Supporting Information

Palladium-Catalyzed, Ring-Forming Aromatic C-H Alkylations with Unactivated Alkyl Halides

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General Methods

Proton and carbon magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were obtained using a Bruker model AVANCE III 400 or 600 (^{1}H NMR at 400 MHz or 600 MHz and ^{13}C NMR at 100 MHz) spectrometer with solvent resonance as internal reference (^{1}H NMR: $CDCl_3$ at 7.28 ppm, ^{13}C NMR: $CDCl_3$ at 77.00 ppm). ^{1}H NMR data are reported as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, bs = broad singlet), coupling constants (Hz), and integration. Mass spectra were obtained using a Micromass (now Waters Corporation) Quattro-II, Triple Quadrupole Mass Spectrometer, with a Z-spray nano-Electrospray source design, in combination with an Advion NanoMate chip-based electrospray sample introduction system or a Perkin Elmer Flexar SQ300 MS LC Detector.

Optical rotation measurements were obtained using a Jasco DIP-1000 Digital Polarimeter. Infrared (IR) Spectra were obtained using a Jasco 260 Plus Fourier transform infrared spectrometer. HPLC spectra were obtained using an Agilent 1200 series HPLC with detection at 210, 230, 250 and 254 nm using a Chiralpak IA & IC columns using a flow rate of 1mL per minute. The solvent system used for HPLC resolution of enantiomers was hexanes (A1) and isopropanol (B2). Flash Chromatography was performed using SiliaFlash P60 silica gel (40-63μm) purchased from Silicycle. Visualization was achieved using a short wave UV light (254 nm) and aqueous basic potassium permanganate solution. Tetrahydrofuran (THF), diethyl ether (Et_2O), dichloromethane (DCM), toluene, acetonitrile (MeCN), and dimethylformamide (DMF) were dried by passage through a column of neutral alumina under nitrogen prior to use. Acetone, 1,4-dioxane and tert-butylbenzene were dried over 3Å molecular sieves and degassed with argon prior to use. All other reagents were obtained from commercial sources and used without further purification unless otherwise noted.

Substrate Preparation

General Procedure A: Sulfonation of Anilines[1].
To a 0°C solution of aniline (1 equiv) and pyridine (1.1 equiv) in CH_2Cl_2 (0.35 M) was added methanesulfonyl chloride (1 equiv). The reaction mixture was allowed to warm to ambient temperature and was stirred at ambient temperature for 16 hours. The reaction was quenched with 3N NaOH and the aqueous layer was extracted with CH_2Cl_2 (3x). The aqueous layer was acidified with conc. HCl and filtered through a fritted funnel. The recovered white precipitate was dried under vacuum.

General Procedure B: Alkylation of Methanesulfonamides.[2]
To a solution of methanesulfonamide (1 equiv) in acetonitrile (0.15 M) was added K_2CO_3 (3 equiv) and alkyl halide (8 equiv). The reaction mixture was heated to reflux and stirred for 20 hours before being quenched with H_2O and extracted with Et_2O (3x). The organic layers were combined and dried over $MgSO_4$, filtered and concentrated. The crude product was purified by flash chromatography.

General Procedure C. Epoxidation of Terminal Alkenes.
To a room temperature solution of alkene (1 equiv) in DCM (0.3 M) was added mCPBA (70%, 2 equiv) portionwise. The reaction mixture was stirred at room temperature for 48 hours, and was quenched with saturated $NaHSO_3$ solution. The aqueous layer was extracted with DCM (3x) and the combined organic layer was washed with saturated $NaHCO_3$ and H_2O, dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography.

General Procedure D: Opening of Terminal Epoxides with Super Hydride.
To a solution of epoxide (1 equiv) in THF (0.15 M) at -78°C was added Super-Hydride solution by syringe pump over 30 minutes (1M in THF, 1.2 equiv). The reaction mixture was stirred, warming to room temperature for 1 hour. The solution was quenched with saturated NH_4Cl and extracted with Et_2O (3x). The organic layers were dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography.

General Procedure E: Iodination of Primary and Secondary Alcohols.
To a solution of triphenylphosphine (1.05 equiv) and imidazole (1.05 equiv) in toluene (0.2 M) was added iodine (1.05 M) and stirred for 30 minutes at room temperature. The alcohol (1 equiv) was then added, and the reaction mixture was heated to 80°C and stirred for 16 hours. The solution was then quenched with H_2O, extracted with Et_2O (3x), and washed with saturated $Na_2S_2O_3$. The organic extracts were then dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography. As a precaution, alkyl iodide products were stored in the dark, under inert atmosphere, at -40°C upon purification.

General Procedure F: Bromination of Primary and Secondary Alcohols.

To a solution of secondary alcohol (1 equiv) in Et_2O (1.0 M) was added phosphorus tribromide (0.5 equiv) dropwise. The reaction mixture was stirred at room temperature for 1 hour, and was then quenched with H_2O. The aqueous layer was back extracted with Et_2O (3x) and the combined organic layers were washed with saturated $NaHCO_3$, dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography

General Procedure G: Alkylation of Triethyl Methanetricarboxylate.
To a solution of sodium hydride (60 %, 1.02 equiv) in 1:1 DMF:Toluene (0.3 M) was added triethyl methanetricarboxylate (1 equiv). The solution was stirred for 30 minutes at room temperature before the addition of benzyl bromide (1.02 equiv). The reaction mixture was heated to reflux and stirred for 20 hours. The reaction was quenched with H_2O, extracted with EtOAc (5x) and washed with H_2O, sat'd $NaHCO_3$, and brine. The organic layer was then dried over $MgSO_4$, filtered, and concentrated.

General Procedure H: Decarboxylation of Benzyl Triesters.
To a solution of sodium hydride (60%, 1.1 equiv) in THF (0.4 M) was added ethanol (1.2 equiv) and stirred for 30 minutes at room temperature. Benzyl triester (1 equiv) was then added, and the solution was heated to reflux and stirred for 16 hours. The reaction mixture was quenched with 1N HCl, extracted with Et_2O, and washed with H_2O, sat'd $NaHCO_3$, and brine. The organic layer was then dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography

General Procedure I: Alkylation of Diethyl Benzylmalonates.
To a solution of sodium hydride (60%, 1.3 equiv) in THF (0.3 M) was added diethyl benzylmalonate (1 equiv). The solution was stirred for 30 minutes at room temperature and 1,2-dibromoethane (10 equiv) was then added. The reaction mixture was heated to reflux, stirred for 24 hours. The reaction was quenched with H_2O, extracted with Et_2O (3x), washed with brine, Dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography.

General Procedure J: Iodination of Primary Bromides and Chlorides.
To a solution of primary halide (1 equiv) in acetone (0.3 M) was added NaI (3 equiv) and 15-crown-5 (10 mol %). The solution was heated to reflux and stirred for 20 hours. The reaction mixture was quenched with H_2O, extracted with DCM (3x), and washed with sat'd $Na_2S_2O_3$ and brine. The organic layer was dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography. As a precaution, alkyl iodide products were stored in the dark, under inert atmosphere, at -40°C upon purification.

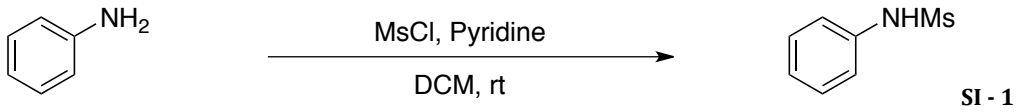
General Procedure K: Iodoalkylation of Diethylbenzylmalonates.
To a solution of sodium hydride (60%, 1.1 equiv) in THF (0.2 M) was added diethyl benzylmalonate (1 equiv). The solution was stirred for 30 minutes at room temperature before the addition of diiodomethane (2 equiv). The reaction mixture was heated to reflux and stirred for 20 hours. The reaction was quenched with H_2O, extracted with Et_2O, and

washed with brine. The organic layer was dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography. As a precaution, alkyl iodide products were stored in the dark, under inert atmosphere, at -40°C upon purification.

General Procedure L: Epoxylkylation or Alkylation of Indoles and Pyrroles.
To a solution of indole or pyrrole (1 equiv) in DMF (0.3 M) was added KOH (1.1 equiv). The solution was stirred for 15 minutes at room temperature before the addition of alkyl halide (1.1 equiv). The reaction mixture was heated to 80°C and stirred for 16 hours, before being quenched with H_2O, extracted with Et_2O (3x), and washed with brine. The organic layer was dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography.

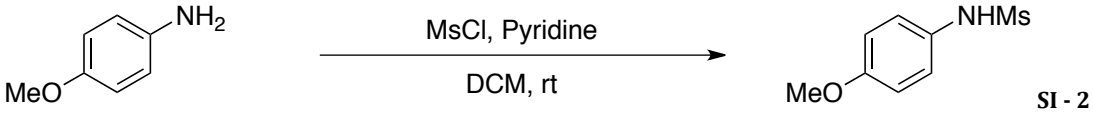
General Procedure M: Alkylation of Indoles and Pyrroles with Dihaloalkanes.
To a solution of indole or pyrrole (1 equiv) in DMSO (0.5 M) was added KOH (1.3 equiv). The solution was sonicated for 10 minutes before the addition of alkyl bromide (3 equiv). The reaction mixture was stirred for 20 hours at room temperature, and was then quenched with H_2O, extracted with Et_2O (3x), and washed with brine. The organic layer was dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography.

General Procedure N: Iodination of Primary Alkyl Chlorides.
To a solution of primary halide (1 equiv) in acetonitrile (0.15 M) was added NaI (4.5 equiv). The solution was heated to reflux and stirred for 16 hours. The reaction mixture was quenched with H_2O, extracted with Et_2O (3x), and washed with sat'd $Na_2S_2O_3$ and brine. The organic layer was dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography. As a precaution, alkyl iodide products were stored in the dark, under inert atmosphere, at -40°C upon purification.



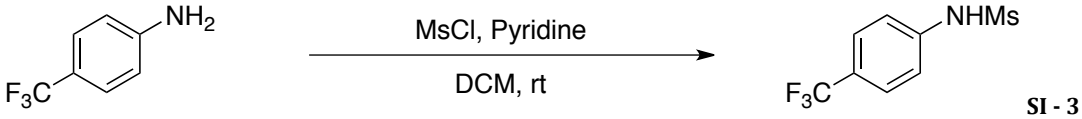
SI - 1

(SI-1): N-phenylmethanesulfonamide. Aniline (4.2 g, 45 mmol) was sulfonated with methanesulfonyl chloride (5.2 g, 45 mmol) according to General Procedure A. The crude product was isolated as a pure white solid (90% Yield). All physical and spectroscopic data were in accordance with the literature data.[3]



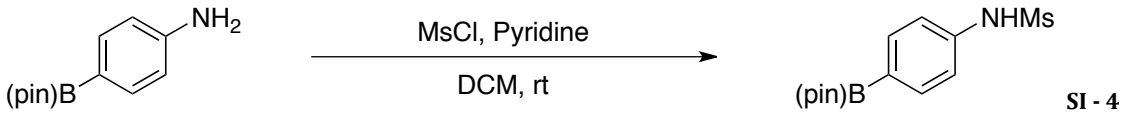
SI - 2

(SI-2): N-(4-methoxyphenyl)methanesulfonamide. p-Anisidine (5.0 g, 40.5 mmol) was sulfonated with methanesulfonyl chloride (4.6 g, 40.5 mmol) according to General Procedure A. The crude product was isolated as a pure white solid (83% Yield). All physical and spectroscopic data were in accordance with the literature data.[3]



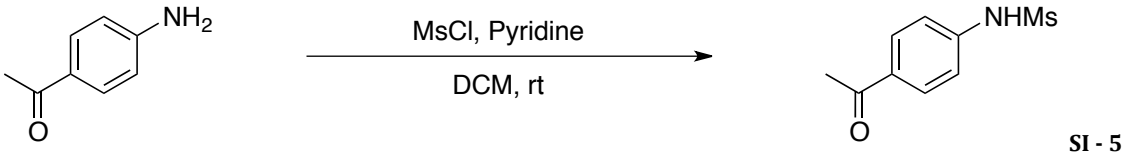
SI - 3

(SI-3): N-(4-trifluoromethylphenyl)methanesulfonamide. p-Trifluoromethylaniline (10.0 g, 62 mmol) was sulfonated with methanesulfonyl chloride (7.1 g, 62 mmol) according to General Procedure A. The crude product was isolated as a pure white solid (82% Yield). All physical and spectroscopic data were in accordance with the literature data.[4]



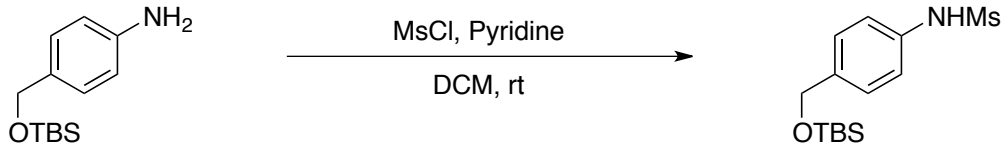
SI - 4

(SI-4): N-(4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanesulfonamide. p-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (5.0 g, 23 mmol) was sulfonated with methanesulfonyl chloride (2.6 g, 23 mmol) according to General Procedure A. The crude product was isolated as a pure white solid (91% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.82 (d, J = 8.4 Hz, 2H), 7.22 (d, J = 8.4 Hz, 2H), 3.05 (s, 3H), 1.37 (s, 12H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 139.40, 136.46, 118.57, 83.95, 39.52, 24.86. **IR** (Thin Film, cm^{-1}): 3253, 2979, 1608, 1361, 1332, 1143, 967, 857. **LRMS** (ESI): Calculated for $[C_{13}H_{20}BNO_4SNa]^+$ 320.17, found 320.31.



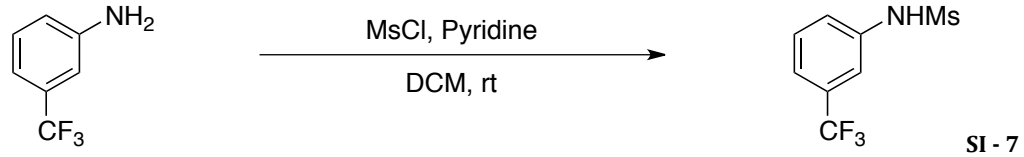
SI - 5

(SI-5): N-(4-acetylphenyl)methanesulfonamide. 4'-aminoacetophenone (9.0 g, 66.5 mmol) was sulfonated with methanesulfonyl chloride (7.6 g, 66.5 mmol) according to General Procedure A. The crude product was isolated as a pure white solid (85% Yield). All physical and spectroscopic data were in accordance with the literature data.[5]



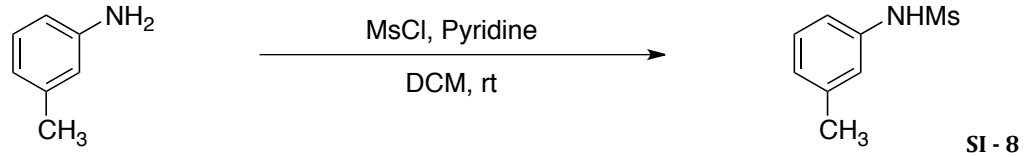
SI - 6

(SI-6): N-(4-((tert-butyldimethylsilyloxy)methyl)phenyl)methanesulfonamide. 4-((tert-butyldimethylsilyloxy)methyl)aniline (10 g, 42.2 mmol) was sulfonated with methanesulfonyl chloride (4.8 g, 42.2 mmol) according to General Procedure A. The crude product was isolated as a pure white solid (88% Yield). **^{1}H-NMR** (600 MHz, D_2O): δ 7.13 (d, J = 8.4 Hz, 2H), 6.89 (d, J = 8.4 Hz, 2H), 2.76 (s, 3H), 0.80 (s, 9H), 0.02 (s, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 145.80, 132.22, 128.41, 121.97, 65.27, 38.43, 25.24, 17.74, -6.04. **IR** (Thin Film, cm^{-1}): 2930, 1505, 1256, 1197, 1092, 999, 837, 775. **LRMS** (ESI): Calculated for $[C_{14}H_{25}NO_3SSiNa]^+$ 338.49, found 338.38.



SI - 7

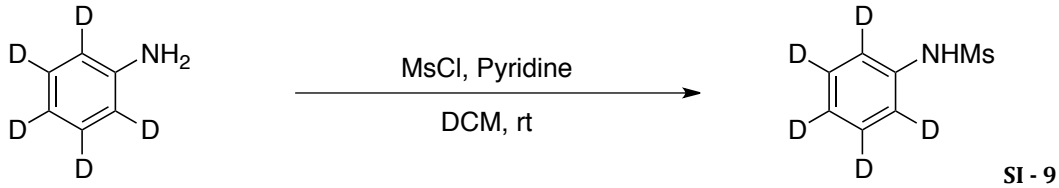
(SI-7): N-(3-trifluoromethylphenyl)methanesulfonamide. m-Trifluoromethylaniline (7.3 g, 45 mmol) was sulfonated with methanesulfonyl chloride (5.2 g, 45 mmol) according to General Procedure A. The crude product was isolated as a pure white solid (52% Yield). All physical and spectroscopic data were in accordance with the literature data.[3]



SI - 8

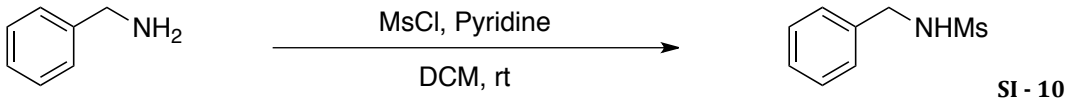
(SI-8): N-(3-tolyl)methanesulfonamide. m-Toluidine (4.8 g, 45 mmol) was sulfonated with methanesulfonyl chloride (5.2 g, 45 mmol) according to General Procedure A. The crude

product was isolated as a pure white solid (98% Yield). All physical and spectroscopic data were in accordance with the literature data.[3]



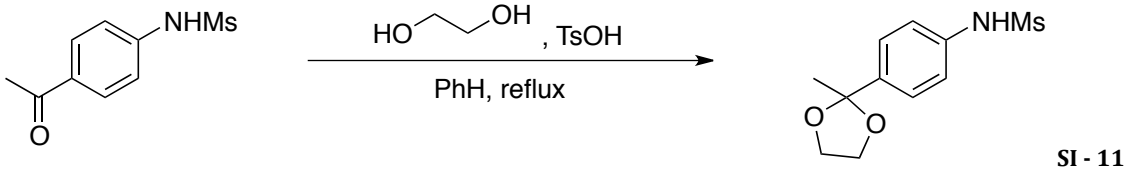
SI - 9

(SI-9): N-(d_5-phenyl)methanesulfonamide. Aniline-2,3,4,5,6-d_5 (2.0 g, 20. mmol) was sulfonated with methanesulfonyl chloride (2.3 g, 20 mmol) according to General Procedure A. The crude product was isolated as a pure white solid (94% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 6.33 (bs, 1H) 3.04 (s, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 136.51, 126.39, 129.23, 129.06, 124.95, 120.48, 120.31, 120.15, 39.30. **IR** (Thin Film, cm^{-1}): 3263, 1565, 1381, 1308, 1149, 911, 770, 555, 512. **LRMS** (ESI): Calculated for $[C_7H_4D_5NO_2SH]^+$ 177.07, found 177.08.



SI - 10

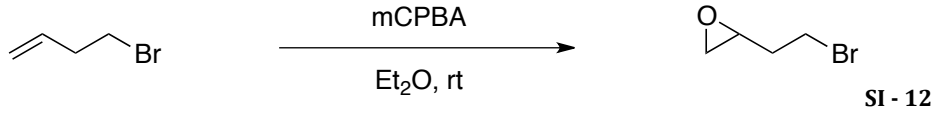
(SI-10): N-benzylmethanesulfonamide. Benzylamine (7.1 g, 66. mmol) was sulfonated with methanesulfonyl chloride (7.2 g, 66 mmol) according to General Procedure A. The crude product was isolated as a pure white solid (99% Yield). All physical and spectroscopic data were in accordance with the literature data.[6]



SI - 11

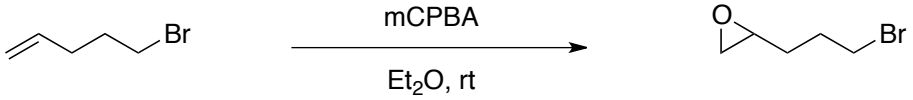
(SI-11): N-(4-(2-methyl-1,3-dioxolan-2-yl)phenyl)methanesulfonamide. To a solution of sulfonamide SI-5 (10.0 g, 46.9 mmol, 1 equiv.) in benzene (50 mL, 1.0 M) was added p-toluenesulfonic acid monohydrate (0.89 g, 2.7 mmol, 10 mol%) and ethylene glycol (3.5 g, 56.3 mmol, 1.2 equiv). The reaction mixture was heated to reflux using a Dean Stark apparatus and reflux condenser and stirred for 18 hours before being quenched with saturated $NaHCO_3$. The aqueous layer was extracted with DCM and the combined organic layer was washed with brine, dried over $MgSO_4$, filtered and concentrated. The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide epoxide SI-11 as a white solid (56% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.47 (d, J = 8.4 Hz, 2H), 7.19 (d, J = 8.4 Hz, 2H), 4.04 (m, 2H), 3.78 (m, 2H), 3.03 (s, 3H), 1.64 (s, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 141.17, 130.83, 127.26, 120.89, 108.94, 64.99, 40.01, 28.01. **IR** (Thin Film, cm^{-1}):

3251, 1673, 1603, 1329, 1153, 1037, 970. **LRMS** (ESI): Calculated for $[C_{11}H_{15}NO_4SNa]^+$ 280.30, found 280.31.



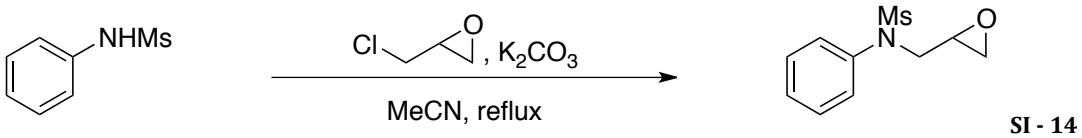
SI - 12

(SI-12): (2-bromoethyl)oxirane. Following General Procedure C, 4-bromo-1-butene (8.0 g, 59.3 mmol) was epoxidized with mCPBA (75%, 20 g, 88.9 mmol). The crude product was isolated as a pure clear oil (89% Yield). All physical and spectroscopic data were in accordance with the literature data.[7]



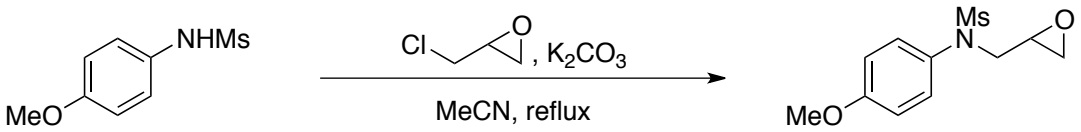
SI - 13

(SI-13): (2-bromoethyl)oxirane. Following General Procedure C, 5-bromo-1-pentene (6.0 g, 40 mmol) was epoxidized with mCPBA (75%, 15 g, 60 mmol). The crude product was isolated as a pure clear oil (97% Yield). All physical and spectroscopic data were in accordance with the literature data.[8]



SI - 14

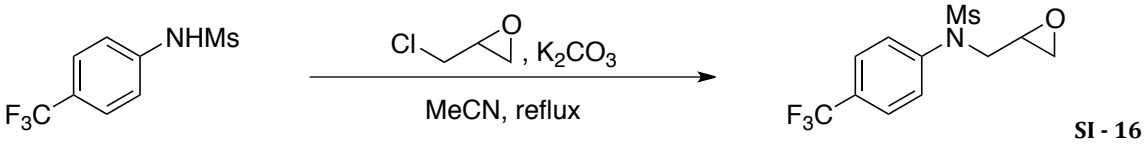
(SI-14): N-(2,3-epoxypropyl)-n-phenylmethanesulfonamide. Following General Procedure B, methanesulfonamide SI-1 (8.6 g, 50 mmol) was alkylated with epichlorohydrin (18.5 g, 200 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (3:1) to provide epoxide SI-14 as a white solid (70% Yield). All physical and spectroscopic data were in accordance with the literature data.[9]



SI - 15

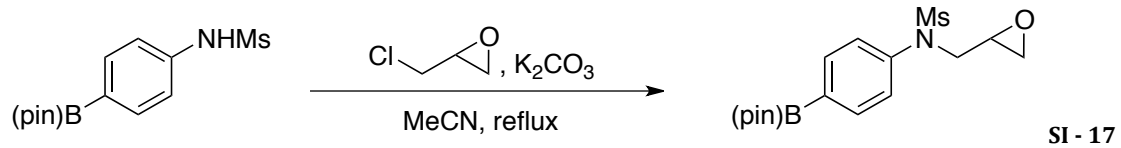
(SI-15): N-(4-anisyl-n-(2,3-epoxypropyl)methanesulfonamide. Following General Procedure B, methanesulfonamide SI-2 (3.2 g, 15.9 mmol) was alkylated with epichlorohydrin (11.7 g, 127 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (3:1) to provide epoxide SI-15 as a white solid (53% Yield). **^{1}H-NMR**

(600 MHz, $CDCl_3$): δ 7.34 (m, 2H), 6.95 (m, 2H), 3.84 (s, 3H), 3.83 (dd, J = 15.0 Hz, 4.2 Hz, 1H), 3.73 (dd, J = 15.0 Hz, 6.0 Hz, 1H), 3.19 (m, 1H), 2.98 (s, 3H), 2.79 (t, J = 4.8 Hz, 1H), 2.54 (m, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 159.51, 131.96, 130.30, 114.82, 55.47, 54.00, 50.30, 45.90, 38.19. **IR** (Thin Film, cm^{-1}): 2933, 1509, 1336, 1251, 1152, 1029, 960, 842. **LRMS** (ESI): Calculated for $[C_{11}H_{15}NO_4SH]^+$ 258.08, found 258.00.



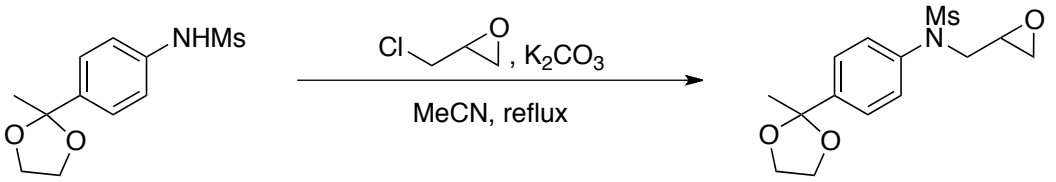
SI - 16

(SI-16): N-(2,3-epoxypropyl)-n-(4-trifluoromethylphenyl)methanesulfonamide. Following General Procedure B, methanesulfonamide SI-3 (6.0 g, 25.0 mmol) was alkylated with epichlorohydrin (18.6 g, 200 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (3:1) to provide epoxide SI-16 as a white solid (77% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.71 (d, J = 8.4 Hz, 2H), 7.58 (d, J = 8.4 Hz, 2H), 4.07 (dd, J = 15.2 Hz, 3.6 Hz, 1H) 3.70 (dd, J = 15.2 Hz, 6.8 Hz, 1H) 3.27 (m, 1H), 3.01 (s, 3H), 2.72 (dd, J = 4.8 Hz, 2.4 Hz, 1H), 2.60 (dd, J = 4.8 Hz, 2.4 Hz, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 128.34, 126.79, 126.77, 53.61, 50.27, 45.75, 38.71. **IR** (Thin Film, cm^{-1}): 2365, 1616, 1325, 1185, 1121, 1069, 511. **LRMS** (ESI): Calculated for $[C_{11}H_{12}F_3NO_3SH]^+$ 296.06, found 296.06.



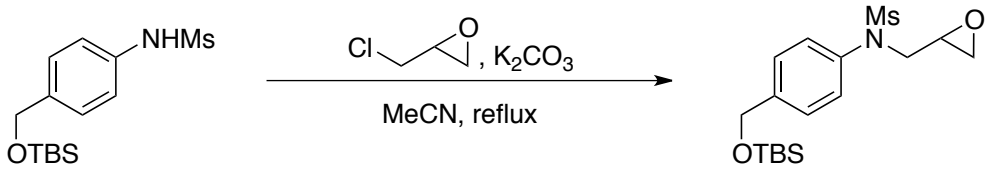
SI - 17

(SI-17): N-(2,3-epoxypropyl)-n-(4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanesulfonamide. Following General Procedure B, methanesulfonamide SI-4 (6.0 g, 20.2 mmol) was alkylated with epichlorohydrin (14.9 g, 162 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (2:1) to provide epoxide SI-17 as a white solid (47% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.89 (d, J = 8.4 Hz, 2H), 7.43 (d, J = 8.4 Hz, 2H), 7.89 (dd, J = 15 Hz, 6.0 Hz, 1H), 3.83 (dd, J = 15, 6.0 Hz, 1H), 3.19 (m, 1H), 2.98 (s, 3H), 2.78 (m, 1H), 2.54 (m, 1H), 1.37 (s, 12H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 142.19, 136.17, 127.49, 84.10, 75.03, 53.54, 50.27, 45.99, 38.39, 24.86. **IR** (Thin Film, cm^{-1}): 3528, 2980, 1605, 1361, 1148, 1093, 961, 857, 658, 550. **LRMS** (ESI): Calculated for $[C_{16}H_{24}BNO_5SNa]^+$ 376.23, found 376.34.



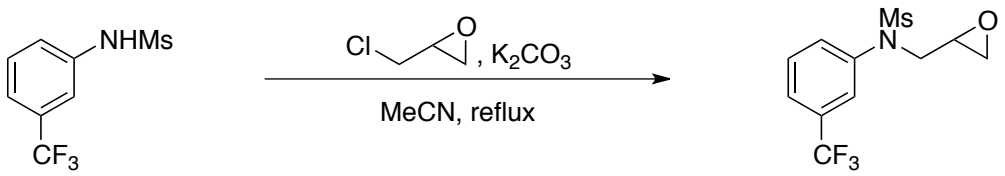
SI - 18

(SI-18): N-(2,3-epoxypropyl)-n-(4-(2-methyl-1,3-dioxolan-2-yl)phenyl)methane sulfonamide. Following General Procedure B, methanesulfonamide SI-11 (6.0 g, 23.3 mmol) was alkylated with epichlorohydrin (17.2 g, 186 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide epoxide SI-18 as a white solid (56% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.53 (d, J = 8.4 Hz, 2H), 7.37 (d, J = 8.4, 2H), 4.05 (m, 2H), 3.87 (dd, J = 14.4 Hz, 3.6 Hz, 1H), 3.80 (m, 2H), 3.73 (dd, J = 15.0 Hz, 6.6 Hz, 1H), 3.18 (m, 1H), 2.98 (s, 3H), 2.79 (t, J = 4.2 Hz, 1H), 2.59 (m, 1H), 1.65 (s, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 144.27, 139.67, 128.89, 127.17, 108.93, 65.05, 54.34, 50.80, 46.45, 38.89, 28.07. **IR** (Thin Film, cm^{-1}): 2989, 1506, 1340, 1155, 1037, 956, 872. **LRMS** (ESI): Calculated for $[C_{14}H_{19}NO_5SNa]^+$ 336.36, found 336.29.



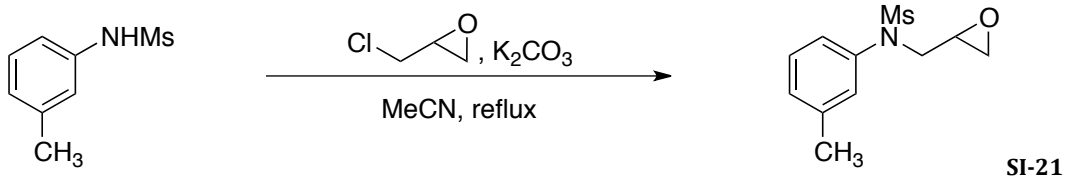
SI - 19

(SI-19): N-(2,3-epoxypropyl)-n-(4-(tert-butyldimethylsilyloxylmethyl)phenyl)methane sulfonamide. Following General Procedure B, methanesulfonamide SI-6 (7.0 g, 22.2 mmol) was alkylated with epichlorohydrin (16.5 g, 178 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide epoxide SI-19 as a white solid (59% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.40 (m, 4H), 4.78 (s, 2H), 3.86 (dd, J = 15.0 Hz, 4.2 Hz, 1H), 3.79 (dd, J = 14.4 Hz, 6.0 Hz, 1H), 3.20 (m, 1H), 2.99 (s, 3H), 2.80 (t, J = 4.2 Hz, 1H), 2.55 (m, 1H), 0.98 (s, 9H), 0.14 (s, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 142.03, 138.16, 128.55, 127.08, 64.26, 53.87, 50.30, 46.01, 38.30, 25.94, 18.41, -5.29. **IR** (Thin Film, cm^{-1}): 2931, 1509, 1342, 1255, 1155, 1089, 840, 777. **LRMS** (ESI): Calculated for $[C_{17}H_{29}NO_4SSiNa]^+$ 394.56, found 394.39.



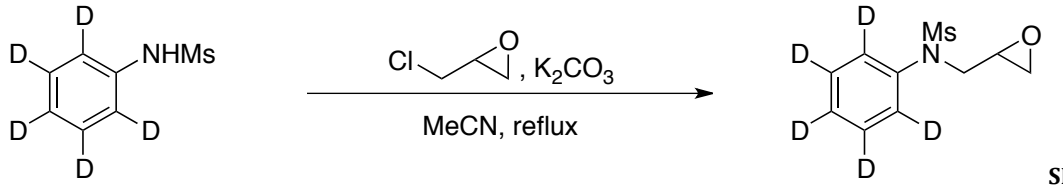
SI - 20

(SI-20): N-(2,3-epoxypropyl)-n-(3-trifluoromethylphenyl)methanesulfonamide. Following General Procedure B, methanesulfonamide SI-7 (4.0 g, 16.7.0 mmol) was alkylated with epichlorohydrin (12.4 g, 134 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (3:1) to provide epoxide SI-20 as a white solid (51 % Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.70-7.64 (m, 3H), 7.59 (t, J = 7.6 Hz, 1H), 4.03 (dd, J = 14.4 Hz, 2.4 Hz, 1H), 3.71 (dd, J = 15.2 Hz, 6.0 Hz, 1H), 3.22 (m, 1H), 3.02 (s, 3H), 2.83 (dd, J = 4.0 Hz, 4.0 Hz, 1H), 2.59 (dd, J = 2.4 Hz, 2.4 Hz, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 140.37, 132.19, 132.08, 131.97, 130.23, 125.15, 125.13, 125.08, 125.05, 124.28, 122.47, 53.77, 50.77, 50.18, 45.70, 38.60. **IR** (Thin Film, cm^{-1}): 3068, 3010, 2934, 1593, 1491, 1445, 1331, 1158, 919, 809, 757, 700, 539. **LRMS** (ESI): Calculated for $[C_{11}H_{12}F_3NO_3SH]^+$ 296.06, found 295.99.



SI-21

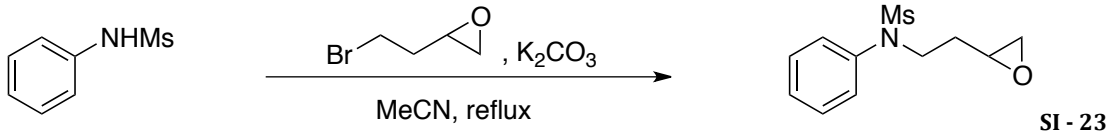
(SI-21): N-(2,3-epoxypropyl)-n-(3-tolyl)methanesulfonamide. Following General Procedure B, methanesulfonamide SI-8 (5.0 g, 27.0 mmol) was alkylated with epichlorohydrin (19.9 g, 216 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (3:1) to provide epoxide SI-21 as a white solid (69% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.33 (t, J = 8.4 Hz, 1H) 7.25-7.18 (m, 3H) 3.86 (dd, J = 14.8 Hz, 4.0 Hz, 1H), 3.77 (dd, J = 14.8 Hz, 6.0 Hz, 1H) 3.20 (m, 1H), 3.00 (s, 3H), 2.79 (dd, J = 4.0 Hz, 4.0 Hz, 1H) 2.56 (dd, J = 2.4 Hz, 2.4 Hz, 1H), 2.40 (s, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 139.72, 139.48, 129.43, 129.35, 129.27, 125.42, 53.80, 50.27, 45.93, 38.32, 21.30. **IR** (Thin Film, cm^{-1}): 3005, 2929, 1605, 1487, 1337, 1155, 1074, 961, 825, 706, 612, 516. **LRMS** (ESI): Calculated for $[C_{11}H_{15}NO_3SH]^+$ 242.08, found 242.12.



SI -22

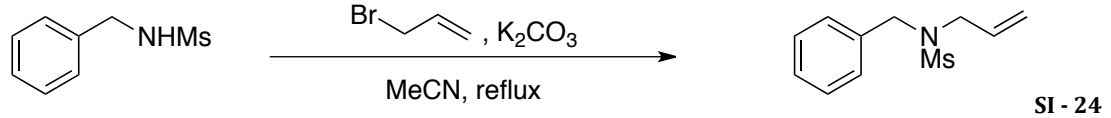
(SI-22): N-(2,3-epoxypropyl)-n-(perdeuterophenyl)methanesulfonamide. Following General Procedure B, methanesulfonamide SI-9 (2.5 g, 14.2 mmol) was alkylated with epichlorohydrin (10.5 g, 113 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (3:1) to provide epoxide SI-22 as a white solid (61% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 3.90 (dd, J = 14.8 Hz, 4.4 Hz, 1H), 3.79 (dd, J = 14.8 Hz, 6.0 Hz, 1H), 3.21 (m, 1H), 3.00 (s, 3H), 2.80 (dd, J = 4.4 Hz, 4.4 Hz, 1H), 2.56 (dd, J = 4.8 Hz, 2.4 Hz, 1H). **^{13}C-**

NMR (100 MHz, $CDCl_3$): δ 53.82, 50.29, 45.94, 38.34. **IR** (Thin Film, cm^{-1}): 1382, 1336, 1152, 958, 815, 525. **LRMS** (ESI): Calculated for $[C_{10}H_8D_5NO_3SH]^+$ 233.10, found 233.11.



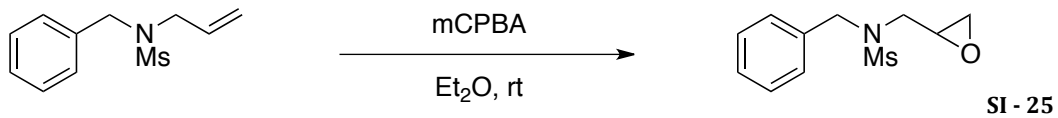
SI - 23

(SI-23): N-(3,4-epoxybutyl)-n-phenylmethanesulfonamide. Following General Procedure B, methanesulfonamide SI-1 (2.3 g, 13.3 mmol) was alkylated with (2-bromoethyl)oxirane (3.0 g, 19.9 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (3:1) to provide epoxide SI-23 as a white solid (62% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.50-7.33 (m, 5H), 3.89 (td, J = 7.2 Hz, 2.4 Hz, 2H), 2.99 (m, 1H), 2.93 (s, 3H) 2.78 (dd, J = 4.8 Hz, 4.4 Hz, 1H), 2.48 (dd, J = 4.8 Hz, 2.4 Hz, 1H) 1.87 (m, 1H), 1.69 (m, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 138.99, 129.61, 128.50, 128.28, 49.80, 48.02, 46.90, 37.03, 32.01. **IR** (Thin Film, cm^{-1}): 2930, 1491, 1336, 1153, 1074, 961, 769, 700, 543, 521. **LRMS** (ESI): Calculated for $[C_{11}H_{15}NO_3SH]^+$ 242.08, found 242.12.



SI - 24

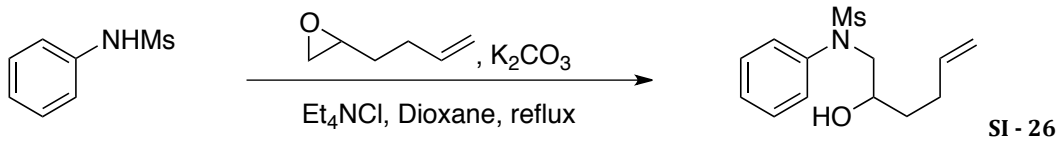
(SI-24): N-allyl-n-benzylmethanesulfonamide. Following General Procedure B, methanesulfonamide SI-10 (5.0 g, 27.0 mmol) was alkylated with allyl bromide (3.4 g, 28.3 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (6:1) to provide alkene SI-24 as a clear oil (75% Yield). All physical and spectroscopic data were in accordance with the literature data.[6]



SI - 25

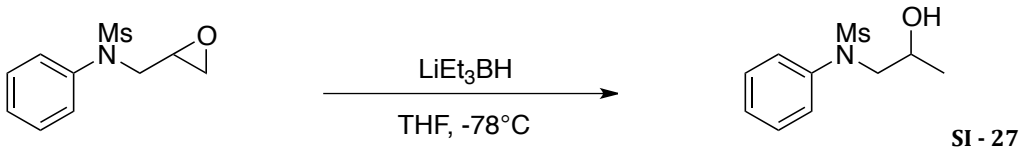
(SI-25): N-benzyl-n-(2,3-epoxypropyl)methanesulfonamide. Following General Procedure C, methanesulfonamide SI-24 (2.5 g, 11.1 mmol) was epoxidized with mCPBA (75%, 5.5 g, 22.2 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (3:1) to provide epoxide SI-25 as a white solid (56% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.47-7.29 (m, 5H), 4.56 (d, J = 3.2 Hz, 2H), 3.54 (dd, J = 14.8 Hz, 2.8 Hz, 1H), 3.16 (dd, J = 21.6 Hz, 6.8 Hz, 1H), 3.11 (m, 1H), 2.96 (s, 3H), 2.77 (dd, J = 4.4 Hz, 4.4 Hz, 1H), 2.48 (dd, J = 4.8 Hz, 2.4 Hz, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 135.64, 128.79, 128.59,

128.16, 51.63, 50.08, 49.21, 45.39, 39.59. **IR** (Thin Film, cm^{-1}): 3007, 2929, 1722, 1329, 1255, 1149, 1027, 965, 935, 792, 700, 515. **LRMS** (ESI): Calculated for $[C_{11}H_{15}NO_3SH]^+$ 242.08, found 242.12.



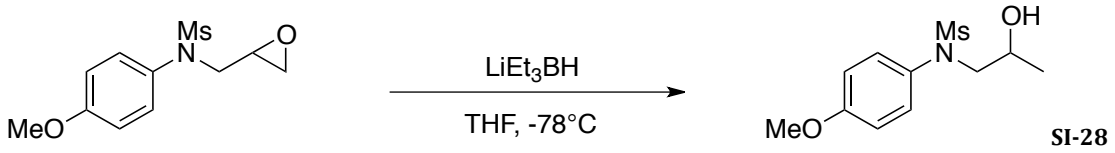
SI - 26

(SI-26): N-(2-hydroxyhex-5-enyl)-n-phenylmethanesulfonamide. To a solution of sulfonamide SI-1 (4.0 g, 23.4 mmol, 1 equiv.) in 1,4-dioxane (120 mL, 0.2 M) was added K_2CO_3 (3.2 g, 23.4 mmol, 1 equiv.) and Et_4NCl (3.9 g, 23.4 mmol, 1 equiv.) and set to stir for 10 minutes at room temperature. 1,2-epoxy-5-hexene (2.3 g, 23.4 mmol, 1 equiv.) was then added, and the solution was heated to reflux and stirred for 24 hours before being quenched with water. The aqueous layer was extracted with Et_2O (3x), and the combined organic layer was washed with brine, dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide epoxide SI-26 as a white solid (32% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.43 (m, 2H), 7.37 (m, 3H), 5.75 (m, 1H), 4.98 (dd, J = 25.8 Hz, 10.2 Hz, 2H), 3.77 (dd, J = 13.8 Hz, 8.4 Hz, 1H), 3.70 (m, 1H), 3.61 (dd, J = 13.8 Hz, 3.0 Hz, 1H), 2.94 (s, 3H), 2.18 (m, 1H), 2.16 (m, 1H), 2.08 (m, 1H), 1.53 (m, 2H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 140.24, 138.43, 130.22, 129.09, 128.92, 115.62, 69.76, 57.80, 37.86, 33.96, 30.15. **IR** (Thin Film, cm^{-1}): 3514, 2930, 1492, 1336, 1153, 965, 777, 698, 544. **LRMS** (ESI): Calculated for $[C_{13}H_{19}NO_3SNa]^+$ 292.35, found 292.38.



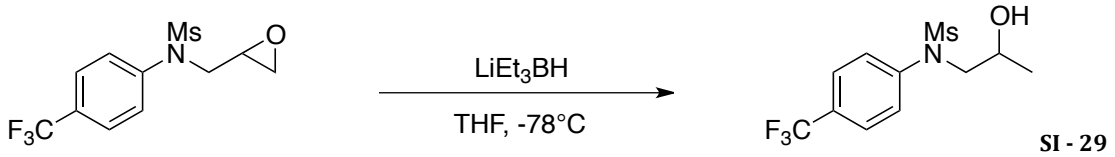
SI - 27

(SI-27): N-(2-hydroxypropyl)-n-phenylmethanesulfonamide. Following General Procedure D, epoxide SI-14 (3.5 g, 15.3 mmol) was reduced with super hydride (1M in THF, 18.4 mL, 18.4 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (3:1) to provide secondary alcohol SI-27 as a white solid (83% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.45 (m, 2H), 7.39 (m, 3H), 3.88 (m, 1H), 3.77 (dd, J = 8.4 Hz, 7.8 Hz, 1H), 3.57 (dd, J = 14.4 Hz, 3.6 Hz, 1H), 2.97 (s, 3H), 1.19 (d, J = 6.0 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 139.72, 129.71, 128.62, 128.42 65.80, 58.53, 37.37, 20.37. **IR** (Thin Film, cm^{-1}): 3511, 2974, 2931, 1491, 1333, 1152, 1070, 968, 866, 778, 698, 544. **LRMS** (ESI): Calculated for $[C_{10}H_{15}NO_3SH]^+$ 230.08, found 230.09.



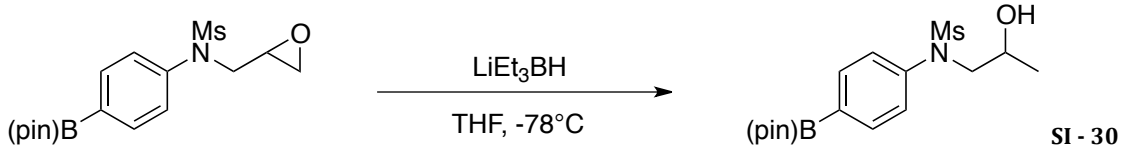
SI-28

(SI-28): N-(2-hydroxypropyl)-n-(4-methoxyphenyl)methanesulfonamide. Following General Procedure D, epoxide SI-15 (2.4 g, 9.1 mmol) was reduced with super hydride (1M in THF, 10.9 mL, 10.9 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide secondary alcohol SI-28 as a white solid (73% Yield). **^{1}H-NMR** (400 MHz, $CDCl_3$): δ 7.22 (m, 2H), 6.85 (m, 2H), 3.79 (m, 1H), 3.77 (m, 3H), 3.64 (dd, J = 14.4 Hz, 8.4 Hz, 1H), 3.42 (dd, J = 14.4 Hz, 3.6 Hz, 1H), 2.87 (s, 3H), 2.14 (m, 1H), 1.10 (d, J = 6.0 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 159.38, 132.02, 129.91, 114.80, 65.63, 58.63, 55.43, 387.20, 20.29. **IR** (Thin Film, cm^{-1}): 3515, 2932, 1509, 1330, 1250, 1151, 1029, 970, 837. **LRMS** (ESI): Calculated for $[C_{11}H_{17}NO_4SH]^+$ 260.10, found 260.17.



SI - 29

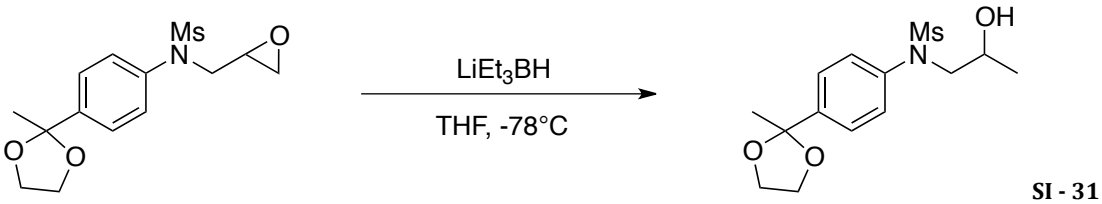
(SI-29): N-(2-hydroxypropyl)-n-(4-trifluoromethylphenyl)methanesulfonamide. Following General Procedure D, epoxide SI-16 (4.0 g, 13.6 mmol) was reduced with super hydride (1M in THF, 16.3 mL, 16.3 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide secondary alcohol SI-29 as a white solid (55% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.71 (d, J = 8.4 Hz, 2H), 7.55 (d, J = 8.4 Hz, 2H), 3.91 (m, 1H), 3.79 (dd, J = 14.4 Hz, 8.4 Hz, 1H), 3.65 (dd, J = 14.4 Hz, 3.6 Hz, 1H), 3.00 (s, 3H), 1.98 (bs, 1H), 1.22 (d, J = 6.0 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 143.14, 128.61, 126.84, 126.82, 126.80, 65.95, 58.21, 37.92, 20.63. **IR** (Thin Film, cm^{-1}): 3505, 1615, 1325, 1159, 1126, 1070, 1017, 970, 873, 788, 525. **LRMS** (ESI): Calculated for $[C_{11}H_{14}F_3NO_3SH]^+$ 298.07, found 298.09.



SI - 30

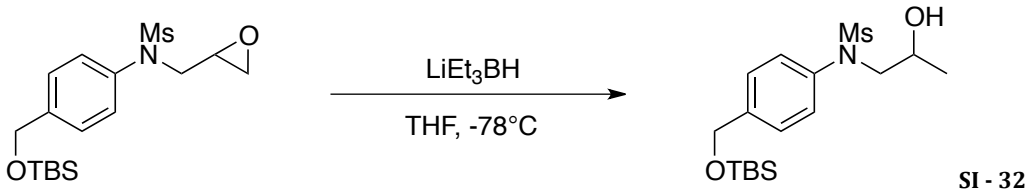
(SI-30): N-(2-hydroxypropyl)-n-(4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl) phenyl)methanesulfonamide. Following General Procedure D, epoxide SI-17 (1.5 g, 4.2 mmol) was reduced with super hydride (1M in THF, 5.1 mL, 5.1 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide secondary

alcohol SI-30 as a white solid (60% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.89 (d, J = 8.4 Hz, 2H), 7.41 (d, J = 8.4 Hz, 2H), 3.88 (m, 1H), 3.79 (dd, J = 14.4 Hz, 8.4 Hz, 1H), 3.62 (dd, J = 14.4, 3.6 Hz, 1H), 2.96 (s, 3H), 1.37 (s, 12H), 1.19 (d, J = 6.0 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 143.71, 137.66, 129.01, 90.06, 85.56, 67.35, 59.77, 54.98, 38.85, 26.29, 26.26, 21.82. **IR** (Thin Film, cm^{-1}): 3504, 2978, 1605, 1361, 1146, 1092, 966, 857, 657. **LRMS** (ESI): Calculated for $[C_{16}H_{26}BNO_5SNa]^+$ 378.25, found 378.36.



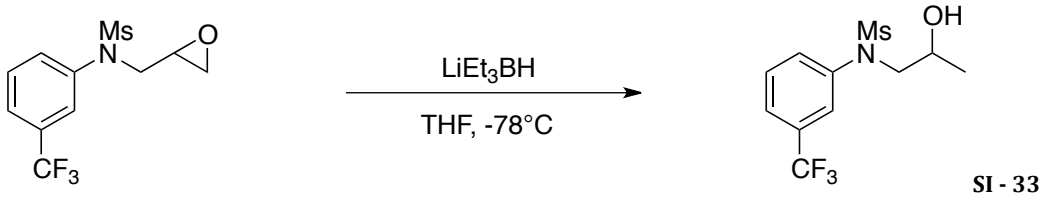
SI - 31

SI-31): N-(2-hydroxypropyl)-n-(4-(2-methyl-1,3-dioxolan-2-yl)phenyl)methane sulfonamide. Following General Procedure D, epoxide SI-18 (2.5 g, 8.0 mmol) was reduced with super hydride (1M in THF, 9.6 mL, 9.6 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide secondary alcohol SI-31 as a white solid (70% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.53 (d, J = 8.4 Hz, 2H), 7.34 (d, J = 8.4 Hz, 2H), 4.05 (m, 2H), 3.85 (m, 1H), 3.79 (m, 2H), 3.73 (dd, J = 14.4 Hz, 6.0 Hz, 1H), 3.55 (dd, J = 14.4 Hz, 3.6 Hz, 1H), 2.92 (s, 3H), 2.08 (bs, 1H), 1.64 (s, 3H), 1.17 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 144.29, 139.71, 128.83, 127.20, 108.91, 66.31, 65.05, 59.07, 37.87, 28.06, 20.84. **IR** (Thin Film, cm^{-1}): 3504, 2981, 1506, 1336, 1155, 1037, 969, 871. **LRMS** (ESI): Calculated for $[C_{14}H_{21}NO_5SNa]^+$ 338.37, found 338.32.



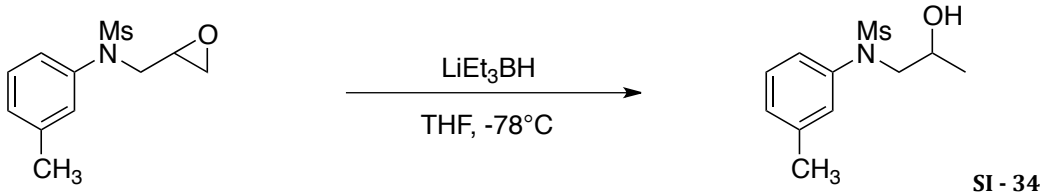
SI - 32

SI-32): N-(2-hydroxypropyl)-n-(4-(tert-butyldimethylsilyloxylmethyl)phenyl)methane sulfonamide. Following General Procedure D, epoxide SI-19 (4.2 g, 11.3 mmol) was reduced with super hydride (1M in THF, 13.6 mL, 13.6 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide secondary alcohol SI-32 as a white solid (69% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.41 (d, J = 8.4 Hz, 2H), 7.37 (d, J = 8.4 Hz, 2H), 4.78 (s, 2H), 3.87 (m, 1H), 3.77 (dd, J = 14.4 Hz, 8.4 Hz, 1H), 3.57 (dd, J = 14.4 Hz, 3.0 Hz, 1H), 2.97 (s, 3H), 1.20 (d, J = 6.6 Hz, 3H), 0.98 (s, 9H), 0.14 (s, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 142.00, 138.26, 128.44, 127.14, 65.83, 64.24, 58.60, 37.32, 25.94, 20.38, 18.42, -5.29. **IR** (Thin Film, cm^{-1}): 3515, 2931, 1509, 1338, 1255, 1155, 1090, 969, 839, 778. **LRMS** (ESI): Calculated for $[C_{17}H_{31}NO_4SSiNa]^+$ 396.57, found 396.43.



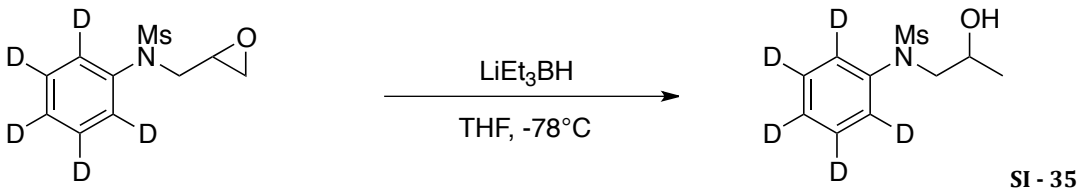
SI - 33

(SI-33): N-(2-hydroxypropyl)-n-(3-trifluoromethylphenyl)methanesulfonamide. Following General Procedure D, epoxide SI-20 (1.9 g, 6.3 mmol) was reduced with super hydride (1M in THF, 7.5 mL, 7.5 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (2:1) to provide secondary alcohol SI-33 as a white solid (62% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.64 (m, 4H), 3.92 (m, 1H), 3.79 (dd, J = 14.0 Hz, 6.6 Hz, 1H), 3.63 (dd, J = 14.0 Hz, 3.6 Hz, 1H), 3.00 (s, 3H), 1.97 (d, J = 4.4 Hz, 1H), 1.22 (d, J = 6.0 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 171.05, 139.66, 139.51, 129.40, 129.24, 129.00, 125.44, 65.42, 60.28, 37.35, 20.86. **IR** (Thin Film, cm^{-1}): 3502, 2930, 1333, 1153, 1074, 970, 757, 514. **LRMS** (ESI): Calculated for $[C_{11}H_{14}F_3NO_3SH]^+$ 298.07, found 298.06.



SI - 34

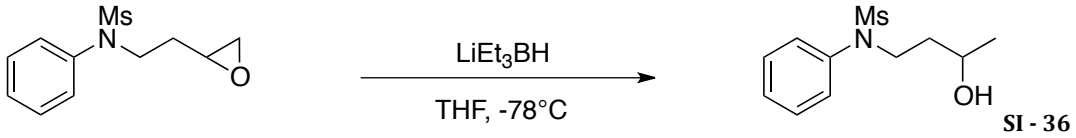
(SI-34): N-(2-hydroxypropyl)-n-(3-tolyl)methanesulfonamide. Following General Procedure D, epoxide SI-21 (2.5 g, 10.4 mmol) was reduced with super hydride (1M in THF, 12.4 mL, 12.4 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (2:1) to provide secondary alcohol SI-34 as a white solid (58% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.31 (m, 1H), 7.20 (m, 2H), 3.87 (m, 1H), 3.76 (dd, J = 13.8 Hz, 8.4 Hz, 1H), 3.57 (dd, J = 13.8 Hz, 3.6 Hz, 1H), 2.97 (s, 3H), 2.40 (s, 3H), 1.20 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 139.86, 139.60, 129.46, 129.42, 129.30, 125.32, 65.81, 58.59, 37.36. **IR** (Thin Film, cm^{-1}): 3507, 2973, 2929, 2360, 1605, 1333, 1154, 1074, 970, 709, 515. **LRMS** (ESI): Calculated for $[C_{11}H_{17}NO_3SH]^+$ 244.10, found 244.11.



SI - 35

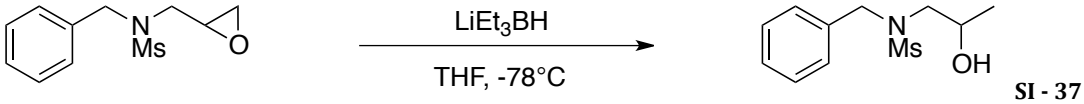
(SI-35): N-(2-hydroxypropyl)-n-(perdeuterophenyl)methanesulfonamide. Following General Procedure D, epoxide SI-22 (1.8 g, 7.5 mmol) was reduced with super hydride (1M in

THF, 9.0 mL, 9.0 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (2:1) to provide secondary alcohol SI-35 as a white solid (57% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 3.87 (m, 1H), 3.77 (dd, J = 14.4 Hz, 8.4 Hz, 1H), 3.58 (dd, J = 14.4 Hz, 3.6 Hz, 1H), 2.97 (s, 3H), 2.19 (d, J = 4.2 Hz, 1H), 1.19 (d, J = 6.0 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 139.58, 129.37, 129.21, 129.05, 128.34, 128.18, 128.02, 65.79, 58.49, 37.34, 20.35. **IR** (Thin Film, cm^{-1}): 3509, 2973, 2932, 1563, 1378, 1329, 1153, 1059, 971, 814, 763. **LRMS** (ESI): Calculated for $[C_{10}H_{10}D_5NO_3SH]^+$ 235.12, found 235.08.



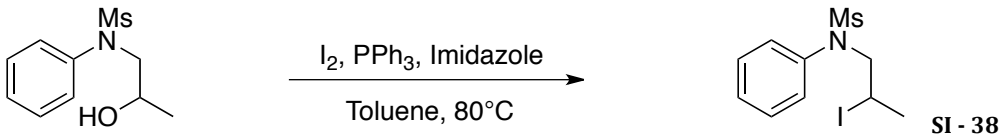
SI - 36

(SI-36): N-(3-hydroxybutyl)-n-phenylmethanesulfonamide. Following General Procedure D, epoxide SI-23 (2.0 g, 8.3 mmol) was reduced with super hydride (1M in THF, 9.9 mL, 9.9 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide secondary alcohol SI-36 as a white solid (53% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.44 (m, 2H), 7.37 (m, 3H), 4.05 (m, 1H), 4.02-3.97 (m, 1H), 3.73-3.69 (m, 1H), 2.93 (s, 3H), 2.27 (d, J = 4.2 Hz, 1H), 1.63-1.59 (m, 1H), 1.54-1.52 (m, 1H), 1.22 (d, J = 6.0 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 138.87, 129.60, 128.57, 128.28, 64.15, 47.80, 37.44, 36.91, 23.20. **IR** (Thin Film, cm^{-1}): 3506, 2930, 1492, 1332, 1153, 1075, 959, 775, 699, 543. **LRMS** (ESI): Calculated for $[C_{11}H_{17}NO_3SH]^+$ 244.10, found 244.16.



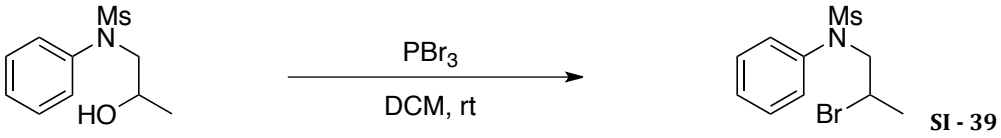
SI - 37

(SI-37): N-benzyl-n-(2-hydroxypropyl)methanesulfonamide. Following General Procedure D, epoxide SI-25 (1.0 g, 4.1 mmol) was reduced with super hydride (1M in THF, 4.9 mL, 4.9 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide secondary alcohol SI-37 as a white solid (76% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.40 (m, 3H), 7.35 (m, 1H), 4.55 (d, J = 15.00 Hz, 1H), 4.45 (d, J = 15.0 Hz, 1H), 3.27 (dd, J = 15.0 Hz, 9.0 Hz, 1H), 3.12 (dd, J = 15.0 Hz, 2.4 Hz, 1H), 2.93 (s, 3H), 1.12 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 135.89, 128.90, 128.49, 128.22, 65.74, 54.88, 52.39, 38.81, 20.80. **IR** (Thin Film, cm^{-1}): 3504, 2930, 1321, 1145, 1022, 958, 795, 700, 518. **LRMS** (ESI): Calculated for $[C_{11}H_{17}NO_3SH]^+$ 244.10, found 244.09.



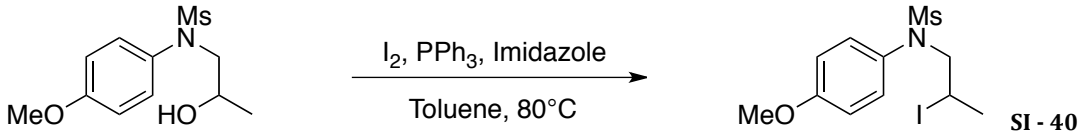
SI - 38

(SI-38): N-(2-iodopropyl)-n-phenylmethanesulfonamide. Secondary alcohol SI-27 (1.0 g, 4.3 mmol) was iodinated with molecular iodine (1.2 g, 4.6 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (7:1) to provide secondary iodide SI-38 as a white solid (62% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.47-7.44 (m, 2H), 7.41-7.38 (m, 3H), 4.13 (dd, J = 13.8 Hz, 6.6 Hz, 1H), 4.02 (m, 1H), 3.90 (dd, J = 13.8 Hz, 8.4 Hz, 1H), 2.94 (s, 3H), 1.93 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 138.93, 129.80, 128.59, 128.55, 60.29, 37.56, 24.93, 23.14. **IR** (Thin Film, cm^{-1}): 2925, 1593, 1491, 1341, 1153, 1059, 964, 843, 776, 697, 541. **LRMS** (ESI): Calculated for $[C_{10}H_{14}INO_2SH]^+$ 339.99, found 339.91.



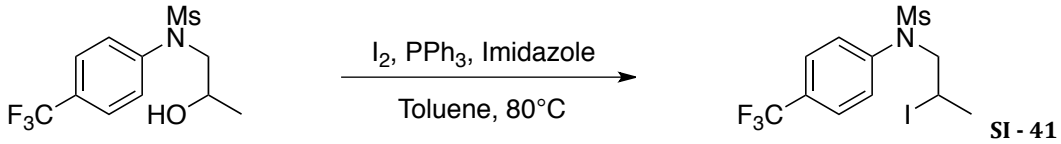
SI - 39

(SI-39): N-(2-bromopropyl)-n-phenylmethanesulfonamide. Secondary alcohol SI-28 (1.5 g, 6.3 mmol) was brominated with phosphorus tribromide (0.3 mL, 3.2 mmol) following General Procedure F. The crude product was purified by flash chromatography using hexanes/ethyl acetate (7:1) to provide secondary bromide SI-39 as a white solid (46% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.47-7.44 (m, 2H), 7.42-7.38 (m, 3H), 4.07 (dd, J = 13.2 Hz, 6.6 Hz, 1H), 4.02 (m, 1H), 3.90 (dd, J = 13.8 Hz, 7.2 Hz, 1H), 2.96 (s, 3H), 1.73 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 139.08, 129.78, 128.66, 128.60, 58.70, 46.05, 37.77, 22.91. **IR** (Thin Film, cm^{-1}): 2981, 2929, 2360, 1593, 1492, 1341, 1156, 1067, 965, 849, 777, 698, 542. **LRMS** (ESI): Calculated for $[C_{10}H_{14}BrNO_2SH]^+$ 292.00, found 291.98.



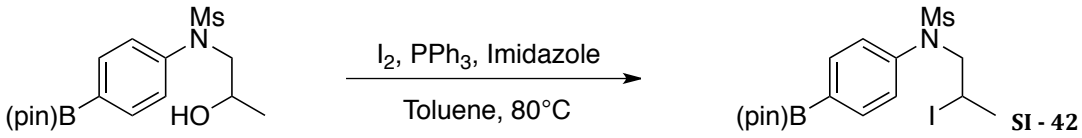
SI - 40

(SI-40): N-(2-iodopropyl)-n-(4-methoxyphenyl)methanesulfonamide. Secondary alcohol SI-29 (1.6 g, 6.2 mmol) was iodinated with molecular iodine (1.7 g, 6.5 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (4:1) to provide secondary iodide SI-40 as a white solid (72% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 3.32 (m, 2H), 6.95 (m, 2H), 4.07 (dd, J = 13.8 Hz, 6.6 Hz, 1H), 4.00 (m, 1H), 3.84 (s, 3H), 3.82 (dd, J = 13.8 Hz, 8.4 Hz, 1H), 2.93 (s, 3H), 1.93 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 159.54, 131.21, 129.90, 114.93, 60.45, 55.50, 37.47, 24.91, 23.34. **IR** (Thin Film, cm^{-1}): 2929, 2838, 1606, 1509, 1448, 1339, 1251, 1153, 966, 843, 759, 545. **LRMS** (ESI): Calculated for $[C_{11}H_{16}INO_3SH]^+$ 370.00, found 369.95.



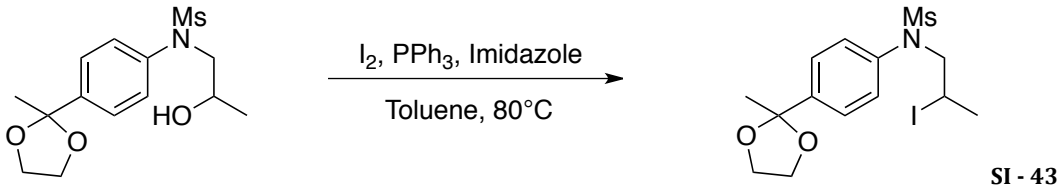
SI - 41

(SI-41): N-(2-iodopropyl)-n-(4-trifluoromethylphenyl)methanesulfonamide. Secondary alcohol SI-30 (1.4 g, 4.7 mmol) was iodinated with molecular iodine (1.3 g, 5.0 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (4:1) to provide secondary iodide SI-41 as a white solid (64% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.73 (d, J = 8.4 Hz, 2H), 7.55 (d, J = 8.4 Hz, 2H), 4.14 (dd, J = 13.8 Hz, 6.6 Hz, 1H), 4.01 (m, 1H), 3.93 (dd, J = 13.8 Hz, 7.8 Hz, 1H), 2.96 (s, 3H), 1.92 (d, J = 7.2 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 142.28, 128.56, 126.94, 126.92, 126.89, 60.03, 37.92, 24.94, 22.50. **IR** (Thin Film, cm^{-1}): 2928, 1615, 1325, 1158, 1068, 965, 853, 785, 602, 522. **LRMS** (ESI): Calculated for $[C_{11}H_{13}F_3INO_2SH]^+$ 407.97, found 408.02.



SI - 42

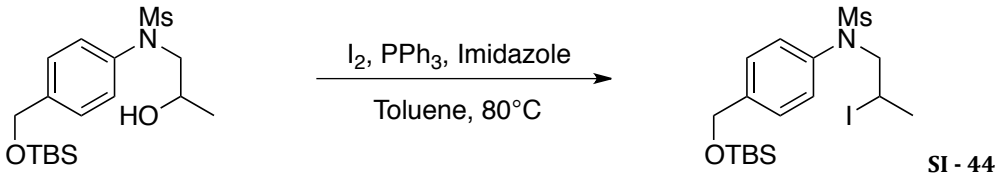
(SI-42): N-(2-iodopropyl)-n-(4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl) methanesulfonamide. Secondary alcohol SI-31 (0.7 g, 2.0 mmol) was iodinated with molecular iodine (0.53 g, 2.1 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (5:1) to provide secondary iodide SI-42 as a white solid (56% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.89 (d, J = 8.4 Hz, 2H), 7.41 (d, J = 8.4 Hz, 2H), 4.15 (dd, J = 13.8, 6.6 Hz, 1H), 4.01 (m, 1H), 3.92 (dd, J = 13.8, 9.0 Hz, 1H), 2.93 (s, 3H), 1.92 (d, J = 7.2 Hz, 3H), 1.37 (s, 12H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 141.50, 136.25, 127.47, 84.15, 60.11, 37.59, 24.96, 24.86, 24.85, 22.99. **IR** (Thin Film, cm^{-1}): 2978, 2360, 1605, 1359, 1150, 1093, 963, 856, 657. **LRMS** (ESI): Calculated for $[C_{16}H_{25}BINO_4SNa]^+$ 488.14, found 488.32.



SI - 43

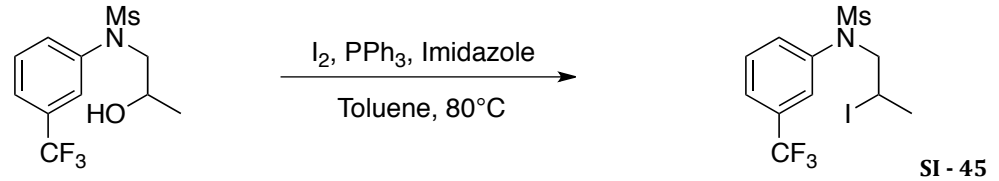
(SI-43): N-(2-iodopropyl)-n-(4-(2-methyl-1,3-dioxolan-2-yl)phenyl)methane sulfonamide. Secondary alcohol SI-32 (1.5 g, 4.8 mmol) was iodinated with molecular iodine (1.3 g, 5.0 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (5:1) to provide secondary iodide SI-43 as a white solid (64% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.54 (d, J = 8.4 Hz, 2H), 7.34 (d, J = 8.4

Hz, 2H), 4.09 (dd, J = 13.8 Hz, 6.6 Hz, 1H), 4.06 (m, 2H), 3.98 (m, 1H), 3.87 (dd, J = 13.8 Hz, 8.4 Hz, 1H), 3.81 (m, 2H), 2.93 (s, 3H), 1.92 (d, J = 7.2 Hz 3H), 1.65 (s, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 138.87, 128.79, 127.29, 125.62, 108.91, 65.10, 60.79, 38.08, 28.06, 25.38, 23.57. **IR** (Thin Film, cm^{-1}): 2985, 1505, 1341, 1154, 1038, 966, 872, 731. **LRMS** (ESI): Calculated for $[C_{14}H_{20}INO_4SNa]^+$ 448.27, found 448.25.



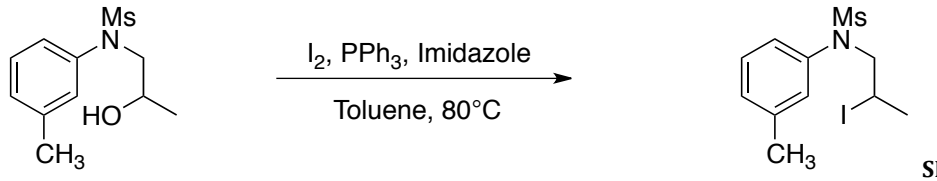
SI - 44

(SI-44): N-(2-iodopropyl)-n-(4-(tert-butyldimethylsilyloxymethyl)phenyl)methane sulfonamide. Secondary alcohol SI-33 (2.0 g, 5.4 mmol) was iodinated with molecular iodine (1.5 g, 5.7 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (5:1) to provide secondary iodide SI-44 as a white solid (65% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.41 (d, J = 8.4 Hz, 2H), 7.37 (d, J = 8.4 Hz, 2H), 4.78 (s, 2H), 4.12 (dd, J = 13.8 Hz, 6.0 Hz, 1H), 4.01 (m, 1H), 3.89 (dd, J = 14.4 Hz, 8.4 Hz, 1H), 2.95 (s, 3H), 1.94 (d, J = 6.6 Hz, 3H), 0.99 (s, 9H), 0.15 (s, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 142.17, 137.44, 128.38, 127.17, 64.22, 60.35, 37.53, 25.95, 24.95, 23.21, 18.43, -5.29. **IR** (Thin Film, cm^{-1}): 2929, 1509, 1343, 1254, 1155, 1091, 966, 839, 777. **LRMS** (ESI): Calculated for $[C_{17}H_{30}INO_3SSiNa]^+$ 506.47, found 506.38.



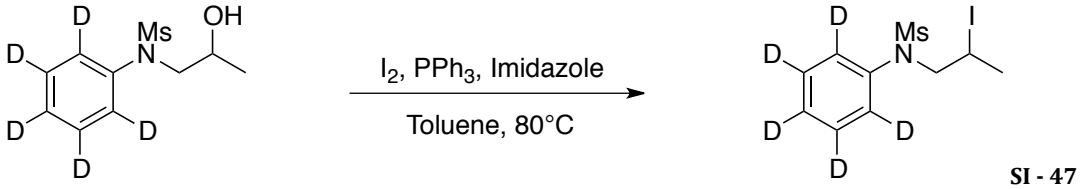
SI - 45

(SI-45): N-(2-iodopropyl)-n-(3-trifluoromethylphenyl)methanesulfonamide. Secondary alcohol SI-34 (0.4 g, 1.3 mmol) was iodinated with molecular iodine (0.4 g, 1.4 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (7:1) to provide secondary iodide SI-45 as a white solid (77% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.68-7.58 (m, 4H), 4.12 (dd, J = 13.8 Hz, 6.6 Hz, 1H), 4.02 (m, 1H), 3.91 (dd, J = 13.8 Hz, 7.8 Hz, 1H), 2.97 (s, 3H), 1.93 (d, J = 7.2 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 139.80, 132.20, 130.42, 125.37, 125.08, 60.26, 37.90, 24.97, 22.63. **IR** (Thin Film, cm^{-1}): 2927, 1593, 1491, 1447, 1328, 1156, 1069, 966, 810, 700, 539. **LRMS** (ESI): Calculated for $[C_{11}H_{13}F_3INO_2SH]^+$ 407.97, found 407.95.



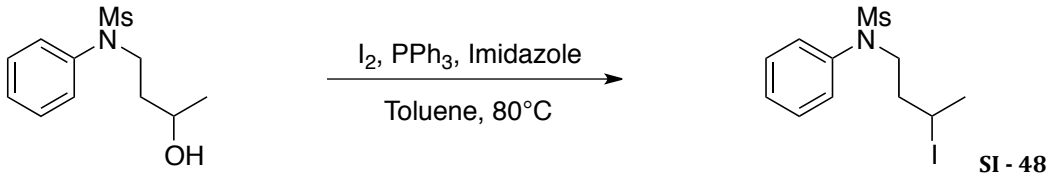
SI - 46

(SI-46): N-(2-iodopropyl)-n-(3-tolyl)methanesulfonamide. Secondary alcohol SI-35 (0.5 g, 2.1 mmol) was iodinated with molecular iodine (0.6 g, 2.2 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (7:1) to provide secondary iodide SI-46 as a white solid (54% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.33 (t, J = 7.8 Hz, 1H), 7.21-7.17 (m, 3H), 4.11 (dd, J = 13.8 Hz, 6.6 Hz, 1H), 4.02 (m, 1H), 3.88 (dd, J = 13.8 Hz, 8.4 Hz, 1H), 2.94 (s, 3H), 2.41 (s, 3H), 1.94 (d, J = 7.2 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 139.91, 138.82, 129.50, 129.43, 129.29, 125.28, 60.33, 37.58, 24.94, 23.26, 21.35. **IR** (Thin Film, cm^{-1}): 2923, 1604, 1486, 1340, 1153, 1065, 966, 808, 690. **LRMS** (ESI): Calculated for $[C_{11}H_{16}INO_2SH]^+$ 354.00, found 354.07.



SI - 47

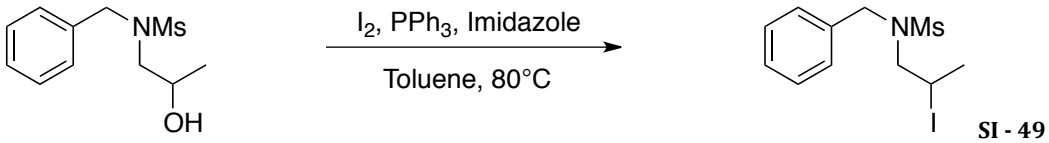
(SI-47): N-(2-iodopropyl)-n-(perdeuterophenyl)methanesulfonamide. Secondary alcohol SI-36 (1.0 g, 4.3 mmol) was iodinated with molecular iodine (1.1 g, 4.5 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (7:1) to provide secondary iodide SI-47 as a white solid (51% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 4.13 (dd, J = 13.8 Hz, 6.6 Hz, 1H), 4.02 (m, 1H), 3.90 (dd, J = 13.8 Hz, 8.4 Hz, 1H), 2.94 (s, 3H), 1.93 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 138.80, 129.46, 129.30, 129.13, 128.27, 128.11, 127.95, 60.28, 37.53, 24.92, 23.14. **IR** (Thin Film, cm^{-1}): 2925, 2360, 1562, 1339, 1153, 1053, 968, 812, 762, 520. **LRMS** (ESI): Calculated for $[C_{10}H_9D_5INO_2SH]^+$ 345.02, found 344.97.



SI - 48

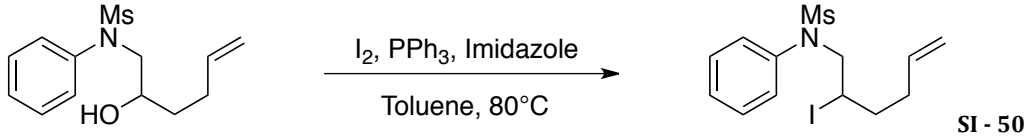
(SI-48): N-(3-iodobutyl)-n-phenylmethanesulfonamide. Secondary alcohol SI-37 (1.0 g, 4.1 mmol) was iodinated with molecular iodine (1.1 g, 4.3 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide secondary iodide SI-48 as a white solid (64% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ

7.45 (t, J = 7.2 Hz, 2H), 7.38 (m, 3H), 4.19 (m, 1H), 3.88 (m, 1H), 3.79 (m, 1H), 2.91 (s, 3H), 2.04 (m, 1H), 1.93 (d, J = 6.6 Hz, 3H), 1.89 (m, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 139.08, 129.63, 128.32, 128.29, 51.09, 41.63, 36.83, 28.80, 24.53. **IR** (Thin Film, cm^{-1}): 2922, 1491, 1339, 1151, 1078, 958, 766, 698, 542, 520. **LRMS** (ESI): Calculated for $[C_{11}H_{16}INO_2SH]^+$ 354.00, found 354.06.



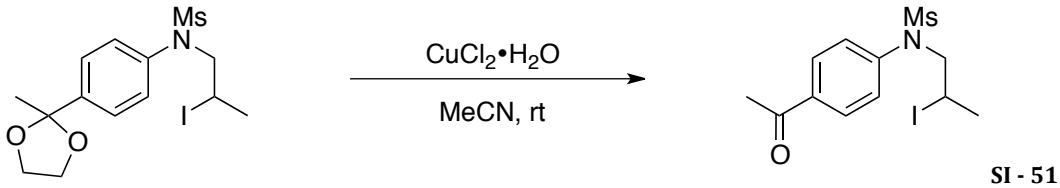
SI - 49

(SI-49): N-benzyl-n-(2-iodopropyl)methanesulfonamide. Secondary alcohol SI-38 (0.75 g, 3.1 mmol) was iodinated with molecular iodine (0.79 g, 3.2 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (7:1) to provide secondary iodide SI-49 as a white solid (84% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.42-7.35 (m, 4H), 4.60 (d, J = 15.0 Hz, 1H), 4.36 (d, J = 15.0 Hz, 1H), 4.11 (m, 1H), 3.57 (dd, J = 15.0 Hz, 7.2 Hz, 1H), 3.49 (dd, J = 14.4 Hz, 7.8 Hz, 1H), 2.91 (s, 3H), 1.81 (d, J = 6.0 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 135.40, 128.94, 128.69, 128.40, 57.48, 52.69, 39.55, 25.18, 23.73. **IR** (Thin Film, cm^{-1}): 2923, 1451, 1329, 1147, 1023, 962, 790, 700. **LRMS** (ESI): Calculated for $[C_{11}H_{16}INO_2SH]^+$ 354.00, found 354.07.



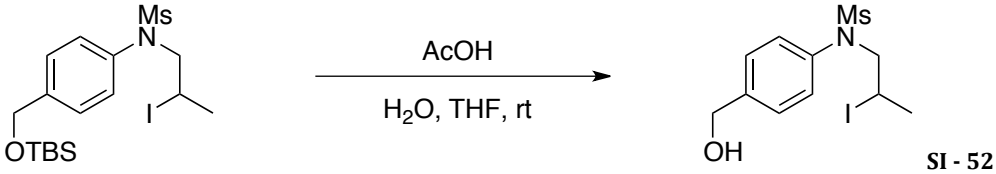
SI - 50

(SI-50): N-(2-iodohex-5-enyl)-n-phenylmethanesulfonamide. Secondary alcohol SI-26 (1.0 g, 3.7 mmol) was iodinated with molecular iodine (1.0 g, 3.9 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide secondary iodide SI-50 as a white solid (57% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.45 (m, 2H), 7.40 (m, 3H), 5.71 (m, 1H), 5.04 (m, 2H), 4.17 (dd, J = 13.8 Hz, 6.0 Hz, 1H), 4.04 (dd, J = 13.8 Hz, 8.4 Hz, 1H), 3.97 (m, 1H), 2.94 (s, 3H), 2.31 (m, 1H), 2.12 (m, 1H), 2.01 (m, 1H), 1.84 (m, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 138.83, 136.38, 129.78, 128.61, 128.50, 115.94, 58.68, 37.40, 35.11, 33.13, 32.28. **IR** (Thin Film, cm^{-1}): 2927, 1593, 1491, 1342, 1154, 962, 775, 697, 542. **LRMS** (ESI): Calculated for $[C_{13}H_{18}INO_2SNa]^+$ 402.25, found 402.23.



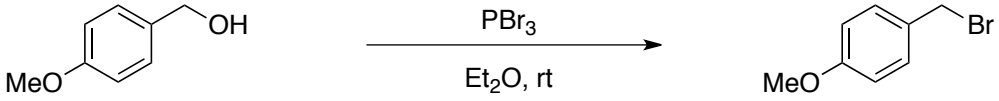
SI - 51

(SI-51): N-(4-acetylphenyl)-n-(2-iodopropyl)methanesulfonamide. To a solution of acetal SI-43 (1.2 g, 2.8 mmol) in acetonitrile (50 ml, 0.05 M) was added copper (II) chloride (0.97 g, 5.6 mmol). The reaction solution was stirred for 3 hours at room temperature before being quenched with water. The aqueous layer was extracted with Et_2O (3x), and the combined aqueous layer was washed with brine, dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide secondary iodide SI-51 as a white solid (89% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 8.01 (d, J = 8.4 Hz, 2H), 7.49 (d, J = 8.4 Hz, 2H), 4.13 (dd, J = 14.4 Hz, 6.6 Hz, 1H), 4.00 (m, 1H), 3.91 (dd, J = 14.4, 7.8 Hz, 1H), 2.93 (s, 3H), 2.61 (s, 3H), 1.89 (d, J = 7.2 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 197.32, 143.69, 137.04, 130.31, 128.58, 60.39, 38.40, 27.19, 25.47, 23.12. **IR** (Thin Film, cm^{-1}): 2925, 1683, 1600, 1343, 1266, 1155, 963, 732, 599. **LRMS** (ESI): Calculated for $[C_{12}H_{16}INO_3SNa]^+$ 404.22, found 404.23.



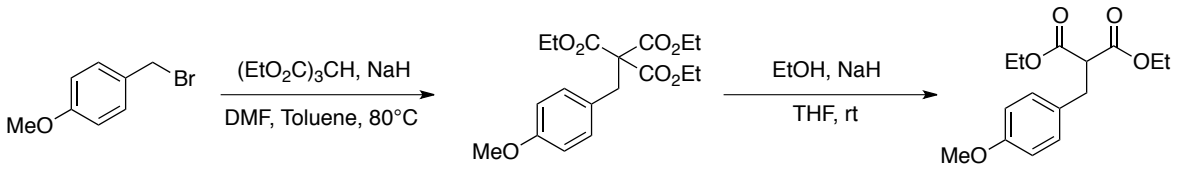
SI - 52

(SI-52): N-(4-(hydroxymethyl)phenyl)-n-(2-iodopropyl)methanesulfonamide. To a solution of acetic acid, water, and THF (3:1:1, 50 mL, 0.03 M) was added silyl ether SI-44 (0.75g, 1.5 mmol). The reaction mixture was stirred at room temperature for 15 hours before being quenched with $NaHCO_3$. The aqueous layer was extracted with Et_2O (3x), and the combined organic layer was washed with brine, dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide secondary iodide SI-52 as a white solid (72% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.47 (d, J = 8.4 Hz, 2H), 7.41 (d, J = 8.4 Hz, 2H), 4.76 (s, 2H), 4.12 (dd, J = 13.8 Hz, 6.6 Hz, 1H), 4.02 (m, 1H), 3.88 (dd, J = 13.8 Hz, 8.4 Hz, 1H), 2.95 (s, 3H), 1.94 (d, J = 6.6 Hz, 3H), 1.75 (bs, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 141.37, 138.17, 128.65, 128.18, 64.54, 60.29, 37.58, 24.93, 23.04. **IR** (Thin Film, cm^{-1}): 3516, 2924, 1509, 1336, 1152, 1056, 966, 731. **LRMS** (ESI): Calculated for $[C_{11}H_{16}INO_3SNa]^+$ 392.21, found 392.29.



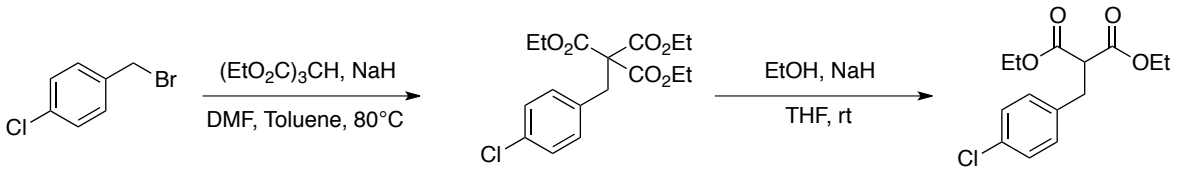
SI - 53

(SI-53): 4-Methoxybenzyl bromide. 4-Methoxybenzyl alcohol (10.0 g, 72.4 mmol) was brominated with phosphorus tribromide (3.6 mL, 38.1 mmol) following General Procedure F. The crude product was purified by flash chromatography using hexanes/ethyl acetate (19:1) to provide benzyl bromide SI-53 as a clear oil (88% Yield). All physical and spectroscopic data were in accordance with the literature data.



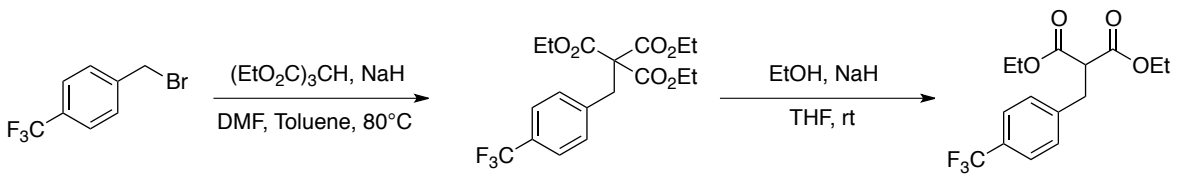
SI - 54

(SI-54): Diethyl (4-methoxybenzyl)malonate. Triethyl methanetricarboxylate (6.8 g, 29.4 mmol) was alkylated with (4-methoxybenzyl) bromide (6.0 g, 30.0 mmol) following General Procedure G. The crude intermediate was then decarboxylated without further purification following General Procedure H. The crude product was purified by flash chromatography using hexanes/ethyl acetate (7:1) to provide diethyl benzylmalonate SI-54 as a pale yellow oil (81% yield). All physical and spectroscopic data were in accordance with literature data.[10]



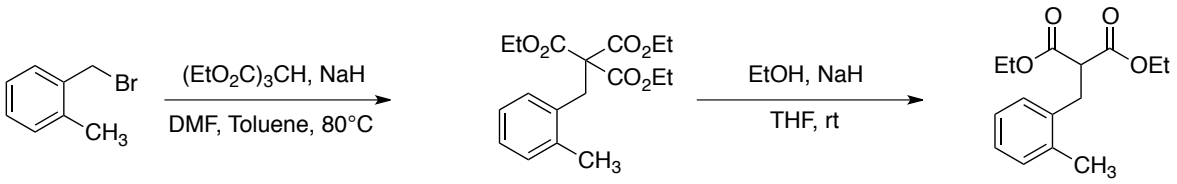
SI - 55

(SI-55): Diethyl (4-chlorobenzyl)malonate. Triethyl methanetricarboxylate (7.5 g, 32.2 mmol) was alkylated with 4-chlorobenzyl bromide (6.7 g, 32.8 mmol) following General Procedure G. The crude intermediate was then decarboxylated without further purification following General Procedure H. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide diethyl benzylmalonate SI-55 as a pale yellow oil (71% yield). All physical and spectroscopic data were in accordance with literature data.[11]



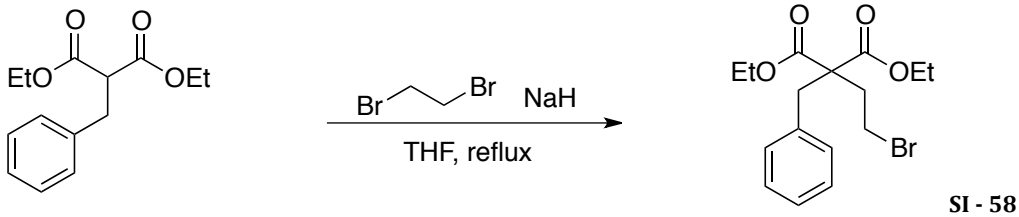
SI - 56

(SI-56): Diethyl (4-trifluoromethylbenzyl)malonate. Triethyl methanetricarboxylate (5.3 g, 22.7 mmol) was alkylated with 4-trifluoromethylbenzyl bromide (5.5 g, 23.2 mmol) following General Procedure G. The crude intermediate was then decarboxylated without further purification following General Procedure H. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide diethyl benzylmalonate SI-56 as a pale yellow oil (80% yield). All physical and spectroscopic data were in accordance with literature data.[10]



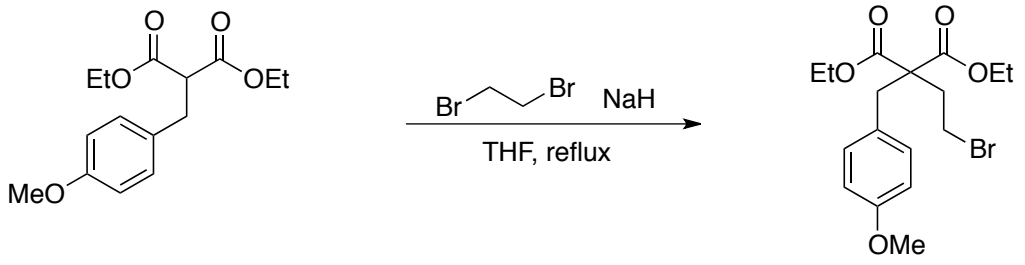
SI - 57

(SI-57): Diethyl (2-methylbenzyl)malonate. Triethyl methanetricarboxylate (8.6 g, 37.1 mmol) was alkylated with 2-methylbenzyl bromide (7.0 g, 37.8 mmol) following General Procedure G. The crude intermediate was then decarboxylated without further purification following General Procedure H. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide diethyl benzylmalonate SI-57 as a pale yellow oil (78% yield). All physical and spectroscopic data were in accordance with literature data.[12]



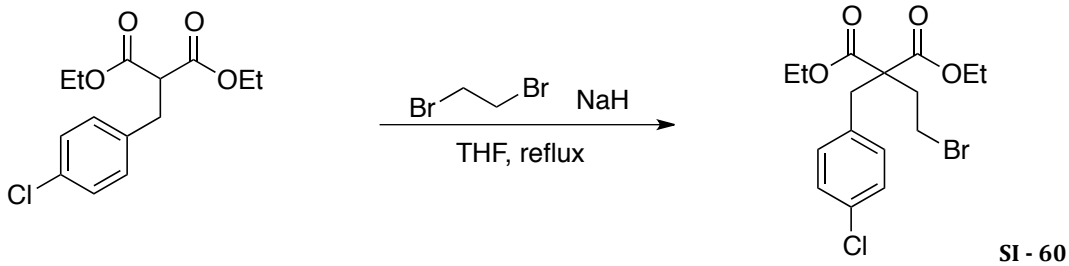
SI - 58

(SI-58): Diethyl benzyl(2-bromoethyl)malonate. Diethyl benzylmalonate (5.1 g, 20.4 mmol) was alkylated with dibromoethane (38.3 g, 204 mmol) following General Procedure I. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide bromide SI-58 as a clear oil (64% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.32-7.26 (m, 3H), 7.11 (d, J = 7.2 Hz, 2H), 4.24 (m, 4H), 3.41 (dd, J = 8.4 Hz, 8.4 Hz, 2H), 3.28 (s, 2H), 2.38 (dd, J = 8.4 Hz, 8.4 Hz, 2H), 1.29 (t, J = 7.1 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 170.24, 135.27, 129.83, 128.45, 127.23, 61.66, 61.64, 58.88, 39.22, 36.06, 27.23, 13.99. **IR** (Thin Film, cm^{-1}): 2980, 1729, 1449, 1261, 1186, 1094, 1035, 861, 701. **LRMS** (ESI): Calculated for $[C_{16}H_{21}BrO_4H]^+$ 357.07, found 357.15.



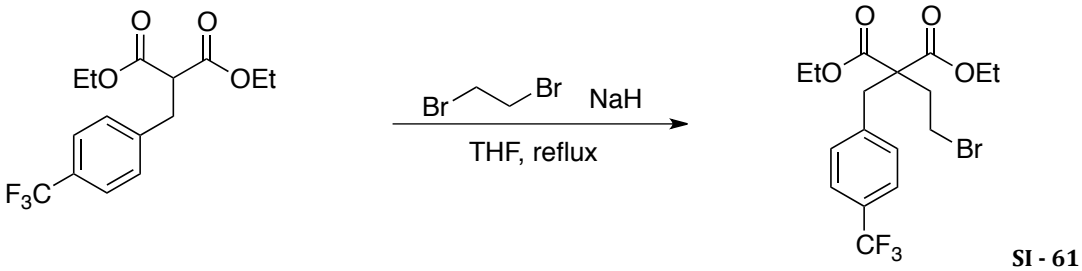
SI - 59

(SI-59): Diethyl (2-bromoethyl)(4-methoxybenzyl)malonate. Diethyl benzylmalonate SI-54 (6.1 g, 21.8 mmol) was alkylated with dibromoethane (40.9 g, 218 mmol) following General Procedure I. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide bromide SI-59 as a clear oil (52% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.02 (d, J = 8.6 Hz, 2H), 6.83 (d, J = 8.6 Hz, 2H), 4.23 (m, 4H), 3.80 (s, 3H), 3.40 (dd, J = 7.8 Hz, 7.2 Hz, 2H), 3.21 (s, 2H), 3.36 (dd, J = 7.8 Hz, 7.2 Hz, 2H), 1.29 (t, J = 7.1 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 170.32, 158.71, 130.84, 127.14, 113.84, 61.60, 58.98, 55.19, 55.16, 38.45, 36.07, 27.32, 14.01. **IR** (Thin Film, cm^{-1}): 2979, 1729, 1612, 1512, 1445, 1248, 1181, 1033, 845. **LRMS** (ESI): Calculated for $[C_{17}H_{23}BrO_4H]^+$ 387.08, found 387.01.



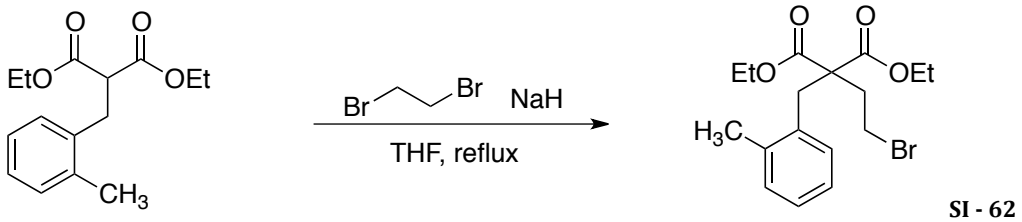
SI - 60

(SI-60): Diethyl (2-bromoethyl)(4-chlorobenzyl)malonate. Diethyl benzylmalonate SI-55 (2.5 g, 8.8 mmol) was alkylated with dibromoethane (16.5 g, 88 mmol) following General Procedure I. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide bromide SI-60 as a clear oil (48% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.27 (d, J = 8.4 Hz, 2H), 7.05 (d, J = 8.4 Hz, 2H), 4.23 (m, 4H), 3.39 (dd, J = 7.8 Hz, 7.8 Hz, 2H), 3.24 (s, 2H), 2.36 (dd, J = 7.8 Hz, 7.8 Hz, 2H), 1.28 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 170.03, 133.81, 133.21, 131.20, 128.62, 61.76, 58.80, 38.70, 36.24, 26.99, 13.99. **IR** (Thin Film, cm^{-1}): 2981, 1729, 1491, 1446, 1261, 1186, 1095, 1015, 861. **LRMS** (ESI): Calculated for $[C_{16}H_{20}BrClO_4H]^+$ 391.03, found 391.15.



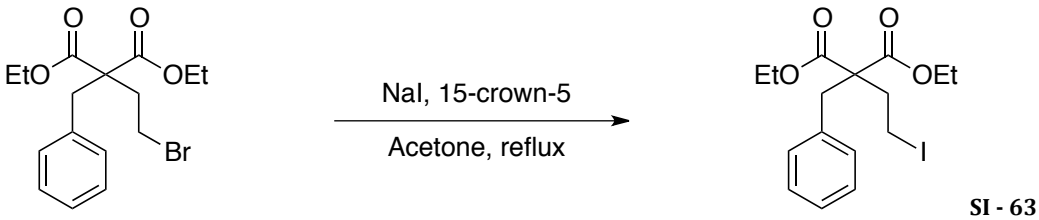
SI - 61

(SI-61): Diethyl (2-bromoethyl)(4-trifluoromethylbenzyl)malonate. Diethyl benzylmalonate SI-56 (1.5 g, 3.5 mmol) was alkylated with dibromoethane (1.6 g, 10.6 mmol) following General Procedure I. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide bromide SI-61 as a clear oil (62% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.56 (d, J = 8.4 Hz, 2H), 7.25 (d, J = 8.4 Hz), 4.22 (m, 4H), 3.40 (m, 2H), 3.32 (s, 2H), 2.37 (m, 2H), 1.27 (t, 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 169.90, 139.58, 130.26, 125.36, 125.33, 61.85, 58.76, 39.14, 36.37, 26.83, 13.95. **IR** (Thin Film, cm^{-1}): 2983, 1730, 1619, 1448, 1326, 1165, 1120, 1019, 857. **LRMS** (ESI): Calculated for $[C_{17}H_{20}BrF_3O_4H]^+$ 425.06, found 425.14.



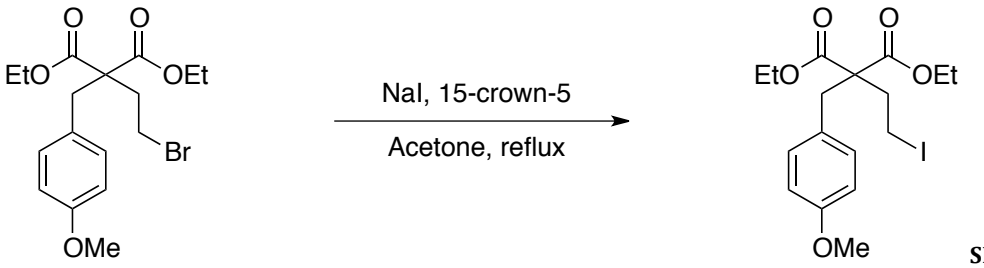
SI - 62

(SI-62): Diethyl (2-bromoethyl)(2-methylbenzyl)malonate. Diethyl benzylmalonate SI-57 (4.0 g, 15.1 mmol) was alkylated with dibromoethane (28.4 g, 151 mmol) following General Procedure I. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide bromide SI-62 as a clear oil (73% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.14 (m, 3H), 7.06 (d, J = 7.8 Hz, 1H), 4.21 (m, 4H), 3.39 (m, 2H), 3.35 (s, 2H), 2.42 (m, 2H), 2.34 (s, 3H), 1.26 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 170.57, 137.12, 134.03, 130.74, 129.82, 127.06, 125.90, 61.65, 58.98, 36.78, 35.64, 27.52, 19.97, 13.92. **IR** (Thin Film, cm^{-1}): 2980, 1729, 1447, 1245, 1217, 1159, 1054, 862, 742. **LRMS** (ESI): Calculated for $[C_{17}H_{23}BrO_4H]^+$ 371.09, found 371.12.



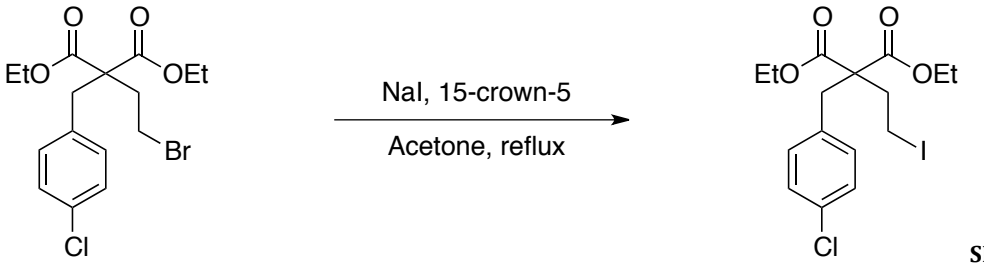
SI - 63

(SI-63): Diethyl benzyl(2-iodoethyl)malonate. Primary bromide SI-58 (3.0 g, 8.4 mmol) was iodinated with sodium iodide (3.8 g, 25.2 mmol) following General Procedure J. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide iodide SI-63 as a clear oil (85% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.29 (m, 3H), 7.10 (d, J = 6.6 Hz, 2H), 4.32 (m, 4H), 3.26 (s, 2H), 3.15 (m, 2H), 2.42 (m, 2H), 1.29 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 170.10, 135.31, 129.78, 128.47, 127.23, 61.62, 60.46, 38.82, 37.46, 14.02, -2.32. **IR** (Thin Film, cm^{-1}): 2980, 1728, 1611, 1512, 1248, 1181, 1030, 842. **LRMS** (ESI): Calculated for $[C_{16}H_{21}IO_4H]^+$ 405.06, found 405.20.



SI - 64

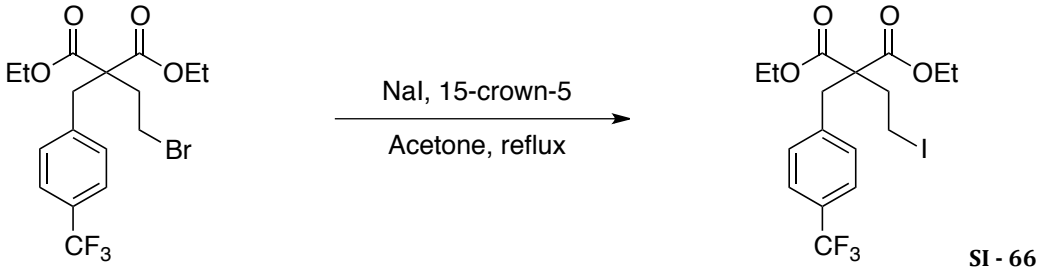
(SI-64): Diethyl (2-iodoethyl)(4-methoxybenzyl)malonate. Primary bromide SI-59 (1.8 g, 4.7 mmol) was iodinated with sodium iodide (2.1 g, 14.1 mmol) following General Procedure J. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide iodide SI-64 as a clear oil (45% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.00 (d, J = 9.0 Hz, 2H), 6.83 (d, J = 9.0 Hz, 2H), 4.22 (m, 4H), 3.80 (s, 3H), 3.19 (s, 2H), 3.14 (m, 2H), 2.40 (m, 2H), 1.28 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 170.17, 158.70, 130.78, 127.16, 113.85, 61.56, 60.54, 55.18, 38.04, 37.46, 14.04, -2.18. **IR** (Thin Film, cm^{-1}): 2980, 1769, 1728, 1611, 1512, 1445, 1248, 1180, 1029, 839. **LRMS** (ESI): Calculated for $[C_{17}H_{23}IO_5H]^+$ 435.07, found 435.07.



SI - 65

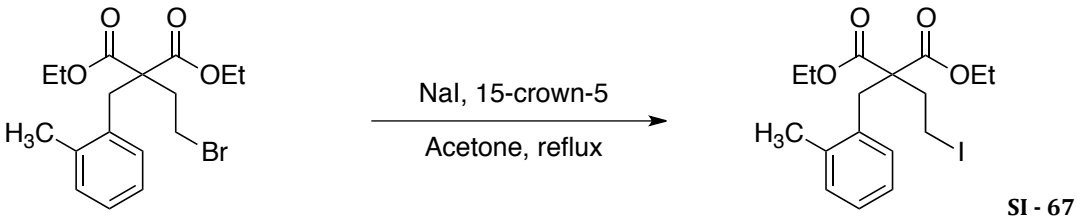
(SI-65): Diethyl (4-chlorobenzyl)(2-iodoethyl)malonate. Primary bromide SI-60 (1.0 g, 2.6 mmol) was iodinated with sodium iodide (1.2 g, 7.7 mmol) following General Procedure J. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide iodide SI-65 as a clear oil (58% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.26 (d, J = 6.0 Hz, 2H), 7.03 (d, J = 6.0 Hz, 2H), 4.21 (m, 4H), 3.21 (s, 2H), 3.12 (m, 2H), 2.39 (m, 2H), 1.27 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 169.85, 133.82, 133.17, 131.12, 128.60, 61.71,

60.34, 38.28, 37.64, 14.00, -2.67. **IR** (Thin Film, cm^{-1}): 2981, 1773, 1728, 1491, 1186, 1094, 1028, 859. **LRMS** (ESI): Calculated for $[C_{16}H_{20}ClIO_4H]^+$ 439.02, found 438.96.



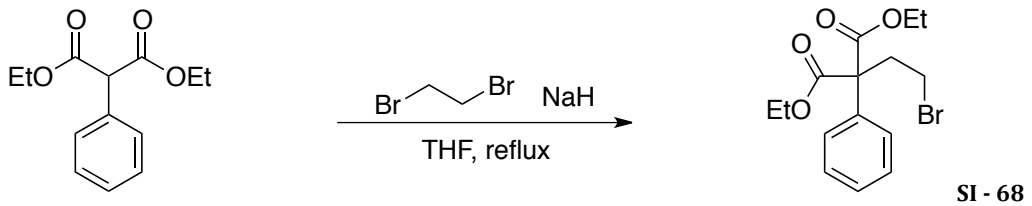
SI - 66

(SI-66): Diethyl (2-iodoethyl)(4-trifluoromethylbenzyl)malonate. Primary bromide SI-61 (1.5 g, 3.5 mmol) was iodinated with sodium iodide (1.6 g, 10.6 mmol) following General Procedure J. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide iodide SI-66 as a clear oil (62% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.56 (d, J = 8.4 Hz, 2H), 7.23 (d, J = 8.4 Hz, 2H), 4.22 (m, 4H), 3.30 (s, 2H), 3.13 (m, 2H), 2.41 (m, 2H), 1.26 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 169.73, 139.60, 130.20, 125.35, 125.32, 61.80, 60.31, 38.72, 37.79, 13.96, -2.92. **IR** (Thin Film, cm^{-1}): 3468, 2983, 1729, 1619, 1447, 1326, 1263, 1165, 1119, 1067, 1021, 858. **LRMS** (ESI): Calculated for $[C_{17}H_{20}F_3IO_4H]^+$ 473.05, found 473.17.



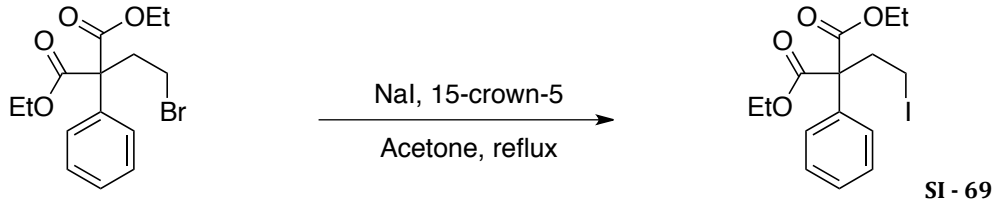
SI - 67

(SI-67): Diethyl (2-iodoethyl)(2-methylbenzyl)malonate. Primary bromide SI-62 (3.0 g, 8.1 mmol) was iodinated with sodium iodide (3.6 g, 24.2 mmol) following General Procedure J. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide iodide SI-67 as a clear oil (74% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.13 (m, 3H), 7.05 (d, J = 7.2 Hz, 1H), 4.21 (m, 4H), 3.33 (s, 2H), 3.14 (m, 2H), 2.47 (m, 2H), 2.33 (s, 3H), 1.25 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 170.41, 137.08, 134.04, 130.72, 129.84, 127.04, 125.88, 61.59, 60.42, 38.23, 35.29, 19.89, 13.92, -1.82. **IR** (Thin Film, cm^{-1}): 2979, 1729, 1447, 1237, 1194, 1035, 862, 747. **LRMS** (ESI): Calculated for $[C_{17}H_{23}IO_4H]^+$ 419.07, found 419.18.



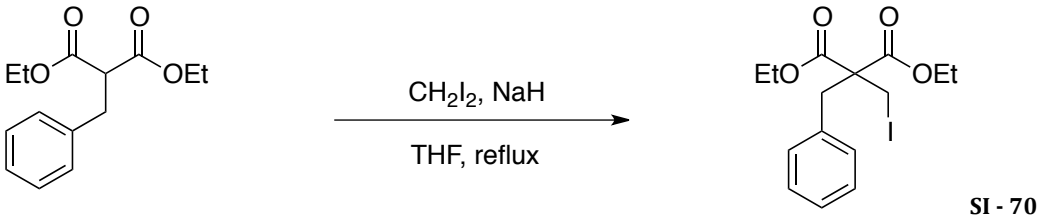
SI - 68

(SI-68): Diethyl (2-bromoethyl)phenylmalonate. Diethyl phenylmalonate (5.9 g, 25.0 mmol) was alkylated with dibromoethane (47.0 g, 250 mmol) following General Procedure I. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide bromide SI-68 as a clear oil (59% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.37 (m, 5H), 4.28 (m, 4H), 3.30 (m, 2H), 2.87 (m, 2H), 1.28 (t, J = 6.6 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 169.83, 135.87, 128.49, 127.90, 127.70, 62.96, 61.99, 39.54, 27.66, 13.96. **IR** (Thin Film, cm^{-1}): 2982, 1732, 1447, 1252, 1094, 1026, 860, 698. **LRMS** (ESI): Calculated for $[C_{15}H_{19}BrO_4H]^+$ 343.06, found 343.09.



SI - 69

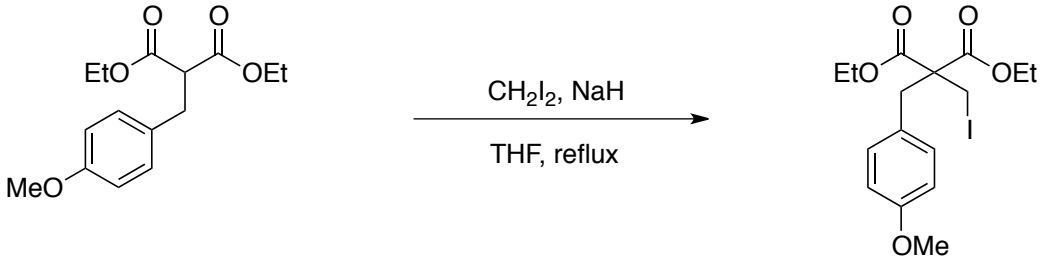
(SI-69): Diethyl (2-iodoethyl)phenylmalonate. Primary bromide SI-68 (3.0 g, 8.7 mmol) was iodinated with sodium iodide (3.9 g, 26.1 mmol) following General Procedure J. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide iodide SI-69 as a clear oil (65% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.35 (m, 5H), 4.27 (m, 4H), 3.07 (m, 2H), 2.90 (m, 2H), 1.28 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 169.67, 135.74, 128.45, 127.83, 127.71, 64.37, 61.92, 41.05, 13.94, -1.44. **IR** (Thin Film, cm^{-1}): 2979, 1775, 1727, 1448, 1371, 1214, 1162, 1024, 698. **LRMS** (ESI): Calculated for $[C_{15}H_{19}IO_4H]^+$ 391.04, found 391.07.



SI - 70

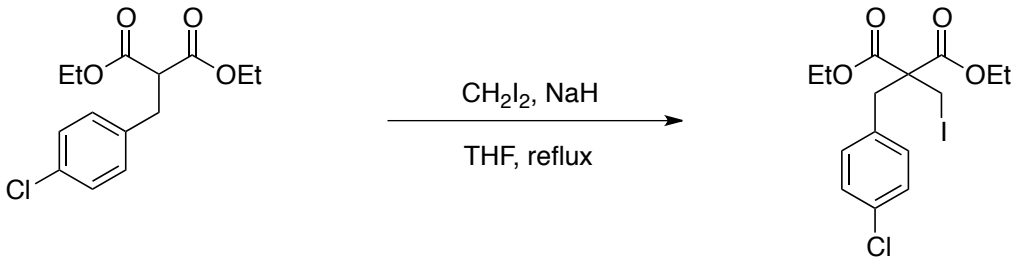
(SI-70): Diethyl benzyl(iodomethyl)malonate. Diethyl benzylmalonate (1.5 g, 5.8 mmol) was alkylated with diiodomethane (3.1 g, 11.6 mmol) following General Procedure K. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide iodide SI-70 as a clear oil (68% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.28 (m, 3H), 7.20

(m, 2H), 4.24 (m, 4H), 3.47 (s, 2H), 3.39 (s, 2H), 1.28 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 168.20, 135.18, 129.58, 128.50, 127.38, 62.06, 59.41, 37.97, 14.01, 7.08. **IR** (Thin Film, cm^{-1}): 2981, 1734, 1443, 1271, 1183, 1032, 862, 741, 702. **LRMS** (ESI): Calculated for $[C_{15}H_{19}IO_4H]^+$ 391.04, found 391.15.



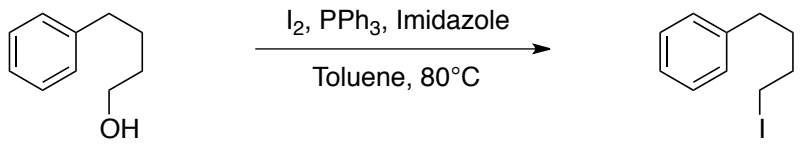
SI - 71

(SI-71): Diethyl (iodomethyl)(4-methoxybenzyl)malonate. Diethyl benzylmalonate (4.5 g, 16.2 mmol) was alkylated with diiodomethane (8.6 g, 32.3 mmol) following General Procedure K. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide iodide SI-71 as a clear oil (60% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.12 (d, J = 8.4 Hz, 2H), 6.83 (d, J = 8.4 Hz, 2H), 4.23 (m, 4H), 3.79 (s, 3H), 3.47 (s, 2H), 3.34 (s, 2H), 1.29 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 168.25, 158.85, 130.58, 127.01, 113.87, 61.98, 59.41, 55.13, 37.17, 14.01, 7.16. **IR** (Thin Film, cm^{-1}): 2981, 2835, 1732, 1612, 1512, 1453, 1249, 1182, 1104, 1032, 948, 575. **LRMS** (ESI): Calculated for $[C_{16}H_{21}IO_5H]^+$ 421.05, found 421.09.



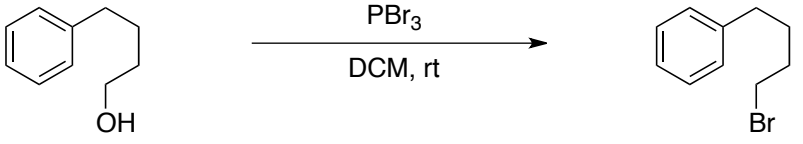
SI - 72

(SI-72): Diethyl (4-chlorobenzyl)(iodomethyl)malonate. Diethyl benzylmalonate (2.0 g, 7.0 mmol) was alkylated with diiodomethane (3.5 g, 14.0 mmol) following General Procedure K. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide iodide SI-72 as a clear oil (85% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.27 (d, J = 8.4 Hz, 2H), 7.15 (d, J = 8.4 Hz, 2H), 4.27 (m, 4H), 3.45 (s, 2H), 3.37 (s, 2H), 1.29 (t, J = 7.2 Hz). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 168.01, 133.71, 133.37, 130.96, 128.69, 62.19, 59.31, 37.45, 14.02, 6.81. **IR** (Thin Film, cm^{-1}): 2981, 1732, 1491, 1267, 1182, 1096, 1033, 851, 828, 576. **LRMS** (ESI): Calculated for $[C_{15}H_{18}ClIO_4H]^+$ 425.00, found 425.06.



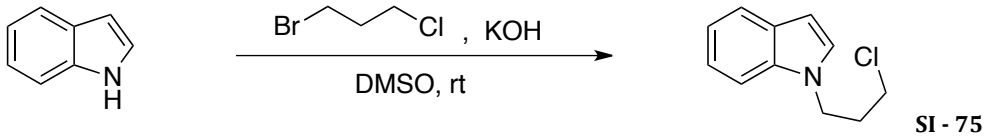
SI - 73

(SI-73): (4-iodobutyl)benzene. 4-Phenyl-1-butanol (2.0 g, 13.3 mmol) was iodinated with molecular iodine (3.6 g, 14.0 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide primary iodide SI-73 as a clear oil (52% Yield). All physical and spectroscopic data were in accordance with the literature data.[13]



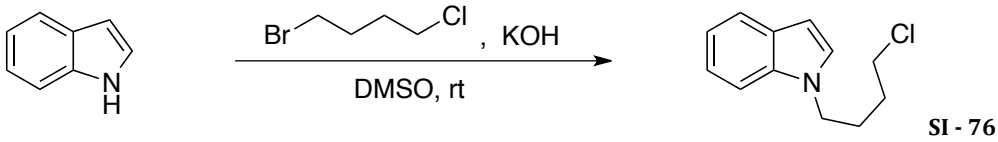
SI - 74

(SI-74): (4-bromobutyl)benzene. 4-Phenyl-1-Butanol (2.0 g, 13.3 mmol) was brominated with phosphorus tribromide (0.7 mL, 6.7 mmol) following General Procedure F. The crude product was purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide primary bromide SI-74 as a clear oil (57% Yield). All physical and spectroscopic data were in accordance with the literature data.[14]



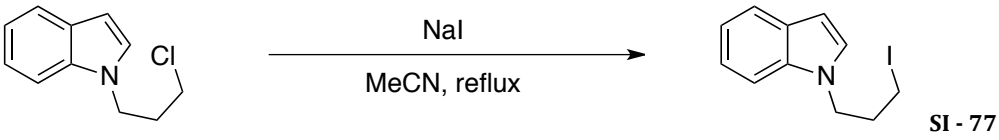
SI - 75

(SI-75): N-(3-chloropropyl)indole. Indole (3.0 g, 25.6 mmol) was alkylated with 1-bromo-3-chloropropane (12.1 g, 76.8 mmol) following General Procedure M. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide chloride SI-75 as a clear oil (72% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.66 (d, J = 7.8 Hz, 1H), 7.40 (d, J = 8.4 Hz, 1H), 7.24 (t, J = 7.2 Hz, 1H), 7.15 (m, 2H), 6.53 (d, J = 3.0 Hz, 1H), 4.38 (t, J = 6.6 Hz, 2H), 3.48 (t, J = 6.0 Hz, 2H), 2.30 (t, J = 6.6 Hz, 2H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 128.68, 128.03, 121.62, 121.07, 119.47, 109.22, 101.48, 42.83, 41.86, 32.59. **IR** (Thin Film, cm^{-1}): 2943, 1711, 1610, 1463, 1362, 1239, 1161, 740, 651. **LRMS** (ESI): Calculated for $[C_{11}H_{12}ClNH]^+$ 196.08, found 196.11.



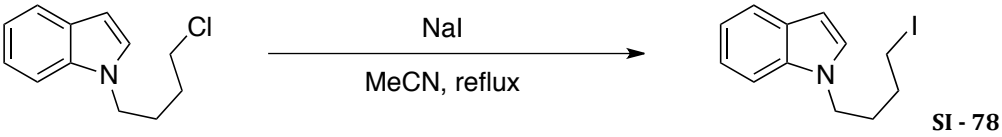
SI - 76

(SI-76): N-(4-chlorobutyl)indole. Indole (3.0 g, 25.6 mmol) was alkylated with 1-bromo-4-chlorobutane (13.3 g, 76.8 mmol) following General Procedure M. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide chloride SI-76 as a clear oil (61% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.66 (d, J = 7.8 Hz, 1H), 7.37 (d, J = 8.4 Hz, 1H), 7.24 (t, J = 7.8 Hz, 1H), 7.13 (m, 2H), 6.53 (d, J = 3.0 Hz, 1H), 4.20 (t, J = 6.6 Hz, 2H), 3.54 (t, J = 6.0 Hz, 2H), 2.05 (m, 2H), 1.80 (m, 2H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 135.88, 128.60, 127.59, 121.50, 121.04, 119.33, 109.22, 101.28, 45.61, 44.43, 29.84, 27.60. **IR** (Thin Film, cm^{-1}): 3420, 2955, 2360, 1637, 1462, 1314, 781, 739. **LRMS** (ESI): Calculated for $[C_{12}H_{14}ClNH]^+$ 208.09, found 208.14.



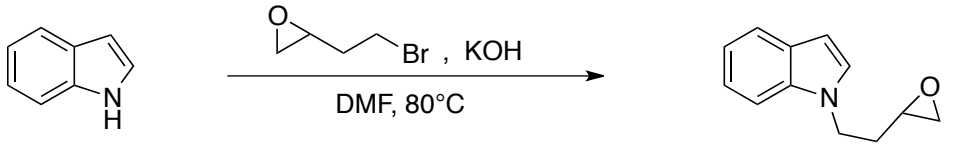
SI - 77

(SI-77): N-(3-iodopropyl)indole. Primary chloride SI-75 (2.5 g, 12.9 mmol) was iodinated with sodium iodide (8.7 g, 58.1 mmol) following General Procedure M. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide iodide SI-77 as a white powder (59% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.68 (d, J = 7.8 Hz, 1H), 7.42 (d, J = 8.4 Hz, 1H), 7.27 (m, 1H), 7.17 (m, 1H), 6.55 (d, J = 3.0 Hz, 1H), 4.31 (t, J = 6.0 Hz, 2H), 3.10 (t, J = 6.0 Hz, 2H), 2.34 (m, 2H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 135.84, 128.75, 128.00, 121.68, 121.14, 119.55, 109.34, 101.59, 46.10, 33.42, 3.24. **IR** (Thin Film, cm^{-1}): 3049, 2935, 1510, 1461, 1314, 1209, 1166, 745. **LRMS** (ESI): Calculated for $[C_{11}H_{12}INH]^+$ 286.01, found 286.09.



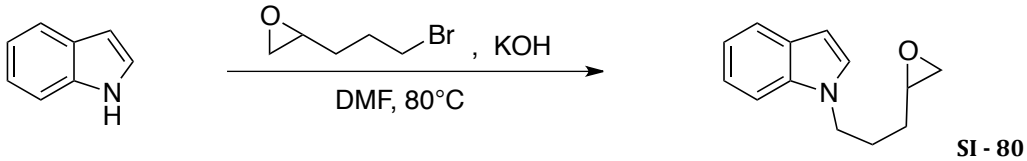
SI - 78

(SI-78): N-(4-iodobutyl)indole. Primary chloride SI-76 (2.5 g, 12.0 mmol) was iodinated with sodium iodide (8.1 g, 54.2 mmol) following General Procedure M. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide iodide SI-78 as a clear oil (66% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.67 (d, J = 8.4 Hz, 1H), 7.37 (d, J = 8.4 Hz, 1H), 7.25 (t, J = 8.4 Hz, 1H), 7.15 (t, J = 7.2 Hz, 1H), 7.11 (d, J = 3.0 Hz, 1H), 6.54 (t, J = 3.0 Hz, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 135.83, 128.57, 127.56, 121.49, 121.02, 119.32, 109.21, 101.29, 45.25, 31.08, 30.62, 5.76. **IR** (Thin Film, cm^{-1}): 3049, 2935, 1509, 1462, 1315, 1237, 1203, 1167, 741. **LRMS** (ESI): Calculated for $[C_{12}H_{14}INH]^+$ 300.03, found 300.11.



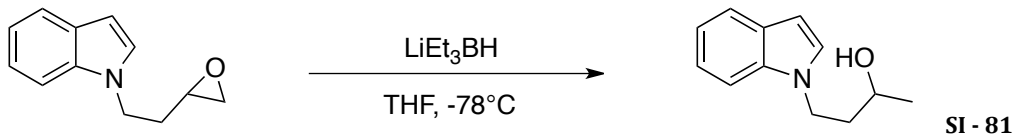
SI - 79

(SI-79): N-(3,4-epoxybutyl)indole. Indole (6.0 g, 51 mmol) was alkylated with (2-bromoethyl)oxirane (5.2 g, 56 mmol) following General Procedure L. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide epoxide SI-79 as a clear oil (45% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.66 (d, J = 7.6 Hz, 1H), 7.40 (d, 8.0 Hz, 1H), 7.25 (t, J = 7.6 Hz, 1H), 7.15 (m, 2H), 6.54 (d, J = 3.2 Hz, 1H), 3.45 (m, 2H), 2.90 (m, 1H), 2.76 (m, 1H), 2.42 (m, 1H), 2.22 (m, 1H), 1.92 (m, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 136.35, 128.58, 128.25, 121.81, 119.66, 109.27, 101.94. **IR** (Thin Film, cm^{-1}): 3053, 2924, 1511, 1462, 1316, 1255, 1201, 909, 850, 743. **LRMS** (ESI): Calculated for $[C_{12}H_{13}NOH]^+$ 174.13, found 174.03.



SI - 80

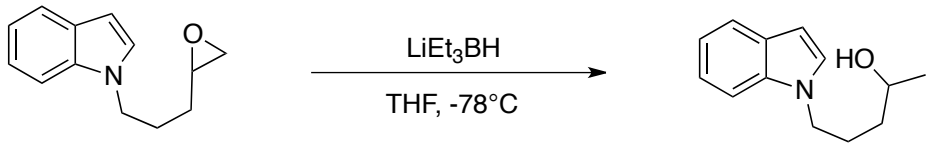
(SI-80): N-(4,5-epoxypentyl)indole. Indole (2.3 g, 20.0 mmol) was alkylated with (4-bromopropyl)oxirane (3.6 g, 22.0 mmol) following General Procedure L. The crude product was purified by flash chromatography using hexanes/ethyl acetate (7:1) to provide epoxide SI-80 as a clear oil (52% yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.65 (d, J = 7.8 Hz, 1H), 7.37 (d, J = 8.4 Hz, 1H), 7.23 (t, J = 6.6 Hz, 1H), 7.13 (m, 2H), 6.52 (d, J = 3.0 Hz, 1H), 4.23 (m, 2H), 2.93 (m, 1H), 2.76 (m, 1H), 2.48 (m, 1H), 2.06-2.02 (m, 2H), 1.75-1.68 (m, 1H), 1.52-1.46 (m, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 135.87, 128.59, 127.74, 121.43, 120.99, 119.27, 109.27, 101.14, 51.77, 46.77, 45.88, 29.67, 26.80. **IR** (Thin Film, cm^{-1}): 2938, 1509, 1462, 1315, 1183, 918, 837, 741. **LRMS** (ESI): Calculated for $[C_{13}H_{15}NOH]^+$ 202.13, found 202.12.



SI - 81

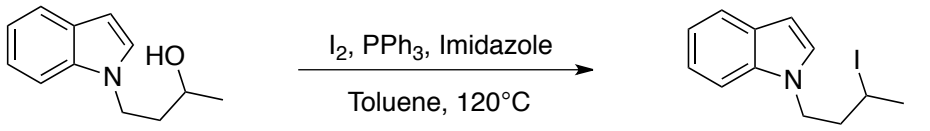
(SI-81): N-(3-hydroxybutyl)indole. Following General Procedure D, epoxide SI-79 (1.6 g, 8.9 mmol) was reduced with super hydride (1M in THF, 10.7 mL, 10.7 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (5:1) to provide secondary alcohol SI-81 as a clear oil (79% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.64 (d, J = 8.0 Hz, 1H),

7.38 (d, J = 8.0 Hz, 1H), 4.19 (m, 2H), 3.82 (m, 1H), 2.01 (m, 1H), 1.93 (m, 1H), 1.19 (d, J = 6.0 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 136.26, 128.61, 128.48, 121.64, 121.00, 119.51, 109.47, 101.56, 67.25, 60.38, 53.79, 20.44. **IR** (Thin Film, cm^{-1}): 3381, 2970, 1511, 1461, 1314, 1206, 1081, 938, 837, 741. **LRMS** (ESI): Calculated for $[C_{12}H_{15}NOH]^+$ 189.12, found 189.05.



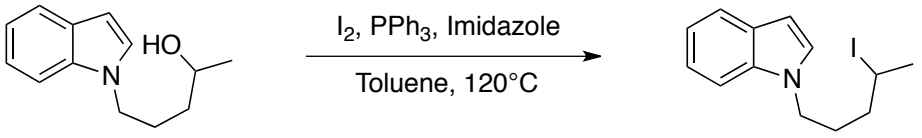
SI - 82

(SI-82): N-(4-hydroxypentyl)indole. Following General Procedure D, epoxide SI-80 (2.0 g, 9.9 mmol) was reduced with super hydride (1M in THF, 11.9 mL, 11.9 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide secondary alcohol SI-82 as a clear oil (70% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.65 (d, J = 7.8 Hz, 1H), 7.37 (d, J = 8.4 Hz, 1H), 7.23 (t, J = 6.6 Hz, 1H), 7.13 (m, 2H), 6.51 (d, J = 3.0 Hz, 1H), 4.19 (m, 2H), 3.82 (m, 1H), 2.01 (m, 1H), 1.92 (m, 1H), 1.19 (d, J = 6.0 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 143.12, 135.80, 128.63, 127.69, 121.23, 119.00, 109.07, 101.03, 67.75, 67.02, 46.10, 23.73. **IR** (Thin Film, cm^{-1}): 3388, 2965, 1702, 1464, 1368, 1133, 741. **LRMS** (ESI): Calculated for $[C_{13}H_{17}NOH]^+$ 204.14, found 204.23.



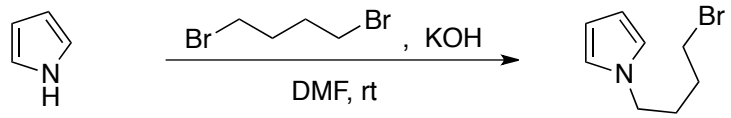
SI - 83

(SI-83): N-(3-iodobutyl)indole. Secondary alcohol SI-81 (1.21 g, 6.9 mmol) was iodinated with molecular iodine (1.84 g, 7.2 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide secondary iodide SI-83 as a clear oil (89% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.66 (d, J = 7.2 Hz, 1H), 7.42 (d, J = 8.4 Hz, 1H), 7.24 (t, J = 7.2 Hz, 1H), 7.14 (m, 2H), 6.52 (d, J = 3.0 Hz, 1H), 4.40 (m, 1H), 4.29 (m, 1H), 3.97 (m, 1H), 2.24 (m, 1H), 2.14 (m, 1H), 1.95 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 132.15, 132.09, 127.94, 121.63, 121.10, 119.49, 109.35, 101.47, 46.61, 42.61, 29.10, 26.28. **IR** (Thin Film, cm^{-1}): 3051, 2921, 1460, 1315, 1192, 1116, 741. **LRMS** (ESI): Calculated for $[C_{12}H_{14}INH]^+$ 300.03, found 300.05.



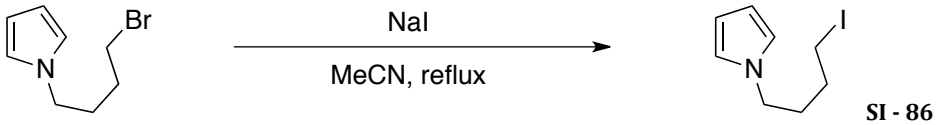
SI - 84

(SI-84): N-(4-iodopentyl)indole. Secondary alcohol SI-82 (1.0 g, 4.9 mmol) was iodinated with molecular iodine (1.3 g, 5.2 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (9:1) to provide secondary iodide SI-84 as a clear oil (45% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.67 (d, J = 7.8 Hz, 1H), 7.38 (d, J = 8.4 Hz, 1H), 7.25 (t, J = 8.4 Hz, 1H), 7.14 (t, J = 7.2 Hz, 1H), 7.12 (d, J = 3.0 Hz, 1H), 6.54 (d, J = 3.0 Hz, 1H), 4.17 (m, 2H), 4.15 (m, 1H), 2.11 (m, 1H), 1.99 (m, 1H), 1.91 (d, J = 7.2 Hz, 3H), 1.84 (m, 1H), 1.63 (m, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 135.87, 128.57, 127.56, 121.49, 121.01, 119.31, 109.24, 101.26, 45.40, 39.86, 30.54, 28.98, 28.92. **IR** (Thin Film, cm^{-1}): 3048, 2934, 1611, 1461, 1373, 1232, 1155, 1012, 742. **LRMS** (ESI): Calculated for $[C_{13}H_{16}INH]^+$ 314.04, found 314.14.



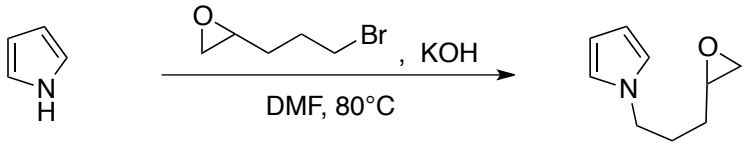
SI - 85

(SI-85): N-(4-bromobutyl)pyrrole. Pyrrole (3.0 g, 44.7 mmol) was alkylated with 1,4-dibromobutane (28.9 g, 134 mmol) following General Procedure M. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide bromide SI-85 as a clear oil (45% yield). All physical and spectroscopic data were in accordance with the literature data.[15]



SI - 86

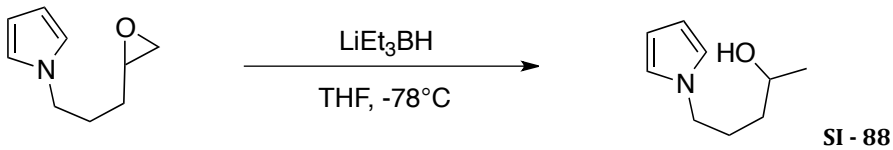
(SI-86): N-(4-iodobutyl)pyrrole. Primary chloride SI-85 (2.0 g, 9.9 mmol) was iodinated with sodium iodide (6.7 g, 44.6 mmol) following General Procedure M. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide iodide SI-86 as a clear oil (50% yield). All physical and spectroscopic data were in accordance with the literature data.[16]



SI - 87

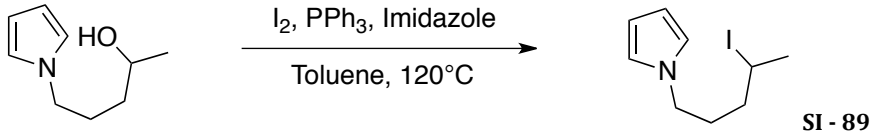
(SI-87): N-(4,5-epoxypentyl)pyrrole. Pyrrole (1.3 g, 20 mmol) was alkylated with (4-bromopropyl)oxirane (3.6 g, 22 mmol) following General Procedure L. The crude product was purified by flash chromatography using hexanes/ethyl acetate (7:1) to provide epoxide SI-87

as a clear oil (58% yield). All physical and spectroscopic data were in accordance with the literature data.[17]



SI - 88

(SI-88): N-(4-hydroxypentyl)pyrrole. Following General Procedure D, epoxide SI-87 (0.6 g, 4.0 mmol) was reduced with super hydride (1M in THF, 4.8 mL, 4.8 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide secondary alcohol SI-88 as a clear oil (70% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 6.68 (m, 2H), 6.16 (m, 2H), 3.93 (m, 2H), 3.82 (m, 1H), 1.96-1.91 (m, 1H), 1.86-1.82 (m, 1H), 1.45 (m, 2H), 1.21 (d, J = 6.0 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 120.44, 107.92, 67.69, 49.53, 36.17, 27.81, 23.69. **IR** (Thin Film, cm^{-1}): 3372, 2928, 1673, 1501, 1375, 1281, 1089, 725. **LRMS** (ESI): Calculated for $[C_9H_{15}NOH]^+$ 154.13, found 154.19.



SI - 89

(SI-89): N-(4-iodopentyl)pyrrole. Secondary alcohol SI-88 (0.5 g, 3.2 mmol) was iodinated with molecular iodine (0.86 g, 3.4 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (7:1) to provide secondary iodide SI-89 as a clear oil (57% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 6.67 (m, 2H), 6.17 (m, 2H), 4.15 (m, 1H), 3.94 (t, J = 7.2 Hz, 2H), 2.02 (m, 1H), 1.93 (d, J = 6.6 Hz, 3H), 1.89 (m, 1H), 1.79 (m, 1H), 1.61 (m, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 120.41, 108.12, 48.61, 39.68, 31.75, 29.02, 28.94. **IR** (Thin Film, cm^{-1}): 2924, 1500, 1444, 1375, 1280, 1141, 1088, 723, 617.

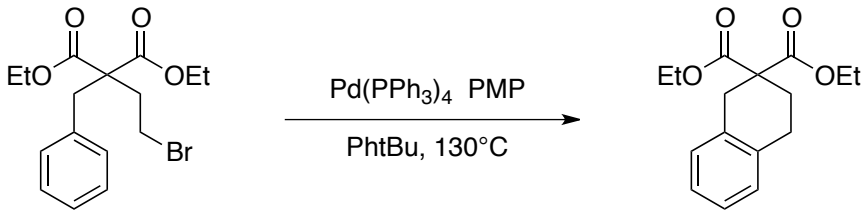
Palladium-Catalyzed Reactions

C-H Alkylation Procedure A:
To a one-dram vial in a glove box under argon atmosphere was added primary or secondary iodide (0.25 mmol, 1 equiv) and dissolved in 1,4-Dioxane (0.5 M). $Pd(PPh_3)_4$ (10 mol%) and K_3PO_4 (2 equiv) were then added. The reaction vial was removed from the glove box and heated in a pie block to 100°C, stirring for 6-24 hours. The reaction mixture was allowed to cool to ambient temperature, was quenched with 1N HCl and the aqueous layer was extracted with CH_2Cl_2. The combined organic layer was dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography.

C-H Alkylation Procedure B:
To a one-dram vial in a glove box was added primary iodide (0.25 mmol, 1 equiv) and dissolved in tert-butylbenzene (0.5 M). $Pd(PPh_3)_4$ (10 mol%) and K_3PO_4 (2 equiv) were then added. The reaction vial was removed from the glove box and heated in a pie block to 100°C, stirring for 24 hours. The reaction mixture was allowed to cool to ambient temperature, was quenched with 1N HCl and the aqueous layer was extracted with CH_2Cl_2. The combined organic layer was dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography.

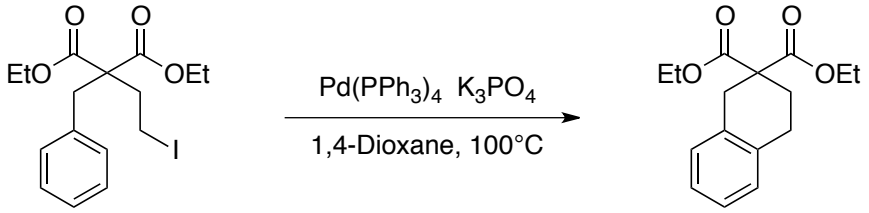
C-H Alkylation Procedure C:
To a one-dram vial in a glove box was added primary bromide (0.25 mmol, 1 equiv) and dissolved in tert-butylbenzene (0.5 M). $Pd(PPh_3)_4$ (10 mol%) and 1,2,2,6,6-pentamethylpiperidine (2 equiv) were then added. The reaction vial was removed from the glove box and heated in a pie block to 130°C, stirring for 48 hours. The reaction mixture was allowed to cool to ambient temperature, was quenched with 1N HCl and the aqueous layer was extracted with CH_2Cl_2. The combined organic layer was dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography.

C-H Alkylation Procedure D:
To a one-dram vial in a glove box was added primary or secondary bromide (0.25 mmol, 1 equiv) and dissolved in tert-butylbenzene (0.5 M). $Pd(PPh_3)_4$ (10 mol%) and K_3PO_4 (2 equiv) were then added. The reaction vial was removed from the glove box and heated in a pie block to 130°C, stirring for 48 hours. The reaction mixture was allowed to cool to ambient temperature, was quenched with 1N HCl and the aqueous layer was extracted with CH_2Cl_2. The combined organic layer was dried over $MgSO_4$, filtered, and concentrated. The crude product was purified by flash chromatography.



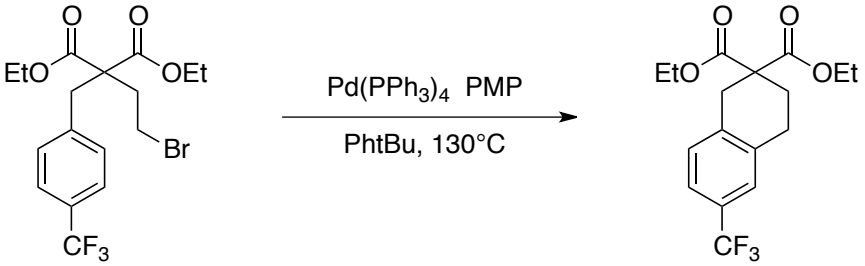
SI - 90

Diethyl benzyl(2-bromoethyl)malonate. Primary bromide SI-58 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure C. The crude product was purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide tetrahydronaphthalene product SI-90 as a clear oil (62.6 mg, 91% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.13 (m, 3H), 7.07 (m, 1H), 4.21 (q, J = 7.2 Hz, 4H), 3.29 (s, 2H), 2.86 (t, J = 6.6 Hz, 2H), 2.35 (t, J = 6.6 Hz, 2H), 1.25 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 171.34, 134.63, 133.59, 128.80, 128.57, 126.02, 125.93, 61.38, 53.61, 34.64, 28.08, 25.92, 13.99. **IR** (Thin Film, cm^{-1}): 2980, 1732, 1451, 1226, 1175, 1083, 861, 745. **LRMS** (ESI): Calculated for $[C_{16}H_{20}O_4H]^+$ 277.15, found 277.06.



SI - 90

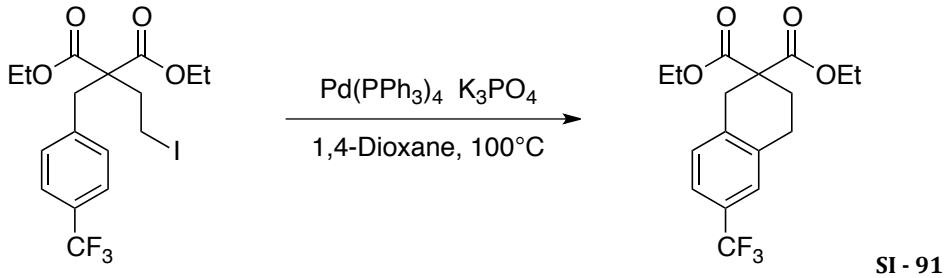
Diethyl benzyl(2-iodoethyl)malonate. Primary iodide SI-63 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide tetrahydronaphthalene product SI-90 as a clear oil (58.7 mg, 85% Yield).



SI - 91

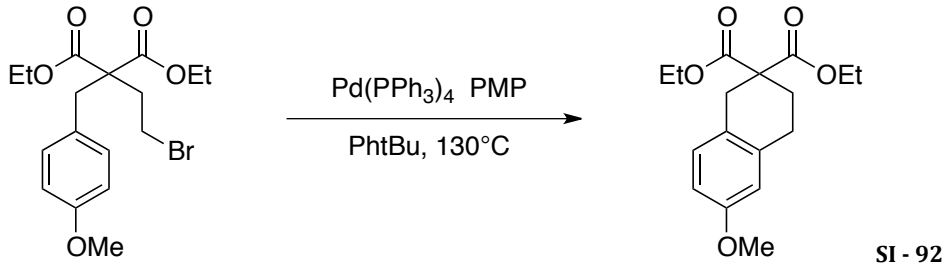
Diethyl (2-bromoethyl)(4-trifluoromethylbenzyl)malonate. Primary bromide SI-61 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure C. The crude product was purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide tetrahydronaphthalene product SI-91 as a clear oil (79.4 mg, 92% Yield). **^{1}H-NMR** (600 MHz,

$CDCl_3$): δ 7.39 (m, 1H), 7.28 (s, 1H), 7.25 (d, J = 8.4 Hz, 1H), 4.21 (q, J = 7.2 Hz, 4H), 3.32 (s, 2H), 2.90 (t, J = 6.6 Hz, 2H), 2.37 (t, J = 6.6 Hz, 2H), 1.26 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 170.99, 137.82, 135.35, 129.23, 129.04, 128.27, 125.50, 125.47, 125.45, 125.12, 123.32, 122.74, 122.71, 61.61, 53.36, 34.60, 27.78, 25.94, 13.99. **IR** (Thin Film, cm^{-1}): 2983, 1733, 1443, 1330, 1267, 1163, 1124, 1020, 859, 824. **LRMS** (ESI): Calculated for $[C_{17}H_{19}F_3O_4H]^+$ 345.33, found 345.19.



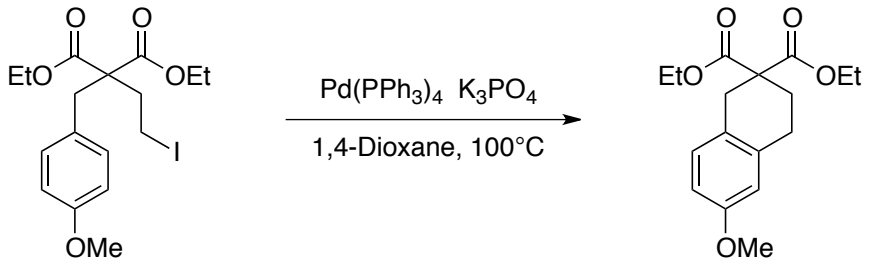
SI - 91

Diethyl (2-iodoethyl)(4-trifluoromethylbenzyl)malonate. Primary iodide SI-66 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide tetrahydronaphthalene product SI-91 as a clear oil (58.5 mg, 68% Yield).



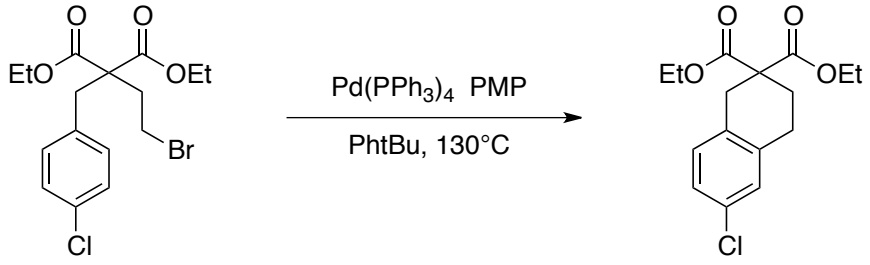
SI - 92

Diethyl (2-bromoethyl)(4-methoxybenzyl)malonate. Primary bromide SI-59 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure C. The crude product was purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide tetrahydronaphthalene product SI-92 as a clear oil (59.8 mg, 78% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.05 (d, J = 8.4 Hz, 1H), 6.72 (m, 1H), 6.61 (s, 1H), 4.20 (q, J = 7.2 Hz, 4H), 3.78 (s, 3H), 3.22 (s, 2H), 2.84 (s, J = 7.0 Hz, 2H), 2.32 (t, J = 7.0 Hz, 2H), 1.25 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 171.38, 157.80, 135.73, 129.69, 125.69, 113.11, 112.41, 61.37, 55.17, 53.77, 33.95, 28.03, 26.25, 14.02. **IR** (Thin Film, cm^{-1}): 2980, 1732, 1612, 1504, 1445, 1225, 1051, 858, 808. **LRMS** (ESI): Calculated for $[C_{17}H_{22}O_5H]^+$ 307.16, found 307.22.



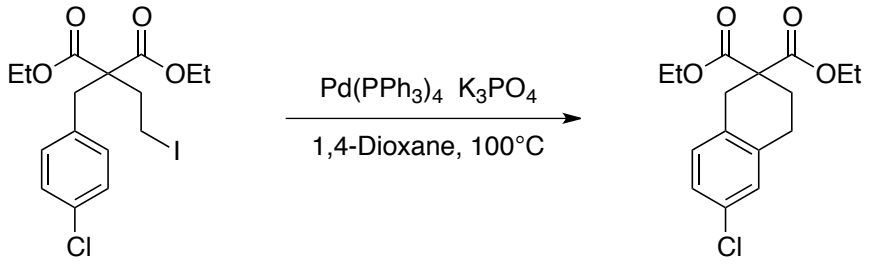
SI - 92

Diethyl (2-iodoethyl)(4-methoxybenzyl)malonate. Primary iodide SI-64 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide tetrahydronaphthalene product SI-92 as a clear oil (50.6 mg, 66% Yield).



SI - 93

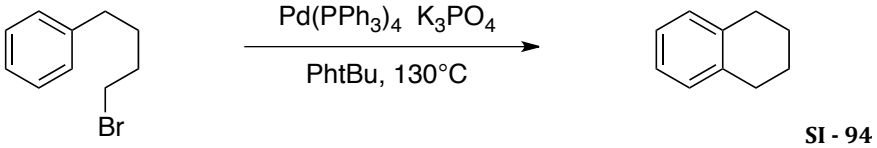
Diethyl (2-bromoethyl)(4-chlorobenzyl)malonate. Primary bromide SI-60 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure C. The crude product was purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide tetrahydronaphthalene product SI-93 as a clear oil (58.4 mg, 75% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.10 (m, 1H), 7.06 (m, 2H), 4.20 (q, J = 7.2 Hz, 4H), 3.23 (s, 2H), 2.83 (t, J = 6.6 Hz, 2H), 2.32 (t, J = 6.6 Hz, 2H), 1.25 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 171.08, 136.47, 132.12, 131.55, 130.08, 128.38, 126.17, 61.52, 53.46, 34.15, 27.73, 25.84, 14.00, 13.97. **IR** (Thin Film, cm^{-1}): 2981, 1732, 1486, 1263, 1180, 1087, 1019, 858, 809. **LRMS** (ESI): Calculated for $[C_{16}H_{19}ClO_4H]^+$ 311.11, found 311.08.



SI - 93

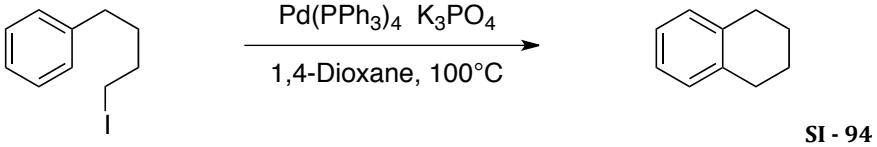
Diethyl (4-chlorobenzyl)(2-iodoethyl)malonate. Primary iodide SI-65 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash

chromatography using hexanes/ethyl acetate (40:1) to provide tetrahydronaphthalene product SI-93 as a clear oil (45.8 mg, 59% Yield).



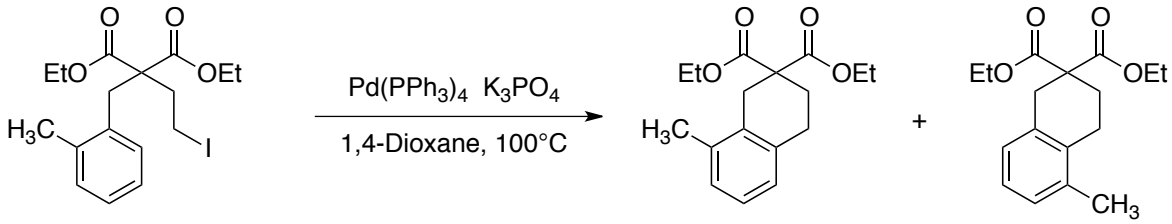
SI - 94

(4-bromobutyl)benzene. Primary bromide SI-74 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure D. The yield of the crude product was determined via gas chromatography using cyclooctane as internal standard (89% Yield). All physical and spectroscopic data were in accordance with the literature data.



SI - 94

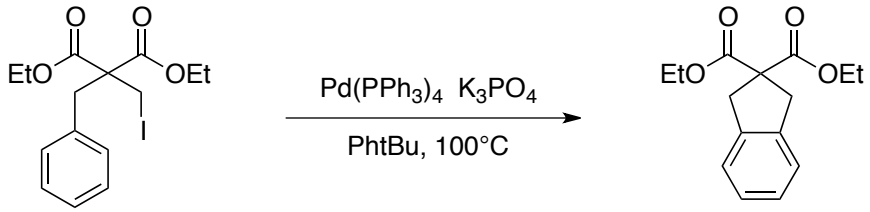
(4-iodobutyl)benzene. Primary iodide SI-73 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The yield of the crude product was determined via gas chromatography using cyclooctane as internal standard (51% Yield). All physical and spectroscopic data were in accordance with the literature data.



SI - 95A **SI - 95B**

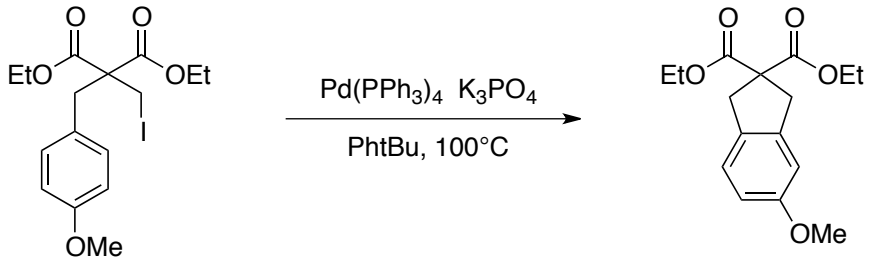
Diethyl (2-iodoethyl)(2-methylbenzyl)malonate. Primary iodide SI-67 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide a 50:50 mixture of tetrahydronaphthalene products SI-95A and SI-95B as a clear oil (54.4 mg, 75% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.04 (m, 2H), 7.01 (m, 3H), 6.94 (m, 1H), 4.20 (m, 8H), 3.29 (s, 2H), 3.15 (s, 2H), 2.83 (t, J = 6.6 Hz, 2H), 2.73 (t, J = 6.6 Hz, 2H), 2.37 (t, J = 6.6 Hz, 2H), 2.32 (t, J = 6.6 Hz, 2H), 2.30 (s, 3H), 2.21 (s, 3H), 1.25 (m, 12H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 171.58, 171.36, 136.28, 136.13, 134.62, 133.38, 133.06, 132.16, 127.60, 127.51, 126.64, 126.36, 125.65, 125.61, 61.43, 61.36, 53.87, 53.27, 35.18, 31.89, 28.18, 27.70, 26.32, 23.69, 19.59,

19.41, 14.00. **IR** (Thin Film, cm^{-1}): 2978, 2935, 1733, 1463, 1257, 1176, 1090, 1024, 862, 767. **LRMS** (ESI): Calculated for $[C_{17}H_{22}O_4H]^+$ 291.16, found 291.05.



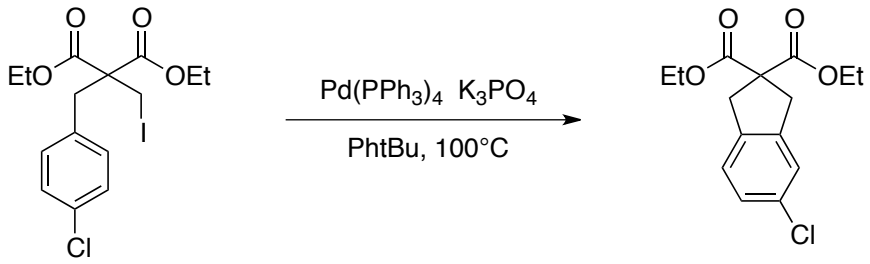
SI - 96

Diethyl benzyl(iodomethyl)malonate. Primary iodide SI-70 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure B. The yield of the crude product was determined by NMR spectroscopy using 1,3,5-trimethoxybenzene as internal standard (88% Yield). The crude product was then purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide indane product SI-96 as a clear oil. **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.21 (m, 2H), 7.18 (m, 2H), 4.23 (q, J = 6.6 Hz, 4H), 3.62 (s, 4H), 1.28 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 171.67, 139.98, 126.87, 124.18, 61.68, 60.30, 40.47, 14.02. **IR** (Thin Film, cm^{-1}): 2980, 2929, 1732, 1461, 1280, 1246, 1188, 1068, 861, 740. **LRMS** (ESI): Calculated for $[C_{15}H_{18}O_4H]^+$ 263.13, found 263.16.



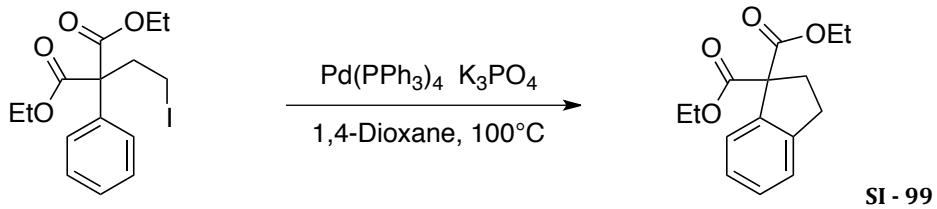
SI - 97

Diethyl (iodomethyl)(4-methoxybenzyl)malonate. Primary iodide SI-71 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure B. The yield of the crude product was determined by NMR spectroscopy using 1,3,5-trimethoxybenzene as internal standard (66% Yield). The crude product was then purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide indane product SI-97 as a clear oil. **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.10 (d, J = 7.8 Hz, 1H), 6.76 (s, 1H), 6.74 (m, 1H), 4.22 (q, J = 7.2 Hz, 4H), 3.79 (s, 3H), 3.58 (s, 2H), 3.54 (s, 2H), 1.28 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 171.67, 159.12, 141.47, 131.90, 124.74, 113.01, 109.50, 61.66, 60.79, 55.38, 40.61, 39.66, 14.02. **IR** (Thin Film, cm^{-1}): 3231, 3019, 1455, 1302, 1135, 1061, 972, 737, 700, 524. **LRMS** (ESI): Calculated for $[C_{16}H_{20}O_5H]^+$ 293.14, found 293.23.



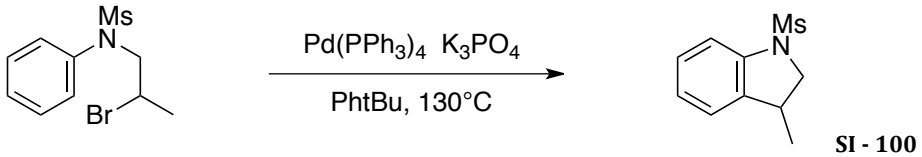
SI - 98

(4-chlorobenzyl)(iodomethyl)malonate. Primary iodide SI-72 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure B. The yield of the crude product was determined by NMR spectroscopy using 1,3,5-trimethoxybenzene as internal standard (74% Yield). The crude product was then purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide indane product SI-98 as a clear oil. **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.19 (s, 1H), 7.14 (m, 2H), 4.23 (q, J = 7.2 Hz, 4H), 3.58 (s, 2H), 3.56 (s, 2H), 1.28 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 171.28, 141.97, 138.47, 132.60, 127.10, 125.24, 124.43, 61.82, 40.22, 39.85, 13.99. **IR** (Thin Film, cm^{-1}): 2982, 1732, 1473, 1274, 1245, 1189, 1069, 962. **LRMS** (ESI): Calculated for $[C_{15}H_{17}ClO_4H]^+$ 297.09, found 297.13.



SI - 99

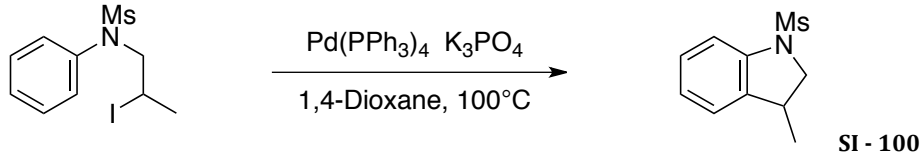
Diethyl (2-iodoethyl)phenylmalonate. Primary iodide SI-69 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide indane product SI-99 as a clear oil (54.7 mg, 83% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.59 (d, J = 7.2 Hz, 1H), 7.25 (m, 2H), 4.23 (m, 4H), 3.05 (t, J = 7.2 Hz, 2H), 2.72 (t, J = 7.2 Hz, 2H), 1.28 (t, J = 7.2 Hz, 6H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 170.77, 136.92, 128.13, 128.06, 127.38, 63.10, 61.40, 31.39, 28.85, 14.00, 13.95, 9.29. **IR** (Thin Film, cm^{-1}): 2980, 1731, 1238, 1025, 698, 509. **LRMS** (ESI): Calculated for $[C_{15}H_{18}O_4H]^+$ 263.13, found 263.17.



SI - 100

N-(2-bromopropyl)-n-phenylmethanesulfonamide. Secondary bromide SI-39 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure D. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide indoline product SI-

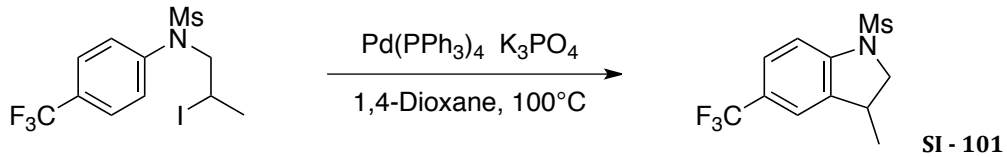
100 as a pale orange solid (28.5 mg, 54% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.42 (d, J = 7.8 Hz, 1H), 7.22 (m, 2H), 7.08 (t, J = 7.2 Hz, 2H), 4.16 (m, 1H), 3.50 (m, 2H), 2.90 (s, 3H), 1.38 (d, J = 6.0 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 141.47, 136.26, 128.14, 124.21, 123.75, 113.50, 58.03, 34.74, 34.27, 19.47. **IR** (Thin Film, cm^{-1}): 3249, 1617, 1520, 1479, 1327, 1147, 979, 916, 844. **LRMS** (ESI): Calculated for $[C_{10}H_{13}NO_2SH]^+$ 212.08, found 212.07.



SI - 100

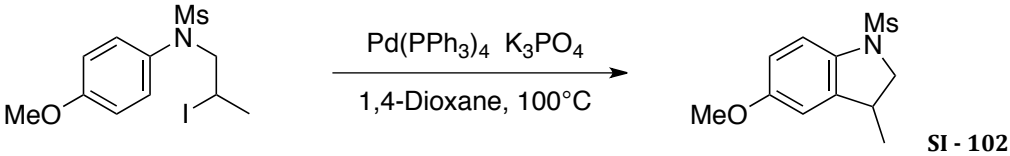
N-(2-iodopropyl)-n-phenylmethanesulfonamide. Secondary iodide SI-38 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide indoline product SI-100 as a pale orange solid (43.5 mg, 82% Yield).

Iodide SI-38 (338 mg, 1.0 mmol) was set up to react with $Pd(PPh_3)_4$ (116 mg, 0.1 mmol) and K_3PO_4 (424 mg, 2.0 mmol) in 1,4-dioxane (2.0 mL 0.5 M) following C-H Alklation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (10:1) to provide indoline product SI-100 as a pale orange solid (177 mg, 84% Yield).



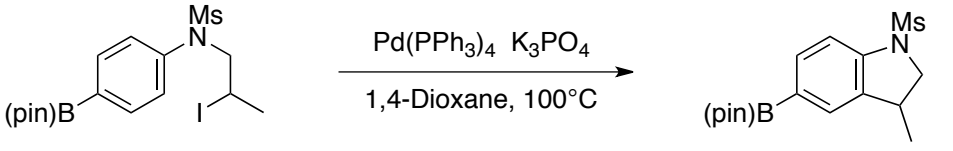
SI - 101

N-(2-iodopropyl)-n-(4-trifluoromethylphenyl)methanesulfonamide. Secondary iodide SI-41 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide indoline product SI-101 as a pale orange solid (48.8 mg, 70% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.50 (m, 2H), 7.44 (s, 1H), 4.23 (m, 1H), 3.59 (m, 1H), 3.54 (m, 1H), 2.95 (s, 3H), 1.42 (s, J = 7.2 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 144.43, 136.87, 126.01, 125.90, 125.87, 125.80, 125.07, 123.27, 121.45, 121.43, 112.98, 58.16, 35.08, 34.51, 19.43. **IR** (Thin Film, cm^{-1}): 2931, 1617, 1492, 1338, 1161, 1119, 985, 833, 770, 551. **LRMS** (ESI): Calculated for $[C_{11}H_{12}F_3NO_2SH]^+$ 280.06, found 280.11.



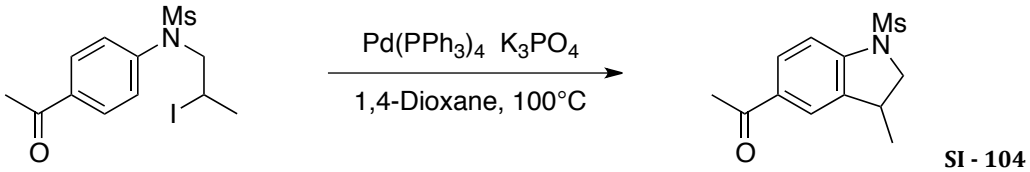
SI - 102

N-(2-iodopropyl)-n-(4-methoxyphenyl)methanesulfonamide. Secondary iodide SI-40 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide indoline product SI-85 as a pale orange solid (39.6 mg, 66% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.35 (d, J = 8.4 Hz, 1H), 6.78 (s, 1H), 6.76 (s, J = 8.4 Hz, 1H), 4.17 (m, 1H), 3.82 (s, 3H), 3.49 (m, 2H), 2.85 (s, 3H), 1.38 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 156.90, 138.10, 134.97, 114.77, 112.70, 110.54, 58.38, 55.71, 35.04, 33.76, 19.27. **IR** (Thin Film, cm^{-1}): 2964, 1596, 1485, 1344, 1232, 1159, 1032, 1159, 1032, 982, 850, 770. **LRMS** (ESI): Calculated for $[C_{11}H_{15}NO_3SH]^+$ 242.09, found 242.02.



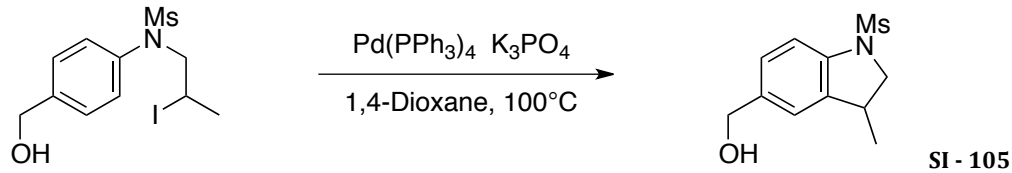
SI - 103

N-(2-iodopropyl)-n-(4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl) methanesulfonamide. Secondary iodide SI-42 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide indoline product SI-85 as a pale orange solid (60.4 mg, 72% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.72 (d, J = 7.8 Hz, 1H), 7.68 (s, 1H), 7.42 (d, J = 7.8 Hz, 1H), 4.17 (dd, J = 9.6 Hz, 9.0 Hz, 1H), 3.51 (m, 2H), 2.90 (s, 3H), 1.40 (d, J = 6.6 Hz, 3H), 1.37 (s, 12H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 135.56, 135.42, 130.54, 112.59, 83.81, 58.15, 34.53, 34.48, 24.89, 24.79, 19.53. **IR** (Thin Film, cm^{-1}): 2976, 1608, 1351, 1161, 1122, 963, 861, 772. **LRMS** (ESI): Calculated for $[C_{16}H_{24}BNO_4SNa]^+$ 360.23, found 360.44.



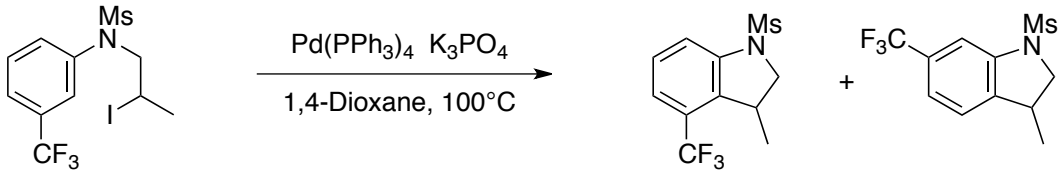
SI - 104

N-(4-acetylphenyl)-n-(2-iodopropyl)methanesulfonamide. Secondary iodide SI-51 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide indoline product SI-104 as a pale orange solid (48.5 mg, 77% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.86 (d, J = 8.4 Hz, 1H), 7.84 (s, 1H), 7.44 (d, J = 8.4 Hz, 1H), 4.23 (t, J = 9.0 Hz, 1H), 3.58 (dd, J = 9.6 Hz, 7.2 Hz, 1H), 3.52 (m, 1H), 2.96 (s, 3H), 2.59 (s, 3H), 1.42 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 196.65, 145.61, 136.71, 133.00, 129.93, 124.31, 112.31, 58.26, 35.27, 34.29, 26.49, 19.52. **IR** (Thin Film, cm^{-1}): 2965, 1675, 1604, 1483, 1351, 1258, 1161, 985, 771. **LRMS** (ESI): Calculated for $[C_{12}H_{15}NO_3SNa]^+$ 276.31, found 276.30.



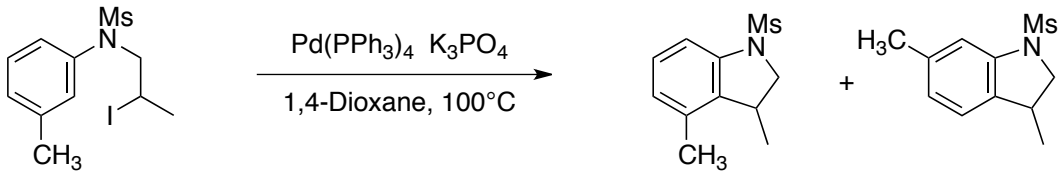
SI - 105

N-(4-(hydroxymethyl)phenyl)-n-(2-iodopropyl)methanesulfonamide. Secondary iodide SI-52 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide indoline product SI-105 as a pale orange solid (34.5 mg, 57% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.40 (d, J = 8.4 Hz, 1H), 7.25 (s, 1H), 7.22 (d, J = 8.4 Hz, 1H), 4.68 (s, 2H), 4.18 (t, J = 8.4 Hz, 1H), 3.51 (m, 2H), 2.89 (s, 3H), 1.68 (bs, 1H), 1.38 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 141.10, 136.79, 128.62, 127.21, 123.27, 113.48, 65.02, 58.24, 34.71, 34.23, 19.43. **IR** (Thin Film, cm^{-1}): 3522, 2928, 1485, 1343, 1159, 985, 771, 557. **LRMS** (ESI): Calculated for $[C_{11}H_{15}NO_3SNa]^+$ 264.80, found 264.35.



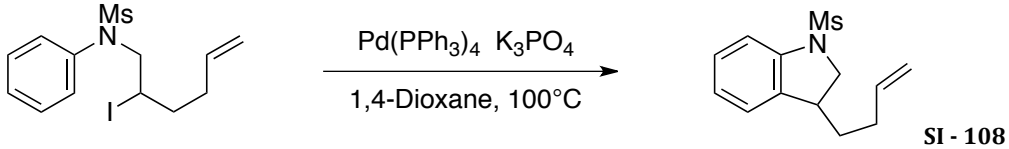
SI - 106A **SI - 106B**

N-(2-iodopropyl)-n-(3-trifluoromethylphenyl)methanesulfonamide. Secondary iodide SI-45 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide indoline products SI-106A and SI-106B as pale orange solids (56.7 mg, 81% Yield, 2.4:1 A:B). **SI-106A: ^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.63 (d, J = 8.4 Hz, 1H), 7.36 (t, J = 7.8 Hz), 7.31 (d, J = 7.2 Hz), 3.94 (dd, J = 10.2 Hz, 8.4 Hz, 1H), 3.84 (dd, J = 9.6 Hz, 1.8 Hz, 1H), 3.68 (m, 1H), 2.94 (s, 3H), 1.36 (d, J = 7.2 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 142.54, 134.38, 128.90, 127.36, 127.15, 124.87, 123.06, 120.81, 120.78, 120.75, 120.72, 116.49, 58.31, 34.72, 34.31, 21.09. **IR** (Thin Film, cm^{-1}): 2934, 1596, 1453, 1353, 1318, 1252, 1162, 1122, 997, 801, 549. **LRMS** (ESI): Calculated for $[C_{11}H_{12}F_3NO_2SH]^+$ 280.06, found 280.10. **SI-106B: ^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.65 (s, 1H), 7.35 (d, J = 7.8 Hz, 1H), 7.30 (d, J = 7.8 Hz, 1H), 4.22 (m, 1H), 3.58 (m, 1H), 3.54 (m, 1H), 2.95 (s, 3H), 1.41 (d, J = 7.2 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 142.04, 124.55, 120.85, 110.18, 58.04, 34.96, 34.69, 19.38. **IR** (Thin Film, cm^{-1}): 2933, 1432, 1351, 1321, 1276, 1162, 1123, 991, 824, 551. **LRMS** (ESI): Calculated for $[C_{11}H_{12}F_3NO_2SH]^+$ 280.06, found 280.11.



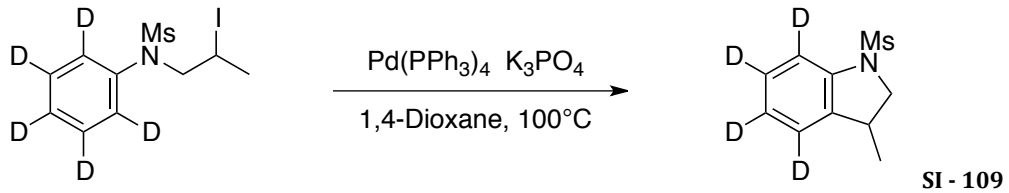
SI - 107A **SI - 107B**

N-(2-iodopropyl)-n-(3-tolyl)methanesulfonamide. Secondary iodide SI-46 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The yield of the crude product was determined by NMR spectroscopy using 1,3,5-trimethoxybenzene as internal standard (91% Yield, 2.0:1 A:B). The crude product was then purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide a mixture of indoline products SI-107A and SI-107B as a pale orange solid**.** **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.24 (s, 2H), 7.13 (t, J = 9.2 Hz, 1H), 7.07 (d, J = 7.6 Hz, 1H), 6.87 (t, J = 7.6 Hz, 2H), 4.15 (m, 1H), 3.92 (m, 1H), 3.74 (m, 1H), 3.47 (m, 3H), 2.89 (s, 3H), 2.88 (s, 3H), 2.36 (s, 3H), 2.32 (s, 3H), 1.34 (d, J = 6.4 Hz, 3H), 1.30 (d, J = 6.4 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 138.31, 134.68, 133.43, 128.25, 125.23, 124.46, 123.86, 114.19, 110.85, 58.36, 57.99, 34.42, 34.08, 21.57, 19.76, 19.59, 18.20. **IR** (Thin Film, cm^{-1}): 2964, 2927, 1610, 1455, 1346, 1246, 1159, 1077, 956, 771, 550. **LRMS** (ESI): Calculated for $[C_{11}H_{15}NO_2SH]^+$ 226.09, found 226.00.



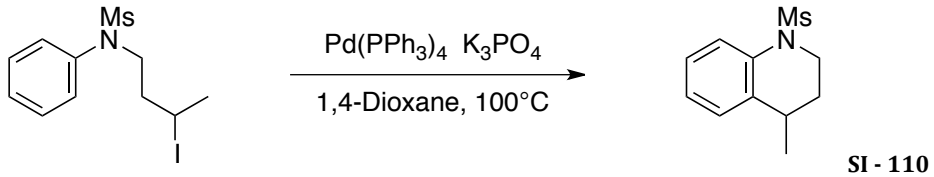
SI - 108

N-(2-iodohex-5-enyl)-n-phenylmethanesulfonamide. Secondary iodide SI-50 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (10:1) to provide indoline product SI-108 as a pale orange solid (50.1 mg, 80% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.42 (d, J = 8.4 Hz, 1H), 7.23 (m, 2H), 7.08 (t, J = 7.2 Hz, 1H), 5.85 (m, 1H), 5.09 (dd, J = 26.4 Hz, 10.2 Hz, 2H), 4.10 (t, J = 9.6 Hz, 1H), 3.65 (m, 1H), 3.41 (m, 1H), 2.90 (s, 3H), 2.20 (m, 2H), 1.96 (m, 1H), 1.69 (m, 1H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 141.63, 137.40, 134.88, 128.28, 124.63, 123.60, 115.61, 113.41, 56.18, 39.35, 34.23, 33.91, 31.13. **IR** (Thin Film, cm^{-1}): 2927, 1593, 1491, 1342, 1154, 962, 775, 697, 542. **LRMS** (ESI): Calculated for $[C_{13}H_{17}NO_2SNa]^+$ 274.33, found 274.38.



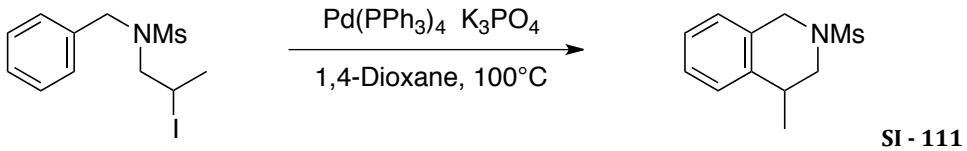
SI - 109

N-(2-iodopropyl)-n-(perdeuterophenyl)methanesulfonamide. Secondary iodide SI-47 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was then purified by flash chromatography using hexanes/ethyl acetate (40:1) to provide indoline product SI-109 as a pale orange solid**. ^{1}H-NMR** (600 MHz, $CDCl_3$): δ 4.16 (m, 1H), 3.50 (m, 2H), 2.89 (s, 3H), 1.38 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 141.40, 136.16, 127.79, 127.63, 127.47, 123.97, 123.81, 123.65, 123.41, 123.25, 123.09, 113.30, 113.13, 112.97, 58.04, 34.72, 34.23, 19.46. **IR** (Thin Film, cm^{-1}): 2965, 2874, 2283, 1582, 1454, 1399, 1346, 1228, 1159, 1078, 975, 768. **LRMS** (ESI): Calculated for $[C_{10}H_9D_4NO_2SH]^+$ 216.10, found 216.16.



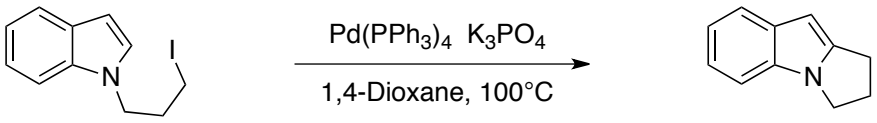
SI - 110

N-(3-iodobutyl)-n-phenylmethanesulfonamide. Secondary iodide SI-48 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide tetrahydroquinoline product SI-110 as a pale orange solid (32.0 mg, 57% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.73 (m, 1H), 7.27 (m, 1H), 7.21 (m, 1H), 7.14 (m, 1H), 3.85 (m, 2H), 3.00 (m, 1H), 2.93 (s, 3H), 2.12 (m, 1H), 1.39 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 136.28, 134.16, 128.53, 126.86, 124.59, 122.49, 44.16, 38.69, 30.69, 30.29, 22.23. **IR** (Thin Film, cm^{-1}): 2931, 2360, 1487, 1339, 1156, 957, 839, 773 **LRMS** (ESI): Calculated for $[C_{11}H_{15}NO_2SH]^+$ 226.09, found 226.09.



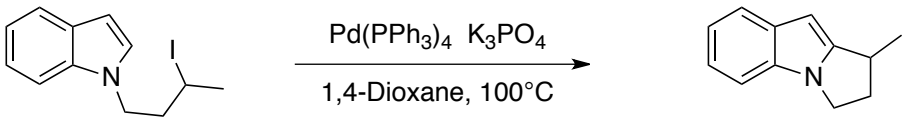
SI - 111

N-benzyl-n-(2-iodopropyl)methanesulfonamide. Secondary iodide SI-49 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide tetrahydroisoquinoline product SI-111 as a pale orange solid (34.2 mg, 61% Yield). **^{1}H-NMR** (600 MHz, $CDCl_3$): δ 7.28-7.22 (m, 3H), 7.11 (d, J = 7.2 Hz, 1H), 4.55 (d, J = 15.0 Hz, 1H), 4.38 (d, J = 15.0 Hz, 1H), 3.50 (m, 1H), 3.56 (m, 1H), 3.14 (m, 1H), 3.87 (s, 3H), 1.39 (d, J = 6.6 Hz, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$): δ 138.60, 131.09, 127.92, 127.15, 126.46, 126.24, 49.72, 47.62, 35.25, 32.93, 20.14. **IR** (Thin Film, cm^{-1}): 2965, 2928, 1454, 1329, 1156, 1037, 961, 808, 754, 519. **LRMS** (ESI): Calculated for $[C_{11}H_{15}NO_2SH]^+$ 226.09, found 226.09.



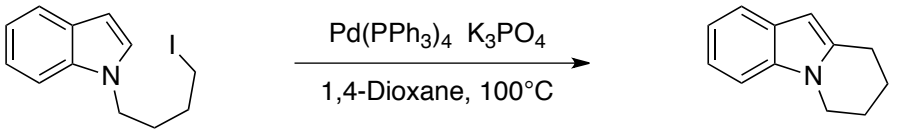
SI - 112

N-(3-iodopropyl)indole. Primary iodide SI-77 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The yield of the crude product was determined by NMR spectroscopy using 1,3,5-trimethoxybenzene as internal standard (51% Yield). All physical and spectroscopic data were in accordance with the literature data.[18]



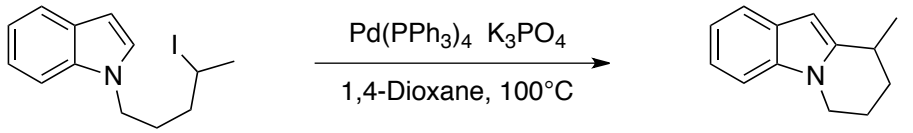
SI - 113

N-(3-iodobutyl)indane. Secondary iodide SI-83 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The yield of the crude product was determined by NMR spectroscopy using 1,3,5-trimethoxybenzene as internal standard (71% Yield). All physical and spectroscopic data were in accordance with the literature data.[19]



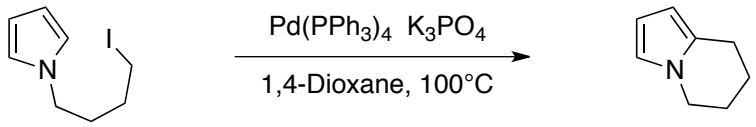
SI - 114

N-(4-iodobutyl)indane. Primary iodide SI-78 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The yield of the crude product was determined by NMR spectroscopy using 1,3,5-trimethoxybenzene as internal standard (70% Yield). All physical and spectroscopic data were in accordance with the literature data.[20]



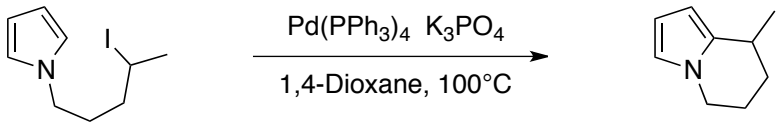
SI - 115

N-(4-iodopentyl)indane. Secondary iodide SI-84 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The yield of the crude product was determined by NMR spectroscopy using 1,3,5-trimethoxybenzene as internal standard (90% Yield). All physical and spectroscopic data were in accordance with the literature data.[19]



SI - 116

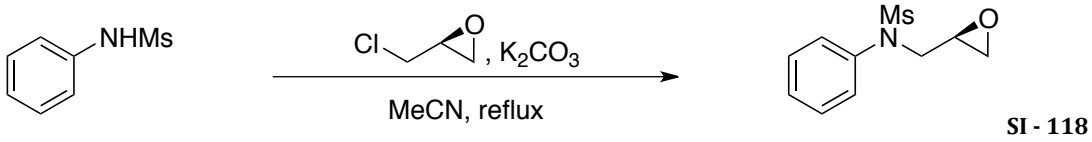
N-(4-iodobutyl)pyrrole. Primary iodide SI-86 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The yield of the crude product was determined by NMR spectroscopy using 1,3,5-trimethoxybenzene as internal standard (64% Yield). All physical and spectroscopic data were in accordance with the literature data.[21]



SI - 117

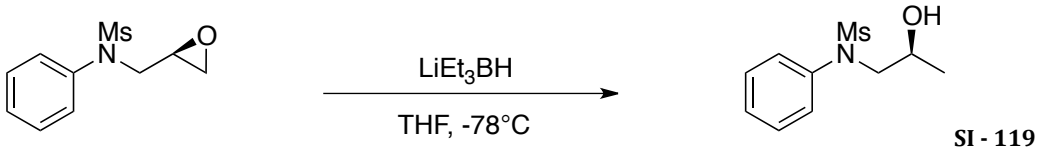
N-(4-iodopentyl)pyrrole. Secondary iodide SI-89 was made to react with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The yield of the crude product was determined by NMR spectroscopy using 1,3,5-trimethoxybenzene as internal standard (95% Yield). All physical and spectroscopic data were in accordance with the literature data.[16]

Stereochemical Experiments



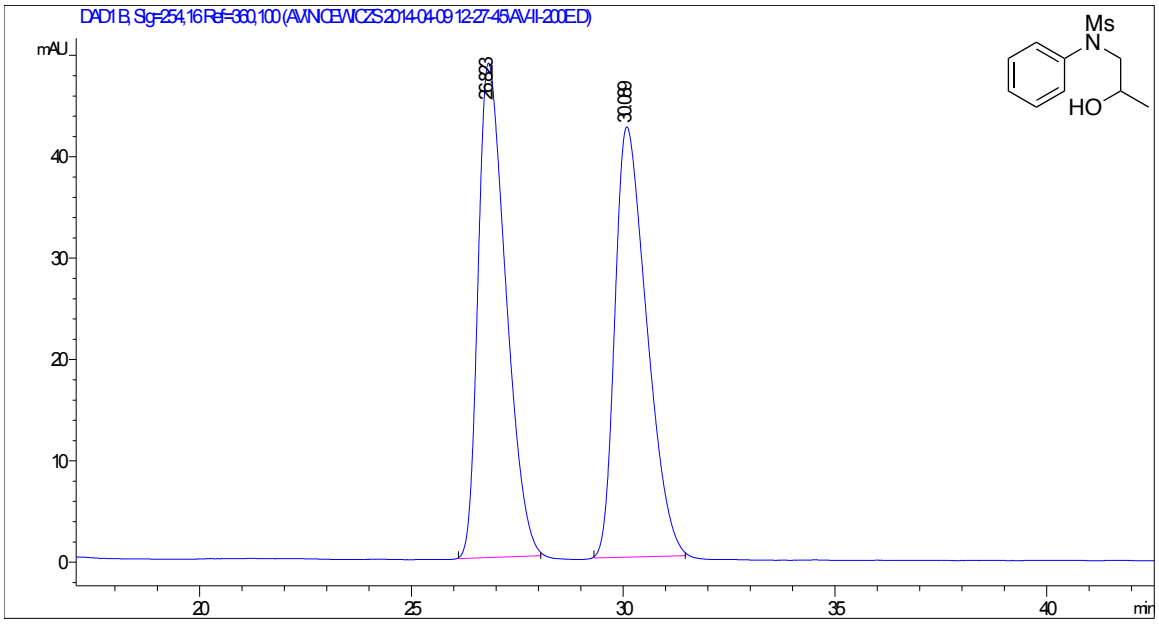
SI - 118

(SI-118): N-((S)-2,3-epoxypropyl)-n-phenylmethanesulfonamide. Following General Procedure B, methanesulfonamide SI-1 (3.0 g, 17.5 mmol) was alkylated with S-(+)-epichlorohydrin (6.5 g, 70 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (3:1) to provide epoxide SI-118 as a white solid (61% Yield).



SI - 119

(SI-119): N-((S)-2-hydroxypropyl)-n-phenylmethanesulfonamide. Following General Procedure D, epoxide SI-118 (2.45 g, 10.7 mmol) was reduced with super hydride (1M in THF, 12.9 mL, 12.9 mmol). The crude product was purified by flash chromatography using hexanes/ethyl acetate (1:1) to provide secondary alcohol SI-119 as a white solid (58% Yield). **Chiral HPLC** (Column IC, 75:25 A1:B2)**:** ee = 88.3%.



#	Time	Area	Height	Width	Area %	Symmetry
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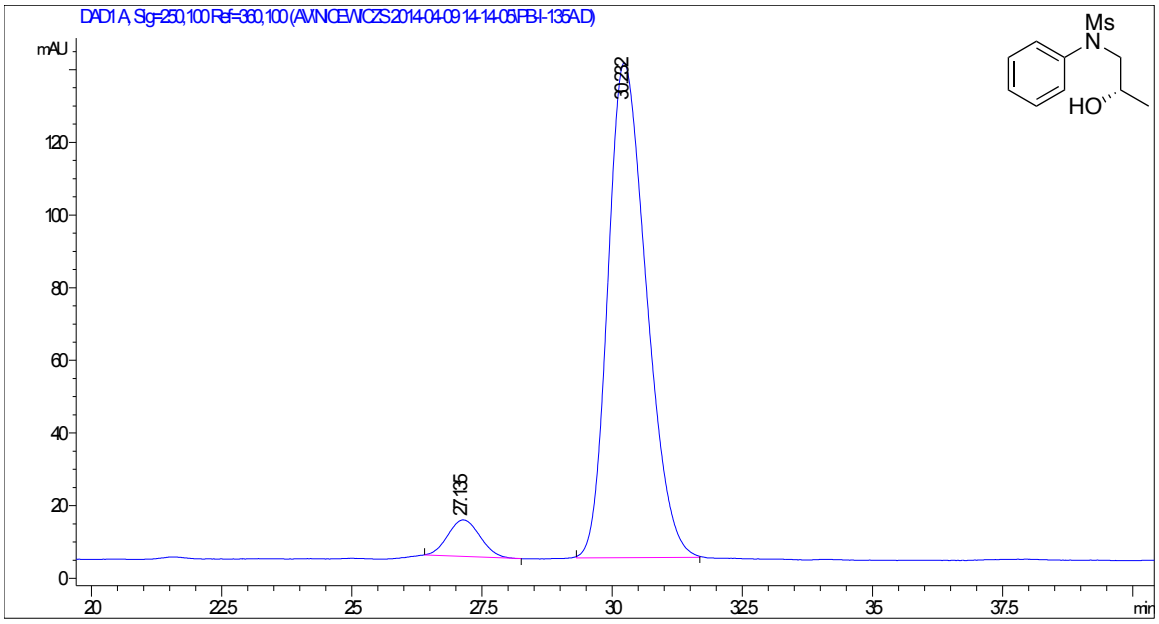
2	30.089	2212.3	42.5	0.7798	49.87	0.572



#	Time	Area	Height	Width	Area %	Symmetry
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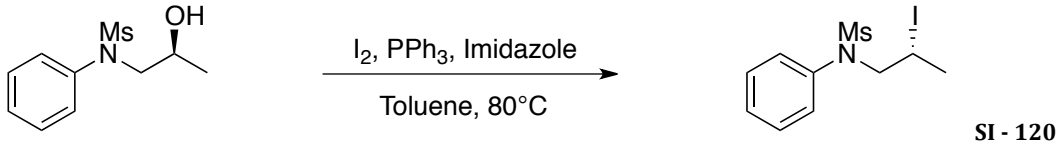
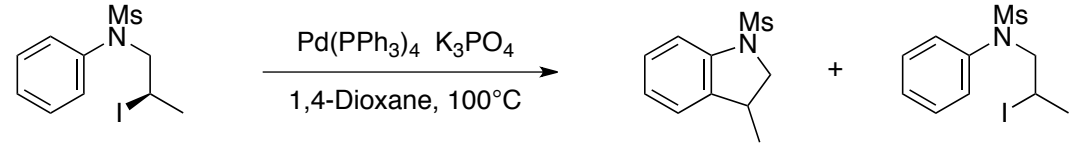


SI - 120

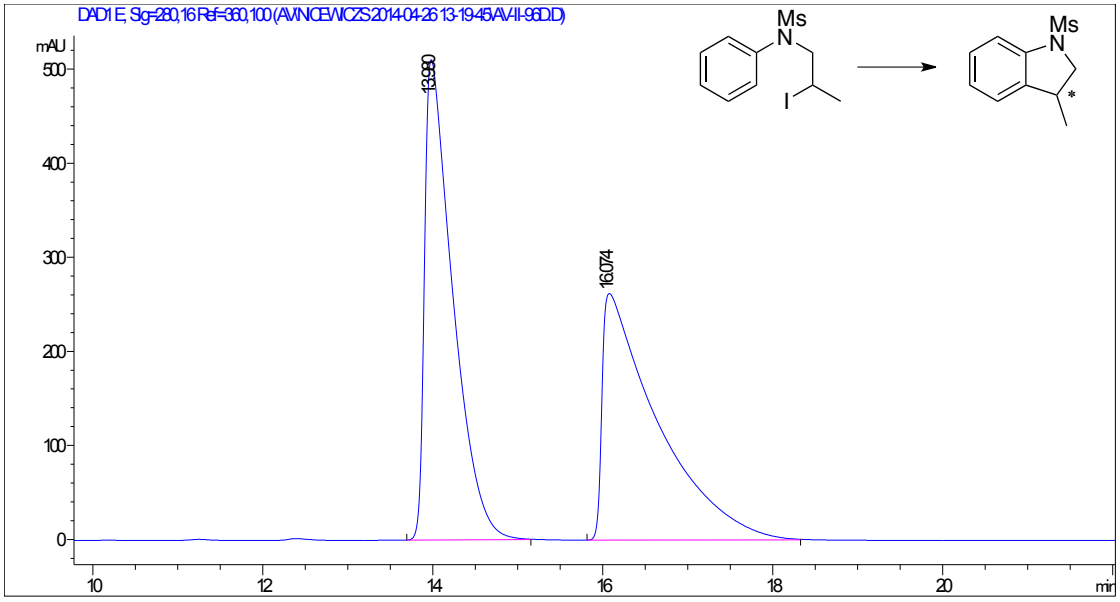
(SI-120): N-((R)-2-iodopropyl)-n-phenylmethanesulfonamide. Secondary alcohol SI-119 (1.4 g, 6.2 mmol) was iodinated with molecular iodine (1.7 g, 6.5 mmol) following General Procedure E. The crude product was purified by flash chromatography using hexanes/ethyl acetate (3:1) to provide secondary iodide SI-120 as a white solid (52% Yield). **Optical Rotation:** α_D^{20} = + 0.4196.



α_D^{20} = + 0.4196 ee = 0% α_D^{20} = - 0.0054

Secondary iodide SI-120 was made to react incompletely with $Pd(PPh_3)_4$ following C-H Alkylation Procedure A. The crude product was purified by flash chromatography using hexanes/ethyl acetate (20:1) to provide indoline cyclization product and unreacted starting material. The enantiomeric excess of the indoline product was determined to be 0% by chiral

HPLC analysis using 90:10 A1:B2 mobile phase and column IA. The recovered starting material was also determined to have racemized by measurement of its optical rotation (α_D^{20} = - 0.0054). By contrast, stereochemistry of the starting material was retained when iodide SI-120 was treated with potassium iodide in the absence of palladium (α_D^{20} = + 0.4226).



#	Time	Area	Height	Width	Area %	Symmetry
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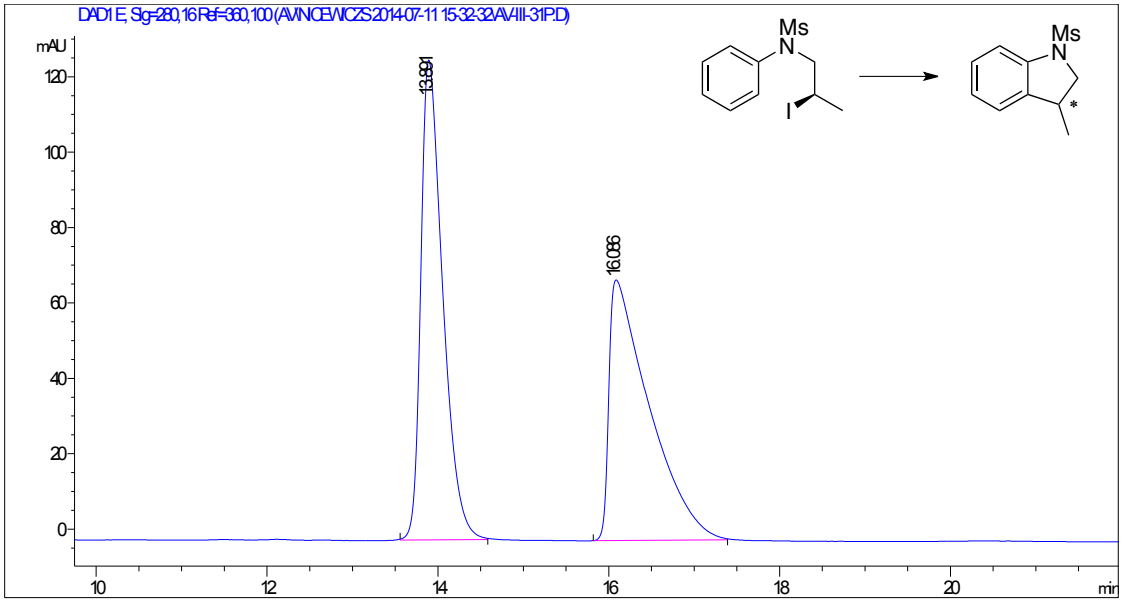
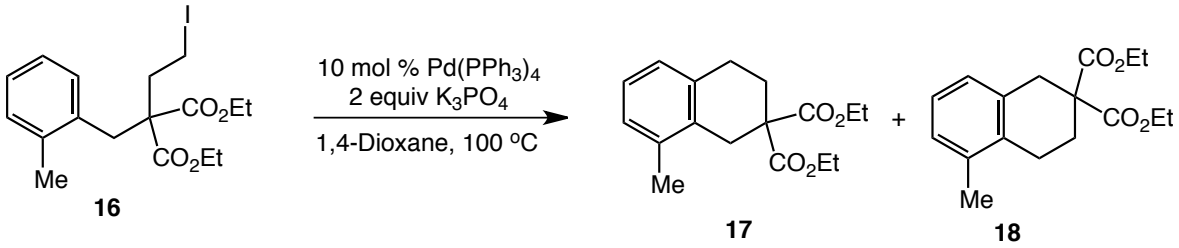
2	16.074	11839.4	262.2	0.6029	49.986	0.133



#	Time	Area	Height	Width	Area %	Symmetry
1	13.891	2270.8	127.4	0.27	50.05	0.535
2	16.086	2266.3	69.2	0.4483	49.95	0.2

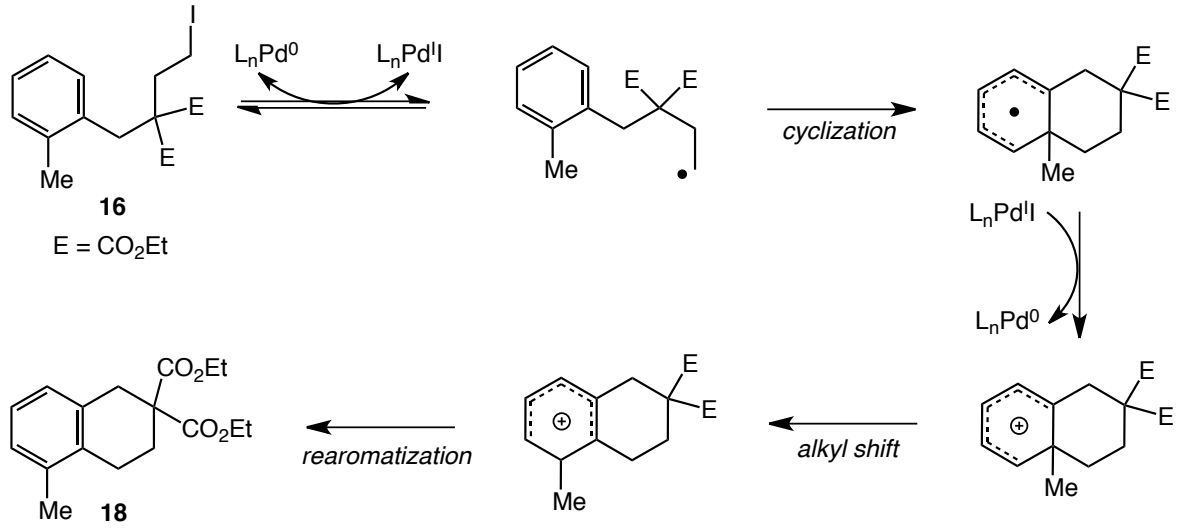
Proposed Rearrangement Mechanism

The following mechanism is proposed as an explanation for the formation of two products in equal quantities by *ortho*-substituted aromatic substrate **16**. Upon activation of the alkyl iodide, radical addition occurs irreversibly at both available sites with no regioselectivity. In each case, Pd^{I} oxidizes the alkyl radical to a cationic species. While one regioisomer can rearomatize upon oxidation, forming the expected product **17**, the intermediate forming a quaternary carbon center is not able to. This intermediate instead undergoes a 1,2-methyl shift, forming a cation that is then capable of rearomatization, forming the observed rearrangement product, **18**.



*Mechanism accounting for product **18**:*

75% combined yield, **17:18** = 50:50



References

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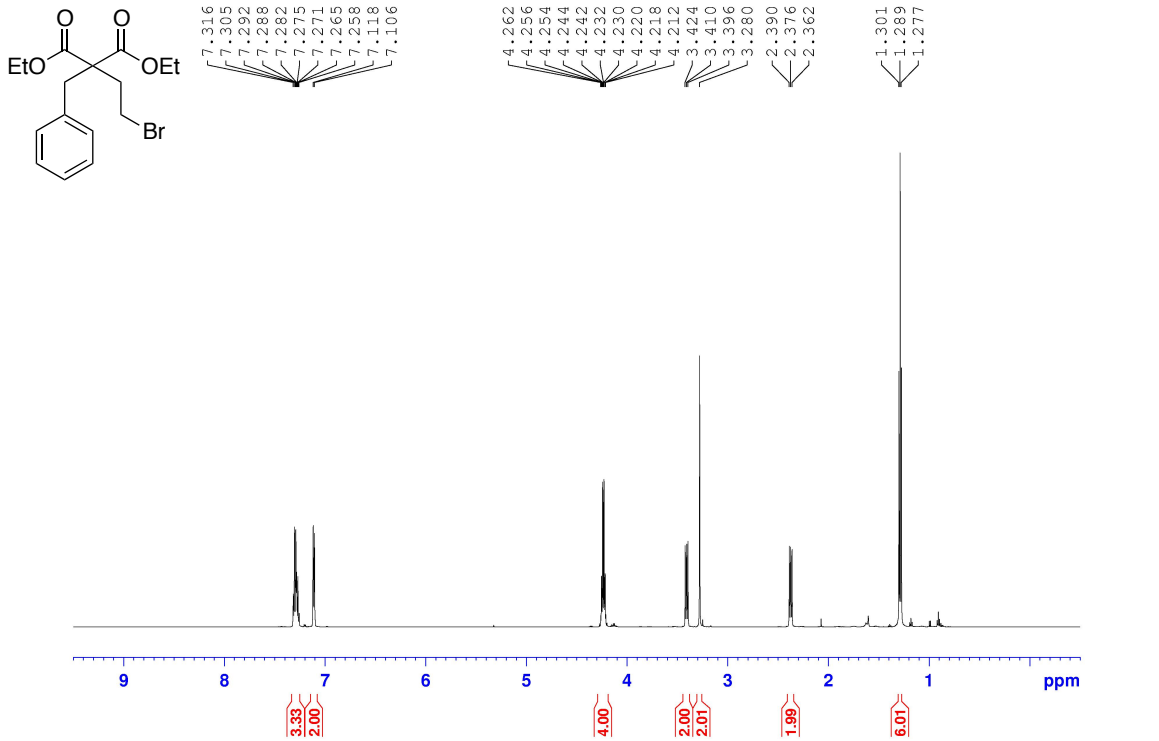
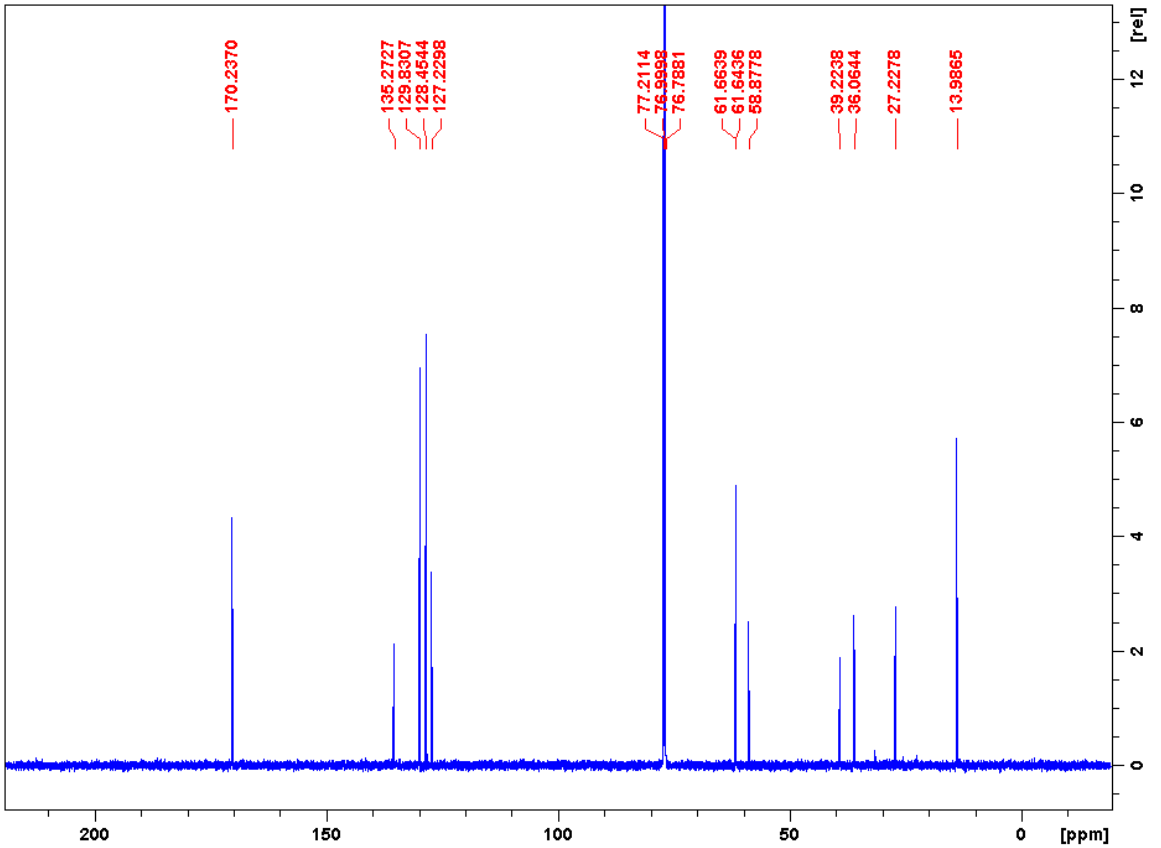
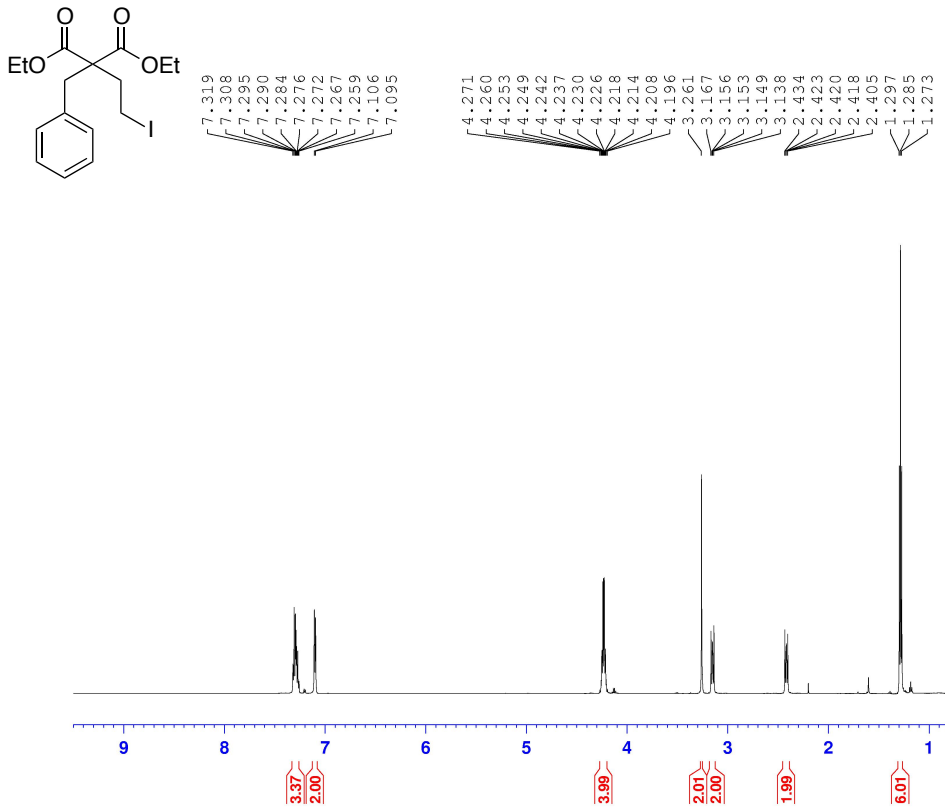
^{1}H and ^{13}C NMR Spectra



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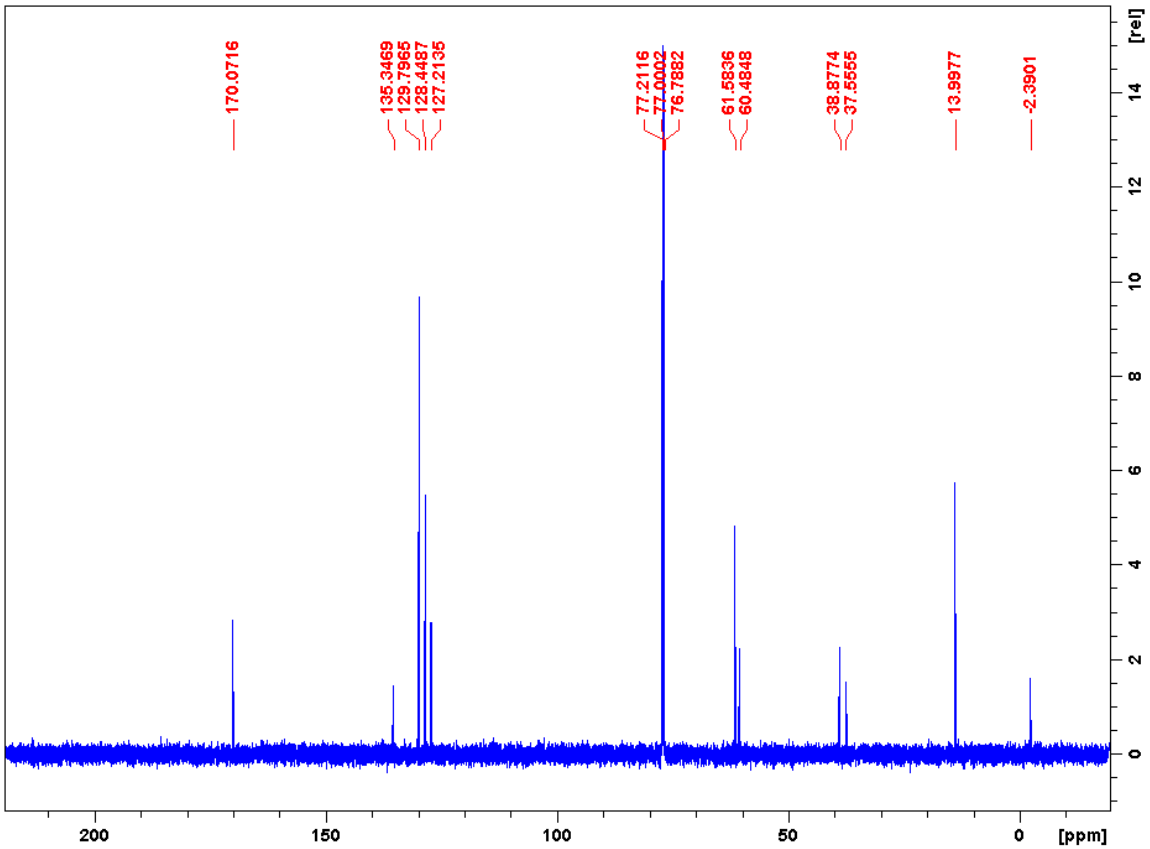
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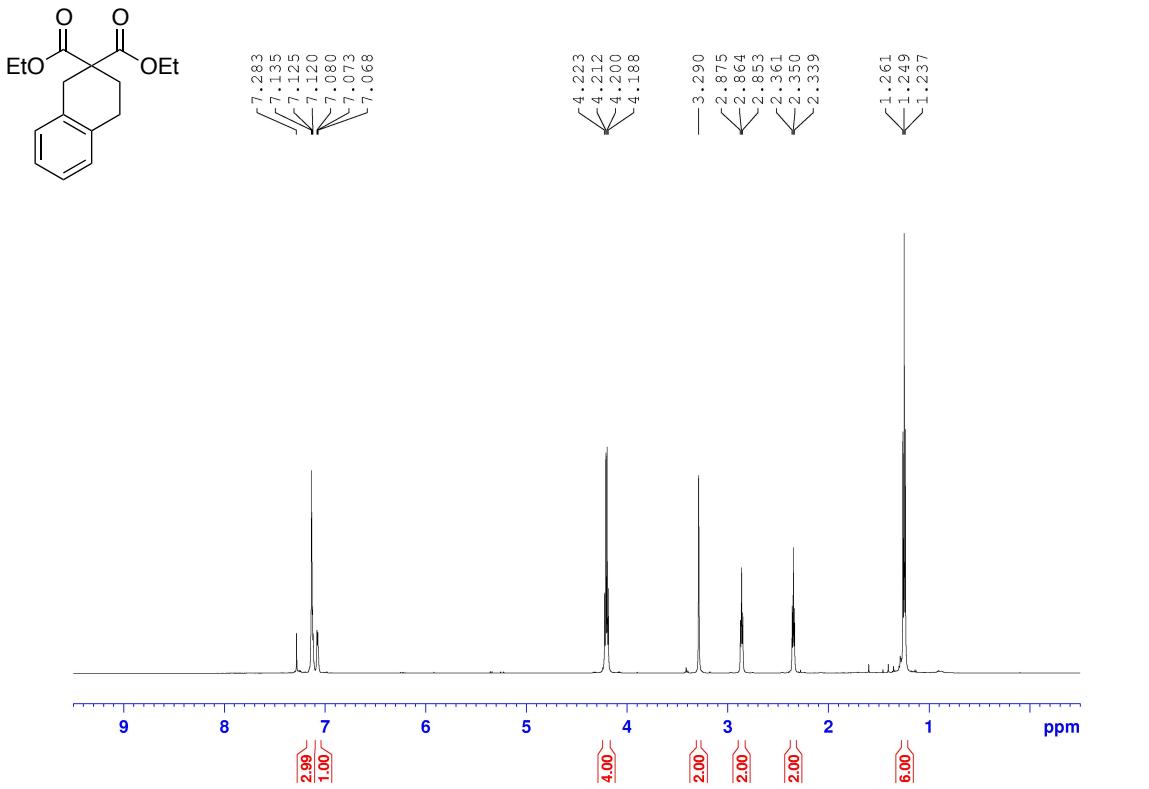
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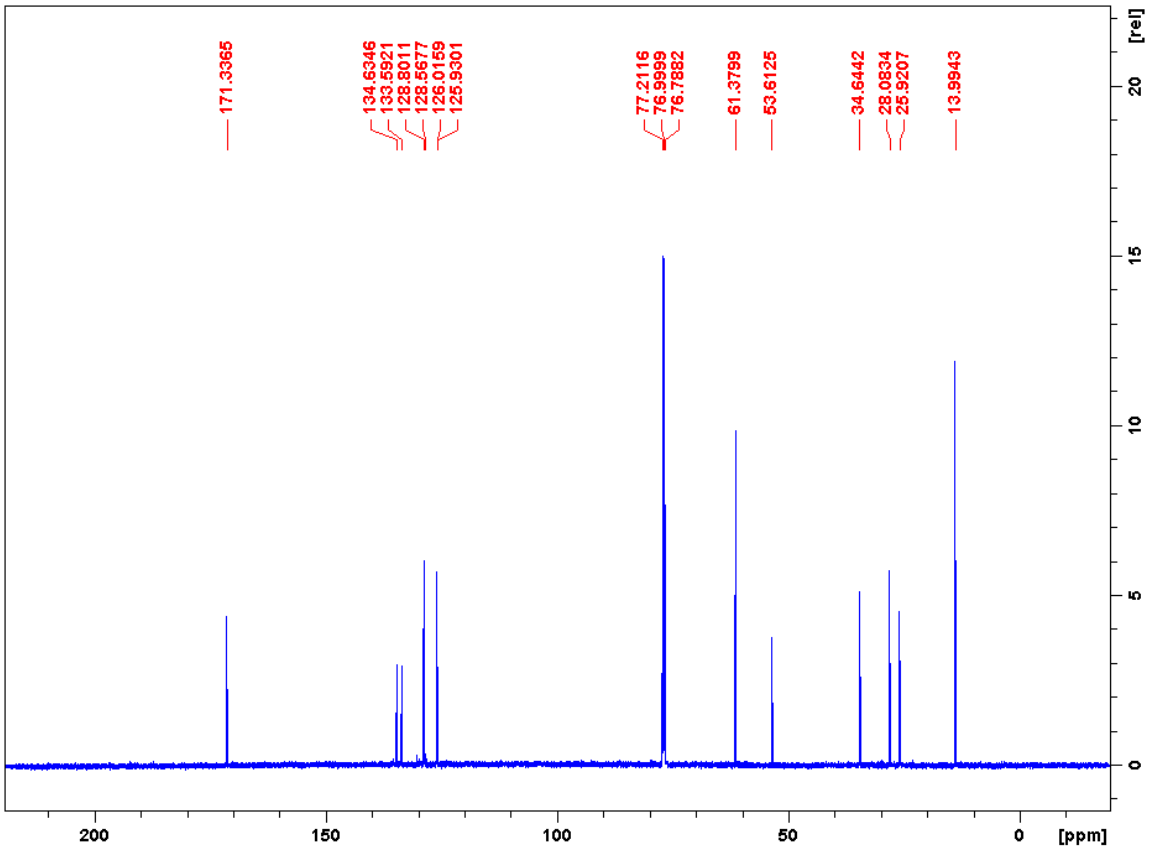
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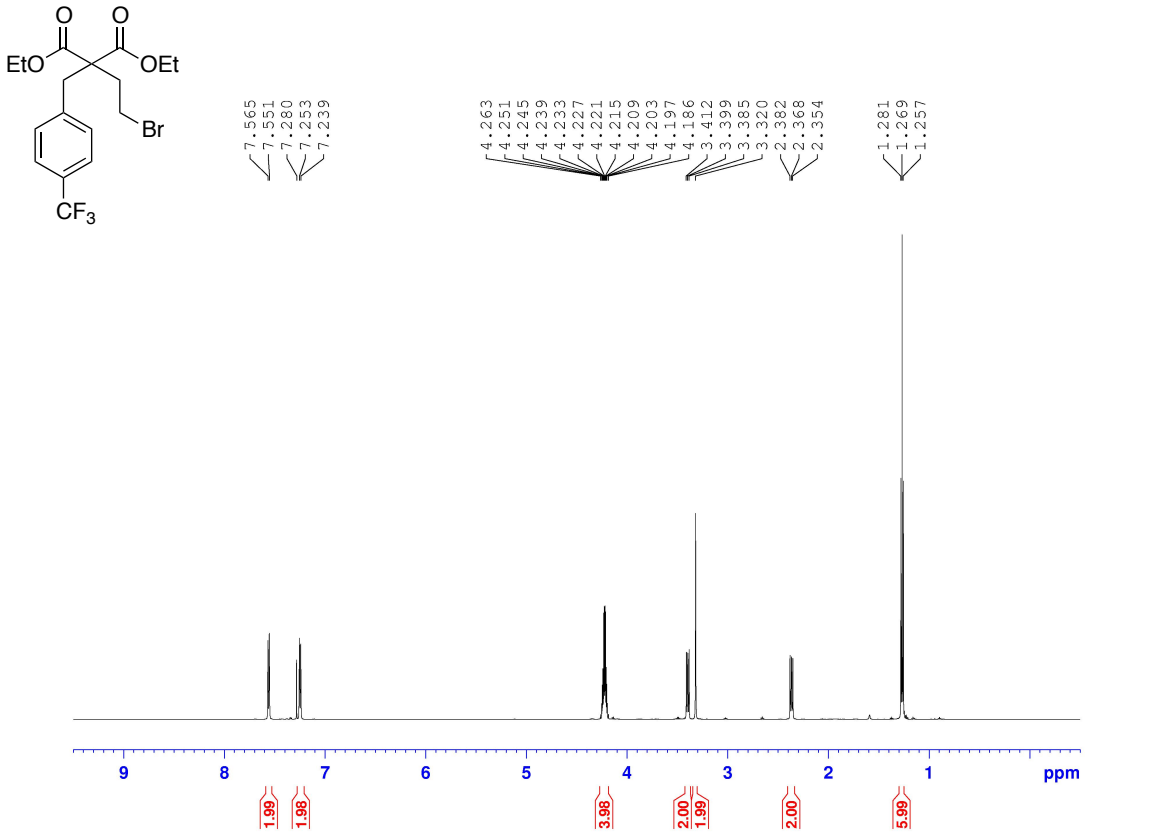
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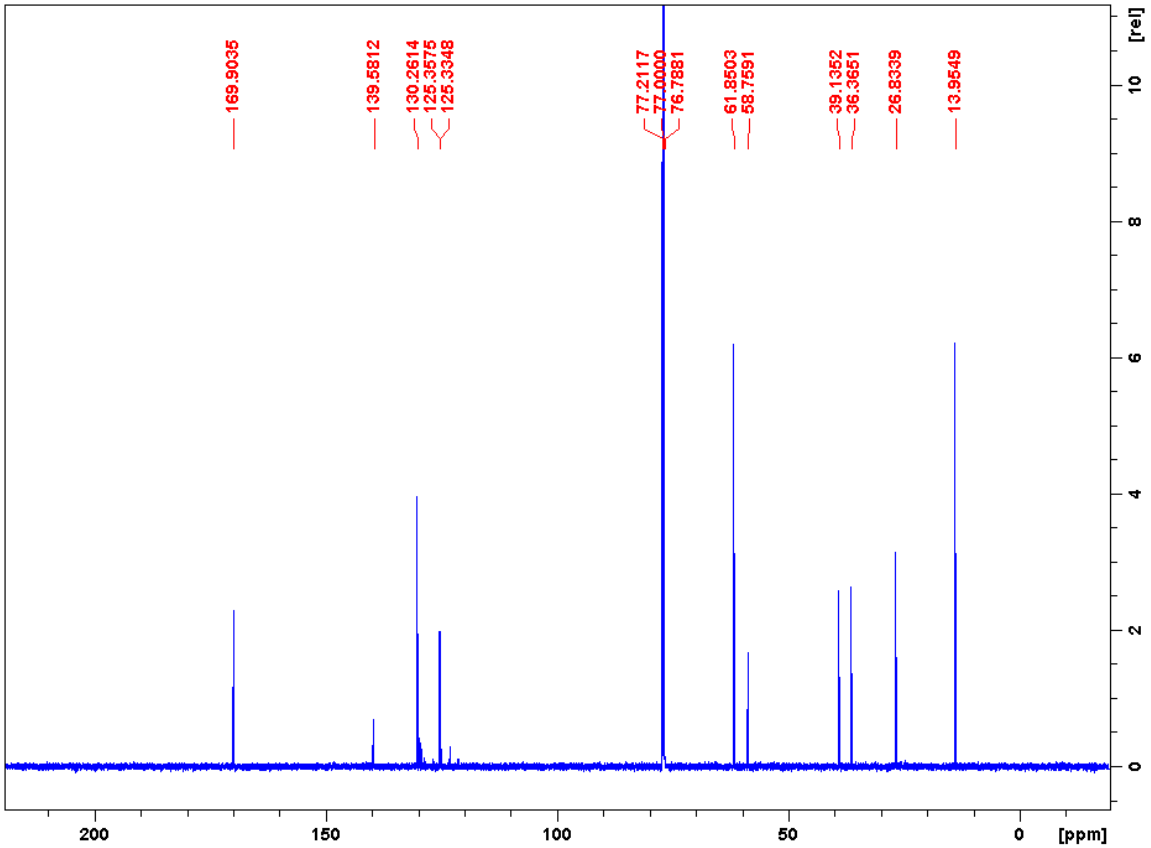
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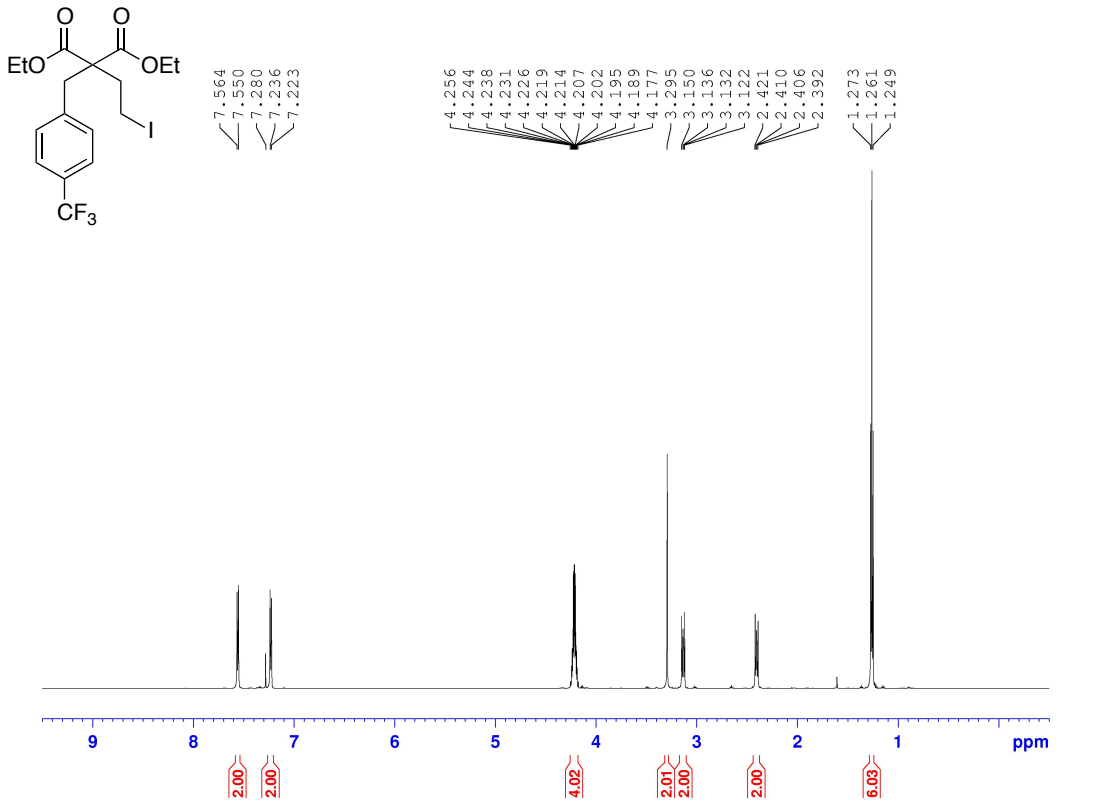
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2.00
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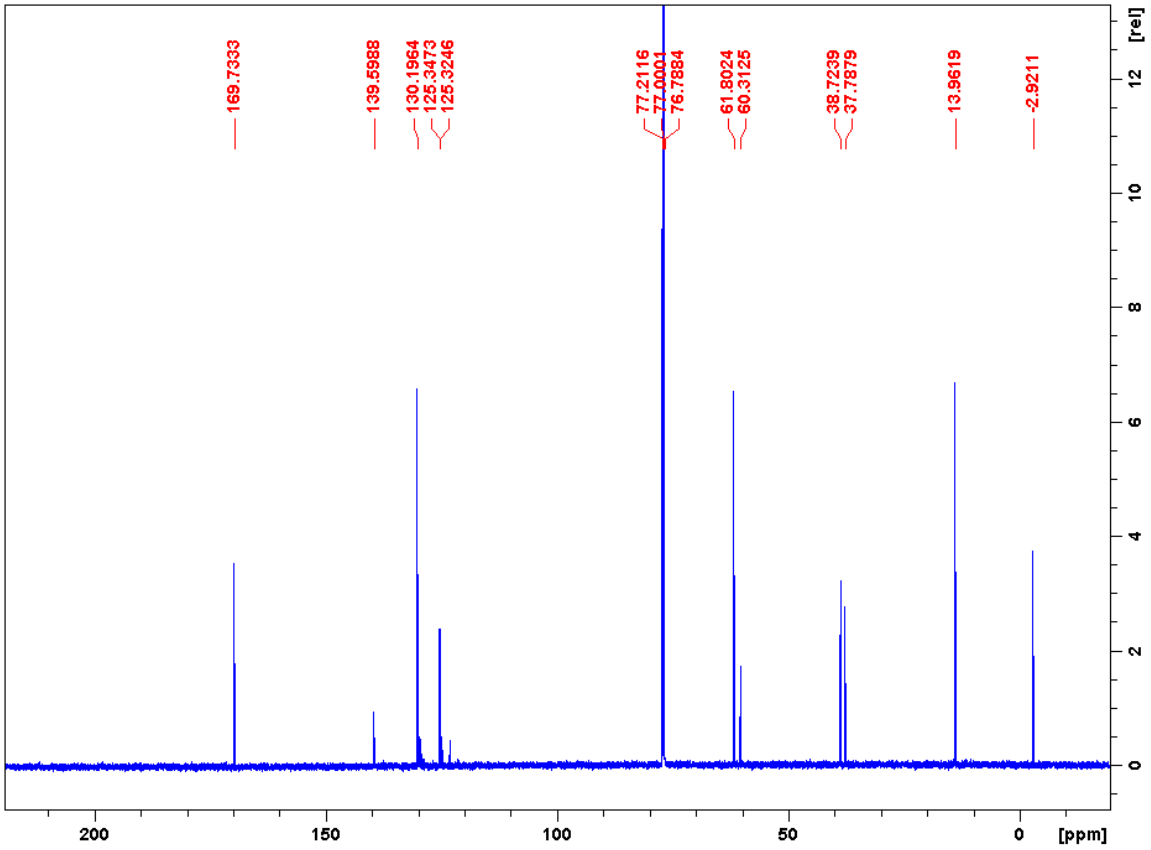
2.01
2.00
2.00
6.03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60.3125
38.7239
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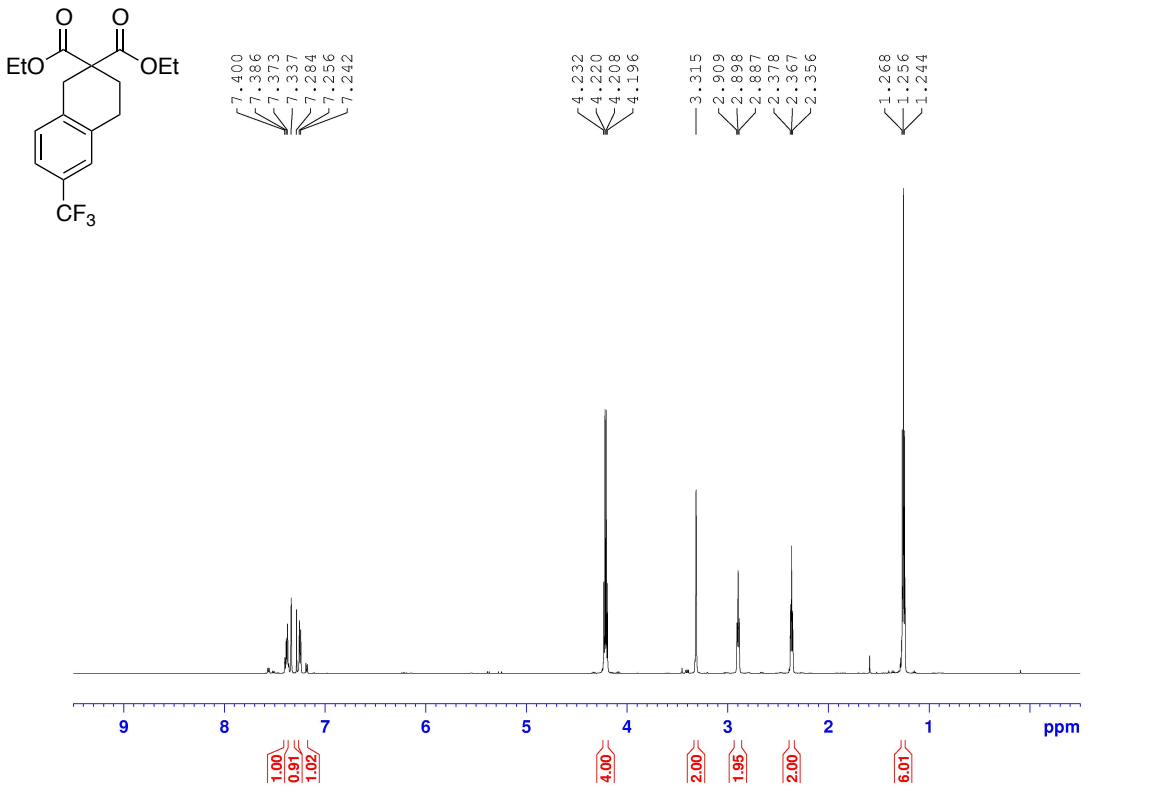
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O
EtO
OEt
CF3
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7.284
7.256
7.242
4.232
4.220
4.208
4.196
3.315
2.909
2.898
2.887
2.378
2.367
2.356
1.268
1.256
1.244
9
8
7
6
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4
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2
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ppm
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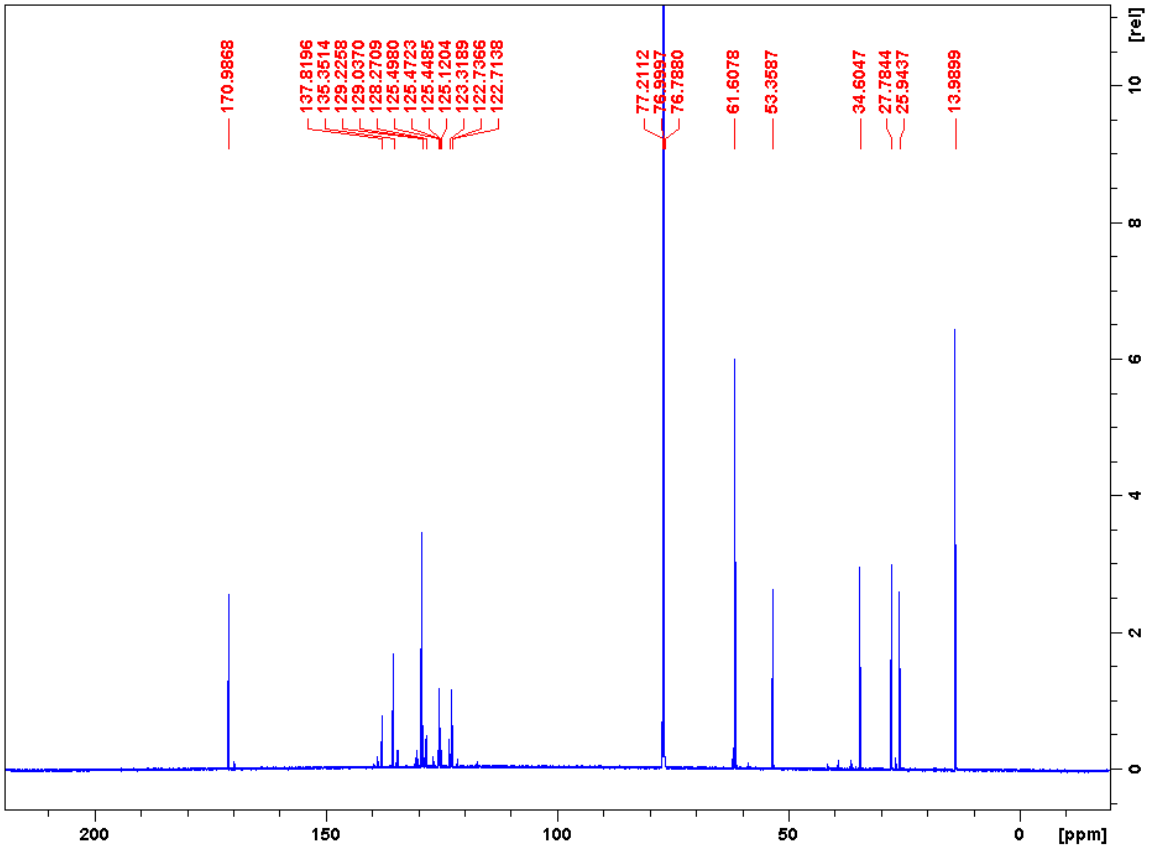
1.02
4.00
2.00
1.95
2.00
6.01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125.4485
125.1204
123.3189
122.7366
122.7138
77.2112
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76.7880
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53.3587
34.6047
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25.9437
13.9899
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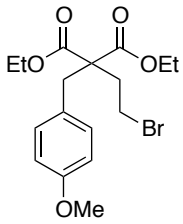
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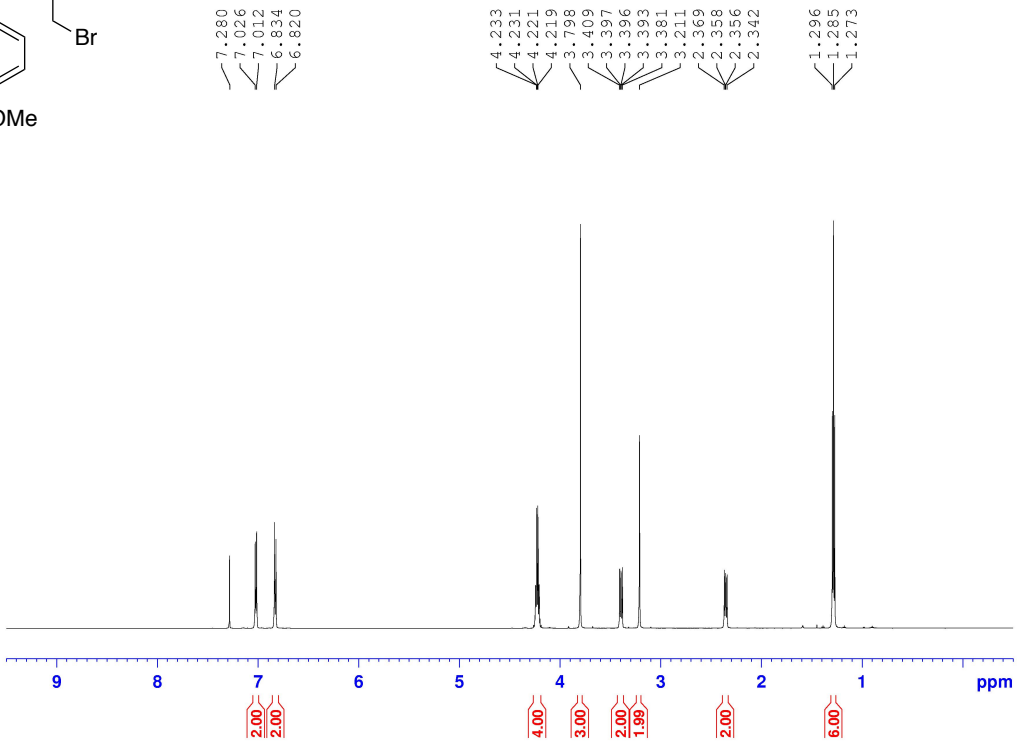
O
EtO
OEt
Br
OMe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4.231
4.221
4.219
3.798
3.409
3.397
3.396
3.393
3.381
3.211
2.369
2.358
2.356
2.342
1.296
1.285
1.273
9
8
7
6
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4
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2
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ppm
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2.00
4.00
3.00
2.00
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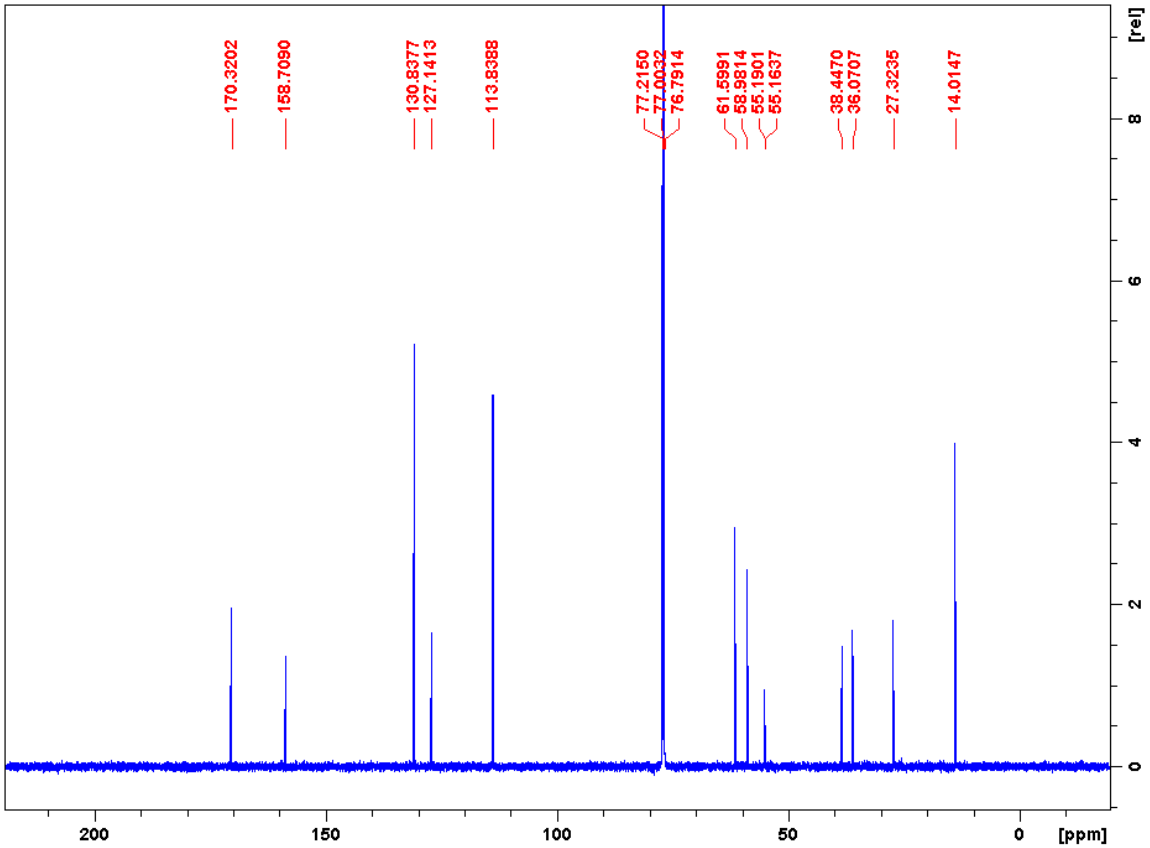
2.00
6.00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77.0032
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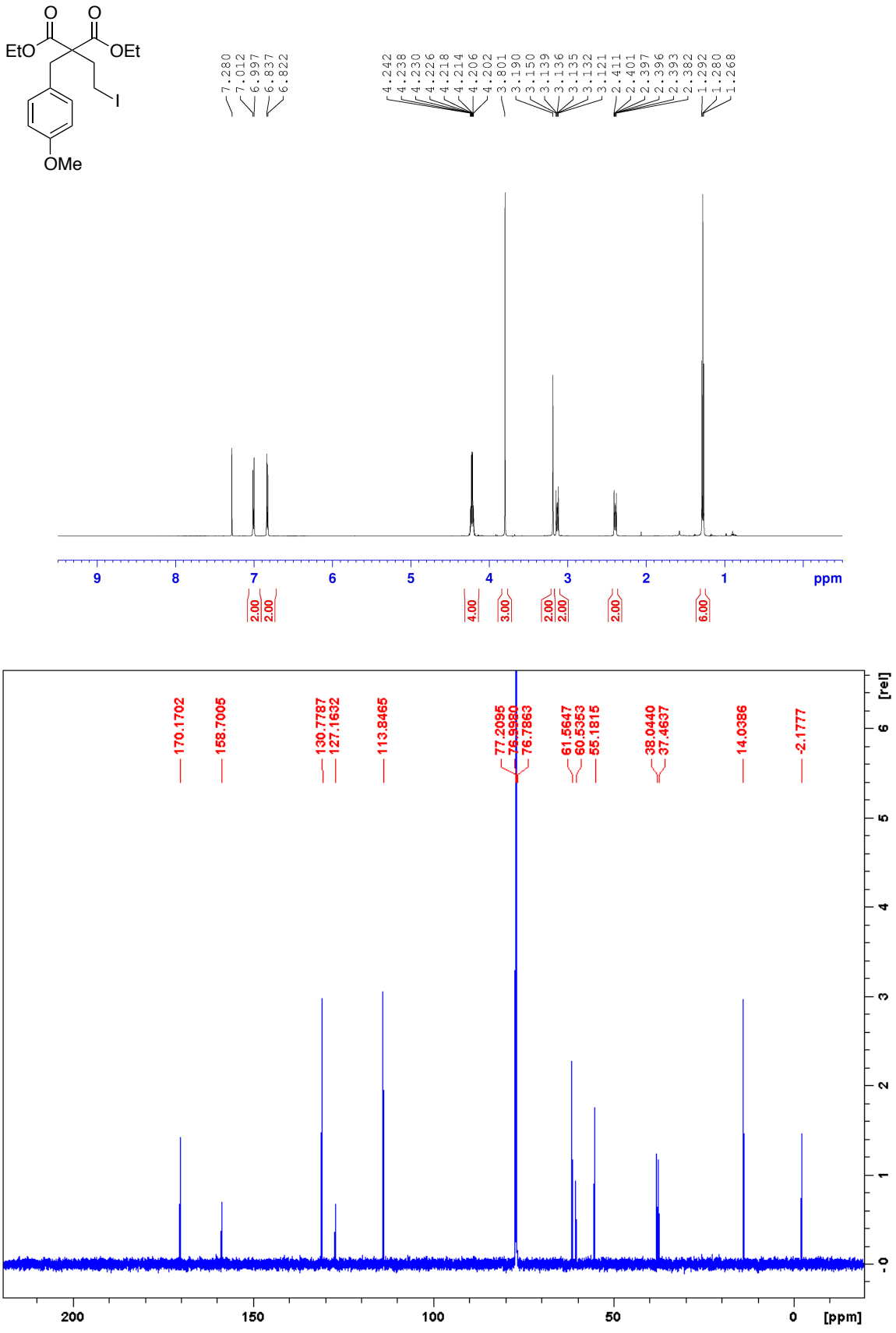
EtO
OEt
I
OMe
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7.012
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6.837
6.822
4.242
4.238
4.230
4.226
4.218
4.214
4.206
4.202
3.801
3.190
3.150
3.139
3.136
3.135
3.132
3.121
2.411
2.401
2.397
2.396
2.393
2.382
1.292
1.280
1.268
9
8
7
6
5
4
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4.00
3.00
2.00
2.00
2.00
6.00
170.1702
158.7005
130.7787
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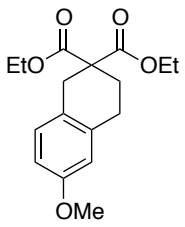
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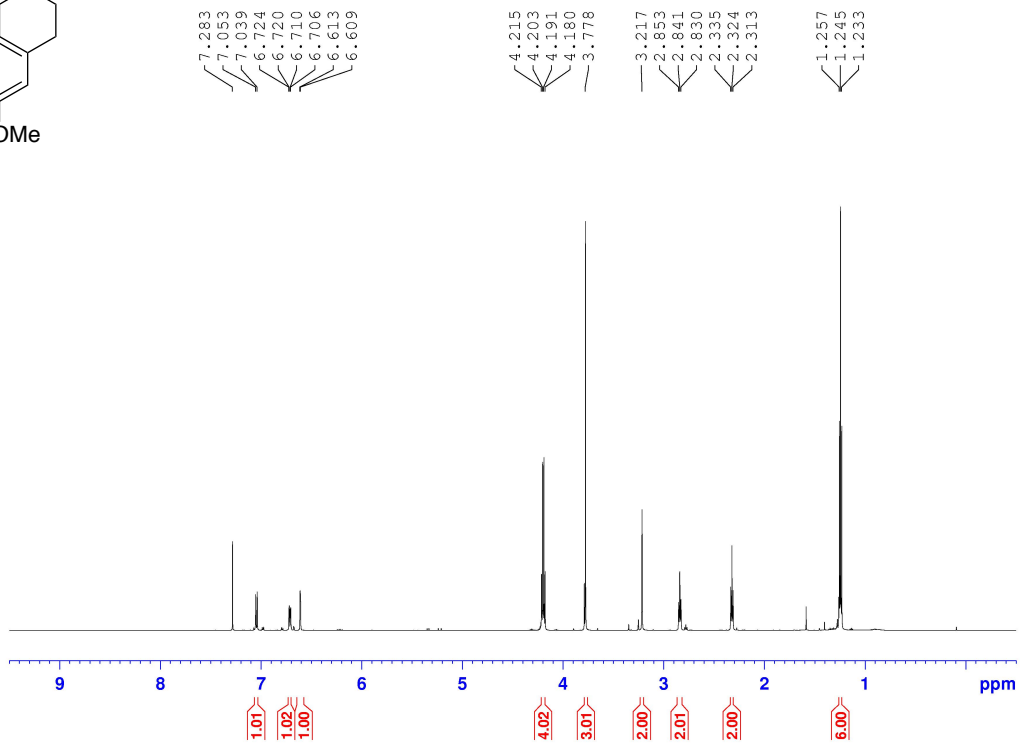
O
EtO
OEt
OMe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7.039
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6.710
6.706
6.613
6.609
4.215
4.203
4.191
4.180
3.778
3.217
2.853
2.841
2.830
2.335
2.324
2.313
1.257
1.245
1.233
9
8
7
6
5
4
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ppm
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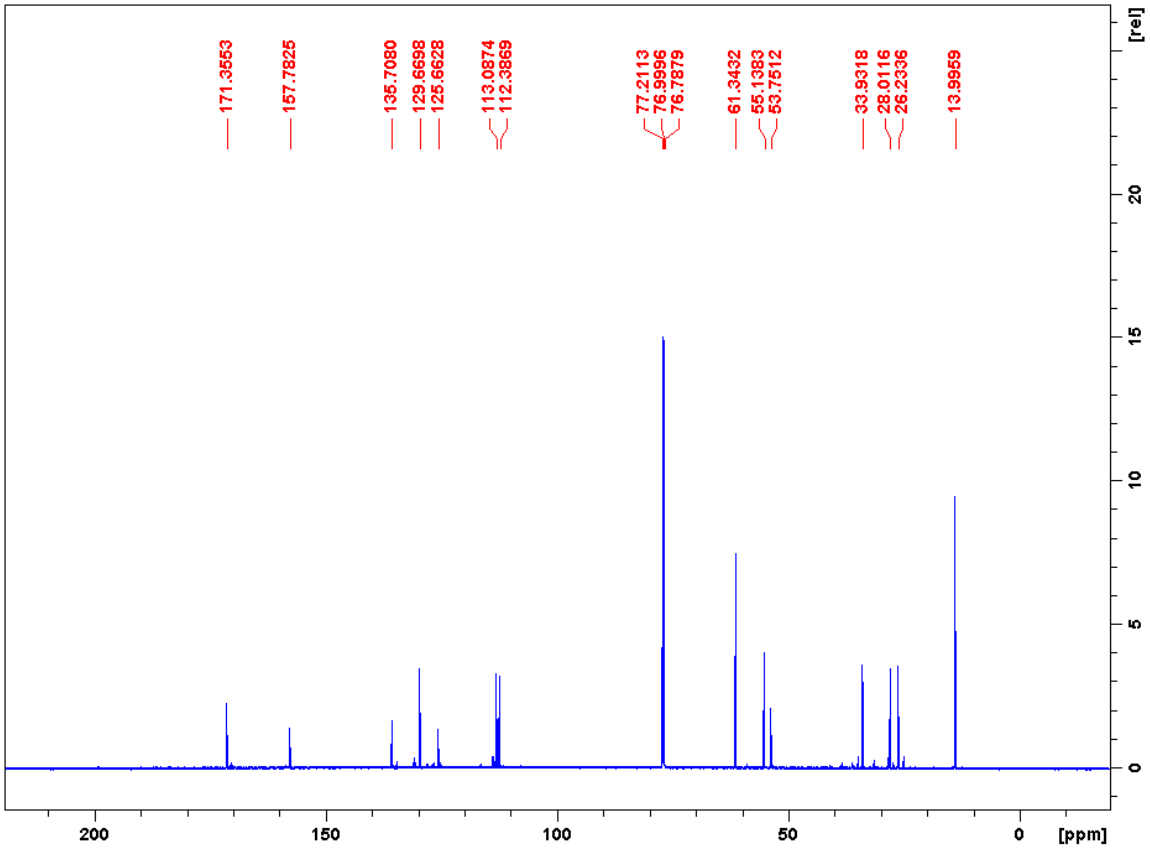
1.02
1.00
4.02
3.01
2.00
2.01
2.00
6.00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112.3869
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76.9996
76.7879
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53.7512
33.9318
28.0116
26.2336
13.9959
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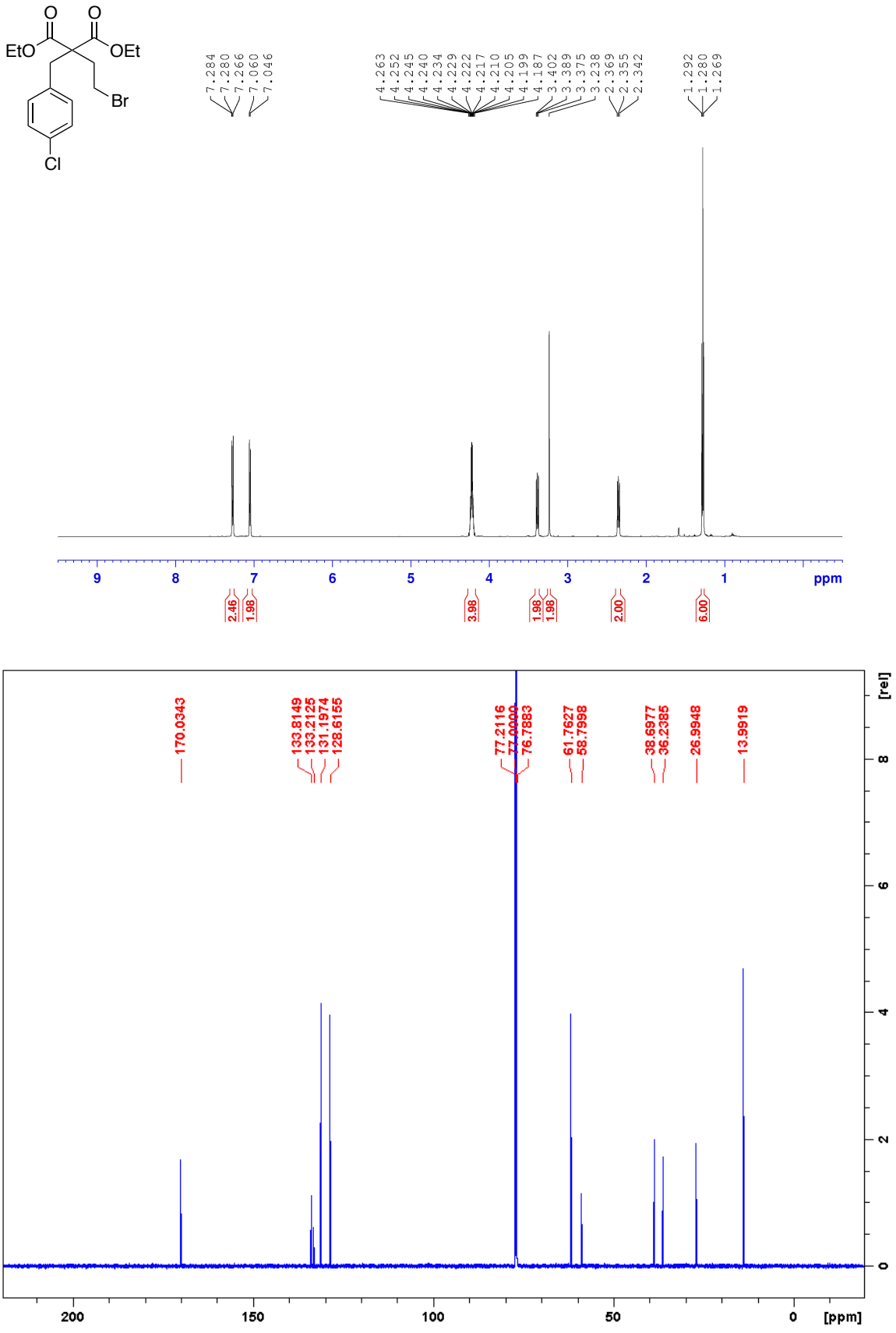
150
100
50
0
[ppm]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OEt
Br
Cl
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7.046
4.263
4.252
4.245
4.240
4.234
4.229
4.222
4.217
4.210
4.205
4.199
4.187
3.402
3.389
3.375
3.238
2.369
2.355
2.342
1.292
1.280
1.269
9
8
7
6
5
4
3
2
1
ppm
2.46
1.98
3.98
1.98
1.98
2.00
6.00
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133.2125
131.1974
128.6155
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77.0000
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13.9919
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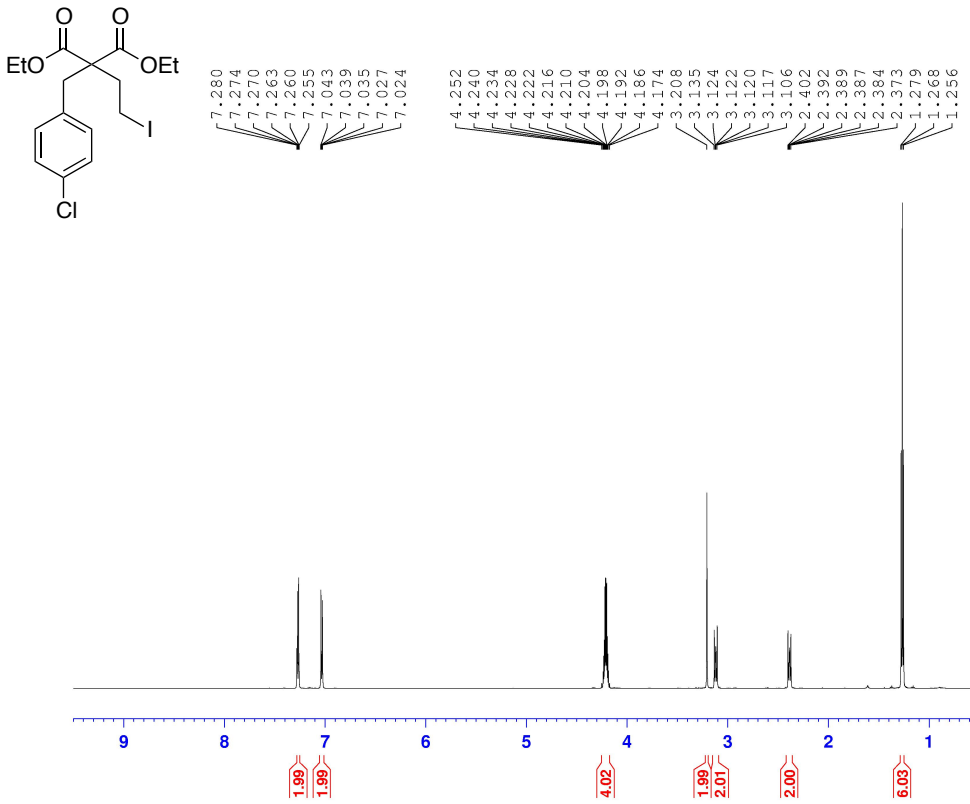
EtO
O
O
OEt
I
Cl
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7.270
7.263
7.260
7.255
7.043
7.039
7.035
7.027
7.024
4.252
4.240
4.234
4.228
4.222
4.216
4.210
4.204
4.198
4.192
4.186
4.174
3.208
3.135
3.124
3.122
3.120
3.117
3.106
2.402
2.392
2.389
2.387
2.384
2.373
1.279
1.268
1.256
9
8
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6
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4
3
2
1
ppm
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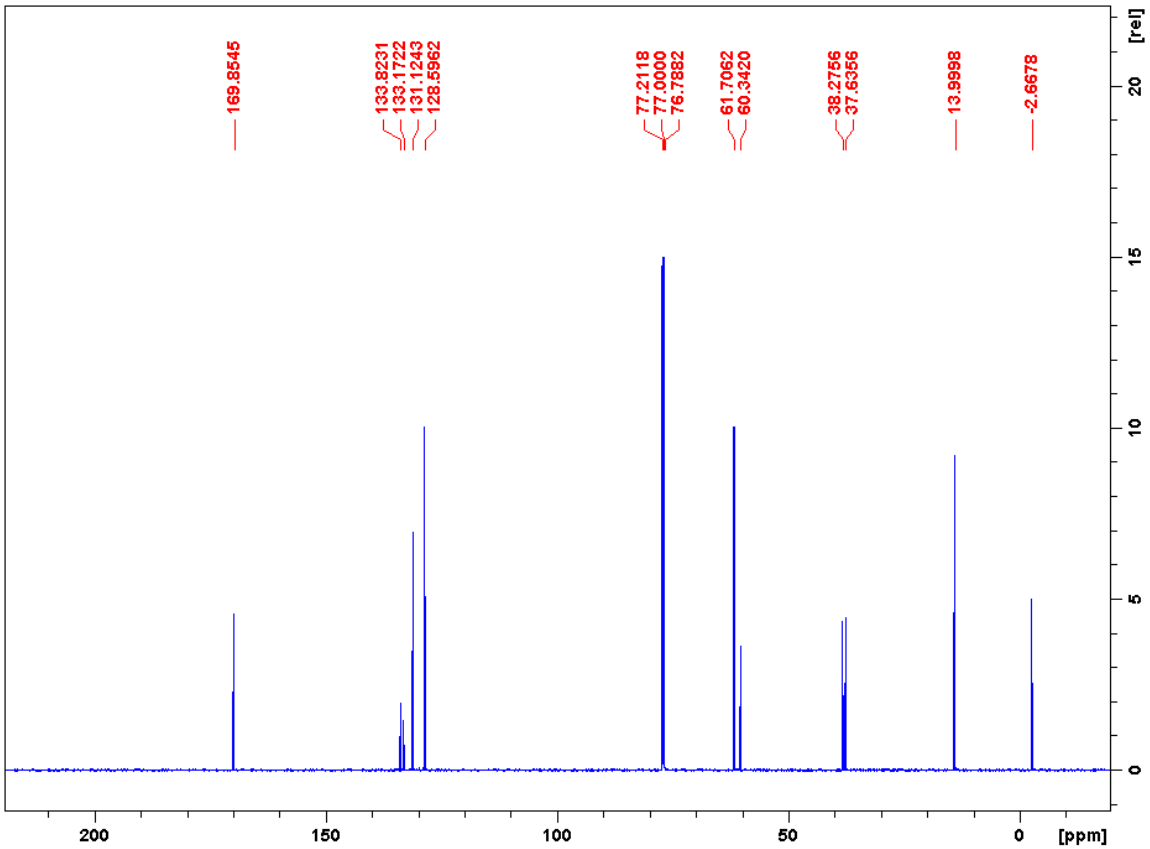
1.99
4.02
1.99
2.01
2.00
6.03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77.0000
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61.7062
60.3420
38.2756
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-2.6678
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5
0
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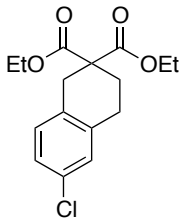
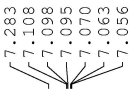
150
100
50
0
[ppm]


O
O
EtO
OEt
Cl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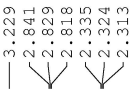
7.070
7.063
7.056


4.220
4.208
4.196
4.184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2.829
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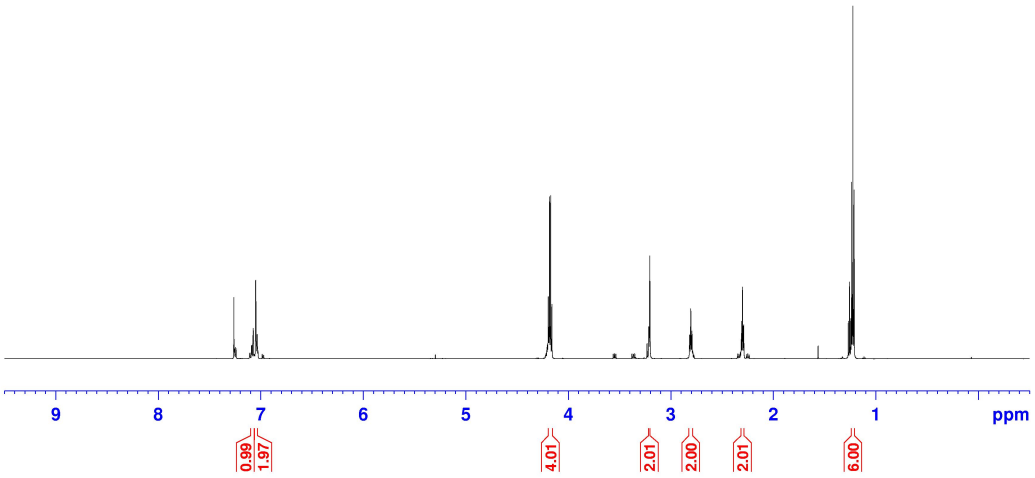
2.335
2.324
2.313


1.259
1.248
1.236


9
8
7
6
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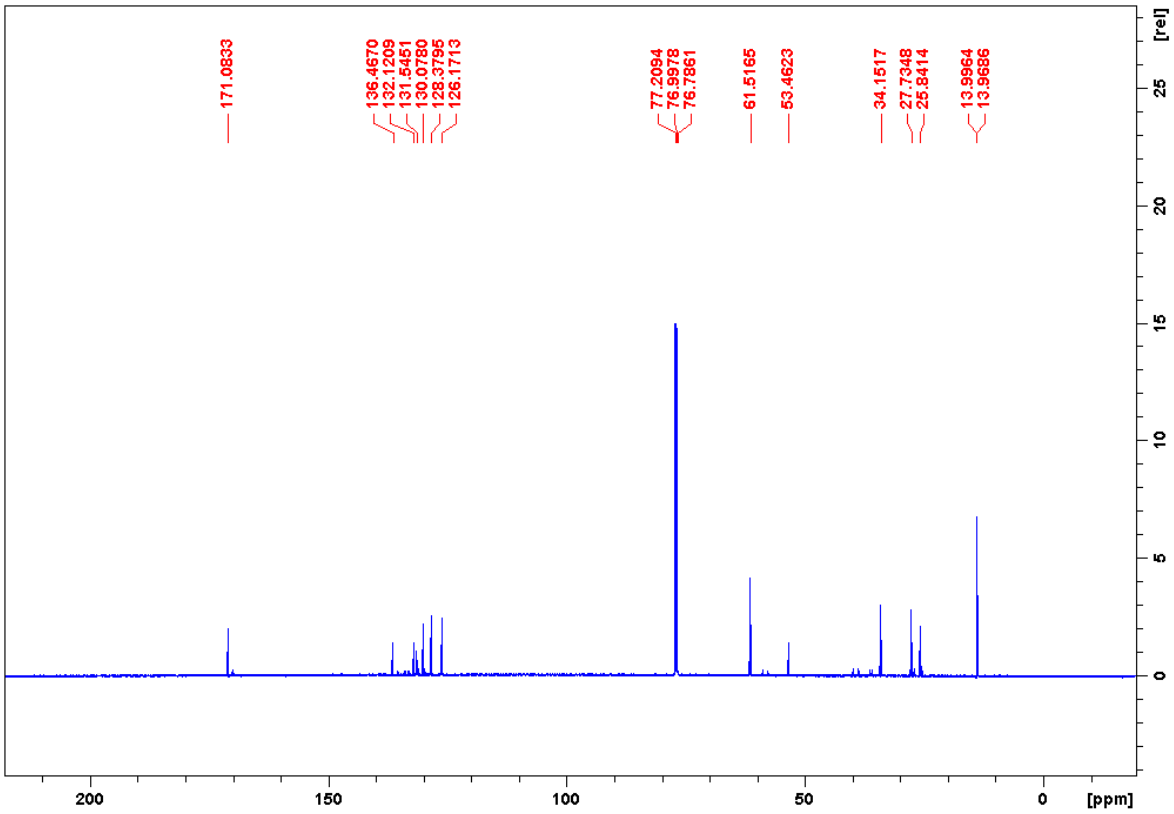
4
3
2
1
ppm
0.99
1.97
4.01
2.01
2.00
2.01
6.00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130.0780
128.3795
126.1713
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76.9978
76.7861
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53.4623
34.1517
27.7348
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13.9686
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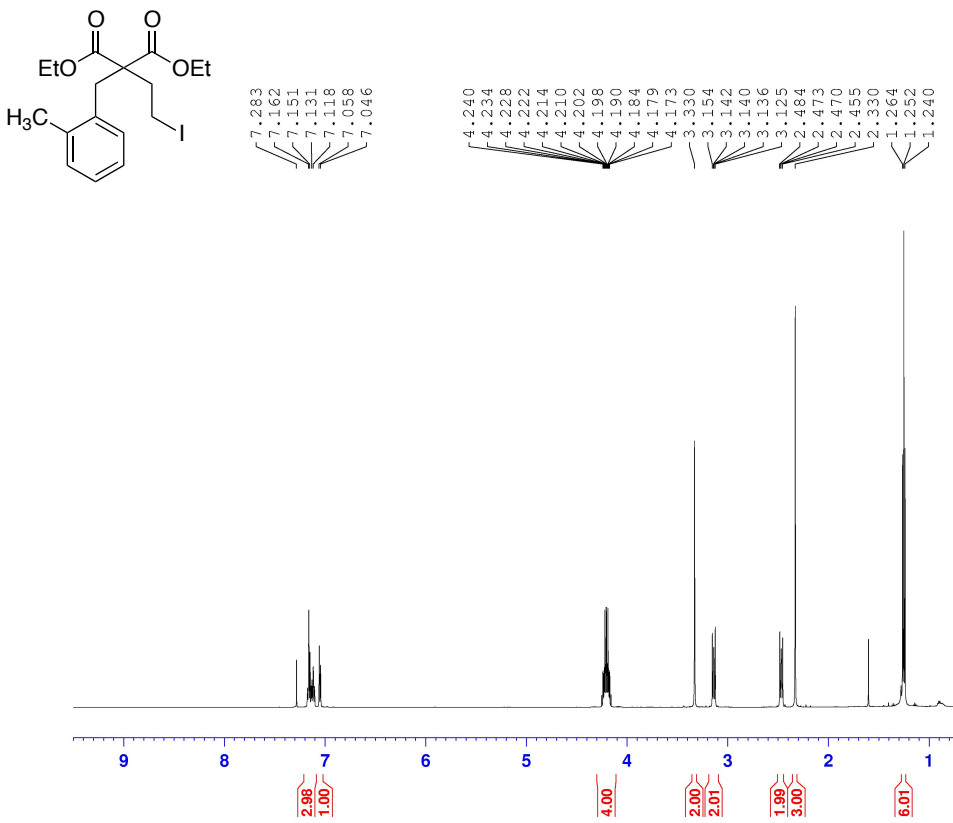
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O
O
OEt
H3C
I
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7.131
7.118
7.058
7.046
4.240
4.234
4.228
4.222
4.214
4.210
4.202
4.198
4.190
4.184
4.179
4.173
3.330
3.154
3.142
3.140
3.136
3.125
2.484
2.473
2.470
2.455
2.330
1.264
1.252
1.240
9
8
7
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ppm
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2.00
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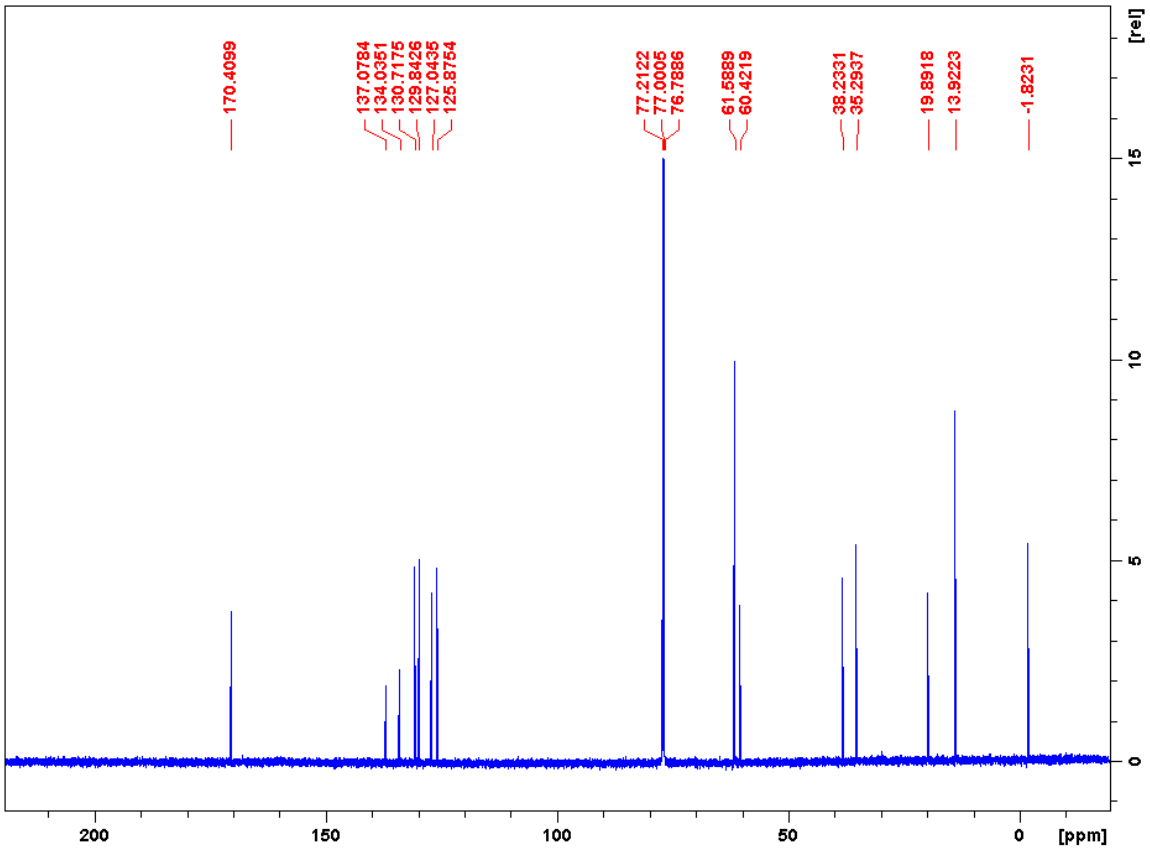
1.99
3.00
6.01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125.8754
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77.0005
76.7886
61.5889
60.4219
38.2331
35.2937
19.8918
13.9223
-1.8231
[rel]
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5
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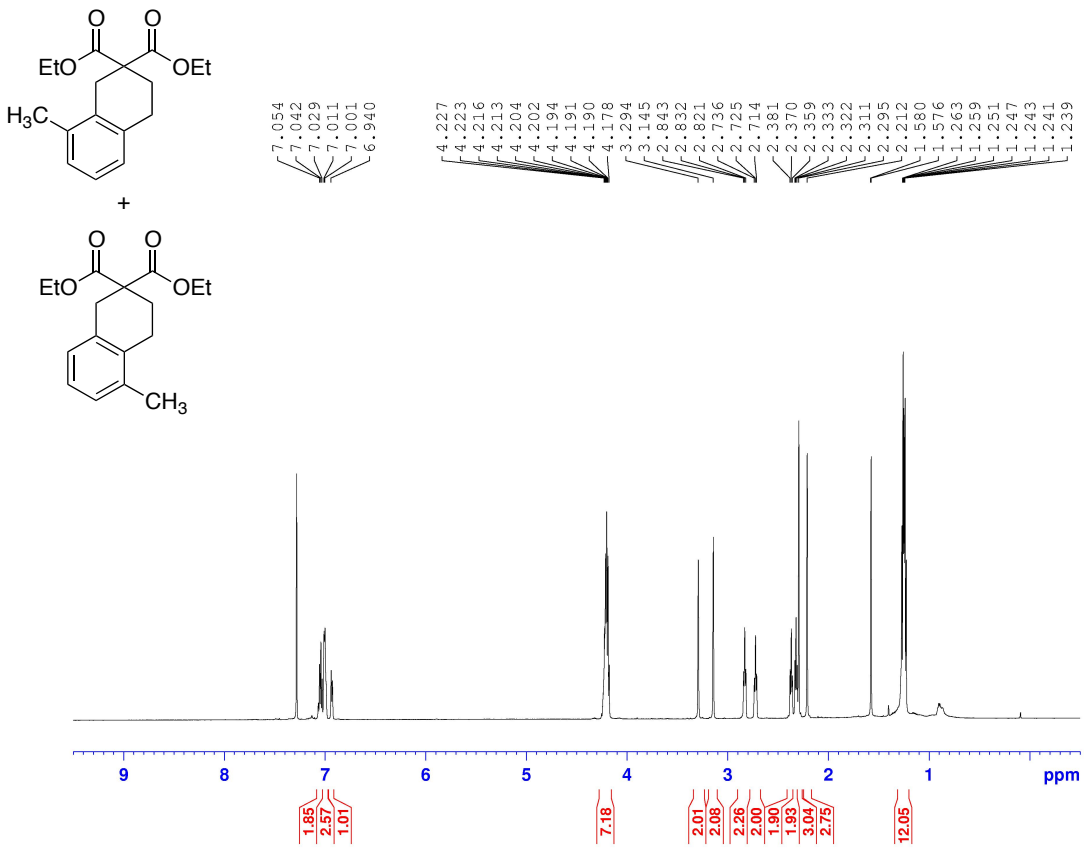
50
0
[ppm]


EtO
OEt
O
O
H3C
+
EtO
OEt
O
O
CH3
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7.042
7.029
7.011
7.001
6.940
4.227
4.223
4.216
4.213
4.204
4.202
4.194
4.191
4.190
4.178
3.294
3.145
2.843
2.832
2.821
2.736
2.725
2.714
2.381
2.370
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2.333
2.322
2.311
2.295
2.212
1.580
1.576
1.263
1.259
1.251
1.247
1.243
1.241
1.239
9
8
7
6
5
4
3
2
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ppm
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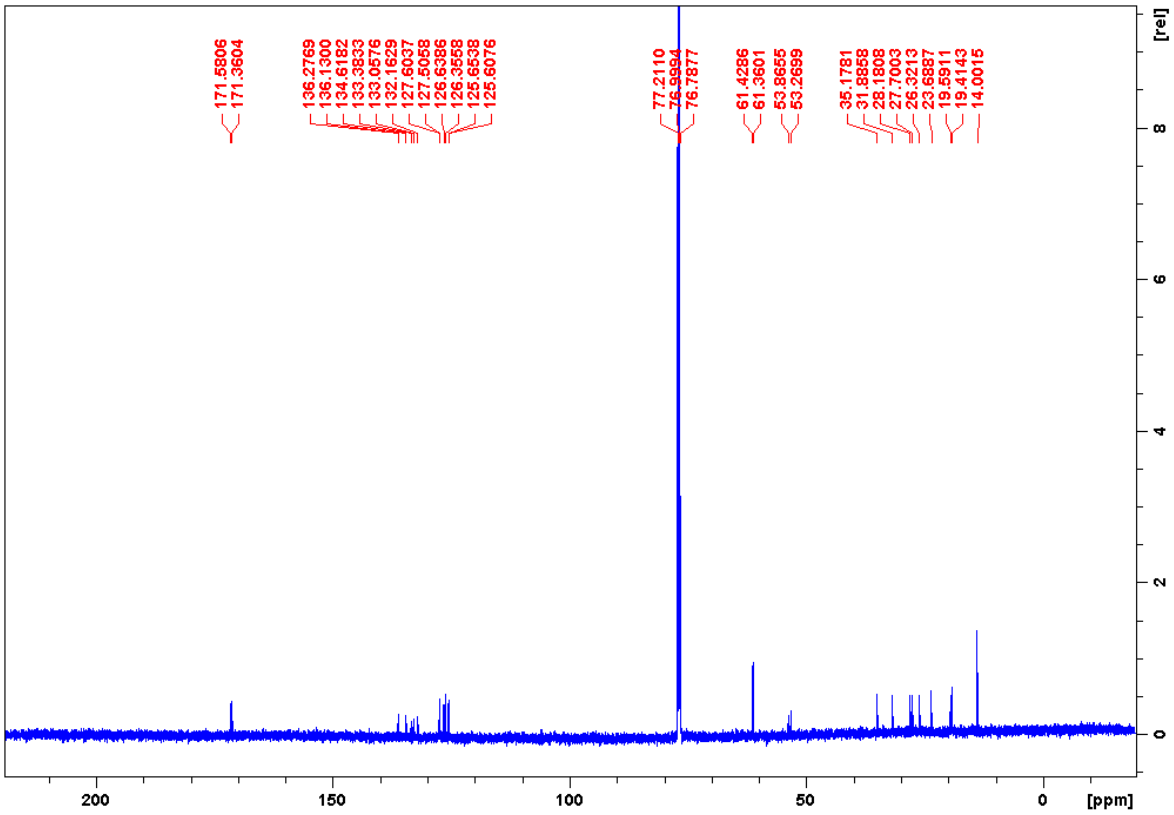
2.75
12.05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126.3558
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125.6076
77.2110
76.9994
76.7877
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61.3601
53.8655
53.2699
35.1781
31.8858
28.1808
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26.3213
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14.0015
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8
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50
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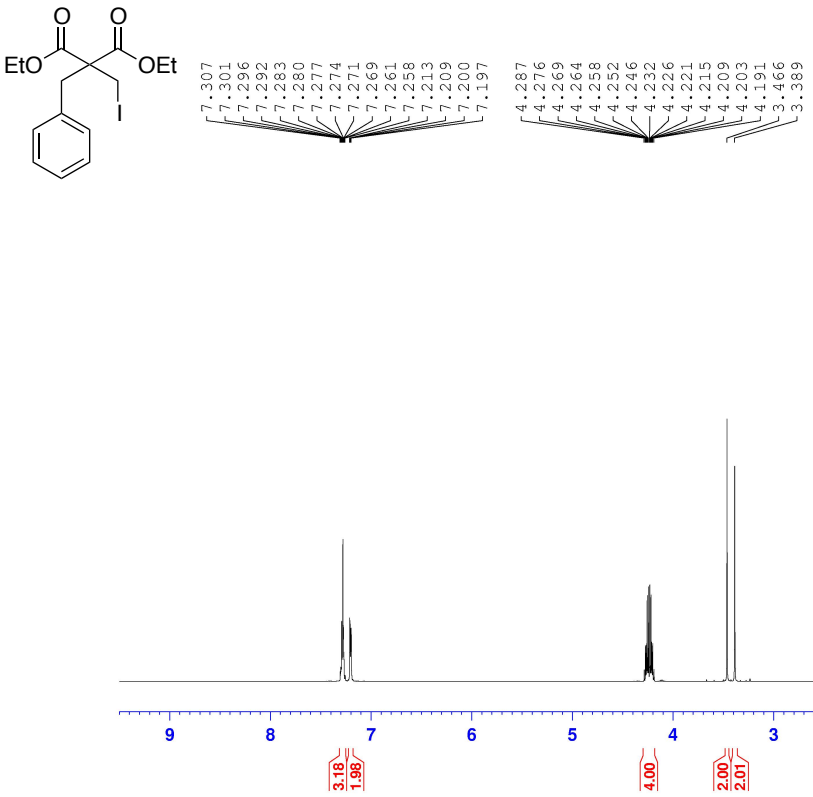
[ppm]


EtO
O
O
OEt
I
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7.296
7.292
7.283
7.280
7.277
7.274
7.271
7.269
7.261
7.258
7.213
7.209
7.200
7.197
4.287
4.276
4.269
4.264
4.258
4.252
4.246
4.232
4.226
4.221
4.215
4.209
4.203
4.191
3.466
3.389
1.292
1.281
1.269
9
8
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5
4
3
2
1
ppm
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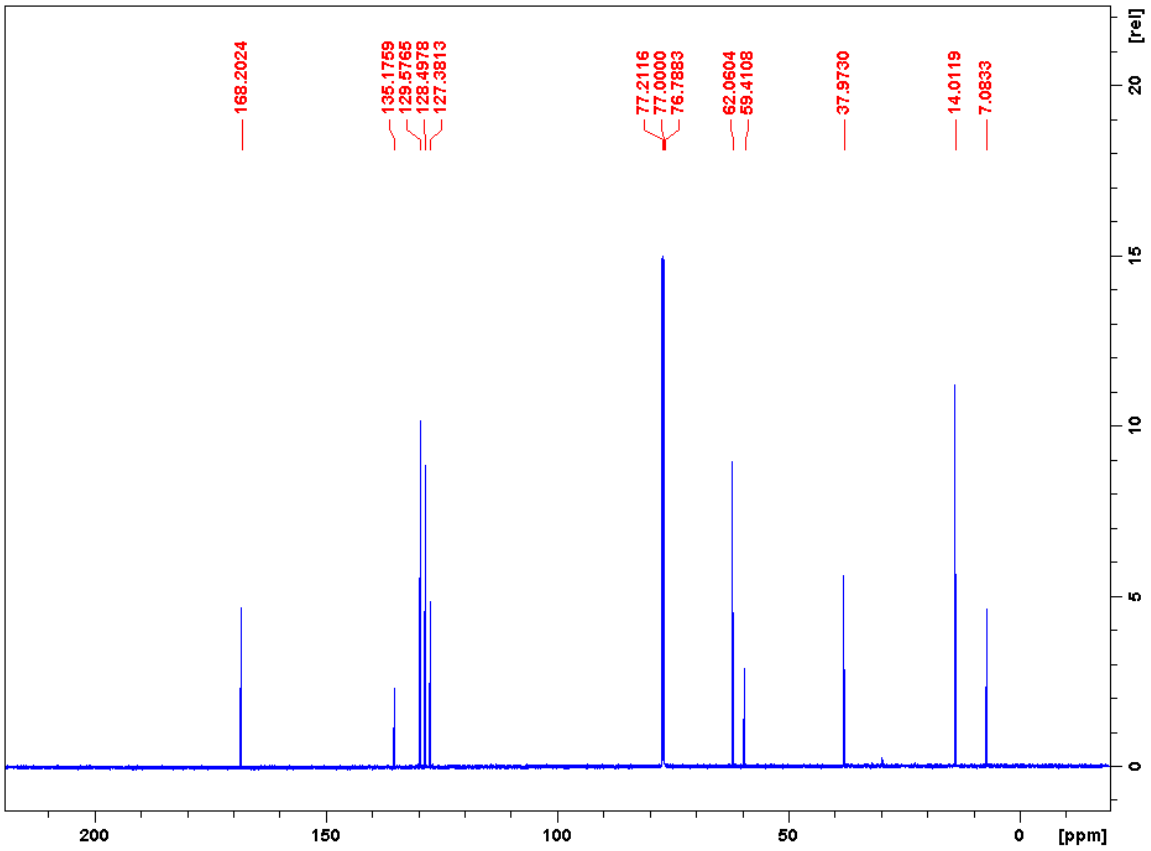
2.01
6.01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7.0833
[rel]
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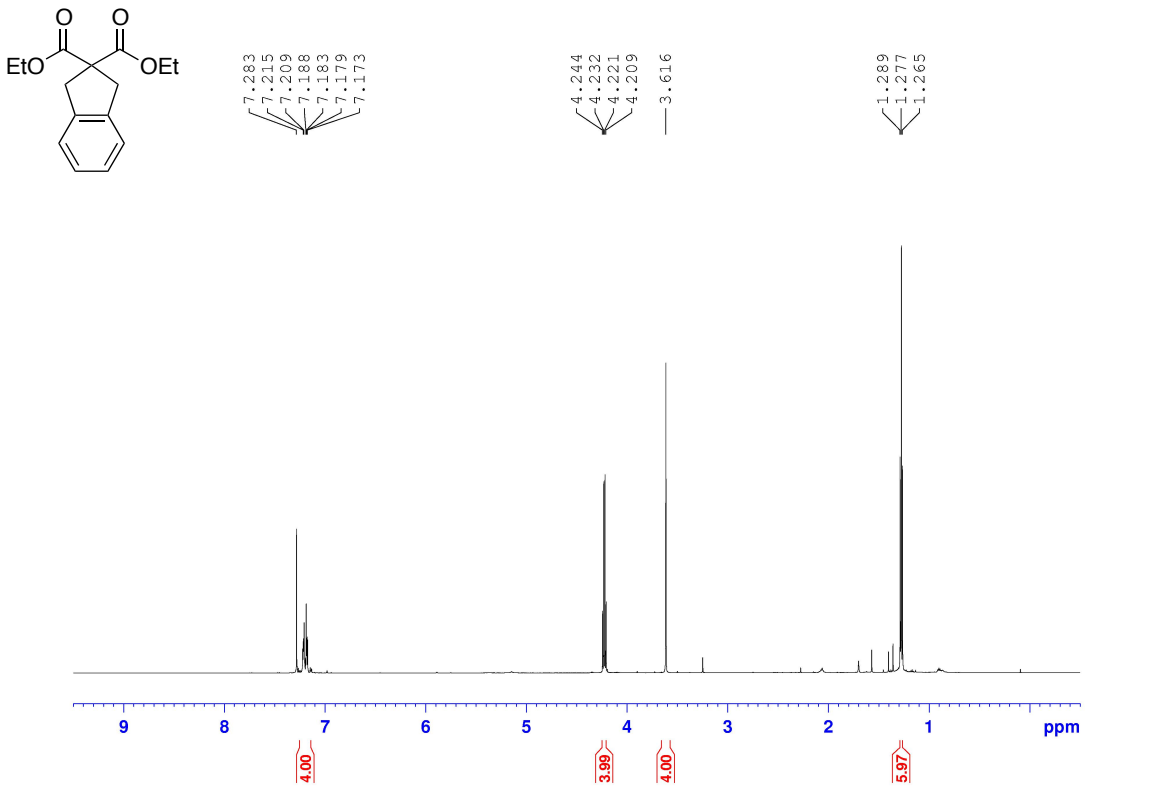
15
10
5
0
200
150
100
50
0
[ppm]


O
O
EtO
OEt
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7.209
7.188
7.183
7.179
7.173
4.244
4.232
4.221
4.209
3.616
1.289
1.277
1.265
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8
7
6
5
4
3
2
1
ppm
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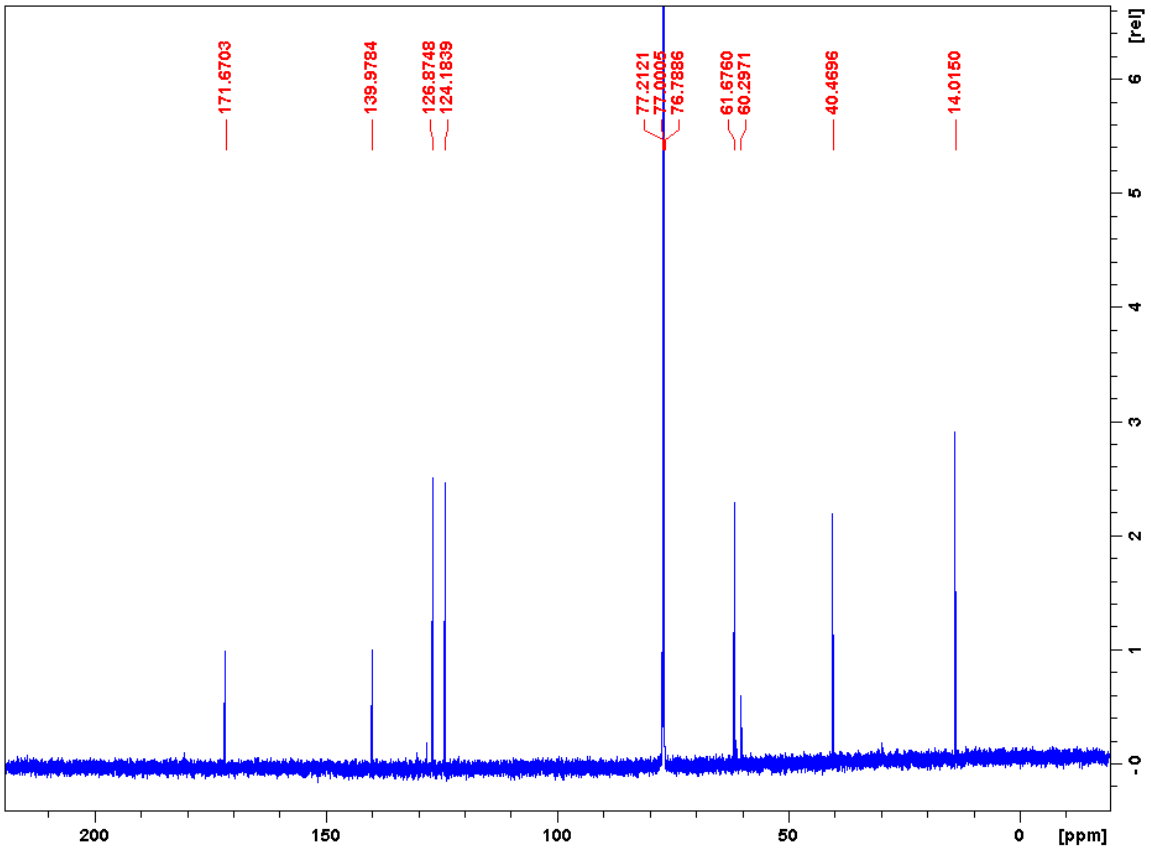
3.99
4.00
5.97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60.2971
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14.0150
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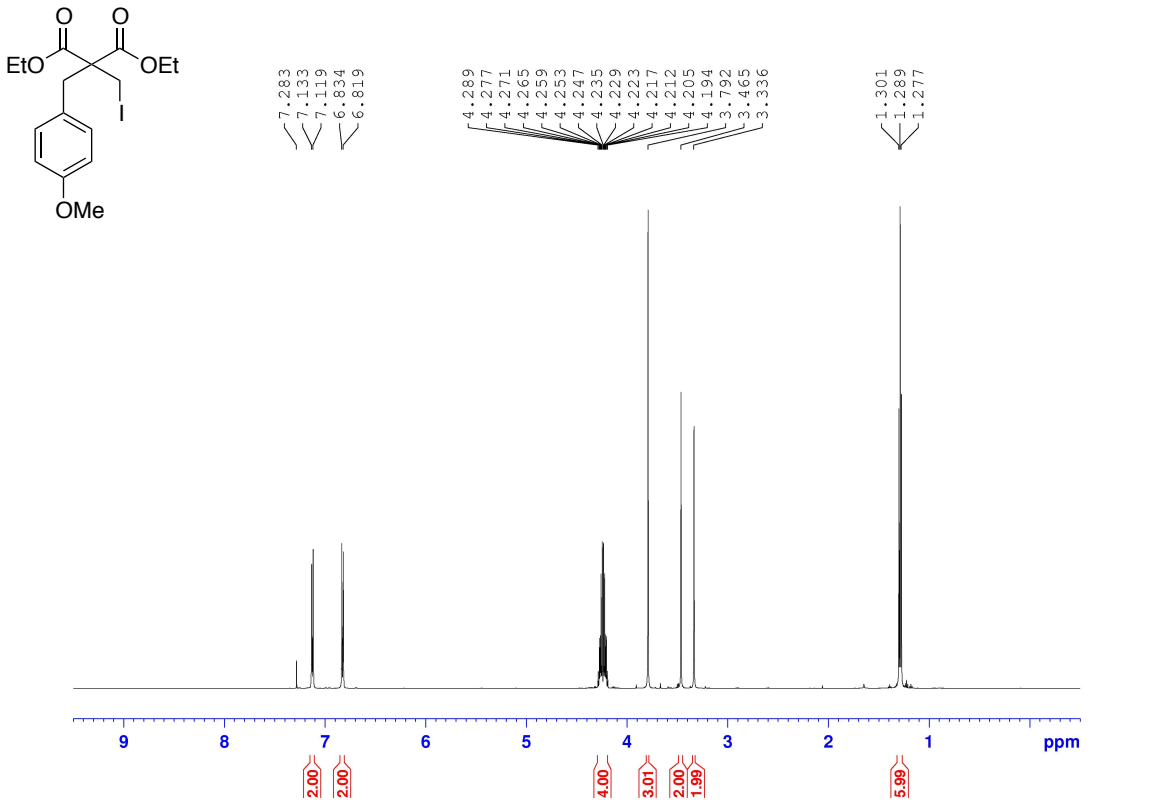
EtO
OEt
I
OMe
7.283
7.133
7.119
6.834
6.819
4.289
4.277
4.271
4.265
4.259
4.253
4.247
4.235
4.229
4.223
4.217
4.212
4.205
4.194
3.792
3.465
3.336
1.301
1.289
1.277
9
8
7
6
5
4
3
2
1
ppm
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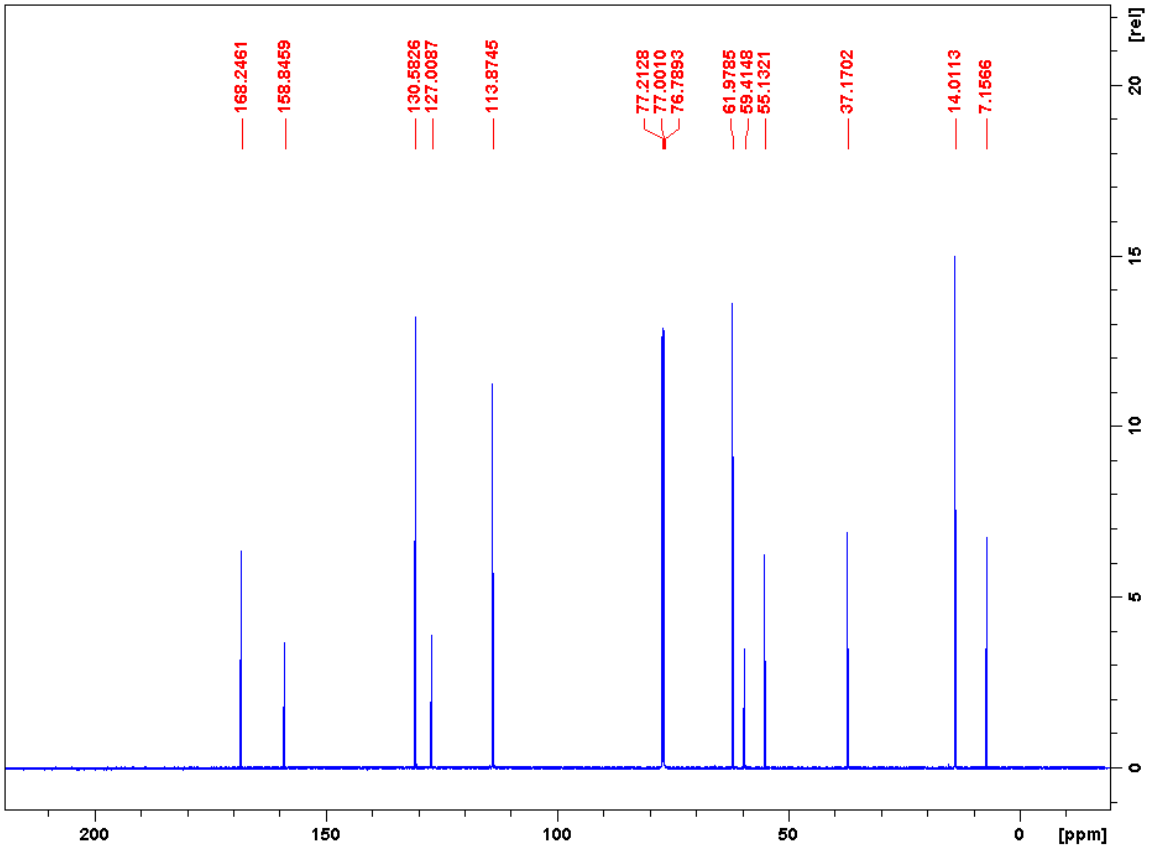
2.00
4.00
3.01
2.00
1.99
5.99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77.0010
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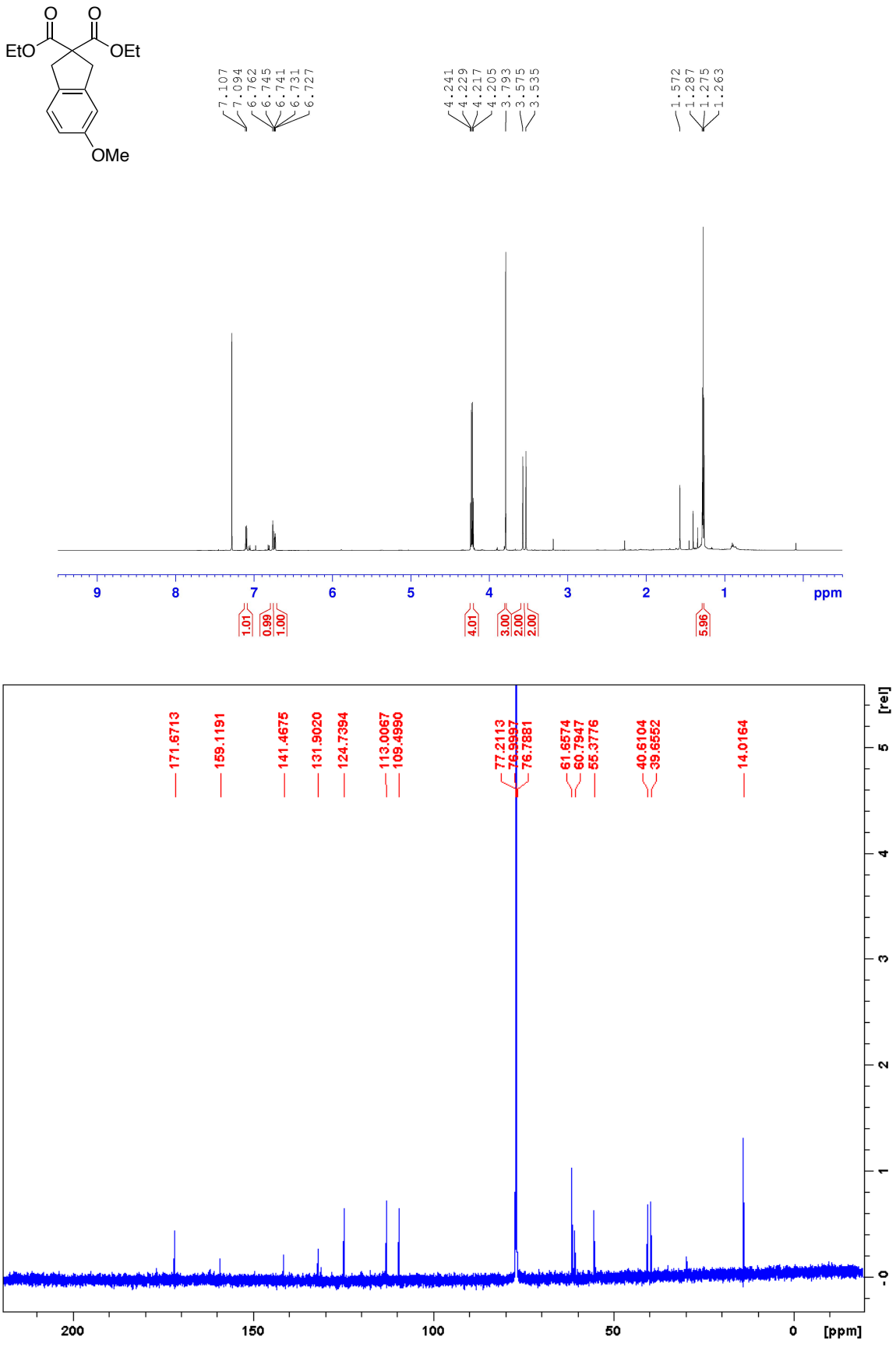
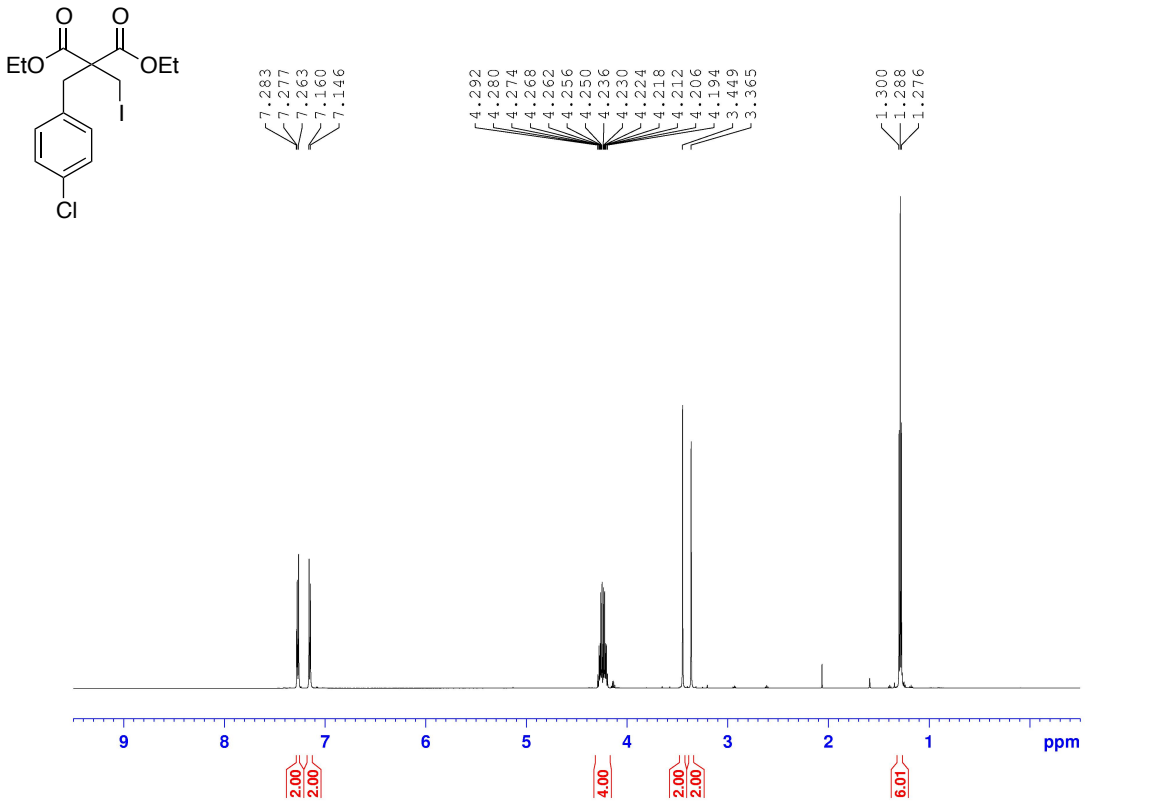
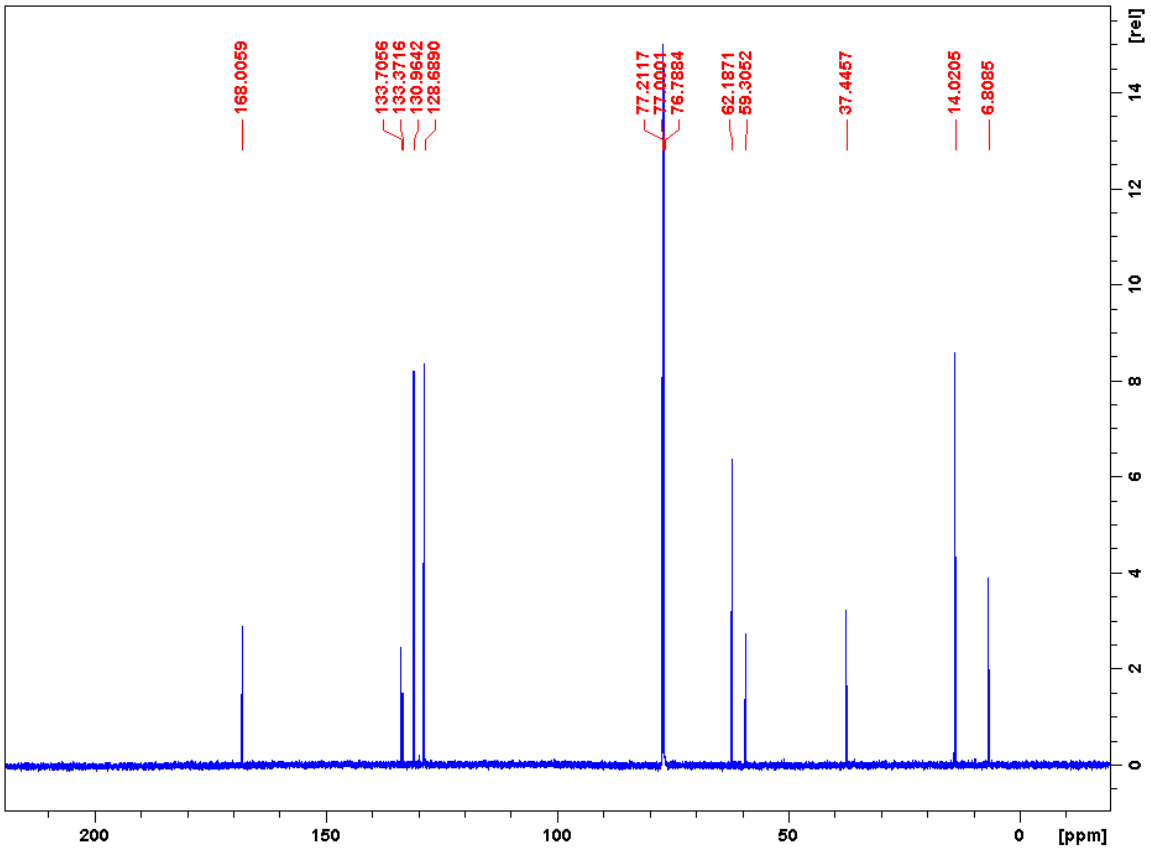
59.4148
55.1321
37.1702
14.0113
7.1566
[rel]
20
15
10
5
0
200
150
100
50
0
[ppm]


EtO
OEt
OMe
7.107
7.094
6.762
6.745
6.741
6.731
6.727
4.241
4.229
4.217
4.205
3.793
3.575
3.535
1.572
1.287
1.275
1.263
9
8
7
6
5
4
3
2
1
ppm
1.01
0.99
1.00
4.01
3.00
2.00
2.00
5.96
171.6713
159.1191
141.4675
131.9020
124.7394
113.0067
109.4990
77.2113
76.9997
76.7881
61.6574
60.7947
55.3776
40.6104
39.6552
14.0164
[rel]
200
150
100
50
0
[ppm]


EtO
OEt
I
Cl
7.283
7.277
7.263
7.160
7.146
4.292
4.280
4.274
4.268
4.262
4.256
4.250
4.236
4.230
4.224
4.218
4.212
4.206
4.194
3.449
3.365
1.300
1.288
1.276
9
8
7
6
5
4
3
2
1
ppm
2.00
2.00
4.00
2.00
2.00
6.01


168.0059
133.7056
133.3716
130.9642
128.6890
77.2117
77.0001
76.7884
62.1871
59.3062
37.4457
14.0205
6.8085
[rel]
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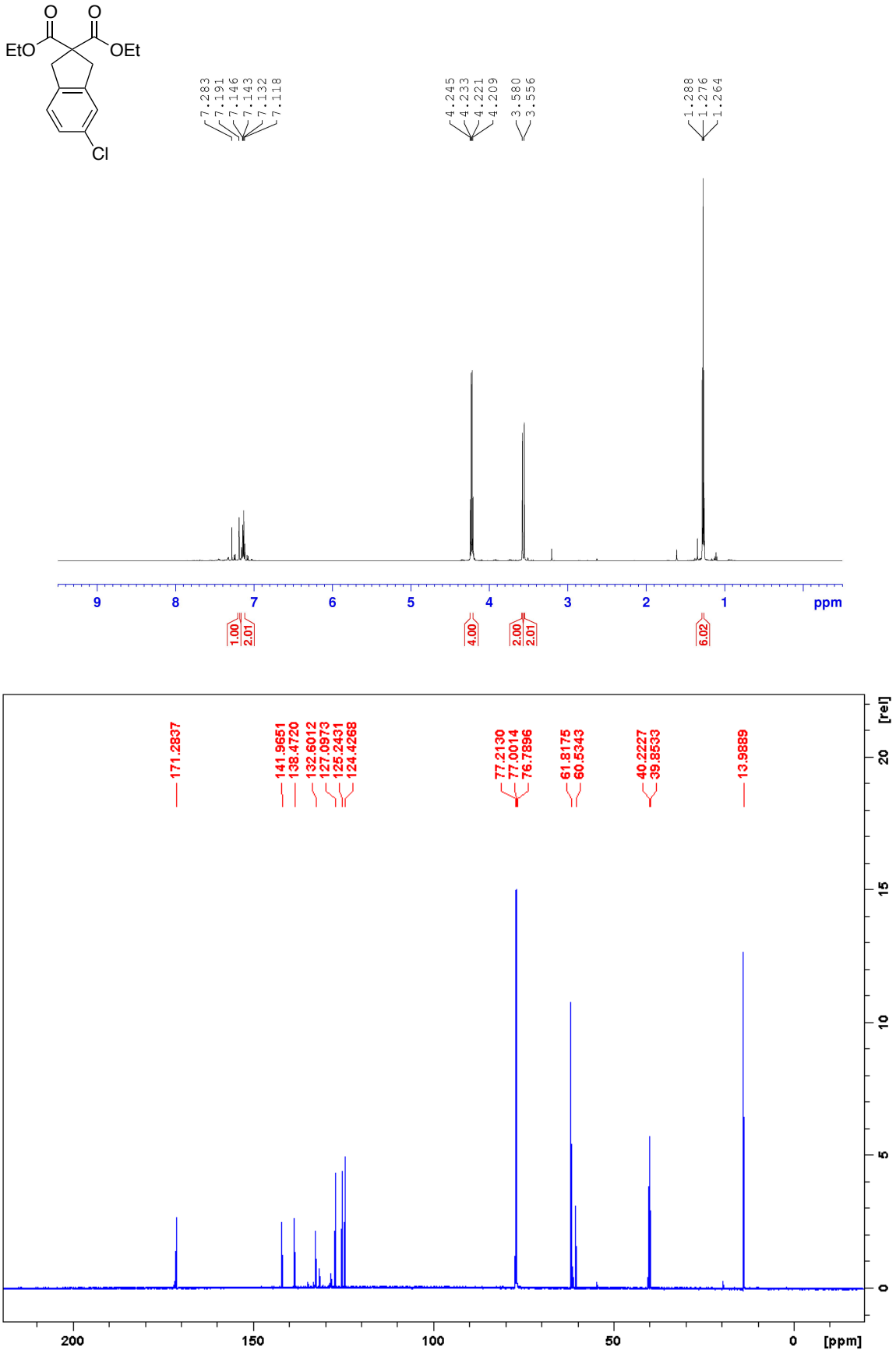
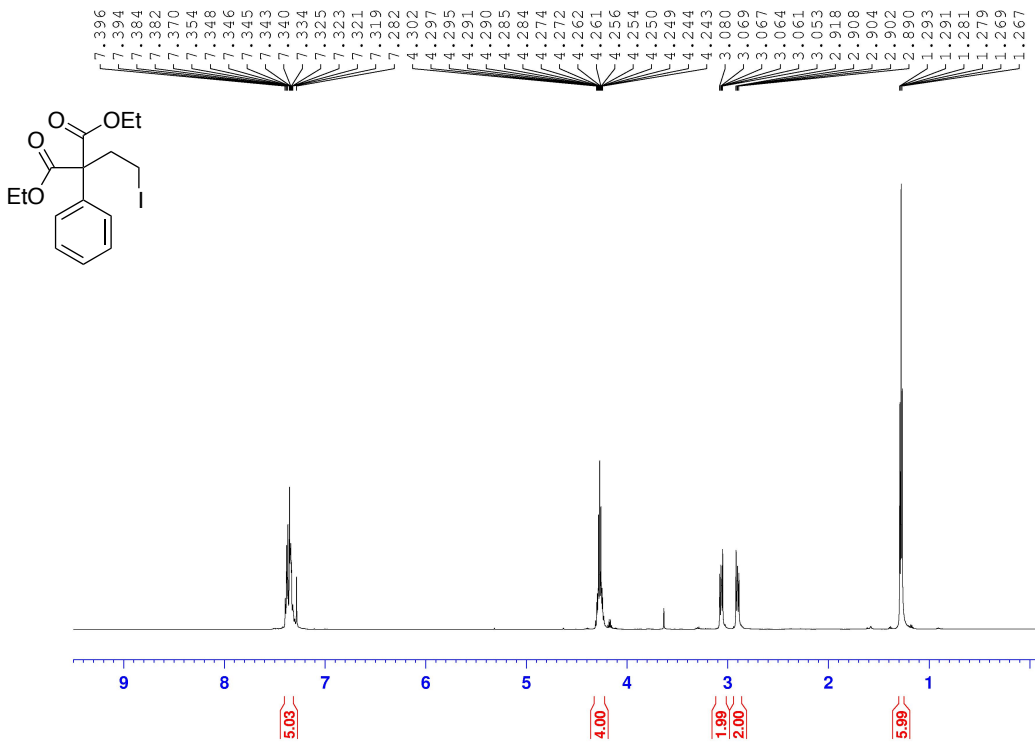
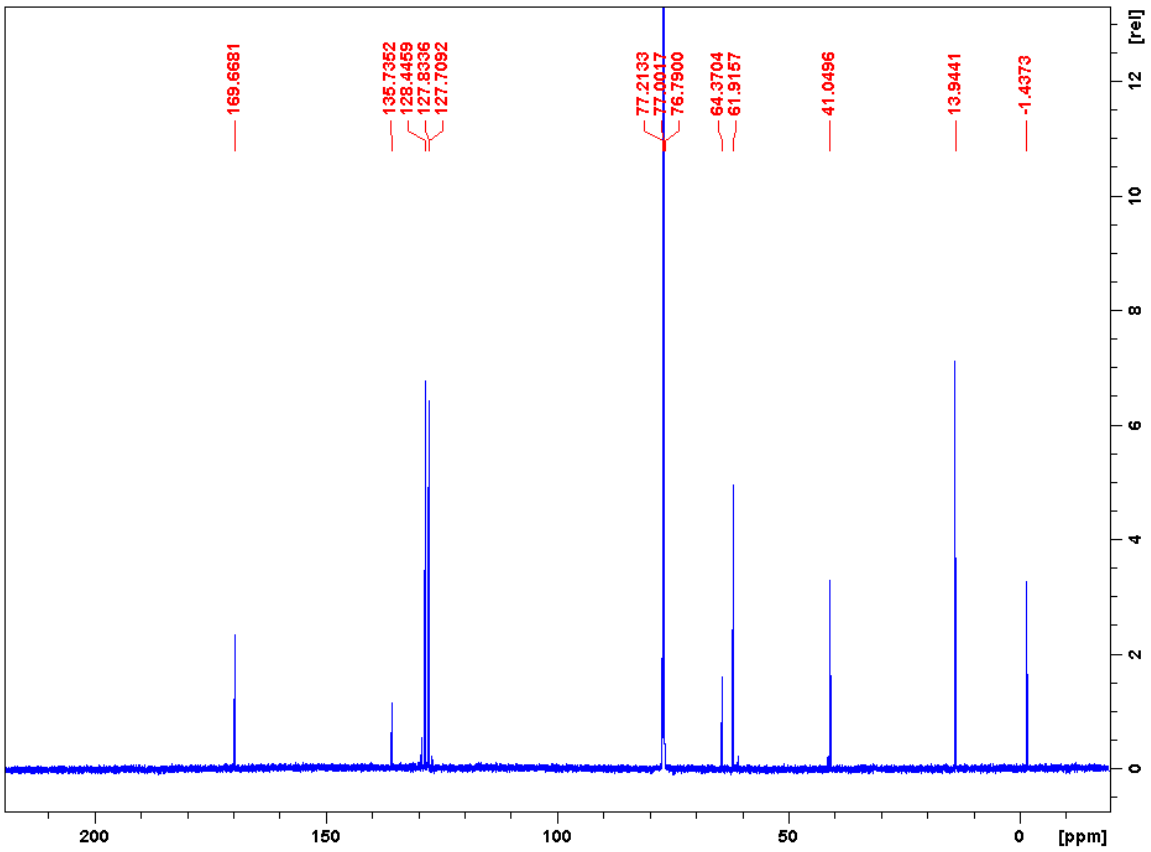
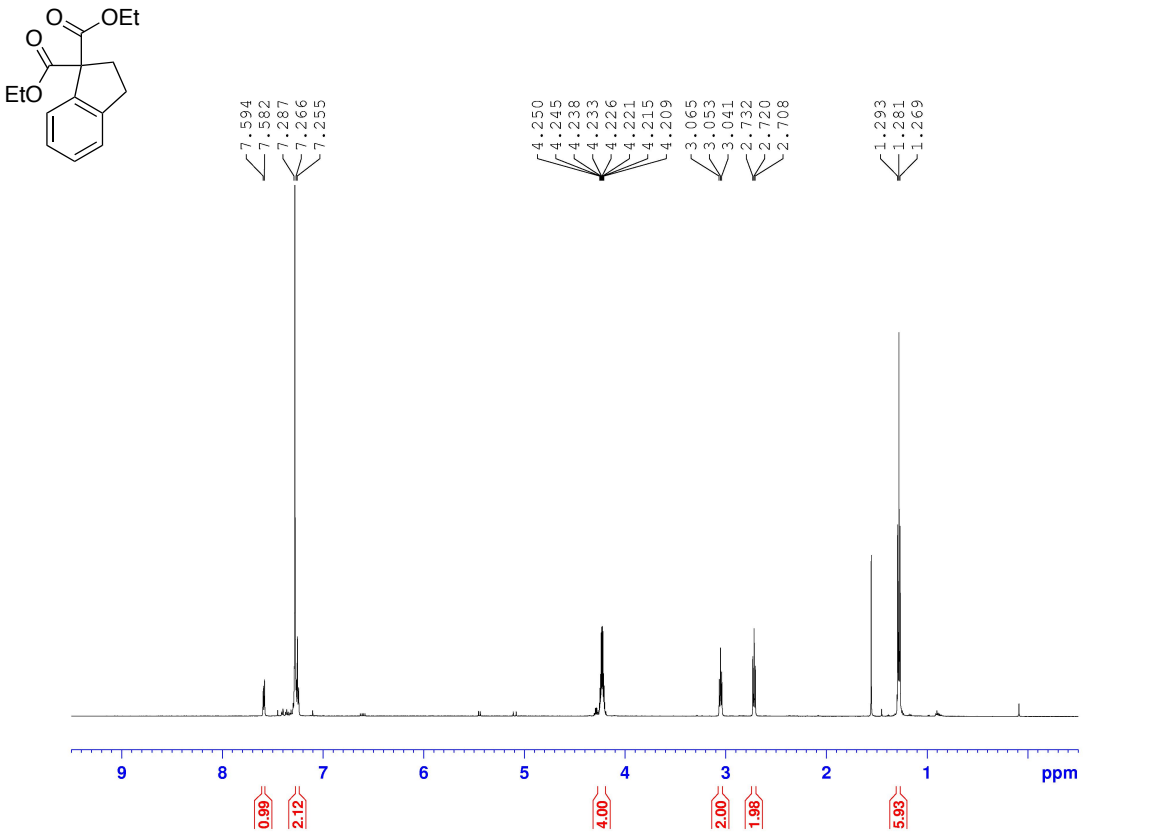
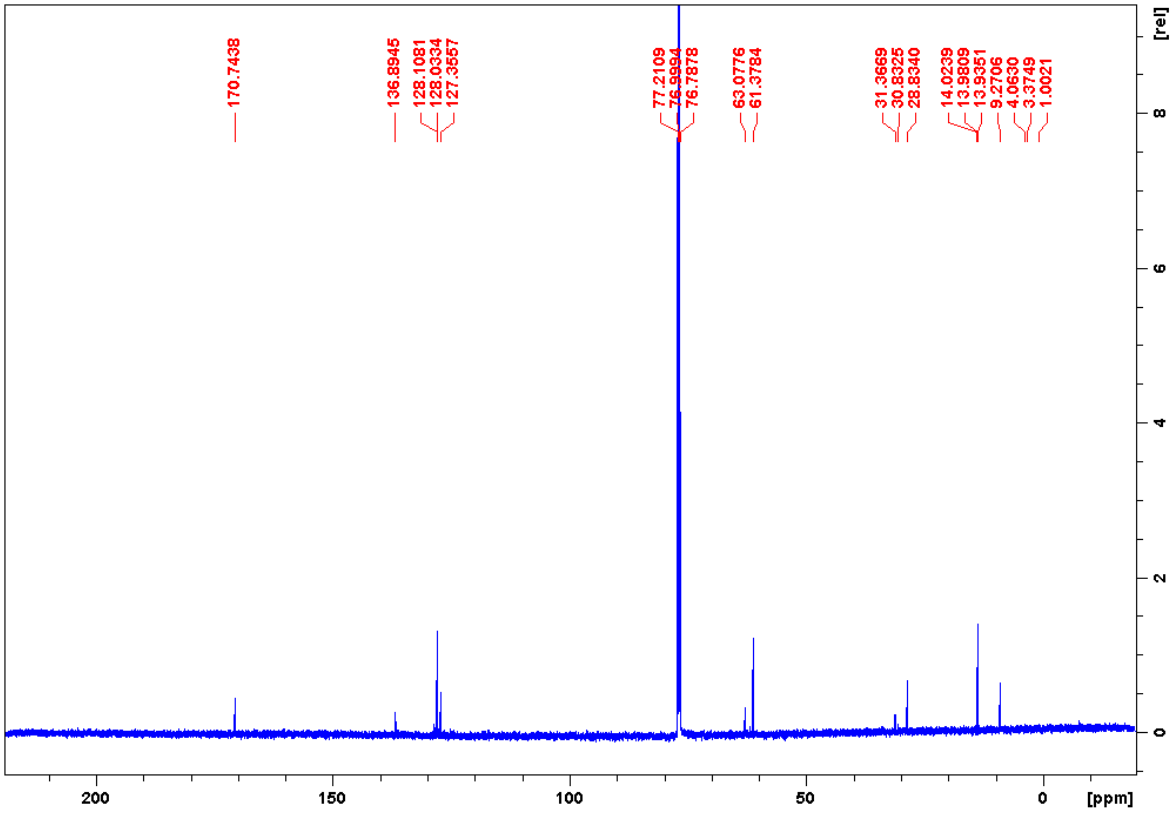
150
100
50
0
[ppm]

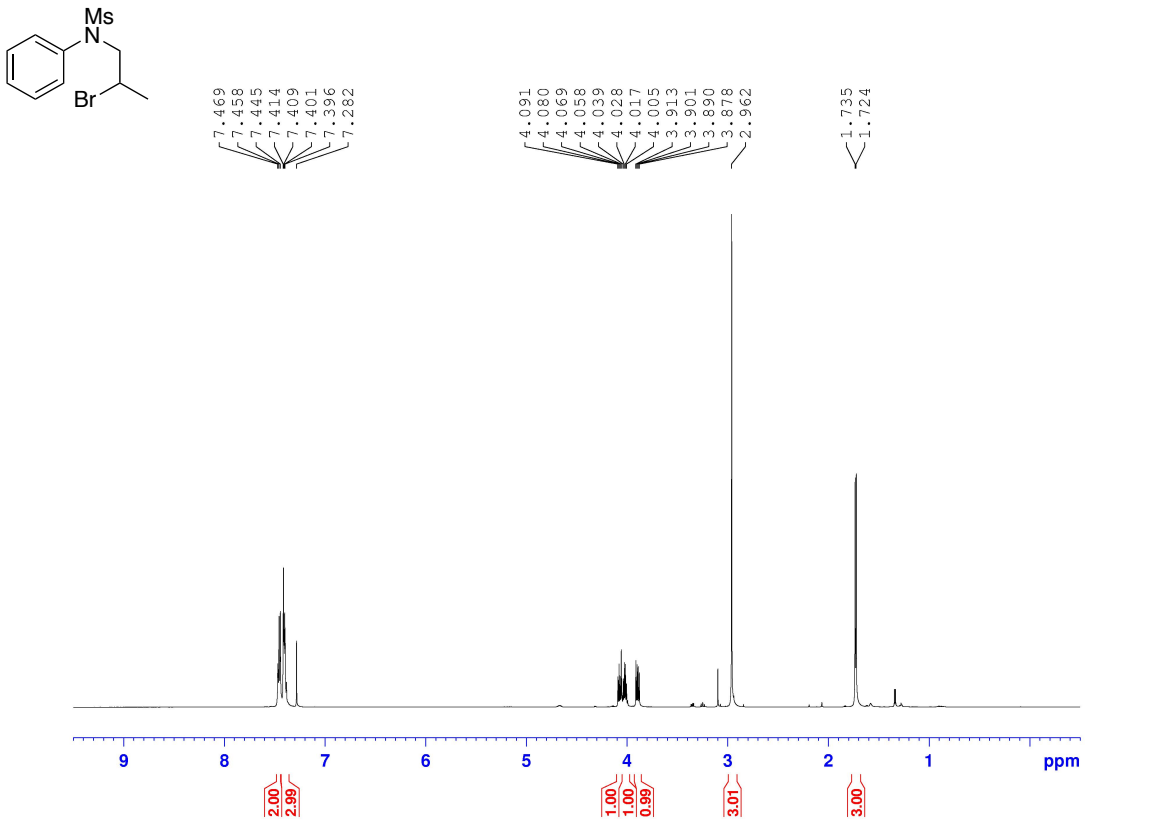

O
O
EtO
OEt
Cl
7.283
7.191
7.146
7.143
7.132
7.118
4.245
4.233
4.221
4.209
3.580
3.556
1.288
1.276
1.264
9
8
7
6
5
4
3
2
1
ppm
1.00
2.01
4.00
2.00
2.01
6.02
171.2837
141.9651
138.4720
132.6012
127.0973
125.2431
124.4268
77.2130
77.0014
76.7896
61.8175
60.5343
40.2227
39.8533
13.9889
[rel]
20
15
10
5
0
200
150
100
50
0
[ppm]

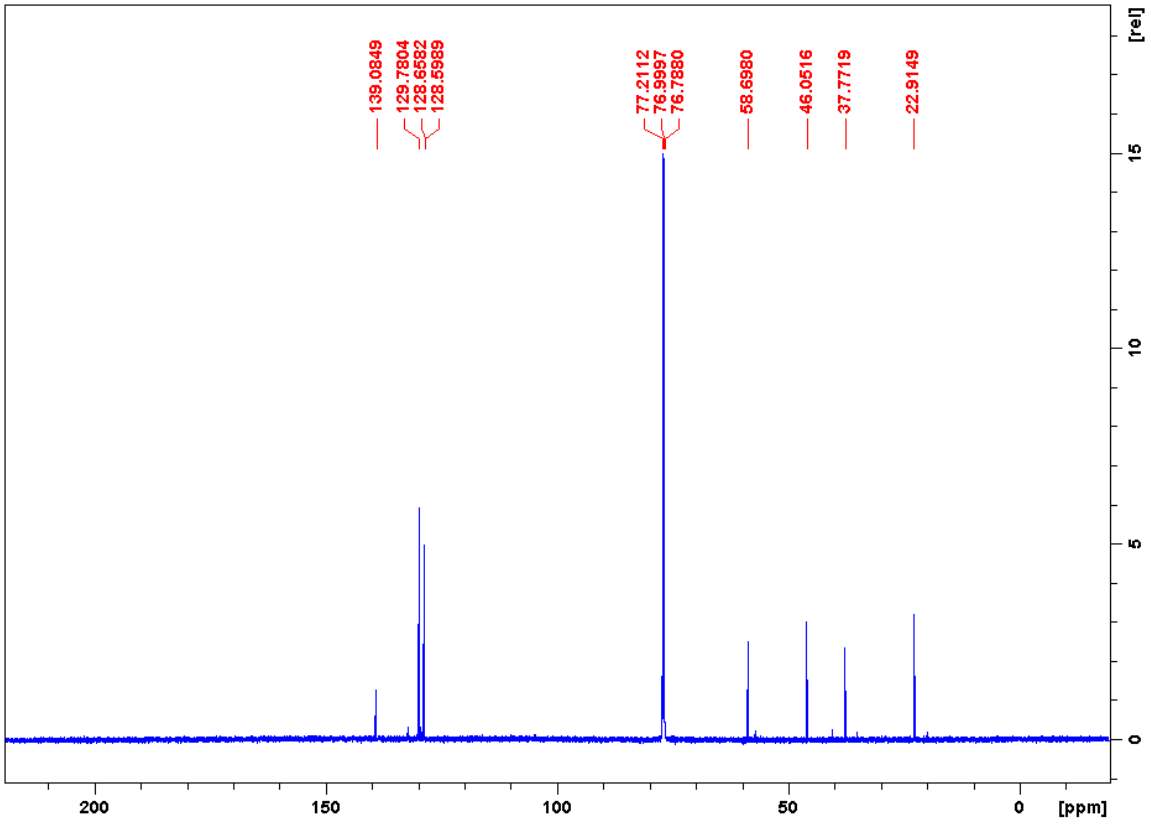

7.396
7.394
7.384
7.382
7.370
7.354
7.348
7.346
7.345
7.343
7.340
7.334
7.325
7.323
7.321
7.319
7.282
4.302
4.297
4.295
4.291
4.290
4.285
4.284
4.274
4.272
4.262
4.261
4.256
4.254
4.250
4.249
4.244
4.243
3.080
3.069
3.067
3.064
3.061
3.053
2.918
2.908
2.904
2.902
2.890
1.293
1.291
1.281
1.279
1.269
1.267
O
OEt
O
EtO
I
9
8
7
6
5
4
3
2
1
ppm
5.03
4.00
1.99
2.00
5.99

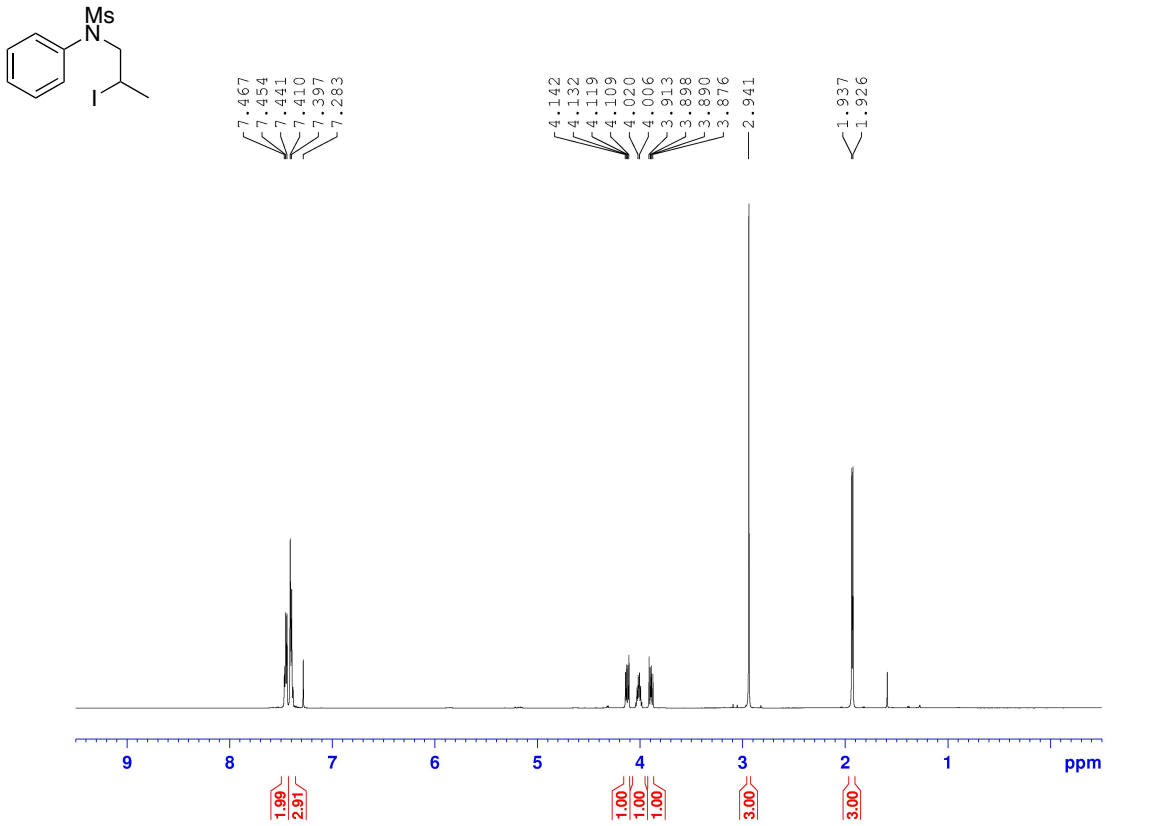

169.6681
135.7352
128.4459
127.8336
127.7092
77.2133
77.0017
76.7900
64.3704
61.9157
41.0496
13.9441
-1.4373
[rel]
12
10
8
6
4
2
0
200
150
100
50
0
[ppm]

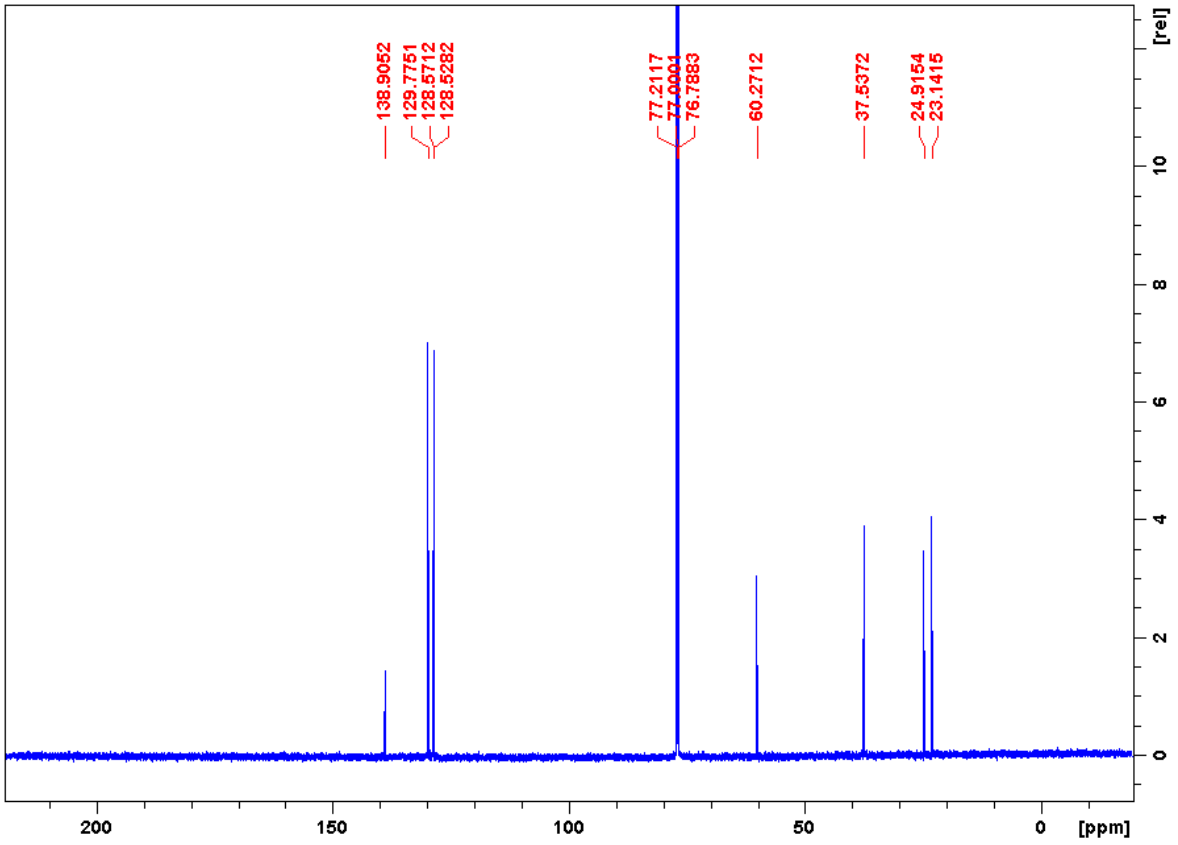

O
OEt
O
EtO
7.594
7.582
7.287
7.266
7.255
4.250
4.245
4.238
4.233
4.226
4.221
4.215
4.209
3.065
3.053
3.041
2.732
2.720
2.708
1.293
1.281
1.269
9
8
7
6
5
4
3
2
1
ppm
0.99
2.12
4.00
2.00
1.98
5.93

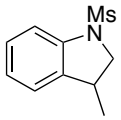

170.7438
136.8945
128.1081
128.0334
127.3557
77.2109
76.9954
76.7878
63.0776
61.3784
31.3669
30.8325
28.8340
14.0239
13.9809
13.9351
9.2706
4.0630
3.3749
1.0021
[rel]
200
150
100
50
0
[ppm]

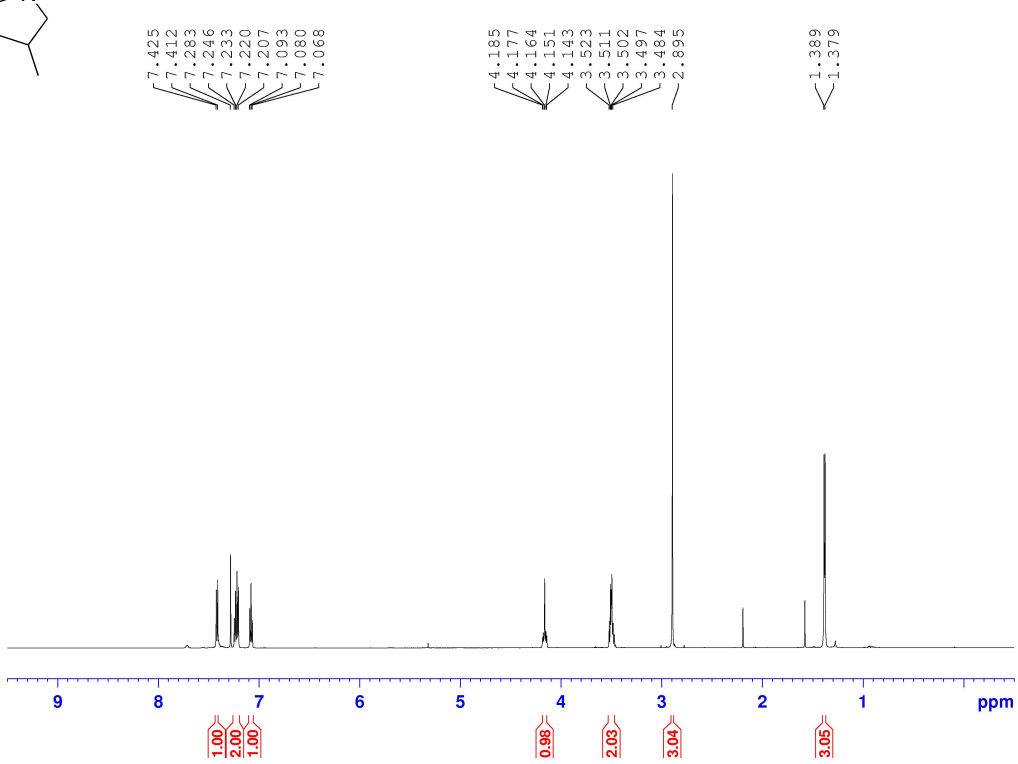

Ms
N
Br
7.469
7.458
7.445
7.414
7.409
7.401
7.396
7.282
4.091
4.080
4.069
4.058
4.039
4.028
4.017
4.005
3.913
3.901
3.890
3.878
2.962
1.735
1.724
9
8
7
6
5
4
3
2
1
ppm
2.00
2.99
1.00
1.00
0.99
3.01
3.00

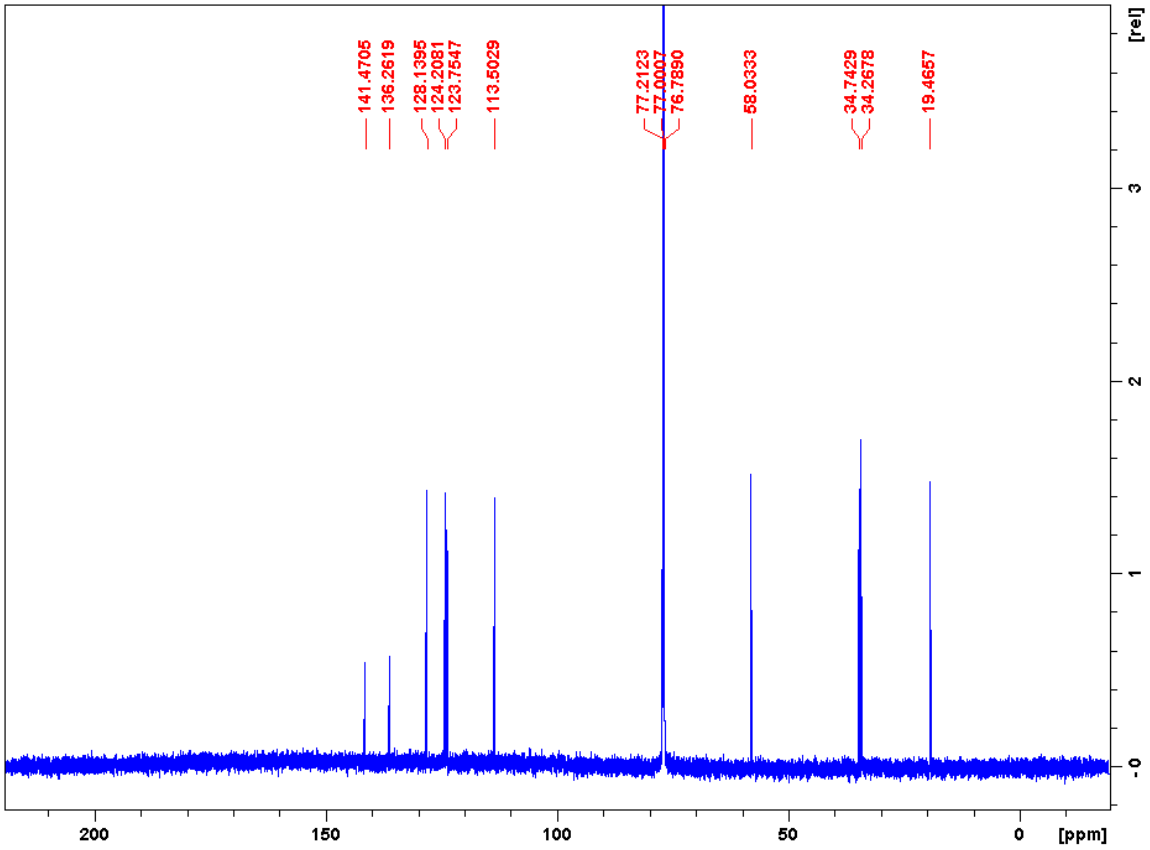

139.0849
129.7804
128.6582
128.5989
77.2112
76.9997
76.7880
58.6980
46.0516
37.7719
22.9149
[rel]
15
10
5
0
200
150
100
50
0
[ppm]

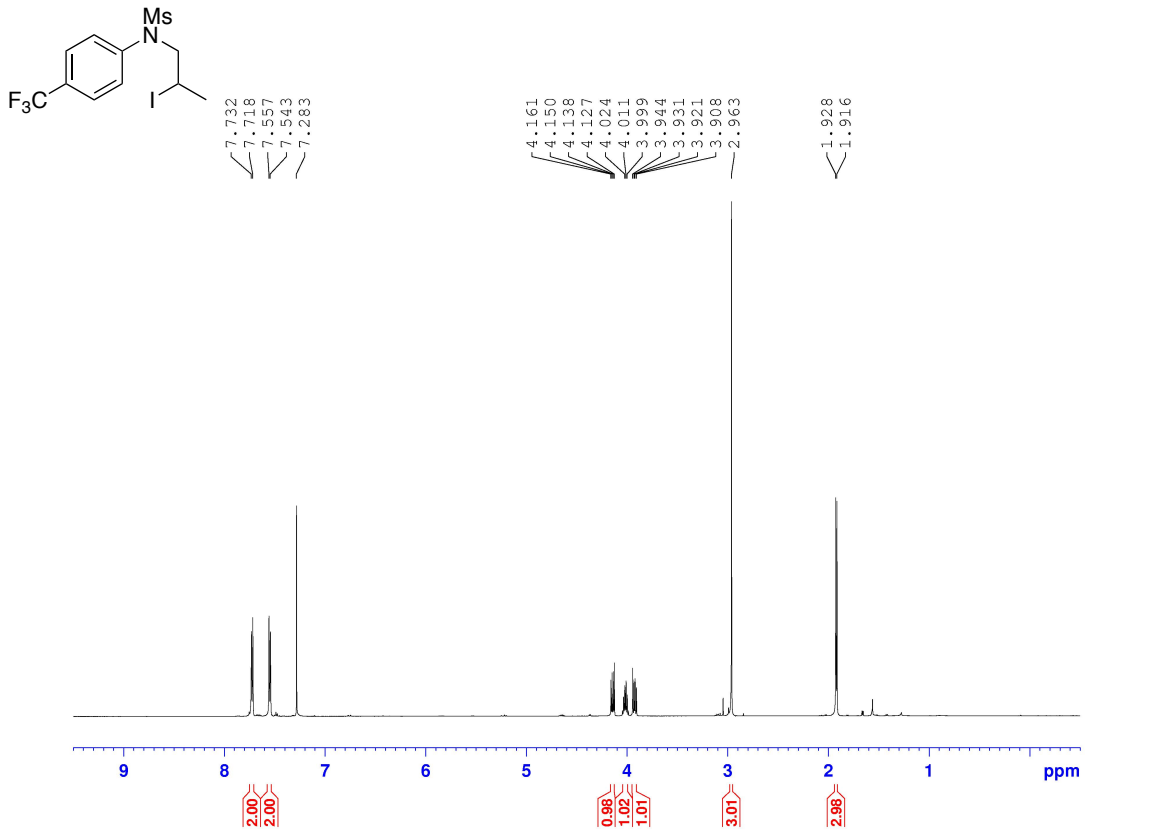

Ms
N
I
7.467
7.454
7.441
7.410
7.397
7.283
4.142
4.132
4.119
4.109
4.020
4.006
3.913
3.898
3.890
3.876
2.941
1.937
1.926
9
8
7
6
5
4
3
2
1
ppm
1.99
2.91
1.00
1.00
1.00
3.00
3.00

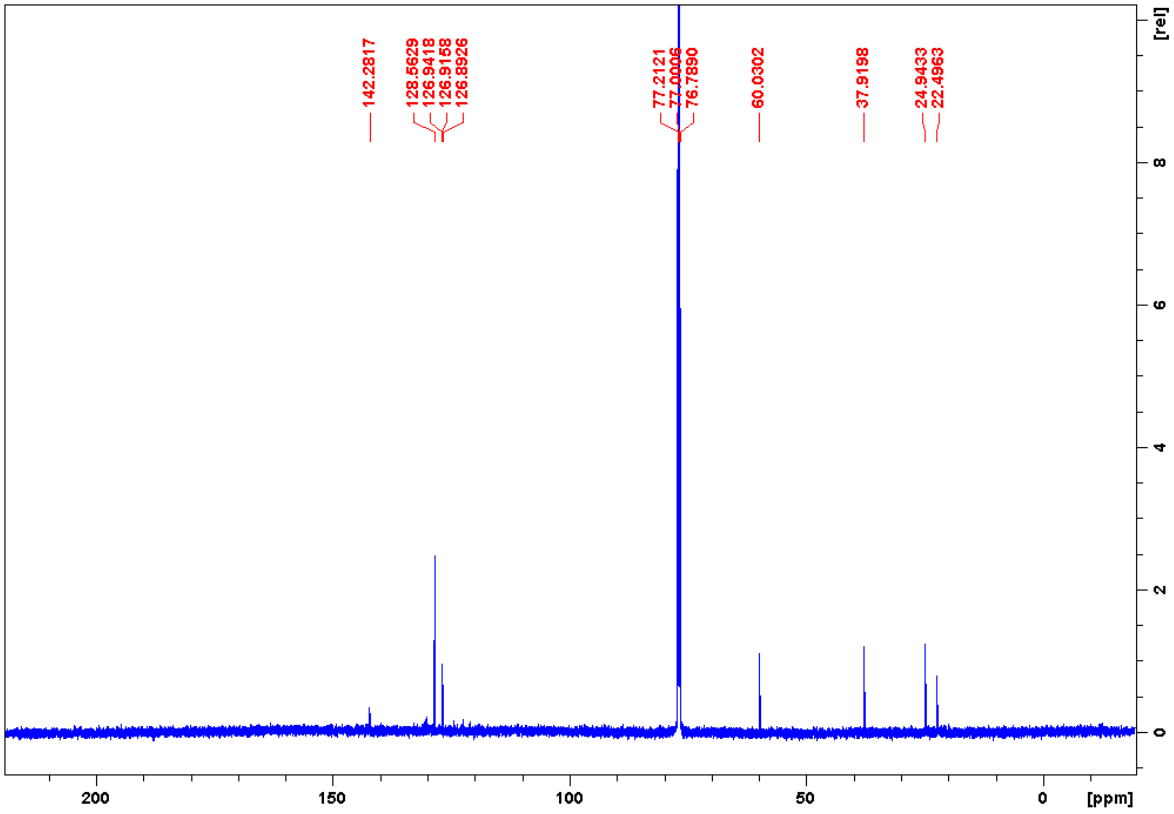

138.9052
129.7751
128.5712
128.5282
77.2117
77.0001
76.7883
60.2712
37.5372
24.9154
23.1415
[rel]
200
150
100
50
0
[ppm]

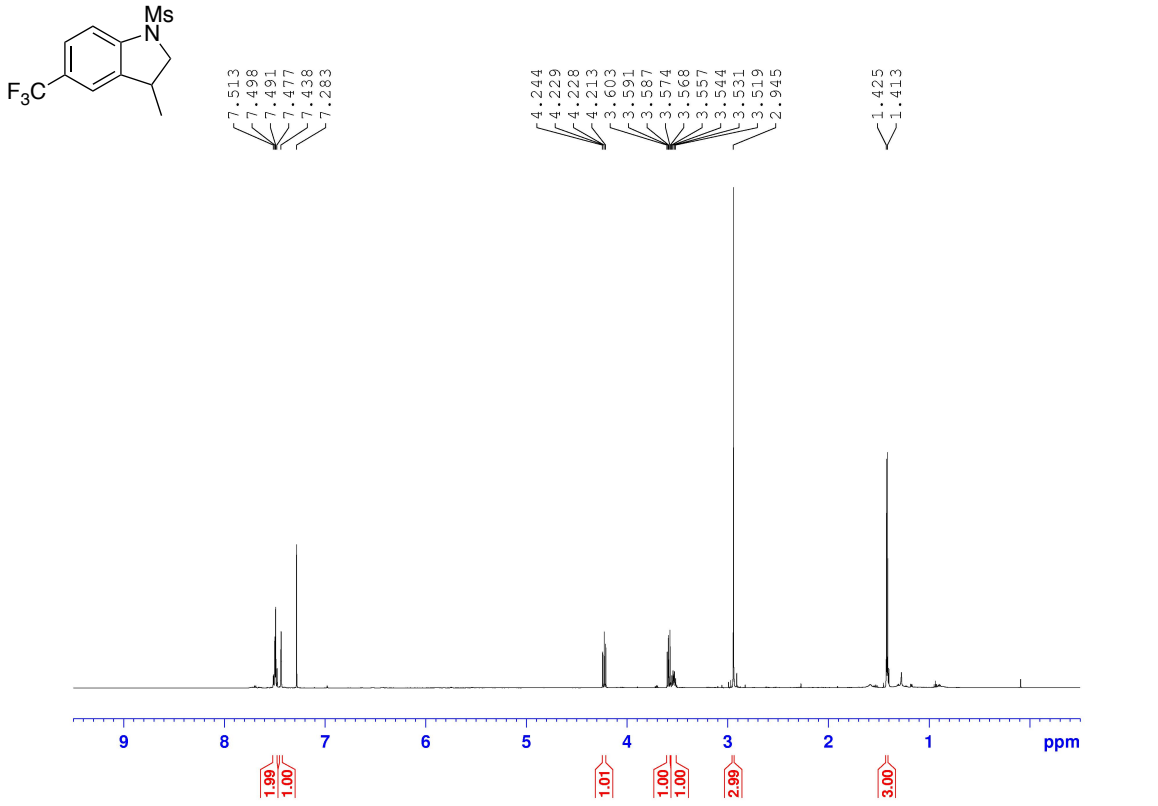

Ms
N


7.425
7.412
7.283
7.246
7.233
7.220
7.207
7.093
7.080
7.068
4.185
4.177
4.164
4.151
4.143
3.523
3.511
3.502
3.497
3.484
2.895
1.389
1.379
9
8
7
6
5
4
3
2
1
ppm
1.00
2.00
1.00
0.98
2.03
3.04
3.05


141.4705
136.2619
128.1395
124.2081
123.7547
113.5029
77.2123
77.0007
76.7890
58.0333
34.7429
34.2678
19.4657
[rel]
3
2
1
-0
200
150
100
50
0
[ppm]


Ms
N
F3C
I
7.732
7.718
7.557
7.543
7.283
4.161
4.150
4.138
4.127
4.024
4.011
3.999
3.944
3.931
3.921
3.908
2.963
1.928
1.916
9
8
7
6
5
4
3
2
1
ppm
2.00
2.00
0.98
1.02
1.01
3.01
2.98


142.2817
128.5629
126.9418
126.9158
126.8926
77.2121
77.0006
76.7890
60.0302
37.9198
24.9433
22.4963
[rel]
200
150
100
50
0
[ppm]


Ms
N
F3C
7.513
7.498
7.491
7.477
7.438
7.283
4.244
4.229
4.228
4.213
3.603
3.591
3.587
3.574
3.568
3.557
3.544
3.531
3.519
2.945
1.425
1.413
9
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4
3
2
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ppm
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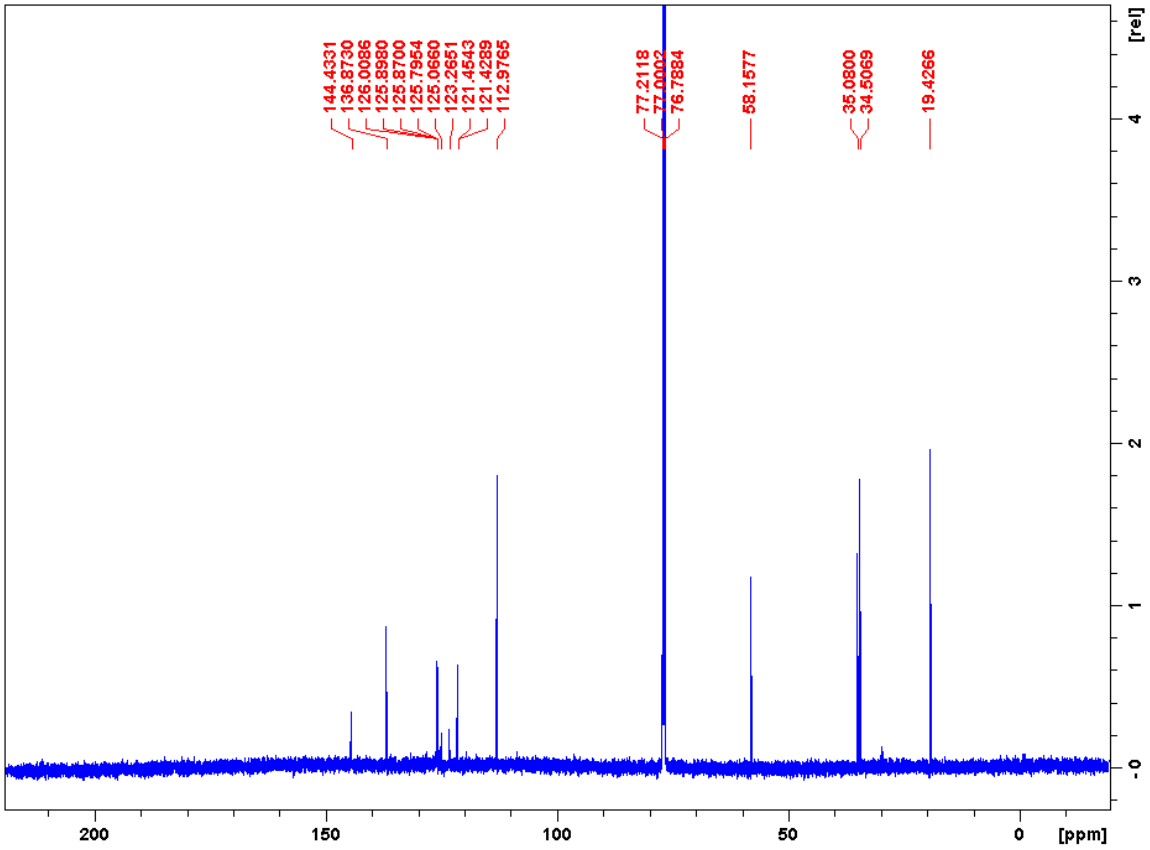
1.00
1.01
1.00
1.00
2.99
3.00


144.4331
136.8730
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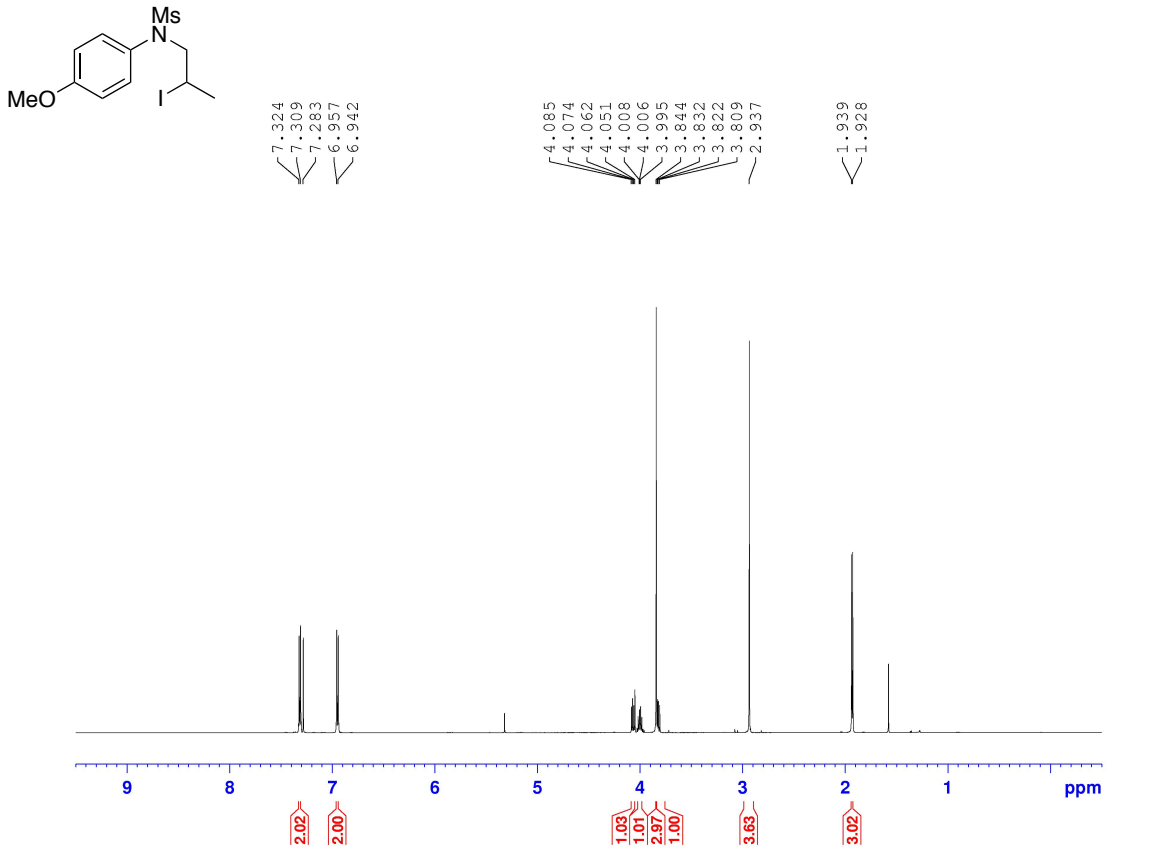
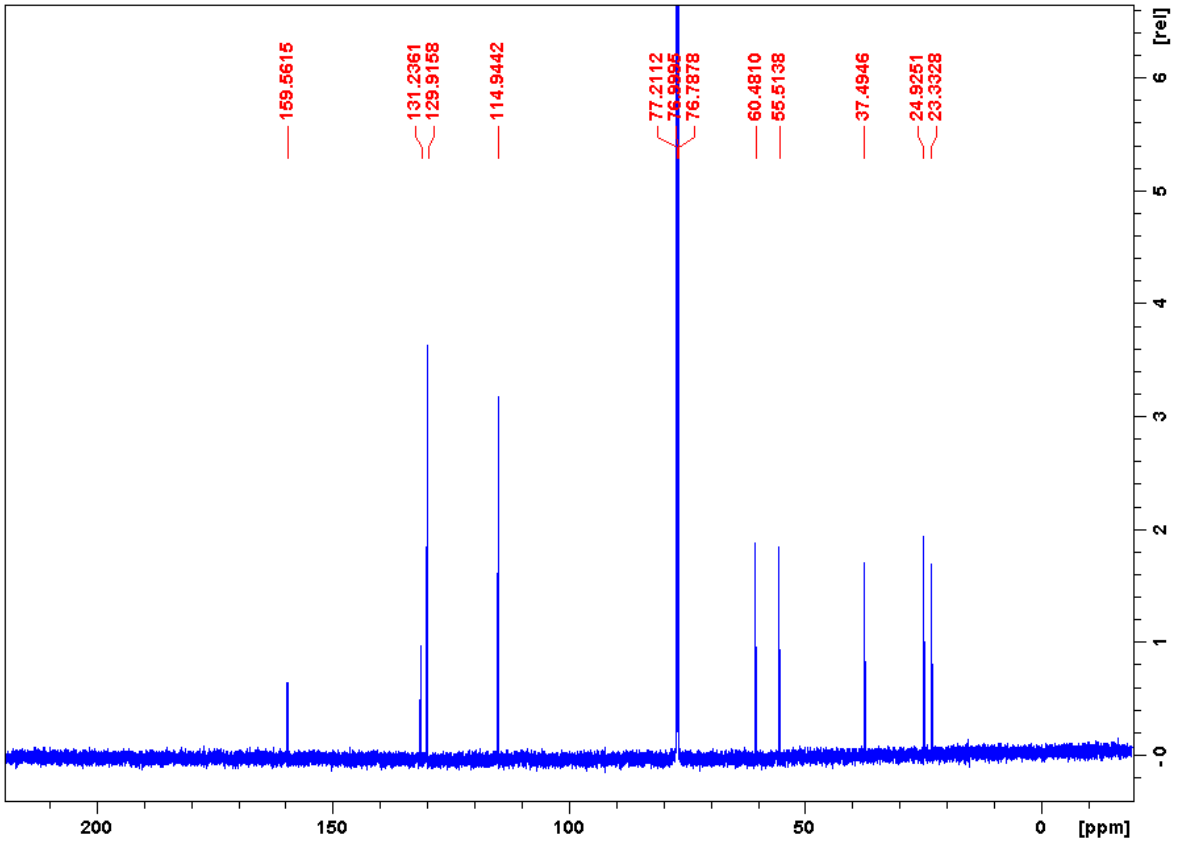
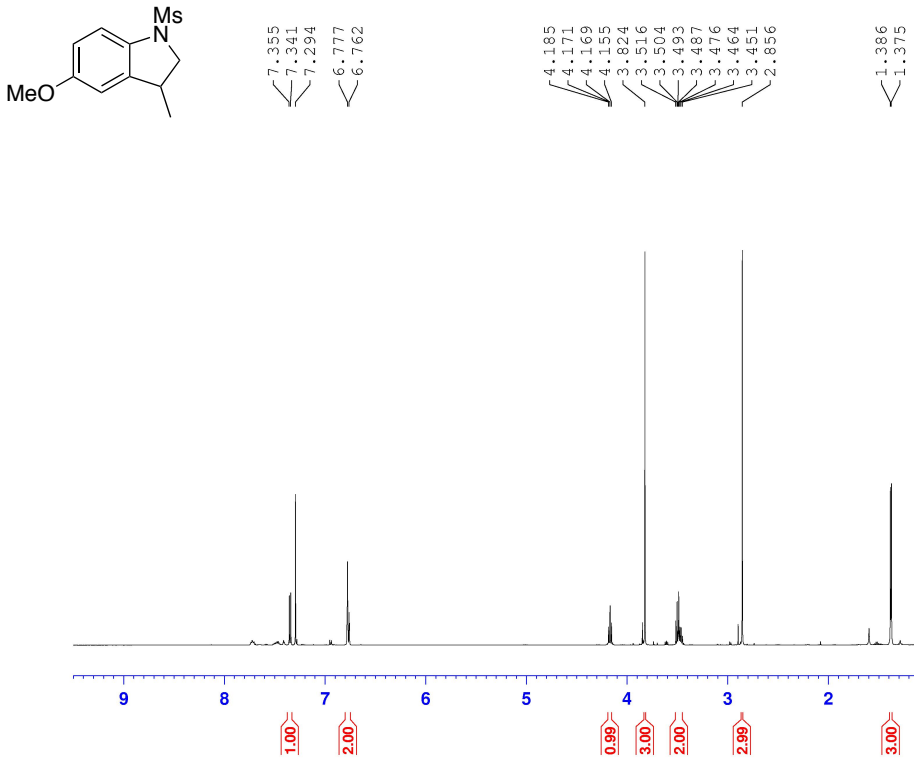
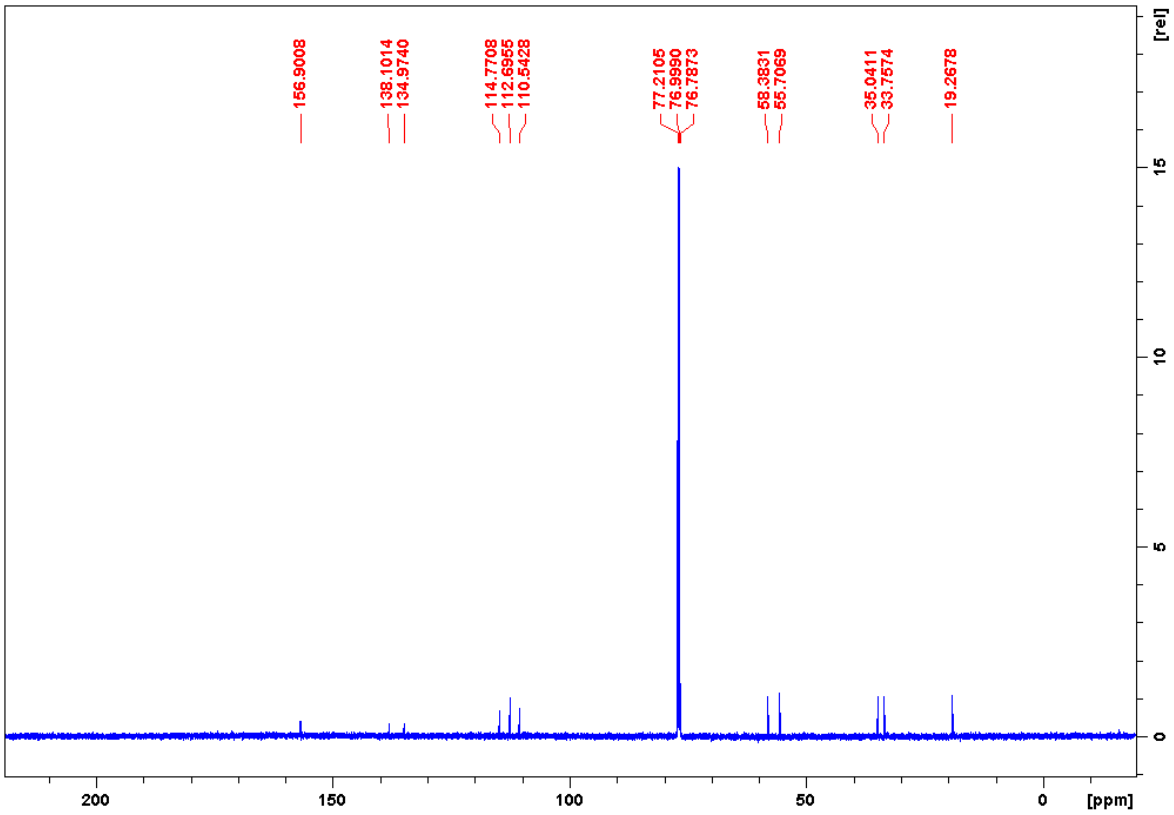
125.8980
125.8700
125.7954
125.0660
123.2651
121.4543
121.4289
112.9765
77.2118
77.0002
76.7884
58.1577
35.0800
34.5069
19.4266
[rel]
4
3
2
1
-0
200
150
100
50
0
[ppm]


Ms
N
MeO
I
7.324
7.309
7.283
6.957
6.942
4.085
4.074
4.062
4.051
4.008
4.006
3.995
3.844
3.832
3.822
3.809
2.937
1.939
1.928
9
8
7
6
5
4
3
2
1
ppm
2.02
2.00
1.03
1.01
2.97
1.00
3.63
3.02


159.5615
131.2361
129.9158
114.9442
77.2112
76.7878
60.4810
55.5138
37.4946
24.9251
23.3328
[rel]
200
150
100
50
0
[ppm]


Ms
N
MeO
7.355
7.341
7.294
6.777
6.762
4.185
4.171
4.169
4.155
3.824
3.516
3.504
3.493
3.487
3.476
3.464
3.451
2.856
1.386
1.375
9
8
7
6
5
4
3
2
1
ppm
1.00
2.00
0.99
3.00
2.00
2.99
3.00


156.9008
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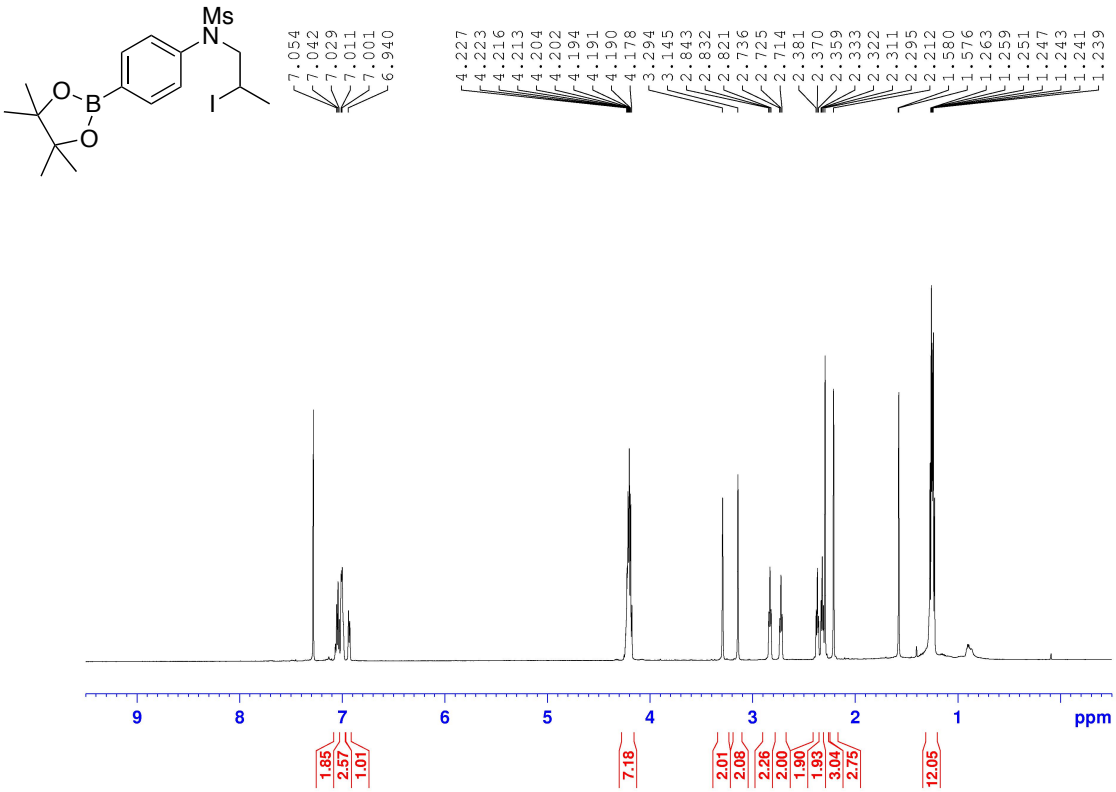
134.9740
114.7708
112.6955
110.5428
77.2105
76.9990
76.7873
58.3831
55.7069
35.0411
33.7574
19.2678
[rel]
15
10
5
0
200
150
100
50
0
[ppm]


Ms
N
O
B
O
I
7.054
7.042
7.029
7.011
7.001
6.940
4.227
4.223
4.216
4.213
4.204
4.202
4.194
4.191
4.190
4.178
3.294
3.145
2.843
2.832
2.821
2.736
2.725
2.714
2.381
2.370
2.359
2.333
2.322
2.311
2.295
2.212
1.580
1.576
1.263
1.259
1.251
1.247
1.243
1.241
1.239
9
8
7
6
5
4
3
2
1
ppm
1.85
2.57
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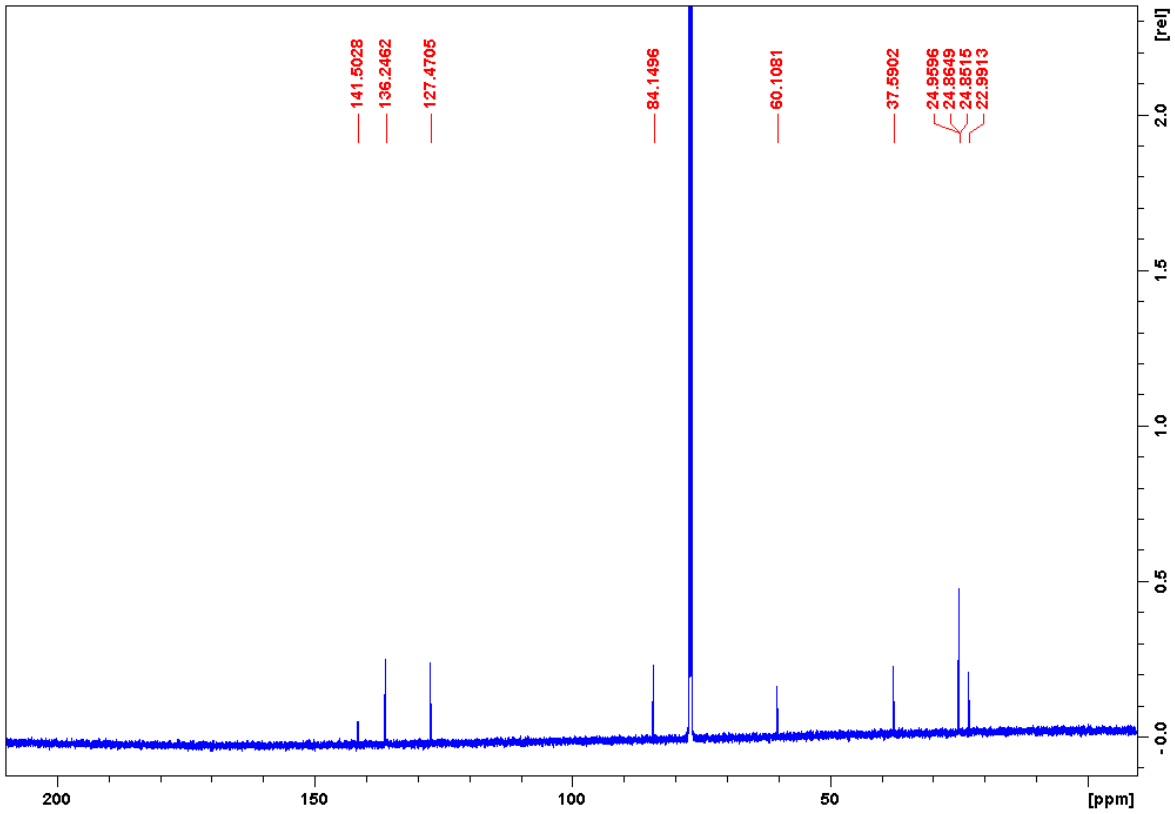
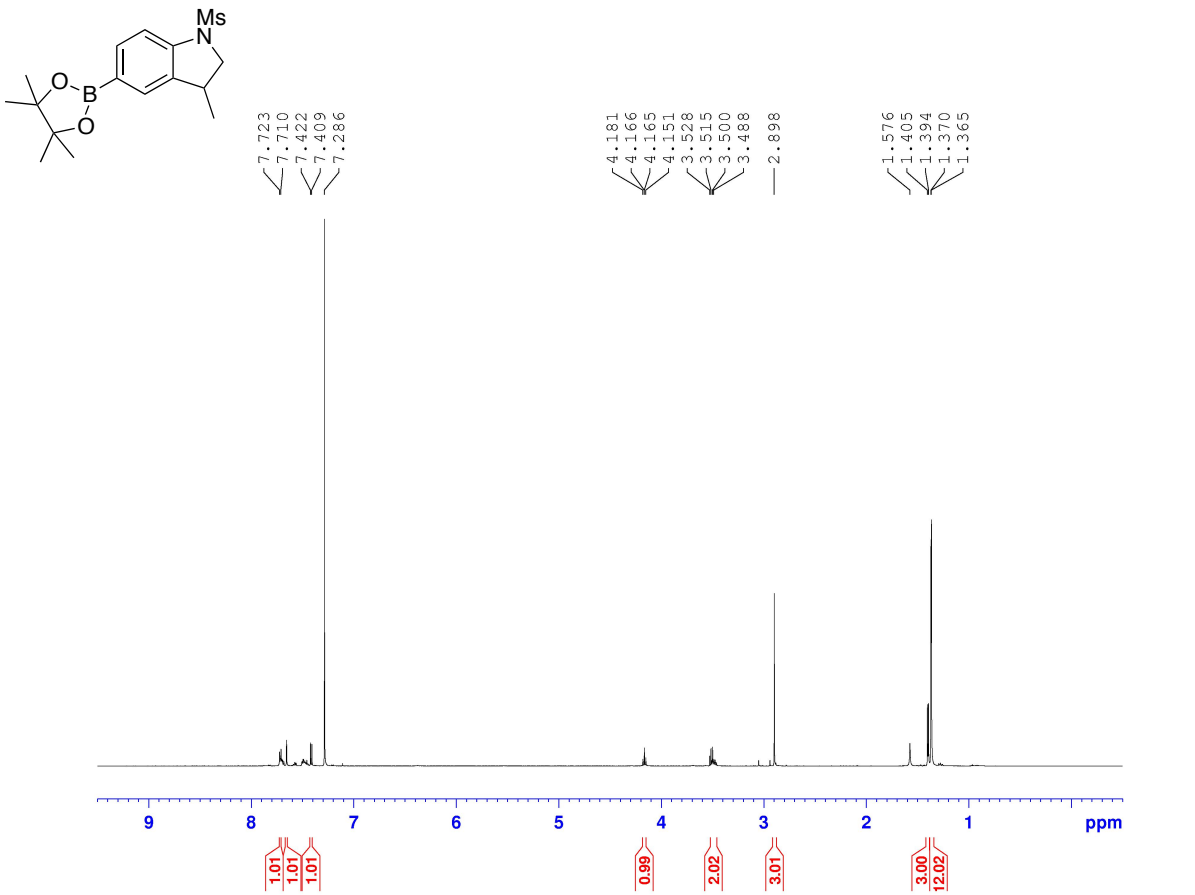
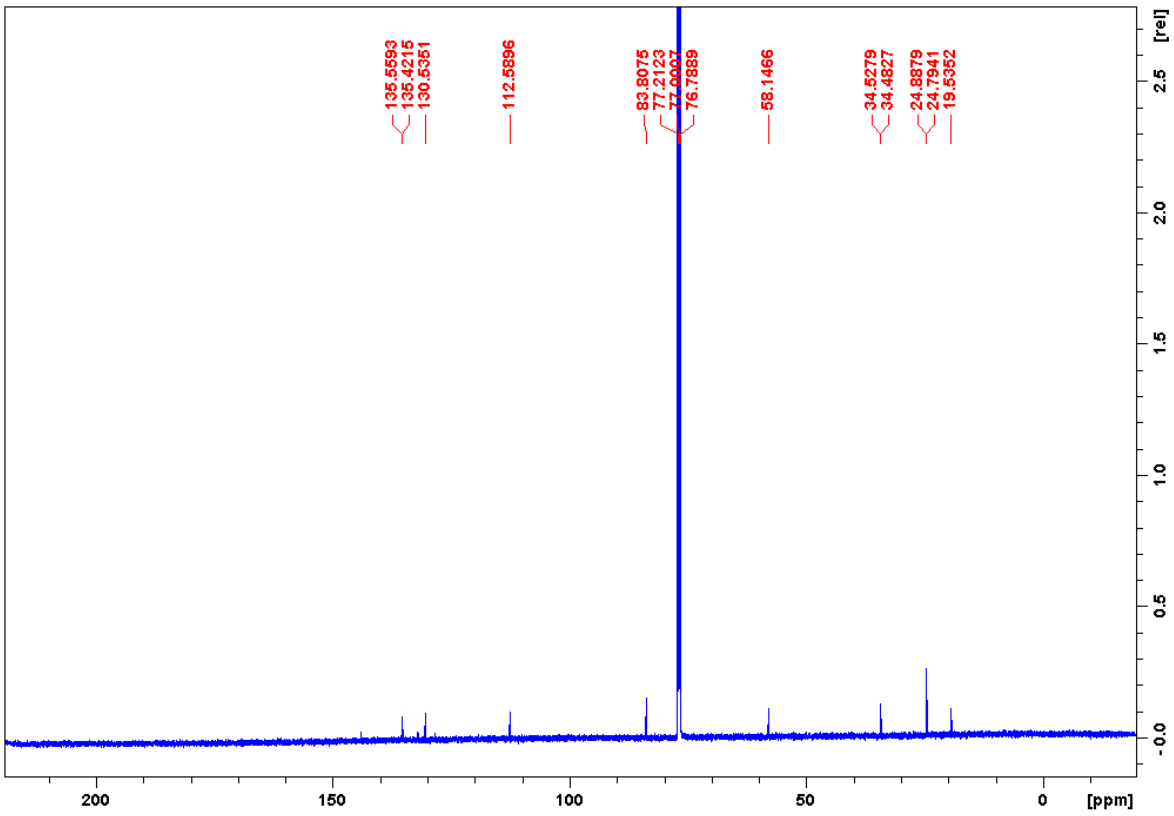
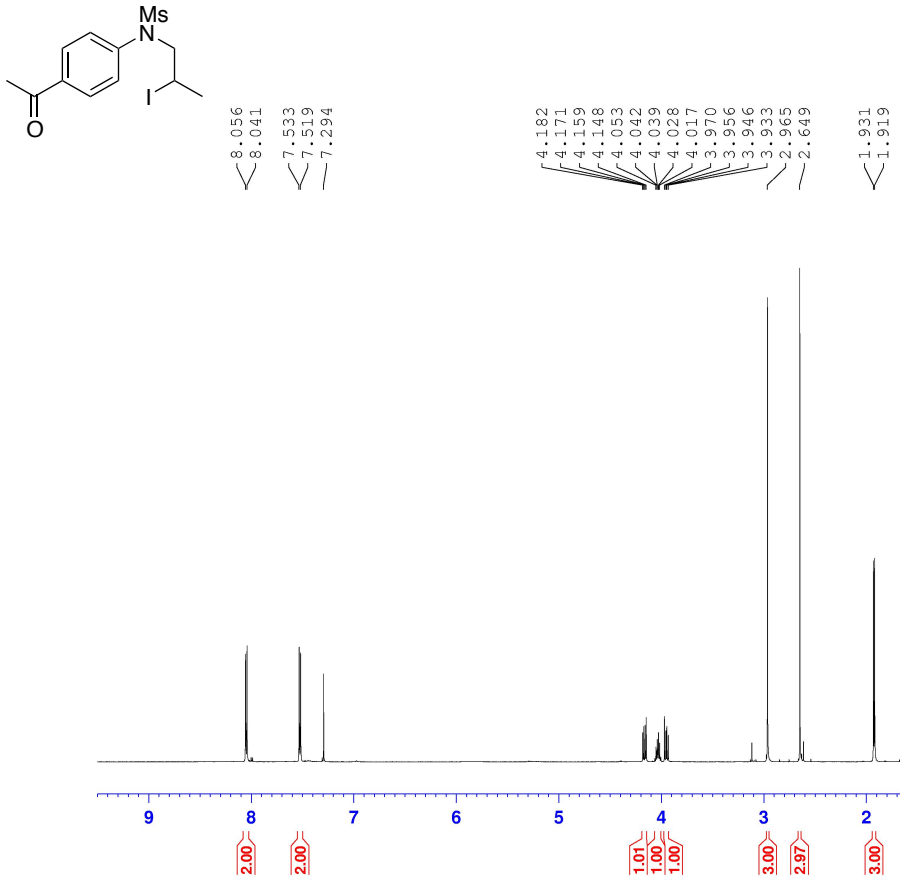
2.01
2.08
2.26
2.00
1.90
1.93
3.04
2.75
12.05


141.5028
136.2462
127.4705
84.1496
60.1081
37.5902
24.9596
24.8649
24.8515
22.9913
[rel]
2.0
1.5
1.0
0.5
-0.0
200
150
100
50
[ppm]


Ms
N
O
B
O
7.723
7.710
7.422
7.409
7.286
4.181
4.166
4.165
4.151
3.528
3.515
3.500
3.488
2.898
1.576
1.405
1.394
1.370
1.365
9
8
7
6
5
4
3
2
1
ppm
1.01
1.01
1.01
0.99
2.02
3.01
3.00
12.02


135.5593
135.4215
130.5351
112.5896
83.8075
77.2123
77.0007
76.7889
58.1466
34.5279
34.4827
24.8879
24.7941
19.5362
[rel]
2.5
2.0
1.5
1.0
0.5
-0.0
200
150
100
50
0
[ppm]


Ms
N
I
O
8.056
8.041
7.533
7.519
7.294
4.182
4.171
4.159
4.148
4.053
4.042
4.039
4.028
4.017
3.970
3.956
3.946
3.933
2.965
2.649
1.931
1.919
9
8
7
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1.00
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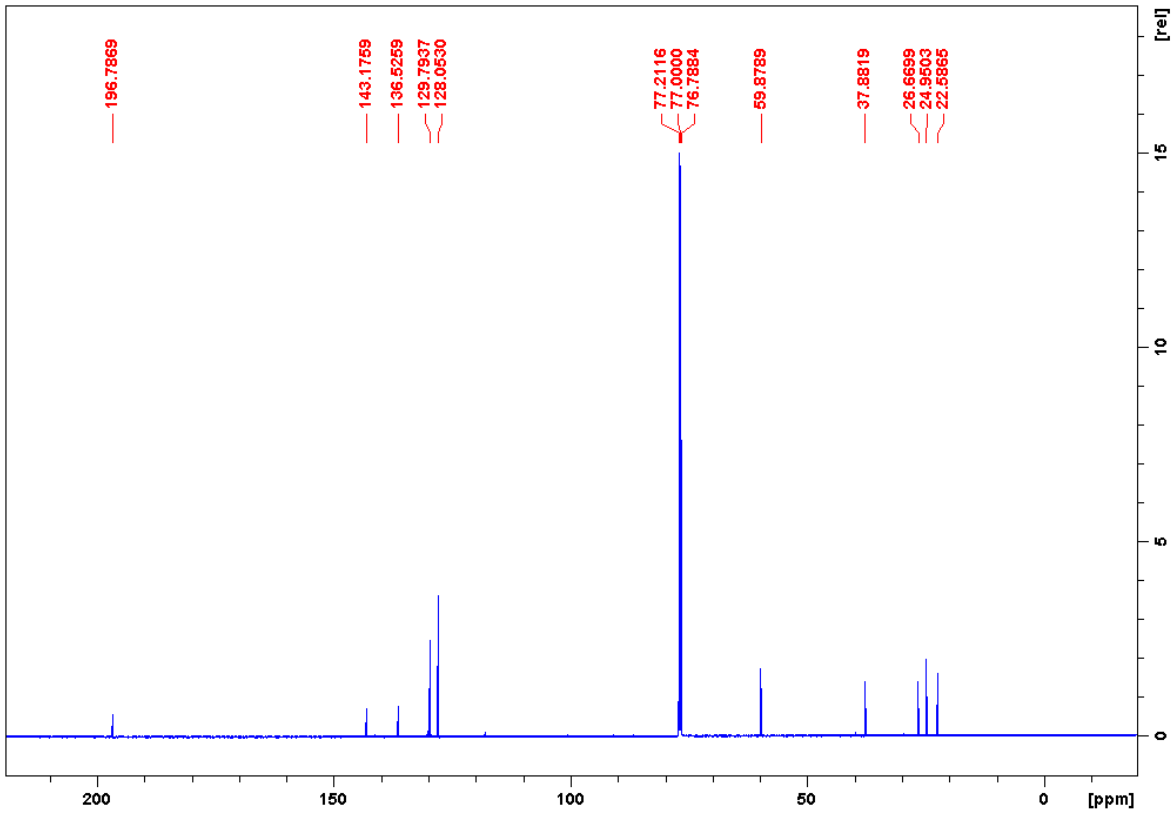
2.97
3.00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77.0000
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59.8789
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24.9503
22.5865
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50
0
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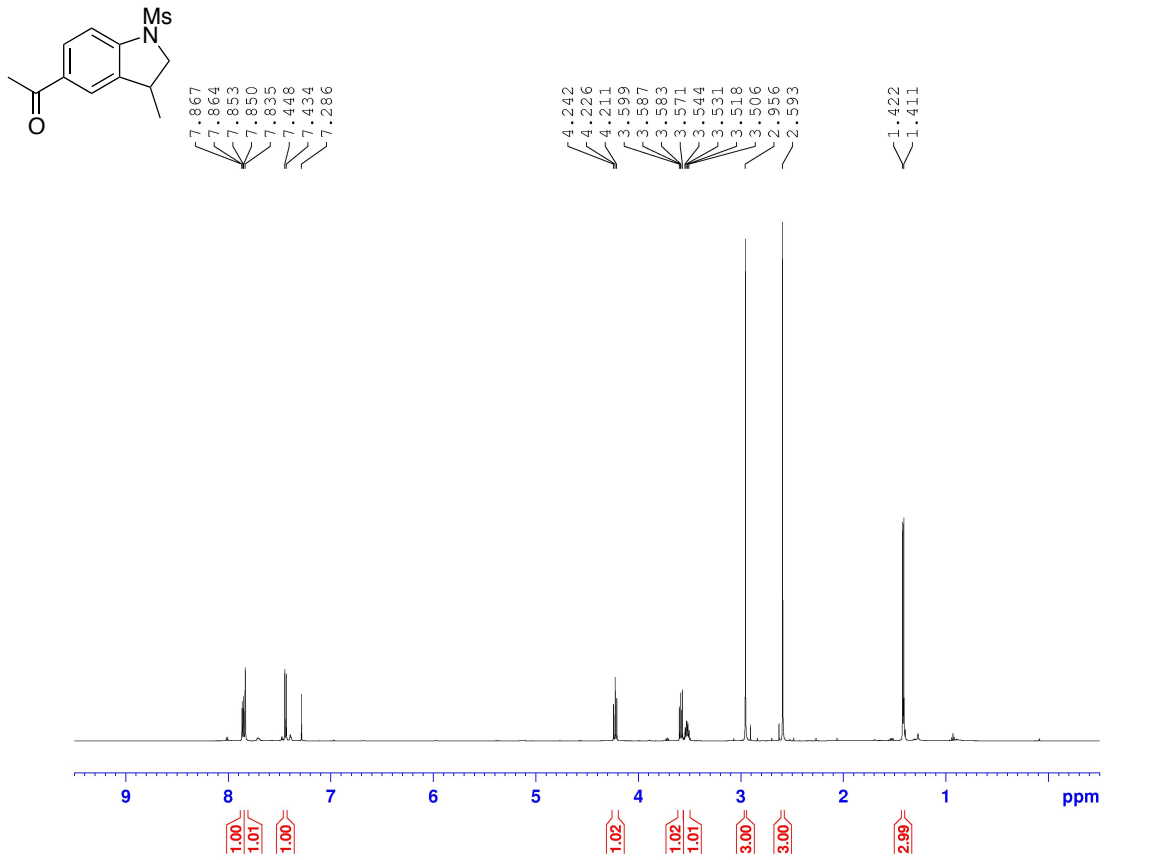
Ms
N
O
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7.850
7.835
7.448
7.434
7.286
4.242
4.226
4.211
3.599
3.587
3.583
3.571
3.544
3.531
3.518
3.506
2.956
2.593
1.422
1.411
9
8
7
6
5
4
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ppm
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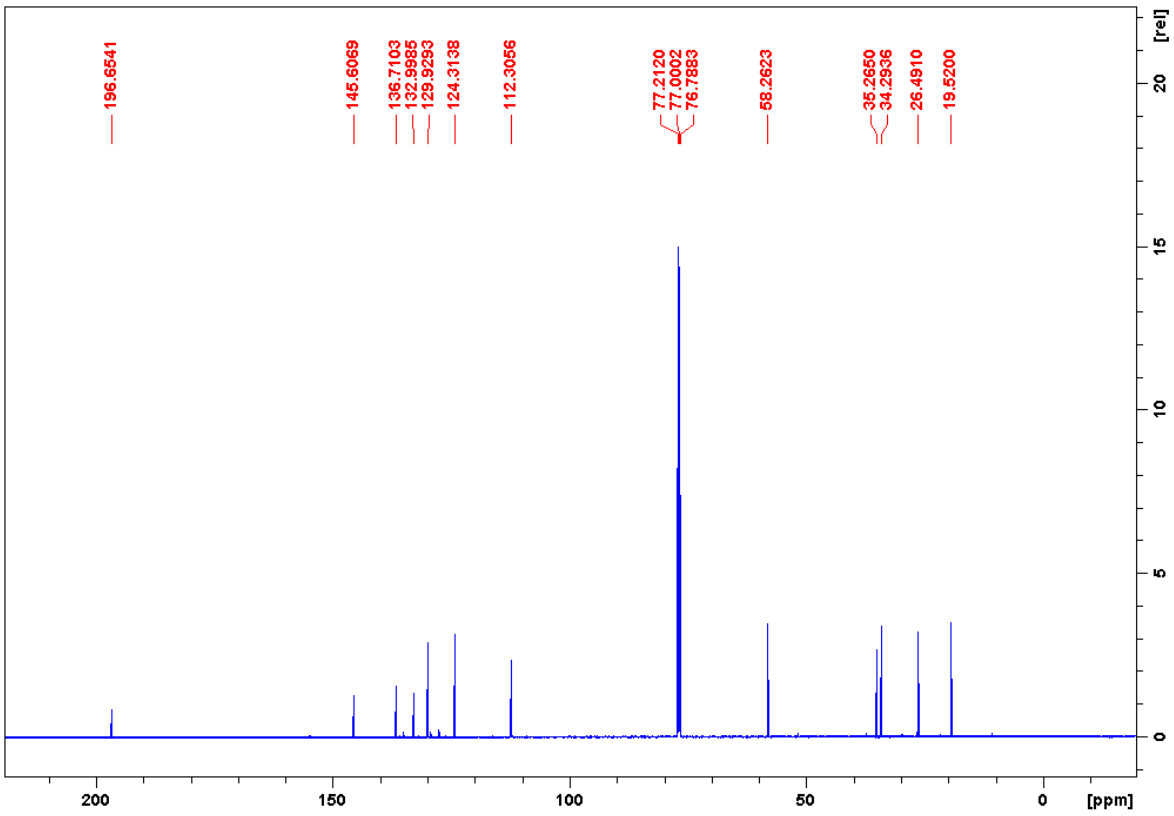
1.00
1.02
1.02
1.01
3.00
3.00
2.99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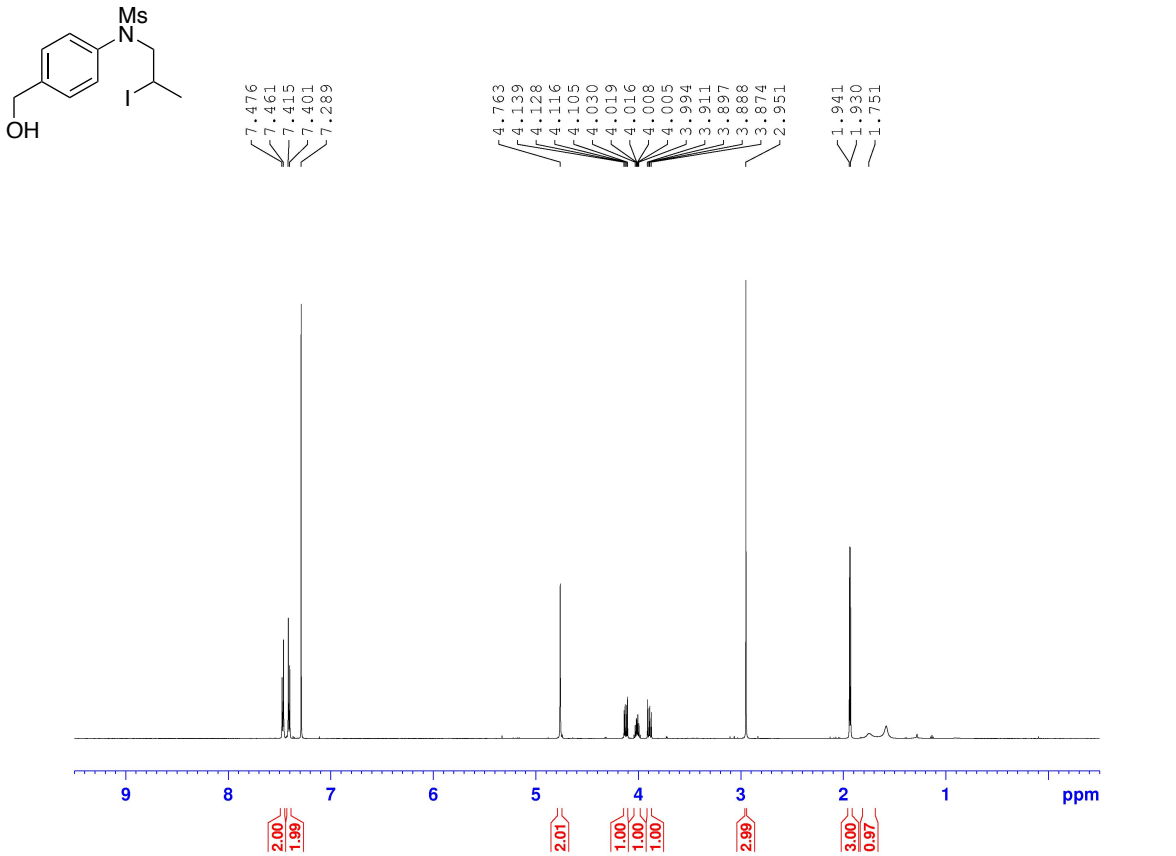
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N
I
OH
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7.401
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4.763
4.139
4.128
4.116
4.105
4.030
4.019
4.016
4.008
4.005
3.994
3.911
3.897
3.888
3.874
2.951
1.941
1.930
1.751
9
8
7
6
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ppm
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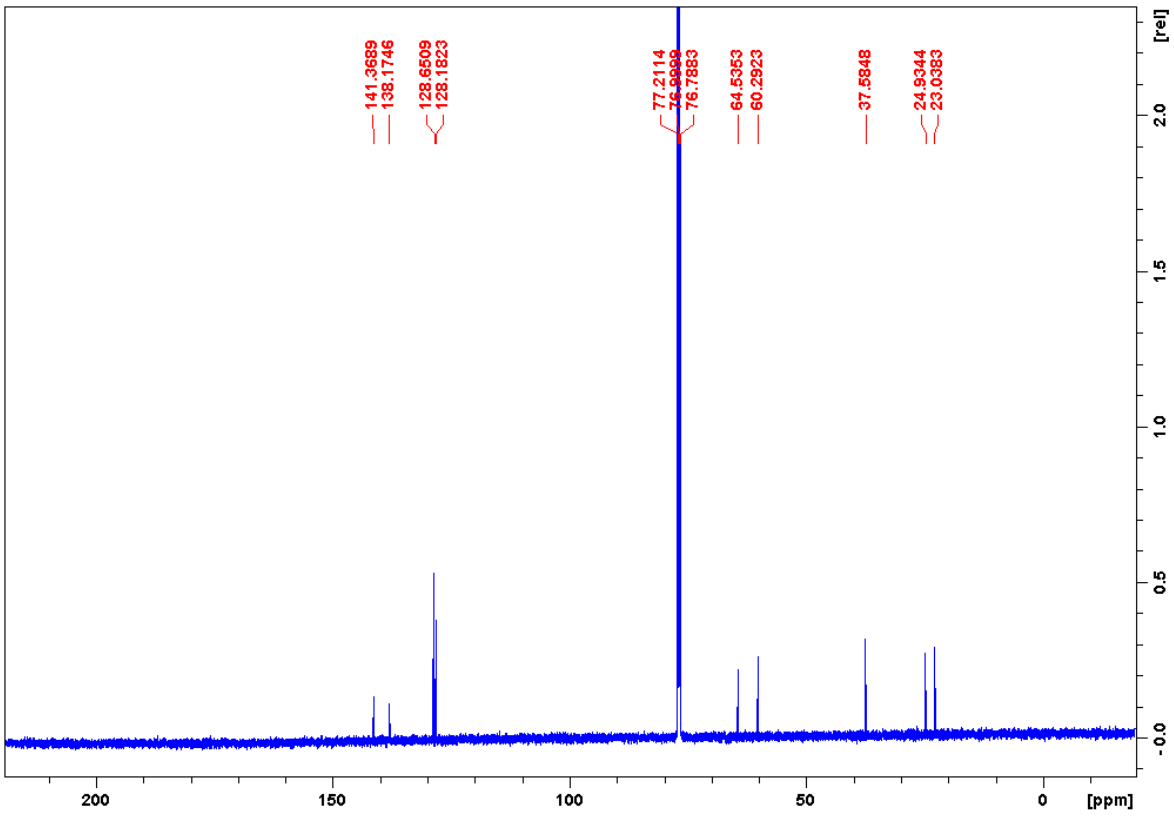
1.99
2.01
1.00
1.00
1.00
2.99
3.00
0.97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76.7883
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60.2923
37.5848
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1.0
0.5
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150
100
50
0
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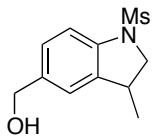
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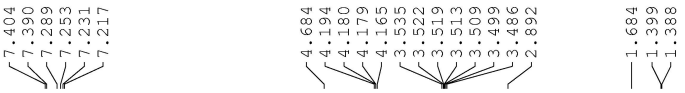
OH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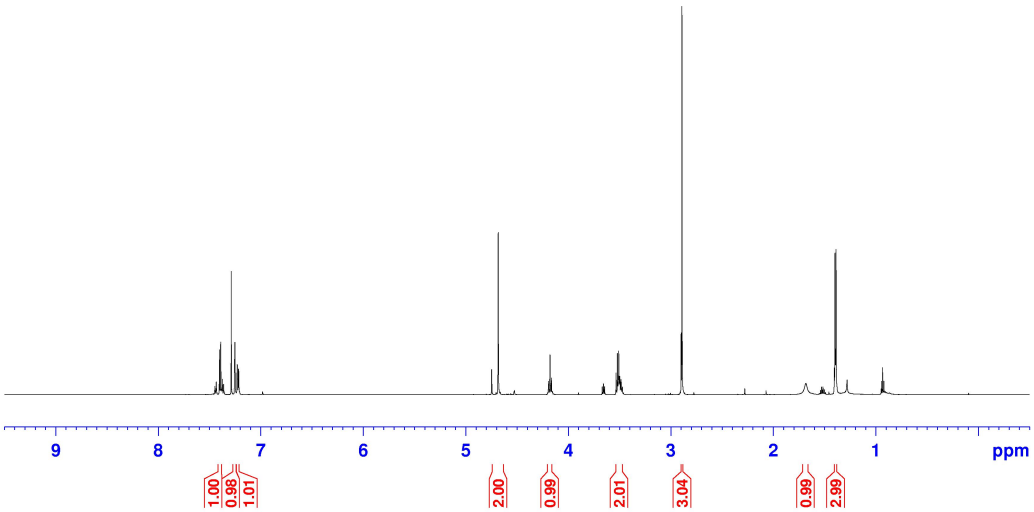
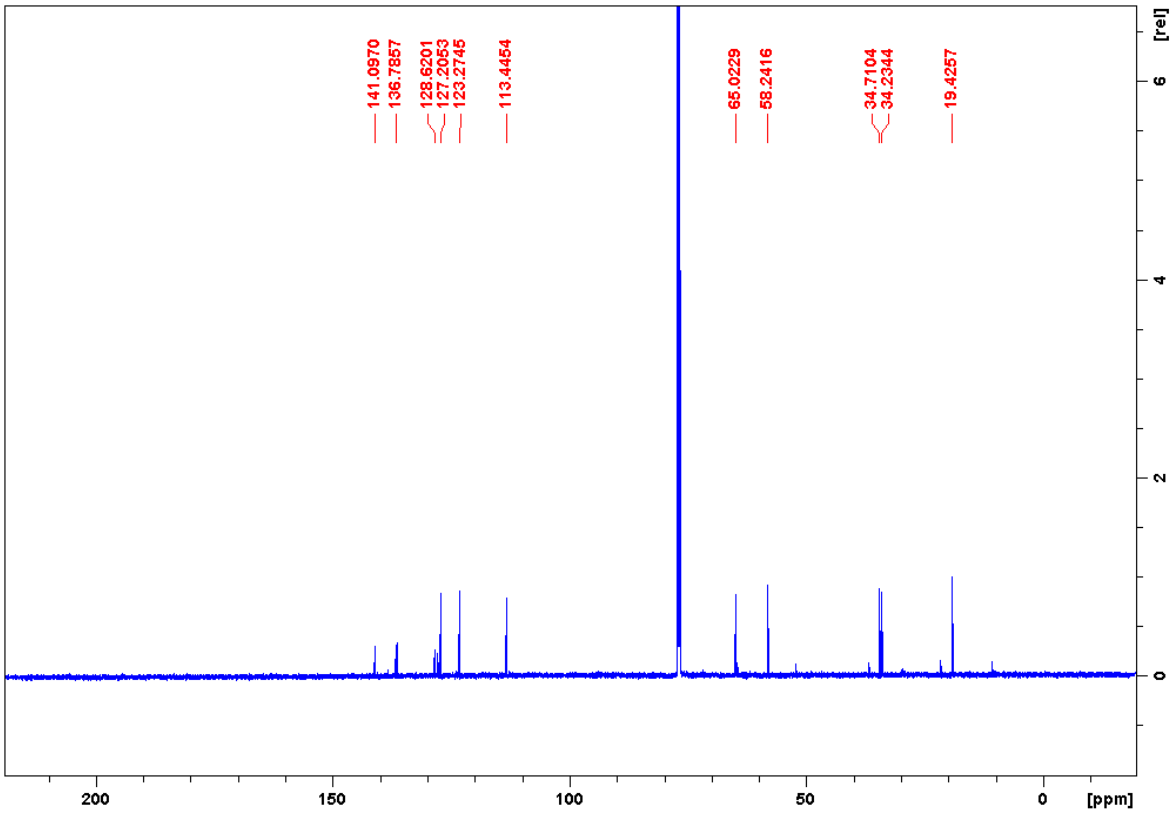
7.390
7.289
7.253
7.231
7.217
4.684
4.194
4.180
4.179
4.165
3.535
3.522
3.519
3.513
3.509
3.499
3.486
2.892
1.684
1.399
1.388


9
8
7
6
5
4
3
2
1
ppm
1.00
0.98
1.01
2.00
0.99
2.01
3.04
0.99
2.99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128.6201
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123.2745
113.4454
65.0229
58.2416
34.7104
34.2344
19.4257
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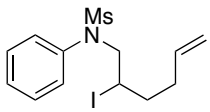
6
4
2
0
200
150
100
50
0
[ppm]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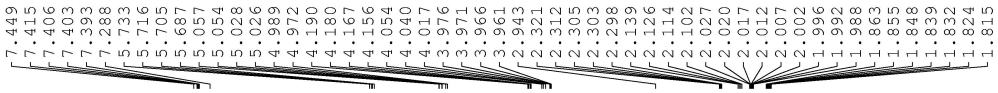
N
I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7.406
7.403
7.393
7.288
5.733
5.716
5.705
5.687
5.057
5.054
5.028
5.026
4.989
4.972
4.190
4.180
4.167
4.156
4.054
4.040
4.017
3.976
3.971
3.966
3.961
2.943
2.321
2.312
2.305
2.303
2.298
2.139
2.126
2.114
2.102
2.027
2.020
2.017
2.012
2.007
2.002
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1.992
1.988
1.863
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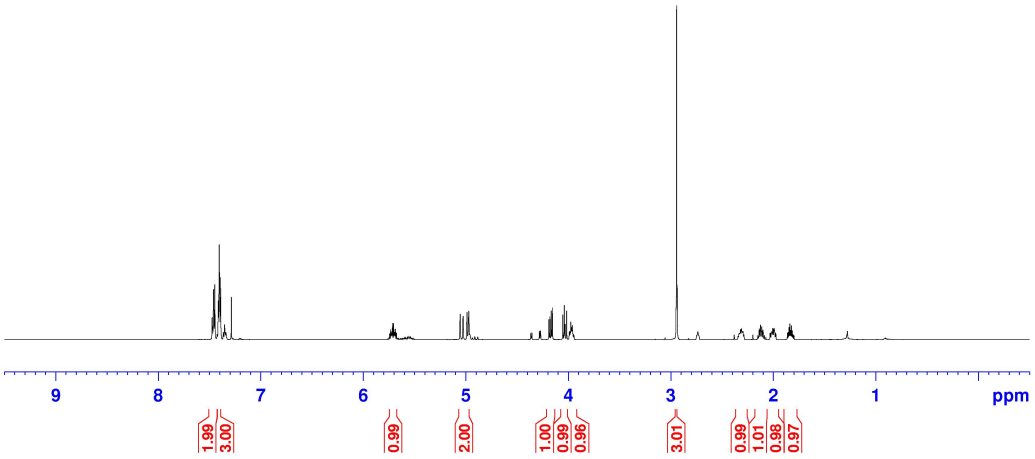
1.848
1.839
1.832
1.824
1.815


9
8
7
6
5
4
3
2
1
ppm
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3.00
0.99
2.00
1.00
0.99
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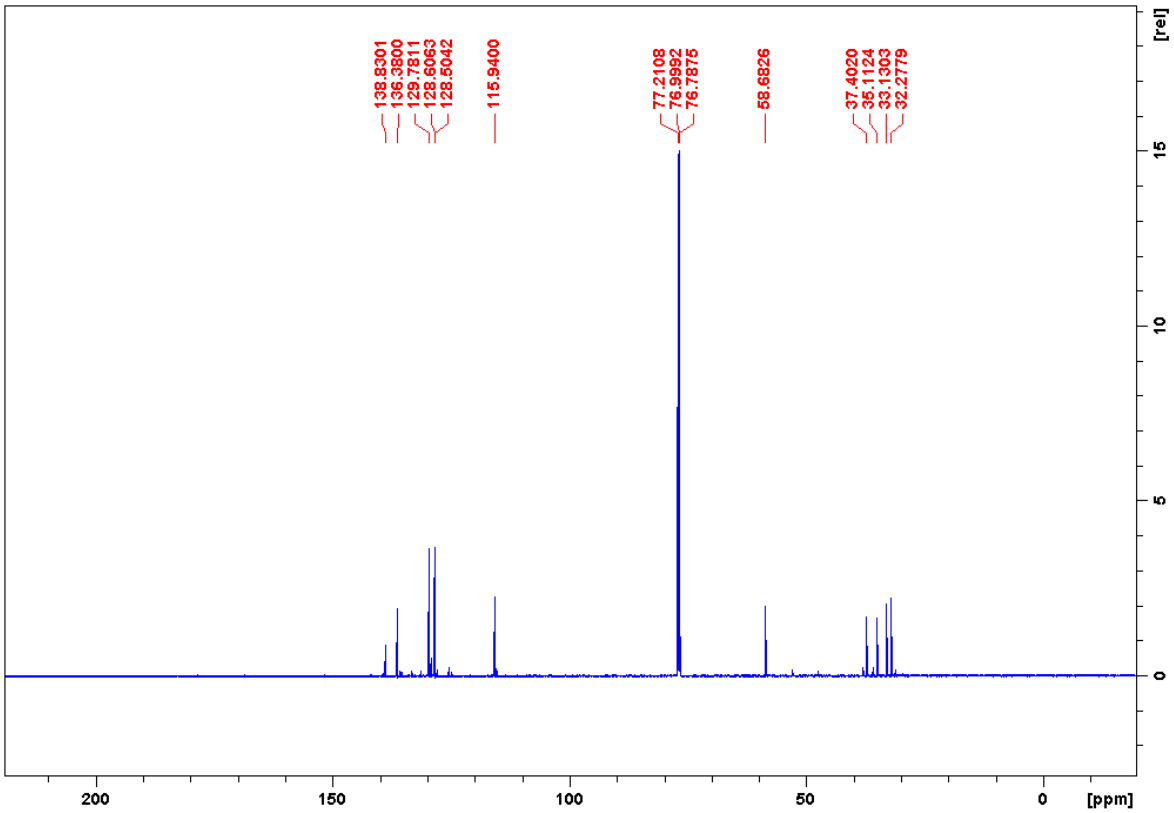
3.01
0.99
1.01
0.98
0.97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129.7811
128.6063
128.5042
115.9400
77.2108
76.9992
76.7875
58.6826
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35.1124
33.1303
32.2779
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5
0
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100
50
0
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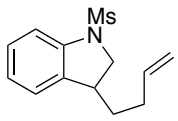
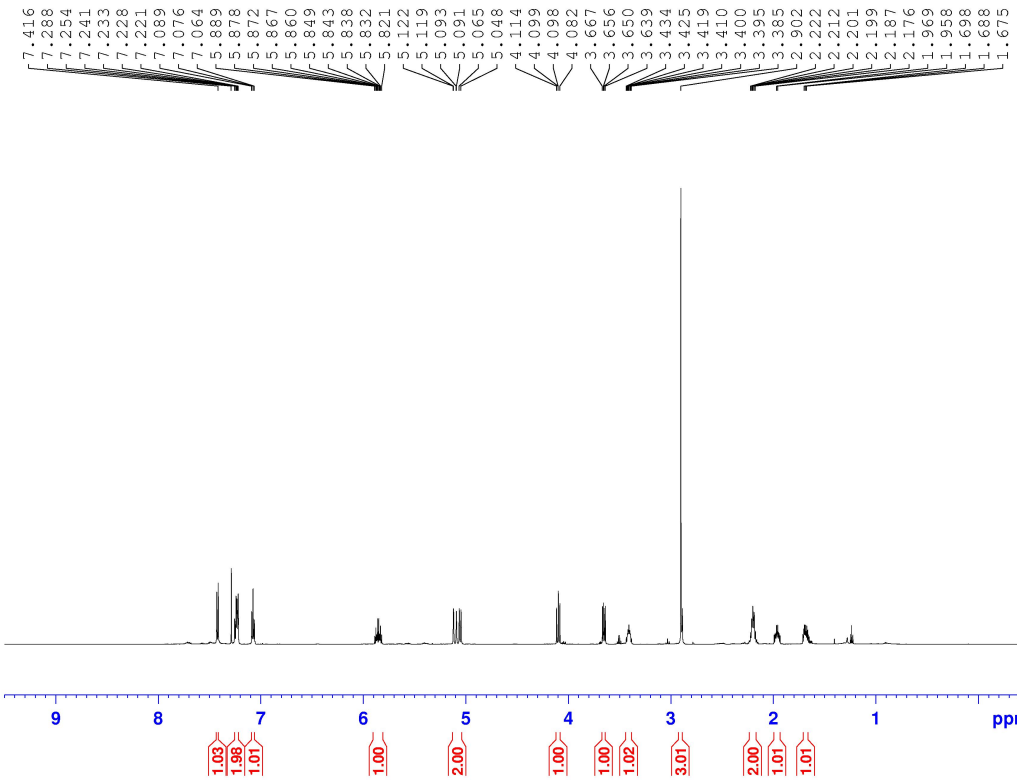

Ms
N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7.254
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7.233
7.228
7.221
7.089
7.076
7.064
5.889
5.878
5.872
5.867
5.860
5.849
5.843
5.838
5.832
5.821
5.122
5.119
5.093
5.091
5.065
5.048
4.114
4.099
4.098
4.082
3.667
3.656
3.650
3.639
3.434
3.425
3.419
3.410
3.400
3.395
3.385
2.902
2.222
2.212
2.201
2.199
2.187
2.176
1.969
1.958
1.698
1.688
1.675
9
8
7
6
5
4
3
2
1
ppm
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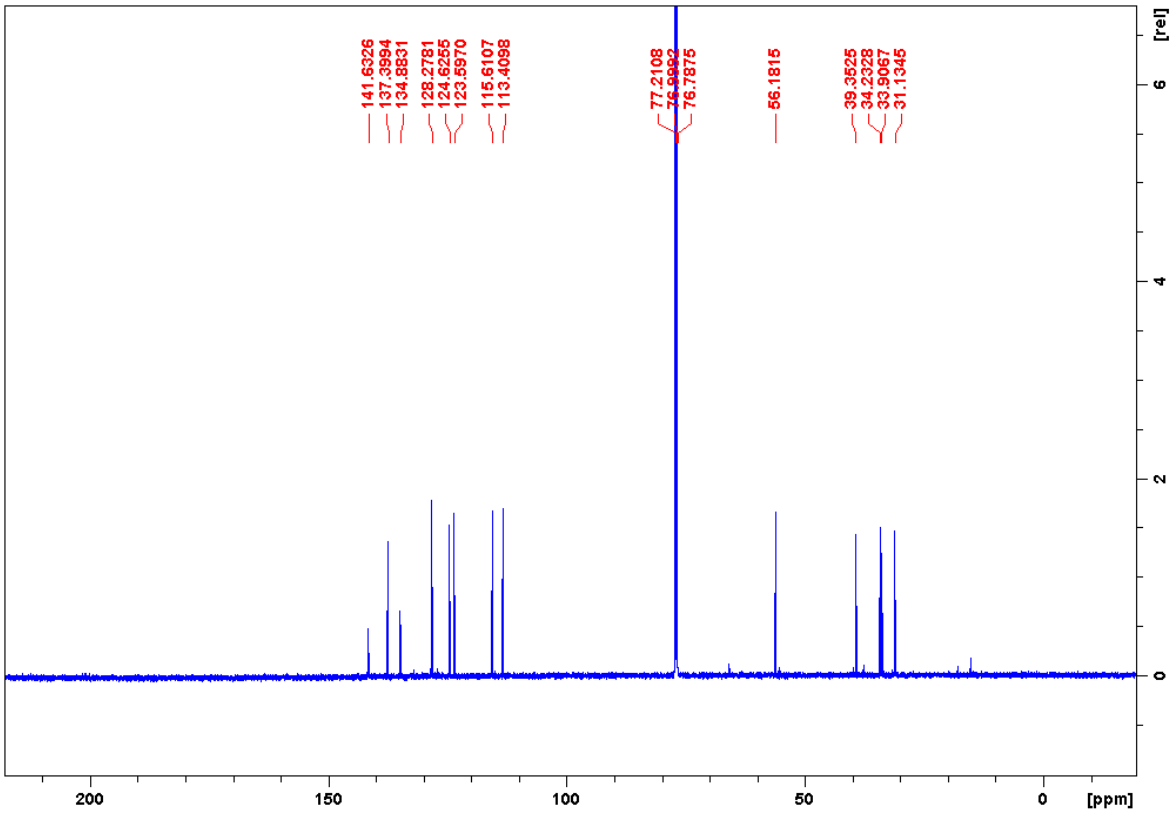
1.98
1.01
1.00
2.00
1.00
1.00
1.02
3.01
2.00
1.01
1.01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115.6107
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77.2108
76.7875
56.1815
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33.9067
31.1345
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2
0
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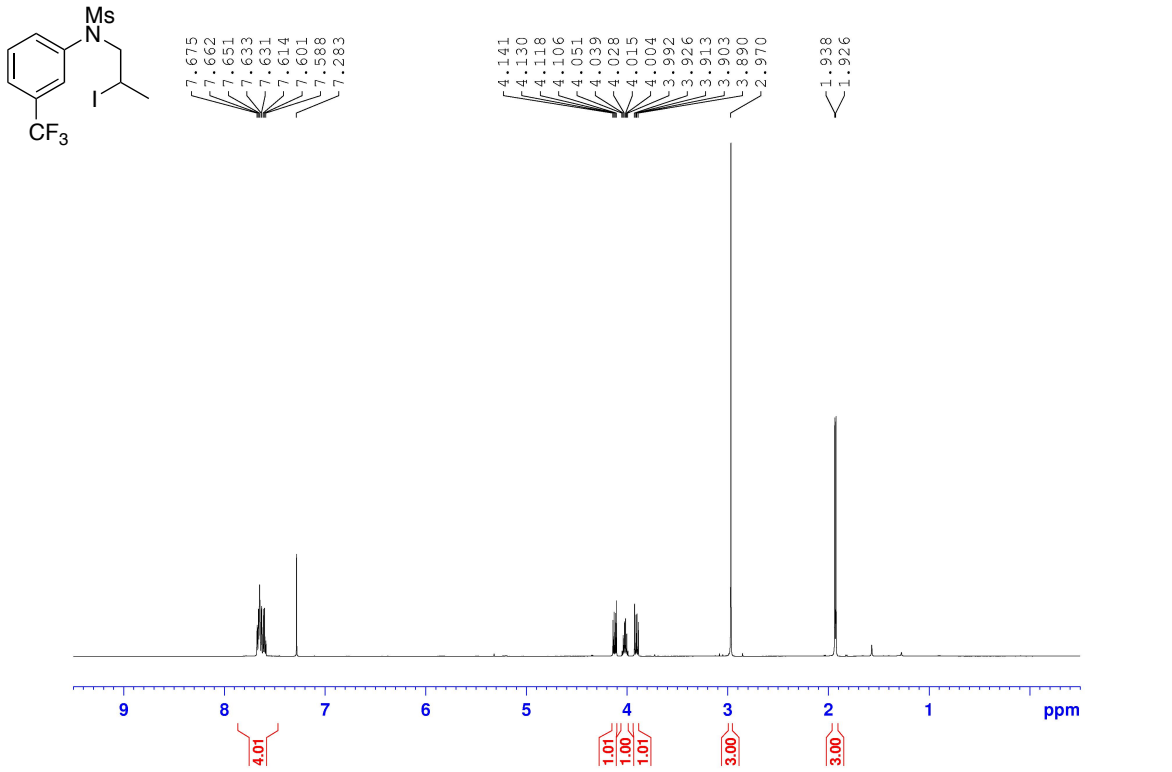
150
100
50
0
[ppm]


Ms
N
I
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7.662
7.651
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7.631
7.614
7.601
7.588
7.283
4.141
4.130
4.118
4.106
4.051
4.039
4.028
4.015
4.004
3.992
3.926
3.913
3.903
3.890
2.970
1.938
1.926
9
8
7
6
5
4
3
2
1
ppm
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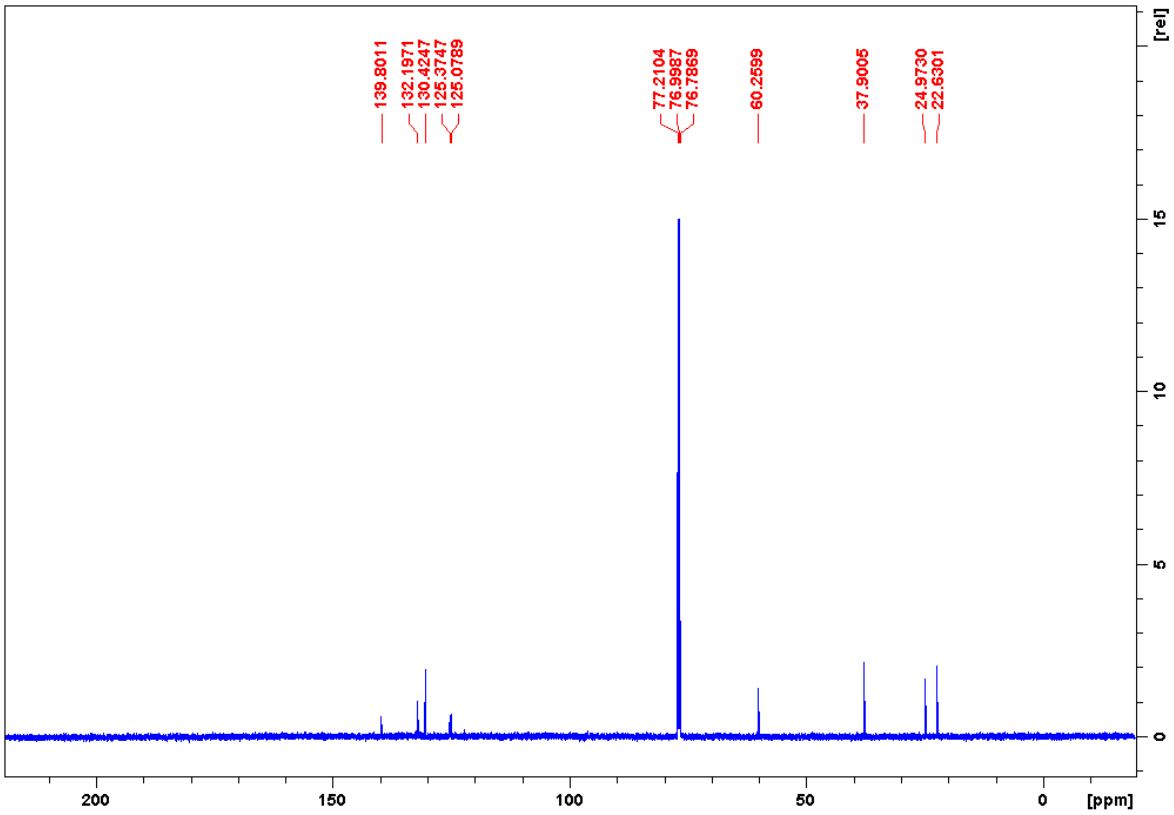
1.01
1.00
1.01
3.00
3.00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22.6301
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0
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100
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0
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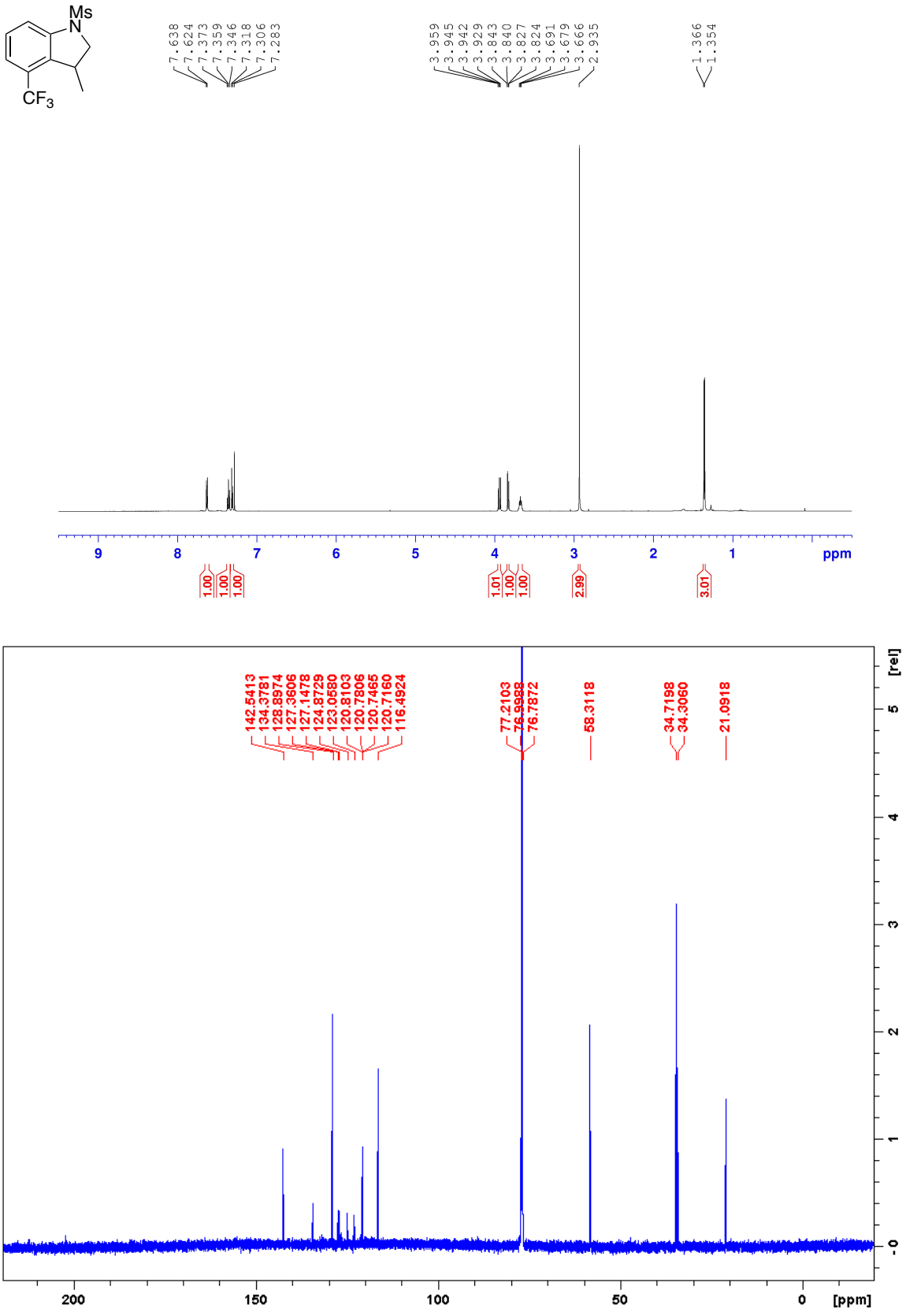
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N
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7.283
3.959
3.945
3.942
3.929
3.843
3.840
3.827
3.824
3.691
3.679
3.666
2.935
1.366
1.354
9
8
7
6
5
4
3
2
1
ppm
1.00
1.00
1.00
1.01
1.00
1.00
2.99
3.01
142.5413
134.3781
128.8974
127.3606
127.1478
124.8729
123.0580
120.8103
120.7806
120.7465
120.7160
116.4924
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34.3060
21.0918
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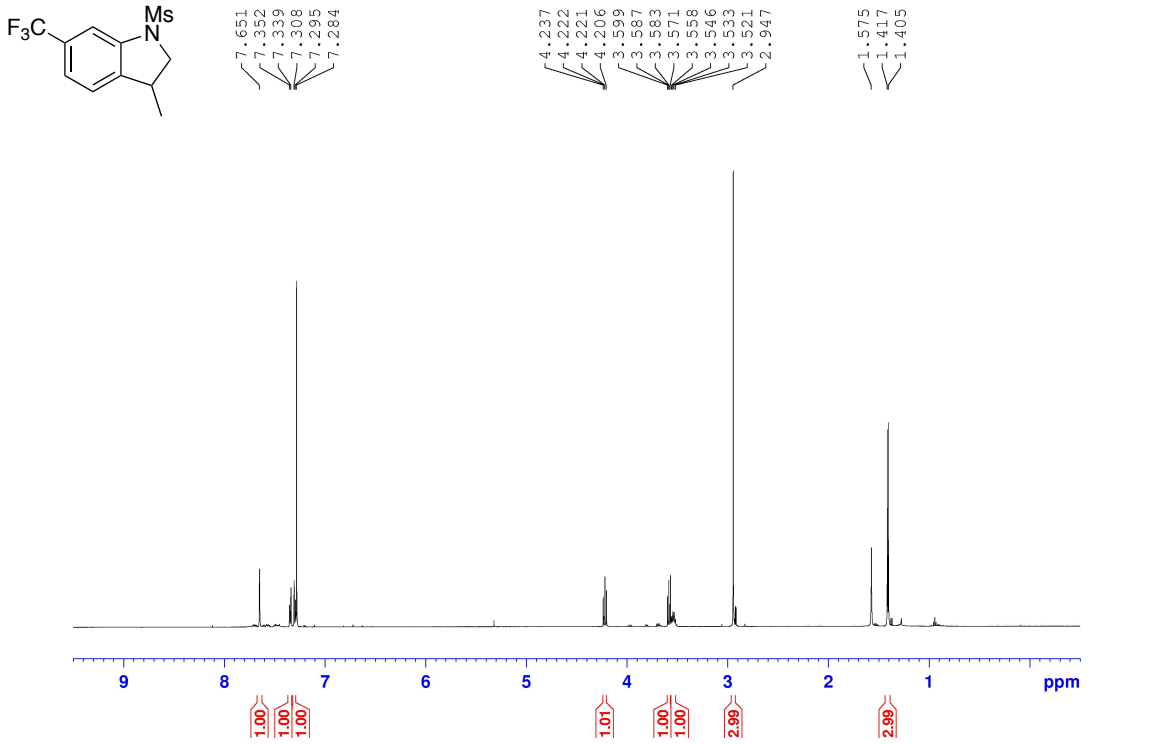
50
0
[ppm]


F3C
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N
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7.284
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4.222
4.221
4.206
3.599
3.587
3.583
3.571
3.558
3.546
3.533
3.521
2.947
1.575
1.417
1.405
9
8
7
6
5
4
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2
1
ppm
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1.00
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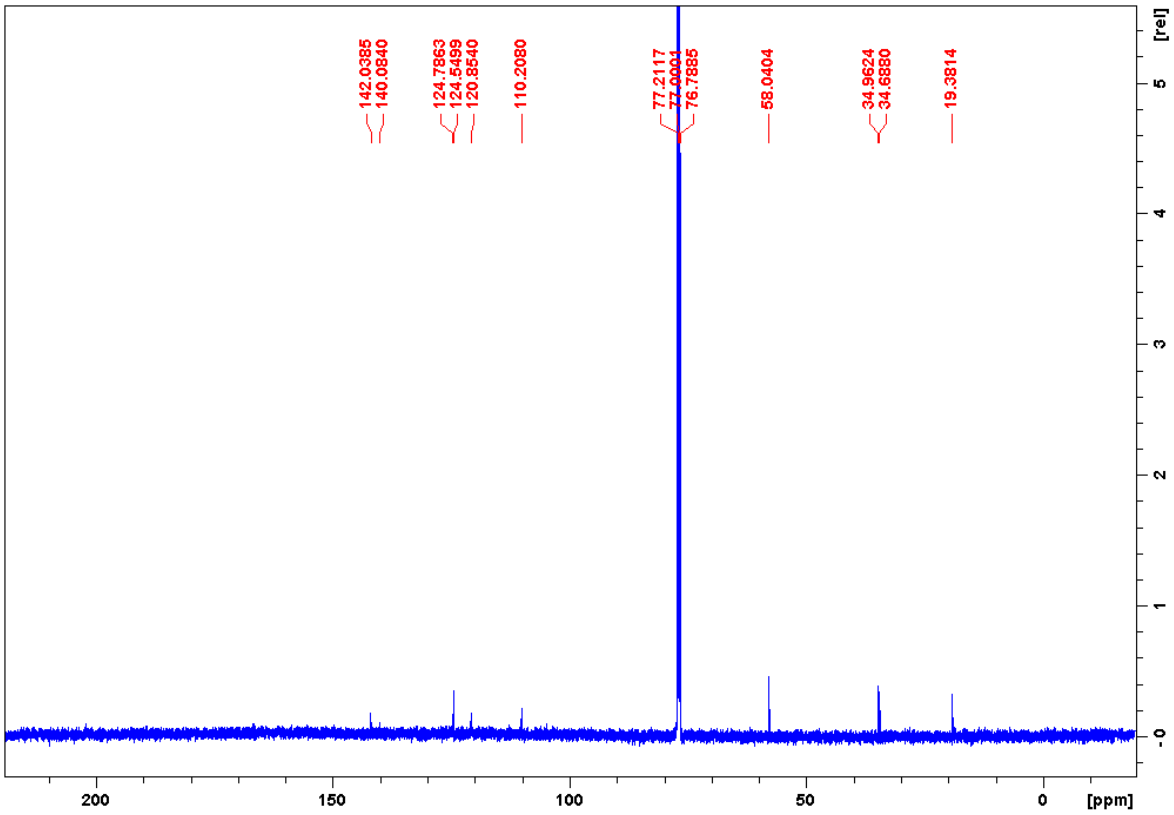
1.01
1.00
1.00
2.99
2.99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77.2117
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76.7885
58.0404
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34.6880
19.3814
200
150
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0
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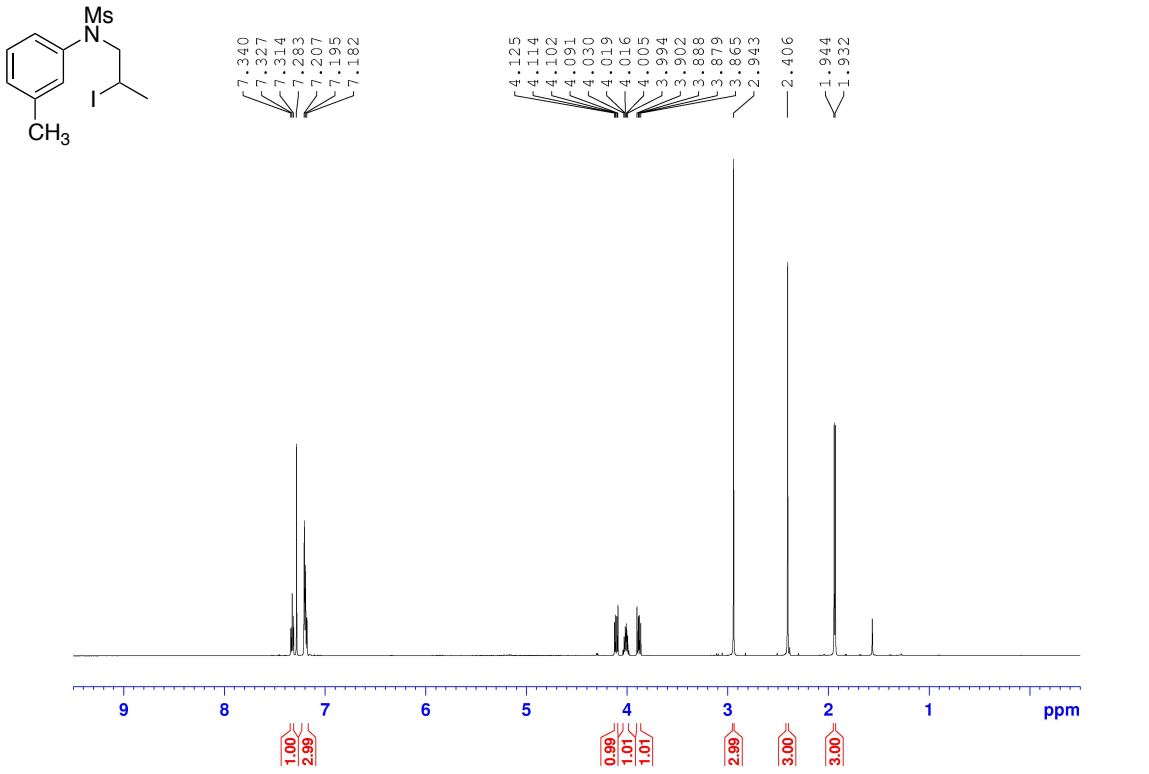
[rel]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I
CH3
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7.207
7.195
7.182
4.125
4.114
4.102
4.091
4.030
4.019
4.016
4.005
3.994
3.902
3.888
3.879
3.865
2.943
2.406
1.944
1.932
9
8
7
6
5
4
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2
1
ppm
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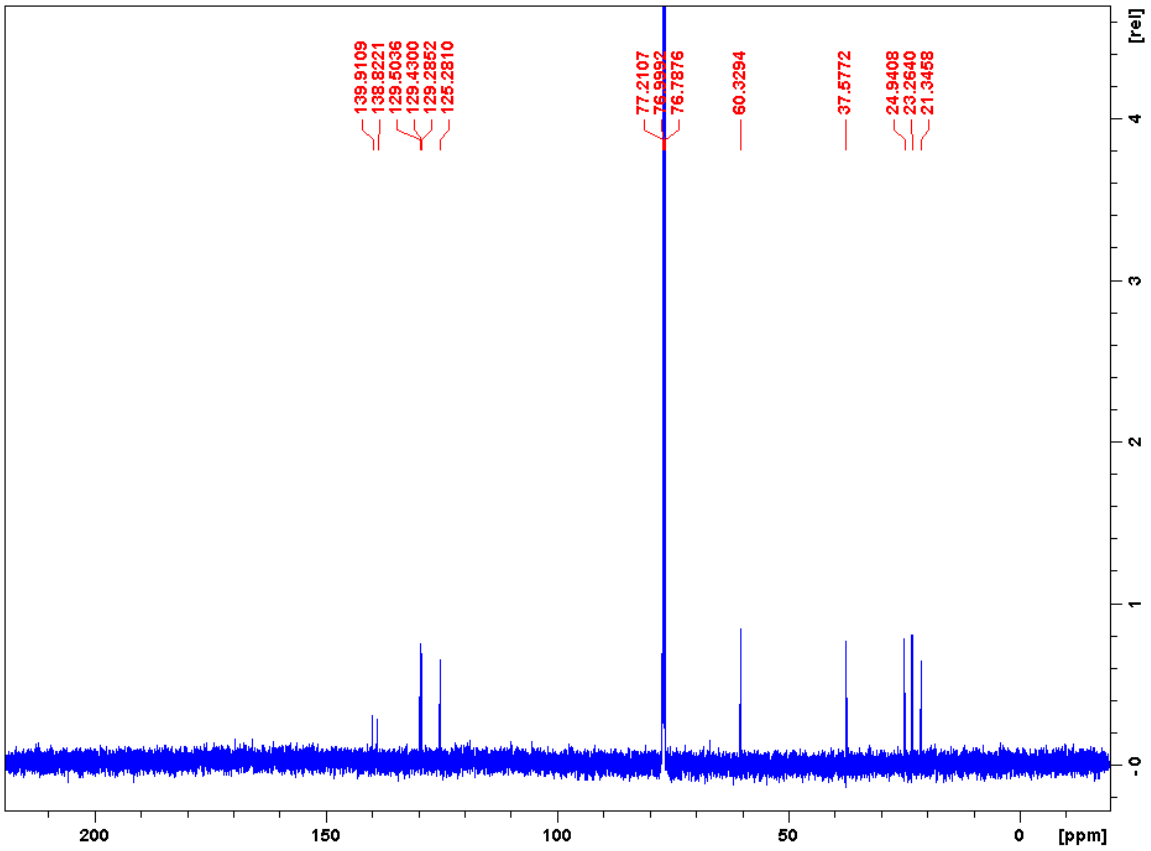
1.01
1.01
2.99
3.00
3.00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129.2852
125.2810
77.2107
76.9992
76.7876
60.3294
37.5772
24.9408
23.2640
21.3458
[rel]
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2
1
-0
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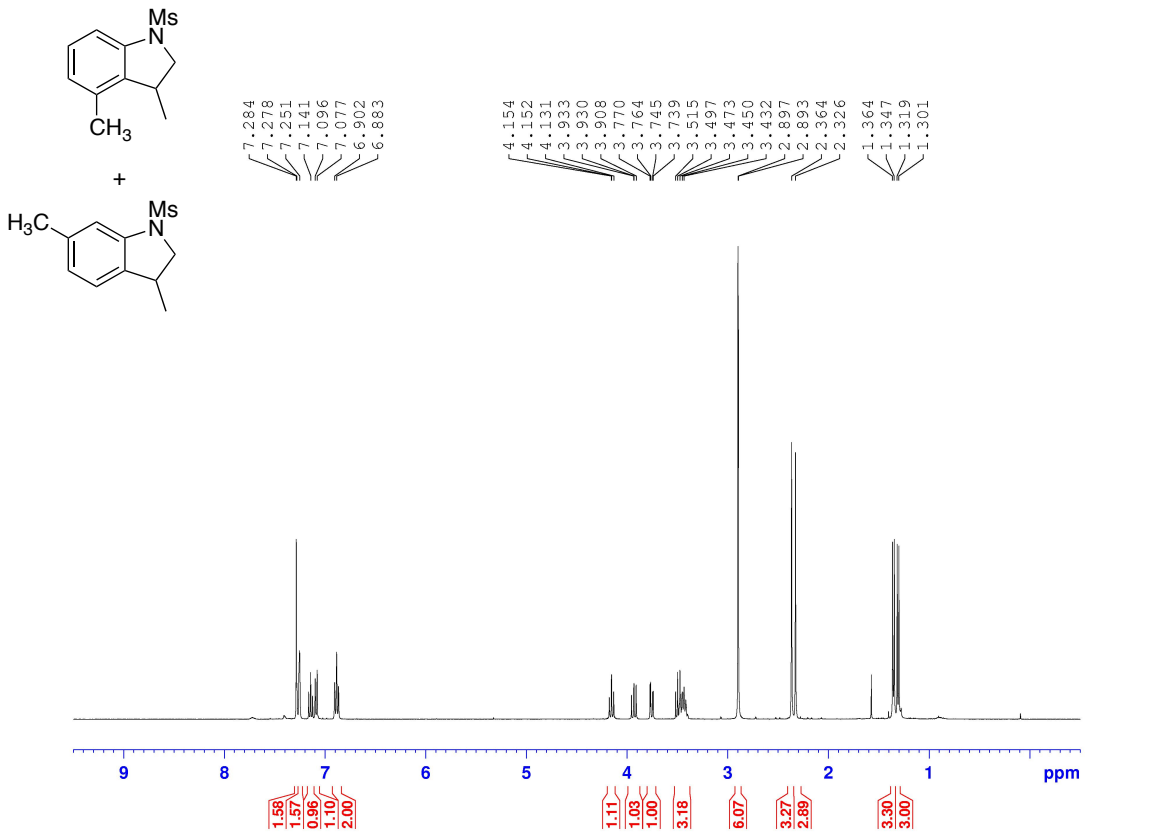
150
100
50
0
[ppm]


Ms
N
CH3
+
H3C
Ms
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7.141
7.096
7.077
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6.883
4.154
4.152
4.131
3.933
3.930
3.908
3.770
3.764
3.745
3.739
3.515
3.497
3.473
3.450
3.432
2.897
2.893
2.364
2.326
1.364
1.347
1.319
1.301
9
8
7
6
5
4
3
2
1
ppm
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1.57
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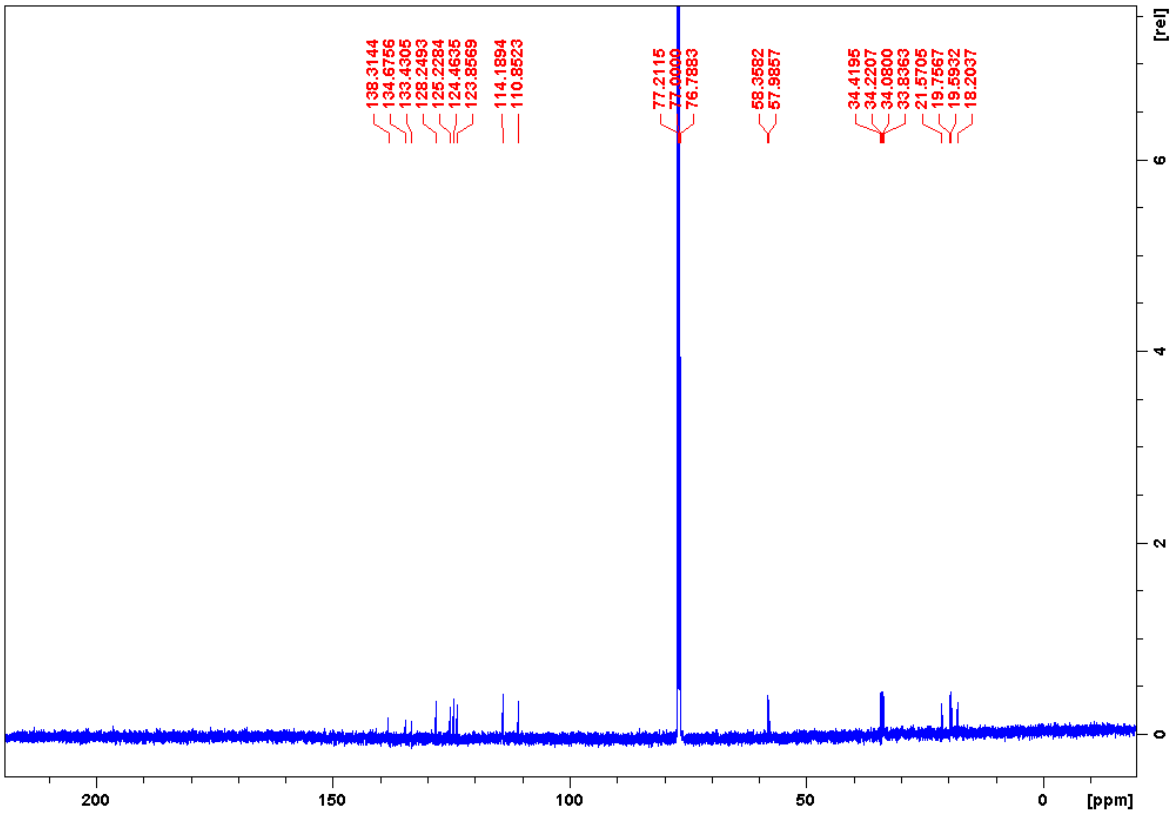
3.00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123.8569
114.1894
110.8523
77.2115
77.0000
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33.8363
21.5705
19.7567
19.5932
18.2037
[rel]
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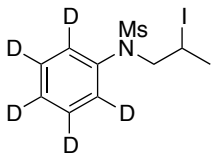
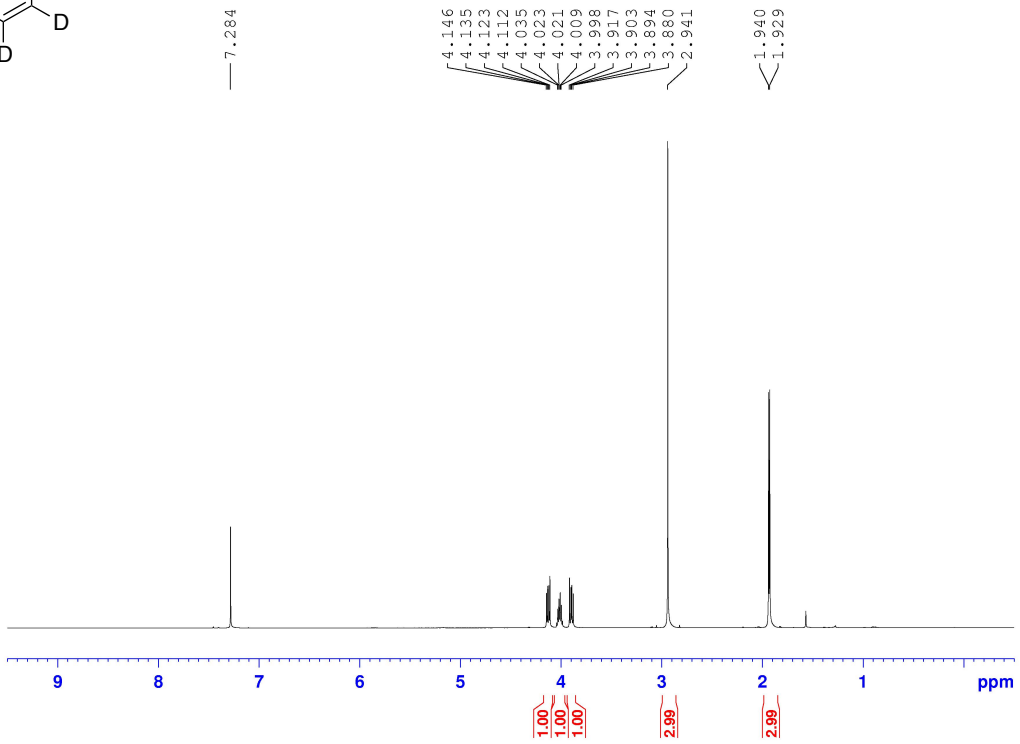
4
2
0
200
150
100
50
0
[ppm]


D
Ms
I
D
N
D
D
D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4.112
4.035
4.023
4.021
4.009
3.998
3.917
3.903
3.894
3.880
2.941
1.940
1.929
9
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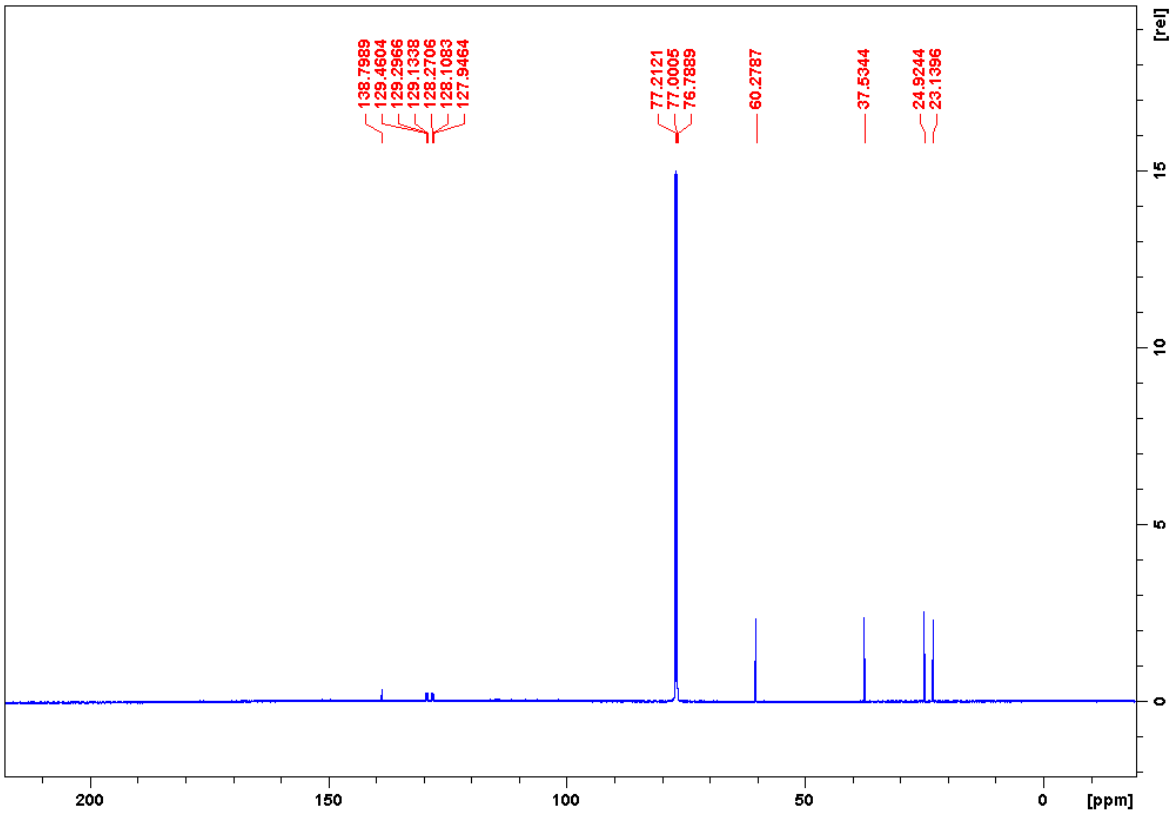
7
6
5
4
3
2
1
ppm
1.00
1.00
1.00
2.99
2.99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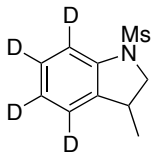
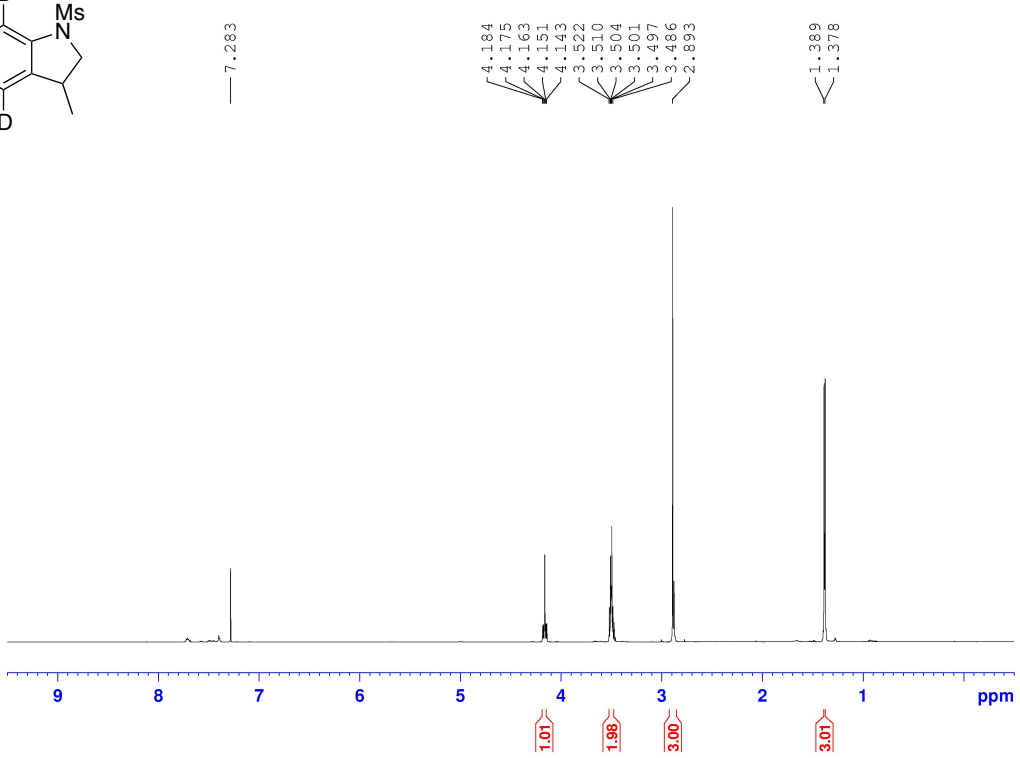
129.2966
129.1338
128.2706
128.1083
127.9464
77.2121
77.0005
76.7889
60.2787
37.5344
24.9244
23.1396
[rel]
15
10
5
0
200
150
100
50
0
[ppm]


D
D
Ms
N
D
D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4.175
4.163
4.151
4.143
3.522
3.510
3.504
3.501
3.497
3.486
2.893
1.389
1.378
9
8
7
6
5
4
3
2
1
ppm
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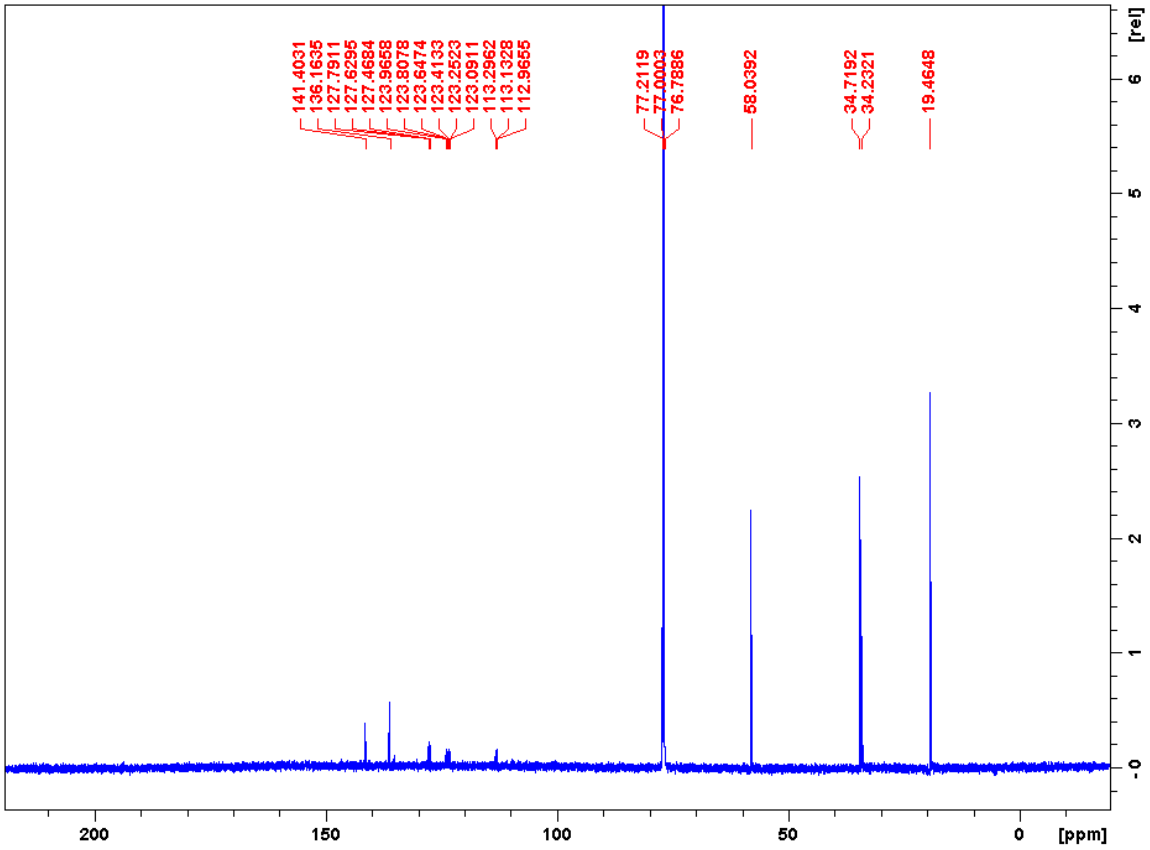
1.98
3.00
3.01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127.6295
127.4684
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123.8078
123.6474
123.4133
123.2523
123.0911
113.2962
113.1328
112.9655
77.2119
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76.7886
58.0392
34.7192
34.2321
19.4648
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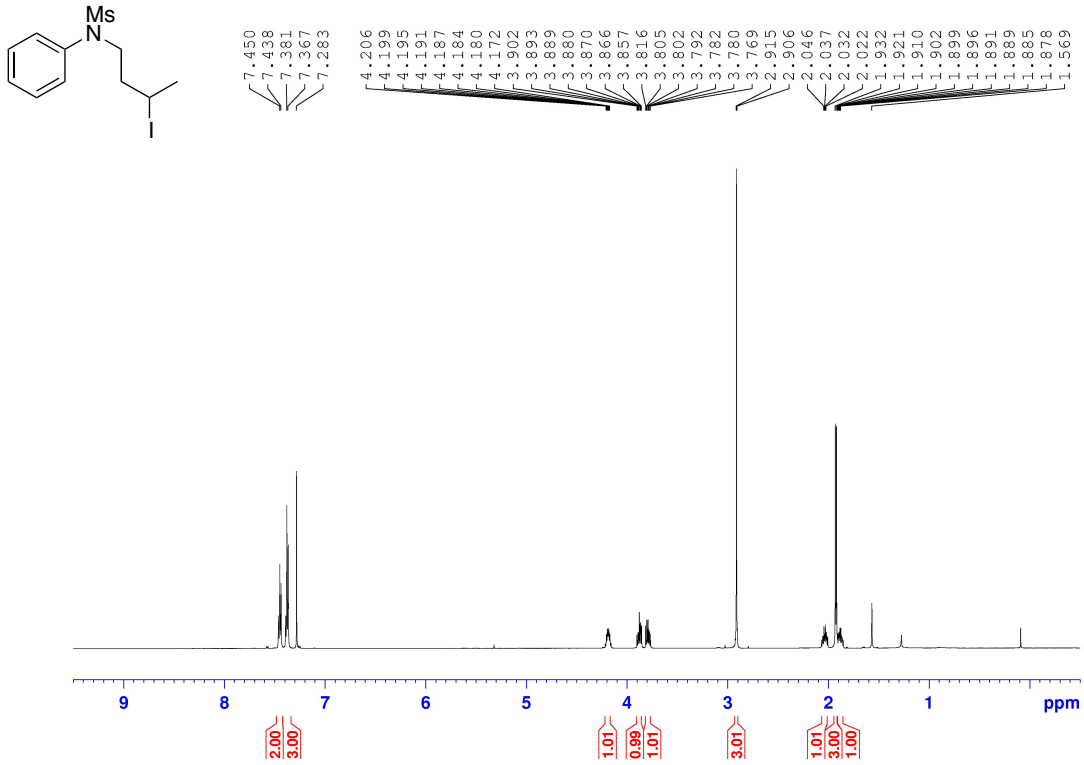
Ms
N
I
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7.438
7.381
7.367
7.283
4.206
4.199
4.195
4.191
4.187
4.184
4.180
4.172
3.902
3.893
3.889
3.880
3.870
3.866
3.857
3.816
3.805
3.802
3.792
3.782
3.780
3.769
2.915
2.906
2.046
2.037
2.032
2.022
1.932
1.921
1.910
1.902
1.899
1.896
1.891
1.889
1.885
1.878
1.569
9
8
7
6
5
4
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ppm
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1.01
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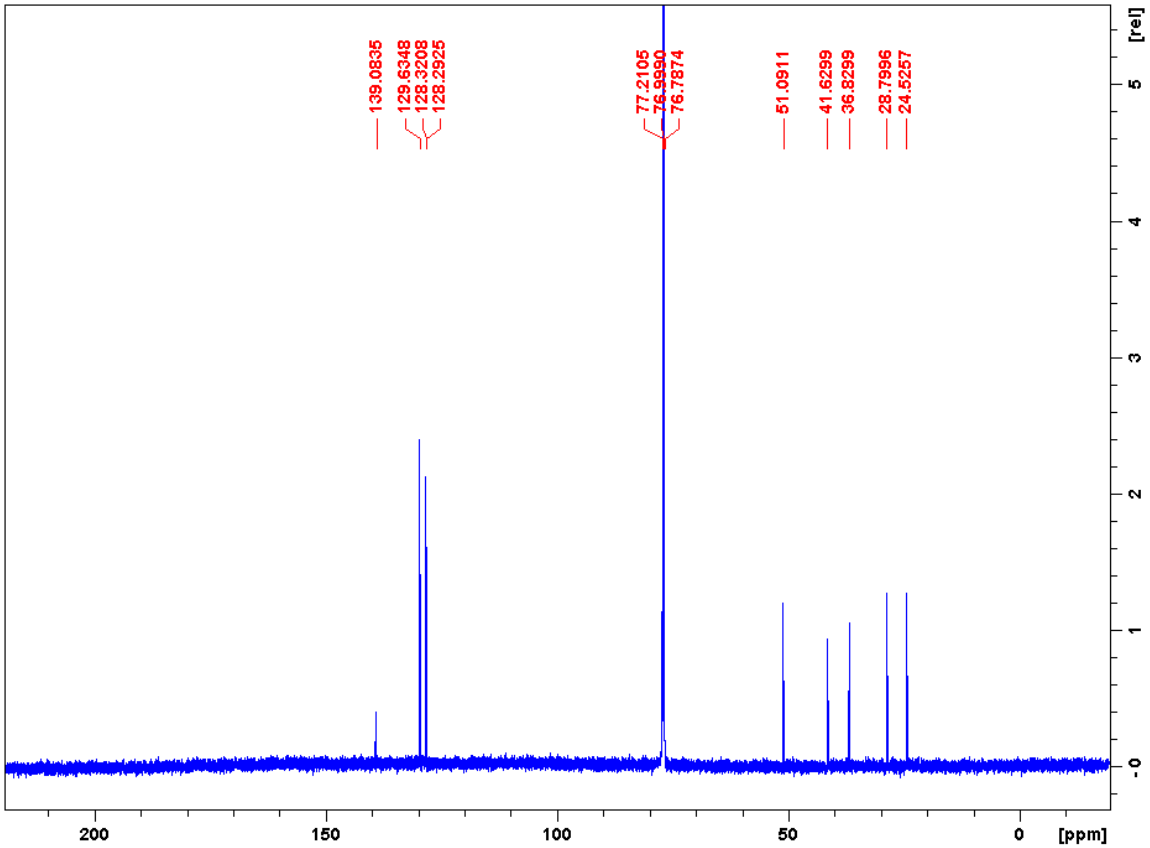
1.00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129.6348
128.3208
128.2925
77.2105
76.9990
76.7874
51.0911
41.6299
36.8299
28.7996
24.5257
200
150
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0
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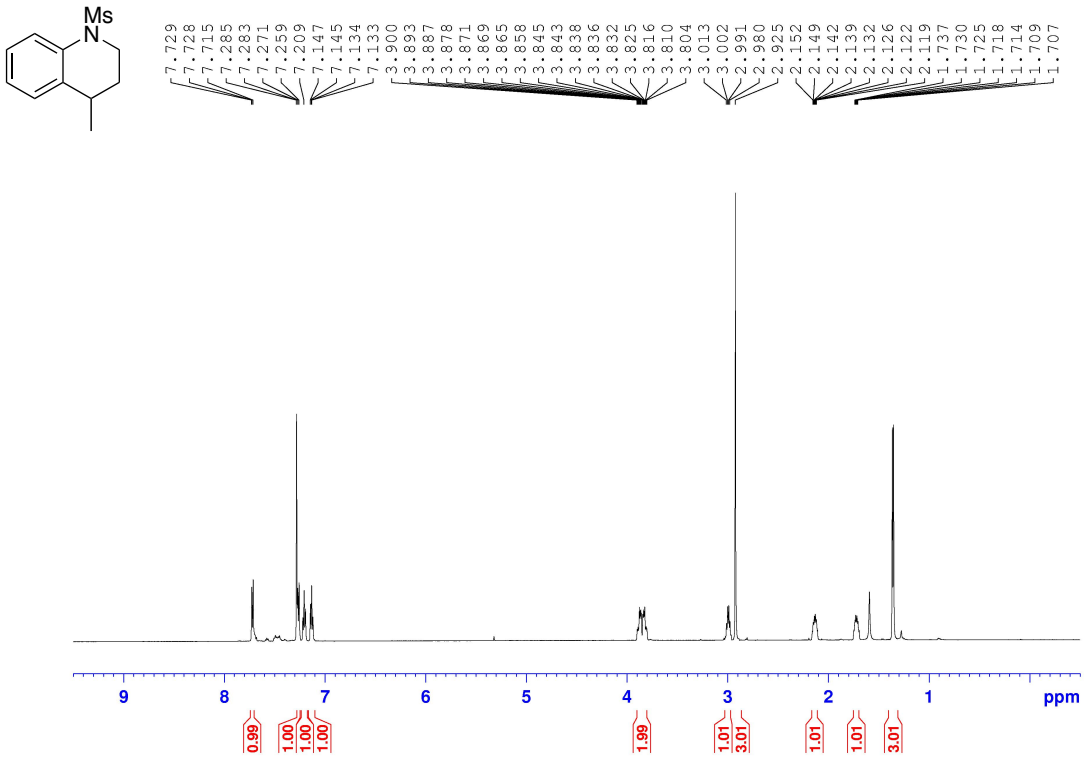
[rel]


Ms
N
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7.728
7.715
7.285
7.283
7.271
7.259
7.209
7.147
7.145
7.134
7.133
3.900
3.893
3.887
3.878
3.871
3.869
3.865
3.858
3.845
3.843
3.838
3.836
3.832
3.825
3.816
3.810
3.804
3.013
3.002
2.991
2.980
2.925
2.152
2.149
2.142
2.139
2.132
2.126
2.122
2.119
1.737
1.730
1.725
1.718
1.714
1.709
1.707
9
8
7
6
5
4
3
2
1
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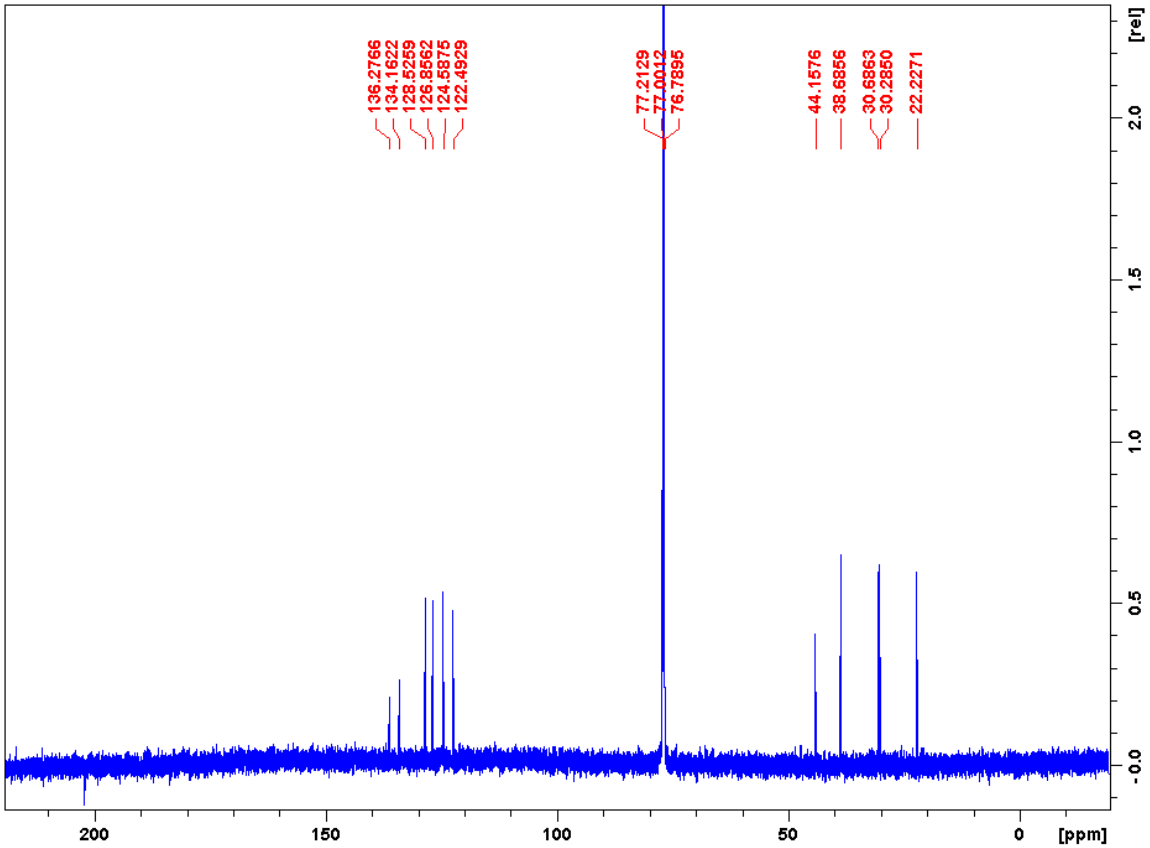
1.00
1.00
1.00
1.99
1.01
3.01
1.01
1.01
3.01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134.1622
128.5259
126.8562
124.5875
122.4929
77.2129
77.0012
76.7895
44.1576
38.6856
30.6863
30.2850
22.2271
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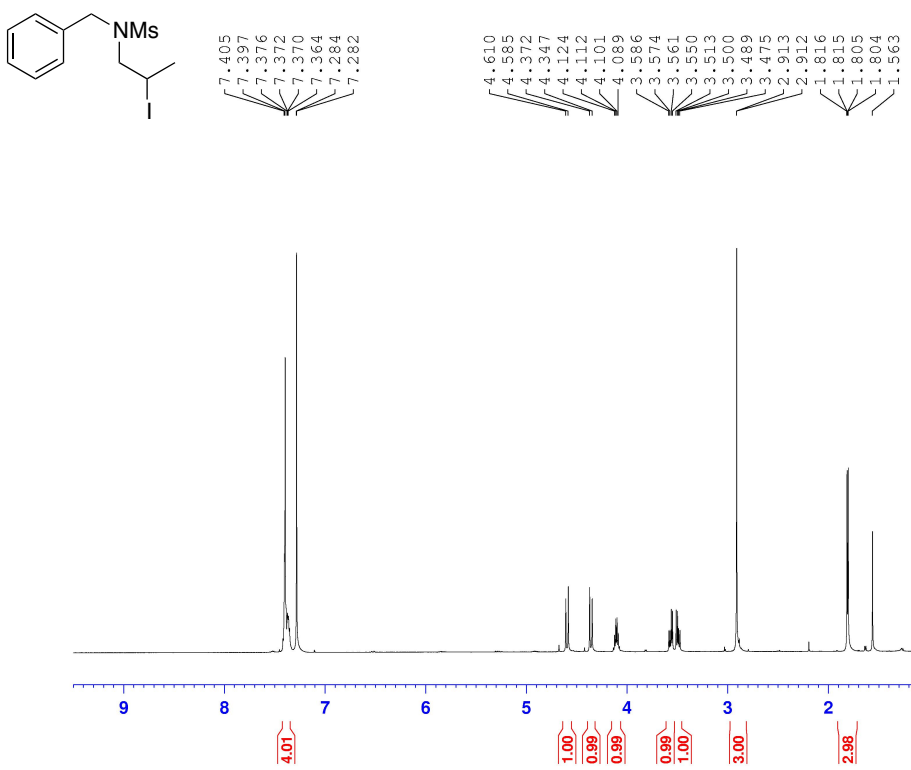
1.5
1.0
0.5
-0.0
200
150
100
50
0
[ppm]


NMs
I
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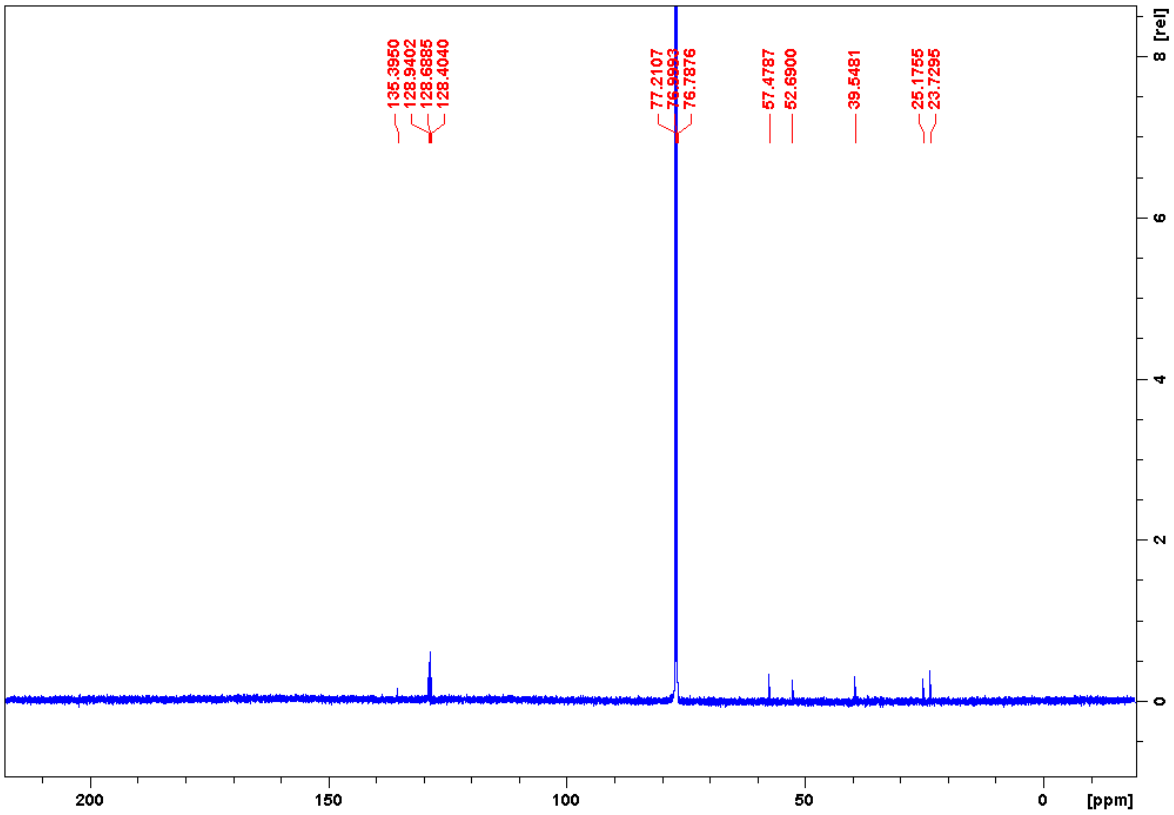
7.397
7.376
7.372
7.370
7.364
7.284
7.282
4.610
4.585
4.372
4.347
4.124
4.112
4.101
4.089
3.586
3.574
3.561
3.550
3.513
3.500
3.489
3.475
2.913
2.912
1.816
1.815
1.805
1.804
1.563
9
8
7
6
5
4
3
2
1
ppm
4.01
1.00
0.99
0.99
0.99
1.00
3.00
2.98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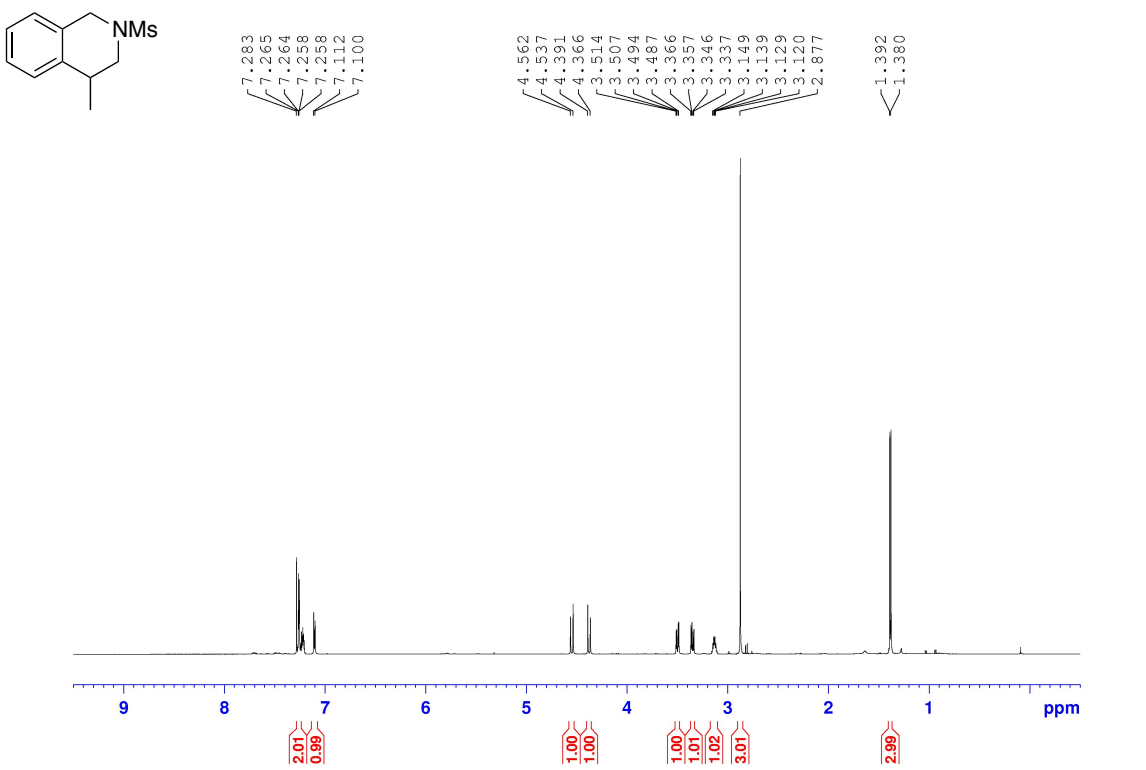
128.6885
128.4040
77.2107
76.9993
76.7876
57.4787
52.6900
39.5481
25.1755
23.7295
8 [rel]
6
4
2
0
200
150
100
50
0
[ppm]


NMs
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7.264
7.258
7.258
7.112
7.100
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4.537
4.391
4.366
3.514
3.507
3.494
3.487
3.366
3.357
3.346
3.337
3.149
3.139
3.129
3.120
2.877
1.392
1.380
9
8
7
6
5
4
3
2
1
ppm
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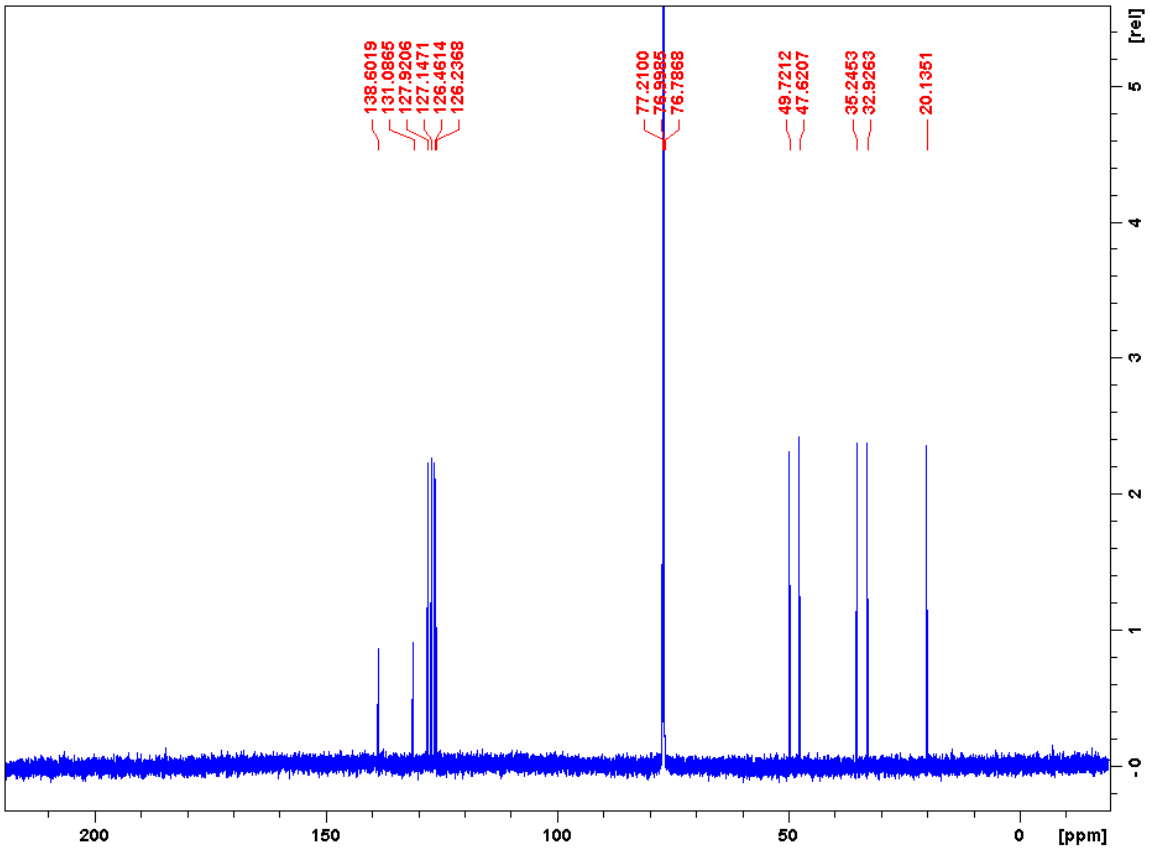
0.99
1.00
1.00
1.00
1.01
1.02
3.01
2.99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127.9206
127.1471
126.4614
126.2368
77.2100
76.9985
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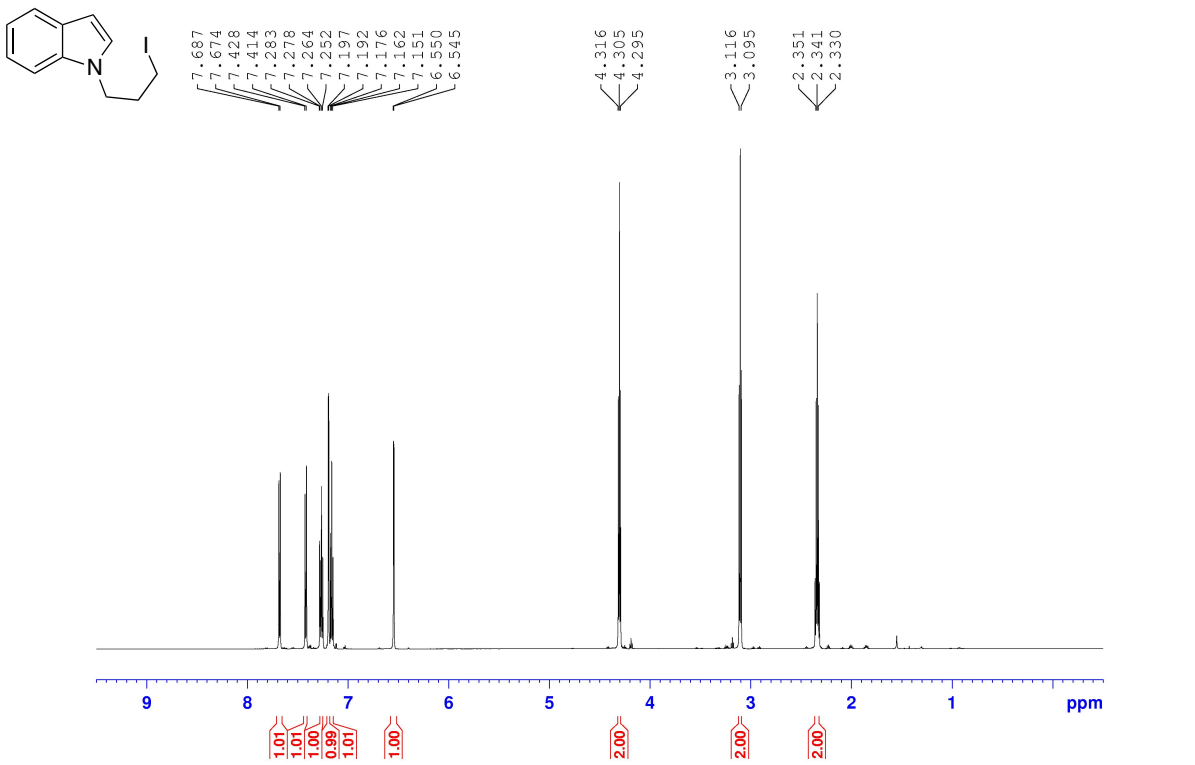
49.7212
47.6207
35.2453
32.9263
20.1351
[rel]
200
150
100
50
0
[ppm]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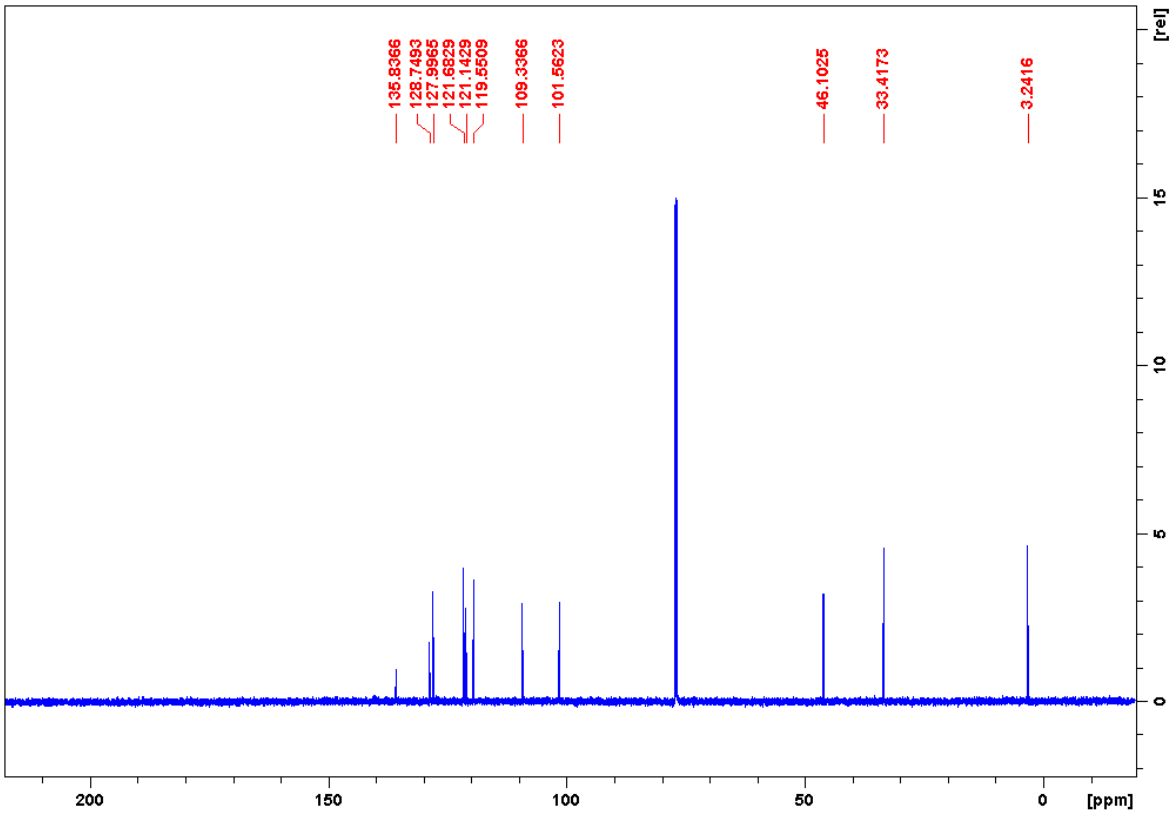
7.428
7.414
7.283
7.278
7.264
7.252
7.197
7.192
7.176
7.162
7.151
6.550
6.545
4.316
4.305
4.295
3.116
3.095
2.351
2.341
2.330
9
8
7
6
5
4
3
2
1
ppm
1.01
1.01
1.00
0.99
1.01
1.00
2.00
2.00
2.00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33.4173
3.2416
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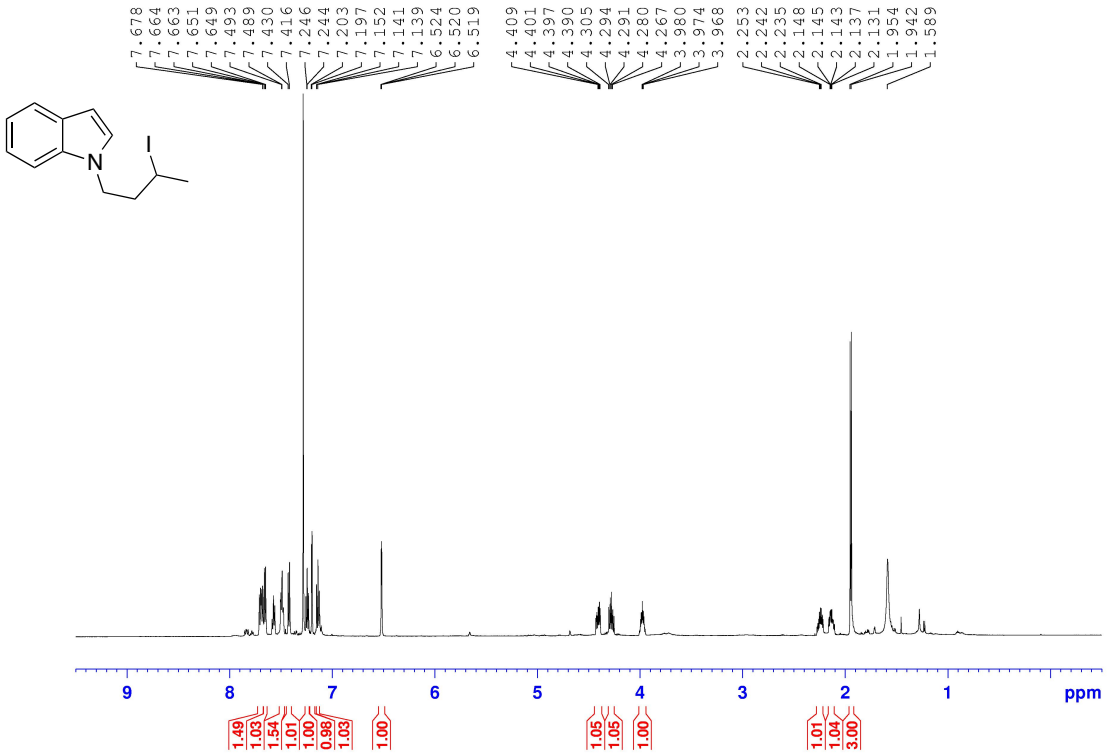
10
5
0
200
150
100
50
0
[ppm]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7.649
7.493
7.489
7.430
7.416
7.246
7.244
7.203
7.197
7.152
7.141
7.139
6.524
6.520
6.519
4.409
4.401
4.397
4.390
4.305
4.294
4.291
4.280
4.267
3.980
3.974
3.968
2.253
2.242
2.235
2.148
2.145
2.143
2.137
2.131
1.954
1.942
1.589
I
N
9
8
7
6
5
4
3
2
1
ppm
1.49
1.03
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1.00
0.98
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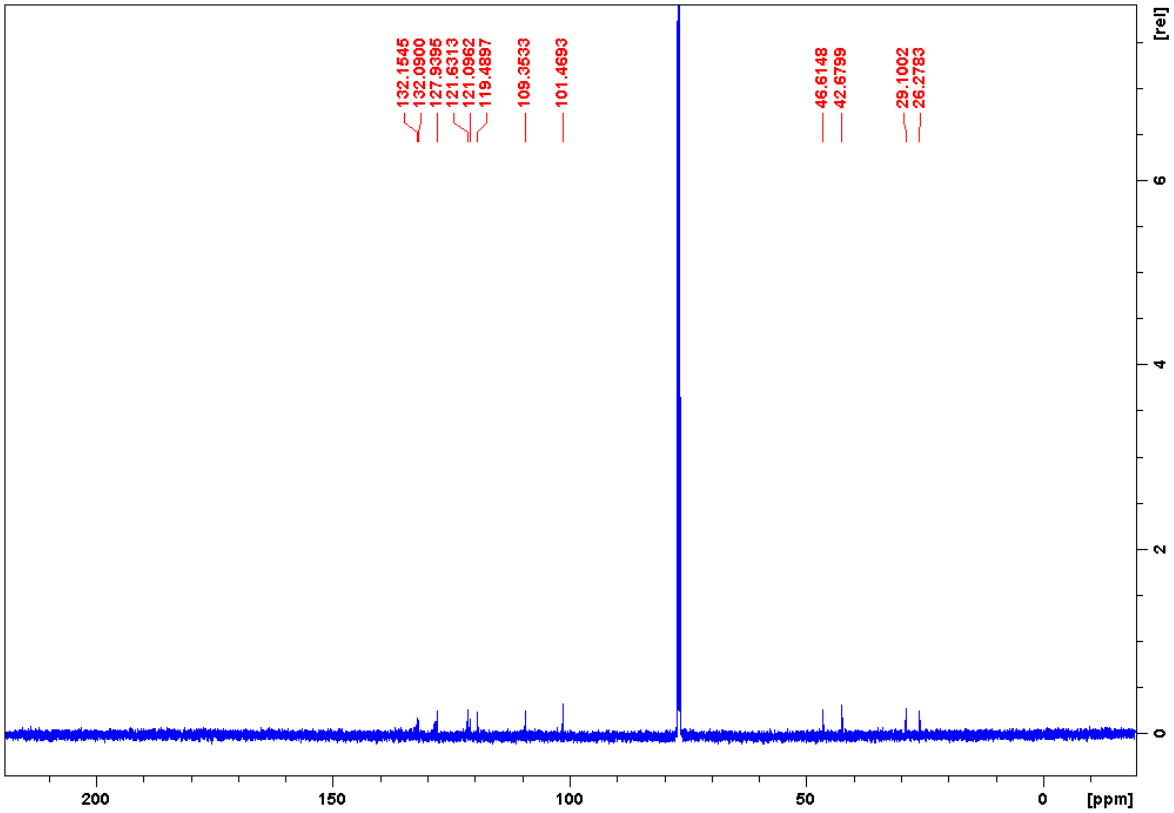
1.00
1.05
1.05
1.00
1.01
1.04
3.00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29.1002
26.2783
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2
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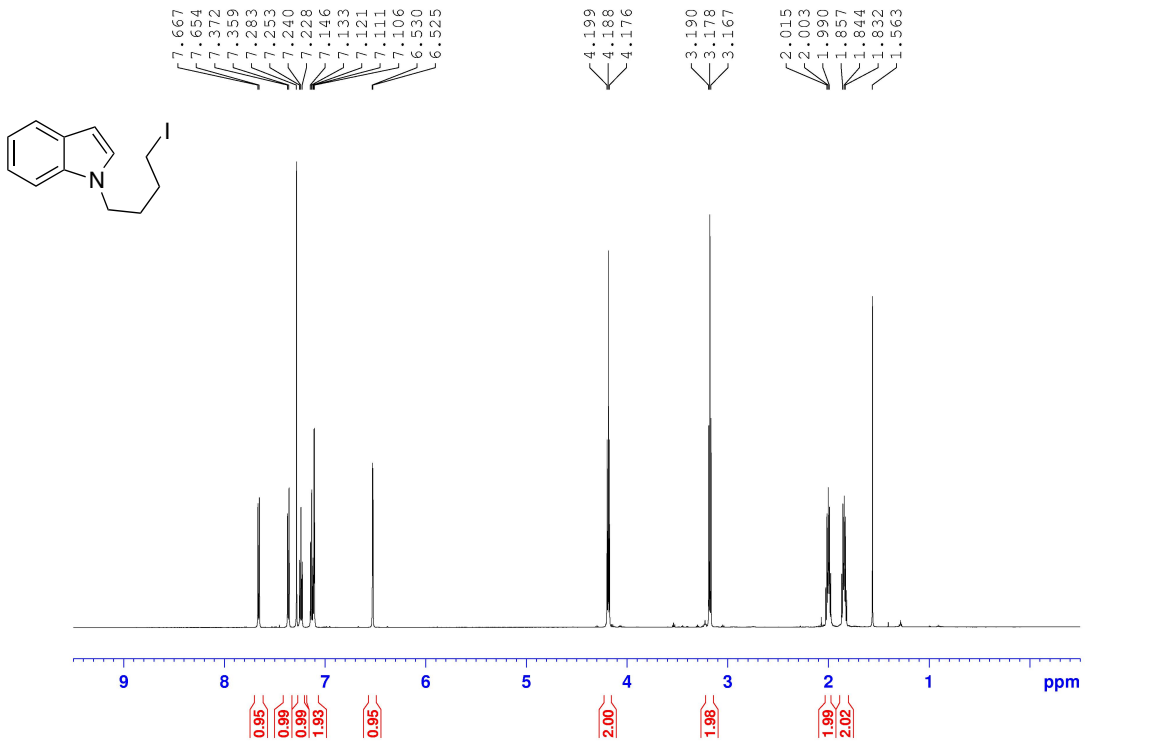
150
100
50
0
[ppm]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7.372
7.359
7.283
7.253
7.240
7.228
7.146
7.133
7.121
7.111
7.106
6.530
6.525
4.199
4.188
4.176
3.190
3.178
3.167
2.015
2.003
1.990
1.857
1.844
1.832
1.563
I
N
9
8
7
6
5
4
3
2
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ppm
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0.99
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0.95
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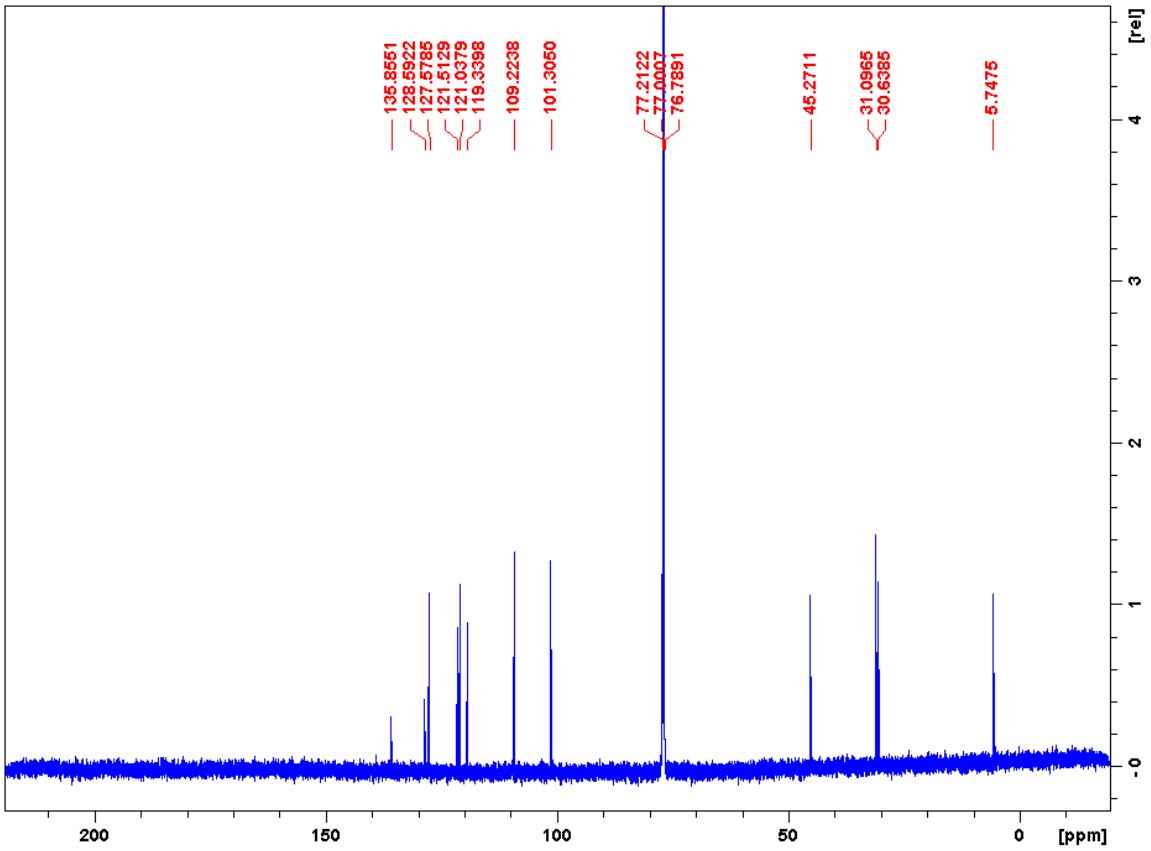
1.98
1.99
2.02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109.2238
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77.2122
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76.7891
45.2711
31.0965
30.6385
5.7475
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50
0
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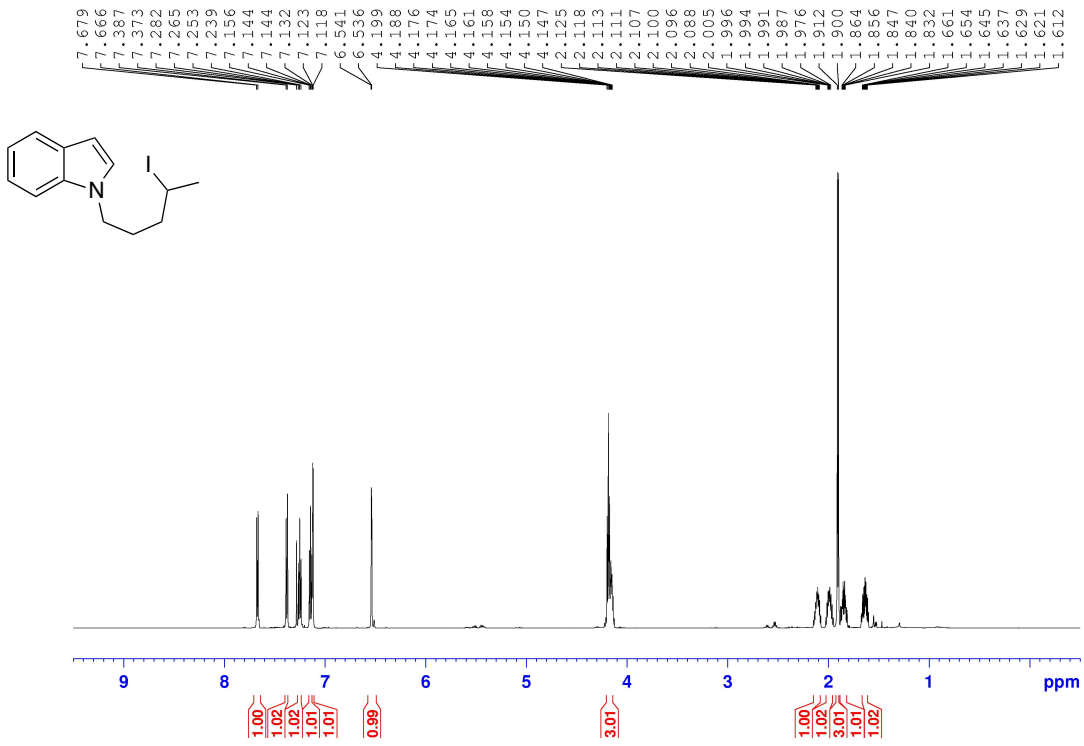
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7.144
7.132
7.123
7.118
6.541
6.536
4.199
4.188
4.176
4.174
4.165
4.161
4.158
4.154
4.150
4.147
2.125
2.118
2.113
2.111
2.107
2.100
2.096
2.088
2.005
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1.994
1.991
1.987
1.976
1.912
1.900
1.864
1.856
1.847
1.840
1.832
1.661
1.654
1.645
1.637
1.629
1.621
1.612
I
N
9
8
7
6
5
4
3
2
1
ppm
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1.00
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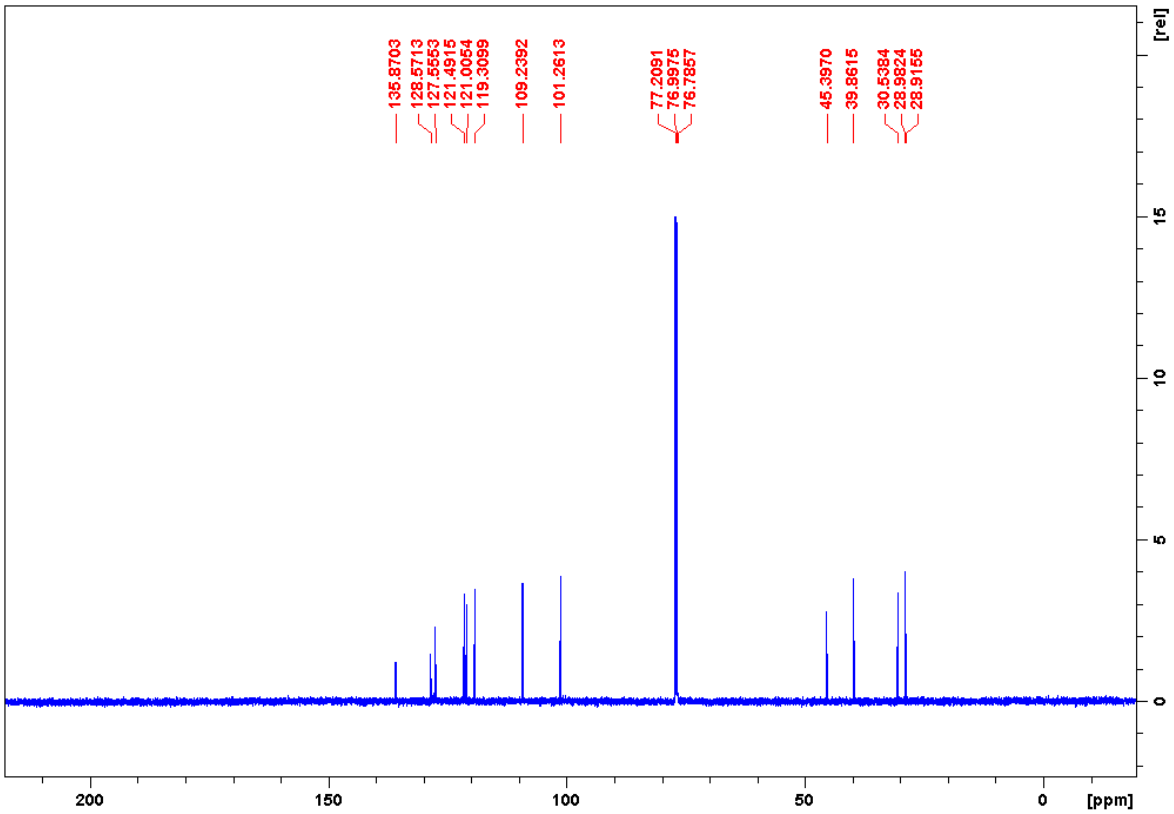
3.01
1.01
1.02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77.2091
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76.7857
45.3970
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28.9824
28.9155
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15
10
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0
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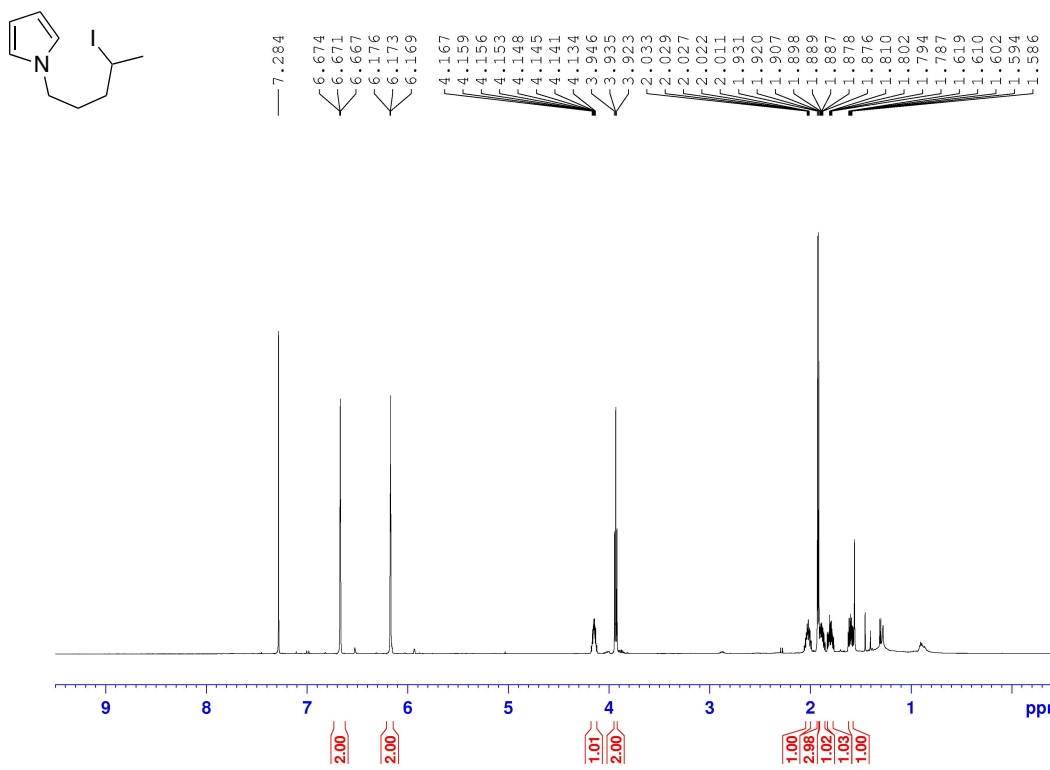
100
50
0
[ppm]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6.173
6.169
4.167
4.159
4.156
4.153
4.148
4.145
4.141
4.134
3.946
3.935
3.923
2.033
2.029
2.027
2.022
2.011
1.931
1.920
1.907
1.898
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1.887
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1.794
1.787
1.619
1.610
1.602
1.594
1.586
9
8
7
6
5
4
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ppm
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2.00
1.00
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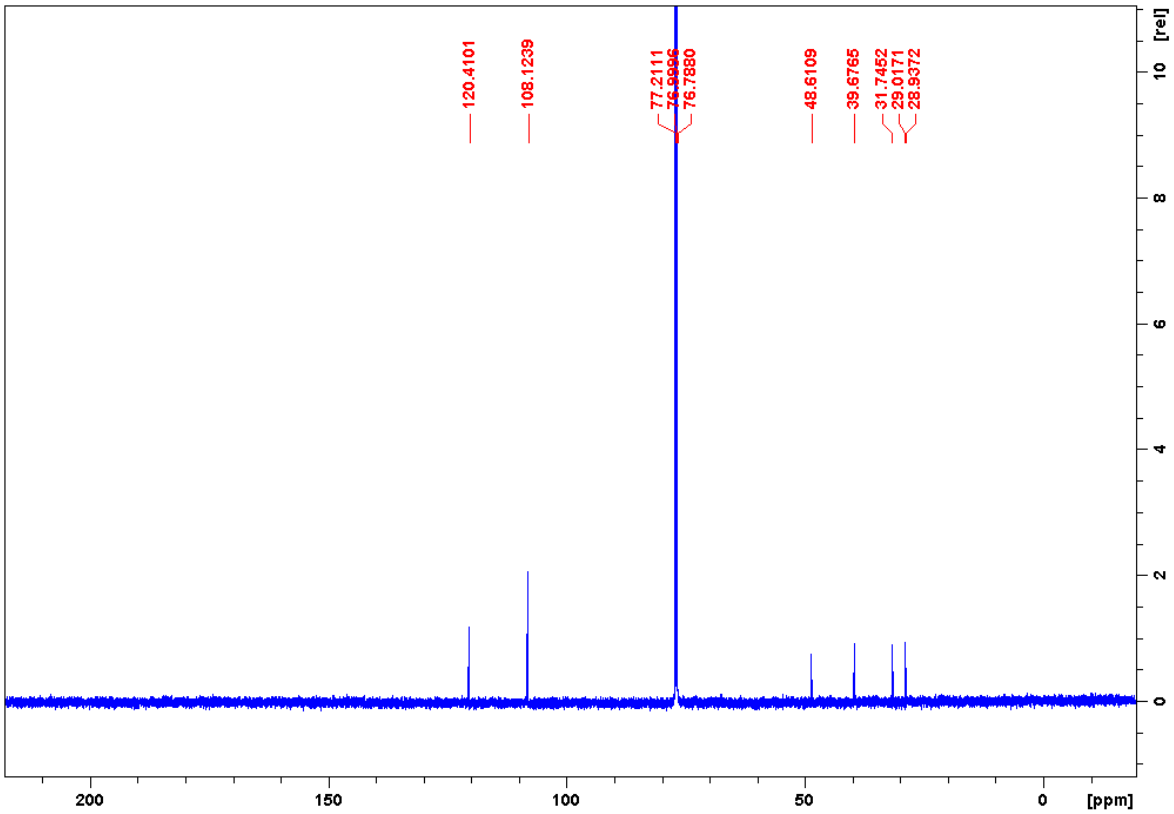
1.03
1.00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31.7452
29.0171
28.9372
10
8
6
4
2
0
[rel]
200
150
100
50
0
[ppm]