Supporting Information

NHC-catalyzed Aldol-Like Reactions of Allenoates with Isatins: Regiospecific Syntheses of γ-Functionalized Allenoates

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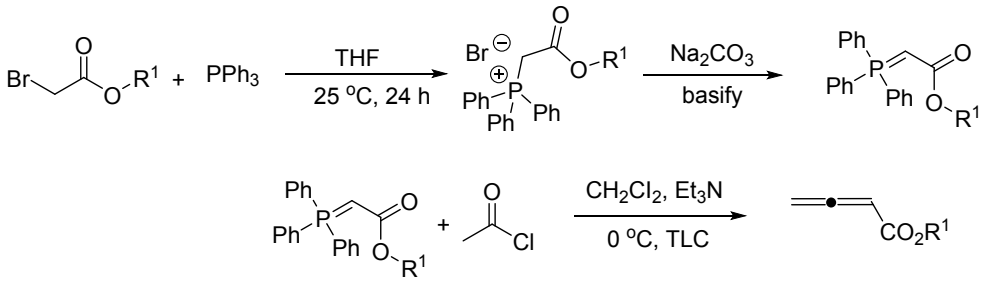
1. General Information

Common reagents and materials were purchased from commercial sources and purified by recrystallization or distillation. Melting points were determined in open capillaries and were uncorrected. ^{1}H NMR spectra were measured on a Bruker DPX 400 MHz spectrometer in $CDCl_3$or DMSO with chemical shift (δ) given in ppm relative to TMS as internal standard. Highresolution mass spectra (HRMS) were obtained on a micrOTOF-QⅡ HRMS/MS instrument (Bruker) with the technique of electrospray ionization. Optical rotation values were measured with instruments operating at λ = 589 nm, corresponding to the sodium D line at the temperatures indicated.TLC was carried out on SiO_2 (silica gel 60 F254, Merck), and the spots were located with UV light.

2. Synthesis of Allenoates (1a-1e)

Allenoates**1a-1e** were prepared according to the literature[1].

1a-1d:

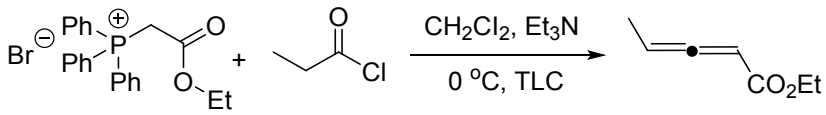


1a: R^1 = Et **1b:** R^1 = ^{i}Pr **1c:** R^1 = ^{n}Bu **1d:** R^1 = Bn

To a solution of PPh_3 (26.2 g, 100 mmol) in THF (150 mL), alkyl/aryl bromoacetate (100 mmol, 1.0 equiv.) was added over 20 minutes. The reaction mixture was stirred at room temperature for 24 hours and the precipitate filtered, washed with cold Et_2O and dried. The collected phosphonium salt was dissolved in CH_2Cl_2 (100 mL) and saturated aqueous Na_2CO_3 (150 mL) was added. The mixture

was stirred at room temperature for 2 hours and separated the organic layer, then extracted water layer with CH_2Cl_2 (20 mL), washed the combined organic layer with saturated aqueous NaCl (50 mL), and dried with Na_2SO_4. The Na_2SO_4 was filtered and washed with CH_2Cl_2. The filtrate was evaporated to 100 mL and directly engaged in the next step. To the solution of stabilized ylide, and triethylamine (14 mL, 100 mmol, 1 equiv.) at 0 °C , acetyl chloride (10 mL, 110 mmol, 1.1 equiv.) in solution in CH_2Cl_2 (20 mL) was added dropwise. After completion of the reaction (TLC), the solution was concentrated to afford a gummy residue. This was treated with Pet-EtOAc 20: 1 (petro ether: ethyl acetate =20: 1, 250 mL, 30-60 °C boiling range Pet) and silica gel (100-200 section, 100 g), stirred vigorously for 1hour. The mixture was filtered and washed with Pet-EtOAc 20: 1, filtrate evaporated and to a flash column chromatography (eluent Pet-EtOAc 20: 1, 30-60 °C boiling range Pet) to afford the pure product **1a-1d** as colorlessor yellow oil.

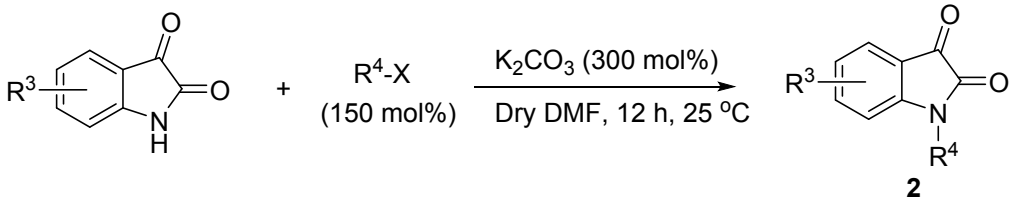
1e:



CH_2Cl_2 (50 mL) and triethylamine (14 mL, 2.0 equiv.) were added to the corresponding phosphonium salt. After stirring for 1 h, the propionyl chloride (1.1 equiv.) in solution in CH_2Cl_2 (10 mL) was added dropwise over 30 min. The mixture was stirred overnight and handled with the same process as mentioned in synthesis of **1e.**

3. Synthesis of N-protected Isatins (2a-2q)

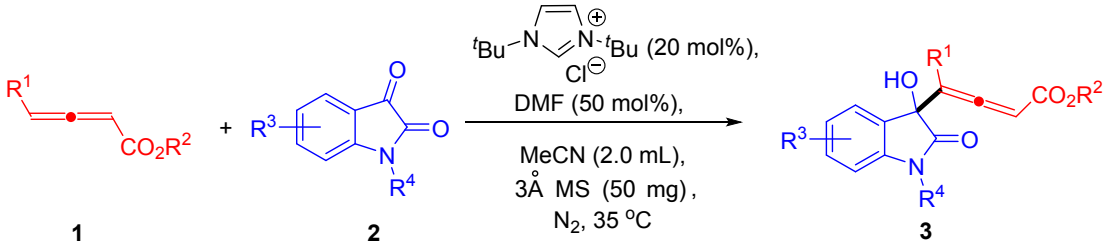
N-protected isatin derivatives **2** were prepared using reported procedures[2-4] from commercially available isatins with different alkyl halides in the presence of K_2CO_3 in DMF at room temperature for 8 h.



2

2a: R^3 = H, R^4 = Bn;
2b: R^3 = 5-Me, R^4 = Bn;
2c: R^3 = 5-MeO, R^4 = Bn;
2d: R^3 = 7-Me, R^4 = Bn;
2e: R^3 = 5-Me, R^4 = 4-$FC_6H_4CH_2$;
2f: R^3 = 5-Me, R^4 = 4-$BrC_6H_4CH_2$;
2g: R^3 = 5-Me, R^4 = 4-$MeC_6H_4CH_2$;
2h: R^3 = 5-MeO, R^4 = 4-$ClC_6H_4CH_2$;
2i: R^3 = 5-MeO, R^4 = 4-$BrC_6H_4CH_2$;
2j: R^3 = 5-MeO, R^4 = 4-$MeC_6H_4CH_2$;
2k: R^3 = 7-Me, R^4 = 4-$MeC_6H_4CH_2$;
2l: R^3 = H, R^4 = 4-FC_6H_4CH2;
2m: R^3 = H, R^4 = 4-$ClC_6H_4CH_2$;
2n: R^3 = H, R^4 = 4-$BrC_6H_4CH_2$;
2o: R^3 = H, R^4 = 4-$MeC_6H_4CH_2$;
2p: R^3 = H, R^4 = Me;
2q: R^3 = H, R^4 = Allyl.

4. General Procedure for the Synthesis of Products

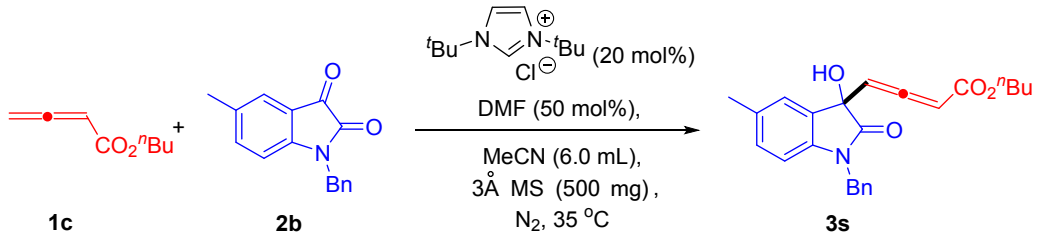


1 **2** **3**

An oven-dried 10 mL Schlenk tube equipped with a magnetic stir bar was charged with imidazolium salt **A** (4.3 mg, 0.02 mmol), isatins **2** (0.10 mmol) and 3Å MS (50 mg). Freshly distilled MeCN (1.5 mL), DMF (3.9 μL, 0.05mmol), allenoates **1** (0.20 mmol) ware added into the mixture with a syringe. Then tube was closed with a septum, evacuated, and refilled with nitrogen. The mixture was stirred at 35 °C until completion (monitored by TLC). After removal of the solvent under reduced pressure, the resulted crude residue was purified by column chromatography (silicagel, mixtures of petroleum ether/ethyl acetate, 3:1-5:1, v/v) to afford the desired product **3**.

4.1 1.0 mmol Scale Synthesis of **3s**

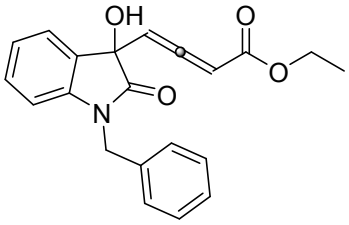
Synthesis of **3s** (1.0 mmol)



Imidazolium salt **A** (43.4 mg, 0.2 mmol), isatin **2b** (1.0 mmol) and 3Å MS (500 mg) were placed into an oven-dried 25 mL flask equipped with a magnetic stir bar. Freshly distilled MeCN (6.0 mL), DMF (39.0 μL, 0.5 mmol) and allenoate **1c** (2.0 mmol) were added into the mixture with a syringe. Then the flask was closed with a septum, evacuated, and refilled with nitrogen. The mixture was stirred at 35 °C until the consumption of the starting materials (monitored by TLC). Then the solvent was removed under reduced pressure and the resulted crude residue was purified by column chromatography (silicagel, mixtures of petroleum ether/ethyl acetate, 3:1 v/v) to afford the desired product **3s** (yield: 79%, 322.1 mg).

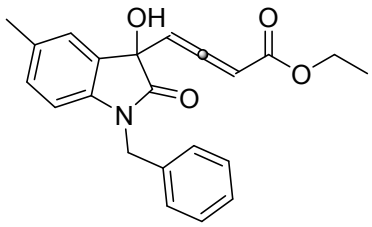
5. Characterization Data of Products

ethyl 4-(1-benzyl-3-hydroxy-2-oxoindolin-3-yl)buta-2,3-dienoate(3a)



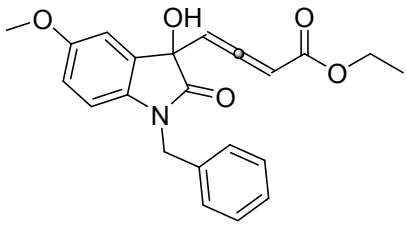
White solid (25.1 mg, 72% yield), m.p.: 112-113 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ7.45 (t, J = 7.4 Hz, 1H), 7.32 – 7.24 (m, 5H), 7.19 (td, J = 7.9, 2.8 Hz, 1H), 7.10 – 7.00 (m, 1H), 6.70 (d, J = 7.8 Hz, 1H), 6.00 (d, J = 6.1 Hz, 1H), 5.80 (d, J = 6.1 Hz, 1H), 4.98 (dd, J = 15.8, 2.4 Hz, 1H), 4.77 (dd, J = 15.7, J_2 = 6.3 Hz, 1H), 4.20 – 4.03 (m, 2H), 1.18 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.44, 175.83, 164.90, 141.88, 135.03, 129.95, 128.75, 128.71, 127.65, 127.06, 124.78, 123.23, 109.62, 97.68, 91.72, 74.82, 61.08, 43.84, 13.98. HRMS (ESI) calcd for $[C_{21}H_{19}NO_4Na, M+Na]^+$: 372.1206, found: 372.1217.

ethyl 4-(1-benzyl-3-hydroxy-5-methyl-2-oxoindolin-3-yl)buta-2,3-dienoate (3b)



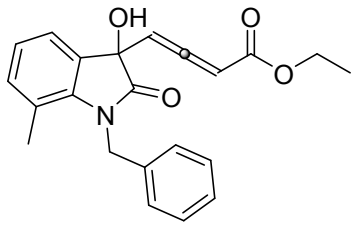
White solid (28.7 mg, 79% yield), m.p.: 152-153 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.36 – 7.26 (m, 4H), 7.17 (s, 1H), 7.03 (d, J = 8.2 Hz, 1H), 6.89 – 6.69 (m, 2H), 6.16 (d, J = 6.1 Hz, 1H), 5.92 (d, J = 6.2 Hz, 1H), 4.86 (q, J = 15.9 Hz, 2H), 4.12 – 3.99 (m, 2H), 2.25 (s, 3H), 1.13 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.73, 175.77, 164.80, 139.59, 135.18, 133.12, 130.36, 128.78, 128.68, 127.68, 127.13, 125.56, 109.47, 97.91, 92.71, 74.57, 61.10, 43.93, 20.97, 14.09. HRMS (ESI) calcd for $[C_{22}H_{21}NO_4Na, M+Na]^+$: 386.1363, found: 386.1359.

ethyl 4-(1-benzyl-3-hydroxy-5-methoxy-2-oxoindolin-3-yl)buta-2,3-dienoate (3c)



White solid (28.5 mg, 75% yield), m.p.: 122-123 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ7.28 (d, J = 7.1 Hz, 2H), 7.23 (d, J = 6.7 Hz, 3H), 7.09 (s, 1H), 6.71 (d, J = 8.5 Hz, 1H), 6.58 (d, J = 8.5 Hz, 1H), 6.02 (d, J = 6.1 Hz, 1H), 5.80 (d, J = 6.1 Hz, 1H), 4.94 (dd, J = 15.7, 6.3 Hz, 1H), 4.74 (dd, J = 15.7, 2.1 Hz, 1H), 4.15 – 4.07 (m, 2H), 3.71 (d, J = 9.6 Hz, 3H), 1.23 – 1.14 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.40, 175.72, 164.93, 156.23, 135.07, 129.94, 129.80, 128.68, 127.57, 127.01, 115.06, 111.31, 110.21, 97.73, 91.60, 75.19, 61.08, 55.57, 43.84, 13.94. HRMS (ESI) calcd for $[C_{22}H_{21}NO_5Na, M+Na]^+$: 402.1312, found: 402.1329.

ethyl 4-(1-benzyl-3-hydroxy-7-methyl-2-oxoindolin-3-yl)buta-2,3-dienoate (3d)



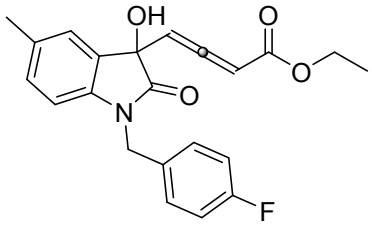
White solid (23.0 mg, 63% yield), m.p.: 150-151 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.38 – 7.27 (m, 3H), 7.21 (d, J = 7.6 Hz, 1H), 7.16 (d, J = 7.5 Hz, 1H), 7.04 – 6.82 (m, 3H), 6.32 (d, J = 6.1 Hz, 1H), 5.84 (d, J = 6.0 Hz, 1H), 5.22 – 5.05 (m, 2H), 4.21 – 3.99 (m, 2H), 2.18 (s, 3H), 1.14 (q, J = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6)

δ 210.86, 176.14, 164.44, 139.70, 137.81, 133.40, 130.80, 128.85, 127.13, 125.45, 122.84, 122.70, 119.76, 98.36, 90.71, 73.68, 60.57, 44.11, 18.09, 14.08. HRMS (ESI) calcd for $[C_{22}H_{21}NO_4Na, M+Na]^+$: 386.1363, found: 386.1365.

ethyl

4-(1-(4-fluorobenzyl)-3-hydroxy-5-methyl-2-oxoindolin-3-yl)buta-2,3-dienoate

(3e)

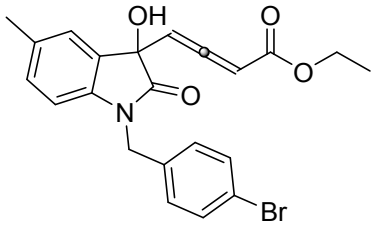


White solid (24.9 mg, 65% yield), m.p.: 141-142 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.35 (dd, J = 8.4, 5.5 Hz, 2H), 7.19 – 7.11 (m, 2H), 7.05 (d, J = 7.9 Hz, 1H), 6.76 (d, J = 5.9 Hz, 2H), 6.15 (d, J = 6.1 Hz, 1H), 5.92 (d, J = 6.0 Hz, 1H), 4.96 – 4.73 (m, 2H), 4.14 – 3.90 (m, 2H), 2.25 (s, 3H), 1.13 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 211.55, 175.23, 164.44, 161.51 (d, J = 243.2 Hz), 139.29, 132.37 (d, J = 3.0 Hz), 131.72, 130.17, 129.76, 129.26 (d, J = 8.1 Hz), 125.32, 115.43 (d, J = 21.3 Hz), 109.20, 98.28, 91.24, 74.11, 60.51, 41.97, 20.69, 14.07. HRMS (ESI) calcd for $[C_{22}H_{20}FNO_4Na, M+Na]^+$: 404.1268, found: 404.1274.

ethyl

4-(1-(4-bromobenzyl)-3-hydroxy-5-methyl-2-oxoindolin-3-yl)buta-2,3-dienoate

(3f)

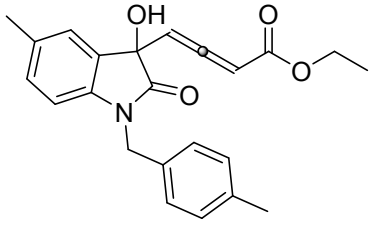


White solid (26.6 mg, 60% yield), m.p.: 109-110 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.52 (dd, J = 8.3, 3.7 Hz, 2H), 7.31 – 7.14 (m, 2H), 7.04 (d, J = 8.0 Hz, 1H), 6.93 – 6.66 (m, 2H), 6.26 (d, J = 6.0 Hz, 1H), 5.80 (d, J = 6.0 Hz, 1H), 4.93 – 4.71 (m, 2H), 4.13 – 4.00 (m, 2H), 2.24 (d, J = 9.7 Hz, 3H), 1.14 (t, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 210.82, 175.05, 164.41, 139.17, 135.71, 131.56, 130.17, 129.97, 129.79, 129.37, 125.40, 120.56, 109.16, 98.07, 90.68, 74.43, 60.55, 42.04, 20.65, 14.12. HRMS (ESI) calcd for $[C_{22}H_{20}BrNO_4Na, M+Na]^+$: 464.0468, found: 464.0469.

ethyl

4-(3-hydroxy-5-methyl-1-(4-methylbenzyl)-2-oxoindolin-3-yl)buta-2,3-dienoate

(3g)

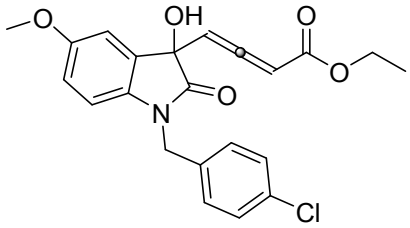


White solid (28.6 mg, 76% yield), m.p.: 110-111 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.26 – 7.15 (m, 2H), 7.13 (t, J = 6.7 Hz, 2H), 7.04 (d, J = 7.9 Hz, 1H), 6.93 – 6.70 (m, 2H), 6.27 (d, J = 6.0 Hz, 1H), 5.78 (d, J = 6.0 Hz, 1H), 4.95 – 4.68 (m, 2H), 4.17 – 4.00 (m, 2H), 2.25 (d, J = 9.8 Hz, 6H), 1.15 (t, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 210.85, 175.04, 164.42, 139.46, 136.59, 133.12, 131.44, 130.20, 129.97, 129.72, 129.21, 127.12, 125.35, 109.25, 98.14, 90.65, 74.48, 60.55, 42.46, 20.73, 14.12. HRMS (ESI) calcd for [$C_{23}H_{23}NO_4Na$, M+Na]$^+$: 400.1519, found: 400.1517.

ethyl

4-(1-(4-chlorobenzyl)-3-hydroxy-5-methoxy-2-oxoindolin-3-yl)buta-2,3-dienoate

(3h)

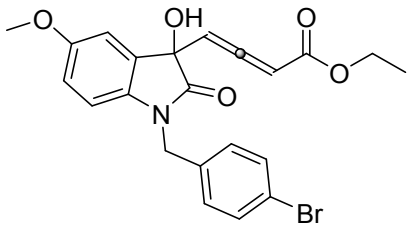


White solid (29.1 mg, 70% yield), m.p.: 97-98 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.48 – 7.22 (m, 4H), 7.02 – 6.94 (m, 1H), 6.89 – 6.76 (m, 2H), 6.29 (d, J = 6.0 Hz, 1H), 5.82 (d, J = 6.0 Hz, 1H), 4.94 – 4.76 (m, 2H), 4.11 – 4.00 (m, 2H), 3.69 (d, J = 8.2 Hz, 3H), 1.12 (q, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 210.91, 174.88, 164.50, 155.63, 135.31, 134.77, 132.11, 131.06, 129.08, 128.67, 114.47, 111.56, 110.02, 98.03, 90.73, 74.64, 60.64, 55.55, 42.05, 14.04. HRMS (ESI) calcd for [$C_{22}H_{20}ClNO_5Na$, M+Na]$^+$: 436.0922, found: 436.0929.

ethyl

4-(1-(4-bromobenzyl)-3-hydroxy-5-methoxy-2-oxoindolin-3-yl)buta-2,3-dienoate

(3i)

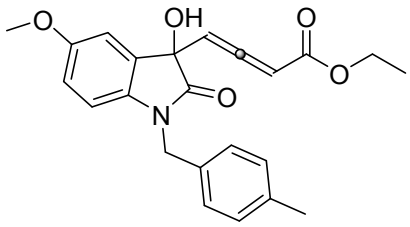


White solid (26.6 mg, 58% yield), m.p.: 121-122 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.52 (d, J = 8.0 Hz, 2H), 7.24 (d, J= 8.0 Hz, 2H), 6.99 (d, J = 15.6 Hz, 1H), 6.80 (s, 2H), 6.29 (d, J = 6.0 Hz, 1H), 5.83 (d, J = 6.0 Hz, 1H), 4.84 (q, J = 16.0 Hz, 2H), 4.08 (q, J = 5.9 Hz, 2H), 3.69 (s, 3H), 1.14 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 210.88, 174.86, 164.48, 155.61, 135.73, 134.74, 131.58, 131.04, 129.41, 120.59, 114.45, 111.54, 110.01, 98.02, 90.73, 74.62, 60.63, 55.55, 42.10, 14.05. HRMS (ESI) calcd for $[C_{22}H_{20}BrNO_5Na, M+Na]^+$: 480.0417, found: 480.0416.

ethyl

4-(3-hydroxy-5-methoxy-1-(4-methylbenzyl)-2-oxoindolin-3-yl)buta-2,3-dienoate

(3j)

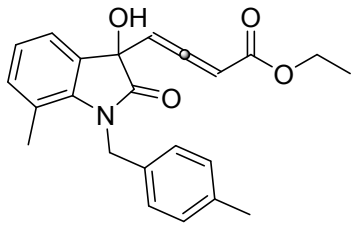


White solid (28.7 mg, 73% yield), m.p.: 105-106 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.27 – 7.09 (m, 4H), 7.03 – 6.94 (m, 1H), 6.92 – 6.71 (m, 2H), 6.30 (d, J = 6.0 Hz, 1H), 5.80 (d, J = 6.0 Hz, 1H), 4.93 – 4.66 (m, 2H), 4.14 – 4.02 (m, 2H), 3.70 (d, J = 8.1 Hz, 3H), 2.26 (s, 3H), 1.13 (q, J = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 210.92, 174.85, 164.51, 155.53, 136.63, 135.04, 133.15, 131.03, 129.24, 127.18, 114.42, 111.50, 110.10, 98.08, 90.69, 74.66, 60.64, 55.53, 42.51, 20.74, 14.05. HRMS (ESI) calcd for $[C_{23}H_{23}NO_5Na, M+Na]^+$: 416.1468, found: 416.1463.

ethyl

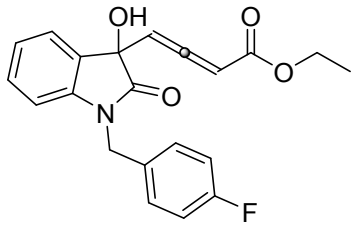
4-(3-hydroxy-7-methyl-1-(4-methylbenzyl)-2-oxoindolin-3-yl)buta-2,3-dienoate

(3k)



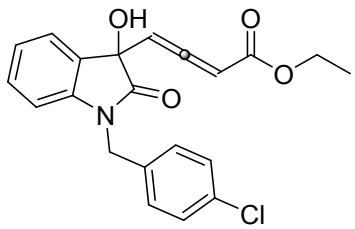
White solid (23.0 mg, 61% yield), m.p.: 131-132 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.27 (d, J = 7.5 Hz, 1H), 7.17 – 7.02 (m, 4H), 6.98 – 6.83 (m, 2H), 6.31 (d, J = 6.0 Hz, 1H), 5.95 (d, J = 6.1 Hz, 1H), 5.17 – 4.97 (m, 2H), 4.19 – 4.00 (m, 2H), 2.26 (s, 3H), 2.18 (s, 3H), 1.14 (q, J = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 210.86, 176.15, 164.43, 139.78, 136.24, 134.76, 133.38, 130.79, 129.41, 125.42, 122.83, 122.71, 119.79, 98.43, 90.69, 73.71, 60.57, 43.92, 20.69, 18.13, 14.09. HRMS (ESI) calcd for $[C_{23}H_{23}NO_4Na, M+Na]^+$: 400.1519, found: 400.1511.

ethyl 4-(1-(4-fluorobenzyl)-3-hydroxy-2-oxoindolin-3-yl)buta-2,3-dienoate (3l)



White solid (22.0 mg, 61% yield), m.p.: 113-114 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.44 – 7.31 (m, 3H), 7.25 (t, J = 7.8 Hz, 1H), 7.16 – 7.03 (m, 2H), 6.96 – 6.82 (m, 2H), 6.20 (d, J = 6.1 Hz, 1H), 5.92 (d, J = 6.0 Hz, 1H), 4.97 – 4.79 (m, 2H), 4.16 – 3.94 (m, 2H), 1.10 (q, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 211.64, 175.35, 164.37, 161.58 (d, J = 243.0 Hz), 141.71, 132.32 (d, J = 3.1 Hz), 130.05, 129.69, 129.32 (d, J = 8.1 Hz), 124.78, 122.68, 115.48 (d, J = 21.4 Hz), 109.43, 98.21, 91.23, 74.06, 60.52, 42.02, 14.04. HRMS (ESI) calcd for $[C_{21}H_{18}FNO_4Na, M+Na]^+$: 390.1112, found: 390.1110.

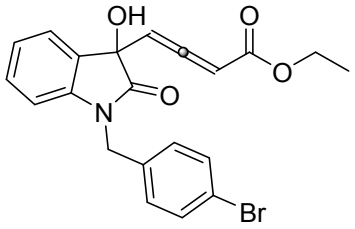
ethyl 4-(1-(4-chlorobenzyl)-3-hydroxy-2-oxoindolin-3-yl)buta-2,3-dienoate (3m)



White solid (24.5 mg, 64% yield), m.p.: 129-130 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.41 – 7.31 (m, 4H), 7.25 (t, J = 7.7 Hz, 1H), 7.05 (q, J = 7.1 Hz, 1H), 6.94 – 6.84 (m, 2H), 6.28 (d, J = 6.1 Hz, 1H), 5.81 (d, J = 6.1 Hz, 1H), 4.99 – 4.74 (m, 2H), 4.16 – 3.94 (m, 2H), 1.10 (q, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 211.61,

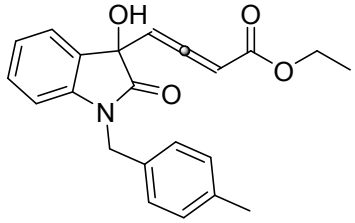
175.34, 164.40, 141.63, 135.20, 132.12, 130.02, 129.70, 129.14, 128.66, 124.77, 122.72, 109.41, 98.18, 91.22, 74.03, 60.51, 42.04, 14.04. HRMS (ESI) calcd for $[C_{21}H_{18}ClNO_4Na, M+Na]^+$: 406.0816, found: 406.0819.

ethyl 4-(1-(4-bromobenzyl)-3-hydroxy-2-oxoindolin-3-yl)buta-2,3-dienoate (3n)



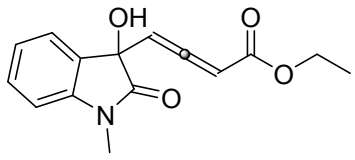
White solid (31.8 mg, 74% yield), m.p.: 135-136 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.53 (d, J = 8.2 Hz, 2H), 7.36 (d, J = 7.0 Hz, 1H), 7.25 (d, J = 7.6 Hz, 2H), 7.05 (t, J = 7.4 Hz, 1H), 6.96 – 6.83 (m, 2H), 6.28 (d, J = 6.0 Hz, 1H), 5.81 (d, J = 6.1 Hz, 1H), 4.96 – 4.74 (m, 2H), 4.15 – 3.97 (m, 2H), 1.12 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.52, 175.73, 164.96, 141.61, 134.12, 131.94, 130.10, 128.84, 128.68, 124.94, 123.56, 121.66, 109.46, 97.75, 92.46, 74.51, 61.23, 43.27, 14.04. HRMS (ESI) calcd for $[C_{21}H_{18}BrNO_4Na, M+Na]^+$: 450.0311, found: 450.0334.

ethyl 4-(3-hydroxy-1-(4-methylbenzyl)-2-oxoindolin-3-yl)buta-2,3-dienoate (3o)



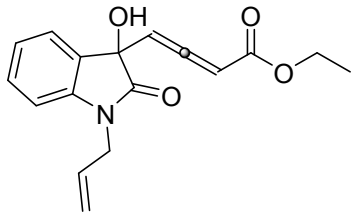
White solid (24.8 mg, 68% yield), m.p.: 111-112 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.34 (d, J = 7.3 Hz, 1H), 7.26 – 7.08 (m, 4H), 7.03 (q, J = 7.1 Hz, 1H), 6.92 – 6.81 (m, 2H), 6.28 (d, J = 6.0 Hz, 1H), 5.91 (d, J = 6.1 Hz, 1H), 4.91 – 4.72 (m, 2H), 4.13 – 3.97 (m, 2H), 2.26 (s, 3H), 1.11 (q, J = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 211.62, 175.27, 164.38, 141.85, 136.63, 133.05, 130.00, 129.65, 129.23, 127.21, 124.68, 122.54, 109.51, 98.18, 91.18, 74.30, 60.53, 42.48, 20.73, 14.04. HRMS (ESI) calcd for $[C_{22}H_{21}NO_4Na, M+Na]^+$: 386.1363, found: 386.1370.

ethyl 4-(3-hydroxy-1-methyl-2-oxoindolin-3-yl)buta-2,3-dienoate (3p)



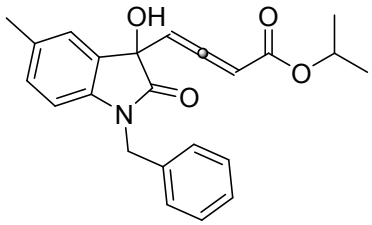
Yellow oil (14.7 mg, 54% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.40 (m, 1H), 7.33 (t, J = 7.3 Hz, 1H), 7.13 – 7.05 (m, 1H), 6.83 (d, J = 7.8 Hz, 1H), 5.89 (d, J = 6.1 Hz, 1H), 5.80 (d, J = 6.1 Hz, 1H), 4.27 – 4.07 (m, 2H), 3.19 (d, J = 3.4 Hz, 3H), 1.28 – 1.20 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.94, 174.74, 163.95, 141.92, 129.24, 127.69, 123.83, 122.45, 107.65, 96.77, 90.87, 73.68, 60.15, 25.46, 13.10. HRMS (ESI) calcd for $[C_{15}H_{15}NO_4Na, M+Na]^+$: 296.0893, found: 296.0888.

ethyl 4-(1-allyl-3-hydroxy-2-oxoindolin-3-yl)buta-2,3-dienoate (3q)



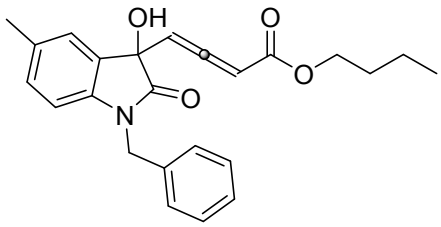
Yellow oil (18.6 mg, 62% yield), ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.40 – 7.25 (m, 2H), 7.07 (q, J = 7.2 Hz, 1H), 6.95 (d, J = 7.8 Hz, 1H), 6.86 (s, 1H), 6.14 (d, J = 6.1 Hz, 1H), 5.90 (d, J = 6.2 Hz, 1H), 5.22 – 5.08 (m, 2H), 4.42 – 4.20 (m, 2H), 4.17 – 3.97 (m, 2H), 1.20 – 1.06 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.80, 175.55, 164.87, 141.94, 130.68, 129.96, 128.66, 124.81, 123.27, 117.62, 109.44, 97.72, 91.67, 74.42, 61.06, 42.33, 13.99. HRMS (ESI) calcd for $[C_{17}H_{17}NO_4Na, M+Na]^+$: 322.1050, found: 322.1056.

isopropyl 4-(1-benzyl-3-hydroxy-5-methyl-2-oxoindolin-3-yl)buta-2,3-dienoate (3r)



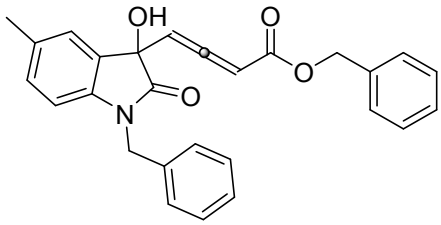
White solid (30.2 mg, 80% yield), m.p.: 101-102 ^{o}C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.33 (d, J = 4.7 Hz, 2H), 7.31 – 7.25 (m, 2H), 7.18 (s, 1H), 7.04 (d, J = 7.9 Hz, 1H), 6.90 – 6.72 (m, 2H), 6.26 (d, J = 6.0 Hz, 1H), 5.73 (d, J = 6.0 Hz, 1H), 4.96 – 4.74 (m, 3H), 2.24 (d, J = 9.3 Hz, 3H), 1.14 (dt, J = 11.5, 6.2 Hz, 6H). ^{13}C NMR (100 MHz, DMSO-d_6)δ 210.71, 175.15, 163.97, 139.46, 136.20, 131.48, 130.00, 129.78, 128.68, 127.43, 127.20, 127.10, 125.34, 109.25, 98.12, 90.97, 74.50, 68.00, 42.67, 21.54, 20.67. HRMS (ESI) calcd for $[C_{23}H_{23}NO_4Na, M+Na]^+$: 400.1519, found: 400.1523.

butyl 4-(1-benzyl-3-hydroxy-5-methyl-2-oxoindolin-3-yl)buta-2,3-dienoate (3s)



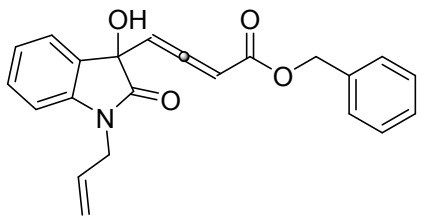
White solid (33.4 mg, 85% yield), m.p.: 77-78 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.35 – 7.25 (m, 4H), 7.20 (s, 1H), 7.04 (d, J = 7.5 Hz, 1H), 6.92 (s, 1H), 6.78 – 6.71 (m, 1H), 6.29 (d, J = 5.9 Hz, 1H), 5.79 (d, J = 5.9 Hz, 1H), 4.96 – 4.76 (m, 2H), 4.11 – 3.94 (m, 2H), 2.24 (d, J = 7.7 Hz, 3H), 1.48 (dt, J = 13.0, 6.8 Hz, 2H), 1.23 (dq, J = 14.3, 7.2 Hz, 2H), 0.84 (q, J = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 210.86, 175.09, 164.53, 139.45, 136.21, 131.53, 130.10, 129.77, 128.67, 127.42, 127.12, 125.28, 109.25, 98.04, 90.62, 74.51, 64.24, 42.72, 30.27, 20.66, 18.61, 13.63. HRMS (ESI) calcd for [$C_{24}H_{25}NO_4Na$, M+Na]$^+$: 414.1676, found: 414.1680.

benzyl 4-(1-benzyl-3-hydroxy-5-methyl-2-oxoindolin-3-yl)buta-2,3-dienoate (3t)



White solid (31.1 mg, 73% yield), m.p.: 122-123 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.34 (t, J = 5.7 Hz, 3H), 7.29 (d, J = 6.8 Hz, 6H), 7.15 (s, 1H), 7.03 (d, J = 7.9 Hz, 1H), 6.92 (s, 1H), 6.75 (d, J = 7.8 Hz, 1H), 6.31 (d, J = 6.0 Hz, 1H), 5.88 (d, J = 6.0 Hz, 1H), 5.13 (s, 2H), 4.84 (q, J = 16.0 Hz, 2H), 2.15 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 211.14, 175.04, 164.36, 139.40, 136.17, 135.96, 131.59, 129.82, 128.68, 128.54, 128.16, 127.98, 127.66, 127.43, 127.09, 125.33, 109.26, 98.13, 90.51, 74.45, 66.05, 42.67, 20.62. HRMS (ESI) calcd for [$C_{27}H_{23}NO_4Na$, M+Na]$^+$: 448.1519, found: 448.1493.

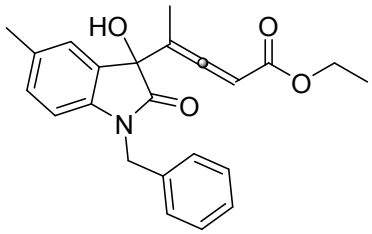
benzyl 4-(1-allyl-3-hydroxy-2-oxoindolin-3-yl)buta-2,3-dienoate (3u)



Yellow oil (22.5 mg, 62% yield), ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.43 – 7.20 (m, 7H), 7.04 – 6.76 (m, 3H), 6.15 (d,J = 6.1 Hz, 1H), 5.99 (d, J = 6.1 Hz, 1H), 5.21 – 5.01 (m, 4H), 4.26 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 211.90, 174.92, 164.28, 141.94, 136.02, 131.60, 129.74, 128.52, 128.09, 128.02, 127.77, 124.71, 122.48,

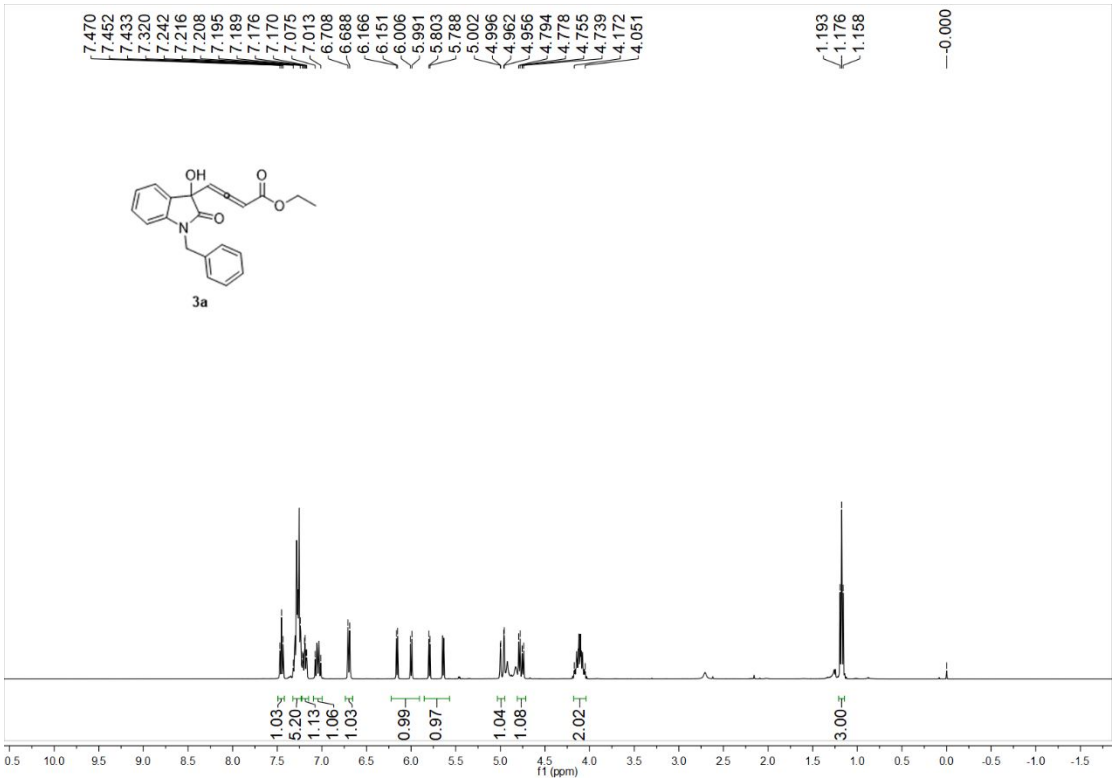
116.74, 109.43, 98.22, 90.98, 73.90, 65.93, 41.45. HRMS (ESI) calcd for $[C_{22}H_{19}NO_4Na, M+Na]^+$: 384.1206, found: 384.1200.

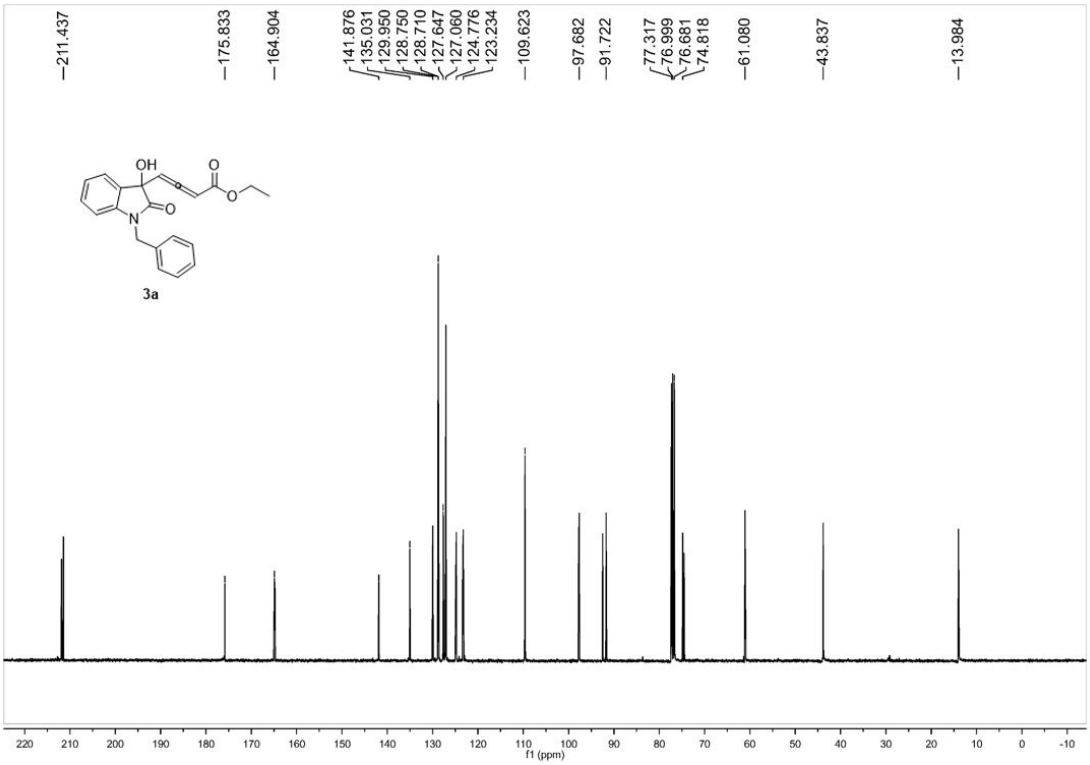
ethyl 4-(1-benzyl-3-hydroxy-5-methyl-2-oxoindolin-3-yl)penta-2,3-dienoate (3v)

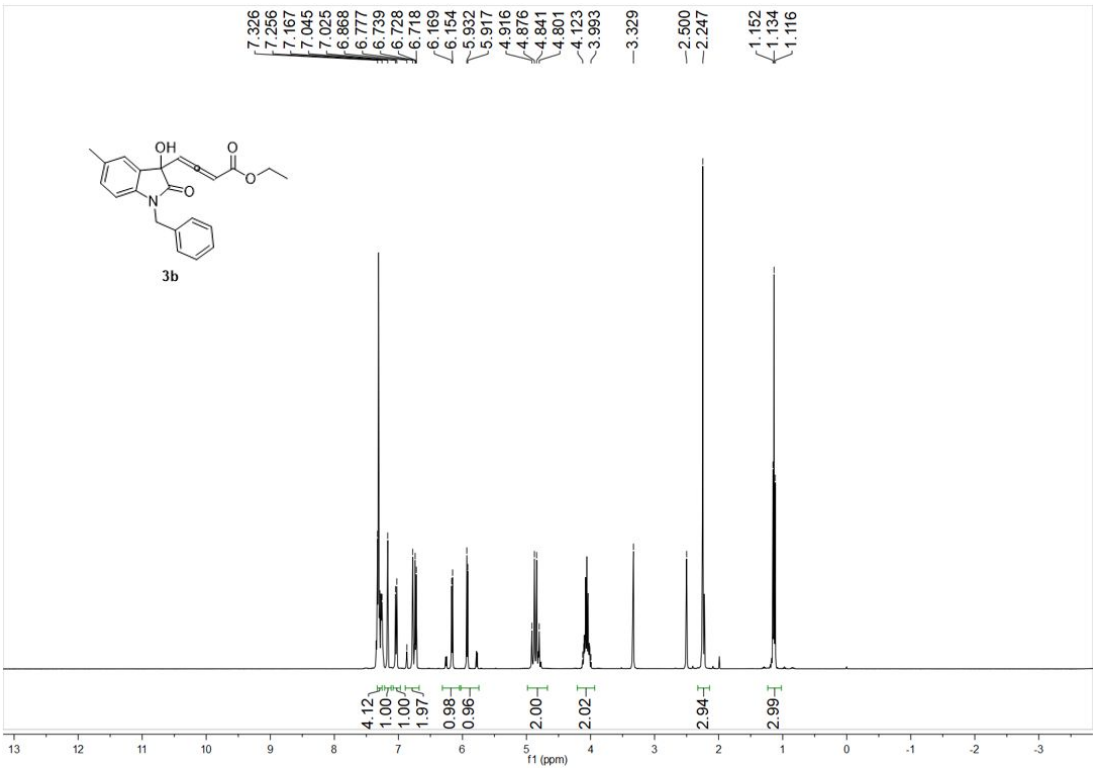


White solid (31.4 mg, 83% yield), m.p.: 126-127 ^oC, ^1H NMR (400 MHz, DMSO-d_6) δ 7.33 (d, J = 3.9 Hz, 2H), 7.30 – 7.24 (m, 2H), 7.19 (s, 1H), 7.04 (dd, J = 14.6, 8.0 Hz, 1H), 6.82 – 6.68 (m, 2H), 5.81 (s, 1H), 4.95 – 4.73 (m, 2H), 4.22 – 3.94 (m, 2H), 2.26 (s, 3H), 1.97 (s, 3H), 1.21 (t, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 210.24, 175.20, 165.13, 140.10, 136.29, 131.82, 130.19, 129.95, 128.68, 127.34, 127.13, 125.07, 109.23, 106.25, 90.63, 76.15, 60.46, 42.87, 20.64, 14.23, 13.24. HRMS (ESI) calcd for $[C_{23}H_{23}NO_4Na, M+Na]^+$: 400.1519, found: 400.1518.

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



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6.169
6.154
5.932
5.917
4.916
4.876
4.841
4.801
4.123
3.993
3.329
2.500
2.247
1.152
1.134
1.116
OH
O
O
N
O
3b
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1.00
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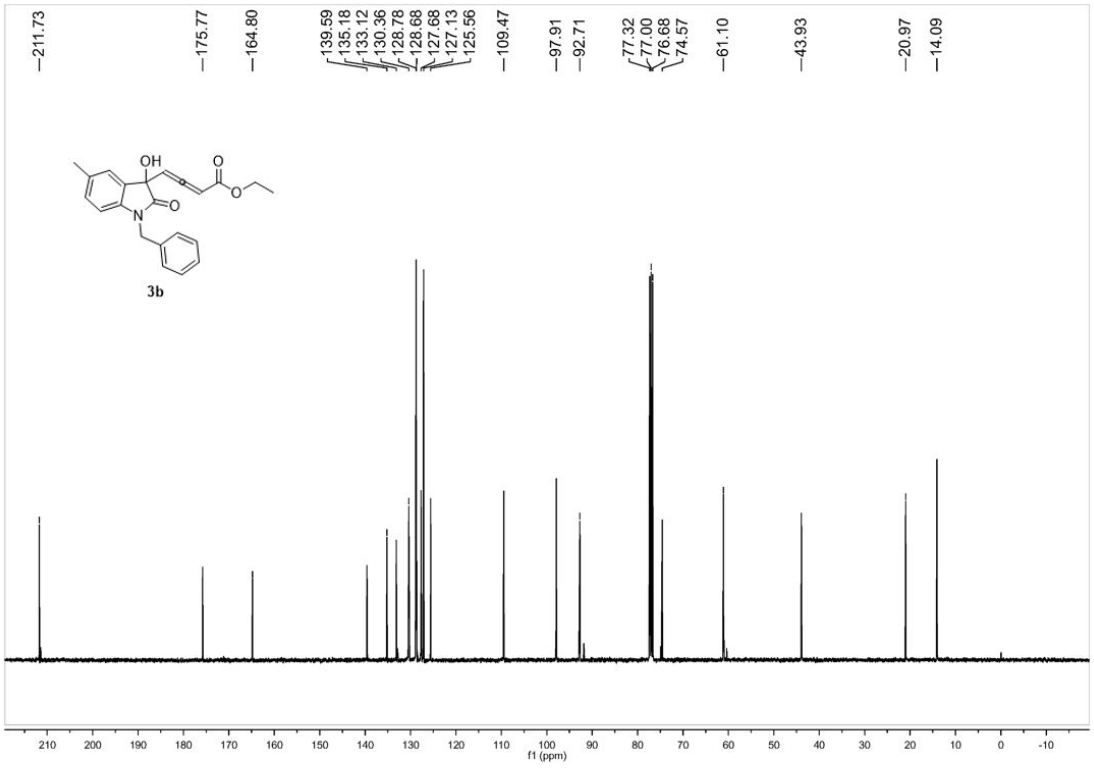
0.98
0.96
2.00
2.02
2.94
2.99
f1 (ppm)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175.77
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133.12
130.36
128.78
128.68
127.68
127.13
125.56
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97.91
92.71
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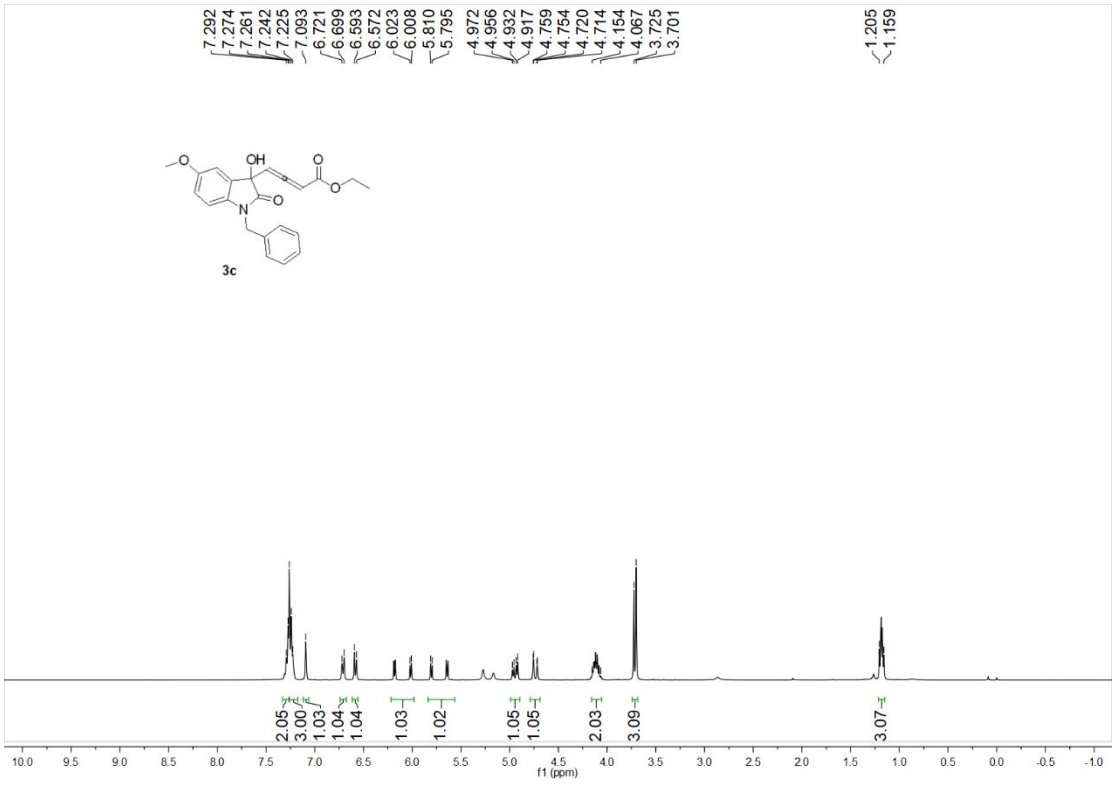
OH
O
O
N
O
3b
f1 (ppm)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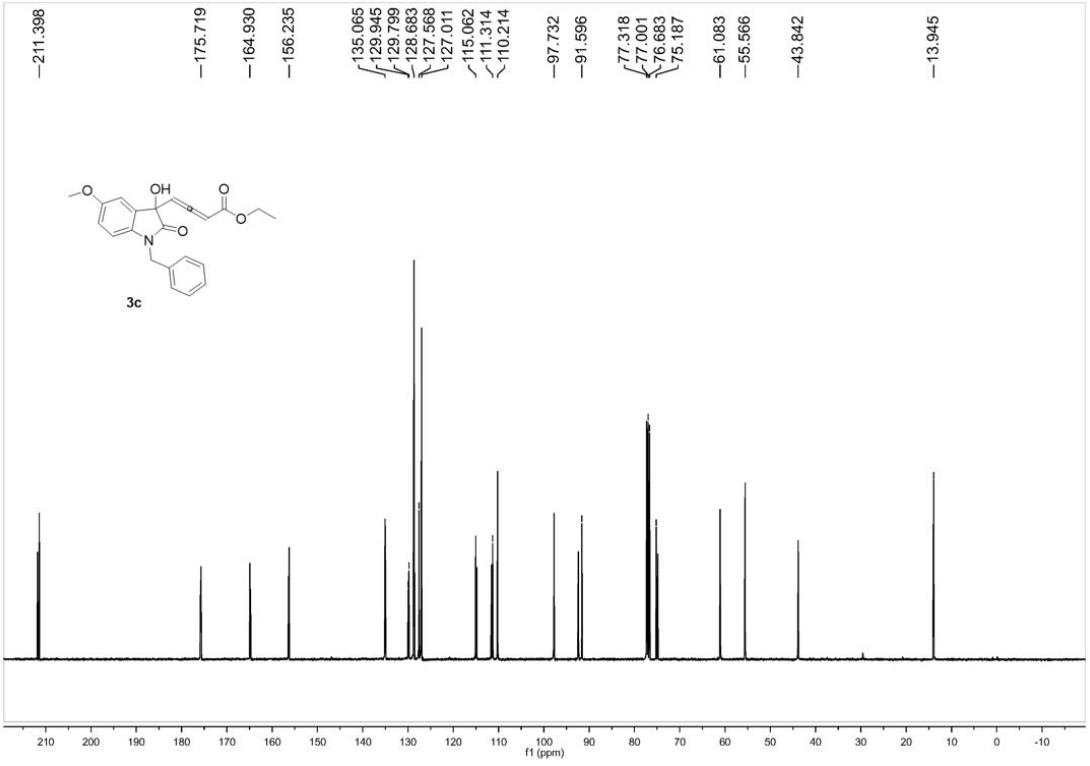
1.02
1.05
1.05
2.03
3.09
3.07
f1 (ppm)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127.568
127.011
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97.732
91.596
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OH
O
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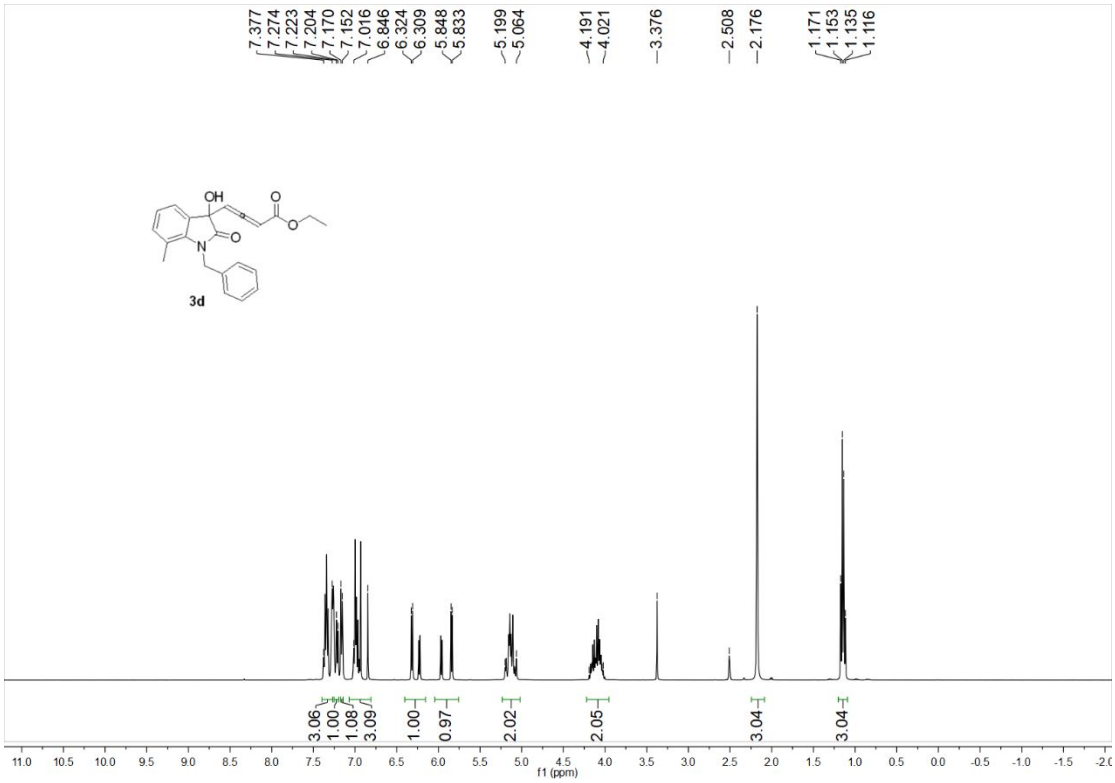
O
3c
f1 (ppm)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1.153
1.135
1.116
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N
O
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1.08
3.09
1.00
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2.05
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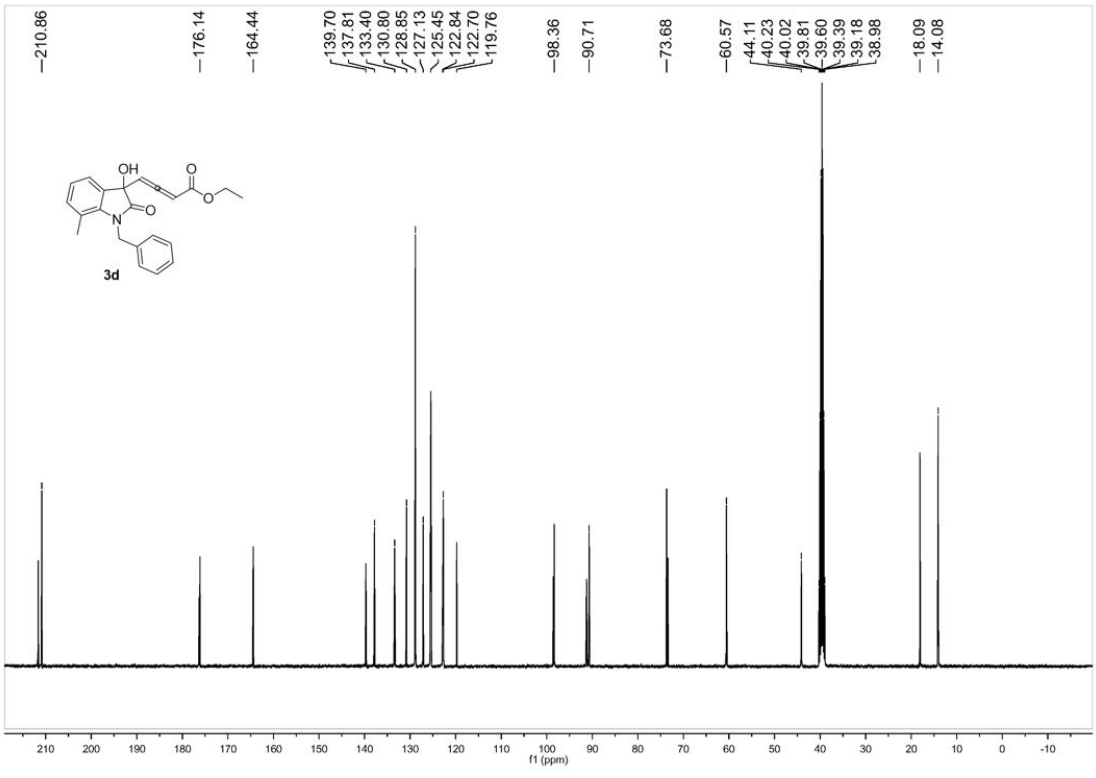
3.04
f1 (ppm)


210.86
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137.81
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130.80
128.85
127.13
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98.36
90.71
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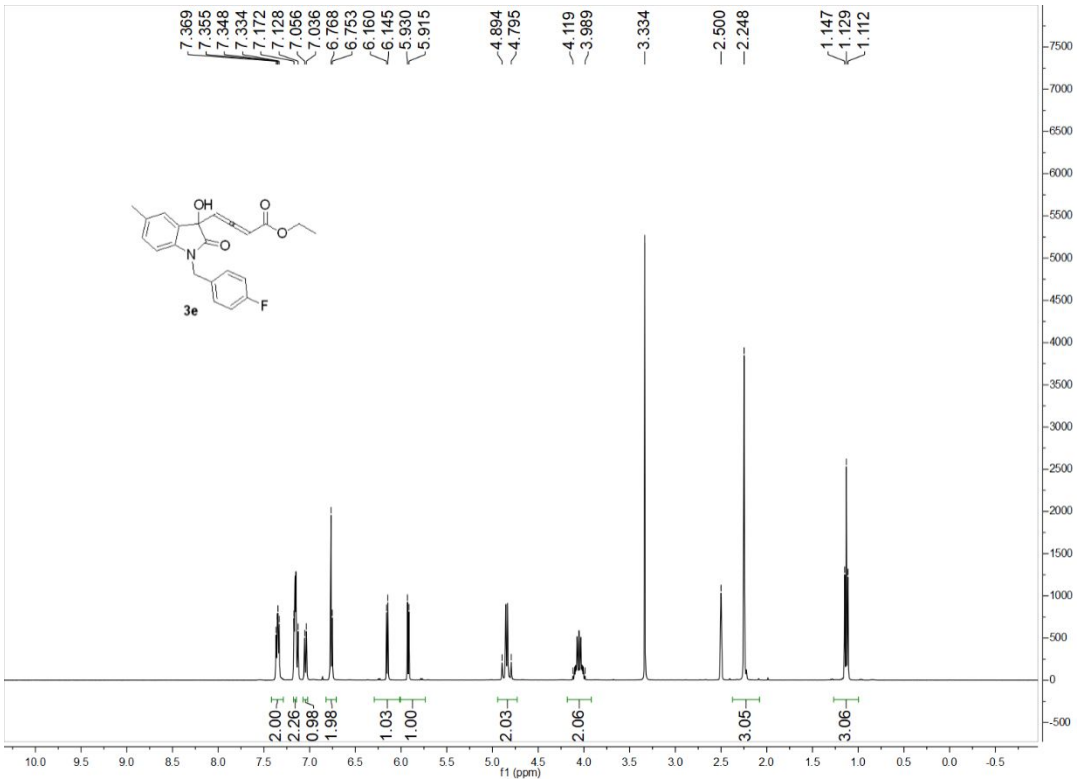
N
O
3d
f1 (ppm)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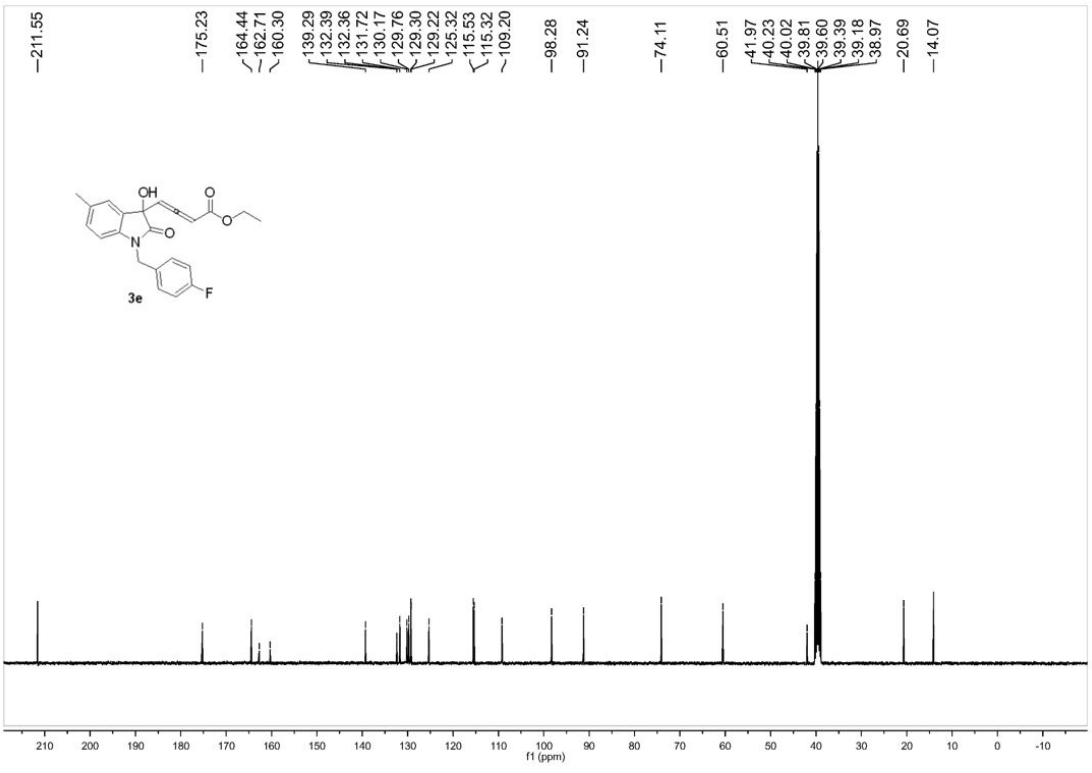
7.128
7.056
7.036
6.768
6.753
6.160
6.145
5.930
5.915
4.894
4.795
4.119
3.989
3.334
2.500
2.248
1.147
1.129
1.112
OH
O
O
N
O
F
3e
2.00
2.26
0.98
1.98
1.03
1.00
2.03
2.06
3.05
3.06
f1 (ppm)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132.36
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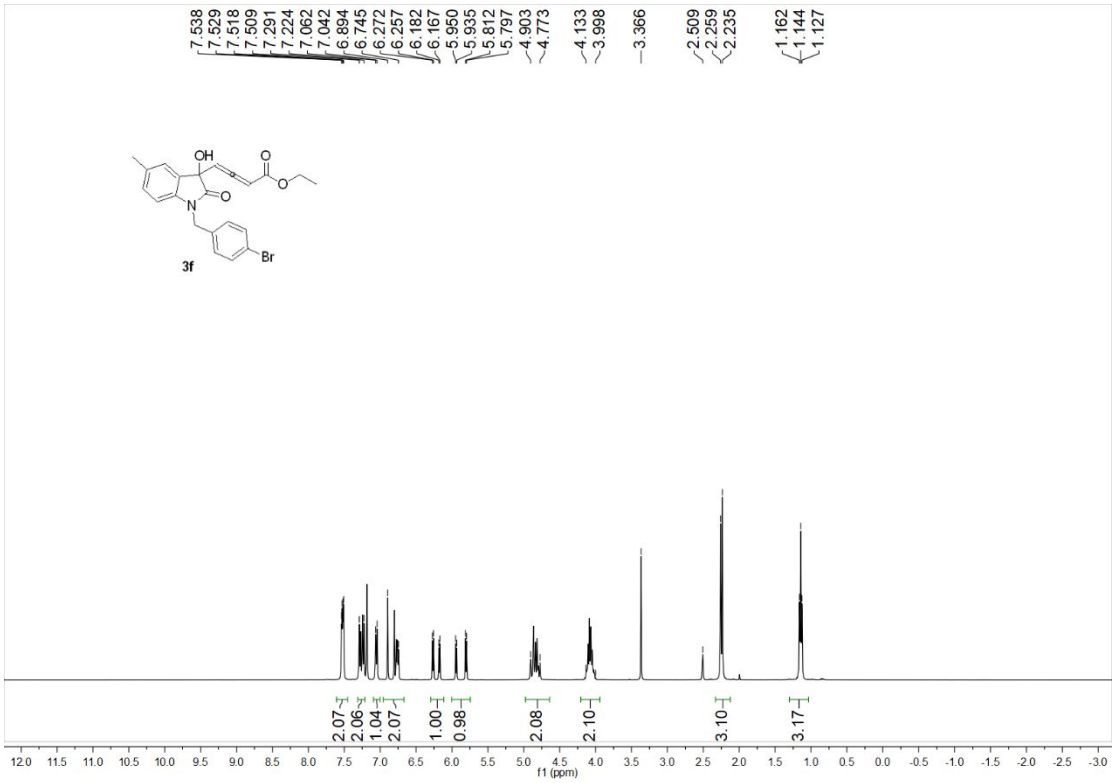
129.30
129.22
125.32
115.53
115.32
109.20
98.28
91.24
74.11
60.51
41.97
40.23
40.02
39.81
39.60
39.39
39.18
38.97
20.69
14.07
OH
O
O
N
O
F
3e
f1 (ppm)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6.167
5.950
5.935
5.812
5.797
4.903
4.773
4.133
3.998
3.366
2.509
2.259
2.235
1.162
1.144
1.127
OH
O
O
N
O
Br
3f
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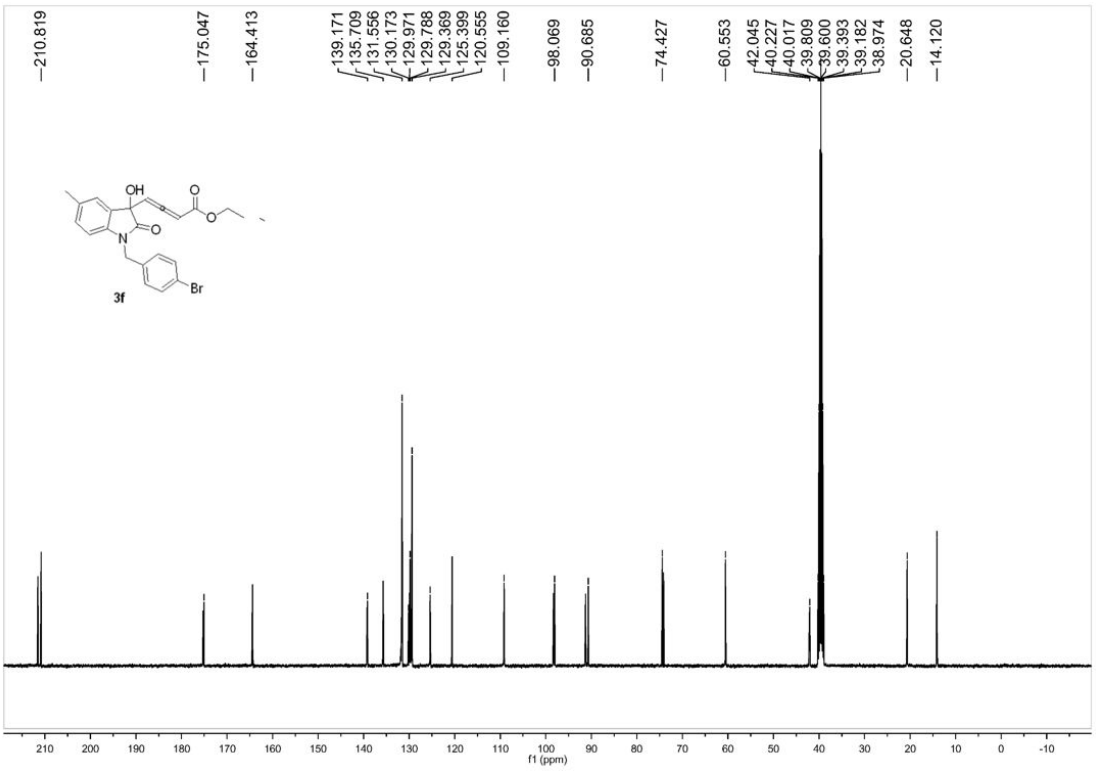
2.06
1.04
2.07
1.00
0.98
2.08
2.10
3.10
3.17
f1 (ppm)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98.069
90.685
74.427
60.553
42.045
40.227
40.017
39.809
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39.182
38.974
20.648
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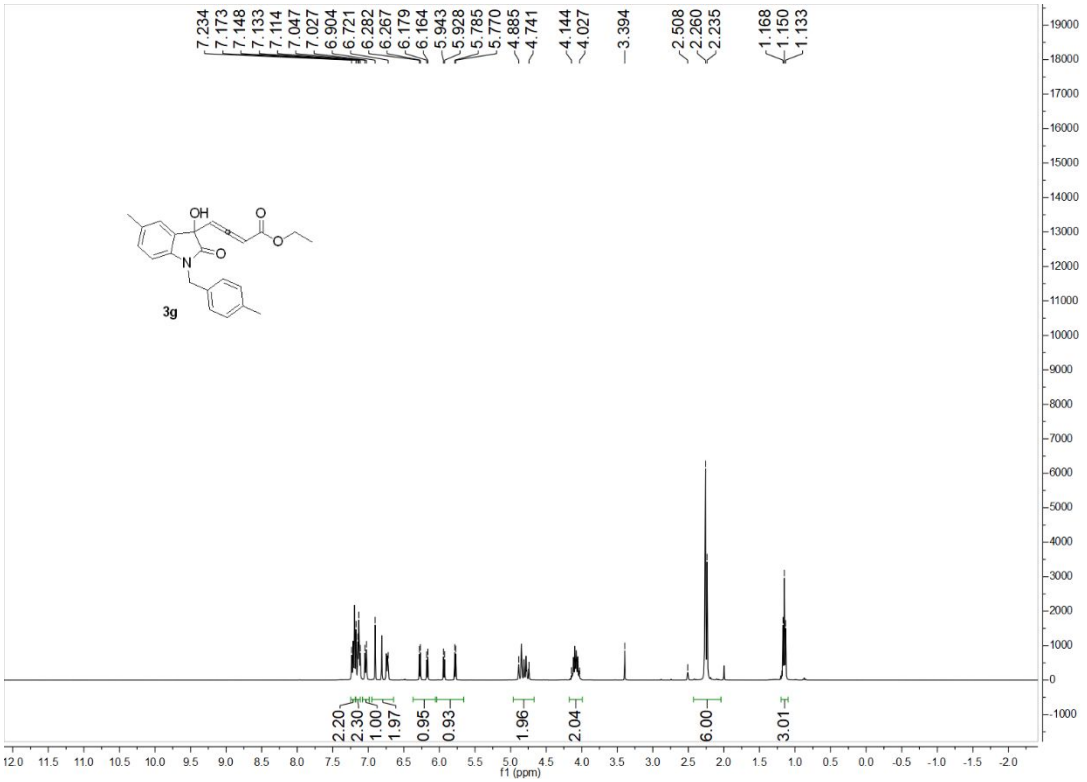
OH
O
O
N
O
Br
3f
f1 (ppm)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6.179
6.164
5.943
5.928
5.785
5.770
4.885
4.741
4.144
4.027
3.394
2.508
2.260
2.235
1.168
1.150
1.133
OH
O
O
N
O
3g
2.20
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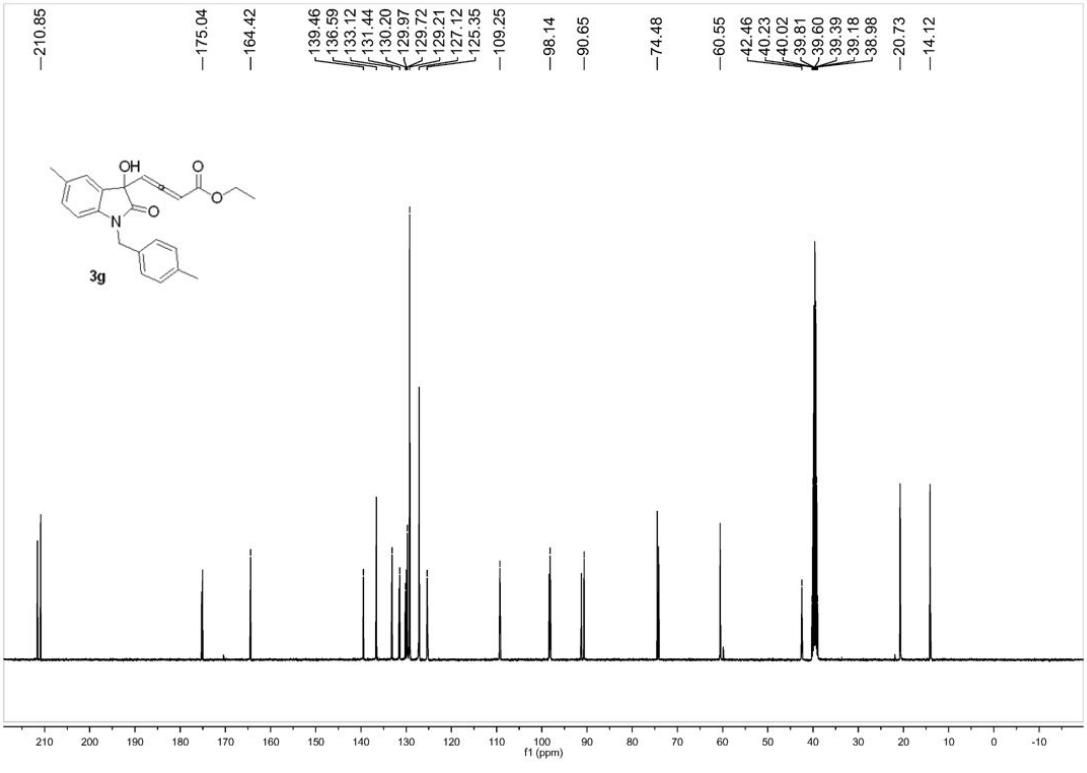
0.93
1.96
2.04
6.00
3.01
f1 (ppm)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98.14
90.65
74.48
60.55
42.46
40.23
40.02
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39.18
38.98
20.73
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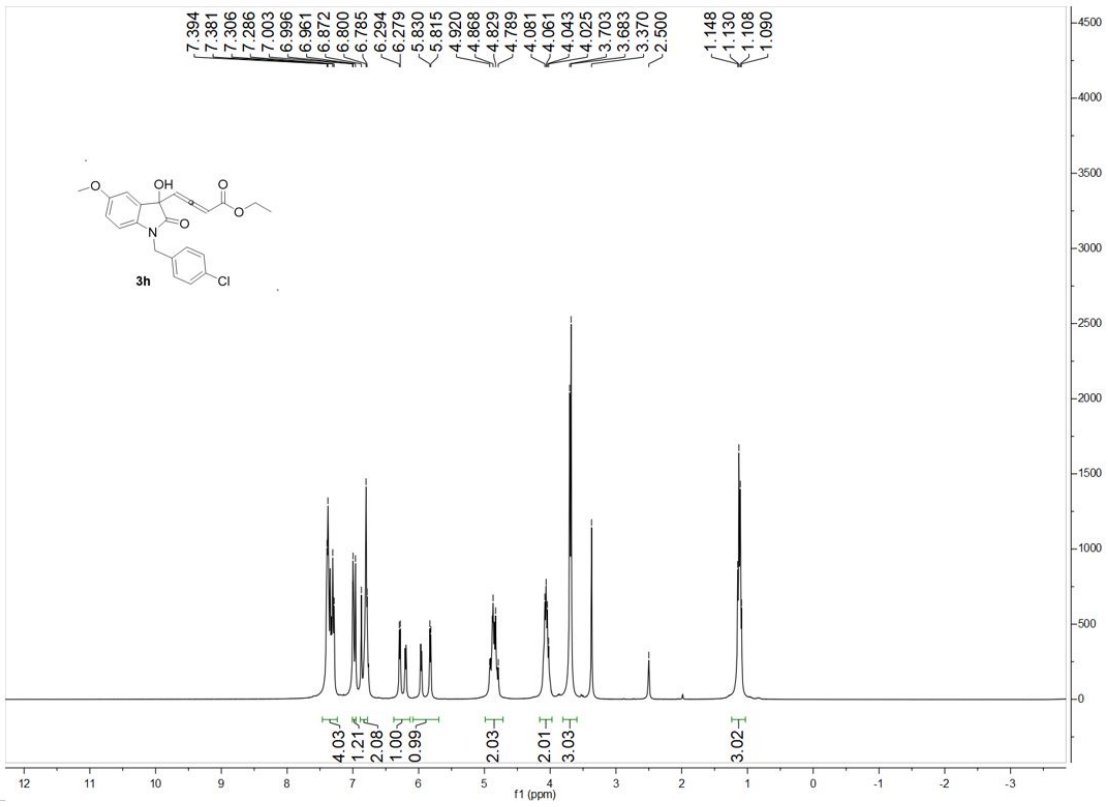
OH
O
O
N
O
3g
f1 (ppm)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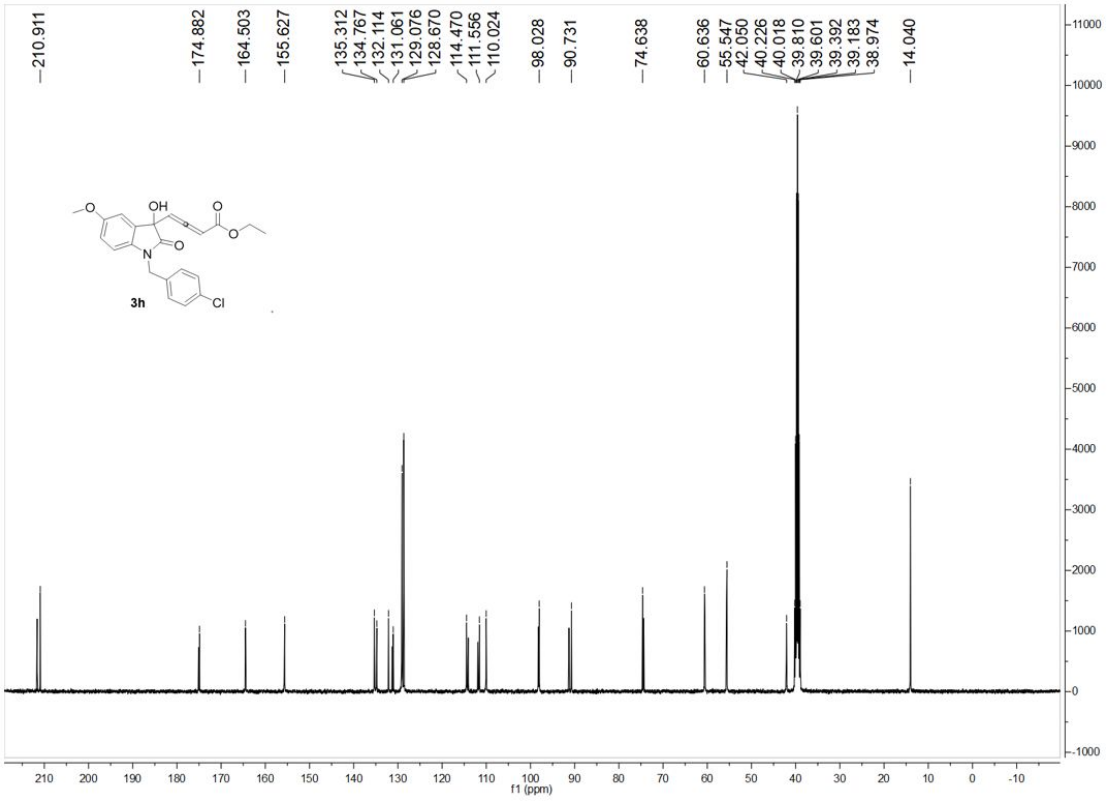
6.785
6.294
6.279
5.830
5.815
4.920
4.868
4.829
4.789
4.081
4.061
4.043
4.025
3.703
3.683
3.370
2.500
1.148
1.130
1.108
1.090
OH
O
O
O
N
Cl
3h
4.03
1.21
2.08
1.00
0.99
2.03
2.01
3.03
3.02
f1 (ppm)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131.061
129.076
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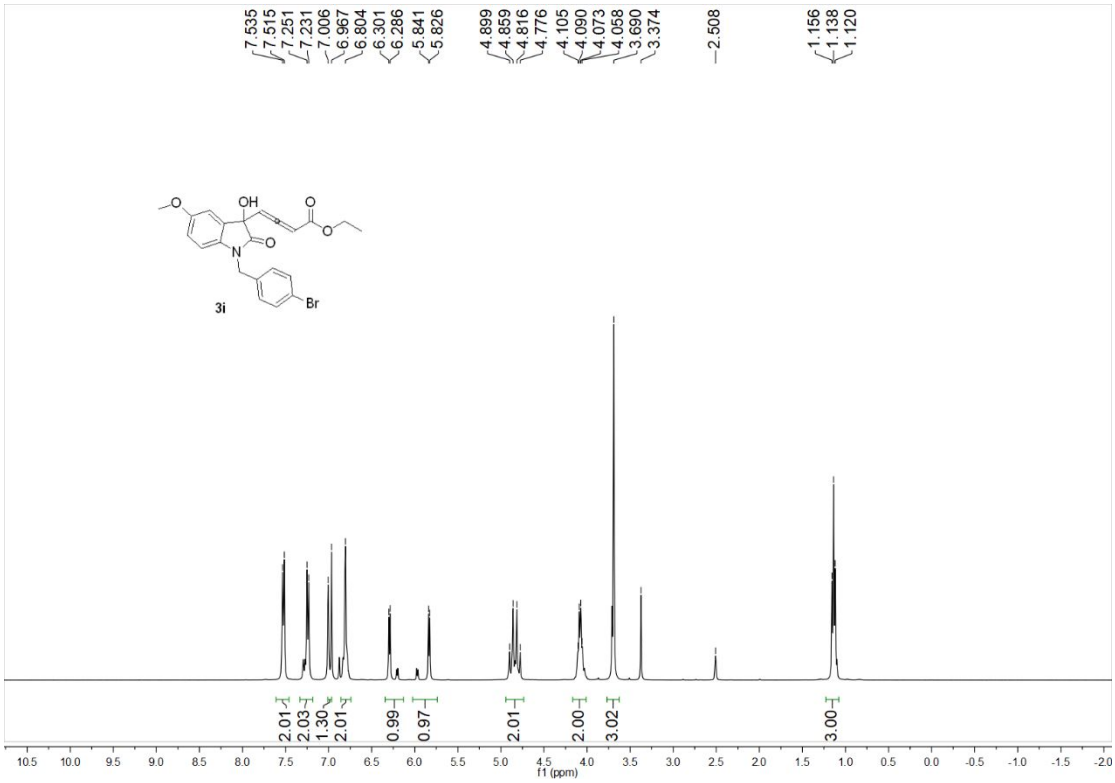
114.470
111.556
110.024
98.028
90.731
74.638
60.636
55.547
42.050
40.226
40.018
39.810
39.601
39.392
39.183
38.974
14.040
OH
O
O
O
N
Cl
3h
f1 (ppm)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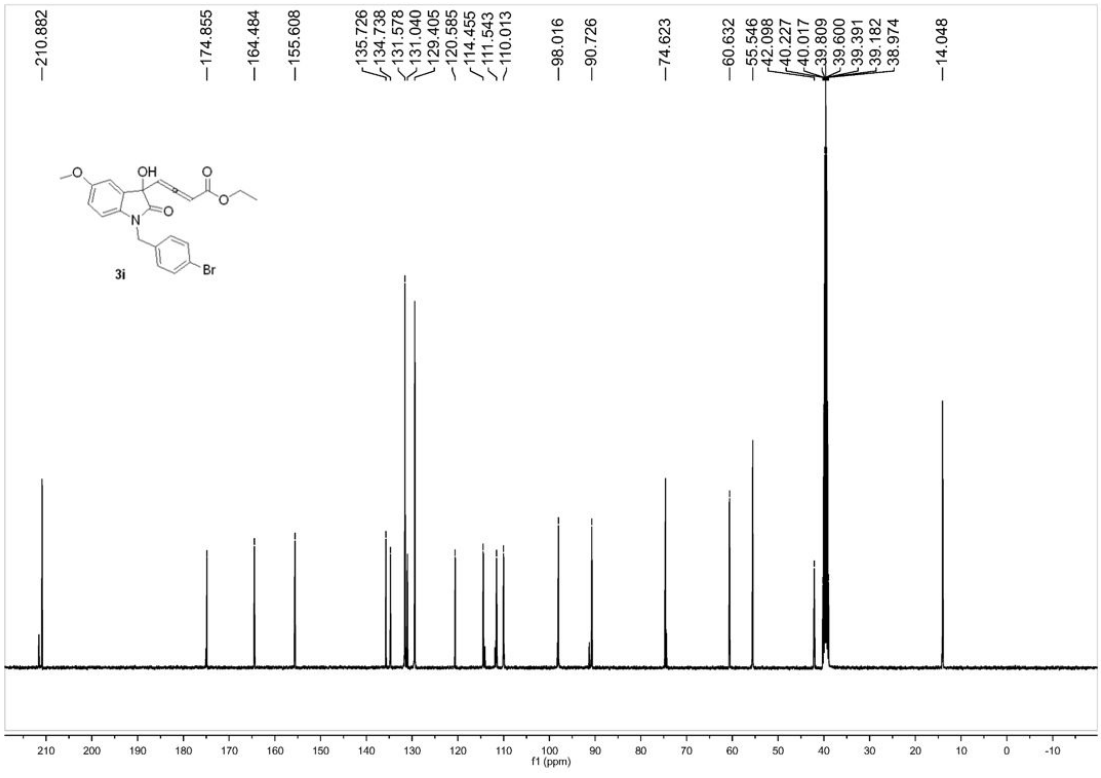
6.804
6.301
6.286
5.841
5.826
4.899
4.859
4.816
4.776
4.105
4.090
4.073
4.058
3.690
3.374
2.508
1.156
1.138
1.120
OH
O
O
O
N
O
Br
3i
2.01
2.03
1.30
2.01
0.99
0.97
2.01
2.00
3.02
3.00
f1 (ppm)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131.040
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114.455
111.543
110.013
98.016
90.726
74.623
60.632
55.546
42.098
40.227
40.017
39.809
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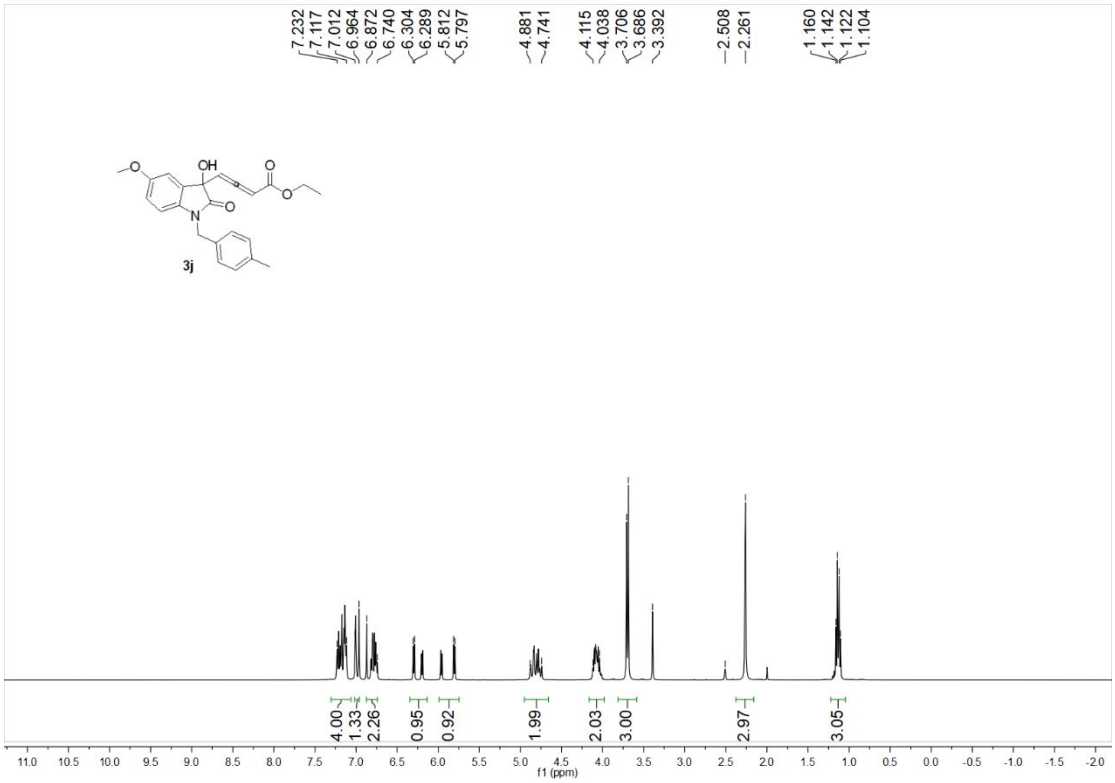
39.391
39.182
38.974
14.048
OH
O
O
O
N
O
Br
3i
f1 (ppm)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6.289
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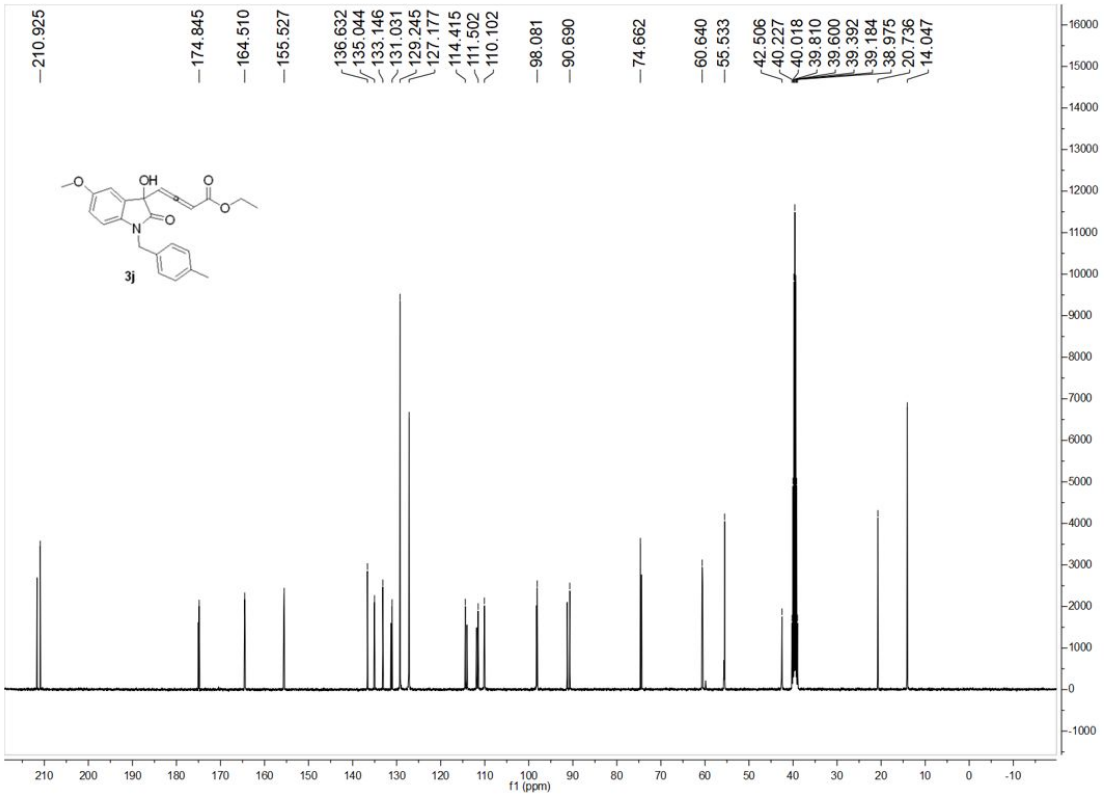
5.797
4.881
4.741
4.115
4.038
3.706
3.686
3.392
2.508
2.261
1.160
1.142
1.122
1.104
OH
O
O
O
N
3j
4.00
1.33
2.26
0.95
0.92
1.99
2.03
3.00
2.97
3.05
f1 (ppm)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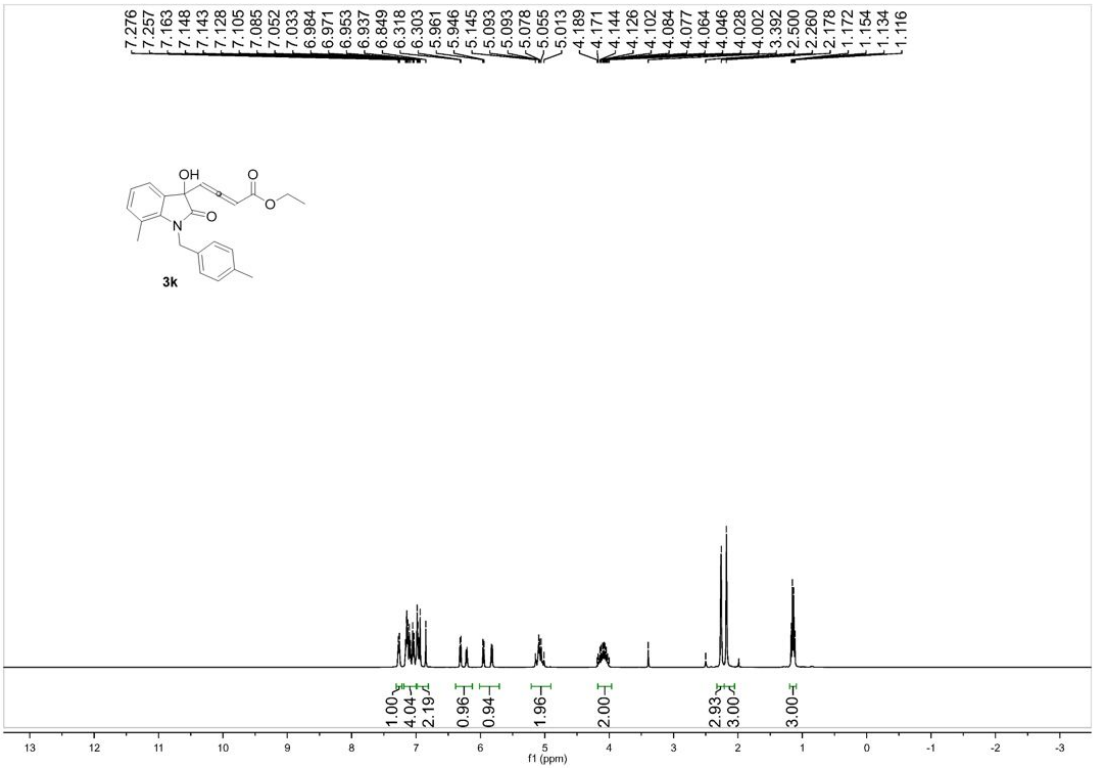
129.245
127.177
114.415
111.502
110.102
98.081
90.690
74.662
60.640
55.533
42.506
40.227
40.018
39.810
39.600
39.392
39.184
38.975
20.736
14.047
OH
O
O
O
N
3j
f1 (ppm)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7.085
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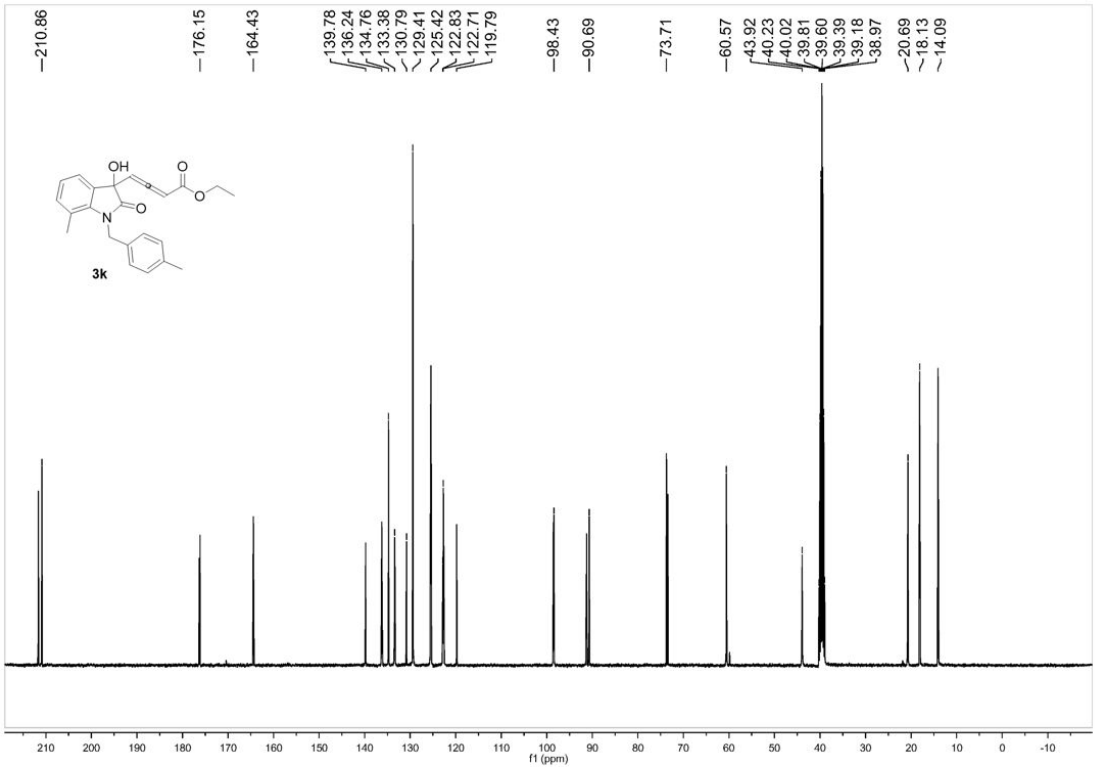
7.033
6.984
6.971
6.953
6.937
6.849
6.318
6.303
5.961
5.946
5.145
5.093
5.093
5.078
5.055
5.013
4.189
4.171
4.144
4.126
4.102
4.084
4.077
4.064
4.046
4.028
4.002
3.392
2.500
2.260
2.178
1.172
1.154
1.134
1.116
OH
O
O
N
O
3k
1.00
4.04
2.19
0.96
0.94
1.96
2.00
2.93
3.00
3.00
f1 (ppm)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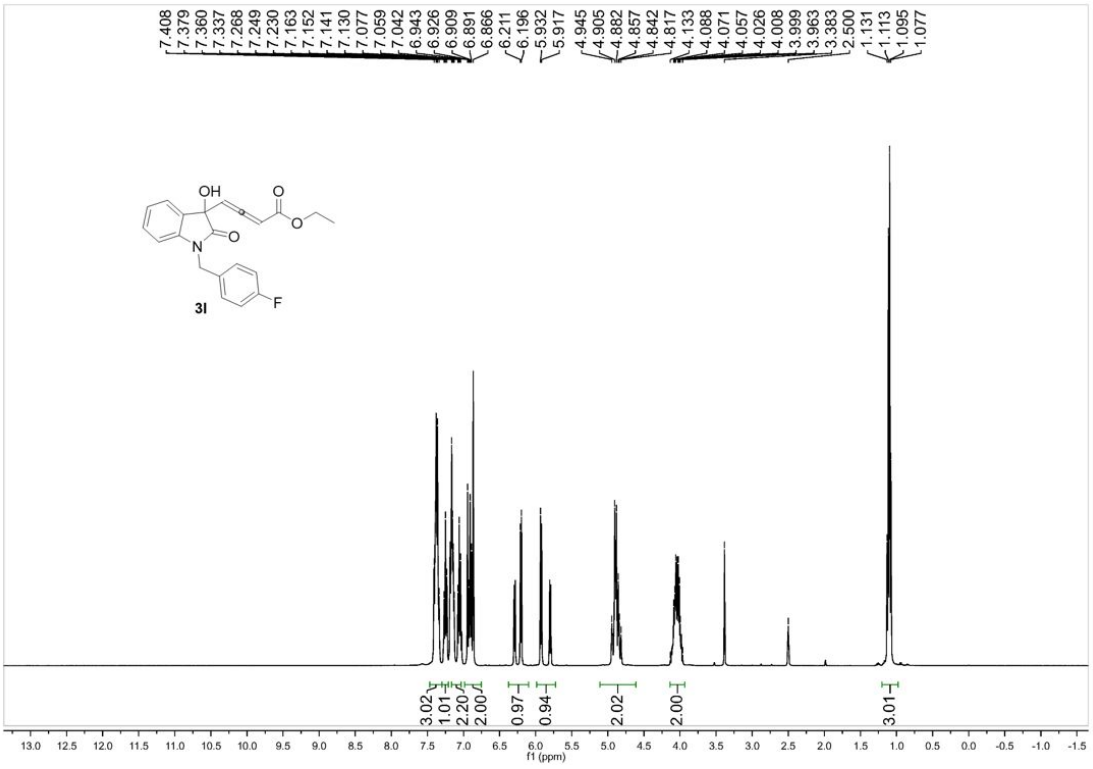
130.79
129.41
125.42
122.83
122.71
119.79
98.43
90.69
73.71
60.57
43.92
40.23
40.02
39.81
39.60
39.39
39.18
38.97
20.69
18.13
14.09
OH
O
O
N
O
3k
f1 (ppm)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7.141
7.130
7.077
7.059
7.042
6.943
6.926
6.909
6.891
6.866
6.211
6.196
5.932
5.917
4.945
4.905
4.882
4.857
4.842
4.817
4.133
4.088
4.071
4.057
4.026
4.008
3.999
3.963
3.383
2.500
1.131
1.113
1.095
1.077
OH
O
O
N
O
F
3l
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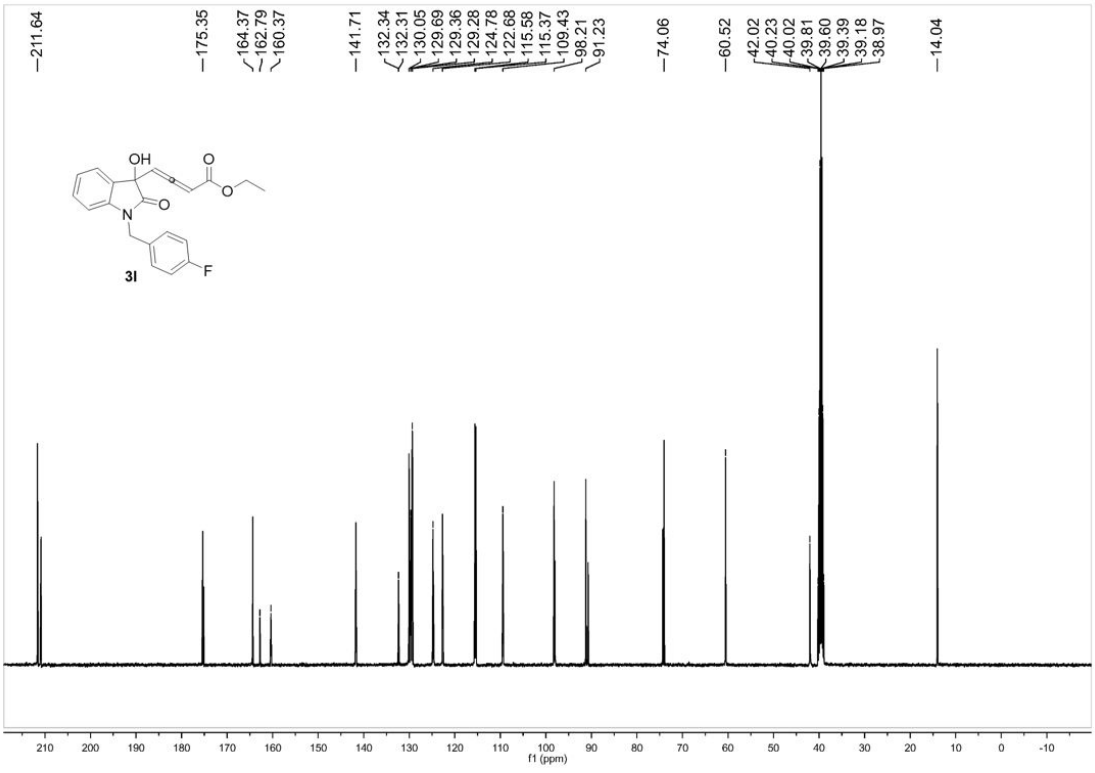
2.00
3.01
f1 (ppm)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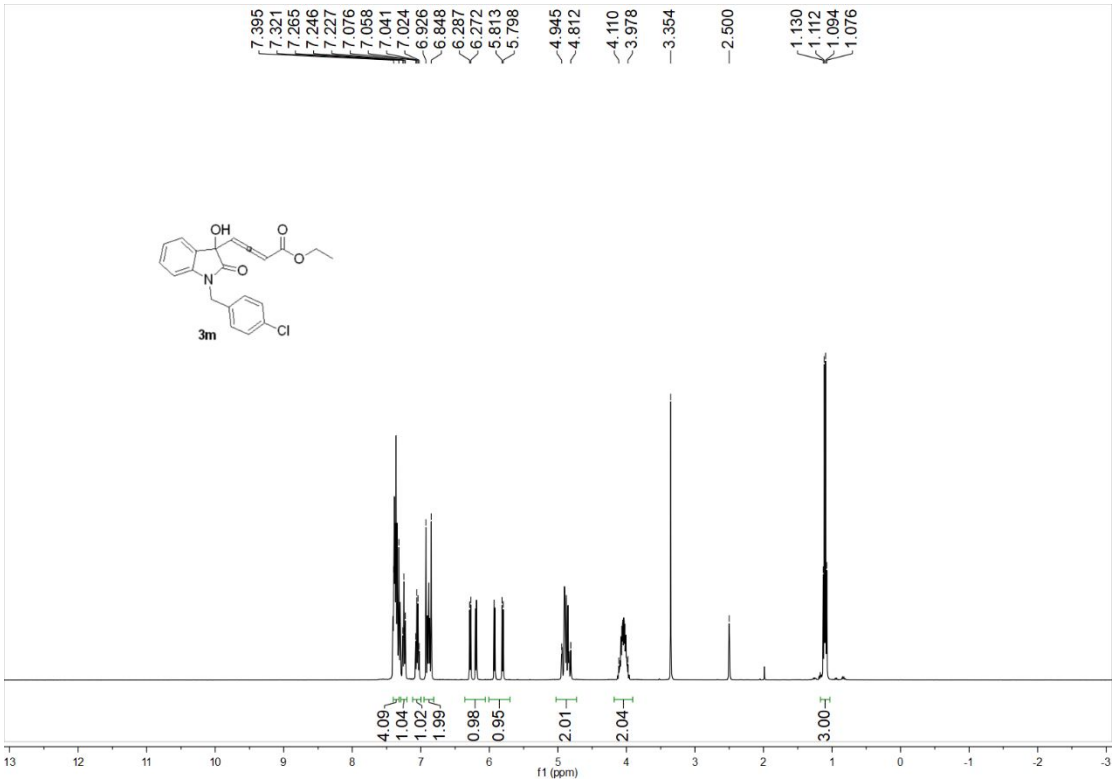
132.34
132.31
130.05
129.69
129.36
129.28
124.78
122.68
115.58
115.37
109.43
98.21
91.23
74.06
60.52
42.02
40.23
40.02
39.81
39.60
39.39
39.18
38.97
14.04
OH
O
O
N
O
F
3l
f1 (ppm)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5.813
5.798
4.945
4.812
4.110
3.978
3.354
2.500
1.130
1.112
1.094
1.076
OH
O
O
N
O
Cl
3m
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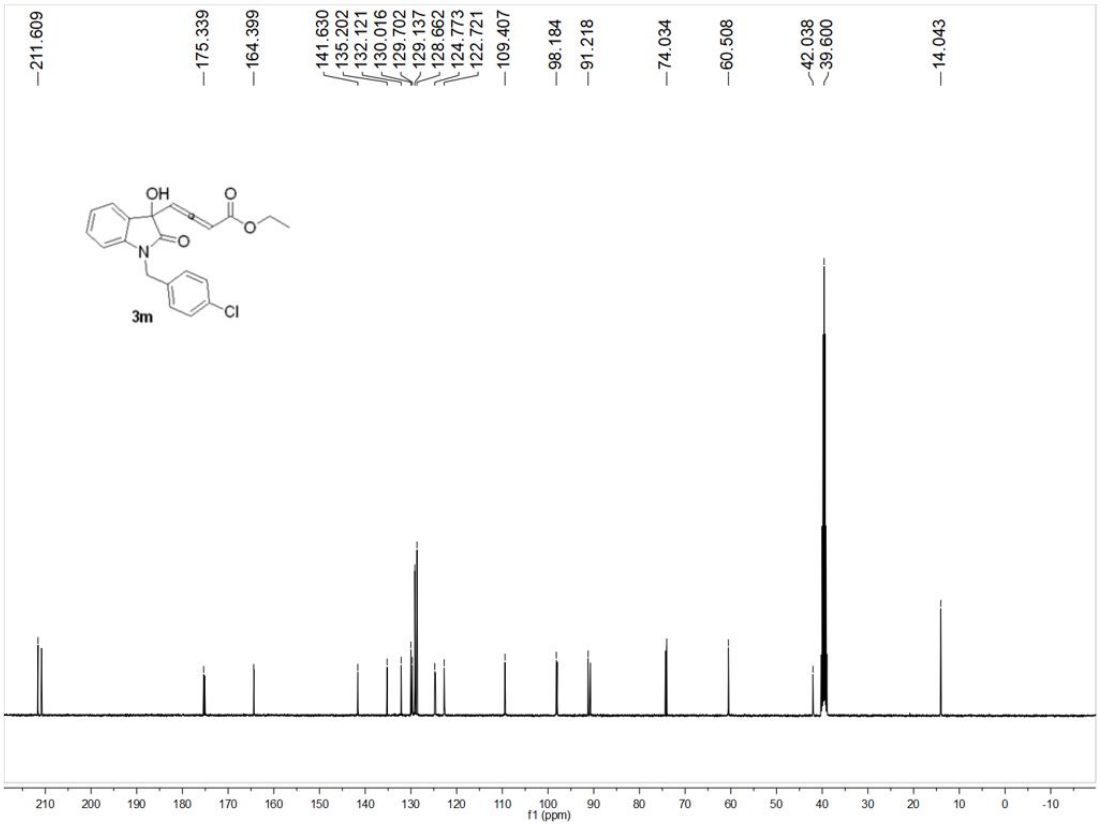
1.04
1.02
1.99
0.98
0.95
2.01
2.04
3.00
f1 (ppm)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128.662
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109.407
98.184
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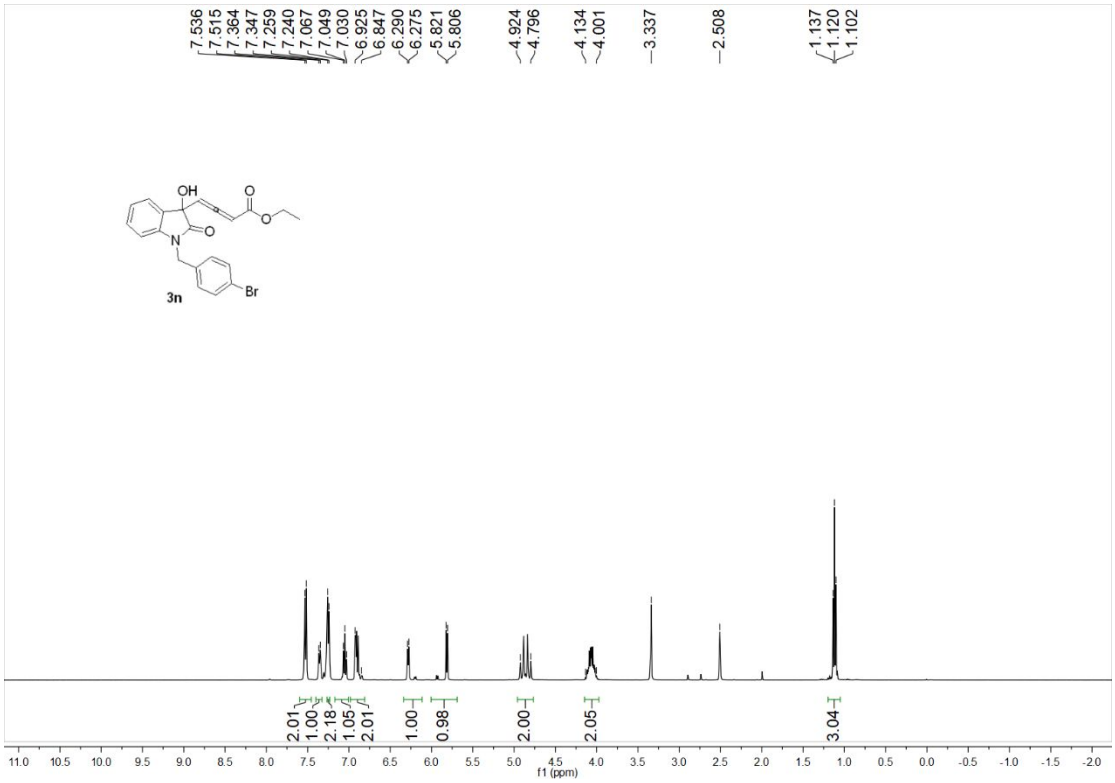
60.508
42.038
39.600
14.043
OH
O
O
N
O
Cl
3m
f1 (ppm)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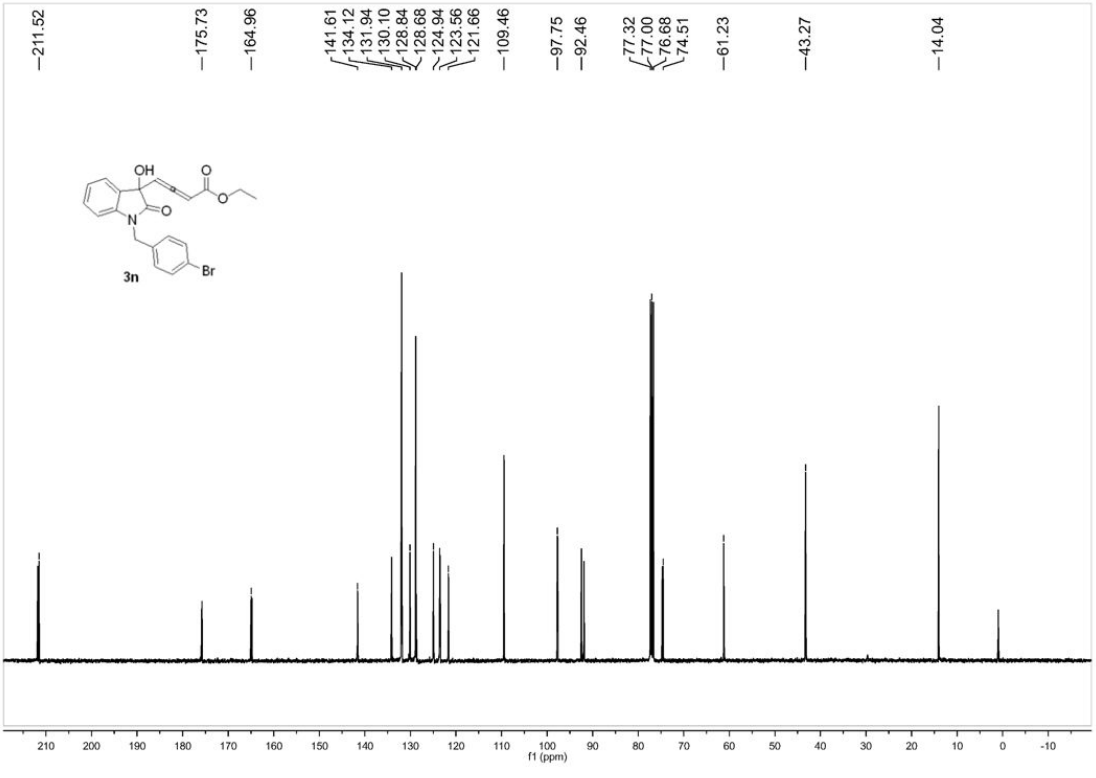
6.290
6.275
5.821
5.806
4.924
4.796
4.134
4.001
3.337
2.508
1.137
1.120
1.102
OH
O
O
N
O
Br
3n
2.01
1.00
2.18
1.05
2.01
1.00
0.98
2.00
2.05
3.04
f1 (ppm)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123.56
121.66
109.46
97.75
92.46
77.32
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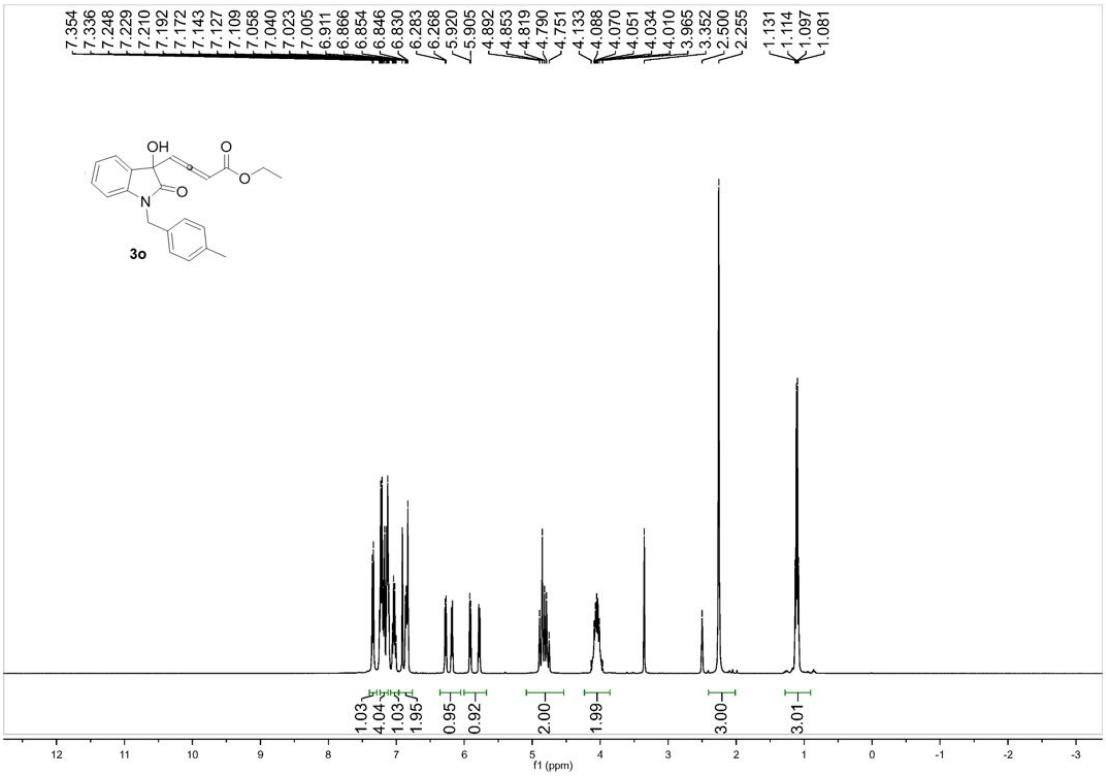
76.68
74.51
61.23
43.27
14.04
OH
O
O
N
O
Br
3n
f1 (ppm)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7.040
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7.005
6.911
6.866
6.854
6.846
6.830
6.283
6.268
5.920
5.905
4.892
4.853
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4.790
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4.070
4.051
4.034
4.010
3.965
3.352
2.500
2.255
1.131
1.114
1.097
1.081
OH
O
O
N
O
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1.03
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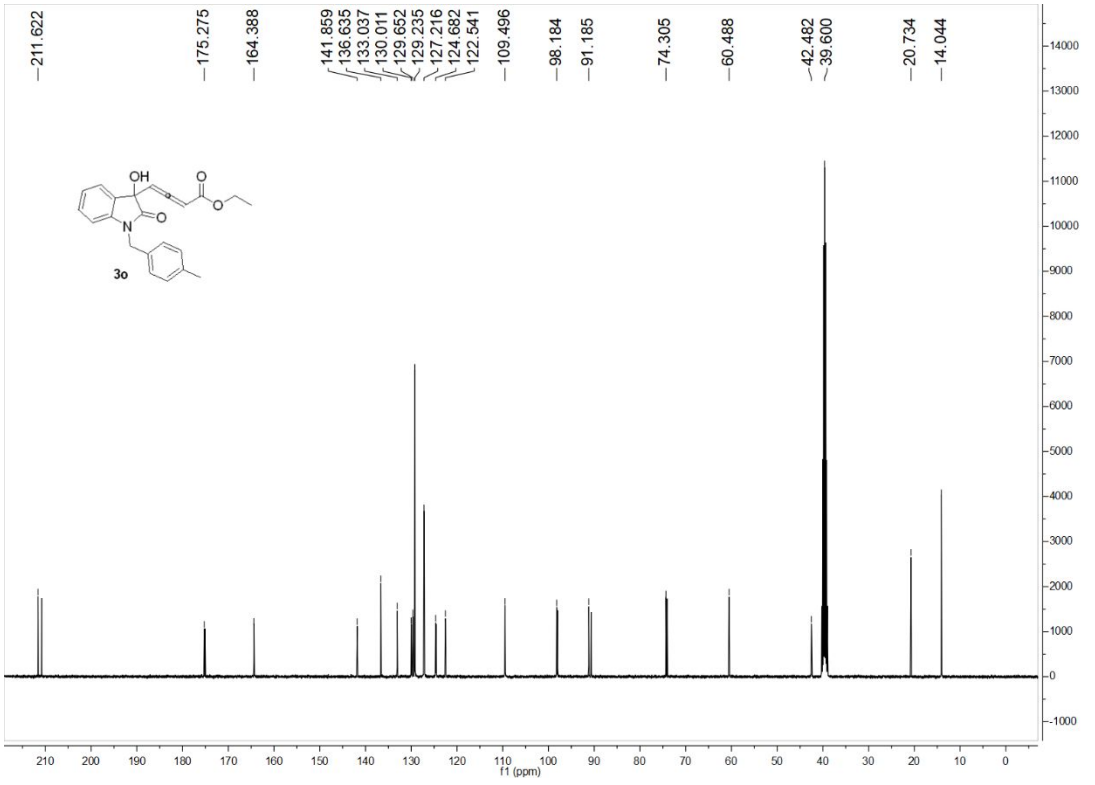
1.99
3.00
3.01
f1 (ppm)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127.216
124.682
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109.496
98.184
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42.482
39.600
20.734
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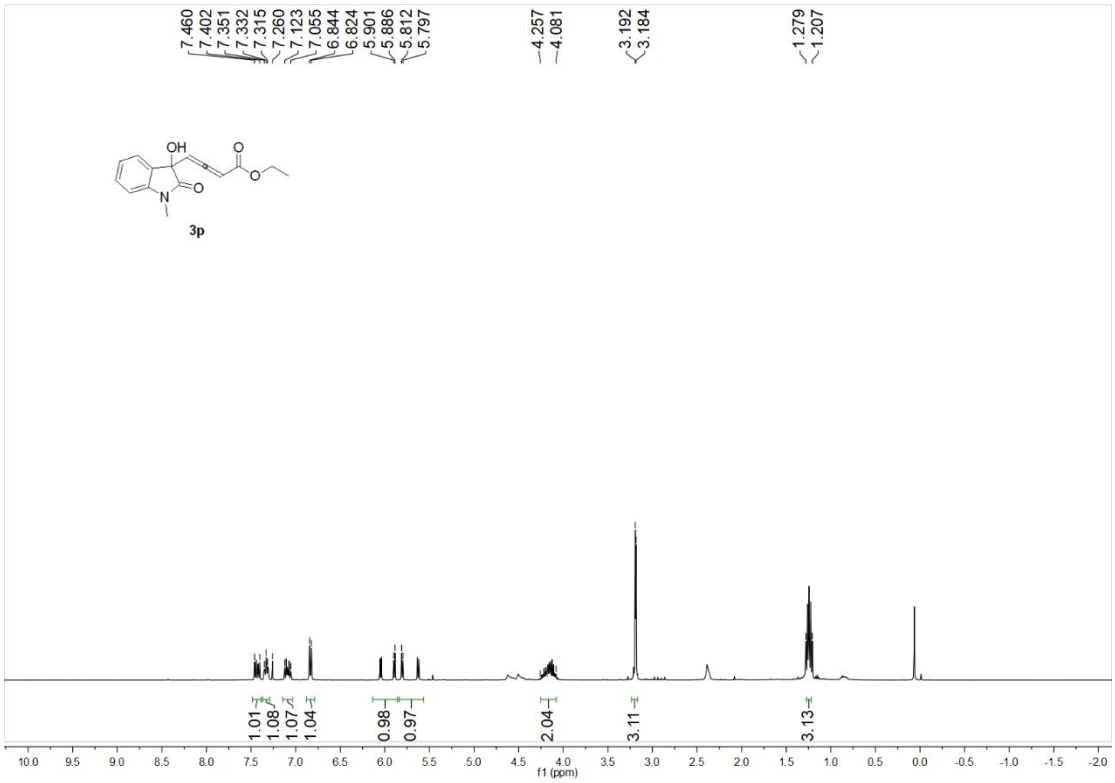
OH
O
O
N
O
3o
f1 (ppm)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6.844
6.824
5.901
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5.812
5.797
4.257
4.081
3.192
3.184
1.279
1.207
OH
O
O
N
3p
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1.08
1.07
1.04
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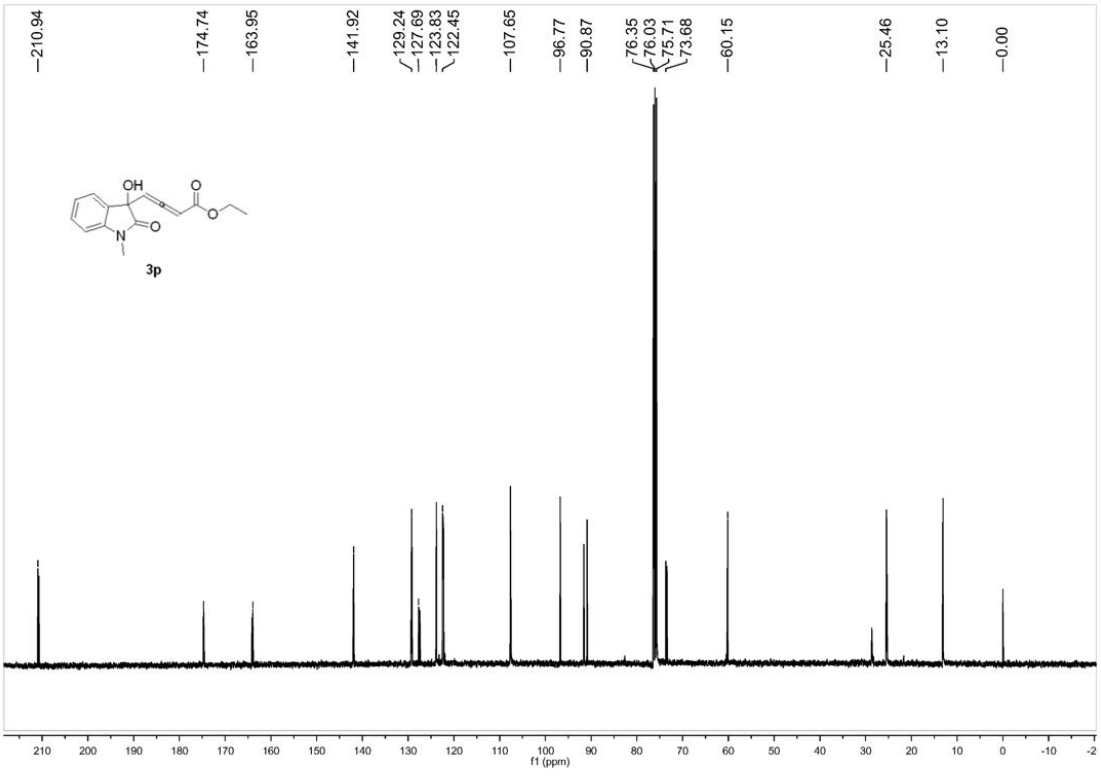
0.97
2.04
3.11
3.13
f1 (ppm)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90.87
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60.15
25.46
13.10
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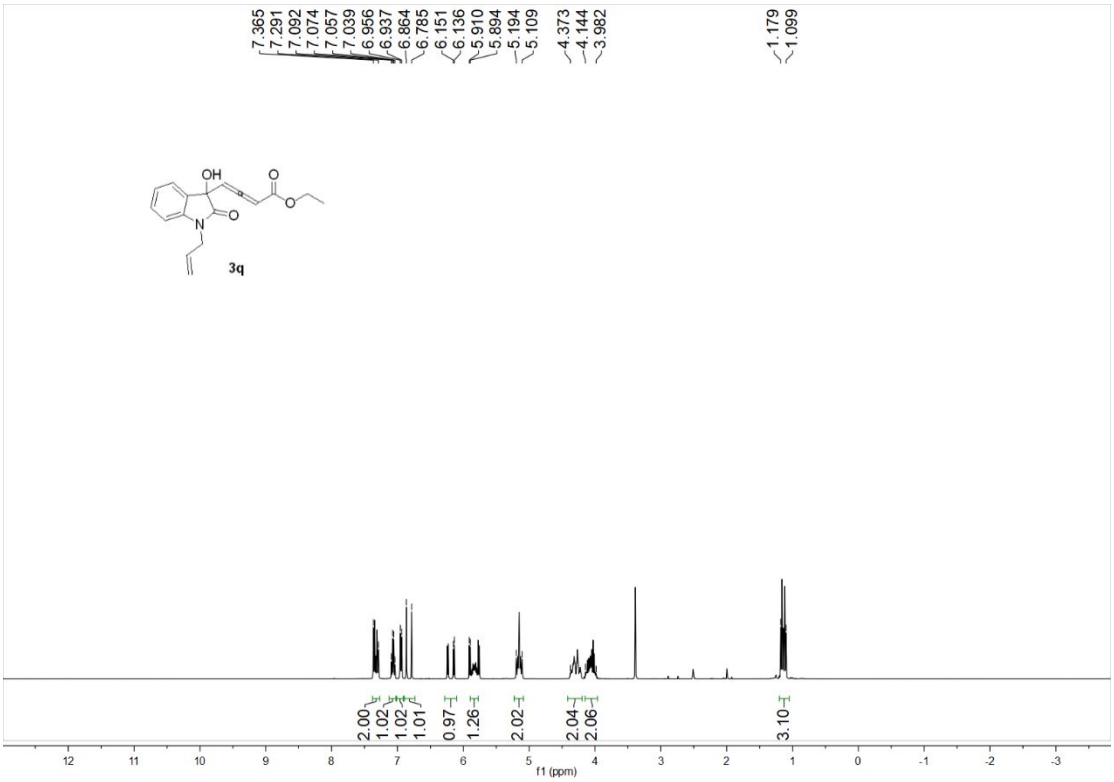
OH
O
O
N
3p
f1 (ppm)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6.151
6.136
5.910
5.894
5.194
5.109
4.373
4.144
3.982
1.179
1.099
OH
O
O
N
O
3q
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1.02
1.01
0.97
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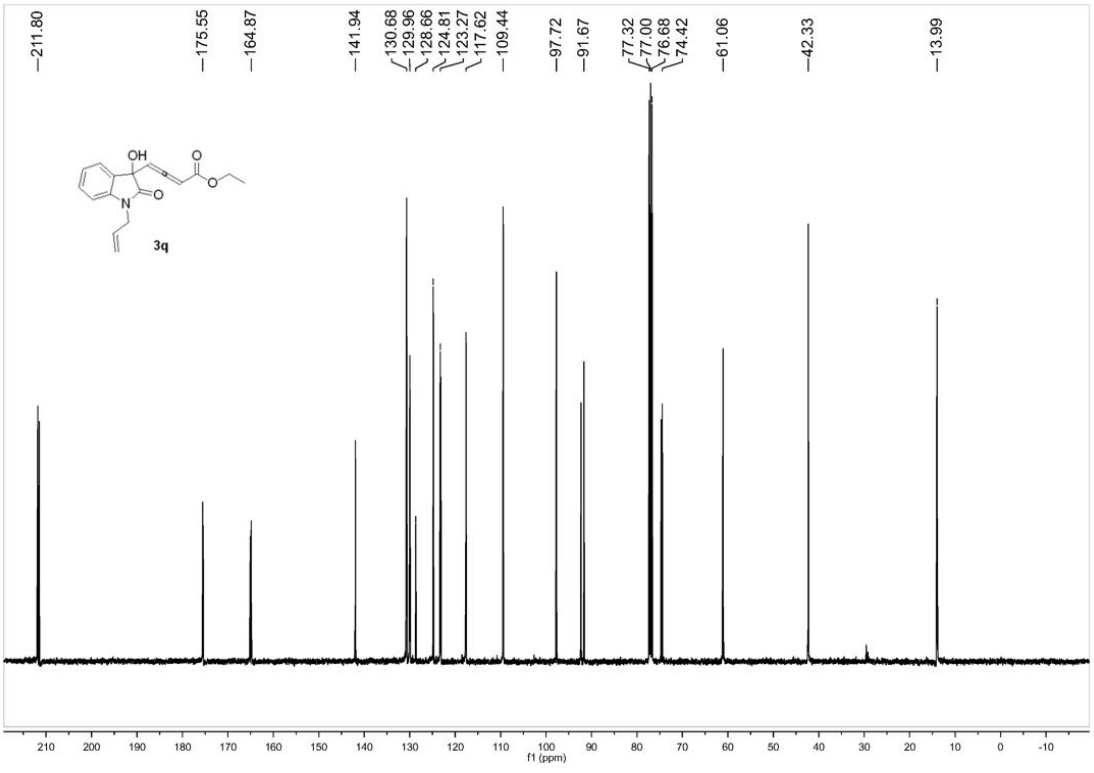
2.04
2.06
3.10
f1 (ppm)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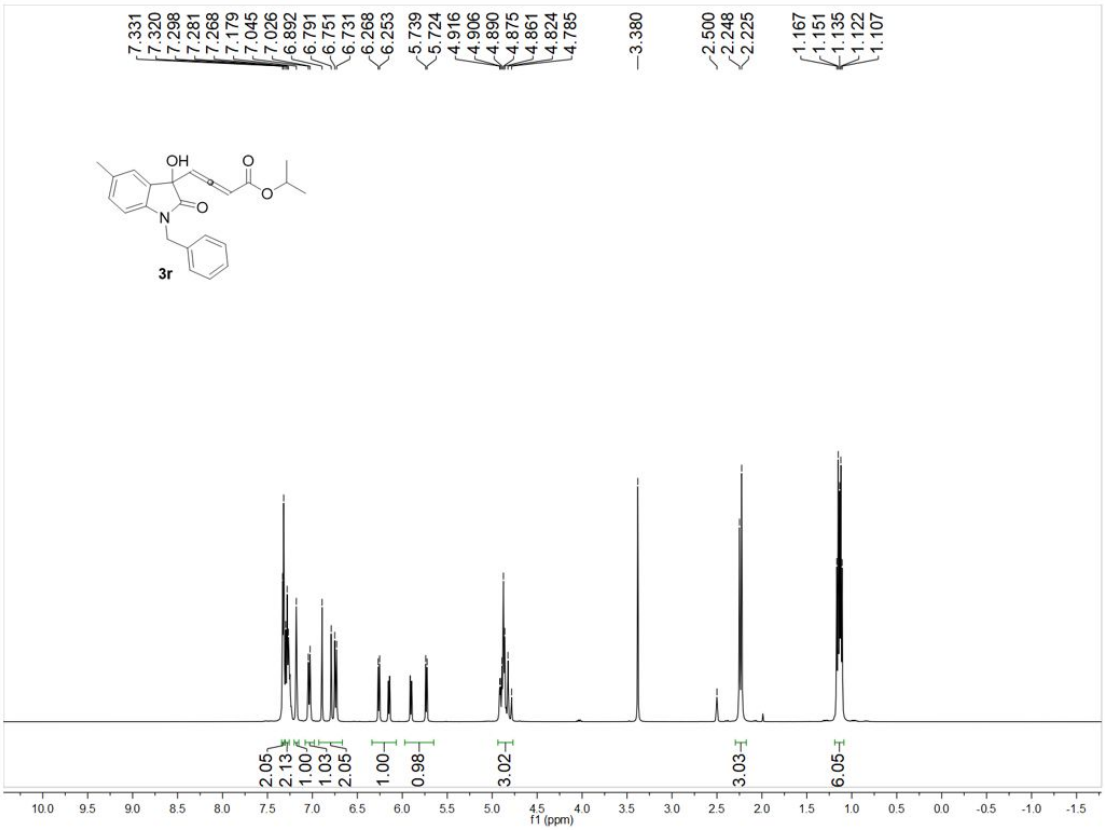
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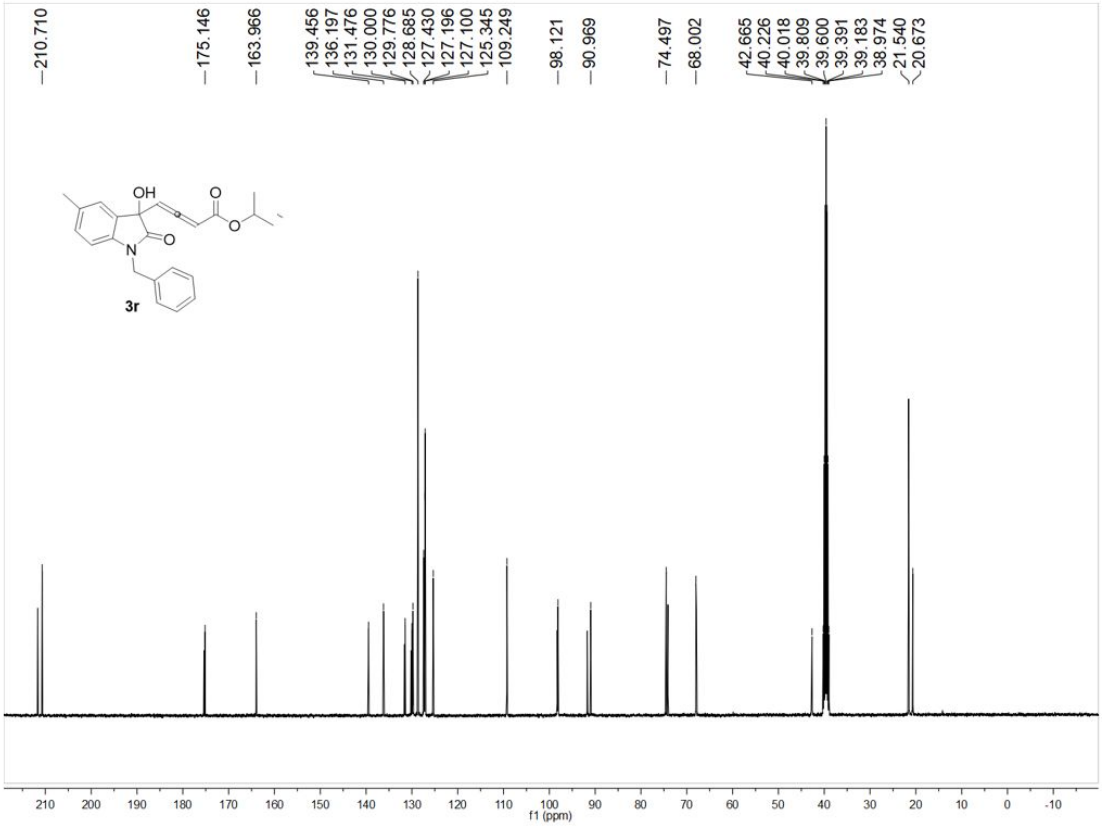
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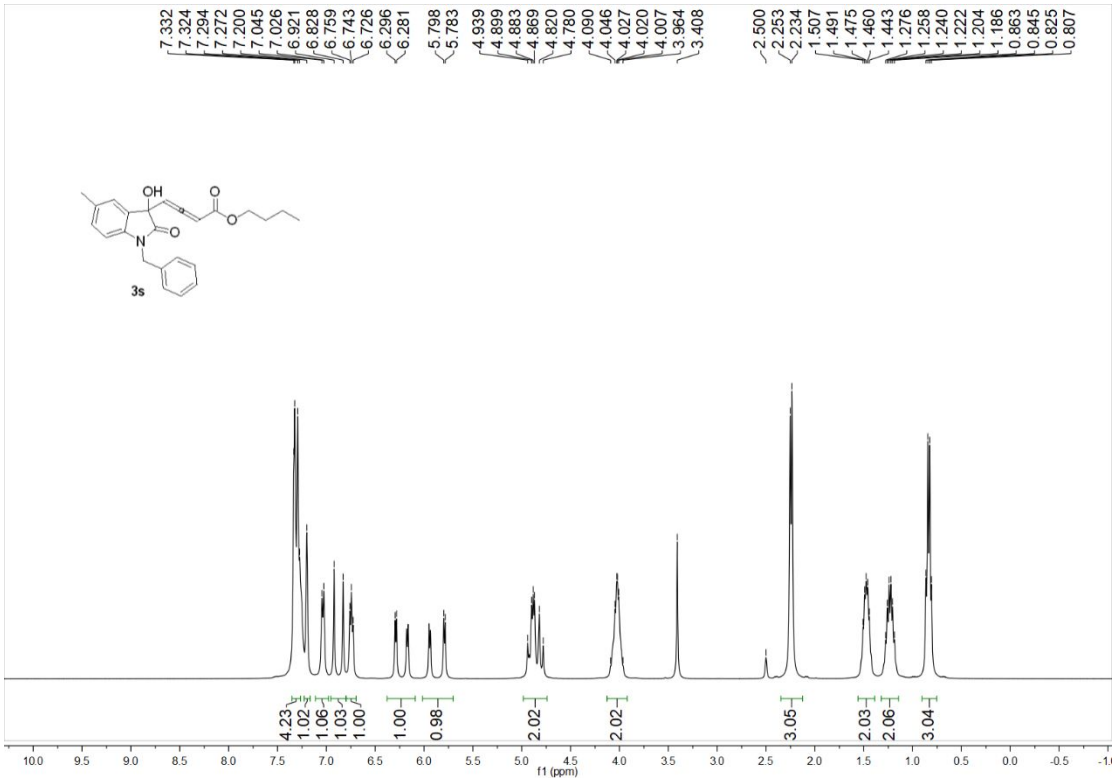
f1 (ppm)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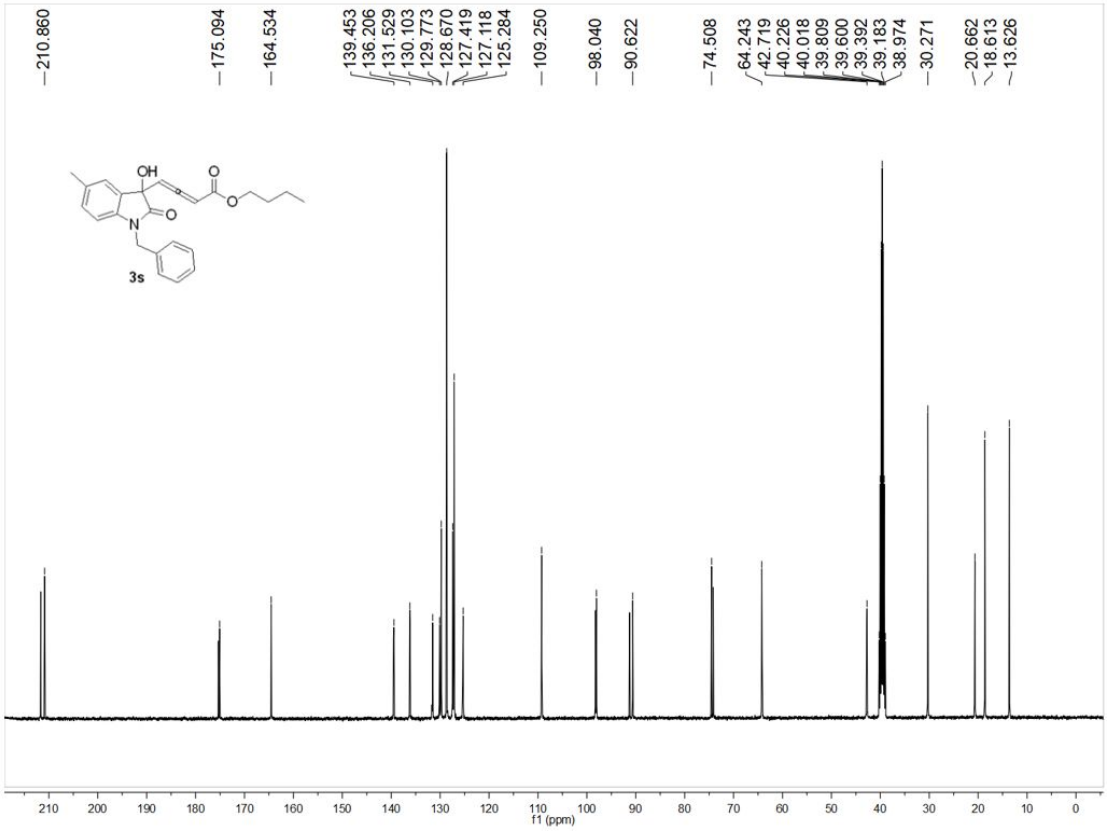
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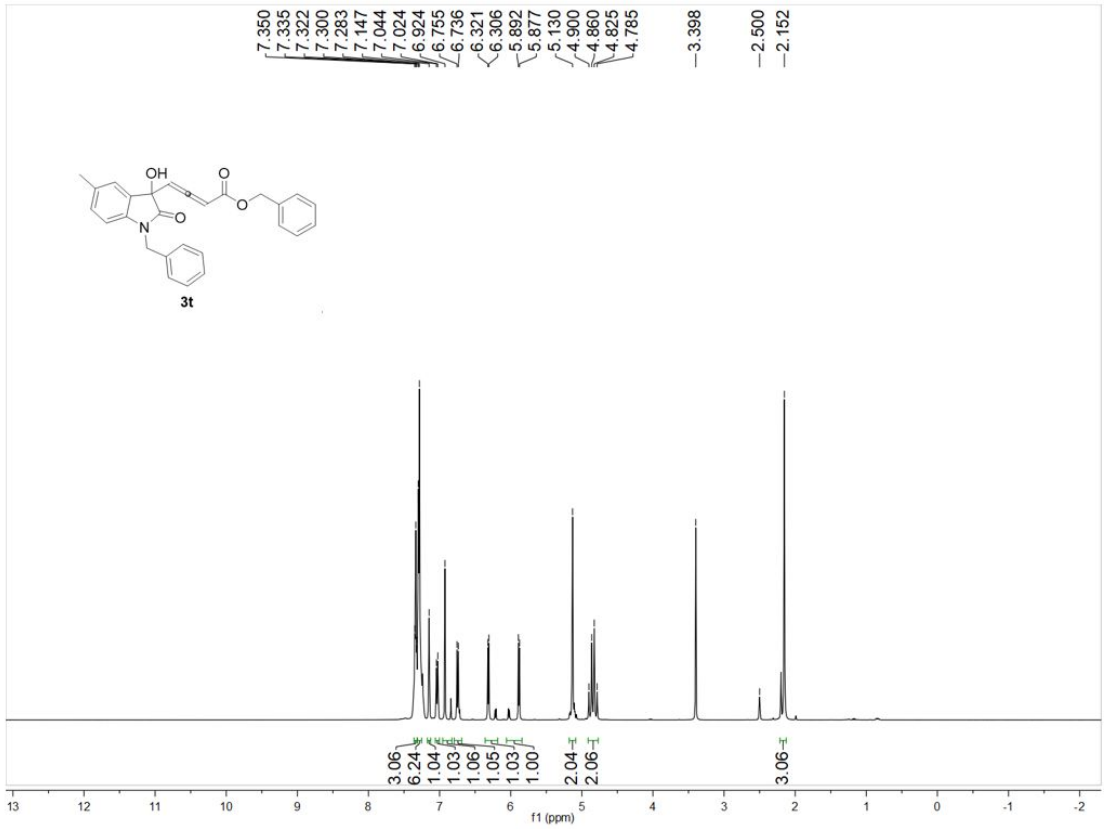
f1 (ppm)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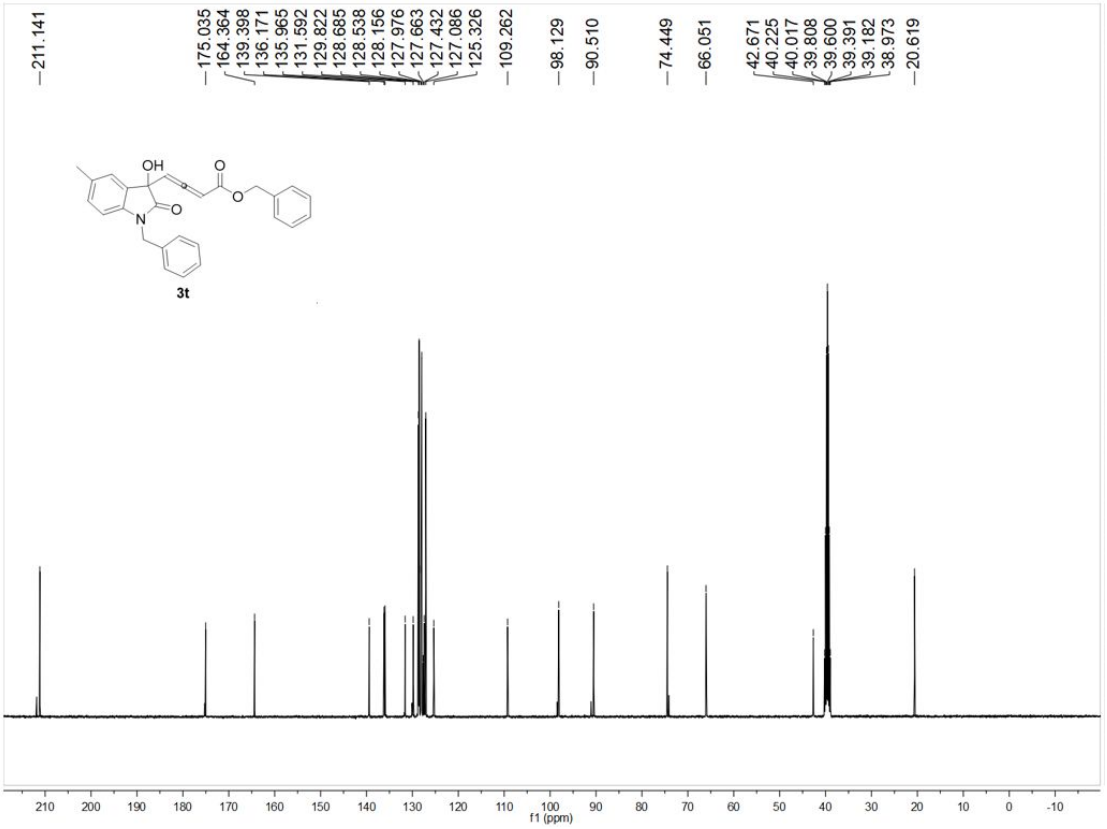
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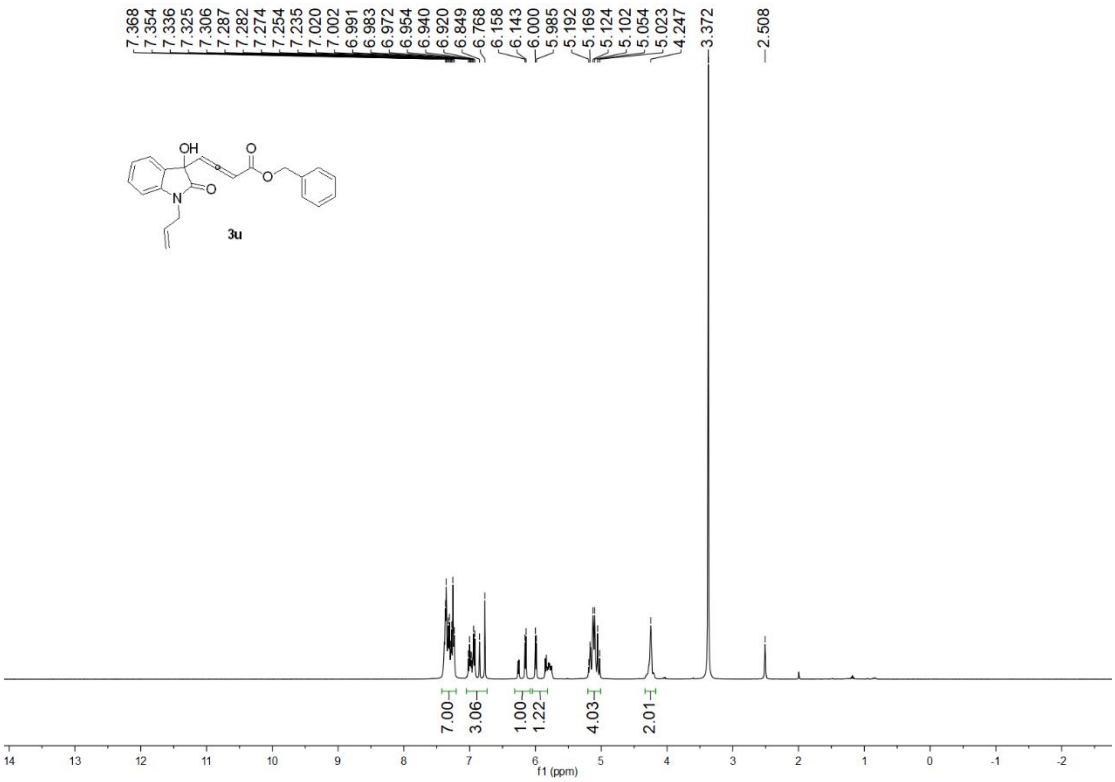
3t
f1 (ppm)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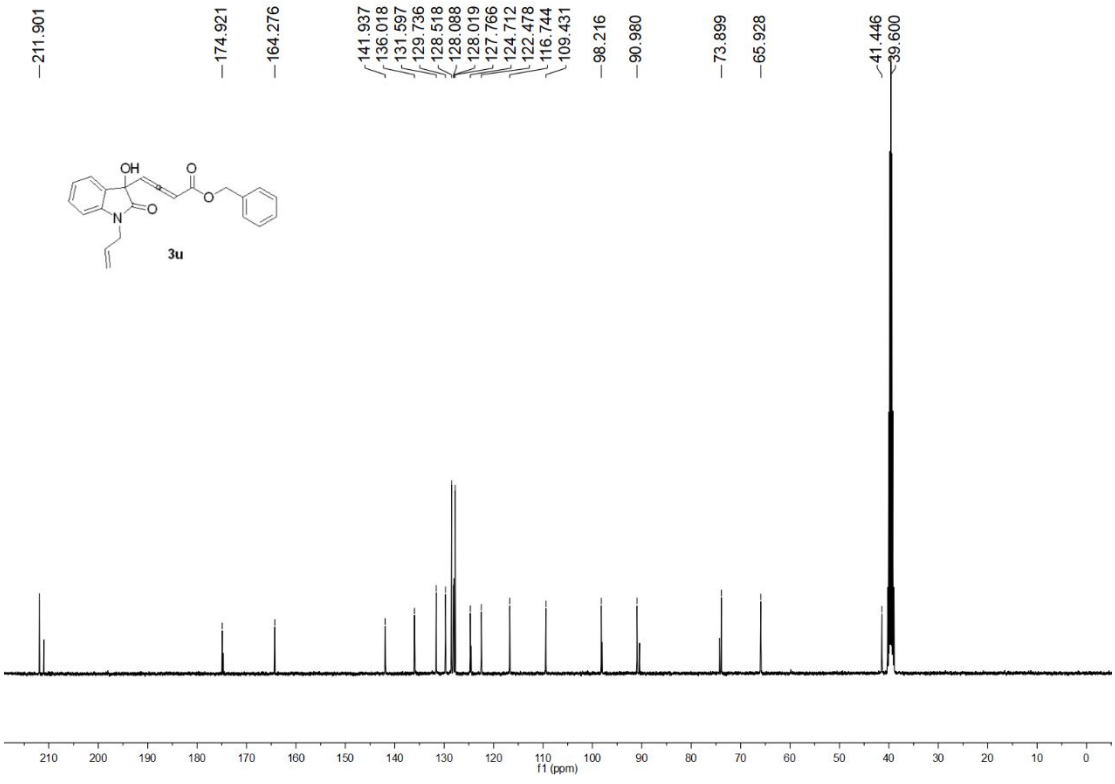
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128.019
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122.478
116.744
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90.980
73.899
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41.446
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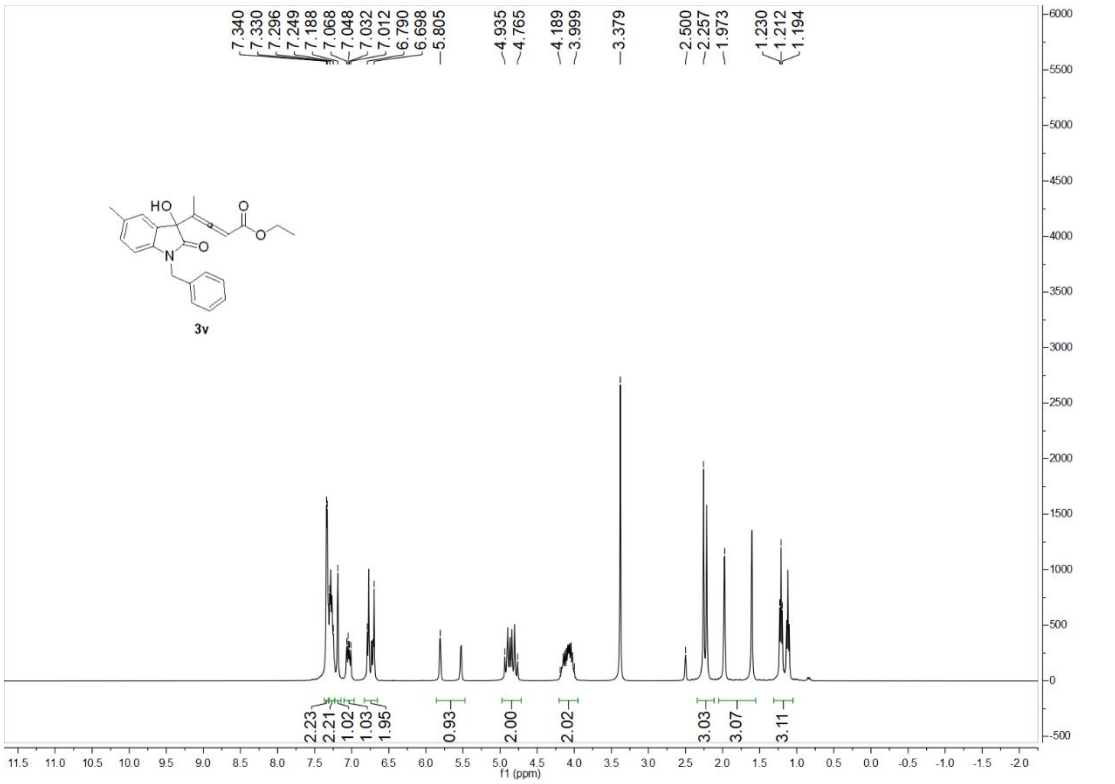
N
3u
f1 (ppm)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1.230
1.212
1.194
HO
O
O
N
O
3v
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1.03
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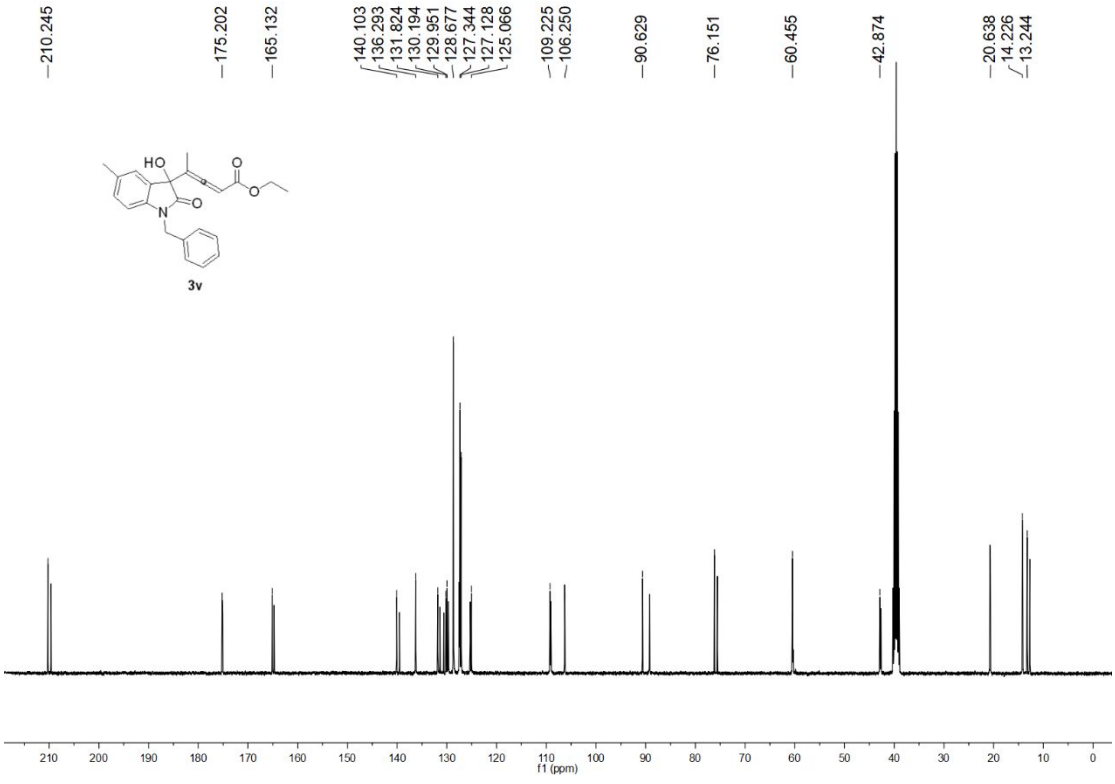
f1 (ppm)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106.250
90.629
76.151
60.455
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20.638
14.226
13.244
HO
O
O
N
O
3v
f1 (ppm)

7. DFT Study on Mechanism

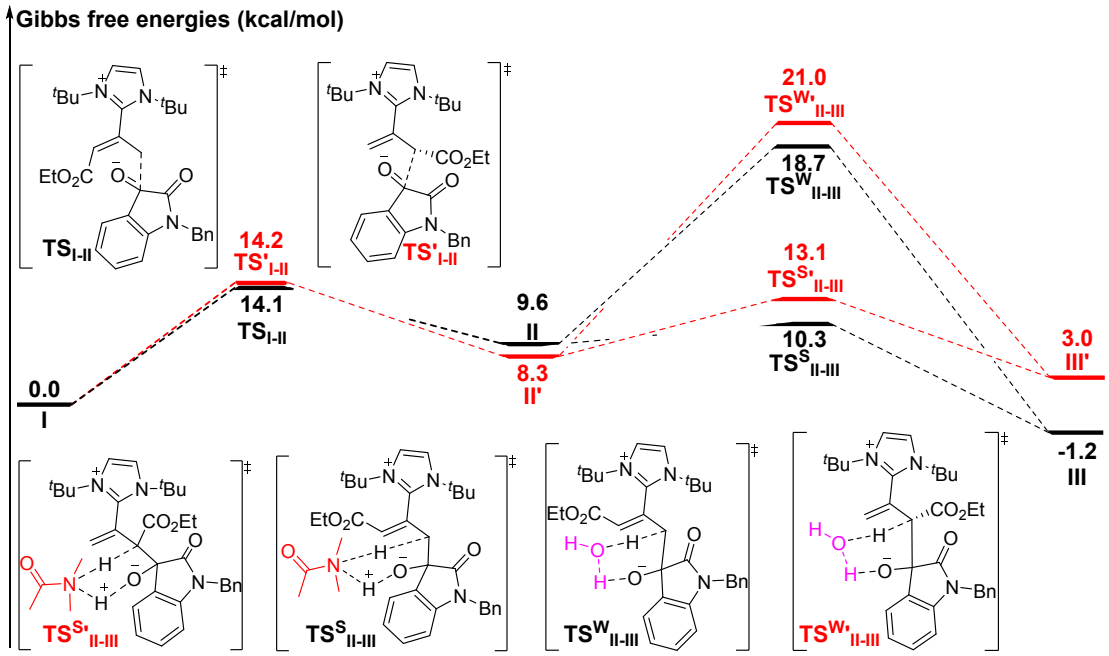

Figure S1. Energy profiles on the competing reaction pathways (All the energies were computed at the M06-2X-GD3/6-311++G(2df, 2pd)/IEF-PCM$_{MeCN}$//M06-2X/6-31G**/IEF-PCM$_{MeCN}$ level of theory)

As shown in Figure S1, there are two competing reaction pathways associated with the structural transformations from **I** and **2a** to **III** or **III′**. The energy barrier associated with $\mathbf{TS_{I\text{-}II}}$ (14.1 kcal/mol) is very close to that via $\mathbf{TS'_{I\text{-}II}}$ (14.2 kcal/mol) for the C-C bond formation step, but the energy of **II** is 1.3 kcal/mol higher than that of **II′**. In the following step, we have considered the possible DMF·H$^+$ and water-mediated [1,3]-proton transfer pathways based on the model pioneered by Yu.[5] Obviously, the energy barriers of DMF·H$^+$-mediated [1,3]-proton transfer pathways via $\mathbf{TS^S_{II\text{-}III}}$ (10.3 kcal/mol) and $\mathbf{TS^{S'}_{II\text{-}III}}$ (13.1 kcal/mol) are lower than those of the pathways via $\mathbf{TS^W_{II\text{-}III}}$ (18.7 kcal/mol) and $\mathbf{TS^{W'}_{II\text{-}III}}$ (21.0 kcal/mol). Noteworthy, the energy of **III** is 4.2 kcal/mol lower than that of **III′**, indicating the pathway associated with formation of **III** is more energetically favorable in thermodynamics. All the calculations are consistent with the experimental observations.

Computational Methods:

The DFT calculations were performed using the Gaussian 09 program[6]. All structures were optimized at the M06-2X[7-9]/6-31G** level, and the corresponding vibrational frequencies were calculated at the same level. The structures discussed in this paper were fully optimized in MeCN solvent using the integral equation formalism polarizable continuum model (IEF-PCM)[10,11]. Then, frequency calculations at the same level of theory were carried out to identify all of the stationary points as minima (zero imaginary frequency) or transition state (only one frequency), and to provide the zero-point and thermal corrections. Furthermore, the energies were then refined at the M06-2X-GD3/6-311++G(2df, 2pd)/IEF-PCM$_{MeCN}$ level. The relative Gibbs free energies discussed were obtained by the addition of the corrections at the M06-2X/6-31G**/IEF-PCM$_{MeCN}$ level to the corresponding single-point energy at M06-2X-GD3/6-311++G(2df, 2pd)/IEF-PCM$_{MeCN}$ level.

Geometrical Coordinates of the Listed Complexes

2a

Total energy=	-783.135523		
Zero-point correction=			0.227694 (Hartree/Particle)
Thermal correction to Energy=			0.241491
Thermal correction to Enthalpy=			0.242435
Thermal correction to Gibbs Free Energy=			0.185107
Sum of electronic and zero-point Energies=			-782.907829
Sum of electronic and thermal Energies=			-782.894032
Sum of electronic and thermal Enthalpies=			-782.893088
Sum of electronic and thermal Free Energies=			-782.950415
C	2.29050600	0.33336600	0.19683600
C	1.03554800	0.47989500	-0.41499700
C	0.51307300	1.73271400	-0.69089400
C	1.29216700	2.83944800	-0.33593400
C	2.54271200	2.70594600	0.27236900
C	3.05423700	1.43821800	0.54582600
C	2.53305500	-1.10673900	0.34417300
C	1.26525200	-1.79344800	-0.25613300
H	-0.46033200	1.85560100	-1.15247100
H	0.90614400	3.83315300	-0.53926000
H	3.11193600	3.59078700	0.53227800
H	4.02254700	1.30485600	1.01739400

O	3.46569000	-1.71418100	0.80978200
O	1.05287300	-2.98331500	-0.32368200
N	0.45339600	-0.77475600	-0.68047400
C	-0.84213600	-0.96766400	-1.30404600
H	-0.93421900	-2.04573500	-1.46750500
H	-0.84673700	-0.47845600	-2.28401200
C	-1.98536500	-0.45229300	-0.45377500
C	-3.05604400	0.21285800	-1.05143200
C	-1.99128800	-0.65540500	0.92745400
C	-4.12572800	0.66300400	-0.27997100
H	-3.05121500	0.38211300	-2.12524500
C	-3.05685100	-0.20271600	1.69946100
H	-1.15638900	-1.16654700	1.40000800
C	-4.12774400	0.45644500	1.09709100
H	-4.95259400	1.18050100	-0.75552500
H	-3.05193100	-0.36446300	2.77255500
H	-4.95784400	0.80967500	1.70013600

DMF·H$^+$

Total energy= -248.815732
Zero-point correction= 0.117376 (Hartree/Particle)
Thermal correction to Energy= 0.123636
Thermal correction to Enthalpy= 0.124580
Thermal correction to Gibbs Free Energy= 0.087872
Sum of electronic and zero-point Energies= -248.698357
Sum of electronic and thermal Energies= -248.692096
Sum of electronic and thermal Enthalpies= -248.691152
Sum of electronic and thermal Free Energies= -248.727860

C	-1.00686900	-0.00004300	0.40960200
O	-2.00709700	0.00018500	-0.22171900
H	-0.89578400	-0.00046600	1.50201600
N	0.32099800	0.00003400	-0.29558100
C	1.08734100	1.24650000	0.04076800
H	1.29233600	1.24675700	1.11065700
H	2.01819300	1.22578600	-0.52234000
H	0.48903100	2.11066000	-0.24127600
C	1.08705600	-1.24660800	0.04064800
H	0.48875100	-2.11065200	-0.24175000
H	2.01806200	-1.22591700	-0.52216400
H	1.29173100	-1.24712100	1.11059500
H	0.10229700	0.00014800	-1.29903400

I

Total energy= -924.220883

Zero-point correction= 0.433369 (Hartree/Particle)

Thermal correction to Energy= 0.456405

Thermal correction to Enthalpy= 0.457349

Thermal correction to Gibbs Free Energy= 0.381753

Sum of electronic and zero-point Energies= -923.787514

Sum of electronic and thermal Energies= -923.764479

Sum of electronic and thermal Enthalpies= -923.763535

Sum of electronic and thermal Free Energies= -923.839131

C	0.95027900	-0.00010800	0.21335500
C	2.06640100	0.67492500	-1.57686900
C	2.06620100	-0.67546400	-1.57687000
H	2.50081900	1.35385100	-2.28680900
H	2.50037900	-1.35450800	-2.28684700
N	1.37932700	-1.09181200	-0.45575200
N	1.37968700	1.09147200	-0.45571800
C	1.23058400	-2.54623600	-0.08136400
C	2.18839000	-2.85200100	1.07148500
C	-0.21941900	-2.85708200	0.28963600
C	1.61389600	-3.39987100	-1.29382100
H	3.21676900	-2.60572600	0.79115800
H	1.91409500	-2.28804600	1.96413400
H	2.13813700	-3.92035700	1.29959400
H	-0.89599600	-2.47239600	-0.47802400
H	-0.32787700	-3.94261000	0.35737100
H	-0.49603900	-2.41700800	1.24573600
H	1.43426100	-4.44404600	-1.03162800
H	1.00193200	-3.15875700	-2.16747100
H	2.67183900	-3.30644600	-1.55124600
C	1.23138400	2.54594900	-0.08133000
C	-0.21857800	2.85733200	0.28935900
C	2.18906800	2.85138300	1.07171500
C	1.61526000	3.39945600	-1.29369600
H	-0.89514800	2.47286600	-0.47842200
H	-0.49556200	2.41738200	1.24540900
H	-0.32665700	3.94290300	0.35704900
H	3.21740900	2.60468100	0.79162100
H	2.13919900	3.91976500	1.29978200
H	1.91435700	2.28755700	1.96431800
H	1.43599100	4.44369200	-1.03149900
H	2.67321400	3.30561200	-1.55092700
H	1.00335400	3.15861500	-2.16746100
C	0.17623800	-0.00005000	1.49539800
C	-1.24758800	0.00019300	1.41850200

H	-1.80713900	0.00020500	2.34652500
C	0.92670200	-0.00027900	2.62934400
H	2.00961900	-0.00043800	2.59359500
H	0.45145300	-0.00028000	3.60504400
C	-1.95013600	0.00034200	0.20733300
O	-1.49588500	0.00027900	-0.95255300
O	-3.32174200	0.00054800	0.39428800
C	-4.10126900	0.00062000	-0.79416800
C	-5.55888300	0.00036700	-0.38045500
H	-3.85954200	-0.87984500	-1.40006700
H	-3.85978600	0.88134200	-1.39980700
H	-6.20343500	0.00045000	-1.26282200
H	-5.78934000	-0.88586800	0.21623100
H	-5.78955800	0.88632600	0.21655400

TS_{I-II}

Total energy= -1707.357033

Zero-point correction= 0.662380 (Hartree/Particle)

Thermal correction to Energy= 0.699701

Thermal correction to Enthalpy= 0.700645

Thermal correction to Gibbs Free Energy= 0.592653

Sum of electronic and zero-point Energies= -1706.694652

Sum of electronic and thermal Energies= -1706.657332

Sum of electronic and thermal Enthalpies= -1706.656388

Sum of electronic and thermal Free Energies= -1706.764380

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C	5.02296300	-0.69972200	1.03399000
C	5.18762000	-0.70199300	-0.30432300
H	5.71978400	-0.95979700	1.81094000
H	6.05723600	-0.95765700	-0.88120400
N	4.00121200	-0.28711700	-0.87154300
N	3.73460400	-0.28345700	1.29958000
C	3.85626900	-0.18169900	-2.38007900
C	3.40367000	-1.53942100	-2.91929800
C	2.89474000	0.93188900	-2.80354700
C	5.23918200	0.16159200	-2.95319200
H	4.06811700	-2.33513400	-2.57121800
H	2.38127700	-1.76573900	-2.61457800
H	3.44030100	-1.51319100	-4.01160800
H	3.16755400	1.88376400	-2.34128300
H	2.98872900	1.03635100	-3.88714600
H	1.85344300	0.70915200	-2.57622800
H	5.11576800	0.37729700	-4.01587300
H	5.66220000	1.04623000	-2.46971200

H	5.94596800	-0.66703500	-2.87779100
C	3.26752200	-0.22194500	2.73824200
C	4.34074600	0.53059700	3.53425900
C	1.94430100	0.51099100	2.88734600
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H	1.13044700	0.01559200	2.36301300
H	1.70500900	0.50681900	3.95493400
H	2.01675400	1.54993900	2.55972000
H	2.84665400	-1.66258100	4.27407000
H	2.34228100	-2.17062300	2.64917700
H	4.07196500	-2.21274900	3.12076300
C	1.69418300	0.33839000	-0.15673600
C	1.43290400	1.68108100	-0.05762800
H	2.17871500	2.35197000	0.35272000
C	0.83925200	-0.70762300	-0.61584700
H	1.32241400	-1.66258100	-0.79724100
H	0.07668200	-0.42200600	-1.33105700
C	0.23684700	2.30010500	-0.59902100
O	-0.59714000	1.77257500	-1.32092000
O	0.16319600	3.61025500	-0.26540400
C	-0.95090300	4.32673400	-0.80817000
C	-0.81120900	5.77103700	-0.37937100
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H	-0.94833500	4.22307600	-1.89753400
H	-1.64488600	6.35795900	-0.77133100
H	-0.81264100	5.85159500	0.71011000
H	0.12105300	6.19565200	-0.75906700
C	-1.20377100	-2.35358300	-0.12150500
C	-2.26709200	-1.56500300	-0.58311700
C	-3.16971900	-2.04147900	-1.52495000
C	-2.98664100	-3.34887000	-1.98781400
C	-1.94254800	-4.14897500	-1.52277400
C	-1.03973900	-3.64883200	-0.57813600
C	-0.41918300	-1.54899100	0.86923600
C	-1.19550300	-0.21885300	0.93791000
H	-3.99360000	-1.42985500	-1.87816700
H	-3.68006800	-3.74816300	-2.72126800
H	-1.83311500	-5.16142900	-1.89665000
H	-0.21868800	-4.25537600	-0.20610800
O	0.23156000	-2.02200800	1.82241300
O	-0.97551800	0.74383500	1.65530800

N	-2.24401700	-0.31416000	0.03976500
C	-3.15721000	0.76829100	-0.24635000
H	-3.09146600	1.03326100	-1.30735300
H	-2.78116100	1.62359600	0.32344200
C	-4.58739900	0.45470100	0.14195500
C	-4.87090800	-0.21015400	1.33704800
C	-5.64232600	0.85304900	-0.67968300
C	-6.18774700	-0.46863800	1.70567100
H	-4.05041200	-0.52889100	1.97519200
C	-6.96221600	0.59825200	-0.31158400
H	-5.42848400	1.36225900	-1.61618100
C	-7.23780100	-0.06400400	0.88187700
H	-6.39592700	-0.98738000	2.63616900
H	-7.77392800	0.91058500	-0.96102900
H	-8.26464600	-0.26871100	1.16741200

TS'_{I-II}

Total energy= -1707.360634
Zero-point correction= 0.663566 (Hartree/Particle)
Thermal correction to Energy= 0.700221
Thermal correction to Enthalpy= 0.701165
Thermal correction to Gibbs Free Energy= 0.596215
Sum of electronic and zero-point Energies= -1706.697069
Sum of electronic and thermal Energies= -1706.660413
Sum of electronic and thermal Enthalpies= -1706.659469
Sum of electronic and thermal Free Energies= -1706.764419

C	-3.02912900	-0.81025000	-0.19610400
C	-4.84282900	-1.91739300	0.44083700
C	-5.23087700	-0.68267700	0.05939300
H	-5.44477800	-2.72818300	0.80454700
H	-6.21873200	-0.26245000	0.04210600
N	-4.10974300	0.00109700	-0.35184300
N	-3.47917200	-2.00098700	0.27446100
C	-4.21171300	1.41344900	-0.89628200
C	-3.84275100	2.40036000	0.21105700
C	-3.35108700	1.58121300	-2.14959100
C	-5.66885400	1.66514200	-1.30710800
H	-4.46429900	2.22726300	1.09406200
H	-2.79345800	2.33852600	0.49259200
H	-4.03240700	3.41539300	-0.14956600
H	-3.59729200	0.81251200	-2.88795900
H	-3.58417800	2.55786500	-2.58087100
H	-2.28249300	1.54945800	-1.95811900

H	-5.70558100	2.63931500	-1.79760200
H	-6.02654800	0.91378100	-2.01589300
H	-6.34362600	1.71285500	-0.44979000
C	-2.70699600	-3.25675500	0.64379200
C	-1.89154600	-3.76262500	-0.54897700
C	-1.82411600	-2.94225700	1.84301900
C	-3.71264500	-4.34633900	1.02911400
H	-2.50234400	-3.78670400	-1.45642700
H	-0.99809600	-3.16253400	-0.70644200
H	-1.57739800	-4.78599700	-0.32658000
H	-2.44151100	-2.64327700	2.69652000
H	-1.28230400	-3.85282700	2.11740900
H	-1.08936600	-2.15636400	1.64978300
H	-3.13572700	-5.23785000	1.28096900
H	-4.29951500	-4.07927200	1.91137400
H	-4.38224800	-4.60291200	0.20310100
C	-1.62144200	-0.45009500	-0.55219500
C	-0.86966400	0.53049000	0.30463900
H	-1.44489900	0.83902900	1.17540200
C	-1.16248600	-0.91973800	-1.71909200
H	-1.77424500	-1.55179200	-2.35420000
H	-0.17424400	-0.64947200	-2.07207900
C	-0.39686100	1.71838800	-0.45732600
O	0.11460700	1.70333700	-1.56237300
O	-0.53910900	2.85300200	0.25061500
C	0.13018100	4.00661400	-0.28193300
C	-0.08247300	5.13756900	0.69848000
H	-0.28337100	4.23352500	-1.26927300
H	1.19126200	3.76145000	-0.40022800
H	0.40665500	6.04358000	0.33336100
H	-1.14822400	5.34504300	0.82381700
H	0.34300400	4.87908900	1.67128300
C	1.53222900	1.06105000	1.32376900
C	2.46463200	0.92627400	0.29072000
C	3.48517900	1.84755600	0.09545400
C	3.55936700	2.92251500	0.98927900
C	2.65133400	3.05637400	2.03924700
C	1.62757100	2.11621800	2.20976800
C	0.55461200	-0.10702700	1.27777000
C	1.23229300	-1.00459200	0.20128100
H	4.21292400	1.72935300	-0.70090100
H	4.34919100	3.65684000	0.86599800
H	2.74246400	3.89095100	2.72715700
H	0.90940600	2.20667100	3.02025600

O	0.12929300	-0.62915000	2.36623100
O	0.97268000	-2.16390400	-0.07908000
N	2.21628500	-0.26087800	-0.41705100
C	3.02885600	-0.75252700	-1.51041300
H	3.11346900	0.03062100	-2.27145700
H	2.47235700	-1.58957300	-1.94356800
C	4.40334500	-1.21104400	-1.06808000
C	5.55439300	-0.73895100	-1.69660000
C	4.52288800	-2.12999000	-0.02178300
C	6.81342500	-1.17869300	-1.28849500
H	5.46586000	-0.02046100	-2.50805200
C	5.77772000	-2.56838100	0.38804900
H	3.62255700	-2.50118600	0.46211200
C	6.92667000	-2.09278800	-0.24497300
H	7.70361200	-0.80209300	-1.78227200
H	5.86213600	-3.28343000	1.20031200
H	7.90529200	-2.43418000	0.07670900

II

Total energy= -1707.367135
Zero-point correction= 0.665761 (Hartree/Particle)
Thermal correction to Energy= 0.702829
Thermal correction to Enthalpy= 0.703773
Thermal correction to Gibbs Free Energy= 0.597046
Sum of electronic and zero-point Energies= -1706.701374
Sum of electronic and thermal Energies= -1706.664306
Sum of electronic and thermal Enthalpies= -1706.663361
Sum of electronic and thermal Free Energies= -1706.770089

C	2.79003200	0.12235900	-0.60674700
C	3.69118600	0.68571900	-2.54480400
C	4.35364900	1.35687800	-1.58187400
H	3.82930200	0.70648100	-3.61141200
H	5.16883000	2.05296900	-1.66839300
N	3.80859000	0.98767900	-0.37072600
N	2.72976400	-0.09544300	-1.93752500
C	4.43771100	1.48691800	0.91512200
C	4.01915800	2.94450500	1.11614100
C	4.07707300	0.63157200	2.13000600
C	5.96157900	1.39799300	0.73679600
H	4.28192400	3.55033000	0.24481000
H	2.94586400	3.03778200	1.29513500
H	4.54682600	3.34683300	1.98456300
H	4.33425700	-0.41726000	1.96739900
H	4.67554600	1.00426400	2.96443500

H	3.03155700	0.70547400	2.42259600
H	6.43043600	1.63996900	1.69255900
H	6.26052500	0.38653000	0.45016400
H	6.34461100	2.10731900	0.00179800
C	1.84326600	-0.94507600	-2.83552300
C	2.78362600	-1.81792200	-3.67522000
C	0.87753500	-1.84588000	-2.08040200
C	1.04056100	0.02517700	-3.70765700
H	3.42519900	-1.23915300	-4.34339100
H	3.41261100	-2.43815500	-3.03048600
H	2.17156000	-2.47639500	-4.29619000
H	0.23402000	-1.26106200	-1.42576600
H	0.26234600	-2.33492900	-2.84202100
H	1.38981600	-2.63163900	-1.52197100
H	0.42315500	-0.55957800	-4.39511700
H	0.40133100	0.62796900	-3.05945100
H	1.68917600	0.66809300	-4.30889500
C	1.88953800	-0.38637400	0.46363900
C	1.97964100	-1.67549400	0.80122900
H	2.66417200	-2.33934600	0.28210600
C	0.97805900	0.64300400	1.09384200
H	1.47513600	1.61595100	1.03388500
H	0.80569800	0.40349300	2.14485200
C	1.09990200	-2.31627600	1.81350800
O	0.67982100	-1.80532700	2.82883900
O	0.83937700	-3.57645000	1.45481900
C	-0.13237100	-4.25912000	2.26611400
C	-0.37070100	-5.61314100	1.63742500
H	-1.03902300	-3.64801000	2.28803700
H	0.25321300	-4.34084700	3.28640300
H	-1.10722000	-6.16743200	2.22324500
H	-0.75022000	-5.50093400	0.61935100
H	0.55434600	-6.19323500	1.60536700
C	-1.15063600	1.98806600	0.87971800
C	-2.42665500	1.55813300	1.25235400
C	-3.41123500	2.43678400	1.67957700
C	-3.07569200	3.79413800	1.75207600
C	-1.80543300	4.24139900	1.39697100
C	-0.83788900	3.33267400	0.94643100
C	-0.35249200	0.80960000	0.30522900
C	-1.33576500	-0.36431600	0.63046500
H	-4.40633000	2.09239200	1.94372900
H	-3.82259900	4.50624800	2.08889600
H	-1.57006900	5.29904400	1.45850600

H	0.14494100	3.68313600	0.63844500
O	-0.16346500	0.89339100	-1.02282700
O	-1.18277900	-1.55527900	0.39597200
N	-2.51656800	0.16070500	1.11941600
C	-3.76567000	-0.56139100	1.06542900
H	-4.36018000	-0.34905800	1.96013900
H	-3.50529000	-1.62393300	1.08533500
C	-4.56278500	-0.23989600	-0.18807300
C	-3.93525500	0.24443600	-1.33909300
C	-5.94105900	-0.46240400	-0.20341200
C	-4.68377000	0.49341000	-2.48803100
H	-2.86368200	0.44070800	-1.33925300
C	-6.68612800	-0.21660300	-1.35351700
H	-6.43323400	-0.83013000	0.69381800
C	-6.05759700	0.26316600	-2.50095300
H	-4.19011300	0.87305700	-3.37738200
H	-7.75723200	-0.39272100	-1.35132000
H	-6.63563300	0.46227400	-3.39770300

II′

Total energy= -1707.367589

Zero-point correction= 0.663964 (Hartree/Particle)

Thermal correction to Energy= 0.701318

Thermal correction to Enthalpy= 0.702263

Thermal correction to Gibbs Free Energy= 0.594689

Sum of electronic and zero-point Energies= -1706.703625

Sum of electronic and thermal Energies= -1706.666271

Sum of electronic and thermal Enthalpies= -1706.665327

Sum of electronic and thermal Free Energies= -1706.772900

C	-3.11241200	-0.61088700	-0.25879200
C	-4.78906200	-1.45379700	0.91395100
C	-5.06402200	-0.15222300	0.69550500
H	-5.35801300	-2.19057200	1.45277100
H	-5.91776000	0.42348400	1.00282400
N	-4.03226500	0.37036400	-0.05471200
N	-3.58555100	-1.74313400	0.30549300
C	-4.08613300	1.80176500	-0.55467000
C	-3.46471100	2.73188800	0.49022300
C	-3.41018100	1.95537600	-1.91838700
C	-5.56734200	2.16980300	-0.73431800
H	-3.89069000	2.54036800	1.47893600
H	-2.37929900	2.63648600	0.53838500
H	-3.69525900	3.76468000	0.21422500
H	-3.79884500	1.22654700	-2.63449700

H	-3.64562300	2.95747400	-2.28388800
H	-2.32727000	1.86554200	-1.88169300
H	-5.61261200	3.13455600	-1.24237800
H	-6.09034200	1.43185600	-1.34812500
H	-6.08807000	2.28663600	0.21797000
C	-3.06069900	-3.16643900	0.41436700
C	-1.83060400	-3.43994300	-0.44059600
C	-2.72433200	-3.39399300	1.89015400
C	-4.19319500	-4.08905800	-0.05569900
H	-2.05017200	-3.34735600	-1.50614200
H	-0.99613100	-2.79922200	-0.15862700
H	-1.55998100	-4.48302400	-0.24876600
H	-3.60075400	-3.25545600	2.52991300
H	-2.37821400	-4.42376400	2.01452900
H	-1.92914600	-2.70349300	2.17771500
H	-3.81404600	-5.11352300	-0.06049400
H	-5.06789900	-4.06846700	0.59749300
H	-4.50348900	-3.83245900	-1.07248700
C	-1.79762500	-0.38788700	-0.91577700
C	-0.81956200	0.43832000	-0.11223400
H	-1.33503400	0.89935600	0.73095500
C	-1.60013500	-0.84623800	-2.15217400
H	-2.38123700	-1.39027600	-2.67397300
H	-0.65979400	-0.67947700	-2.66050600
C	-0.12801300	1.50897700	-0.90634200
O	0.34659000	1.37455600	-2.01763300
O	-0.02534700	2.65152300	-0.21229200
C	0.81521200	3.66517100	-0.78867700
C	0.87632300	4.80834500	0.19851900
H	0.39559700	3.96926400	-1.75212600
H	1.80337700	3.22774300	-0.96655600
H	1.50784600	5.60633800	-0.19835700
H	-0.12172400	5.21427200	0.38150500
H	1.29863800	4.46511200	1.14634800
C	1.16768400	0.47638700	1.44511800
C	2.35093500	0.65541800	0.72270300
C	3.31947700	1.57100300	1.10974400
C	3.07505200	2.30691500	2.27762300
C	1.91289100	2.11872500	3.02273100
C	0.94632100	1.19546300	2.60062100
C	0.26260500	-0.52414400	0.72205500
C	1.24438600	-1.01995000	-0.39611900
H	4.23819600	1.70002800	0.54570400
H	3.81551700	3.02730600	2.61152600

H	1.75802900	2.69136900	3.93165100
H	0.02929700	1.04147300	3.16396900
O	-0.37951900	-1.42160400	1.42012400
O	1.08103000	-1.93866000	-1.18263000
N	2.36588400	-0.21520400	-0.37820700
C	3.39401300	-0.23820500	-1.39387800
H	3.55279400	0.78153300	-1.76487500
H	2.98764800	-0.83663500	-2.21535400
C	4.69925700	-0.83096700	-0.90639900
C	5.91072500	-0.17857900	-1.13060000
C	4.69783600	-2.05864700	-0.23940500
C	7.10938500	-0.74589400	-0.69961200
H	5.91638000	0.77974900	-1.64445700
C	5.89189100	-2.62572100	0.19341500
H	3.75143000	-2.56539900	-0.06592600
C	7.10186500	-1.96979500	-0.03664600
H	8.04683500	-0.22863200	-0.87773800
H	5.88096800	-3.58004000	0.71056900
H	8.03336400	-2.41120000	0.30298300

TS^{W}_{II-III}

Total energy= -1783.756090

Zero-point correction= 0.685536 (Hartree/Particle)

Thermal correction to Energy= 0.724430

Thermal correction to Enthalpy= 0.725374

Thermal correction to Gibbs Free Energy= 0.615422

Sum of electronic and zero-point Energies= -1783.070554

Sum of electronic and thermal Energies= -1783.031660

Sum of electronic and thermal Enthalpies= -1783.030715

Sum of electronic and thermal Free Energies= -1783.140668

C	3.01249100	0.17052500	0.26958200
C	4.71353600	-0.25891800	1.61932800
C	5.05006300	-0.69211400	0.38855500
H	5.27311300	-0.29304800	2.53764200
H	5.95603900	-1.16646700	0.05833100
N	4.00364600	-0.40032800	-0.45860500
N	3.45422200	0.29851000	1.53705400
C	4.08379800	-0.78235300	-1.92168200
C	3.67405600	-2.24779200	-2.07725100
C	3.22922000	0.11611300	-2.81768500
C	5.54688400	-0.60298100	-2.35801300
H	4.21863200	-2.87944200	-1.37053100
H	2.60399600	-2.37007000	-1.90878600
H	3.91681500	-2.56796700	-3.09458900

H	3.45720600	1.17266900	-2.65578800
H	3.48152200	-0.13399100	-3.85107000
H	2.16110500	-0.04681400	-2.68910400
H	5.59301100	-0.71682300	-3.44252600
H	5.91749900	0.39259000	-2.09935400
H	6.21050900	-1.35716200	-1.93105000
C	2.84654200	0.90027600	2.78042900
C	1.52246600	1.59462700	2.50887000
C	2.63171400	-0.24376600	3.77405200
C	3.84658900	1.92944100	3.32048300
H	1.63524100	2.43666600	1.82312900
H	0.77098900	0.91218400	2.11801200
H	1.16803700	1.98397000	3.46763600
H	3.56666800	-0.75713300	4.01296500
H	2.22293300	0.16540000	4.70140300
H	1.92062000	-0.96049800	3.35955000
H	3.40184700	2.41562400	4.19200800
H	4.79036600	1.48118400	3.63806700
H	4.05321000	2.69322800	2.56585800
C	1.65416700	0.44589000	-0.30969000
C	0.84504600	-0.78965700	-0.56041400
H	1.67894500	-1.88377200	-0.07144500
C	1.44183000	1.70721800	-0.72643400
H	2.18648900	2.48086500	-0.55833600
C	-1.17580800	-2.17242200	-0.17303800
C	-2.37821600	-1.61815200	-0.62235100
C	-3.34485900	-2.37629000	-1.26561300
C	-3.07435300	-3.73848100	-1.44663600
C	-1.88577700	-4.30756700	-0.99593500
C	-0.92110800	-3.51679600	-0.35647700
C	-0.31379500	-1.07625300	0.42409400
C	-1.30695700	0.10505600	0.44070700
H	-4.27847100	-1.93746800	-1.60318900
H	-3.81225400	-4.36052100	-1.94340300
H	-1.70618000	-5.36731700	-1.14332200
H	0.01418800	-3.94121800	-0.00353400
O	0.13975500	-1.34269900	1.73127100
O	-1.15917800	1.20147500	0.95748800
N	-2.41134900	-0.25592200	-0.29794900
C	-3.47364300	0.65749400	-0.65097200
H	-3.66448700	0.58858200	-1.72790800
H	-3.08323200	1.65800000	-0.44152000
C	-4.74750900	0.40921500	0.13031000
C	-4.68973500	0.22841200	1.51445500

C	-5.98573700	0.37713100	-0.50952000
C	-5.85383100	0.02018300	2.24674600
H	-3.72420000	0.25414700	2.01390700
C	-7.15444800	0.17143800	0.22284600
H	-6.03576400	0.50999100	-1.58753600
C	-7.09040900	-0.00854300	1.60177400
H	-5.79815900	-0.11944600	3.32174100
H	-8.11266900	0.14471400	-0.28637200
H	-7.99882600	-0.17386800	2.17208400
O	2.22915200	-2.54915800	0.73559100
H	2.25216600	-3.45478400	0.40500800
H	0.92118400	-1.94464200	1.59317900
H	0.40721100	-0.72332600	-1.55953100
C	0.22047600	2.15754700	-1.42915100
O	-0.55025900	1.46968200	-2.06761200
O	0.08067300	3.48813700	-1.30772500
C	-1.06298000	4.05792700	-1.96250200
C	-1.00031700	5.55482100	-1.75744800
H	-1.96921500	3.62336600	-1.52901700
H	-1.03566500	3.78604600	-3.02155500
H	-1.85438700	6.03104200	-2.24372300
H	-1.02584100	5.79944700	-0.69323700
H	-0.08333900	5.96335500	-2.18820500

$TS^{W\prime}_{II\text{-}III}$

Total energy= -1783.750824

Zero-point correction= 0.685860 (Hartree/Particle)

Thermal correction to Energy= 0.725060

Thermal correction to Enthalpy= 0.726004

Thermal correction to Gibbs Free Energy= 0.613785

Sum of electronic and zero-point Energies= -1783.064964

Sum of electronic and thermal Energies= -1783.025764

Sum of electronic and thermal Enthalpies= -1783.024820

Sum of electronic and thermal Free Energies= -1783.137039

C	-2.96338800	-0.82131100	-0.21495300
C	-3.95041300	-2.34895400	1.04840600
C	-4.67138900	-1.21419100	1.14190500
H	-4.11688700	-3.30514800	1.51267400
H	-5.56531300	-1.02615200	1.70627400
N	-4.08065800	-0.27580700	0.32851500
N	-2.90766200	-2.11624000	0.17884900
C	-4.68972600	1.09605100	0.13814100
C	-3.93868400	2.12884800	0.97806900
C	-4.70058800	1.46872000	-1.34710700

C	-6.14622800	1.04001500	0.61847000
H	-3.82614900	1.77394600	2.00419700
H	-2.95545400	2.33908600	0.56134400
H	-4.51792400	3.05704600	0.97523500
H	-5.12421000	0.65608300	-1.94536200
H	-5.33932400	2.34826800	-1.46589500
H	-3.70709200	1.72394800	-1.70688100
H	-6.60874600	1.99597700	0.36702000
H	-6.71054100	0.24816100	0.11813100
H	-6.22563300	0.91881800	1.70157700
C	-2.07678400	-3.31217300	-0.24450200
C	-1.07499800	-3.00881100	-1.34866400
C	-1.34345100	-3.83896900	0.99184800
C	-3.06517400	-4.36057700	-0.77887600
H	-1.57390000	-2.73252100	-2.27969000
H	-0.37335900	-2.22949000	-1.06914500
H	-0.52243000	-3.93617300	-1.52671800
H	-2.02983200	-4.04851600	1.81615600
H	-0.84685600	-4.77594600	0.72567300
H	-0.59030200	-3.12114800	1.31839100
H	-2.49160700	-5.20053400	-1.17799600
H	-3.73214400	-4.75202400	-0.00831100
H	-3.66816600	-3.93870100	-1.58783900
C	-1.93370500	-0.06218600	-0.99774600
C	-0.97587700	0.84625200	-0.23463400
H	-1.49625000	0.80721900	0.99594700
C	-1.98336400	-0.14180800	-2.32764000
H	-2.74145100	-0.72959300	-2.83827800
H	-1.26819200	0.39551000	-2.94240700
C	-0.83368900	2.15710800	-0.90393700
O	-1.72887600	2.83366700	-1.38794000
O	0.44293000	2.59206000	-0.92617500
C	0.67629600	3.92677600	-1.38588000
C	2.14281100	4.21512100	-1.14697100
H	0.02845200	4.61256200	-0.83178800
H	0.40824700	3.99531400	-2.44468200
H	2.38588000	5.22962500	-1.47112100
H	2.38049500	4.11392500	-0.08438800
H	2.76599700	3.51118700	-1.70541400
C	1.24383200	1.05579600	1.10159700
C	2.54963400	1.03792600	0.60188600
C	3.60475700	1.66974900	1.23864800
C	3.31778600	2.36729700	2.41874200
C	2.02220100	2.41548800	2.92252800

C	0.97623000	1.75120700	2.26442500
C	0.35791900	0.19516700	0.19935500
C	1.33909400	-0.13016100	-0.95637900
H	4.61277000	1.62955700	0.83789600
H	4.12046900	2.87708800	2.94196600
H	1.81734400	2.96723000	3.83400300
H	-0.03262500	1.79711700	2.65659200
O	0.07745400	-1.02989400	0.84938100
O	1.09094900	-0.72922700	-1.98789000
N	2.58249400	0.33931600	-0.61329800
C	3.77739000	0.09273700	-1.38403300
H	4.27874100	1.04307300	-1.60237000
H	3.44105900	-0.33330000	-2.33418700
C	4.73662000	-0.85364100	-0.68648700
C	4.26797200	-1.83249300	0.19170300
C	6.10562700	-0.76730700	-0.94381800
C	5.15706200	-2.71822000	0.79562000
H	3.20495000	-1.89174000	0.41240500
C	6.99488600	-1.65493800	-0.34304400
H	6.47701100	0.00036900	-1.61812900
C	6.52195100	-2.63395100	0.52827700
H	4.78245200	-3.47327400	1.47949400
H	8.05748400	-1.57709200	-0.55019900
H	7.21407900	-3.32372200	1.00037900
O	-1.81223500	0.11802400	2.07095600
H	-1.66424400	0.61108800	2.88508800
H	-0.63542500	-0.75247600	1.52552800

$TS^{S}_{II\text{-}III}$

Total energy= -1956.209144

Zero-point correction= 0.780448 (Hartree/Particle)

Thermal correction to Energy= 0.824448

Thermal correction to Enthalpy= 0.825393

Thermal correction to Gibbs Free Energy= 0.704820

Sum of electronic and zero-point Energies= -1955.428696

Sum of electronic and thermal Energies= -1955.384695

Sum of electronic and thermal Enthalpies= -1955.383751

Sum of electronic and thermal Free Energies= -1955.504323

C	0.78646000	1.55183100	0.49243900
C	0.04132400	3.59192100	0.06317700
C	-0.51989300	3.18431100	1.22124600
H	-0.07518500	4.52239400	-0.46486500
H	-1.20186800	3.70469800	1.86982700
N	-0.04247300	1.92133300	1.49846400

N	0.86702700	2.58111000	-0.38201600
C	-0.18938400	1.37350500	2.91268200
C	0.11608600	-0.11648500	3.05112300
C	0.79598700	2.17230700	3.77175400
C	-1.63183900	1.62424300	3.36056400
H	-0.46493700	-0.71716200	2.35731800
H	1.17315900	-0.33555700	2.91278200
H	-0.15719700	-0.39742600	4.07090000
H	0.57407300	3.24226900	3.74475400
H	0.72254400	1.82981400	4.80710300
H	1.82081600	2.01147100	3.42502000
H	-1.78066000	1.14071200	4.32784900
H	-1.85890600	2.68351800	3.49463000
H	-2.33878500	1.20079200	2.64466700
C	1.81593500	2.86366700	-1.53027600
C	2.79420900	3.93000300	-1.02550100
C	2.59008800	1.62278100	-1.95373000
C	1.00245100	3.38900800	-2.71570800
H	2.28390100	4.86571100	-0.78441500
H	3.32568400	3.57814200	-0.13717900
H	3.52616700	4.13358000	-1.81106900
H	1.90467200	0.80071100	-2.16597400
H	3.12930400	1.87183700	-2.87154200
H	3.31408400	1.32361500	-1.19551400
H	1.70070800	3.63542000	-3.51918800
H	0.31229300	2.62478800	-3.07621200
H	0.45064000	4.30015300	-2.47590100
C	1.39418900	0.18145800	0.42266000
C	2.67664100	0.10401700	0.95489000
H	3.17723500	1.00762100	1.28155300
C	0.59656800	-0.86593700	-0.07624300
H	0.84066900	-1.85541200	0.30802000
H	1.57557800	-1.44080600	-1.39197700
C	3.36428600	-1.14090600	1.15680600
O	2.92389800	-2.26380100	0.90873500
O	4.60657400	-0.96969700	1.66434700
C	5.36438000	-2.16978200	1.86701000
C	6.71875800	-1.76103600	2.40303200
H	5.44565300	-2.70351900	0.91557400
H	4.82917400	-2.81802300	2.56802100
H	7.33413700	-2.64777400	2.57090400
H	7.23403800	-1.11079900	1.69223600
H	6.61414400	-1.22794700	3.35086700
C	-2.04609500	1.24476900	-1.27165100

C	-2.60508500	0.65439800	-0.12486900
C	-3.75726600	1.21008100	0.45011300
C	-4.26993600	2.36906100	-0.11901800
C	-3.69130200	2.97845700	-1.24612700
C	-2.57839900	2.40440400	-1.83907200
C	-0.94426400	0.40231300	-1.69583200
C	-0.79389500	-0.74461900	-0.65301700
H	-4.24406900	0.74588900	1.30154600
H	-5.15733500	2.81372600	0.32095400
H	-4.12821100	3.88230800	-1.65393700
H	-2.12465000	2.83184400	-2.72832200
O	-0.24925200	0.46809800	-2.69202600
O	-1.07816800	-1.91444000	-1.40617300
N	-1.88977000	-0.44470500	0.29619600
C	-2.47376200	-1.45981300	1.15415800
H	-2.60900300	-1.05175600	2.16416300
H	-1.72812200	-2.25812600	1.26500000
C	-3.80213700	-2.03615200	0.69052900
C	-4.14584500	-2.13444700	-0.65893300
C	-4.70446000	-2.48807900	1.65628400
C	-5.36964000	-2.68578800	-1.03266400
H	-3.45144900	-1.78241500	-1.41520800
C	-5.92448800	-3.04519700	1.28300700
H	-4.45021300	-2.39996600	2.70986100
C	-6.26070000	-3.14462500	-0.06527500
H	-5.62767000	-2.75444900	-2.08479800
H	-6.61513600	-3.39297400	2.04459600
H	-7.21391900	-3.57128200	-0.36044000
C	3.58032100	-1.70907200	-2.01027500
O	4.38733900	-2.49058800	-1.61577100
H	3.78308600	-0.67782800	-2.32884600
N	2.15602000	-2.06075700	-2.13139000
C	1.89840000	-3.47982900	-1.76769800
H	0.82983900	-3.65004500	-1.88665200
H	2.46424100	-4.12495700	-2.43907400
H	2.21452300	-3.62595600	-0.73673900
C	1.63784300	-1.73383400	-3.49661200
H	1.91682600	-0.71391000	-3.75870400
H	2.06155000	-2.44338100	-4.20738000
H	0.55285700	-1.80595900	-3.45412400
H	-1.03622900	-2.68063800	-0.81559200

$TS^{S'}_{II\text{-}III}$

Total energy= -1956.214467

Zero-point correction= 0.780373 (Hartree/Particle)
Thermal correction to Energy= 0.822755
Thermal correction to Enthalpy= 0.823699
Thermal correction to Gibbs Free Energy= 0.709883
Sum of electronic and zero-point Energies= -1955.434093
Sum of electronic and thermal Energies= -1955.391712
Sum of electronic and thermal Enthalpies= -1955.390768
Sum of electronic and thermal Free Energies= -1955.504584

C	-2.07093800	-0.45848400	0.76409300
C	-3.02545000	-2.41267600	0.35137900
C	-2.20234500	-2.57259400	1.40933900
H	-3.65644800	-3.13495100	-0.13622200
H	-2.00844600	-3.45405600	1.99460700
N	-1.62489100	-1.35171100	1.68052400
N	-2.95769100	-1.09341500	-0.04300500
C	-0.99381400	-1.13091500	3.04786000
C	-0.18673500	0.15664100	3.15765700
C	-2.16014300	-1.08900800	4.04034000
C	-0.05954800	-2.30536400	3.34058300
H	0.62791900	0.17332700	2.43334200
H	-0.79919000	1.05092700	3.05604200
H	0.25427100	0.16684200	4.15745500
H	-2.73303800	-2.01949600	4.02618300
H	-1.76474500	-0.94241400	5.04842400
H	-2.82944200	-0.25649500	3.80502700
H	0.41022500	-2.12985200	4.31042000
H	-0.57371900	-3.26588500	3.40075500
H	0.72370700	-2.36758700	2.58315700
C	-3.95980700	-0.61098500	-1.08667900
C	-5.34398600	-0.79154500	-0.45133500
C	-3.79077600	0.84918800	-1.50216300
C	-3.81435000	-1.48735000	-2.33482400
H	-5.57164300	-1.84157600	-0.25365600
H	-5.41362500	-0.23258200	0.48583500
H	-6.09686200	-0.40539300	-1.14265900
H	-2.75851600	1.07713200	-1.76672900
H	-4.40979400	0.98999700	-2.39232300
H	-4.14021400	1.54168000	-0.73738300
H	-4.63436800	-1.24103900	-3.01341200
H	-2.87070700	-1.27306500	-2.83888000
H	-3.88052600	-2.55511100	-2.11781500
C	-1.64577700	0.96689600	0.67378000
C	-2.54127000	1.84802000	1.14071400
H	-3.48525200	1.49840400	1.54992300

C	-0.28139000	1.34966300	0.12276000
H	-0.52557600	2.21895500	-0.76534300
C	-0.13775800	-1.97426300	-1.29284000
C	0.77966500	-2.07092300	-0.23817300
C	1.20400200	-3.33562900	0.19277100
C	0.65950200	-4.45206800	-0.42967700
C	-0.27053600	-4.35382800	-1.47765800
C	-0.66162900	-3.10360500	-1.92719100
C	-0.31912300	-0.56233000	-1.57530700
C	0.56832400	0.25537000	-0.57650600
H	1.95292300	-3.45584900	0.96725900
H	0.98008000	-5.43544600	-0.10017000
H	-0.66118300	-5.25314500	-1.93888300
H	-1.34943100	-2.99126800	-2.75886400
O	-0.97805400	-0.03437400	-2.44891900
O	1.53009600	0.96769100	-1.32073400
N	1.18243900	-0.82734000	0.23798900
C	2.51762500	-0.71447300	0.81519900
H	2.59326400	-1.45489300	1.62076400
H	2.60053600	0.26051900	1.28857100
C	3.69707000	-0.89501600	-0.13206700
C	3.60217100	-1.44838800	-1.41228100
C	4.95588400	-0.49297300	0.32728700
C	4.73564900	-1.57703500	-2.21706900
H	2.64919600	-1.80066600	-1.79778000
C	6.08682900	-0.62747900	-0.46978600
H	5.04802400	-0.06716100	1.32313800
C	5.98001800	-1.16829300	-1.75078200
H	4.63770200	-2.00395100	-3.20994900
H	7.05178400	-0.30266500	-0.09397400
H	6.85975400	-1.26794800	-2.37782500
C	-1.90267100	3.92700400	-1.23726300
O	-1.99092100	4.83629300	-0.44908000
H	-2.76935200	3.48606200	-1.75580100
N	-0.69061800	3.27543100	-1.55724800
C	0.51261500	4.07460700	-1.22944700
H	1.36822700	3.39655000	-1.21952700
H	0.65620800	4.84872900	-1.98690400
H	0.37414500	4.53617900	-0.25432500
C	-0.64416800	2.80486000	-2.96268900
H	-1.56422200	2.27633700	-3.20843000
H	-0.51192200	3.65996400	-3.63098100
H	0.19082500	2.11315600	-3.05550600
H	2.10977900	0.34814000	-1.78861400

H	-2.35303600	2.91255100	1.15528000
C	0.42326800	2.27576800	1.08086400
O	-0.15238800	3.13738700	1.71729900
O	1.75642000	2.16700300	1.10890700
C	2.45250900	3.15498100	1.89414200
C	3.90981700	2.75387300	1.92897400
H	2.01038300	3.19021800	2.89248300
H	2.30657500	4.13211100	1.42293700
H	4.49330600	3.53240000	2.42498500
H	4.04164600	1.82310400	2.48702400
H	4.29849000	2.61659300	0.91670600

III

Total energy= -1707.378847

Zero-point correction= 0.663150 (Hartree/Particle)

Thermal correction to Energy= 0.701397

Thermal correction to Enthalpy= 0.702341

Thermal correction to Gibbs Free Energy= 0.590588

Sum of electronic and zero-point Energies= -1706.715697

Sum of electronic and thermal Energies= -1706.677450

Sum of electronic and thermal Enthalpies= -1706.676506

Sum of electronic and thermal Free Energies= -1706.788259

C	2.13316800	-1.26756000	-0.26071700
C	2.41351600	-3.46553900	-0.27192700
C	2.64905400	-3.01710800	-1.52070400
H	2.44122200	-4.46943700	0.11458700
H	2.91215300	-3.56474800	-2.40880100
N	2.49827200	-1.64478400	-1.50528400
N	2.11515000	-2.37056600	0.51529100
C	2.64346300	-0.87858000	-2.79705100
C	1.48959800	-1.32328400	-3.70100700
C	2.61703800	0.63663500	-2.61677300
C	4.00109900	-1.25644100	-3.40120900
H	1.57293600	-2.37992400	-3.97028200
H	0.53746200	-1.17166100	-3.18704000
H	1.50382100	-0.73615900	-4.62307100
H	3.41233700	0.97310900	-1.95038200
H	2.77160700	1.07484500	-3.60593900
H	1.66659700	0.99091200	-2.22077000
H	4.13939500	-0.68979000	-4.32501300
H	4.81008200	-0.99985800	-2.71199200
H	4.07386300	-2.31603300	-3.65349800
C	1.80294500	-2.58714100	1.97754800
C	2.99533600	-3.33831300	2.58102200

C	1.60375500	-1.29182200	2.75754000
C	0.52097400	-3.42190600	2.03379700
H	3.15442000	-4.31760400	2.12497900
H	3.90986600	-2.74781900	2.47633700
H	2.80465400	-3.49684300	3.64496800
H	0.72503600	-0.74921300	2.41331300
H	1.44772200	-1.57892100	3.80098600
H	2.48097300	-0.64611200	2.69649500
H	0.26020300	-3.60003500	3.08053100
H	-0.29328800	-2.87178600	1.55711000
H	0.64611000	-4.39344300	1.54773800
C	1.87183500	0.13341200	0.18736600
C	3.07028700	0.77962100	0.62023600
H	3.99731800	0.21999300	0.58978000
C	0.61208700	0.65261600	0.12223800
H	0.49167800	1.67908100	0.44936900
C	3.12415500	2.11668600	1.05477200
O	2.19898400	2.93608200	1.15480800
O	4.41116700	2.49997300	1.39552200
C	4.55608300	3.84799200	1.82135300
C	6.01960000	4.06416400	2.14930600
H	3.92108400	4.03667400	2.69442900
H	4.22191200	4.52853200	1.02960400
H	6.18707800	5.09241800	2.47903300
H	6.33846500	3.38843400	2.94702900
H	6.64159400	3.87607700	1.27040700
C	-1.43941900	0.90129800	-1.28609000
C	-2.55492200	1.40713500	-0.61109400
C	-3.44188000	2.29115600	-1.20511300
C	-3.18508900	2.66546200	-2.52826000
C	-2.08479900	2.16568400	-3.21929600
C	-1.19883800	1.27913600	-2.59466700
C	-0.65993000	-0.00704800	-0.34287500
C	-1.64042400	-0.07377600	0.87236900
H	-4.30933700	2.66829900	-0.67408500
H	-3.86308500	3.35381600	-3.02228400
H	-1.91165900	2.46430200	-4.24744000
H	-0.34074100	0.89142300	-3.13467300
O	-0.40596500	-1.29787000	-0.84895300
O	-1.56596600	-0.82458600	1.82892200
N	-2.61619200	0.86946900	0.68748800
C	-3.71366300	1.07893200	1.61524700
H	-3.88245200	2.15448600	1.72672400
H	-3.37117300	0.68683000	2.57666900

C	-4.98378500	0.38070300	1.17576100
C	-4.96316800	-0.99373400	0.92107500
C	-6.17631500	1.08580700	1.02444800
C	-6.12079800	-1.65044600	0.51813900
H	-4.03422900	-1.54449800	1.04899500
C	-7.33901900	0.42813300	0.62326700
H	-6.19669400	2.15499300	1.22121200
C	-7.31205800	-0.93972100	0.36790600
H	-6.09700000	-2.71791400	0.32345300
H	-8.26235900	0.98634700	0.50621900
H	-8.21505100	-1.45280900	0.05304200
H	-1.23820300	-1.67650000	-1.16221100

III′

Total energy= -1707.378862

Zero-point correction= 0.664239 (Hartree/Particle)

Thermal correction to Energy= 0.701746

Thermal correction to Enthalpy= 0.702690

Thermal correction to Gibbs Free Energy= 0.595497

Sum of electronic and zero-point Energies= -1706.714623

Sum of electronic and thermal Energies= -1706.677116

Sum of electronic and thermal Enthalpies= -1706.676172

Sum of electronic and thermal Free Energies= -1706.783364

C	-2.95789100	-0.47002300	0.06389900
C	-3.54105800	-2.49768200	0.74324900
C	-3.76996600	-1.64469100	1.76079000
H	-3.69223800	-3.56180300	0.69200100
H	-4.15258800	-1.83881200	2.74733600
N	-3.43035800	-0.37798200	1.32624300
N	-3.05802600	-1.75957900	-0.31987600
C	-3.47656700	0.77220800	2.29954900
C	-2.33839300	0.54791900	3.29909500
C	-3.33475400	2.13635500	1.62938800
C	-4.83858100	0.73453900	3.00297100
H	-2.47433100	-0.38874900	3.84724400
H	-1.38172800	0.50765800	2.77459000
H	-2.32051800	1.36847500	4.02129900
H	-4.16386800	2.33447800	0.94891900
H	-3.34649700	2.88315900	2.42800600
H	-2.40338200	2.23177200	1.07214800
H	-4.91623400	1.61346700	3.64714900
H	-5.65036400	0.76870500	2.27155800
H	-4.96731900	-0.14443000	3.63764400
C	-2.65890200	-2.47849700	-1.58659600

C	-2.29025500	-1.54142300	-2.73275400
C	-1.45318100	-3.35219700	-1.22963200
C	-3.85843500	-3.32826500	-2.02300900
H	-3.13219600	-0.91336600	-3.02509100
H	-1.43182100	-0.91815500	-2.48351400
H	-2.01812200	-2.18043600	-3.57747700
H	-1.70017300	-4.07679100	-0.44848700
H	-1.13838200	-3.90499500	-2.11882900
H	-0.62971200	-2.71814300	-0.89524800
H	-3.60995900	-3.81738000	-2.96779100
H	-4.10976100	-4.11170900	-1.30494000
H	-4.73732300	-2.69694300	-2.18088100
C	-2.51526500	0.66874500	-0.79691400
C	-1.11711600	1.04002300	-0.85437900
C	-3.56563000	1.21758700	-1.46093900
H	-4.55891000	0.80242100	-1.32137900
H	-3.43748400	2.05322700	-2.13113900
C	-0.71273300	2.00655900	-1.80926300
O	-1.39972600	2.69991000	-2.56857200
O	0.66388200	2.12254000	-1.85295800
C	1.21569500	3.02707300	-2.79716600
C	2.71145600	2.78182100	-2.80333600
H	0.97800000	4.05777100	-2.50841500
H	0.77335600	2.85330500	-3.78298400
H	3.21412900	3.47489200	-3.48214000
H	3.12200300	2.91351100	-1.79722300
H	2.92209900	1.75883300	-3.12899000
C	0.86700100	1.30628900	0.79391300
C	2.21647800	1.04502300	0.52756800
C	3.24442400	1.70285000	1.18582500
C	2.88708100	2.65972900	2.14279800
C	1.55189100	2.94169700	2.41418900
C	0.53176700	2.26397600	1.73185900
C	-0.00088200	0.38709200	-0.06436100
C	1.09638900	-0.27967800	-0.96549600
H	4.28533300	1.48421700	0.97024300
H	3.66904400	3.19101800	2.67580200
H	1.29816500	3.69342200	3.15397600
H	-0.50820500	2.50022000	1.93300800
O	-0.53217400	-0.66763400	0.74131000
O	0.91093400	-1.07044000	-1.87128300
N	2.33045500	0.08650000	-0.48790500
C	3.58477700	-0.37128300	-1.04452400
H	4.18599500	0.49500000	-1.34602500

H	3.32420400	-0.93152000	-1.94771900
C	4.36515700	-1.24091800	-0.08032600
C	5.72922600	-1.03379700	0.12060500
C	3.72268400	-2.27266000	0.60873200
C	6.44601400	-1.84777000	0.99665100
H	6.23284300	-0.22777100	-0.40737700
C	4.43515700	-3.08443700	1.48537000
H	2.65846900	-2.43601300	0.45454700
C	5.80011700	-2.87342300	1.68140100
H	7.50662200	-1.67454700	1.14848500
H	3.92679700	-3.88329500	2.01586000
H	6.35621500	-3.50488500	2.36674000
H	0.13578600	-0.90982600	1.39691900

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