Supporting Information

Alder–Ene Reactions Driven by High Steric Strain and Bond Angle Distortion to Form Benzocyclobutenes

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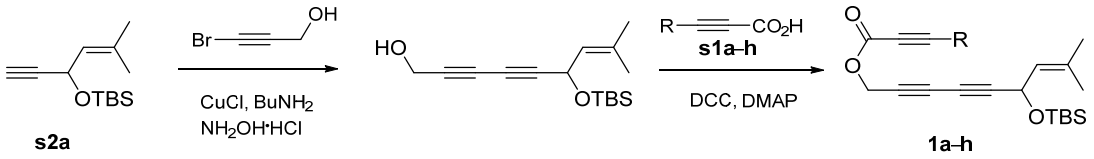
Table of Contents

Materials and Methods

Reactions were carried out in oven-dried glassware unless otherwise noted. Compounds were purchased from Aldrich, Acros, TCI America or Oakwood unless otherwise noted. Toluene, dichloromethane, triethylamine and acetonitrile were distilled over calcium hydride (CaH_2) under nitrogen. Tetrahydrofuran was dried over sodiumbenzophenone ketyl. Column chromatography was performed using silica gel 60 Å (32–63 mesh) purchased from Silicycle Inc. Analytical thin layer chromatography (TLC) was performed on 0.25 mm E. Merck precoated silica gel 60 (particle size 0.040–0.063 mm). Yields refer to chromatographically and spectroscopically pure isolated compounds unless otherwise stated. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AV–500 spectrometer. ^{1}H NMR chemical shifts (δ) are reported in parts per million (ppm) downfield of TMS and are referenced relative to the residual proteated solvent peak ($CDCl_3$ (7.26 ppm)). ^{13}C chemical shifts (δ) are reported in parts per million downfield of TMS and are referenced to the carbon resonance of the solvent ($CDCl_3$ (77.2 ppm)). Multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), quin (quintet), sext (sextet) or m (multiplet). ^{1}H NMR signals that fall within a ca. 0.3 ppm range are generally reported as a multiplet, with a range of chemical shift values corresponding to the peak or center of the peak. Coupling constants, *J*, are reported in Hz (Hertz). Electrospray ionization (ESI) and Electron impact (EI) mass spectra were recorded on a Waters Micromass Q-Tof Ultima and Micromass 70–VSE, respectively in the University of Illinois at Urbana-Champaign.

Experimental Details

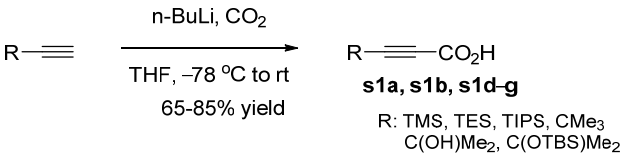
Preparation of triyne 1a–h[1]



In a schlenk flask containing CuCl (80.5 mg, 0.81 mmol) was added 10ml (30% aqueous $BuNH_2$ solution) under nitrogen flow. A pinch of $NH_2OH{\cdot}HCl$ was added until the blue color disappeared. Alkyne **s2a** (700 mg, 3.1 mmol) in CH_2Cl_2 was added at 0 °C to the flask and the solution became yellow. A solution of propargyl alcohol bromide (505 mg, 3.7 mmol) in CH_2Cl_2 was added dropwise at 0 °C. The reaction mixture was stirred for 15 min at room temperature. The nitrogen flow was removed, and the biphasic reaction mixture was transferred to a separatory funnel. Dichloromethane layer was separated and dried over anhydrous Na_2SO_4. After filtration, the organic layer was concentrated, and the crude material was purified by column chromatography (SiO_2, hexanes–EtOAc, 5:1) to obtain the diyne (713 mg, 82%) as yellow oil. The diyne (116 mg, 0.5 mmol) was dissolved in CH_2Cl_2 and cooled to 0 °C. The corresponding carboxylic acid (0.6 mmol), DCC (0.75 mmol) and DMAP (0.05 mmol) was added and the mixture was stirred for 1 h at 0 °C. The precipitate was filtered over a short pad of silica, concentrated

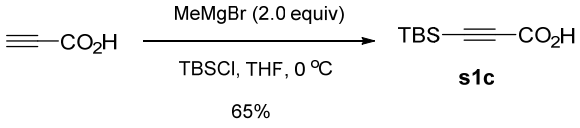
and purified by column chromatography (SiO_2, hexanes–EtOAc, 5:1) to obtain the triyne **1a–h** (65–88% yield) as colorless oil.

Preparation of carboxylic acids s1a, s1b, s1d–g



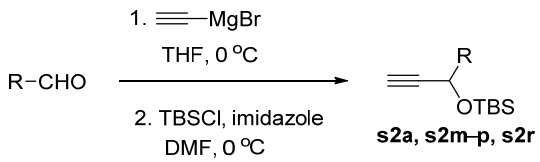
Alkyne (5.0–6.0 mmol) was dissolved in anhydrous THF under N_2 and cooled to –78 °C and *n*-BuLi (2.5 M in hexanes) (1.2 equiv) was added dropwise. The mixture was stirred at –78 °C for 45 min. CO_2 generated from dry ice was dried by passing through a tube containing drierite was bubbled into the reaction mixture for 30 minutes at –78 °C. The reaction was stirred at the same temp for another 30 min and then slowly warmed to room temperature. The reaction was quenched by adding 30 mL 1.0 M HCl. Ethyl acetate (30 mL) was added and the mixture transferred to a separatory funnel. The organic layer was washed with 30 mL water (x1) and 30 mL brine (x2), dried over anhydrous Na_2SO_4, filtered and concentrated. The carboxylic acid was used directly without further purification. In case of alkyne with free alcohol 2.2 equiv of *n*-BuLi was used.

Preparation of carboxylic acid s1c



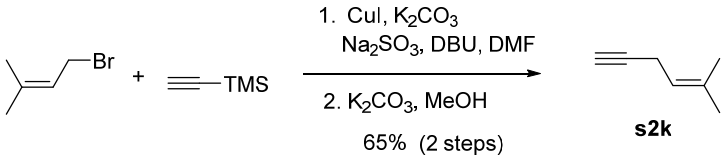
Propiolic acid (500 mg, 7.1 mmol) was dissolved in anhydrous THF under N_2 and cooled to 0 °C. MeMgBr (3.0M in Et_2O) (5.41 mL, 2.2 equiv) was added dropwise and white precipitate was formed due to formation of carboxylate salts. The mixture was stirred at 0 °C for 30 min followed by addition of TBSCl (1.2 g, 1.2 equiv). The mixture was stirred at 0 °C for another 30 min and slowly warmed to room temp. 1.0 M HCl (10 mL) was added to quench the reaction. Ethyl acetate (30 mL) was added and the mixture was transferred to a separatory funnel. The organic layer was washed with 15 ml water (x1) and 15 ml brine (x2), dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (SiO_2, hexanes–EtOAc, 3:1) to obtain the carboxylic acid **s1c** (850 mg, 65%) as a white solid.

Preparation of alkyne s2a, s2m-p, s2u



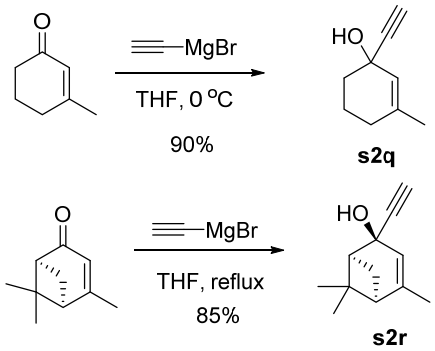
Commercially available aldehydes (prenal, tiglic aldehyde, crotonaldehyde) were used directly for synthesizing **s2a**, **s2m**, and **s2n**. Geranial, neral and but-2-ynal were obtained by oxidation of their corresponding alcohols using MnO_2 and used for synthesizing **s2o**, **s2p**, and **s2u**. The aldehyde (2.0–5.0 mmol) was dissolved in dry THF under N_2 and cooled to 0 °C. Ethynyl magnesium bromide (0.5 M in THF) (1.1 equiv) was added dropwise and stirred for 30 min. The reaction was quenched with NH_4Cl and extracted with EtOAc. The organic layer was washed with water (x1) followed by brine (x1), dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (SiO_2, hexanes–EtOAc, 5:1) to obtain the propargyl alcohols as colorless oils. The propargyl alcohols (2.0–5.0 mmol) was dissolved in DMF (0.5 mL/mmol) and cooled to 0 °C. TBSCl (1.2 equiv) and imidazole (1.4 equiv) was added and the reaction was stirred for 30 min. The reaction mixture was diluted with hexanes and filtered over silica, concentrated and the alkyne obtained was used for subsequent steps without further purification.

Preparation of alkyne s2k



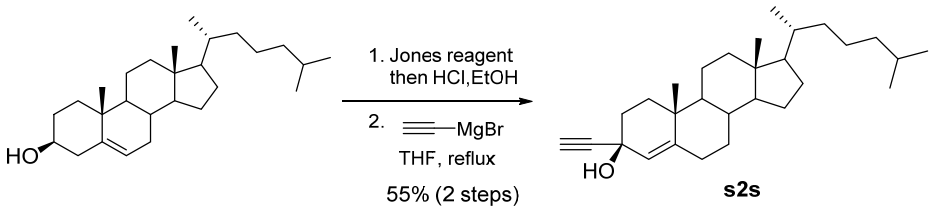
The alkyne **s2k** was synthesized by following literature procedures.[2]

Preparation of alkyne s2q, s2r



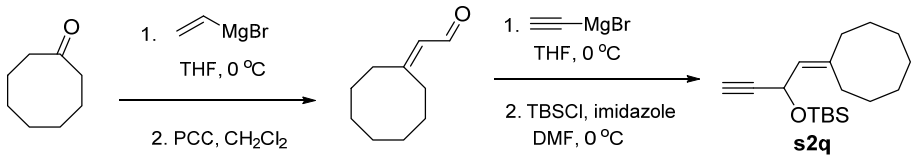
The alkyne **s2q** and **s2r** were prepared by following typical procedure of adding ethynyl magnesium bromide as described above. For **s2r**, reaction conditions involved refluxing under THF for 14 h.

Preparation of alkyne s2s



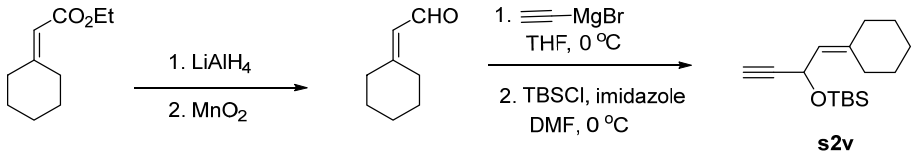
Cholesterol (1.0 g, 2.5mmol) was dissolved in acetone (50 mL) and cooled to 0 °C followed by dropwise addition of Jones reagent (2.7 M) (1.5 mL, 3 mmol). After stirring for 30 min the reaction was quenched by adding 10 mL EtOH and 1 N HCl (10 mL) was added and the mixture was heated at 50 °C for 15 min. The reaction was cooled and solvent was removed under reduced pressure. The residue was diluted with EtOAc and washed with satd. $NaHCO_3$ (x1) followed by brine (x1). The organic layer was dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (SiO_2, hexanes–EtOAc, 10:1) to give pure 4-cholestan-3-one (750 mg, 74%), which was further converted to **s2s** following method described above. The reaction required 14 h under refluxing THF for complete conversion.

Preparation of alkyne s2t



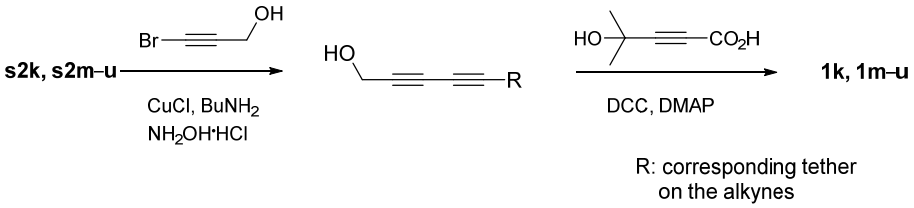
After the preparation of the enal following literature proceudures,[3] the enal was converted to **s2t** by the typical procedure described above.

Preparation of alkyne s2v



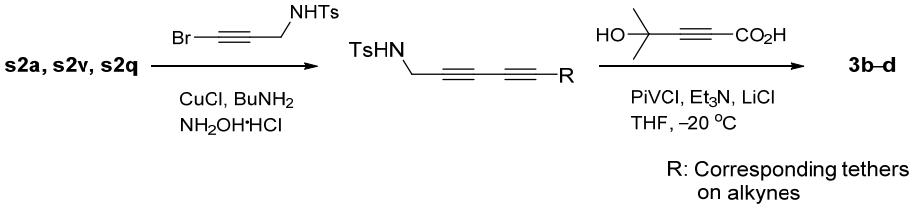
After the preparation of the enal from cyclohexanone (3 steps) following literature proceudures,[4] the enal was converted to **s2v** by the typical procedure described above.

Preparation of triyne 1k, 1m–u



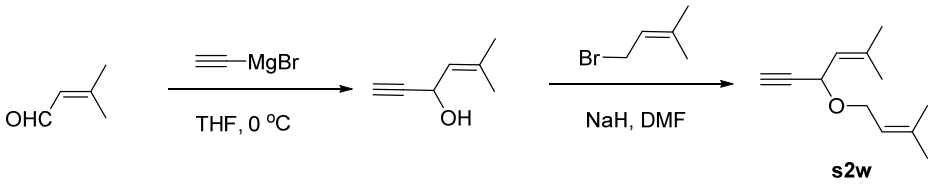
The triynes **1k** and **1m–u** was prepared from the respective alkynes **s2k** and **s2m-u** following the method described above for preparation of related triynes **1a–h**.

Preparation of imide-tethered triyne 3b–d[5]



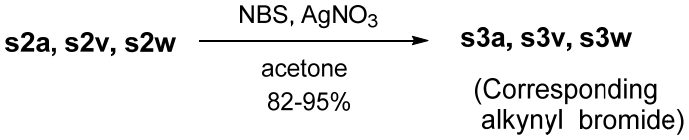
The corresponding diynes were prepared by following typical procedure for a Cadiot–Chodkiewicz coupling described above. The carboxylic acid (1.2 equiv) was dissolved in THF under N_2 and cooled to –20 °C. To it was added pivaloyl chloride (1.4 equiv) followed by Et_3N (2.5 equiv) and, the mixture was stirred for 2 h at –20 °C. To this solution, LiCl (1.5 equiv) and the diyne (0.5–1.5 mmol) were added. The reaction mixture was allowed to warm to room temp and stirred for another 15 min. The mixture was concentrated, and the residue was directly purified through column chromatography. For **3b** and **3c**(SiO_2, hexanes–EtOAc, 5:1) and for **3d** (SiO_2, hexanes–EtOAc, 2:1) was used as eluting solvent in column chromatography.

Preparation of alkyne s2w



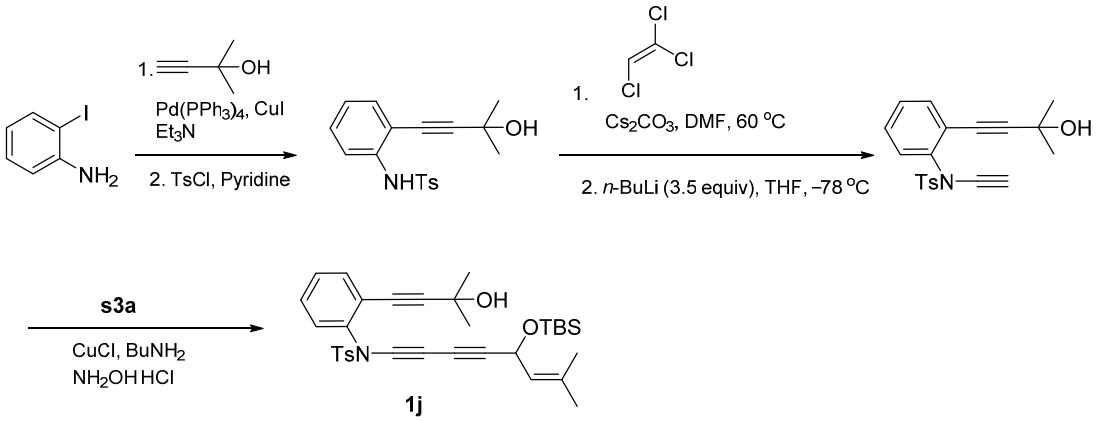
The alkyne **s2w** was prepared by adding ethynyl magnesium bromide as described above followed by a typical Williamson's ether synthesis.

Preparation of alkynyl bromide s3a, s3v and s3w



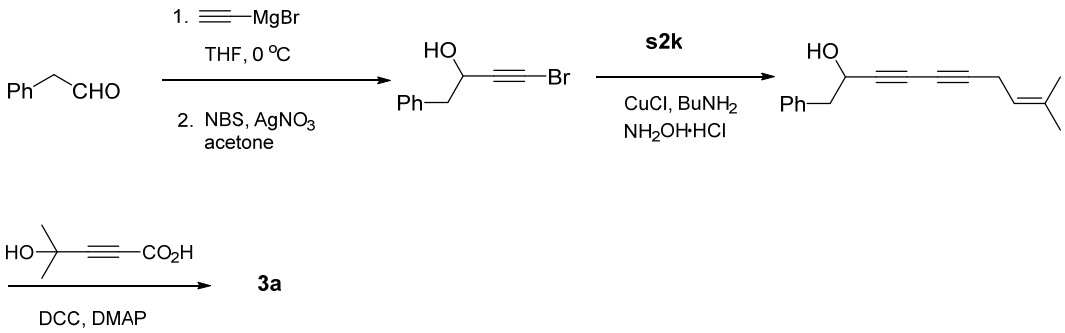
To an acetone solution of alkynes **s2a**, **s2v** and **s2w** (0.5–1.0 mmol) was added $AgNO_3$ (0.1 equiv) followed by *N*-bromosuccinimide (1.4 equiv) under N_2. The reaction was stirred under dark in a round bottom flask covered with aluminium foil for 2 h. After completion the acetone was removed under reduced pressure. The residue was dissolved in hexanes filtered over silica and concentrated obtaining the corresponding alkynyl bromides **s3a**, **s3v** and **s3w** were obtained as colorless oil (82–95% yield), which were directly used without further purification.

Preparation of triyne 1j



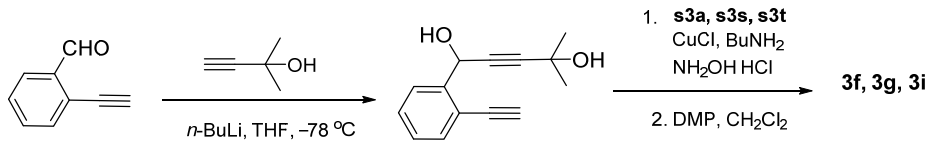
The triyne **1j** was synthesized by following literature procedure for related compounds.[6]

Preparation of triyne 3a



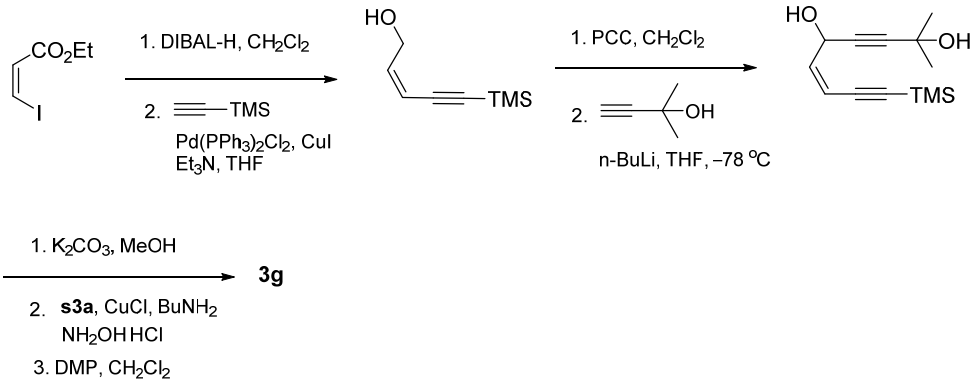
The triyne **3a** was synthesized by following the procedure

Preparation of benzene-tethered triyne 3f, 3g, 3i[7]



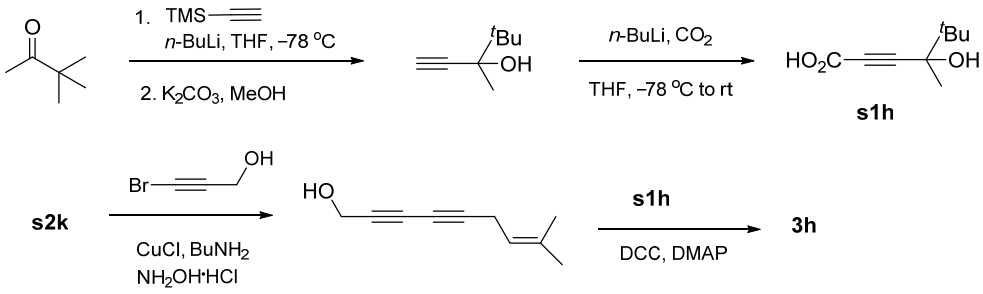
The benzene tethered triynes **3f**, **3g**, and **3i** were synthesized by following literature procedures involving alkynyl anion addition to the aldehyde followed by typical coupling with alkynyl bromides **s3a**, **s3s**, and **s3t** respectively and oxidation using DMP. Oxidation with MnO_2 was also tried but gave significantly low yield.

Preparation of Enone-tethered triyne 3g[7]



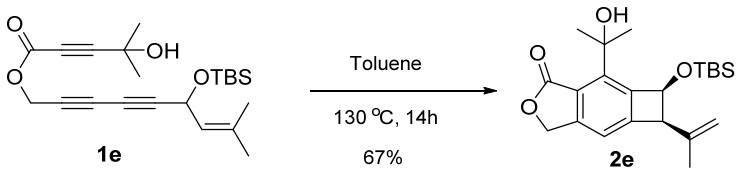
The triyne **3g** was prepared following literature procedure starting from the vinylic iodide involving the reduction to alcohol using DIBAL-H, a Sonogashira coupling, oxidation to aldehyde, alkynyl anion addition, TMS-deprotection, coupling of alkynyl bromide and DMP oxidation.

Preparation of 3h



The triyne **3h** was prepared starting from pinacolone following standard reaction condition described above for synthesizing related triynes.

Preparation of 2e (1.0 mmol scale) via intramolecular Alder-Ene reaction



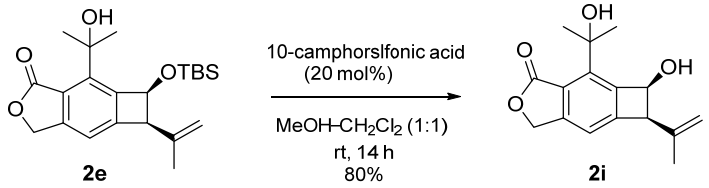
1e 2e

A toluene solution (0.05 M) of the triyne (400 mg, 1.0 mmol) was heated in a Schlenk tube at 130 °C for 14 h. After completion, the reaction was cooled to room temperature and toluene was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, hexanes–EtOAc, 6:1) to obtain **2e** (268 mg, 67% yield) as white solid with complete *cis*-diastereoselectivity.

General procedure for Alder-Ene reactions to generate benzocyclobutenes

A toluene solution (0.05 M) of the triyne (0.1–0.3 mmol) was heated in a Schlenk tube at 130 °C for ester-tethered and 90 °C for imide, benzene and enone tether for 14 h. After completion, the reaction was cooled to room temperature and the solvent was removed under reduced pressure. The residue was then purified by column chromatography. The yield, solvent system used for purification, and physical property of the isolated compounds are given in the characterization data.

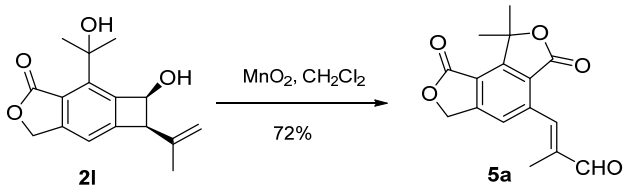
TBS-deprotection with 2e



2e 2i

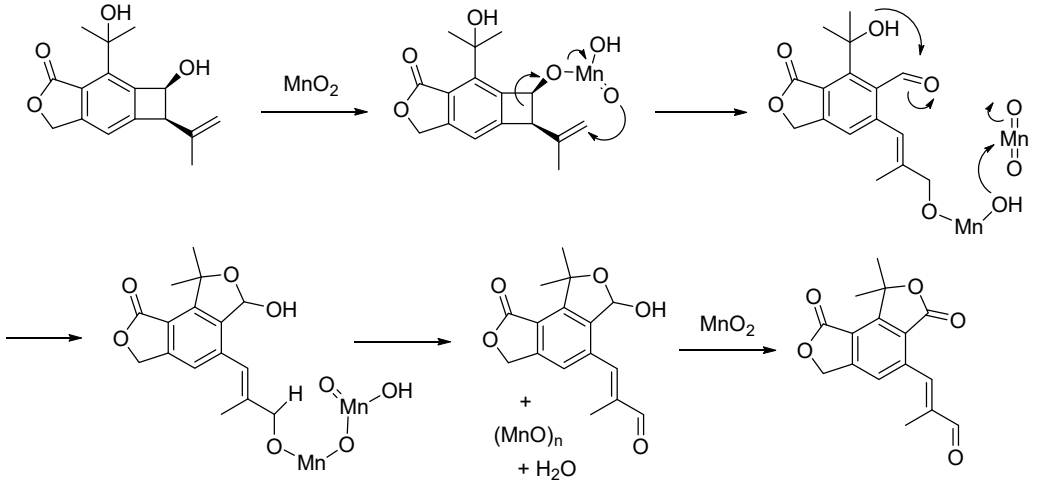
Benzocyclobutene **2e** (230 mg, 0.6 mmol) was dissolved in MeOH–CH_2Cl_2 (1:1), and 10-camphorsulfonic acid (30 mg, 0.12 mmol) was added, and the mixture was stirred at rt for 14 h. The solvent was removed under reduced pressure, and the residue was directly purified by flash column chromatography (hexanes–EtOAc, 2:1) to give compound **2i** (130 mg, 80 %) as white solid.

MnO_2-mediated ring cleavage and allylic oxidation of 2l

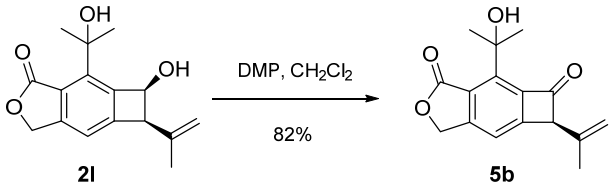


Benzocyclobutenol **2l** (30 mg, 0.1 mmol) was dissolved in CH_2Cl_2, and MnO_2 (48 mg, 0.5 mmol) was added and stirred for 15 min. The mixture was filtered over a short pad of celite, concentrated and the residue was purified by column chromatography (SiO_2, hexanes–EtOAc, 5:1 → 2:1) to afford **5a** (22 mg, 72%) as white solid.

Proposed Mechanism for MnO_2-mediated oxidation to generate 5a

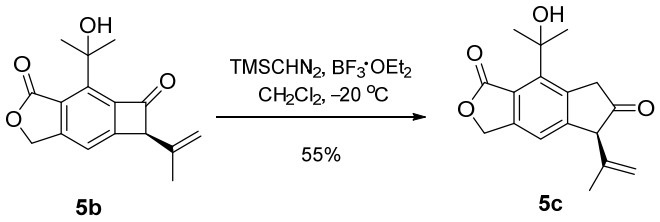


DMP oxidation of 2l



Benzocyclobutenol **2l** (65 mg, 0.2 mmol) was dissolved in CH_2Cl_2 and DMP (110 mg, 0.25 mmol) was added and stirred at room temp for 3 h. After completion, $Na_2S_2O_3$ solution (1 mL), saturated $NaHCO_3$ (1 mL) and water (1 mL) were added, and the mixture was stirred vigorously until two distinct layers were formed. The mixture was diluted with CH_2Cl_2 and organic layer was separated and washed with water (x1) and brine (x1), dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (SiO_2, hexanes–EtOAc, 5:1 → 2:1) to give ketone **5b** (53 mg, 82%) as white solid.

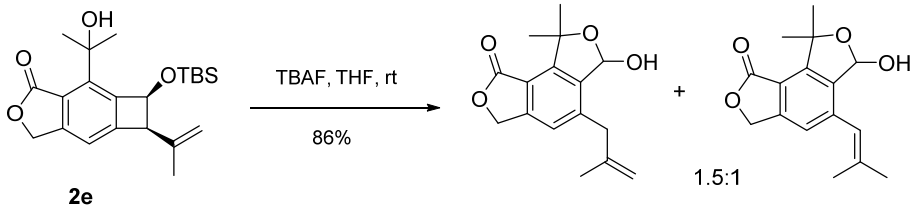
One-carbon homologation of 5b



5b **5c**

Benzocyclobutenone **5b** (20 mg, 0.06 mmol) was dissolved in dry CH_2Cl_2 under N_2 and cooled –20 °C. $TMSCHN_2$ (2.0 M in hexanes, 0.04 mL, 0.07 mmol) and $BF_3.OEt_2$ (0.01 ml) were added dropwise. The mixture was stirred at –20 °C for 20 min. After completion, the reaction was quenched with saturated NH_4Cl and extracted with CH_2Cl_2. The organic layer was washed with water (x1) and brine (x1), dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (SiO_2, hexanes–EtOAc, 5:1 → 3:1) to give ketone **5c** (12 mg, 55%) as colorless oil.

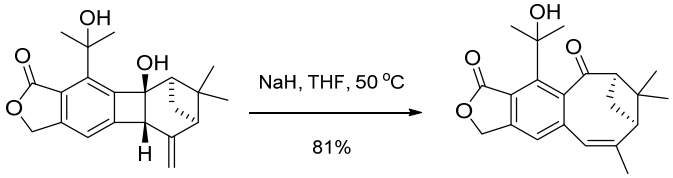
TBAF-induced ring cleavage of 2e



2e **5d**

To a THF solution of **2e** (60 mg, 0.15 mmol) was added TBAF (1.0 M in THF) (0.18 ml) and the mixture was stirred for 20 min at room temperature. The reaction was quenched with satd. NH_4Cl and extracted with EtOAc. The organic layer was washed with water (x1) and brine (x1), dried over anhydrous Na_2SO_4, filtered, concentrated and purified by column chromatography (gradient elution, hexanes–EtOAc, 5:1 to 3:1) to give a mixture of isomeric alkenes **5d** (35 mg, 86%) as colorless oil.

Ring expansion of 2r



2r **5e**

To a THF solution of **2r** (30 mg, 0.10 mmol) was added NaH (60% in mineral oil, 3 mg, 0.12 mmol) under N_2 and the mixture was stirred for 30 min at 50 °C. The reaction was filtered over a short pad of celite,

concentrated and purified by column chromatography (hexanes–EtOAc, 4:1) to give a mixture of isomeric alkenes **5e** (35 mg, 81%) as colorless oil.

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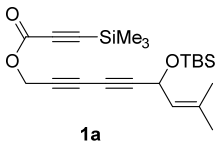
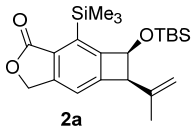
7 T. R. Hoye, B. Baire, D. Niu, D, P. H. Willoughby, B. P. Woods, *Nature*, **2012**, *490*, 208–212.

Characterization Data



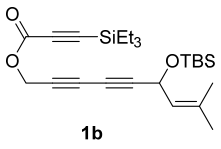
1a

1a: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.27 (d, *J* = 8.2 Hz, 1H), 5.08 (d, *J* = 8.2 Hz, 1H), 4.81 (s, 2H), 1.72 (s, 3H), 1.67 (s, 3H), 0.89 (s, 9H), 0.25 (s, 9H), 0.12 (s, 3H), 0.10 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 151.9, 135.3, 124.6, 95.9, 93.5, 81.4, 71.8, 71.7, 67.4, 60.4, 53.6, 25.7, 18.2, –0.95, –4.5, –4.7; **HRMS** (ESI) calcd for $C_{22}H_{34}O_3NaSi$ $[M+Na]^+$ 425.1944, found 425.1964.



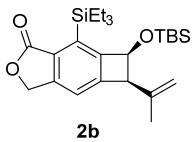
2a

2a: white solid; 25 mg (45% yield, 10:1 *dr*); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 50:1 → 20:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.17 (s, 1H), 5.29–5.21 (m, 2H), 5.19 (s, 1H), 4.94 (s, 1H), 4.89 (s, 1H), 3.80 (s, 1H), 1.77 (s, 3H), 0.91 (s, 9H), 0.43 (s, 9H), 0.17 (s, 3H), 0.12 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 153.9, 150.6, 147.9, 142.7, 138.8, 129.6, 119.9, 117.3, 112.8, 76.3, 69.4, 59.7, 25.9, 20.7, 17.9, –0.28, –3.4, –4.75; **HRMS** (ESI) calcd for $C_{22}H_{34}O_3NaSi$ $[M+Na]^+$ 425.1944, found 425.1945.



1b

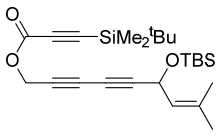
1b: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.27 (d, *J* = 8.1 Hz, 1H), 5.08 (d, *J* = 8.1 Hz, 1H), 4.81 (s, 2H), 1.72 (s, 3H), 1.66 (s, 3H), 1.01 (t, *J* = 8.0 Hz, 9H), 0.88 (s, 9H), 0.67 (q, *J* = 8.0 Hz, 6H), 0.11 (s, 3H), 0.09 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 151.9, 135.2, 124.6, 94.7, 94.1, 81.3, 71.8, 71.7, 67.4, 60.3, 53.6, 25.7, 25.5, 18.2, 7.2, 3.7, –4.5, –4.6; **HRMS** (ESI) calcd for $C_{25}H_{40}O_3NaSi_2$ $[M+Na]^+$ 467.2414, found 467.2403.



2b

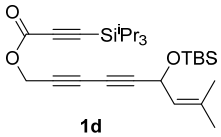
2b: white solid; 32 mg (48% yield, 7:1 *dr*); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 50:1 → 20:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.16 (s, 1H), 5.28–5.19 (m, 2H), 5.17 (s, 1H), 4.95 (s, 1H), 4.91 (s, 1H), 3.79 (s, 1H), 1.70 (s, 3H), 1.11–0.91 (m, 6H), 0.94–0.86 (m, 18H), 0.20 (s, 3H), 0.15 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 171.9,

155.2, 150.7, 148.1, 142.6, 136.8, 129.9, 123.5, 119.9, 117.1, 113.1, 76.1, 68.4, 59.8, 25.8, 7.6, 3.0, –3.5, –5.1; **HRMS** (ESI) calcd for $C_{25}H_{40}O_3NaSi_2$ $[M+Na]^+$ 467.2414, found 467.2398.



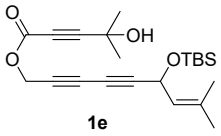
1c

1c: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.26 (dt, *J* = 1.5, 8.5 Hz, 1H), 5.08 (d, *J* = 8.0 Hz, 1H), 4.80 (s, 2H), 1.72 (s, 3H), 1.68 (s, 3H), 0.96 (s, 9H), 0.88 (s, 9H), 0.18 (s, 6H), 0.11 (s, 3H), 0.09 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 151.8, 135.2, 124.6, 94.6, 94.3, 81.3, 71.8, 67.4, 60.4, 53.6, 25.9, 25.7, 25.5, 18.2, 16.5, –4.5, –4.7, –5.3; **HRMS** (ESI) calcd for $C_{25}H_{40}O_3NaSi_2$ $[M+Na]^+$ 467.2414, found 467.2415.



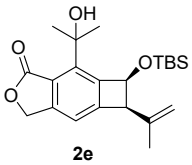
1d

1d: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.27 (d, *J* = 7.5 Hz, 1H), 5.08 (d, *J* = 8.0 Hz, 1H), 4.81 (s, 2H), 1.72 (s, 3H), 1.66 (s, 3H), 1.34–1.26 (m, 3H), 1.10 (s, 18H), 0.88 (s, 9H), 0.11 (s, 3H), 0.10 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 151.9, 135.2, 124.6, 95.6, 93.3, 81.3, 71.9, 71.7, 67.5, 60.4, 53.5, 25.7, 25.5, 18.4, 10.9, –4.7, –4.5; **HRMS** (ESI) calcd for $C_{28}H_{46}O_3NaSi_2$ $[M+Na]^+$ 509.2883, found 509.2891.



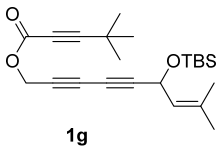
1e

1e: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.26 (d, *J* = 8.4 Hz, 1H), 5.08 (d, *J* = 7.1 Hz, 1H), 4.81 (s, 2H), 2.5 (br s, 1H, OH), 1.71 (s, 3H), 1.65 (s, 3H), 1.55 (s, 6H), 0.87 (s, 9H), 0.10 (s, 3H), 0.09 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.5, 135.3, 124.6, 92.7, 81.4, 73.2, 71.9, 71.7, 67.4, 64.9, 60.3, 53.7, 30.4, 25.7, 25.5, 18.2, –4.7, –4.5; **HRMS** (ESI) calcd for $C_{22}H_{33}O_4Si$ $[M+H]^+$ 389.2148, found 389.2132.



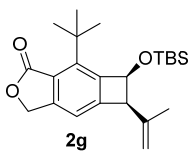
2e

2e: white solid; 268 mg (67% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 6:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7. 10 (s, 1H), 6.14 (s, 1H, OH), 5.36–5.24 (m, 2H), 5.22 (s, 1H), 4.96 (s, 1H), 4.90 (s, 1H), 3.78 (s, 1H), 1.79 (s, 3H), 1.71 (s, 3H), 1.67 (s, 3H), 0.91 (s, 9H), 0.18 (s, 3H), 0.14 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 173.5, 152.9, 150.5, 148.3, 143.3, 141.9, 121.4, 115.7, 113.7, 75.5, 72.3, 70.1, 59.9, 30.9, 28.5, 25.8, 20.3, 17.8, –3.7, –5.3; **HRMS** (ESI) calcd for $C_{22}H_{33}O_4Si$ $[M+H]^+$ 389.2148, found 389.2158.



1g

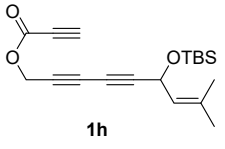
1g: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.26 (d, *J* = 8.7 Hz, 1H), 5.08 (d, *J* = 8.1 Hz, 1H), 4.79 (s, 2H), 2.5 (br s, 1H, OH), 1.71 (s, 3H), 1.65 (s, 3H), 1.28 (s, 9H), 0.88 (s, 9H), 0.11 (s, 3H), 0.09 (s, 3H) **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.9, 135.2, 124.7, 98.3, 81.2, 72.0, 71.6, 67.5, 60.4, 53.4, 30.0, 29.8, 27.6, 25.8, 25.5, 18.2, -4.5, -4.7; **HRMS** (ESI) calcd for $C_{23}H_{34}O_3NaSi$ $[M+Na]^+$ 409.2175, found 409.2187.



2g
dr: 5:1

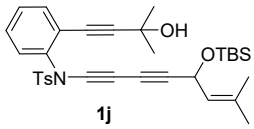
2g: colorless oil; 22 mg (49% yield, 5:1 dr); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 20:1 → 10:1); **^{1}H NMR** ($CDCl_3$, 500 MHz) (for major diasteomer): δ 7. 02 (s, 1H), 5.22 (s, 1H), 5.20–5.17 (m, 2H), 4.95 (s, 1H), 4.90 (s, 1H), 3.75 (s, 1H), 1.73 (s, 3H), 1.59 (s, 9H), 0.92 (s, 9H), 0.15 (s, 3H), 0.13 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz) (all

discernable signals for both : δ 170.6, 152.7, 151.0, 150.8, 144.6, 142.5, 122.5, 116.5, 114.8, 114.5, 113.1, 76.6, 75.9, 68.3, 68.2, 59.4, 56.3, 36.3, 30.6, 30.2, 25.9, 25.8, 20.4, 17.9, –3.7, –5.1; **HRMS** (ESI) calcd for $C_{23}H_{35}O_3Si$ $[M+H]^+$ 387.2355, found 387.2354.



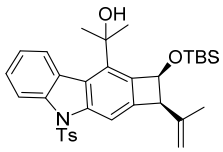
1h

1h: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.27 (dt, *J* = 1.6, 8.3 Hz, 1H), 5.09 (d, *J* = 8.5 Hz, 1H), 4.84 (s, 2H), 2.95 (s, 1H), 1.72 (s, 3H), 1.67 (s, 3H), 0.89 (s, 9H), 0.12 (s, 3H), 0.10 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 151.8, 135.3, 124.6, 81.5, 76.1, 73.8, 72.1, 71.4, 67.4, 60.4, 53.9, 25.8, 25.4, 18.2, –4.5, –4.7; **HRMS** (ESI) calcd for $C_{19}H_{26}O_3NaSi$ $[M+Na]^+$ 353.1549, found 353.1554.



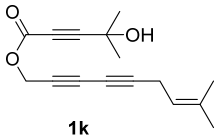
1j

1j: yellow oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.68 (d, *J* = 8.1 Hz, 2H), 7.43–7.38 (m, 1H), 7.35–7.28 (m, 2H), 7.27–7.23 (m, 1H), 5.26 (d, *J* = 8.1 Hz, 1H), 5.11 (d, *J* = 9.22 Hz, 1H), 2.45 (s, 1H), 2.04 (br s, 1H, OH), 1.70 (s, 3H), 1.64 (s, 3H), 1.47 (s, 6H), 0.88 (s, 9H), 0.10 (s, 3H), 0.08 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 145.3, 138.2, 134.5, 134.4, 133.4, 129.9, 129.2, 128.9, 128.4, 125.1, 122.4, 100.7, 84.1, 77.4, 70.5, 68.1, 60.7, 58.3, 30.9, 25.8, 25.5, 21.7, 18.2, -4.4, -4.6; **HRMS** (ESI) calcd for $C_{33}H_{41}NO_4NaSSi$ $[M+Na]^+$ 598.2423, found 598.2411.



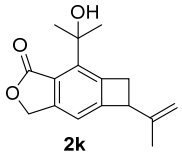
2j
dr 5:1

2j: yellow solid; 11 mg (28% yield, 5:1 dr); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 10:1); **^{1}H NMR** ($CDCl_3$, 500 MHz) (for major diasteomer): δ 8.45 (d, *J* =7.9 Hz, 2H), 8.16 (s, 1H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.45 (t, *J* = 8.1 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 2H), 5.34–5.32 (m, 1H), 5.01–4.98 (m, 2H), 3.92 (s, 1H), 1.90 (s, 3H), 1.85 (s, 3H), 1.76 (s, 3H), 0.95 (s, 9H), 0.22 (s, 3H), 0.19 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz) (all discernable signals for both isomers): δ 144.9, 143.4, 143.0, 141.3, 140.9, 138.4, 137.7, 135.0, 129.7, 129.6, 126.6, 126.3, 126.0, 125.5, 123.2, 116.1, 114.8, 113.2, 109.5, 76.0, 73.4, 59.6, 57.2, 31.2, 29.7, 28.2, 25.8, 25.9, 21.5, 20.0, -3.5, -5.1; **HRMS** (ESI) calcd for $C_{33}H_{41}NO_4NaSSi$ $[M+Na]^+$ 598.2423, found 598.2419.



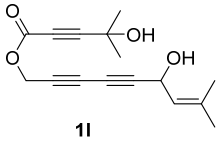
1k

1k: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.16–5.09 (m, 1H), 4.79 (s, 2H), 2.97–2.92 (m, 2H), 1.70 (s, 3H), 1.61 (s, 3H), 1.55 (s, 6H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.6, 135.4, 116.6, 92.6, 81.0, 73.2, 68.3, 65.0, 63.6, 53.9, 30.4, 25.4, 18.3, 17.7; **HRMS** (ESI) calcd for $C_{16}H_{18}O_3Na$ $[M+Na]^+$ 281.1154, found 281.1153.

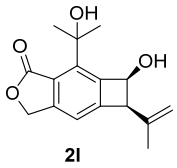


2k

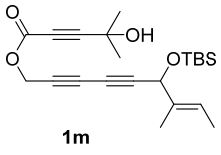
2k: white solid; 32 mg (72% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 6:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.11 (s, 1H), 6.31 (s, 1H, OH), 5.32 (s, 2H), 4.85 (s, 1H), 4.83 (s, 1H), 4.02–3.97 (m, 1H), 3.58 (dd, J= 8.3,5.5 Hz, 1H), 3.15–3.11 (m, 1H), 1.79 (s, 3H), 1.64 (s, 3H), 1.63 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 174.1, 155.5, 148.9, 146.0, 143.9, 140.4, 121.2, 115.3, 110.9, 71.9, 70.3, 47.6, 38.0, 30.2, 30.1, 20.4; **HRMS** (ESI) calcd for $C_{16}H_{18}O_3Na$ $[M+Na]^+$ 281.1154, found 281.1152.



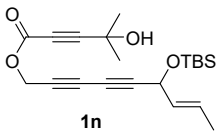
1l: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.37–5.27 (m, 1H), 5.14–5.08 (d, *J* = 8.3 Hz, 1H), 4.82 (s, 2H), 1.75 (s, 3H), 2.33 (br s, 1H, OH), 2.04 (br s, 1H, OH), 1.71 (s, 3H), 1.66 (s, 6H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.5, 138.4, 123.2, 92.7, 80.6, 73.2, 72.2, 71.5, 68.1, 65.1, 59.4, 53.7, 30.4, 25.6, 18.2; **HRMS** (ESI) calcd for $C_{16}H_{18}O_4Na$ $[M+Na]^+$ 297.1103, found 297.1096.



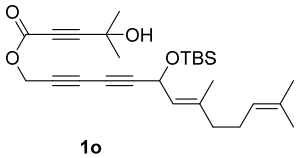
2l: white solid; 15 mg (30% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 2:1) **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.18 (s, 1H), 5.57 (br s, 1H, OH), 537–5.27 (m, 2H), 4.99 (s, 1H), 4.87 (s, 1H), 4.75 (s, 1H), 3.85 (br s, 1H, OH), 3.77 (s, 1H), 1.86 (s, 3H), 1.75 (s, 3H), 1.69 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 172.9, 152.1, 150.6, 147.6, 143.3, 142.4, 121.1, 116.5, 111.4, 76.8, 72.8, 69.9, 59.4, 30.5, 29.3, 21.2; **HRMS** (ESI) calcd for $C_{16}H_{19}O_4$ $[M+H]^+$ 275.1283, found 275.1283.



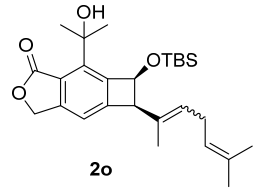
1m: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.62–5.53 (m, 1H), 4.82 (s, 2H), 4.75 (s, 1H), 1.67 (s, 3H), 1.61 (d, *J* = 6.3 Hz, 3H), 1.56 (s, 6H), 0.89 (s, 9H), 0.11 (s, 3H), 0.08 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.0, 134.6, 121.8, 92.7, 80.9, 73.2, 71.8, 71.5, 68.7, 68.2, 65.0, 53.7, 30.4, 25.7, 18.2, 13.2, 11.8, –4.70, –5.02; **HRMS** (ESI) calcd for $C_{22}H_{32}O_4NaSi$ $[M+Na]^+$ 411.1968, found 411.1973.



1n: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.81–5.72 (m, 1H), 5.52–5.45 (m, 1H), 4.86 (d, *J* = 5.6 Hz, 1H), 4.81 (s, 2H), 2.46 (s, 1H, OH), 1.70 (d, *J* = 6.5 Hz, 3H), 1.56 (s, 6H), 0.89 (s, 9H), 0.11 (s, 3H), 0.10 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.5, 129.8, 127.9, 92.7, 80.5, 73.2, 71.8, 71.7, 68.6, 65.0, 63.8, 53.7, 30.4, 25.7, 18.3, 17.4, –4.6, –4.8; **HRMS** (ESI) calcd for $C_{21}H_{30}O_4NaSi$ $[M+Na]^+$ 397.1811, found 397.1806.

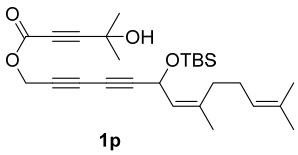


1o: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.28–5.24 (m, 1H), 5.11–5.03 (m, 1H), 4.81 (s, 2H), 2.38 (s, 1H, OH), 2.12–2.05 (m, 2H), 2.04–1.98 (m, 2H), 1.67 (s, 3H), 1.65 (s, 3H), 1.59 (s, 3H), 1.56 (s, 6H), 0.88 (s, 9H), 0.1 (s, 3H), 0.09 (s, 3H) **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.5, 138.5, 131.9, 124.5, 123.6, 92.7, 81.4, 73.2, 71.9, 71.6, 67.3, 65.0, 60.4, 53.7, 39.2, 30.2, 26.1, 25.74, 25.67, 18.2, 17.7, 16.6, –4.5, –4.7; **HRMS** (ESI) calcd for $C_{27}H_{40}O_4NaSi$ $[M+Na]^+$ 479.2594, found 479.2590.



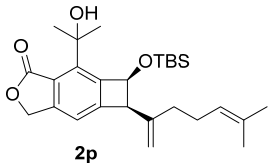
2o: white solid; 32 mg (67% yield, 2.5:1 E/Z); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 10:1 → 6:1). **^{1}H NMR** ($CDCl_3$, 500 MHz) **Major isomer:** δ 7.02 (s, 1H), 6.13 (s, 1H, OH), 5.39 (t, *J* = 7.4 Hz, 1H), 5.33 (s, 1H), 5.32–5.28 (m, 2H), 5.14 (t, *J* = 6.1 Hz, 1H), 4.21 (s, 1H), 2.80–2.72 (m, 2H), 1.80 (s, 3H), 1.73 (s, 3H), 1.68 (s, 3H), 1.65 (s, 3H), 1.58 (s, 3H), 0.93 (s, 9H), 0.17 (s, 3H), 0.12 (s, 3H); **Minor isomer:** 7.09 (s, 1H), 6.13 (s, 1H), 5.39 (t, *J* = 7.4 Hz, 1H), 5.33 (s, 1H), 5.32–5.28 (m,

2H), 5.14 (t, *J* = 6.1 Hz, 1H, OH), 3.73 (s, 1H), 2.98–2.87 (m, 2H), 1.80 (s, 3H), 1.70 (s, 3H), 1.68 (s, 3H), 1.64 (s, 3H), 1.57 (s, 3H), 0.92 (s, 9H), 0.17 (s, 3H), 0.13 (s, 3H) **^{13}C NMR** ($CDCl_3$, 500 MHz) (all discernable signals for both isomers): δ 173.4, 153.5, 150.6, 148.1, 143.5, 132.2, 131.3, 130.9, 127.7, 122.5, 122.2, 121.3, 115.7, 75.4, 73.8, 72.3, 70.0, 61.5, 54.4, 31.0, 28.7, 28.6, 27.2, 27.0, 25.8, 25.7, 19.8, 17.8, 13.8, –3.7, –4.3, –5.2,–5.3; **HRMS** (ESI) calcd for $C_{27}H_{41}O_4Si$ $[M+H]^+$ 457.2774, found 457.2779.



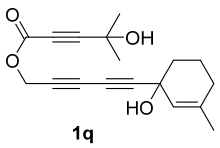
1p

1p: Colorless oil **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.27 (d, *J* = 8.6 Hz, 1H), 5.12–5.06 (m, 2H), 4.81 (s, 2H), 2.38 (s, 1H, OH), 2.13–1.96 (m, 4H), 1.72 (s, 3H), 1.69 (s, 3H), 1.61 (s, 3H), 1.56 (s, 6H), 0.88 (s, 9H), 0.10 (s, 3H), 0.09 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.5, 138.7, 132.4, 125.1, 123.5, 92.6, 81.5, 73.2, 71.9, 71.6, 67.4, 65.0, 60.1, 53.7, 32.5, 30.6, 30.4, 26.3, 25.7, 23.2, 18.2, 17.7, –4.4, –4.6; **HRMS** (ESI) calcd for $C_{27}H_{40}O_4NaSi$ $[M+Na]^+$ 479.2594, found 479.2601.



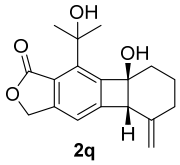
2p

2p: white solid; 28 mg (62% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 10:1 → 6:1 **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.09 (s, 1H), 6.12 (s, 1H, OH), 5.35–5.26 (m, 2H), 5.04 (s, 1H), 5.11–5.05 (m, 1H), 4.99 (s, 1H), 4.95 (s, 1H), 3.79 (s, 1H), 2.23–2.09 (m, 2H), 2.07–1.98 (m, 2H), 1.80 (s, 3H), 1.68 (s, 6H), 1.59 (s, 3H), 0.92 (s, 9H), 0.18 (s, 3H), 0.14 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 173.4, 153.3, 150.4, 148.4, 146.1, 143.4, 132.2, 123.4, 121.4, 115.6, 112.1, 75.9, 72.3, 70.0, 59.4, 34.0, 30.9, 28.6, 26.5, 25.8, 25.6, 17.7, –3.7, –5.2; **HRMS** (ESI) calcd for $C_{27}H_{41}O_4Si$ $[M+H]^+$ 457.2774, found 457.2779.



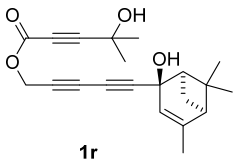
1q

1q: colorless oil**; ^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.73 (s, 1H), 4.81 (s, 2H), 1.98–1.86 (m, 3H), 1.85–1.71 (m, 3H), 1.69 (s, 3H), 1.56 (s, 6H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.5, 139.5, 123.7, 92.8, 83.9, 73.1, 72.3, 71.6, 67.0, 66.3, 64.9, 53.7, 37.2, 30.4, 29.6, 23.4, 19.2; **HRMS** (ESI) calcd for $C_{18}H_{20}O_4Na$ $[M+Na]^+$ 323.1259, found 323.1257.



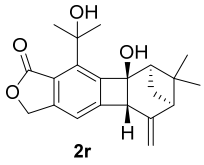
2q

2q: white solid; 22 mg (56% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 4:1 → 2:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.15 (s, 1H), 5.26 (s, 2H), 5.02 (s, 1H), 4.93 (s, 1H), 3.87 (s, 1H), 3.51 (br s, 1H, OH), 2.20–2.12 (m, 2H), 1.96–1.88 (m, 2H), 1.78 (s, 6H), 1.72–1.64 (m, 2H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 184.2, 152.7, 150.5, 147.0, 145.7, 144.5, 120.8, 115.6, 112.5, 81.5, 73.1, 69.4, 57.6, 34.8, 30.5, 30.1, 28.5, 19.0; **HRMS** (ESI) calcd for $C_{18}H_{20}O_4Na$ $[M+Na]^+$ 323.1259, found 323.1268.

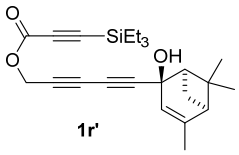


1r

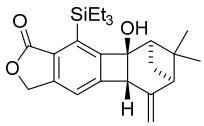
1r: yellow oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.29 (s, 1H), 4.79 (s, 2H), 3.11 (br s, 1H, OH), 2.55 (br s, 1H, OH), 2.52–2.47 (m, 1H), 2.33–2.28 (m, 1H), 1.98–1.95 (m, 1H), 1.71 (s, 3H), 1.59 (d, *J* = 9.0 Hz, 1H), 1.53 (s, 6H), 1.33 (s, 3H), 1.00 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.6, 148.6, 118.7, 93.1, 83.7, 73.1, 72.9, 72.3, 71.7, 67.1, 64.9, 53.7, 52.5, 47.6, 42.0, 36.3, 30.4, 26.9, 22.9, 22.6; **HRMS** (ESI) calcd for $C_{21}H_{24}O_4Na$ $[M+Na]^+$ 363.1572, found 363.1576.



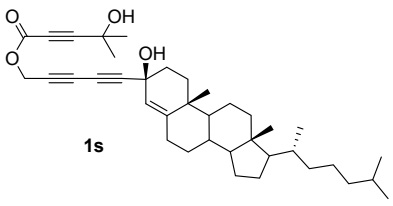
2r: pale-yellow solid; 50 mg (68% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 4:1 → 2:1) **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.15 (s, 1H), 5.25 (s, 2H), 4.97 (s, 1H), 4.85 (s, 1H), 4.01 (s, 1H), 3.48 (br s, 1H, OH), 2.6–2.52 (m, 2H), 2.25–2.17 (m, 2H), 1.73 (s, 6H), 1.38 (s, 3H), 1.06 (s, 3H), 0.57–0.52 (m, 1H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 172.1, 155.5, 150.5, 149.1, 146.8, 144.8, 120.7, 113.9, 109.1, 83.9, 72.9, 69.4, 53.5. 53.3, 48.9, 41.3, 30.5, 30.3, 27.6, 26.9, 23.9; **HRMS** (ESI) calcd for $C_{21}H_{25}O_4$ $[M+H]^+$ 341.1766, found 341.1762.



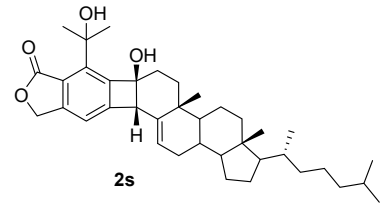
1r': yellow oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.28 (s, 1H), 4.79 (s, 2H), 2.54–2.48 (m, 1H), 2.35–2.30 (m, 1H), 2.19 (br s, 1H, OH), 2.01–1.97 (m, 1H), 1.73 (d, *J* = 1.3 Hz, 3H), 1.61 (d, *J* = 9.6 Hz, 1H), 1.34 (s, 1H), 1.03–0.95 (m, 12H), 0.66 (q, *J* = 7.8 Hz, 6H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 151.8, 148.5, 118.8, 94.7, 94.1, 83.5, 72.9, 72.4, 71.6, 67.2, 53.5, 52.6, 47.6, 41.6 36.3, 26.9, 23.0, 22.6, 7.2, 3.7; **HRMS** (ESI) calcd for $C_{24}H_{32}O_4NaSi$ $[M+Na]^+$ 419.2018, found 419.2013.



2r': pale-yellow solid; 42 mg (46% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 10:1 → 5:1) **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.22 (s, 1H), 5.23 (s, 2H), 4.95 (s, 1H), 4.84 (s, 1H), 3.97 (s, 1H), 2.63–2.51 (m, 2H), 240 (s, 1H, OH), 2.21–2.13 (m, 1H), 1.40 (s, 3H), 1.13–1.04 (m, 3H), 1.08 (s, 3H), 1.02–0.93 (m, 3H), 0.89–0.83 (m, 9H), 0.49 (d, *J* = 10.9, 1H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 171.8, 156.5, 152.9, 149.4, 148.5, 136.4, 130.0, 128.6, 115.5, 108.8, 84.9, 69.1, 54.3, 53.3, 48.6, 41.3, 27.5, 27.0, 23.9, 7.7, 3.1; **HRMS** (ESI) calcd for $C_{24}H_{32}O_4NaSi$ $[M+Na]^+$ 419.2018, found 419.2018.

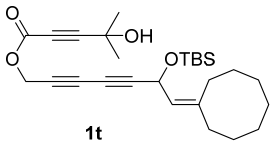


1s: ^{1}H NMR ($CDCl_3$, 500 MHz): δ 5.23 (s, 1H), 4.82 (s, 2H), 2.60 (br s, 1H, OH), 2.46 (br s, 1H, OH), 2.18–2.11 (m, 1H), 2.04–1.95 (m, 3H), 1.95–1.88 (m, 1H), 1.86–1.76 (m, 3H), 1.64–1.65 (m, 4H), 1.57 (d, *J* = 3.3 Hz, 1H), 1.56 (s, 6H), 1.38–1.28 (m, 6H), 1.26–1.21 (m, 3H), 1.16–1.03 (m, 6H), 1.02 (s, 3H), 0.89 (d, *J* = 6.6 Hz, 3H), 0.85 (dd, *J* = 1.9, 4.7 Hz, 6H), 0.66 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.6, 148.9, 121.8, 92.9, 83.6, 73.1, 72.3, 71.8, 67.4, 67.3, 64.9, 56.2, 55.9, 53.9, 53.7, 42.5, 39.7, 39.5, 37.5, 36.2, 35.8, 34.8, 34.5, 33.9, 32.6, 32.1, 30.6, 30.5, 30.4, 28.2, 28.0, 24.2, 23.8, 23.3, 22.8, 22.5, 21.1, 18.7, 18.5, 11.9; **HRMS** (ESI) calcd for $C_{38}H_{54}O_4Na$ $[M+Na]^+$ 597.3920, found 597.3923.



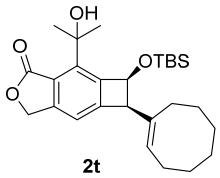
2s: white solid; 12 mg (42% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 5:1 → 3:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.23 (s, 1H), 5.58–5.53 (m, 1H), 3.90 (s, 1H), 2.8–1.94 (m, 3H), 1.76 (d, *J* = 4.8 Hz, 6H), 1.71–1.64 (m, 3H), 1.55–1.48 (m, 7H), 1.42–1.24 (m, 6H), 1.15 (s, 3H), 1.13–1.05 (m, 6H), 1.02–0.95 (m, 3H), 0.91 (d, *J* = 6.4 Hz, 3H),

0.86 (dd, *J* = 2.6, 4.5 Hz, 6H), 0.71 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 172.2, 153.8, 150.2, 146.9, 141.4, 130.2, 128.5, 122.1, 117.0, 81.5, 72.8, 69.4, 56.9, 56.1, 53.9, 48.2, 42.5, 39.9, 39.5, 36.7, 36.2, 35.8, 32.9, 32.6, 32.2, 31.3, 30.5, 30.3, 28.3, 28.0, 24.1, 23.8, 22.8, 22.7, 22.5, 21.5, 18.7, 12.0; **HRMS** (ESI) calcd for $C_{38}H_{55}O_4$ $[M+H]^+$ 575.4100, found 575.4088.



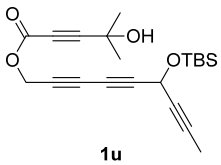
1t

1t: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.26 (d, *J* = 8.2 Hz, 1H), 5.13 (d, *J* = 8.1 Hz, 1H), 4.82 (s, 2H), 2.32 (s, 1H, OH), 2.26–2.18 (m, 1H), 2.18–2.10 (m, 3H), 1.72–1.58 (m, 4H), 1.56 (s, 6H), 1.52–1.39 (m, 6H), 0.88 (s, 9H), 0.12 (s, 3H), 0.10 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.5, 144.8, 124.4, 92.6, 81.4, 73.2, 71.9, 71.5, 67.5, 65.0, 60.1, 53.8, 36.9, 30.4, 29.5, 27.1, 27.0, 26.4, 25.7, 25.5, 18.2, –4.4, –4.6; **HRMS** (ESI) calcd for $C_{27}H_{40}O_4NaSi$ $[M+Na]^+$ 479.2594, found 479.2602.



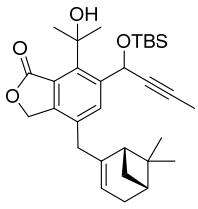
2t

2t: white solid; 37 mg (69% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 10:1 → 6:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.08 (s, 1H), 6.17 (s, 1H, OH), 5.59 (t, *J* = 8.2 Hz, 1H), 5.35–525 (m, 2H), 5.21 (s, 1H), 3.75 (s, 1H), 2.19–2.13 (m, 2H), 213–2.07 (m, 2H), 1.80 (s, 3H), 1.67 (s, 3H), 162–1.59 (m, 1H), 1.57–1.45 (m, 7H), 0.92 (s, 9H), 0.17 (s, 3H), 0.12 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 173.5, 154.1, 150.3, 148.2, 143.5, 137.5, 128.3, 121.3, 115.9, 76.0, 72.3, 70.0, 60.7, 30.9, 30.1, 29.2, 28.5, 27.3, 26.4, 26.2, 26.2, 25.8, 17.9, –3.5, –5.2; **HRMS** (ESI) calcd for $C_{27}H_{40}O_4NaSi$ $[M+Na]^+$ 479.2594, found 479.2601.



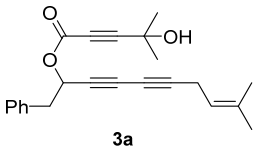
1u

1u: yellow oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.20–5.16 (m, 1H), 4.81 (s, 2H), 2.53 (s, 1H, OH), 1.83 (d, *J* = 2.2 Hz, 3H), 1.55 (s, 6H), 0.89 (s, 9H), 0.15 (s, 3H), 0.14 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.5, 92.8, 81.4, 78.1, 75.9, 73.1, 72.4, 71.4, 66.8, 65.0, 53.6, 53.4, 30.4, 25.6, 18.2, 3.6, –4.6; **HRMS** (ESI) calcd for $C_{21}H_{28}O_4NaSi$ $[M+Na]^+$ 395.1655, found 395.1664.



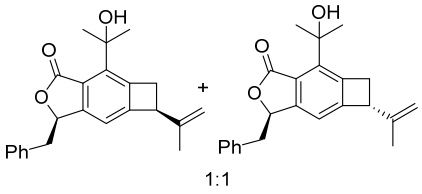
2u'

2u': pale-yellow oil; 35 mg (76% yield, 1:1 diastereomeric mixture); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 3:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.96 (s, 1H), 6.31 (s, 1H), 6.12–6.08 (m, 1H), 5.22 (s, 2H), 3.32–3.14 (m, 2H), 2.36–2.29 (m, 1H), 2.29–2.15 (m, 1H), 2.11–2.04 (m, 1H), 2.02–1.95 (m, 1H), 1.84 (s, 3H), 1.81 (s, 3H), 1.80 (s, 3H), 1.25–1.17 (m, 1H), 1.22 (s, 3H), 1.12 (dd, *J* = 9, 17 Hz, 1H), 0.89 (s, 9H), 0.75 (s, 3H), 0.18 (s, 3H), 0.11–0.07 (m, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz) (all discernable signal for both isomer): δ 173.9, 147.8, 146.5, 146.4, 144.7, 144.5, 141.6, 136.2, 136.1, 131.8, 122.8, 118.9, 118.8, 82.7, 82.6, 81.0, 74.0, 68.3, 45.7, 45.5, 40.6, 40.5, 39.4, 39.2, 38.1, 31.7, 31.3, 26.1, 25.7, 20.8, 18.2, 3.7, –4.3, –4.8; **HRMS** (ESI) calcd for $C_{31}H_{45}O_4Si$ $[M+H]^+$ 509.3087, found 509.3075.



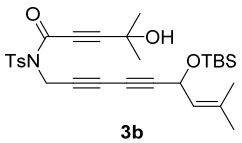
3a

3a: yellow oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.34–7.28 (m, 2H), 7.28–7.22 (m, 3H), 5.60 (t, *J* = 5.4 Hz, 1H), 5.15–5.09 (m, 1H), 3.15–3.04 (m, 2H), 2.96 (d, *J* = 5.0 Hz, 2H), 2.40 (br s, 1H, OH), 1.71 (s, 3H), 1.62 (s, 3H), 1.56 (s, 6H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.2, 135.0, 129.6, 128.5, 127.3, 116.7, 92.4, 81.1, 73.5, 72.2, 71.3, 66.7, 65.0, 63.7, 40.9, 30.5, 25.5, 23.9, 18.4, 17.7; **HRMS** (ESI) calcd for $C_{23}H_{24}O_3Na$ $[M+Na]^+$ 371.1623, found 371.1609.



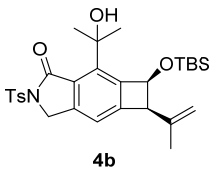
4a

4a: 62% total yield; Purification: Column Chromatography (SiO_2, hexanes–EtOAc, 10:1 → 6:1); **Diastereomer 1:** white solid; 16 mg; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.32–7.26 (m, 2H), 7.27–7.24 (m, 1H), 7.23–7.19 (m, 2H), 6.88 (s, 1H, OH), 6.32 (s, 1H), 5.71–5.63 (m, 1H), 4.83 (s, 1H), 4.79 (s, 1H), 4.00–3.96 (m, 1H), 3.57 (dd, J= 6.0, 8.5 Hz, 1H), 3.18 (d, *J* = 6.3 Hz, 2H), 3.10 (d, *J* = 13.5 Hz, 1H), 1.76 (s, 3H), 1.61 (s, 3H), 1.57 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 173.1, 155.2, 151.7, 145.9, 143.9, 140.5, 135.1, 129.6, 128.6, 127.2, 115.4, 110.9, 81.7, 71.8, 47.7, 41.3, 38.0, 30.1, 30.0, 20.3; **HRMS** (ESI) calcd for $C_{23}H_{24}O_3Na$ $[M+Na]^+$ 371.1623, found 371.1618. **Diastereomer 2:** white solid; 16 mg; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.30–7.22 (m, 2H), 7.18 (d, *J* = 7.3 Hz, 2H), 6.70 (s, 1H), 6.31 (s, 1H, OH), 5.65 (t, *J* = 6.2 Hz, 1H), 4.86 (s, 1H), 4.79 (s, 1H), 3.94–3.90 (m, 1H), 3.55 (dd, *J* = 5.6, 8.4 Hz, 1H), 3.30 (dd, *J* = 8.1, 5.3 Hz, 2H), 3.15–3.03 (m, 2H), 1.77 (s, 3H), 1.59 (s, 3H), 1.56 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 173.1, 154.9, 151.5, 145.8, 144.1, 140.4, 134.8, 129.7, 128.5, 127.3, 115.7, 110.8, 81.5, 71.8, 47.6, 41.2, 38.1, 30.1, 30.0, 20.3; **HRMS** (ESI) calcd for $C_{23}H_{24}O_3Na$ $[M+Na]^+$ 371.1623, found 371.1627. All attempts to confirm to assign stereochemistry to each diastereomers by nOe failed.



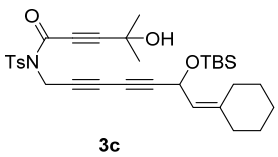
3b

3b: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.97 (d, *J* = 8.1 Hz, 2H), 7.34 (d, J = 8.1 Hz, 2H), 5.27 (d, *J* = 7.2 Hz, 1H), 5.08 (d, *J* = 8.1 Hz, 1H), 4.94 (s, 2H), 2.44 (s, 3H), 1.74 (s, 3H), 1.68 (s, 3H), 1.54 (s, 6H), 0.90 (s, 9H), 0.12 (s, 3H), 0.11 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 151.4, 145.6, 135.3, 135.1, 129.6, 128.9, 124.7, 99.1, 80.4, 74.5, 73.1, 69.4, 67.5, 65.2, 60.4, 36.9, 30.2, 25.8. 25.6, 21.7, 18.2, –4.5, –4.6; **HRMS** (ESI) calcd for $C_{29}H_{39}NO_5NaSiS$ $[M+Na]^+$ 564.2216, found 564.2231.



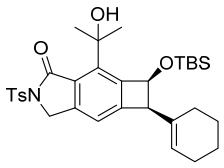
4b

4b: white solid; 46 mg (72% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 4:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.98 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.10 (s, 1H), 6.26 (s, 1H, OH), 5.18 (s, 1H), 4.93 (s, 1H), 4.98 (s, 1H), 4.87 (s, 2H), 3.75 (s, 1H), 2.41 (s, 3H), 1.73 (s, 3H), 1.68 (s, 3H), 1.60 (s, 3H), 0.89 (s, 9H), 0.15 (s, 3H), 0.12 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 168.9, 152.5, 148.2, 145.5, 145.1, 143.2, 141.9, 134.8, 129.8, 125.9, 117.2, 113.6, 75.8, 72.1, 60.1, 50.0, 31.0, 28.5, 25.7, 21.7, 20.3, 17.8, –3.7, –5.3; **HRMS** (ESI) calcd for $C_{29}H_{40}NO_5SiS$ $[M+H]^+$ 542.2396, found 542.2385.



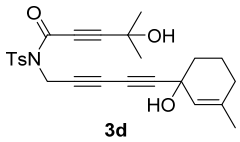
3c

3c: yellow oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.97 (d, *J* = 8.1 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 5.23 (d, *J* = 7.2 Hz, 1H), 5.15 (d, *J* = 8.1 Hz, 1H), 4.84 (s, 2H), 2.44 (s, 3H), 2.30 (br s, 1H) 2.18–2.12 (m, 2H), 2.12–2.06 (m, 2H), 1.60–1.51 (m, 6H), 1.59–1.51 (m, 6H), 0.93–0.87 (m, 9H), 0.14–0.08 (m, 6H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 151.4, 145.6, 143.0, 135.1, 129.6, 128.9, 121.4, 99.1, 80.7, 74.5, 73.1, 69.4, 67.3, 65.2, 59.5, 36.7, 30.2, 29.3, 28.1, 27.4, 26.5, 25.8, 21.7, 18.2, –4.4, –4.6; **HRMS** (ESI) calcd for $C_{32}H_{43}NO_5NaSiS$ $[M+Na]^+$ 604.2529, found 604.2541.



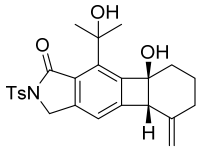
4c

4c: white solid; 28 mg (56% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 4:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.98 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 7.08 (s, 1H), 6.25 (s, 1H, OH), 5.59 (s, 1H), 5.15 (s, 1H), 4.91–4.81 (m, 2H), 3.66 (s, 1H), 2.42 (s, 3H), 1.88–1.77 (m, 2H), 1.73 (s, 3H), 1.64–1.53 (m, 9H), 0.89 (s, 9H), 0.14 (s, 3H), 0.11 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 168.8, 153.0, 148.0, 145.5, 144.9, 143.4, 134.8, 134.6, 129.8, 128.3, 125.7, 125.0, 117.2, 75.7, 72.1, 60.4, 50.0, 31.0, 28.6, 26.4, 25.8, 25.2, 22.7, 22.3, 21.7, 17.9, –3.7, –5.2; **HRMS** (ESI) calcd for $C_{32}H_{44}NO_5SiS$ $[M+H]^+$ 582.2709, found 582.2723.



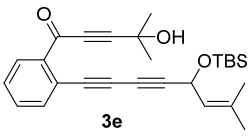
3d

3d: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.95 (d, *J* = 8.2 Hz, 2H), 7.33 (d, *J* = 8.1 Hz, 2H), 5.43 (s, 1H), 4.81 (s, 2H), 3.05 (br s, 1H), 2.43 (s, 3H), 1.97–1.89 (m, 3H), 1.86–1.74 (m, 3H), 1.69 (s, 3H), 1.52 (s, 6H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 151.4, 145.6, 139.5, 135.1, 129.6, 128.9, 123.8, 99.3, 82.9, 74.4, 73.8, 69.2, 67.1, 66.3, 65.2, 37.2, 36.9, 30.2, 29.7, 23.5, 21.7, 19.2; **HRMS** (ESI) calcd for $C_{25}H_{27}NO_5NaS$ $[M+Na]^+$ 476.1521, found 476.1519.



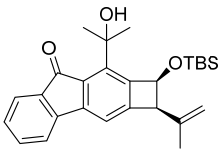
4d

4d: white solid; 23 mg (42% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 4:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.00 (d, *J* = 7.5 Hz, 2H), 7.34 (d, *J* = 7.6, 2H), 7.13 (s, 1H), 5.00 (s, 1H), 4.91 (s, 1H), 4.84 (s, 2H), 3.83 (s, 1H), 3.19 (s, 1H, OH), 2.43 (s, 3H), 2.30–2.22 (m, 1H), 2.18–2.07 (m, 2H), 1.94–1.85 (m, 1H), 1.70 (s, 3H), 1.69 (s, 3H), 1.66–1.61 (m, 2H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 167.6, 152.2, 145.6, 145.4, 145.1, 144.1, 139.6, 135.1, 129.8, 128.3, 128.0, 117.1, 112.5, 109.9, 109.6, 81.9, 58.0, 49.5, 34.7, 30.5, 28.4, 21.7, 19.0; **HRMS** (ESI) calcd for $C_{27}H_{26}NO_5S$ $[M+H]^+$ 476.1532, found 476.1531.



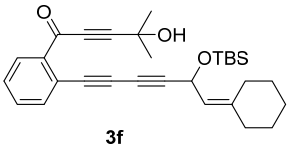
3e

3e: yellow oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.00 (d, *J* = 8.1 Hz, 1H), 7.60 (d, *J* = 8.2 Hz, 1H), 7.49 (t, *J* = 6.3 Hz, 1H), 7.43 (t, *J* = 6.5 Hz, 1H), 5.33–5.28 (m, 1H), 5.18 (d, *J* = 8.3 Hz, 1H), 2.44 (br s, 1H, OH), 1.73 (s, 3H), 1.69 (s, 3H), 1.64 (s, 6H), 0.90 (s, 9H), 0.14 (s, 3H), 0.12 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 176.7, 139.0, 135.6, 135.0, 132.6, 131.2, 128.8, 124.8, 121.7, 98.9, 86.0, 80.9, 79.9, 76.3, 68.7, 65.3, 60.7, 30.6, 25.8, 25.6, 18.3, –4.5, –4.6; **HRMS** (ESI) calcd for $C_{27}H_{35}O_3Si$ $[M+NH]^+$ 435.2355, found 435.2362.



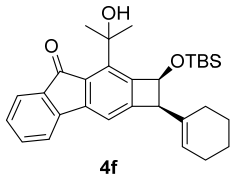
4e

4e: yellow solid; 42 mg (87% yield, 6:1 *dr*); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 10:1); **Major diastereomer:** **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.59 (d, *J* = 7.3 Hz, 1H), 7.47–7.40 (m, 2H), 7.27–7.23 (m, 2H), 7.18 (s, 1H), 6.26 (s, 1H, OH), 5.17 (s, 1H), 4.96 (s, 1H), 4.93 (s, 1H), 3.72 (s, 1H), 1.76 (s, 3H), 1.74 (s, 3H), 1.63 (s, 3H), 0.92 (s, 9H), 0.17 (s, 3H), 0.15 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 196.7, 153.7, 149.3, 148.6, 144.2, 143.9, 142.3, 135.1, 133.5, 129.2, 124.6, 119.8, 116.5, 114.6, 113.5, 75.9, 72.3, 59.9, 30.5, 28.3, 25.8, 20.3, 17.9, –3.6, –5.2; **HRMS** (ESI) calcd for $C_{27}H_{35}O_3Si$ $[M+H]^+$ 435.2355, found 435.2341.



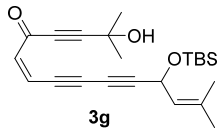
3f

3f: yellow oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.00 (d, *J* = 7.3 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 6.8 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 5.26 (s, 2H), 2.30 (s, 1H, OH), 2.21–2.14 (m, 2H), 2.13–2.07 (m, 2H), 1.64 (s, 6H), 1.61–1.49 (m, 6H), 0.90 (s, 9H), 0.14 (s, 3H), 0.12 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 176.7, 142.8, 139.1, 135.7, 132.6, 131.1, 128.8, 121.5, 98.9, 86.4, 81.0, 76.3, 68.5, 65.3, 59.8, 36.8, 30.7, 29.4, 28.1, 27.4, 26.5, 25.8, 18.3, –4.4, –4.6; **HRMS** (ESI) calcd for $C_{30}H_{38}O_3NaSi$ $[M+Na]^+$ 497.2488, found 497.2493.



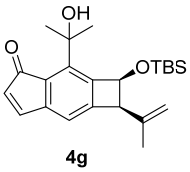
4f

4f: yellow solid; 36 mg (76% yield, 10:1 *dr*); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 10:1); **Major diastereomer:** **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.56 (d, *J* = 7.2 Hz, 1H), 7.47–7.39 (m, 2H), 7.27–7.23 (m, 1H), 7.18 (s, 1H), 6.27 (s, 1H, OH), 5.95 (s, 1H), 5.15–5.13 (m, 1H), 3.63 (s, 1H), 2.11–2.04 (m, 2H), 1.95–1.89 (m, 2H), 1.76 (s, 3H), 1.63 (s, 3H), 1.65–1.58 (m, 4H), 0.92 (s, 9H), 0.17 (s, 3H), 0.14 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 196.8, 154.3, 149.2, 148.5, 144.3, 144.1, 135.1, 134.8, 133.6, 129.8, 129.2, 124.8, 124.5, 119.8, 114.7, 75.9, 72.4, 60.3, 30.5, 28.3, 26.4, 25.8, 25.3, 22.8, 22.4, 17.9 – 3.7, –5.1; **HRMS** (ESI) calcd for $C_{30}H_{39}O_3Si$ $[M+H]^+$ 475.2668, found 475.2658.



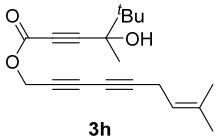
3g

3g: yellow oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 6.44 (d, *J* = 11.9 Hz, 1H), 6.35 (d, *J* = 11.6 Hz, 1H), 5.27 (d, *J* = 7.6 Hz, 1H), 5.17 (d, *J* = 8.3 Hz, 1H), 2.20 (s, 1H, OH), 1.73 (s, 3H), 1.68 (s, 3H), 1.60 (s, 6H), 0.89 (s, 9H), 0.11 (s, 3H), 0.10 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 174.7, 139.7, 135.5, 124.4, 121.9, 98.0, 89.9, 86.9, 81.4, 74.6, 68.2, 65.2, 60.7, 30.6, 25.7, 25.6, 18.3, –4.6, –4.7; **HRMS** (ESI) calcd for $C_{23}H_{32}O_3NaSi$ $[M+Na]^+$ 407.2018, found 407.2008.

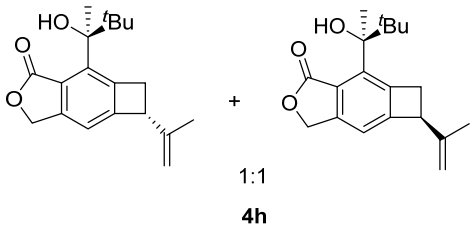


4g

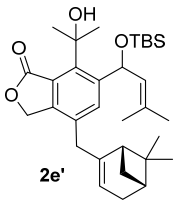
4g: yellow oil; 36 mg (56% yield, 10:1 *dr*); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 10:1); The major diastereomer could be completely separated from minor; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.44 (d, *J* = 5.8 Hz, 1H), 6.71 (s, 1H, OH), 5.87 (s, 1H), 5.81 (d, *J* = 5.8 Hz, 1H), 5.09 (s, 1H), 4.84 (s, 1H), 4.89 (s, 1H), 3.65 (s, 1H), 1.70 (s, 6H), 1.58 (s, 3H), 0.92 (s, 9H), 0.16 (s, 3H), 0.14 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 201.2, 152.3, 150.5, 148.3, 148.2, 144.3, 142.3, 126.7, 125.8, 117.4, 113.4, 75.8, 72.3, 59.8, 30.4, 28.1, 25.8, 20.2, 17.9, –3.7, –5.2; **HRMS** (ESI) calcd for $C_{23}H_{32}O_3NaSi$ $[M+Na]^+$ 407.2018, found 407.2008.



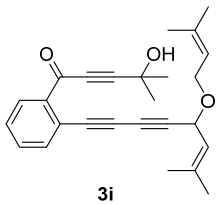
3h: colorless oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 5.13 (t, *J* = 7.3 Hz, 1H), 4.79 (s, 2H), 2.96 (d, *J* = 6.8 Hz, 1H), 2.11 (br s, 1H, OH), 1.70 (s, 3H), 1.62 (s, 3H), 1.48 (s, 3H), 1.05 (s, 9H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 152.5, 135.4, 116.7, 92.2, 80.9, 75.2, 74.1, 72.5, 68.4, 63.7, 53.8, 38.3, 25.5, 24.9, 24.1, 18.4, 17.7; **HRMS** (ESI) calcd for $C_{19}H_{25}O_3$ $[M+H]^+$ 301.1804, found 301.1816.



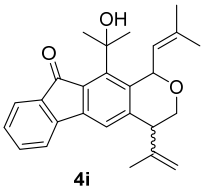
4h: 87% total yield; Purification: Column Chromatography (SiO_2, hexanes–EtOAc, 10:1 → 6:1); **Diastereomer 1:** white solid; 18 mg; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.17 (s, 1H, OH), 7.12 (s, 1H), 5.31 (s, 2H), 4.84 (d, *J* = 7.1 Hz, 2H), 3.99–3.95 (m, 1H), 3.58 (dd, J = 5.6, 8.3 Hz, 1H), 3.21 (dd, J = 2.6, 11.3 Hz), 1.77 (s, 3H), 1.60 (s, 3H), 0.97 (s, 9H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 174.3, 154.5, 148.3, 145.4, 144.0, 143.5, 122.9, 115.1, 111.0, 80.9, 69.9, 46.8, 41.7, 39.5, 25.7, 24.4, 20.2. **HRMS** (ESI) calcd for $C_{19}H_{25}O_3$ $[M+H]^+$ 301.1804, found 301.1807. **Diastereomer 2:** white solid; 20 mg; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.17 (s, 1H, OH), 7.11 (s, 1H), 5.35–5.27 (m, 2H), 4.86–4.81 (m, 2H), 3.99–3.95 (m, 1H), 3.67 (dd, J = 5.8, 7.9 Hz, 1H), 3.13 (dd, J = 2.8, 11.2 Hz), 1.77 (s, 3H), 1.59 (s, 3H), 0.97 (s, 9H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 174.3, 154.6, 148.3, 145.4, 144.2, 143.7, 122.9, 115.1, 111.0, 80.8, 69.9, 46.8, 41.8, 39.2, 25.8, 24.4, 20.2; **HRMS** (ESI) calcd for $C_{19}H_{25}O_3$ $[M+H]^+$ 301.1804, found 301.1801. All attempts to confirm to assign stereochemistry to each diastereomers by nOe failed.



2e': colorless oil; 24 mg (76% yield, 1:1 diastereomeric mixture); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 4:1); **^{1}H NMR** (both isomers) ($CDCl_3$, 500 MHz): δ 7.79 (s, 1H), 7.60 (s, 1H), 6.39 (s, 2H), 6.36 (s, 2H), 6.02 (d, *J* = 4.4 Hz, 1H), 6.00 (d, J = 4.5 Hz, 2H), 5.21–5.19 (m, 4H), 3.29–3.17 (m, 4H), 2.37–2.31 (m, 2H), 2.27–2.18 (m, 4H), 2.11–2.06 (m, 2H), 2.00–1.95 (m, 2H), 1.86 (s, 6H), 1.78 (s, 6H), 1.73–1.68 (m, 12H), 1.23 (s, 6H), 1.14–1.09 (m, 2H), 0.84 (s, 18H), 0.76 (s, 3H), 0.75 (s, 3H), 0.09–0.06 (m, 6H), –0.10 (s, 3H), –0.12 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz) (all discernable signal for both isomer): δ 174.0, 147.0, 147.4, 147.2, 147.1, 144.7, 144.5, 144.3, 144.2, 137.0, 136.9, 134.1, 131.5, 129.5, 129.4, 122.8, 122.7, 119.0, 118.7, 111.4, 73.6, 68.8, 68.6, 68.3, 68.2, 45.8, 45.6, 40.6, 40.5, 39.4, 39.2, 38.1, 31.7, 31.4, 31.3, 31.2, 26.2, 25.9, 25.8, 20.9, 20.8, 19.0, 18.1, –4.1, –4.3, –4.4; ; **HRMS** (ESI) calcd for $C_{32}H_{48}O_4NaSi$ $[M+Na]^+$ 547.3220, found 547.3197.

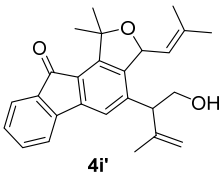


3i: yellow oil; **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.01 (d, *J* = 7.6 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.5, 1H), 5.38 (m, 2H), 4.90 (d, *J* = 8.6 Hz, 1H), 4.18 (dd, *J* = 6.8, 4.7 Hz, 1H), 4.02 (dd, *J* = 7.4, 3.6 Hz, 1H), 1.76 (s, 3H), 1.75 (s, 3H), 1.71 (s. 6H), 1.64 (s, 6H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 176.6, 139.1, 138.3, 135.7, 132.6, 131.3, 128.9, 121.8, 121.6, 120.4, 98.8, 84.2, 80.9, 79.7, 76.2, 70.0, 65.6, 65.3, 64.7, 30.6, 26.1, 25.8, 25.7, 18.4, 18.2; **HRMS** (ESI) calcd for $C_{26}H_{29}O_3$ $[M+H]^+$ 389.2117, found 389.2121.



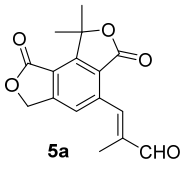
4i

4i: yellow oil; 24 mg (28% yield, 1:1 diastereomeric mixture); formed along with **4i'**; Purification: Column Chromatography (SiO_2, hexanes–EtOAc, 20:1 → 10:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.60 (d, *J* = 7.8 Hz, 2H), 7.48 (t, *J* = 6.7 Hz, 1H), 7.31 (s, 1H), 7.29–7.26 (m, 2H), 7.24 (s, 1H), 6.06 (d, *J* = 6.9 Hz, 1H), 6.01 (d, *J* = 9.6 Hz, 1H), 5.25–5.19 (m, 2H), 5.13 (s, 1H), 5.00–4.98 (m, 1H), 4.96 (s, 1H), 4.87 (s, 1H), 4.14–4.09 (m, 1H), 4.02–3.96 (m, 1H), 3.83–3.77 (m, 1H), 3.67–3.56 (m, 3H), 1.93–1.90 (m, 3H), 1.87 (s, 3H), 1.80–1.77 (m, 9H), 1.71–1.68 (m, 6H), 1.64 (s, 6H), 1.58 (s, 1H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 196.9, 193.1, 146.5, 147.6, 146.1, 145.9, 144.6, 144.2, 143.8, 143.1, 142.5, 140.2, 139.5, 136.7, 135.0, 134.5, 134.2, 133.9, 129.1, 126.7, 126.2, 124.7, 120.6, 120.1, 119.6, 118.2, 115.1, 111.9, 85.9, 78.2, 74.5, 71.1, 64.8, 63.1, 49.5, 48.1, 30.5, 30.1, 28.5, 27.1, 26.0, 23.2, 19.9, 18.8, 18.0; **HRMS** (ESI) calcd for $C_{26}H_{29}O_3$ $[M+H]^+$ 389.2117, found 389.2123.



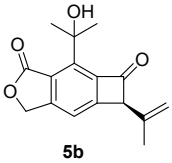
4i'

4i': yellow oil; 24 mg (28% yield); formed along with **4i**; Purification: Column Chromatography (SiO_2, hexanes–EtOAc, 20:1 → 10:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.60 (d, *J* = 7.2 Hz, 1H), 7.46–7.43 (m, 2H), 7.27–7.23 (m, 2H), 6.06 (d, J = 6.6 Hz, 1H), 5.25 (d, *J* = 6.7 HZ, 1H), 5.04 (s, 1H), 4.91 (s, 1H), 3.97 (dd, *J* = 3.8, 6.8 Hz, 1H), 3.79–3.72 (m, 2H), 1.88 (s, 3H), 1.79 (s, 3H), 1.78 (s, 3H), 1.72 (s, 3H), 1.66 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 196.8, 151.6, 145.2, 144.6, 144.3, 143.2, 139.9, 139.3, 135.0, 133.9, 130.6, 129.1, 127.2, 124.7, 120.7, 119.6, 116.0, 74.7, 71.1, 62.7, 48.6, 30.7, 30.4, 25.6, 20.1, 18.8; **HRMS** (ESI) calcd for $C_{26}H_{29}O_3$ $[M+H]^+$ 389.2117, found 389.2131.



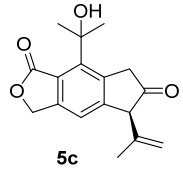
5a

5a: white solid; 22 mg (72% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc 5:1 → 2:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 9.76 (s, 1H), 8.27 (s, 1H), 7.69 (s, 1H), 5.51 (s, 1H), 5.29 (s, 1H), 2.06 (s, 3H), 1.89 (s, 6H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 194.8, 167.8, 167.6, 155.2, 152.8, 142.8, 141.2, 140.7, 125.4, 123.1, 120.2, 85.7, 70.3, 25.7, 11.3; **HRMS** (ESI) calcd for $C_{16}H_{15}O_3$ $[M+H]^+$ 389.2117, found 389.2131.



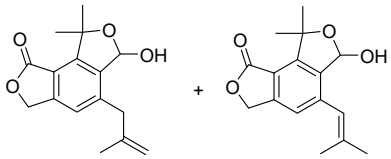
5b

5b: white solid; 53 mg (82% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 5:1 → 2:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.53 (s, 1H), 6.11 (s, 1H), 5.43 (s, 2H), 5.00 (s, 1H), 4.81 (s, 1H), 4.73 (s, 1H), 1.85 (s, 3H), 1.78 (s, 3H), 1.77 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 186.3, 172.3, 159.7, 155.3, 150.9, 145.4, 139.7, 123.8, 116.3, 113.4, 72.1, 70.1, 69.0, 30.2, 30.1, 21.3; **HRMS** (ESI) calcd for $C_{16}H_{17}O_4$ $[M+H]^+$ 273.1127, found 273.1133.



5c

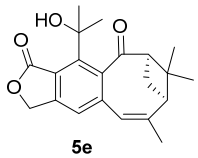
5c: colorless oil; 12 mg (55% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 5:1 → 3:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.50 (s, 1H), 5.32 (s, 2H), 4.98 (s, 1H), 4.82 (s, 1H), 4.70 (s, 1H), 3.31 (s, 2H), 1.87 (s, 3H), 1.80 (s, 3H), 1.79 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 185.6, 168.3, 159.3, 155.3, 149.4, 147.1, 140.2, 123.5, 116.3, 113.0, 77.0, 68.8, 68.3, 50.4, 25.2, 24.9, 21.4; **HRMS** (ESI) calcd for $C_{17}H_{18}O_4Na$ $[M+H]^+$ 273.1127, found 273.1133.



5d

1.5:1

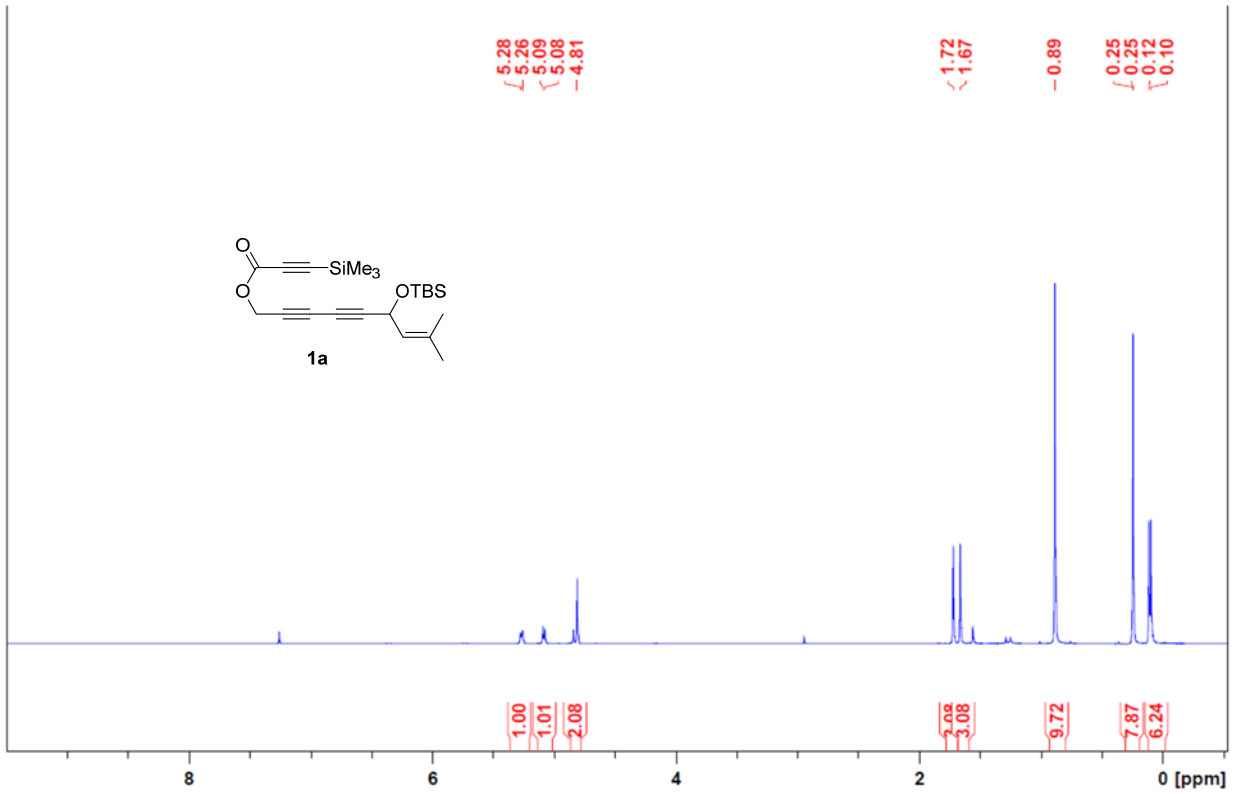
5d: colorless oil; 35 mg (86% yield, inseparable mixture (1.5:1) of isomeric alkenes); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 5:1 → 3:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): **Major isomer:** δ 7.24 (s, 1H), 6.54 (d, *J* = 5.7 Hz, 1H), 5.31 (s, 2H), 4.91 (s, 1H), 4.69 (s, 1H), 3.88 (d, *J* = 5.6 Hz, 1H, OH), 3.66 (d, *J* = 15.4 Hz , 1H), 3.45 (d, *J* = 15.7, 1H), 1.79 (s, 3H), 1.72 (s, 3H), 1.70 (s, 3H); **Minor isomer:** δ 7.28 (s, 1H), 6.48 (s, 1H), 6.46 (d, *J* = 5.2 Hz, 1H), 5.33 (s, 2H), 3.76 (d, *J* = 5.1 Hz, 1H, OH), 1.96 (s, 3H), 1.88 (s, 3H), 1.79 (s, 3H), 1.69 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz) (all discernable signal for both isomer): δ 169.5, 169.4, 149.5, 149.1, 147.2, 146.9, 142.1, 143.7, 139.3, 138.6, 122.4, 121.6, 120.6, 117.4, 113.6, 99.1, 98.8, 87.1, 87.0, 69.9, 69.8, 40.6, 29.3, 27.5, 27.1, 22.5, 20.0 ; **HRMS** (ESI) calcd for $C_{16}H_{19}O_4$ $[M+H]^+$ 275.1283, found 275.1281.

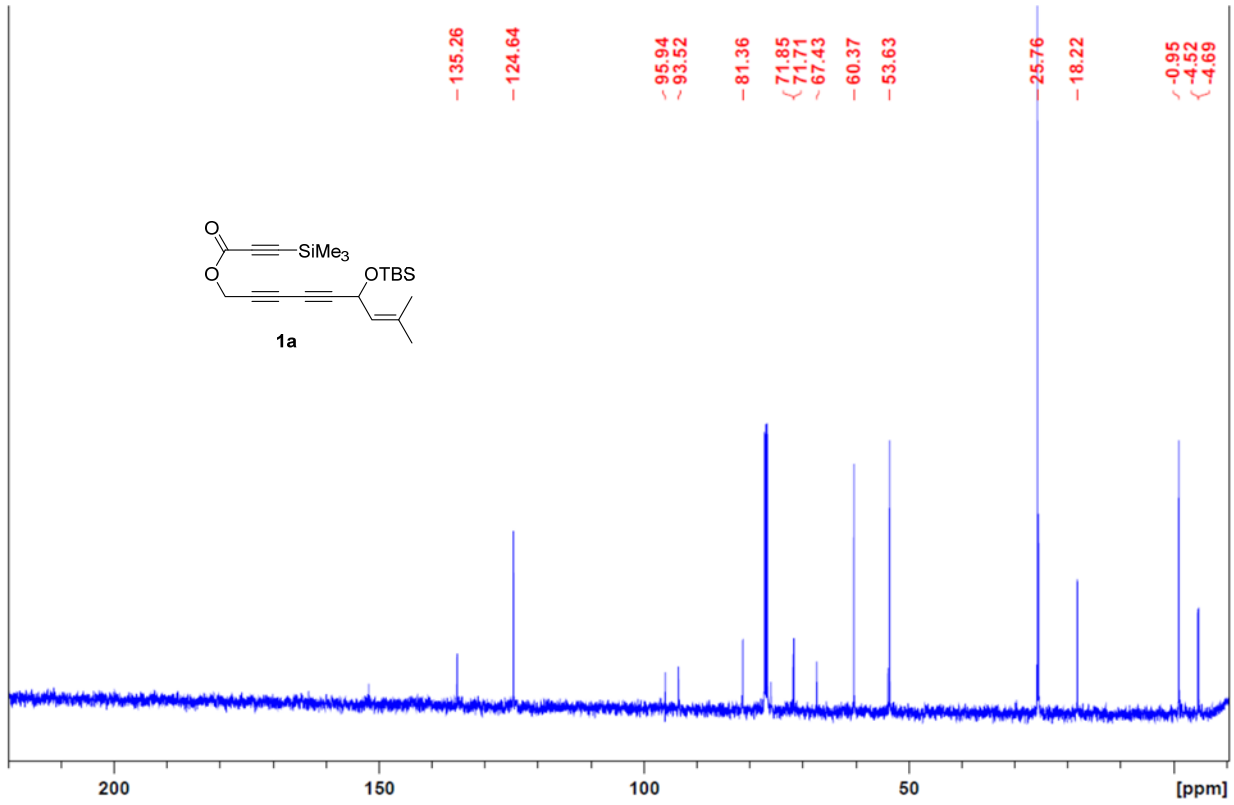


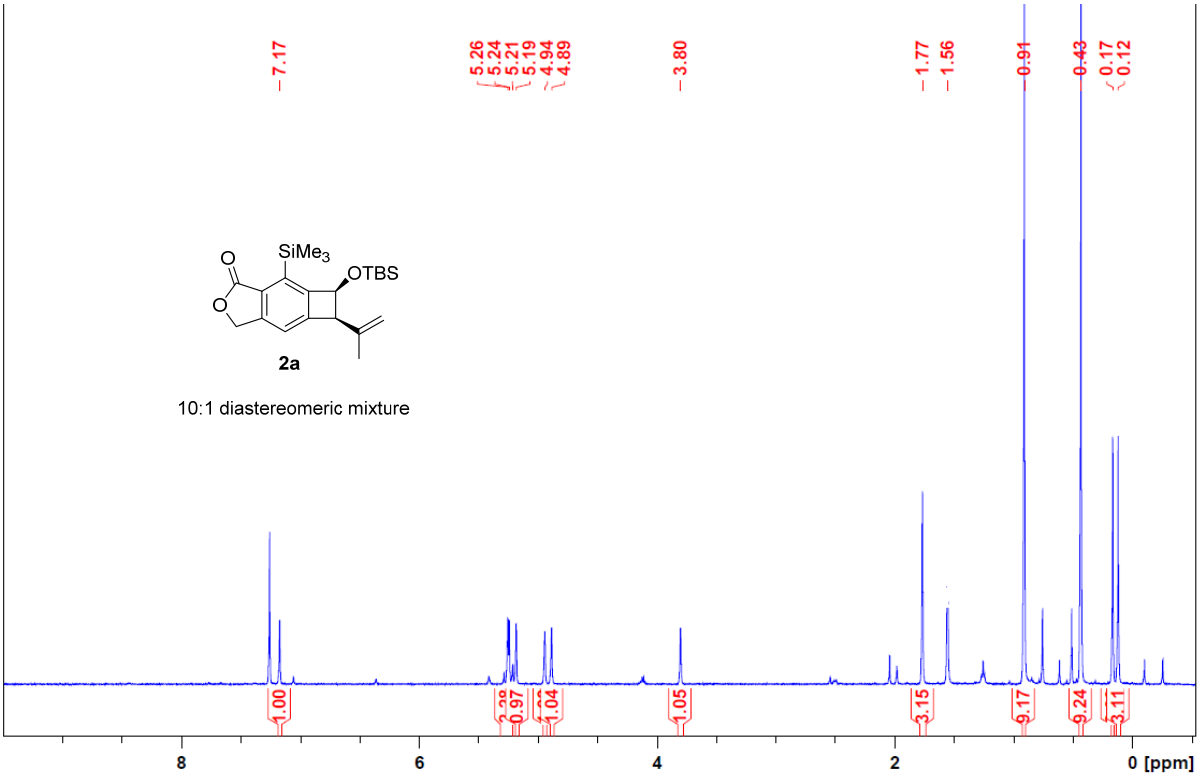
5e

5e: colorless oil; 35 mg (81% yield); Purification: Flash Chromatography (SiO_2, hexanes–EtOAc, 4:1); **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.23 (s, 1H), 7.22 (s, 1H), 6.11 (s, 2H), 2.94–2.88 (m, 2H), 2.87–2.82 (m, 2H), 2.65–2.59 (m, 1H), 2.25 (d, *J* = 10.8 Hz, 1H), 2.00 (s, 3H), 1.68 (s, 3H), 1.67 (s, 3H), 1.56 (s, 3H), 1.44 (s, 3H); **^{13}C NMR** ($CDCl_3$, 500 MHz): δ 201.0, 173.5, 165.9, 150.9, 148.7, 140.8, 131.4, 127.7, 122.3, 121.4, 71.9, 50.5, 39.9, 30.2, 29.9, 27.3, 26.6, 22.0, 21.8; **HRMS** (ESI) calcd for $C_{21}H_{25}O_4$ $[M+H]^+$ 341.1753, found 371.1766.

^{1}H, ^{13}C NMRs, and Selected nOE Spectra



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3.80
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1.56
0.91
0.43
0.17
0.12
SiMe3
OTBS
O
O
2a
10:1 diastereomeric mixture
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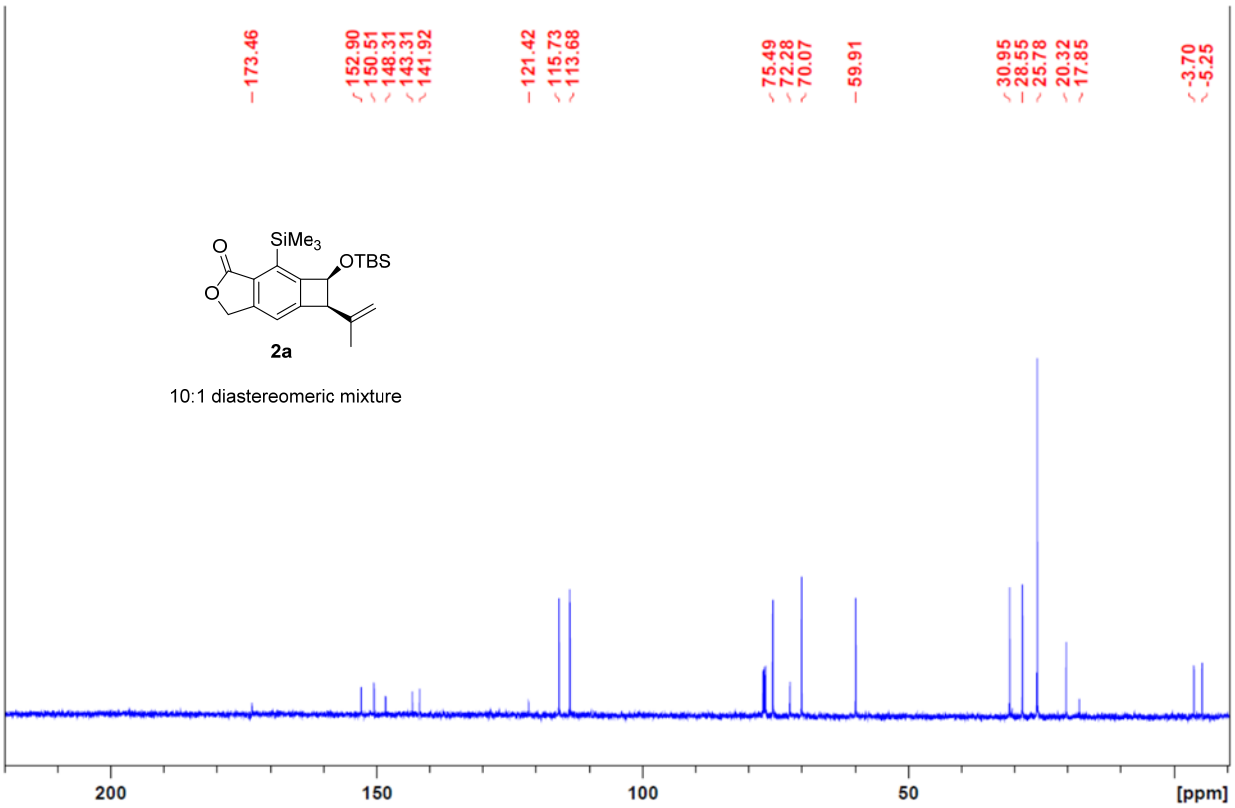
1.04
1.05
3.15
9.17
9.24
3.11
8
6
4
2
0 [ppm]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30.95
28.55
25.78
20.32
17.85
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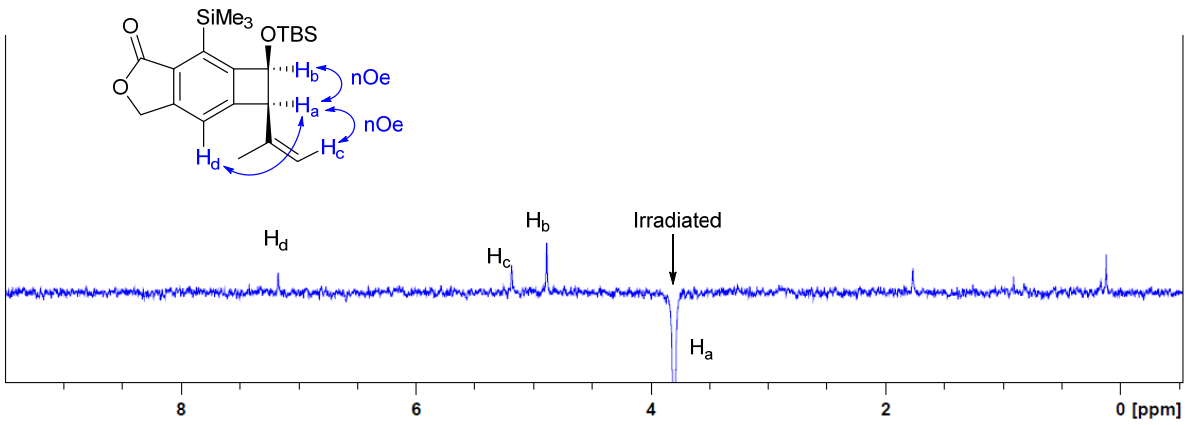
SiMe3
OTBS
O
O
2a
10:1 diastereomeric mixture
200
150
100
50
[ppm]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OTBS
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O
Hb
Ha
Hc
Hd
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nOe
Hd
Hc
Hb
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Ha
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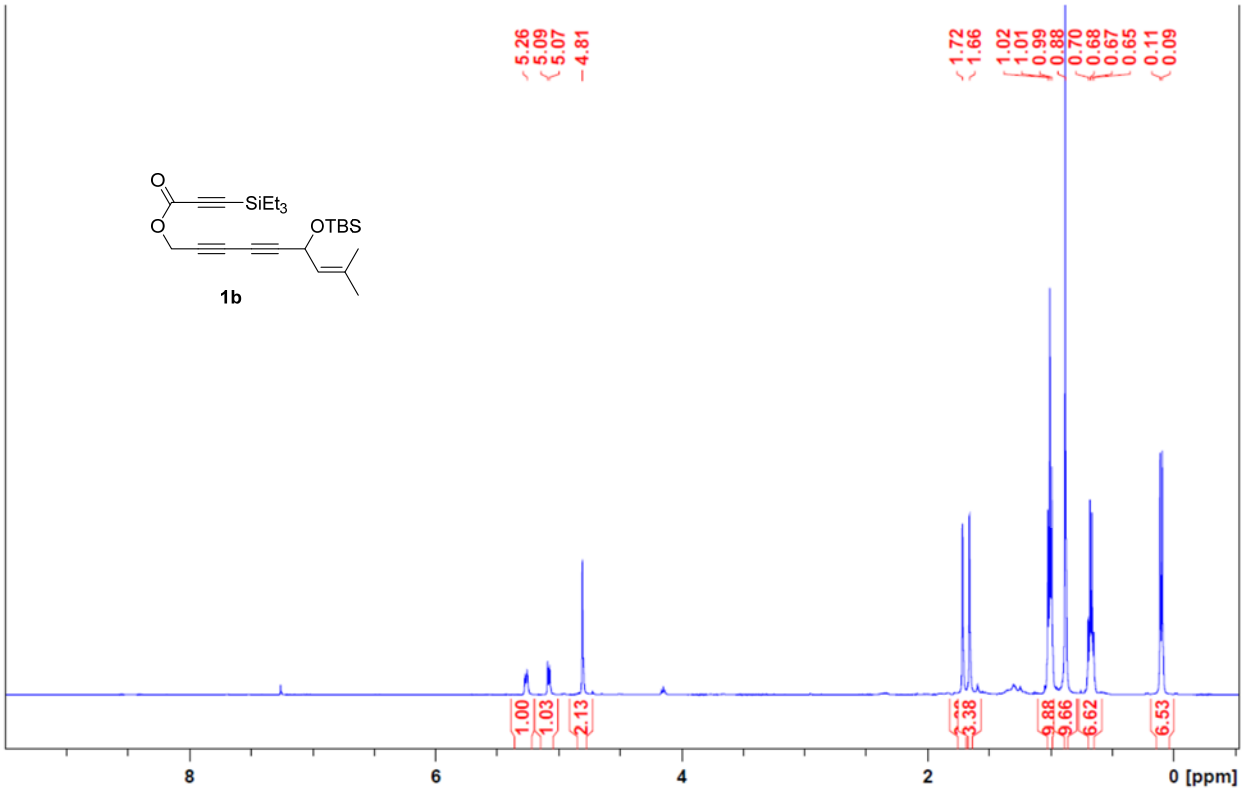
6
4
2
0 [ppm]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0.88
0.70
0.68
0.67
0.65
0.11
0.09
SiEt3
OTBS
1b
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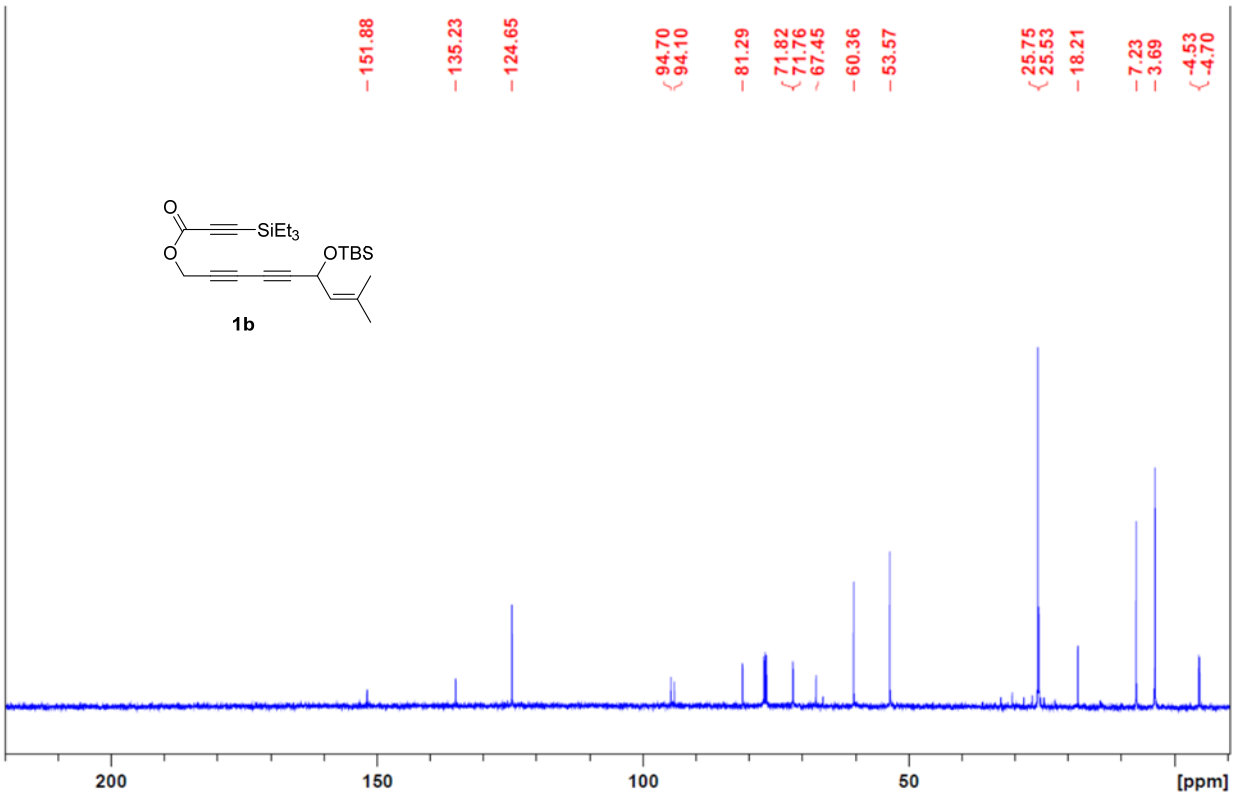
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SiEt3
OTBS
1b
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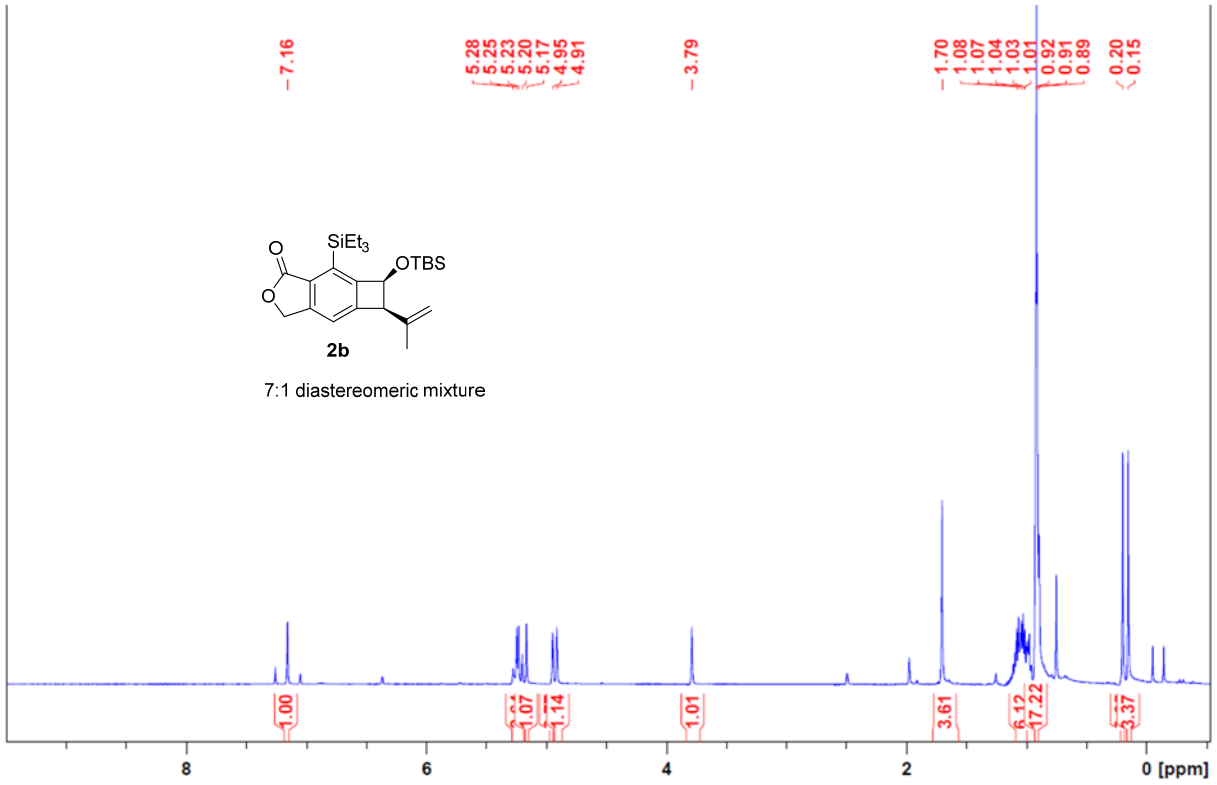
50
[ppm]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4.91
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1.08
1.07
1.04
1.03
1.01
0.92
0.91
0.89
0.20
0.15
SiEt3
OTBS
O
O
2b
7:1 diastereomeric mixture
1.00
1.07
1.14
1.01
3.61
6.12
17.22
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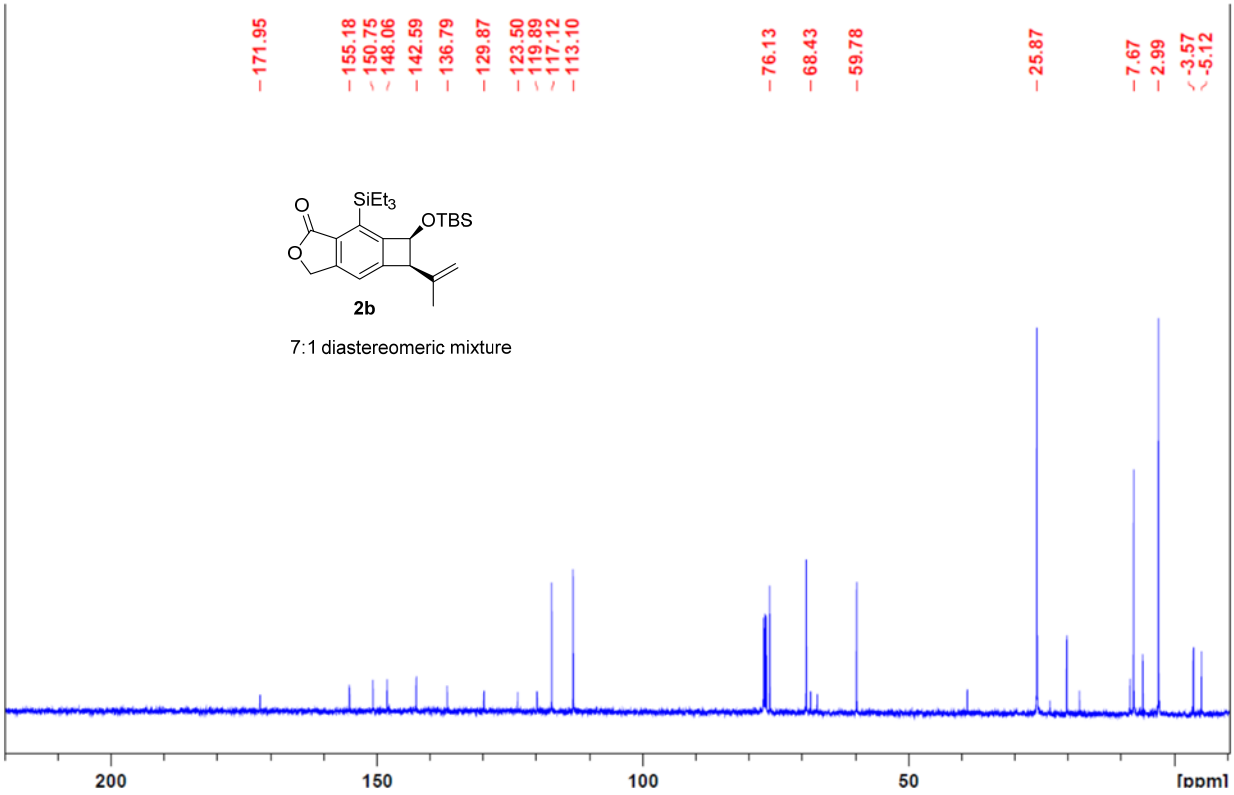
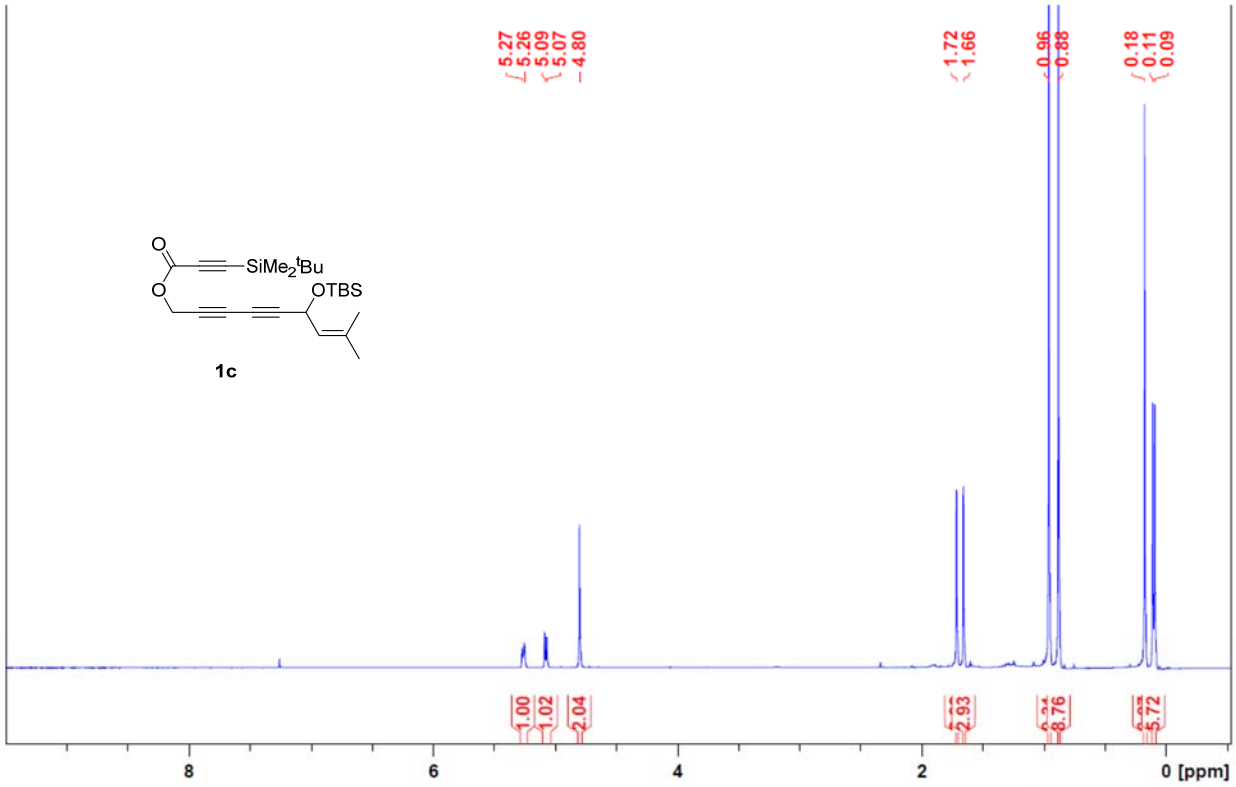
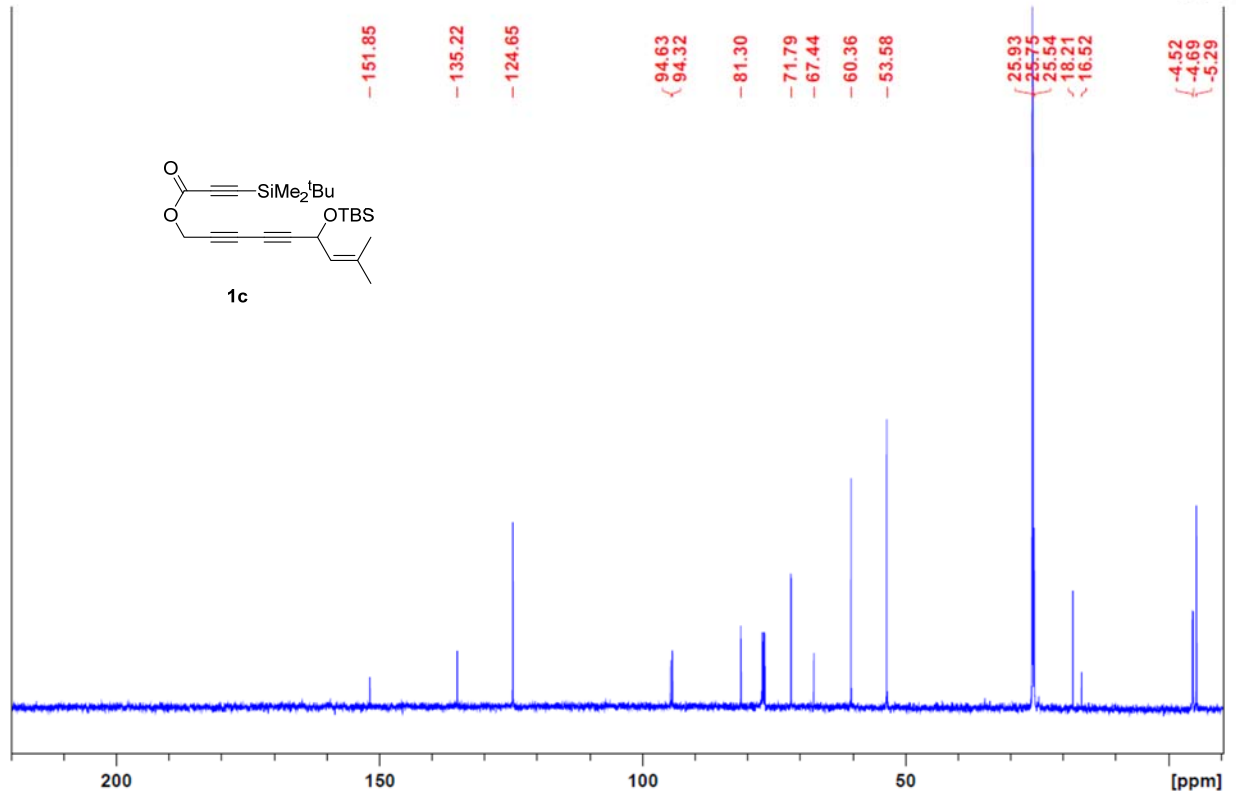
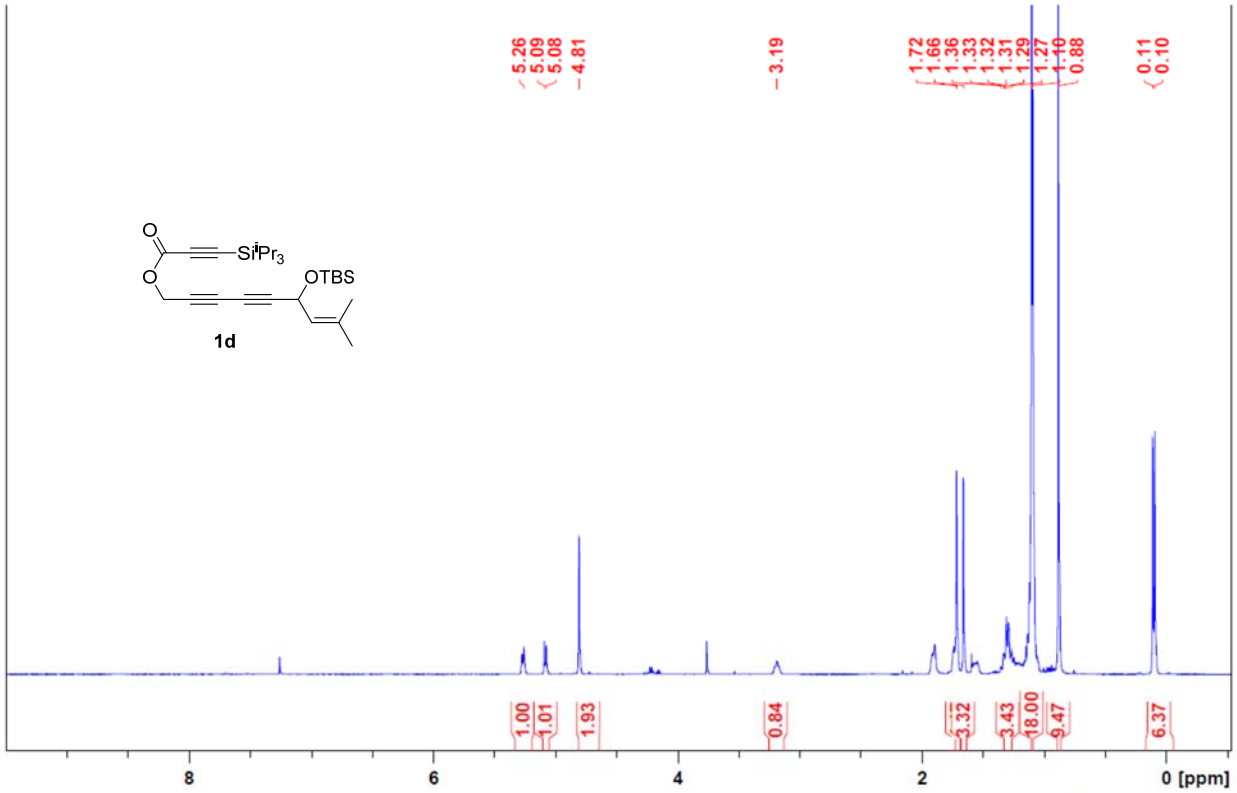
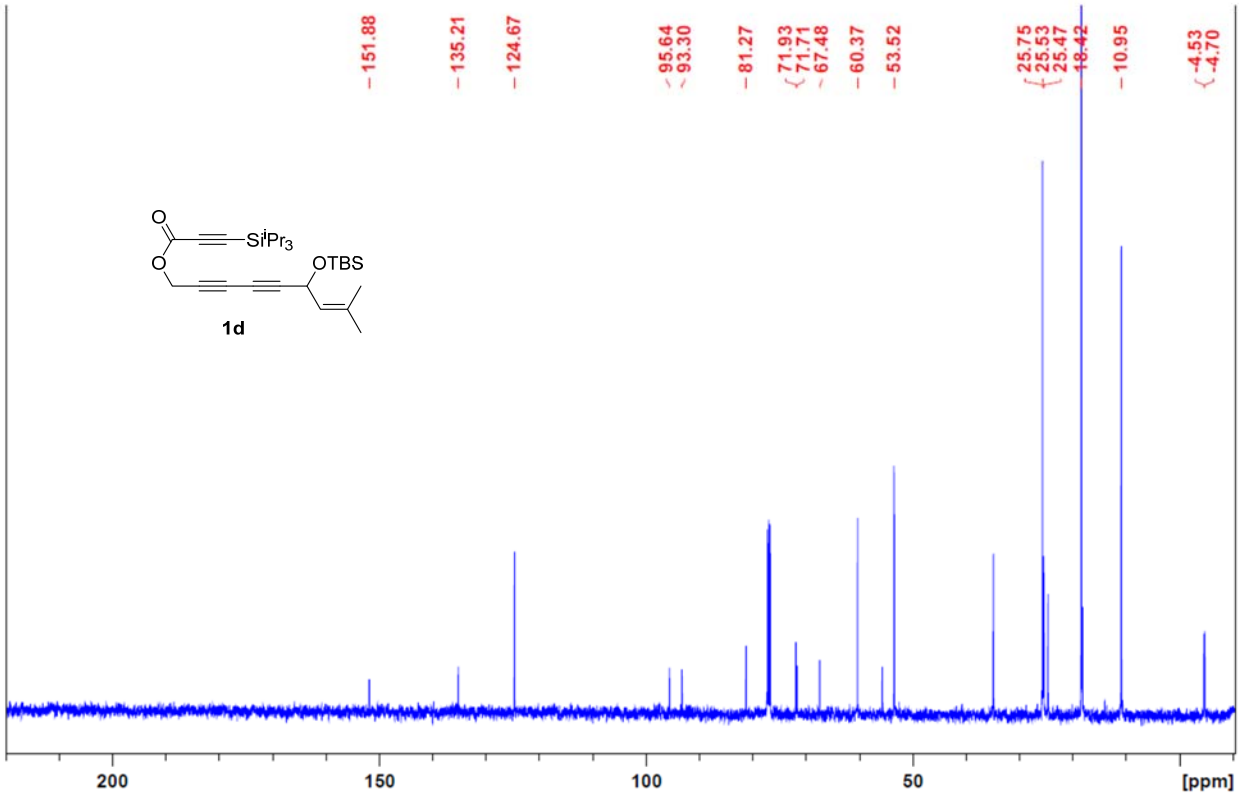
8
6
4
2
0 [ppm]

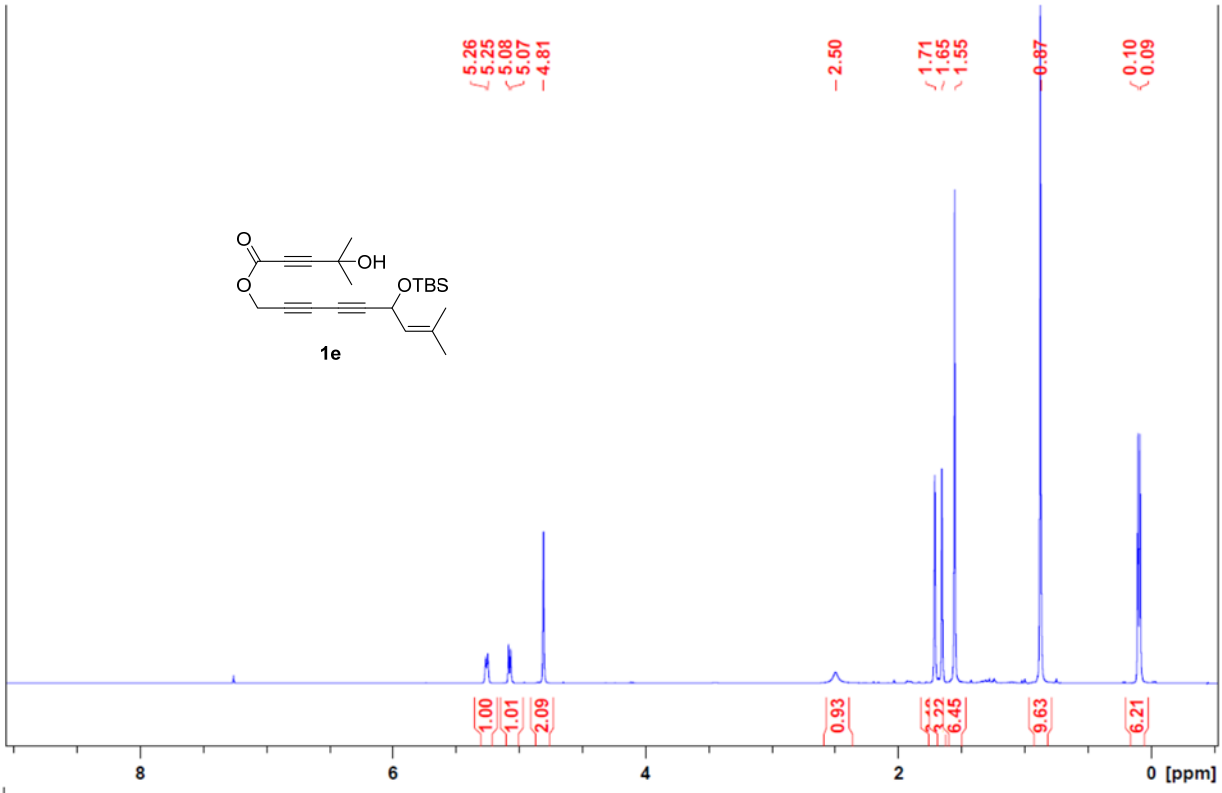

171.95
155.18
150.75
148.06
142.59
136.79
129.87
123.50
119.89
117.12
113.10
76.13
68.43
59.78
25.87
7.67
2.99
-3.57
-5.12
SiEt3
OTBS
O
O
2b
7:1 diastereomeric mixture
200
150
100
50
[ppm]

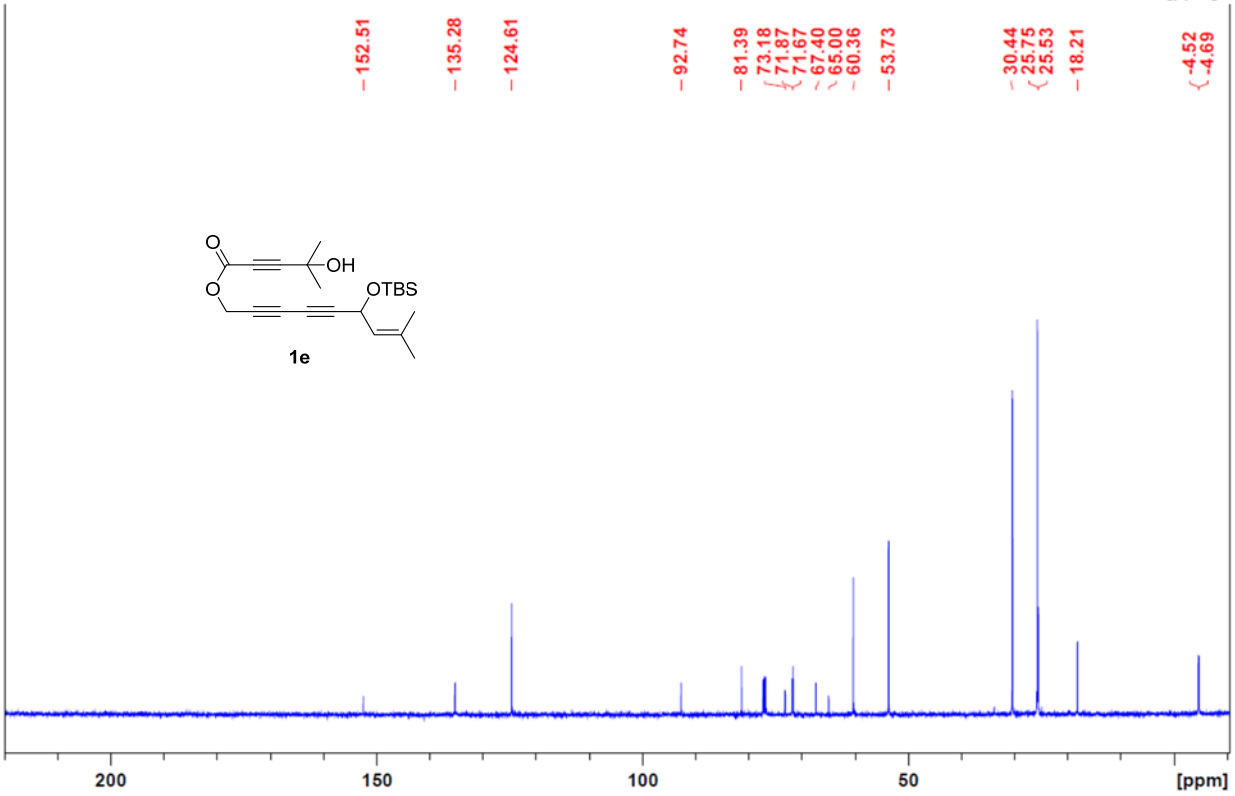

5.27
5.26
5.09
5.07
4.80
1.72
1.66
0.96
0.88
0.18
0.11
0.09
1.00
1.02
2.04
2.93
8.76
5.72
8
6
4
2
0 [ppm]
SiMe2tBu
OTBS
1c

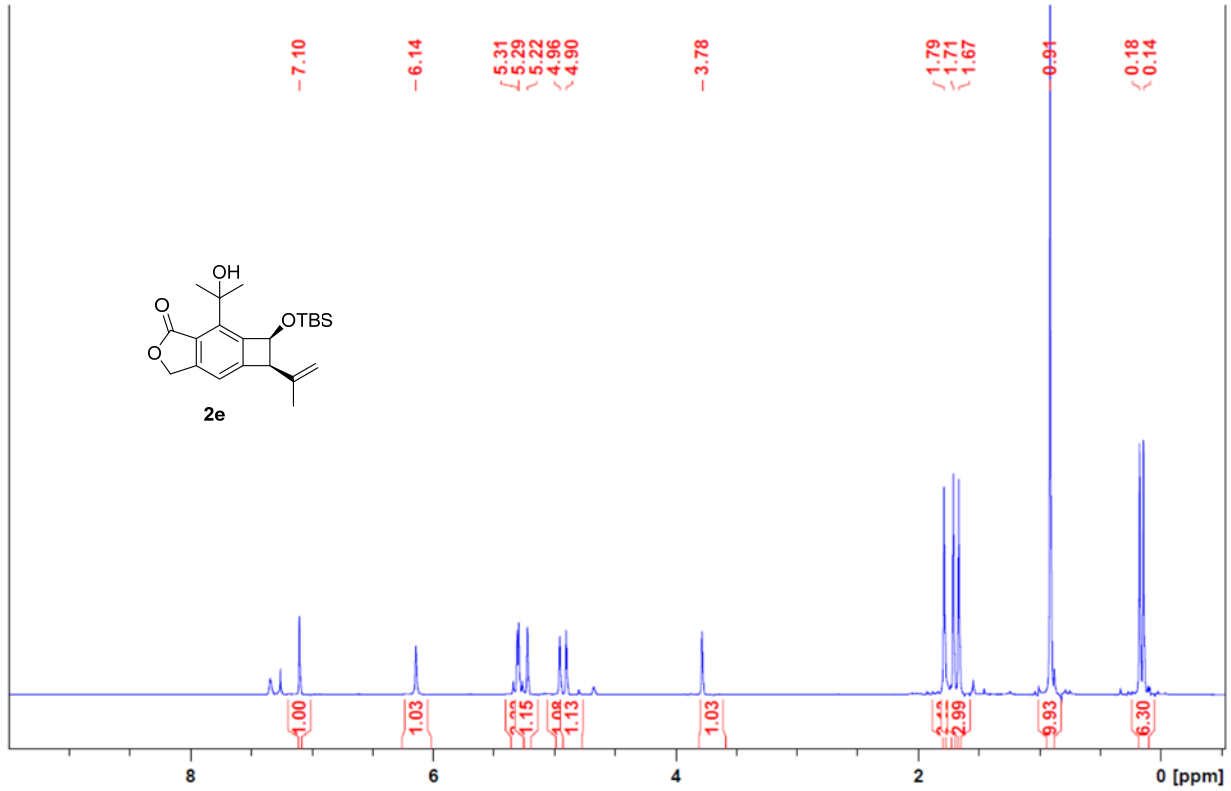

151.85
135.22
124.65
94.63
94.32
81.30
71.79
67.44
60.36
53.58
25.93
25.75
25.54
18.21
16.52
-4.52
-4.69
-5.29
200
150
100
50
[ppm]
SiMe2tBu
OTBS
1c

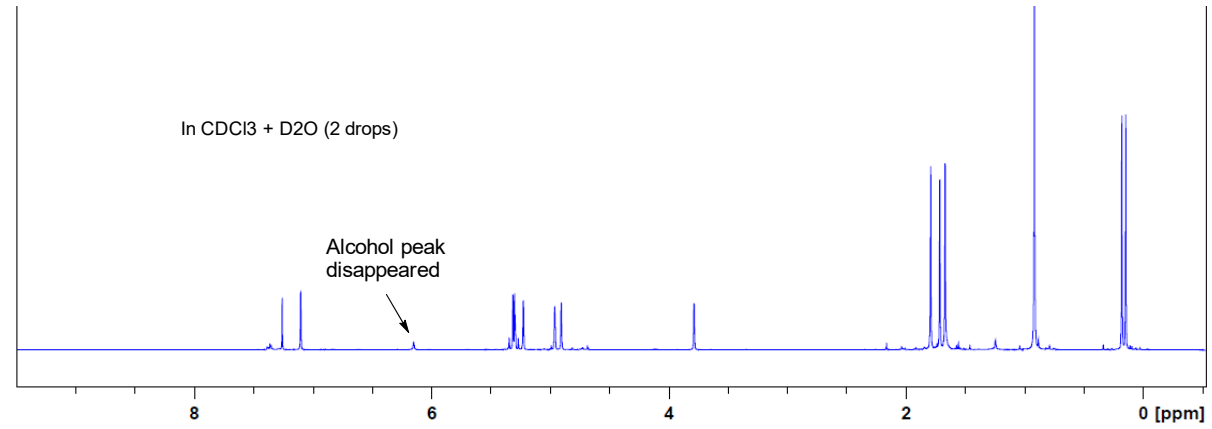

5.26
5.09
5.08
4.81
3.19
1.72
1.66
1.36
1.33
1.32
1.31
1.29
1.27
1.10
0.88
0.11
0.10
1.00
1.01
1.93
0.84
3.32
3.43
18.00
9.47
6.37
8
6
4
2
0 [ppm]
OTBS
1d

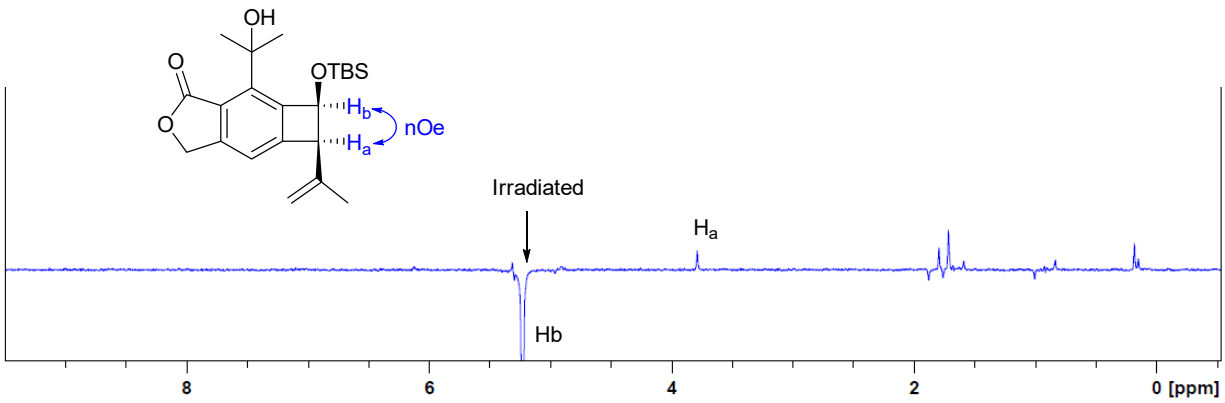

151.88
135.21
124.67
95.64
93.30
81.27
71.93
71.71
67.48
60.37
53.52
25.75
25.53
25.47
18.42
10.95
-4.53
-4.70
200
150
100
50
[ppm]
OTBS
1d

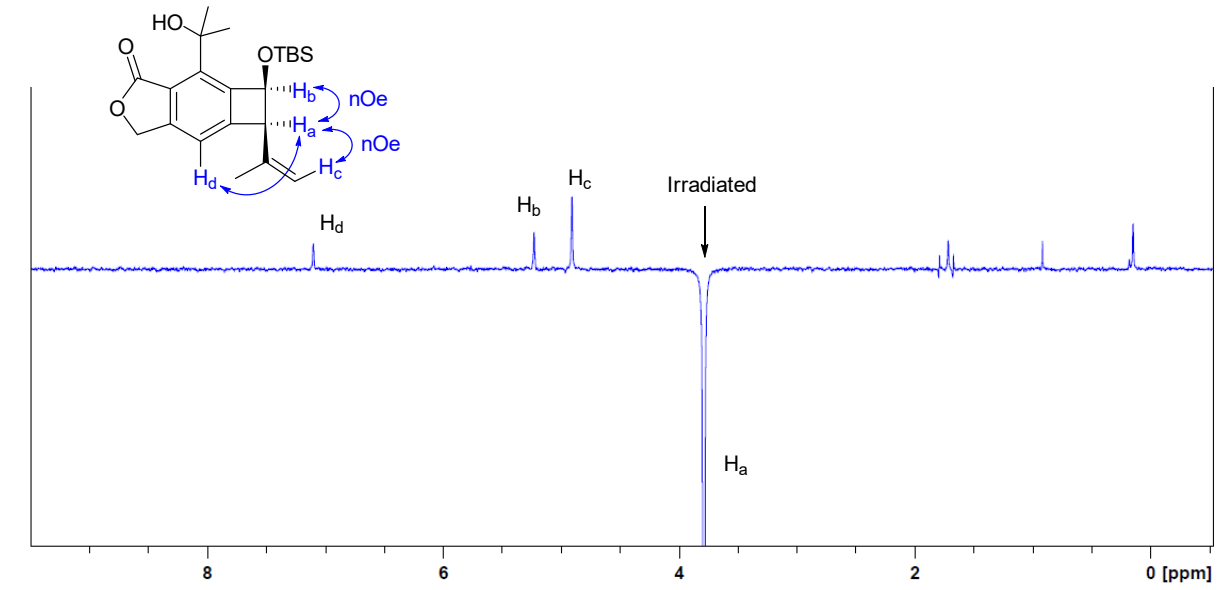

5.26
5.25
5.08
5.07
4.81
2.50
1.71
1.65
1.55
0.87
0.10
0.09
OH
OTBS
1e
1.00
1.01
2.09
0.93
6.45
9.63
6.21
8
6
4
2
0
[ppm]

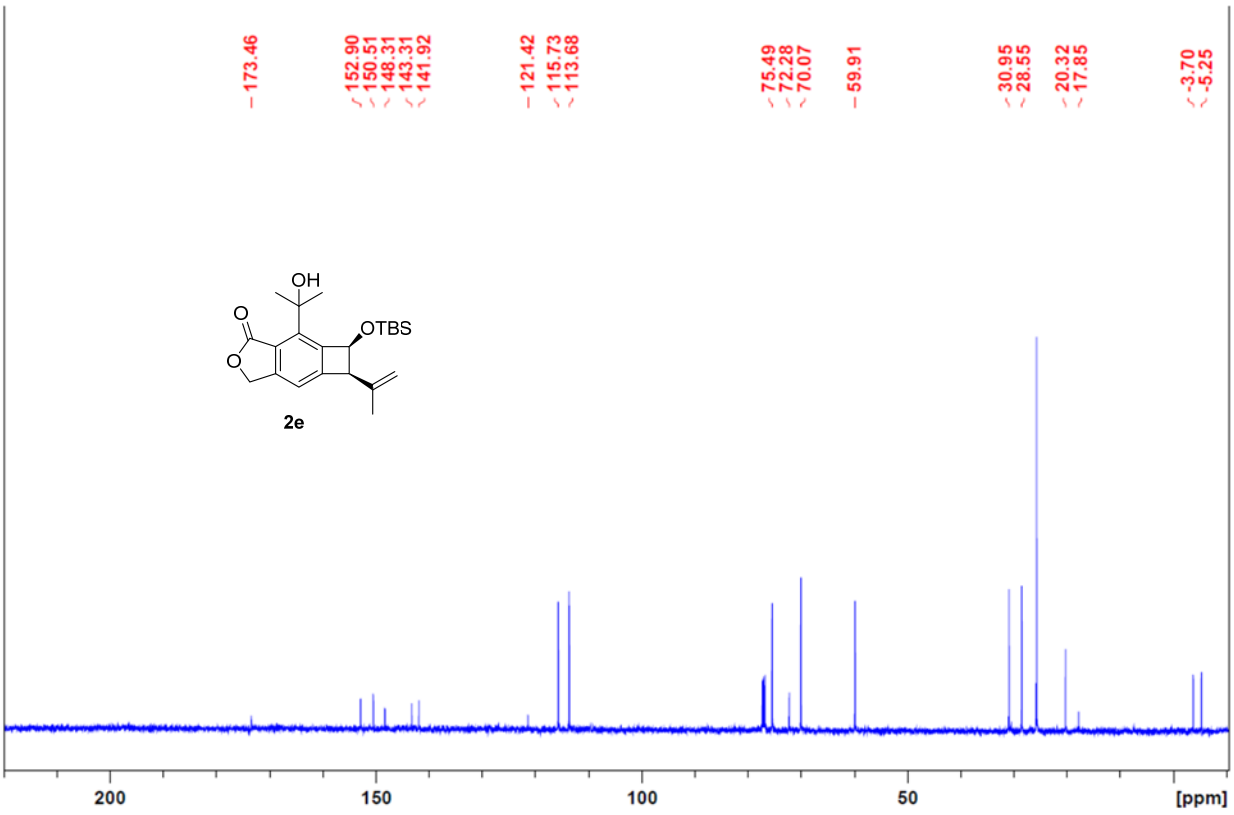

152.51
135.28
124.61
92.74
81.39
73.18
71.87
71.67
67.40
65.00
60.36
53.73
30.44
25.75
25.53
18.21
-4.52
-4.69
OH
OTBS
1e
200
150
100
50
[ppm]

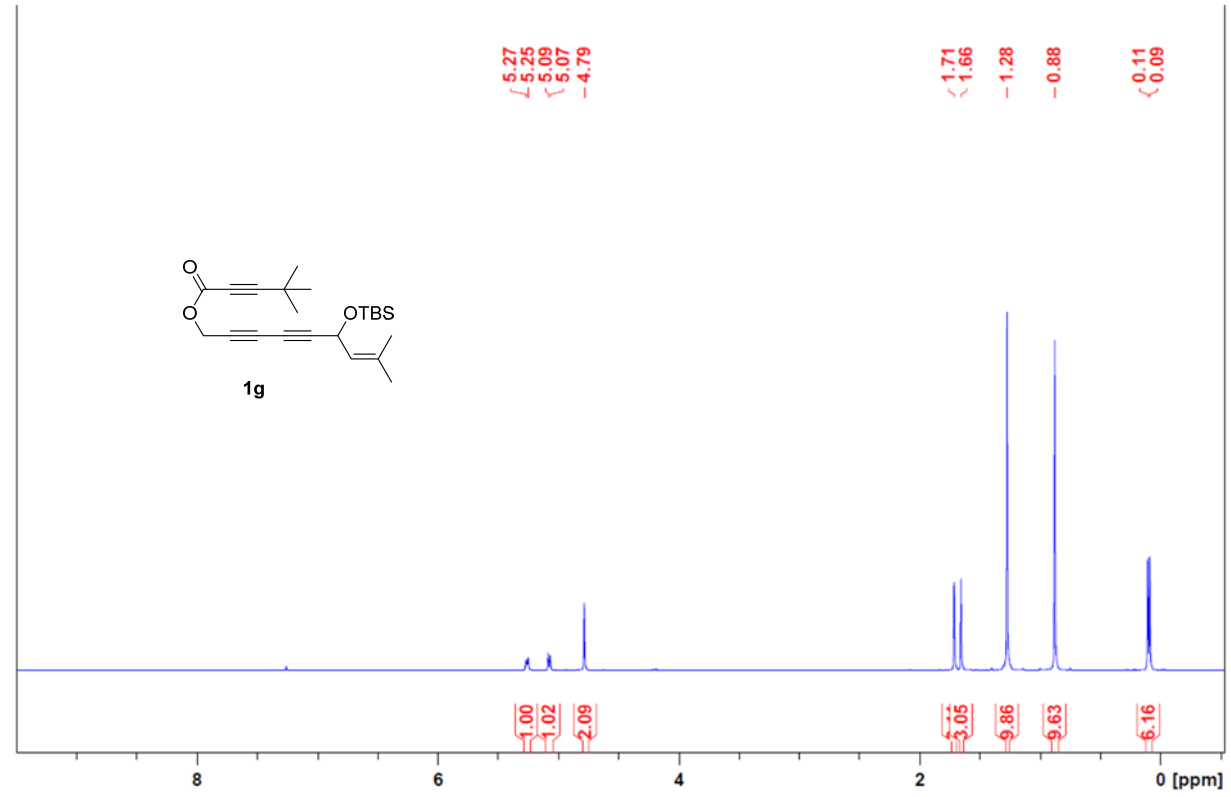

7.10
6.14
5.31
5.29
5.22
4.96
4.90
3.78
1.79
1.71
1.67
0.91
0.18
0.14
OH
O
O
OTBS
2e
1.00
1.03
1.15
1.08
1.13
1.03
2.99
9.93
6.30
8
6
4
2
0 [ppm]

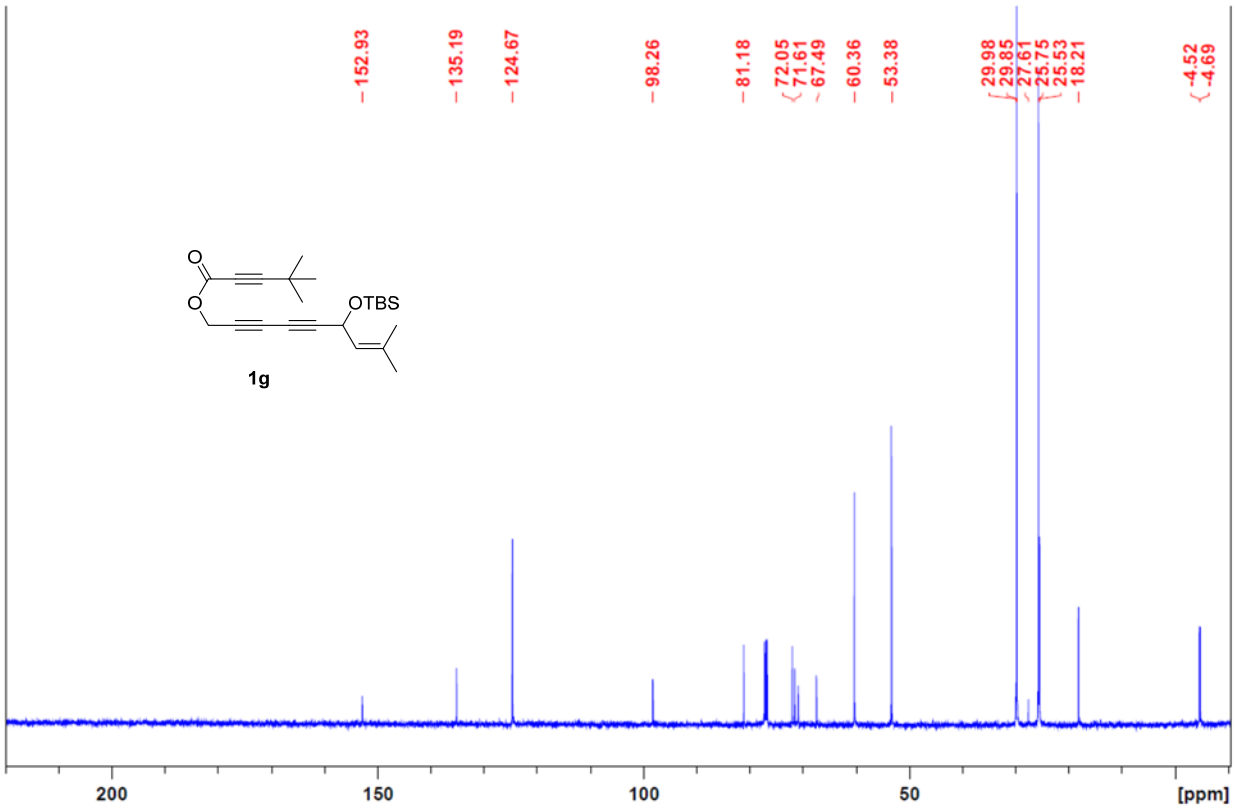

In CDCl3 + D2O (2 drops)
Alcohol peak
disappeared
8
6
4
2
0 [ppm]

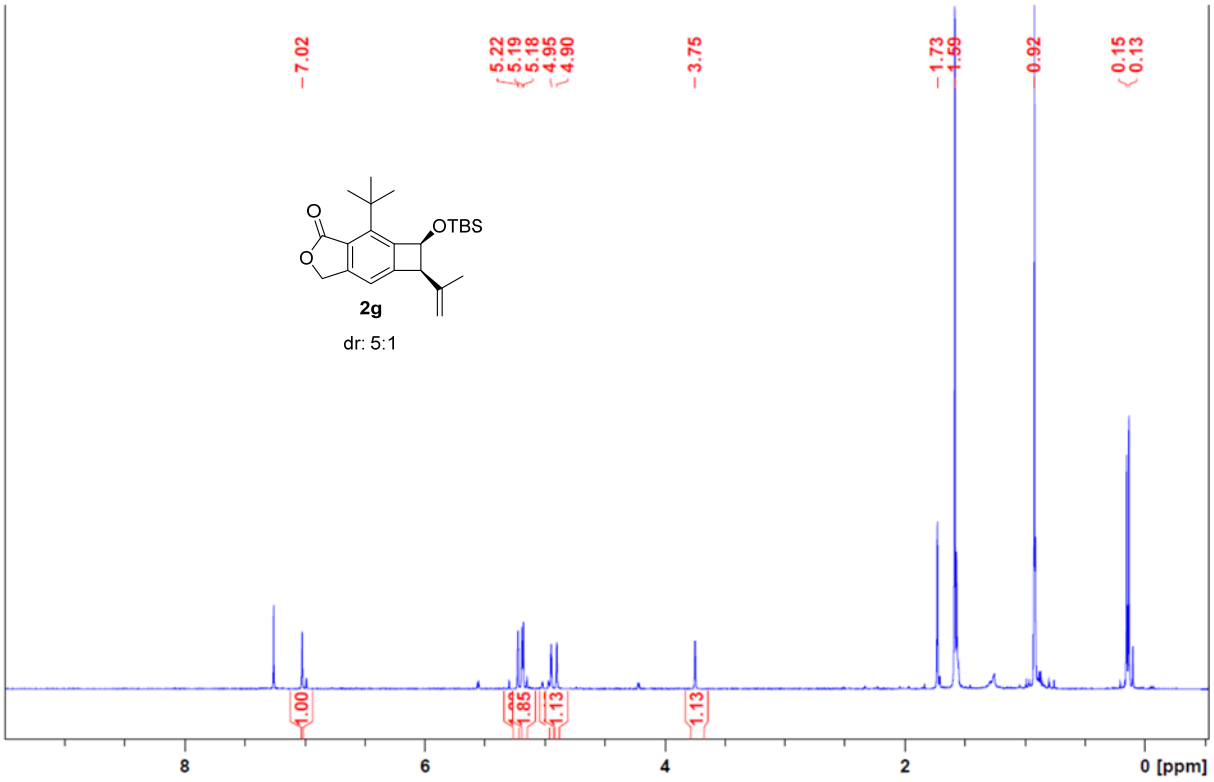

OH
O
O
OTBS
Hb
Ha
nOe
Irradiated
Ha
Hb
8
6
4
2
0 [ppm]

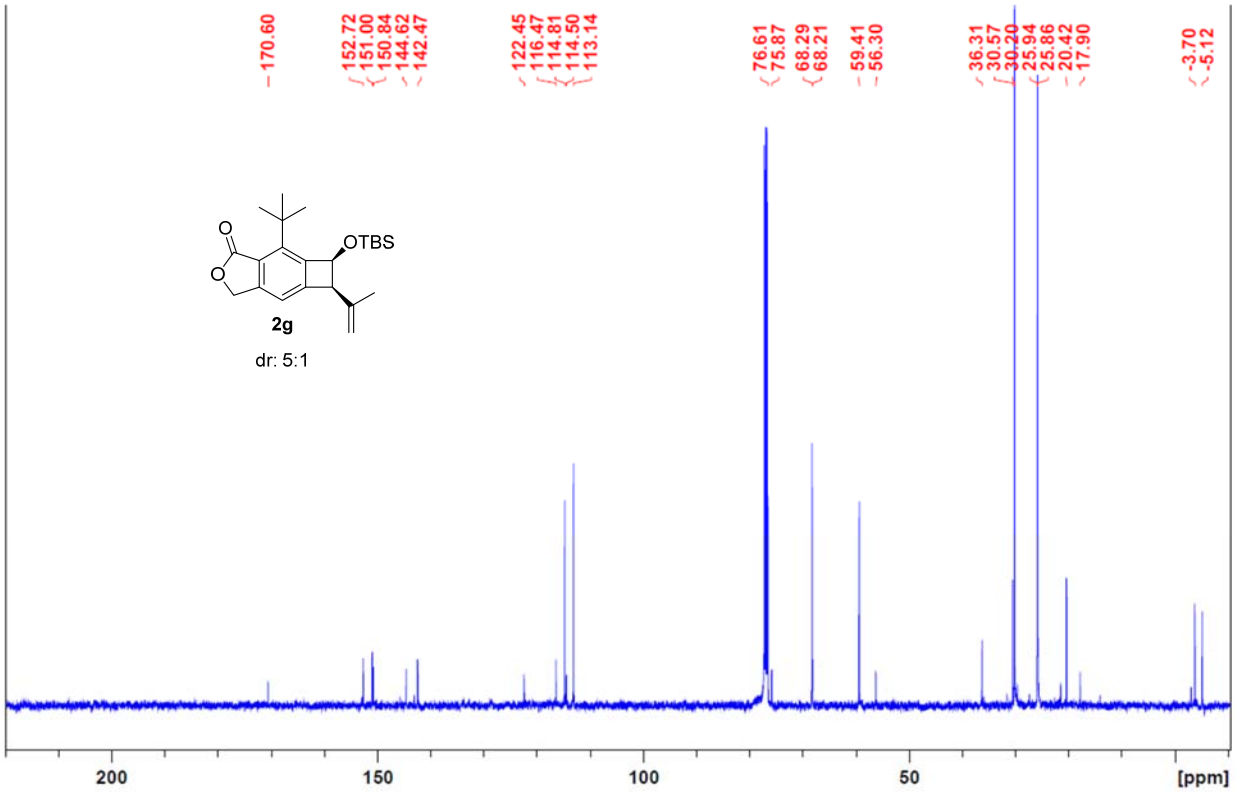

HO
O
O
OTBS
Hb
Ha
Hc
Hd
nOe
nOe
Irradiated
Hd
Hb
Hc
Ha
8
6
4
2
0 [ppm]

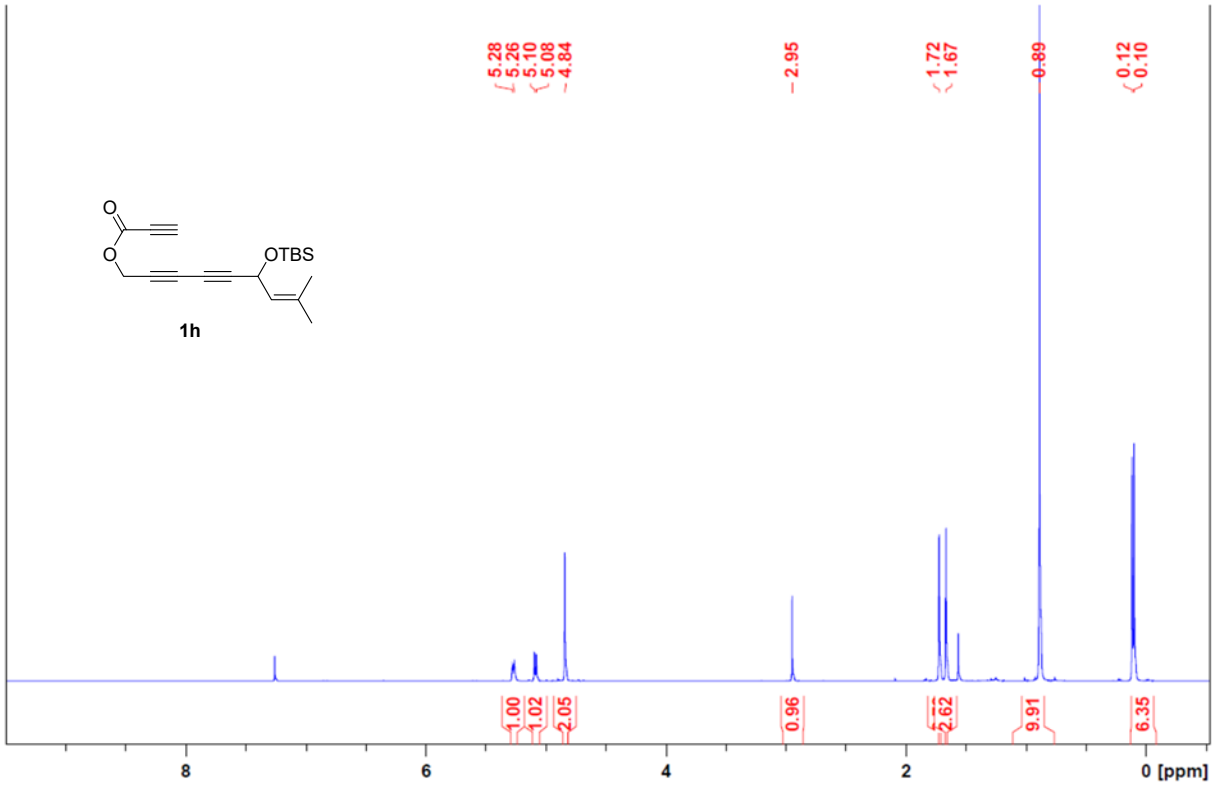

173.46
152.90
150.51
148.31
143.31
141.92
121.42
115.73
113.68
75.49
72.28
70.07
59.91
30.95
28.55
20.32
17.85
-3.70
-5.25
OH
O
O
OTBS
2e
200
150
100
50
[ppm]

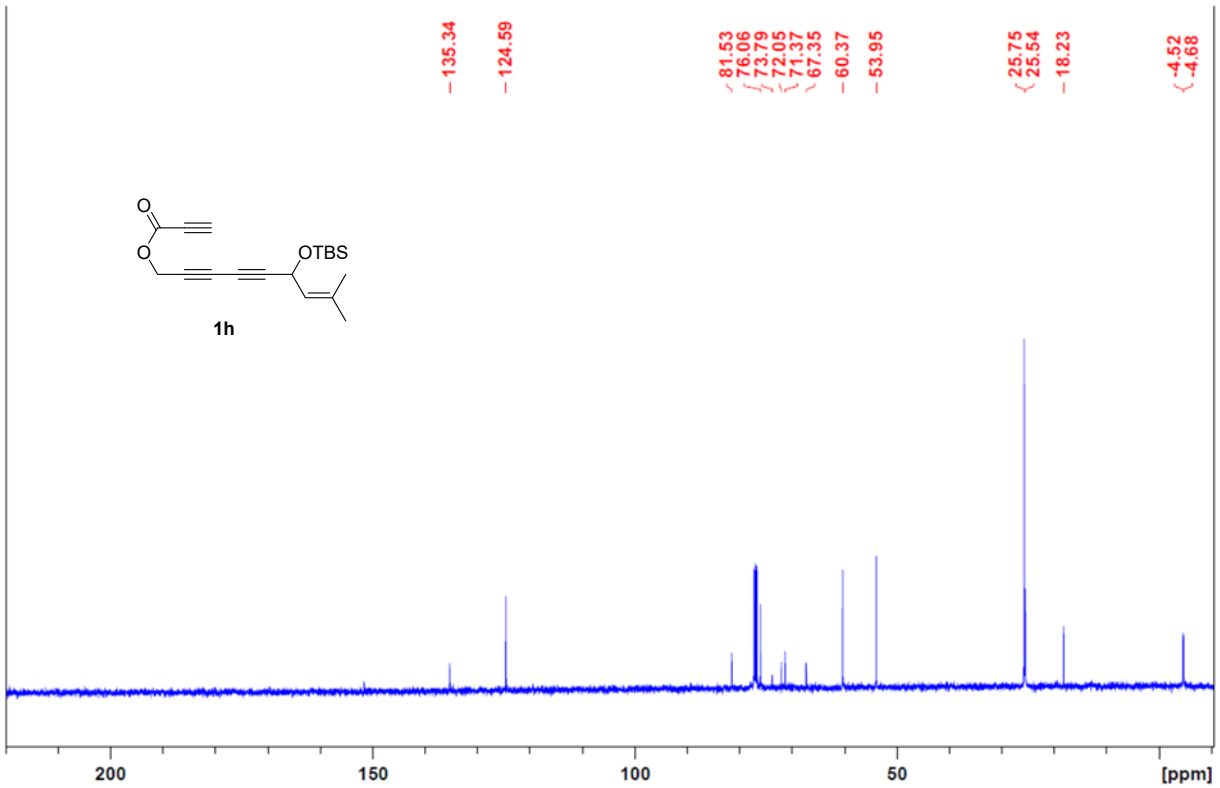

5.27
5.25
5.09
5.07
4.79
1.71
1.66
1.28
0.88
0.11
0.09
OTBS
1g
1.00
1.02
2.09
3.05
9.86
9.63
6.16
8
6
4
2
0 [ppm]

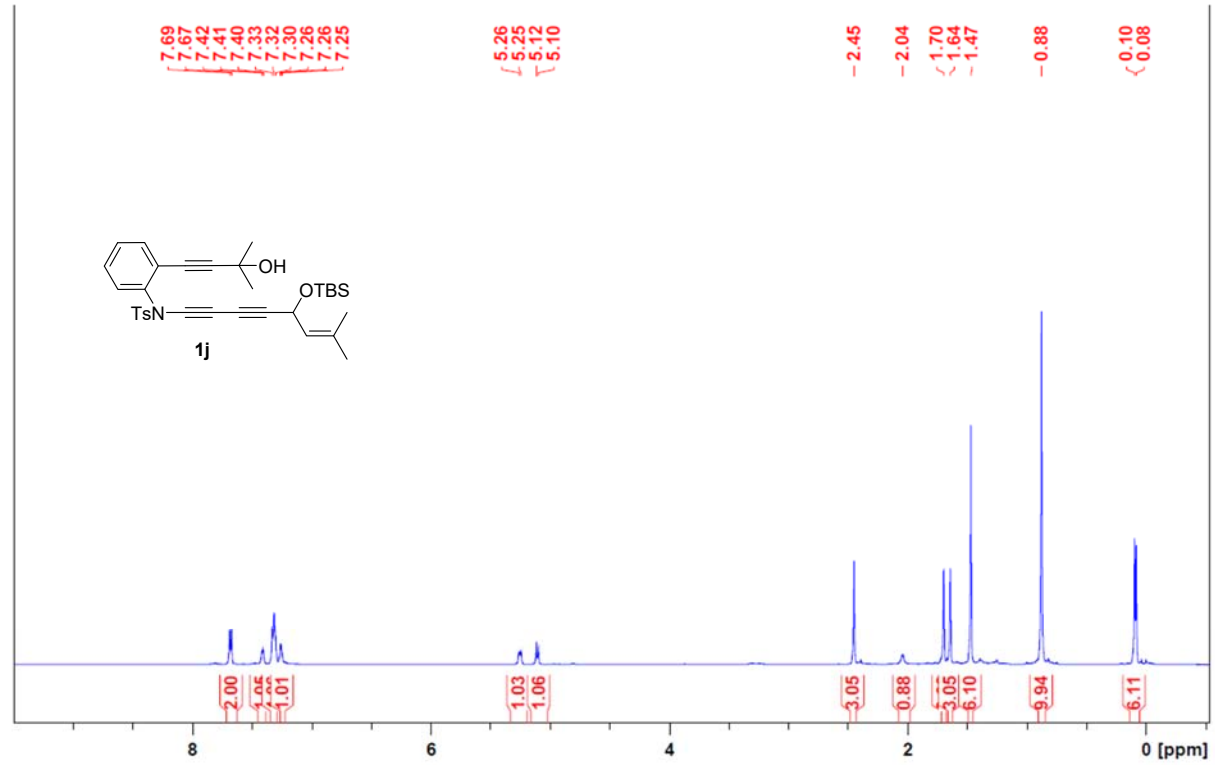

152.93
135.19
124.67
98.26
81.18
72.05
71.61
67.49
60.36
53.38
29.98
29.85
27.61
25.75
25.53
18.21
-4.52
-4.69
OTBS
1g
200
150
100
50
[ppm]

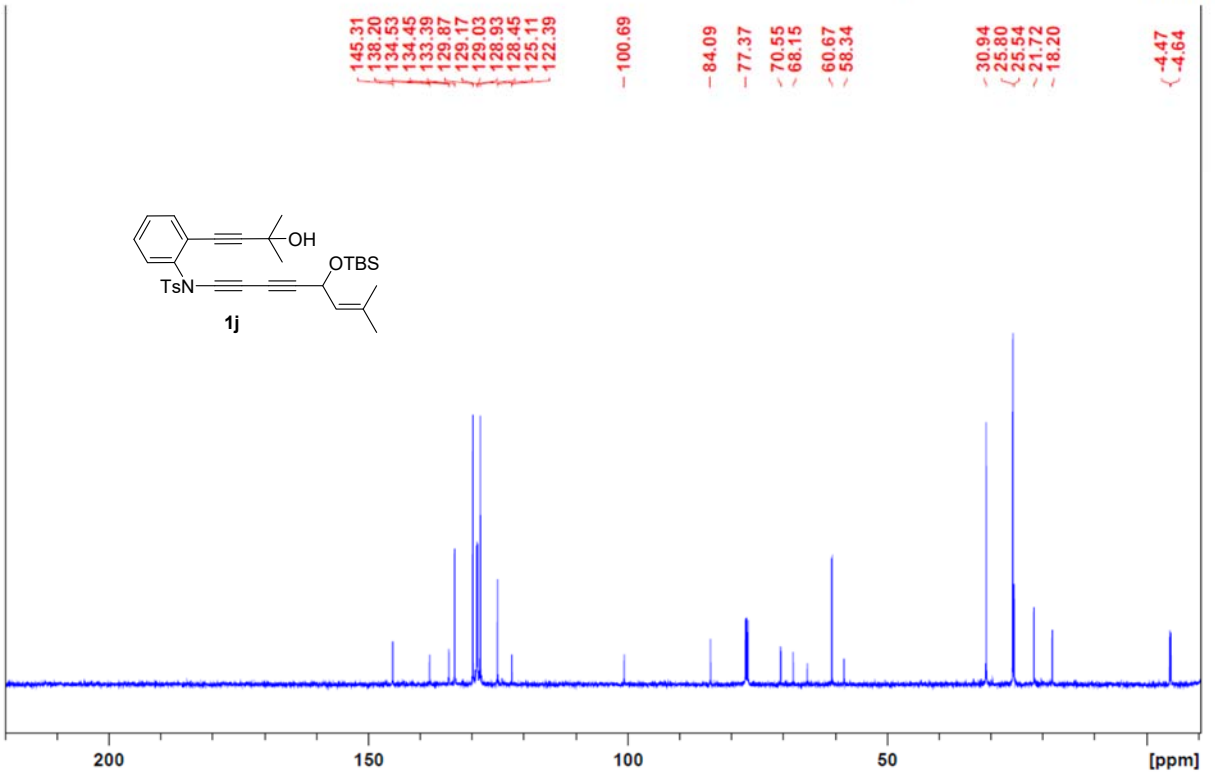

7.02
5.22
5.19
5.18
4.95
4.90
3.75
1.73
1.59
0.92
0.15
0.13
OTBS
2g
dr: 5:1
1.00
1.85
1.13
1.13
8
6
4
2
0 [ppm]

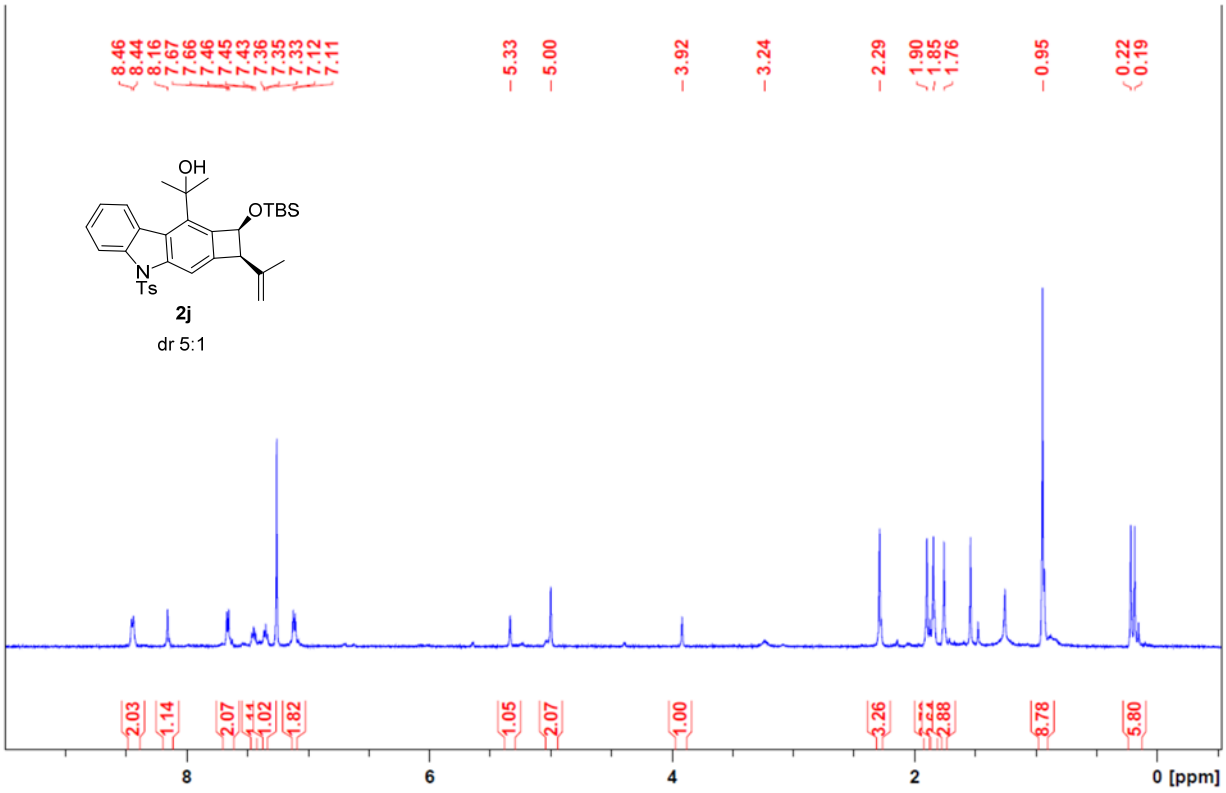

170.60
152.72
151.00
150.84
144.62
142.47
122.45
116.47
114.81
114.50
113.14
76.61
75.87
68.29
68.21
59.41
56.30
36.31
30.57
30.20
25.94
25.86
20.42
17.90
-3.70
-5.12
OTBS
2g
dr: 5:1
200
150
100
50
[ppm]

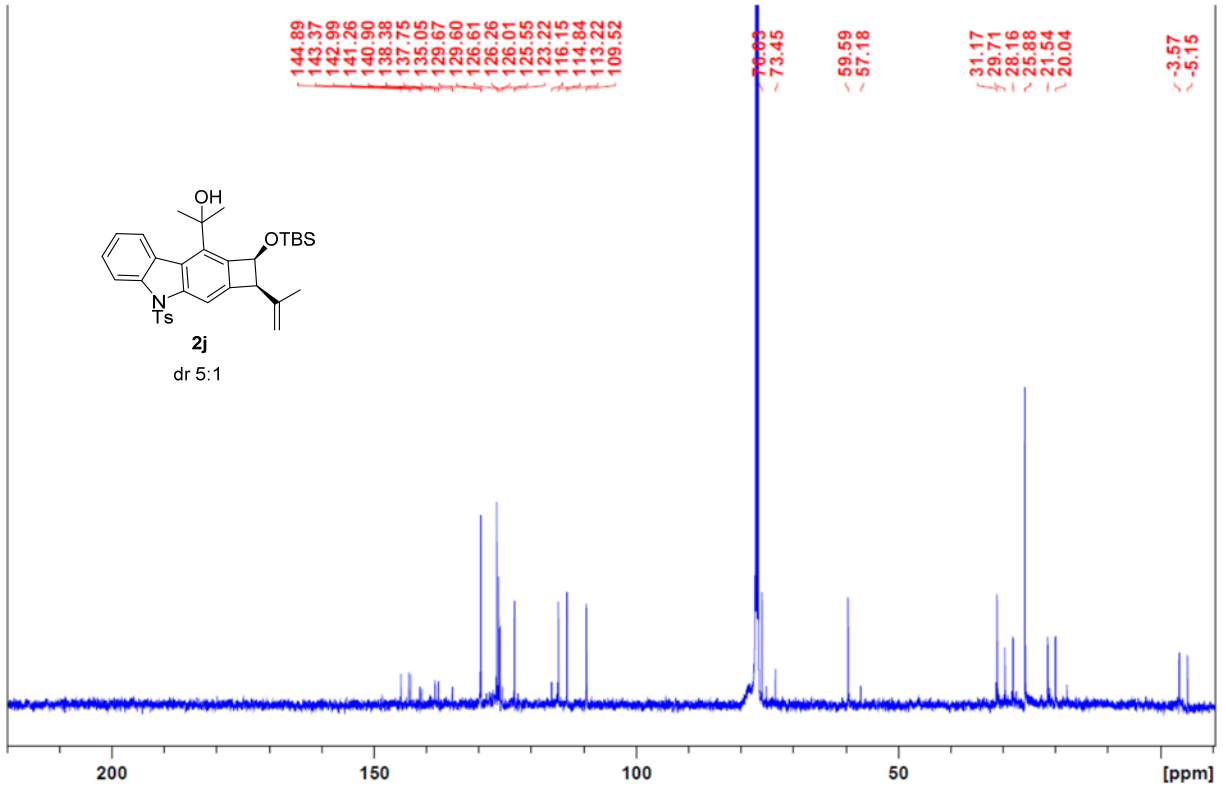

5.28
5.26
5.10
5.08
4.84
2.95
1.72
1.67
0.89
0.12
0.10
OTBS
1h
1.00
1.02
2.05
0.96
2.62
9.91
6.35
8
6
4
2
0 [ppm]

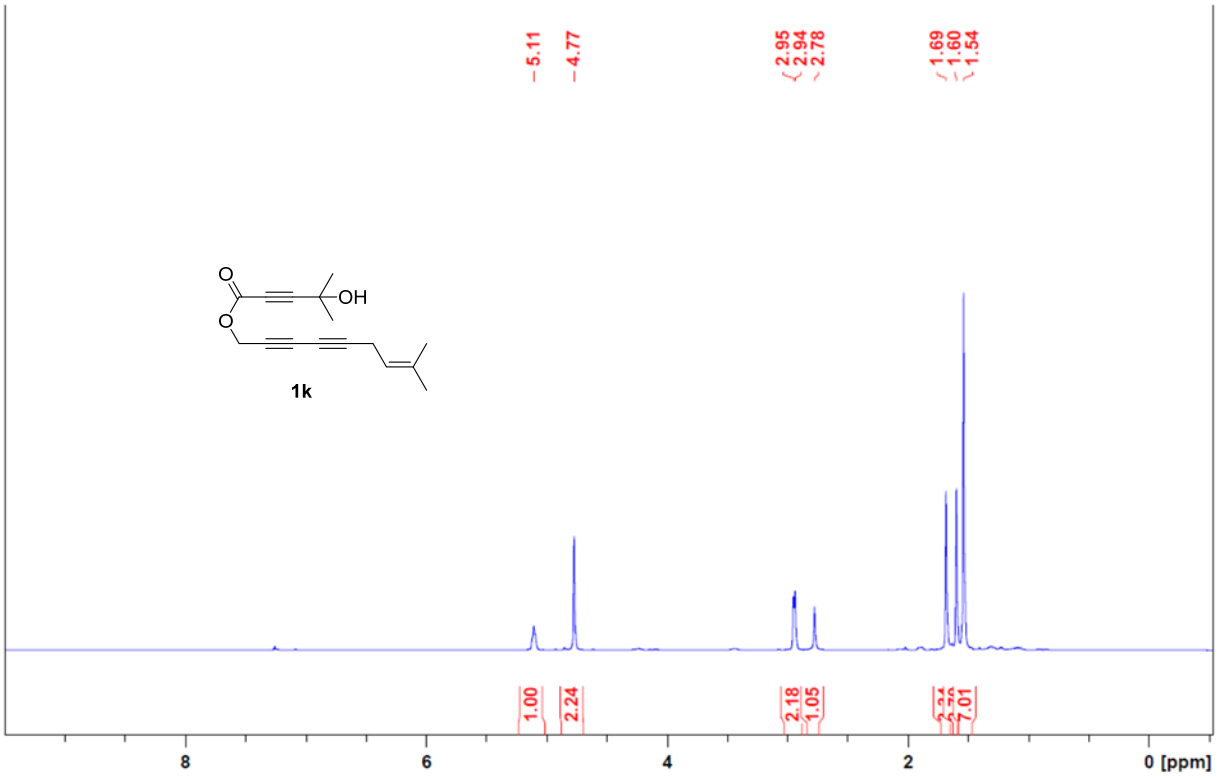

135.34
124.59
81.53
76.06
73.79
72.05
71.37
67.35
60.37
53.95
25.75
25.54
18.23
-4.52
-4.68
OTBS
1h
200
150
100
50
[ppm]

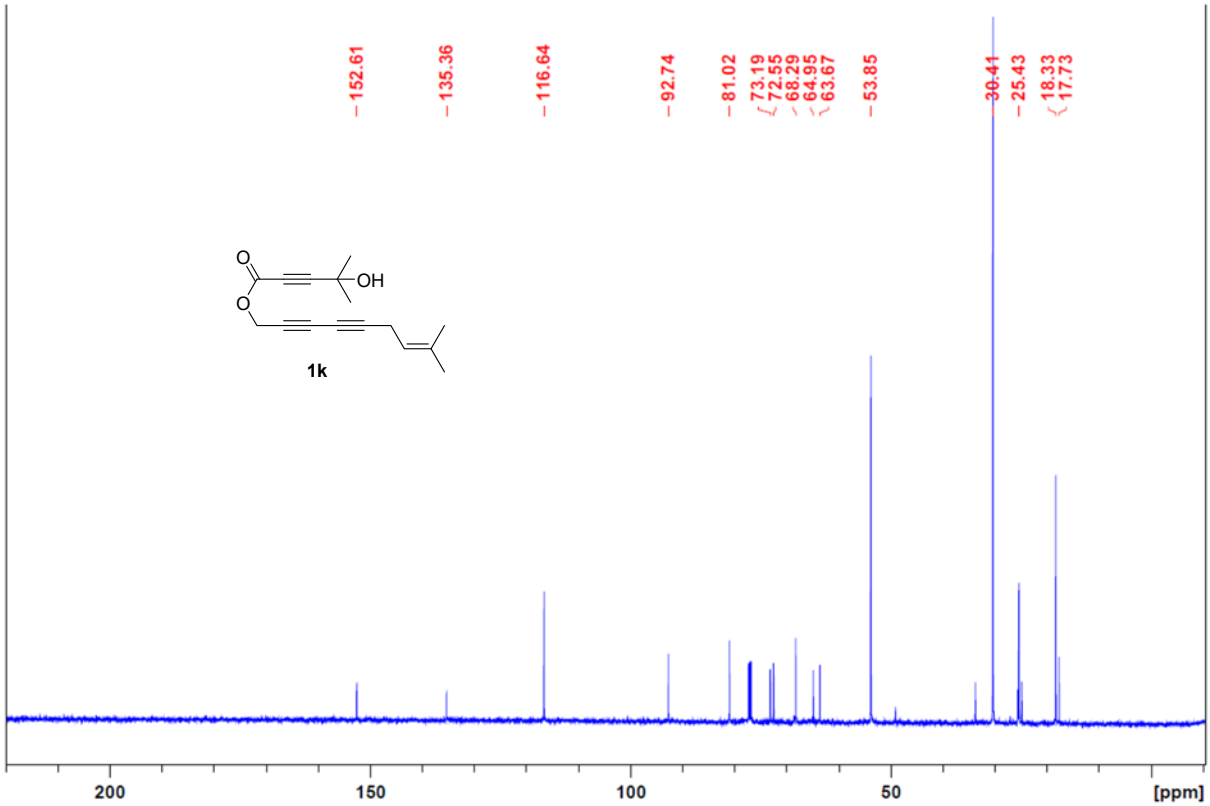

7.69
7.67
7.42
7.41
7.40
7.33
7.32
7.30
7.26
7.26
7.25
5.26
5.25
5.12
5.10
2.45
2.04
1.70
1.64
1.47
0.88
0.10
0.08
OH
OTBS
TsN
1j
2.00
1.01
1.03
1.06
3.05
0.88
3.05
6.10
9.94
6.11
8
6
4
2
0 [ppm]

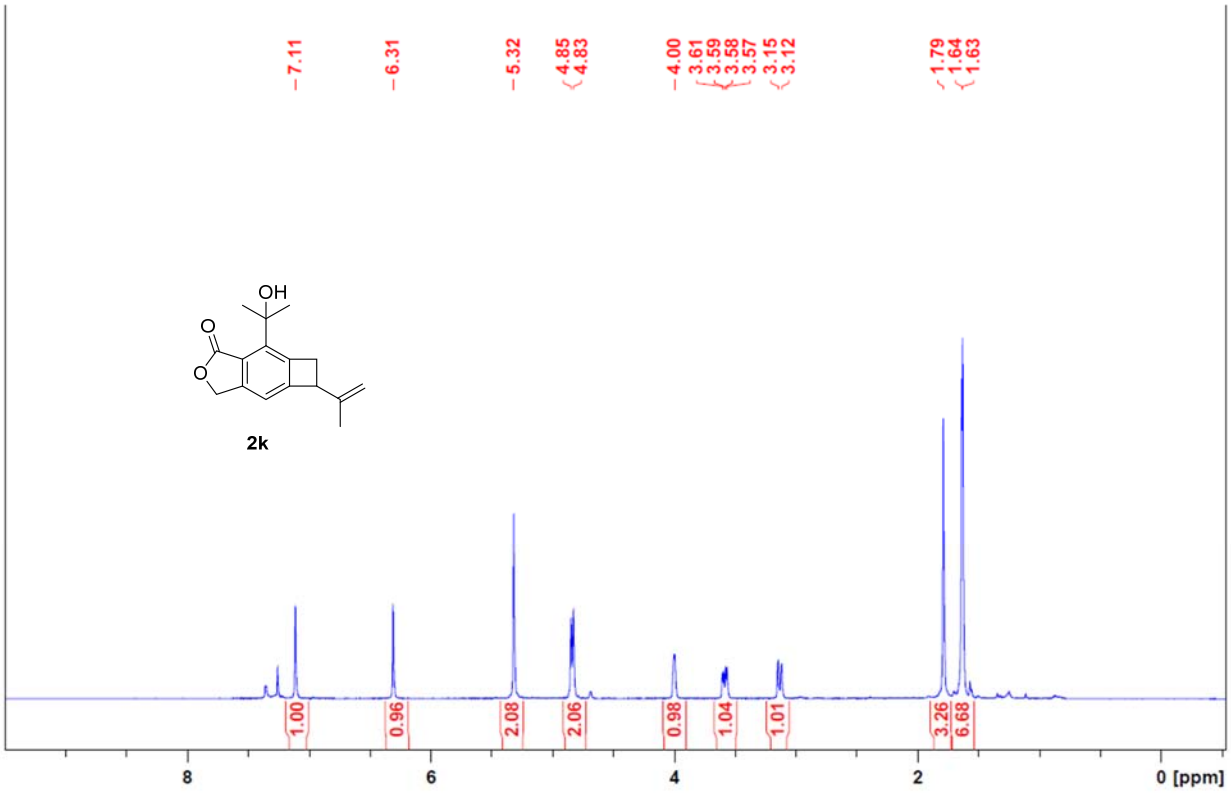

145.31
138.20
134.53
134.45
133.39
129.87
129.17
129.03
128.93
128.45
125.11
122.39
100.69
84.09
77.37
70.55
68.15
60.67
58.34
30.94
25.80
25.54
21.72
18.20
-4.47
-4.64
OH
OTBS
TsN
1j
200
150
100
50
[ppm]

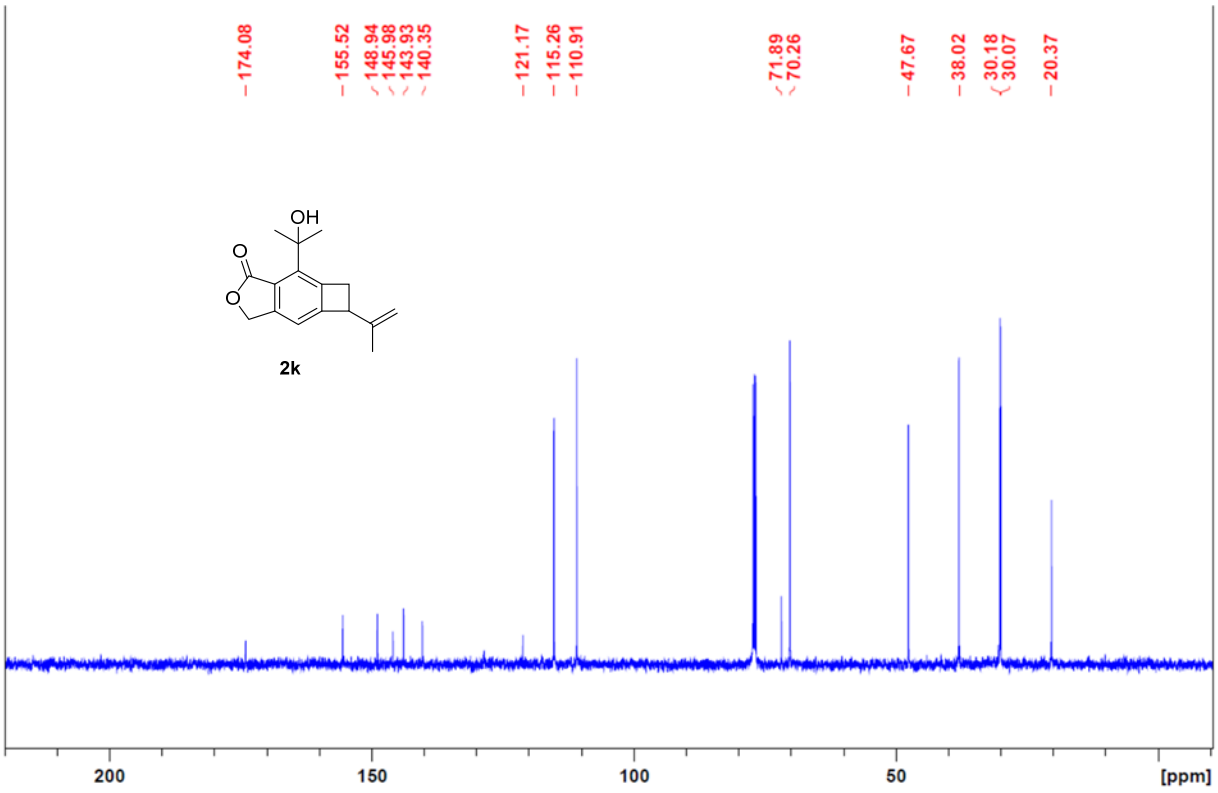

8.46
8.44
8.16
7.67
7.66
7.46
7.45
7.43
7.36
7.35
7.33
7.12
7.11
5.33
5.00
3.92
3.24
2.29
1.90
1.85
1.76
0.95
0.22
0.19
OH
OTBS
N
Ts
2j
dr 5:1
2.03
1.14
2.07
1.02
1.82
1.05
2.07
1.00
3.26
2.88
8.78
5.80
8
6
4
2
0 [ppm]

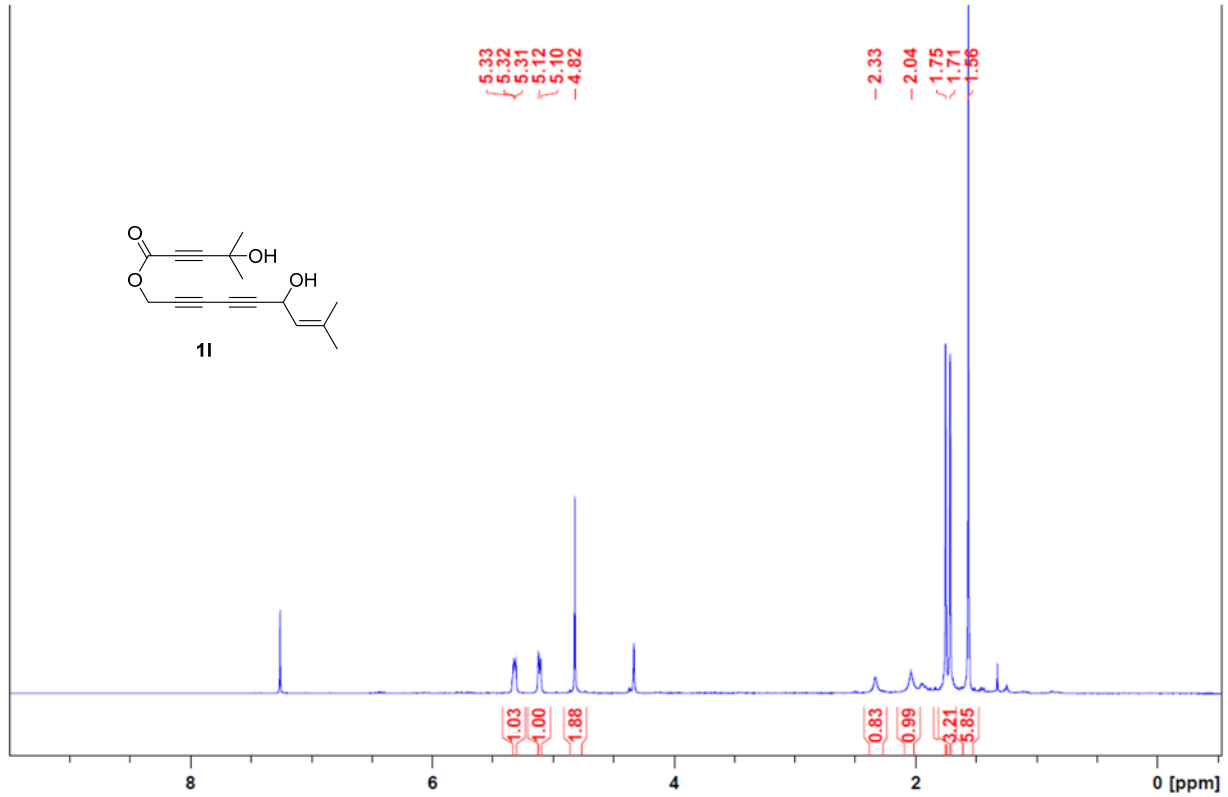

144.89
143.37
142.99
141.26
140.90
138.38
137.75
135.05
129.67
129.60
126.61
126.26
126.01
125.55
123.22
116.15
114.84
113.22
109.52
73.45
59.59
57.18
31.17
29.71
28.16
25.88
21.54
20.04
-3.57
-5.15
OH
OTBS
N
Ts
2j
dr 5:1
200
150
100
50
[ppm]

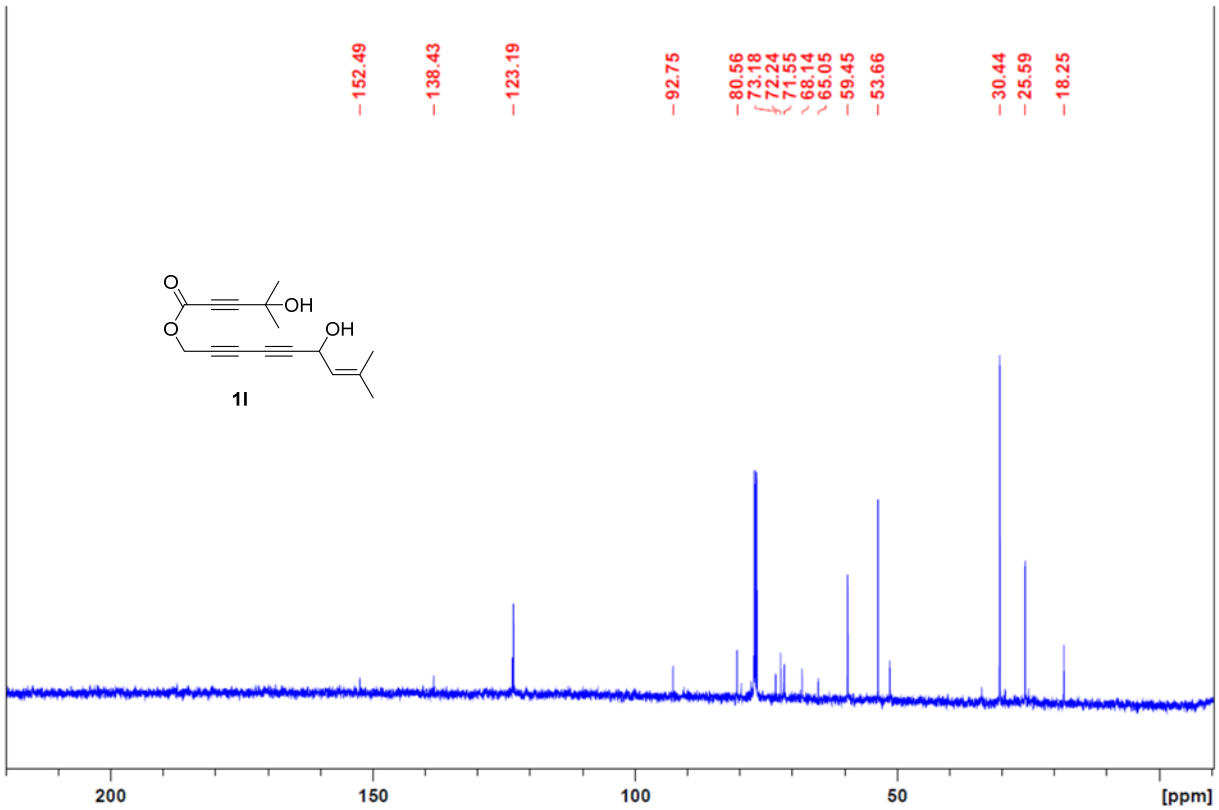

5.11
4.77
2.95
2.94
2.78
1.69
1.60
1.54
OH
1k
1.00
2.24
2.18
1.05
7.01
8
6
4
2
0 [ppm]

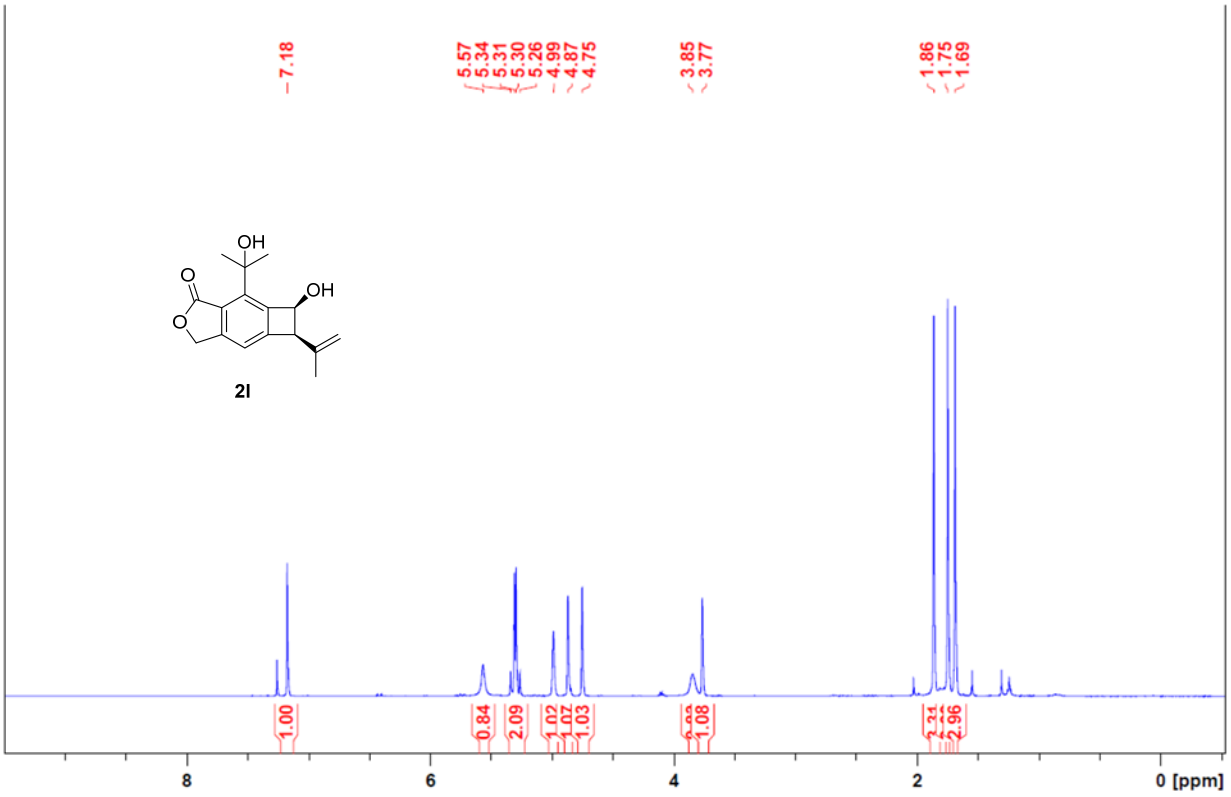

152.61
135.36
116.64
92.74
81.02
73.19
72.55
68.29
64.95
63.67
53.85
30.41
25.43
18.33
17.73
OH
1k
200
150
100
50
[ppm]

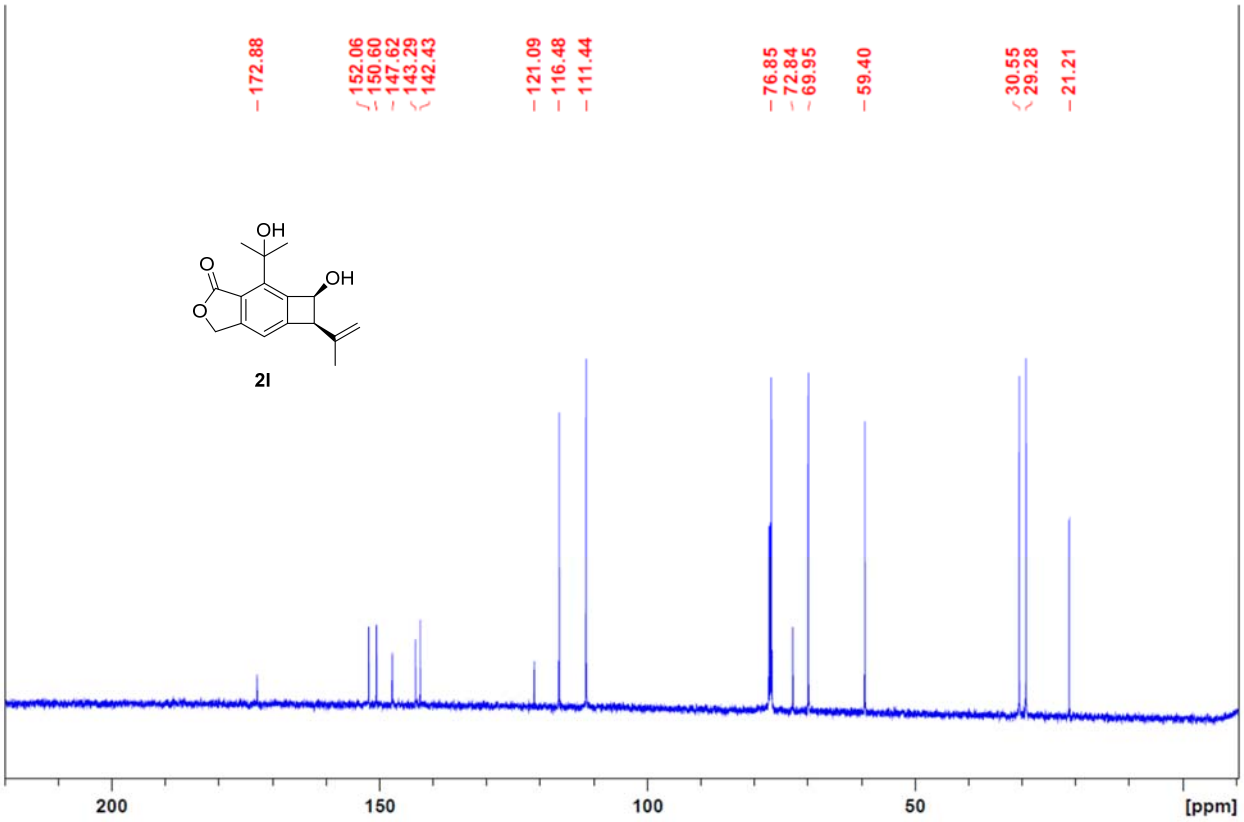

7.11
6.31
5.32
4.85
4.83
4.00
3.61
3.59
3.58
3.57
3.15
3.12
1.79
1.64
1.63
OH
O
O
2k
1.00
0.96
2.08
2.06
0.98
1.04
1.01
3.26
6.68
8
6
4
2
0 [ppm]

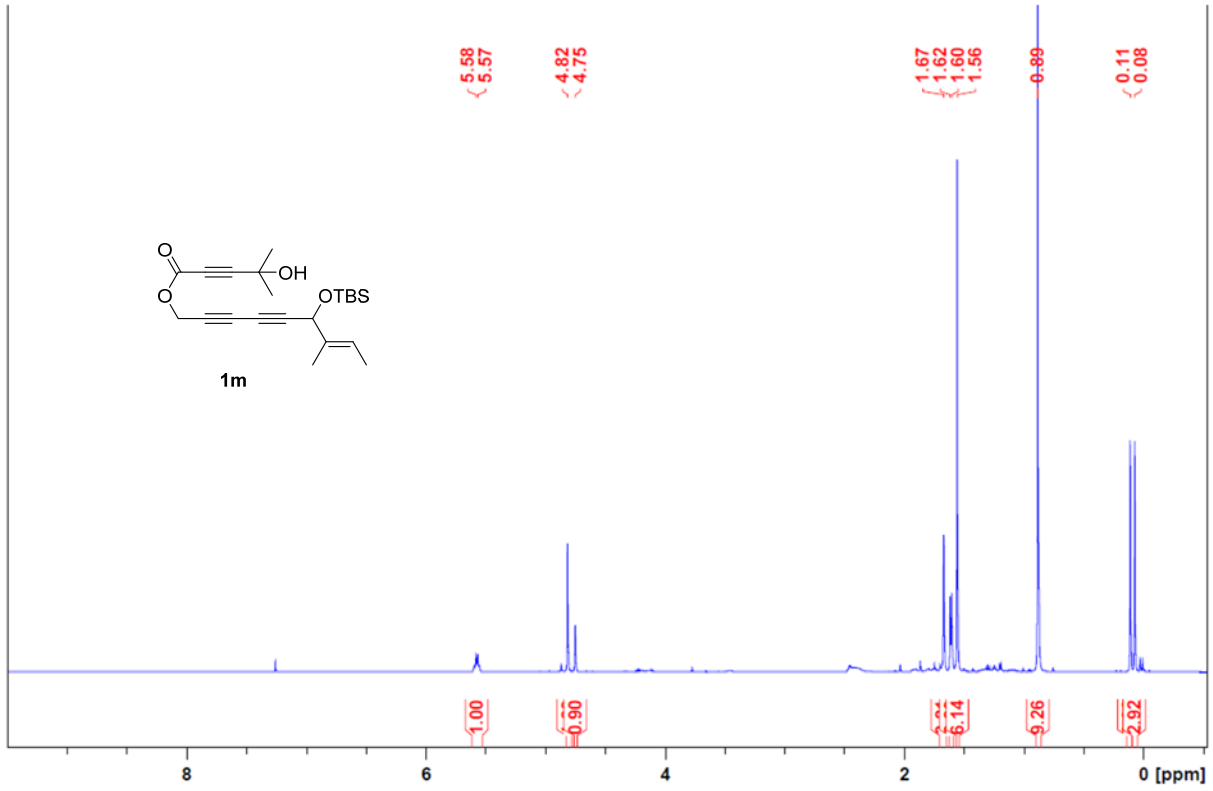

174.08
155.52
148.94
145.98
143.93
140.35
121.17
115.26
110.91
71.89
70.26
47.67
38.02
30.18
30.07
20.37
OH
O
O
2k
200
150
100
50
[ppm]

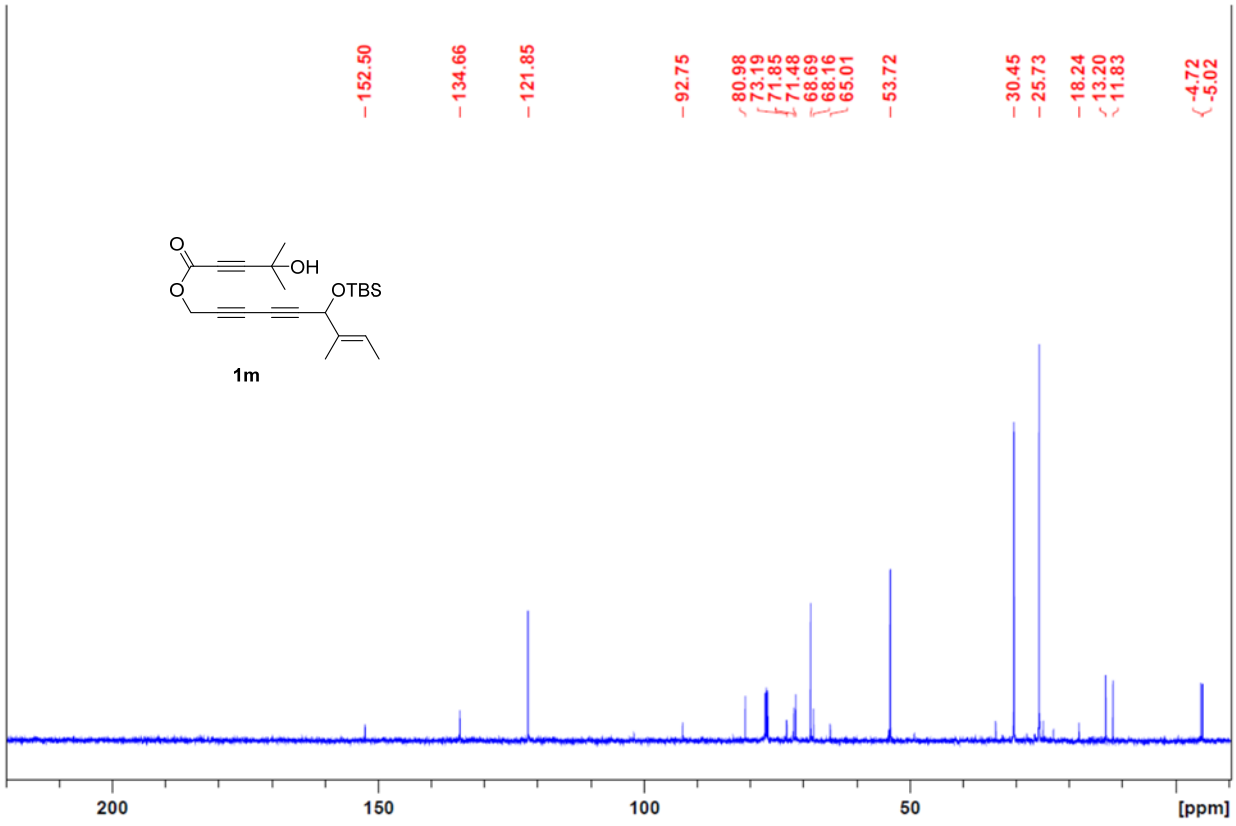

5.33
5.32
5.31
5.12
5.10
4.82
2.33
2.04
1.75
1.71
1.56
OH
OH
1l
1.03
1.00
1.88
0.83
0.99
3.21
5.85
8
6
4
2
0 [ppm]


152.49
138.43
123.19
92.75
80.56
73.18
72.24
71.55
68.14
65.05
59.45
53.66
30.44
25.59
18.25
OH
OH
1l
200
150
100
50
[ppm]


7.18
5.57
5.34
5.31
5.30
5.26
4.99
4.87
4.75
3.85
3.77
1.86
1.75
1.69
OH
O
O
OH
2l
1.00
0.84
2.09
1.02
1.02
1.03
6.00
1.08
2.24
2.96
8
6
4
2
0 [ppm]


172.88
152.06
150.60
147.62
143.29
142.43
121.09
116.48
111.44
76.85
72.84
69.95
59.40
30.55
29.28
21.21
OH
O
O
OH
2l
200
150
100
50
[ppm]


5.58
5.57
4.82
4.75
1.67
1.62
1.60
1.56
0.89
0.11
0.08
OH
OTBS
1m
1.00
0.90
6.14
9.26
2.92
8
6
4
2
0 [ppm]


152.50
134.66
121.85
92.75
80.98
73.19
71.85
71.48
68.69
68.16
65.01
53.72
30.45
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OTBS
1m
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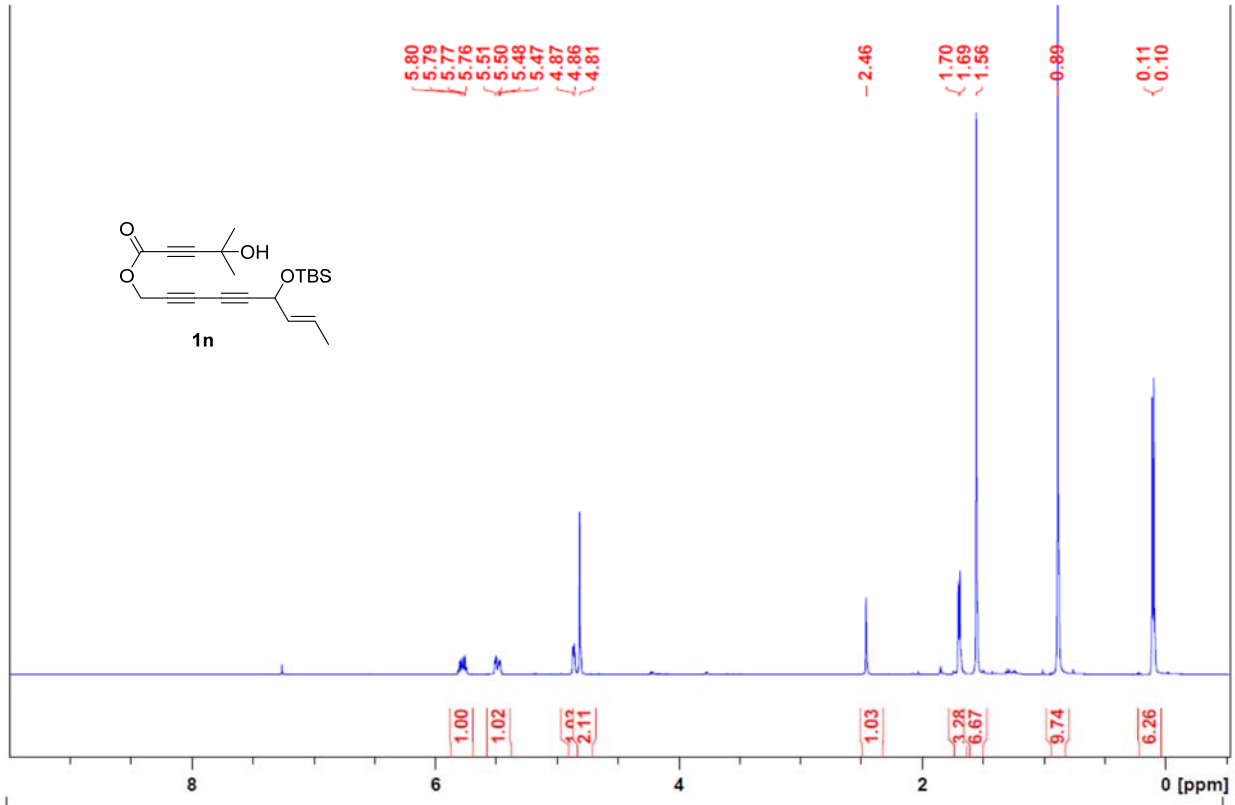
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5.47
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4.86
4.81
2.46
1.70
1.69
1.56
0.89
0.11
0.10
OH
OTBS
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2.11
1.03
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6.26
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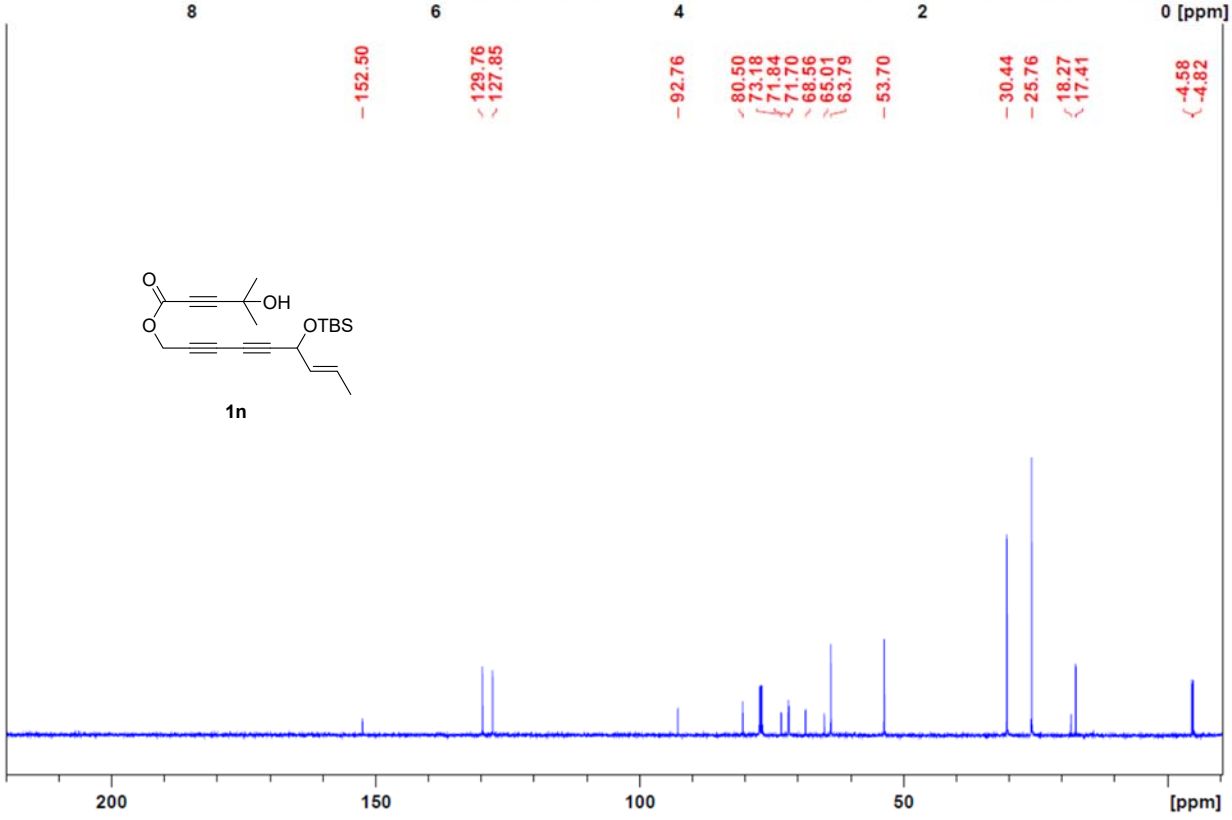
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63.79
53.70
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17.41
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OTBS
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100
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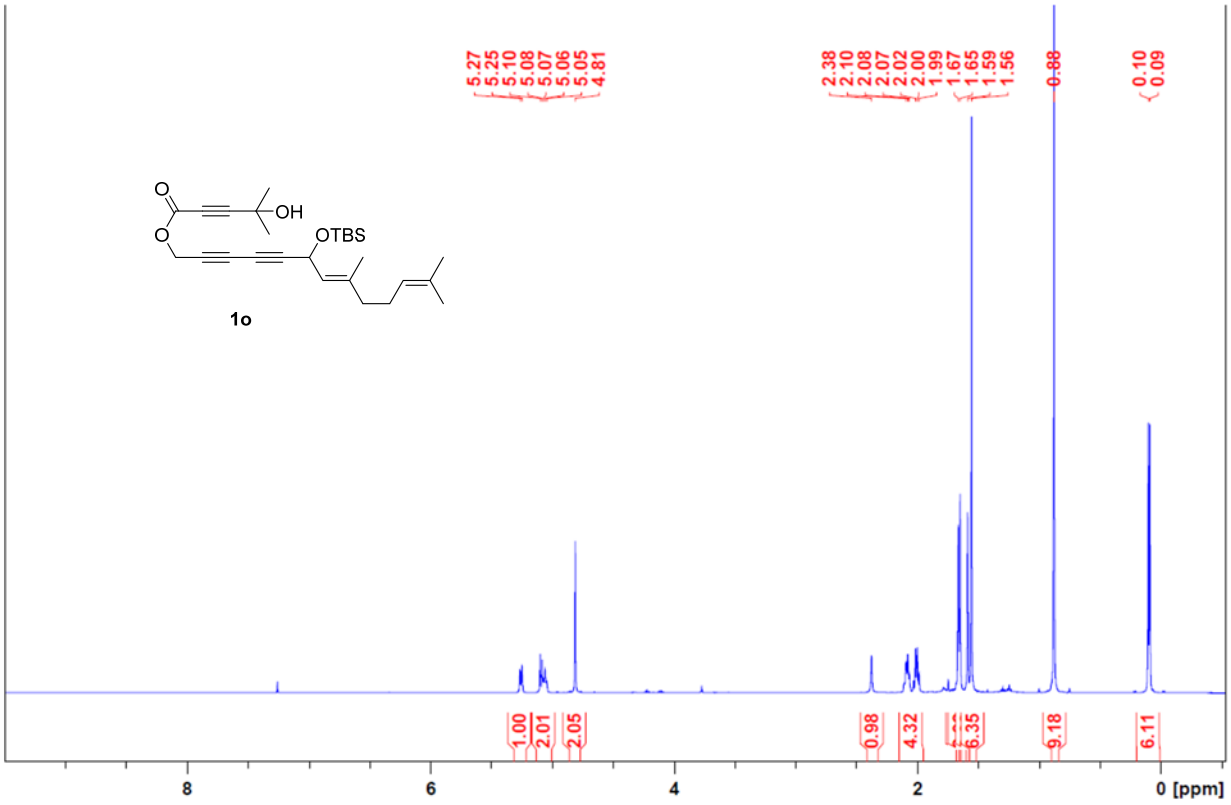
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5.06
5.05
4.81
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2.10
2.08
2.07
2.02
2.00
1.99
1.67
1.65
1.59
1.56
0.88
0.10
0.09
OH
OTBS
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2.05
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6.11
8
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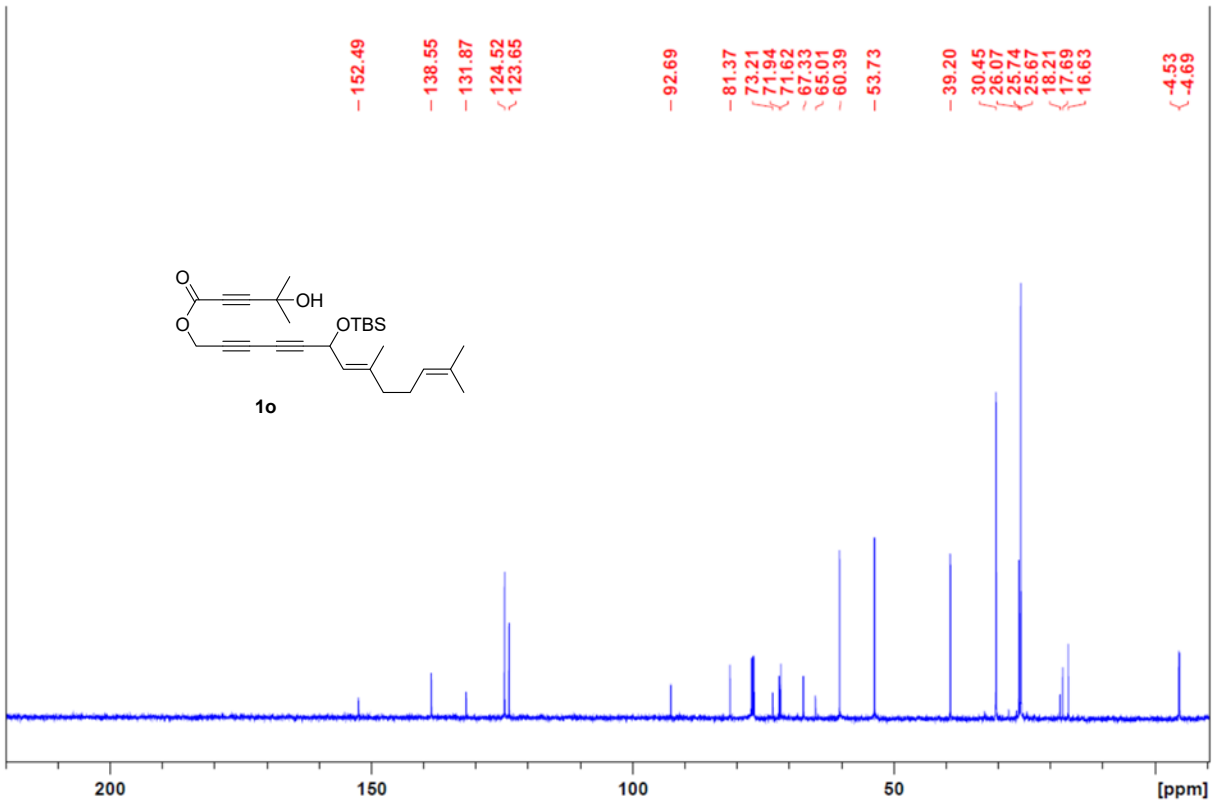
4
2
0 [ppm]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67.33
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53.73
39.20
30.45
26.07
25.74
25.67
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16.63
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-4.69
OH
OTBS
1o
200
150
100
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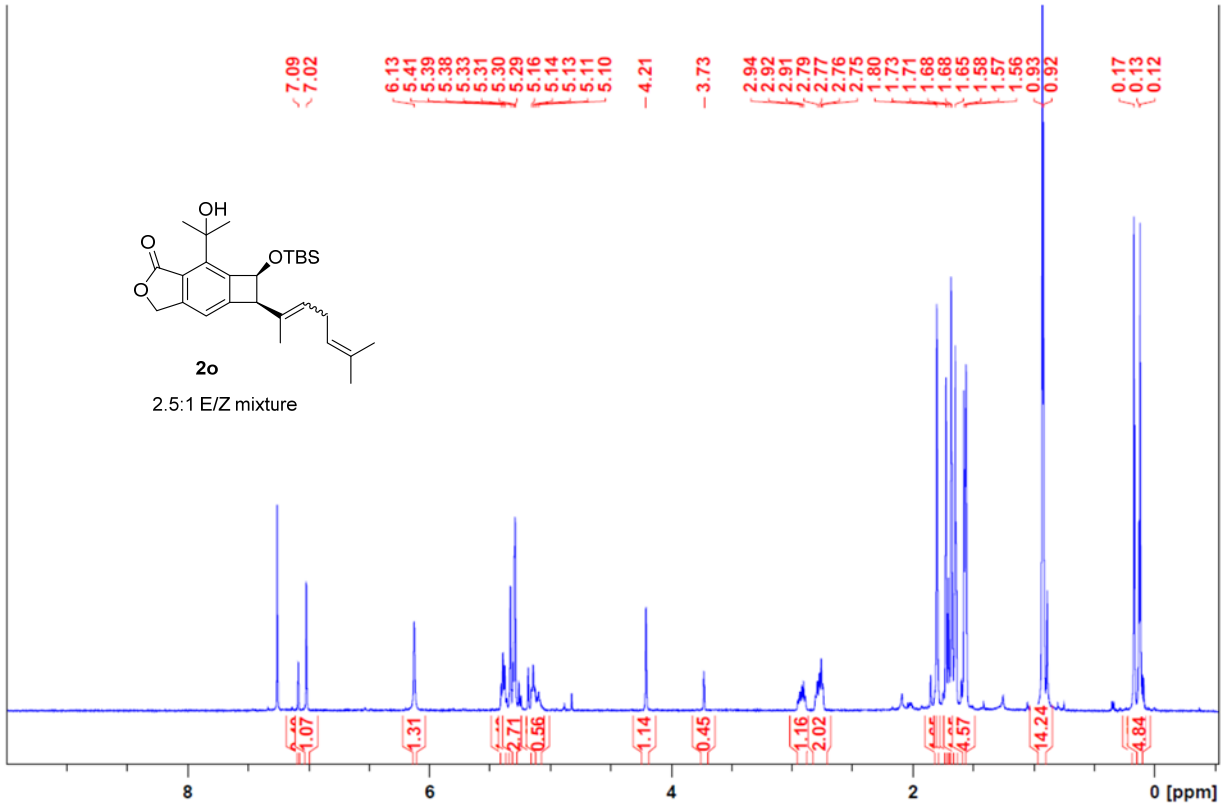
[ppm]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5.38
5.33
5.31
5.30
5.29
5.16
5.14
5.13
5.11
5.10
4.21
3.73
2.94
2.92
2.91
2.79
2.77
2.76
2.75
1.80
1.73
1.71
1.68
1.68
1.65
1.58
1.57
1.56
0.93
0.92
0.17
0.13
0.12
OH
O
O
OTBS
2o
2.5:1 E/Z mixture
1.07
1.31
2.71
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0.45
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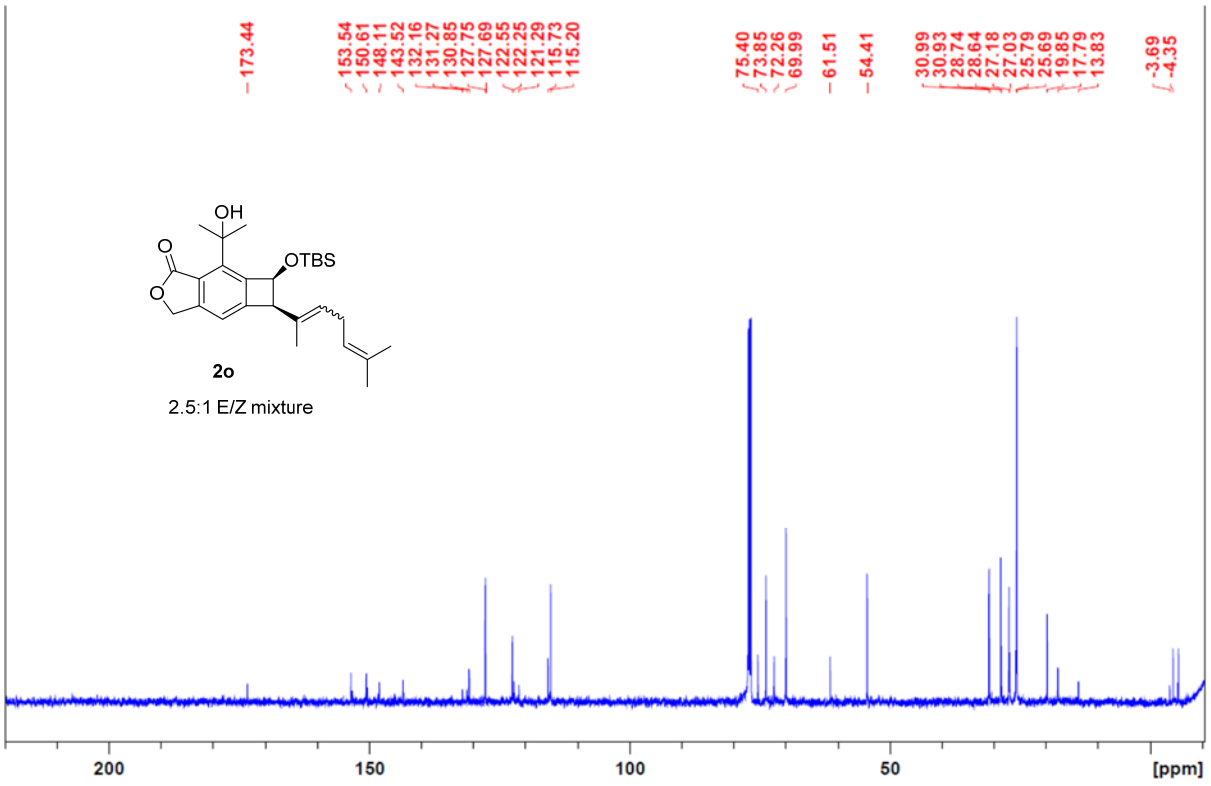
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127.69
122.55
122.25
121.29
115.73
115.20
75.40
73.85
72.26
69.99
61.51
54.41
30.99
30.93
28.74
28.64
27.18
27.03
25.79
25.69
19.85
17.79
13.83
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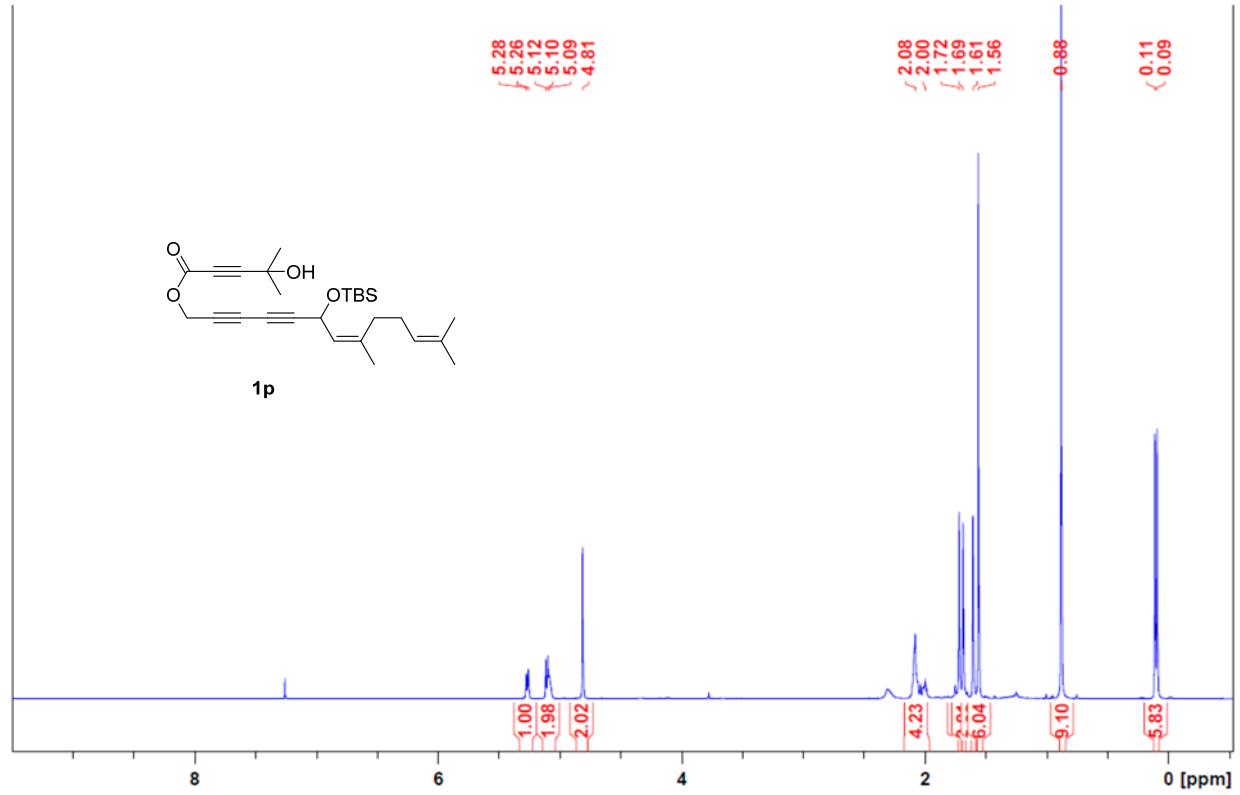
OH
O
O
OTBS
2o
2.5:1 E/Z mixture
200
150
100
50
[ppm]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4.81
2.08
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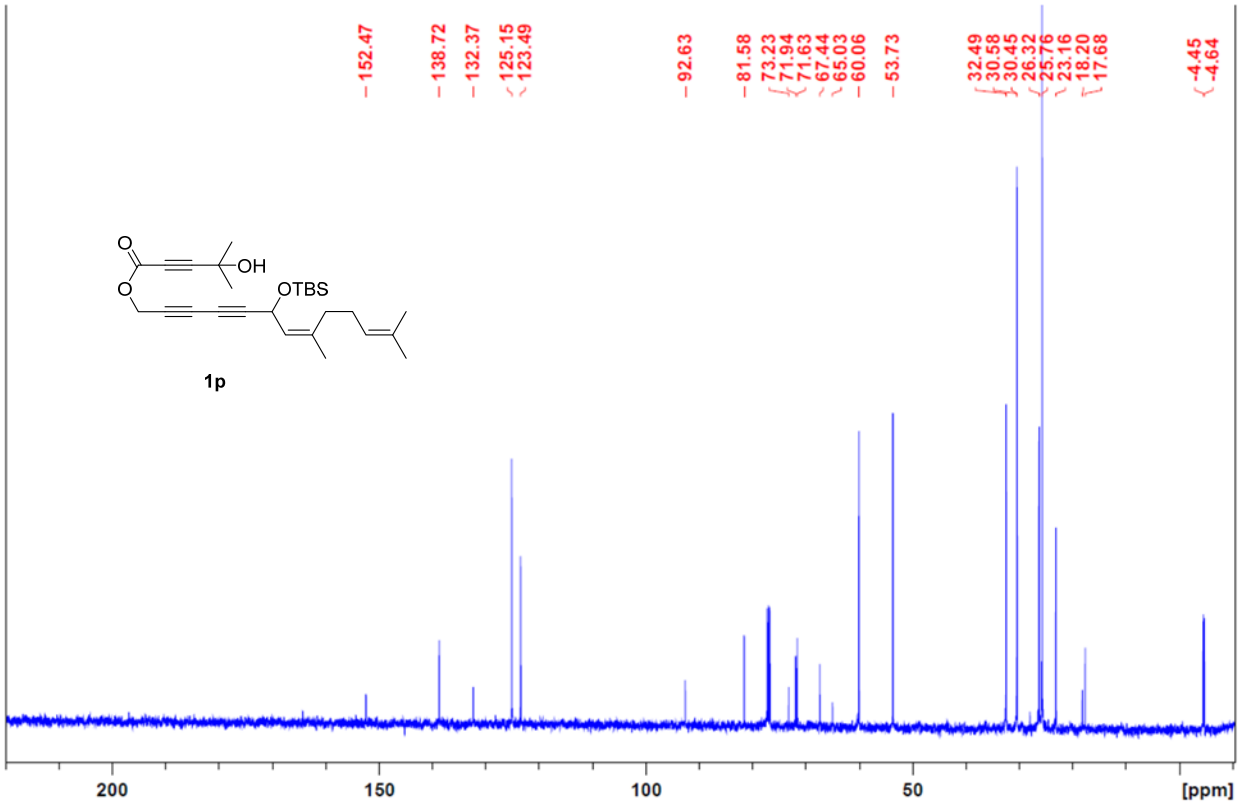
1.69
1.61
1.56
0.88
0.11
0.09
OH
OTBS
1p
1.00
1.98
2.02
4.23
6.04
9.10
5.83
8
6
4
2
0 [ppm]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92.63
81.58
73.23
71.94
71.63
67.44
65.03
60.06
53.73
32.49
30.58
30.45
26.32
25.76
23.16
18.20
17.68
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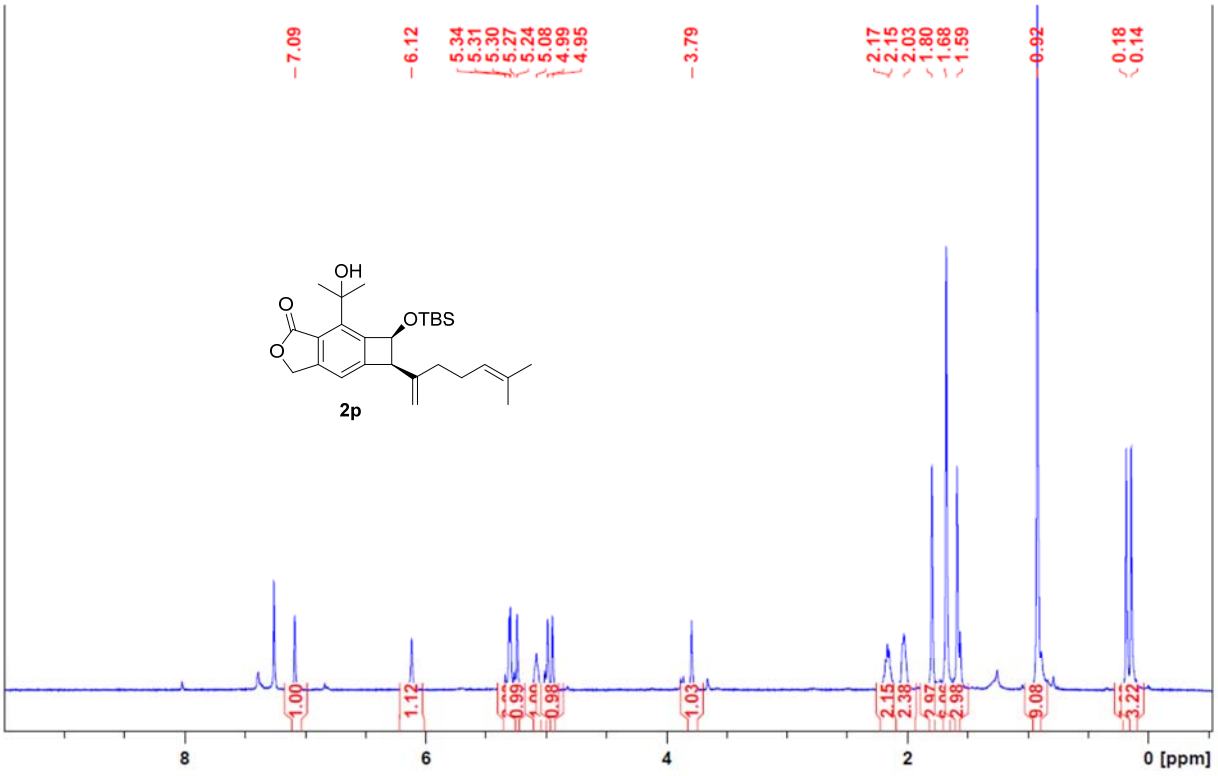
-4.64
OH
OTBS
1p
200
150
100
50
[ppm]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6.12
5.34
5.31
5.30
5.27
5.24
5.08
4.99
4.95
3.79
2.17
2.15
2.03
1.80
1.68
1.59
0.92
0.18
0.14
OH
O
O
OTBS
2p
1.00
1.12
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1.03
2.15
2.38
2.98
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3.22
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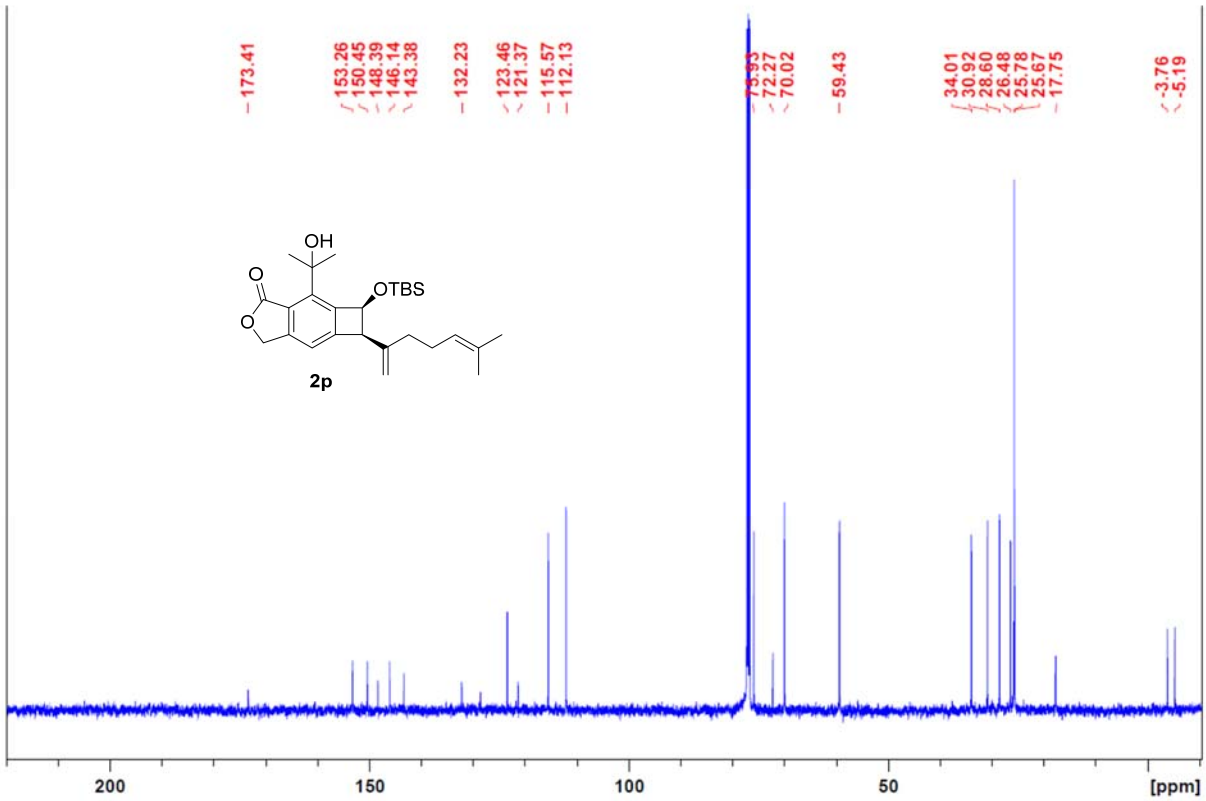
4
2
0 [ppm]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150.45
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146.14
143.38
132.23
123.46
121.37
115.57
112.13
73.93
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70.02
59.43
34.01
30.92
28.60
26.48
25.78
25.67
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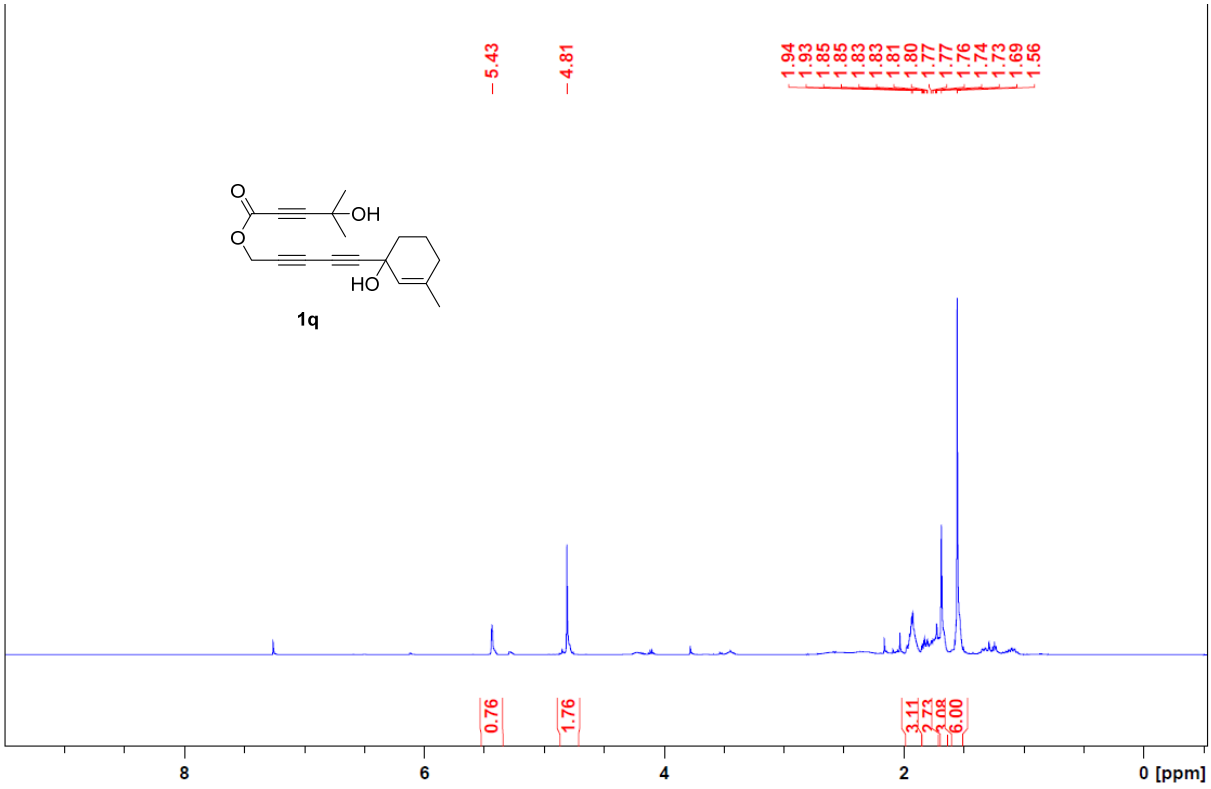
-3.76
-5.19
OH
O
O
OTBS
2p
200
150
100
50
[ppm]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1.93
1.85
1.85
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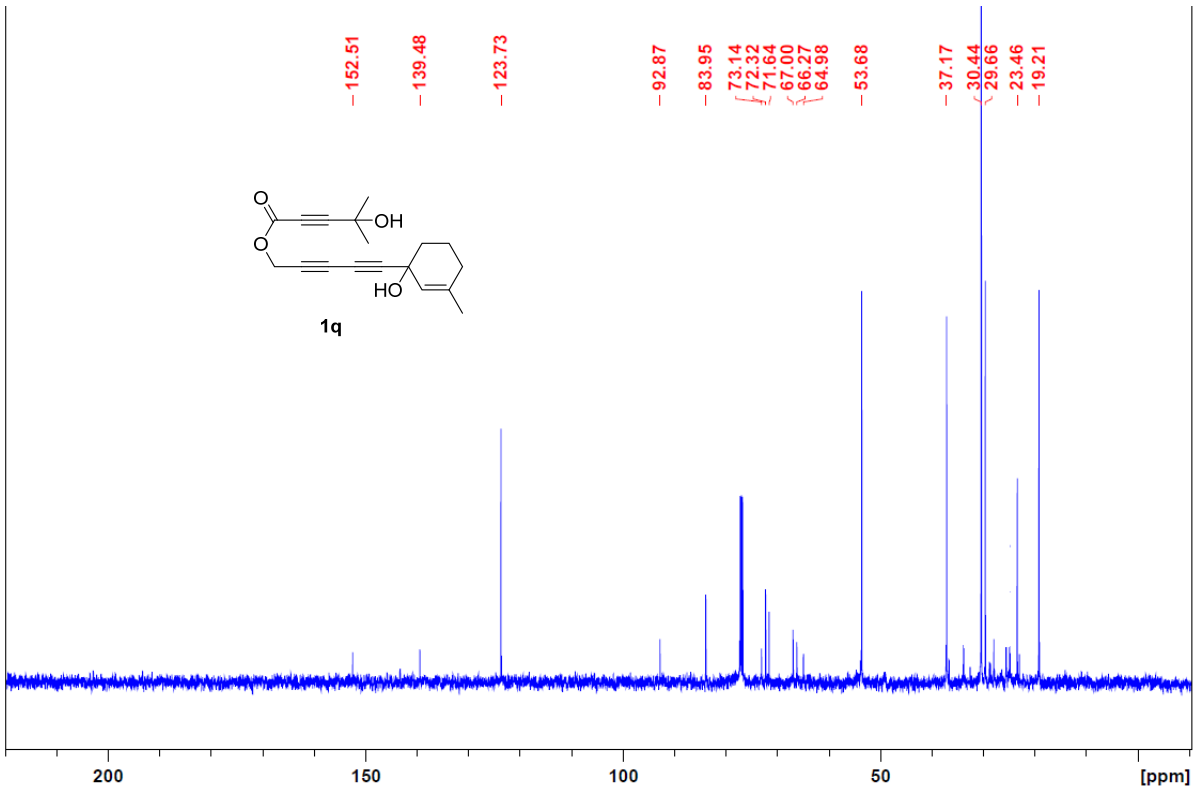
1.83
1.81
1.80
1.77
1.77
1.76
1.74
1.73
1.69
1.56
OH
HO
1q
0.76
1.76
3.11
2.73
2.08
6.00
8
6
4
2
0 [ppm]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71.64
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66.27
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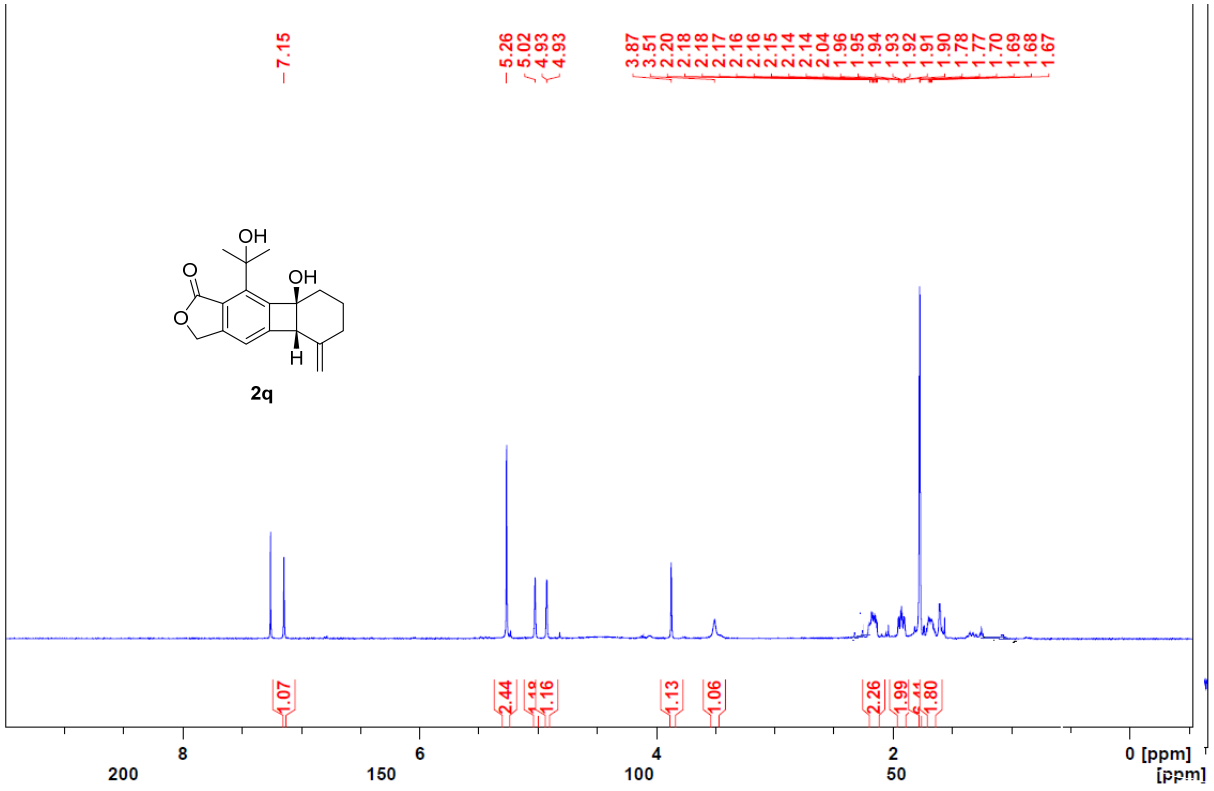
30.44
29.66
23.46
19.21
OH
HO
1q
200
150
100
50
[ppm]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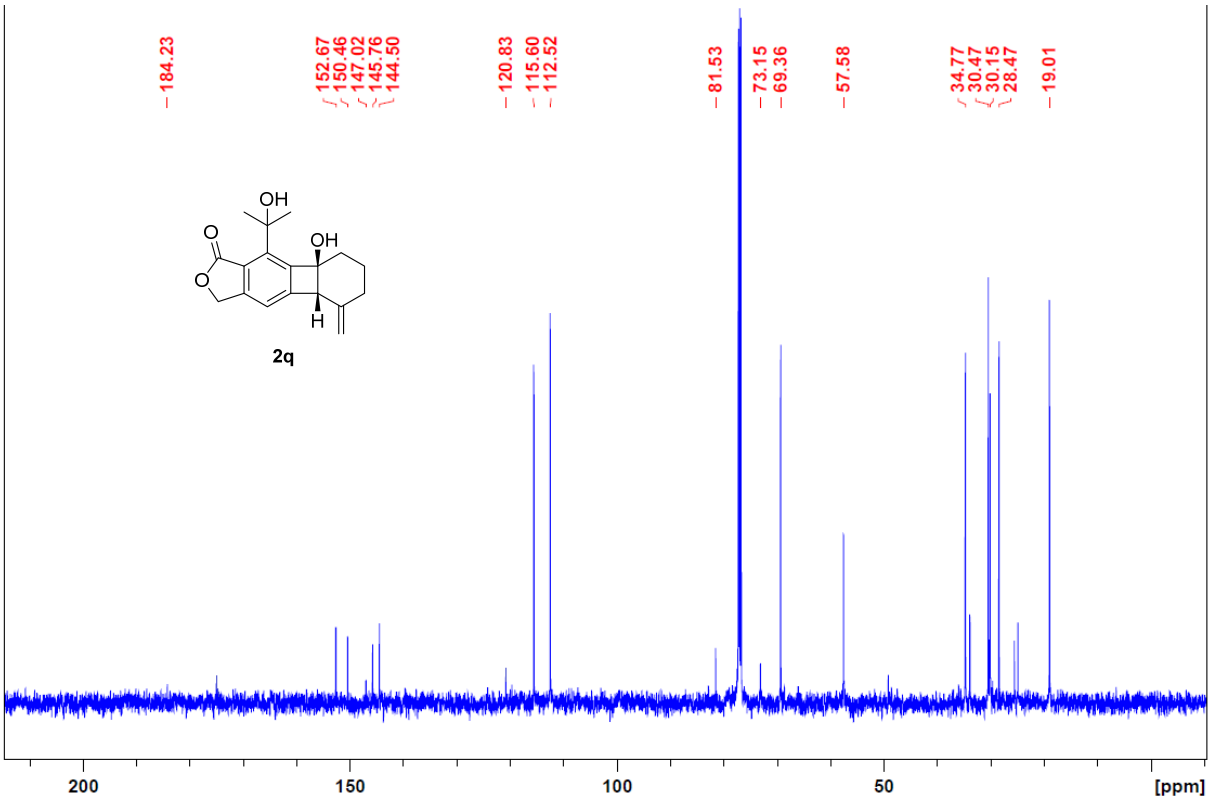
4.93
3.87
3.51
2.20
2.18
2.18
2.17
2.16
2.16
2.15
2.14
2.14
2.04
1.96
1.95
1.94
1.93
1.92
1.91
1.90
1.78
1.77
1.70
1.69
1.68
1.67
OH
O
OH
O
H
2q
1.07
2.44
1.16
1.13
1.06
2.26
1.99
1.80
8
6
4
2
0 [ppm]
200
150
100
50
[ppm]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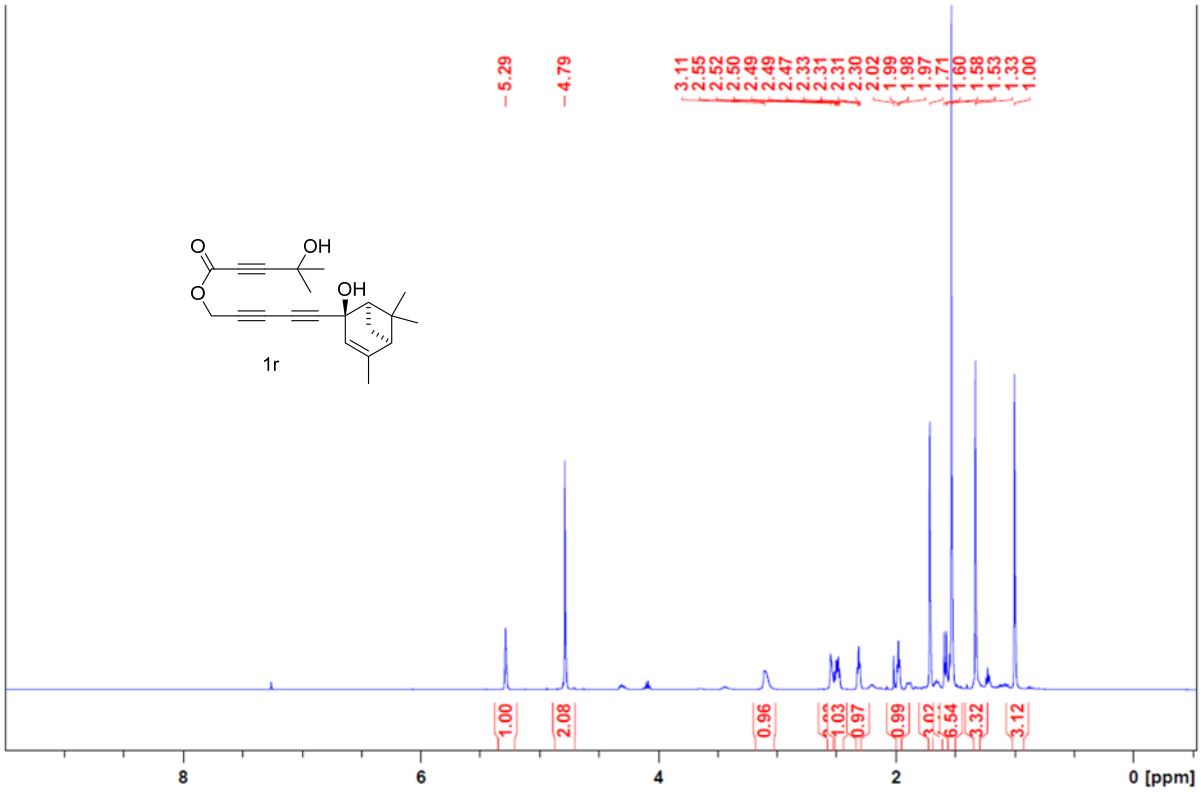
145.76
144.50
120.83
115.60
112.52
81.53
73.15
69.36
57.58
34.77
30.47
30.15
28.47
19.01
OH
O
OH
O
H
2q
200
150
100
50
[ppm]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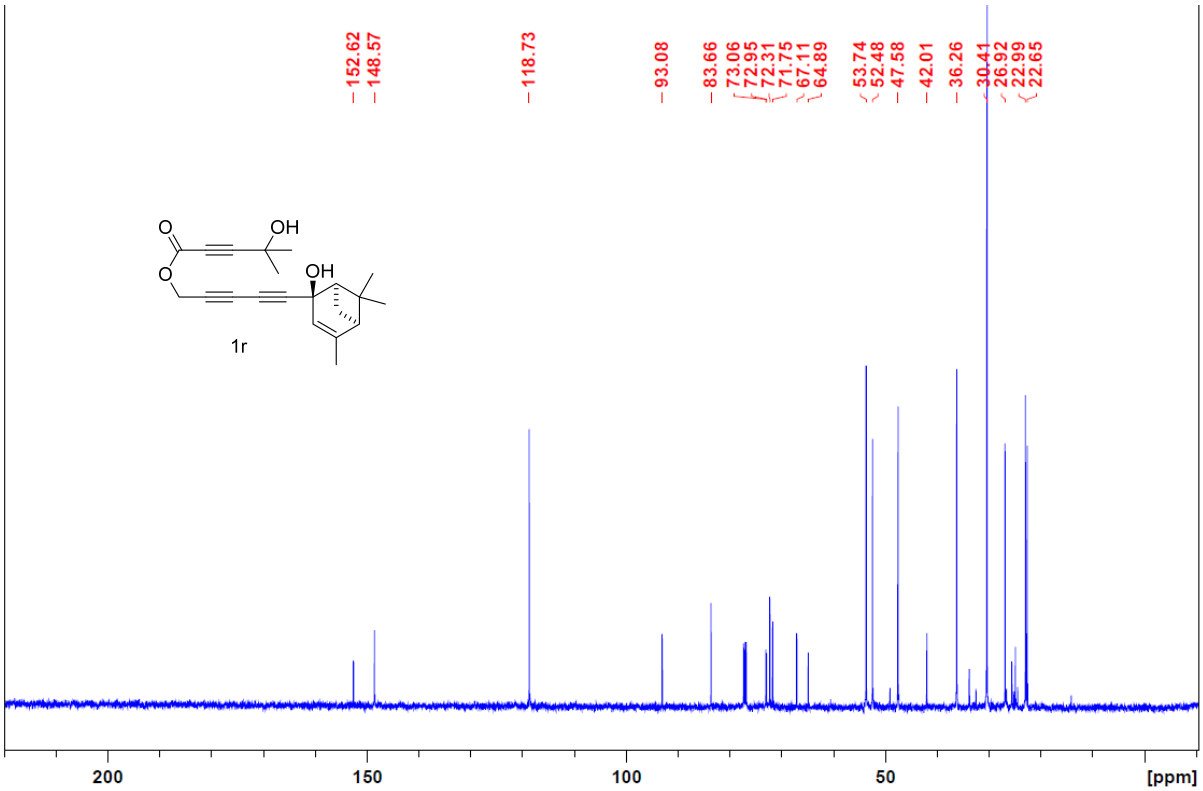
2.50
2.49
2.49
2.47
2.33
2.31
2.31
2.30
2.02
1.99
1.98
1.97
1.71
1.60
1.58
1.53
1.33
1.00
OH
O
O
OH
1r
1.00
2.08
0.96
1.03
0.97
0.99
3.32
3.12
8
6
4
2
0 [ppm]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73.06
72.95
72.31
71.75
67.11
64.89
53.74
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47.58
42.01
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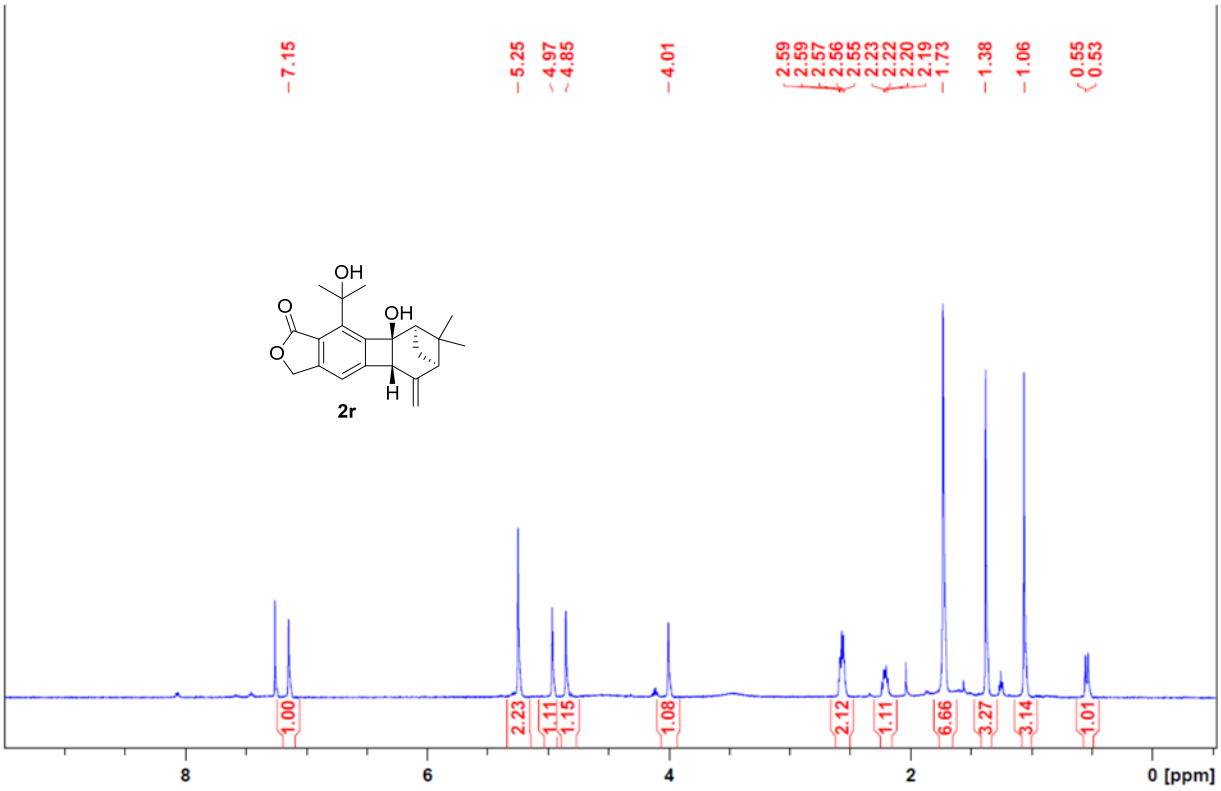
26.92
22.99
22.65
OH
O
O
OH
1r
200
150
100
50
[ppm]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2.59
2.57
2.56
2.55
2.23
2.22
2.20
2.19
1.73
1.38
1.06
0.55
0.53
OH
O
OH
O
H
2r
1.00
2.23
1.11
1.15
1.08
2.12
1.11
6.66
3.27
3.14
1.01
8
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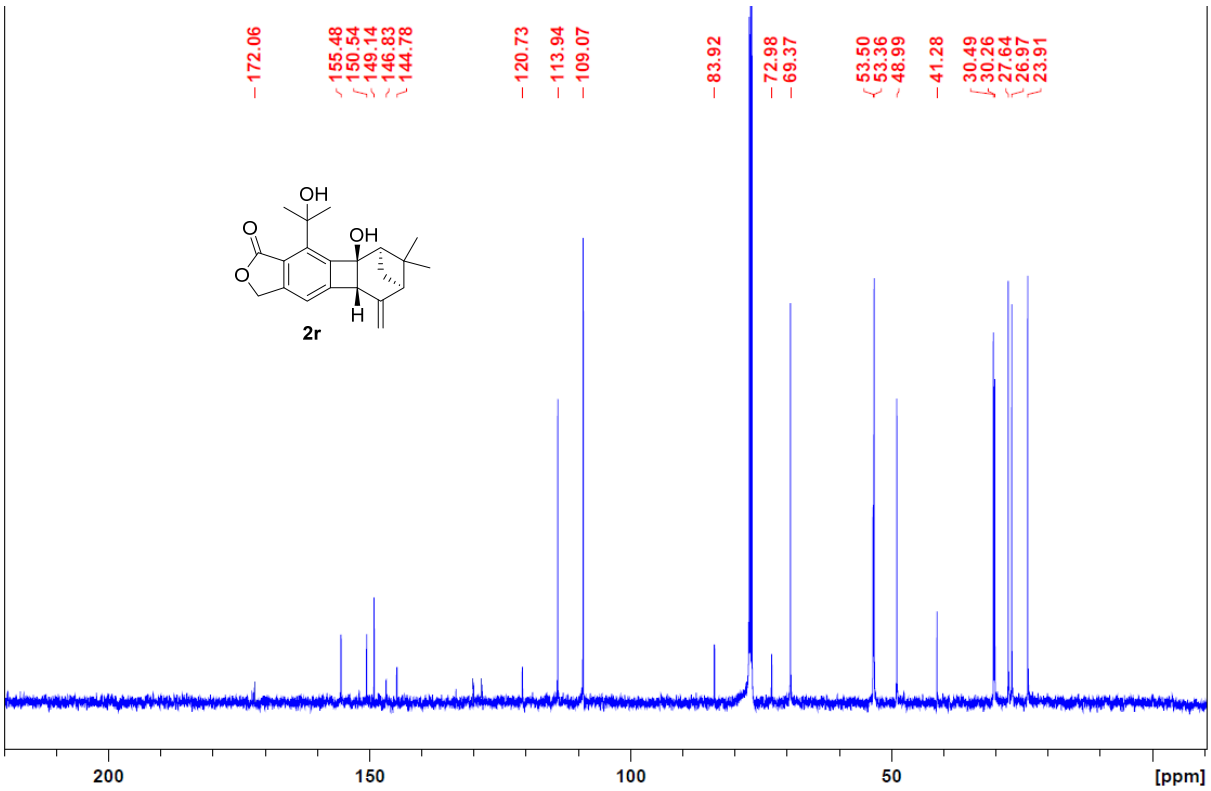
4
2
0 [ppm]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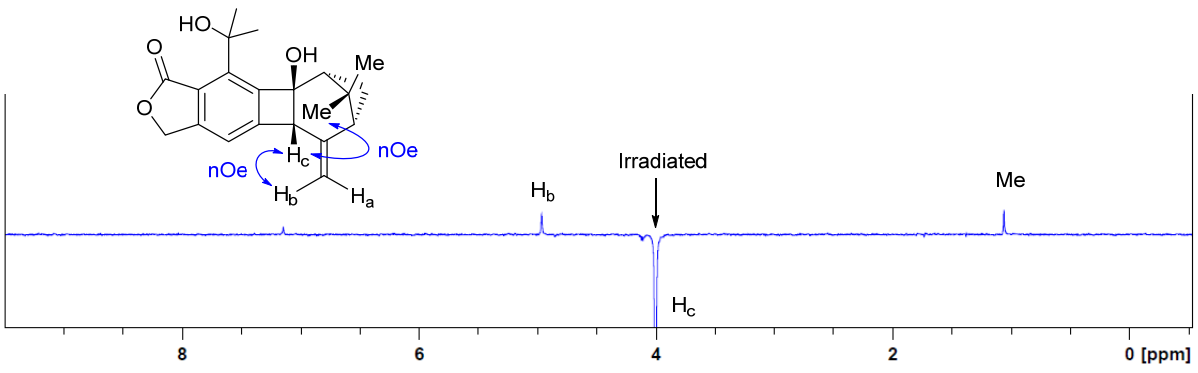
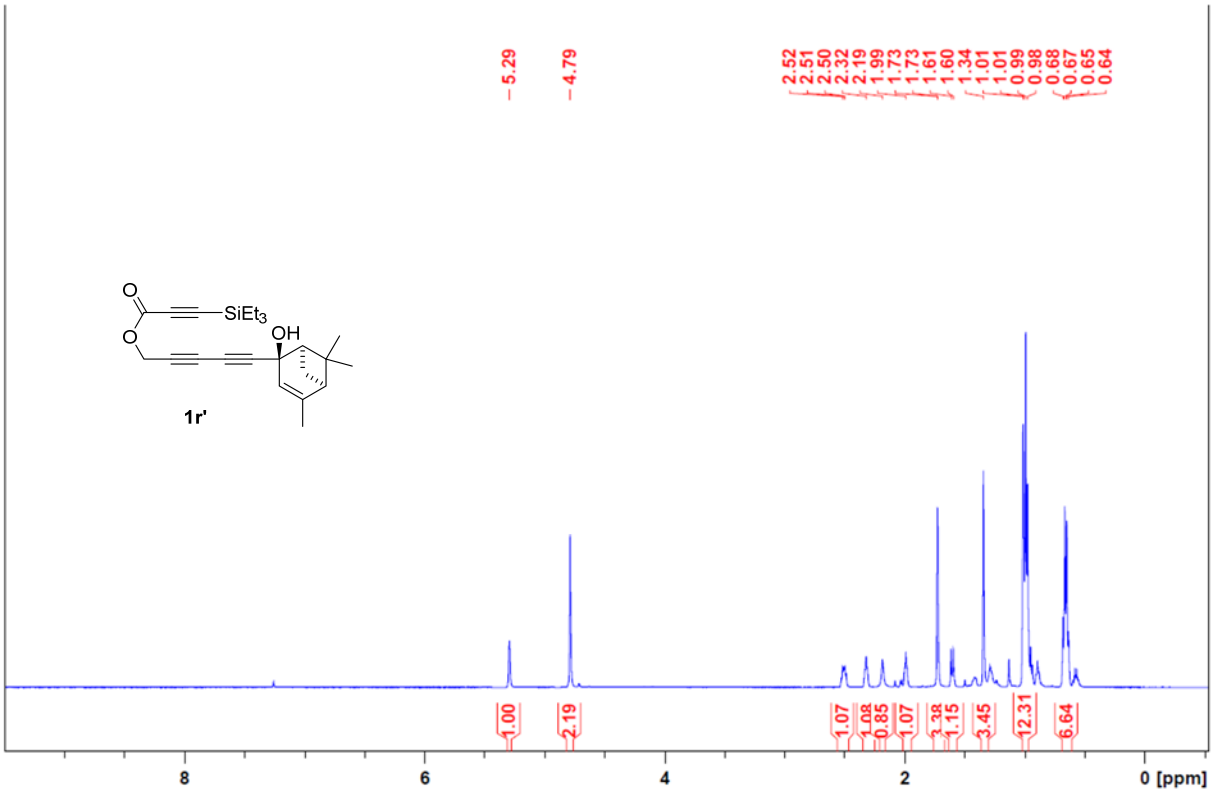
146.83
144.78
120.73
113.94
109.07
83.92
72.98
69.37
53.50
53.36
48.99
41.28
30.49
30.26
27.64
26.97
23.91
OH
O
OH
O
H
2r
200
150
100
50
[ppm]


HO
O
O
OH
Me
Me
nOe
nOe
Hc
Hb
Ha
Irradiated
Hb
Me
Hc
8
6
4
2
0 [ppm]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2.32
2.19
1.99
1.73
1.73
1.61
1.60
1.34
1.01
1.01
0.99
0.98
0.68
0.67
0.65
0.64
SiEt3
OH
1r'
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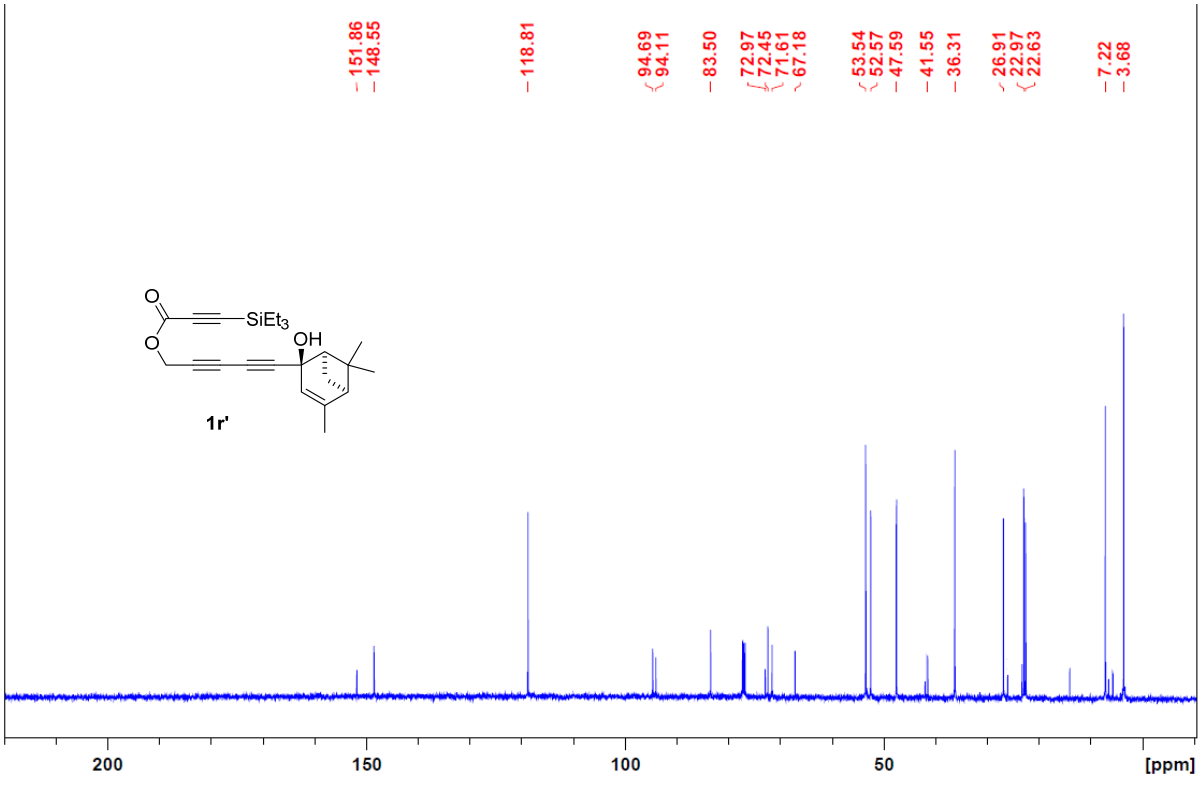
0.85
1.07
1.15
3.45
12.31
6.64
8
6
4
2
0 [ppm]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67.18
53.54
52.57
47.59
41.55
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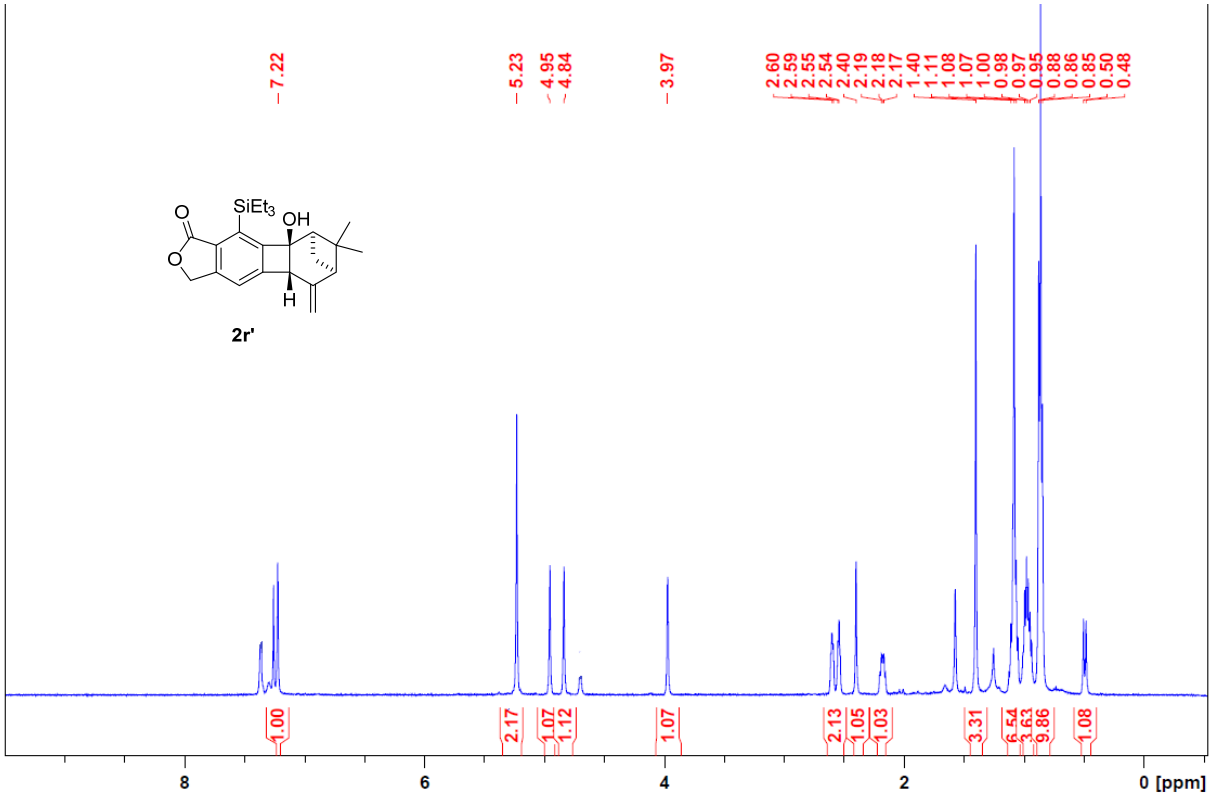
26.91
22.97
22.63
7.22
3.68
SiEt3
OH
1r'
200
150
100
50
[ppm]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2.55
2.54
2.40
2.19
2.18
2.17
1.40
1.11
1.08
1.07
1.00
0.98
0.97
0.95
0.88
0.86
0.85
0.50
0.48
SiEt3
OH
O
O
H
2r'
1.00
2.17
1.07
1.12
1.07
2.13
1.05
1.03
3.31
6.54
3.63
9.86
1.08
8
6
4
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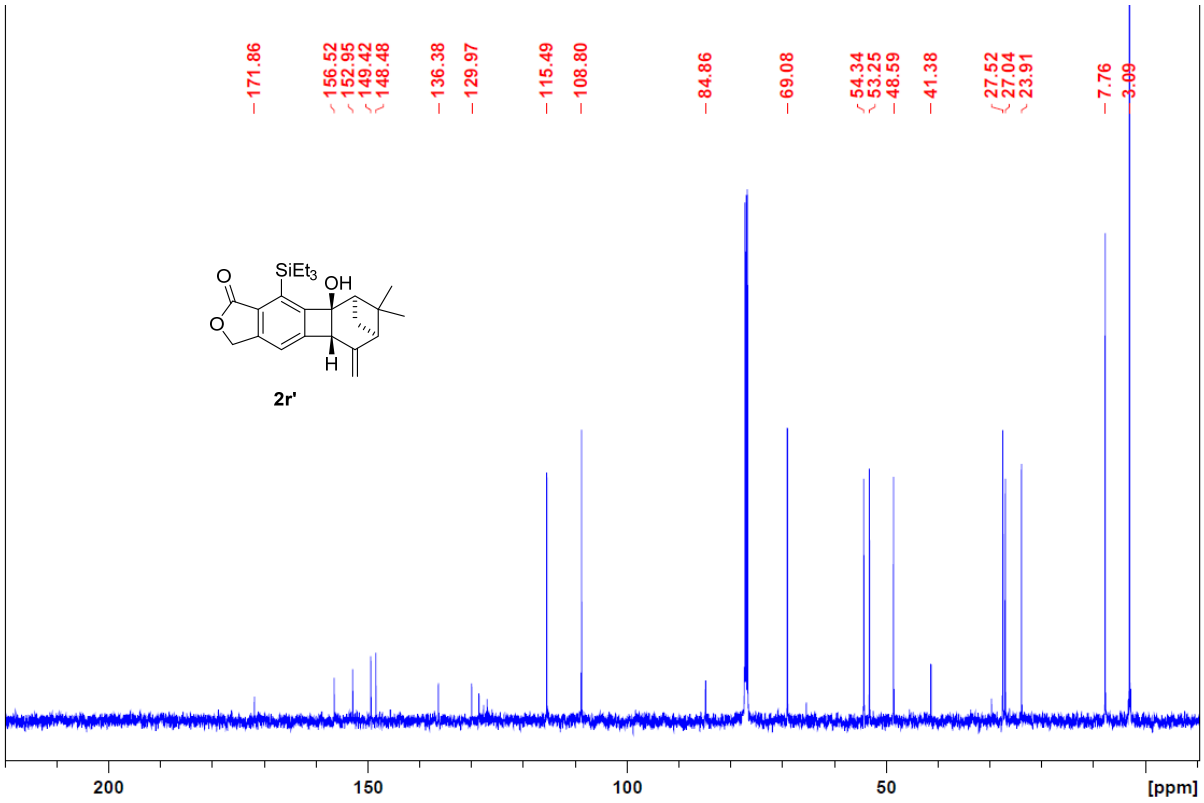
0 [ppm]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53.25
48.59
41.38
27.52
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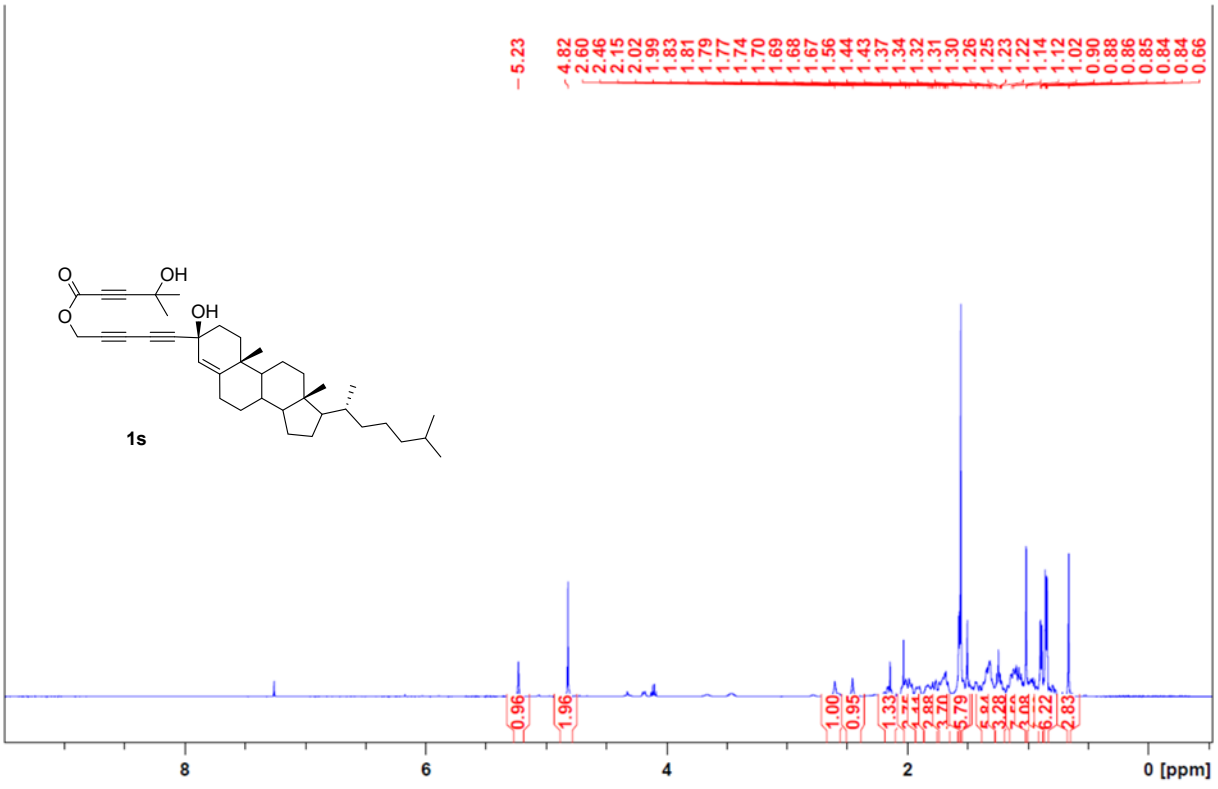
7.76
3.09
SiEt3
OH
O
O
H
2r'
200
150
100
50
[ppm]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1.81
1.79
1.77
1.74
1.70
1.69
1.68
1.67
1.56
1.44
1.43
1.37
1.34
1.32
1.31
1.30
1.26
1.25
1.23
1.22
1.14
1.12
1.02
0.90
0.88
0.86
0.85
0.84
0.84
0.66
O
OH
O
OH
1s
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1.00
0.95
1.33
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2.83
8
6
4
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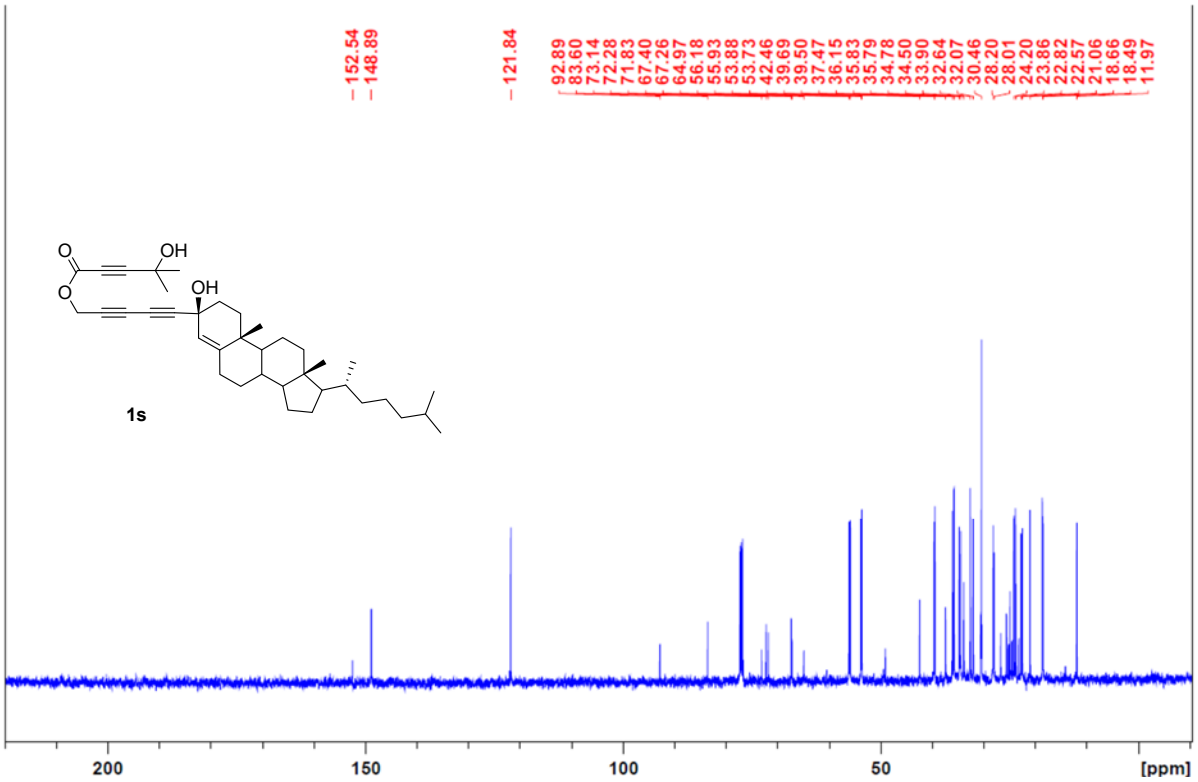
0 [ppm]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71.83
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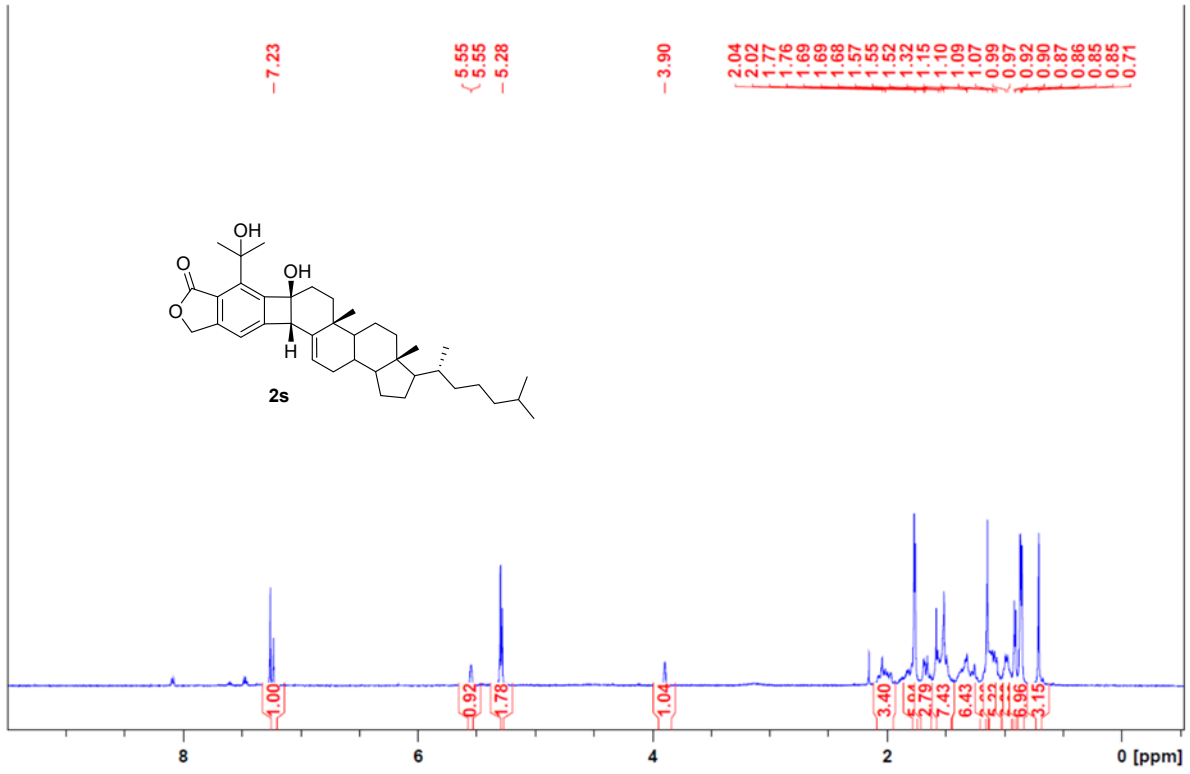
67.26
64.97
56.18
55.93
53.88
53.73
42.46
39.69
39.50
37.47
36.15
35.83
35.79
34.78
34.50
33.90
32.64
32.07
30.46
28.20
28.01
24.20
23.86
22.82
22.57
21.06
18.66
18.49
11.97
O
OH
O
OH
1s
200
150
100
50
[ppm]


7.23
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5.55
5.28
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2.04
2.02
1.77
1.76
1.69
1.69
1.68
1.57
1.55
1.52
1.32
1.15
1.10
1.09
1.07
0.99
0.97
0.92
0.90
0.87
0.86
0.85
0.71
OH
O
O
OH
H
2s
1.00
0.92
1.78
1.04
3.40
2.79
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8
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4
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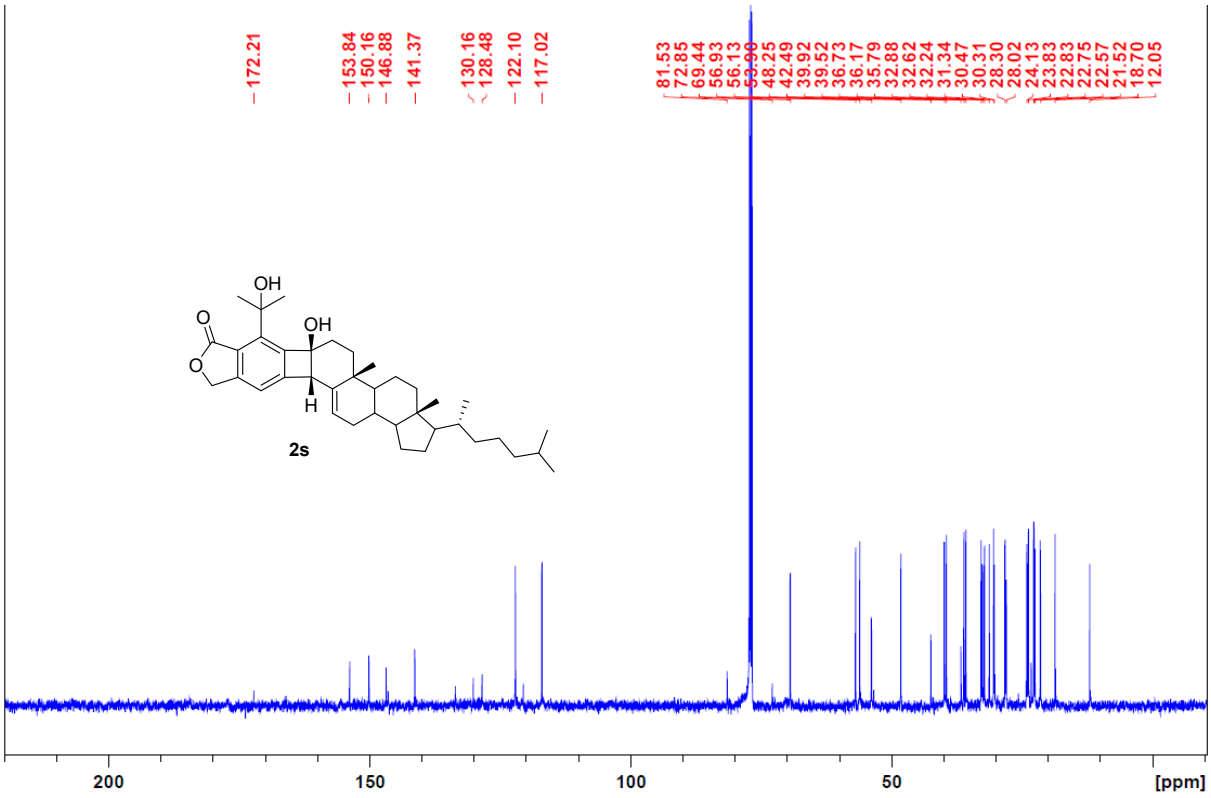
0 [ppm]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130.16
128.48
122.10
117.02
81.53
72.85
69.44
56.93
56.13
53.90
48.25
42.49
39.92
39.52
36.73
36.17
35.79
32.88
32.62
32.24
31.34
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30.31
28.30
28.02
24.13
23.83
22.83
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OH
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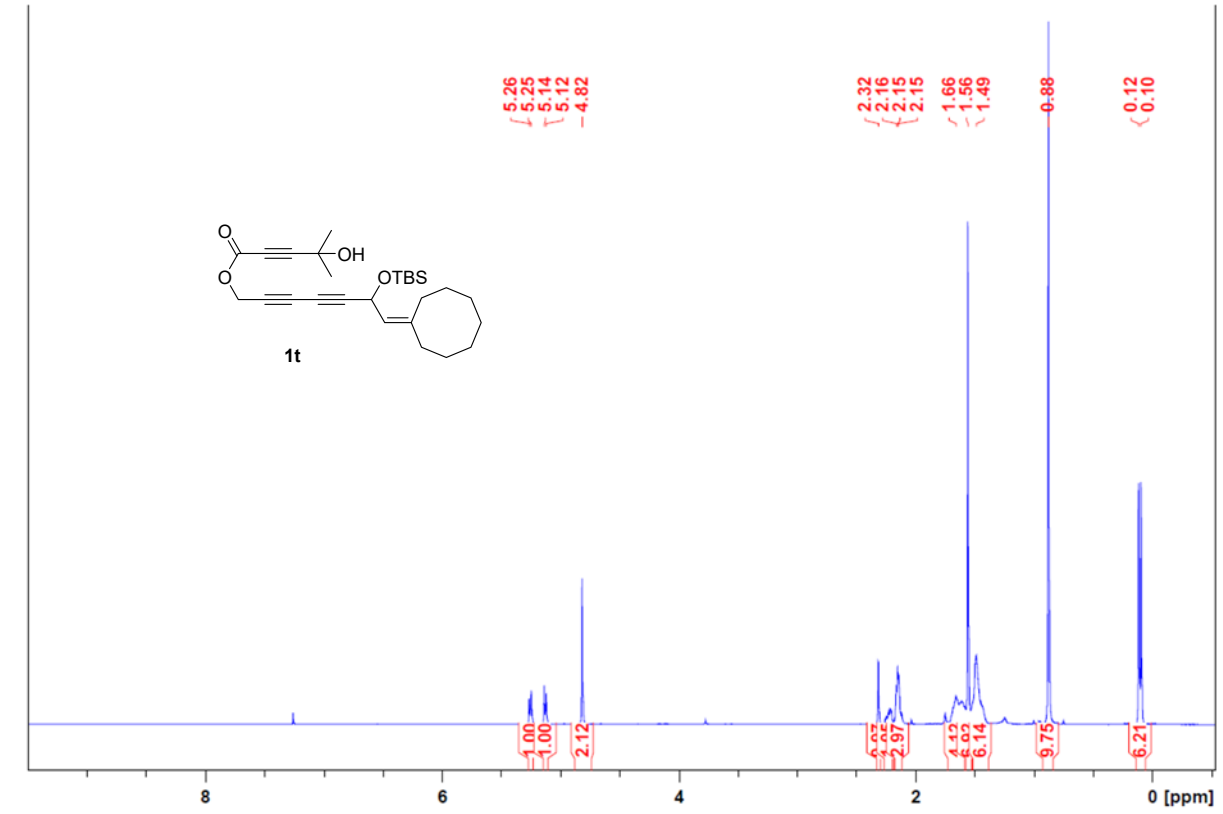
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2.15
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1.56
1.49
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0.12
0.10
O
OH
O
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1.00
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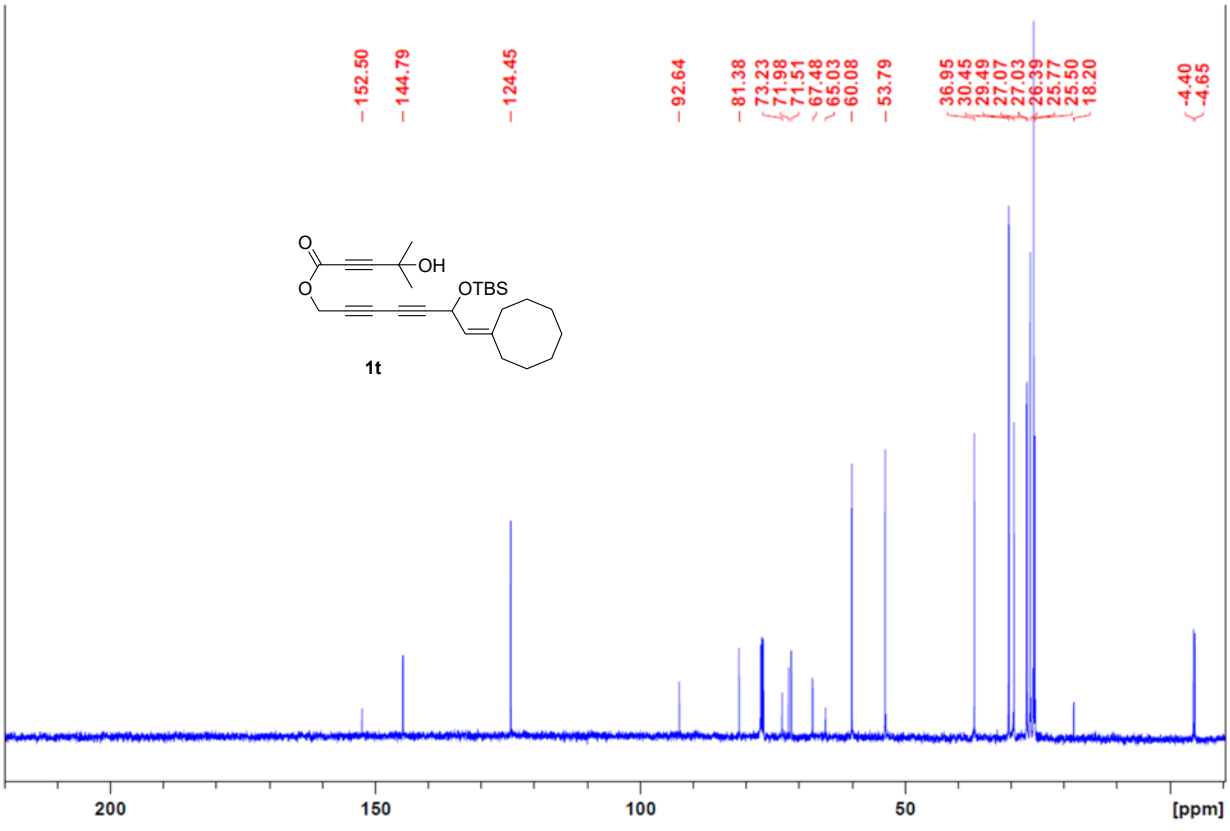
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53.79
36.95
30.45
29.49
27.07
27.03
26.39
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OH
O
OTBS
1t
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100
50
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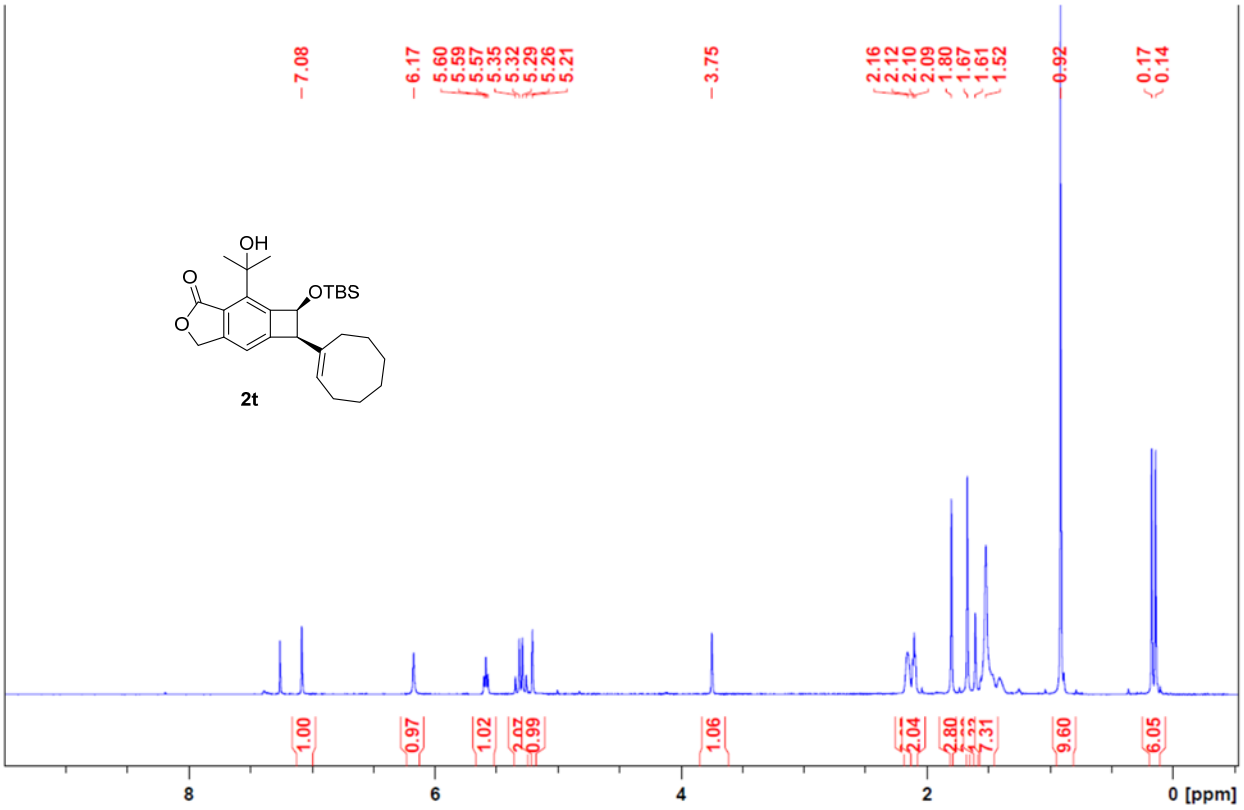
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5.29
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5.21
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2.16
2.12
2.10
2.09
1.80
1.67
1.61
1.52
0.92
0.17
0.14
OH
O
O
OTBS
2t
1.00
0.97
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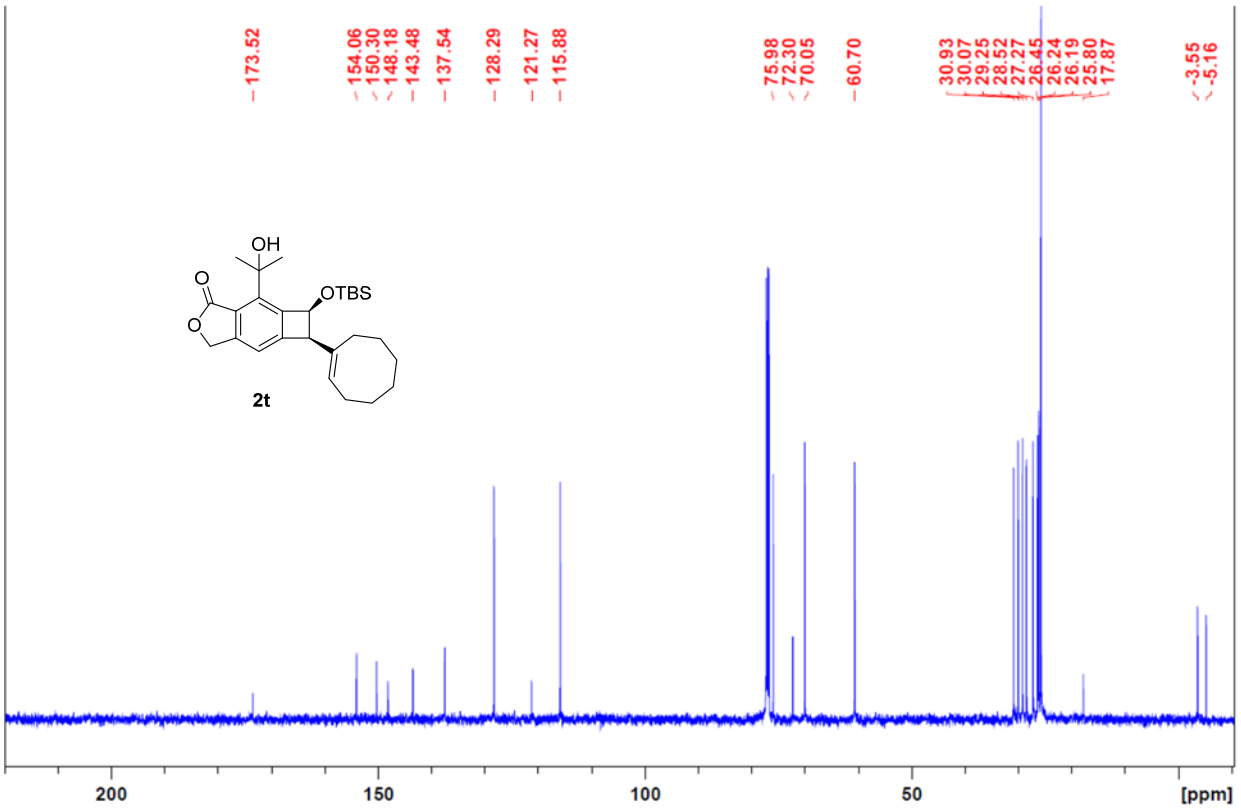
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70.05
60.70
30.93
30.07
29.25
28.52
27.27
26.45
26.24
26.19
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-5.16
OH
O
O
OTBS
2t
200
150
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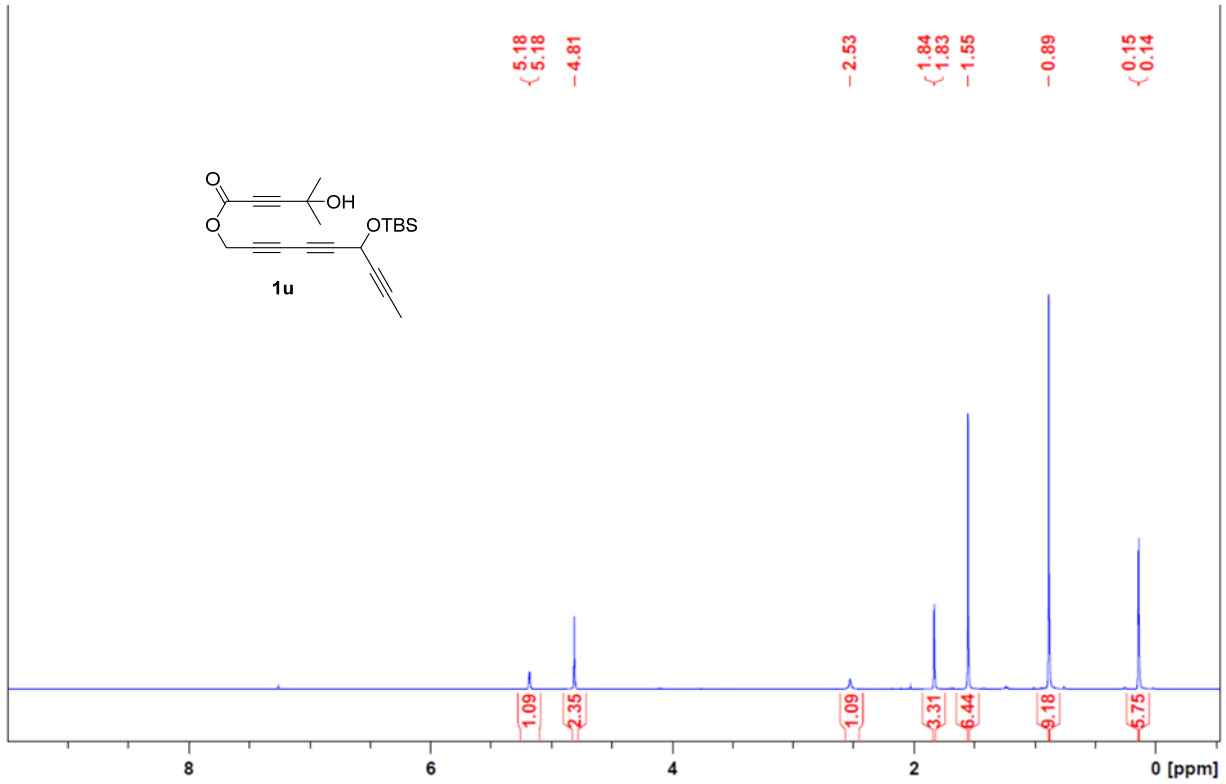
50
[ppm]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1.83
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0.14
OH
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5.75
8
6
4
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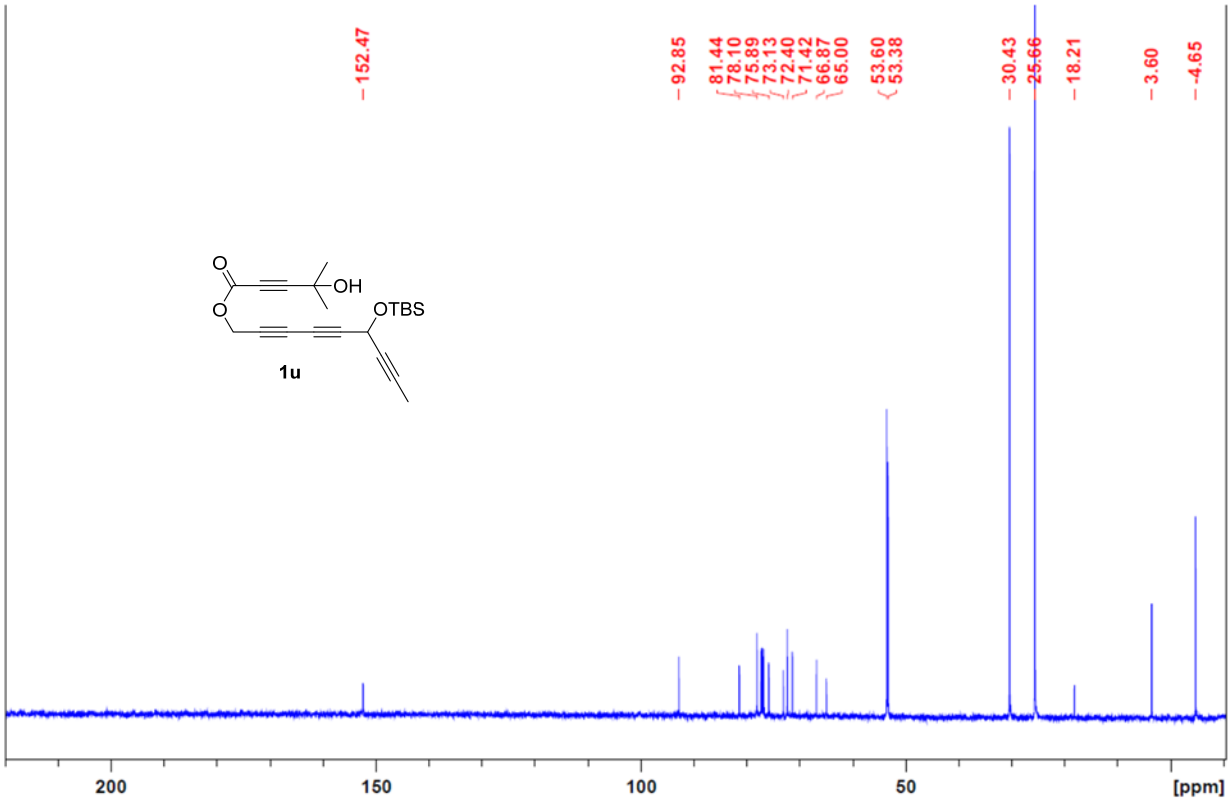
0 [ppm]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OTBS
1u
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150
100
50
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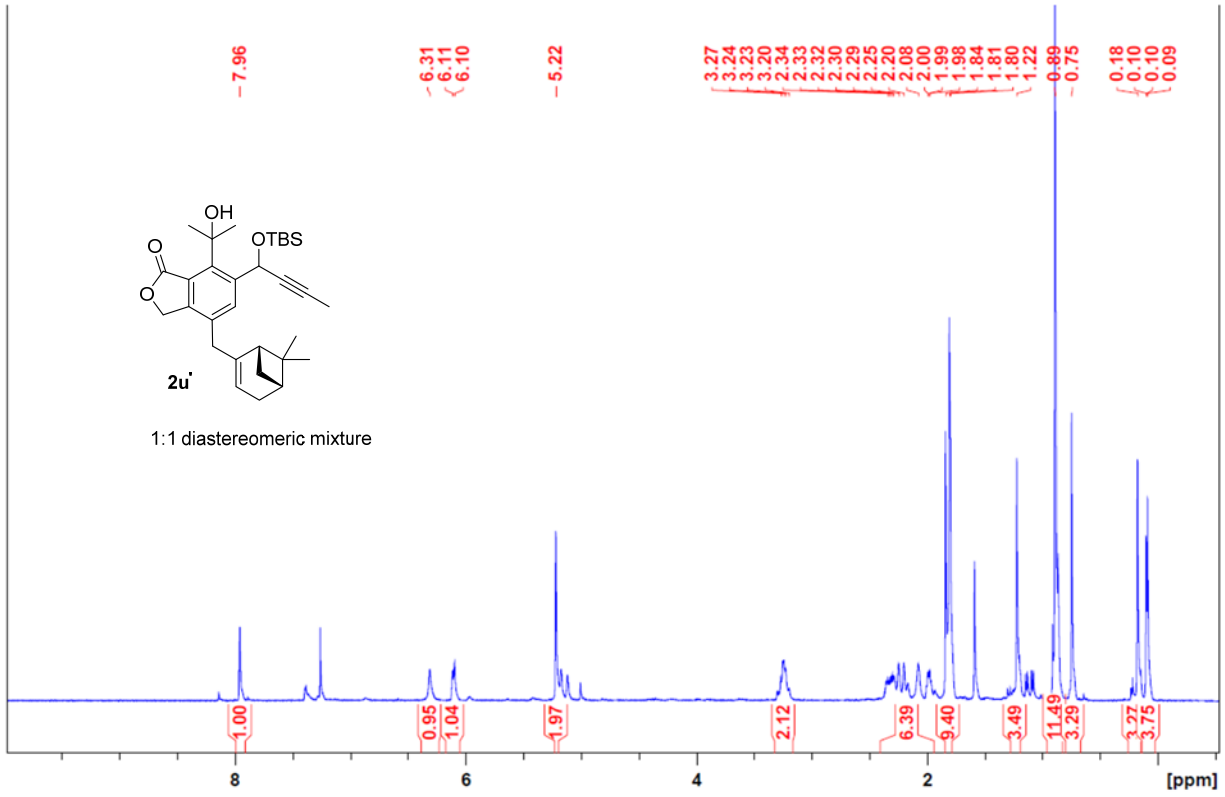
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3.23
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2.34
2.33
2.32
2.30
2.29
2.25
2.20
2.08
2.00
1.99
1.98
1.84
1.81
1.80
1.22
0.89
0.75
0.18
0.10
0.10
0.09
OH
OTBS
O
O
2u'
1:1 diastereomeric mixture
1.00
0.95
1.04
1.97
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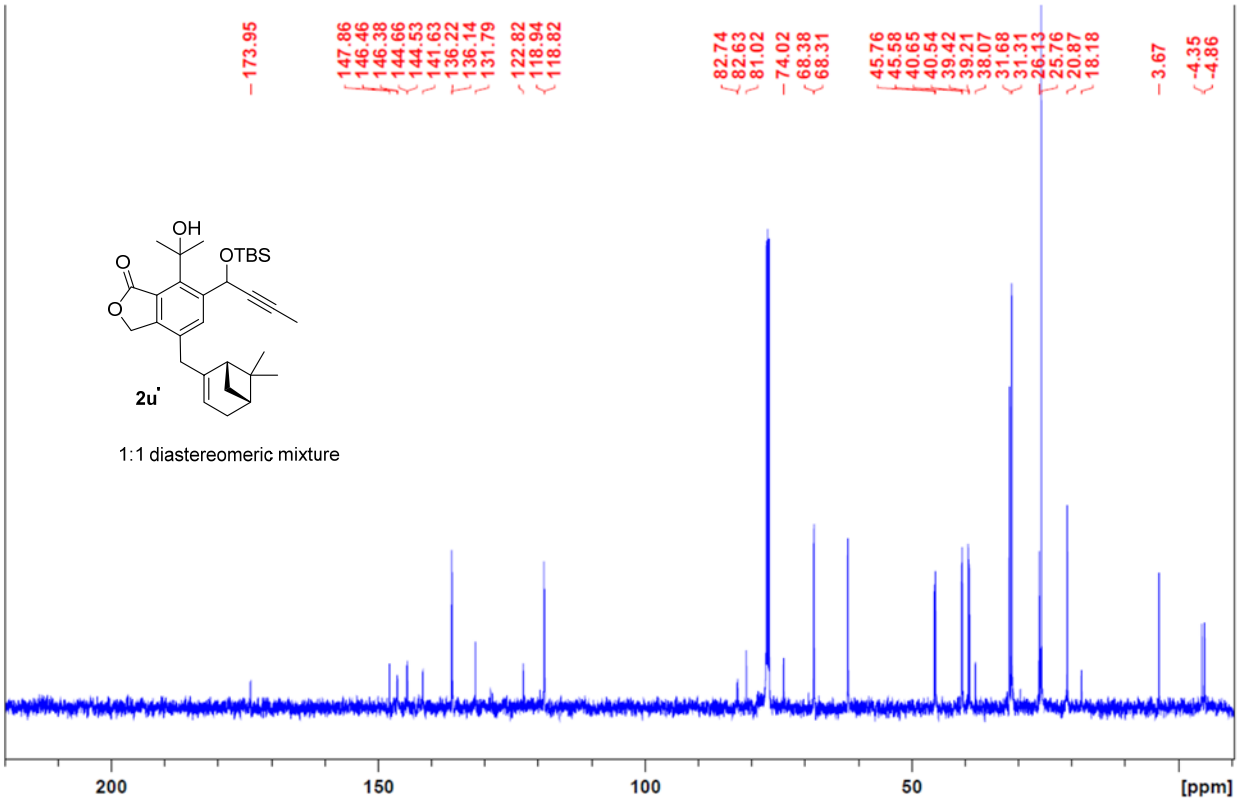
9.40
3.49
11.49
3.29
3.27
3.75
8
6
4
2
[ppm]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136.22
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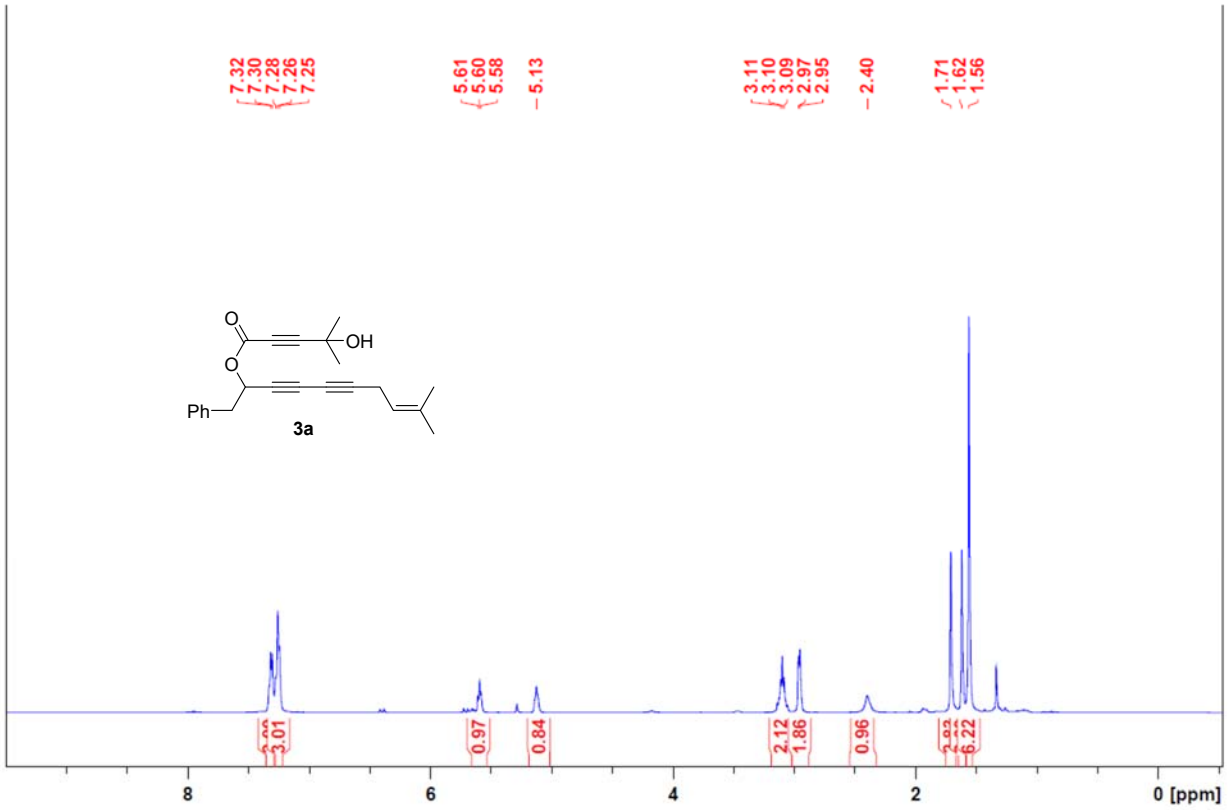
131.79
122.82
118.94
118.82
82.74
82.63
81.02
74.02
68.38
68.31
45.76
45.58
40.65
40.54
39.42
39.21
38.07
31.68
31.31
26.13
25.76
20.87
18.18
3.67
-4.35
-4.86
OH
OTBS
O
O
2u'
1:1 diastereomeric mixture
200
150
100
50
[ppm]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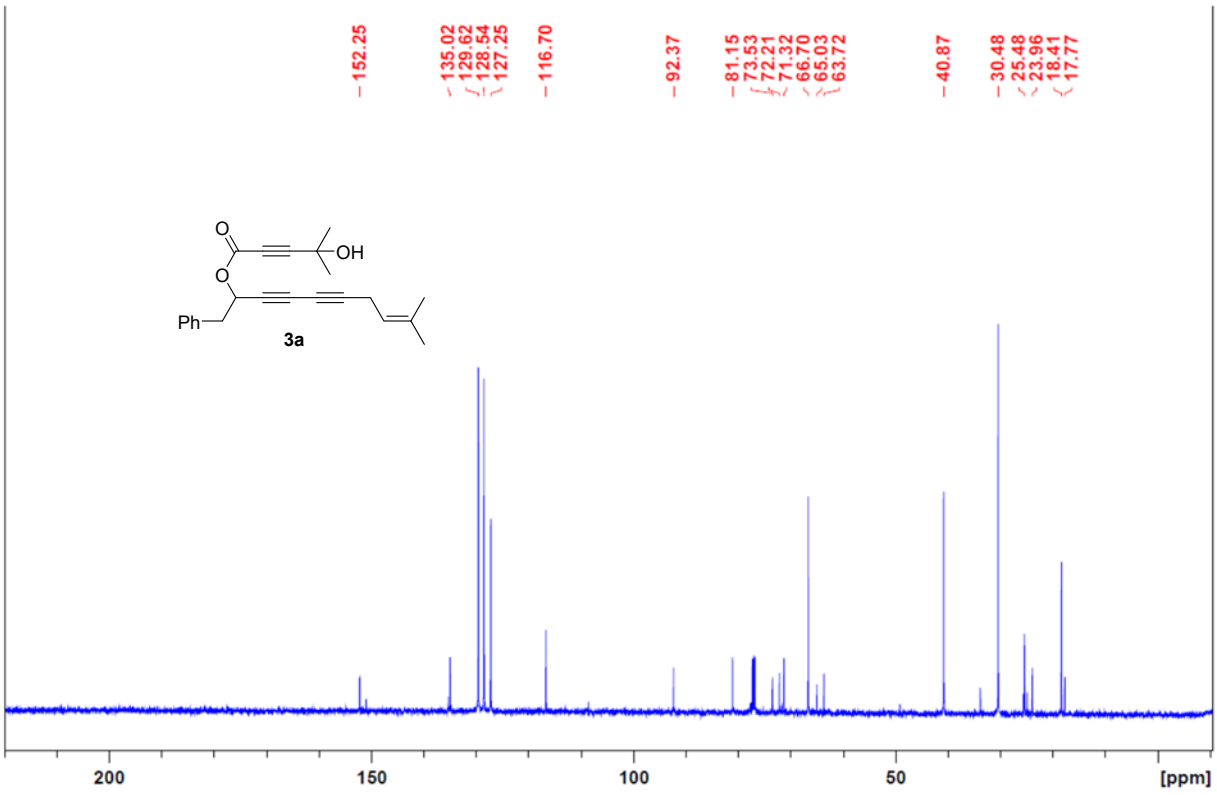
7.26
7.25
5.61
5.60
5.58
5.13
3.11
3.10
3.09
2.97
2.95
2.40
1.71
1.62
1.56
O
OH
O
Ph
3a
3.01
0.97
0.84
2.12
1.86
0.96
8
6
4
2
0 [ppm]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127.25
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81.15
73.53
72.21
71.32
66.70
65.03
63.72
40.87
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25.48
23.96
18.41
17.77
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OH
O
Ph
3a
200
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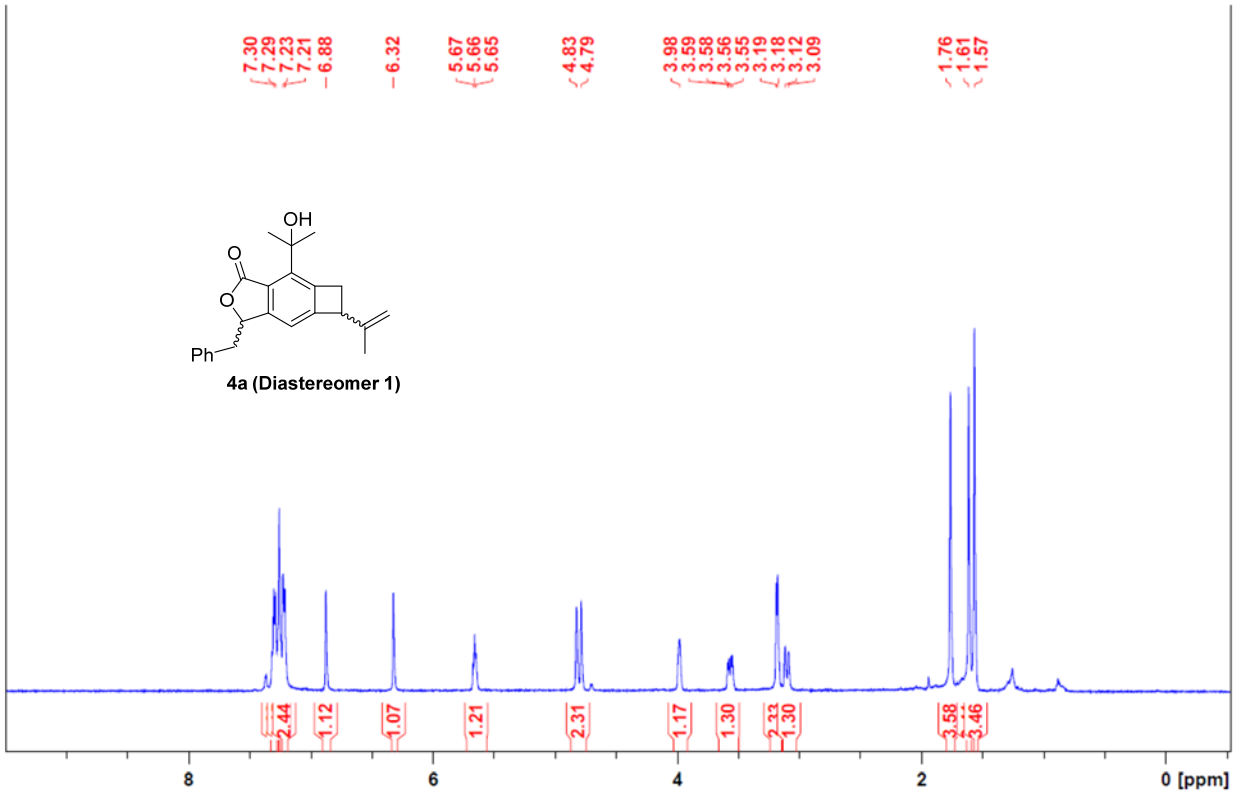
100
50
[ppm]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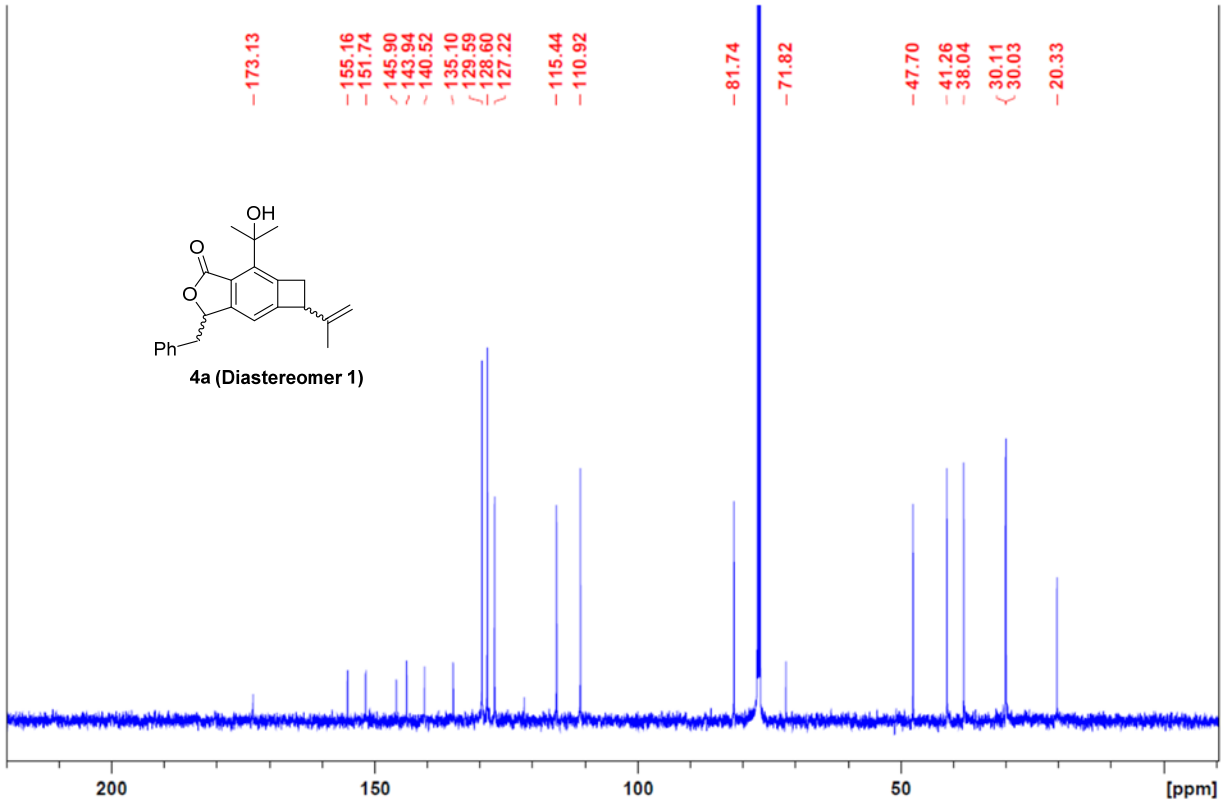
6.32
5.67
5.66
5.65
4.83
4.79
3.98
3.59
3.58
3.56
3.55
3.19
3.18
3.12
3.09
1.76
1.61
1.57
OH
O
O
Ph
4a (Diastereomer 1)
2.44
1.12
1.07
1.21
2.31
1.17
1.30
2.33
1.30
2.58
3.46
8
6
4
2
0 [ppm]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135.10
129.59
128.60
127.22
115.44
110.92
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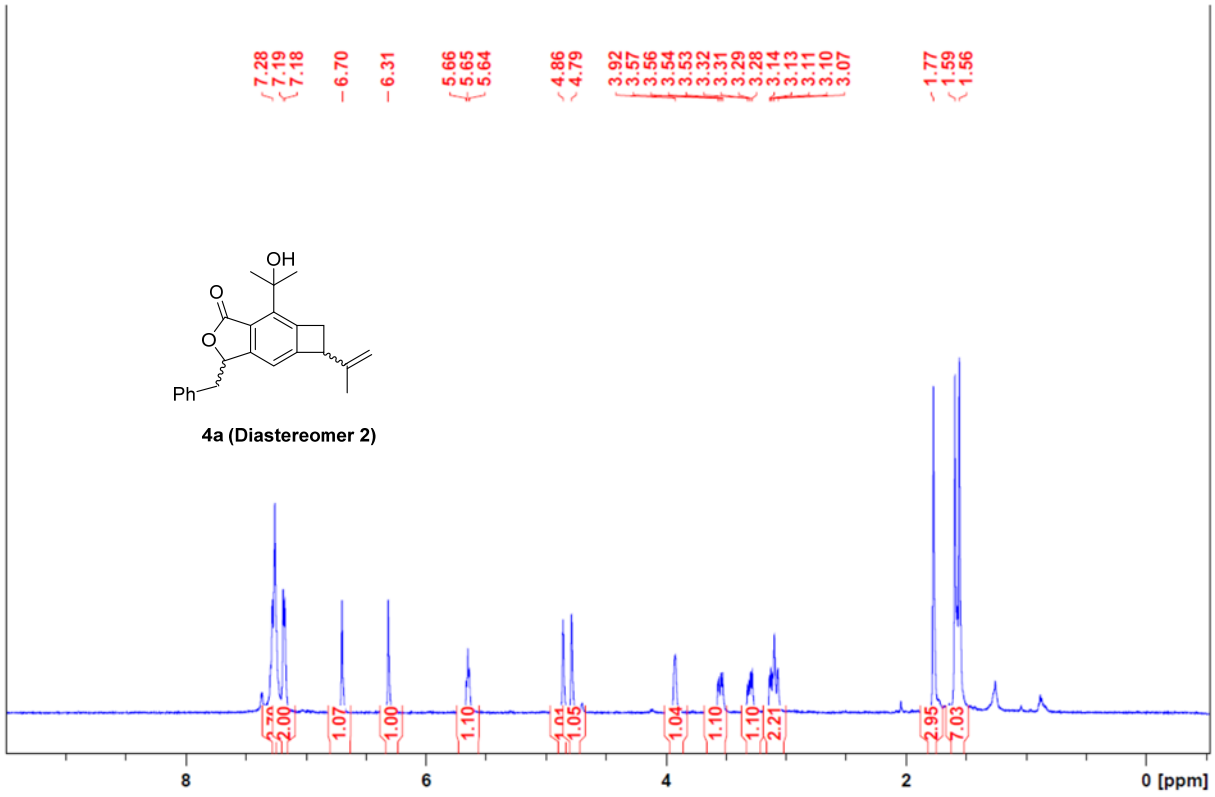
71.82
47.70
41.26
38.04
30.11
30.03
20.33
OH
O
O
Ph
4a (Diastereomer 1)
200
150
100
50
[ppm]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7.19
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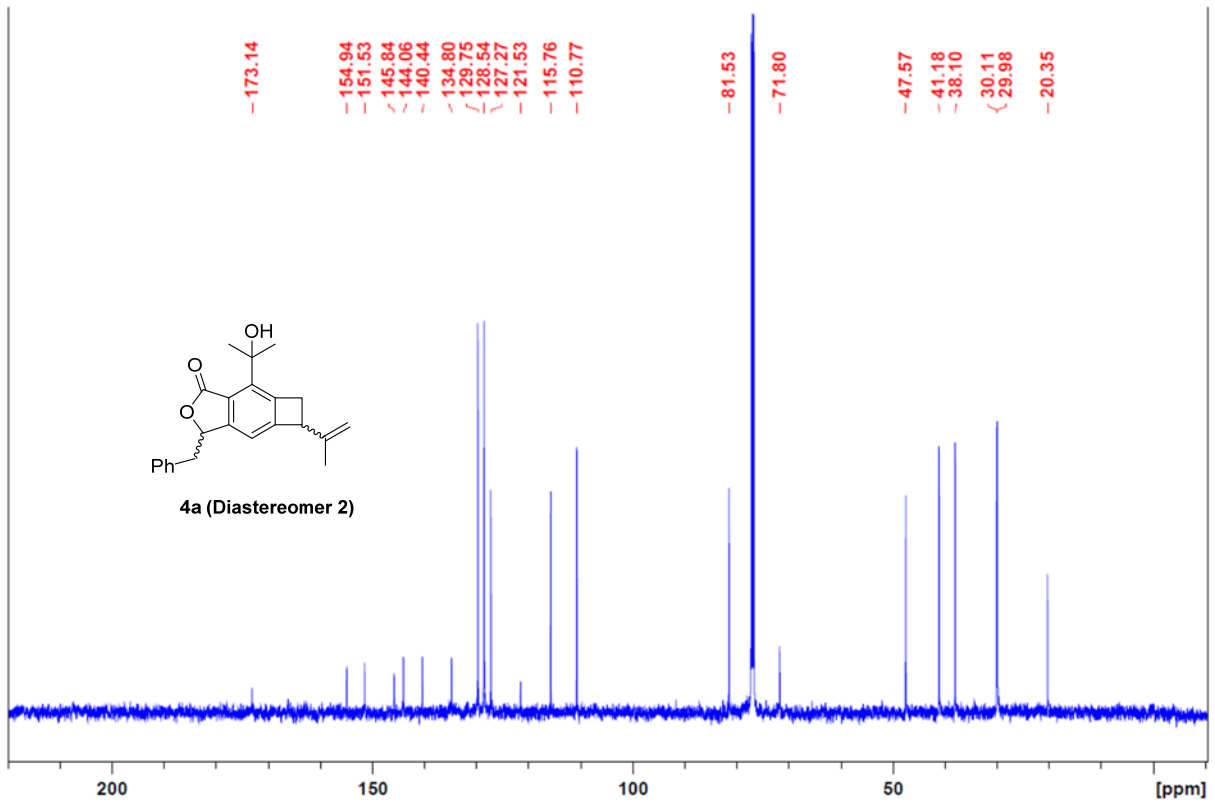
6.70
6.31
5.66
5.65
5.64
4.86
4.79
3.92
3.57
3.56
3.54
3.53
3.32
3.31
3.29
3.28
3.14
3.13
3.11
3.10
3.07
1.77
1.59
1.56
OH
O
O
Ph
4a (Diastereomer 2)
2.00
1.07
1.00
1.10
1.05
1.04
1.10
1.10
2.21
2.95
7.03
8
6
4
2
0 [ppm]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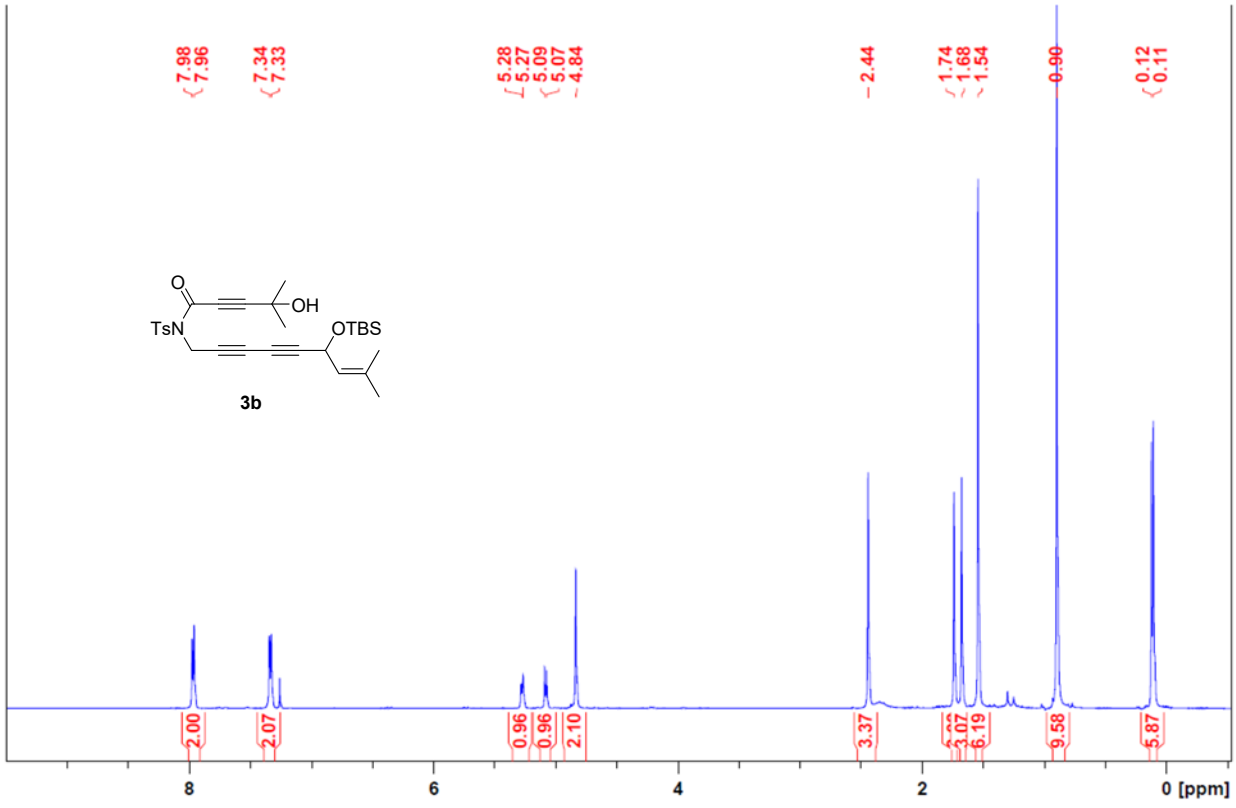
128.54
127.27
121.53
115.76
110.77
81.53
71.80
47.57
41.18
38.10
30.11
29.98
20.35
OH
O
O
Ph
4a (Diastereomer 2)
200
150
100
50
[ppm]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7.96
7.34
7.33
5.28
5.27
5.09
5.07
4.84
2.44
1.74
1.68
1.54
0.90
0.12
0.11
O
OH
TsN
OTBS
3b
2.00
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2.10
3.37
3.07
6.19
9.58
5.87
8
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4
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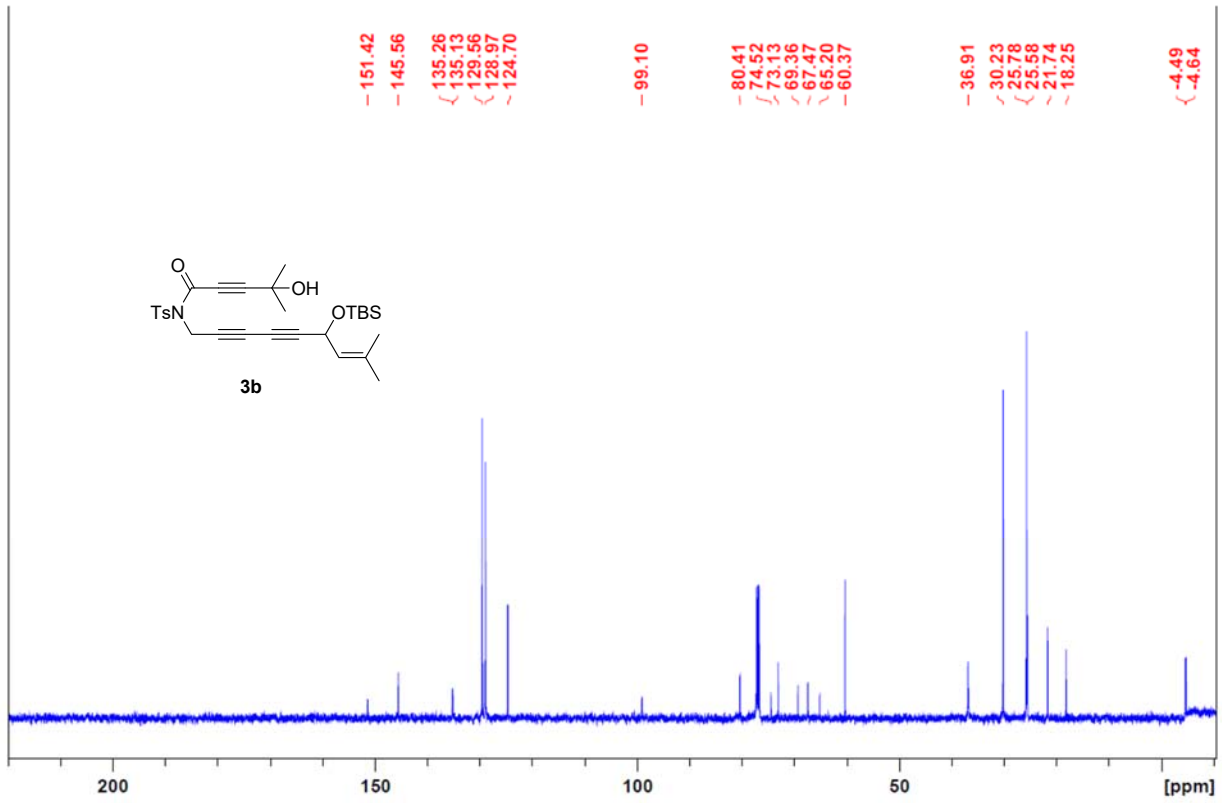
0 [ppm]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80.41
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65.20
60.37
36.91
30.23
25.78
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-4.64
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OH
TsN
OTBS
3b
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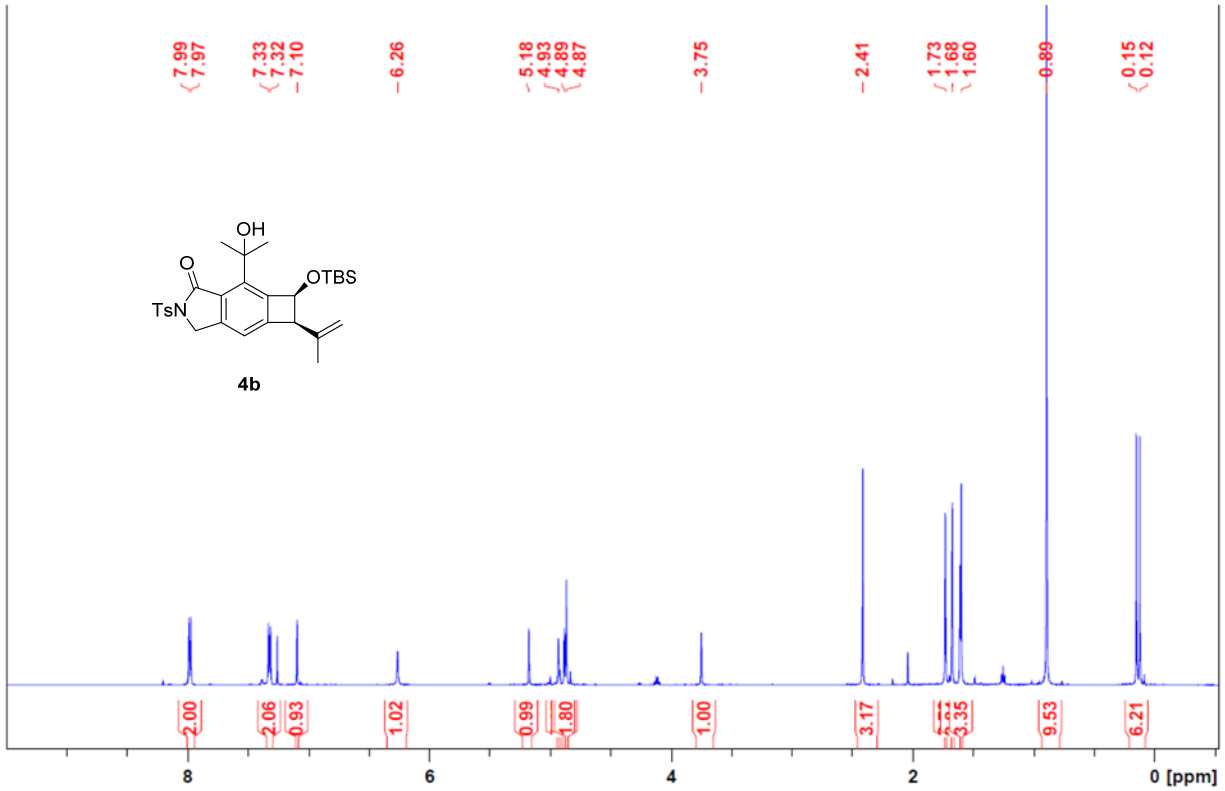
150
100
50
[ppm]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3.75
2.41
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1.68
1.60
0.89
0.15
0.12
OH
O
TsN
OTBS
4b
2.00
2.06
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1.00
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6.21
8
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4
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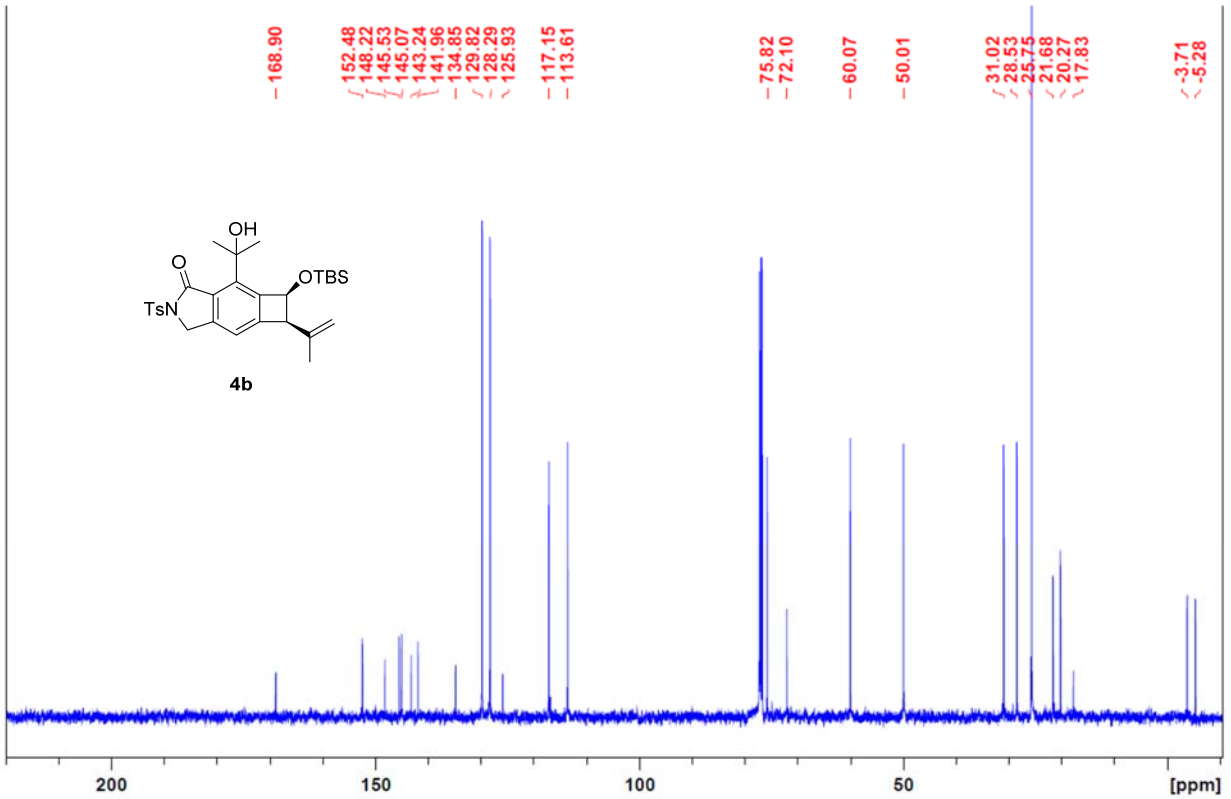
0 [ppm]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128.29
125.93
117.15
113.61
75.82
72.10
60.07
50.01
31.02
28.53
25.75
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20.27
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-5.28
OH
O
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OTBS
4b
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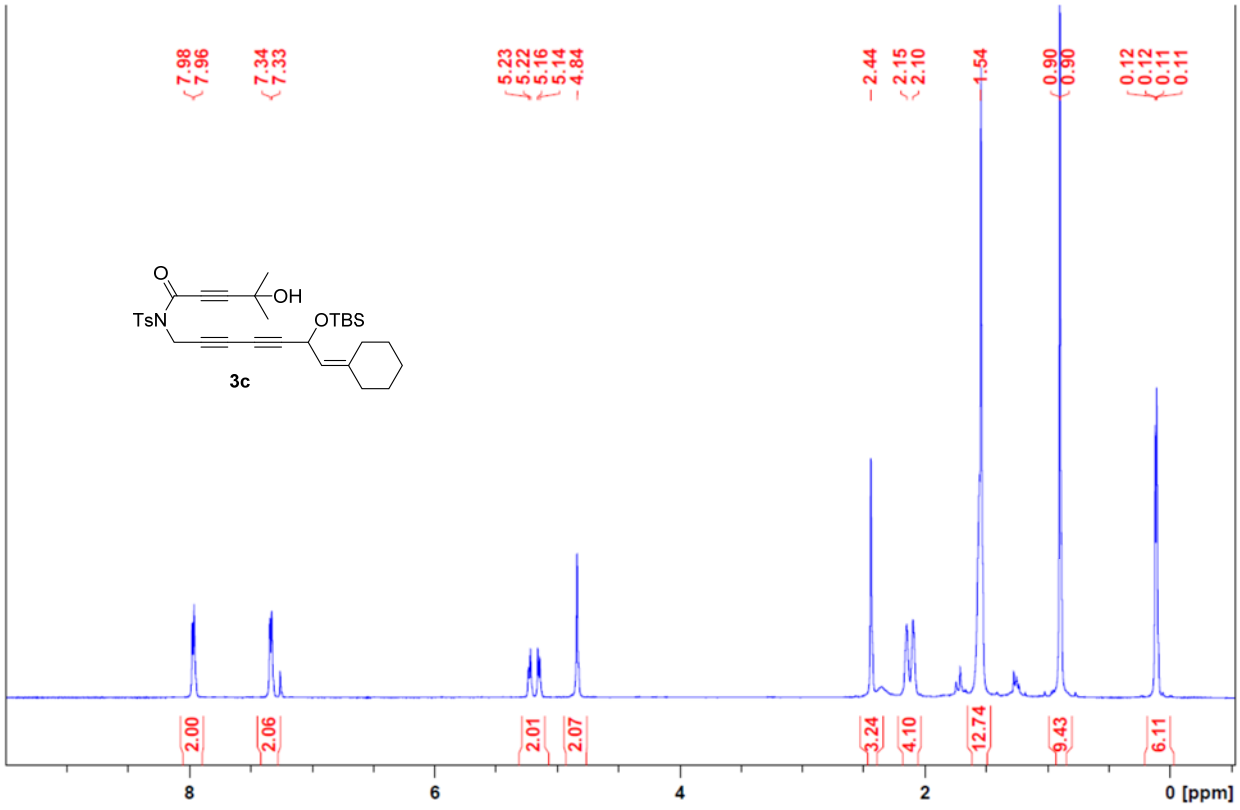
100
50
[ppm]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5.14
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2.44
2.15
2.10
1.54
0.90
0.90
0.12
0.12
0.11
0.11
O
OH
TsN
OTBS
3c
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3.24
4.10
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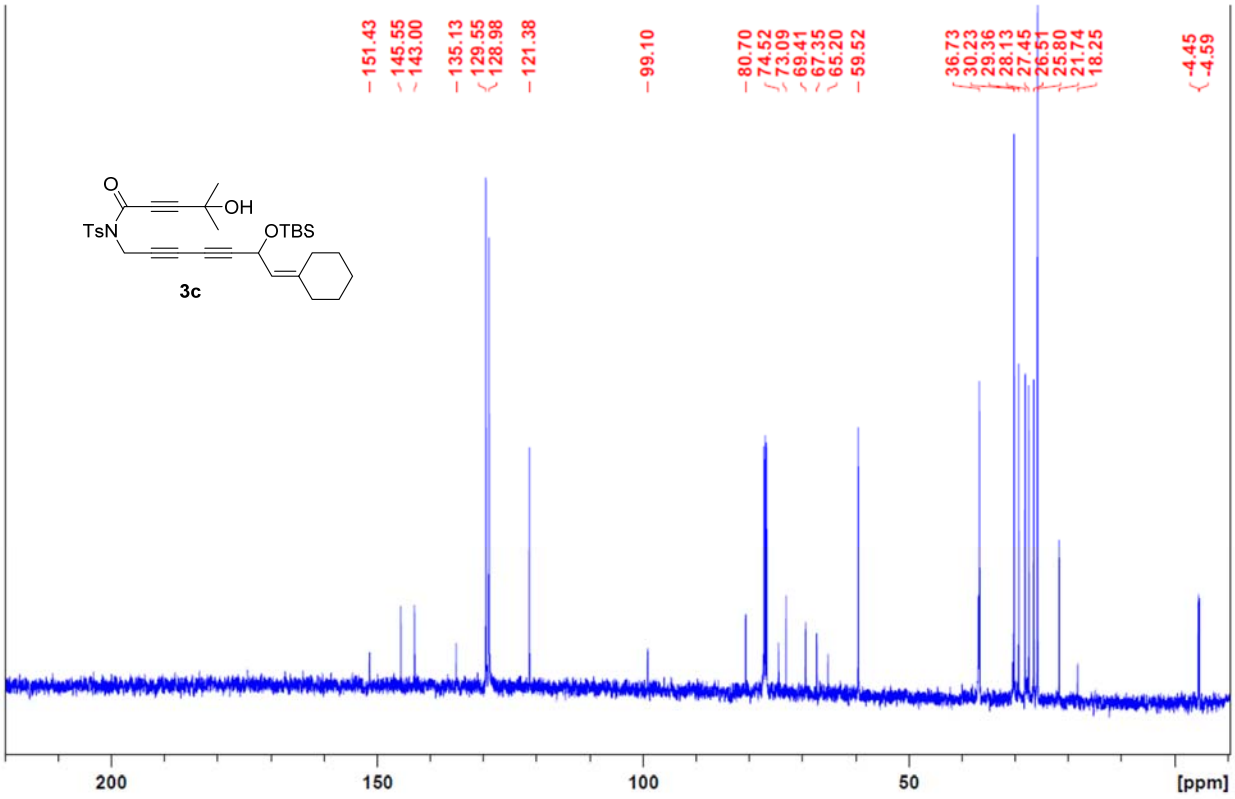
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74.52
73.09
69.41
67.35
65.20
59.52
36.73
30.23
29.36
28.13
27.45
26.51
25.80
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-4.59
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OH
TsN
OTBS
3c
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150
100
50
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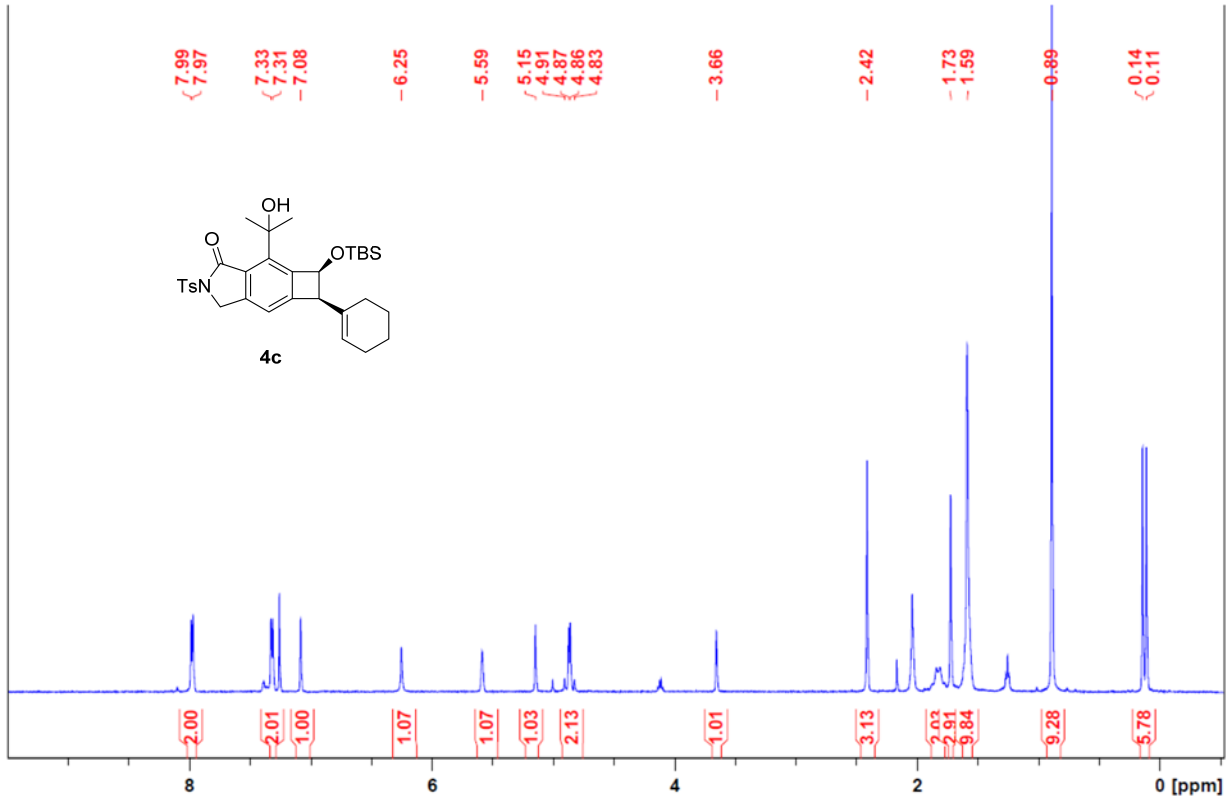
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4.87
4.86
4.83
3.66
2.42
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1.59
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0.14
0.11
OH
O
OTBS
TsN
4c
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2.01
1.00
1.07
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1.01
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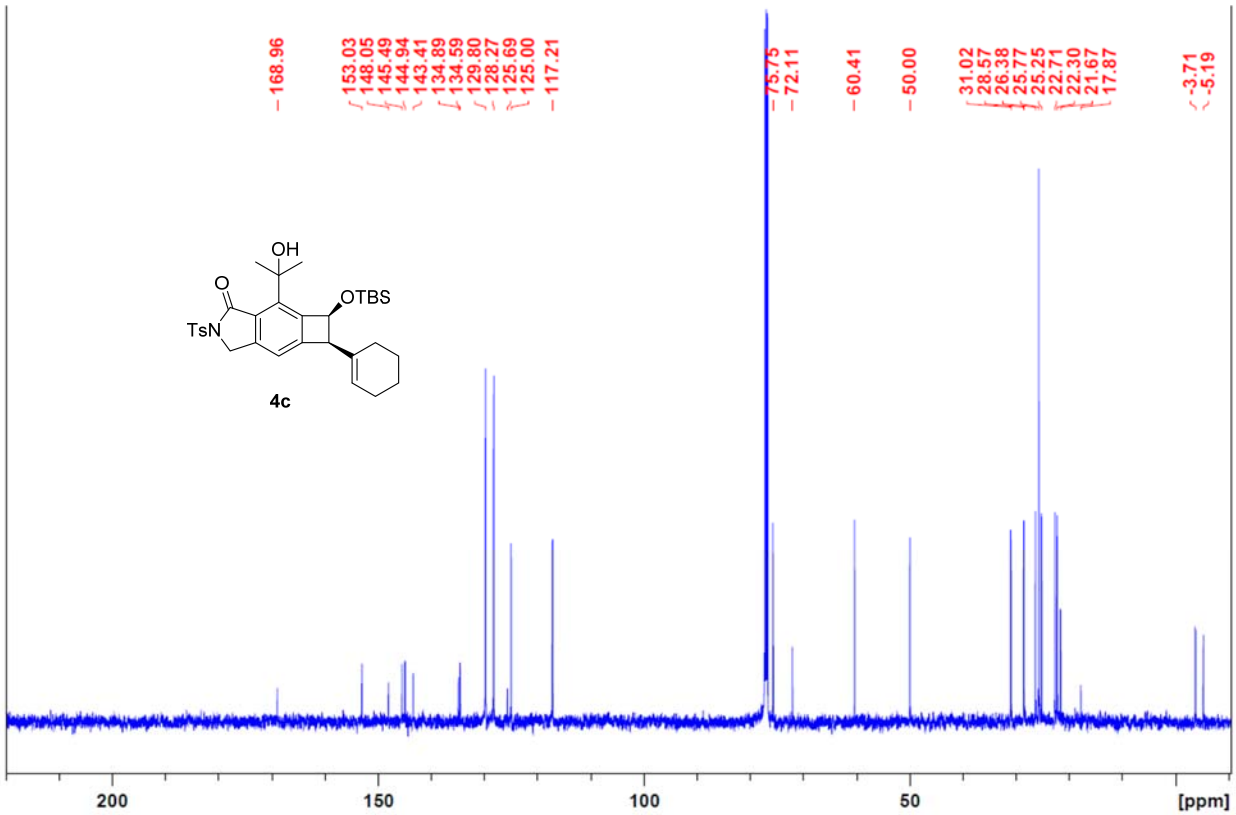
0 [ppm]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145.49
144.94
143.41
134.89
134.59
129.80
128.27
125.69
125.00
117.21
75.75
72.11
60.41
50.00
31.02
28.57
26.38
25.77
25.25
22.71
22.30
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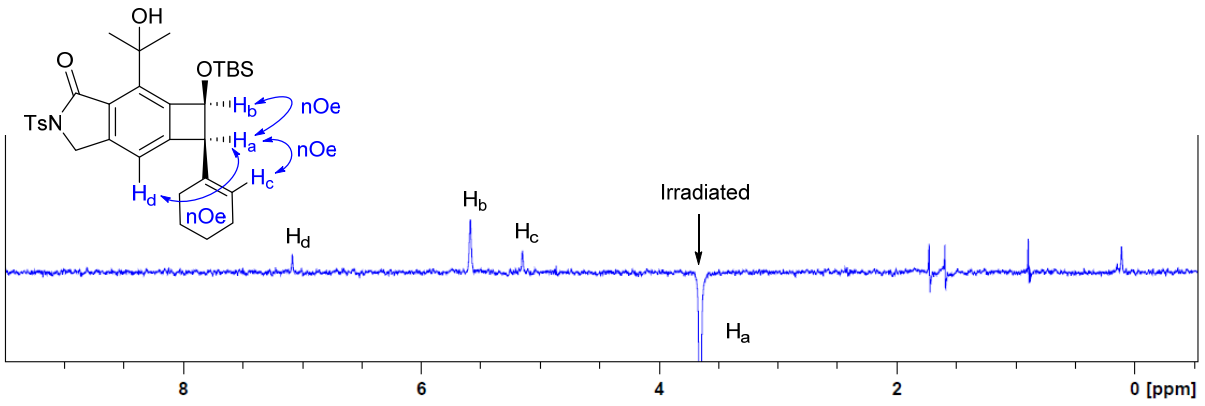
-3.71
-5.19
OH
O
OTBS
TsN
4c
200
150
100
50
[ppm]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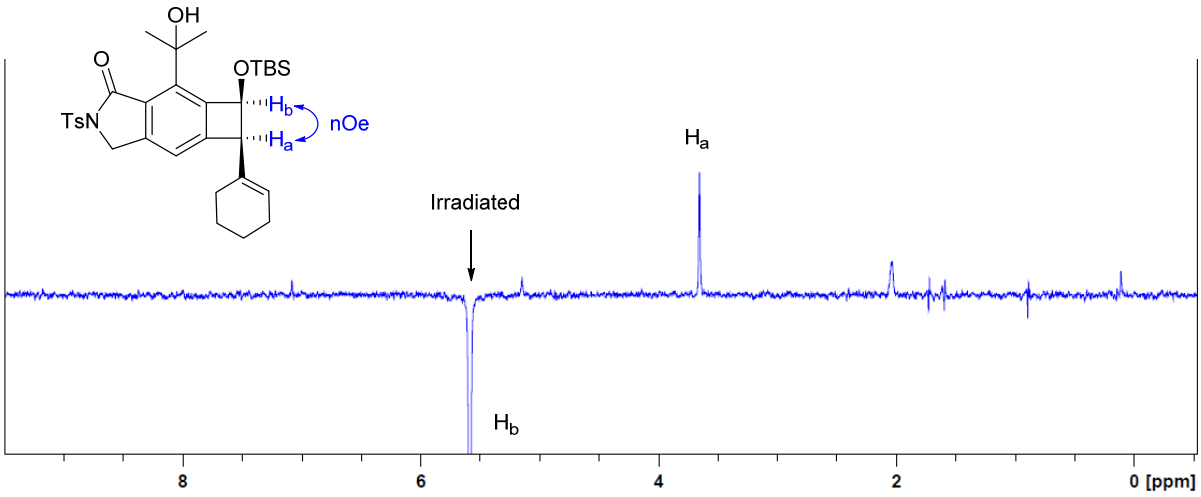
OTBS
TsN
Hb
nOe
Ha
nOe
Hc
Hd
nOe
Hd
Hb
Hc
Irradiated
Ha
8
6
4
2
0 [ppm]


OH
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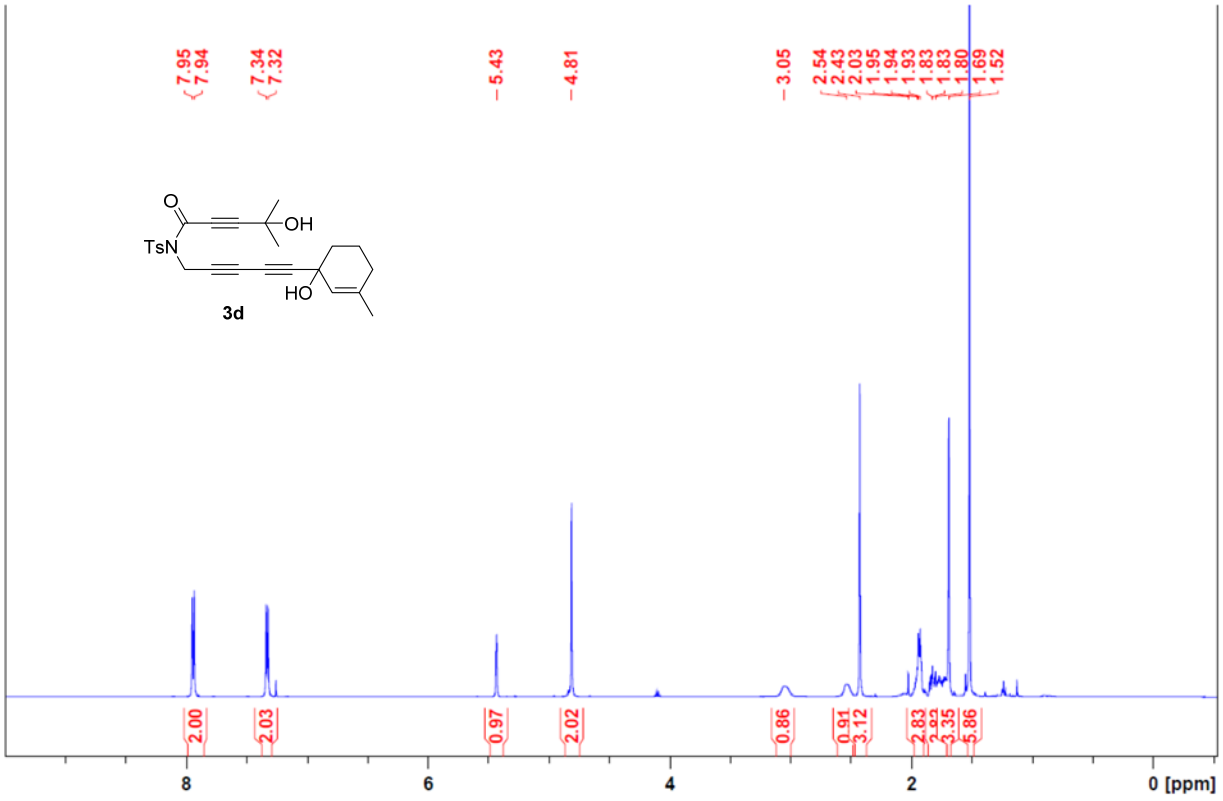
OTBS
TsN
Hb
nOe
Ha
Ha
Irradiated
Hb
8
6
4
2
0 [ppm]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2.54
2.43
2.03
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1.94
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1.83
1.83
1.80
1.69
1.52
O
OH
TsN
HO
3d
2.00
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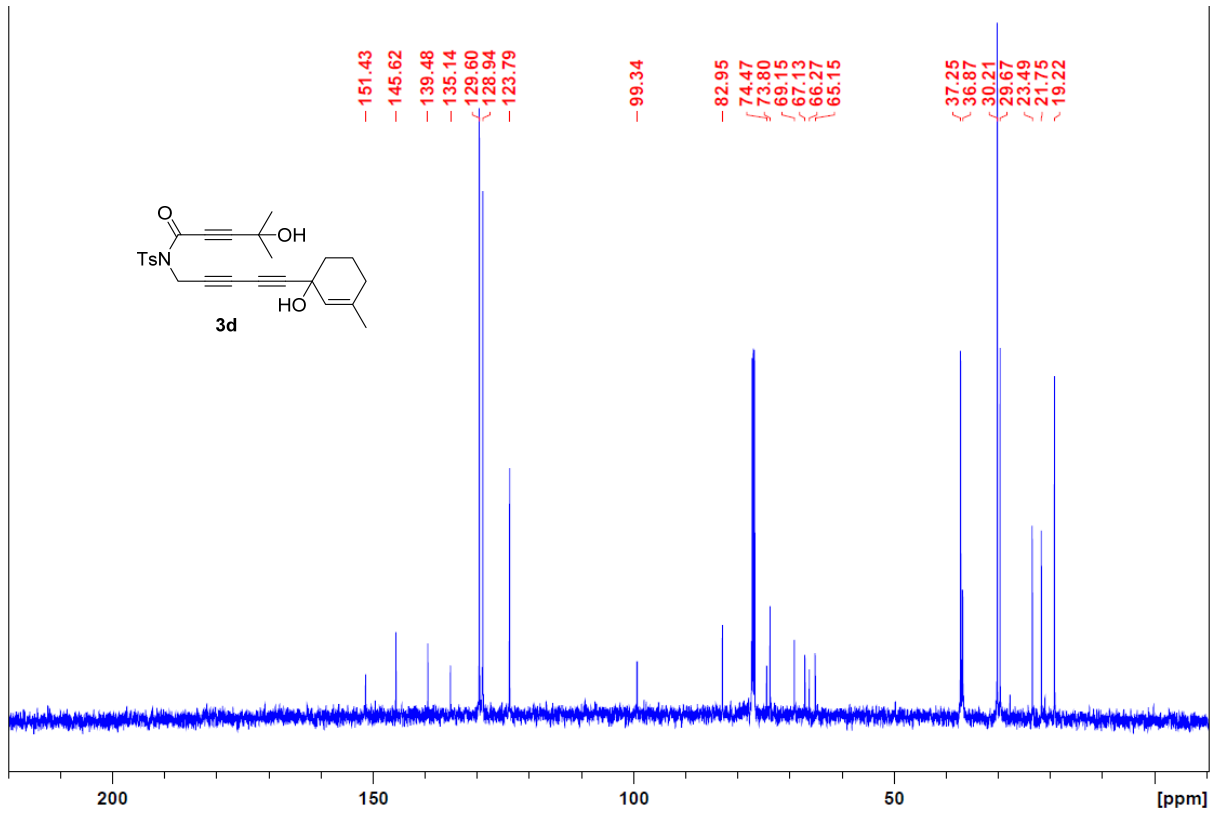
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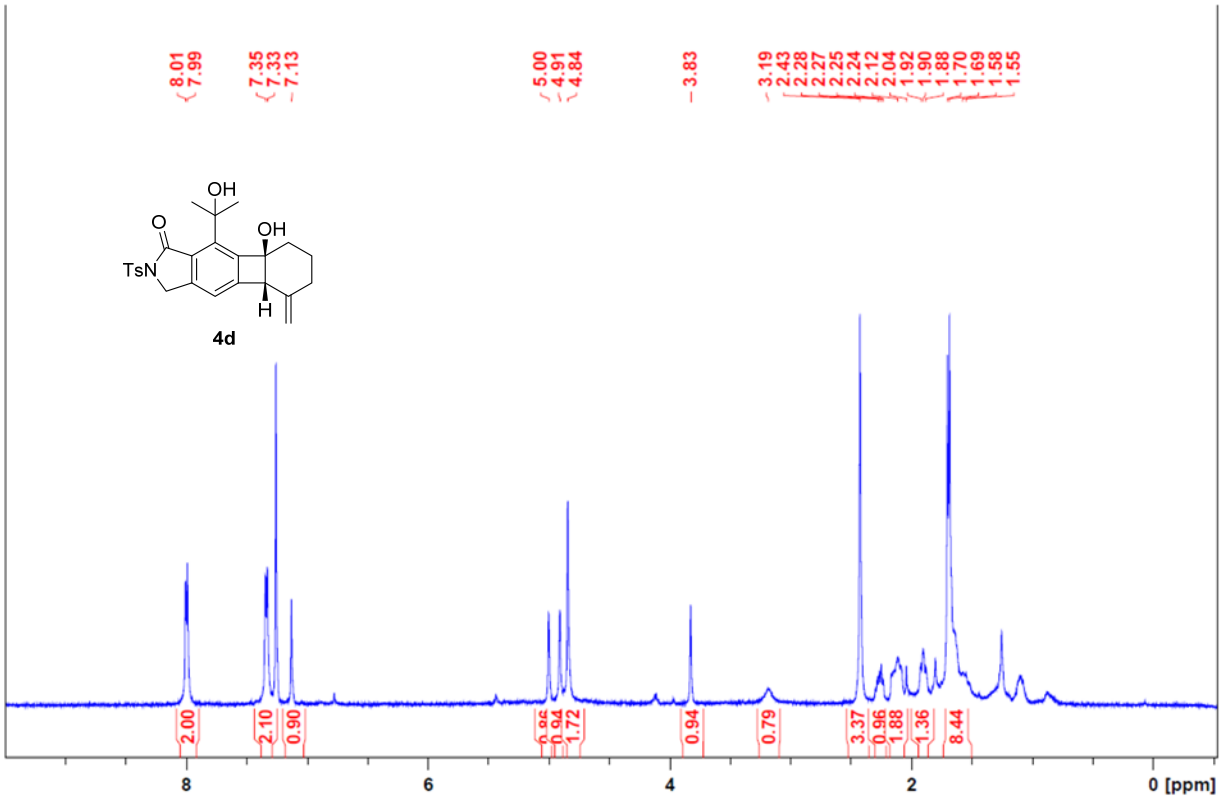
69.15
67.13
66.27
65.15
37.25
36.87
30.21
29.67
23.49
21.75
19.22
O
OH
TsN
HO
3d
200
150
100
50
[ppm]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4.84
3.83
3.19
2.43
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2.27
2.25
2.24
2.12
2.04
1.92
1.90
1.88
1.70
1.69
1.58
1.55
OH
O
OH
TsN
H
4d
2.00
2.10
0.90
1.72
0.94
0.79
3.37
0.96
1.88
1.36
8.44
8
6
4
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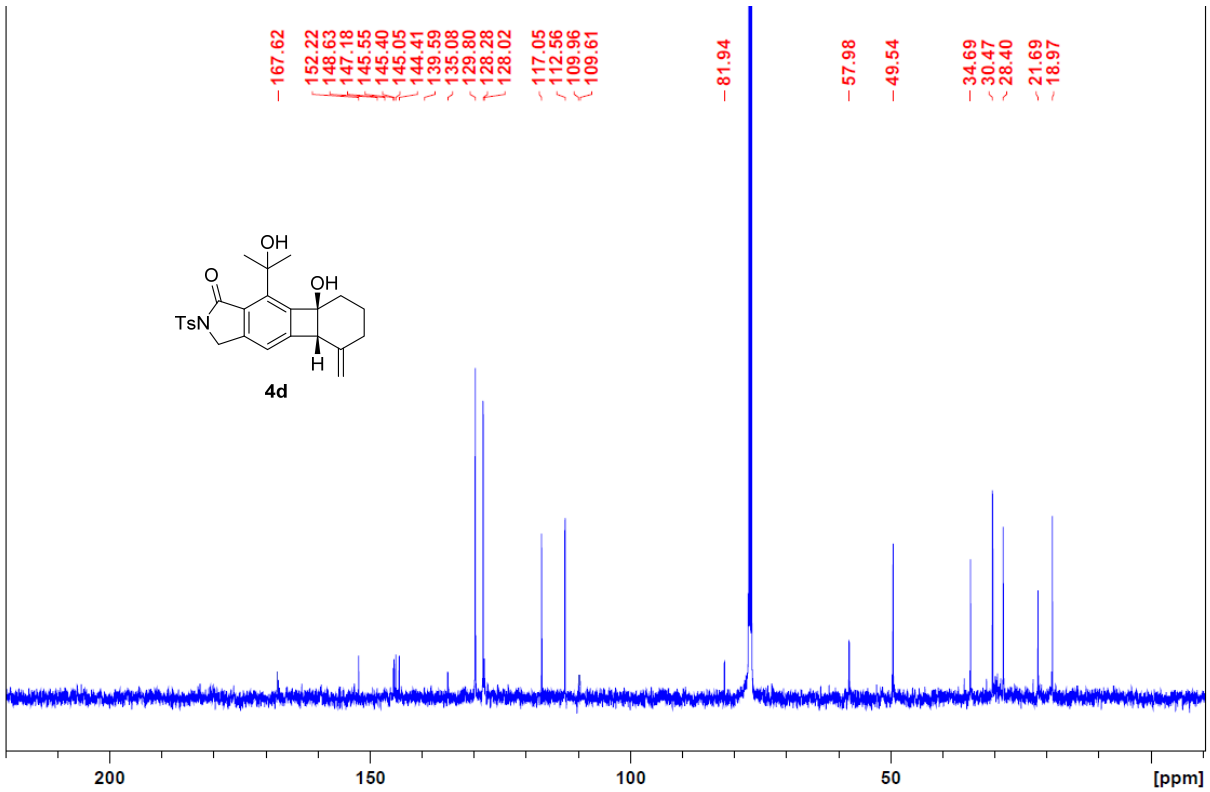
0 [ppm]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128.02
117.05
112.56
109.96
109.61
81.94
57.98
49.54
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OH
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H
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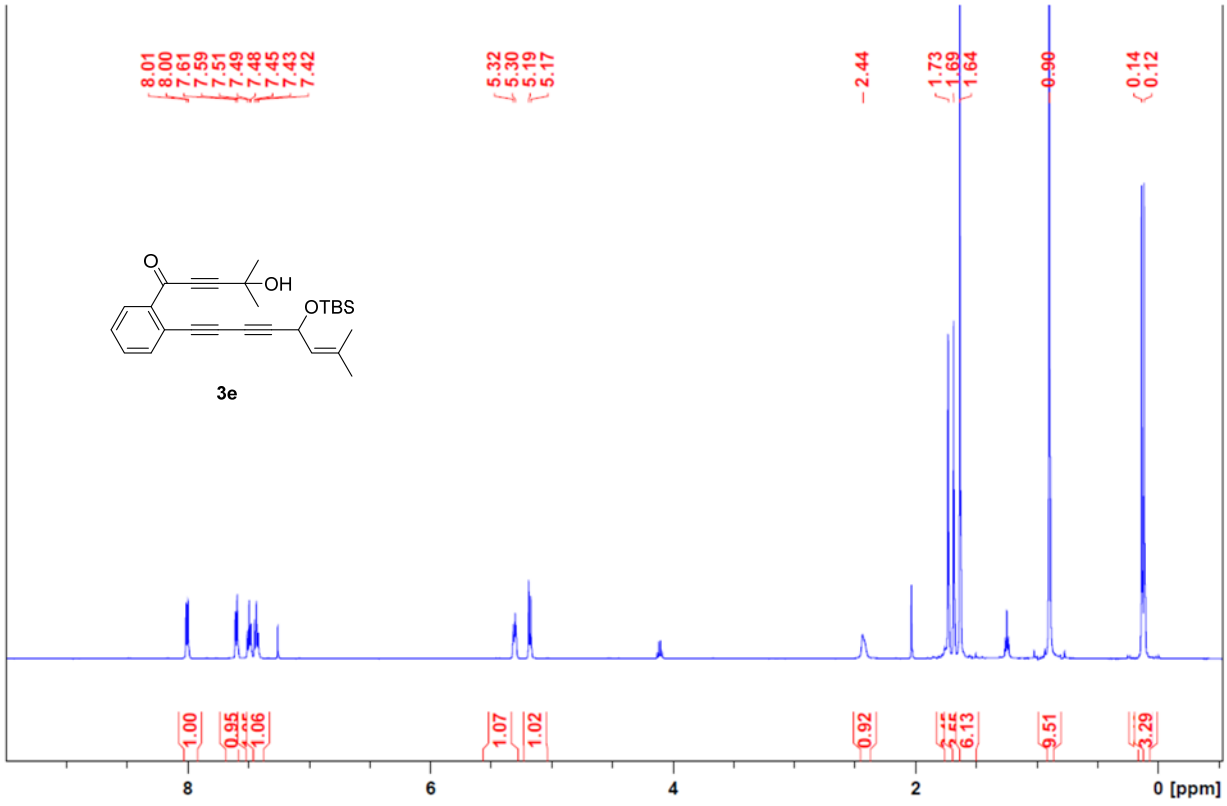
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5.17
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1.69
1.64
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0.12
O
OH
OTBS
3e
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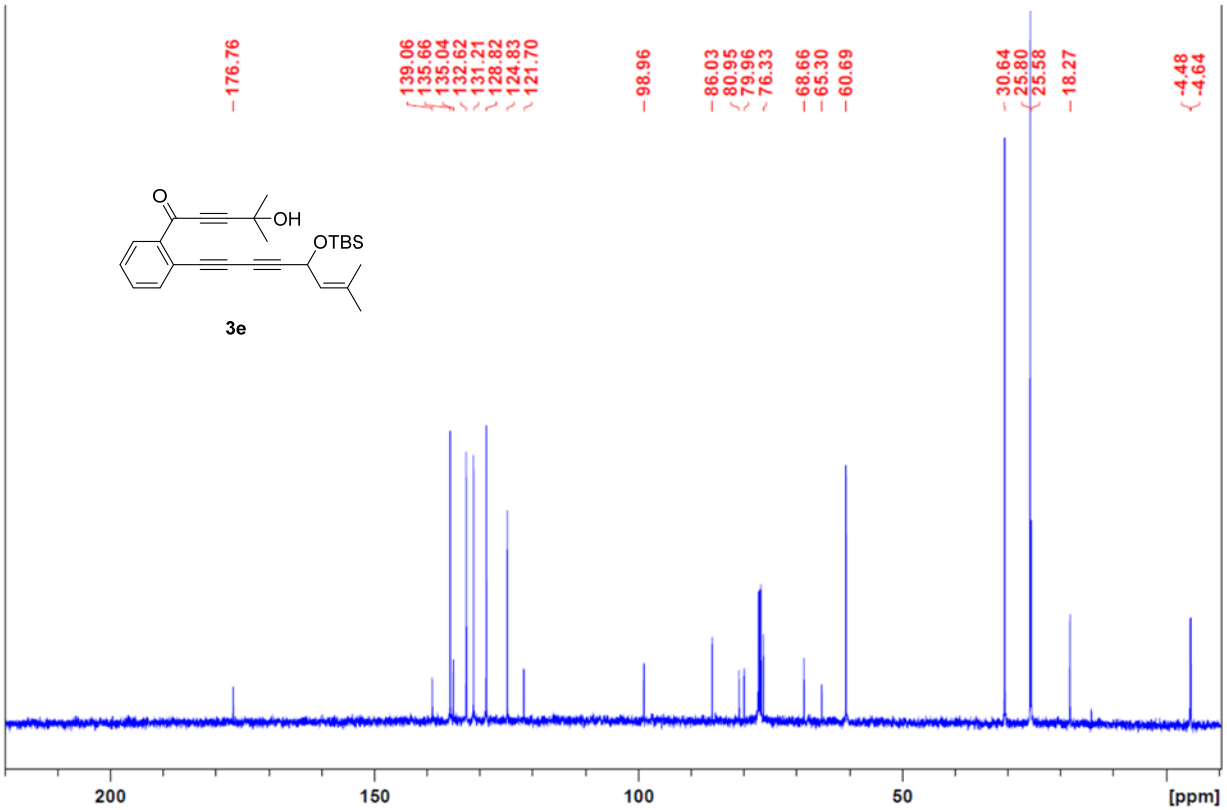
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98.96
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80.95
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76.33
68.66
65.30
60.69
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O
OH
OTBS
3e
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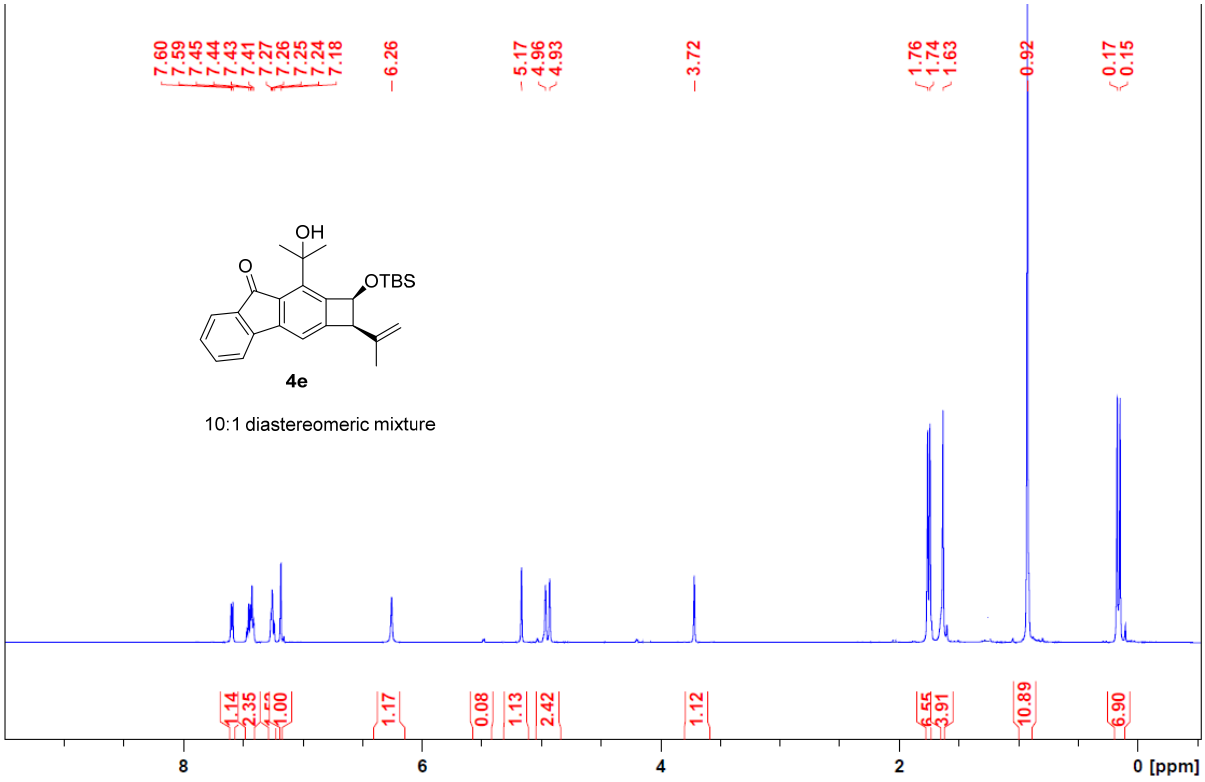
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5.17
4.96
4.93
3.72
1.76
1.74
1.63
0.92
0.17
0.15
OH
O
OTBS
4e
10:1 diastereomeric mixture
1.14
2.35
1.00
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2.42
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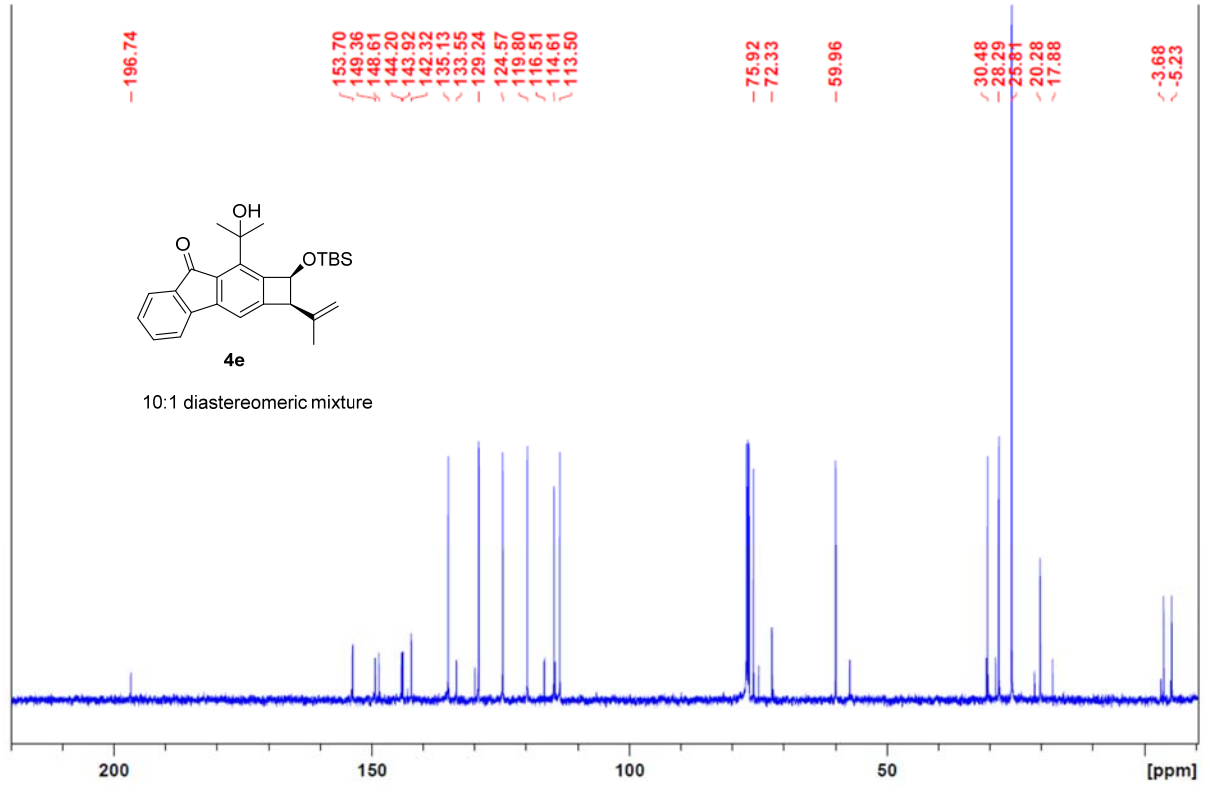
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119.80
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113.50
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59.96
30.48
28.29
25.81
20.28
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OH
O
OTBS
4e
10:1 diastereomeric mixture
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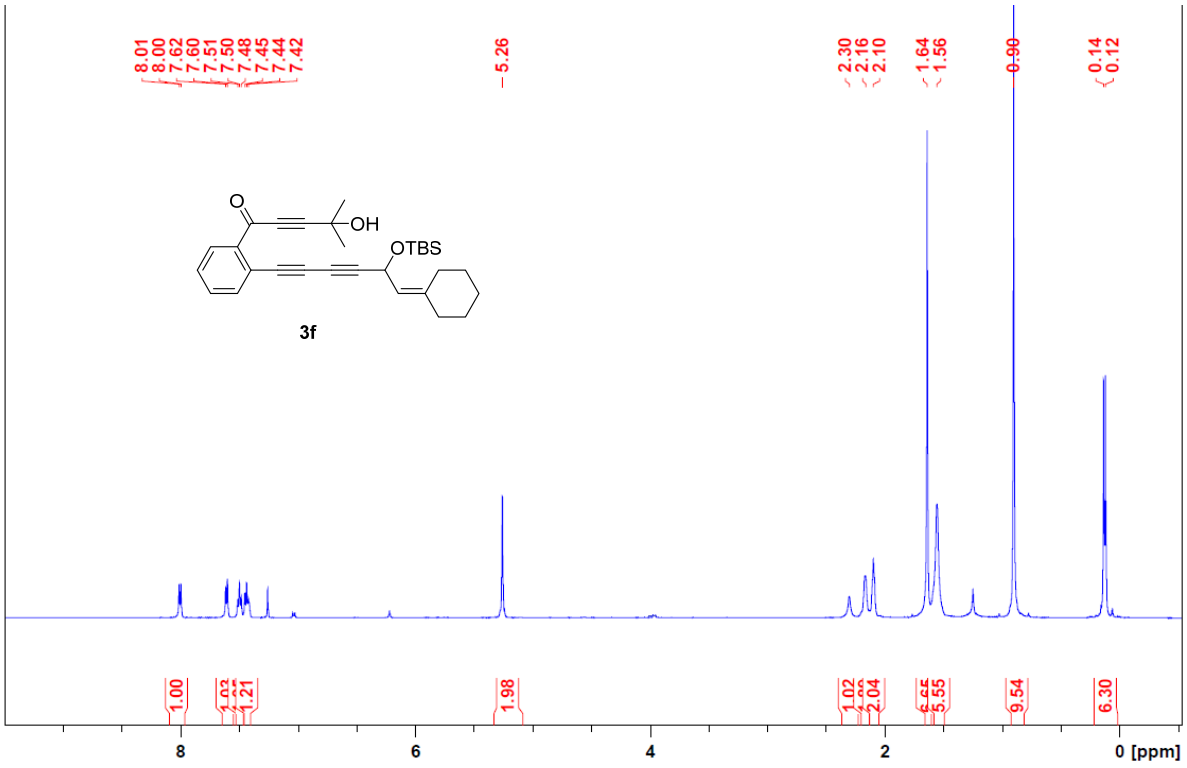
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7.50
7.48
7.45
7.44
7.42
5.26
2.30
2.16
2.10
1.64
1.56
0.00
0.14
0.12
O
OH
OTBS
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1.98
1.02
2.04
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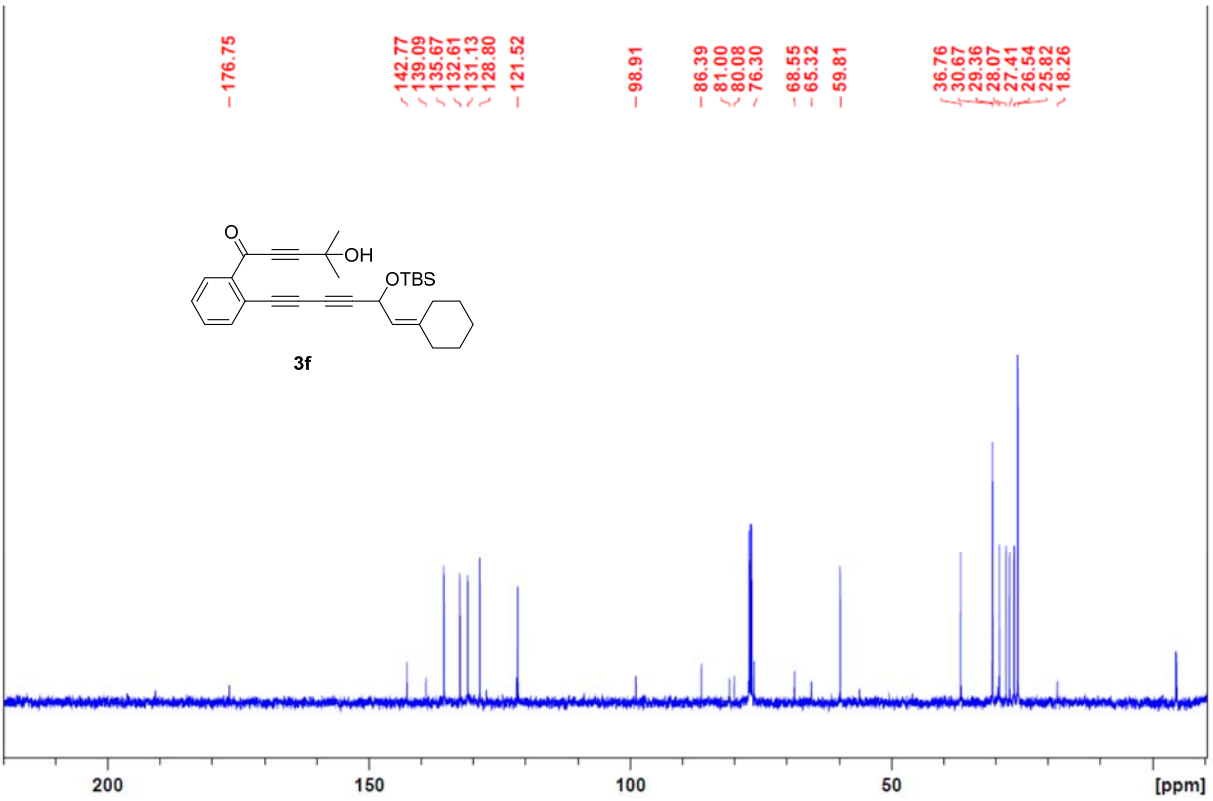
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80.08
76.30
68.55
65.32
59.81
36.76
30.67
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26.54
25.82
18.26
O
OH
OTBS
3f
200
150
100
50
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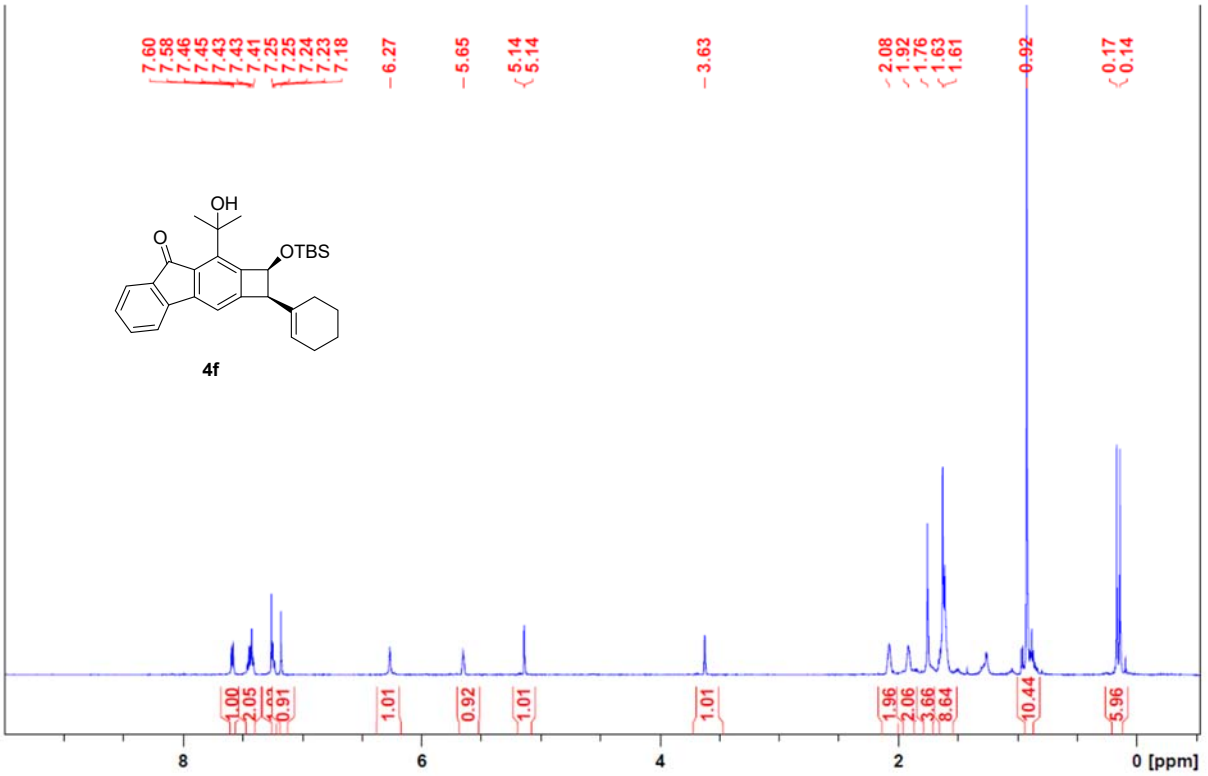
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7.43
7.41
7.25
7.25
7.24
7.23
7.18
6.27
5.65
5.14
5.14
3.63
2.08
1.92
1.76
1.63
1.61
0.92
0.17
0.14
OH
O
OTBS
4f
1.00
2.05
0.91
1.01
0.92
1.01
1.01
1.96
2.06
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8
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4
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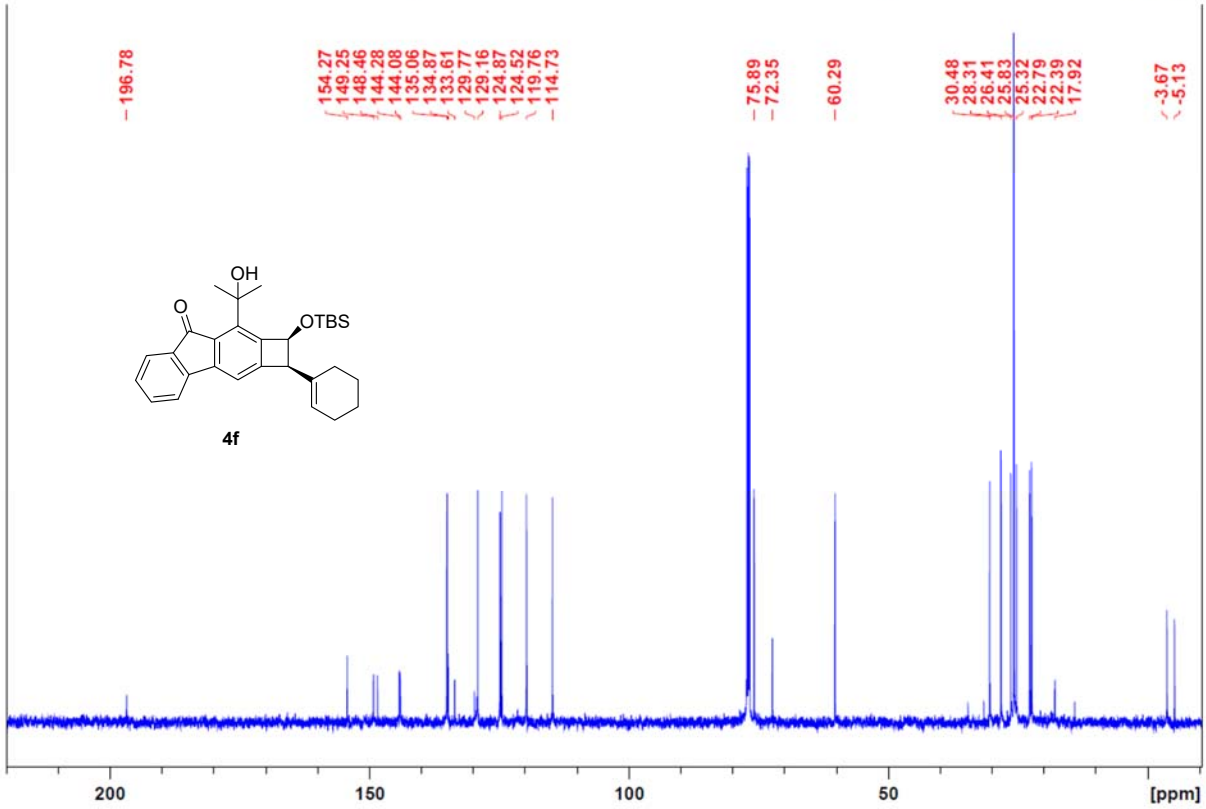
0 [ppm]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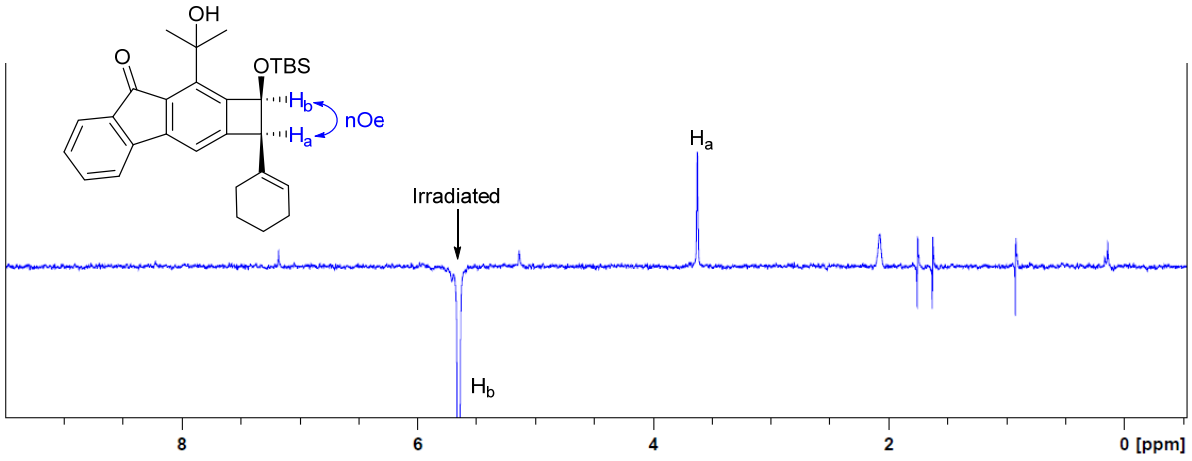
133.61
129.77
129.16
124.87
124.52
119.76
114.73
75.89
72.35
60.29
30.48
28.31
26.41
25.83
25.32
22.79
22.39
17.92
-3.67
-5.13
OH
O
OTBS
4f
200
150
100
50
[ppm]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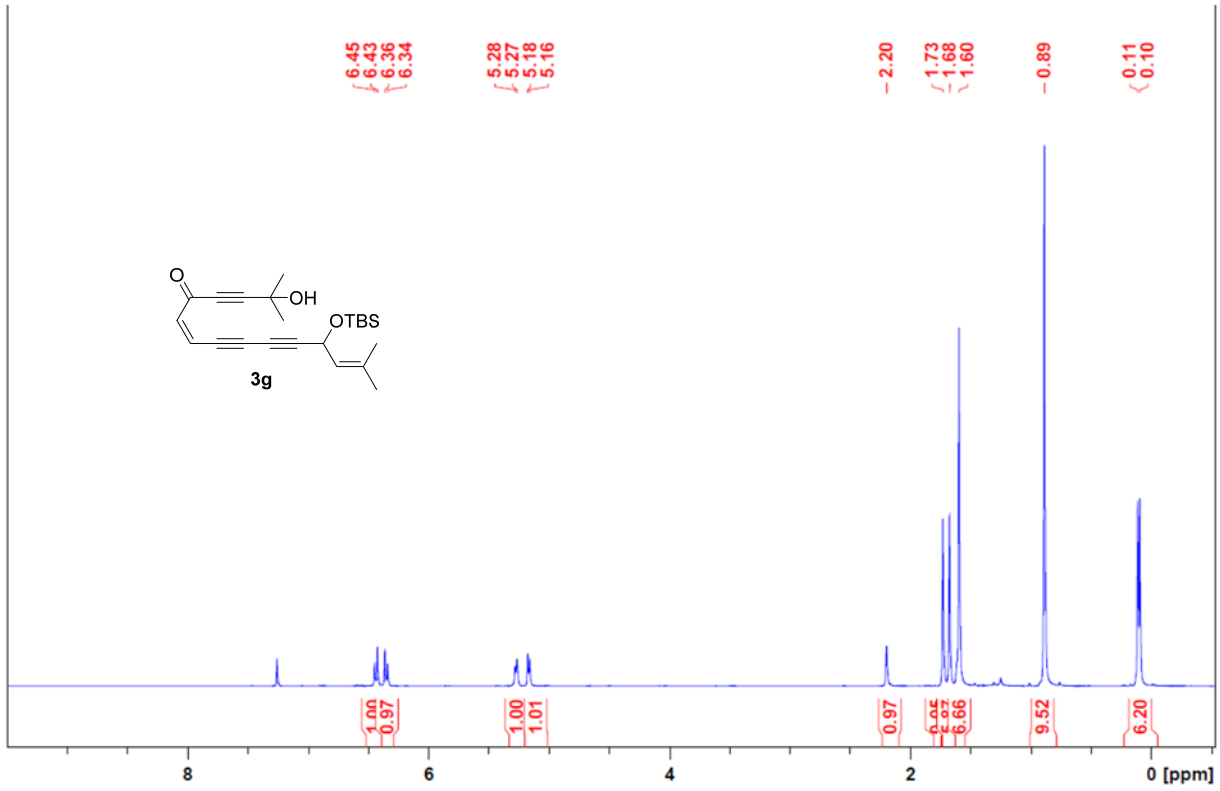
OTBS
Hb
Ha
nOe
Irradiated
Ha
Hb
8
6
4
2
0 [ppm]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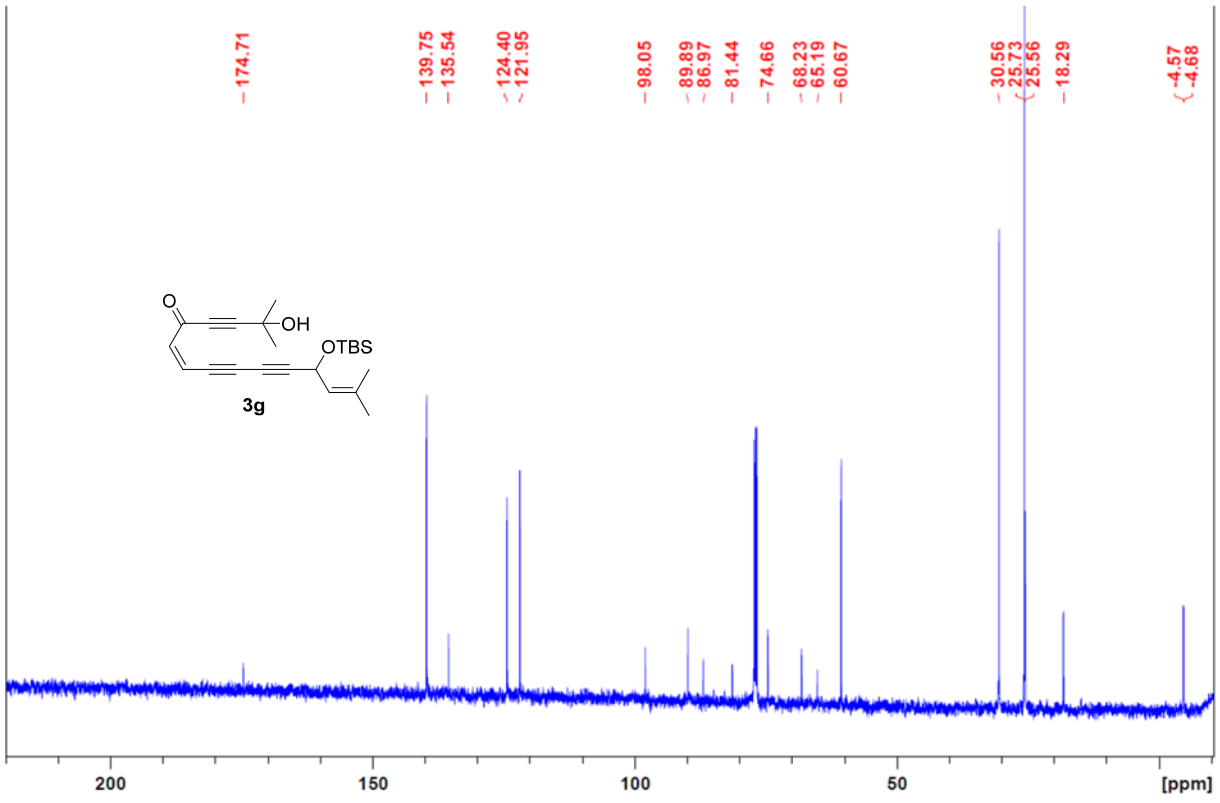
6.43
6.36
6.34
5.28
5.27
5.18
5.16
2.20
1.73
1.68
1.60
0.89
0.11
0.10
O
OH
OTBS
3g
1.00
0.97
1.00
1.01
0.97
6.66
9.52
6.20
8
6
4
2
0 [ppm]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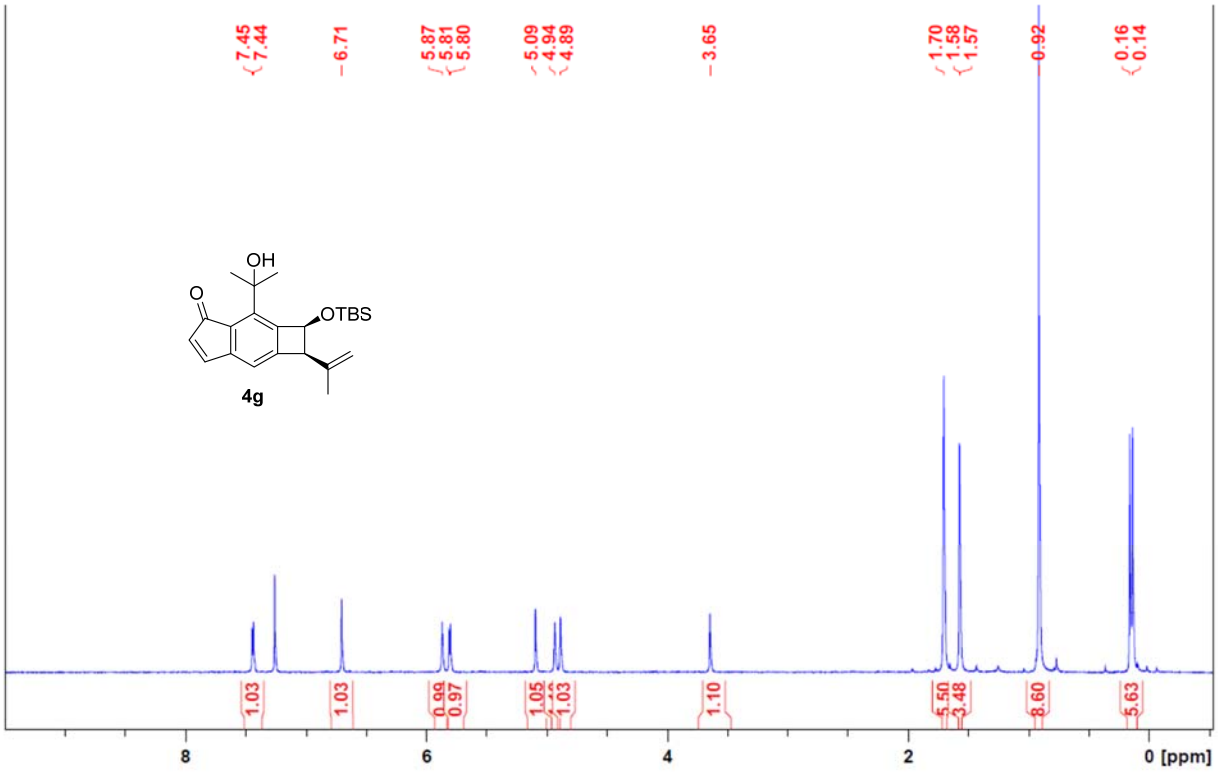
86.97
81.44
74.66
68.23
65.19
60.67
30.56
25.73
25.56
18.29
-4.57
-4.68
O
OH
OTBS
3g
200
150
100
50
[ppm]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7.44
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5.81
5.80
5.09
4.94
4.89
3.65
1.70
1.58
1.57
0.92
0.16
0.14
OH
O
OTBS
4g
1.03
1.03
0.99
0.97
1.05
1.03
1.10
5.50
3.48
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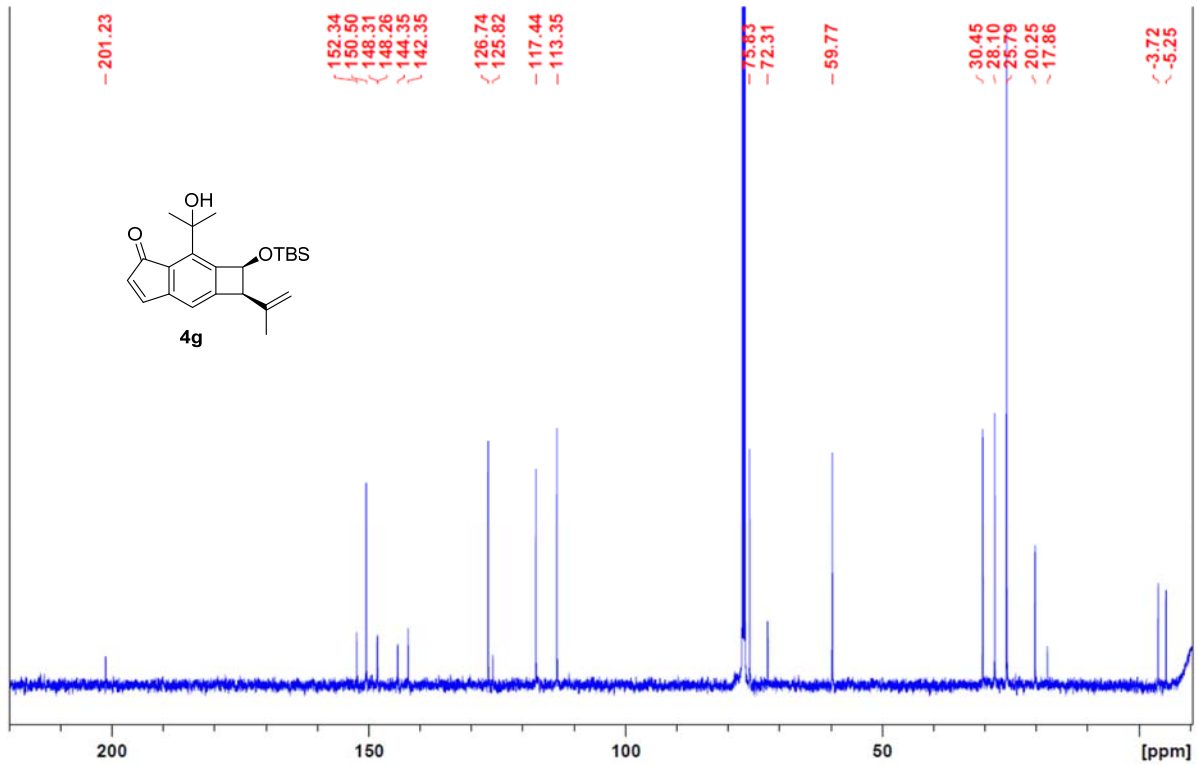
5.63
8
6
4
2
0 [ppm]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142.35
126.74
125.82
117.44
113.35
75.83
72.31
59.77
30.45
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17.86
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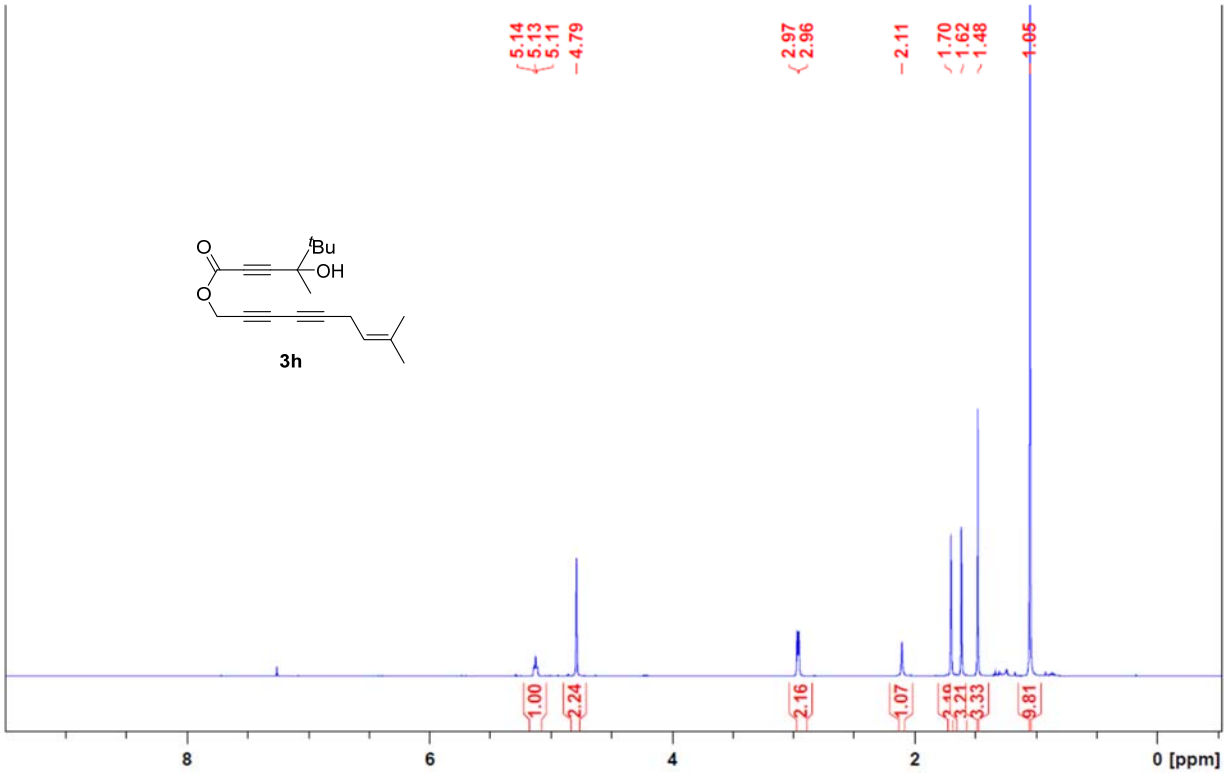
-5.25
OH
O
OTBS
4g
200
150
100
50
[ppm]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5.13
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1.62
1.48
1.00
2.24
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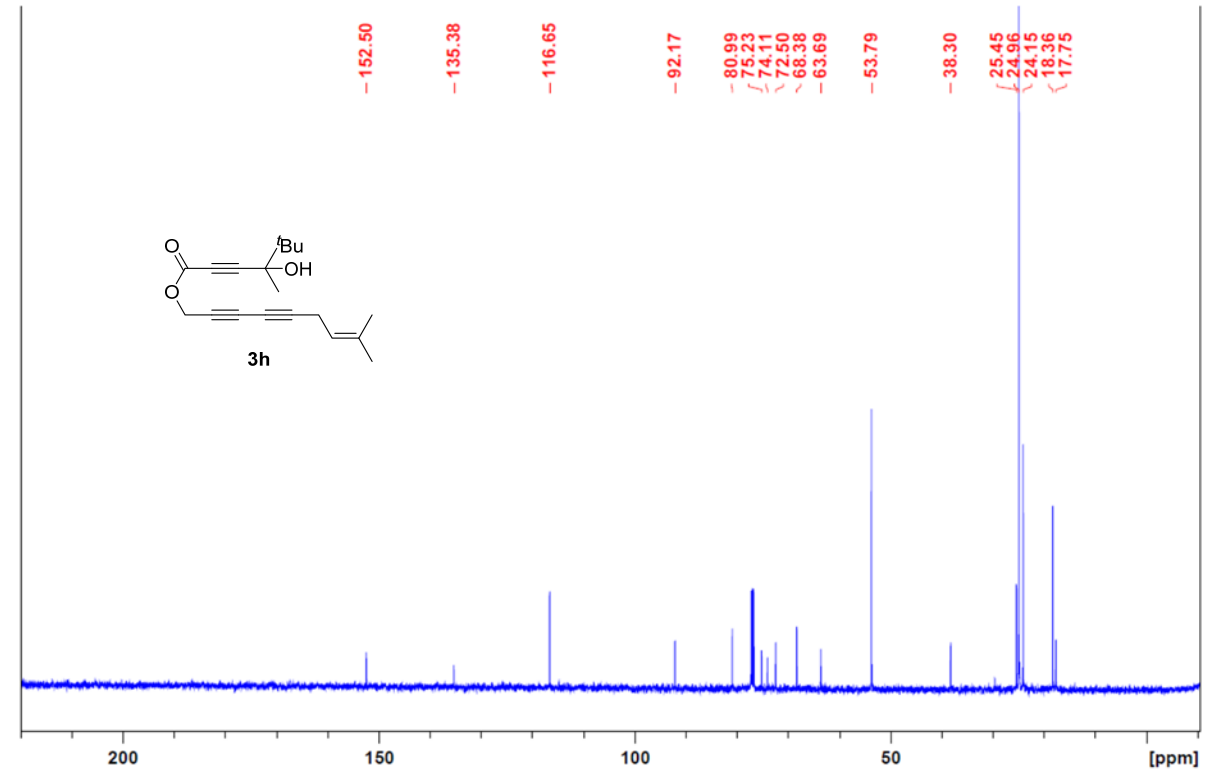
1.07
3.21
3.33
9.81
8
6
4
2
0 [ppm]
tBu
OH
O
O
3h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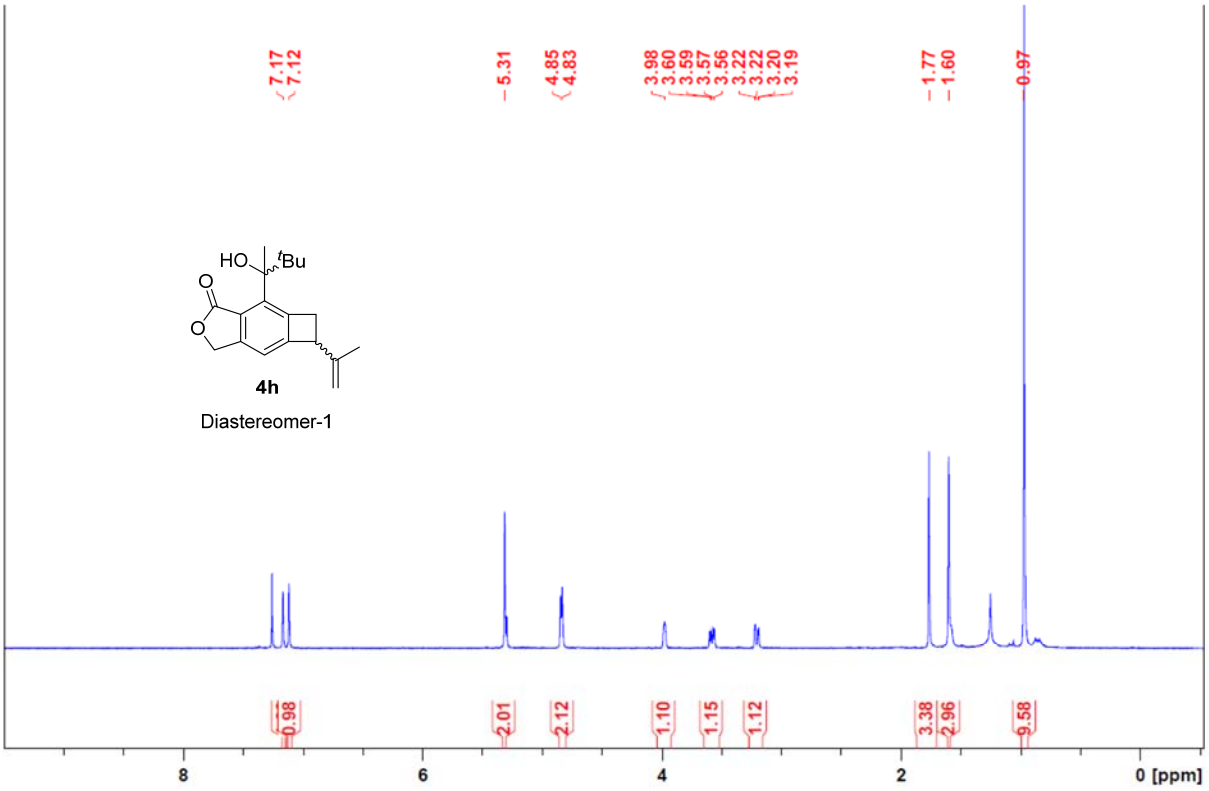
75.23
74.11
72.50
68.38
63.69
53.79
38.30
25.45
24.96
24.15
18.36
17.75
200
150
100
50
[ppm]
tBu
OH
O
O
3h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3.19
1.77
1.60
0.97
HO
tBu
O
O
4h
Diastereomer-1
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1.15
1.12
3.38
2.96
9.58
8
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4
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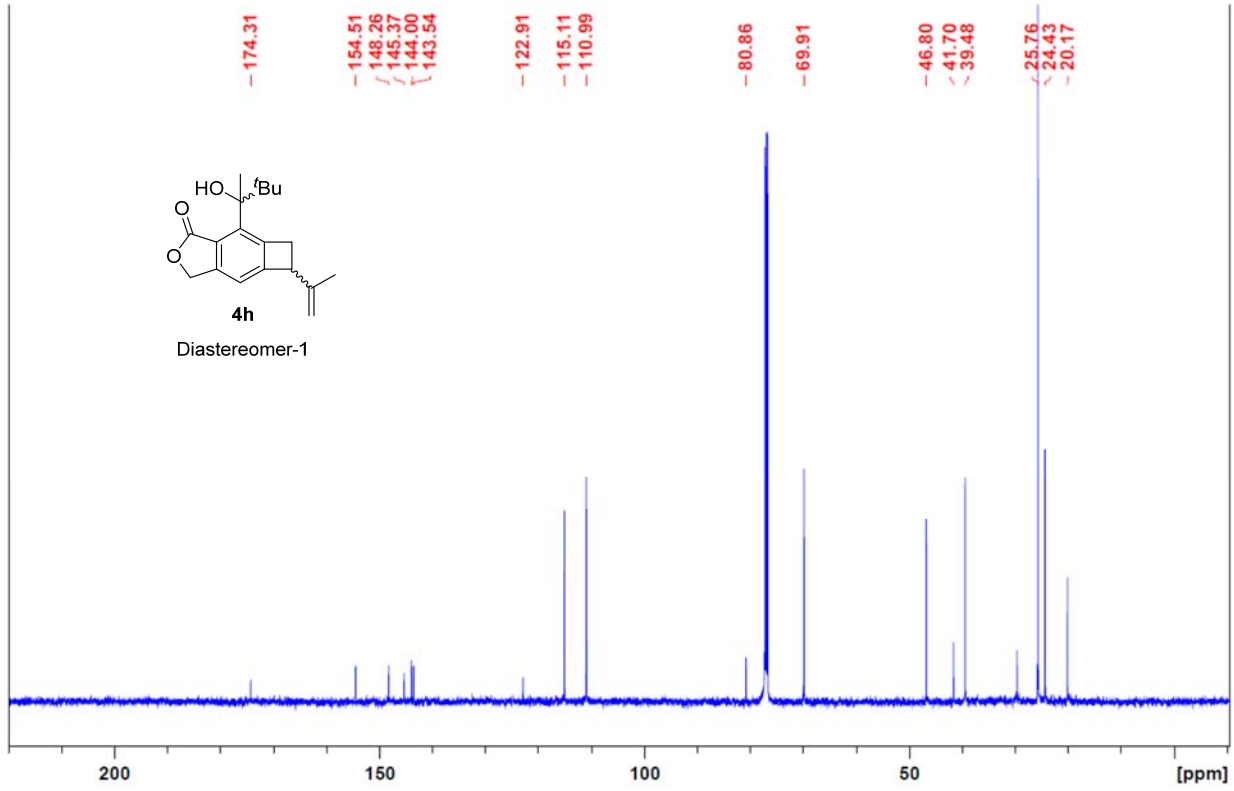
0 [ppm]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46.80
41.70
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20.17
HO
tBu
O
O
4h
Diastereomer-1
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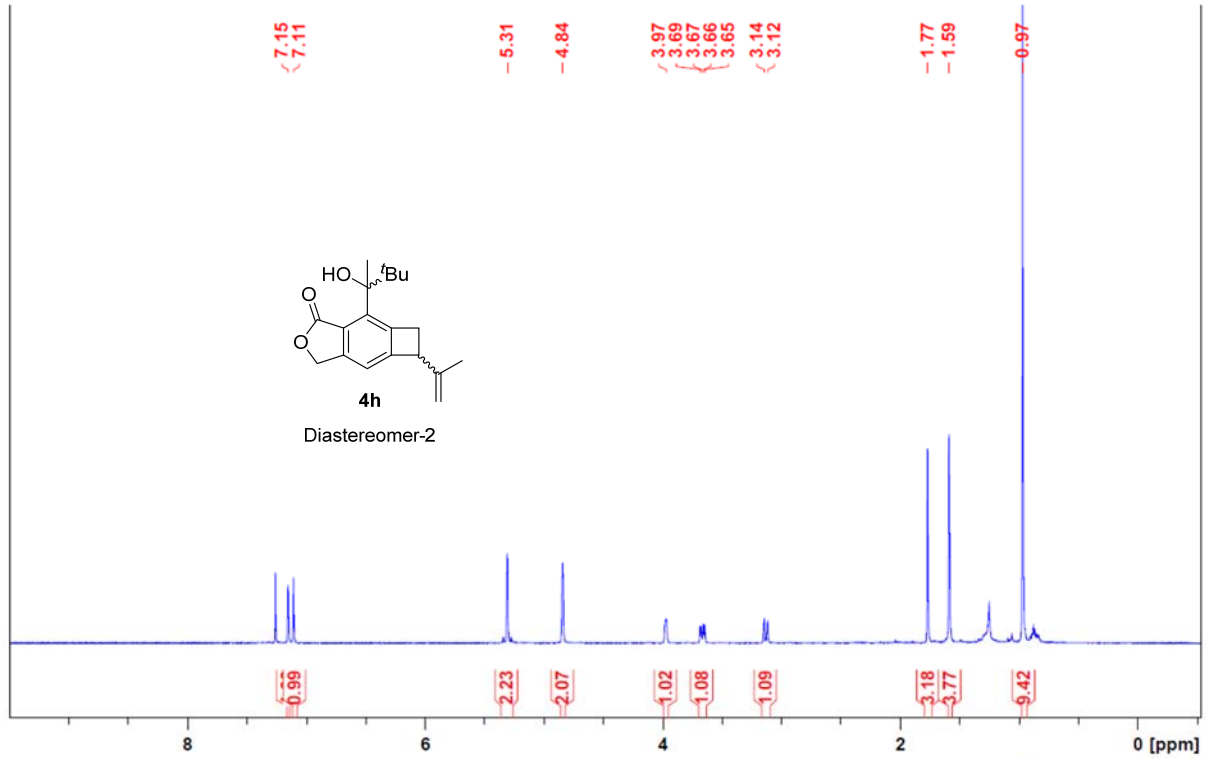
150
100
50
[ppm]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3.69
3.67
3.66
3.65
3.14
3.12
1.77
1.59
0.97
HO
tBu
O
O
4h
Diastereomer-2
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1.02
1.08
1.09
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9.42
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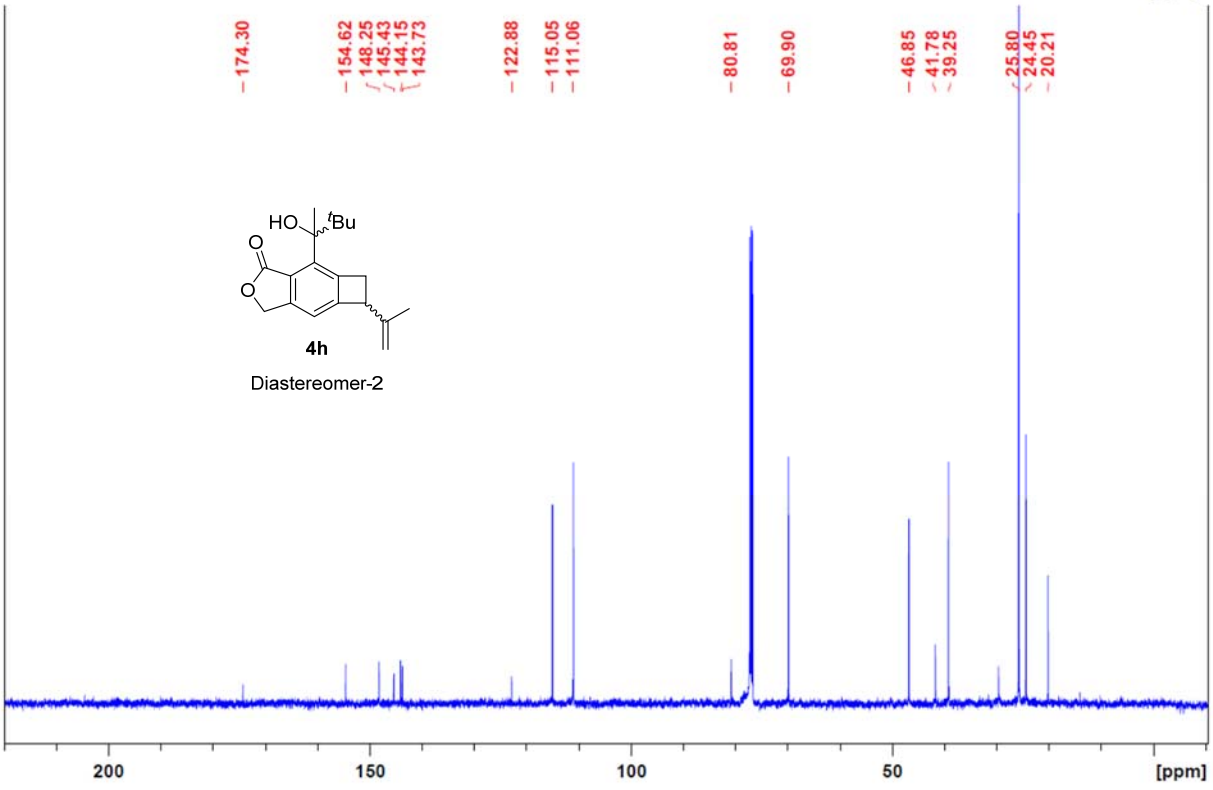
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111.06
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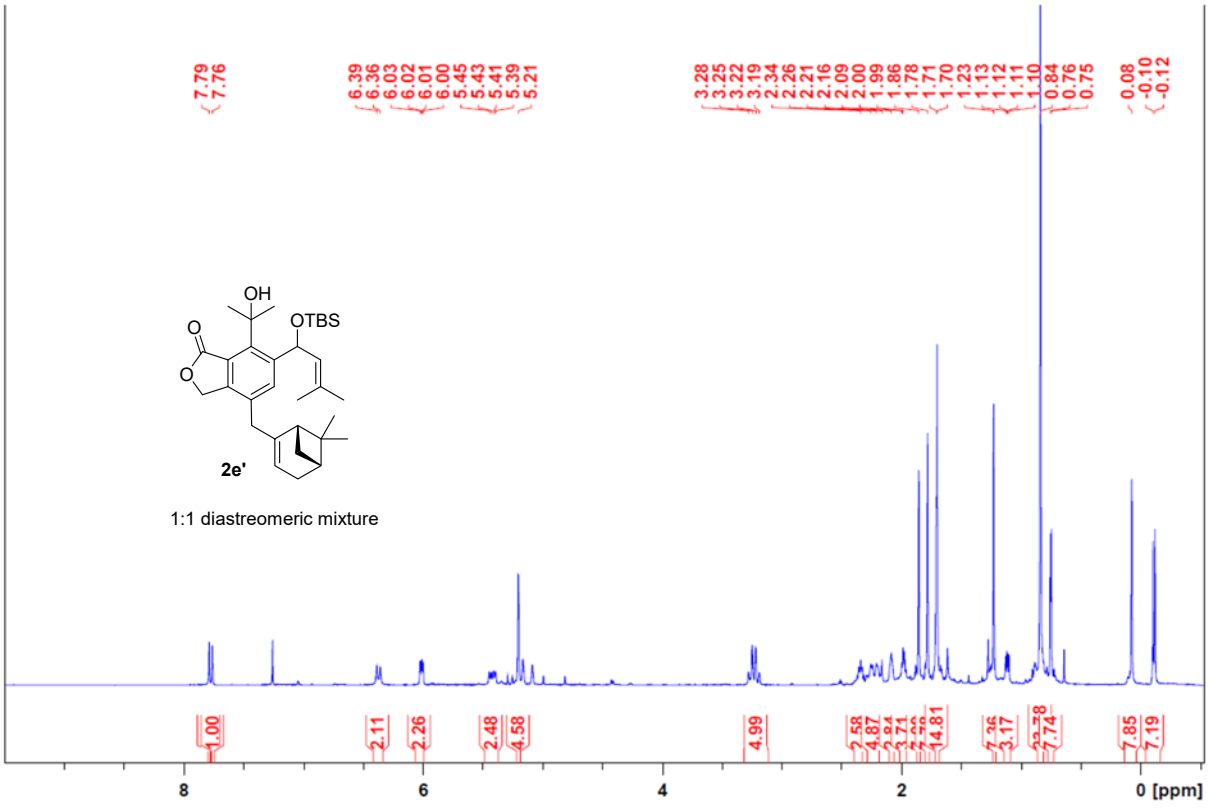
69.90
46.85
41.78
39.25
25.80
24.45
20.21
HO
tBu
O
O
4h
Diastereomer-2
200
150
100
50
[ppm]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OTBS
O
O
2e'
1:1 diastreomeric mixture
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6
4
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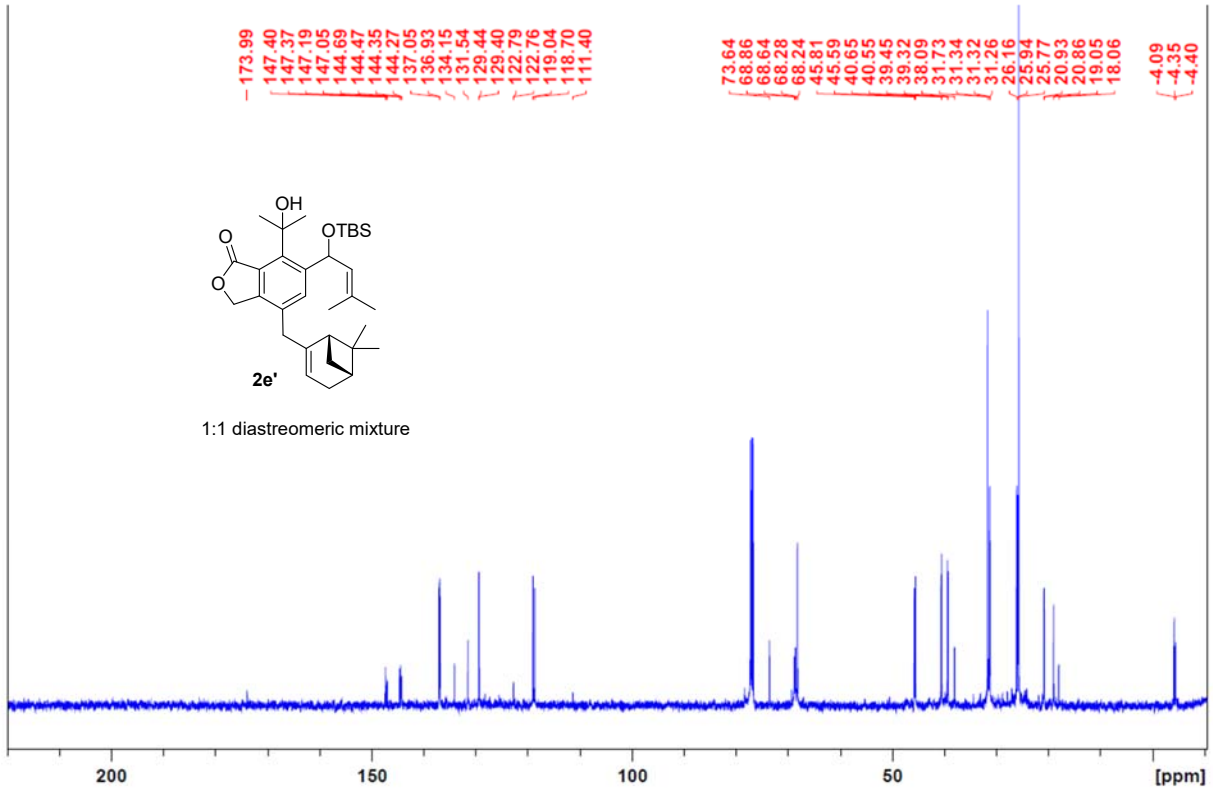
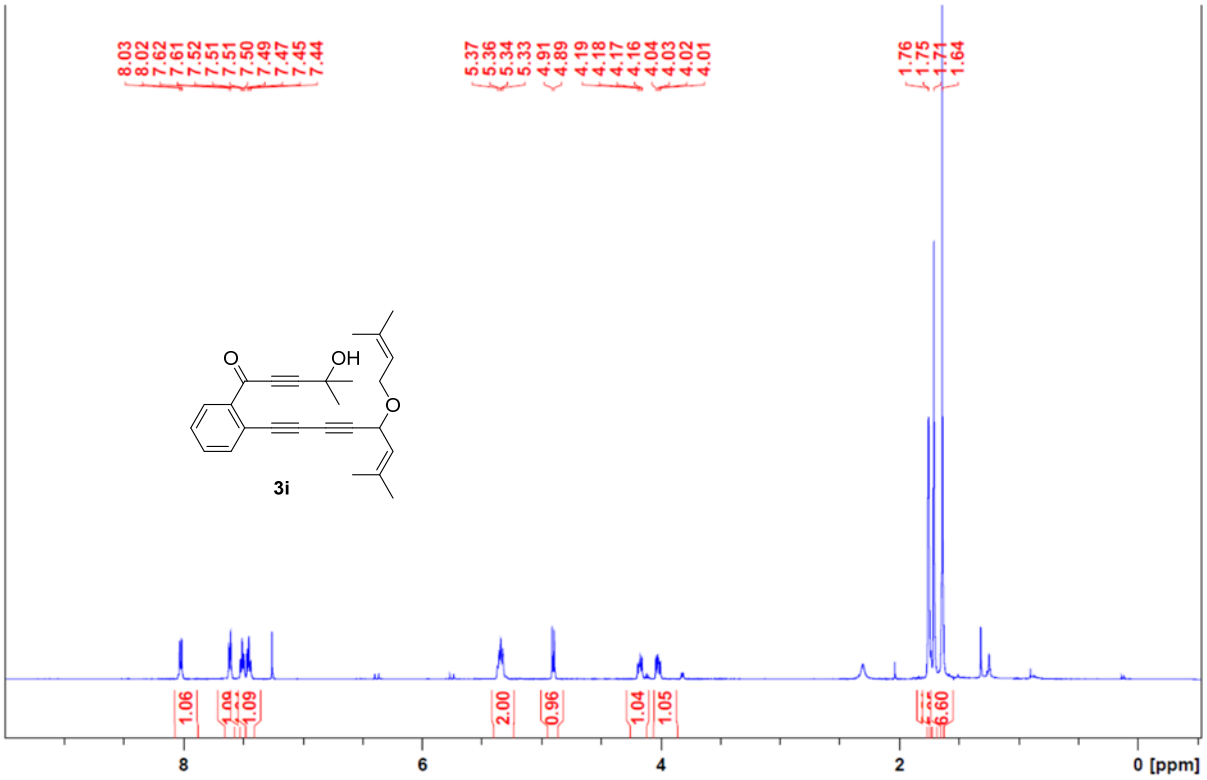

OH
OTBS
O
O
2e'
1:1 diastreomeric mixture
200
150
100
50
[ppm]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5.36
5.34
5.33
4.91
4.89
4.19
4.18
4.17
4.16
4.04
4.03
4.02
4.01
1.76
1.75
1.71
1.64
O
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O
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1.09
2.00
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1.05
6.60
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4
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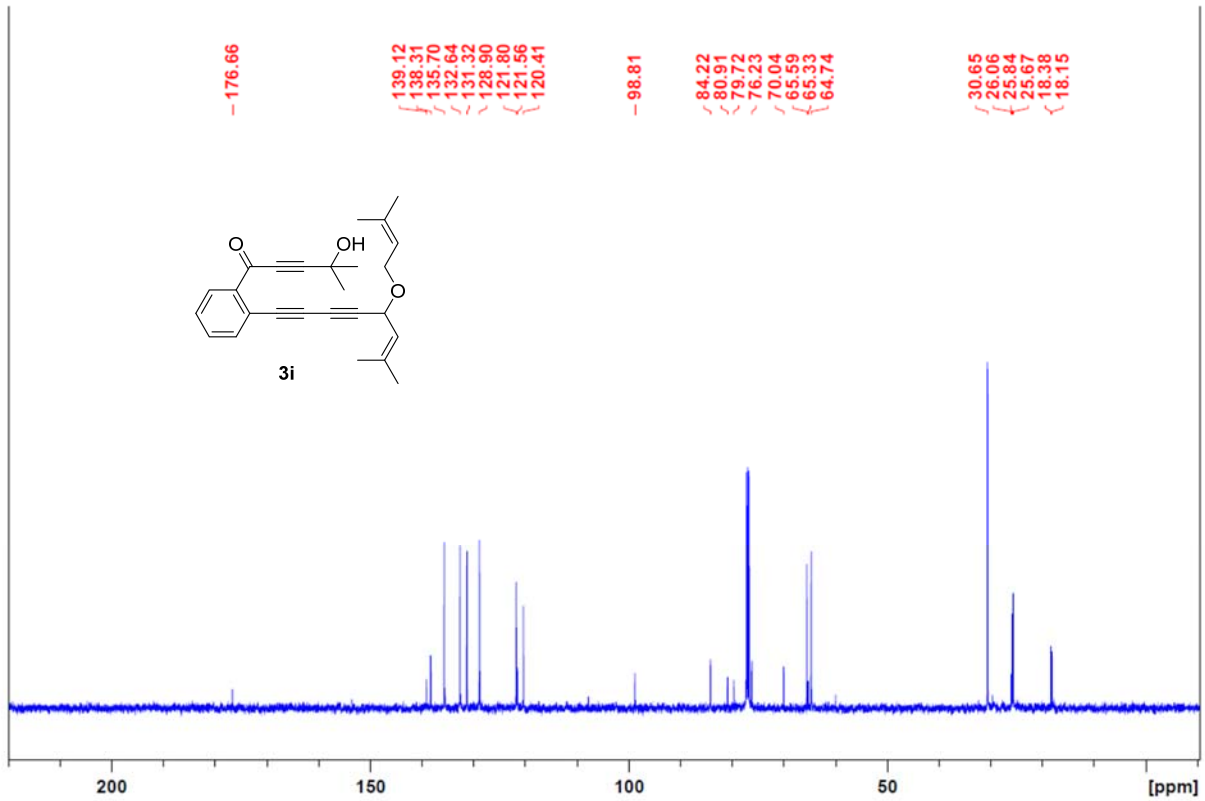
0 [ppm]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120.41
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80.91
79.72
76.23
70.04
65.59
65.33
64.74
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25.67
18.38
18.15
O
OH
O
3i
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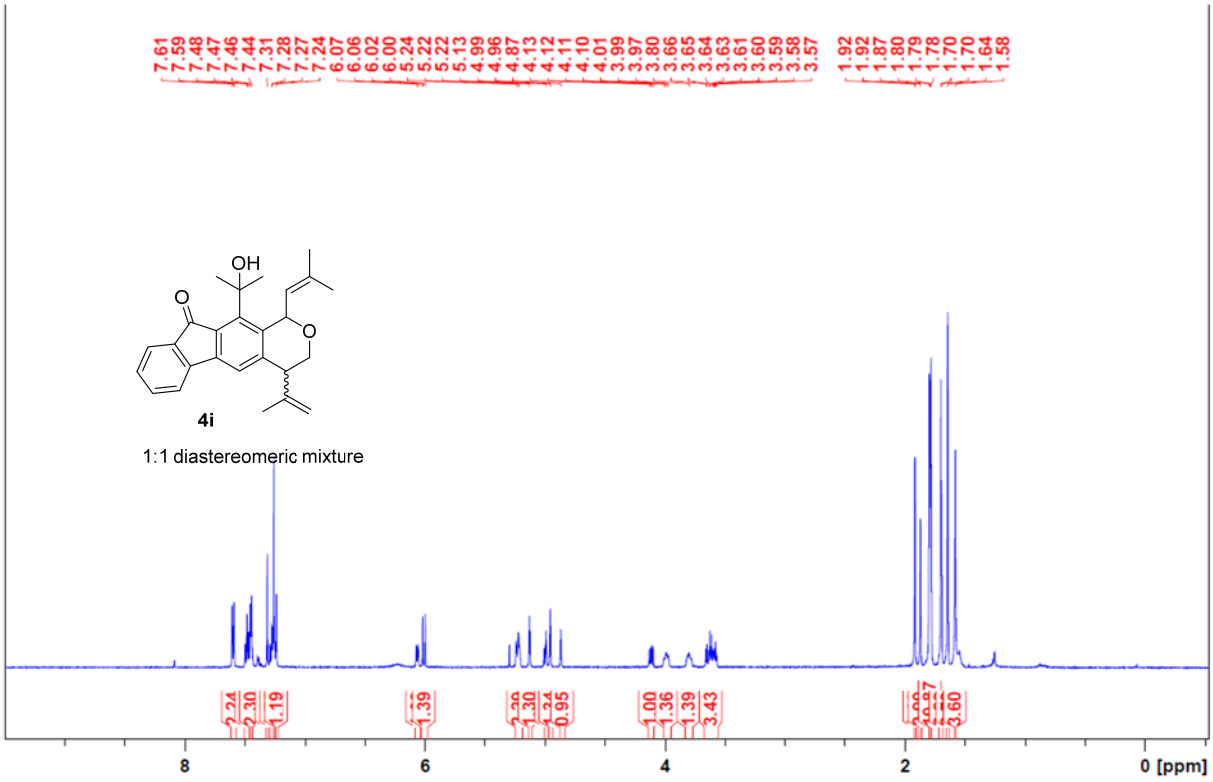
150
100
50
[ppm]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7.47
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7.44
7.31
7.28
7.27
7.24
6.07
6.06
6.02
6.00
5.24
5.22
5.22
5.13
4.99
4.96
4.87
4.13
4.12
4.11
4.10
4.01
3.99
3.97
3.80
3.66
3.65
3.64
3.63
3.61
3.60
3.59
3.58
3.57
1.92
1.92
1.87
1.80
1.79
1.78
1.70
1.70
1.64
1.58
OH
O
O
4i
1:1 diastereomeric mixture
2.24
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1.00
1.36
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3.60
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4
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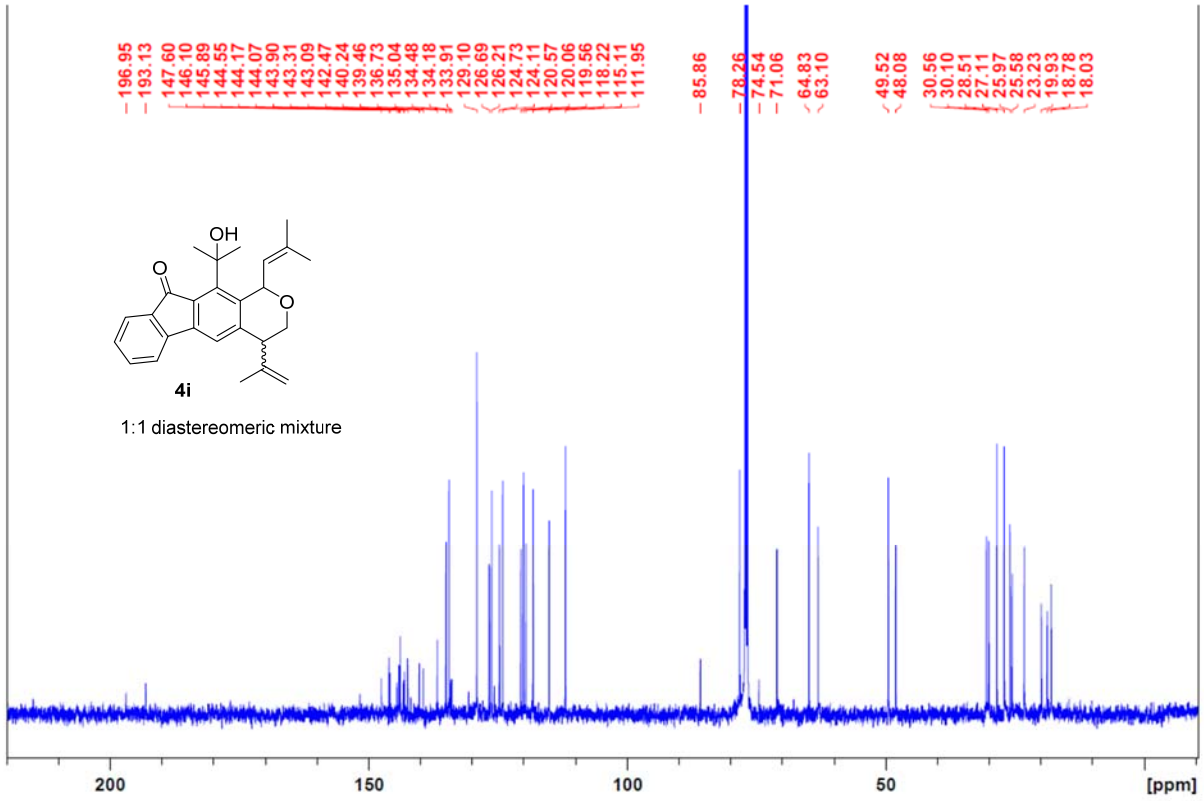
0 [ppm]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143.31
143.09
142.47
140.24
139.46
136.73
135.04
134.48
134.18
133.91
129.10
126.69
126.21
124.73
124.11
120.57
120.06
119.56
118.22
115.11
111.95
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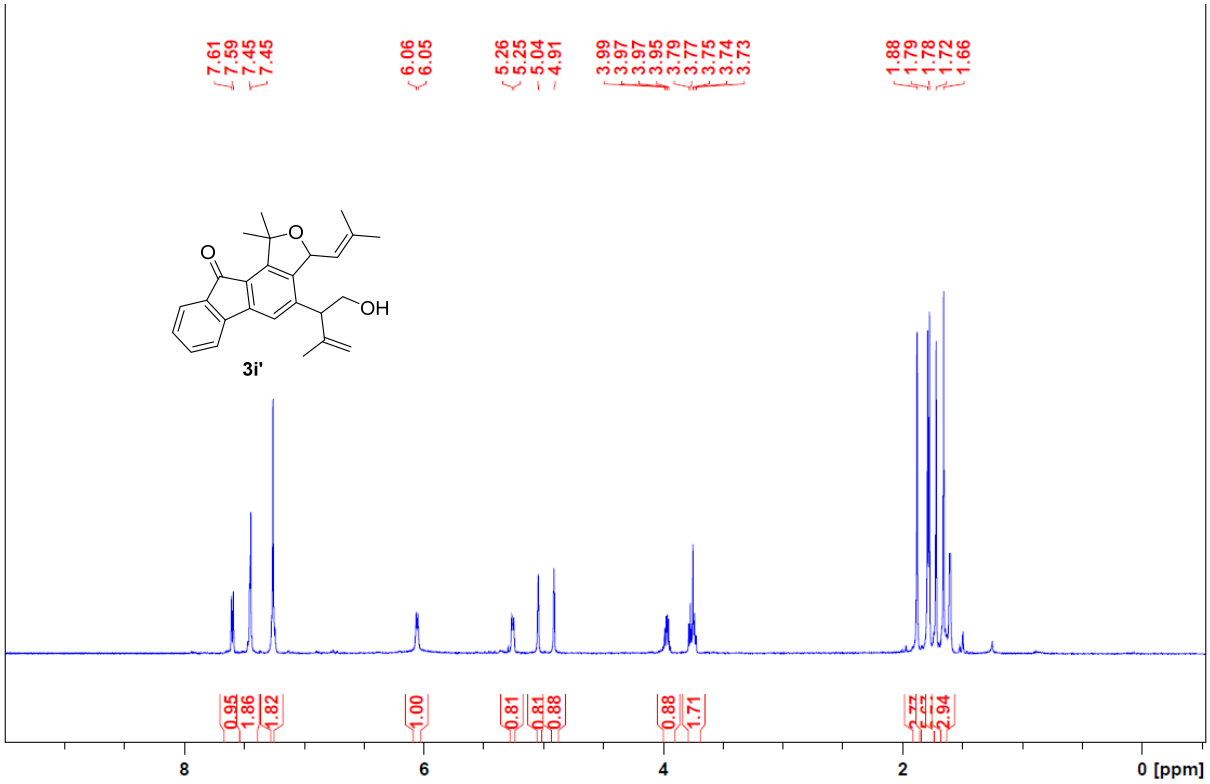
30.10
28.51
27.11
25.97
25.58
23.23
19.93
18.78
18.03
OH
O
O
4i
1:1 diastereomeric mixture
200
150
100
50
[ppm]


7.61
7.59
7.45
7.45
6.06
6.05
5.26
5.25
5.04
4.91
3.99
3.97
3.97
3.95
3.79
3.77
3.75
3.74
3.73
1.88
1.79
1.78
1.72
1.66
O
OH
3i'
0.95
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0.81
0.81
0.88
0.88
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2.94
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4
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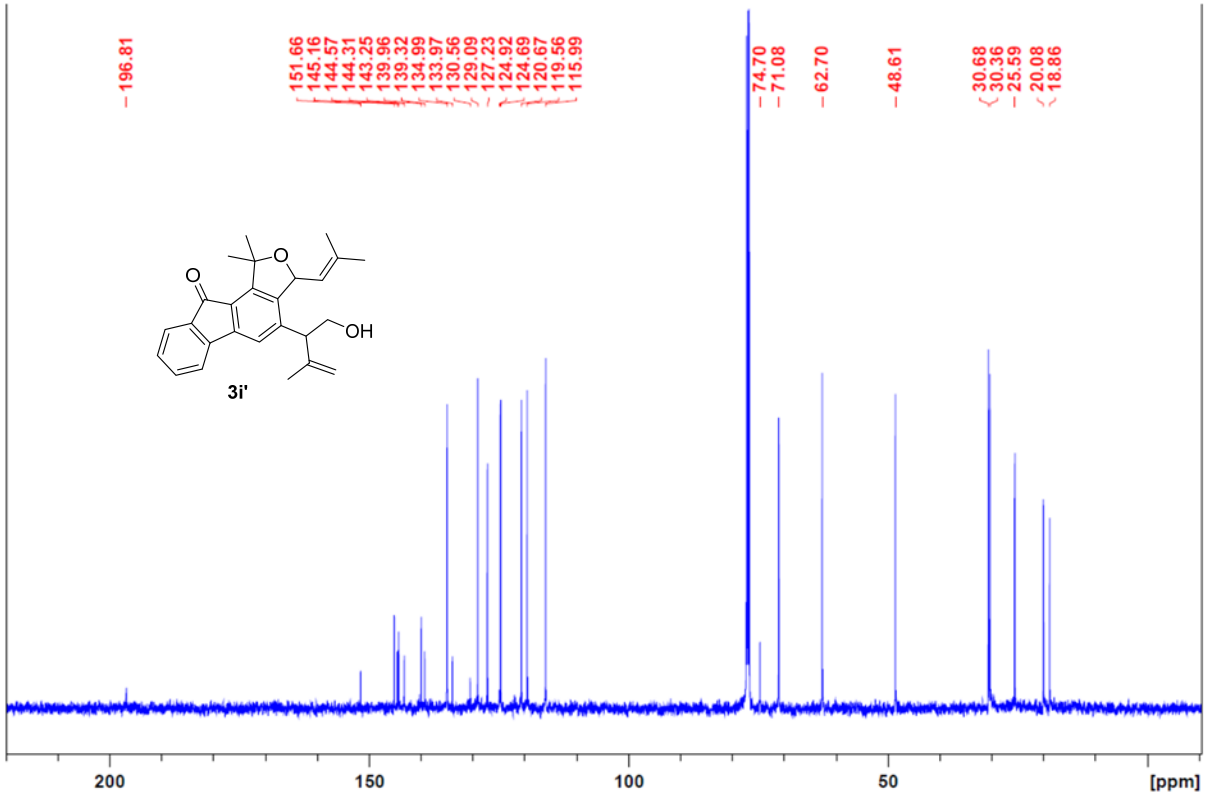
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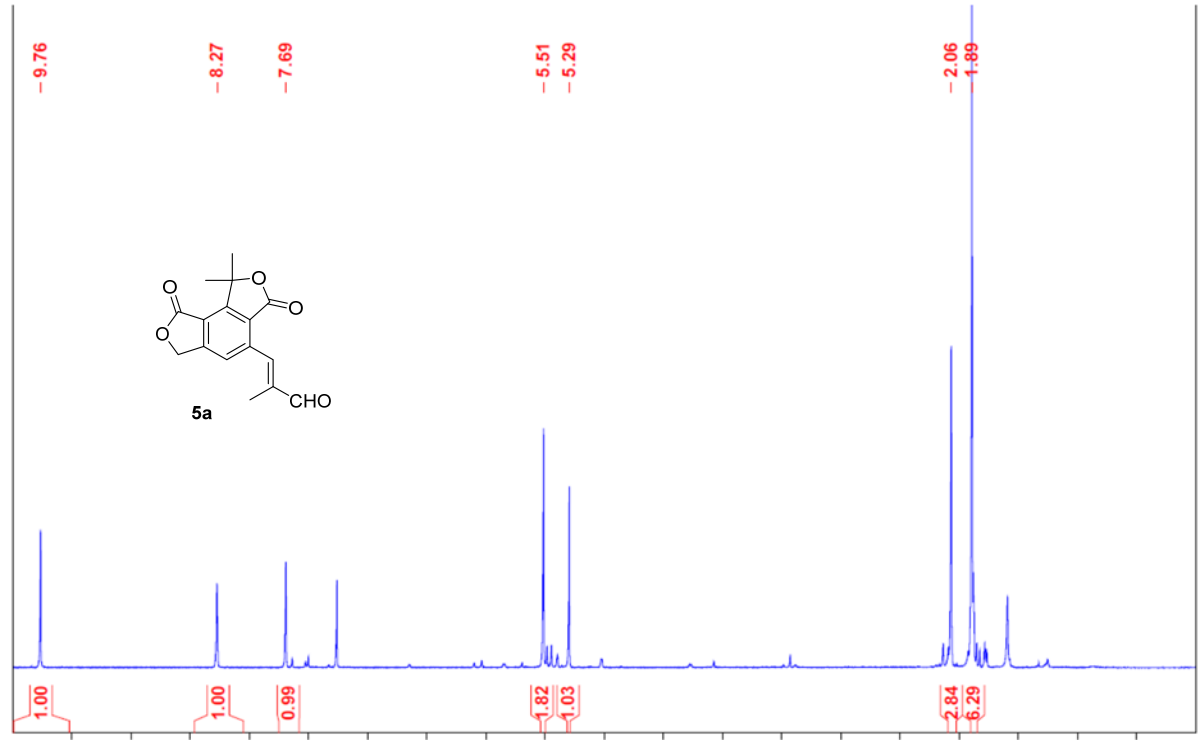
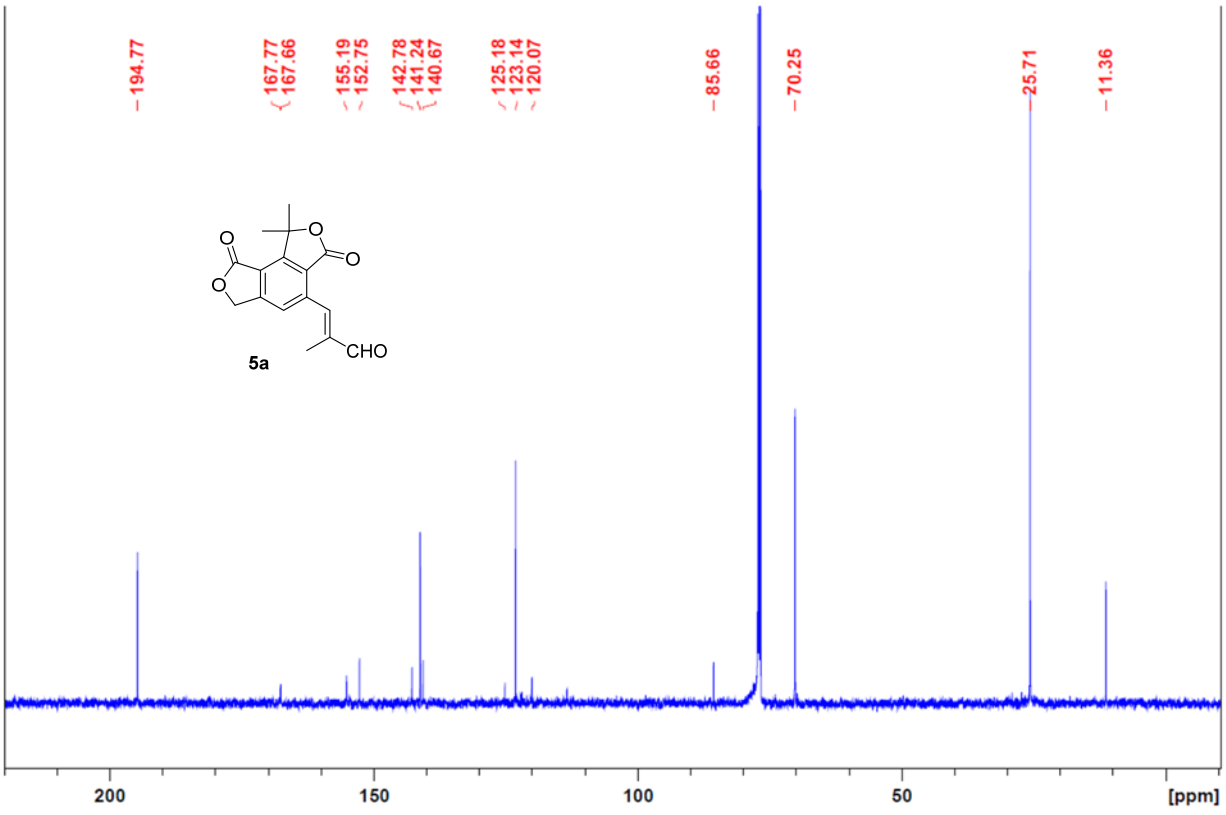
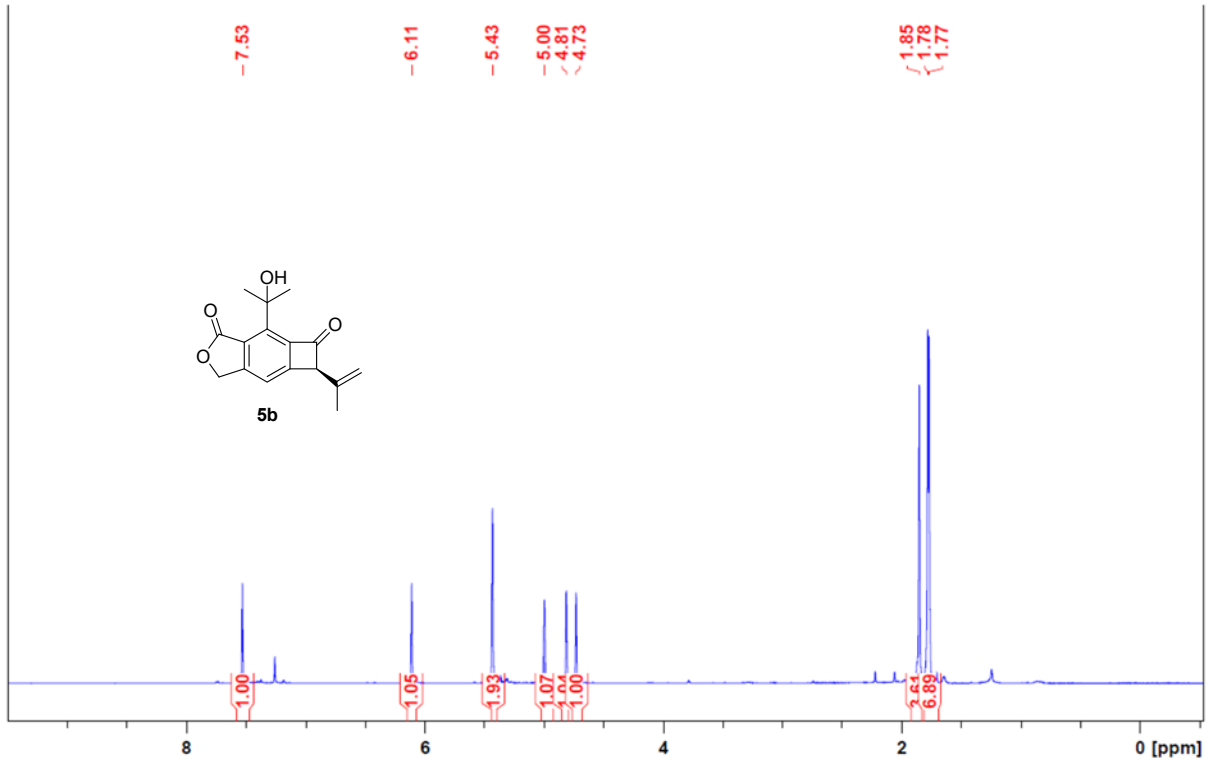
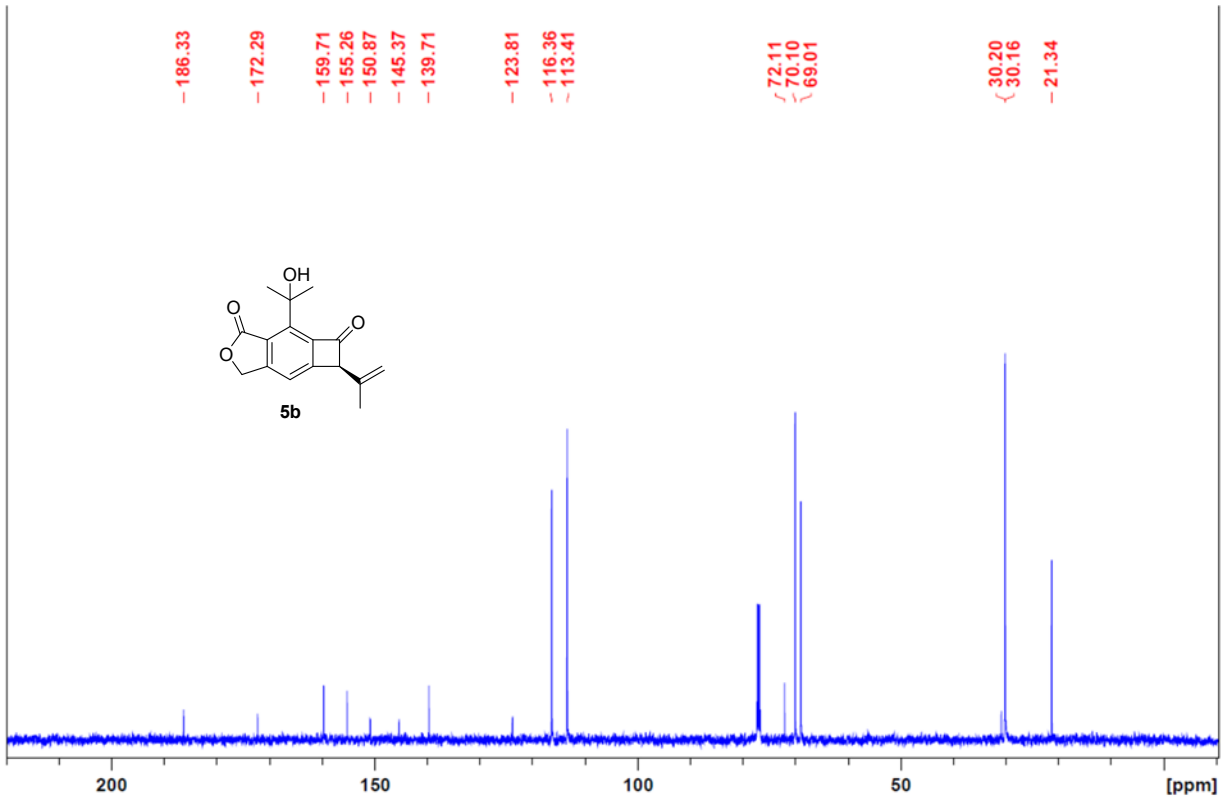
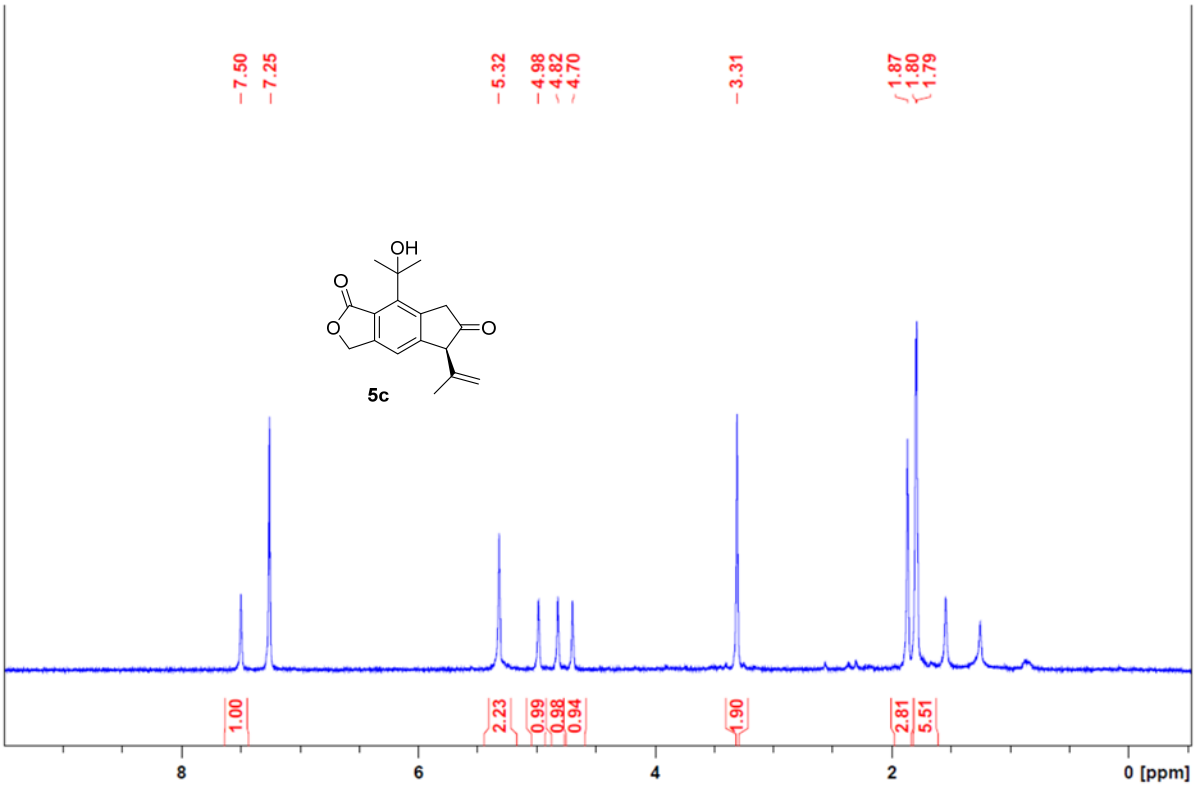
130.56
129.09
127.23
124.92
124.69
120.67
119.56
115.99
74.70
71.08
62.70
48.61
30.68
30.36
25.59
20.08
18.86
O
OH
3i'
200
150
100
50
[ppm]

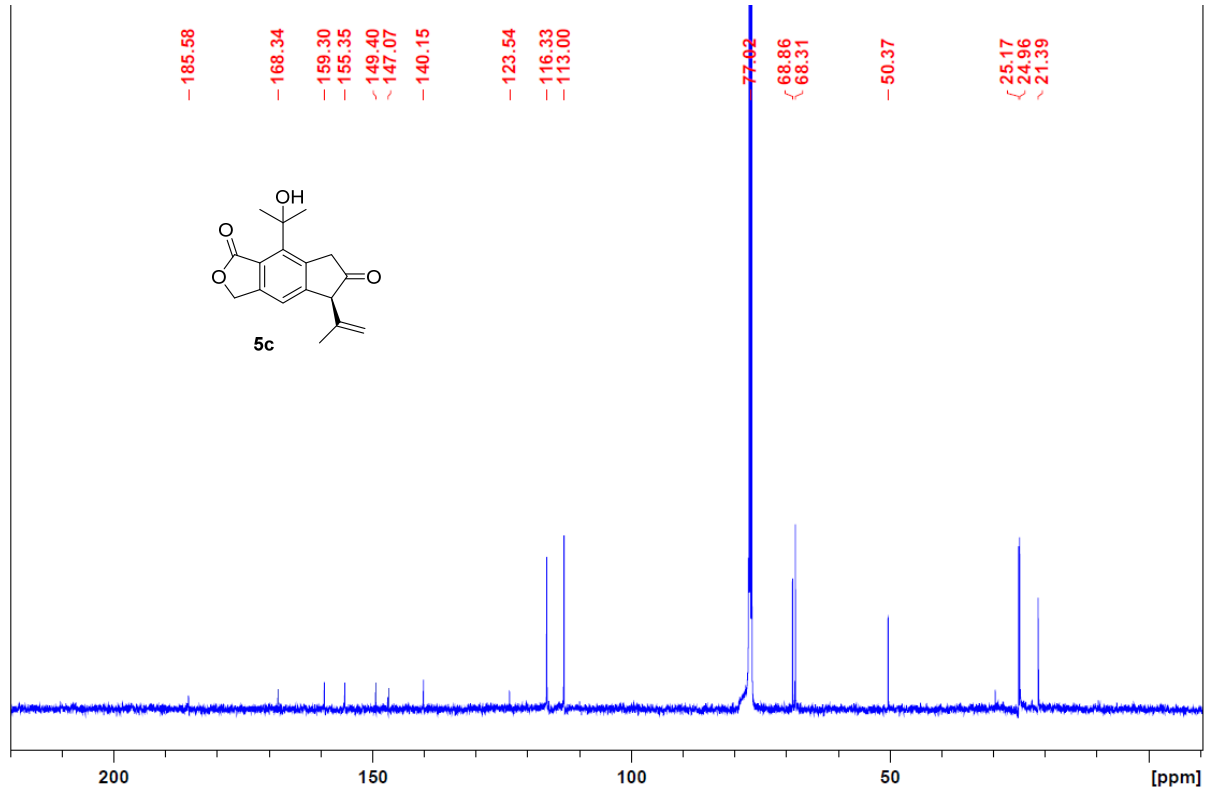

9.76
8.27
7.69
5.51
5.29
2.06
1.89
1.00
1.00
0.99
1.82
1.03
2.84
6.29
5a

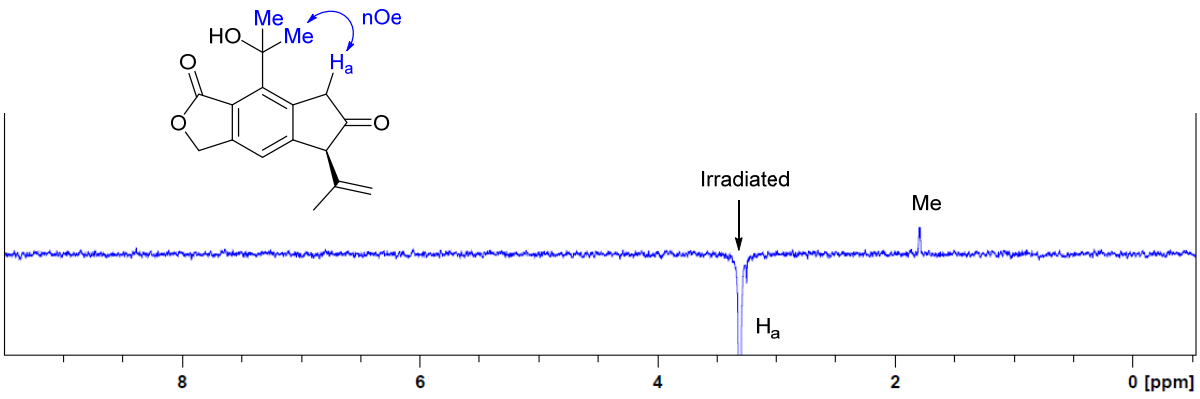

194.77
167.77
167.66
155.19
152.75
142.78
141.24
140.67
125.18
123.14
120.07
85.66
70.25
25.71
11.36
5a
200
150
100
50
[ppm]

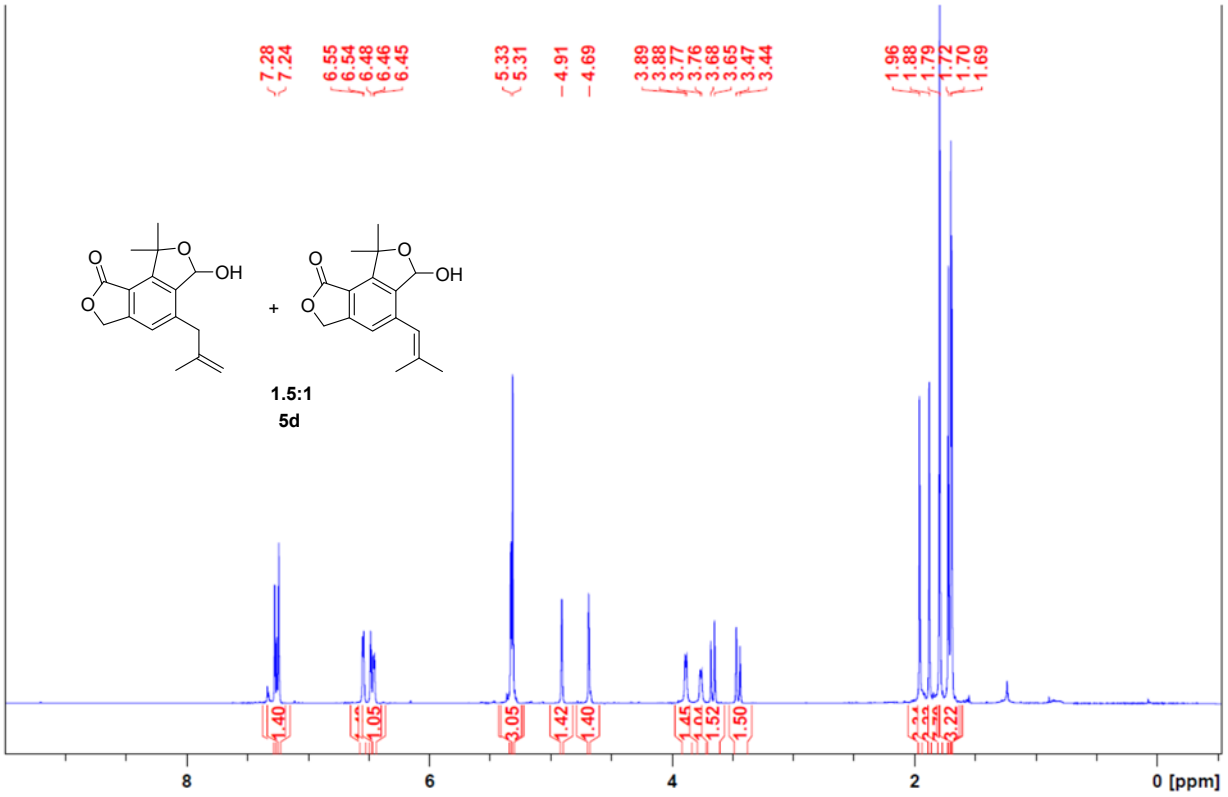

7.53
6.11
5.43
5.00
4.81
4.73
1.85
1.78
1.77
OH
O
O
O
5b
1.00
1.05
1.93
1.07
1.04
1.00
2.64
6.89
8
6
4
2
0 [ppm]

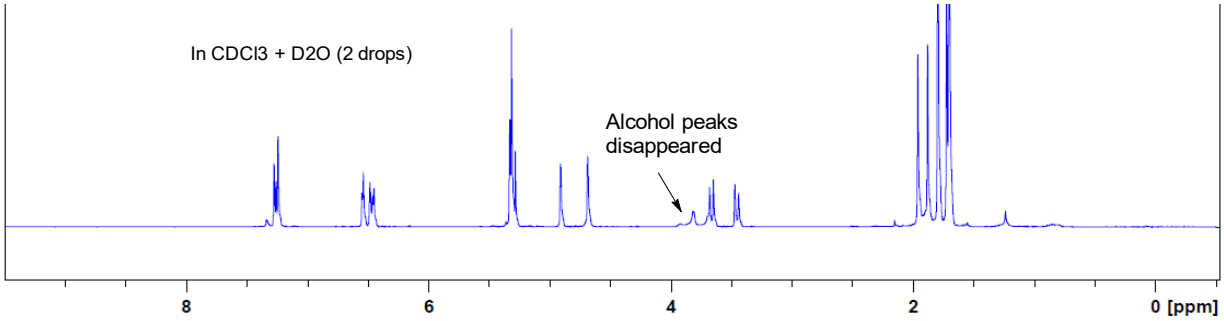

186.33
172.29
159.71
155.26
150.87
145.37
139.71
123.81
116.36
113.41
72.11
70.10
69.01
30.20
30.16
21.34
OH
O
O
O
5b
200
150
100
50
[ppm]

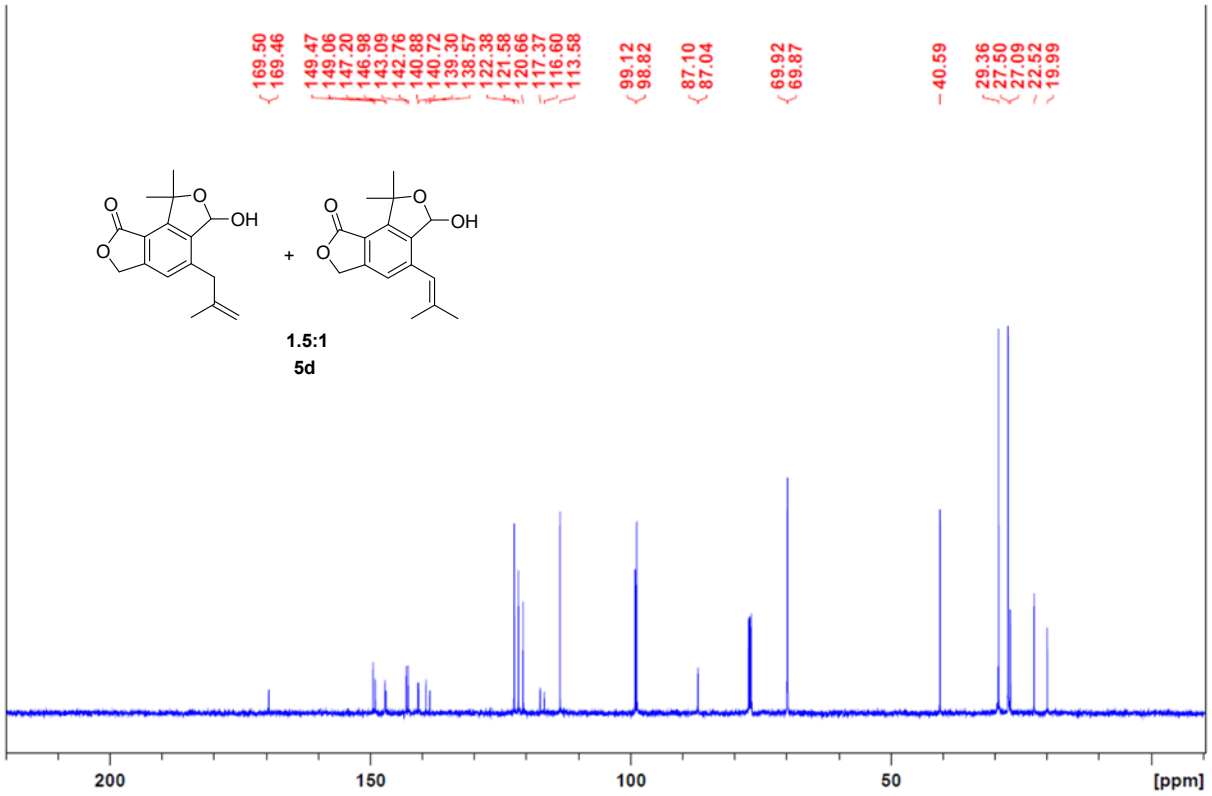

7.50
7.25
5.32
4.98
4.82
4.70
3.31
1.87
1.80
1.79
OH
O
O
O
5c
1.00
2.23
0.99
0.98
0.94
1.90
2.81
5.51
8
6
4
2
0 [ppm]

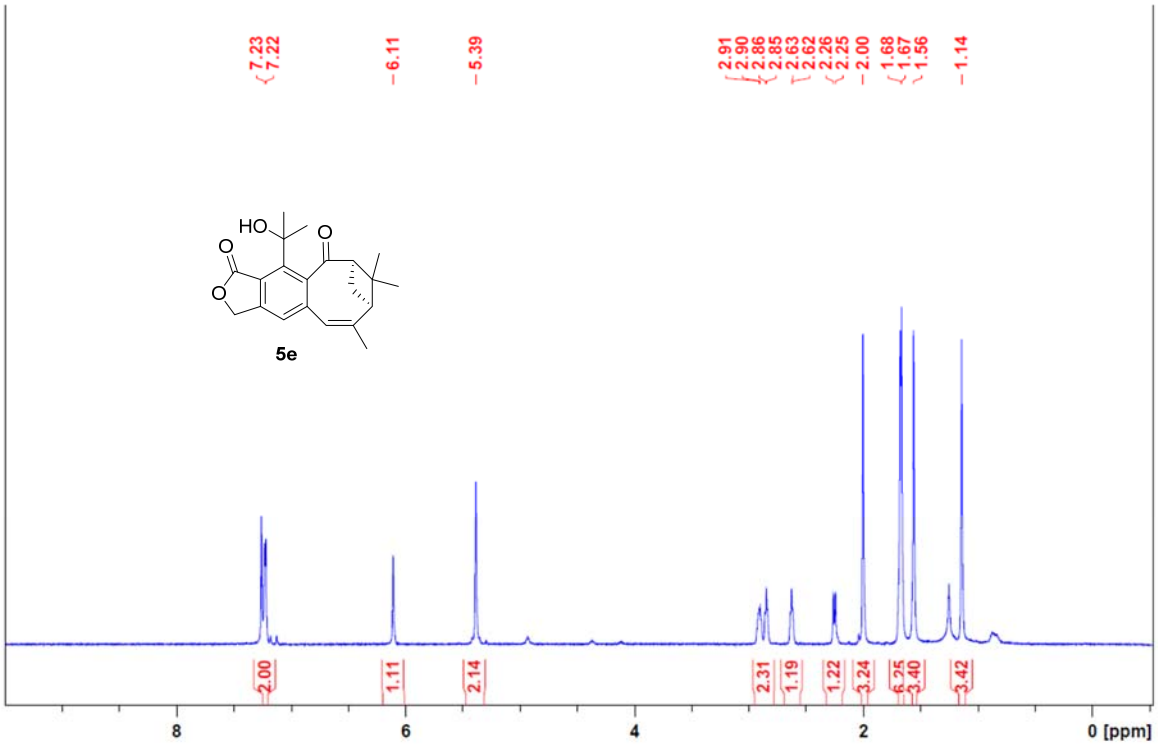

185.58
168.34
159.30
155.35
149.40
147.07
140.15
123.54
116.33
113.00
77.02
68.86
68.31
50.37
25.17
24.96
21.39
OH
O
O
O
5c
200
150
100
50
[ppm]

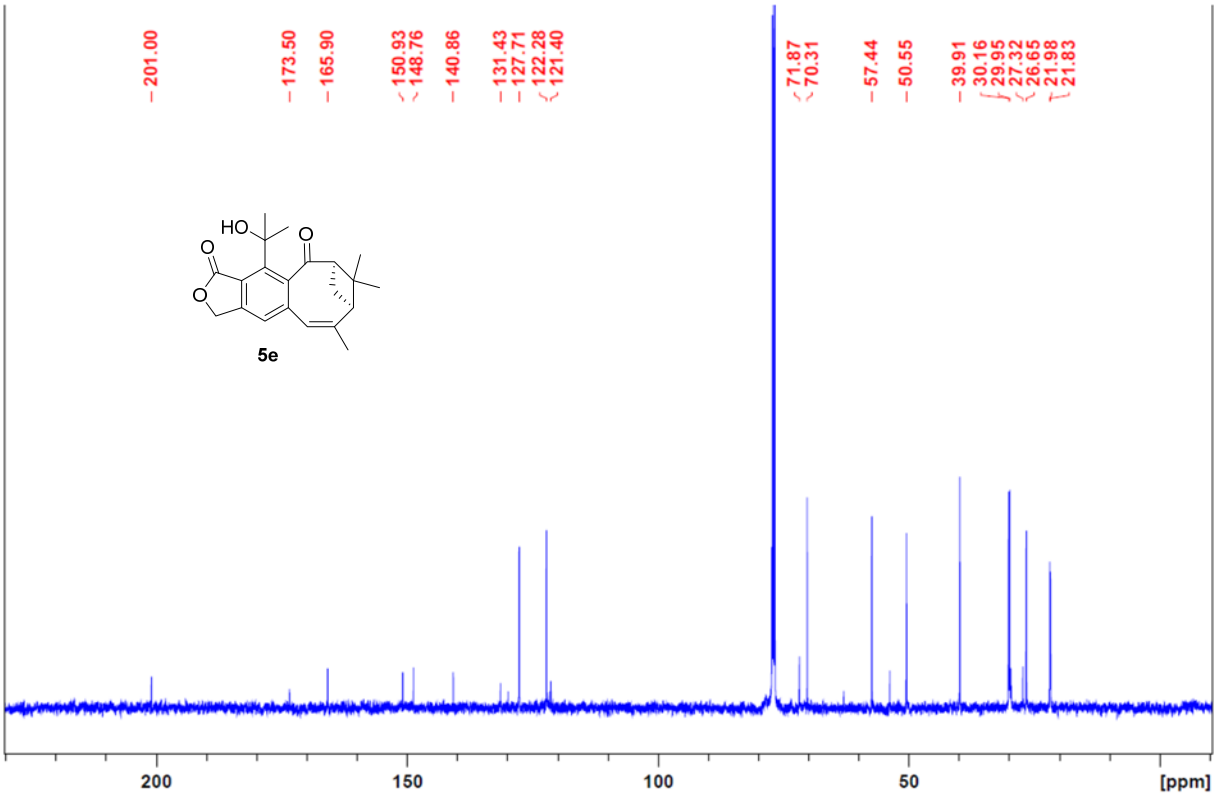

Me
nOe
HO
Me
Ha
O
O
O
Irradiated
Me
Ha
8
6
4
2
0 [ppm]


7.28
7.24
6.55
6.54
6.48
6.46
6.45
5.33
5.31
4.91
4.69
3.89
3.88
3.77
3.76
3.68
3.65
3.47
3.44
1.96
1.88
1.79
1.72
1.70
1.69
OH
OH
1.5:1
5d
1.40
1.05
3.05
1.42
1.40
1.45
1.04
1.52
1.50
3.22
8
6
4
2
0 [ppm]


In CDCl3 + D2O (2 drops)
Alcohol peaks
disappeared
8
6
4
2
0 [ppm]

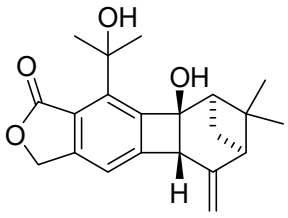

169.50
169.46
149.47
149.06
147.20
146.98
143.09
142.76
140.88
140.72
139.30
138.57
122.38
121.58
120.66
117.37
116.60
113.58
99.12
98.82
87.10
87.04
69.92
69.87
40.59
29.36
27.50
27.09
22.52
19.99
OH
OH
1.5:1
5d
200
150
100
50
[ppm]


7.23
7.22
6.11
5.39
2.91
2.90
2.86
2.85
2.63
2.62
2.26
2.25
2.00
1.68
1.67
1.56
1.14
HO
O
O
O
5e
2.00
1.11
2.14
2.31
1.19
1.22
3.24
6.25
3.40
3.42
8
6
4
2
0 [ppm]

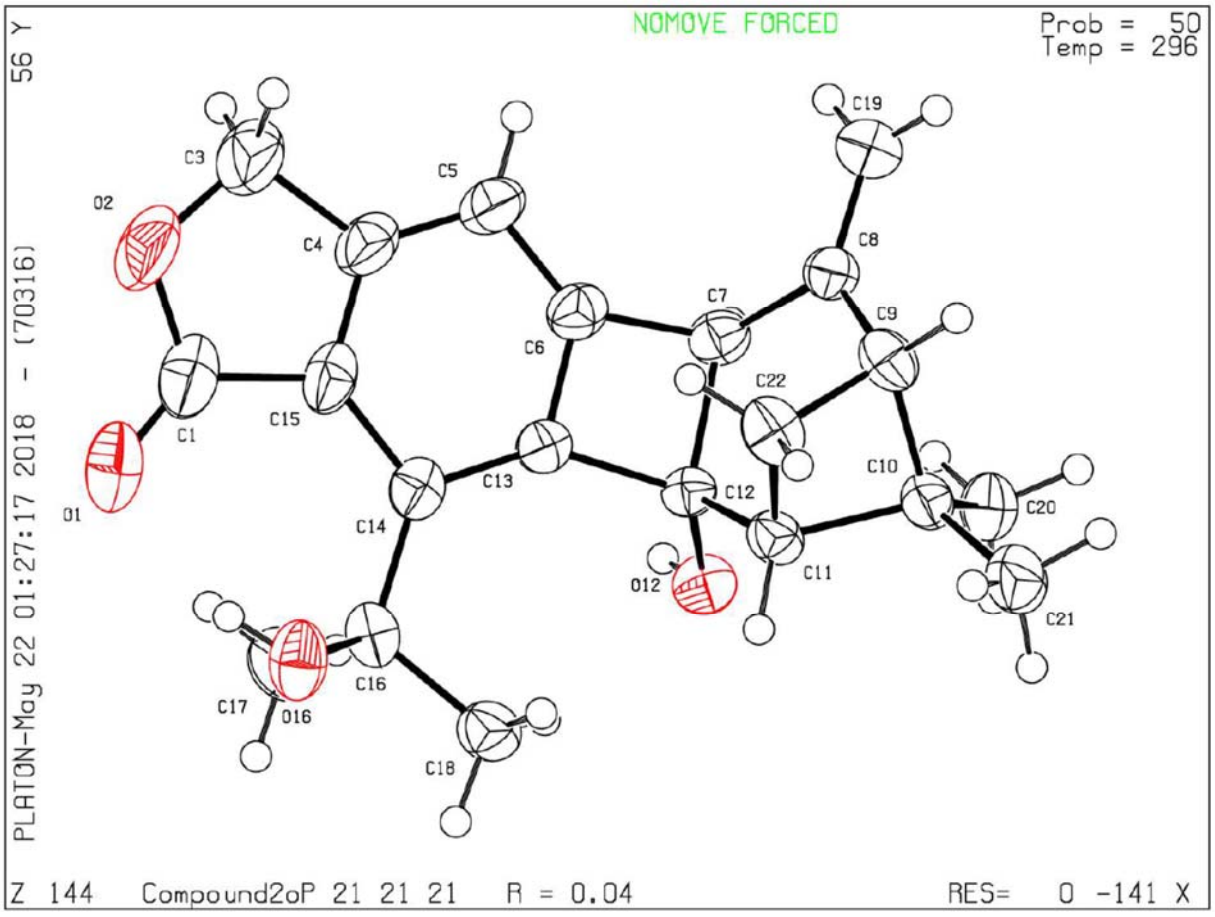

201.00
173.50
165.90
150.93
148.76
140.86
131.43
127.71
122.28
121.40
71.87
70.31
57.44
50.55
39.91
30.16
29.95
27.32
26.65
21.98
21.83
HO
O
O
O
5e
200
150
100
50
[ppm]

X–ray Crystallographic data for compound 2o

CCDC **1843923** contain the supplementary crystallographic data for compound **2o**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.



2o



Data for DFT calculations

1. Computational Details

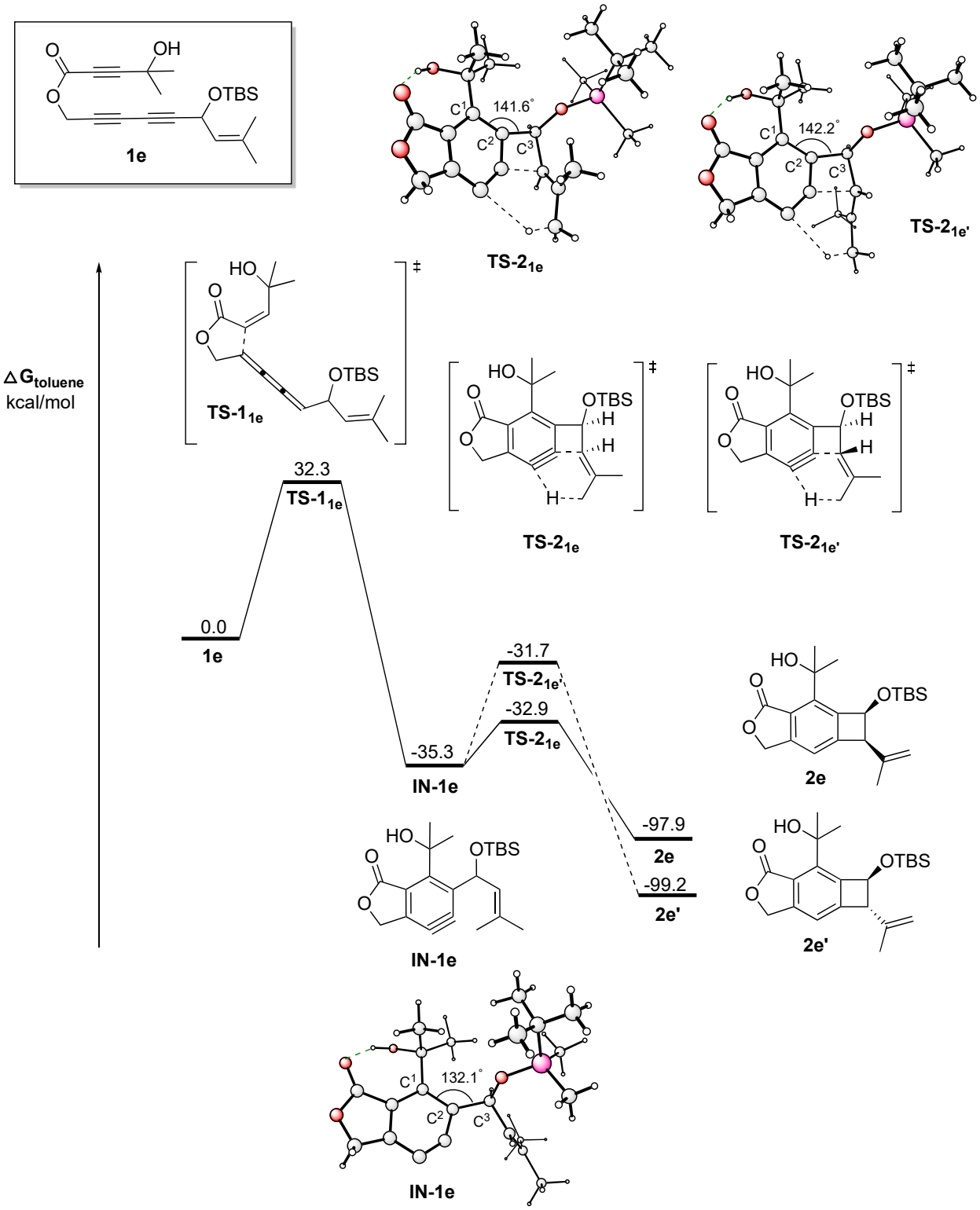
All DFT calculations were carried out with the Gaussian 09 suite of computational programs.[1] The geometries of all stationary points were optimized using the B3LYP hybrid functional[2] at the basis set level of 6-31G(d). Frequencies were analytically computed at the same level of theory to obtain the free energies and to confirm whether the structures are minima (no imaginary frequency) or transition states (only one imaginary frequency). The solvent effect of toluene was evaluated by using the SMD polarizable continuum model by carrying out single point calculations at the M06/6-311++G(d,p) level.[3] All transition state structures were confirmed to connect the proposed reactants and products by intrinsic reaction coordinate (IRC) calculations. The energies given in the text are Gibbs free energies corrected with solvation effects. All these are relative to the energies of the corresponding substrate.

[1] Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, **2009**.

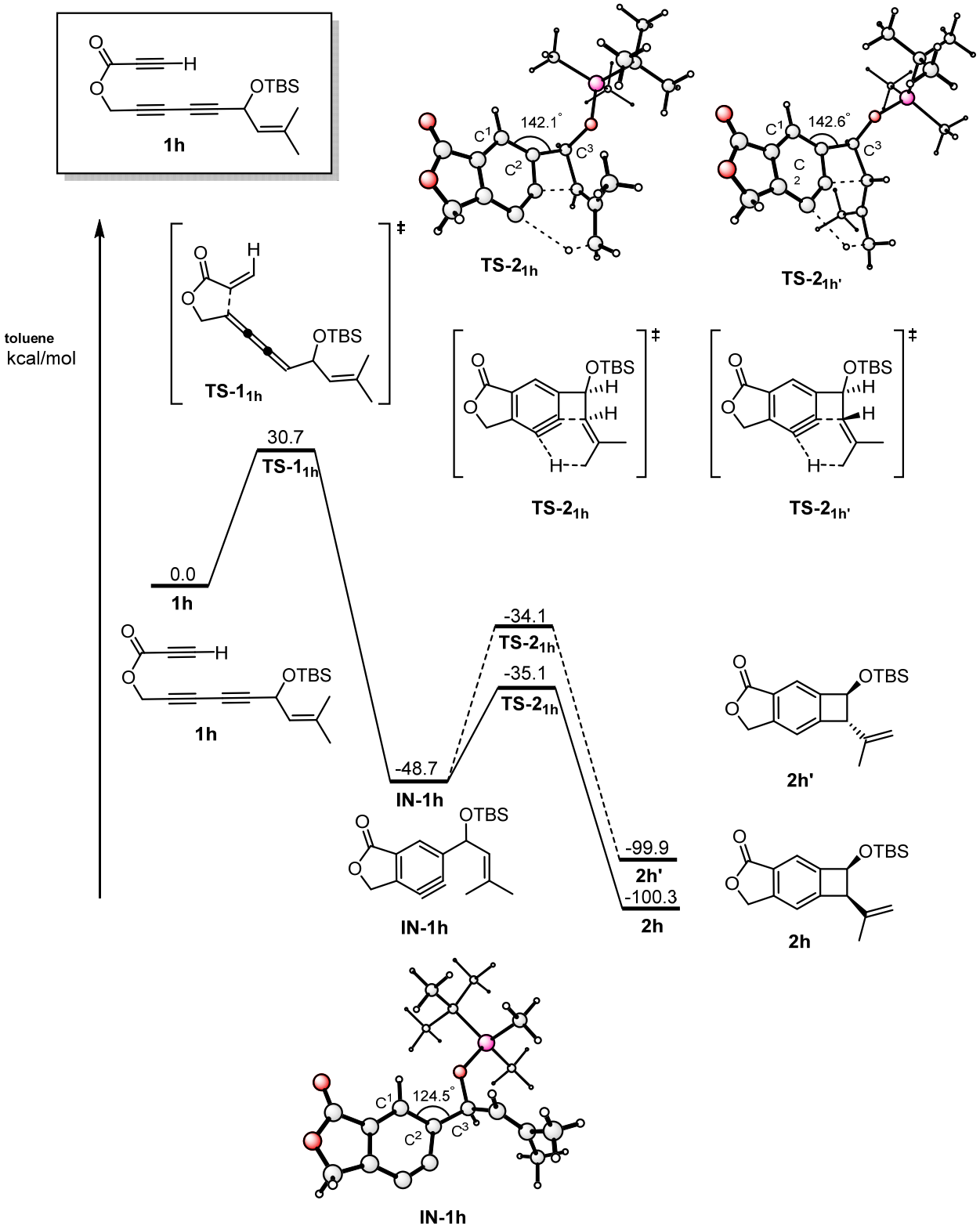
[2] (a) Becke, A. D. J. *Chem. Phys.* **1993**, *98*, 5648. (b) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 1372. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

[3] (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157.

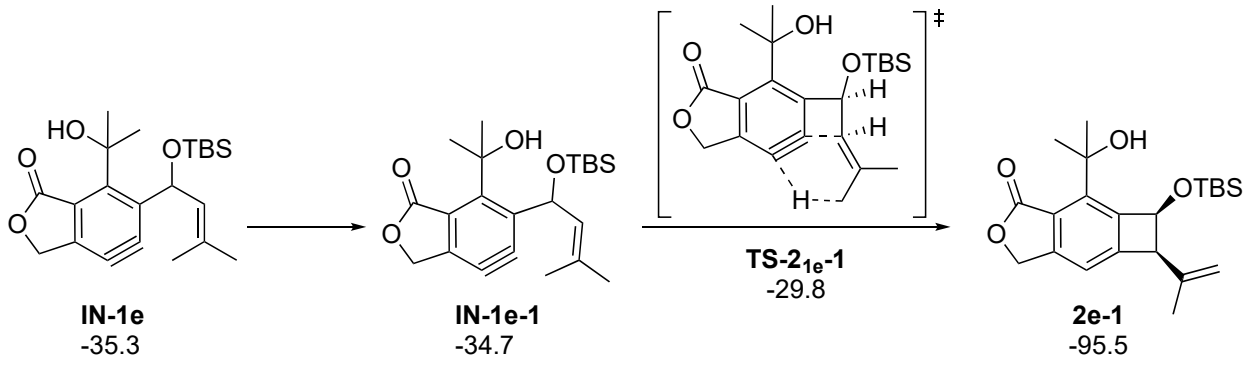
2. Reaction profile for 1e



3. Reaction profile for 1h



4. Comparison of the reaction without hydrogen bonding for IN-1e

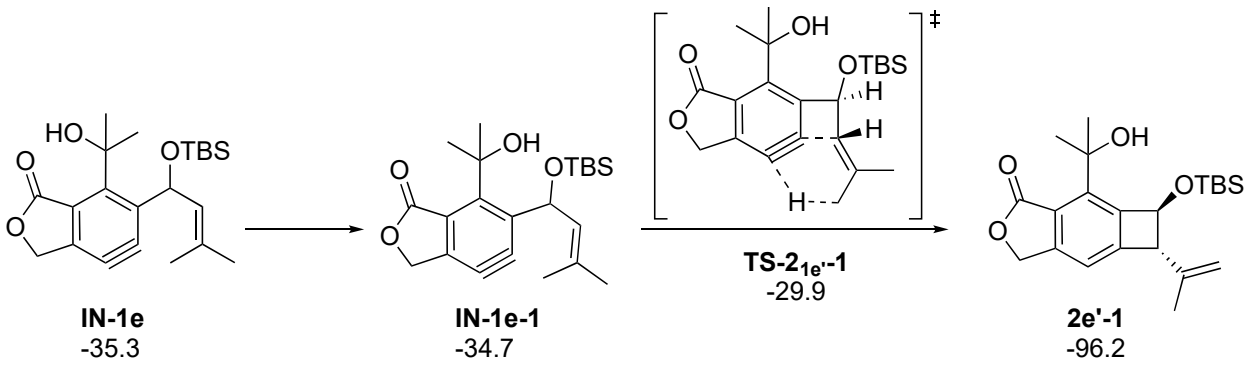


IN-1e
-35.3

IN-1e-1
-34.7

TS-2$_{1e}$-1
-29.8

2e-1
-95.5



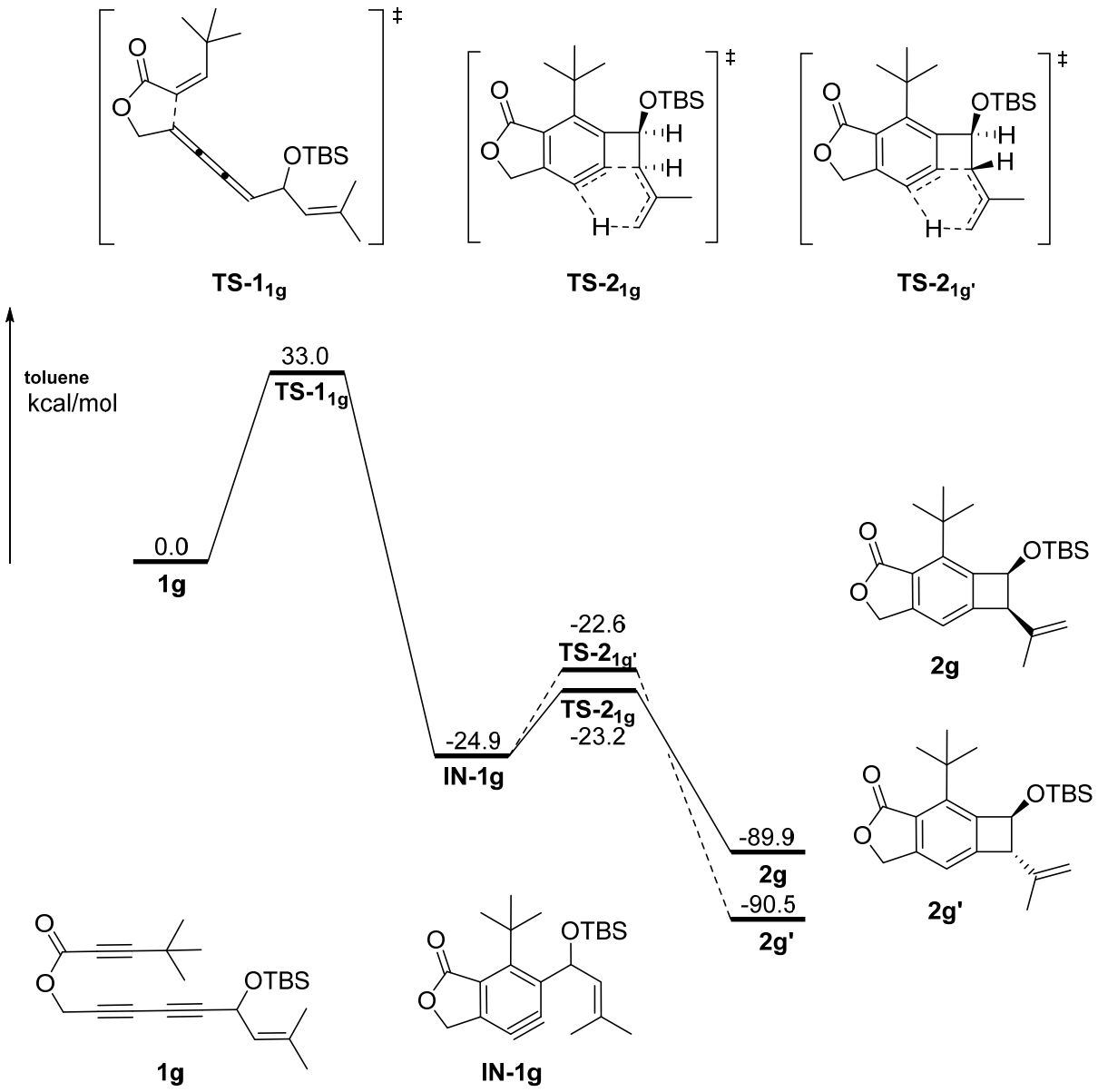
IN-1e
-35.3

IN-1e-1
-34.7

TS-2$_{1e'}$-1
-29.9

2e'-1
-96.2

5. Reaction profile for 1g (*t*-butyl substituted substrate)



6. Calculated Energy Values

Table S1. Energies (in Hartree) calculated at SMD-M06/6-311++G(d,p)//B3LYP/6-31G(d)

Species	E_0[a]	H_{298}[b]	G_{298}[c]	E[d]	G_{Sol}[e]
1e	-1447.365375	-1447.329308	-1447.439061	-1447.330252	-1447.39734543
TS-1_{1e}	-1447.325627	-1447.290548	-1447.396384	-1447.291492	-1447.34114204
IN-1e	-1447.433618	-1447.401206	-1447.495928	-1447.402150	-1447.46500117
TS-2_{1e}	-1447.422274	-1447.390901	-1447.484143	-1447.391845	-1447.46068623
2e	-1447.537567	-1447.506475	-1447.597295	-1447.507419	-1447.57016603
TS-$2_{1e'}$	-1447.424417	-1447.392854	-1447.485024	-1447.393798	-1447.45956518
2e'	-1447.541054	-1447.509590	-1447.602361	-1447.510535	-1447.57001507
1h	-1254.289172	-1254.258565	-1254.355942	-1254.259509	-1254.28800903
TS-1_{1h}	-1254.247490	-1254.217869	-1254.309956	-1254.218813	-1254.24141752
IN-1h	-1254.380471	-1254.352562	-1254.439719	-1254.353506	-1254.37803205
TS-2_{1h}	-1254.352709	-1254.326015	-1254.410066	-1254.326959	-1254.35756375
2h	-1254.468509	-1254.442058	-1254.524947	-1254.443002	-1254.46612864
TS-$2_{1h'}$	-1254.353525	-1254.326896	-1254.409497	-1254.327841	-1254.35719017
2h'	-1254.470143	-1254.443661	-1254.526190	-1254.444606	-1254.46600106
IN-1e-1	-1447.437869	-1447.405392	-1447.499792	-1447.406337	-1447.46448820
TS-2_{1e}-1	-1447.423750	-1447.392393	-1447.483469	-1447.393337	-1447.45787739
TS-$2_{1e'}$-1	-1447.425236	-1447.393828	-1447.484677	-1447.394772	-1447.45813213
2e-1	-1447.539281	-1447.508081	-1447.598921	-1447.509025	-1447.56636819
2e'-1	-1447.541852	-1447.510608	-1447.601546	-1447.511552	-1447.56749431

1g	-1411.446725	-1411.410458	-1411.520813	-1411.411402	-1411.47246507
TS-1$_{1g}$	-1411.402272	-1411.367148	-1411.472765	-1411.368092	-1411.42138399
IN-1g	-1411.497052	-1411.464106	-1411.559780	-1411.465051	-1411.52856100
TS-2$_{1g}$	-1411.487610	-1411.455751	-1411.549598	-1411.456696	-1411.52564579
2g	-1411.604476	-1411.572764	-1411.665136	-1411.573708	-1411.63660189
TS-2$_{1g'}$	-1411.489703	-1411.457561	-1411.551098	-1411.458505	-1411.52461829
2g'	-1411.607558	-1411.575653	-1411.669046	-1411.576598	-1411.63655990

[a] Sum of electronic and zero-point energies
[b] Sum of electronic and thermal enthalpies
[c] Sum of electronic and thermal free energies
[d] Electronic energies
[e] Single point energies in solution

5. Cartesian Coordinates for All Species

1e

O	-0.09613300	-0.69891800	-0.42611100
C	0.40141500	-1.91919500	-0.08785800
O	1.53146600	-2.21239700	-0.39880200
C	-1.44093100	-0.33088900	-0.04504800
H	-1.70012900	0.47621400	-0.73682300
H	-2.12316900	-1.16934700	-0.22681500
C	-1.54186800	0.12455000	1.33624100
C	-1.62151800	0.51238600	2.48611100
C	-1.71706500	0.94765500	3.77658000
C	-1.80207500	1.33425000	4.92694800
C	-1.91224100	1.78215300	6.32446900
H	-1.37966400	1.04854300	6.94513600
C	-3.36666900	1.85754100	6.73743100
H	-3.90366700	2.66739000	6.24664600
C	-4.01962100	1.06816500	7.60352400
C	-3.42004600	-0.10442800	8.34124500
H	-3.58444200	-0.00326900	9.42240800
H	-3.91278100	-1.03864800	8.03889800
H	-2.34748600	-0.23032500	8.17405500
C	-5.48167000	1.30763800	7.89744600
H	-6.08365300	0.42483000	7.64091000
H	-5.64134500	1.49314800	8.96858100
H	-5.87642500	2.16218200	7.34015200
C	-0.47498600	-2.82130000	0.63239800
C	-1.13895000	-3.62935500	1.24629600
O	-1.30108700	3.06629900	6.44205700
Si	-0.33937600	3.61535700	7.71669700
C	-1.40407900	3.95152200	9.24203800
H	-1.92990500	3.04178500	9.55518200
H	-0.79707200	4.29125400	10.09012100
H	-2.16368600	4.71561600	9.04370600
C	0.95366300	2.30280900	8.14970400
H	1.63842700	2.67491300	8.92141500
H	0.49438300	1.38959600	8.54805300
H	1.55478000	2.01959600	7.27858700
C	0.45597700	5.20971400	7.02870300
C	1.35392100	5.86192300	8.10279000
H	2.17480000	5.20270000	8.41229000
H	1.80943600	6.78202200	7.70936800
H	0.78921800	6.13956700	9.00157800
C	1.31029400	4.87314800	5.78757500
H	0.71087500	4.40167100	5.00133100
H	1.75142200	5.78943500	5.36930300
H	2.13841600	4.19588100	6.03091100
C	-0.65056900	6.20638400	6.61997800
H	-0.20457000	7.12070100	6.20222900
H	-1.31433600	5.78049000	5.85989900
H	-1.26772800	6.50787700	7.47543900
C	-1.90046000	-4.62826900	2.02582500
C	-1.60608300	-4.42807800	3.52545500
H	-1.90762100	-3.43060000	3.86077500
H	-2.15597300	-5.18250200	4.09689700
H	-0.53566400	-4.54467200	3.72767000
C	-3.40246500	-4.51344800	1.73119800
H	-3.78060800	-3.52859100	2.02018100
H	-3.59016600	-4.67211700	0.66589800
H	-3.93570200	-5.28323900	2.29757500
O	-1.53401700	-5.95076300	1.61498500
H	-0.57214000	-6.03754300	1.71912000

TS-1_{1e}

O	-4.68166000	0.39807200	2.08614300
C	-4.80058700	-0.94141100	2.08208300
O	-5.61498800	-1.50883700	1.38778500
C	-3.66304800	0.90147500	2.95279700
H	-2.98003500	1.50129100	2.34336700
H	-4.14536000	1.55193100	3.69014000
C	-2.93104400	-0.22320300	3.63290400
C	-1.94377900	-0.25826300	4.41866800
C	-0.95758600	-0.66479800	5.23485200
C	-0.04411000	-1.00698900	5.98039700
C	1.02966700	-1.40394400	6.90480500
H	0.55071800	-1.63336100	7.86889300
C	1.99101800	-0.24863600	7.15461300
H	1.95083900	0.16150900	8.16171600
C	2.85039900	0.28561000	6.27364300

C	3.00108400	-0.16892200	4.84477100
H	2.82276900	0.67047100	4.15880400
H	4.02965100	-0.50877700	4.66148600
H	2.32568000	-0.98393500	4.58536500
C	3.75889100	1.41767600	6.68615400
H	4.81394800	1.13691300	6.56364300
H	3.59604300	2.29969900	6.05145900
H	3.60374800	1.71306800	7.72827500
C	-3.85194500	-1.63732300	2.99578400
C	-3.76269600	-2.86420900	3.24531900
C	-4.12528200	-4.28427000	3.08145300
C	-3.14827700	-4.93957000	2.08253800
H	-2.12151100	-4.93115700	2.46383600
H	-3.46126400	-5.97530500	1.91627200
H	-3.16990000	-4.41173800	1.12395400
C	-4.15253400	-5.04669600	4.41375400
H	-4.83546900	-4.55823200	5.11402600
H	-4.51214700	-6.06467200	4.23204400
H	-3.15410800	-5.09357800	4.85824500
O	-5.46772600	-4.33751900	2.57254100
H	-5.58942600	-3.59077100	1.95224000
O	1.72953100	-2.55969700	6.44539100
Si	1.17054200	-4.15740500	6.48822300
C	0.08044400	-4.40804800	8.01441600
H	-0.83967600	-3.81439300	7.95413100
H	-0.22263400	-5.45850600	8.10125300
H	0.59523200	-4.13674500	8.94325200
C	0.16061800	-4.53572500	4.93681300
H	-0.70552900	-3.86797000	4.86734900
H	0.75383000	-4.40016800	4.02541700
H	-0.20892600	-5.56873600	4.94670800
C	2.76549500	-5.20932500	6.56237200
C	2.40836300	-6.71155300	6.54934700
H	1.87716200	-7.00210500	5.63463600
H	3.32250400	-7.32027200	6.60093400
H	1.78294500	-6.99511700	7.40518300
C	3.65815700	-4.88947900	5.34359800
H	3.93473200	-3.82986500	5.31362900
H	4.58701200	-5.47686300	5.38673800
H	3.16287700	-5.13488000	4.39613300
C	3.54770500	-4.88454400	7.85320700
H	4.47978700	-5.46682500	7.89100900
H	3.81511500	-3.82322800	7.90544600
H	2.97337700	-5.13293700	8.75432900

IN-1e

O	-2.44036800	-0.80328800	-0.46501100
C	-1.65134200	-1.08313600	0.61002900
O	-0.62946200	-1.72217300	0.44249700
C	-3.58332400	-0.02270700	-0.08945100
H	-3.57393500	0.91112900	-0.66309500
H	-4.49067000	-0.58107600	-0.34769200
C	-3.41517200	0.18664100	1.38100600
C	-4.15245800	0.88770500	2.32900600
C	-3.65165000	0.87045600	3.47680100
C	-2.56217000	0.33544900	4.13105000
C	-2.35379200	0.65598300	5.61392600
H	-2.15961100	-0.26208200	6.16839100
C	-3.61147400	1.31390600	6.13598000
H	-3.76259700	2.32400800	5.75459000
C	-4.52869100	0.79988200	6.97256500
C	-4.47871800	-0.58232000	7.57639600
H	-4.58400200	-0.52870400	8.66811600
H	-5.32178800	-1.18581600	7.21322200
H	-3.56022200	-1.12911900	7.35171100
C	-5.74486500	1.60642500	7.36100800
H	-6.66769600	1.08968200	7.06392200
H	-5.79746400	1.73552200	8.45079500
H	-5.74607800	2.59746200	6.89763000
C	-2.24934300	-0.46791700	1.83412200
C	-1.79795800	-0.44362700	3.19784400
O	-1.22048300	1.52503600	5.73105500
Si	-0.65600700	2.29407000	7.13161700
C	-1.74557800	3.77195800	7.58588900
H	-2.75509900	3.45007900	7.86033400
H	-1.32816700	4.31730400	8.44107000
H	-1.83512000	4.47893400	6.75295300
C	-0.63805500	1.06902200	8.57351300
H	-0.18486100	1.52068100	9.46444200
H	-1.65489300	0.76504900	8.84814900
H	-0.07006300	0.16189400	8.33764300
C	1.10864400	2.88928000	6.68107800

C	1.65696400	3.78309800	7.81617000
H	1.70469800	3.25275100	8.77591400
H	2.67875100	4.11161600	7.57810600
H	1.05119600	4.68524400	7.96020400
C	2.06173300	1.68908700	6.49786700
H	1.73226900	1.02091700	5.69534900
H	3.07061400	2.04118000	6.23760800
H	2.15310800	1.09361900	7.41448800
C	1.07017600	3.70809900	5.37247100
H	2.08064300	4.05285900	5.10878000
H	0.68879400	3.11501400	4.53446200
H	0.43679800	4.59915500	5.46552100
C	-0.50128300	-1.23764600	3.58097500
C	0.71892100	-0.42440100	3.09932900
H	0.74033500	0.55922700	3.57852200
H	1.63543600	-0.96618300	3.35836800
H	0.70134500	-0.28480700	2.01530900
C	-0.34271400	-1.56002700	5.07168200
H	-0.16584200	-0.67347400	5.67961200
H	-1.20975000	-2.11382300	5.44563200
H	0.52550000	-2.21930700	5.15679300
O	-0.54127700	-2.52543200	2.98514400
H	-0.36403200	-2.42135000	2.02794000

TS-2$_{1e}$

O	-3.86874800	-0.63942000	-0.15097100
C	-2.63909600	-0.69194200	0.42651300
O	-1.66832200	-1.01246300	-0.23767100
C	-4.86249900	-0.21546900	0.79823000
H	-5.34761900	0.68876600	0.41361100
H	-5.61906200	-1.00400100	0.88523600
C	-4.11111500	0.02326600	2.07796600
C	-4.63478200	0.52140300	3.29392300
C	-3.59927900	0.60081100	4.09873700
C	-2.22975500	0.35446700	4.06025100
C	-1.80875500	0.64281300	5.49898100
H	-1.48049700	-0.27060300	6.01150000
C	-3.26025900	0.96674900	5.94710500
H	-3.76429600	0.18069600	6.50786300
C	-3.94064800	2.15792600	5.77428800
C	-3.35612700	3.40984200	5.18839100
H	-3.95997900	3.72813000	4.32925100
H	-3.41934700	4.21422600	5.93437400
H	-2.31835700	3.29193300	4.88361800
C	-5.41823200	2.15241700	5.97284000
H	-5.81895600	3.15231600	6.16208000
H	-5.83925700	1.78175000	5.01020500
H	-5.74486200	1.46642400	6.75969400
C	-2.75377900	-0.28859300	1.85346200
C	-1.74026300	-0.17688300	2.85512400
O	-0.85018800	1.66553000	5.66944200
Si	0.01037800	1.98445700	7.09876900
C	-1.15921300	2.67324700	8.41660400
H	-1.96739200	1.96691500	8.64108600
H	-0.62224600	2.85852900	9.35465300
H	-1.62140000	3.61727500	8.10695700
C	0.77987400	0.38666400	7.75374200
H	1.38632100	0.59313500	8.64417100
H	0.01495900	-0.34088600	8.05119900
H	1.42771300	-0.09719700	7.01498100
C	1.32964100	3.26731000	6.58677400
C	2.14026100	3.69425100	7.83194600
H	2.66141500	2.84796900	8.29664600
H	2.90667700	4.42951300	7.54893600
H	1.50961800	4.16295200	8.59752800
C	2.29337600	2.65987700	5.54449700
H	1.76664000	2.35697400	4.63298400
H	3.05510200	3.39865700	5.25725500
H	2.82280300	1.78220600	5.93442000
C	0.65626000	4.51476000	5.97396900
H	1.41836500	5.25455400	5.68999200
H	0.08681200	4.26500900	5.07190100
H	-0.02504800	5.00594200	6.67971200
C	-0.26517000	-0.57268600	2.60905500
C	0.43763900	0.56909600	1.84376800
H	0.40776200	1.50494400	2.41355900
H	1.48342800	0.29374200	1.66796600
H	-0.03979800	0.73774700	0.87377400
C	0.47926000	-0.86698100	3.91550300
H	0.56313500	0.01758500	4.54847500
H	-0.02039100	-1.67052300	4.46696300
H	1.48422400	-1.21456000	3.65892300

O	-0.18300900	-1.79217300	1.88630800
H	-0.51861400	-1.62278600	0.98119000

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O	-3.29492800	-1.16048900	-0.30717500
C	-2.25916200	-1.24874200	0.57549300
O	-1.22254900	-1.79080900	0.24310800
C	-4.40502500	-0.46376100	0.27462300
H	-4.63745400	0.40210300	-0.35625800
H	-5.27247300	-1.13445400	0.27431700
C	-3.94822000	-0.08612400	1.65508700
C	-4.63493300	0.64779300	2.62106700
C	-3.90069600	0.86831800	3.77539300
C	-2.60840700	0.36888800	3.98755600
C	-2.56953800	0.91889300	5.42468400
H	-2.68375200	0.11175500	6.16251400
C	-4.00392000	1.57649600	5.11612300
H	-4.78424200	1.17541900	5.77472500
C	-4.11384900	3.08448900	5.07804700
C	-3.28810900	3.82935800	4.05743600
H	-3.40746600	4.91142000	4.16794200
H	-2.22656700	3.58006100	4.15578100
H	-3.58431600	3.55671000	3.03632500
C	-4.95136100	3.71848000	5.90803300
H	-5.05540300	4.80062200	5.89440400
H	-5.64048700	1.02829400	2.46290600
H	-5.56409600	3.18130900	6.62795600
C	-2.64859700	-0.58103000	1.84724600
C	-1.91141200	-0.40342700	3.05148800
O	-1.51671300	1.77602200	5.78132600
Si	-0.97251000	2.06426700	7.36489900
C	-2.40132600	2.62199900	8.46836100
H	-3.13539700	1.81637800	8.59417900
H	-2.03845300	2.88587100	9.46955700
H	-2.92967200	3.48611100	8.05458700
C	-0.26194300	0.47194700	8.09856800
H	-0.02828400	0.61276700	9.16091700
H	-0.98198100	-0.35293500	8.03545500
H	0.65370000	0.14467900	7.59498700
C	0.36830300	3.41527900	7.17250300
C	1.08345000	3.62012300	8.52685200
H	1.58642300	2.70830800	8.87044000
H	1.85162300	4.40123900	8.43571000
H	0.39080700	3.93963500	9.31575600
C	1.40447600	2.98347200	6.11317000
H	0.93981000	2.83485400	5.13246200
H	2.18141200	3.75393000	6.00292100
H	1.91016100	2.05002100	6.38919000
C	-0.27033300	4.75123300	6.73707900
H	0.50308700	5.52583300	6.63134500
H	-0.78193300	4.66222800	5.77257700
H	-0.99929800	5.11568900	7.47083000
C	-0.49874400	-0.98746100	3.26387900
C	0.53064100	-0.08983100	2.54485700
H	0.51067300	0.93160800	2.94116500
H	1.53271100	-0.50640600	2.69405200
H	0.33248700	-0.05039300	1.46931500
C	-0.15172300	-1.09711600	4.75010900
H	-0.11618400	-0.11855300	5.22913500
H	-0.87970500	-1.73095500	5.26739300
H	0.82879100	-1.57456200	4.83643000
O	-0.43074500	-2.32506700	2.78660100
H	-0.48393800	-2.29511800	1.81005100

TS-$2_{1e'}$

O	-2.59568600	-1.33598100	-0.16467300
C	-1.78333100	-1.38969100	0.92525900
O	-0.71101900	-1.96522800	0.85584200
C	-3.79441900	-0.59738200	0.12589300
H	-3.86688500	0.23860900	-0.57924400
H	-4.65642700	-1.25659800	-0.02903300
C	-3.64623700	-0.15186100	1.55316400
C	-4.55564300	0.61401800	2.31821500
C	-3.97001200	0.80641100	3.47072700
C	-2.80681800	0.40761800	4.12150600
C	-2.93821500	1.09990800	5.47550300
H	-3.07382900	0.39909400	6.30871500
C	-4.25313800	1.81477500	5.07188200
H	-4.10699200	2.84053300	4.73928800
C	-5.54070900	1.33514300	5.20482500
C	-5.88618800	0.01913000	5.83737100
H	-6.67333700	0.16872700	6.58750800

H	-6.29832900	-0.66026600	5.07894000
H	-5.03885500	-0.47462600	6.31660900
C	-6.62472000	2.00929400	4.43758200
H	-6.53800600	1.61725700	3.39694300
H	-7.62316700	1.77106900	4.81487700
H	-6.49776100	3.09444200	4.38326500
C	-2.42033200	-0.64662100	2.04429500
C	-1.94195300	-0.40426000	3.37073800
O	-1.90342700	2.01532900	5.76028100
Si	-1.65884100	2.82709800	7.22800800
C	-3.14055800	3.94249100	7.60578400
H	-4.06952900	3.36401900	7.67732400
H	-3.00565800	4.45709400	8.56486300
H	-3.28643000	4.70881600	6.83600500
C	-1.47938700	1.56510000	8.62424100
H	-1.25435600	2.06488000	9.57424800
H	-2.40442000	0.99510900	8.77507100
H	-0.67659700	0.84654400	8.42665700
C	-0.06589500	3.84055600	6.94304500
C	0.22142600	4.71874400	8.18195600
H	0.36850600	4.11982500	9.08958700
H	1.14101400	5.30056800	8.02689900
H	-0.58522500	5.43556300	8.37903300
C	1.13389500	2.89796100	6.70769700
H	0.98555100	2.26118200	5.82870400
H	2.04904700	3.48397400	6.54076500
H	1.31915600	2.24525900	7.56951800
C	-0.23960100	4.75043800	5.70716600
H	0.67641500	5.33288500	5.53287200
H	-0.44223800	4.16707300	4.80263600
H	-1.05990100	5.46758600	5.83654900
C	-0.60636500	-0.97637400	3.90294600
C	0.56089700	-0.12907800	3.35484600
H	0.46806100	0.91828400	3.66343400
H	1.50672300	-0.52959100	3.73629400
H	0.58906400	-0.16820500	2.26173600
C	-0.56372900	-1.00669300	5.43458600
H	-0.58931000	-0.00444400	5.86476900
H	-1.39700400	-1.59898900	5.82773400
H	0.36565600	-1.49850500	5.73608500
O	-0.46576400	-2.33906300	3.52738000
H	-0.34245600	-2.36597900	2.55533900

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O	-2.57195200	-1.57640400	-0.15451000
C	-1.72646100	-1.55246600	0.91537500
O	-0.64708900	-2.10894400	0.85086100
C	-3.77165900	-0.84192100	0.12537400
H	-3.87534900	-0.05169400	-0.62734100
H	-4.62449700	-1.52441600	0.02976800
C	-3.58957800	-0.31245200	1.51985600
C	-4.45141000	0.50335700	2.25320500
C	-3.95358800	0.85438000	3.49792400
C	-2.72800800	0.40156300	4.00137000
C	-2.93617200	1.12015400	5.34041300
H	-3.11077600	0.43186400	6.17739100
C	-4.29924600	1.68963800	4.72428200
H	-4.18000100	2.76147900	4.53201200
C	-5.60632000	1.43464100	5.43664600
C	-5.96754100	0.00198000	5.75106200
H	-5.22181400	-0.47279000	6.40201300
H	-6.93738500	-0.06096600	6.25299300
H	-6.01415600	-0.60551300	4.83846200
C	-6.41859800	2.45023700	5.75603100
H	-5.40829200	0.84303900	1.86593400
H	-7.36503000	2.28574600	6.26522300
H	-6.16922000	3.48061200	5.51557900
C	-2.35137800	-0.76005200	2.00806300
C	-1.85913600	-0.44185300	3.30451900
O	-1.96646900	2.08176300	5.67162600
Si	-1.80267600	2.89014600	7.15019200
C	-3.26914900	4.04890500	7.42763000
H	-4.21512600	3.49535000	7.42566800
H	-3.18865600	4.56177500	8.39385000
H	-3.33260700	4.81651500	6.64781200
C	-1.74274600	1.62608600	8.55601200
H	-1.56620900	2.12154300	9.51848400
H	-2.69045500	1.08144800	8.64717300
H	-0.94771400	0.88651700	8.41054800
C	-0.16617300	3.86160400	6.97255100
C	0.06555800	4.72637100	8.23198900
H	0.14100500	4.11953800	9.14313000

H	1.00666300	5.28693700	8.13860600
H	-0.73503800	5.46086400	8.38299100
C	1.02234900	2.89129300	6.80544900
H	0.91044300	2.26063900	5.91666400
H	1.96040800	3.45446200	6.69550000
H	1.13995300	2.23121300	7.67352300
C	-0.23911300	4.78224700	5.73472900
H	0.70076400	5.34154800	5.62024500
H	-0.40134700	4.20891900	4.81556800
H	-1.04722100	5.51951500	5.81837800
C	-0.51633600	-0.96738500	3.85406300
C	0.63325300	-0.12787800	3.25763400
H	0.52894600	0.93069700	3.52060900
H	1.58689600	-0.49796700	3.64955700
H	0.65473500	-0.21460200	2.16679400
C	-0.47085000	-0.91305400	5.38474700
H	-0.53180300	0.11049800	5.75779000
H	-1.28535600	-1.50753500	5.81172800
H	0.47401800	-1.35680100	5.71161000
O	-0.35271300	-2.34590200	3.54659300
H	-0.21966700	-2.42081300	2.58000800

1h

O	-2.95247800	-1.10587600	-1.02967500
C	-2.62958500	-2.41895500	-0.91169700
O	-3.46811900	-3.26687200	-1.09835400
C	-1.97003500	-0.07947700	-0.75082400
H	-1.00129100	-0.36308700	-1.17752800
H	-2.34079600	0.79412700	-1.29513400
C	-1.84226700	0.21070900	0.67103900
C	-1.74251000	0.45074400	1.85889200
C	-1.62225400	0.72083700	3.19149600
C	-1.51626100	0.95973100	4.37941900
C	-1.41344600	1.26435700	5.81495100
H	-2.33792800	0.90948500	6.29049000
C	-1.25851300	2.75614700	6.02305800
H	-0.29208100	3.13234200	5.69159700
C	-2.15201500	3.61184300	6.54293600
C	-3.53865800	3.24730600	7.01513000
H	-3.69893600	3.59748500	8.04354300
H	-4.29595900	3.74644600	6.39535000
H	-3.74730300	2.17514400	6.98682300
C	-1.81496300	5.07844500	6.67279900
H	-2.52116900	5.69456700	6.09917200
H	-1.89182700	5.40802600	7.71806100
H	-0.80427600	5.29966200	6.31746500
C	-1.25189600	-2.74397800	-0.57946700
C	-0.12618700	-3.08838800	-0.30729400
O	-0.29249200	0.55878300	6.34466600
Si	-0.08010400	0.02441300	7.93241500
C	0.53800000	1.43631200	9.02600700
H	-0.17241600	2.27080200	9.01653000
H	0.66046800	1.11423500	10.06734300
H	1.50271100	1.82272500	8.67864900
C	-1.72446700	-0.61385400	8.61789500
H	-1.58155200	-1.05639900	9.61124100
H	-2.45756600	0.19381700	8.73328700
H	-2.16949700	-1.38170900	7.97506800
C	1.22134500	-1.36700600	7.77078000
C	1.59204800	-1.91504400	9.16576200
H	0.72610800	-2.34278400	9.68680600
H	2.34114200	-2.71477200	9.07434700
H	2.02311900	-1.13992900	9.81135400
C	0.65209400	-2.51262400	6.90688600
H	0.36454700	-2.15956900	5.91039700
H	1.40435500	-3.30450500	6.77772600
H	-0.22956300	-2.97515400	7.36792500
C	2.49154700	-0.81067900	7.09153000
H	3.24284000	-1.60601500	6.97872400
H	2.27332200	-0.41203000	6.09500400
H	2.95351800	-0.00893500	7.68097700
H	0.86380000	-3.40189700	-0.05957900

TS-1$_{1h}$

O	-0.50520700	-2.02758000	0.02673400
C	0.38528400	-1.59892500	0.95650700
O	1.19911200	-2.34584900	1.43018000
C	-1.43034900	-1.05289700	-0.45682300
H	-1.32459100	-1.00532400	-1.54661900
H	-2.44114800	-1.40468900	-0.21910300
C	-1.16265200	0.27420600	0.16583700
C	-1.54695100	1.48468500	0.17786700

C	-1.13443300	2.56129700	0.88014600
C	-0.52992500	3.29452900	1.65904400
C	0.09747200	4.32461300	2.50154100
H	-0.70468100	4.87765100	3.00758900
C	0.92759600	5.26125400	1.65086800
H	1.82427800	4.79133200	1.25006500
C	0.66354200	6.54040700	1.34033500
C	-0.55758500	7.31105100	1.77974800
H	-0.26572300	8.25378800	2.26140800
H	-1.16805000	7.58393100	0.90819800
H	-1.20089300	6.76250400	2.47161300
C	1.61009200	7.32144500	0.46006800
H	1.10164300	7.66678000	-0.45065800
H	1.97188500	8.22177900	0.97535400
H	2.47756400	6.72635700	0.15996000
C	0.23255400	-0.15030800	1.29649600
C	0.78007400	0.67060200	2.06382300
O	0.90558500	3.66289300	3.48706100
Si	1.49989900	4.38163800	4.90691700
C	3.12521500	5.27380800	4.54875600
H	2.96771200	6.09358700	3.83926500
H	3.55842400	5.70024200	5.46186800
H	3.86752800	4.59650600	4.11184400
C	0.23099900	5.62138900	5.56510700
H	0.56071100	6.02796500	6.52873400
H	0.10314900	6.47307800	4.88673800
H	-0.75308600	5.16450500	5.72116800
C	1.75169800	2.92709600	6.12227400
C	2.26771300	3.46997100	7.47412700
H	1.55692100	4.16272700	7.94123400
H	2.42373500	2.64156000	8.17957500
H	3.22714000	3.99162400	7.37072400
C	0.41366100	2.19110600	6.35074400
H	0.00237900	1.79690100	5.41493300
H	0.55704900	1.34278400	7.03520600
H	-0.34279000	2.84659400	6.79991500
C	2.78690800	1.92559100	5.56402200
H	2.93574900	1.09961400	6.27407500
H	2.46249800	1.48174100	4.61622000
H	3.76578600	2.39143600	5.39784700
H	1.12610600	1.49346600	2.65841500

IN-1h

O	-0.54414900	-1.59579500	-0.01066000
C	0.14634100	-0.98852800	1.01947400
O	0.87843800	-1.60416600	1.75132200
C	-1.34947200	-0.65167000	-0.73877700
H	-1.03445700	-0.65841500	-1.78889100
H	-2.39664800	-0.97250800	-0.68895500
C	-1.09859800	0.65936700	-0.05400600
C	-1.48662800	1.98350500	-0.16269600
C	-1.06695400	2.87654300	0.60710300
C	-0.18693500	2.80832700	1.68349600
C	0.25812600	3.97998600	2.54411100
H	-0.64813600	4.43883300	2.96116300
C	1.00936400	4.98650900	1.70041100
H	1.98885400	4.62976500	1.38264000
C	0.60325500	6.20354700	1.30499500
C	-0.73217900	6.82709800	1.63240900
H	-0.59358000	7.82113600	2.07827700
H	-1.31875600	6.97734400	0.71575900
H	-1.33953500	6.23091500	2.31739000
C	1.49678500	7.06327400	0.44213200
H	1.01019000	7.29752300	-0.51479000
H	1.70454200	8.02599000	0.92923600
H	2.45200500	6.57517400	0.22708000
C	-0.19816100	0.45427700	1.00458500
C	0.25347500	1.47688700	1.85346500
O	1.06735700	3.47923100	3.59849100
Si	1.55545800	4.31070400	4.98851700
C	3.12277300	5.30488300	4.63700700
H	2.93650400	6.05713200	3.86254500
H	3.47436200	5.82901200	5.53420600
H	3.93710600	4.66159800	4.28521100
C	0.18026600	5.48548900	5.54268100
H	0.44462000	5.96756300	6.49167400
H	0.01633100	6.28503400	4.81069400
H	-0.77334400	4.96609900	5.69190500
C	1.87275900	2.93359400	6.27685100
C	2.35537500	3.55869700	7.60388700
H	1.60951900	4.23724700	8.03641400
H	2.54807400	2.77230600	8.34765800

H	3.28871800	4.12122400	7.47882700
C	0.57045600	2.14473300	6.53117200
H	0.18355600	1.69712100	5.60910400
H	0.75017200	1.32951200	7.24684200
H	-0.21804600	2.78023100	6.95346900
C	2.95427500	1.96173400	5.75606100
H	3.13055000	1.16083300	6.48843600
H	2.65624400	1.48741200	4.81439600
H	3.91382400	2.46595400	5.58788400
H	0.94910000	1.25610100	2.65564100

TS-2$_{1h}$

O	-2.99731300	-1.64598900	0.35335400
C	-2.09714100	-1.54984500	1.38784900
O	-1.05988800	-2.16838200	1.40474200
C	-4.14500200	-0.80563100	0.58905800
H	-4.22683700	-0.08766300	-0.23551500
H	-5.04280800	-1.43513500	0.58712800
C	-3.89503400	-0.14108600	1.92055000
C	-4.68810500	0.80664700	2.61510500
C	-4.03972900	1.08086100	3.73315700
C	-2.83059100	0.71673000	4.32023000
C	-2.90955800	1.41162700	5.66979600
H	-3.03295300	0.68634600	6.48729000
C	-4.30641400	2.01167900	5.34052200
H	-5.15155000	1.54141900	5.84111700
C	-4.56623900	3.15144600	4.59190800
C	-3.52053300	4.06936800	4.03343900
H	-3.63872800	4.14740300	2.94520700
H	-3.68401800	5.07665300	4.44179400
H	-2.50744100	3.75418900	4.27436900
C	-5.96053200	3.35800300	4.11219000
H	-6.15078200	4.38985200	3.80477500
H	-6.05853900	2.69745300	3.21698800
H	-6.71754900	3.03896500	4.83461400
C	-2.65295300	-0.60530700	2.38296500
C	-2.07887500	-0.21225100	3.60589400
O	-1.90962700	2.35082400	5.99316400
Si	-0.62571500	2.06738400	7.06657900
C	-1.32981500	1.65413900	8.77224100
H	-1.95691700	2.46407200	9.16107900
H	-1.94086700	0.74353700	8.74854500
H	-0.52509500	1.47730100	9.49597800
C	0.40684000	0.61152300	6.44988600
H	1.26226200	0.42159700	7.10933600
H	-0.18650900	-0.31071900	6.42112800
H	0.79495200	0.78722000	5.44048600
C	0.35672600	3.70480200	7.07347800
C	1.55840400	3.58285000	8.03722500
H	2.25216200	2.78894600	7.73464200
H	2.12870400	4.52249800	8.05267300
H	1.24347600	3.37912900	9.06816700
C	0.87883000	4.01508500	5.65397600
H	0.06028900	4.11703900	4.93276300
H	1.44163300	4.95957300	5.65348400
H	1.55389800	3.23382000	5.28475200
C	-0.55067900	4.86275500	7.54203400
H	0.00468100	5.81158600	7.52762000
H	-1.42587700	4.97927400	6.89325700
H	-0.91028400	4.71213200	8.56720600
H	-1.12640200	-0.61608300	3.93545800

2h

O	-3.13331800	-1.25520300	-0.25772400
C	-2.08667400	-1.17508700	0.63528500
O	-0.99633900	-1.63066800	0.39802500
C	-4.31448500	-0.63481500	0.27697300
H	-4.62308500	0.16741700	-0.40405500
H	-5.11441800	-1.38432300	0.30965100
C	-3.92013400	-0.13220400	1.64297700
C	-4.66808000	0.55287900	2.60656300
C	-3.95721200	0.87409100	3.75836200
C	-2.61713200	0.51871600	3.95681000
C	-2.58691500	1.06829400	5.37545500
H	-2.58969300	0.26317300	6.12545100
C	-4.09833100	1.56872300	5.11245400
H	-4.80856200	1.07822000	5.78960900
C	-4.34932200	3.05873800	5.12705600
C	-3.68126300	3.89982600	4.06782500
H	-3.89472800	4.96281100	4.21570400
H	-2.59595600	3.75380100	4.08214000
H	-4.02663500	3.61883700	3.06449000

C	-5.14705300	3.59369000	6.05971100
H	-5.33537200	4.66352300	6.10279500
H	-5.71067400	0.81963100	2.45247800
H	-5.64119200	2.98334100	6.81195400
C	-2.57644900	-0.46630200	1.83993100
C	-1.86781500	-0.16103700	3.00896800
O	-1.61069200	2.03014500	5.66859400
Si	-0.80643800	2.17391400	7.15207200
C	-2.07048700	2.40357800	8.53757900
H	-2.76740700	3.21691800	8.30853700
H	-2.66398700	1.49268800	8.68496300
H	-1.58270100	2.62932300	9.49361800
C	0.18259200	0.59233400	7.46541700
H	0.70005600	0.63016700	8.43162000
H	-0.47053800	-0.28893000	7.48564700
H	0.93642400	0.42478800	6.68792800
C	0.33118300	3.69427000	6.94693400
C	1.21299200	3.85002000	8.20585900
H	1.86141300	2.98002000	8.36581400
H	1.86642300	4.72837400	8.10510800
H	0.61535700	3.99496100	9.11474400
C	1.23955100	3.51150100	5.71168400
H	0.65372700	3.39636800	4.79334500
H	1.89181700	4.38784200	5.58606300
H	1.89002600	2.63321600	5.80625800
C	-0.51393100	4.97336600	6.76447500
H	0.14218300	5.84765000	6.64349200
H	-1.15400200	4.91488100	5.87732800
H	-1.15808000	5.16665600	7.63080300
H	-0.82568600	-0.44338600	3.12511200

TS-2$_{1h'}$

O	-2.45177800	-1.45720300	0.08622400
C	-1.63560600	-1.32267700	1.18530300
O	-0.52812000	-1.80151600	1.23175600
C	-3.71336800	-0.79334500	0.29659900
H	-3.84519800	-0.03982600	-0.48903000
H	-4.51715500	-1.53310500	0.20121300
C	-3.63022200	-0.19510000	1.67849300
C	-4.59623400	0.53951300	2.40849800
C	-4.04767900	0.86301800	3.56190800
C	-2.84606700	0.58856000	4.21138700
C	-3.03359300	1.31379000	5.52887700
H	-3.16356800	0.63343900	6.38157300
C	-4.38407800	1.91883000	5.03362000
H	-4.29064300	2.93675400	4.65849800
C	-5.65834400	1.38737400	5.20517000
C	-5.94290900	0.11712500	5.94936900
H	-6.75303500	0.29000000	6.66952400
H	-6.30115800	-0.65168400	5.25109700
H	-5.07994000	-0.27961500	6.48705700
C	-6.74580600	1.91670500	4.34504500
H	-6.56288800	1.45698300	3.33762200
H	-7.74277200	1.62433600	4.68529200
H	-6.69851500	3.00130000	4.20963500
C	-2.36719700	-0.52539300	2.19563600
C	-1.92043400	-0.14247100	3.47474500
O	-2.04950200	2.27686300	5.80499100
Si	-1.73512400	3.01443000	7.29493500
C	-3.16347000	4.17128000	7.74214500
H	-4.11129600	3.62281600	7.80994700
H	-2.99770200	4.65225500	8.71372600
H	-3.29338300	4.96343600	6.99618500
C	-1.57524700	1.69144300	8.63654900
H	-1.30107800	2.14578400	9.59629000
H	-2.51937500	1.15649100	8.79695000
H	-0.80914200	0.94802200	8.38985500
C	-0.10476400	3.96174900	7.00189900
C	0.29923800	4.72804800	8.28051100
H	0.47006200	4.05516200	9.13021900
H	1.23521300	5.27931400	8.11215700
H	-0.45916700	5.46222600	8.57973000
C	1.01621700	2.96674900	6.62938300
H	0.77108700	2.40364100	5.72227500
H	1.95640200	3.50545500	6.44348600
H	1.20934400	2.24532900	7.43297100
C	-0.28660100	4.96659200	5.84322900
H	0.65507400	5.50142700	5.65398800
H	-0.57656600	4.46299400	4.91476600
H	-1.04898200	5.72205900	6.07047900
H	-0.92796200	-0.40463000	3.82826400

2h'

O	-2.39251700	-1.65179500	0.05988000
C	-1.55549900	-1.44372900	1.13508800
O	-0.44083700	-1.89933400	1.18602700
C	-3.65793000	-1.00025800	0.25967700
H	-3.81519700	-0.28991700	-0.56087500
H	-4.44874600	-1.75870300	0.21399100
C	-3.55697700	-0.33239200	1.60806000
C	-4.48777400	0.44547300	2.30589400
C	-4.03087900	0.91440100	3.53288800
C	-2.76527100	0.61101100	4.04852100
C	-3.02366400	1.33975400	5.35898300
H	-3.16729600	0.65140100	6.20330700
C	-4.42589800	1.79440300	4.72051600
H	-4.35760200	2.85834000	4.46790700
C	-5.70517700	1.52251700	5.47262400
C	-6.03138100	0.08596400	5.80569000
H	-6.97304700	0.01002900	6.35712600
H	-6.11703300	-0.52238100	4.89638700
H	-5.24604300	-0.37889500	6.41639000
C	-6.51528800	2.52881300	5.82511700
H	-5.47315800	0.67243800	1.90668600
H	-7.43577100	2.35505800	6.37705700
H	-6.28961300	3.56115500	5.56968700
C	-2.28420900	-0.60881700	2.11733700
C	-1.83261000	-0.14936800	3.36139500
O	-2.11408600	2.35375000	5.68309700
Si	-1.86157200	3.06261600	7.19669800
C	-3.26813300	4.26249900	7.58645900
H	-4.23536500	3.74594300	7.57598300
H	-3.14560800	4.71565600	8.57778100
H	-3.31912400	5.07432200	6.85202900
C	-1.80540100	1.71824500	8.52647100
H	-1.55592100	2.15052800	9.50307600
H	-2.77426200	1.21678100	8.63848900
H	-1.05600900	0.95090300	8.30213100
C	-0.18638700	3.96128600	7.00806000
C	0.16779800	4.70416500	8.31480900
H	0.26481000	4.01960200	9.16686000
H	1.13006300	5.22495200	8.20724300
H	-0.58232800	5.46108100	8.57557200
C	0.92357800	2.93633200	6.68994000
H	0.71345000	2.38888500	5.76447800
H	1.88929000	3.44676500	6.56356200
H	1.04748800	2.20193500	7.49552300
C	-0.27080700	4.98188800	5.85216200
H	0.69720100	5.48624500	5.71844000
H	-0.52845800	4.49705500	4.90424500
H	-1.01837700	5.76103500	6.04649000
H	-0.83715800	-0.38951400	3.72268400

IN-1e-1

O	-1.85927200	-1.26565600	-0.54201900
C	-1.26711900	-1.27850400	0.69664400
O	-0.22564200	-1.87163600	0.85105600
C	-3.08061500	-0.52098300	-0.53860700
H	-3.00102300	0.29656400	-1.26513700
H	-3.90048300	-1.18012000	-0.84844500
C	-3.21535500	-0.04177000	0.87058900
C	-4.17427700	0.71662900	1.52901300
C	-3.95010800	0.92345900	2.74268600
C	-2.98953800	0.59702400	3.67566400
C	-3.15149400	1.05841700	5.12697000
H	-3.02184500	0.20203400	5.78897900
C	-4.51793200	1.67715800	5.28879100
H	-4.63264500	2.62777600	4.76721600
C	-5.56933900	1.18563500	5.96606600
C	-5.58151900	-0.12070300	6.72121700
H	-5.91699700	0.03610500	7.75502300
H	-6.29924100	-0.81607900	6.26494900
H	-4.61009300	-0.61819700	6.75130400
C	-6.87938900	1.93605900	5.99209700
H	-7.68705600	1.32686700	5.56377500
H	-7.17797900	2.16738200	7.02376500
H	-6.82771800	2.87412100	5.43139100
C	-2.12113000	-0.48788700	1.64479200
C	-1.97017200	-0.19657600	3.04111400
O	-2.11067300	2.02030100	5.41858600
Si	-1.92156700	2.91596700	6.85639000
C	-3.09472700	4.39629800	6.86694500
H	-4.14003800	4.07210500	6.85557100
H	-2.94690300	5.00690700	7.76575000

H	-2.93431900	5.04164400	5.99553500
C	-2.26097800	1.80329700	8.34521700
H	-1.98931000	2.30767500	9.28069000
H	-3.32264000	1.53976500	8.41293000
H	-1.68629100	0.87173200	8.29073800
C	-0.09748100	3.50179600	6.81071200
C	0.11666900	4.58513500	7.89268900
H	-0.12606100	4.22039800	8.89927800
H	1.17028100	4.89821000	7.90920300
H	-0.48570000	5.48177300	7.70603600
C	0.86644700	2.32936900	7.09943500
H	0.76058900	1.50392200	6.38689100
H	1.90869600	2.67522000	7.04289100
H	0.71538900	1.91707300	8.10424800
C	0.23160600	4.10484000	5.42794000
H	1.27112400	4.46242900	5.40603200
H	0.11370000	3.36981600	4.62463900
H	-0.41289300	4.96047300	5.19050600
C	-0.74203400	-0.71802500	3.85031700
C	-0.72748300	-2.25379100	3.88817300
H	-0.59131500	-2.68490600	2.89791100
H	0.10149900	-2.56977300	4.52979400
H	-1.65865300	-2.62212500	4.33115800
C	0.56346900	-0.12891500	3.28109900
H	0.75425200	-0.45110400	2.25793800
H	0.52735600	0.96697100	3.31237200
H	1.39160100	-0.46272500	3.91509600
O	-0.82671700	-0.35032300	5.22623700
H	-0.87948700	0.62313300	5.27899200

TS-2_{1e}-1

O	-3.38337900	-0.98147900	-0.31289000
C	-2.28993000	-0.98094300	0.51068200
O	-1.23661300	-1.44554400	0.13307100
C	-4.51483000	-0.37883600	0.33237700
H	-4.84692700	0.47778600	-0.26599500
H	-5.33085400	-1.11063600	0.36669200
C	-4.03195100	0.02013500	1.69945300
C	-4.77638400	0.69074800	2.70026200
C	-3.94745300	0.82262600	3.71575200
C	-2.61979300	0.51727900	3.99498800
C	-2.51448500	0.90306100	5.46072700
H	-2.39686600	0.01579100	6.09335300
C	-3.99735900	1.37079800	5.51425300
H	-4.68518800	0.69834600	6.02553900
C	-4.50441500	2.58708400	5.08130300
C	-3.67869400	3.72587000	4.56015900
H	-4.00939000	3.98871200	3.54733700
H	-3.85980400	4.60863400	5.18930000
H	-2.61187100	3.51128000	4.55447100
C	-5.97883100	2.69985400	4.90498000
H	-6.31965700	3.73813000	4.86784500
H	-6.18866700	2.22287700	3.91779000
H	-6.54703300	2.14805200	5.65946700
C	-2.67521900	-0.35445200	1.80806400
C	-1.90019000	-0.13919600	2.98699300
O	-1.51815400	1.85989100	5.78251200
Si	-0.89572600	2.09700800	7.35555700
C	-2.17127600	3.05231600	8.37232900
H	-3.13620500	2.53106300	8.37923200
H	-1.84892200	3.15606900	9.41513200
H	-2.34226400	4.05924000	7.97439000
C	-0.56417900	0.41415900	8.14386400
H	0.08767500	0.51706500	9.02010300
H	-1.48542300	-0.07222700	8.48595500
H	-0.07137300	-0.25833800	7.43278700
C	0.70778100	3.10492500	7.09879800
C	1.15507300	3.69481100	8.45644300
H	1.33604300	2.91610900	9.20869500
H	2.09625500	4.24915000	8.33412400
H	0.41680400	4.39362300	8.86750900
C	1.83953100	2.20421400	6.55592600
H	1.57915900	1.71764500	5.60959800
H	2.74433200	2.80300400	6.37911000
H	2.10546100	1.41283800	7.26621400
C	0.46044900	4.26287000	6.10762400
H	1.37148700	4.86812700	5.99720500
H	0.18476100	3.89379500	5.11391400
H	-0.33687400	4.93544000	6.44869500
C	-0.42859500	-0.53466300	3.19926500
C	-0.23376000	-2.05270600	3.10058800
H	-0.45799100	-2.40928500	2.09479800

H	0.80755200	-2.29103100	3.34170000
H	-0.87801700	-2.56153800	3.82501600
C	0.49090400	0.22172500	2.22479700
H	0.27903900	-0.04741500	1.18847600
H	0.36455900	1.30531900	2.34373800
H	1.53166800	-0.03048900	2.45437700
O	-0.04382400	-0.21032700	4.54582900
H	-0.20471200	0.73796700	4.69304600

TS-2$_{1e'}$-1

O	-2.75457200	-1.49711500	-0.14556500
C	-1.86211400	-1.43217200	0.89161300
O	-0.77808500	-1.96502900	0.80113900
C	-3.96662200	-0.79875900	0.17265600
H	-4.12628600	-0.01280100	-0.57521400
H	-4.80523400	-1.50300100	0.11495900
C	-3.76149700	-0.25429700	1.55861600
C	-4.68118600	0.49112200	2.33332300
C	-4.06372800	0.77342200	3.45542600
C	-2.84662200	0.45830000	4.04961900
C	-2.97308400	1.15584200	5.39386900
H	-3.06401600	0.45392100	6.22978300
C	-4.32203200	1.80835400	4.98848300
H	-4.22348200	2.82889500	4.62271600
C	-5.59474300	1.29916600	5.20058900
C	-5.87347000	0.01154000	5.91681900
H	-6.65109400	0.17525400	6.67387000
H	-6.27359300	-0.72764400	5.20927200
H	-4.99731600	-0.41790300	6.40575000
C	-6.71383700	1.88296600	4.41683100
H	-6.60918000	1.44190800	3.39286900
H	-7.69777100	1.61535100	4.81133700
H	-6.63871500	2.96848000	4.30360200
C	-2.47749300	-0.64248000	1.99671300
C	-1.95293200	-0.29901600	3.28027900
O	-1.95880800	2.10983800	5.66209900
Si	-1.67994000	2.82969500	7.18195100
C	-3.05461900	4.08094300	7.52563800
H	-4.04199600	3.60563900	7.48061400
H	-2.95047700	4.52045300	8.52468500
H	-3.04808800	4.90069900	6.79807300
C	-1.68531700	1.48187900	8.50483000
H	-1.30238000	1.86651400	9.45796900
H	-2.69408900	1.09701400	8.69692500
H	-1.05508800	0.63672800	8.20589100
C	0.02586800	3.67276700	7.00957400
C	0.24098700	4.63718200	8.19794900
H	0.20056100	4.11960600	9.16509300
H	1.23105900	5.10895900	8.12640200
H	-0.50300300	5.44235800	8.21589600
C	1.15516600	2.61782400	7.01812400
H	1.05070400	1.87571700	6.21870900
H	2.12955100	3.10870100	6.88338800
H	1.19449100	2.07167300	7.96810600
C	0.08747400	4.47549900	5.69185000
H	1.06114200	4.97732700	5.59927600
H	-0.04114100	3.83018600	4.81661600
H	-0.68523600	5.25336500	5.64840800
C	-0.56350300	-0.67039300	3.83018700
C	-0.40128900	-2.19078500	3.95362300
H	-0.43745100	-2.66946200	2.97464400
H	0.56567600	-2.40362200	4.42165500
H	-1.18879400	-2.59967100	4.59510800
C	0.55311800	-0.04586900	2.97555300
H	0.54615100	-0.44296100	1.95877000
H	0.43679500	1.04439400	2.93234300
H	1.51919000	-0.27055800	3.43999200
O	-0.44592400	-0.18751500	5.17720900
H	-0.59436200	0.77505300	5.17222600

2e-1

O	-3.27474600	-1.13341100	-0.33820300
C	-2.19268500	-1.09393200	0.50599300
O	-1.12127600	-1.52578100	0.15001000
C	-4.43125200	-0.55963600	0.27926600
H	-4.77925600	0.27604100	-0.34001100
H	-5.22350900	-1.31767500	0.30921300
C	-3.97705900	-0.13095100	1.64673100
C	-4.72490100	0.50500700	2.63920000
C	-4.00033600	0.78741400	3.78662200
C	-2.65767000	0.43075600	3.95059200
C	-2.63095400	0.91602800	5.39886700

H	-2.63074900	0.07430900	6.10286800
C	-4.13417700	1.43581100	5.16009700
H	-4.84566500	0.92741900	5.82259600
C	-4.40061400	2.92357400	5.20079200
C	-3.67830200	3.80363400	4.21031600
H	-3.92819000	4.85751800	4.36577100
H	-2.59348800	3.68417500	4.29877400
H	-3.94506300	3.53884100	3.17906600
C	-5.27503000	3.42151000	6.08355000
H	-5.48785300	4.48629700	6.13637400
H	-5.77119300	0.76596500	2.50344800
H	-5.80912600	2.78535000	6.78536200
C	-2.61980400	-0.46435700	1.78945100
C	-1.88393500	-0.20515000	2.97712100
O	-1.63189400	1.85066400	5.74922400
Si	-1.02311800	2.06522900	7.33120000
C	-2.30766300	2.94942900	8.39444700
H	-3.25386800	2.39683300	8.40603600
H	-1.96200500	3.03665600	9.43169500
H	-2.52677200	3.95595800	8.02270300
C	-0.63535700	0.36902300	8.06618400
H	0.01120600	0.46569100	8.94716300
H	-1.54201500	-0.15546000	8.39071200
H	-0.12256900	-0.26569900	7.33500100
C	0.55309300	3.12525700	7.10379300
C	0.98689000	3.68490100	8.47850700
H	1.19224000	2.88819000	9.20528300
H	1.91164100	4.26968900	8.37194100
H	0.23010100	4.34855400	8.91296500
C	1.71116900	2.27718100	6.53294200
H	1.46551800	1.81533600	5.57058400
H	2.59839500	2.90782100	6.37754100
H	2.00017300	1.46999800	7.21616800
C	0.27146400	4.30671800	6.15049400
H	1.16498200	4.94091600	6.05842800
H	0.00357100	3.96124900	5.14622800
H	-0.54489600	4.94403100	6.51304700
C	-0.40193400	-0.52915100	3.22232100
C	-0.13167300	-2.03726300	3.13247300
H	-0.30656600	-2.40983300	2.12291600
H	0.91236100	-2.22072500	3.40652400
H	-0.76972200	-2.57477700	3.84143000
C	0.49741100	0.26911400	2.26050500
H	0.32128900	-0.01147400	1.22028300
H	0.31754300	1.34535000	2.37446100
H	1.54400900	0.06798100	2.51157400
O	-0.06206200	-0.18567400	4.57177900
H	-0.31035800	0.74175800	4.73590300

2e'-1

O	-2.72124200	-1.71826700	-0.13347200
C	-1.81243300	-1.59170900	0.88815700
O	-0.72534700	-2.11445600	0.81056600
C	-3.93142000	-1.01439600	0.16357800
H	-4.10430400	-0.27006100	-0.62320700
H	-4.76356500	-1.72893300	0.14887500
C	-3.70904900	-0.39961300	1.51763500
C	-4.58435400	0.40719000	2.24809400
C	-4.06446100	0.83291400	3.46034800
C	-2.80292600	0.45060400	3.92587300
C	-2.99132100	1.16977500	5.25671000
H	-3.12965300	0.47665000	6.09419400
C	-4.37927600	1.70914300	4.67159100
H	-4.26942700	2.77259000	4.43200900
C	-5.65605000	1.48376300	5.44470100
C	-6.01420700	0.06280900	5.81029800
H	-6.95978700	0.02061900	6.35858600
H	-6.10905500	-0.56505000	4.91528300
H	-5.24218800	-0.40353100	6.43622400
C	-6.44236800	2.51564400	5.77653700
H	-5.56821300	0.68371300	1.87832600
H	-7.36529100	2.37479900	6.33367800
H	-6.19460900	3.53691900	5.49796200
C	-2.42456400	-0.75625800	1.96141400
C	-1.90170500	-0.34409200	3.21696100
O	-2.01381000	2.14165300	5.56975200
Si	-1.78234400	2.83981600	7.10613500
C	-3.15628500	4.09370500	7.42852900
H	-4.14127900	3.61955400	7.34677300
H	-3.07712100	4.52042200	8.43553400
H	-3.12521900	4.92215500	6.71121800
C	-1.82999500	1.47342300	8.40952000

H	-1.46764200	1.84169100	9.37711500
H	-2.84716100	1.09664600	8.56950800
H	-1.19983000	0.62669700	8.11465300
C	-0.06663000	3.67861500	7.00230100
C	0.11072900	4.62724400	8.20941400
H	0.03553400	4.09704600	9.16762100
H	1.10403600	5.09708100	8.17833500
H	-0.63180700	5.43385600	8.21272300
C	1.06116800	2.62298500	7.03562900
H	0.98627800	1.89351600	6.22155300
H	2.04041000	3.11501200	6.94559700
H	1.06448800	2.06147700	7.97751300
C	0.04127900	4.49901300	5.69863300
H	1.01969300	4.99761700	5.64344200
H	-0.06264400	3.86608100	4.81102100
H	-0.72667200	5.28069600	5.64100600
C	-0.51340300	-0.67447300	3.78873600
C	-0.32833100	-2.18629500	3.97618700
H	-0.34605000	-2.70761000	3.01869500
H	0.63690300	-2.36208100	4.46225900
H	-1.11480100	-2.58100000	4.62761200
C	0.59635000	-0.06968000	2.90931000
H	0.59851600	-0.50644700	1.90860700
H	0.46664800	1.01630900	2.82346600
H	1.56374100	-0.26273900	3.38452300
O	-0.40934200	-0.13507800	5.11266500
H	-0.61256800	0.81761000	5.08412100

1g

O	-0.04989400	-0.73666400	-0.40876800
C	0.44079200	-1.96161800	-0.06450300
O	1.57516000	-2.25062700	-0.36414800
C	-1.39418200	-0.36258400	-0.03886800
H	-1.64837000	0.44105800	-0.73678800
H	-2.07846800	-1.20008400	-0.21703400
C	-1.50332200	0.10279200	1.33910500
C	-1.58885400	0.49669000	2.48649400
C	-1.69062400	0.93741800	3.77472400
C	-1.78049600	1.32729600	4.92360100
C	-1.89344500	1.77223800	6.32156000
H	-1.34531200	1.04750800	6.93902900
C	-3.34696100	1.82175700	6.74156500
H	-3.90008200	2.62381600	6.25588000
C	-3.98236100	1.01857000	7.60802300
C	-3.35930400	-0.14606300	8.33895100
H	-3.52218600	-0.05261100	9.42105300
H	-3.83568800	-1.08786000	8.03386900
H	-2.28518600	-0.25160900	8.16794100
C	-5.44703700	1.23158400	7.90930400
H	-6.03467300	0.33904000	7.65307800
H	-5.60508400	1.41143200	8.98167600
H	-5.85928300	2.08056000	7.35616500
C	-0.44882500	-2.86009300	0.64053400
C	-1.12379900	-3.66170800	1.25129500
O	-1.30413400	3.06694700	6.43971000
Si	-0.35036100	3.62906000	7.71425600
C	-1.42273600	3.96832000	9.23365100
H	-1.94616600	3.05779400	9.54845600
H	-0.82090400	4.31463600	10.08277600
H	-2.18470300	4.72827700	9.02846800
C	0.94885900	2.32696500	8.16020200
H	1.62805300	2.70809800	8.93241000
H	0.49383800	1.41330000	8.56232500
H	1.55535300	2.04215300	7.29333800
C	0.43916500	5.22435400	7.02120400
C	1.33063600	5.88597500	8.09489300
H	2.15390400	5.23229500	8.40974200
H	1.78268800	6.80662300	7.69870300
H	0.76198000	6.16475500	8.99086900
C	1.29862600	4.88621500	5.78409200
H	0.70353600	4.40867700	4.99823900
H	1.73695600	5.80262000	5.36309300
H	2.12892900	4.21357800	6.03270800
C	-0.67110000	6.21352200	6.60447400
H	-0.22854500	7.12780400	6.18294600
H	-1.33075800	5.78029600	5.84494800
H	-1.29190100	6.51648300	7.45677500
C	-1.93756900	-4.62392800	2.00971600
C	-1.66373500	-4.41258000	3.51923200
H	-1.92421400	-3.39509600	3.82754700
H	-2.26637600	-5.11795800	4.10311800
H	-0.60830900	-4.58222300	3.75449100
C	-3.43528800	-4.37877300	1.70988000

H	-3.73200200	-3.36372400	1.99351800
H	-3.65128800	-4.51587500	0.64508200
H	-4.04795100	-5.08837800	2.27778500
C	-1.54417500	-6.06248700	1.59956300
H	-2.14137300	-6.78510200	2.16770300
H	-1.72349900	-6.23072400	0.53272100
H	-0.48550500	-6.25267900	1.80181400

TS-1_{1g}

O	-2.83019900	-0.62642200	-0.25953200
C	-4.10690400	-0.84550100	0.12124300
O	-5.04898700	-0.49945200	-0.54009400
C	-1.85686100	-1.10177300	0.67419100
H	-1.19695500	-1.79715000	0.14597300
H	-1.26792400	-0.24308300	1.01430300
C	-2.57171100	-1.77837500	1.81946700
C	-2.11455100	-2.38436900	2.86198100
C	-2.62845900	-2.99406300	3.95086000
C	-3.11565600	-3.54675400	4.93580700
C	-3.69805600	-4.20744400	6.11321900
H	-4.58489400	-4.76362400	5.77045700
C	-4.18873800	-3.20551400	7.15171500
H	-5.26299300	-3.22115800	7.32697200
C	-3.43410800	-2.35333600	7.86151800
C	-1.93793700	-2.22945400	7.73049500
H	-1.66277500	-1.20138900	7.45791100
H	-1.45549200	-2.43731700	8.69547800
H	-1.51954800	-2.91026400	6.98926400
C	-4.06704400	-1.43758800	8.88041200
H	-3.65457600	-1.62198200	9.88193300
H	-3.85410000	-0.38553000	8.64543600
H	-5.15300000	-1.56362300	8.93105500
C	-4.16009100	-1.56413300	1.45702500
C	-5.20067600	-1.88704500	2.10022800
C	-6.47229600	-2.21208700	2.72847800
C	-7.60803000	-1.73989700	1.76786500
H	-7.53903500	-2.24265800	0.79925800
H	-8.57897300	-1.97626900	2.22007900
H	-7.55280000	-0.66176600	1.59511700
C	-6.58225400	-3.74283000	2.94173000
H	-5.77366900	-4.09976600	3.58675800
H	-7.54446900	-3.97899200	3.41044900
H	-6.52274700	-4.27724100	1.98827800
O	-2.77075300	-5.12687500	6.70519500
Si	-2.57517400	-6.74391200	6.25385800
C	-4.20310600	-7.66479000	6.54952600
H	-5.00337600	-7.28216800	5.90338600
H	-4.09890500	-8.73394500	6.32815800
H	-4.54168600	-7.56785900	7.58708400
C	-2.12022700	-6.88830600	4.42552100
H	-2.90652800	-6.47066300	3.78591300
H	-1.19516000	-6.35037300	4.19273000
H	-1.98591600	-7.93783800	4.13582500
C	-1.17974800	-7.37802500	7.39549200
C	-0.92476800	-8.87798600	7.13080500
H	-0.62497000	-9.07000600	6.09297100
H	-0.11359500	-9.24549900	7.77575400
H	-1.80978500	-9.49079300	7.34317400
C	0.11889700	-6.58808100	7.12442400
H	-0.01812100	-5.51469700	7.29561400
H	0.92123100	-6.93348300	7.79272300
H	0.47300100	-6.72139200	6.09495200
C	-1.58405200	-7.18498600	8.87305800
H	-0.78012300	-7.53462900	9.53719200
H	-1.77534900	-6.13130600	9.10305500
H	-2.48694300	-7.75334100	9.12858200
C	-6.60252900	-1.47282600	4.08379700
H	-5.78614700	-1.74698000	4.75816300
H	-6.58287800	-0.38755700	3.94184300
H	-7.55588600	-1.74139400	4.55350700

IN-1g

O	-1.56846400	-0.41616300	-0.77204300
C	-1.01131600	-0.65907100	0.45912600
O	0.06058900	-1.21480300	0.51476700
C	-2.80712000	0.28598500	-0.66264000
H	-2.73183700	1.23097100	-1.21398000
H	-3.60300900	-0.31641800	-1.11762300
C	-2.98998200	0.47958300	0.80678900
C	-3.97879200	1.12648800	1.54211200
C	-3.76651500	1.11926900	2.77458700
C	-2.84234500	0.64113800	3.67719800

C	-3.03203200	1.01150300	5.15380300
H	-2.85922200	0.15108100	5.79643200
C	-4.44856000	1.50794300	5.34180000
H	-4.63404200	2.47842500	4.88075300
C	-5.46100000	0.89936100	5.98174500
C	-5.37803900	-0.44673100	6.65947100
H	-5.72953800	-0.37737000	7.69751500
H	-6.03811400	-1.16651600	6.15629700
H	-4.37232700	-0.87276000	6.67090300
C	-6.82449800	1.54562500	6.04423700
H	-7.58448300	0.90045700	5.58248800
H	-7.13819800	1.69942600	7.08594800
H	-6.84472900	2.51289300	5.53348200
C	-1.92657800	-0.11272900	1.52294300
C	-1.82287000	-0.08904700	2.96442600
O	-2.07881400	2.03383600	5.46787400
Si	-1.93463300	2.93058400	6.89516800
C	-3.27815100	4.25745800	7.01075700
H	-4.27061100	3.80832400	7.11988600
H	-3.11219400	4.90742000	7.87859300
H	-3.29570400	4.89321500	6.11806500
C	-2.06982300	1.78438200	8.39465600
H	-1.90754800	2.33796600	9.32753000
H	-3.06750200	1.33369600	8.45618000
H	-1.33671100	0.97053900	8.36028500
C	-0.20551500	3.74422300	6.76713600
C	0.00796500	4.70453600	7.95842600
H	-0.04519600	4.18547500	8.92395100
H	1.00222000	5.16957500	7.89602900
H	-0.72904100	5.51614000	7.97258900
C	0.90444800	2.67227100	6.79107800
H	0.81704900	1.97616300	5.94993000
H	1.89391400	3.14743200	6.72299700
H	0.88996600	2.08468500	7.71750000
C	-0.10150700	4.54280900	5.44950900
H	0.89113100	5.00827900	5.36303200
H	-0.24700600	3.89849900	4.57579600
H	-0.84399900	5.34889600	5.39860000
C	0.68015000	-0.15612300	3.33178700
H	0.67788500	0.87465500	3.70424000
H	1.50205300	-0.69158000	3.82259700
H	0.88094900	-0.14960800	2.26166500
C	-0.74549600	-0.89616500	5.21634500
H	-0.72718100	0.09507900	5.67034300
H	-1.62551700	-1.44761900	5.56554200
H	0.13226300	-1.44123500	5.58008700
C	-0.66187100	-0.84973000	3.67642500
C	-0.67314300	-2.33688000	3.23224300
H	-0.50476700	-2.46572900	2.16616500
H	0.12616200	-2.87177600	3.75900200
H	-1.62480800	-2.80765800	3.50750600

TS-2$_{1g}$

O	-3.74606600	-0.37928200	-0.38048900
C	-2.55721000	-0.62181400	0.25500000
O	-1.65444500	-1.15694300	-0.34974100
C	-4.66580300	0.29380300	0.48522800
H	-4.94906300	1.24909300	0.02742600
H	-5.57001700	-0.31820500	0.59000000
C	-3.93220000	0.46908700	1.78329200
C	-4.42080900	1.12999600	2.93499200
C	-3.43030800	1.07267900	3.78719500
C	-2.13266800	0.57707700	3.86765400
C	-1.75030900	0.88630600	5.31996900
H	-1.60169400	-0.03287500	5.90049500
C	-3.13758600	1.47388600	5.67412000
H	-3.80091600	0.80855900	6.22490400
C	-3.59975400	2.74234300	5.39703400
C	-2.79216200	3.84720900	4.77887500
H	-3.30099900	4.21002900	3.87702200
H	-2.74733000	4.69262100	5.47945500
H	-1.77818900	3.54261200	4.52856400
C	-5.06581400	2.99676000	5.52026500
H	-5.29465000	4.05739200	5.65916700
H	-5.50359100	2.66834300	4.55212800
H	-5.53905100	2.41020200	6.31300600
C	-2.65130000	-0.11113700	1.66036300
C	-1.68868500	-0.13005600	2.72790900
O	-0.65446800	1.76044800	5.50709500
Si	0.17578100	1.97606900	6.97291700
C	-0.99419600	2.68145100	8.28240000
H	-1.80103200	1.97721200	8.51853200

H	-0.45735500	2.88131400	9.21790500
H	-1.45907200	3.61928200	7.95926300
C	0.83342800	0.31471900	7.59138200
H	1.32239200	0.43529100	8.56554600
H	0.02697100	-0.41559900	7.72907000
H	1.56194800	-0.12572300	6.90239700
C	1.59070700	3.19215300	6.55234300
C	2.50504500	3.35743100	7.78700300
H	2.97381800	2.41118800	8.08276700
H	3.31602600	4.06554800	7.56521300
H	1.96287900	3.75035100	8.65627700
C	2.42713000	2.64889100	5.37375500
H	1.82099100	2.53341500	4.46890000
H	3.24818300	3.34183100	5.14040100
H	2.87834300	1.67562500	5.60228800
C	1.01804200	4.57185500	6.16278200
H	1.83441700	5.26726100	5.92047600
H	0.37013400	4.50777300	5.28148800
H	0.43816700	5.02319700	6.97712600
C	0.57614500	-0.16062900	1.60461900
H	0.76595100	0.87903100	1.89769700
H	1.54261100	-0.67764400	1.55429800
H	0.13281000	-0.17664300	0.60871500
C	0.41442100	-0.84829800	3.99269600
H	0.62155900	0.16590900	4.33813700
H	-0.14289700	-1.38004600	4.77282300
H	1.37203200	-1.36678100	3.87072100
C	-0.33145400	-0.86073600	2.64499000
C	-0.54764300	-2.34856000	2.27231200
H	-0.98912900	-2.46569300	1.28385200
H	0.42023200	-2.86482900	2.27320500
H	-1.18909100	-2.84209400	3.01281400

2g

O	-3.86270600	-0.49669100	-0.38840700
C	-2.61025000	-0.56066200	0.17165900
O	-1.66h516100	-0.87646400	-0.51251900
C	-4.83443700	-0.07629000	0.56928400
H	-5.31937500	0.83565400	0.19987900
H	-5.59937600	-0.85740800	0.66205900
C	-4.06327300	0.14099700	1.83869500
C	-4.55816600	0.59097100	3.06027000
C	-3.58287200	0.73729900	4.03003100
C	-2.23051400	0.41957400	3.83780600
C	-1.90126500	0.73845300	5.31548300
H	-1.72030200	-0.17978300	5.89256300
C	-3.43353500	1.18557100	5.47112700
H	-3.96828800	0.55379400	6.19139200
C	-3.73554400	2.63788200	5.76694700
C	-3.30343300	3.67044000	4.75450200
H	-3.51266600	4.68365000	5.11096400
H	-2.23305900	3.58488600	4.54121300
H	-3.82870900	3.52986000	3.80102300
C	-4.40111300	2.97365600	6.87898000
H	-4.63852700	4.00917600	7.11026900
H	-5.60790600	0.82445600	3.21760100
H	-4.73435800	2.22781200	7.59667000
C	-2.71250600	-0.17509800	1.61610100
C	-1.71180200	-0.08863200	2.63458700
O	-0.92325100	1.70585300	5.59954600
Si	-0.04306300	1.81014400	7.04757200
C	-1.20805400	1.88341800	8.53371300
H	-1.77364800	0.94878500	8.63615100
H	-0.64258000	2.02081200	9.46389900
H	-1.93307200	2.69821100	8.44828900
C	1.05505600	0.28203400	7.24299500
H	1.56138800	0.29626800	8.21586200
H	0.46772100	-0.64315000	7.20043500
H	1.82290600	0.21953500	6.46494200
C	1.00072500	3.40267800	6.87025500
C	2.01465700	3.47909500	8.03459000
H	2.72362700	2.64256900	8.02146200
H	2.60302100	4.40509500	7.96379300
H	1.52065800	3.48514400	9.01461900
C	1.77007700	3.39055800	5.53187300
H	1.08810100	3.36276100	4.67531800
H	2.38741600	4.29597300	5.43964100
H	2.44400500	2.52865800	5.45165700
C	0.09492300	4.65190700	6.91599400
H	0.69988900	5.56326200	6.80231300
H	-0.64753300	4.64660700	6.11057200
H	-0.44312300	4.73439100	7.86786000

C	0.44903600	0.41150700	1.41914100
H	0.43150500	1.44964800	1.77175100
H	1.49872100	0.11263800	1.30889200
H	-0.02111400	0.35981800	0.43669400
C	0.53904900	-0.43856600	3.76012000
H	0.56121600	0.57679500	4.15866600
H	0.11892600	-1.10130600	4.52528000
H	1.57145500	-0.76003700	3.58104800
C	-0.24708900	-0.52140900	2.43986500
C	-0.18291500	-1.99527200	1.96820600
H	-0.64579000	-2.13874600	0.99276000
H	0.86711200	-2.30199700	1.89081800
H	-0.66924800	-2.65554400	2.69672100

TS-2$_{1g'}$

O	-2.42208200	-0.90498000	-0.42336000
C	-1.59541200	-1.04105100	0.66134300
O	-0.52094000	-1.58410000	0.52934400
C	-3.62098300	-0.20631900	-0.07388300
H	-3.70331500	0.69000000	-0.70044200
H	-4.48385700	-0.85079700	-0.28190900
C	-3.47909100	0.11490000	1.38519900
C	-4.41175900	0.80410200	2.19464900
C	-3.83831400	0.91493400	3.35807300
C	-2.68352900	0.48480600	4.00199400
C	-2.84290300	1.09290200	5.39893100
H	-2.93855700	0.34607800	6.19664100
C	-4.18402400	1.78441100	5.05926200
H	-4.08054600	2.83878300	4.81186400
C	-5.44542200	1.23878600	5.13238200
C	-5.73305000	-0.14683300	5.63231300
H	-6.52755600	-0.10771800	6.38853100
H	-6.11136600	-0.76720300	4.80848500
H	-4.86425900	-0.64534300	6.06619300
C	-6.56113800	1.93740100	4.43237800
H	-6.47095800	1.64543000	3.36146300
H	-7.54675100	1.62884100	4.79264000
H	-6.47601700	3.02705100	4.47747700
C	-2.25437300	-0.41126500	1.84888300
C	-1.80226900	-0.27951800	3.20836900
O	-1.85362000	2.04704200	5.72735400
Si	-1.62286700	2.76019500	7.24646100
C	-3.21716100	3.59906700	7.83001500
H	-4.04352800	2.88204800	7.90592400
H	-3.08024800	4.03943200	8.82520500
H	-3.53686000	4.40046000	7.15447800
C	-1.15490800	1.42989000	8.50624900
H	-0.98383700	1.87069000	9.49589300
H	-1.95551300	0.68858700	8.61925400
H	-0.24586200	0.89180800	8.21710200
C	-0.22182700	4.02660800	6.95813100
C	0.08701200	4.76787000	8.27744100
H	0.41859400	4.08293500	9.06770200
H	0.89331200	5.49876600	8.12279200
H	-0.78280500	5.31999900	8.65439400
C	1.05380200	3.30673500	6.46994300
H	0.88367200	2.77856300	5.52529600
H	1.86021900	4.03510500	6.30241800
H	1.42206600	2.57789300	7.20229800
C	-0.65824200	5.05033600	5.88769500
H	0.15080600	5.77001900	5.69690100
H	-0.89986300	4.56144600	4.93755300
H	-1.53641000	5.62670100	6.20405000
C	0.72823800	-0.29369700	3.11210100
H	0.76382900	0.77994400	3.33231100
H	1.63520300	-0.75281000	3.52495300
H	0.73900000	-0.43709700	2.03102200
C	-0.39883100	-0.77219100	5.28648300
H	-0.33737800	0.27636400	5.58221600
H	-1.23940100	-1.23937500	5.81402600
H	0.51458200	-1.27366400	5.62540700
C	-0.52025800	-0.93938500	3.75901100
C	-0.55333000	-2.46383400	3.48547200
H	-0.55636200	-2.69167200	2.42070900
H	0.33698300	-2.92809400	3.92711300
H	-1.43404000	-2.92080600	3.95345700

2g'

O	-2.40885000	-1.10921900	-0.43514800
C	-1.55738700	-1.18677600	0.63997000
O	-0.48456000	-1.72986200	0.51671700
C	-3.60156200	-0.40064300	-0.09700200

H	-3.69895500	0.46165300	-0.76796400
H	-4.46252900	-1.06085600	-0.26050500
C	-3.42949300	-0.00838000	1.34206700
C	-4.31173500	0.73290200	2.12628500
C	-3.84000200	0.97384000	3.40395500
C	-2.62241500	0.48241600	3.89196100
C	-2.85924600	1.11592100	5.27625400
H	-3.01214800	0.38589100	6.08151700
C	-4.22877400	1.68965200	4.68842500
H	-4.15100200	2.77830100	4.59697400
C	-5.53489600	1.31944000	5.35110200
C	-5.84112800	-0.14917600	5.52860100
H	-5.08468600	-0.65028100	6.14680600
H	-6.81398700	-0.29607100	6.00650600
H	-5.84968100	-0.67213600	4.56411600
C	-6.39307800	2.26857500	5.74539100
H	-5.26378400	1.09950500	1.75154900
H	-7.34019300	2.02183900	6.21894900
H	-6.18153900	3.32547400	5.60451200
C	-2.20009500	-0.50504900	1.80803600
C	-1.73876800	-0.31316700	3.14794900
O	-1.92989900	2.10214900	5.65452200
Si	-1.75792400	2.80192500	7.18427700
C	-3.34766600	3.69184300	7.68849200
H	-4.20972300	3.01552300	7.65925200
H	-3.27046900	4.08387500	8.70998600
H	-3.56999700	4.53516100	7.02471600
C	-1.38286800	1.45657600	8.46013100
H	-1.23780300	1.89261800	9.45601500
H	-2.21055500	0.74133000	8.54138100
H	-0.47989600	0.89024300	8.20765700
C	-0.30542100	4.02955700	6.97616000
C	-0.06450900	4.77429600	8.30764200
H	0.20275300	4.08849100	9.12129600
H	0.76496900	5.48785800	8.20033300
H	-0.94486000	5.34601800	8.62600700
C	0.98265100	3.27825000	6.57739800
H	0.86499400	2.75086100	5.62420800
H	1.81639100	3.98622100	6.46328500
H	1.28252100	2.54322300	7.33453600
C	-0.64539900	5.05576500	5.87357400
H	0.19145300	5.75516200	5.73218400
H	-0.83637600	4.56489100	4.91300800
H	-1.52885800	5.65450600	6.12744000
C	0.78530200	-0.29758900	3.03188400
H	0.80964000	0.78536000	3.20210500
H	1.70086400	-0.72566700	3.45818500
H	0.79099300	-0.49019300	1.95828900
C	-0.32870700	-0.67186700	5.23529000
H	-0.30338900	0.39364400	5.47091200
H	-1.15452000	-1.13200100	5.79063000
H	0.60075400	-1.12423800	5.59890300
C	-0.44903400	-0.92886300	3.72050000
C	-0.45654900	-2.46577500	3.52684800
H	-0.45234100	-2.75164000	2.47572500
H	0.43951500	-2.89083500	3.99494700
H	-1.33055100	-2.91269500	4.01650900