Supporting Information

Formal Oxo- and Aza-[3+2] Reactions of α-Enaminones and Quinones: A Double Divergent Process and the Functions of Chiral Phosphoric Acid and Molecular Sieves

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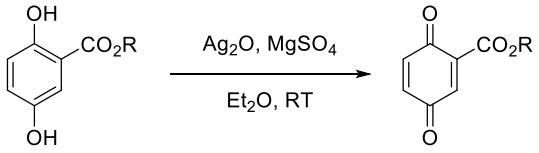
1. General remarks

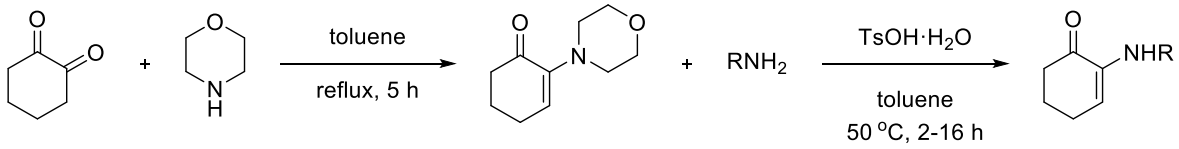
^{1}H NMR spectra were recorded on commercial instruments (400 MHz or 500 MHz). Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$, δ = 7.26). Spectra are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), integration, and assignment. ^{13}C NMR spectra were collected on commercial instruments (101 MHz or 126 MHz) with complete proton decoupling. Chemical shifts are reported in ppm from the tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$, δ = 77.0). The enantiomeric excesses were determined by HPLC analysis employing a chiral stationary phase column specified in the individual experiment, by comparing the samples with the appropriate racemic mixtures. Optical rotations were measured on a commercial polarimeter and reported as follows: $[\alpha]^T_D$ (c = g/100 mL, solvent). ESI-HRMS spectra were recorded using a commercial apparatus and methanol or acetonitrile was used to dissolve the sample. Unless otherwise indicated, reagents obtained from commercial sources were used without further purification. Solvents were dried and distilled prior to use according to the standard methods. 4 Å M.S. was purchased from ACROS Organics and used as received.

2. Preparation of the quinone esters and α-enaminones

All quinone esters and α-enaminones were prepared according to the previous reports.[1,2]

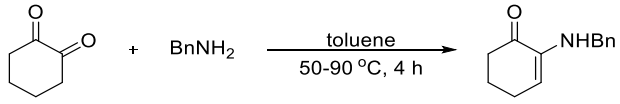


Silver oxide (3.0 mmol) and magnesium sulfate (3.0 mmol) were added to a solution of 1,4-dihydroxybenzene-2-carboxylate (1.0 mmol) in diethyl ether (20 mL). The reaction mixture was stirred at room temperature for 2 h. After filtration, the filtrate was evaporated in vacuo to furnish the desired quinone ester.



A 250 mL three-necked bottom flask was equipped with a Dean-Stark trap, condenser, stir bar, and gas inlet (argon atmosphere). The flask was charged with of 1,2-cyclohexanedione (4.48 g, 40 mmol), morpholine (4.4 mL, 50 mmol), and toluene (100 mL). The resulting yellow solution was heated at reflux for 5 h. The brown solution was decanted from thick oil and rinsed with toluene. The solution was concentrated under high vacuum to afford a brown solid. The compound could be directly used without further purification.

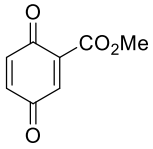
A mixture of substituted aniline (10 mmol), 2-morpholinocyclohex-2-enone (1.81 g, 10 mmol), and *p*-toluenesulfonic acid monohydrate (1.90 g, 10 mmol) in toluene (25 mL) was heated at 50 °C under argon for 2-16 h. The mixture was then cooled down to room temperature, diluted with EtOAc, and washed with saturated aqueous $NaHCO_3$. The separated organic layer was dried with Na_2SO_4, filtered, and concentrated under vacuum. Purification of the crude residue by column chromatography using a mixture of hexane and EtOAc as eluent gave the title product.



1,2-cyclohexanedione (1.12 g, 10 mmol) is added to toluene (10 mL).The mixture is heated to 50 °C under stirring and added benzylamine (0.6 g, 5 mmol). The mixture is stirred at 90 °C for 4 hours. After cooling to room temperature, the solvent is removed in vacuo and the crude is purified by a silica gel column that is eluted with hexane/EtOAc to give 2-(benzylamino)cyclohex-2-en-1-one.

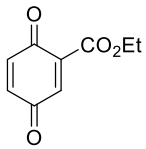
3. Characterization of the quinone ester and α-enaminones

methyl 3,6-dioxocyclohexa-1,4-diene-1-carboxylate **1a**



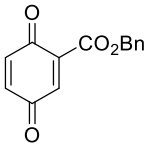
(**$C_8H_6O_4$**) orange solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.10 (s, 1H), 6.82 (s, 2H), 3.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.81, 182.96, 163.11, 136.96, 136.92, 136.55, 136.13, 53.14.

ethyl 3,6-dioxocyclohexa-1,4-diene-1-carboxylate **1b**



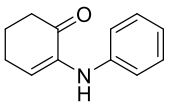
(**$C_9H_8O_4$**) orange oil; ^{1}H NMR (500 MHz, cdcl$_3$) δ 7.05 (d, *J* = 2.0 Hz, 1H), 6.84 – 6.76 (m, 2H), 4.33 (q, *J* = 7.1 Hz, 2H), 1.33 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, cdcl$_3$) δ 186.93, 183.07, 162.60, 137.30, 136.88, 136.09, 136.05, 62.40, 14.03.

benzyl 3,6-dioxocyclohexa-1,4-diene-1-carboxylate **1c**



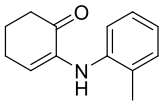
(**$C_{14}H_{10}O_4$**) orange solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.34 (m, 5H), 7.17 – 7.08 (m, 1H), 6.83 (d, *J* = 1.5 Hz, 2H), 5.35 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.82, 182.92, 162.43, 136.94, 136.52, 136.12, 134.58, 128.73, 128.42, 68.02.

2-(phenylamino)cyclohex-2-en-1-one **2a**



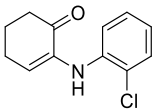
(**$C_{12}H_{13}NO$**) yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.22 (m, 2H), 7.07 – 7.01 (m, 2H), 6.95 – 6.88 (m, 1H), 6.43 (t, *J* = 4.8 Hz, 1H), 6.35 (s, 1H), 2.60 – 2.53 (m, 2H), 2.46 (dd, *J* = 11.0, 5.8 Hz, 2H), 2.02 (dt, *J* = 12.3, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.58, 141.90, 136.15, 129.21, 121.04, 118.63, 116.43, 37.70, 24.57, 22.92.

2-(*o*-tolylamino)cyclohex-2-en-1-one **2b**



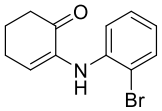
(**$C_{13}H_{15}NO$**) yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 – 7.12 (m, 3H), 6.92 (td, *J* = 7.3, 1.6 Hz, 1H), 6.12 (t, *J* = 4.8 Hz, 2H), 2.58 (dd, *J* = 8.5, 4.9 Hz, 2H), 2.43 (dd, *J* = 10.9, 5.9 Hz, 2H), 2.23 (s, 3H), 2.02 (dt, *J* = 12.3, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.66, 140.03, 136.80, 130.91, 129.29, 126.53, 122.06, 119.56, 116.07, 37.76, 24.53, 23.09, 17.81.

2-((2-chlorophenyl)amino)cyclohex-2-en-1-one **2c**



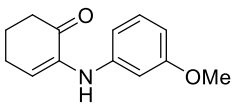
(**$C_{12}H_{12}ClNO$**) yellow oil; ^{1}H NMR (400 MHz, cdcl$_3$) δ 7.33 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.26 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.18 – 7.11 (m, 1H), 6.88 – 6.71 (m, 2H), 6.44 (t, *J* = 4.7 Hz, 1H), 2.61 – 2.52 (m, 2H), 2.46 (dd, *J* = 10.8, 5.9 Hz, 2H), 2.01 (dt, *J* = 12.3, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 195.13, 138.61, 135.43, 129.88, 127.24, 123.41, 121.00, 118.94, 117.29, 37.62, 24.63, 22.77.

2-((2-bromophenyl)amino)cyclohex-2-en-1-one **2d**



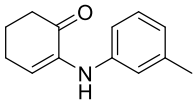
(**$C_{12}H_{12}BrNO$**) yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.47 (m, 1H), 7.28 – 7.14 (m, 2H), 6.84 – 6.68 (m, 2H), 6.41 (t, *J* = 4.7 Hz, 1H), 2.55 (t, *J* = 6.7 Hz, 2H), 2.44 (dd, *J* = 11.1, 5.6 Hz, 2H), 2.05 – 1.96 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.08, 139.70, 135.51, 133.15, 127.93, 121.55, 118.92, 117.55, 114.12, 37.62, 24.64, 22.79.

2-((3-methoxyphenyl)amino)cyclohex-2-en-1-one **2e**



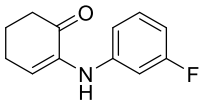
(**$C_{13}H_{15}NO_2$**) yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (t, *J* = 8.1 Hz, 1H), 6.65 – 6.57 (m, 2H), 6.48 – 6.43 (m, 2H), 6.38 (s, 1H), 3.78 (s, 3H), 2.59 – 2.51 (m, 2H), 2.45 (dd, *J* = 11.0, 5.7 Hz, 2H), 2.01 (dt, *J* = 12.5, 6.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.48, 160.49, 143.25, 136.03, 129.95, 117.34, 111.06, 106.04, 104.32, 55.19, 37.66, 24.61, 22.86.

2-(*m*-tolylamino)cyclohex-2-en-1-one **2f**



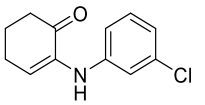
(**$C_{13}H_{15}NO$**) yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 – 7.10 (m, 1H), 6.85 (d, *J* = 6.2 Hz, 2H), 6.74 (d, *J* = 7.4 Hz, 1H), 6.41 (t, *J* = 4.8 Hz, 1H), 6.32 (s, 1H), 2.60 – 2.52 (m, 2H), 2.46 (dd, *J* = 11.0, 5.7 Hz, 2H), 2.31 (s, 3H), 2.02 (dt, *J* = 12.4, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.59, 141.85, 139.08, 136.32, 129.02, 121.95, 119.43, 116.32, 115.69, 37.72, 24.59, 22.94, 21.53.

2-((3-fluorophenyl)amino)cyclohex-2-en-1-one **2g**



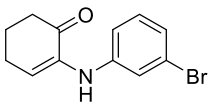
(**$C_{12}H_{12}FNO$**) yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (td, *J* = 8.3, 6.9 Hz, 1H), 6.78 – 6.70 (m, 2H), 6.54 (tdd, *J* = 8.4, 2.4, 0.9 Hz, 1H), 6.49 (s, 1H), 6.43 (t, *J* = 4.8 Hz, 1H), 2.57 – 2.48 (m, 2H), 2.43 (dd, *J* = 11.1, 5.8 Hz, 2H), 1.98 (dt, *J* = 12.3, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.25, 164.72, 162.30, 143.88, 143.78, 135.51, 130.37, 130.27, 118.46, 113.64, 113.62, 107.22, 107.01, 104.49, 104.24, 37.54, 24.57, 22.73.

2-((3-chlorophenyl)amino)cyclohex-2-en-1-one **2h**



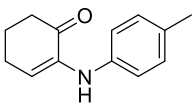
(**$C_{12}H_{12}ClNO$**) yellowish solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (t, *J* = 8.1 Hz, 1H), 7.03 (t, *J* = 2.1 Hz, 1H), 6.86 (dddd, *J* = 7.8, 4.6, 2.0, 0.8 Hz, 2H), 6.45 (t, *J* = 4.8 Hz, 1H), 6.41 (s, 1H), 2.62 – 2.52 (m, 2H), 2.48 (dd, *J* = 11.0, 5.8 Hz, 2H), 2.02 (dt, *J* = 12.3, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.30, 143.27, 135.56, 134.80, 130.22, 120.69, 118.26, 117.56, 116.35, 37.57, 24.58, 22.76.

2-((3-bromophenyl)amino)cyclohex-2-en-1-one **2i**



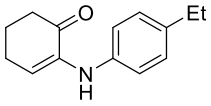
(**$C_{12}H_{12}BrNO$**) yellowish solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (s, 1H), 7.10 (t, *J* = 8.0 Hz, 1H), 7.00 (d, *J* = 7.8 Hz, 1H), 6.91 (d, *J* = 7.0 Hz, 1H), 6.44 (t, *J* = 4.7 Hz, 1H), 6.40 (s, 1H), 2.64 – 2.52 (m, 2H), 2.48 (dd, *J* = 10.9, 5.6 Hz, 2H), 2.02 (dt, *J* = 12.4, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.29, 143.42, 135.54, 130.51, 123.63, 122.93, 120.51, 118.21, 116.82, 37.56, 24.58, 22.76.

2-(*p*-tolylamino)cyclohex-2-en-1-one **2j**



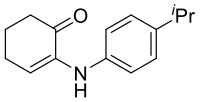
(**$C_{13}H_{15}NO$**) yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.1 Hz, 2H), 6.99 – 6.88 (m, 2H), 6.32 (t, *J* = 4.8 Hz, 1H), 6.24 (s, 1H), 2.60 – 2.51 (m, 2H), 2.43 (dd, *J* = 11.0, 5.8 Hz, 2H), 2.29 (s, 3H), 2.01 (dt, *J* = 12.3, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.73, 139.27, 136.85, 130.81, 129.72, 119.40, 115.31, 37.75, 24.53, 23.01, 20.67.

2-((4-ethylphenyl)amino)cyclohex-2-en-1-one **2k**



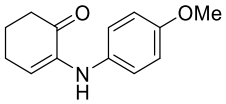
(**$C_{14}H_{17}NO$**) yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 – 7.06 (m, 2H), 7.02 – 6.91 (m, 2H), 6.34 (t, *J* = 4.8 Hz, 1H), 6.28 (s, 1H), 2.69 – 2.52 (m, 4H), 2.43 (dd, *J* = 11.1, 5.7 Hz, 2H), 2.01 (dt, *J* = 12.4, 6.1 Hz, 2H), 1.22 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.61, 139.49, 137.27, 136.74, 128.53, 119.35, 115.36, 37.75, 28.14, 24.55, 23.02, 15.75.

2-((4-isopropylphenyl)amino)cyclohex-2-en-1-one **2l**



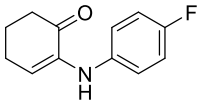
(**$C_{15}H_{19}NO$**) yellow solid; ^{1}H NMR (400 MHz, cdcl$_3$) δ 7.14 (d, *J* = 8.2 Hz, 2H), 6.98 (d, *J* = 8.2 Hz, 2H), 6.35 (t, *J* = 4.6 Hz, 1H), 6.28 (s, 1H), 2.93 – 2.79 (m, 1H), 2.61 – 2.50 (m, 2H), 2.43 (dd, *J* = 10.7, 5.4 Hz, 2H), 2.01 (dt, *J* = 12.3, 6.0 Hz, 2H), 1.24 (s, 3H), 1.23 (s, 3H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 195.60, 141.89, 139.59, 136.71, 127.07, 119.24, 115.40, 37.75, 33.39, 24.55, 24.10, 23.02.

2-((4-methoxyphenyl)amino)cyclohex-2-en-1-one **2m**



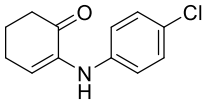
(**$C_{13}H_{15}NO_2$**) yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 – 6.94 (m, 2H), 6.89 – 6.79 (m, 2H), 6.14 (t, *J* = 4.8 Hz, 1H), 6.09 (s, 1H), 3.78 (s, 3H), 2.60 – 2.50 (m, 2H), 2.39 (dd, *J* = 11.2, 5.7 Hz, 2H), 2.06 – 1.92 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.67, 154.89, 137.72, 134.87, 122.19, 114.50, 114.07, 55.52, 37.78, 24.45, 23.12.

2-((4-fluorophenyl)amino)cyclohex-2-en-1-one **2n**



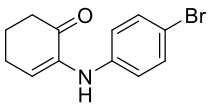
(**$C_{12}H_{12}FNO$**) yellowish solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 – 6.82 (m, 4H), 6.34 – 6.05 (m, 2H), 2.59 – 2.52 (m, 2H), 2.42 (dd, *J* = 11.0, 5.8 Hz, 2H), 2.01 (dt, *J* = 12.3, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.50, 158.98, 156.56, 136.93, 121.15, 121.07, 115.92, 115.70, 115.29, 37.68, 24.45, 22.98.

2-((4-chlorophenyl)amino)cyclohex-2-en-1-one **2o**



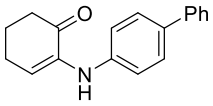
(**$C_{12}H_{12}ClNO$**) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.11 (m, 2H), 7.00 – 6.89 (m, 2H), 6.35 (t, *J* = 4.7 Hz, 2H), 2.61 – 2.51 (m, 2H), 2.44 (dd, *J* = 11.0, 5.7 Hz, 2H), 2.01 (dt, *J* = 12.4, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.38, 140.51, 135.98, 129.14, 125.58, 119.65, 116.97, 37.61, 24.54, 22.84.

2-((4-bromophenyl)amino)cyclohex-2-en-1-one **2p**



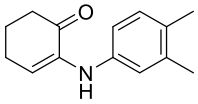
(**$C_{12}H_{12}BrNO$**) yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.30 (m, 2H), 7.00 – 6.84 (m, 2H), 6.38 (t, *J* = 4.8 Hz, 1H), 6.35 (s, 1H), 2.63 – 2.51 (m, 2H), 2.46 (dd, *J* = 11.0, 5.7 Hz, 2H), 2.02 (dt, *J* = 12.5, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.38, 140.99, 135.86, 132.07, 119.95, 117.20, 112.86, 37.60, 24.55, 22.82.

2-([1,1'-biphenyl]-4-ylamino)cyclohex-2-en-1-one **2q**



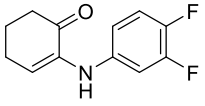
(**$C_{18}H_{17}NO$**) yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.54 (m, 2H), 7.54 – 7.48 (m, 2H), 7.45 – 7.38 (m, 2H), 7.33 – 7.27 (m, 1H), 7.15 – 7.08 (m, 2H), 6.48 (dd, *J* = 12.5, 7.8 Hz, 2H), 2.63 – 2.55 (m, 2H), 2.49 (dd, *J* = 11.0, 5.6 Hz, 2H), 2.04 (dt, *J* = 12.3, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.54, 141.27, 140.74, 136.08, 133.76, 128.71, 127.84, 126.63, 126.54, 118.63, 116.87, 37.69, 24.63, 22.90.

2-((3,4-dimethylphenyl)amino)cyclohex-2-en-1-one **2r**



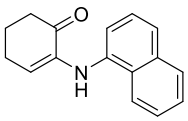
(**$C_{14}H_{17}NO$**) yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.03 (d, *J* = 7.9 Hz, 1H), 6.88 – 6.75 (m, 2H), 6.32 (t, *J* = 4.7 Hz, 1H), 6.21 (s, 1H), 2.61 – 2.51 (m, 2H), 2.43 (dd, *J* = 11.0, 5.6 Hz, 2H), 2.23 (s, 3H), 2.20 (s, 3H), 2.01 (dt, *J* = 12.4, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.65, 139.58, 137.42, 136.84, 130.17, 129.59, 120.97, 116.75, 115.20, 37.77, 24.55, 23.03, 19.95, 18.98.

2-((3,4-difluorophenyl)amino)cyclohex-2-en-1-one **2s**



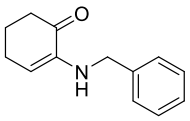
(**$C_{12}H_{11}F_2NO$**) yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.03 (dd, *J* = 18.9, 9.0 Hz, 1H), 6.87 (ddd, *J* = 12.3, 6.9, 2.7 Hz, 1H), 6.72 – 6.65 (m, 1H), 6.32 (dd, *J* = 10.7, 6.0 Hz, 2H), 2.61 – 2.52 (m, 2H), 2.45 (dd, *J* = 11.0, 5.7 Hz, 2H), 2.02 (dt, *J* = 12.5, 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.28, 151.72, 151.53, 149.27, 149.13, 146.25, 146.10, 143.83, 143.66, 138.54, 136.08, 117.62, 117.60, 117.44, 117.42, 117.07, 114.55, 114.53, 114.49, 107.63, 107.43, 37.55, 24.47, 22.81.

2-(naphthalen-1-ylamino)cyclohex-2-en-1-one **2t**



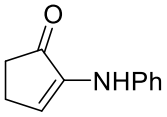
(**$C_{16}H_{15}NO$**) red oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 7.96 (m, 1H), 7.85 (dd, *J* = 6.0, 3.0 Hz, 1H), 7.56 (d, *J* = 8.1 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.33 (d, *J* = 7.4 Hz, 1H), 6.76 (s, 1H), 6.14 (t, *J* = 4.6 Hz, 1H), 2.63 (t, *J* = 6.2 Hz, 2H), 2.44 – 2.35 (m, 2H), 2.08 – 1.99 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.66, 137.58, 134.63, 128.49, 127.98, 126.10, 125.80, 125.74, 123.00, 121.98, 116.76, 116.63, 37.77, 24.49, 23.14.

2-(benzylamino)cyclohex-2-en-1-one **2u**



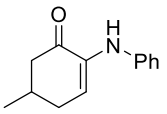
(**$C_{13}H_{15}NO$**) yellowish solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.23 (m, 5H), 5.44 (t, *J* = 4.7 Hz, 1H), 4.64 (s, 1H), 4.09 (s, 2H), 2.50 (dd, *J* = 8.4, 4.9 Hz, 2H), 2.34 (dd, *J* = 11.0, 5.7 Hz, 2H), 1.95 (dt, *J* = 12.4, 6.1 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 195.79, 140.38, 139.06, 128.52, 127.39, 127.09, 111.73, 47.56, 37.93, 24.51, 23.50.

2-(phenylamino)cyclopent-2-en-1-one **2v**



(**$C_{11}H_{11}NO$**) yellowish solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.26 (m, 2H), 7.10 – 7.00 (m, 2H), 6.93 (t, *J* = 7.4 Hz, 1H), 6.74 (t, *J* = 3.2 Hz, 1H), 6.25 (s, 1H), 2.68 – 2.60 (m, 2H), 2.51 – 2.44 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 204.68, 141.71, 140.07, 129.34, 124.57, 120.85, 116.57, 32.37, 23.94.

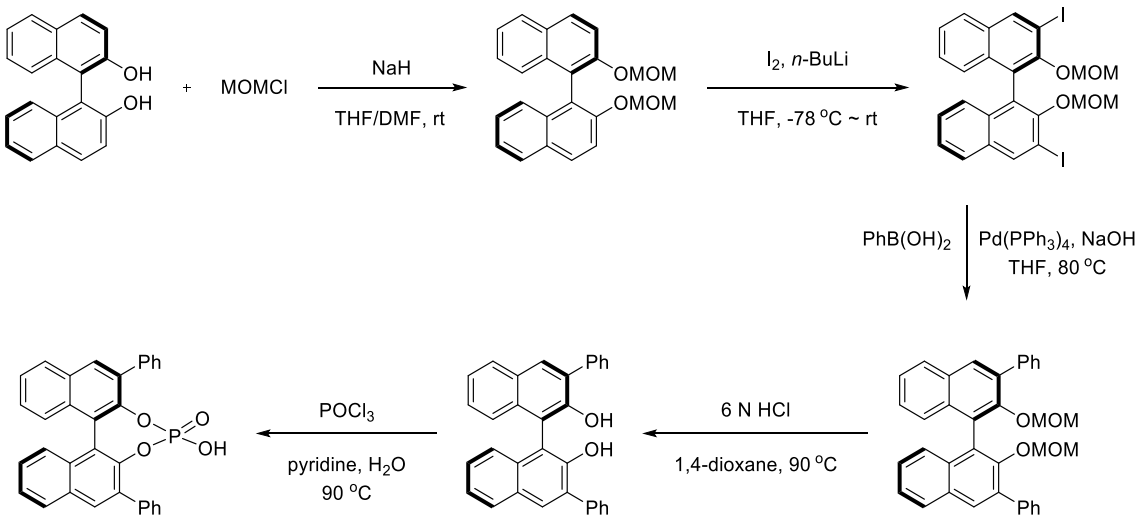
4-methyl-2-(phenylamino)cyclohex-2-en-1-one **2w**



(**$C_{13}H_{15}NO$**) yellowish solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.24 (m, 2H), 7.07 – 7.00 (m, 2H), 6.92 (ddd, *J* = 8.4, 2.1, 1.0 Hz, 1H), 6.39 (dd, *J* = 6.4, 3.2 Hz, 1H), 6.35 (s, 1H), 2.70 – 2.60 (m, 1H), 2.56 – 2.45 (m, 1H), 2.31 – 2.22 (m, 2H), 2.20 – 2.13 (m, 1H), 1.10 (d, *J* = 6.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 195.67, 141.96, 136.05, 129.21, 121.05, 118.63, 115.47, 45.66, 32.91, 30.59, 21.15.

4. Preparation of chiral phosphoric acids

Chiral phosphoric acids were synthesized by using the literature method.[3]



1) NaH (2.0 g, 60% in oil, 50.0 mmol) was added portionwise to a precooled (0 °C) reaction flask filled with dry THF (75 mL) and DMF (35 mL). To the mixture with stirring, was added a solution of (*R*)-2,2′-dihydroxy-1,1′-binaphthyl (5.73 g, 20.0 mmol) in THF (25 mL) in a dropping funnel. After the addition, the mixture was stirred at room temperature for 2 h. Then to this, chloromethyl methyl ether (3.8 mL, 50.0 mmol) was slowly added from the dropping funnel. After the addition, the reaction mixture was stirred for 6 h. Saturated aqueous NH_4Cl was added to the flask, then the residue was extracted with EtOAc. The organic layers were combined, washed with brine, dried over Na_2SO_4, and concentrated. Crude product was

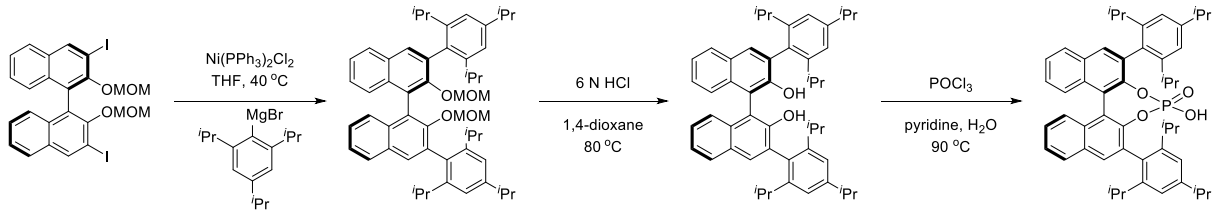
purified by column chromatography and crystallized from DCM/hexane to give a white crystalline (*R*)-2,2′-Bis(methoxymethoxy)-1,1′-binaphthyl product.

2) To a solution of (*R*)-2,2′-Bis(methoxymethoxy)-1,1′-binaphthyl (7.28 g, 19.4 mmol) in 100 mL anhydrous THF, *n*-butyllithium (23 mL, 2.5 M in hexanes, 58.2 mmol) was added slowly at -78 °C. The reaction mixture stirred at same temperature for 30 minutes followed by 2 hours at 0 °C; then again cooled back to -78 °C and solid iodine (14.8 g, 58.2 mmol) was added in one portion. The stirring was continued at room temperature for 2 hours before quenching excess of iodine with 50 mL of a saturated sodium thiosulfate solution. The crude product was isolated by extraction with EtOAc. The combined organic layers washed with brine; dried over Na_2SO_4 and concentrated under reduced pressure. The crude material was purified by flash column chromatography on silica gel using hexane/EtOAc as eluent isolating (*R*)-3,3′-Diiodo-2,2′-Bis(methoxymethoxy-1,1′-binaphthyl as a pale yellow solid.

3) Argon gas was purged for 10 minutes through a solution of (*R*)-3,3′-Diiodo-2,2′-Bis(methoxymethoxy-1,1′-binaphthyl (3.0 g, 4.79 mmol), $Pd(PPh_3)_4$ (276 mg, 0.239 mmol, 5 mol %), $PhB(OH)_2$ (1.28 g, 10.5 mmol) and NaOH (1.15 g, 28.7 mmol) in THF-H_2O (3:1, 60 mL, degassed with argon for 20 minutes). Then reaction mixture was stirred at 80 °C for 6 h. After complete consumption of starting material, the mixture was cooled to room temperature and extracted with EtOAc. Combined organic layer was washed with water, brine and dried over Na_2SO_4. After evaporation of solvent, residual material was purified by column chromatography on silica gel using hexane/EtOAc as eluent isolating (*R*)-2,2′-bis(methoxymethoxy)-3,3′-diphenyl-1,1′-binaphthalene as white solid.

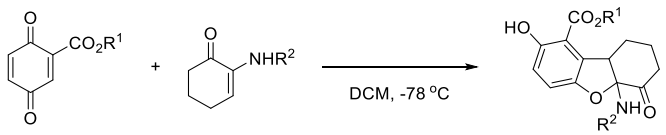
4) To a solution of (*R*)-2,2′-bis(methoxymethoxy)-3,3′-diphenyl-1,1′-binaphthalene (2.1 g, 4.0 mmol) in 30 mL dioxane, aq. HCl (6 N, 6 mL) was added at room temperature. Reaction mixture was warmed to 90 °C and stirred for 3 h at the same temperature then cooled to room temperature and solvent was evaporated under reduced pressure. Residual material was diluted with DCM and washed with $NaHCO_3$, water and brine. Organic layer dried over Na_2SO_4, volatiles were removed under reduced pressure. The crude compound was purified by column chromatography on silica gel using hexane/EtOAc as eluent to isolate (*R*)-3,3'-diphenyl-[1,1'-binaphthalene]-2,2'-diol as white solid.

5) To a solution of (*R*)-3,3'-diphenyl-[1,1'-binaphthalene]-2,2'-diol (2.18 g, 5.0 mmol) in 20 mL pyridine, $POCl_3$ (1.0 mL, 11.0 mmol) was added slowly at room temperature under nitrogen atmosphere. Stirring was continued at same temperature for 10 minutes and then at 90 °C for 2 hours. Reaction mixture was cooled to room temperature before slow addition of water (20 mL) and again stirred at 90 °C for additional 2 hours. After cooling to room temperature, crude product was isolated by extraction with DCM. Combined organic layer washed with aq. HCl (2 x 50 mL, 2 N), brine then dried over Na_2SO_4 and evaporated under reduced pressure. Crude product was purified by column chromatography on silica gel using DCM/MeOH as eluent. Then the product was dissolved in DCM, washed with 6 N aq. HCl, organic layers were combined and concentrated. The product was purified by crystallization in DCM/EtOH/hexane to afford the (4*R*)-4-hydroxy-2,6-diphenyldinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepine 4-oxide.



1) To a well-stirred suspension of (*R*)-3,3′-Diiodo-2,2′-Bis(methoxymethoxy-1,1′-binaphthyl (3.13 g, 5.0 mmol) and $NiCl_2(Ph_3P)_2$ (327 mg, 0.5 mmol, 10 mol%) in anhydrous THF (20 mL) was slowly added to the Grignard solution over 5 minutes. The resultant brown solution was stirred at 40 °C for 16 h, after which the mixture was poured over saturated aqueous NH_4Cl. The aqueous layer was extracted with EtOAc, and the combined organic extracts were dried over anhydrous Na_2SO_4, filtered and concentrated *in vacuo.* The crude residue was purified by flash chromatography on silica gel.
2) To a solution of (*R*)-2,2′-bis(methoxymethoxy)-3,3′-bis(2,4,6-triisopropylphenyl)-1,1′-binaphthalene (3.1 g, 4.0 mmol) in 30 mL dioxane, aq. HCl (6 N, 6 mL) was added at room temperature. Reaction mixture was warmed to 90 °C and stirred for 3 h at the same temperature then cooled to room temperature and solvent was evaporated under reduced pressure. Residual material was diluted with DCM and washed with $NaHCO_3$, water and brine. Organic layer dried over Na_2SO_4, volatiles were removed under reduced pressure. The crude compound was purified by column chromatography on silica gel using hexane/EtOAc as eluent to isolate (*R*)-3,3'-bis(2,4,6-triisopropylphenyl)-[1,1'-binaphthalene]-2,2'-diol.
3) To a solution of (*R*)-3,3'-bis(2,4,6-triisopropylphenyl)-[1,1'-binaphthalene]-2,2'-diol (1.38 g, 2.0 mmol) in 20 mL pyridine, $POCl_3$ (0.5 mL, 5.0 mmol) was added slowly at room temperature under nitrogen atmosphere. Stirring was continued at same temperature for 10 minutes and then at 90 °C for 2 hours. Reaction mixture was cooled to room temperature before slow addition of water (20 mL) and again stirred at 90 °C for additional 2 hours. After cooling to room temperature, crude product was isolated by extraction with DCM. Combined organic layer washed with aq. HCl (2 x 30 mL, 2 N), brine then dried over Na_2SO_4 and evaporated under reduced pressure. Crude product was purified by column chromatography on silica gel using DCM/MeOH as eluent. Then the product was dissolved in DCM, washed with 6 N aq. HCl, organic layers were combined and concentrated. The product was purified by crystallization in $CHCl_3/CH_3CN$ to afford the (*R*)-TRIP.

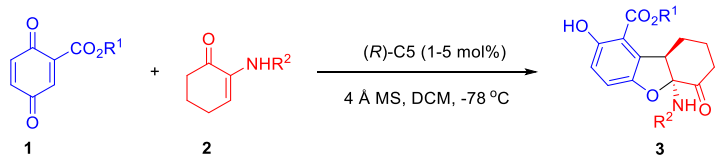
5. General procedure for the preparation of the racemic products



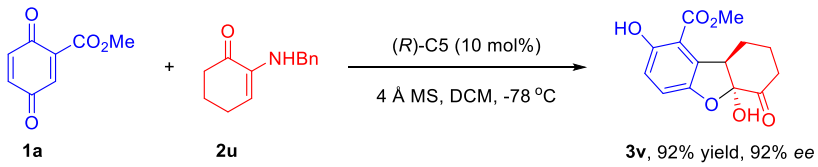
In an oven dried Schlenk tube substituted α-enaminone **2** (0.1 mmol) was dissolved in anhydrous DCM (1 mL). The solution was stirred for 5 min at -78 °C, and then 2-alkoxycarbonyl-1,4-benzoquinone **1** (0.1 mmol) was added to the mixture. After stirred at -78 °C for several hours (monitored by TLC), then the mixture was purified by silica gel column chromatography (hexane/DCM/EtOAc = 4/2/1 to 12/2/1) to afford pure racemic product **3a**–**u**.

In an oven dried Schlenk tube 2-(benzylamino)cyclohex-2-en-1-one **2u** (0.1 mmol) was dissolved in anhydrous DCM (1 mL). The solution was stirred for 5 min at -78 °C, and then methyl 3,6-dioxocyclohexa-1,4-diene-1-carboxylate **1a** (0.1 mmol) was added to the mixture. After stirred at -78 °C for 16 hours (monitored by TLC), then the mixture was purified by silica gel column chromatography (first run: hexane/DCM/EtOAc = 6/2/1; second run: hexane/DCM = 1/6) to afford pure racemic product **3v**.

6. General procedure for the enantioselective preparation of products

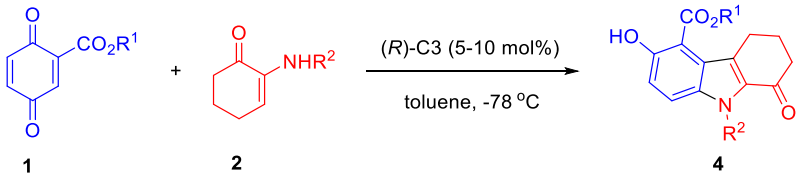


In an oven dried Schlenk tube chiral phosphoric acid C5 (1–5 mol%), 4 Å M.S. (5–20 mg), and substituted α-enaminone **2** (0.11 mmol) were dissolved in anhydrous DCM (0.5 mL). The solution was stirred for 5 min at -78 °C, and then a solution of 2-alkoxycarbonyl-1,4-benzoquinone **1** (0.1 mmol) in DCM (0.5 mL) was added to the mixture. After stirred at -78 °C for several hours (monitored by TLC), then the mixture was purified by silica gel column chromatography (hexane/DCM/EtOAc = 4/2/1 to 12/2/1) to afford pure product **3a**–**u**.



In an oven dried Schlenk tube chiral phosphoric acid C5 (10 mol%), 4 Å M.S. (20 mg), and 2-(benzylamino)cyclohex-2-en-1-one **2u** (0.11 mmol) were dissolved in anhydrous DCM (0.5 mL). The solution was stirred for 5 min at -78 °C, and then a solution of methyl 3,6-dioxocyclohexa-1,4-diene-1-carboxylate **1a** (0.1 mmol) in DCM (0.5 mL) was added to the mixture. After stirred at -78 °C for 16 hours (monitored by TLC), then the mixture was purified by silica gel column chromatography (first run: hexane/DCM/EtOAc = 6/2/1; second run: hexane/DCM = 1/4) to afford pure product **3v**.

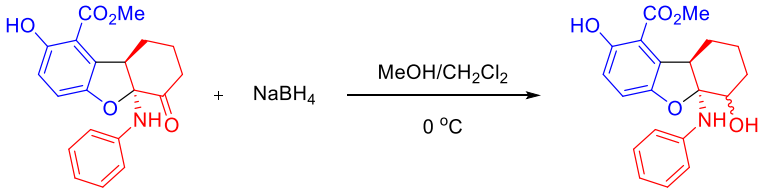
7. General procedure for the preparation of indole derivatives



1 2 4

In an oven dried Schlenk tube chiral phosphoric acid C3 (5–10 mol%), and substituted α-enaminone **2** (0.1 mmol) were dissolved in anhydrous toluene (0.5 mL). The solution was stirred for 5 min at -78 °C, and then a solution of 2-alkoxycarbonyl-1,4-benzoquinone **1** (0.1 mmol) in toluene (0.5 mL) was added to the mixture. After stirred at -78 °C for several hours (monitored by TLC), then the mixture was purified by silica gel column chromatography (first run: hexane/DCM/EtOAc = 4/2/1 to 12/2/1; second run: hexane/DCM = 1/4) to afford pure product **4a**–**r**.

8. Experimental procedure for the transformations of the product



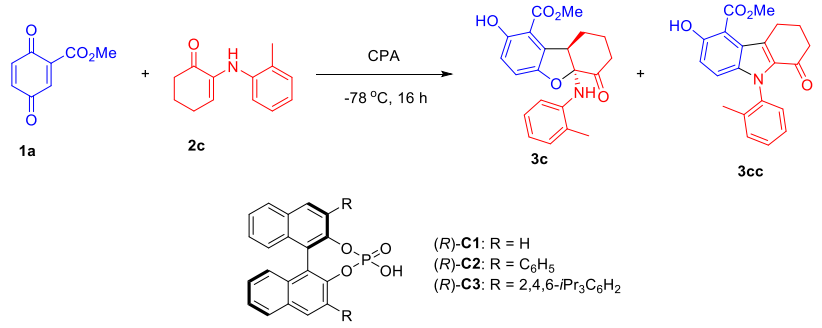
3a, 99% *ee*

5, 93% yield
75:25 d.r., 97%/99% *ee*

To a solution of adduct **3a** (70.6 mg, 0.2 mmol, 1.0 equiv) in MeOH/DCM (1/1, 2.0 mL) was added $NaBH_4$ (7.6 mg, 0.2 mmol, 1.0 equiv) at 0 °C. The mixture was allowed to stir at 0 °C for 1 h. The mixture was quenched by saturated NH_4Cl aq. and extracted with EtOAc three times (10 mL), dried with Na_2SO_4,

filtered and the solvent was removed in vacuo. The residue was purified by column chromatography on silica gel (hexane: ethyl acetate = 2:1) to afford **5** (65.9 mg, 93% yield).

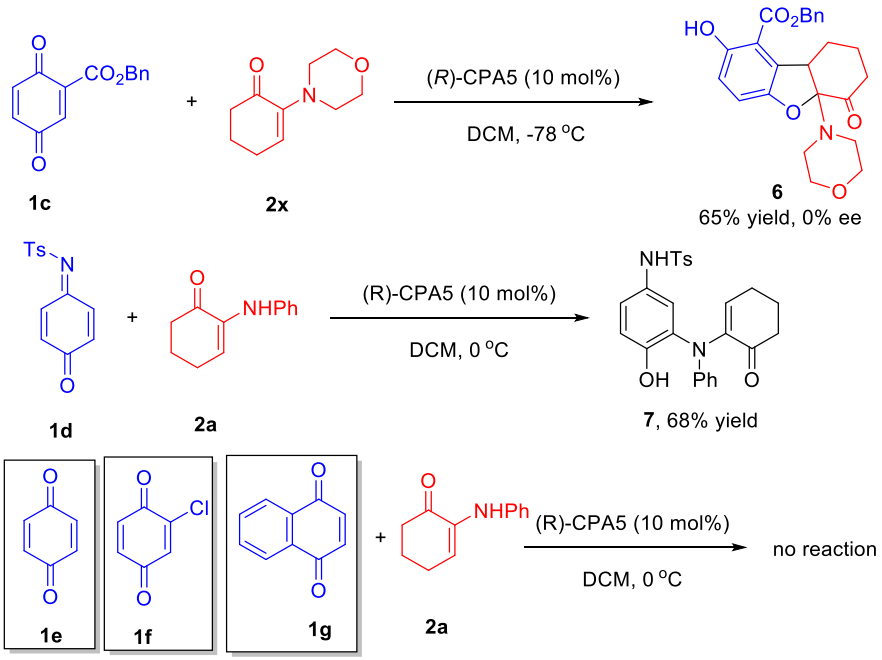
9. Extra optimization of the reaction conditions (Table S1)



Entry	Cat. (10 mol%)	solvent	additives	Yield of 3c [%][b]	Yield of 3cc [%][b]
1	CPA1	toluene	-	64	<5
2	CPA2	toluene	-	32	<5
3	CPA3	toluene	-	57	<5
4	CPA3	DCM	-	75	5
5	CPA3	DCM	$Fe(OTf)_3$ (10 mol%)	43	<5
6	CPA3	DCM	$Y(OTf)_3$ (10 mol%)	64	<5
7	CPA3	DCM	$Zn(OTf)_2$ (10 mol%)	43	<5
8	CPA3	DCM	$In(OTf)_3$ (10 mol%)	38	<5
9	CPA3	THF	$Y(OTf)_3$ (10 mol%)	53	5
10	CPA3	DCM	PhCOOH (20 mol%)	78	10
11	CPA3	DCM	$NaHCO_3$ (20 mol%)	79	<5
12	CPA3	DCM	Et_3N (20 mol%)	18	<5
13	CPA3	DCM	2,6-lutidine (20 mol%)	73	<5
14	CPA3	DCM	DABCO (20 mol%)	44	<5
15	CPA3	DCM	H_2O (5 μL)	71	5
16	CPA3	DCM	4 Å MS (5 mg)	82	<5

[a] Unless specified otherwise, all reactions were performed with catalyst (10 mol %), **1a** (0.1 mmol), **2c** (0.1 mmol) in 1.0 mL solvent at -78 °C. [b] ^1H NMR yield.

10. Screening of other substrates



11. X-ray crystallographic analysis

a) The configuration of **3a** was determined to be (5a*S*, 9a*R*) by X-ray analysis.

Table S2. **Crystal data and structure refinement for 3a.**

Identification code	**3a**	
Empirical formula	$C_{20}H_{19}NO_5$	
Formula weight	353.36	
Temperature	100.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 8.94010(10) Å	α = 90°.
	b = 10.34330(10) Å	β = 103.4510(10)°.
	c = 9.39150(10) Å	γ = 90°.
Volume	844.611(16) Å^3	
Z	2	

Density (calculated)	1.389 Mg/m^3
Absorption coefficient	0.830 mm^{-1}
F(000)	372
Crystal size	0.1 x 0.05 x 0.04 mm^3
Theta range for data collection	4.842 to 77.758°.
Index ranges	-11<=h<=11, -12<=k<=12, -11<=l<=11
Reflections collected	24355
Independent reflections	3535 [R(int) = 0.0204]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.89379
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3535 / 1 / 237
Goodness-of-fit on F^2	1.068
Final R indices [I>2sigma(I)]	R1 = 0.0257, wR2 = 0.0666
R indices (all data)	R1 = 0.0257, wR2 = 0.0666
Absolute structure parameter	0.00(3)
Extinction coefficient	n/a
Largest diff. peak and hole	0.156 and -0.184 $e.Å^{-3}$

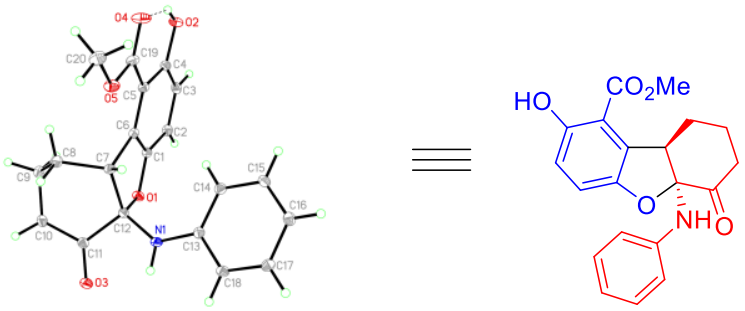


Figure S1. Crystallographic Data for **3a**.

Single crystal of **3a** [$\mathbf{C_{20}H_{19}NO_5}$] was obtained from the mixed solvents of ethyl acetate and *n*-hexane. CCDC 1919282 contains the supplementary crystallographic data which can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.

b) The configuration of **4v** was determined to be (5a*S*, 9a*R*) by X-ray analysis.

***Table S3*. Crystal data and structure refinement for 3v.**

Identification code	**3v**
Empirical formula	$C_{14}H_{14}O_6$
Formula weight	278.25
Temperature	100.00(10) K
Wavelength	1.54184 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 7.17307(3) Å α = 90°.
	b = 9.46902(5) Å β = 90°.
	c = 36.9162(2) Å γ = 90°.
Volume	2507.42(2) Å3
Z	8
Density (calculated)	1.474 Mg/m^3
Absorption coefficient	0.986 mm^{-1}
F(000)	1168
Crystal size	0.09 x 0.05 x 0.035 mm^3
Theta range for data collection	4.792 to 74.474°.
Index ranges	-7<=h<=8, -11<=k<=11, -46<=l<=46
Reflections collected	52023
Independent reflections	5118 [R(int) = 0.0357]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.84005
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5118 / 39 / 369
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0311, wR2 = 0.0804
R indices (all data)	R1 = 0.0314, wR2 = 0.0806
Absolute structure parameter	0.01(3)
Extinction coefficient	0.00095(17)
Largest diff. peak and hole	0.848 and -0.347 $e.Å^{-3}$

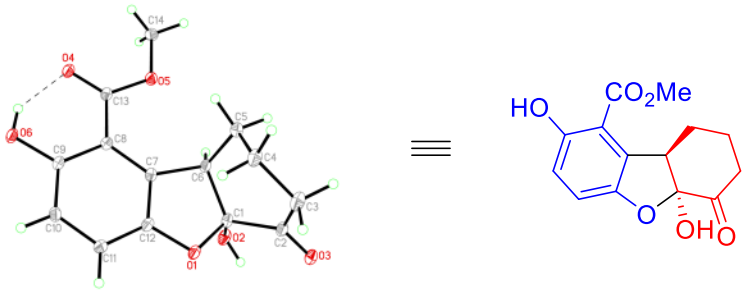


Figure S2. Crystallographic Data for **3v**.

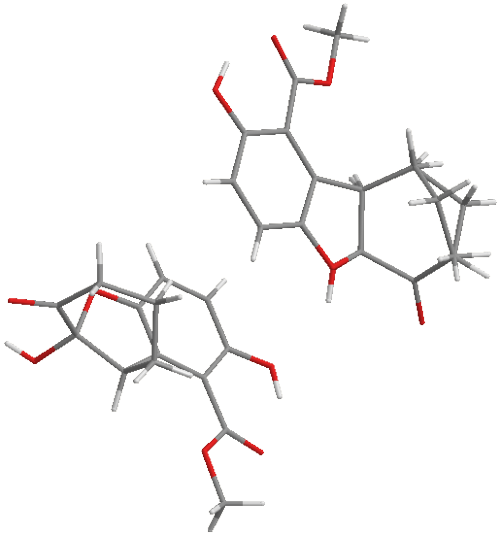


Figure S3. Filp of the cyclohexanone in **3v**.

Although the -CH_2-CH_2- fragment of the cyclohexanone part is disordered over two positions, the structure and absolute configuration of **3v** is determined. The single crystal of **3v** [$\mathbf{C_{14}H_{14}O_6}$] was obtained from the mixed solvents of ethyl acetate and *n*-hexane. CCDC 1921254 contains the supplementary crystallographic data which can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.

c) The configuration of **4a** was determined by X-ray analysis.

***Table S4*. Crystal data and structure refinement for 4a.**

Identification code	**4a**
Empirical formula	$C_{20}H_{17}NO_4$
Formula weight	335.35
Temperature	100.00(10) K
Wavelength	1.54184 Å
Crystal system	Monoclinic

Space group	P 1 21/c 1
Unit cell dimensions	a = 12.27300(10) Å α = 90°.
	b = 13.85930(10) Å β = 103.9840(10)°.
	c = 19.0331(2) Å γ = 90°.
Volume	3141.49(5) $Å^3$
Z	8
Density (calculated)	1.418 Mg/m^3
Absorption coefficient	0.814 mm^{-1}
F(000)	1408
Crystal size	0.1 x 0.05 x 0.04 mm^3
Theta range for data collection	3.712 to 77.708°.
Index ranges	-15<=h<=15, -15<=k<=17, -24<=l<=24
Reflections collected	29255
Independent reflections	6612 [R(int) = 0.0265]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.82155
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6612 / 0 / 455
Goodness-of-fit on F^2	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.1040
R indices (all data)	R1 = 0.0420, wR2 = 0.1063
Extinction coefficient	n/a
Largest diff. peak and hole	0.319 and -0.307 $e.Å^{-3}$

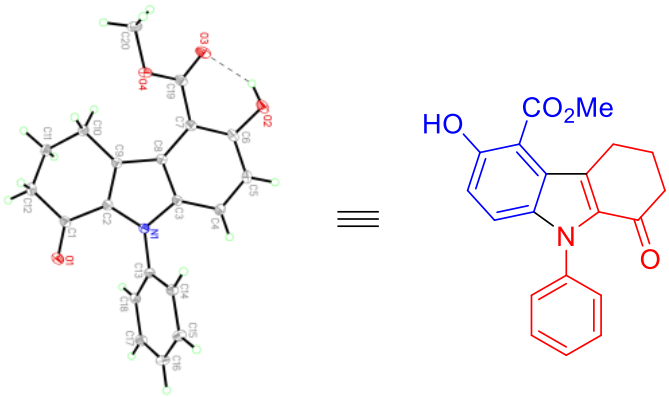


Figure S4. Crystallographic Data for **4a**.

Single crystal of **4a** [$C_{20}H_{17}NO_4$] was obtained from the mixed solvents of ethyl acetate and *n*-hexane. CCDC 1919286 contains the supplementary crystallographic data which can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.

12. Mechanism study

a) Control NMR experiments.

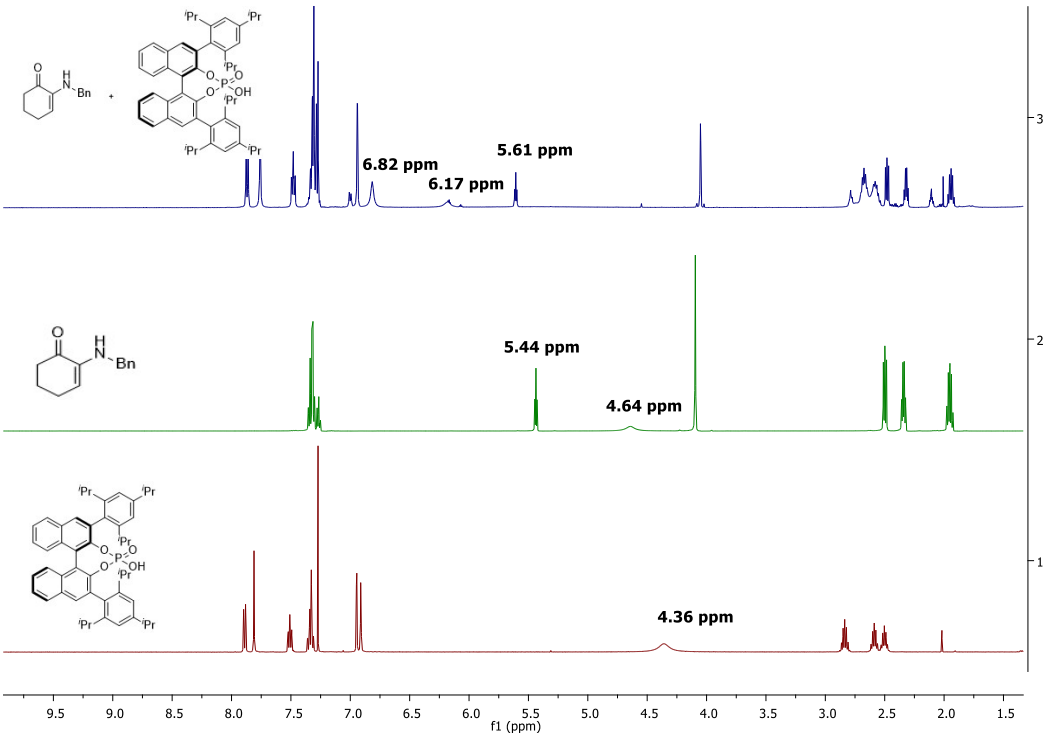


Figure S5. ^{1}H NMR spectra for the investigation of the interaction of phosphoric acid with α-enaminone in $CDCl_3$.

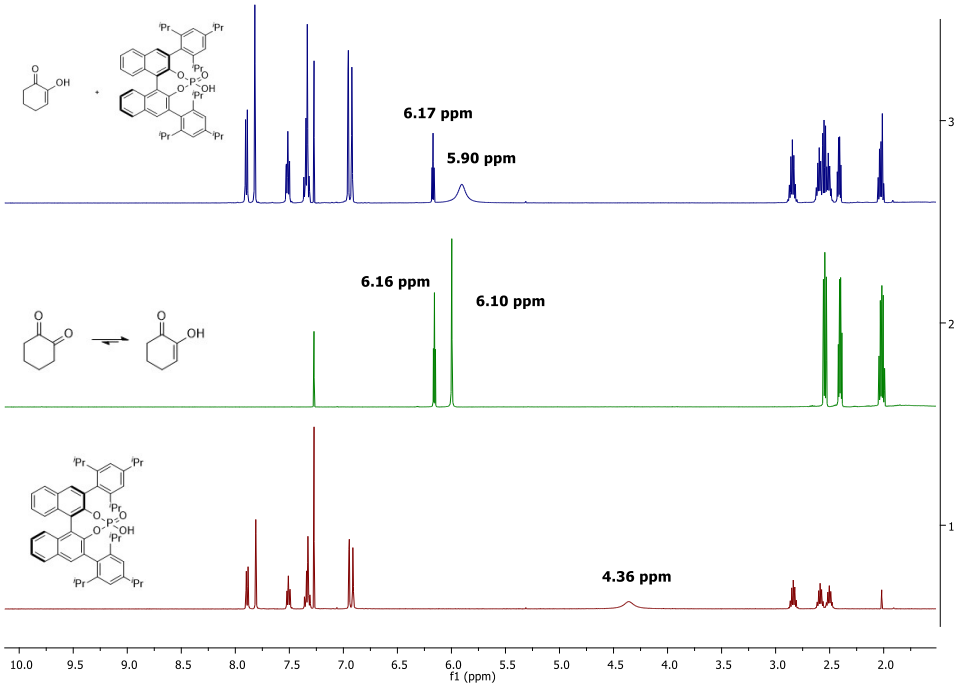


Figure S6. ^{1}H NMR spectra for the investigation of the interaction of phosphoric acid with1,2-cyclohexanedione in $CDCl_3$.

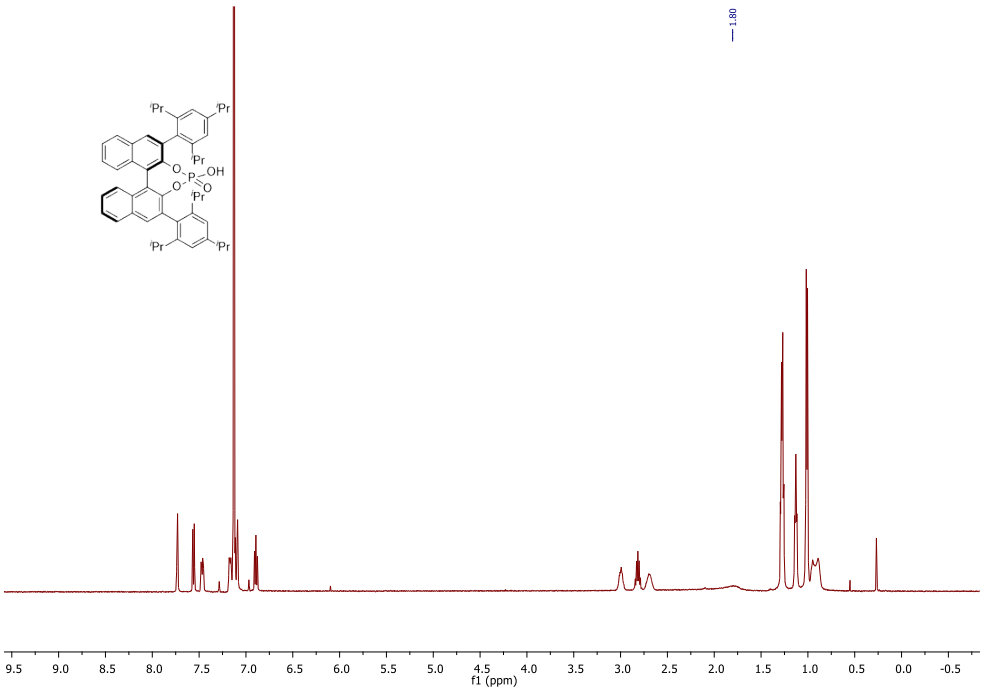


Figure S7. ^{1}H NMR spectra of CPA5 in C_6D_6.

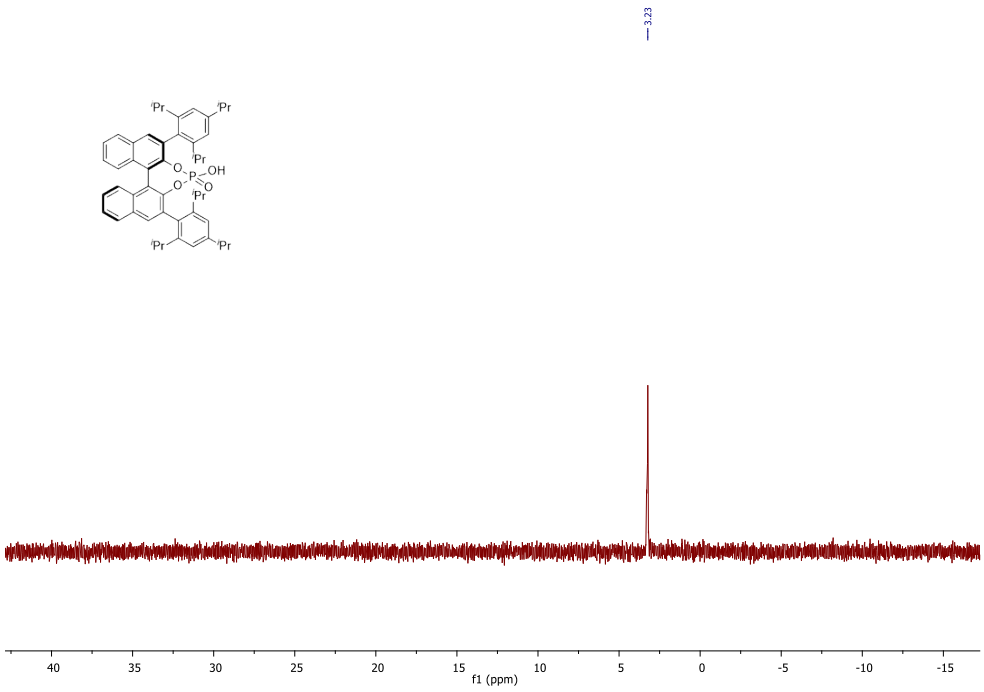


Figure S8. ^{31}P NMR spectra of CPA5 in C_6D_6.

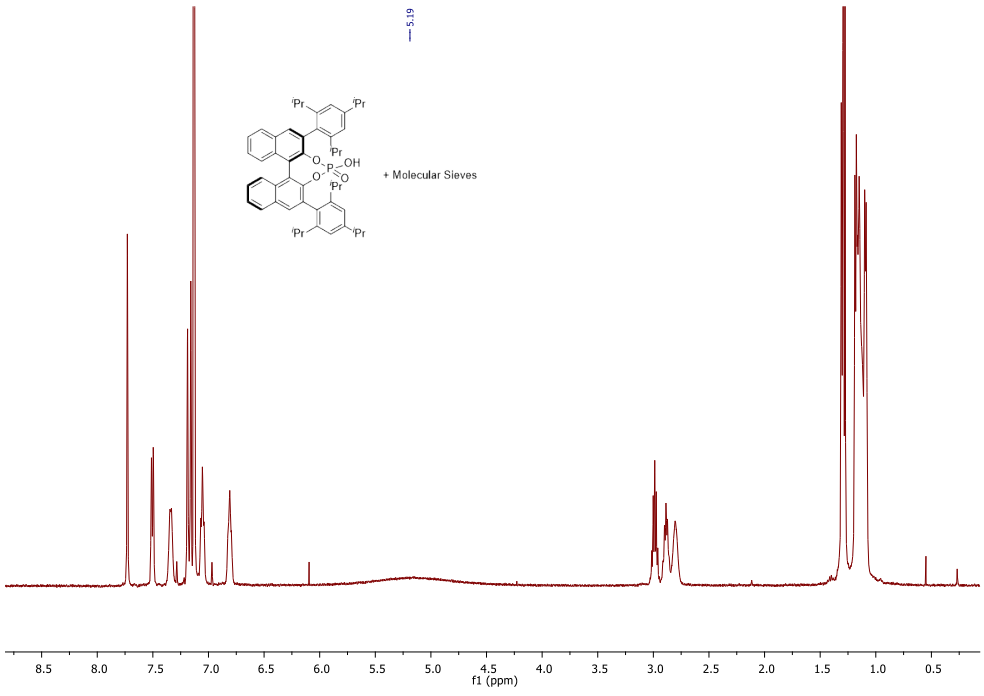


Figure S9. ^{1}H NMR spectra of CPA5 and molecular sieves in C_6D_6.

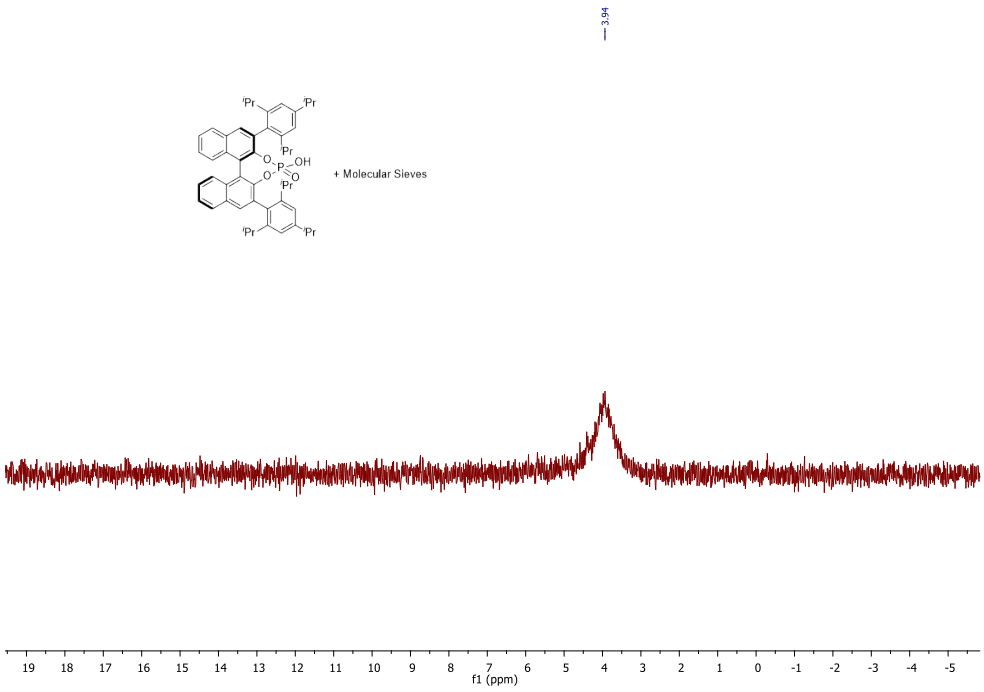


Figure S10. ^{31}P NMR spectra of CPA5 and molecular sieves in C_6D_6.

b) Potential reaction products of the α-enaminones and quinones.

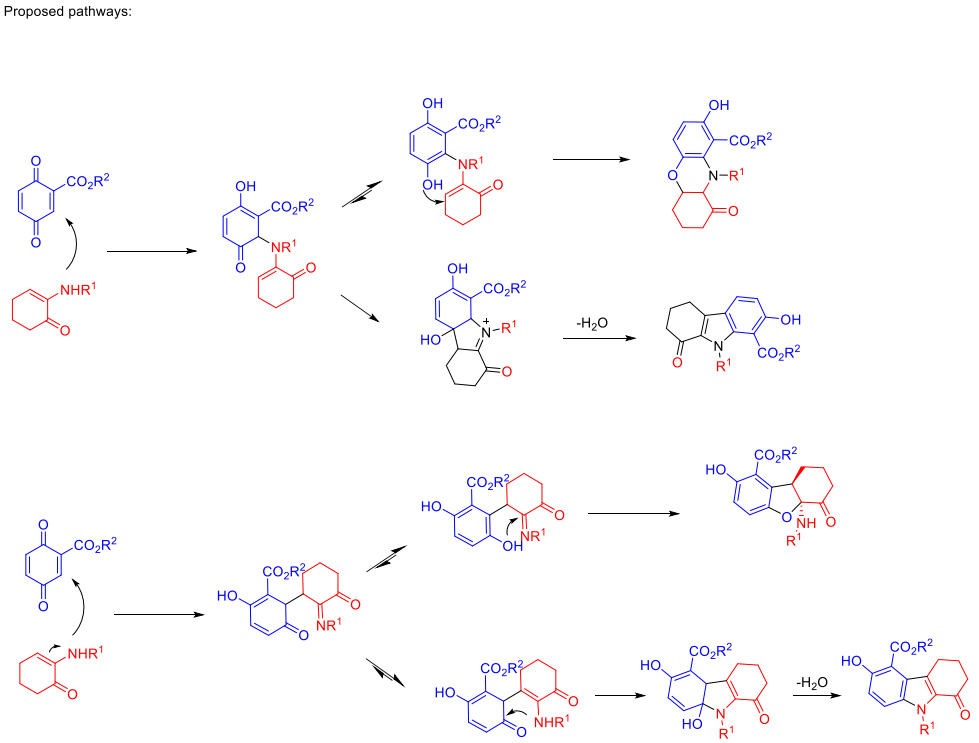


Figure S11. Possible reaction pathways to diverse products.

c) Proposed Mechanism.

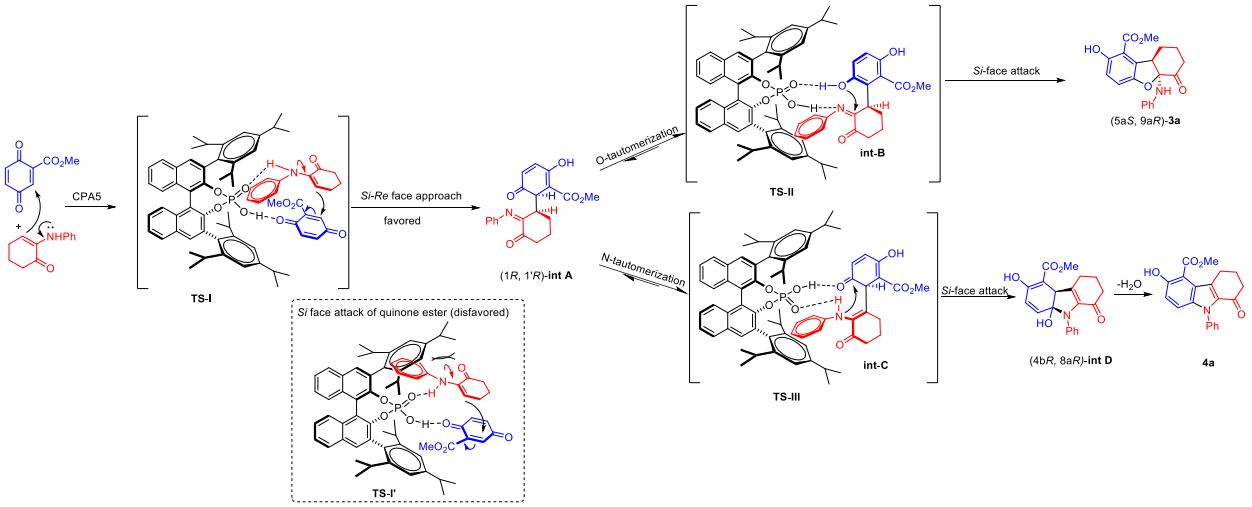


Figure S12. Proposed Mechanism.

13. DFT calculations

Computational method: calculations are done with the Gaussian 16 software package.[4] Geometry optimizations and frequency calculations were performed with B3LYP[5] functional and 6-31G(d) basis set. Frequency calculations confirm that local minima have zero imaginary frequency and transition states have one imaginary frequency. Single-point energies are then performed with B3LYP-D3[6] with a Becke-Johnson[7] (BJ) damping function and the 6-311+G(d,p) basis set and CPCM[8] continuum solvent model with dichloromethane.

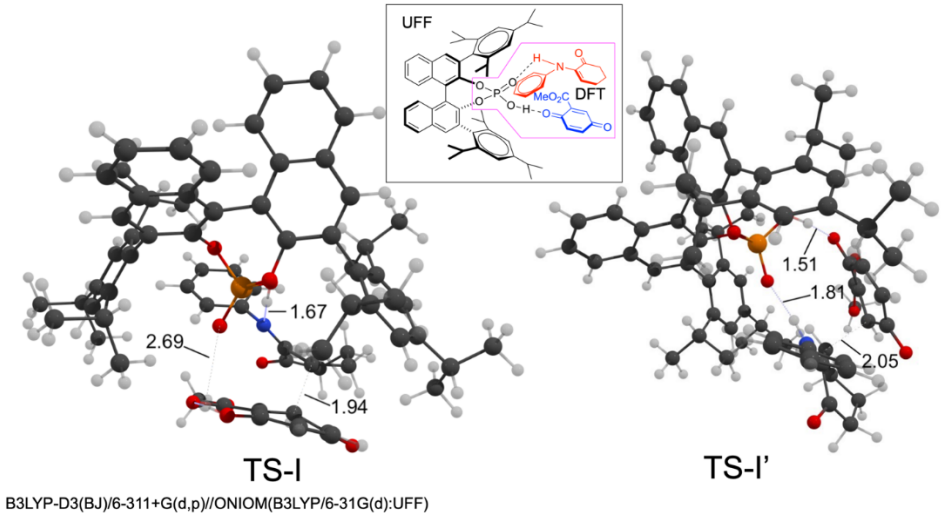


Figure S13. Optimized geometries and the key bond lengths of TS-I and TS-I' with CPA5. The higher layer with DFT method and the lower layer with UFF is shown in the figure.

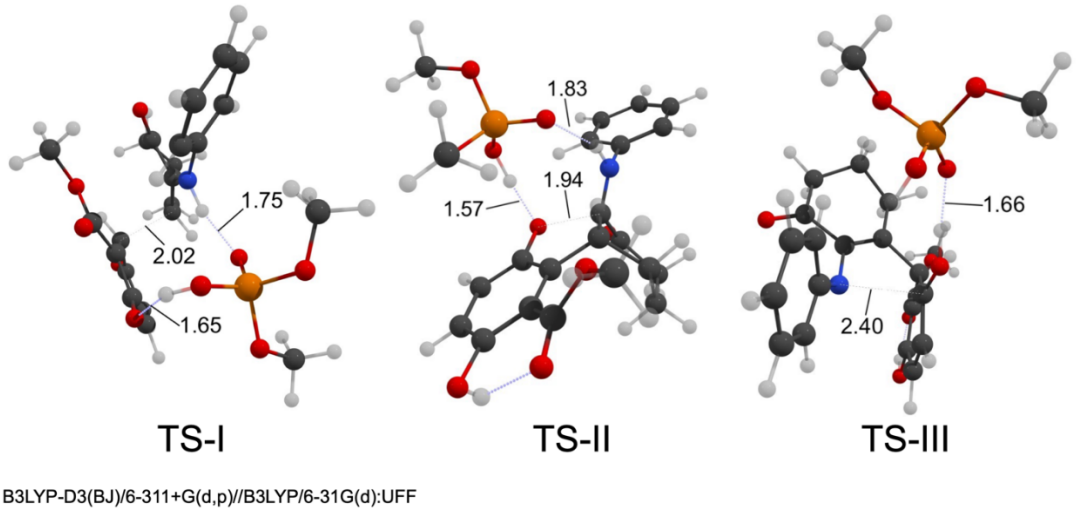


Figure S14. Optimized geometries and the key bond lengths of TS-I, TS-II and TS-III with truncated phosphoric acid catalyst.

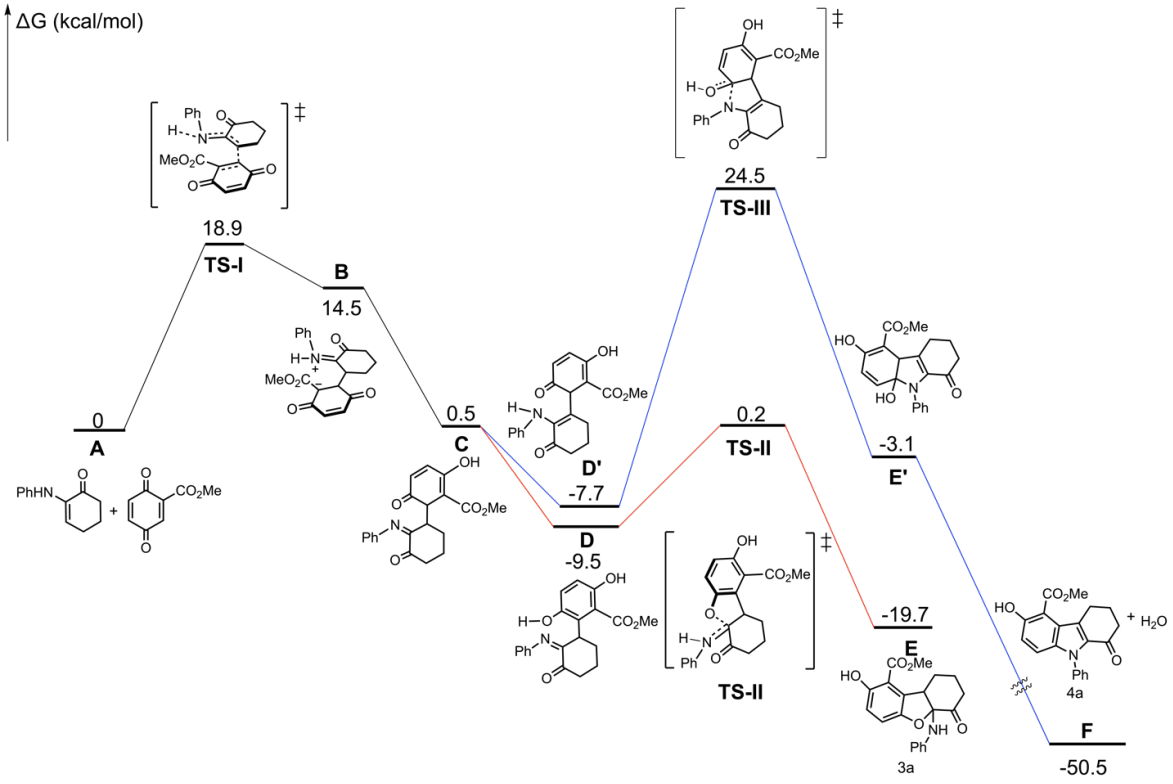


Figure S15. Possible background reaction mechanism without catalyst.

2a

H	-0.232173000000	2.088912000000	-0.542382000000
N	-0.203377000000	1.087079000000	-0.408171000000
C	1.057839000000	0.582300000000	-0.064891000000
C	1.406038000000	-0.806134000000	-0.518093000000
C	2.759239000000	-1.333503000000	-0.054191000000
C	3.837167000000	-0.244696000000	-0.107906000000
H	3.007052000000	-2.198630000000	-0.675842000000
H	2.648063000000	-1.694372000000	0.980386000000
H	4.803256000000	-0.643212000000	0.222422000000
H	3.965339000000	0.082678000000	-1.148207000000
C	-1.451369000000	0.509323000000	-0.114107000000
C	-2.599827000000	1.090791000000	-0.676551000000
C	-1.600472000000	-0.594943000000	0.737711000000
C	-3.862902000000	0.575769000000	-0.398675000000
H	-2.491556000000	1.943297000000	-1.343856000000
C	-2.867875000000	-1.115065000000	0.993587000000
H	-0.729698000000	-1.041414000000	1.205038000000
C	-4.007878000000	-0.536301000000	0.433646000000
H	-4.737665000000	1.042734000000	-0.844140000000
H	-2.962198000000	-1.975546000000	1.651183000000
H	-4.992723000000	-0.943155000000	0.643789000000
C	1.994784000000	1.355967000000	0.533126000000
H	1.703984000000	2.351556000000	0.869715000000
C	3.427987000000	0.956416000000	0.753260000000
H	4.087320000000	1.812890000000	0.558106000000
H	3.570698000000	0.715238000000	1.820211000000
O	0.653444000000	-1.473758000000	-1.205089000000

1a

O	0.063344000000	2.457507000000	-0.313454000000
C	0.643115000000	1.399507000000	-0.127208000000
C	2.129467000000	1.343129000000	-0.113763000000
C	-0.087470000000	0.098852000000	0.040055000000
C	2.801745000000	0.183977000000	-0.032599000000
H	2.626204000000	2.305033000000	-0.203814000000
C	0.596953000000	-1.060567000000	0.095491000000
C	2.082158000000	-1.108205000000	0.062686000000
H	3.886653000000	0.129764000000	-0.042695000000
H	0.094314000000	-2.018737000000	0.183610000000
C	-1.579138000000	0.134228000000	0.195154000000
O	-2.177408000000	0.973062000000	0.827638000000
O	-2.160893000000	-0.915319000000	-0.423385000000
C	-3.590118000000	-0.997785000000	-0.267538000000
H	-4.067739000000	-0.102119000000	-0.672228000000
H	-3.891953000000	-1.883105000000	-0.826977000000
H	-3.854520000000	-1.097478000000	0.788386000000
O	2.678304000000	-2.176772000000	0.116708000000

CPA (simplified with OMe)

O	-0.790141000000	-1.229927000000	1.075298000000
H	-0.377853000000	-2.079541000000	1.301173000000
O	0.947413000000	0.522622000000	0.753586000000
P	0.040609000000	-0.502996000000	-0.106261000000
O	0.774693000000	-1.377194000000	-1.040280000000
O	-1.079554000000	0.400488000000	-0.810474000000

C	2.036088000000	1.186641000000	0.082909000000
H	2.596929000000	1.712447000000	0.857308000000
H	2.676646000000	0.457555000000	-0.419784000000
H	1.655234000000	1.907590000000	-0.648605000000
C	-1.947548000000	1.250161000000	-0.038998000000
H	-2.538535000000	1.816798000000	-0.760180000000
H	-2.606895000000	0.646186000000	0.590548000000
H	-1.365197000000	1.935183000000	0.584956000000

B

O	2.404520000000	-2.056162000000	1.872399000000
H	2.468481000000	0.461122000000	1.438732000000
O	1.655032000000	-0.316785000000	-1.030679000000
H	-0.028623000000	0.651212000000	-0.786355000000
O	3.284570000000	1.565671000000	-1.593875000000
P	2.970862000000	0.284863000000	-0.676154000000
O	3.169276000000	0.790362000000	0.812882000000
O	4.236025000000	-0.695176000000	-0.872791000000
C	4.409586000000	2.416347000000	-1.308330000000
H	4.420776000000	3.178867000000	-2.088641000000
H	4.291330000000	2.884971000000	-0.327869000000
H	5.343570000000	1.845496000000	-1.333363000000
C	4.346883000000	-1.426011000000	-2.105548000000
H	5.227691000000	-2.062504000000	-2.006389000000
H	3.456481000000	-2.040180000000	-2.268309000000
H	4.479703000000	-0.743082000000	-2.951804000000
N	-0.987302000000	0.947416000000	-0.595355000000
C	-1.962268000000	0.113445000000	-1.158758000000

C	-3.260752000000	-0.042100000000	-0.427325000000
C	-4.293956000000	-0.989255000000	-1.027584000000
C	-4.104759000000	-1.246075000000	-2.524245000000
H	-5.288029000000	-0.597554000000	-0.786588000000
H	-4.187536000000	-1.938382000000	-0.480254000000
H	-4.809674000000	-2.011018000000	-2.869945000000
H	-4.319525000000	-0.329573000000	-3.089723000000
C	-1.149526000000	2.317264000000	-0.337714000000
C	-2.294690000000	3.039734000000	-0.712973000000
C	-0.102290000000	3.006045000000	0.304701000000
C	-2.394933000000	4.400269000000	-0.429403000000
H	-3.102005000000	2.540627000000	-1.237163000000
C	-0.208659000000	4.369437000000	0.569274000000
H	0.789012000000	2.462665000000	0.603642000000
C	-1.357415000000	5.079216000000	0.211927000000
H	-3.293053000000	4.936089000000	-0.727052000000
H	0.615144000000	4.878135000000	1.064240000000
H	-1.440008000000	6.141326000000	0.424186000000
C	-1.681381000000	-0.702014000000	-2.206960000000
H	-0.680835000000	-0.658528000000	-2.634626000000
C	1.328905000000	-2.425609000000	1.421765000000
C	1.242835000000	-3.672165000000	0.616658000000
C	0.048616000000	-1.697330000000	1.683422000000
C	0.075983000000	-4.151483000000	0.158000000000
H	2.192371000000	-4.169403000000	0.440970000000
C	-1.122673000000	-2.202219000000	1.243679000000
C	-1.193408000000	-3.441448000000	0.431008000000
H	0.002017000000	-5.063682000000	-0.427205000000

H	-2.060127000000	-1.692917000000	1.438145000000
C	0.080950000000	-0.386230000000	2.404193000000
O	1.023955000000	0.391910000000	2.401916000000
O	-1.060785000000	-0.150425000000	3.044275000000
C	-1.228167000000	1.172453000000	3.602146000000
H	-1.178195000000	1.916269000000	2.805282000000
H	-2.217161000000	1.161437000000	4.057551000000
H	-0.453693000000	1.364834000000	4.348078000000
O	-2.266352000000	-3.851029000000	-0.005127000000
C	-2.659556000000	-1.677012000000	-2.799898000000
H	-2.477054000000	-1.758012000000	-3.879108000000
H	-2.490361000000	-2.685904000000	-2.387973000000
O	-3.449800000000	0.483044000000	0.661390000000

TS1

O	1.206736000000	-2.303047000000	1.815579000000
H	2.262588000000	-1.044307000000	1.663343000000
O	1.791852000000	-0.703126000000	-1.099450000000
H	0.372681000000	0.240652000000	-0.693265000000
O	4.253317000000	0.114237000000	-0.874745000000
P	3.074718000000	-0.829568000000	-0.330029000000
O	2.998063000000	-0.518082000000	1.216067000000
O	3.755561000000	-2.275270000000	-0.424559000000
C	3.991834000000	1.487110000000	-1.213482000000
H	3.821410000000	2.076843000000	-0.308771000000
H	4.883688000000	1.849149000000	-1.727943000000
H	3.123199000000	1.564041000000	-1.873466000000
C	3.904396000000	-2.897514000000	-1.711440000000

H	2.945749000000	-2.928524000000	-2.237699000000
H	4.641894000000	-2.355471000000	-2.311927000000
H	4.259333000000	-3.911659000000	-1.521407000000
N	-0.355611000000	0.972405000000	-0.569370000000
C	-1.602889000000	0.655828000000	-0.918628000000
C	-2.740820000000	1.636612000000	-0.715178000000
C	-4.063199000000	1.254703000000	-1.356642000000
C	-3.859011000000	0.354277000000	-2.576485000000
H	-4.593616000000	2.183873000000	-1.588397000000
H	-4.664427000000	0.730173000000	-0.597808000000
H	-4.822340000000	0.119957000000	-3.042789000000
H	-3.262331000000	0.887257000000	-3.329731000000
C	0.197707000000	2.267393000000	-0.286814000000
C	0.047950000000	3.320659000000	-1.196430000000
C	0.995403000000	2.420981000000	0.850441000000
C	0.669439000000	4.540952000000	-0.946758000000
H	-0.546843000000	3.179634000000	-2.093373000000
C	1.611033000000	3.651694000000	1.091996000000
H	1.114769000000	1.598329000000	1.547058000000
C	1.450014000000	4.712421000000	0.200167000000
H	0.548275000000	5.357717000000	-1.652830000000
H	2.217453000000	3.773902000000	1.985039000000
H	1.933004000000	5.666411000000	0.392217000000
C	-1.908535000000	-0.687728000000	-1.296146000000
H	-1.031140000000	-1.263262000000	-1.585804000000
C	0.095607000000	-2.385123000000	1.248313000000
C	-0.145841000000	-3.634490000000	0.470623000000
C	-0.975502000000	-1.420071000000	1.305508000000

C	-1.312186000000	-3.923030000000	-0.129695000000
H	0.699190000000	-4.317490000000	0.453497000000
C	-2.134335000000	-1.604857000000	0.492500000000
C	-2.442579000000	-2.986500000000	-0.019858000000
H	-1.496371000000	-4.859588000000	-0.648782000000
H	-3.034817000000	-1.086537000000	0.801886000000
C	-0.899838000000	-0.280087000000	2.227578000000
O	0.044991000000	0.036236000000	2.932724000000
O	-2.071798000000	0.428785000000	2.231235000000
C	-2.097531000000	1.578068000000	3.089443000000
H	-1.385983000000	2.331916000000	2.744841000000
H	-3.113824000000	1.967788000000	3.022490000000
H	-1.857035000000	1.294004000000	4.117028000000
O	-3.585634000000	-3.313954000000	-0.323263000000
C	-3.151348000000	-0.938519000000	-2.152916000000
H	-2.851221000000	-1.513883000000	-3.036530000000
H	-3.862984000000	-1.575666000000	-1.614072000000
O	-2.606889000000	2.651066000000	-0.056510000000

C

O	-0.104483000000	3.060996000000	1.792115000000
H	-0.442772000000	2.310558000000	2.346241000000
O	-1.468793000000	1.085687000000	-1.128868000000
H	-0.947371000000	0.269930000000	-0.845278000000
O	-3.842039000000	0.426571000000	-0.730306000000
P	-2.699165000000	1.441310000000	-0.177696000000
O	-2.506593000000	1.398553000000	1.287173000000
O	-3.139182000000	2.896623000000	-0.704928000000

C	-4.984267000000	0.176357000000	0.107062000000
H	-5.530269000000	-0.648631000000	-0.354925000000
H	-4.667513000000	-0.097697000000	1.116199000000
H	-5.629576000000	1.060710000000	0.153877000000
C	-3.346733000000	3.139817000000	-2.103728000000
H	-3.707641000000	4.166828000000	-2.187112000000
H	-2.408312000000	3.029624000000	-2.655229000000
H	-4.094527000000	2.451990000000	-2.511913000000
N	0.009822000000	-1.163194000000	-0.545136000000
C	1.289803000000	-1.136277000000	-0.644598000000
C	2.213061000000	-2.350825000000	-0.606410000000
C	2.870007000000	-2.637039000000	-1.952440000000
C	2.767771000000	-1.437515000000	-2.908472000000
H	2.389723000000	-3.534047000000	-2.367978000000
H	3.913547000000	-2.907931000000	-1.750921000000
H	3.473493000000	-1.560606000000	-3.737029000000
H	1.765574000000	-1.392494000000	-3.354956000000
C	-0.790962000000	-2.304582000000	-0.272782000000
C	-0.523218000000	-3.247570000000	0.732224000000
C	-1.969692000000	-2.418092000000	-1.029942000000
C	-1.410105000000	-4.303276000000	0.944448000000
H	0.366093000000	-3.147182000000	1.338663000000
C	-2.834613000000	-3.489287000000	-0.824773000000
H	-2.196062000000	-1.660893000000	-1.773069000000
C	-2.558827000000	-4.436933000000	0.163957000000
H	-1.197293000000	-5.024943000000	1.728470000000
H	-3.733346000000	-3.574864000000	-1.429355000000
H	-3.241729000000	-5.264690000000	0.333858000000

C	1.978140000000	0.159343000000	-1.063534000000
H	1.195464000000	0.787647000000	-1.500434000000
C	0.902883000000	2.610833000000	1.049579000000
C	1.411739000000	3.602667000000	0.101584000000
C	1.486781000000	1.371063000000	1.154211000000
C	2.550251000000	3.405965000000	-0.591225000000
H	0.852715000000	4.532395000000	0.041097000000
C	2.568476000000	0.965170000000	0.177143000000
C	3.325046000000	2.162863000000	-0.409564000000
H	2.985543000000	4.173978000000	-1.223573000000
H	3.308522000000	0.327074000000	0.667032000000
C	1.073636000000	0.502589000000	2.251298000000
O	0.184008000000	0.767955000000	3.058388000000
O	1.807988000000	-0.629459000000	2.334064000000
C	1.513306000000	-1.489593000000	3.446560000000
H	0.450044000000	-1.738859000000	3.468306000000
H	2.120971000000	-2.379618000000	3.285698000000
H	1.783027000000	-0.998615000000	4.385884000000
O	4.495280000000	2.082289000000	-0.755280000000
C	3.062920000000	-0.140919000000	-2.142105000000
H	3.126808000000	0.708542000000	-2.828382000000
H	4.049469000000	-0.216505000000	-1.669791000000
O	2.431528000000	-3.011409000000	0.389526000000

Int A

O	-1.949450000000	-3.277507000000	-0.972128000000
H	-1.245340000000	-3.502799000000	-0.302065000000
N	1.039112000000	0.213584000000	-0.880551000000

C	0.361418000000	1.011689000000	-0.142887000000
C	0.906707000000	1.937265000000	0.935965000000
C	0.656580000000	3.418972000000	0.666274000000
C	-0.312763000000	3.648734000000	-0.501244000000
H	1.634012000000	3.888525000000	0.489871000000
H	0.270223000000	3.855554000000	1.596349000000
H	-0.638688000000	4.694713000000	-0.516006000000
H	0.196474000000	3.465602000000	-1.456973000000
C	2.413361000000	-0.084253000000	-0.815893000000
C	3.146991000000	-0.347226000000	0.355151000000
C	3.054794000000	-0.215562000000	-2.062691000000
C	4.492649000000	-0.705739000000	0.268046000000
H	2.661542000000	-0.268746000000	1.317930000000
C	4.404567000000	-0.542151000000	-2.137391000000
H	2.468875000000	-0.048660000000	-2.961473000000
C	5.130653000000	-0.793410000000	-0.969550000000
H	5.045879000000	-0.913539000000	1.180329000000
H	4.886699000000	-0.620630000000	-3.108205000000
H	6.180362000000	-1.068192000000	-1.026081000000
C	-1.111214000000	1.220583000000	-0.506071000000
H	-1.176361000000	0.921232000000	-1.557492000000
C	-2.266200000000	-1.996544000000	-0.765042000000
C	-3.339757000000	-1.500310000000	-1.623281000000
C	-1.702382000000	-1.194197000000	0.196652000000
C	-3.924516000000	-0.306910000000	-1.400112000000
H	-3.683660000000	-2.174986000000	-2.402615000000
C	-2.095617000000	0.262359000000	0.297943000000
C	-3.493308000000	0.537450000000	-0.264379000000

H	-4.784558000000	0.032410000000	-1.969672000000
H	-2.094564000000	0.584082000000	1.342754000000
C	-0.748769000000	-1.798533000000	1.117604000000
O	-0.366546000000	-2.973943000000	1.053300000000
O	-0.337682000000	-0.966486000000	2.088753000000
C	0.573865000000	-1.511793000000	3.058886000000
H	1.414197000000	-1.999039000000	2.560785000000
H	0.911882000000	-0.656654000000	3.642041000000
H	0.057489000000	-2.240119000000	3.690467000000
O	-4.201230000000	1.439000000000	0.160187000000
C	-1.521262000000	2.713658000000	-0.362806000000
H	-2.284210000000	2.954401000000	-1.108534000000
H	-1.996577000000	2.882131000000	0.611676000000
O	1.498377000000	1.553328000000	1.928605000000

E

O	1.363322000000	-3.322291000000	-2.814535000000
H	2.080123000000	-2.667048000000	-2.998337000000
O	-2.303585000000	0.750644000000	0.933687000000
H	-1.380093000000	0.710674000000	0.525706000000
O	-3.219452000000	-0.281764000000	-1.140432000000
P	-3.391075000000	-0.302199000000	0.463387000000
O	-3.376050000000	-1.666906000000	1.060262000000
O	-4.780411000000	0.423236000000	0.796368000000
C	-3.723750000000	-1.384129000000	-1.919420000000
H	-3.448956000000	-1.172617000000	-2.953870000000
H	-3.267156000000	-2.320883000000	-1.592718000000
H	-4.813123000000	-1.452704000000	-1.833876000000

C	-5.032115000000	1.769224000000	0.355934000000
H	-6.054697000000	2.000835000000	0.658095000000
H	-4.333949000000	2.462256000000	0.832630000000
H	-4.940740000000	1.843778000000	-0.732202000000
N	0.273064000000	1.215390000000	0.219030000000
C	1.256231000000	0.726265000000	0.883745000000
C	2.513778000000	1.525733000000	1.224732000000
C	3.147305000000	1.274134000000	2.591553000000
C	2.482802000000	0.170553000000	3.423539000000
H	3.166671000000	2.237998000000	3.116529000000
H	4.198482000000	1.022915000000	2.394906000000
H	3.143151000000	-0.113543000000	4.250663000000
H	1.556310000000	0.544786000000	3.880720000000
C	0.250245000000	2.476887000000	-0.439436000000
C	0.909118000000	2.666835000000	-1.660939000000
C	-0.580514000000	3.485026000000	0.066807000000
C	0.754724000000	3.865743000000	-2.352688000000
H	1.532850000000	1.873922000000	-2.060083000000
C	-0.709341000000	4.690702000000	-0.622437000000
H	-1.114319000000	3.318459000000	0.997501000000
C	-0.046960000000	4.885789000000	-1.835128000000
H	1.271873000000	4.005152000000	-3.298186000000
H	-1.338948000000	5.475584000000	-0.211594000000
H	-0.158013000000	5.821666000000	-2.375410000000
C	1.072691000000	-0.655515000000	1.509016000000
H	0.154445000000	-0.557060000000	2.100424000000
C	0.861645000000	-3.037104000000	-1.598210000000
C	-0.234533000000	-3.812889000000	-1.190854000000

C	1.389961000000	-2.035892000000	-0.730386000000
C	-0.824624000000	-3.586666000000	0.033925000000
H	-0.591490000000	-4.583623000000	-1.865986000000
C	0.736667000000	-1.771181000000	0.517080000000
C	-0.358084000000	-2.565567000000	0.880902000000
H	-1.674181000000	-4.178853000000	0.360365000000
C	2.612719000000	-1.368757000000	-1.212614000000
O	3.026386000000	-1.437232000000	-2.373310000000
O	3.327812000000	-0.696300000000	-0.287892000000
C	4.558118000000	-0.111494000000	-0.769035000000
H	4.349727000000	0.654941000000	-1.517058000000
H	5.027142000000	0.335128000000	0.106314000000
H	5.194156000000	-0.886047000000	-1.201466000000
C	2.161424000000	-1.036679000000	2.536987000000
H	1.775089000000	-1.867769000000	3.135796000000
H	3.068801000000	-1.388693000000	2.035980000000
O	2.982954000000	2.343992000000	0.457542000000
O	-0.981897000000	-2.350850000000	2.081814000000
H	-1.946144000000	-2.220330000000	1.894664000000

E’

O	2.882377000000	1.454861000000	-2.851779000000
H	3.736228000000	1.238695000000	-2.386733000000
O	-2.562176000000	1.014822000000	-0.472161000000
H	-0.807453000000	0.732787000000	0.221211000000
O	-5.087353000000	0.842360000000	-0.811816000000
P	-3.717644000000	0.078726000000	-0.479927000000
O	-3.687170000000	-1.107806000000	-1.539090000000

O	-3.957681000000	-0.693591000000	0.914597000000
C	-6.319846000000	0.113652000000	-0.953234000000
H	-7.100848000000	0.861836000000	-1.098130000000
H	-6.271149000000	-0.549476000000	-1.821237000000
H	-6.529179000000	-0.471414000000	-0.052209000000
C	-3.772413000000	0.035142000000	2.150051000000
H	-4.046482000000	-0.656163000000	2.948460000000
H	-2.730978000000	0.343954000000	2.265918000000
H	-4.428365000000	0.911176000000	2.183631000000
N	0.177218000000	0.634316000000	0.484466000000
C	0.507747000000	-0.603093000000	1.089812000000
C	0.267777000000	-0.771951000000	2.559539000000
C	0.786592000000	-2.059455000000	3.182240000000
C	0.481790000000	-3.245278000000	2.259603000000
H	0.331405000000	-2.169783000000	4.170584000000
H	1.873846000000	-1.963649000000	3.324914000000
H	0.842983000000	-4.181604000000	2.700142000000
H	-0.606252000000	-3.343144000000	2.151781000000
C	0.781510000000	1.838468000000	0.868294000000
C	2.060605000000	1.876772000000	1.447951000000
C	0.120706000000	3.050709000000	0.597600000000
C	2.652861000000	3.098735000000	1.762032000000
H	2.588329000000	0.948331000000	1.648748000000
C	0.727924000000	4.263656000000	0.908918000000
H	-0.869926000000	3.022104000000	0.151824000000
C	1.996218000000	4.301206000000	1.495133000000
H	3.641345000000	3.107766000000	2.215161000000
H	0.200122000000	5.190039000000	0.695309000000

H	2.464086000000	5.250769000000	1.738737000000
C	0.930909000000	-1.642821000000	0.332347000000
C	1.981210000000	0.564331000000	-2.434433000000
C	0.659506000000	0.752504000000	-3.011130000000
C	2.238778000000	-0.463495000000	-1.556094000000
C	-0.378008000000	-0.056102000000	-2.713750000000
H	0.548123000000	1.595244000000	-3.686960000000
C	-0.211709000000	-1.193069000000	-1.813337000000
H	-1.368609000000	0.107601000000	-3.124061000000
C	3.610042000000	-0.624668000000	-1.093012000000
O	4.538487000000	0.142529000000	-1.374554000000
O	3.813267000000	-1.716083000000	-0.327191000000
C	5.163624000000	-1.913487000000	0.129674000000
H	5.490244000000	-1.065454000000	0.736196000000
H	5.136296000000	-2.826121000000	0.725456000000
H	5.841895000000	-2.027780000000	-0.719368000000
C	1.106940000000	-3.039218000000	0.874948000000
H	0.669497000000	-3.746675000000	0.158617000000
H	2.183952000000	-3.261240000000	0.898752000000
O	-0.327671000000	0.073006000000	3.209505000000
O	-1.143196000000	-1.968285000000	-1.556201000000
H	-2.775835000000	-1.508946000000	-1.622956000000
C	1.157301000000	-1.457879000000	-1.179630000000
H	1.459427000000	-2.442423000000	-1.567765000000

TSII

O	-5.067814000000	-0.189894000000	-1.554862000000
H	-5.395524000000	-0.528230000000	-0.678555000000

O	0.714105000000	1.772847000000	1.533111000000
H	1.501555000000	0.141900000000	1.239288000000
O	1.215356000000	2.204975000000	-1.022437000000
N	1.807371000000	-0.676065000000	0.675380000000
C	0.853098000000	-1.249670000000	-0.069230000000
C	1.291077000000	-2.490908000000	-0.872741000000
C	0.696667000000	-3.820979000000	-0.446287000000
C	-0.751552000000	-3.717631000000	0.045207000000
H	1.328781000000	-4.185476000000	0.385205000000
H	0.821719000000	-4.525213000000	-1.272516000000
H	-1.419218000000	-3.492005000000	-0.805503000000
H	-1.070483000000	-4.684902000000	0.450411000000
C	3.241800000000	-0.780574000000	0.474070000000
C	3.997013000000	-1.459451000000	1.468835000000
C	3.858488000000	-0.160331000000	-0.635339000000
C	5.383807000000	-1.530280000000	1.336889000000
H	3.491143000000	-1.925598000000	2.323200000000
C	5.244428000000	-0.233037000000	-0.749750000000
H	3.265256000000	0.368476000000	-1.394259000000
C	6.013663000000	-0.917179000000	0.226842000000
H	5.975427000000	-2.060857000000	2.108710000000
H	5.735125000000	0.240120000000	-1.620622000000
H	7.093317000000	-0.975505000000	0.133831000000
C	-0.557867000000	-1.212390000000	0.556171000000
H	-0.526906000000	-0.519020000000	1.402421000000
C	-3.718383000000	-0.224901000000	-1.521391000000
C	-3.054455000000	0.179600000000	-2.685162000000
C	-2.965024000000	-0.620298000000	-0.373198000000

C	-1.672521000000	0.207393000000	-2.741718000000
H	-3.652804000000	0.488611000000	-3.536053000000
C	-1.546637000000	-0.690797000000	-0.476980000000
C	-0.916605000000	-0.223204000000	-1.628995000000
H	-1.146392000000	0.539666000000	-3.631258000000
C	-3.731640000000	-0.768955000000	0.874811000000
O	-4.952667000000	-0.937378000000	0.931554000000
O	-3.001510000000	-0.619437000000	2.002099000000
C	-3.725593000000	-0.704772000000	3.237114000000
H	-4.215695000000	-1.677219000000	3.338202000000
H	-2.981129000000	-0.561996000000	4.022078000000
H	-4.492955000000	0.081243000000	3.285511000000
C	-0.886520000000	-2.629593000000	1.103376000000
H	-0.201153000000	-2.842925000000	1.937867000000
H	-1.886879000000	-2.627337000000	1.537028000000
O	2.123688000000	-2.407562000000	-1.746063000000
P	0.630402000000	2.695429000000	0.365782000000
O	-0.881359000000	3.129101000000	-0.012740000000
O	1.423380000000	4.056373000000	0.654474000000
O	0.432821000000	-0.189215000000	-1.633447000000
H	0.906581000000	1.274679000000	-1.313339000000
C	1.538774000000	5.072027000000	-0.369339000000
H	2.113038000000	4.691138000000	-1.218032000000
H	0.545766000000	5.396421000000	-0.695636000000
H	2.069174000000	5.906189000000	0.096250000000
C	-1.865157000000	3.221374000000	1.023457000000
H	-2.798825000000	3.503168000000	0.532810000000
H	-1.980864000000	2.252983000000	1.528247000000

H	-1.594854000000	3.991563000000	1.756960000000

TSIII

O	4.941270000000	1.673644000000	-1.024200000000
H	5.458520000000	0.950548000000	-0.575890000000
O	-3.535214000000	0.051513000000	-1.138086000000
H	-2.895102000000	0.745633000000	-0.858595000000
N	0.613958000000	1.604374000000	0.694860000000
C	0.608762000000	0.354766000000	1.270820000000
C	0.113347000000	0.180749000000	2.690121000000
C	0.253902000000	-1.204460000000	3.311664000000
C	0.175278000000	-2.318233000000	2.269676000000
H	-0.509910000000	-1.291725000000	4.091160000000
H	1.230645000000	-1.237376000000	3.820204000000
H	0.309437000000	-3.297666000000	2.744871000000
H	-0.813746000000	-2.317298000000	1.795728000000
C	-0.520943000000	2.376070000000	0.632498000000
C	-1.850783000000	1.909033000000	0.823540000000
C	-0.361609000000	3.735677000000	0.263451000000
C	-2.942526000000	2.766133000000	0.667508000000
H	-2.008736000000	0.896012000000	1.182317000000
C	-1.455393000000	4.573099000000	0.092171000000
H	0.651266000000	4.103250000000	0.129744000000
C	-2.758358000000	4.097670000000	0.288168000000
H	-3.947546000000	2.391770000000	0.852393000000
H	-1.295866000000	5.612046000000	-0.186796000000
H	-3.611901000000	4.757991000000	0.164737000000
C	1.186574000000	-0.708015000000	0.629565000000

C	3.681896000000	1.233773000000	-1.133123000000
C	2.802305000000	2.121605000000	-1.849337000000
C	3.249510000000	-0.007397000000	-0.690057000000
C	1.496767000000	1.803293000000	-2.046503000000
H	3.233151000000	3.040269000000	-2.233110000000
C	1.781720000000	-0.419027000000	-0.770003000000
C	0.940221000000	0.626511000000	-1.467453000000
H	0.824145000000	2.452925000000	-2.596659000000
H	1.708874000000	-1.348495000000	-1.357840000000
C	4.278361000000	-0.950805000000	-0.283659000000
O	5.464772000000	-0.656403000000	-0.078391000000
O	3.860597000000	-2.231741000000	-0.204252000000
C	4.867812000000	-3.198040000000	0.136819000000
H	5.321413000000	-2.958962000000	1.101816000000
H	4.345740000000	-4.154215000000	0.182427000000
H	5.649294000000	-3.222409000000	-0.626992000000
O	-0.284164000000	0.315857000000	-1.855715000000
C	1.250888000000	-2.099940000000	1.201198000000
H	1.134670000000	-2.827955000000	0.388420000000
H	2.239243000000	-2.301913000000	1.639779000000
O	-0.332988000000	1.113882000000	3.335125000000
P	-3.089334000000	-1.443799000000	-0.760156000000
O	-3.452686000000	-1.698674000000	0.770670000000
O	-4.182267000000	-2.318025000000	-1.529821000000
O	-1.661202000000	-1.773041000000	-1.034615000000
H	-0.633758000000	-0.534387000000	-1.459574000000
C	-4.777070000000	-1.454154000000	1.286790000000
H	-4.998500000000	-0.383868000000	1.260478000000

H	-5.518879000000	-2.008781000000	0.707056000000
H	-4.763442000000	-1.808687000000	2.317383000000
C	-4.188273000000	-2.344618000000	-2.973086000000
H	-3.212420000000	-2.663670000000	-3.349359000000
H	-4.951920000000	-3.068513000000	-3.259099000000
H	-4.441634000000	-1.356389000000	-3.366593000000

F

O	4.893234000000	0.216686000000	1.875950000000
H	5.335320000000	-0.091822000000	1.048727000000
O	-0.629488000000	1.687292000000	-1.614204000000
H	-1.454972000000	-0.064145000000	-1.257522000000
O	-1.423814000000	2.125926000000	0.864580000000
N	-1.749535000000	-0.842112000000	-0.663878000000
C	-0.720425000000	-1.314706000000	0.183478000000
C	-1.000312000000	-2.761688000000	0.676950000000
C	-1.135292000000	-3.779929000000	-0.442039000000
C	-0.160330000000	-3.467362000000	-1.600935000000
H	-2.176284000000	-3.777890000000	-0.789299000000
H	-0.939990000000	-4.760442000000	0.003628000000
H	0.149859000000	-4.399587000000	-2.085684000000
H	-0.659984000000	-2.860099000000	-2.363280000000
C	-3.120189000000	-0.799404000000	-0.315667000000
C	-4.021456000000	-0.376849000000	-1.309123000000
C	-3.619784000000	-1.157958000000	0.946169000000
C	-5.386903000000	-0.324476000000	-1.049611000000
H	-3.636276000000	-0.092670000000	-2.285123000000
C	-4.995832000000	-1.121529000000	1.185787000000

H	-2.946173000000	-1.439189000000	1.746610000000
C	-5.887445000000	-0.706965000000	0.198313000000
H	-6.064672000000	0.009039000000	-1.831298000000
H	-5.364570000000	-1.406250000000	2.167914000000
H	-6.954744000000	-0.673750000000	0.397423000000
C	0.675565000000	-1.299770000000	-0.560615000000
H	0.584374000000	-0.631357000000	-1.424043000000
C	3.568669000000	0.022808000000	1.722366000000
C	2.750306000000	0.361046000000	2.813253000000
C	2.990444000000	-0.476882000000	0.517706000000
C	1.373400000000	0.211922000000	2.744942000000
H	3.231070000000	0.747312000000	3.705506000000
C	1.591481000000	-0.689048000000	0.484125000000
C	0.825892000000	-0.312385000000	1.575750000000
H	0.733184000000	0.481685000000	3.578371000000
C	3.883103000000	-0.623215000000	-0.643801000000
O	5.113476000000	-0.608180000000	-0.579764000000
O	3.248715000000	-0.706082000000	-1.827756000000
C	4.097445000000	-0.806645000000	-2.986989000000
H	4.722493000000	-1.701044000000	-2.928841000000
H	3.416592000000	-0.864091000000	-3.836117000000
H	4.739552000000	0.073700000000	-3.065507000000
C	1.065814000000	-2.712335000000	-1.065660000000
H	1.829607000000	-2.613402000000	-1.838282000000
H	1.515626000000	-3.286790000000	-0.243830000000
O	-1.017738000000	-3.052349000000	1.852556000000
P	-0.709644000000	2.630243000000	-0.466545000000
O	0.728399000000	3.119389000000	0.081932000000

O	-1.524395000000	3.956333000000	-0.838027000000
O	-0.533627000000	-0.461550000000	1.383652000000
H	-1.196968000000	1.190715000000	1.102421000000
C	1.807732000000	3.299556000000	-0.853062000000
H	1.587745000000	4.117144000000	-1.547916000000
H	2.685972000000	3.551732000000	-0.256686000000
H	1.984453000000	2.378118000000	-1.413660000000
C	-1.813722000000	4.953575000000	0.159871000000
H	-0.890833000000	5.311454000000	0.626854000000
H	-2.305132000000	5.773926000000	-0.365383000000
H	-2.480909000000	4.542541000000	0.921729000000

F’

O	-4.459296000000	-1.102343000000	-2.235231000000
H	-4.973485000000	-0.304974000000	-1.924880000000
O	1.586626000000	1.260198000000	1.070788000000
H	1.291963000000	0.414951000000	0.624316000000
N	0.613683000000	-1.149401000000	-0.077773000000
C	-0.167948000000	-1.473405000000	1.085275000000
C	0.083685000000	-2.534922000000	2.087170000000
C	-0.941517000000	-2.616702000000	3.221982000000
C	-1.726821000000	-1.325054000000	3.464570000000
H	-0.405489000000	-2.949560000000	4.116941000000
H	-1.631685000000	-3.432201000000	2.957046000000
H	-2.493695000000	-1.485459000000	4.231118000000
H	-1.048533000000	-0.550584000000	3.845816000000
C	1.893115000000	-1.698795000000	-0.420813000000
C	2.878115000000	-1.808342000000	0.576374000000

C	2.245460000000	-2.006590000000	-1.744419000000
C	4.151480000000	-2.274008000000	0.268742000000
H	2.645891000000	-1.533744000000	1.597716000000
C	3.531701000000	-2.462826000000	-2.042447000000
H	1.546754000000	-1.850754000000	-2.553810000000
C	4.489325000000	-2.613161000000	-1.043218000000
H	4.886923000000	-2.362107000000	1.063893000000
H	3.777007000000	-2.697161000000	-3.075158000000
H	5.486143000000	-2.973321000000	-1.281413000000
C	-1.344808000000	-0.801432000000	1.065009000000
C	-3.250901000000	-1.006150000000	-1.680249000000
C	-2.323298000000	-2.075076000000	-2.041855000000
C	-2.861474000000	0.005297000000	-0.834290000000
C	-1.012419000000	-1.975975000000	-1.788592000000
H	-2.745165000000	-2.930873000000	-2.560917000000
C	-1.472003000000	-0.026490000000	-0.235281000000
C	-0.411671000000	-0.737104000000	-1.130126000000
H	-0.334233000000	-2.767943000000	-2.085639000000
H	-1.133846000000	1.006389000000	-0.073080000000
C	-3.811218000000	1.056297000000	-0.532149000000
O	-4.961370000000	1.116164000000	-0.992216000000
O	-3.344045000000	1.997144000000	0.316734000000
C	-4.237957000000	3.086407000000	0.597883000000
H	-5.155656000000	2.721279000000	1.066252000000
H	-3.690764000000	3.739729000000	1.277809000000
H	-4.494134000000	3.618050000000	-0.321896000000
O	0.126537000000	0.036166000000	-2.142923000000
C	-2.362659000000	-0.829390000000	2.159923000000

H	-2.790759000000	0.173403000000	2.282427000000
H	-3.204686000000	-1.479301000000	1.872117000000
O	0.972729000000	-3.367502000000	1.994492000000
P	1.775854000000	2.452228000000	0.034641000000
O	1.680781000000	3.768923000000	0.939610000000
O	3.319808000000	2.309618000000	-0.397673000000
O	0.816139000000	2.498466000000	-1.103507000000
H	0.332691000000	0.944620000000	-1.810379000000
C	2.470207000000	3.897599000000	2.137591000000
H	3.534601000000	3.778353000000	1.913626000000
H	2.281645000000	4.902359000000	2.518415000000
H	2.160954000000	3.152770000000	2.875789000000
C	3.780499000000	2.981542000000	-1.587135000000
H	3.797156000000	4.065738000000	-1.433756000000
H	4.793499000000	2.618929000000	-1.766085000000
H	3.136673000000	2.738807000000	-2.435740000000

Int D

O	-2.881309000000	2.552087000000	-1.756389000000
H	-3.757308000000	2.142934000000	-1.507939000000
N	1.312418000000	-0.045695000000	0.532784000000
C	0.727341000000	-1.224523000000	0.033438000000
C	1.463669000000	-2.482263000000	-0.236673000000
C	0.620715000000	-3.574489000000	-0.891725000000
C	-0.794620000000	-3.646643000000	-0.301571000000
H	1.161776000000	-4.518467000000	-0.778289000000
H	0.563792000000	-3.357766000000	-1.970017000000
H	-1.374276000000	-4.431664000000	-0.801418000000

H	-0.722646000000	-3.928834000000	0.757131000000
C	2.667725000000	0.343373000000	0.299420000000
C	3.297041000000	0.131082000000	-0.935156000000
C	3.367913000000	0.991428000000	1.324976000000
C	4.613587000000	0.542063000000	-1.131576000000
H	2.753544000000	-0.356614000000	-1.738502000000
C	4.679025000000	1.420167000000	1.114114000000
H	2.875116000000	1.147632000000	2.277308000000
C	5.309323000000	1.192675000000	-0.109870000000
H	5.093824000000	0.361250000000	-2.089666000000
H	5.213090000000	1.920631000000	1.917658000000
H	6.334674000000	1.516215000000	-0.266997000000
C	-0.623856000000	-1.161686000000	-0.018149000000
C	-1.950654000000	1.902352000000	-1.054265000000
C	-0.595636000000	2.410560000000	-1.243315000000
C	-2.213042000000	0.880544000000	-0.170540000000
C	0.419508000000	2.020067000000	-0.459059000000
H	-0.468498000000	3.167724000000	-2.011804000000
C	-1.073344000000	0.178423000000	0.542321000000
C	0.263901000000	0.987915000000	0.636528000000
H	1.409215000000	2.450995000000	-0.572294000000
H	-1.382729000000	0.001091000000	1.582837000000
C	-3.601383000000	0.544722000000	0.082581000000
O	-4.566620000000	1.046328000000	-0.513608000000
O	-3.786553000000	-0.367513000000	1.062369000000
C	-5.154318000000	-0.690110000000	1.365311000000
H	-5.656931000000	-1.102212000000	0.486723000000
H	-5.105335000000	-1.430528000000	2.164105000000

H	-5.693405000000	0.200209000000	1.698674000000
C	-1.521071000000	-2.296002000000	-0.409324000000
H	-2.421695000000	-2.295862000000	0.214423000000
H	-1.875325000000	-2.142211000000	-1.442716000000
O	2.642148000000	-2.646974000000	0.036135000000
O	0.414532000000	1.630664000000	1.902272000000
H	-0.122330000000	2.440670000000	1.880282000000

3a

O	-4.728886000000	0.389746000000	-1.322418000000
H	-4.720860000000	1.205301000000	-0.764792000000
N	1.536502000000	-0.512512000000	-1.135075000000
C	0.896205000000	-1.240208000000	-0.057369000000
C	1.898214000000	-2.095800000000	0.780581000000
C	1.501370000000	-2.462164000000	2.196474000000
C	0.825037000000	-1.289067000000	2.924139000000
H	2.394065000000	-2.827473000000	2.713151000000
H	0.790912000000	-3.300299000000	2.133509000000
H	0.545560000000	-1.598484000000	3.938069000000
H	1.535341000000	-0.458818000000	3.039760000000
C	2.525631000000	0.470212000000	-0.966057000000
C	2.908806000000	1.005610000000	0.274922000000
C	3.146265000000	0.973940000000	-2.125996000000
C	3.866818000000	2.019634000000	0.343511000000
H	2.484774000000	0.624744000000	1.197075000000
C	4.107612000000	1.973977000000	-2.045586000000
H	2.855337000000	0.573684000000	-3.094556000000
C	4.473980000000	2.513490000000	-0.808544000000

H	4.146606000000	2.412733000000	1.317828000000
H	4.570754000000	2.339172000000	-2.958718000000
H	5.222257000000	3.298057000000	-0.747127000000
C	-0.106957000000	-0.332109000000	0.722240000000
H	0.272780000000	0.688318000000	0.759398000000
C	-3.549041000000	-0.233610000000	-1.138725000000
C	-3.345402000000	-1.426152000000	-1.852568000000
C	-2.532852000000	0.266289000000	-0.268284000000
C	-2.153344000000	-2.132938000000	-1.748198000000
H	-4.145461000000	-1.768480000000	-2.500099000000
C	-1.332703000000	-0.467907000000	-0.165125000000
C	-1.169124000000	-1.627664000000	-0.904680000000
H	-1.987378000000	-3.046951000000	-2.309289000000
H	1.742344000000	-1.147321000000	-1.898601000000
C	-2.791144000000	1.532092000000	0.436453000000
O	-3.836665000000	2.177110000000	0.338731000000
O	-1.780756000000	1.961148000000	1.214991000000
C	-2.000115000000	3.215933000000	1.886402000000
H	-2.172078000000	4.012358000000	1.158704000000
H	-2.862487000000	3.147504000000	2.553847000000
H	-1.086915000000	3.401971000000	2.451632000000
O	0.061803000000	-2.229059000000	-0.710005000000
C	-0.419534000000	-0.832561000000	2.156957000000
H	-0.939576000000	-0.032001000000	2.691717000000
H	-1.119137000000	-1.676630000000	2.097458000000
O	2.936919000000	-2.454668000000	0.269111000000

4a

O	-3.198049000000	-3.226168000000	-0.272038000000
H	-4.000047000000	-2.644833000000	-0.305247000000
N	1.291712000000	-0.081472000000	0.016773000000
C	0.761342000000	1.198546000000	-0.040461000000
C	1.553274000000	2.433221000000	-0.046152000000
C	0.720717000000	3.710407000000	-0.104792000000
C	-0.583689000000	3.522578000000	-0.888791000000
H	1.352472000000	4.497616000000	-0.527833000000
H	0.494084000000	4.005398000000	0.931914000000
H	-1.156021000000	4.457788000000	-0.896430000000
H	-0.343323000000	3.289054000000	-1.934733000000
C	2.670203000000	-0.474898000000	0.080016000000
C	3.368126000000	-0.388314000000	1.286656000000
C	3.288386000000	-0.996179000000	-1.058478000000
C	4.694033000000	-0.812344000000	1.347636000000
H	2.871690000000	0.018386000000	2.161890000000
C	4.614537000000	-1.426040000000	-0.989156000000
H	2.732323000000	-1.053280000000	-1.989461000000
C	5.318876000000	-1.333086000000	0.211760000000
H	5.239517000000	-0.737369000000	2.284116000000
H	5.096331000000	-1.828052000000	-1.876054000000
H	6.352266000000	-1.664498000000	0.263461000000
C	-0.630404000000	1.136592000000	-0.112429000000
C	-2.127433000000	-2.418285000000	-0.181862000000
C	-0.873395000000	-3.079567000000	-0.139749000000
C	-2.218184000000	-1.007689000000	-0.093529000000
C	0.301550000000	-2.372611000000	-0.038805000000
H	-0.881556000000	-4.163458000000	-0.179070000000

C	-0.992732000000	-0.251298000000	-0.061616000000
C	0.235045000000	-0.970018000000	-0.017678000000
H	1.259228000000	-2.880705000000	0.005443000000
C	-3.566855000000	-0.457688000000	0.081534000000
O	-4.609168000000	-1.088156000000	-0.129599000000
O	-3.611598000000	0.794963000000	0.566090000000
C	-4.926090000000	1.334693000000	0.783719000000
H	-5.464853000000	0.739901000000	1.525383000000
H	-4.763100000000	2.348817000000	1.149515000000
H	-5.498541000000	1.346955000000	-0.147096000000
C	-1.444196000000	2.390996000000	-0.302826000000
H	-2.294485000000	2.194891000000	-0.961200000000
H	-1.875610000000	2.713572000000	0.655268000000
O	2.776189000000	2.456364000000	0.014639000000

TS-I (uncatalyzed)

O	-0.273396000000	-3.352585000000	-0.424366000000
H	0.304414000000	-0.647407000000	-1.321517000000
N	0.770777000000	0.163836000000	-0.926983000000
C	-0.056352000000	1.180587000000	-0.638023000000
C	0.365576000000	2.328062000000	0.232419000000
C	-0.715443000000	3.354081000000	0.520509000000
C	-1.660739000000	3.515453000000	-0.673129000000
H	-0.213859000000	4.285891000000	0.798125000000
H	-1.277641000000	3.013991000000	1.403622000000
H	-2.391079000000	4.308382000000	-0.477192000000
H	-1.082900000000	3.828271000000	-1.553620000000
C	2.185424000000	-0.029354000000	-0.828028000000

C	3.101144000000	0.979493000000	-1.148701000000
C	2.622831000000	-1.325002000000	-0.521586000000
C	4.462352000000	0.692193000000	-1.128374000000
H	2.755116000000	1.970583000000	-1.412255000000
C	3.991075000000	-1.593079000000	-0.501508000000
H	1.904548000000	-2.104137000000	-0.279109000000
C	4.913118000000	-0.589974000000	-0.800837000000
H	5.173837000000	1.474410000000	-1.377012000000
H	4.329842000000	-2.593366000000	-0.248929000000
H	5.977895000000	-0.804856000000	-0.787314000000
C	-1.451592000000	0.973931000000	-0.942787000000
H	-1.579252000000	0.346379000000	-1.826906000000
C	-1.177269000000	-2.515534000000	-0.299525000000
C	-2.415464000000	-2.705225000000	-1.121144000000
C	-1.136450000000	-1.333267000000	0.549582000000
C	-3.443874000000	-1.840310000000	-1.128636000000
H	-2.424377000000	-3.617080000000	-1.713298000000
C	-2.070480000000	-0.259012000000	0.326520000000
C	-3.408794000000	-0.632852000000	-0.280259000000
H	-4.353820000000	-2.008766000000	-1.698642000000
H	-2.211180000000	0.408848000000	1.171318000000
C	-0.129993000000	-1.209620000000	1.605517000000
O	0.673065000000	-2.048180000000	1.970546000000
O	-0.188850000000	0.038684000000	2.191135000000
C	0.795669000000	0.275090000000	3.207255000000
H	0.764072000000	-0.514076000000	3.962100000000
H	1.796065000000	0.314318000000	2.767932000000
H	0.541257000000	1.241237000000	3.645453000000

O	-4.409378000000	0.043523000000	-0.080806000000
C	-2.386169000000	2.194385000000	-0.956030000000
H	-2.888833000000	2.242428000000	-1.928224000000
H	-3.185563000000	2.051104000000	-0.220830000000
O	1.493383000000	2.430649000000	0.686712000000

B(uncatalyzed)

O	-2.328472000000	0.840237000000	2.032560000000
H	-0.024287000000	-2.360132000000	-0.147081000000
N	-0.231779000000	-1.432538000000	-0.532914000000
C	0.876711000000	-0.815133000000	-0.933974000000
C	2.102108000000	-1.651194000000	-0.788273000000
C	3.400484000000	-0.984247000000	-1.171520000000
C	3.156080000000	-0.026371000000	-2.348039000000
H	4.132861000000	-1.763319000000	-1.402655000000
H	3.775198000000	-0.428142000000	-0.299111000000
H	4.103749000000	0.409548000000	-2.682990000000
H	2.759431000000	-0.601263000000	-3.196049000000
C	-1.605140000000	-1.173954000000	-0.825748000000
C	-2.558639000000	-1.480679000000	0.150875000000
C	-1.993378000000	-0.706294000000	-2.088068000000
C	-3.910149000000	-1.306531000000	-0.142480000000
H	-2.238283000000	-1.789437000000	1.140708000000
C	-3.347992000000	-0.534439000000	-2.363361000000
H	-1.247555000000	-0.517633000000	-2.853898000000
C	-4.308825000000	-0.835091000000	-1.393932000000
H	-4.649196000000	-1.524062000000	0.622200000000
H	-3.652685000000	-0.182047000000	-3.344728000000

H	-5.363649000000	-0.700526000000	-1.615015000000
C	0.945401000000	0.626619000000	-1.149356000000
H	0.018853000000	1.000366000000	-1.587986000000
C	-1.376674000000	1.323990000000	1.406019000000
C	-1.617133000000	2.614070000000	0.681501000000
C	-0.042111000000	0.770458000000	1.318678000000
C	-0.650049000000	3.321716000000	0.074059000000
H	-2.641487000000	2.973549000000	0.741350000000
C	0.937719000000	1.330551000000	0.373571000000
C	0.735887000000	2.823606000000	0.073994000000
H	-0.819145000000	4.299485000000	-0.369724000000
H	1.961049000000	1.200576000000	0.722450000000
C	0.341450000000	-0.355631000000	2.163792000000
O	-0.346316000000	-0.990369000000	2.944058000000
O	1.681709000000	-0.671302000000	1.971508000000
C	2.156582000000	-1.792393000000	2.725733000000
H	1.832995000000	-2.729917000000	2.260726000000
H	3.246051000000	-1.728798000000	2.704265000000
H	1.782417000000	-1.750152000000	3.750393000000
O	1.686657000000	3.548657000000	-0.178789000000
C	2.180367000000	1.099673000000	-1.965418000000
H	1.835763000000	1.607142000000	-2.872973000000
H	2.713238000000	1.859299000000	-1.386149000000
O	2.001540000000	-2.819612000000	-0.424545000000

TS-III (without catalyst)

O	3.257702000000	-2.299439000000	-1.693207000000
H	4.024492000000	-1.701148000000	-1.449813000000

N	-1.497484000000	-0.197391000000	-0.773794000000
C	-0.749781000000	0.955036000000	-0.565948000000
C	-1.287727000000	2.225440000000	-1.192257000000
C	-0.332585000000	3.415587000000	-1.240186000000
C	0.543270000000	3.480202000000	0.014256000000
H	-0.931288000000	4.318417000000	-1.384114000000
H	0.297978000000	3.296296000000	-2.136324000000
H	1.234566000000	4.327737000000	-0.052184000000
H	-0.097865000000	3.646994000000	0.891075000000
C	-2.742278000000	-0.315542000000	-0.186519000000
C	-3.176521000000	0.461746000000	0.932614000000
C	-3.614407000000	-1.323334000000	-0.658426000000
C	-4.422228000000	0.235103000000	1.521521000000
H	-2.530611000000	1.259420000000	1.298960000000
C	-4.850351000000	-1.548531000000	-0.059626000000
H	-3.278086000000	-1.908756000000	-1.507566000000
C	-5.259346000000	-0.770635000000	1.028587000000
H	-4.736697000000	0.847179000000	2.358600000000
H	-5.498862000000	-2.327082000000	-0.452380000000
H	-6.233461000000	-0.943737000000	1.487889000000
C	0.454143000000	0.952687000000	0.062623000000
C	2.213050000000	-1.897253000000	-0.963328000000
C	1.040249000000	-2.737906000000	-1.105000000000
C	2.245280000000	-0.853023000000	-0.057089000000
C	-0.037538000000	-2.559081000000	-0.294633000000
H	1.086169000000	-3.539828000000	-1.835686000000
C	0.970531000000	-0.384261000000	0.643500000000
C	-0.122117000000	-1.447532000000	0.595459000000

H	-0.888408000000	-3.239893000000	-0.314835000000
H	1.218223000000	-0.215085000000	1.711005000000
C	3.552043000000	-0.305365000000	0.265922000000
O	4.589641000000	-0.536532000000	-0.371379000000
O	3.583275000000	0.459935000000	1.384876000000
C	4.868676000000	0.972932000000	1.757157000000
H	5.562613000000	0.150936000000	1.966807000000
H	5.281307000000	1.598300000000	0.961135000000
H	4.697967000000	1.563229000000	2.663179000000
O	-0.920922000000	-1.623934000000	1.660350000000
C	1.326075000000	2.179366000000	0.185221000000
H	1.835444000000	2.170144000000	1.159942000000
H	2.138916000000	2.136086000000	-0.570361000000
O	-2.408687000000	2.285996000000	-1.669389000000
H	-1.218710000000	-0.759489000000	2.028133000000

TS-II (without catalyst)

O	4.995666000000	1.497643000000	-0.101695000000
H	5.287661000000	0.549174000000	-0.031516000000
H	-1.565033000000	-0.834637000000	-1.711559000000
N	-1.922546000000	-0.540940000000	-0.780695000000
C	-1.003544000000	-0.042438000000	0.056585000000
C	-1.520658000000	0.352741000000	1.454638000000
C	-1.029120000000	-0.483380000000	2.622357000000
C	0.416872000000	-0.967395000000	2.466087000000
H	-1.695730000000	-1.365017000000	2.668750000000
H	-1.195027000000	0.088698000000	3.538567000000
H	1.109118000000	-0.111574000000	2.559676000000

H	0.660173000000	-1.662003000000	3.278396000000
C	-3.358298000000	-0.333574000000	-0.712506000000
C	-4.172350000000	-1.463349000000	-0.426668000000
C	-3.915342000000	0.933252000000	-0.996493000000
C	-5.558978000000	-1.313118000000	-0.408850000000
H	-3.711663000000	-2.436430000000	-0.216864000000
C	-5.301461000000	1.066207000000	-0.982283000000
H	-3.276479000000	1.797959000000	-1.223771000000
C	-6.129665000000	-0.047448000000	-0.686723000000
H	-6.196514000000	-2.190689000000	-0.183793000000
H	-5.746314000000	2.056633000000	-1.192622000000
H	-7.209534000000	0.059295000000	-0.672847000000
C	0.398932000000	-0.672884000000	-0.081024000000
H	0.408223000000	-1.262095000000	-1.003306000000
C	3.646938000000	1.500446000000	-0.166766000000
C	3.027813000000	2.753909000000	-0.232352000000
C	2.853432000000	0.312316000000	-0.197277000000
C	1.652277000000	2.862773000000	-0.331151000000
H	3.656964000000	3.637986000000	-0.222301000000
C	1.434987000000	0.436942000000	-0.190573000000
C	0.854093000000	1.697573000000	-0.317435000000
H	1.162115000000	3.828627000000	-0.404393000000
C	3.592483000000	-0.945663000000	-0.393787000000
O	4.797369000000	-1.092718000000	-0.172157000000
O	2.861817000000	-1.946423000000	-0.933074000000
C	3.563185000000	-3.171064000000	-1.188372000000
H	3.980415000000	-3.583963000000	-0.265601000000
H	2.821780000000	-3.848036000000	-1.615932000000

H	4.384781000000	-3.000161000000	-1.898850000000
C	0.617697000000	-1.641744000000	1.114536000000
H	-0.091121000000	-2.477756000000	1.013171000000
H	1.610403000000	-2.086921000000	1.042927000000
O	-2.334680000000	1.236624000000	1.592476000000
O	-0.489190000000	1.757731000000	-0.436167000000

D(without catalyst)

O	3.695336000000	-2.197683000000	-1.578042000000
H	3.844337000000	-1.331138000000	-2.011316000000
N	-1.864600000000	-0.159030000000	0.656374000000
C	-0.921225000000	0.642447000000	0.325489000000
C	-1.044987000000	1.774976000000	-0.685576000000
C	-0.862626000000	3.153487000000	-0.062814000000
C	-0.014746000000	3.084001000000	1.223552000000
H	-1.862382000000	3.567921000000	0.129529000000
H	-0.399135000000	3.791408000000	-0.823931000000
H	0.444861000000	4.059042000000	1.416802000000
H	-0.647581000000	2.859206000000	2.092225000000
C	-3.146800000000	-0.258001000000	0.065872000000
C	-3.362983000000	-0.402745000000	-1.313690000000
C	-4.238340000000	-0.324007000000	0.948082000000
C	-4.661019000000	-0.579367000000	-1.793971000000
H	-2.520450000000	-0.381453000000	-1.992791000000
C	-5.531148000000	-0.473536000000	0.455231000000
H	-4.055091000000	-0.247332000000	2.015950000000
C	-5.747710000000	-0.604607000000	-0.919337000000
H	-4.818918000000	-0.696200000000	-2.862650000000

H	-6.369172000000	-0.504859000000	1.146196000000
H	-6.755282000000	-0.738169000000	-1.303063000000
C	0.408278000000	0.600375000000	1.117196000000
H	0.105303000000	0.437685000000	2.159590000000
C	2.732892000000	-2.036253000000	-0.635335000000
C	2.209014000000	-3.202095000000	-0.067105000000
C	2.296714000000	-0.765100000000	-0.174280000000
C	1.207467000000	-3.111896000000	0.879798000000
H	2.593779000000	-4.159100000000	-0.403665000000
C	1.199090000000	-0.669974000000	0.730538000000
C	0.669026000000	-1.870524000000	1.245609000000
H	0.770514000000	-4.001128000000	1.322758000000
C	3.212279000000	0.330798000000	-0.587929000000
O	3.662411000000	0.460762000000	-1.722132000000
O	3.661357000000	1.079070000000	0.436704000000
C	4.637263000000	2.079838000000	0.094577000000
H	4.220551000000	2.801348000000	-0.613571000000
H	4.891914000000	2.567065000000	1.035950000000
H	5.519268000000	1.613808000000	-0.350581000000
C	1.062105000000	1.998415000000	1.062233000000
H	1.828668000000	2.069946000000	1.836073000000
H	1.564003000000	2.169977000000	0.104654000000
O	-1.253526000000	1.598550000000	-1.869488000000
O	-0.367960000000	-1.894538000000	2.142117000000
H	-1.099196000000	-1.331508000000	1.785110000000

D’(without catalyst)

O	-2.608370000000	-2.353585000000	0.381469000000
H	-2.574910000000	-2.325612000000	-0.614220000000
H	0.117205000000	1.742856000000	1.933397000000
N	-0.043127000000	1.171699000000	1.107429000000
C	1.170002000000	1.050124000000	0.360175000000
C	1.845194000000	2.323076000000	-0.036069000000
C	3.078710000000	2.200756000000	-0.915092000000
C	3.913050000000	0.982398000000	-0.506678000000
H	3.641141000000	3.136867000000	-0.851054000000
H	2.740120000000	2.092732000000	-1.957345000000
H	4.788438000000	0.877374000000	-1.157714000000
H	4.290269000000	1.131137000000	0.513273000000
C	-1.236177000000	1.579319000000	0.463222000000
C	-1.436285000000	1.424519000000	-0.915988000000
C	-2.281965000000	2.098451000000	1.243637000000
C	-2.655144000000	1.780131000000	-1.493670000000
H	-0.634698000000	1.033327000000	-1.534468000000
C	-3.493600000000	2.453053000000	0.657427000000
H	-2.136901000000	2.222443000000	2.314814000000
C	-3.692624000000	2.295153000000	-0.716346000000
H	-2.789486000000	1.652929000000	-2.564912000000
H	-4.287448000000	2.856795000000	1.280734000000
H	-4.639149000000	2.570910000000	-1.171862000000
C	1.722664000000	-0.159256000000	0.115635000000
C	-1.386588000000	-2.039369000000	0.815207000000
C	-1.263972000000	-2.041666000000	2.267219000000
C	-0.313858000000	-1.758842000000	0.000732000000
C	-0.098456000000	-1.778725000000	2.886312000000

H	-2.170402000000	-2.270568000000	2.820509000000
C	1.126259000000	-1.475821000000	2.129718000000
H	-0.004211000000	-1.781188000000	3.968220000000
C	-0.512350000000	-1.879042000000	-1.435030000000
O	-1.590251000000	-2.154033000000	-1.977061000000
O	0.604866000000	-1.679122000000	-2.167327000000
C	0.450291000000	-1.822370000000	-3.590608000000
H	-0.279282000000	-1.103831000000	-3.971655000000
H	1.437892000000	-1.627735000000	-4.009541000000
H	0.118931000000	-2.833419000000	-3.839710000000
C	3.074246000000	-0.300198000000	-0.542364000000
H	3.614660000000	-1.111096000000	-0.038569000000
H	2.919790000000	-0.637240000000	-1.578094000000
O	1.409846000000	3.400307000000	0.341665000000
O	2.189548000000	-1.261849000000	2.694703000000
C	1.053877000000	-1.459658000000	0.586031000000
H	1.725180000000	-2.274520000000	0.277789000000

TS-I with CPA5

O	-0.785341000000	-1.671803000000	-3.720798000000
H	-0.072963000000	-2.251396000000	-3.342066000000
O	-0.552246000000	-0.034817000000	0.966190000000
H	-0.789867000000	-1.019841000000	0.948211000000
O	0.556587000000	-0.582137000000	-1.331927000000
N	-1.204432000000	-2.610227000000	1.251221000000
C	-2.367000000000	-3.109818000000	1.031467000000
C	-2.851992000000	-4.454602000000	1.579710000000
C	-4.331009000000	-4.499634000000	1.943148000000

C	-4.897748000000	-3.087319000000	2.119154000000
H	-4.433554000000	-5.125352000000	2.835379000000
H	-4.855532000000	-5.020275000000	1.137740000000
H	-5.951998000000	-3.133280000000	2.422100000000
H	-4.358397000000	-2.580499000000	2.938030000000
C	-0.232051000000	-3.148140000000	2.132901000000
C	-0.517733000000	-3.336698000000	3.495490000000
C	1.069971000000	-3.322490000000	1.660666000000
C	0.491493000000	-3.757849000000	4.362473000000
H	-1.514813000000	-3.146428000000	3.872293000000
C	2.062209000000	-3.766068000000	2.533306000000
H	1.295712000000	-3.101074000000	0.612967000000
C	1.777196000000	-3.981396000000	3.877703000000
H	0.271480000000	-3.894933000000	5.418908000000
H	3.063651000000	-3.936909000000	2.160237000000
H	2.564806000000	-4.314986000000	4.552015000000
C	-3.349944000000	-2.355641000000	0.200862000000
H	-2.946062000000	-1.383980000000	-0.079167000000
C	-1.905934000000	-1.970849000000	-3.078922000000
C	-3.040791000000	-1.120021000000	-3.437600000000
C	-2.054970000000	-3.015838000000	-2.185223000000
C	-4.291596000000	-1.396879000000	-3.014790000000
H	-2.817744000000	-0.288379000000	-4.102950000000
C	-3.361496000000	-3.224559000000	-1.533661000000
C	-4.552618000000	-2.581597000000	-2.180162000000
H	-5.141241000000	-0.817497000000	-3.337537000000
H	-3.569064000000	-4.259908000000	-1.273028000000
C	-0.915263000000	-3.903402000000	-1.959336000000

O	0.200949000000	-3.730640000000	-2.453290000000
O	-1.210924000000	-4.960580000000	-1.182473000000
C	-0.106957000000	-5.834973000000	-0.859690000000
H	-0.603805000000	-6.622401000000	-0.095675000000
H	0.285339000000	-6.362231000000	-1.905298000000
H	0.784707000000	-5.161561000000	-0.334433000000
O	-5.695334000000	-2.995666000000	-1.986268000000
C	-4.758262000000	-2.287229000000	0.813686000000
H	-5.001416000000	-1.235424000000	0.995354000000
H	-5.502389000000	-2.653288000000	0.096317000000
O	-2.106883000000	-5.413177000000	1.697956000000
P	0.405248000000	0.379212000000	-0.222694000000
O	-0.194321000000	1.800015000000	-0.767308000000
O	1.767936000000	0.730032000000	0.615204000000
C	-0.160950000000	2.839859000000	0.134395000000
C	2.621821000000	1.593485000000	-0.028408000000
C	-1.383526000000	3.392217000000	0.592008000000
C	1.028813000000	3.399777000000	0.487735000000
C	2.290015000000	2.906053000000	-0.148996000000
C	3.886218000000	1.123591000000	-0.457399000000
C	-1.380696000000	4.462035000000	1.411759000000
C	1.047921000000	4.444459000000	1.449811000000
C	3.155505000000	3.779199000000	-0.859182000000
C	4.765203000000	1.966499000000	-1.034039000000
H	-2.319867000000	4.900254000000	1.728282000000
C	-0.178800000000	4.994114000000	1.887201000000
C	2.243516000000	4.955661000000	2.003721000000
C	2.807288000000	5.110755000000	-1.178834000000

C	4.417854000000	3.298862000000	-1.279119000000
H	5.739105000000	1.602146000000	-1.340064000000
C	-0.175011000000	6.057387000000	2.805543000000
C	2.207238000000	5.967187000000	2.887906000000
H	3.207008000000	4.540285000000	1.739801000000
H	1.837539000000	5.514666000000	-0.919528000000
C	3.675443000000	5.904751000000	-1.828587000000
C	5.300418000000	4.162086000000	-1.949292000000
H	-1.106370000000	6.498201000000	3.141479000000
C	0.986450000000	6.529493000000	3.286387000000
H	3.131028000000	6.351399000000	3.301808000000
H	3.397249000000	6.924247000000	-2.064173000000
C	4.937418000000	5.428193000000	-2.210946000000
H	6.275521000000	3.812986000000	-2.268510000000
H	0.981501000000	7.345156000000	3.998308000000
H	5.620969000000	6.086293000000	-2.732282000000
C	4.261555000000	-0.305728000000	-0.287803000000
C	4.566276000000	-0.821260000000	1.004967000000
C	4.375325000000	-1.152810000000	-1.429412000000
C	4.953826000000	-2.167843000000	1.128891000000
C	4.798109000000	-2.481609000000	-1.255374000000
C	5.062733000000	-3.004198000000	0.014008000000
H	5.195860000000	-2.569425000000	2.106725000000
H	4.912177000000	-3.123091000000	-2.118187000000
C	-2.692710000000	2.815239000000	0.175081000000
C	-3.168234000000	3.001606000000	-1.155604000000
C	-3.530303000000	2.175024000000	1.138403000000
C	-4.464181000000	2.563934000000	-1.486242000000

C	-4.836265000000	1.805126000000	0.770749000000
C	-5.313540000000	2.001539000000	-0.529337000000
H	-4.837305000000	2.710389000000	-2.491469000000
H	-5.497090000000	1.373345000000	1.509757000000
C	5.471343000000	-4.456517000000	0.188612000000
H	5.588703000000	-4.684666000000	1.272705000000
C	4.401527000000	-5.409120000000	-0.354465000000
H	3.409240000000	-5.175418000000	0.095231000000
H	4.315807000000	-5.332333000000	-1.459638000000
H	4.657612000000	-6.458011000000	-0.093364000000
C	6.832915000000	-4.724457000000	-0.462697000000
H	7.596955000000	-4.035287000000	-0.053463000000
H	7.154928000000	-5.767260000000	-0.255119000000
H	6.776051000000	-4.581582000000	-1.563212000000
C	4.523850000000	0.043330000000	2.266343000000
H	4.211827000000	1.079931000000	2.033389000000
C	5.915649000000	0.162928000000	2.900294000000
H	6.276155000000	-0.817694000000	3.276050000000
H	6.640646000000	0.550064000000	2.152567000000
H	5.884628000000	0.874152000000	3.753334000000
C	3.504473000000	-0.498435000000	3.278847000000
H	2.512680000000	-0.628152000000	2.796463000000
H	3.827647000000	-1.475660000000	3.694893000000
H	3.389015000000	0.217361000000	4.120447000000
C	4.053678000000	-0.672146000000	-2.846212000000
H	3.585922000000	0.332857000000	-2.826059000000
C	5.331470000000	-0.559191000000	-3.686750000000
H	5.091950000000	-0.143980000000	-4.688975000000

H	6.057800000000	0.120909000000	-3.195679000000
H	5.811127000000	-1.552247000000	-3.819728000000
C	3.035014000000	-1.588686000000	-3.538564000000
H	2.197972000000	-1.810769000000	-2.850030000000
H	2.626160000000	-1.089221000000	-4.442814000000
H	3.494832000000	-2.549397000000	-3.852100000000
C	-6.751765000000	1.672771000000	-0.893989000000
H	-6.911651000000	1.859910000000	-1.979478000000
C	-7.725868000000	2.581571000000	-0.135184000000
H	-7.487395000000	3.647714000000	-0.337719000000
H	-8.767096000000	2.388857000000	-0.471212000000
H	-7.668697000000	2.403498000000	0.959882000000
C	-7.078373000000	0.196503000000	-0.645651000000
H	-6.328165000000	-0.446122000000	-1.146711000000
H	-7.089132000000	-0.037387000000	0.439501000000
H	-8.078057000000	-0.046219000000	-1.064743000000
C	-2.348275000000	3.717240000000	-2.231107000000
H	-1.363286000000	4.038112000000	-1.842742000000
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H	-2.993844000000	2.525487000000	-3.961371000000
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H	-1.580350000000	1.851533000000	-3.065137000000
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H	-3.252009000000	5.657031000000	-1.819115000000
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H	-3.997280000000	4.786751000000	-3.217031000000
C	-3.074888000000	1.906039000000	2.575410000000
H	-1.994850000000	2.129871000000	2.692203000000

C	-3.833644000000	2.798713000000	3.566649000000
H	-4.917173000000	2.554481000000	3.576463000000
H	-3.430349000000	2.656355000000	4.591965000000
H	-3.717282000000	3.867918000000	3.296610000000
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H	-2.801438000000	-0.226870000000	2.184495000000
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TS-I’ with CPA5

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N	2.265870000000	2.070255000000	1.510786000000
C	3.607071000000	2.024955000000	1.373368000000
C	4.461512000000	2.695008000000	2.436729000000
C	5.983405000000	2.842758000000	2.216221000000
C	6.496335000000	2.170704000000	0.892498000000
H	6.466726000000	2.388018000000	3.164266000000
H	6.221706000000	3.992531000000	2.243190000000
H	6.395512000000	2.892332000000	0.040601000000
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C	1.795657000000	4.409254000000	2.121935000000
C	-0.473806000000	3.543074000000	3.499315000000
H	0.084531000000	1.558045000000	2.878315000000
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C	2.095790000000	1.594328000000	-2.485782000000
C	1.478860000000	2.822905000000	-1.909824000000
C	3.527797000000	1.437366000000	-2.377934000000
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O	3.813223000000	-0.060759000000	-4.257471000000
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H	5.657065000000	-1.589528000000	-3.885682000000
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C	5.699535000000	0.904494000000	0.588340000000
H	5.814860000000	0.164693000000	1.389067000000
H	6.075799000000	0.441530000000	-0.332940000000
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H	7.094103000000	-5.240114000000	-0.128914000000

H	6.009301000000	-4.930319000000	1.285560000000
C	6.112964000000	-2.671320000000	-0.436462000000
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H	6.263504000000	-2.435238000000	0.641831000000
H	7.127595000000	-2.745598000000	-0.918266000000
C	0.517541000000	-4.730846000000	-1.834325000000
H	-0.510712000000	-4.630833000000	-1.448187000000
C	0.585765000000	-3.953486000000	-3.155666000000
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H	-0.271925000000	-4.266625000000	-3.812287000000
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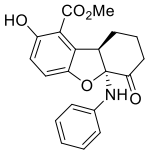
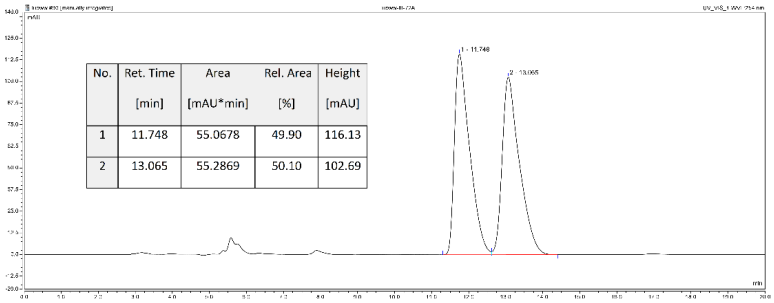
C	2.246886000000	-3.615901000000	3.865167000000
H	3.346612000000	-3.773581000000	3.893918000000
H	1.930769000000	-3.193937000000	4.849235000000
H	1.757673000000	-4.599947000000	3.736501000000
C	2.521416000000	-1.284133000000	2.923246000000
H	2.319001000000	-0.644734000000	2.027278000000
H	2.084453000000	-0.771331000000	3.805658000000
H	3.618160000000	-1.374482000000	3.060158000000
O	-0.871931000000	0.328344000000	-1.883499000000
H	-0.003051000000	0.522993000000	-2.415483000000

14. Analytical and spectral characterization data of the products

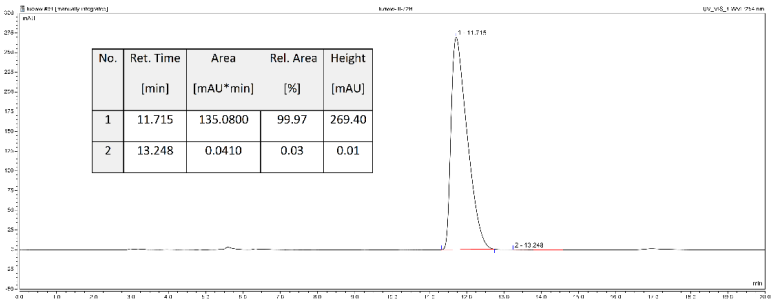
methyl (5a*S*,9a*R*)-2-hydroxy-6-oxo-5a-(phenylamino)-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3a**



(**$C_{20}H_{19}NO_5$**) The title compound **3a** was obtained as a white solid in 34.7 mg, 98% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = +14.7 (*c* 0.50 in $CHCl_3$). HPLC analysis: Chiralcel ADH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 11.7 min (major), t_2 = 13.2 min (minor). ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.64 (s, 1H), 7.15 – 7.08 (m, 2H), 7.02 (d, *J* = 8.8 Hz, 1H), 6.93 (d, *J* = 8.8 Hz, 1H), 6.81 (tt, *J* = 7.5, 1.0 Hz, 1H), 6.66 – 6.58 (m, 2H), 5.73 (s, 1H), 4.29 (t, *J* = 4.0 Hz, 1H), 3.93 (s, 3H), 2.91 – 2.81 (m, 1H), 2.60 – 2.51 (m, 1H), 2.05 – 2.00 (m, 1H), 1.85 – 1.62 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 202.92, 170.02, 157.39, 151.85, 141.50, 129.17, 128.20, 120.14, 118.42, 117.64, 117.35, 108.59, 96.73, 52.46, 49.90, 34.14, 27.11, 18.36. ESI-HRMS: calcd for $C_{20}H_{20}NO_5^+$ ([M+H$^+$]) 354.1336, found 354.1364.

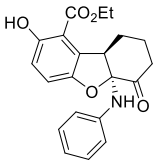


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	11.748	55.0678	49.90	116.13
2	13.065	55.2869	50.10	102.69

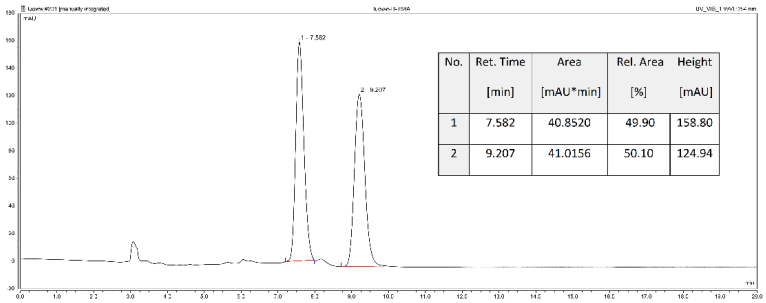


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	11.715	135.0800	99.97	269.40
2	13.248	0.0410	0.03	0.01

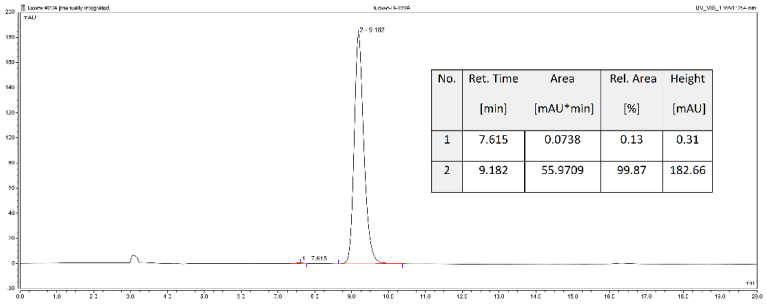
ethyl (5a*S*,9a*R*)-2-hydroxy-6-oxo-5a-(phenylamino)-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3b**



(**$C_{21}H_{21}NO_5$**) The title compound **3b** was obtained as a yellowish solid in 36.4 mg, 99% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = -12.9 (*c* 0.43 in $CHCl_3$). HPLC analysis: Chiralcel ADH, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 7.6 min (major), t_2 = 9.2 min (minor). ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.72 (s, 1H), 7.14 – 7.07 (m, 2H), 7.01 (d, *J* = 8.8 Hz, 1H), 6.91 (d, *J* = 8.8 Hz, 1H), 6.81 (tt, *J* = 7.5, 1.0 Hz, 1H), 6.65 – 6.61 (m, 2H), 5.64 (s, 1H), 4.51 – 4.34 (m, 2H), 4.27 (t, *J* = 4.3 Hz, 1H), 2.92 – 2.82 (m, 1H), 2.57 (dt, *J* = 25.6, 8.7 Hz, 1H), 2.09 – 2.00 (m, 1H), 1.79 (dddd, *J* = 13.5, 11.0, 5.1, 3.0 Hz, 2H), 1.75 – 1.65 (m, 1H), 1.36 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 203.12, 169.59, 157.49, 151.79, 141.55, 129.07, 128.31, 120.35, 118.33, 117.79, 117.48, 108.71, 96.77, 61.84, 50.21, 34.53, 27.42, 18.32, 14.04. ESI-HRMS: calcd for $C_{21}H_{22}NO_5^+$ ([M+H$^+$]) 368.1492, found 368.1497.

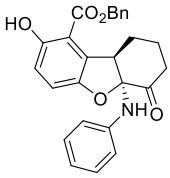


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	7.582	40.8520	49.90	158.80
2	9.207	41.0156	50.10	124.94

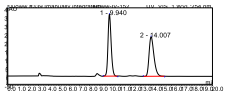


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	7.615	0.0738	0.13	0.31
2	9.182	55.9709	99.87	182.66

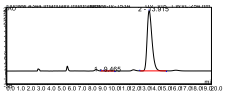
benzyl (5aS,9aR)-2-hydroxy-6-oxo-5a-(phenylamino)-5a,6,7,8,9,9a-hexahydrodibenzo[b,d]furan-1-carboxylate **3c**



(**$C_{26}H_{23}NO_5$**) The title compound **3c** was obtained as a colorless syrup in 35.2 mg, 82% yield, >95:5 d.r., 99% *ee*. HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 9.5 min (minor), t_2 = 13.9 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.61 (s, 1H), 7.35 – 7.26 (m, 4H), 7.14 – 7.03 (m, 2H), 7.00 (d, *J* = 8.8 Hz, 1H), 6.93 – 6.78 (m, 2H), 6.67 – 6.56 (m, 2H), 5.54 (s, 1H), 5.35 (s, 2H), 5.29 (s, 1H), 4.15 (t, *J* = 4.3 Hz, 1H), 2.87 – 2.73 (m, 1H), 2.57 – 2.42 (m, 1H), 1.80 (dt, *J* = 7.7, 3.4 Hz, 1H), 1.68 – 1.48 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 203.13, 169.32, 157.50, 151.64, 141.48, 134.40, 129.00, 128.85, 128.79, 128.62, 120.66, 118.39, 118.27, 117.68, 108.43, 96.85, 67.60, 50.01, 34.69, 27.52, 18.23.

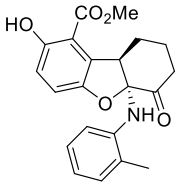


	Retention Time	Area	% Area	Height
1	9.940	130.4815	50.52	363.11
2	14.007	127.7838	49.48	232.44

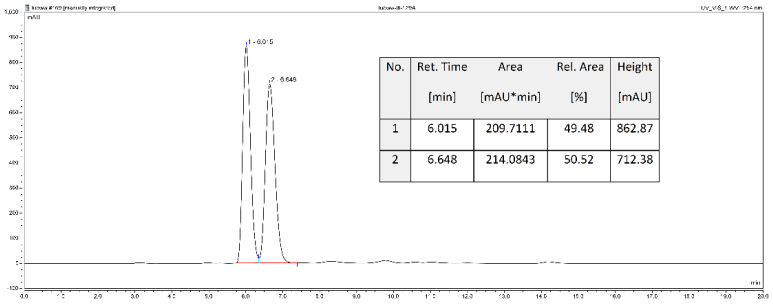


	Retention Time	Area	% Area	Height
1	9.465	0.1256	0.10	0.36
2	13.915	129.6234	99.90	236.21

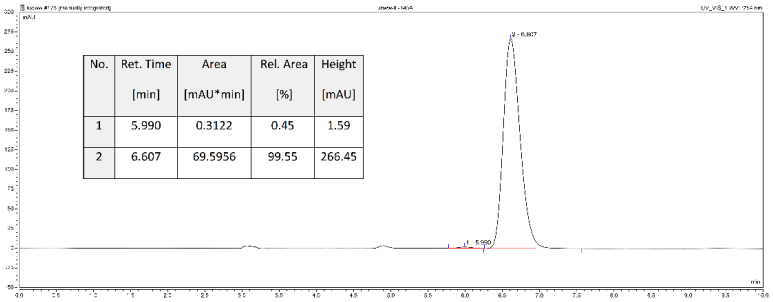
methyl (5a*S*,9a*R*)-2-hydroxy-6-oxo-5a-(*o*-tolylamino)-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3d**



(**$C_{21}H_{21}NO_5$**) The title compound **3d** was obtained as a colorless syrup in 35.2 mg, 96% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = +39.9 (*c* 0.34 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 6.0 min (minor), t_2 = 6.6 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.62 (s, 1H), 7.10 (d, *J* = 7.4 Hz, 1H), 7.02 (d, *J* = 8.8 Hz, 1H), 6.93 (dd, *J* = 8.8, 0.5 Hz, 1H), 6.89 (ddd, *J* = 8.6, 7.6, 1.2 Hz, 1H), 6.74 (td, *J* = 7.4, 1.0 Hz, 1H), 6.40 – 6.33 (m, 1H), 5.72 (s, 1H), 4.30 (t, *J* = 3.9 Hz, 1H), 3.91 (s, 3H), 2.92 – 2.79 (m, 1H), 2.60 – 2.48 (m, 1H), 2.27 (s, 3H), 2.11 – 1.99 (m, 1H), 1.85 – 1.62 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.88, 170.03, 157.35, 151.85, 139.47, 130.66, 128.22, 126.76, 125.89, 120.00, 118.44, 117.57, 115.68, 108.62, 96.68, 52.41, 49.30, 33.74, 27.00, 18.34, 17.97. ESI-HRMS: calcd for $C_{21}H_{22}NO_5^+$ ([M+H$^+$]) 368.1492, found 368.1497.

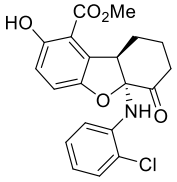


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	6.015	209.7111	49.48	862.87
2	6.648	214.0843	50.52	712.38

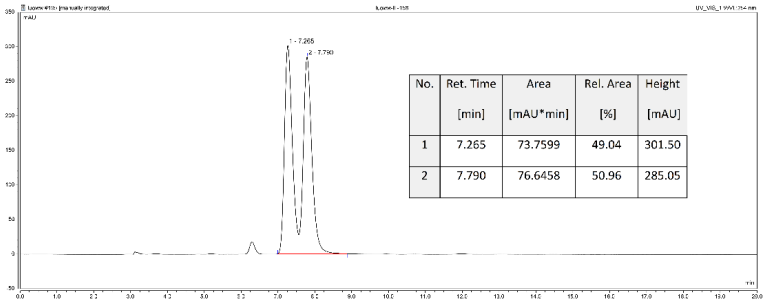


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	5.990	0.3122	0.45	1.59
2	6.607	69.5956	99.55	266.45

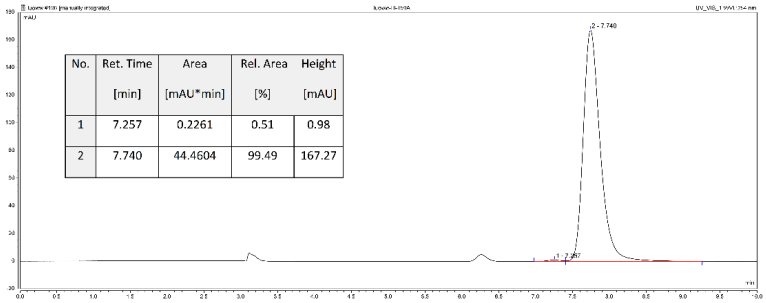
methyl (5a*S*,9a*R*)-5a-((2-chlorophenyl)amino)-2-hydroxy-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3e**



(**$C_{20}H_{18}ClNO_5$**) The title compound **3e** was obtained as a colorless syrup in 33.0 mg, 85% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = -26.9 (*c* 0.33 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 7.3 min (minor), t_2 = 7.7 min (major). ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.64 (s, 1H), 7.29 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.05 (d, *J* = 8.8 Hz, 1H), 6.98 – 6.92 (m, 2H), 6.73 (td, *J* = 7.7, 1.4 Hz, 1H), 6.51 (dd, *J* = 8.2, 1.4 Hz, 1H), 6.25 (s, 1H), 4.22 (t, *J* = 4.2 Hz, 1H), 3.95 (s, 3H), 2.92 – 2.82 (m, 1H), 2.58 (ddd, *J* = 17.0, 9.4, 7.7 Hz, 1H), 2.01 (ddd, *J* = 9.7, 5.7, 2.4 Hz, 1H), 1.90 – 1.77 (m, 2H), 1.76 – 1.66 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 202.78, 169.90, 157.60, 151.69, 138.42, 129.58, 127.93, 127.41, 121.96, 120.08, 118.64, 117.77, 116.18, 108.60, 96.33, 52.50, 51.10, 34.17, 27.04, 18.44. ESI-HRMS: calcd for $C_{20}H_{19}{}^{35}ClNO_5^+$ ([M+H$^+$]) 388.0946, found 388.0909.

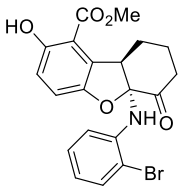


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	7.265	73.7599	49.04	301.50
2	7.790	76.6458	50.96	285.05

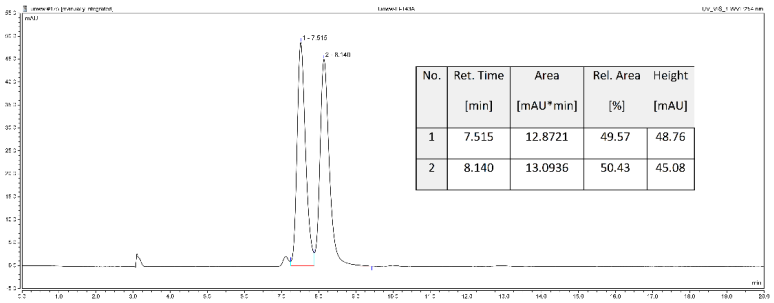


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	7.257	0.2261	0.51	0.98
2	7.740	44.4604	99.49	167.27

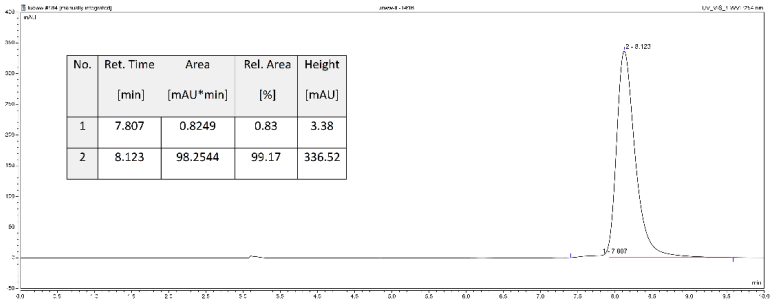
methyl (5a*S*,9a*R*)-5a-((2-bromophenyl)amino)-2-hydroxy-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3f**



(**$C_{20}H_{18}BrNO_5$**) The title compound **3f** was obtained as a white solid in 35.2 mg, 81% yield, >95:5 d.r., 98% *ee*. $[\alpha]_D^{25}$ = -21.6 (*c* 0.34 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 7.8 min (minor), t_2 = 8.1 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.63 (s, 1H), 7.46 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.04 (d, *J* = 8.9 Hz, 1H), 7.01 – 6.90 (m, 2H), 6.65 (td, *J* = 7.7, 1.5 Hz, 1H), 6.50 (dd, *J* = 8.2, 1.4 Hz, 1H), 6.26 (s, 1H), 4.21 (t, *J* = 4.1 Hz, 1H), 3.94 (s, 3H), 2.90 – 2.79 (m, 1H), 2.57 (ddd, *J* = 16.9, 9.4, 7.6 Hz, 1H), 2.06 – 1.95 (m, 1H), 1.88 – 1.66 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.69, 169.89, 157.58, 151.68, 139.46, 132.88, 128.10, 127.93, 120.57, 118.63, 117.74, 116.25, 112.59, 108.58, 96.44, 52.50, 50.99, 34.07, 27.00, 18.44. ESI-HRMS: calcd for $C_{20}H_{19}{}^{79}BrNO_5^+$ ([M+H$^+$]) 432.0441, found 432.0431.

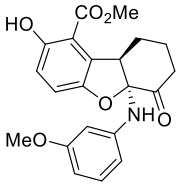


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	7.515	12.8721	49.57	48.76
2	8.140	13.0936	50.43	45.08

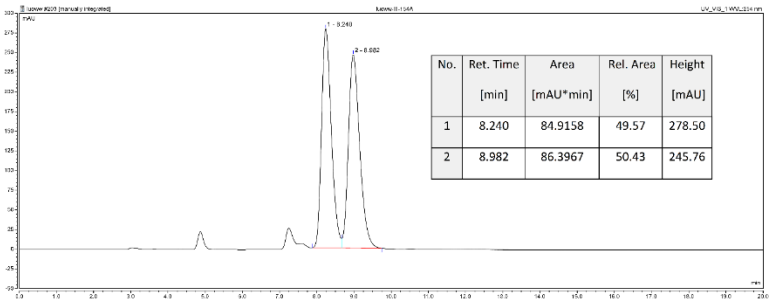


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	7.807	0.8249	0.83	3.38
2	8.123	98.2544	99.17	336.52

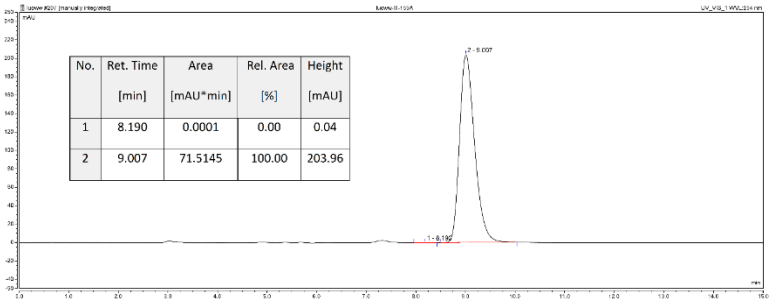
methyl (5a*S*,9a*R*)-2-hydroxy-5a-((3-methoxyphenyl)amino)-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3g**



(**$C_{21}H_{21}NO_6$**) The title compound **3g** was obtained as a colorless syrup in 38.0 mg, 99% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = +7.3 (*c* 0.43 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 8.2 min (minor), t_2 = 9.0 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 7.08 – 6.96 (m, 2H), 6.93 (dd, *J* = 8.8, 0.6 Hz, 1H), 6.36 (ddd, *J* = 8.3, 2.4, 0.8 Hz, 1H), 6.21 (ddd, *J* = 8.0, 2.2, 0.8 Hz, 1H), 6.12 (t, *J* = 2.3 Hz, 1H), 5.80 (s, 1H), 4.28 (d, *J* = 3.4 Hz, 1H), 3.92 (s, 3H), 3.51 (s, 3H), 2.91 – 2.80 (m, 1H), 2.60 – 2.48 (m, 1H), 2.08 – 1.99 (m, 1H), 1.85 – 1.62 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.71, 169.96, 160.41, 157.43, 151.91, 142.72, 129.95, 128.17, 118.46, 117.61, 109.75, 108.49, 106.29, 102.43, 96.50, 54.73, 52.47, 49.83, 34.03, 27.09, 18.20. ESI-HRMS: calcd for $C_{21}H_{22}NO_6^+$ ([M+H$^+$]) 384.1442, found 384.1454.

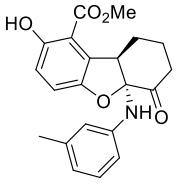


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	8.240	84.9158	49.57	278.50
2	8.982	86.3967	50.43	245.76

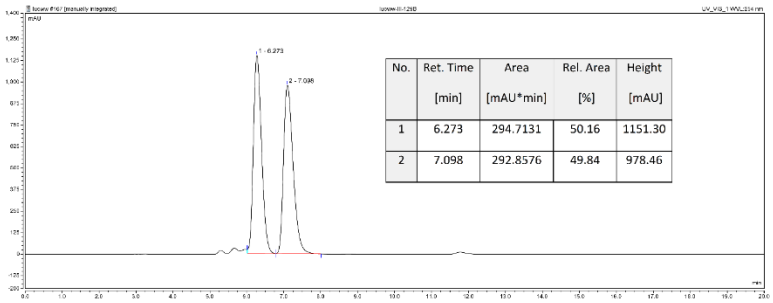


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	8.190	0.0001	0.00	0.04
2	9.007	71.5145	100.00	203.96

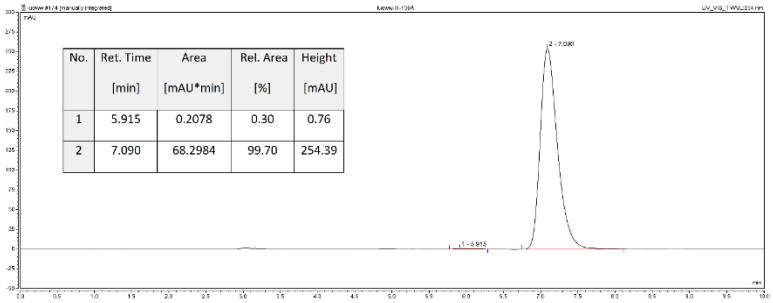
methyl (5a*S*,9a*R*)-2-hydroxy-6-oxo-5a-(*m*-tolylamino)-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3h**



(**$C_{21}H_{21}NO_5$**) The title compound **3h** was obtained as a yellow syrup in 33.4 mg, 91% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = +3.2 (*c* 0.36 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 5.9 min (minor), t_2 = 7.1 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.61 (s, 1H), 7.04 – 6.89 (m, 3H), 6.62 (dd, *J* = 8.1, 0.6 Hz, 1H), 6.46 (s, 1H), 6.36 (dd, *J* = 8.0, 2.2 Hz, 1H), 5.65 (s, 1H), 4.26 (d, *J* = 3.9 Hz, 1H), 3.92 (s, 3H), 2.91 – 2.78 (m, 1H), 2.59 – 2.48 (m, 1H), 2.16 (s, 3H), 2.05 – 1.95 (m, 1H), 1.83 – 1.64 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.95, 170.02, 157.35, 151.86, 141.39, 138.90, 128.97, 128.34, 121.04, 118.58, 118.33, 117.61, 114.25, 108.43, 96.77, 52.42, 49.95, 34.27, 27.17, 21.47, 18.34. ESI-HRMS: calcd for $C_{21}H_{22}NO_5^+$ ([M+H$^+$]) 368.1492, found 368.1509.

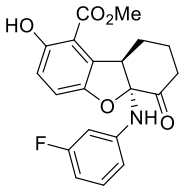


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	6.273	294.7131	50.16	1151.30
2	7.098	292.8576	49.84	978.46

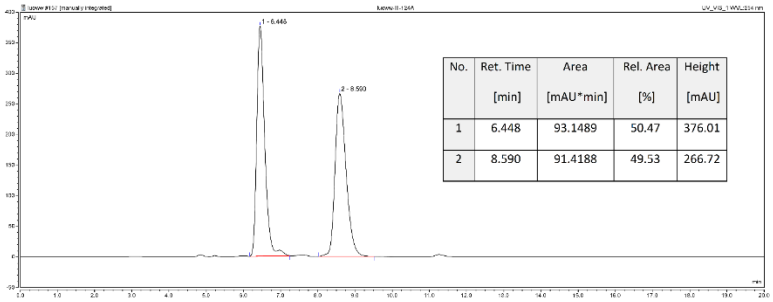


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	5.915	0.2078	0.30	0.76
2	7.090	68.2984	99.70	254.39

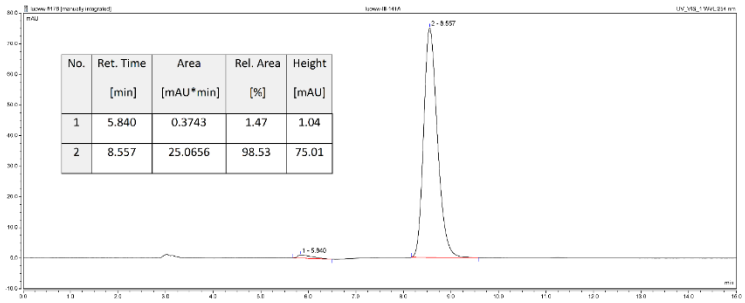
methyl (5a*S*,9a*R*)-5a-((3-fluorophenyl)amino)-2-hydroxy-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3i**



(**$C_{20}H_{18}FNO_5$**) The title compound **3i** was obtained as a yellowish syrup in 36.6 mg, 99% yield, >95:5 d.r., 97% *ee*. $[\alpha]_D^{25}$ = +2.9 (*c* 0.37 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 5.8 min (minor), t_2 = 8.6 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.61 (s, 1H), 7.08 – 6.98 (m, 2H), 6.93 (dd, *J* = 8.8, 0.4 Hz, 1H), 6.53 – 6.43 (m, 1H), 6.38 – 6.25 (m, 2H), 5.75 (s, 1H), 4.21 (d, *J* = 3.7 Hz, 1H), 3.93 (s, 3H), 2.91 – 2.79 (m, 1H), 2.60 – 2.48 (m, 1H), 2.00 (dt, *J* = 4.9, 2.8 Hz, 1H), 1.84 – 1.62 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.82, 169.87, 164.65, 162.23, 157.58, 151.67, 143.53, 143.42, 130.31, 130.21, 127.87, 118.64, 117.68, 112.61, 112.58, 108.54, 106.67, 106.46, 104.27, 104.02, 96.30, 52.48, 50.42, 34.19, 27.09, 18.29. ESI-HRMS: calcd for $C_{20}H_{19}FNO_5^+$ ([M+H$^+$]) 372.1242, found 372.1239.

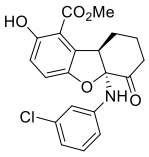


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	6.448	93.1489	50.47	376.01
2	8.590	91.4188	49.53	266.72

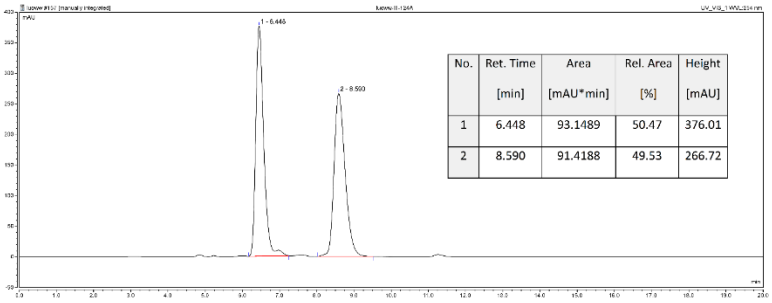


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	5.840	0.3743	1.47	1.04
2	8.557	25.0656	98.53	75.01

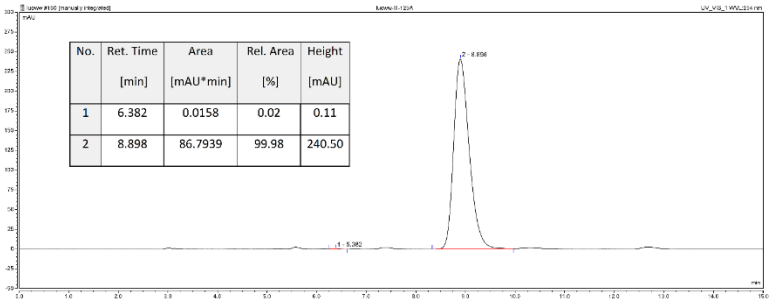
methyl (5a*S*,9a*R*)-5a-((3-chlorophenyl)amino)-2-hydroxy-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3j**



(**$C_{20}H_{18}ClNO_5$**) The title compound **3j** was obtained as a white solid in 38.3 mg, 99% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = -15.3 (*c* 0.42 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 6.4 min (minor), t_2 = 8.9 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.62 (s, 1H), 7.07 – 6.86 (m, 3H), 6.76 (ddd, *J* = 8.0, 1.9, 0.9 Hz, 1H), 6.62 (t, *J* = 2.1 Hz, 1H), 6.43 (ddd, *J* = 8.2, 2.3, 0.9 Hz, 1H), 5.67 (s, 1H), 4.19 (t, *J* = 4.2 Hz, 1H), 3.94 (s, 3H), 2.91 – 2.79 (m, 1H), 2.54 (dt, *J* = 17.2, 8.5 Hz, 1H), 2.03 – 1.94 (m, 1H), 1.85 – 1.60 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.82, 169.86, 157.59, 151.61, 142.97, 134.67, 130.09, 127.98, 120.04, 118.62, 117.69, 117.51, 115.15, 108.43, 96.30, 52.49, 50.46, 34.42, 27.21, 18.29. ESI-HRMS: calcd for $C_{20}H_{19}{}^{35}ClNO_5^+$ ([M+H$^+$]) 388.0946, found 388.0930.

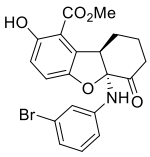


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	6.448	93.1489	50.47	376.01
2	8.590	91.4188	49.53	266.72



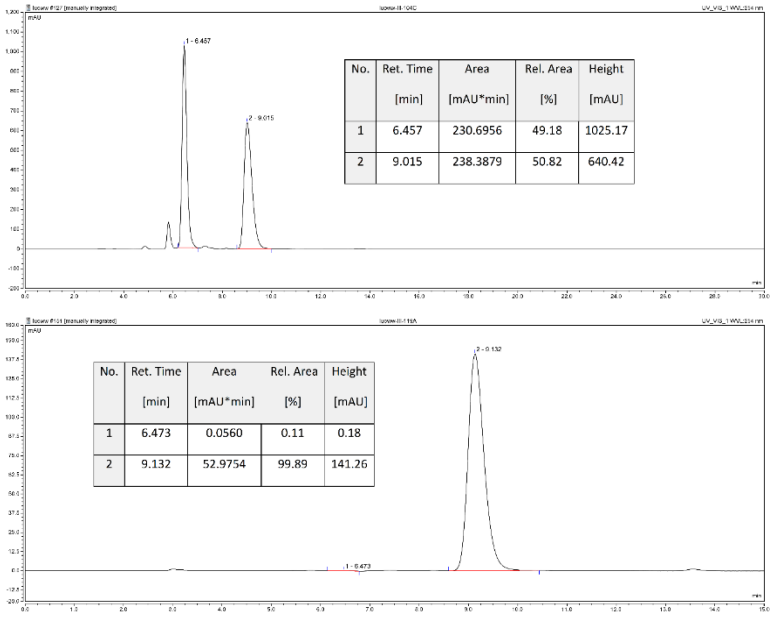
No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	6.382	0.0158	0.02	0.11
2	8.898	86.7939	99.98	240.50

methyl (5a*S*,9a*R*)-5a-((3-bromophenyl)amino)-2-hydroxy-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3k**



(**$C_{20}H_{18}BrNO_5$**) The title compound **3k** was obtained as a yellow syrup in 42.7 mg, 99% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = -31.3 (*c* 0.45 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 6.5 min (minor), t_2 = 9.1 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.63 (s, 1H), 7.02 (d, *J* = 8.8 Hz, 1H), 6.96 – 6.87 (m, 3H), 6.78 (t, *J* = 1.9 Hz, 1H), 6.51 – 6.44 (m, 1H), 5.68 (s, 1H), 4.19 (t, *J* = 4.2 Hz, 1H), 3.94 (s, 3H), 2.92 – 2.77 (m, 1H),

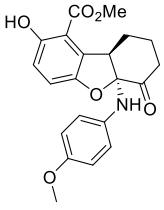
2.54 (dt, *J* = 17.1, 8.5 Hz, 1H), 2.03 – 1.94 (m, 1H), 1.84 – 1.63 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.81, 169.87, 157.61, 151.59, 143.10, 130.36, 128.02, 122.93, 122.78, 120.49, 118.61, 117.68, 115.64, 108.39, 96.26, 52.51, 50.41, 34.49, 27.26, 18.27. ESI-HRMS: calcd for $C_{20}H_{19}{}^{79}BrNO_5^+$ ([M+H$^+$]) 432.0441, found 432.0431.



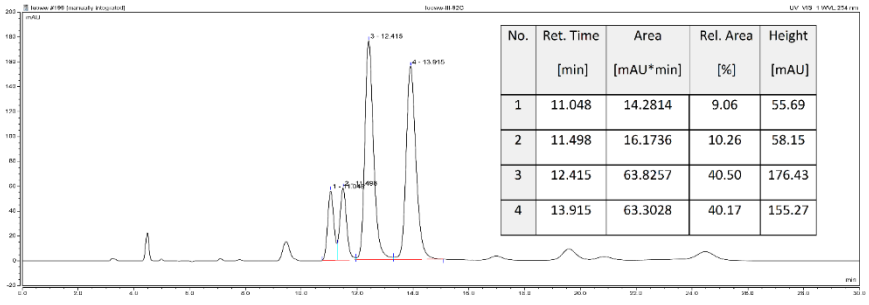
No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	6.457	230.6956	49.18	1025.17
2	9.015	238.3879	50.82	640.42

No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	6.473	0.0560	0.11	0.18
2	9.132	52.9754	99.89	141.26

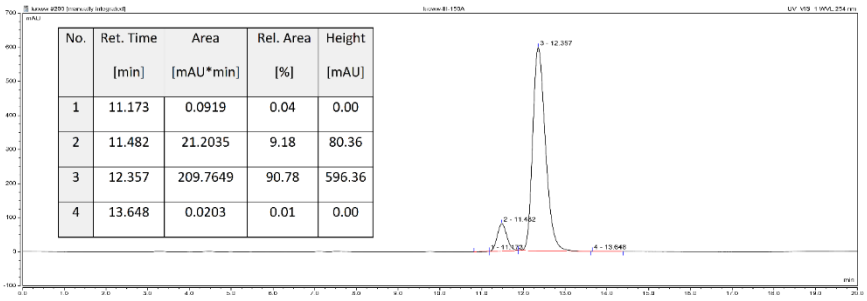
methyl (5a*S*,9a*R*)-2-hydroxy-5a-((4-methoxyphenyl)amino)-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3l**



(**$C_{21}H_{21}NO_6$**) The title compound **3l** was obtained as a red syrup in 37.6 mg, 98% yield, 91:9 d.r., 99% *ee*. $[\alpha]_D^{25}$ = -13.2 (*c* 0.37 in $CHCl_3$). HPLC analysis: Chiralcel IC, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 11.2 min, t_2 = 11.5 min, t_3 = 12.4 min, t_4 = 13.6 min. ^{1}H NMR of the major diastereomer (400 MHz, $CDCl_3$) δ 10.54 (s, 1H), 6.97 (d, *J* = 8.8 Hz, 1H), 6.86 (dd, *J* = 8.8, 0.5 Hz, 1H), 6.64 (s, 4H), 5.33 (s, 1H), 4.17 (t, *J* = 4.5 Hz, 1H), 3.91 (s, 3H), 3.68 (s, 3H), 2.85 – 2.75 (m, 1H), 2.58 – 2.48 (m, 1H), 1.92 (ddd, *J* = 10.0, 3.5, 1.6 Hz, 1H), 1.86 – 1.68 (m, 3H). ^{13}C NMR of the major diastereomer (101 MHz, $CDCl_3$) δ 203.00, 170.00, 157.14, 154.66, 151.64, 134.38, 128.64, 121.44, 118.10, 117.46, 114.29, 108.41, 97.44, 55.44, 52.37, 49.55, 34.82, 27.55, 18.36. ESI-HRMS: calcd for $C_{21}H_{22}NO_6^+$ ([M+H$^+$]) 384.1442, found 384.1444.

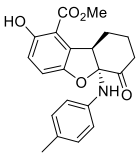


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	11.048	14.2814	9.06	55.69
2	11.498	16.1736	10.26	58.15
3	12.415	63.8257	40.50	176.43
4	13.915	63.3028	40.17	155.27

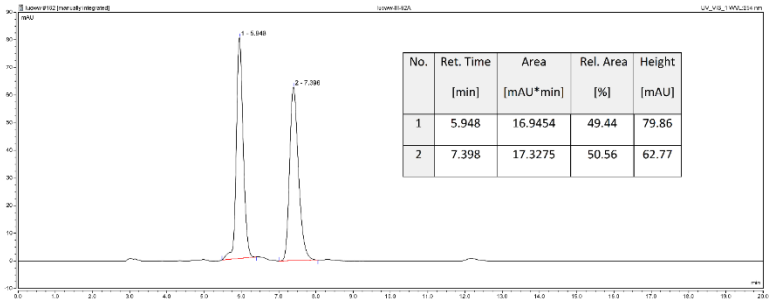


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	11.173	0.0919	0.04	0.00
2	11.482	21.2035	9.18	80.36
3	12.357	209.7649	90.78	596.36
4	13.648	0.0203	0.01	0.00

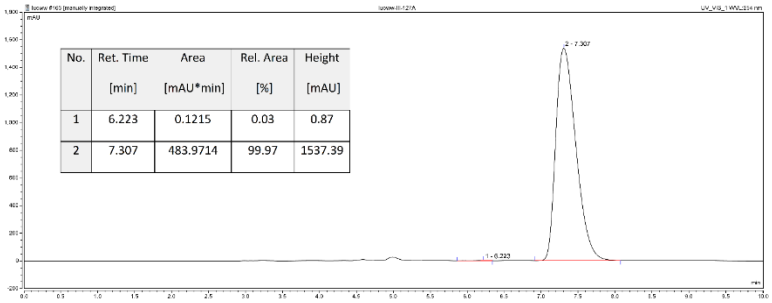
methyl (5a*S*,9a*R*)-2-hydroxy-6-oxo-5a-(*p*-tolylamino)-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3m**



(**$C_{21}H_{21}NO_5$**) The title compound **3m** was obtained as a brown solid in 34.8 mg, 95% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = -8.3 (*c* 0.45 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 6.2 min (minor), t_2 = 7.3 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 6.99 (d, *J* = 8.8 Hz, 1H), 6.96 – 6.82 (m, 3H), 6.58 – 6.48 (m, 2H), 5.57 (s, 1H), 4.25 (t, *J* = 4.2 Hz, 1H), 3.92 (s, 3H), 2.89 – 2.76 (m, 1H), 2.54 (dt, *J* = 25.1, 8.4 Hz, 1H), 2.20 (s, 3H), 2.03 – 1.95 (m, 1H), 1.76 (dddd, *J* = 18.8, 7.3, 5.9, 2.9 Hz, 2H), 1.70 – 1.59 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.94, 170.03, 157.28, 151.84, 138.82, 129.77, 129.64, 128.34, 118.28, 117.99, 117.57, 108.53, 97.01, 52.41, 49.76, 34.31, 27.21, 20.45, 18.34. ESI-HRMS: calcd for $C_{21}H_{22}NO_5^+$ ([M+H$^+$]) 368.1492, found 368.1497.

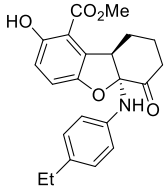


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	5.948	16.9454	49.44	79.86
2	7.398	17.3275	50.56	62.77

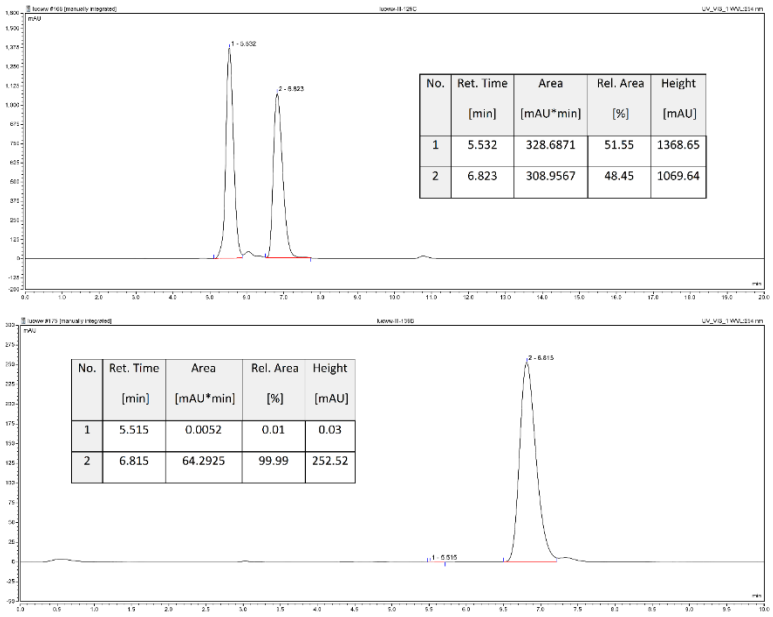


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	6.223	0.1215	0.03	0.87
2	7.307	483.9714	99.97	1537.39

methyl (5a*S*,9a*R*)-5a-((4-ethylphenyl)amino)-2-hydroxy-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3n**



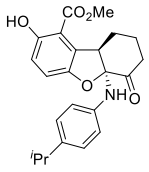
(**$C_{22}H_{23}NO_5$**) The title compound **3n** was obtained as a yellow syrup in 34.7 mg, 91% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = -17.0 (*c* 0.35 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 5.5 min (minor), t_2 = 6.8 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.61 (s, 1H), 7.00 (d, *J* = 8.8 Hz, 1H), 6.92 (dd, *J* = 12.2, 8.6 Hz, 3H), 6.58 – 6.51 (m, 2H), 5.61 (s, 1H), 4.27 (t, *J* = 3.8 Hz, 1H), 3.92 (s, 3H), 2.88 – 2.77 (m, 1H), 2.52 (dq, *J* = 17.9, 7.5 Hz, 3H), 2.05 – 1.96 (m, 1H), 1.82 – 1.62 (m, 3H), 1.14 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.91, 170.04, 157.29, 151.87, 139.04, 136.21, 128.48, 128.31, 118.29, 117.82, 117.58, 108.55, 96.97, 52.40, 49.71, 34.22, 27.92, 27.17, 18.36, 15.70. ESI-HRMS: calcd for $C_{22}H_{24}NO_5^+$ ([M+H$^+$]) 382.1649, found 382.1617.



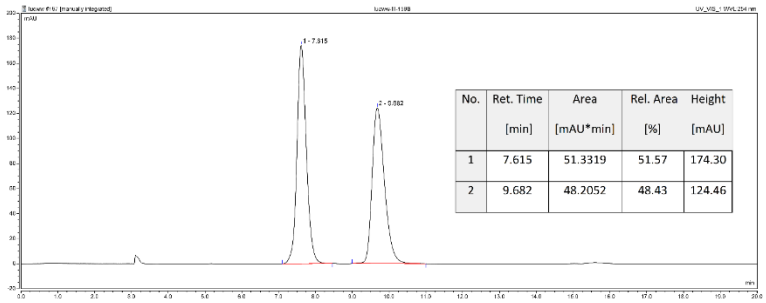
No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	5.532	328.6871	51.55	1368.65
2	6.823	308.9567	48.45	1069.64

No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	5.515	0.0052	0.01	0.03
2	6.815	64.2925	99.99	252.52

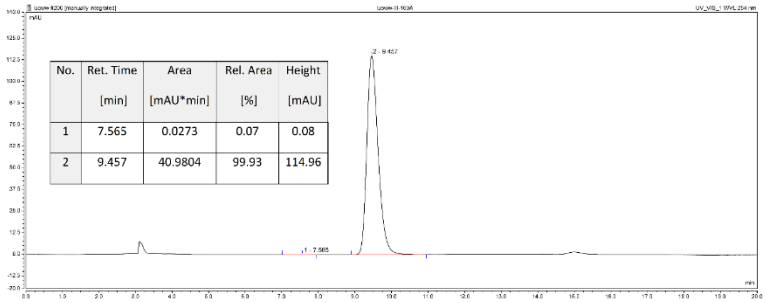
methyl (5a*S*,9a*R*)-2-hydroxy-5a-((4-isopropylphenyl)amino)-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3o**



(**$C_{23}H_{25}NO_5$**) The title compound **3o** was obtained as a colorless syrup in 34.5 mg, 87% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = -7.4 (*c* 0.42 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 7.6 min (minor), t_2 = 9.5 min (major). ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.62 (s, 1H), 7.03 – 6.96 (m, 3H), 6.92 (d, *J* = 8.8 Hz, 1H), 6.58 – 6.54 (m, 2H), 5.65 (s, 1H), 4.30 (t, *J* = 4.0 Hz, 1H), 3.94 (s, 3H), 2.88 – 2.81 (m, 1H), 2.78 (dt, *J* = 13.8, 6.9 Hz, 1H), 2.59 – 2.50 (m, 1H), 2.02 (ddd, *J* = 9.0, 5.1, 2.2 Hz, 1H), 1.85 – 1.72 (m, 2H), 1.71 – 1.63 (m, 1H), 1.18 (s, 3H), 1.16 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 202.87, 170.07, 157.31, 151.91, 140.77, 139.11, 128.28, 127.08, 118.31, 117.61, 117.57, 108.57, 96.92, 52.42, 49.62, 34.13, 33.20, 27.12, 24.11, 24.05, 18.38. ESI-HRMS: calcd for $C_{23}H_{26}NO_5^+$ ([M+H$^+$]) 396.1805, found 396.1833.

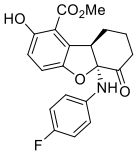


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	7.615	51.3319	51.57	174.30
2	9.682	48.2052	48.43	124.46

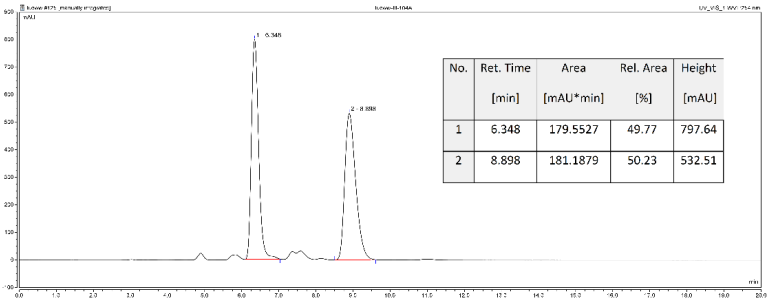


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	7.565	0.0273	0.07	0.08
2	9.457	40.9804	99.93	114.96

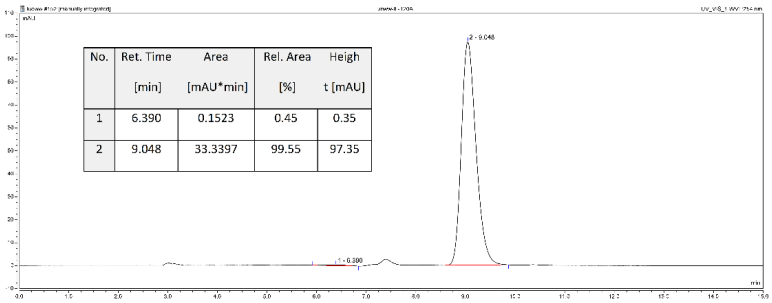
methyl (5a*S*,9a*R*)-5a-((4-fluorophenyl)amino)-2-hydroxy-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3p**



(**$C_{20}H_{18}FNO_5$**) The title compound **3p** was obtained as a yellow solid in 34.6 mg, 93% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = +16.4 (*c* 0.34 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 6.4 min (minor), t_2 = 9.0 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.57 (s, 1H), 6.99 (d, *J* = 8.8 Hz, 1H), 6.89 (dd, *J* = 8.8, 0.5 Hz, 1H), 6.82 – 6.74 (m, 2H), 6.60 (ddd, *J* = 6.8, 5.3, 3.0 Hz, 2H), 5.49 (s, 1H), 4.19 – 4.14 (m, 1H), 3.92 (s, 3H), 2.87 – 2.75 (m, 1H), 2.60 – 2.46 (m, 1H), 2.01 – 1.89 (m, 1H), 1.86 – 1.72 (m, 2H), 1.72 – 1.59 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.91, 169.88, 158.89, 157.35, 156.51, 151.59, 137.48, 137.45, 128.27, 120.13, 120.05, 118.39, 117.56, 115.68, 115.46, 108.44, 96.95, 52.44, 49.93, 34.58, 27.38, 18.31. ESI-HRMS: calcd for $C_{20}H_{19}FNO_5^+$ ([M+H$^+$]) 372.1242, found 372.1228.

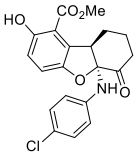


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	6.348	179.5527	49.77	797.64
2	8.898	181.1879	50.23	532.51

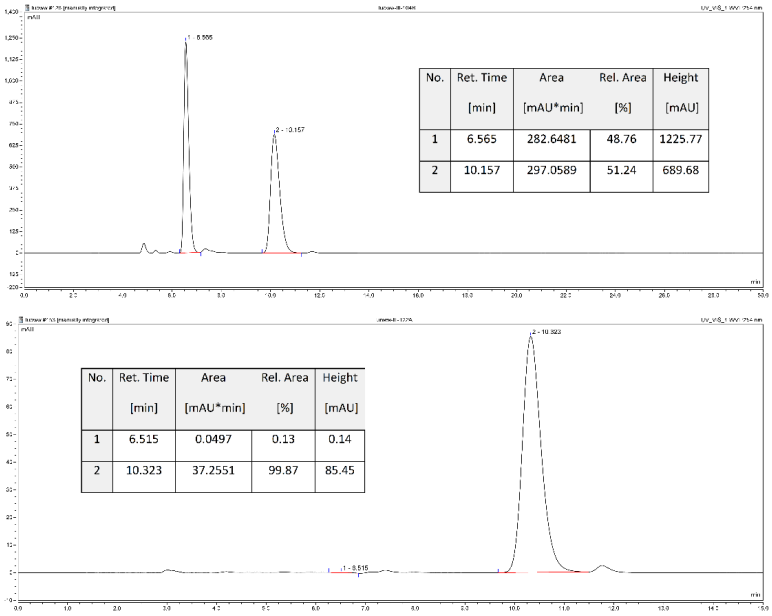


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Heigh t [mAU]
1	6.390	0.1523	0.45	0.35
2	9.048	33.3397	99.55	97.35

methyl (5a*S*,9a*R*)-5a-((4-chlorophenyl)amino)-2-hydroxy-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3q**



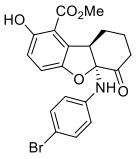
(**$C_{20}H_{18}FNO_5$**) The title compound **3q** was obtained as a yellowish syrup in 38.0 mg, 99% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = -17.6 (*c* 0.34 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 6.5 min (minor), t_2 = 10.3 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 7.03 (ddd, *J* = 16.1, 8.0, 6.0 Hz, 3H), 6.91 (dd, *J* = 8.8, 0.5 Hz, 1H), 6.58 – 6.46 (m, 2H), 5.66 (s, 1H), 4.18 (d, *J* = 3.7 Hz, 1H), 3.93 (s, 3H), 2.89 – 2.78 (m, 1H), 2.53 (dt, *J* = 17.1, 8.4 Hz, 1H), 2.03 – 1.96 (m, 1H), 1.83 – 1.59 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.82, 169.86, 157.50, 151.65, 140.22, 129.02, 127.97, 125.11, 118.59, 118.57, 117.64, 108.51, 96.49, 52.49, 50.19, 34.26, 27.15, 18.27. ESI-HRMS: calcd for $C_{20}H_{19}{}^{35}ClNO_5^+$ ([M+H$^+$]) 388.0946, found 388.0930.



No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	6.565	282.6481	48.76	1225.77
2	10.157	297.0589	51.24	689.68

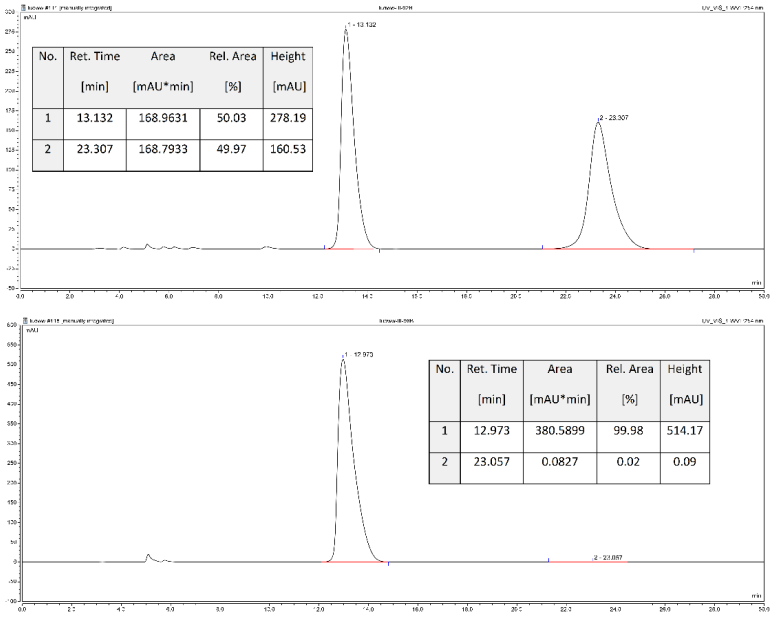
No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	6.515	0.0497	0.13	0.14
2	10.323	37.2551	99.87	85.45

methyl (5a*S*,9a*R*)-5a-((4-bromophenyl)amino)-2-hydroxy-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3r**



(**$C_{20}H_{18}BrNO_5$**) The title compound **3r** was obtained as a yellow solid in 43.0 mg, 99% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = -17.0 (*c* 0.84 in $CHCl_3$). HPLC analysis: Chiralcel ADH, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 13.0 min (major), t_2 = 23.1 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.61 (s, 1H), 7.23 – 7.13 (m, 2H), 7.00 (d, *J* = 8.8 Hz, 1H), 6.91 (d, *J* = 8.8 Hz, 1H), 6.52 – 6.39 (m, 2H), 5.67 (s, 1H), 4.17 (d, *J* = 3.5 Hz, 1H), 3.93 (s, 3H), 2.90 – 2.78 (m, 1H), 2.53 (dt,

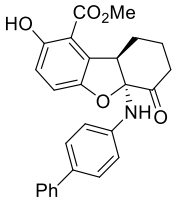
J = 17.1, 8.4 Hz, 1H), 2.00 (ddd, *J* = 9.9, 5.6, 3.9 Hz, 1H), 1.83 – 1.57 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.81, 169.85, 157.53, 151.65, 140.74, 131.93, 127.92, 118.83, 118.61, 117.65, 112.30, 108.51, 96.40, 52.51, 50.23, 34.22, 27.12, 18.27. ESI-HRMS: calcd for $C_{20}H_{19}{}^{79}BrNO_5^+$ ([M+H$^+$]) 432.0441, found 432.0466.



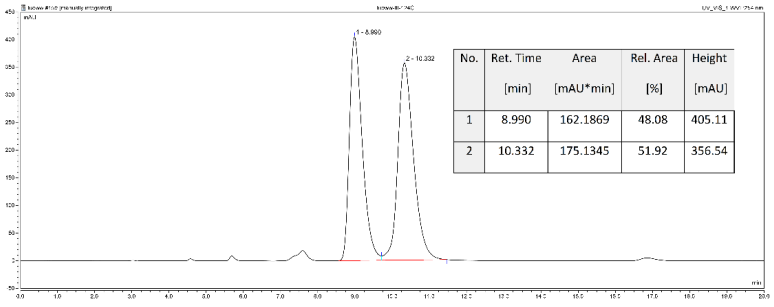
No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	13.132	168.9631	50.03	278.19
2	23.307	168.7933	49.97	160.53

No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	12.973	380.5899	99.98	514.17
2	23.057	0.0827	0.02	0.09

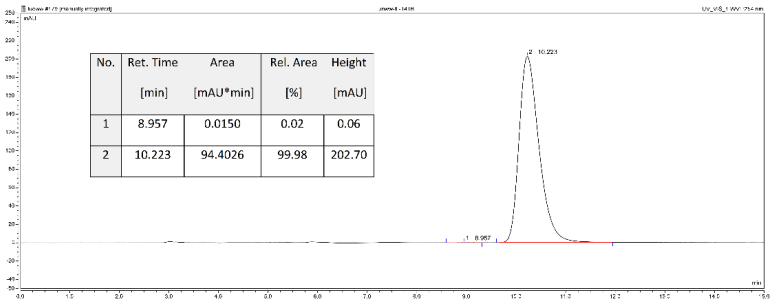
methyl (5a*S*,9a*R*)-5a-([1,1'-biphenyl]-4-ylamino)-2-hydroxy-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3s**



(**$C_{26}H_{23}NO_5$**) The title compound **3s** was obtained as a yellowish solid in 42.4 mg, 99% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = -53.9 (*c* 0.47 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 9.0 min (minor), t_2 = 10.2 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.65 (s, 1H), 7.53 – 7.47 (m, 2H), 7.37 (ddd, *J* = 8.0, 4.4, 2.0 Hz, 4H), 7.30 – 7.23 (m, 1H), 7.05 (d, *J* = 8.8 Hz, 1H), 6.95 (d, *J* = 8.9 Hz, 1H), 6.70 – 6.64 (m, 2H), 5.82 (s, 1H), 4.31 (d, *J* = 3.6 Hz, 1H), 3.94 (s, 3H), 2.88 (ddd, *J* = 17.1, 9.9, 2.9 Hz, 1H), 2.57 (dt, *J* = 17.0, 8.3 Hz, 1H), 2.10 – 2.00 (m, 1H), 1.83 – 1.63 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.88, 170.00, 157.48, 151.88, 140.95, 140.70, 132.86, 128.66, 128.12, 127.83, 126.49, 126.42, 118.53, 117.69, 117.36, 108.61, 96.62, 52.48, 50.06, 34.13, 27.11, 18.33. ESI-HRMS: calcd for $C_{26}H_{24}NO_5^+$ ([M+H$^+$]) 430.1649, found 430.1665.

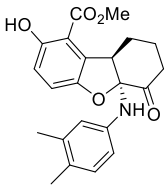


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	8.990	162.1869	48.08	405.11
2	10.332	175.1345	51.92	356.54

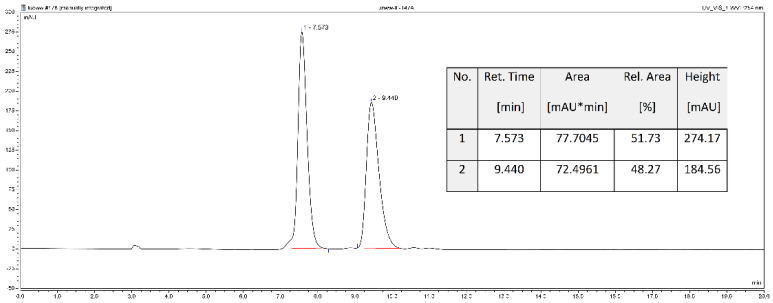


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	8.957	0.0150	0.02	0.06
2	10.223	94.4026	99.98	202.70

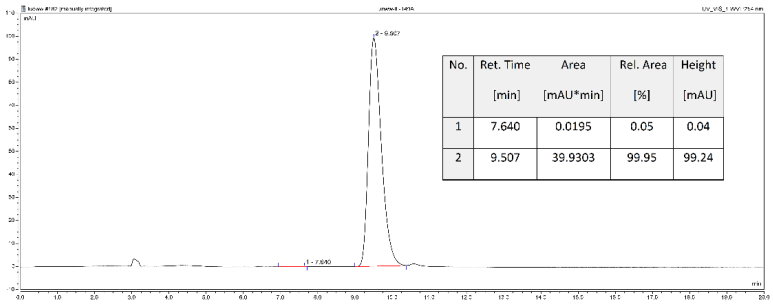
methyl (5a*S*,9a*R*)-5a-((3,4-dimethylphenyl)amino)-2-hydroxy-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3t**



(**$C_{22}H_{23}NO_5$**) The title compound **3t** was obtained as a colorless syrup in 36.6 mg, 96% yield, >95:5 d.r., 99% *ee*. $[\alpha]_D^{25}$ = -21.4 (*c* 0.39 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 7.6 min (minor), t_2 = 9.5 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.61 (s, 1H), 7.00 (d, *J* = 8.8 Hz, 1H), 6.90 (d, *J* = 8.8 Hz, 1H), 6.83 (d, *J* = 8.1 Hz, 1H), 6.47 (d, *J* = 2.4 Hz, 1H), 6.33 (dd, *J* = 8.1, 2.5 Hz, 1H), 5.54 (s, 1H), 4.25 (t, *J* = 4.3 Hz, 1H), 3.92 (s, 3H), 2.88 – 2.78 (m, 1H), 2.54 (dt, *J* = 17.1, 8.4 Hz, 1H), 2.10 (s, 3H), 2.07 (s, 3H), 2.03 – 1.94 (m, 1H), 1.83 – 1.62 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.99, 170.06, 157.27, 151.88, 139.13, 137.22, 130.10, 128.50, 128.49, 119.82, 118.21, 117.58, 115.07, 108.41, 97.04, 52.40, 49.83, 34.43, 27.26, 19.91, 18.73, 18.36. ESI-HRMS: calcd for $C_{22}H_{24}NO_5^+$ ([M+H$^+$]) 382.1649, found 382.1617.

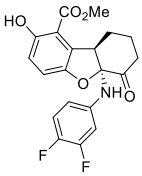


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	7.573	77.7045	51.73	274.17
2	9.440	72.4961	48.27	184.56

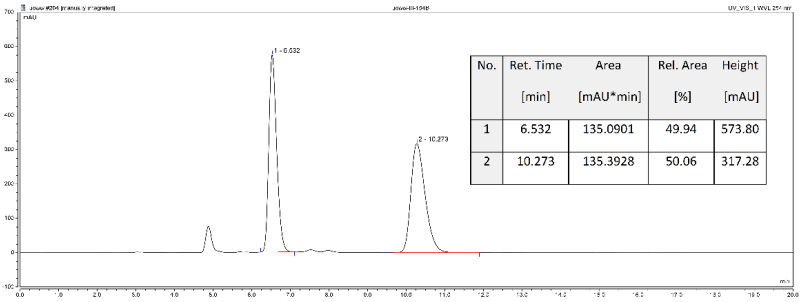


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	7.640	0.0195	0.05	0.04
2	9.507	39.9303	99.95	99.24

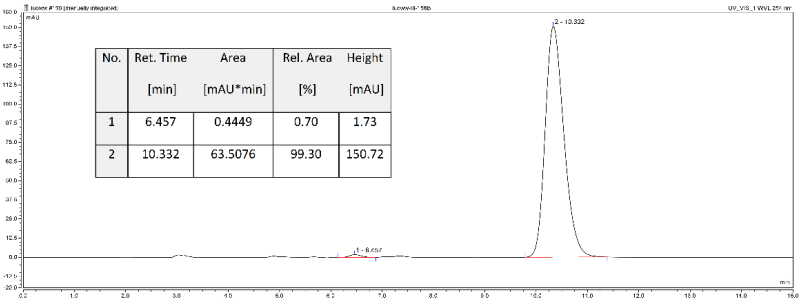
methyl (5a*S*,9a*R*)-5a-((3,4-difluorophenyl)amino)-2-hydroxy-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3u**



(**$C_{20}H_{17}F_2NO_5$**) The title compound **3u** was obtained as a white solid in 38.7 mg, 99% yield, >95:5 d.r., 98% *ee*. $[\alpha]_D^{25}$ = +2.7 (*c* 0.43 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 6.5 min (minor), t_2 = 10.3 min (major). ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.59 (s, 1H), 7.02 (d, *J* = 8.8 Hz, 1H), 6.95 – 6.83 (m, 2H), 6.47 (ddd, *J* = 12.4, 6.8, 2.8 Hz, 1H), 6.34 – 6.29 (m, 1H), 5.52 (s, 1H), 4.15 (t, *J* = 4.4 Hz, 1H), 3.95 (s, 3H), 2.89 – 2.79 (m, 1H), 2.55 (dt, *J* = 25.5, 8.6 Hz, 1H), 2.03 – 1.94 (m, 1H), 1.85 – 1.74 (m, 2H), 1.73 – 1.63 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 202.88, 169.79, 157.57, 151.48, 151.29, 151.18, 149.33, 149.23, 145.90, 145.80, 143.99, 143.88, 138.54, 138.52, 138.48, 138.45, 127.96, 118.65, 117.69, 117.38, 117.36, 117.23, 117.22, 113.46, 113.43, 113.41, 113.39, 108.47, 107.29, 107.12, 96.56, 52.50, 50.54, 34.58, 27.30, 18.30. ESI-HRMS: calcd for $C_{20}H_{18}F_2NO_5^+$ ([M+H$^+$]) 390.1148, found 390.1148.

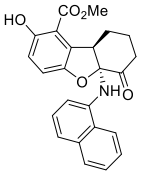


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	6.532	135.0901	49.94	573.80
2	10.273	135.3928	50.06	317.28

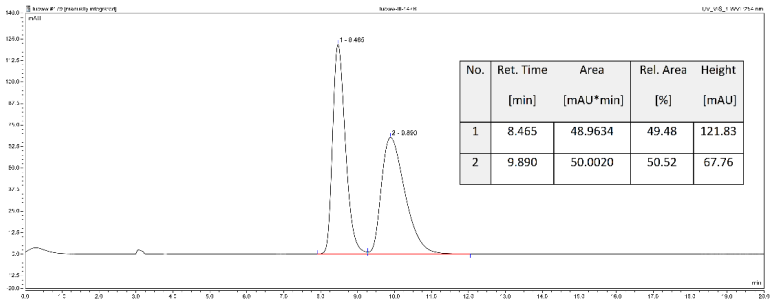


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	6.457	0.4449	0.70	1.73
2	10.332	63.5076	99.30	150.72

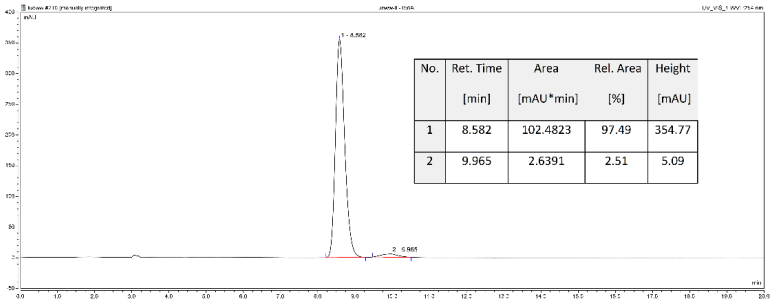
methyl (5a*S*,9a*R*)-2-hydroxy-5a-(naphthalen-1-ylamino)-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[*b*,*d*]furan-1-carboxylate **3v**



(**$C_{24}H_{21}NO_5$**) The title compound **3v** was obtained as a yellow syrup in 37.2 mg, 92% yield, >95:5 d.r., 95% *ee*. $[\alpha]_D^{25}$ = -0.5 (*c* 0.38 in $CHCl_3$). HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 8.6 min (major), t_2 = 10.0 min (minor). ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.58 (s, 1H), 8.28 – 8.23 (m, 1H), 8.01 – 7.95 (m, 1H), 7.59 – 7.51 (m, 3H), 7.25 (dd, *J* = 9.0, 3.0 Hz, 1H), 7.19 (d, *J* = 8.1 Hz, 1H), 7.01 (d, *J* = 9.0 Hz, 1H), 6.78 (d, *J* = 8.1 Hz, 1H), 6.48 (s, 1H), 5.88 (t, *J* = 4.8 Hz, 1H), 3.91 (s, 3H), 2.66 – 2.59 (m, 2H), 2.37 (dd, *J* = 11.0, 5.8 Hz, 2H), 2.04 (dt, *J* = 12.4, 6.1 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 195.66, 170.03, 157.79, 150.15, 149.35, 138.57, 132.96, 130.02, 127.60, 127.22, 126.68, 126.21, 122.66, 122.42, 119.32, 119.04, 118.87, 115.59, 112.63, 111.93, 52.42, 37.78, 24.41, 23.23. ESI-HRMS: calcd for $C_{24}H_{22}NO_5^+$ ([M+H$^+$]) 404.1492, found 404.1486.

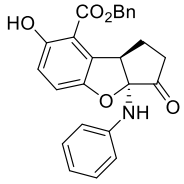


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	8.465	48.9634	49.48	121.83
2	9.890	50.0020	50.52	67.76

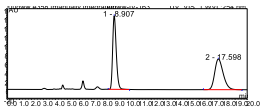


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	8.582	102.4823	97.49	354.77
2	9.965	2.6391	2.51	5.09

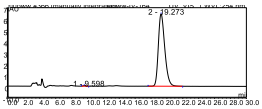
benzyl 7-hydroxy-3-oxo-3a-(phenylamino)-2,3,3a,8b-tetrahydro-1H-cyclopenta[b]benzofuran-8-carboxylate **3w**



(**$C_{25}H_{21}NO_5$**) The title compound **3w** was obtained as a yellowish solid in 8.1 mg (0.05 mmol scale), 39% yield, >95:5 d.r., 99% *ee*. HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 9.6 min (minor), t_2 = 19.3 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.72 (s, 1H), 7.42 – 7.29 (m, 5H), 7.16 – 7.10 (m, 2H), 6.93 (dt, *J* = 8.9, 4.7 Hz, 2H), 6.84 (ddd, *J* = 7.6, 2.1, 1.0 Hz, 1H), 6.57 – 6.47 (m, 2H), 5.52 (d, *J* = 11.9 Hz, 1H), 5.27 (d, *J* = 11.9 Hz, 2H), 4.48 (d, *J* = 8.4 Hz, 1H), 2.38 – 2.30 (m, 2H), 2.09 – 2.01 (m, 1H), 1.92 – 1.79 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 205.93, 169.38, 157.65, 151.12, 141.80, 134.43, 129.42, 128.98, 128.95, 128.79, 128.53, 120.27, 118.68, 117.73, 116.19, 108.52, 97.15, 67.77, 47.05, 33.77, 27.30.

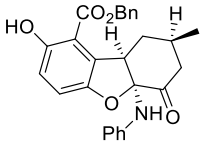


	Retention Time	Area	% Area	Height
1	8.907	57.1129	50.48	164.14
2	17.598	56.0254	49.52	68.46

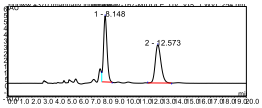


	Retention Time	Area	% Area	Height
1	9.598	0.1730	0.29	0.49
2	19.273	60.4397	99.71	64.59

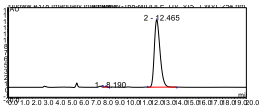
benzyl (5aS,8*R*,9a*R*)-2-hydroxy-8-methyl-6-oxo-5a-(phenylamino)-5a,6,7,8,9,9a-hexahydrodibenzo[b,d]furan-1-carboxylate **3x**



(**$C_{27}H_{25}NO_5$**) The title compound **3x** was obtained as a white solid in 31.4 mg, 71% yield, >95:5 d.r. (isolated major diastereomer), 99% *ee*. HPLC analysis: Chiralcel ODH, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 8.2 min (minor), t_2 = 12.5 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.46 (s, 1H), 7.42 (s, 5H), 7.11 – 7.03 (m, 2H), 6.95 (d, *J* = 8.8 Hz, 1H), 6.83 (s, 1H), 6.80 – 6.71 (m, 3H), 5.47 (d, *J* = 11.7 Hz, 1H), 5.28 (d, *J* = 11.8 Hz, 1H), 4.88 (s, 1H), 3.89 (dd, *J* = 11.3, 5.6 Hz, 1H), 2.72 (ddd, *J* = 15.4, 6.5, 1.7 Hz, 1H), 2.12 (dd, *J* = 15.4, 9.6 Hz, 1H), 1.99 (dddd, *J* = 13.8, 5.5, 3.7, 1.7 Hz, 1H), 1.85 – 1.72 (m, 1H), 1.01 (dt, *J* = 13.8, 11.4 Hz, 1H), 0.81 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 203.41, 169.20, 157.00, 149.85, 142.02, 134.43, 130.27, 129.18, 129.16, 128.92, 128.74, 121.99, 120.44, 118.50, 117.56, 108.33, 96.69, 67.80, 51.80, 44.24, 36.89, 28.93, 22.19.

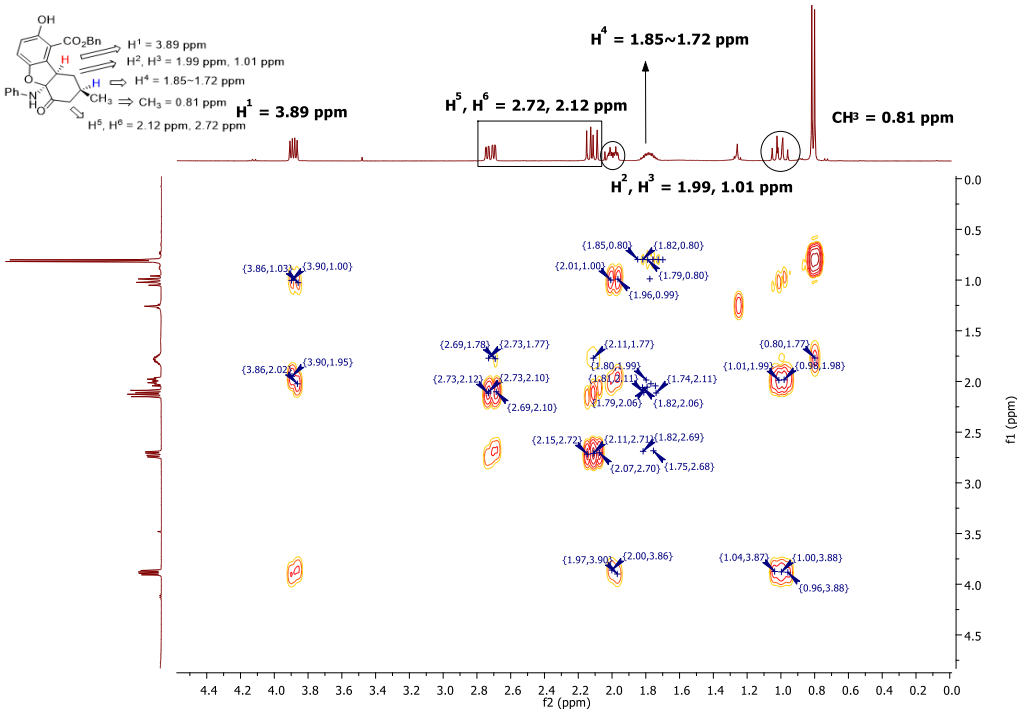


	Retention Time	Area	% Area	Height
1	8.148	17.3516	50.97	51.60
2	12.573	16.6924	49.03	29.87

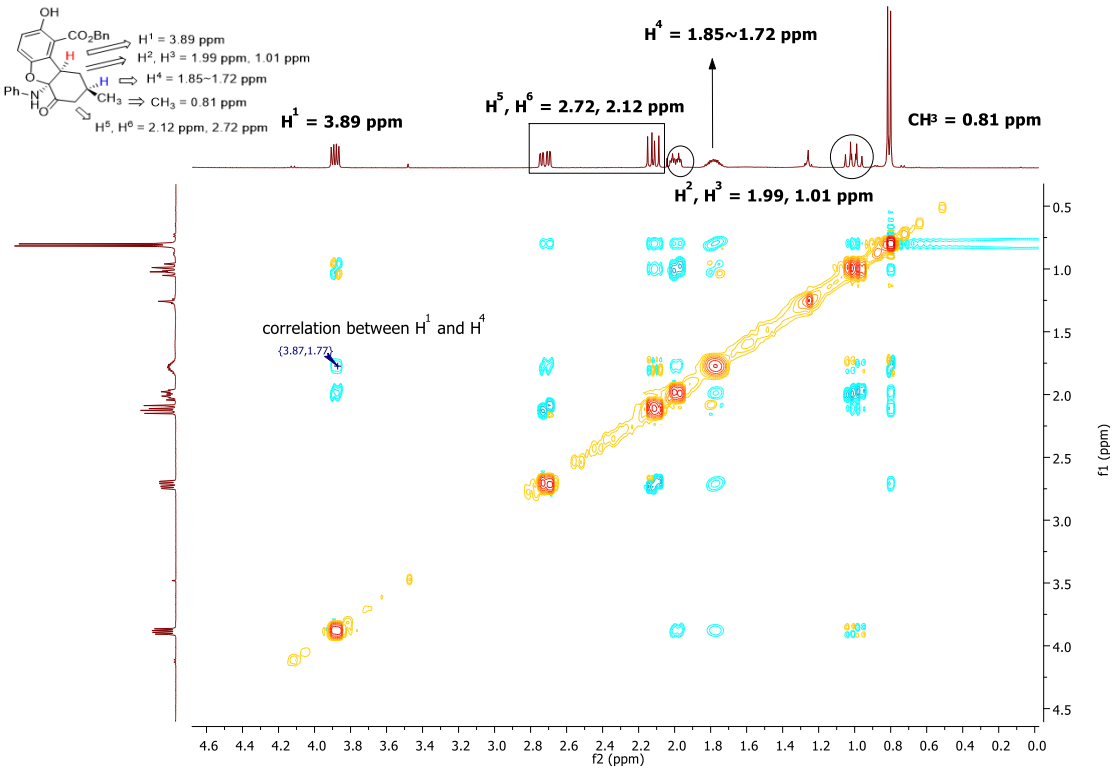


	Retention Time	Area	% Area	Height
1	8.190	0.1804	0.24	0.68
2	12.465	75.2476	99.76	135.42

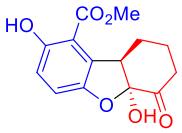
2D COSY spectrum of product



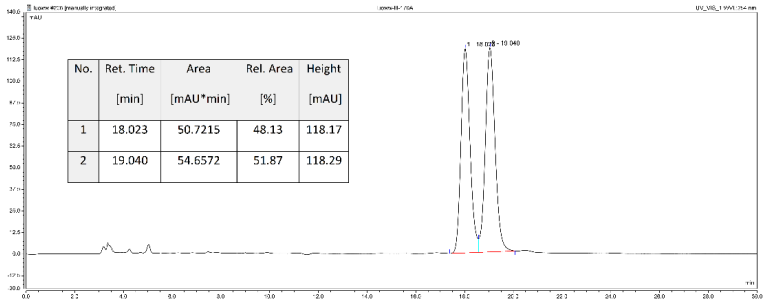
2D NOESY spectrum of product: the proton H^1 is correlated to proton H^4, suggesting a *cis*-configuration of the methyl group and phenyl group.



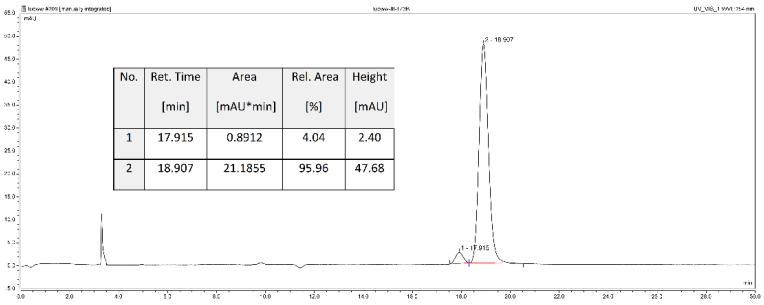
methyl 2-(2,3-dioxocyclohexyl)-3,6-dihydroxybenzoate **3z**



(**$C_{14}H_{14}O_6$**) The title compound **3z** was obtained as a yellowish solid in 25.8 mg, 92% yield, 92% *ee*. $[\alpha]_D^{25}$ = +152.5 (*c* 0.25 in $CHCl_3$). HPLC analysis: Chiralcel IC, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 17.9 min (minor), t_2 = 18.9 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.63 (s, 1H), 7.02 (dd, *J* = 25.1, 7.2 Hz, 1H), 6.87 (t, *J* = 8.0 Hz, 1H), 5.02 (s, 1H), 3.96 (s, 3H), 3.89 (t, *J* = 6.4 Hz, 1H), 2.70 (dd, *J* = 15.6, 8.6 Hz, 1H), 2.65 – 2.52 (m, 1H), 2.20 – 2.07 (m, 1H), 1.90 – 1.77 (m, 1H), 1.77 – 1.70 (m, 1H), 1.70 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 204.26, 170.00, 157.70, 149.78, 130.09, 118.26, 117.75, 108.81, 102.97, 52.36, 51.72, 36.69, 29.39, 19.94. ESI-HRMS: calcd for $C_{14}H_{15}O_6^+$ ([M+H$^+$]) 279.0863, found 279.0827.

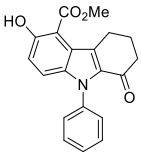


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	18.023	50.7215	48.13	118.17
2	19.040	54.6572	51.87	118.29



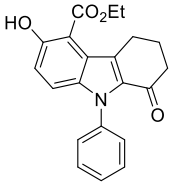
No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	17.915	0.8912	4.04	2.40
2	18.907	21.1855	95.96	47.68

methyl 6-hydroxy-1-oxo-9-phenyl-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4a**



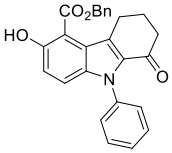
(**$C_{20}H_{17}NO_4$**) The title compound **4a** was obtained as a yellowish solid in 33.3 mg, 99% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.05 (s, 1H), 7.57 – 7.44 (m, 3H), 7.31 – 7.25 (m, 2H), 7.21 (d, *J* = 9.1 Hz, 1H), 6.99 (d, *J* = 9.2 Hz, 1H), 4.07 (s, 3H), 3.18 (t, *J* = 6.1 Hz, 2H), 2.60 (dd, *J* = 7.5, 5.5 Hz, 2H), 2.22 – 2.14 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.78, 171.01, 159.48, 137.88, 135.45, 132.62, 129.06, 128.83, 128.25, 127.93, 121.91, 119.85, 118.65, 104.04, 51.88, 39.18, 26.24, 24.70. ESI-HRMS: calcd for $C_{20}H_{18}NO_4^+$ ([M+H$^+$]) 336.1230, found 336.1231.

ethyl 6-hydroxy-1-oxo-9-phenyl-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4b**



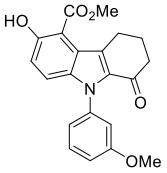
(**$C_{21}H_{19}NO_4$**) The title compound **4b** was obtained as a yellow solid in 29.7 mg, 85% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.16 (s, 1H), 7.53 – 7.45 (m, 3H), 7.30 – 7.25 (m, 2H), 7.21 (d, *J* = 9.1 Hz, 1H), 6.99 (d, *J* = 9.1 Hz, 1H), 4.58 (q, *J* = 7.2 Hz, 2H), 3.22 (t, *J* = 6.1 Hz, 2H), 2.61 (dd, *J* = 7.5, 5.5 Hz, 2H), 2.21 – 2.15 (m, 2H), 1.53 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.75, 170.74, 159.53, 137.92, 135.47, 132.51, 129.05, 128.90, 128.23, 127.94, 121.87, 119.67, 118.75, 104.49, 61.63, 39.21, 26.72, 24.70, 14.45. ESI-HRMS: calcd for $C_{21}H_{20}NO_4^+$ ([M+H$^+$]) 350.1387, found 350.1382.

benzyl 6-hydroxy-1-oxo-9-phenyl-2,3,4,9-tetrahydro-1H-carbazole-5-carboxylate **4c**



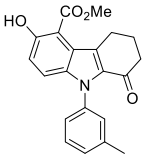
(**$C_{26}H_{21}NO_4$**) The title compound **4c** was obtained as a colorless syrup in 38.4 mg, 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.13 (s, 1H), 7.58 – 7.35 (m, 8H), 7.23 (ddd, *J* = 20.3, 10.3, 5.0 Hz, 3H), 6.98 (d, *J* = 9.2 Hz, 1H), 5.52 (s, 2H), 2.95 (t, *J* = 6.1 Hz, 2H), 2.49 (dd, *J* = 7.5, 5.6 Hz, 2H), 1.99 (dt, *J* = 12.6, 6.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.79, 170.50, 159.77, 137.88, 135.46, 134.84, 132.49, 129.30, 129.06, 129.03, 128.87, 128.75, 128.21, 127.91, 121.86, 119.89, 118.69, 104.28, 67.39, 39.12, 26.82, 24.52.

methyl 6-hydroxy-9-(3-methoxyphenyl)-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4d**



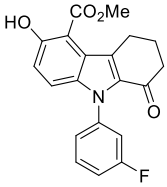
(**$C_{21}H_{19}NO_5$**) The title compound **4d** was obtained as a colorless syrup in 34.8 mg, 95% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.04 (s, 1H), 7.43 – 7.37 (m, 1H), 7.24 (d, *J* = 9.1 Hz, 1H), 7.05 – 6.96 (m, 2H), 6.86 (ddd, *J* = 7.8, 1.9, 0.9 Hz, 1H), 6.82 – 6.78 (m, 1H), 4.06 (s, 3H), 3.83 (s, 3H), 3.17 (t, *J* = 6.1 Hz, 2H), 2.64 – 2.57 (m, 2H), 2.22 – 2.14 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.61, 170.99, 160.05, 159.48, 138.97, 135.43, 132.62, 129.67, 128.82, 121.89, 120.24, 119.93, 118.66, 113.92, 113.82, 104.03, 55.41, 51.85, 39.17, 26.22, 24.68. ESI-HRMS: calcd for $C_{21}H_{20}NO_5^+$ ([M+H$^+$]) 366.1336, found 366.1335.

methyl 6-hydroxy-1-oxo-9-(*m*-tolyl)-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4e**



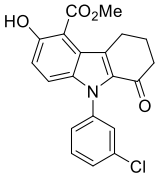
(**$C_{21}H_{19}NO_4$**) The title compound **4e** was obtained as a colorless syrup in 32.1 mg, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.04 (s, 1H), 7.41 – 7.34 (m, 1H), 7.27 (dd, *J* = 7.3, 1.0 Hz, 1H), 7.20 (d, *J* = 9.1 Hz, 1H), 7.08 – 7.03 (m, 2H), 6.97 (d, *J* = 9.2 Hz, 1H), 4.05 (s, 3H), 3.16 (t, *J* = 6.1 Hz, 2H), 2.59 (dd, *J* = 7.4, 5.6 Hz, 2H), 2.41 (s, 3H), 2.23 – 2.11 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.73, 171.02, 159.45, 138.99, 137.78, 135.51, 132.64, 129.05, 128.80, 128.67, 128.43, 124.92, 121.82, 119.96, 118.55, 103.98, 51.83, 39.19, 26.22, 24.69, 21.36. ESI-HRMS: calcd for $C_{21}H_{20}NO_4^+$ ([M+H$^+$]) 350.1387, found 350.1382.

methyl 9-(3-fluorophenyl)-6-hydroxy-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4f**



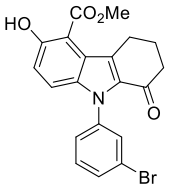
(**$C_{20}H_{16}FNO_4$**) The title compound **4f** was obtained as a yellowish solid in 19.1 mg, 54% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.03 (s, 1H), 7.47 (td, *J* = 8.2, 6.3 Hz, 1H), 7.25 – 7.15 (m, 2H), 7.08 (ddd, *J* = 7.9, 1.9, 0.9 Hz, 1H), 7.05 – 6.98 (m, 2H), 4.07 (s, 3H), 3.17 (t, *J* = 6.1 Hz, 2H), 2.61 (dd, *J* = 7.4, 5.6 Hz, 2H), 2.23 – 2.15 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.67, 170.89, 163.67, 161.70, 159.54, 139.34, 139.26, 135.23, 132.53, 130.14, 130.07, 129.32, 123.87, 123.84, 122.15, 119.50, 118.95, 115.74, 115.56, 115.52, 115.36, 104.21, 51.90, 39.06, 26.19, 24.63. ESI-HRMS: calcd for $C_{20}H_{17}FNO_4^+$ ([M+H$^+$]) 354.1136, found 354.1118.

methyl 9-(3-chlorophenyl)-6-hydroxy-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4g**



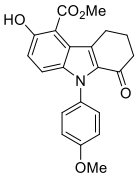
(**$C_{20}H_{16}ClNO_4$**) The title compound **4g** was obtained as a yellow syrup in 25.2 mg, 68% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.03 (s, 1H), 7.49 – 7.38 (m, 2H), 7.27 (ddd, *J* = 3.7, 2.8, 0.7 Hz, 1H), 7.22 – 7.14 (m, 2H), 7.00 (d, *J* = 9.2 Hz, 1H), 4.05 (s, 3H), 3.16 (t, *J* = 6.1 Hz, 2H), 2.64 – 2.54 (m, 2H), 2.17 (p, *J* = 6.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.67, 170.87, 159.53, 139.02, 135.21, 134.51, 132.50, 129.94, 129.36, 128.53, 128.29, 126.35, 122.18, 119.45, 118.95, 104.22, 51.90, 39.04, 26.18, 24.61. ESI-HRMS: calcd for $C_{20}H_{17}{}^{35}ClNO_4^+$ ([M+H$^+$]) 370.0841, found 370.0874.

methyl 9-(3-bromophenyl)-6-hydroxy-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4h**



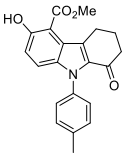
(**$C_{20}H_{16}BrNO_4$**) The title compound **4h** was obtained as a yellow syrup in 21.9 mg, 53% yield. ^{1}H NMR (500 MHz, cdcl$_3$) δ 11.04 (s, 1H), 7.61 (ddd, *J* = 8.1, 1.9, 1.0 Hz, 1H), 7.44 (t, *J* = 1.9 Hz, 1H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.26 – 7.16 (m, 2H), 7.02 (d, *J* = 9.1 Hz, 1H), 4.07 (s, 3H), 3.17 (t, *J* = 6.1 Hz, 2H), 2.64 – 2.57 (m, 2H), 2.18 (dt, *J* = 12.6, 6.3 Hz, 2H). ^{13}C NMR (126 MHz, cdcl$_3$) δ 190.68, 170.88, 159.56, 139.14, 135.23, 132.51, 131.44, 131.12, 130.22, 129.36, 126.85, 122.32, 122.19, 119.47, 118.98, 104.23, 51.91, 39.05, 26.19, 24.62. ESI-HRMS: calcd for $C_{20}H_{17}{}^{79}BrNO_4^+$ ([M+H$^+$]) 414.0335, found 414.0301.

methyl 6-hydroxy-9-(4-methoxyphenyl)-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4i**



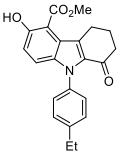
(**$C_{21}H_{19}NO_5$**) The title compound **4i** was obtained as a yellow syrup in 35.5 mg, 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.03 (s, 1H), 7.21 – 7.13 (m, 3H), 7.02 – 6.94 (m, 3H), 4.05 (s, 3H), 3.87 (s, 3H), 3.15 (t, *J* = 6.1 Hz, 2H), 2.58 (dd, *J* = 7.5, 5.5 Hz, 2H), 2.20 – 2.11 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.92, 171.02, 159.45, 159.22, 135.74, 132.66, 130.56, 128.89, 128.53, 121.71, 119.90, 118.55, 114.23, 103.97, 55.48, 51.82, 39.23, 26.21, 24.70. ESI-HRMS: calcd for $C_{21}H_{20}NO_5^+$ ([M+H$^+$]) 366.1336, found 366.1335.

methyl 6-hydroxy-1-oxo-9-(*p*-tolyl)-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4j**



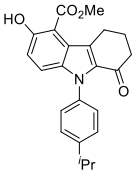
(**$C_{21}H_{19}NO_4$**) The title compound **4j** was obtained as a yellow solid in 30.7 mg, 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.04 (s, 1H), 7.29 (d, *J* = 8.3 Hz, 2H), 7.20 (d, *J* = 9.2 Hz, 1H), 7.16 – 7.11 (m, 2H), 6.97 (d, *J* = 9.2 Hz, 1H), 4.05 (s, 3H), 3.16 (t, *J* = 6.1 Hz, 2H), 2.59 (dd, *J* = 7.4, 5.6 Hz, 2H), 2.45 (s, 3H), 2.16 (dt, *J* = 12.6, 6.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.78, 171.02, 159.45, 138.08, 135.53, 135.23, 132.64, 129.71, 128.63, 127.59, 121.80, 119.92, 118.53, 103.98, 51.83, 39.22, 26.23, 24.70, 21.29. ESI-HRMS: calcd for $C_{21}H_{19}NO_4^+$ ([M+H$^+$]) 350.1387, found 350.1382.

methyl 9-(4-ethylphenyl)-6-hydroxy-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4k**



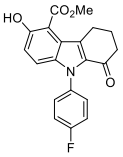
(**$C_{22}H_{21}NO_4$**) The title compound **4k** was obtained as a white solid in 34.0 mg, 94% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.04 (s, 1H), 7.34 – 7.29 (m, 2H), 7.22 (d, *J* = 9.1 Hz, 1H), 7.19 – 7.14 (m, 2H), 6.97 (d, *J* = 9.2 Hz, 1H), 4.05 (s, 3H), 3.16 (t, *J* = 6.1 Hz, 2H), 2.75 (q, *J* = 7.6 Hz, 2H), 2.59 (dd, *J* = 7.5, 5.5 Hz, 2H), 2.22 – 2.11 (m, 2H), 1.32 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.79, 171.02, 159.45, 144.22, 135.56, 135.38, 132.64, 128.63, 128.45, 127.64, 121.79, 119.99, 118.52, 103.97, 51.82, 39.21, 28.57, 26.23, 24.70, 15.33. ESI-HRMS: calcd for $C_{22}H_{22}NO_4^+$ ([M+H$^+$]) 364.1543, found 364.1563.

methyl 6-hydroxy-9-(4-isopropylphenyl)-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4l**



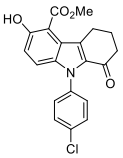
(**$C_{23}H_{23}NO_4$**) The title compound **4l** was obtained as a yellow solid in 33.6 mg, 89% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.05 (s, 1H), 7.37 – 7.33 (m, 2H), 7.24 (d, *J* = 9.1 Hz, 1H), 7.20 – 7.15 (m, 2H), 6.98 (d, *J* = 9.2 Hz, 1H), 4.06 (s, 3H), 3.18 (t, *J* = 6.1 Hz, 2H), 3.07 – 2.98 (m, 1H), 2.60 (dd, *J* = 7.3, 5.7 Hz, 2H), 2.22 – 2.13 (m, 2H), 1.34 (s, 3H), 1.33 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.83, 171.04, 159.47, 148.78, 135.59, 135.42, 132.65, 128.65, 127.64, 127.03, 121.80, 120.06, 118.53, 103.97, 51.84, 39.20, 33.87, 26.24, 24.71, 23.98. ESI-HRMS: calcd for $C_{23}H_{24}NO_4^+$ ([M+H$^+$]) 378.1700, found 378.1692.

methyl 9-(4-fluorophenyl)-6-hydroxy-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4m**



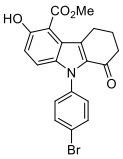
(**$C_{20}H_{16}FNO_4$**) The title compound **4m** was obtained as a yellow solid in 32.1 mg, 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.03 (s, 1H), 7.27 – 7.12 (m, 5H), 6.99 (d, *J* = 9.1 Hz, 1H), 4.05 (s, 3H), 3.16 (t, *J* = 6.1 Hz, 2H), 2.59 (dd, *J* = 7.4, 5.6 Hz, 2H), 2.22 – 2.11 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.87, 170.92, 163.38, 160.91, 159.49, 135.49, 133.84, 133.80, 132.58, 129.66, 129.58, 129.00, 121.97, 119.52, 118.83, 116.13, 115.90, 104.13, 51.88, 39.13, 26.18, 24.65. ESI-HRMS: calcd for $C_{20}H_{17}FNO_4^+$ ([M+H$^+$]) 354.1136, found 354.1118.

methyl 9-(4-chlorophenyl)-6-hydroxy-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4n**



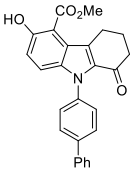
(**$C_{20}H_{16}ClNO_4$**) The title compound **4n** was obtained as a yellowish solid in 34.5 mg, 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.02 (s, 1H), 7.49 – 7.42 (m, 2H), 7.23 – 7.13 (m, 3H), 6.99 (d, *J* = 9.2 Hz, 1H), 4.05 (s, 3H), 3.16 (t, *J* = 6.0 Hz, 2H), 2.59 (dd, *J* = 7.2, 5.8 Hz, 2H), 2.22 – 2.12 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.80, 170.87, 159.51, 136.40, 135.26, 134.04, 132.48, 129.28, 129.25, 122.13, 119.44, 118.91, 104.19, 51.89, 39.09, 26.19, 24.62. ESI-HRMS: calcd for $C_{20}H_{17}{}^{35}ClNO_4^+$ ([M+H$^+$]) 370.0841, found 370.0874.

methyl 9-(4-bromophenyl)-6-hydroxy-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4o**



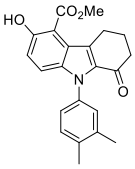
(**$C_{20}H_{16}BrNO_4$**) The title compound **4o** was obtained as a yellow solid in 37.9 mg, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.02 (s, 1H), 7.65 – 7.57 (m, 2H), 7.20 – 7.11 (m, 3H), 6.99 (d, *J* = 9.2 Hz, 1H), 4.05 (s, 3H), 3.15 (t, *J* = 6.0 Hz, 2H), 2.59 (dd, *J* = 7.4, 5.6 Hz, 2H), 2.21 – 2.11 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.79, 170.86, 159.51, 136.92, 135.19, 132.44, 132.26, 129.58, 129.33, 122.16, 122.09, 119.44, 118.93, 104.20, 51.90, 39.08, 26.19, 24.62. ESI-HRMS: calcd for $C_{20}H_{17}{}^{79}BrNO_4^+$ ([M+H$^+$]) 414.0335, found 414.0301.

methyl 9-([1,1'-biphenyl]-4-yl)-6-hydroxy-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4p**



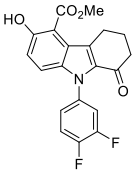
(**$C_{26}H_{21}NO_4$**) The title compound **4p** was obtained as a yellow solid in 37.0 mg, 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.06 (s, 1H), 7.75 – 7.63 (m, 4H), 7.52 – 7.45 (m, 2H), 7.42 – 7.31 (m, 3H), 7.28 (t, *J* = 8.5 Hz, 1H), 7.01 (d, *J* = 9.2 Hz, 1H), 4.07 (s, 3H), 3.19 (t, *J* = 6.0 Hz, 2H), 2.67 – 2.57 (m, 2H), 2.27 – 2.13 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.87, 170.99, 159.52, 141.07, 140.29, 137.02, 135.47, 132.62, 129.06, 128.85, 128.21, 127.73, 127.59, 127.23, 122.03, 119.89, 118.74, 104.10, 51.88, 39.20, 26.26, 24.69. ESI-HRMS: calcd for $C_{26}H_{22}NO_4^+$ ([M+H$^+$]) 412.1543, found 412.1577.

methyl 9-(3,4-dimethylphenyl)-6-hydroxy-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4q**



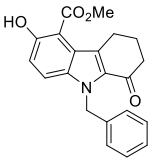
(**$C_{22}H_{21}NO_4$**) The title compound **4q** was obtained as a yellow solid in 33.0 mg, 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.04 (s, 1H), 7.22 (dd, *J* = 12.2, 8.5 Hz, 2H), 7.04 – 6.94 (m, 3H), 4.05 (s, 3H), 3.16 (t, *J* = 6.1 Hz, 2H), 2.59 (dd, *J* = 7.4, 5.6 Hz, 2H), 2.34 (s, 3H), 2.30 (s, 3H), 2.21 – 2.12 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.76, 171.05, 159.44, 137.41, 136.74, 135.61, 135.47, 132.67, 130.15, 128.71, 128.50, 125.08, 121.72, 120.06, 118.45, 103.93, 51.80, 39.24, 26.23, 24.71, 19.91, 19.59. ESI-HRMS: calcd for $C_{22}H_{22}NO_4^+$ ([M+H$^+$]) 364.1543, found 364.1563.

methyl 9-(3,4-difluorophenyl)-6-hydroxy-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4r**



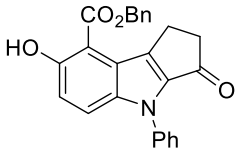
(**$C_{20}H_{15}F_2NO_4$**) The title compound **4r** was obtained as a white solid in 29.8 mg, 80% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.03 (s, 1H), 7.32 – 7.27 (m, 1H), 7.18 (d, *J* = 9.1 Hz, 1H), 7.15 – 7.10 (m, 1H), 7.06 – 7.00 (m, 2H), 4.07 (s, 3H), 3.17 (t, *J* = 6.1 Hz, 2H), 2.65 – 2.56 (m, 2H), 2.23 – 2.14 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.81, 170.83, 159.56, 151.17, 149.17, 149.06, 135.28, 134.12, 132.49, 129.47, 124.44, 124.41, 124.39, 124.36, 122.18, 119.21, 119.11, 117.78, 117.64, 117.48, 117.34, 104.30, 51.93, 39.03, 26.16, 24.60. ESI-HRMS: calcd for $C_{20}H_{16}F_2NO_4^+$ ([M+H$^+$]) 372.1042, found 372.1060.

methyl 9-benzyl-6-hydroxy-1-oxo-2,3,4,9-tetrahydro-1*H*-carbazole-5-carboxylate **4s**



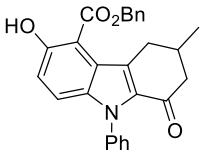
(**$C_{21}H_{19}NO_4$**) The title compound **4s** was obtained as a yellowish solid in 10.8 mg, 31% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.98 (s, 1H), 7.47 (d, *J* = 9.2 Hz, 1H), 7.27 – 7.18 (m, 3H), 7.08 – 6.95 (m, 3H), 5.87 (s, 2H), 4.03 (s, 3H), 3.12 (t, *J* = 6.1 Hz, 2H), 2.63 (dd, *J* = 7.5, 5.5 Hz, 2H), 2.18 – 2.09 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.69, 170.95, 159.13, 137.97, 134.23, 131.49, 128.59, 128.31, 127.23, 126.35, 121.81, 118.99, 118.61, 104.31, 51.79, 47.84, 39.57, 26.25, 24.75. ESI-HRMS: calcd for $C_{21}H_{20}NO_4^+$ ([M+H$^+$]) 350.1387, found 350.1382.

benzyl 7-hydroxy-3-oxo-4-phenyl-1,2,3,4-tetrahydrocyclopenta[b]indole-8-carboxylate **4t**



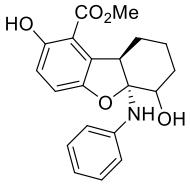
(**$C_{25}H_{19}NO_4$**) The title compound **4t** was obtained as a yellowish solid in 7.9 mg (0.05 mmol scale), 40% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.55 (s, 1H), 7.57 (d, *J* = 9.2 Hz, 1H), 7.51 (tt, *J* = 4.0, 2.1 Hz, 4H), 7.45 – 7.36 (m, 6H), 7.05 (d, *J* = 9.2 Hz, 1H), 5.54 (s, 2H), 3.10 – 3.04 (m, 2H), 2.85 – 2.80 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.90, 170.80, 160.31, 145.14, 138.88, 135.44, 135.05, 129.25, 129.06, 128.86, 128.79, 127.90, 126.47, 120.70, 120.64, 119.05, 103.59, 67.21, 41.18, 23.91.

benzyl 6-hydroxy-3-methyl-1-oxo-9-phenyl-2,3,4,9-tetrahydro-1H-carbazole-5-carboxylate **4u**

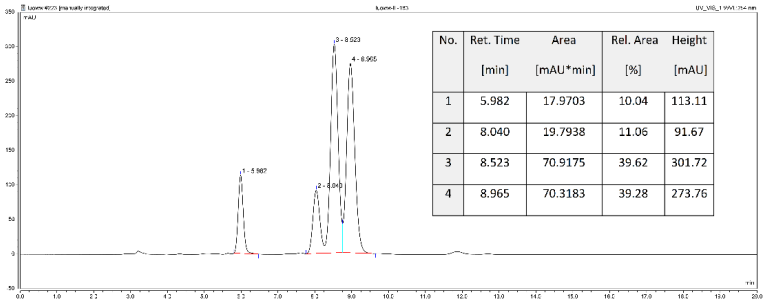


(**$C_{27}H_{23}NO_4$**) The title compound **4u** was obtained as a yellow syrup in 20.3 mg, 48% yield (First run: flash column chromatography conditions: hexane/EtOAc = 1:6; Second run: preparative thin layer chromatography conditions: hexane/acetone = 1/4). ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.18 (s, 1H), 7.56 – 7.39 (m, 7H), 7.26 – 7.22 (m, 2H), 7.20 (d, *J* = 9.2 Hz, 1H), 6.99 (d, *J* = 9.1 Hz, 1H), 5.53 (d, *J* = 11.8 Hz, 1H), 5.47 (d, *J* = 11.8 Hz, 1H), 3.08 – 3.01 (m, 1H), 2.51 – 2.42 (m, 2H), 2.23 (dd, *J* = 19.9, 8.0 Hz, 2H), 0.94 (d, *J* = 6.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.53, 170.65, 159.83, 137.79, 135.68, 134.71, 132.39, 129.71, 129.01, 128.98, 128.83, 128.62, 128.21, 127.92, 121.73, 119.90, 118.65, 104.25, 67.69, 47.20, 35.36, 32.03, 21.38.

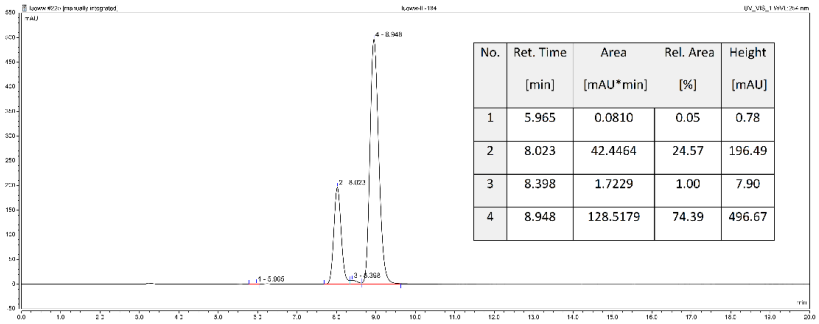
methyl (5aS,9aR)-2,6-dihydroxy-5a-(phenylamino)-5a,6,7,8,9,9a-hexahydrodibenzo[b,d]furan-1-carboxylate **5**



(**$C_{20}H_{21}NO_5$**) The title compound **5** was obtained as a yellow syrup in 65.9 mg, 93% yield, 75:25 d.r., 97/99% *ee*. $[\alpha]_D^{25}$ = -194.4 (*c* 0.60 in $CHCl_3$). HPLC analysis: Chiralcel IC, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 6.0 min, t_2 = 8.0 min, t_3 = 8.4 min, t_4 = 8.9 min. ^{1}H NMR of the major diastereomer (500 MHz, $CDCl_3$) δ10.50 (s, 1H), 7.22 – 7.10 (m, 2H), 7.00 – 6.88 (m, 2H), 6.86 – 6.72 (m, 3H), 4.90 (s, 1H), 4.25 (dd, *J* = 9.3, 4.4 Hz, 1H), 3.95 (s, 3H), 3.91 (dd, *J* = 7.5, 5.3 Hz, 1H), 2.46 (s, 1H), 2.05 – 1.97 (m, 1H), 1.96 – 1.86 (m, 1H), 1.81 – 1.42 (m, 4H). ^{13}C NMR of the major diastereomer (126 MHz, $CDCl_3$) δ 170.24, 156.60, 150.87, 142.92, 130.94, 129.06, 120.45, 119.27, 118.43, 117.61, 117.36, 109.04, 99.96, 70.47, 52.30, 48.06, 25.70, 25.13, 17.88. ESI-HRMS: calcd for $C_{20}H_{22}NO_5^+$ ([M+H$^+$]) 356.1492, found 356.1523.

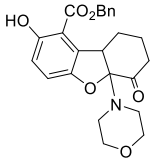


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	5.982	17.9703	10.04	113.11
2	8.040	19.7938	11.06	91.67
3	8.523	70.9175	39.62	301.72
4	8.965	70.3183	39.28	273.76

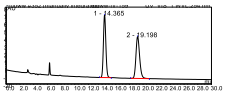


No.	Ret. Time [min]	Area [mAU*min]	Rel. Area [%]	Height [mAU]
1	5.965	0.0810	0.05	0.78
2	8.023	42.4464	24.57	196.49
3	8.398	1.7229	1.00	7.90
4	8.948	128.5179	74.39	496.67

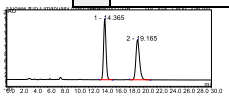
benzyl 2-hydroxy-5a-morpholino-6-oxo-5a,6,7,8,9,9a-hexahydrodibenzo[b,d]furan-1-carboxylate **6**



(**$C_{24}H_{25}NO_6$**) The title compound **6** was obtained as a yellow syrup in 27.3 mg, 65% yield, >95:5 d.r., 0% *ee*. HPLC analysis: Chiralcel IC, n-hexane/2-propanol = 70/30, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 14.4 min, t_2 = 19.2 min. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.48 (s, 1H), 7.49 – 7.36 (m, 5H), 7.05 (d, *J* = 8.9 Hz, 1H), 6.83 (d, *J* = 8.7 Hz, 1H), 5.49 (d, *J* = 11.7 Hz, 1H), 5.28 (d, *J* = 11.7 Hz, 1H), 3.86 (dd, *J* = 10.7, 4.2 Hz, 1H), 3.68 – 3.57 (m, 4H), 2.77 – 2.64 (m, 3H), 2.47 – 2.31 (m, 3H), 1.82 (ddd, *J* = 13.4, 8.8, 4.3 Hz, 1H), 1.76 – 1.67 (m, 1H), 1.64 – 1.53 (m, 1H), 1.18 (ddd, *J* = 15.1, 9.1, 4.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 206.96, 169.25, 156.97, 151.80, 134.41, 129.18, 129.17, 128.94, 127.74, 117.99, 117.38, 107.98, 104.40, 67.83, 66.84, 51.26, 46.50, 34.81, 27.46, 20.37.

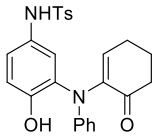


	Retention Time	Area	% Area	Height
1	14.365	34.0645	49.89	81.83
2	19.198	34.2156	50.11	54.73



	Retention Time	Area	% Area	Height
1	14.365	72.5150	50.65	173.52
2	19.165	70.6633	49.35	114.25

N-(4-hydroxy-3-((6-oxocyclohex-1-en-1-yl)(phenyl)amino)phenyl)-4-methylbenzenesulfonamide **7**



(**$C_{25}H_{24}N_2O_4S$**) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.3 Hz, 2H), 7.26 (dd, *J* = 4.5, 3.9 Hz, 2H), 7.15 – 7.04 (m, 4H), 6.95 – 6.88 (m, 2H), 6.74 – 6.68 (m, 2H), 6.43 (t, *J* = 4.7 Hz, 1H), 6.37 (s, 1H), 6.13 (s, 1H), 2.59 – 2.51 (m, 2H), 2.49 – 2.32 (m, 5H), 2.00 (dt, *J* = 12.5, 6.1 Hz, 2H).

15. References

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4. Gaussian 16, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.
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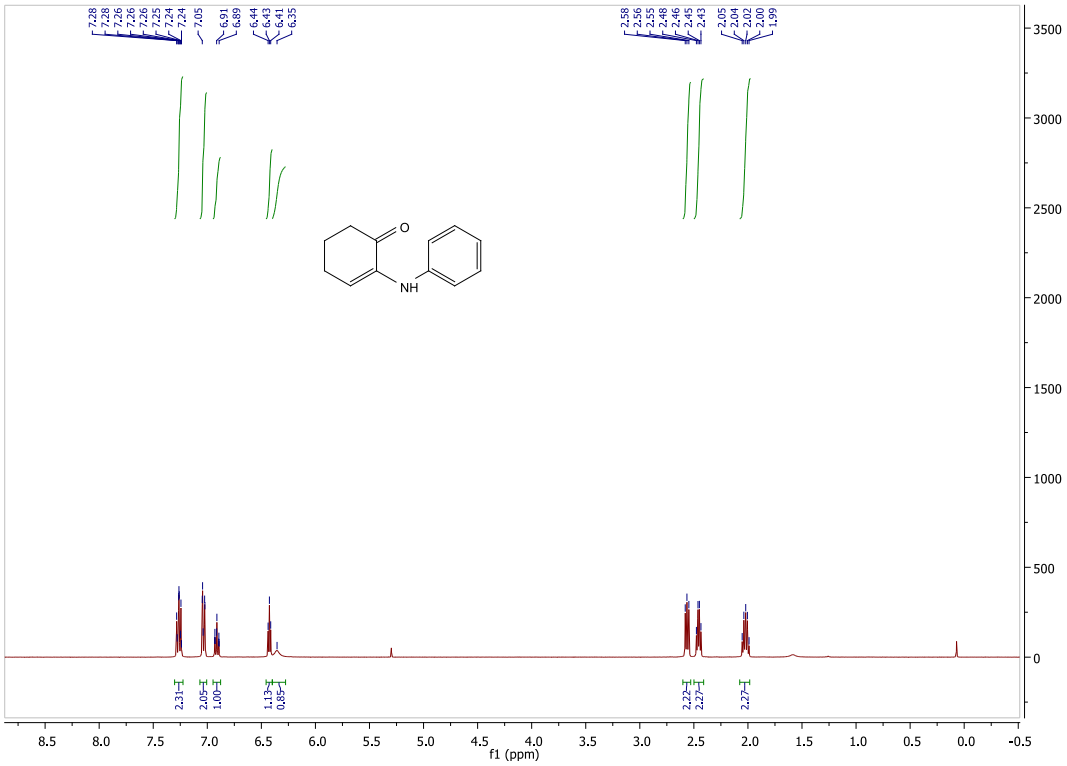
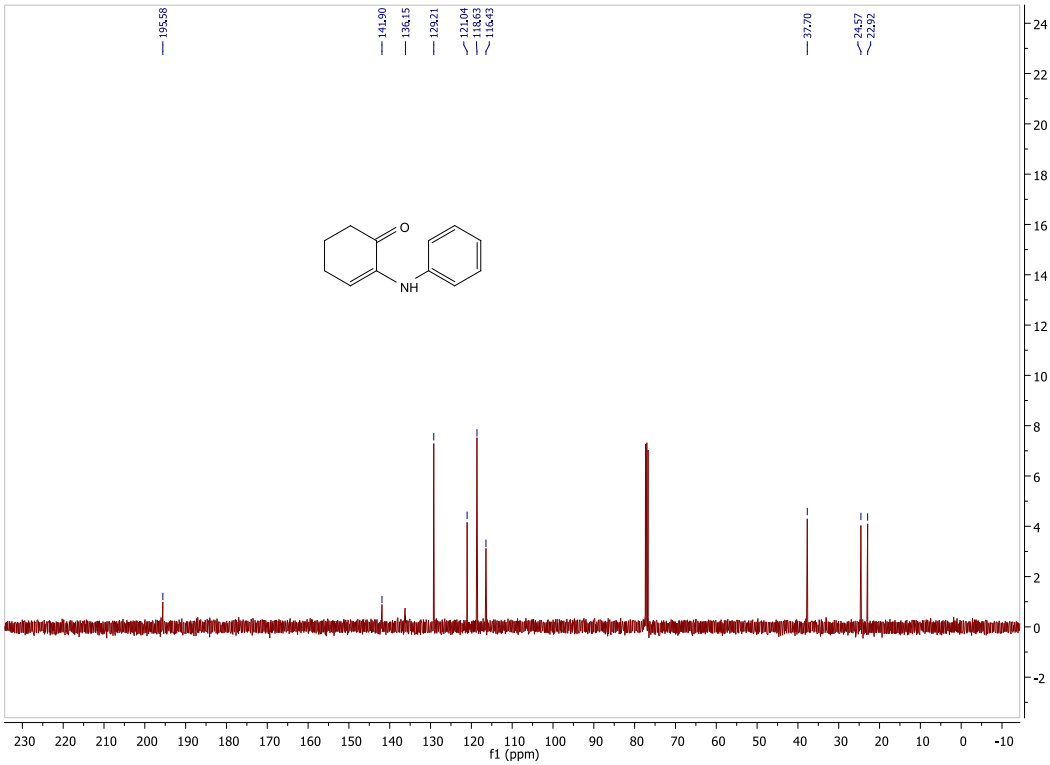
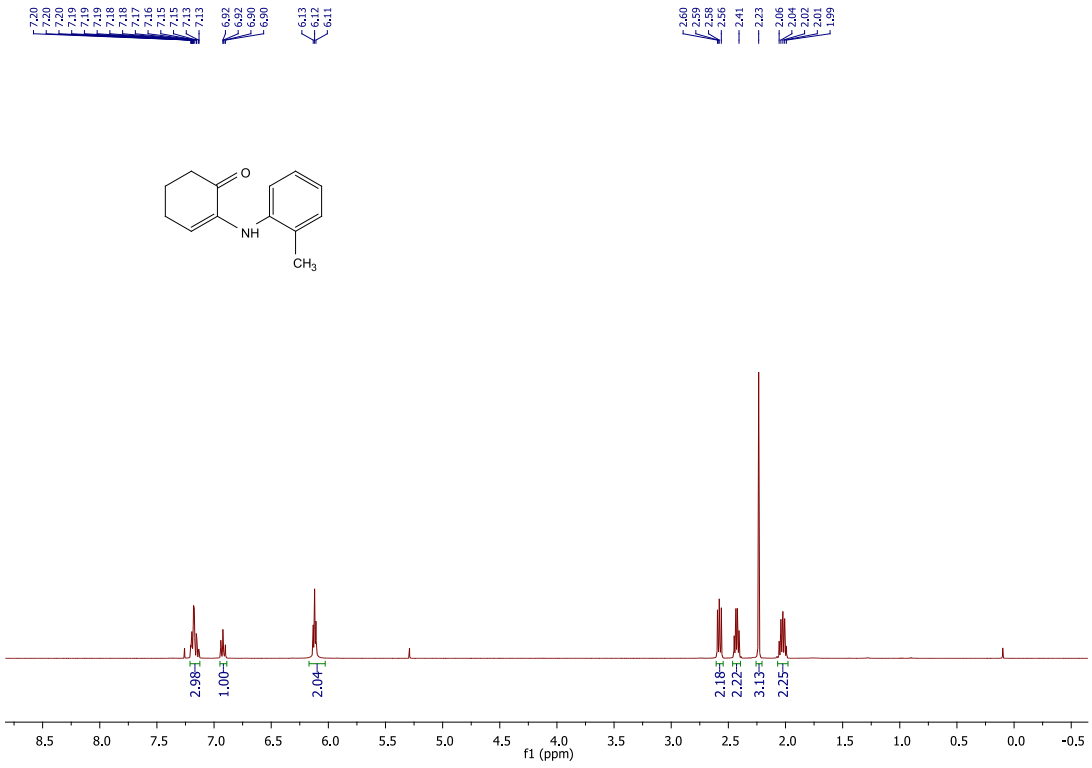
16. Copies of NMR spectra






7.20
7.20
7.20
7.19
7.19
7.19
7.18
7.18
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6.92
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6.90
6.90
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6.11
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2.41
2.23
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2.02
2.01
1.99
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NH
CH3
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2.04
2.18
2.22
3.13
2.25
8.5
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7.0
6.5
6.0
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5.0
4.5
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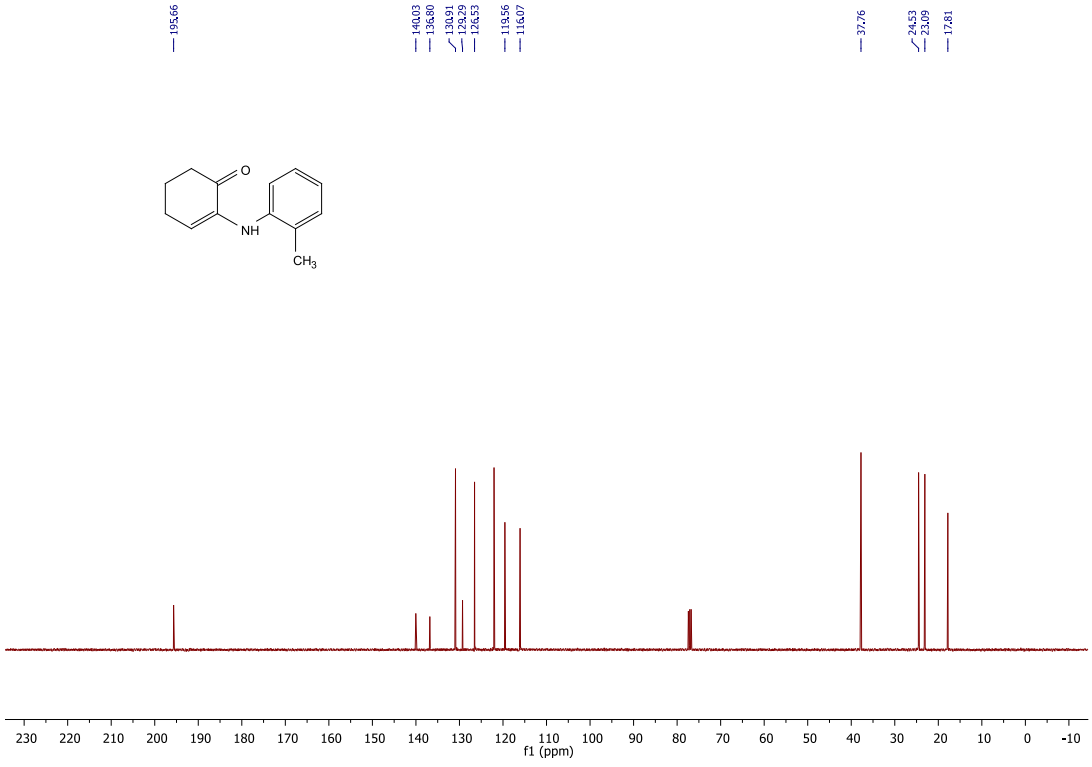
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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140.03
136.80
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126.53
119.56
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24.53
23.09
17.81
O
NH
CH3
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.35
7.34
7.33
7.32
7.27
7.27
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7.25
7.17
7.16
7.15
7.15
7.14
7.13
7.13
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6.78
6.45
6.44
6.42


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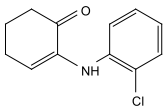
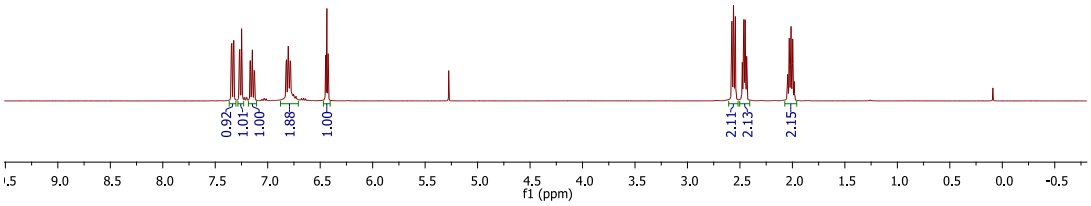

O
NH
Cl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2.13
2.15
f1 (ppm)

195.13


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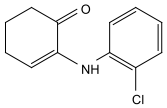
118.94
117.29


37.62
24.63
22.77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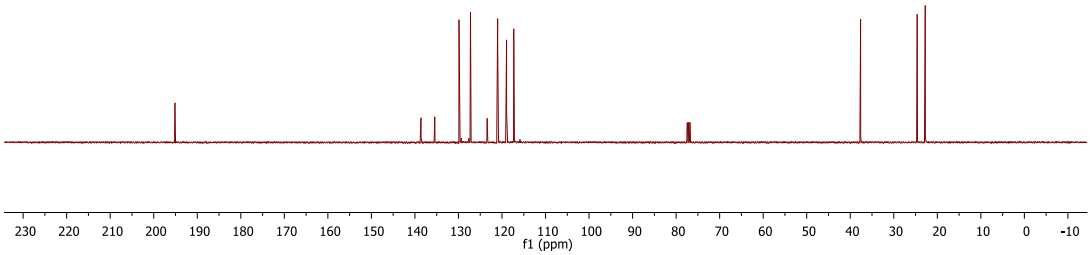
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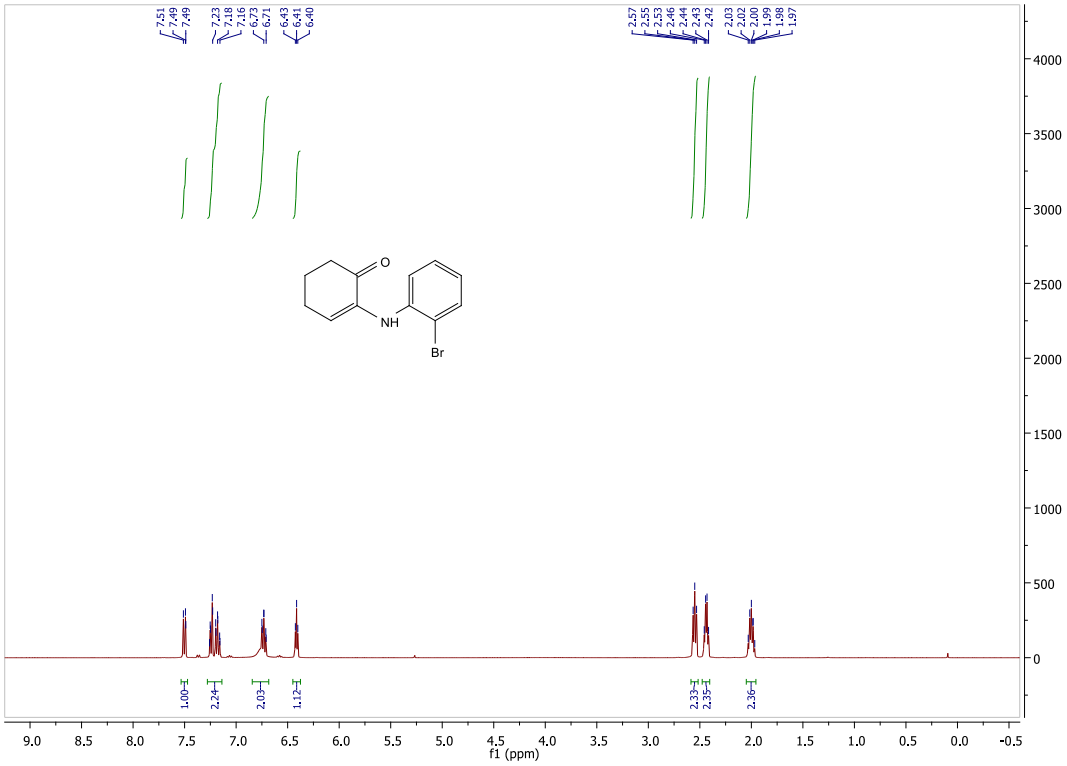
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2.57
2.55
2.53
2.46
2.44
2.43
2.42
2.03
2.02
2.00
1.99
1.98
1.97
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NH
Br
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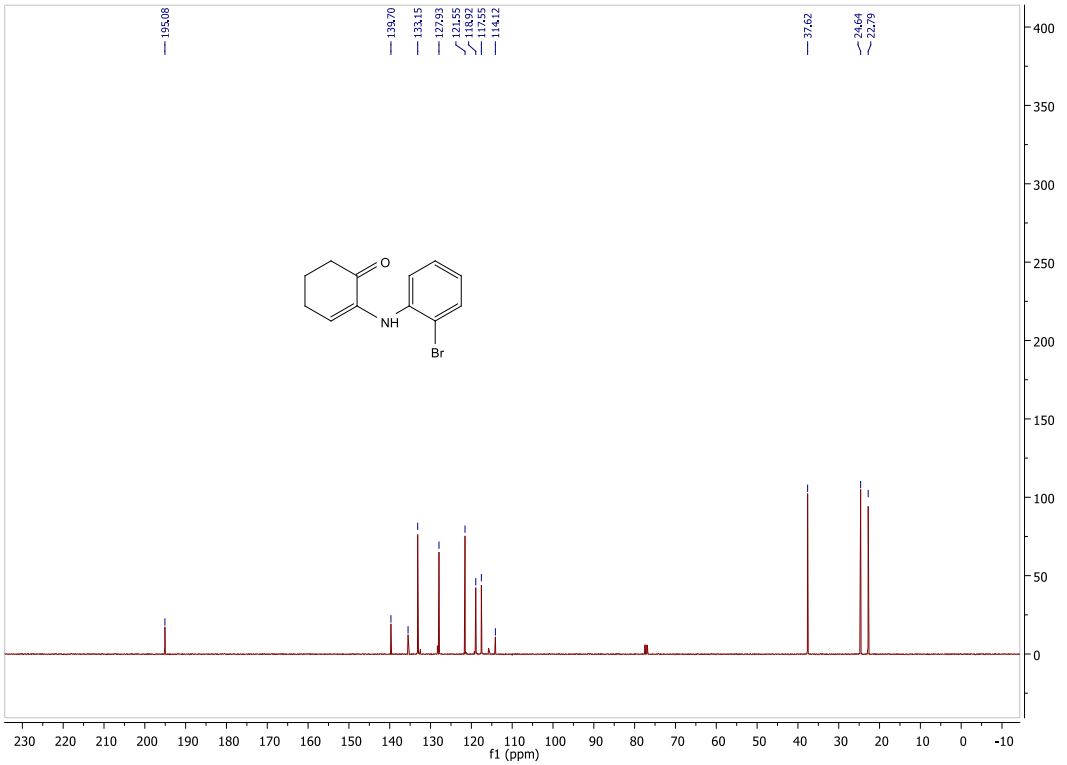
2.24
2.03
1.12
2.33
2.35
2.36
f1 (ppm)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114.12
37.62
24.64
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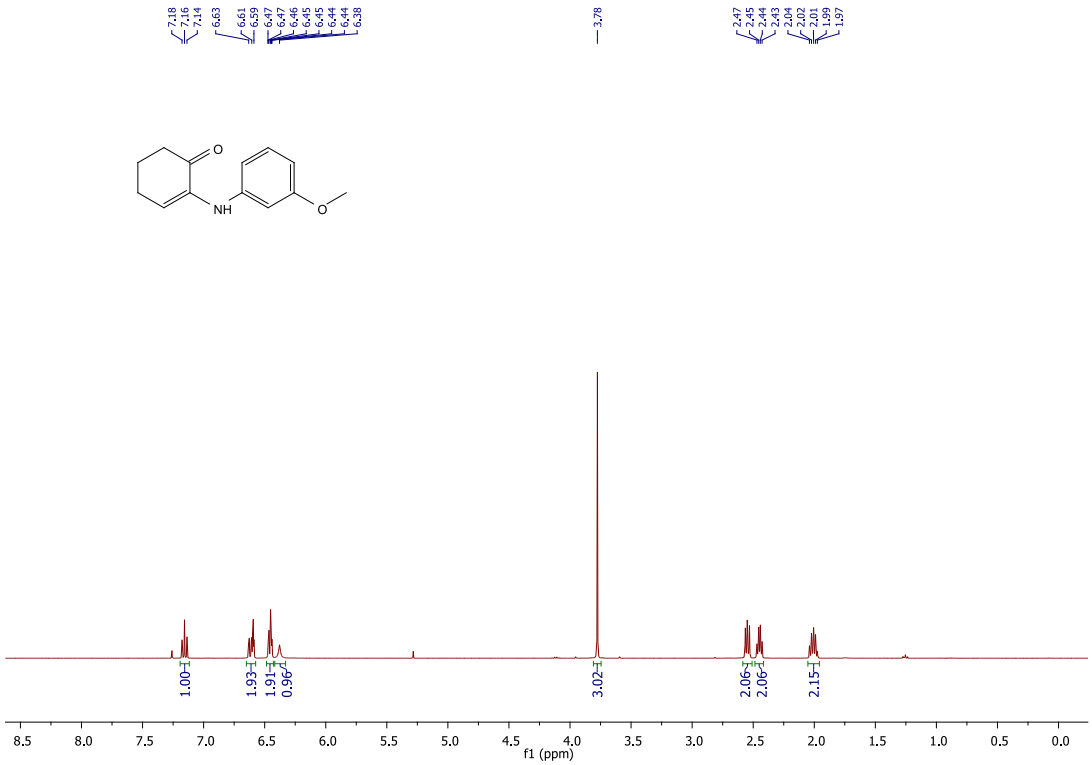
NH
Br
f1 (ppm)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6.47
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6.45
6.44
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3.78
2.47
2.45
2.44
2.43
2.04
2.02
2.01
1.99
1.97
O
NH
O
1.00
1.93
1.91
0.96
3.02
2.06
2.06
2.15
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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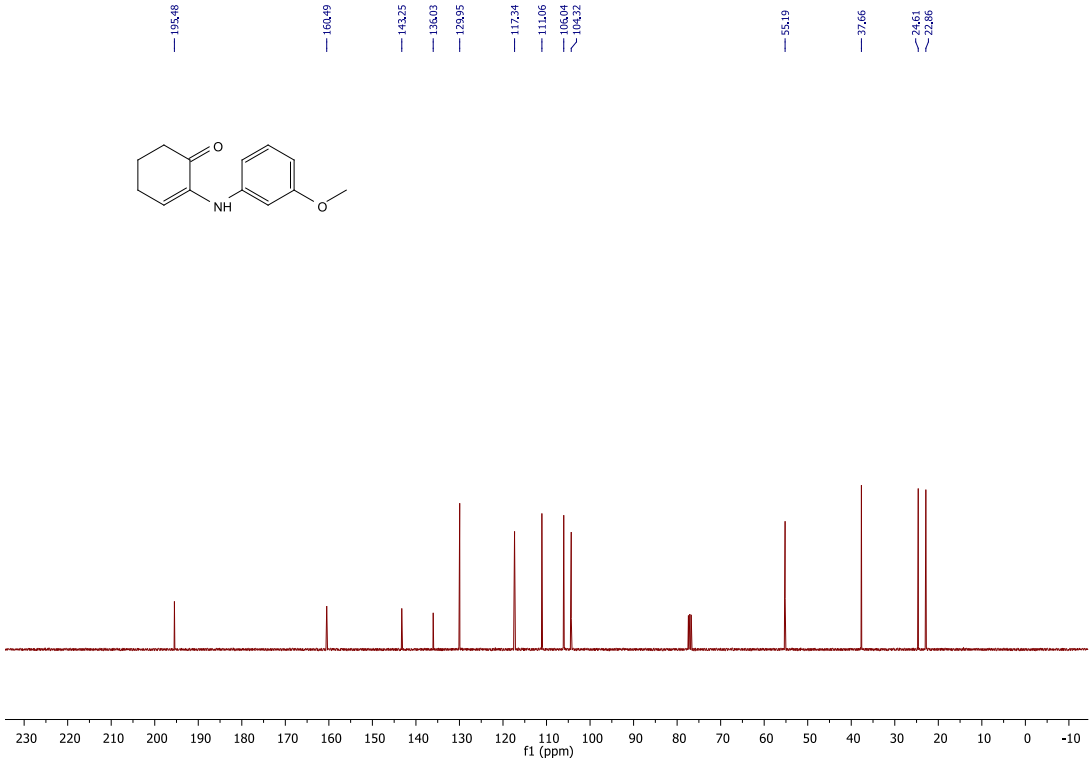
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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111.06
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24.61
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NH
O
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220
210
200
190
180
170
160
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120
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100
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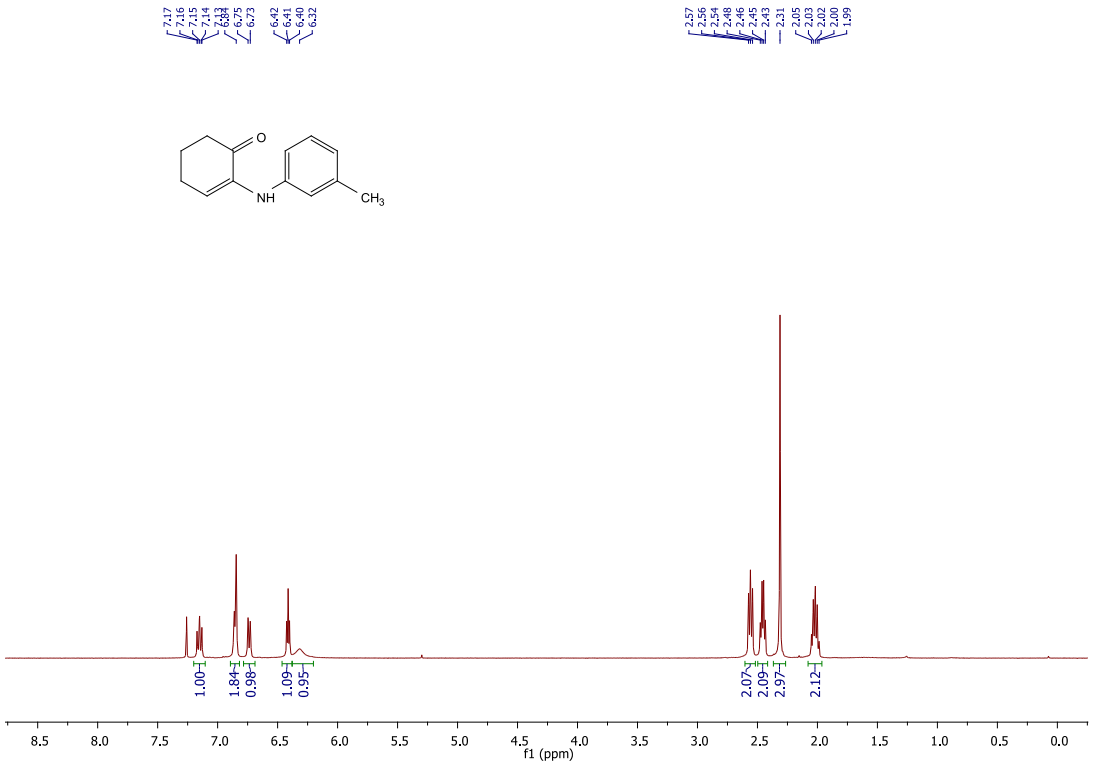
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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6.32
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2.56
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2.46
2.45
2.43
2.31
2.05
2.03
2.02
2.00
1.99
O
NH
CH3
1.00
1.84
0.98
1.09
0.95
2.07
2.09
2.97
2.12
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
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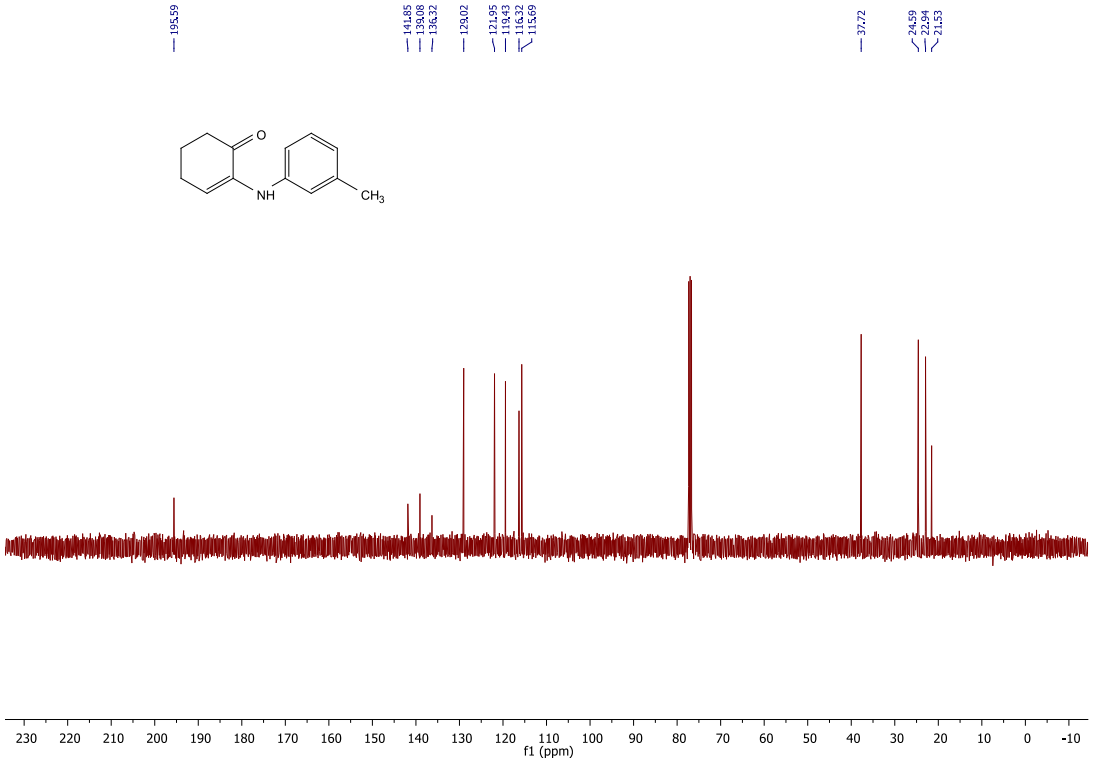
f1 (ppm)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24.59
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21.53
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NH
CH3
230
220
210
200
190
180
170
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100
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80
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60
50
40
30
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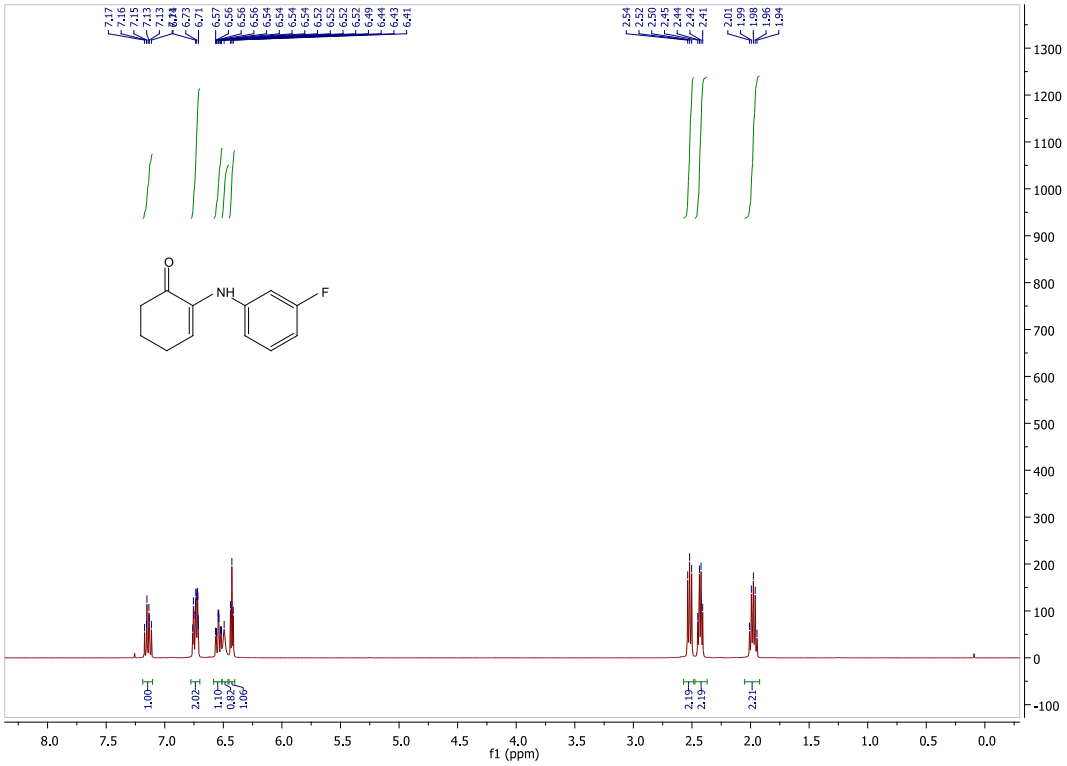
-10
f1 (ppm)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6.71
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6.56
6.56
6.56
6.54
6.54
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6.54
6.52
6.52
6.52
6.49
6.44
6.43
6.41
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2.52
2.50
2.45
2.44
2.42
2.41
2.01
1.99
1.98
1.96
1.94
O
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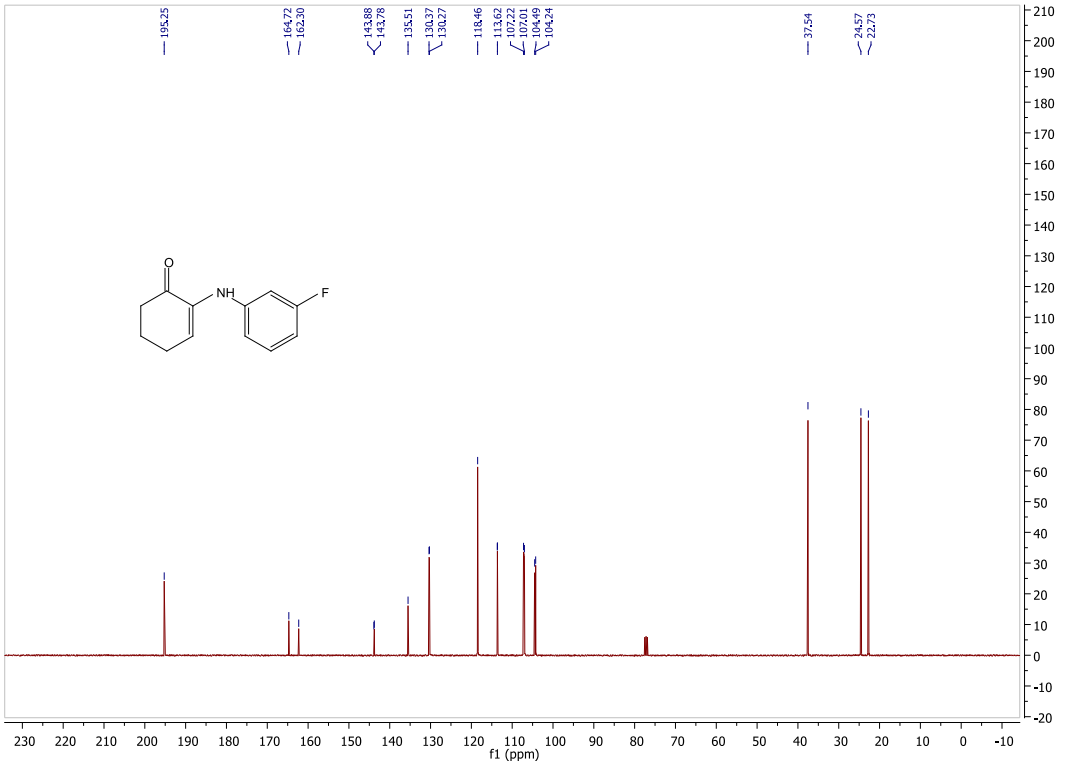
F
1.00
2.02
1.10
0.82
1.06
2.19
2.19
2.21
f1 (ppm)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162.30
143.88
143.78
135.51
130.37
130.27
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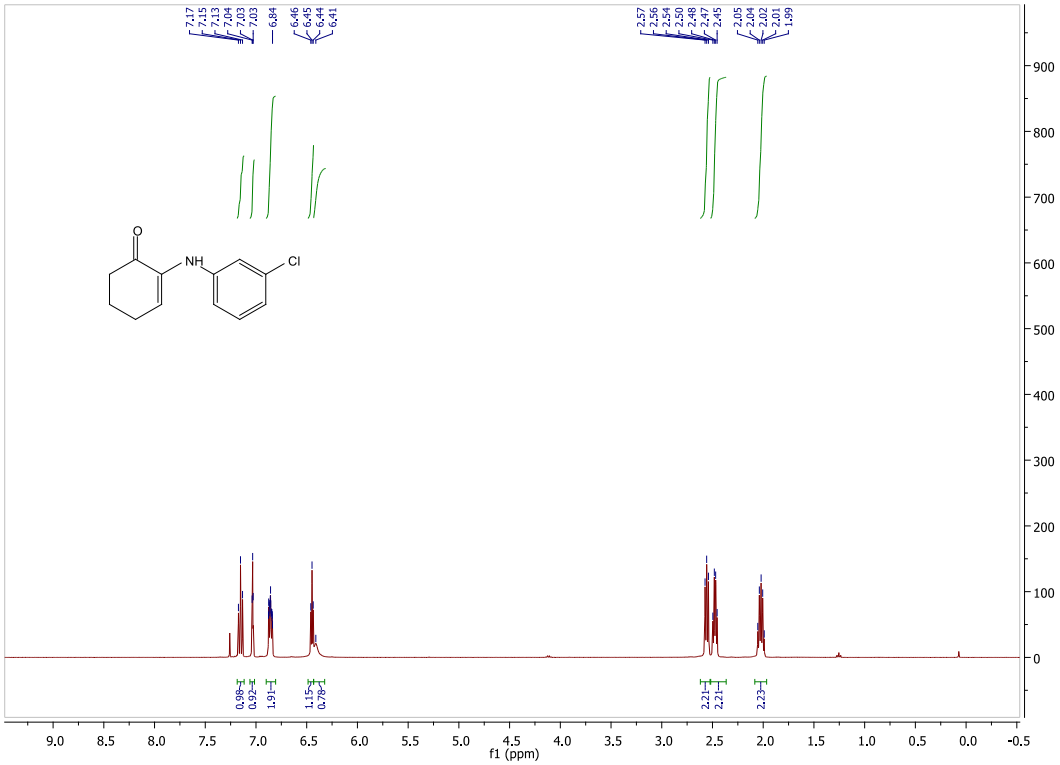
113.62
107.22
107.01
104.49
104.24
37.54
24.57
22.73
O
NH
F
f1 (ppm)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7.03
7.03
6.84
6.46
6.45
6.44
6.41
2.57
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2.54
2.50
2.48
2.47
2.45
2.05
2.04
2.02
2.01
1.99
O
NH
Cl
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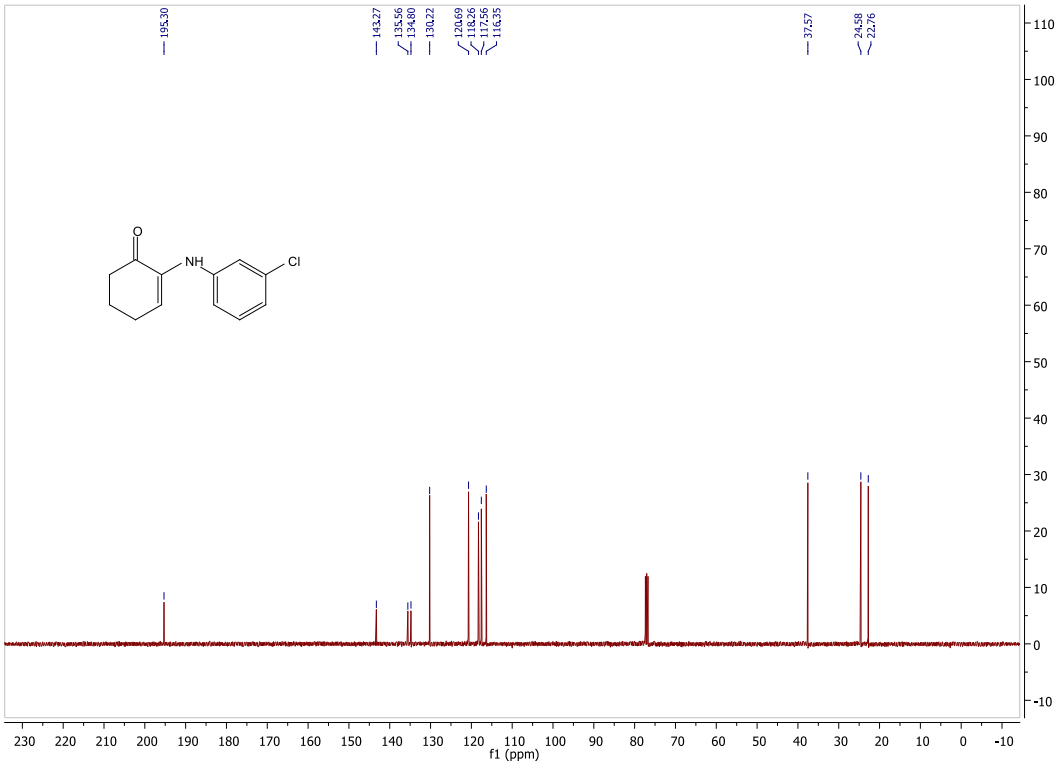
0.92
1.91
1.15
0.78
2.21
2.21
2.23
f1 (ppm)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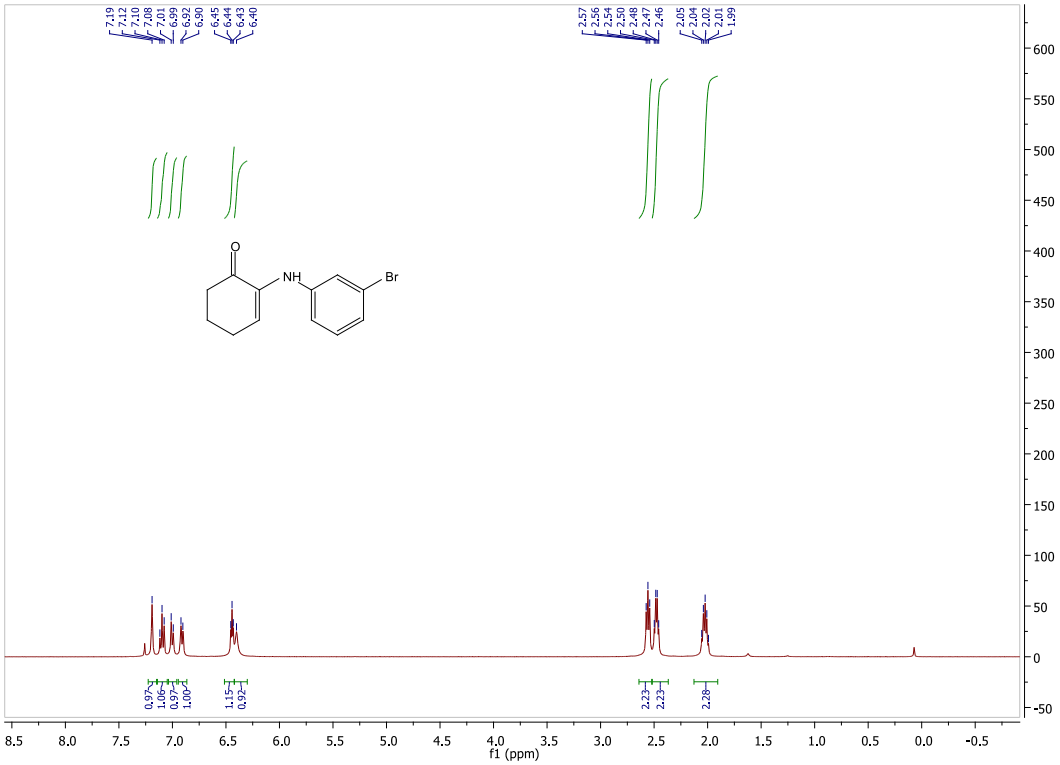
37.57
24.58
22.76
O
NH
Cl
f1 (ppm)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7.10
7.08
7.01
6.99
6.92
6.90
6.45
6.44
6.43
6.40
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2.56
2.54
2.50
2.48
2.47
2.46
2.05
2.04
2.02
2.01
1.99
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NH
Br
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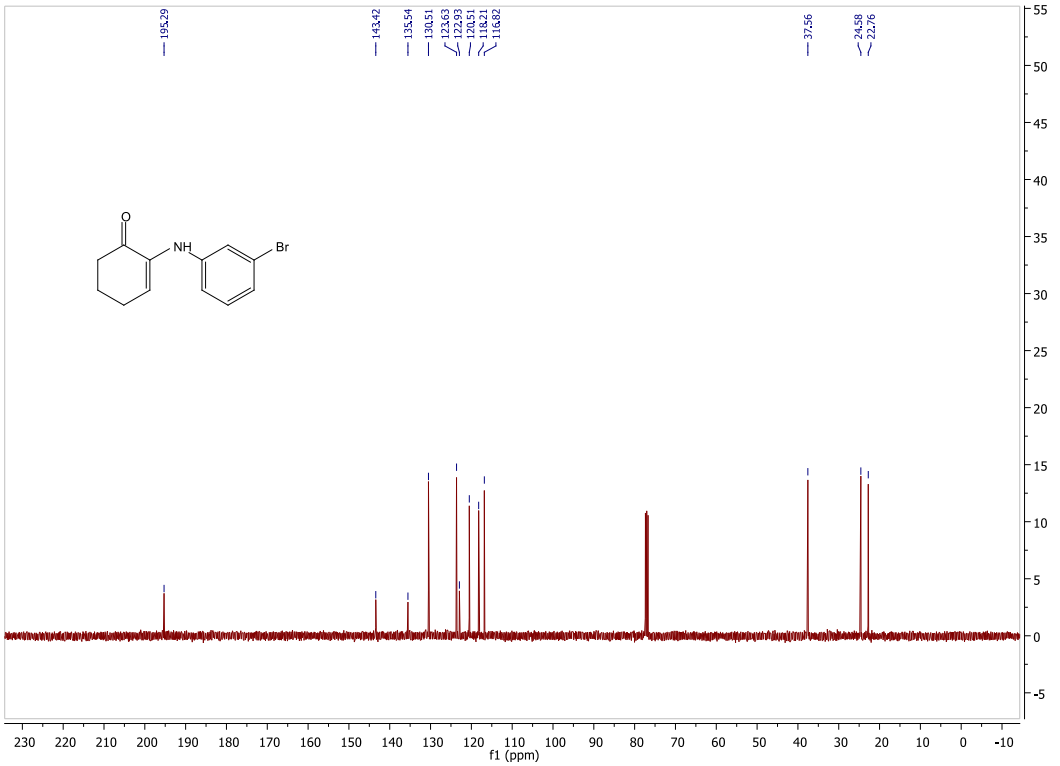
1.06
0.97
1.00
1.15
0.92
2.23
2.23
2.28
f1 (ppm)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143.42
135.54
130.51
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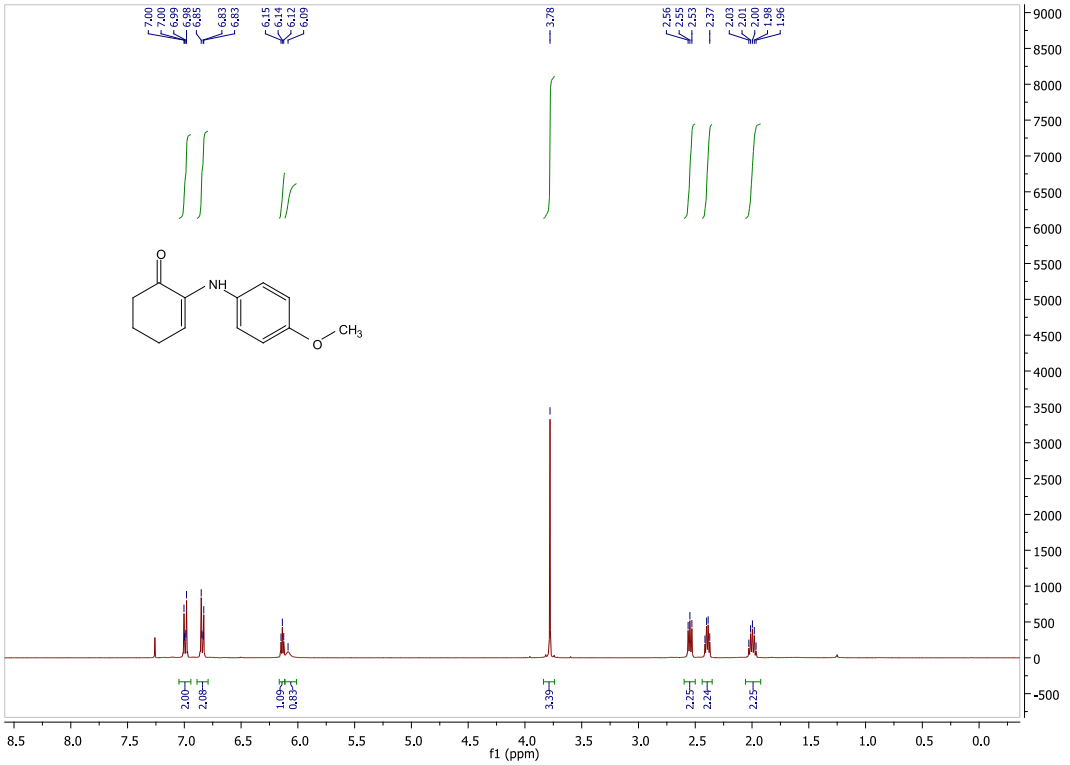
122.93
120.51
118.21
116.82
37.56
24.58
22.76
O
NH
Br
f1 (ppm)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6.83
6.15
6.14
6.12
6.09
3.78
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2.55
2.53
2.37
2.03
2.01
2.00
1.98
1.96
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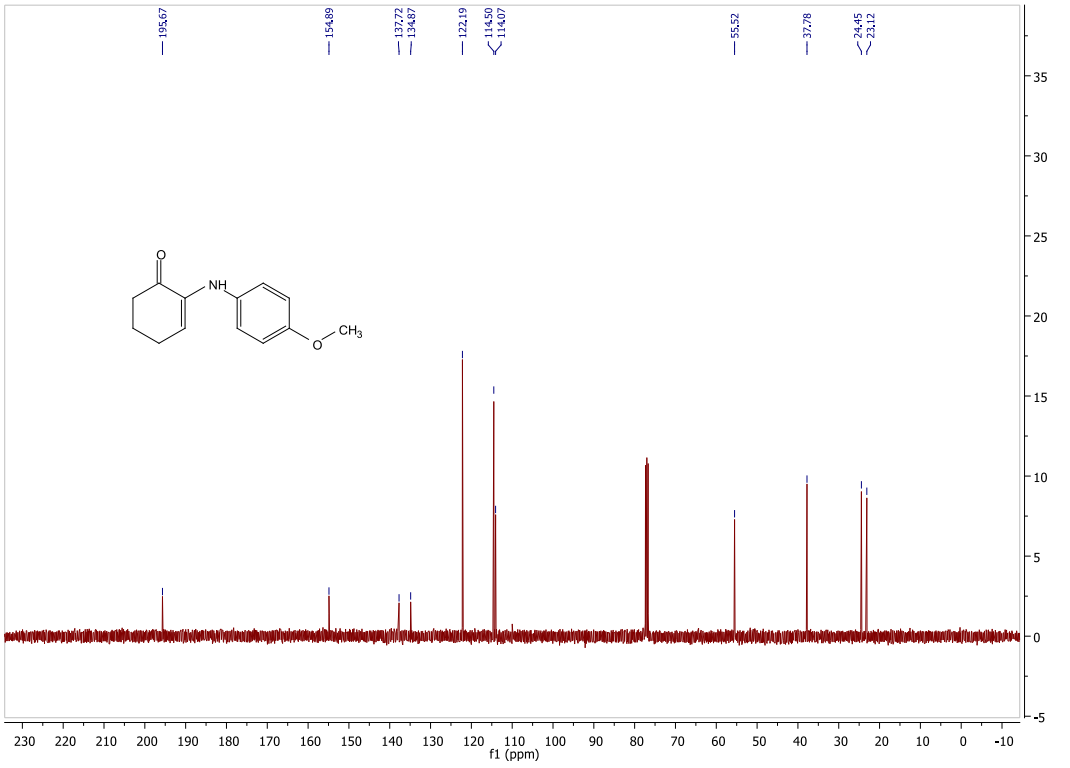
NH
O
CH3
2.00
2.08
1.09
0.83
3.39
2.25
2.24
2.25
f1 (ppm)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114.07
55.52
37.78
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23.12
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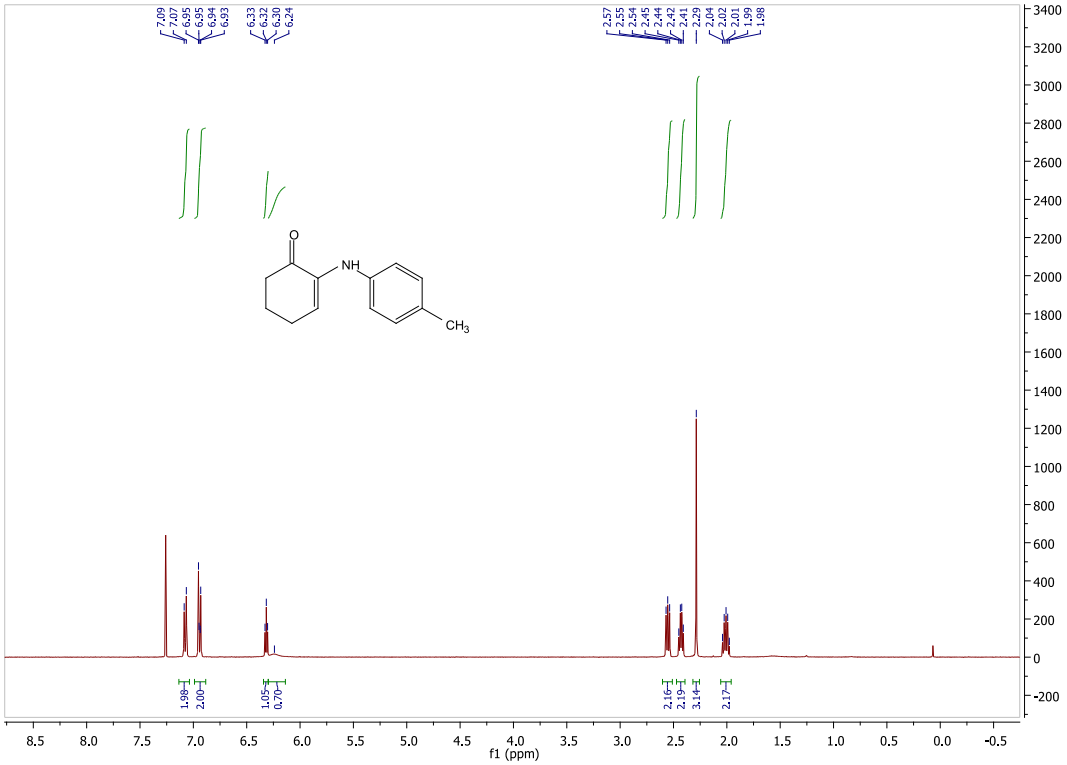
O
CH3
f1 (ppm)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7.07
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6.95
6.94
6.93
6.33
6.32
6.30
6.24
2.57
2.55
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2.45
2.44
2.42
2.41
2.29
2.04
2.02
2.01
1.99
1.98
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CH3
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2.00
1.05
0.70
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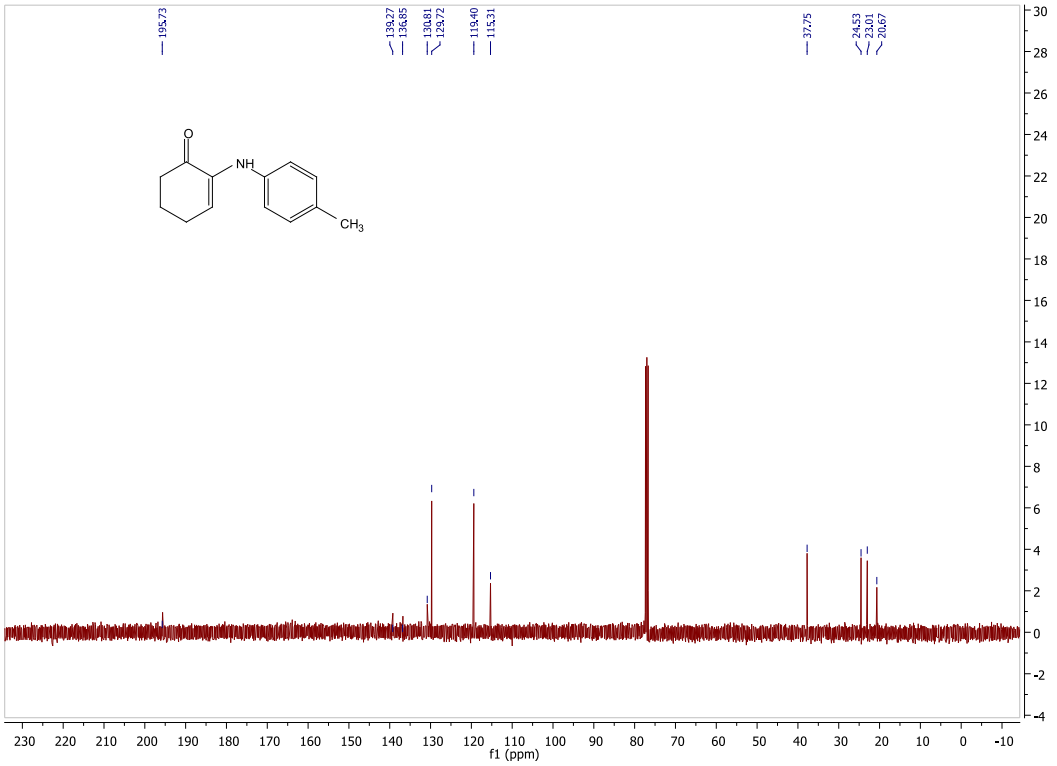
2.19
3.14
2.17
f1 (ppm)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23.01
20.67
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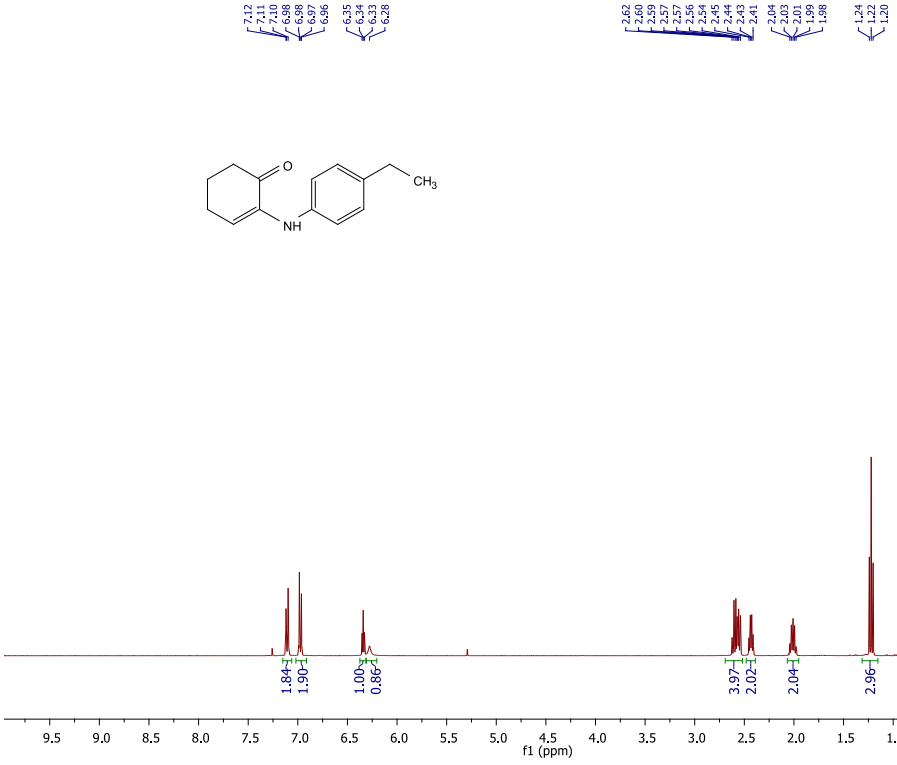
CH3
f1 (ppm)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6.97
6.96
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6.28
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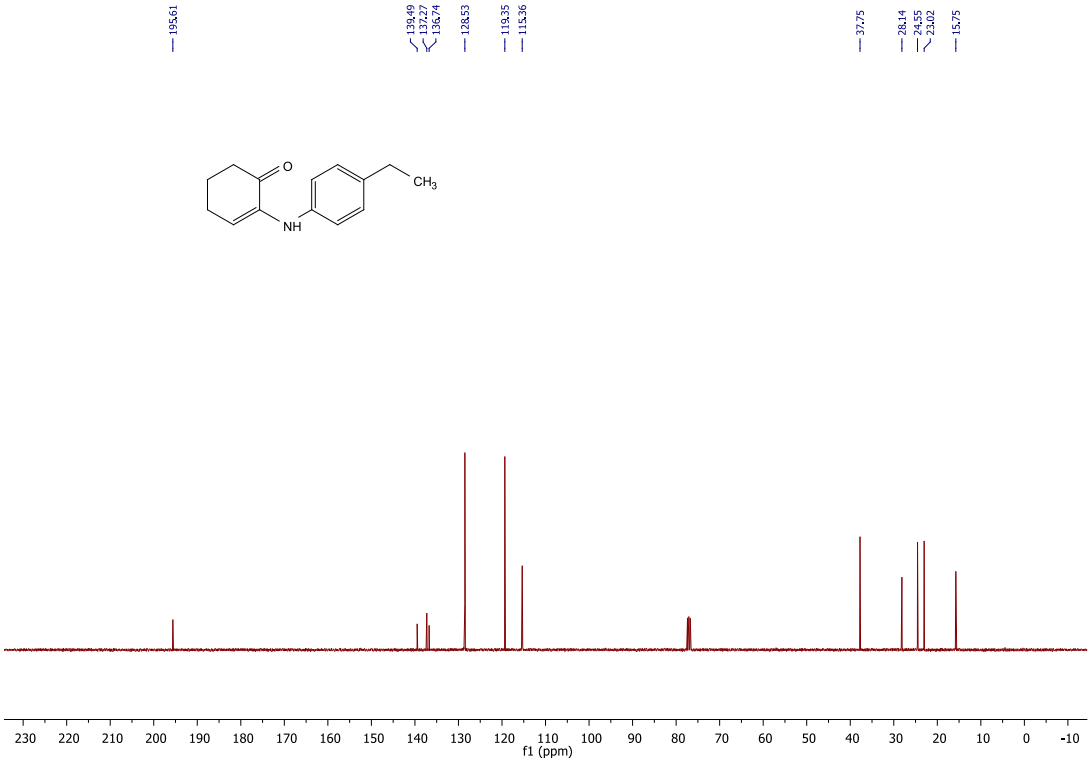
2.54
2.45
2.44
2.43
2.41
2.04
2.03
2.01
1.99
1.98
1.24
1.22
1.20
O
CH3
NH
1.84
1.90
1.00
0.86
3.97
2.02
2.04
2.96
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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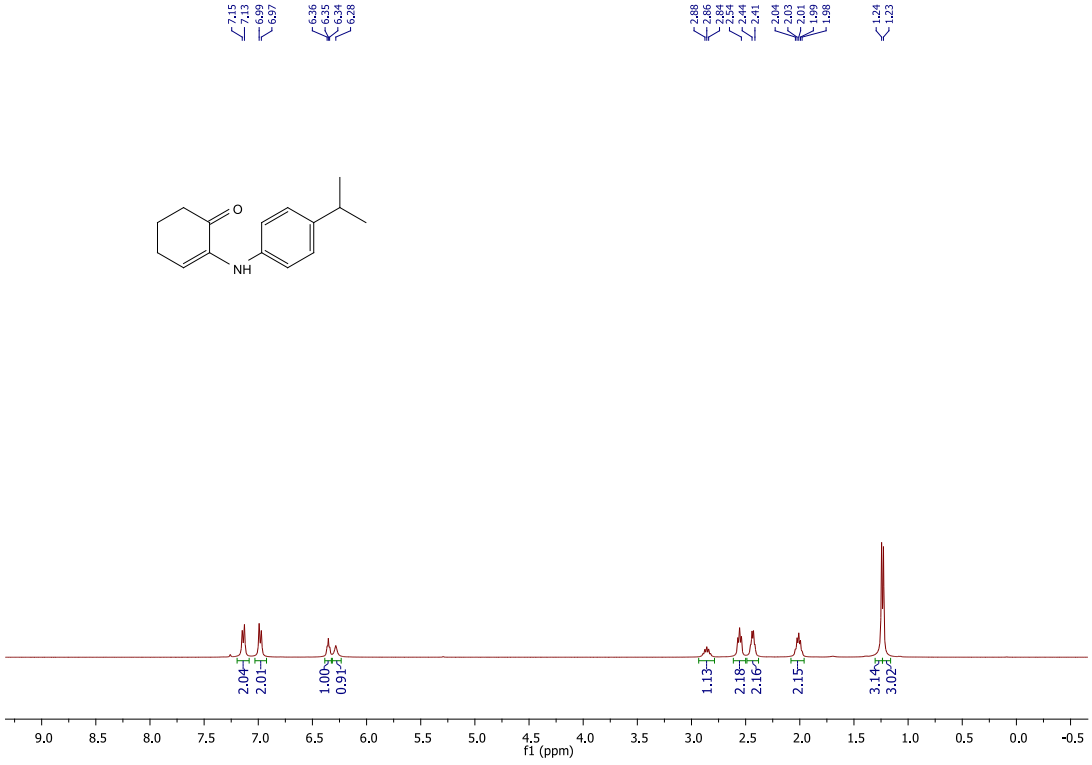
15.75
O
CH3
NH
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.28
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2.86
2.84
2.54
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2.41
2.04
2.03
2.01
1.99
1.98
1.24
1.23
O
NH
2.04
2.01
1.00
0.91
1.13
2.18
2.16
2.15
3.14
3.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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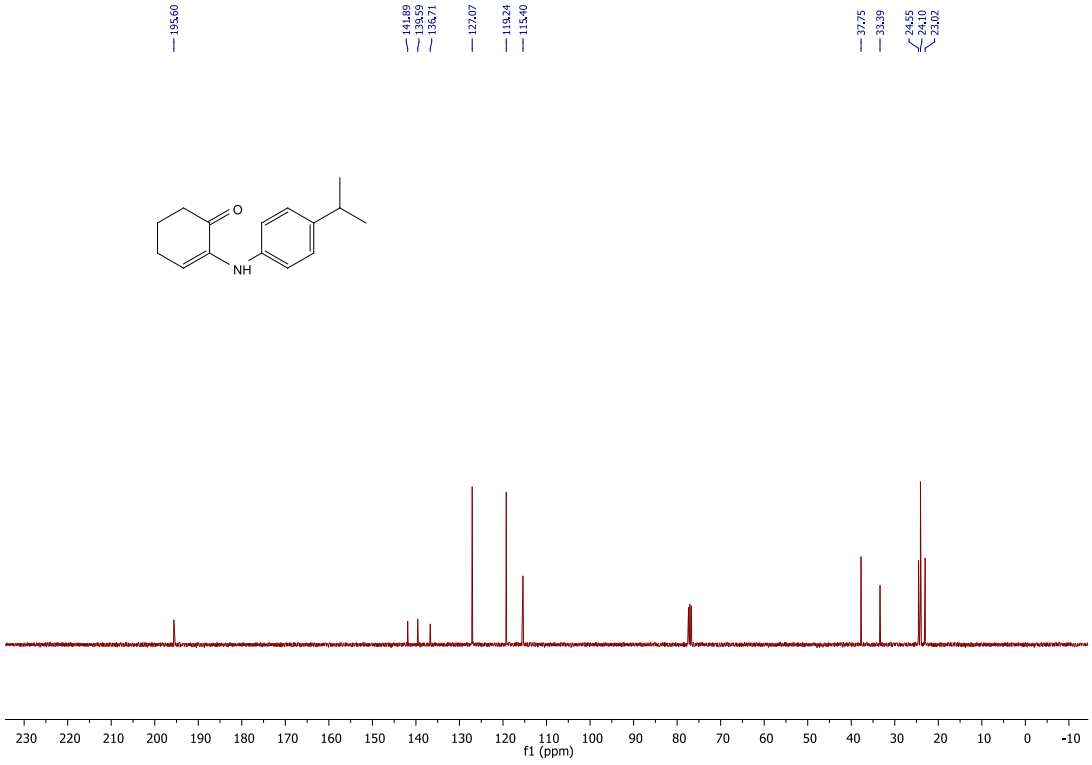
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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119.24
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37.75
33.39
24.55
24.10
23.02
O
NH
230
220
210
200
190
180
170
160
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140
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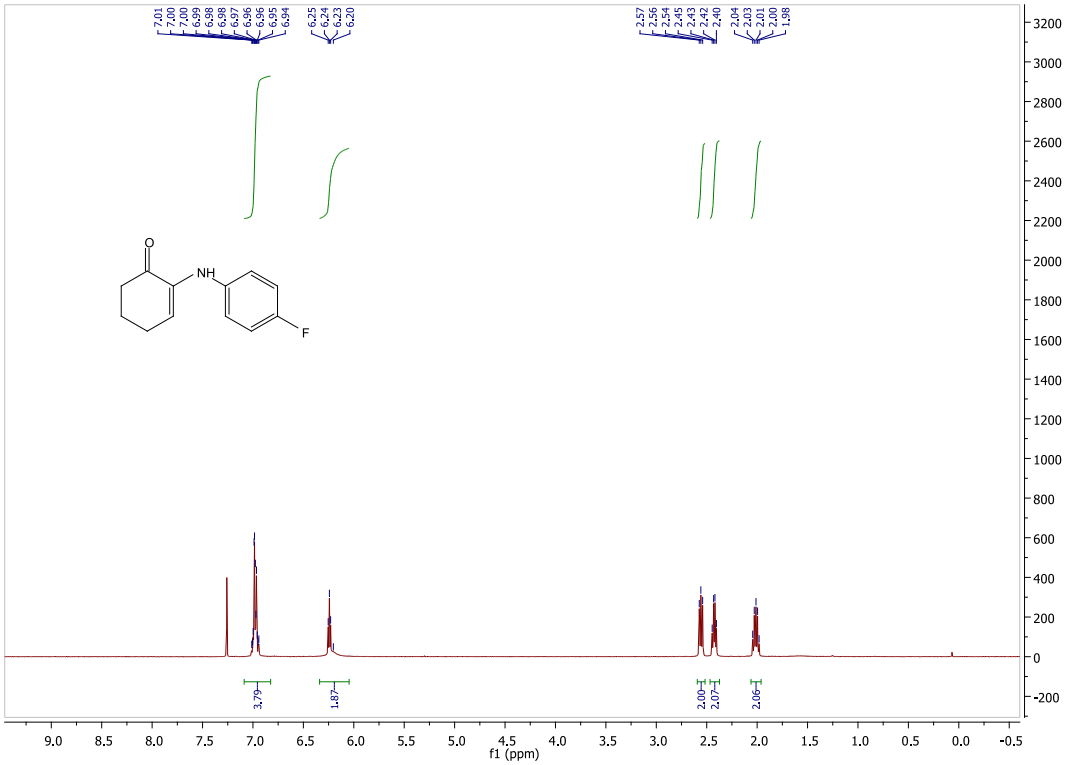
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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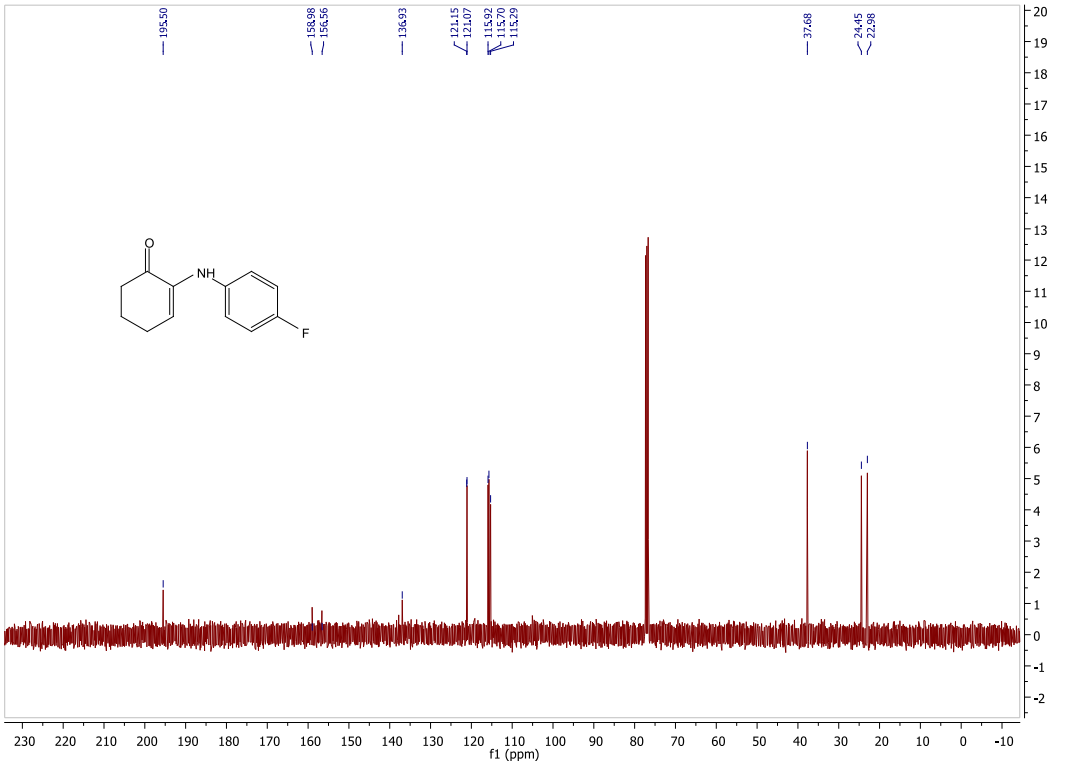
6.94
6.25
6.24
6.23
6.20
2.57
2.56
2.54
2.45
2.43
2.42
2.40
2.04
2.03
2.01
2.00
1.98
O
NH
F
3.79
1.87
2.00
2.07
2.06
f1 (ppm)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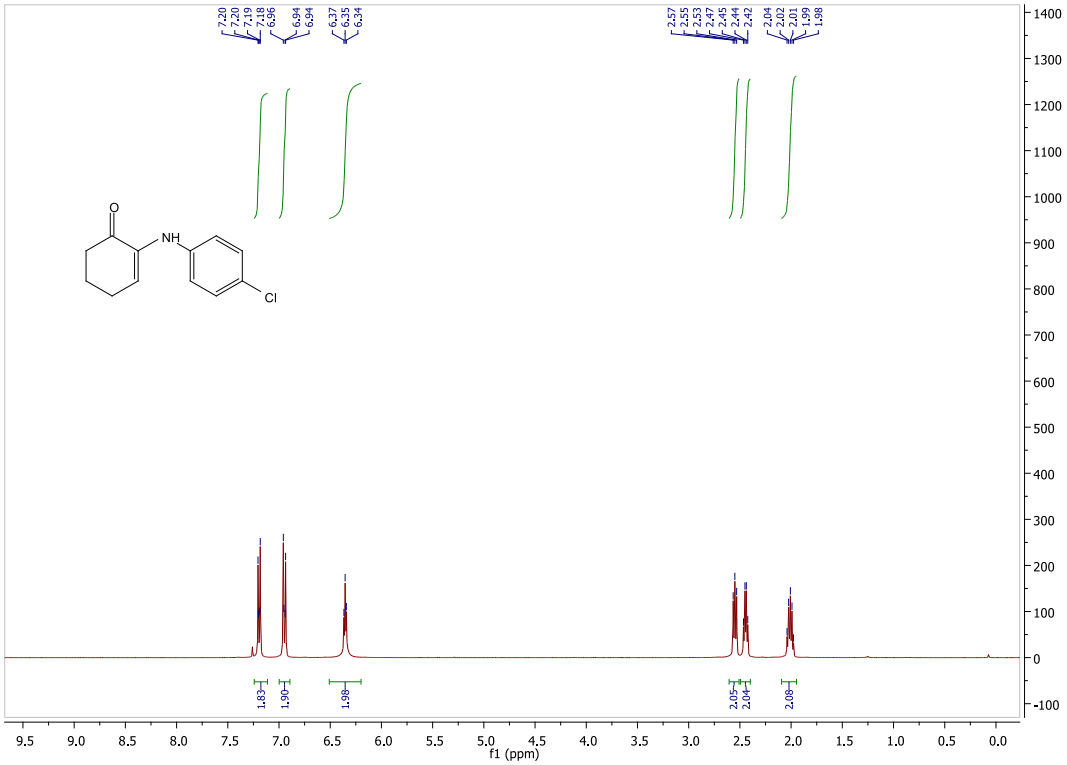
24.45
22.98
O
NH
F
f1 (ppm)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6.94
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6.34
2.57
2.55
2.53
2.47
2.45
2.44
2.42
2.04
2.02
2.01
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O
NH
Cl
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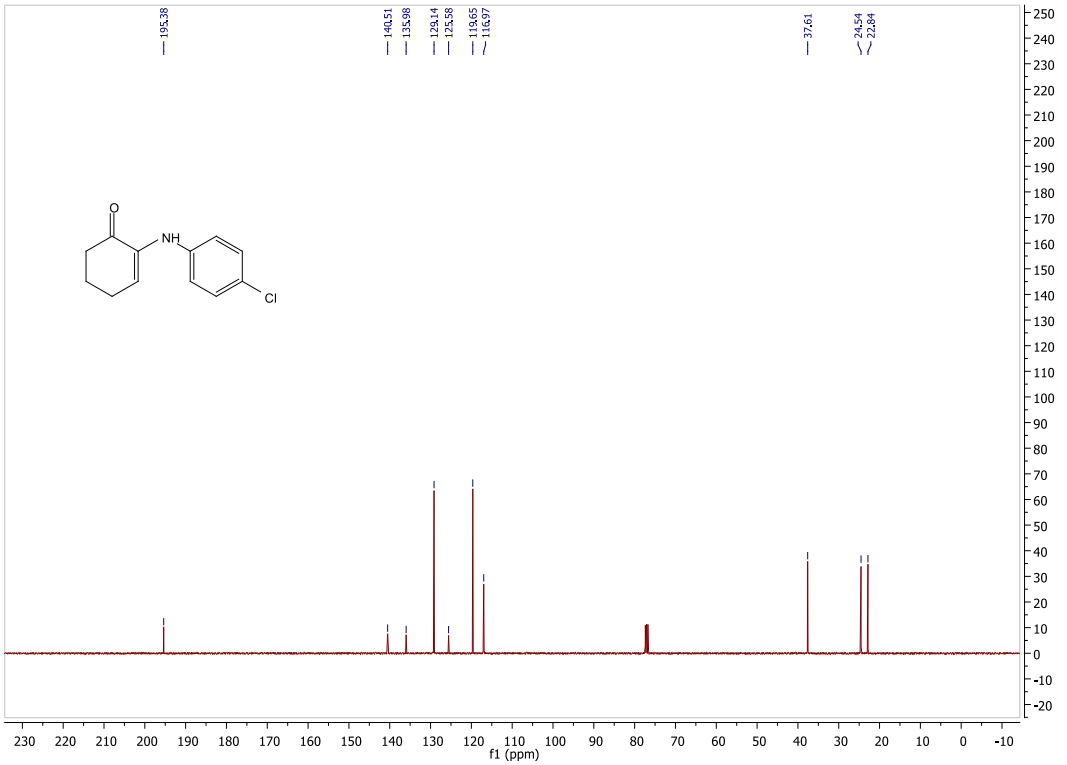
2.05
2.04
2.08
f1 (ppm)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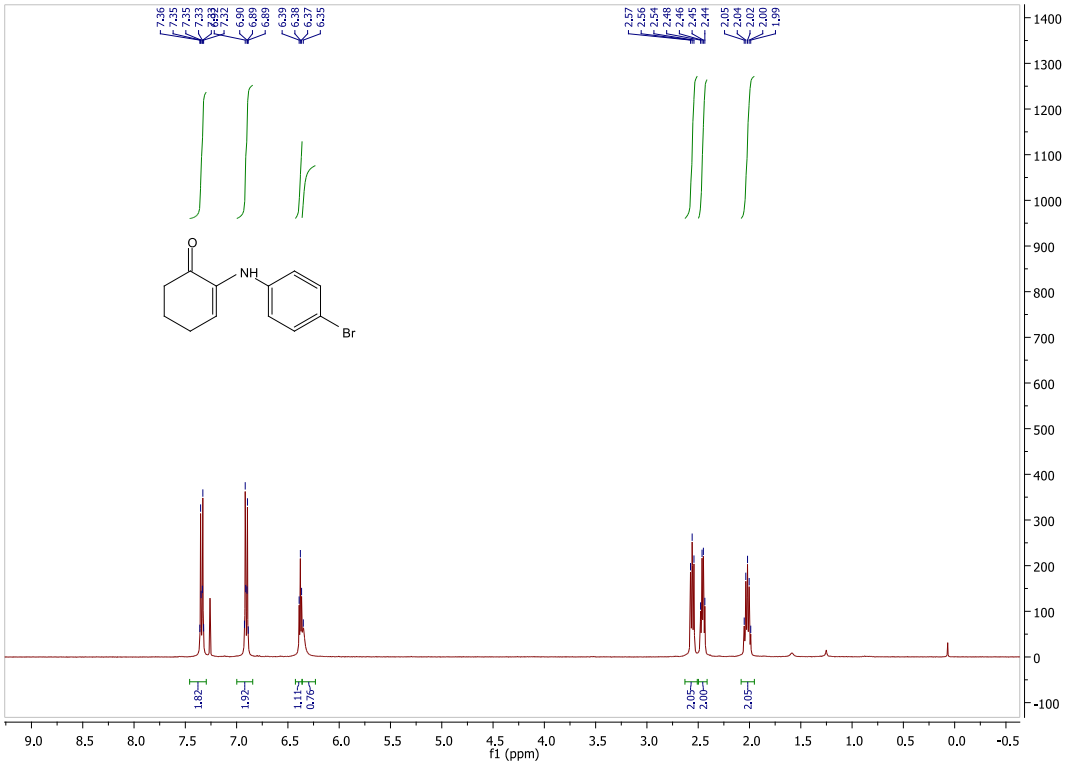
NH
Cl
f1 (ppm)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6.38
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6.35
2.57
2.56
2.54
2.48
2.46
2.45
2.44
2.05
2.04
2.02
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NH
Br
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1.92
1.11
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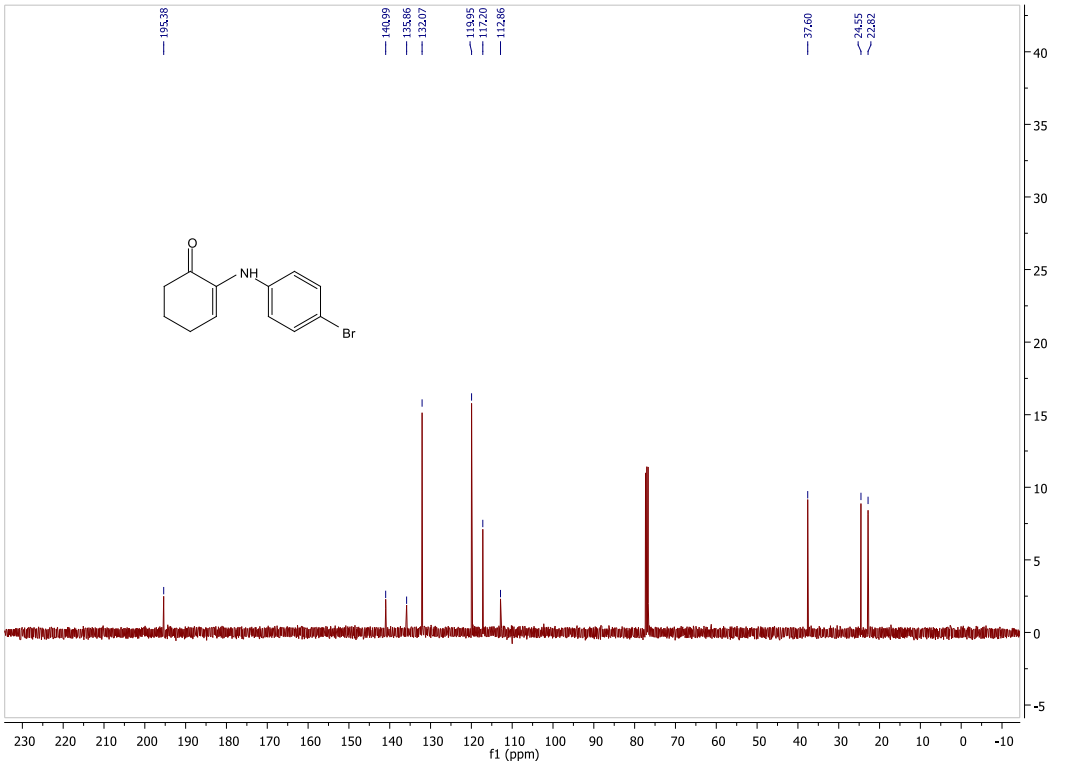
2.05
2.00
2.05
f1 (ppm)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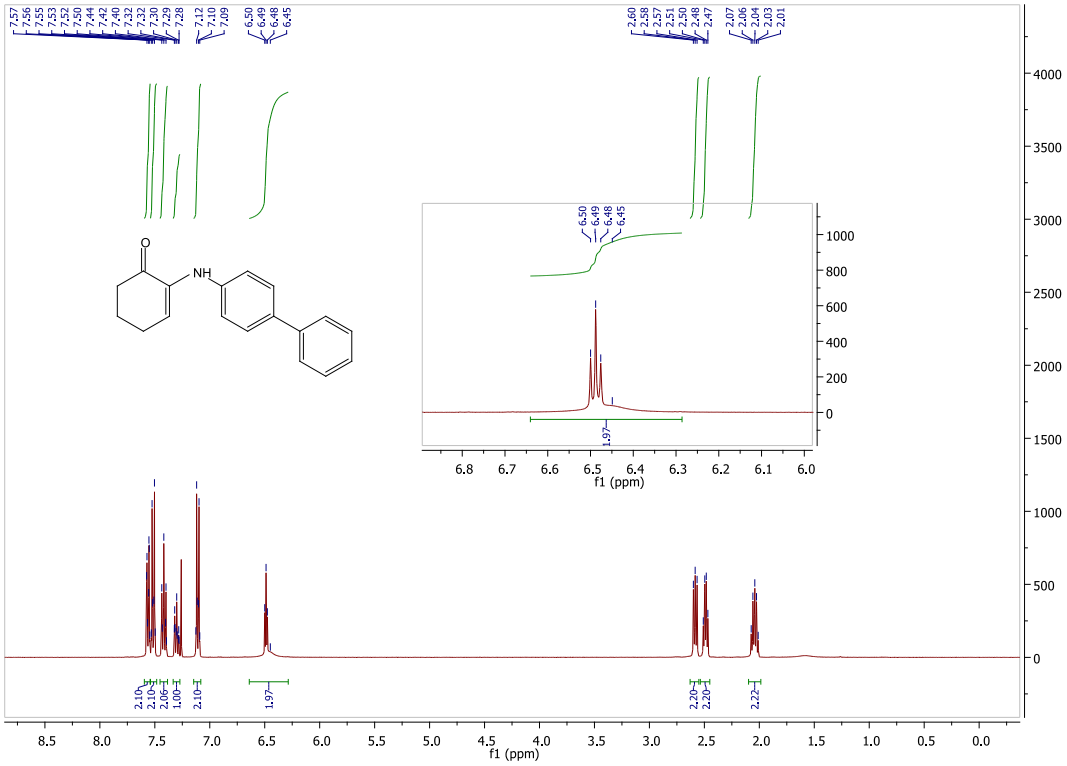
24.55
22.82
O
NH
Br
f1 (ppm)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7.10
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6.45
2.60
2.58
2.57
2.51
2.50
2.48
2.47
2.07
2.06
2.04
2.03
2.01
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NH
f1 (ppm)
2.10
2.16
2.05
1.00
2.10
1.97
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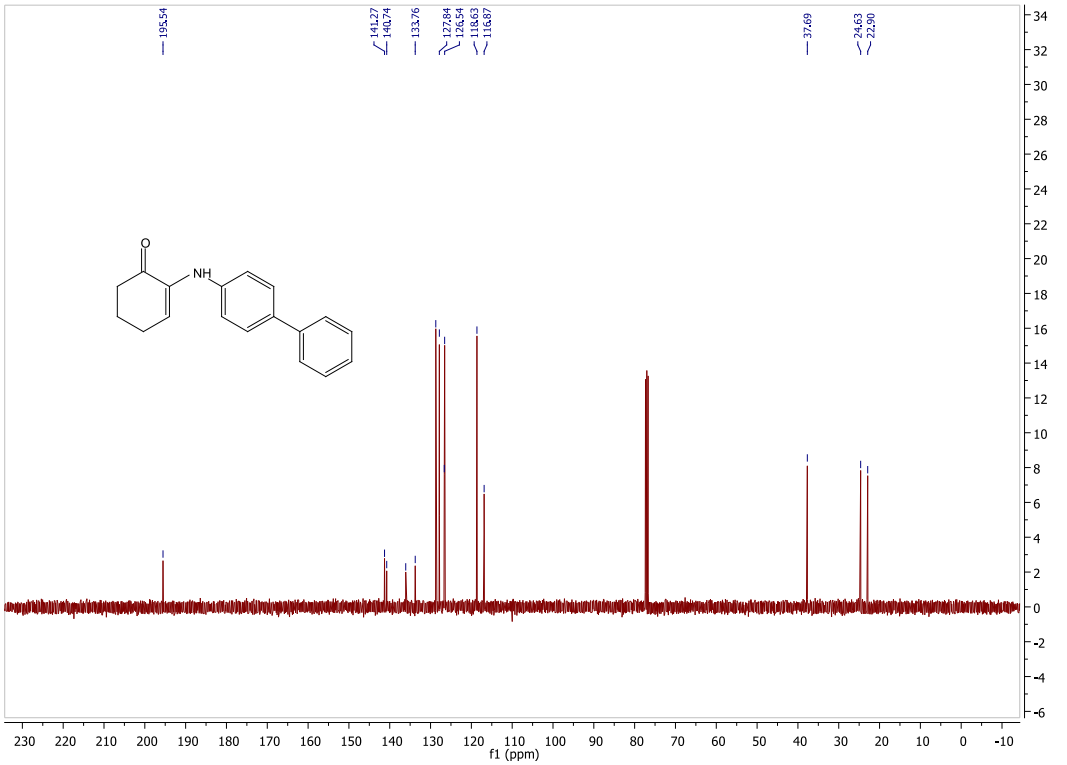
2.20
2.22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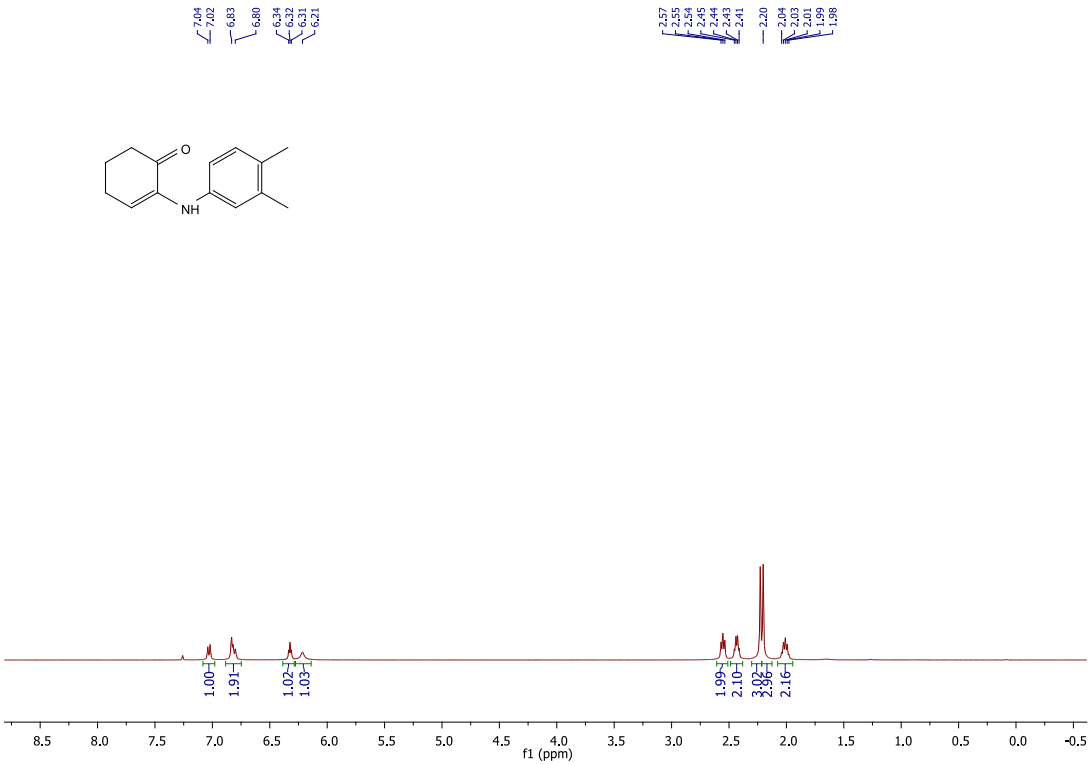
22.90
O
NH
f1 (ppm)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2.43
2.41
2.20
2.04
2.03
2.01
1.99
1.98
O
NH
1.00
1.91
1.02
1.03
1.99
2.10
3.02
2.96
2.16
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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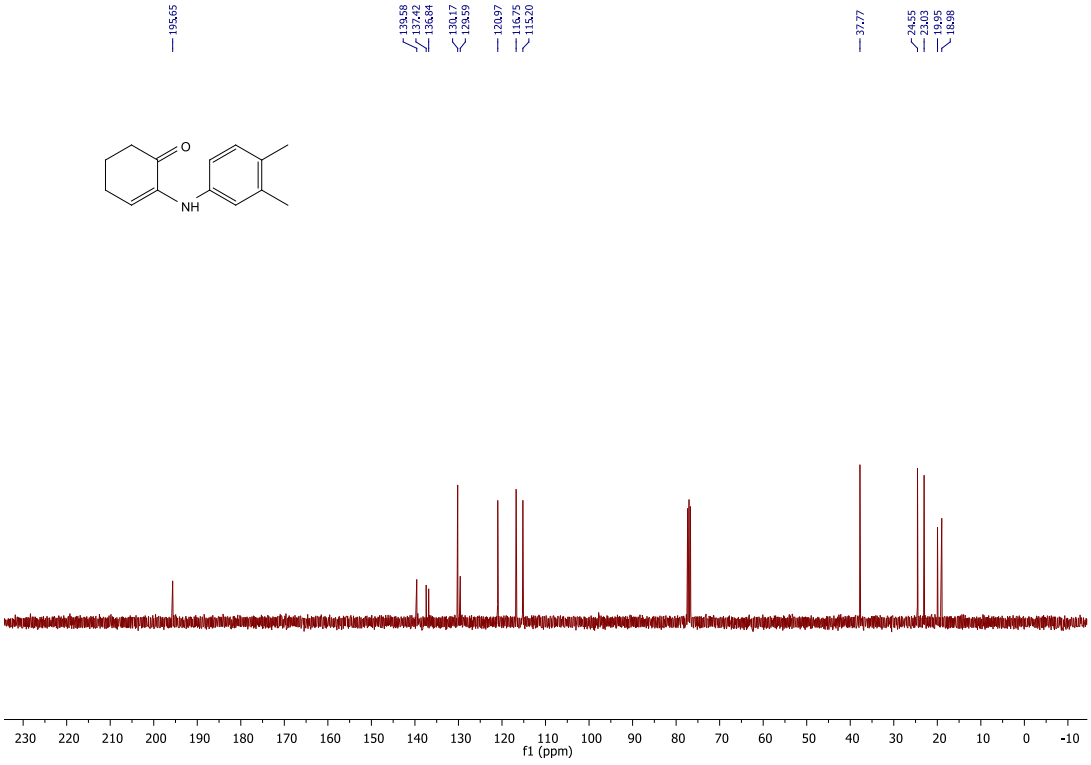
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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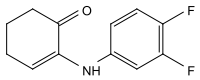
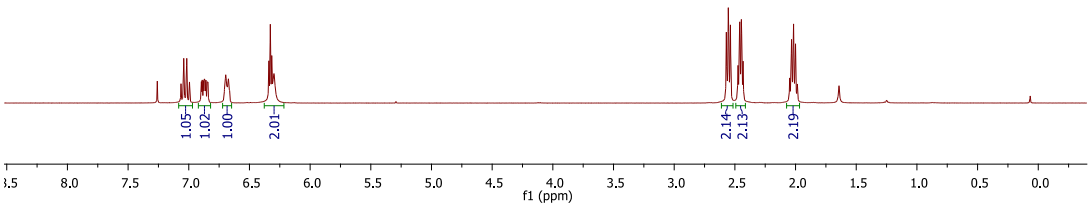
139.58
137.42
136.84
130.17
129.59
120.97
116.75
115.20
37.77
24.55
23.03
19.95
18.98
O
NH
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

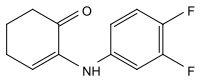

7.06
7.04
7.02
6.90
6.89
6.88
6.87
6.87
6.86
6.85
6.84
6.66
6.34
6.33
6.32
6.30

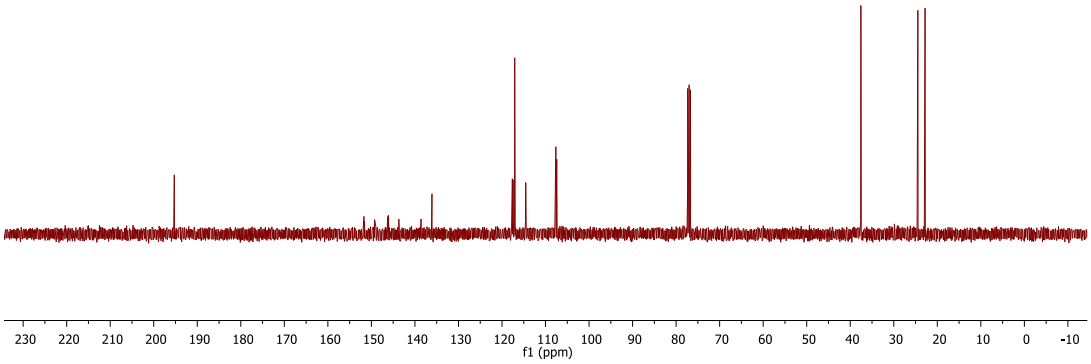

2.57
2.55
2.54
2.47
2.46
2.45
2.43
2.05
2.03
2.02
2.00
1.99

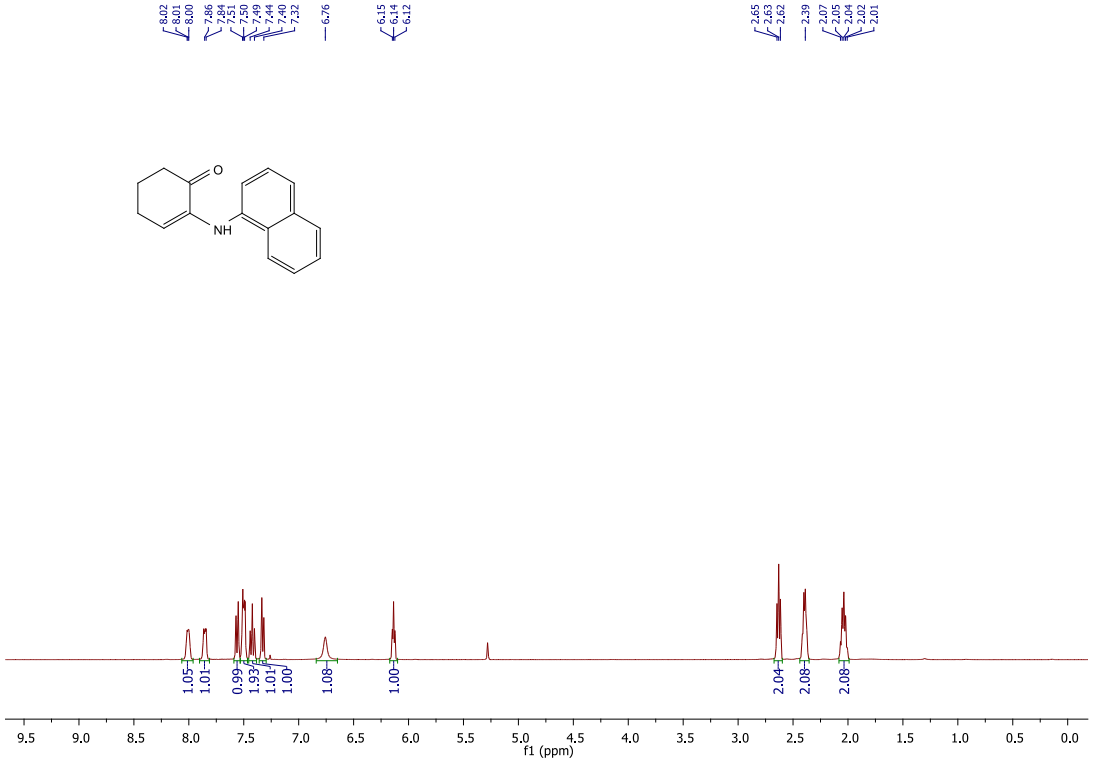

O
F
NH
F

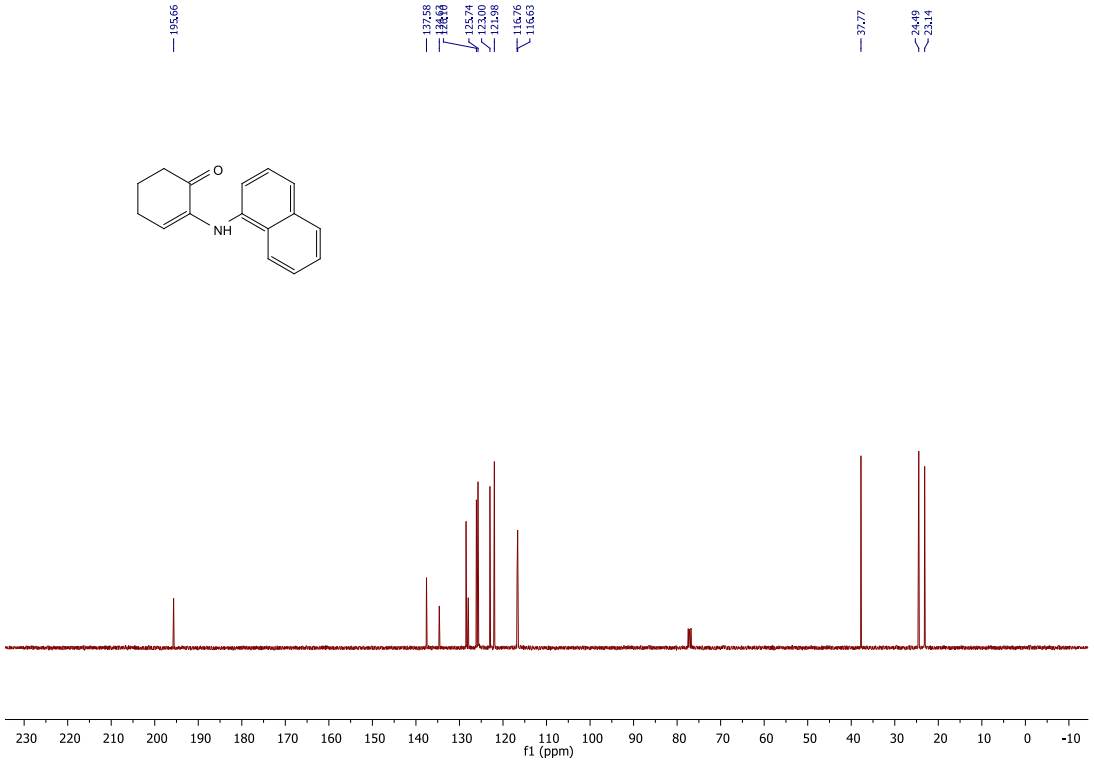

1.05
1.02
1.00
2.01
2.14
2.13
2.19
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

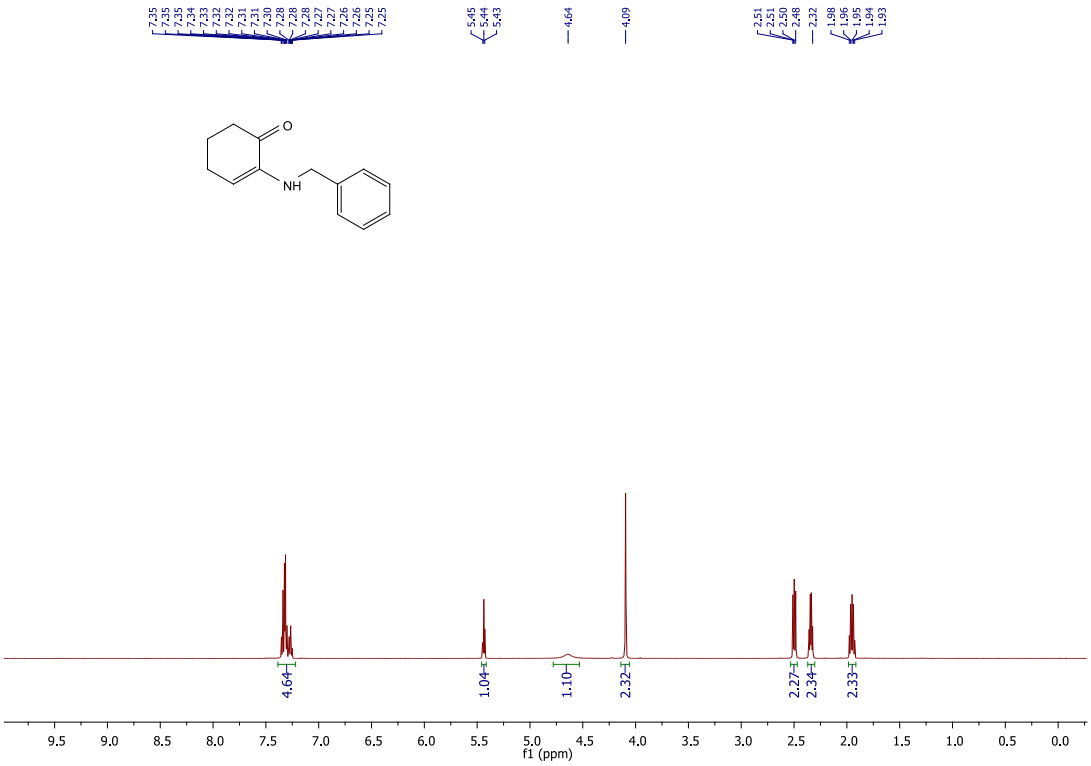

195.28
151.72
151.53
149.27
149.13
146.25
146.10
143.83
143.66
138.54
136.08
117.62
117.07
114.55
114.53
114.49
107.63
107.43
37.55
24.47
22.81

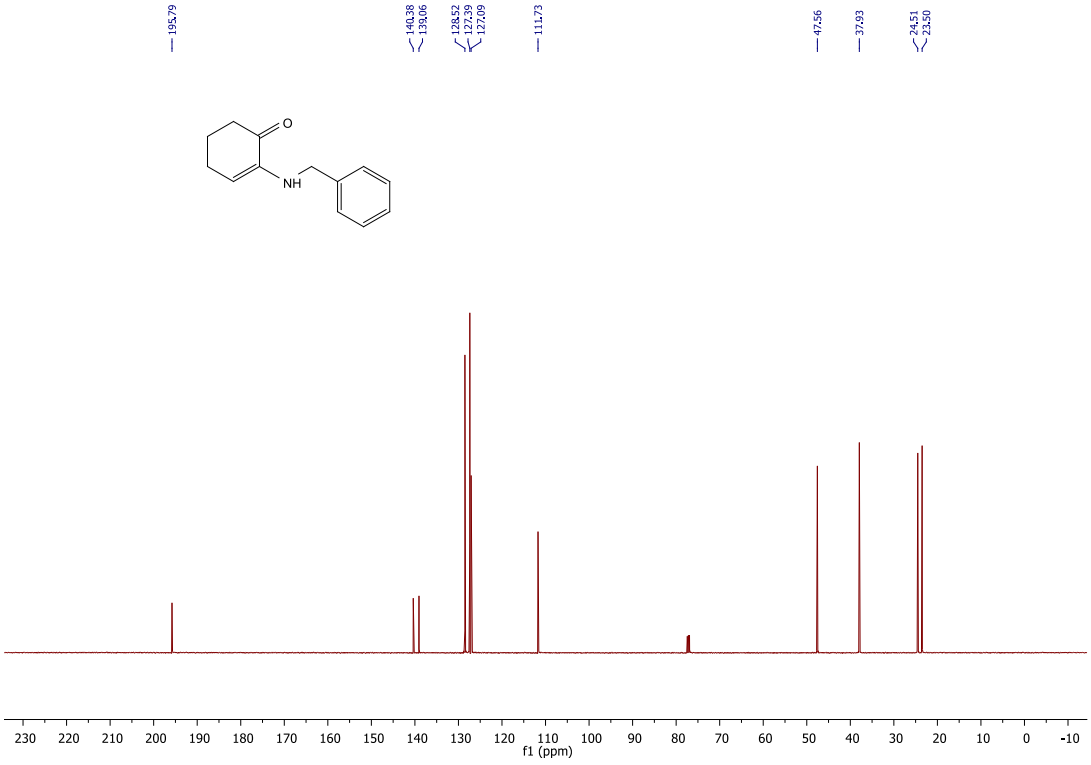

O
F
NH
F

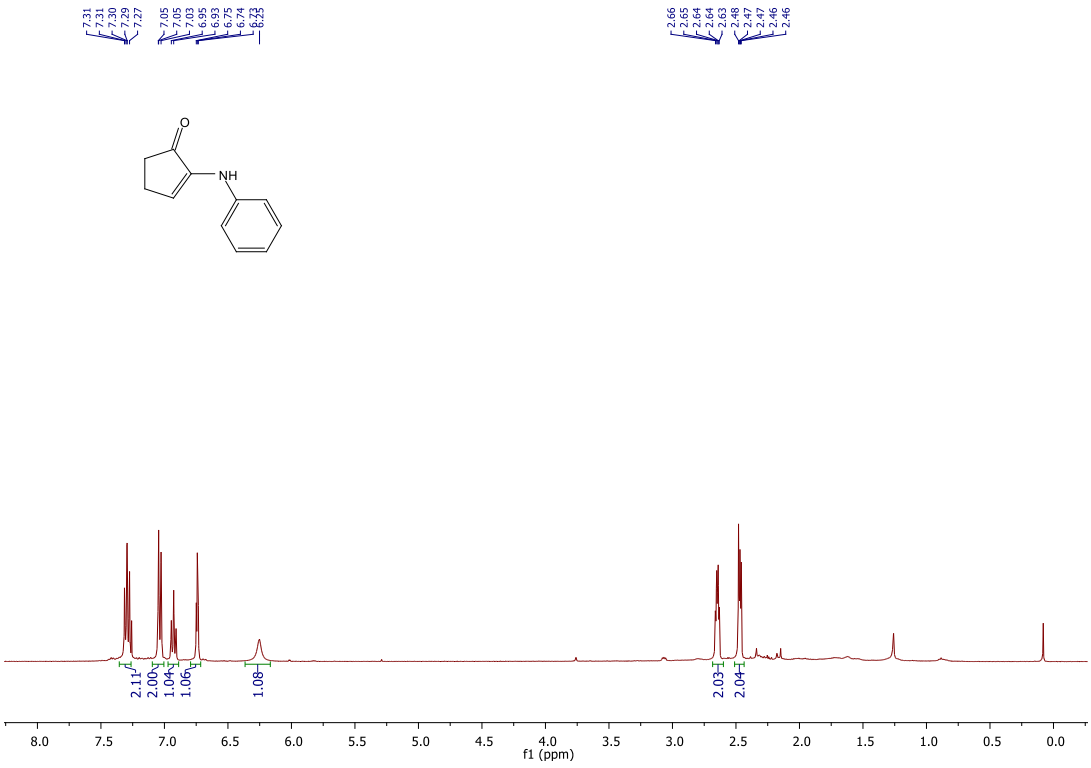

230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

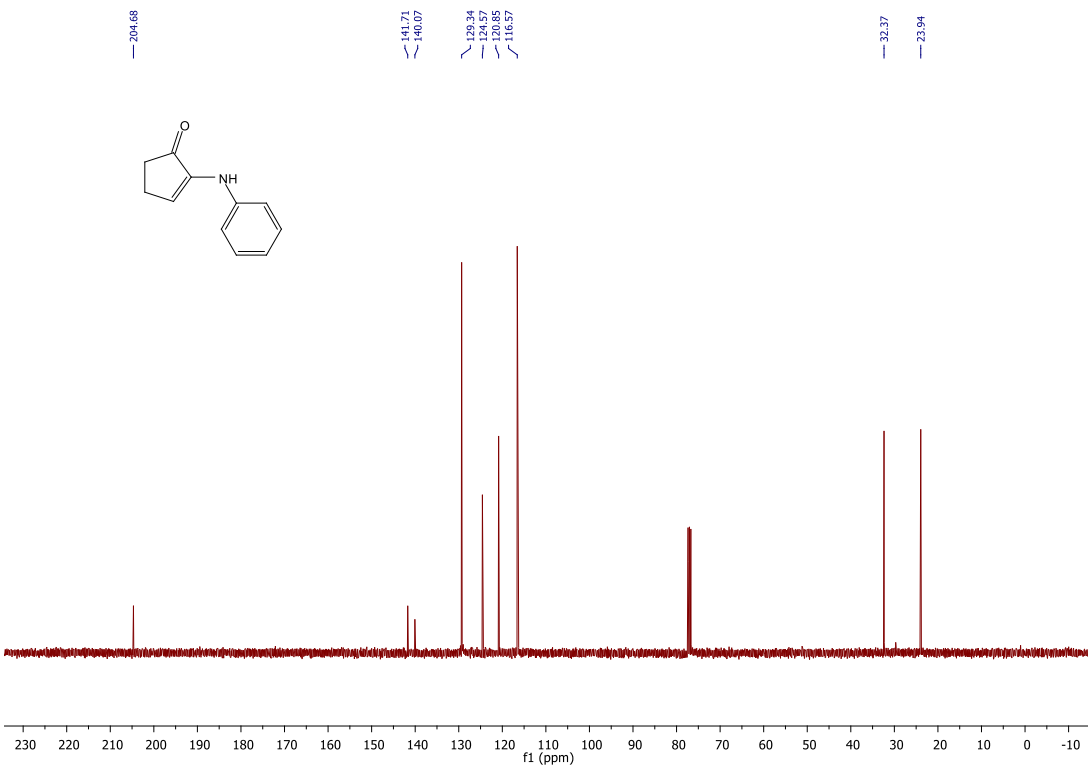

8.02
8.01
8.00
7.86
7.84
7.51
7.50
7.49
7.44
7.40
7.32
6.76
6.15
6.14
6.12
2.65
2.63
2.62
2.39
2.07
2.05
2.04
2.02
2.01
O
NH
1.05
1.01
0.99
1.93
1.01
1.00
1.08
1.00
2.04
2.08
2.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

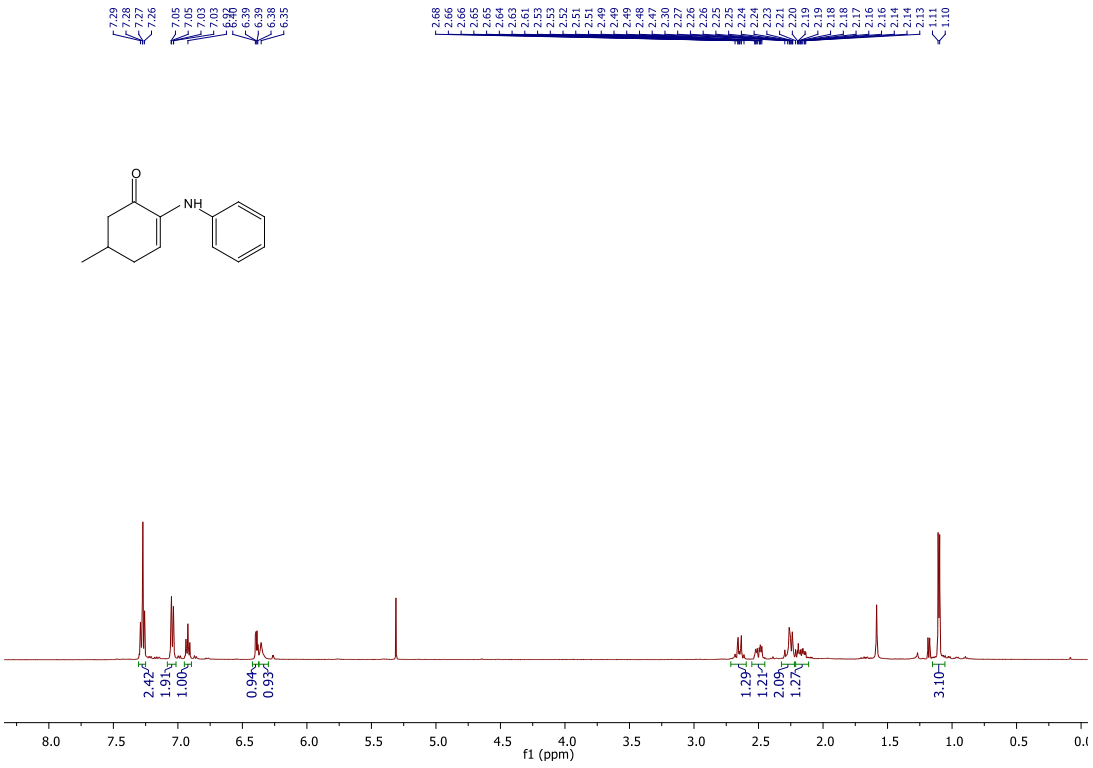

195.66
137.58
125.74
123.00
121.98
116.76
116.63
37.77
24.49
23.14
O
NH
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

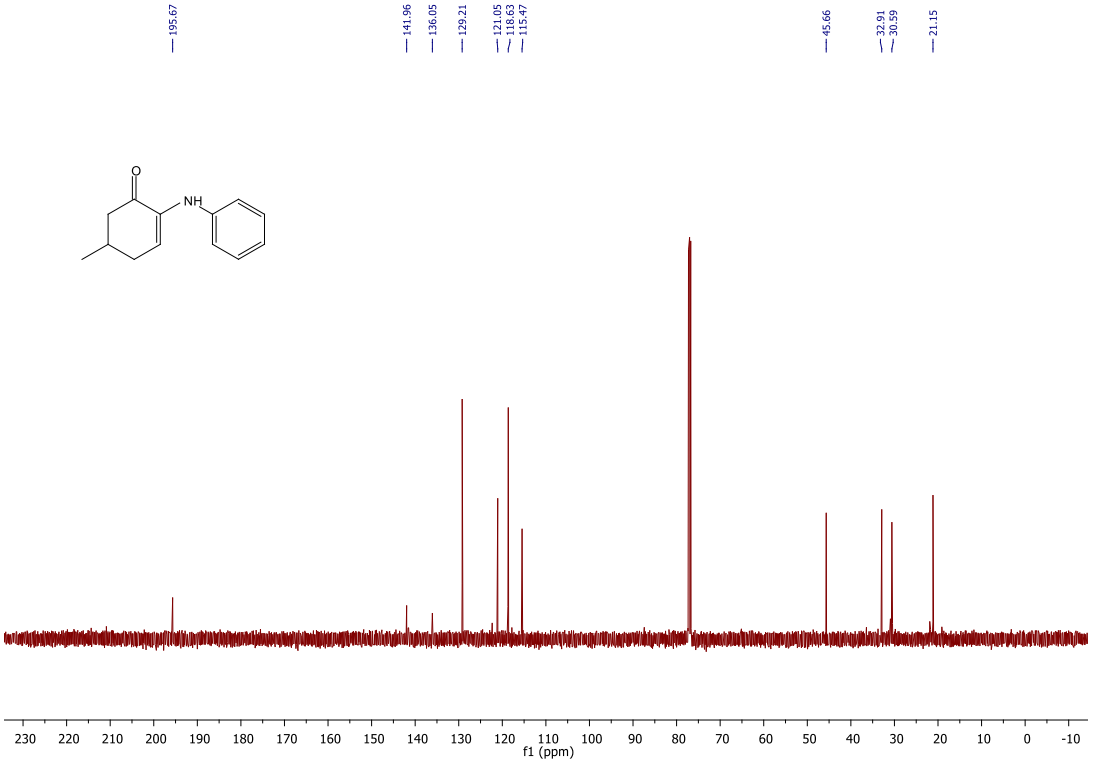

7.35
7.35
7.35
7.34
7.33
7.32
7.32
7.31
7.31
7.30
7.28
7.28
7.28
7.27
7.27
7.26
7.26
7.25
7.25
7.25
5.45
5.44
5.43
4.64
4.09
2.51
2.51
2.50
2.48
2.32
1.98
1.96
1.95
1.94
1.93
O
NH
4.64
1.04
1.10
2.32
2.27
2.34
2.33
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

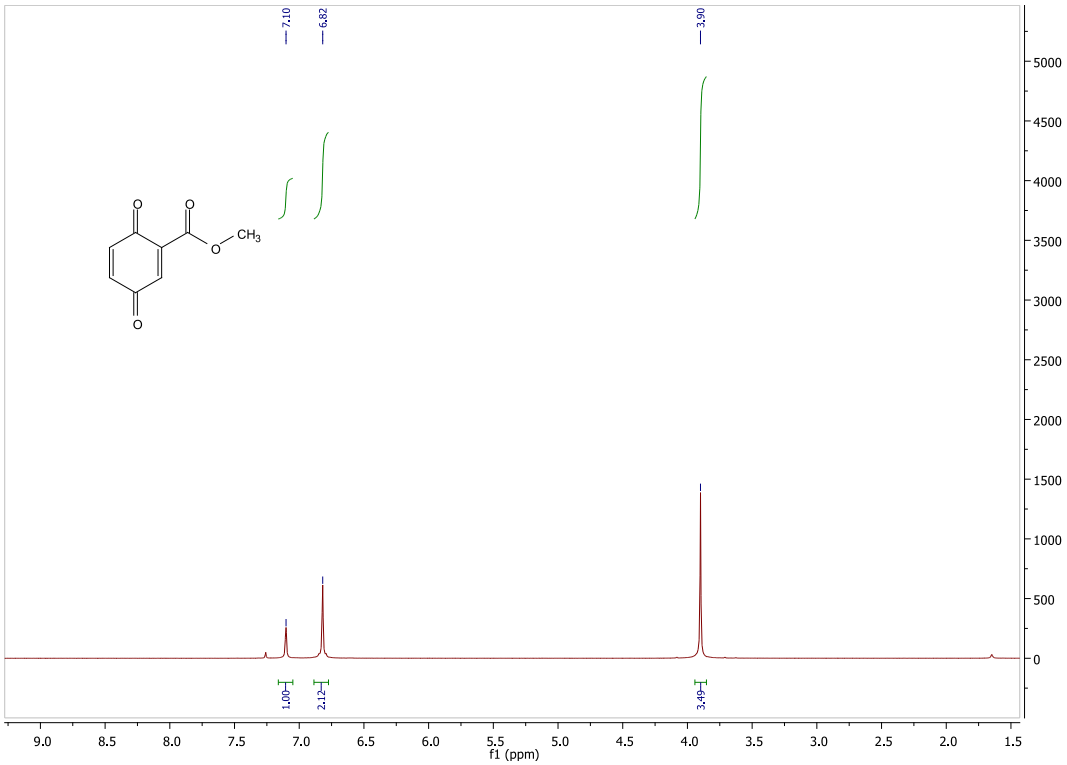

195.79
140.38
139.06
128.52
127.39
127.09
111.73
47.56
37.93
24.51
23.50
O
NH
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

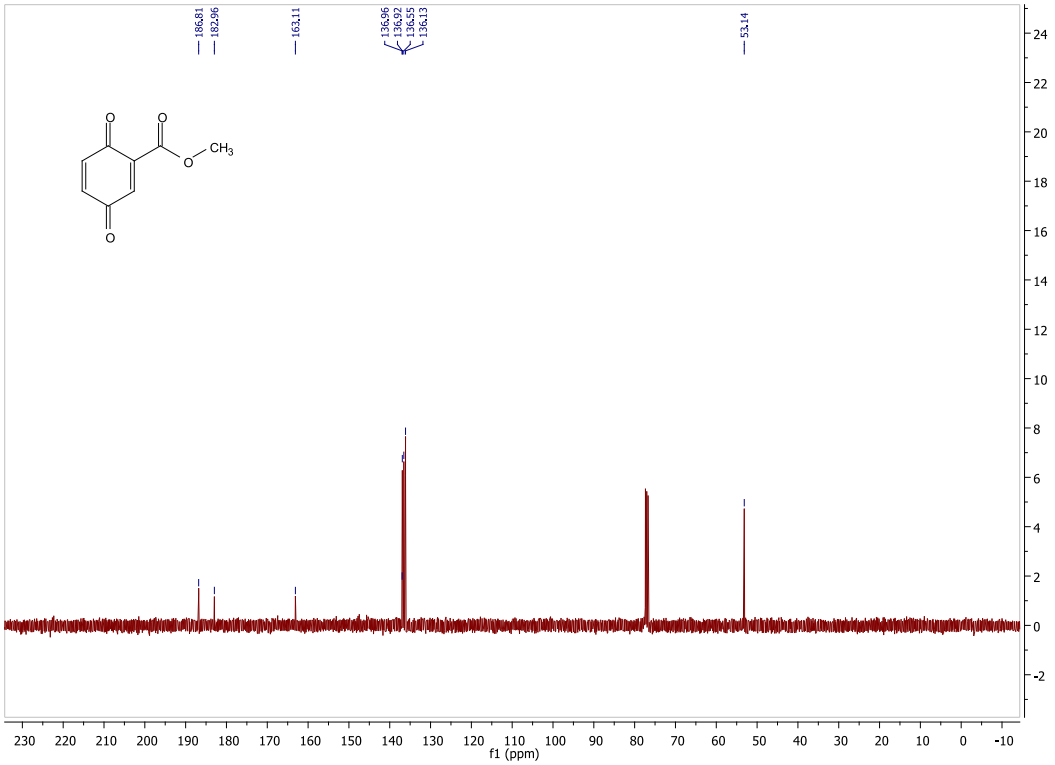

7.31
7.31
7.30
7.29
7.27
7.05
7.05
7.03
6.95
6.93
6.75
6.74
6.23
6.23
2.66
2.65
2.64
2.64
2.63
2.48
2.47
2.47
2.46
2.46
O
NH
2.11
2.00
1.04
1.06
1.08
2.03
2.04
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

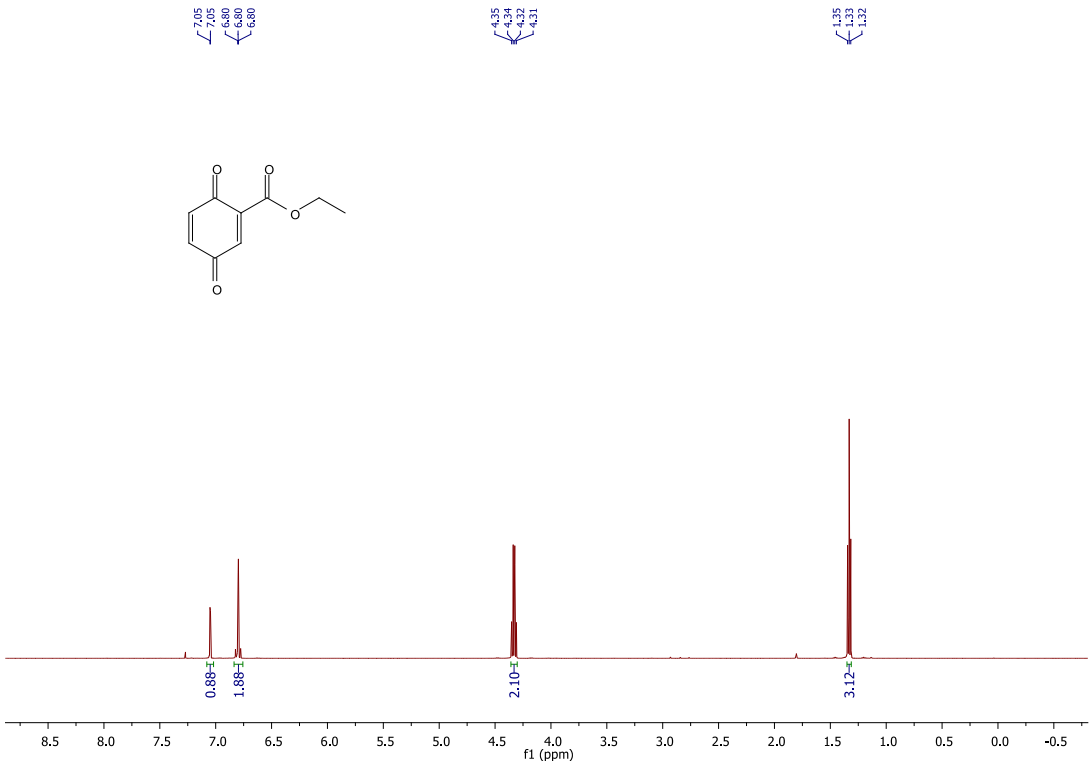

204.68
141.71
140.07
129.34
124.57
120.85
116.57
32.37
23.94
O
NH
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.29
7.28
7.27
7.26
7.05
7.05
7.03
7.03
6.40
6.39
6.39
6.38
6.35
2.68
2.66
2.66
2.65
2.65
2.64
2.63
2.61
2.53
2.53
2.52
2.51
2.51
2.49
2.49
2.49
2.48
2.47
2.30
2.27
2.26
2.26
2.25
2.25
2.24
2.24
2.23
2.21
2.20
2.19
2.19
2.18
2.18
2.17
2.16
2.16
2.14
2.14
2.13
2.11
1.10
O
NH
2.42
1.91
1.00
0.94
0.93
1.29
1.21
2.09
1.27
3.10
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


195.67
141.96
136.05
129.21
121.05
118.63
115.47
45.66
32.91
30.59
21.15
O
NH
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.10
6.82
3.90
1.00
2.12
3.49
f1 (ppm)


186.81
182.96
163.11
136.96
136.92
136.55
136.13
53.14
f1 (ppm)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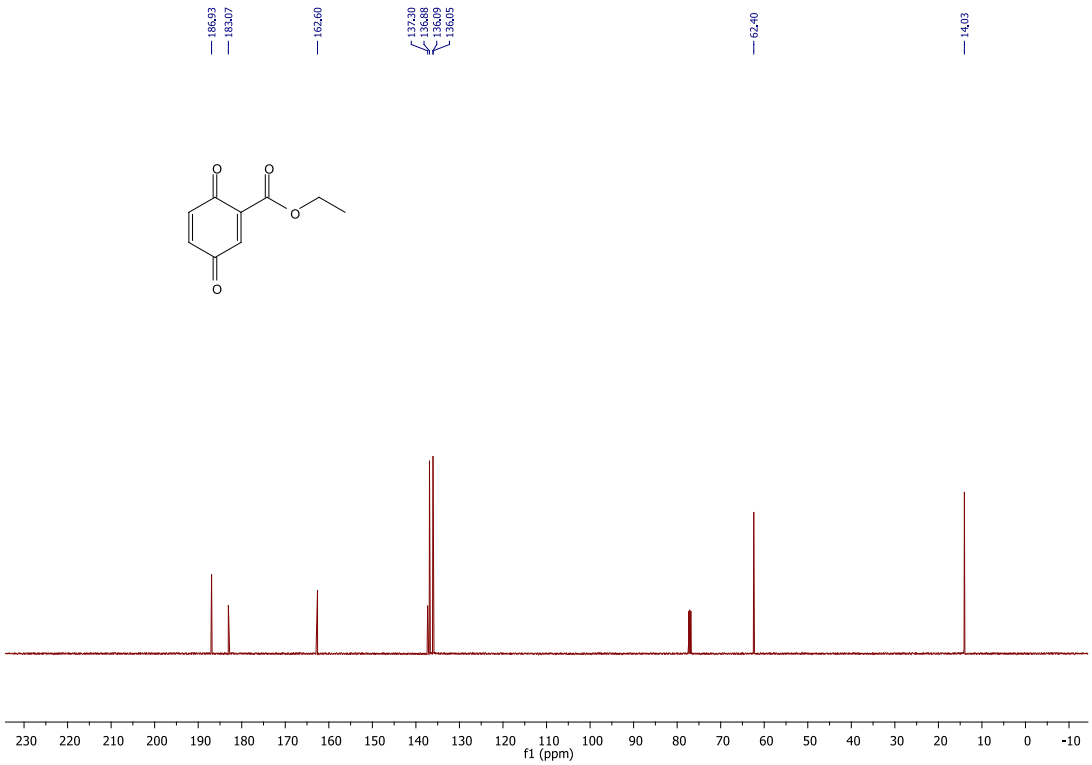
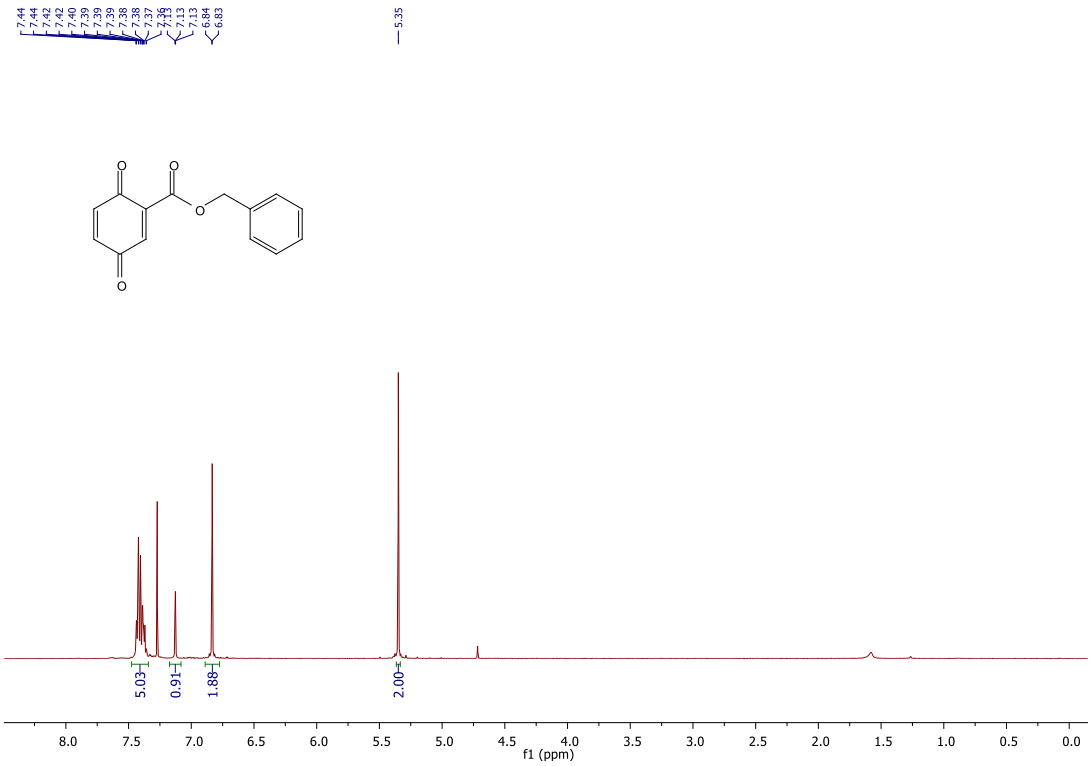
7.05
6.80
6.80
6.80
4.35
4.34
4.32
4.31
1.35
1.33
1.32
O
O
O
O
0.88
1.88
2.10
3.12
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


186.93
183.07
162.60
137.30
136.88
136.09
136.05
62.40
14.03
O
O
O
O
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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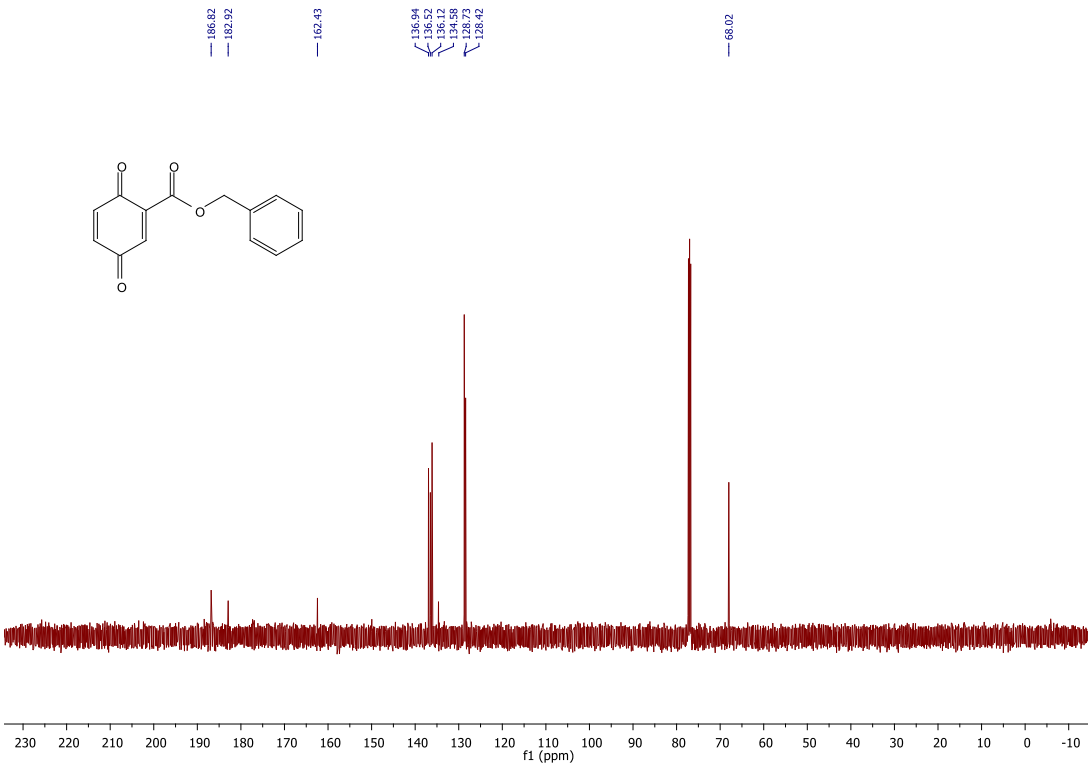
7.44
7.42
7.42
7.40
7.39
7.39
7.39
7.38
7.38
7.37
7.36
7.13
7.13
6.84
6.83
5.35
O
O
O
O
5.03
0.91
1.88
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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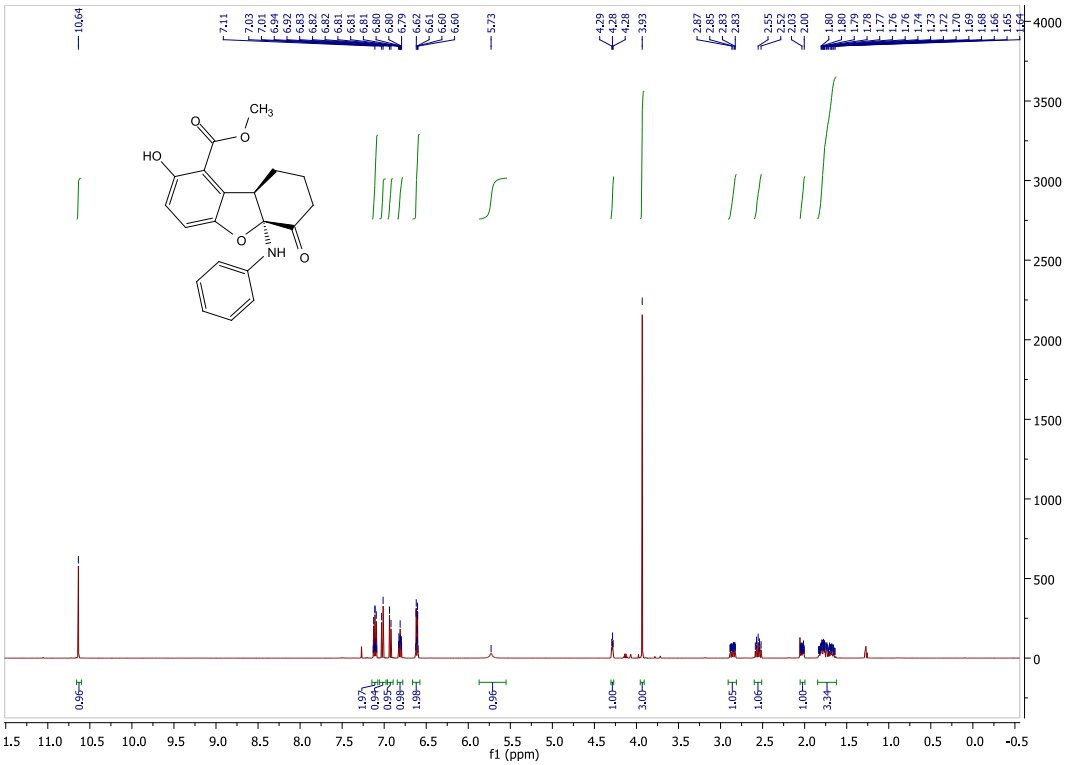
162.43
136.94
136.52
136.12
134.58
128.73
128.42
68.02
O
O
O
O
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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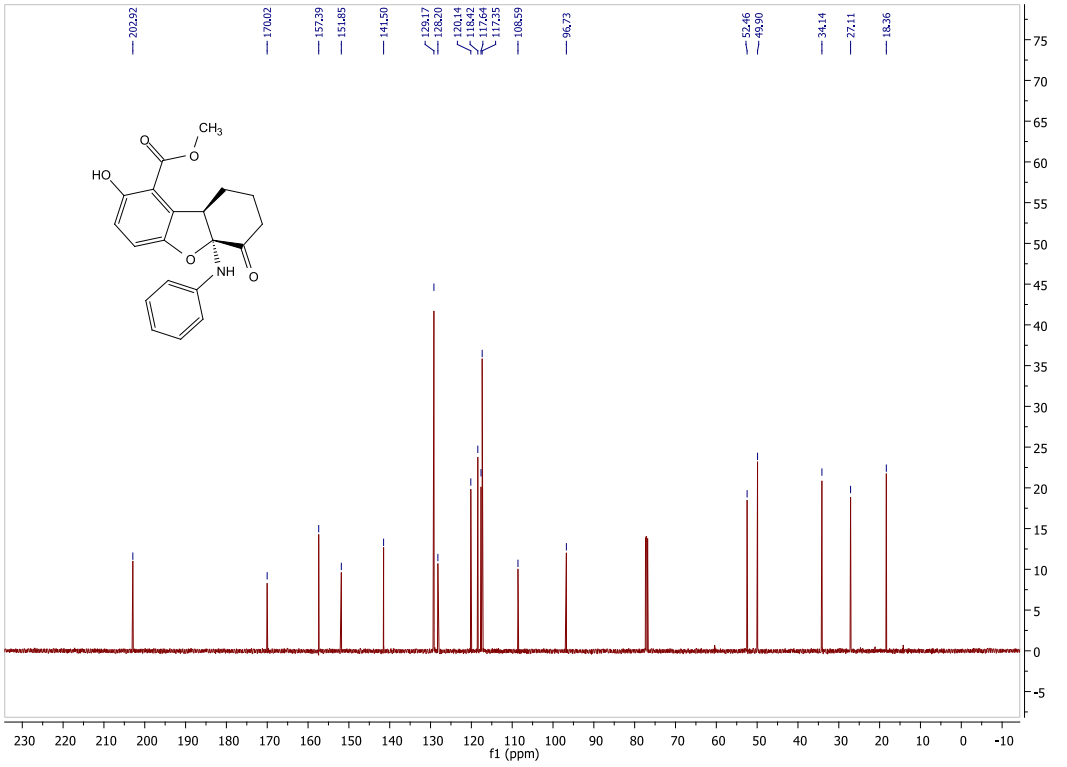
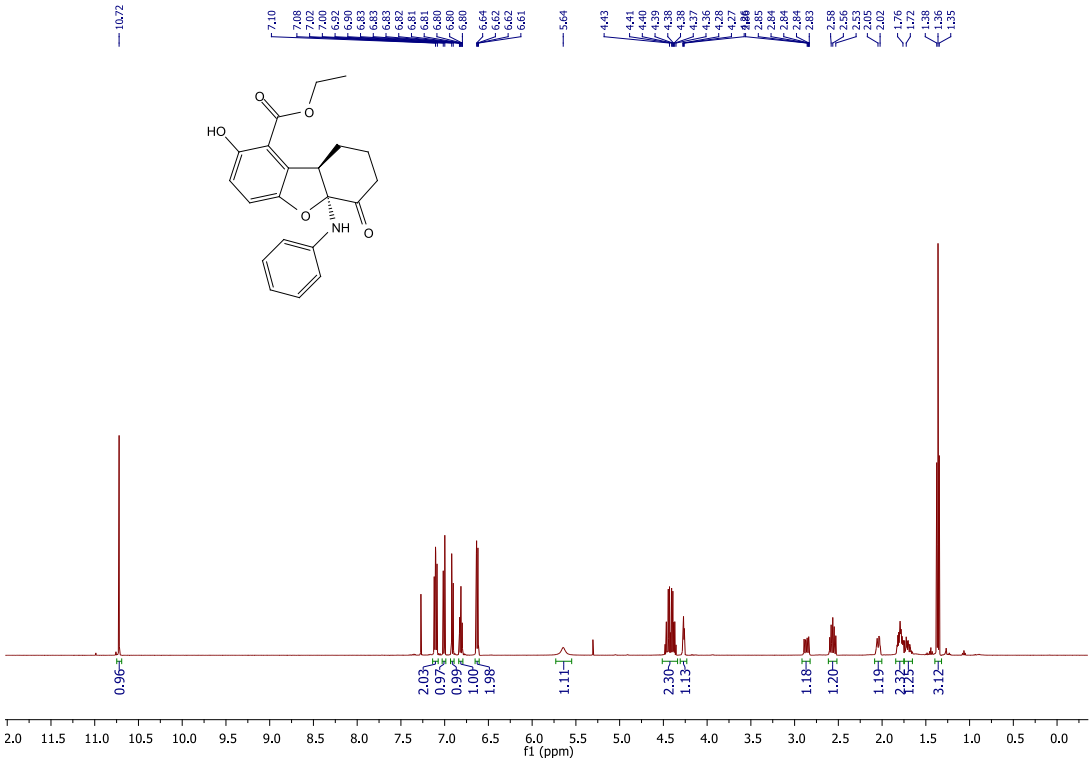
7.01
6.94
6.92
6.83
6.82
6.82
6.81
6.81
6.81
6.80
6.80
6.79
6.62
6.61
6.60
6.60
5.73
4.29
4.28
4.28
3.93
2.87
2.85
2.83
2.83
2.55
2.53
2.03
2.00
1.80
1.80
1.79
1.78
1.77
1.76
1.75
1.74
1.73
1.72
1.70
1.69
1.68
1.66
1.65
1.64
CH3
O
O
HO
O
NH
O
0.96
1.97
0.94
0.95
0.98
1.98
0.96
1.00
3.00
1.05
1.06
1.00
3.34
f1 (ppm)


202.92
170.02
157.39
151.85
141.50
129.17
128.20
120.14
118.42
117.64
117.35
108.59
96.73
52.46
49.90
34.14
27.11
18.36
CH3
O
O
HO
O
NH
O
f1 (ppm)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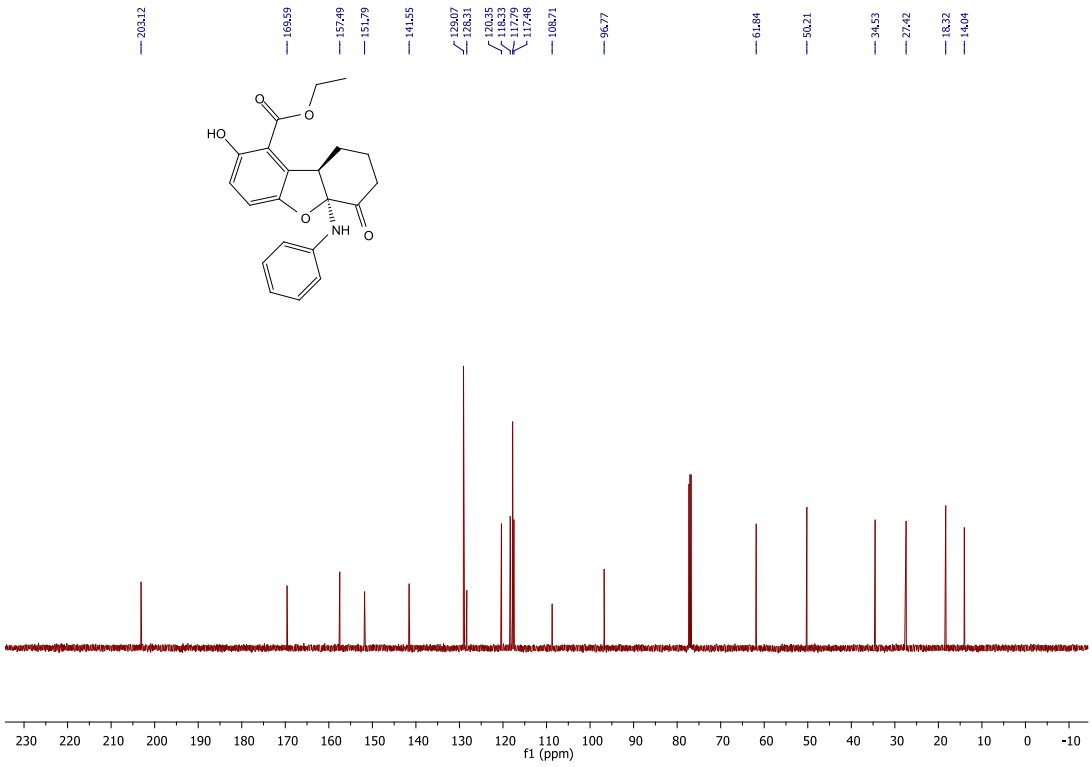
7.10
7.08
7.02
7.00
6.92
6.90
6.83
6.83
6.82
6.81
6.81
6.80
6.80
6.80
6.64
6.62
6.62
6.61
5.64
4.43
4.41
4.40
4.39
4.38
4.38
4.37
4.36
4.28
4.27
2.85
2.84
2.84
2.84
2.83
2.58
2.56
2.53
2.05
2.02
1.76
1.72
1.38
1.36
1.35
HO
O
O
O
NH
O
0.96
2.03
0.97
0.99
1.00
1.98
1.11
2.30
1.13
1.18
1.20
1.19
1.32
1.25
3.12
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


203.12
169.59
157.49
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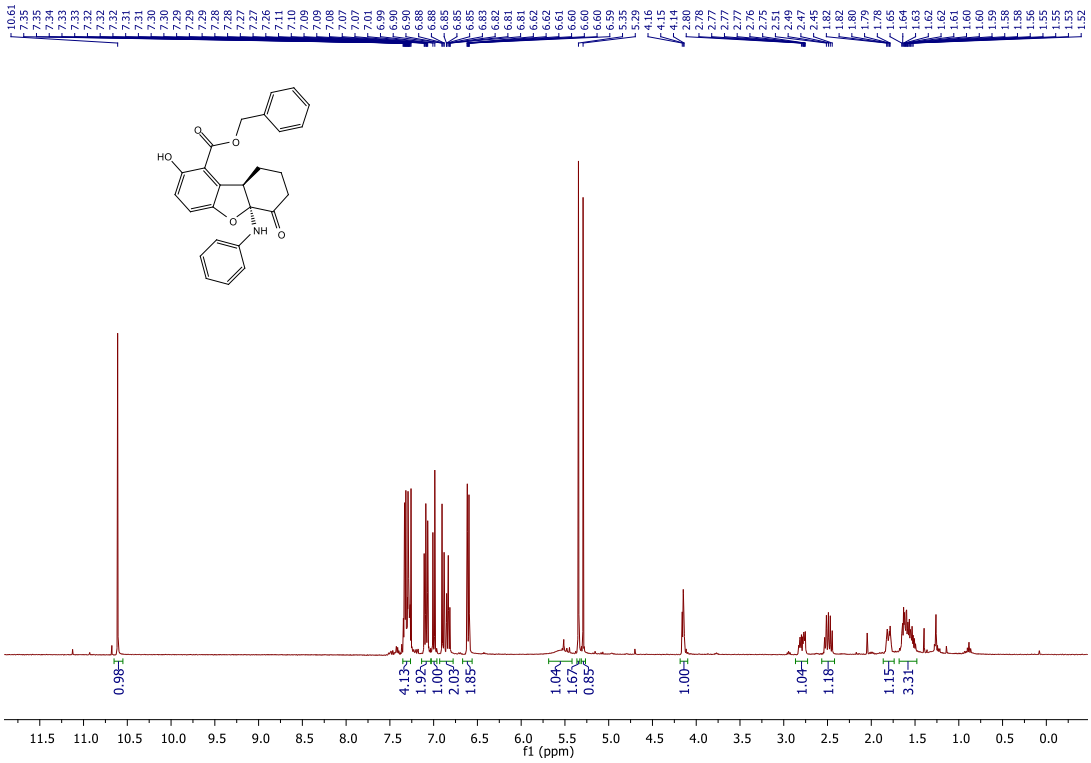
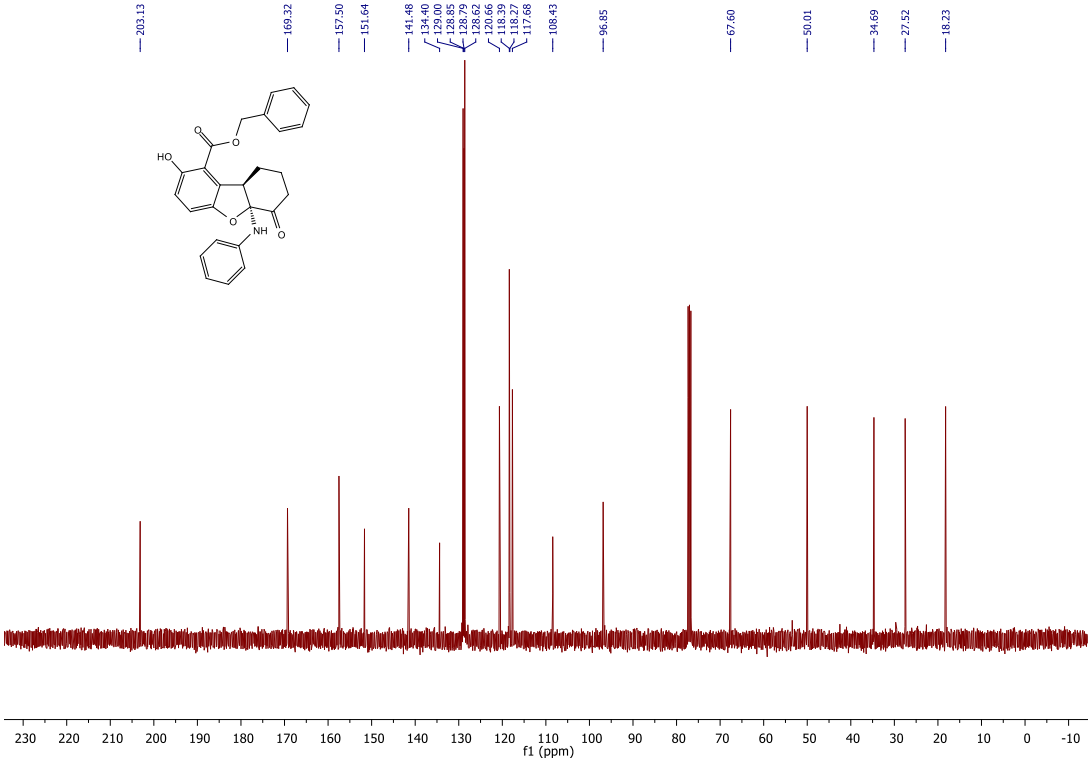
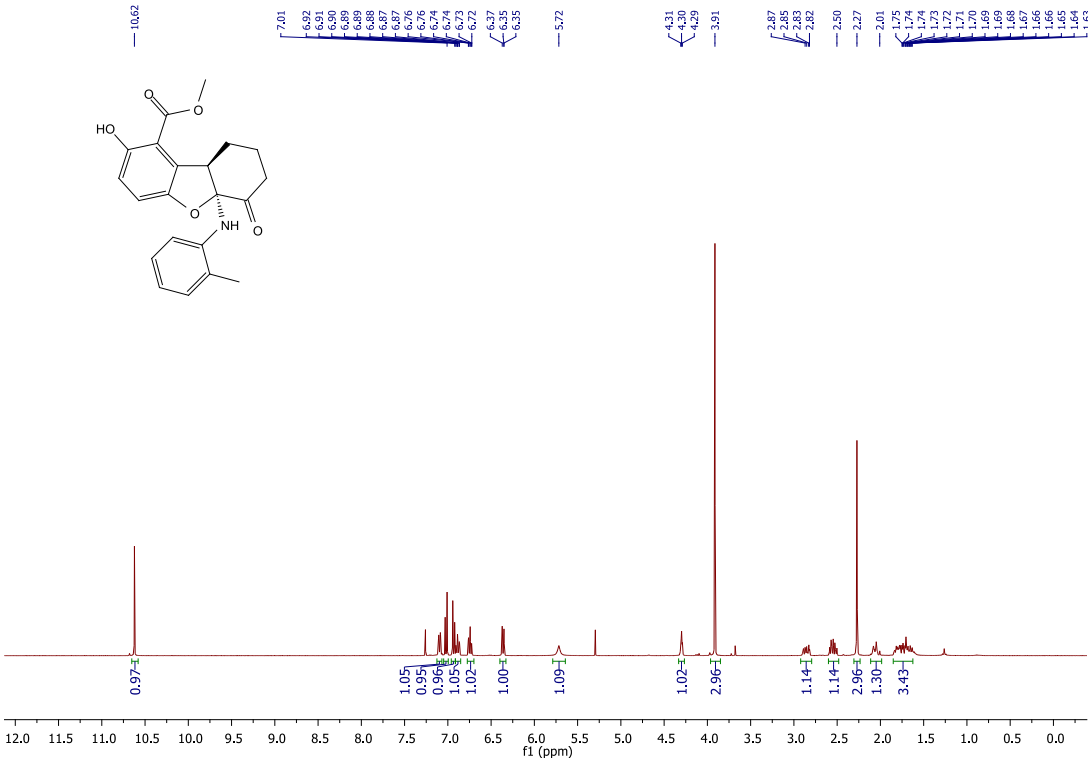
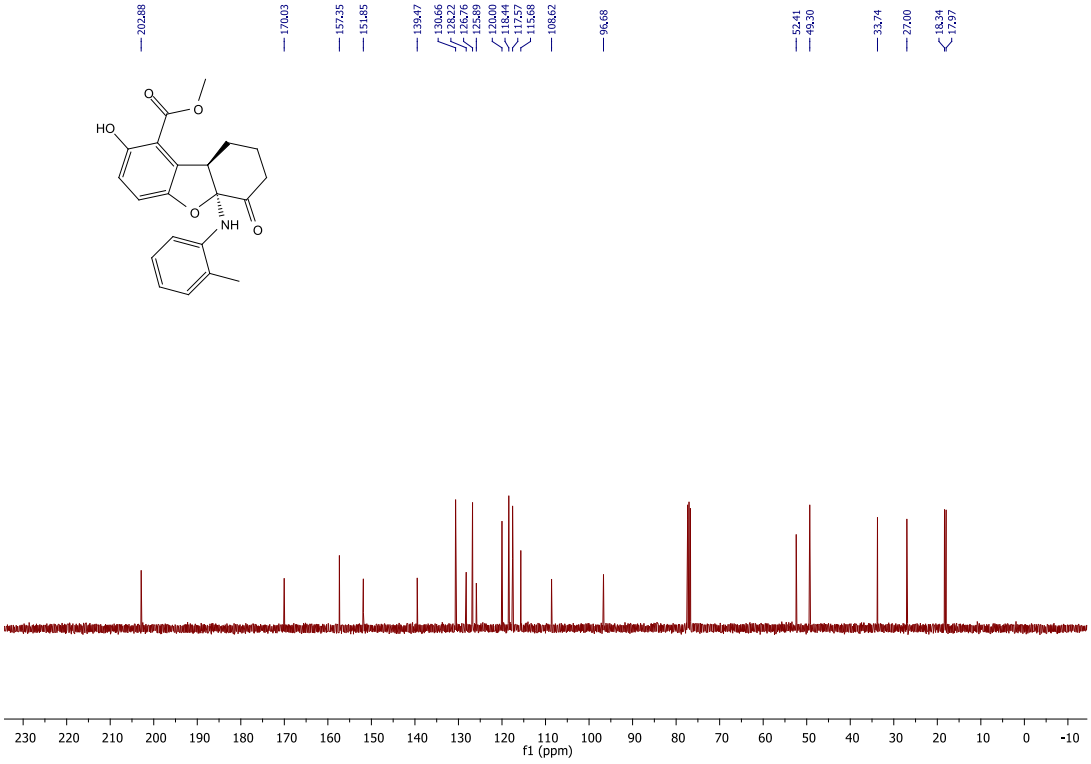
141.55
129.07
128.31
120.35
118.23
117.29
117.48
108.71
96.77
61.84
50.21
34.53
27.42
18.32
14.04
HO
O
O
O
NH
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


HO
O
O
NH
O
0.98
4.13
1.92
1.00
2.03
1.85
1.04
1.67
0.85
1.00
1.04
1.18
1.15
3.31
f1 (ppm)


203.13
169.32
157.50
151.64
141.48
134.40
129.00
128.85
128.79
128.62
120.66
118.39
113.27
117.68
108.43
96.85
67.60
50.01
34.69
27.52
18.23
HO
O
O
NH
O
f1 (ppm)


10.62
7.01
6.92
6.91
6.90
6.89
6.89
6.88
6.87
6.87
6.87
6.76
6.76
6.74
6.74
6.73
6.72
6.37
6.35
6.35
5.72
4.31
4.30
4.29
3.91
2.87
2.85
2.83
2.82
2.50
2.27
2.01
1.75
1.74
1.74
1.73
1.72
1.71
1.70
1.69
1.69
1.68
1.67
1.66
1.66
1.65
1.64
1.63
HO
O
O
O
NH
O
0.97
1.05
0.95
0.96
1.05
1.02
1.00
1.09
1.02
2.96
1.14
1.14
2.96
1.30
3.43
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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108.62
96.68
52.41
49.30
33.74
27.00
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O
NH
O
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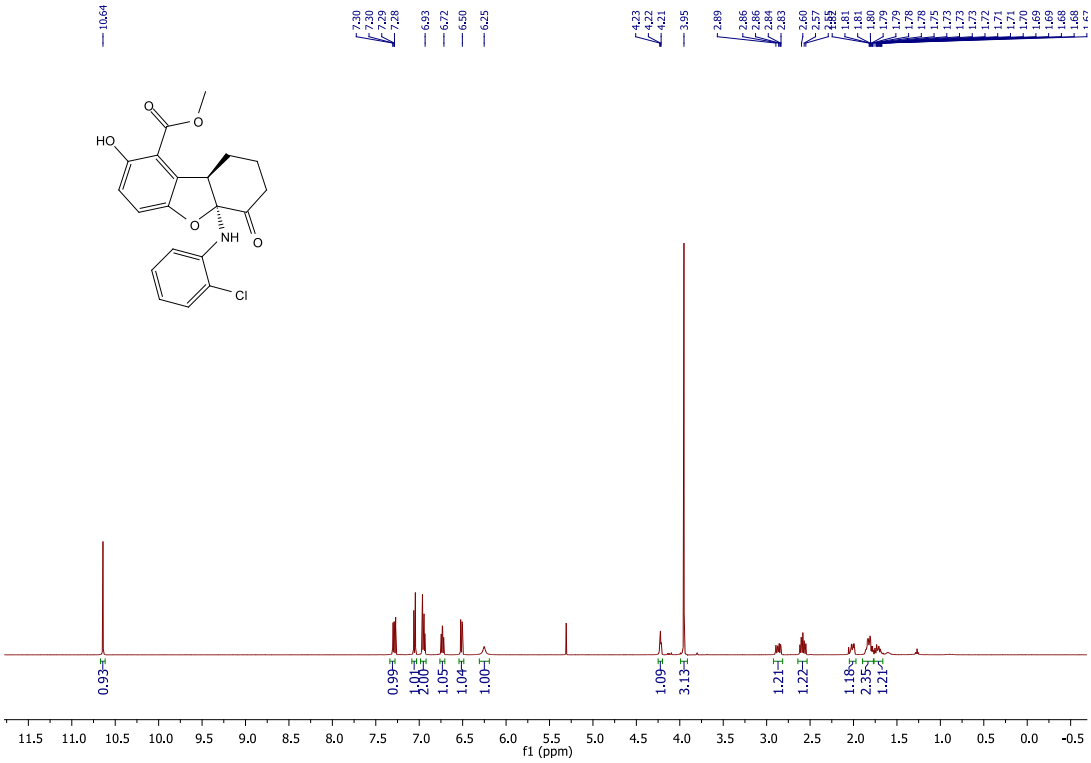
f1 (ppm)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2.86
2.84
2.83
2.60
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1.81
1.80
1.79
1.79
1.78
1.78
1.75
1.73
1.73
1.73
1.72
1.71
1.71
1.70
1.69
1.69
1.68
1.68
HO
O
O
O
NH
O
Cl
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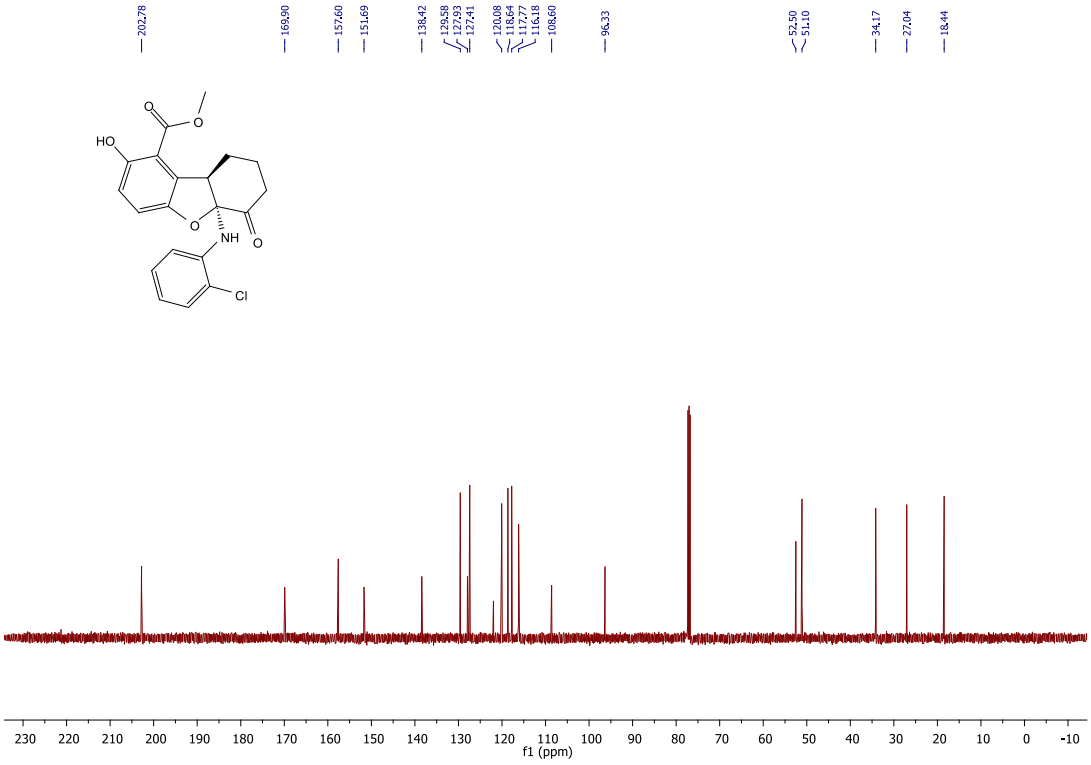
2.00
1.05
1.04
1.00
1.09
3.13
1.21
1.22
1.18
2.35
1.21
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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51.10
34.17
27.04
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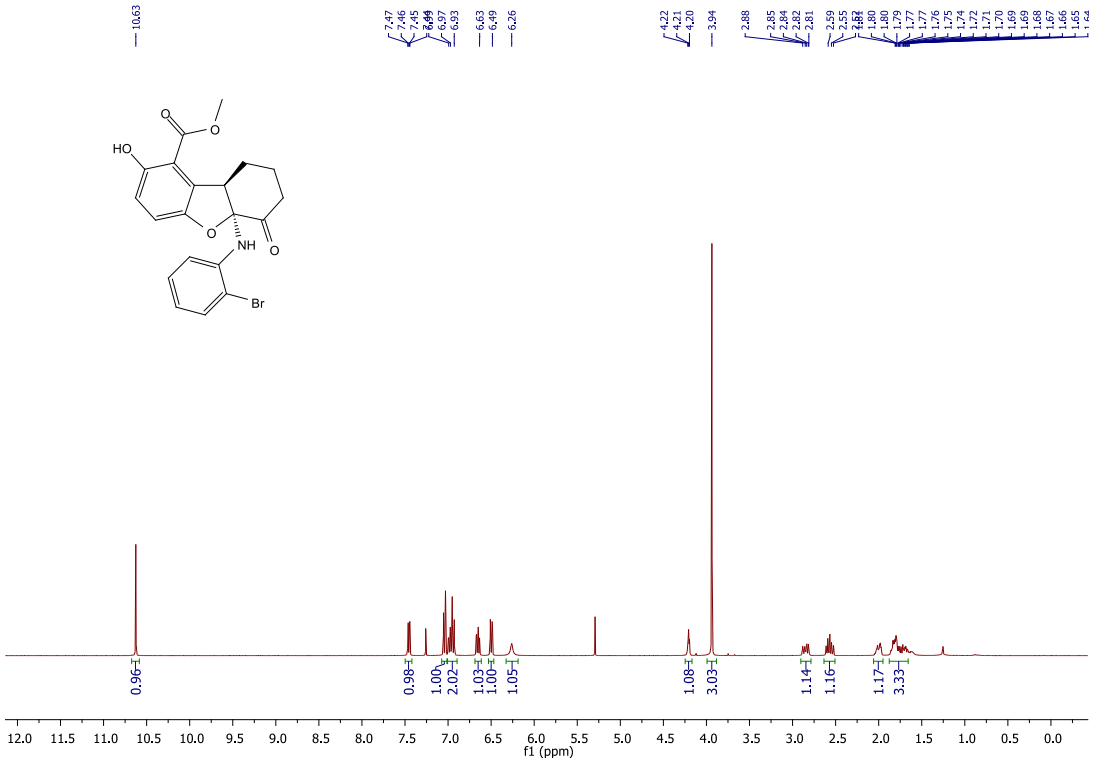
NH
O
Cl
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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2.85
2.84
2.82
2.81
2.59
2.55
1.80
1.79
1.77
1.76
1.75
1.74
1.72
1.71
1.70
1.69
1.68
1.67
1.66
1.65
1.64
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O
NH
O
Br
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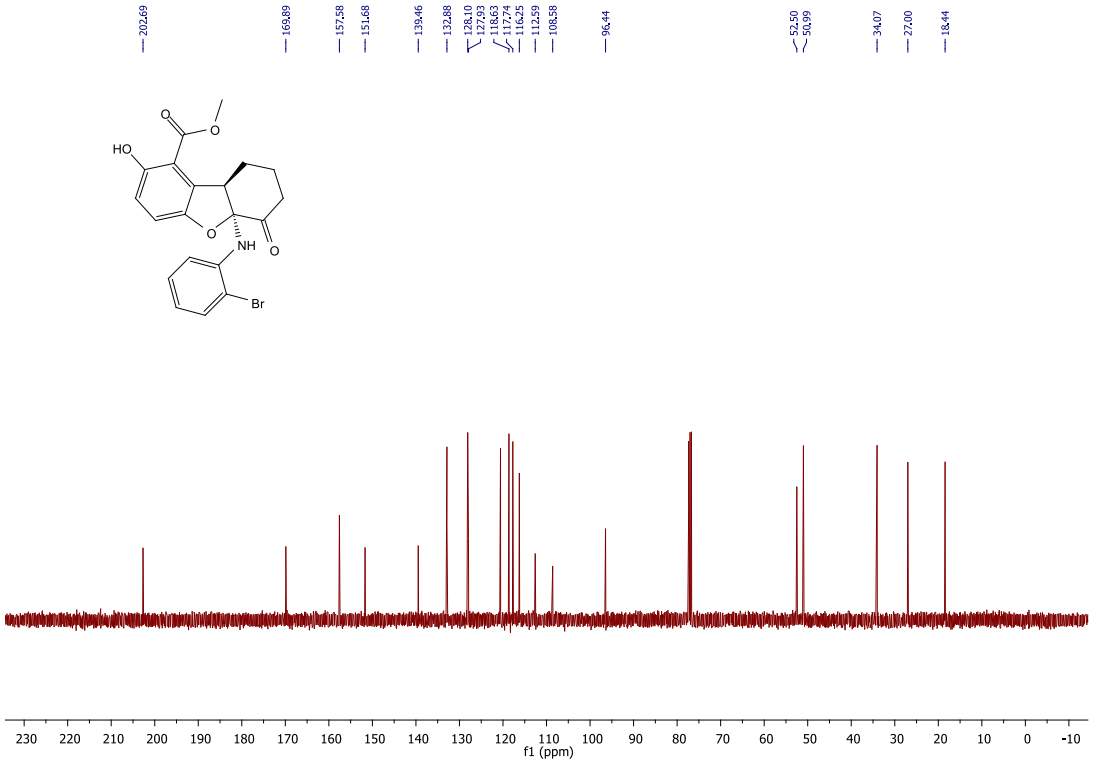
0.98
1.00
2.02
1.03
1.00
1.05
1.08
3.03
1.14
1.16
1.17
3.33
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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108.58
96.44
52.50
50.99
34.07
27.00
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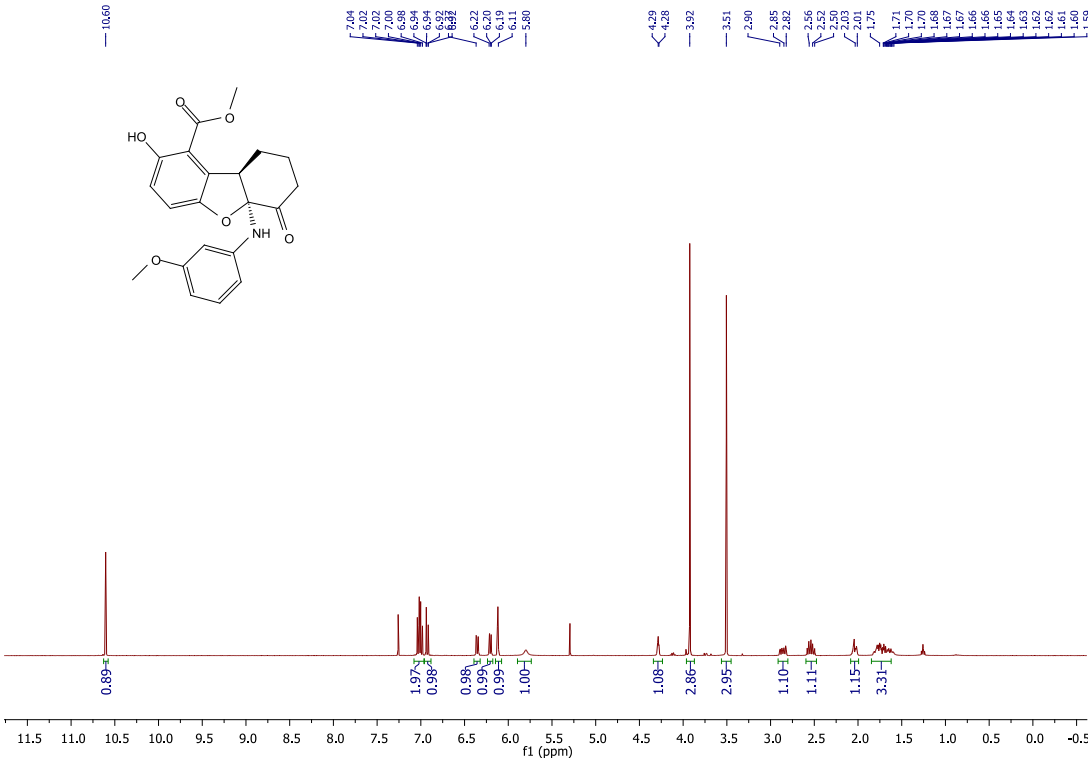
HO
O
O
NH
O
Br
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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5.80
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4.28
3.92
3.51
2.90
2.85
2.82
2.56
2.52
2.50
2.03
2.01
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1.71
1.70
1.70
1.68
1.67
1.67
1.66
1.66
1.65
1.64
1.63
1.62
1.62
1.61
1.60
HO
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O
O
NH
O
O
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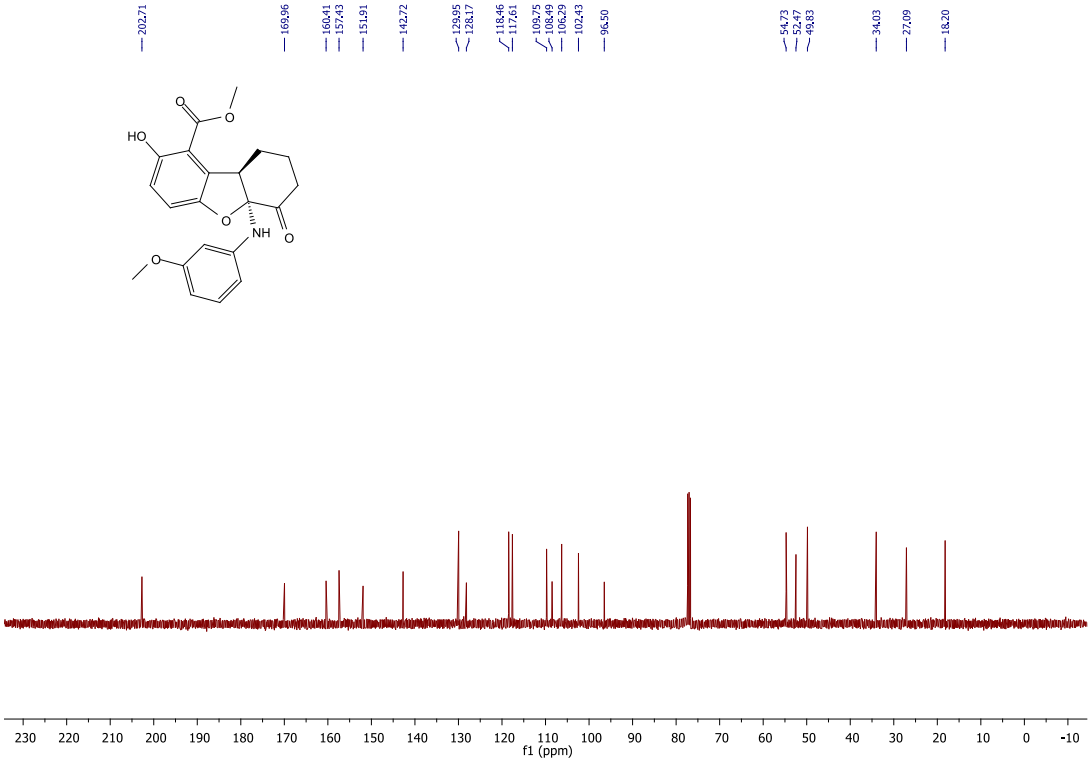
0.98
0.98
0.99
0.99
1.00
1.08
2.86
2.95
1.10
1.11
1.15
3.31
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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52.47
49.83
34.03
27.09
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O
NH
O
O
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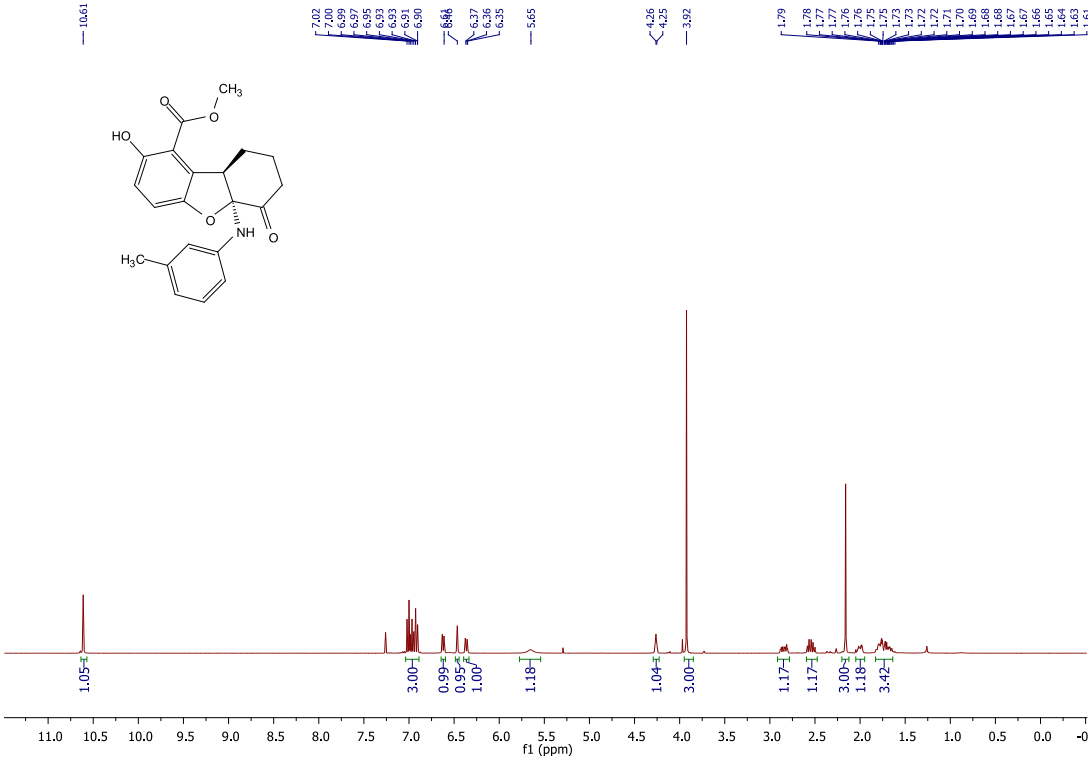
f1 (ppm)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1.68
1.67
1.67
1.66
1.65
1.64
1.63
1.61
CH3
O
O
HO
O
NH
O
H3C
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3.00
0.99
0.95
1.00
1.18
1.04
3.00
1.17
1.17
3.00
1.18
3.42
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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3.0
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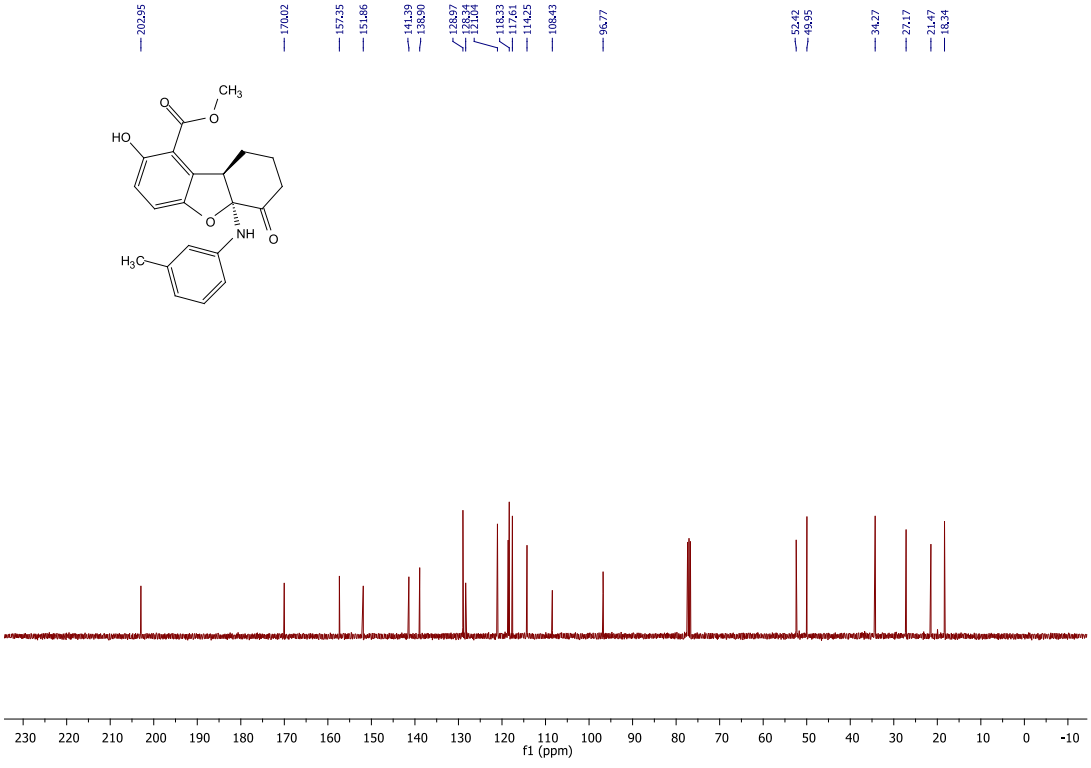
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)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96.77
52.42
49.95
34.27
27.17
21.47
18.34
CH3
O
O
HO
O
NH
O
H3C
230
220
210
200
190
180
170
160
150
140
130
120
110
100
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80
70
60
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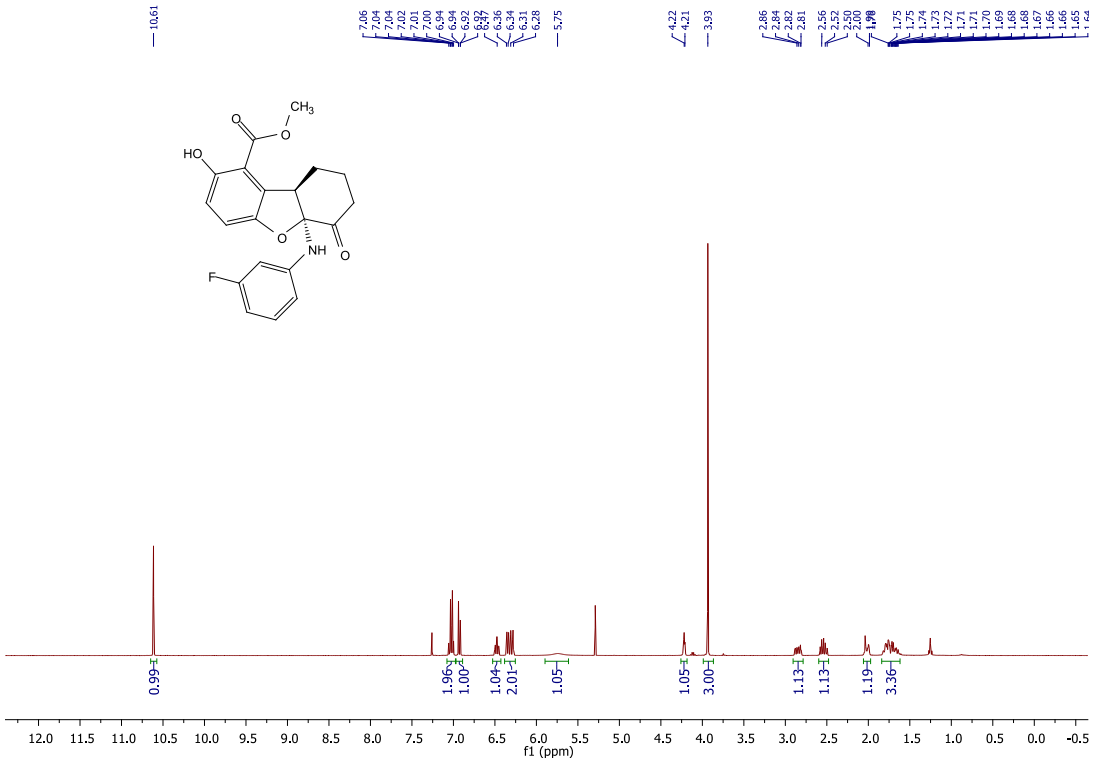
40
30
20
10
0
-10
f1 (ppm)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5.75
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4.21
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2.82
2.81
2.56
2.52
2.50
2.00
1.78
1.75
1.75
1.74
1.73
1.72
1.71
1.71
1.70
1.69
1.68
1.68
1.67
1.66
1.66
1.65
1.64
CH3
O
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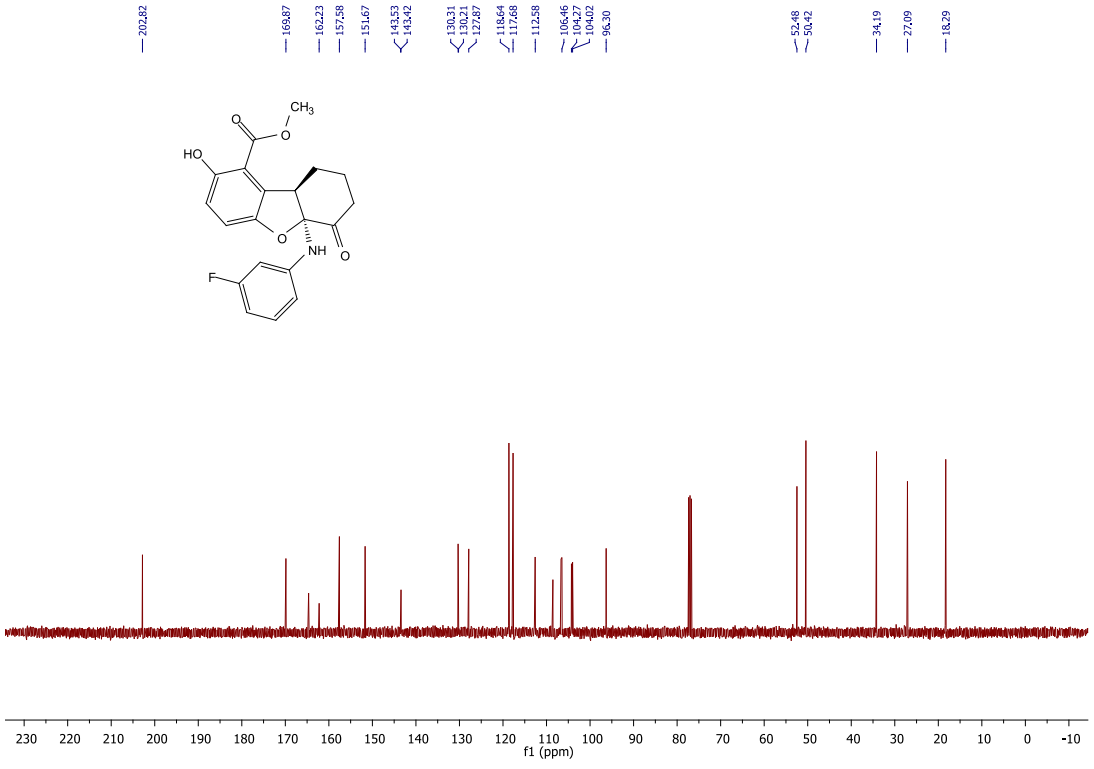
HO
O
NH
O
F
0.99
1.96
1.00
1.04
2.01
1.05
1.05
3.00
1.13
1.13
1.19
3.36
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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104.02
96.30
52.48
50.42
34.19
27.09
18.29
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HO
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NH
O
F
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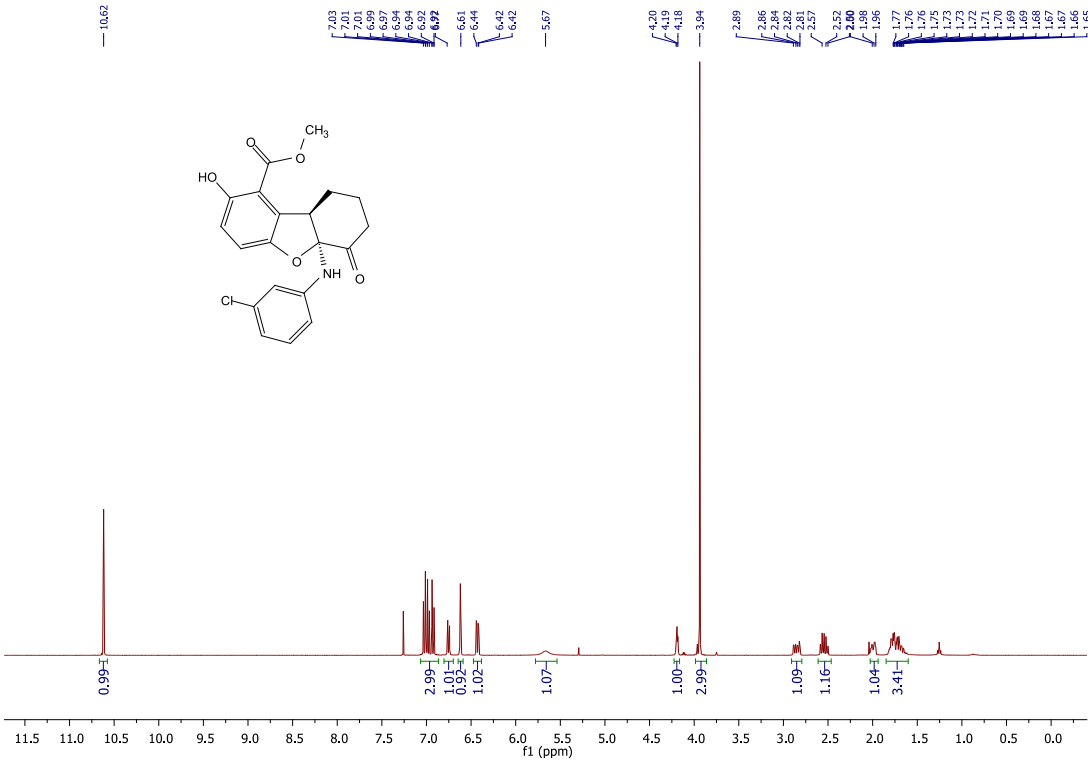
f1 (ppm)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6.42
5.67
4.20
4.19
4.18
3.94
2.89
2.86
2.84
2.82
2.81
2.57
2.52
2.00
1.98
1.96
1.77
1.76
1.76
1.75
1.73
1.73
1.72
1.71
1.70
1.69
1.69
1.68
1.67
1.67
1.66
HO
O
O
CH3
O
NH
O
Cl
0.99
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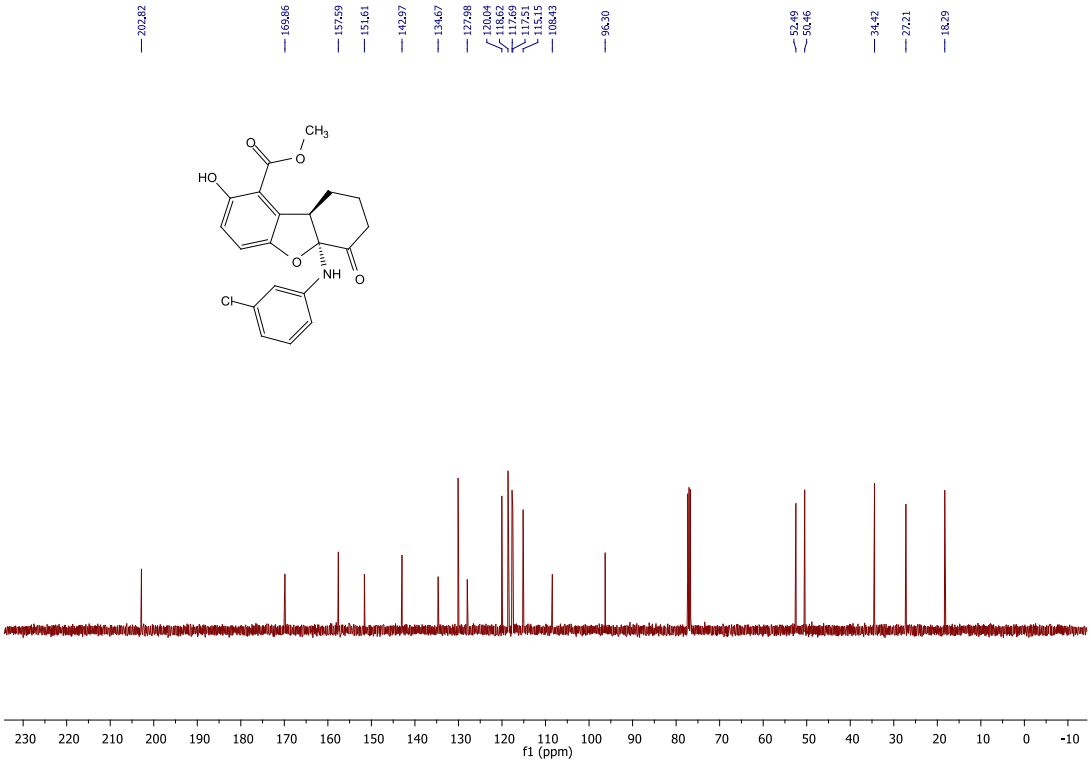
f1 (ppm)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27.21
18.29
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CH3
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NH
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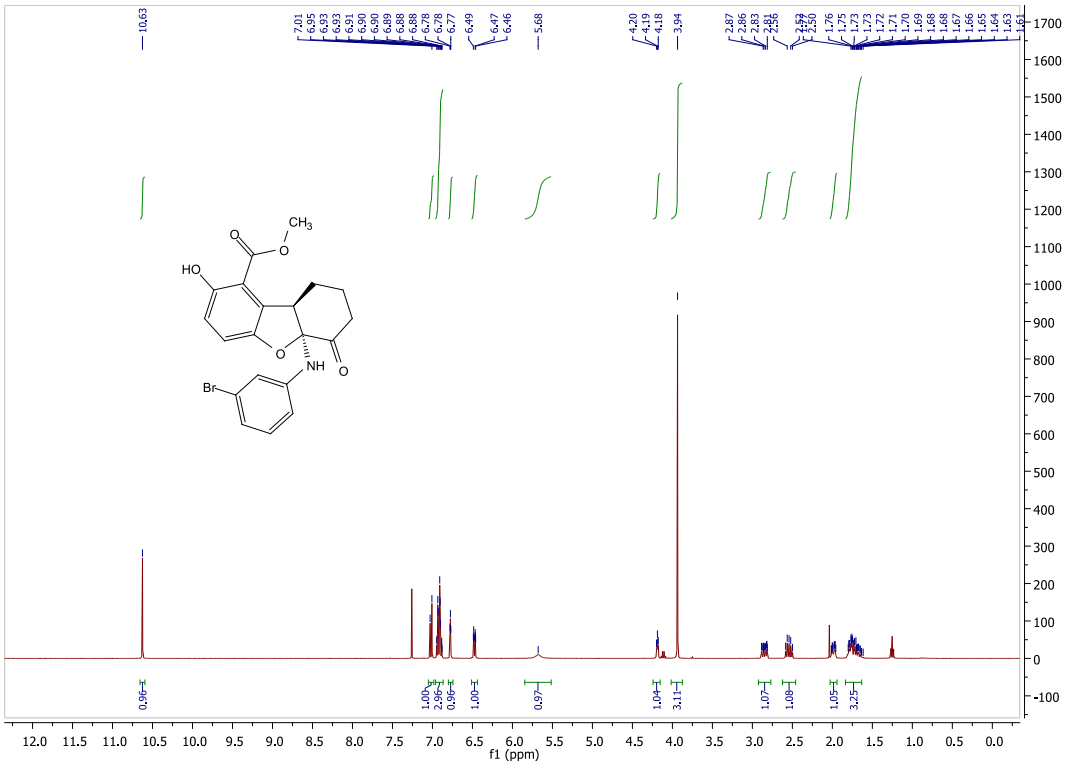
Cl
f1 (ppm)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4.18
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1.65
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1.63
1.61
CH3
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HO
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NH
O
Br
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1.08
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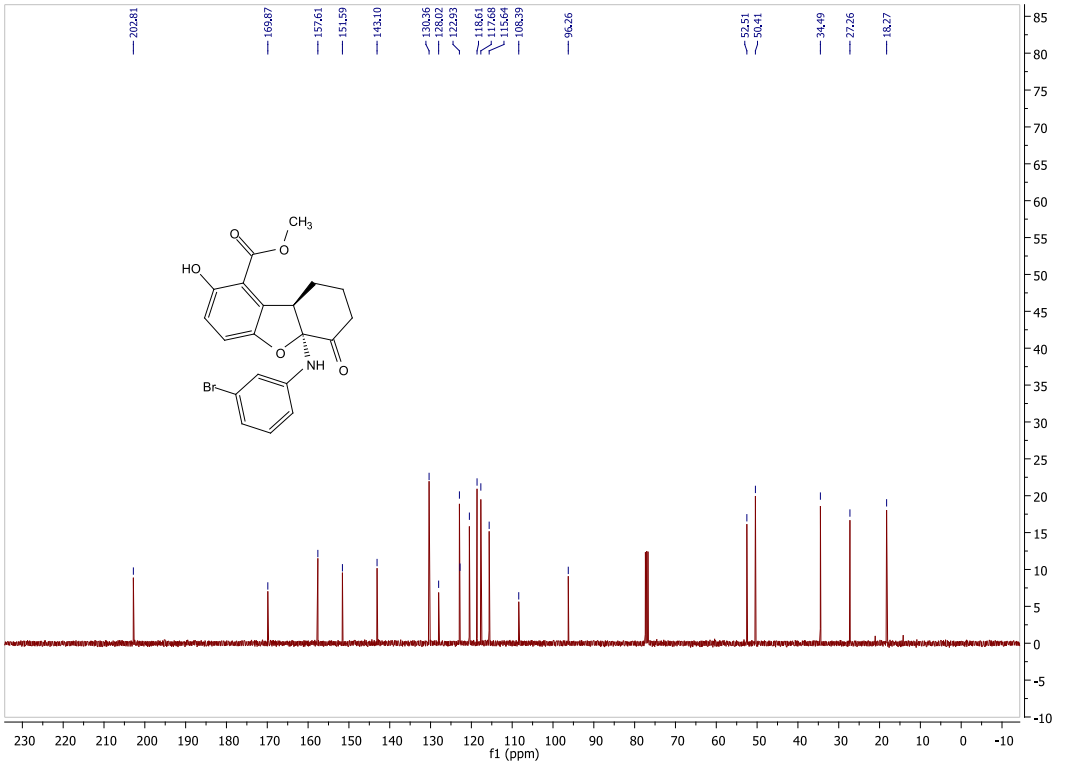
f1 (ppm)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27.26
18.27
CH3
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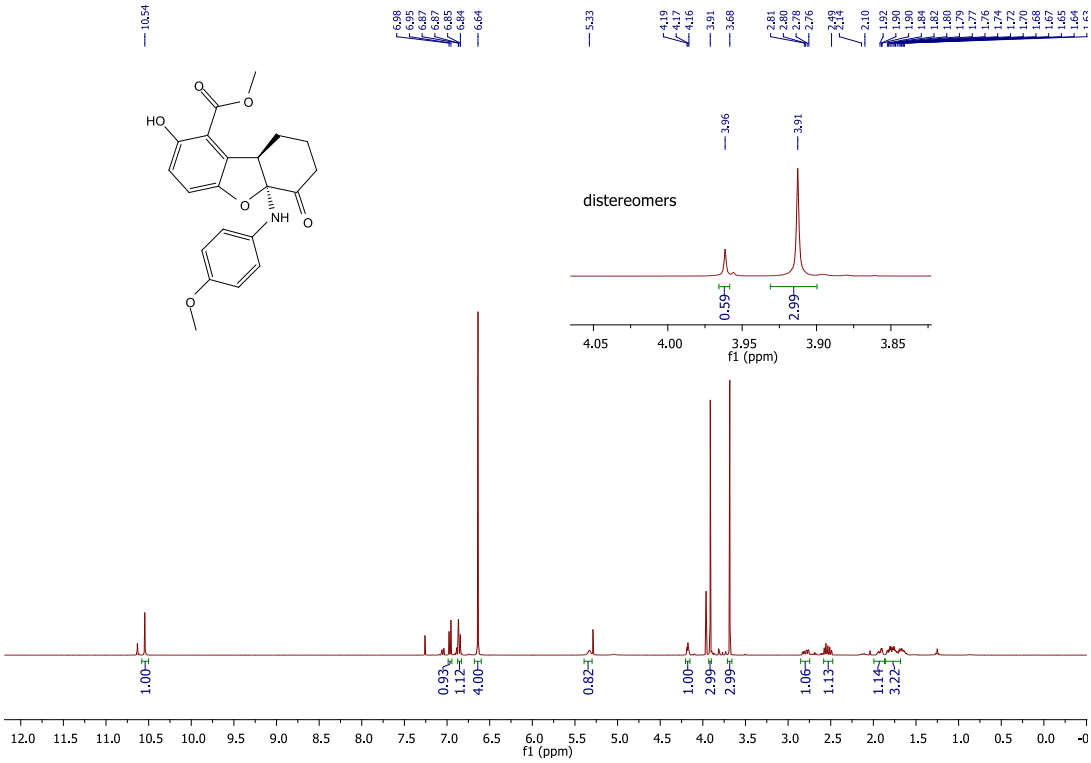
O
HO
O
NH
O
Br
f1 (ppm)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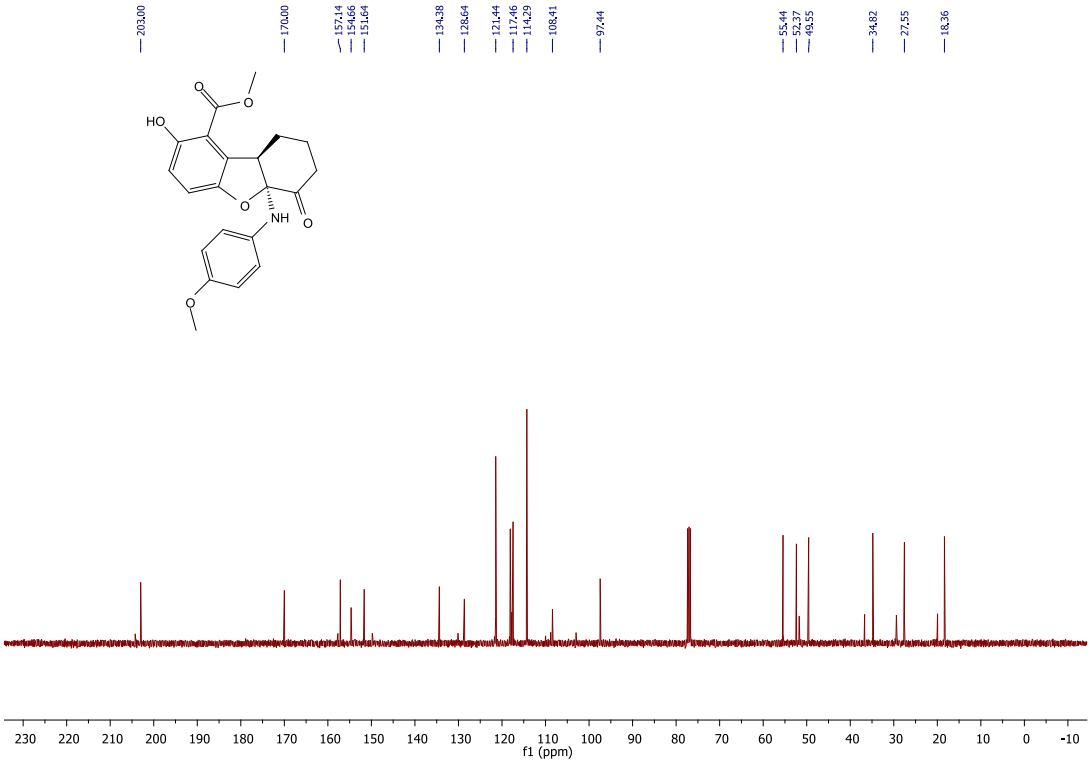
f1 (ppm)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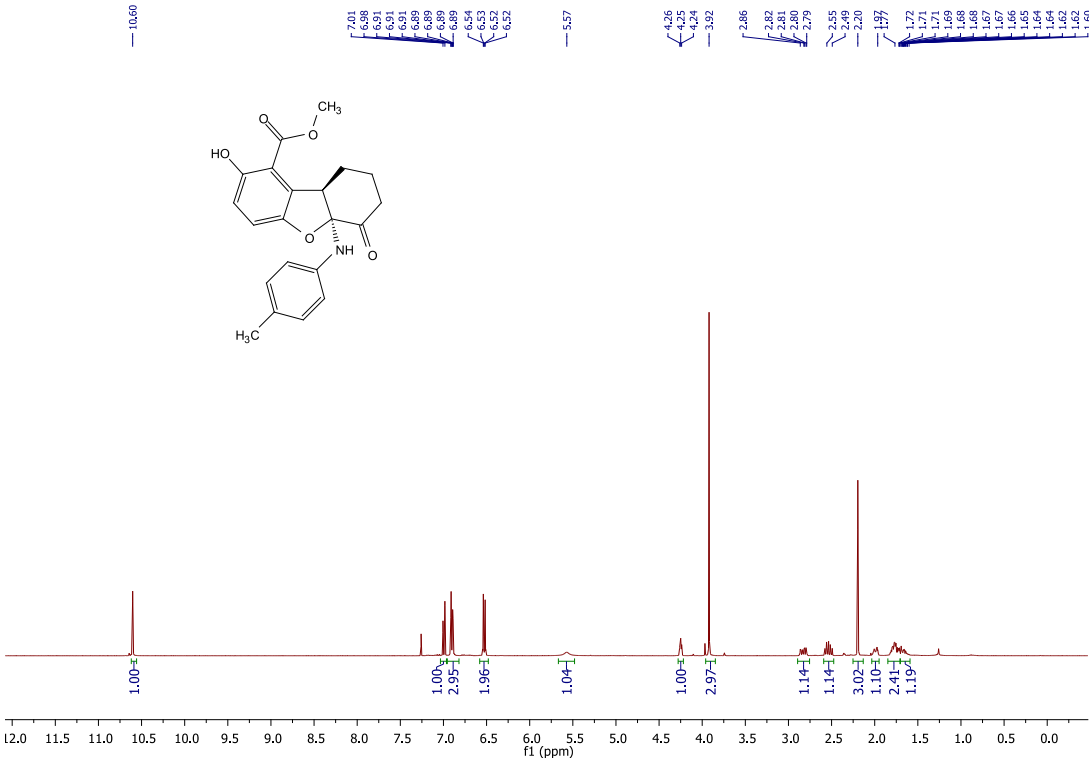
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5.57
4.26
4.25
4.24
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1.69
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1.68
1.67
1.67
1.66
1.65
1.64
1.64
1.62
1.62
1.61
HO
O
O
CH3
O
NH
O
H3C
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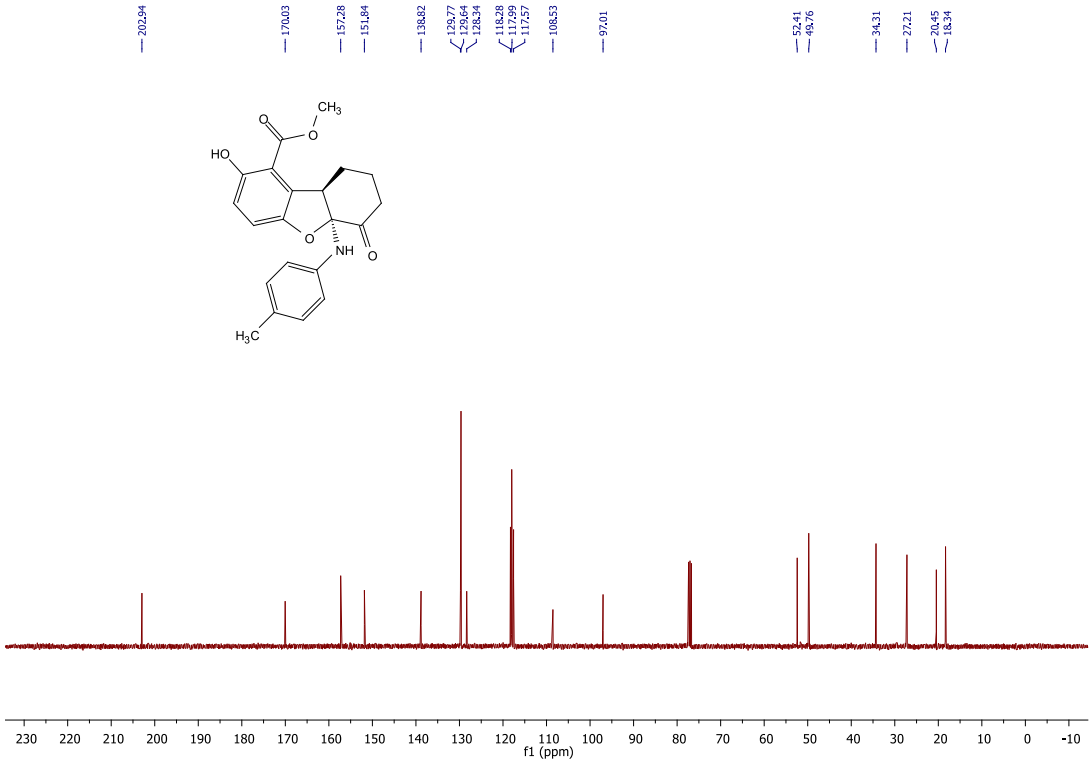
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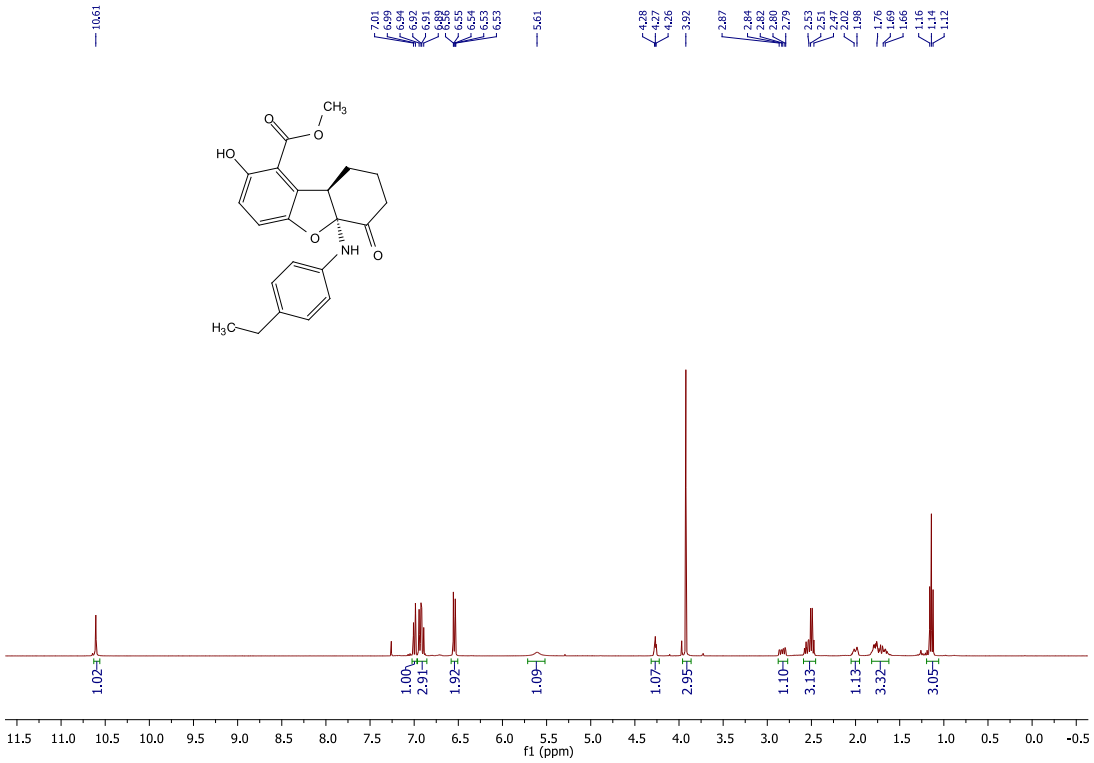
CH3
O
NH
O
H3C
f1 (ppm)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2.80
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2.53
2.51
2.47
2.02
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1.76
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1.16
1.14
1.12
HO
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O
CH3
NH
O
H3C
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1.13
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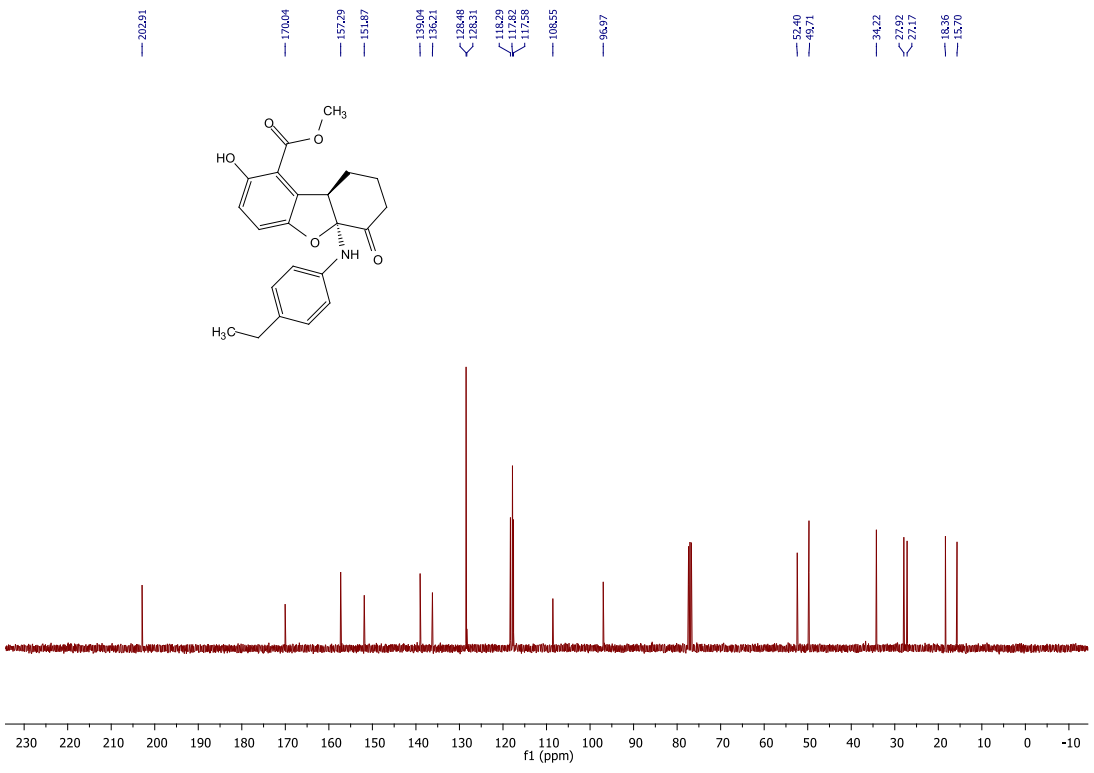
3.05
f1 (ppm)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96.97
52.40
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27.17
18.36
15.70
HO
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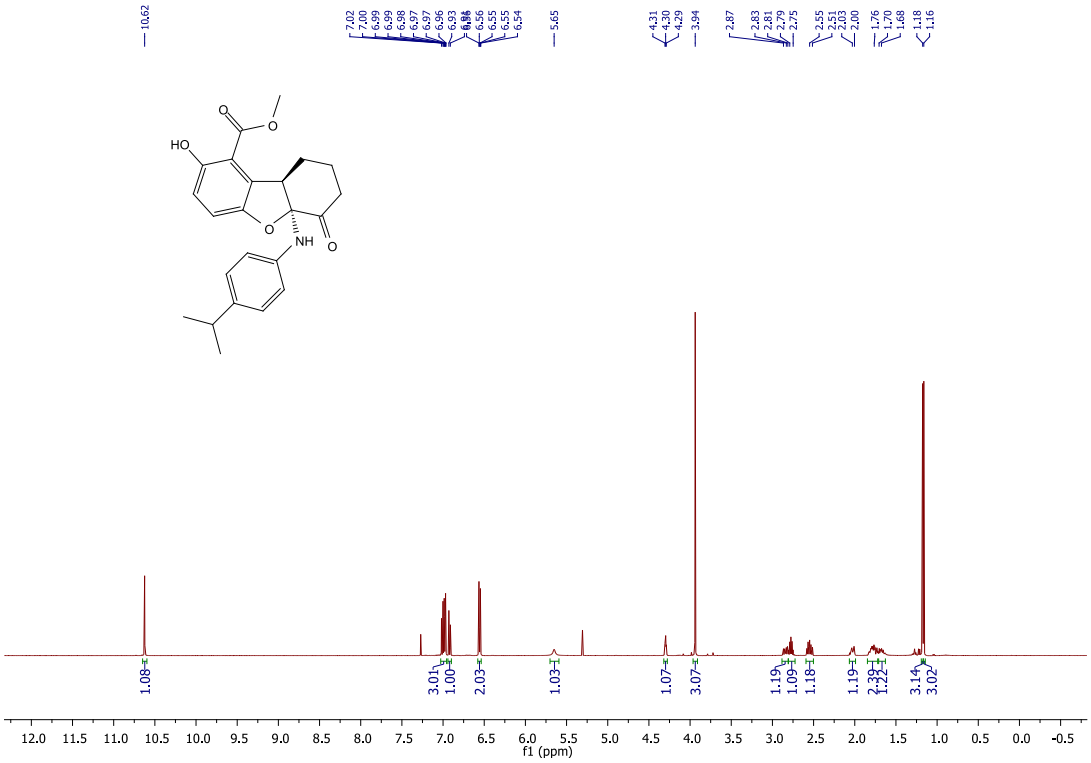
O
CH3
NH
O
H3C
f1 (ppm)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6.54
5.65
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4.30
4.29
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1.16
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NH
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3.01
1.00
2.03
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1.22
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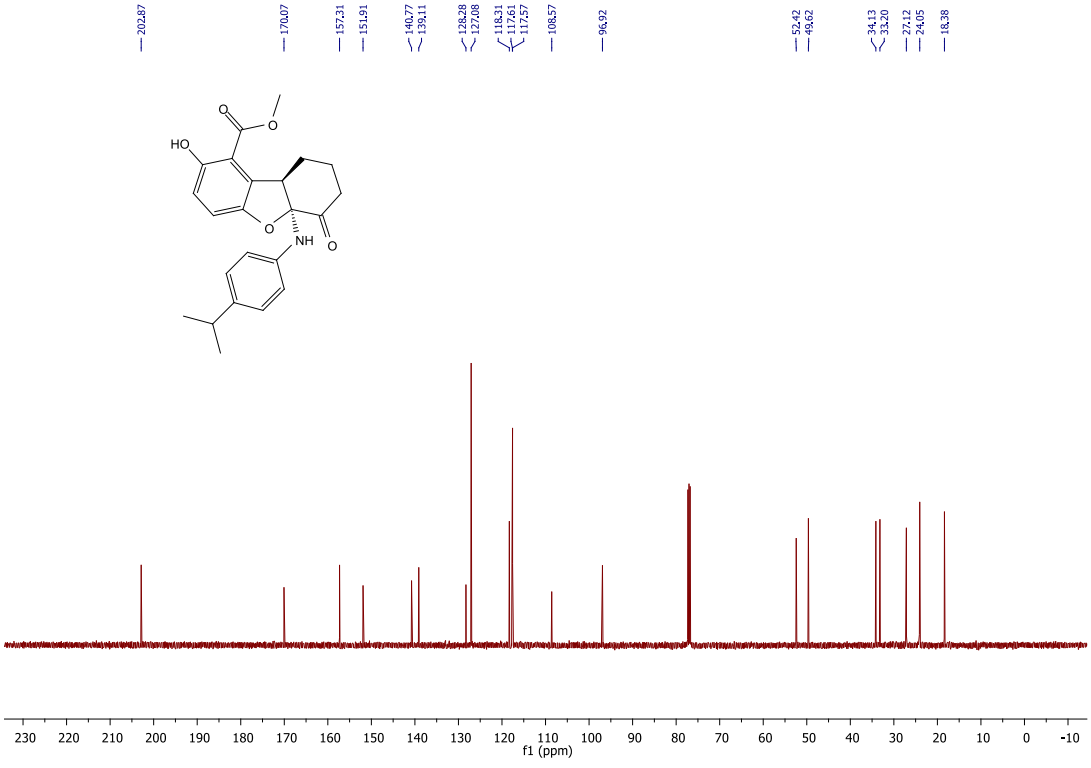
3.02
f1 (ppm)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24.05
18.38
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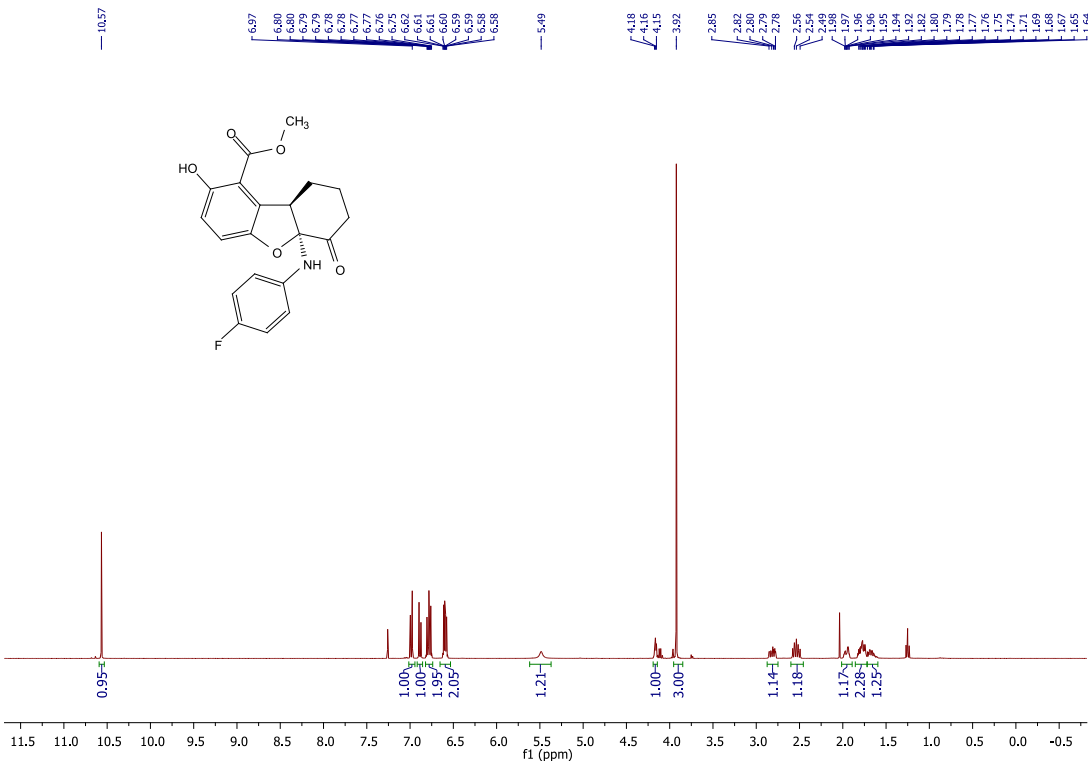
O
NH
O
f1 (ppm)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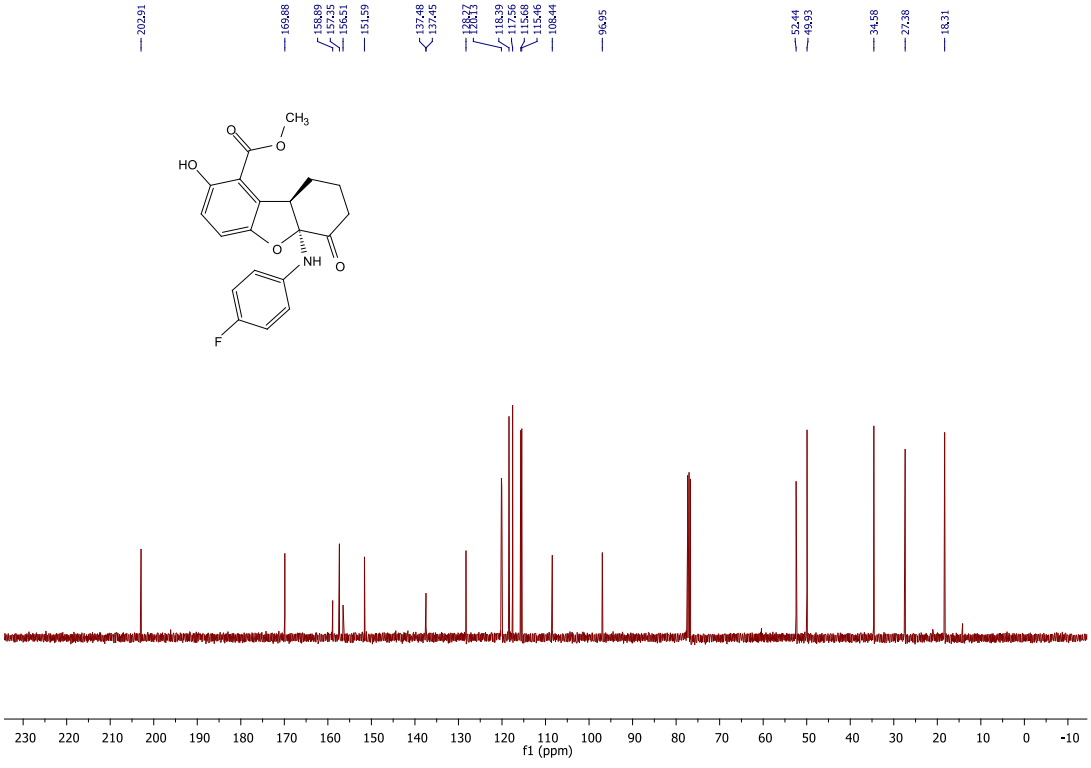
6.79
6.78
6.78
6.78
6.77
6.77
6.77
6.76
6.75
6.62
6.61
6.61
6.60
6.59
6.59
6.58
6.58
5.49
4.18
4.16
4.15
3.92
2.85
2.82
2.80
2.79
2.78
2.56
2.54
2.49
1.98
1.97
1.96
1.96
1.95
1.94
1.92
1.82
1.80
1.79
1.78
1.77
1.76
1.75
1.74
1.71
1.69
1.68
1.67
1.65
1.64
CH3
O
O
HO
O
NH
O
F
0.95
1.00
1.00
1.95
2.05
1.21
1.00
3.00
1.14
1.18
1.17
2.28
1.25
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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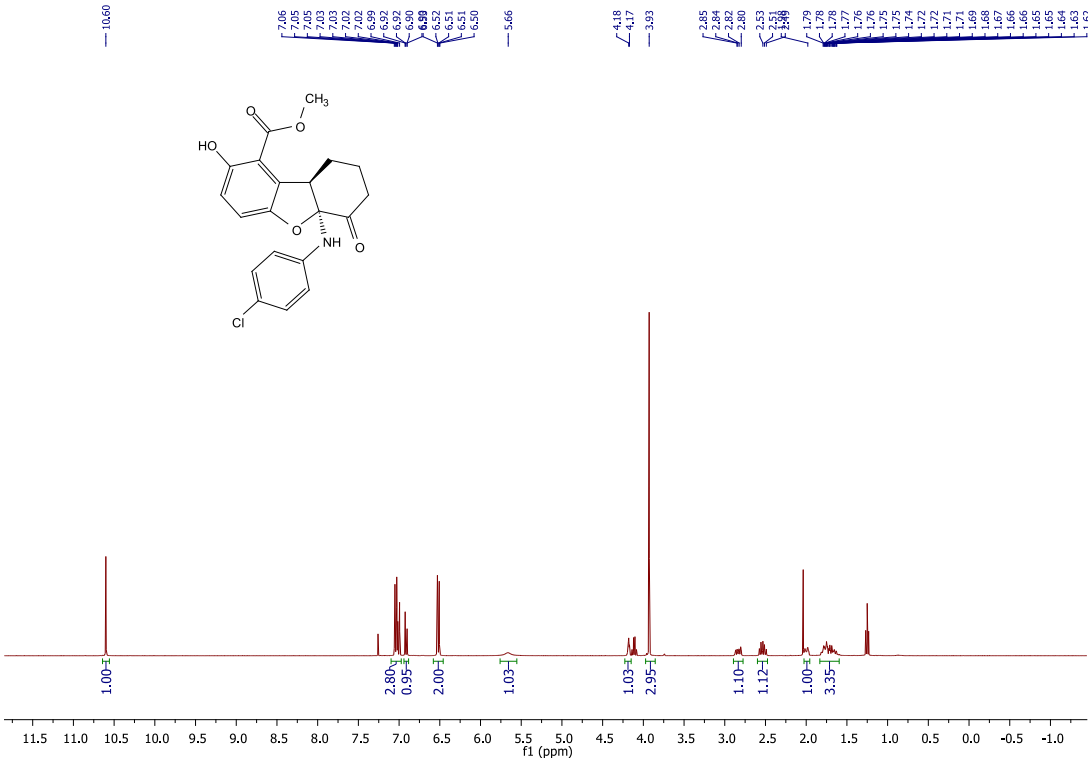
117.56
115.68
115.46
108.44
96.95
52.44
49.93
34.58
27.38
18.31
CH3
O
O
HO
O
NH
O
F
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.52
6.51
6.51
6.50
5.66
4.18
4.17
3.93
2.85
2.84
2.82
2.80
2.53
1.79
1.78
1.78
1.77
1.76
1.76
1.75
1.75
1.74
1.72
1.72
1.72
1.71
1.71
1.69
1.68
1.67
1.66
1.66
1.65
1.65
1.64
1.63
HO
O
O
CH3
O
NH
O
Cl
1.00
2.80
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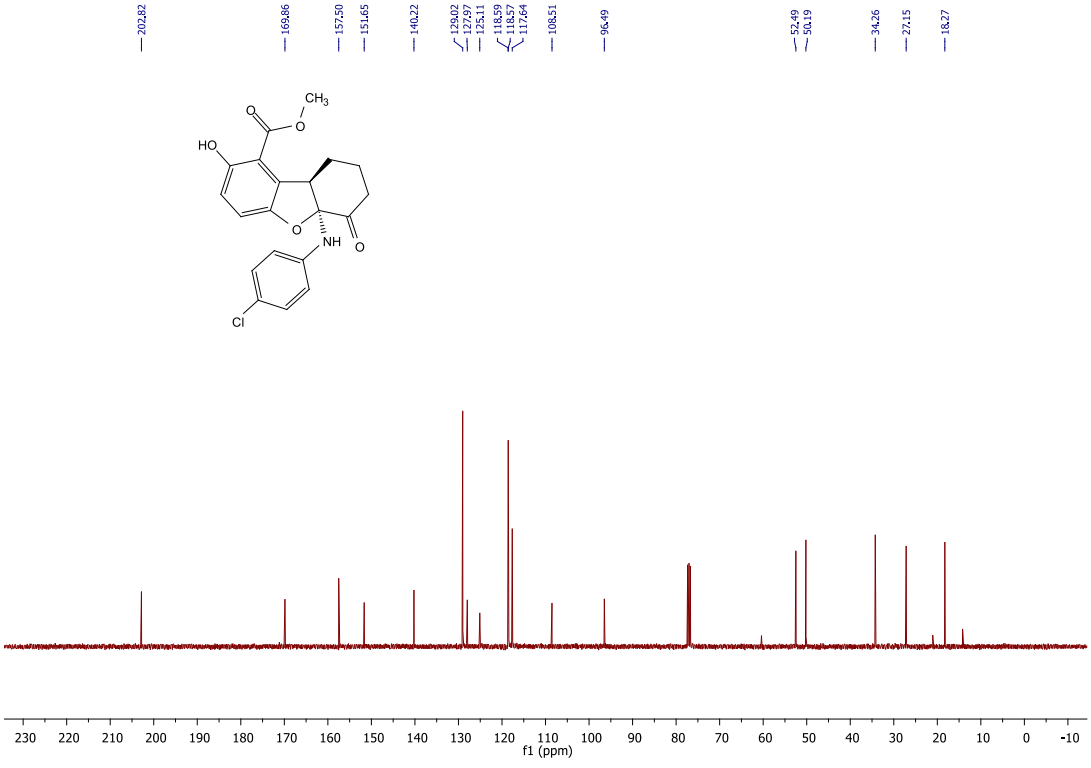
2.00
1.03
1.03
2.95
1.10
1.12
1.00
3.35
f1 (ppm)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34.26
27.15
18.27
HO
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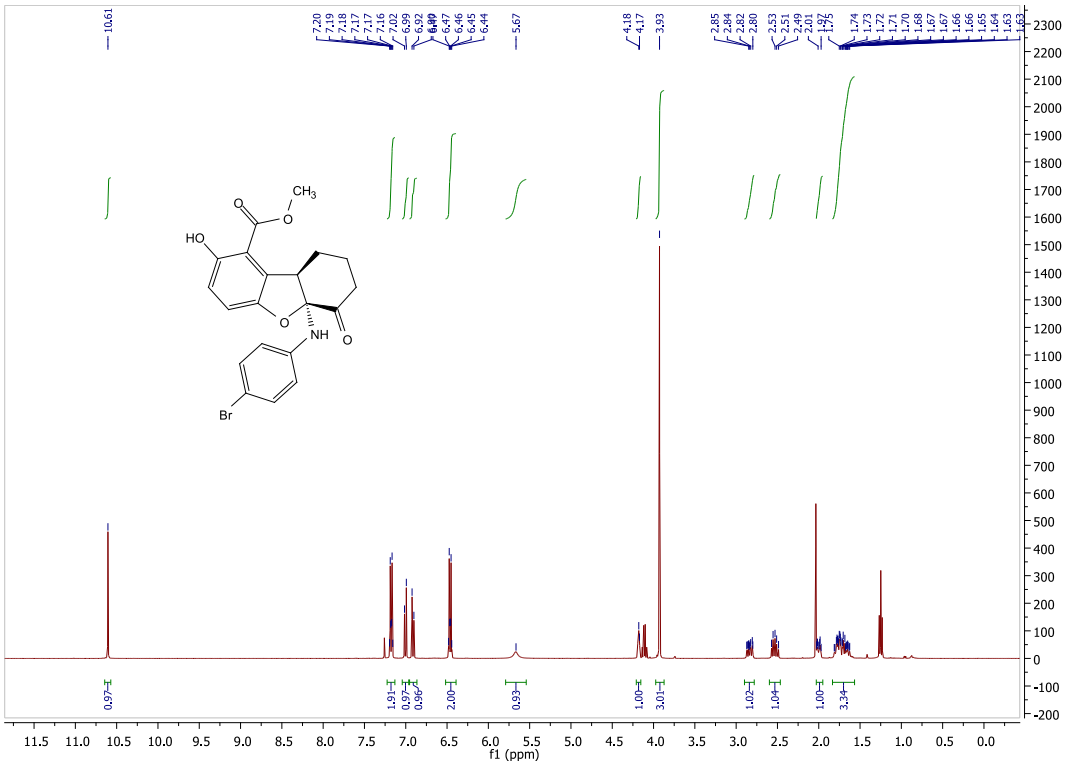
O
CH3
O
NH
O
Cl
f1 (ppm)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6.46
6.45
6.44
5.67
4.18
4.17
3.93
2.85
2.84
2.82
2.80
2.53
2.51
2.49
2.01
1.97
1.75
1.74
1.73
1.72
1.71
1.70
1.68
1.67
1.67
1.66
1.66
1.65
1.64
1.63
1.63
0.97
1.91
0.97
0.96
2.00
0.93
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1.04
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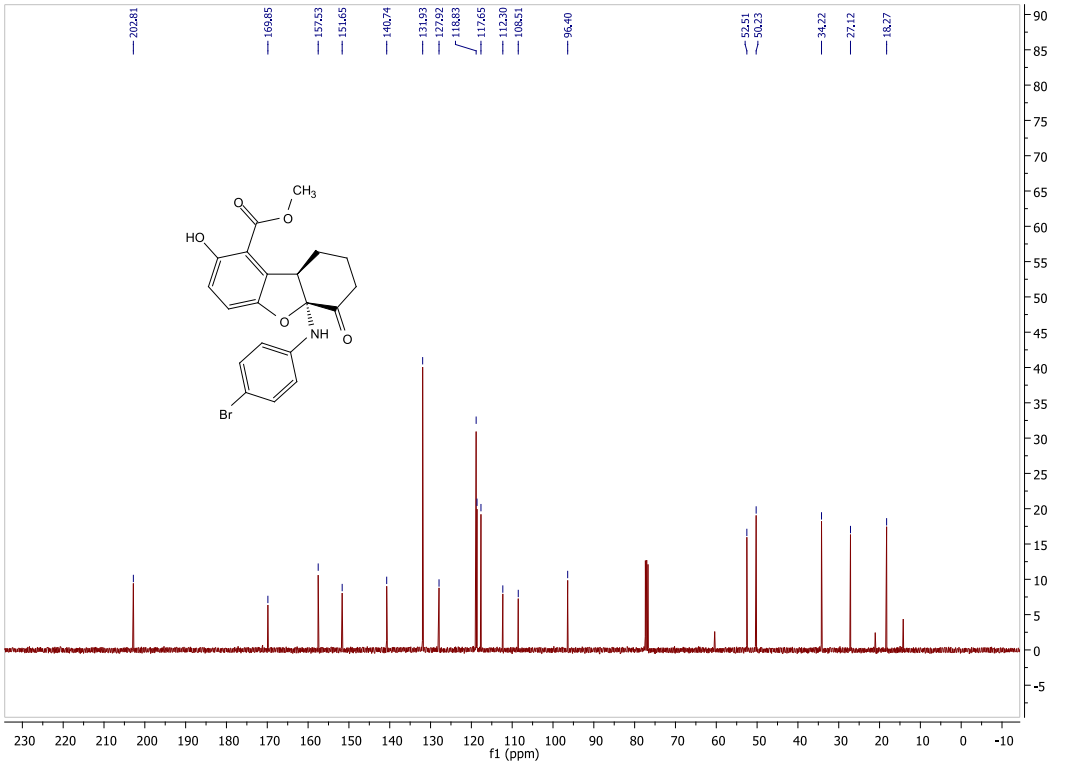
3.34
HO
O
O
CH3
O
NH
O
Br
f1 (ppm)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108.51
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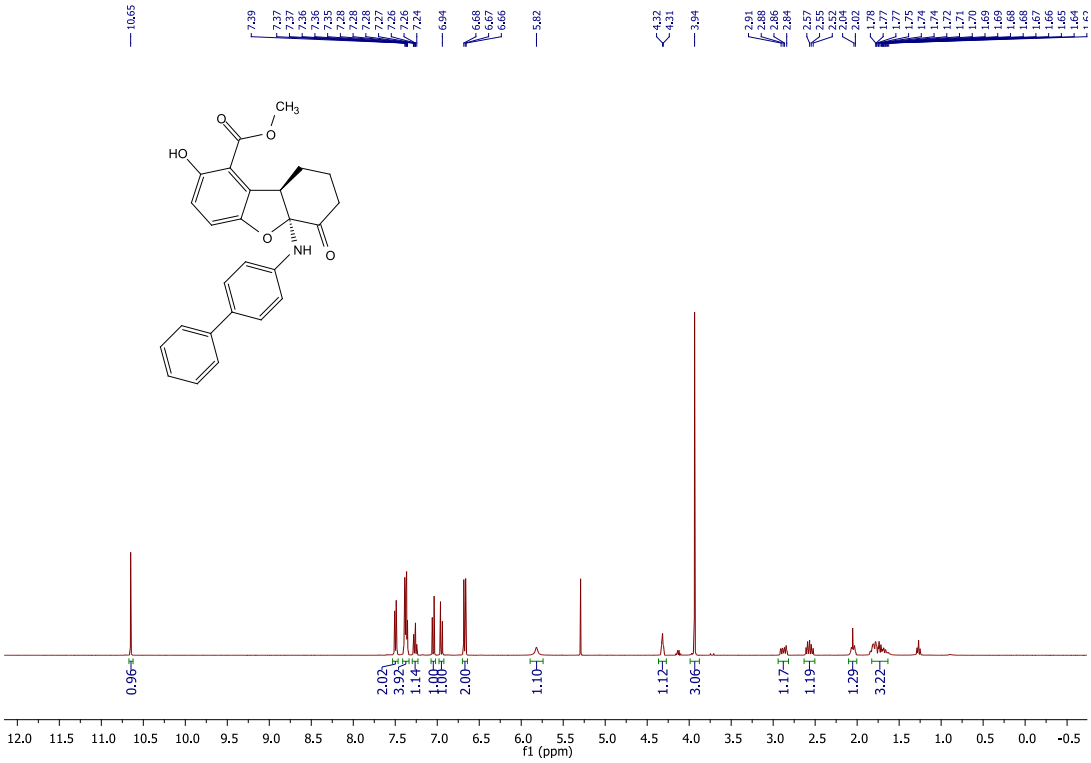
34.22
27.12
18.27
HO
O
O
CH3
O
NH
O
Br
f1 (ppm)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7.28
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7.26
7.26
7.24
6.94
6.68
6.67
6.66
5.82
4.32
4.31
3.94
2.91
2.88
2.86
2.84
2.57
2.55
2.52
2.04
2.02
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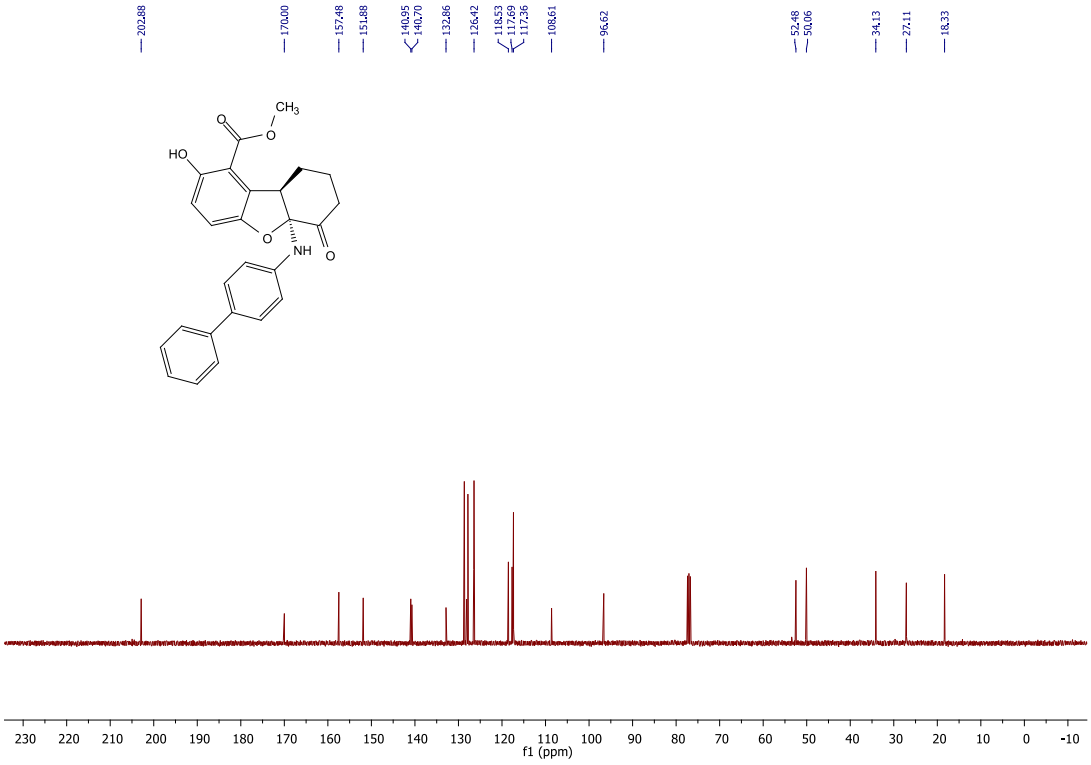
1.69
1.69
1.68
1.68
1.67
1.66
1.65
1.64
HO
O
O
CH3
O
NH
O
0.96
2.02
3.92
1.14
1.00
1.00
2.00
1.10
1.12
3.06
1.17
1.19
1.29
3.22
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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117.69
117.36
108.61
96.62
52.48
50.06
34.13
27.11
18.33
HO
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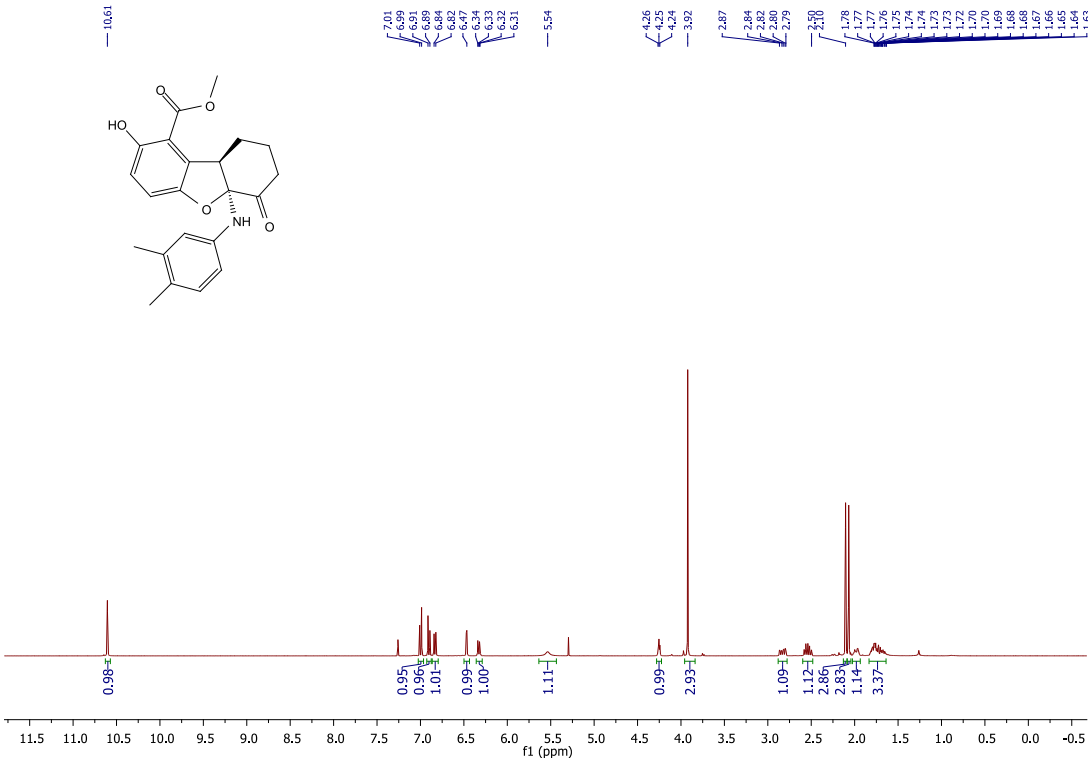
O
CH3
O
NH
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.47
6.34
6.33
6.32
6.31
5.54
4.26
4.25
4.24
3.92
2.87
2.84
2.82
2.80
2.79
2.10
1.78
1.77
1.77
1.76
1.75
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1.73
1.73
1.72
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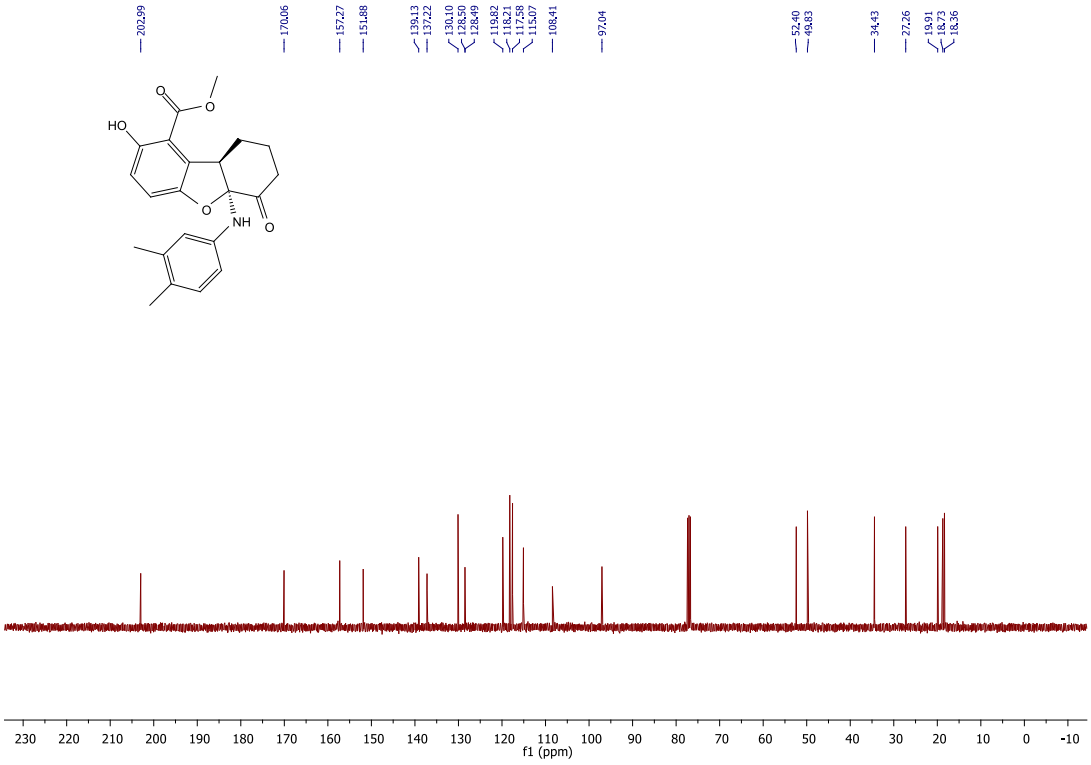
1.70
1.69
1.68
1.68
1.67
1.66
1.65
1.64
HO
O
O
NH
O
0.98
0.95
0.96
1.01
0.99
1.00
1.11
0.99
2.93
1.09
1.12
2.86
2.83
1.14
3.37
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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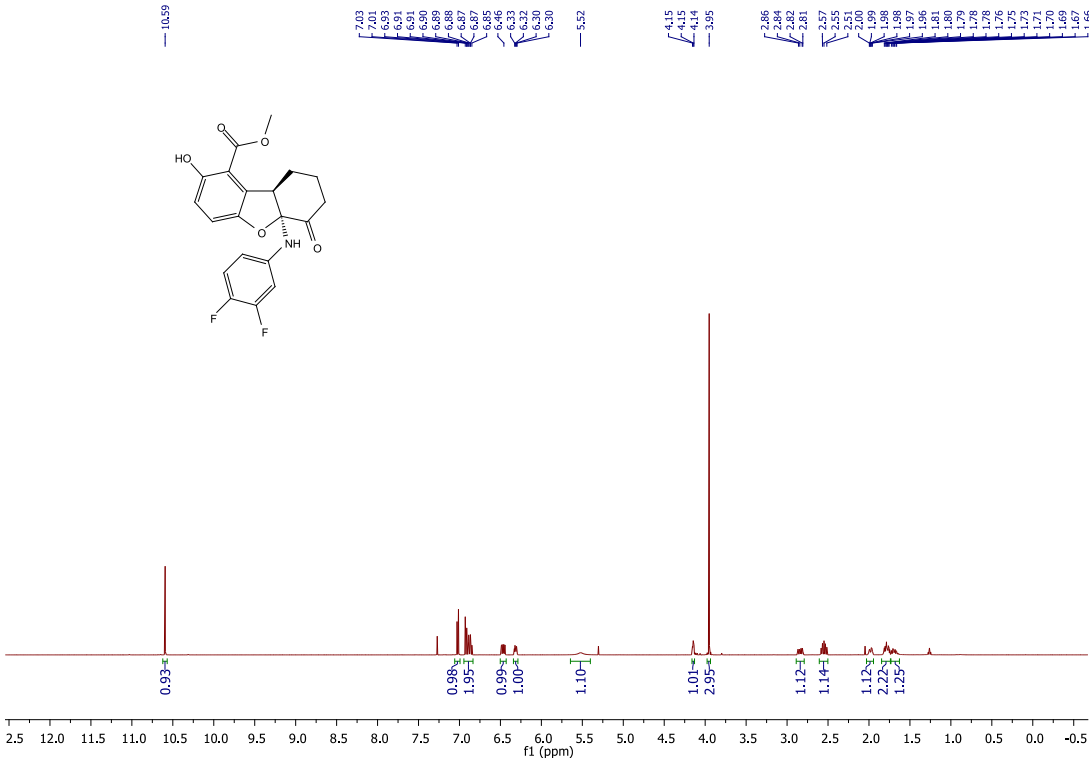
137.22
130.10
128.50
128.49
115.82
116.21
117.58
115.07
108.41
97.04
52.40
49.83
34.43
27.26
19.91
18.73
18.36
HO
O
O
NH
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.89
6.88
6.87
6.87
6.55
6.46
6.33
6.32
6.30
6.30
5.52
4.15
4.15
4.14
3.95
2.86
2.84
2.82
2.81
2.57
2.55
2.51
2.00
1.99
1.98
1.98
1.97
1.96
1.81
1.80
1.79
1.78
1.78
1.76
1.75
1.73
1.71
1.70
1.69
1.67
1.64
HO
O
O
O
NH
O
F
F
0.93
0.98
1.95
0.99
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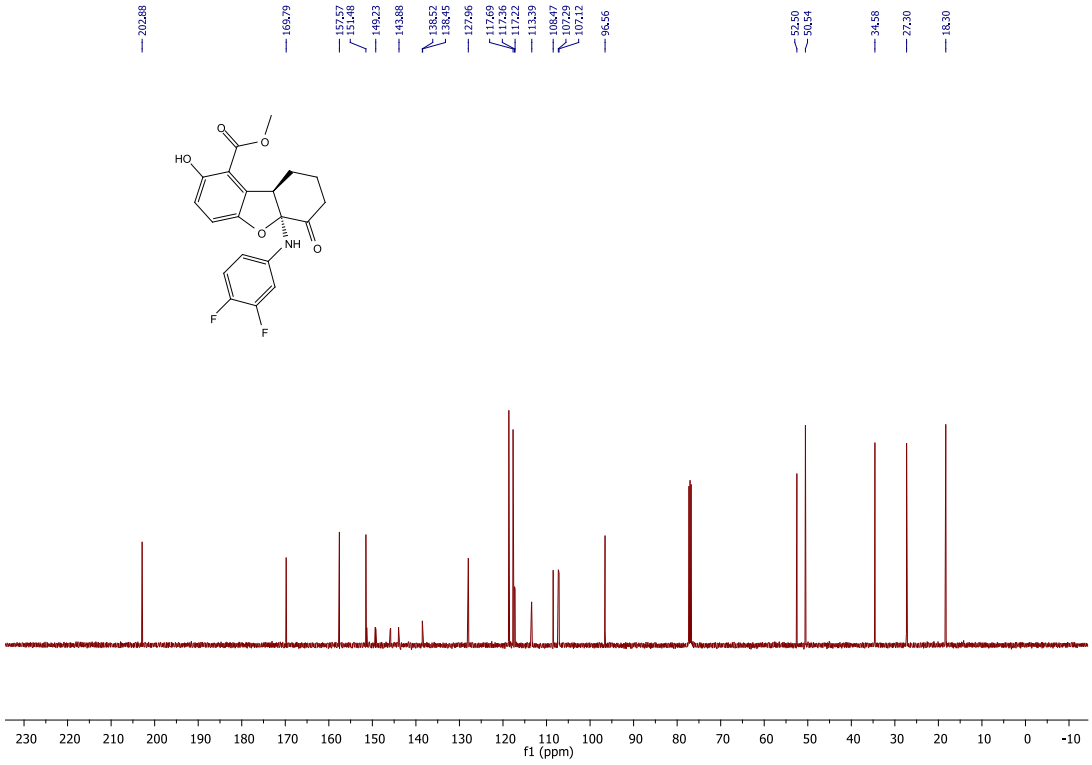
1.10
1.01
2.95
1.12
1.14
1.12
2.22
1.25
f1 (ppm)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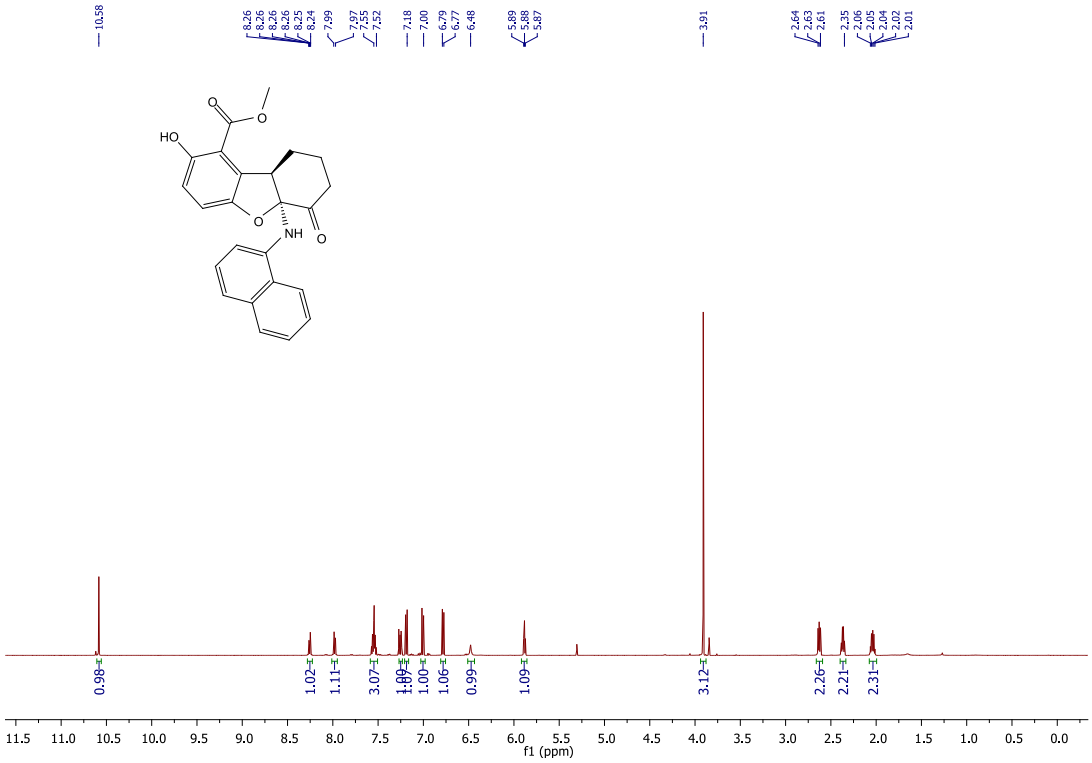
138.45
127.96
117.69
117.36
117.22
113.39
108.47
107.29
107.12
96.56
52.50
50.54
34.58
27.30
18.30
HO
O
O
O
NH
O
F
F
f1 (ppm)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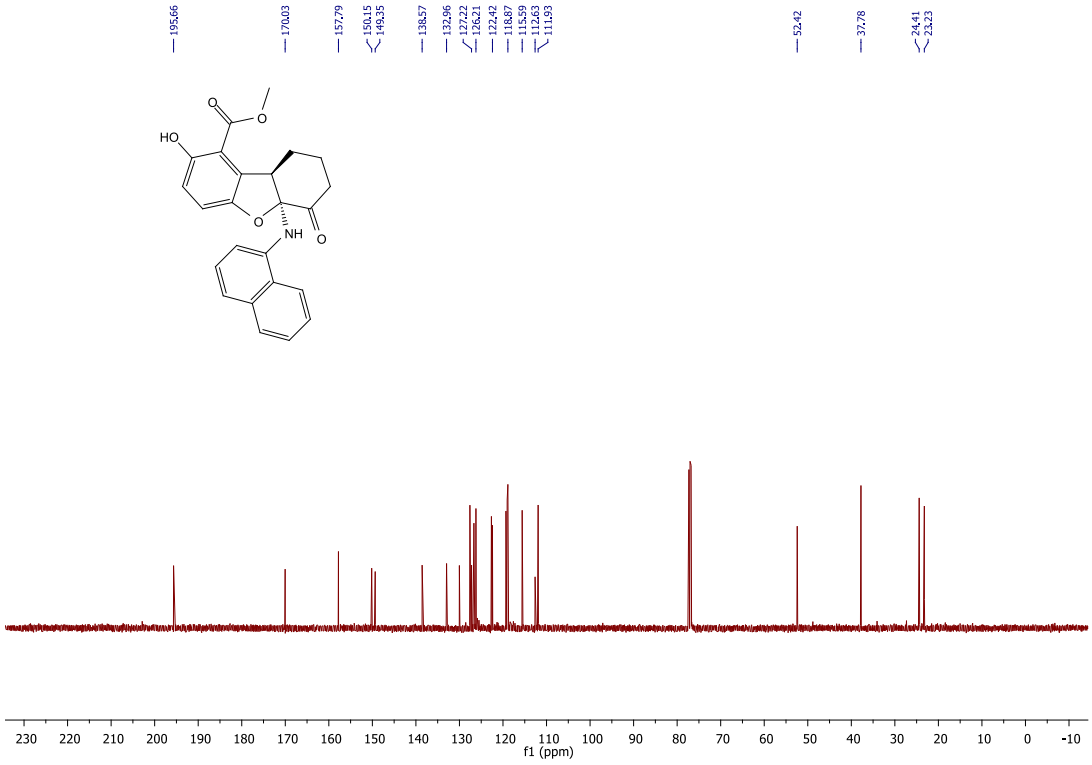
8.26
8.26
8.26
8.25
8.24
7.99
7.97
7.55
7.52
7.18
7.00
6.79
6.77
6.48
5.89
5.88
5.87
3.91
2.64
2.63
2.61
2.35
2.06
2.05
2.04
2.02
2.01
HO
O
O
O
NH
O
0.98
1.02
1.11
3.07
1.00
1.06
0.99
1.09
3.12
2.26
2.21
2.31
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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138.57
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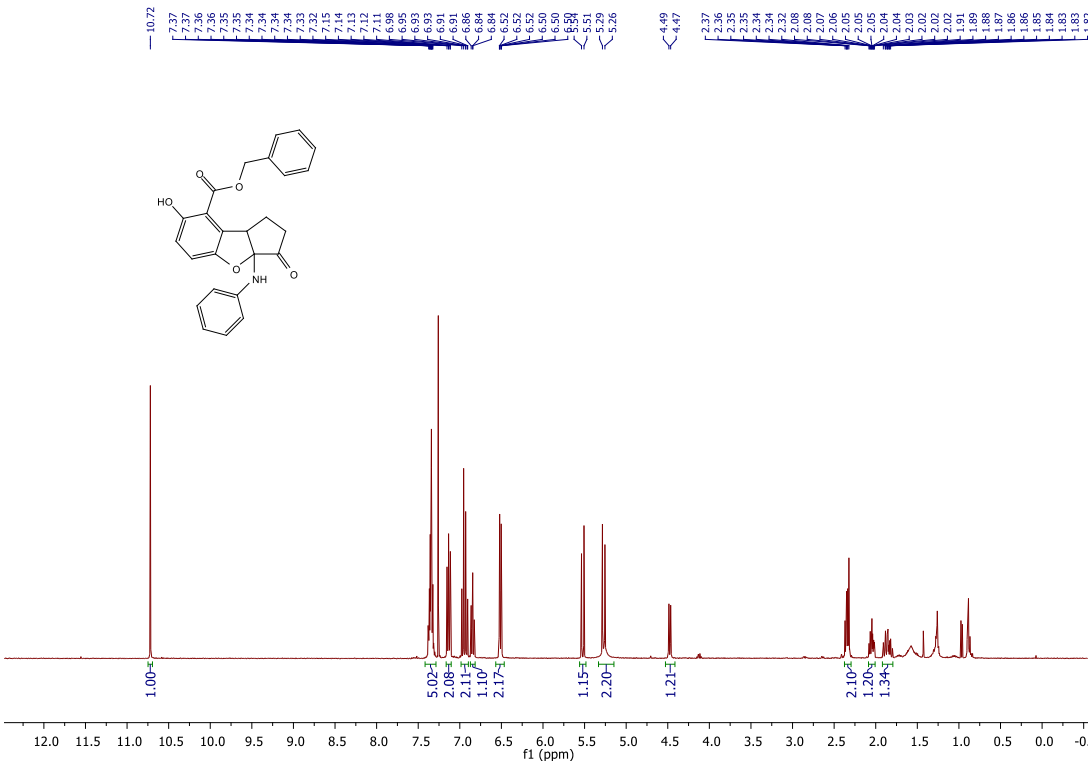
127.22
126.21
122.42
118.87
115.59
112.63
111.93
52.42
37.78
24.41
23.23
HO
O
O
O
NH
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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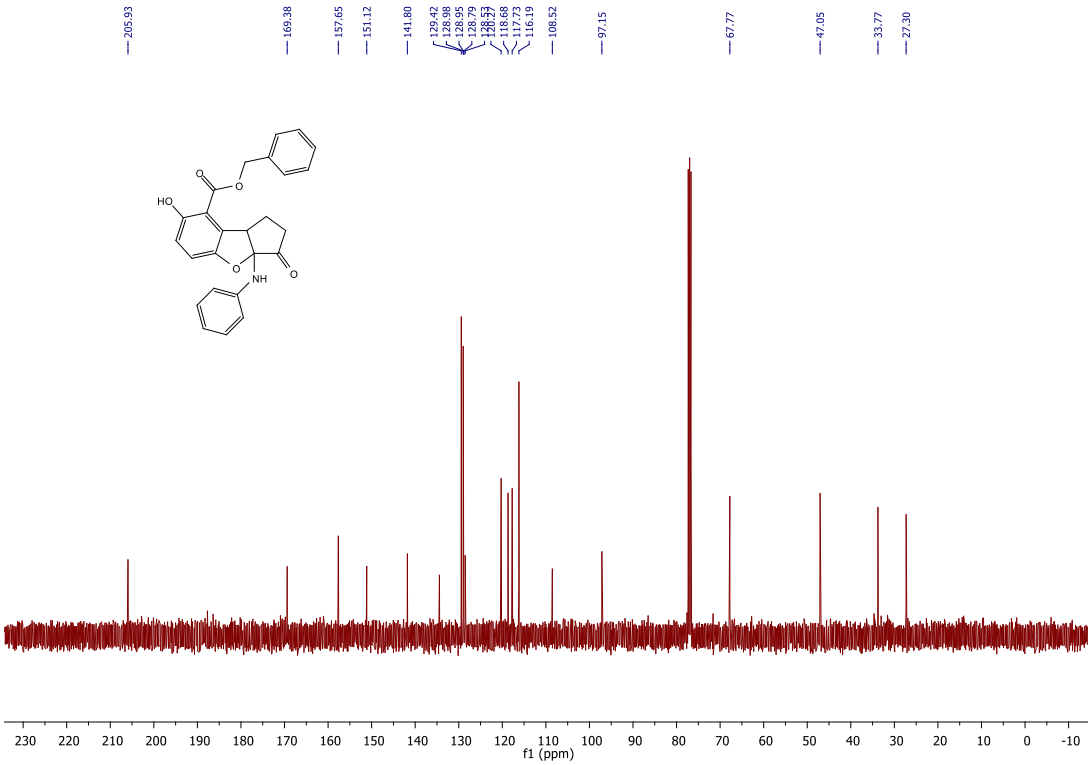
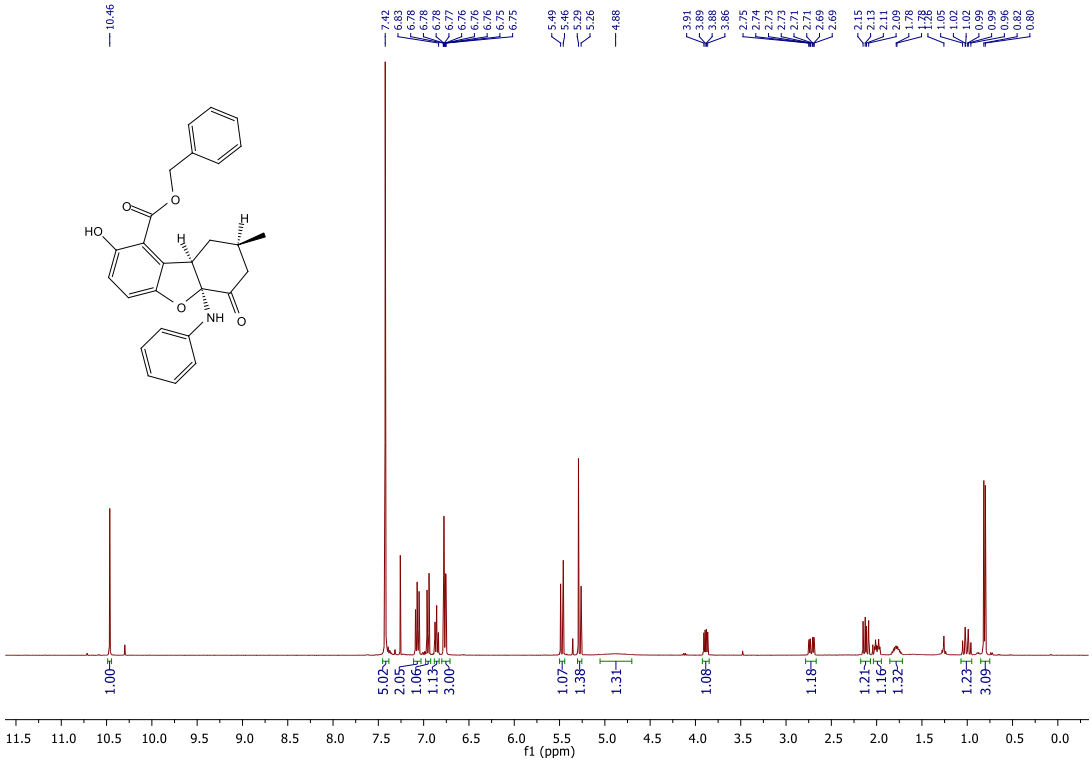
O
NH
O
f1 (ppm)


HO
O
O
NH
O
f1 (ppm)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6.75
5.49
5.46
5.29
5.26
4.88
3.91
3.89
3.88
3.86
2.75
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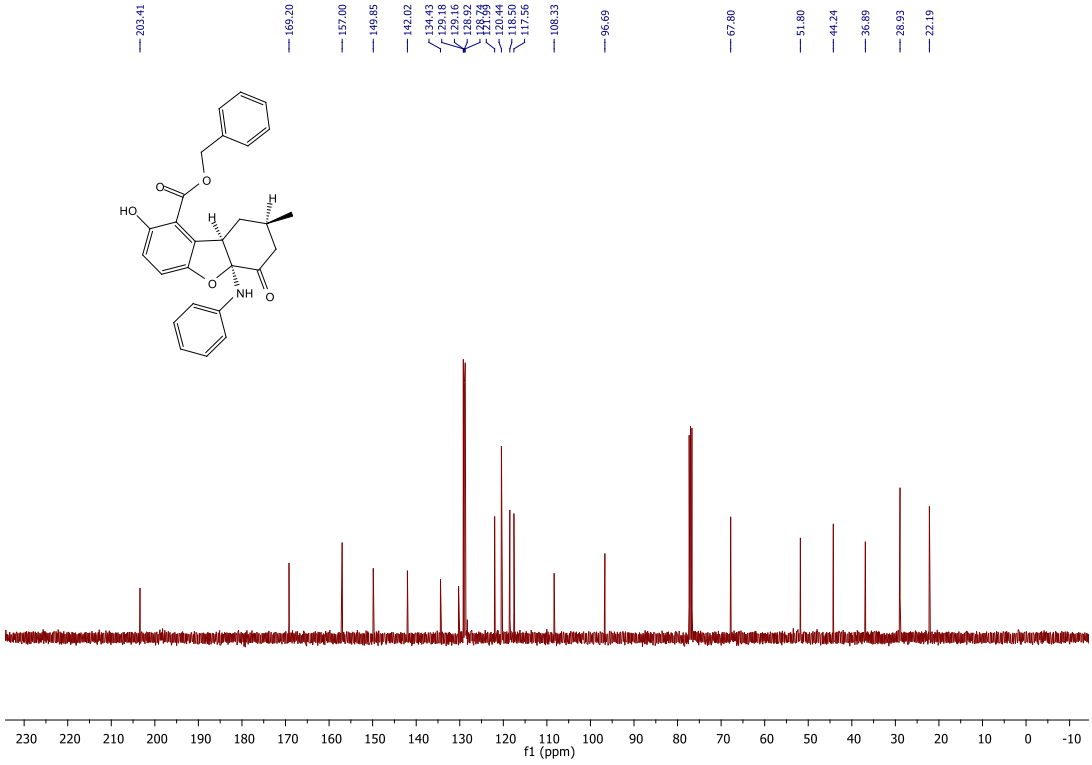
2.73
2.73
2.71
2.71
2.69
2.69
2.15
2.13
2.11
2.09
1.78
1.28
1.05
1.02
1.02
0.99
0.99
0.96
0.82
0.80
HO
O
O
H
H
O
NH
O
1.00
5.02
2.05
1.06
1.13
3.00
1.07
1.38
1.31
1.08
1.18
1.21
1.16
1.32
1.23
3.09
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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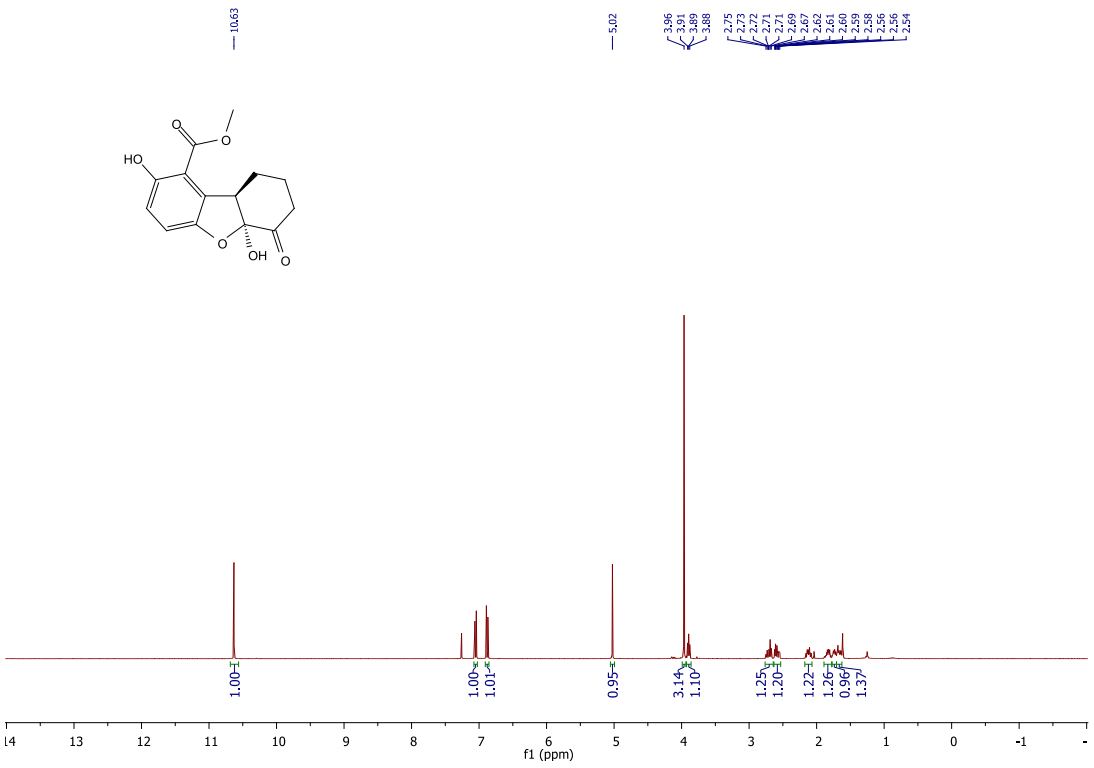
129.16
128.92
120.44
118.50
117.56
108.33
96.69
67.80
51.80
44.24
36.89
28.93
22.19
HO
O
O
H
H
O
NH
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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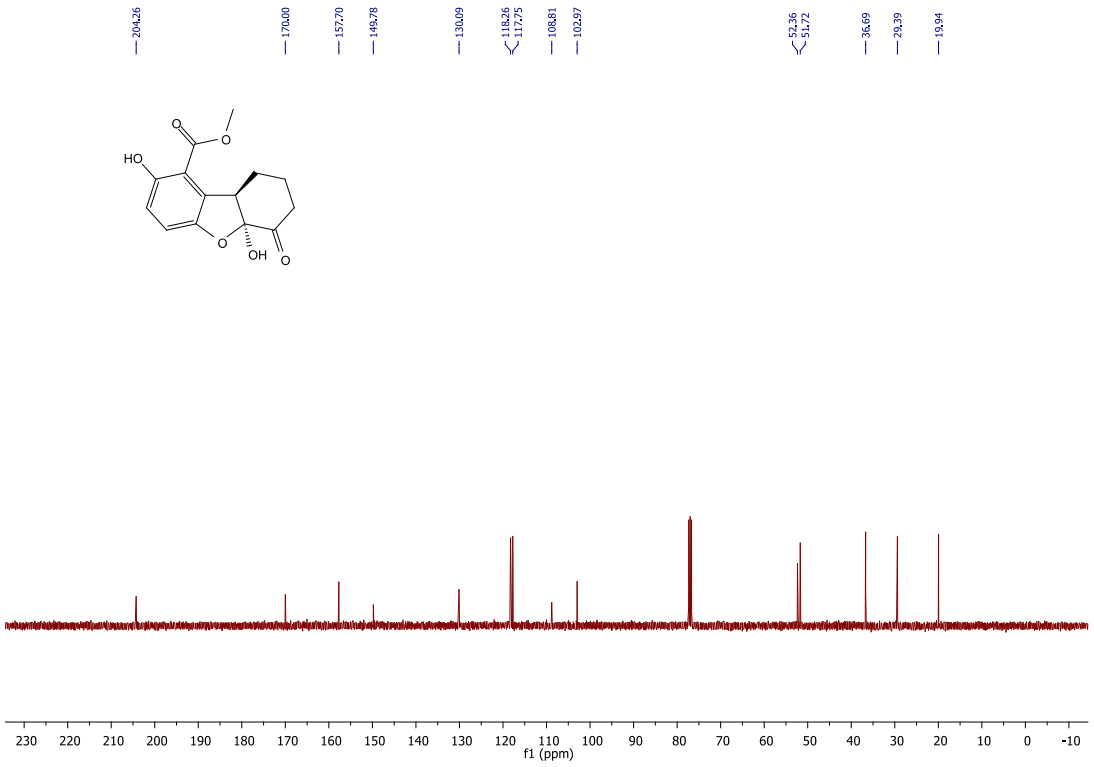
2.71
2.71
2.69
2.67
2.62
2.61
2.60
2.59
2.58
2.56
2.56
2.54
HO
O
O
OH
O
1.00
1.00
1.01
0.95
3.14
1.10
1.25
1.20
1.22
1.26
0.96
1.37
f1 (ppm)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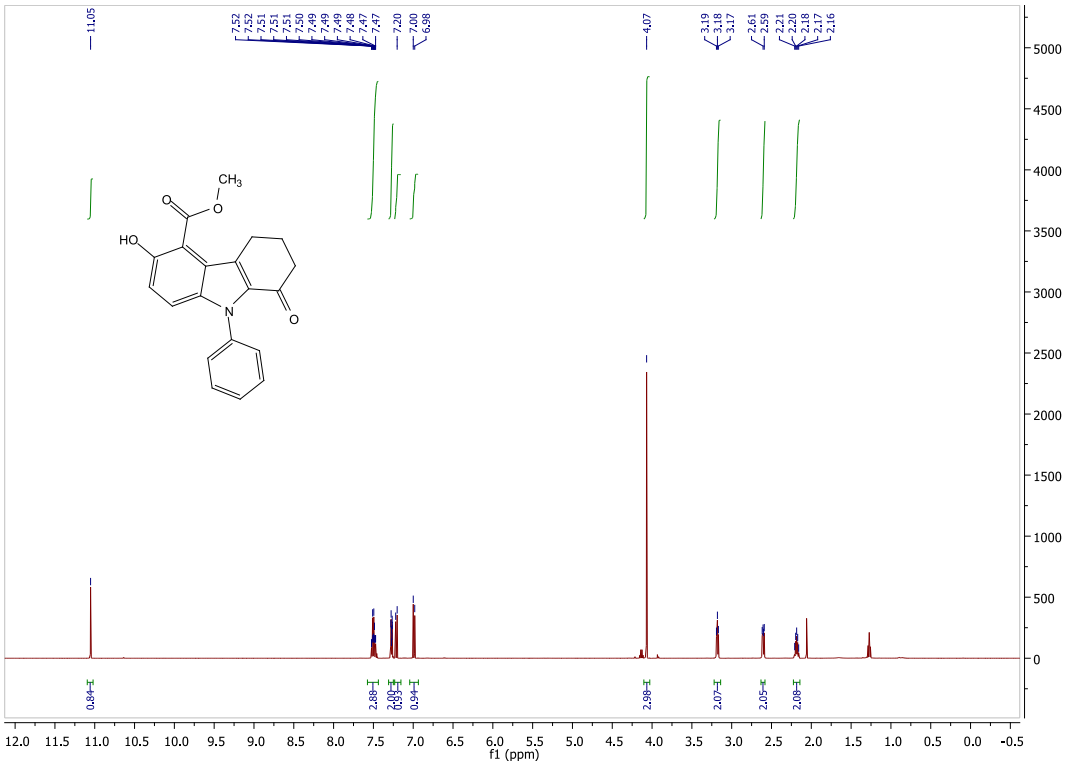
36.69
29.39
19.94
HO
O
O
OH
O
f1 (ppm)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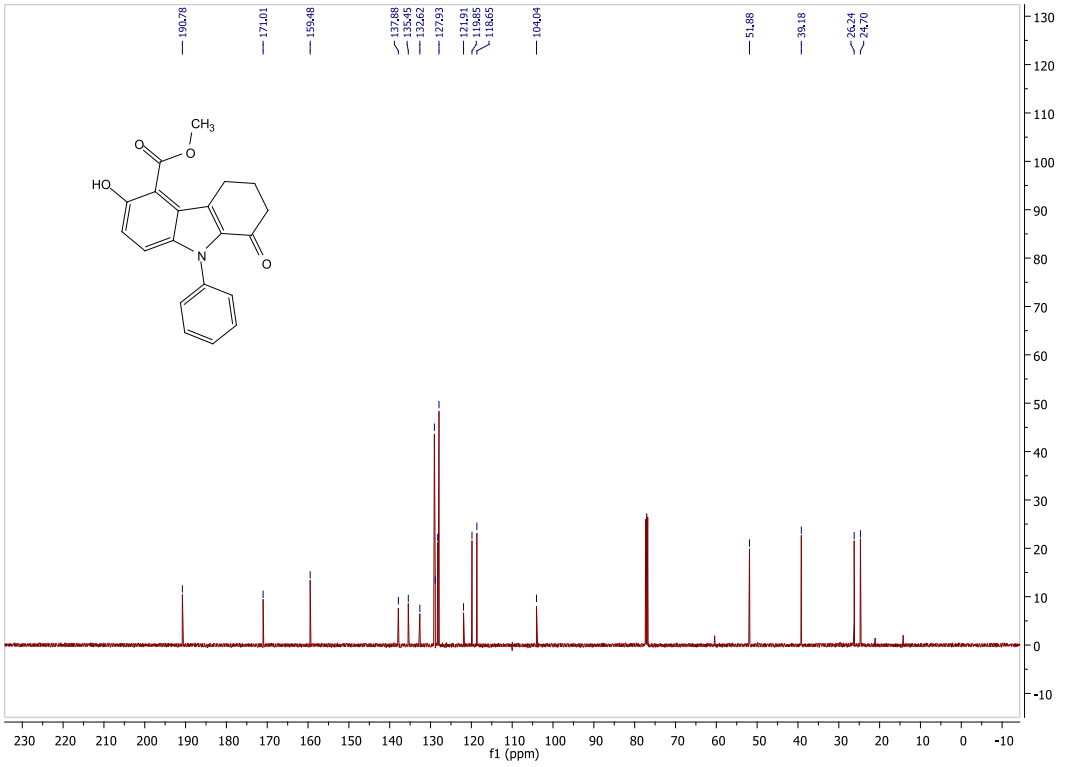
7.49
7.48
7.47
7.47
7.20
7.00
6.98
4.07
3.19
3.18
3.17
2.61
2.59
2.21
2.20
2.18
2.17
2.16
CH3
O
O
HO
N
O
0.84
2.88
0.94
2.98
2.07
2.05
2.08
f1 (ppm)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127.93
121.91
119.85
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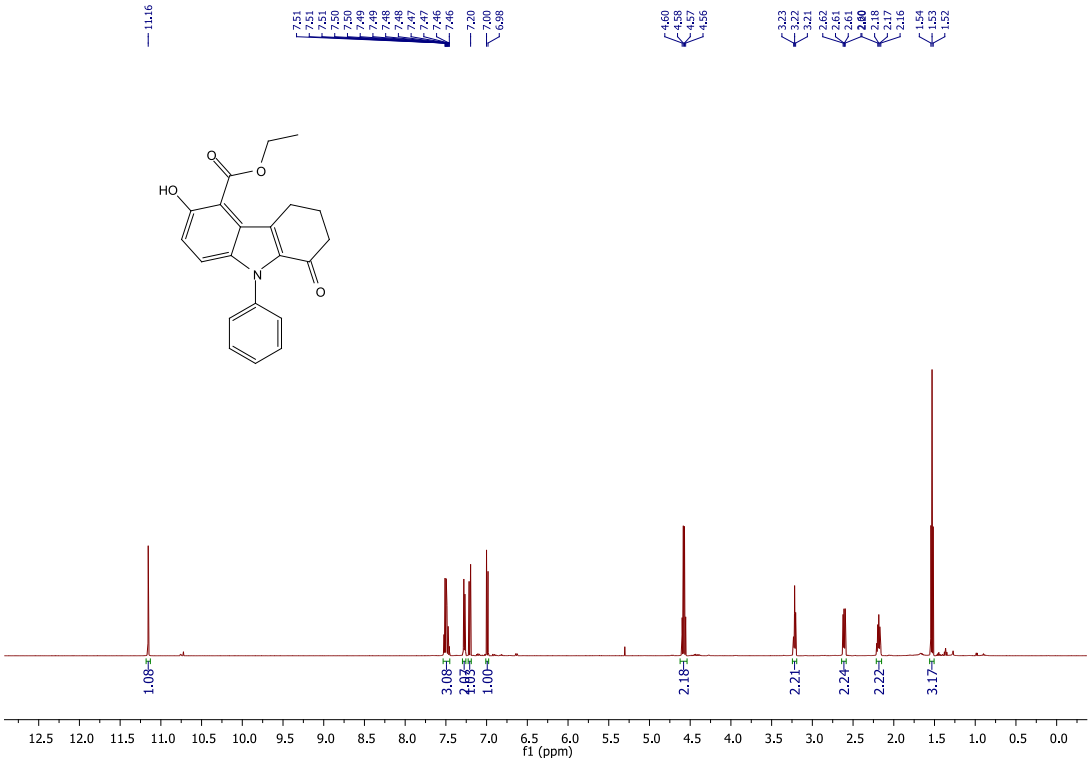
51.88
39.18
26.24
24.70
CH3
O
O
HO
N
O
f1 (ppm)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7.51
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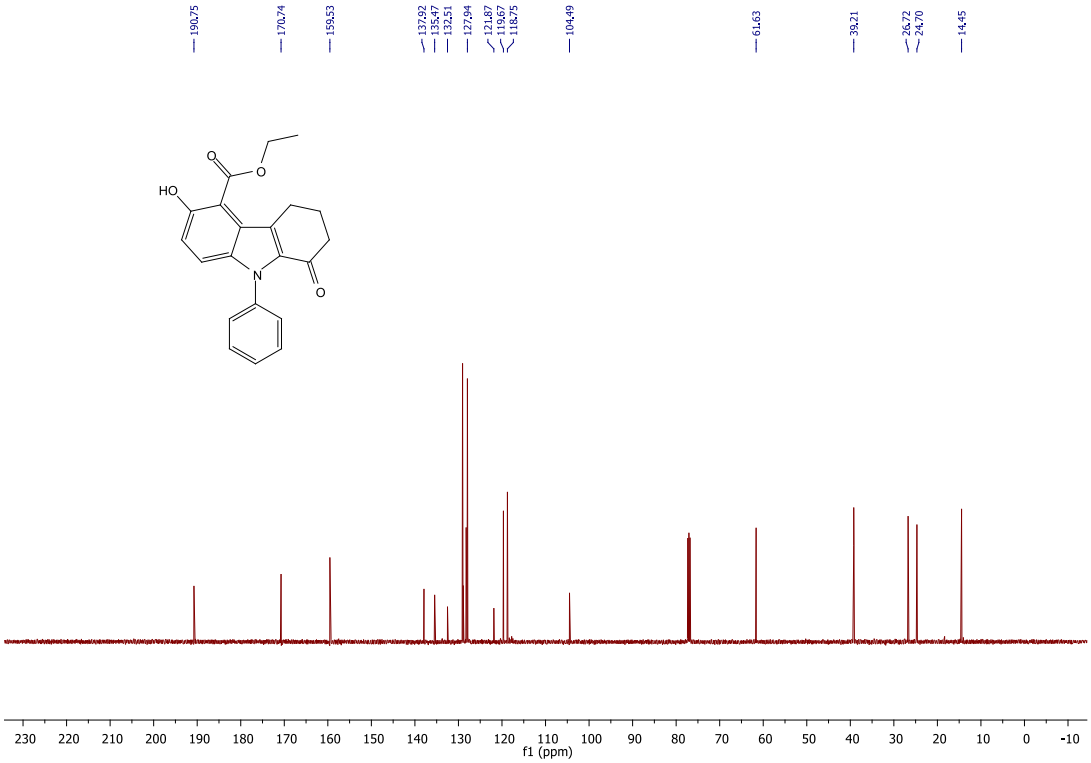
7.47
7.47
7.46
7.46
7.20
7.00
6.98
4.60
4.58
4.57
4.56
3.23
3.22
3.21
2.62
2.61
2.61
2.60
2.18
2.17
2.16
1.54
1.53
1.52
HO
O
O
N
O
1.08
3.08
2.13
2.03
1.00
2.18
2.21
2.24
2.22
3.17
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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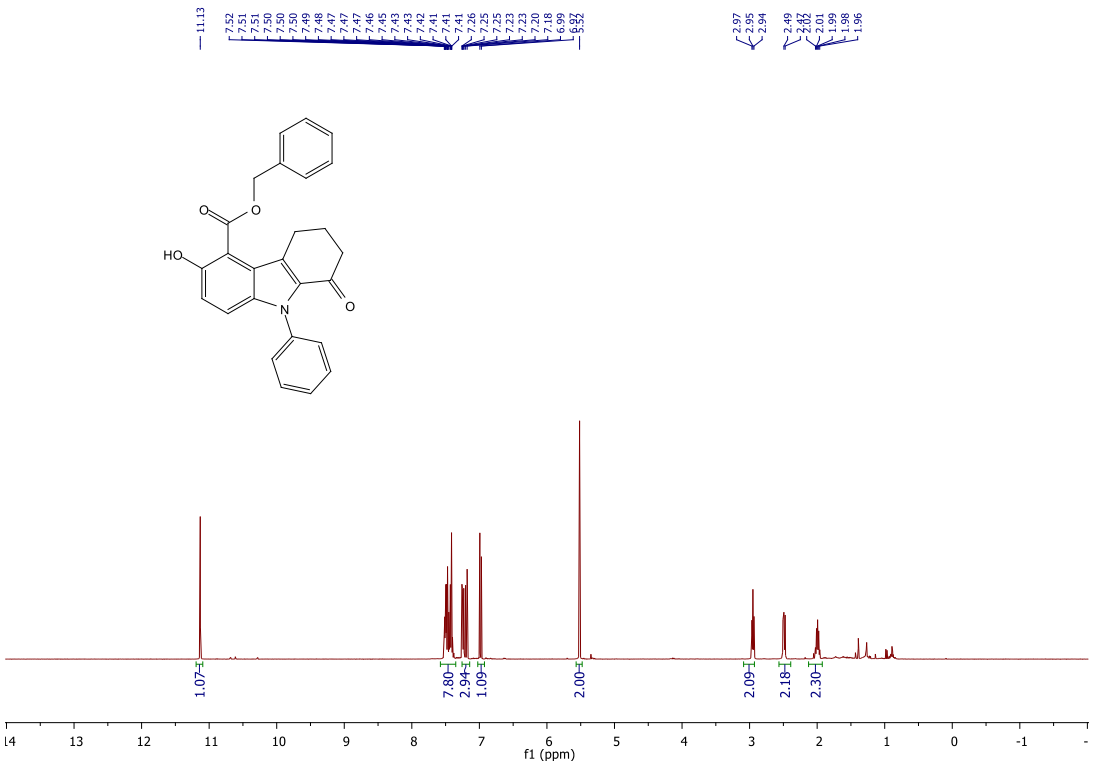
132.51
127.94
121.87
119.67
118.75
104.49
61.63
39.21
26.72
24.70
14.45
HO
O
O
N
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.51
7.50
7.50
7.50
7.49
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7.47
7.47
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7.46
7.45
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7.43
7.42
7.41
7.41
7.41
7.26
7.25
7.23
7.23
7.20
7.18
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6.97
2.97
2.95
2.94
2.49
2.42
2.04
2.01
1.99
1.98
1.96
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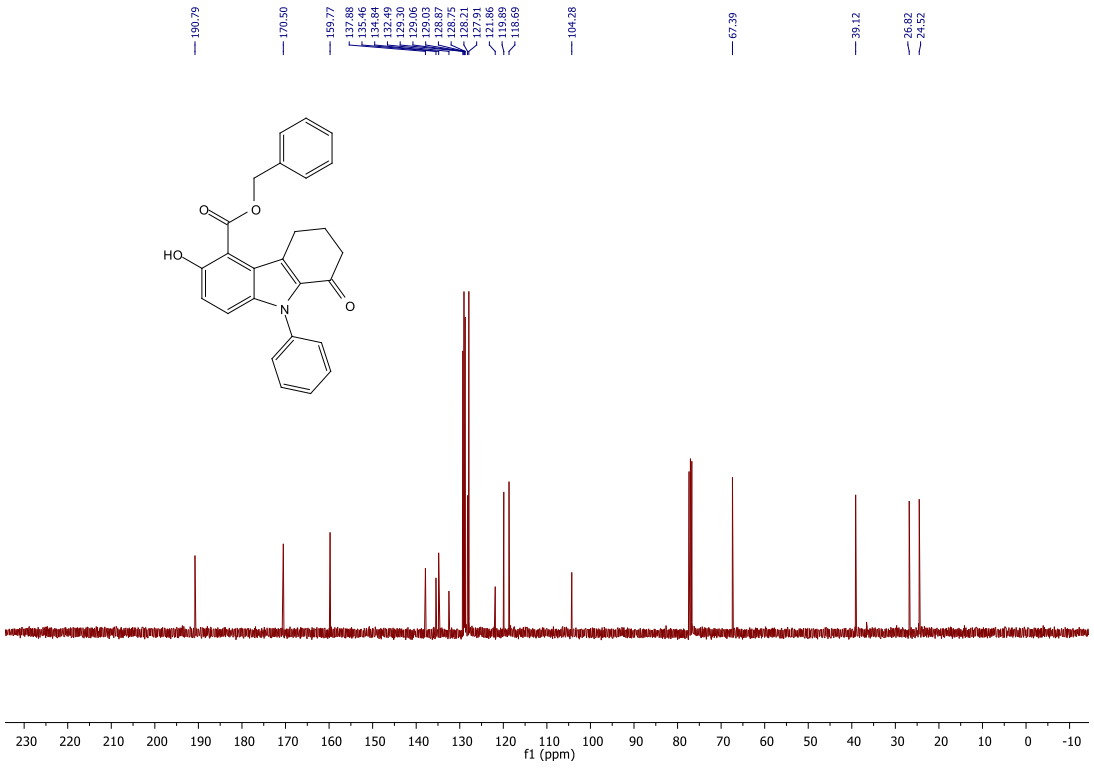
2.09
2.18
2.30
f1 (ppm)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128.75
128.21
127.91
121.86
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104.28
67.39
39.12
26.82
24.52
HO
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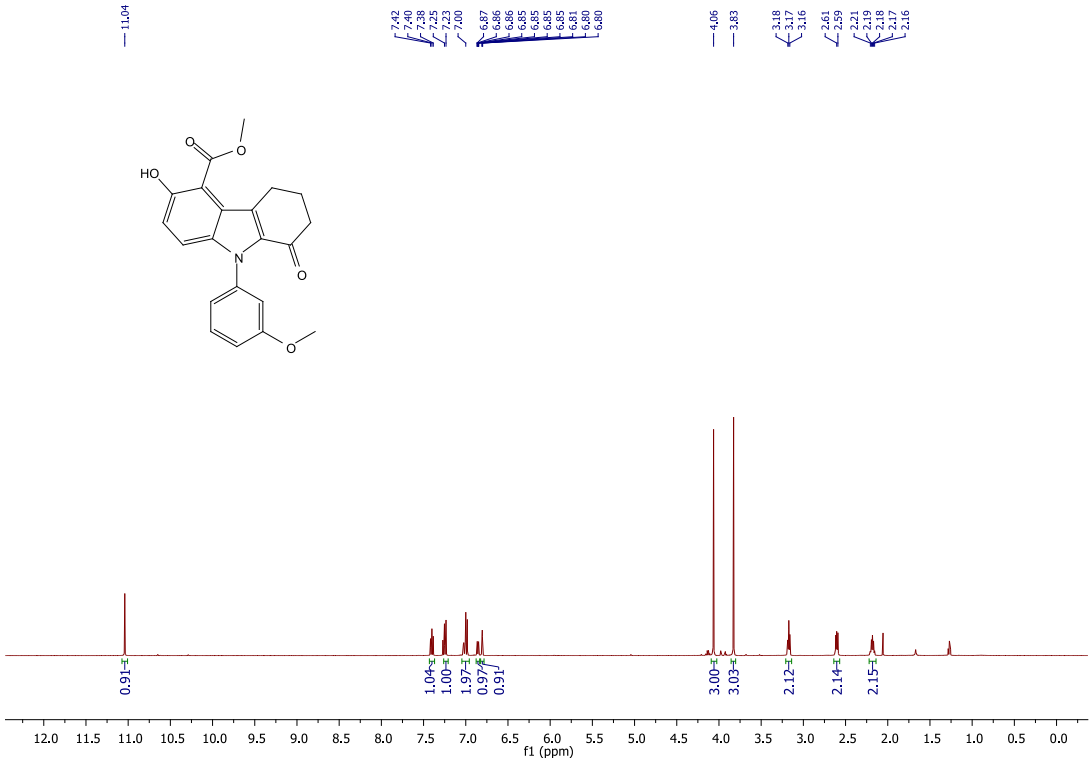
O
N
O
f1 (ppm)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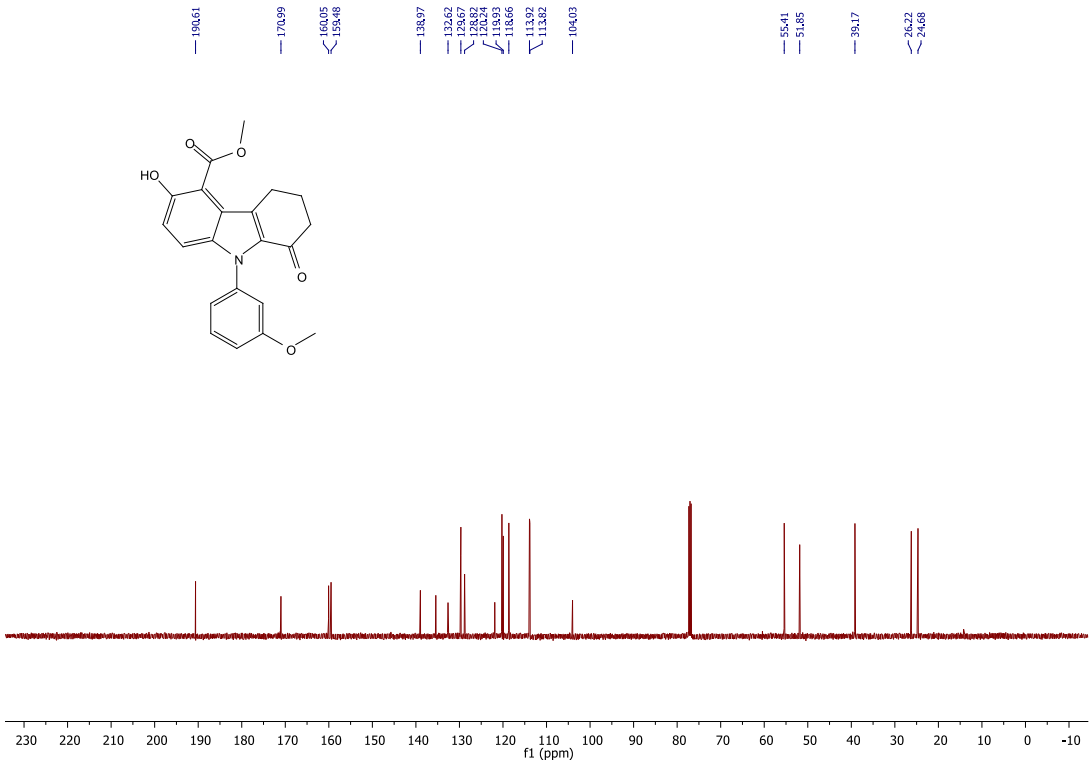
6.86
6.85
6.85
6.85
6.85
6.81
6.80
6.80
4.06
3.83
3.18
3.17
3.16
2.61
2.59
2.21
2.19
2.18
2.17
2.16
HO
O
O
N
O
O
0.91
1.04
1.00
1.97
0.97
0.91
3.00
3.03
2.12
2.14
2.15
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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119.93
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113.92
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104.03
55.41
51.85
39.17
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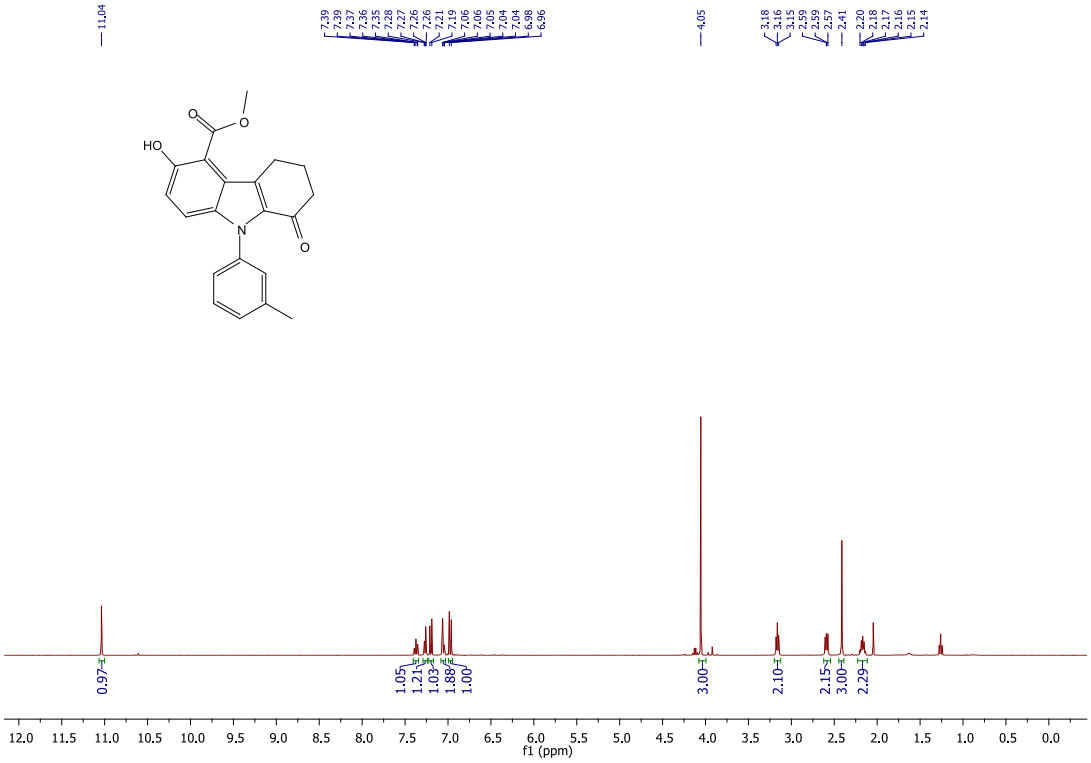
f1 (ppm)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7.19
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7.06
7.05
7.04
7.04
6.98
6.96
4.05
3.18
3.16
3.15
2.59
2.59
2.57
2.41
2.20
2.18
2.17
2.16
2.15
2.14
HO
O
O
N
O
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1.03
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1.00
3.00
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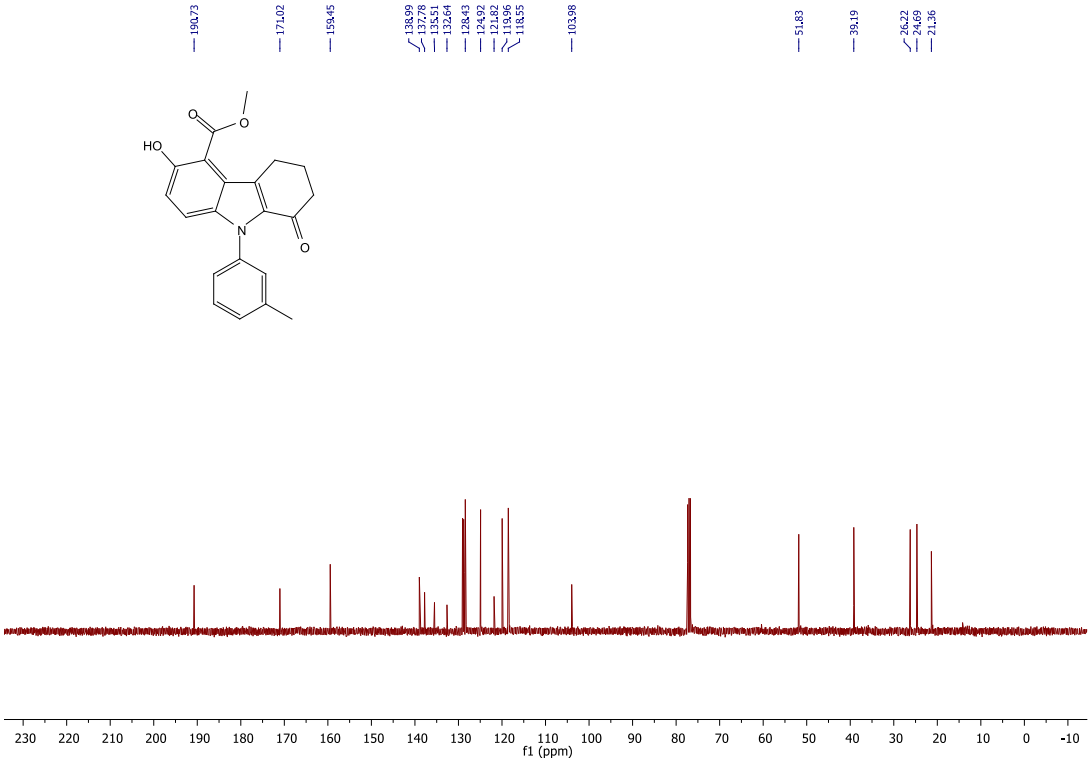
2.15
3.00
2.29
f1 (ppm)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121.82
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51.83
39.19
26.22
24.69
21.36
HO
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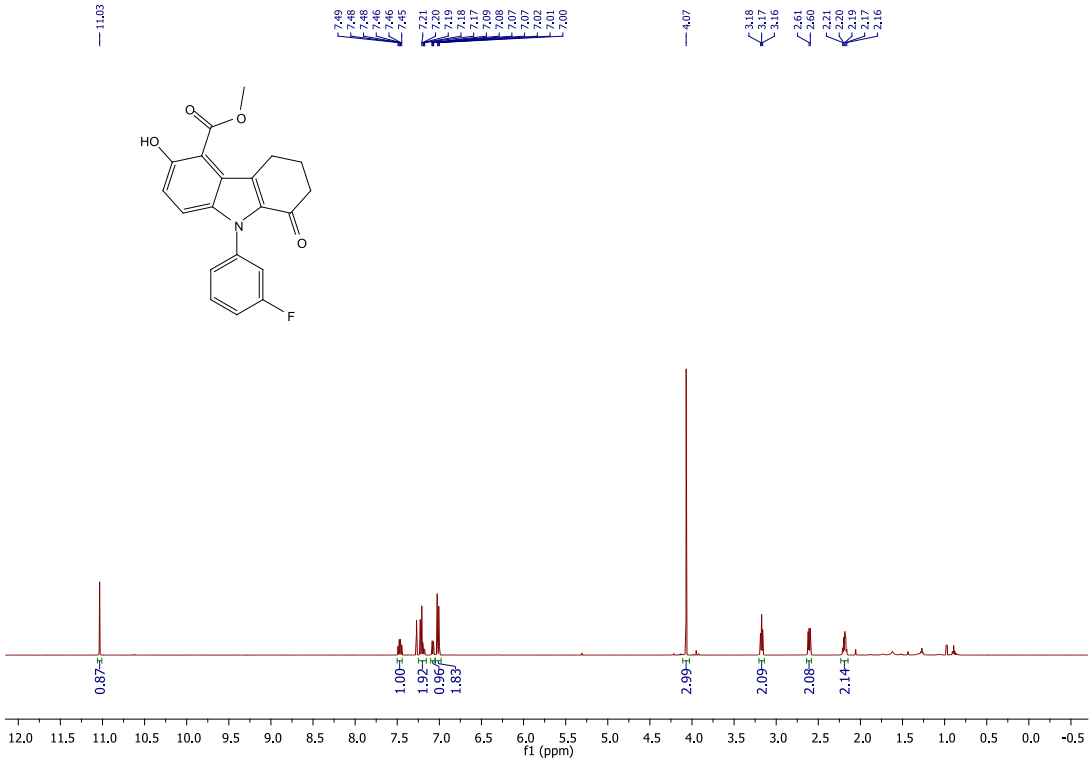
O
N
O
f1 (ppm)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7.19
7.18
7.17
7.09
7.08
7.07
7.07
7.02
7.01
7.00
4.07
3.18
3.17
3.16
2.61
2.60
2.21
2.20
2.19
2.17
2.16
HO
O
O
N
O
F
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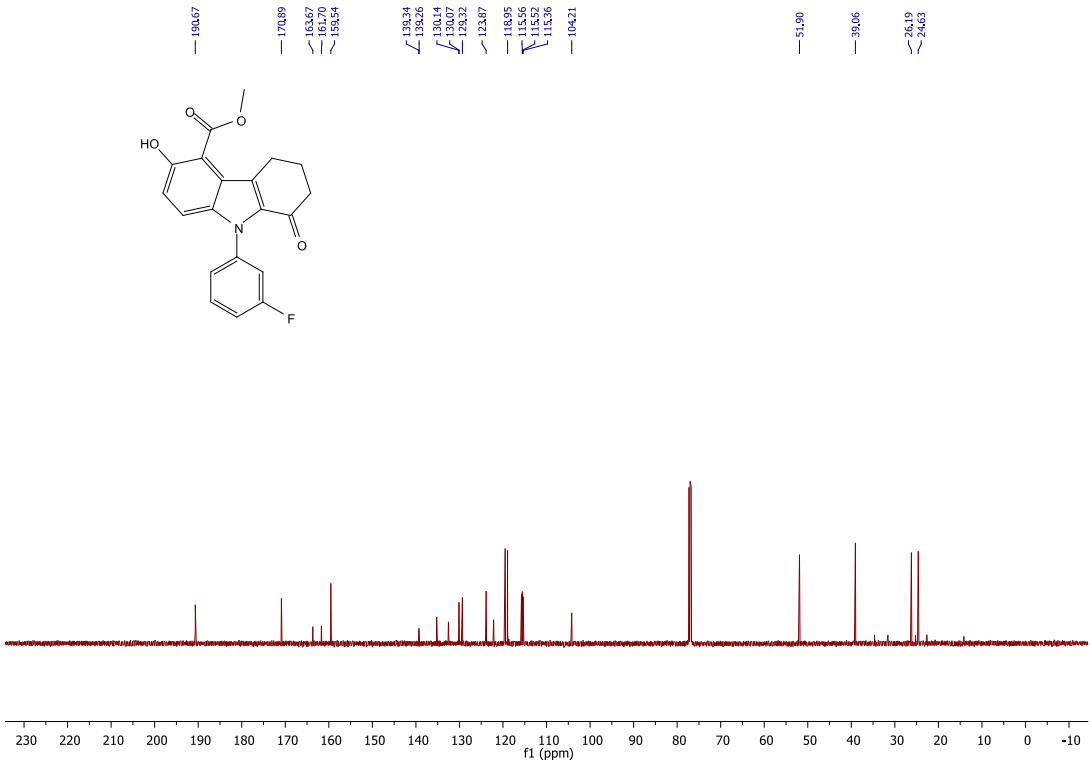
1.00
1.92
0.96
1.83
2.99
2.09
2.08
2.14
f1 (ppm)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115.56
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104.21
51.90
39.06
26.19
24.63
HO
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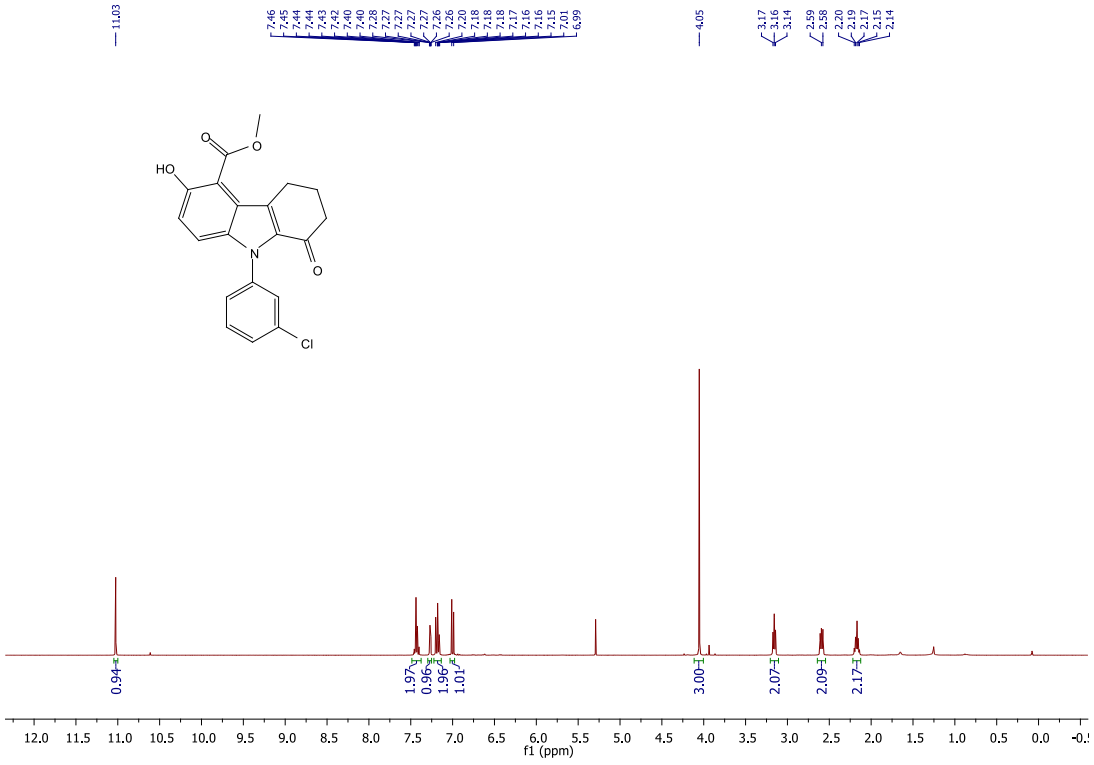
O
N
O
F
f1 (ppm)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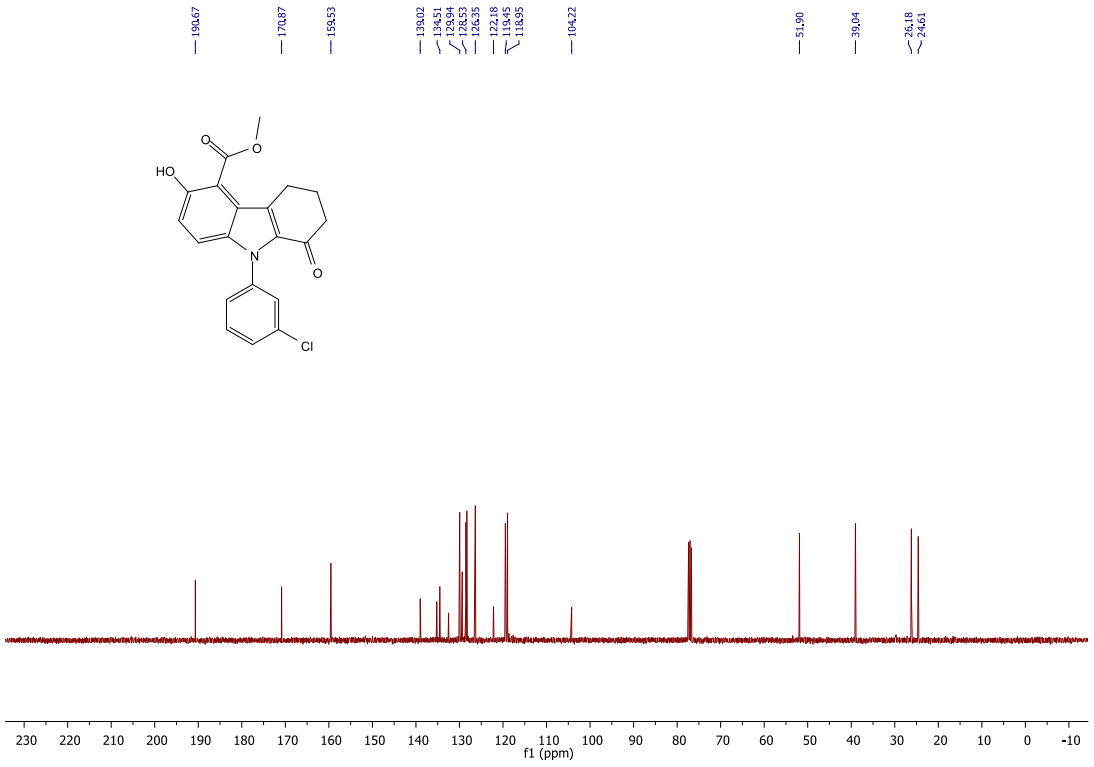
7.27
7.26
7.26
7.20
7.18
7.18
7.18
7.17
7.16
7.16
7.15
7.01
6.99
4.05
3.17
3.16
3.14
2.59
2.58
2.20
2.19
2.17
2.15
2.14
HO
O
O
N
O
Cl
0.94
1.97
0.96
1.96
1.01
3.00
2.07
2.09
2.17
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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134.51
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122.18
119.45
118.95
104.22
51.90
39.04
26.18
24.61
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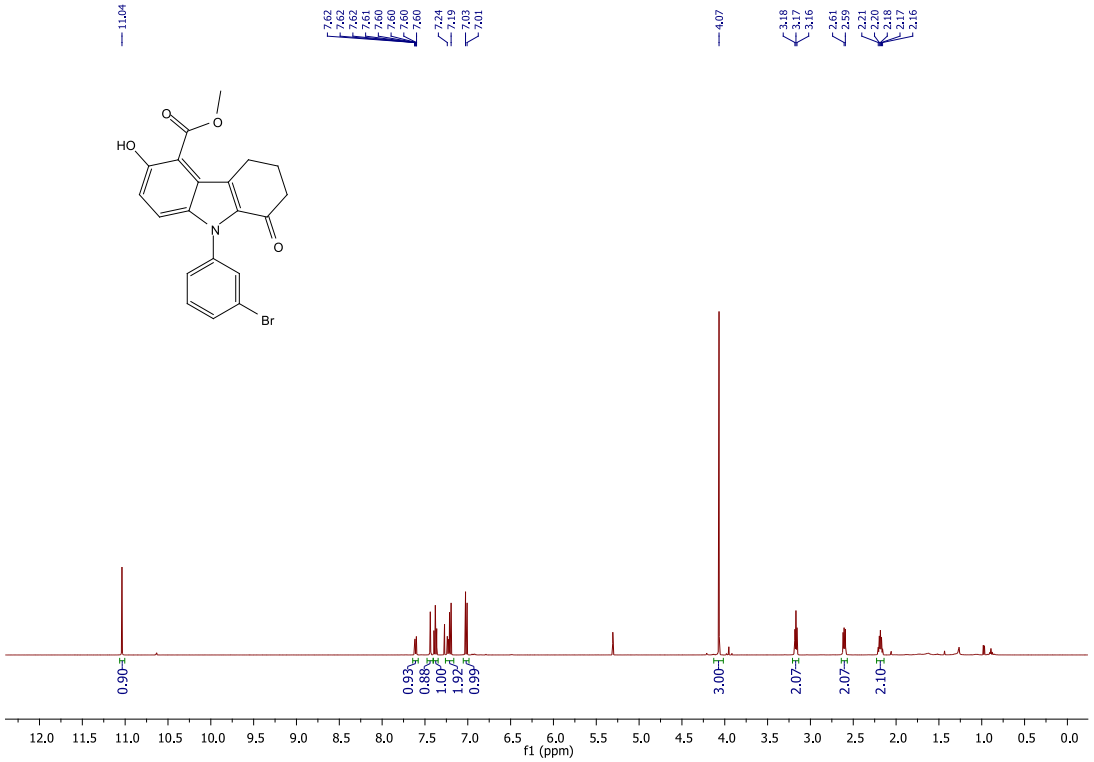
O
O
N
O
Cl
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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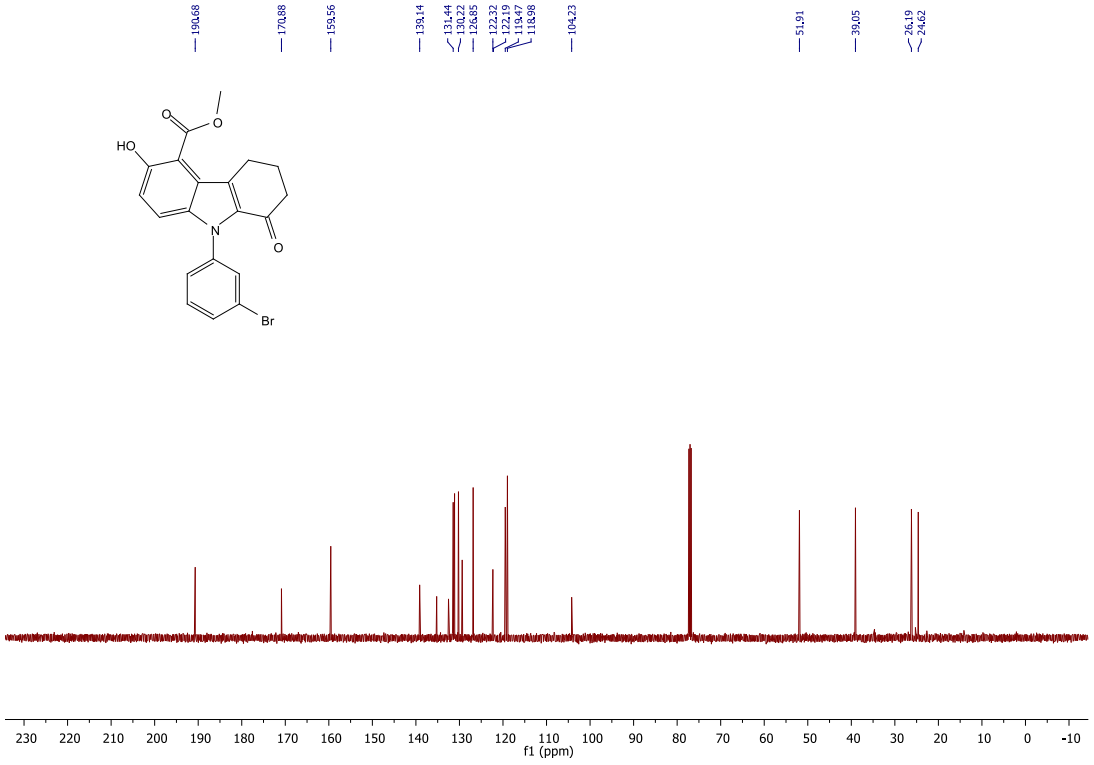
7.60
7.60
7.60
7.24
7.19
7.03
7.01
4.07
3.18
3.17
3.16
2.61
2.59
2.21
2.20
2.18
2.17
2.16
HO
O
O
N
O
Br
0.90
0.93
0.88
1.00
1.92
0.99
3.00
2.07
2.07
2.10
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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122.19
119.47
114.98
104.23
51.91
39.05
26.19
24.62
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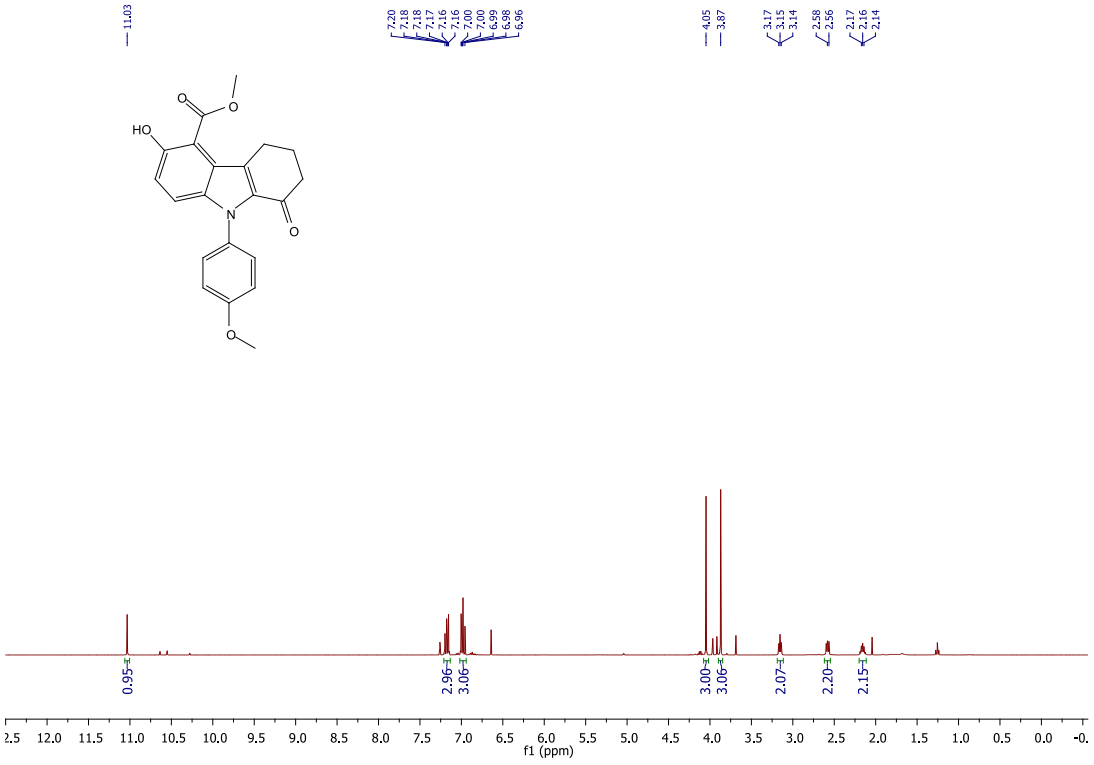
O
N
O
Br
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.16
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7.00
6.99
6.98
6.96
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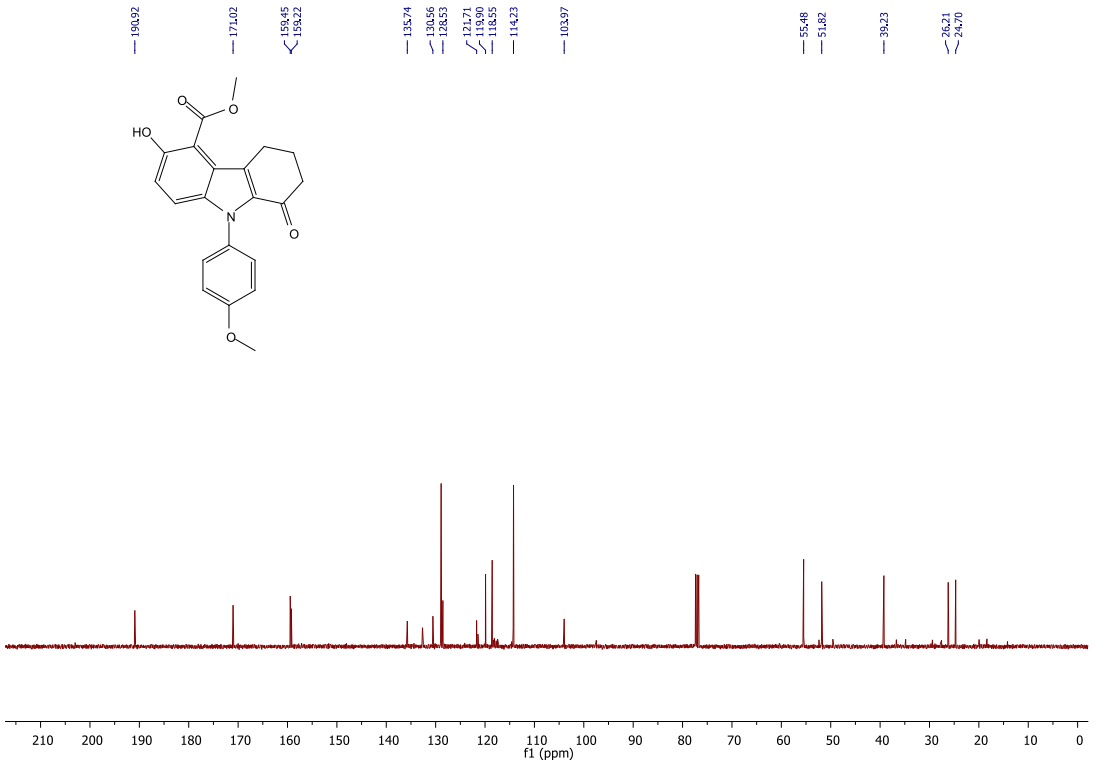
3.87
3.17
3.15
3.14
2.58
2.56
2.17
2.16
2.14
HO
O
O
N
O
O
0.95
2.96
3.06
3.00
3.06
2.07
2.20
2.15
f1 (ppm)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118.55
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24.70
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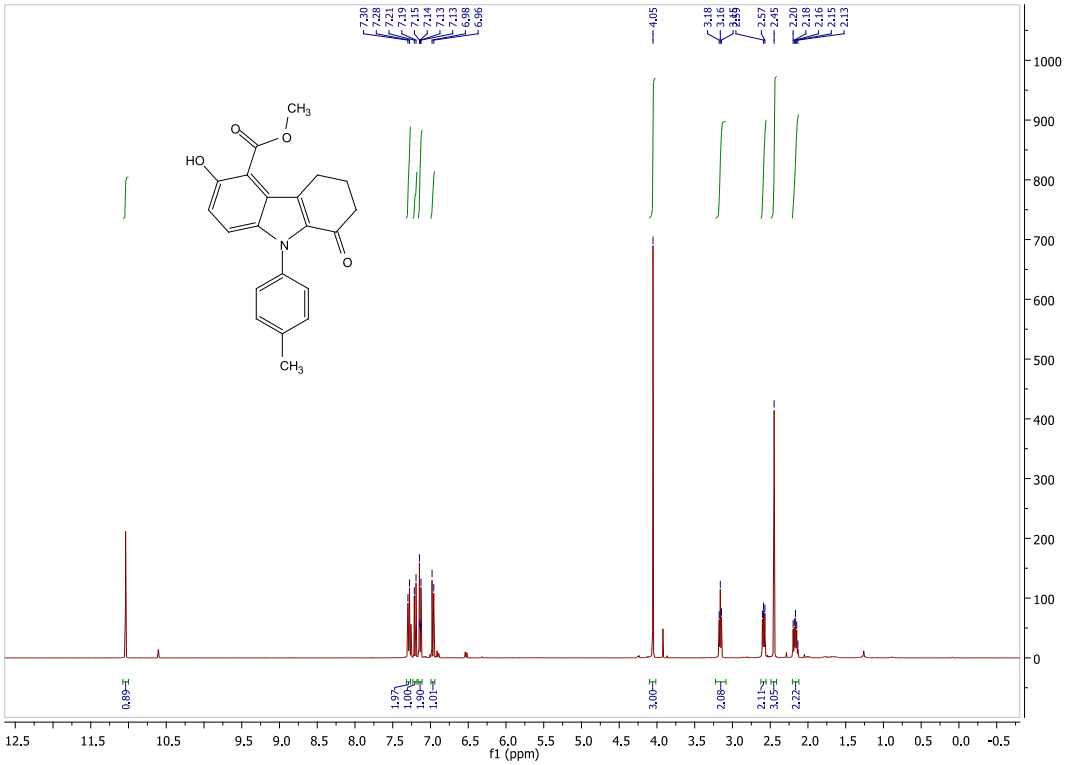
O
N
O
O
f1 (ppm)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7.13
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6.96
4.05
3.18
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2.57
2.45
2.20
2.18
2.16
2.15
2.13
CH3
O
O
HO
N
O
CH3
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3.00
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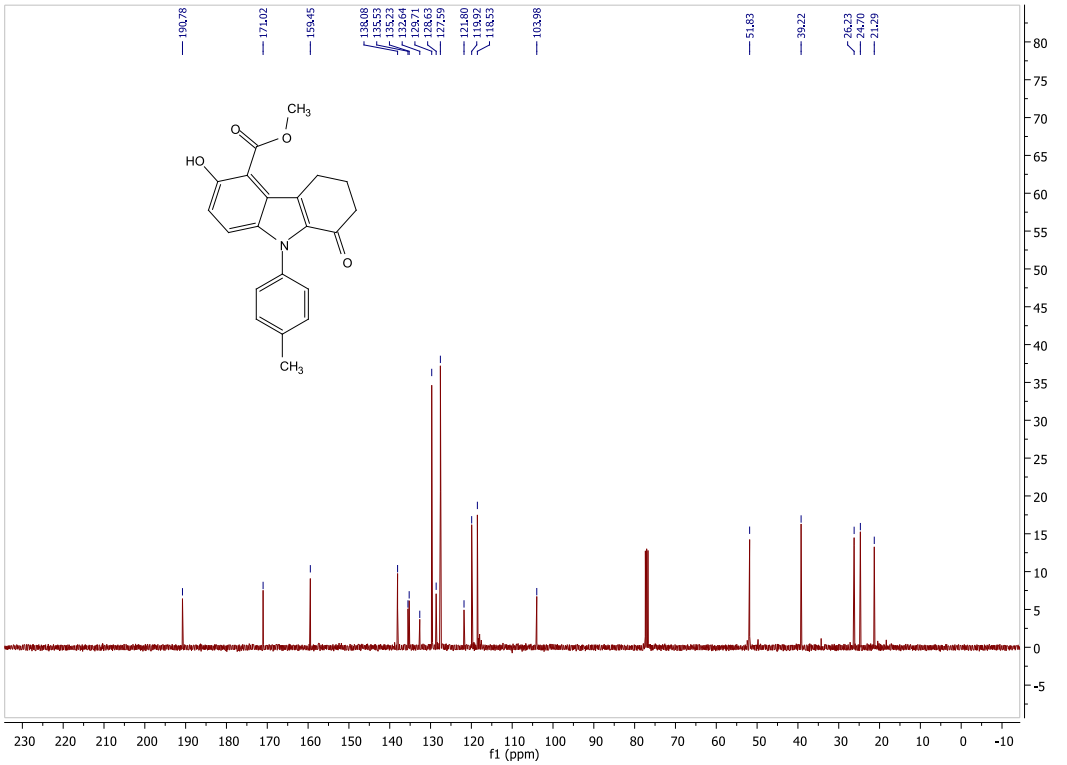
2.11
3.05
2.22
f1 (ppm)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26.23
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21.29
CH3
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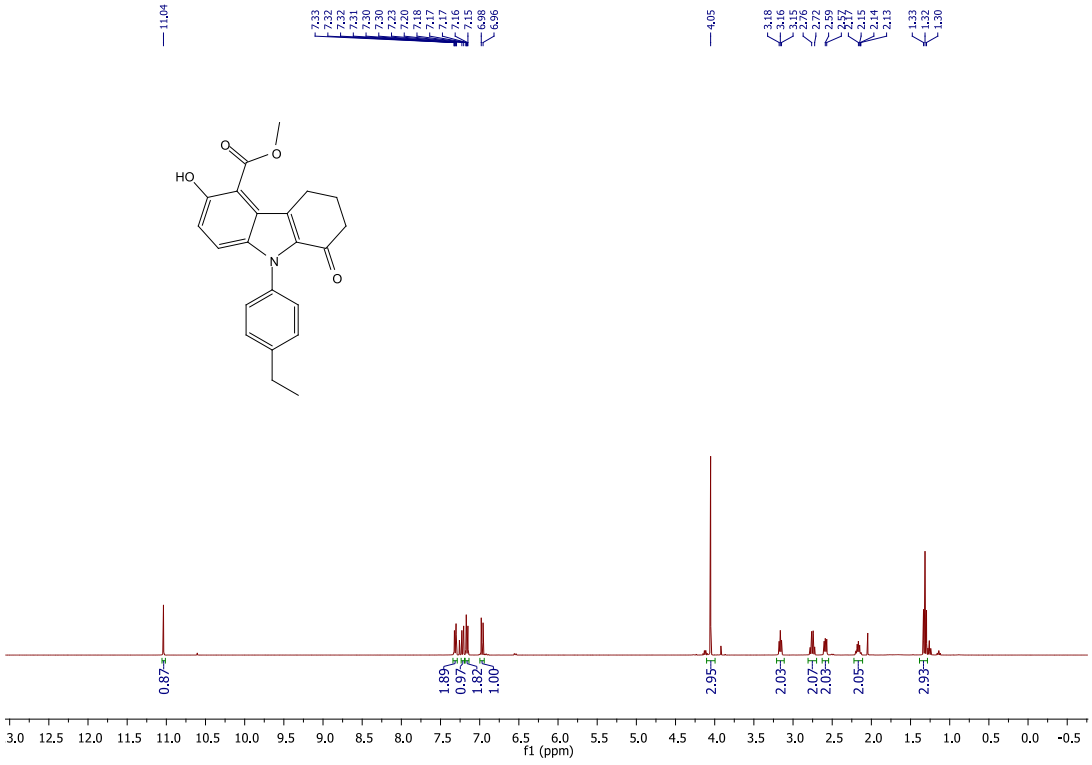
O
HO
N
O
CH3
f1 (ppm)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7.16
7.15
6.98
6.96
4.05
3.18
3.16
3.15
2.76
2.72
2.59
2.57
2.17
2.15
2.14
2.13
1.33
1.32
1.30
HO
O
O
N
O
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1.89
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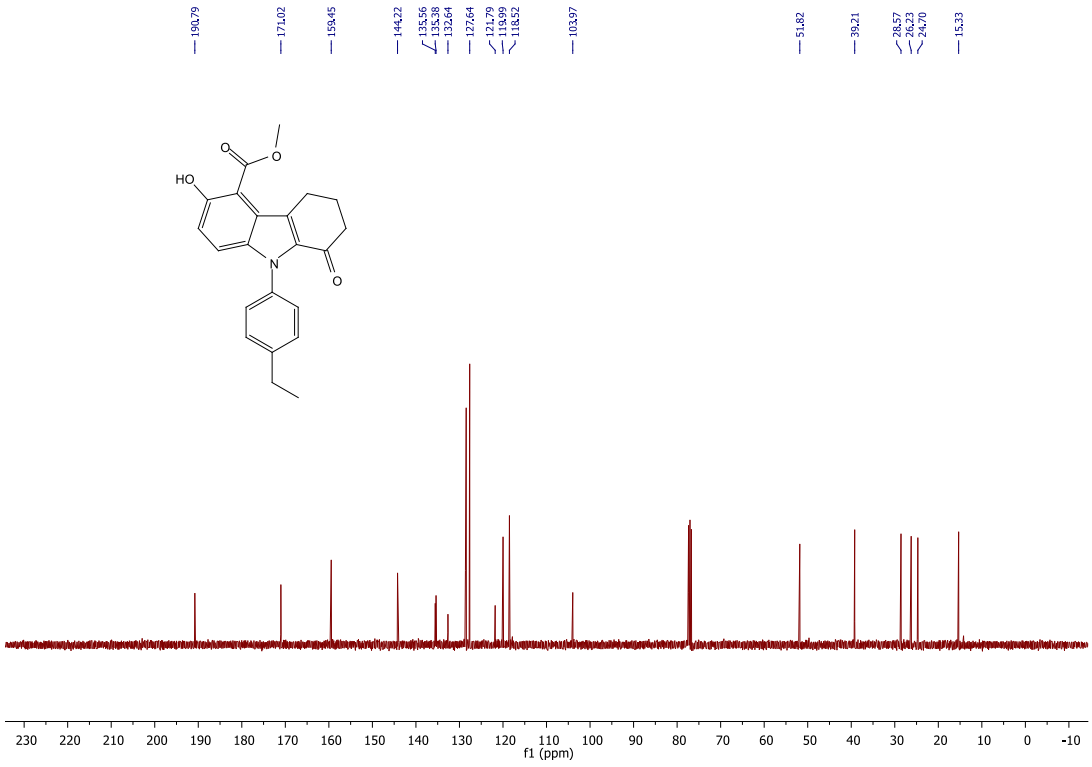
1.82
1.00
2.95
2.03
2.07
2.03
2.05
2.93
f1 (ppm)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39.21
28.57
26.23
24.70
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HO
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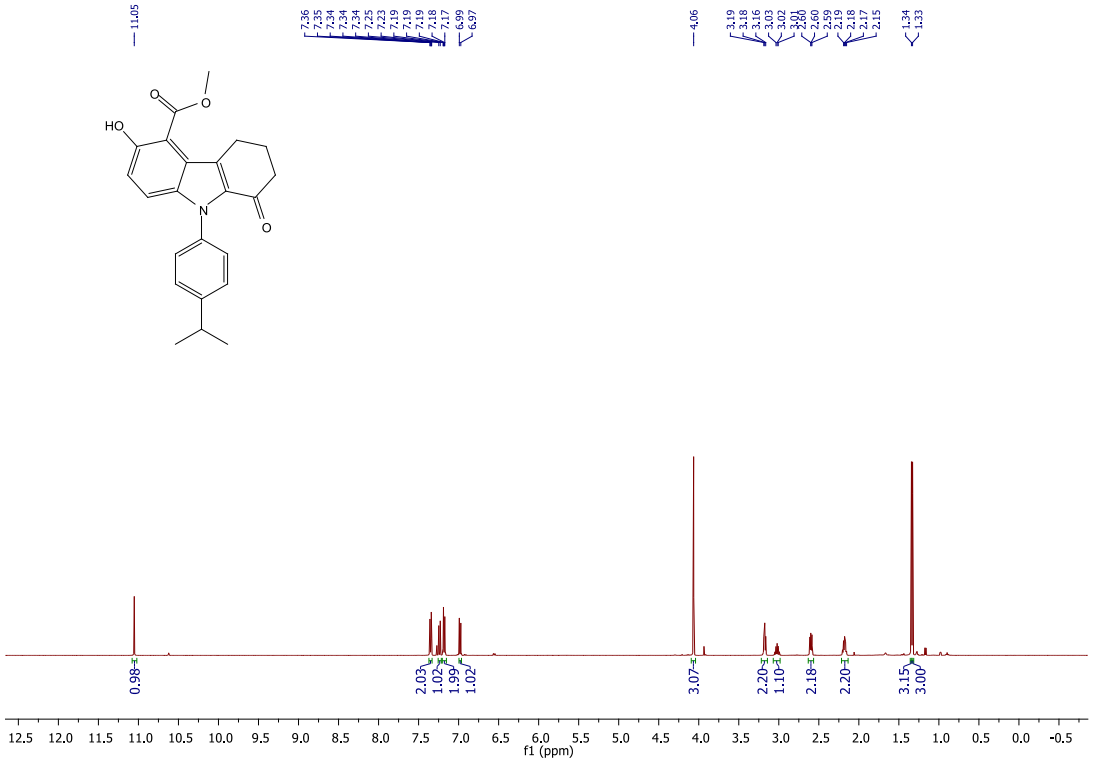
O
N
O
f1 (ppm)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7.17
6.99
6.97
4.06
3.19
3.18
3.16
3.03
3.02
3.01
2.60
2.59
2.19
2.18
2.17
2.15
1.34
1.33
HO
O
O
N
O
0.98
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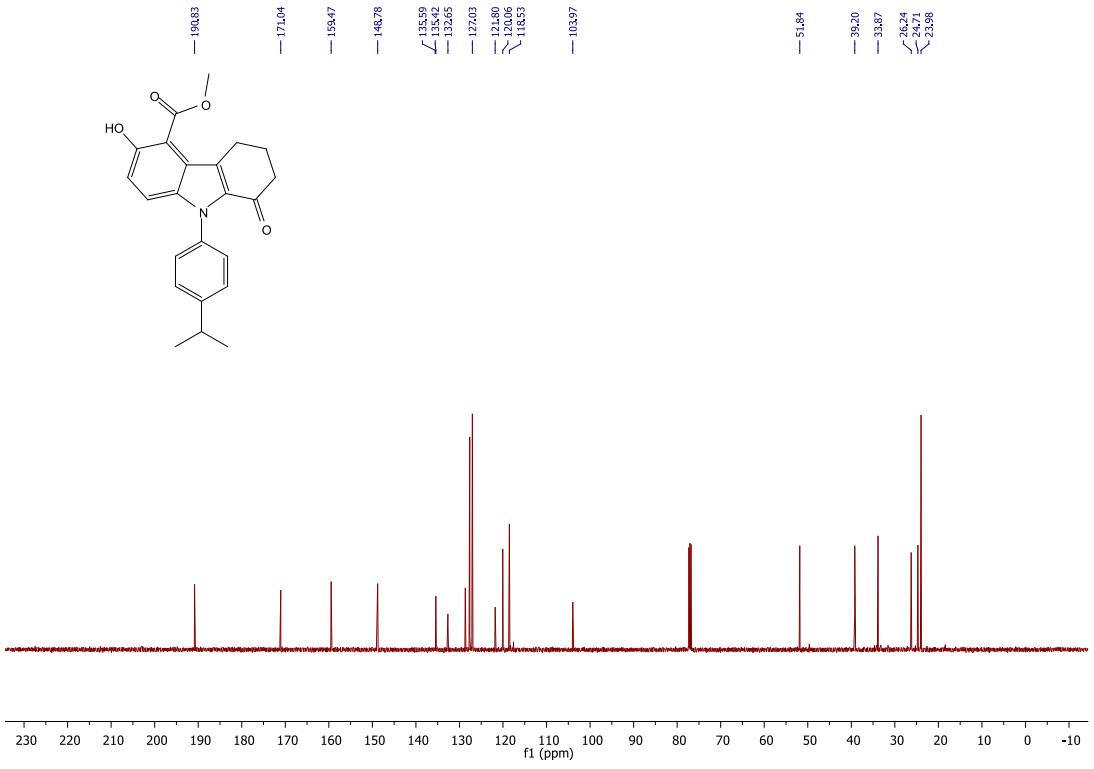
1.02
1.99
1.02
3.07
2.20
1.10
2.18
2.20
3.15
3.00
f1 (ppm)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120.06
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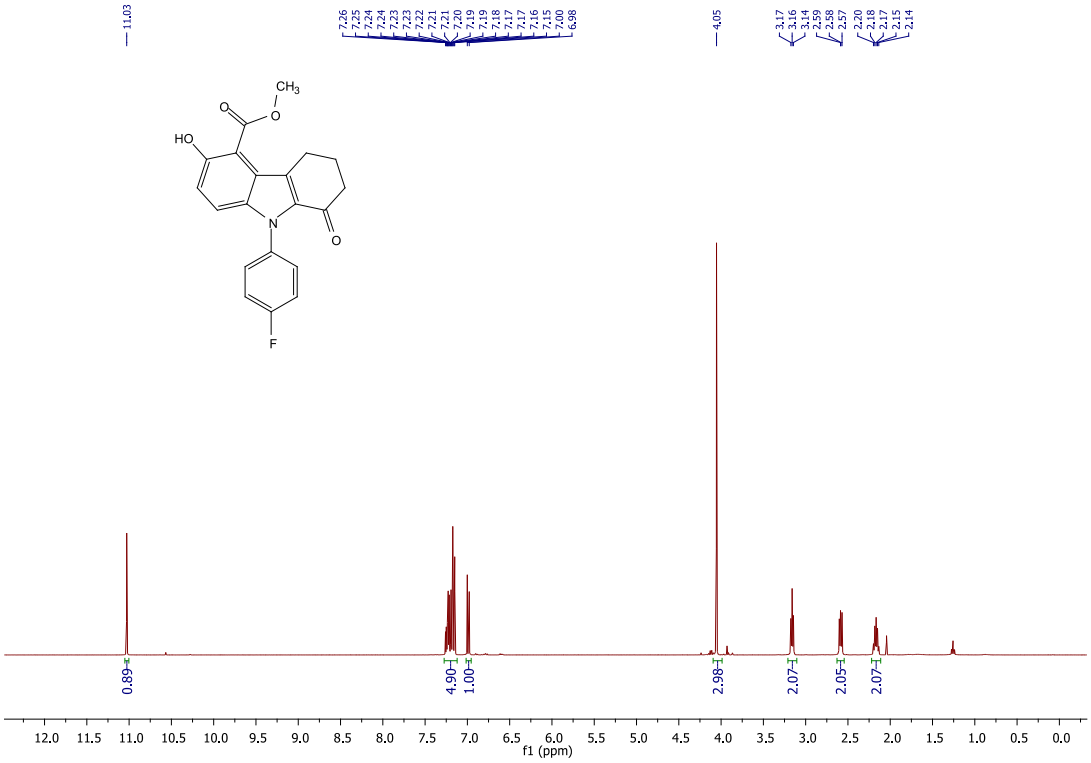
39.20
33.87
26.24
24.71
23.98
HO
O
O
N
O
f1 (ppm)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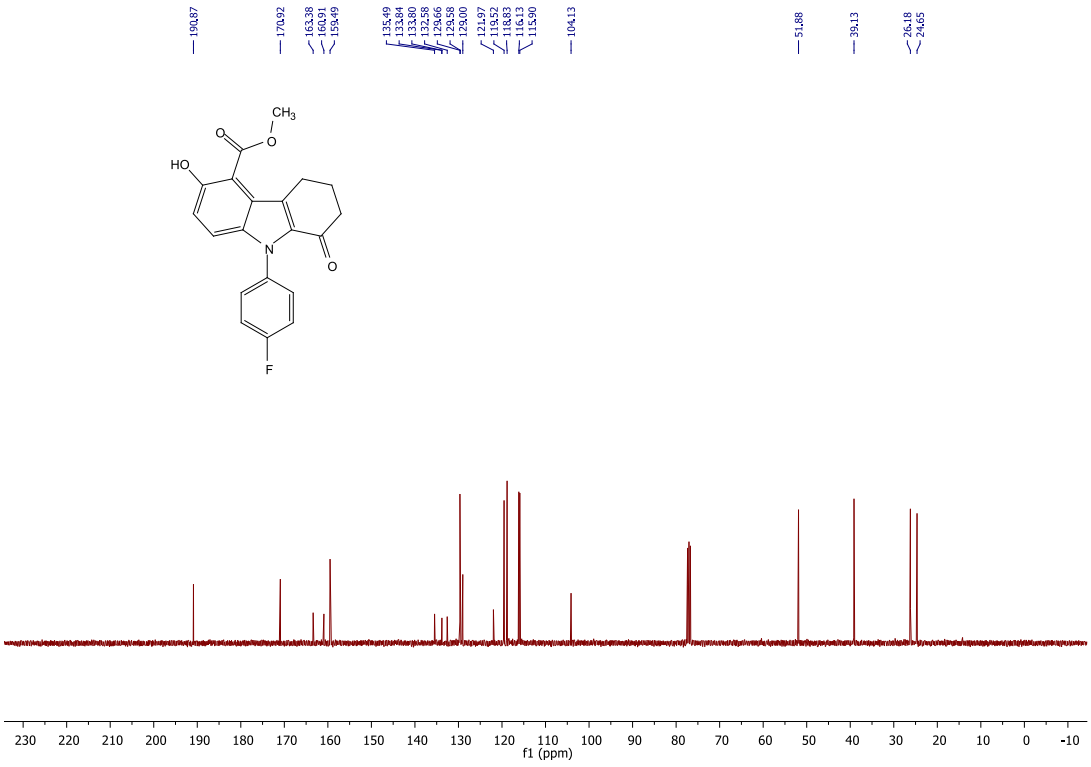
7.19
7.19
7.18
7.17
7.17
7.16
7.15
7.00
6.98
4.05
3.17
3.16
3.14
2.59
2.58
2.57
2.20
2.18
2.17
2.15
2.14
CH3
O
O
HO
N
O
F
0.89
4.90
1.00
2.98
2.07
2.05
2.07
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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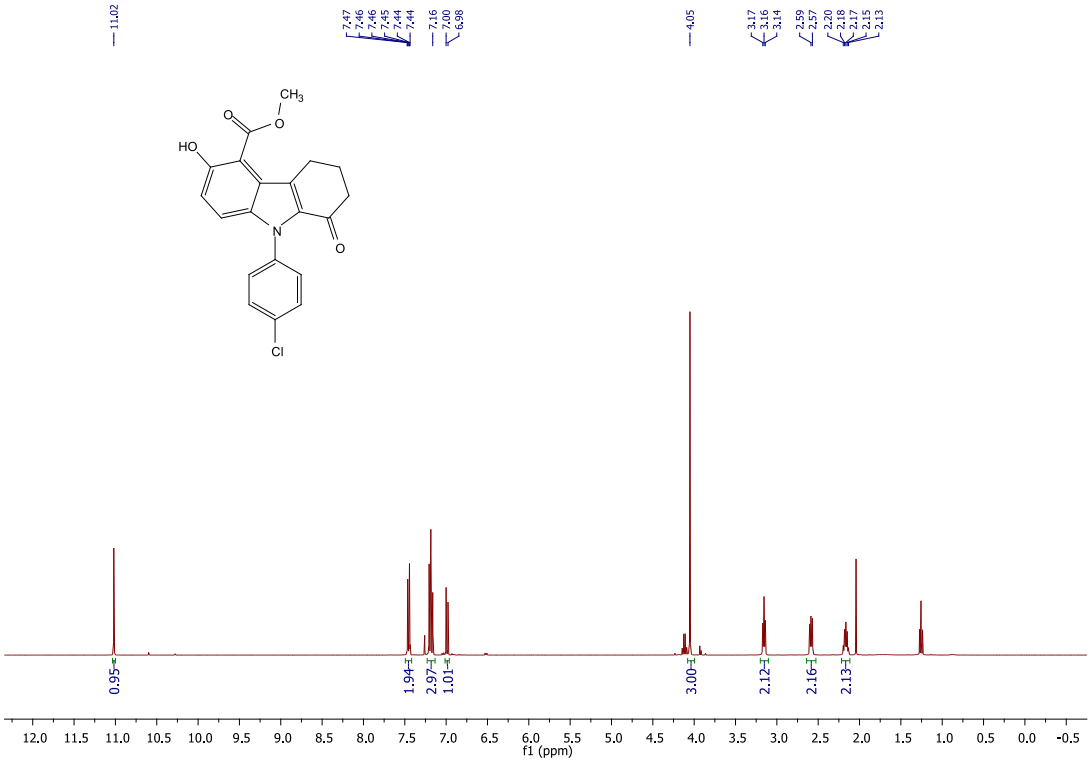
129.00
121.97
119.52
118.83
116.13
115.90
104.13
51.88
39.13
26.18
24.65
CH3
O
O
HO
N
O
F
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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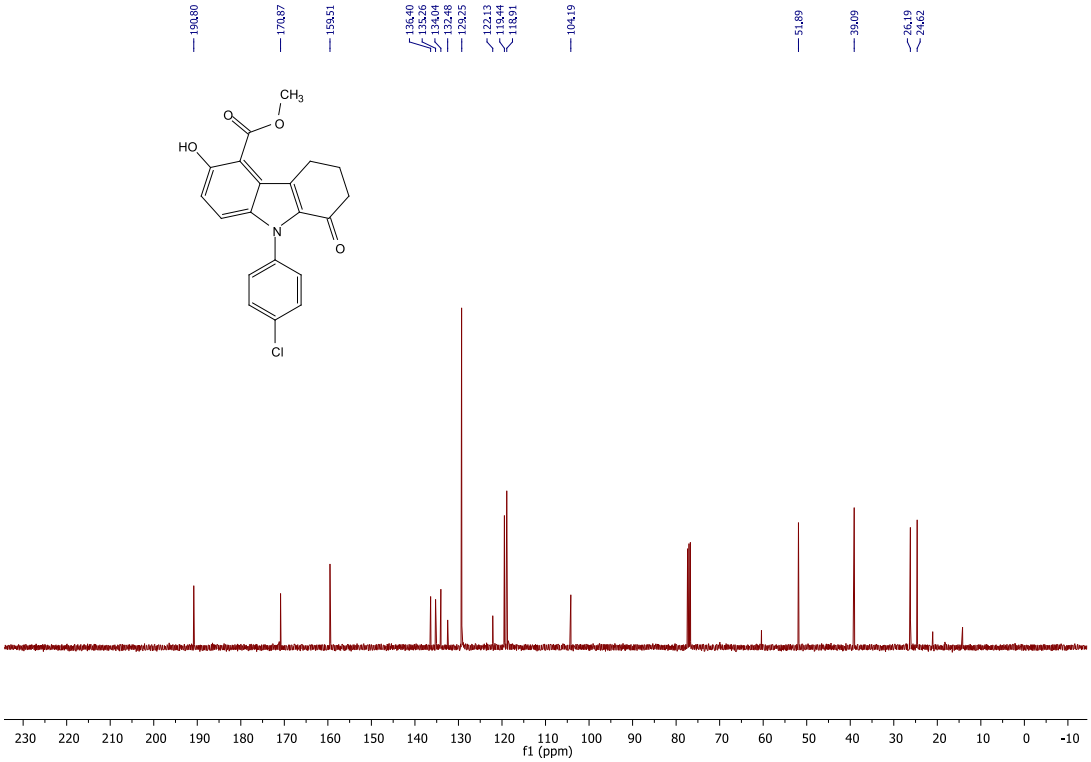
3.14
2.59
2.57
2.20
2.18
2.17
2.15
2.13
CH3
O
O
HO
N
O
Cl
0.95
1.94
2.97
1.01
3.00
2.12
2.16
2.13
f1 (ppm)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39.09
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CH3
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HO
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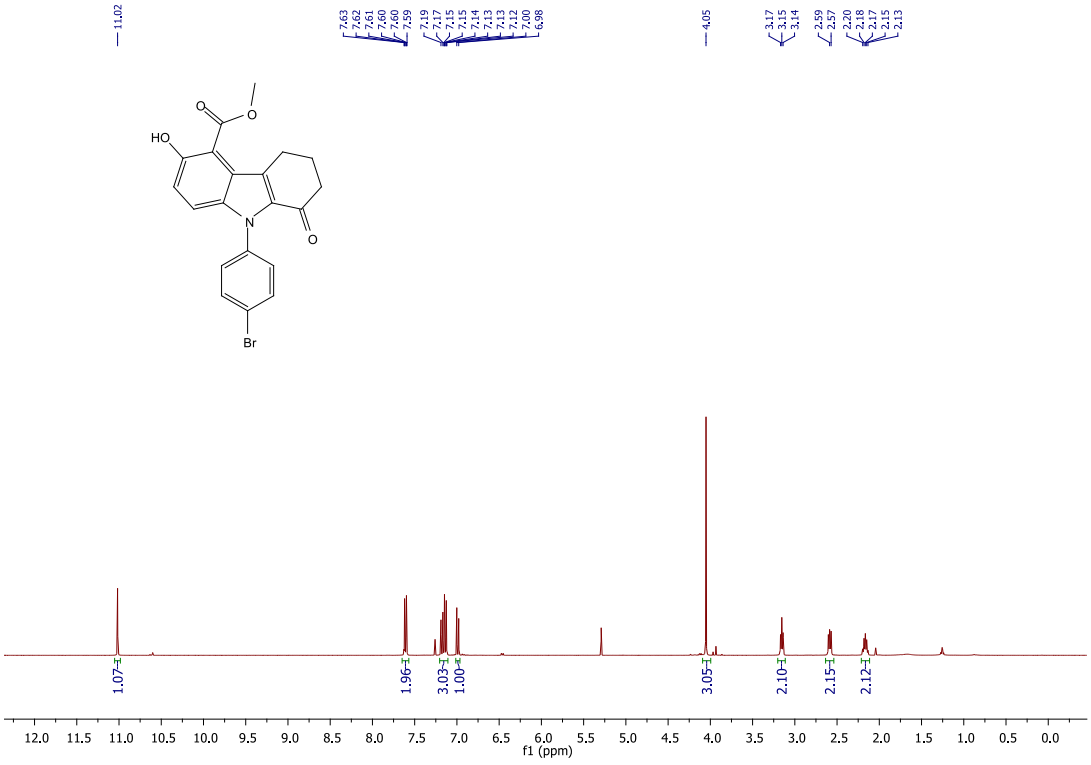
O
Cl
f1 (ppm)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7.14
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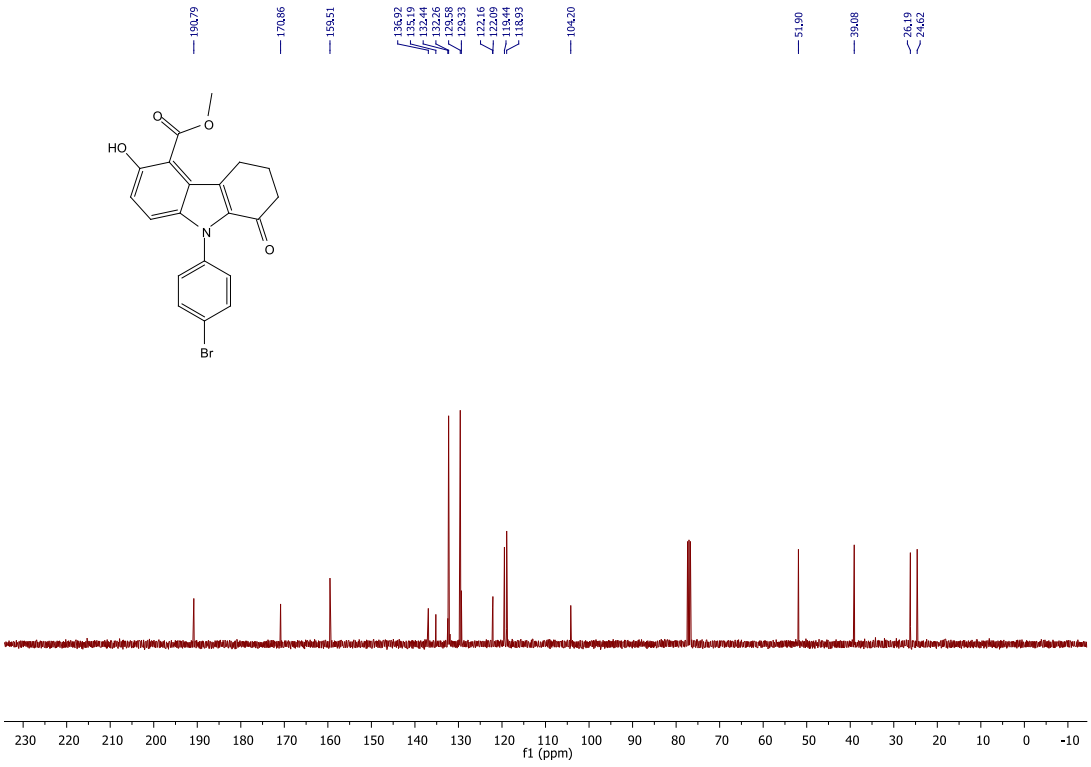
7.13
7.12
7.00
6.98
4.05
3.17
3.15
3.14
2.59
2.57
2.20
2.18
2.17
2.15
2.13
HO
O
O
N
O
Br
1.07
1.96
3.03
1.00
3.05
2.10
2.15
2.12
f1 (ppm)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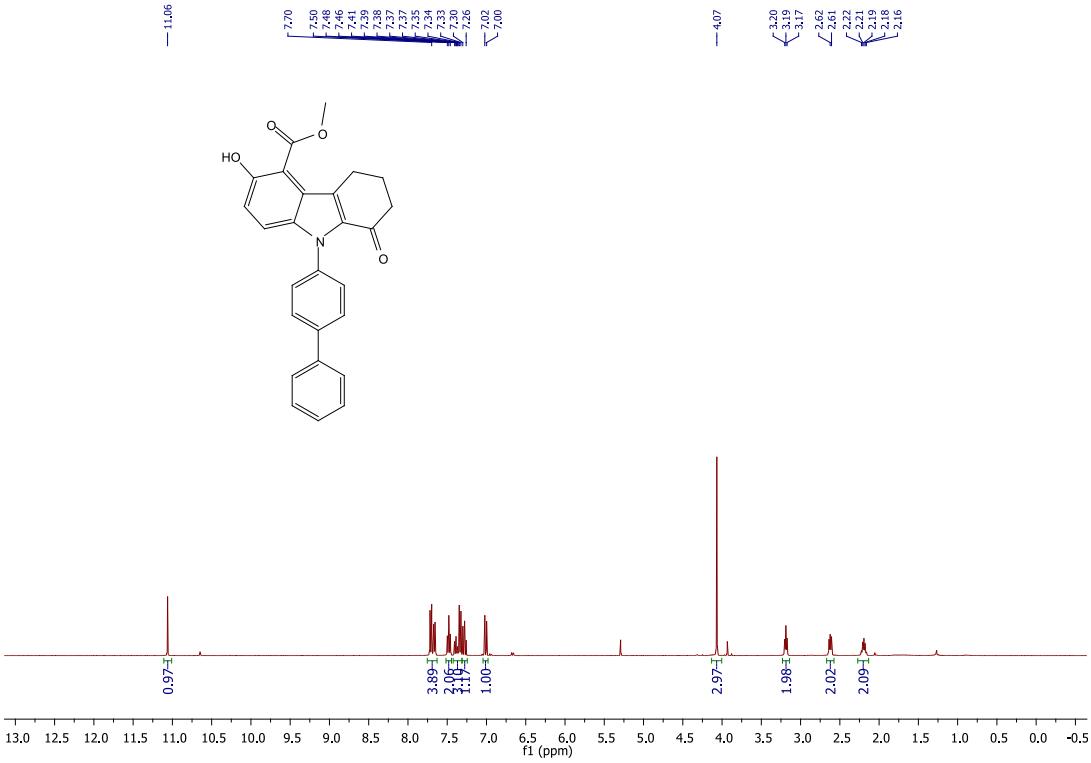
51.90
39.08
26.19
24.62
HO
O
O
N
O
Br
f1 (ppm)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7.30
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7.02
7.00
4.07
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3.19
3.17
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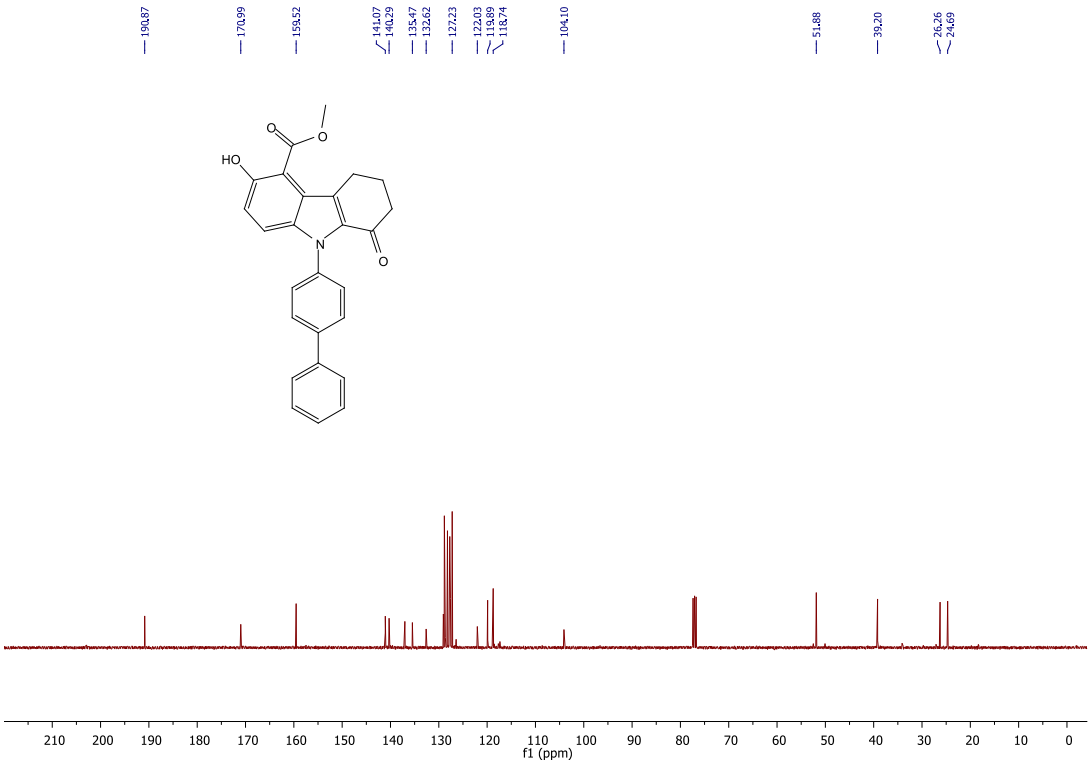
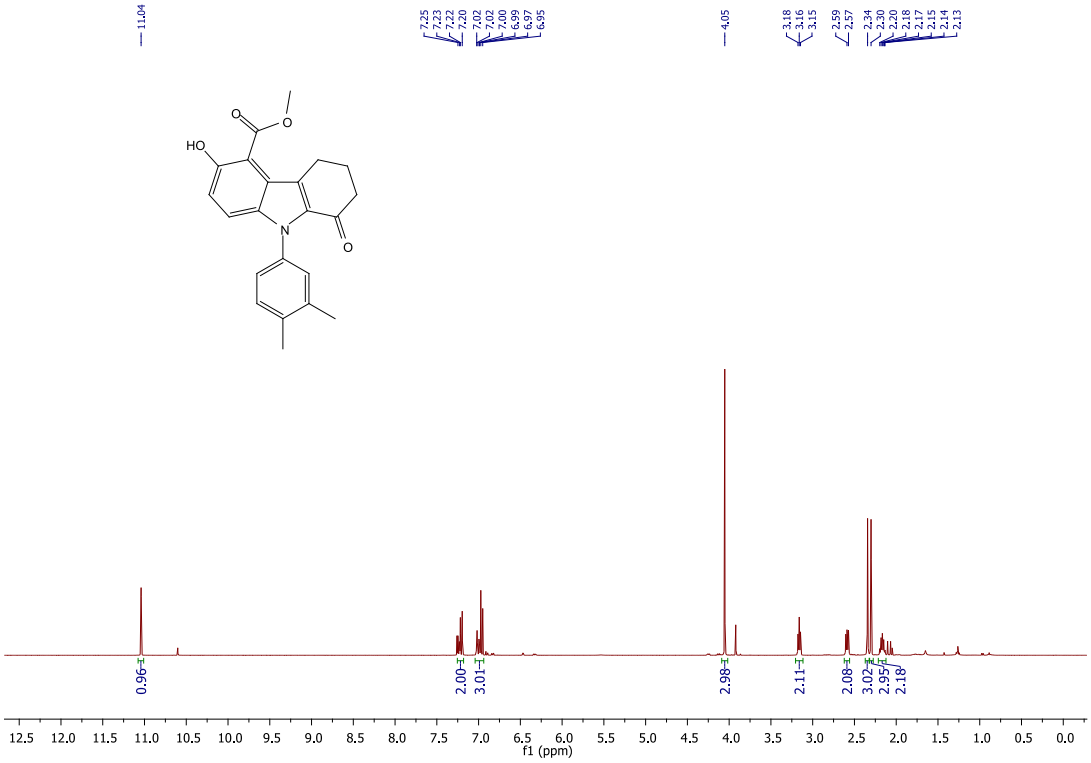
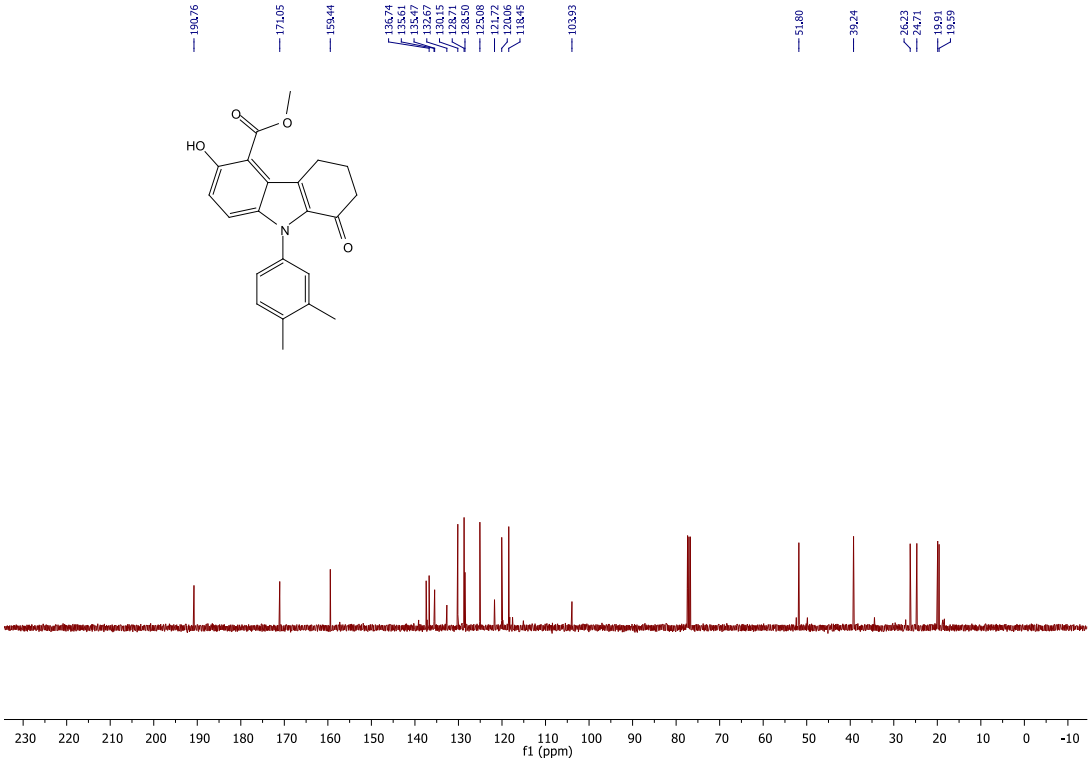
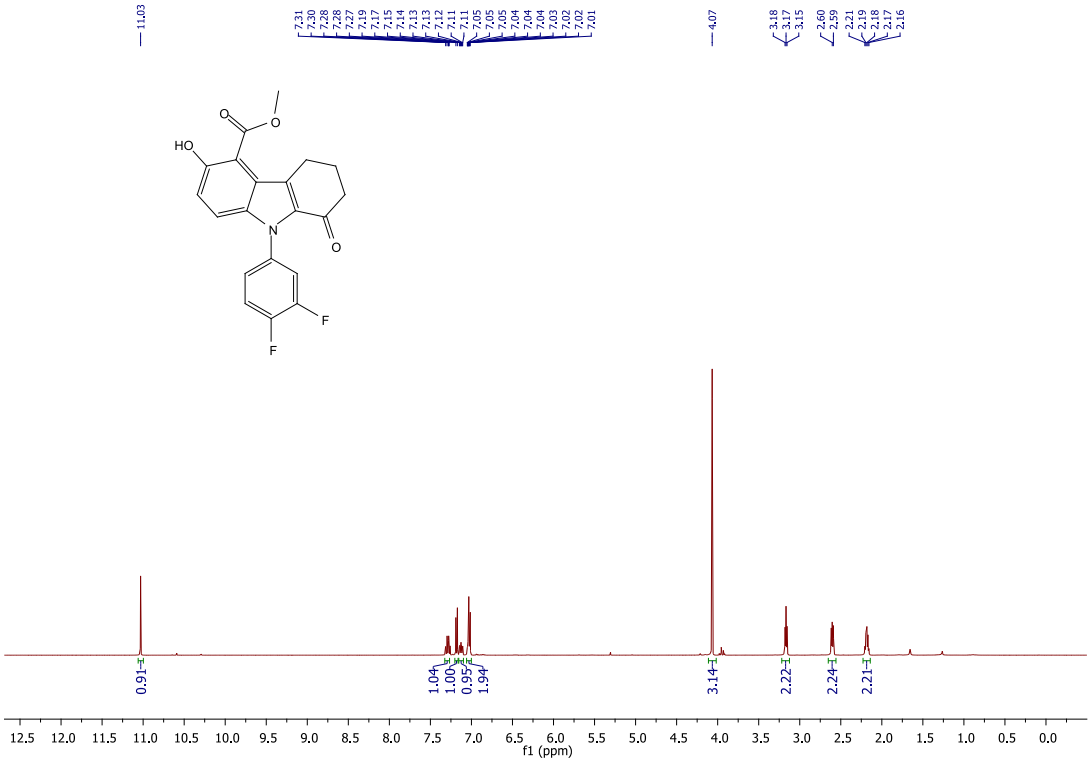
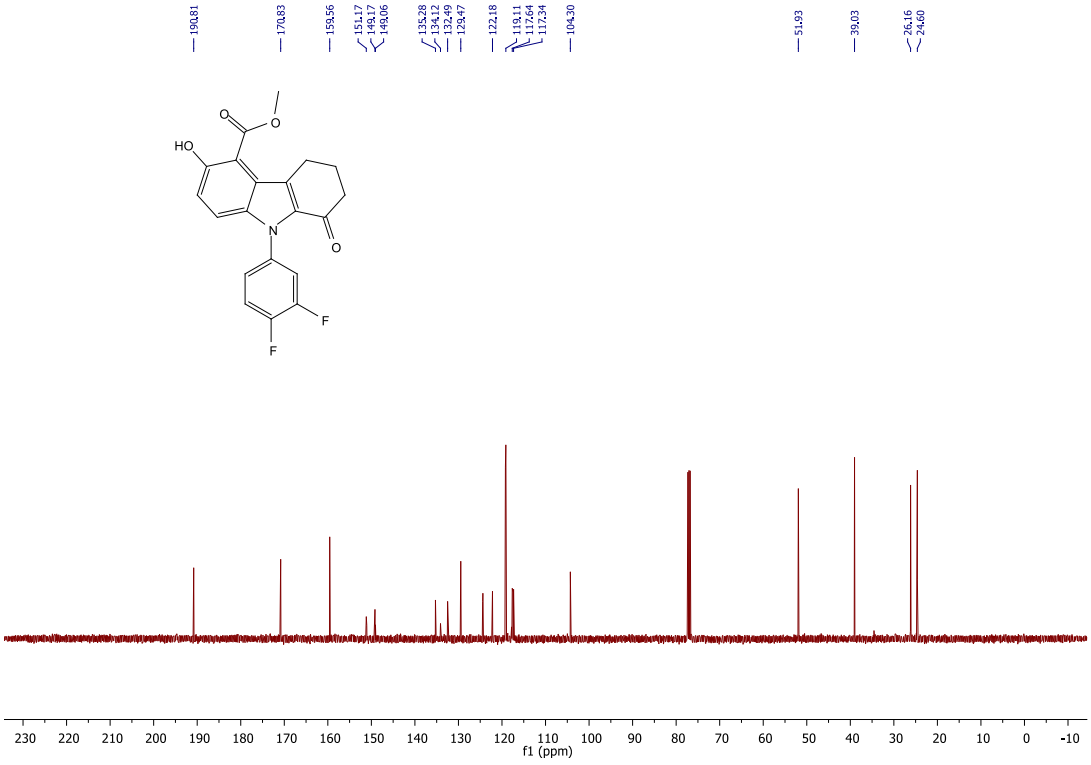
2.61
2.22
2.21
2.19
2.18
2.16
HO
O
O
N
O
0.97
3.89
2.06
2.17
1.11
1.00
2.97
1.98
2.02
2.09
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

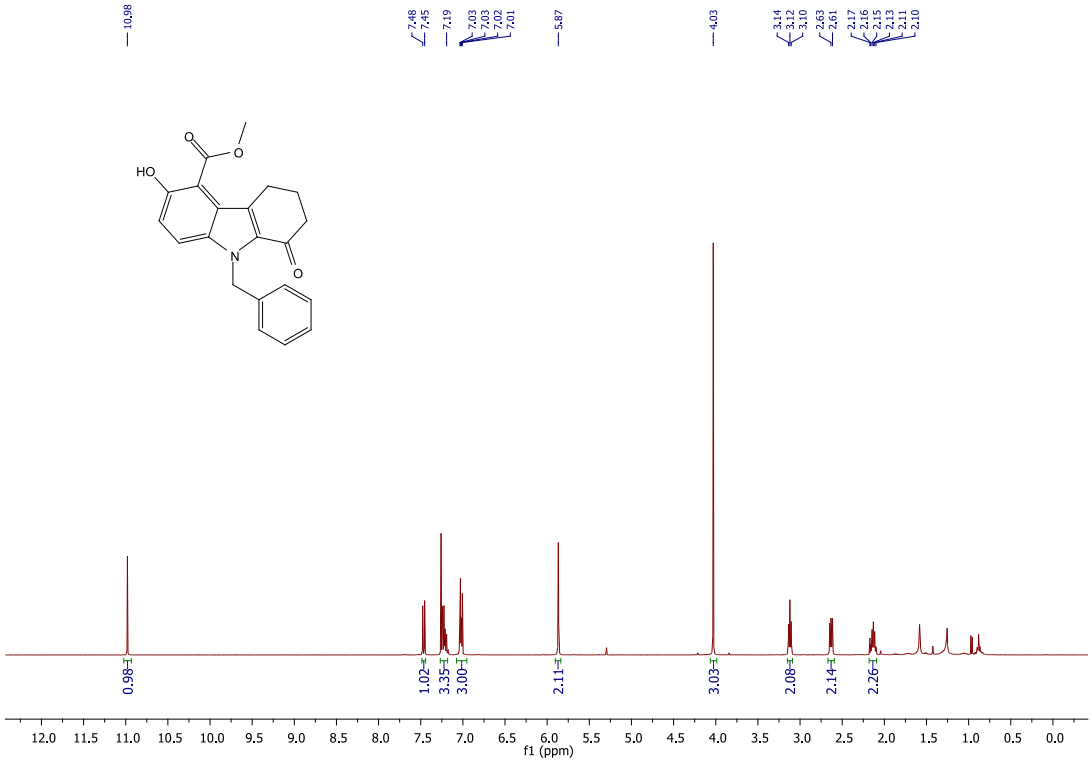

190.87
170.99
159.52
141.07
140.29
135.47
132.62
127.23
122.03
119.89
118.74
104.10
51.88
39.20
26.26
24.69
HO
O
O
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

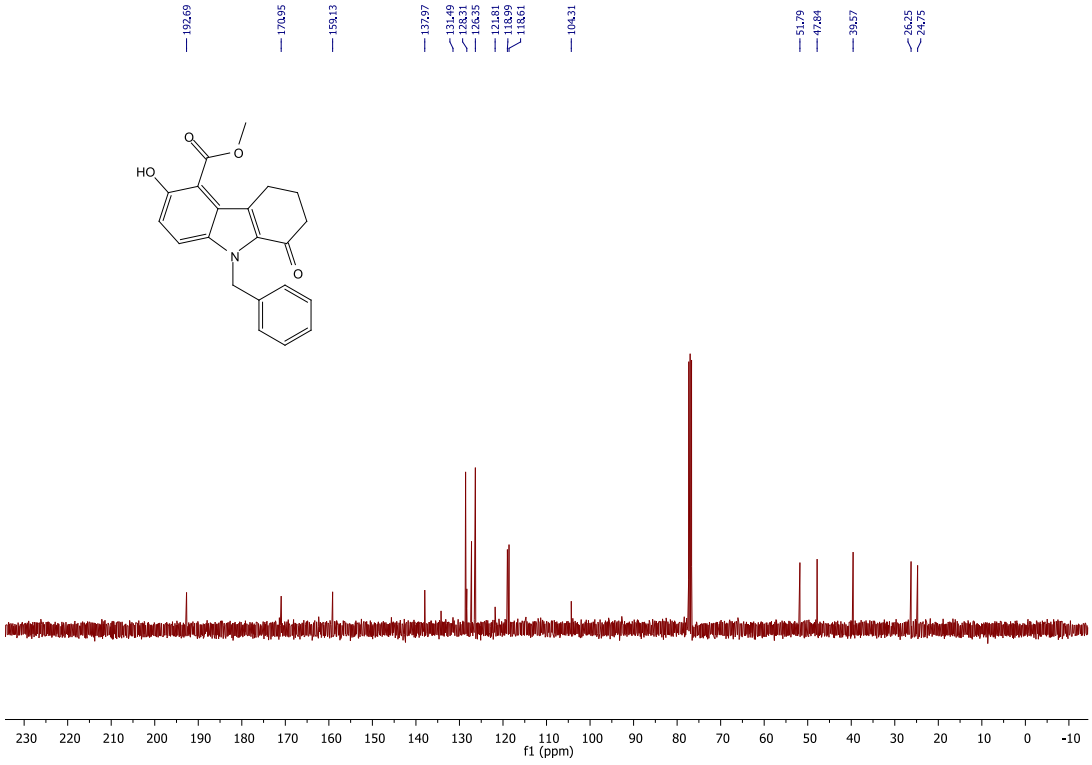

11.04
7.25
7.23
7.22
7.20
7.02
7.02
7.00
6.99
6.97
6.95
4.05
3.18
3.16
3.15
2.59
2.57
2.34
2.30
2.20
2.18
2.17
2.15
2.14
2.13
HO
O
O
N
O
0.96
2.00
3.01
2.98
2.11
2.08
3.02
2.95
2.18
f1 (ppm)

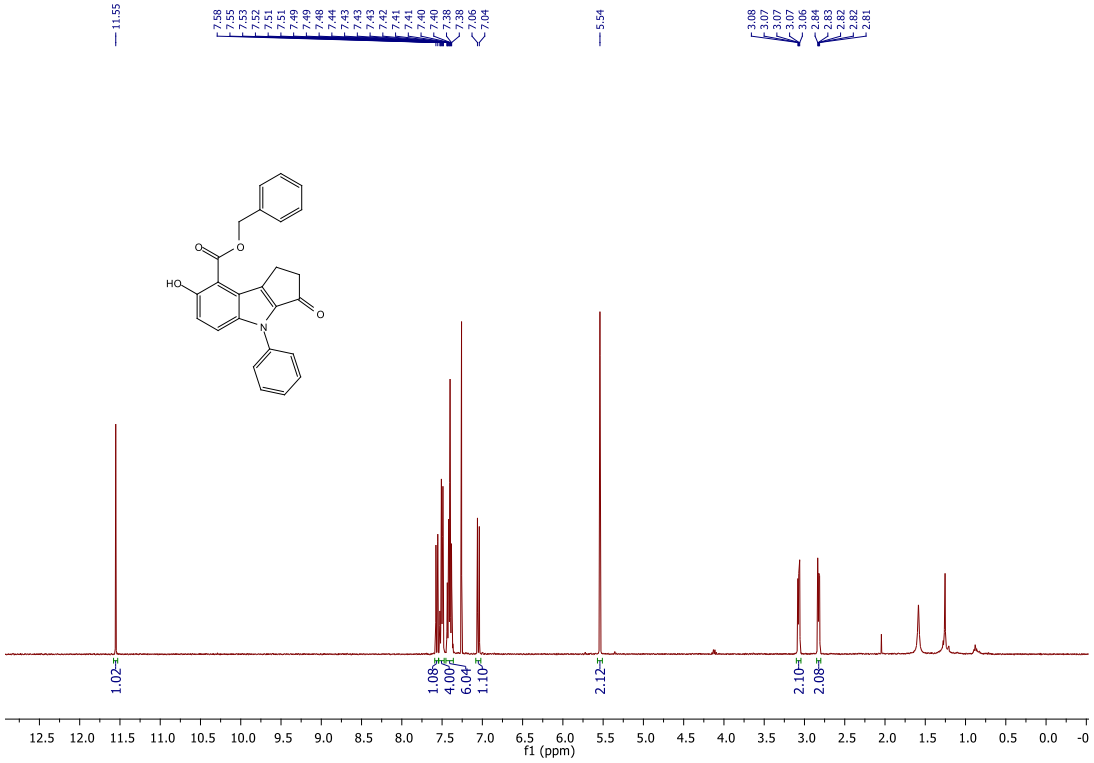

190.76
171.05
159.44
136.74
136.61
135.47
132.67
130.15
128.71
128.50
125.08
121.72
120.06
118.45
103.93
51.80
39.24
26.23
24.71
19.91
19.59
HO
O
O
N
O
f1 (ppm)

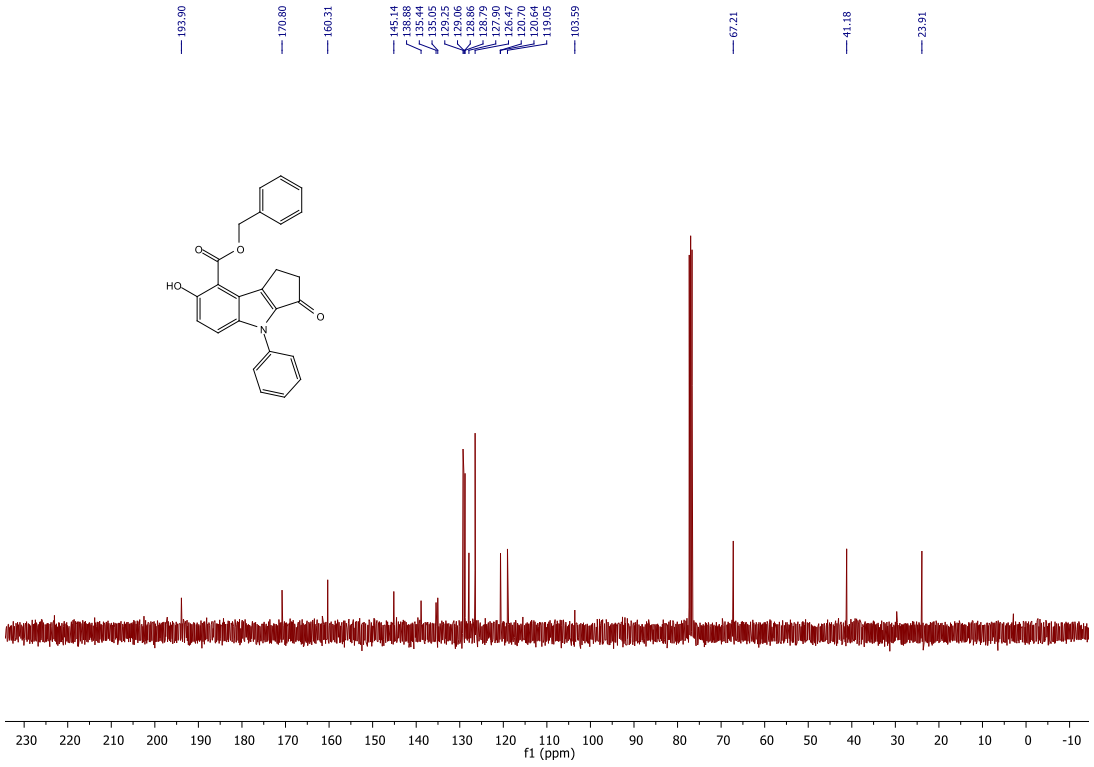

11.03
7.31
7.30
7.28
7.28
7.27
7.19
7.17
7.15
7.14
7.13
7.13
7.12
7.11
7.11
7.05
7.05
7.05
7.04
7.04
7.04
7.03
7.02
7.02
7.01
4.07
3.18
3.17
3.15
2.60
2.59
2.21
2.19
2.18
2.17
2.16
HO
O
O
N
O
F
F
0.91
1.04
1.00
0.95
1.94
3.14
2.22
2.24
2.21
f1 (ppm)

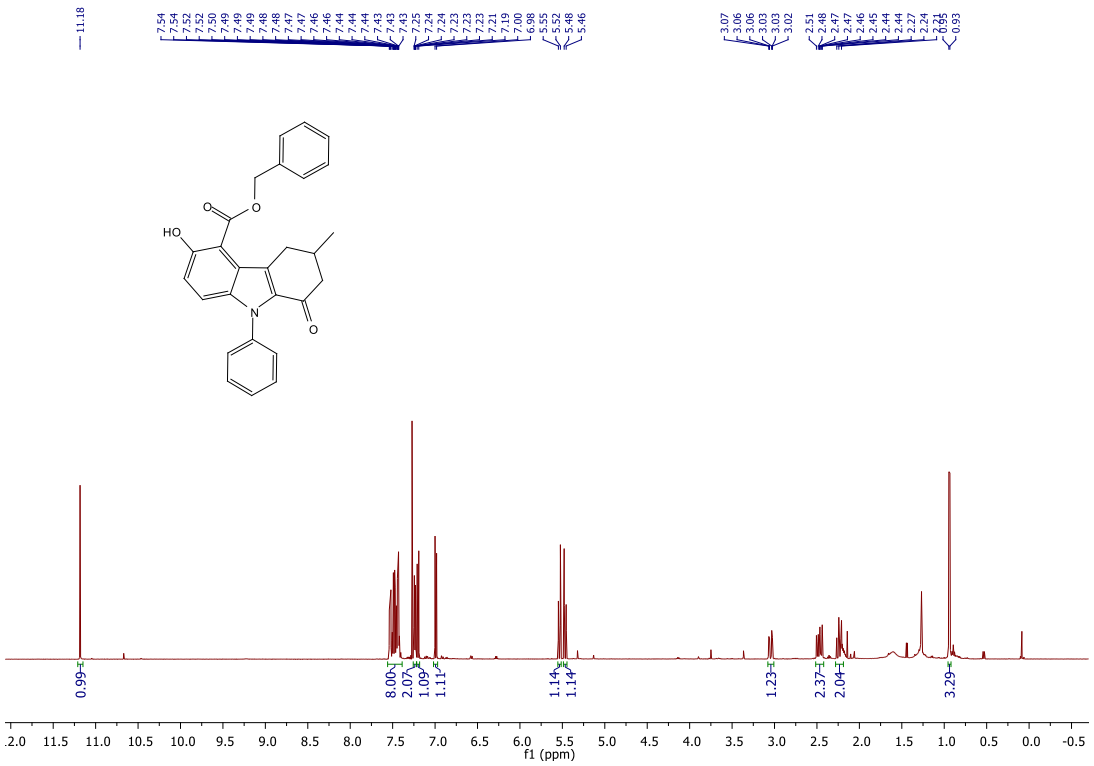

190.81
170.83
159.56
151.17
149.17
149.06
135.28
134.12
132.49
129.47
122.18
119.11
117.64
117.34
104.30
51.93
39.03
26.16
24.60
HO
O
O
N
O
F
F
f1 (ppm)

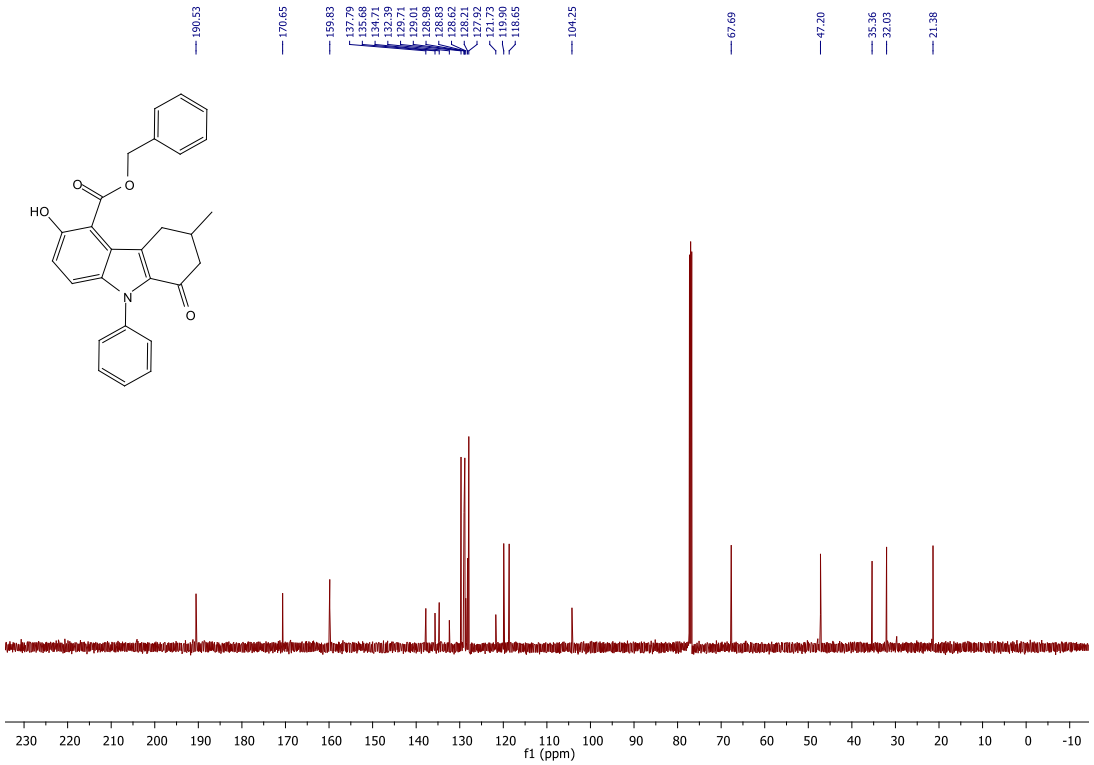

10.98
7.48
7.45
7.19
7.03
7.03
7.02
7.01
5.87
4.03
3.14
3.12
3.10
2.63
2.61
2.17
2.16
2.15
2.13
2.11
2.10
HO
O
O
N
O
0.98
1.02
3.35
3.00
2.11
3.03
2.08
2.14
2.26
f1 (ppm)

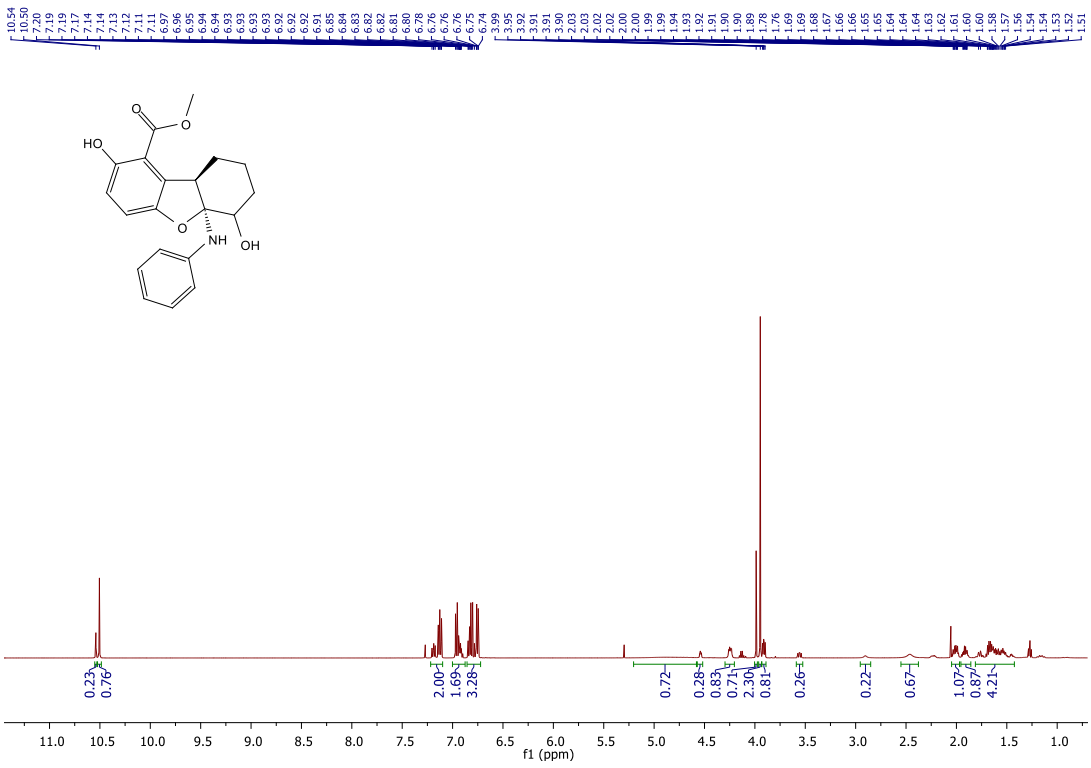

192.69
170.95
159.13
137.97
131.49
128.31
126.35
121.81
118.99
118.61
104.31
51.79
47.84
39.57
26.25
24.75
HO
O
O
N
O
f1 (ppm)

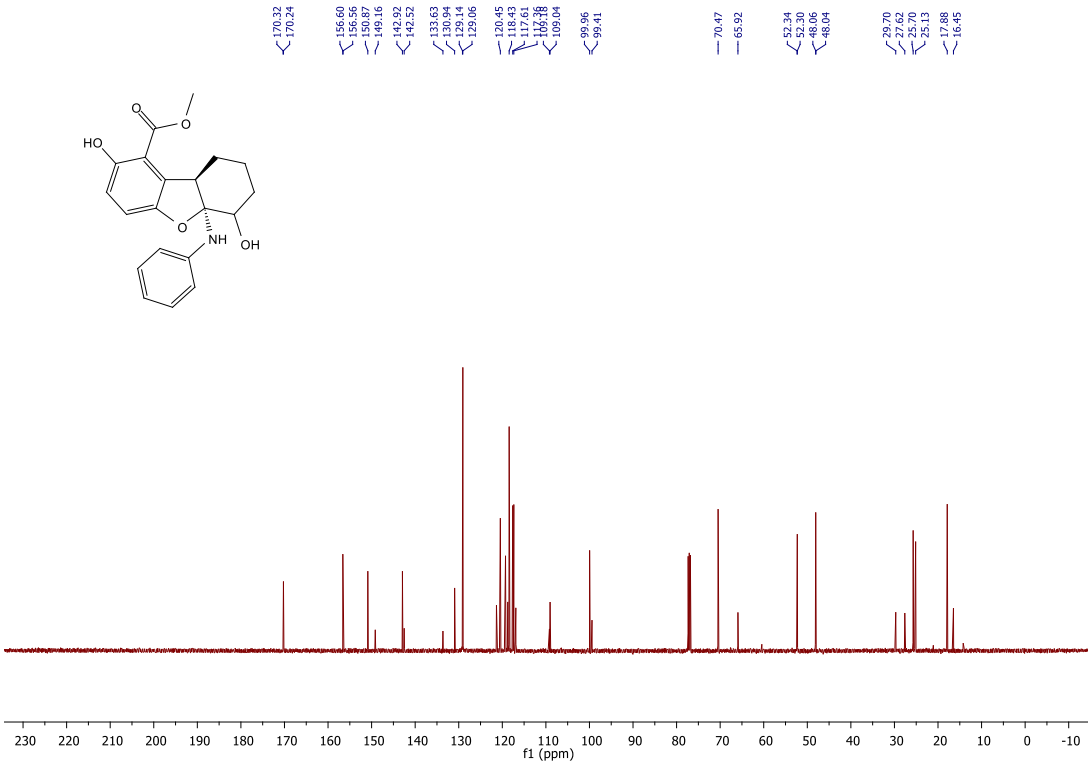

11.55
7.58
7.55
7.53
7.52
7.51
7.51
7.49
7.49
7.48
7.44
7.43
7.43
7.43
7.42
7.41
7.41
7.40
7.40
7.38
7.38
7.06
7.04
5.54
3.08
3.07
3.07
3.07
3.06
2.84
2.83
2.82
2.82
2.81
HO
O
O
O
N
1.02
1.08
4.00
6.04
1.10
2.12
2.10
2.08
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

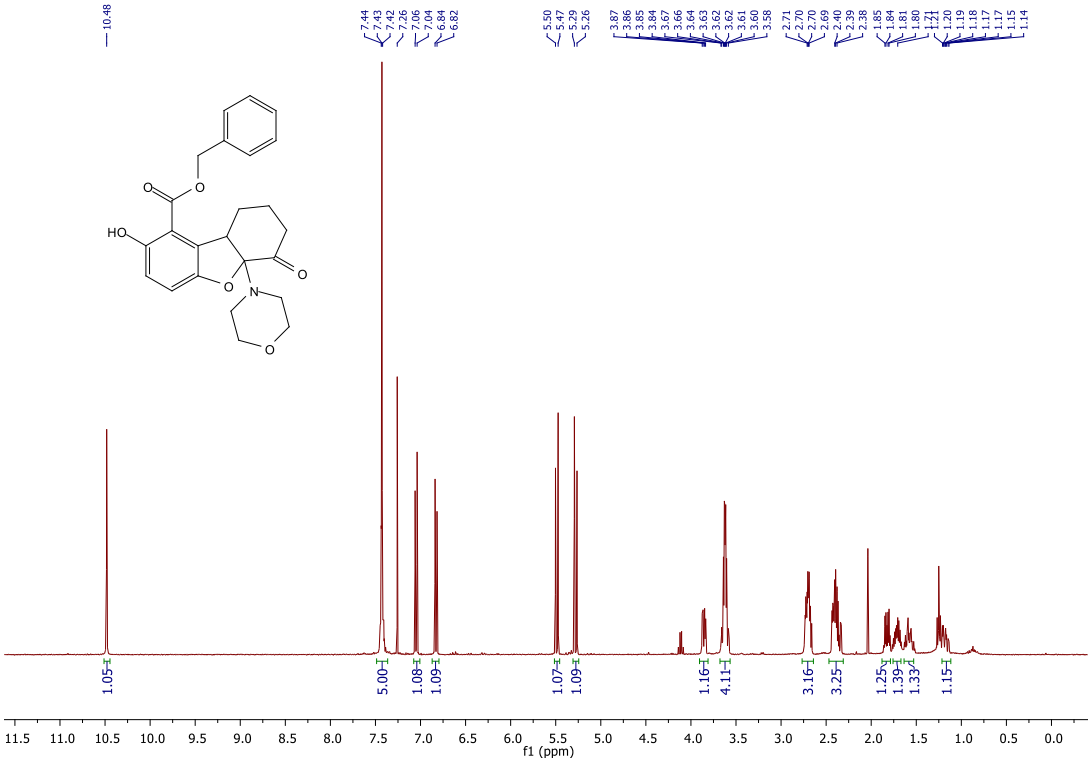

193.90
170.80
160.31
145.14
138.88
135.44
135.05
129.25
129.06
128.86
128.79
127.90
126.47
120.70
120.64
119.05
103.59
67.21
41.18
23.91
HO
O
O
O
N
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

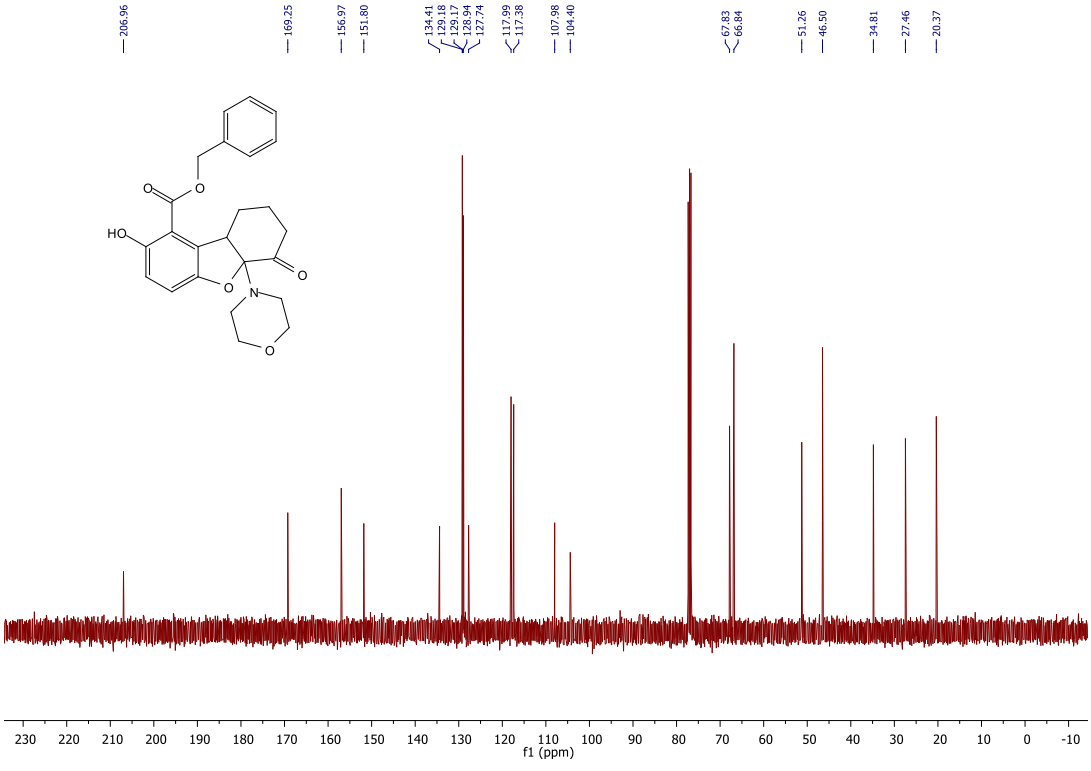

11.18
7.54 7.54 7.52 7.52 7.50 7.49 7.49 7.49 7.48 7.48 7.47 7.47 7.46 7.46 7.44 7.44 7.44 7.43 7.43 7.25 7.24 7.24 7.23 7.23 7.23 7.21 7.19 7.00 6.98 5.55 5.52 5.48 5.46
3.07 3.06 3.06 3.03 3.03 3.02 2.51 2.48 2.47 2.47 2.46 2.45 2.44 2.44 2.27 2.24 1.31 0.95 0.93
HO
O
O
N
O
0.99 8.00 2.07 1.09 1.11 1.14 1.14 1.23 2.37 2.04 3.29
f1 (ppm)

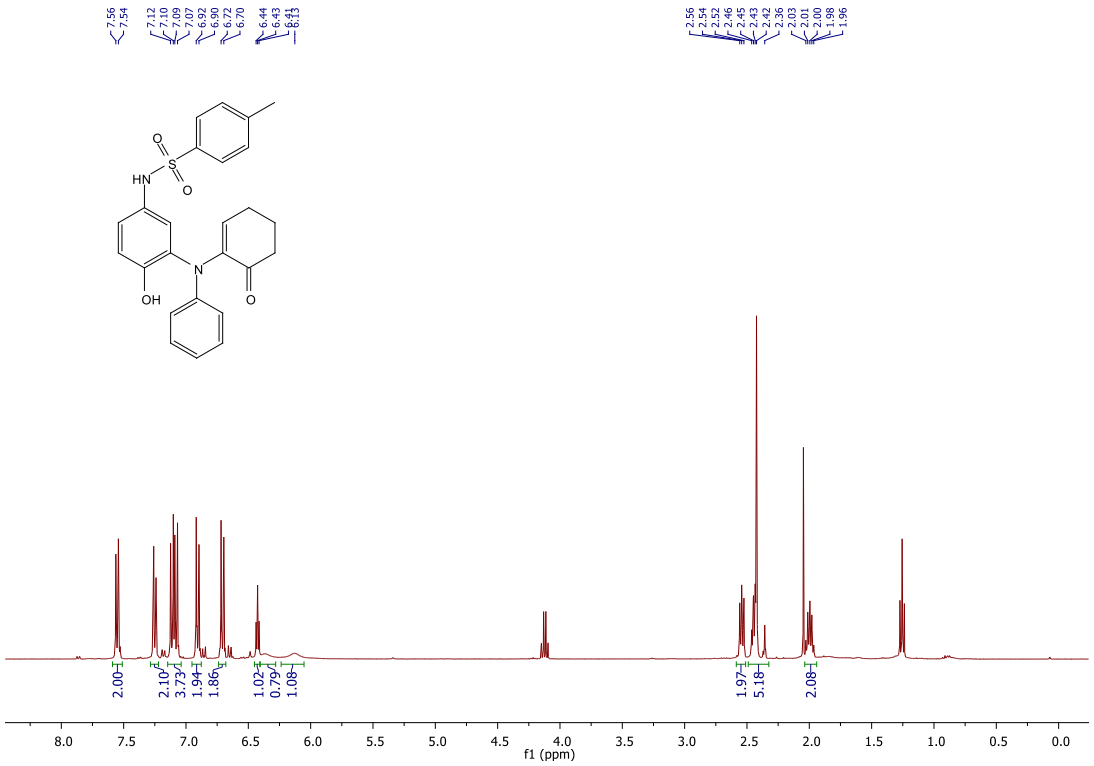

190.53 170.65 159.83 137.79 135.68 134.71 131.39 129.71 129.01 128.98 128.83 128.62 128.21 127.92 121.73 119.90 118.65 104.25 67.69 47.20 35.36 32.03 21.38
HO
O
O
N
O
f1 (ppm)


HO
O
O
NH
OH
0.23
0.76
2.00
1.69
3.28
0.72
0.28
0.83
0.71
2.30
0.81
0.26
0.22
0.67
1.07
0.87
4.21
f1 (ppm)


HO
O
O
NH
OH
f1 (ppm)


10.48
7.44
7.43
7.42
7.26
7.06
7.04
6.84
6.82
5.50
5.47
5.29
5.26
3.87
3.86
3.85
3.84
3.67
3.66
3.64
3.63
3.62
3.62
3.61
3.60
3.58
2.71
2.70
2.70
2.69
2.40
2.39
2.38
1.85
1.84
1.81
1.80
1.21
1.20
1.19
1.18
1.17
1.17
1.15
1.14
HO
O
O
O
O
N
O
1.05
5.00
1.08
1.09
1.07
1.09
1.16
4.11
3.16
3.25
1.25
1.39
1.33
1.15
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


206.96
169.25
156.97
151.80
134.41
129.18
129.17
128.94
127.74
117.99
117.38
107.98
104.40
67.83
66.84
51.26
46.50
34.81
27.46
20.37
HO
O
O
O
O
N
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.56
7.54
7.12
7.10
7.09
7.07
6.92
6.90
6.72
6.70
6.44
6.43
6.41
6.13
2.56
2.54
2.52
2.46
2.45
2.43
2.42
2.36
2.03
2.01
2.00
1.98
1.96
HN
S
O
O
N
OH
O
2.00
2.10
3.79
1.94
1.86
1.02
0.79
1.08
1.97
5.18
2.08
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)