Supporting Information

Co^{III}-Carbene Radical Approach to Substituted *1*H-Indenes

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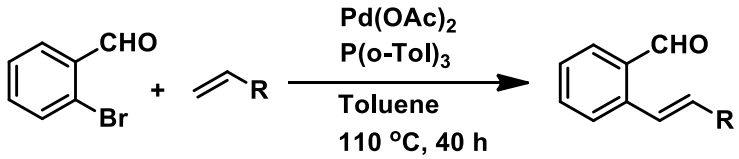
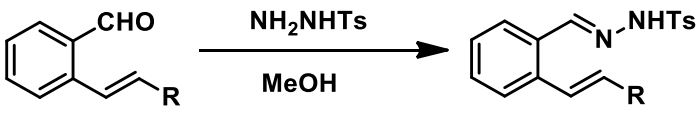
EXPERIMENTAL SECTION

General Considerations: All manipulations were performed under a nitrogen atmosphere using standard Schlenk techniques. All solvents used for catalysis were dried over and distilled from sodium (toluene) or CaH_2 (dichloromethane, hexane, ethyl acetate, methanol). The catalyst [Co^{II}(MeTAA)] has been synthesized according to literature procedures.[1] All chemicals were purchased from commercial suppliers (either from Sigma-Aldrich or Fluorochem) and used without further purification. NMR spectra (^1H and ^{13}C) were measured on a Bruker AV400 (100 MHz for ^{13}C). Unless noted otherwise, the NMR spectra were measured in $CDCl_3$. Individual peaks are reported as: multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), integration, coupling constant in Hz. Mass spectra of the newly synthesized compounds were recorded on an Agilent-5973 GC-MS spectrometer, and the corresponding HRMS data were recorded on a JEOL AccuTOF 4G via direct injection probe using CSI (Cold Spray Ionization). EPR spectra were recorded on a Bruker EMXplus spectrometer at room temperature (298 K).

General Procedure for the synthesis of the aldehyde precursors:[2] The *o*-bromobenzaldehyde (1.0 equiv.) was dissolved in toluene (2 mL/mmol aldehyde). $Pd(OAc)_2$ (0.02 equiv.), $P(o\text{-}tol)_3$ (0.04 equiv.), the required Heck acceptor (1.5 equiv.) and Et_3N (0.4 mL/mmol aldehyde) were added, and the reaction mixture was placed under an N_2 atmosphere and heated to reflux (115°C, oil bath) for 40 h. The reaction was then cooled to RT, diluted with H_2O and extracted with CH_2Cl_2. The organic phase was dried ($MgSO_4$), filtered and concentrated, and the crude material was purified by flash chromatography.



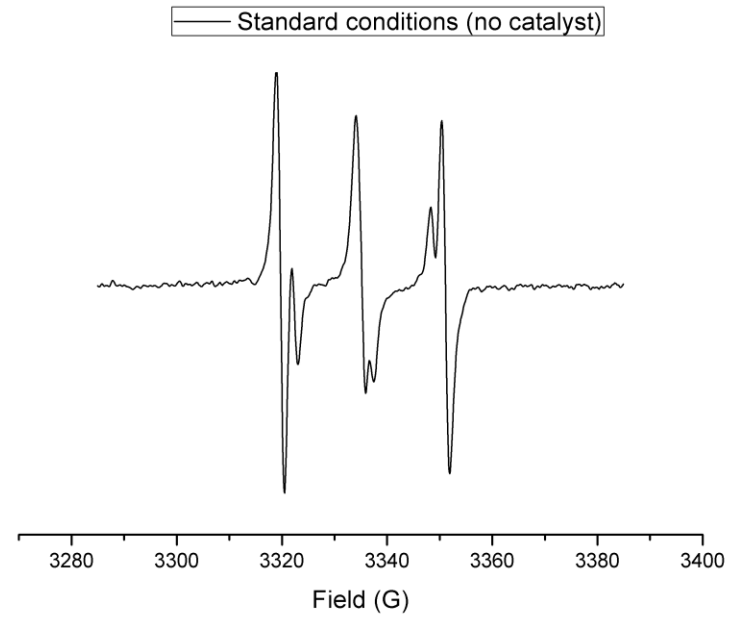
General Procedure for Synthesis of the N-tosylhydrazone substrates:[3] An equimolar mixture of corresponding aldehyde and N-tosyl hydrazide were placed in a round bottom flask and dissolved in methanol (2 mL/mmol). The reaction mixture was stirred overnight at room temperature. The white precipitate was collected by filtration, and washed with methanol and hexane to obtain the pure product.

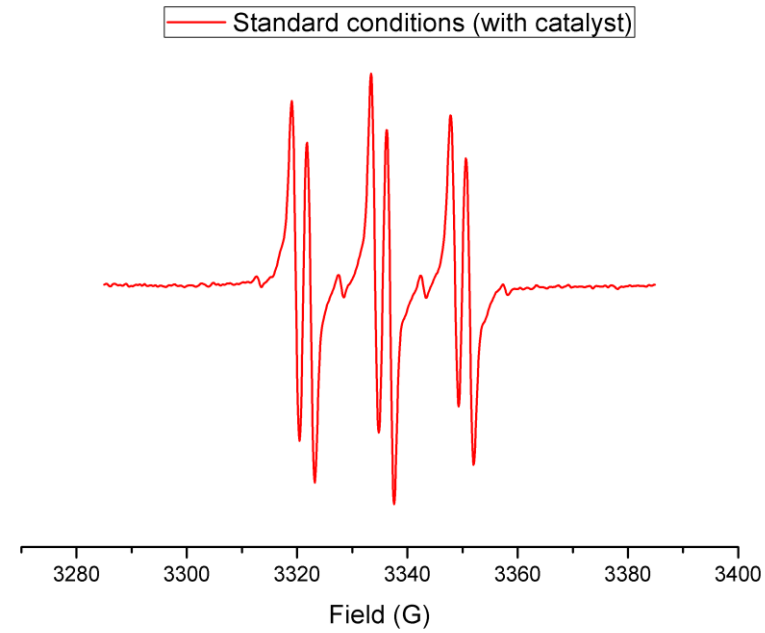


General Procedure for Synthesis of 1*H*-Indenes: Under a nitrogen atmosphere, the respective cinnamyl N-tosylhydrazone (**1a−r**) (0.2 mmol) was added to a flame-dried Schlenk tube. The tube was capped with a Teflon screw cap, evacuated, and backfilled with nitrogen. Base LiO^tBu (1.2 equiv; 0.22 mmol), [Co^{II}(MeTAA)] catalyst (5 mol%) and benzene (anhydrous and degassed, 3 mL) were added inside the glove box. The Schlenk tube was then placed in an oil bath and heated to the desired temperature under nitrogen for a set

period. After the reaction finished, the resulting mixture was concentrated and the residue was purified by flash chromatography (silica gel).

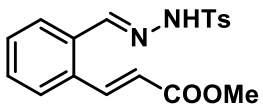
EPR Spectra of Catalytic Reaction Mixtures: X-band EPR spectrum of a carbon radical (probably Co^{III}-carbene radical intermediate) trapped with PBN; *Settings*: microwave frequency: 9.36607 GHz; power: 6.33 mW; modulation amplitude: 1.0G); *Reaction conditions:* N-tosylhydrazone (0.2 mmol, 1.0 equiv), LiOtBu (0.24 mmol, 1.2 equiv), [Co(MeTAA)] (5 mol%), PBN (0.4 mmol, 2.0 equiv), benzene (3 mL), 60 ^{0}C, 30 min.





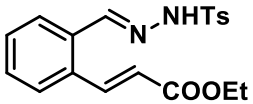
Characterization of N-tosylhydrazone substrates and 1*H*-indene products:

(*E*)-Methyl 3-(2-((*E*)-(2-tosylhydrazono)methyl)phenyl)acrylate (1a):



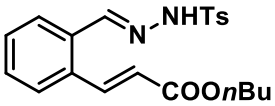
Yield = 82%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.17 (d, *J* = 15.8 Hz, 1H), 8.09 (d, *J* = 8.3 Hz, 2H), 7.77 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.42 (s, 1H), 7.36 (s, 1H), 7.17 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.05 (t, *J* = 8.1 Hz, 1H), 6.96 (t, *J* = 9.5 Hz, 3H), 6.28 (d, *J* = 15.8 Hz, 1H), 3.65 (s, 3H), 1.97 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 167.11, 144.74, 144.07, 141.55, 135.23, 133.56, 131.81, 130.06, 129.87, 129.57, 127.88, 127.17, 126.92, 126.70, 120.91, 51.83, 21.48.

(*E*)-Mthyl 3-(2-((*E*)-(2-tosylhydrazono)methyl)phenyl)acrylate (1b):



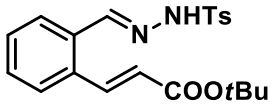
Yield = 85%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.20 (s, 1H), 8.12 (d, *J* = 15.8 Hz, 1H), 7.90 (d, *J* = 8.1 Hz, 2H), 7.83 – 7.57 (m, 2H), 7.49 (dd, *J* = 5.3, 3.6 Hz, 1H), 7.38 – 7.30 (m, 2H), 7.27 (d, *J* = 8.2 Hz, 2H), 6.30 (d, *J* = 15.8 Hz, 1H), 4.27 (q, *J* = 7.0 Hz, 2H), 2.37 (s, 3H), 1.34 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 166.85, 144.99, 143.95, 141.46, 135.33, 133.58, 131.94, 129.97, 129.81, 129.54, 127.88, 127.14, 121.25, 60.82, 21.45, 21.18, 14.15.

(*E*)-Butyl 3-(2-((*E*)-(2-tosylhydrazono)methyl)phenyl)acrylate (1c):



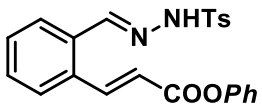
Yield = 86%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.98 (s, 1H), 8.22 (s, 1H), 8.10 (d, *J* = 15.8 Hz, 1H), 7.91 (d, *J* = 8.3 Hz, 2H), 7.80 (dd, *J* = 6.1, 3.1 Hz, 1H), 7.54 – 7.48 (m, 1H), 7.36 (dd, *J* = 5.7, 3.5 Hz, 2H), 7.29 (d, *J* = 8.3 Hz, 2H), 4.22 (t, *J* = 6.7 Hz, 2H), 2.39 (s, 3H), 1.70 (p, *J* = 6.8 Hz, 2H), 1.43 (h, *J* = 7.4 Hz, 2H), 0.96 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 166.90, 144.71, 144.00, 141.19, 135.26, 133.60, 131.89, 130.03, 129.84, 129.56, 127.89, 127.61, 127.12, 121.37, 64.74, 30.57, 21.47, 19.06, 13.63.

(*E*)-tert-Butyl 3-(2-((*E*)-(2-tosylhydrazono)methyl)phenyl)acrylate (1d):



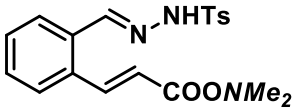
Yield = 81%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.85 (s, 1H), 8.19 (s, 1H), 7.99 (d, *J* = 15.8 Hz, 1H), 7.91 (d, *J* = 8.3 Hz, 2H), 7.79 (dd, *J* = 5.7, 3.5 Hz, 1H), 7.49 (dd, *J* = 5.6, 3.5 Hz, 1H), 7.36 (dd, *J* = 5.9, 3.4 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 6.24 (d, *J* = 15.7 Hz, 1H), 2.39 (s, 3H), 1.55 (s, 9H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 166.03, 144.78, 144.01, 140.15, 135.23, 133.91, 131.70, 130.02, 129.58, 129.55, 127.90, 127.55, 127.19, 123.42, 81.04, 28.05, 21.47.

(*E*)-Phenyl 3-(2-((*E*)-(2-tosylhydrazono)methyl)phenyl)acrylate (1e):



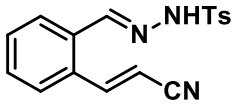
Yield = 89%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.53 (s, 1H), 8.29 (d, *J* = 15.8 Hz, 1H), 8.11 (s, 1H), 7.95 – 7.86 (m, 2H), 7.74 (dd, *J* = 5.8, 3.4 Hz, 1H), 7.59 (dd, *J* = 5.7, 3.4 Hz, 1H), 7.42 (dd, *J* = 10.3, 5.2 Hz, 4H), 7.27 (d, *J* = 7.9 Hz, 3H), 7.20 (d, *J* = 7.7 Hz, 2H), 6.51 (d, *J* = 15.8 Hz, 1H), 2.38 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 165.04, 150.57, 144.86, 144.16, 143.40, 135.10, 133.39, 131.89, 130.15, 129.61, 129.37, 128.29, 127.89, 127.43, 125.81, 121.49, 120.43, 21.47.

(*E*)-N'-(2-((*E*)-3-((Dimethylamino)oxy)-3-oxoprop-1-en-1-yl)benzylidene)-4-methylbenzenesulfonohydrazide (1f):



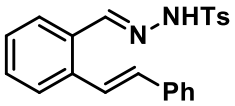
Yield = 76%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 9.33 (s, 1H), 8.27 (s, 1H), 7.88 (d, *J* = 8.4 Hz, 4H), 7.46 (dd, *J* = 5.8, 3.2 Hz, 1H), 7.36 (dd, *J* = 5.4, 3.8 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 6.74 (d, *J* = 15.3 Hz, 1H), 3.17 (s, 3H), 3.09 (s, 3H), 2.39 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 166.27, 144.21, 143.60, 138.70, 135.75, 134.66, 132.11, 129.78, 129.43, 129.25, 127.76, 126.95, 126.63, 121.21, 37.43, 36.06, 21.43.

(*E*)-N'-(2-((*E*)-2-Cyanovinyl)benzylidene)-4-methylbenzenesulfonohydrazide (1g):



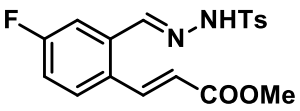
Yield = 80%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.07 (s, 1H), 8.02 – 7.77 (m, 4H), 7.62 – 7.52 (m, 1H), 7.51 – 7.38 (m, 4H), 7.28 (d, *J* = 0.9 Hz, 2H), 5.76 (d, *J* = 16.5 Hz, 1H), 2.46 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 148.86, 145.05, 143.87, 135.66, 132.45, 131.90, 130.39, 129.70, 129.49, 127.75, 126.86, 117.89, 98.53, 21.48.

(*E*)-4-Methyl-N'-(2-((*E*)-styryl)benzylidene)benzenesulfonohydrazide (1h):



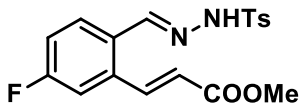
Yield = 92%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.13 (s, 1H), 7.89 – 7.74 (m, 3H), 7.71 (d, *J* = 7.9 Hz, 1H), 7.56 (dd, *J* = 13.0, 7.7 Hz, 4H), 7.44 – 7.29 (m, 5H), 7.24 (d, *J* = 8.4 Hz, 2H), 6.92 (d, *J* = 16.1 Hz, 1H), 2.40 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 146.92, 144.12, 137.26, 136.96, 135.10, 132.61, 130.23, 130.13, 129.55, 128.66, 128.08, 127.98, 127.87, 127.46, 126.90, 126.70, 125.61, 21.47.

(*E*)-Methyl 3-(4-fluoro-2-((*E*)-(2-tosylhydrazono)methyl)phenyl)acrylate (1i):



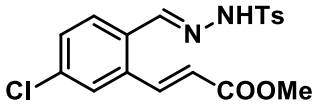
Yield = 79%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.26 (s, 1H), 8.09 (s, 1H), 8.05 (d, *J* = 15.8 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 2H), 7.80 (dd, *J* = 8.8, 5.7 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.24 – 7.17 (m, 1H), 7.10 (td, *J* = 8.3, 2.6 Hz, 1H), 6.32 (d, *J* = 15.8 Hz, 1H), 3.86 (s, 3H), 2.43 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 167.04, 144.32, 142.73, 142.70, 140.00, 135.04, 134.18, 134.10, 129.67, 129.29, 129.20, 127.88, 120.81, 117.69, 117.47, 113.70, 113.47, 51.92, 21.51.

(*E*)-Methyl 3-(5-fluoro-2-((*E*)-(2-tosylhydrazono)methyl)phenyl)acrylate (1j):



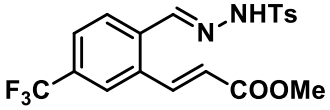
Yield = 80%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.19 (s, 1H), 8.09 (d, *J* = 1.5 Hz, 1H), 7.99 (d, *J* = 15.7 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 2H), 7.53 (dd, *J* = 9.2, 3.8 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.11 (t, *J* = 8.3 Hz, 1H), 6.29 (d, *J* = 15.7 Hz, 1H), 3.84 (s, 3H), 2.44 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 167.04, 144.32, 142.73, 142.70, 140.00, 135.04, 134.18, 134.10, 129.67, 129.29, 129.20, 127.88, 120.81, 117.69, 117.47, 113.70, 113.47, 51.92, 21.51.

(*E*)-Methyl 3-(5-chloro-2-((*E*)-(2-tosylhydrazono)methyl)phenyl)acrylate (1k):



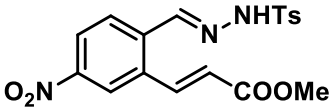
Yield = 86%; **^{1}H NMR (400 MHz, $CDCl_3$):** Yield = 86%;δ 8.18 (s, 1H), 8.06 (s, 1H), 8.00 (d, *J* = 15.8 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 2.3 Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 3H), 6.32 (d, *J* = 15.8 Hz, 1H), 3.85 (s, 3H), 2.44 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 166.90, 144.34, 142.73, 140.04, 136.15, 135.02, 133.26, 131.82, 130.16, 129.68, 128.46, 127.88, 127.20, 121.38, 51.95, 21.52.

(*E*)-Methyl 3-(2-((*E*)-(2-tosylhydrazono)methyl)-5-(trifluoromethyl)phenyl)acrylate (1l):



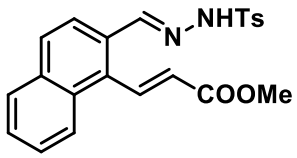
Yield = 84%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.24 (s, 1H), 8.08 (d, *J* = 17.1 Hz, 2H), 8.00 (s, 1H), 7.93 (d, *J* = 8.3 Hz, 2H), 7.63 (d, *J* = 1.2 Hz, 2H), 7.36 (d, *J* = 8.1 Hz, 2H), 6.38 (d, *J* = 15.9 Hz, 1H), 3.87 (s, 3H), 2.44 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 166.53, 144.50, 142.85, 140.05, 136.69, 134.88, 132.32, 131.56, 129.69, 127.94, 124.71, 123.21, 52.03, 21.50.

(*E*)-Methyl 3-(5-nitro-2-((*E*)-(2-tosylhydrazono)methyl)phenyl)acrylate (1m):



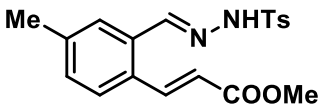
Yield = 82%; **^{1}H NMR (400 MHz, DMSO-d_6):** δ 11.85 (s, 1H), 8.39 (d, *J* = 2.4 Hz, 1H), 8.30 (s, 1H), 8.18 (dd, *J* = 8.6, 2.4 Hz, 1H), 8.07 (d, *J* = 15.9 Hz, 1H), 7.99 (d, *J* = 8.6 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 6.67 (d, *J* = 15.8 Hz, 1H), 3.79 (s, 3H), 2.36 (s, 3H); **^{13}C NMR (100 MHz, DMSO-d_6):** δ 166.22, 148.33, 144.11, 143.51, 139.58, 139.06, 136.24, 133.61, 130.10, 129.98, 127.57, 124.60, 124.23, 122.17, 52.23, 21.36.

(*E*)-Methyl 3-(2-((*E*)-(2-tosylhydrazono)methyl)naphthalen-1-yl)acrylate (1n):



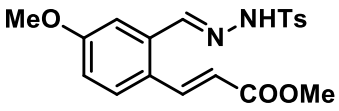
Yield = 78%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.23 (d, *J* = 16.1 Hz, 1H), 8.18 (s, 1H), 8.14 (s, 1H), 8.05 (d, *J* = 8.8 Hz, 1H), 8.00 – 7.95 (m, 1H), 7.93 (d, *J* = 8.3 Hz, 2H), 7.87 – 7.79 (m, 2H), 7.60 – 7.50 (m, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 6.09 (d, *J* = 16.1 Hz, 1H), 3.89 (s, 3H), 2.42 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 166.35, 145.65, 144.09, 140.71, 135.31, 133.74, 133.13, 130.96, 129.58, 129.47, 129.04, 128.91, 128.37, 127.92, 127.84, 127.56, 127.26, 127.00, 124.98, 122.95, 52.02, 21.47.

(*E*)-Methyl 3-(4-methyl-2-((*E*)-(2-tosylhydrazono)methyl)phenyl)acrylate (1o):



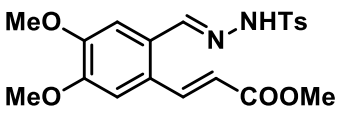
Yield = 93%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.21 (s, 1H), 8.14 – 8.06 (m, 2H), 7.92 (d, *J* = 8.0 Hz, 2H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 3H), 7.21 (d, *J* = 8.1 Hz, 1H), 6.31 (d, *J* = 15.9 Hz, 1H), 3.85 (s, 3H), 2.42 (s, 3H), 2.38 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 167.20, 145.00, 144.01, 141.64, 140.37, 135.24, 133.42, 130.88, 129.54, 129.20, 127.88, 127.82, 127.59, 120.62, 51.82, 21.47, 21.26.

(*E*)-Methyl 3-(4-methoxy-2-((*E*)-(2-tosylhydrazono)methyl)phenyl)acrylate (1p):



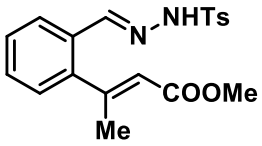
Yield = 89%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.40 (s, 1H), 8.18 (s, 1H), 8.01 (d, *J* = 15.7 Hz, 1H), 7.95 – 7.89 (m, 2H), 7.50 (d, *J* = 8.7 Hz, 1H), 7.36 – 7.30 (m, 3H), 6.94 (dd, *J* = 8.7, 2.7 Hz, 1H), 6.25 (d, 15.7 Hz, 1H), 3.88 (s, 3H), 3.83 (s, 3H), 2.42 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 167.57, 160.87, 144.22, 144.10, 140.51, 135.21, 133.53, 129.56, 128.48, 127.88, 126.18, 118.36, 117.43, 110.57, 55.43, 51.77, 21.47.

(*E*)-Methyl 3-(4,5-dimethoxy-2-((*E*)-(2-tosylhydrazono)methyl)phenyl)acrylate (1q):



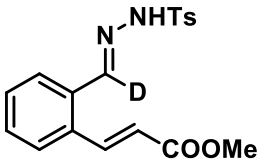
Yield = 88%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.25 (s, 1H), 8.18 (s, 1H), 7.99 (d, *J* = 15.7 Hz, 1H), 7.91 (d, *J* = 8.4 Hz, 2H), 7.40 – 7.30 (m, 3H), 6.96 (s, 1H), 6.26 (d, *J* = 15.5 Hz, 1H), 3.96 (s, 3H), 3.93 (s, 3H), 3.84 (s, 3H), 2.43 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 167.38, 150.82, 150.77, 144.16, 144.08, 140.14, 135.26, 129.53, 127.89, 126.79, 125.88, 118.59, 108.26, 108.11, 56.00, 55.85, 51.83, 21.48.

(*E*)-Methyl 3-(2-((*E*)-(2-tosylhydrazono)methyl)phenyl)but-2-enoate (1r):



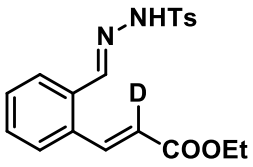
Yield = 86%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.24 (s, 1H), 7.95 – 7.82 (m, 4H), 7.42 – 7.30 (m, 4H), 7.15 (dd, *J* = 7.1, 1.8 Hz, 1H), 5.70 (s, 1H), 4.22 (q, *J* = 7.1 Hz, 2H), 2.43 (s, 3H), 2.40 (s, 3H), 1.32 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 166.29, 155.31, 145.37, 143.98, 143.75, 135.37, 129.88, 129.59, 129.53, 128.01, 127.81, 127.37, 126.44, 121.07, 60.19, 21.54, 21.49, 14.13.

1a-D:



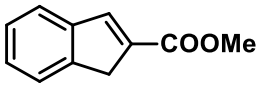
Yield = 83%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.58 (s, 1H), 8.12 (d, *J* = 15.8 Hz, 1H), 7.92 (d, *J* = 8.3 Hz, 2H), 7.85 – 7.75 (m, 1H), 7.57 – 7.46 (m, 1H), 7.43 – 7.34 (m, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 6.33 (d, *J* = 15.8 Hz, 1H), 3.85 (s, 3H), 2.41 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 167.11, 144.15, 141.43, 135.18, 133.57, 131.69, 130.14, 129.92, 129.61, 127.91, 127.76, 127.18, 121.00, 106.18, 106.17, 51.87, 21.50.

1b-D:



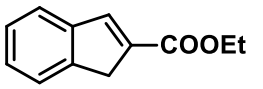
Yield = 88%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.51 (d, *J* = 3.0 Hz, 1H), 8.16 (d, *J* = 2.5 Hz, 1H), 8.10 (s, 1H), 7.92 (d, *J* = 7.9 Hz, 2H), 7.87 – 7.75 (m, 1H), 7.59 – 7.47 (m, 1H), 7.39 (dt, *J* = 5.9, 3.9 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 4.30 (d, *J* = 7.0 Hz, 2H), 2.42 (d, *J* = 3.2 Hz, 3H), 1.36 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 144.69, 144.22, 140.97, 135.11, 133.78, 131.53, 130.19, 129.77, 129.61, 127.92, 127.87, 127.30, 60.74, 21.50, 14.19.

Methyl 1*H*-indene-2-carboxylate (2a):



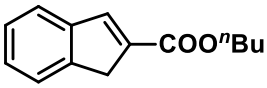
Yield = 86%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.75 (s, 1H), 7.54 (q, *J* = 4.7 Hz, 2H), 7.42 – 7.31 (m, 2H), 3.98 – 3.79 (s, 3H), 3.71 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 165.35, 144.67, 142.59, 141.12, 136.93, 127.47, 126.76, 124.17, 123.29, 51.53, 38.25; **HRMS (EI, m/z):** Calculated for [M^+] $C_{11}H_{10}O_2$: 174.0681; found: 174.0671.

Ethyl 1*H*-indene-2-carboxylate (2b):



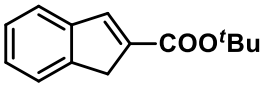
Yield = 78%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.75 (s, 1H), 7.54 (dd, *J* = 7.8, 3.9 Hz, 2H), 7.40 – 7.30 (m, 2H), 4.33 (q, *J* = 7.1 Hz, 2H), 3.72 (s, 2H), 1.39 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 164.96, 144.68, 142.66, 140.85, 137.38, 127.38, 126.73, 124.15, 123.22, 60.31, 38.25, 14.29; **HRMS (EI, m/z):** Calculated for [M^+] $C_{12}H_{12}O_2$: 188.0837, found: 188.0834.

***n*-Butyl 1*H*-indene-2-carboxylate (2c):**



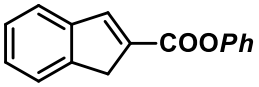
Yield = 80%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.79 – 7.70 (m, 1H), 7.54 (d, *J* = 3.3 Hz, 2H), 7.41 – 7.31 (m, 2H), 4.28 (t, *J* = 6.6 Hz, 2H), 3.71 (s, 2H), 1.75 (dd, *J* = 8.5, 6.4 Hz, 2H), 1.55 – 1.42 (m, 2H), 1.01 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 165.02, 144.68, 142.67, 140.79, 137.41, 127.36, 126.72, 124.14, 123.21, 64.21, 38.25, 30.71, 19.18, 13.68, 0.92; **HRMS (EI, m/z):** Calculated for [M^+] $C_{14}H_{16}O_2$, 216.1150, found: 216.1155.

***tert*-Butyl 1*H*-indene-2-carboxylate (2d):**



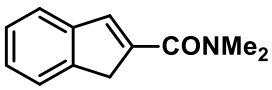
Yield = 76%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.64 (d, *J* = 2.1 Hz, 1H), 7.56 – 7.45 (m, 2H), 7.34 (dd, *J* = 5.6, 3.1 Hz, 2H), 3.66 (d, *J* = 2.0 Hz, 2H), 1.59 (s, 9H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 164.39, 144.64, 142.82, 140.00, 139.23, 127.10, 126.62, 124.08, 123.03, 105.97, 80.36, 38.27, 28.16. **HRMS (EI, m/z):** Calculated for [M^+] $C_{14}H_{16}O_2$: 216.1150, found: 216.1151.

Phenyl 1*H*-indene-2-carboxylate (2e):



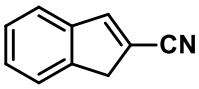
Yield = 82%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.99 (d, *J* = 2.0 Hz, 1H), 7.60 (ddd, *J* = 9.6, 6.0, 2.8 Hz, 2H), 7.50 – 7.37 (m, 4H), 7.30 (d, *J* = 7.7 Hz, 1H), 7.26 – 7.19 (m, 2H), 3.85 (d, *J* = 2.0 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 163.18, 150.70, 144.98, 142.92, 142.43, 136.25, 129.34, 127.91, 126.92, 125.63, 124.28, 123.59, 121.60, 38.39. **HRMS (EI, m/z):** Calculated for [M^+] $C_{16}H_{12}O_2$: 236.0837, found: 236.0832.

N,N-Dimethyl-1*H*-indene-2-carboxamide (2f):



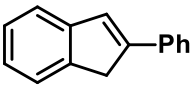
Yield = 98%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.51 (d, *J* = 7.0 Hz, 1H), 7.46 (d, *J* = 7.2 Hz, 1H), 7.37 – 7.27 (m, 2H), 7.04 (s, 1H), 3.78 (s, 2H), 3.15 (d, *J* = 13.5 Hz, 6H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 167.99, 143.16, 143.05, 140.63, 133.42, 126.59, 126.10, 123.82, 122.08, 40.48, 38.99, 35.37. **HRMS (EI, m/z):** Calculated for [M^+] $C_{12}H_{13}NO$: 187.0997, found: 187.1005.

1*H*-Indene-2-carbonitrile (2g):



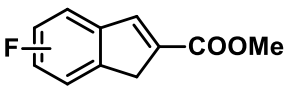
Yield = 52%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.64 (d, *J* = 2.2 Hz, 1H), 7.59 – 7.48 (m, 2H), 7.47 – 7.33 (m, 2H), 3.72 (d, *J* = 2.0 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 146.13, 142.99, 141.29, 128.27, 127.37, 124.00, 123.16, 116.99, 114.09, 40.82; **HRMS (EI, m/z):** Calculated for [M^+] $C_{10}H_7N$: 141.0578, found: 141.0578.

2-Phenyl-1H-indene (2h):



Yield = 85%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.73 – 7.66 (m, 2H), 7.53 (d, *J* = 7.4 Hz, 1H), 7.45 (td, *J* = 7.6, 5.8 Hz, 3H), 7.37 – 7.31 (m, 2H), 7.29 (s, 1H), 7.25 (td, *J* = 7.4, 1.2 Hz, 1H), 3.85 (d, *J* = 1.5 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 146.33, 145.28, 143.07, 135.90, 128.61, 128.58, 127.45, 126.55, 126.51, 126.44, 125.57, 125.49, 124.68, 123.60, 120.91, 38.91; **HRMS (EI, m/z):** Calculated for [M^+] $C_{15}H_{12}$: 192.0939, found: 192.0936.

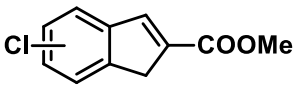
Methyl 6-fluoro-1H-indene-2-carboxylate (2i):



Yield = 87%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.69 (d, *J* = 6.1 Hz, 1H), 7.46 (td, *J* = 8.8, 5.0 Hz, 1H), 7.23 (ddd, *J* = 8.5, 5.9, 2.4 Hz, 1H), 7.12 – 7.00 (m, 1H), 3.87 (d, *J* = 3.4 Hz, 3H), 3.70 (d, *J* = 2.0 Hz, 1H), 3.67 (s, 1H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 165.02, 164.98, 164.14, 163.38, 161.68, 160.96, 146.96, 146.87, 144.21, 144.12, 140.25, 140.23, 140.19, 139.93, 139.91, 139.11, 138.61, 138.58, 136.75, 136.71, 125.08, 124.99, 124.24, 124.15, 114.57, 114.34, 114.28, 114.05, 111.92, 111.69, 110.07, 109.84, 51.65, 51.56, 38.47, 38.44, 37.69; **HRMS (EI, m/z):** Calculated for [M^+] $C_{11}H_9FO_2$: 192.0587, found: 192.0593.

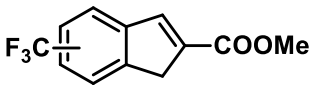
Methyl 5-chloro-1*H*-indene-2-carboxylate (2j):

Yield = 82%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.68 (d, *J* = 10.6 Hz, 1H), 7.52 (d, *J* = 2.0 Hz, 1H), 7.45 (dd, *J* = 8.1, 4.4 Hz, 1H), 7.33 (ddd, *J* = 8.0, 4.5, 1.9 Hz, 1H), 3.87 (d, *J* = 1.8 Hz, 3H), 3.73 – 3.64 (m, 2H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 165.00, 146.18, 144.16, 142.69, 141.04, 140.12, 139.87, 138.71, 137.32, 133.70, 132.74, 127.41, 127.19, 125.12, 124.62, 124.02, 123.23, 51.68, 51.64, 38.23, 37.93; **HRMS (EI, m/z):** Calculated for [M^+] $C_{11}H_9ClO_2$: 208.0291, found: 208.0294.



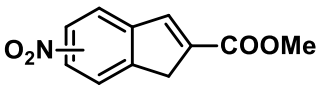
Methyl 5-(trifluoromethyl)-1*H*-indene-2-carboxylate (2k):

Yield = 84%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.89 – 7.71 (m, 2H), 7.63 (d, *J* = 1.4 Hz, 2H), 3.89 (d, *J* = 1.0 Hz, 3H), 3.77 (d, *J* = 1.9 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 164.81, 164.75, 147.94, 145.76, 144.65, 142.99, 139.82, 139.72, 138.83, 125.66, 124.43, 124.27- 124.03 (m, 1C), 123.30, 121.06, 121.03, 120.03, 119.99, 51.78, 51.75, 38.45, 38.40; **HRMS (EI, m/z):** Calculated for [M^+] $C_{12}H_9F_3O_2$: 242.0555, found: 242.0557.



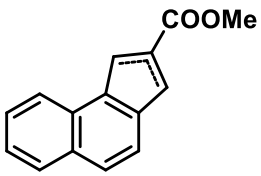
Methyl 5-nitro-1*H*-indene-2-carboxylate (2l):

Yield = 84%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.39 (s, 1H), 8.32 – 8.24 (m, 1H), 7.82 – 7.74 (m, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 3.91 (dd, *J* = 2.3, 0.9 Hz, 3H), 3.87 – 3.81 (m, 2H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 164.32, 150.92, 148.57, 147.23, 145.04, 143.69, 142.47, 140.08, 139.23, 139.06, 124.64, 123.35, 122.97, 122.54, 119.48, 118.15, 51.91, 38.79, 38.59; **HRMS (EI, m/z):** Calculated for [M^+] $C_{11}H_9NO_4$: 219.0532, found: 219.0536.



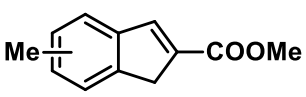
Methyl 3*H*-cyclopenta *α*-naphthalene-2-carboxylate (2m):

Yield = 93%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.15 (d, *J* = 8.8 Hz, 1H), 7.99 (d, *J* = 7.5 Hz, 1H), 7.91 (dd, *J* = 13.6, 7.8 Hz, 1H), 7.83 (dd, *J* = 14.9, 7.7 Hz, 2H), 7.68 – 7.47 (m, 3H), 4.00 (d, *J* = 1.9 Hz, 1H), 3.92 (d, *J* = 4.3 Hz, 3H), 3.84 (d, *J* = 2.0 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 165.22, 165.15, 143.48, 142.53, 141.86, 139.96, 138.86, 138.77, 136.69, 136.37, 132.75, 132.47, 129.77, 128.77, 128.46, 128.13, 127.79, 126.60, 126.47, 125.92, 125.47, 123.80, 123.33, 122.37, 121.24, 51.56, 51.54, 39.51, 37.41; **HRMS (EI, m/z):** Calculated for [M^+] $C_{15}H_{12}O_2$: 224.0837, found: 224.0837.

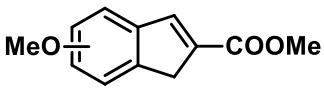


Methyl 5-methyl-1H-indene-2-carboxylate (2n):

Yield = 88%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.71 (d, *J* = 7.0 Hz, 1H), 7.42 (t, *J* = 7.3 Hz, 1H), 7.35 (s, 1H), 7.18 (dd, *J* = 8.0, 3.8 Hz, 1H), 3.87 (t, *J* = 1.3 Hz, 3H), 3.72 – 3.63 (m, 2H), 2.44 (d, *J* = 5.7 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 165.45, 145.09, 142.83, 141.80, 141.16, 139.99, 137.70, 137.06, 136.44, 135.84, 128.47, 127.66, 124.97, 123.81, 122.95, 51.48, 38.01, 21.61, 21.26; **HRMS (EI, m/z):** Calculated for [M^+] $C_{12}H_{12}O_2$: 188.0837, found: 188.0837.

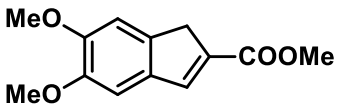


Methyl 6-methoxy-*1*H-indene-2-carboxylate (2o):



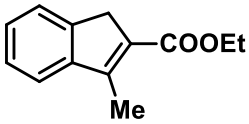
Yield = 72%; **^{1}H NMR (400 MHz, CDCl3):** δ 7.70 (d, *J* = 2.0 Hz, 1H), 7.42 (dd, *J* = 10.8, 8.2 Hz, 1H), 7.14 – 7.03 (m, 1H), 6.98 – 6.86 (m, 1H), 3.89 – 3.83 (m, 6H), 3.66 (dd, *J* = 12.5, 1.9 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 165.39, 165.28, 160.02, 147.00, 143.82, 141.04, 138.13, 136.89, 135.63, 134.54, 124.66, 123.97, 114.27, 113.12, 109.94, 107.92, 55.42, 51.53, 51.40, 38.30, 37.54; **HRMS (EI, m/z):** Calculated for [M+] $C_{12}H_{12}O_3$: 204.0786, found: 204.0792.

Methyl 5,6-dimethoxy-1*H*-indene-2-carboxylate (2p):



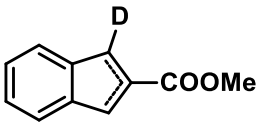
Yield = 70%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.70 – 7.63 (m, 1H), 7.08 (s, 1H), 7.04 (s, 1H), 3.95 (s, 3H), 3.93 (s, 3H), 3.84 (s, 3H), 3.64 (d, *J* = 1.1 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 165.25, 149.64, 148.57, 141.36, 138.19, 135.12, 107.42, 105.83, 56.01, 51.38, 38.26; **HRMS (EI, m/z):** Calculated for [M+] $C_{13}H_{14}O_4$: 234.0892, found: 234.0897.

Ethyl 3-methyl-1*H*-indene-2-carboxylate (3):



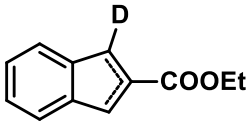
Yield = 95%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.52 (dddd, *J* = 8.5, 5.3, 2.8, 0.8 Hz, 2H), 7.42 – 7.33 (m, 2H), 4.33 (q, *J* = 7.1 Hz, 2H), 3.69 (d, *J* = 2.5 Hz, 2H), 2.58 (t, *J* = 2.4 Hz, 3H), 1.40 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 165.90, 151.20, 145.21, 143.38, 129.74, 127.49, 126.44, 123.84, 120.98, 106.12, 59.83, 38.67, 14.34, 12.32; **HRMS (EI, m/z):** Calculated for [M+] $C_{13}H_{14}O_2$: 202.0994, found: 202.0977.

Methyl 1*H*, 1*D*-indene-2-carboxylate (2a-D):



Yield = 88%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.76 (s, 1H), 7.54 (q, *J* = 4.6 Hz, 2H), 7.36 (dd, *J* = 5.4, 3.2 Hz, 2H), 3.87 (s, 3H), 3.71 (s, 1H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 165.35, 144.67, 142.59, 141.19, 141.12, 136.93, 127.47, 126.76, 124.17, 123.28, 51.53, 38.26; **^{2}H NMR (60 MHz, $CDCl_3$):** δ 7.54, 3.46; **HRMS (EI, m/z):** Calculated for [M+] $C_{11}H_9DO_2$: 175.0744, found: 175.0762.

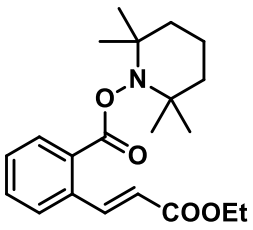
Ethyl 1*H*, 1*D*-indene-2-carboxylate (2b-D):



Yield = 85%; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.88 – 7.63 (m, 1H), 7.62 – 7.46 (m, 2H), 7.43 – 7.30 (m, 2H), 4.33 (q, *J* = 7.1 Hz, 2H), 3.71 (s, 1H), 1.39 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 164.97, 144.68, 142.66, 140.85, 137.38, 127.38, 126.73, 124.15, 123.22, 60.31, 38.25, 14.28; **^{2}H NMR (60 MHz, $CHCl_3$):** δ 8.24, 4.16; **HRMS (EI, m/z):** Calculated for [M+] $C_{12}H_{11}DO_2$: 189.0900, found: 189.0924.

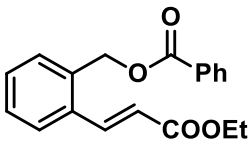
Synthetic procedure for compound 5 and 7: Under a nitrogen atmosphere, cinnamyl N-tosylhydrazone (**1a-b**) (0.1 mmol) and TEMPO/DBP (0.2 mmol) were added to a flame-dried Schlenk tube. The tube was capped with a Teflon screw cap, evacuated, and backfilled with nitrogen. Base LiO^{t}Bu (1.2 equiv; 0.12 mmol), [Co^{II}(MeTAA)] catalyst (5 mol %) and and benzene (anhydrous and degassed, 2 mL) were added inside the glove box. The Schlenk tube was then placed in an oil bath and heated to the desired temperature under nitrogen for a set period. After the reaction finished, the resulting mixture was concentrated and the residue was purified by flash chromatography (silica gel).

(*E*)-2,2,6,6-Tetramethylpiperidin-1-yl 2-(3-ethoxy-3-oxoprop-1-en-1-yl)benzoate (5):

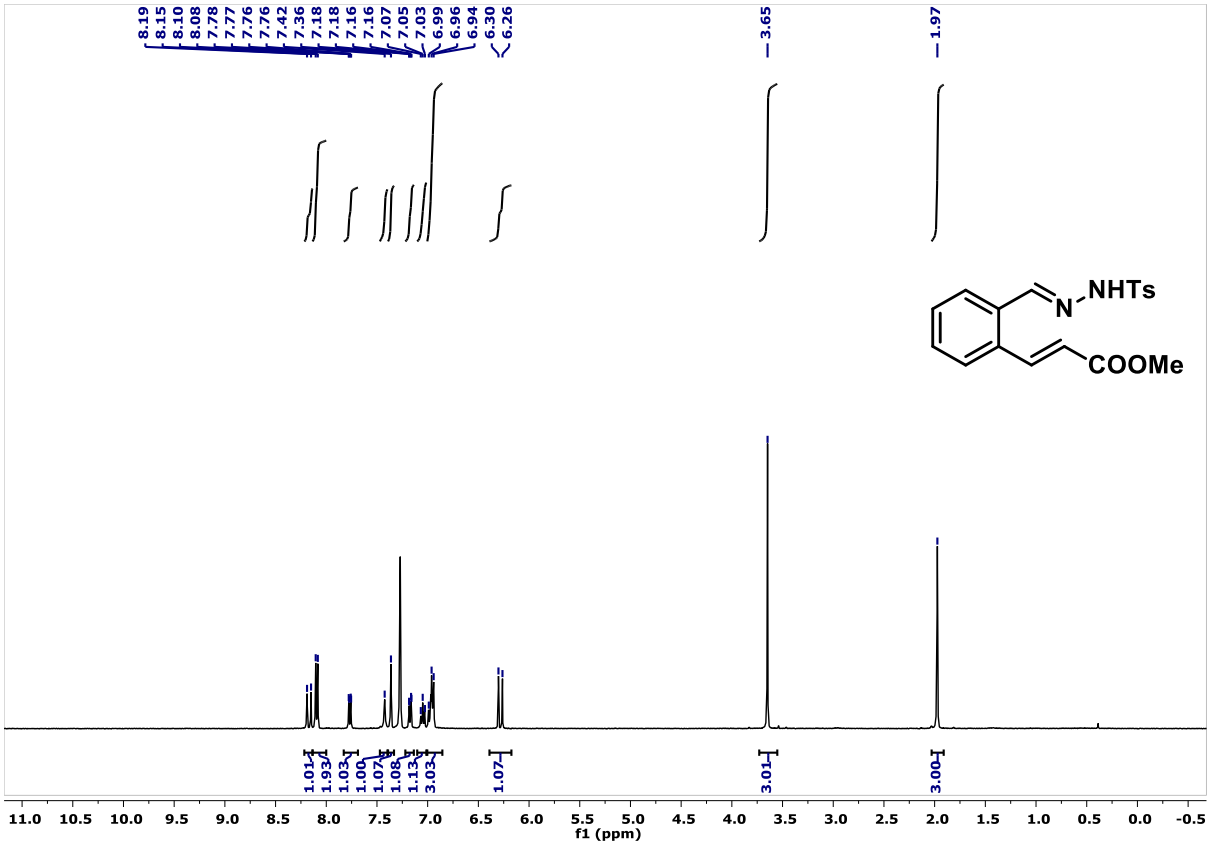


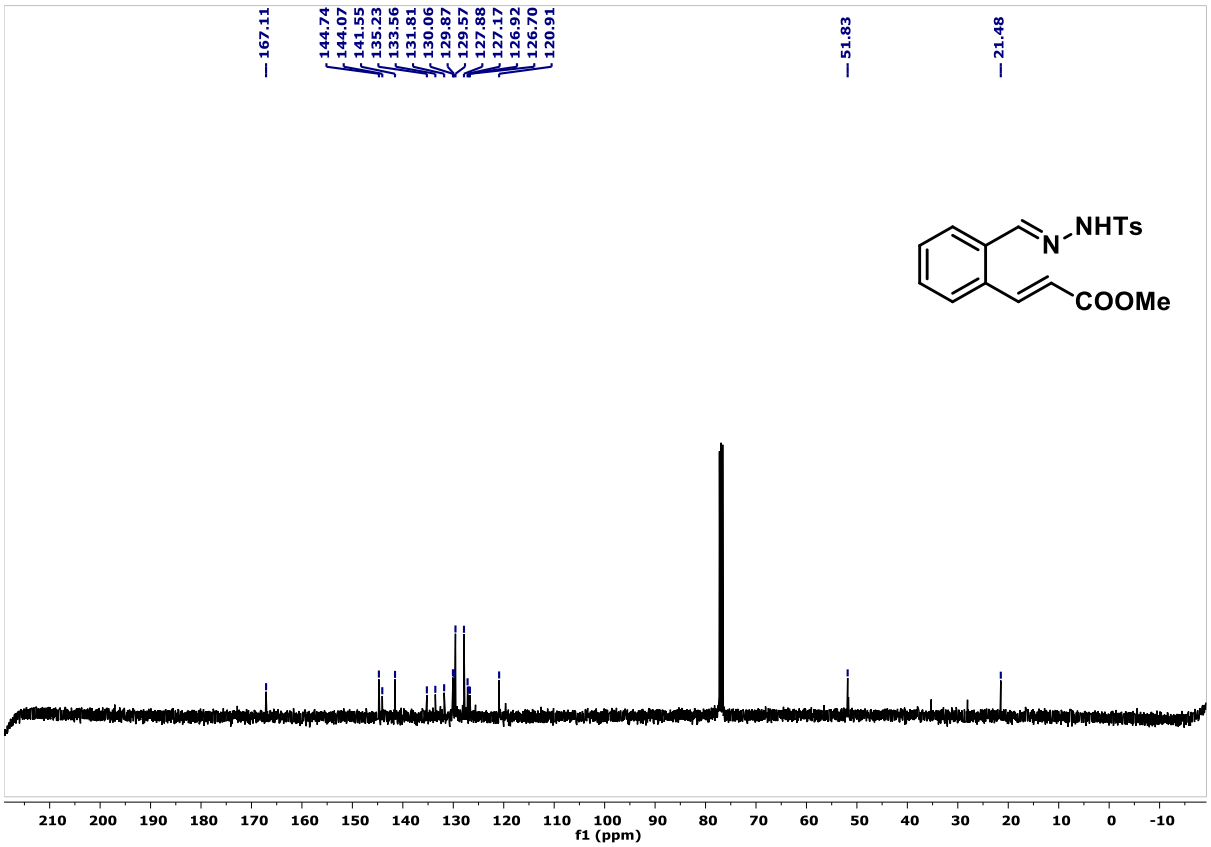
Yield = 14%; **^{1}H NMR (400 MHz, CDCl$_3$):** δ 8.44 (d, *J* = 15.9 Hz, 1H), 7.98 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.61 – 7.54 (m, 1H), 7.48 (td, *J* = 7.6, 1.4 Hz, 1H), 6.35 (d, *J* = 15.9 Hz, 1H), 3.81 (s, 3H), 1.86 – 1.62 (m, 5H), 1.48 (dd, *J* = 7.8, 5.2 Hz, 1H), 1.27 (s, 6H), 1.18 (s, 6H); **^{13}C NMR (100 MHz, CDCl$_3$):** δ 166.74, 166.70, 143.50, 136.14, 132.04, 130.01, 129.72, 129.30, 127.79, 120.78, 60.33, 51.59, 39.09, 31.88, 20.84, 16.88; **HRMS (GC, m/z):** Calculated for [M+] $C_{20}H_{27}NO_4$: 345.1940, found: 345.

(*E*)-2-(3-ethoxy-3-oxoprop-1-en-1-yl)benzyl benzoate (7):



Yield = 08%; **^{1}H NMR (400 MHz, CDCl$_3$):** δ 8.13 (d, *J* = 15.8 Hz, 1H), 8.10 – 8.03 (m, 2H), 7.69 – 7.63 (m, 1H), 7.61 – 7.52 (m, 2H), 7.48 – 7.38 (m, 4H), 6.45 (d, *J* = 15.8 Hz, 1H), 5.53 (s, 2H), 3.82 (s, 3H); **^{13}C NMR (100 MHz, CDCl$_3$):** δ 166.90, 166.06, 141.27, 134.73, 133.87, 133.02, 130.03, 129.99, 129.74, 129.61, 128.87, 128.29, 126.82, 120.33, 64.26, 51.68, 29.60; **HRMS (GC, m/z):** Calculated for [M+] $C_{18}H_{16}O_4$: 296.1049, found: 296.


8.19
8.15
8.10
8.08
7.78
7.77
7.76
7.76
7.42
7.36
7.18
7.18
7.16
7.16
7.07
7.05
7.03
6.99
6.96
6.94
6.30
6.26
3.65
1.97
NHTs
N
COOMe
1.01
1.93
1.03
1.00
1.07
1.08
1.13
3.03
1.07
3.01
3.00
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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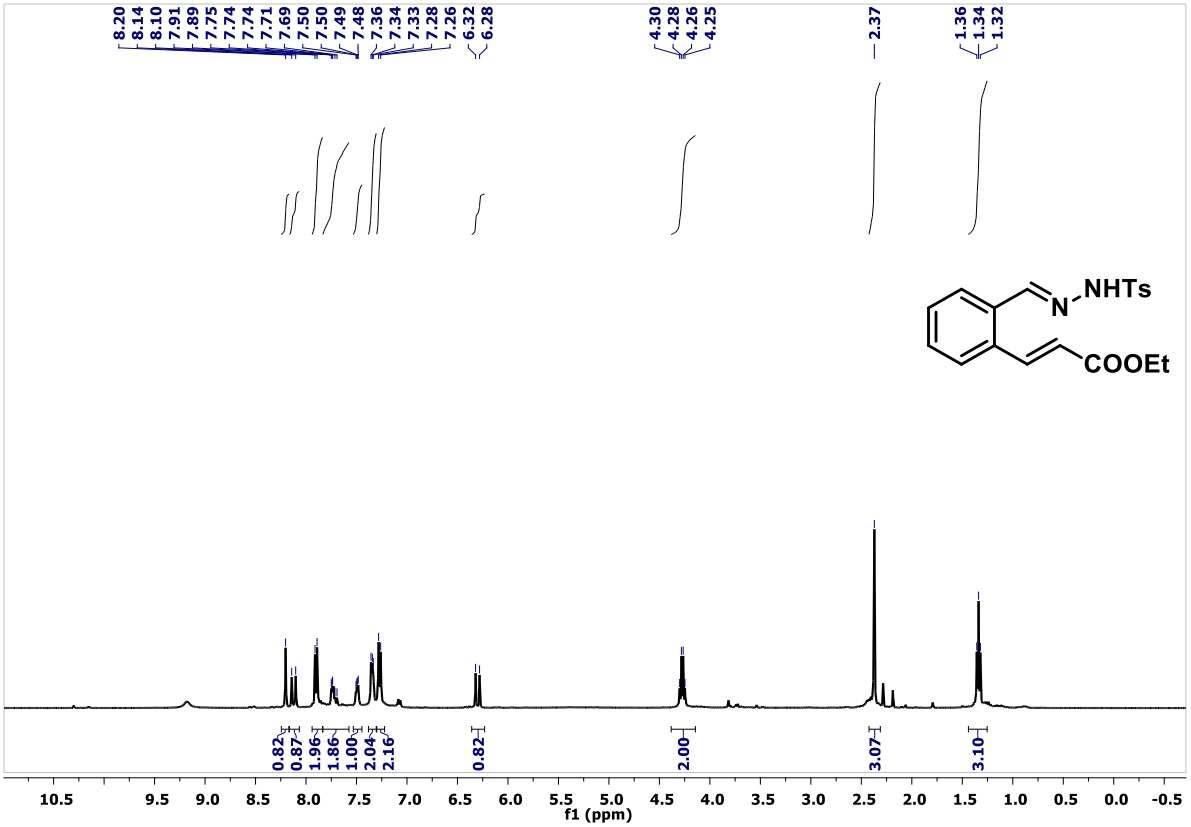
144.07
141.55
135.23
133.56
131.81
130.06
129.87
129.57
127.88
127.17
126.92
126.70
120.91
51.83
21.48
NHTs
N
COOMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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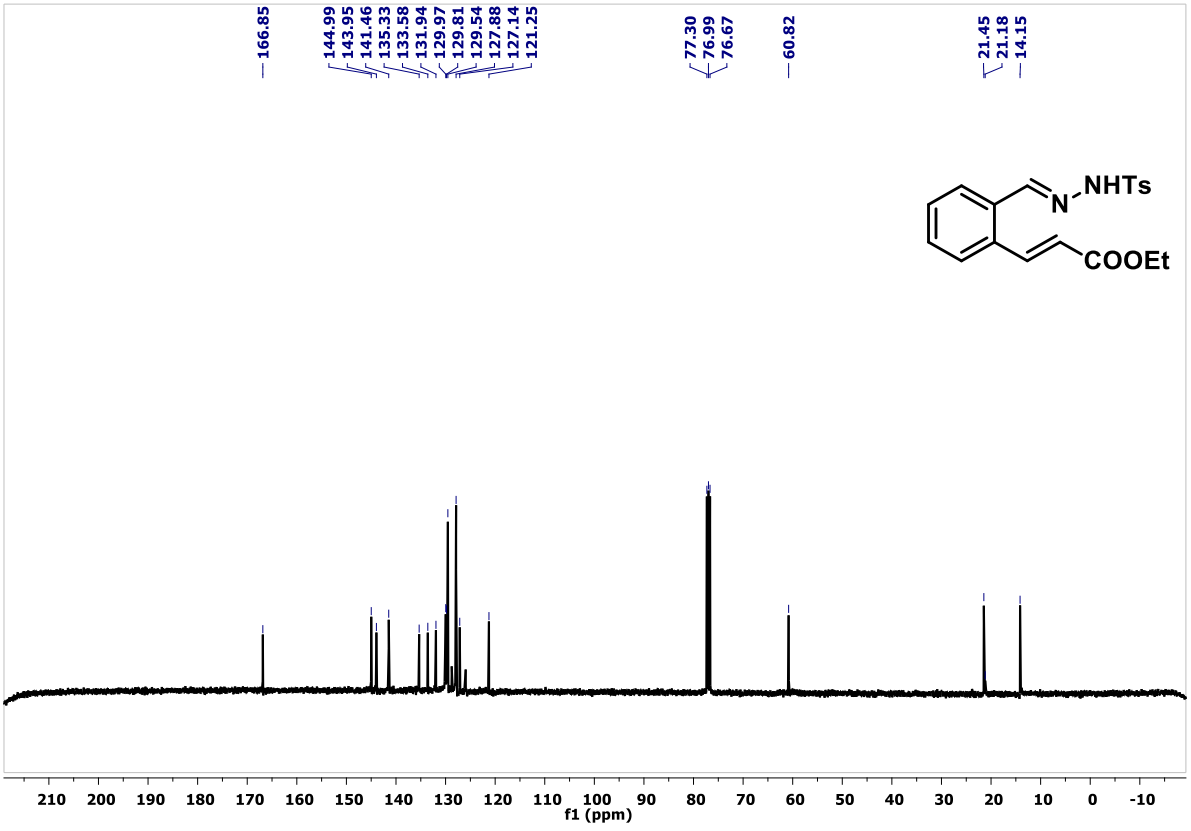
7.89
7.75
7.74
7.74
7.71
7.69
7.50
7.50
7.49
7.48
7.36
7.34
7.33
7.28
7.26
6.32
6.28
4.30
4.28
4.26
4.25
2.37
1.36
1.34
1.32
NHTs
COOEt
0.82
0.87
1.96
1.86
1.00
2.04
2.16
0.82
2.00
3.07
3.10
f1 (ppm)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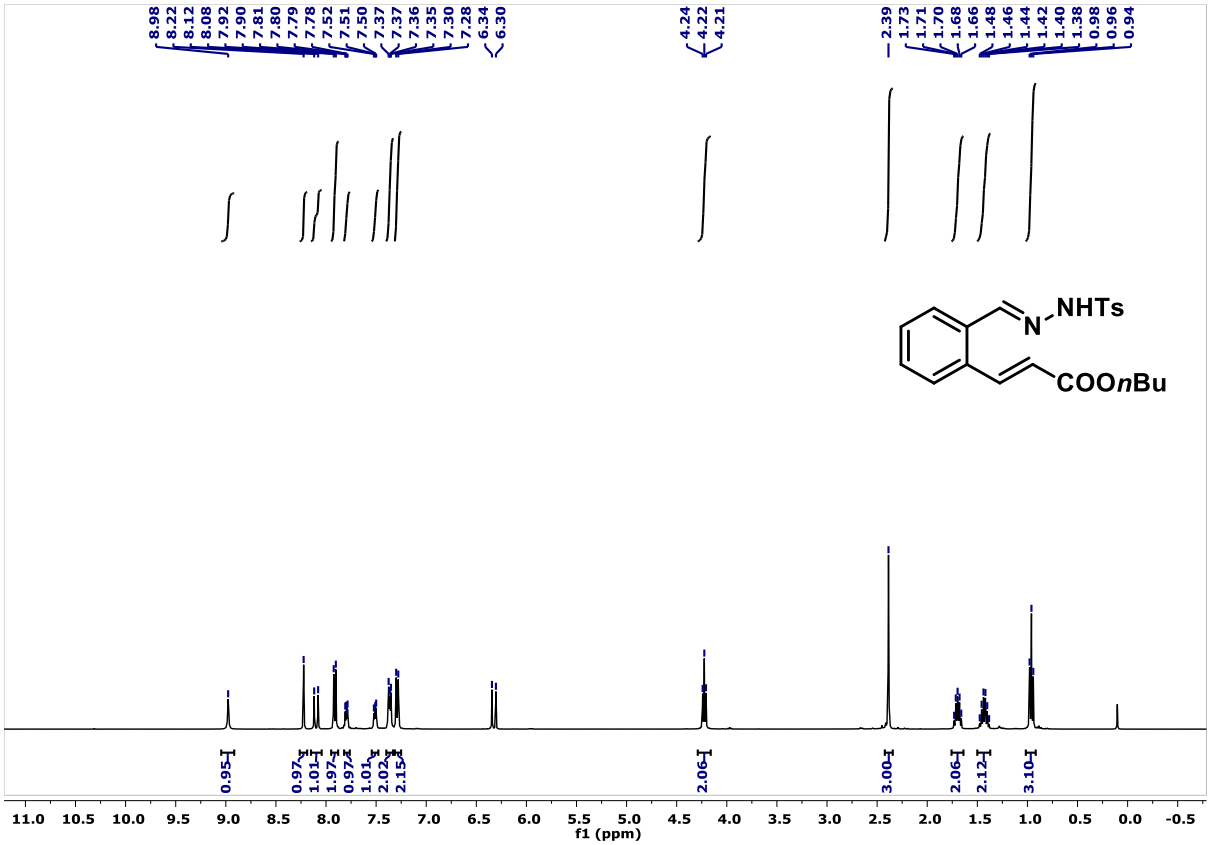
141.46
135.33
133.58
131.94
129.97
129.81
129.54
127.88
127.14
121.25
77.30
76.99
76.67
60.82
21.45
21.18
14.15
NHTs
COOEt
f1 (ppm)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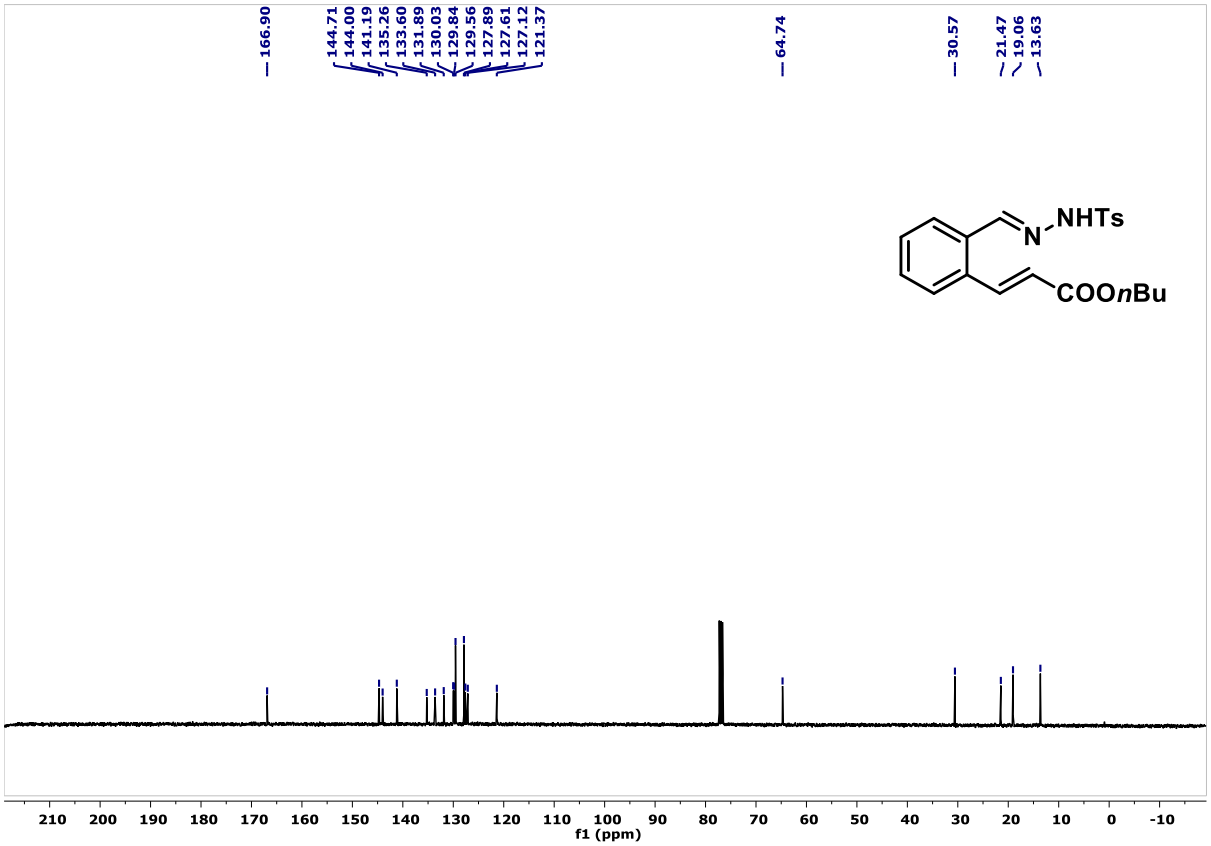
8.08
7.92
7.90
7.81
7.80
7.79
7.78
7.52
7.51
7.50
7.37
7.37
7.36
7.35
7.30
7.28
6.34
6.30
4.24
4.22
4.21
2.39
1.73
1.71
1.70
1.68
1.66
1.48
1.46
1.44
1.42
1.40
1.38
0.98
0.96
0.94
NHTs
N
COOnBu
0.95
0.97
1.01
1.97
0.97
1.01
2.02
2.15
2.06
3.00
2.06
2.12
3.10
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 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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135.26
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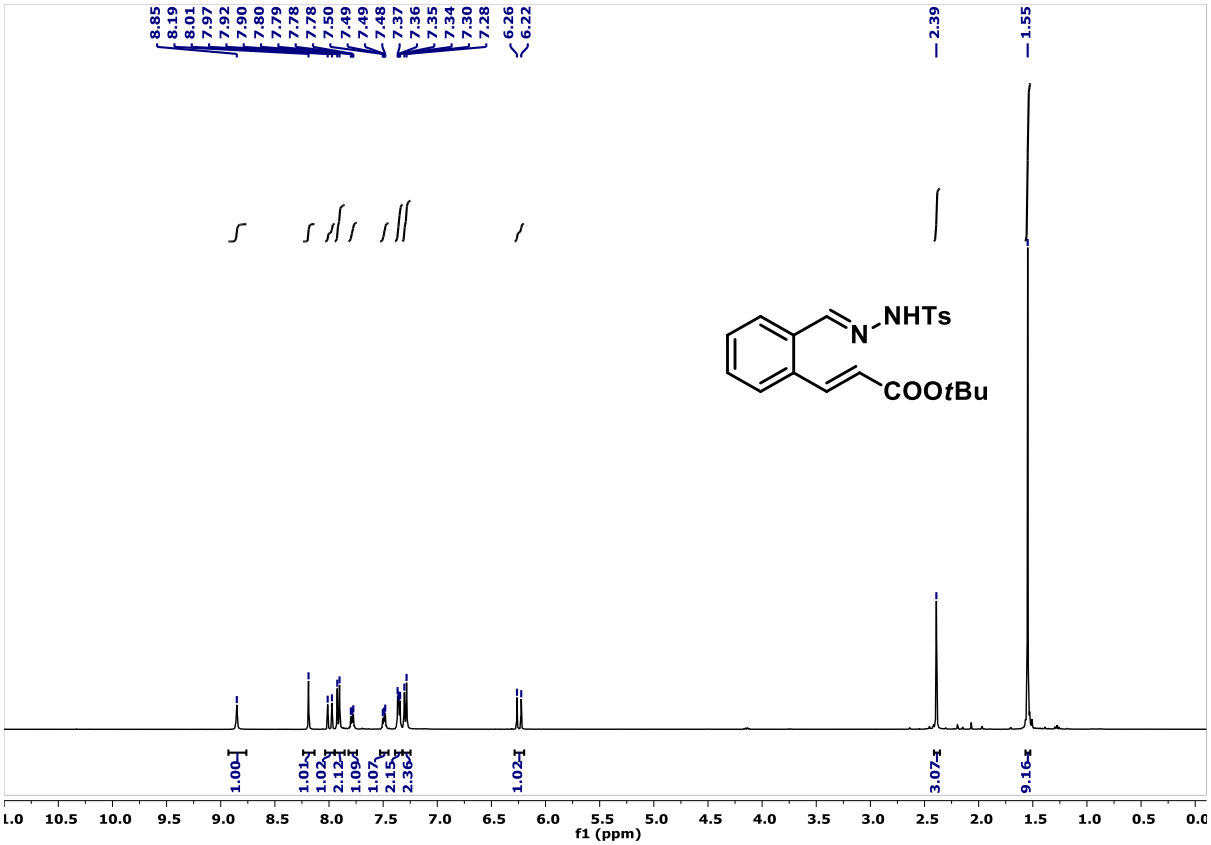
131.89
130.03
129.84
129.56
127.89
127.61
127.12
121.37
64.74
30.57
21.47
19.06
13.63
NHTs
N
COOnBu
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.01
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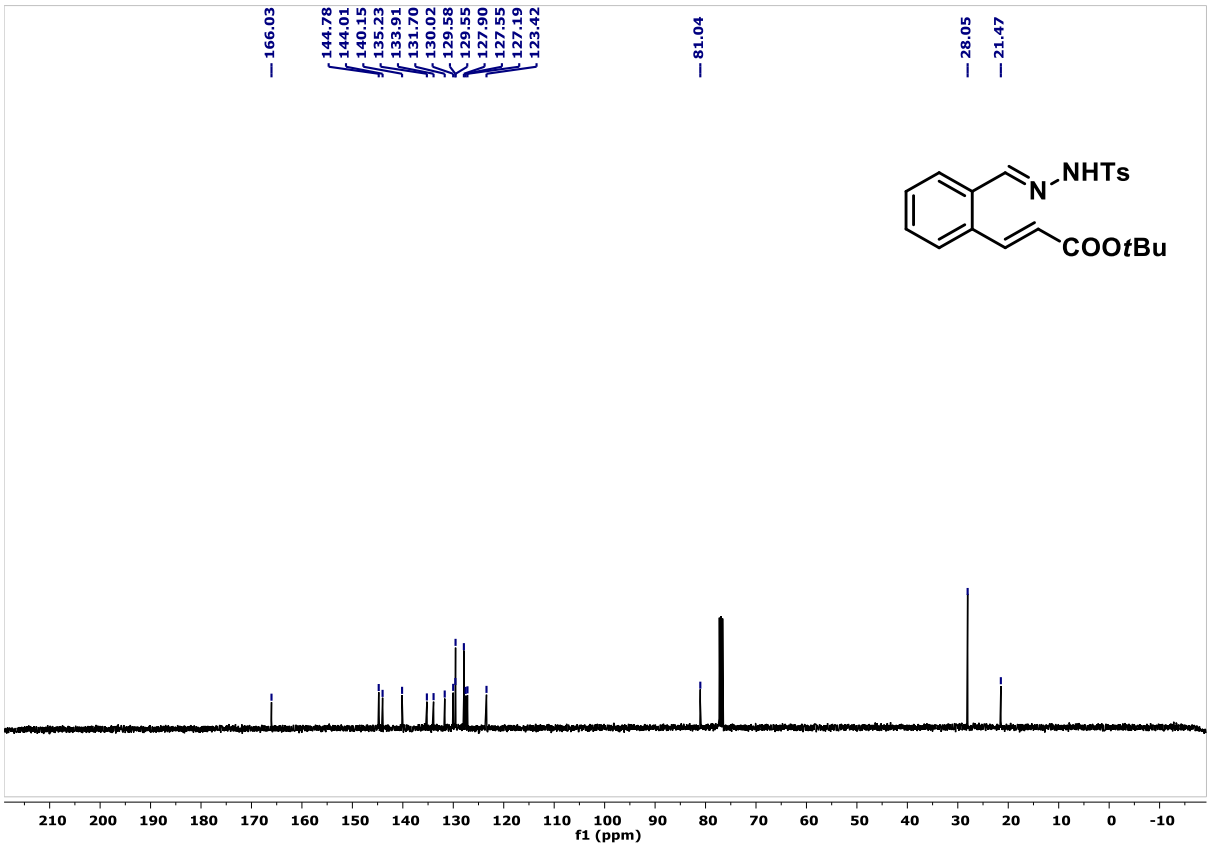
7.90
7.80
7.79
7.78
7.78
7.50
7.49
7.49
7.48
7.37
7.36
7.35
7.34
7.30
7.28
6.26
6.22
2.39
1.55
NHTs
N
COOtBu
1.00
1.01
1.02
2.12
1.09
1.07
2.15
2.36
1.02
3.07
9.16
f1 (ppm)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144.78
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140.15
135.23
133.91
131.70
130.02
129.58
129.55
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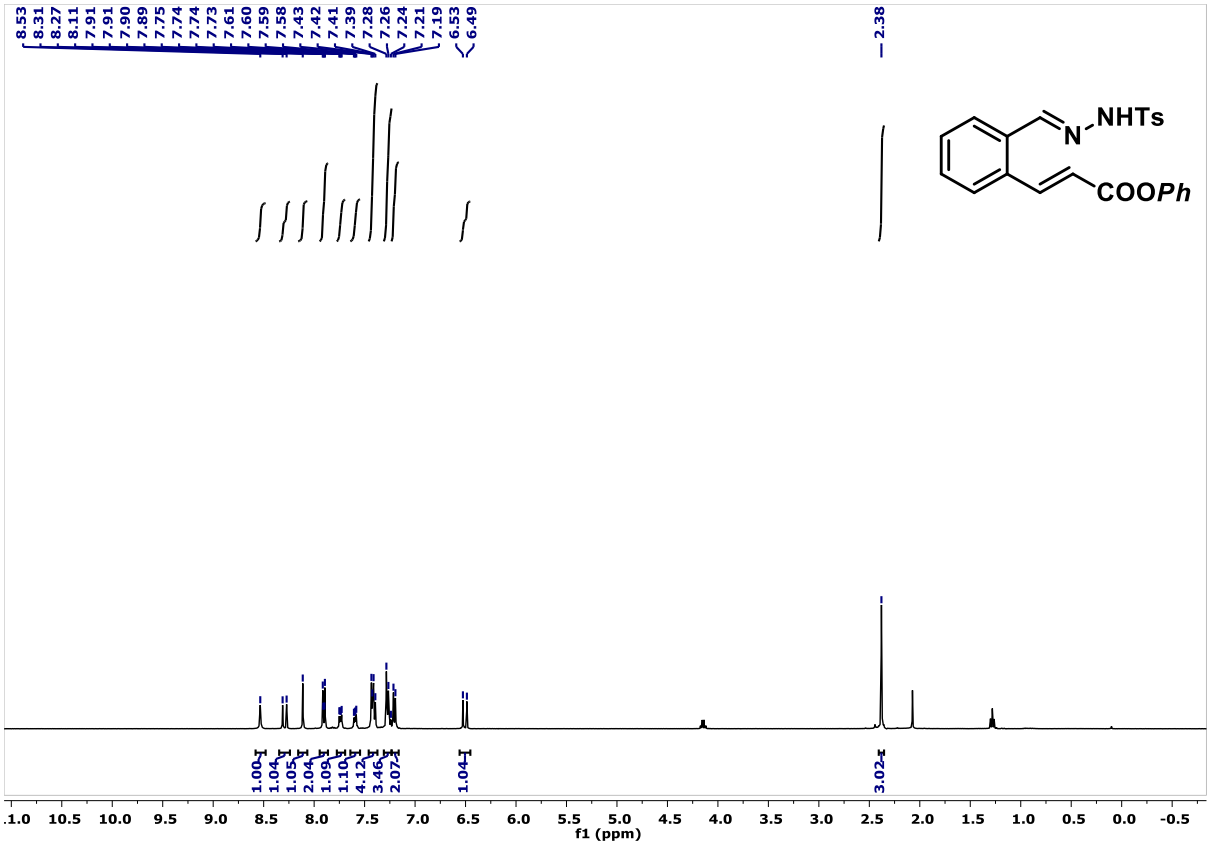
127.19
123.42
81.04
28.05
21.47
NHTs
N
COOtBu
f1 (ppm)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7.91
7.90
7.89
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7.74
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7.58
7.43
7.42
7.41
7.39
7.28
7.26
7.24
7.21
7.19
6.53
6.49
2.38
NHTs
N
COOPh
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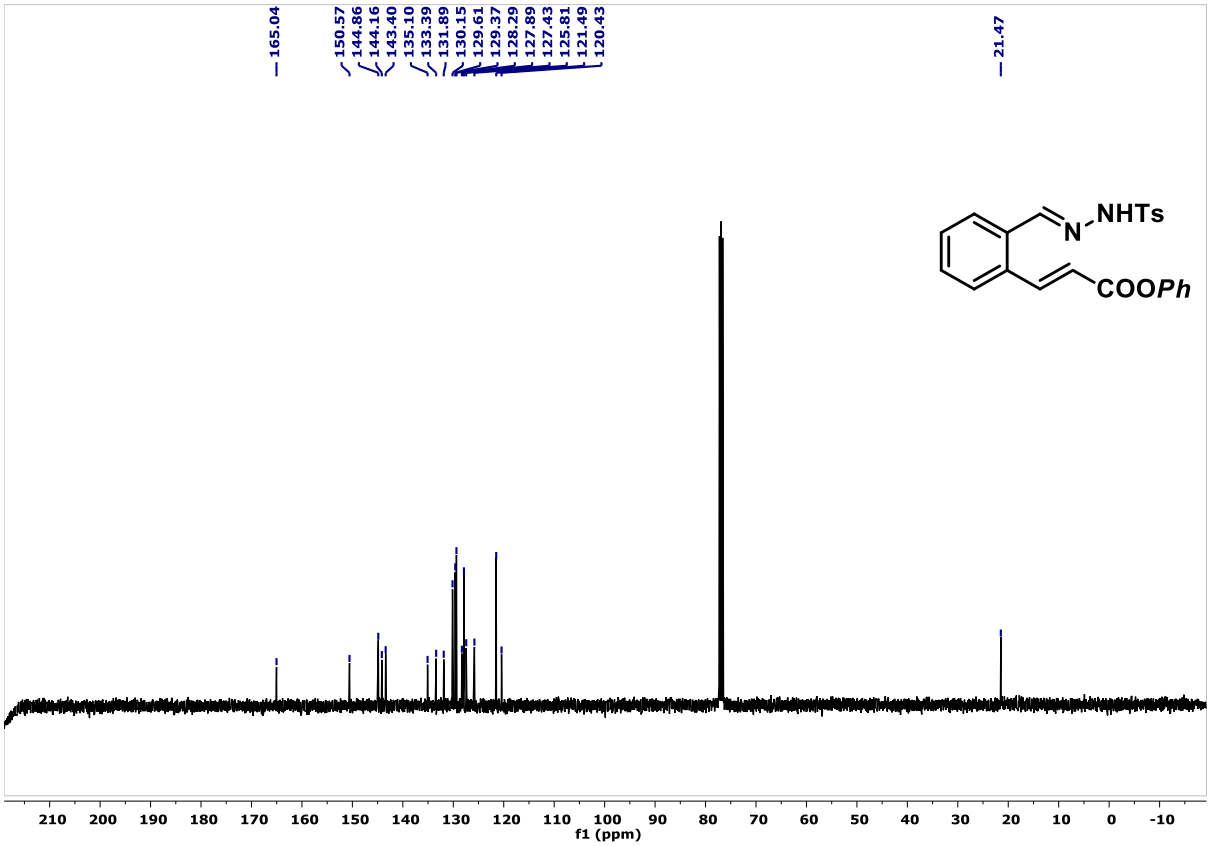
1.05
2.04
1.09
1.10
4.12
3.46
2.07
1.04
3.02
f1 (ppm)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128.29
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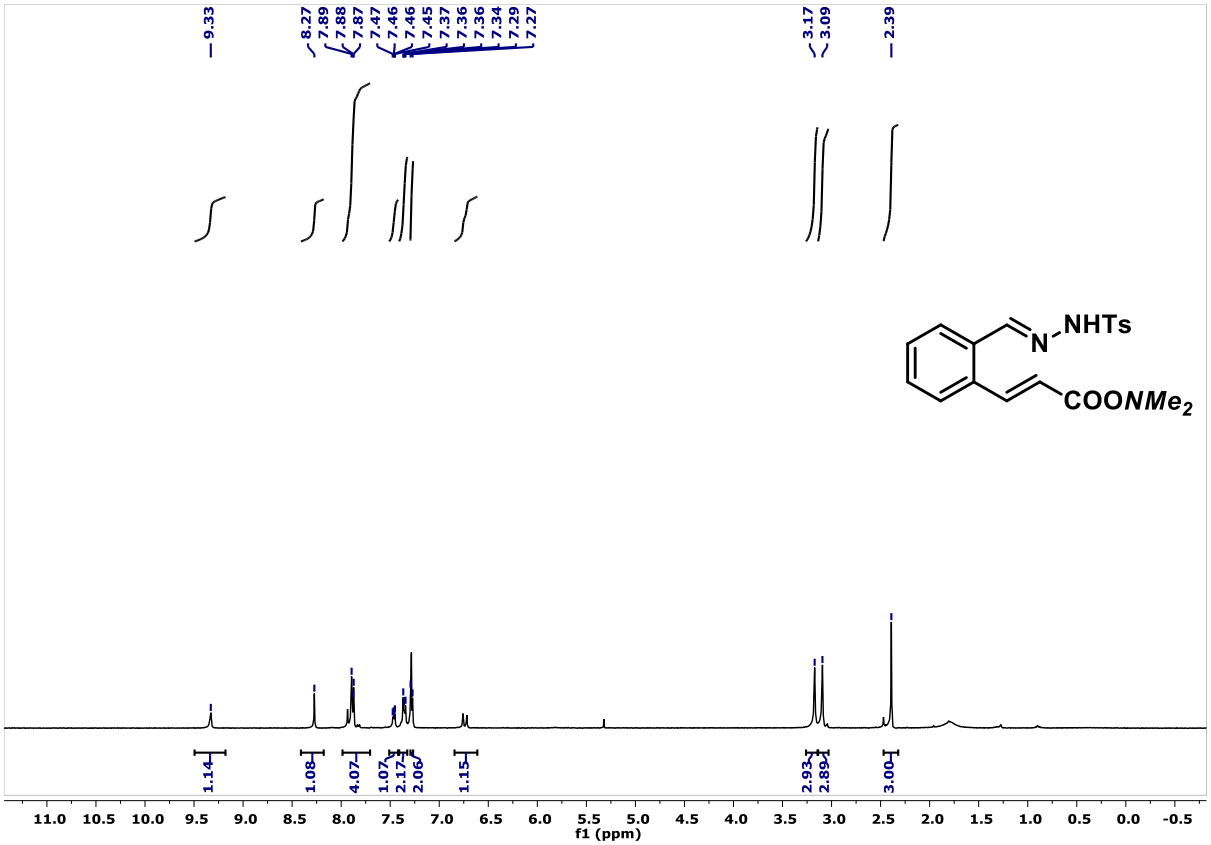
120.43
21.47
NHTs
N
COOPh
f1 (ppm)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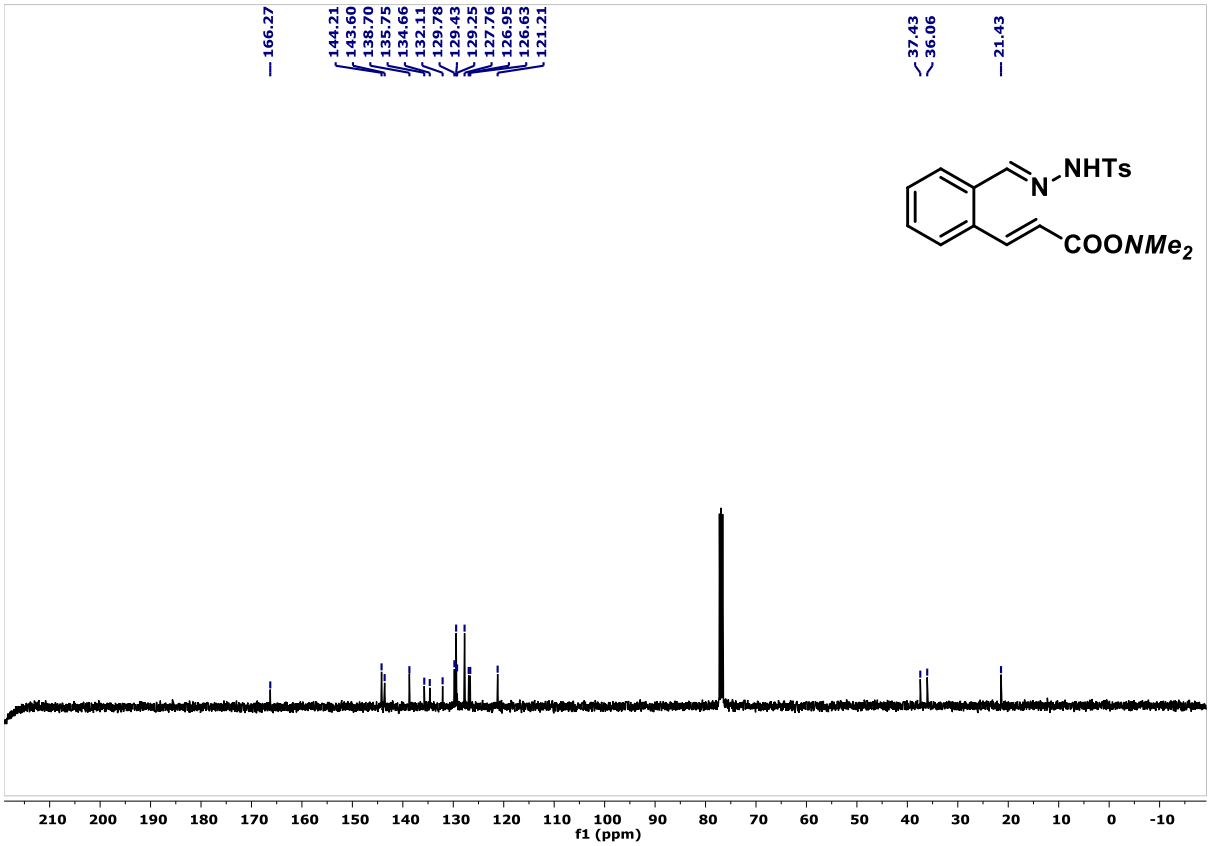
7.47
7.46
7.46
7.45
7.37
7.36
7.36
7.34
7.29
7.27
3.17
3.09
2.39
NHTs
N
COONMe2
1.14
1.08
4.07
1.07
2.17
2.06
1.15
2.93
2.89
3.00
f1 (ppm)


166.27
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138.70
135.75
134.66
132.11
129.78
129.43
129.25
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126.95
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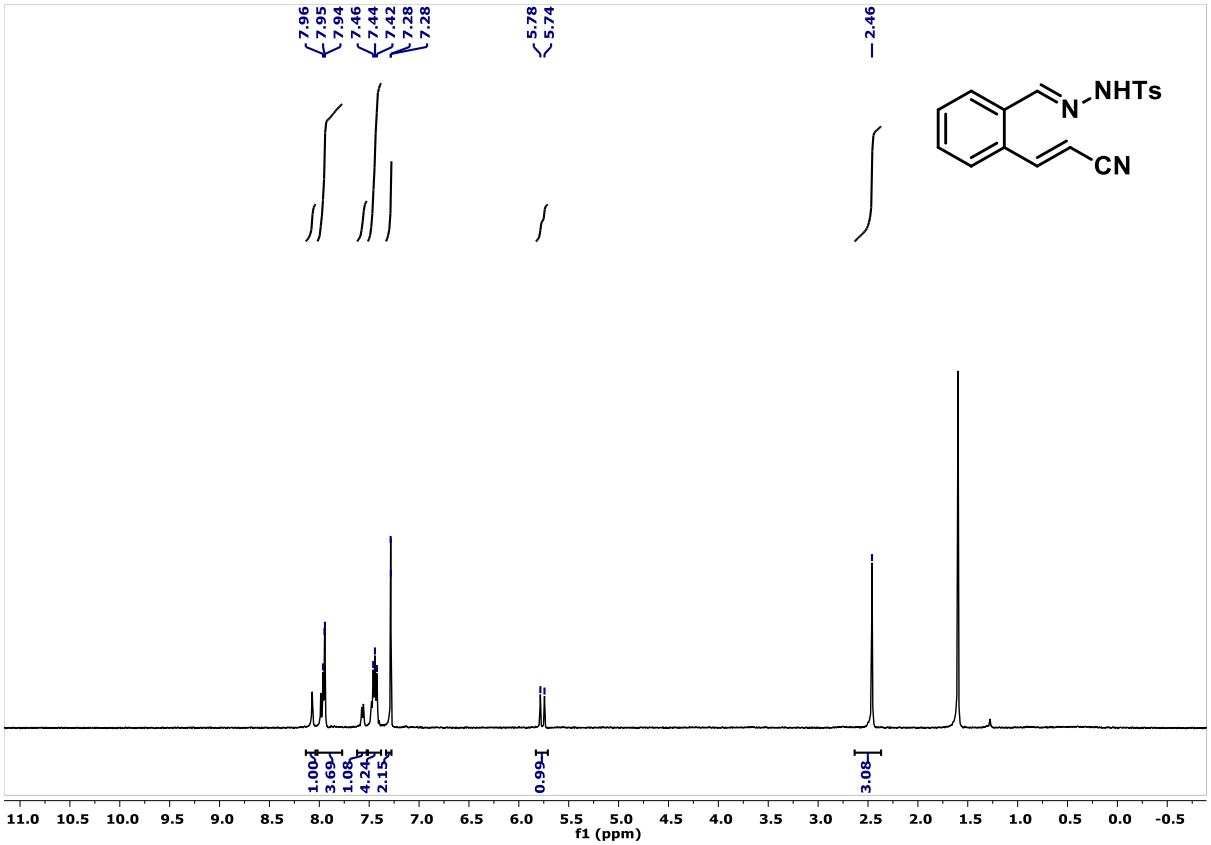
21.43
NHTs
N
COONMe2
f1 (ppm)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7.46
7.44
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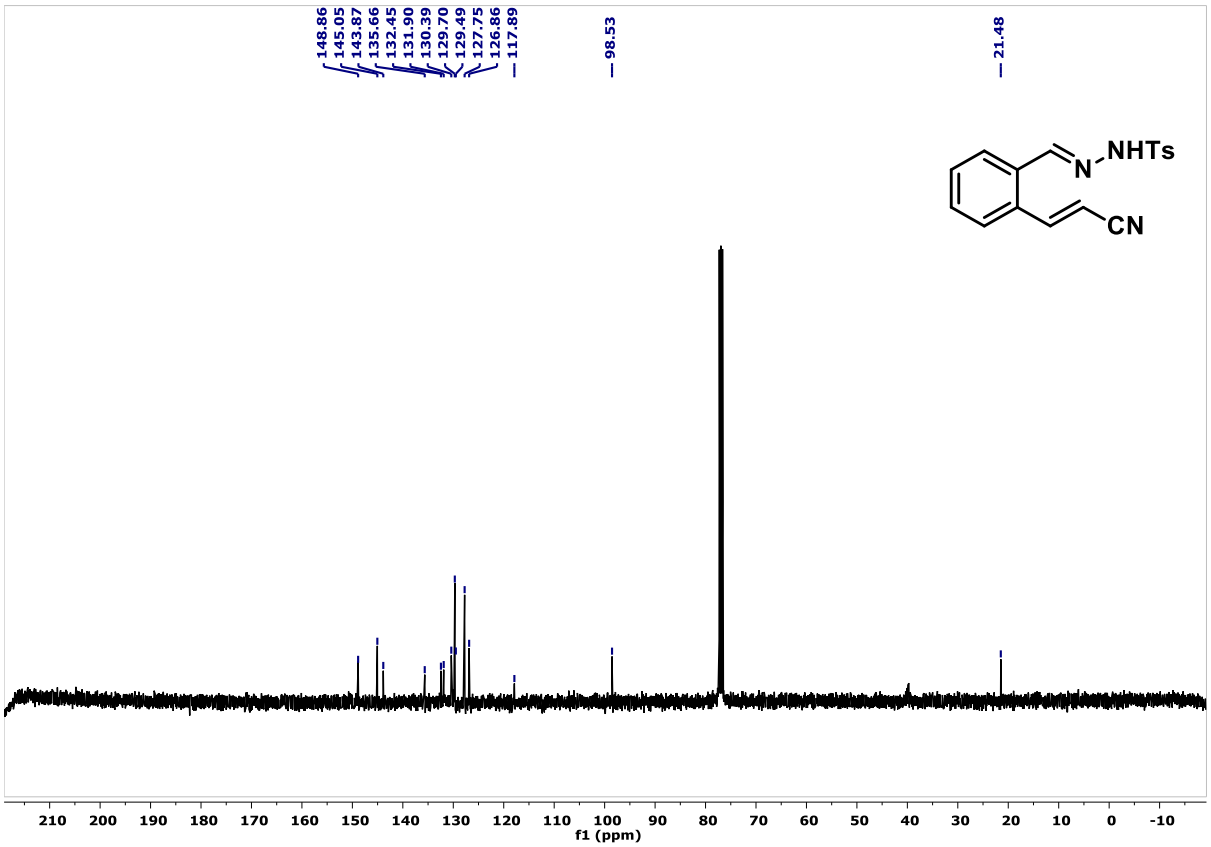
7.28
7.28
5.78
5.74
2.46
NHTs
N
CN
1.00
3.69
1.08
4.24
2.15
0.99
3.08
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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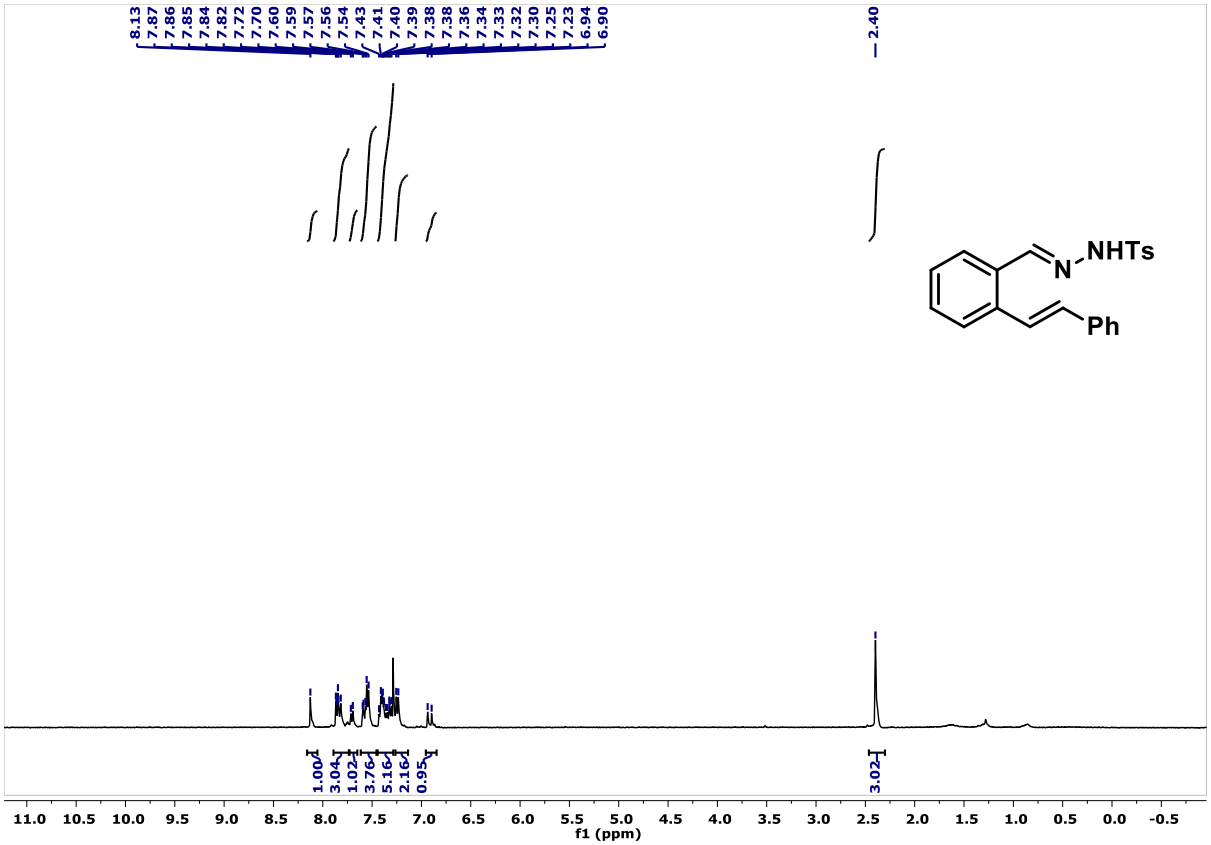
f1 (ppm)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7.84
7.82
7.72
7.70
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7.59
7.57
7.56
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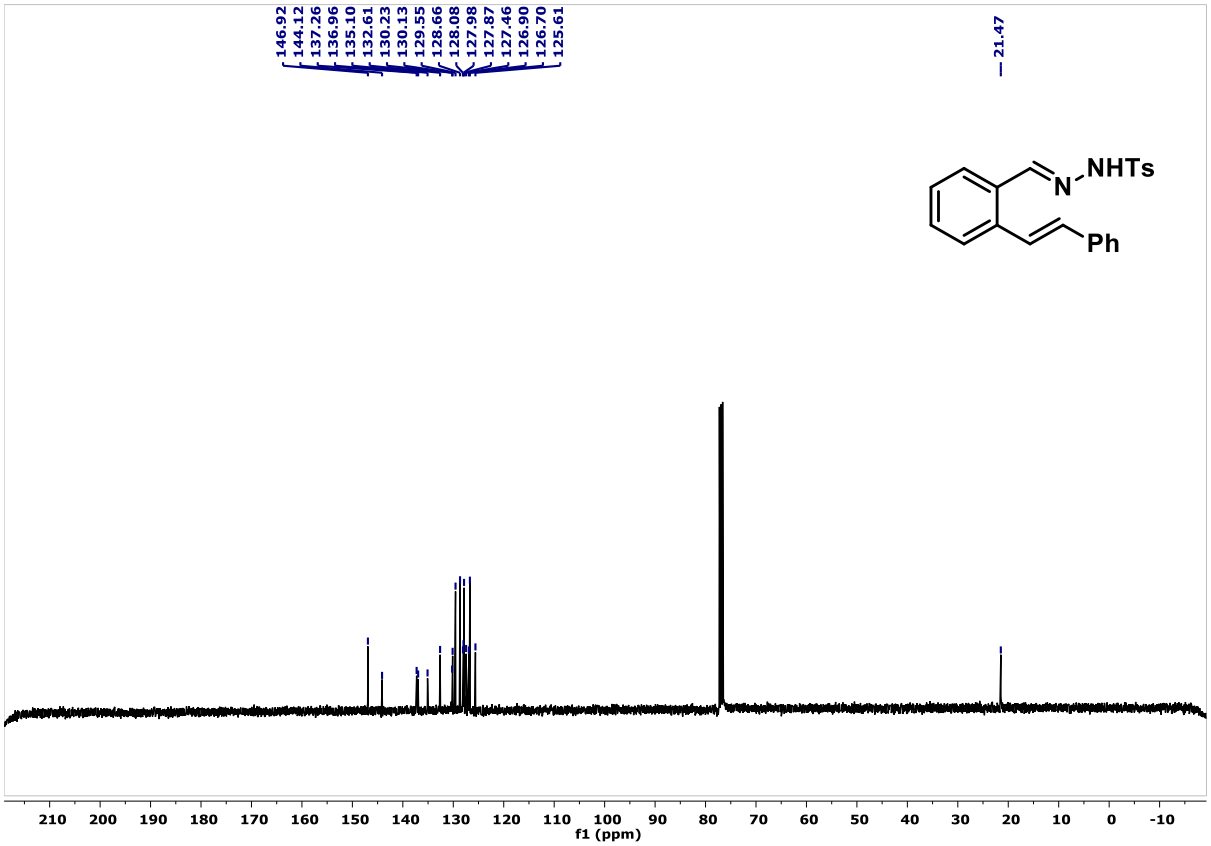
7.43
7.41
7.40
7.39
7.38
7.38
7.36
7.34
7.33
7.32
7.30
7.25
7.23
6.94
6.90
2.40
NHTs
N
Ph
1.00
3.04
1.02
3.76
5.16
2.16
0.95
3.02
f1 (ppm)


146.92
144.12
137.26
136.96
135.10
132.61
130.23
130.13
129.55
128.66
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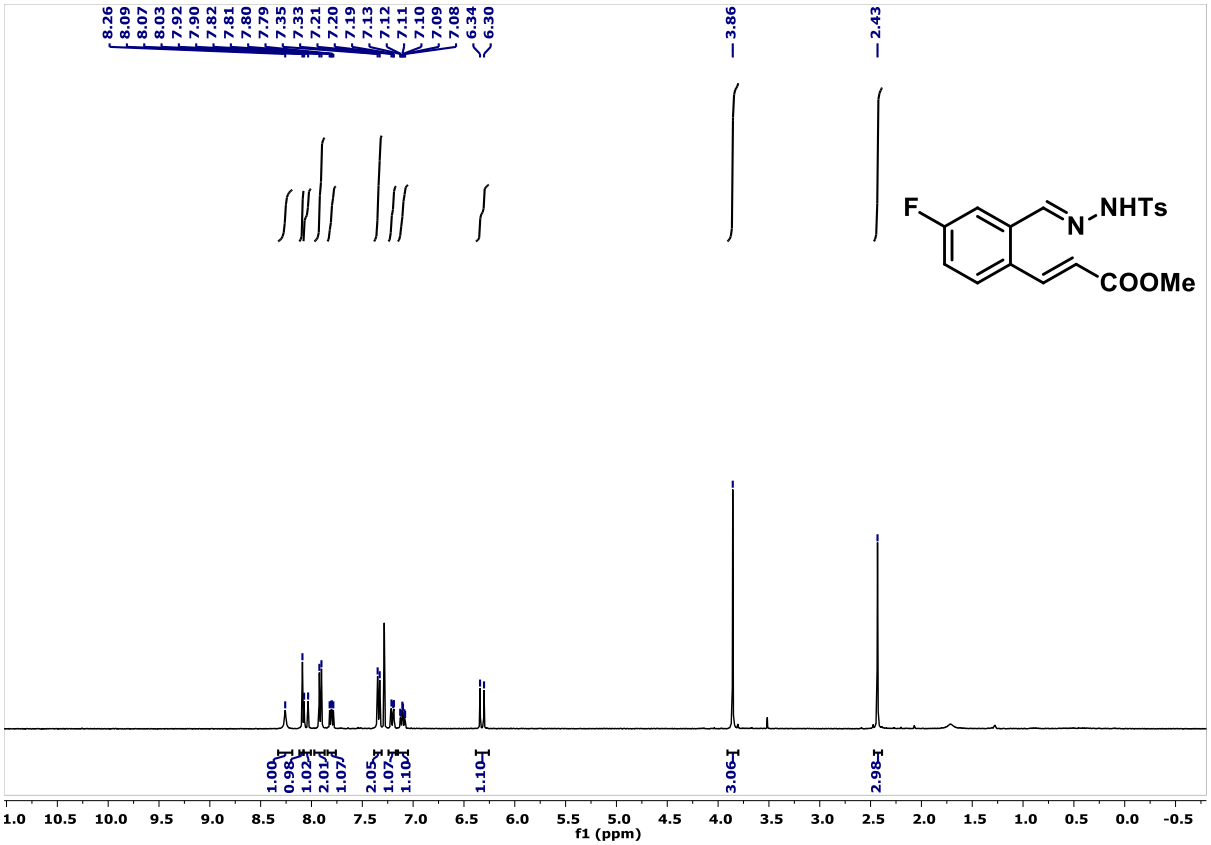
127.87
127.46
126.90
126.70
125.61
21.47
NHTs
N
Ph
f1 (ppm)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8.09
8.07
8.03
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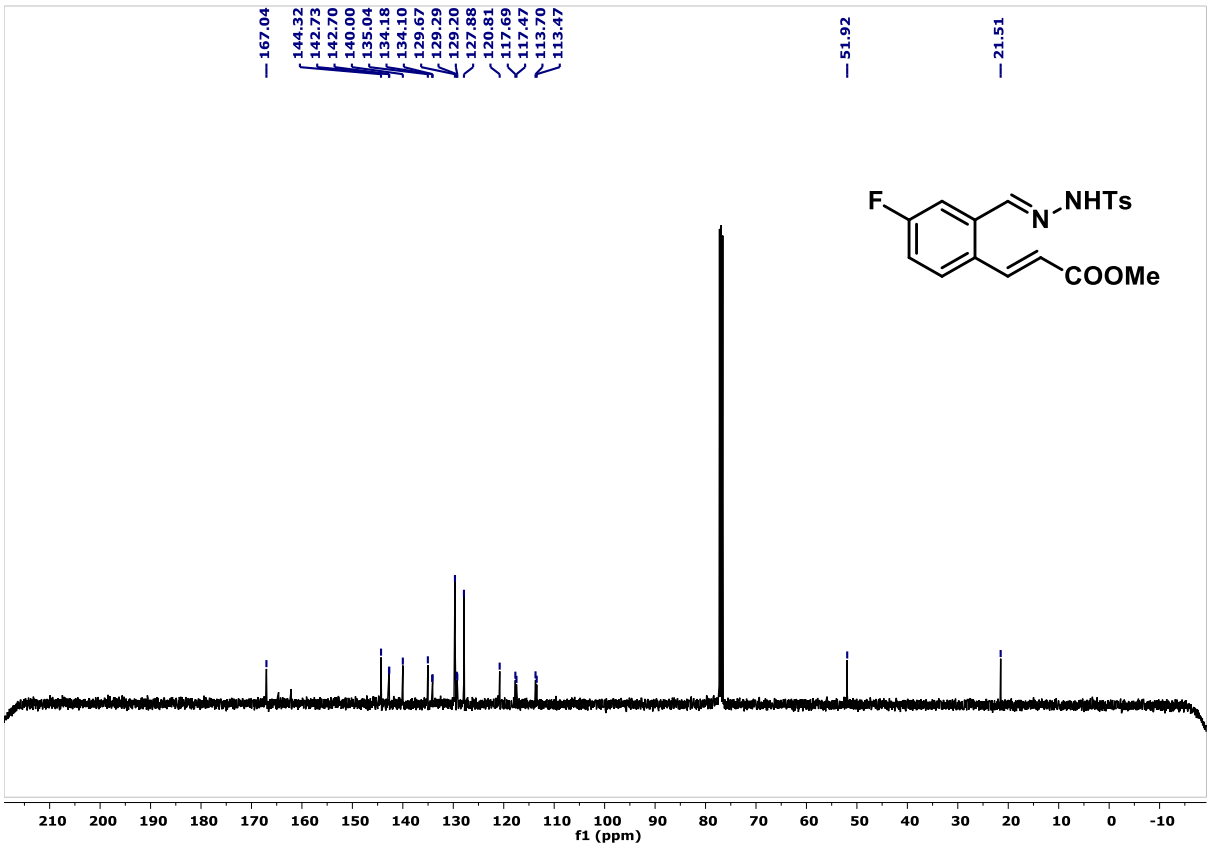
7.90
7.82
7.81
7.80
7.79
7.35
7.33
7.21
7.20
7.19
7.13
7.12
7.11
7.10
7.09
7.08
6.34
6.30
3.86
2.43
F
N
NHTs
COOMe
1.00
0.98
1.02
2.01
1.07
2.05
1.07
1.04
1.10
3.06
2.98
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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142.70
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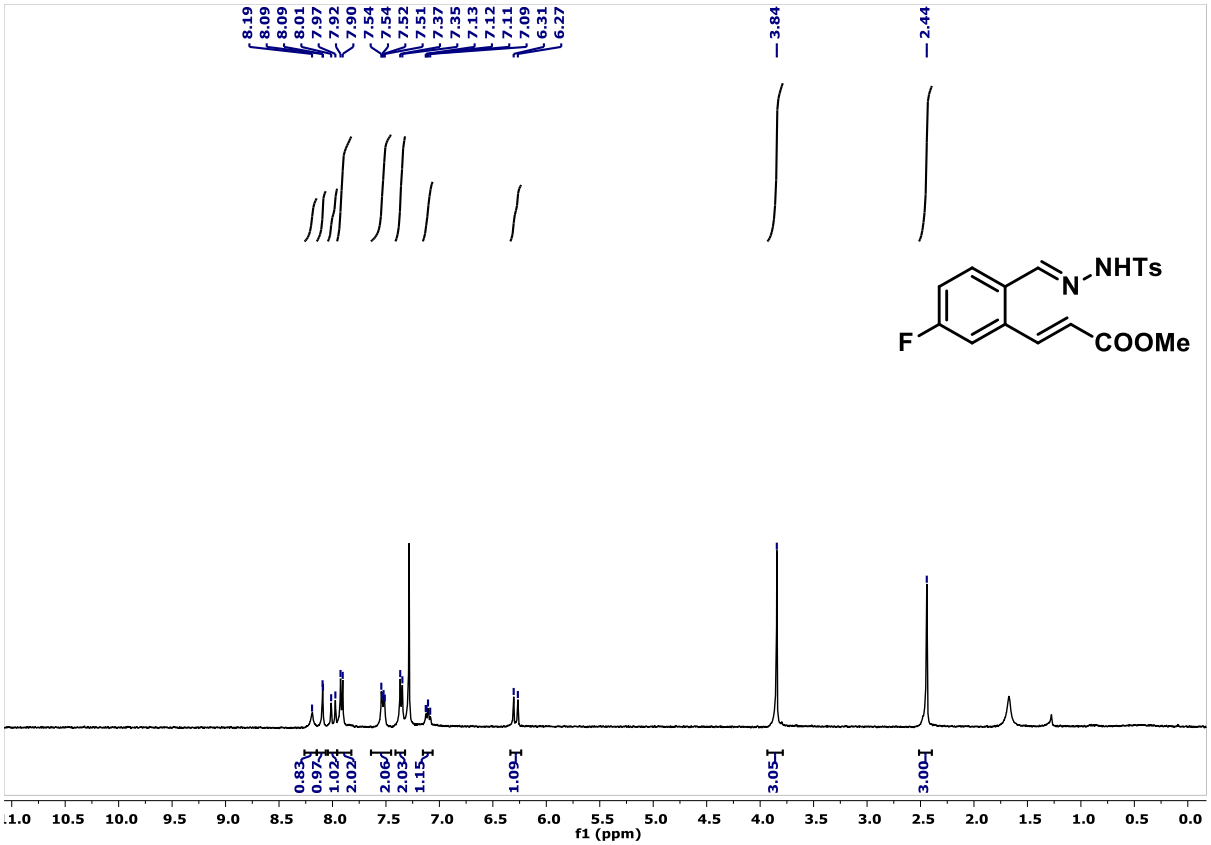
135.04
134.18
134.10
129.67
129.29
129.20
127.88
120.81
117.69
117.47
113.70
113.47
51.92
21.51
F
N
NHTs
COOMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.09
8.09
8.01
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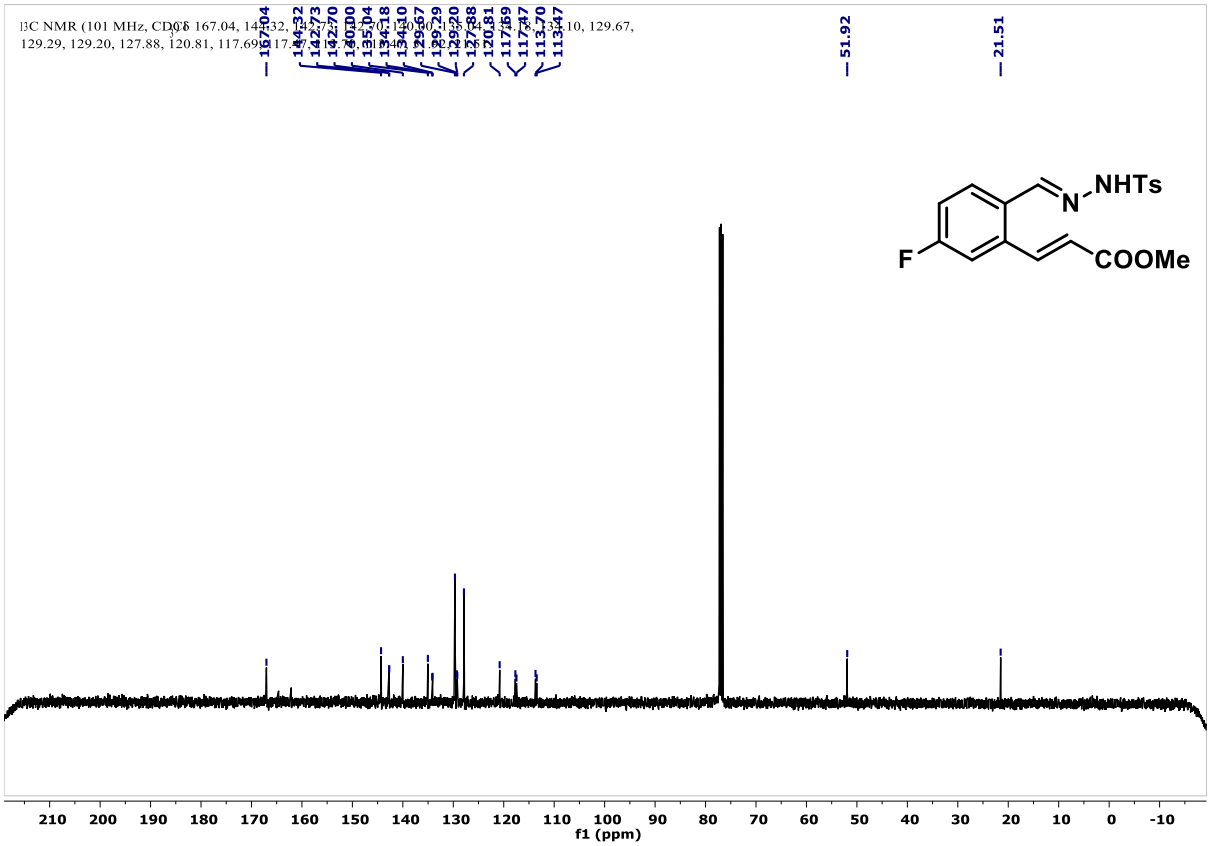
7.92
7.90
7.54
7.54
7.52
7.51
7.37
7.35
7.13
7.12
7.11
7.09
6.31
6.27
3.84
2.44
NHTs
N
F
COOMe
0.83
0.97
1.02
2.02
2.06
2.03
1.15
1.09
3.05
3.00
f1 (ppm)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142.73
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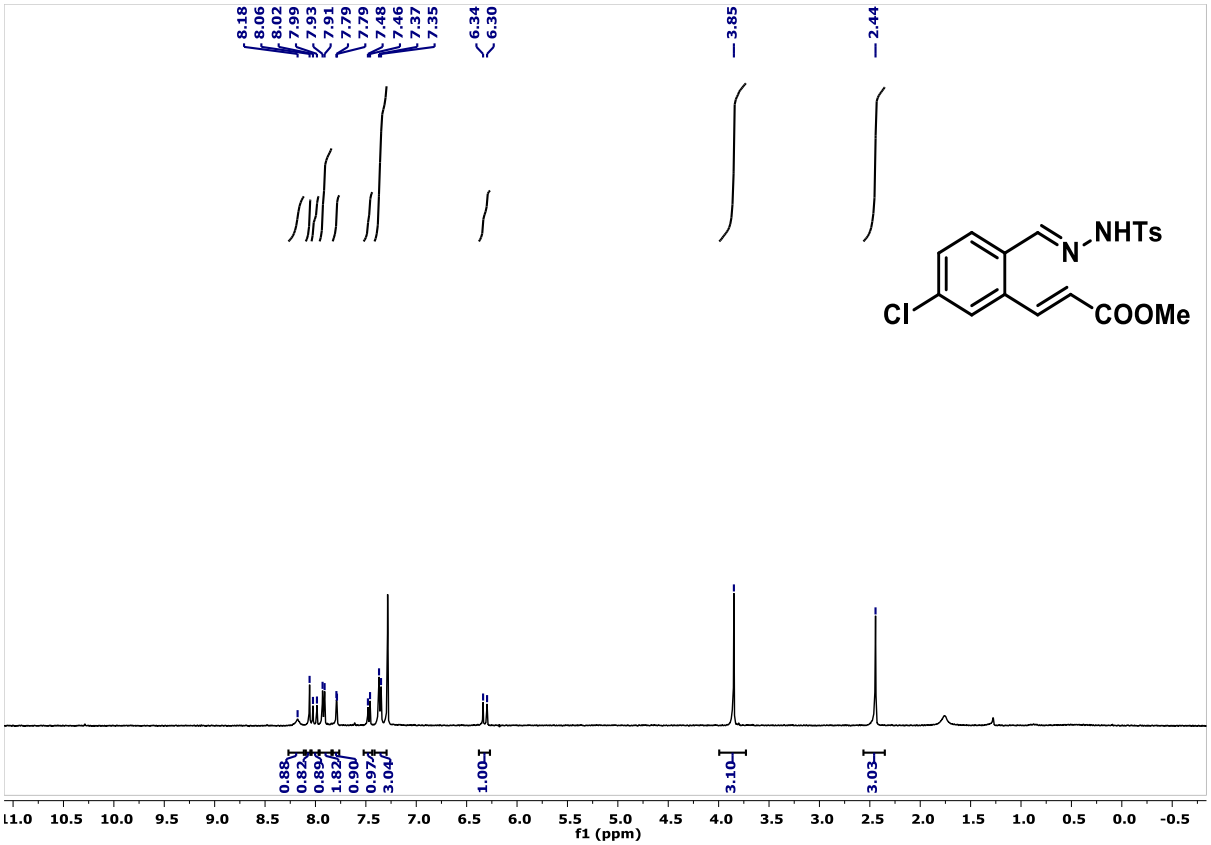
135.04
134.18
134.10
129.67
129.29
129.20
127.88
120.81
117.69
117.47
113.70
113.47
51.92
21.51
NHTs
N
F
COOMe
f1 (ppm)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8.06
8.02
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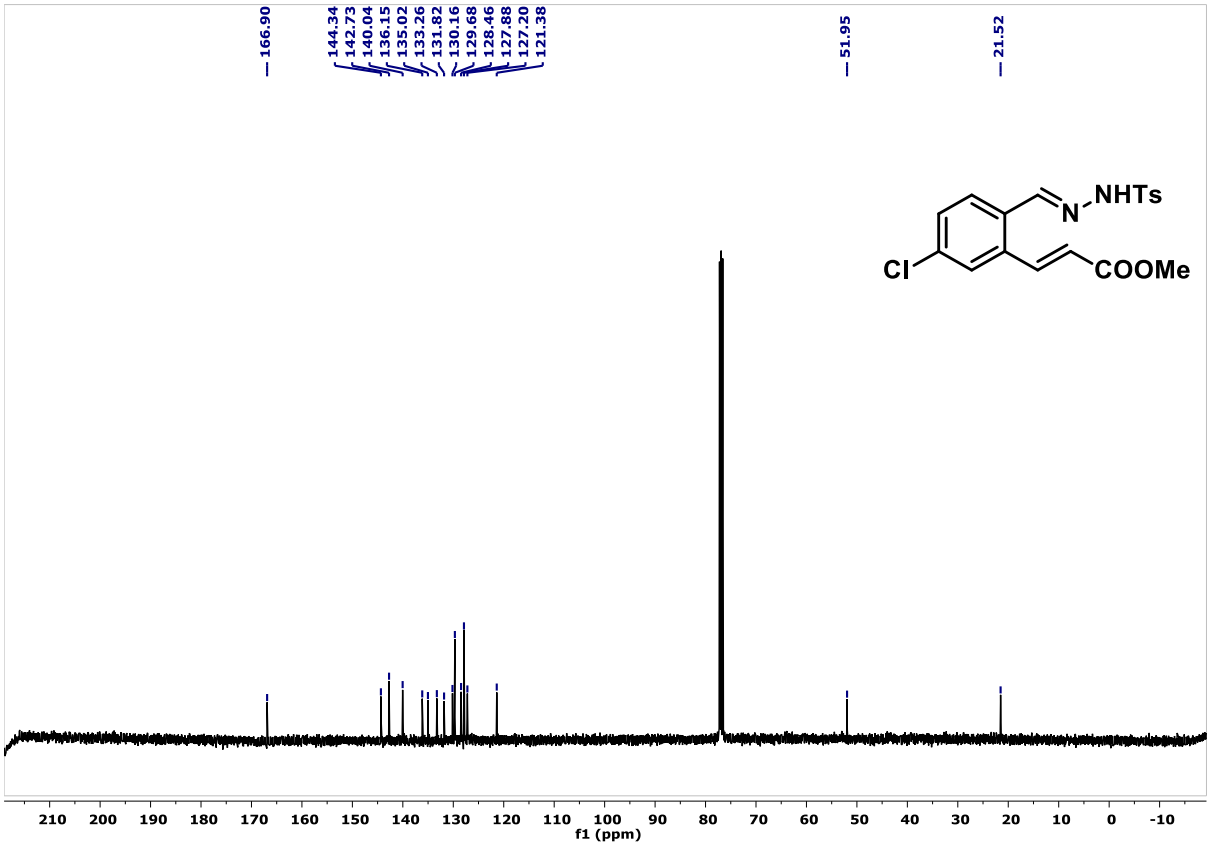
7.91
7.79
7.79
7.48
7.46
7.37
7.35
6.34
6.30
3.85
2.44
NHTs
N
Cl
COOMe
0.88
0.82
0.89
1.82
0.90
0.97
3.04
1.00
3.10
3.03
f1 (ppm)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142.73
140.04
136.15
135.02
133.26
131.82
130.16
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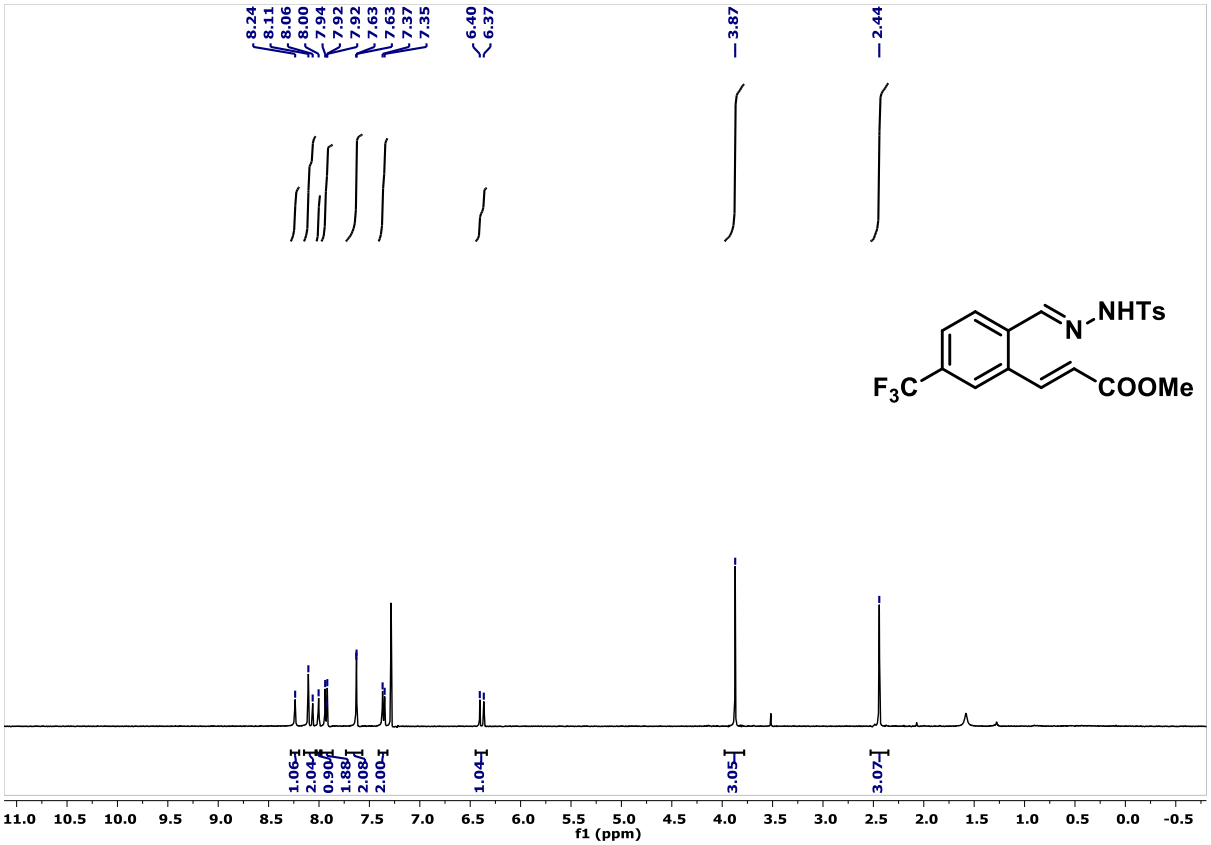
128.46
127.88
127.20
121.38
51.95
21.52
NHTs
N
Cl
COOMe
f1 (ppm)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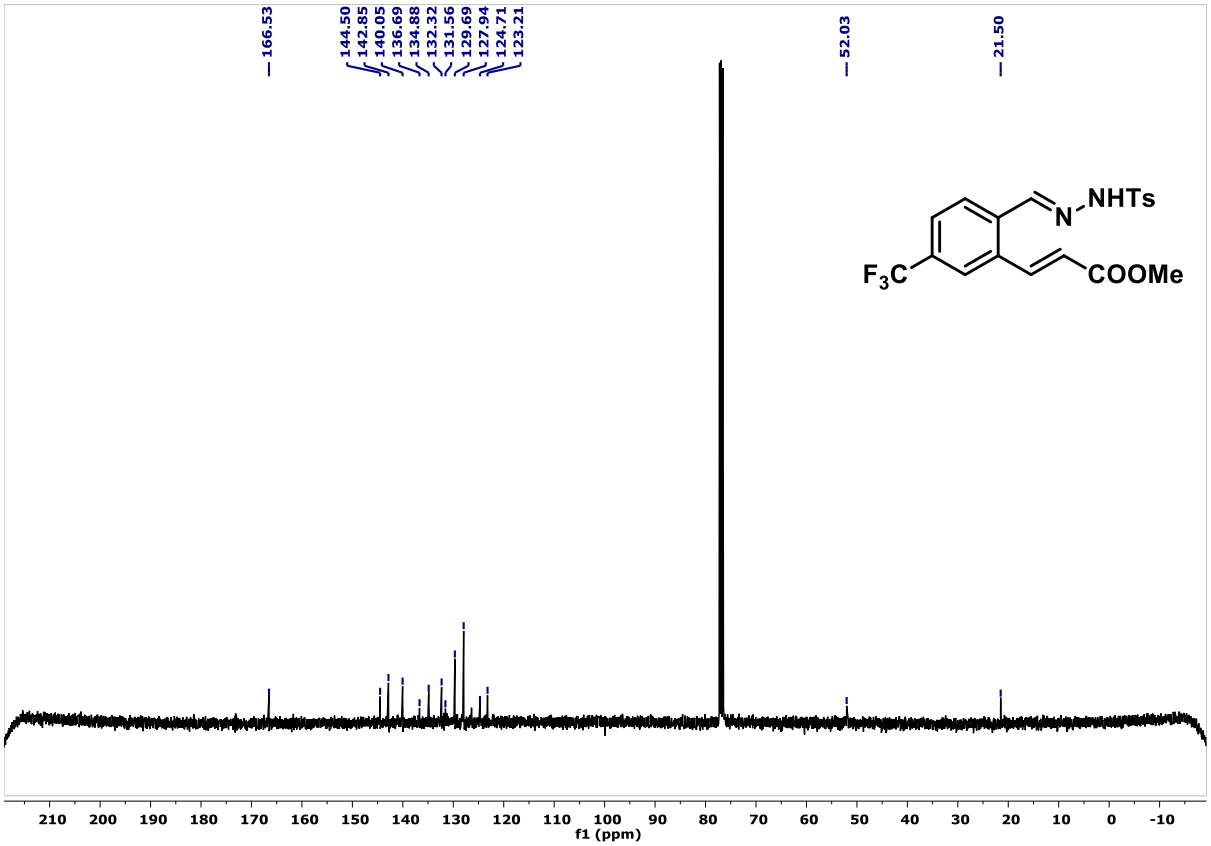
8.11
8.06
8.00
7.94
7.92
7.92
7.63
7.63
7.37
7.35
6.40
6.37
3.87
2.44
NHTs
N
F3C
COOMe
1.06
2.04
0.90
1.88
2.08
2.00
1.04
3.05
3.07
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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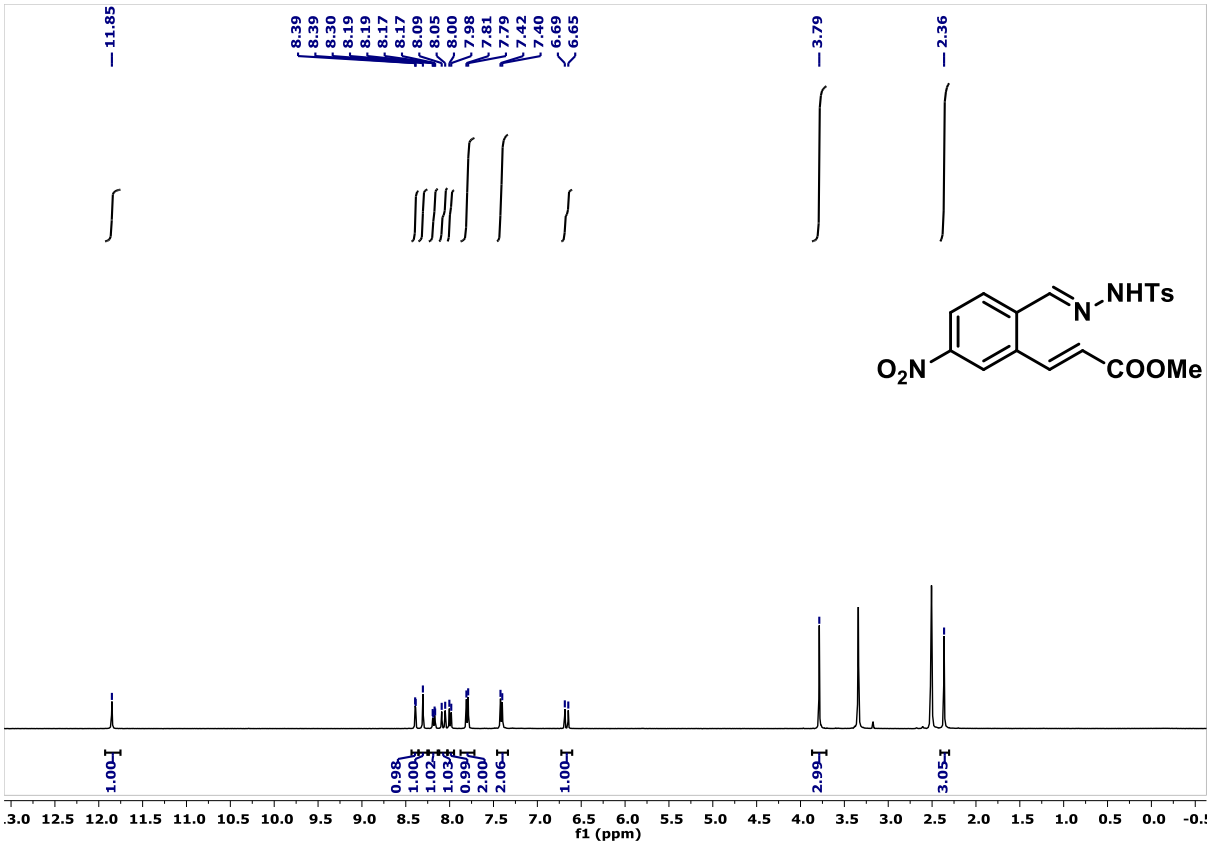
142.85
140.05
136.69
134.88
132.32
131.56
129.69
127.94
124.71
123.21
52.03
21.50
NHTs
N
F3C
COOMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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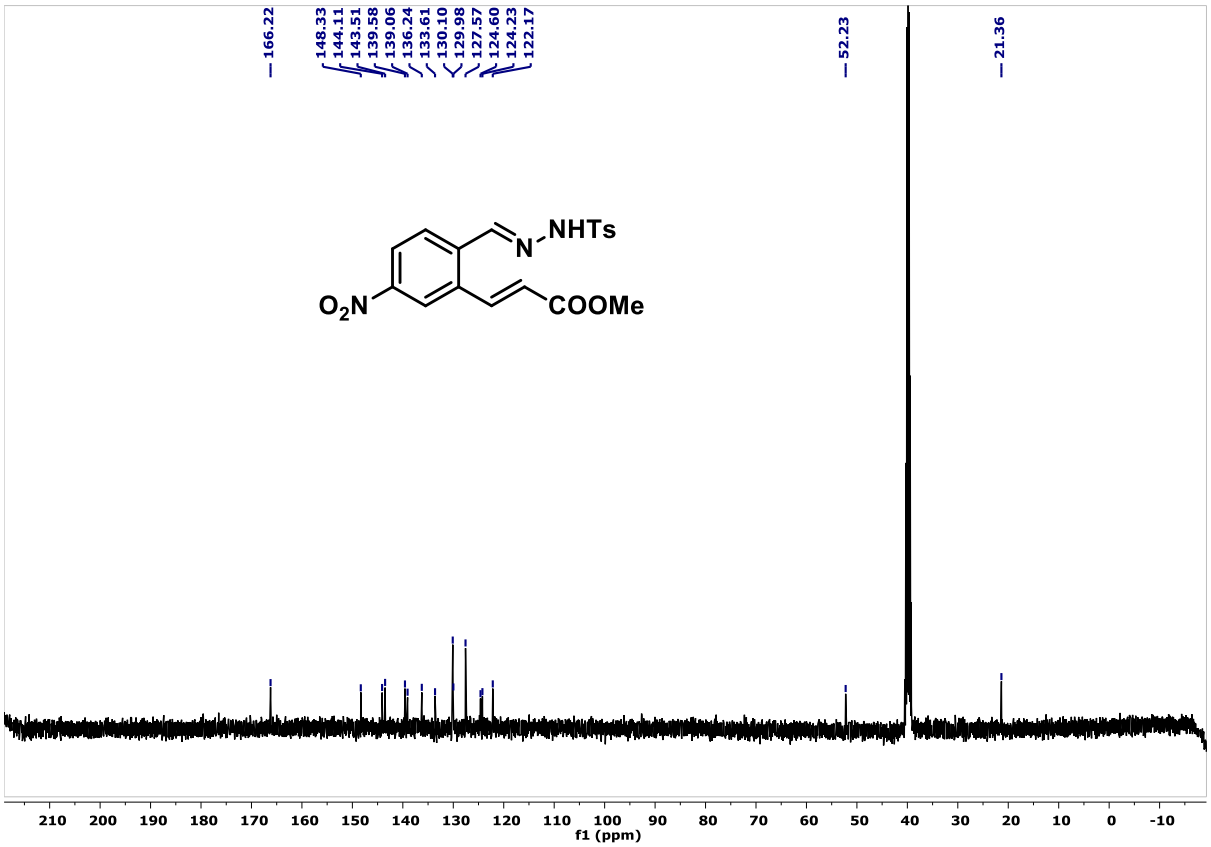
8.39
8.39
8.30
8.19
8.19
8.17
8.17
8.09
8.05
8.00
7.98
7.81
7.79
7.42
7.40
6.69
6.65
3.79
2.36
NHTs
N
O2N
COOMe
1.00
0.98
1.00
1.02
1.03
0.99
2.00
2.06
1.00
2.99
3.05
f1 (ppm)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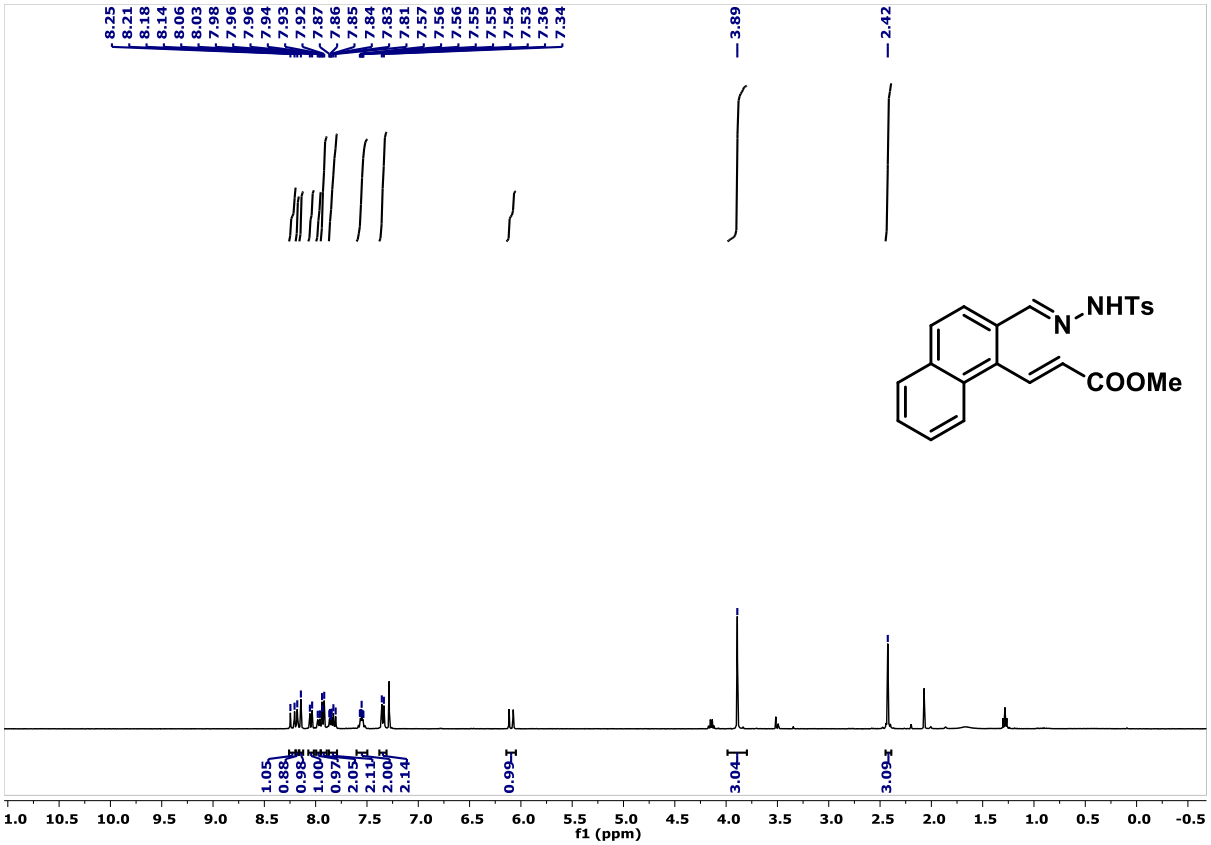
148.33
144.11
143.51
139.58
139.06
136.24
133.61
130.10
129.98
127.57
124.60
124.23
122.17
52.23
21.36
NHTs
N
O2N
COOMe
f1 (ppm)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8.21
8.18
8.14
8.06
8.03
7.98
7.96
7.96
7.94
7.93
7.92
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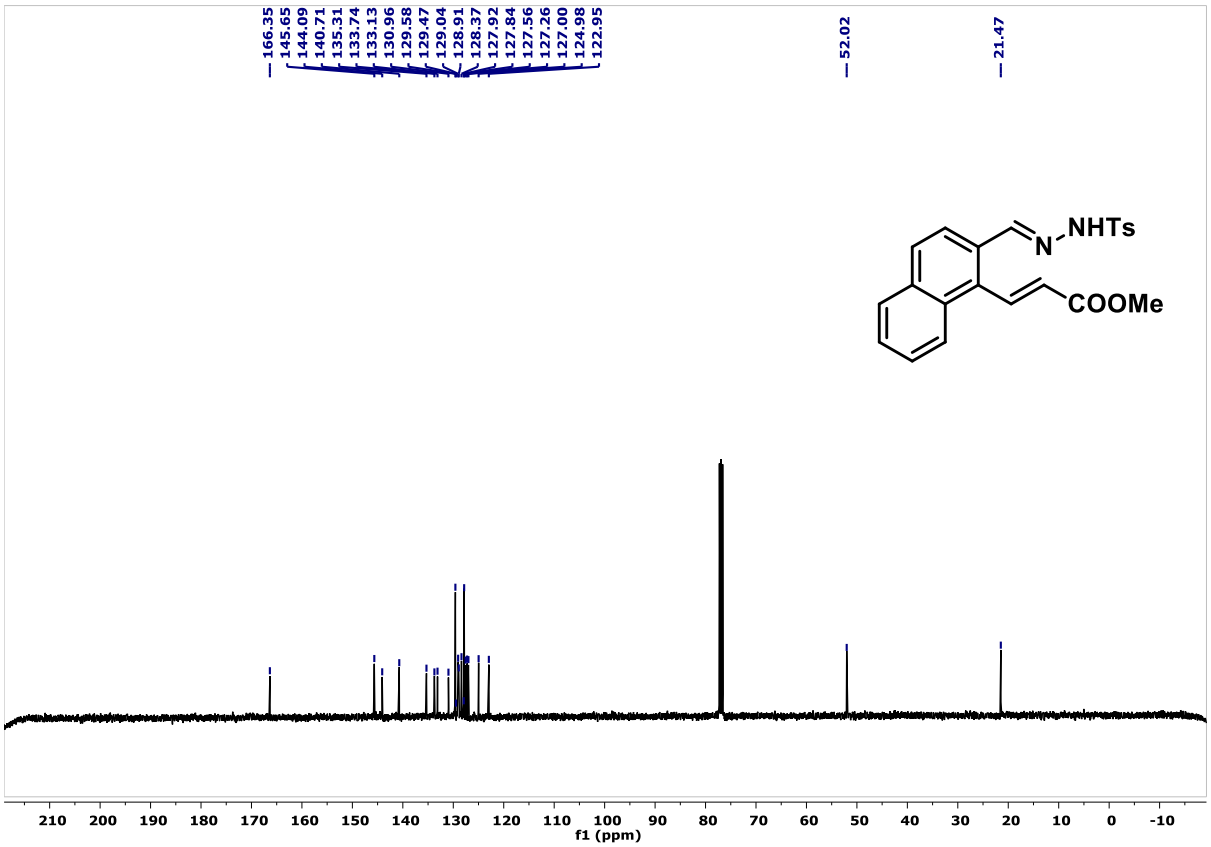
7.86
7.85
7.84
7.83
7.81
7.57
7.56
7.56
7.55
7.55
7.54
7.53
7.36
7.34
3.89
2.42
NHTs
N
COOMe
1.05
0.88
0.98
1.00
0.97
2.05
2.11
2.00
2.14
0.99
3.04
3.09
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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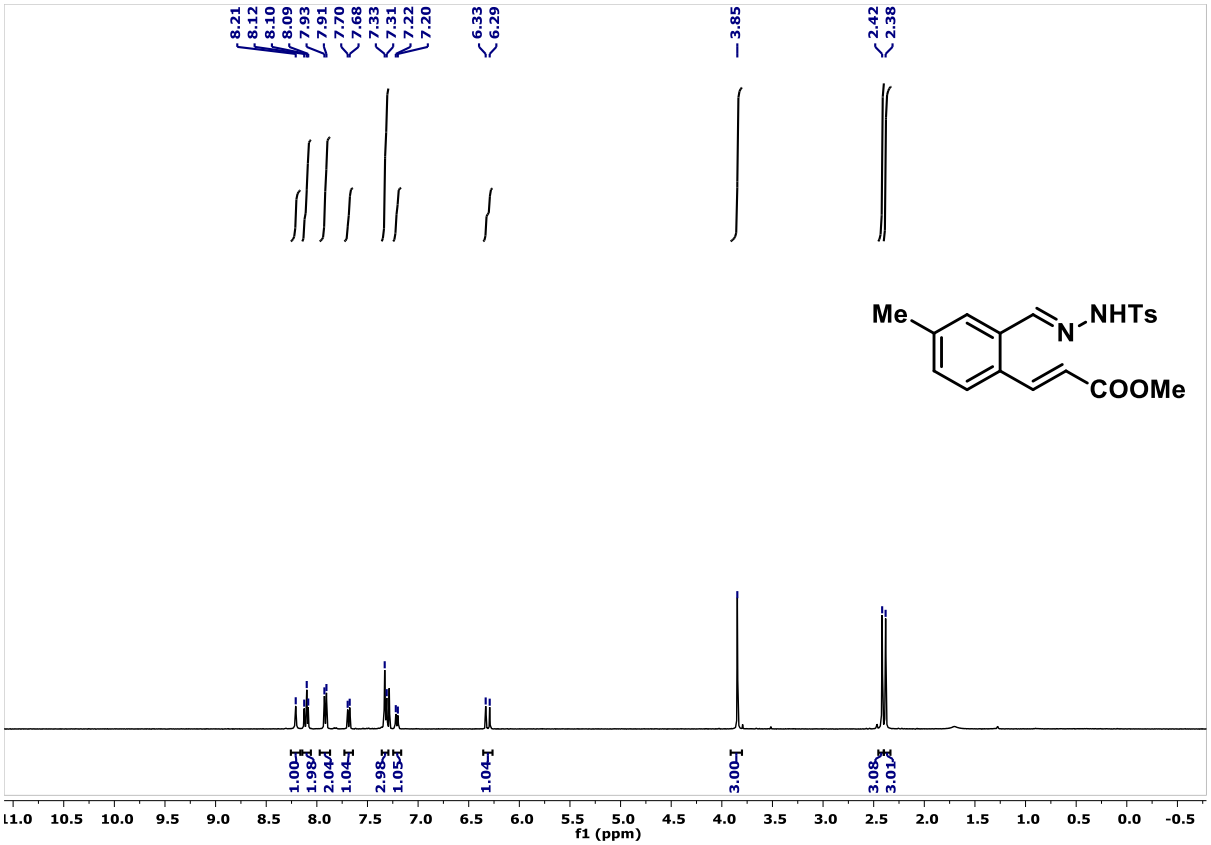
145.65
144.09
140.71
135.31
133.74
133.13
130.96
129.58
129.47
129.04
128.91
128.37
127.92
127.84
127.56
127.26
127.00
124.98
122.95
52.02
21.47
NHTs
N
COOMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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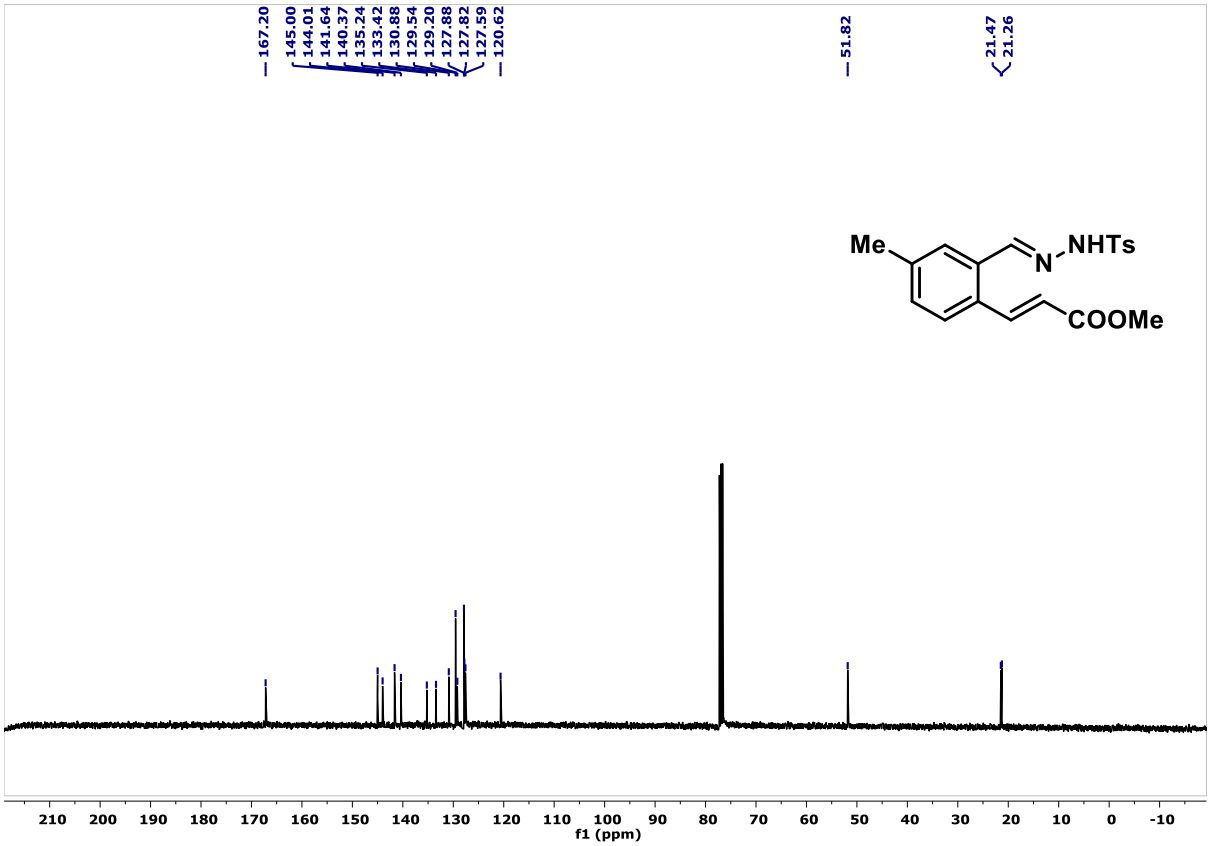
8.12
8.10
8.09
7.93
7.91
7.70
7.68
7.33
7.31
7.22
7.20
6.33
6.29
3.85
2.42
2.38
Me
NHTs
N
COOMe
1.00
1.98
2.04
1.04
2.98
1.05
1.04
3.00
3.08
3.01
f1 (ppm)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133.42
130.88
129.54
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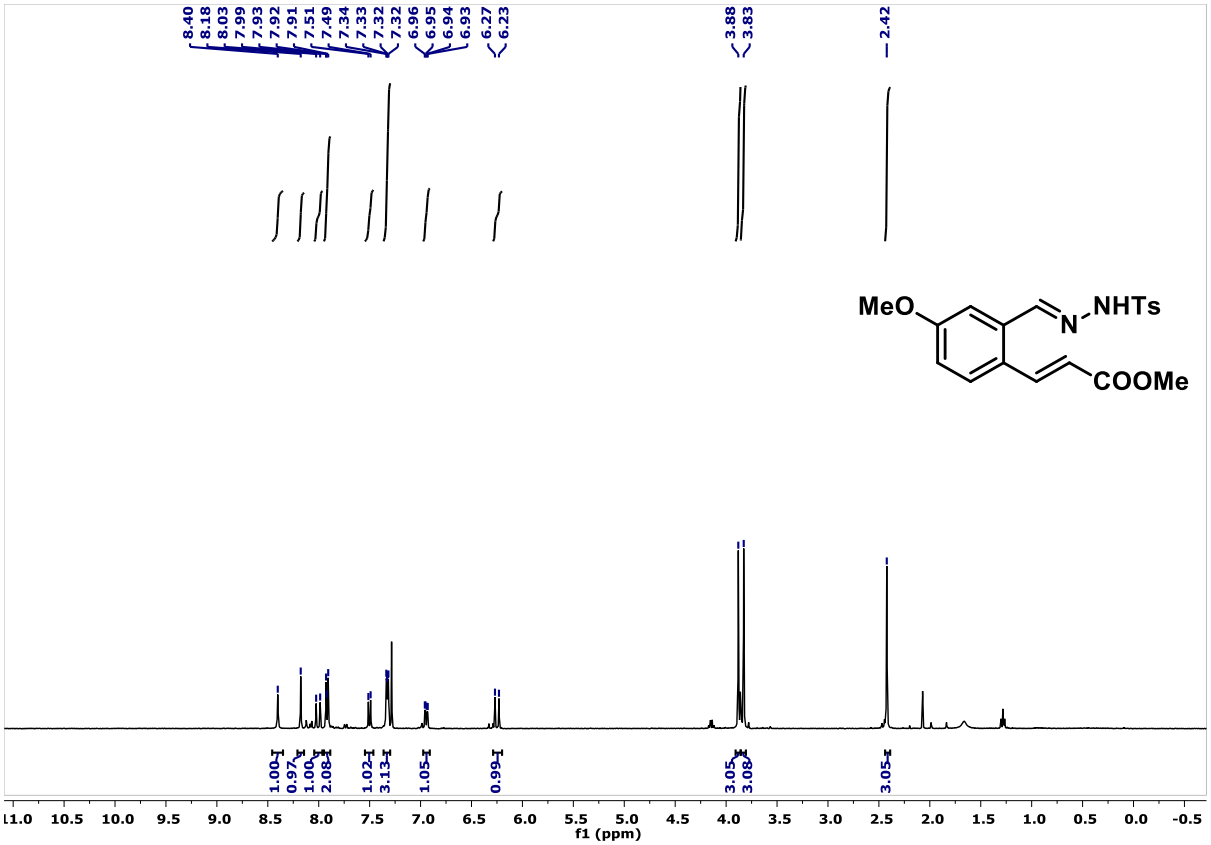
127.82
127.59
120.62
51.82
21.47
21.26
Me
NHTs
N
COOMe
f1 (ppm)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8.18
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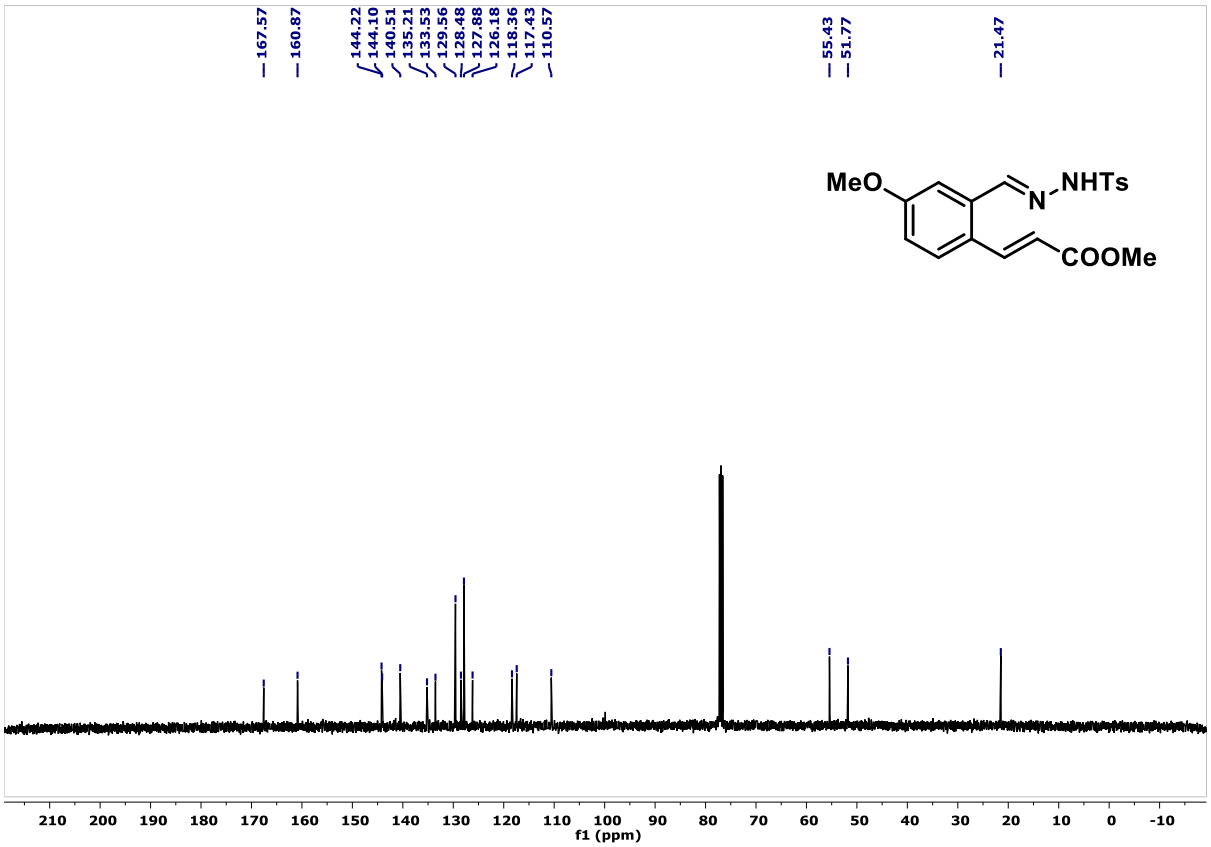
7.92
7.91
7.51
7.49
7.34
7.33
7.32
7.32
6.96
6.95
6.94
6.93
6.27
6.23
3.88
3.83
2.42
MeO
N
NHTs
COOMe
1.00
0.97
1.00
2.08
1.02
3.13
1.05
0.99
3.05
3.08
3.05
f1 (ppm)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160.87
144.22
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133.53
129.56
128.48
127.88
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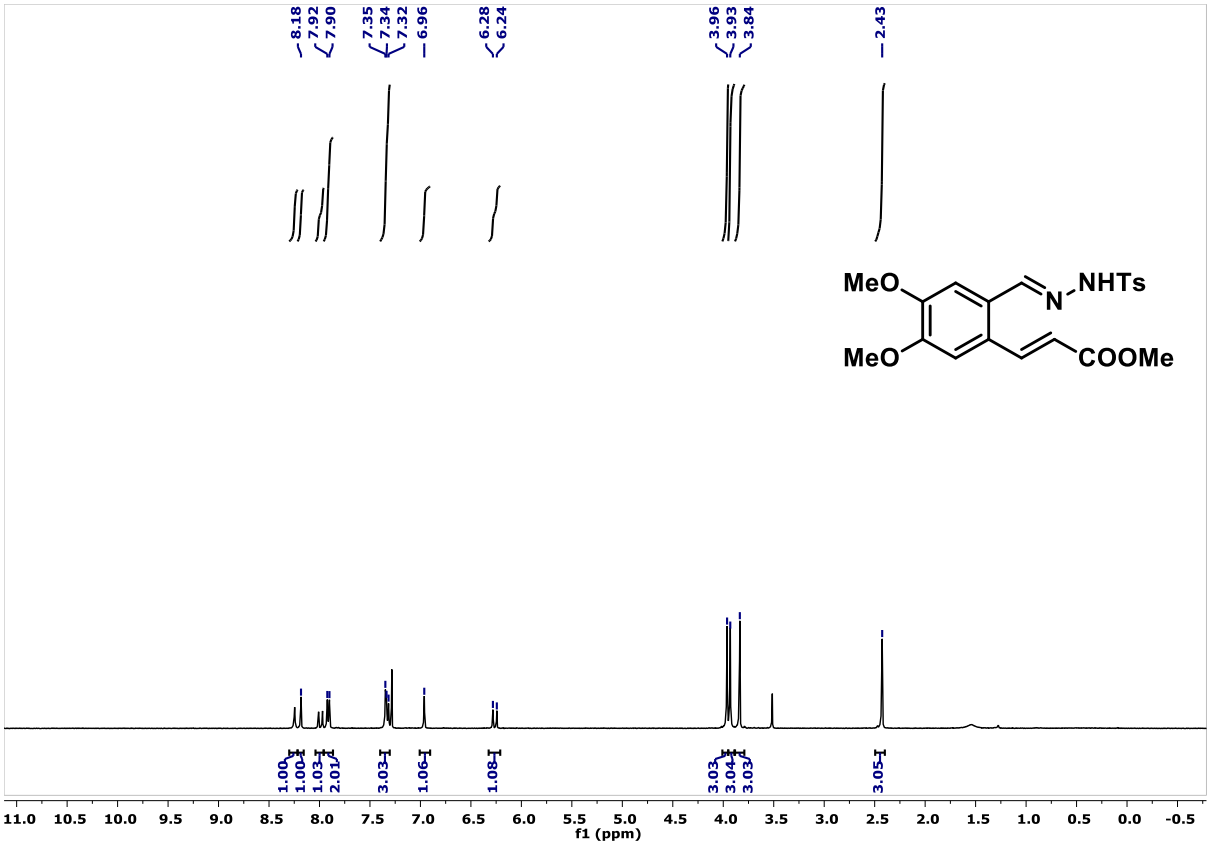
117.43
110.57
55.43
51.77
21.47
MeO
N
NHTs
COOMe
f1 (ppm)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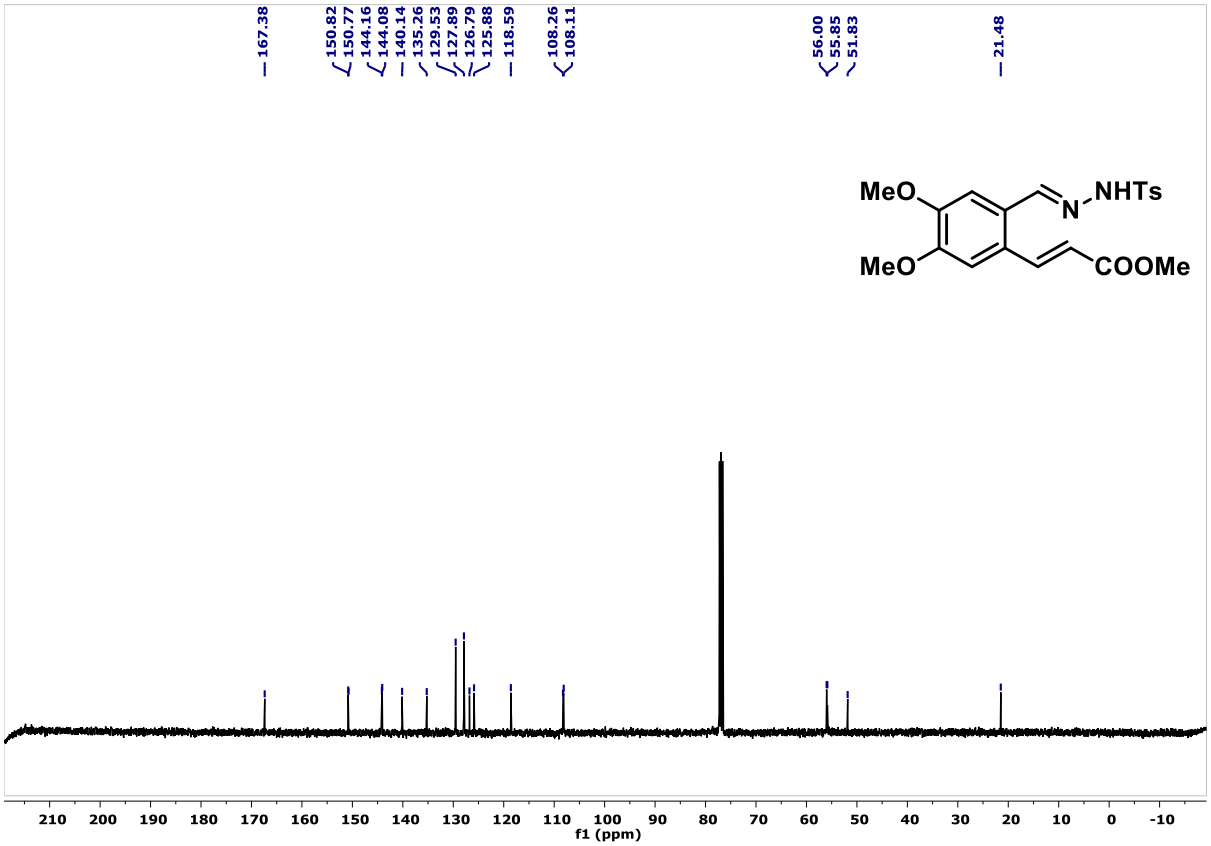
7.92
7.90
7.35
7.34
7.32
6.96
6.28
6.24
3.96
3.93
3.84
2.43
MeO
MeO
N
NHTs
COOMe
1.00
1.00
1.03
2.01
3.03
1.06
1.08
3.03
3.04
3.03
3.05
f1 (ppm)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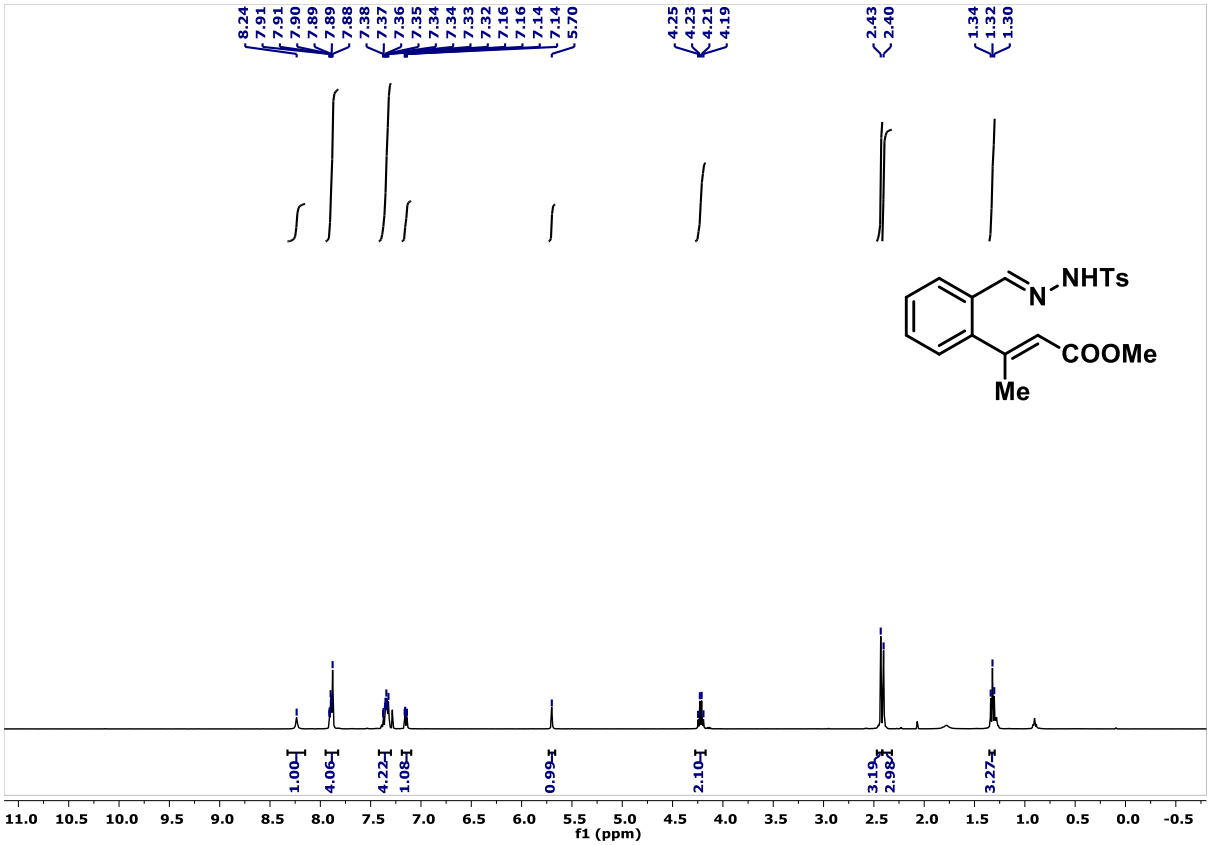
140.14
135.26
129.53
127.89
126.79
125.88
118.59
108.26
108.11
56.00
55.85
51.83
21.48
MeO
MeO
N
NHTs
COOMe
f1 (ppm)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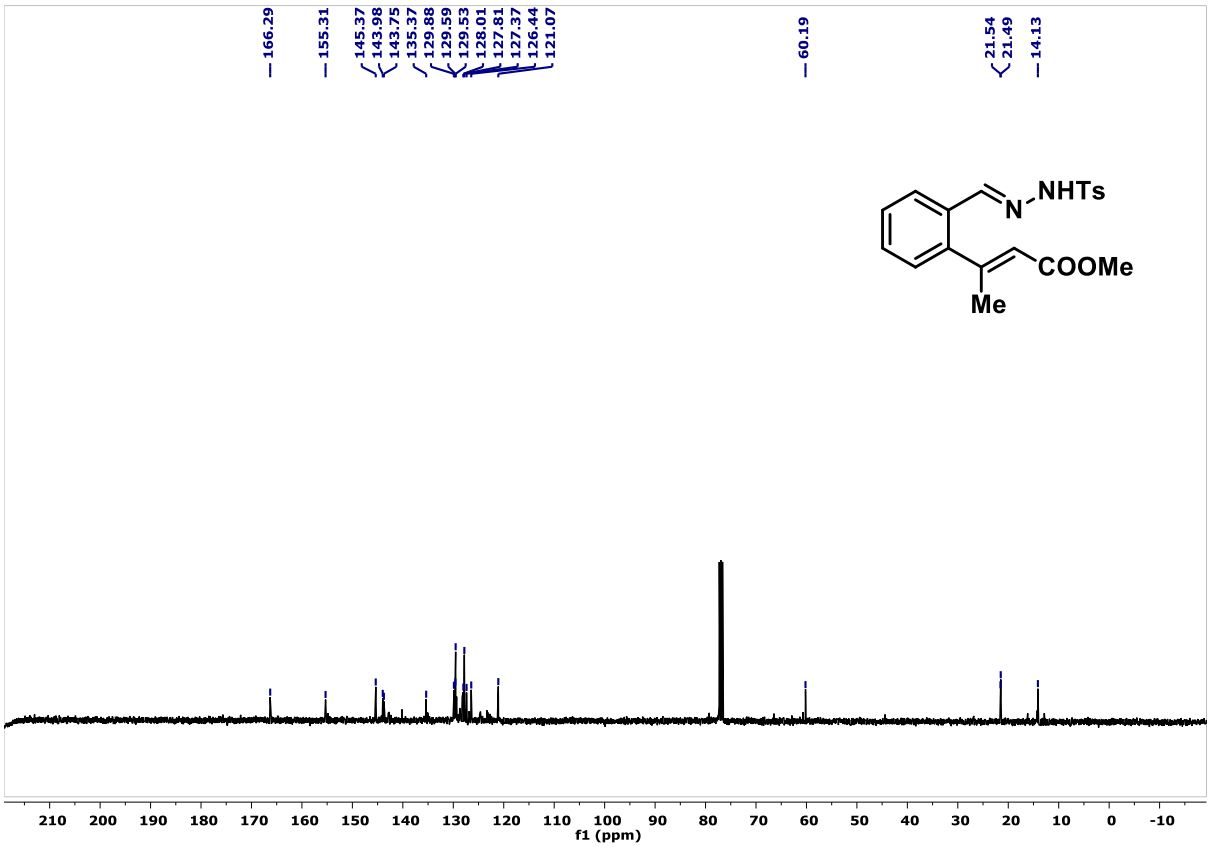
7.91
7.90
7.89
7.89
7.88
7.38
7.37
7.36
7.35
7.34
7.34
7.33
7.32
7.16
7.16
7.14
7.14
5.70
4.25
4.23
4.21
4.19
2.43
2.40
1.34
1.32
1.30
NHTs
N
COOMe
Me
1.00
4.06
4.22
1.08
0.99
2.10
3.19
2.98
3.27
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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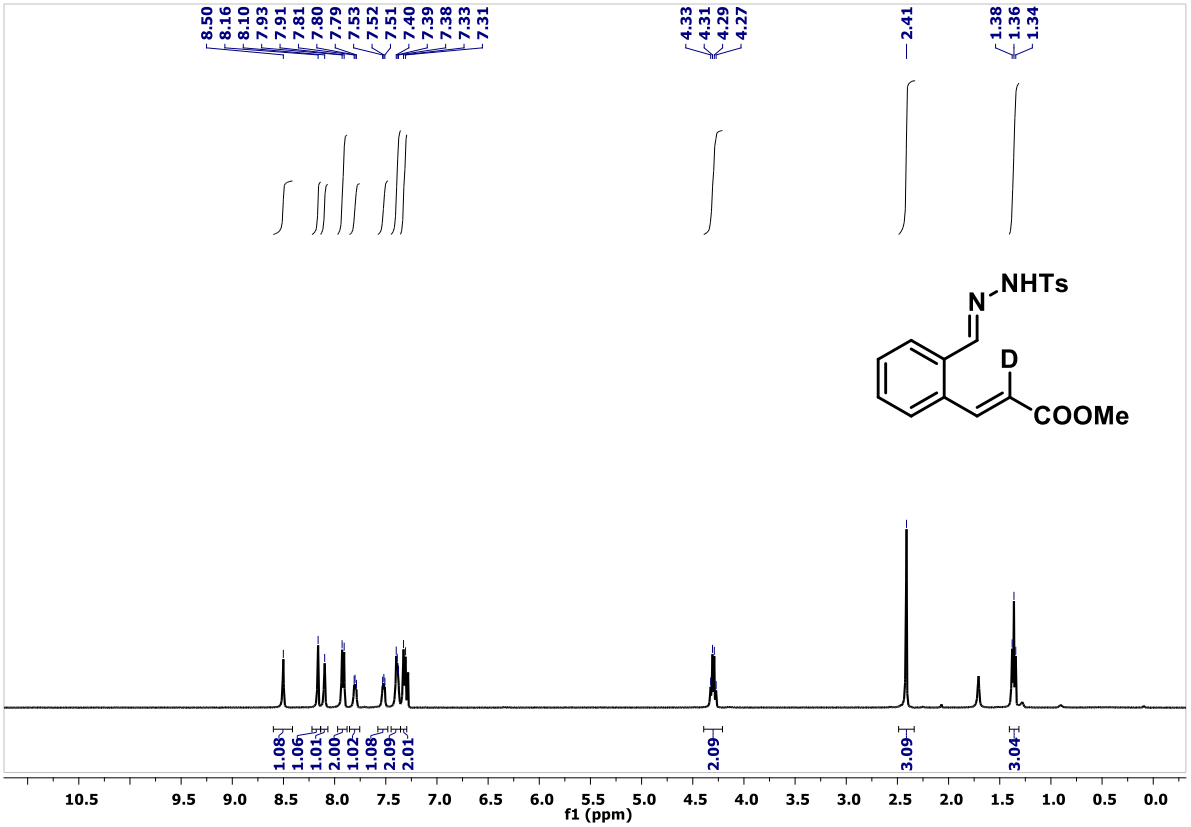
129.59
129.53
128.01
127.81
127.37
126.44
121.07
60.19
21.54
21.49
14.13
NHTs
N
COOMe
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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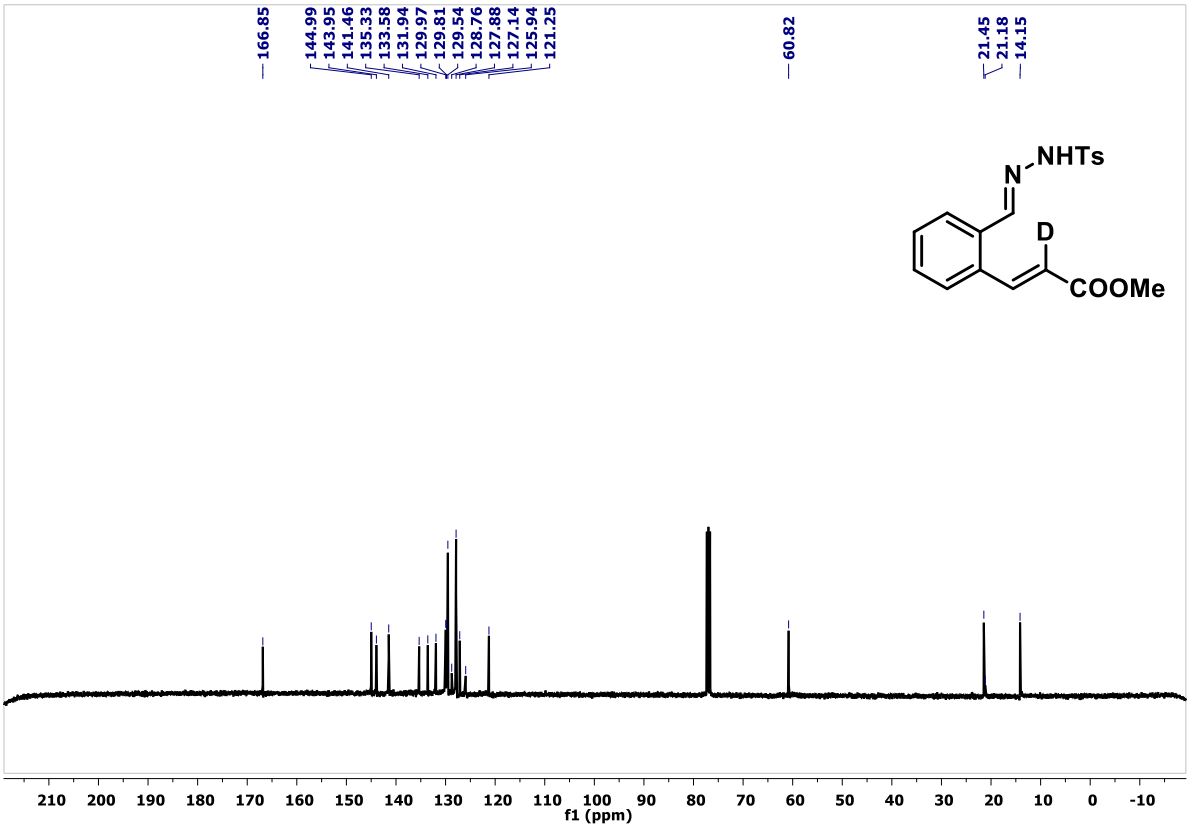
7.80
7.79
7.53
7.52
7.51
7.40
7.39
7.38
7.33
7.31
4.33
4.31
4.29
4.27
2.41
1.38
1.36
1.34
NHTs
N
D
COOMe
1.08
1.06
1.01
2.00
1.02
1.08
2.09
2.01
2.09
3.09
3.04
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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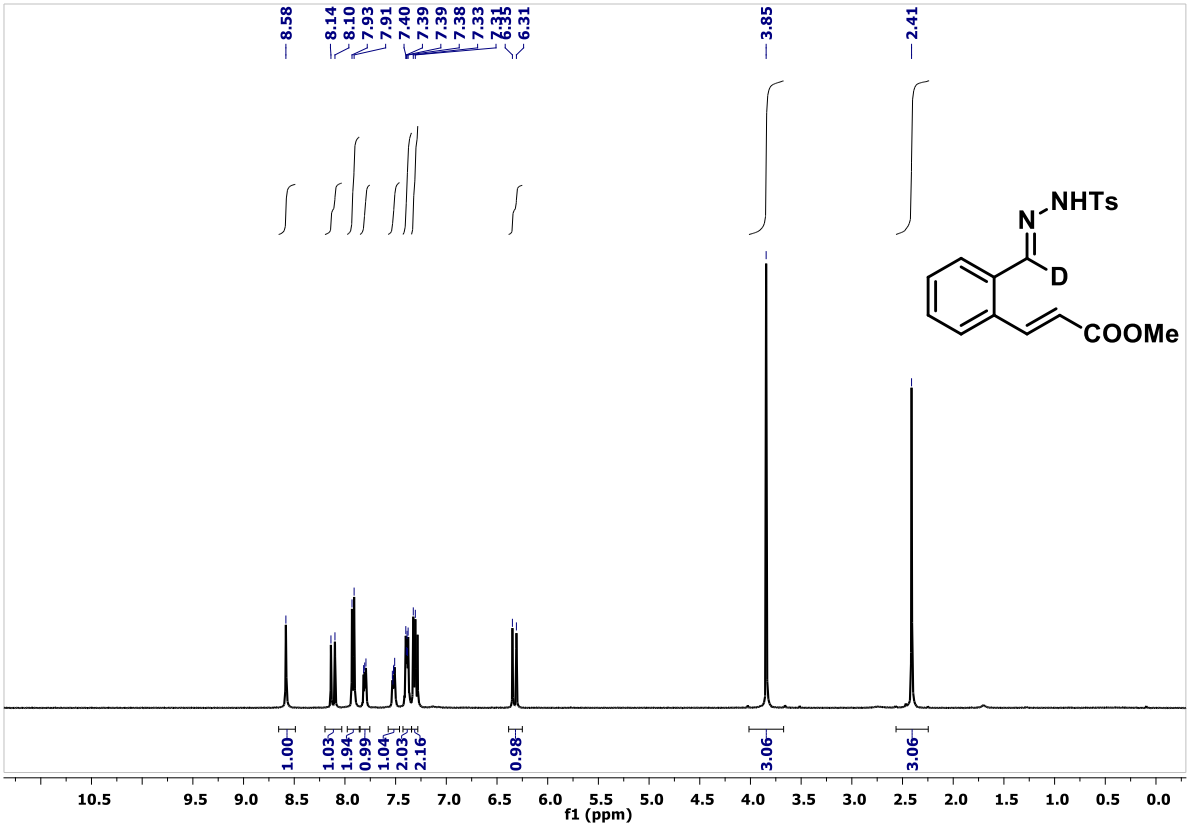
133.58
131.94
129.97
129.81
129.54
128.76
127.88
127.14
125.94
121.25
60.82
21.45
21.18
14.15
NHTs
N
D
COOMe
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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8.10
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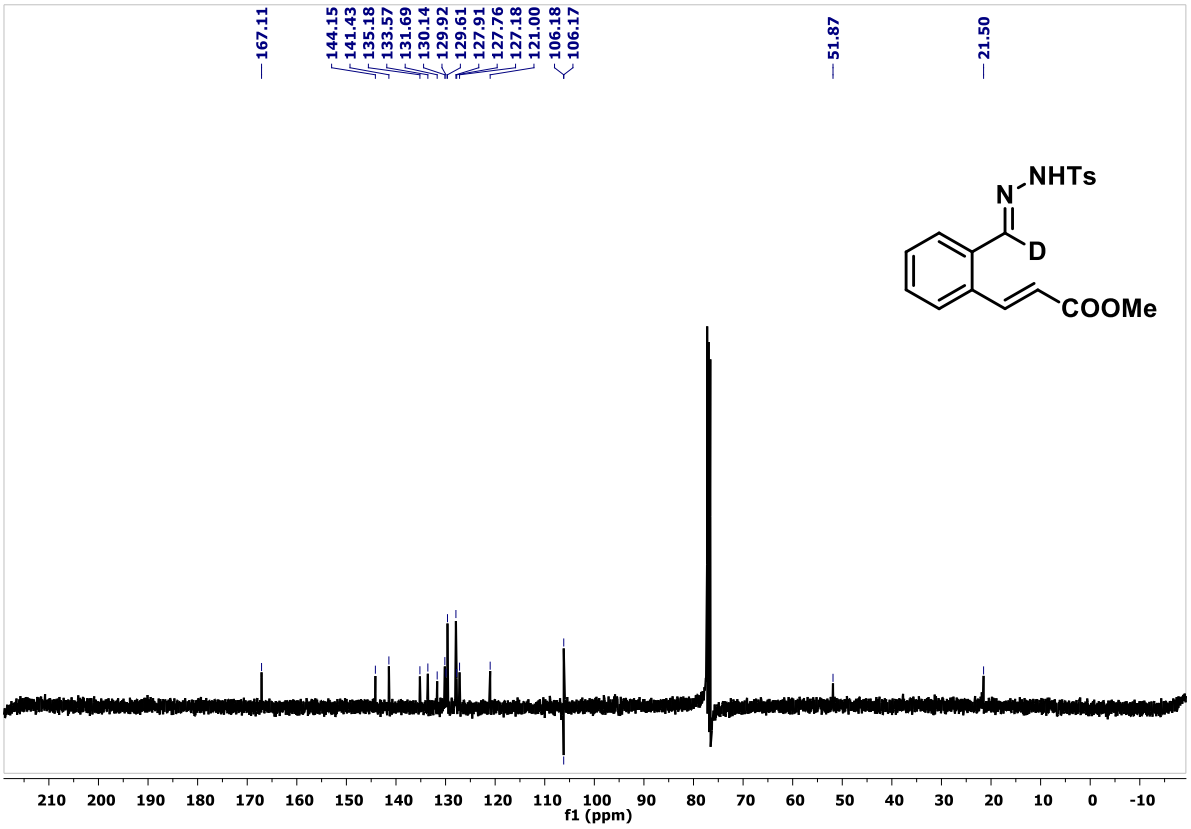
7.40
7.39
7.39
7.38
7.33
6.35
6.31
3.85
2.41
NHTs
N
D
COOMe
1.00
1.03
1.94
0.99
1.04
2.03
2.16
0.98
3.06
3.06
f1 (ppm)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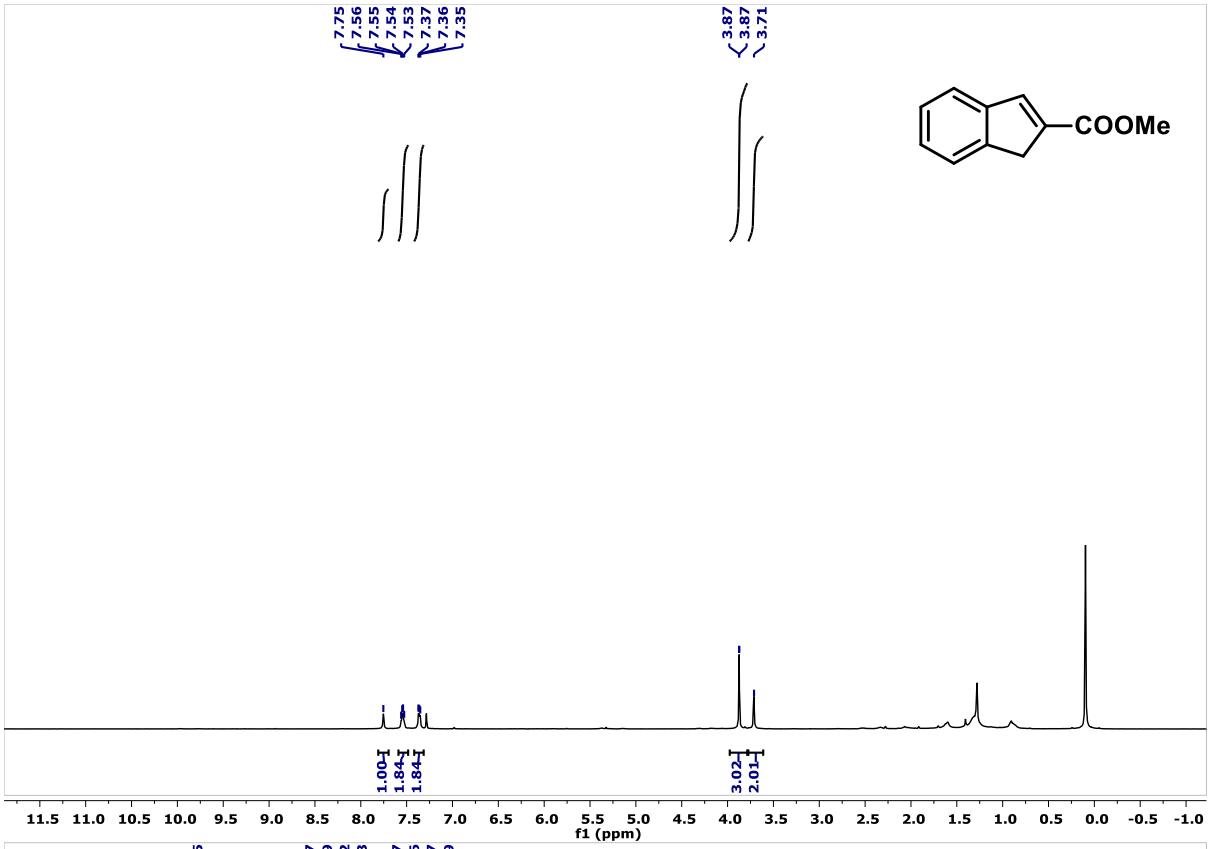
135.18
133.57
131.69
130.14
129.92
129.61
127.91
127.76
127.18
121.00
106.18
106.17
51.87
21.50
NHTs
N
D
COOMe
f1 (ppm)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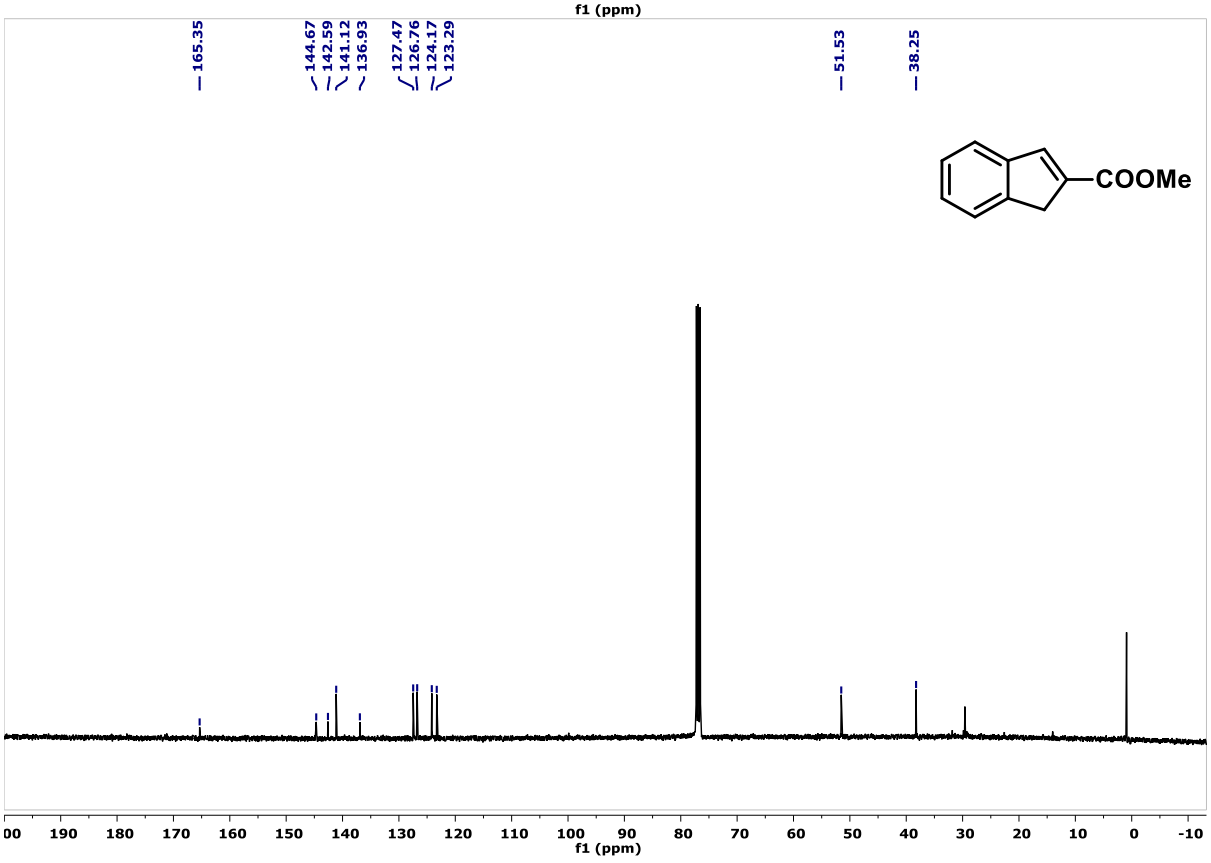
7.55
7.54
7.53
7.37
7.36
7.35
3.87
3.87
3.71
COOMe
1.00
1.84
1.84
3.02
2.01
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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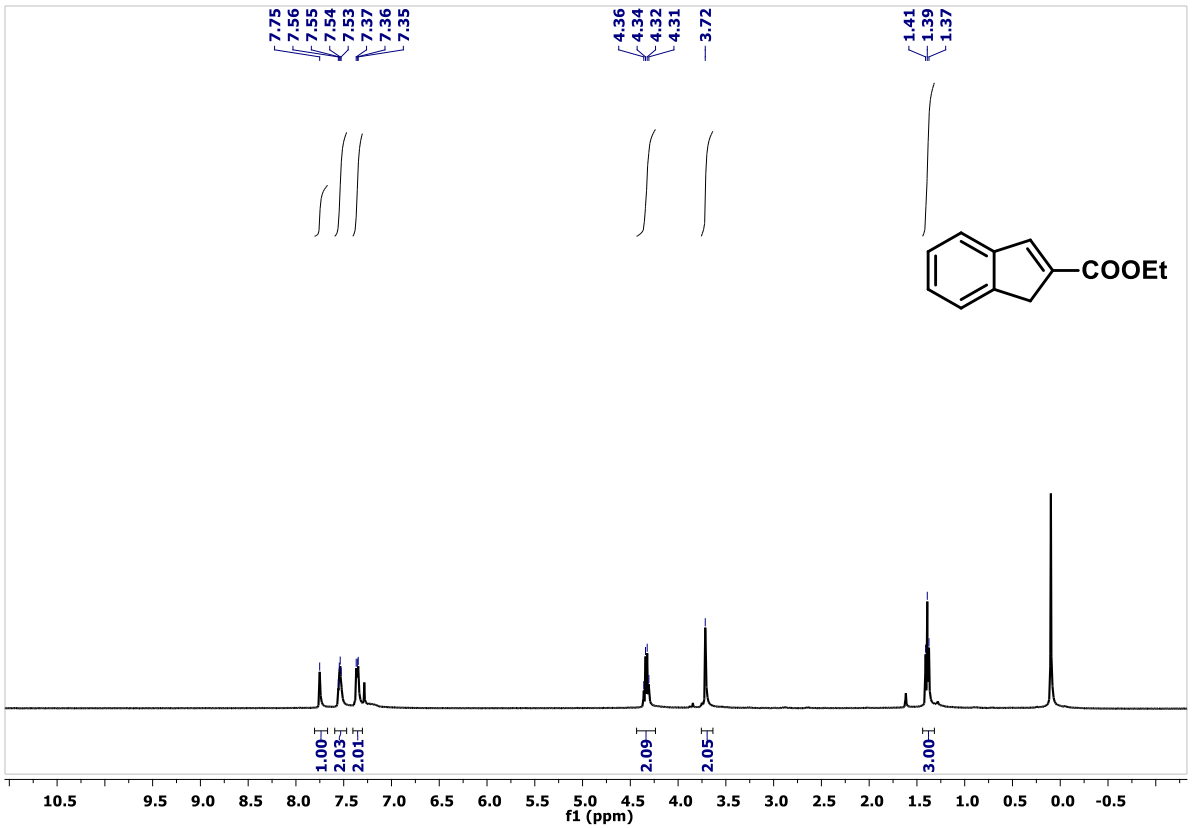
144.67
142.59
141.12
136.93
127.47
126.76
124.17
123.29
51.53
38.25
COOMe
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.75
7.56
7.55
7.54
7.53
7.37
7.36
7.35
4.36
4.34
4.32
4.31
3.72
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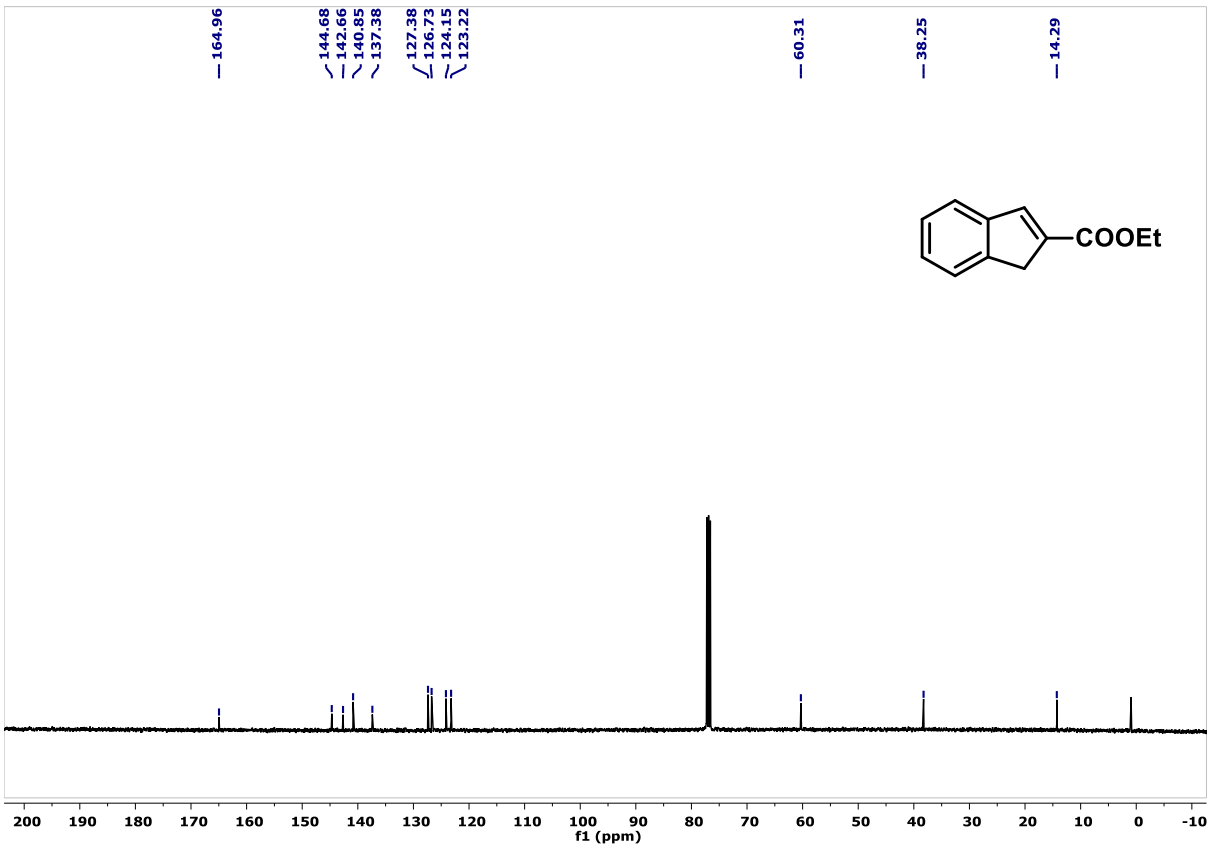
1.39
1.37
COOEt
1.00
2.03
2.01
2.09
2.05
3.00
f1 (ppm)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124.15
123.22
60.31
38.25
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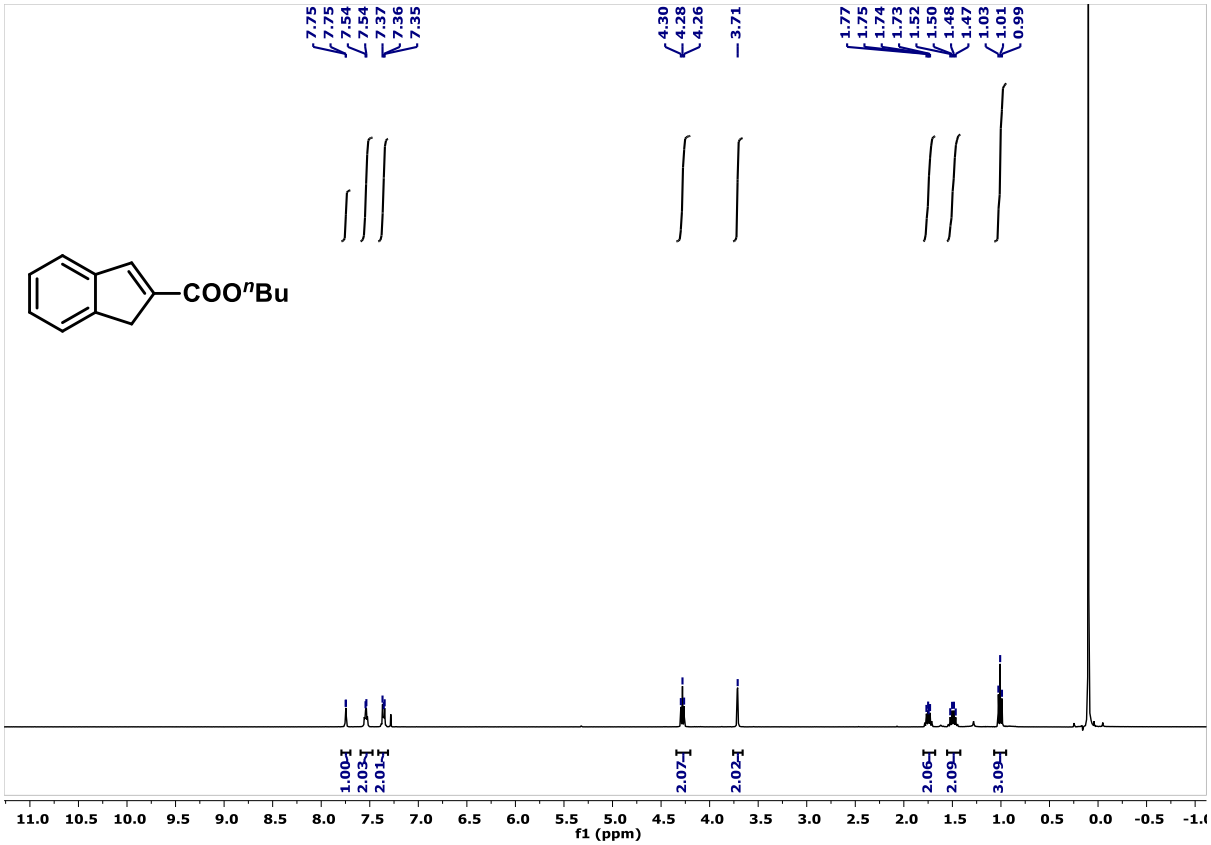
COOEt
f1 (ppm)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1.75
1.74
1.73
1.52
1.50
1.48
1.47
1.03
1.01
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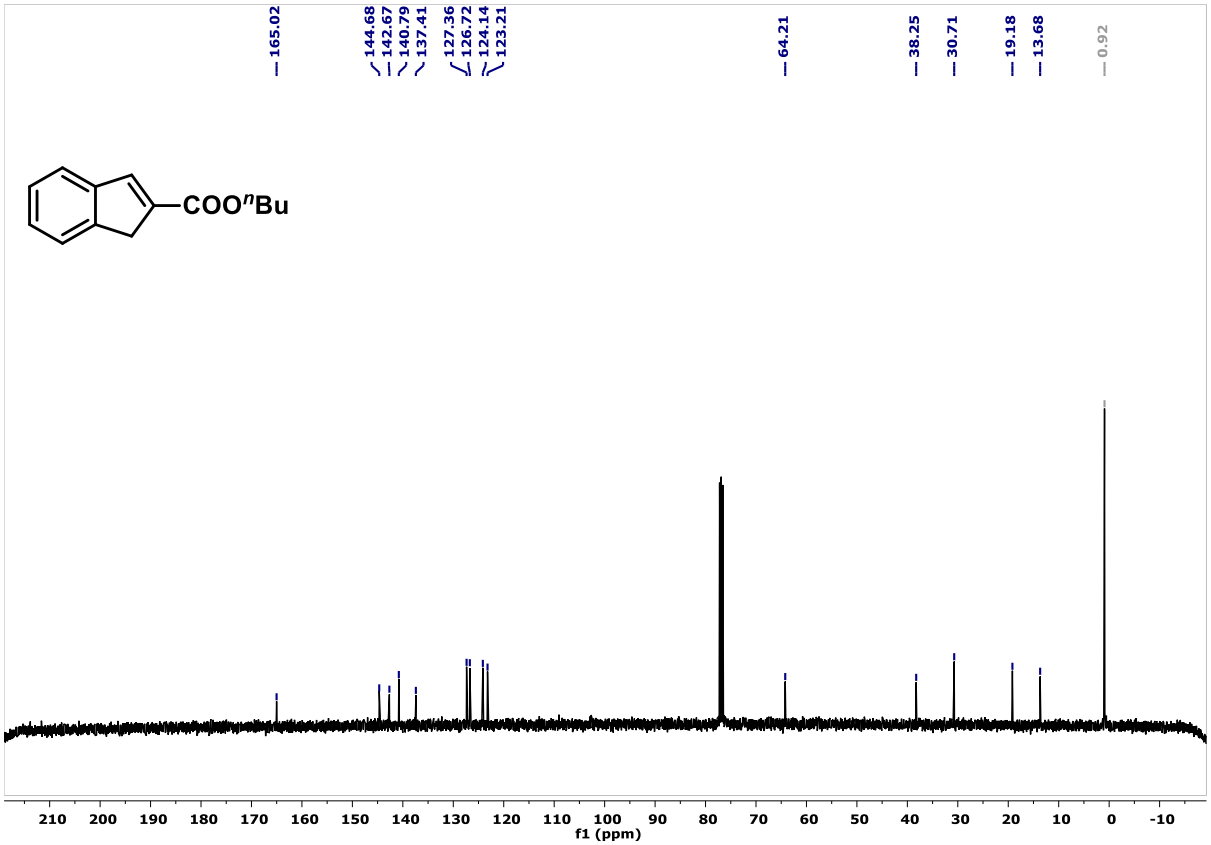
COO^{n}Bu
1.00
2.03
2.01
2.07
2.02
2.06
2.09
3.09
f1 (ppm)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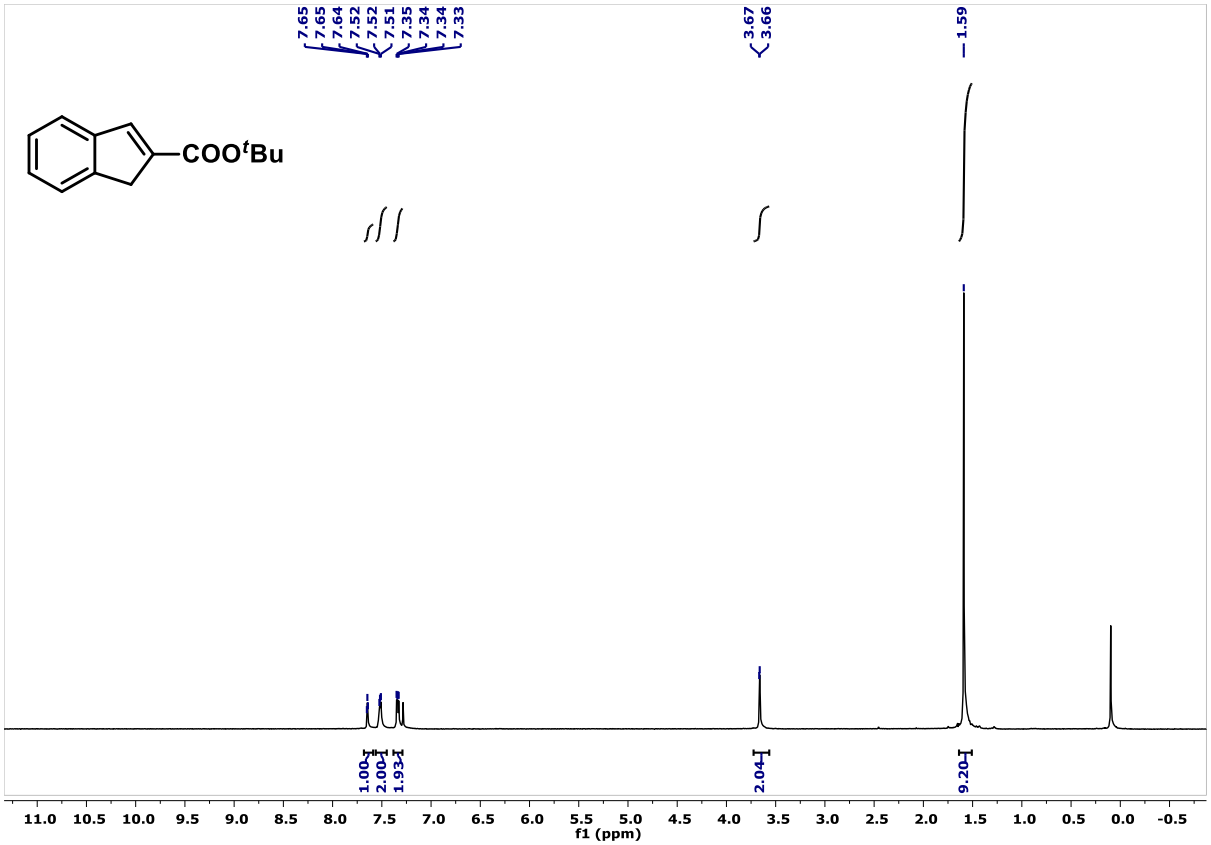
19.18
13.68
0.92
COO^{n}Bu
f1 (ppm)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7.34
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2.00
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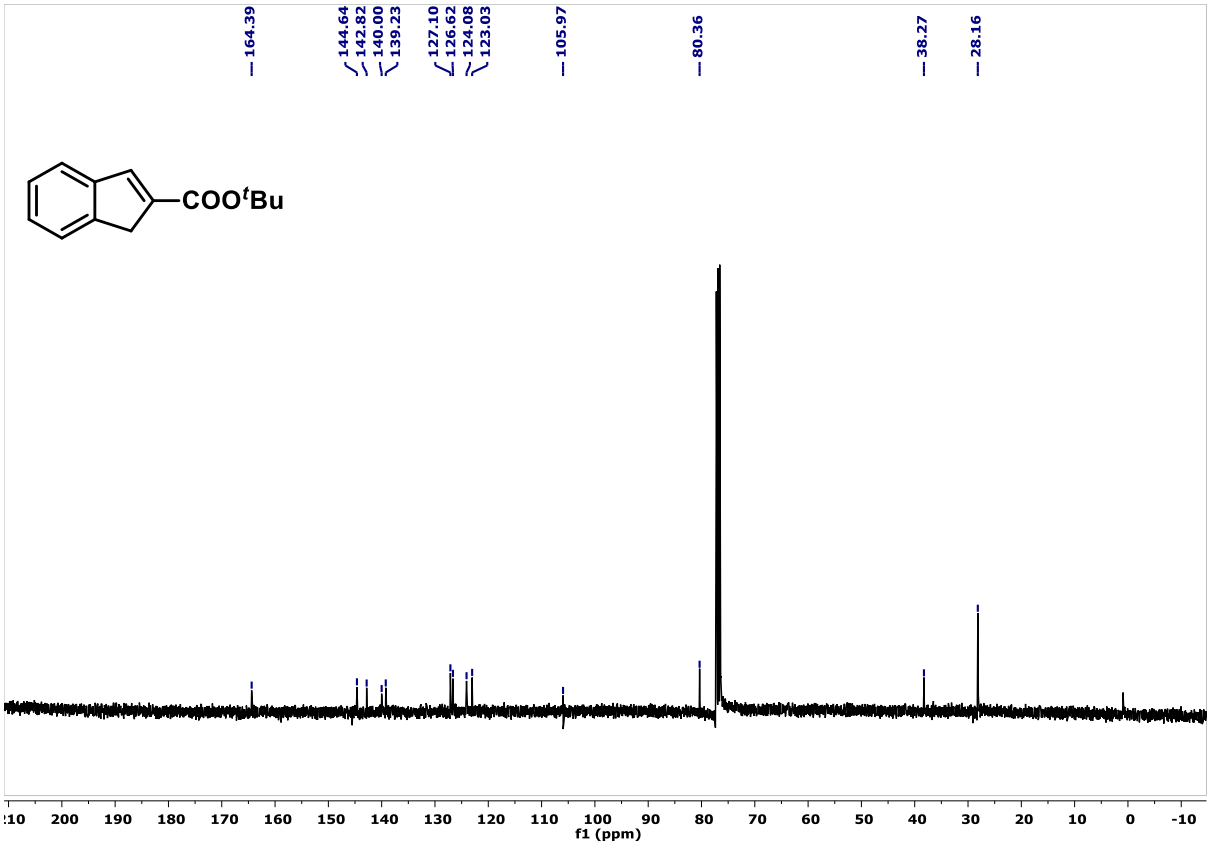
2.04
9.20
f1 (ppm)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38.27
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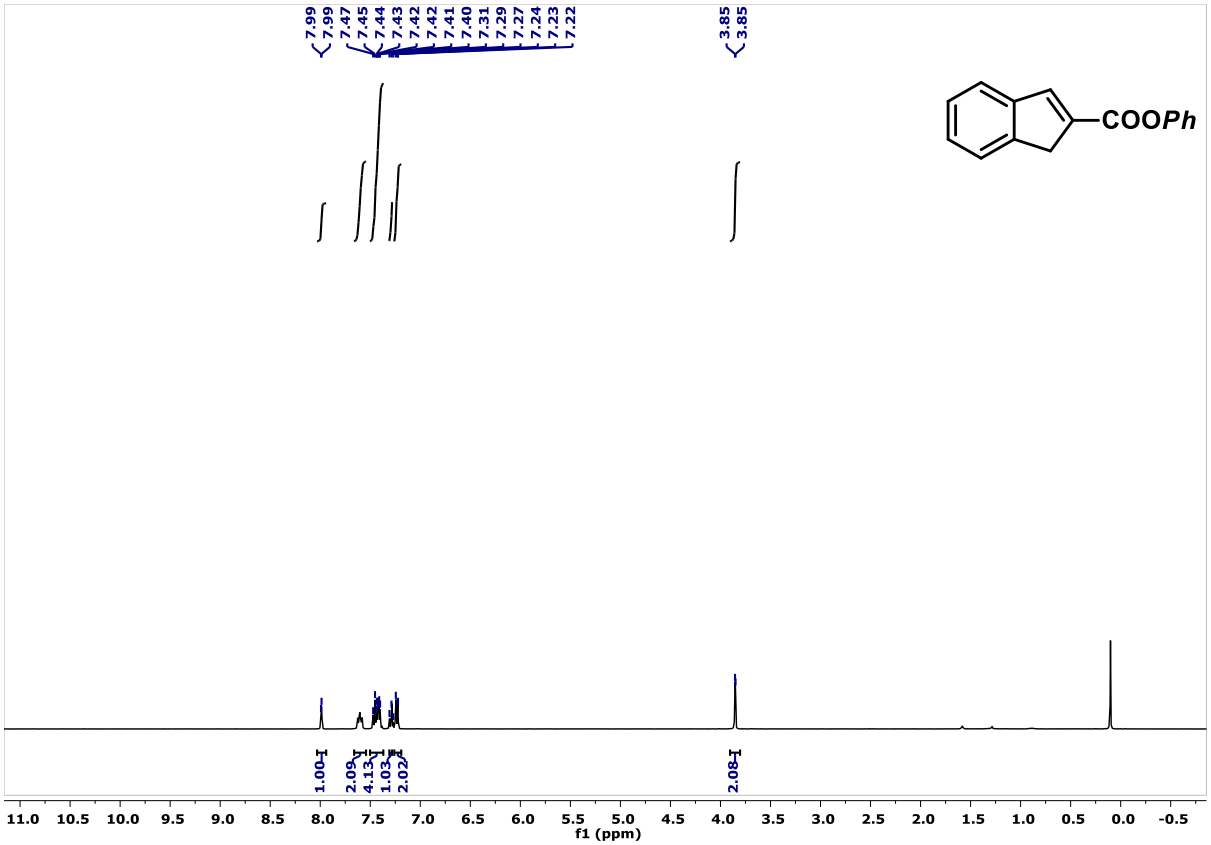
COO^{t}Bu
f1 (ppm)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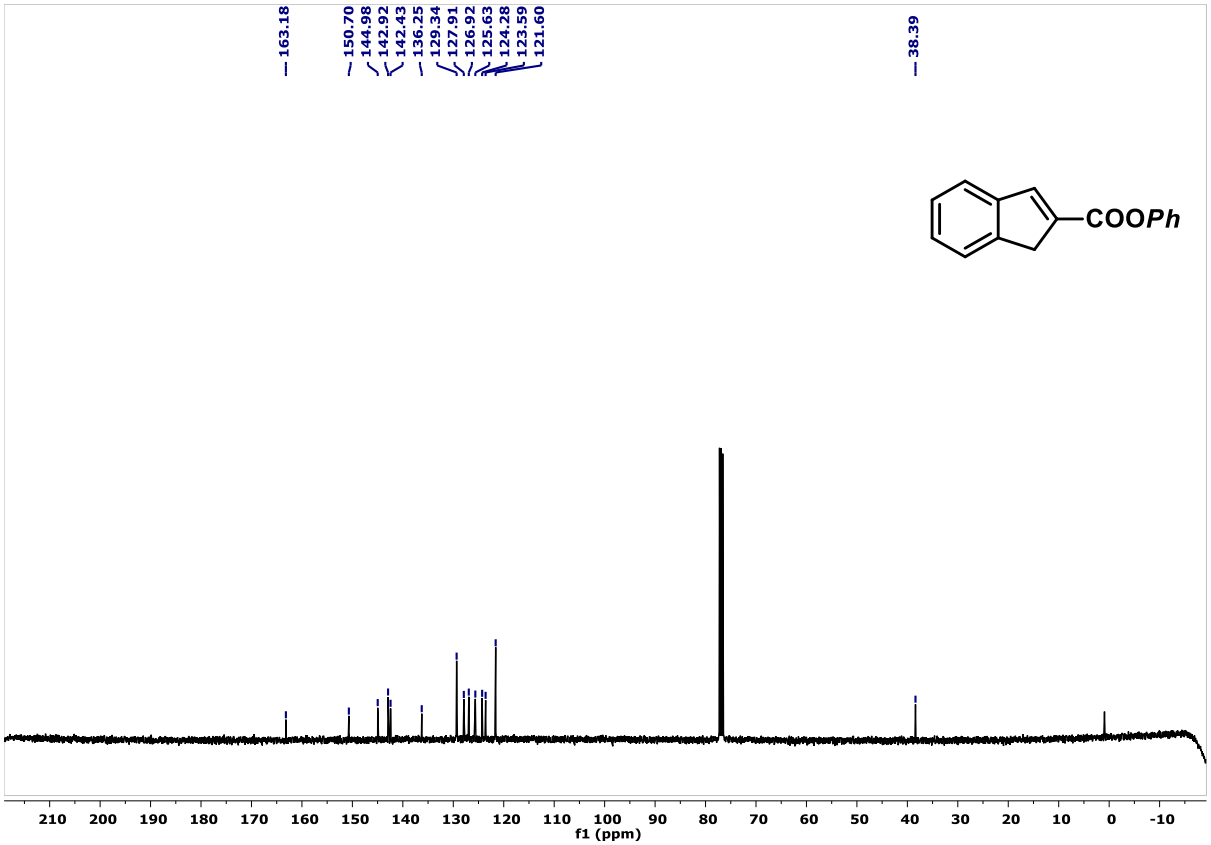
7.31
7.29
7.27
7.24
7.23
7.22
3.85
3.85
COOPh
1.00
2.09
4.13
1.03
2.02
2.08
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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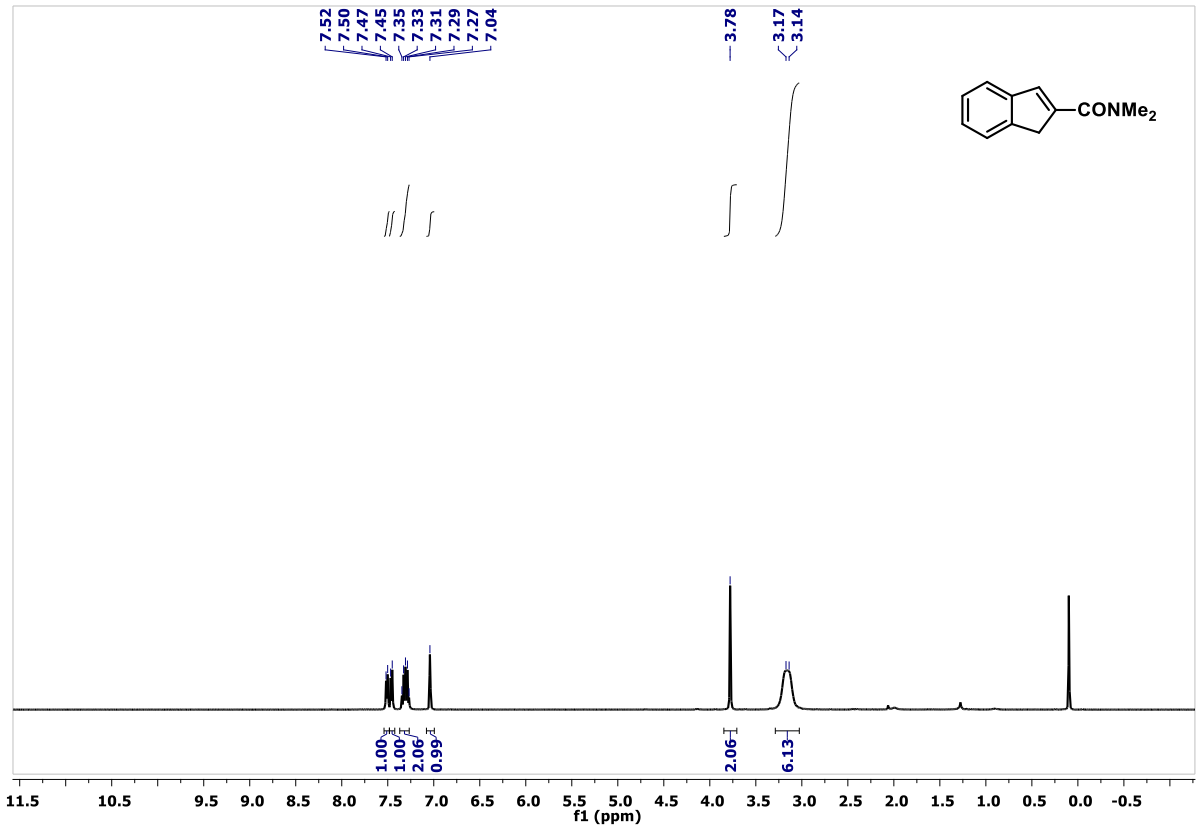
38.39
COOPh
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.29
7.27
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3.14
CONMe2
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1.00
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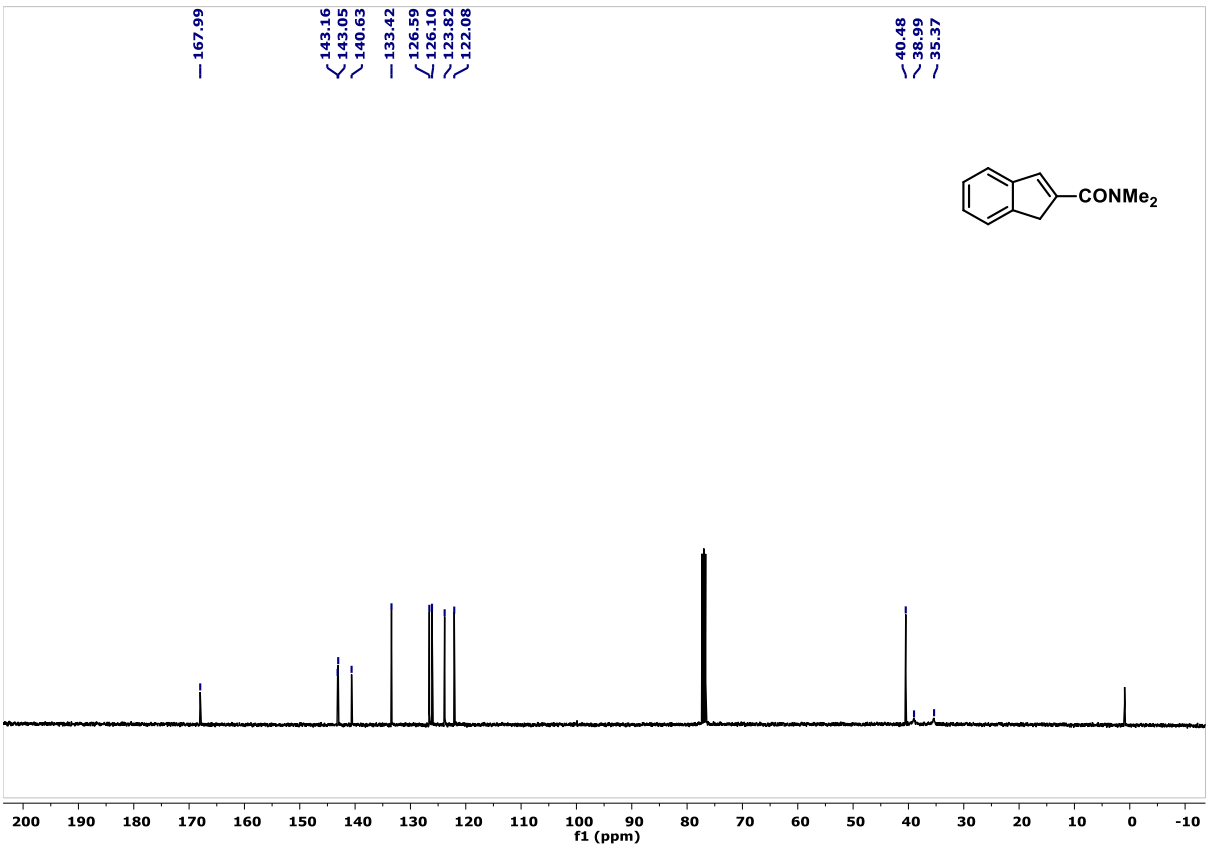
0.99
2.06
6.13
f1 (ppm)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140.63
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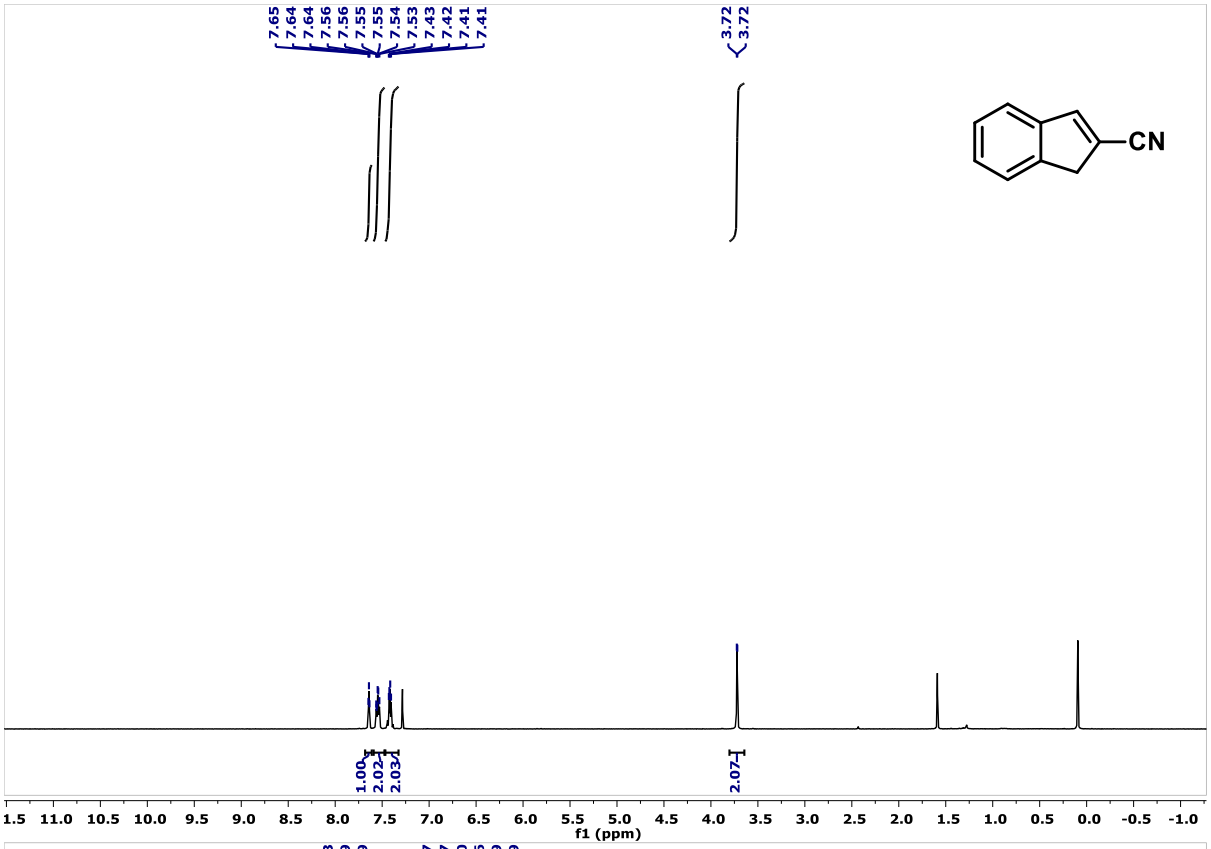
126.59
126.10
123.82
122.08
40.48
38.99
35.37
CONMe2
f1 (ppm)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7.56
7.55
7.55
7.54
7.53
7.43
7.42
7.41
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CN
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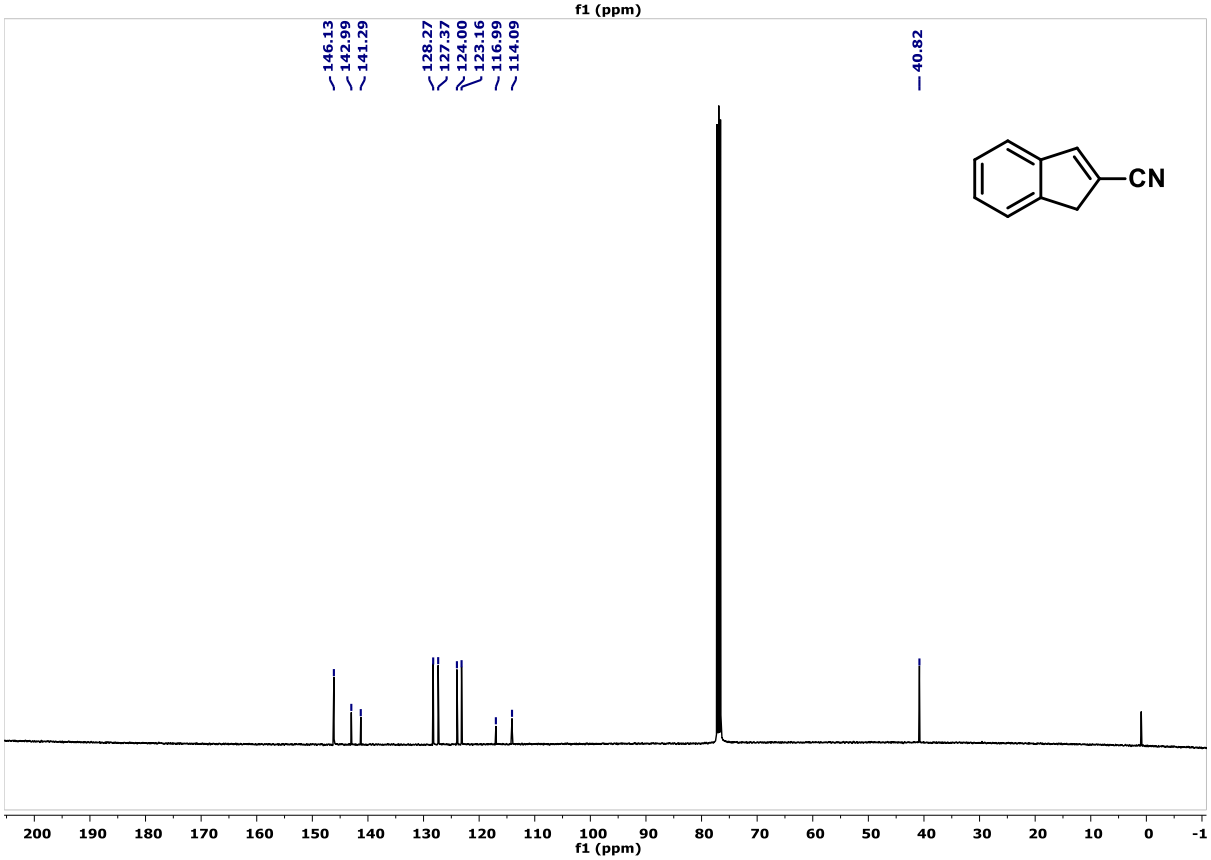
2.02
2.03
2.07
f1 (ppm)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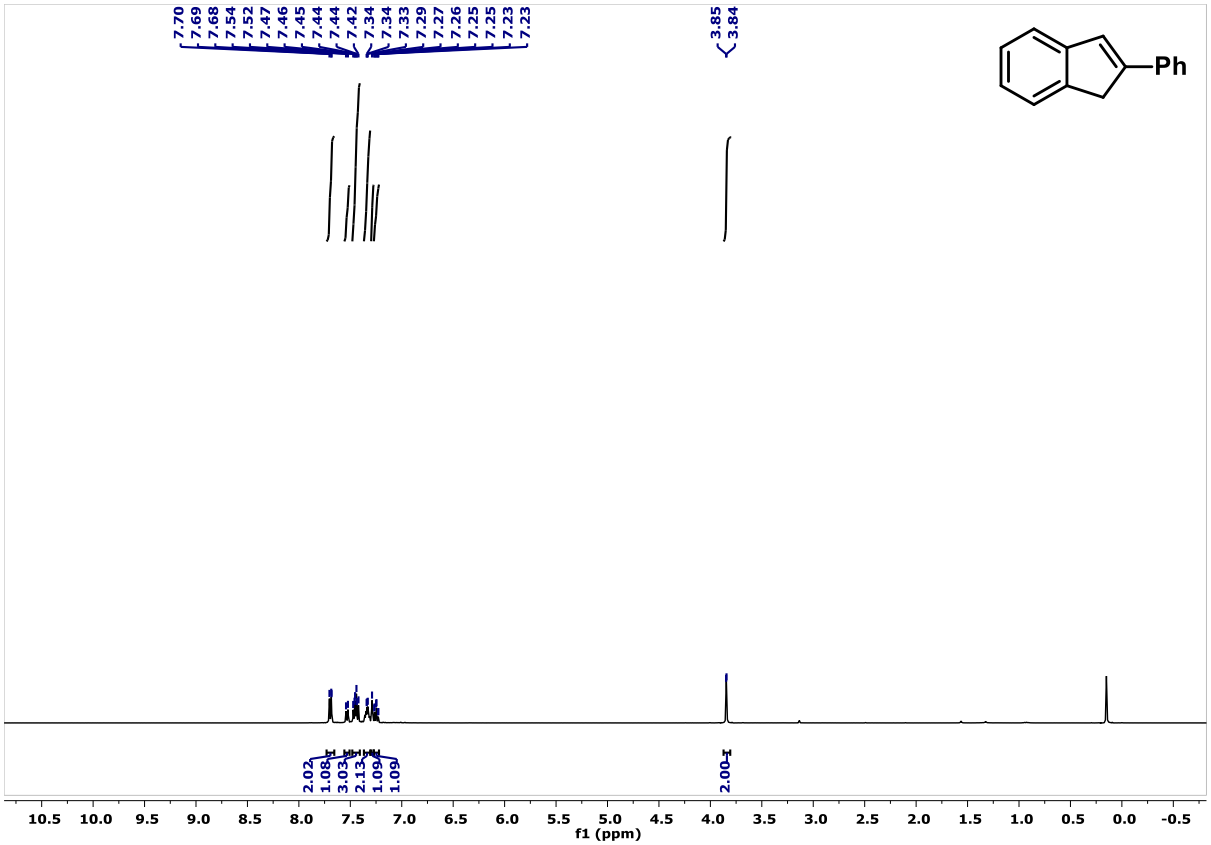
124.00
123.16
116.99
114.09
40.82
CN
f1 (ppm)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7.44
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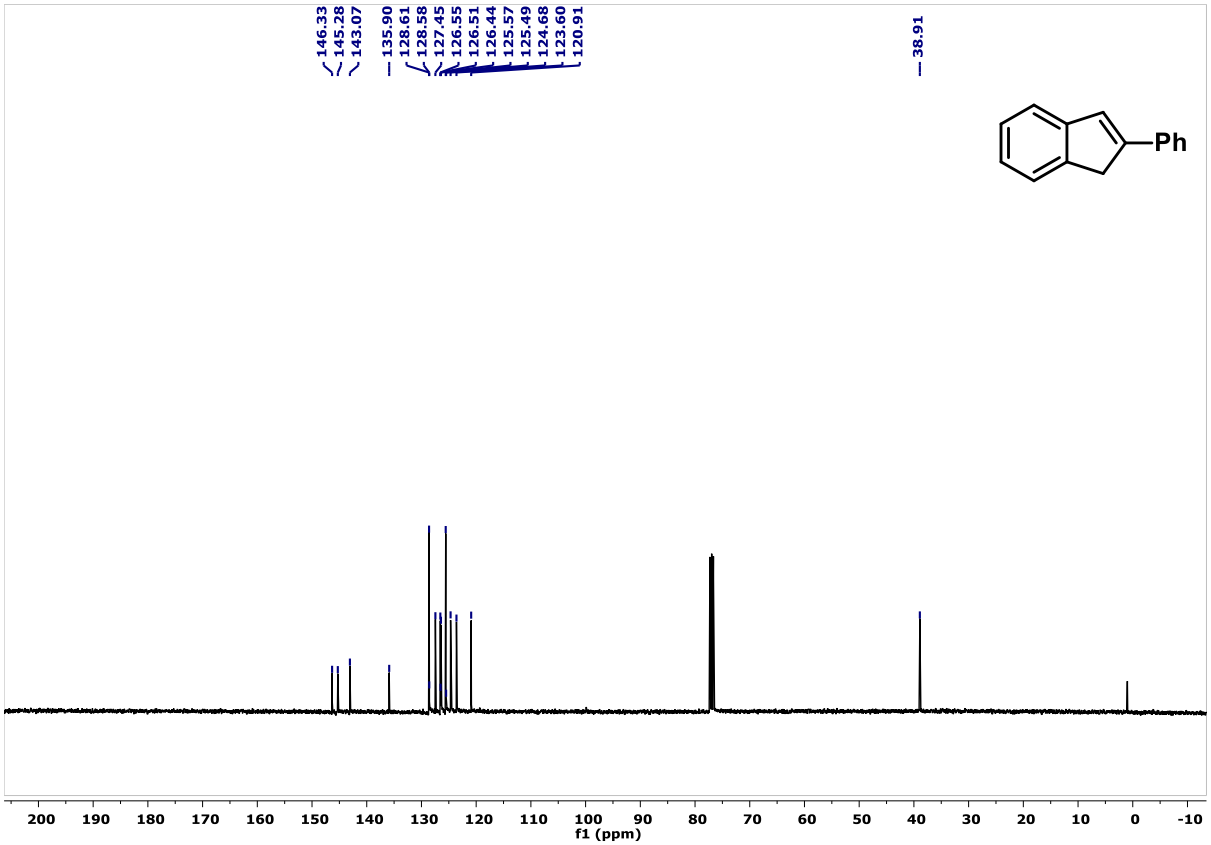
7.34
7.33
7.29
7.27
7.26
7.25
7.25
7.23
7.23
3.85
3.84
Ph
2.02
1.08
3.03
2.13
1.09
1.09
2.00
f1 (ppm)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128.58
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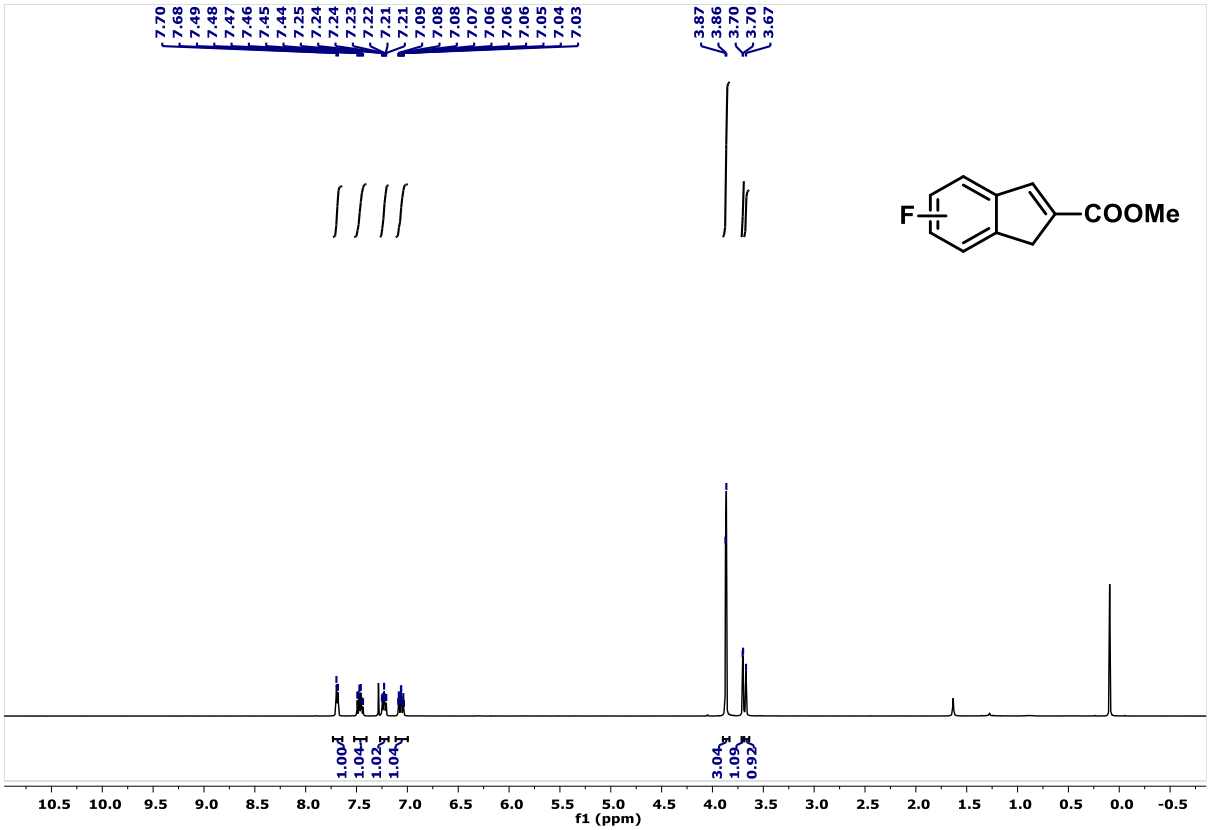
123.60
120.91
38.91
Ph
f1 (ppm)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7.21
7.21
7.09
7.08
7.08
7.07
7.06
7.06
7.06
7.05
7.04
7.03
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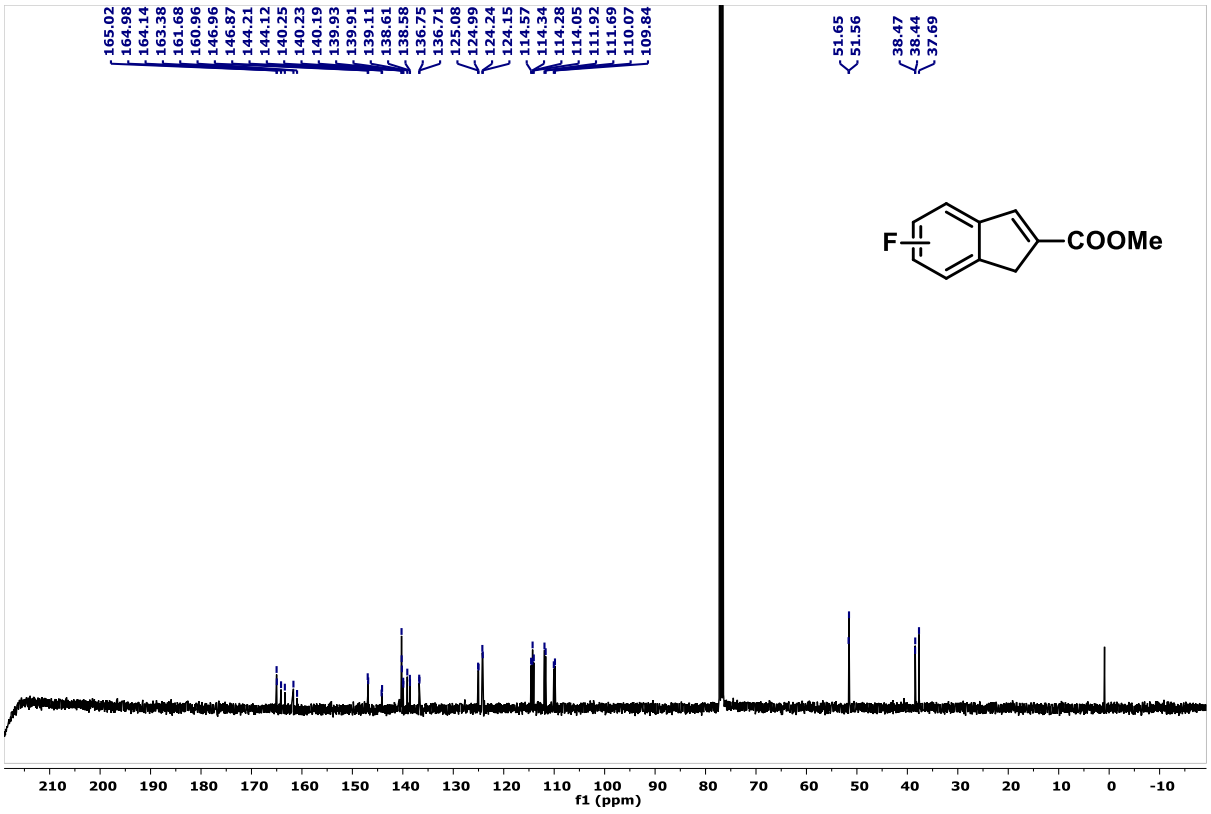
3.86
3.70
3.70
3.67
F
COOMe
1.00
1.04
1.02
1.04
3.04
1.09
0.92
f1 (ppm)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140.23
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139.93
139.91
139.11
138.61
138.58
136.75
136.71
125.08
124.99
124.24
124.15
114.57
114.34
114.28
114.05
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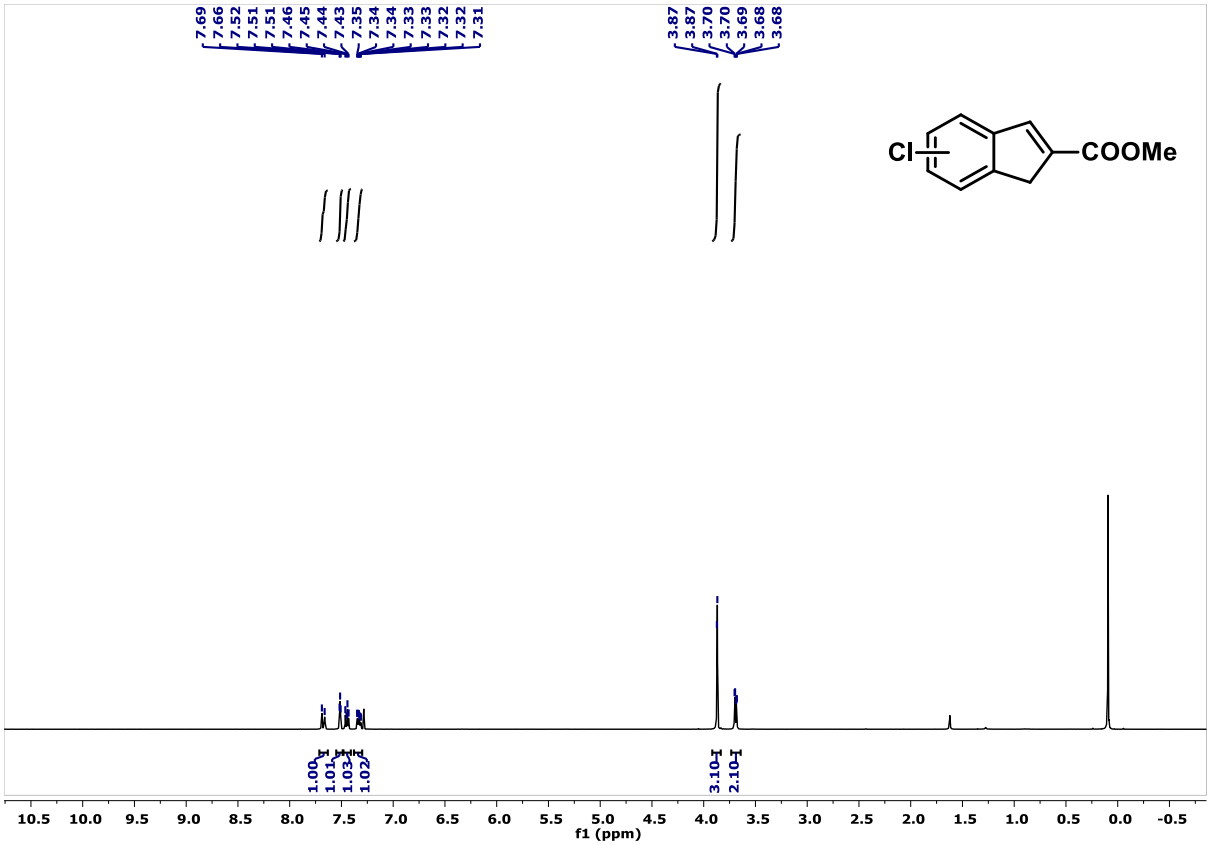
51.56
38.47
38.44
37.69
F
COOMe
f1 (ppm)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7.33
7.33
7.32
7.32
7.31
3.87
3.87
3.70
3.70
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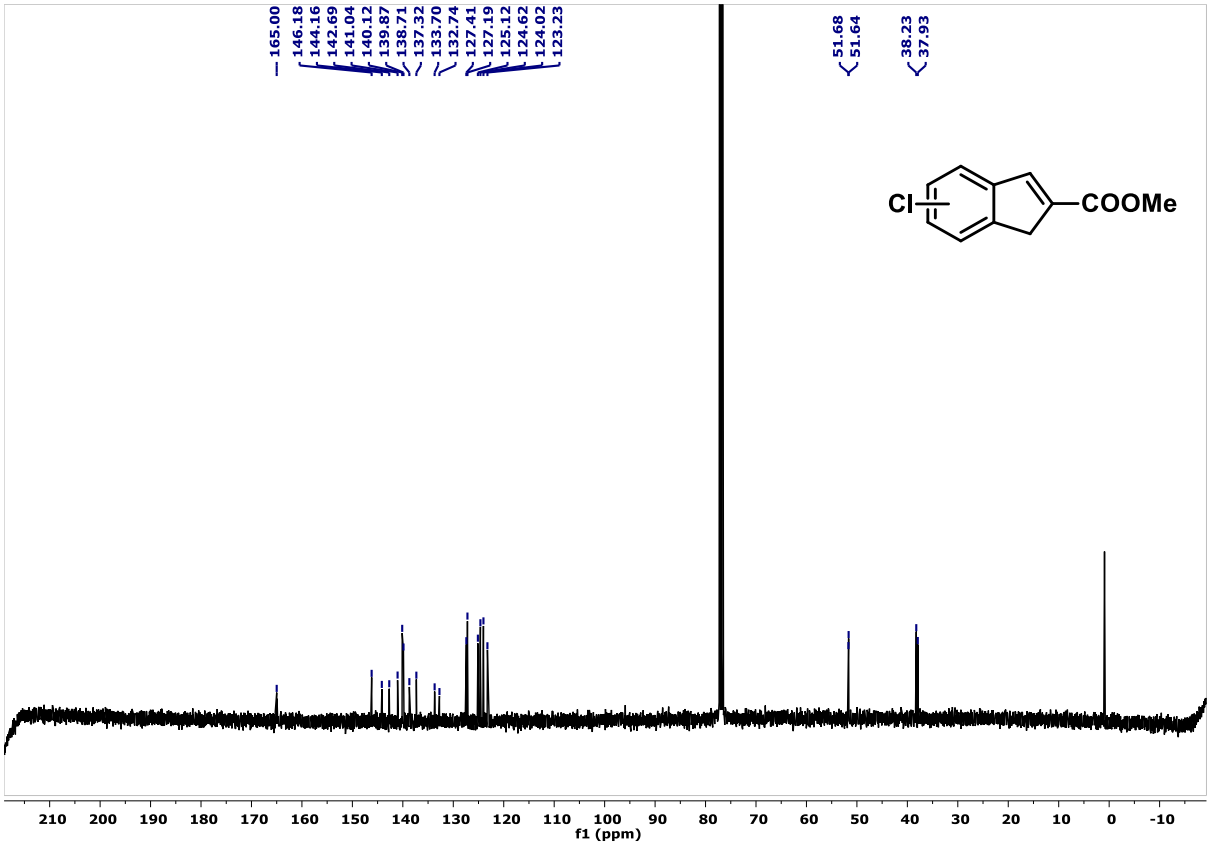
3.68
Cl
COOMe
1.00
1.01
1.03
1.02
3.10
2.10
f1 (ppm)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132.74
127.41
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124.02
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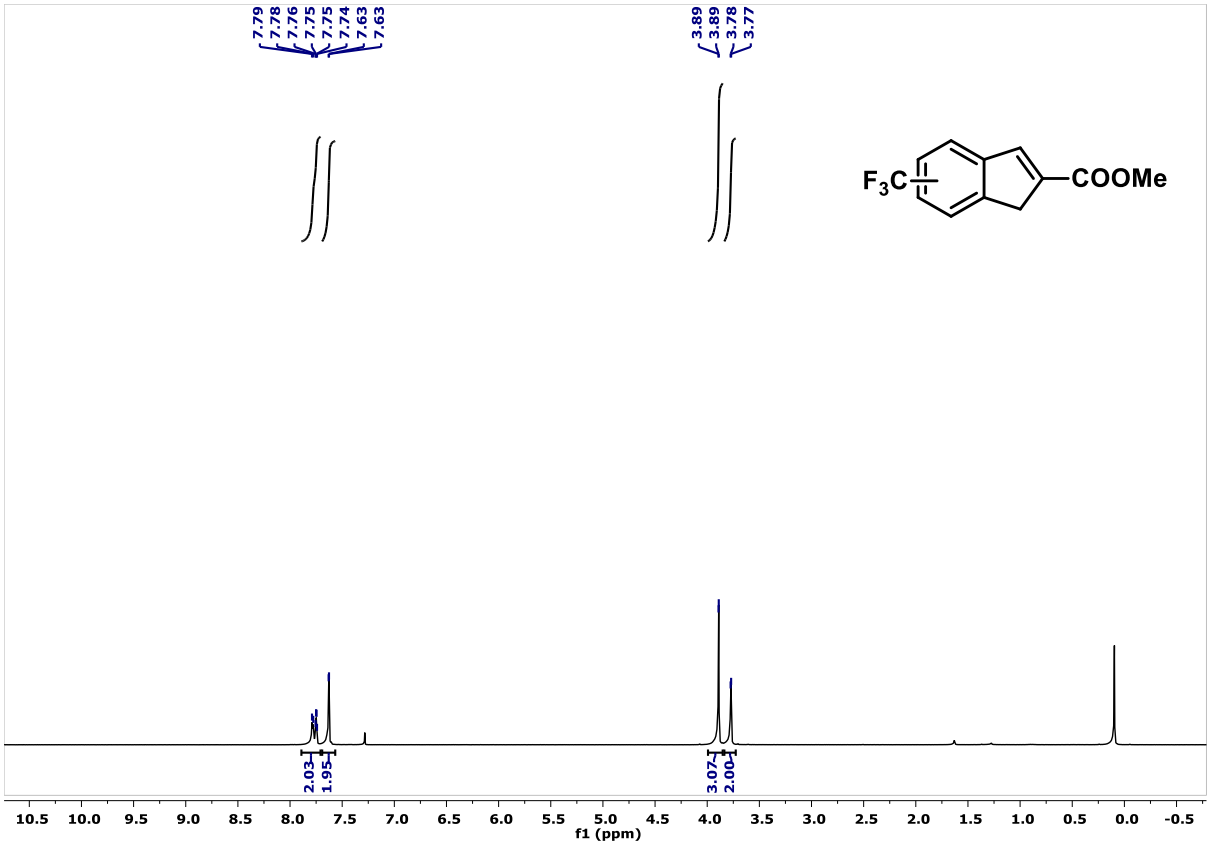
38.23
37.93
Cl
COOMe
f1 (ppm)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7.63
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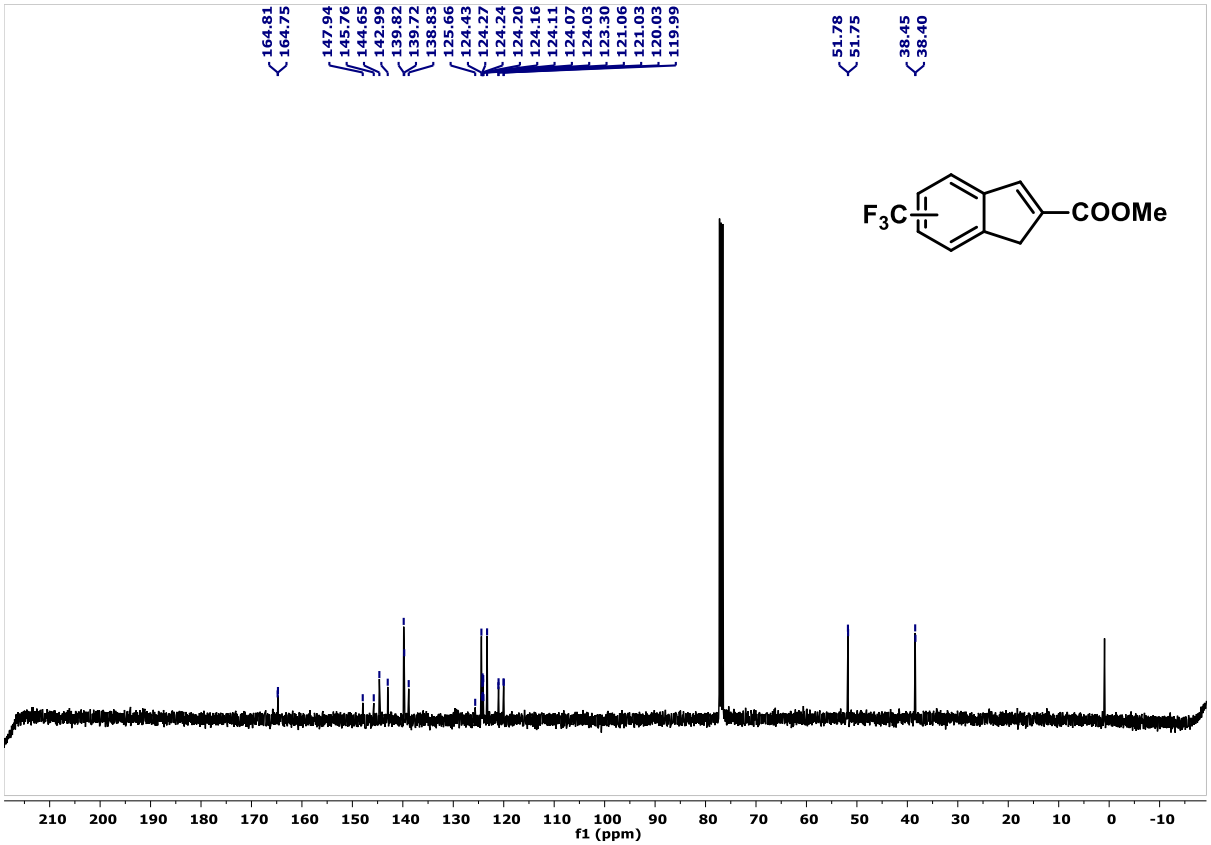
3.89
3.78
3.77
F3C
COOMe
2.03
1.95
3.07
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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124.27
124.24
124.20
124.16
124.11
124.07
124.03
123.30
121.06
121.03
120.03
119.99
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51.75
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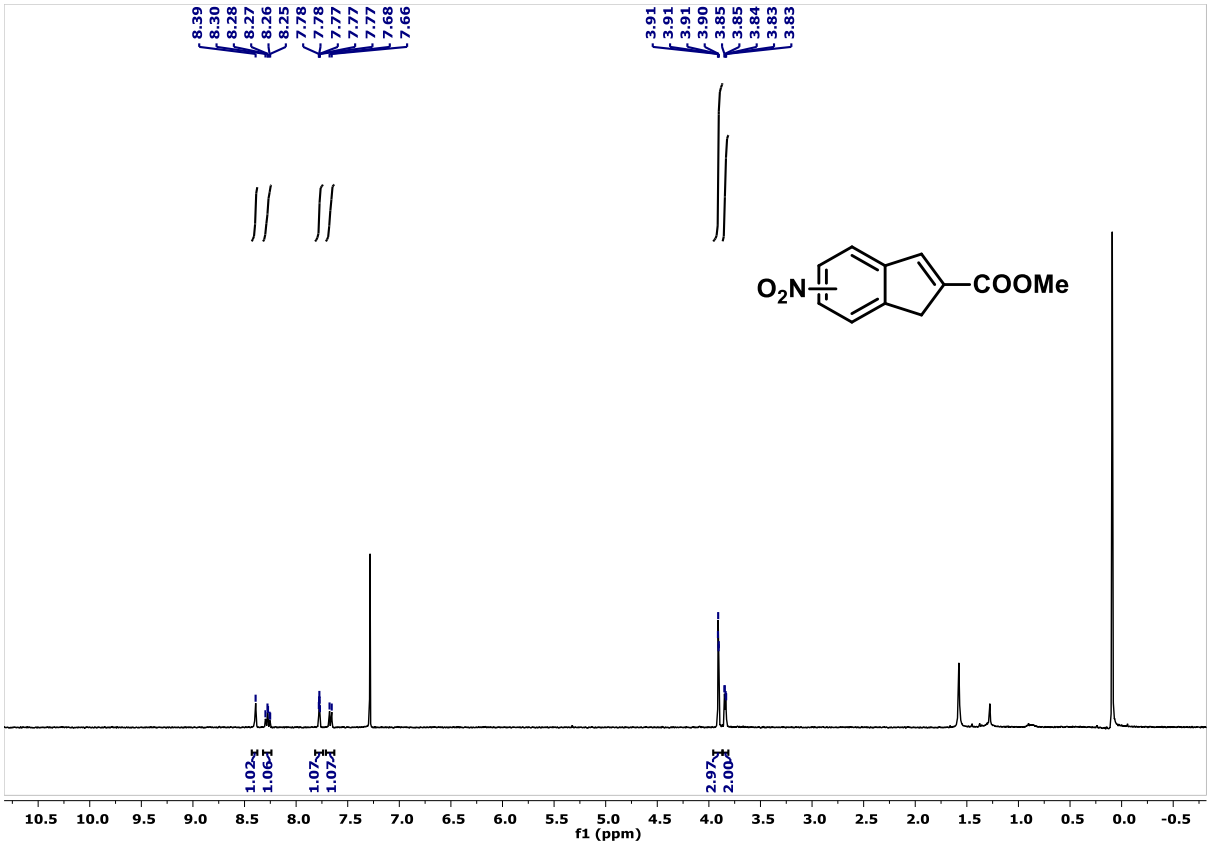
38.40
F3C
COOMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.66
3.91
3.91
3.91
3.90
3.85
3.85
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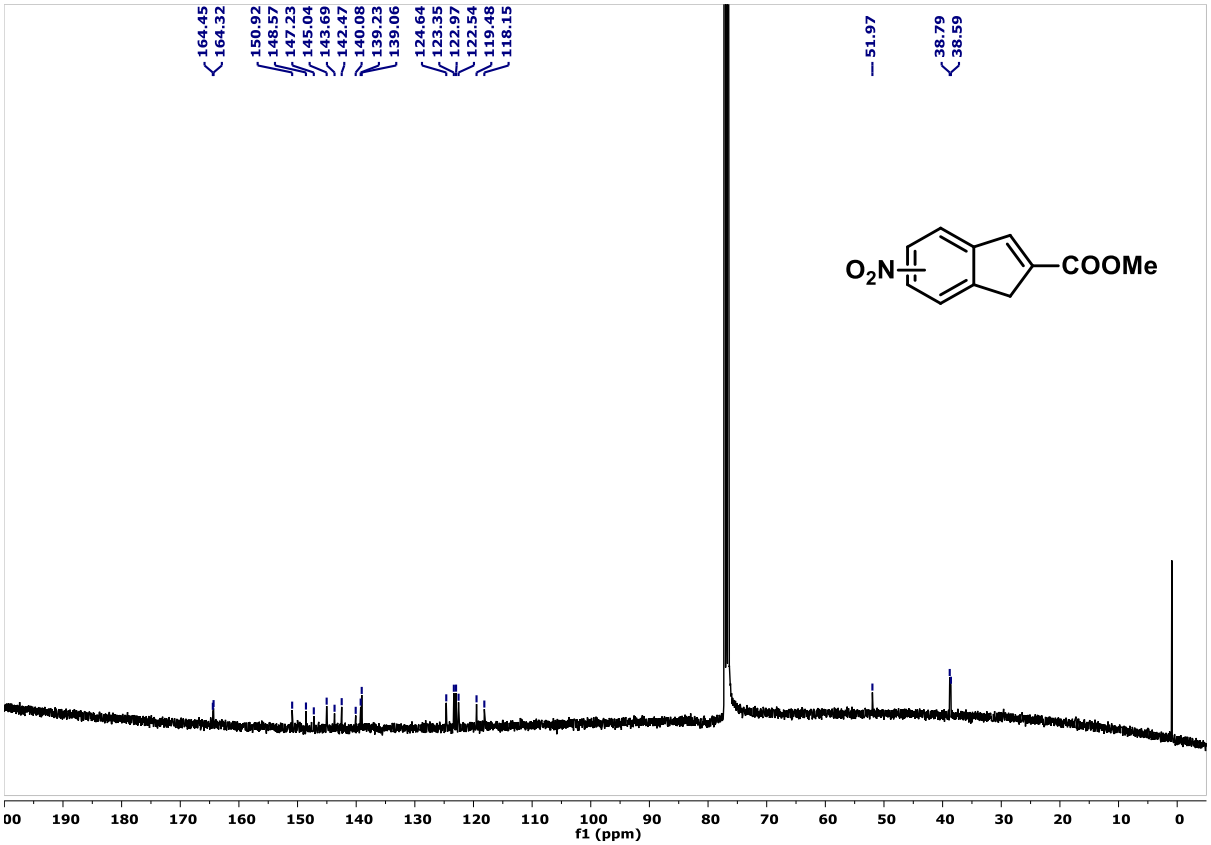
3.83
3.83
O2N
COOMe
1.02
1.06
1.07
1.07
2.97
2.00
f1 (ppm)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139.23
139.06
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122.54
119.48
118.15
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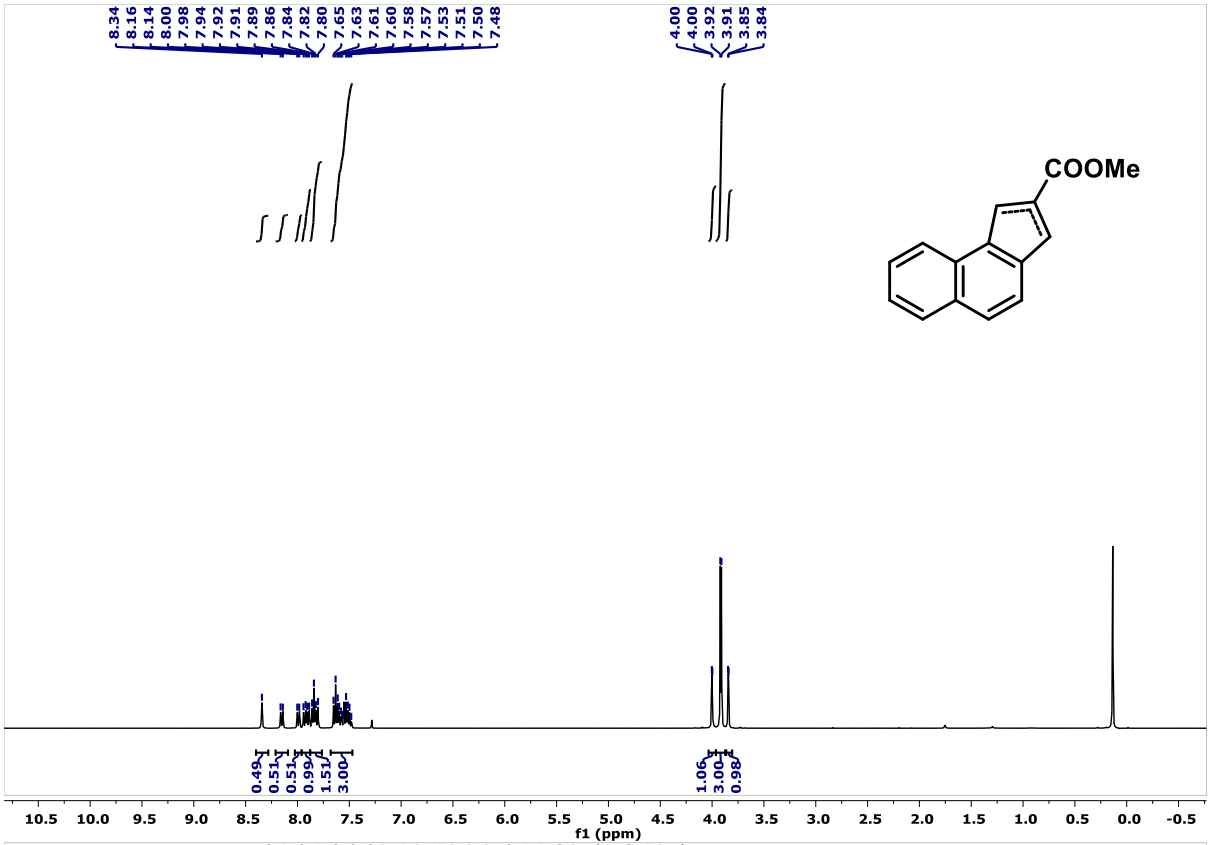
38.59
O2N
COOMe
f1 (ppm)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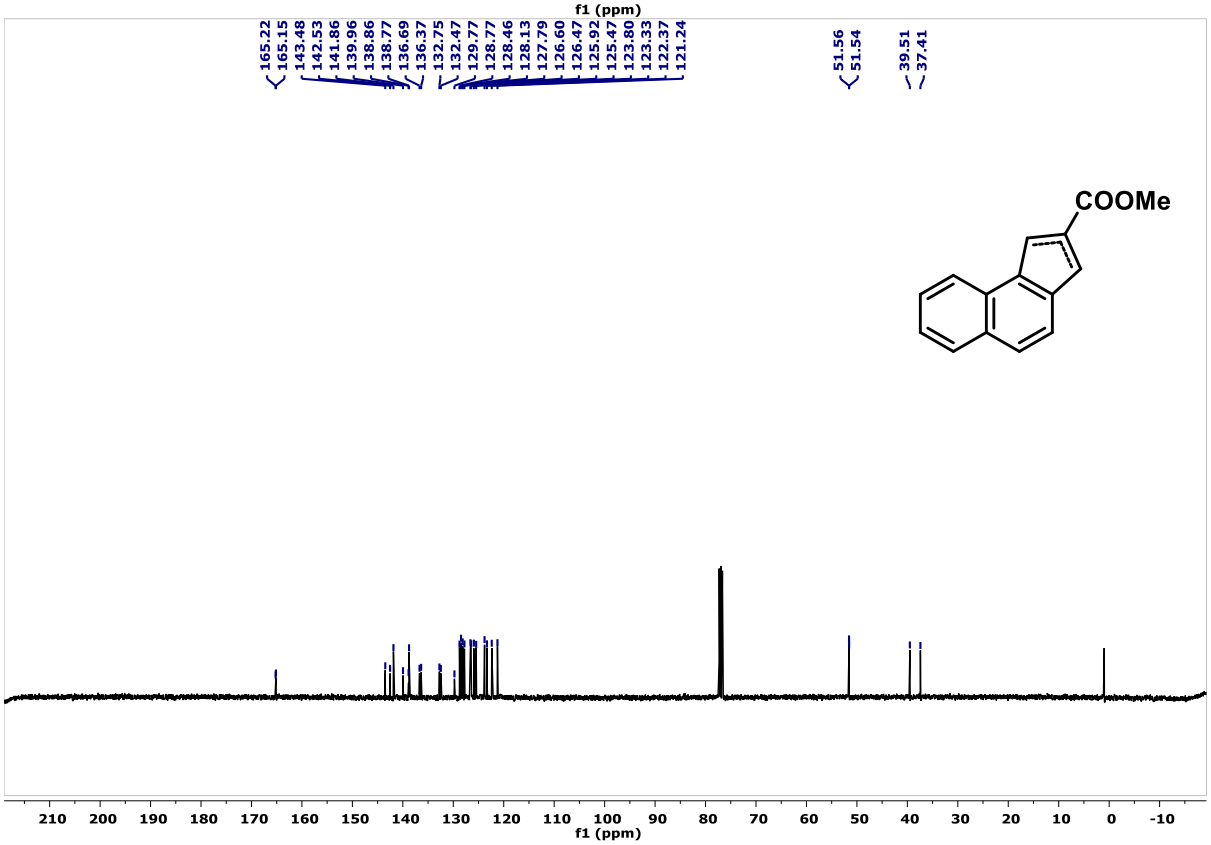
7.65
7.63
7.61
7.60
7.58
7.57
7.53
7.51
7.50
7.48
4.00
4.00
3.92
3.91
3.85
3.84
COOMe
0.49
0.51
0.51
0.99
1.51
3.00
1.06
3.00
0.98
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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132.47
129.77
128.77
128.46
128.13
127.79
126.60
126.47
125.92
125.47
123.80
123.33
122.37
121.24
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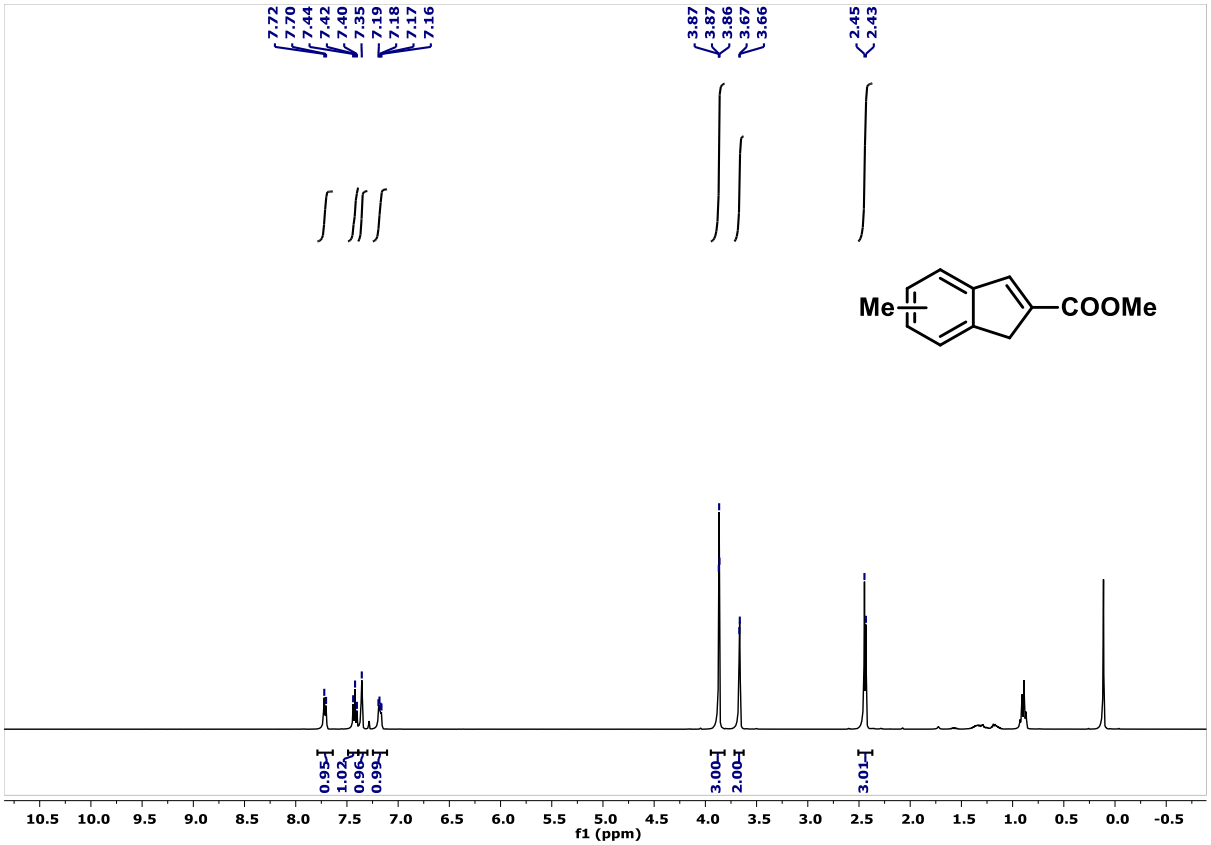
39.51
37.41
COOMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.16
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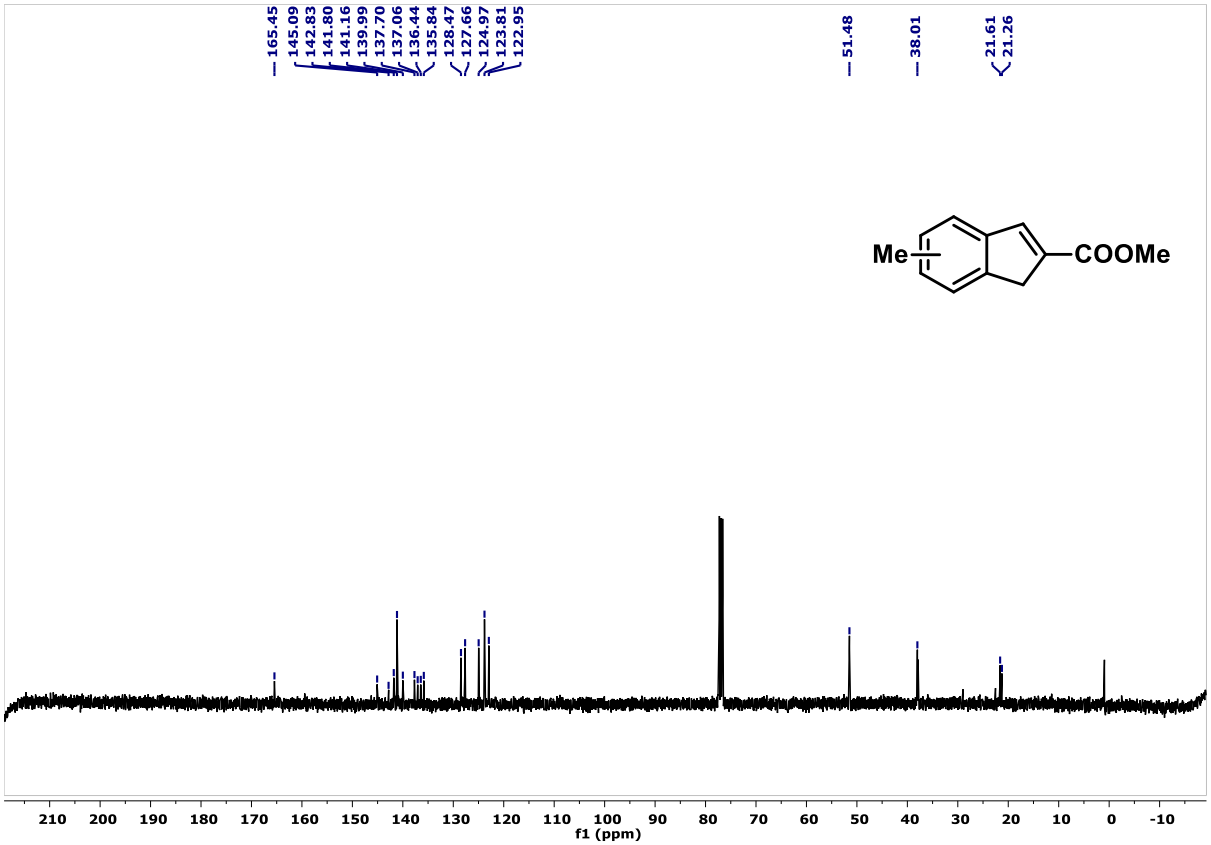
3.87
3.86
3.67
3.66
2.45
2.43
Me
COOMe
0.95
1.02
0.96
0.99
3.00
2.00
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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137.70
137.06
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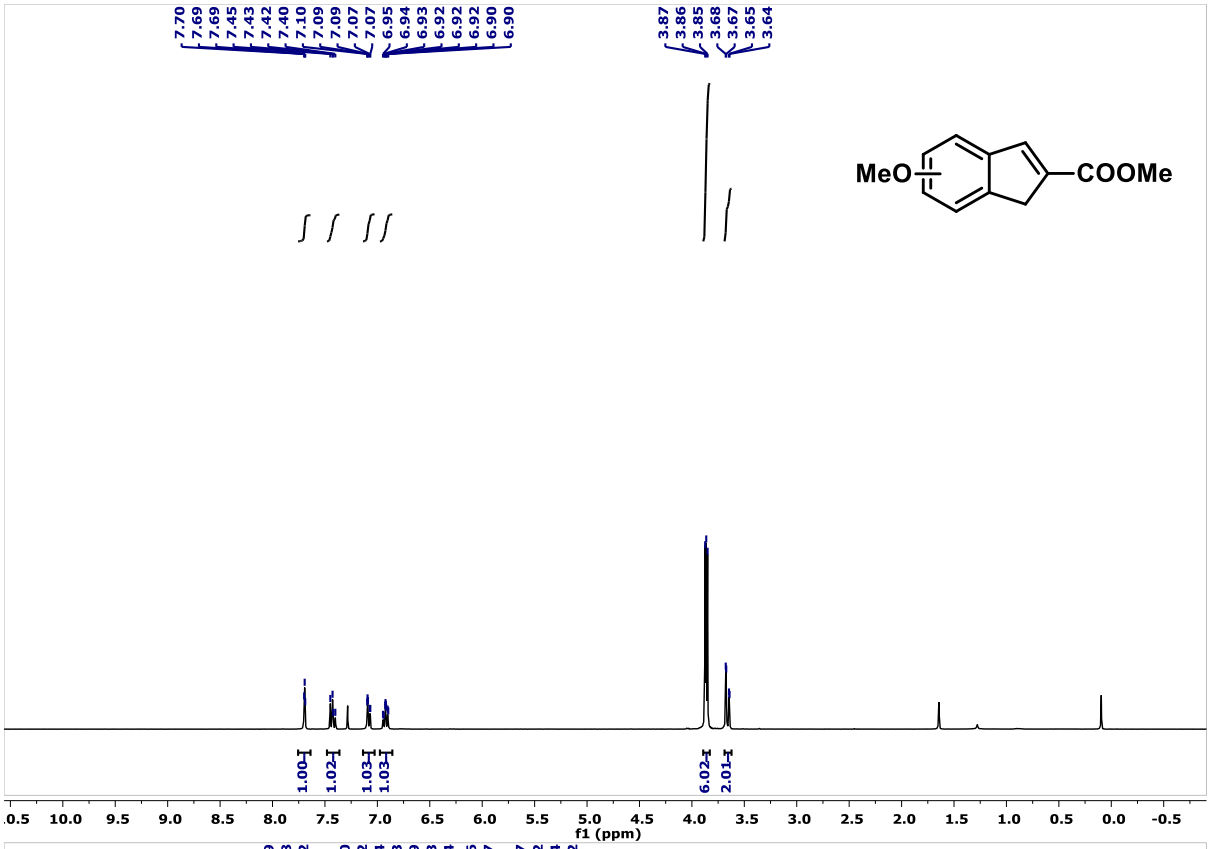
135.84
128.47
127.66
124.97
123.81
122.95
51.48
38.01
21.61
21.26
Me
COOMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.09
7.07
7.07
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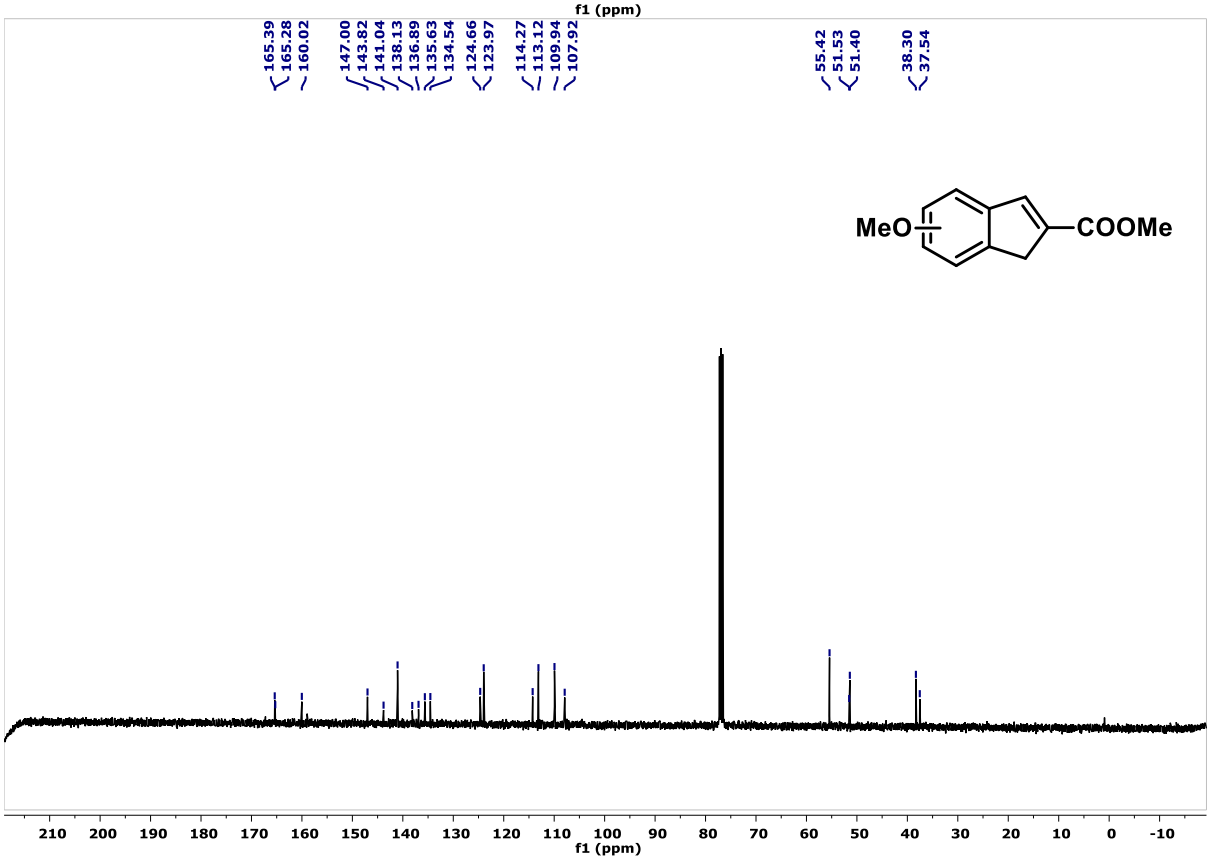
6.94
6.93
6.92
6.92
6.90
6.90
3.87
3.86
3.85
3.68
3.67
3.65
3.64
MeO
COOMe
1.00
1.02
1.03
1.03
6.02
2.01
f1 (ppm)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134.54
124.66
123.97
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113.12
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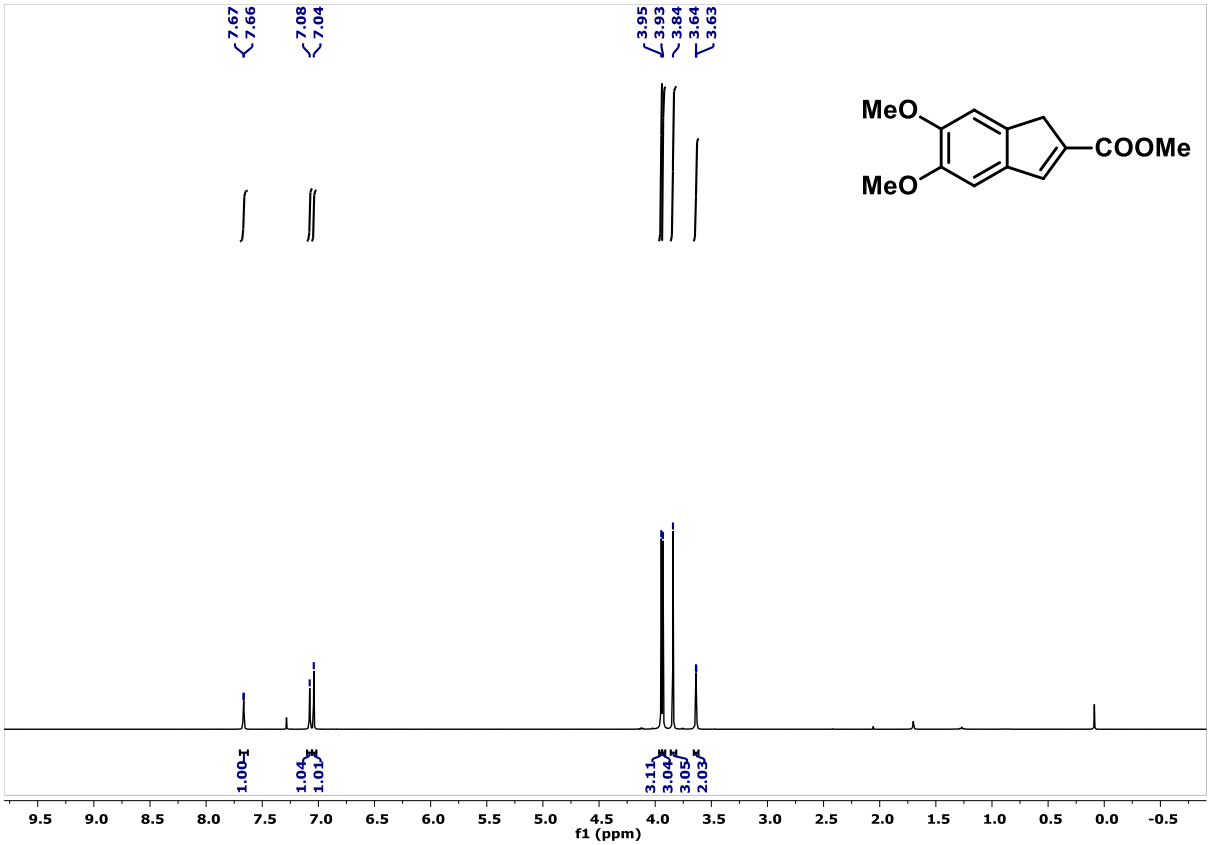
107.92
55.42
51.53
51.40
38.30
37.54
MeO
COOMe
f1 (ppm)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3.84
3.64
3.63
MeO
MeO
COOMe
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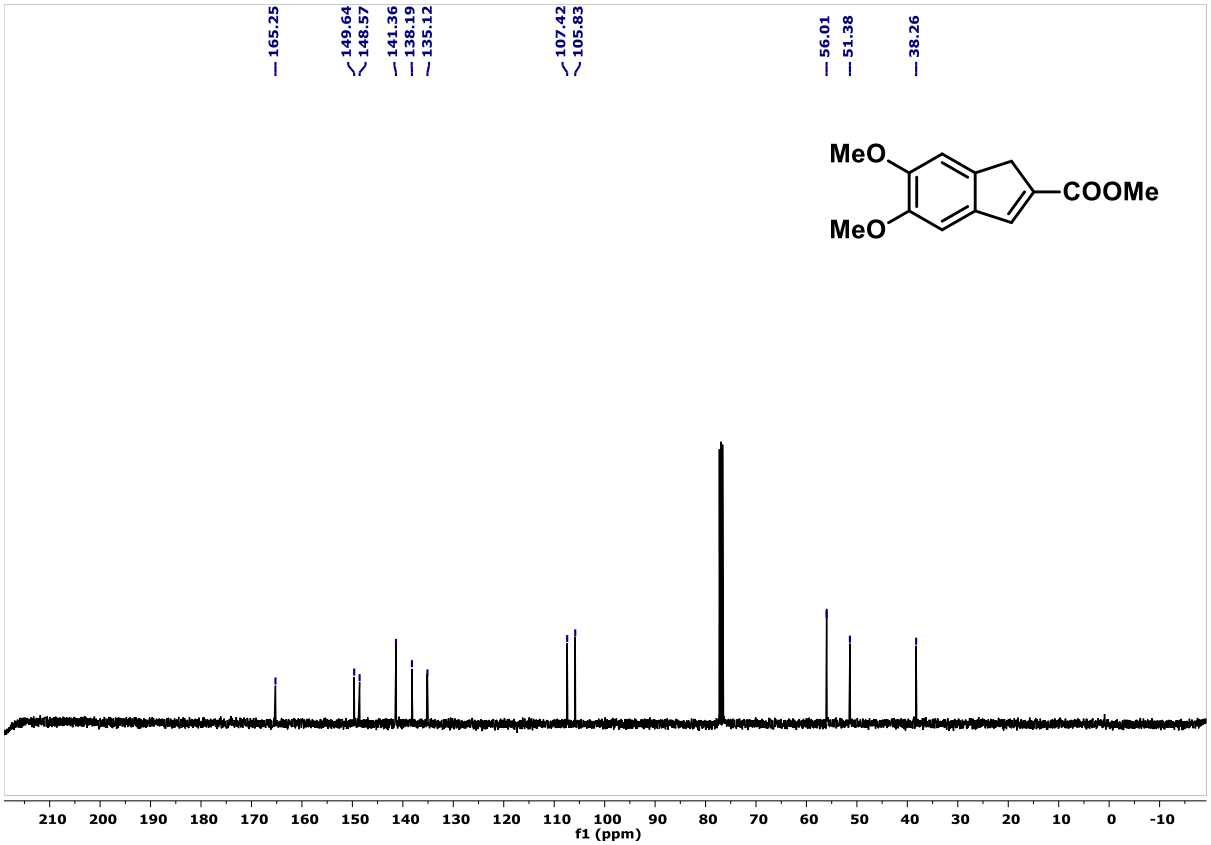
1.04
1.01
3.11
3.04
3.05
2.03
f1 (ppm)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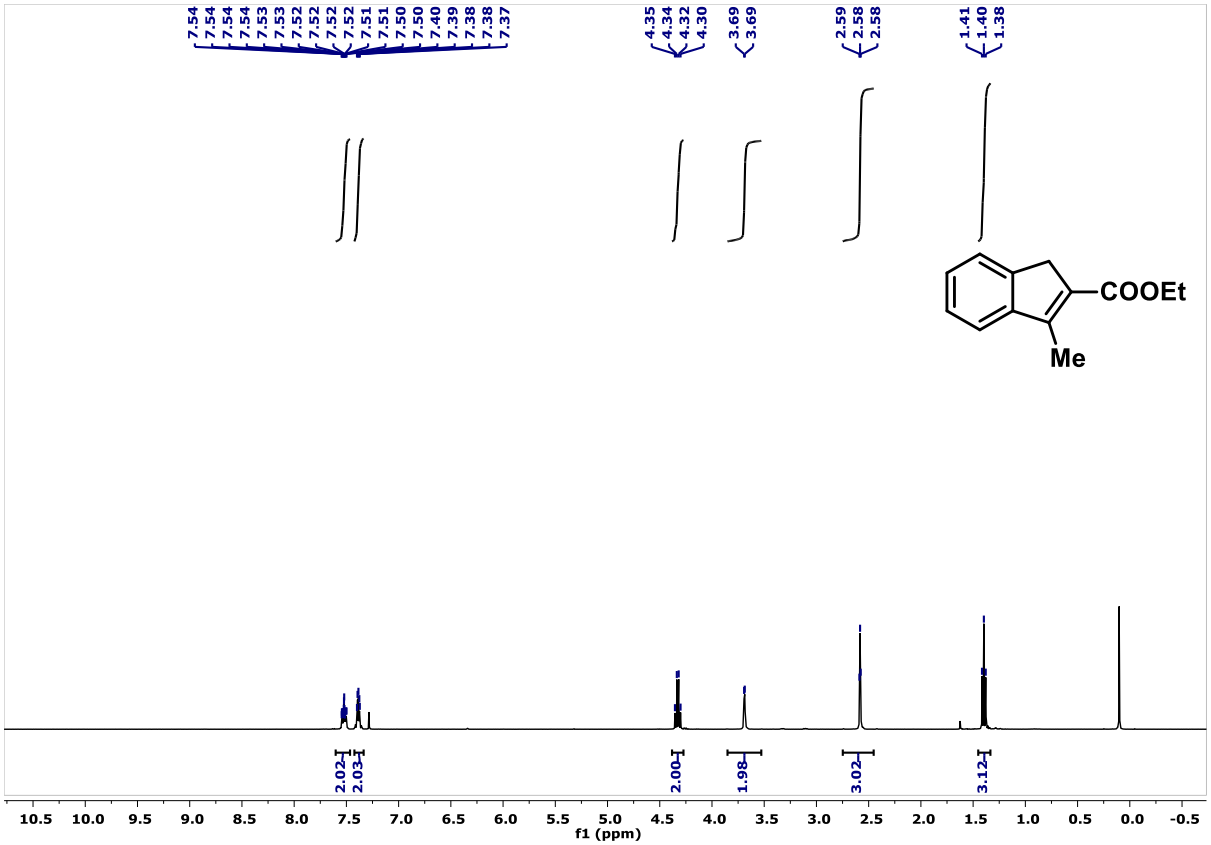
56.01
51.38
38.26
MeO
MeO
COOMe
f1 (ppm)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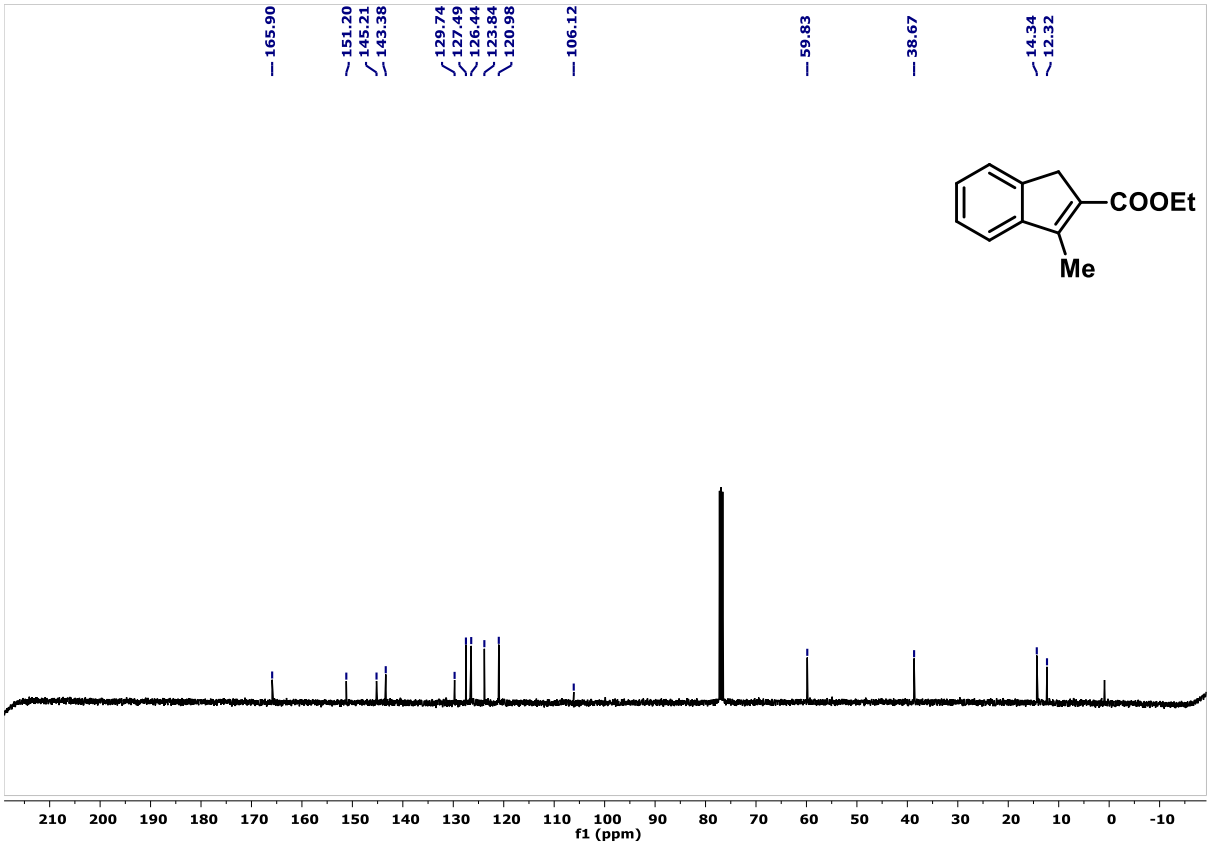
4.30
3.69
3.69
2.59
2.58
2.58
1.41
1.40
1.38
COOEt
Me
2.02
2.03
2.00
1.98
3.02
3.12
f1 (ppm)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127.49
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123.84
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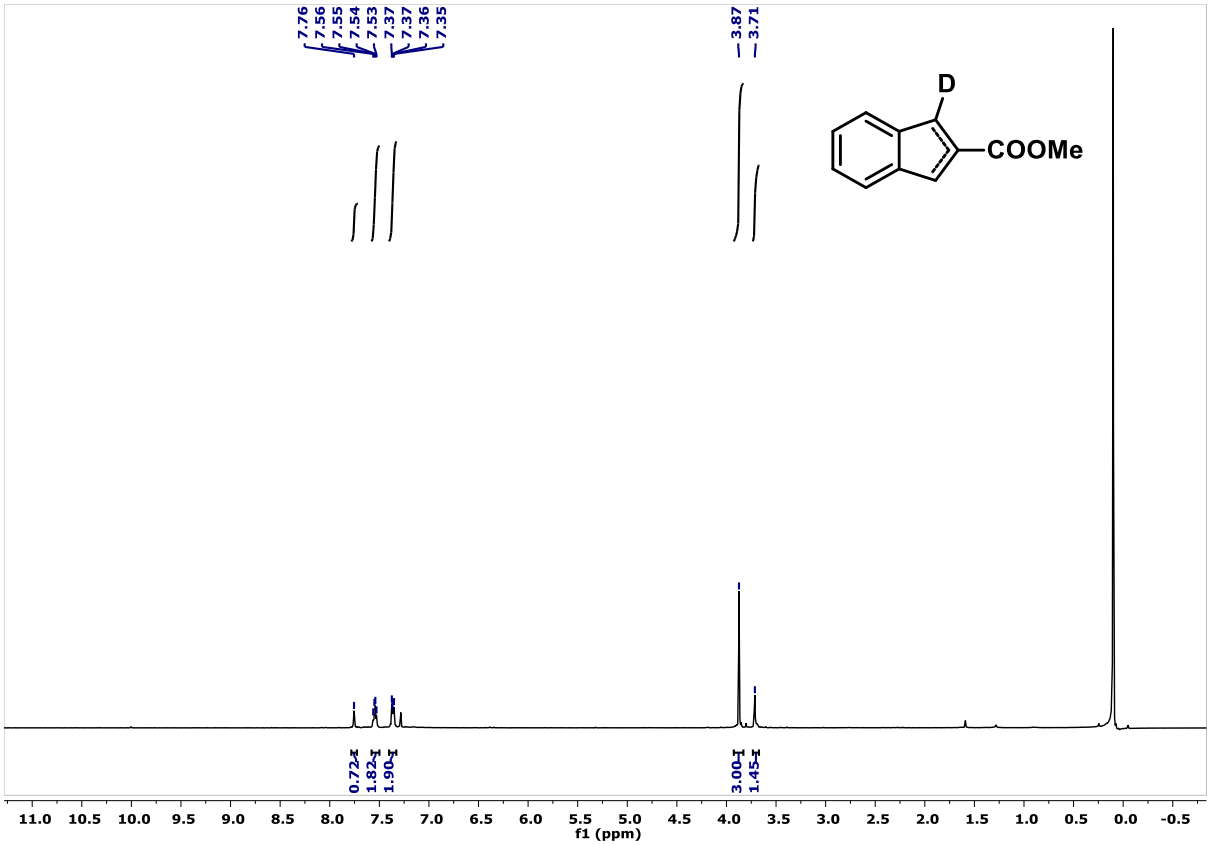
14.34
12.32
COOEt
Me
f1 (ppm)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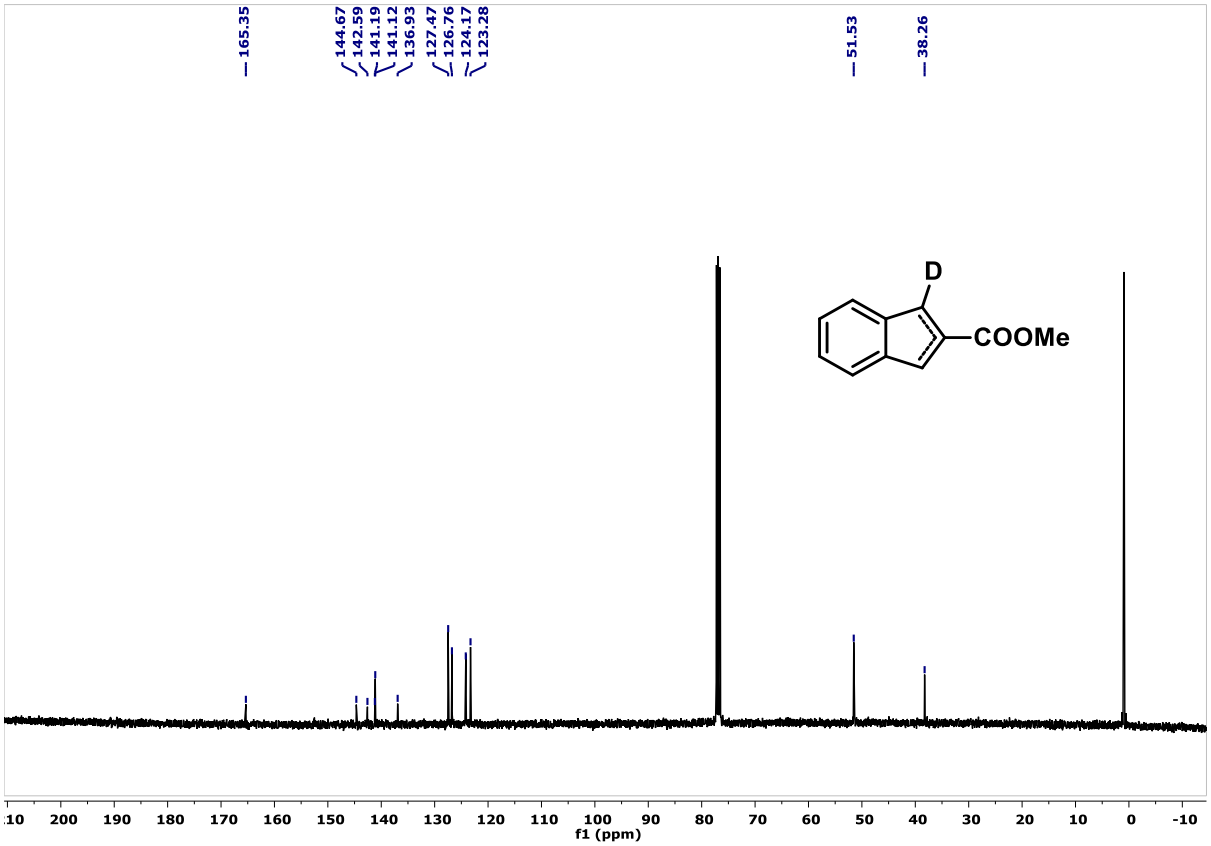
7.55
7.54
7.53
7.37
7.37
7.36
7.35
3.87
3.71
D
COOMe
0.72
1.82
1.90
3.00
1.45
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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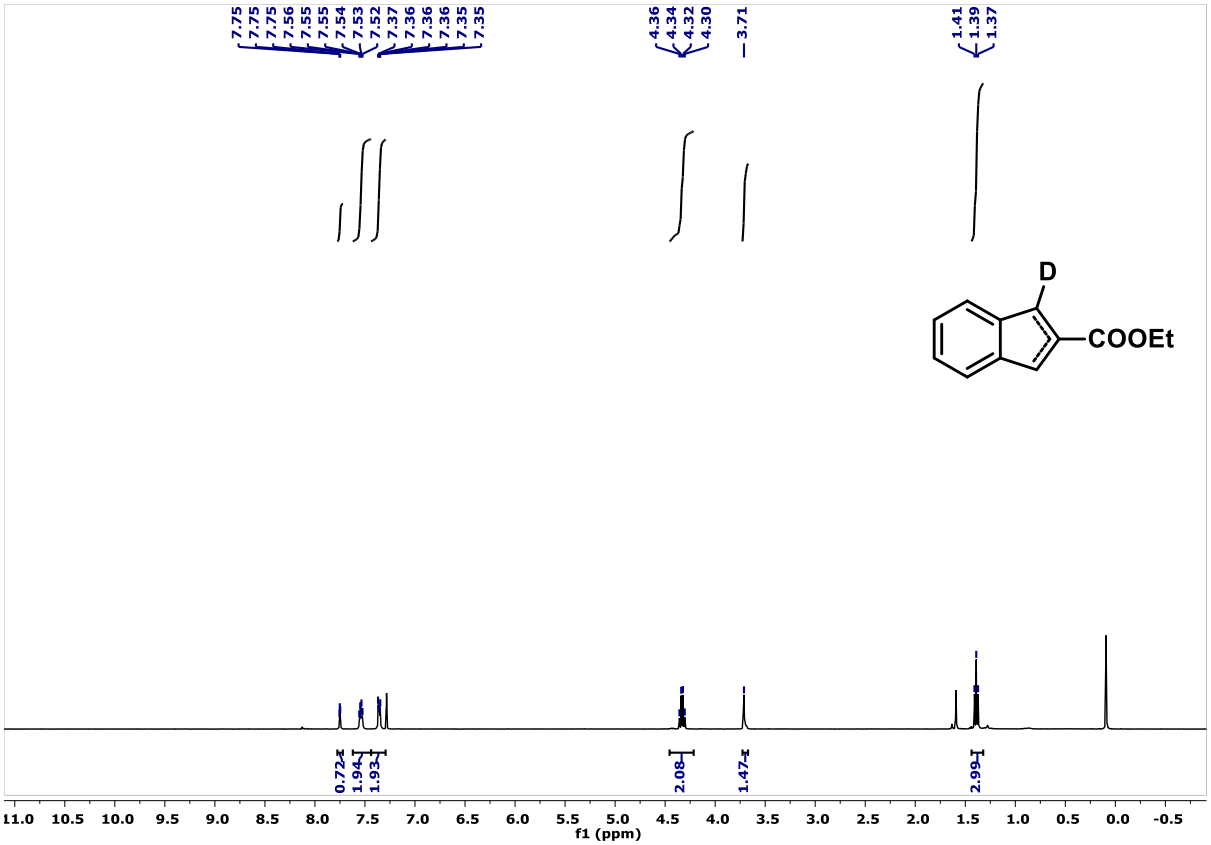
D
COOMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.55
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7.35
7.35
4.36
4.34
4.32
4.30
3.71
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D
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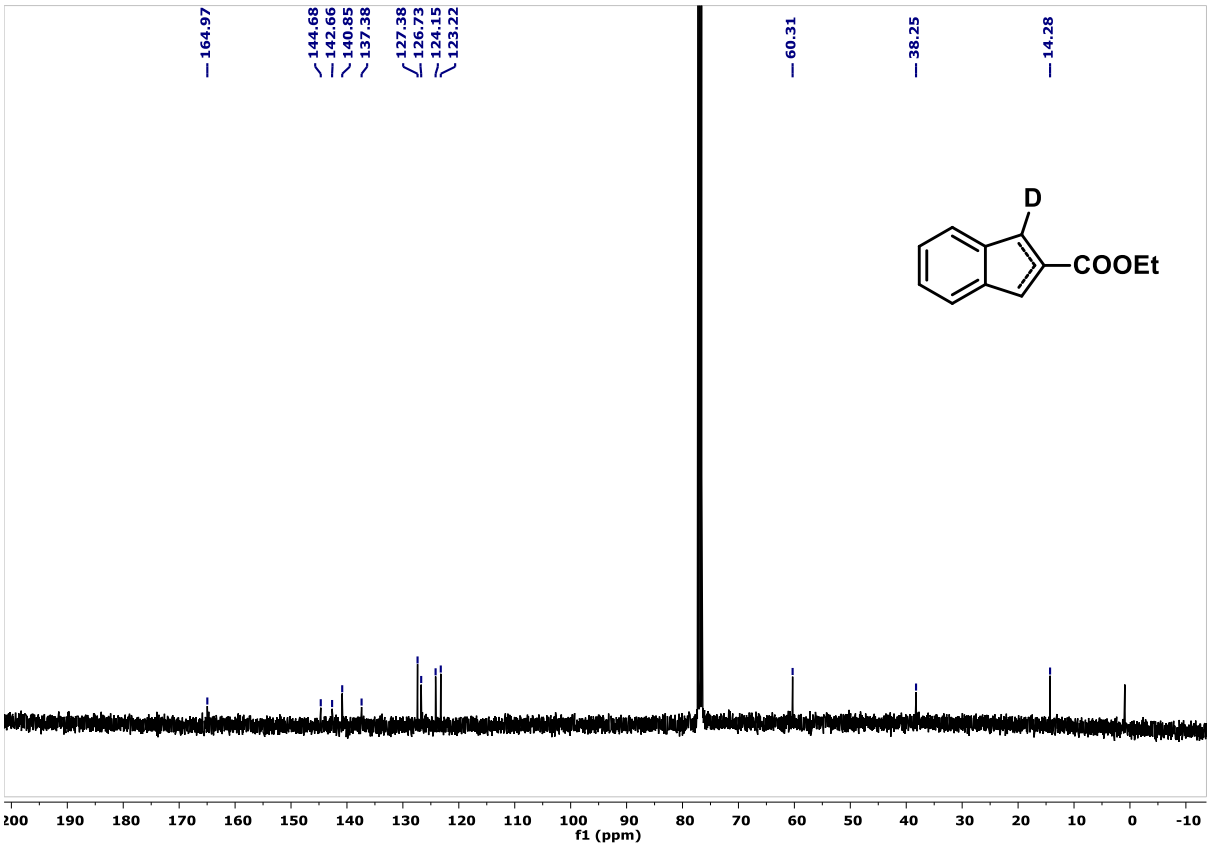
1.47
2.99
f1 (ppm)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60.31
38.25
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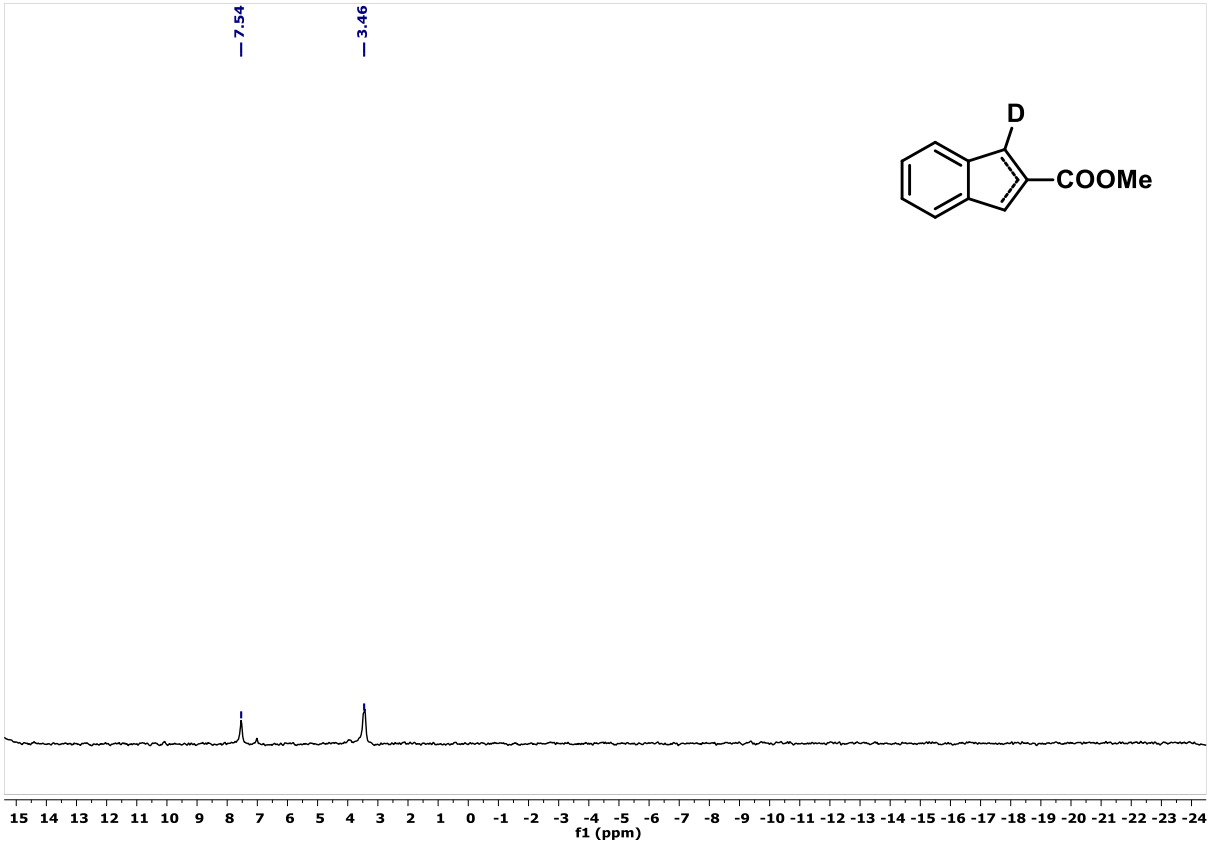
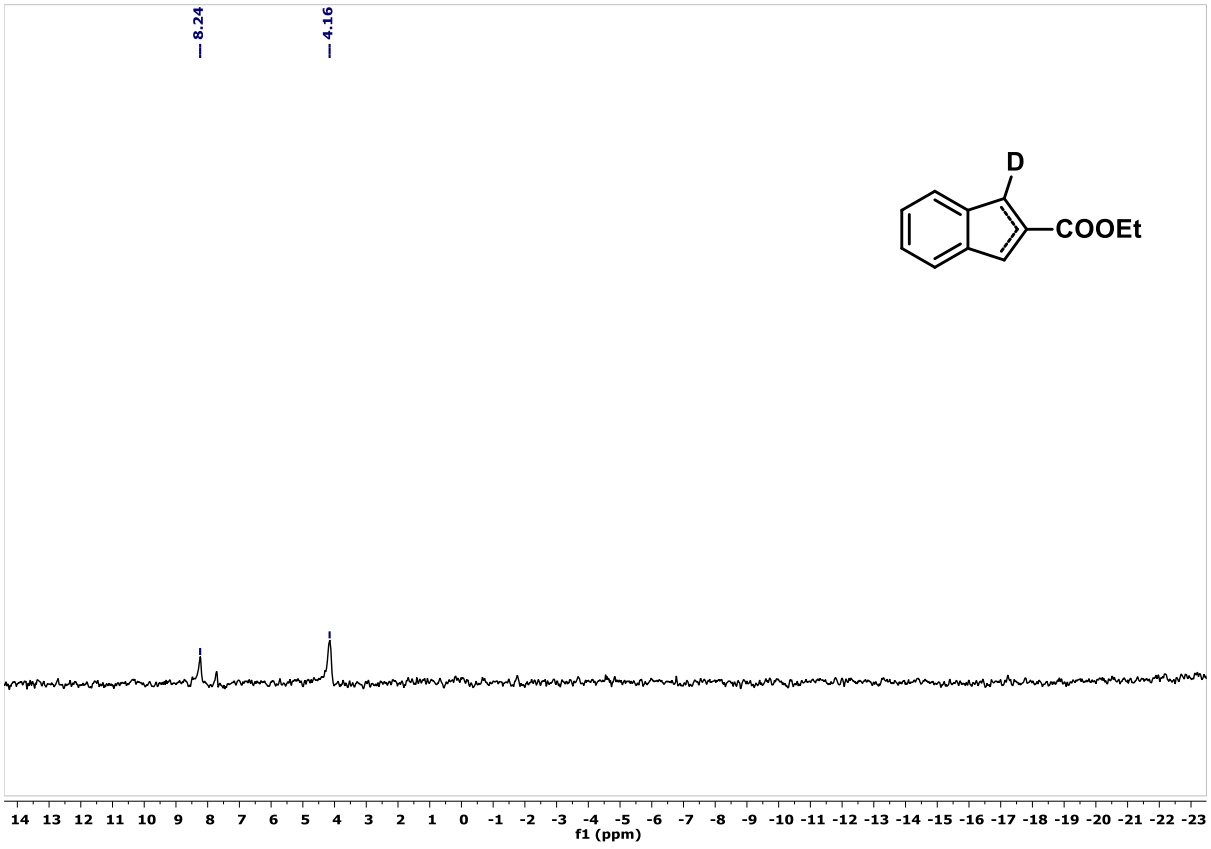
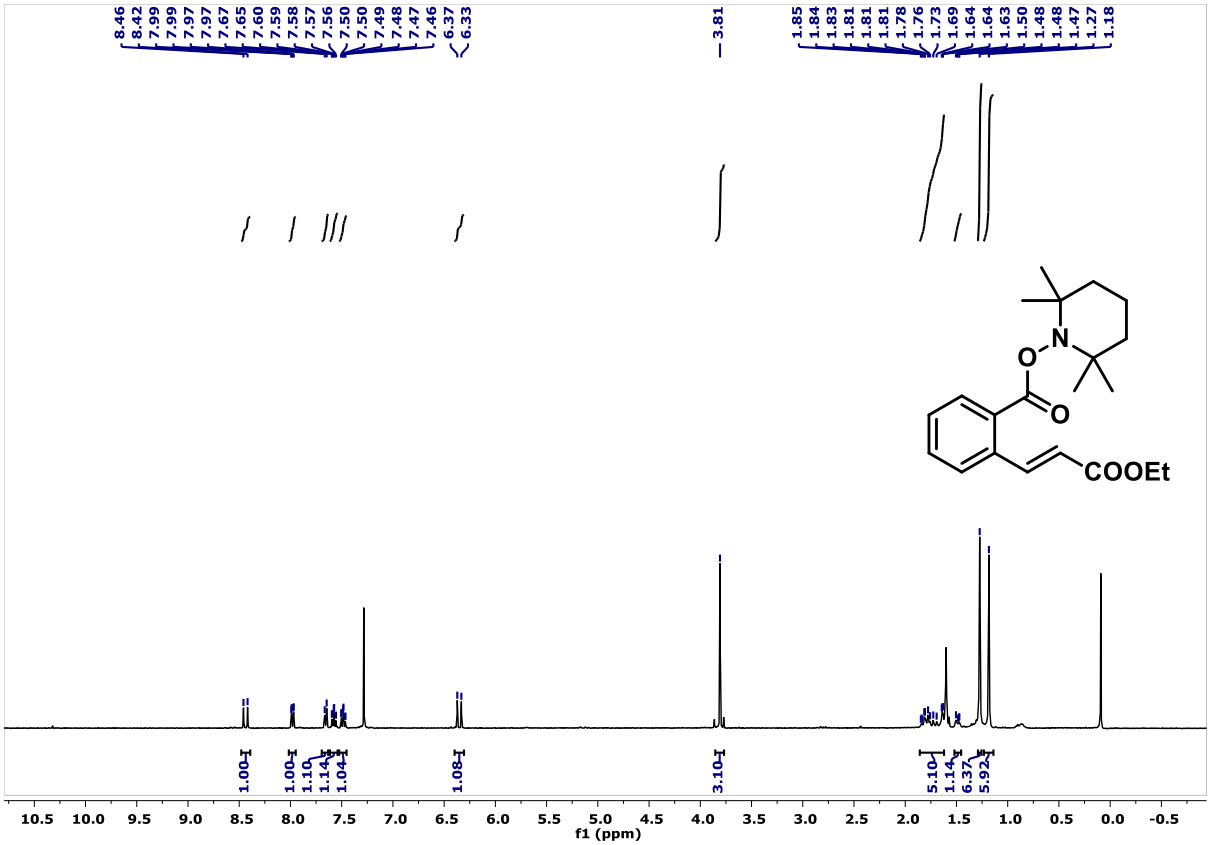
D
COOEt
f1 (ppm)

^{2}H NMR spectra of 2a-D and 2b-D:



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7.48
7.47
7.46
6.37
6.33
3.81
1.85
1.84
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1.81
1.81
1.81
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1.76
1.73
1.69
1.64
1.64
1.63
1.50
1.48
1.48
1.47
1.27
1.18
O
N
O
O
COOEt
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1.00
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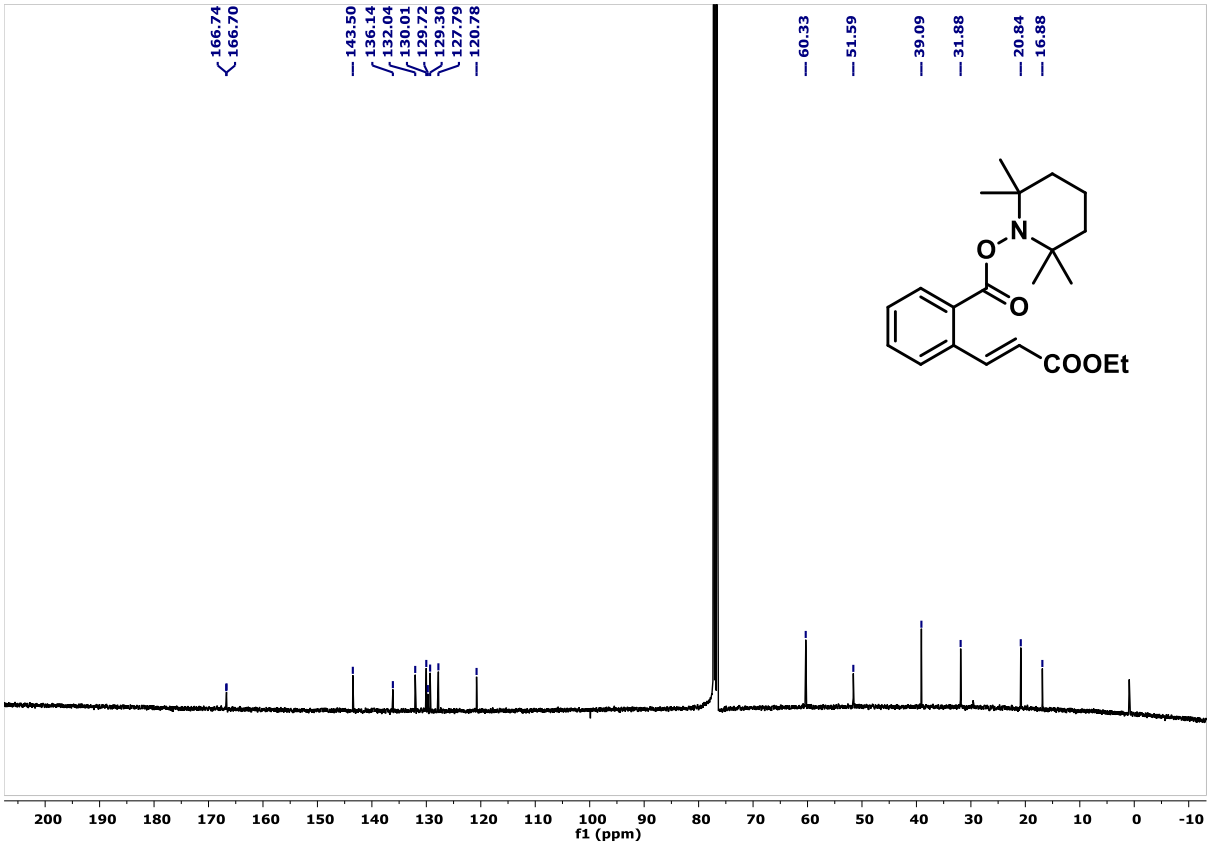
1.14
1.04
1.08
3.10
5.10
1.14
6.37
5.92
f1 (ppm)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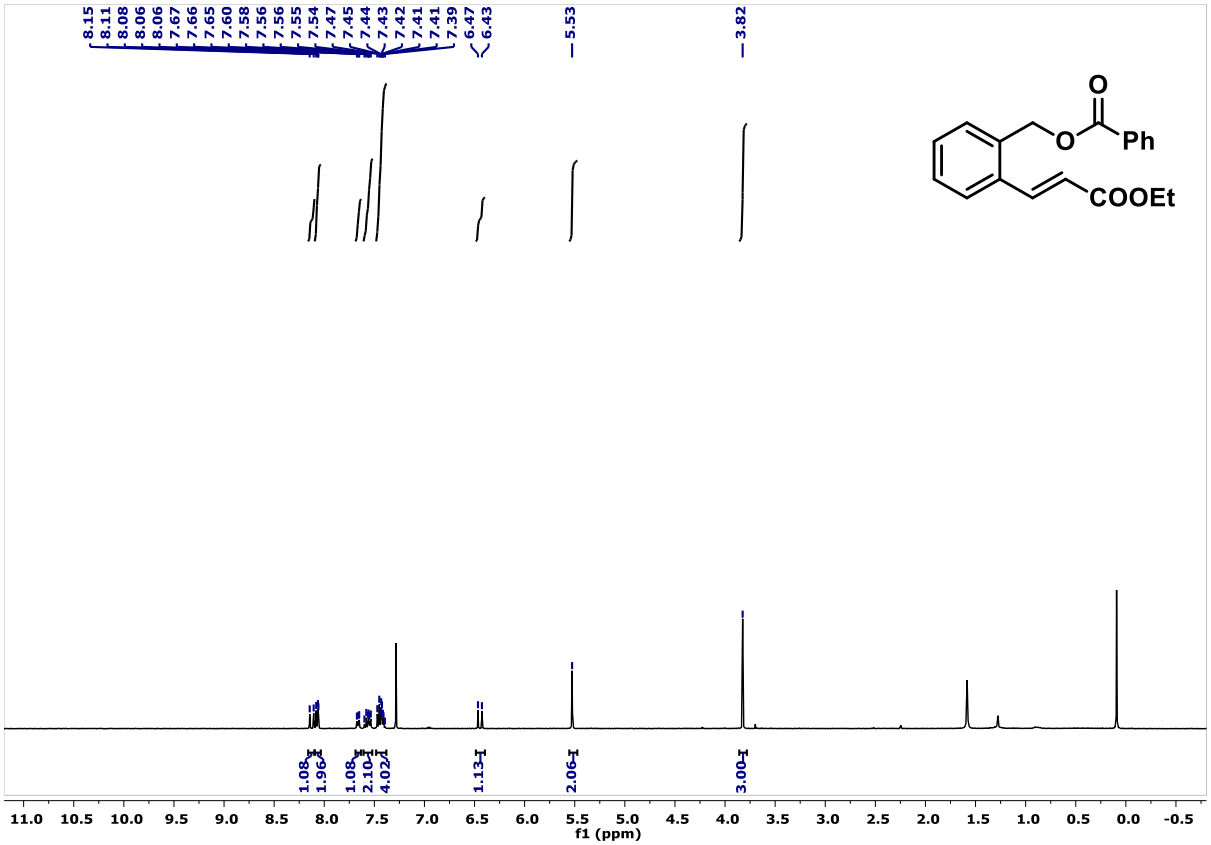
129.30
127.79
120.78
60.33
51.59
39.09
31.88
20.84
16.88
O
N
O
O
COOEt
f1 (ppm)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7.65
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7.56
7.56
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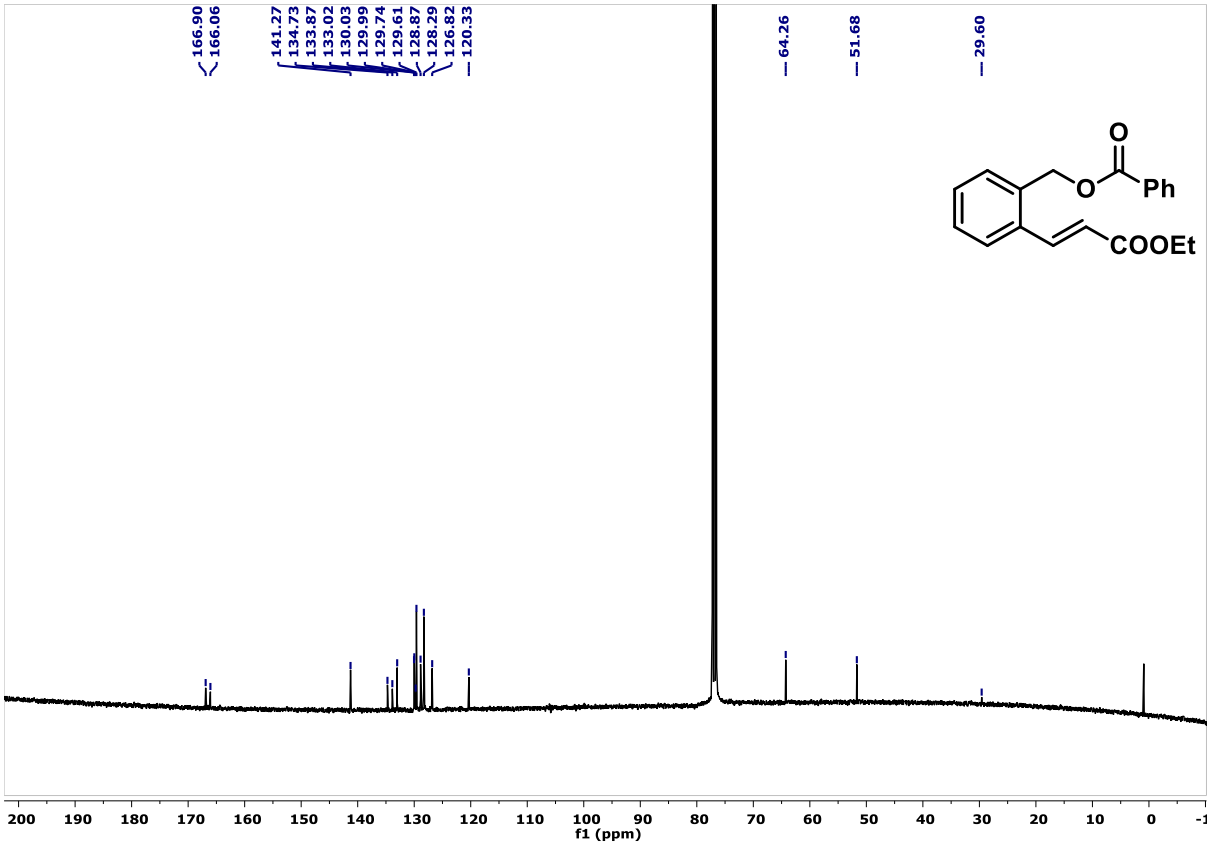
7.54
7.47
7.45
7.44
7.43
7.42
7.41
7.41
7.39
6.47
6.43
5.53
3.82
O
O
Ph
COOEt
1.08
1.96
1.08
2.10
4.02
1.13
2.06
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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166.06
141.27
134.73
133.87
133.02
130.03
129.99
129.74
129.61
128.87
128.29
126.82
120.33
64.26
51.68
29.60
O
O
Ph
COOEt
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

COMPUTATIONAL SECTION

Geometry optimizations were carried out with the Turbomole program package[4] coupled to the PQS Baker optimizer[5] via the BOpt package.[6] We used unrestricted ri-DFT-D3 calculations at the BP86 level,[7] in combination with the def2-TZVP basis set,[8] and a small (m4) grid size. Grimme's dispersion corrections[9] (version 3, disp3, 'zero damping') were used to include Van der Waals interactions. All minima (no imaginary frequencies) and transition states (one imaginary frequency) were characterized by calculating the Hessian matrix. ZPE and gas-phase thermal corrections (entropy and enthalpy, 298 K, 1 bar) from these analyses were calculated. The nature of the transition states was confirmed by following the intrinsic reaction coordinate. The relative (free) energies obtained from these calculations and the energy diagram are reported in Figure S1 and Table S1.

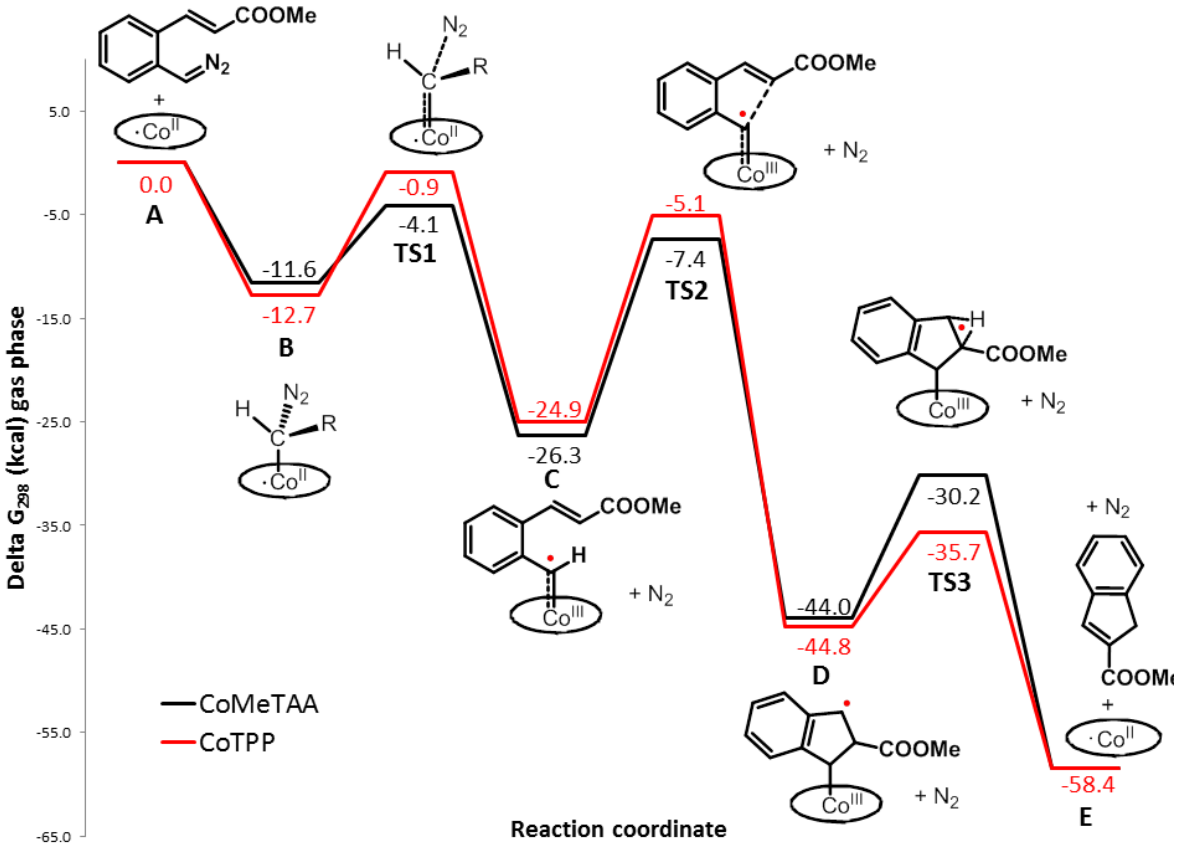

Figure S1 – Energy Diagram for the computed mechanism for catalytic indene synthesis using [Co(MeTAA)] (black) and [Co(TPP)] (red).

Table S1 – Energies of the optimized geometries

SPECIES	$<S^2>$	SCF (au)	ZPE (au)	SCF+ZPE (au)	ENTHALPY (au)	FREE ENERGY (298) (au)	FREE ENERGY (298) (kcal)
N_2	0.00	-109.58042	0.00535	-109.5751	-109.57176	-109.5935	-68770.96
CoTPP	0.76	-3296.5797	0.58059	-3295.999	-3295.96046	-3296.07171	-2068316.21
CoMeTAA	0.76	-2454.2354	0.38508	-2453.85	-2453.82584	-2453.89959	-1539845.23
Diazo compound	0.00	-685.41364	0.18475	-685.2289	-685.21353	-685.2717	-430014.48
Indene	0.00	-575.91128	0.17761	-575.7337	-575.72146	-575.77127	-361301.92
Non-Aromatic Indene (**E'**)	0.00	-575.86602	0.17639	-575.6896	-575.6773	-575.728	-361274.77
Indene H-shift non-aromatic to aromatic TS (**TS4**)	0.00	-575.84726	0.17323	-575.674	-575.662	-575.71148	-361264.41
CoMeTAA diazo (**B**)	0.76	-3139.6934	0.5717	-3139.122	-3139.08156	-3139.1897	-1969871.26
CoMeTAA N_2 loss from diazo TS (**TS1**)	0.77	-3139.6801	0.5695	-3139.111	-3139.07098	-3139.17783	-1969863.81
CoMeTAA carbene complex (**C**)	0.76	-3030.1157	0.56258	-3029.553	-3029.51546	-3029.61968	-1901115.04
CoMeTAA carbene cyclization TS (**TS2**)	0.76	-3030.0842	0.5597	-3029.524	-3029.48723	-3029.58951	-1901096.10
CoMeTAA gama radical after cyclization (**D**)	0.77	-3030.1473	0.56414	-3029.583	-3029.54643	-3029.64788	-1901132.73
CoMeTAA H-shift gama radical to beta radical TS (**TS3**)	0.76	-3030.1199	0.55965	-3029.56	-3029.52312	-3029.62584	-1901118.90
CoTPP diazo (**B**)	0.76	-3982.042	0.76761	-3981.274	-3981.21985	-3981.36368	-2498343.41
CoTPP N_2 loss from diazo TS (**TS1**)	0.77	-3982.024	0.76583	-3981.258	-3981.20443	-3981.34485	-2498331.59
CoTPP carbene complex (**C**)	0.76	-3872.459	0.7575	-3871.702	-3871.64982	-3871.78967	-2429584.68
CoTPP carbene cyclization TS (**TS2**)	0.76	-3872.428	0.75457	-3871.673	-3871.6221	-3871.75805	-2429564.84
CoTPP gama radical after cyclization (**D**)	0.80	-3872.493	0.7583	-3871.734	-3871.68277	-3871.82132	-2429604.54
CoTPP H-shift gama radical to beta radical TS (**TS3**)	0.76	-3872.477	0.75557	-3871.722	-3871.67103	-3871.80674	-2429595.39

Coordinates (pdb format) for all optimized geometries

N_2

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END
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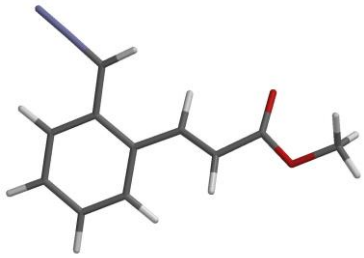
Diazo compound



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ATOM      3  C   111     1        -0.131   -0.617    0.833  1.00  0.00
ATOM      4  C   111     1        -0.220    1.390    2.228  1.00  0.00
ATOM      5  C   111     1         0.704    0.835    3.104  1.00  0.00
ATOM      6  C   111     1         0.810   -1.147    1.740  1.00  0.00
ATOM      7  H   111     1        -0.607    2.390    2.428  1.00  0.00
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ATOM      9  H   111     1         1.183   -2.157    1.571  1.00  0.00
ATOM     10  H   111     1         1.947   -0.885    3.551  1.00  0.00
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ATOM     12  H   111     1        -1.577   -1.179   -0.716  1.00  0.00
ATOM     13  C   111     1         0.083   -2.399   -0.925  1.00  0.00
ATOM     14  H   111     1         1.092   -2.697   -0.638  1.00  0.00
ATOM     15  C   111     1        -0.535   -3.118   -2.053  1.00  0.00
ATOM     16  O   111     1        -1.638   -2.906   -2.534  1.00  0.00
ATOM     17  O   111     1         0.313   -4.084   -2.521  1.00  0.00
ATOM     18  C   111     1        -0.199   -4.845   -3.636  1.00  0.00
ATOM     19  H   111     1        -1.128   -5.362   -3.358  1.00  0.00
ATOM     20  H   111     1         0.587   -5.567   -3.883  1.00  0.00
ATOM     21  H   111     1        -0.405   -4.187   -4.491  1.00  0.00
ATOM     22  C   111     1        -1.580    1.296    0.142  1.00  0.00
ATOM     23  H   111     1        -1.839    0.872   -0.824  1.00  0.00
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ATOM     25  N   111     1        -2.616    3.463    0.635  1.00  0.00
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CONECT    2    5    6   10
CONECT    3    6   11
CONECT    4    5    7
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CONECT    6    9
CONECT   11   12   13
CONECT   13   14   15
CONECT   15   16   17
CONECT   17   18
CONECT   18   19   20   21
CONECT   22   23   24
CONECT   24   25
END
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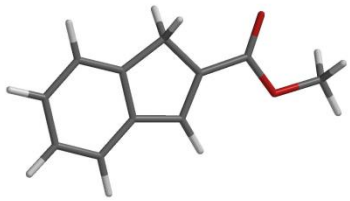
Indene



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ATOM      4  C   111     1        -0.144  -1.152   1.350  1.00  0.00
ATOM      5  C   111     1         0.291   1.096   2.077  1.00  0.00
ATOM      6  C   111     1        -0.063   0.752   3.389  1.00  0.00
ATOM      7  C   111     1        -0.502  -1.502   2.676  1.00  0.00
ATOM      8  H   111     1         0.600   2.118   1.854  1.00  0.00
ATOM      9  H   111     1        -0.025   1.510   4.172  1.00  0.00
ATOM     10  H   111     1        -0.739  -0.818   4.724  1.00  0.00
ATOM     11  C   111     1        -0.281  -2.367   0.472  1.00  0.00
ATOM     12  H   111     1         0.667  -2.654  -0.012  1.00  0.00
ATOM     13  H   111     1        -1.002  -2.222  -0.349  1.00  0.00
ATOM     14  C   111     1        -0.751  -3.427   1.437  1.00  0.00
ATOM     15  C   111     1        -0.869  -2.908   2.691  1.00  0.00
ATOM     16  H   111     1        -1.191  -3.464   3.570  1.00  0.00
ATOM     17  C   111     1        -1.017  -4.799   0.996  1.00  0.00
ATOM     18  O   111     1        -0.886  -5.189  -0.155  1.00  0.00
ATOM     19  O   111     1        -1.433  -5.604   2.020  1.00  0.00
ATOM     20  C   111     1        -1.709  -6.967   1.635  1.00  0.00
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CONECT    4    7   11
CONECT    5    6    8
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CONECT    7   15
CONECT   11   12   13   14
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CONECT   15   16
CONECT   17   18   19
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CONECT   20   21   22   23
END
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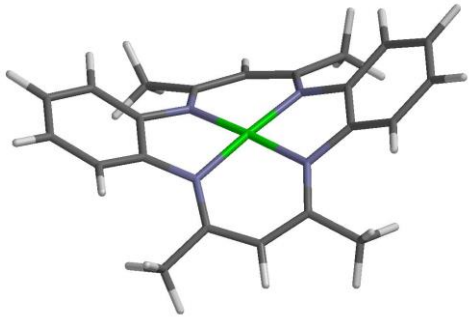
CoMeTAA



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ATOM      4  C   111     1        1.543   0.702  -4.198  1.00  0.00
ATOM      5  C   111     1        2.306   2.994  -4.062  1.00  0.00
ATOM      6  C   111     1        1.804   3.083  -2.758  1.00  0.00
ATOM      7  H   111     1        1.527  -0.241  -4.737  1.00  0.00
ATOM      8  H   111     1        2.834   3.845  -4.494  1.00  0.00
ATOM      9  H   111     1        1.991   3.984  -2.180  1.00  0.00
ATOM     10  C   111     1       -0.178  -1.338  -2.671  1.00  0.00
ATOM     11  C   111     1       -0.541  -2.431  -1.868  1.00  0.00
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ATOM     16  C   111     1        1.367  -3.072   2.076  1.00  0.00
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ATOM     27  C   111     1        0.289   2.937  -0.085  1.00  0.00
ATOM     28  N   111     1        0.689   1.899  -0.841  1.00  0.00
ATOM     29  N   111     1        0.453  -0.269  -2.153  1.00  0.00
ATOM     30  N   111     1        0.385  -1.696   0.216  1.00  0.00
ATOM     31  C   111     1        1.004   0.789  -2.911  1.00  0.00
ATOM     32  N   111     1        0.618   0.473   1.528  1.00  0.00
ATOM     33 CO   111     1        0.608   0.095  -0.314  1.00  0.00
ATOM     34  C   111     1        0.014   4.306  -0.671  1.00  0.00
ATOM     35  H   111     1       -0.772   4.796  -0.083  1.00  0.00
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ATOM     37  H   111     1        0.744   2.081   4.146  1.00  0.00
ATOM     38  H   111     1       -0.493   0.820   3.959  1.00  0.00
ATOM     39  H   111     1       -0.897   2.531   3.666  1.00  0.00
ATOM     40  C   111     1       -0.614  -1.395  -4.120  1.00  0.00
ATOM     41  H   111     1       -1.522  -2.006  -4.198  1.00  0.00
ATOM     42  H   111     1        0.146  -1.862  -4.765  1.00  0.00
ATOM     43  H   111     1       -0.828  -0.397  -4.521  1.00  0.00
ATOM     44  C   111     1       -0.728  -3.937   0.094  1.00  0.00
ATOM     45  H   111     1       -1.621  -4.273  -0.449  1.00  0.00
ATOM     46  H   111     1       -0.986  -3.820   1.154  1.00  0.00
ATOM     47  H   111     1        0.019  -4.741   0.016  1.00  0.00
ATOM     48  H   111     1       -0.317   4.244  -1.715  1.00  0.00
ATOM     49  H   111     1        0.899   4.958  -0.636  1.00  0.00
CONECT    1    2
CONECT    2    4    5
CONECT    3    6   28   31
CONECT    4    7   31
CONECT    5    6    8
CONECT    6    9
CONECT   10   11   29   40
CONECT   11   12   13
CONECT   13   30   44
CONECT   14   16   17   30
CONECT   15   18   19   23
CONECT   16   19   20
CONECT   17   18   32
CONECT   18   21
CONECT   19   22
CONECT   24   25   32   36
CONECT   25   26   27
CONECT   27   28   34
CONECT   28   33
CONECT   29   31   33
CONECT   30   33
CONECT   32   33
```

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CONECT   34   35   48   49
CONECT   36   37   38   39
CONECT   40   41   42   43
CONECT   44   45   46   47
END
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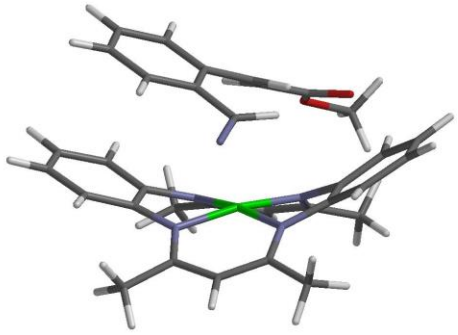
CoMeTAA diazo (B)



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ATOM      1  H   111     1        2.769   1.590  -5.832  1.00  0.00
ATOM      2  C   111     1        2.324   1.727  -4.846  1.00  0.00
ATOM      3  C   111     1        1.235   2.047  -2.285  1.00  0.00
ATOM      4  C   111     1        1.648   0.658  -4.244  1.00  0.00
ATOM      5  C   111     1        2.476   2.937  -4.169  1.00  0.00
ATOM      6  C   111     1        1.949   3.094  -2.881  1.00  0.00
ATOM      7  H   111     1        1.613  -0.302  -4.752  1.00  0.00
ATOM      8  H   111     1        3.046   3.751  -4.618  1.00  0.00
ATOM      9  H   111     1        2.153   3.998  -2.311  1.00  0.00
ATOM     10  C   111     1       -0.156  -1.278  -2.621  1.00  0.00
ATOM     11  C   111     1       -0.555  -2.308  -1.751  1.00  0.00
ATOM     12  H   111     1       -1.141  -3.107  -2.204  1.00  0.00
ATOM     13  C   111     1       -0.268  -2.464  -0.382  1.00  0.00
ATOM     14  C   111     1        0.841  -1.646   1.640  1.00  0.00
ATOM     15  C   111     1        1.937  -1.562   4.228  1.00  0.00
ATOM     16  C   111     1        1.244  -2.824   2.285  1.00  0.00
ATOM     17  C   111     1        1.005  -0.394   2.309  1.00  0.00
ATOM     18  C   111     1        1.572  -0.374   3.590  1.00  0.00
ATOM     19  C   111     1        1.773  -2.784   3.579  1.00  0.00
ATOM     20  H   111     1        1.204  -3.774   1.759  1.00  0.00
ATOM     21  H   111     1        1.802   0.574   4.068  1.00  0.00
ATOM     22  H   111     1        2.097  -3.710   4.056  1.00  0.00
ATOM     23  H   111     1        2.401  -1.520   5.214  1.00  0.00
ATOM     24  C   111     1        0.274   1.916   1.963  1.00  0.00
ATOM     25  C   111     1        0.034   2.996   1.093  1.00  0.00
ATOM     26  H   111     1       -0.376   3.895   1.550  1.00  0.00
ATOM     27  C   111     1        0.283   3.069  -0.289  1.00  0.00
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ATOM     28  N   111     1        0.773   2.018  -0.958  1.00  0.00
ATOM     29  N   111     1        0.501  -0.199  -2.173  1.00  0.00
ATOM     30  N   111     1        0.393  -1.526   0.314  1.00  0.00
ATOM     31  C   111     1        1.084   0.804  -2.968  1.00  0.00
ATOM     32  N   111     1        0.680   0.718   1.512  1.00  0.00
ATOM     33  C   111     1       -0.096   4.351  -0.996  1.00  0.00
ATOM     34  H   111     1       -0.930   4.825  -0.462  1.00  0.00
ATOM     35  C   111     1       -0.023   2.170   3.425  1.00  0.00
ATOM     36  H   111     1        0.878   2.489   3.970  1.00  0.00
ATOM     37  H   111     1       -0.419   1.277   3.925  1.00  0.00
ATOM     38  H   111     1       -0.758   2.979   3.513  1.00  0.00
ATOM     39  C   111     1       -0.572  -1.417  -4.069  1.00  0.00
ATOM     40  H   111     1       -1.491  -2.015  -4.129  1.00  0.00
ATOM     41  H   111     1        0.193  -1.937  -4.666  1.00  0.00
ATOM     42  H   111     1       -0.756  -0.441  -4.536  1.00  0.00
ATOM     43  C   111     1       -0.822  -3.712   0.275  1.00  0.00
ATOM     44  H   111     1       -1.716  -4.041  -0.270  1.00  0.00
ATOM     45  H   111     1       -1.095  -3.534   1.322  1.00  0.00
ATOM     46  H   111     1       -0.102  -4.544   0.250  1.00  0.00
ATOM     47  H   111     1       -0.402   4.159  -2.032  1.00  0.00
ATOM     48  H   111     1        0.742   5.061  -1.017  1.00  0.00
ATOM     49 CO   111     1        0.727   0.233  -0.326  1.00  0.00
ATOM     50  C   111     1        3.830  -0.118   0.752  1.00  0.00
ATOM     51  C   111     1        5.041  -0.162   3.298  1.00  0.00
ATOM     52  C   111     1        4.023   1.101   1.464  1.00  0.00
ATOM     53  C   111     1        4.219  -1.330   1.351  1.00  0.00
ATOM     54  C   111     1        4.816  -1.357   2.605  1.00  0.00
ATOM     55  C   111     1        4.642   1.041   2.730  1.00  0.00
ATOM     56  H   111     1        4.035  -2.272   0.833  1.00  0.00
ATOM     57  H   111     1        5.101  -2.312   3.045  1.00  0.00
ATOM     58  H   111     1        4.836   1.975   3.258  1.00  0.00
ATOM     59  H   111     1        5.523  -0.172   4.275  1.00  0.00
ATOM     60  C   111     1        3.593   2.377   0.915  1.00  0.00
ATOM     61  H   111     1        3.516   2.487  -0.171  1.00  0.00
ATOM     62  C   111     1        3.246   3.461   1.644  1.00  0.00
ATOM     63  H   111     1        3.198   3.435   2.733  1.00  0.00
ATOM     64  C   111     1        2.862   4.718   0.999  1.00  0.00
ATOM     65  O   111     1        2.930   4.979  -0.196  1.00  0.00
ATOM     66  O   111     1        2.406   5.615   1.928  1.00  0.00
ATOM     67  C   111     1        1.980   6.881   1.390  1.00  0.00
ATOM     68  H   111     1        2.783   7.348   0.804  1.00  0.00
ATOM     69  H   111     1        1.724   7.498   2.258  1.00  0.00
ATOM     70  H   111     1        1.101   6.749   0.743  1.00  0.00
ATOM     71  N   111     1        3.149  -1.224  -1.261  1.00  0.00
ATOM     72  N   111     1        3.029  -2.207  -1.821  1.00  0.00
ATOM     73  C   111     1        3.167  -0.101  -0.555  1.00  0.00
ATOM     74  H   111     1        3.175   0.781  -1.198  1.00  0.00
CONECT    1    2
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CONECT    2    4    5
CONECT    3    6   28   31
CONECT    4    7   31
CONECT    5    6    8
CONECT    6    9
CONECT   10   11   29   39
CONECT   11   12   13
CONECT   13   30   43
CONECT   14   16   17   30
CONECT   15   18   19   23
CONECT   16   19   20
CONECT   17   18   32
CONECT   18   21
CONECT   19   22
CONECT   24   25   32   35
CONECT   25   26   27
CONECT   27   28   33
CONECT   28   49
CONECT   29   31   49
CONECT   30   49
CONECT   32   49
CONECT   33   34   47   48
CONECT   35   36   37   38
CONECT   39   40   41   42
CONECT   43   44   45   46
CONECT   50   52   53   73
CONECT   51   54   55   59
CONECT   52   55   60
CONECT   53   54   56
CONECT   54   57
CONECT   55   58
CONECT   60   61   62
CONECT   62   63   64
CONECT   64   65   66
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CONECT   71   72   73
CONECT   73   74
END
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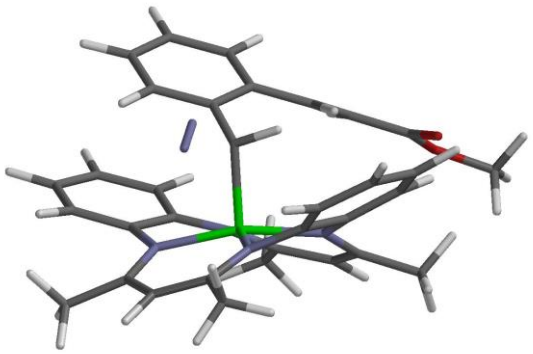
CoMeTAA N_2 loss from diazo TS (TS1)



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ATOM      1  H   111     1         2.665   1.649  -5.907  1.00  0.00
ATOM      2  C   111     1         2.248   1.772  -4.907  1.00  0.00
ATOM      3  C   111     1         1.246   2.055  -2.313  1.00  0.00
ATOM      4  C   111     1         1.632   0.681  -4.285  1.00  0.00
ATOM      5  C   111     1         2.389   2.986  -4.233  1.00  0.00
ATOM      6  C   111     1         1.910   3.124  -2.927  1.00  0.00
ATOM      7  H   111     1         1.625  -0.282  -4.786  1.00  0.00
ATOM      8  H   111     1         2.919   3.816  -4.701  1.00  0.00
ATOM      9  H   111     1         2.116   4.028  -2.358  1.00  0.00
ATOM     10  C   111     1        -0.045  -1.315  -2.597  1.00  0.00
ATOM     11  C   111     1        -0.423  -2.346  -1.718  1.00  0.00
ATOM     12  H   111     1        -0.988  -3.158  -2.172  1.00  0.00
ATOM     13  C   111     1        -0.175  -2.483  -0.343  1.00  0.00
ATOM     14  C   111     1         0.855  -1.656   1.715  1.00  0.00
ATOM     15  C   111     1         1.865  -1.538   4.336  1.00  0.00
ATOM     16  C   111     1         1.208  -2.829   2.398  1.00  0.00
ATOM     17  C   111     1         1.015  -0.396   2.368  1.00  0.00
ATOM     18  C   111     1         1.546  -0.356   3.663  1.00  0.00
ATOM     19  C   111     1         1.690  -2.770   3.708  1.00  0.00
ATOM     20  H   111     1         1.173  -3.788   1.891  1.00  0.00
ATOM     21  H   111     1         1.784   0.597   4.124  1.00  0.00
ATOM     22  H   111     1         1.979  -3.692   4.215  1.00  0.00
ATOM     23  H   111     1         2.298  -1.485   5.335  1.00  0.00
ATOM     24  C   111     1         0.299   1.904   1.965  1.00  0.00
ATOM     25  C   111     1         0.069   2.975   1.086  1.00  0.00
ATOM     26  H   111     1        -0.358   3.871   1.533  1.00  0.00
ATOM     27  C   111     1         0.319   3.046  -0.294  1.00  0.00
ATOM     28  N   111     1         0.835   2.009  -0.968  1.00  0.00
ATOM     29  N   111     1         0.584  -0.211  -2.170  1.00  0.00
ATOM     30  N   111     1         0.483  -1.546   0.364  1.00  0.00
ATOM     31  C   111     1         1.108   0.811  -2.991  1.00  0.00
ATOM     32  N   111     1         0.735   0.706   1.539  1.00  0.00
ATOM     33  C   111     1        -0.098   4.317  -0.999  1.00  0.00
ATOM     34  H   111     1        -0.938   4.771  -0.458  1.00  0.00
ATOM     35  C   111     1        -0.057   2.159   3.414  1.00  0.00
ATOM     36  H   111     1         0.820   2.491   3.989  1.00  0.00
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ATOM     37  H   111     1       -0.461   1.263   3.903  1.00  0.00
ATOM     38  H   111     1       -0.805   2.959   3.470  1.00  0.00
ATOM     39  C   111     1       -0.456  -1.491  -4.042  1.00  0.00
ATOM     40  H   111     1       -1.340  -2.138  -4.096  1.00  0.00
ATOM     41  H   111     1        0.343  -1.976  -4.623  1.00  0.00
ATOM     42  H   111     1       -0.691  -0.532  -4.521  1.00  0.00
ATOM     43  C   111     1       -0.776  -3.708   0.317  1.00  0.00
ATOM     44  H   111     1       -1.648  -4.041  -0.260  1.00  0.00
ATOM     45  H   111     1       -1.096  -3.499   1.346  1.00  0.00
ATOM     46  H   111     1       -0.066  -4.547   0.348  1.00  0.00
ATOM     47  H   111     1       -0.408   4.121  -2.033  1.00  0.00
ATOM     48  H   111     1        0.724   5.045  -1.023  1.00  0.00
ATOM     49 CO   111     1        0.903   0.207  -0.316  1.00  0.00
ATOM     50  C   111     1        3.662  -0.074   0.746  1.00  0.00
ATOM     51  C   111     1        5.025  -0.245   3.214  1.00  0.00
ATOM     52  C   111     1        3.999   1.109   1.463  1.00  0.00
ATOM     53  C   111     1        4.003  -1.318   1.305  1.00  0.00
ATOM     54  C   111     1        4.682  -1.408   2.516  1.00  0.00
ATOM     55  C   111     1        4.676   0.996   2.693  1.00  0.00
ATOM     56  H   111     1        3.717  -2.226   0.777  1.00  0.00
ATOM     57  H   111     1        4.929  -2.388   2.925  1.00  0.00
ATOM     58  H   111     1        4.959   1.906   3.224  1.00  0.00
ATOM     59  H   111     1        5.560  -0.309   4.162  1.00  0.00
ATOM     60  C   111     1        3.616   2.412   0.936  1.00  0.00
ATOM     61  H   111     1        3.519   2.518  -0.148  1.00  0.00
ATOM     62  C   111     1        3.311   3.498   1.676  1.00  0.00
ATOM     63  H   111     1        3.283   3.470   2.765  1.00  0.00
ATOM     64  C   111     1        2.908   4.753   1.033  1.00  0.00
ATOM     65  O   111     1        2.925   5.001  -0.166  1.00  0.00
ATOM     66  O   111     1        2.479   5.656   1.969  1.00  0.00
ATOM     67  C   111     1        2.022   6.913   1.432  1.00  0.00
ATOM     68  H   111     1        2.809   7.390   0.832  1.00  0.00
ATOM     69  H   111     1        1.769   7.529   2.300  1.00  0.00
ATOM     70  H   111     1        1.137   6.762   0.798  1.00  0.00
ATOM     71  N   111     1        3.401  -1.355  -1.501  1.00  0.00
ATOM     72  N   111     1        2.901  -1.862  -2.388  1.00  0.00
ATOM     73  C   111     1        2.854   0.012  -0.487  1.00  0.00
ATOM     74  H   111     1        3.197   0.792  -1.187  1.00  0.00
CONECT    1    2
CONECT    2    4    5
CONECT    3    6   28   31
CONECT    4    7   31
CONECT    5    6    8
CONECT    6    9
CONECT   10   11   29   39
CONECT   11   12   13
CONECT   13   30   43
CONECT   14   16   17   30
CONECT   15   18   19   23
CONECT   16   19   20
CONECT   17   18   32
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CONECT   18   21
CONECT   19   22
CONECT   24   25   32   35
CONECT   25   26   27
CONECT   27   28   33
CONECT   28   49
CONECT   29   31   49
CONECT   30   49
CONECT   32   49
CONECT   33   34   47   48
CONECT   35   36   37   38
CONECT   39   40   41   42
CONECT   43   44   45   46
CONECT   49   73
CONECT   50   52   53   73
CONECT   51   54   55   59
CONECT   52   55   60
CONECT   53   54   56
CONECT   54   57
CONECT   55   58
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CONECT   62   63   64
CONECT   64   65   66
CONECT   66   67
CONECT   67   68   69   70
CONECT   71   72
CONECT   73   74
END
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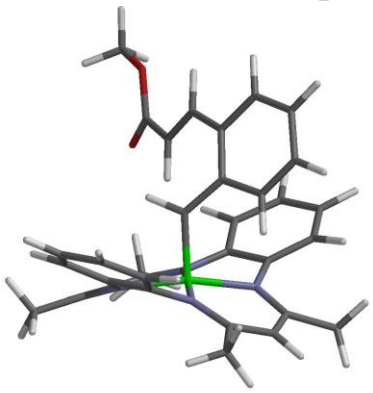
CoMeTAA carbene complex (C)



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ATOM      1  H   111     1       1.859   2.445  -6.022  1.00  0.00
ATOM      2  C   111     1       1.545   2.425  -4.979  1.00  0.00
ATOM      3  C   111     1       0.805   2.346  -2.274  1.00  0.00
ATOM      4  C   111     1       1.107   1.224  -4.416  1.00  0.00
ATOM      5  C   111     1       1.637   3.576  -4.194  1.00  0.00
ATOM      6  C   111     1       1.288   3.531  -2.842  1.00  0.00
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ATOM      7  H   111     1        1.131   0.320  -5.017  1.00  0.00
ATOM      8  H   111     1        2.025   4.502  -4.619  1.00  0.00
ATOM      9  H   111     1        1.455   4.408  -2.222  1.00  0.00
ATOM     10  C   111     1       -0.128  -1.110  -2.841  1.00  0.00
ATOM     11  C   111     1       -0.209  -2.293  -2.091  1.00  0.00
ATOM     12  H   111     1       -0.655  -3.142  -2.607  1.00  0.00
ATOM     13  C   111     1        0.235  -2.551  -0.782  1.00  0.00
ATOM     14  C   111     1        1.315  -1.768   1.272  1.00  0.00
ATOM     15  C   111     1        2.730  -1.704   3.702  1.00  0.00
ATOM     16  C   111     1        1.987  -2.909   1.735  1.00  0.00
ATOM     17  C   111     1        1.368  -0.576   2.043  1.00  0.00
ATOM     18  C   111     1        2.099  -0.549   3.237  1.00  0.00
ATOM     19  C   111     1        2.669  -2.879   2.953  1.00  0.00
ATOM     20  H   111     1        2.070  -3.795   1.113  1.00  0.00
ATOM     21  H   111     1        2.239   0.388   3.769  1.00  0.00
ATOM     22  H   111     1        3.206  -3.769   3.282  1.00  0.00
ATOM     23  H   111     1        3.313  -1.666   4.623  1.00  0.00
ATOM     24  C   111     1        0.309   1.616   2.023  1.00  0.00
ATOM     25  C   111     1       -0.054   2.778   1.321  1.00  0.00
ATOM     26  H   111     1       -0.489   3.576   1.920  1.00  0.00
ATOM     27  C   111     1        0.074   3.043  -0.051  1.00  0.00
ATOM     28  N   111     1        0.522   2.117  -0.915  1.00  0.00
ATOM     29  N   111     1        0.375   0.025  -2.331  1.00  0.00
ATOM     30  N   111     1        0.715  -1.579   0.007  1.00  0.00
ATOM     31  C   111     1        0.716   1.171  -3.071  1.00  0.00
ATOM     32  N   111     1        0.800   0.537   1.398  1.00  0.00
ATOM     33 CO   111     1        0.785   0.280  -0.487  1.00  0.00
ATOM     34  C   111     1        2.614   0.144  -0.805  1.00  0.00
ATOM     35  H   111     1        2.828  -0.500  -1.663  1.00  0.00
ATOM     36  C   111     1       -0.409   4.401  -0.516  1.00  0.00
ATOM     37  H   111     1       -1.185   4.762   0.171  1.00  0.00
ATOM     38  C   111     1        0.041   1.626   3.514  1.00  0.00
ATOM     39  H   111     1        0.886   2.048   4.077  1.00  0.00
ATOM     40  H   111     1       -0.152   0.618   3.901  1.00  0.00
ATOM     41  H   111     1       -0.833   2.257   3.718  1.00  0.00
ATOM     42  C   111     1       -0.719  -1.167  -4.235  1.00  0.00
ATOM     43  H   111     1       -1.538  -1.897  -4.249  1.00  0.00
ATOM     44  H   111     1        0.020  -1.495  -4.981  1.00  0.00
ATOM     45  H   111     1       -1.111  -0.193  -4.552  1.00  0.00
ATOM     46  C   111     1        0.088  -3.979  -0.309  1.00  0.00
ATOM     47  H   111     1       -0.708  -4.472  -0.881  1.00  0.00
ATOM     48  H   111     1       -0.159  -4.034   0.759  1.00  0.00
ATOM     49  H   111     1        1.022  -4.535  -0.481  1.00  0.00
ATOM     50  H   111     1       -0.826   4.359  -1.529  1.00  0.00
ATOM     51  H   111     1        0.400   5.146  -0.515  1.00  0.00
ATOM     52  C   111     1        3.686   0.594  -0.018  1.00  0.00
ATOM     53  C   111     1        5.958   1.718   1.280  1.00  0.00
ATOM     54  C   111     1        4.956  -0.118  -0.003  1.00  0.00
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ATOM     55  C   111     1        3.596   1.795   0.749  1.00  0.00
ATOM     56  C   111     1        4.698   2.345   1.374  1.00  0.00
ATOM     57  C   111     1        6.066   0.510   0.605  1.00  0.00
ATOM     58  H   111     1        2.636   2.308   0.777  1.00  0.00
ATOM     59  H   111     1        4.596   3.284   1.922  1.00  0.00
ATOM     60  H   111     1        7.028  -0.010   0.582  1.00  0.00
ATOM     61  H   111     1        6.833   2.163   1.753  1.00  0.00
ATOM     62  C   111     1        5.134  -1.489  -0.425  1.00  0.00
ATOM     63  H   111     1        6.173  -1.835  -0.431  1.00  0.00
ATOM     64  C   111     1        4.179  -2.427  -0.681  1.00  0.00
ATOM     65  H   111     1        3.122  -2.184  -0.624  1.00  0.00
ATOM     66  C   111     1        4.418  -3.848  -0.891  1.00  0.00
ATOM     67  O   111     1        3.530  -4.700  -0.876  1.00  0.00
ATOM     68  O   111     1        5.734  -4.171  -1.098  1.00  0.00
ATOM     69  C   111     1        5.991  -5.577  -1.265  1.00  0.00
ATOM     70  H   111     1        7.072  -5.661  -1.424  1.00  0.00
ATOM     71  H   111     1        5.443  -5.974  -2.131  1.00  0.00
ATOM     72  H   111     1        5.688  -6.140  -0.371  1.00  0.00
CONECT    1    2
CONECT    2    4    5
CONECT    3    6   28   31
CONECT    4    7   31
CONECT    5    6    8
CONECT    6    9
CONECT   10   11   29   42
CONECT   11   12   13
CONECT   13   30   46
CONECT   14   16   17   30
CONECT   15   18   19   23
CONECT   16   19   20
CONECT   17   18   32
CONECT   18   21
CONECT   19   22
CONECT   24   25   32   38
CONECT   25   26   27
CONECT   27   28   36
CONECT   28   33
CONECT   29   31   33
CONECT   30   33
CONECT   32   33
CONECT   33   34
CONECT   34   35   52
CONECT   36   37   50   51
CONECT   38   39   40   41
CONECT   42   43   44   45
CONECT   46   47   48   49
CONECT   52   54   55
CONECT   53   56   57   61
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CONECT   54   57   62
CONECT   55   56   58
CONECT   56   59
CONECT   57   60
CONECT   62   63   64
CONECT   64   65   66
CONECT   66   67   68
CONECT   68   69
CONECT   69   70   71   72
END
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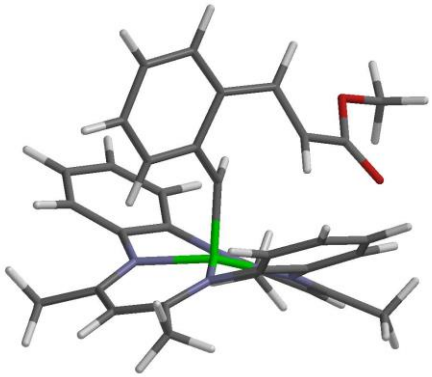
CoMeTAA carbene cyclization TS (TS2)



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ATOM      1  H   111     1        2.612   1.858  -5.861  1.00  0.00
ATOM      2  C   111     1        2.183   1.894  -4.860  1.00  0.00
ATOM      3  C   111     1        1.156   1.963  -2.250  1.00  0.00
ATOM      4  C   111     1        1.712   0.718  -4.272  1.00  0.00
ATOM      5  C   111     1        2.160   3.095  -4.148  1.00  0.00
ATOM      6  C   111     1        1.668   3.126  -2.841  1.00  0.00
ATOM      7  H   111     1        1.820  -0.221  -4.807  1.00  0.00
ATOM      8  H   111     1        2.570   4.004  -4.589  1.00  0.00
ATOM      9  H   111     1        1.743   4.044  -2.264  1.00  0.00
ATOM     10  C   111     1        0.272  -1.518  -2.701  1.00  0.00
ATOM     11  C   111     1        0.018  -2.625  -1.881  1.00  0.00
ATOM     12  H   111     1       -0.431  -3.484  -2.377  1.00  0.00
ATOM     13  C   111     1        0.283  -2.792  -0.514  1.00  0.00
ATOM     14  C   111     1        1.270  -1.948   1.551  1.00  0.00
ATOM     15  C   111     1        2.504  -1.824   4.074  1.00  0.00
ATOM     16  C   111     1        1.828  -3.101   2.126  1.00  0.00
ATOM     17  C   111     1        1.349  -0.714   2.255  1.00  0.00
ATOM     18  C   111     1        1.989  -0.660   3.499  1.00  0.00
ATOM     19  C   111     1        2.420  -3.038   3.390  1.00  0.00
ATOM     20  H   111     1        1.898  -4.014   1.545  1.00  0.00
ATOM     21  H   111     1        2.145   0.297   3.990  1.00  0.00
ATOM     22  H   111     1        2.870  -3.937   3.811  1.00  0.00
ATOM     23  H   111     1        3.017  -1.768   5.035  1.00  0.00
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ATOM     24  C   111     1        0.339   1.491   2.028  1.00  0.00
ATOM     25  C   111     1       -0.008   2.594   1.223  1.00  0.00
ATOM     26  H   111     1       -0.503   3.417   1.737  1.00  0.00
ATOM     27  C   111     1        0.197   2.768  -0.152  1.00  0.00
ATOM     28  N   111     1        0.752   1.810  -0.915  1.00  0.00
ATOM     29  N   111     1        0.762  -0.367  -2.210  1.00  0.00
ATOM     30  N   111     1        0.796  -1.806   0.238  1.00  0.00
ATOM     31  C   111     1        1.174   0.737  -2.977  1.00  0.00
ATOM     32  N   111     1        0.880   0.383   1.509  1.00  0.00
ATOM     33 CO   111     1        1.019   0.004  -0.352  1.00  0.00
ATOM     34  C   111     1        2.860   0.006  -0.531  1.00  0.00
ATOM     35  H   111     1        3.154  -0.294  -1.543  1.00  0.00
ATOM     36  C   111     1       -0.310   4.063  -0.752  1.00  0.00
ATOM     37  H   111     1       -1.163   4.426  -0.165  1.00  0.00
ATOM     38  C   111     1       -0.010   1.598   3.497  1.00  0.00
ATOM     39  H   111     1        0.817   2.029   4.081  1.00  0.00
ATOM     40  H   111     1       -0.252   0.620   3.930  1.00  0.00
ATOM     41  H   111     1       -0.875   2.263   3.617  1.00  0.00
ATOM     42  C   111     1       -0.136  -1.655  -4.153  1.00  0.00
ATOM     43  H   111     1       -0.947  -2.390  -4.233  1.00  0.00
ATOM     44  H   111     1        0.693  -2.017  -4.779  1.00  0.00
ATOM     45  H   111     1       -0.483  -0.702  -4.572  1.00  0.00
ATOM     46  C   111     1       -0.116  -4.123   0.080  1.00  0.00
ATOM     47  H   111     1       -0.958  -4.538  -0.488  1.00  0.00
ATOM     48  H   111     1       -0.411  -4.033   1.132  1.00  0.00
ATOM     49  H   111     1        0.723  -4.830   0.009  1.00  0.00
ATOM     50  H   111     1       -0.629   3.930  -1.793  1.00  0.00
ATOM     51  H   111     1        0.459   4.850  -0.734  1.00  0.00
ATOM     52  C   111     1        3.833   0.724   0.223  1.00  0.00
ATOM     53  C   111     1        5.999   2.255   1.177  1.00  0.00
ATOM     54  C   111     1        5.188   0.190   0.188  1.00  0.00
ATOM     55  C   111     1        3.599   1.956   0.872  1.00  0.00
ATOM     56  C   111     1        4.664   2.715   1.334  1.00  0.00
ATOM     57  C   111     1        6.263   1.028   0.608  1.00  0.00
ATOM     58  H   111     1        2.583   2.340   0.933  1.00  0.00
ATOM     59  H   111     1        4.478   3.686   1.794  1.00  0.00
ATOM     60  H   111     1        7.287   0.656   0.531  1.00  0.00
ATOM     61  H   111     1        6.823   2.875   1.534  1.00  0.00
ATOM     62  C   111     1        5.291  -1.148  -0.199  1.00  0.00
ATOM     63  H   111     1        6.249  -1.575  -0.508  1.00  0.00
ATOM     64  C   111     1        4.101  -1.944  -0.176  1.00  0.00
ATOM     65  H   111     1        3.497  -1.915   0.733  1.00  0.00
ATOM     66  C   111     1        3.830  -3.080  -1.021  1.00  0.00
ATOM     67  O   111     1        2.966  -3.944  -0.836  1.00  0.00
ATOM     68  O   111     1        4.648  -3.102  -2.139  1.00  0.00
ATOM     69  C   111     1        4.405  -4.200  -3.032  1.00  0.00
ATOM     70  H   111     1        5.111  -4.070  -3.860  1.00  0.00
ATOM     71  H   111     1        3.369  -4.183  -3.402  1.00  0.00
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ATOM     72  H   111     1        4.576  -5.164  -2.529  1.00  0.00
CONECT    1    2
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CONECT    3    6   28   31
CONECT    4    7   31
CONECT    5    6    8
CONECT    6    9
CONECT   10   11   29   42
CONECT   11   12   13
CONECT   13   30   46
CONECT   14   16   17   30
CONECT   15   18   19   23
CONECT   16   19   20
CONECT   17   18   32
CONECT   18   21
CONECT   19   22
CONECT   24   25   32   38
CONECT   25   26   27
CONECT   27   28   36
CONECT   28   33
CONECT   29   31   33
CONECT   30   33
CONECT   32   33
CONECT   33   34
CONECT   34   35   52
CONECT   36   37   50   51
CONECT   38   39   40   41
CONECT   42   43   44   45
CONECT   46   47   48   49
CONECT   52   54   55
CONECT   53   56   57   61
CONECT   54   57   62
CONECT   55   56   58
CONECT   56   59
CONECT   57   60
CONECT   62   63   64
CONECT   64   65   66
CONECT   66   67   68
CONECT   68   69
CONECT   69   70   71   72
END
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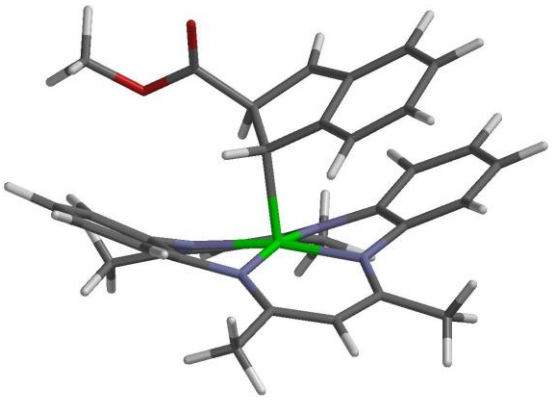
CoMeTAA gama radical after cyclization (D)



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ATOM      1   H   111     1         2.661   1.552  -6.034  1.00  0.00
ATOM      2   C   111     1         2.302   1.667  -5.011  1.00  0.00
ATOM      3   C   111     1         1.439   1.927  -2.349  1.00  0.00
ATOM      4   C   111     1         1.732   0.573  -4.356  1.00  0.00
ATOM      5   C   111     1         2.464   2.879  -4.340  1.00  0.00
ATOM      6   C   111     1         2.054   3.001  -3.010  1.00  0.00
ATOM      7   H   111     1         1.708  -0.387  -4.859  1.00  0.00
ATOM      8   H   111     1         2.953   3.721  -4.831  1.00  0.00
ATOM      9   H   111     1         2.273   3.919  -2.471  1.00  0.00
ATOM     10   C   111     1         0.228  -1.480  -2.633  1.00  0.00
ATOM     11   C   111     1        -0.068  -2.543  -1.761  1.00  0.00
ATOM     12   H   111     1        -0.605  -3.377  -2.210  1.00  0.00
ATOM     13   C   111     1         0.211  -2.677  -0.390  1.00  0.00
ATOM     14   C   111     1         1.320  -1.850   1.615  1.00  0.00
ATOM     15   C   111     1         2.540  -1.769   4.140  1.00  0.00
ATOM     16   C   111     1         1.791  -3.026   2.215  1.00  0.00
ATOM     17   C   111     1         1.480  -0.608   2.289  1.00  0.00
ATOM     18   C   111     1         2.109  -0.584   3.540  1.00  0.00
ATOM     19   C   111     1         2.381  -2.987   3.481  1.00  0.00
ATOM     20   H   111     1         1.766  -3.966   1.671  1.00  0.00
ATOM     21   H   111     1         2.347   0.363   4.014  1.00  0.00
ATOM     22   H   111     1         2.761  -3.908   3.925  1.00  0.00
ATOM     23   H   111     1         3.054  -1.726   5.101  1.00  0.00
ATOM     24   C   111     1         0.773   1.701   1.992  1.00  0.00
ATOM     25   C   111     1         0.582   2.817   1.156  1.00  0.00
ATOM     26   H   111     1         0.240   3.723   1.655  1.00  0.00
ATOM     27   C   111     1         0.748   2.917  -0.233  1.00  0.00
ATOM     28   N   111     1         1.107   1.862  -0.985  1.00  0.00
ATOM     29   N   111     1         0.813  -0.351  -2.205  1.00  0.00
ATOM     30   N   111     1         0.836  -1.712   0.302  1.00  0.00
ATOM     31   C   111     1         1.277   0.686  -3.034  1.00  0.00
ATOM     32   N   111     1         1.114   0.501   1.505  1.00  0.00
ATOM     33  CO   111     1         1.159   0.051  -0.362  1.00  0.00
ATOM     34   C   111     1         3.199  -0.150  -0.697  1.00  0.00
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ATOM     35  C   111     1        0.396   4.259  -0.846  1.00  0.00
ATOM     36  H   111     1       -0.357   4.755  -0.222  1.00  0.00
ATOM     37  C   111     1        0.480   1.924   3.462  1.00  0.00
ATOM     38  H   111     1        1.377   2.244   4.012  1.00  0.00
ATOM     39  H   111     1        0.095   1.017   3.945  1.00  0.00
ATOM     40  H   111     1       -0.267   2.721   3.565  1.00  0.00
ATOM     41  C   111     1       -0.240  -1.657  -4.063  1.00  0.00
ATOM     42  H   111     1       -1.098  -2.341  -4.083  1.00  0.00
ATOM     43  H   111     1        0.546  -2.100  -4.692  1.00  0.00
ATOM     44  H   111     1       -0.542  -0.705  -4.515  1.00  0.00
ATOM     45  C   111     1       -0.312  -3.935   0.273  1.00  0.00
ATOM     46  H   111     1       -1.217  -4.270  -0.251  1.00  0.00
ATOM     47  H   111     1       -0.560  -3.767   1.328  1.00  0.00
ATOM     48  H   111     1        0.414  -4.760   0.225  1.00  0.00
ATOM     49  H   111     1       -0.007   4.149  -1.861  1.00  0.00
ATOM     50  H   111     1        1.266   4.930  -0.901  1.00  0.00
ATOM     51  C   111     1        3.967   0.090   0.517  1.00  0.00
ATOM     52  C   111     1        5.474   0.047   2.878  1.00  0.00
ATOM     53  C   111     1        4.576  -1.133   0.971  1.00  0.00
ATOM     54  C   111     1        4.138   1.275   1.239  1.00  0.00
ATOM     55  C   111     1        4.892   1.251   2.412  1.00  0.00
ATOM     56  C   111     1        5.318  -1.140   2.183  1.00  0.00
ATOM     57  H   111     1        3.650   2.192   0.902  1.00  0.00
ATOM     58  H   111     1        5.033   2.169   2.985  1.00  0.00
ATOM     59  H   111     1        5.759  -2.067   2.551  1.00  0.00
ATOM     60  H   111     1        6.047   0.059   3.806  1.00  0.00
ATOM     61  C   111     1        4.322  -2.148   0.045  1.00  0.00
ATOM     62  C   111     1        3.565  -1.598  -1.128  1.00  0.00
ATOM     63  C   111     1        4.414  -1.504  -2.396  1.00  0.00
ATOM     64  O   111     1        5.565  -1.128  -2.466  1.00  0.00
ATOM     65  O   111     1        3.671  -1.860  -3.488  1.00  0.00
ATOM     66  C   111     1        4.347  -1.685  -4.753  1.00  0.00
ATOM     67  H   111     1        3.658  -2.076  -5.510  1.00  0.00
ATOM     68  H   111     1        5.295  -2.238  -4.769  1.00  0.00
ATOM     69  H   111     1        4.547  -0.619  -4.931  1.00  0.00
ATOM     70  H   111     1        3.314   0.605  -1.483  1.00  0.00
ATOM     71  H   111     1        4.634  -3.186   0.130  1.00  0.00
ATOM     72  H   111     1        2.682  -2.199  -1.379  1.00  0.00
CONECT    1    2
CONECT    2    4    5
CONECT    3    6   28   31
CONECT    4    7   31
CONECT    5    6    8
CONECT    6    9
CONECT   10   11   29   41
CONECT   11   12   13
CONECT   13   30   45
CONECT   14   16   17   30
```

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CONECT   15   18   19   23
CONECT   16   19   20
CONECT   17   18   32
CONECT   18   21
CONECT   19   22
CONECT   24   25   32   37
CONECT   25   26   27
CONECT   27   28   35
CONECT   28   33
CONECT   29   31   33
CONECT   30   33
CONECT   32   33
CONECT   33   34
CONECT   34   51   62   70
CONECT   35   36   49   50
CONECT   37   38   39   40
CONECT   41   42   43   44
CONECT   45   46   47   48
CONECT   51   53   54
CONECT   52   55   56   60
CONECT   53   56   61
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CONECT   56   59
CONECT   61   62   71
CONECT   62   63   72
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CONECT   65   66
CONECT   66   67   68   69
END
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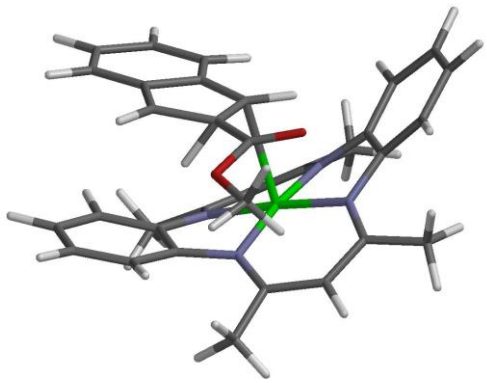
CoMeTAA H-shift gama radical to beta radical TS (TS3)



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ATOM      1  H   111     1        2.961   2.454  -5.808  1.00  0.00
ATOM      2  C   111     1        2.517   2.414  -4.813  1.00  0.00
ATOM      3  C   111     1        1.465   2.267  -2.209  1.00  0.00
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ATOM      4  C   111     1        1.946   1.221  -4.361  1.00  0.00
ATOM      5  C   111     1        2.573   3.525  -3.972  1.00  0.00
ATOM      6  C   111     1        2.071   3.445  -2.669  1.00  0.00
ATOM      7  H   111     1        2.008   0.332  -4.981  1.00  0.00
ATOM      8  H   111     1        3.056   4.445  -4.305  1.00  0.00
ATOM      9  H   111     1        2.215   4.285  -1.996  1.00  0.00
ATOM     10  C   111     1        0.322  -1.051  -3.083  1.00  0.00
ATOM     11  C   111     1       -0.000  -2.246  -2.407  1.00  0.00
ATOM     12  H   111     1       -0.542  -2.989  -2.991  1.00  0.00
ATOM     13  C   111     1        0.298  -2.608  -1.086  1.00  0.00
ATOM     14  C   111     1        1.445  -2.095   1.010  1.00  0.00
ATOM     15  C   111     1        2.792  -2.414   3.459  1.00  0.00
ATOM     16  C   111     1        1.950  -3.350   1.394  1.00  0.00
ATOM     17  C   111     1        1.626  -0.973   1.881  1.00  0.00
ATOM     18  C   111     1        2.320  -1.153   3.086  1.00  0.00
ATOM     19  C   111     1        2.605  -3.511   2.617  1.00  0.00
ATOM     20  H   111     1        1.909  -4.185   0.701  1.00  0.00
ATOM     21  H   111     1        2.575  -0.294   3.698  1.00  0.00
ATOM     22  H   111     1        3.011  -4.487   2.884  1.00  0.00
ATOM     23  H   111     1        3.350  -2.522   4.389  1.00  0.00
ATOM     24  C   111     1        0.860   1.340   2.022  1.00  0.00
ATOM     25  C   111     1        0.574   2.559   1.385  1.00  0.00
ATOM     26  H   111     1        0.227   3.362   2.035  1.00  0.00
ATOM     27  C   111     1        0.703   2.891   0.025  1.00  0.00
ATOM     28  N   111     1        1.078   1.983  -0.887  1.00  0.00
ATOM     29  N   111     1        0.892  -0.020  -2.453  1.00  0.00
ATOM     30  N   111     1        0.901  -1.753  -0.240  1.00  0.00
ATOM     31  C   111     1        1.386   1.140  -3.079  1.00  0.00
ATOM     32  N   111     1        1.196   0.243   1.327  1.00  0.00
ATOM     33 CO   111     1        1.130   0.109  -0.570  1.00  0.00
ATOM     34  C   111     1        3.756   0.184  -0.900  1.00  0.00
ATOM     35  C   111     1        0.324   4.307  -0.357  1.00  0.00
ATOM     36  H   111     1       -0.457   4.668   0.326  1.00  0.00
ATOM     37  C   111     1        0.690   1.324   3.527  1.00  0.00
ATOM     38  H   111     1        1.634   1.558   4.042  1.00  0.00
ATOM     39  H   111     1        0.339   0.350   3.891  1.00  0.00
ATOM     40  H   111     1       -0.039   2.090   3.818  1.00  0.00
ATOM     41  C   111     1       -0.083  -0.989  -4.540  1.00  0.00
ATOM     42  H   111     1       -0.962  -1.626  -4.701  1.00  0.00
ATOM     43  H   111     1        0.718  -1.364  -5.194  1.00  0.00
ATOM     44  H   111     1       -0.328   0.033  -4.855  1.00  0.00
ATOM     45  C   111     1       -0.165  -3.983  -0.648  1.00  0.00
ATOM     46  H   111     1       -1.056  -4.264  -1.223  1.00  0.00
ATOM     47  H   111     1       -0.416  -4.009   0.420  1.00  0.00
ATOM     48  H   111     1        0.598  -4.754  -0.833  1.00  0.00
ATOM     49  H   111     1       -0.055   4.365  -1.384  1.00  0.00
ATOM     50  H   111     1        1.174   5.001  -0.270  1.00  0.00
ATOM     51  C   111     1        4.265   0.728   0.297  1.00  0.00
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ATOM     52  C   111     1         5.307   1.242   2.854  1.00  0.00
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ATOM     54  C   111     1         4.181   2.038   0.832  1.00  0.00
ATOM     55  C   111     1         4.696   2.279   2.088  1.00  0.00
ATOM     56  C   111     1         5.391  -0.048   2.372  1.00  0.00
ATOM     57  H   111     1         3.684   2.823   0.262  1.00  0.00
ATOM     58  H   111     1         4.629   3.280   2.517  1.00  0.00
ATOM     59  H   111     1         5.829  -0.846   2.973  1.00  0.00
ATOM     60  H   111     1         5.701   1.477   3.844  1.00  0.00
ATOM     61  C   111     1         4.766  -1.541   0.371  1.00  0.00
ATOM     62  C   111     1         4.008  -1.227  -0.875  1.00  0.00
ATOM     63  C   111     1         3.713  -2.119  -2.024  1.00  0.00
ATOM     64  O   111     1         3.502  -1.739  -3.159  1.00  0.00
ATOM     65  O   111     1         3.646  -3.423  -1.630  1.00  0.00
ATOM     66  C   111     1         3.201  -4.333  -2.662  1.00  0.00
ATOM     67  H   111     1         3.188  -5.322  -2.192  1.00  0.00
ATOM     68  H   111     1         3.890  -4.320  -3.517  1.00  0.00
ATOM     69  H   111     1         2.196  -4.044  -3.001  1.00  0.00
ATOM     70  H   111     1         3.424   0.718  -1.783  1.00  0.00
ATOM     71  H   111     1         5.059  -2.542   0.673  1.00  0.00
ATOM     72  H   111     1         3.350  -1.679   0.075  1.00  0.00
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CONECT    2    4    5
CONECT    3    6   28   31
CONECT    4    7   31
CONECT    5    6    8
CONECT    6    9
CONECT   10   11   29   41
CONECT   11   12   13
CONECT   13   30   45
CONECT   14   16   17   30
CONECT   15   18   19   23
CONECT   16   19   20
CONECT   17   18   32
CONECT   18   21
CONECT   19   22
CONECT   24   25   32   37
CONECT   25   26   27
CONECT   27   28   35
CONECT   28   33
CONECT   29   31   33
CONECT   30   33
CONECT   32   33
CONECT   34   51   62   70
CONECT   35   36   49   50
CONECT   37   38   39   40
CONECT   41   42   43   44
CONECT   45   46   47   48
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CONECT    51    53    54
CONECT    52    55    56    60
CONECT    53    56    61
CONECT    54    55    57
CONECT    55    58
CONECT    56    59
CONECT    61    62    71
CONECT    62    63    72
CONECT    63    64    65
CONECT    65    66
CONECT    66    67    68    69
END
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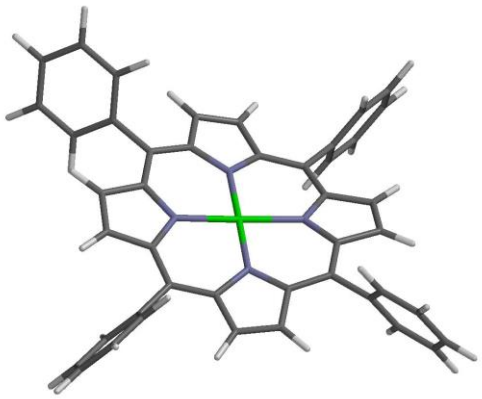
CoTPP



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ATOM      4  C   111     1       -0.871  -0.890   0.920  1.00  0.00
ATOM      5  C   111     1       -1.452   0.425   0.824  1.00  0.00
ATOM      6  H   111     1       -2.510   0.641   0.928  1.00  0.00
ATOM      7  C   111     1       -0.434   1.289   0.555  1.00  0.00
ATOM      8  C   111     1       -1.627  -2.055   1.035  1.00  0.00
ATOM      9  N   111     1        0.302  -3.602   0.918  1.00  0.00
ATOM     10  C   111     1        0.384  -4.986   0.850  1.00  0.00
ATOM     11  C   111     1       -0.934  -5.567   0.798  1.00  0.00
ATOM     12  H   111     1       -1.139  -6.629   0.713  1.00  0.00
ATOM     13  C   111     1       -1.824  -4.543   0.904  1.00  0.00
ATOM     14  H   111     1       -2.907  -4.593   0.930  1.00  0.00
ATOM     15  C   111     1       -1.057  -3.325   0.962  1.00  0.00
ATOM     16  C   111     1        2.040   1.059   0.285  1.00  0.00
ATOM     17  H   111     1        6.493  -0.066   0.687  1.00  0.00
ATOM     18  C   111     1        5.410  -0.111   0.655  1.00  0.00
ATOM     19  C   111     1        4.630  -1.284   0.951  1.00  0.00
ATOM     20  H   111     1        4.751   1.889   0.000  1.00  0.00
ATOM     21  N   111     1        3.278  -1.025   0.784  1.00  0.00
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ATOM     22  C   111    1        3.210   0.315   0.426  1.00  0.00
ATOM     23  C   111    1        4.533   0.872   0.307  1.00  0.00
ATOM     24  C   111    1        1.557  -5.735   0.933  1.00  0.00
ATOM     25  H   111    1        6.032  -5.173   1.888  1.00  0.00
ATOM     26  C   111    1        4.998  -4.987   1.618  1.00  0.00
ATOM     27  C   111    1        3.995  -5.891   1.444  1.00  0.00
ATOM     28  H   111    1        4.037  -6.970   1.547  1.00  0.00
ATOM     29  C   111    1        2.806  -5.144   1.125  1.00  0.00
ATOM     30  N   111    1        3.077  -3.784   1.101  1.00  0.00
ATOM     31  C   111    1        4.437  -3.684   1.364  1.00  0.00
ATOM     32  C   111    1        5.191  -2.513   1.301  1.00  0.00
ATOM     33 CO   111    1        1.790  -2.310   0.888  1.00  0.00
ATOM     34  C   111    1        1.481  -7.223   0.884  1.00  0.00
ATOM     35  C   111    1        1.373 -10.033   0.787  1.00  0.00
ATOM     36  C   111    1        2.033  -7.923  -0.200  1.00  0.00
ATOM     37  C   111    1        0.878  -7.952   1.922  1.00  0.00
ATOM     38  C   111    1        0.824  -9.346   1.874  1.00  0.00
ATOM     39  C   111    1        1.978  -9.318  -0.250  1.00  0.00
ATOM     40  H   111    1        2.506  -7.361  -1.007  1.00  0.00
ATOM     41  H   111    1        0.458  -7.413   2.772  1.00  0.00
ATOM     42  H   111    1        0.358  -9.898   2.691  1.00  0.00
ATOM     43  H   111    1        2.407  -9.846  -1.102  1.00  0.00
ATOM     44  H   111    1        1.331 -11.123   0.750  1.00  0.00
ATOM     45  C   111    1        2.133   2.507  -0.056  1.00  0.00
ATOM     46  C   111    1        2.280   5.242  -0.703  1.00  0.00
ATOM     47  C   111    1        1.657   2.976  -1.290  1.00  0.00
ATOM     48  C   111    1        2.680   3.428   0.851  1.00  0.00
ATOM     49  C   111    1        2.753   4.785   0.530  1.00  0.00
ATOM     50  C   111    1        1.731   4.333  -1.613  1.00  0.00
ATOM     51  H   111    1        1.229   2.264  -1.997  1.00  0.00
ATOM     52  H   111    1        3.044   3.070   1.815  1.00  0.00
ATOM     53  H   111    1        3.177   5.489   1.248  1.00  0.00
ATOM     54  H   111    1        1.361   4.681  -2.578  1.00  0.00
ATOM     55  H   111    1        2.337   6.302  -0.954  1.00  0.00
ATOM     56  C   111    1       -3.108  -1.930   1.174  1.00  0.00
ATOM     57  C   111    1       -5.895  -1.672   1.445  1.00  0.00
ATOM     58  C   111    1       -3.671  -1.518   2.391  1.00  0.00
ATOM     59  C   111    1       -3.959  -2.207   0.093  1.00  0.00
ATOM     60  C   111    1       -5.343  -2.081   0.228  1.00  0.00
ATOM     61  C   111    1       -5.056  -1.390   2.526  1.00  0.00
ATOM     62  H   111    1       -3.012  -1.299   3.232  1.00  0.00
ATOM     63  H   111    1       -3.524  -2.520  -0.857  1.00  0.00
ATOM     64  H   111    1       -5.992  -2.297  -0.622  1.00  0.00
ATOM     65  H   111    1       -5.479  -1.071   3.480  1.00  0.00
ATOM     66  H   111    1       -6.977  -1.572   1.551  1.00  0.00
ATOM     67  C   111    1        6.659  -2.574   1.552  1.00  0.00
ATOM     68  C   111    1        9.432  -2.656   2.026  1.00  0.00
ATOM     69  C   111    1        7.214  -1.924   2.665  1.00  0.00
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ATOM     70  C   111     1        7.515  -3.262   0.677  1.00  0.00
ATOM     71  C   111     1        8.890  -3.303   0.912  1.00  0.00
ATOM     72  C   111     1        8.590  -1.966   2.902  1.00  0.00
ATOM     73  H   111     1        6.554  -1.385   3.347  1.00  0.00
ATOM     74  H   111     1        7.090  -3.760  -0.196  1.00  0.00
ATOM     75  H   111     1        9.542  -3.837   0.219  1.00  0.00
ATOM     76  H   111     1        9.004  -1.460   3.776  1.00  0.00
ATOM     77  H   111     1       10.507  -2.687   2.210  1.00  0.00
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CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8   15   56
CONECT    9   10   15   33
CONECT   10   11   24
CONECT   11   12   13
CONECT   13   14   15
CONECT   16   22   45
CONECT   17   18
CONECT   18   19   23
CONECT   19   21   32
CONECT   20   23
CONECT   21   22   33
CONECT   22   23
CONECT   24   29   34
CONECT   25   26
CONECT   26   27   31
CONECT   27   28   29
CONECT   29   30
CONECT   30   31   33
CONECT   31   32
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CONECT   35   38   39   44
CONECT   36   39   40
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CONECT   47   50   51
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CONECT   49   53
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CONECT   57   60   61   66
CONECT   58   61   62
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CONECT   60   64
CONECT   61   65
CONECT   67   69   70
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CONECT   71   75
CONECT   72   76
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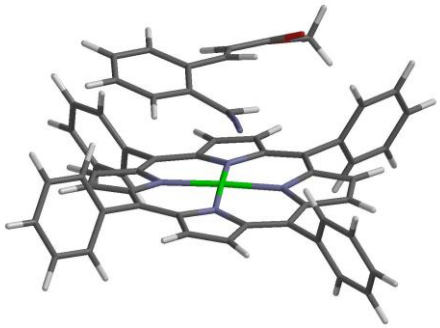
CoTPP diazo (B)



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ATOM      3  H   111     1       -0.482   2.362   0.409  1.00  0.00
ATOM      4  C   111     1       -0.871  -0.890   0.920  1.00  0.00
ATOM      5  C   111     1       -1.452   0.425   0.824  1.00  0.00
ATOM      6  H   111     1       -2.510   0.641   0.928  1.00  0.00
ATOM      7  C   111     1       -0.434   1.289   0.555  1.00  0.00
ATOM      8  C   111     1       -1.627  -2.055   1.035  1.00  0.00
ATOM      9  N   111     1        0.302  -3.602   0.918  1.00  0.00
ATOM     10  C   111     1        0.384  -4.986   0.850  1.00  0.00
ATOM     11  C   111     1       -0.934  -5.567   0.798  1.00  0.00
ATOM     12  H   111     1       -1.139  -6.629   0.713  1.00  0.00
ATOM     13  C   111     1       -1.824  -4.543   0.904  1.00  0.00
ATOM     14  H   111     1       -2.907  -4.593   0.930  1.00  0.00
ATOM     15  C   111     1       -1.057  -3.325   0.962  1.00  0.00
ATOM     16  C   111     1        2.040   1.059   0.285  1.00  0.00
ATOM     17  H   111     1        6.493  -0.066   0.687  1.00  0.00
ATOM     18  C   111     1        5.410  -0.111   0.655  1.00  0.00
ATOM     19  C   111     1        4.630  -1.284   0.951  1.00  0.00
ATOM     20  H   111     1        4.751   1.889   0.000  1.00  0.00
ATOM     21  N   111     1        3.278  -1.025   0.784  1.00  0.00
ATOM     22  C   111     1        3.210   0.315   0.426  1.00  0.00
ATOM     23  C   111     1        4.533   0.872   0.307  1.00  0.00
ATOM     24  C   111     1        1.557  -5.735   0.933  1.00  0.00
ATOM     25  H   111     1        6.032  -5.173   1.888  1.00  0.00
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ATOM     26  C   111     1        4.998  -4.987   1.618  1.00  0.00
ATOM     27  C   111     1        3.995  -5.891   1.444  1.00  0.00
ATOM     28  H   111     1        4.037  -6.970   1.547  1.00  0.00
ATOM     29  C   111     1        2.806  -5.144   1.125  1.00  0.00
ATOM     30  N   111     1        3.077  -3.784   1.101  1.00  0.00
ATOM     31  C   111     1        4.437  -3.684   1.364  1.00  0.00
ATOM     32  C   111     1        5.191  -2.513   1.301  1.00  0.00
ATOM     33 CO   111     1        1.790  -2.310   0.888  1.00  0.00
ATOM     34  C   111     1        1.481  -7.223   0.884  1.00  0.00
ATOM     35  C   111     1        1.373 -10.033   0.787  1.00  0.00
ATOM     36  C   111     1        2.033  -7.923  -0.200  1.00  0.00
ATOM     37  C   111     1        0.878  -7.952   1.922  1.00  0.00
ATOM     38  C   111     1        0.824  -9.346   1.874  1.00  0.00
ATOM     39  C   111     1        1.978  -9.318  -0.250  1.00  0.00
ATOM     40  H   111     1        2.506  -7.361  -1.007  1.00  0.00
ATOM     41  H   111     1        0.458  -7.413   2.772  1.00  0.00
ATOM     42  H   111     1        0.358  -9.898   2.691  1.00  0.00
ATOM     43  H   111     1        2.407  -9.846  -1.102  1.00  0.00
ATOM     44  H   111     1        1.331 -11.123   0.750  1.00  0.00
ATOM     45  C   111     1        2.133   2.507  -0.056  1.00  0.00
ATOM     46  C   111     1        2.280   5.242  -0.703  1.00  0.00
ATOM     47  C   111     1        1.657   2.976  -1.290  1.00  0.00
ATOM     48  C   111     1        2.680   3.428   0.851  1.00  0.00
ATOM     49  C   111     1        2.753   4.785   0.530  1.00  0.00
ATOM     50  C   111     1        1.731   4.333  -1.613  1.00  0.00
ATOM     51  H   111     1        1.229   2.264  -1.997  1.00  0.00
ATOM     52  H   111     1        3.044   3.070   1.815  1.00  0.00
ATOM     53  H   111     1        3.177   5.489   1.248  1.00  0.00
ATOM     54  H   111     1        1.361   4.681  -2.578  1.00  0.00
ATOM     55  H   111     1        2.337   6.302  -0.954  1.00  0.00
ATOM     56  C   111     1       -3.108  -1.930   1.174  1.00  0.00
ATOM     57  C   111     1       -5.895  -1.672   1.445  1.00  0.00
ATOM     58  C   111     1       -3.671  -1.518   2.391  1.00  0.00
ATOM     59  C   111     1       -3.959  -2.207   0.093  1.00  0.00
ATOM     60  C   111     1       -5.343  -2.081   0.228  1.00  0.00
ATOM     61  C   111     1       -5.056  -1.390   2.526  1.00  0.00
ATOM     62  H   111     1       -3.012  -1.299   3.232  1.00  0.00
ATOM     63  H   111     1       -3.524  -2.520  -0.857  1.00  0.00
ATOM     64  H   111     1       -5.992  -2.297  -0.622  1.00  0.00
ATOM     65  H   111     1       -5.479  -1.071   3.480  1.00  0.00
ATOM     66  H   111     1       -6.977  -1.572   1.551  1.00  0.00
ATOM     67  C   111     1        6.659  -2.574   1.552  1.00  0.00
ATOM     68  C   111     1        9.432  -2.656   2.026  1.00  0.00
ATOM     69  C   111     1        7.214  -1.924   2.665  1.00  0.00
ATOM     70  C   111     1        7.515  -3.262   0.677  1.00  0.00
ATOM     71  C   111     1        8.890  -3.303   0.912  1.00  0.00
ATOM     72  C   111     1        8.590  -1.966   2.902  1.00  0.00
ATOM     73  H   111     1        6.554  -1.385   3.347  1.00  0.00
```

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ATOM     74  H   111     1         7.090  -3.760  -0.196  1.00  0.00
ATOM     75  H   111     1         9.542  -3.837   0.219  1.00  0.00
ATOM     76  H   111     1         9.004  -1.460   3.776  1.00  0.00
ATOM     77  H   111     1        10.507  -2.687   2.210  1.00  0.00
CONECT    1    2    7   16
CONECT    2    4   33
CONECT    3    7
CONECT    4    5    8
CONECT    5    6    7
CONECT    8   15   56
CONECT    9   10   15   33
CONECT   10   11   24
CONECT   11   12   13
CONECT   13   14   15
CONECT   16   22   45
CONECT   17   18
CONECT   18   19   23
CONECT   19   21   32
CONECT   20   23
CONECT   21   22   33
CONECT   22   23
CONECT   24   29   34
CONECT   25   26
CONECT   26   27   31
CONECT   27   28   29
CONECT   29   30
CONECT   30   31   33
CONECT   31   32
CONECT   32   67
CONECT   34   36   37
CONECT   35   38   39   44
CONECT   36   39   40
CONECT   37   38   41
CONECT   38   42
CONECT   39   43
CONECT   45   47   48
CONECT   46   49   50   55
CONECT   47   50   51
CONECT   48   49   52
CONECT   49   53
CONECT   50   54
CONECT   56   58   59
CONECT   57   60   61   66
CONECT   58   61   62
CONECT   59   60   63
CONECT   60   64
CONECT   61   65
CONECT   67   69   70
```

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CONECT   68   71   72   77
CONECT   69   72   73
CONECT   70   71   74
CONECT   71   75
CONECT   72   76
END
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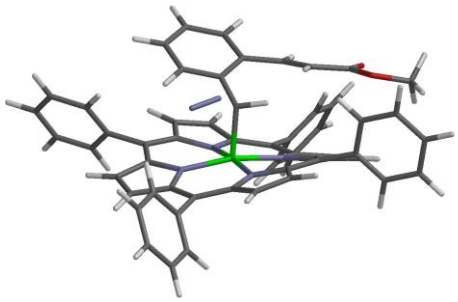
CoTPP N2 loss from diazo TS (TS1)



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HEADER BOpt - Pdb
ATOM      1  C   111     1        3.274   0.494  -1.205  1.00  0.00
ATOM      2  C   111     1        4.021   2.665  -2.866  1.00  0.00
ATOM      3  C   111     1        3.245   0.351  -2.628  1.00  0.00
ATOM      4  C   111     1        3.706   1.723  -0.670  1.00  0.00
ATOM      5  C   111     1        4.099   2.786  -1.478  1.00  0.00
ATOM      6  C   111     1        3.577   1.468  -3.421  1.00  0.00
ATOM      7  H   111     1        3.706   1.843   0.412  1.00  0.00
ATOM      8  H   111     1        4.425   3.722  -1.022  1.00  0.00
ATOM      9  H   111     1        3.499   1.374  -4.506  1.00  0.00
ATOM     10  H   111     1        4.289   3.501  -3.512  1.00  0.00
ATOM     11  C   111     1        2.869  -0.852  -3.370  1.00  0.00
ATOM     12  H   111     1        2.435  -0.661  -4.357  1.00  0.00
ATOM     13  C   111     1        3.048  -2.152  -3.058  1.00  0.00
ATOM     14  H   111     1        3.523  -2.484  -2.138  1.00  0.00
ATOM     15  C   111     1        2.595  -3.213  -3.972  1.00  0.00
ATOM     16  O   111     1        2.057  -3.066  -5.060  1.00  0.00
ATOM     17  O   111     1        2.849  -4.433  -3.415  1.00  0.00
ATOM     18  C   111     1        2.353  -5.571  -4.144  1.00  0.00
ATOM     19  H   111     1        2.430  -6.415  -3.450  1.00  0.00
ATOM     20  H   111     1        2.959  -5.746  -5.044  1.00  0.00
ATOM     21  H   111     1        1.310  -5.407  -4.448  1.00  0.00
ATOM     22  N   111     1        3.899  -0.683   1.056  1.00  0.00
ATOM     23  N   111     1        3.964  -0.107   2.036  1.00  0.00
ATOM     24  C   111     1        2.743  -0.540  -0.293  1.00  0.00
ATOM     25  H   111     1        2.845  -1.565  -0.650  1.00  0.00
ATOM     26  C   111     1        0.663   2.417  -0.753  1.00  0.00
ATOM     27  N   111     1        0.366   1.075  -0.940  1.00  0.00
ATOM     28  H   111     1        0.704   4.199  -2.119  1.00  0.00
ATOM     29  C   111     1       -0.071   0.979  -2.252  1.00  0.00
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ATOM     30  C   111     1        0.005   2.263  -2.901  1.00  0.00
ATOM     31  H   111     1       -0.247   2.447  -3.940  1.00  0.00
ATOM     32  C   111     1        0.484   3.147  -1.982  1.00  0.00
ATOM     33  C   111     1       -0.482  -0.189  -2.897  1.00  0.00
ATOM     34  N   111     1        0.314  -1.701  -1.109  1.00  0.00
ATOM     35  C   111     1        0.515  -3.074  -1.083  1.00  0.00
ATOM     36  C   111     1       -0.051  -3.686  -2.256  1.00  0.00
ATOM     37  H   111     1       -0.036  -4.748  -2.468  1.00  0.00
ATOM     38  C   111     1       -0.603  -2.687  -2.999  1.00  0.00
ATOM     39  H   111     1       -1.127  -2.772  -3.944  1.00  0.00
ATOM     40  C   111     1       -0.310  -1.450  -2.323  1.00  0.00
ATOM     41  C   111     1        1.021   2.999   0.463  1.00  0.00
ATOM     42  H   111     1        1.155   1.874   4.937  1.00  0.00
ATOM     43  C   111     1        1.148   1.820   3.854  1.00  0.00
ATOM     44  C   111     1        1.135   0.597   3.094  1.00  0.00
ATOM     45  H   111     1        1.156   3.911   3.155  1.00  0.00
ATOM     46  N   111     1        1.059   0.874   1.734  1.00  0.00
ATOM     47  C   111     1        1.098   2.255   1.644  1.00  0.00
ATOM     48  C   111     1        1.156   2.845   2.957  1.00  0.00
ATOM     49  C   111     1        1.165  -3.779  -0.069  1.00  0.00
ATOM     50  H   111     1        2.020  -3.311   4.432  1.00  0.00
ATOM     51  C   111     1        1.792  -3.105   3.392  1.00  0.00
ATOM     52  C   111     1        1.854  -3.955   2.328  1.00  0.00
ATOM     53  H   111     1        2.121  -5.007   2.317  1.00  0.00
ATOM     54  C   111     1        1.432  -3.206   1.172  1.00  0.00
ATOM     55  N   111     1        1.158  -1.891   1.518  1.00  0.00
ATOM     56  C   111     1        1.374  -1.824   2.882  1.00  0.00
ATOM     57  C   111     1        1.289  -0.668   3.659  1.00  0.00
ATOM     58  C   111     1        1.534  -5.206  -0.297  1.00  0.00
ATOM     59  C   111     1        2.282  -7.876  -0.769  1.00  0.00
ATOM     60  C   111     1        2.884  -5.551  -0.462  1.00  0.00
ATOM     61  C   111     1        0.564  -6.218  -0.358  1.00  0.00
ATOM     62  C   111     1        0.935  -7.544  -0.596  1.00  0.00
ATOM     63  C   111     1        3.256  -6.876  -0.697  1.00  0.00
ATOM     64  H   111     1        3.640  -4.766  -0.421  1.00  0.00
ATOM     65  H   111     1       -0.485  -5.958  -0.214  1.00  0.00
ATOM     66  H   111     1        0.170  -8.321  -0.640  1.00  0.00
ATOM     67  H   111     1        4.309  -7.125  -0.832  1.00  0.00
ATOM     68  H   111     1        2.572  -8.911  -0.955  1.00  0.00
ATOM     69  C   111     1        1.290   4.460   0.533  1.00  0.00
ATOM     70  C   111     1        1.843   7.218   0.679  1.00  0.00
ATOM     71  C   111     1        2.545   4.920   0.968  1.00  0.00
ATOM     72  C   111     1        0.312   5.407   0.186  1.00  0.00
ATOM     73  C   111     1        0.586   6.774   0.258  1.00  0.00
ATOM     74  C   111     1        2.821   6.286   1.038  1.00  0.00
ATOM     75  H   111     1        3.303   4.191   1.257  1.00  0.00
ATOM     76  H   111     1       -0.673   5.060  -0.129  1.00  0.00
ATOM     77  H   111     1       -0.188   7.495  -0.009  1.00  0.00
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ATOM     78  H   111     1        3.803   6.624   1.372  1.00  0.00
ATOM     79  H   111     1        2.057   8.287   0.734  1.00  0.00
ATOM     80  C   111     1       -1.055  -0.079  -4.267  1.00  0.00
ATOM     81  C   111     1       -2.142   0.183  -6.851  1.00  0.00
ATOM     82  C   111     1       -2.227   0.668  -4.481  1.00  0.00
ATOM     83  C   111     1       -0.437  -0.697  -5.368  1.00  0.00
ATOM     84  C   111     1       -0.978  -0.563  -6.649  1.00  0.00
ATOM     85  C   111     1       -2.767   0.797  -5.761  1.00  0.00
ATOM     86  H   111     1       -2.713   1.145  -3.628  1.00  0.00
ATOM     87  H   111     1        0.466  -1.292  -5.222  1.00  0.00
ATOM     88  H   111     1       -0.482  -1.046  -7.492  1.00  0.00
ATOM     89  H   111     1       -3.681   1.374  -5.907  1.00  0.00
ATOM     90  H   111     1       -2.563   0.284  -7.852  1.00  0.00
ATOM     91  C   111     1        1.479  -0.789   5.131  1.00  0.00
ATOM     92  C   111     1        1.858  -1.049   7.905  1.00  0.00
ATOM     93  C   111     1        0.522  -1.443   5.924  1.00  0.00
ATOM     94  C   111     1        2.632  -0.273   5.745  1.00  0.00
ATOM     95  C   111     1        2.819  -0.402   7.122  1.00  0.00
ATOM     96  C   111     1        0.709  -1.569   7.302  1.00  0.00
ATOM     97  H   111     1       -0.372  -1.850   5.449  1.00  0.00
ATOM     98  H   111     1        3.382   0.219   5.124  1.00  0.00
ATOM     99  H   111     1        3.723  -0.002   7.584  1.00  0.00
ATOM    100  H   111     1       -0.046  -2.074   7.907  1.00  0.00
ATOM    101  H   111     1        2.005  -1.149   8.981  1.00  0.00
ATOM    102 CO   111     1        0.877  -0.403   0.258  1.00  0.00
CONECT    1    3    4   24
CONECT    2    5    6   10
CONECT    3    6   11
CONECT    4    5    7
CONECT    5    8
CONECT    6    9
CONECT   11   12   13
CONECT   13   14   15
CONECT   15   16   17
CONECT   17   18
CONECT   18   19   20   21
CONECT   22   23
CONECT   24   25  102
CONECT   26   27   32   41
CONECT   27   29  102
CONECT   28   32
CONECT   29   30   33
CONECT   30   31   32
CONECT   33   40   80
CONECT   34   35   40  102
CONECT   35   36   49
CONECT   36   37   38
CONECT   38   39   40
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CONECT   41   47   69
CONECT   42   43
CONECT   43   44   48
CONECT   44   46   57
CONECT   45   48
CONECT   46   47  102
CONECT   47   48
CONECT   49   54   58
CONECT   50   51
CONECT   51   52   56
CONECT   52   53   54
CONECT   54   55
CONECT   55   56  102
CONECT   56   57
CONECT   57   91
CONECT   58   60   61
CONECT   59   62   63   68
CONECT   60   63   64
CONECT   61   62   65
CONECT   62   66
CONECT   63   67
CONECT   69   71   72
CONECT   70   73   74   79
CONECT   71   74   75
CONECT   72   73   76
CONECT   73   77
CONECT   74   78
CONECT   80   82   83
CONECT   81   84   85   90
CONECT   82   85   86
CONECT   83   84   87
CONECT   84   88
CONECT   85   89
CONECT   91   93   94
CONECT   92   95   96  101
CONECT   93   96   97
CONECT   94   95   98
CONECT   95   99
CONECT   96  100
END
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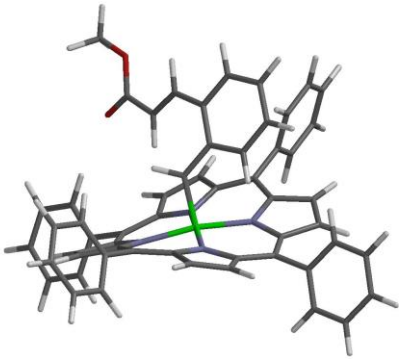
CoTPP carbene complex (C)



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ATOM      1  C   111     1         2.502   0.107  -0.641  1.00  0.00
ATOM      2  H   111     1         2.687   0.052  -1.715  1.00  0.00
ATOM      3  C   111     1         3.516  -0.302   0.251  1.00  0.00
ATOM      4  C   111     1         5.660  -0.934   2.026  1.00  0.00
ATOM      5  C   111     1         4.574  -1.207  -0.164  1.00  0.00
ATOM      6  C   111     1         3.575   0.206   1.583  1.00  0.00
ATOM      7  C   111     1         4.607  -0.099   2.448  1.00  0.00
ATOM      8  C   111     1         5.635  -1.455   0.740  1.00  0.00
ATOM      9  H   111     1         2.795   0.897   1.894  1.00  0.00
ATOM     10  H   111     1         4.614   0.328   3.452  1.00  0.00
ATOM     11  H   111     1         6.438  -2.121   0.416  1.00  0.00
ATOM     12  H   111     1         6.486  -1.169   2.698  1.00  0.00
ATOM     13  C   111     1         4.612  -1.973  -1.393  1.00  0.00
ATOM     14  H   111     1         5.567  -2.480  -1.562  1.00  0.00
ATOM     15  C   111     1         3.646  -2.226  -2.318  1.00  0.00
ATOM     16  H   111     1         2.636  -1.833  -2.239  1.00  0.00
ATOM     17  C   111     1         3.837  -3.086  -3.486  1.00  0.00
ATOM     18  O   111     1         2.965  -3.325  -4.316  1.00  0.00
ATOM     19  O   111     1         5.097  -3.615  -3.586  1.00  0.00
ATOM     20  C   111     1         5.306  -4.461  -4.732  1.00  0.00
ATOM     21  H   111     1         6.346  -4.800  -4.660  1.00  0.00
ATOM     22  H   111     1         5.147  -3.902  -5.665  1.00  0.00
ATOM     23  H   111     1         4.619  -5.318  -4.715  1.00  0.00
ATOM     24  C   111     1         0.745   2.417  -2.441  1.00  0.00
ATOM     25  N   111     1         0.398   1.135  -2.050  1.00  0.00
ATOM     26  H   111     1         0.658   3.518  -4.392  1.00  0.00
ATOM     27  C   111     1        -0.046   0.501  -3.200  1.00  0.00
ATOM     28  C   111     1        -0.030   1.422  -4.309  1.00  0.00
ATOM     29  H   111     1        -0.347   1.176  -5.317  1.00  0.00
ATOM     30  C   111     1         0.486   2.596  -3.846  1.00  0.00
ATOM     31  C   111     1        -0.307  -0.865  -3.333  1.00  0.00
ATOM     32  N   111     1         0.362  -1.436  -1.023  1.00  0.00
ATOM     33  C   111     1         0.736  -2.630  -0.421  1.00  0.00
ATOM     34  C   111     1         0.580  -3.721  -1.346  1.00  0.00
ATOM     35  H   111     1         0.827  -4.755  -1.133  1.00  0.00
ATOM     36  C   111     1         0.051  -3.202  -2.490  1.00  0.00
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ATOM     37  H   111     1       -0.215  -3.727  -3.400  1.00  0.00
ATOM     38  C   111     1       -0.025  -1.775  -2.311  1.00  0.00
ATOM     39  C   111     1        1.178   3.435  -1.588  1.00  0.00
ATOM     40  H   111     1        0.931   4.428   2.914  1.00  0.00
ATOM     41  C   111     1        0.944   3.901   1.965  1.00  0.00
ATOM     42  C   111     1        0.638   2.504   1.802  1.00  0.00
ATOM     43  H   111     1        1.591   5.390   0.471  1.00  0.00
ATOM     44  N   111     1        0.752   2.143   0.469  1.00  0.00
ATOM     45  C   111     1        1.116   3.303  -0.201  1.00  0.00
ATOM     46  C   111     1        1.280   4.385   0.734  1.00  0.00
ATOM     47  C   111     1        1.102  -2.761   0.917  1.00  0.00
ATOM     48  H   111     1        0.320  -0.456   4.833  1.00  0.00
ATOM     49  C   111     1        0.499  -0.698   3.791  1.00  0.00
ATOM     50  C   111     1        0.850  -1.901   3.251  1.00  0.00
ATOM     51  H   111     1        1.007  -2.848   3.757  1.00  0.00
ATOM     52  C   111     1        0.911  -1.718   1.825  1.00  0.00
ATOM     53  N   111     1        0.631  -0.407   1.495  1.00  0.00
ATOM     54  C   111     1        0.434   0.246   2.704  1.00  0.00
ATOM     55  C   111     1        0.390   1.631   2.866  1.00  0.00
ATOM     56  C   111     1        1.662  -4.040   1.429  1.00  0.00
ATOM     57  C   111     1        2.807  -6.403   2.425  1.00  0.00
ATOM     58  C   111     1        2.995  -4.053   1.874  1.00  0.00
ATOM     59  C   111     1        0.907  -5.221   1.499  1.00  0.00
ATOM     60  C   111     1        1.478  -6.395   1.994  1.00  0.00
ATOM     61  C   111     1        3.563  -5.229   2.365  1.00  0.00
ATOM     62  H   111     1        3.582  -3.134   1.820  1.00  0.00
ATOM     63  H   111     1       -0.134  -5.207   1.176  1.00  0.00
ATOM     64  H   111     1        0.879  -7.306   2.050  1.00  0.00
ATOM     65  H   111     1        4.602  -5.227   2.699  1.00  0.00
ATOM     66  H   111     1        3.251  -7.322   2.810  1.00  0.00
ATOM     67  C   111     1        1.610   4.726  -2.193  1.00  0.00
ATOM     68  C   111     1        2.440   7.137  -3.378  1.00  0.00
ATOM     69  C   111     1        2.806   4.787  -2.925  1.00  0.00
ATOM     70  C   111     1        0.831   5.887  -2.069  1.00  0.00
ATOM     71  C   111     1        1.244   7.085  -2.657  1.00  0.00
ATOM     72  C   111     1        3.219   5.985  -3.511  1.00  0.00
ATOM     73  H   111     1        3.410   3.884  -3.027  1.00  0.00
ATOM     74  H   111     1       -0.108   5.840  -1.516  1.00  0.00
ATOM     75  H   111     1        0.625   7.978  -2.557  1.00  0.00
ATOM     76  H   111     1        4.154   6.018  -4.072  1.00  0.00
ATOM     77  H   111     1        2.763   8.073  -3.837  1.00  0.00
ATOM     78  C   111     1       -0.783  -1.365  -4.655  1.00  0.00
ATOM     79  C   111     1       -1.694  -2.252  -7.159  1.00  0.00
ATOM     80  C   111     1       -2.078  -1.049  -5.094  1.00  0.00
ATOM     81  C   111     1        0.057  -2.125  -5.484  1.00  0.00
ATOM     82  C   111     1       -0.401  -2.565  -6.728  1.00  0.00
ATOM     83  C   111     1       -2.532  -1.492  -6.338  1.00  0.00
ATOM     84  H   111     1       -2.728  -0.454  -4.451  1.00  0.00
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ATOM     85  H   111     1        1.066  -2.369  -5.147  1.00  0.00
ATOM     86  H   111     1        0.262  -3.153  -7.365  1.00  0.00
ATOM     87  H   111     1       -3.543  -1.245  -6.666  1.00  0.00
ATOM     88  H   111     1       -2.047  -2.598  -8.131  1.00  0.00
ATOM     89  C   111     1        0.227   2.212   4.228  1.00  0.00
ATOM     90  C   111     1       -0.077   3.357   6.778  1.00  0.00
ATOM     91  C   111     1       -0.922   2.951   4.546  1.00  0.00
ATOM     92  C   111     1        1.227   2.062   5.202  1.00  0.00
ATOM     93  C   111     1        1.076   2.629   6.469  1.00  0.00
ATOM     94  C   111     1       -1.075   3.518   5.814  1.00  0.00
ATOM     95  H   111     1       -1.698   3.077   3.789  1.00  0.00
ATOM     96  H   111     1        2.128   1.501   4.953  1.00  0.00
ATOM     97  H   111     1        1.864   2.509   7.213  1.00  0.00
ATOM     98  H   111     1       -1.977   4.084   6.048  1.00  0.00
ATOM     99  H   111     1       -0.195   3.801   7.768  1.00  0.00
ATOM    100 CO   111     1        0.682   0.355  -0.294  1.00  0.00
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CONECT    5    8   13
CONECT    6    7    9
CONECT    7   10
CONECT    8   11
CONECT   13   14   15
CONECT   15   16   17
CONECT   17   18   19
CONECT   19   20
CONECT   20   21   22   23
CONECT   24   25   30   39
CONECT   25   27  100
CONECT   26   30
CONECT   27   28   31
CONECT   28   29   30
CONECT   31   38   78
CONECT   32   33   38  100
CONECT   33   34   47
CONECT   34   35   36
CONECT   36   37   38
CONECT   39   45   67
CONECT   40   41
CONECT   41   42   46
CONECT   42   44   55
CONECT   43   46
CONECT   44   45  100
CONECT   45   46
CONECT   47   52   56
CONECT   48   49
CONECT   49   50   54
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CONECT   55   89
CONECT   56   58   59
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CONECT   58   61   62
CONECT   59   60   63
CONECT   60   64
CONECT   61   65
CONECT   67   69   70
CONECT   68   71   72   77
CONECT   69   72   73
CONECT   70   71   74
CONECT   71   75
CONECT   72   76
CONECT   78   80   81
CONECT   79   82   83   88
CONECT   80   83   84
CONECT   81   82   85
CONECT   82   86
CONECT   83   87
CONECT   89   91   92
CONECT   90   93   94   99
CONECT   91   94   95
CONECT   92   93   96
CONECT   93   97
CONECT   94   98
END
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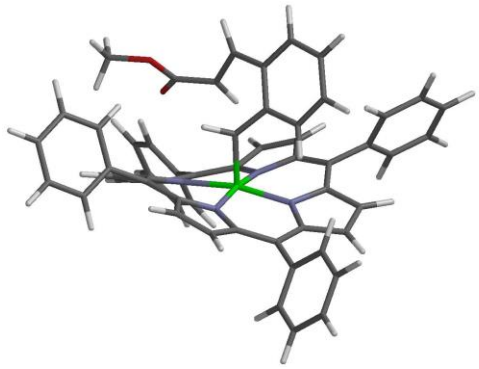
CoTPP carbene cyclization TS (TS2)



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ATOM      1  C   111     1        2.692  -0.041  -0.441  1.00  0.00
ATOM      2  H   111     1        3.016   0.738  -1.143  1.00  0.00
ATOM      3  C   111     1        3.670  -0.621   0.419  1.00  0.00
ATOM      4  C   111     1        5.842  -1.518   2.007  1.00  0.00
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ATOM      5  C   111     1        4.855  -1.206  -0.192  1.00  0.00
ATOM      6  C   111     1        3.606  -0.562   1.834  1.00  0.00
ATOM      7  C   111     1        4.671  -0.983   2.608  1.00  0.00
ATOM      8  C   111     1        5.938  -1.617   0.638  1.00  0.00
ATOM      9  H   111     1        2.735  -0.114   2.305  1.00  0.00
ATOM     10  H   111     1        4.615  -0.889   3.693  1.00  0.00
ATOM     11  H   111     1        6.826  -2.045   0.169  1.00  0.00
ATOM     12  H   111     1        6.665  -1.856   2.638  1.00  0.00
ATOM     13  C   111     1        4.820  -1.319  -1.585  1.00  0.00
ATOM     14  H   111     1        5.746  -1.437  -2.154  1.00  0.00
ATOM     15  C   111     1        3.573  -1.198  -2.247  1.00  0.00
ATOM     16  H   111     1        2.729  -1.796  -1.888  1.00  0.00
ATOM     17  C   111     1        3.417  -0.702  -3.602  1.00  0.00
ATOM     18  O   111     1        2.542  -1.026  -4.400  1.00  0.00
ATOM     19  O   111     1        4.386   0.233  -3.920  1.00  0.00
ATOM     20  C   111     1        4.255   0.785  -5.244  1.00  0.00
ATOM     21  H   111     1        5.072   1.508  -5.345  1.00  0.00
ATOM     22  H   111     1        3.282   1.286  -5.355  1.00  0.00
ATOM     23  H   111     1        4.338  -0.000  -6.008  1.00  0.00
ATOM     24  C   111     1        1.076   1.899  -2.573  1.00  0.00
ATOM     25  N   111     1        0.623   0.683  -2.113  1.00  0.00
ATOM     26  H   111     1        0.970   2.935  -4.560  1.00  0.00
ATOM     27  C   111     1        0.039   0.053  -3.201  1.00  0.00
ATOM     28  C   111     1        0.049   0.939  -4.337  1.00  0.00
ATOM     29  H   111     1       -0.388   0.713  -5.303  1.00  0.00
ATOM     30  C   111     1        0.746   2.053  -3.968  1.00  0.00
ATOM     31  C   111     1       -0.303  -1.299  -3.239  1.00  0.00
ATOM     32  N   111     1        0.407  -1.766  -0.911  1.00  0.00
ATOM     33  C   111     1        0.737  -2.932  -0.235  1.00  0.00
ATOM     34  C   111     1        0.626  -4.060  -1.122  1.00  0.00
ATOM     35  H   111     1        0.866  -5.085  -0.860  1.00  0.00
ATOM     36  C   111     1        0.126  -3.587  -2.303  1.00  0.00
ATOM     37  H   111     1       -0.111  -4.144  -3.204  1.00  0.00
ATOM     38  C   111     1        0.016  -2.157  -2.177  1.00  0.00
ATOM     39  C   111     1        1.626   2.916  -1.778  1.00  0.00
ATOM     40  H   111     1        1.169   4.314   2.615  1.00  0.00
ATOM     41  C   111     1        1.189   3.714   1.711  1.00  0.00
ATOM     42  C   111     1        0.755   2.342   1.628  1.00  0.00
ATOM     43  H   111     1        2.098   5.005   0.171  1.00  0.00
ATOM     44  N   111     1        0.913   1.879   0.335  1.00  0.00
ATOM     45  C   111     1        1.447   2.930  -0.389  1.00  0.00
ATOM     46  C   111     1        1.663   4.060   0.477  1.00  0.00
ATOM     47  C   111     1        0.959  -2.997   1.142  1.00  0.00
ATOM     48  H   111     1       -0.045  -0.378   4.816  1.00  0.00
ATOM     49  C   111     1        0.211  -0.702   3.813  1.00  0.00
ATOM     50  C   111     1        0.506  -1.966   3.386  1.00  0.00
ATOM     51  H   111     1        0.534  -2.883   3.966  1.00  0.00
ATOM     52  C   111     1        0.718  -1.892   1.966  1.00  0.00
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ATOM     53  N   111     1        0.574  -0.588   1.531  1.00  0.00
ATOM     54  C   111     1        0.322   0.167   2.668  1.00  0.00
ATOM     55  C   111     1        0.375   1.565   2.728  1.00  0.00
ATOM     56  C   111     1        1.377  -4.271   1.784  1.00  0.00
ATOM     57  C   111     1        2.240  -6.637   3.033  1.00  0.00
ATOM     58  C   111     1        2.632  -4.329   2.413  1.00  0.00
ATOM     59  C   111     1        0.557  -5.410   1.797  1.00  0.00
ATOM     60  C   111     1        0.986  -6.585   2.418  1.00  0.00
ATOM     61  C   111     1        3.061  -5.505   3.030  1.00  0.00
ATOM     62  H   111     1        3.269  -3.442   2.404  1.00  0.00
ATOM     63  H   111     1       -0.428  -5.362   1.329  1.00  0.00
ATOM     64  H   111     1        0.335  -7.461   2.427  1.00  0.00
ATOM     65  H   111     1        4.042  -5.539   3.507  1.00  0.00
ATOM     66  H   111     1        2.574  -7.556   3.517  1.00  0.00
ATOM     67  C   111     1        2.319   4.031  -2.474  1.00  0.00
ATOM     68  C   111     1        3.680   6.064  -3.863  1.00  0.00
ATOM     69  C   111     1        3.498   3.746  -3.186  1.00  0.00
ATOM     70  C   111     1        1.827   5.346  -2.477  1.00  0.00
ATOM     71  C   111     1        2.504   6.355  -3.166  1.00  0.00
ATOM     72  C   111     1        4.174   4.756  -3.872  1.00  0.00
ATOM     73  H   111     1        3.881   2.724  -3.184  1.00  0.00
ATOM     74  H   111     1        0.896   5.567  -1.953  1.00  0.00
ATOM     75  H   111     1        2.106   7.371  -3.166  1.00  0.00
ATOM     76  H   111     1        5.092   4.521  -4.412  1.00  0.00
ATOM     77  H   111     1        4.208   6.853  -4.400  1.00  0.00
ATOM     78  C   111     1       -0.910  -1.894  -4.460  1.00  0.00
ATOM     79  C   111     1       -2.107  -3.061  -6.722  1.00  0.00
ATOM     80  C   111     1       -2.182  -2.488  -4.372  1.00  0.00
ATOM     81  C   111     1       -0.238  -1.906  -5.693  1.00  0.00
ATOM     82  C   111     1       -0.836  -2.486  -6.814  1.00  0.00
ATOM     83  C   111     1       -2.778  -3.062  -5.496  1.00  0.00
ATOM     84  H   111     1       -2.701  -2.488  -3.412  1.00  0.00
ATOM     85  H   111     1        0.766  -1.488  -5.746  1.00  0.00
ATOM     86  H   111     1       -0.299  -2.498  -7.764  1.00  0.00
ATOM     87  H   111     1       -3.769  -3.510  -5.413  1.00  0.00
ATOM     88  H   111     1       -2.571  -3.512  -7.601  1.00  0.00
ATOM     89  C   111     1        0.149   2.257   4.027  1.00  0.00
ATOM     90  C   111     1       -0.280   3.613   6.456  1.00  0.00
ATOM     91  C   111     1       -0.935   3.137   4.174  1.00  0.00
ATOM     92  C   111     1        1.021   2.074   5.113  1.00  0.00
ATOM     93  C   111     1        0.808   2.746   6.318  1.00  0.00
ATOM     94  C   111     1       -1.150   3.808   5.379  1.00  0.00
ATOM     95  H   111     1       -1.611   3.288   3.330  1.00  0.00
ATOM     96  H   111     1        1.877   1.408   4.998  1.00  0.00
ATOM     97  H   111     1        1.499   2.598   7.149  1.00  0.00
ATOM     98  H   111     1       -2.001   4.483   5.479  1.00  0.00
ATOM     99  H   111     1       -0.447   4.137   7.397  1.00  0.00
ATOM    100 CO   111     1        0.817   0.028  -0.290  1.00  0.00
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CONECT    4    7    8   12
CONECT    5    8   13
CONECT    6    7    9
CONECT    7   10
CONECT    8   11
CONECT   13   14   15
CONECT   15   16   17
CONECT   17   18   19
CONECT   19   20
CONECT   20   21   22   23
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CONECT   26   30
CONECT   27   28   31
CONECT   28   29   30
CONECT   31   38   78
CONECT   32   33   38  100
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CONECT   36   37   38
CONECT   39   45   67
CONECT   40   41
CONECT   41   42   46
CONECT   42   44   55
CONECT   43   46
CONECT   44   45  100
CONECT   45   46
CONECT   47   52   56
CONECT   48   49
CONECT   49   50   54
CONECT   50   51   52
CONECT   52   53
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CONECT   55   89
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CONECT   57   60   61   66
CONECT   58   61   62
CONECT   59   60   63
CONECT   60   64
CONECT   61   65
CONECT   67   69   70
CONECT   68   71   72   77
CONECT   69   72   73
CONECT   70   71   74
CONECT   71   75
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CONECT   79   82   83   88
CONECT   80   83   84
CONECT   81   82   85
CONECT   82   86
CONECT   83   87
CONECT   89   91   92
CONECT   90   93   94   99
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CONECT   92   93   96
CONECT   93   97
CONECT   94   98
END
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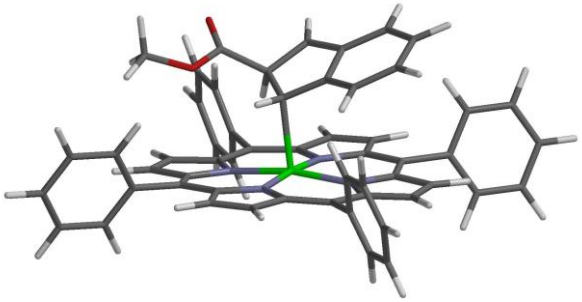
CoTPP gama radical after cyclization (D)



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ATOM      1  C   111     1         3.330  -0.270  -0.721  1.00  0.00
ATOM      2  C   111     1         4.074   0.776  -0.083  1.00  0.00
ATOM      3  C   111     1         5.558   2.467   1.604  1.00  0.00
ATOM      4  C   111     1         4.785   0.245   1.067  1.00  0.00
ATOM      5  C   111     1         4.204   2.138  -0.409  1.00  0.00
ATOM      6  C   111     1         4.924   2.970   0.432  1.00  0.00
ATOM      7  C   111     1         5.507   1.128   1.923  1.00  0.00
ATOM      8  H   111     1         3.701   2.536  -1.290  1.00  0.00
ATOM      9  H   111     1         5.001   4.033   0.202  1.00  0.00
ATOM     10  H   111     1         6.016   0.737   2.806  1.00  0.00
ATOM     11  H   111     1         6.100   3.160   2.250  1.00  0.00
ATOM     12  C   111     1         4.656  -1.136   1.086  1.00  0.00
ATOM     13  C   111     1         3.759  -1.557  -0.032  1.00  0.00
ATOM     14  C   111     1         4.228  -2.724  -0.890  1.00  0.00
ATOM     15  O   111     1         4.835  -3.685  -0.456  1.00  0.00
ATOM     16  O   111     1         3.774  -2.623  -2.159  1.00  0.00
ATOM     17  C   111     1         3.950  -3.806  -2.974  1.00  0.00
ATOM     18  H   111     1         3.432  -3.587  -3.913  1.00  0.00
ATOM     19  H   111     1         3.492  -4.672  -2.479  1.00  0.00
ATOM     20  H   111     1         5.017  -4.001  -3.144  1.00  0.00
ATOM     21  H   111     1         3.211  -0.276  -1.803  1.00  0.00
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ATOM     22  H   111     1         5.061  -1.826   1.822  1.00  0.00
ATOM     23  H   111     1         2.892  -2.043   0.456  1.00  0.00
ATOM     24  C   111     1         1.008   2.018  -2.716  1.00  0.00
ATOM     25  N   111     1         0.961   0.715  -2.238  1.00  0.00
ATOM     26  H   111     1         0.840   2.944  -4.753  1.00  0.00
ATOM     27  C   111     1         0.802  -0.069  -3.373  1.00  0.00
ATOM     28  C   111     1         0.737   0.750  -4.556  1.00  0.00
ATOM     29  H   111     1         0.580   0.374  -5.562  1.00  0.00
ATOM     30  C   111     1         0.866   2.042  -4.150  1.00  0.00
ATOM     31  C   111     1         0.658  -1.456  -3.396  1.00  0.00
ATOM     32  N   111     1         0.794  -1.756  -0.944  1.00  0.00
ATOM     33  C   111     1         0.774  -2.893  -0.149  1.00  0.00
ATOM     34  C   111     1         0.577  -4.074  -0.948  1.00  0.00
ATOM     35  H   111     1         0.515  -5.083  -0.553  1.00  0.00
ATOM     36  C   111     1         0.494  -3.664  -2.244  1.00  0.00
ATOM     37  H   111     1         0.360  -4.271  -3.132  1.00  0.00
ATOM     38  C   111     1         0.634  -2.229  -2.239  1.00  0.00
ATOM     39  C   111     1         1.121   3.170  -1.942  1.00  0.00
ATOM     40  H   111     1         1.703   4.496   2.428  1.00  0.00
ATOM     41  C   111     1         1.530   3.899   1.539  1.00  0.00
ATOM     42  C   111     1         1.447   2.461   1.520  1.00  0.00
ATOM     43  H   111     1         1.393   5.334  -0.129  1.00  0.00
ATOM     44  N   111     1         1.233   1.994   0.232  1.00  0.00
ATOM     45  C   111     1         1.198   3.138  -0.552  1.00  0.00
ATOM     46  C   111     1         1.372   4.320   0.255  1.00  0.00
ATOM     47  C   111     1         0.984  -2.932   1.230  1.00  0.00
ATOM     48  H   111     1         1.795  -0.152   4.816  1.00  0.00
ATOM     49  C   111     1         1.614  -0.531   3.815  1.00  0.00
ATOM     50  C   111     1         1.424  -1.820   3.420  1.00  0.00
ATOM     51  H   111     1         1.427  -2.721   4.024  1.00  0.00
ATOM     52  C   111     1         1.191  -1.788   1.998  1.00  0.00
ATOM     53  N   111     1         1.256  -0.488   1.515  1.00  0.00
ATOM     54  C   111     1         1.512   0.289   2.635  1.00  0.00
ATOM     55  C   111     1         1.611   1.677   2.659  1.00  0.00
ATOM     56  C   111     1         1.090  -4.265   1.893  1.00  0.00
ATOM     57  C   111     1         1.345  -6.766   3.144  1.00  0.00
ATOM     58  C   111     1         2.267  -5.017   1.746  1.00  0.00
ATOM     59  C   111     1         0.043  -4.779   2.671  1.00  0.00
ATOM     60  C   111     1         0.170  -6.024   3.293  1.00  0.00
ATOM     61  C   111     1         2.392  -6.260   2.370  1.00  0.00
ATOM     62  H   111     1         3.087  -4.621   1.143  1.00  0.00
ATOM     63  H   111     1        -0.871  -4.195   2.785  1.00  0.00
ATOM     64  H   111     1        -0.653  -6.415   3.894  1.00  0.00
ATOM     65  H   111     1         3.314  -6.831   2.252  1.00  0.00
ATOM     66  H   111     1         1.444  -7.737   3.632  1.00  0.00
ATOM     67  C   111     1         1.215   4.487  -2.635  1.00  0.00
ATOM     68  C   111     1         1.434   6.974  -3.934  1.00  0.00
ATOM     69  C   111     1         2.372   4.819  -3.357  1.00  0.00
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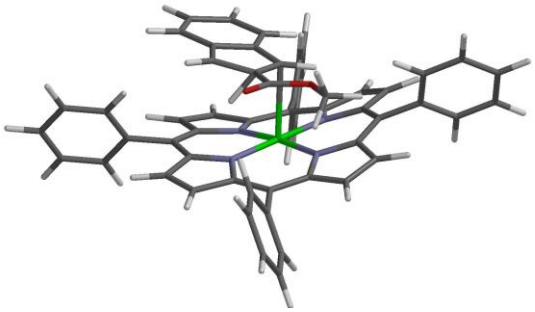
ATOM     71  C   111     1         0.275   6.653  -3.220  1.00  0.00
ATOM     72  C   111     1         2.482   6.052  -4.001  1.00  0.00
ATOM     73  H   111     1         3.189   4.096  -3.409  1.00  0.00
ATOM     74  H   111     1        -0.736   5.164  -2.018  1.00  0.00
ATOM     75  H   111     1        -0.549   7.365  -3.168  1.00  0.00
ATOM     76  H   111     1         3.391   6.296  -4.554  1.00  0.00
ATOM     77  H   111     1         1.518   7.938  -4.436  1.00  0.00
ATOM     78  C   111     1         0.514  -2.136  -4.714  1.00  0.00
ATOM     79  C   111     1         0.249  -3.428  -7.201  1.00  0.00
ATOM     80  C   111     1        -0.700  -2.737  -5.083  1.00  0.00
ATOM     81  C   111     1         1.591  -2.185  -5.614  1.00  0.00
ATOM     82  C   111     1         1.461  -2.827  -6.847  1.00  0.00
ATOM     83  C   111     1        -0.831  -3.379  -6.316  1.00  0.00
ATOM     84  H   111     1        -1.542  -2.693  -4.391  1.00  0.00
ATOM     85  H   111     1         2.532  -1.706  -5.336  1.00  0.00
ATOM     86  H   111     1         2.309  -2.860  -7.533  1.00  0.00
ATOM     87  H   111     1        -1.784  -3.836  -6.588  1.00  0.00
ATOM     88  H   111     1         0.146  -3.929  -8.164  1.00  0.00
ATOM     89  C   111     1         1.857   2.353   3.966  1.00  0.00
ATOM     90  C   111     1         2.312   3.616   6.435  1.00  0.00
ATOM     91  C   111     1         0.817   3.025   4.625  1.00  0.00
ATOM     92  C   111     1         3.128   2.322   4.558  1.00  0.00
ATOM     93  C   111     1         3.354   2.949   5.785  1.00  0.00
ATOM     94  C   111     1         1.042   3.653   5.852  1.00  0.00
ATOM     95  H   111     1        -0.173   3.048   4.166  1.00  0.00
ATOM     96  H   111     1         3.937   1.808   4.037  1.00  0.00
ATOM     97  H   111     1         4.348   2.921   6.233  1.00  0.00
ATOM     98  H   111     1         0.222   4.168   6.355  1.00  0.00
ATOM     99  H   111     1         2.488   4.106   7.394  1.00  0.00
ATOM    100 CO   111     1         1.196   0.099  -0.373  1.00  0.00
CONECT    1    2   13   21  100
CONECT    2    4    5
CONECT    3    6    7   11
CONECT    4    7   12
CONECT    5    6    8
CONECT    6    9
CONECT    7   10
CONECT   12   13   22
CONECT   13   14   23
CONECT   14   15   16
CONECT   16   17
CONECT   17   18   19   20
CONECT   24   25   30   39
CONECT   25   27  100
CONECT   26   30
CONECT   27   28   31
CONECT   28   29   30
```

```
CONECT   31   38   78
CONECT   32   33   38  100
CONECT   33   34   47
CONECT   34   35   36
CONECT   36   37   38
CONECT   39   45   67
CONECT   40   41
CONECT   41   42   46
CONECT   42   44   55
CONECT   43   46
CONECT   44   45  100
CONECT   45   46
CONECT   47   52   56
CONECT   48   49
CONECT   49   50   54
CONECT   50   51   52
CONECT   52   53
CONECT   53   54  100
CONECT   54   55
CONECT   55   89
CONECT   56   58   59
CONECT   57   60   61   66
CONECT   58   61   62
CONECT   59   60   63
CONECT   60   64
CONECT   61   65
CONECT   67   69   70
CONECT   68   71   72   77
CONECT   69   72   73
CONECT   70   71   74
CONECT   71   75
CONECT   72   76
CONECT   78   80   81
CONECT   79   82   83   88
CONECT   80   83   84
CONECT   81   82   85
CONECT   82   86
CONECT   83   87
CONECT   89   91   92
CONECT   90   93   94   99
CONECT   91   94   95
CONECT   92   93   96
CONECT   93   97
CONECT   94   98
END
```

CoTPP H-shift gama radical to beta radical TS (TS3)



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HEADER BOpt - Pdb
ATOM      1  C   111     1         3.715  -0.431  -1.156  1.00  0.00
ATOM      2  C   111     1         4.135   0.874  -0.826  1.00  0.00
ATOM      3  C   111     1         5.060   3.243   0.363  1.00  0.00
ATOM      4  C   111     1         4.756   0.859   0.485  1.00  0.00
ATOM      5  C   111     1         4.004   2.103  -1.525  1.00  0.00
ATOM      6  C   111     1         4.458   3.258  -0.929  1.00  0.00
ATOM      7  C   111     1         5.210   2.068   1.068  1.00  0.00
ATOM      8  H   111     1         3.519   2.121  -2.502  1.00  0.00
ATOM      9  H   111     1         4.342   4.213  -1.443  1.00  0.00
ATOM     10  H   111     1         5.665   2.069   2.059  1.00  0.00
ATOM     11  H   111     1         5.394   4.184   0.801  1.00  0.00
ATOM     12  C   111     1         4.768  -0.471   0.958  1.00  0.00
ATOM     13  C   111     1         4.095  -1.294  -0.076  1.00  0.00
ATOM     14  C   111     1         4.096  -2.774  -0.041  1.00  0.00
ATOM     15  O   111     1         4.412  -3.438   0.933  1.00  0.00
ATOM     16  O   111     1         3.704  -3.299  -1.227  1.00  0.00
ATOM     17  C   111     1         3.640  -4.743  -1.256  1.00  0.00
ATOM     18  H   111     1         3.253  -4.992  -2.249  1.00  0.00
ATOM     19  H   111     1         2.955  -5.109  -0.480  1.00  0.00
ATOM     20  H   111     1         4.638  -5.173  -1.097  1.00  0.00
ATOM     21  H   111     1         3.282  -0.770  -2.090  1.00  0.00
ATOM     22  H   111     1         5.183  -0.884   1.872  1.00  0.00
ATOM     23  H   111     1         3.405  -0.934   0.916  1.00  0.00
ATOM     24  C   111     1         0.773   2.098  -2.610  1.00  0.00
ATOM     25  N   111     1         0.913   0.780  -2.209  1.00  0.00
ATOM     26  H   111     1         0.628   3.105  -4.611  1.00  0.00
ATOM     27  C   111     1         0.978   0.045  -3.384  1.00  0.00
ATOM     28  C   111     1         0.926   0.922  -4.527  1.00  0.00
ATOM     29  H   111     1         0.986   0.600  -5.561  1.00  0.00
ATOM     30  C   111     1         0.748   2.186  -4.048  1.00  0.00
ATOM     31  C   111     1         0.984  -1.348  -3.463  1.00  0.00
ATOM     32  N   111     1         0.832  -1.725  -1.023  1.00  0.00
ATOM     33  C   111     1         0.623  -2.866  -0.263  1.00  0.00
ATOM     34  C   111     1         0.387  -4.002  -1.118  1.00  0.00
ATOM     35  H   111     1         0.176  -5.007  -0.767  1.00  0.00
ATOM     36  C   111     1         0.527  -3.567  -2.402  1.00  0.00
ATOM     37  H   111     1         0.433  -4.136  -3.321  1.00  0.00
```

```
ATOM     38  C   111     1        0.808  -2.155  -2.336  1.00  0.00
ATOM     39  C   111     1        0.760   3.205  -1.761  1.00  0.00
ATOM     40  H   111     1        2.118   4.361   2.471  1.00  0.00
ATOM     41  C   111     1        1.768   3.789   1.619  1.00  0.00
ATOM     42  C   111     1        1.722   2.349   1.553  1.00  0.00
ATOM     43  H   111     1        1.208   5.288   0.104  1.00  0.00
ATOM     44  N   111     1        1.291   1.937   0.300  1.00  0.00
ATOM     45  C   111     1        1.042   3.108  -0.400  1.00  0.00
ATOM     46  C   111     1        1.309   4.258   0.428  1.00  0.00
ATOM     47  C   111     1        0.783  -2.963   1.120  1.00  0.00
ATOM     48  H   111     1        2.129  -0.413   4.723  1.00  0.00
ATOM     49  C   111     1        1.862  -0.734   3.722  1.00  0.00
ATOM     50  C   111     1        1.460  -1.971   3.314  1.00  0.00
ATOM     51  H   111     1        1.343  -2.869   3.911  1.00  0.00
ATOM     52  C   111     1        1.194  -1.886   1.905  1.00  0.00
ATOM     53  N   111     1        1.417  -0.588   1.447  1.00  0.00
ATOM     54  C   111     1        1.815   0.129   2.571  1.00  0.00
ATOM     55  C   111     1        2.029   1.508   2.624  1.00  0.00
ATOM     56  C   111     1        0.589  -4.294   1.763  1.00  0.00
ATOM     57  C   111     1        0.226  -6.822   2.937  1.00  0.00
ATOM     58  C   111     1        1.692  -5.023   2.235  1.00  0.00
ATOM     59  C   111     1       -0.696  -4.846   1.885  1.00  0.00
ATOM     60  C   111     1       -0.876  -6.101   2.469  1.00  0.00
ATOM     61  C   111     1        1.509  -6.280   2.818  1.00  0.00
ATOM     62  H   111     1        2.692  -4.600   2.130  1.00  0.00
ATOM     63  H   111     1       -1.553  -4.280   1.517  1.00  0.00
ATOM     64  H   111     1       -1.881  -6.516   2.562  1.00  0.00
ATOM     65  H   111     1        2.375  -6.839   3.176  1.00  0.00
ATOM     66  H   111     1        0.085  -7.803   3.394  1.00  0.00
ATOM     67  C   111     1        0.575   4.565  -2.344  1.00  0.00
ATOM     68  C   111     1        0.248   7.153  -3.398  1.00  0.00
ATOM     69  C   111     1        1.591   5.159  -3.110  1.00  0.00
ATOM     70  C   111     1       -0.604   5.288  -2.110  1.00  0.00
ATOM     71  C   111     1       -0.767   6.572  -2.634  1.00  0.00
ATOM     72  C   111     1        1.429   6.443  -3.635  1.00  0.00
ATOM     73  H   111     1        2.513   4.603  -3.287  1.00  0.00
ATOM     74  H   111     1       -1.393   4.832  -1.510  1.00  0.00
ATOM     75  H   111     1       -1.692   7.120  -2.445  1.00  0.00
ATOM     76  H   111     1        2.229   6.892  -4.226  1.00  0.00
ATOM     77  H   111     1        0.121   8.157  -3.807  1.00  0.00
ATOM     78  C   111     1        1.148  -2.022  -4.780  1.00  0.00
ATOM     79  C   111     1        1.513  -3.347  -7.236  1.00  0.00
ATOM     80  C   111     1        0.179  -1.932  -5.791  1.00  0.00
ATOM     81  C   111     1        2.299  -2.794  -5.014  1.00  0.00
ATOM     82  C   111     1        2.482  -3.449  -6.233  1.00  0.00
ATOM     83  C   111     1        0.361  -2.589  -7.010  1.00  0.00
ATOM     84  H   111     1       -0.727  -1.351  -5.608  1.00  0.00
ATOM     85  H   111     1        3.049  -2.870  -4.224  1.00  0.00
```

```
ATOM     86  H   111     1        3.385  -4.038  -6.401  1.00  0.00
ATOM     87  H   111     1       -0.405  -2.514  -7.785  1.00  0.00
ATOM     88  H   111     1        1.654  -3.859  -8.188  1.00  0.00
ATOM     89  C   111     1        2.552   2.084   3.893  1.00  0.00
ATOM     90  C   111     1        3.579   3.134   6.297  1.00  0.00
ATOM     91  C   111     1        1.795   2.980   4.665  1.00  0.00
ATOM     92  C   111     1        3.824   1.709   4.357  1.00  0.00
ATOM     93  C   111     1        4.335   2.231   5.546  1.00  0.00
ATOM     94  C   111     1        2.305   3.503   5.855  1.00  0.00
ATOM     95  H   111     1        0.794   3.255   4.329  1.00  0.00
ATOM     96  H   111     1        4.404   0.995   3.772  1.00  0.00
ATOM     97  H   111     1        5.328   1.931   5.885  1.00  0.00
ATOM     98  H   111     1        1.701   4.194   6.444  1.00  0.00
ATOM     99  H   111     1        3.977   3.543   7.227  1.00  0.00
ATOM    100 CO   111     1        1.170   0.096  -0.386  1.00  0.00
CONECT    1    2   13   21
CONECT    2    4    5
CONECT    3    6    7   11
CONECT    4    7   12
CONECT    5    6    8
CONECT    6    9
CONECT    7   10
CONECT   12   13   22
CONECT   13   14   23
CONECT   14   15   16
CONECT   16   17
CONECT   17   18   19   20
CONECT   24   25   30   39
CONECT   25   27  100
CONECT   26   30
CONECT   27   28   31
CONECT   28   29   30
CONECT   31   38   78
CONECT   32   33   38  100
CONECT   33   34   47
CONECT   34   35   36
CONECT   36   37   38
CONECT   39   45   67
CONECT   40   41
CONECT   41   42   46
CONECT   42   44   55
CONECT   43   46
CONECT   44   45  100
CONECT   45   46
CONECT   47   52   56
CONECT   48   49
CONECT   49   50   54
CONECT   50   51   52
```

```
CONECT   52   53
CONECT   53   54  100
CONECT   54   55
CONECT   55   89
CONECT   56   58   59
CONECT   57   60   61   66
CONECT   58   61   62
CONECT   59   60   63
CONECT   60   64
CONECT   61   65
CONECT   67   69   70
CONECT   68   71   72   77
CONECT   69   72   73
CONECT   70   71   74
CONECT   71   75
CONECT   72   76
CONECT   78   80   81
CONECT   79   82   83   88
CONECT   80   83   84
CONECT   81   82   85
CONECT   82   86
CONECT   83   87
CONECT   89   91   92
CONECT   90   93   94   99
CONECT   91   94   95
CONECT   92   93   96
CONECT   93   97
CONECT   94   98
END
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