SUPPORTING INFORMATION FOR

On the Mechanism of the Dyotropic Expansion of Hydrindanes into Decalins

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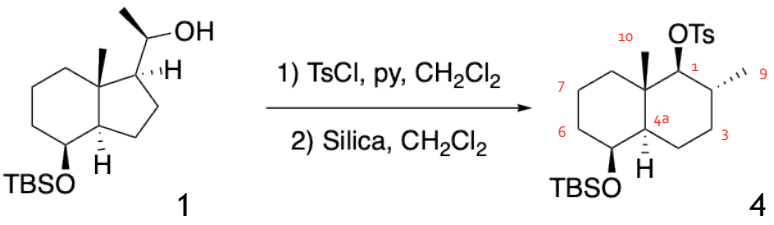
Experimental procedure

General: Solvents were purified and dried by standard procedures before use. Melting points are uncorrected. ^{1}H NMR and ^{13}C NMR spectra were recorded with a Bruker ARX-400 spectrometer (400 MHz for ^{1}H NMR, 100.61 MHz for ^{13}C NMR) using TMS as internal standard (Chemical shifts in δ values, J in Hz).

Flash chromatography (FC) was performed on silica gel (Silica Gel 40-63 µm (VWR Chemicals), silicaFlash P60 40-63 µm (Silicycle) and Silica Gel 2-5 mm (VWR Chemicals)); analytical TLC was performed on plates precoated with silica gel (Merck 60 F254, 0.25mm); mass spectra (FAB, EI) were recorded using FISONS VG and electron spray ionization (ESI-MS) spectroscopy was recorded using Bruker FTMS APEXIII. Melting points were obtained in open capillary tubes and are not corrected. Optical rotations were obtained using a Jasco P-2000 polarimeter. IR spectra were recorded with a JASCO FT/I(R)-6100 spectrophotometer.

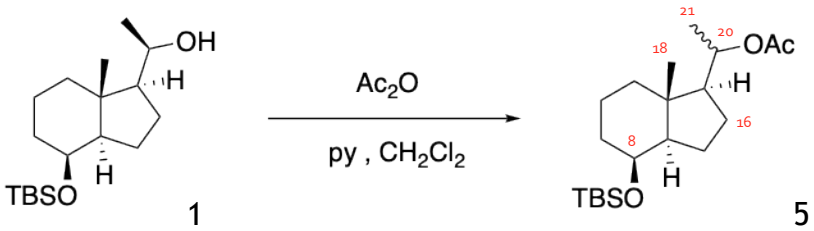
1. Synthesis of (1*S*,2*R*,4a*R*,5*S*,8a*S*)-5-((*tert*-butyldimethylsilyl)oxy)-2,8a-dimethyldecahydronaphthalen-1-yl 4-methylbenzenesulfonate (4)



To a solution of alcohol **1** (85 mg, 0.27 mmol) in CH_2Cl_2 (2 mL) at 0 ºC were added pyridine (0.44 mL, 5.44 mmol) and TsCl (518 mg, 2.72 mmol). After stirring the mixture at this temperature for 4 h, H_2O (5 ml) was added and the product was extracted with CH_2Cl_2 (3x15 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give a residue. To a solution of the residue in CH_2Cl_2 was added silica and stirred for 4 h. Then the mixture was concentrated and chromatographed on silica gel using 2% EtOAc/Hexane as eluent, affording mesylate **4** (105 mg, 83%) as a white solid (Mp: 59-61 ºC); Rf: 0.75 (10% EtOAc/Hexane).

IR (ATR, cm^{-1}): 2946, 2928, 2854, 1358, 1173, 1076, 1029, 906, 804. **$[\alpha]^{22}_D$**= +39.9 (c 1.00, $CHCl_3$). **^{1}H-NMR ($CDCl_3$, δ):** 7.79 (d, J = 8.0 Hz, 2H, 2H-Ts), 7.32 (d, J = 7.9 Hz, 2H, 2H-Ts), 4.12 (d, J = 10.7 Hz, 1H, H-1), 3.82 (s, 1H, H-5), 2.45 (s, 3H, Me-Ts), 1.91 (m, 1H), 1.80 (s, 2H), 1.65 (s, 3H), 1.52 (m, 2H), 1.35 (m, 2H), 1.08 (m, 2H), 1.03 (s, 3H, H-10), 0.88 (s, 9H, ^{t}Bu-TBS), 0.84 (d, J = 6.4 Hz, 3H, H-9), 0.01 (s, 3H, Me-TBS), 0.00 (s, 3H, Me-TBS) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 143.9 (C-Ts), 135.5 (C-Ts), 129.4 (CH-Ts), 127.4 (CH-Ts), 98.6 (CH-1), 71.4 (CH-5), 47.9 (CH-4a), 39.4 (C-8a), 37.7 (CH_2), 34.1 (CH_2), 33.7 (CH_2), 32.9 (CH-2), 25.8 (CH_3-^{t}Bu), 25.6 (CH_2), 21.6 (Me-Ts), 19.7 (CH_3-9), 18.0 (C-^{t}Bu), 16.4 (CH_2), 14.0 (CH_3-10), -4.6 (Me-TBS), -5.1 (Me-TBS) ppm. **MS (ESI) [m/z, (%)]:** 163.15 (45), 295.26 (100), 489.24 ([M]$^+$, 8). **HRMS (ESI):** 489.2465 calculated for $C_{25}H_{42}NaO_4SSi$, found 489.2451.

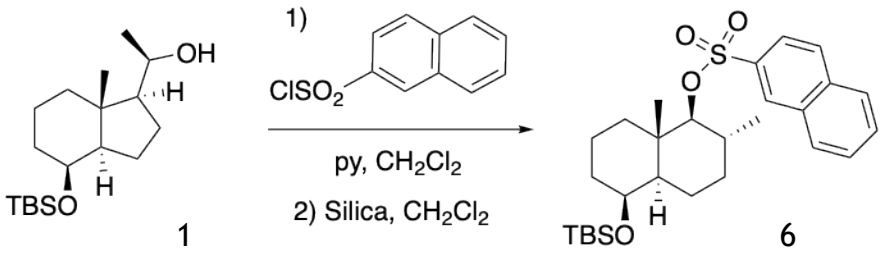
2. Synthesis of 1-((1*S*,3a*R*,4*S*,7a*R*)-4-((*tert*-butyldimethylsilyl)oxy)-7a-methyloctahydro-1*H*-inden-1-yl)ethyl acetate (5)



To a solution of alcohol **1** (101 mg, 0.27 mmol) in CH_2Cl_2 (2 mL) at 0 ºC were added pyridine (0.44 mL, 5.44 mmol) and TsCl (518 mg, 2.72 mmol). After stirring the mixture at this temperature for 24 h, H_2O (2 ml) was added and the product was extracted with CH_2Cl_2 (3x5 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give a residue which was chromatographed on silica gel using 1% EtOAc/Hexane as eluent, affording acetate **5** (30 mg, 25%) as a colourless oil; Rf: 0.80 (10% EtOAc/Hexane).

IR (ATR, cm^{-1}): 2945, 2928, 2855, 1351, 1073, 929, 774. **^{1}H-NMR ($CDCl_3$, δ):** 4.84 (m, 1H), 4.03 (s, 1H), 2.03 (s, 3H, Me-Ac), 1.80 (m, 3H), 1.69 (m, 3H), 1.54 (m, 3H), 1.40 (m, 4H), 1.28 (m, 2H), 1.15 (d, J = 6.1 Hz, 3H, CH_3-9), 0.89 (s, 9H, ^{t}Bu-TBS), 0.02 (s, 3H, Me-TBS), 0.01 (s, 3H, Me-TBS) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 170.5 (CO-Ac), 72.7 (CH-20), 69.1 (CH-8), 55.6 (CH), 52.5 (CH), 41.9 (C-13), 40.2 (CH_2), 34.5 (CH_2), 25.8 (Me-^{t}Bu), 24.6 (CH_2), 23.0 (CH_2), 21.6 (CH), 19.8 (CH_2-21), 18.0 (C-^{t}Bu), 17.6 (CH_2), 14.4 (CH_3-18), -4.8 (Me-TBS), -5.2 (Me-TBS) ppm. **MS (ESI) [m/z, (%)]:** 295.26 (100), 355.26 ([M+1]$^{+}$, 17). **HRMS (ESI):** 355.2663 calculated for $C_{20}H_{39}O_3Si$, found 355.2667.

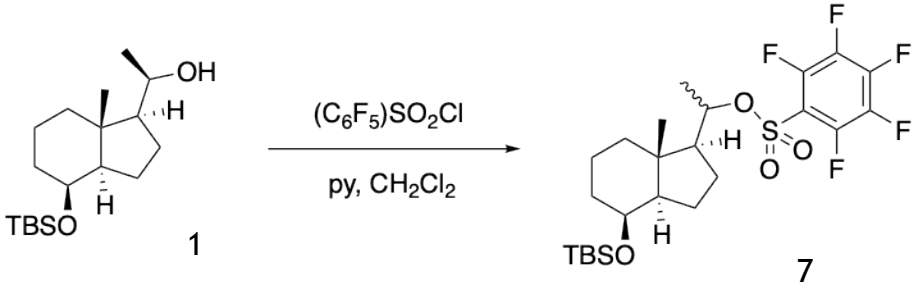
3. Synthesis of (1*S*,2*R*,4a*R*,5*S*,8a*S*)-5-((*tert*-butyldimethylsilyl)oxy)-2,8a-dimethyldecahydronaphthalen-1-yl naphthalene-2-sulfonate (6)



To a solution of alcohol **1** (77 mg, 0.24 mmol) in CH_2Cl_2 (2 mL) at r.t. were added Et_3N (0.33 mL, 2.40 mmol) and naphthalene-2-sulfonyl chloride (544 mg, 2.40 mmol). After stirring at the same temperature for 4 days, H_2O (2 ml) was added and the product was extracted with CH_2Cl_2 (3x5 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give a residue. To a solution of the residue in CH_2Cl_2 was added silica and stirred for 2 days. Then the mixture was concentrated and chromatographed on silica gel using 2% EtOAc/Hexane as eluent, affording compound **6** (85 mg, 70%) as a white solid (Mp: 65-68 ºC); Rf: 0.47 (10% EtOAc/Hexane).

IR (ATR, cm^{-1}): 2950, 2930, 2856, 1351, 1073, 930, 775. **$[\alpha]^{22}_D$**= +42.5 (c 1.00, $CHCl_3$). **^{1}H-NMR ($CDCl_3$, δ):** 8.47 (s, 1H, H-Ar), 7.98 (m, 2H, H-Ar), 7.92 (m, 2H, H-Ar), 7.66 (m, 2H, H-Ar), 4.21 (d, J = 9.9 Hz, 1H, H-1), 3.83 (s, 1H, H-5), 1.93 (m, 1H), 1.82 (m, 1H), 1.62 (m, 4H), 1.30 (m, 3H), 1.11 (m, 2H), 1.06 (s, 3H, CH_3-10), 0.92 (m, 1H), 0.88 (s, 9H, ^{t}Bu-TBS), 0.84 (d, J = 1.6 Hz, 3H, H-9), 0.01 (s, 6H) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 135.4 (C-Ar), 135.0 (C-Ar), 131.9 (C-Ar), 129.4 (CH-Ar), 129.2 (CH-Ar), 128.9 (CH-Ar), 128.5 (CH-Ar), 127.9 (CH-Ar), 127.5 (CH-Ar), 122.7 (CH-Ar), 99.1 (CH-1), 71.4 (CH-5), 47.9 (CH-4a), 39.5 (CH-8a), 37.8 (CH_2), 34.1 (CH_2), 33.7 (CH_2), 33.0 (CH-2), 25.8 (CH_3-^{t}Bu), 25.6 (CH_2), 19.8 (CH_3-9), 18.0 (C-^{t}Bu), 16.4 (CH_2), 14.0 (CH_3-10), -4.6 (Me-TBS), -5.1 (Me-TBS) ppm. **MS (ESI) [m/z, (%)]:** 295.25 (100), 525.24 ([M+Na]$^+$, 12). **HRMS (ESI):** 525.2465 calculated for $C_{28}H_{42}NaO_4SSi$, found 525.2460.

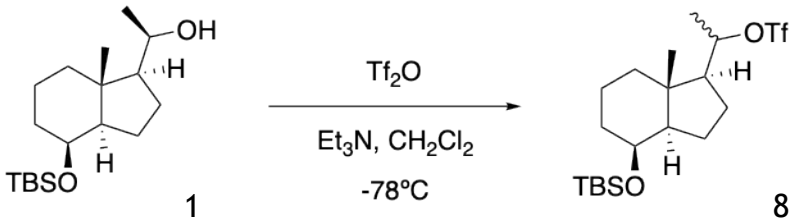
4. Synthesis of 1-((1*S*,3a*R*,4*S*,7a*S*)-4-((*tert*-butyldimethylsilyl)oxy)-7a-methyloctahydro-1*H*-inden-1-yl)ethyl 2,3,4,5,6-pentafluorobenzenesulfonate (7)



To a solution of alcohol **1** (83 mg, 0.26 mmol) in CH_2Cl_2 (2 mL) at r.t. were added Et_3N (0.12 mL, 0.79 mmol), a catalytic amount of 4-dimethylaminopyridine (DMAP) and $(C_6F_5)SO_2Cl$ (0.11 ml, 0.79 mmol). After stirring the mixture at this temperature for 22 h., H_2O (3 mL) was added and the product was extracted with CH_2Cl_2 (3x5 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give a residue which was chromatographed on silica gel using 3% EtOAc/Hexane as eluent, affording compound **7** (50 mg, 35%) as a colourless oil; Rf: 0.77 (10% EtOAc/Hexane).

IR (ATR, cm^{-1}): 2950, 2932, 2881, 1501, 1402, 1184, 1104, 995, 567, 550. **^{1}H-NMR ($CDCl_3$, δ):** 4.48 (m, 1H, H-20), 4.03/4.01 (s, 1H, H-8), 1.67 (m, 4H), 1.42 (m, 5H), 1.35 (m, 3H), 1.27 (m, 3H), 1.04/0.95 (d, J = 1.6 Hz, 3H, CH_3-21), 0.89 (s, 9H, ^{t}Bu-TBS), 0.01 (m, 6H, Me-TBS) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 147.6 (C-Ar), 145.8 (C-Ar), 143.1 (C-Ar), 139.3 (C-Ar), 136.8 (C-Ar), 83.1 (CH-20), 80.9 (CH-20), 69.1 (CH-8), 68.9 (CH-8), 56.6 (CH), 56.4 (CH), 52.6 (CH), 52.5 (CH), 42.03(C-13), 41.8 (C-13), 39.8 (CH_2), 39.5 (CH_2), 34.4 (CH_2), 34.2 (CH_2), 25.7 (CH_3-^{t}Bu), 25.0 (CH_2), 24.7 (CH_2), 23.0 (CH_2), 22.8 (CH_2), 22.0 (CH), 20.9 (CH_3-21), 18.0 (C-^{t}Bu), 17.5 (CH_2), 17.3 (CH_2), 14.3 (CH_3-18), 13.8 (CH_3-18), -4.8 (Me-TBS), -5.3 (Me-TBS) ppm. **MS (ESI) [m/z, (%)]:** 295.24 (100), 543.20 ($[M+1]^+$, 65), 590.21 (19). **HRMS (ESI):** 543.2018 calculated for $C_{24}H_{36}F_5O_4SSi$, found 543.2028.

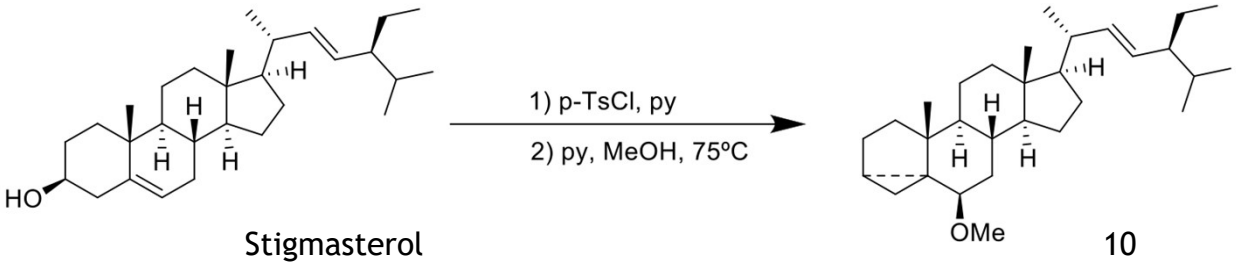
5. Synthesis of 1-((1*S*,3a*R*,4*S*,7a*S*)-4-((*tert*-butyldimethylsilyl)oxy)-7a-methyloctahydro-1*H*-inden-1-yl)ethyl trifluoromethanesulfonate (8)



To a solution of alcohol **1** (73 mg, 0.23 mmol) in CH_2Cl_2 (3 mL) at -78 °C were added Et_3N (0.33 mL, 2.35 mmol) and Tf_2O (0.11 ml, 0.70 mmol). After stirring the mixture at this temperature for 3 h, H_2O (2 mL) was added and the product was extracted with CH_2Cl_2 (3x5 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give a residue which was chromatographed on silica gel using 3% EtOAc/Hexane as eluent, affording compound **8** (20 mg, 25%) as a colourless oil; Rf: 0.73 (10% EtOAc/Hexane).

IR (ATR, cm^{-1}): 2953, 2930, 2856, 1196, 1131, 849. ^{1}H-NMR ($CDCl_3$, δ): 4.54 (m, 1H, H-20), 4.11 (s, 1H, H-8), 4.04 (s, 1H, H-8), 2.12 (m, 1H), 1.90 (m, 3H), 1.70 (m, 4H), 1.46 (d, J = 1.6 Hz, 3H, H-21), 1.40 (m, 4H), 1.37 (d, J = 1.6 Hz, 3H, H-21), 1.27 (m, 3H), 1.03 (s, 3H, CH_3-18), 0.99 (s, 3H, CH_3-18), 0.90 (s, 9H, CH_3-18), 0.03 (s, 3H, Me-TBS), 0.01 (s, 3H, Me-TBS) ppm. ^{13}C-NMR ($CDCl_3$, δ): 83.8 (CH-20), 81.9 (CH-20), 69.0 (CH-8), 56.6 (CH), 56.2 (CH), 52.6 (CH), 52.5 (CH), 42.1 (C-13), 39.5 (CH_2), 39.4 (CH_2), 34.4 (CH_2), 34.3 (CH_2), 25.8 (CH_3-^{t}Bu), 24.9 (CH_2), 23.0 (CH_2), 22.9 (CH_2), 21.8 (CH), 20.8 (CH_3-21), 18.0 (C-^{t}Bu), 17.6 (CH_2), 17.5 (CH_2), 17.4 (CH_2), 14.2 (CH_3-18), 13.9 (CH_3-18), -4.8 (Me-TBS), -5.2 (Me-TBS) ppm. MS (ESI) [m/z, (%)]: 295.24 (100), 445.20 ([M+1]$^+$, 5), 492.22 (25). HRMS (ESI): 445.2050 calculated for $C_{19}H_{36}F_3O_4SSi$, found 445.2057.

6. Synthesis of (1a*R*,3a*R*,3b*S*,5a*R*,6*R*,8a*S*,8b*S*,10*R*,10a*R*)-6-((2*R*,5*S*,*E*)-5-ethyl-6-methylhept-3-en-2-yl)-10-methoxy-3a,5a-dimethylhexadecahydrocyclopenta[*a*]cyclopropa[2,3]cyclopenta [1,2-*f*]naphthalene (10)



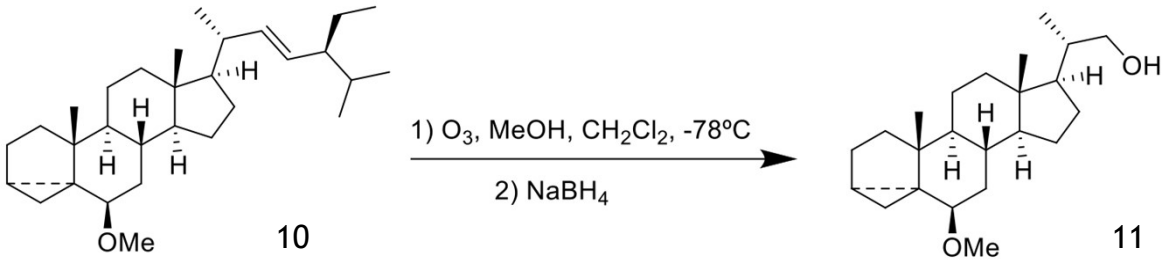
Stigmasterol 10

To a solution of Stigmasterol (988 mg, 2.39 mmol) in pyridine (15 mL) at 0 ºC was added p-TsCl (1.14 g, 5.97 mmol). After 21 h. under stirring, a saturated solution of $NaHCO_3$ (5 mL) and H_2O (10 mL) were added. The mixture was extracted with CH_2Cl_2 (3x15 mL), dried over Na_2SO_4, filtered and concentrated to give a residue. A solution of residue (524 mg, 0.92 mmol) and pyridine (0.22 mL, 2.77 mmol) in MeOH (8 mL) was heated to 75 ºC for 3h, then the solvent was evaporated and concentrated to give a residue which was chromatographed on silica gel using 2% EtOAc/Hexane as eluent, affording compound 10 (217 mg, 71%) as a colourless oil; Rf: 0.87 (10% EtOAc/Hexane).

IR (ATR, cm^{-1}): 2953, 2930, 2867, 1456, 1382, 1098, 970. $[\alpha]^{23}_D$= +10.02 (c 1.3, $CHCl_3$). ^{1}H-NMR ($CDCl_3$, δ): 5.18 (1H, dd, J=15.1/8.5Hz, H-22), 5.04 (1H, dd, J=15.1/8.6Hz, H-23), 3.35 (3H, s, CH_3O), 2.79 (1H, t, J=2.6Hz, H-6), 1.98 (3H, m), 1.75 (3H, m), 1.56 (6H, m),1.44 (3H, m), 1.29 (3H, s, H-18), 1.14 (6H, m), 1.04 (3H, d, J=6.9Hz, H-21), 0.85 (12H, m), 0.76 (3H, s, H-19), 0.67 (1H, t, J=4.3Hz, H-4), 0.46 (1H, dd, J=8.0/5.0Hz, H-4) ppm. ^{13}C-NMR ($CDCl_3$, δ): 138.4 (CH-22), 129.3 (CH-23), 82.5 (CH-6), 56.7 (CH_3O), 56.6 (CH), 56.2 (CH), 51.3

(CH), 48.1 (CH), 43.4 (C-10), 42.7 (C-13), 40.5 (CH), 40.2 (CH_2), 35.3 (C-5), 35.1 (CH_2), 33.4 (CH_2), 31.9 (CH), 30.5 (CH), 29.0 (CH_2), 25.4 (CH_2), 25.0 (CH_2), 24.3 (CH_2), 22.8 (CH_2), 21.5 (CH-3), 21.2 (CH_3-26/27), 21.1 (CH_3-26/27), 19.3 (CH_3-18), 19.0 (CH_3-21), 13.1 (CH_2-4), 12.5 (CH_3-19/29), 12.3 (CH_3-19/29) ppm. **MS (FAB) [m/z, (%)]:** 427.4 (M^++1, 17), 395.4 (M^+-MeO, 34). **HRMS (FAB):** 427.3940 calculated for $C_{30}H_{51}O$, found 427.3961.

7. Synthesis of (*S*)-2-((1a*R*,3a*R*,3b*S*,5a*S*,6*R*,8a*S*,8b*S*,10*R*,10a*R*)-10-methoxy-3a,5a-dimethylhexadecahydrocyclopenta[*a*]cyclopropa[2,3]cyclopenta[1,2-*f*]naphthalen-6-yl)propan-1-ol (11)

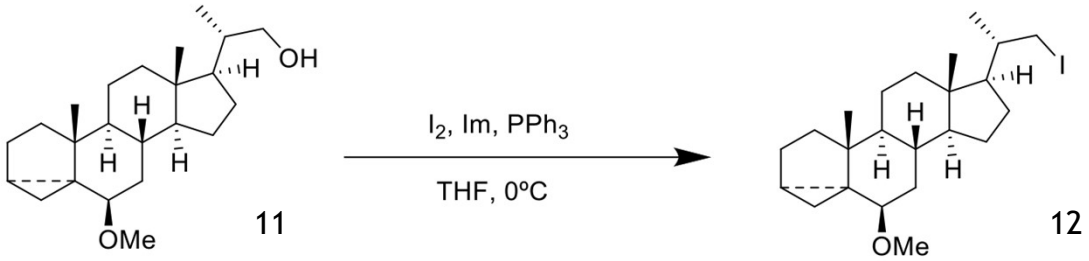


10 11

To a solution of compound **10** (415 mg, 0.97 mmol) in CH_2Cl_2 (30 ml) and MeOH (15 ml), was passed a current of O_3 (1.0 mL/min, 0.4 A), when the color of mixture change to blue that means a saturated solution of O_3 flux was sttoped. After passing a flow of Ar was added $NaBH_4$ (365 mg, 9.73 mmol) in small portions, and after 3 h. under stirring was added a 5% solution of HCl (20 mL) and the mixture was extracted with CH_2Cl_2 (2x30 ml). The combined organic layers was dried over Na_2SO_4 and the solvent evaporated under reduced pressure to give a residue which was chromatographed on silica gel using 12% EtOAc/Hexane as eluent, affording iodide **11** (304 mg, 90%) as a colourless liquid, Rf: 0.35 (20% AcOEt/Hexano).

IR (ATR, cm^{-1}): 3379, 2931, 2924, 2866, 1617, 1455, 1373, 1269, 736. **$[\alpha]^{23}_D$**= +33.53 (c 1.2, $CHCl_3$). **^{1}H-NMR ($CDCl_3$, δ):** 3.65 (1H, dd, J=10.5/3.2Hz, H-22), 3.38 (1H, dd, J=10.4/6.9Hz, H-22), 3.34 (3H, s, CH_3O), 2.79 (1H, t, J=2.5Hz, H-6), 1.87 (3H, m), 1.57 (3H, m), 1.39 (3H, m), 1.18 (6H, m), 1.06 (3H, d, J=6.6Hz, CH_3-21), 1.04 (3H, s, CH_3-18), 0.87 (6H, m), 0.75 (3H, s, CH_3-19), 0.66 (1H, dd, J=8.3/3.5Hz, H-4), 0.45 (1H, dd, J=8.1/5.1Hz, H-4) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 82.4 (CH-6), 68.0 (CH_2-22), 56.5 (CH_3O), 56.3 (CH), 52.6 (CH), 48.0 (CH), 43.4 (C-10), 42.9 (C-13), 40.1 (CH_2), 38.8 (CH), 35.3 (C-5), 35.1 (CH_2), 33.4 (CH_2), 30.5 (CH), 27.8 (CH_2), 25.0 (CH_2), 24.3 (CH_2), 22.8 (CH_2), 21.5 (CH-3), 19.3 (CH_3-18), 16.7 (CH_3-21), 13.1 (CH_2-4), 12.3 (CH_3-19) ppm. **MS (IE) [m/z, (%)]:** 347.3 (M+1, 8), 346.3 (M^+, 34), 315.3 (M^+-OMe, 15). **HRMS (IE):** 346.2872 calculated for $C_{23}H_{38}O_2$, found 346.2873.

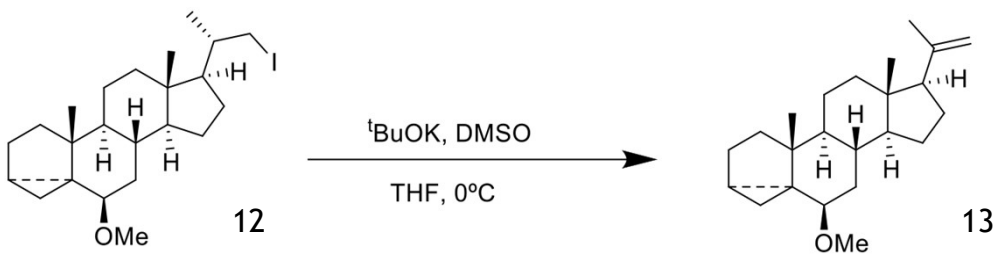
8. Synthesis of (1a*R*,3a*R*,3b*S*,5a*S*,6*R*,8a*S*,8b*S*,10*R*,10a*R*)-6-((*S*)-1-iodopropan-2-yl)-10-methoxy-3a,5a-dimethylhexadecahydrocyclopenta[*a*]cyclopropa[2,3]cyclopenta[1,2-*f*]naphthalene (12)



To a solution of diol **11** (561 mg, 1.62 mmol) in THF (5 mL) at room temperature were added siquentially PPh_3 (637 mg, 2.43 mmol) and imidazole (331 mg, 4.86 mmol). After cooling the mixture to 0 ºC, I_2 (576 mg, 2.27 mmol) was added and stirring continued for 20 min. The reaction was quenched with an aqueous saturated solution of $NaHCO_3$ (5 mL) and the product extracted with EtOAc (3x20 mL). The organic phase was washed with a 10% aqueous solution of $Na_2S_2O_3$ (10 mL) and brine (10 mL), dried over Na_2SO_4, filtered and concentrated to give a residue which was chromatographed on silica gel using 1% EtOAc/Hexane as eluent, affording iodide **12** (532 mg, 72%) as a colourless liquid, Rf: 0.76 (20% AcOEt/Hexano).

IR (ATR, cm^{-1}): 2927, 2864, 1455, 1377, 1095, 1017. **$[\alpha]^{21}_D$**= +17.62 (c 1.00, $CHCl_3$). **^{1}H-NMR ($CDCl_3$, δ):** 3.36 (1H, d, J=2.0Hz, H-22), 3.34 (3H, s, CH_3O), 3.19 (1H, dd, J=9.3/4.3Hz, H-22), 2.79 (1H, t, J=3.0Hz, H-6), 1.92 (3H, m), 1.70 (3H, m), 1.54 (1H, m), 1.44 (1H, m), 1.20 (6H,m), 1.10 (3H, dd, J=3.4/1.5Hz, CH_3-21), 1.04 (3H, s, CH_3-18), 0.86 (6H, m), 0.78 (3H, s, CH_3-19), 0.67 (1H, t, J=4.4Hz, H-4), 0.45 (1H, dd, J=8.1/4.9Hz, H-4) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 82.4 (CH-6), 56.6 (CH_3O), 56.2 (CH), 55.5 (CH), 47.9 (CH), 43.4 (C-10), 42.8 (C-13), 40.0 (CH_2), 36.9 (CH), 35.3 (C-5), 35.1 (CH_2), 33.4 (CH_2), 30.5 (CH), 27.7 (CH_2), 25.0 (CH_2), 24.1 (CH_2), 22.7 (CH_2), 21.5 (CH-3), 21.5 (CH_2-22), 20.8 (CH_3-18), 19.3 (CH_3-21), 13.1 (CH_2-4), 13.1 (CH_3-19) ppm. **MS (ESI) [m/z, (%)]:** 591.37 (30), 425.17 (M^+-OMe, 100). **HRMS (ESI):** 425.1699 calculadred for $C_{22}H_{34}I$, found 425.1685.

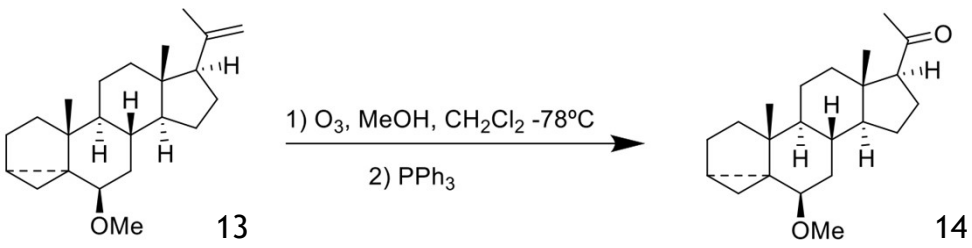
9. Synthesis of (1a*R*,3a*R*,3b*S*,5a*S*,6*R*,8a*S*,8b*S*,10*R*,10a*R*)-10-methoxy-3a,5a-dimethyl-6-(prop-1-en-2-yl)hexadecahydrocyclopenta[*a*]cyclopropa[2,3]cyclopenta[1,2-*f*]naphthalene (13)



To a solution of iodine **12** (532 mg, 1.16 mmol) in THF (7 mL) at 0 ºC were added ^{t}BuOK (260 mg, 2.32 mmol) and DMSO (3 mL). After 4h. under stirring the reaction was quenched with H_2O (10 mL) and the product extracted with EtOAc (3x10 mL). The organic phase were dried over Na_2SO_4, filtered and concentrated to give a residue which was chromatographed on silica gel using 1% EtOAc/Hexane as eluent, affording alkene **13** (325 mg, 85%) as a colourless oil, Rf: 0.67 (10% AcOEt/Hexano).

IR (ATR, cm^{-1}): 2951, 2929, 2868, 1640, 1453, 1098, 855. **[α]$^{21}_{D}$**= +20.95 (c 1.00, $CHCl_3$). **^{1}H-NMR ($CDCl_3$, δ):** 4.79 (1H, d, J=54.6Hz, H-22), 3.79 (3H, s, CH_3O), 2.79 (1H, t, J=2.9Hz, H-6), 2.05 (1H, t, J=9.3Hz), 1.90 (1H, m), 1.77 (3H, s, CH_3-21), 1.71 (3H, m), 1.48 (6H, m), 1.18 (6H,m) 1.04 (3H, s, CH_3-18), 0.88 (3H, m), 0.67 (1H, dd, J=5.1/3.8Hz, H-4), 0.64 (3H, s, CH_3-19), 0.45 (1H, dd, J=8.0/5.1Hz, H-4) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 145.7 (C-20), 110.7 (CH_2-22), 82.4 (CH-6), 57.4 (CH), 56.6 (CH_3O), 56.4 (CH), 48.3 (CH), 43.5 (C-10), 43.5 (C-13), 39.2 (CH_2), 35.3 (C-5), 35.1 (CH_2), 33.4 (CH_2), 30.8 (CH), 25.5 (CH_2), 25.0 (CH_2), 24.7 (CH_3-21), 24.2 (CH_2), 22.8 (CH_2), 21.5 (CH-3), 19.3 (CH_3-18), 13.1 (CH_2-4), 13.1 (CH_3-19) ppm. **EM (ESI) [m/z, (%)]:** 425.17 (40), 297.26 (M^+-OMe, 100). **EMAR (ESI):** 297.2576 calculated for $C_{22}H_{33,}$ found 297.2564.

10. Synthesis of 1-((1a*R*,3a*R*,3b*S*,5a*S*,6*S*,8a*S*,8b*S*,10*R*,10a*R*)-10-methoxy-3a,5a-dimethylhexadecahydrocyclopenta[*a*]cyclopropa[2,3]cyclopenta[1,2-*f*]naphthalen-6-yl)ethan-1-one (14)



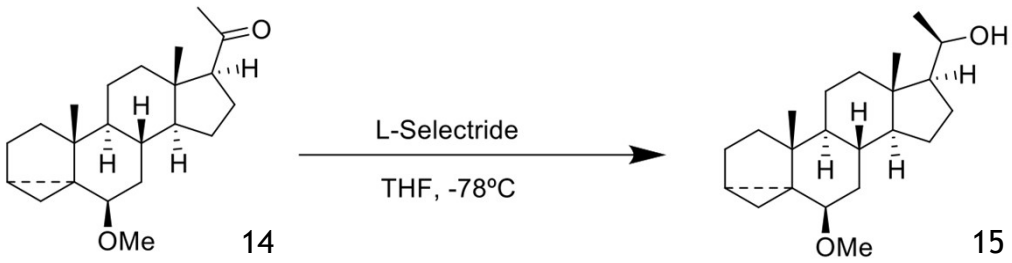
13 14

To a solution of compound **13** (325 mg, 0.99 mmol) in CH_2Cl_2 (20 mL) and MeOH (4 mL), was passed a current of O_3 (1.0 ml/min, 0.40 A), after 10 min. the O_3 flux was sttoped when the color of mixture change to blue that means a saturated solution of O_3. After passing a flow of Ar was added PPh_3 (648 mg, 2.47 mmol) in

small portions, and then 5 min. under stirring was added a saturated solution of NH_4Cl (15 ml) and the mixture was extracted with CH_2Cl_2 (2x30 ml). The combined organic layers was dried over Na_2SO_4 and the solvent evaporated under reduced pressure to give a residue which was chromatographed on silica gel using 10% EtOAc/Hexane as eluent, affording ketone **14**(240 mg, 74%) as a colourless oil, Rf: 0.35 (10% AcOEt/Hexano).

IR (ATR, cm^{-1}): 2930, 2869, 2847, 1704, 1453, 1354, 1097, 1016. **$[\alpha]^{21}_D$= +63.71** (c 1.00, $CHCl_3$). **^{1}H-NMR ($CDCl_3$, δ):** 3.31 (3H, s, CH_3O), 2.76 (1H, t, J=2.9Hz, H-6), 2.52 (1H, t, J=9.0Hz, H-17), 2.16 (1H, m), 2.10 (3H, s, CH_3-21), 2.02 (1H, m), 1.89 (1H, m), 1.69 (3H, m), 1.47 (6H, m), 1.18 (3H, m), 1.01 (3H, s, CH_3-18), 0.86 (3H, m), 0.65 (3H, s, CH_3-19), 0.64 (1H, t, J=3.1Hz, H-4), 0.44 (1H, m, H-4) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 209.5 (C-20), 82.2 (CH-6), 63.9 (CH-17), 56.7 (CH), 56.6 (CH_3O), 47.9 (CH), 44.4 (C-10), 43.4 (C-13), 39.3 (CH_2), 35.2 (C-5), 35.1 (CH_2), 33.4 (CH_2), 31.5 (CH_3-21), 30.5 (CH), 24.9 (CH_2), 24.4 (CH_2), 22.8 (CH_2), 22.8 (CH_2), 21.4 (CH-3), 19.3 (CH_3-18), 13.6 (CH_3-19), 13.1 (CH_2-4) ppm. **MS (ESI) [m/z, (%)]:** 425.17 (100), 299.24 (M^+-OMe, 35). **HRMS (ESI):** 299.2369 calculated for $C_{21}H_{31}O$, found 299.2365.

11. Synthesis of (*R*)-1-((1a*R*,3a*R*,3b*S*,5a*S*,6*S*,8a*S*,8b*S*,10*R*,10a*R*)-10-methoxy-3a,5a-dimethylhexadecahydrocyclopenta[*a*]cyclopropa[2,3]cyclopenta[1,2-*f*]naphthalen-6-yl)ethan-1-ol (15)

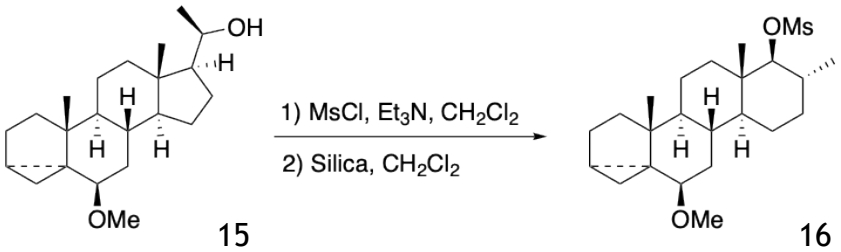


To a solution of ketone **14** (240 mg, 0.72 mmol) in THF (3 mL) cooled to -78ºC was added a solution 1 M of L-Selectride in THF (1.82 mL, 1.82 mmol) and was stirred for 3 h. Then, over the solution was added a saturated solution of NH_4Cl (5 ml) and extracted with EtOAc (2x10 ml). The combined organic layers was dried over Na_2SO_4 and the solvent evaporated under reduced pressure to give a residue which was chromatographed on silica gel using 6% EtOAc/Hexane as eluent, affording alcohol **15** (169 mg, 70%) as a colourless oil, Rf: 0.45 (20% AcOEt/Hexano).

IR (ATR, cm^{-1}): 3329, 2953, 2929, 2856, 1455, 1373, 1098, 1015. **$[\alpha]^{22}_D$= +6.57** (c 1.00, $CHCl_3$). **^{1}H-NMR ($CDCl_3$, δ):** 3.75 (1H, m, H-20), 3.33 (3H, s, CH_3O), 2.78 (1H, t, J=2.9Hz, H-6), 2.06 (1H, m), 1.89 (1H,m), 1.77 (2H, m),

1.66 (2H, m), 1.53 (2H, m), 1.44 (2H, m), 1.26 (6H, m), 1.14 (3H, d, J=6.1Hz, CH_3-21), 1.09 (1H, m), 1.04 (3H, s, CH_3-18), 0.87 (3H, m), 0.81 (3H, s, CH_3-19), 0.66 (1H, t, J=4.6Hz, H-4), 0.44 (1H, dd, J=8.0/5.1Hz, H-4) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 82.4 (CH-6), 70.5 (CH-20), 58.6 (CH-17), 56.6 (CH_3O), 56.0 (CH) 48.1 (CH), 43.4 (C-10), 42.7 (C-13), 40.4 (CH_2), 35.3 (C-5), 35.2 (CH_2), 33.4 (CH_2), 30.4 (CH), 25.7 (CH_2), 25.0 (CH_2), 24.4 (CH_2), 23.6 (CH_3-21), 22.6 (CH_2), 21.5 (CH-3), 19.3 (CH_3-18), 13.1 (CH_2-4), 12.8 (CH_3-19) ppm. **MS (ESI) [m/z, (%)]:** 425.17 (100), 301.25 (M^+-OMe, 33), 283.24 (M^+-OMe-OH, 71). **HRMS (ESI):** 301.2526 calculated for $C_{21}H_{33}O$, found 301.2521.

12. Synthesis of (1a*R*,3a*R*,3b*S*,5a*S*,6*S*,7*R*,9a*S*,9b*R*,11*R*,11a*R*)-11-methoxy-3a,5a,7-trimethylhexadecahydro-1*H*-cyclopropa[2,3]cyclopenta[1,2-*a*]phenanthren-6-yl methanesulfonate (16)



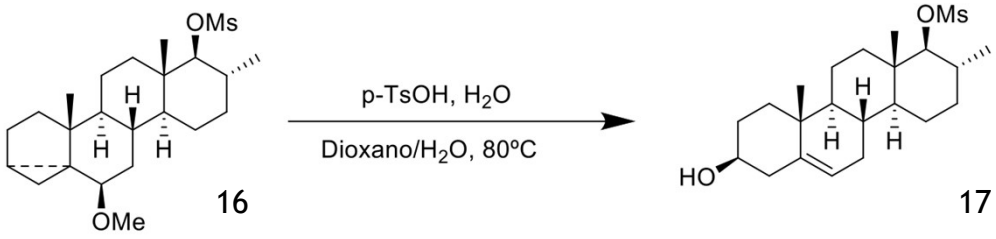
15 16

To a solution of alcohol **15** (84 mg, 0.25 mmol) in CH_2Cl_2 (2 mL) at -78 ºC were added Et_3N (0.11 mL, 0.76 mmol), DMAP (in catalytic amount) and MsCl (0.06 mL, 0.76 mmol). After stirring the mixture at this temperature for 2 h, H_2O (5 ml) was added and the product was extracted with CH_2Cl_2 (3x15 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give a residue. To a solution of the residue in CH_2Cl_2 was added silica and stirred for 1 h. Then the mixture was concentrated and chromatographed on silica gel using 7% EtOAc/Hexane as eluent, affording mesylate **16** (62 mg, 74%) as a colourless oil; Rf: 0.46 (20% EtOAc/Hexane).

IR (ATR, cm^{-1}): 2957, 2929, 2854, 1458, 1340, 1174, 1009, 917. **[α]$^{22}_D$**= +99.25 (c 1.00, $CHCl_3$). **^{1}H-NMR ($CDCl_3$, δ):** 4.11 (1H, d, J=10.8Hz, H-20), 3.32 (3H, s, CH_3O), 3.05 (3H, s, Ms-CH_3), 2.80 (1H, t, J=3.0Hz, H-6), 2.07 (1H, m), 1.89 (3H, m), 1.69 (3H, m), 1.51 (3H, m), 1.27 (3H, m), 1.09 (1H, m), 1.02 (3H, s, CH_3-18), 1.00 (3H, d, J=5.4Hz, CH_3-21), 0.93 (3H, s, CH_3-19), 0.85 (5H, m), 0.66 (1H, t, J=4.4Hz, H-4), 0.45 (1H, dd, J =8.1/5.1Hz, H-4) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 98.1 (CH-20), 82.2 (CH-6), 56.6 (CH_3O), 50.3 (CH-14), 47.2 (CH), 43.5 (C-10), 39.5 (C-13), 38.8 (CH_3-Ms), 38.0 (CH_2), 34.6 (C-5), 34.5 (CH_2), 33.6 (CH_2), 33.3 (CH_2), 32.4 (CH), 30.5 (CH), 24.9

(CH_2), 23.0 (CH_2), 21.7 (CH_2), 21.2 (CH-3), 19.7 (CH_3-21), 19.3 (CH_3-18), 13.2 (CH_2-4), 12.6 (CH_3-19) ppm. **MS (ESI) [m/z, (%)]:** 379.23 (M^+-OMe, 100), 283.24 (40). **HRMS (ESI):** 379.2301 calculated for $C_{22}H_{35}O_3S$, found 379.2295.

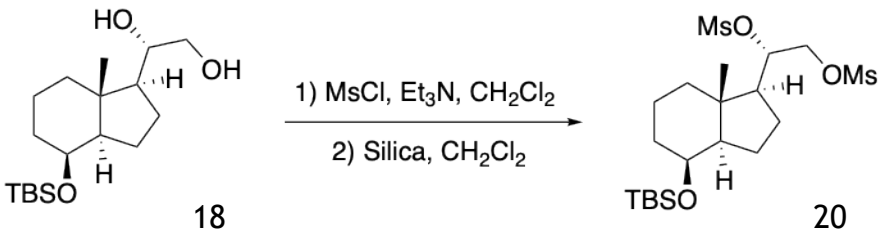
13. Synthesis of (1*S*,2*R*,4a*S*,4b*R*,8*S*,10a*R*,10b*S*,12a*S*)-8-hydroxy-2,10a,12a-trimethyl-1,2,3,4,4a,4b,5,7,8,9,10,10a,10b,11,12,12a-hexadecahydrochrysen-1-yl methanesulfonate (17)



To a solution of compound **16** (98 mg, 2.4 mmol) in dioxane (4 mL) and H_2O (1 mL) was added p-TsOH (in catalytic amount). The mixture was kept und stirring at 80 ºC for 2 h. After that, H_2O (5 mL) was added and it was extracted with CH_2Cl_2 (3x5 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give a residue which was chromatographed on silica gel using 70% EtOAc/Hexane as eluent, affording mesylate **17** (82 mg, 87%) as a white solid (Mp: 127-129 ºC); Rf: 0.47 (70% EtOAc/Hexane).

IR (ATR, cm^{-1}): 3515, 2930, 2873, 2853, 1336, 1171, 1043, 916. **$[\alpha]^{22}_D$**= +63.50 (c 1.00, $CHCl_3$). **^{1}H-NMR ($CDCl_3$, δ):** 5.34 (1H, t, J=2.5Hz, H-6), 4.12 (1H, d, J=10.8Hz, H-20), 3.53 (1H, m, H-3), 3.07 (3H, s, Ms-CH_3), 2.22 (3H, m), 1.88 (7H, m), 1.51 (7H, m), 1.19 (3H, m), 1.03 (3H, d, J=6.5Hz, CH_3-21), 0.99 (3H, s, CH_3-18), 0.91 (3H, s, CH_3-19), 0.83 (1H, m) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 140.5 (C-5), 121.2 (CH-6), 97.8 (CH-20), 71.6 (CH-3), 50.7 (CH-14), 49.2 (CH), 41.9 (CH_2), 39.1 (C-10), 38.8 (Ms-CH_3), 37.2 (CH_2), 36.8 (CH_2), 36.7 (C-13), 33.6 (CH_2), 32.5 (CH), 31.9 (CH_2), 31.5 (CH_2), 31.4 (CH), 23.3 (CH_2), 19.8 (CH_2), 19.7 (CH_3-21), 19.3 (CH_3-18), 12.3 (CH_3-19) ppm. **MS (ESI) [m/z, (%)]:** 603.87 (50), 379.23 (M^+-OH, 100), 283.24 (34). **HRMS (ESI):** 379.2301 calculated for $C_{22}H_{35}O_3S$, found 379.2296.

14. Synthesis of (*S*)-1-((1*S*,3a*R*,4*S*,7a*S*)-4-((*tert*-butyldimethylsilyl)oxy)-7a-methyloctahydro-1*H*-inden-1-yl)ethane-1,2-diyl dimethanesulfonate (18)

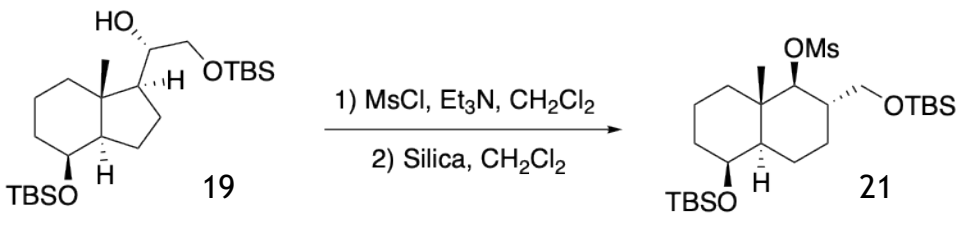


18 20

To a solution of diol **18** (40 mg, 0.12 mmol) in CH_2Cl_2 (2 mL) at 0 ºC were added Et_3N (0.10 mL, 0.73 mmol), DMAP (in catalytic amount) and MsCl (57 µL, 0.73 mmol). After stirring the mixture at this temperature for 3 h, H_2O (3 mL) was added and the product was extracted with CH_2Cl_2 (3x5 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give a residue which was dissolved in CH_2Cl_2, added silica and stirred for 16 h. Then the mixture was concentrated and chromatographed on silica gel using 25% EtOAc/Hexane as eluent, affording mesylate **20** (52 mg, 90%) as a colourless oil; Rf: 0.40 (30% EtOAc/Hexane).

IR (ATR, cm^{-1}): 2929, 2850, 1460, 1329, 1137, 1072, 777, 695. **$[\alpha]^{22}_D$**= +10.3 (c 1.00, $CHCl_3$). **^{1}H-NMR ($CDCl_3$, δ):** 4.89 (m, 1H, H-20), 4.63 (dd, J = 11.8, 2.1 Hz, 1H, H-21), 4.20 (dd, J = 11.8, 3.5 Hz, 1H, H-21), 4.04 (s, 1H, H-8), 3.12 (s, 3H, Me-Ms), 3.10 (s, 3H, Me-Ms), 1.95 (m, 2H), 1.88 (m, 2H), 1.79 (m, 2H), 1.65 (m, 2H), 1.50 (m, 2H), 1.33 (m, 2H), 1.06 (s, 3H, CH_3-18), 0.89 (s, 9H, ^{t}Bu-TBS), 0.03 (s, 3H, Me-TBS), 0.01 (s, 3H, Me-TBS) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 80.0 (CH-20), 70.1 (CH_2-21), 68.8 (CH-8), 52.3 (CH-17), 49.6 (CH-14), 41.9 (C-13), 39.5 (Me-Ms), 39.2 (CH_2), 37.5 (Me-Ms), 34.2 (CH_2), 25.8 (Me-^{t}Bu), 24.0 (CH_2), 22.8 (CH_2), 18.0 (C-^{t}Bu), 17.4 (CH_2), 13.9 (CH_3-18), -4.8 (Me-TBS), -5.2 (Me-TBS) ppm. **MS (ESI) [m/z, (%)]:** 507.18 ([M+Na]$^+$, 100). **HRMS (ESI):** 507.1877 calculated for $C_{20}H_{40}O_7S_2Si$, found 507.1884.

15. Synthesis of (1*S*,2*S*,4a*R*,5*S*,8a*S*)-5-((*tert*-butyldimethylsilyl)oxy)-2-(((*tert*-butyldimethylsilyl)oxy)methyl)-8a-methyldecahydronaphthalen-1-yl methanesulfonate (19)

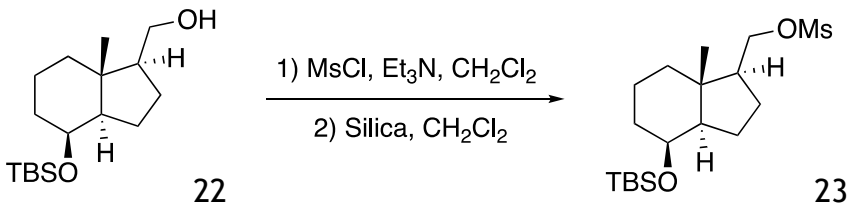


19 21

To a solution of alcohol **19** (36 mg, 0.08 mmol) in CH_2Cl_2 (2 mL) at 0 ºC were added Et_3N (34 µL, 0.24 mmol), DMAP (in catalytic amount) and MsCl (19 µL, 0.24 mmol). After stirring the mixture at this temperature for 2 h, H_2O (2 ml) was added and the product was extracted with CH_2Cl_2 (3x5 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give a residue. To a solution of the residue in CH_2Cl_2 was added silica and stirred for 16 h. Then the mixture was concentrated and chromatographed on silica gel using 3% EtOAc/Hexane as eluent, affording mesylate **21** (27 mg, 65%) as a colourless oil; Rf: 0.35 (10% EtOAc/Hexane).

IR (ATR, cm^{-1}): 2930, 2853, 1453, 1330, 1159, 1076, 907, 769. **$[\alpha]^{17}_D$**= +64.2 (c 1.00, $CHCl_3$). **^{1}H-NMR ($CDCl_3$, δ):** 4.34 (d, J = 10.9 Hz, 1H, H-1), 3.84 (s, 1H, H-5), 3.60 (m, 1H, H-9), 3.47 (m, 1H, H-9), 3.07 (s, 3H, Me-Ms), 2.10 (m, 1H), 2.01 (m, 1H), 1.92 (m, 1H), 1.82 (m, 2H), 1.63 (m, 4H), 1.29 (m, 3H), 1.10 (s, 3H, CH_3-10), 0.91 (s, 18H, ^{t}Bu-TBS), 0.05 (s, 12H, Me-TBS) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 92.1 (CH-1), 71.4 (CH-5), 66.5 (CH_2-9), 47.6 (CH-4a), 39.9 (CH-2), 39.2 (C-8a), 38.4 (Me-Ms), 37.5 (CH_2), 34.0 (CH_2), 32.5 (CH_2), 25.9 (CH_3-^{t}Bu), 25.8 (CH_3-^{t}Bu), 25.1 (CH_2), 18.0 (C-^{t}Bu), 16.4 (CH_2), 13.95 (CH_3-10), -4.6 (CH_3-Si), -5.1 (CH_3-Si), -5.3 (CH_3-Si), -5.5 (CH_3-Si) ppm. **MS (ESI) [m/z, (%)]:** 521.31 ([M+1]$^+$, 100). **HRMS (ESI):** 521.3147 calculated for $C_{25}H_{53}O_5SSi_2$, found 521.3155.

16. Synthesis of ((1S,3aR,4S,7aR)-4-((tert-butyldimethylsilyl)oxy)-7a-methyloctahydro-1H-inden-1-yl)methyl methanesulfonate (23)

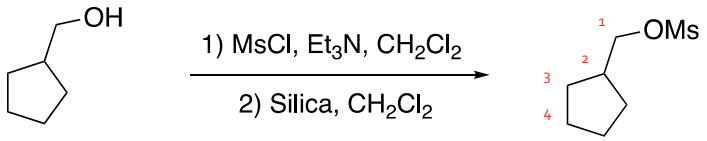


22 23

To a solution of alcohol **22** (77 mg, 0.25 mmol) in CH_2Cl_2 (3 mL) at 0 ºC were added Et_3N (107 µL, 0.77 mmol) and MsCl (60 µL, 0.77 mmol). After stirring the mixture at this temperature for 2 h, H_2O (2 ml) was added and the product was extracted with CH_2Cl_2 (3x5 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give a residue. To a solution of the residue in CH_2Cl_2 was added silica and stirred for 16 h. Then the mixture was concentrated and chromatographed on silica gel using 5% EtOAc/Hexane as eluent, affording mesylate **23** (84 mg, 90%) as a colourless oil; Rf: 0.51 (10% EtOAc/Hexane).

IR (ATR, cm^{-1}): 2929, 2854, 1455, 1320, 1149, 1086, 903, 769. **$[\alpha]^{15}_D$**= +14.2 (c 1.00, $CHCl_3$). **^{1}H-NMR ($CDCl_3$, δ):** 4.27 (m, 1H, H-20), 4.15 (m, 1H, H-20), 4.05 (s, 1H, H-8), 3.01 (s, 3H, Me-Ms), 1.74 (m, 6H), 1.44 (m, 3H), 1.34 (m, 2H), 1.17 (m, 1H), 0.96 (s, 3H, CH_3-18), 0.90 (s, 9H, ^{t}Bu-TBS), 0.04 (s, 3H, CH_3-Si), 0.02 (s, 3H, CH_3-Si) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 71.6 (CH_2-20), 68.9 (CH-8), 52.5 (CH-17), 49.6 (CH-14), 41.7 (C-13), 39.2 (CH_2), 37.3 (CH_3-Ms), 34.4 (CH_2), 25.8 (CH_3-^{t}Bu), 24.4 (CH_2), 23.2 (CH_2), 18.0 (C-^{t}Bu), 17.4 (CH_2), 14.4 (CH_3-18), -4.8 (CH_3-Si), -5.2 (CH_3-Si) ppm. **MS (ESI) [m/z, (%)]:** 377.22 ([M+1]$^+$, 100). **HRMS (ESI):** 377.2176 calculated for $C_{18}H_{37}O_4SSi$, found 377.2180.

17. Synthesis of cyclopentylmethyl methanesulfonate (2')

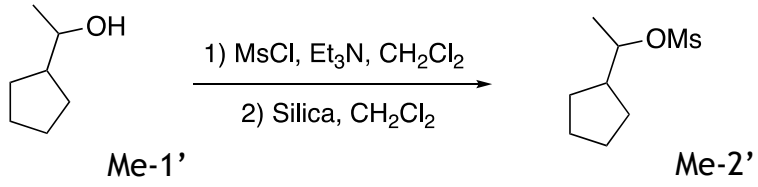


1' 2'

To a solution of alcohol **1'** (186 mg, 1.85 mmol) in CH_2Cl_2 (3 mL) at 0 ºC were added Et_3N (0.77 mL, 5.55 mmol) and MsCl (0.43 mL, 5.55 mmol). After stirring the mixture at this temperature for 1 h, H_2O (5 mL) was added and the product was extracted with CH_2Cl_2 (3x10 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give a residue. To a solution of the residue in CH_2Cl_2 was added silica and stirred for 16 h. Then the mixture was concentrated and chromatographed on silica gel using 10% EtOAc/Hexane as eluent, affording mesylate **2'** (315 mg, 95%) as a colourless oil; Rf: 0.40 (10% EtOAc/Hexane).

IR (ATR, cm^{-1}): 2930, 2854, 1454, 1249, 1006, 927, 859. **^{1}H-NMR ($CDCl_3$, δ):** 4.08 (d, *J*=7.2 Hz, 2H, H-1), 2.99 (s, 3H, Me-Ms), 2.28 (p, *J*=7.5 Hz, 1H, H-2), 1.78 (m, 2H), 1.60 (m, 4H), 1.28 (m, 2H) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 73.9 (CH_2-1), 52.6 (CH-2), 37.2 (Me-Ms), 29.0 (CH_2), 25.3 (CH_2) ppm. **MS (ESI) [m/z, (%)]:** 179.07 ($[M+1]^+$, 100). **HRMS (ESI):** 179.0742 calculated for $C_7H_{15}O_3S$, found 179.0751.

18. Synthesis of 1-cyclopentylethyl methanesulfonate (Me-2')



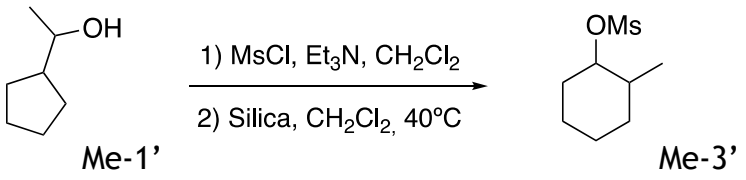
Me-1' Me-2'

To a solution of alcohol **Me-1'** (27 mg, 0.24 mmol) in CH_2Cl_2 (2 mL) at 0 ºC were added Et_3N (100 µL, 0.72 mmol) and MsCl (55 µL, 0.72 mmol). After stirring the mixture at this temperature for 2 h, H_2O (2 ml) was added and the product was extracted with CH_2Cl_2 (3x5 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give a residue. To a solution of the residue in CH_2Cl_2 was added silica and stirred for 16 h. Then the mixture was concentrated and chromatographed on silica gel using 15% EtOAc/Hexane as eluent, affording mesylate **Me-2'** (39 mg, 86%) as a colourless oil; Rf: 0.53 (20% EtOAc/Hexane).

IR (ATR, cm^{-1}): 2929, 2850, 1364, 1201, 1060, 876, 762. **^{1}H-NMR ($CDCl_3$, δ):** 4.65 (m, 1H, H-1), 3.00 (s, 3H, Me-Ms), 2.07 (p, *J*=7.5 Hz, 1H, H-2), 1.80 (m, 2H), 1.62 (m, 4H), 1.43 (d, *J*=6.3 Hz, 3H, H-1'), 1.26 (m, 2H) ppm. **^{13}C-NMR ($CDCl_3$, δ):** 84.1 (CH-1), 52.6 (CH-2), 38.7 (Me-Ms), 29.1 (CH_2), 28.8 (CH_2), 25.5 (CH_2), 25.3 (CH_2),

20.4 (CH_3-1') ppm. **MS (ESI) [m/z, (%)]:** 193.09 ([M+1]$^+$, 100). **HRMS (ESI):** 193.0893 calculated for $C_8H_{17}O_3S$, found 193.0889.

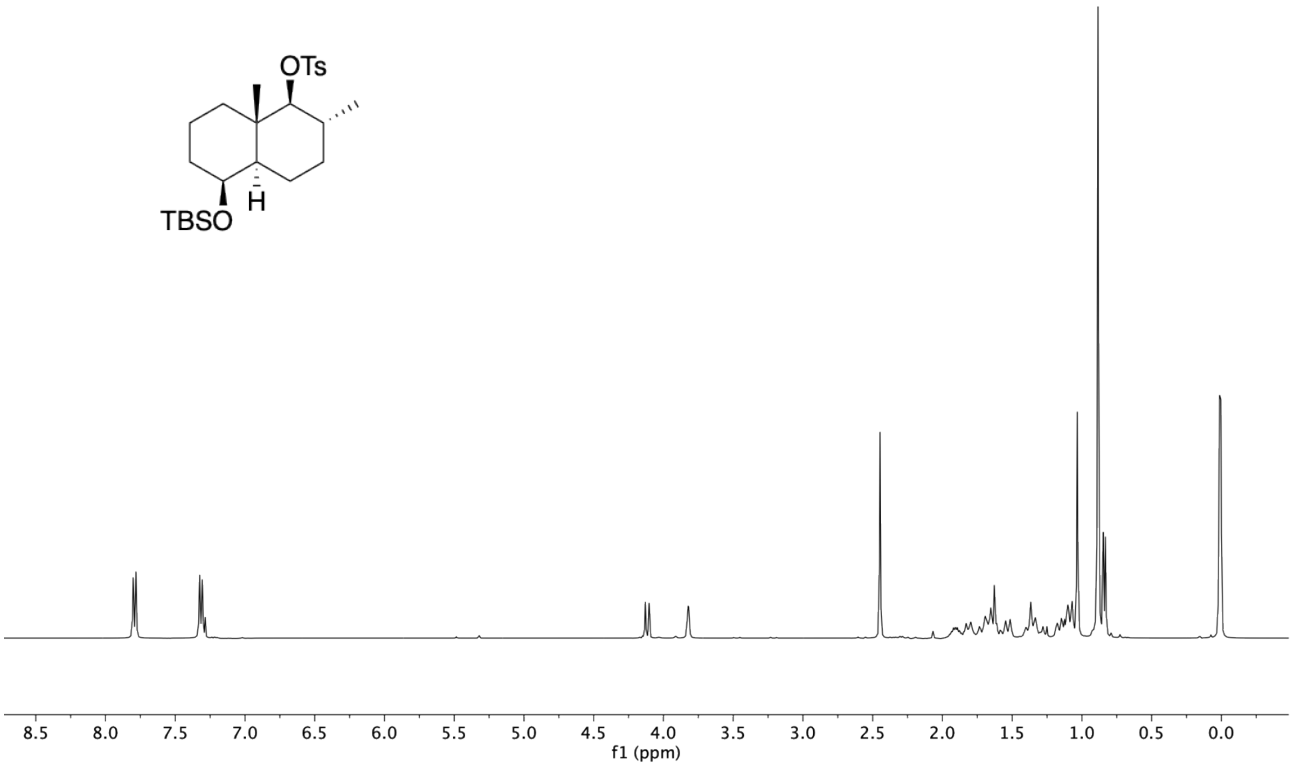
19. Synthesis of 2-methylcyclohexyl methanesulfonate (Me-3')



Me-1' Me-3'

To a solution of alcohol **Me-1'** (27 mg, 0.24 mmol) in CH_2Cl_2 (2 mL) at 0 ºC were added Et_3N (100 µL, 0.72 mmol) and MsCl (55 µL, 0.72 mmol). After stirring the mixture at this temperature for 2 h, H_2O (2 ml) was added and the product was extracted with CH_2Cl_2 (3x5 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated to give a residue. To a solution of the residue in CH_2Cl_2 was added silica and stirred for 16 h. at reflux. Then the mixture was concentrated and chromatographed on silica gel using 15% EtOAc/Hexane as eluent, affording mesylate **Me-3´** (38 mg, 85%) as a colourless oil; Rf: 0.50 (20% EtOAc/Hexane).

IR (ATR, cm^{-1}): 2931, 2848, 1364, 1205, 1059, 876, 760. **^{1}H-NMR ($CDCl_3$, δ):** 4.26 (td, *J*=10.4/4.4 Hz, 1H, H-1), 3.03 (s, 3H, Me-Ms), 2.23 (dt, *J*=12.4/4.4 Hz, 1H, H-2), 1.82 (m, 2H), 1.62 (m, 3H), 1.30 (m, 2H), 1.11 (m, 1H), 1.05 (d, *J*=6.4/1.4 Hz, 3H, CH_3-2') ppm. **^{13}C-NMR ($CDCl_3$, δ):** 87.9 (CH-1), 38.7 (Me-Ms), 37.6 (CH-2), 33.5 (CH_2), 33.2 (CH_2), 31.6 (CH_2), 24.9 (CH_2), 24.7 (CH_2), 18.72 (CH_3-2') ppm. **MS (ESI) [m/z, (%)]:** 193.09 ([M+1]$^+$, 100). **HRMS (ESI):** 193.0893 calculated for $C_8H_{17}O_3S$, found 193.0879.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TBSO
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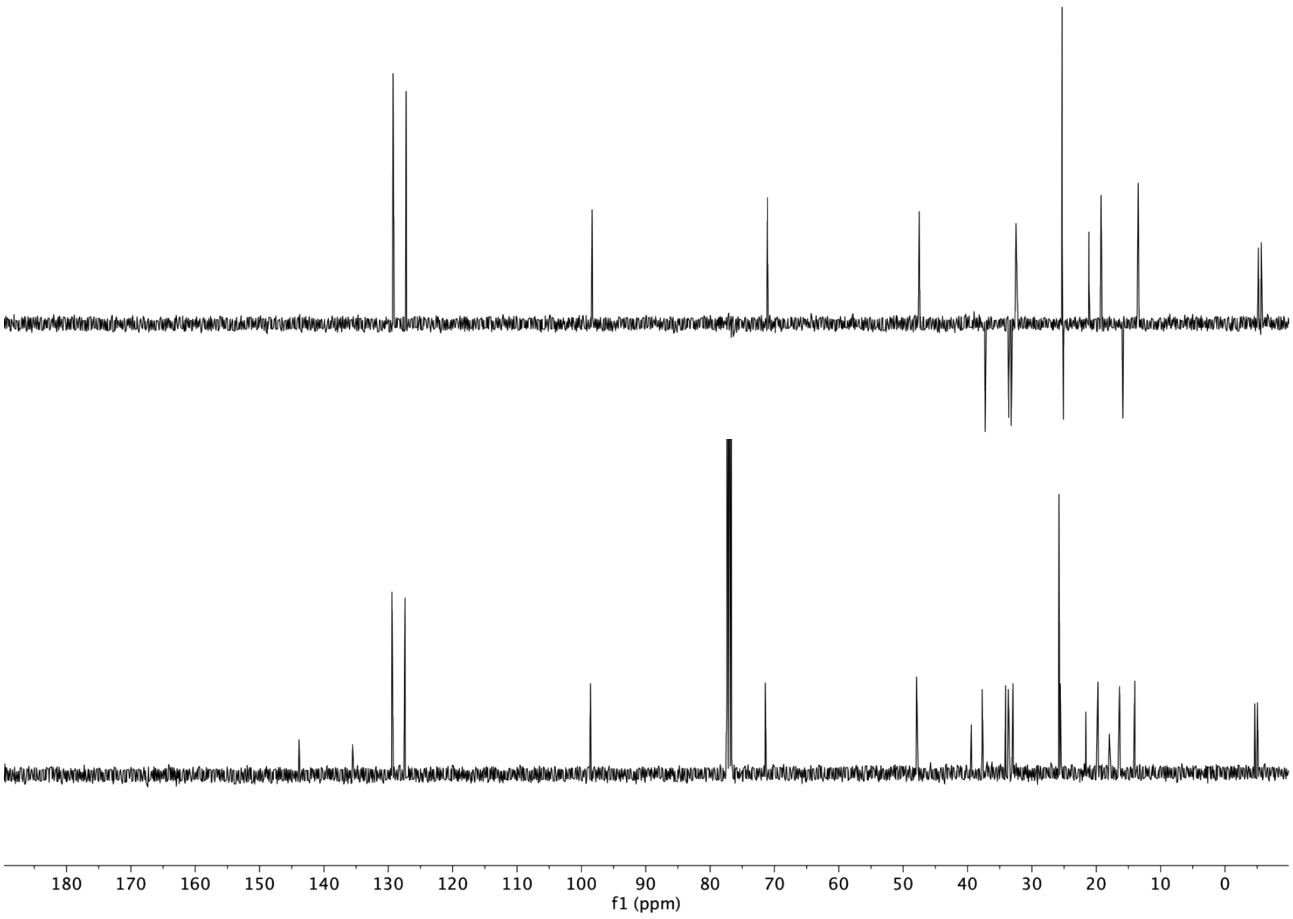
f1 (ppm)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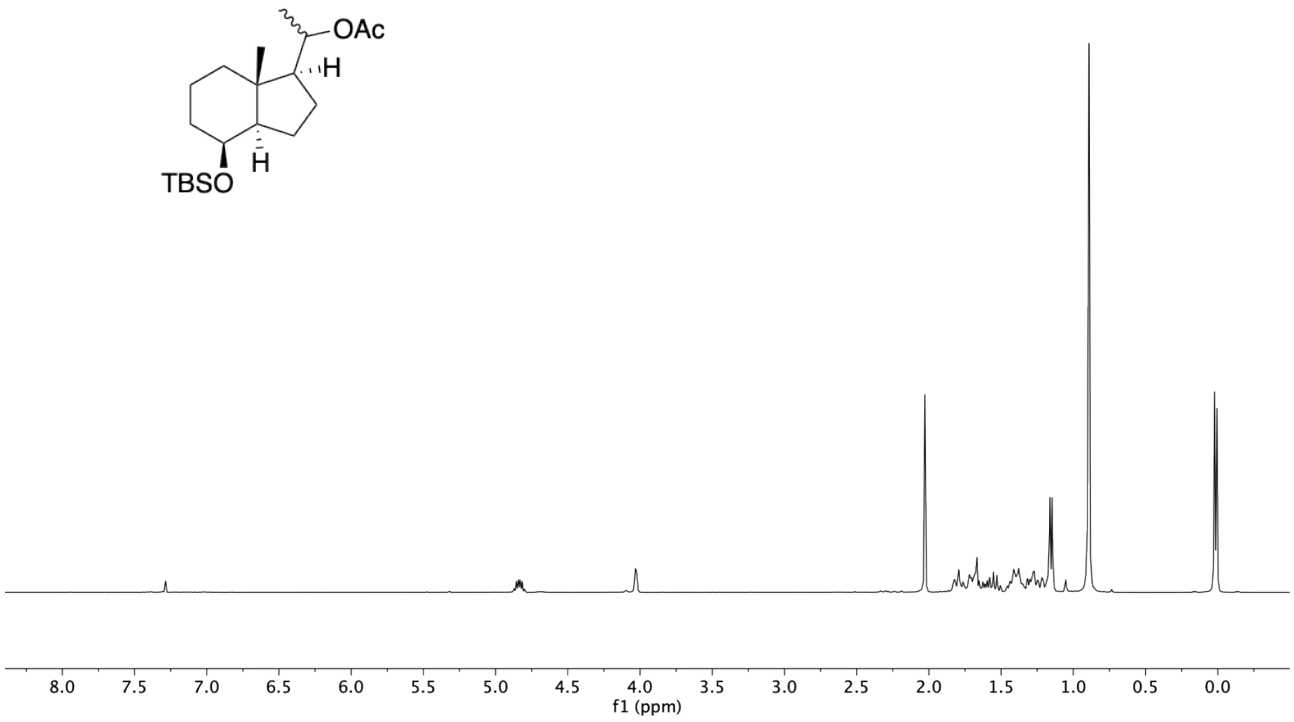
f1 (ppm)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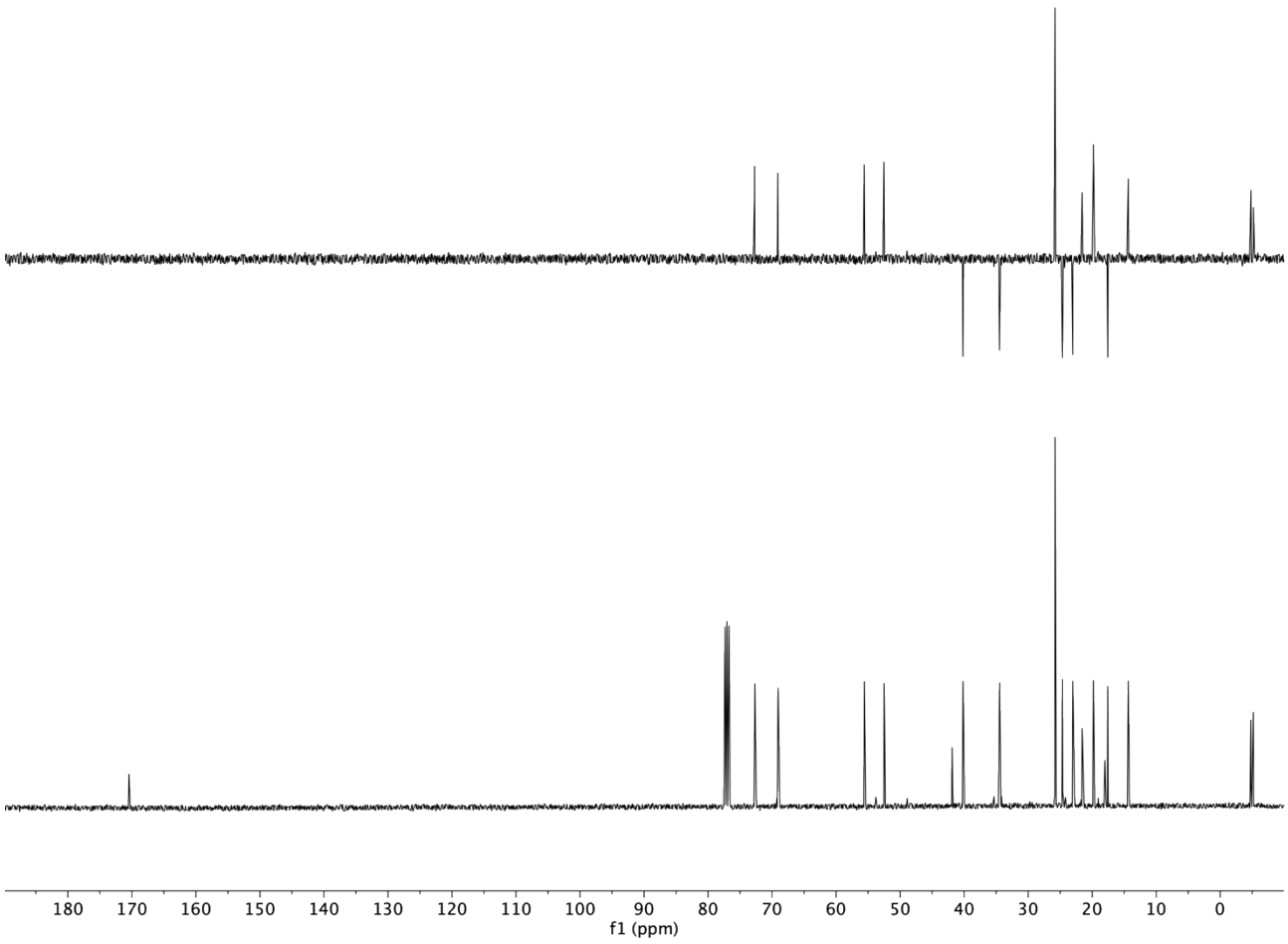
f1 (ppm)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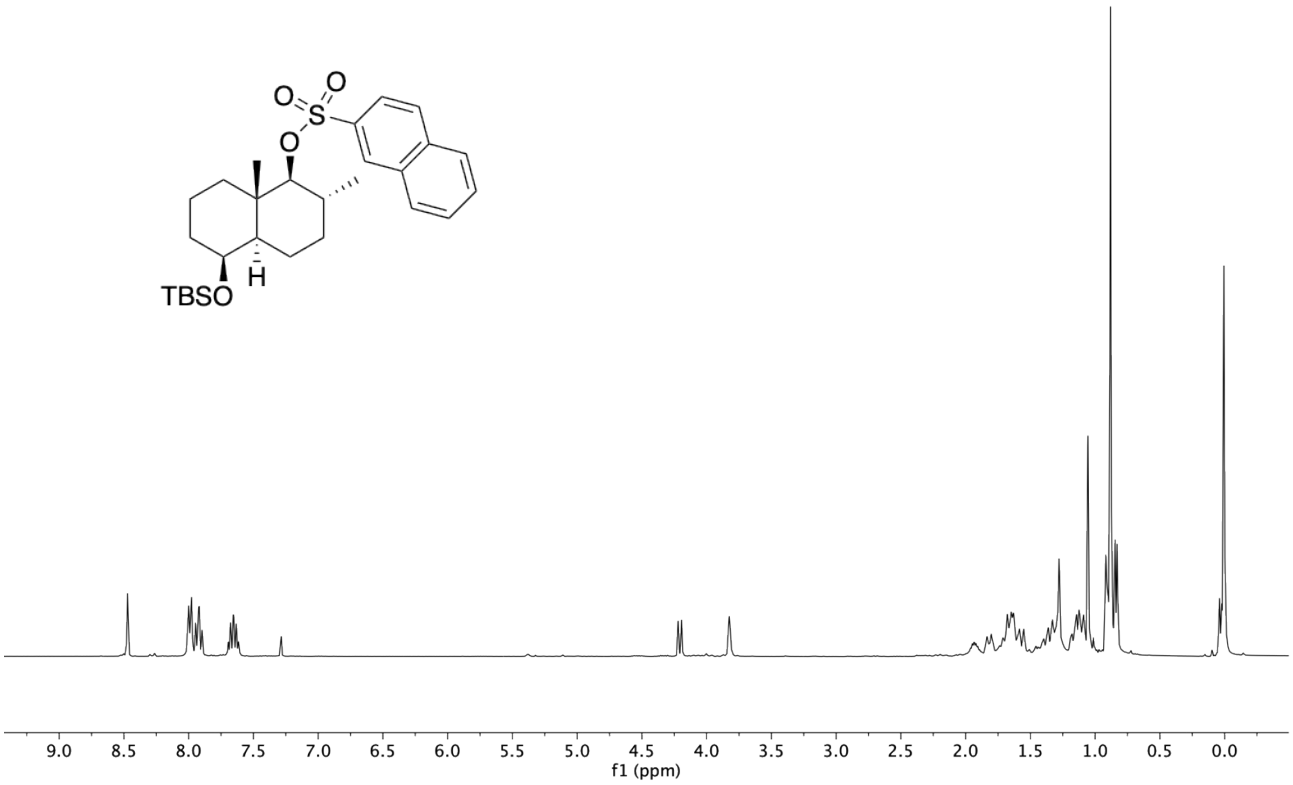
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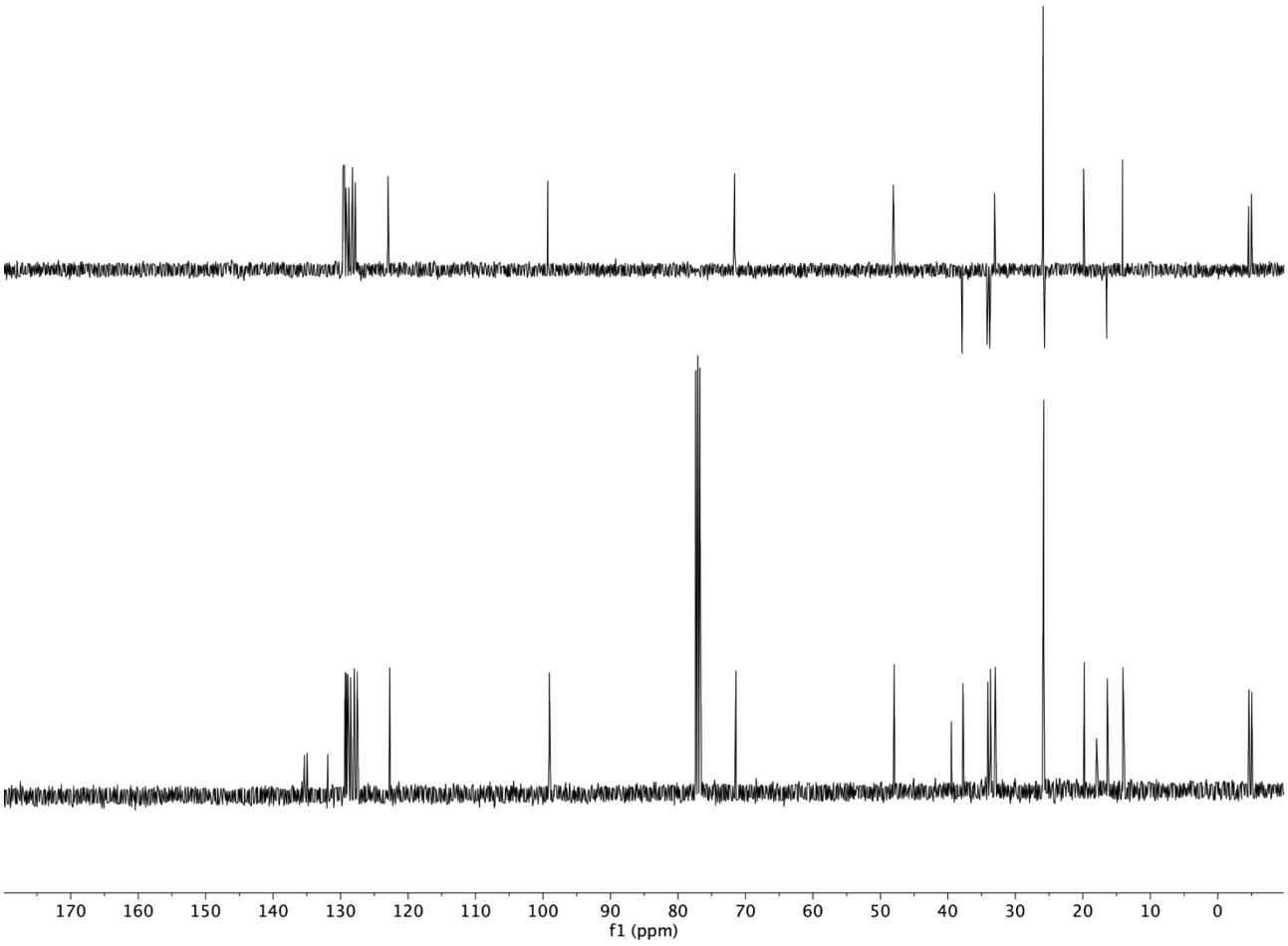
f1 (ppm)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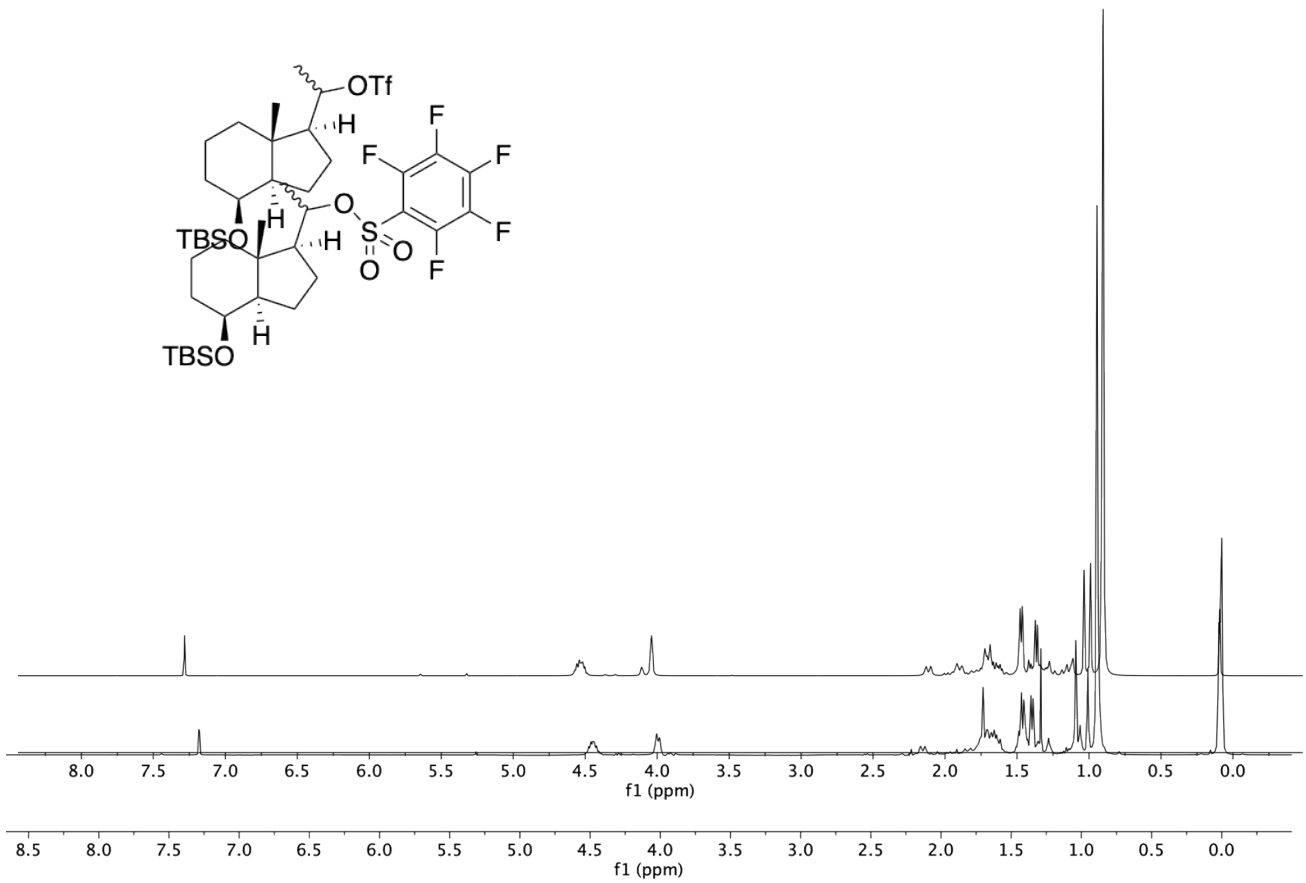
f1 (ppm)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F
F
F
F
F
O
S
O
O
H
TBSO
H
TBSO
H
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f1 (ppm)
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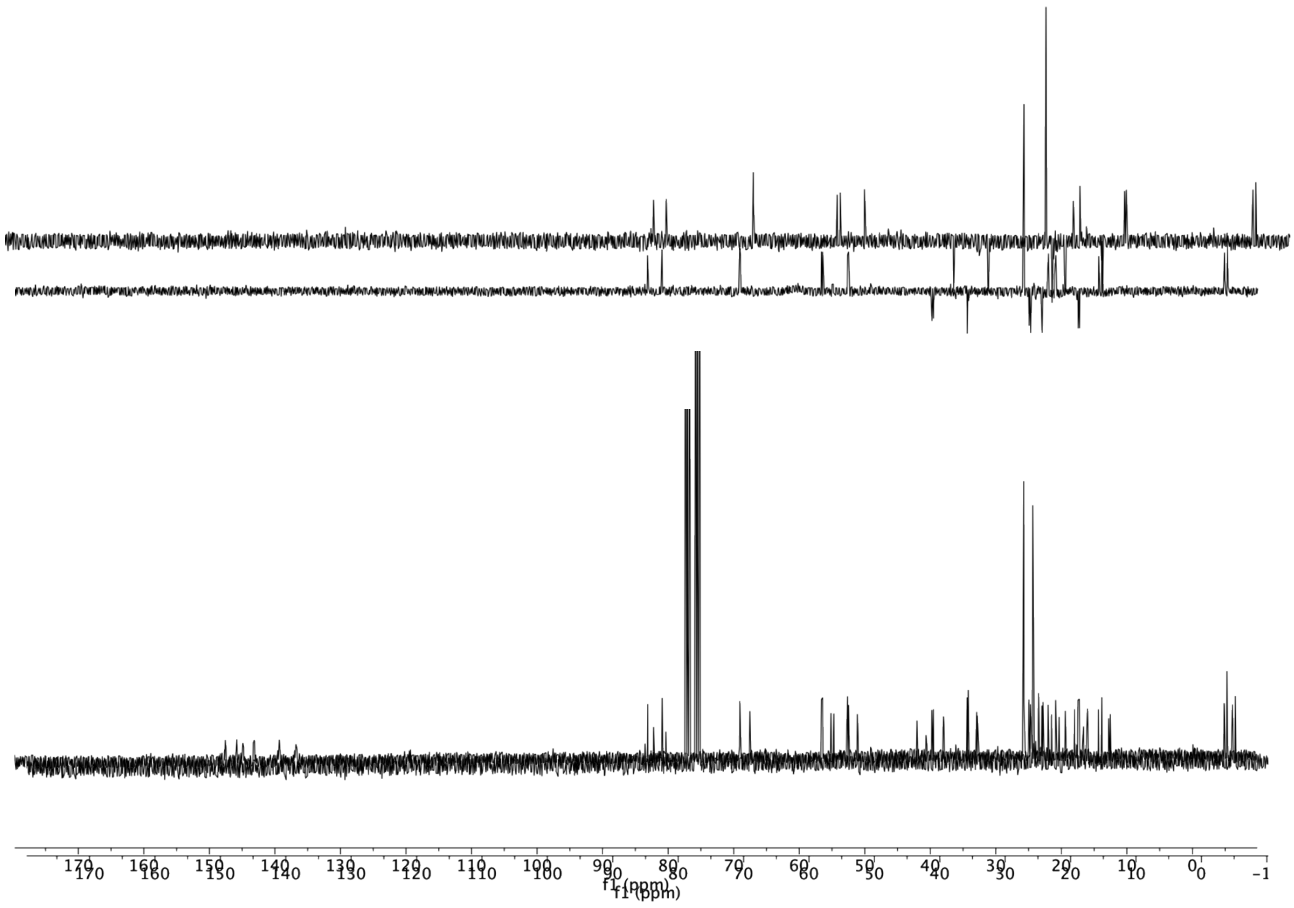
f1 (ppm)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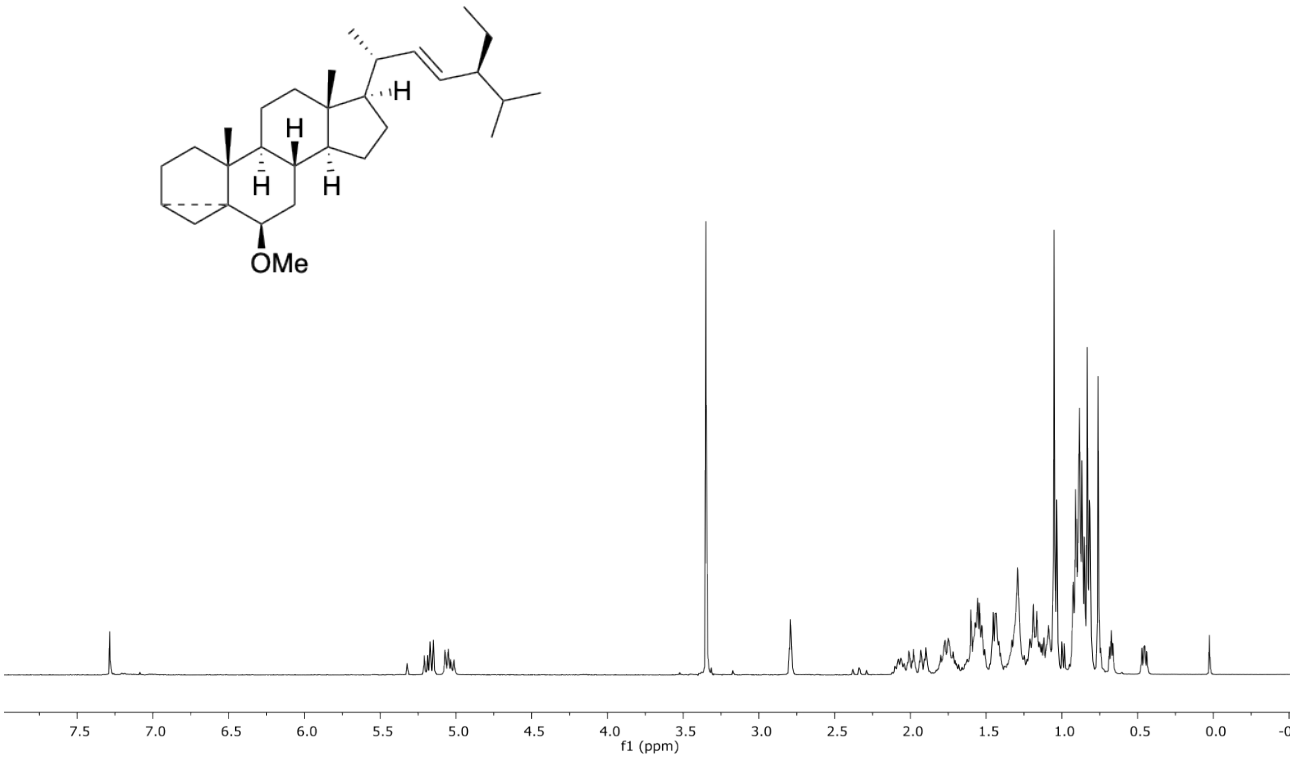
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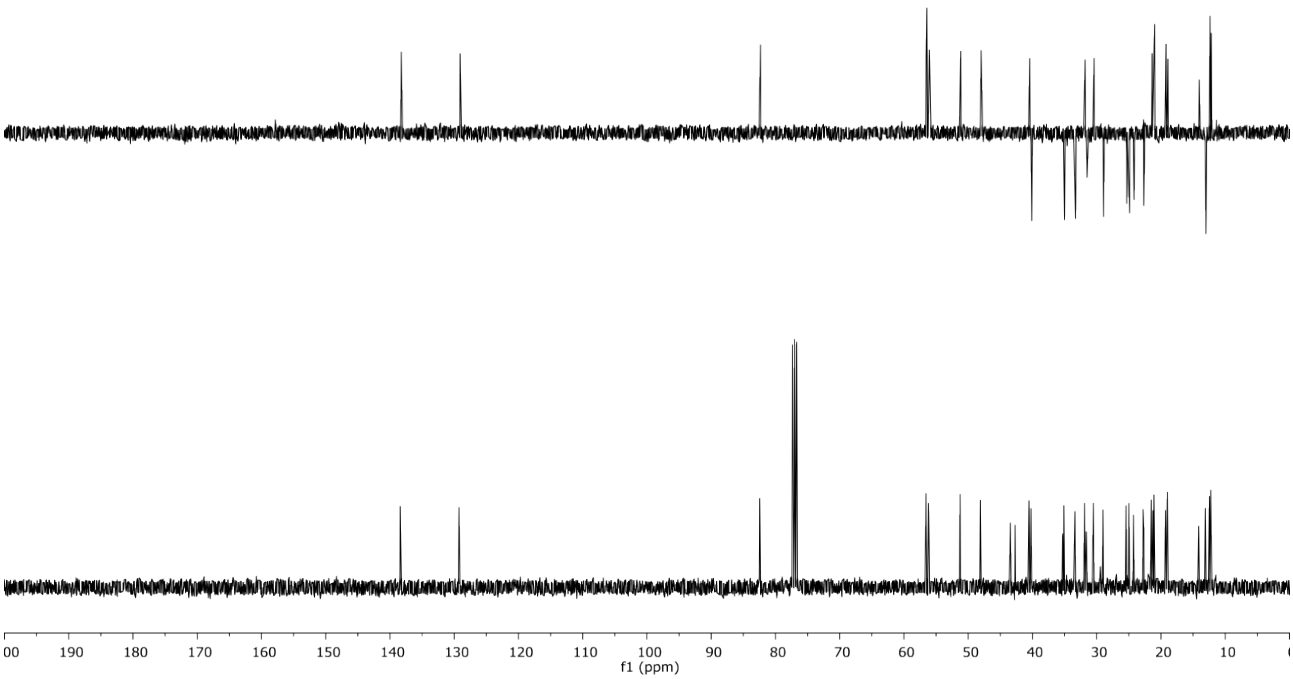
f1 (ppm)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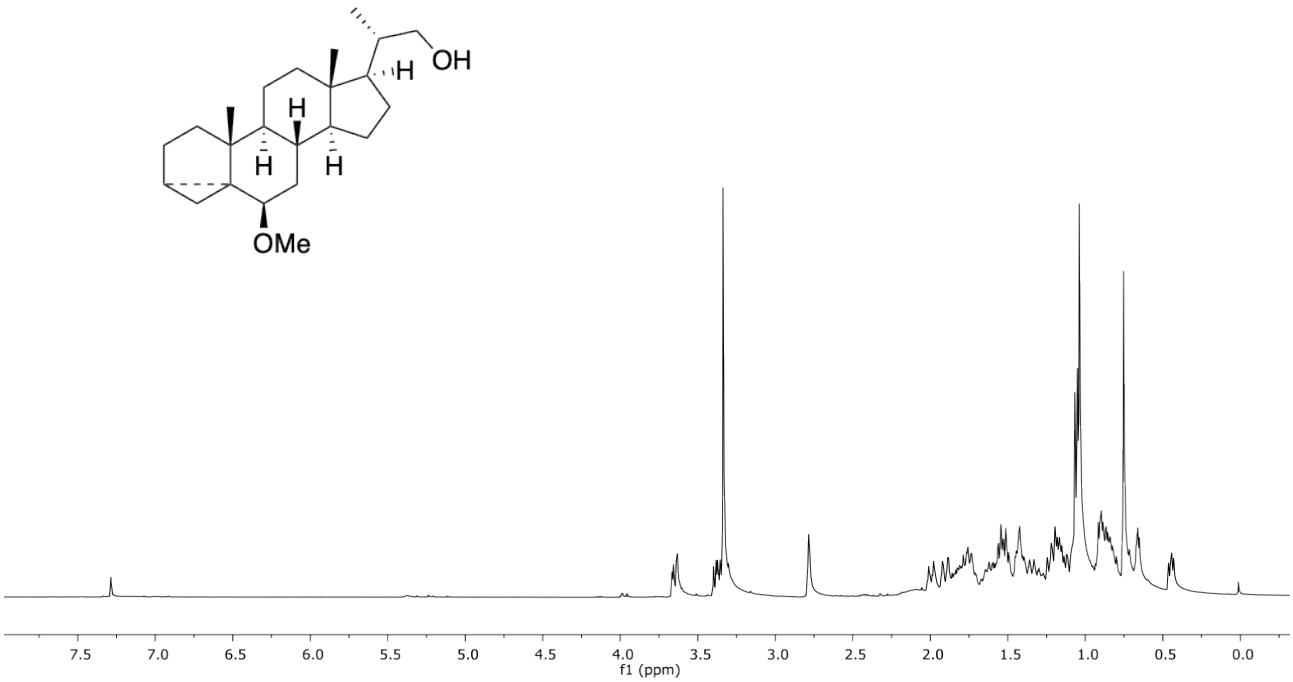
f1 (ppm)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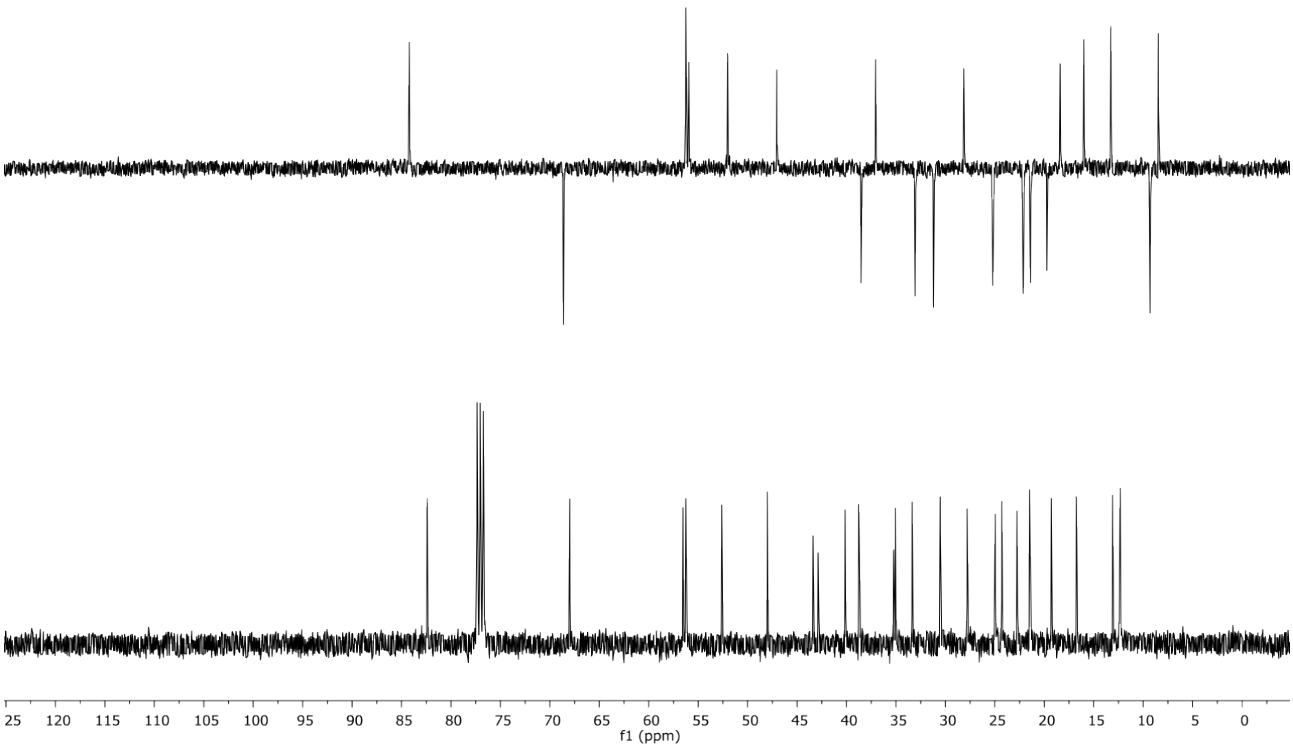
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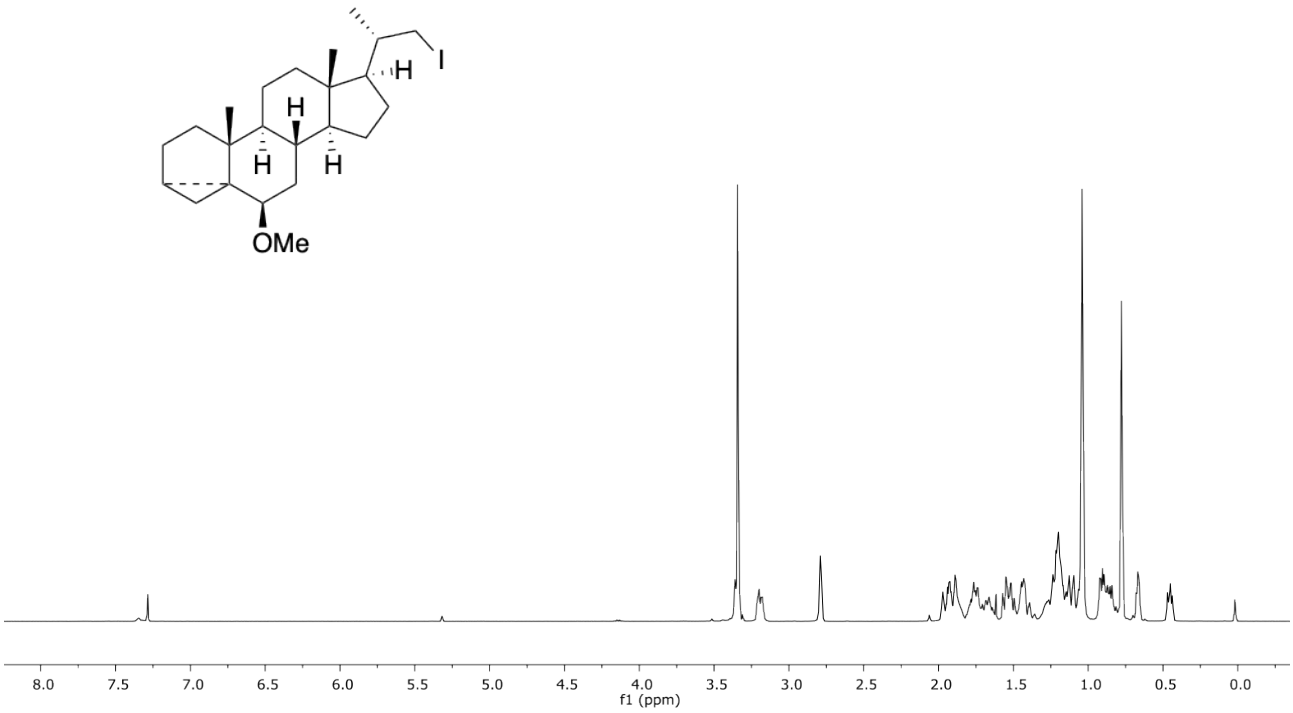
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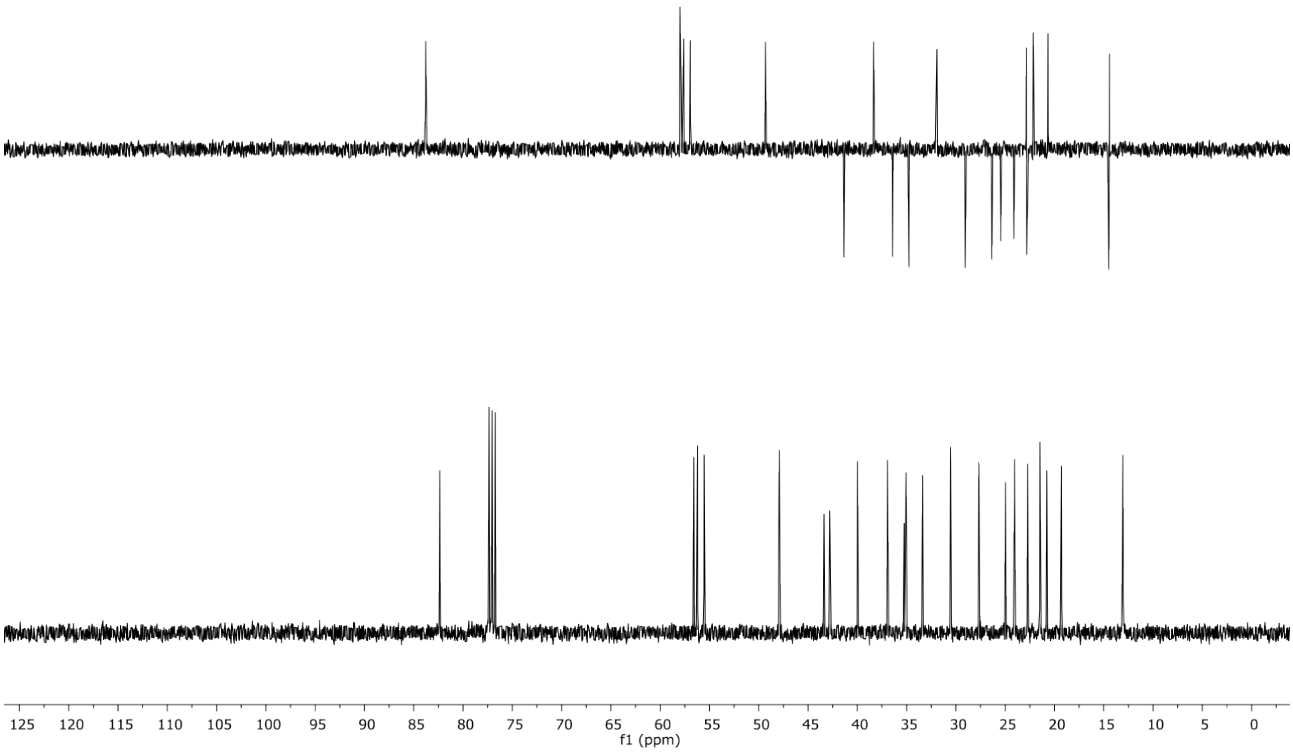
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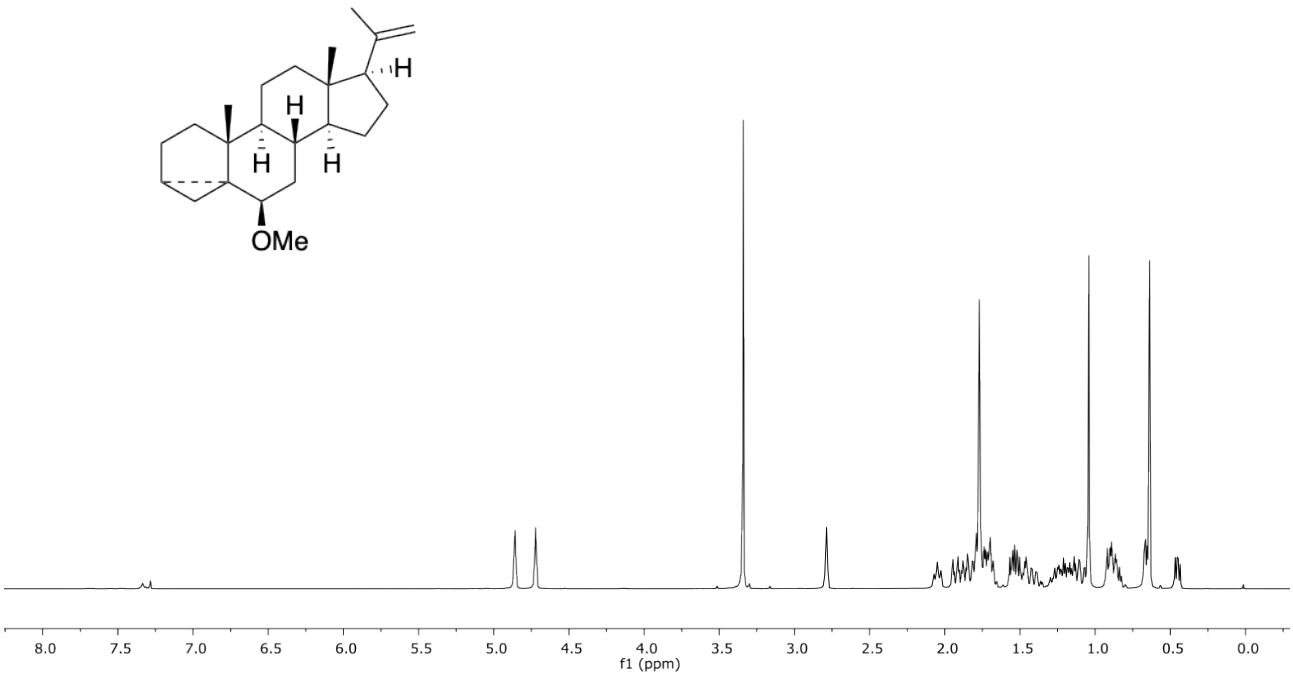
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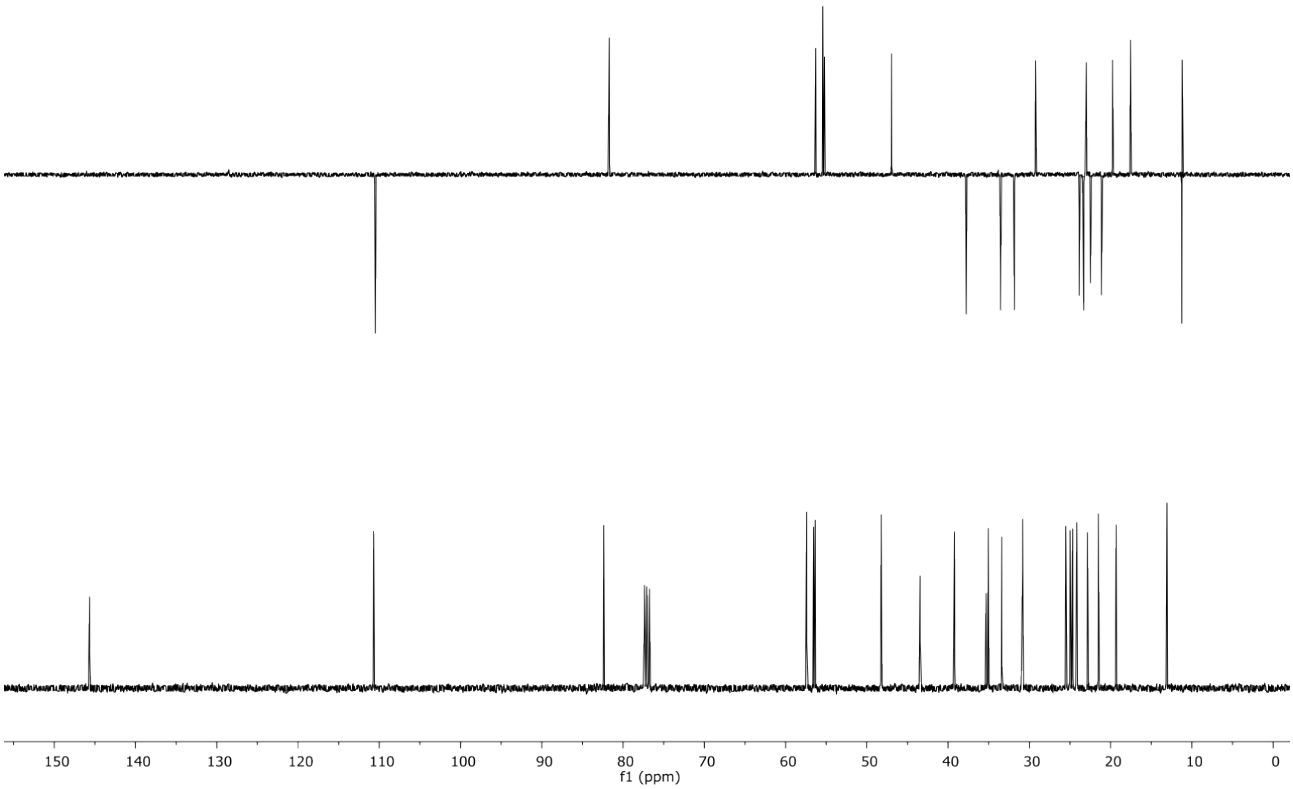
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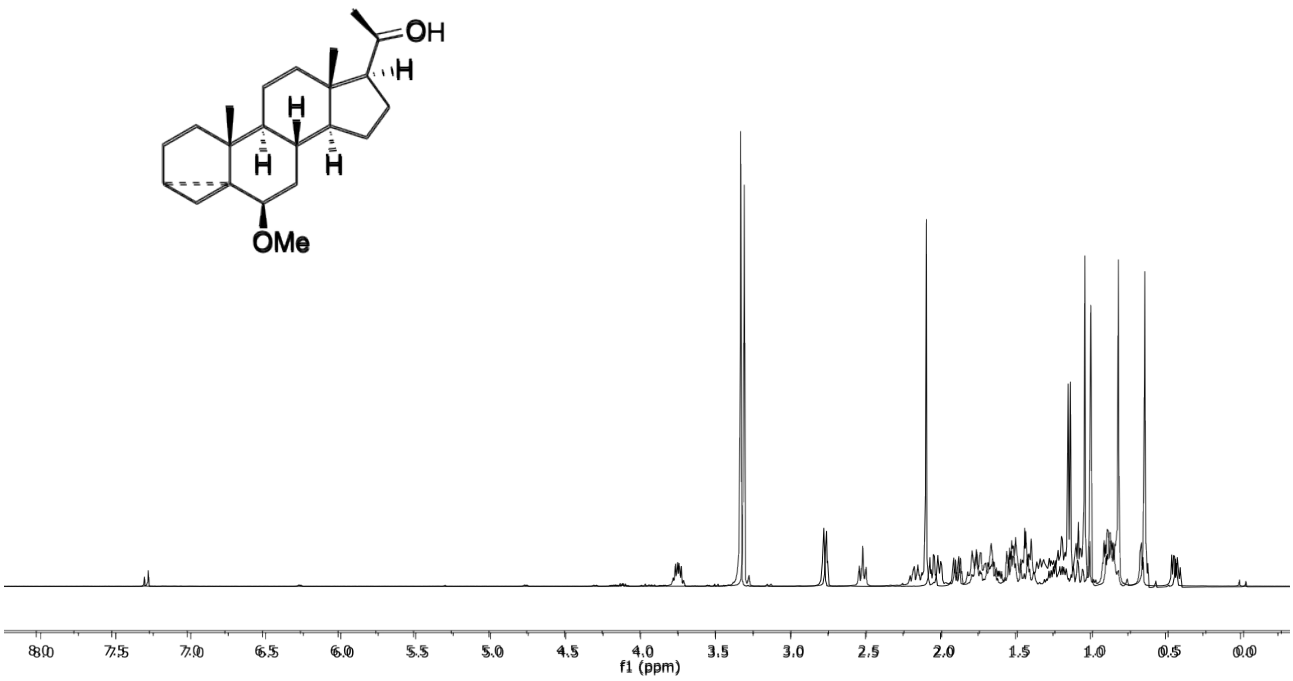
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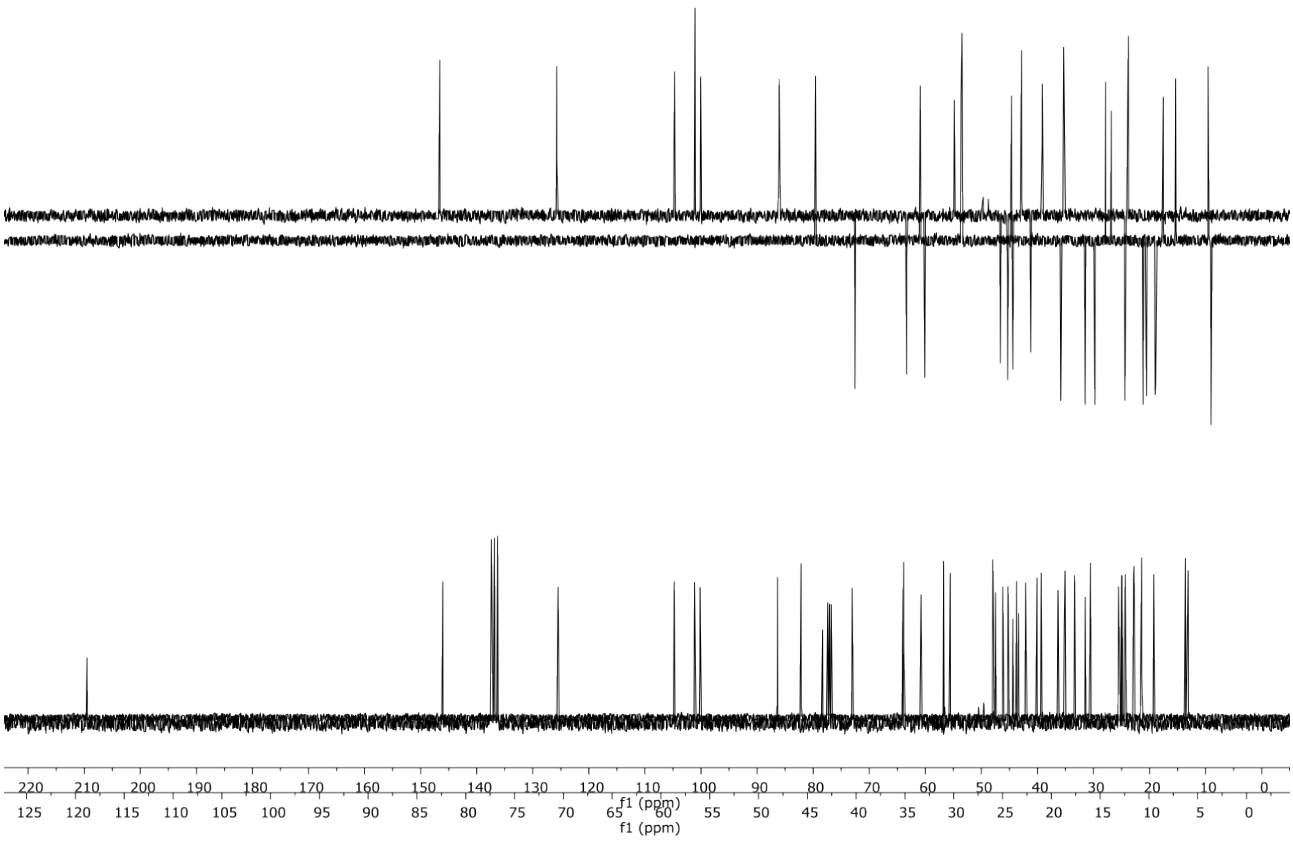
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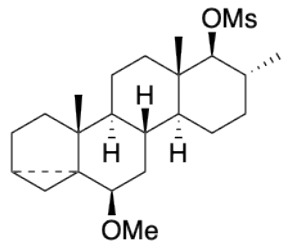
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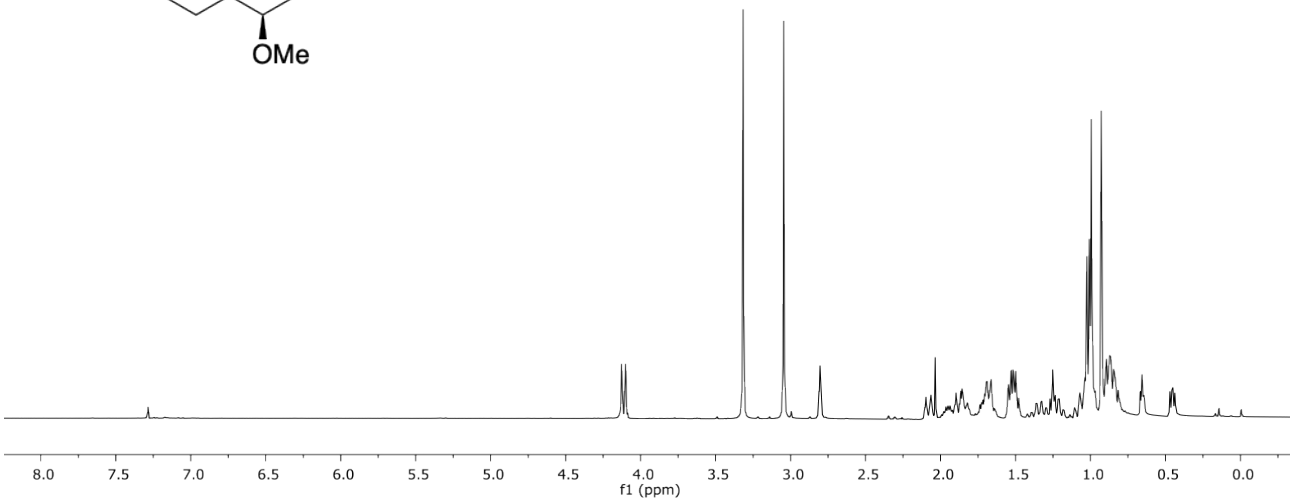
H
OMe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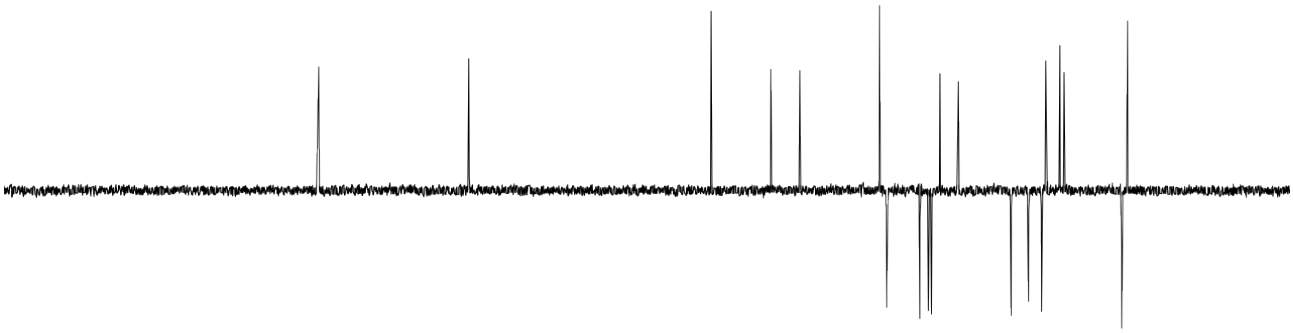

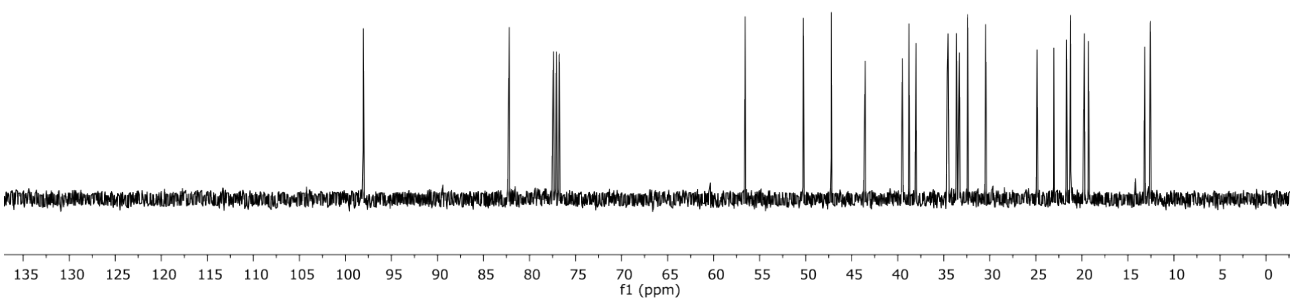
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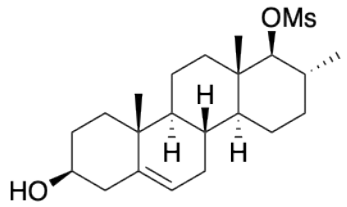
OMs
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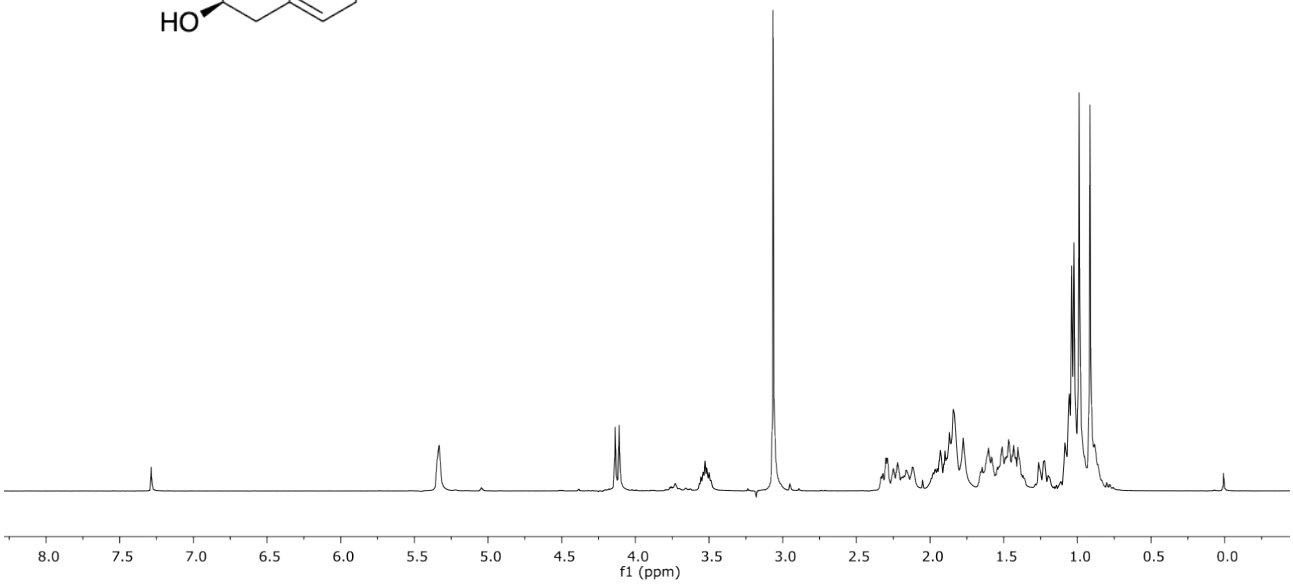
HO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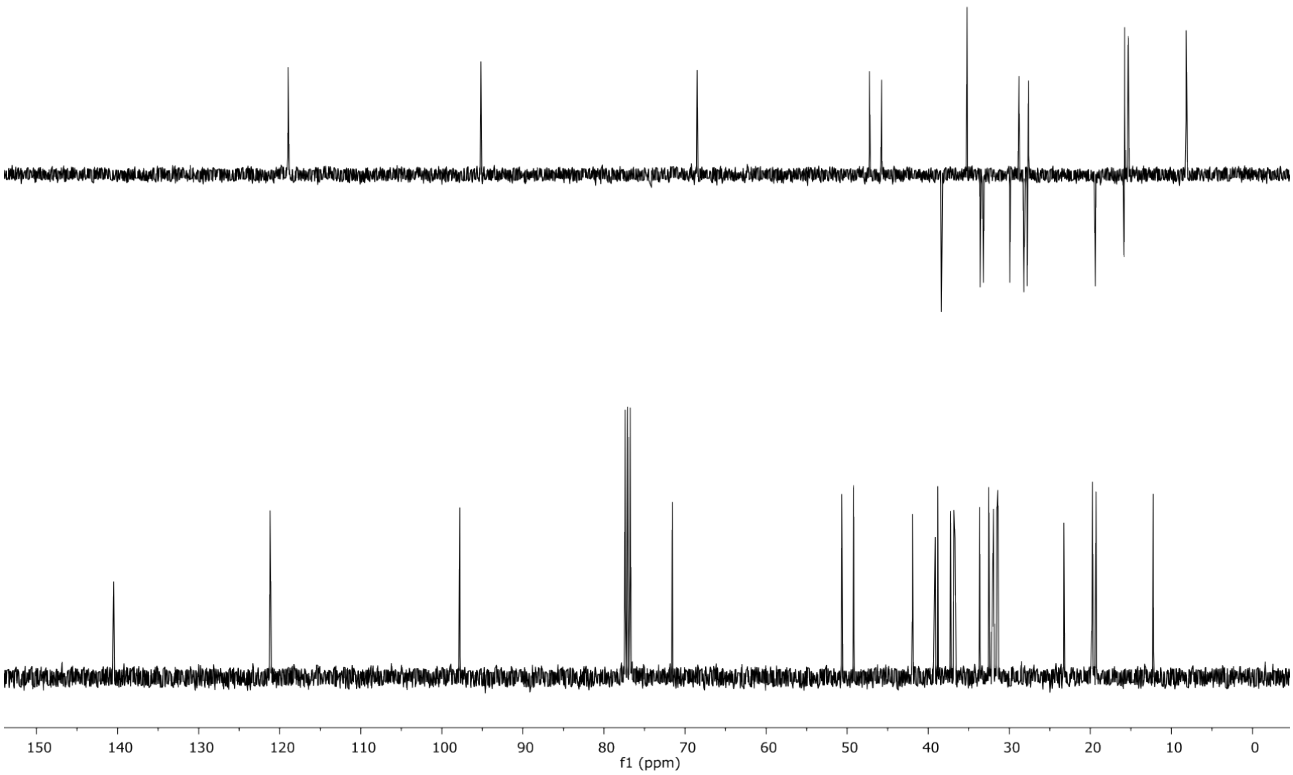
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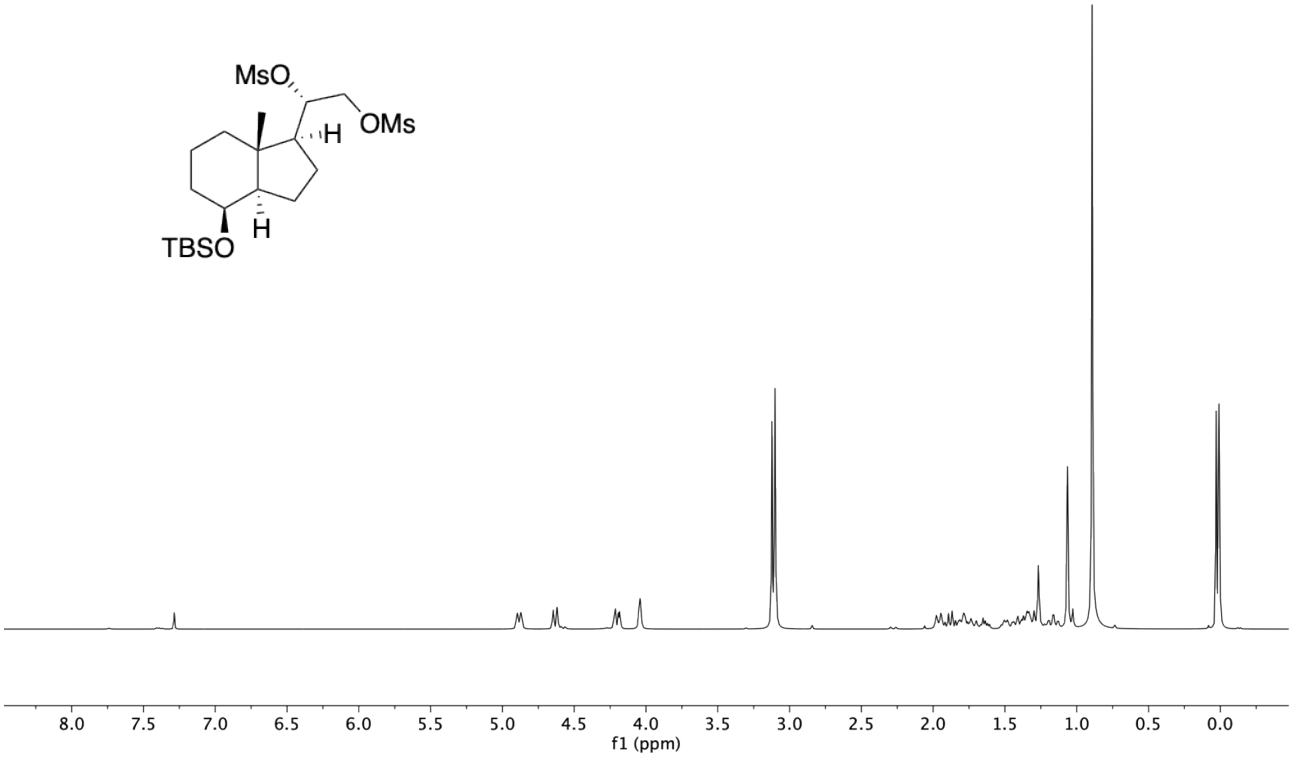
f1 (ppm)


MsO
OMs
H
H
TBSO
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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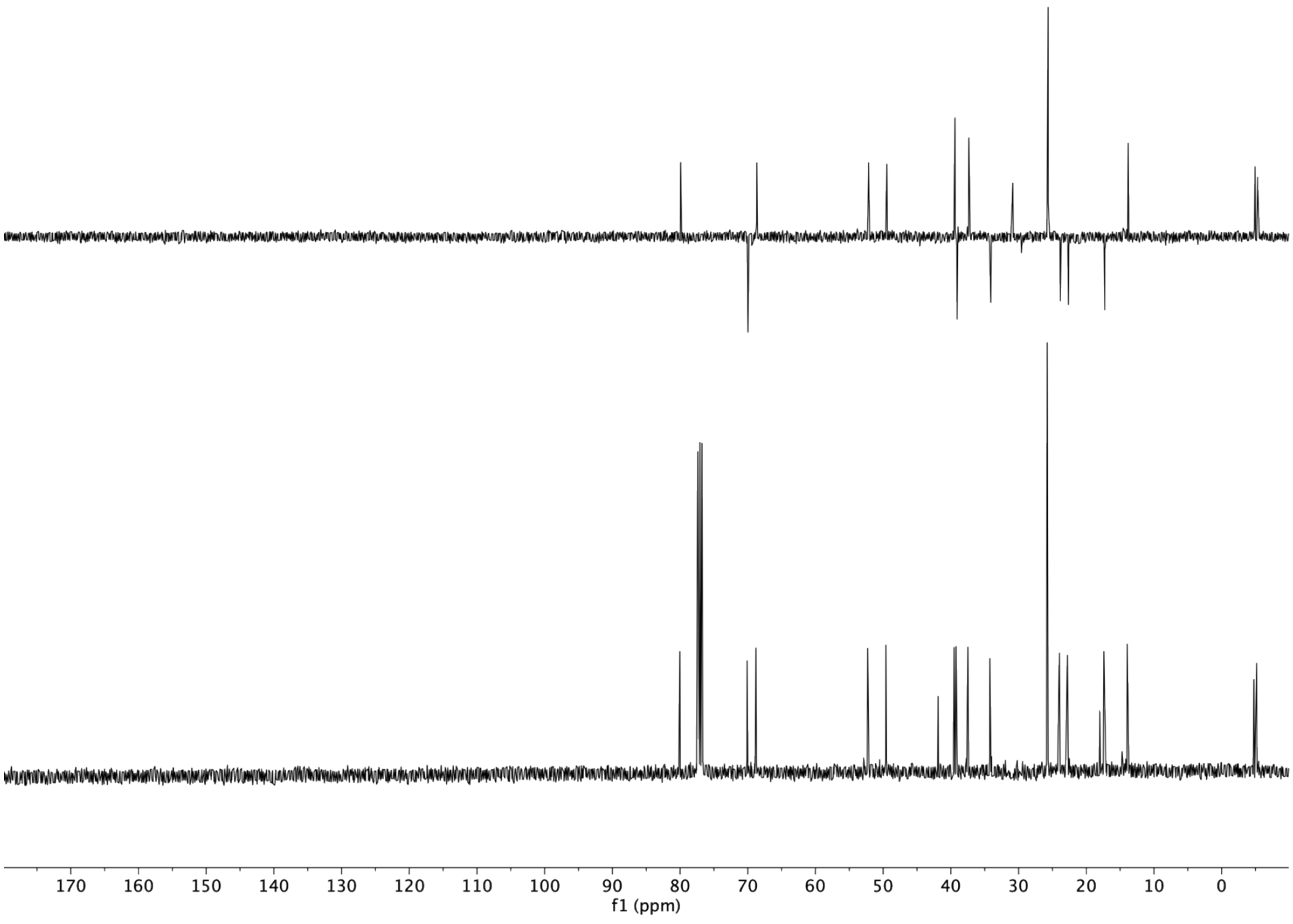
0.0
f1 (ppm)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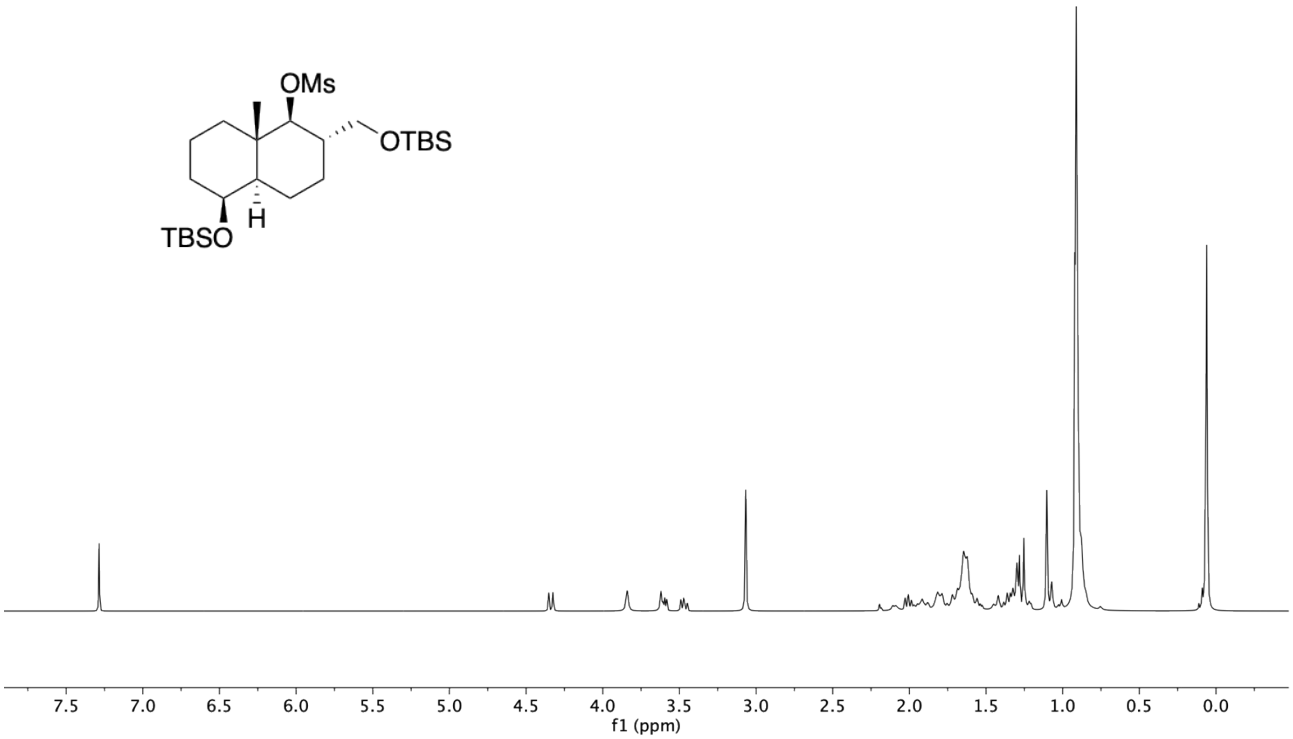
OMs
OTBS
TBSO
H
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7.0
6.5
6.0
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3.0
2.5
2.0
1.5
1.0
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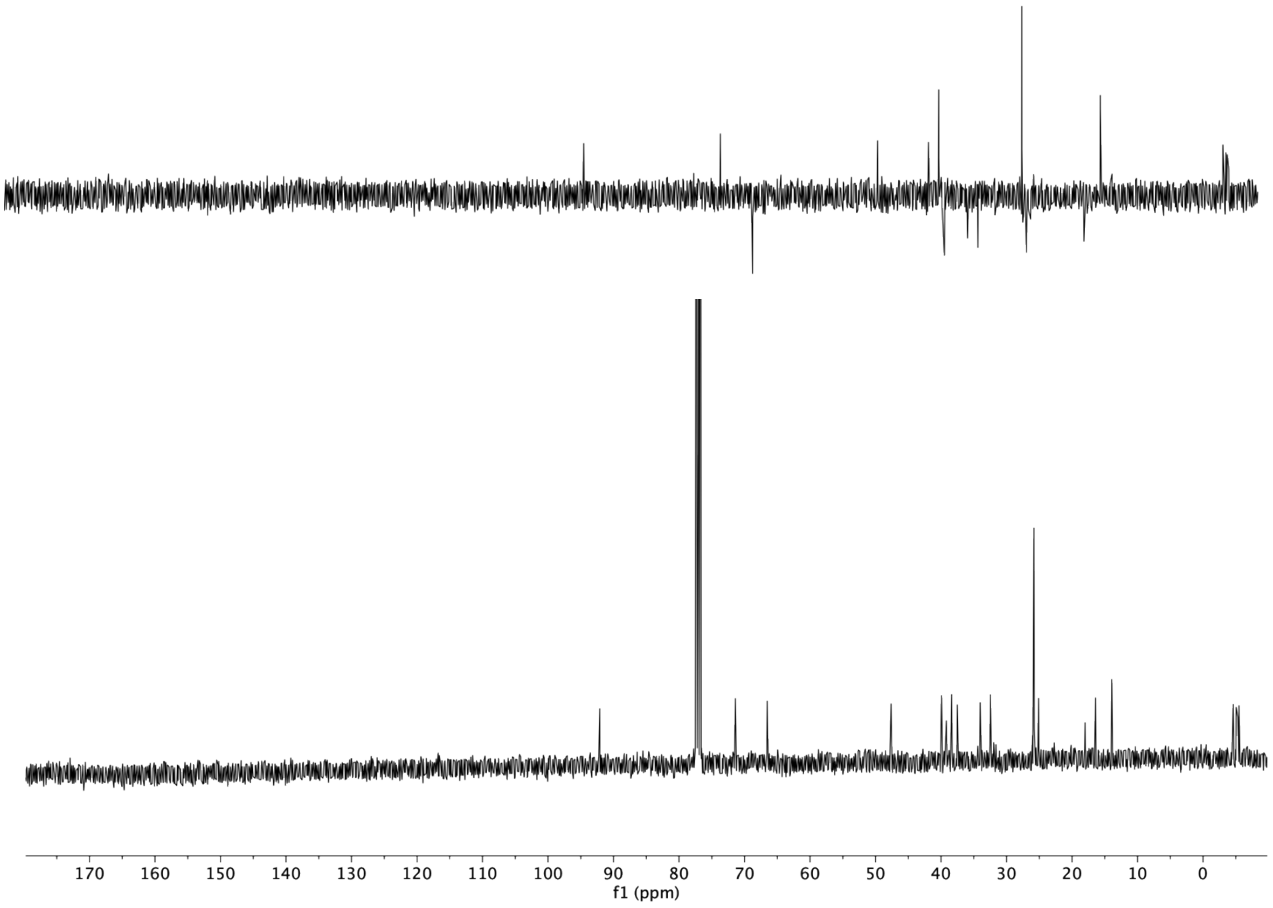
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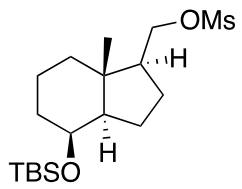
f1 (ppm)


OMs
H
H
TBSO

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6.5
6.0
5.5
5.0
4.5
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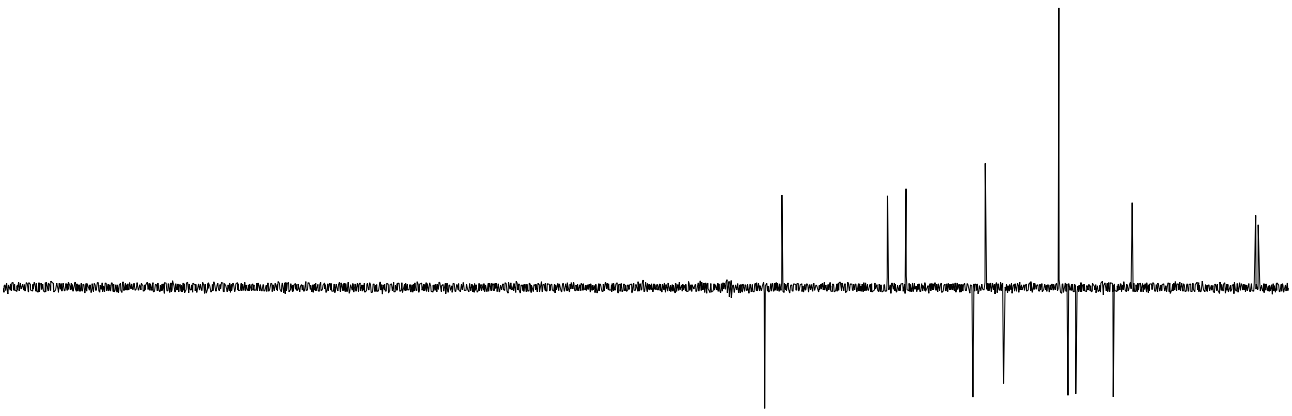
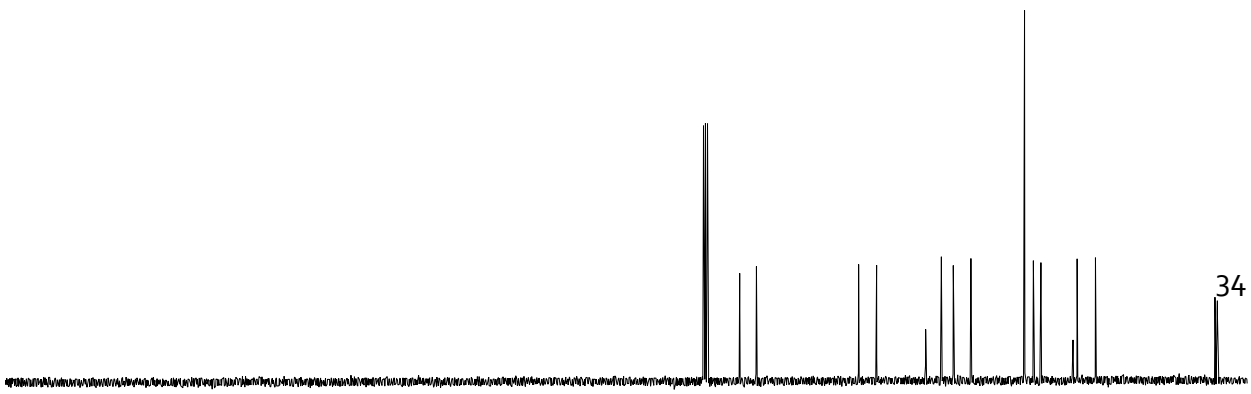
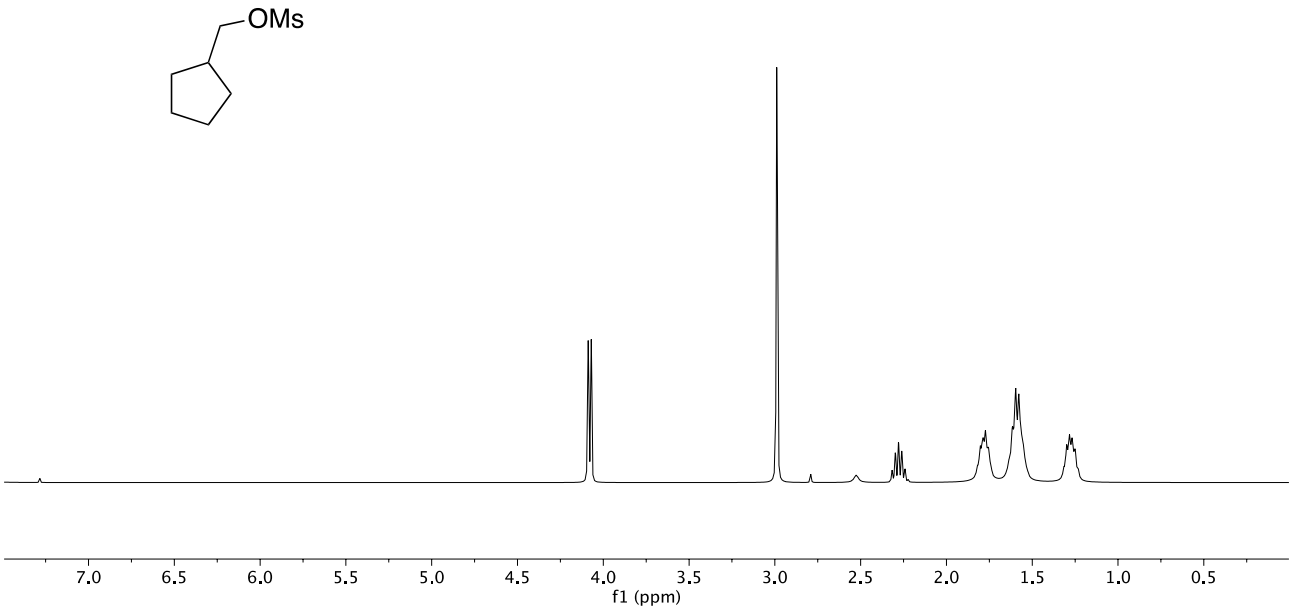
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)






OMs
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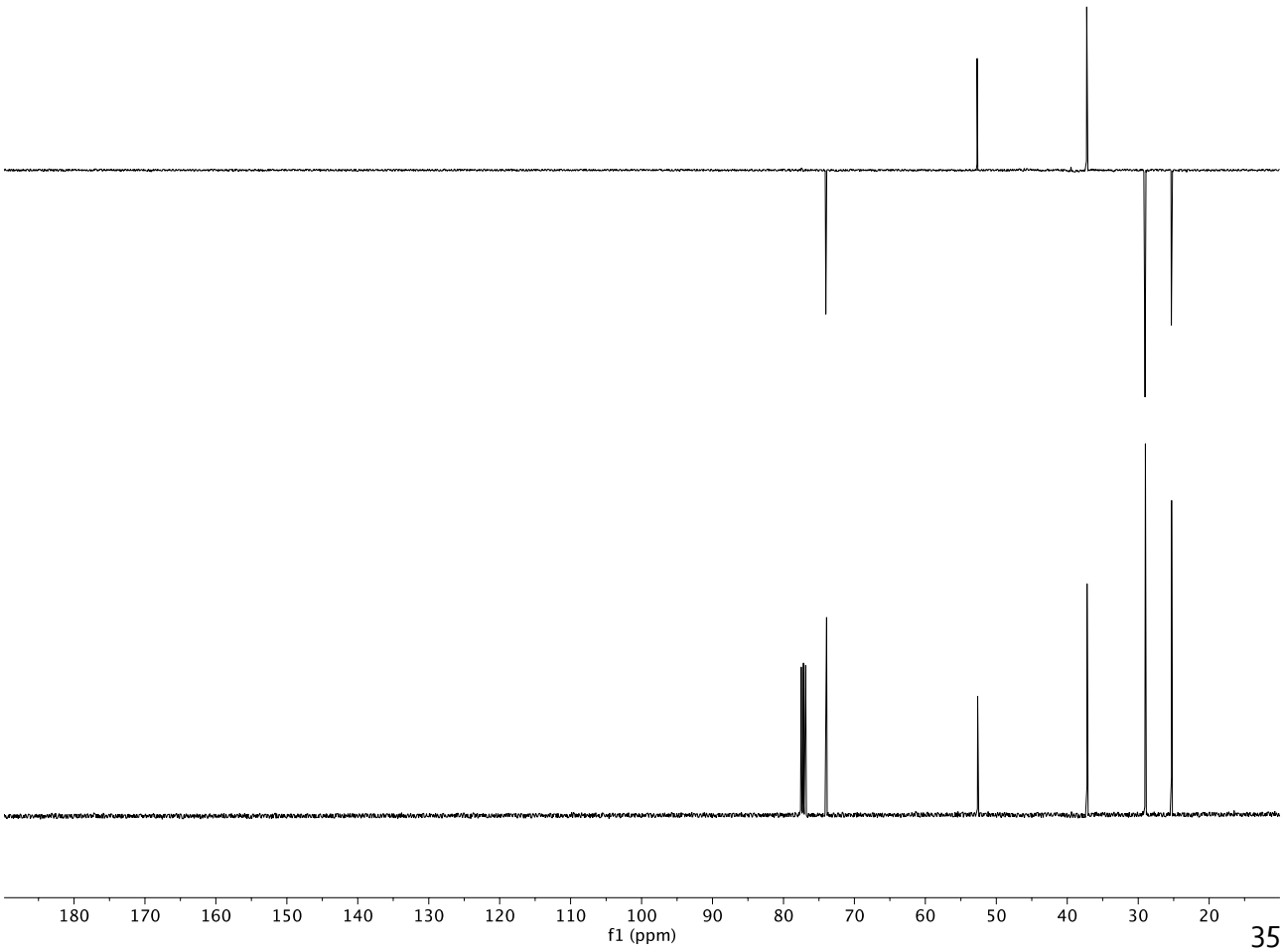
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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50
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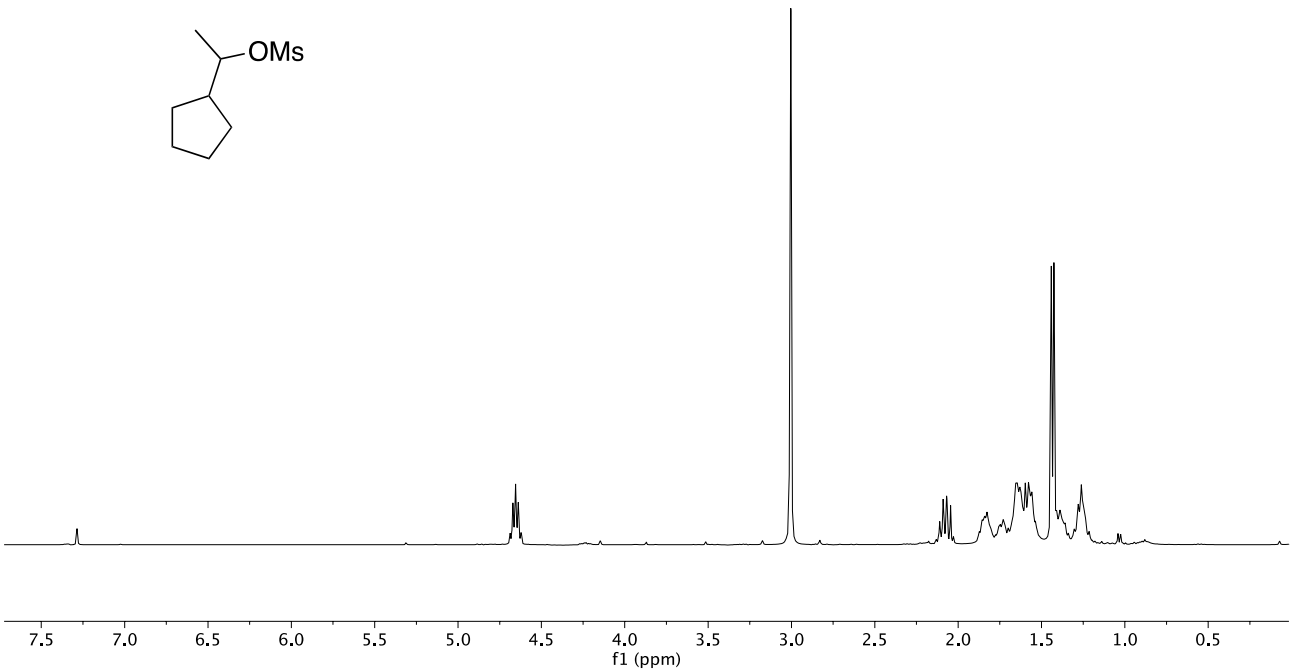
30
20
f1 (ppm)


OMs
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6.0
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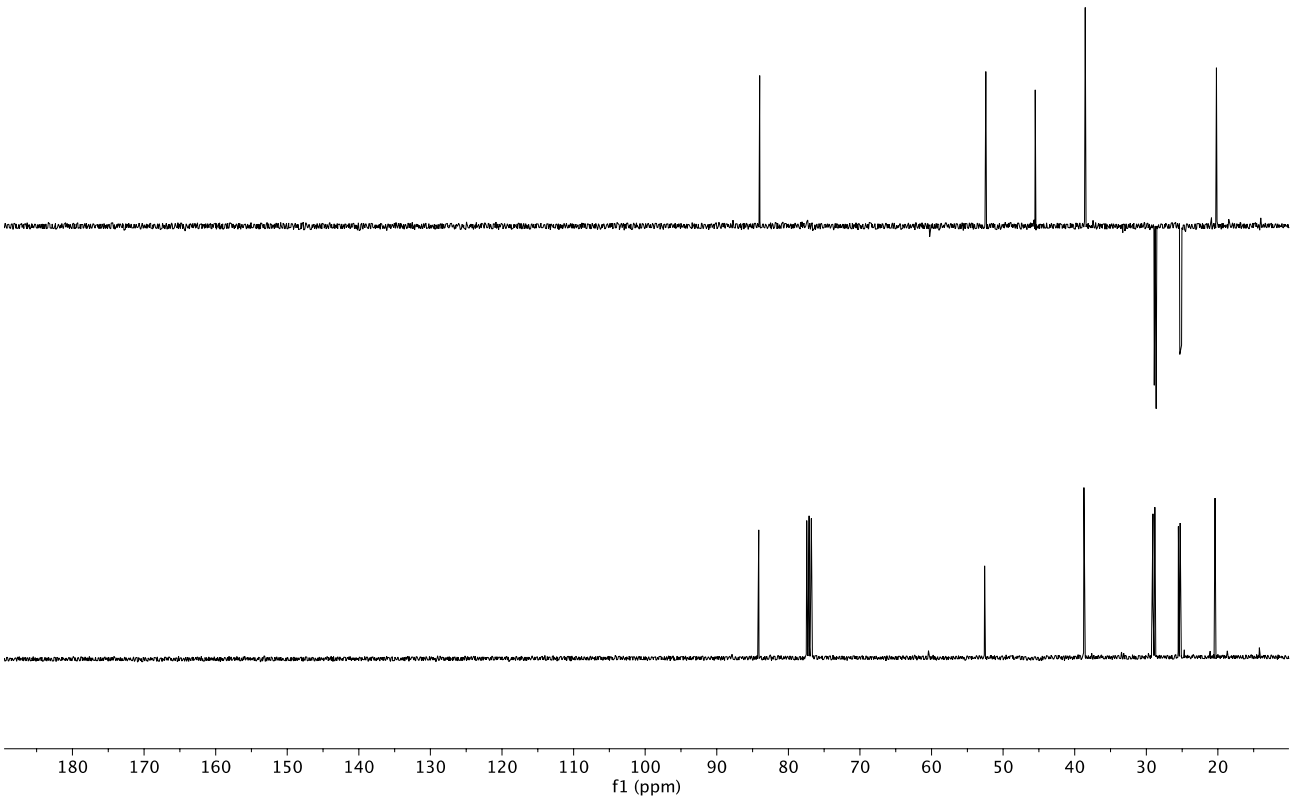
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


180
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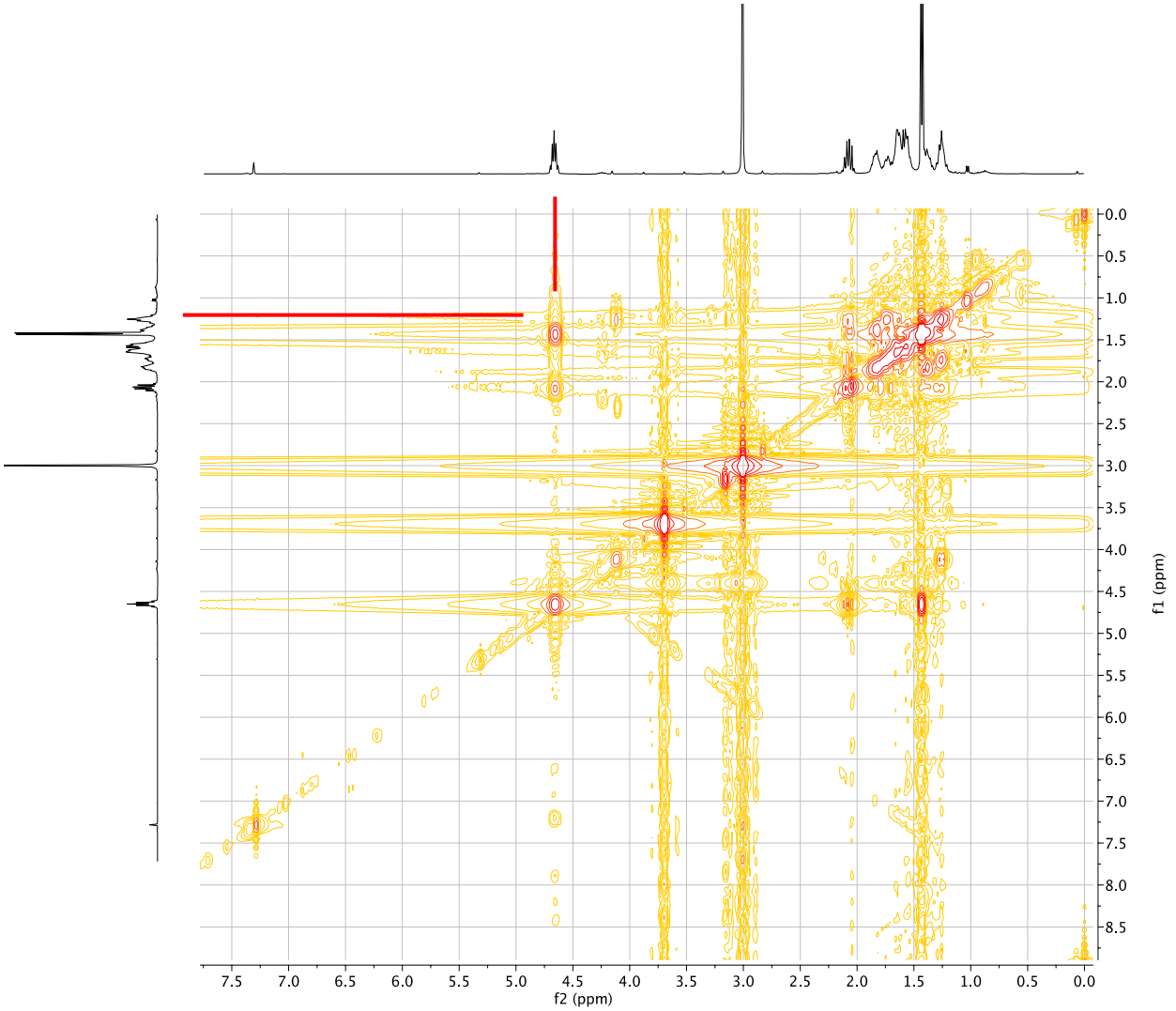
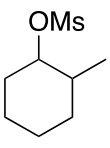
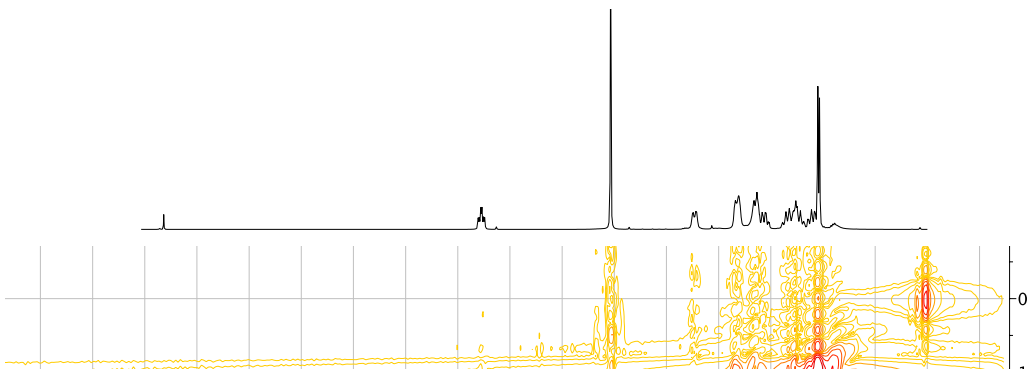
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


f2 (ppm)
f1 (ppm)


OMs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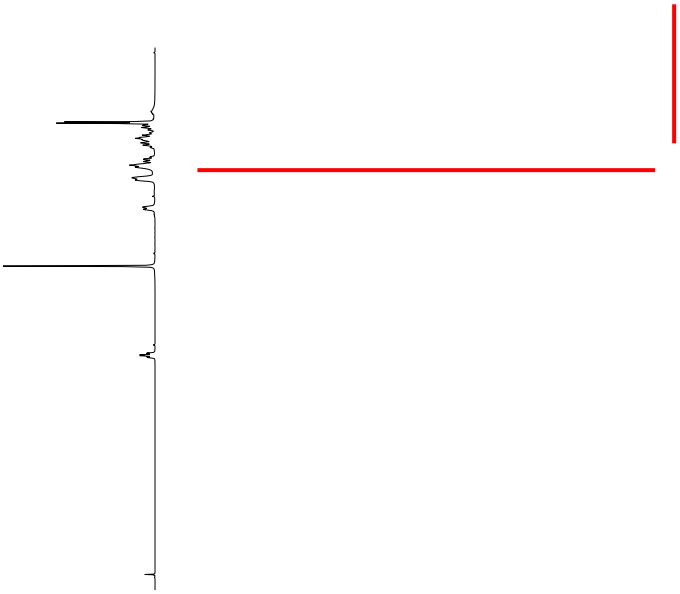
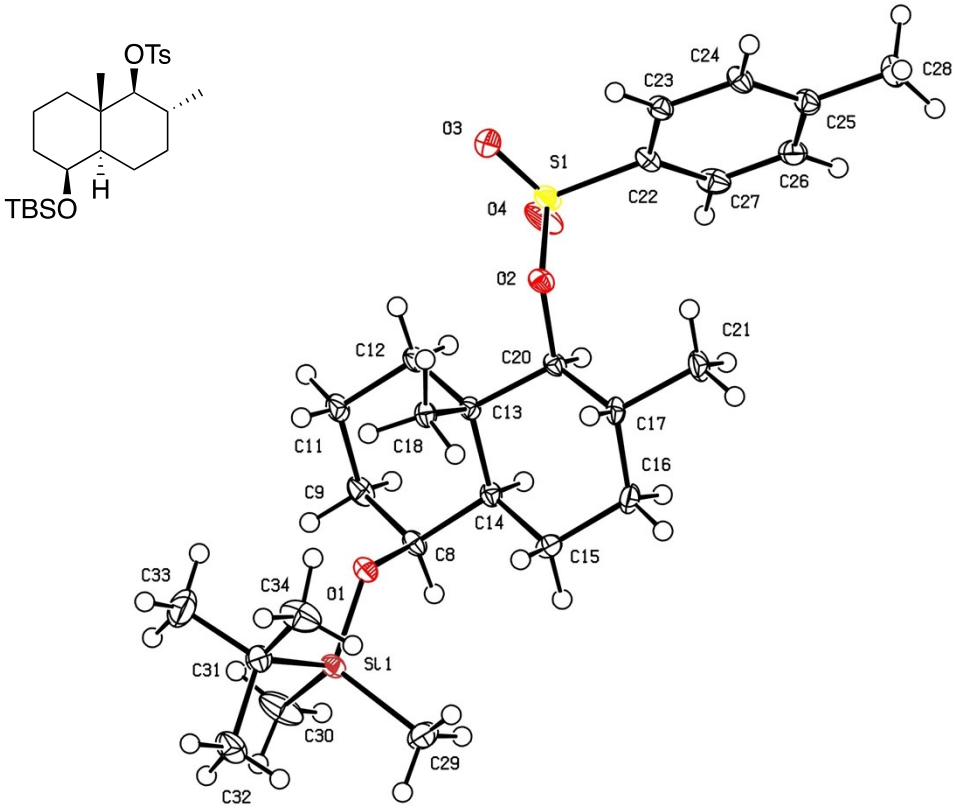


A single crystal of **4** has been analysed by X-ray diffraction and a summary of the crystallographic data and the structure refinement parameters is reported in Table 1. Crystallographic data have been collected at 100 K using a Bruker D8 Venture diffractometer with a Photon II CMOS detector and Mo-Kα radiation (λ = 0.71073 Å) generated by an Incoatec high brillance microfocus source equipped with Incoatec Helios multilayer optics.

The software APEX3 has been used for collecting frames of data, indexing reflections, and the determination of lattice parameters, SAINT for integration of intensity of reflections, and SADABS for scaling and empirical absorption correction. The structure has been solved by dual-space algorithm using the program SHELXT. All non-hydrogen atoms have been refined with anisotropic thermal parameters by full-matrix least-squares calculations on F^2 using the program SHELXL with OLEX2. Hydrogen atoms have been inserted at calculated positions and constrained with isotropic thermal parameters. The sample has crystallized in the chiral space group P1. The absolute configuration has been determined by anomalous dispersion effects in diffraction

measurements on the crystal [Flack parameter = 0.037(18)]. The asymmetric unit consists of four independent molecules. Drawings were produced with PLATON.



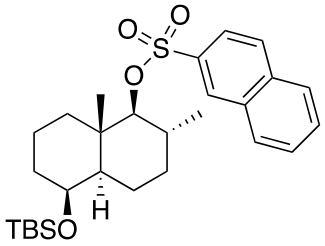
Identification code	32068101_0m	
Empirical formula	C25 H42 O4 S Si	
Formula weight	466.73	
Temperature	100.0 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 9.9546(9) Å	a= 93.903(4)°.
	b = 11.1380(11) Å	b= 95.575(4)°.
	c = 24.037(2) Å	g = 90.203(4)°.
Volume	2646.2(4) $Å^3$	
Z	4	
Density (calculated)	1.172 Mg/m^3	
Absorption coefficient	0.194 mm^{-1}	
F(000)	1016	

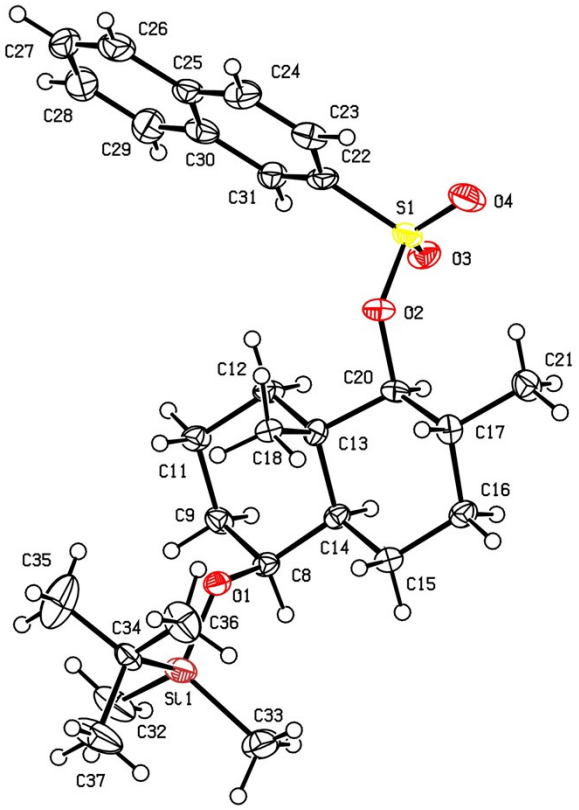
Crystal size	0.252 x 0.167 x 0.057 mm^3
Theta range for data collection	2.056 to 28.387°.
Index ranges	-13<=h<=13, -14<=k<=14, -32<=l<=32
Reflections collected	197680
Independent reflections	25989 [R(int) = 0.0527]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.6713
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	25989 / 3 / 1149
Goodness-of-fit on F^2	1.115
Final R indices [I>2sigma(I)]	R1 = 0.0428, wR2 = 0.0988
R indices (all data)	R1 = 0.0455, wR2 = 0.1002
Absolute structure parameter	0.037(18)
Extinction coefficient	n/a
Largest diff. peak and hole	0.490 and -0.312 $e.Å^{-3}$

Table 1. Crystal data and structure refinement for **4**.

A single crystal of **6** has been analysed by X-ray diffraction and a summary of the crystallographic data and the structure refinement parameters is reported in Table 2. Crystallographic data have been collected at 100 K using a Bruker D8 Venture diffractometer with a Photon II CMOS detector and Mo-Kα radiation (λ = 0.71073 Å) generated by an Incoatec high brillance microfocus source equipped with Incoatec Helios multilayer optics.

The software APEX3 has been used for collecting frames of data, indexing reflections, and the determination of lattice parameters, SAINT for integration of intensity of reflections, and SADABS for scaling and empirical absorption correction. The structure has been solved by dual-space algorithm using the program SHELXT. All non-hydrogen atoms have been refined with anisotropic thermal parameters by full-matrix least-squares calculations on F^2 using the program SHELXL with OLEX2. Hydrogen atoms have been inserted at calculated positions and constrained with isotropic thermal parameters. The sample has crystallized in the chiral space group P21. The absolute configuration has been determined by anomalous dispersion effects in diffraction measurements on the crystal using Bayesian statistics on Bijvoet differences [P2(true) = 1.000, P3(true) = 1.000, P3(rac-twin) = 0.1 x 10-10 and P3(false) = 0.3 x 10-51]. The asymmetric unit consists of two independent molecules; in one molecule, the TBS group is disordered over two positions, the site occupation factors have been refined converging to 63:37. Drawings have been produced with PLATON.





Empirical formula	
Formula weight	502.76
Temperature	100.0 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 1 21 1
Unit cell dimensions	a = 7.2736(9) Å a= 90°.

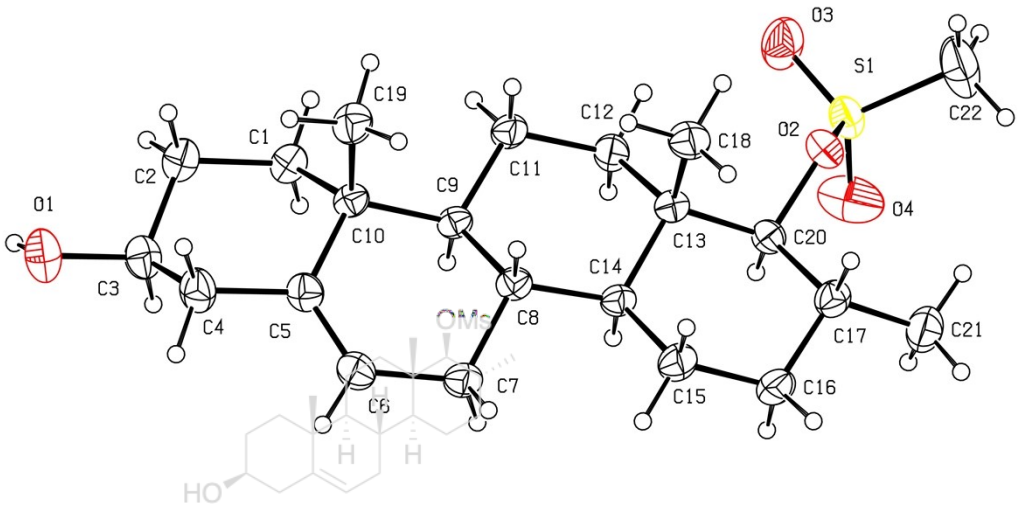
	b = 19.217(2) Å	b= 91.946(5)°.
	c = 19.825(2) Å	g = 90°.
Volume	2769.4(5) Å^3	
Z	4	
Density (calculated)	1.206 Mg/m^3	
Absorption coefficient	0.191 mm^{-1}	
F(000)	1088	
Crystal size	0.293 x 0.217 x 0.021 mm^3	
Theta range for data collection	2.056 to 25.349°.	
Index ranges	-8<=h<=8, -23<=k<=23, -23<=l<=23	
Reflections collected	57153	
Independent reflections	9530 [R(int) = 0.0942]	
Completeness to theta = 25.242°	97.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.5112	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9530 / 2 / 678	
Goodness-of-fit on F^2	1.099	
Final R indices [I>2sigma(I)]	R1 = 0.0711, wR2 = 0.1814	
R indices (all data)	R1 = 0.0841, wR2 = 0.1919	
Absolute structure parameter	0.05(8)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.685 and -0.412 e.Å^{-3}	

Table 2. Crystal data and structure refinement for **6**.

A single crystal of **17** was analysed by X-ray diffraction and a summary of the crystallographic data and the structure refinement parameters is reported in Table 3. Crystallographic data were collected at room temperature using a Bruker Smart 6000 CCD detector and Cu-Kα radiation (λ = 1.54178 Å) generated by a Incoatec microfocus source equipped with Incoatec Quazar MX optics.

The software APEX3 was used for collecting frames of data, indexing reflections, and the determination of lattice parameters, SAINT for integration of intensity of reflections, and SADABS for scaling and empirical absorption correction. The structure was solved by dual-space algorithm using the program SHELXT. All non-hydrogen atoms were refined with anisotropic thermal parameters by full-matrix least- squares calculations on F^2 using the program SHELXL with OLEX2. Hydrogen atoms were inserted at calculated positions and constrained with isotropic thermal parameters except for the hydrogen atoms of the hydroxyl

groups, which were located from a Fourier-difference map and refined isotropically. The asymmetric unit consists of two independent molecules. The absolute configuration has been established by anomalous dispersion effects in diffraction measurements on the crystal [Flack parameter = -0.020(11)]. Drawings were produced with PLATON.



Empirical formula	C22 H30 O4 S	
Formula weight	396.57	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 9.8554(2) Å	a= 90°.
	b = 15.7898(4) Å	b= 90°.
	c = 26.9608(6) Å	g = 90°.
Volume	4195.50(17) $Å^3$	
Z	8	
Density (calculated)	1.256 Mg/m^3	
Absorption coefficient	1.561 mm^{-1}	
F(000)	1728	

Crystal size	0.161 x 0.135 x 0.031 mm^3
Theta range for data collection	3.243 to 71.378°.
Index ranges	-11<=h<=11, -19<=k<=18, -26<=l<=32
Reflections collected	24881
Independent reflections	7895 [R(int) = 0.0454]
Completeness to theta = 67.679°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7535 and 0.5853
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7895 / 2 / 503
Goodness-of-fit on F^2	1.062
Final R indices [I>2sigma(I)]	R1 = 0.0489, wR2 = 0.1318
R indices (all data)	R1 = 0.0526, wR2 = 0.1390
Absolute structure parameter	-0.020(11)
Extinction coefficient	n/a
Largest diff. peak and hole	0.302 and -0.296 $e.Å^{-3}$

Table 3. Crystal data and structure refinement for **17**.

Hexane Neutral
Naphthyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1477.28090
ΔU: -1477.25806
ΔH: -1477.25712
ΔG: -1477.33389
Num. Imaginary Frequencies: 0

C	-2.826439	-0.387761	-0.012658
C	-2.765190	-1.870055	-0.466024
C	-3.717474	-2.785122	0.290207
C	-5.153126	-2.271609	0.112439
C	-5.297467	-0.786115	0.466421
C	-4.265358	0.108149	-0.240637
C	-1.272872	-2.198945	-0.504481
H	-3.114294	-1.868433	-1.518667
H	-3.449509	-2.827330	1.361747
H	-3.636428	-3.818531	-0.092120
H	-5.445994	-2.416299	-0.945097
H	-5.856758	-2.871071	0.716266
H	-5.206289	-0.659623	1.560147
H	-6.313907	-0.441938	0.206734
H	-4.473230	0.110791	-1.328270
H	-4.392582	1.146484	0.107551
C	-2.429068	-0.209434	1.462628
C	-1.741694	0.193380	-0.960132
H	-1.053978	-3.034008	-1.189787
H	-0.915027	-2.502815	0.494313

C	-0.613031	-0.872391	-0.951051
C	-1.219162	1.621751	-0.794393
H	-2.192807	0.197234	-1.970191
H	-0.146561	-0.951992	-1.946858
H	0.186451	-0.581200	-0.253704
H	-2.516726	0.847811	1.761258
H	-3.070987	-0.799286	2.136268
H	-1.385643	-0.506519	1.653366
H	-0.499006	1.788129	-1.614962
C	-2.264279	2.724069	-0.840296
O	-0.494869	1.737871	0.455343
H	-1.767029	3.705575	-0.894516
H	-2.913067	2.604615	-1.723628
H	-2.892176	2.702628	0.063641
S	0.901851	2.533872	0.525934
C	2.058359	1.278104	0.045860
O	0.907652	3.579394	-0.481809
O	1.077225	2.837371	1.927136
C	2.455939	1.183577	-1.309291
C	3.258899	0.139478	-1.695269
C	3.692783	-0.838439	-0.757840
C	3.298283	-0.716213	0.607699
C	2.469107	0.369144	0.990288
H	2.130203	1.942568	-2.023793
H	3.577694	0.051338	-2.737837
C	4.514219	-1.935024	-1.138550
H	2.150743	0.473060	2.030965
C	4.919529	-2.861834	-0.208871
H	4.818523	-2.029032	-2.185092
H	5.550253	-3.701729	-0.513331
C	4.527001	-2.738944	1.148443
C	3.736009	-1.690023	1.548064
H	4.858345	-3.484437	1.876443
H	3.430307	-1.589461	2.593527

Naphthyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: 0
ΔU: 0
ΔH: 0
ΔG: 0
Num. Imaginary Frequencies: 0

C	-2.837467	0.676047	0.044705
C	-4.348597	1.035387	0.015041
C	-4.602191	2.506946	0.305984
C	-3.874212	3.353663	-0.748747
C	-2.386893	2.997825	-0.880829
C	-2.134195	1.493893	-1.056477
C	-5.023403	-0.030112	0.869713
H	-4.687354	0.856438	-1.025796
H	-4.255867	2.764392	1.323081
H	-5.685736	2.717810	0.276851
H	-4.369977	3.190641	-1.724481
H	-3.985285	4.426927	-0.517902
H	-1.838658	3.369769	0.002309
H	-1.956873	3.532647	-1.744675
H	-2.524459	1.172067	-2.040320
H	-1.059363	1.260399	-1.060901
C	-2.172685	0.928636	1.405952
C	-2.864877	-0.805899	-0.287391
H	-6.117413	-0.052401	0.730808
H	-4.835736	0.125406	1.943748
C	-4.451922	-1.370394	0.407933
C	-2.636505	-1.858958	0.591016
H	-2.913985	-1.061293	-1.350883
H	-4.896873	-1.760901	-0.517253
H	-4.583446	-2.154332	1.171491
H	-1.169862	0.470496	1.405467
H	-2.073543	2.004815	1.608310
H	-2.737580	0.499027	2.250343
O	0.073280	-1.369907	1.157758
H	-2.392715	-1.624840	1.630029
C	-2.457172	-3.269601	0.147312
H	-2.864225	-3.981219	0.882439
H	-2.897389	-3.447591	-0.846194
H	-1.365643	-3.438246	0.067587
S	0.559266	-1.632262	-0.221265
O	0.827685	-3.058718	-0.477964
O	-0.293486	-1.004121	-1.259759
C	2.141446	-0.804094	-0.357452
C	2.738001	-0.691601	-1.639868
C	3.962347	-0.088152	-1.769629
C	4.647565	0.432125	-0.633916
C	4.039557	0.315995	0.649828
C	2.769659	-0.316745	0.758707
H	2.208716	-1.083333	-2.512077
H	4.429059	0.003418	-2.755357
C	5.916338	1.064704	-0.738760
H	2.287287	-0.414702	1.734723
C	6.551384	1.557765	0.376756
H	6.382110	1.152769	-1.725305
H	7.528021	2.041494	0.282694
C	5.946780	1.441883	1.653174
C	4.719991	0.835598	1.785050
H	6.461571	1.836597	2.533926
H	4.249426	0.742440	2.768703

Tosyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1363.09811
ΔU: -1363.07605
ΔH: -1363.07511
ΔG: -1363.15016
Num. Imaginary Frequencies: 0

C	-2.474434	0.059258	0.028496
C	-2.747190	1.562057	0.299963
C	-3.914902	2.129862	-0.493864
C	-5.181966	1.328406	-0.164273
C	-4.985248	-0.183498	-0.332398
C	-3.747289	-0.718728	0.406382
C	-1.373510	2.225378	0.201600
H	-3.047343	1.616595	1.366200
H	-3.703560	2.094362	-1.578224
H	-4.065564	3.194666	-0.240452
H	-5.462211	1.536880	0.886014
H	-6.028270	1.668050	-0.786741
H	-4.905506	-0.425316	-1.407450
H	-5.882332	-0.714992	0.030638
H	-3.909692	-0.627999	1.497972
H	-3.639153	-1.794760	0.191781
C	-2.099475	-0.213131	-1.438391
C	-1.250348	-0.130892	0.965135
H	-1.332765	3.170501	0.767443
H	-1.133838	2.469678	-0.847701
C	-0.404853	1.154363	0.757881
C	-0.412657	-1.410488	0.935096
H	-1.651391	-0.106692	1.995795
H	0.063433	1.466696	1.706012
H	0.416674	0.966356	0.050758
H	-1.955871	-1.292965	-1.605726
H	-2.881328	0.130037	-2.134611
H	-1.157099	0.278833	-1.727137
H	0.362612	-1.295150	1.713257
C	-1.165596	-2.705227	1.193150
O	0.261799	-1.528307	-0.341179
H	-0.448929	-3.530985	1.327399
H	-1.783064	-2.618875	2.102450
H	-1.821578	-2.949516	0.343497
S	1.804081	-1.985684	-0.414665
C	2.647529	-0.440930	-0.225974
O	2.106667	-2.827955	0.729423
O	1.978331	-2.462965	-1.766923
C	3.127965	-0.064894	1.025167
C	3.693925	1.199239	1.178859
C	3.784889	2.087636	0.101154
C	3.301346	1.674443	-1.149932
C	2.735342	0.417197	-1.323020
H	3.062185	-0.757093	1.867815
H	4.071580	1.499954	2.160691
C	4.416149	3.445276	0.264913
H	3.369137	2.353563	-2.005242
H	2.357522	0.099975	-2.298051
H	3.882021	4.208595	-0.324648
H	4.423176	3.763130	1.319775
H	5.463423	3.429257	-0.087093

Tosyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1363.02036
ΔU: -1362.99762
ΔH: -1362.99668
ΔG: -1363.07313
Num. Imaginary Frequencies: 1
Imaginary Frequency: -311.2132

C	-1.701559	0.716472	0.023103
C	-3.044456	1.488591	-0.095041
C	-2.900100	2.960841	0.260964
C	-1.880011	3.604056	-0.690466
C	-0.545626	2.847442	-0.737407
C	-0.708354	1.340347	-0.977077
C	-4.062379	0.629535	0.645065
H	-3.328173	1.448471	-1.166222
H	-2.580701	3.073848	1.312714
H	-3.875411	3.470383	0.169079
H	-2.318402	3.621243	-1.706281
H	-1.706548	4.656364	-0.407541
H	0.011327	3.018094	0.200383
H	0.087593	3.265722	-1.538148
H	-1.084397	1.170038	-2.002910
H	0.262976	0.829691	-0.914242
C	-1.112317	0.726576	1.442127
C	-2.109732	-0.685615	-0.391649
H	-5.101772	0.925566	0.424423
H	-3.933965	0.689878	1.737388
C	-3.853840	-0.802678	0.153527
C	-2.268763	-1.778706	0.450989
H	-2.137538	-0.886686	-1.465965
H	-4.300524	-1.015429	-0.826977
H	-4.275515	-1.539688	0.855347
H	-0.298656	-0.013878	1.500716
H	-0.704135	1.714453	1.698746
H	-1.852552	0.476017	2.220329
O	0.319091	-2.244374	1.045757
H	-2.074777	-1.646264	1.517457
C	-2.441497	-3.176009	-0.038126
H	-3.167596	-3.734828	0.573542
H	-2.721838	-3.212637	-1.101746
H	-1.451726	-3.645683	0.082571
S	1.056873	-2.158767	-0.245981
O	1.852910	-3.349026	-0.551889
O	0.178106	-1.719630	-1.360989
C	2.218066	-0.803434	-0.024298
C	2.745086	-0.162380	-1.146586
C	3.638777	0.892189	-0.985510
C	4.025783	1.326657	0.290469
C	3.488896	0.668268	1.402045
C	2.593630	-0.391263	1.251189
H	2.434777	-0.482545	-2.144748
H	4.042350	1.394855	-1.870915
C	5.014310	2.453884	0.452486
H	3.773172	0.991305	2.409078
H	2.170263	-0.896384	2.122824
H	4.941720	2.914451	1.451492
H	6.049939	2.087643	0.330042
H	4.853791	3.241868	-0.302602

Hexane Protonated

Naphthyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1477.62394
ΔU: -1477.60090
ΔH: -1477.59995
ΔG: -1477.67483
Num. Imaginary Frequencies: 0

C	-2.956215	-0.357861	-0.063920
C	-2.923536	-1.904225	-0.192048
C	-4.065811	-2.602313	0.531244
C	-5.399742	-2.086568	-0.025854
C	-5.494868	-0.555953	-0.016912
C	-4.283731	0.131204	-0.670301
C	-1.480096	-2.291157	0.130264
H	-3.072437	-2.111862	-1.270838
H	-4.002701	-2.429385	1.621040
H	-3.993531	-3.694446	0.385852
H	-5.503812	-2.444884	-1.067350
H	-6.245231	-2.516345	0.537720
H	-5.605190	-0.198864	1.022581
H	-6.412653	-0.240056	-0.541635
H	-4.283371	-0.089784	-1.755060
H	-4.397567	1.223490	-0.569596
C	-2.826225	0.114657	1.394240
C	-1.670081	-0.037553	-0.872957
H	-1.202268	-3.255602	-0.322766
H	-1.338304	-2.395000	1.219125
C	-0.644795	-1.113771	-0.426614
C	-1.086838	1.367170	-0.924053
H	-1.917735	-0.228838	-1.933942
H	-0.001570	-1.411938	-1.270966
H	0.022851	-0.715477	0.352591
H	-2.894680	1.214040	1.456363
H	-3.626902	-0.293606	2.029482
H	-1.866947	-0.179603	1.850535
H	-0.212123	1.334269	-1.593637
C	-2.013011	2.491749	-1.333277
O	-0.557037	1.722389	0.435772
H	-1.449237	3.420293	-1.517549
H	-2.528145	2.214884	-2.266603
H	-2.773192	2.679559	-0.560778
S	0.863028	2.264992	0.730483
C	2.068253	1.194080	0.086886
O	1.032147	3.536303	-0.194566
O	0.961450	2.527379	2.132610
C	2.445364	1.222174	-1.283064
C	3.316765	0.262019	-1.726188
C	3.834924	-0.735338	-0.851581
C	3.453611	-0.727504	0.525207
C	2.553831	0.262938	0.982687
H	2.078996	1.997627	-1.957952
H	3.632150	0.263668	-2.772822
C	4.733103	-1.734696	-1.306334
H	2.251867	0.274121	2.033371
C	5.223763	-2.676830	-0.432852
H	5.032384	-1.743436	-2.357678
H	5.916831	-3.442297	-0.791637
C	4.845470	-2.666778	0.933101
C	3.979403	-1.712055	1.406006
H	5.248965	-3.423571	1.610384
H	3.686013	-1.697659	2.459129
H	0.499402	4.301926	0.112314

Naphthyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1477.61358
ΔU: -1477.58975
ΔH: -1477.58880
ΔG: -1477.66645
Num. Imaginary Frequencies: 1
Imaginary Frequency: -116.3482

C	1.566741	-1.204396	-0.033486
C	2.460418	-2.462212	-0.238717
C	1.726825	-3.744679	0.125269
C	0.481235	-3.877690	-0.765119
C	-0.412678	-2.629998	-0.751469
C	0.364976	-1.328719	-0.993549
C	3.783642	-2.123721	0.437652
H	2.675017	-2.516472	-1.324642
H	1.452094	-3.742016	1.195023
H	2.390806	-4.612606	-0.027615
H	0.817314	-4.065728	-1.801839
H	-0.106319	-4.760563	-0.463787
H	-0.960511	-2.566647	0.204983
H	-1.189819	-2.723393	-1.528302
H	0.739017	-1.316602	-2.034156
H	-0.307626	-0.465451	-0.886419
C	1.094971	-1.030415	1.419785
C	2.494114	-0.077393	-0.444731
H	4.588041	-2.822147	0.153275
H	3.710907	-2.144897	1.536511
C	4.171658	-0.733903	-0.054903
C	3.193248	0.762902	0.415054
H	2.521239	0.170818	-1.513507
H	4.551720	-0.699420	-1.085602
H	4.949599	-0.266603	0.572135
H	0.696770	-0.014596	1.566598
H	0.295478	-1.742451	1.667823
H	1.897319	-1.185716	2.159070
O	0.787605	2.492752	1.326665
H	3.035919	0.641193	1.491770
C	3.888875	2.010838	-0.018387
H	4.783739	2.205284	0.592054
H	4.150218	1.992630	-1.087492
H	3.174462	2.834606	0.143745
S	0.142429	2.846665	0.076634
O	-0.462992	4.313152	0.323365
O	0.914719	2.868963	-1.156266
C	-1.261694	1.806681	-0.169710
C	-1.776930	1.656281	-1.482190
C	-2.780266	0.746680	-1.697009
C	-3.288263	-0.053278	-0.634279
C	-2.771533	0.128024	0.682893
C	-1.752147	1.090733	0.895574
H	-1.355866	2.232782	-2.308549
H	-3.185648	0.609323	-2.703212
C	-4.284190	-1.043338	-0.849156
H	-1.338934	1.230670	1.897317
C	-4.736294	-1.816058	0.193723
H	-4.683560	-1.184078	-1.857412
H	-5.501639	-2.576599	0.017117
C	-4.221388	-1.635138	1.502211
C	-3.262118	-0.682257	1.743425
H	-4.595440	-2.256454	2.320079
H	-2.862754	-0.534938	2.751066
H	-0.610275	4.780837	-0.519576

Tosyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1363.44519
ΔU: -1363.42284
ΔH: -1363.42190
ΔG: -1363.49580
Num. Imaginary Frequencies: 0

C	2.429356	0.063089	-0.016143
C	2.697112	1.460978	-0.634213
C	3.672452	2.309862	0.167780
C	5.004483	1.557646	0.293978
C	4.831233	0.131346	0.830120
C	3.773904	-0.681440	0.063722
C	1.309226	2.013087	-0.962505
H	3.192367	1.260730	-1.605237
H	3.259504	2.544321	1.166033
H	3.832869	3.278595	-0.336986
H	5.474282	1.509232	-0.706415
H	5.703136	2.116445	0.939558
H	4.562909	0.170070	1.901175
H	5.796507	-0.401005	0.782298
H	4.137893	-0.872758	-0.963796
H	3.662336	-1.665883	0.548740
C	1.787961	0.155688	1.378508
C	1.412268	-0.456988	-1.067373
H	1.347967	2.763998	-1.767042
H	0.865378	2.508932	-0.082322
C	0.494695	0.759910	-1.363736
C	0.657338	-1.762858	-0.879574
H	1.996509	-0.659575	-1.984651
H	0.202090	0.772532	-2.426166
H	-0.438309	0.707303	-0.781315
H	1.636801	-0.849611	1.806441
H	2.422433	0.715198	2.082403
H	0.807008	0.658813	1.354628
H	-0.006470	-1.901164	-1.747552
C	1.470647	-3.016916	-0.649321
O	-0.265810	-1.649225	0.313475
H	0.825748	-3.910313	-0.683642
H	2.228237	-3.109714	-1.443775
H	1.989463	-2.983847	0.320227
S	-1.796926	-1.880932	0.204261
C	-2.585174	-0.341727	0.227333
O	-2.183777	-2.735265	-0.881489
O	-2.104348	-2.434471	1.642743
C	-3.400934	-0.017024	-0.857641
C	-3.942515	1.262741	-0.908697
C	-3.677089	2.204779	0.094301
C	-2.848492	1.836027	1.170815
C	-2.294806	0.569730	1.251535
H	-3.605152	-0.744678	-1.646182
H	-4.584438	1.533097	-1.751071
C	-4.280885	3.579114	0.044682
H	-2.632771	2.561442	1.959599
H	-1.646606	0.299168	2.088094
H	-3.554089	4.345273	0.359635
H	-4.642826	3.828016	-0.964306
H	-5.140632	3.636484	0.736157
H	-1.574524	-3.226764	1.878043

Tosyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1363.42970
ΔU: -1363.40690
ΔH: -1363.40596
ΔG: -1363.48127
Num. Imaginary Frequencies: 1
Imaginary Frequency: -104.5958

C	-1.808526	0.670815	0.025652
C	-3.169130	1.413718	-0.086148
C	-3.056866	2.889938	0.262766
C	-2.052676	3.549738	-0.694676
C	-0.702227	2.822808	-0.748484
C	-0.836435	1.311363	-0.985495
C	-4.158455	0.526433	0.660014
H	-3.457121	1.364146	-1.155270
H	-2.745144	3.019287	1.314661
H	-4.043158	3.374643	0.164727
H	-2.494351	3.558315	-1.708539
H	-1.897544	4.604533	-0.413823
H	-0.140806	3.006431	0.184182
H	-0.085730	3.251742	-1.556128
H	-1.214707	1.134085	-2.009328
H	0.152596	0.832135	-0.925626
C	-1.209781	0.702525	1.440215
C	-2.196453	-0.741256	-0.381740
H	-5.207446	0.786328	0.441481
H	-4.031823	0.587252	1.752248
C	-3.912330	-0.896819	0.158628
C	-2.315502	-1.842297	0.459535
H	-2.213957	-0.942518	-1.459014
H	-4.359920	-1.131365	-0.816233
H	-4.299727	-1.651059	0.864164
H	-0.332319	0.037969	1.493233
H	-0.877754	1.714914	1.708488
H	-1.917965	0.385874	2.222862
O	0.531970	-2.330214	1.038666
H	-2.118949	-1.702582	1.527043
C	-2.439043	-3.247291	-0.022444
H	-3.100730	-3.843752	0.624544
H	-2.772143	-3.303457	-1.070313
H	-1.424820	-3.676200	0.048091
S	1.202248	-2.056778	-0.218797
O	2.184086	-3.311027	-0.428625
O	0.419278	-1.885844	-1.433797
C	2.277994	-0.675122	-0.021724
C	2.670035	0.052527	-1.146691
C	3.503616	1.152075	-0.977608
C	3.952177	1.534906	0.295238
C	3.539380	0.782782	1.404051
C	2.707482	-0.322512	1.257648
H	2.307663	-0.220889	-2.140604
H	3.807824	1.730600	-1.854577
C	4.876225	2.710696	0.461927
H	3.874334	1.067780	2.405436
H	2.384813	-0.898530	2.127997
H	5.927418	2.385020	0.362924
H	4.764812	3.174899	1.454707
H	4.693985	3.478561	-0.306947
H	2.487128	-3.369190	-1.353570

DCM Neutral

Naphthyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1477.28671
ΔU: -1477.26384
ΔH: -1477.26290
ΔG: -1477.33981
Num. Imaginary Frequencies: 0

C	-2.835731	-0.383333	-0.015452
C	-2.768643	-1.876680	-0.430158
C	-3.745526	-2.769310	0.321567
C	-5.173463	-2.254879	0.091734
C	-5.320275	-0.760697	0.405688
C	-4.265695	0.111850	-0.295423
C	-1.277439	-2.212491	-0.418737
H	-3.088082	-1.899420	-1.491653
H	-3.507779	-2.786425	1.400976
H	-3.658513	-3.811801	-0.033949
H	-5.437445	-2.423701	-0.969767
H	-5.895903	-2.836609	0.690799
H	-5.257160	-0.608304	1.498187
H	-6.327745	-0.418793	0.110288
H	-4.443295	0.087463	-1.387953
H	-4.398363	1.158994	0.023136
C	-2.477992	-0.169741	1.465295
C	-1.722205	0.169145	-0.946631
H	-1.044146	-3.064906	-1.077404
H	-0.949002	-2.492290	0.597185
C	-0.599091	-0.900367	-0.879974
C	-1.199399	1.599341	-0.804605
H	-2.144371	0.149953	-1.968545
H	-0.106986	-1.006002	-1.860752
H	0.181954	-0.595542	-0.167715
H	-2.578403	0.894330	1.735688
H	-3.136410	-0.744925	2.135672
H	-1.439285	-0.460577	1.689595
H	-0.460998	1.743302	-1.612624
C	-2.239728	2.702511	-0.896414
O	-0.498216	1.745810	0.460616
H	-1.740359	3.682226	-0.961710
H	-2.867816	2.563859	-1.791504
H	-2.888624	2.701717	-0.007146
S	0.903026	2.524401	0.537051
C	2.059630	1.275760	0.048092
O	0.918446	3.589786	-0.451622
O	1.073213	2.820281	1.943469
C	2.448680	1.186063	-1.310497
C	3.253127	0.145617	-1.703386
C	3.696254	-0.832514	-0.770074
C	3.308456	-0.715946	0.598236
C	2.476968	0.364863	0.988531
H	2.115963	1.942008	-2.024818
H	3.564541	0.060578	-2.748213
C	4.519893	-1.924810	-1.159028
H	2.163020	0.459728	2.031201
C	4.933139	-2.852793	-0.233396
H	4.818679	-2.014601	-2.207353
H	5.565159	-3.689644	-0.543242
C	4.546779	-2.735674	1.126637
C	3.753751	-1.690912	1.534278
H	4.884262	-3.482716	1.850116
H	3.452198	-1.595340	2.581294

Naphthyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1477.22351
ΔU: -1477.20001
ΔH: -1477.19906
ΔG: -1477.27697
Num. Imaginary Frequencies: 1
Imaginary Frequency: -206.7637

C	-1.735121	1.070420	-0.067012
C	-2.702499	2.277659	-0.198493
C	-1.986437	3.607295	-0.012194
C	-0.888633	3.735044	-1.080120
C	0.057619	2.526697	-1.121464
C	-0.681597	1.183011	-1.185723
C	-3.893084	1.923423	0.685081
H	-3.076903	2.261956	-1.241409
H	-1.556317	3.675949	1.003154
H	-2.704496	4.439930	-0.110208
H	-1.378039	3.838519	-2.066851
H	-0.308153	4.659518	-0.919641
H	0.724198	2.544585	-0.241360
H	0.721496	2.607752	-1.999005
H	-1.191764	1.092605	-2.162740
H	0.031517	0.348875	-1.123190
C	-1.058028	0.981834	1.309594
C	-2.665417	-0.107228	-0.291919
H	-4.769688	2.560780	0.483626
H	-3.659343	2.021583	1.756708
C	-4.266942	0.481512	0.342044
C	-3.136882	-0.972125	0.685784
H	-2.853833	-0.388774	-1.332279
H	-4.842052	0.364332	-0.585842
H	-4.868337	0.015233	1.139921
H	-0.597160	-0.011304	1.422046
H	-0.270635	1.741057	1.419631
H	-1.759726	1.127278	2.147058
O	-0.668305	-2.452733	1.225917
H	-2.812481	-0.815521	1.717896
C	-3.825348	-2.258798	0.388163
H	-4.622208	-2.471956	1.117090
H	-4.220384	-2.291979	-0.638400
H	-3.041705	-3.027744	0.488899
S	-0.099131	-2.700658	-0.122977
O	0.375456	-4.078989	-0.322072
O	-0.977746	-2.215508	-1.214988
C	1.359083	-1.656866	-0.236943
C	1.947088	-1.462069	-1.514388
C	3.010751	-0.608040	-1.654250
C	3.536815	0.095720	-0.532144
C	2.955975	-0.122349	0.750852
C	1.861148	-1.023384	0.869697
H	1.528319	-1.978870	-2.381443
H	3.461704	-0.446763	-2.638138
C	4.616262	1.013220	-0.651970
H	1.399359	-1.188848	1.846301
C	5.093437	1.684115	0.449965
H	5.061643	1.179196	-1.637663
H	5.923301	2.388882	0.345492
C	4.514888	1.467550	1.725839
C	3.471550	0.583645	1.872489
H	4.903130	2.007065	2.594412
H	3.021643	0.413304	2.855381

Tosyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1363.10350
ΔU: -1363.08148
ΔH: -1363.08054
ΔG: -1363.15529
Num. Imaginary Frequencies: 0

C	-2.478746	0.057260	0.030537
C	-2.747850	1.565967	0.271369
C	-3.929319	2.114612	-0.515519
C	-5.190063	1.321183	-0.145026
C	-4.995215	-0.194068	-0.281703
C	-3.744562	-0.712004	0.448195
C	-1.376822	2.227721	0.133617
H	-3.029407	1.645139	1.340874
H	-3.737055	2.053192	-1.602346
H	-4.075861	3.185026	-0.284196
H	-5.451420	1.553687	0.905033
H	-6.047157	1.645995	-0.760732
H	-4.933497	-0.460104	-1.352301
H	-5.885474	-0.717341	0.109167
H	-3.887854	-0.595881	1.539852
H	-3.639967	-1.792694	0.256258
C	-2.129208	-0.248869	-1.435953
C	-1.238183	-0.109424	0.949994
H	-1.327463	3.185237	0.677422
H	-1.155438	2.447646	-0.925160
C	-0.397479	1.170752	0.697833
C	-0.401213	-1.389178	0.939846
H	-1.620623	-0.060709	1.986439
H	0.086279	1.504608	1.630550
H	0.411181	0.967104	-0.019654
H	-1.991543	-1.333141	-1.579997
H	-2.923092	0.078713	-2.126057
H	-1.192310	0.237267	-1.751909
H	0.384220	-1.254683	1.704211
C	-1.151029	-2.677033	1.235723
O	0.260361	-1.539793	-0.345051
H	-0.434939	-3.501584	1.379792
H	-1.755127	-2.567925	2.151230
H	-1.819865	-2.939399	0.401607
S	1.802860	-1.980001	-0.425396
C	2.648981	-0.441600	-0.225180
O	2.116694	-2.843794	0.701292
O	1.971411	-2.451025	-1.783811
C	3.120627	-0.072363	1.032158
C	3.689212	1.189263	1.195093
C	3.791108	2.082076	0.121264
C	3.314783	1.676141	-1.135459
C	2.745317	0.421841	-1.318080
H	3.046331	-0.764150	1.874279
H	4.059040	1.484422	2.181316
C	4.424634	3.436696	0.295970
H	3.389326	2.358704	-1.987141
H	2.371023	0.115080	-2.297676
H	3.902633	4.201674	-0.301864
H	4.418270	3.751993	1.351415
H	5.476470	3.415199	-0.041590

Tosyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1363.03845
ΔU: -1363.01651
ΔH: -1363.01556
ΔG: -1363.08986
Num. Imaginary Frequencies: 2
Imaginary Frequency: -219.1337

C	-1.679890	0.707168	-0.010253
C	-3.000400	1.521022	-0.087547
C	-2.794074	2.986008	0.267665
C	-1.780490	3.596594	-0.712688
C	-0.474614	2.794818	-0.807395
C	-0.701524	1.295491	-1.044865
C	-4.020821	0.688424	0.678958
H	-3.316663	1.493925	-1.149255
H	-2.441856	3.085740	1.310096
H	-3.753177	3.528744	0.203064
H	-2.249206	3.634277	-1.714087
H	-1.559549	4.640188	-0.430569
H	0.119544	2.941734	0.111564
H	0.143729	3.194071	-1.629482
H	-1.124547	1.146650	-2.055854
H	0.252474	0.749199	-1.017945
C	-1.048815	0.701951	1.390809
C	-2.141629	-0.683264	-0.406119
H	-5.056910	1.011527	0.485399
H	-3.863607	0.737465	1.767761
C	-3.868475	-0.745275	0.172447
C	-2.320172	-1.761028	0.450319
H	-2.192448	-0.891439	-1.479078
H	-4.339921	-0.941098	-0.799621
H	-4.298771	-1.474578	0.878176
H	-0.259022	-0.064314	1.432287
H	-0.597539	1.675121	1.630949
H	-1.774897	0.482309	2.190599
O	0.402185	-2.399083	1.046648
H	-2.101613	-1.623722	1.512181
C	-2.521452	-3.161624	-0.016307
H	-3.225905	-3.708057	0.629724
H	-2.846417	-3.208946	-1.066736
H	-1.528707	-3.632828	0.071832
S	1.136383	-2.244955	-0.236415
O	2.035120	-3.371531	-0.535077
O	0.245251	-1.887447	-1.367016
C	2.199957	-0.814525	-0.007464
C	2.710521	-0.154631	-1.127510
C	3.533865	0.954434	-0.962477
C	3.864855	1.428553	0.316336
C	3.352770	0.746474	1.425126
C	2.527770	-0.368915	1.269524
H	2.444079	-0.501842	-2.129322
H	3.925176	1.469541	-1.845995
C	4.731153	2.651755	0.478000
H	3.599849	1.093621	2.433607
H	2.123513	-0.889253	2.141185
H	4.177191	3.564899	0.194933
H	5.623364	2.597452	-0.168756
H	5.068046	2.772791	1.520184

DCM Protonated

Naphthyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1477.65307
ΔU: -1477.62975
ΔH: -1477.62880
ΔG: -1477.70610
Num. Imaginary Frequencies: 0

C	-2.954326	-0.348714	-0.067522
C	-2.927977	-1.898070	-0.144561
C	-4.103956	-2.566396	0.552413
C	-5.410039	-2.063192	-0.077380
C	-5.494127	-0.532445	-0.118822
C	-4.252951	0.127404	-0.743049
C	-1.501806	-2.284303	0.248247
H	-3.034140	-2.138129	-1.221395
H	-4.087157	-2.354745	1.637099
H	-4.032194	-3.663488	0.446987
H	-5.470487	-2.452350	-1.111470
H	-6.282026	-2.471052	0.462687
H	-5.641301	-0.145148	0.905285
H	-6.388620	-0.226894	-0.688791
H	-4.208884	-0.127206	-1.819313
H	-4.363809	1.222505	-0.680737
C	-2.880596	0.172170	1.377944
C	-1.633893	-0.062513	-0.832266
H	-1.211872	-3.260032	-0.172712
H	-1.407096	-2.364780	1.344465
C	-0.635494	-1.123889	-0.297750
C	-1.047104	1.340288	-0.914937
H	-1.835807	-0.296660	-1.894039
H	0.055161	-1.447254	-1.093640
H	-0.013922	-0.704082	0.507430
H	-2.940539	1.273548	1.396606
H	-3.710732	-0.207600	1.993490
H	-1.942773	-0.112564	1.882089
H	-0.160117	1.283768	-1.565448
C	-1.961431	2.449876	-1.385784
O	-0.548387	1.737139	0.443381
H	-1.391997	3.373350	-1.576179
H	-2.443969	2.143000	-2.326980
H	-2.743825	2.661546	-0.642497
S	0.873898	2.275328	0.743142
C	2.071033	1.193072	0.094889
O	1.064458	3.537540	-0.177252
O	0.970651	2.521938	2.149098
C	2.453817	1.236918	-1.272766
C	3.319504	0.276993	-1.727126
C	3.826206	-0.735693	-0.863473
C	3.439268	-0.743866	0.511079
C	2.545460	0.247809	0.979706
H	2.091046	2.020786	-1.939339
H	3.636381	0.289789	-2.772971
C	4.716575	-1.738381	-1.328942
H	2.240578	0.246226	2.029267
C	5.193365	-2.698488	-0.467462
H	5.017485	-1.735550	-2.379851
H	5.878089	-3.467338	-0.834990
C	4.808910	-2.704177	0.897250
C	3.950878	-1.746825	1.380002
H	5.200181	-3.475921	1.564843
H	3.650472	-1.744117	2.431142
H	0.537841	4.316734	0.108725

Naphthyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1477.64288
ΔU: -1477.61876
ΔH: -1477.61781
ΔG: -1477.69657
Num. Imaginary Frequencies: 1
Imaginary Frequency: -125.1712

C	1.534452	-1.206667	-0.044266
C	2.430142	-2.468970	-0.235700
C	1.688962	-3.742813	0.144290
C	0.442259	-3.885657	-0.742566
C	-0.449625	-2.636642	-0.741358
C	0.332279	-1.342722	-1.002799
C	3.754460	-2.135541	0.441944
H	2.645109	-2.535889	-1.320158
H	1.414216	-3.724922	1.213872
H	2.351421	-4.613638	0.001786
H	0.776584	-4.083778	-1.777948
H	-0.146105	-4.764300	-0.429493
H	-0.992259	-2.559315	0.217315
H	-1.229677	-2.737105	-1.514795
H	0.706086	-1.345960	-2.043143
H	-0.336505	-0.475302	-0.906649
C	1.066646	-1.017294	1.408427
C	2.454169	-0.089154	-0.469698
H	4.547329	-2.848786	0.163203
H	3.680419	-2.147485	1.540483
C	4.172557	-0.760280	-0.059470
C	3.210917	0.708046	0.381729
H	2.492646	0.141245	-1.541903
H	4.518810	-0.743252	-1.101932
H	4.980479	-0.313849	0.543323
H	0.682404	0.004688	1.549476
H	0.258945	-1.718010	1.661888
H	1.868906	-1.177419	2.145836
O	0.750222	2.586338	1.349622
H	3.049842	0.603459	1.459274
C	3.908521	1.956957	-0.059771
H	4.809246	2.143153	0.544236
H	4.170572	1.929317	-1.128740
H	3.202098	2.787308	0.100760
S	0.110277	2.918306	0.090820
O	-0.534138	4.369650	0.335331
O	0.891834	2.957412	-1.134714
C	-1.267443	1.841343	-0.163747
C	-1.777973	1.678431	-1.476851
C	-2.753364	0.739393	-1.694927
C	-3.236125	-0.079757	-0.634848
C	-2.725951	0.114224	0.682755
C	-1.736142	1.107154	0.898785
H	-1.376918	2.270591	-2.301848
H	-3.151464	0.591357	-2.702347
C	-4.194966	-1.105367	-0.854367
H	-1.324854	1.251334	1.900551
C	-4.616671	-1.900212	0.185053
H	-4.587651	-1.256347	-1.863803
H	-5.350851	-2.690120	0.004864
C	-4.107662	-1.706470	1.494348
C	-3.185043	-0.718674	1.740059
H	-4.454229	-2.348022	2.308795
H	-2.787027	-0.564441	2.746956
H	-0.711754	4.829430	-0.507036

Tosyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1363.47434
ΔU: -1363.45156
ΔH: -1363.45062
ΔG: -1363.52717
Num. Imaginary Frequencies: 0

C	2.465638	0.072847	-0.016221
C	2.721210	1.478325	-0.621667
C	3.702618	2.321937	0.178595
C	5.039513	1.574284	0.277964
C	4.877942	0.140725	0.798658
C	3.814767	-0.665975	0.034380
C	1.327843	2.027629	-0.927003
H	3.206023	1.290778	-1.600627
H	3.301757	2.539565	1.185450
H	3.852226	3.298254	-0.315608
H	5.494262	1.538653	-0.730166
H	5.745292	2.128283	0.920878
H	4.619942	0.167128	1.872569
H	5.845250	-0.386920	0.733513
H	4.164935	-0.838031	-1.001281
H	3.714532	-1.658743	0.503767
C	1.841752	0.144669	1.387735
C	1.438826	-0.442423	-1.060326
H	1.354062	2.795659	-1.716221
H	0.888287	2.500199	-0.031903
C	0.520165	0.776550	-1.346662
C	0.679047	-1.744689	-0.860387
H	2.014374	-0.647474	-1.982077
H	0.234148	0.800343	-2.410395
H	-0.416131	0.714157	-0.771112
H	1.705285	-0.867190	1.805192
H	2.478535	0.702846	2.091395
H	0.854875	0.635696	1.381914
H	0.031944	-1.897633	-1.737799
C	1.487103	-2.994842	-0.593311
O	-0.258588	-1.600250	0.310394
H	0.838684	-3.885502	-0.619164
H	2.257360	-3.102570	-1.373429
H	1.985188	-2.945269	0.386178
S	-1.782436	-1.875545	0.193838
C	-2.604509	-0.351528	0.210725
O	-2.140377	-2.732434	-0.900547
O	-2.094383	-2.431005	1.625524
C	-3.421159	-0.043775	-0.877243
C	-4.006050	1.217814	-0.919900
C	-3.779849	2.157242	0.093809
C	-2.948268	1.806087	1.173810
C	-2.352420	0.558410	1.246095
H	-3.595021	-0.769204	-1.674615
H	-4.649859	1.474382	-1.764778
C	-4.418375	3.516321	0.050450
H	-2.763680	2.530452	1.971439
H	-1.704246	0.299784	2.086355
H	-3.668500	4.306245	0.222279
H	-4.911951	3.702547	-0.915350
H	-5.176826	3.605013	0.847982
H	-1.549758	-3.210848	1.874230

Tosyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1363.45939
ΔU: -1363.43577
ΔH: -1363.43482
ΔG: -1363.51338
Num. Imaginary Frequencies: 1
Imaginary Frequency: -96.4312

C	-1.765098	0.652050	-0.011010
C	-3.120316	1.411116	-0.070089
C	-2.969522	2.884935	0.274947
C	-1.997416	3.530964	-0.724533
C	-0.660642	2.784805	-0.836865
C	-0.829883	1.276218	-1.065549
C	-4.093234	0.536985	0.712034
H	-3.449855	1.366126	-1.126565
H	-2.609663	3.007459	1.312020
H	-3.951591	3.384834	0.218990
H	-2.482668	3.544951	-1.718338
H	-1.814419	4.583445	-0.450212
H	-0.057580	2.959817	0.071205
H	-0.073520	3.203978	-1.671376
H	-1.260205	1.105047	-2.069497
H	0.151940	0.779377	-1.050315
C	-1.112641	0.682843	1.379965
C	-2.177608	-0.755893	-0.397720
H	-5.144260	0.817999	0.535267
H	-3.922813	0.585203	1.798752
C	-3.896971	-0.885019	0.191937
C	-2.325244	-1.835612	0.464498
H	-2.225383	-0.968289	-1.471670
H	-4.359172	-1.090230	-0.782672
H	-4.301024	-1.638283	0.888759
H	-0.259830	-0.013761	1.412983
H	-0.731844	1.685337	1.619755
H	-1.803765	0.404452	2.191373
O	0.620566	-2.448276	1.041817
H	-2.107402	-1.685554	1.526435
C	-2.466087	-3.248527	0.005848
H	-3.130141	-3.824234	0.668398
H	-2.812933	-3.316629	-1.036671
H	-1.456269	-3.687722	0.071404
S	1.267726	-2.124724	-0.216095
O	2.319810	-3.319268	-0.436616
O	0.471600	-1.983455	-1.425733
C	2.262239	-0.682942	-0.007985
C	2.639660	0.054650	-1.131632
C	3.393565	1.208731	-0.955355
C	3.772529	1.639722	0.324918
C	3.383738	0.873059	1.431896
C	2.631922	-0.287889	1.277080
H	2.331744	-0.257976	-2.132115
H	3.688821	1.792125	-1.832136
C	4.551816	2.914790	0.501708
H	3.671774	1.190560	2.438044
H	2.324829	-0.873200	2.146591
H	5.271552	3.060529	-0.319977
H	5.100744	2.923092	1.456503
H	3.867971	3.782682	0.500252
H	2.640699	-3.347489	-1.357974

DMF Neutral

Naphthyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1477.28846
ΔU: -1477.26557
ΔH: -1477.26462
ΔG: -1477.34150
Num. Imaginary Frequencies: 0

C	-2.838122	-0.381838	-0.017135
C	-2.770719	-1.878552	-0.419504
C	-3.755311	-2.763361	0.331422
C	-5.180336	-2.248089	0.085918
C	-5.326715	-0.751230	0.387043
C	-4.264855	0.113854	-0.312377
C	-1.280347	-2.217300	-0.393544
H	-3.081642	-1.908931	-1.483218
H	-3.526439	-2.772342	1.412876
H	-3.667475	-3.808727	-0.015380
H	-5.435838	-2.424567	-0.976382
H	-5.908711	-2.823711	0.683745
H	-5.272107	-0.590566	1.478854
H	-6.331058	-0.409735	0.080656
H	-4.433547	0.081396	-1.406020
H	-4.398128	1.163638	-0.002844
C	-2.491672	-0.157309	1.464725
C	-1.715978	0.160809	-0.943807
H	-1.043898	-3.074975	-1.044210
H	-0.960664	-2.490014	0.627142
C	-0.595506	-0.910141	-0.859285
C	-1.191864	1.591068	-0.809909
H	-2.129534	0.134037	-1.968912
H	-0.095759	-1.023972	-1.835222
H	0.179856	-0.601314	-0.142497
H	-2.593346	0.909125	1.725596
H	-3.156166	-0.726164	2.134501
H	-1.455157	-0.448306	1.699120
H	-0.446361	1.726613	-1.612714
C	-2.229190	2.695255	-0.918839
O	-0.500130	1.747145	0.461123
H	-1.727938	3.673740	-0.988168
H	-2.849404	2.550066	-1.818275
H	-2.886091	2.702530	-0.035457
S	0.902210	2.520533	0.542771
C	2.059873	1.275135	0.050603
O	0.921794	3.593573	-0.438053
O	1.068681	2.811214	1.951586
C	2.448937	1.189861	-1.308438
C	3.254669	0.151438	-1.704138
C	3.699035	-0.828580	-0.773247
C	3.310646	-0.716687	0.595419
C	2.477507	0.361750	0.988738
H	2.115128	1.946359	-2.021603
H	3.565489	0.069387	-2.749303
C	4.524163	-1.918699	-1.165443
H	2.162655	0.451703	2.031527
C	4.938160	-2.848953	-0.242263
H	4.823149	-2.004971	-2.213957
H	5.571182	-3.684195	-0.554321
C	4.551067	-2.736527	1.118106
C	3.756610	-1.693963	1.528904
H	4.889087	-3.485613	1.839194
H	3.454274	-1.602129	2.575992

Naphthyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1477.22695
ΔU: -1477.20331
ΔH: -1477.20237
ΔG: -1477.28489
Num. Imaginary Frequencies: 1
Imaginary Frequency: -179.6893

C	-2.812397	0.711986	0.020597
C	-4.297339	1.156225	-0.071455
C	-4.474902	2.645077	0.184374
C	-3.660019	3.425289	-0.858365
C	-2.191160	2.983987	-0.927525
C	-2.020233	1.463932	-1.066222
C	-5.057204	0.141652	0.774034
H	-4.607853	0.977276	-1.120104
H	-4.153820	2.904769	1.209063
H	-5.542139	2.916220	0.107396
H	-4.127141	3.269099	-1.848950
H	-3.714820	4.507980	-0.652717
H	-1.656546	3.340749	-0.029766
H	-1.700248	3.476203	-1.784498
H	-2.391281	1.146708	-2.058666
H	-0.958046	1.176613	-1.021485
C	-2.184720	0.952948	1.401526
C	-2.917609	-0.772360	-0.286292
H	-6.143758	0.168205	0.590705
H	-4.903633	0.301800	1.852375
C	-4.541052	-1.233887	0.349646
C	-2.769376	-1.815490	0.618351
H	-2.938433	-1.043287	-1.346543
H	-4.974158	-1.623061	-0.581051
H	-4.734661	-1.994811	1.124293
H	-1.204488	0.450722	1.442341
H	-2.040352	2.026129	1.592550
H	-2.799688	0.565191	2.230253
O	0.077398	-1.457982	1.219153
H	-2.560253	-1.575138	1.663955
C	-2.634318	-3.242946	0.211572
H	-3.129000	-3.915307	0.929033
H	-3.017157	-3.419669	-0.805322
H	-1.552915	-3.466704	0.217394
S	0.592811	-1.787940	-0.131004
O	0.913257	-3.222629	-0.289325
O	-0.246491	-1.262127	-1.231933
C	2.157530	-0.929163	-0.294215
C	2.811338	-0.955846	-1.554476
C	4.017344	-0.321649	-1.709901
C	4.627046	0.369777	-0.622610
C	3.963321	0.392853	0.638842
C	2.713922	-0.276210	0.775221
H	2.344112	-1.478330	-2.393287
H	4.526245	-0.337146	-2.678469
C	5.874313	1.039255	-0.757036
H	2.193360	-0.266714	1.736330
C	6.434892	1.700088	0.311287
H	6.382382	1.020876	-1.726015
H	7.394708	2.211747	0.196519
C	5.774592	1.723031	1.565547
C	4.567076	1.084288	1.725223
H	6.230762	2.252040	2.407075
H	4.054273	1.099757	2.691748

Tosyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1363.10515
ΔU: -1363.08310
ΔH: -1363.08215
ΔG: -1363.15711
Num. Imaginary Frequencies: 0

C	-2.481902	0.057315	0.031813
C	-2.749921	1.568278	0.259379
C	-3.937009	2.108549	-0.524853
C	-5.194862	1.318619	-0.137447
C	-5.000388	-0.197865	-0.260293
C	-3.744485	-0.708129	0.466039
C	-1.380246	2.229244	0.105467
H	-3.023975	1.657997	1.329895
H	-3.752432	2.036040	-1.612367
H	-4.082237	3.181192	-0.303200
H	-5.448697	1.561518	0.912076
H	-6.056350	1.636923	-0.750464
H	-4.946053	-0.474451	-1.328653
H	-5.887651	-0.717440	0.142206
H	-3.879997	-0.581042	1.557387
H	-3.640969	-1.790670	0.284114
C	-2.142688	-0.263155	-1.434047
C	-1.234705	-0.099461	0.944101
H	-1.327729	3.191983	0.639636
H	-1.166212	2.438649	-0.956989
C	-0.396450	1.178496	0.673480
C	-0.397495	-1.378881	0.941552
H	-1.609572	-0.040764	1.982640
H	0.093154	1.521520	1.599728
H	0.407195	0.968262	-0.047730
H	-2.005866	-1.348940	-1.567906
H	-2.941958	0.056738	-2.121553
H	-1.208786	0.221304	-1.761477
H	0.391830	-1.236973	1.700382
C	-1.145309	-2.664248	1.252233
O	0.258625	-1.541373	-0.346456
H	-0.428775	-3.487687	1.400501
H	-1.744445	-2.546484	2.169822
H	-1.818807	-2.934117	0.424258
S	1.800825	-1.977605	-0.430135
C	2.649946	-0.442500	-0.224778
O	2.117663	-2.849558	0.689882
O	1.966411	-2.444746	-1.791218
C	3.119160	-0.077106	1.034908
C	3.691345	1.182303	1.201624
C	3.799303	2.076737	0.129445
C	3.324837	1.674864	-1.129399
C	2.751387	0.422913	-1.315846
H	3.040277	-0.769081	1.876415
H	4.058711	1.474513	2.189566
C	4.436952	3.428635	0.308769
H	3.403405	2.358786	-1.979536
H	2.377905	0.120612	-2.297104
H	3.926799	4.194243	-0.298252
H	4.418677	3.746329	1.363312
H	5.492937	3.400483	-0.015070

Tosyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1363.04357
ΔU: -1363.02081
ΔH: -1363.01986
ΔG: -1363.09633
Num. Imaginary Frequencies: 1
Imaginary Frequency: -194.3648

C	-1.674506	0.702724	-0.018887
C	-2.987381	1.529217	-0.090093
C	-2.764591	2.990261	0.271400
C	-1.746823	3.594536	-0.708821
C	-0.449377	2.779812	-0.812430
C	-0.693621	1.283838	-1.054918
C	-4.013115	0.701838	0.675247
H	-3.306504	1.510422	-1.150897
H	-2.409468	3.082049	1.313512
H	-3.717958	3.543210	0.210584
H	-2.217977	3.642238	-1.708544
H	-1.513374	4.634088	-0.421943
H	0.150233	2.917079	0.104562
H	0.169118	3.176160	-1.635898
H	-1.122815	1.144594	-2.064641
H	0.254779	0.727237	-1.033283
C	-1.040837	0.688115	1.381069
C	-2.149325	-0.682369	-0.416986
H	-5.046730	1.034083	0.485023
H	-3.853194	0.743280	1.763848
C	-3.875382	-0.730465	0.160983
C	-2.339880	-1.757787	0.439304
H	-2.201609	-0.888874	-1.490387
H	-4.347229	-0.917702	-0.812477
H	-4.313758	-1.459358	0.862544
H	-0.257502	-0.084827	1.419932
H	-0.580643	1.656532	1.623507
H	-1.767845	0.473363	2.181118
O	0.429502	-2.432492	1.059160
H	-2.121069	-1.622047	1.501521
C	-2.545088	-3.158160	-0.026720
H	-3.249854	-3.702654	0.620258
H	-2.872501	-3.204897	-1.076436
H	-1.553002	-3.631366	0.059275
S	1.163821	-2.269741	-0.221458
O	2.087695	-3.382172	-0.507472
O	0.273107	-1.942574	-1.360712
C	2.199324	-0.818410	-0.000530
C	2.706593	-0.161545	-1.123678
C	3.504997	0.967036	-0.964523
C	3.812719	1.463806	0.311300
C	3.306300	0.782760	1.424070
C	2.507026	-0.351591	1.274395
H	2.456842	-0.524298	-2.124324
H	3.893094	1.479825	-1.850607
C	4.640504	2.713568	0.469434
H	3.536457	1.146877	2.430488
H	2.105734	-0.868875	2.149192
H	5.062348	2.792292	1.484431
H	5.471392	2.738473	-0.255296
H	4.024244	3.613755	0.292787

DMF Protonated

Naphthyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1477.65989
ΔU: -1477.63642
ΔH: -1477.63547
ΔG: -1477.71492
Num. Imaginary Frequencies: 0

C	-2.953991	-0.348487	-0.069358
C	-2.933398	-1.897819	-0.147406
C	-4.111039	-2.562317	0.550507
C	-5.416220	-2.053301	-0.076727
C	-5.494469	-0.522100	-0.116678
C	-4.251728	0.133090	-0.742609
C	-1.507957	-2.289149	0.243263
H	-3.041514	-2.136744	-1.224266
H	-4.092031	-2.351815	1.635413
H	-4.043951	-3.659677	0.443627
H	-5.479422	-2.440944	-1.111266
H	-6.289046	-2.458455	0.464332
H	-5.638205	-0.135299	0.908143
H	-6.388940	-0.212794	-0.684865
H	-4.210294	-0.121299	-1.819005
H	-4.357463	1.228657	-0.679681
C	-2.876502	0.170878	1.376571
C	-1.634057	-0.066466	-0.836292
H	-1.222560	-3.266253	-0.177896
H	-1.411329	-2.369059	1.339413
C	-0.638604	-1.132262	-0.305342
C	-1.041439	1.333884	-0.917263
H	-1.838598	-0.298636	-1.897801
H	0.046401	-1.458251	-1.104884
H	-0.011602	-0.715403	0.497143
H	-2.934947	1.272317	1.395882
H	-3.705739	-0.208647	1.993695
H	-1.937461	-0.115267	1.877611
H	-0.151978	1.272611	-1.563638
C	-1.949206	2.446425	-1.393640
O	-0.547579	1.726544	0.443353
H	-1.374771	3.365809	-1.587504
H	-2.431677	2.138138	-2.334394
H	-2.730952	2.665713	-0.651840
S	0.870498	2.273680	0.746644
C	2.072516	1.194110	0.099820
O	1.060337	3.534511	-0.172166
O	0.963397	2.515988	2.153828
C	2.460570	1.244215	-1.265972
C	3.328593	0.286896	-1.721569
C	3.831976	-0.729411	-0.860399
C	3.439321	-0.744304	0.512286
C	2.543271	0.245139	0.982193
H	2.098364	2.029798	-1.930766
H	3.648806	0.304166	-2.766275
C	4.724224	-1.730186	-1.327311
H	2.234261	0.238273	2.030465
C	5.197216	-2.694834	-0.468851
H	5.028549	-1.721828	-2.377223
H	5.882969	-3.462262	-0.837522
C	4.806773	-2.707291	0.894323
C	3.946891	-1.752053	1.378229
H	5.194565	-3.482839	1.559608
H	3.640917	-1.754639	2.427744
H	0.523974	4.311460	0.102685

Naphthyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1477.64959
ΔU: -1477.62542
ΔH: -1477.62448
ΔG: -1477.70345
Num. Imaginary Frequencies: 1
Imaginary Frequency: -129.1442

C	1.530006	-1.203945	-0.042824
C	2.431664	-2.464330	-0.227495
C	1.697774	-3.737099	0.170494
C	0.446756	-3.895484	-0.707485
C	-0.451716	-2.651394	-0.711490
C	0.321744	-1.356535	-0.991165
C	3.759720	-2.120308	0.437791
H	2.639016	-2.541435	-1.312486
H	1.428477	-3.709442	1.241287
H	2.363889	-4.605960	0.032908
H	0.775940	-4.100483	-1.743166
H	-0.134860	-4.774498	-0.382648
H	-0.986827	-2.567905	0.250953
H	-1.236917	-2.762857	-1.478303
H	0.687729	-1.367654	-2.034062
H	-0.350192	-0.491328	-0.897821
C	1.073368	-1.000121	1.411459
C	2.438813	-0.088710	-0.488747
H	4.550769	-2.836188	0.160733
H	3.693679	-2.120490	1.536804
C	4.175592	-0.751369	-0.080806
C	3.214005	0.708290	0.346471
H	2.470374	0.126889	-1.564150
H	4.505424	-0.746177	-1.128681
H	4.993422	-0.302085	0.506100
H	0.690736	0.023470	1.545215
H	0.267265	-1.697720	1.678333
H	1.881634	-1.152765	2.143730
O	0.732155	2.613669	1.359090
H	3.061178	0.618187	1.426456
C	3.902340	1.956538	-0.115457
H	4.808273	2.151037	0.478109
H	4.156880	1.916022	-1.186014
H	3.195048	2.787038	0.040780
S	0.080340	2.950603	0.107448
O	-0.598314	4.380803	0.384341
O	0.856555	3.031363	-1.118880
C	-1.274101	1.846400	-0.160263
C	-1.776310	1.680505	-1.476064
C	-2.736844	0.727766	-1.701635
C	-3.211102	-0.102776	-0.646636
C	-2.708577	0.093176	0.673678
C	-1.735276	1.100591	0.897651
H	-1.381796	2.283234	-2.296535
H	-3.128175	0.577512	-2.711344
C	-4.152272	-1.143162	-0.874303
H	-1.330219	1.246329	1.901708
C	-4.563969	-1.950165	0.159814
H	-4.538100	-1.296257	-1.886042
H	-5.283539	-2.751954	-0.026827
C	-4.062178	-1.754635	1.471781
C	-3.157022	-0.752723	1.725444
H	-4.399393	-2.406887	2.281667
H	-2.763455	-0.598242	2.734012
H	-0.819370	4.841221	-0.447564

Tosyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1363.48061
ΔU: -1363.45784
ΔH: -1363.45690
ΔG: -1363.53364
Num. Imaginary Frequencies: 0

C	2.450420	0.069031	-0.014345
C	2.712888	1.465638	-0.637033
C	3.684892	2.321131	0.162168
C	5.020590	1.575266	0.288209
C	4.852518	0.149821	0.828853
C	3.798864	-0.668487	0.063757
C	1.322756	2.009987	-0.965630
H	3.209019	1.264201	-1.607520
H	3.272409	2.553052	1.161093
H	3.840332	3.290243	-0.344554
H	5.486515	1.523976	-0.714200
H	5.719158	2.139145	0.930663
H	4.580641	0.193089	1.898803
H	5.820698	-0.378580	0.784056
H	4.161658	-0.856042	-0.964883
H	3.692422	-1.653959	0.546818
C	1.808935	0.161384	1.380637
C	1.436624	-0.461672	-1.063424
H	1.357432	2.764854	-1.767280
H	0.874154	2.497082	-0.082860
C	0.518955	0.752272	-1.372762
C	0.677631	-1.763610	-0.855474
H	2.022268	-0.675777	-1.976560
H	0.238755	0.760251	-2.438210
H	-0.420577	0.696665	-0.801805
H	1.667508	-0.844291	1.811017
H	2.436249	0.731066	2.083741
H	0.821530	0.650930	1.355424
H	0.038037	-1.927298	-1.736379
C	1.487110	-3.008744	-0.568759
O	-0.266564	-1.608034	0.305081
H	0.841234	-3.900986	-0.594624
H	2.267146	-3.119832	-1.338579
H	1.971318	-2.949810	0.417201
S	-1.790677	-1.879220	0.186890
C	-2.600686	-0.348025	0.213573
O	-2.152392	-2.723547	-0.916085
O	-2.107908	-2.443004	1.612661
C	-3.397991	-0.018121	-0.881923
C	-3.963867	1.252360	-0.920489
C	-3.736282	2.179205	0.104373
C	-2.924811	1.805658	1.191983
C	-2.348524	0.548348	1.260503
H	-3.570298	-0.732950	-1.689045
H	-4.592121	1.526081	-1.771698
C	-4.352009	3.549112	0.064141
H	-2.740013	2.519608	1.998851
H	-1.715625	0.272502	2.106983
H	-3.591398	4.325057	0.251875
H	-4.829806	3.750897	-0.906505
H	-5.119042	3.644161	0.852676
H	-1.561932	-3.222454	1.861845

Tosyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1363.46574
ΔU: -1363.44213
ΔH: -1363.44118
ΔG: -1363.51994
Num. Imaginary Frequencies: 1
Imaginary Frequency: -91.9398

C	-1.756484	0.643089	-0.017038
C	-3.116070	1.395190	-0.074226
C	-2.972423	2.866575	0.284565
C	-2.000490	3.526249	-0.706261
C	-0.659692	2.787630	-0.822095
C	-0.821609	1.280327	-1.063988
C	-4.087076	0.510236	0.698217
H	-3.442481	1.358587	-1.131848
H	-2.616117	2.981560	1.323722
H	-3.956804	3.362185	0.229862
H	-2.483091	3.546600	-1.701225
H	-1.822932	4.577062	-0.421643
H	-0.059575	2.957680	0.088865
H	-0.072819	3.216624	-1.651855
H	-1.248784	1.115906	-2.070303
H	0.162808	0.788349	-1.049766
C	-1.109239	0.667508	1.376641
C	-2.157689	-0.763795	-0.415144
H	-5.138371	0.789679	0.521088
H	-3.918860	0.549133	1.785585
C	-3.886782	-0.906610	0.167354
C	-2.317791	-1.844694	0.442803
H	-2.200290	-0.971197	-1.490306
H	-4.337203	-1.101723	-0.814813
H	-4.299345	-1.666543	0.851979
H	-0.256965	-0.029607	1.409587
H	-0.728690	1.668621	1.622687
H	-1.803702	0.385220	2.183654
O	0.660850	-2.469677	1.066664
H	-2.107281	-1.698836	1.506768
C	-2.445793	-3.257436	-0.022393
H	-3.112073	-3.838281	0.633107
H	-2.785942	-3.322938	-1.067166
H	-1.434082	-3.691332	0.046879
S	1.299877	-2.142287	-0.194569
O	2.377526	-3.316083	-0.403656
O	0.499620	-2.027950	-1.404087
C	2.263090	-0.677448	-0.000890
C	2.633542	0.050757	-1.132931
C	3.354975	1.227210	-0.967981
C	3.707017	1.689801	0.308943
C	3.328355	0.930499	1.424539
C	2.609574	-0.252555	1.281108
H	2.346460	-0.287108	-2.131511
H	3.644076	1.803637	-1.851342
C	4.445631	2.990396	0.473854
H	3.596570	1.272181	2.428215
H	2.308570	-0.831223	2.157111
H	5.157629	3.153616	-0.351198
H	4.996134	3.023362	1.427286
H	3.733372	3.835149	0.468596
H	2.711514	-3.337659	-1.320747

Water Neutral

Naphthyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1477.28878
ΔU: -1477.26588
ΔH: -1477.26494
ΔG: -1477.34180
Num. Imaginary Frequencies: 0

C	-2.838274	-0.381660	-0.017337
C	-2.770867	-1.878734	-0.418369
C	-3.756346	-2.762670	0.332420
C	-5.181023	-2.247284	0.085135
C	-5.327327	-0.750146	0.384903
C	-4.264627	0.114130	-0.314252
C	-1.280600	-2.217839	-0.390763
H	-3.080809	-1.909922	-1.482324
H	-3.528505	-2.770766	1.414106
H	-3.668427	-3.808339	-0.013449
H	-5.435527	-2.424549	-0.977267
H	-5.910089	-2.822238	0.682772
H	-5.273701	-0.588632	1.476645
H	-6.331298	-0.408669	0.077265
H	-4.432301	0.080862	-1.408008
H	-4.397943	1.164185	-0.005639
C	-2.493071	-0.155983	1.464649
C	-1.715168	0.159847	-0.943524
H	-1.043829	-3.076055	-1.040599
H	-0.961928	-2.489818	0.630447
C	-0.594991	-0.911227	-0.856917
C	-1.190952	1.590120	-0.810740
H	-2.127721	0.132123	-1.968977
H	-0.094366	-1.025924	-1.832294
H	0.179666	-0.601973	-0.139537
H	-2.594965	0.910702	1.724478
H	-3.158227	-0.724184	2.134325
H	-1.456796	-0.447014	1.700132
H	-0.444473	1.724559	-1.612794
C	-2.227906	2.694383	-0.921994
O	-0.500517	1.747591	0.461157
H	-1.726456	3.672737	-0.991795
H	-2.846931	2.548305	-1.822087
H	-2.885999	2.702668	-0.039500
S	0.902046	2.519998	0.543599
C	2.059842	1.275058	0.051033
O	0.922407	3.594280	-0.435945
O	1.067900	2.809915	1.952804
C	2.449191	1.190592	-1.308004
C	3.255146	0.152470	-1.704064
C	3.699433	-0.827965	-0.773550
C	3.310634	-0.716933	0.595099
C	2.477225	0.361147	0.988814
H	2.115357	1.947209	-2.021016
H	3.566060	0.070946	-2.749228
C	4.524818	-1.917753	-1.166182
H	2.161983	0.450199	2.031556
C	4.938636	-2.848505	-0.243388
H	4.824087	-2.003384	-2.214658
H	5.571825	-3.683502	-0.555746
C	4.551102	-2.736950	1.116954
C	3.756393	-1.694720	1.528178
H	4.888965	-3.486470	1.837660
H	3.453686	-1.603586	2.575213

Naphthyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1477.22774
ΔU: -1477.20415
ΔH: -1477.20321
ΔG: -1477.28326
Num. Imaginary Frequencies: 1
Imaginary Frequency: -172.6432

C	-2.822849	0.708800	0.019230
C	-4.309910	1.148776	-0.056774
C	-4.489000	2.636612	0.203875
C	-3.687277	3.421118	-0.845864
C	-2.217969	2.984163	-0.931471
C	-2.044268	1.464783	-1.074571
C	-5.058162	0.130045	0.794048
H	-4.630427	0.971046	-1.102569
H	-4.157955	2.895252	1.225657
H	-5.557720	2.904857	0.138506
H	-4.164373	3.265502	-1.831757
H	-3.742827	4.503253	-0.637494
H	-1.674849	3.340936	-0.038834
H	-1.737705	3.479240	-1.792838
H	-2.425065	1.148407	-2.063619
H	-0.980826	1.180368	-1.041168
C	-2.181576	0.949532	1.393953
C	-2.926801	-0.775485	-0.288851
H	-6.146475	0.153241	0.621184
H	-4.894754	0.288278	1.871220
C	-4.541783	-1.242839	0.361379
C	-2.765973	-1.819467	0.612670
H	-2.957459	-1.044589	-1.349401
H	-4.982874	-1.631762	-0.565634
H	-4.724947	-2.006059	1.136419
H	-1.199517	0.450162	1.424458
H	-2.038402	2.022847	1.585114
H	-2.786826	0.558829	2.228399
O	0.087736	-1.463162	1.214343
H	-2.547519	-1.580051	1.656579
C	-2.629495	-3.245847	0.202537
H	-3.116087	-3.920850	0.923007
H	-3.020246	-3.422437	-0.811362
H	-1.547362	-3.465921	0.199650
S	0.599922	-1.781623	-0.139657
O	0.922998	-3.214645	-0.309470
O	-0.243291	-1.249705	-1.234513
C	2.162694	-0.918879	-0.300499
C	2.807728	-0.925112	-1.565565
C	4.013303	-0.289466	-1.718773
C	4.631196	0.383192	-0.624346
C	3.976149	0.386018	0.641880
C	2.727060	-0.284114	0.775775
H	2.334128	-1.432852	-2.409851
H	4.515380	-0.289118	-2.691002
C	5.878249	1.053619	-0.756308
H	2.213203	-0.289697	1.740521
C	6.446812	1.696085	0.318996
H	6.379619	1.050847	-1.728923
H	7.406355	2.208664	0.206172
C	5.795134	1.698891	1.578004
C	4.588022	1.058808	1.735446
H	6.257655	2.213461	2.424987
H	4.081879	1.058819	2.705586

Tosyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1363.10581
ΔU: -1363.08444
ΔH: -1363.08350
ΔG: -1363.15681
Num. Imaginary Frequencies: 1

C	-2.483842	0.056047	0.032910
C	-2.752319	1.569061	0.245918
C	-3.945083	2.099298	-0.536571
C	-5.199427	1.312207	-0.132312
C	-5.003931	-0.205339	-0.239725
C	-3.742566	-0.706193	0.483698
C	-1.384515	2.230024	0.076250
H	-3.019664	1.669987	1.317111
H	-3.767447	2.014975	-1.624399
H	-4.090220	3.174141	-0.325778
H	-5.446693	1.566354	0.916108
H	-6.065266	1.622735	-0.743192
H	-4.956500	-0.493606	-1.305324
H	-5.887833	-0.721422	0.174499
H	-3.870975	-0.567468	1.574470
H	-3.638959	-1.790507	0.312773
C	-2.153861	-0.279706	-1.431607
C	-1.230512	-0.089415	0.938716
H	-1.329929	3.198552	0.599632
H	-1.177421	2.428131	-0.989741
C	-0.395769	1.186783	0.649481
C	-0.391676	-1.367761	0.944174
H	-1.598821	-0.020502	1.978941
H	0.098662	1.540310	1.569187
H	0.403900	0.970011	-0.074239
H	-2.014512	-1.366487	-1.554339
H	-2.959052	0.029802	-2.116947
H	-1.224115	0.204464	-1.771085
H	0.400773	-1.217749	1.698148
C	-1.136340	-2.651195	1.269924
O	0.259152	-1.540928	-0.345503
H	-0.418189	-3.472369	1.422738
H	-1.731562	-2.525526	2.188992
H	-1.813213	-2.929574	0.447538
S	1.801049	-1.976812	-0.431832
C	2.652099	-0.442740	-0.227087
O	2.119736	-2.849583	0.687116
O	1.963634	-2.444374	-1.793284
C	3.118655	-0.075372	1.035186
C	3.693966	1.180464	1.200082
C	3.808541	2.073568	0.124646
C	3.341388	1.669623	-1.133780
C	2.762429	0.417627	-1.318891
H	3.036621	-0.766291	1.877273
H	4.062393	1.473982	2.187481
C	4.422275	3.432884	0.330693
H	3.430011	2.348023	-1.987050
H	2.394743	0.113660	-2.301782
H	4.477871	3.999025	-0.612113
H	3.829044	4.021970	1.051423
H	5.442323	3.344256	0.742116

Tosyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1363.04461
ΔU: -1363.02182
ΔH: -1363.02087
ΔG: -1363.09761
Num. Imaginary Frequencies: 1
Imaginary Frequency: -190.0187

C	-1.675016	0.701033	-0.019647
C	-2.988559	1.526516	-0.091020
C	-2.767101	2.987182	0.272803
C	-1.749005	3.593588	-0.705783
C	-0.450817	2.780059	-0.809653
C	-0.693739	1.284148	-1.054180
C	-4.014291	0.697050	0.672062
H	-3.306653	1.509100	-1.152116
H	-2.413015	3.077863	1.315355
H	-3.720835	3.539433	0.211817
H	-2.219429	3.642351	-1.705778
H	-1.516424	4.632861	-0.417207
H	0.148032	2.916662	0.107953
H	0.167846	3.177981	-1.632251
H	-1.121958	1.145887	-2.064442
H	0.255353	0.728637	-1.032097
C	-1.042610	0.685561	1.380898
C	-2.147957	-0.684144	-0.419610
H	-5.047954	1.028831	0.481446
H	-3.855369	0.736327	1.760874
C	-3.875245	-0.734043	0.155162
C	-2.340588	-1.759616	0.436102
H	-2.197883	-0.890214	-1.493250
H	-4.344434	-0.919505	-0.819909
H	-4.315326	-1.464574	0.853999
H	-0.258653	-0.086752	1.419738
H	-0.583444	1.654123	1.624735
H	-1.770221	0.469530	2.180008
O	0.435882	-2.435820	1.061756
H	-2.124194	-1.623881	1.498841
C	-2.542816	-3.160362	-0.030459
H	-3.248094	-3.705796	0.615121
H	-2.868520	-3.207414	-1.080707
H	-1.550196	-3.632156	0.057115
S	1.172267	-2.273280	-0.217511
O	2.102214	-3.382763	-0.497275
O	0.283378	-1.954889	-1.360477
C	2.200774	-0.816732	0.000754
C	2.706580	-0.160588	-1.123489
C	3.499375	0.972267	-0.966287
C	3.802718	1.474108	0.308611
C	3.297999	0.793630	1.422580
C	2.504476	-0.344982	1.274885
H	2.459865	-0.526910	-2.123591
H	3.886110	1.484561	-1.853229
C	4.623659	2.728589	0.464690
H	3.524680	1.161743	2.428313
H	2.104241	-0.861308	2.150724
H	5.047679	2.809643	1.478587
H	5.452264	2.758596	-0.262413
H	4.001452	3.625048	0.289992

Water Protonated

Naphthyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1477.66110
ΔU: -1477.63853
ΔH: -1477.63759
ΔG: -1477.71196
Num. Imaginary Frequencies: 1

C	-2.953461	-0.348162	-0.069626
C	-2.934730	-1.897486	-0.148258
C	-4.113161	-2.560875	0.549407
C	-5.417794	-2.050024	-0.077502
C	-5.494112	-0.518706	-0.116735
C	-4.250655	0.135214	-0.742567
C	-1.509746	-2.290604	0.242311
H	-3.043102	-2.135820	-1.225211
H	-4.093857	-2.350735	1.634394
H	-4.047392	-3.658303	0.442096
H	-5.481470	-2.437060	-1.112255
H	-6.291115	-2.454392	0.463430
H	-5.637111	-0.132253	0.908338
H	-6.388311	-0.207947	-0.684620
H	-4.209581	-0.118793	-1.819059
H	-4.355028	1.230878	-0.679174
C	-2.875321	0.170456	1.376545
C	-1.633260	-0.067550	-0.836631
H	-1.225556	-3.267970	-0.179140
H	-1.413117	-2.370860	1.338460
C	-0.639073	-1.134638	-0.306154
C	-1.038839	1.332004	-0.917276
H	-1.838062	-0.299206	-1.898146
H	0.044986	-1.461222	-1.106226
H	-0.011158	-0.718674	0.496093
H	-2.933467	1.271893	1.396359
H	-3.704456	-0.209191	1.993819
H	-1.936065	-0.116113	1.876964
H	-0.148495	1.269168	-1.562212
C	-1.944694	2.445123	-1.395928
O	-0.546711	1.724205	0.443875
H	-1.368895	3.362983	-1.592330
H	-2.427781	2.135575	-2.335959
H	-2.725874	2.667558	-0.654474
S	0.870500	2.273836	0.747547
C	2.073729	1.195282	0.101249
O	1.059470	3.534353	-0.171608
O	0.962555	2.515649	2.154873
C	2.463619	1.247031	-1.263917
C	3.331632	0.289797	-1.719766
C	3.832932	-0.728208	-0.859459
C	3.438392	-0.744877	0.512663
C	2.542581	0.244647	0.982892
H	2.102310	2.033545	-1.928084
H	3.653083	0.308221	-2.764061
C	4.724674	-1.729291	-1.326821
H	2.232075	0.236288	2.030693
C	5.195307	-2.695981	-0.469340
H	5.030239	-1.719564	-2.376363
H	5.880534	-3.463706	-0.838400
C	4.802912	-2.710257	0.893306
C	3.943530	-1.754729	1.377620
H	5.188685	-3.487516	1.557786
H	3.635790	-1.758761	2.426610
H	0.514887	4.307945	0.096726

Naphthyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1477.65071
ΔU: -1477.62656
ΔH: -1477.62561
ΔG: -1477.70447
Num. Imaginary Frequencies: 1
Imaginary Frequency: -130.9122

C	1.529983	-1.202478	-0.043291
C	2.433931	-2.461825	-0.225795
C	1.701613	-3.735086	0.173673
C	0.451412	-3.896757	-0.704848
C	-0.449253	-2.654317	-0.710205
C	0.322011	-1.358552	-0.991443
C	3.761464	-2.115258	0.439316
H	2.641667	-2.540169	-1.310544
H	1.431393	-3.706417	1.244216
H	2.369281	-4.603012	0.037669
H	0.781507	-4.101937	-1.740203
H	-0.128745	-4.776557	-0.379456
H	-0.984221	-2.570790	0.252327
H	-1.234306	-2.767937	-1.476876
H	0.687922	-1.370248	-2.034321
H	-0.351217	-0.494250	-0.899034
C	1.073229	-0.996704	1.410693
C	2.436591	-0.087010	-0.491380
H	4.552933	-2.831180	0.163574
H	3.695277	-2.113520	1.538303
C	4.176951	-0.747178	-0.081527
C	3.213794	0.709702	0.342349
H	2.468266	0.126341	-1.567230
H	4.504795	-0.743844	-1.130042
H	4.995837	-0.297234	0.503346
H	0.690765	0.027129	1.543053
H	0.266886	-1.693712	1.678399
H	1.881451	-1.148433	2.143180
O	0.726327	2.620984	1.360175
H	3.060793	0.621611	1.422468
C	3.899849	1.958794	-0.121547
H	4.805527	2.155504	0.471692
H	4.154848	1.916697	-1.191964
H	3.191162	2.788432	0.033190
S	0.072767	2.956561	0.109016
O	-0.612817	4.382984	0.388727
O	0.848465	3.043351	-1.117129
C	-1.276740	1.846426	-0.159926
C	-1.777932	1.679114	-1.475909
C	-2.735358	0.723332	-1.701956
C	-3.207018	-0.109133	-0.647309
C	-2.705241	0.087893	0.673138
C	-1.735580	1.098707	0.897682
H	-1.385345	2.283536	-2.296037
H	-3.125902	0.572065	-2.711813
C	-4.144475	-1.152773	-0.875578
H	-1.331416	1.245567	1.901924
C	-4.553181	-1.961940	0.158052
H	-4.529557	-1.306758	-1.887461
H	-5.269714	-2.766331	-0.029098
C	-4.051924	-1.765489	1.470112
C	-3.150440	-0.760401	1.724390
H	-4.386427	-2.419713	2.279536
H	-2.757044	-0.605452	2.732950
H	-0.838613	4.842689	-0.442345

Tosyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1363.48172
ΔU: -1363.45895
ΔH: -1363.45801
ΔG: -1363.53462
Num. Imaginary Frequencies: 0

C	2.448097	0.068212	-0.014313
C	2.711210	1.463876	-0.638809
C	3.681753	2.320873	0.160572
C	5.017443	1.575562	0.289897
C	4.848813	0.150965	0.832603
C	3.796597	-0.668835	0.067112
C	1.321409	2.007359	-0.970188
H	3.208829	1.261070	-1.608260
H	3.267627	2.554165	1.158498
H	3.837766	3.289271	-0.347412
H	5.484861	1.522704	-0.711756
H	5.714918	2.140677	0.932520
H	4.575046	0.196001	1.902001
H	5.817234	-0.377266	0.790315
H	4.161104	-0.858004	-0.960639
H	3.689540	-1.653517	0.551626
C	1.804460	0.162816	1.379546
C	1.436113	-0.464498	-1.064169
H	1.357077	2.761167	-1.772833
H	0.871289	2.495415	-0.088711
C	0.518716	0.748818	-1.376891
C	0.677094	-1.766394	-0.855307
H	2.023229	-0.679848	-1.976036
H	0.240445	0.755062	-2.442833
H	-0.421928	0.693622	-0.807746
H	1.662479	-0.842133	1.811351
H	2.430573	0.733877	2.082647
H	0.816951	0.652012	1.352022
H	0.038341	-1.931206	-1.736591
C	1.486483	-3.011010	-0.566147
O	-0.267775	-1.609236	0.304172
H	0.840847	-3.903361	-0.592087
H	2.267659	-3.122508	-1.334793
H	1.969041	-2.951082	0.420561
S	-1.791981	-1.879787	0.186400
C	-2.599861	-0.347394	0.214431
O	-2.155003	-2.722220	-0.917607
O	-2.109697	-2.444688	1.611508
C	-3.394227	-0.014411	-0.882271
C	-3.957183	1.257378	-0.920626
C	-3.729281	2.182671	0.105559
C	-2.920655	1.806170	1.194239
C	-2.347384	0.547434	1.262596
H	-3.566279	-0.727878	-1.690616
H	-4.583051	1.533429	-1.772847
C	-4.341517	3.554176	0.065465
H	-2.735555	2.518915	2.002098
H	-1.716429	0.269533	2.109875
H	-3.579178	4.328029	0.254852
H	-4.817380	3.757840	-0.905750
H	-5.109412	3.650629	0.852990
H	-1.562617	-3.223480	1.860774

Tosyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1363.46683
ΔU: -1363.44322
ΔH: -1363.44228
ΔG: -1363.52105
Num. Imaginary Frequencies: 1
Imaginary Frequency: -92.0768

C	-1.754620	0.642887	-0.017717
C	-3.114282	1.395074	-0.075311
C	-2.970734	2.865717	0.286662
C	-1.997426	3.527323	-0.701536
C	-0.656539	2.788804	-0.817318
C	-0.818411	1.282008	-1.062354
C	-4.086351	0.508996	0.694520
H	-3.439465	1.360771	-1.133362
H	-2.615832	2.978564	1.326530
H	-3.955019	3.361507	0.231578
H	-2.478787	3.549765	-1.697045
H	-1.820035	4.577515	-0.414439
H	-0.057469	2.956987	0.094677
H	-0.068691	3.219354	-1.645591
H	-1.244416	1.119615	-2.069475
H	0.165956	0.789861	-1.047822
C	-1.109355	0.665087	1.376958
C	-2.154789	-0.763207	-0.418685
H	-5.137272	0.789426	0.516812
H	-3.919050	0.545826	1.782083
C	-3.886748	-0.907033	0.161594
C	-2.319679	-1.844270	0.438043
H	-2.196193	-0.969254	-1.494167
H	-4.334333	-1.099366	-0.822420
H	-4.302482	-1.667752	0.843432
H	-0.257839	-0.032901	1.410265
H	-0.728258	1.665554	1.624793
H	-1.805289	0.382379	2.182523
O	0.662659	-2.469191	1.071822
H	-2.110859	-1.699875	1.502526
C	-2.446843	-3.256750	-0.028780
H	-3.115283	-3.837558	0.624516
H	-2.784701	-3.321087	-1.074349
H	-1.435646	-3.691437	0.042256
S	1.301874	-2.144830	-0.190159
O	2.380300	-3.318659	-0.395018
O	0.501912	-2.034422	-1.400198
C	2.263559	-0.678385	-0.000162
C	2.634643	0.046948	-1.133877
C	3.352914	1.225717	-0.971246
C	3.700984	1.693482	0.304853
C	3.322243	0.936733	1.422184
C	2.606662	-0.248504	1.281127
H	2.350622	-0.294823	-2.132011
H	3.642342	1.799954	-1.855911
C	4.435027	2.996946	0.467462
H	3.587520	1.282375	2.425280
H	2.305188	-0.824890	2.158458
H	5.141954	3.164336	-0.361071
H	4.990164	3.031062	1.418192
H	3.719010	3.838547	0.467180
H	2.713661	-3.344436	-1.312242

MF Neutral

Naphthyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1477.28895
ΔU: -1477.26605
ΔH: -1477.26511
ΔG: -1477.34197
Num. Imaginary Frequencies: 0

C	-2.838301	-0.381587	-0.017426
C	-2.770896	-1.878795	-0.417960
C	-3.756703	-2.762406	0.332780
C	-5.181249	-2.246982	0.084820
C	-5.327528	-0.749742	0.384091
C	-4.264514	0.114242	-0.314953
C	-1.280669	-2.218041	-0.389747
H	-3.080471	-1.910283	-1.482000
H	-3.529254	-2.770168	1.414555
H	-3.668749	-3.808186	-0.012745
H	-5.435366	-2.424530	-0.977624
H	-5.910575	-2.821692	0.682379
H	-5.274276	-0.587925	1.475810
H	-6.331357	-0.408272	0.075977
H	-4.431803	0.080690	-1.408749
H	-4.397846	1.164392	-0.006662
C	-2.493555	-0.155489	1.464609
C	-1.714837	0.159480	-0.943444
H	-1.043793	-3.076445	-1.039296
H	-0.962374	-2.489761	0.631657
C	-0.594766	-0.911632	-0.856037
C	-1.190590	1.589759	-0.811148
H	-2.127003	0.131370	-1.969026
H	-0.093815	-1.026636	-1.831206
H	0.179611	-0.602222	-0.138414
H	-2.595590	0.911285	1.724052
H	-3.158934	-0.723478	2.134245
H	-1.457358	-0.446515	1.700479
H	-0.443677	1.723721	-1.612862
C	-2.227375	2.694055	-0.923411
O	-0.500725	1.747854	0.461155
H	-1.725838	3.672354	-0.993401
H	-2.845852	2.547598	-1.823809
H	-2.886017	2.702771	-0.041326
S	0.901955	2.519752	0.543978
C	2.059814	1.275028	0.051253
O	0.922718	3.594648	-0.434935
O	1.067495	2.809321	1.953377
C	2.449357	1.190969	-1.307767
C	3.255423	0.152986	-1.703982
C	3.699615	-0.827672	-0.773645
C	3.310553	-0.717078	0.594981
C	2.477012	0.360837	0.988868
H	2.115540	1.947644	-2.020718
H	3.566419	0.071723	-2.749134
C	4.525129	-1.917306	-1.166469
H	2.161528	0.449425	2.031573
C	4.938798	-2.848324	-0.243860
H	4.824586	-2.002611	-2.214913
H	5.572069	-3.683207	-0.556349
C	4.550983	-2.737214	1.116454
C	3.756146	-1.695141	1.527866
H	4.888719	-3.486964	1.836976
H	3.453207	-1.604366	2.574862

Naphthyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1477.22844
ΔU: -1477.20478
ΔH: -1477.20384
ΔG: -1477.28391
Num. Imaginary Frequencies: 1
Imaginary Frequency: -169.7509

C	-2.915331	0.673665	0.010083
C	-4.421845	1.047551	0.045677
C	-4.645658	2.523046	0.339666
C	-3.956311	3.353659	-0.753649
C	-2.479740	2.982414	-0.951939
C	-2.252051	1.473557	-1.127428
C	-5.063161	-0.013022	0.932005
H	-4.807584	0.867822	-0.977503
H	-4.253220	2.784397	1.338801
H	-5.726842	2.744889	0.354662
H	-4.496931	3.188620	-1.704602
H	-4.042744	4.429903	-0.526055
H	-1.888383	3.353636	-0.096649
H	-2.085847	3.506867	-1.839378
H	-2.691795	1.151721	-2.090157
H	-1.178117	1.234115	-1.172740
C	-2.188295	0.929598	1.338598
C	-2.975151	-0.810812	-0.308115
H	-6.160867	-0.036664	0.835601
H	-4.831635	0.139924	1.997351
C	-4.518704	-1.356429	0.445250
C	-2.710338	-1.855172	0.568224
H	-3.068019	-1.070802	-1.367852
H	-5.005217	-1.756228	-0.453942
H	-4.613061	-2.135681	1.220583
H	-1.189178	0.465885	1.300415
H	-2.071222	2.006346	1.528307
H	-2.720318	0.512175	2.209244
O	0.157357	-1.432423	1.180472
H	-2.427403	-1.615136	1.596342
C	-2.538833	-3.269836	0.131413
H	-2.933515	-3.973358	0.880147
H	-3.001449	-3.457297	-0.849912
H	-1.450562	-3.436838	0.039834
S	0.639288	-1.673220	-0.200069
O	0.943433	-3.097029	-0.462367
O	-0.219451	-1.067963	-1.243254
C	2.209942	-0.821093	-0.339271
C	2.812671	-0.724131	-1.621285
C	4.028526	-0.104138	-1.757370
C	4.699015	0.449665	-0.627946
C	4.085780	0.350052	0.655235
C	2.825088	-0.301324	0.770451
H	2.298078	-1.139839	-2.491483
H	4.498274	-0.024551	-2.742392
C	5.958278	1.100614	-0.740948
H	2.343481	-0.383866	1.748210
C	6.578259	1.626685	0.368600
H	6.427366	1.176718	-1.726613
H	7.546857	2.125020	0.270308
C	5.968116	1.527587	1.644497
C	4.750261	0.904068	1.784226
H	6.471424	1.950090	2.518718
H	4.275999	0.825739	2.767209

Tosyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1363.10570
ΔU: -1363.08359
ΔH: -1363.08264
ΔG: -1363.15790
Num. Imaginary Frequencies: 0

C	-2.483199	0.057390	0.032228
C	-2.750900	1.569130	0.254960
C	-3.940085	2.106294	-0.528237
C	-5.196804	1.317646	-0.134577
C	-5.002416	-0.199259	-0.252318
C	-3.744512	-0.706676	0.472560
C	-1.381770	2.229828	0.095181
H	-3.022211	1.662688	1.325811
H	-3.758355	2.029705	-1.615963
H	-4.084892	3.179731	-0.310169
H	-5.447855	1.564380	0.914712
H	-6.059942	1.633533	-0.746537
H	-4.950908	-0.479751	-1.319810
H	-5.888512	-0.717451	0.154530
H	-3.877117	-0.575623	1.563770
H	-3.641331	-1.789858	0.294276
C	-2.147797	-0.268323	-1.433350
C	-1.233569	-0.095769	0.941826
H	-1.328143	3.194411	0.625890
H	-1.170459	2.435513	-0.968557
C	-0.396278	1.181345	0.664435
C	-0.396201	-1.375029	0.941949
H	-1.605677	-0.033414	1.981098
H	0.095564	1.527701	1.588234
H	0.405463	0.968692	-0.058188
H	-2.010540	-1.354545	-1.563389
H	-2.949336	0.048156	-2.119798
H	-1.215390	0.216030	-1.765233
H	0.394400	-1.230528	1.698908
C	-1.143224	-2.659555	1.257788
O	0.258048	-1.541540	-0.347006
H	-0.426436	-3.482506	1.407542
H	-1.740705	-2.538833	2.176042
H	-1.818257	-2.932102	0.431934
S	1.800122	-1.976815	-0.431748
C	2.650400	-0.442860	-0.224567
O	2.117719	-2.851363	0.686154
O	1.964758	-2.442535	-1.793701
C	3.118629	-0.078755	1.035979
C	3.692194	1.179798	1.204008
C	3.802587	2.074685	0.132341
C	3.328967	1.674176	-1.127263
C	2.753980	0.423095	-1.315031
H	3.037932	-0.770793	1.877250
H	4.058592	1.471033	2.192579
C	4.442039	3.425446	0.313380
H	3.409211	2.358473	-1.976912
H	2.380940	0.122211	-2.296884
H	3.939067	4.190656	-0.300019
H	4.415828	3.745821	1.366936
H	5.500658	3.393560	-0.001406

Tosyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1363.04514
ΔU: -1363.02234
ΔH: -1363.02139
ΔG: -1363.09841
Num. Imaginary Frequencies: 1
Imaginary Frequency: -187.4086

C	-1.674521	0.700273	-0.020084
C	-2.988103	1.525660	-0.092245
C	-2.767035	2.985991	0.273165
C	-1.747912	3.593316	-0.703800
C	-0.449560	2.779968	-0.807195
C	-0.692221	1.284228	-1.053176
C	-4.014551	0.695348	0.668965
H	-3.305041	1.509226	-1.153681
H	-2.414144	3.075791	1.316191
H	-3.720717	3.538240	0.211556
H	-2.217312	3.643013	-1.704219
H	-1.515590	4.632300	-0.413979
H	0.148469	2.915827	0.111070
H	0.169781	3.178618	-1.628937
H	-1.119422	1.146821	-2.063978
H	0.257009	0.728925	-1.030427
C	-1.043702	0.684001	1.381180
C	-2.146649	-0.684760	-0.421436
H	-5.048017	1.027250	0.477580
H	-3.856763	0.733322	1.757979
C	-3.875003	-0.735114	0.150660
C	-2.341318	-1.760184	0.433857
H	-2.194806	-0.890513	-1.495242
H	-4.342226	-0.919403	-0.825570
H	-4.316682	-1.466401	0.847727
H	-0.259900	-0.088436	1.420535
H	-0.584670	1.652364	1.626065
H	-1.772306	0.467745	2.179297
O	0.438724	-2.437813	1.063805
H	-2.126792	-1.624477	1.496993
C	-2.542053	-3.161111	-0.033004
H	-3.248170	-3.706789	0.611424
H	-2.866166	-3.208343	-1.083743
H	-1.549326	-3.632400	0.056102
S	1.176650	-2.276017	-0.214567
O	2.110011	-3.383966	-0.490102
O	0.289100	-1.962978	-1.359953
C	2.201153	-0.816441	0.001790
C	2.707018	-0.161678	-1.123230
C	3.496171	0.973962	-0.967511
C	3.795638	1.480016	0.306633
C	3.291110	0.800746	1.421480
C	2.501359	-0.340651	1.275283
H	2.463012	-0.531000	-2.122894
H	3.882824	1.485210	-1.855079
C	4.611872	2.737724	0.461190
H	3.514810	1.172131	2.426666
H	2.101108	-0.855755	2.151827
H	5.039152	2.819422	1.473667
H	5.437575	2.772214	-0.268965
H	3.985064	3.631651	0.289971

MF Protonated

Naphthyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1477.66137
ΔU: -1477.63806
ΔH: -1477.63712
ΔG: -1477.71383
Num. Imaginary Frequencies: 0

C	-2.969436	-0.334938	-0.088530
C	-2.986655	-1.886048	-0.115358
C	-4.203971	-2.497055	0.563143
C	-5.473724	-1.975872	-0.124133
C	-5.510312	-0.445246	-0.215564
C	-4.230914	0.156973	-0.820324
C	-1.585308	-2.299170	0.335998
H	-3.065033	-2.158090	-1.186913
H	-4.215482	-2.251277	1.640730
H	-4.162679	-3.598731	0.493882
H	-5.512643	-2.395316	-1.147430
H	-6.374483	-2.340935	0.399508
H	-5.676789	-0.021615	0.791120
H	-6.377484	-0.132252	-0.822778
H	-4.161029	-0.133998	-1.885917
H	-4.308786	1.256453	-0.796312
C	-2.926342	0.229982	1.341708
C	-1.618382	-0.111977	-0.819482
H	-1.312066	-3.297164	-0.042179
H	-1.526647	-2.343409	1.436867
C	-0.668711	-1.184111	-0.222369
C	-0.985513	1.268679	-0.924619
H	-1.794209	-0.373194	-1.879337
H	0.030640	-1.554199	-0.989534
H	-0.054647	-0.756107	0.584514
H	-2.954803	1.332597	1.323080
H	-3.786006	-0.106864	1.941796
H	-2.012790	-0.063953	1.883682
H	-0.072058	1.159252	-1.530199
C	-1.843831	2.385440	-1.476913
O	-0.536414	1.690867	0.441922
H	-1.237924	3.280278	-1.688488
H	-2.302447	2.051703	-2.420903
H	-2.644271	2.655790	-0.772709
S	0.870050	2.246199	0.781829
C	2.092505	1.193044	0.129092
O	1.063086	3.530117	-0.102854
O	0.936024	2.455677	2.195914
C	2.531418	1.306336	-1.217325
C	3.414451	0.368617	-1.684879
C	3.882054	-0.689887	-0.855052
C	3.437584	-0.768922	0.499511
C	2.527679	0.201377	0.982547
H	2.193520	2.123141	-1.856695
H	3.773564	0.433864	-2.714884
C	4.787668	-1.671985	-1.336037
H	2.181111	0.146474	2.017623
C	5.223995	-2.679819	-0.508311
H	5.131065	-1.614653	-2.372304
H	5.919989	-3.432617	-0.887843
C	4.781962	-2.756049	0.837022
C	3.908138	-1.820337	1.334002
H	5.140785	-3.565392	1.477885
H	3.562005	-1.872203	2.369633
H	0.491089	4.285746	0.160219

Naphthyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1477.65133
ΔU: -1477.62716
ΔH: -1477.62622
ΔG: -1477.70511
Num. Imaginary Frequencies: 1
Imaginary Frequency: -131.7449

C	1.530285	-1.201724	-0.043657
C	2.435388	-2.460496	-0.224952
C	1.703768	-3.734089	0.174814
C	0.454258	-3.897219	-0.704411
C	-0.447499	-2.655593	-0.710521
C	0.322776	-1.359346	-0.992124
C	3.762443	-2.112622	0.440479
H	2.643671	-2.539291	-1.309521
H	1.432730	-3.705128	1.245148
H	2.372242	-4.601529	0.039645
H	0.785148	-4.102286	-1.739533
H	-0.125290	-4.777468	-0.379106
H	-0.982666	-2.572170	0.251920
H	-1.232254	-2.770192	-1.477364
H	0.688996	-1.371208	-2.034874
H	-0.351086	-0.495474	-0.900316
C	1.072985	-0.995186	1.410049
C	2.436018	-0.086030	-0.492361
H	4.554332	-2.828352	0.165459
H	3.695916	-2.110111	1.539438
C	4.177586	-0.744761	-0.081154
C	3.213337	0.710930	0.341055
H	2.468045	0.126383	-1.568386
H	4.505202	-0.742077	-1.129742
H	4.996430	-0.294289	0.503359
H	0.690301	0.028656	1.541700
H	0.266620	-1.692114	1.677908
H	1.881019	-1.146305	2.142859
O	0.723387	2.624647	1.360318
H	3.059899	0.623613	1.421173
C	3.898219	1.960569	-0.123386
H	4.803519	2.158485	0.470030
H	4.153758	1.917946	-1.193663
H	3.188565	2.789563	0.030586
S	0.068942	2.959239	0.109319
O	-0.619970	4.383878	0.390137
O	0.844392	3.048645	-1.116740
C	-1.278152	1.846174	-0.159939
C	-1.778879	1.677896	-1.475958
C	-2.734894	0.720685	-1.701989
C	-3.205299	-0.112457	-0.647319
C	-2.703737	0.085264	0.673110
C	-1.735822	1.097752	0.897687
H	-1.387178	2.282882	-2.296077
H	-3.125102	0.568735	-2.711871
C	-4.141056	-1.157634	-0.875620
H	-1.332035	1.245321	1.901968
C	-4.548227	-1.967682	0.157936
H	-4.525905	-1.312157	-1.887507
H	-5.263362	-2.773307	-0.029262
C	-4.047022	-1.770660	1.469945
C	-3.147240	-0.764046	1.724278
H	-4.380114	-2.425733	2.279266
H	-2.753759	-0.608778	2.732754
H	-0.848598	4.842859	-0.440586

Tosyl-Hydrindane
SCF Energy:
ZPE-corrected Energy: -1363.48230
ΔU: -1363.45953
ΔH: -1363.45859
ΔG: -1363.53512
Num. Imaginary Frequencies: 0

C	2.447751	0.068146	-0.014434
C	2.710904	1.463853	-0.638831
C	3.681273	2.320883	0.160746
C	5.016994	1.575623	0.290239
C	4.848294	0.151026	0.832975
C	3.796280	-0.668834	0.067266
C	1.321112	2.007231	-0.970380
H	3.208679	1.261142	-1.608226
H	3.266987	2.554020	1.158638
H	3.837324	3.289334	-0.347170
H	5.484466	1.522715	-0.711402
H	5.714399	2.140778	0.932942
H	4.574208	0.196166	1.902287
H	5.816771	-0.377161	0.790944
H	4.161023	-0.858010	-0.960403
H	3.689085	-1.653491	0.551793
C	1.803802	0.162622	1.379271
C	1.436095	-0.464676	-1.064562
H	1.356835	2.761364	-1.772742
H	0.870661	2.494768	-0.088784
C	0.518871	0.748708	-1.377831
C	0.677021	-1.766552	-0.855706
H	2.023530	-0.680190	-1.976171
H	0.241608	0.754965	-2.444030
H	-0.422440	0.693244	-0.809808
H	1.661924	-0.842329	1.811051
H	2.429567	0.733954	2.082480
H	0.816107	0.651425	1.351508
H	0.038309	-1.931342	-1.737007
C	1.486301	-3.011152	-0.566126
O	-0.267909	-1.608934	0.303648
H	0.840657	-3.903458	-0.592439
H	2.267881	-3.122470	-1.334397
H	1.967981	-2.951327	0.421010
S	-1.791976	-1.880034	0.186570
C	-2.599768	-0.347432	0.214551
O	-2.155599	-2.722349	-0.917349
O	-2.109197	-2.445015	1.611670
C	-3.394019	-0.014204	-0.882100
C	-3.956750	1.257703	-0.920482
C	-3.728647	2.182917	0.105708
C	-2.920011	1.806285	1.194318
C	-2.347048	0.547384	1.262671
H	-3.565955	-0.727559	-1.690556
H	-4.582493	1.533853	-1.772762
C	-4.340501	3.554640	0.065601
H	-2.734603	2.518970	2.002155
H	-1.715997	0.269588	2.109933
H	-3.577417	4.328315	0.252774
H	-4.818146	3.757589	-0.904891
H	-5.106724	3.652159	0.854609
H	-1.558705	-3.221077	1.862442

Tosyl-TS_expansion
SCF Energy:
ZPE-corrected Energy: -1363.46742
ΔU: -1363.44380
ΔH: -1363.44286
ΔG: -1363.52171
Num. Imaginary Frequencies: 1
Imaginary Frequency: -92.5157

C	-1.753313	0.643126	-0.017983
C	-3.112698	1.395899	-0.076252
C	-2.968757	2.866080	0.287496
C	-1.994114	3.528356	-0.698943
C	-0.653441	2.789351	-0.814276
C	-0.815797	1.282892	-1.061066
C	-4.085937	0.509610	0.691860
H	-3.436887	1.362974	-1.134638
H	-2.614932	2.977627	1.327870
H	-3.952778	3.362350	0.231873
H	-2.474472	3.552147	-1.694900
H	-1.816486	4.578131	-0.410427
H	-0.055159	2.956284	0.098465
H	-0.064630	3.220510	-1.641555
H	-1.240896	1.121760	-2.068763
H	0.168340	0.790268	-1.046048
C	-1.109554	0.663896	1.377433
C	-2.153339	-0.762394	-0.420587
H	-5.136488	0.790989	0.513510
H	-3.919447	0.545284	1.779576
C	-3.887098	-0.906068	0.157917
C	-2.321540	-1.843434	0.435464
H	-2.193792	-0.967742	-1.496247
H	-4.332909	-1.096758	-0.827221
H	-4.305059	-1.667000	0.838154
H	-0.258719	-0.034887	1.411226
H	-0.727879	1.663876	1.626349
H	-1.806652	0.381237	2.181993
O	0.662396	-2.468552	1.074719
H	-2.113987	-1.699851	1.500295
C	-2.448625	-3.255760	-0.032165
H	-3.118987	-3.836137	0.619529
H	-2.784526	-3.319433	-1.078393
H	-1.437982	-3.691388	0.040633
S	1.301998	-2.146322	-0.187646
O	2.380179	-3.320798	-0.390020
O	0.502359	-2.037691	-1.398043
C	2.263620	-0.679493	0.000297
C	2.635930	0.043753	-1.134399
C	3.352932	1.223484	-0.973072
C	3.698436	1.694330	0.302597
C	3.318753	0.939532	1.420919
C	2.604437	-0.246626	1.281198
H	2.353859	-0.300305	-2.132303
H	3.643228	1.796123	-1.858482
C	4.430572	2.999047	0.463728
H	3.582070	1.287539	2.423711
H	2.302003	-0.821330	2.159293
H	5.137373	3.166499	-0.364894
H	4.985409	3.035151	1.414570
H	3.713250	3.839538	0.462318
H	2.712890	-3.349460	-1.307397