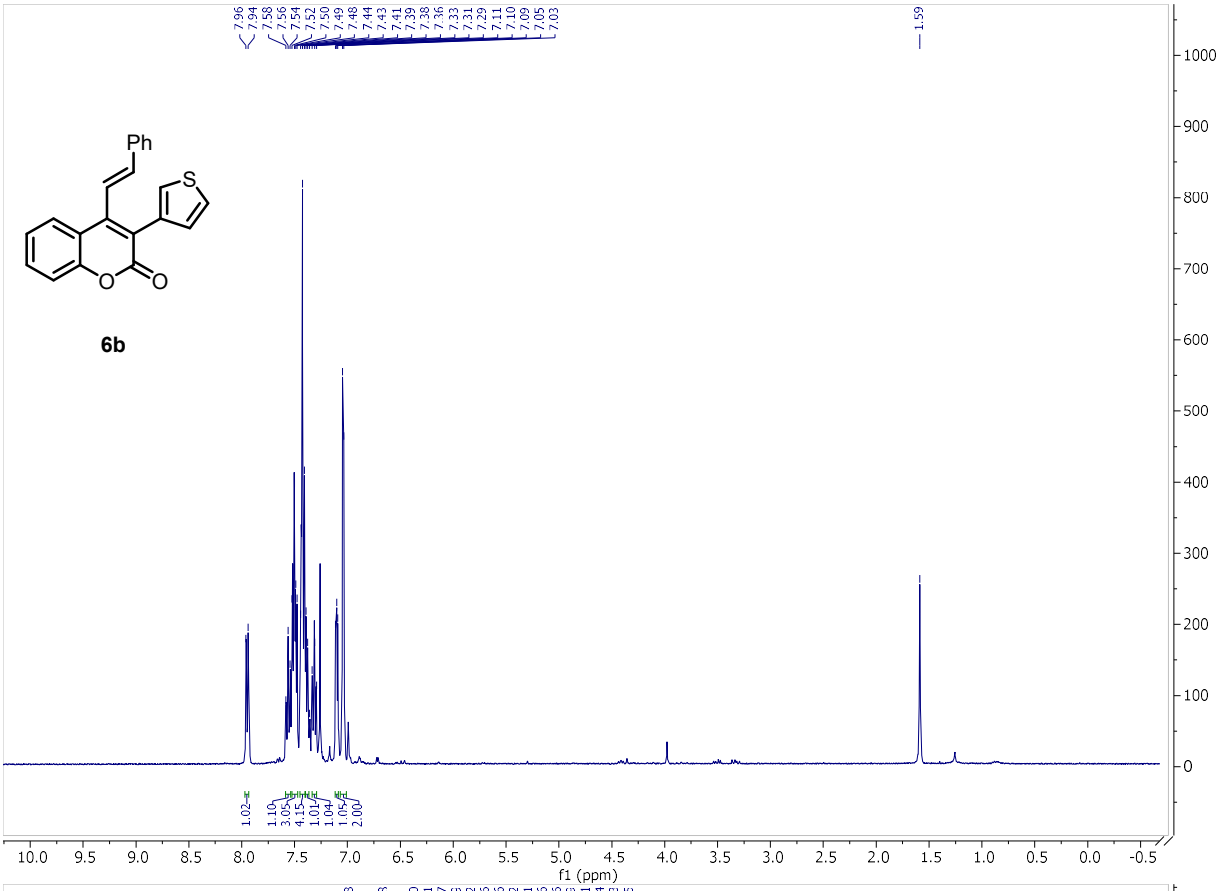
111.41
30.74
Ph
O
O
O
O
6a
f1 (ppm)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7.41
7.39
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7.36
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1.04
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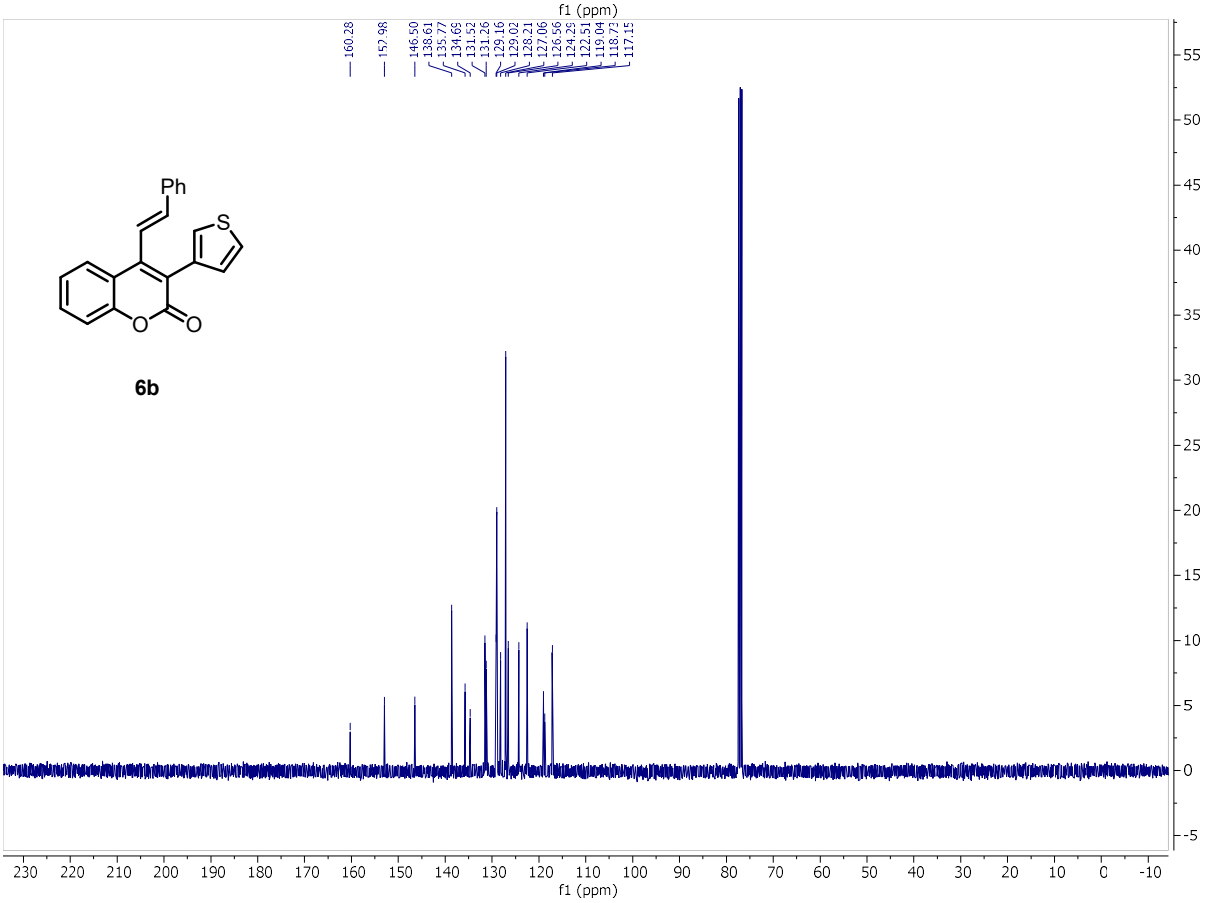
2.00
f1 (ppm)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6b
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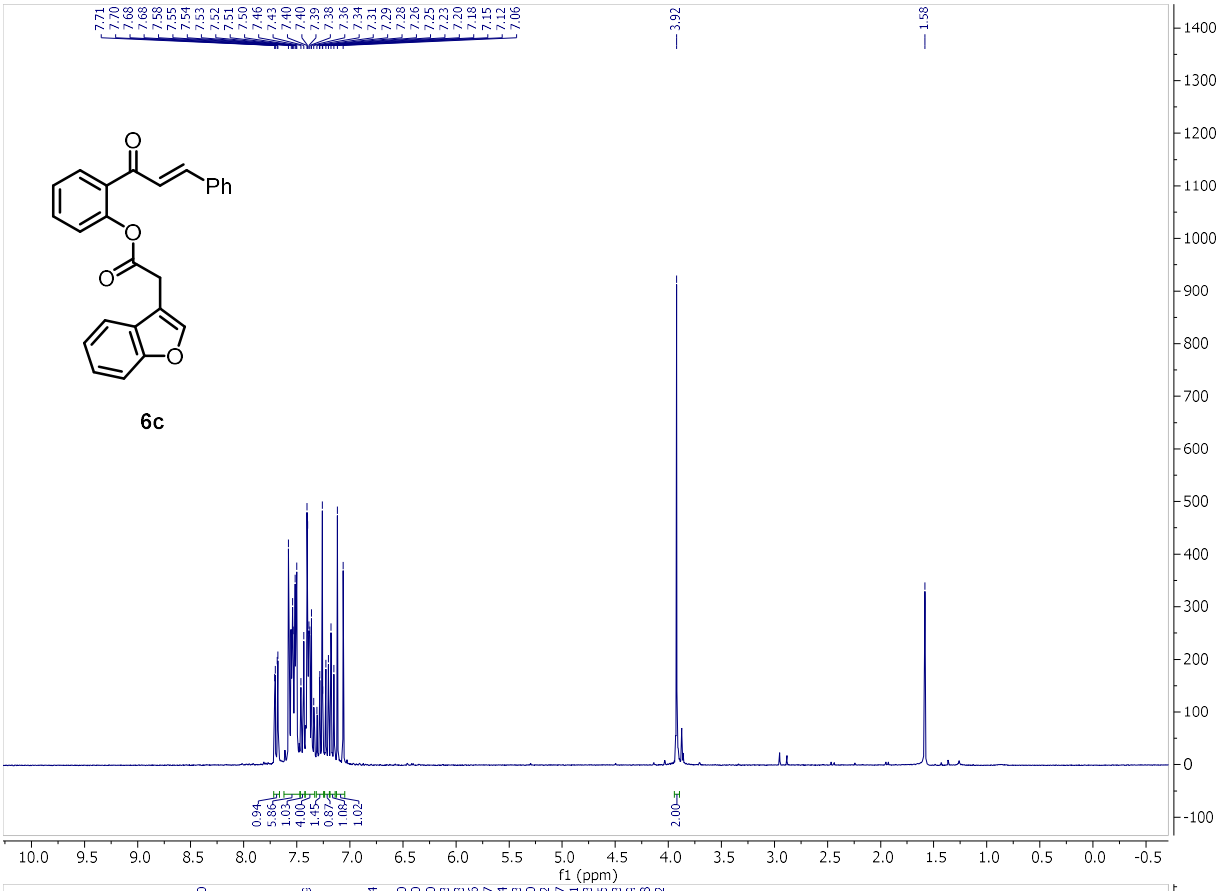
f1 (ppm)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7.23
7.20
7.18
7.15
7.12
7.06
3.92
1.58
Ph
O
O
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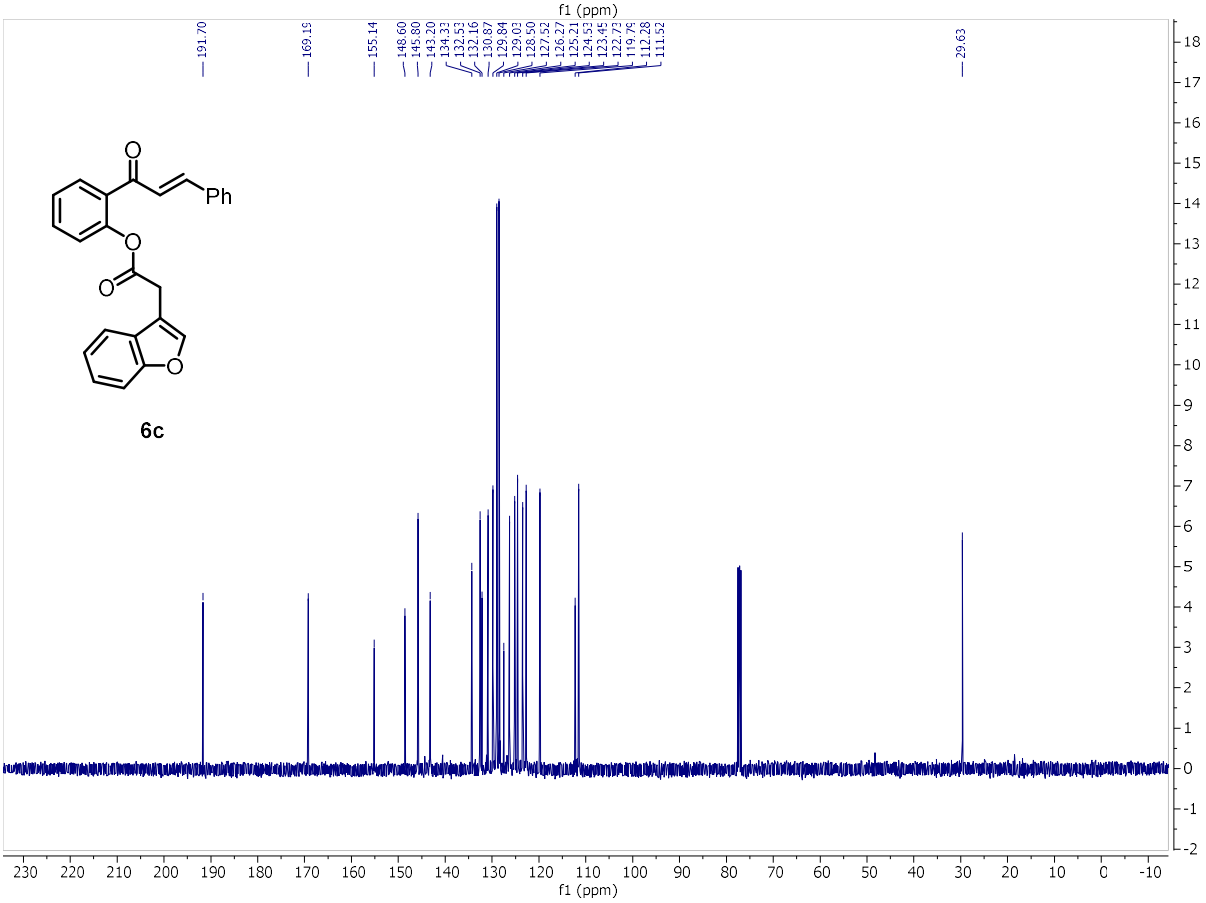
2.00
f1 (ppm)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127.52
126.27
125.21
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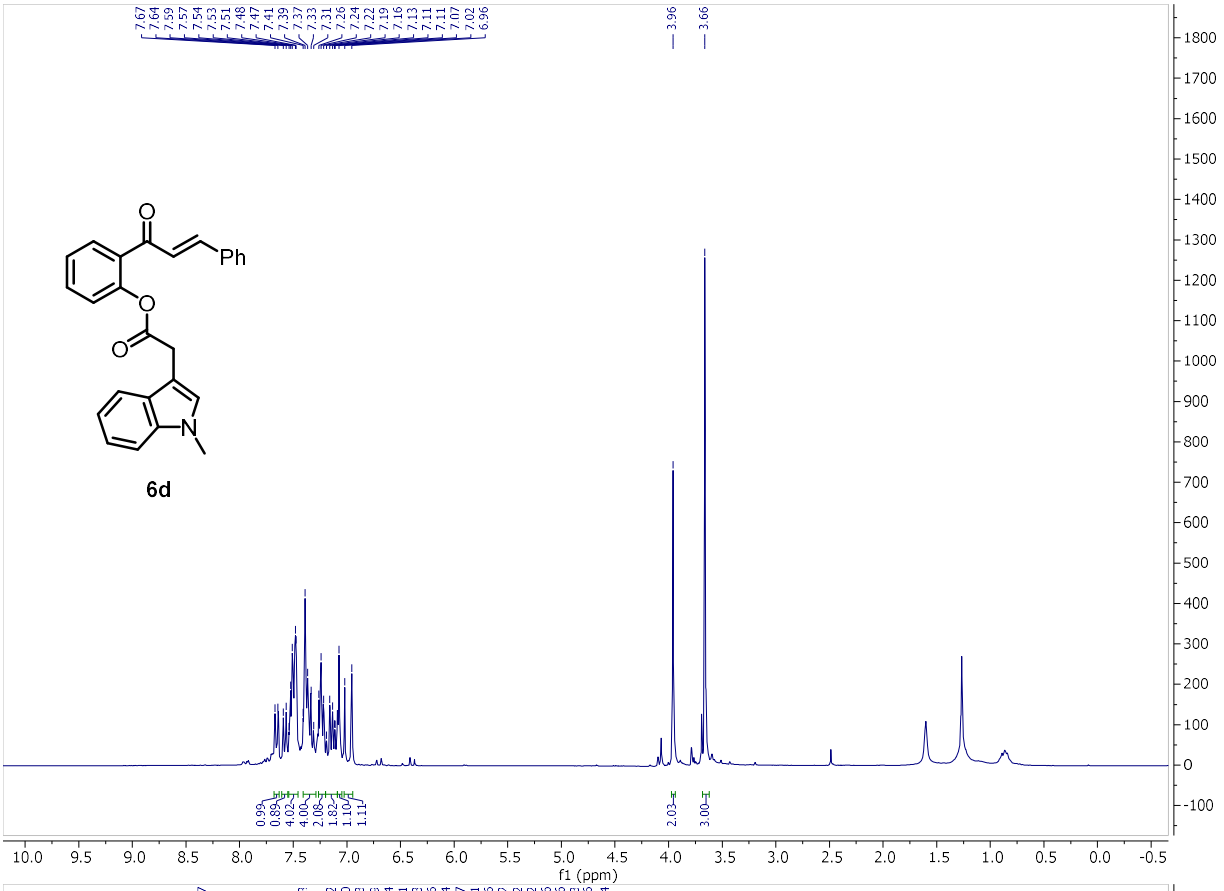
119.75
112.28
111.52
29.63
Ph
O
O
O
O
6c
f1 (ppm)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7.31
7.26
7.24
7.22
7.19
7.16
7.13
7.11
7.11
7.07
7.02
6.96
3.96
3.66
O
Ph
O
O
N
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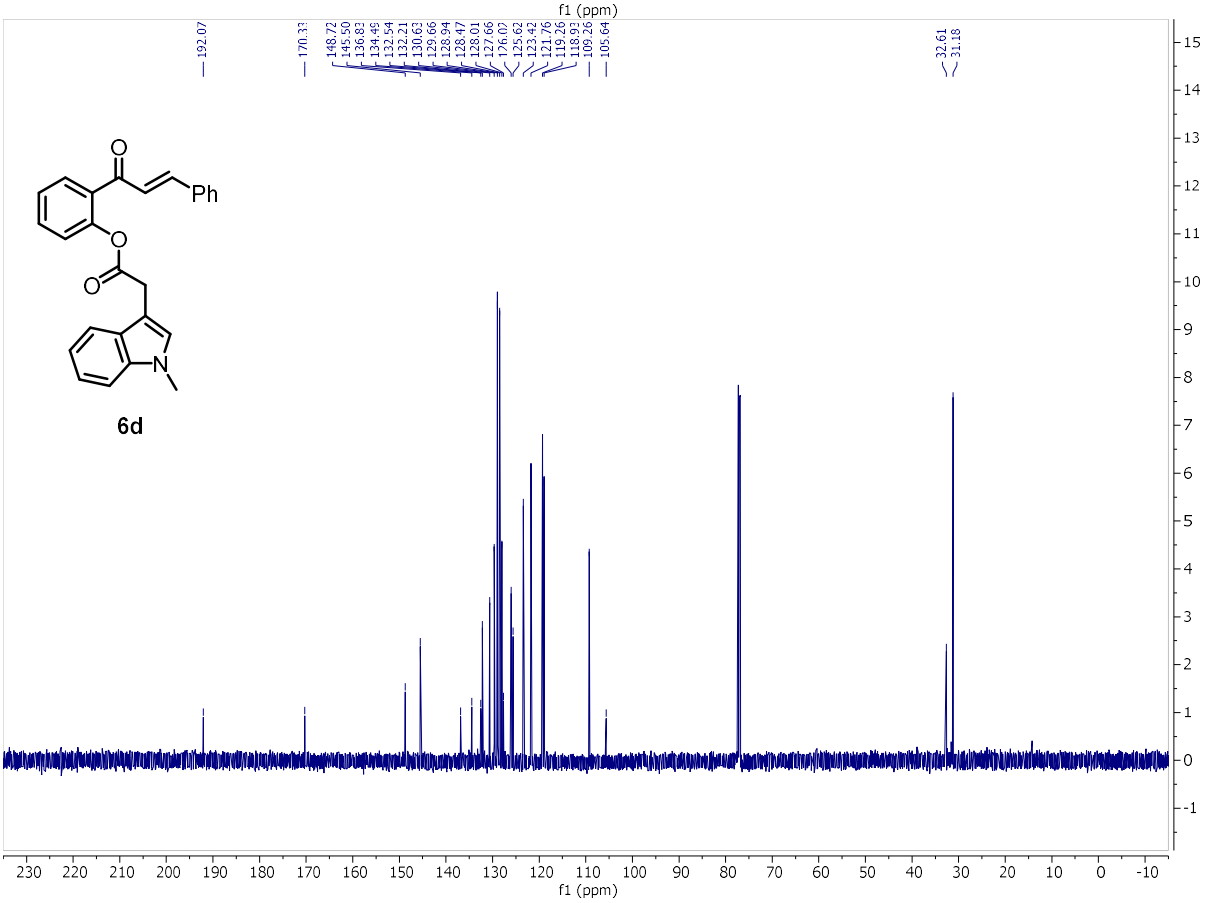
2.08
1.82
1.10
1.11
2.03
3.00
f1 (ppm)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128.94
128.47
128.01
127.66
126.02
125.62
123.42
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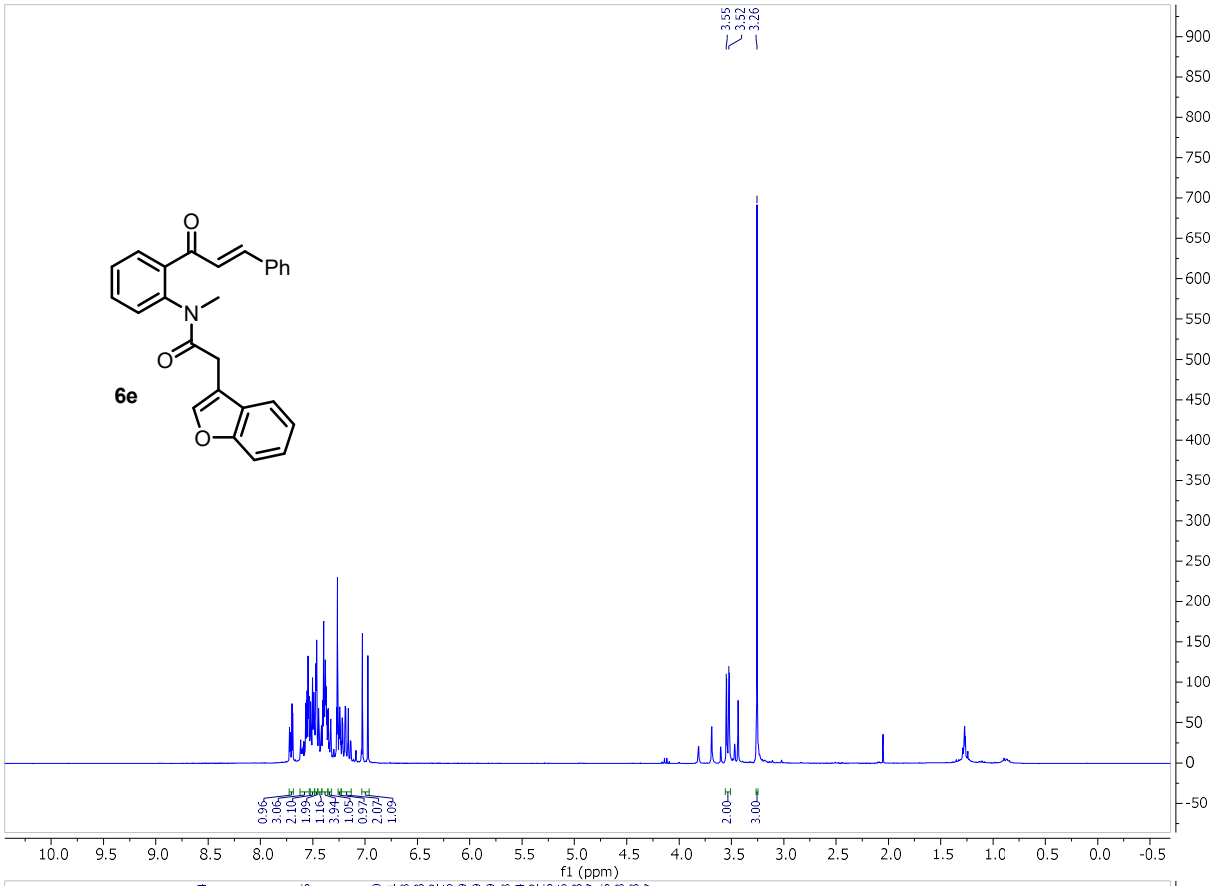
Ph
O
O
N
6d
f1 (ppm)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1.05
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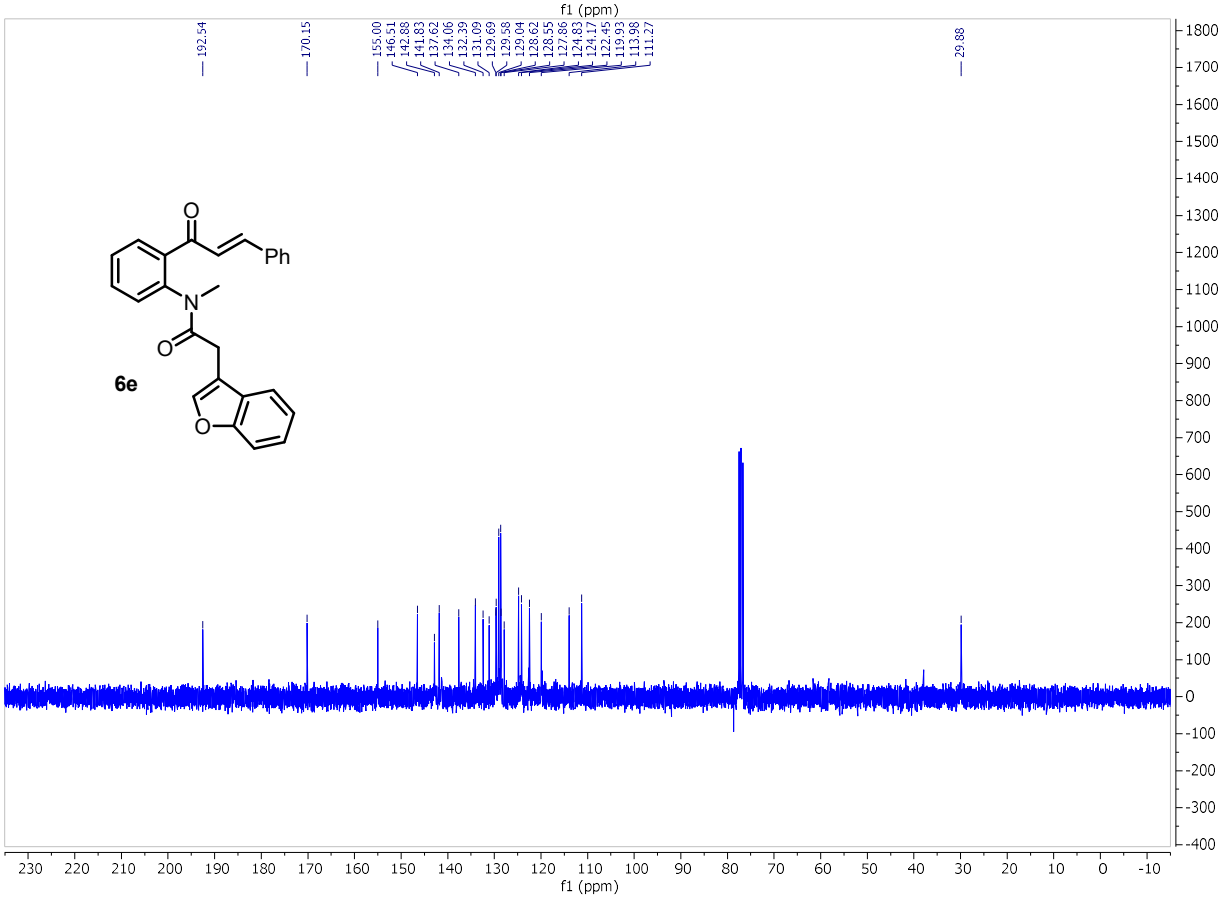
1.09
2.00
3.00
f1 (ppm)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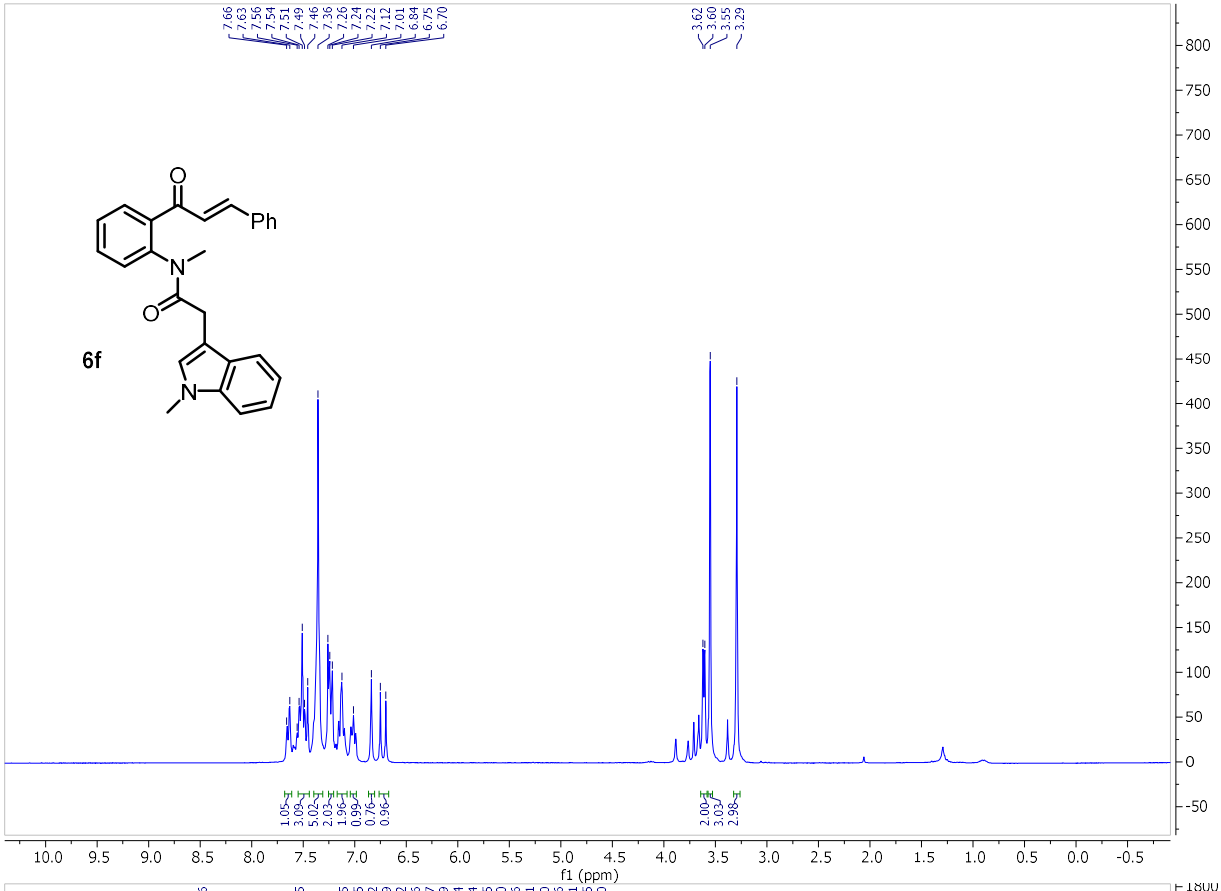
129.58
129.04
128.62
128.55
127.86
124.83
124.17
122.45
119.93
113.98
111.27
29.88
f1 (ppm)

O
Ph
N
O
O

6e

O
Ph
N
O
O

6e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7.56
7.54
7.51
7.49
7.46
7.36
7.26
7.24
7.22
7.12
7.01
6.84
6.75
6.70
3.62
3.60
3.55
3.29
O
Ph
N
O
N
6f
1.05
3.09
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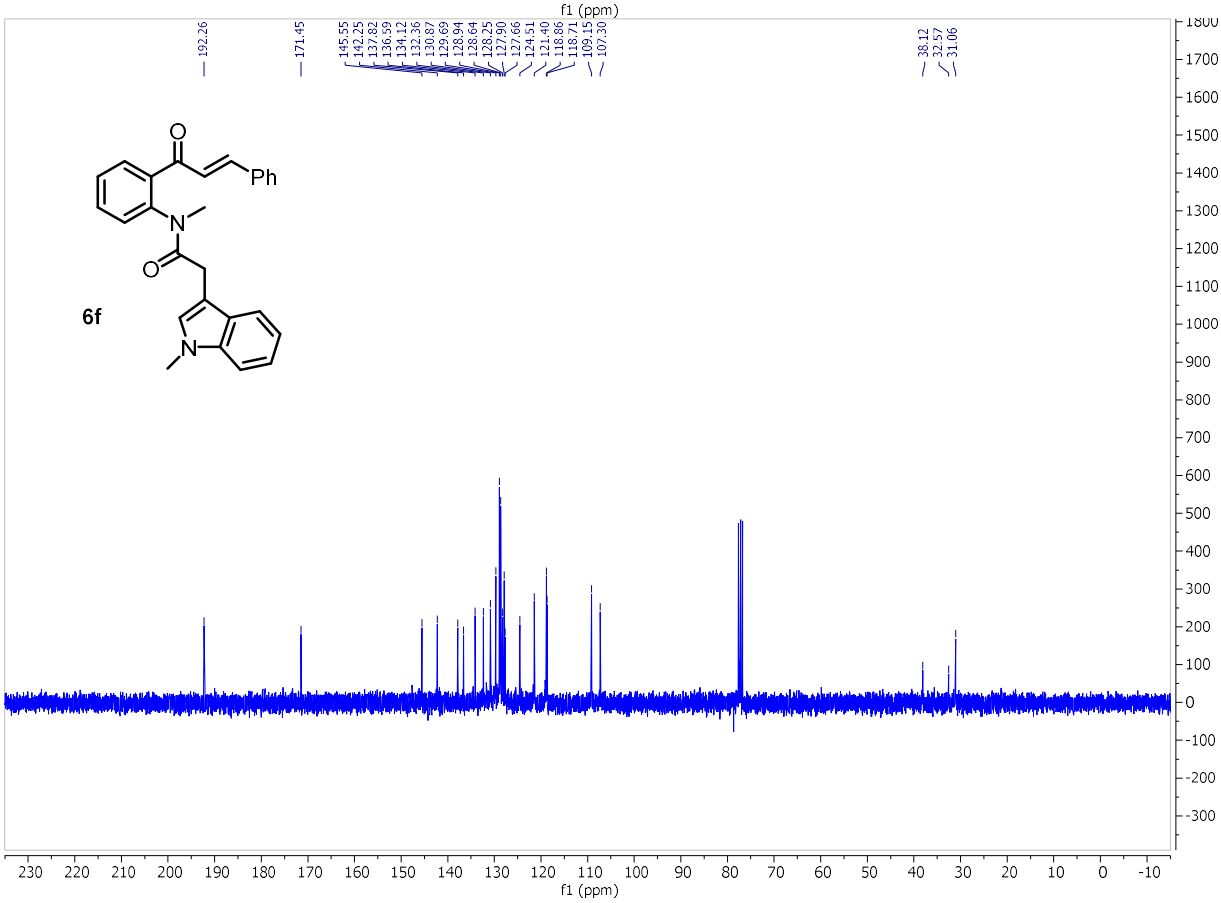
2.03
1.96
0.99
0.76
0.96
2.00
3.03
2.98
f1 (ppm)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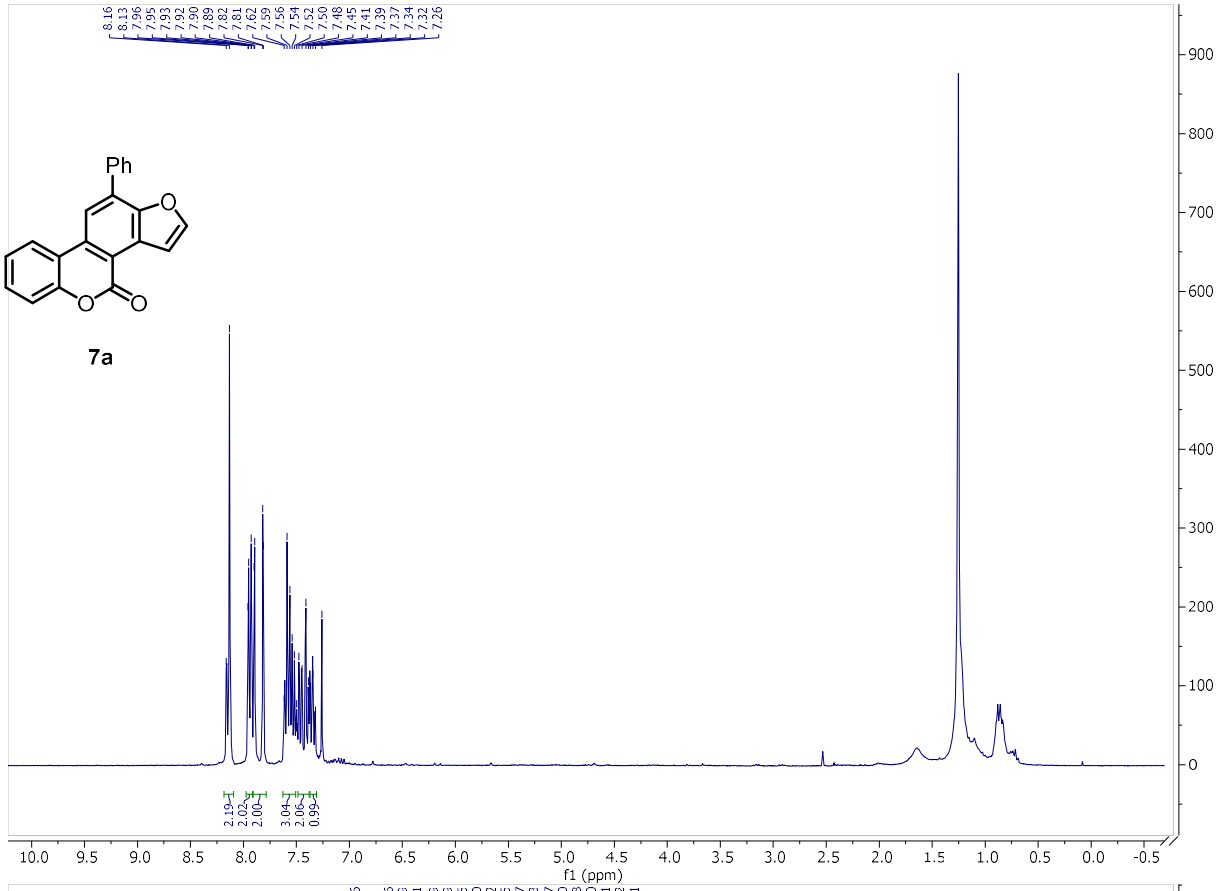
136.59
134.12
132.36
130.87
129.69
128.94
128.64
128.25
127.90
127.66
124.51
121.40
118.86
118.71
109.15
107.30
38.12
32.57
31.06
O
Ph
N
O
N
6f
f1 (ppm)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8.13
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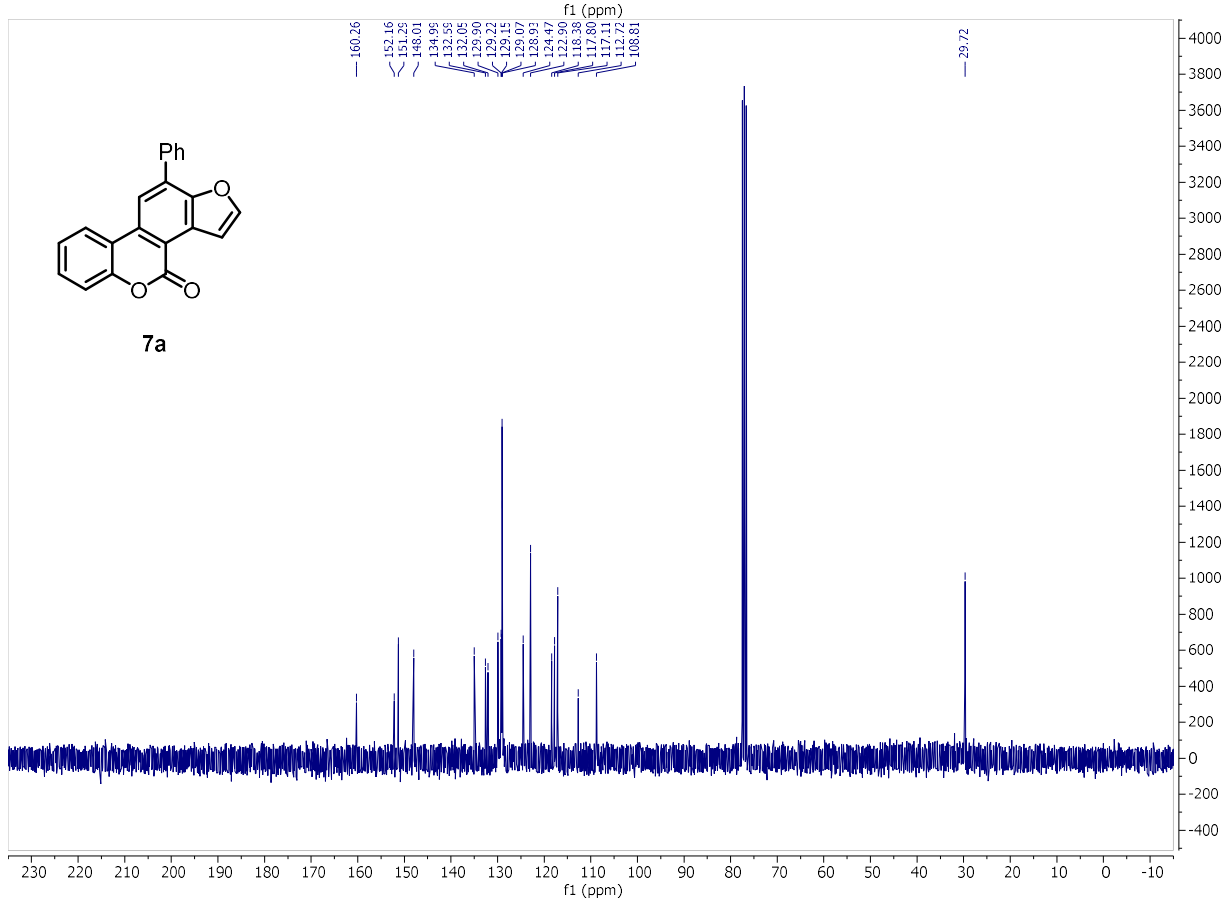
7.95
7.93
7.92
7.90
7.89
7.82
7.81
7.62
7.59
7.56
7.54
7.52
7.50
7.48
7.45
7.41
7.39
7.37
7.34
7.32
7.26
Ph
O
O
O
7a
2.19
2.02
2.00
3.04
2.06
0.99
f1 (ppm)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152.16
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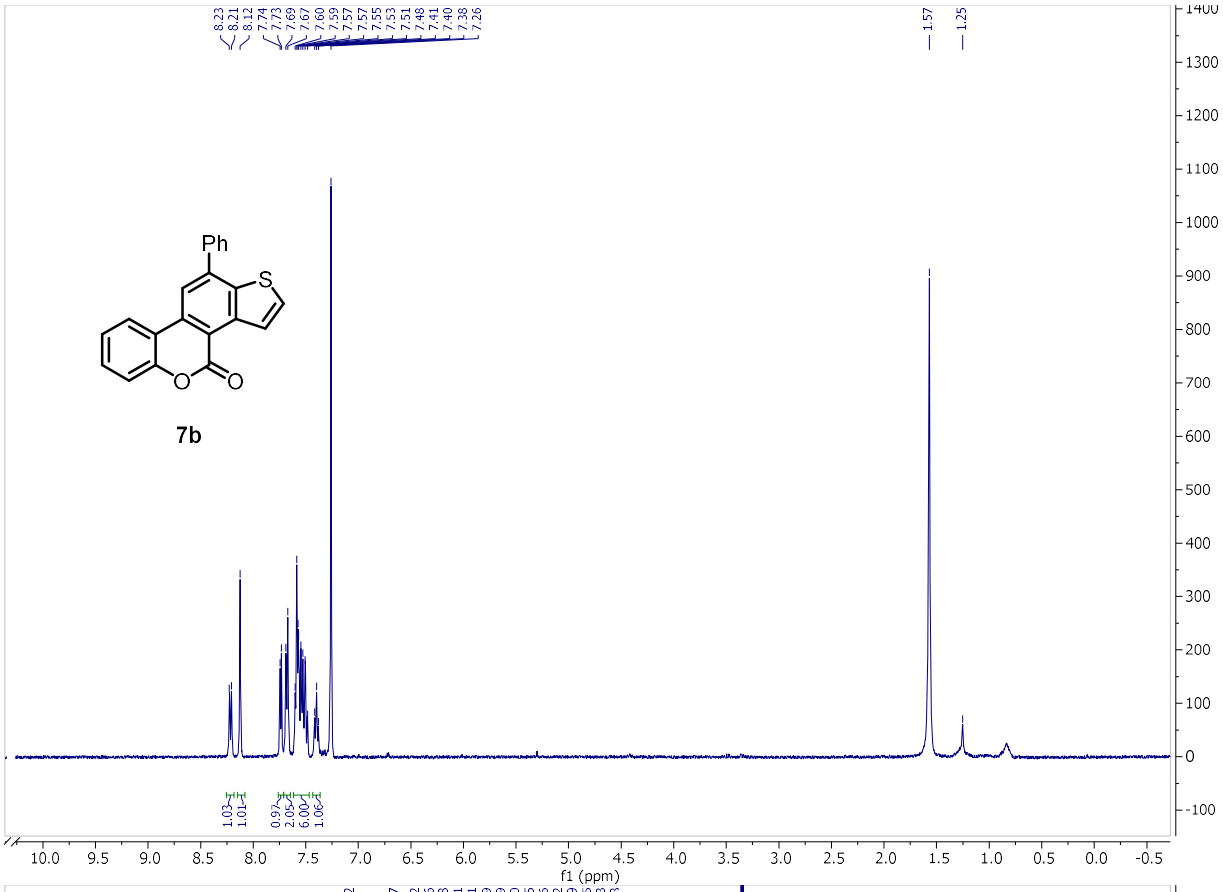
132.55
132.05
129.90
129.22
129.15
129.07
128.91
124.47
122.90
118.38
117.80
117.11
112.72
108.81
29.72
Ph
O
O
O
7a
f1 (ppm)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8.21
8.12
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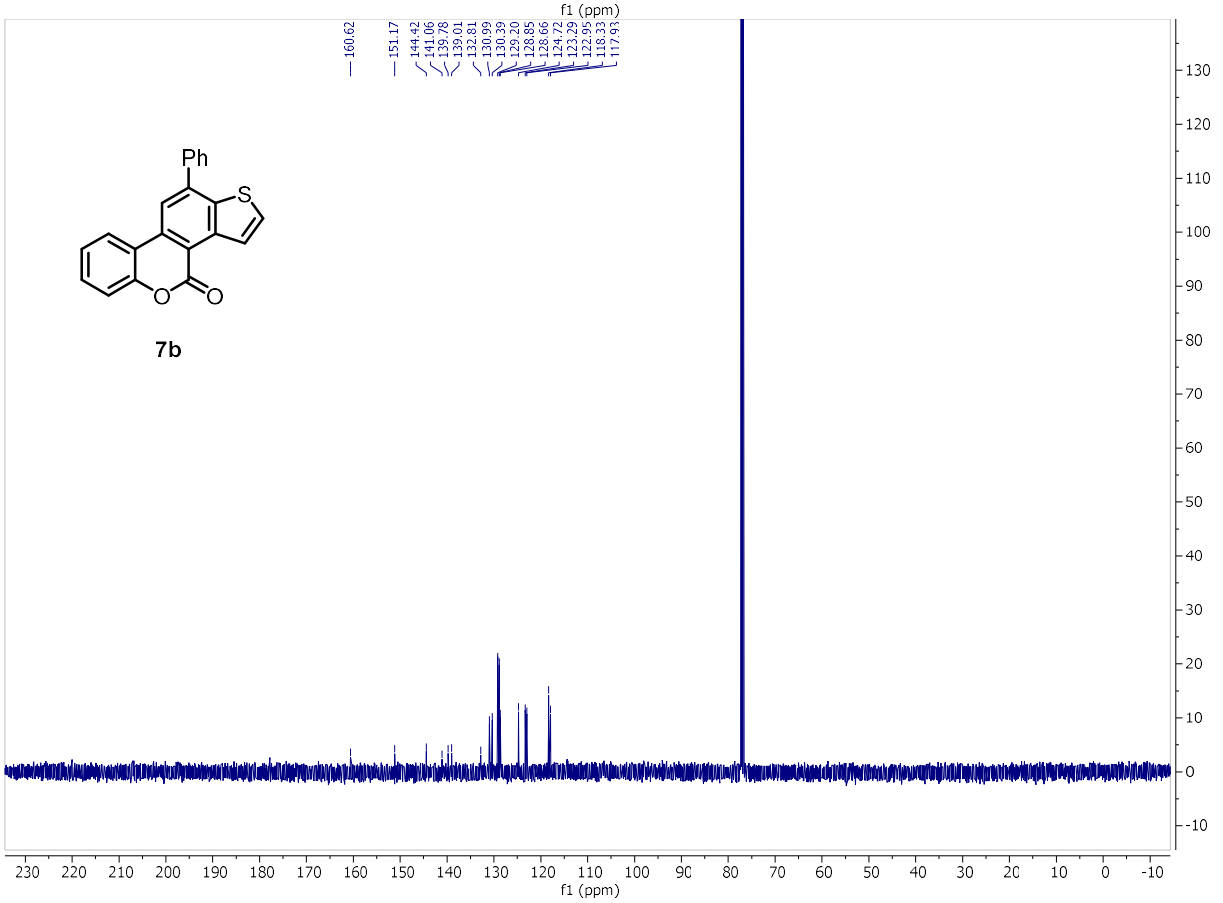
7.67
7.60
7.59
7.57
7.57
7.55
7.53
7.51
7.48
7.41
7.40
7.38
7.26
1.57
1.25
Ph
S
O
O
7b
1.03
1.01
0.97
2.05
6.00
1.06
f1 (ppm)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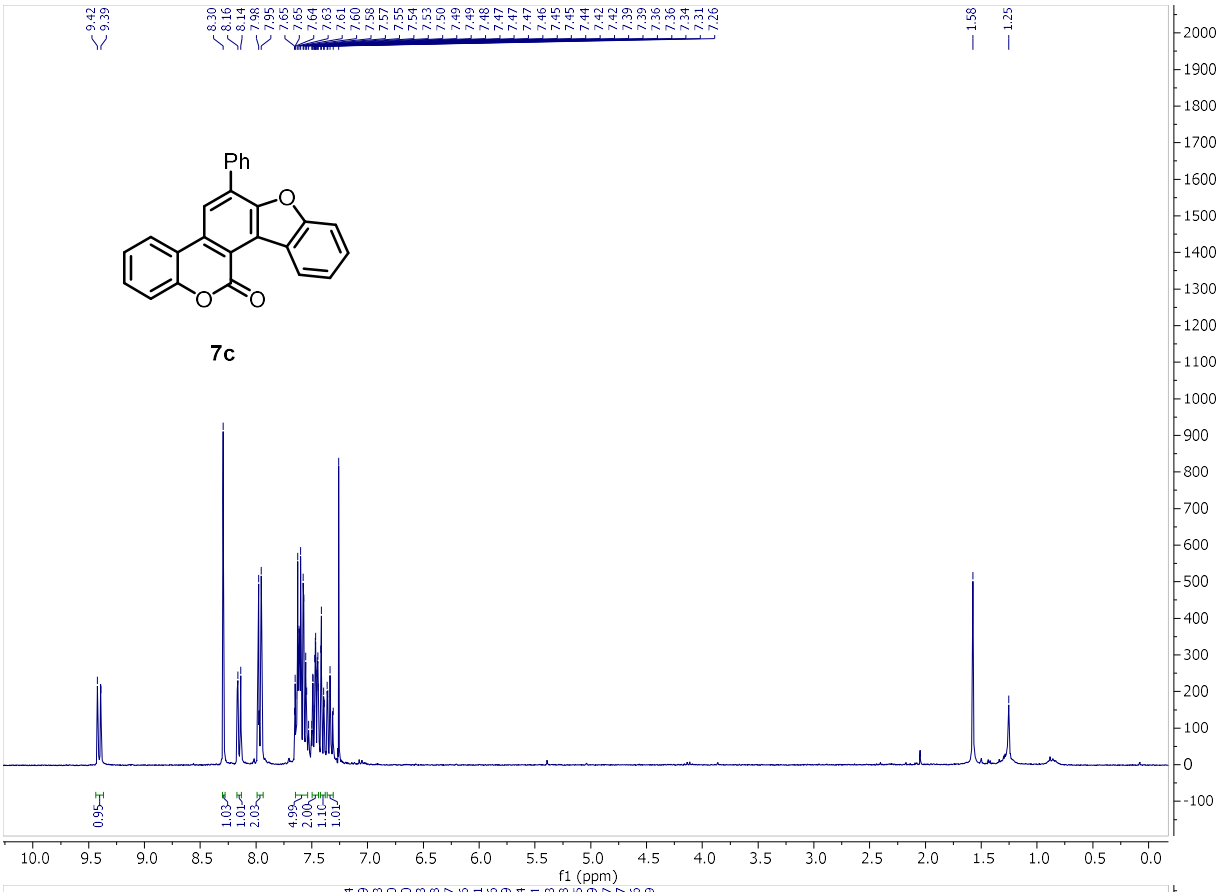
139.01
132.81
130.99
130.39
129.20
128.85
128.66
124.72
123.28
122.93
118.33
117.91
Ph
S
O
O
7b
f1 (ppm)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7.63
7.61
7.60
7.58
7.57
7.55
7.54
7.53
7.50
7.49
7.49
7.48
7.47
7.47
7.47
7.46
7.45
7.45
7.44
7.42
7.42
7.39
7.39
7.36
7.36
7.34
7.31
7.26
1.58
1.25
Ph
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O
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7c
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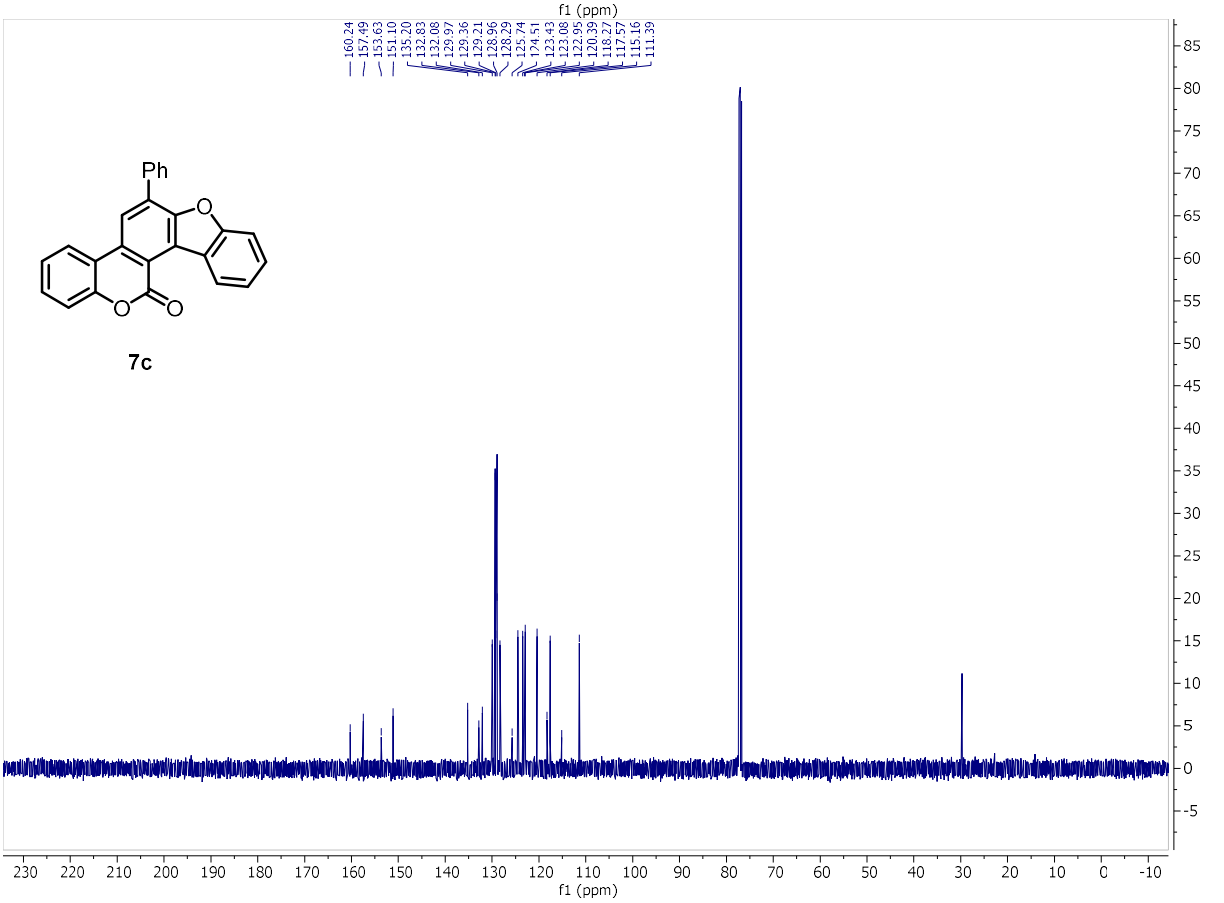
1.03
1.01
2.03
4.99
2.00
1.10
1.01
f1 (ppm)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153.63
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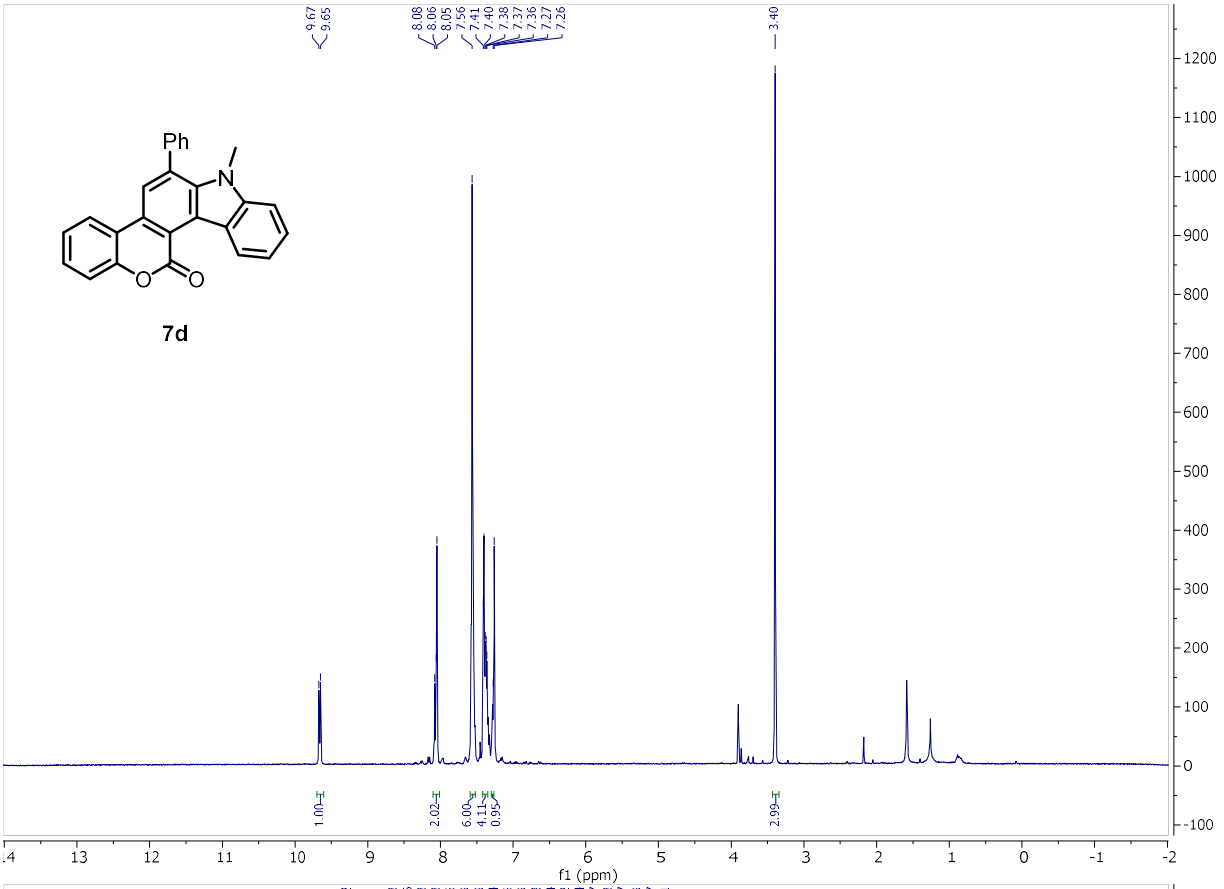
135.20
132.83
132.08
129.97
129.36
129.21
128.96
128.29
125.74
124.51
123.43
123.08
122.95
120.39
118.27
117.57
115.16
111.39
Ph
O
O
O
7c
f1 (ppm)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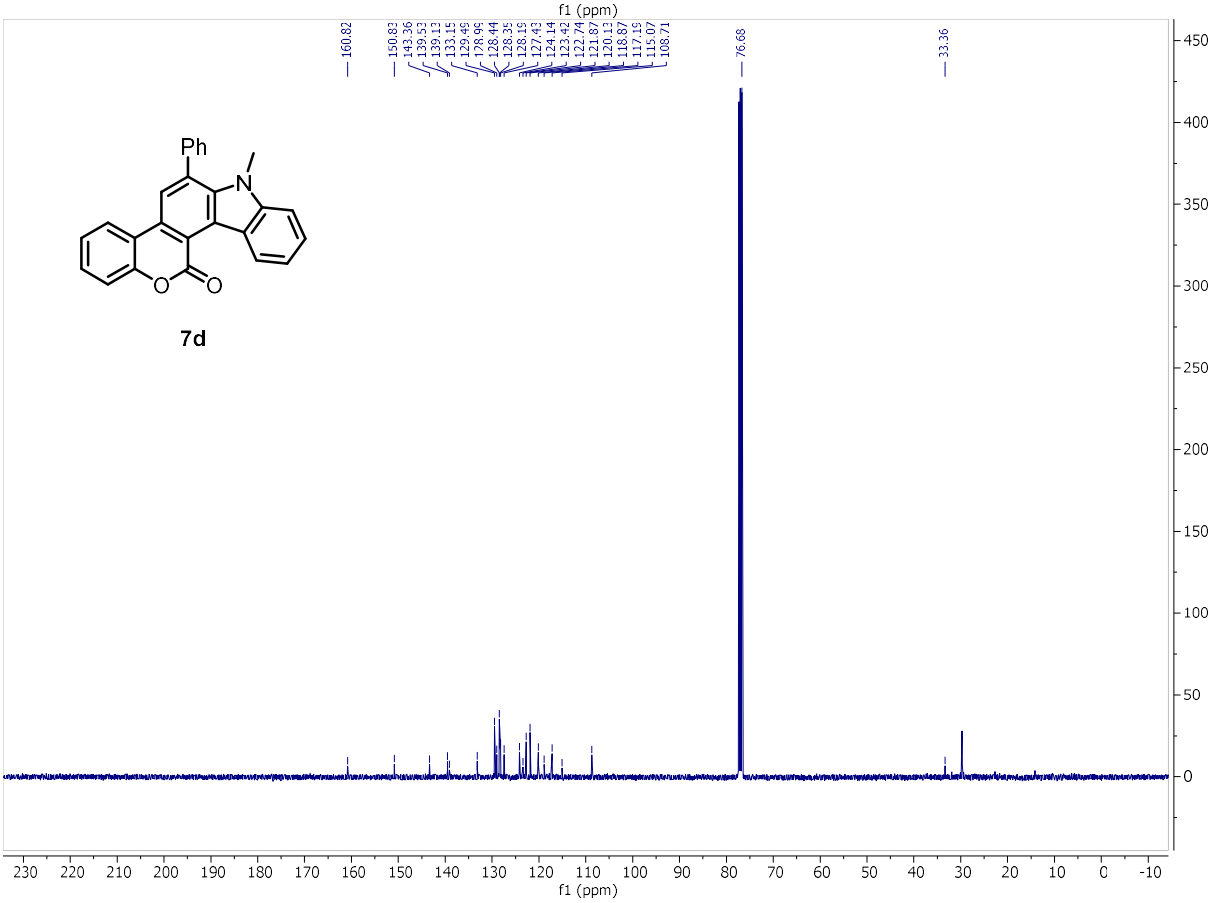
9.65
8.08
8.06
8.05
7.56
7.41
7.40
7.38
7.37
7.36
7.27
7.26
3.40
Ph
N
O
O
1.00
2.02
6.00
4.11
0.95
2.99
f1 (ppm)

7d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143.36
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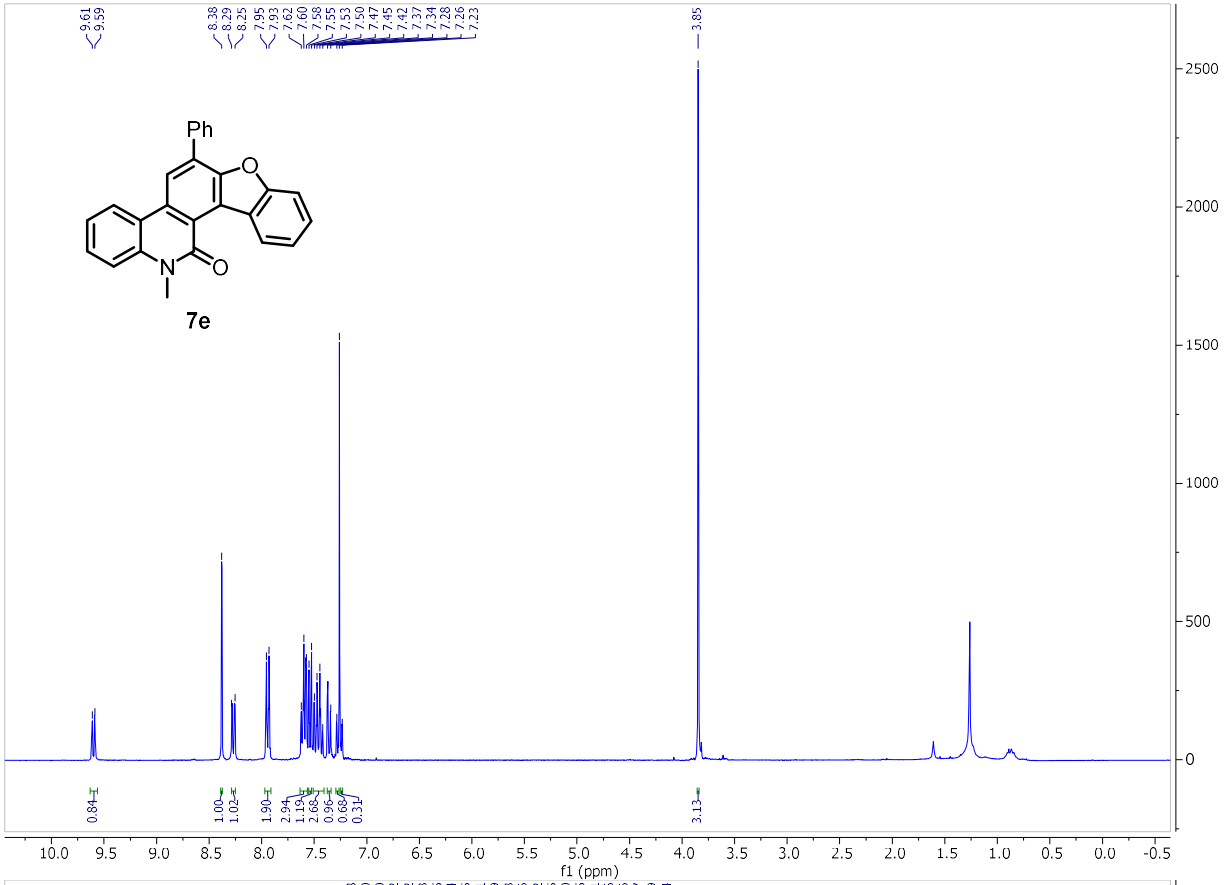
139.13
133.15
129.45
128.96
128.44
128.35
128.15
127.43
124.14
123.42
122.74
121.67
120.13
118.87
117.45
115.07
108.71
76.68
33.36
Ph
N
O
O
f1 (ppm)

7d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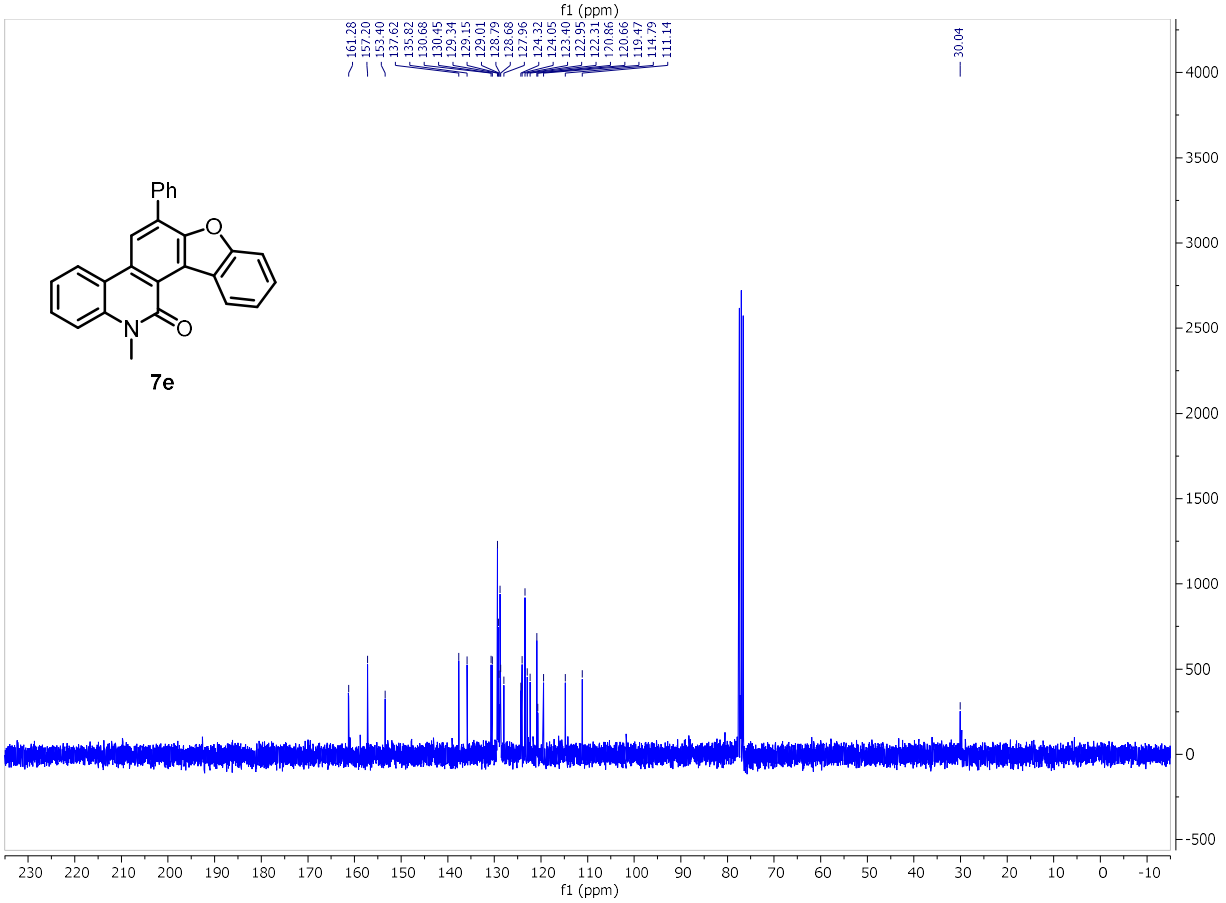
8.29
8.25
7.95
7.93
7.62
7.60
7.58
7.55
7.53
7.50
7.47
7.45
7.42
7.37
7.34
7.28
7.26
7.23
3.85
Ph
O
N
O
7e
0.84
1.00
1.02
1.90
2.94
1.19
2.68
0.96
0.68
0.31
3.13
f1 (ppm)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129.34
129.15
129.01
128.79
128.68
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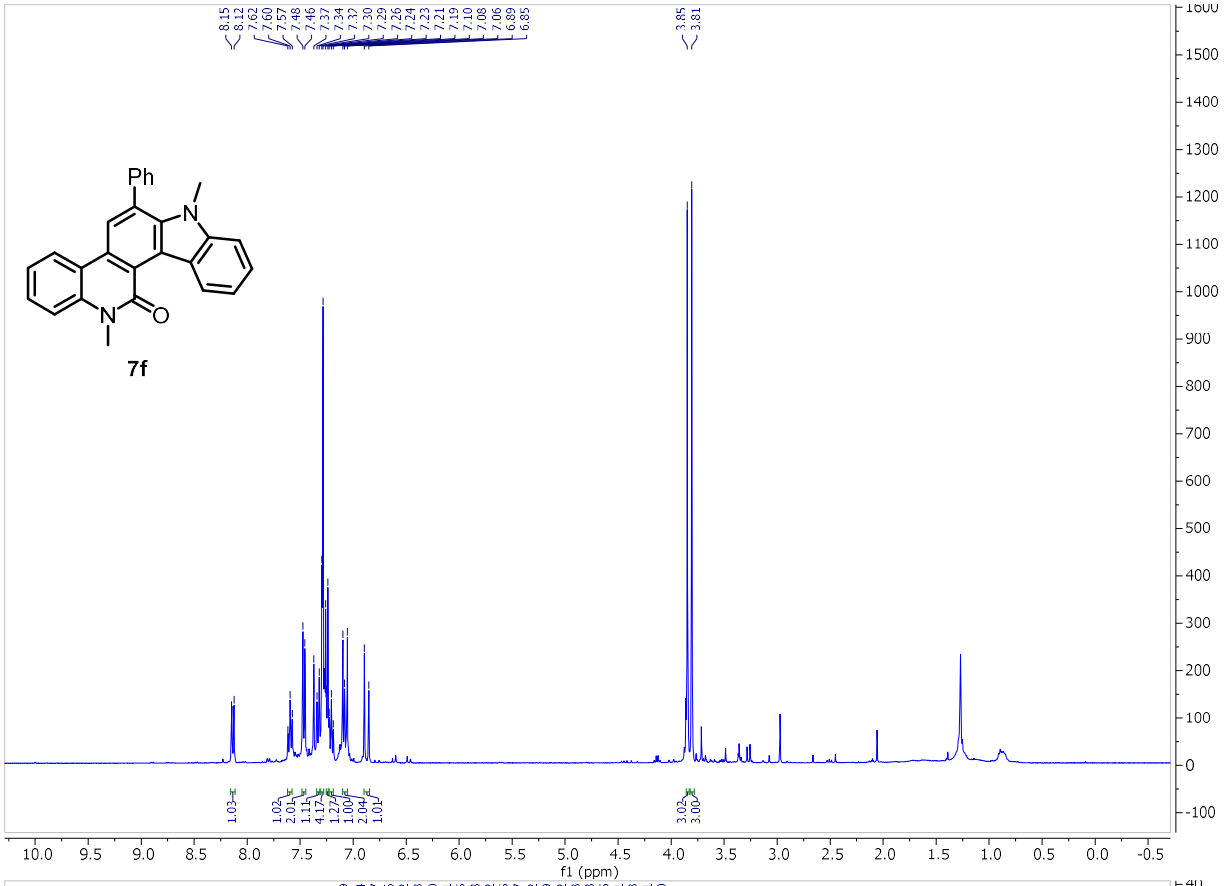
124.32
124.05
123.40
122.95
122.31
120.86
120.66
119.47
114.79
111.14
30.04
Ph
O
N
O
7e
f1 (ppm)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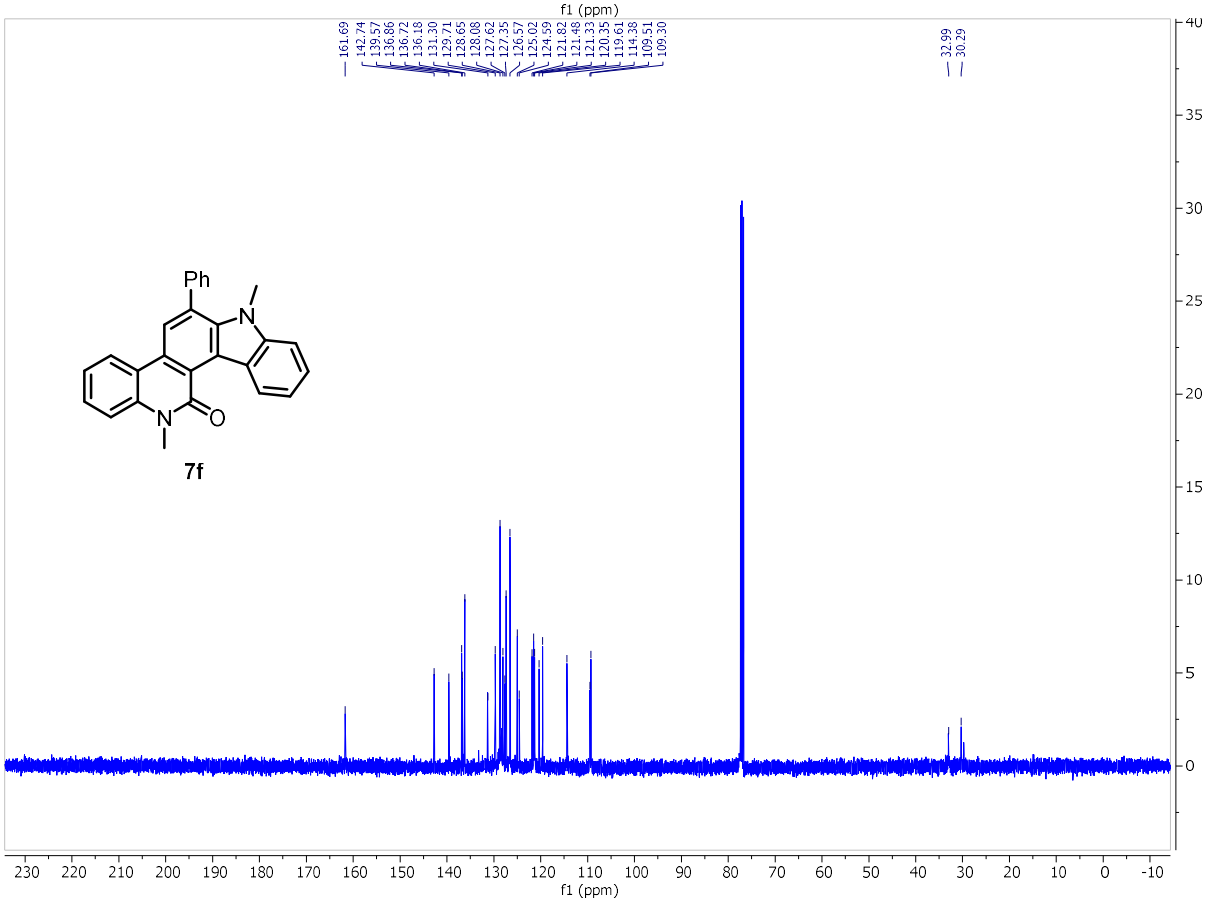
7.57
7.48
7.46
7.37
7.34
7.32
7.30
7.29
7.26
7.24
7.23
7.21
7.19
7.10
7.08
7.06
6.89
6.85
3.85
3.81
Ph
N
N
O
7f
1.03
1.02
2.01
1.11
4.17
1.27
1.00
2.04
1.01
3.03
3.00
f1 (ppm)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136.72
136.18
131.30
129.71
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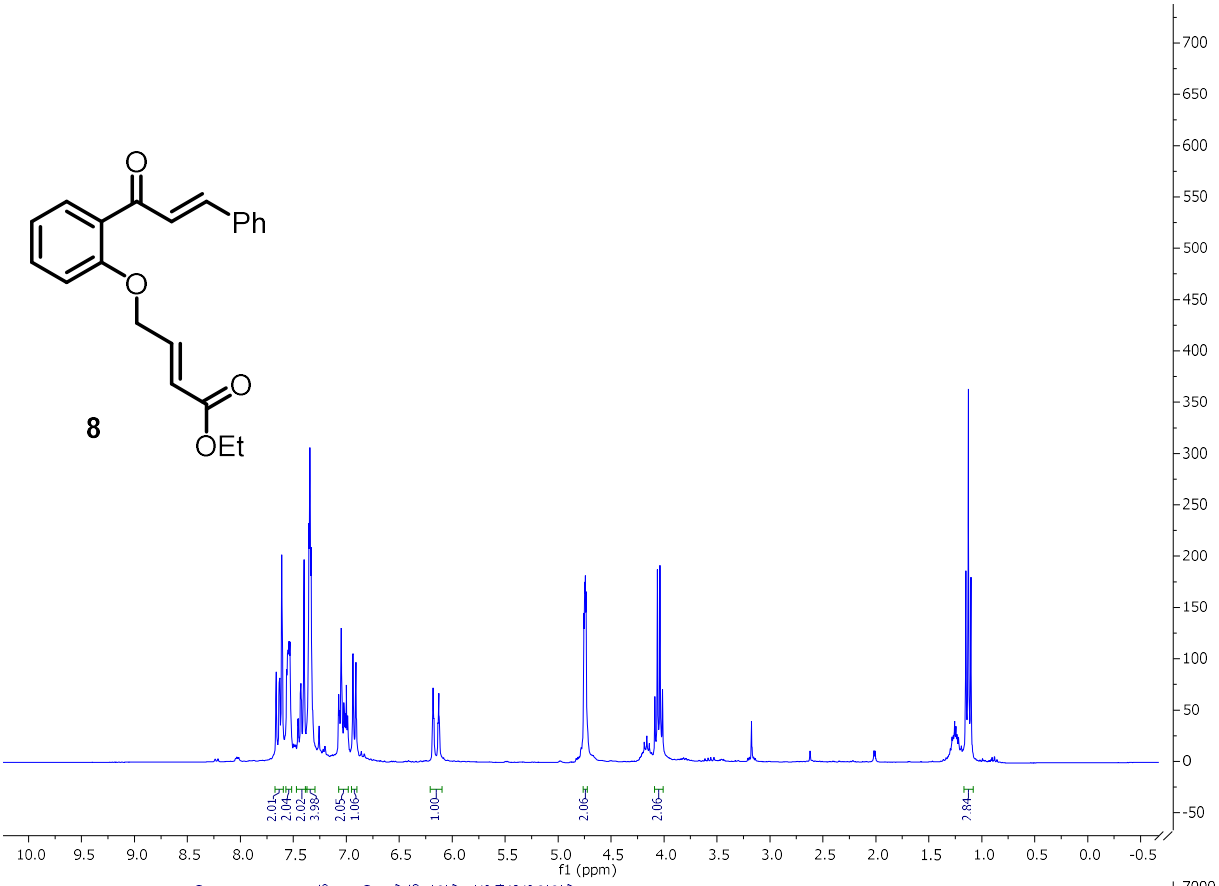
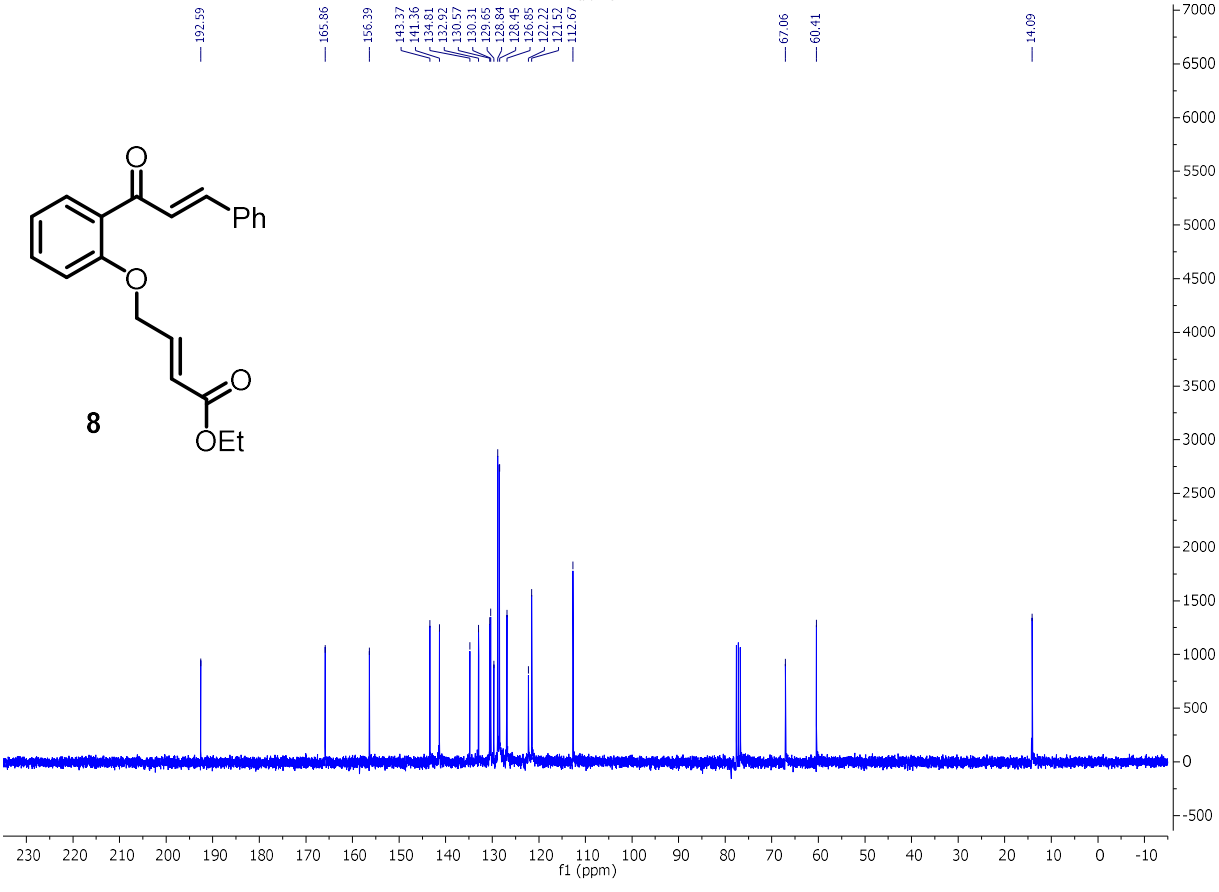
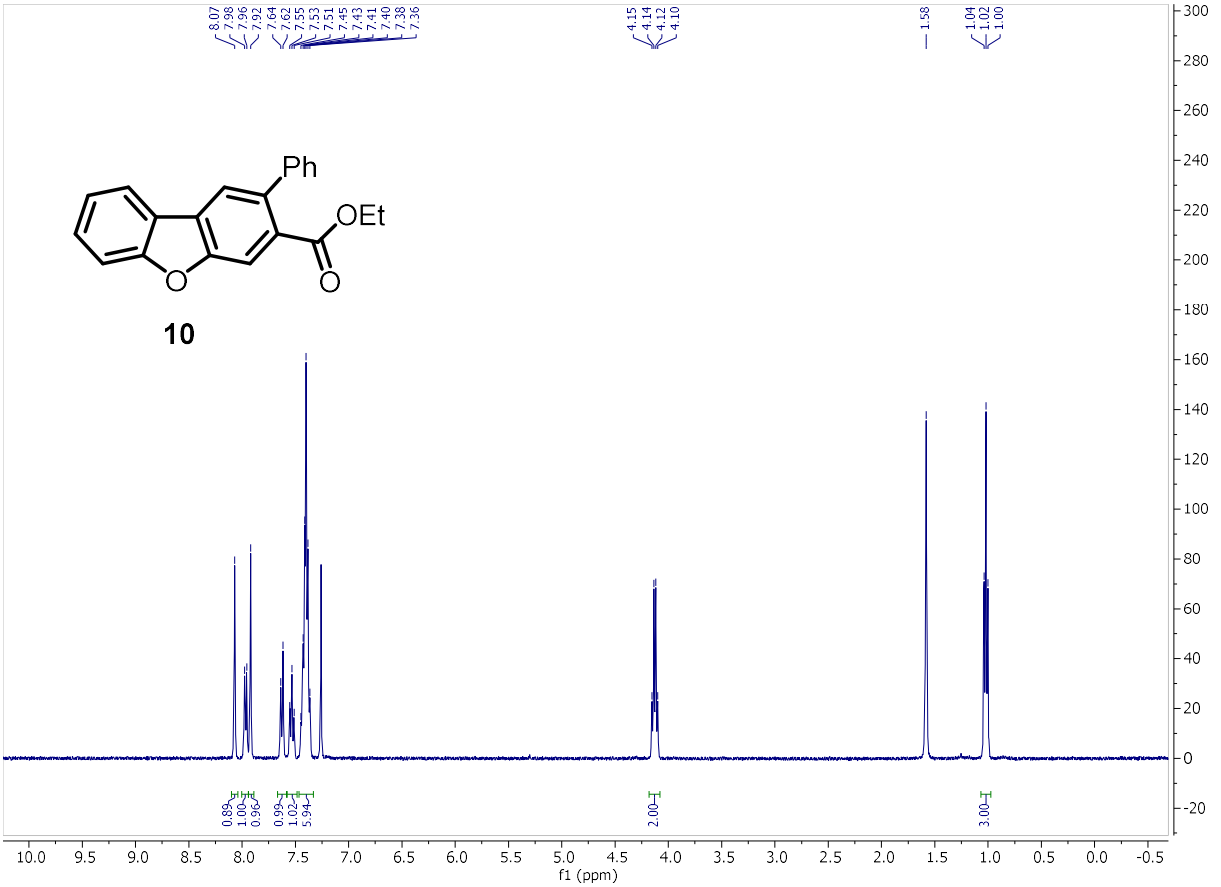
128.08
127.62
127.35
126.57
125.02
124.59
121.82
121.48
121.33
120.35
119.61
114.38
109.51
109.30
32.99
30.29
Ph
N
N
O
7f
f1 (ppm)


O
Ph
O
O
OEt
8
2.01
2.04
2.02
3.90
2.05
1.06
1.00
2.06
2.06
2.84
f1 (ppm)


192.59
165.86
156.39
143.37
141.36
134.81
132.92
130.57
130.31
129.65
128.84
128.45
126.85
122.22
121.52
112.67
67.06
60.41
14.09
O
Ph
O
O
OEt
8
f1 (ppm)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7.96
7.92
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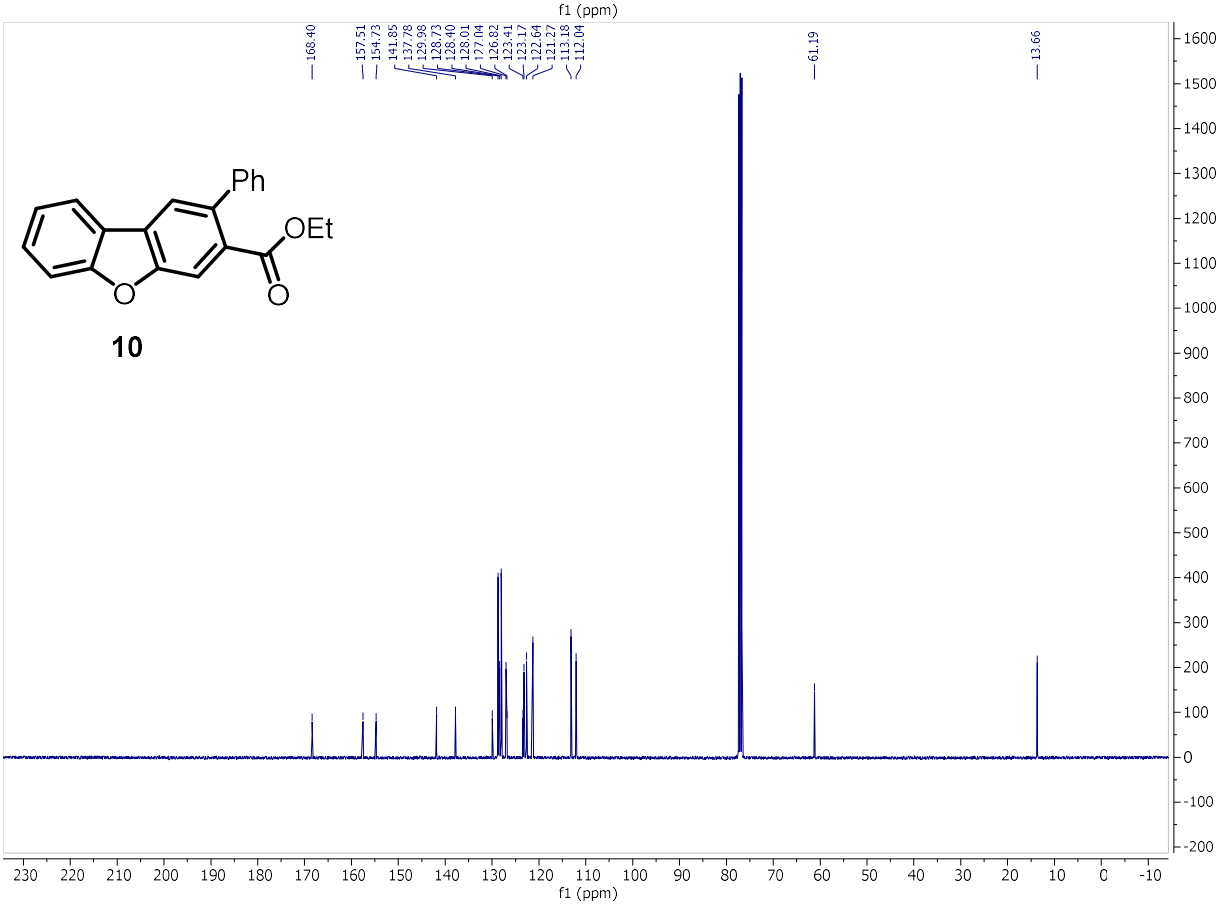
7.62
7.55
7.53
7.51
7.45
7.43
7.41
7.40
7.38
7.36
4.15
4.14
4.12
4.10
1.58
1.04
1.02
1.00
Ph
OEt
O
O
10
0.89
1.00
0.96
0.99
1.02
5.94
2.00
3.00
f1 (ppm)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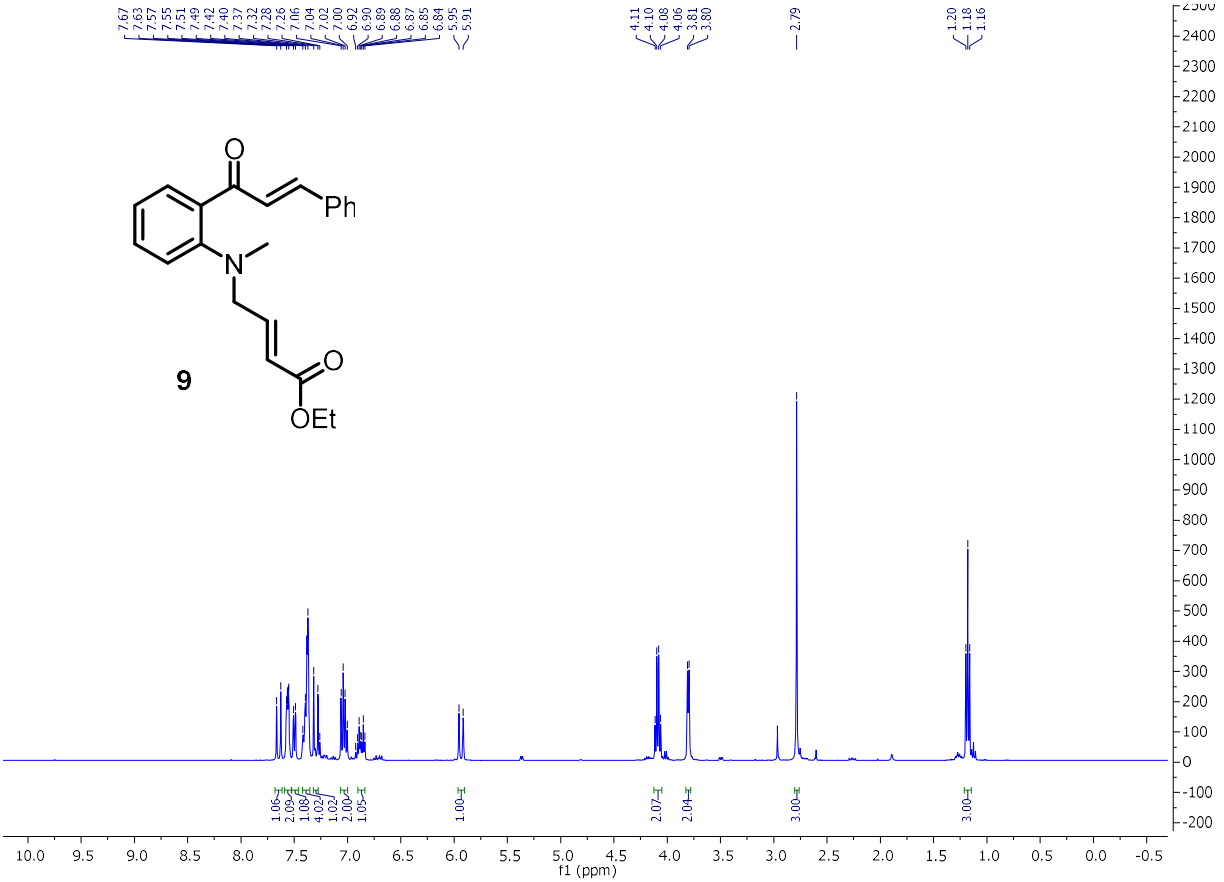
154.73
141.85
137.78
129.98
128.73
128.40
128.01
127.04
126.82
123.41
123.17
122.64
121.27
113.18
112.04
61.19
13.66
Ph
OEt
O
O
10
f1 (ppm)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7.63
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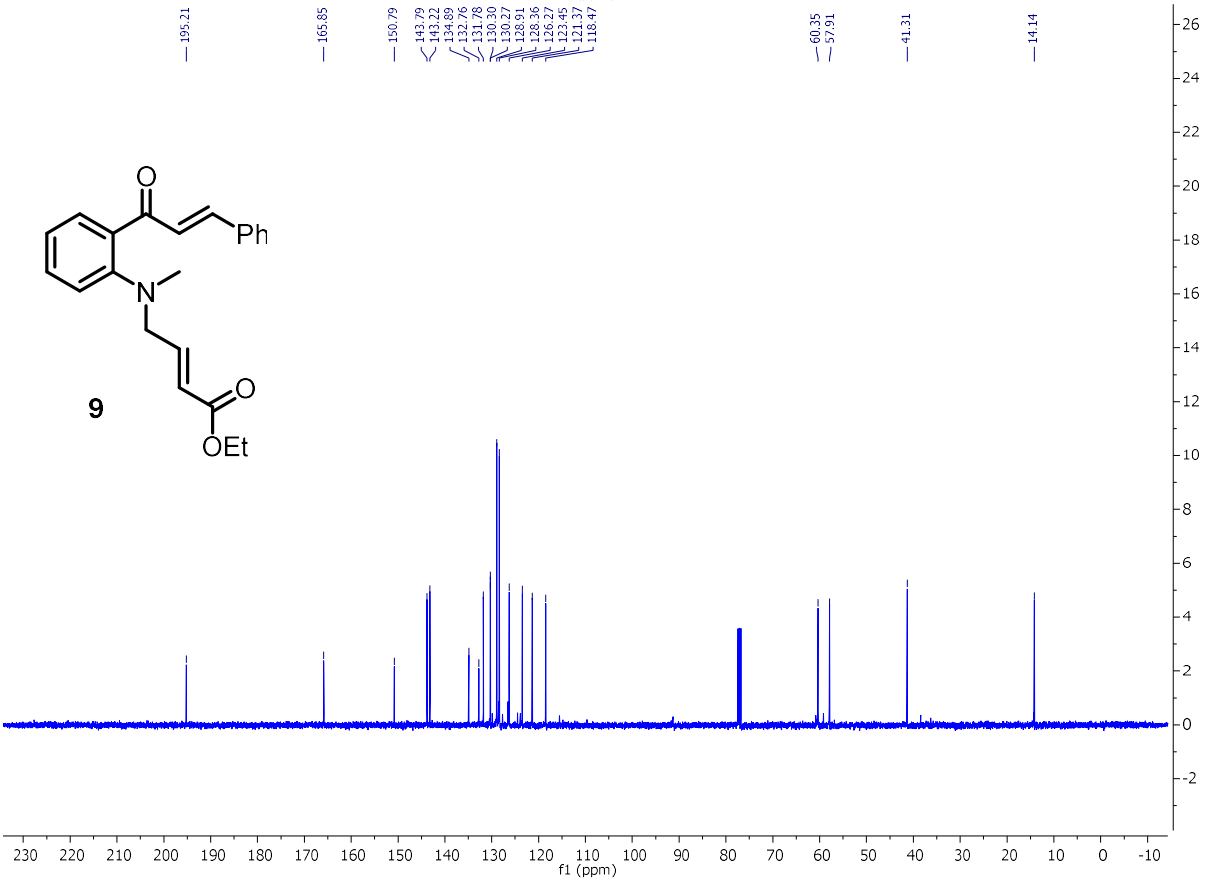
7.49
7.42
7.40
7.37
7.32
7.28
7.26
7.06
7.04
7.02
7.00
6.92
6.90
6.89
6.88
6.87
6.85
6.84
5.95
5.91
4.11
4.10
4.08
4.06
3.81
3.80
2.79
1.20
1.18
1.16
O
Ph
N
O
OEt
9
1.06
2.09
1.08
4.02
1.02
2.00
1.05
1.00
2.07
2.04
3.00
3.00
f1 (ppm)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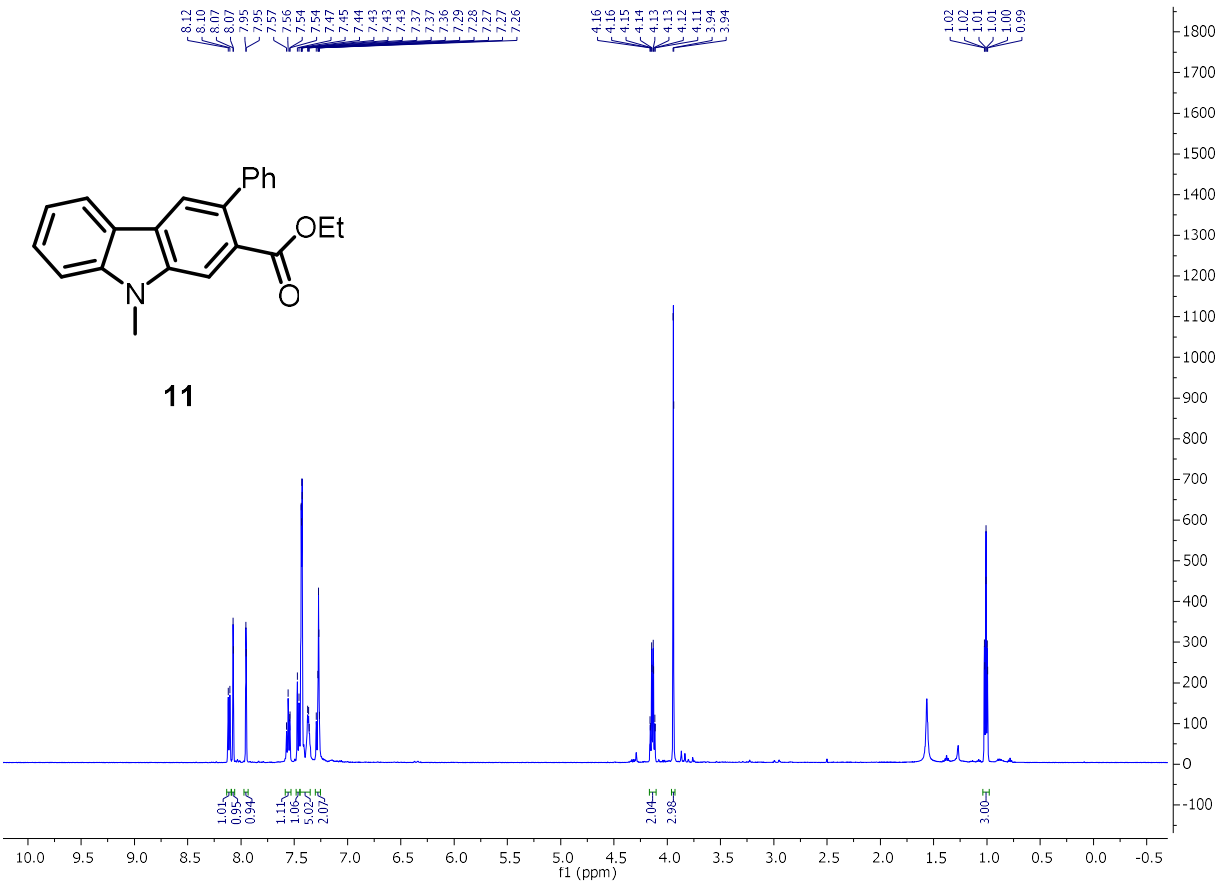
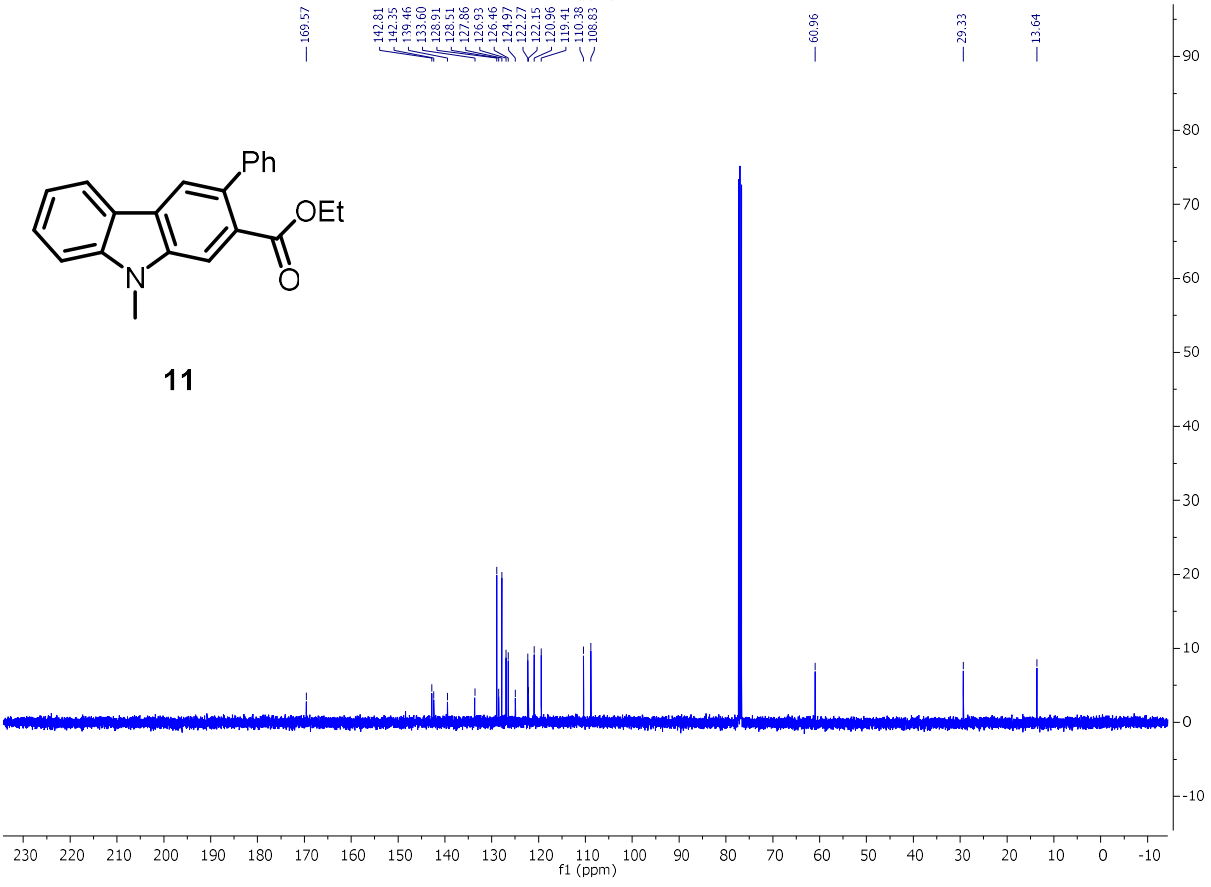
150.79
143.79
143.22
134.89
132.76
131.78
130.30
130.27
128.91
128.36
126.27
123.45
121.37
118.47
60.35
57.91
41.31
14.14
O
Ph
N
O
OEt
9
f1 (ppm)


Ph
OEt
O
N
11
f1 (ppm)


Ph
OEt
O
N
11
f1 (ppm)