Supporting Information

For

Diels-Alder Dimerization of Ene-Allenes and Enyne-Allenes Generated via the Propargylic Alder-Ene Reaction of Diynes and Triynes

Kumudi J. W. Rajapaksa, Duy-Viet Vo, Wu Tong Tong, Yanshu Luo, Eunhye Lee,

Yuanzhi Xia* and Daesung Lee*

[1]Department of Chemistry, University of Illinois Chicago, 845 West Taylor Street, Chicago, Illinois 60607, United States.
[2]College of Chemistry and Materials Engineering, Wenzhou University, 325035 Wenzhou, Zhejiang, P. R. China.

*E-mail: dsunglee@uic.edu (D. L.)

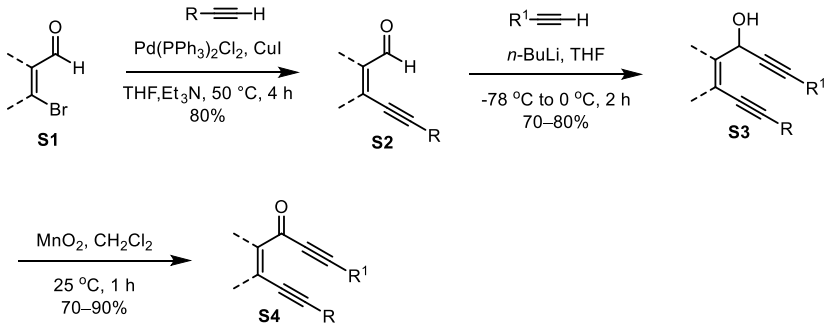
Contents

General Information

All reactions were carried out in oven or flame-dried glassware unless otherwise noted. Reagents which were commercially available, were purchased from Sigma - Aldrich, Alfa Aesar, Acros, and Oakwood Products unless otherwise noted. Known compounds were prepared according to literature procedure. Both toluene and tetrahydrofuran were purchased from Sigma-Aldrich. Piperidine and acetic acid were purchased from Sigma-Aldrich and Fischer Scientific respectively. 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). Yield was calculated on basis of chromatographically and spectroscopically pure isolated compound. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AV-500 spectrometer at 298 K, unless otherwise stated. ^{1}H NMR chemical shifts (δ) were reported in parts per million (ppm) downfield of TMS and were referenced relative to the residual proteated solvent peak ($CDCl_3$ (7.26 ppm)). ^{13}C chemical shifts (δ) were reported in parts per million downfield of TMS and are referenced to the carbon resonance of the solvent ($CDCl_3$, δ 77.2 ppm). Multiplicities in ^{1}H NMR were abbreviated by s (singlet), d (doublet), t (triplet), q (quartet), quin (quintet), sext (sextet), sept (septet) 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) mass spectra were recorded on a Waters Micromass Q-Tof Ultima (Waters Corporation, Milford, MA, USA) at the University of Illinois at Urbana-Champaign.

Experimental Details

Procedure for synthesis of diynone substrates



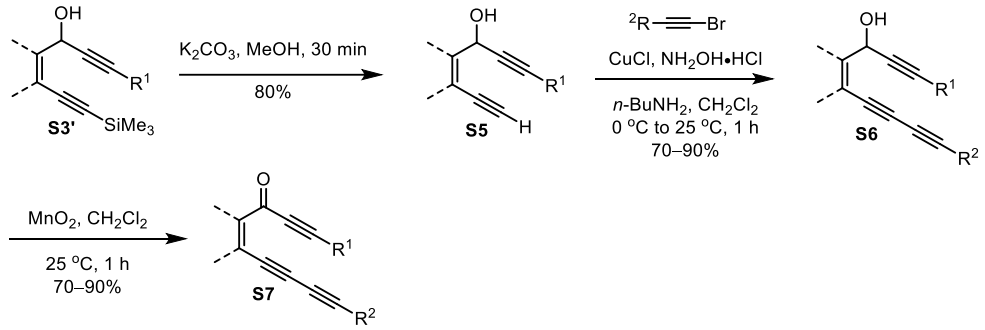
To a stirred solution of **S1** (1.00 g, 5.44 mmol) in THF at 25 °C, $Pd(PPh_3)_2Cl_2$ (0.11 g, 0.16 mmol) and trimethylsilyl acetylene (0.69 g, 7.03 mmol) were added sequentially under N_2 atmosphere. Then CuI (41.4 mg, 0.38 mmol) and Et_3N (1.13 mL, 8.11 mmol) were added, and the reaction mixture was stirred at 50 °C for 4 h. Upon completion of the reaction, the reaction mixture was concentrated under reduced pressure and filtered through silica gel. Purification by flash column chromatography (SiO_2, EtOAc–hexanes, 1:20) provided the enyne **S2** (0.87 g, 80% yield) as white solid.

To a stirred solution of aldehyde **S2** (0.37 g, 2.8 mmol) in THF at –78 °C, *n*-BuLi (2.5 M, 1.25 mL, 1.1 mmol) was added slowly under N_2 atmosphere and the stirring was continued for additional 40 min.

The dry ice bath was removed and the alkynyl substrate (0.130 g, 3.4 mmol) in THF was added. The stirring continued for an additional 1 h at 0 °C. The reaction was quenched by aqueous NH_4Cl and extracted with EtOAc. The combined organic extracts were washed sequentially with water and brine and dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude material was purified by flash column chromatography (SiO_2, EtOAc–hexanes, 2:48 to 3:47) to provide pure product **S4** (0.40–0.50 g, 70–80% yield) as a colorless oil.

To a stirred solution of **S3** (0.25 g, 8.0 mmol) in CH_2Cl_2 at 25 °C**,** MnO_2 (0.69 g, 80.0 mmol) was added, and the mixture was stirred for 1 h. After the completion of the reaction, the reaction mixture was filtered through a celite column. Purification by flash column chromatography (SiO_2, EtOAc–hexanes, 1:49 to 2:48) provided the pure product **S4** (0.17–0.20 g, 70–90% yield) as orange color oil or solid.

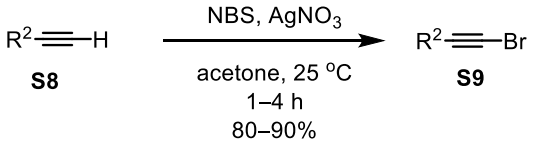
Procedure for synthesis of triynone substrates



To a stirred solution of **S3'** (0.80 g, 3.95 mmol) in methanol at room temperature, K_2CO_3 was added (0.55 g, 3.95 mmol) and kept for 30 mins under N_2 atmosphere. After the reaction was completed, it was quenched by a saturated solution of NH_4Cl and extracted with EtOAc. The combined organic extracts were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude material was purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:49 to 2:48) to provide the pure product **S5** (0.37 g, 80% yield) as a white solid.

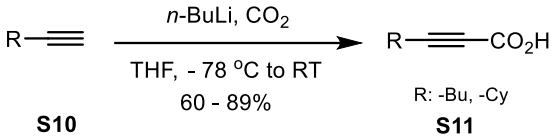
To a mixture of 30% aqueous *n*-$BuNH_2$ (10 mL), CuCl (34 mg,.0.35 mmol) and a pinch of $NH_2OH{\cdot}HCl$ in a two-necked round-bottomed flask, a solution of terminal alkyne **S5** (0.25 g, 1.18 mmol) in CH_2Cl_2 was added slowly at 0 °C under N_2 atmosphere. Then, alkynyl bromide **S9** (0.26 g, 1.41 mmol) diluted in CH_2Cl_2 was added dropwise into the reaction mixture over 30 min. After that, the ice bath was removed and stirring was continued for an additional 25 min at room temperature (TLC monitoring). A pinch of $NH_2OH{\cdot}HCl$ was added several times into the reaction mixture when the solution became blue. The reaction was quenched by a saturated solution of NH_4Cl and extracted with CH_2Cl_2. The combined organic extracts were washed with water and brine sequentially then dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude material was purified by flash column chromatography (SiO_2, EtOAc–hexanes, 2:48 to 3:47) to provide the pure triyne **S6** (0.25–0.33 g, 70–90% yield).

To a stirred solution of **S6** (0.25 g, 8.0 mmol) in CH_2Cl_2 at 25 °C**,** MnO_2 (0.69 g, 80.0 mmol) was added, and the mixture was stirred for 1 h. After the completion of the reaction, the reaction mixture was filtered through a celite column. Purification by flash column chromatography (SiO_2, EtOAc–hexanes, 1:49 to 2:48) provided the pure product **S7** (0.17–0.20 g, 70–90% yield) as orange color oil or solid.

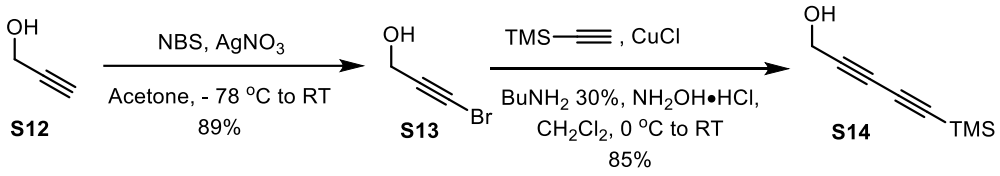


To a stirred solution of alkyne **S8** (1.00 g, 10.0 mmol) in acetone at 25 °C, *N*-bromosuccinimide (2.10 g, 11.7 mmol) and $AgNO_3$ (0.166 g, 1.0 mmol) were sequentially added under N_2 atmosphere in the dark. After addition, the mixture was stirred for 3 h. After completely consuming the alkyne, the reaction mixture was concentrated under reduced pressure and filtered through silica gel. Purification by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10 to 1:6) provided the bromide **S9** (1.4–1.6 g, 80–90% yield) as clear oil.

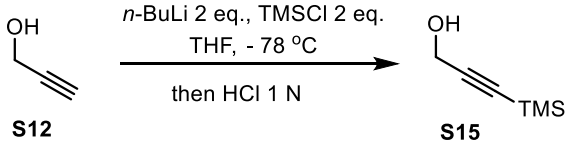
Procedure for synthesis of ester-tethered and amide-tethered alkynyl substrates



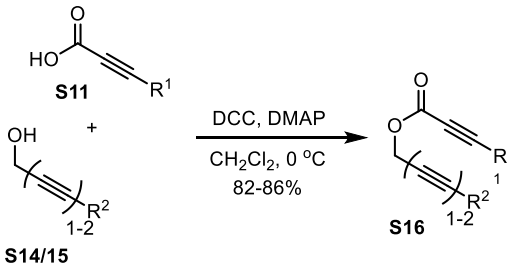
The carboxylic acids **S11** were prepared according to the reported procedure.[2]



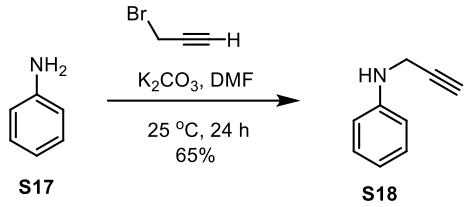
The 1,3-diyne alcohol **S14** was prepared according to the reported procedure.[2]



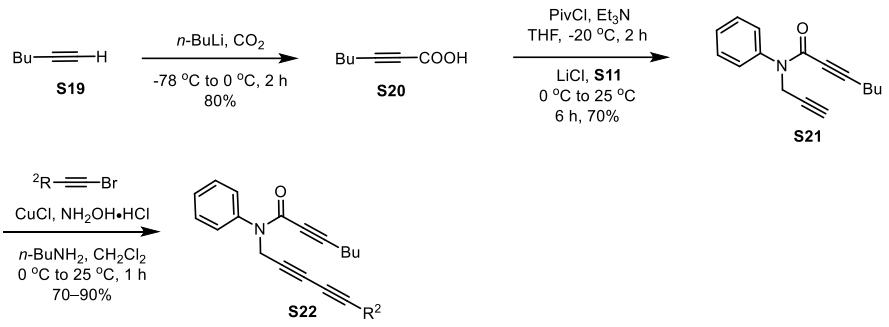
The propragyl alcohol **S15** was prepared according to the reported procedure.[2]



To a solution of alcohol (1.0 mmol, 1 equiv) and carboxylic acid (1.3 mmol, 1.3 equiv) in 5 mL DCM, DCC (1.3 mmol, 1.3 equiv), and DMAP (0.1 mmol, 0.1 equiv) were added sequentially at 0 °C under nitrogen. After completion of the reaction (TLC monitoring approx. 2 h), the precipitate was filtered over a short pad of silica, concentrated the mixture and purified by column chromatography (SiO_2, hexanes–EtOAc, 20:1 to 10:1) to obtain the triyne esters **S16** (82–86% yield) as colorless oils.



To a stirred solution of aniline **S17** (3.1 mL, 33.6 mmol) in DMF at 25 °C, propargyl bromide (2.00 g, 16.8 mmol) and K_2CO_3 (4.64 g, 33.6 mmol) were added under N_2 atmosphere and was stirred for 24 h. After completely consuming propargyl bromide, aqueous workup was done and was extracted with EtOAc. The extract was concentrated under reduced pressure and filtered purification by flash column chromatography (SiO_2, EtOAc–hexanes, 1:49) provided the **S18** (2.60 g, 65% yield) as clear oil.

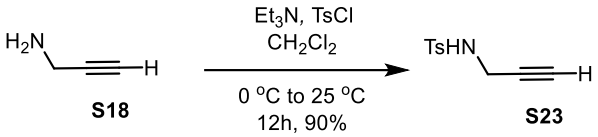


To a stirred solution of **S19** (1.00g, 12.0 mmol) in THF at –78 °C, *n*-BuLi (2.5 M, 5.36 mL, 13.4 mmol) was added slowly under N_2 atmosphere and the stirring was continued for additional 30 min. Then CO_2 was bubbled into the reaction mixture at –78 °C and the dry ice bath was removed. The stirring was continued for an additional 1 h at room temperature. The reaction was quenched by aqueous HCl (1 M) and extracted with EtOAc. The combined organic extracts were washed sequentially with water and brine and dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude material was purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:5) to provide pure product **S20** (1.23 g, 80% yield) as pale-yellow oil.

To a stirred solution of **S20** (0.24 g, 1.92 mmol) in THF at –20 °C under N_2 atmosphere, PivCl (0.28 mL, 2.2 mmol) and Et_3N (0.56 mL, 4.8 mmol) were added, and the mixture was stirred at –20 °C for 2 h. Then LiCl (0.102 g, 2.4 mmol) and the amine **S18** (0.21 g, 1.6 mmol) were added and the dry ice bath was removed and stirring was continued for additional 6 h at room temperature. The reaction was quenched by aqueous NH_4Cl and extracted with EtOAc. The combined organic extracts were washed sequentially with water and brine and dried over anhydrous Na_2SO_4 and concentrated under reduced

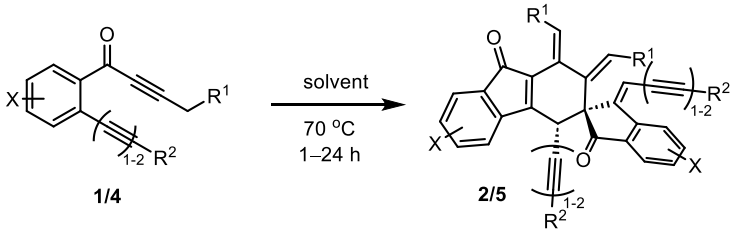
pressure. The crude material was purified by flash column chromatography (SiO_2, EtOAc–hexanes, 2:48 to 3:47) to provide the pure product **S21** (0.23 g, 70% yield) as pale-yellow oil.

To a mixture of 30% aqueous *n*-$BuNH_2$ (10 mL), CuCl (28.5 mg, 0.3 mmol) and a pinch of $NH_2OH{\cdot}HCl$ in a two-necked round-bottomed flask, a solution of amide **S21** (0.23 g, 1.0 mmol) in CH_2Cl_2 was added slowly at 0 °C under N_2 atmosphere. Then, alkynyl bromide (0.21 g, 1.15 mmol) diluted in CH_2Cl_2 was added dropwise into the reaction mixture over 30 min. After that, the ice bath was removed and stirring was continued for an additional 25 min at room temperature (TLC monitoring). A pinch of $NH_2OH{\cdot}HCl$ was added several times into the reaction mixture when the solution became blue. The reaction was quenched by a saturated solution of NH_4Cl and extracted with CH_2Cl_2. The combined organic extracts were washed with water and brine sequentially and dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude material was purified by flash column chromatography (SiO_2, EtOAc–hexanes, 2:48 to 3:47) to provide the pure triyne **S22** (0.20–0.32 g, 70–90% yield) as pale yellow oil.



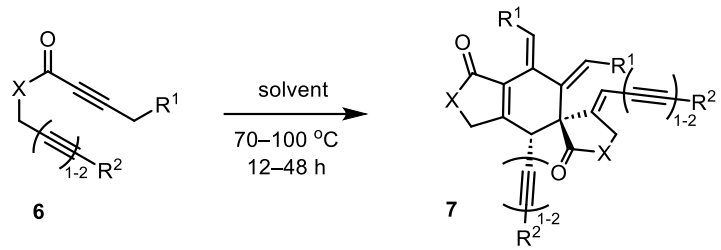
To a stirred solution of **S18** propagyl amine (1.00 g, 18.1 mmol) in CH_2Cl_2 at 0 °C under N_2 atmosphere, Et_3N (2.95 mL, 21.1 mmol) and tosyl chloride (2.88 g, 15.1 mmol) were added, and the mixture was stirred at 25 °C for 12 h. After completion, water was added to the reaction and extracted with CH_2Cl_2. The combined organic extracts were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude material was purified by flash column chromatography (SiO_2, EtOAc–hexanes, 2:48 to 3:47) to provide the pure product **S23** (3.2 g, 90% yield) as a white solid.

General Procedure for synthesis of homodimerized products



A reaction vial was charged with **1a-l**, (25 mg, 0.1 mmol) in toluene. Then, the reaction mixture was stirred at 70 °C for 12–24 h. Upon full conversion of the substrate to the dimer, the crude material was purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10 to 1:9) to provide pure products **2a-l** (6–21 mg, 18–83% yield) as orange solid or oil.

A reaction vial was charged with **4a-i**, (35 mg, 0.1 mmol) in chloroform. Then, the reaction mixture was stirred at 70 °C for 1–3 h. Upon full conversion of the substrate to the dimer, the crude material was purified by flash column chromatography (SiO_2 or basic Al_2O_3, EtOAc–hexanes, 1:10 to 1:9) to provide pure products **5a-i** (8–30 mg, 21–83% yield) as orange oil.



A reaction vial was charged with **6a**—**6e, 6g**, (25 mg, 0.1 mmol) in toluene. Then, the reaction mixture was stirred at 100 °C for 12–24 h. Upon full conversion of the substrate to the dimer, the crude material was purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10 to 1:8) to provide pure products **7a**—**7e, 7g** (9–11 mg, 14–45% yield) as whie solid or colorless oil.

A reaction vial was charged with **6f**, **6h**—**6l**, (33.5 mg, 0.1 mmol) in chloroform. Then, the reaction mixture was stirred at 70 °C for 12–24 h. Upon full conversion of the substrate to the dimer, the crude material was purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10 to 1:8) to provide pure products **7f**, **7h**—**7l** (18–28 mg, 32–79% yield) as colorless oil.

References:

1. K. J. W. Rajapaksa, , H. Y. Wong and D. Lee, *Chem. Eur. J.,* 2024*,* **30***,* e202403270

2. D.-V. Vo, S. Su, R. Karmakar and D. Lee, *Org. Lett.,* 2024, **26**, 1299–1303.

3. V. Bilinski, M. Karpf, and A. S. Dreiding, *Helv. Chim. Acta.,* 1986, **69**, 1734-1741.

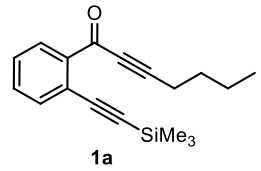
4. F. Bodinier, Y. Sanogo, I. Ardisson, M.-I. Lannou, and G. Sorin, *Chem. Commun.,* 2021, **57**, 3603–3606.

5. H. Hofmeister, K. Annen, H. Laurent and H. Wiechert, *Angew. Chem., Int. Ed*., 1984, **23**, 727.

6. (a) W. Chodkiewicz, *Ann. Chim*., 1957, **2**, 819. (b) P. Cadiot and W. Chodkiewicz, In *Chemistry of Acetylenes,* ed. H. G. Viehe, Marcel Dekker, New York, 1969, pp. 597.

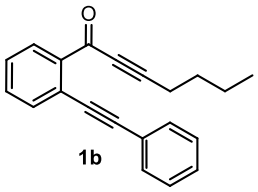
Characterization Data of Substrates

A. Diynones



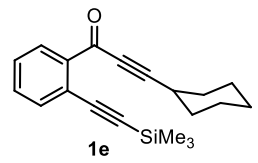
1a

36.7 mg (88% yield), pale yellow oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.98 (d, 1H, *J* = 7.9 Hz), 7.59 (d, 1H, *J* = 7.9 Hz), 7.49 (t, 1H, *J* = 7.6 Hz), 7.41 (t, 1H, *J* = 7.6 Hz), 2.19 (s, 1H), 1.58 (s, 6H), 0.29 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 176.3, 138.0, 135.1, 132.7, 131.2, 128.3, 122.9, 102.5, 102.4, 92.3, 77.4, 75.8, 66.1, 65.7, 30.8, -0.2; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{19}H_{21}O_2Si$ 309.1311; found 309.1309.



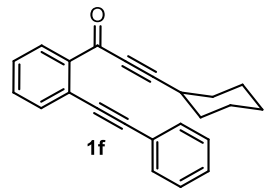
1b

40.8 mg (85% yield), pale yellow oil, purified by flash column chromatography (SiO2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.01 (d, *J* = 7.8 Hz, 1H), 7.46 (d, *J* = 7.7 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 2.43 (t, *J* = 7.2 Hz, 4H), 1.59 (m, *J* = 7.0 Hz, 4H), 1.47 (m, *J* = 22.1, 7.3 Hz, 4H), 0.91 (t, *J* = 7.3 Hz, 6H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 177.39, 164.12, 138.78, 135.02, 132.07, 131.64, 128.08, 122.41, 103.24, 100.75, 96.74, 80.56, 29.79, 22.08, 18.97, 13.53; **HRMS** (ESI) m/z: [M + H]+ calcd for $C_{21}H_{19}O$ 287.1436; found 287.1433.



1e

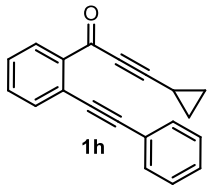
37 mg (88% yield), yellow oil, purified by flash column chromatography (SiO,EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.06 (d, *J* = 7.7 Hz, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.41 – 7.35 (m, 1H), 2.63 (dq, *J* = 9.2, 4.5 Hz, 1H), 1.92 – 1.83 (m, 2H), 1.77 – 1.67 (m, 2H), 1.62 – 1.48 (m, 3H), 1.40 – 1.29 (m, 3H), 0.26 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 177.40, 138.83, 135.06, 132.04, 131.78, 128.05, 122.40, 103.34, 100.64, 100.06, 80.40, 31.64, 29.41, 25.64, 24.72.; **HRMS** (ESI) calcd for $C_{20}H_{25}OSi$ $[M + H]^+$ 309.1675, found 309.1669.



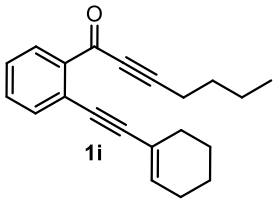
1f

39.9 mg (80% yield), yellow oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.12 (d, *J* = 9.2 Hz, 1H), 7.62 (t, *J* = 6.1 Hz, 3H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.34 (dd, *J* = 5.1, 2.2 Hz, 3H), 2.67 – 2.58 (m, 1H), 1.92 – 1.82 (m, 2H), 1.78 – 1.67 (m, 3H), 1.62 – 1.49 (m, 3H), 1.38 – 1.25 (m, 4H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 177.77, 138.50, 134.23, 132.24, 131.95, 131.84, 128.60, 128.32,

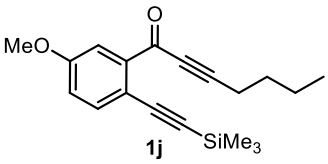
127.86, 123.37, 122.80, 100.44, 95.03, 88.45, 80.64, 31.64, 29.47, 25.64, 24.74; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{23}H_{21}O$ 313.1592; found 313.1594.



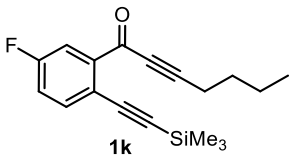
32.8 mg (85% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.04 (d, *J* = 7.8 Hz, 1H), 7.61 (dd, *J* = 7.2, 2.6 Hz, 3H), 7.50 – 7.45 (m, 1H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.33 (dd, *J* = 5.6, 1.7 Hz, 3H), 1.46 – 1.40 (m, 1H), 0.96 – 0.90 (m, 5H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 177.47, 138.55, 134.17, 132.22, 131.91, 131.44, 128.65, 128.36, 127.94, 123.30, 122.72, 101.57, 95.16, 88.37, 76.83, 9.96; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{20}H_{15}O$ 271.1123; found 271.1127.



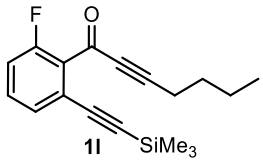
33.9 mg (88% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.06 (d, *J* = 7.9 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 6.33 – 6.27 (m, 1H), 2.46 (t, *J* = 7.2 Hz, 2H), 2.29 (d, *J* = 6.4 Hz, 2H), 2.16 (d, *J* = 6.2 Hz, 2H), 1.72 – 1.58 (m, 7H), 1.48 (p, *J* = 7.3 Hz, 2H), 0.94 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 177.72, 138.12, 136.38, 134.09, 132.11, 131.72, 127.25, 123.40, 121.09, 97.18, 96.68, 85.84, 80.74, 29.84, 28.92, 25.90, 22.32, 22.11, 21.54, 19.03, 13.55; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{21}H_{23}O$ 291.1749; found 291.1747.



17.3 mg (85% yield), pale yellow oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.54 (d, *J* = 2.8 Hz, 1H), 7.50 (d, *J* = 8.5 Hz, 1H), 6.99 (dd, *J* = 8.6, 2.7 Hz, 1H), 3.86 (s, 3H), 2.46 (t, *J* = 7.2 Hz, 2H), 1.63 (p, *J* = 7.2 Hz, 2H), 1.48 (h, *J* = 7.3 Hz, 2H), 0.94 (t, *J* = 7.4 Hz, 3H), 0.26 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 177.38, 159.14, 140.26, 136.45, 118.01, 116.44, 114.68, 103.16, 98.73, 97.04, 80.61, 55.54, 29.78, 22.10, 19.03, 13.53,-0.04; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{19}H_{25}O_2Si$ 313.1624; found 313.1624.



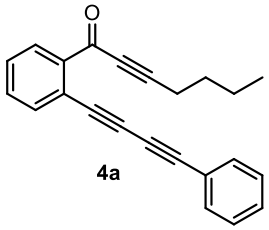
43.8 mg (83% yield), pale yellow oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.71 (dd, *J* = 9.0, 2.8 Hz, 1H), 7.59 – 7.52 (m, 1H), 7.16 (td, *J* = 8.2, 2.8 Hz, 1H), 2.46 (t, *J* = 7.2 Hz, 2H), 1.67 – 1.58 (m, 2H), 1.46 (h, *J* = 7.4 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H), 0.25 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 176.02, 162.61, 160.61, 140.71, 136.94, 119.52, 118.19, 102.07, 100.54, 97.64, 80.20, 29.71, 22.09, 18.99, 13.50; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{18}H_{22}OSiF$ 301.1424; found 301.1423.



1l

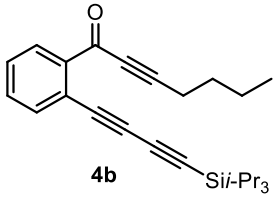
42.3 mg (80% yield), pale yellow oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.37 – 7.27 (m, 2H), 7.07 (t, *J* = 8.8 Hz, 1H), 2.43 (t, *J* = 6.3 Hz, 2H), 1.63 – 1.55 (m, 2H), 1.50 – 1.40 (m, 2H), 0.95 – 0.89 (m, 3H), 0.24 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 175.51, 160.51, 158.50, 131.61, 131.54, 129.30, 129.28, 122.96, 116.59, 116.41, 101.32, 100.74, 98.18, 81.93, 29.62, 22.01, 19.11, 13.50,-0.31; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{18}H_{22}OSiF$ 301.1424; found 301.1421.

B. Triynones



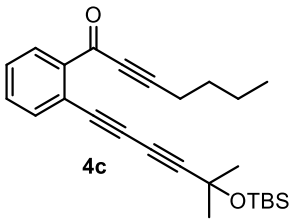
4a

36 mg (83% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.11 (d, *J* = 7.8 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.56–7.48 (m, 3H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.35 (dd, *J* = 12.1, 7.2 Hz, 3H), 2.51 (t, *J* = 7.2 Hz, 2H), 1.66 (p, *J* = 7.2 Hz, 2H), 1.48 (h, *J* = 7.3 Hz, 2H), 0.94 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 176.86, 139.33, 135.59, 132.53, 132.38, 131.71, 129.35, 128.71, 128.48, 121.78, 121.61, 98.04, 83.52, 80.53, 79.89, 79.67, 74.34, 29.78, 22.14, 19.11, 13.56; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{23}H_{19}O$ 311.1436; found 311.1440.



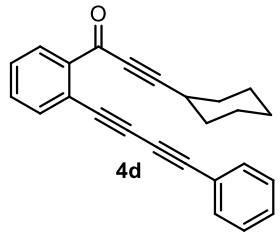
4b

30 mg (85% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.07 (d, *J* = 7.7 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.46 (dt, *J* = 24.9, 6.8 Hz, 2H), 2.54–2.48 (m, 2H), 1.69–1.59 (m, 2H), 1.48 (q, *J* = 7.5 Hz, 2H), 1.10 (s, 21H), 0.94 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 176.86, 139.58, 135.91, 132.29, 131.42, 128.69, 121.52, 98.26, 90.17, 89.75, 80.55, 80.50, 73.59, 29.74, 22.09, 19.10, 18.58, 13.53; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{26}H_{35}OSi$ 391.2457; found 391.2449.

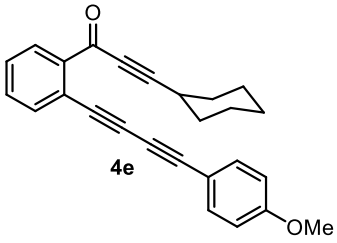


4c

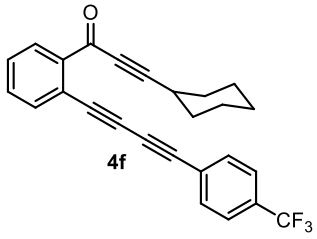
30 mg (85% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.07 (d, *J* = 7.7 Hz, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.50–7.45 (m, 1H), 7.45–7.40 (m, 1H), 2.51 – 2.44 (m, 2H), 1.62 (t, *J* = 7.4 Hz, 2H), 1.50 (s, 9H), 0.96–0.90 (m, 3H), 0.86 (s, 10H), 0.19 (s, 6H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 176.79, 139.36, 135.67, 132.29, 131.63, 128.62, 121.54, 97.78, 89.50, 80.46, 79.17, 76.58, 68.02, 66.87, 32.60, 29.75, 25.68, 22.09, 19.03, 17.91, 13.53, -3.01; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{26}H_{35}O_2Si$ 407.2406; found 407.2387.



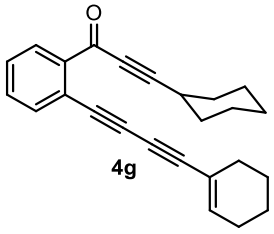
38 mg (85% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.10 (d, *J* = 7.7 Hz, 1H), 7.64 (d, *J* = 6.1 Hz, 1H), 7.55–7.43 (m, 4H), 7.35 (dd, *J* = 12.0, 7.1 Hz, 3H), 2.74–2.65 (m, 1H), 1.98–1.88 (m, 2H), 1.81–1.69 (m, 2H), 1.69–1.48 (m, 4H), 1.36 (d, J = 9.1 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 177.10, 139.57, 135.55, 132.52, 132.33, 131.62, 129.36, 128.73,128.50, 121.78, 121.55, 101.47, 83.53, 80.48, 79.90, 79.71, 74.41, 31.63, 29.57, 25.66, 24.80; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{25}H_{21}O$ 337.1592; found 337.1584.



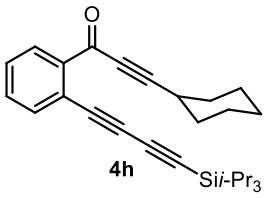
46 mg (83% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.08 (d, *J* = 7.9 Hz, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.55–7.40 (m, 4H), 6.85 (d, *J* = 9.0 Hz, 2H), 3.81 (s, 3H), 2.69 (m, 1H), 1.94 (m, 2H), 1.81–1.70 (m, 2H), 1.63 (m, 2H), 1.53 (s, 1H), 1.35 (m, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 177.13, 160.49, 139.48, 135.45, 134.17, 132.28, 131.55, 128.51, 121.81, 114.22, 113.68, 101.41, 83.90, 80.51, 80.14, 79.41, 73.30, 55.37, 31.63, 29.57, 25.66, 24.81; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{26}H_{23}O_2$ 367.1698; found 367.1689.



44 mg (80% yield), orange solid, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.12 (d, *J* = 7.8 Hz, 1H), 7.60 (dq, *J* = 15.6, 8.0 Hz, 5H), 7.48 (dq, *J* = 15.3, 7.5 Hz, 2H), 2.68 (t, *J* = 9.3 Hz, 1H), 1.91 (dd, *J* = 11.5, 5.8 Hz, 2H), 1.74 (q, *J* = 7.6 Hz, 2H), 1.68–1.47 (m, 4H), 1.35 (t, *J* = 8.4 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 176.85, 139.60, 135.62, 132.71, 132.38, 131.85, 130.62, 129.04, 125.71, 125.40, 125.36, 121.02, 101.38, 81.56, 81.23, 80.31, 78.89, 76.66, 31.61, 29.52, 25.63, 24.75; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{26}H_{20}OF_3$ 405.1466; found 405.1460.

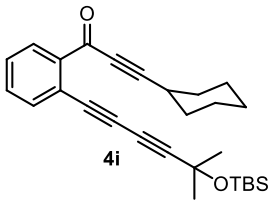


45 mg (70% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.05 (d, *J* = 7.8 Hz, 1H), 7.59 (d, *J* = 7.7 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 6.31 (s, 1H), 2.68 (t, *J* = 11.3 Hz, 1H), 2.14 (q, *J* = 6.0 Hz, 5H), 1.99 – 1.88 (m, 2H), 1.78 (s, 2H), 1.62 (dt, *J* = 23.8, 6.1 Hz, 8H), 1.36 (t, *J* = 10.0 Hz, 4H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 177.20, 139.48, 139.18, 135.40, 132.19, 131.38, 128.37, 121.99, 119.89, 101.41, 85.80, 80.54, 80.26, 78.80, 71.91, 31.61, 29.57, 28.58, 25.98, 25.66, 24.82, 22.11, 21.30; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{25}H_{25}O$ 341.1905; found 341.1894.



4h

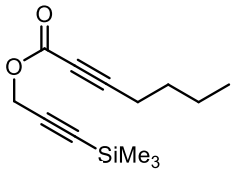
45 mg (80% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.04 (d, *J* = 7.5 Hz, 1H), 7.64 (d, *J* = 9.2 Hz, 1H), 7.52 – 7.40 (m, 2H), 2.74 – 2.64 (m, 1H), 1.92 (d, *J* = 17.8 Hz, 2H), 1.76 (t, *J* = 10.7 Hz, 2H), 1.56 (s, 4H), 1.37 (d, *J* = 10.7 Hz, 3H), 1.11 (s, 21H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 177.19, 139.90, 135.87, 132.20, 131.34, 128.71,121.38, 101.60, 90.12, 89.76, 80.55, 80.47, 73.57, 31.60, 29.53, 25.64, 24.77, 18.59, 11.33; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{28}H_{37}OSi$ 417.2614; found 417.2604.



4i

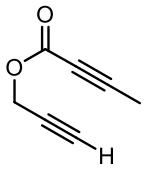
20 mg (85% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.06 (d, *J* = 9.4 Hz, 1H), 7.61 (d, *J* = 7.7 Hz, 1H), 7.51 – 7.41 (m, 2H), 2.72 – 2.64 (m, 1H), 1.97 – 1.88 (m, 2H), 1.81 – 1.72 (m, 2H), 1.67 – 1.54 (m, 4H), 1.51 (s, 6H), 1.35 (d, *J* = 8.2 Hz, 4H), 0.88 (s, 9H), 0.21 (s, 6H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 177.13, 139.66, 135.66, 132.19, 131.51, 128.59, 121.53, 101.28, 89.55, 80.42, 79.26, 76.53, 68.03, 66.88, 32.63, 31.61, 29.52, 25.70, 24.78, 17.93, -3.00; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{28}H_{37}O_2Si$ 433.2563; found 433.2552.

C. Non-aromatic tethered alkynones



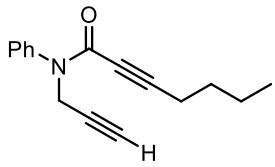
6a

203 mg (86%), colorless oil purified by flash column chromatography (SiO_2, hexanes–EtOAc, 20:1 to 10:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 4.72 (s, 2H), 2.32 (t, *J* = 7.1 Hz, 2H), 1.54 (p, *J* = 7.6 Hz, 2H), 1.42 (h, *J* = 7.1 Hz, 2H), 0.90 (t, *J* = 7.1 Hz, 3H), 0.17 (s, 9H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.9, 98.0, 92.8, 90.9, 72.5, 53.7, 29.4, 21.9, 18.4, 13.4, -0.4. **HRMS** (ESI) m/z: $[M+H]^+$ calcd for $C_{13}H_{21}O_2Si$ 237.1311; Found 237.1306.



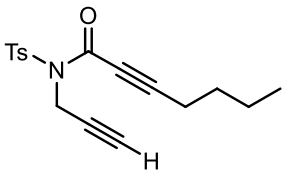
6b

100 mg (83% yield), colorless oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:20). **^{1}H NMR** ($CDCl_3$, 500 MHz): the characterization data of this substrate is consistent with the reported data.[3]



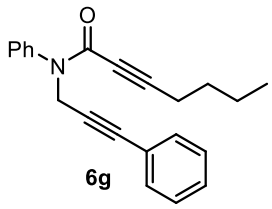
6c

33.1 mg (80% yield), colorless oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.43 – 7.32 (m, 5H), 4.50 (s, 2H), 2.19 (s, 1H), 2.07 (t, *J* = 6.9 Hz, 2H), 1.18 (q, *J* = 7.1 Hz, 2H), 1.08 – 0.99 (m, 3H), 0.72 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 153.96, 141.25, 129.82, 129.07, 128.40, 128.36, 95.08, 78.37, 74.54, 72.40, 37.71, 29.30, 21.42, 18.39, 13.40; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{16}H_{18}NO$ 240.1388; found 240.1393.



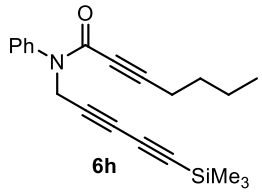
6d

46.2 mg (82% yield), colorless oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:6). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 8.3 Hz, 2H), 4.75 (s, 2H), 2.38 (s, 3H), 2.31 (t, *J* = 7.1 Hz, 2H), 1.49 (p, *J* = 7.2 Hz, 2H), 1.36 (h, *J* = 7.3 Hz, 2H), 0.85 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 151.84, 145.28, 135.47, 129.38, 128.80, 98.05, 78.07, 73.66, 72.95, 36.28, 29.22, 21.89, 21.63, 18.72, 13.42; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{17}H_{20}NO_3S$ 318.1164; found 318.1158.



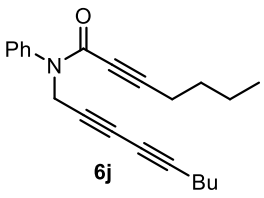
6g

36 mg (80% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.41 (q, *J* = 6.5 Hz, 6H), 7.34 (d, *J* = 9.3 Hz, 2H), 7.27 (d, *J* = 6.1 Hz, 3H), 4.74 (s, 2H), 2.09 (t, *J* = 6.8 Hz, 2H), 1.20 (p, *J* = 7.8 Hz, 2H), 1.05 (p, *J* = 7.5 Hz, 2H), 0.74 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 153.98, 141.33, 131.71, 129.04, 128.66, 128.34, 128.22, 126.63, 122.70, 95.01, 84.33, 83.84, 74.68, 38.47, 29.34, 21.44, 18.42, 13.42; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{22}H_{22}NO$ 316.1701; found 316.1701.



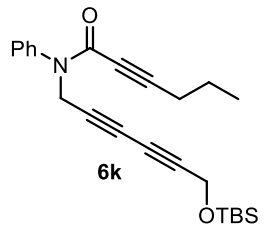
6h

49.5 mg (90% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.40 (q, *J* = 8.3 Hz, 4H), 7.36 – 7.29 (m, 3H), 4.57 (s, 2H), 2.07 (t, *J* = 6.6 Hz, 2H), 1.18 (q, *J* = 7.6 Hz, 2H), 1.05 (d, *J* = 7.4 Hz, 2H), 0.73 (t, *J* = 7.0 Hz, 3H), 0.17 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 153.87, 141.14, 129.20, 128.44, 128.31, 95.31, 87.52, 86.31, 74.40, 72.70, 71.82, 38.43, 29.29, 21.43, 18.39, 13.40, 0.47; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{21}H_{26}NOSi$ 336.1784; found 336.1778.



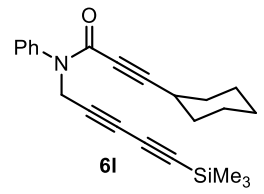
6j

21 mg (79% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.49 – 7.28 (m, 6H), 4.54 (s, 2H), 2.23 (t, *J* = 7.1 Hz, 2H), 2.06 (t, *J* = 6.9 Hz, 2H), 1.47 (p, *J* = 6.9 Hz, 3H), 1.38 (p, *J* = 7.2 Hz, 2H), 1.18 (p, *J* = 7.0 Hz, 2H), 1.03 (p, *J* = 7.3 Hz, 2H), 0.88 (t, *J* = 7.3 Hz, 3H), 0.72 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 153.84, 141.21, 129.12, 128.36, 95.10, 80.38, 74.50, 70.28, 69.21, 64.67, 38.44, 30.14, 29.30, 21.89, 21.42, 18.89, 18.38, 13.50, 13.39; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{22}H_{26}NO$ 320.2014; found 320.2015.



6k

36 mg (80% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.40 (q, *J* = 6.1 Hz, 3H), 7.32 (d, *J* = 6.8 Hz, 2H), 4.58 (s, 2H), 4.34 (s, 3H), 2.07 (t, *J* = 6.9 Hz, 2H), 1.19 (p, *J* = 7.0 Hz, 2H), 1.07 – 1.00 (m, 3H), 0.89 (s, 12H), 0.73 (t, *J* = 7.4 Hz, 3H), 0.10 (s, 6H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 153.89, 141.06, 129.17, 128.46, 128.42, 95.32, 76.97, 74.43, 73.81, 69.14, 68.50, 52.05, 38.38, 29.29, 25.77, 21.42, 18.40, 13.40, -5.19; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{25}H_{34}NO_2Si$ 408.2359; found 408.2353.

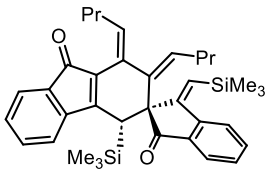


6l

56.4 mg (80% yield), colorless oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.45 – 7.31 (m, 6H), 4.57 (s, 2H), 2.31 (s, 1H), 1.46 (d, *J* = 11.0 Hz, 2H), 1.38 – 1.27 (m, 4H), 1.23 – 1.09 (m, 6H), 0.17 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 154.01, 141.28, 129.20, 128.45, 128.39, 98.66, 87.54, 86.28, 74.51, 72.76, 68.98, 38.40, 30.99, 29.34, 28.60, 25.56, 23.97,0.46; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{23}H_{28}NOSi$ 362.1940; found 362.1938.

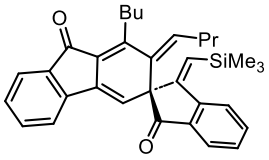
Characterization Data of Products

A. Products from Diynones



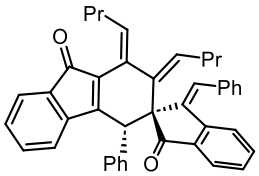
2a

25 mg (68% yield), orange solid, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.80 (dd, *J* = 12.0, 7.8 Hz, 2H), 7.70 (t, *J* = 7.5 Hz, 1H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.37 (dd, *J* = 22.9, 5.6 Hz, 2H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.12 (t, *J* = 7.3 Hz, 1H), 6.69 (d, *J* = 7.2 Hz, 1H), 6.17 (s, 1H), 5.90 – 5.81 (m, 2H), 2.58 – 2.45 (m, 1H), 2.27 (s, 1H), 2.19 (dt, *J* = 13.9, 6.9 Hz, 1H), 1.68 – 1.46 (m, 3H), 1.41 – 1.28 (m, 2H), 1.18 (p, *J* = 7.4 Hz, 2H), 1.02 (t, *J* = 7.4 Hz, 3H), 0.66 (t, *J* = 7.3 Hz, 3H), 0.28 (s, 9H), -0.01 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 202.46, 192.80, 162.28, 155.89, 147.27, 143.88, 139.55, 134.98, 134.22, 133.33, 132.50, 132.40, 130.94, 129.74, 129.42, 128.74, 127.88, 127.24, 125.03, 124.83, 121.86, 119.18, 63.97, 37.08, 32.97, 23.28, 21.89, 14.29, 13.89, 1.16; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{36}H_{45}O_2Si_2$ 565.2958; found 565.2961.



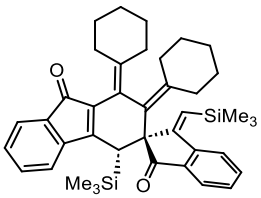
2a'

17 mg (44% yield), yellow oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.96 (d, *J* = 7.7 Hz, 1H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.84 – 7.76 (m, 2H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.50 (d, *J* = 5.9 Hz, 2H), 7.41 – 7.36 (m, 1H), 6.61 (t, *J* = 7.7 Hz, 1H), 5.81 (s, 1H), 5.69 (s, 1H), 3.64 (m, 1H), 3.05 (m, 1H), 1.77 – 1.68 (m, 1H), 1.67 – 1.48 (m, 6H), 1.40 – 1.23 (m, 3H), 0.99 (t, *J* = 7.2 Hz, 3H), 0.70 (t, *J* = 7.4 Hz, 3H), 0.25 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 201.26, 191.46, 158.22, 148.52, 146.86, 142.72, 141.89, 138.58, 135.86, 135.55, 134.95, 133.65, 130.40, 130.15, 128.79, 128.71, 125.24, 125.07, 123.55, 121.07, 116.91, 65.60, 33.31, 32.26, 25.82, 23.01, 22.24, 14.13, 13.79, -0.29; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{33}H_{37}O_2Si$ 493.2563; found 493.2551.



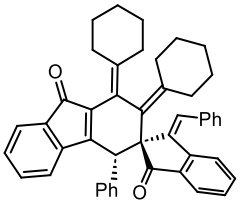
2b

17 mg (47% yield, dr = 3:1), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.83 (d, *J* = 7.4 Hz, 1H), 7.38 (t, *J* = 7.3 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.20 (t, *J* = 7.4 Hz, 4H), 7.12 (d, *J* = 6.1 Hz, 3H), 7.10 – 7.01 (m, 3H), 6.78 (d, *J* = 5.3 Hz, 2H), 6.60 (d, *J* = 5.0 Hz, 1H), 6.19 (s, 1H), 5.97 (t, *J* = 7.6 Hz, 1H), 5.91 (t, *J* = 7.3 Hz, 1H), 4.00 (s, 1H), 2.60 (m, 1H), 2.43 (m, 1H), 1.69 (m, 3H), 1.58 (m, 2H), 1.27 (m, 4H), 1.05 (t, *J* = 7.5 Hz, 3H), 0.71 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 203.88, 194.01, 158.24, 146.58, 143.28, 140.17, 138.40, 137.90, 137.38, 134.45, 133.14, 132.30, 131.89, 130.54, 130.08, 129.71, 129.11, 128.83, 128.53, 128.39, 127.76, 127.41, 125.15, 124.65, 122.50, 119.42, 62.91, 48.27, 32.84, 32.06, 23.34, 22.27, 14.21, 13.82; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{42}H_{37}O_2$ 573.2794; found 573.2797.



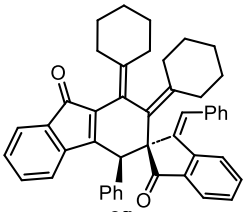
2e

27.5 mg (74% yield), orange solid, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.84 (d, *J* = 7.5 Hz, 1H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.31 (d, *J* = 7.0 Hz, 1H), 7.16 (t, *J* = 8.1 Hz, 1H), 7.08 (t, *J* = 7.4 Hz, 1H), 6.66 (d, *J* = 7.2 Hz, 1H), 6.19 (s, 1H), 2.59 – 2.51 (m, 1H), 2.47 (dd, *J* = 12.6, 7.4 Hz, 1H), 2.27 (s, 1H), 2.23 (q, *J* = 7.2 Hz, 2H), 2.20 – 2.10 (m, 2H), 1.75 (s, 1H), 1.73 – 1.64 (m, 5H), 1.59 (d, *J* = 13.5 Hz, 2H), 1.51 (t, *J* = 6.1 Hz, 2H), 1.46 – 1.33 (m, 5H), 1.33 – 1.24 (m, 2H), 1.11 – 1.01 (m, 1H), 0.27 (s, 9H), -0.05 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 201.80, 193.34, 162.44, 158.23, 146.62, 144.23, 138.06, 137.87, 135.46, 135.26, 134.00, 132.48, 129.61, 128.30, 127.40, 125.06, 124.98, 123.61, 121.77, 118.72, 66.37, 37.74, 34.32, 33.92, 32.92, 31.54, 27.39, 26.95, 26.52, 26.43, 26.33, 26.28, 0.92, -0.14; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{40}H_{49}O_2Si_2$ 617.3271; found 617.3265.



2f

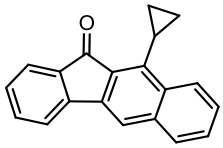
8 mg (27% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.91 (d, *J* = 7.3 Hz, 1H), 7.40 (h, *J* = 7.6 Hz, 3H), 7.30 – 7.18 (m, 6H), 7.12 (t, *J* = 6.9 Hz, 2H), 7.05 (d, *J* = 7.7 Hz, 1H), 6.99 (d, *J* = 7.6 Hz, 1H), 6.74 (d, *J* = 4.5 Hz, 2H), 6.67 (d, *J* = 6.4 Hz, 1H), 6.05 (s, 1H), 3.87 (s, 1H), 2.59 (d, *J* = 13.8 Hz, 1H), 2.50 (t, *J* = 9.7 Hz, 1H), 2.41 (d, *J* = 14.2 Hz, 1H), 2.33 (d, *J* = 11.3 Hz, 1H), 2.12 (d, *J* = 9.5 Hz, 2H), 1.89 (s, 1H), 1.69 (d, *J* = 14.8 Hz, 5H), 1.49 (s, 2H), 1.44 – 1.30 (m, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 202.95, 194.66, 158.89, 145.87, 143.62, 141.83, 139.55, 138.85, 137.99, 137.69, 137.59, 135.44, 134.24, 133.14, 131.85, 129.62, 129.55, 129.07, 128.56, 128.48, 128.15, 128.09, 127.78, 127.64, 127.31, 125.25, 125.15, 123.09, 122.57, 118.30, 65.39, 48.19, 34.04, 33.48, 33.04, 31.83, 27.34, 27.03, 26.47, 26.41, 26.36, 26.28; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{46}H_{41}O_2$ 625.3107; found 625.3107.



2f'

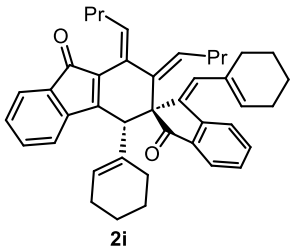
Tentative structure

7 mg (24% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.40 (d, J = 8.2 Hz, 1H), 7.36 (t, J = 6.4 Hz, 3H), 7.31 (d, J = 7.2 Hz, 1H), 7.24 (d, J = 7.1 Hz, 5H), 7.10 (d, J = 14.9 Hz, 2H), 7.04 (q, J = 6.9 Hz, 2H), 6.94 (d, J = 7.6 Hz, 2H), 6.89 (t, J = 7.9 Hz, 2H), 6.53 (d, J = 7.4 Hz, 1H), 4.35 (s, 1H), 2.66 (d, J = 14.2 Hz, 1H), 2.52 (d, J = 13.8 Hz, 1H), 2.32 (d, J = 13.9 Hz, 1H), 2.20 (t, J = 12.4 Hz, 1H), 2.12 – 1.97 (m, 2H), 1.93 – 1.62 (m, 9H), 1.53 – 1.39 (m, 3H), 1.39 – 1.21 (m, 5H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 205.08, 193.84, 160.24, 147.99, 143.50, 143.12, 141.90, 139.99, 138.54, 137.48, 137.16, 133.72, 132.95, 132.25, 132.05, 130.54, 128.70, 128.61, 128.21, 128.07, 127.69, 127.26, 124.46, 123.17, 122.80, 122.62, 122.02, 66.83, 55.66, 33.70, 33.66, 31.73, 28.94, 27.69, 27.53, 27.28, 26.65, 26.44; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{46}H_{41}O_2$ 625.3107; found 625.3102.



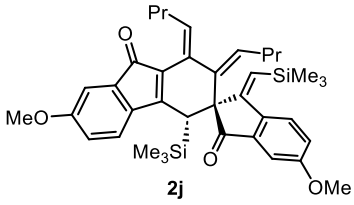
3h

21 mg (63% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.64 (d, *J* = 8.3 Hz, 1H), 7.80 (d, *J* = 5.9 Hz, 2H), 7.76 – 7.68 (m, 2H), 7.52 (dt, *J* = 20.6, 7.1 Hz, 3H), 7.34 (t, *J* = 7.3 Hz, 1H), 2.29 – 2.20 (m, 1H), 1.38 (d, *J* = 7.2 Hz, 2H), 0.73 (d, *J* = 4.7 Hz, 2H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 192.80, 143.83, 143.31, 138.58, 136.48, 136.38, 134.95, 134.49, 131.20, 129.06, 129.03, 128.56, 128.23, 126.43, 124.05, 120.46, 118.17, 9.90, 9.44; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{20}H_{15}O$ 271.1123; found 271.1123.



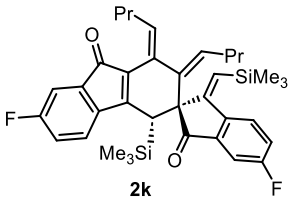
2i

6 mg (18% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.04 (d, *J* = 8.1 Hz, 1H), 7.78 (d, *J* = 8.2 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.43 – 7.37 (m, 2H), 7.20 (t, *J* = 7.4 Hz, 1H), 7.14 (t, *J* = 7.1 Hz, 1H), 6.76 (d, *J* = 6.7 Hz, 1H), 6.07 (s, 1H), 5.86 – 5.77 (m, 3H), 5.32 (s, 1H), 3.19 (s, 1H), 2.47 (dq, *J* = 12.6, 6.5 Hz, 1H), 2.25 (dt, *J* = 15.3, 7.8 Hz, 1H), 2.12 (d, *J* = 27.6 Hz, 4H), 1.92 (s, 3H), 1.83 – 1.66 (m, 7H), 1.64 – 1.54 (m, 3H), 1.54 – 1.44 (m, 6H), 1.40 (d, *J* = 24.7 Hz, 2H), 1.34 – 1.18 (m, 6H), 0.96 (d, *J* = 7.4 Hz, 3H), 0.88 (t, *J* = 6.7 Hz, 2H), 0.68 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 204.12, 194.00, 147.60, 143.70, 138.47, 138.34, 135.08, 135.02, 134.84, 134.30, 133.18, 133.07, 132.69, 132.02, 130.72, 129.26, 129.00, 128.86, 128.61, 128.48, 125.97, 125.34, 124.59, 122.26, 119.07, 62.24, 50.00, 32.63, 32.09, 28.40, 25.75, 25.40, 23.23, 22.81, 22.72, 22.17, 22.11, 21.82, 14.12, 13.81; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{42}H_{45}O_2$ 581.3420; found 581.3418.



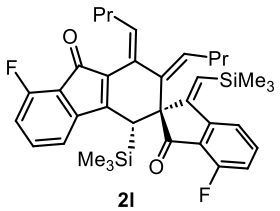
2j

5.4 mg (31% yield), orange solid, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.68 (d, *J* = 8.4 Hz, 1H), 7.31 – 7.23 (m, 5H), 6.98 (s, 1H), 6.60 (s, 2H), 6.00 (s, 1H), 5.81 (q, *J* = 7.3 Hz, 2H), 3.89 (s, 3H), 3.78 (s, 4H), 2.49 (q, *J* = 6.8 Hz, 1H), 2.24 (s, 1H), 2.16 (dq, *J* = 15.3, 8.2 Hz, 1H), 1.69 – 1.45 (m, 4H), 1.26 (dp, *J* = 76.8, 7.4 Hz, 8H), 1.01 (t, *J* = 7.3 Hz, 3H), 0.67 (t, *J* = 7.2 Hz, 3H), 0.26 (s, 9H), -0.01 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 202.56, 192.18, 163.72, 161.08, 155.38, 140.67, 139.36, 136.71, 135.87, 134.83, 133.30, 129.83, 129.28, 127.20, 126.15, 124.26, 123.24, 120.08, 114.94, 110.05, 106.16, 64.49, 55.73, 55.69, 37.51, 33.02, 32.78, 23.30, 21.94, 14.31, 13.93, 1.16,0.01; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{38}H_{49}O_4Si_2$ 625.3169; found 625.3153.



2k

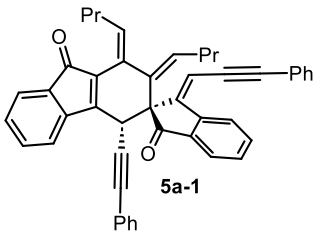
35.3 mg (83% yield), red oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.80 – 7.74 (m, 1H), 7.48 – 7.39 (m, 2H), 7.07 (dd, *J* = 7.2, 2.5 Hz, 1H), 6.89 – 6.82 (m, 1H), 6.68 – 6.62 (m, 1H), 6.13 (s, 1H), 5.84 (dt, *J* = 10.4, 7.4 Hz, 2H), 2.54 – 2.42 (m, 1H), 2.23 (s, 1H), 2.16 (td, *J* = 14.9, 7.4 Hz, 1H), 1.68 – 1.45 (m, 3H), 1.40 – 1.24 (m, 3H), 1.18 (p, *J* = 7.9 Hz, 2H), 1.01 (t, *J* = 7.3 Hz, 3H), 0.67 (t, *J* = 7.3 Hz, 3H), 0.27 (s, 9H), -0.00 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 164.58, 162.57, 162.23, 154.51, 143.31, 139.23, 138.98, 137.06, 134.97, 132.89, 131.24, 129.80, 128.19, 127.00, 126.73, 126.66, 122.19, 122.00, 120.06, 117.71, 117.52, 111.12, 111.00, 110.94, 110.80, 64.56, 37.22, 33.06, 33.01, 23.23, 21.86, 14.28, 13.90, 1.12,-0.09; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{36}H_{43}O_2F_2Si_2$ 601.2770; found 601.2760.



2l

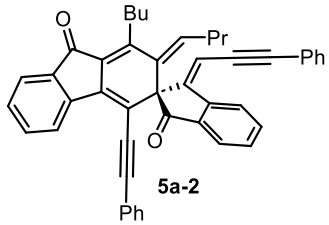
16.9 mg (41% yield), red oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.68 (d, *J* = 4.4 Hz, 2H), 7.56 (d, *J* = 8.1 Hz, 2H), 7.24 – 7.09 (m, 3H), 6.81 (t, *J* = 8.5 Hz, 1H), 6.55 (d, *J* = 7.1 Hz, 1H), 6.22 (s, 1H), 5.85 (p, *J* = 7.7 Hz, 2H), 2.57 – 2.44 (m, 2H), 2.31 (s, 1H), 2.16 (d, *J* = 7.1 Hz, 1H), 1.67 – 1.46 (m, 5H), 1.39 – 1.17 (m, 8H), 1.01 (t, *J* = 6.1 Hz, 3H), 0.69 (t, *J* = 7.3 Hz, 3H), 0.28 (s, 9H), -0.01 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 198.42, 189.06, 160.65, 160.58, 158.55, 158.41, 156.33, 154.73, 149.27, 146.01, 139.09, 136.10, 136.03, 135.75, 135.07, 135.00, 132.81, 131.53, 130.00, 129.35, 129.06, 128.78, 120.90, 118.44, 118.26, 117.09, 116.93, 115.65, 64.47, 37.07, 33.17, 33.05, 23.22, 21.86, 14.27, 13.91, 1.09, -0.13; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{36}H_{43}O_4F_2Si_2$ 633.2668; found 633.2659.

B. Products from Triynones



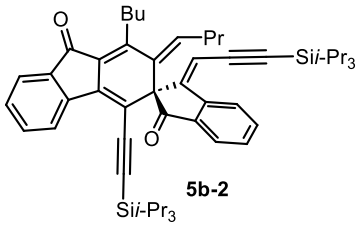
5a-1

9 mg (45% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.77 (d, *J* = 7.9 Hz, 1H), 7.92 (d, *J* = 7.7 Hz, 1H), 7.76 (dd, *J* = 11.1, 7.6 Hz, 2H), 7.59 – 7.46 (m, 4H), 7.37 (dd, *J* = 23.1, 5.6 Hz, 4H), 7.31 – 7.12 (m, 6H), 6.84 (d, *J* = 8.0 Hz, 2H), 6.08 – 6.00 (m, 1H), 5.86 (t, *J* = 7.5 Hz, 1H), 4.39 (s, 1H), 2.38 (h, *J* = 7.8 Hz, 1H), 2.24 (dq, *J* = 14.4, 8.0 Hz, 1H), 1.66 – 1.42 (m, 5H), 1.25 – 1.16 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H), 0.64 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 203.07, 192.96, 155.27, 149.79, 148.27, 142.90, 138.34, 137.06, 135.31, 134.07, 133.74, 131.77, 131.66, 131.47, 131.30, 130.50, 129.93, 129.30, 129.02, 128.71, 128.50, 128.33, 128.07, 124.78, 123.70, 123.16, 122.89, 121.21, 105.60, 98.43, 87.99, 87.45, 84.21, 61.88, 38.81, 32.79, 32.24, 23.14, 22.11, 14.00, 13.72; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{46}H_{37}O_2$ 621.2794; found 621.2785.



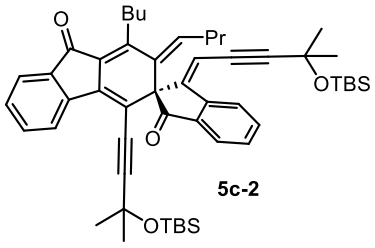
5a-2

9.5 mg (34% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.82 (d, *J* = 8.0 Hz, 1H), 8.55 (d, *J* = 7.9 Hz, 1H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.91 – 7.81 (m, 2H), 7.63 (dt, *J* = 10.5, 7.2 Hz, 2H), 7.55 – 7.50 (m, 2H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.37 (dd, *J* = 5.0, 2.0 Hz, 3H), 7.25 – 7.11 (m, 4H), 6.79 (d, *J* = 6.9 Hz, 2H), 6.62 (t, *J* = 7.8 Hz, 1H), 5.97 (s, 1H), 3.50 (m, 1H), 3.17 (m, 1H), 1.79 – 1.71 (m, 2H), 1.67 – 1.60 (m, 2H), 1.61 – 1.55 (m, 2H), 1.33 (m, 3H), 1.02 (t, *J* = 7.2 Hz, 3H), 0.70 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 202.09, 190.81, 153.48, 148.68, 147.96, 143.94, 141.60, 138.62, 137.63, 135.55, 135.42, 134.05, 133.96, 131.49, 131.07, 130.49, 129.54, 128.86, 128.56, 128.18, 125.11, 124.93, 124.23, 124.10, 123.41, 123.04, 122.54, 105.99, 100.18, 99.68, 87.83, 87.12, 63.10, 32.91, 32.52, 26.12, 23.26, 22.21, 14.04, 13.75; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{46}H_{37}O_2$ 621.2794; found 621.2785.



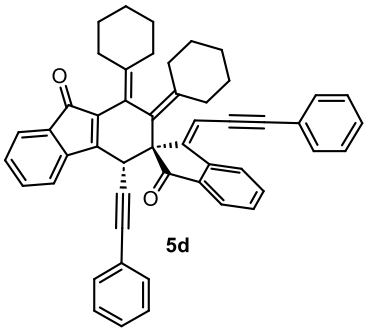
5b-2

11.5 mg (42% yield), orange oil, purified by flash column chromatography (basic Al_2O_3, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.89 (d, *J* = 7.9 Hz, 1H), 8.68 (d, *J* = 7.7 Hz, 1H), 7.86 (dd, *J* = 13.8, 7.6 Hz, 2H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.53 (q, *J* = 7.6 Hz, 2H), 7.45 (t, *J* = 7.3 Hz, 1H), 6.51 (t, *J* = 7.9 Hz, 1H), 5.79 (s, 1H), 3.34 (s, 1H), 3.22 (s, 1H), 1.67 – 1.58 (m, 3H), 1.26 (q, *J* = 7.7 Hz, 3H), 0.99 (t, *J* = 6.9 Hz, 4H), 0.76 (p, *J* = 7.2 Hz, 4H), 0.61 (d, *J* = 7.4 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 201.83, 190.69, 153.90, 148.68, 148.14, 143.76, 141.47, 138.57, 137.37, 135.74, 135.15, 135.00, 133.57, 130.37, 129.53, 125.24, 125.08, 124.72, 124.02, 123.27, 112.32, 106.72, 104.64, 103.39, 103.23, 103.01, 62.43, 32.69, 32.43, 26.11, 23.16, 22.29, 18.65, 18.62, 13.99, 13.70, 11.35, 11.16; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{52}H_{69}O_2Si_2$ 781.4836; found 781.4828.



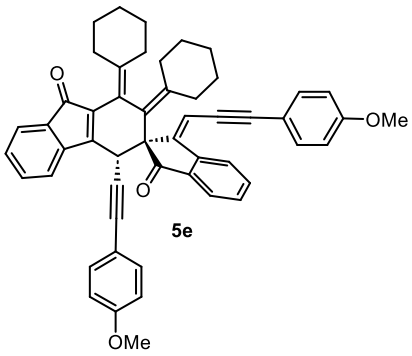
5c-2

17 mg (59% yield), orange oil, purified by flash column chromatography (basic Al_2O_3, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.69 (d, *J* = 8.0 Hz, 1H), 8.55 (d, *J* = 7.9 Hz, 1H), 7.90 (d, *J* = 7.4 Hz, 1H), 7.85 (d, *J* = 7.7 Hz, 1H), 7.75 (d, *J* = 7.9 Hz, 1H), 7.61 – 7.53 (m, 2H), 7.45 (t, *J* = 7.4 Hz, 1H), 6.53 (t, *J* = 7.7 Hz, 1H), 5.71 (s, 1H), 3.46 (s, 1H), 3.14 (s, 1H), 1.70 – 1.50 (m, 15H), 1.26 (d, *J* = 8.3 Hz, 3H), 1.10 (s, 3H), 0.98 (d, *J* = 6.1 Hz, 6H), 0.87 (s, 12H), 0.80 (s, 10H), 0.64 (t, *J* = 7.4 Hz, 3H), 0.13 (d, *J* = 4.9 Hz, 6H), -0.00 (s, 6H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 202.11, 190.81, 153.28, 148.50, 147.90, 143.67, 141.43, 138.53, 137.37, 135.69, 135.18, 134.34, 133.77, 130.42, 129.53, 125.04, 124.64, 124.25, 123.95, 123.29, 111.87, 106.05, 105.24, 104.55, 80.59, 79.23, 67.17, 66.82, 62.75, 32.80, 32.75, 32.42, 32.16, 32.01, 25.99, 25.70, 23.18, 22.23, 17.95, 17.84, 14.06, 13.73, -2.73, -2.80; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{52}H_{69}O_4Si_2$ 813.4734; found 813.4720.



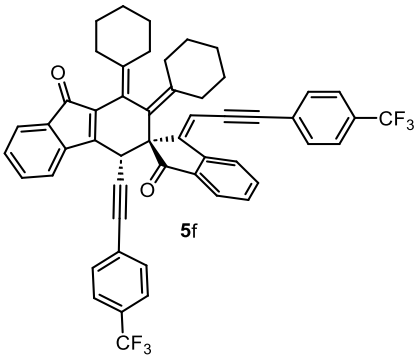
5d

25.7 mg (68% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.78 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.79 – 7.70 (m, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.48 (d, *J* = 4.6 Hz, 2H), 7.43 (d, *J* = 7.2 Hz, 1H), 7.34 (d, *J* = 5.6 Hz, 4H), 7.22 (q, *J* = 7.2 Hz, 2H), 7.16 (q, *J* = 7.1 Hz, 3H), 6.78 (d, *J* = 8.0 Hz, 2H), 5.96 (s, 1H), 4.36 (s, 1H), 2.60 (d, *J* = 13.5 Hz, 1H), 2.45 (d, *J* = 14.1 Hz, 1H), 2.34 (d, *J* = 12.8 Hz, 1H), 2.25 – 2.16 (m, 1H), 1.98 (dt, *J* = 25.5, 11.0 Hz, 2H), 1.86 (d, *J* = 7.3 Hz, 2H), 1.78 (s, 1H), 1.77 – 1.57 (m, 8H), 1.50 (m, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 203.88, 193.08, 156.67, 150.73, 148.48, 143.39, 143.10, 139.88, 138.58, 137.01, 135.21, 133.76, 131.62, 131.47, 131.23, 129.85, 128.64, 128.49, 128.23, 128.06, 124.90, 123.65, 123.25, 122.78, 122.30, 121.76, 120.53, 104.17, 98.12, 88.10, 87.65, 84.51, 64.80, 41.01, 33.74, 33.48, 31.62, 31.58, 28.86, 27.65, 27.58, 26.63, 26.55, 26.31; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{50}H_{41}O_2$ 673.3107; found 673.3093.



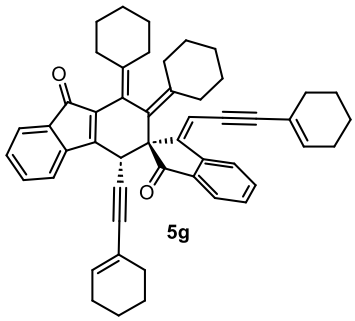
5e

37 mg (58% yield), orange solid, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:8). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.76 (d, *J* = 7.9 Hz, 1H), 7.87 (d, *J* = 7.4 Hz, 1H), 7.76 – 7.70 (m, 2H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.41 (d, *J* = 8.9 Hz, 3H), 7.22 (d, *J* = 7.7 Hz, 1H), 7.15 (t, *J* = 7.5 Hz, 1H), 6.87 (d, *J* = 8.8 Hz, 2H), 6.72 (d, *J* = 8.9 Hz, 2H), 6.67 (d, *J* = 8.8 Hz, 3H), 5.93 (s, 1H), 4.33 (s, 1H), 3.82 (s, 3H), 3.75 (s, 3H), 2.60 (d, *J* = 13.2 Hz, 1H), 2.43 (d, *J* = 13.5 Hz, 1H), 2.33 (d, *J* = 13.4 Hz, 1H), 2.19 (t, *J* = 10.9 Hz, 1H), 1.98 (td, *J* = 23.6, 11.6 Hz, 3H), 1.85 (d, *J* = 12.1 Hz, 2H), 1.78 (d, *J* = 11.6 Hz, 1H), 1.71 (s, 3H), 1.61 (s, 5H), 1.50 (s, 3H), 1.33 (t, *J* = 13.9 Hz, 4H).; **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 204.08, 193.13, 159.94, 159.48, 157.02, 149.86, 148.68, 143.21, 139.74, 138.46, 136.96, 135.07, 133.69, 132.96, 132.64, 131.67, 129.56, 128.77, 128.55, 124.78, 123.55, 122.69, 121.85, 120.59, 115.44, 114.50, 114.15, 113.66, 104.44, 98.26, 87.52, 87.14, 83.04, 64.85, 55.37, 55.25, 41.08, 33.70, 33.46, 31.58, 28.84, 27.64, 27.56, 26.63, 26.56, 26.31; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{52}H_{45}O_4$ 733.3318; found 733.3303.



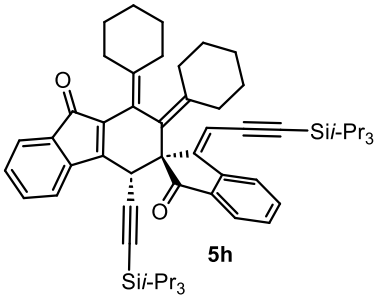
5f

32.6 mg (73% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.71 (d, *J* = 8.0 Hz, 1H), 7.92 (d, *J* = 7.6 Hz, 1H), 7.77 (t, *J* = 7.8 Hz, 1H), 7.64 (d, *J* = 6.2 Hz, 1H), 7.58 (q, *J* = 8.2 Hz, 5H), 7.43 (dd, *J* = 13.4, 7.6 Hz, 3H), 7.25 – 7.16 (m, 2H), 6.86 (d, *J* = 7.9 Hz, 2H), 5.97 (s, 1H), 4.38 (s, 1H), 2.59 (d, *J* = 13.7 Hz, 1H), 2.44 (d, *J* = 13.8 Hz, 1H), 2.34 (d, *J* = 13.9 Hz, 1H), 2.23 (d, *J* = 12.4 Hz, 1H), 1.99 (dt, *J* = 25.7, 12.6 Hz, 2H), 1.82 (d, *J* = 35.6 Hz, 3H), 1.54 (d, *J* = 29.7 Hz, 10H), 1.30 (dd, *J* = 25.6, 15.8 Hz, 8H), 0.96 (d, *J* = 6.6 Hz, 1H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 203.28, 192.83, 155.77, 151.79, 148.10, 143.86, 142.95, 140.18, 138.88, 137.12, 135.31, 133.70, 131.67, 131.55, 131.43, 130.29, 128.81, 128.43, 126.87, 125.87, 125.43, 125.10, 124.74, 123.87, 122.98, 121.53, 120.18, 103.67, 96.67, 90.02, 87.18, 86.37, 64.78, 40.90, 33.78, 33.73, 33.46, 31.60, 28.84, 27.63, 27.54, 26.64, 26.50, 26.24; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{52}H_{39}F_6O_2$ 809.86; found 808.3419.



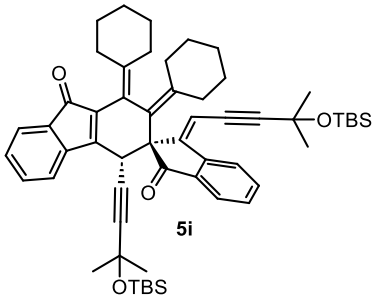
5g

15.2 mg (54% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.63 (d, *J* = 8.0 Hz, 1H), 7.83 (d, *J* = 7.7 Hz, 1H), 7.72 – 7.63 (m, 2H), 7.49 (s, 1H), 7.23 (t, *J* = 7.6 Hz, 2H), 7.14 (t, *J* = 7.4 Hz, 1H), 6.19 (s, 1H), 5.79 (s, 1H), 5.45 (s, 1H), 4.21 (s, 1H), 2.56 (d, *J* = 12.9 Hz, 1H), 2.38 (d, *J* = 13.5 Hz, 1H), 2.29 (d, *J* = 13.8 Hz, 1H), 2.22 (s, 2H), 2.15 (s, 3H), 1.94 (d, *J* = 23.5 Hz, 4H), 1.81 (s, 1H), 1.79 – 1.56 (m, 12H), 1.49 (t, *J* = 10.8 Hz, 11H), 1.36 – 1.13 (m, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 204.23, 193.17, 157.23, 149.62, 148.72, 143.17, 142.97, 139.52, 138.27, 136.83, 136.07, 134.83, 134.42, 133.58, 131.67, 129.31, 128.82, 128.45, 124.76, 123.36, 122.59, 121.87, 121.19, 120.64, 119.90, 104.50, 100.04, 89.42, 85.97, 81.45, 64.74, 53.44, 40.96, 33.64, 33.61, 33.42, 31.54, 29.72, 28.83, 28.20, 27.62, 27.52, 26.59, 26.55, 26.31, 25.92, 25.39, 22.26, 22.02, 21.45, 21.33; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{50}H_{49}O_2$ 681.3733; found 681.3721.



5h

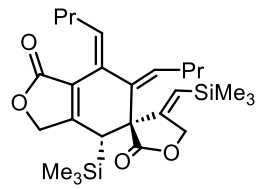
7.5 mg (21% yield), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.67 (d, *J* = 7.9 Hz, 1H), 7.84 (s, 1H), 7.75 (d, *J* = 7.3 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.39 (d, *J* = 7.0 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.18 – 7.12 (m, 1H), 5.70 (s, 1H), 4.10 (s, 1H), 2.51 (d, *J* = 13.1 Hz, 1H), 2.43 – 2.34 (m, 1H), 2.33 – 2.26 (m, 1H), 2.17 (d, *J* = 17.3 Hz, 1H), 2.04 – 1.95 (m, 1H), 1.93 – 1.85 (m, 1H), 1.85 – 1.74 (m, 2H), 1.69 (d, *J* = 12.0 Hz, 2H), 1.63 (s, 3H), 1.55 (d, *J* = 2.2 Hz, 3H), 1.50 – 1.42 (m, 3H), 1.42 – 1.30 (m, 2H), 1.10 (s, 3H), 0.83 (s, 11H), 0.80 (s, 13H), 0.09 – -0.06 (m, 14H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 203.78, 193.04, 156.68, 150.56, 148.41, 143.15, 143.06, 139.68, 138.45, 136.82, 134.97, 133.44, 131.60, 129.74, 128.85, 128.54, 124.63, 123.56, 122.67, 121.73, 120.73, 103.92, 103.70, 92.17, 80.67, 76.63, 67.00, 66.39, 64.16, 40.22, 33.67, 33.52, 33.48, 32.73, 32.65, 32.04, 31.94, 31.47, 29.72, 28.78, 27.56, 27.50, 26.67, 26.53, 26.27, 25.68, 25.65, 17.90, 17.84, -2.79, -2.85, -3.01; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_0H_{49}O_2$ 681.3733; found 681.3721.



5i

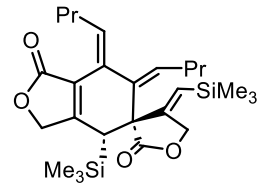
28 mg (83% yield,), orange oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.67 (d, *J* = 7.9 Hz, 1H), 7.84 (s, 1H), 7.75 (d, *J* = 7.3 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.39 (d, *J* = 7.0 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.18 – 7.12 (m, 1H), 5.70 (s, 1H), 4.10 (s, 1H), 2.51 (d, *J* = 13.1 Hz, 1H), 2.43 – 2.34 (m, 1H), 2.33 – 2.26 (m, 1H), 2.17 (d, *J* = 17.3 Hz, 1H), 2.04 – 1.95 (m, 1H), 1.93 – 1.85 (m, 1H), 1.85 – 1.74 (m, 2H), 1.69 (d, *J* = 12.0 Hz, 2H), 1.63 (s, 3H), 1.55 (d, *J* = 2.2 Hz, 3H), 1.50 – 1.42 (m, 3H), 1.42 – 1.30 (m, 2H), 1.10 (s, 3H), 0.83 (s, 11H), 0.80 (s, 13H), 0.09 – -0.06 (m, 14H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 203.78, 193.04, 156.68, 150.56, 148.41, 143.15, 143.06, 139.68, 138.45, 136.82, 134.97, 133.44, 131.60, 129.74, 128.85, 128.54, 124.63, 123.56, 122.67, 121.73, 120.73, 103.92, 103.70, 92.17, 80.67, 76.63, 67.00, 66.39, 64.16, 40.22, 33.67, 33.52, 33.48, 32.73, 32.65, 32.04, 31.94, 31.47, 29.72, 28.78, 27.56, 27.50, 26.67, 26.53, 26.27, 25.68, 25.65, 17.90, 17.84, -2.79, -2.85, -3.01; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{50}H_{49}O_2$ 681.3733; found 681.3721.

C. Products from non-aromatic tethered alkynones



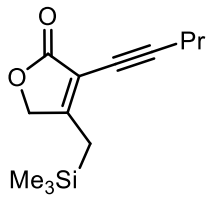
7a

(**7b :** (**7b':7b"**) = 23 : (16:3) mg, 49% : (34%:6%) purified by flash column chromatography (SiO_2, , EtOAc–hexanes, 1:20 to 1:10); **2b**, white solid: **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.97 (t, *J* = 7.5 Hz, 1H), 5.90 (dd, *J* = 9.0, 5.5 Hz, 1H), 5.19 (s, 1H), 5.04 (dd, *J* = 13.6, 2.7 Hz, 1H), 4.93 (dd, *J* = 13.6, 2.0 Hz, 1H), 4.85 (s, 1H), 4.34 (d, *J* = 17.4 Hz, 1H), 2.44 (td, *J* = 16.2, 15.4, 6.4 Hz, 1H), 2.21 (td, *J* = 16.2, 15.4, 6.4 Hz, 1H), 2.07 (s, 1H), 1.85 – 1.74 (m, 1H), 1.51 – 1.42 (m, 2H), 1.42 – 1.32 (m, 2H), 1.32 – 1.22 (m, 1H), 0.98 (t, *J* = 7.4 Hz, 3H), 0.83 (t, *J* = 7.3 Hz, 3H), 0.11 (s, 9H), 0.03 (s, 9H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 175.7, 170.5, 163.9, 156.3, 137.2, 131.0, 129.8, 128.7, 124.3, 121.1, 73.2, 69.6, 54.5, 39.3, 33.0, 32.5, 22.9, 21.9, 14.2, 14.0, -0.2, -0.7. **HRMS** (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{41}O_4Si_2$ 473.2543; found 473.2539.



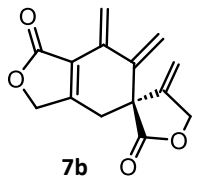
7a'

7b':7b", white solid: **7b'**: **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.76 (t, *J* = 7.6 Hz, 1H), 5.72 (t, *J* = 7.3 Hz, 1H), 5.62 (s, 1H), 4.91 (d, *J* = 13.4, 1H), 4.86 (d, *J* = 13.4, 1H), 4.80 (d, *J* = 17.3 Hz, 1H), 4.67 (d, *J* = 17.2 Hz, 1H), 2.59 (s, 1H), 2.52 (dq, *J* = 15.3, 7.2 Hz, 1H), 2.25 (dt, *J* = 14.4, 7.1 Hz, 1H), 1.74 (q, *J* = 7.4 Hz, 2H), 1.45 (p, *J* = 7.4 Hz, 2H), 1.34 (qd, *J* = 7.2, 4.4 Hz, 2H), 0.97 (t, *J* = 7.4 Hz, 3H), 0.86 (t, *J* = 7.4 Hz, 3H), 0.14 (s, 9H), 0.09 (s, 9H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.3, 170.2, 163.0, 151.2, 136.6, 132.7, 130.3, 129.4, 126.2, 124.0, 71.7, 69.9, 54.5, 38.1, 32.4, 31.6, 23.2, 22.5, 14.2, 13.9, 0.4, -0.7. **HRMS** (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{41}O_4Si_2$ 473.2543; found 473.2542.



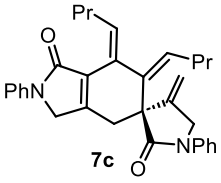
7a"

7d": **^{1}H NMR** (500 MHz, $CDCl_3$) δ 4.55 (s, 1H), 2.21 (s, 2H), 2.05 (t, *J* = 7.2 Hz, 2H), 1.55 – 1.49 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H), 0.12 (s, 9H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 164.8, 136.0, 117.6, 71.7, 66.4, 63.8, 27.8, 22.0, 20.8, 20.4, -1.4. **HRMS** (ESI) m/z: $[M+H]^+$ Calcd for $C_{13}H_{21}O_2Si$ 237.1311; found 237.1309.



7b

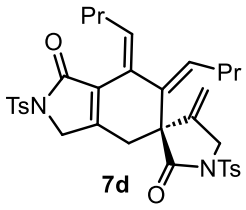
5 mg (14% yield), white solid, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:20 to 1:10); the characterization data of this product is consistent with the reported data.[3]



7c

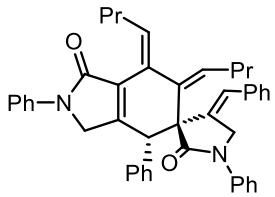
11 mg (33% yield), colorless oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.81 – 7.65 (m, 4H), 7.49 – 7.32 (m, 4H), 7.20 (s, 1H), 7.11 (s, 1H), 5.93 (d, *J* = 27.7 Hz, 2H), 5.01 (s, 1H), 4.90 (s, 1H), 4.65 (d, *J* = 12.7 Hz, 1H), 4.46 (t, *J* = 19.1 Hz, 2H), 4.26 (d, *J* = 19.1 Hz, 1H), 3.01 (d, *J* = 16.8 Hz, 1H), 2.54 (d, *J* = 15.4 Hz, 1H), 2.48 (d, *J* = 6.4 Hz, 1H), 2.39 (d, *J* = 6.7 Hz, 1H), 1.85 (s, 1H), 1.82 – 1.69 (m, 1H), 1.52 (d, *J* = 7.0 Hz, 4H), 1.45 – 1.20 (m, 5H), 0.95 (d, *J* = 5.0 Hz, 3H), 0.80 (s, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 174.52, 167.33, 148.83, 145.68, 139.66,

139.07, 138.96, 134.67, 131.21, 129.97, 129.17, 129.12, 124.94, 123.84, 119.72, 118.82, 108.88, 54.82, 53.52, 51.29, 34.66, 32.56, 31.68, 23.13, 22.21, 13.95; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{32}H_{35}N_2O_2$ 479.2699; found 479.2691.



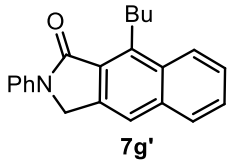
7d

10.9 mg (32% yield), colorless oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:3). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.91 (dd, *J* = 13.9, 8.3 Hz, 5H), 7.32 (t, *J* = 9.2 Hz, 6H), 5.79 (t, *J* = 7.6 Hz, 1H), 5.63 (d, *J* = 7.2 Hz, 1H), 4.87 (s, 1H), 4.61 (d, *J* = 13.3 Hz, 2H), 4.44 (d, *J* = 16.1 Hz, 1H), 4.39 (d, *J* = 19.2 Hz, 1H), 4.23 (d, *J* = 19.3 Hz, 1H), 2.68 (d, *J* = 15.5 Hz, 1H), 2.42 (d, *J* = 7.5 Hz, 9H), 2.38 (d, *J* = 15.6 Hz, 1H), 2.25 – 2.08 (m, 2H), 1.37 (tt, *J* = 13.8, 7.0 Hz, 3H), 1.10 (q, *J* = 7.4 Hz, 2H), 1.02 (q, *J* = 7.3 Hz, 3H), 0.85 (d, *J* = 4.2 Hz, 3H), 0.54 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 173.06, 165.36, 152.61, 145.74, 145.02, 143.61, 137.21, 135.35, 134.38, 133.09, 132.27, 130.11, 129.76, 128.30, 127.90, 110.14, 60.41, 52.61, 49.63, 34.87, 32.36, 31.90, 22.80, 21.70, 13.79, 13.60; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{34}H_{39}N_2O_6S_2$ 635.2250; found 635.2234.



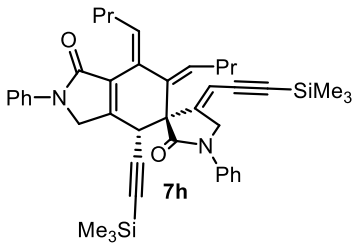
7g

9 mg (27.5% yield), colorless oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.69 (d, *J* = 8.7 Hz, 2H), 7.35 (ddd, *J* = 27.5, 20.4, 7.5 Hz, 12H), 7.22 (d, *J* = 7.9 Hz, 2H), 7.17 – 7.11 (m, 1H), 7.08 (d, *J* = 7.7 Hz, 3H), 6.43 (s, 1H), 6.11 (t, *J* = 7.3 Hz, 1H), 6.01 (t, *J* = 7.1 Hz, 1H), 4.62 (d, *J* = 19.4 Hz, 1H), 4.52 (s, 1H), 4.24 (d, *J* = 19.3 Hz, 1H), 4.16 (d, *J* = 15.0 Hz, 1H), 3.67 (d, *J* = 12.0 Hz, 1H), 2.60 (q, *J* = 7.5 Hz, 1H), 2.38 (dd, *J* = 15.0, 7.4 Hz, 1H), 1.91 – 1.80 (m, 1H), 1.71 (dd, *J* = 14.9, 7.2 Hz, 2H), 1.62 (d, *J* = 6.2 Hz, 2H), 1.53 (s, 1H), 1.33 (dt, *J* = 14.1, 6.8 Hz, 3H), 1.00 (t, *J* = 7.3 Hz, 3H), 0.71 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 173.26, 167.44, 137.67, 134.47, 131.69, 130.32, 129.42, 129.07, 128.87, 128.77, 128.55, 128.40, 128.26, 127.59, 126.03, 125.43, 124.06, 121.09, 119.11, 53.00, 52.91, 51.69, 32.62, 31.72, 23.14, 22.04, 14.07, 14.02; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{44}H_{43}N_2O_2$ 631.3325; found 631.3312.



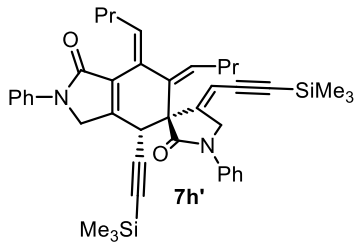
7g'

9 mg (27.5% yield), colorless oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:9). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 8.28 (s, 1H), 7.91 (d, *J* = 8.0 Hz, 3H), 7.78 (s, 1H), 7.58 (d, *J* = 8.6 Hz, 2H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.20 (t, *J* = 6.9 Hz, 1H), 4.95 (s, 2H), 3.81 (t, *J* = 7.6 Hz, 2H), 1.74 (d, *J* = 6.6 Hz, 2H), 1.59 (t, *J* = 7.3 Hz, 2H), 0.99 (t, *J* = 7.4 Hz, 3H); **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{22}H_{22}NO$ 316.1701; found 316.1700.



7h

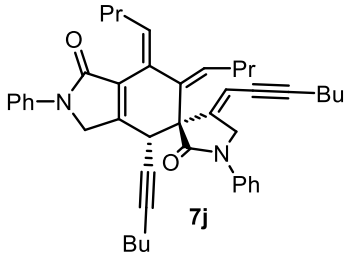
28 mg (60% yield), colorless oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.75 (dd, *J* = 23.9, 8.8 Hz, 3H), 7.43 (dt, *J* = 16.0, 8.1 Hz, 4H), 7.35 – 7.22 (m, 2H), 7.16 (t, *J* = 7.4 Hz, 1H), 6.01 (t, *J* = 7.6 Hz, 1H), 5.89 (t, *J* = 7.3 Hz, 1H), 5.24 (s, 1H), 4.70 (dd, *J* = 15.5, 3.0 Hz, 1H), 4.67 – 4.54 (m, 2H), 4.41 – 4.33 (m, 1H), 4.20 (s, 1H), 2.48 (td, *J* = 14.7, 6.2 Hz, 1H), 2.30 (dt, *J* = 15.0, 7.5 Hz, 1H), 1.85 (dt, *J* = 14.6, 7.5 Hz, 1H), 1.73 (p, *J* = 7.7 Hz, 1H), 1.65 – 1.30 (m, 4H), 0.93 (t, *J* = 7.3 Hz, 2H), 0.81 (t, *J* = 7.4 Hz, 3H), 0.19 (s, 9H), 0.08 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 172.96, 166.73, 150.53, 148.38, 139.63, 139.50, 138.61, 134.83, 131.89, 129.96, 129.76, 129.20, 129.14, 125.43, 124.21, 120.42, 119.12, 105.25, 102.99, 100.16, 98.82, 90.80, 60.03, 53.72, 52.52, 39.44, 32.59, 31.64, 22.94, 22.04, 13.98, 13.95, -0.05, -0.21; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{42}H_{51}N_2O_2Si_2$ 671.3489; found 671.3481.



7h'

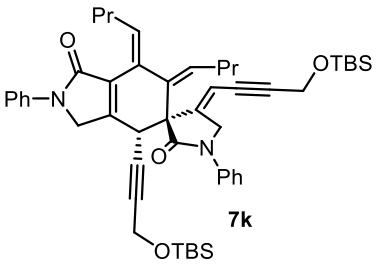
8 mg (18% yield), colorless oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.70 (t, *J* = 9.6 Hz, 3H), 7.45 – 7.33 (m, 5H), 7.18 (d, *J* = 7.2 Hz, 1H), 7.10 (t, *J* = 7.0 Hz, 1H), 5.86 (dt, *J* = 14.2, 6.9 Hz, 2H), 5.74 (s, 1H), 4.68 (s, 2H), 4.46 (s, 2H), 3.70 (s, 1H), 2.49 (q, *J* = 7.2 Hz, 1H), 2.29 (q, *J* = 7.4 Hz, 1H), 2.11 – 2.01 (m, 1H), 1.82 – 1.70 (m, 2H), 1.46 – 1.33 (m, 3H), 0.92 (t, *J* = 7.3 Hz, 4H), 0.80 (t, *J* = 7.3 Hz, 3H), 0.26 (s, 9H), -0.02 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 171.84, 166.80, 151.68, 148.59, 140.42, 139.72, 138.52, 134.11, 131.06, 130.87, 130.11, 129.00, 128.96, 125.04, 123.84, 120.02, 119.22, 105.50, 103.72, 100.18, 98.48, 91.11, 59.49, 52.36, 51.90, 42.48, 32.49, 31.73, 23.03, 21.99, 13.96, 13.84, 0.02, -0.34; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{42}H_{51}N_2O_2Si_2$ 671.3489; found 671.3484.

Tentative structure



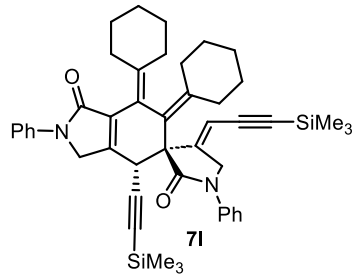
7j

26 mg (79% yield, *dr* = 2:1), colorless oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.77 (dd, *J* = 16.4, 8.2 Hz, 5H), 7.41 (dq, *J* = 16.9, 8.6 Hz, 8H), 6.01 (t, *J* = 7.7 Hz, 1H), 5.88 (t, *J* = 7.3 Hz, 1H), 5.18 (s, 1H), 4.67 (d, *J* = 15.1 Hz, 1H), 4.58 (d, *J* = 16.9 Hz, 2H), 4.36 (d, *J* = 19.9 Hz, 1H), 4.17 (s, 1H), 2.55 – 2.46 (m, 1H), 2.35 (t, *J* = 6.0 Hz, 2H), 2.32 – 2.27 (m, 1H), 2.13 (t, *J* = 5.7 Hz, 3H), 1.91 – 1.82 (m, 1H), 1.74 (ddq, *J* = 22.9, 15.4, 7.7 Hz, 3H), 1.65 – 1.33 (m, 21H), 0.93 (tdd, *J* = 23.4, 10.6, 4.9 Hz, 20H), 0.80 (t, *J* = 7.3 Hz, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 173.40, 166.94, 149.93, 147.56, 140.19, 138.89, 134.36, 131.34, 130.47, 129.78, 129.66, 129.14, 129.08, 125.12, 124.01, 120.15, 118.94, 98.51, 85.68, 76.29, 72.88, 59.90, 53.40, 52.74, 38.61, 32.61, 31.61, 30.78, 30.70, 23.08, 22.97, 22.67, 22.05, 21.93, 19.36, 18.43, 14.00, 13.96, 13.58, 13.52; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{44}H_{51}N_2O_2$ 639.90; found 639.3946.



7k

29 mg (67% yield, *dr* = 1.2:1)), colorless oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.77 (d, *J* = 8.2 Hz, 2H), 7.62 (d, *J* = 8.3 Hz, 2H), 7.32 (d, *J* = 7.2 Hz, 2H), 7.21 (dd, *J* = 21.5, 7.2 Hz, 2H), 7.08 (t, *J* = 7.5 Hz, 1H), 6.03 (t, *J* = 7.5 Hz, 1H), 5.91 (t, *J* = 7.5 Hz, 1H), 5.24 (s, 1H), 4.83 (d, *J* = 15.2 Hz, 2H), 4.59 (d, *J* = 16.7 Hz, 2H), 4.36 (d, *J* = 14.0 Hz, 4H), 4.15 (s, 1H), 2.50 (dq, *J* = 14.5, 6.7 Hz, 1H), 2.30 (d, *J* = 7.4 Hz, 1H), 1.85 (s, 1H), 1.75 (dp, *J* = 24.0, 7.6 Hz, 2H), 1.65 – 1.52 (m, 3H), 1.47 (d, *J* = 7.7 Hz, 3H), 1.37 (t, *J* = 7.3 Hz, 3H), 0.94 (s, 13H), 0.90 (s, 13H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 172.78, 166.73, 150.84, 148.70, 140.44, 139.71, 138.61, 134.79, 131.78, 130.08, 129.98, 129.13, 129.08, 125.28, 124.14, 120.64, 118.99, 104.96, 96.50, 95.81, 84.27, 83.97, 59.25, 52.27, 51.54, 41.61, 38.44, 32.65, 31.75, 25.79, 23.07, 22.02, 13.89, -5.18; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{50}H_{67}N_2O_4Si_2$ 815.4639; found 815.4637.

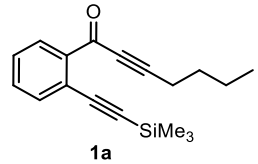


7l

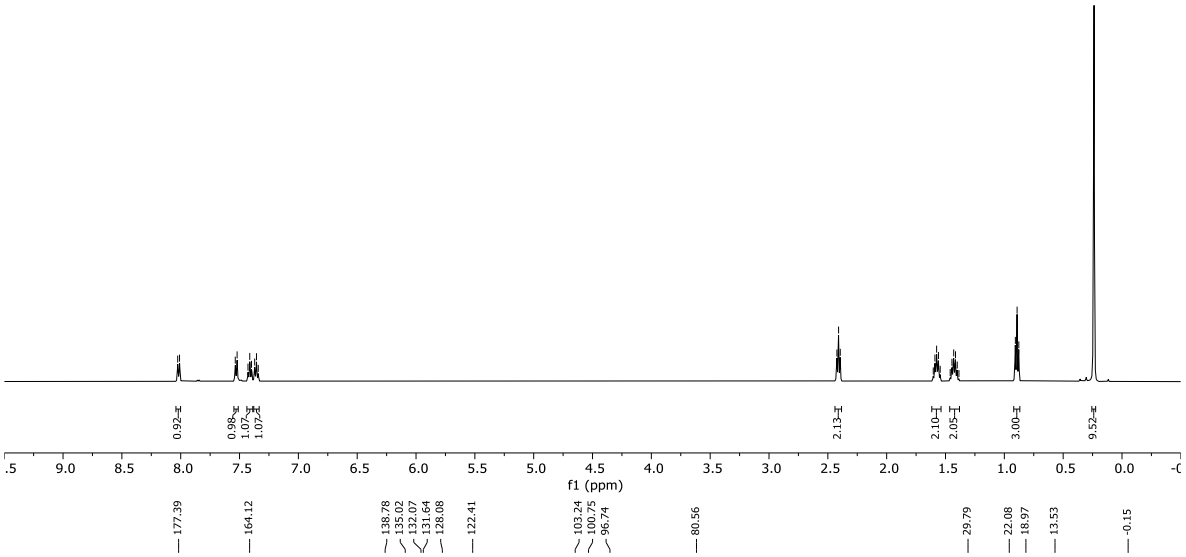
18 mg (32% yield), colorless oil, purified by flash column chromatography (SiO_2, EtOAc–hexanes, 1:10). **^{1}H NMR** ($CDCl_3$, 500 MHz): δ 7.80 (d, *J* = 7.5 Hz, 2H), 7.71 (d, *J* = 7.6 Hz, 2H), 7.50 – 7.33 (m, 5H), 7.29 (d, *J* = 7.3 Hz, 1H), 7.22 (t, *J* = 7.3 Hz, 1H), 7.14 (t, *J* = 7.6 Hz, 1H), 5.19 (s, 1H), 4.70 (d, *J* = 15.6 Hz, 1H), 4.64 – 4.53 (m, 2H), 4.31 (d, *J* = 19.6 Hz, 1H), 4.16 (s, 1H), 2.49 (d, *J* = 13.3 Hz, 1H), 2.46 – 2.34 (m, 2H), 2.25 (t, *J* = 10.2 Hz, 1H), 1.97 (s, 2H), 1.79 (dd, *J* = 49.6, 16.8 Hz, 5H), 1.63 (s, 2H), 1.51 (d, *J* = 7.7 Hz, 3H), 1.46 – 1.35 (m, 2H), 1.28 (d, *J* = 26.4 Hz, 4H), 0.20 (s, 9H), 0.07 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 173.93, 167.06, 151.95, 148.73, 143.90, 140.29, 139.75, 139.04, 138.73, 130.83, 129.24, 129.12, 129.08, 128.57, 125.37, 123.92, 120.73, 120.37, 118.76, 103.57, 102.69, 100.33, 99.30, 90.45, 62.78, 53.93, 52.37, 40.76, 33.44, 33.30, 31.59, 29.34, 28.62, 27.72, 27.37, 26.47, 26.16, 25.97, 0.01, -0.22; **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{46}H_{55}N_2O_2Si_2$ 723.3802; found 723.3796.

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

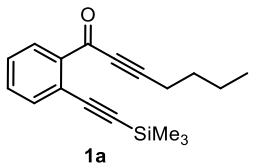
^{1}H NMR ($CDCl_3$, 500 MHz)



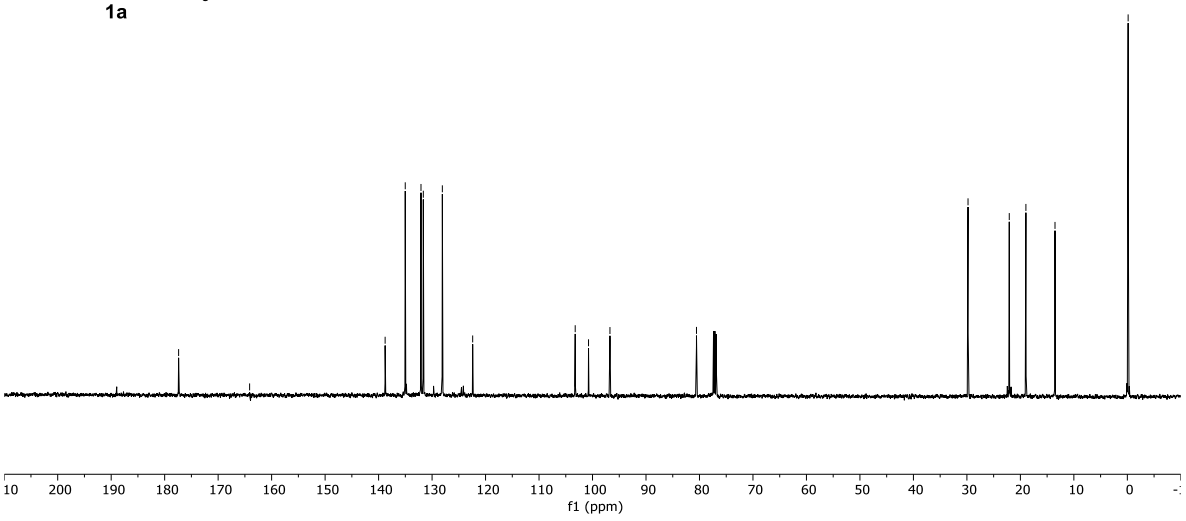
1a



^{13}C NMR ($CDCl_3$, 125 MHz)



1a



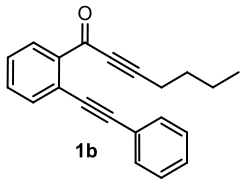
8.12
8.10
7.63
7.62
7.62
7.61
7.51
7.49
7.48
7.42
7.40
7.39
7.34
7.33

2.43
2.41
2.40

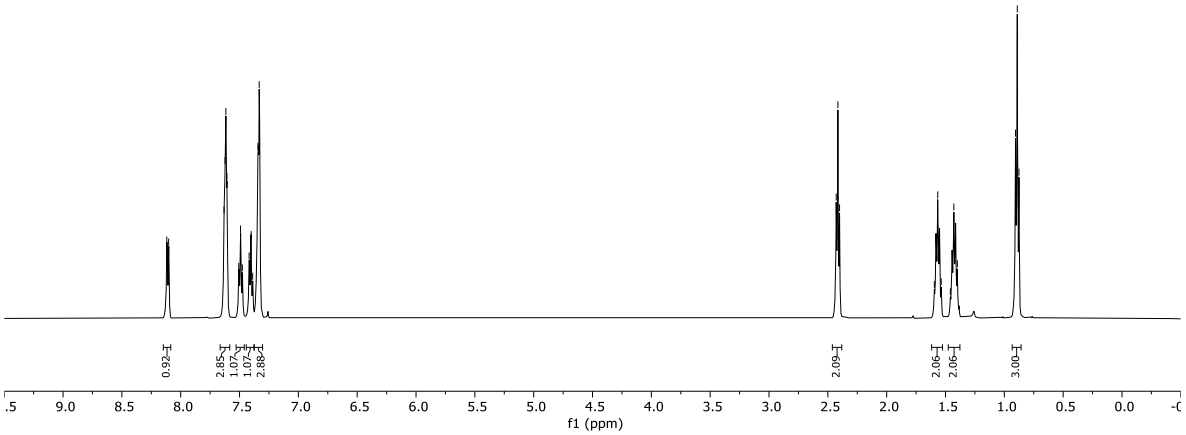
1.60
1.57
1.54
1.46
1.43
1.40

0.90
0.89
0.88

^{1}H NMR ($CDCl_3$, 500 MHz)



1b



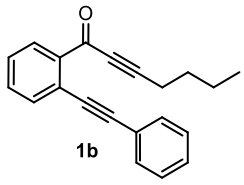
177.65

138.35
134.24
132.32
131.92
131.79
128.64
128.36
127.91
123.34
122.82

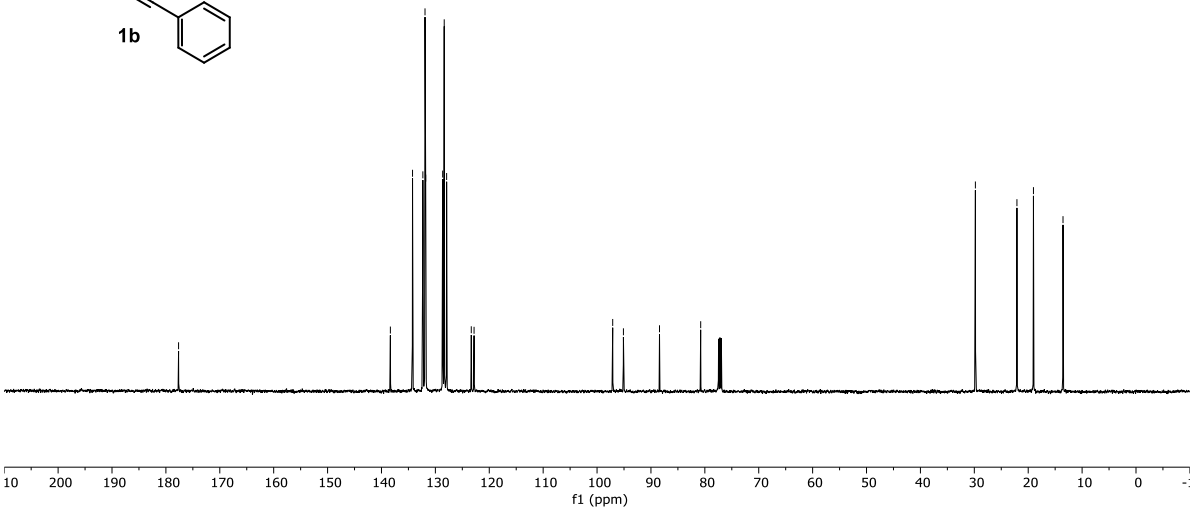
97.10
95.11
88.41
80.77

29.80
22.09
19.03
13.54

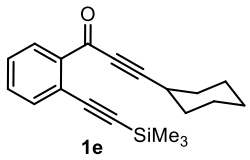
^{13}C NMR ($CDCl_3$, 125 MHz)



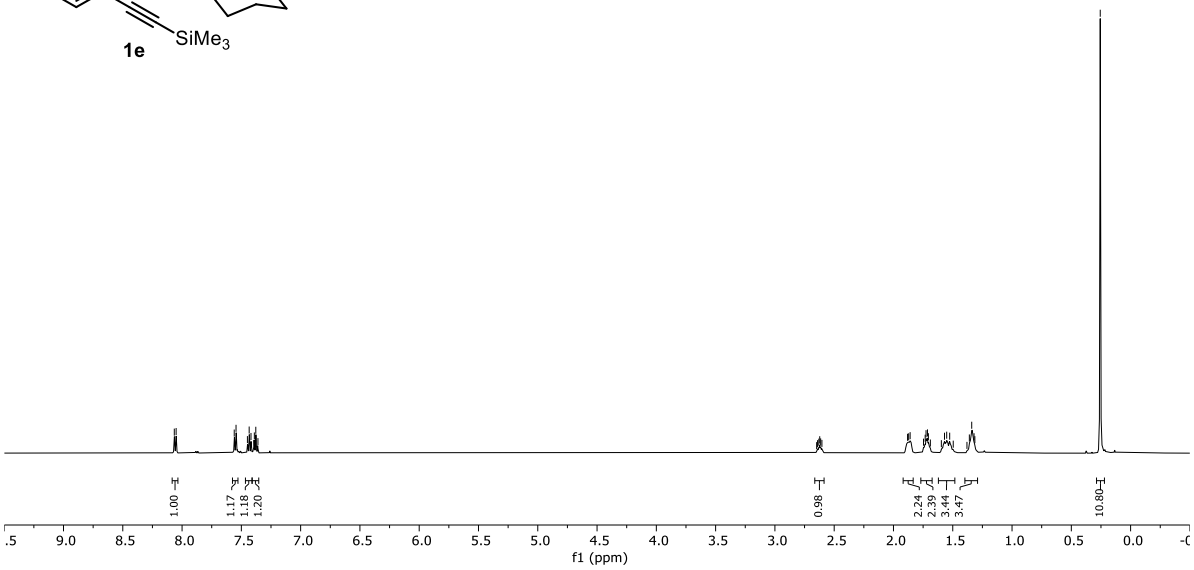
1b



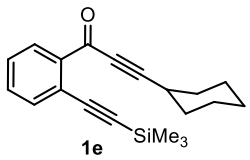
^{1}H NMR ($CDCl_3$, 500 MHz)



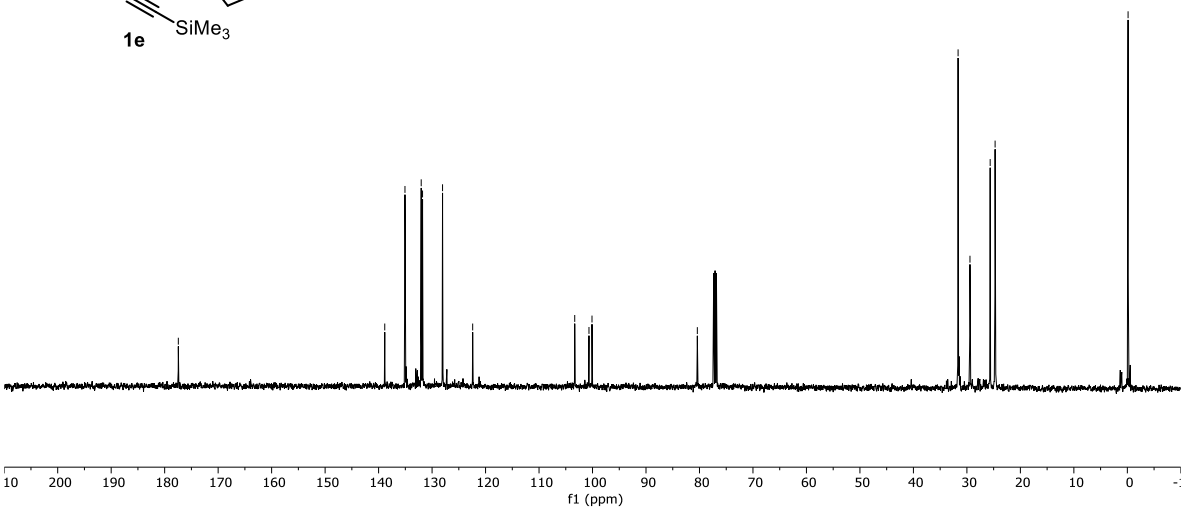
1e



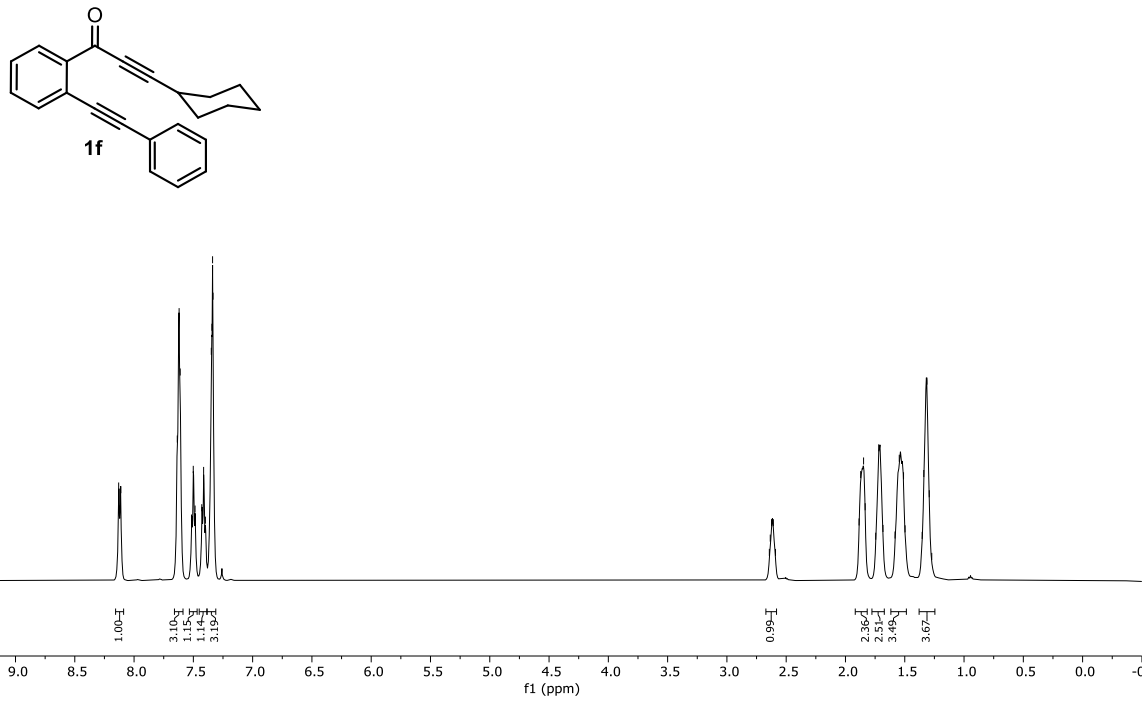
^{13}C NMR ($CDCl_3$, 125 MHz)



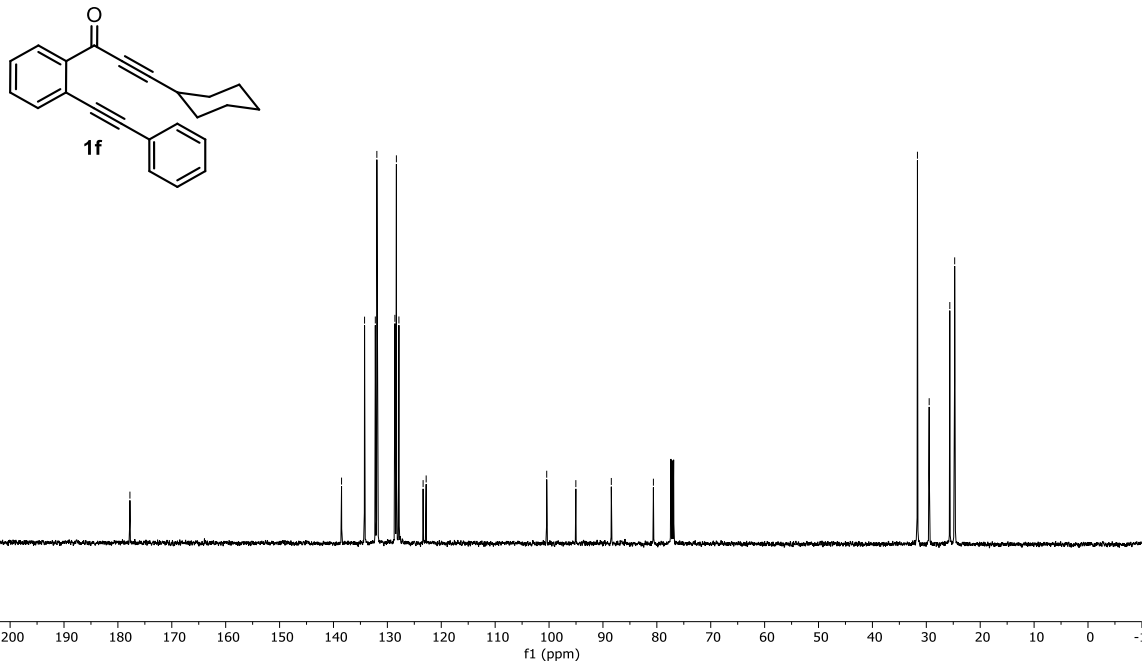
1e



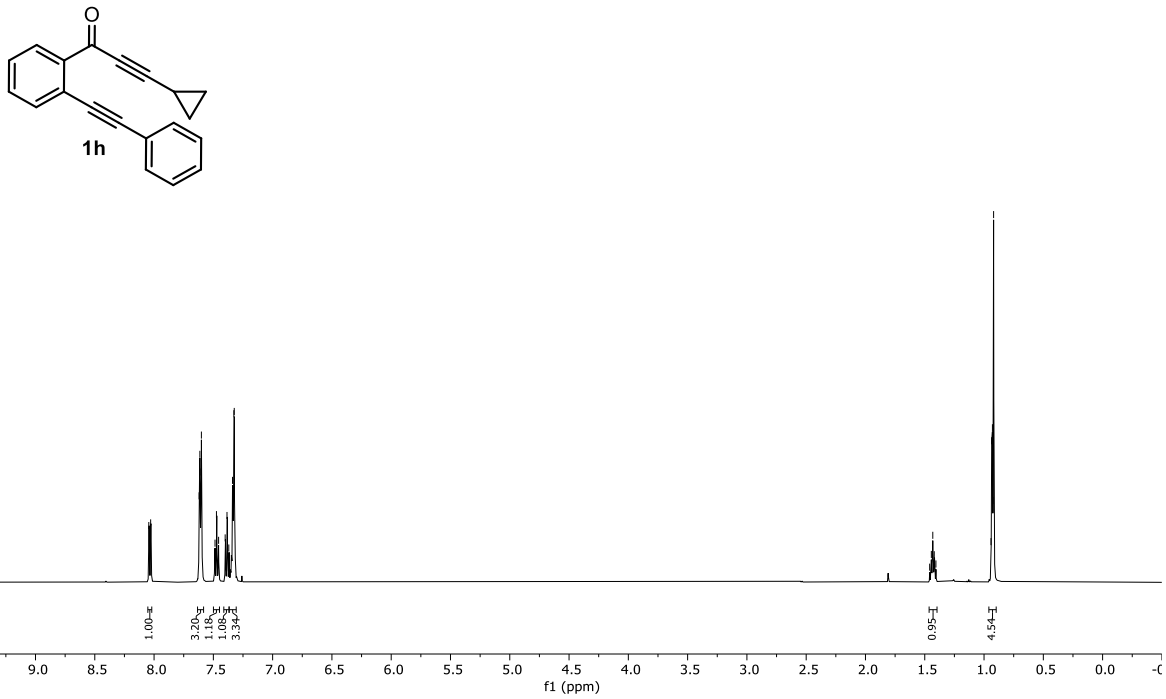
^{1}H NMR ($CDCl_3$, 500 MHz)



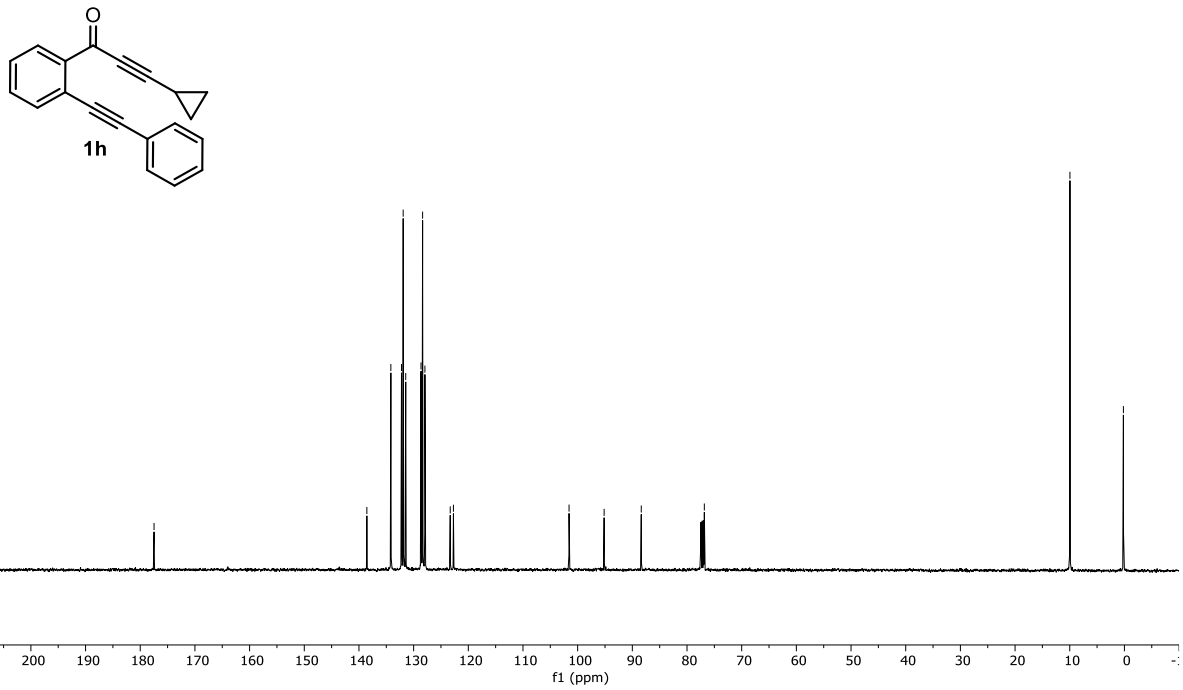
^{13}C NMR ($CDCl_3$, 125 MHz)



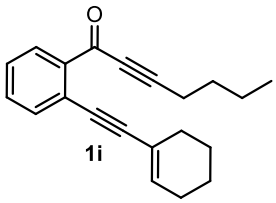
^{1}H NMR ($CDCl_3$, 500 MHz)

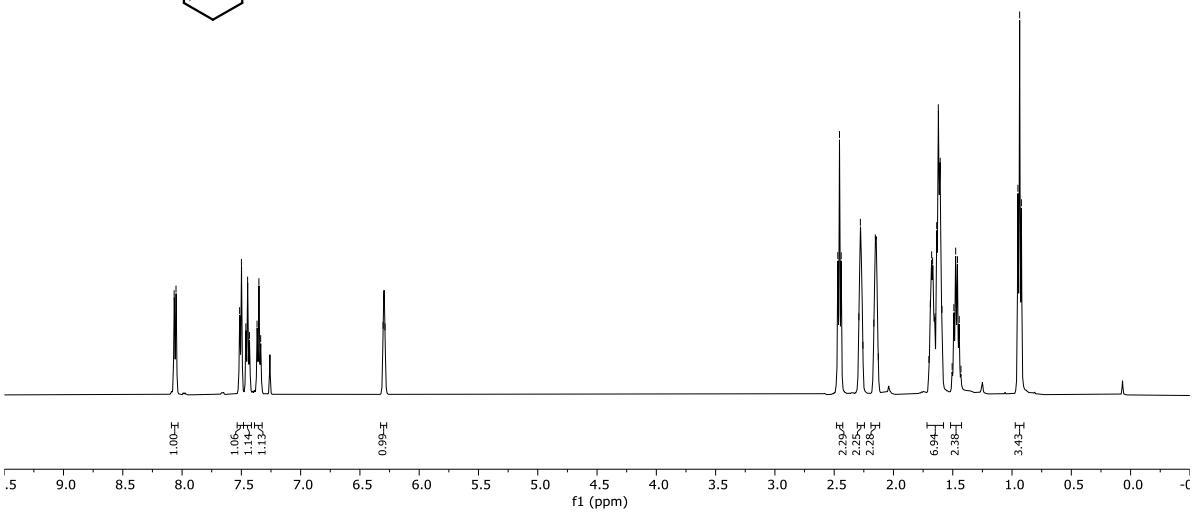


^{13}C NMR ($CDCl_3$, 125 MHz)

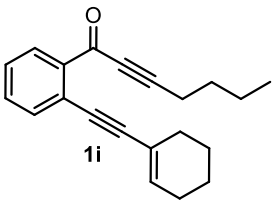


^{1}H NMR ($CDCl_3$, 500 MHz)

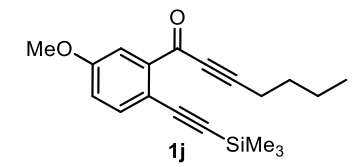




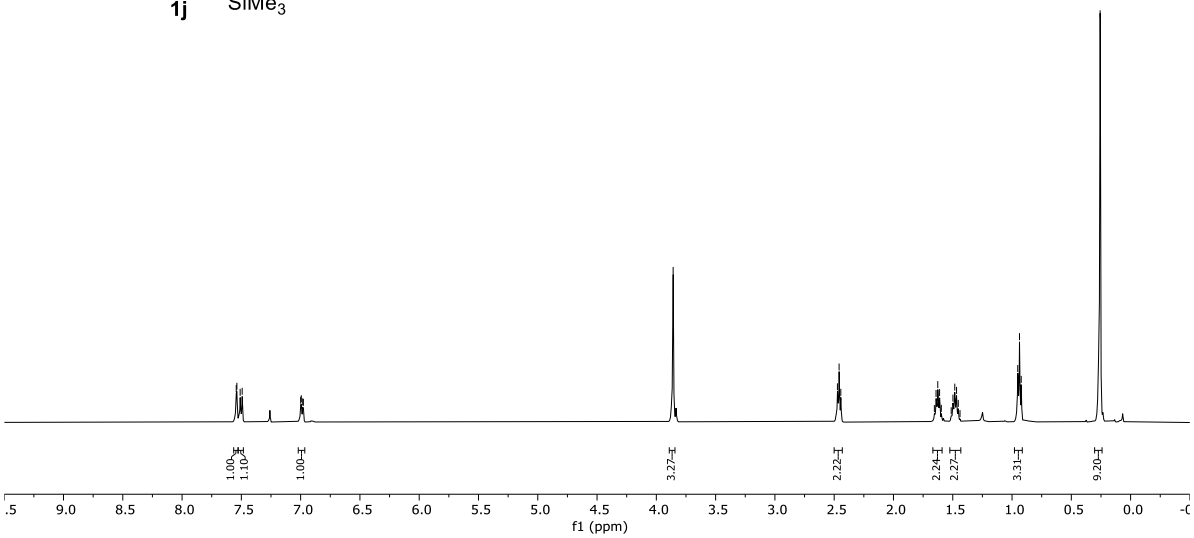
^{13}C NMR ($CDCl_3$, 125 MHz)



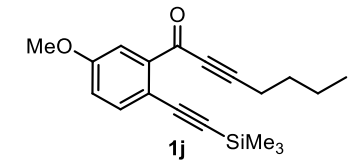
^{1}H NMR ($CDCl_3$, 500 MHz)



1j

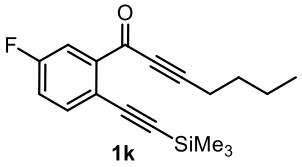


^{13}C NMR ($CDCl_3$, 125 MHz)

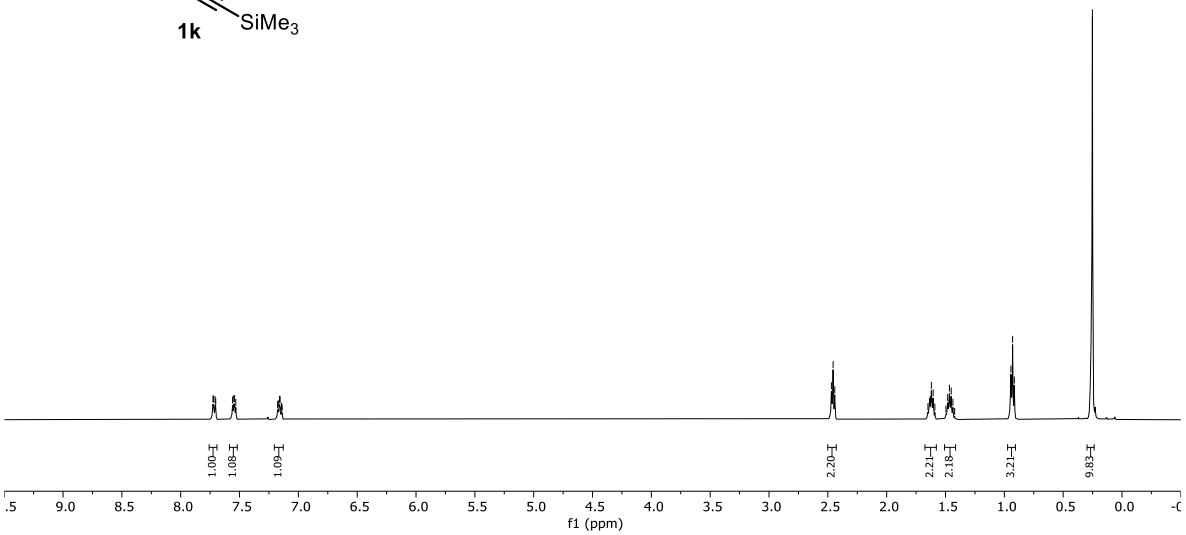


1j

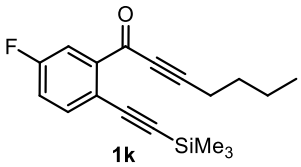
^{1}H NMR ($CDCl_3$, 500 MHz)



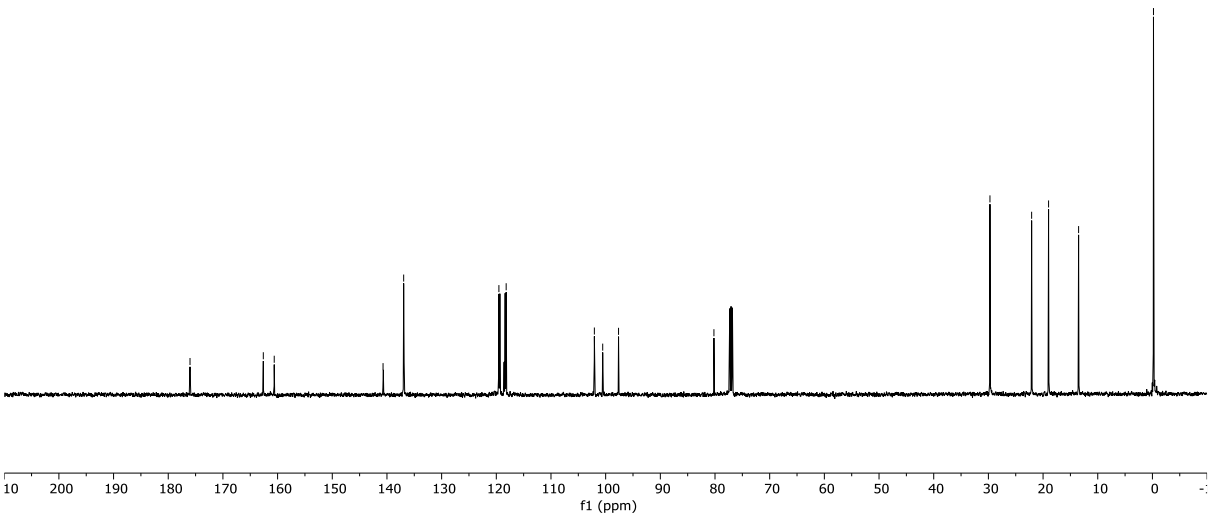
1k



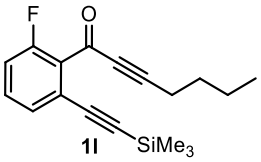
^{13}C NMR ($CDCl_3$, 125 MHz)



1k

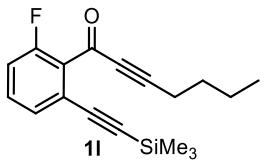


^{1}H NMR ($CDCl_3$, 500 MHz)



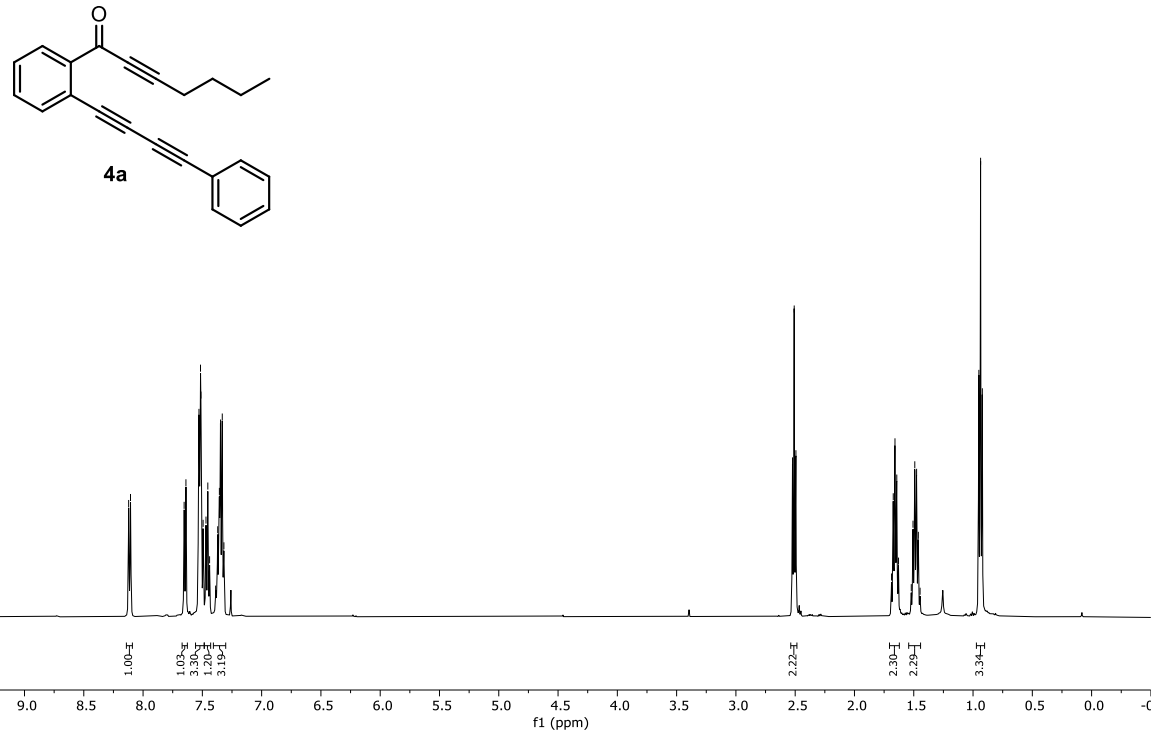
1l

^{13}C NMR ($CDCl_3$, 125 MHz)

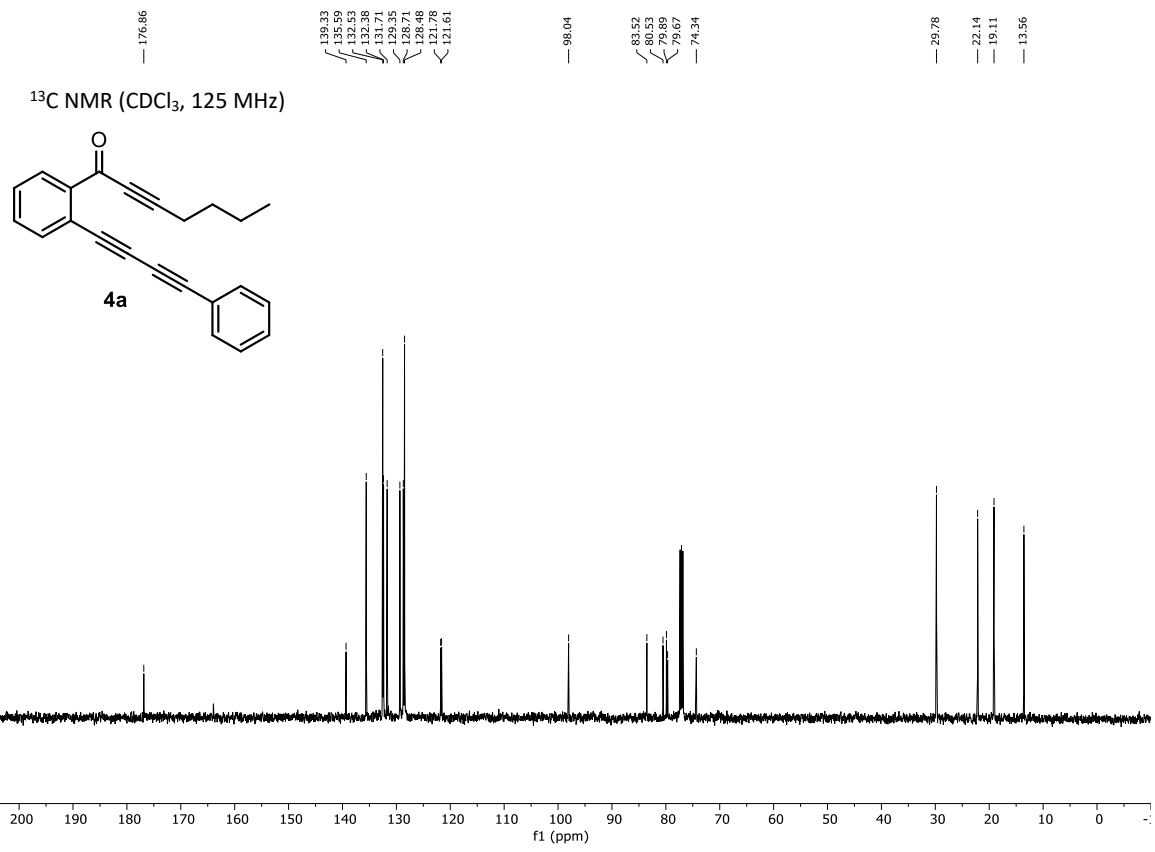


1l

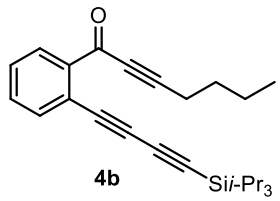
^{1}H NMR ($CDCl_3$, 500 MHz)



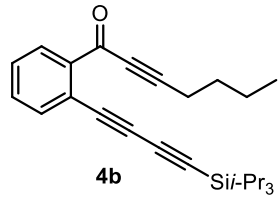
^{13}C NMR ($CDCl_3$, 125 MHz)



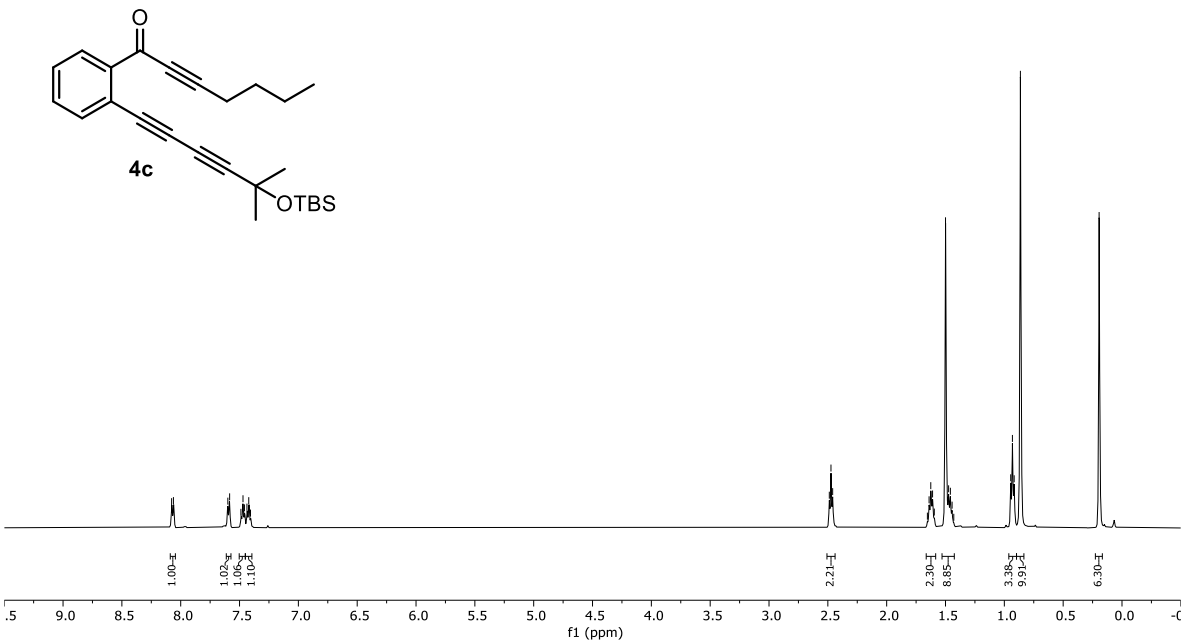
^{1}H NMR ($CDCl_3$, 500 MHz)



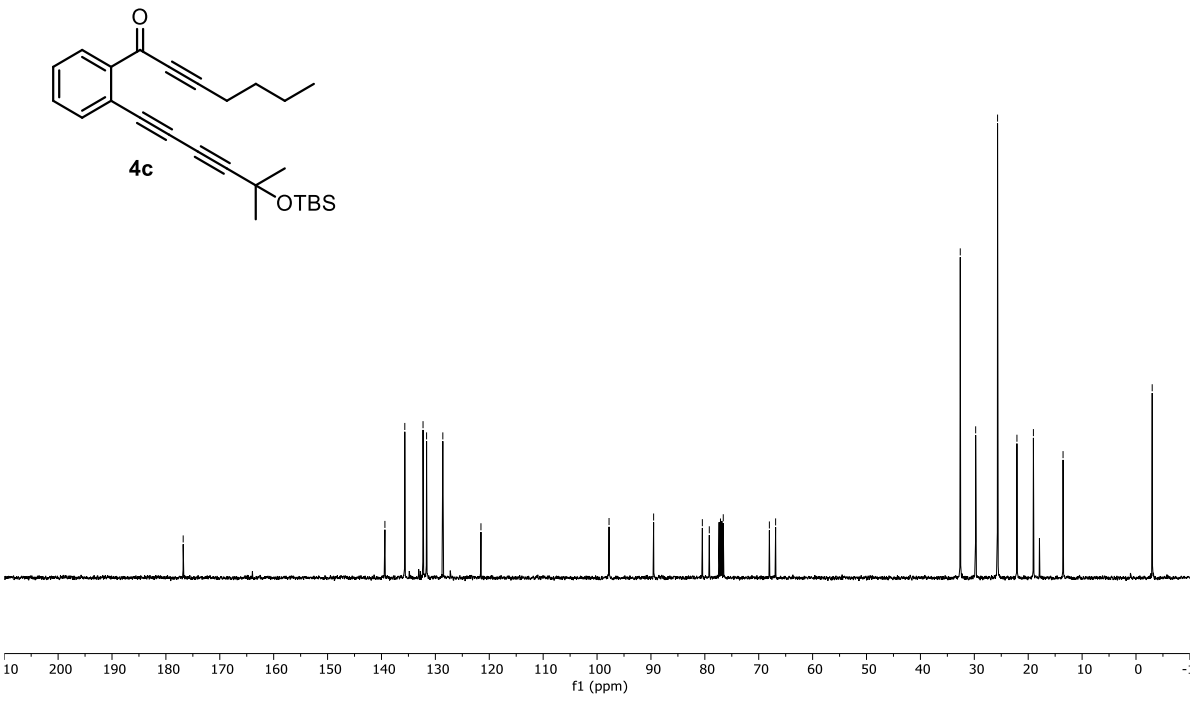
^{13}C NMR ($CDCl_3$, 125 MHz)



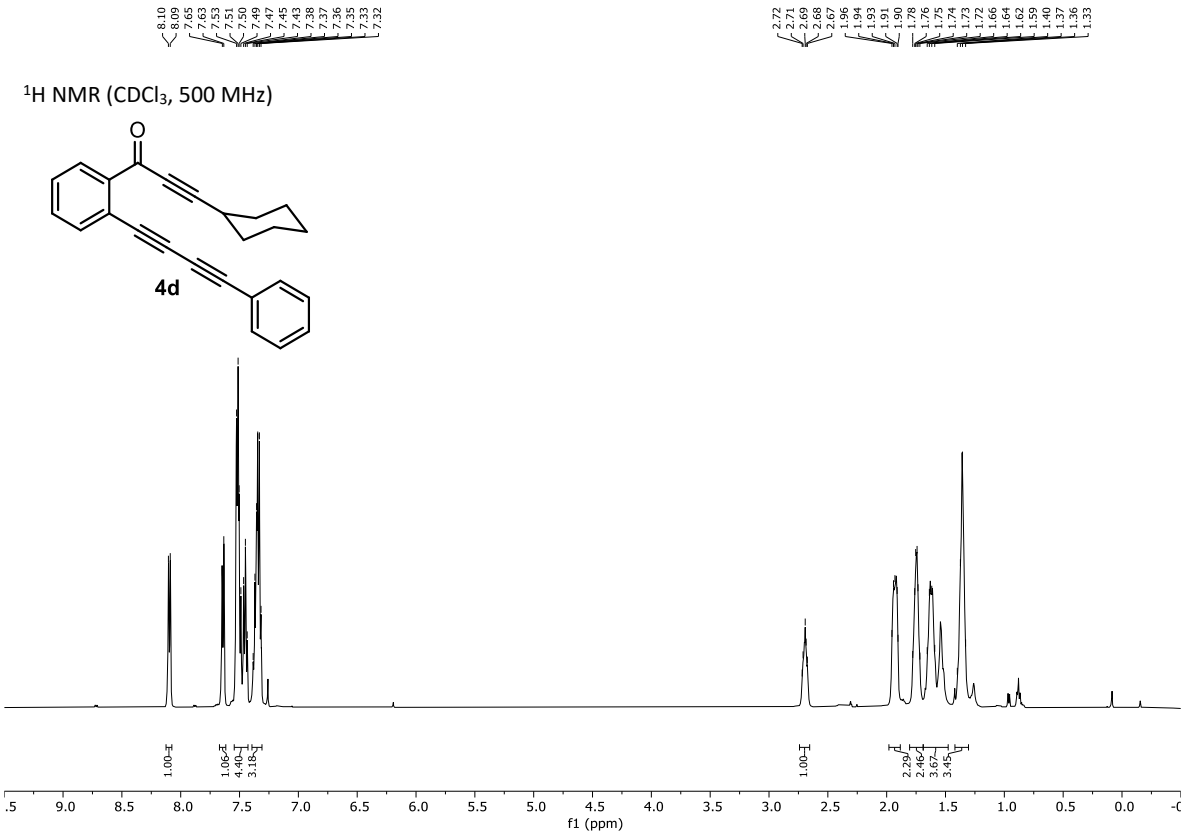
^{1}H NMR ($CDCl_3$, 500 MHz)



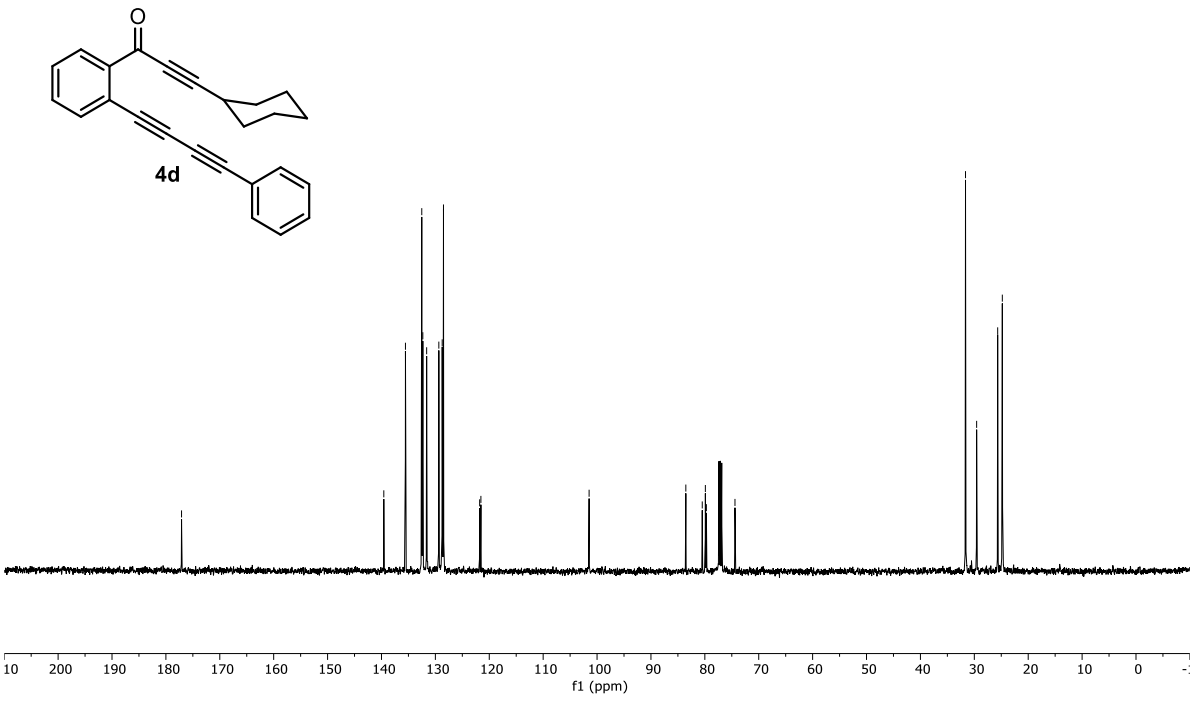
^{13}C NMR ($CDCl_3$, 125 MHz)



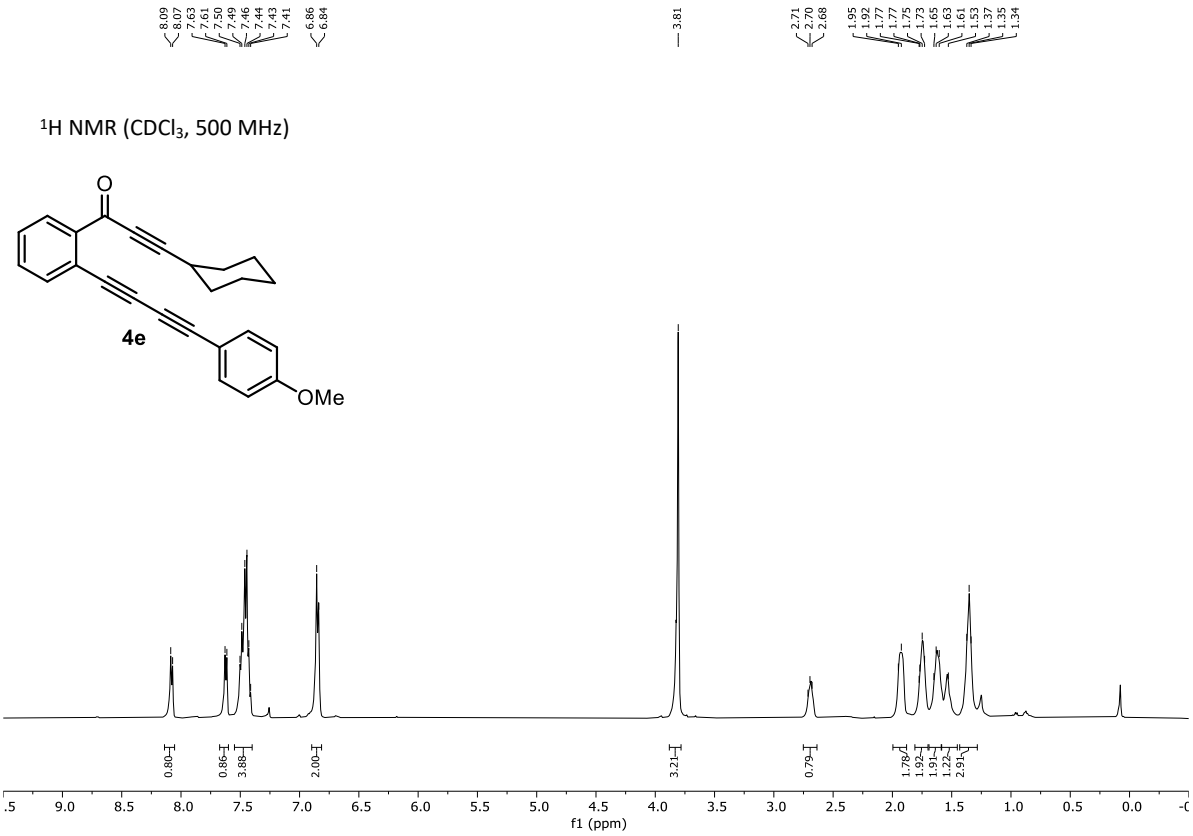
^{1}H NMR ($CDCl_3$, 500 MHz)



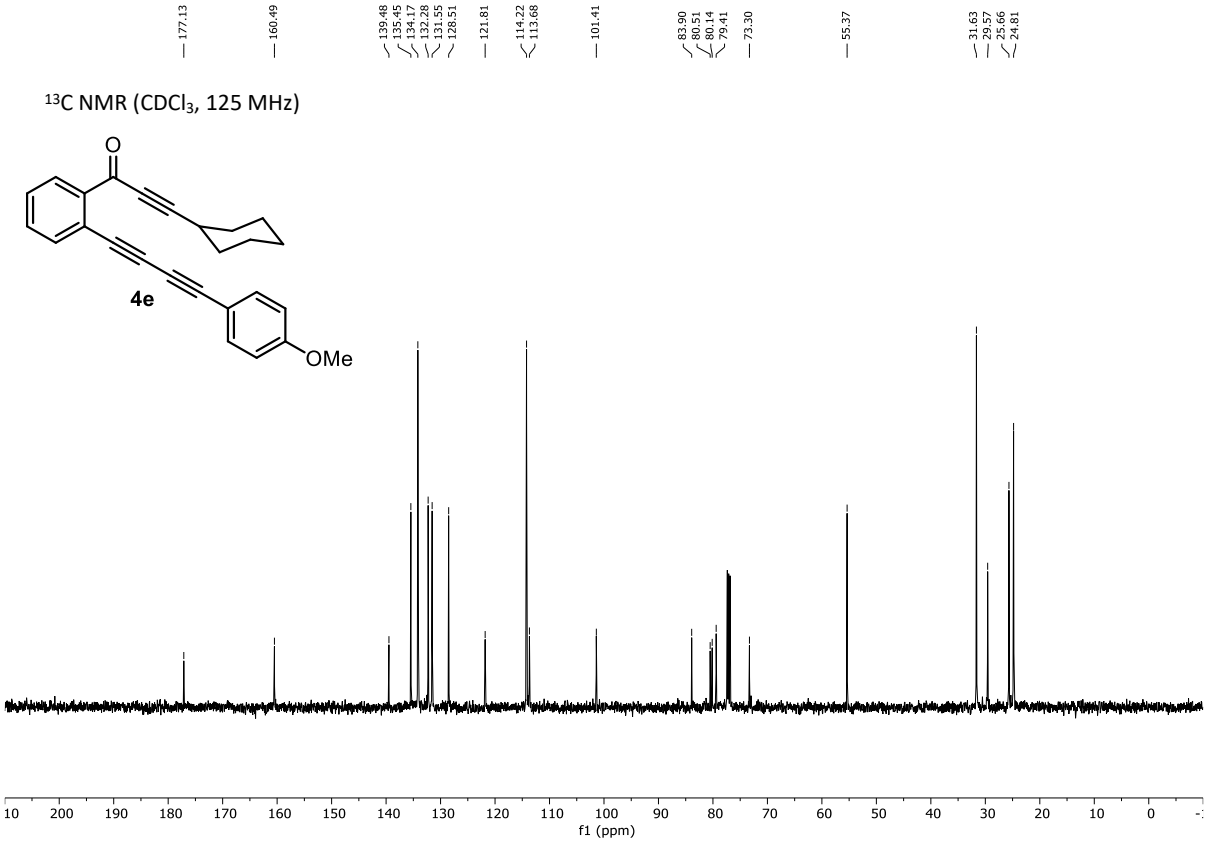
^{13}C NMR ($CDCl_3$, 125 MHz)



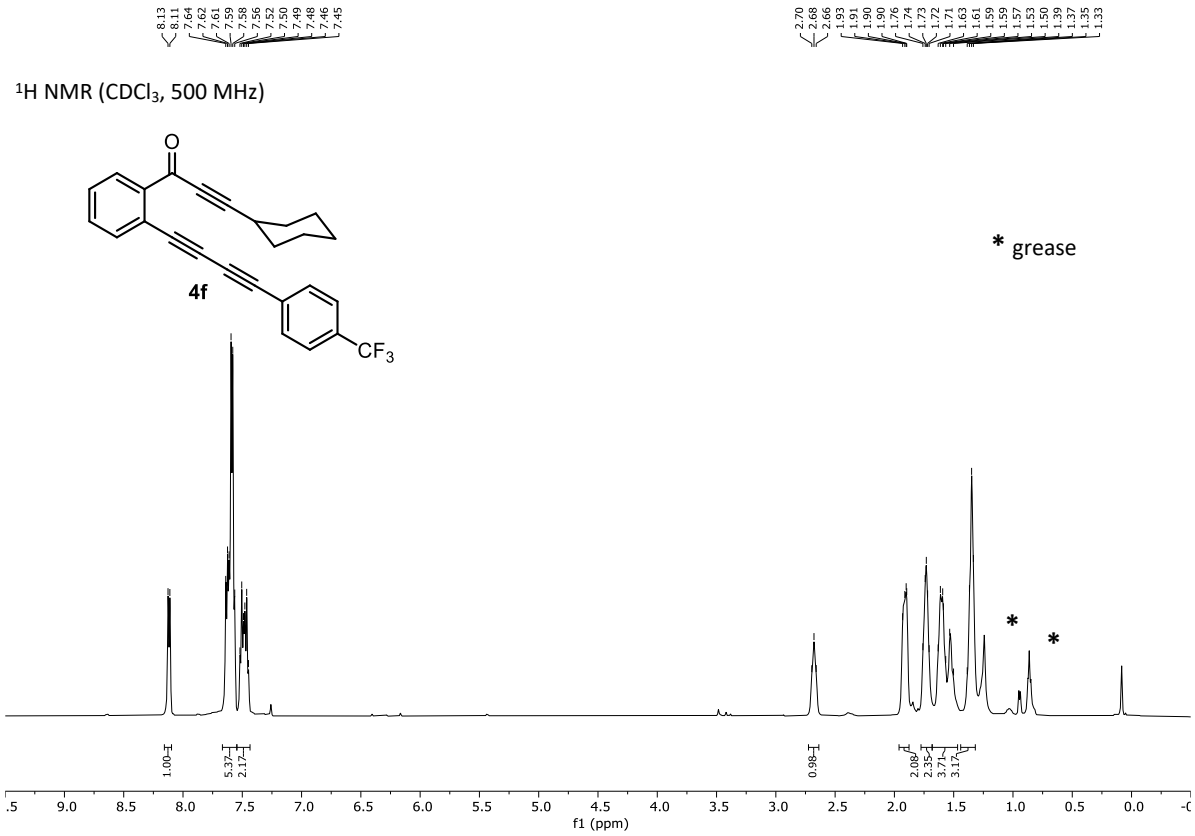
^{1}H NMR ($CDCl_3$, 500 MHz)

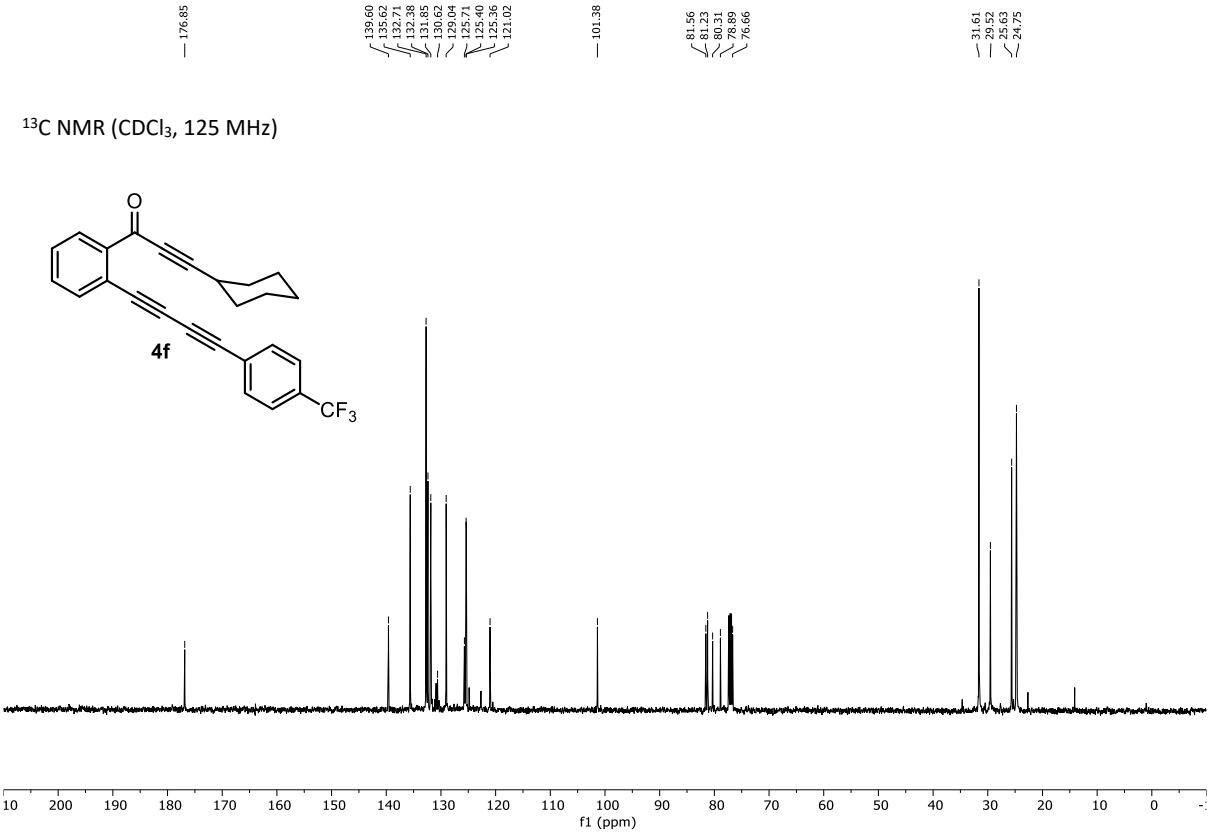


^{13}C NMR ($CDCl_3$, 125 MHz)



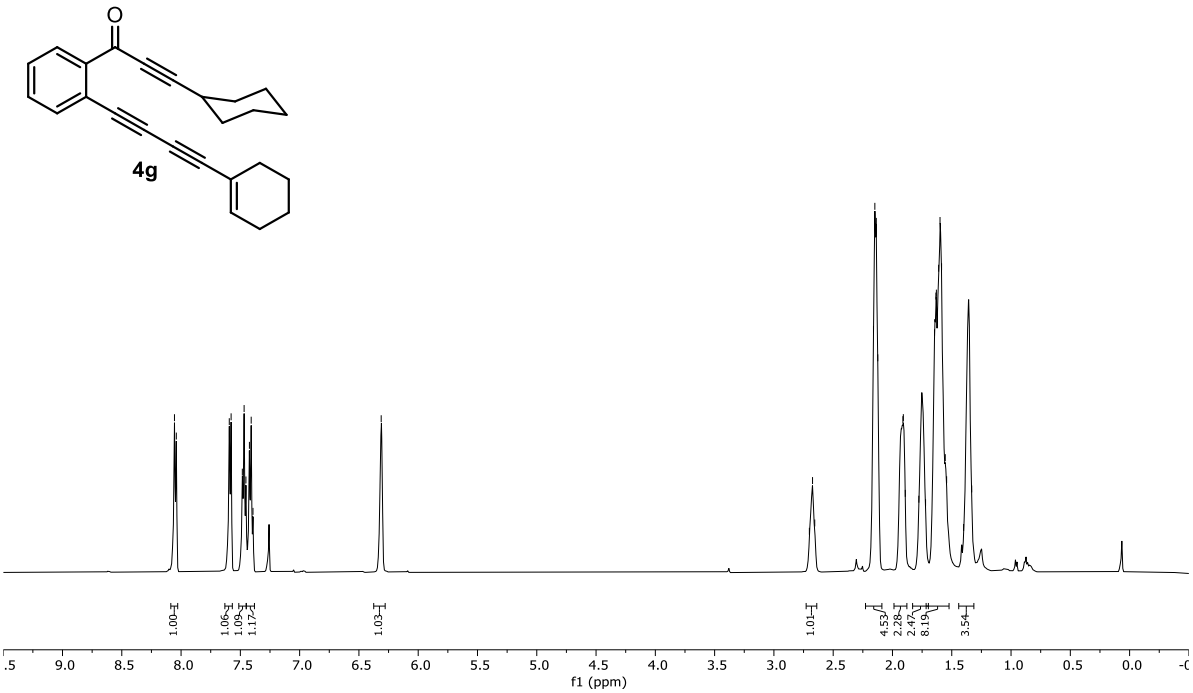
^{1}H NMR ($CDCl_3$, 500 MHz)



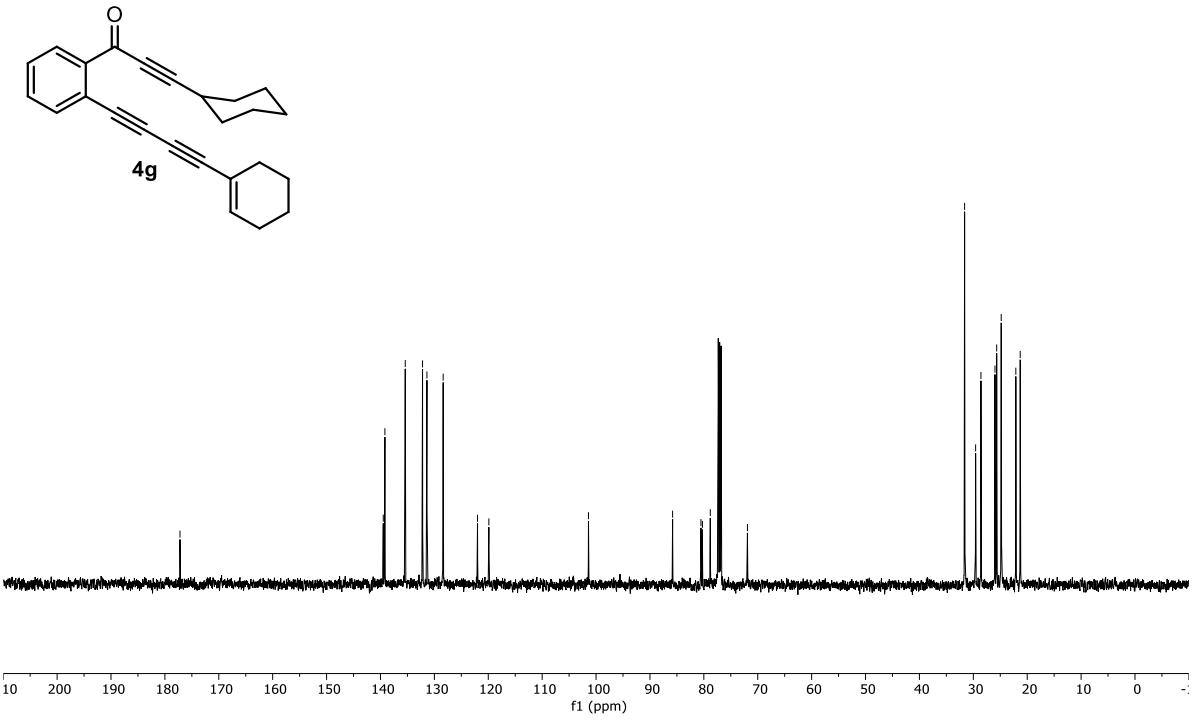


^{13}C NMR ($CDCl_3$, 125 MHz)

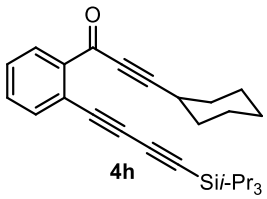
^{1}H NMR ($CDCl_3$, 500 MHz)

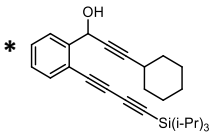


^{13}C NMR ($CDCl_3$, 125 MHz)

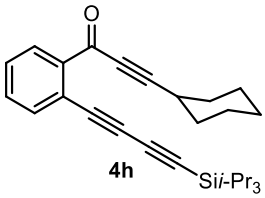


^{1}H NMR ($CDCl_3$, 500 MHz)

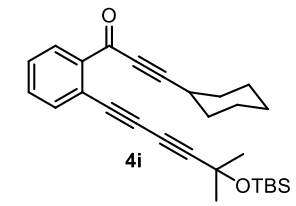




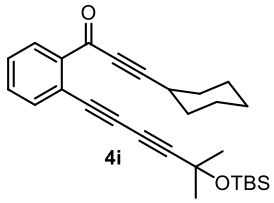
^{13}C NMR ($CDCl_3$, 125 MHz)



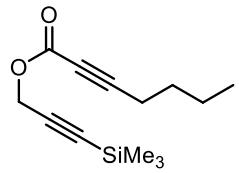
^{1}H NMR ($CDCl_3$, 500 MHz)



^{13}C NMR ($CDCl_3$, 125 MHz)

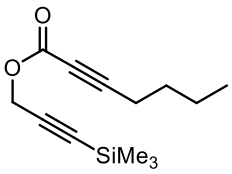


^{1}H NMR ($CDCl_3$, 500 MHz)



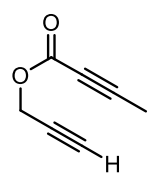
6a

^{13}C NMR ($CDCl_3$, 125 MHz)



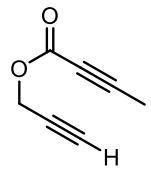
6a

^{1}H NMR ($CDCl_3$, 500 MHz)



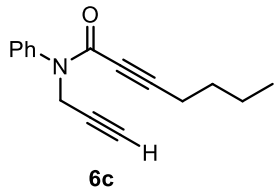
6b

^{13}C NMR ($CDCl_3$, 125 MHz)

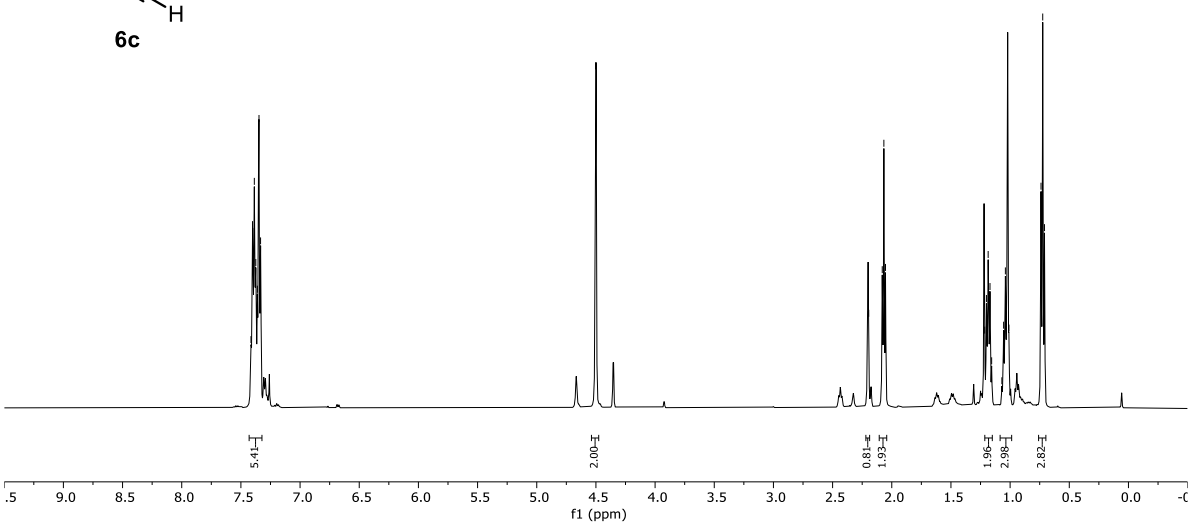


6b

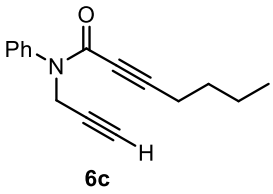
^{1}H NMR ($CDCl_3$, 500 MHz)



6c

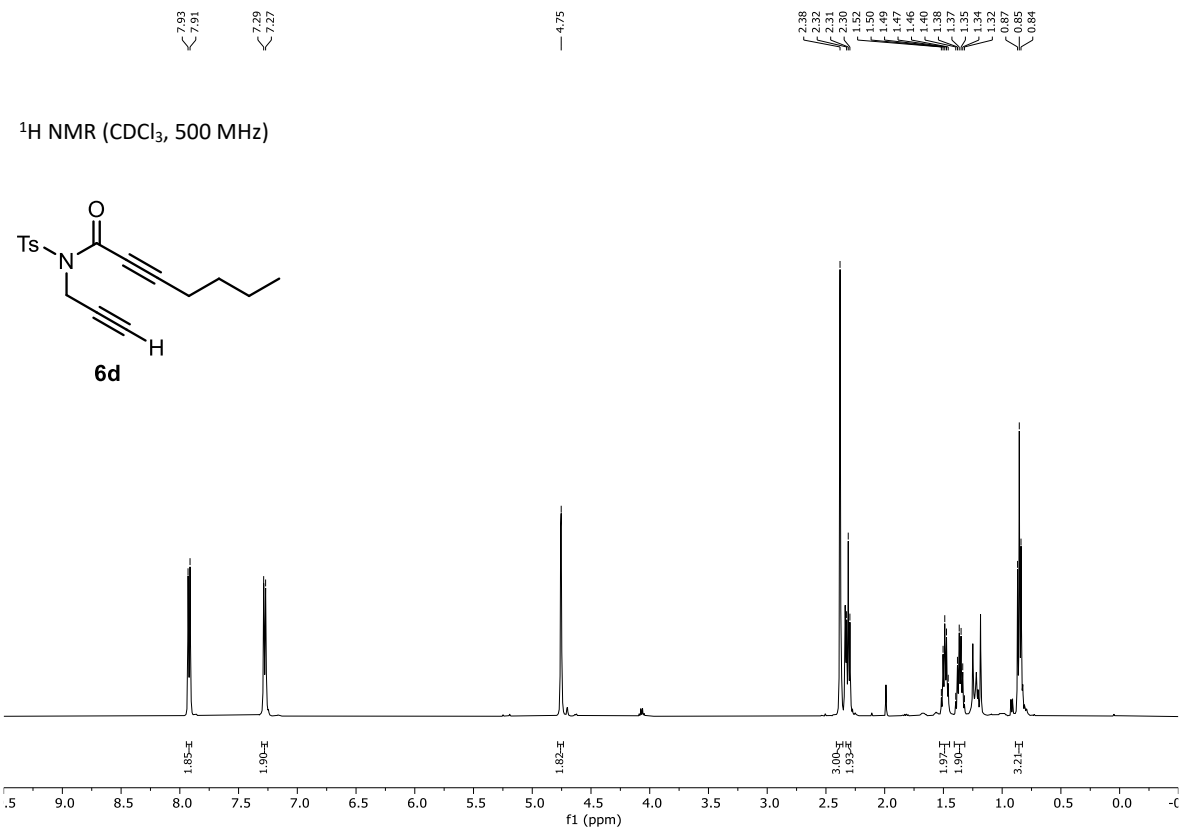


^{13}C NMR ($CDCl_3$, 125 MHz)

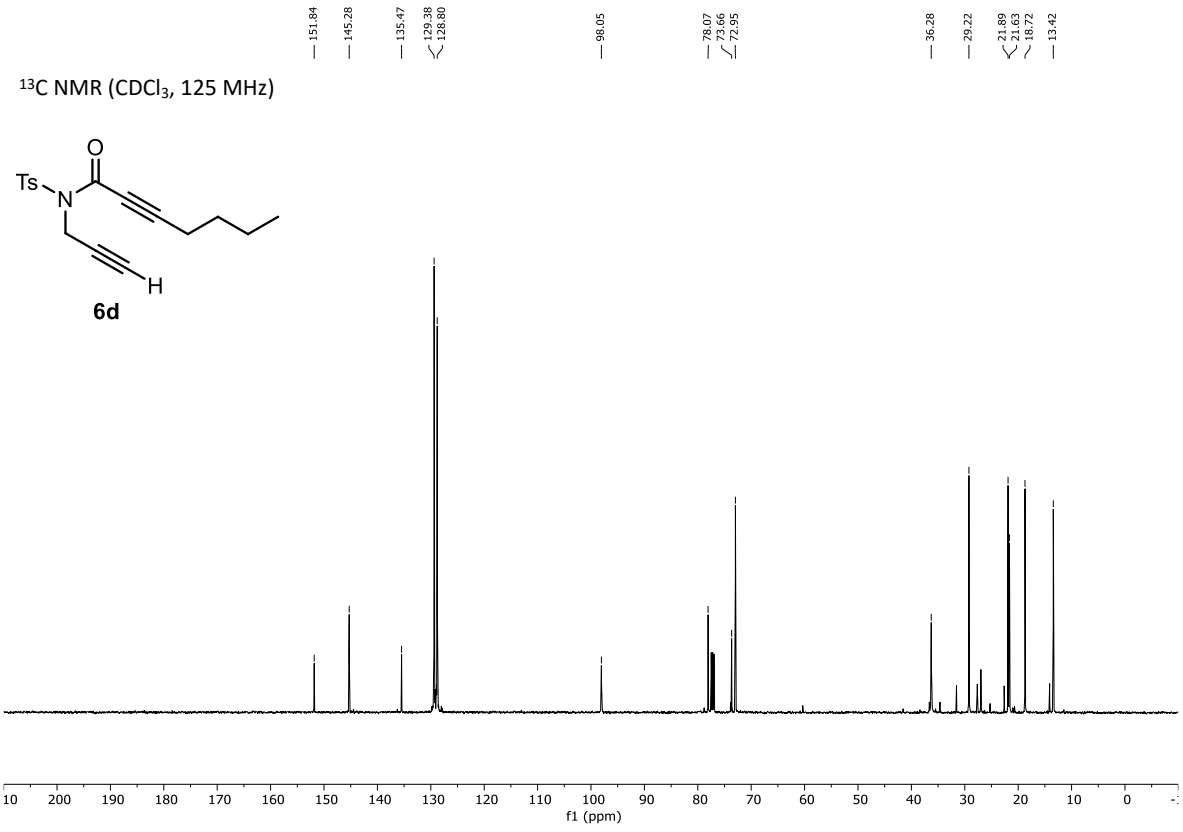


6c

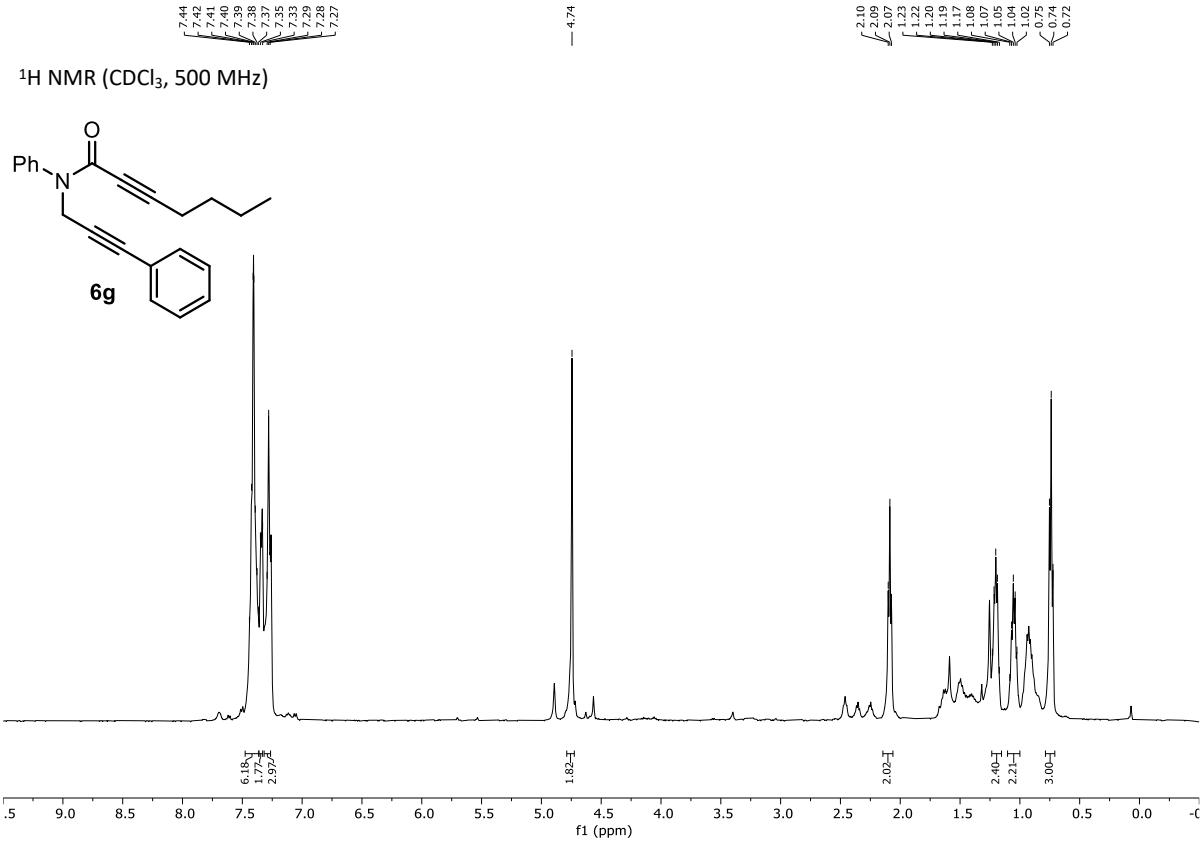
^{1}H NMR ($CDCl_3$, 500 MHz)



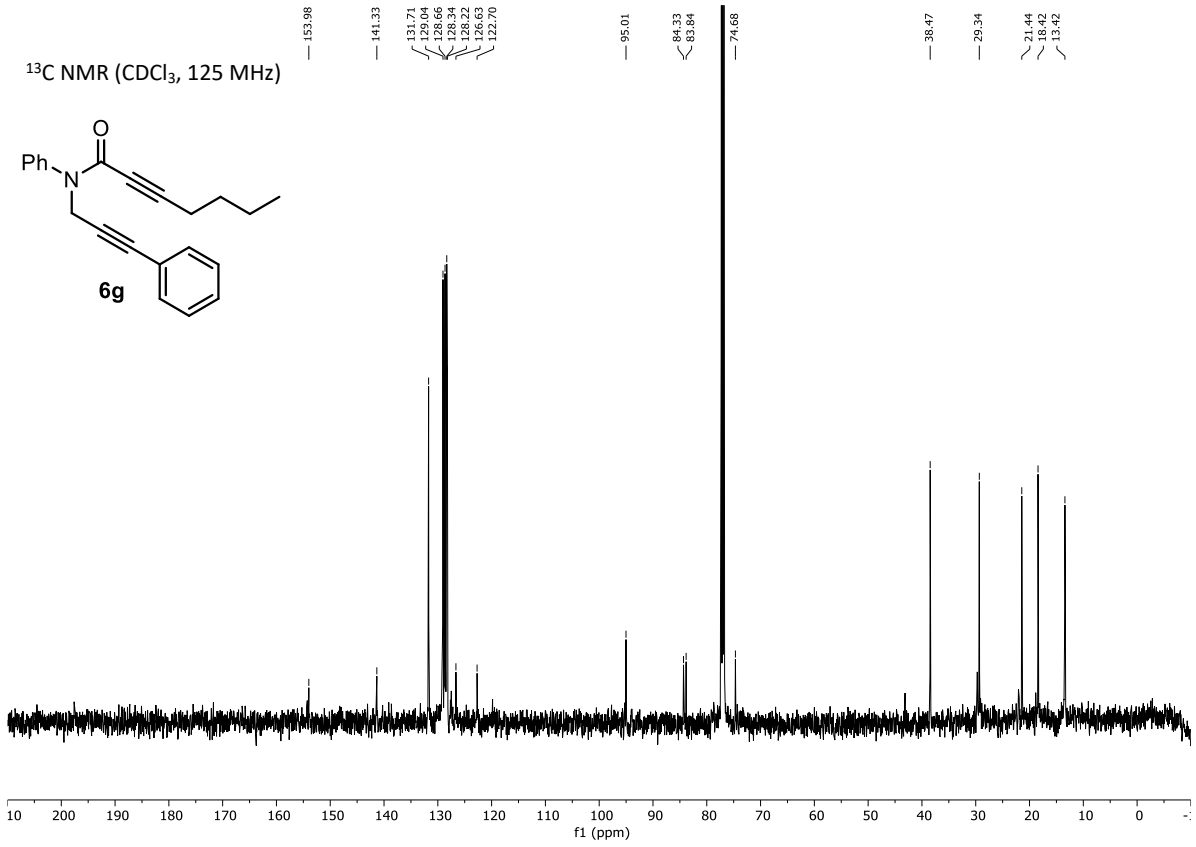
^{13}C NMR ($CDCl_3$, 125 MHz)



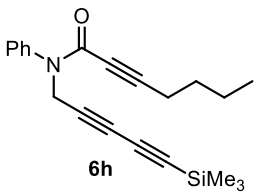
^{1}H NMR ($CDCl_3$, 500 MHz)



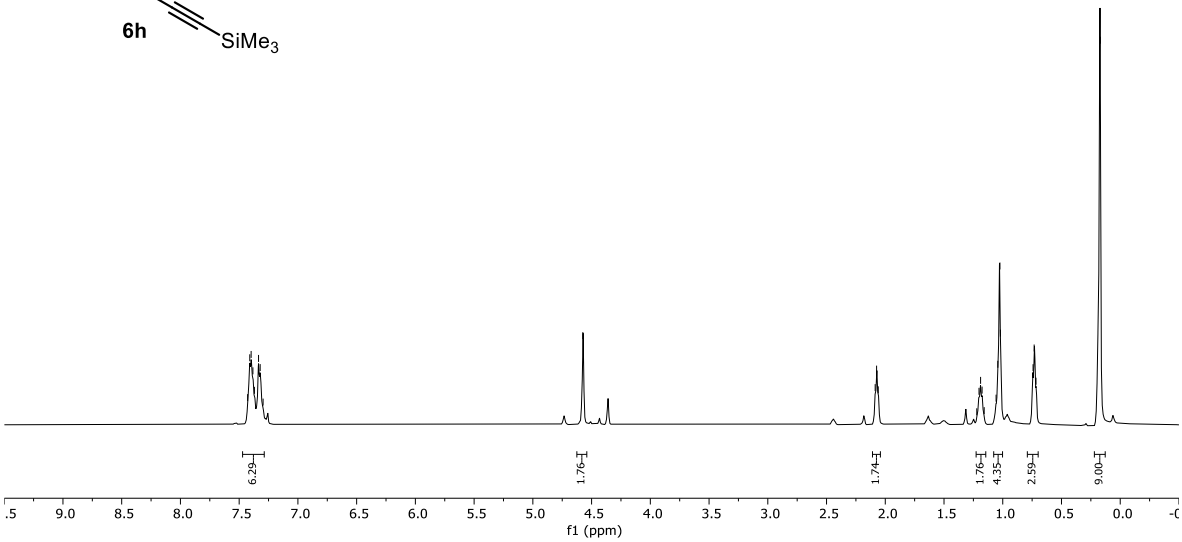
^{13}C NMR ($CDCl_3$, 125 MHz)



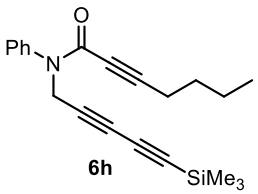
^{1}H NMR ($CDCl_3$, 500 MHz)



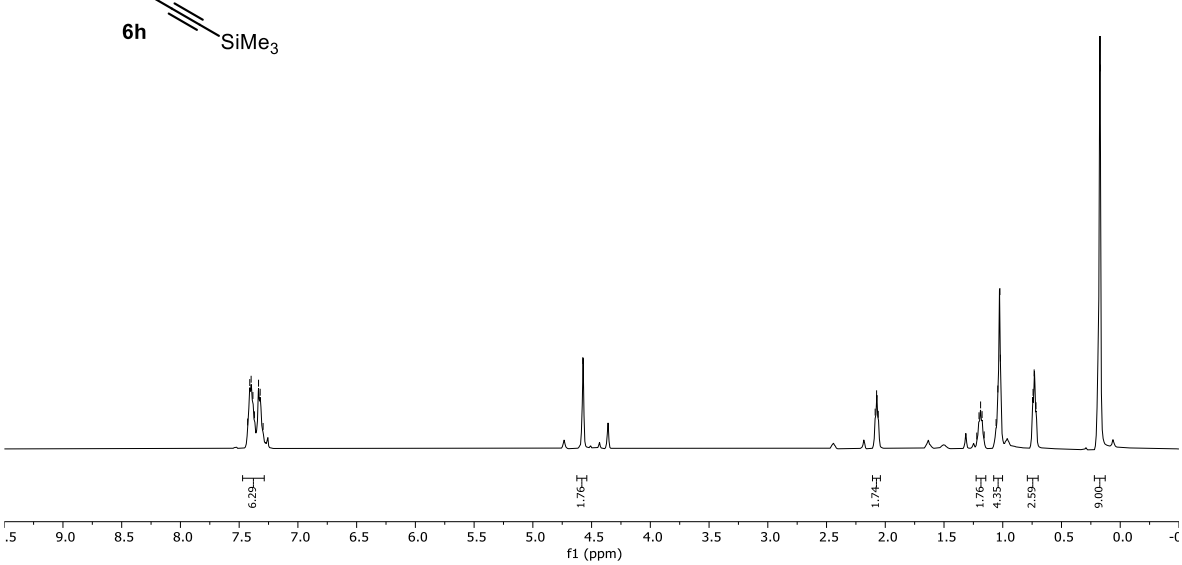
6h



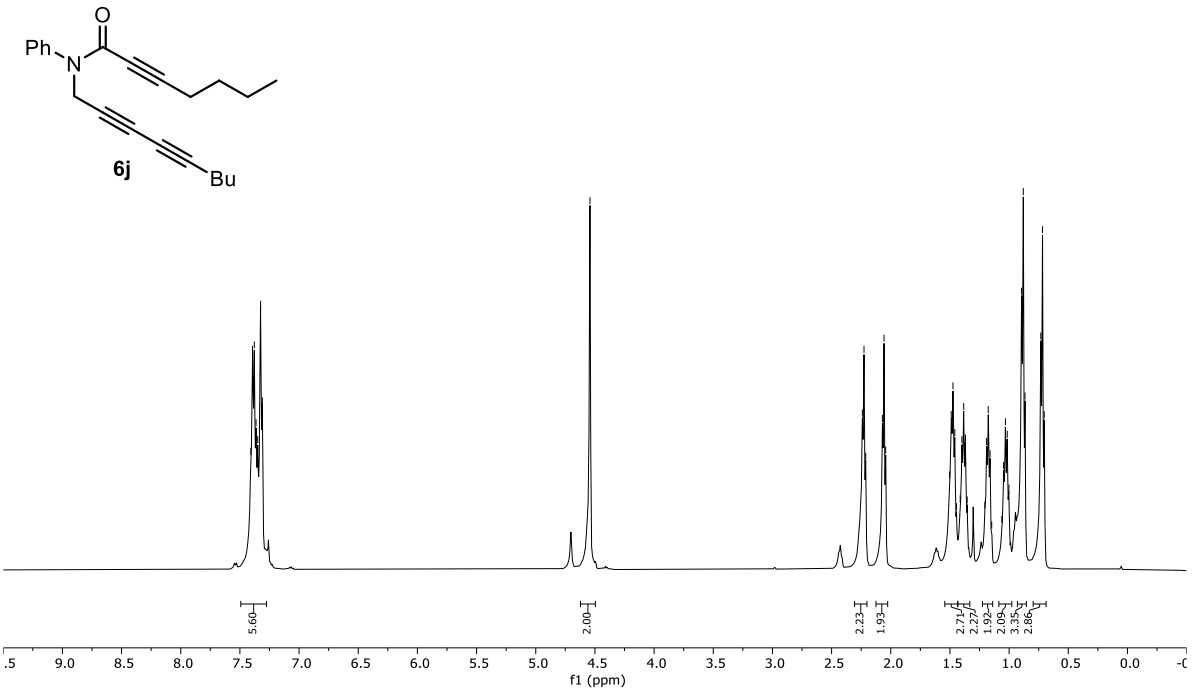
^{13}C NMR ($CDCl_3$, 125 MHz)



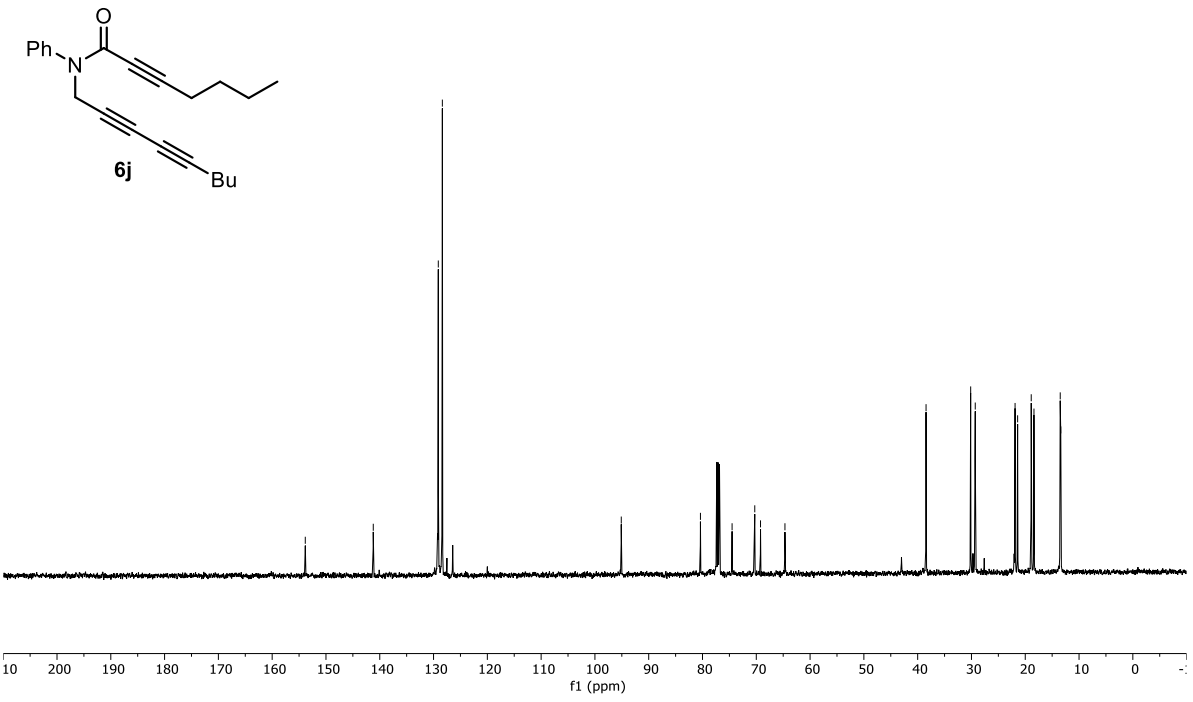
6h



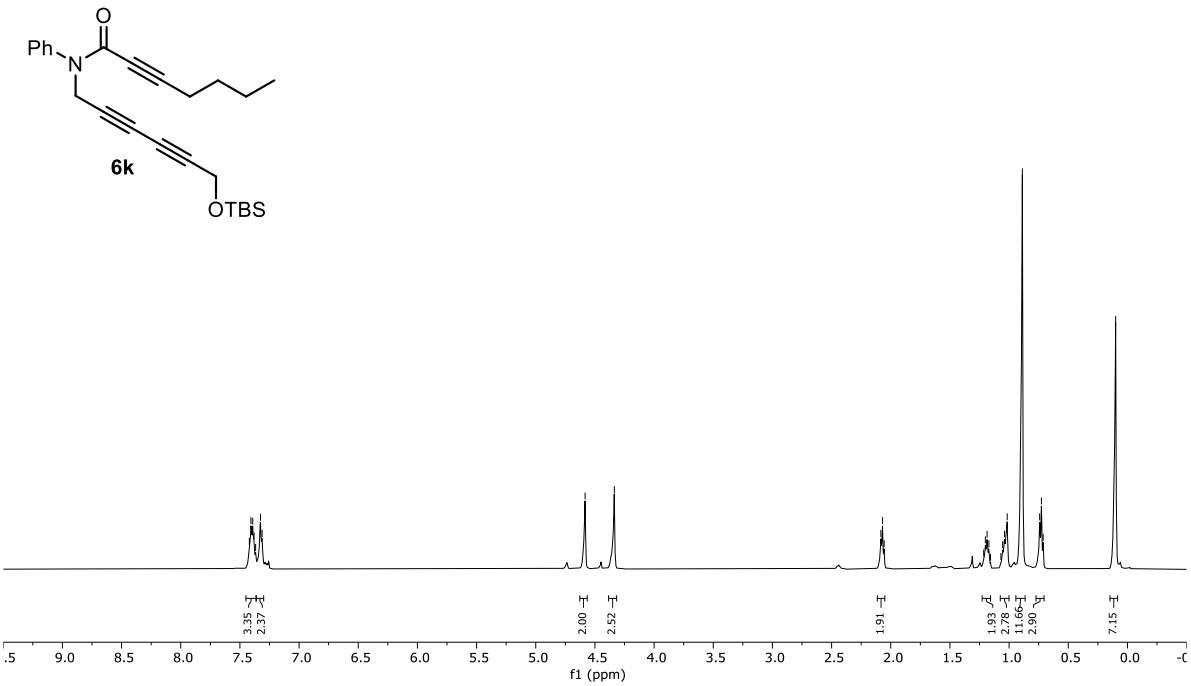
^{1}H NMR ($CDCl_3$, 500 MHz)



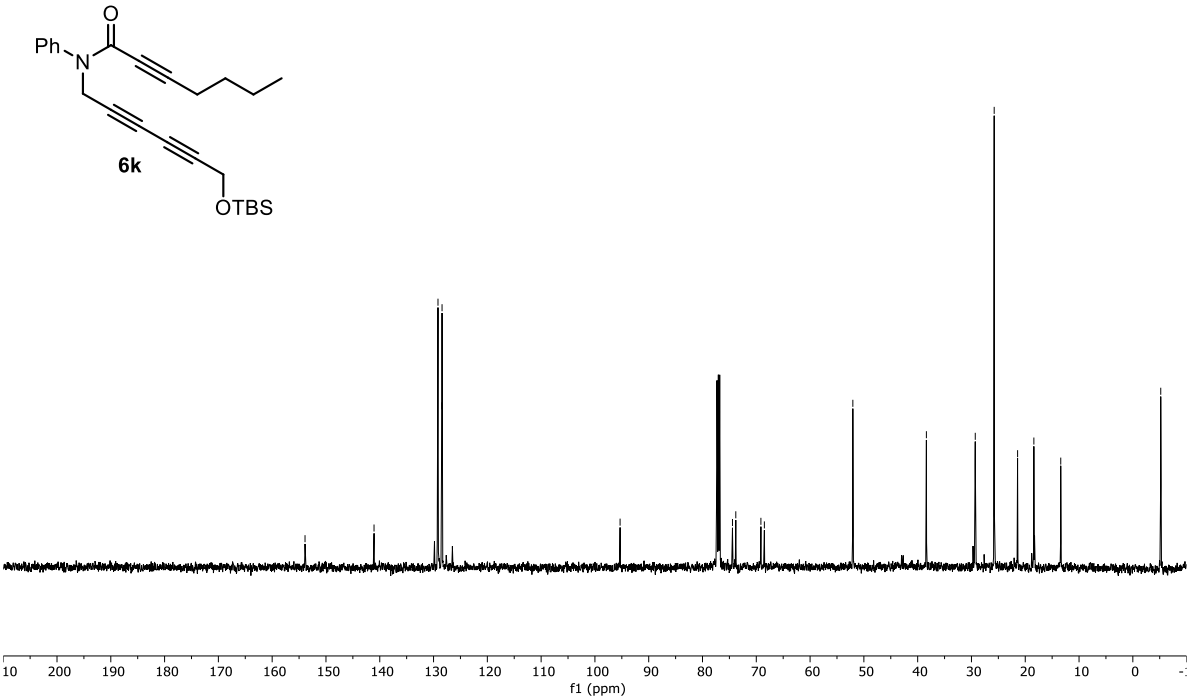
^{13}C NMR ($CDCl_3$, 125 MHz)



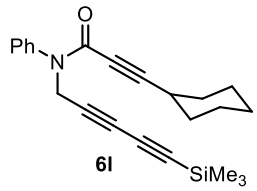
^{1}H NMR ($CDCl_3$, 500 MHz)



^{13}C NMR ($CDCl_3$, 125 MHz)

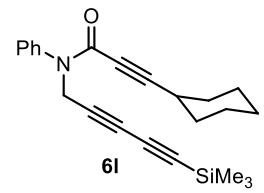


^{1}H NMR ($CDCl_3$, 500 MHz)



6l

^{13}C NMR ($CDCl_3$, 125 MHz)

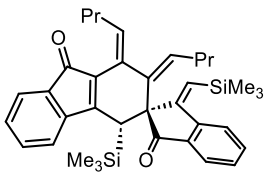


6l

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

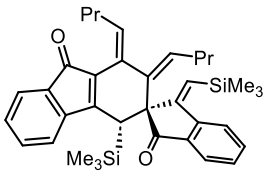
A. Dimerization of diynone

^{1}H NMR ($CDCl_3$, 500 MHz)

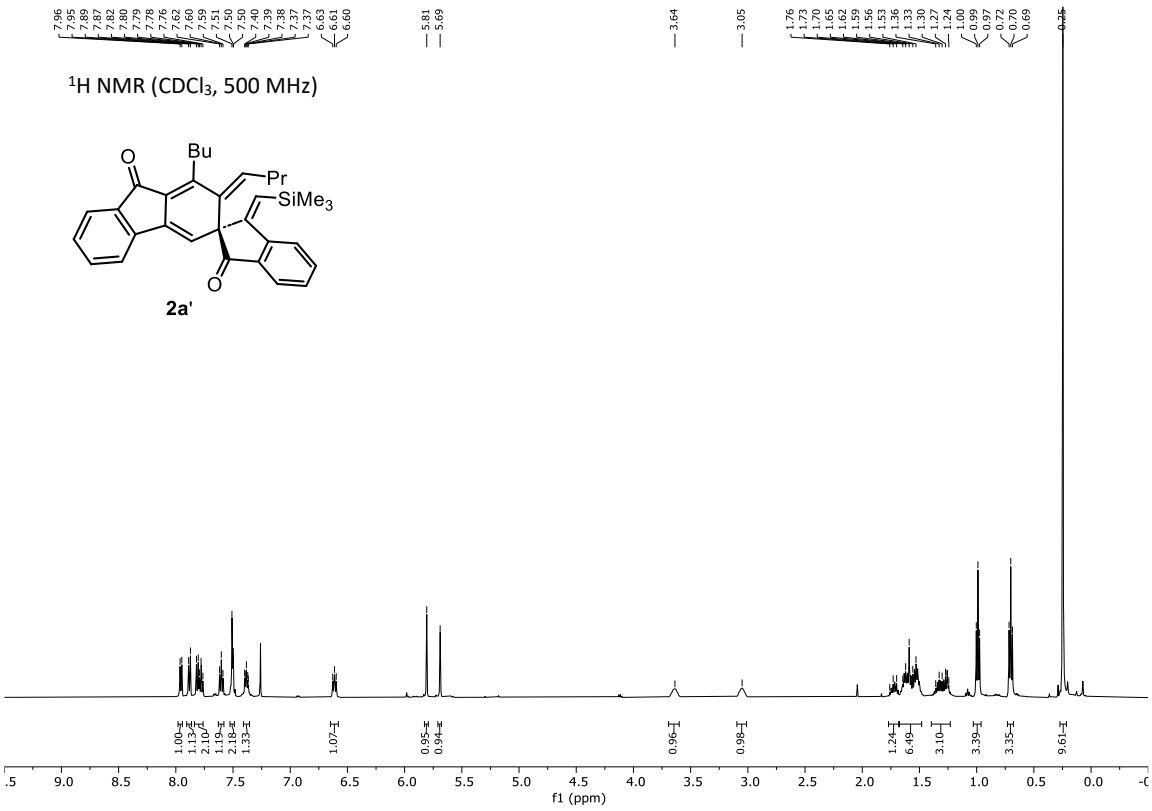


2a

^{13}C NMR ($CDCl_3$, 125 MHz)

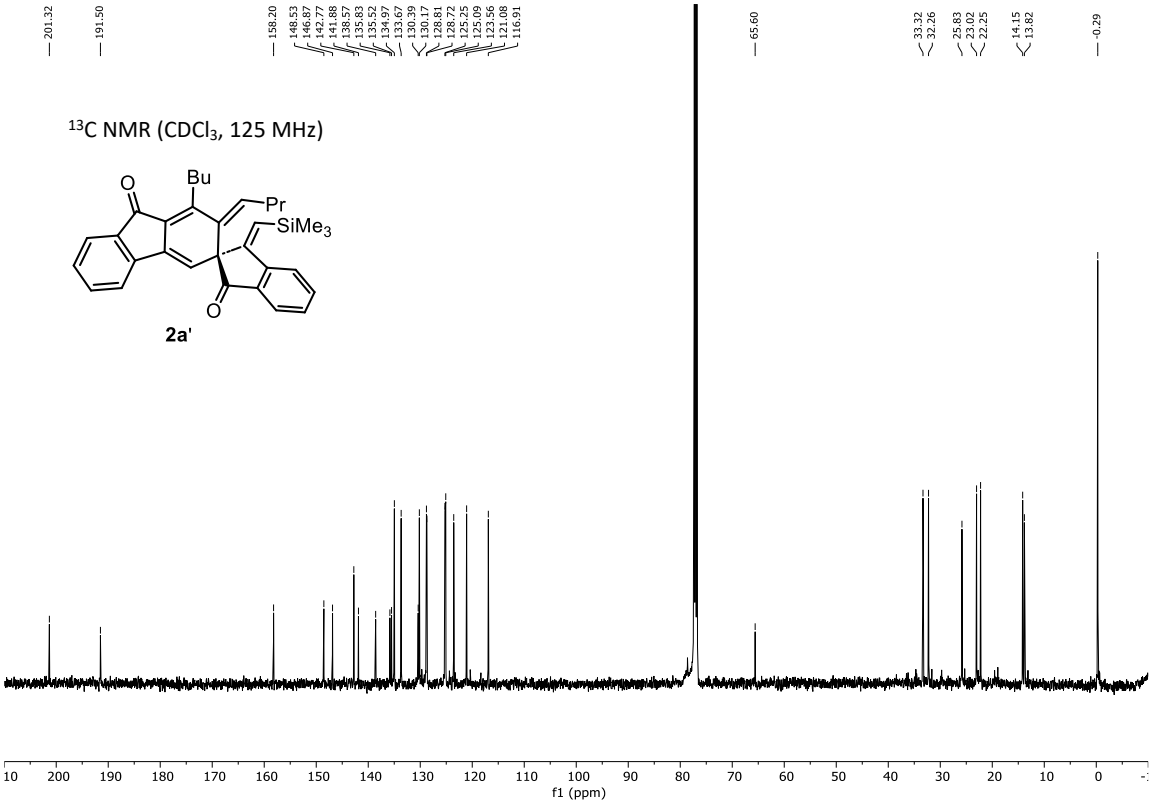


2a



^{1}H NMR ($CDCl_3$, 500 MHz)

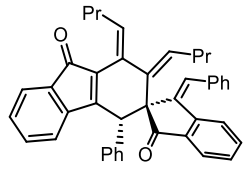
2a'



^{13}C NMR ($CDCl_3$, 125 MHz)

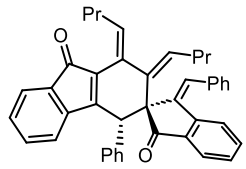
2a'

^{1}H NMR ($CDCl_3$, 500 MHz)



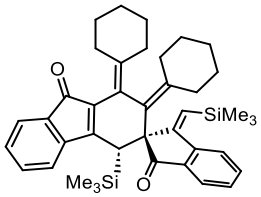
2b (dr = 3:1)

^{13}C NMR ($CDCl_3$, 125 MHz)



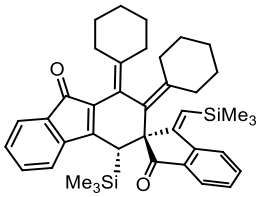
2b (dr = 3:1)

^{1}H NMR ($CDCl_3$, 500 MHz)

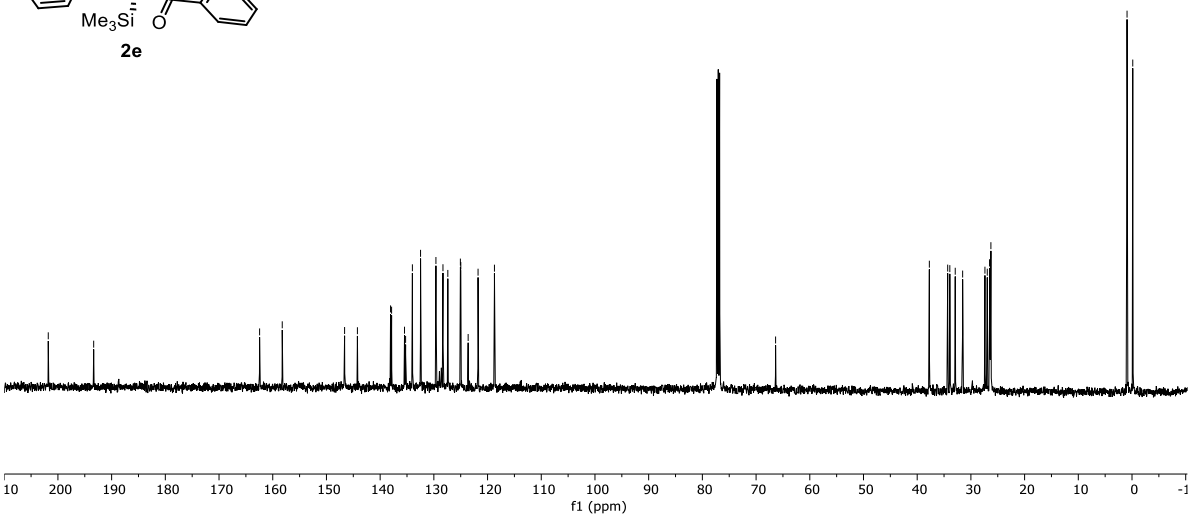


2e

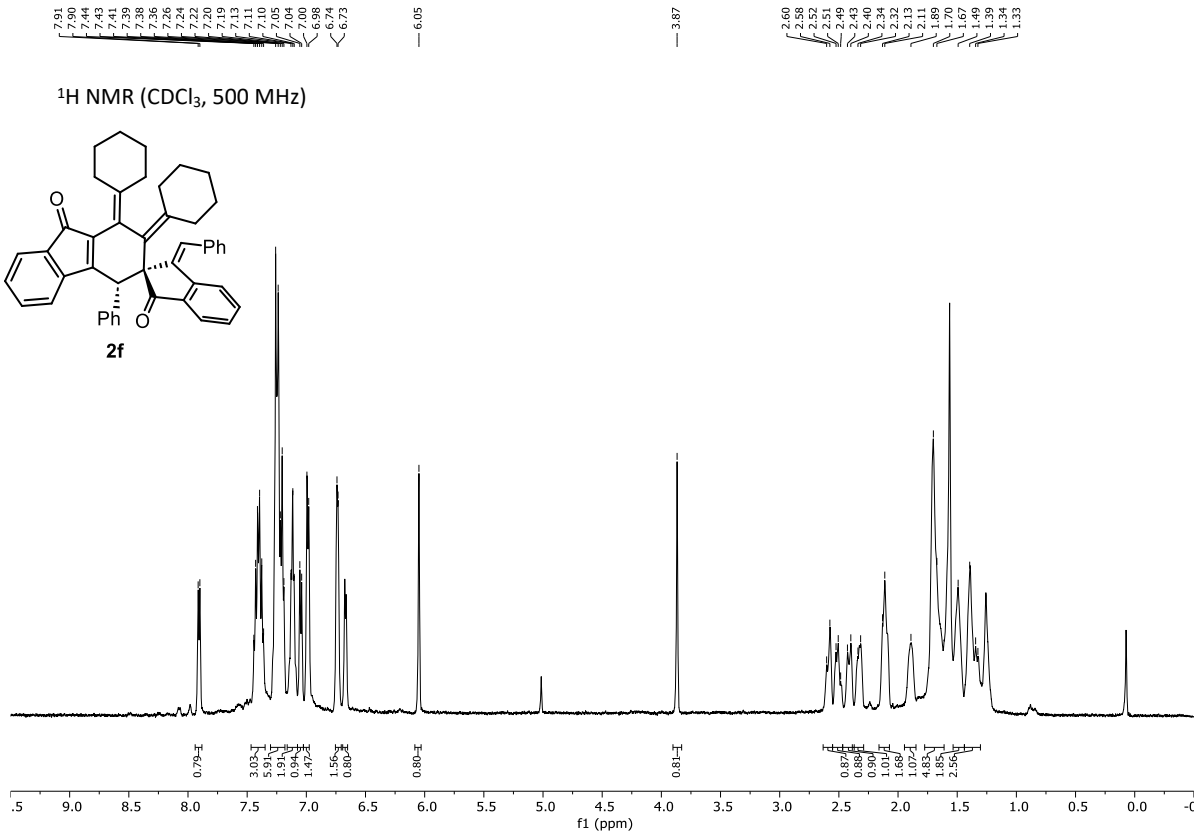
^{13}C NMR ($CDCl_3$, 125 MHz)



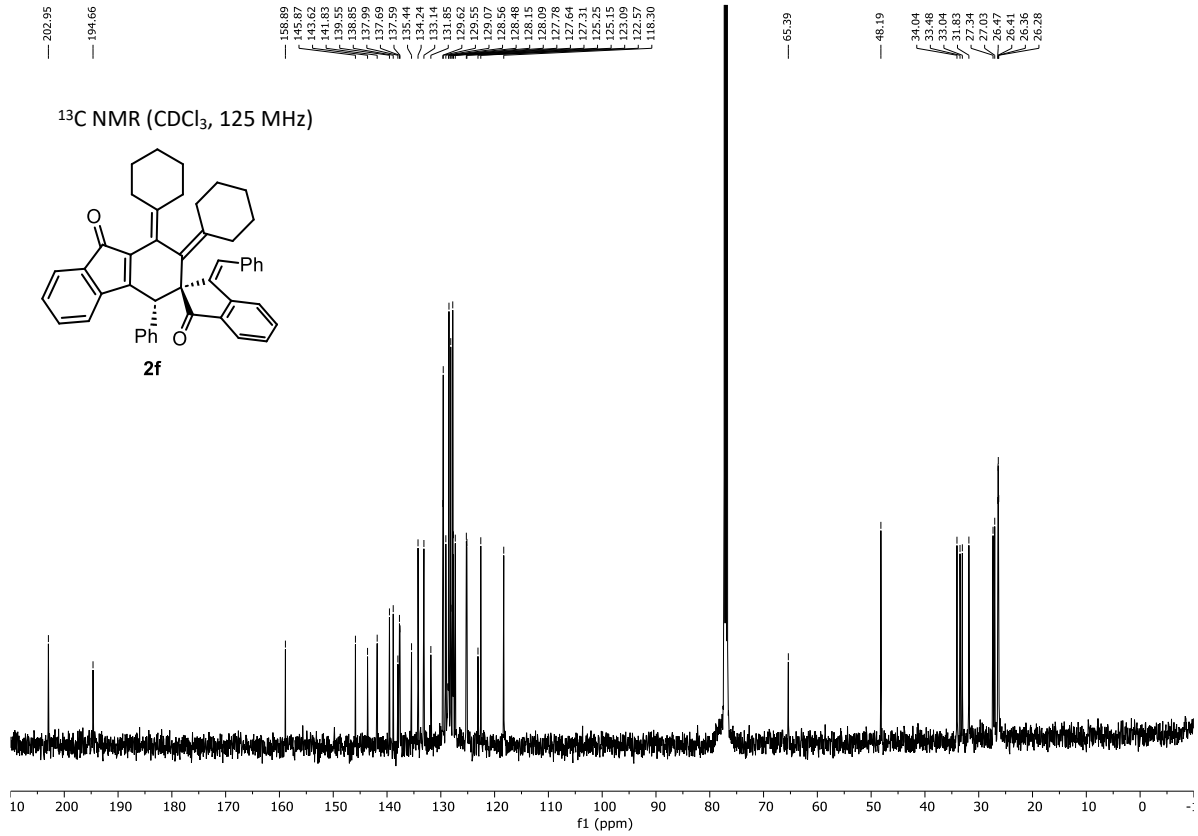
2e



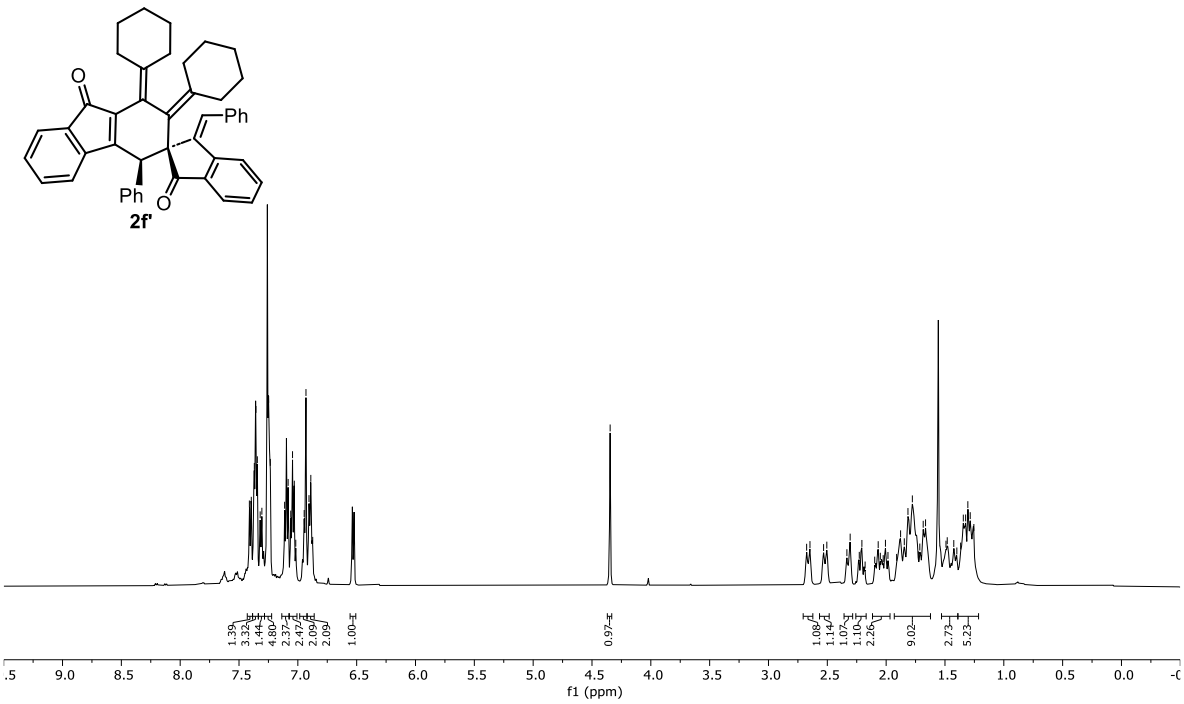
^{1}H NMR ($CDCl_3$, 500 MHz)



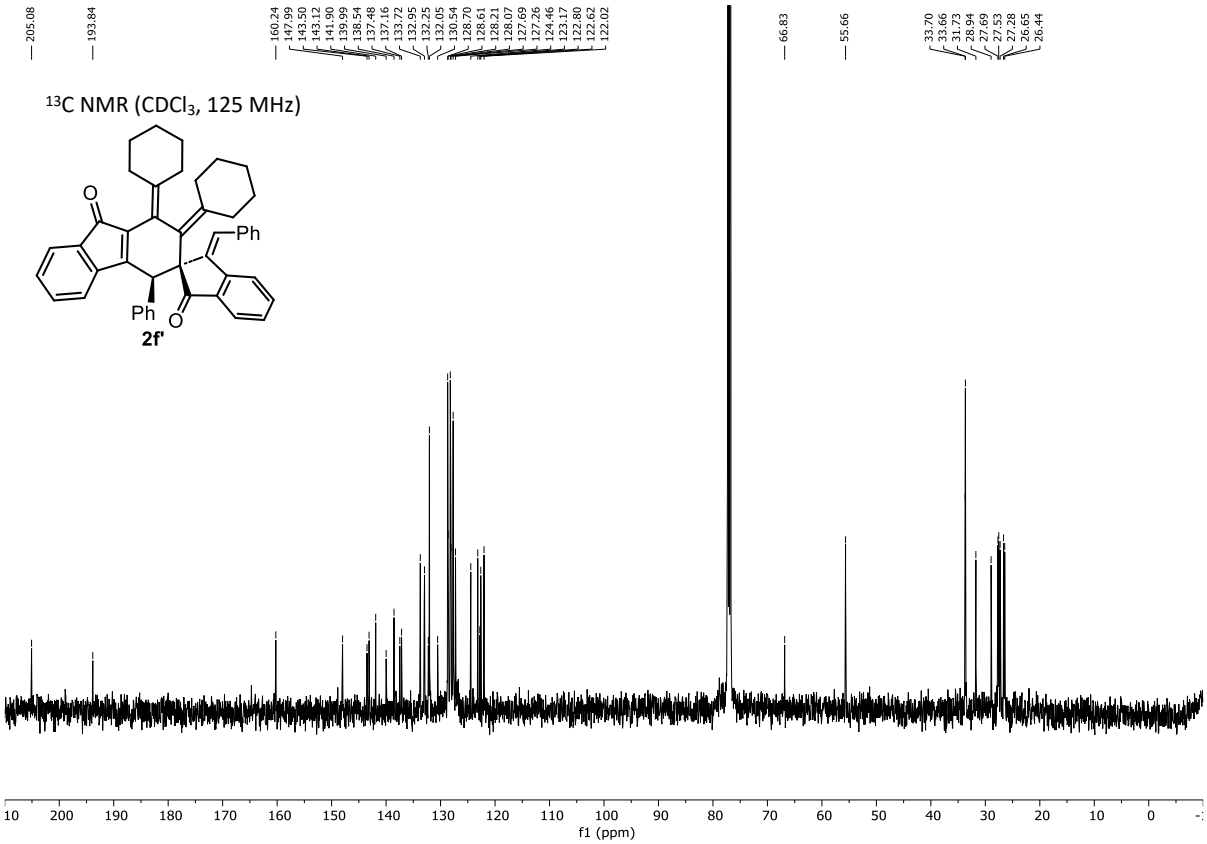
^{13}C NMR ($CDCl_3$, 125 MHz)



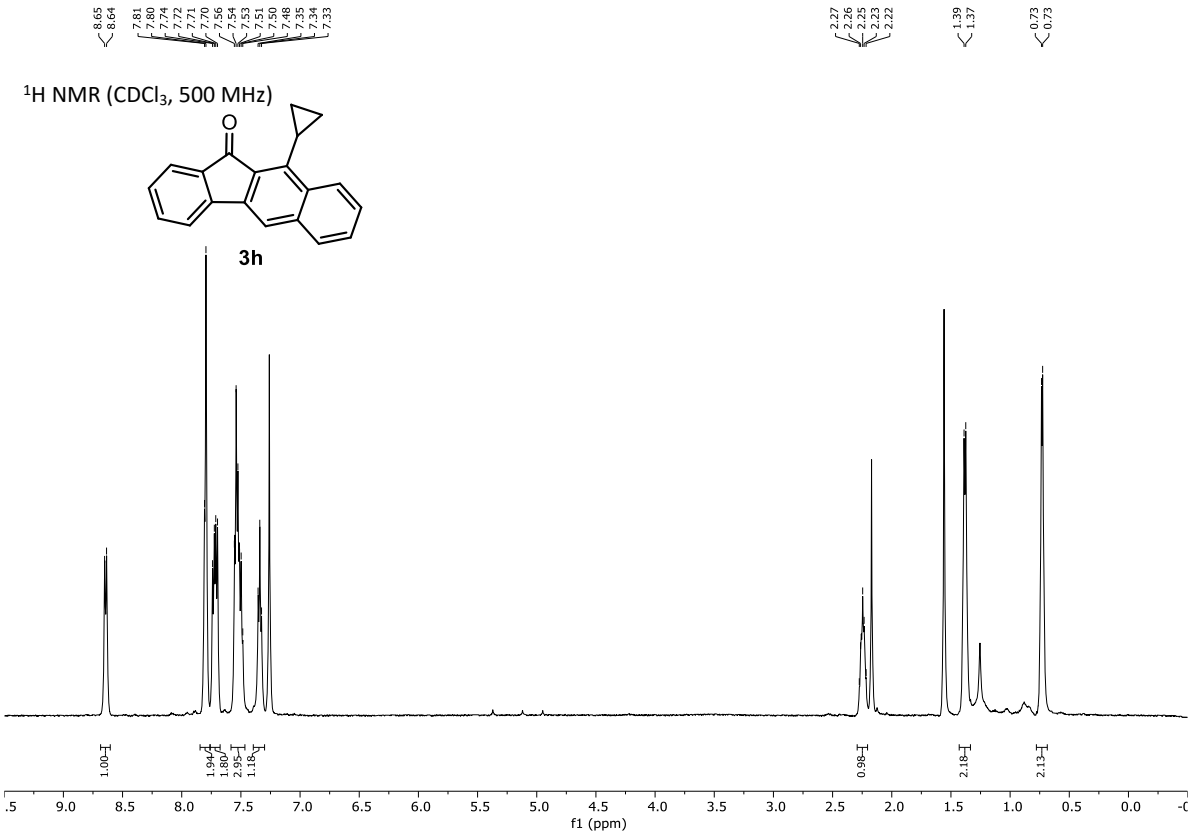
^{1}H NMR ($CDCl_3$, 500 MHz)



^{13}C NMR ($CDCl_3$, 125 MHz)

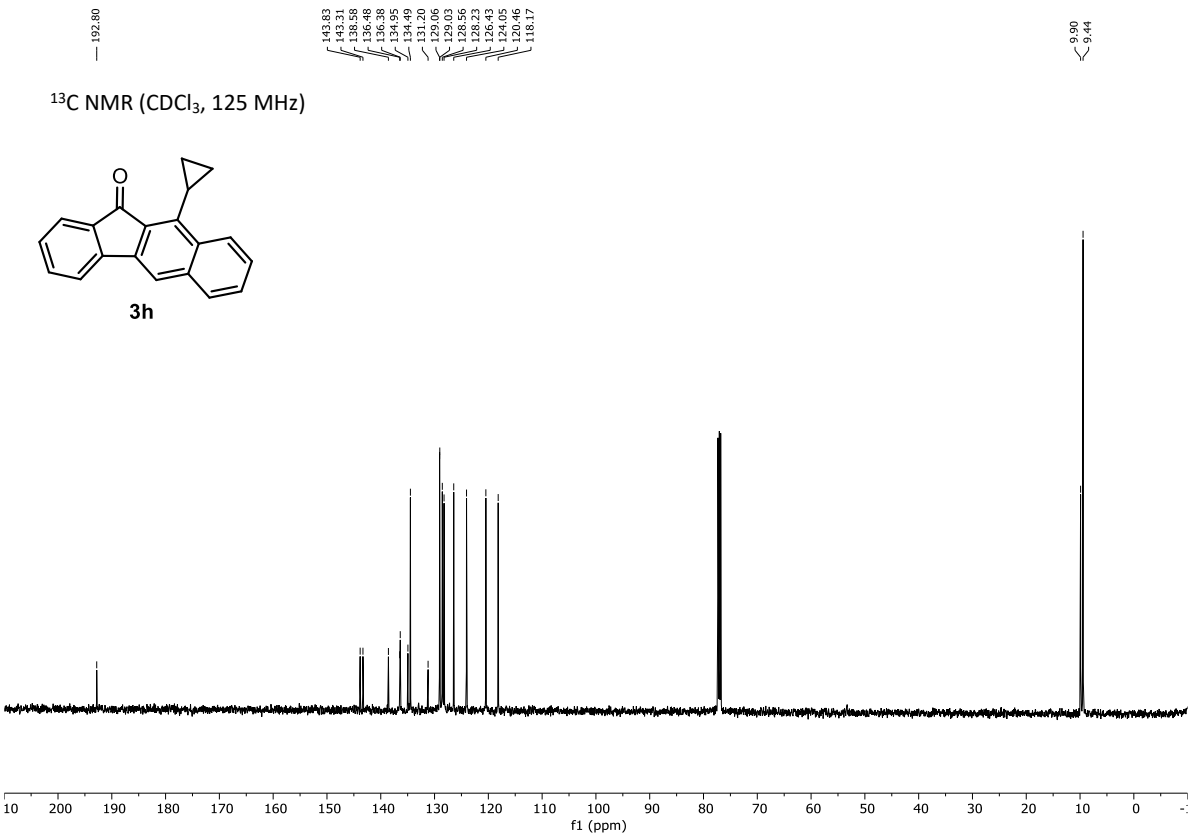


^{1}H NMR ($CDCl_3$, 500 MHz)

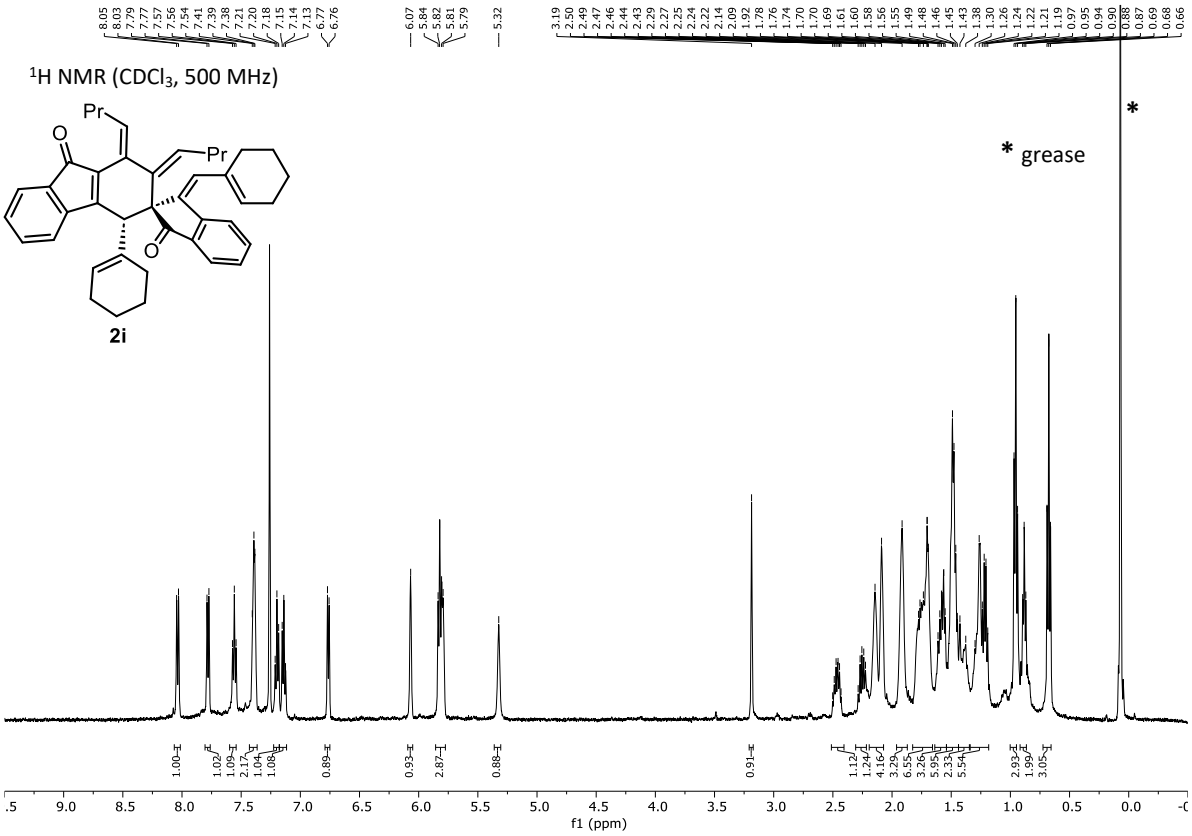


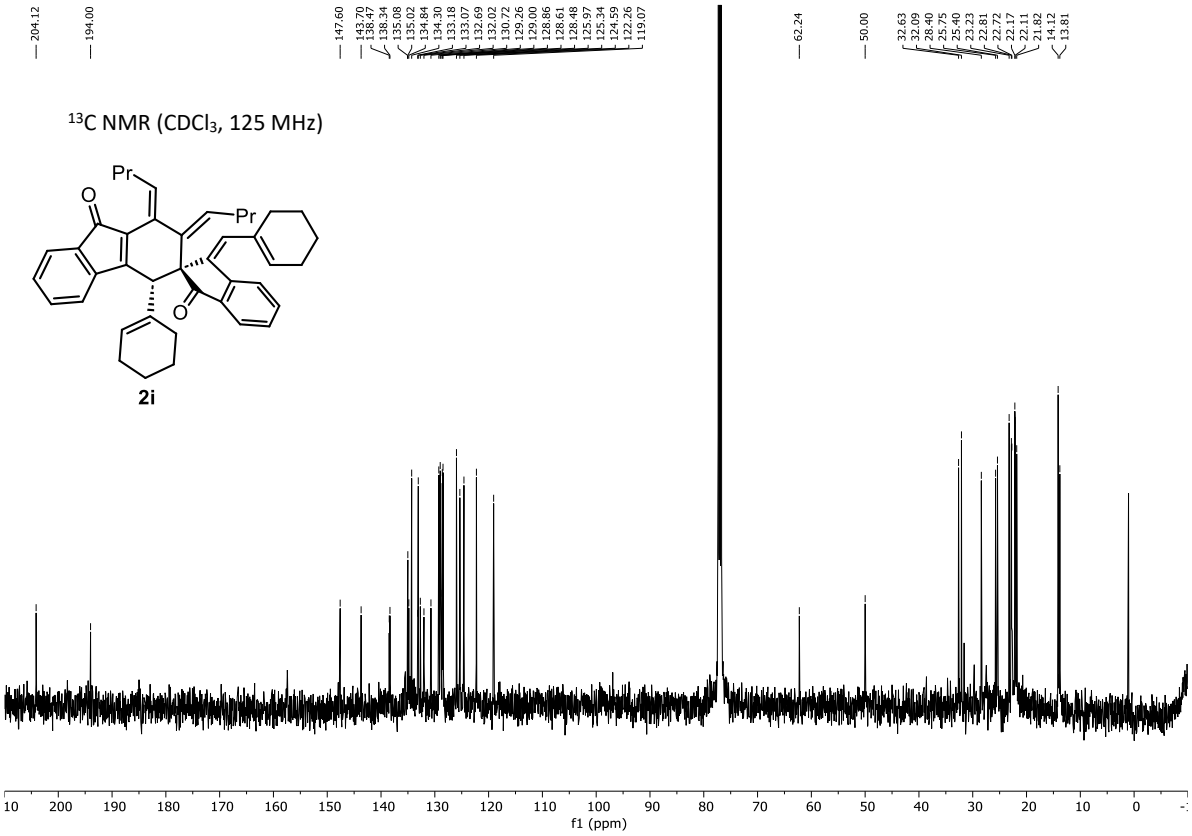
3h

^{13}C NMR ($CDCl_3$, 125 MHz)

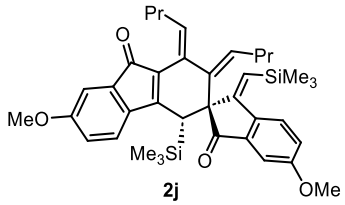


3h

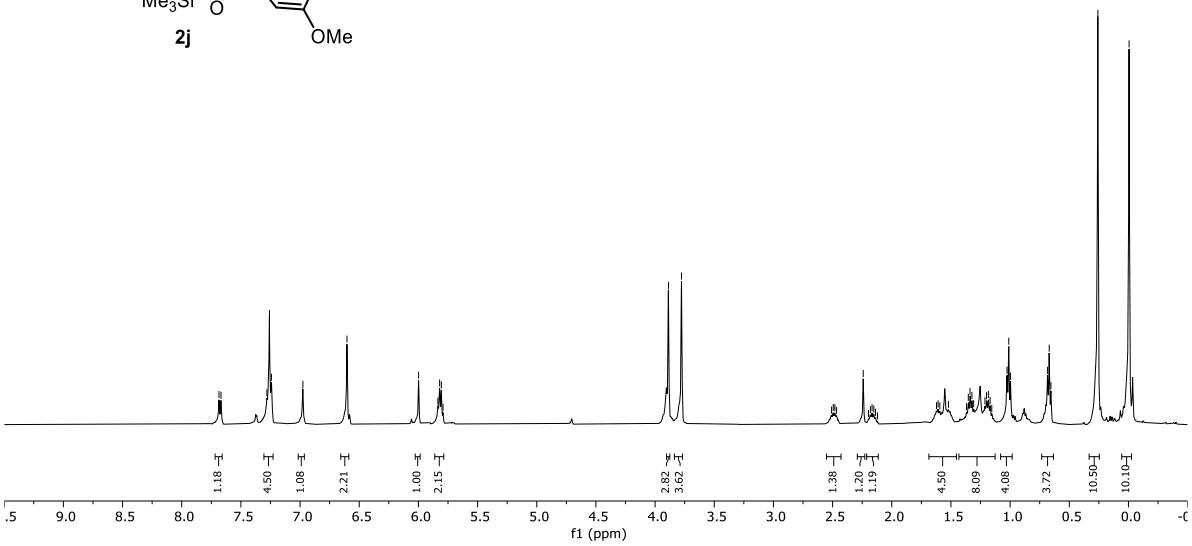

^{1}H NMR ($CDCl_3$, 500 MHz)
Pr
Pr
O
O
2i
* grease
*
f1 (ppm)


^{13}C NMR ($CDCl_3$, 125 MHz)
Pr
Pr
O
O
2i
f1 (ppm)

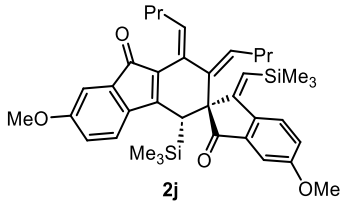
^{1}H NMR ($CDCl_3$, 500 MHz)



2j

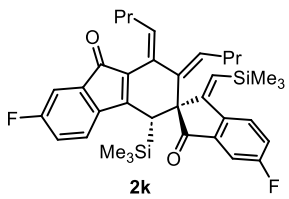


^{13}C NMR ($CDCl_3$, 125 MHz)

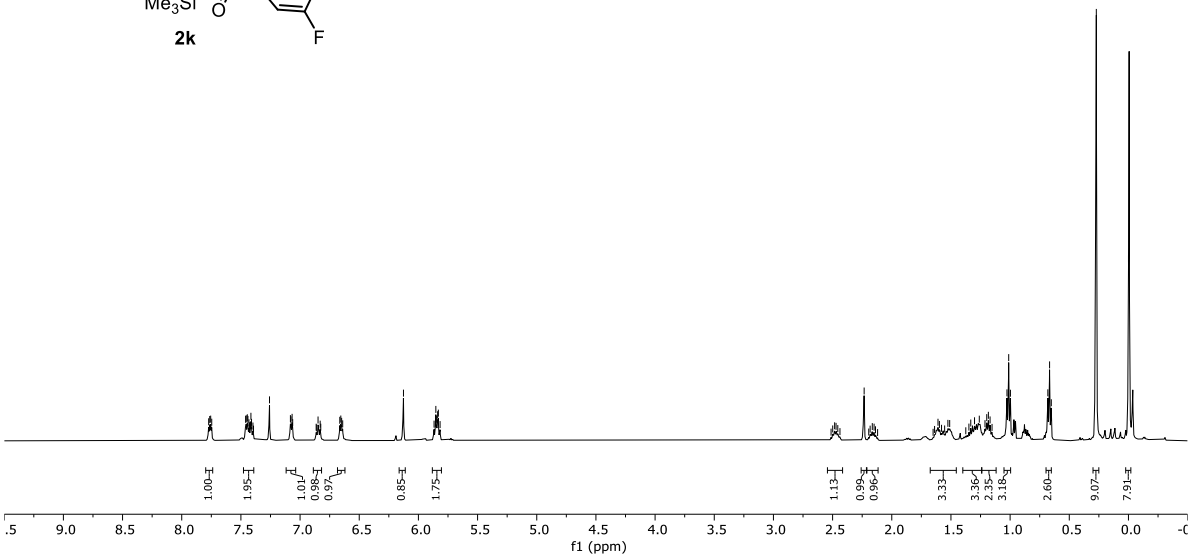


2j

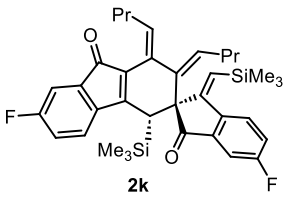
^{1}H NMR ($CDCl_3$, 500 MHz)



2k

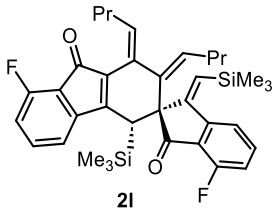


^{13}C NMR ($CDCl_3$, 125 MHz)

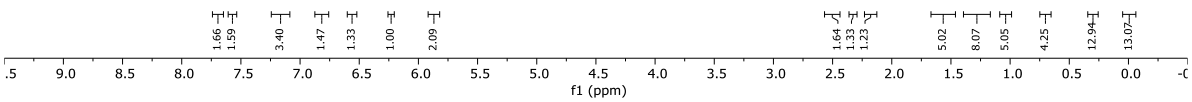


2k

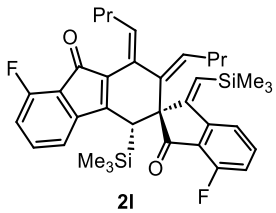
^{1}H NMR ($CDCl_3$, 500 MHz)



2l



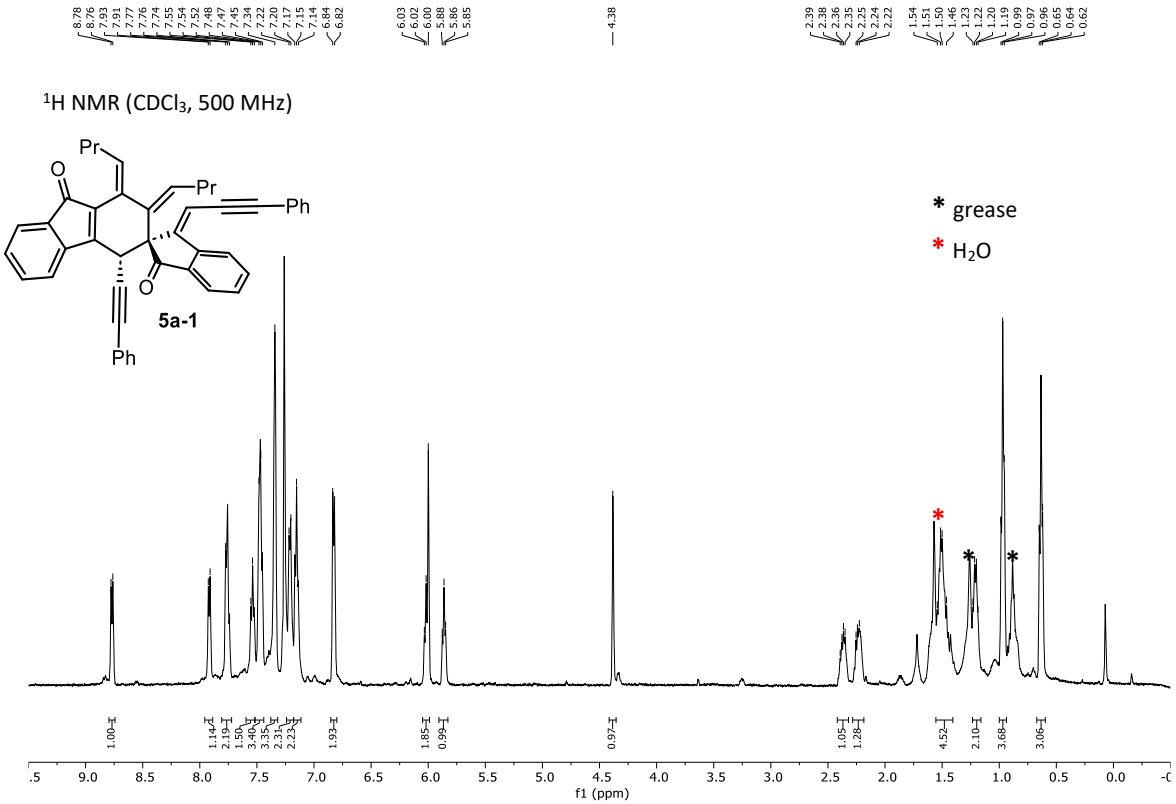
^{13}C NMR ($CDCl_3$, 125 MHz)



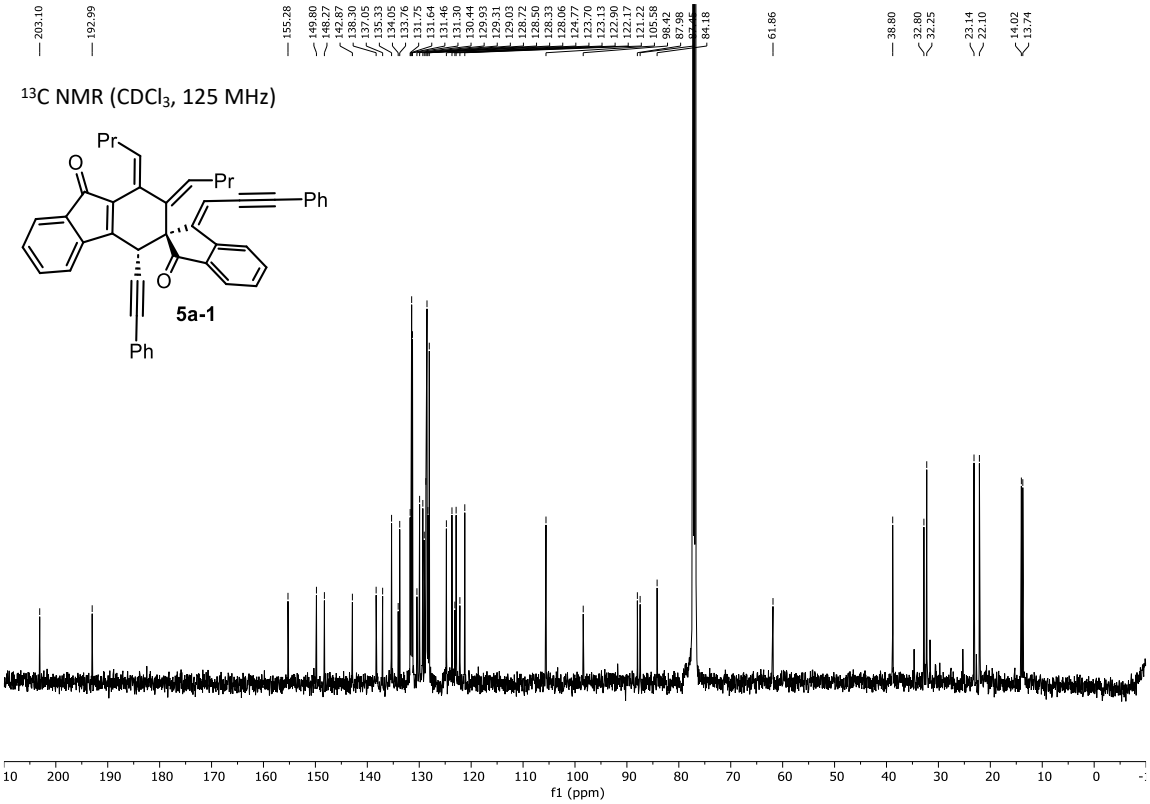
2l

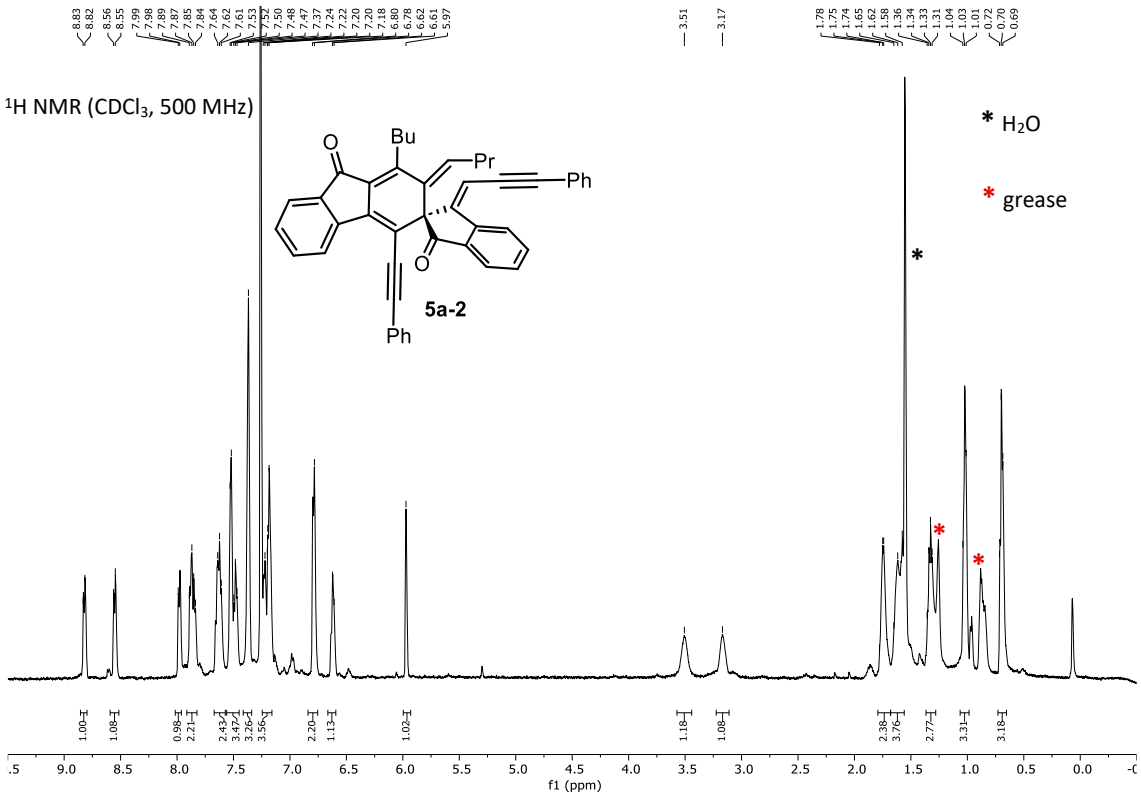
B. Dimerization of triynones

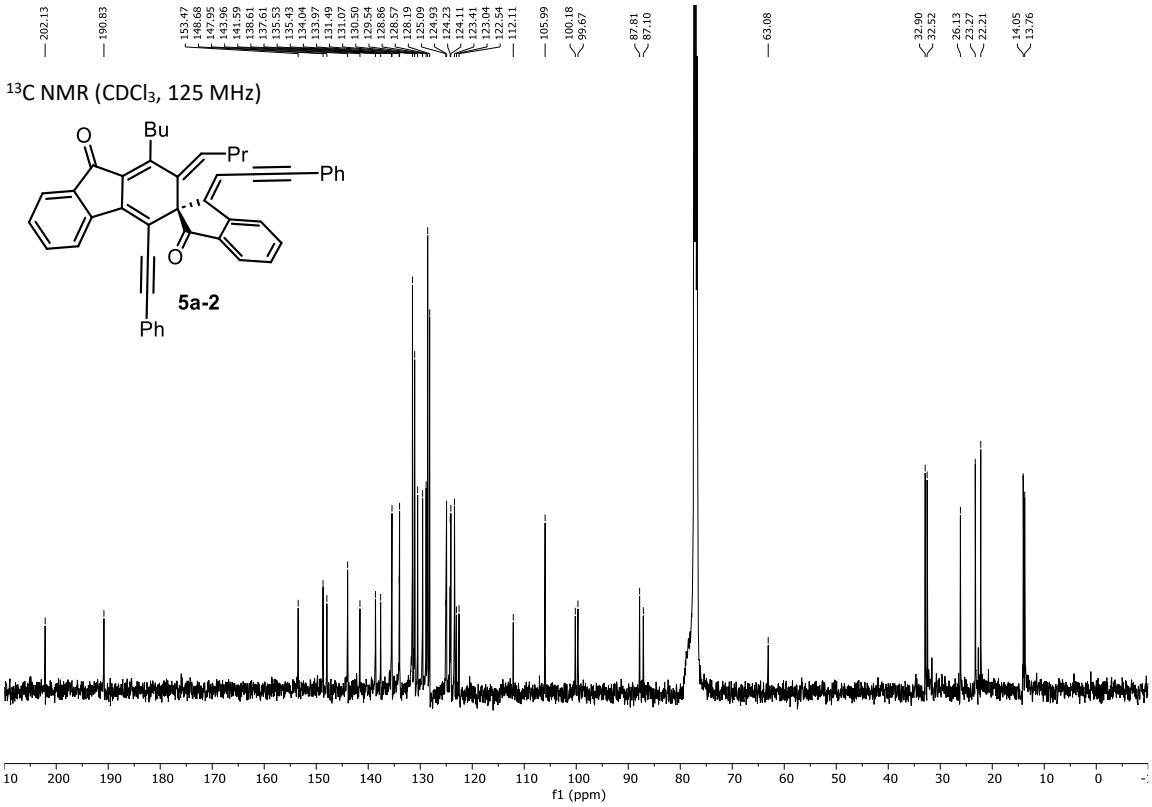
^{1}H NMR ($CDCl_3$, 500 MHz)



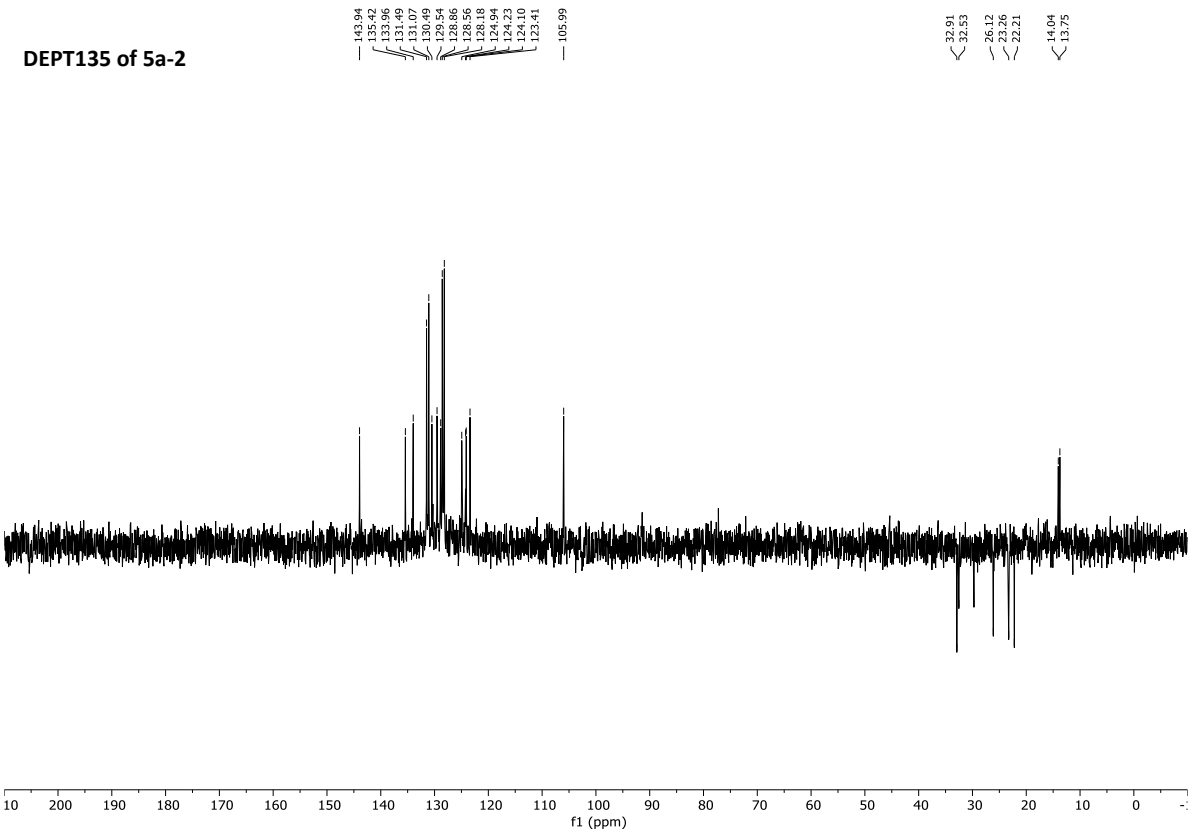
^{13}C NMR ($CDCl_3$, 125 MHz)



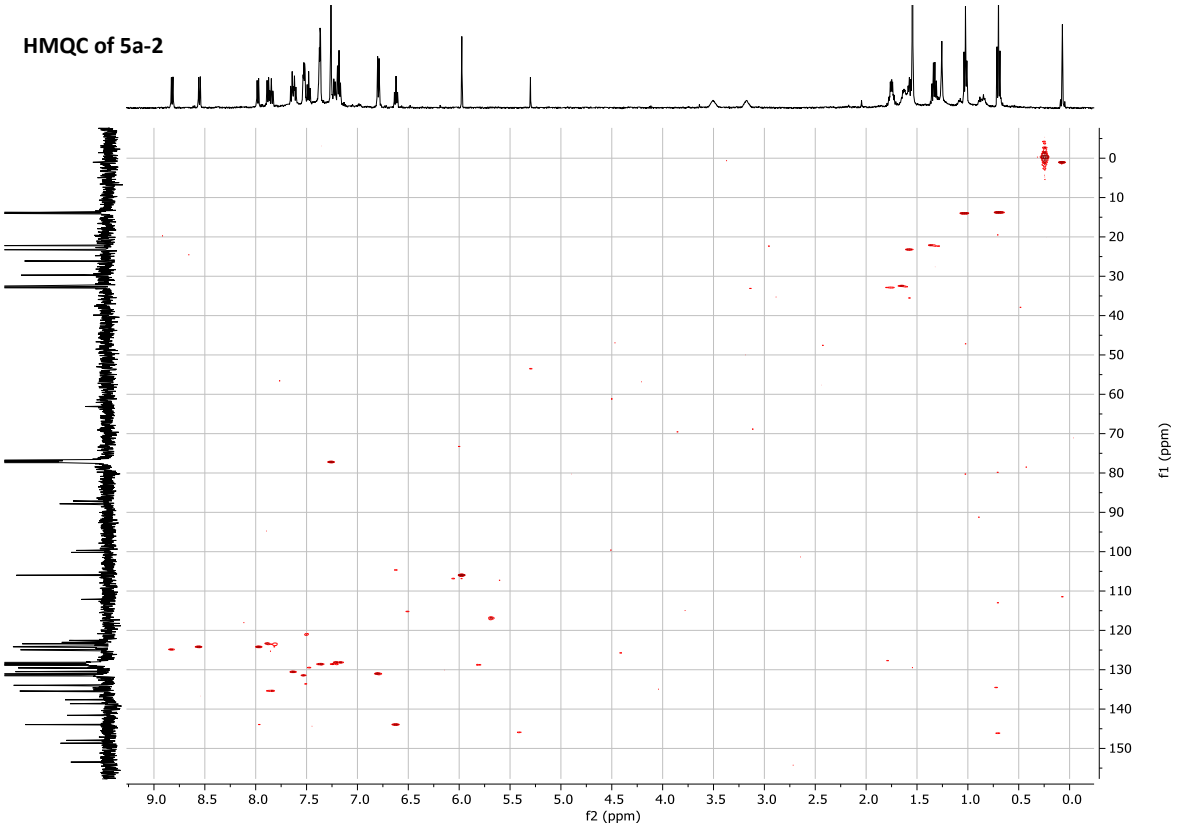

^{1}H NMR ($CDCl_3$, 500 MHz)
* H_2O
* grease
Bu
Pr
Ph
O
O
Ph
5a-2
f1 (ppm)


^{13}C NMR ($CDCl_3$, 125 MHz)
Bu
Pr
Ph
O
O
Ph
5a-2
f1 (ppm)

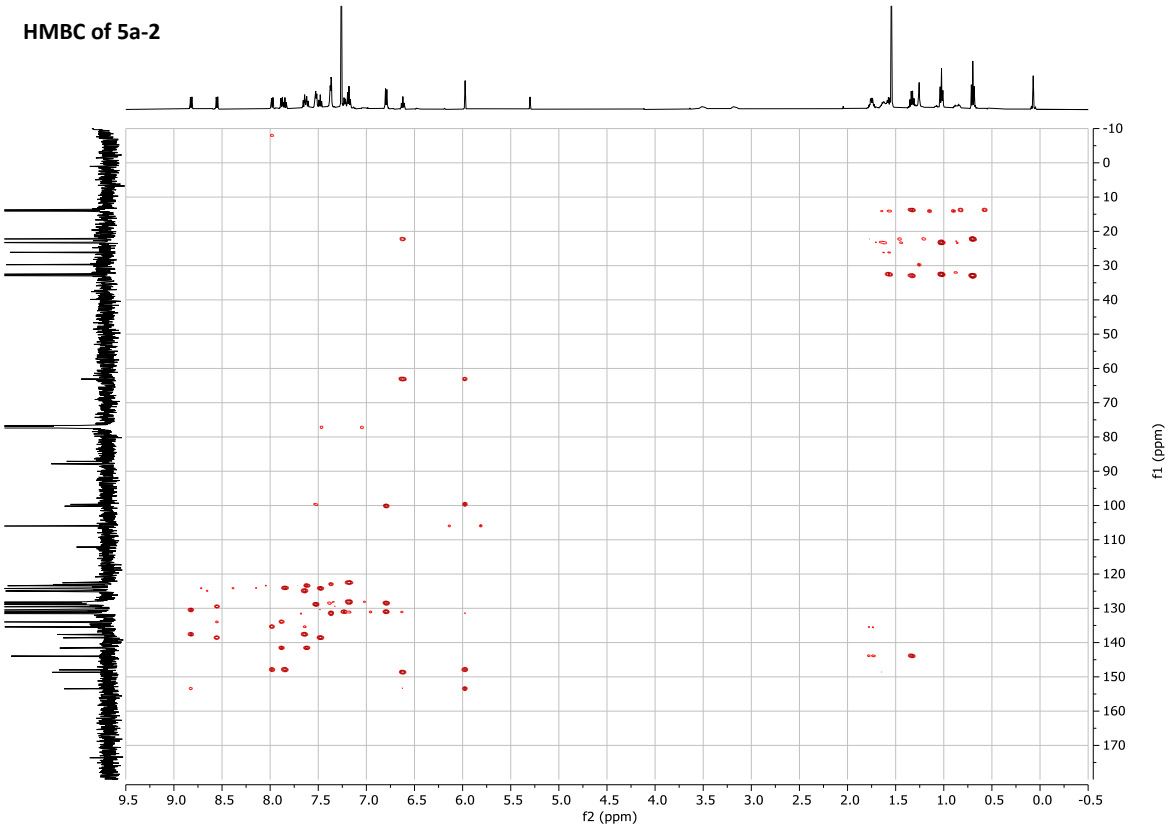
DEPT135 of 5a-2

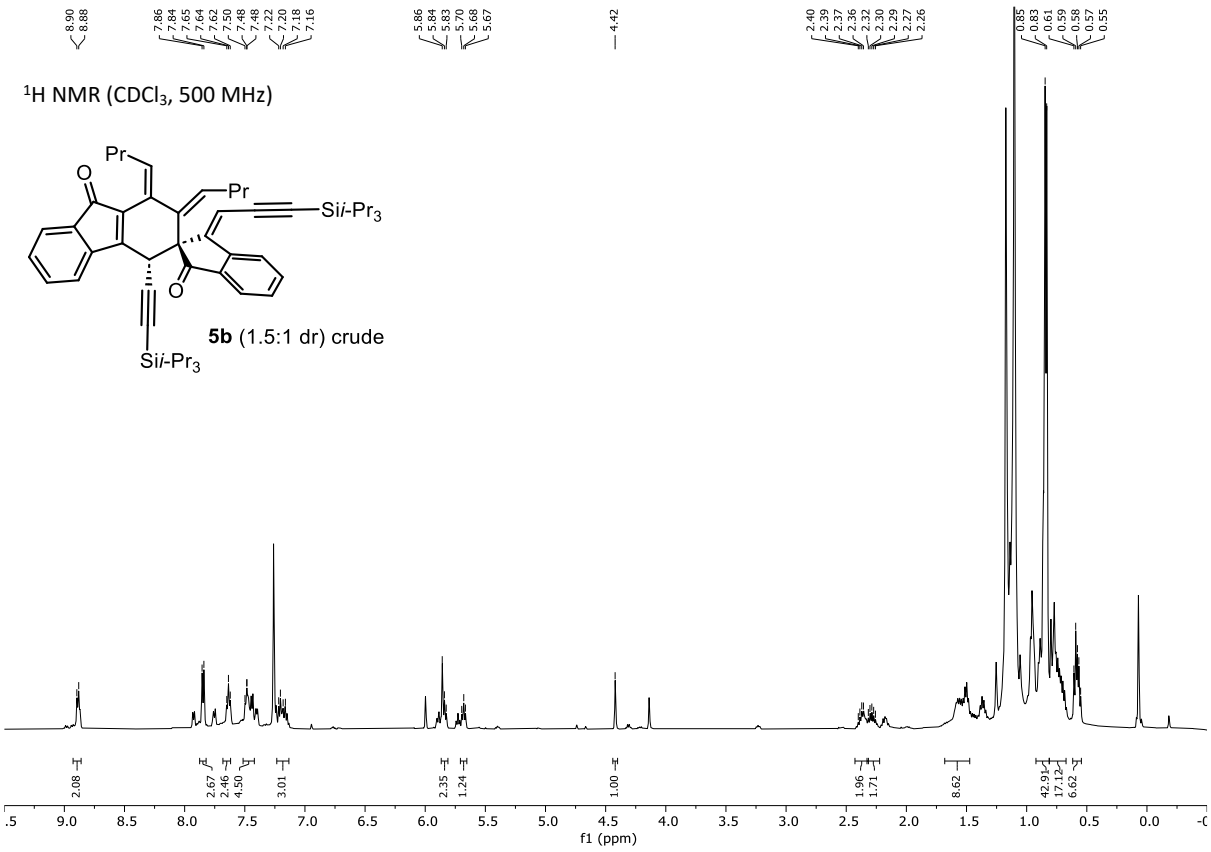


HMQC of 5a-2



HMBC of 5a-2

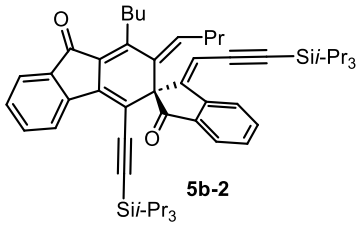




^{1}H NMR ($CDCl_3$, 500 MHz)

5b (1.5:1 dr) crude

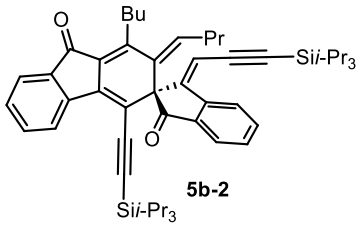
^{1}H NMR ($CDCl_3$, 500 MHz)



5b-2

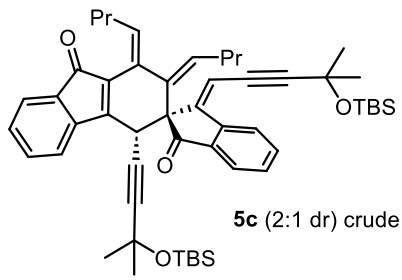
* acetone

^{13}C NMR ($CDCl_3$, 125 MHz)



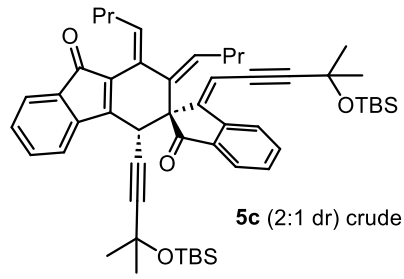
5b-2

^{1}H NMR ($CDCl_3$, 500 MHz)



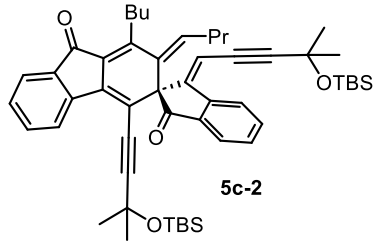
5c (2:1 dr) crude

^{13}C NMR ($CDCl_3$, 125 MHz)



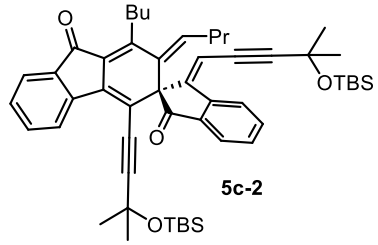
5c (2:1 dr) crude

^{1}H NMR ($CDCl_3$, 500 MHz)



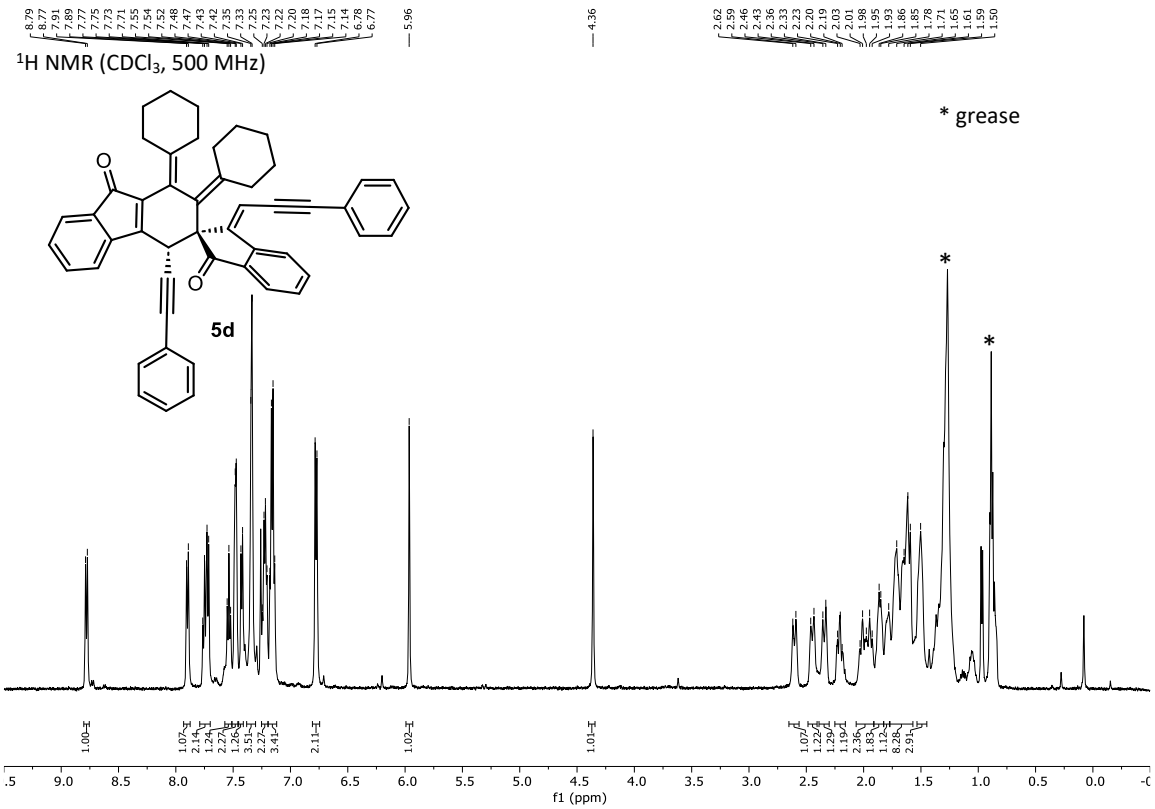
5c-2

^{13}C NMR ($CDCl_3$, 125 MHz)

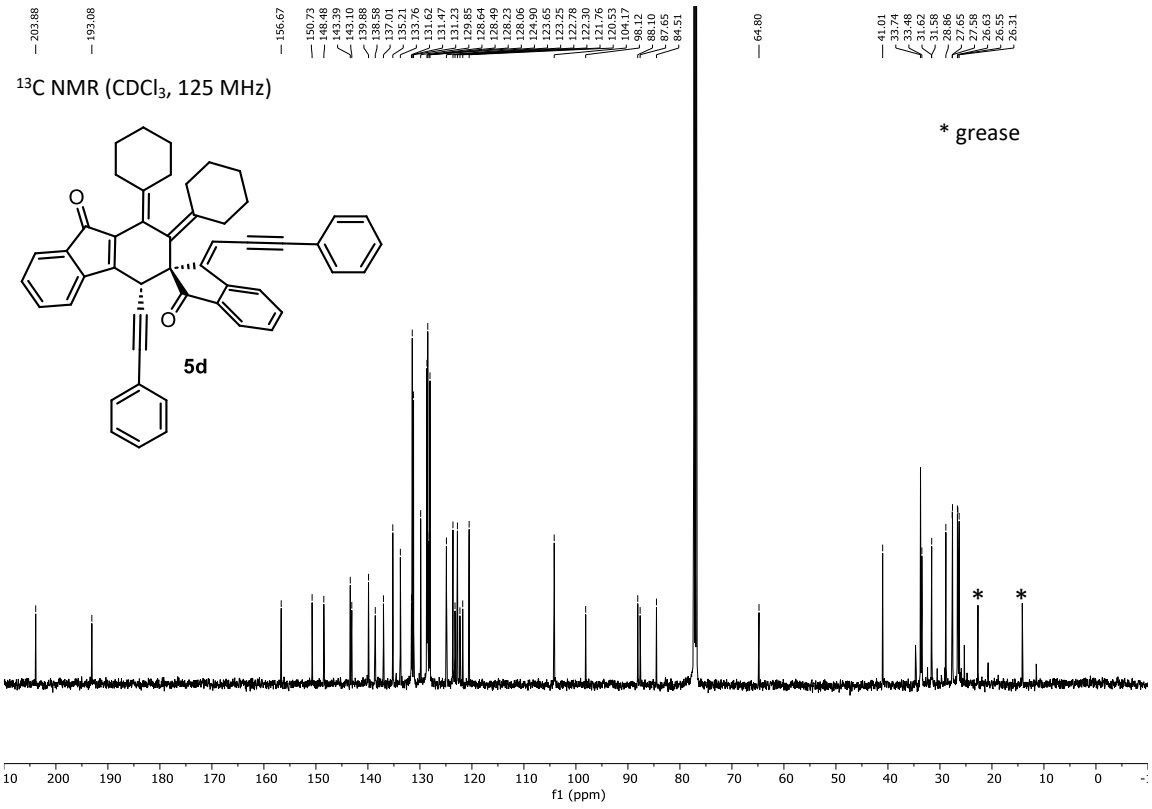


5c-2

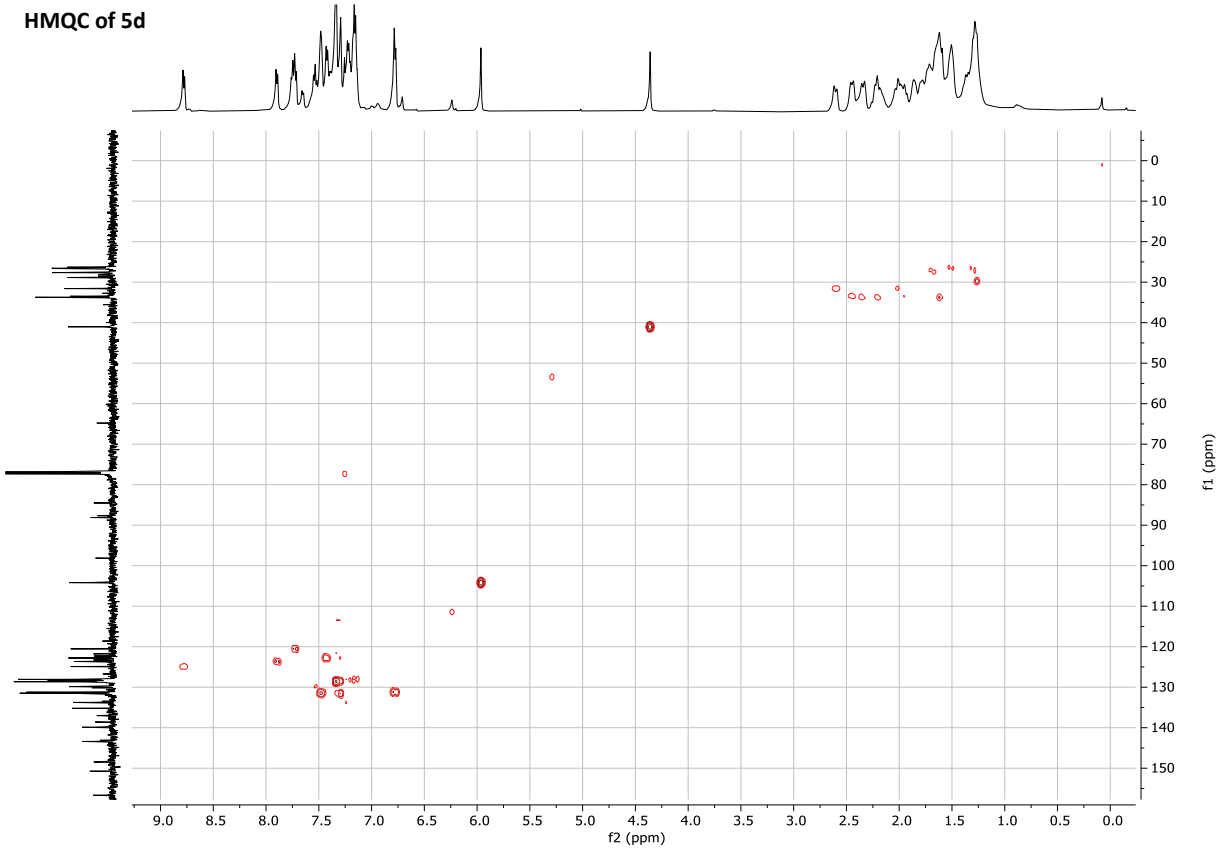
^{1}H NMR ($CDCl_3$, 500 MHz)



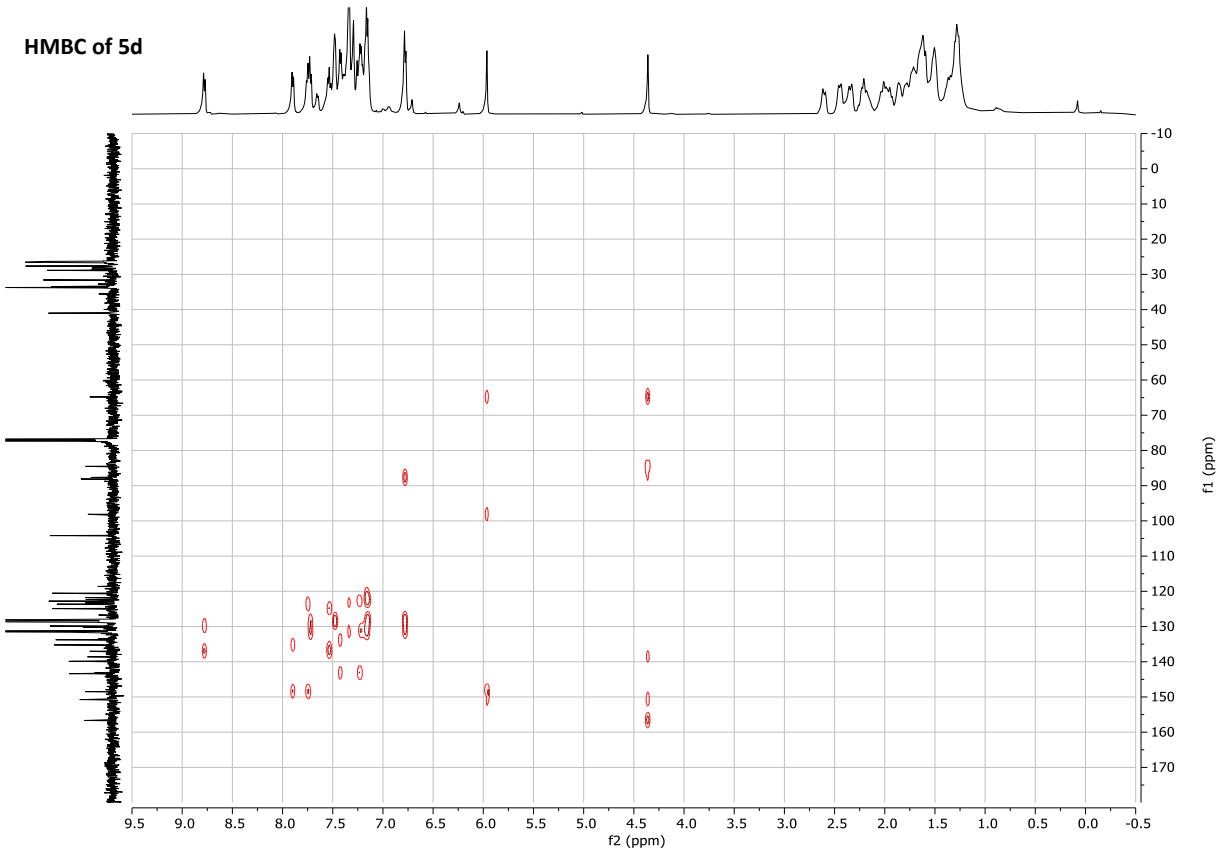
^{13}C NMR ($CDCl_3$, 125 MHz)



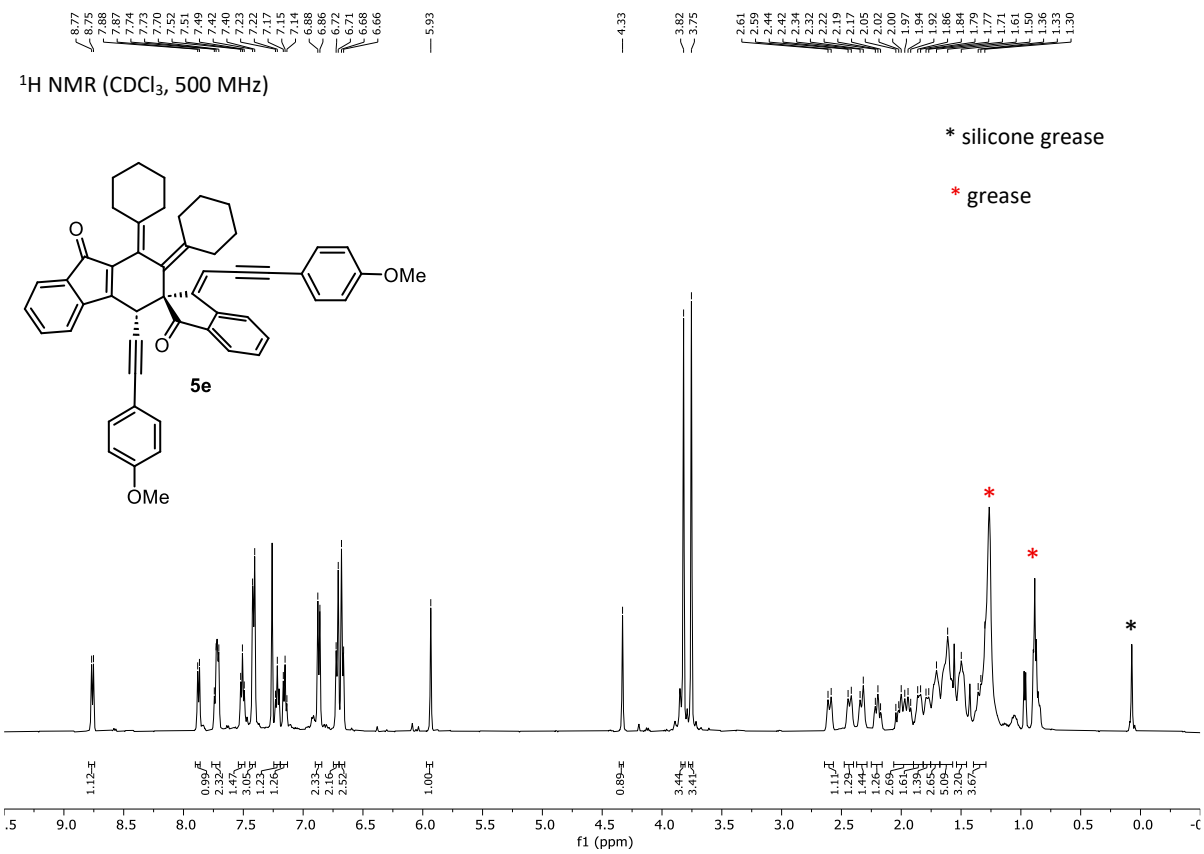
HMQC of 5d



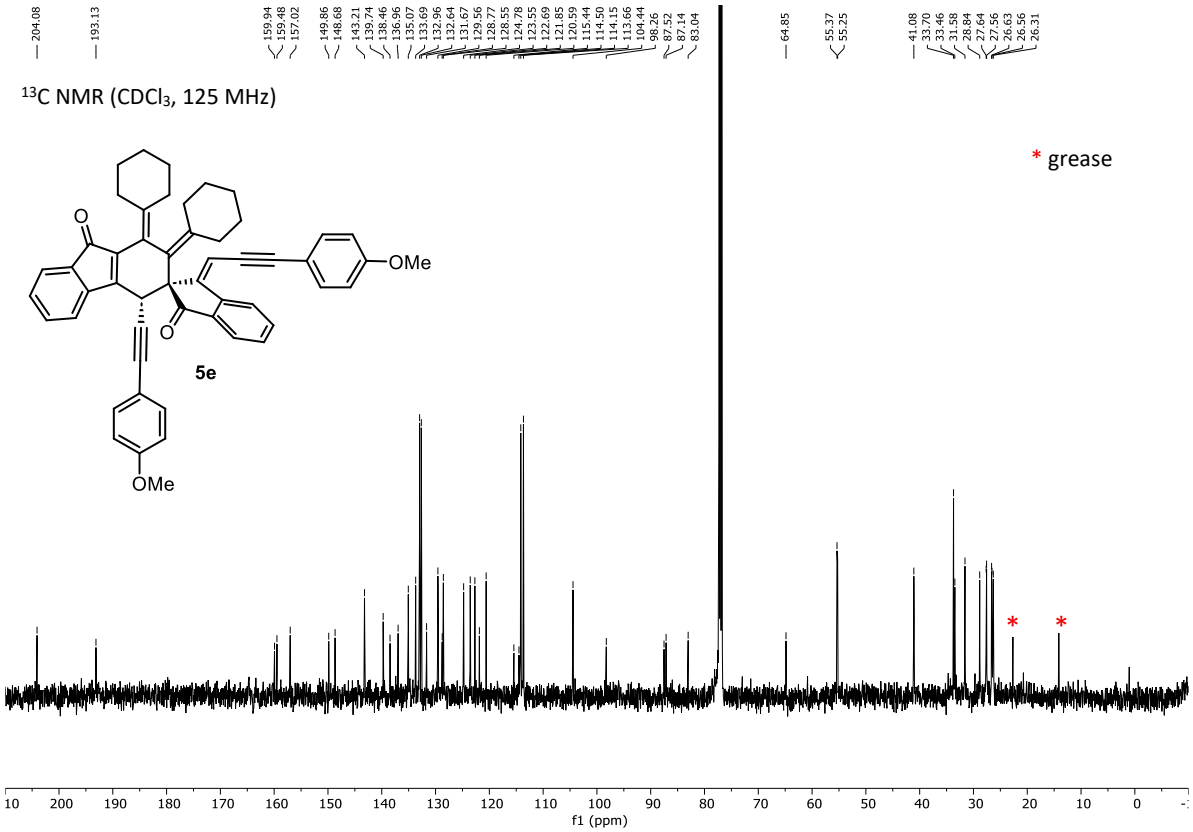
HMBC of 5d



^{1}H NMR ($CDCl_3$, 500 MHz)

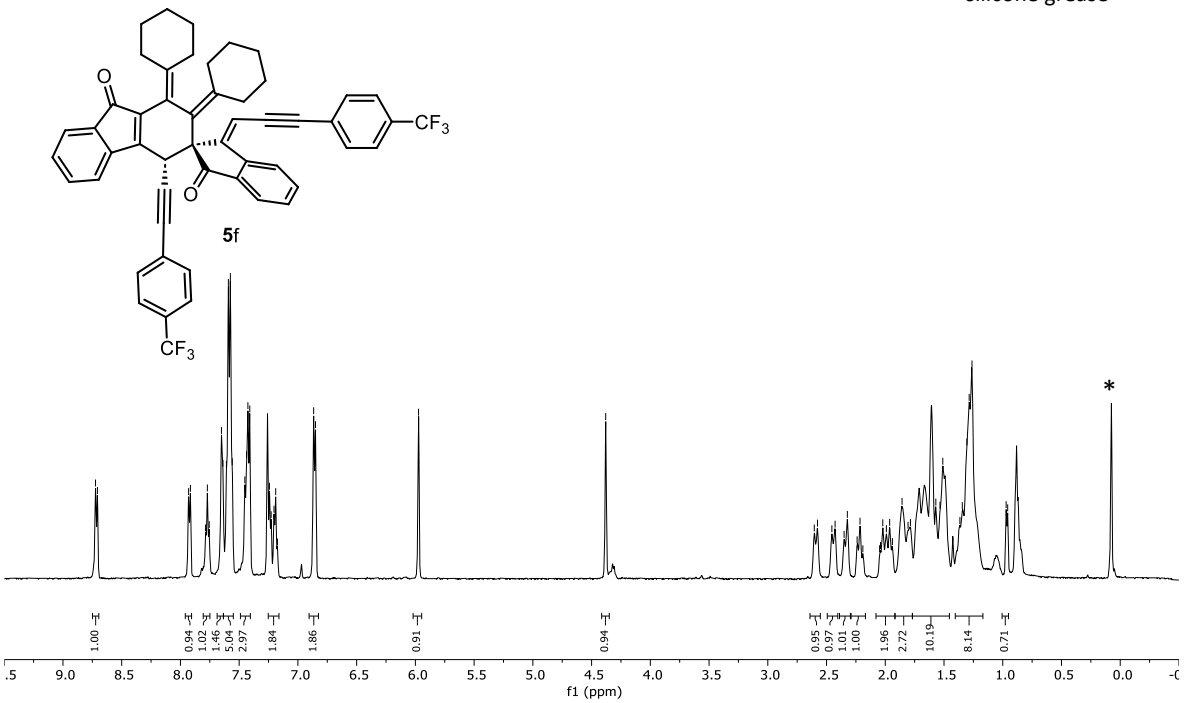


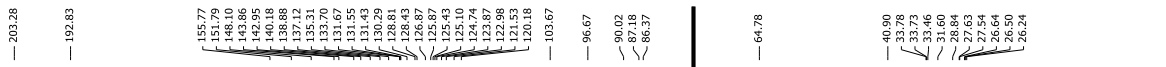
^{13}C NMR ($CDCl_3$, 125 MHz)



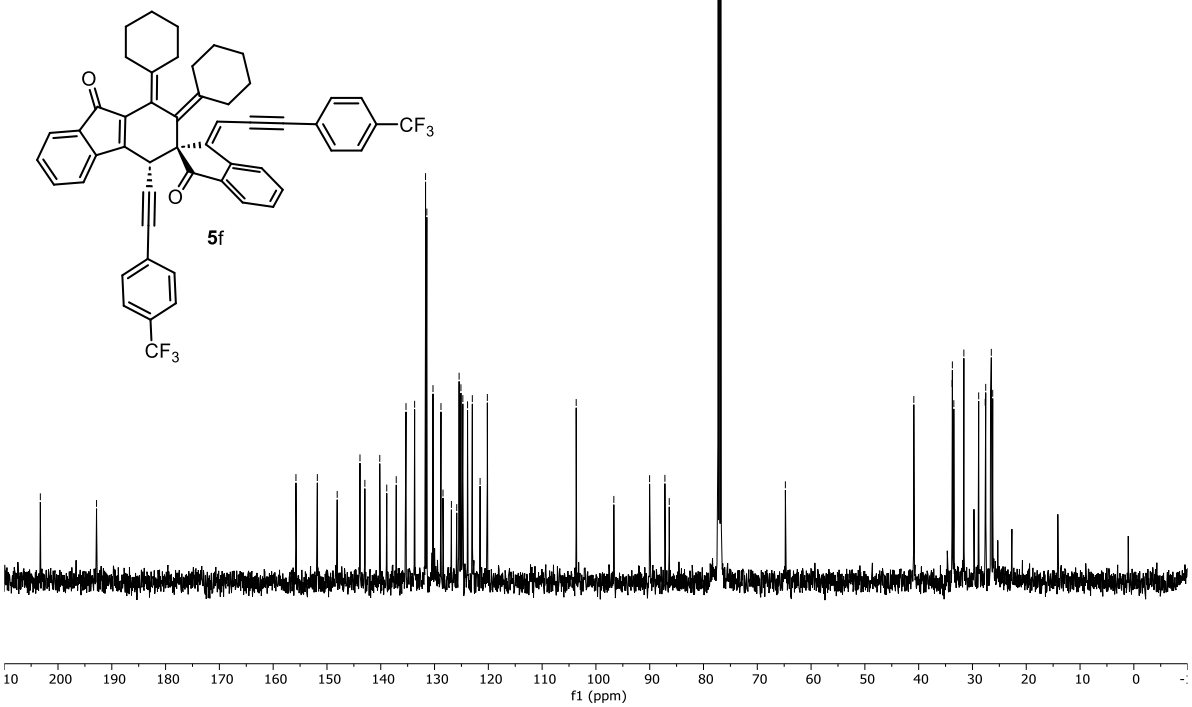
^{1}H NMR ($CDCl_3$, 500 MHz)

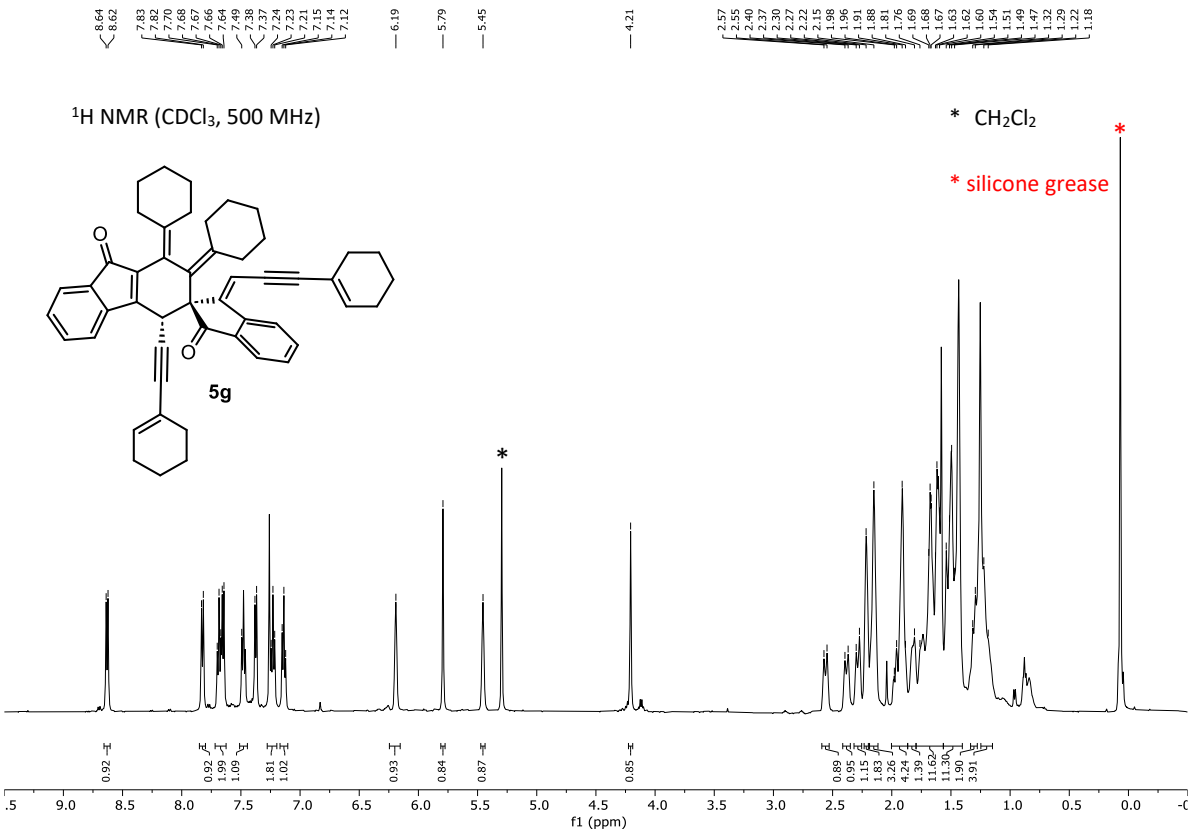
* silicone grease

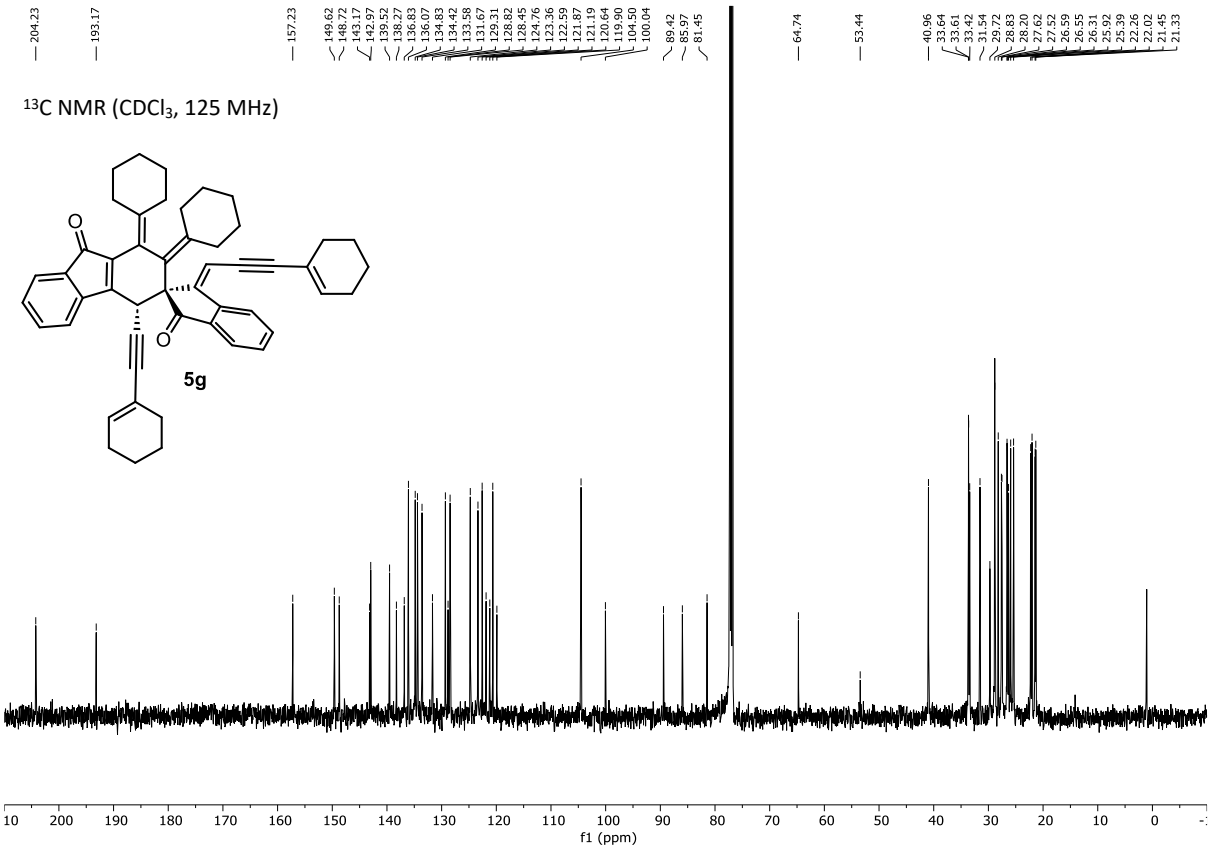




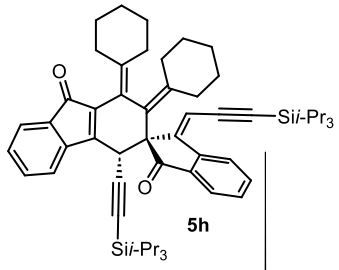
^{13}C NMR ($CDCl_3$, 125 MHz)




^{1}H NMR ($CDCl_3$, 500 MHz)
* CH_2Cl_2
* silicone grease
5g
f1 (ppm)

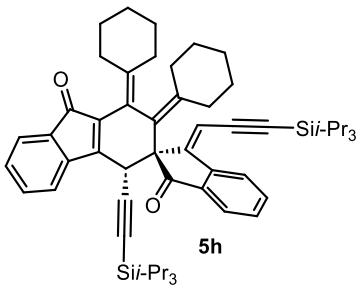

^{13}C NMR ($CDCl_3$, 125 MHz)
5g
f1 (ppm)

^{1}H NMR ($CDCl_3$, 500 MHz)



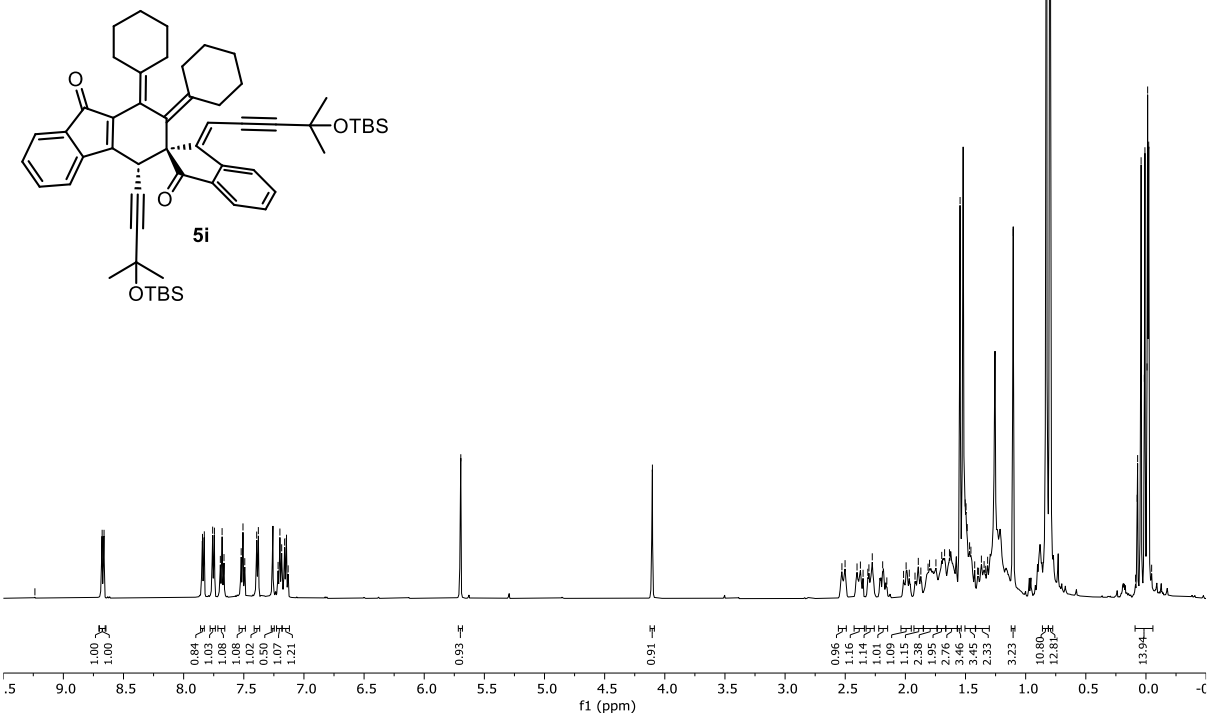
5h

^{13}C NMR ($CDCl_3$, 125 MHz)



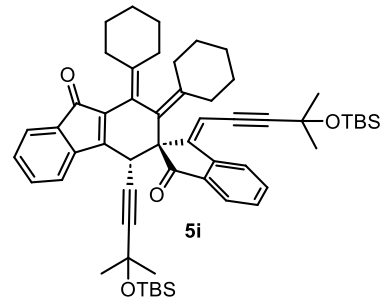
5h

^{1}H NMR ($CDCl_3$, 500 MHz)



5i

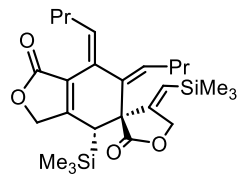
^{13}C NMR ($CDCl_3$, 125 MHz)



5i

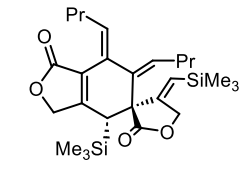
C. Dimerization of non-aromatic tethered alkynes

^{1}H NMR ($CDCl_3$, 500 MHz)



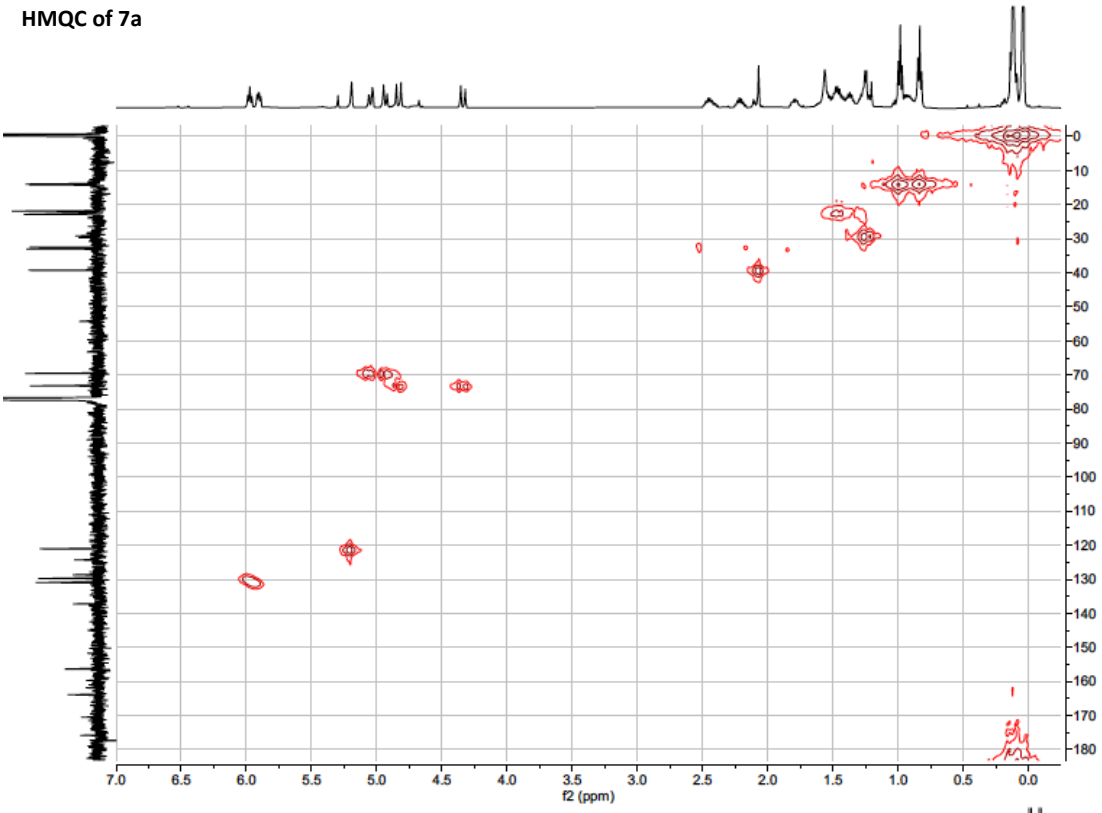
7a

^{13}C NMR ($CDCl_3$, 125 MHz)

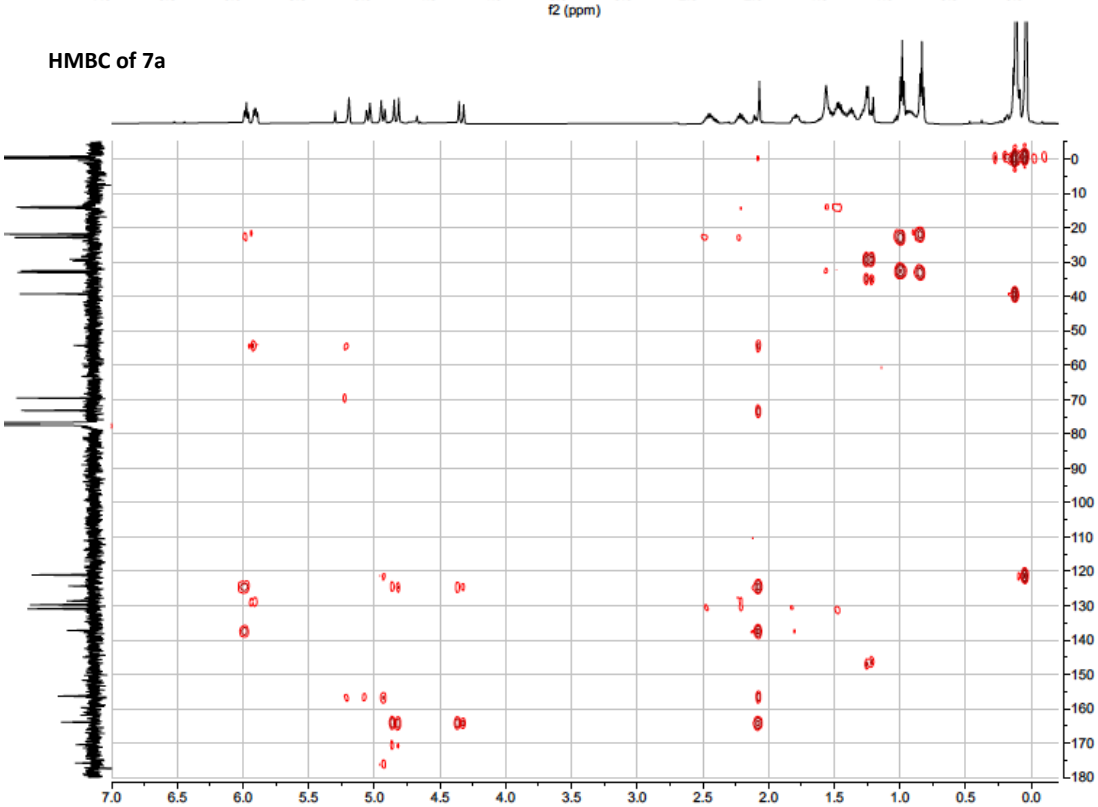


7a

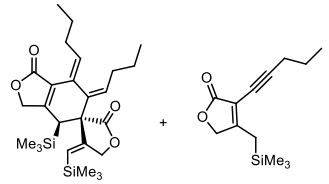
HMQC of 7a



HMBC of 7a

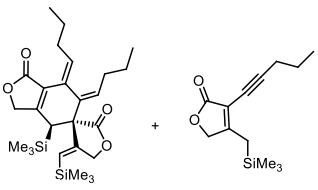


^{1}H NMR ($CDCl_3$, 500 MHz)



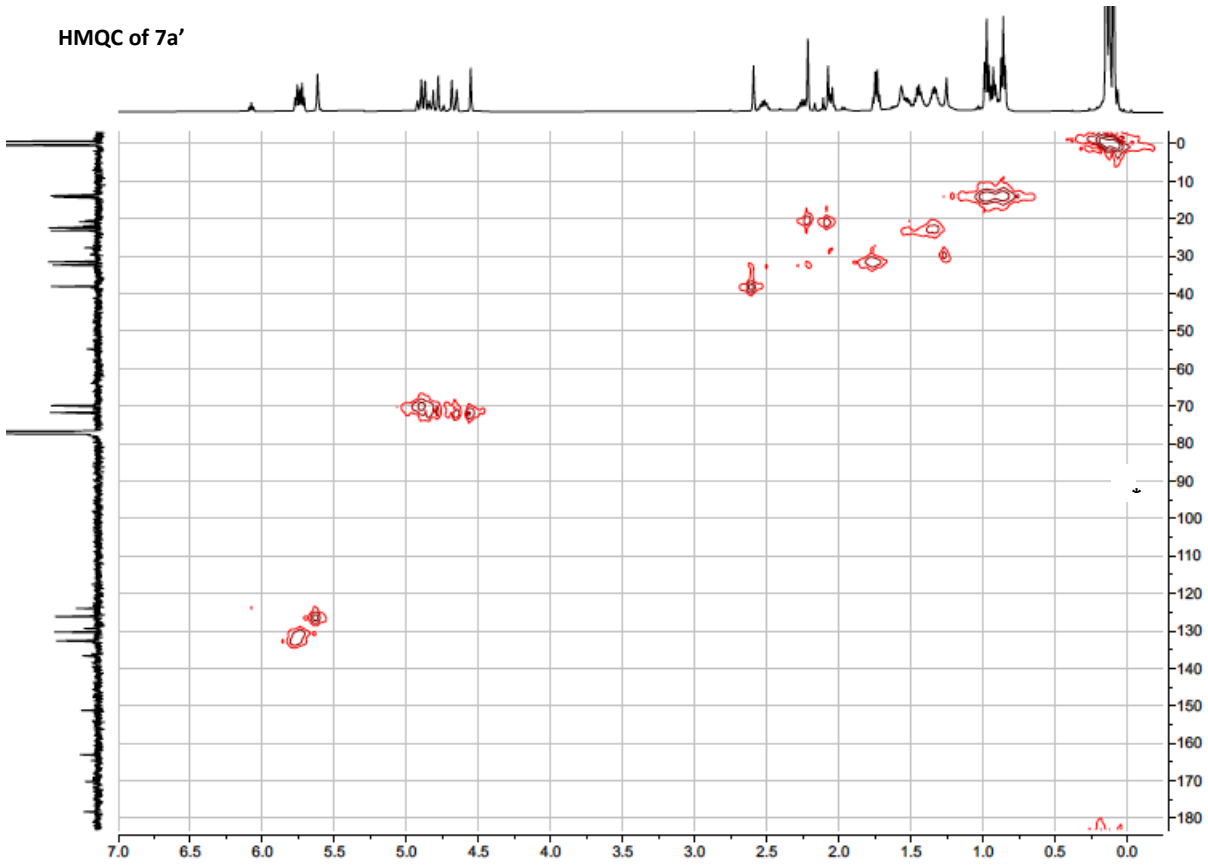
7a' 2.4:1 * **7a''**

^{13}C NMR ($CDCl_3$, 125 MHz)

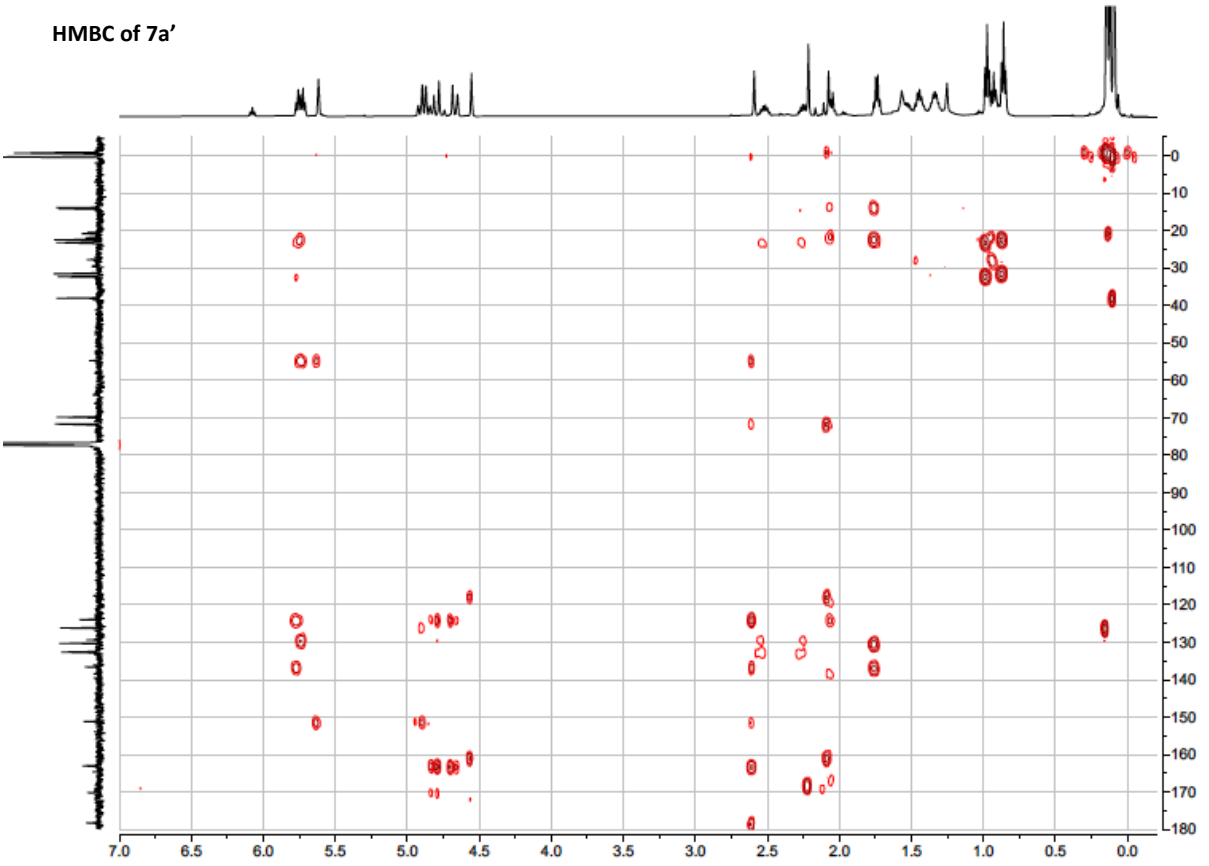


7a' 2.4:1 * **7a''**

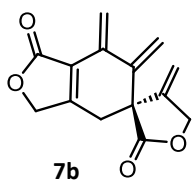
HMQC of 7a'



HMBC of 7a'

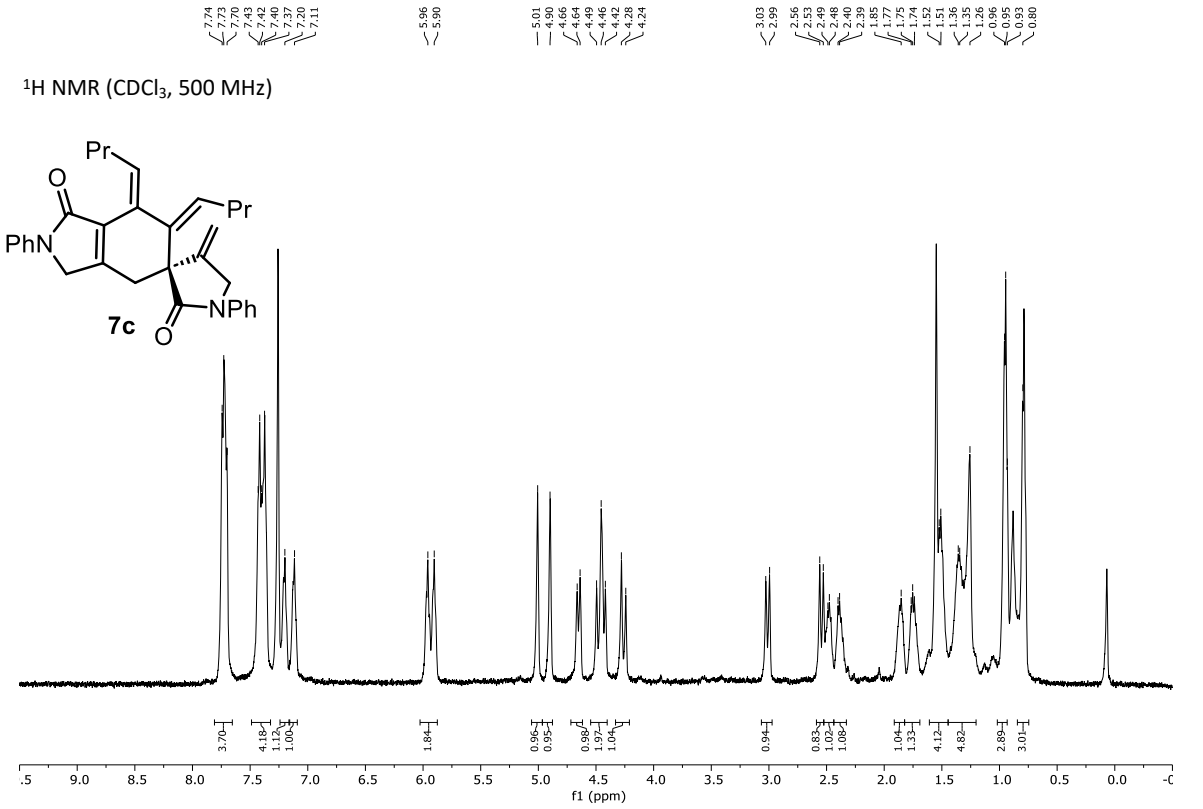


^{1}H NMR ($CDCl_3$, 500 MHz)

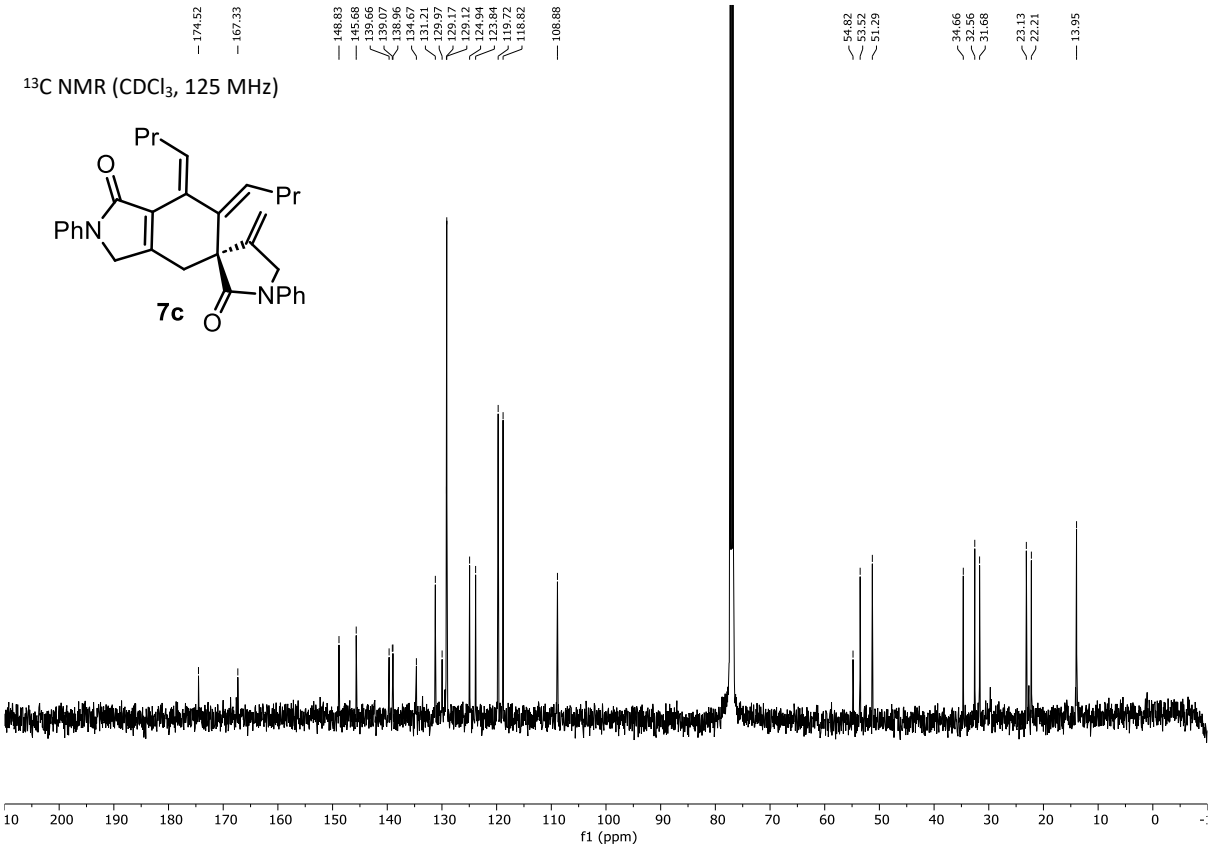


7b

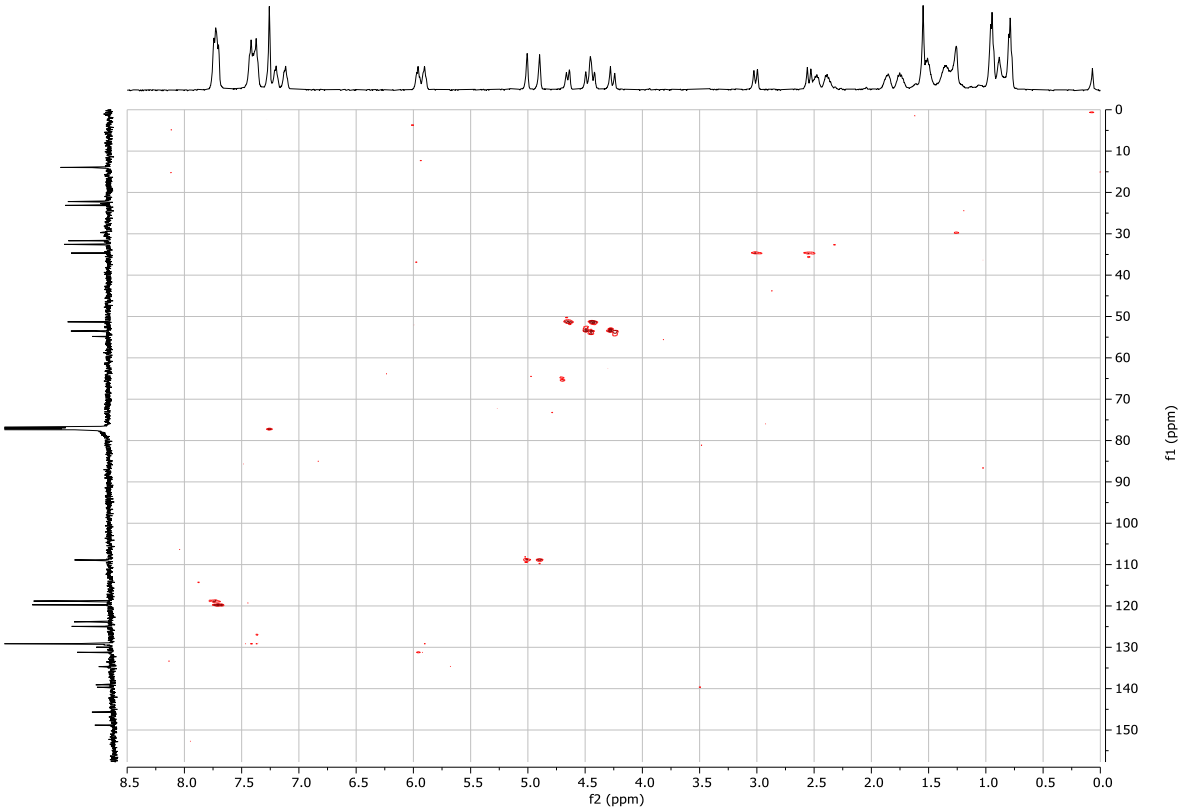
^{1}H NMR ($CDCl_3$, 500 MHz)



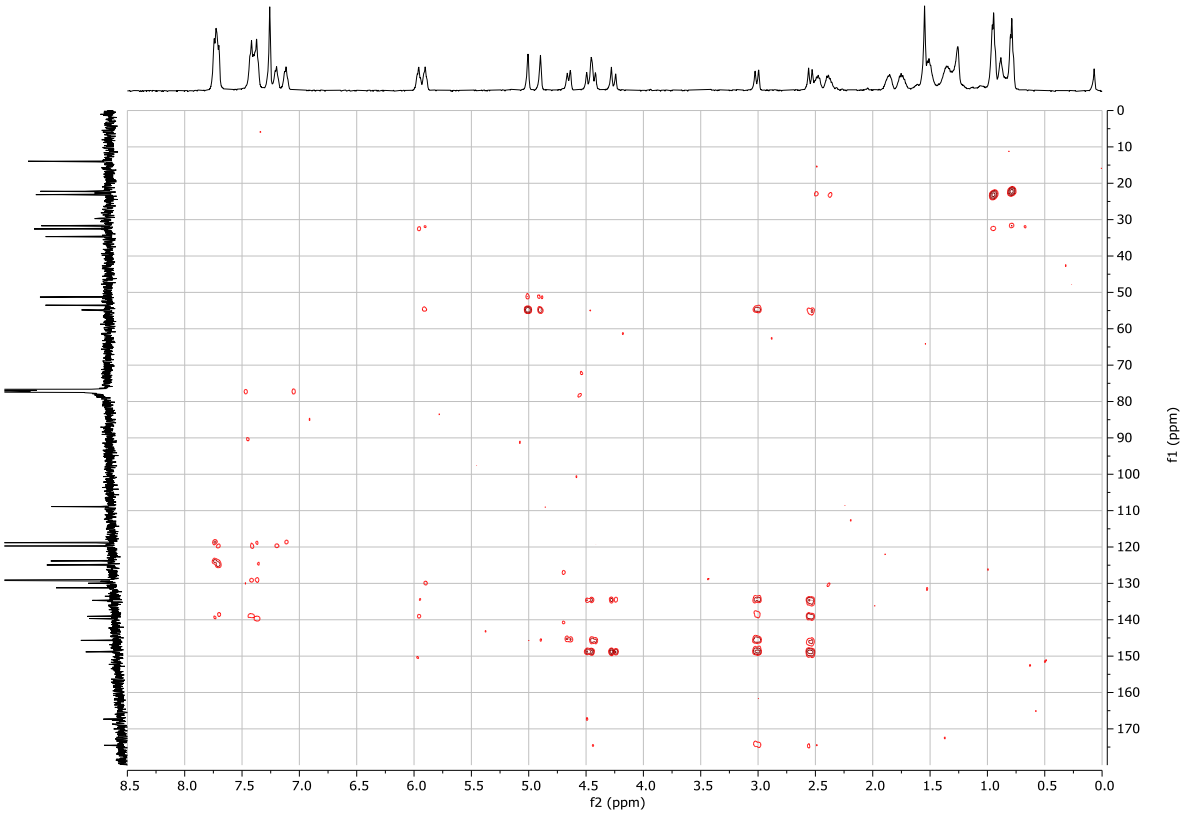
^{13}C NMR ($CDCl_3$, 125 MHz)



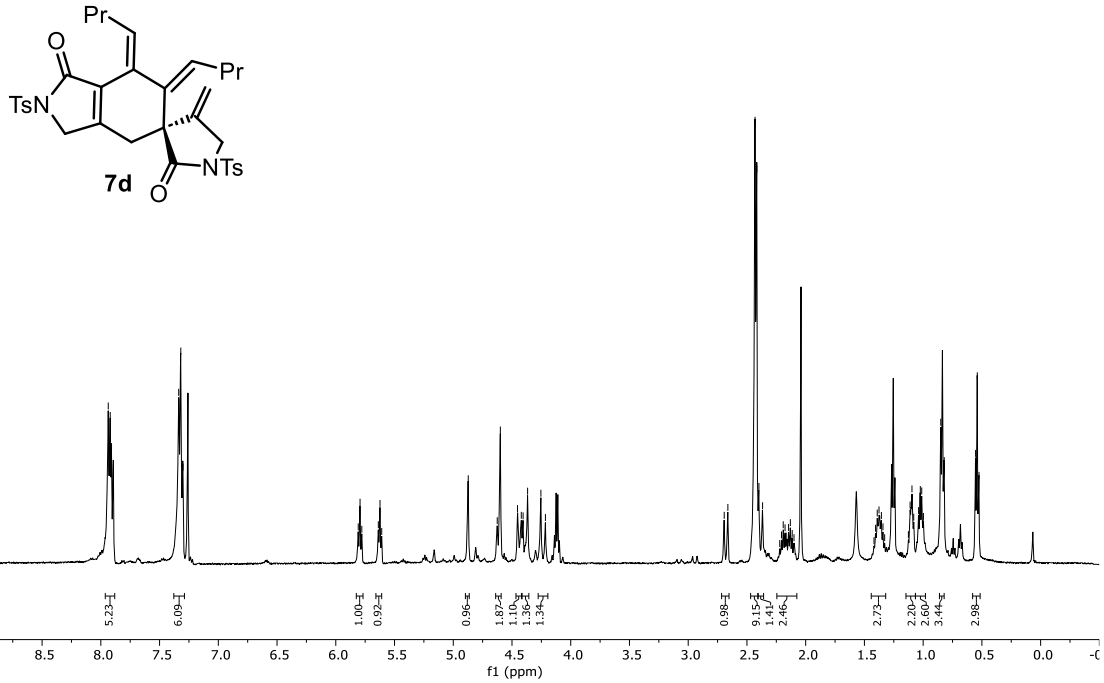
HMQC of 7c



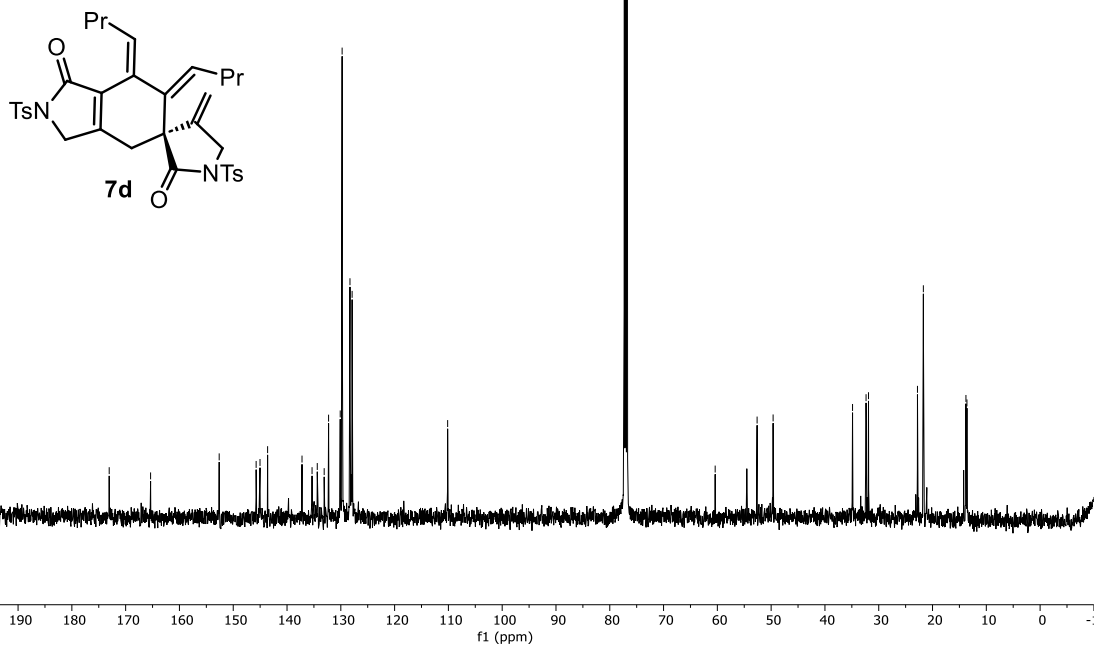
HMBC of 7c

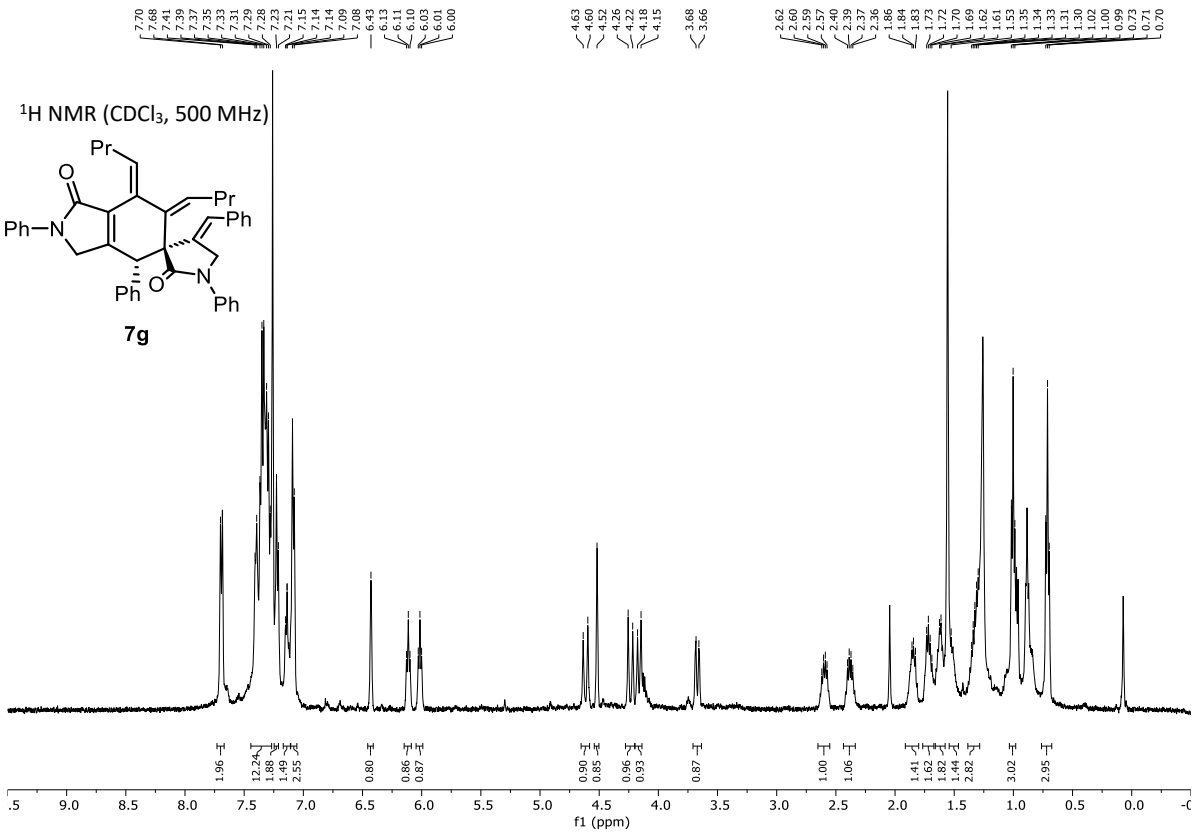


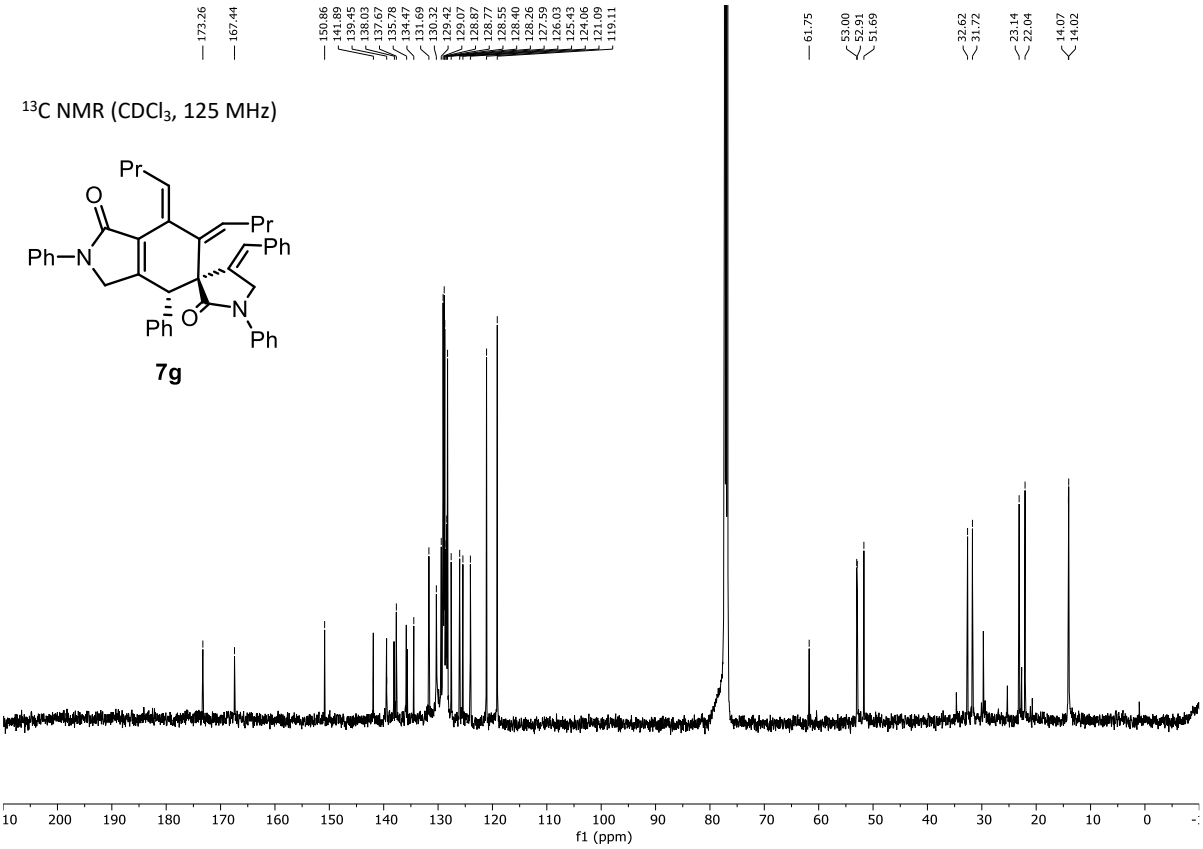
^{1}H NMR ($CDCl_3$, 500 MHz)



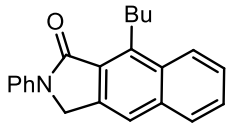
^{13}C NMR ($CDCl_3$, 125 MHz)



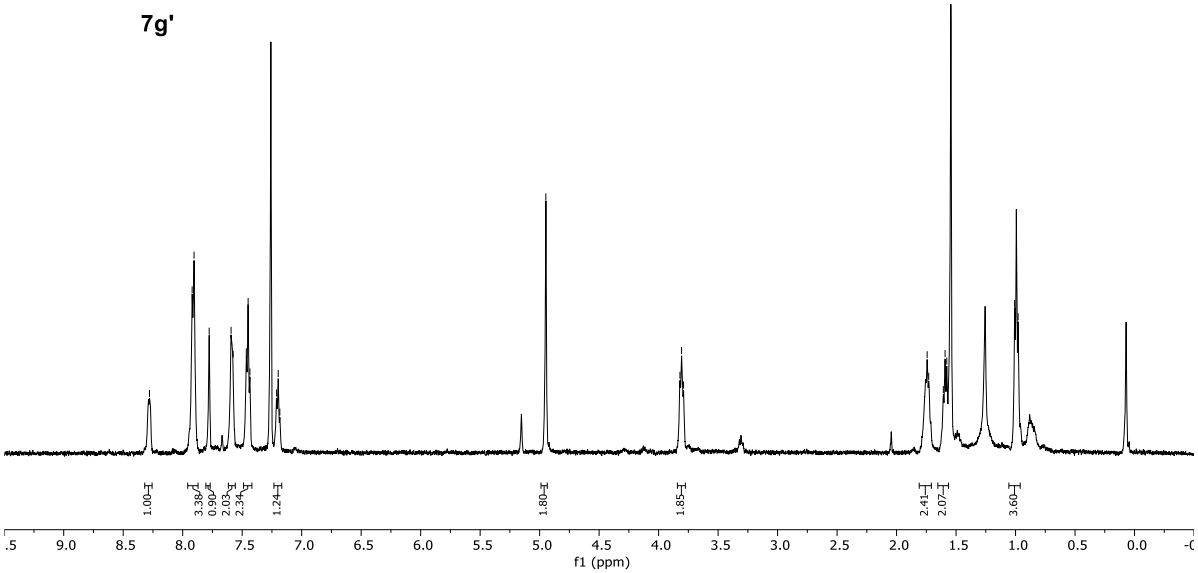

^{1}H NMR ($CDCl_3$, 500 MHz)
Pr
O
Pr
Ph–N
Ph
Ph
O
N
Ph
7g
f1 (ppm)

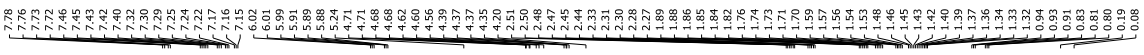

^{13}C NMR ($CDCl_3$, 125 MHz)
Pr
O
Pr
Ph–N
Ph
Ph
O
N
Ph
7g
f1 (ppm)

^{1}H NMR ($CDCl_3$, 500 MHz)

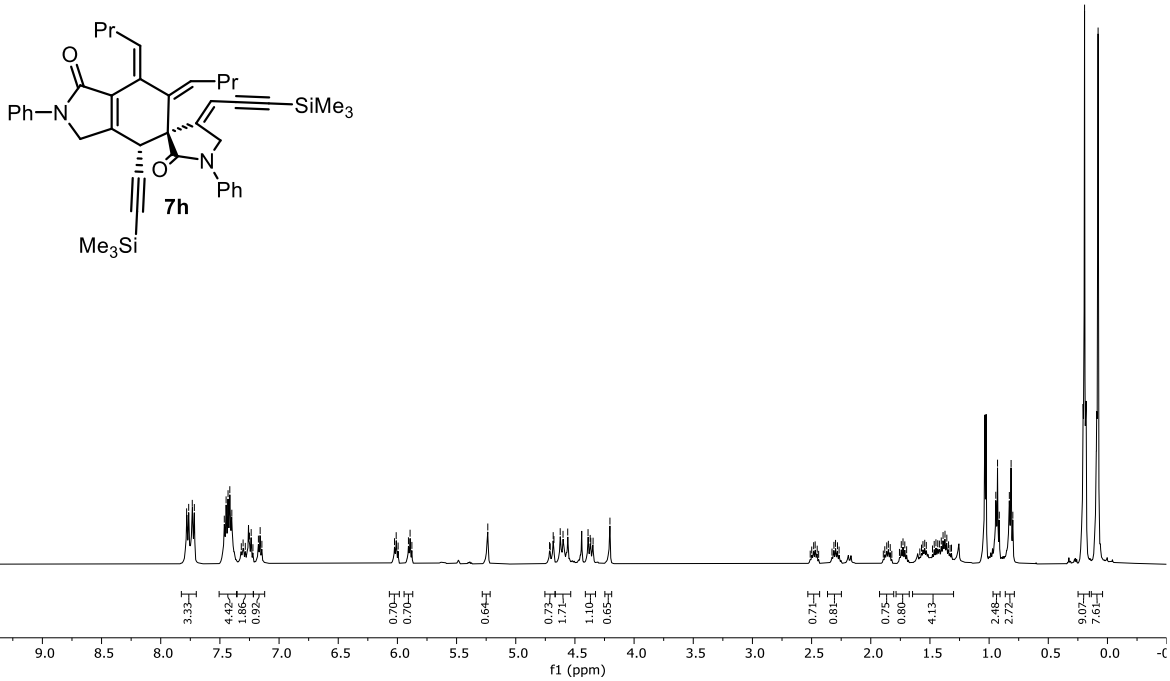


7g'

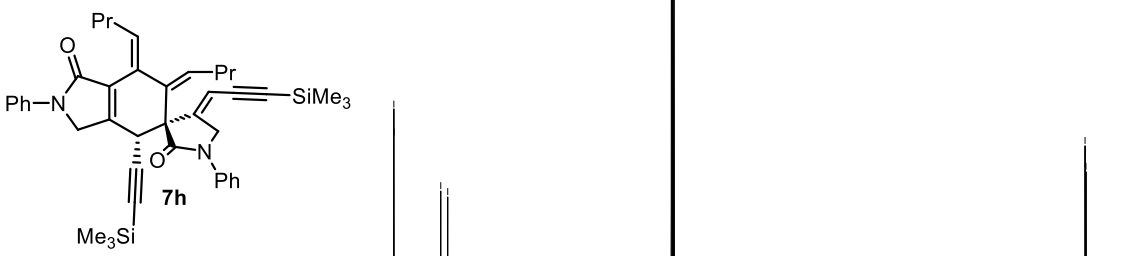


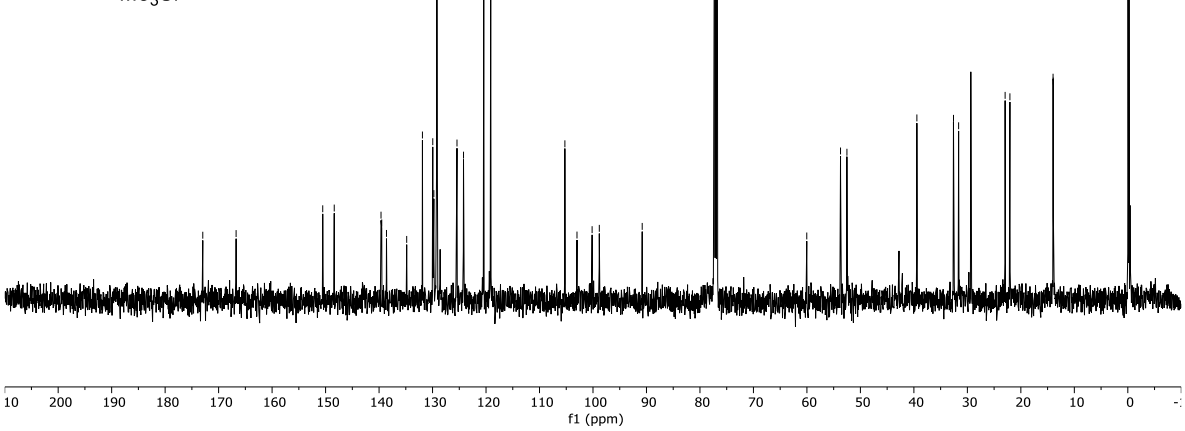


^{1}H NMR ($CDCl_3$, 500 MHz)

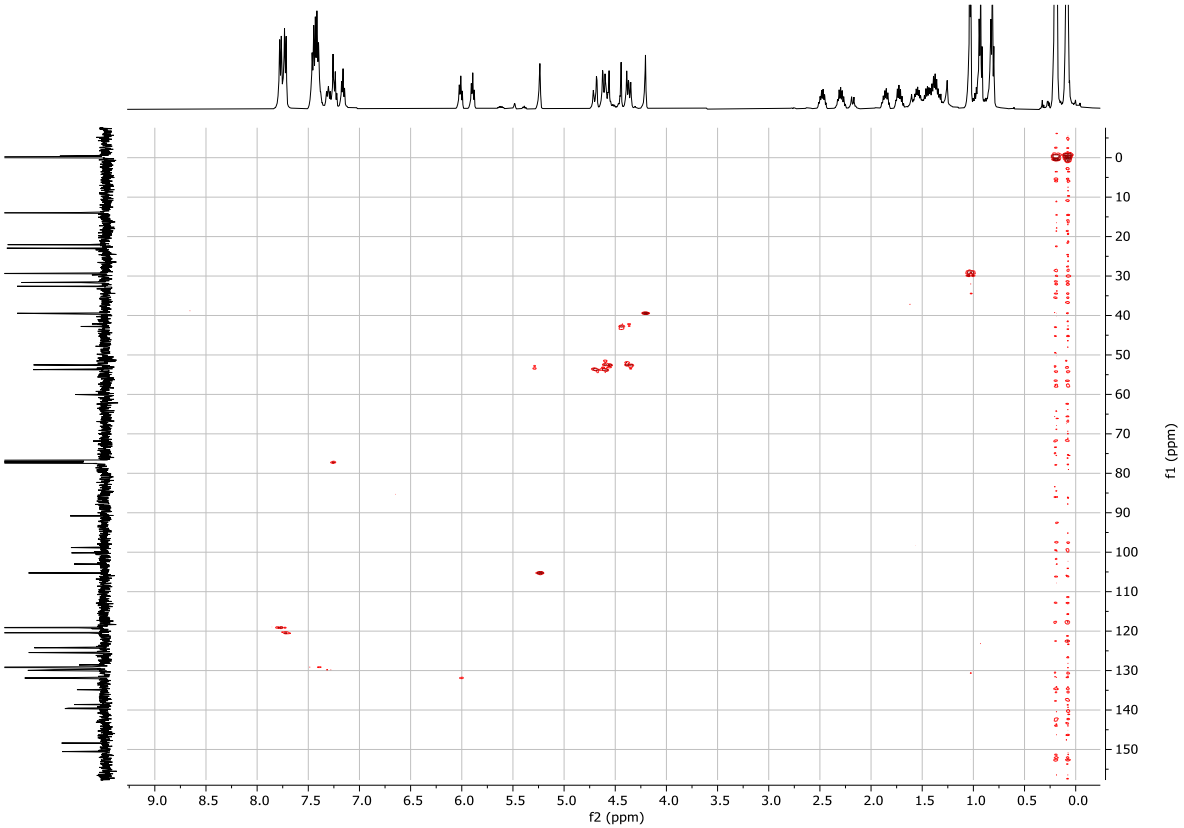


^{13}C NMR ($CDCl_3$, 125 MHz)

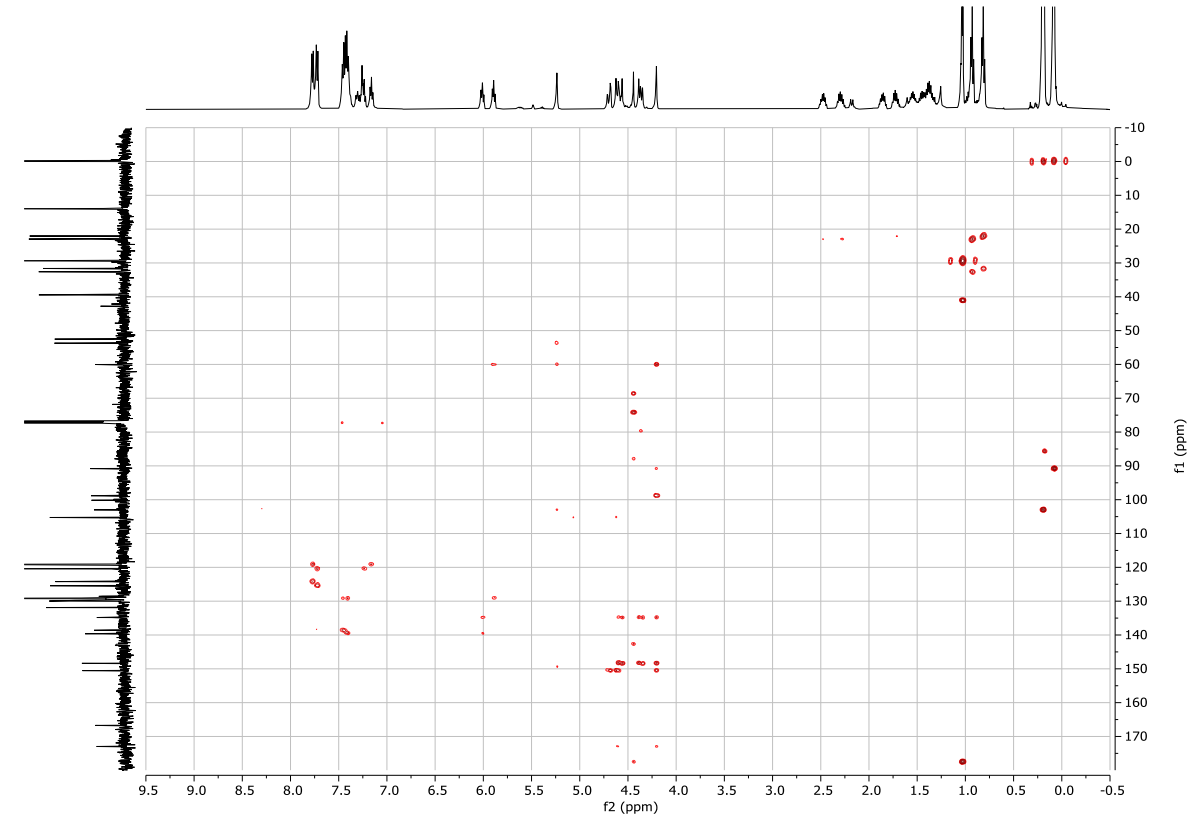




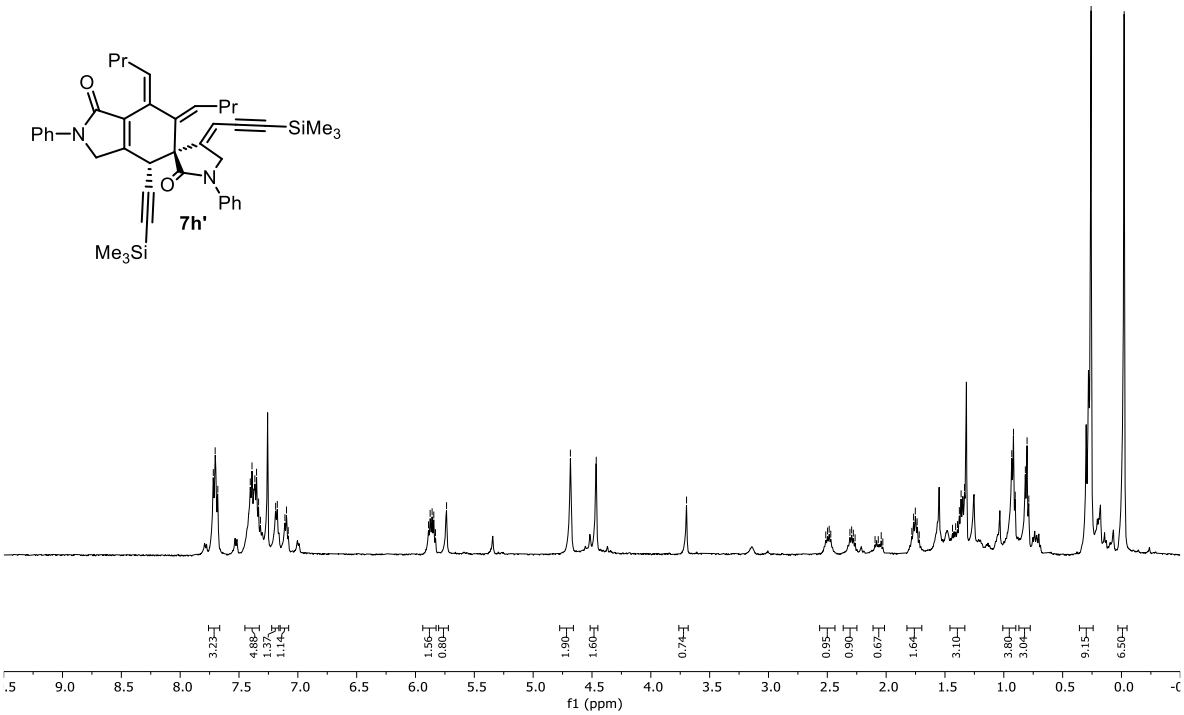
HMQC of 7h



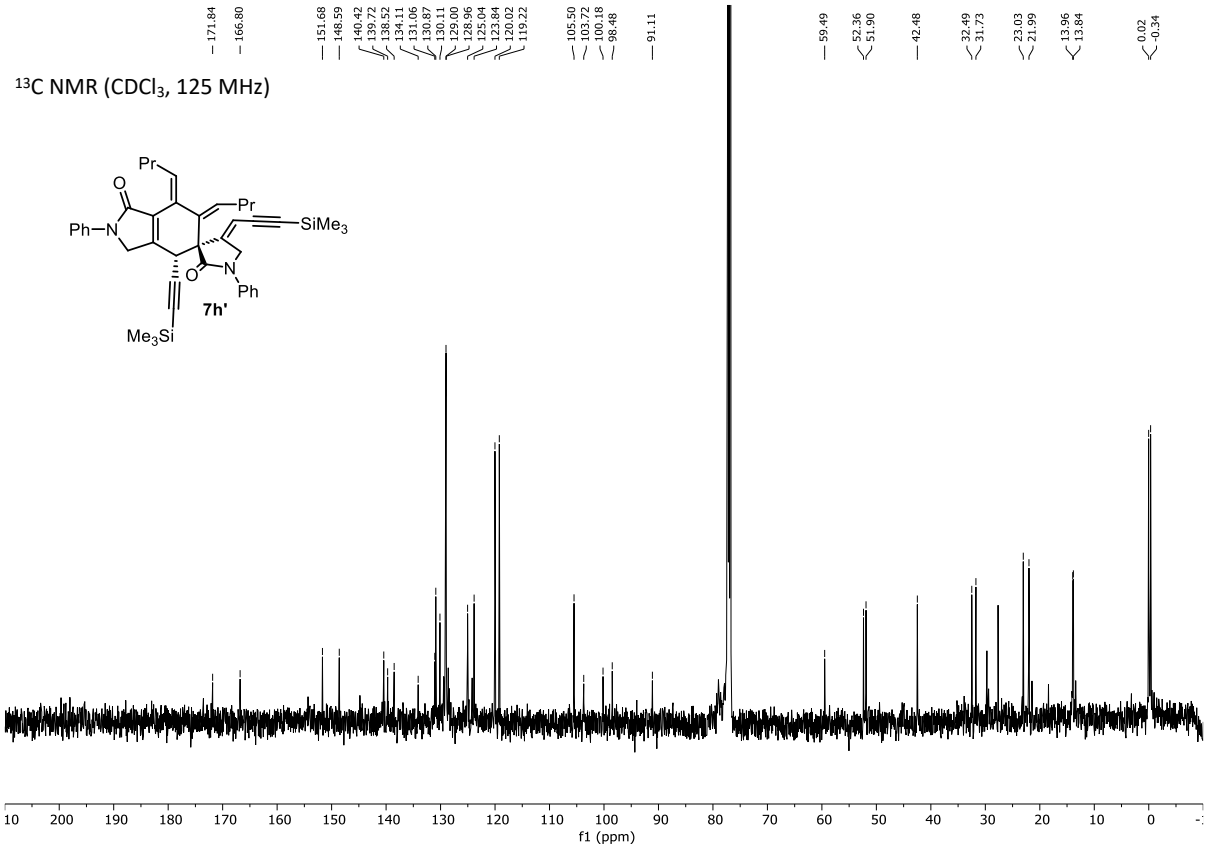
HMBC of 7h



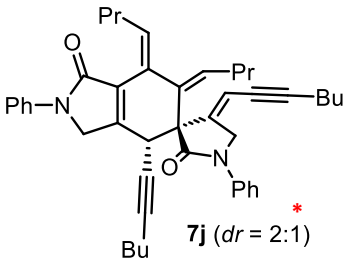
^{1}H NMR ($CDCl_3$, 500 MHz)



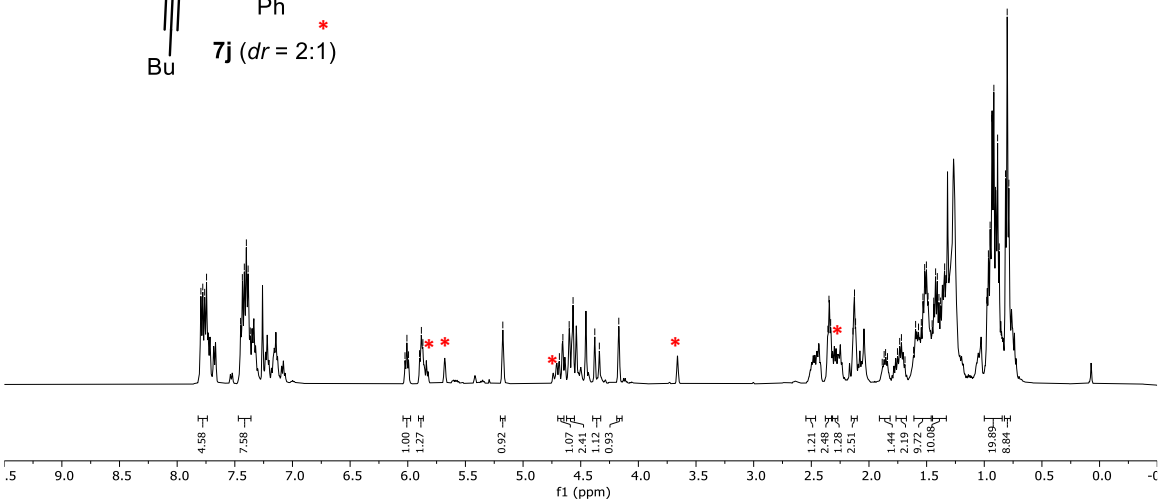
^{13}C NMR ($CDCl_3$, 125 MHz)



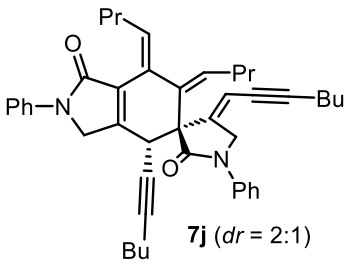
^{1}H NMR ($CDCl_3$, 500 MHz)



7j (*dr* = 2:1)

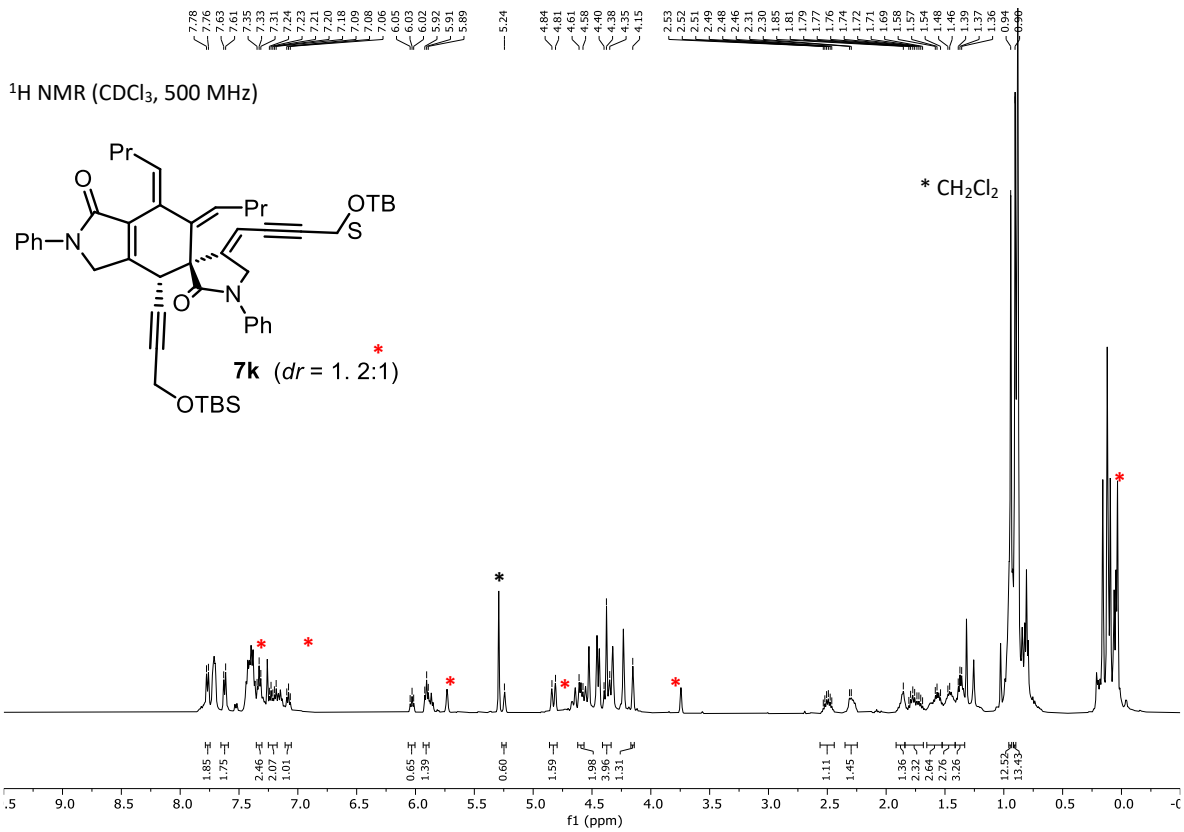


^{13}C NMR ($CDCl_3$, 125 MHz)

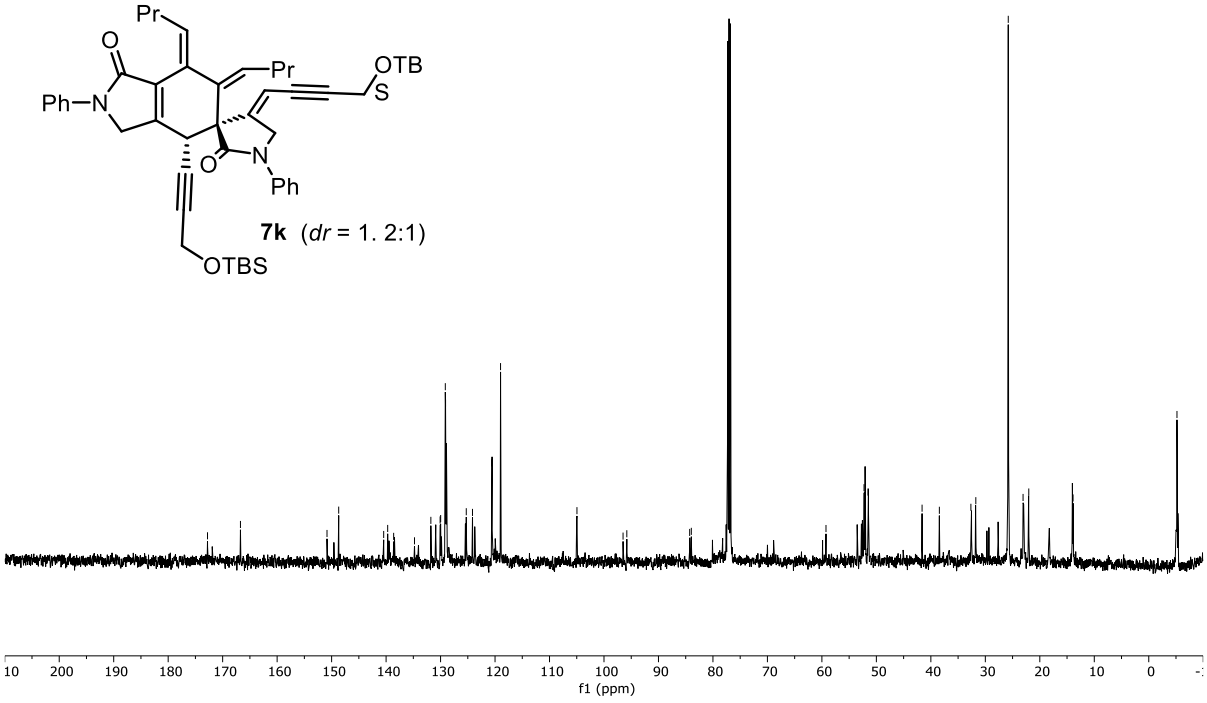


7j (*dr* = 2:1)

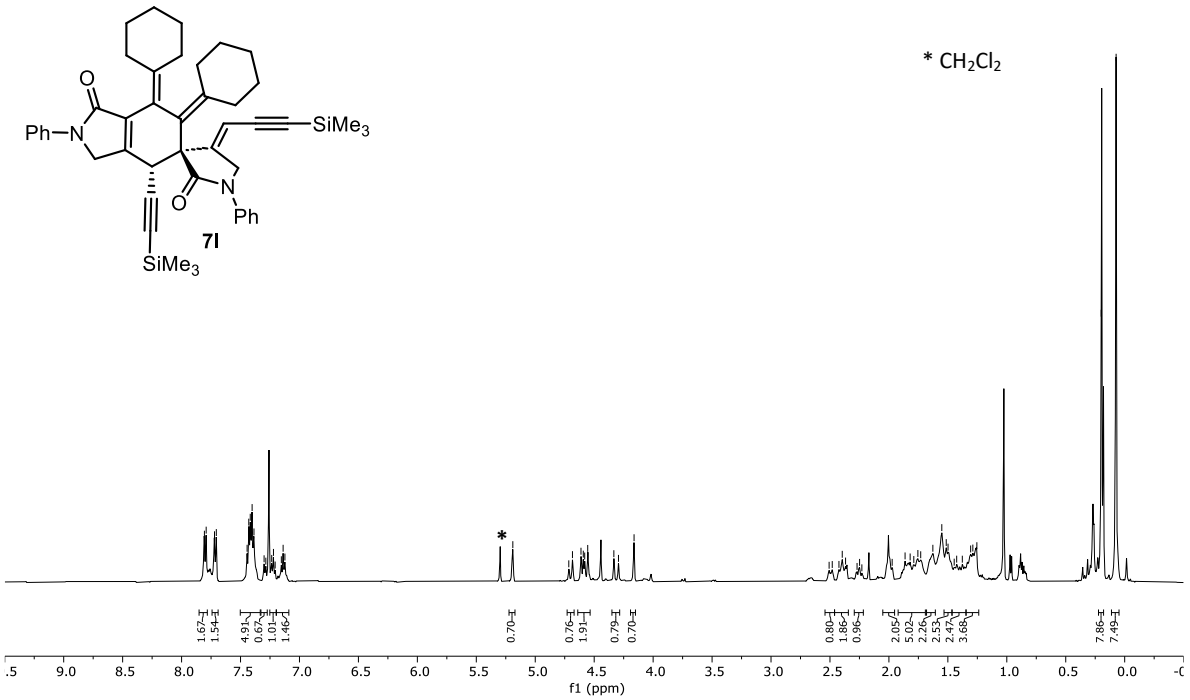
^{1}H NMR ($CDCl_3$, 500 MHz)



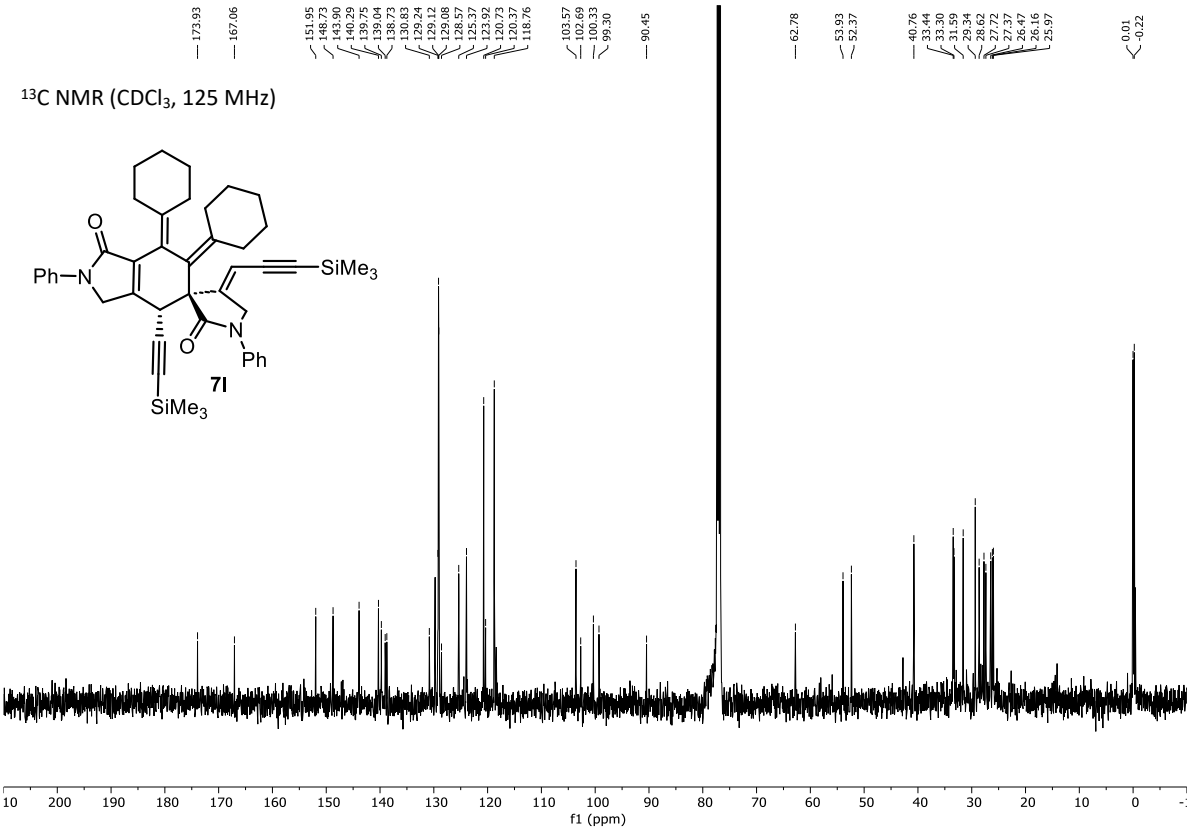
^{13}C NMR ($CDCl_3$, 125 MHz)



^{1}H NMR ($CDCl_3$, 500 MHz)



^{13}C NMR ($CDCl_3$, 125 MHz)



X-ray Crystallographic Data

All X-ray data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Summary of X-ray Crystallographic Data

Crystal data	Compound **2a**
CCDC deposition number	2494308
Chemical formula	$C_{36}H_{44}O_2Si_2$
Formula weight (g/mol)	564.89
Crystal system, space group	Monoclinic, P21/n
Temperature (K)	100
a, b, c (Å)	11.1779(6), 17.3334(9), 17.0876(9)
α, β, *γ* (°)	90, 100.100(1), 90
V (Å^3)	3259.4(3)
Z	4
Radiation type	MoK_α
μ (mm^{-1})	0.138
Crystal size (mm)	0.220 x 0.224 x 0.262
Diffraction measurement device	Bruker APEX-II CCD
Absorption correction	(Same as μ)
T_{min}, T_{max}	0.022, 0.051
F(000)	1216.0
Density (g/cm^3)	1.151
R_{int}	0.0856
$R_1(wR_2)$	0.2057 (8408)
GOF	1.037
N_{ref}	8408
Completeness (%)	99.9
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.521, -0.276

2. Crystal preparation of 2a

The purified product **2a** (10 mg) was dissolved in CH_2Cl_2 (1mL) in a vial. Then hexane (1 mL) was carefully added along the wall without disturbing the CH_2Cl_2 layer. The vial was then caped slightly and stored at 0 ^oC until crystals are formed.

3. X-ray structure determinations

The red block crystal was coated with Paratone-n oil and mounted to the nylon loop. Crystallography data for **2a** was collected at 100 K using a Bruker D8 QUEST ECO diffractometer under its default manufacturer settings. The collected frames were integrated using Bruker *APEX4* software suite. Data reduction was integrated with SAINT+ v.8.40B and scaled with SADABS v.2016 programs in the *APEX4* suite.

Structure solution and refinement were carried out with *SHELX* package using the XPERP utility for the space group determination and the *SHELXT* and *SHELXL* plugins within the *Olex2-1.5* for the structure solution and refinement, respectively.[1,2] Details of the X-ray diffraction experiment conditions and the crystallographic data for **2a** is given in Table xxxx, and CIF file is uploaded as Supporting Information.

4. Crystal Structure of 2a

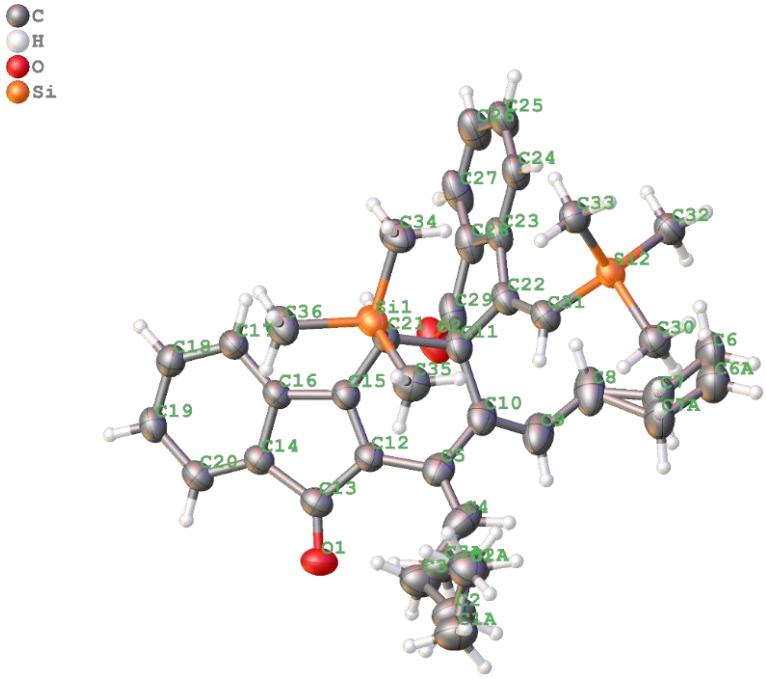


Fig. S1. Molecular structure of **2a**, shows 50% thermal probability ellipsoids. Hydrogen atoms are omitted for clarity.

Selected bond distances (Å):

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C4	C5	1.345(5)	C21	Si1	1.930(3)
C4	C3	1.605(9)	C22	C23	1.474(5)
C4	C3A	1.203(14)	C22	C31	1.339(5)
C5	C10	1.494(5)	C23	C24	1.390(5)
C5	C12	1.465(5)	C23	C28	1.402(5)
C8	C9	1.494(6)	C24	C25	1.383(5)
C8	C7	1.472(18)	C25	C26	1.391(6)
C8	C7A	1.67(3)	C26	C27	1.391(6)
C9	C10	1.341(5)	C27	C28	1.382(5)
C10	C11	1.528(5)	C28	C29	1.476(5)
C11	C21	1.599(5)	C29	O2	1.211(4)
C11	C22	1.541(4)	C30	Si2	1.865(4)
C11	C29	1.543(5)	C31	Si2	1.872(3)
C12	C13	1.486(4)	C32	Si2	1.864(3)
C12	C15	1.355(4)	C33	Si2	1.874(4)
C13	C14	1.492(5)	C34	Si1	1.861(4)
C13	O1	1.216(4)	C35	Si1	1.853(4)
C14	C16	1.405(4)	C36	Si1	1.871(4)
C14	C20	1.373(4)	C1	C2	1.497(7)
C15	C16	1.479(4)	C2	C3	1.520(8)
C15	C21	1.485(4)	C6	C7	1.527(9)
C16	C17	1.367(4)	C1A	C2A	1.499(9)
C17	C18	1.400(5)	C2A	C3A	1.517(11)
C18	C19	1.382(5)	C6A	C7A	1.524(10)

C19	C20	1.404(5)

Selected bond angles (°):

Atom	Atom	Atom	Angle °	Atom	Atom	Atom	Angle °
C5	C4	C3	126.5(5)	C15	C21	C11	109.1(3)
C3A	C4	C5	139.2(10)	C15	C21	Si1	109.1(2)
C4	C5	C10	122.2(4)	C23	C22	C11	105.8(3)
C4	C5	C12	125.6(4)	C31	C22	C11	124.5(3)
C12	C5	C10	112.1(3)	C31	C22	C23	129.6(3)
C9	C8	C7A	103.7(10)	C24	C23	C22	130.7(3)
C7	C8	C9	120.3(10)	C24	C23	C28	119.1(3)
C10	C9	C8	129.3(4)	C28	C23	C22	110.1(3)
C5	C10	C11	118.8(3)	C25	C24	C23	119.4(4)
C9	C10	C5	119.1(4)	C24	C25	C26	120.7(4)
C9	C10	C11	122.0(4)	C25	C26	C27	120.9(4)
C10	C11	C21	114.0(3)	C28	C27	C26	117.9(4)
C10	C11	C22	114.7(3)	C23	C28	C29	109.4(3)
C10	C11	C29	113.0(3)	C27	C28	C23	122.0(4)
C22	C11	C21	110.1(3)	C27	C28	C29	128.7(3)
C22	C11	C29	102.2(3)	C28	C29	C11	106.3(3)
C29	C11	C21	101.4(3)	O2	C29	C11	126.6(4)
C5	C12	C13	130.3(3)	O2	C29	C28	126.9(4)
C15	C12	C5	120.7(3)	C22	C31	Si2	134.3(3)
C15	C12	C13	108.4(3)	C34	Si1	C21	110.44(16)
C12	C13	C14	105.7(3)	C34	Si1	C36	106.18(18)
O1	C13	C12	128.2(3)	C35	Si1	C21	113.09(17)
O1	C13	C14	126.1(3)	C35	Si1	C34	112.40(19)
C16	C14	C13	108.0(3)	C35	Si1	C36	107.10(19)

C20	C14	C13	130.5(3)	C36	Si1	C21	107.19(16)
C20	C14	C16	121.5(3)	C30	Si2	C31	103.08(16)
C12	C15	C16	110.6(3)	C30	Si2	C33	109.38(17)
C12	C15	C21	122.4(3)	C31	Si2	C33	111.73(16)
C16	C15	C21	127.0(3)	C32	Si2	C30	108.50(16)
C14	C16	C15	107.3(3)	C32	Si2	C31	111.68(16)
C17	C16	C14	120.5(3)	C32	Si2	C33	112.03(16)
C17	C16	C15	132.2(3)	C1	C2	C3	113.5(6)
C16	C17	C18	118.3(3)	C2	C3	C4	113.8(6)
C19	C18	C17	121.5(3)	C8	C7	C6	119.2(11)
C18	C19	C20	120.0(3)	C1A	C2A	C3A	113.8(9)
C14	C20	C19	118.2(3)	C4	C3A	C2A	115.6(12)
C11	C21	Si1	119.5(2)	C6A	C7A	C8	104.4(14)

References

1. G. M. Sheldrick, A Short History of SHELX. *Acta Crystallogr. A,* 2008, **64 (1),** 112–122. https://doi.org/10.1107/S0108767307043930.
2. P. Müller, Practical Suggestions for Better Crystal Structures. *Crystallogr. Rev.,* 2009, ***15*** **(1),** 57–83. DOI: .org/10.1080/08893110802547240.

DFT Calculation Data

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).[3] Frequencies were analytically computed at the same level of theory to obtain the Gibbs 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.[4,5] All transition state structures were confirmed to connect the proposed reactants and products by intrinsic reaction coordinate (IRC) calculations. All the energies given in the text are relative free energies corrected with solvation effects.

References

1. Gaussian 09, Revision A.02, 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 and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
2. (a) A. D. Becke*, J. Chem. Phys.* 1993, **98,** 5648. (b) A. D. Becke, *J. Chem. Phys.,* 1993, **98**, 1372. (c) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B,* 1988, **37**, 785. (d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.,* 1994, **98**, 11623.
3. (a) P. J. Hay and W. R. Wadt, *J. Chem. Phys.* 1985, **82**, 270. (b) Wadt, P. J. Hay, *J. Chem. Phys.,* 1985, **82**, 284. (c) P. J. Hay, W, R, Wadt, *J. Chem. Phys.,* 1985, **82**, 299.
4. (a) Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.,* 2008, **120**, 215. (b) Y. Zhao and D. G. Truhlar, *Acc. Chem. Res.,* 2008, **41**, 157.
5. (a) L. Szentpály, P. Fuentealba, H. Preuss and H. Stoll, *Chem. Phys. Lett.,* 1982, **93**, 555. (b) M. Dolg, U. Wedig, H. Stoll and H. Preuss, J. *Chem. Phys.,* 1987, **86**, 866. (c) P. Schwerdtfeger, M. Dolg, W. H. E. Schwarz, G. A. Bowmaker and P. D. W. Boyd, *J. Chem. Phys.,* 1989, **91**, 1762.

2. Calculated energy values

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

Species	G_{298}[a]	E_{298}[b]	E_{sol}[c]	Imaginary Frequency
IN1-1a	-1063.577308	-1063.8725206	-1063.47907631	
TS1-1a	-2127.109808	-2127.7228921	-2126.94661701	-392.8377
TS2-1a	-2127.105407	-2127.7203124	-2126.94407858	-383.9716
TS3-1a	-2127.095126	-2127.710354	-2126.935515	-412.2641
TS4-1a	-2127.099767	-2127.713968	-2126.940091	-414.8113
IN2-1a	-2127.132260	-2127.7544513	-2126.98009914	
TS-IN2-1a	-2127.127565	-2127.7512603	-2126.98136197	-156.7388
2a	-2127.165766	-2127.7896364	-2127.03392390	
1a	-1063.532635	-1063.8201881	-1063.43069294	
TS5-1a	-2127.062291	-2127.6688997	-2126.89210977	-341.9745
IN3-1a	-2127.066944	-2127.6757633	-2126.89899281	
1f	-1063.532635	-1063.8201881	-1063.43069294	
TS0-1f	-963.263776	-963.5744023	-963.099129797	-352.0293
IN1-1f	-963.366195	-963.6812355	-963.2019234	
TS1-1f	-1926.671955	-1927.327091	-1926.38605836	-304.0445
2f-1	-1926.734782	-1927.3987074	-1926.46929618	
TS3-1f	-963.257828	-963.5698681	-963.096287970	-180.8246
IN2-1f	-963.283321	-963.6024724	-963.130713222	
2f-2	-963.434088	-963.7565159	-963.277084107	
1h	-845.409839	-845.6339013	-845.232233821	
TS0-1h	-845.365237	-845.5911069	-845.185069629	-223.5006
IN1-1h	-845.388825	-845.6212425	-845.219678962	
2h-2	-845.541029	-845.7775492	-845.367893431	
TS1-1h	-845.366612	-845.591343	-845.183157911	-216.0208
IN2-1h	-845.454989	-845.6840897	-845.275793608	
TS1-1h(endo)	-1690.858894	-1691.3393894	-1690.53359264	-419.1102

2h-1	-1690.932028	-1691.4220308	-1690.62513580	
IN1-4a	-962.134349	-962.416677	-961.936824511	
exo-TS1	-1924.227808	-1924.812906	-1923.85935503	-413.2256
exo-5a-1	-1924.281302	-1924.8784685	-1923.94050886	
exo-TS2	-2153.462537	-2154.1266888	-2153.20560722	-410.5479
5c-2	-1924.315032	-1924.9135661	-1923.97201651	
endo-TS1	-1924.223377	-1924.8110478	-1923.85995048	-385.9360
IN2-4a	-1924.251244	-1924.8441408	-1923.89451347	
endo-5a-1	-1924.280456	-1924.8774963	-1923.93965048	
4a	-962.072505	-962.3493607	-961.876781122	
TS3-IN1	-1924.150521	-1924.7333635	-1923.78865273	-378.2502
IN5-4a	-1924.246277	-1924.8389022	-1923.89563553	
TS-4a	-962.035068	-962.3138375	-961.8349055	-281.1960

[a] Sum of electronic and thermal free energies

[b] Sum of electronic energies

[c] Single point energies calculated in toluene solution

3. Cartesian Coordinates for All Species

IN1-1a

C	-4.19263600	2.58059500	0.41548200
C	-2.96157600	1.97383400	0.70788700
C	-1.80347600	2.74507400	0.76475700
C	-1.90616900	4.11398800	0.52564800
C	-3.13310700	4.73922000	0.23033700
C	-4.28972700	3.95219700	0.17688000
H	-5.09131300	1.97070000	0.37342100
H	-2.91730800	0.90356200	0.88906300
H	-0.83335700	2.31067500	0.98824100
H	-5.25675700	4.38553900	-0.04551200
C	-0.80552900	5.10860300	0.53704100
C	-2.93354900	6.19585700	0.02351000

C	-3.81652600	7.17475900	-0.27816300
C	-1.46604900	6.42523100	0.21813300
C	-0.80956700	7.56399800	0.13329800
O	0.37367700	4.89581200	0.75857700
C	-0.13759000	8.67997100	0.05879500
H	-3.34634400	8.15958500	-0.36546600
C	0.11875600	9.62577400	1.21397100
H	1.20582000	9.71303100	1.35644300
H	-0.28804100	9.19858000	2.13746300
C	-0.47187500	11.02666600	0.97387300
H	-1.55828800	10.93838000	0.84300600
H	-0.08019400	11.42746100	0.02857900
C	-0.16111100	12.00050700	2.11454000
H	0.92050900	12.12868700	2.24376300
H	-0.59330600	12.98848900	1.92058100
H	-0.56816500	11.63930600	3.06669500
Si	-5.67562800	7.25143200	-0.59095300
C	-6.18788400	6.23668200	-2.11055100
H	-5.68735600	6.61902600	-3.00805300
H	-5.94150500	5.17314800	-2.02897400
H	-7.26975200	6.31692700	-2.27600700
C	-6.67863300	6.74113000	0.93733800
H	-6.47773100	5.71770200	1.27017200
H	-6.45341600	7.40724200	1.77867200
H	-7.75374600	6.82007900	0.73216300
C	-6.04910600	9.07306500	-0.95355900
H	-5.49160100	9.42999400	-1.82811000
H	-7.11565300	9.22531100	-1.15848200

H	-5.78185300	9.71485300	-0.10520600
H	0.27612700	8.97145400	-0.90996700

TS1-1a

C	-8.86177000	-2.27738500	-1.04467200
O	-8.18956400	-1.94969400	-2.01616600
C	-8.50164100	-2.15844800	0.39707600
C	-7.30575200	-1.69717700	0.85847800
C	-6.52091500	-0.70625500	1.23297000
H	-5.49670700	-0.90801200	1.52961500
C	-9.58382600	-2.72601200	1.21832800
C	-9.56610900	-2.72830200	2.57806400
H	-8.66446100	-2.26901700	2.99216200
C	-6.83690300	-5.48877600	2.33094900
C	-6.36268900	-4.09085500	2.13698900
C	-6.02701000	-3.50246100	3.45810600
O	-5.61035900	-2.37581800	3.70854900
C	-6.24060100	-3.46576400	0.93655000
C	-5.72817500	-3.51754000	-0.29045700
H	-6.17445800	-2.93639800	-1.09653800
C	-7.22276200	-6.31461500	1.32694700
H	-7.19776900	-5.83044500	0.34593800
C	-10.20422000	-2.91225000	-1.06199500
C	-10.97929500	-3.23362000	-2.17240500
C	-10.61761300	-3.19741500	0.25440500
C	-12.20691900	-3.86233800	-1.96432200
H	-10.61841900	-2.99538800	-3.16890000
C	-11.84572700	-3.83249400	0.45036900

C	-12.62865600	-4.15941900	-0.66129900
H	-12.83669600	-4.12698300	-2.80910900
H	-12.19834200	-4.08202200	1.44344200
H	-13.58346600	-4.65595500	-0.50905000
C	-6.99325600	0.72561700	1.34763800
H	-6.39118700	1.34346800	0.66393000
H	-8.03404900	0.80599400	1.01366200
C	-6.84920600	1.27747800	2.77828400
H	-5.81022000	1.15440800	3.11089900
H	-7.45776400	0.66848300	3.45834300
C	-7.25861200	2.74972500	2.88238000
H	-8.30383300	2.89432000	2.58222900
H	-7.15256900	3.11831600	3.90886900
H	-6.63827500	3.38205300	2.23510900
C	-6.27955700	-4.58217700	4.44817000
C	-6.09456700	-4.52855200	5.82718900
C	-6.75180400	-5.73641000	3.79600800
C	-6.39561100	-5.66257800	6.58133600
H	-5.72263100	-3.61623400	6.28480200
C	-7.05222800	-6.86661300	4.56210200
C	-6.87166400	-6.81883700	5.94732400
H	-6.26316200	-5.65423900	7.65968000
H	-7.42205000	-7.77567900	4.10446800
H	-7.10565100	-7.69725100	6.54311200
C	-4.46687300	-4.27826300	-0.62857700
H	-3.66006300	-3.55105200	-0.80936600
H	-4.15638000	-4.88941600	0.22631100
C	-4.63029400	-5.15232200	-1.88614300

H	-4.97716600	-4.52712000	-2.71967700
H	-5.41941900	-5.89472900	-1.70903200
C	-3.32979300	-5.86105000	-2.27736100
H	-3.47093700	-6.48050000	-3.17004700
H	-2.53426800	-5.13797700	-2.49493500
H	-2.97412000	-6.51332900	-1.47061400
Si	-7.77905300	-8.11140200	1.20109000
Si	-10.78726900	-3.24719000	3.92416700
C	-12.42352900	-2.29521300	3.77220700
H	-13.10955500	-2.58856900	4.57703100
H	-12.24506100	-1.21760700	3.86803500
H	-12.93810600	-2.45727800	2.81972200
C	-11.08779900	-5.11943900	3.94315600
H	-11.49070400	-5.50757600	3.00196200
H	-10.14731100	-5.64725900	4.13872600
H	-11.79124300	-5.38500300	4.74247800
C	-9.97897000	-2.76165600	5.56500500
H	-9.02741700	-3.28535400	5.71301500
H	-9.77593900	-1.68473200	5.60869900
H	-10.62974000	-3.00920900	6.41257300
C	-9.42729100	-8.43227600	2.08580900
H	-9.75041800	-9.46779100	1.91888700
H	-9.38734900	-8.26768300	3.16739700
H	-10.20675700	-7.77356100	1.68529700
C	-8.05121500	-8.42469300	-0.64771600
H	-7.13110900	-8.26674500	-1.22385300
H	-8.38000500	-9.45506700	-0.82981000
H	-8.81776600	-7.75659600	-1.05857500

C	-6.44346900	-9.31576200	1.80913400
H	-6.78391200	-10.35297300	1.69713000
H	-5.52968100	-9.20247400	1.21373700
H	-6.16868600	-9.16709800	2.85840400

TS2-1a

C	-8.60505600	-3.18485700	-0.74698200
O	-7.90111900	-2.86109000	-1.69433300
C	-8.27651200	-3.07503000	0.71079200
C	-7.07657000	-2.61147800	1.14629000
C	-6.23957800	-1.59497500	1.25680000
H	-5.18268900	-1.77291000	1.44012400
C	-9.38755700	-3.62476700	1.49911700
C	-9.40817000	-3.64357400	2.85901000
H	-8.50790500	-3.21595200	3.30721500
C	-6.89934700	-6.35595200	2.74512400
C	-6.26822500	-5.00226700	2.65765400
C	-5.93014000	-4.53921700	4.02273700
C	-6.05631600	-4.43122100	1.44375600
C	-5.58748900	-4.64576700	0.21728600
H	-5.98776100	-4.09582300	-0.63244000
C	-9.95837100	-3.78716900	-0.79844800
C	-10.71349600	-4.08340600	-1.92947800
C	-10.40918900	-4.06520400	0.50641700
C	-11.96216500	-4.67862200	-1.75406000
H	-10.32106900	-3.85225400	-2.91555000

C	-11.65846000	-4.66746400	0.66900300
C	-12.42265800	-4.96814700	-0.46254900
H	-12.57788200	-4.92413700	-2.61475400
H	-12.04170500	-4.91479000	1.65067300
H	-13.39326900	-5.44032100	-0.33509800
C	-6.67430200	-0.14928600	1.15748600
H	-6.13023000	0.31119200	0.31885700
H	-7.73998100	-0.09990900	0.90799800
C	-6.39445700	0.65959200	2.43699200
H	-5.32739400	0.58274400	2.68822900
H	-6.94233000	0.20551800	3.27316500
C	-6.78407900	2.13452300	2.29789700
H	-7.85263000	2.24300700	2.07606100
H	-6.57709400	2.68835500	3.22042500
H	-6.22651900	2.61730700	1.48607900
C	-6.40380800	-5.61436900	4.94070000
C	-6.37506600	-5.72063500	6.33479100
C	-6.95298500	-6.67383500	4.19572100
C	-6.88019100	-6.87352800	6.94302000
H	-5.97421300	-4.92769700	6.95315600
C	-7.45160500	-7.82824000	4.79331900
C	-7.41280000	-7.92483900	6.18423600
H	-6.85873100	-6.95357300	8.02671400
H	-7.85633200	-8.62274900	4.17279900
H	-7.79488800	-8.81120300	6.68301900
C	-4.46722100	-5.61254800	-0.08142200
H	-3.64817700	-5.07596200	-0.58376100
H	-4.06384800	-6.02294800	0.85064700

C	-4.95705800	-6.75827800	-0.99256800
H	-5.38523700	-6.33329600	-1.91054100
H	-5.77105200	-7.28038000	-0.47770100
C	-3.83444800	-7.73647100	-1.35140500
H	-4.20759800	-8.54417800	-1.99113700
H	-3.02073200	-7.23359200	-1.88885300
H	-3.40580000	-8.19577000	-0.45230400
Si	-10.70293900	-4.12338700	4.15305400
C	-12.28371800	-3.09164400	3.94062100
H	-13.01980300	-3.36429600	4.70760200
H	-12.05993800	-2.02522800	4.06340700
H	-12.75990300	-3.21473300	2.96274200
C	-11.09275400	-5.97850100	4.15433900
H	-11.45188200	-6.35385100	3.19090800
H	-10.19468800	-6.55107600	4.41201200
H	-11.85841700	-6.20315100	4.90790200
C	-9.94343600	-3.67734900	5.82884100
H	-9.02984200	-4.25277700	6.01725500
H	-9.68599100	-2.61253200	5.88259400
H	-10.64388000	-3.88897900	6.64599800
C	-5.26068400	-3.39426400	4.31446900
H	-5.01354100	-2.80566800	3.42955800
O	-7.25962000	-7.08165000	1.82880200
Si	-4.59491300	-2.59642300	5.88925100
C	-5.97723200	-2.04529400	7.06823200
H	-5.55094700	-1.58477600	7.96862100
H	-6.61068800	-1.29357200	6.58216200
H	-6.63253600	-2.86094000	7.39055100

C	-3.67035500	-1.04350800	5.31933100
H	-3.23177100	-0.51142800	6.17210500
H	-2.85266000	-1.29340600	4.63223200
H	-4.33820700	-0.34379500	4.80276700
C	-3.34157500	-3.70766200	6.78363100
H	-2.48599800	-3.91378400	6.12954800
H	-2.95784500	-3.20177000	7.67874800
H	-3.75213700	-4.67264000	7.09651600

TS3-1a

C	-9.92687400	-3.84789500	-0.22897800
O	-9.93075300	-4.03266500	-1.43949200
C	-8.76728900	-3.46779600	0.64104300
C	-7.52148800	-3.29737500	0.12320900
C	-6.91437800	-2.77131600	-0.93750700
H	-5.95376700	-3.16827300	-1.26043300
C	-9.23126600	-3.34644200	2.02989400
C	-8.42112600	-3.05642100	3.08317100
H	-7.37665300	-2.91944200	2.79755500
C	-7.54622000	-6.57593600	1.23643900
C	-6.60083200	-5.58140300	1.75926100
C	-6.30053200	-5.90173000	3.19325400
O	-5.53814900	-5.31183300	3.94798800
C	-6.02992600	-4.49882700	1.17024400
C	-4.84522100	-3.88555200	1.17086700
H	-3.98120900	-4.55560500	1.20953900
C	-7.97190200	-6.61887500	-0.05433700
H	-7.57163500	-5.80851500	-0.66631600

C	-11.10245500	-3.88515300	0.67720400
C	-12.42785500	-4.14578400	0.34144100
C	-10.69859700	-3.60737500	1.99624500
C	-13.38288400	-4.13763000	1.35809000
H	-12.69331500	-4.34525600	-0.69292300
C	-11.66346800	-3.59872600	3.00560400
C	-12.99612500	-3.86629000	2.67720900
H	-14.42632000	-4.33776500	1.13117900
H	-11.40075200	-3.38891100	4.03465300
H	-13.74645500	-3.86094500	3.46355100
C	-7.43745900	-1.58546800	-1.71249400
H	-7.58069300	-1.91153200	-2.75400600
H	-8.42463200	-1.29811000	-1.33640100
C	-6.48915600	-0.37218500	-1.69789800
H	-5.49258500	-0.68463400	-2.04010600
H	-6.36436300	-0.02545500	-0.66372500
C	-6.99516200	0.77932800	-2.57231400
H	-7.97870600	1.12932500	-2.23629500
H	-6.30879400	1.63296900	-2.54140100
H	-7.09497900	0.46779200	-3.61923000
C	-7.09893700	-7.11372600	3.50308100
C	-7.16197500	-7.80814600	4.70793700
C	-7.84793200	-7.49238000	2.37292400
C	-8.01053000	-8.91213000	4.79241100
H	-6.55756700	-7.48350600	5.55024800
C	-8.70100300	-8.59344200	2.47202100
C	-8.77450800	-9.29228600	3.68098500
H	-8.08476800	-9.47660000	5.71770100

H	-9.31243600	-8.90936000	1.63619000
H	-9.44059600	-10.14770600	3.75829900
C	-4.50110700	-2.42503400	1.14132100
H	-3.99542000	-2.17376600	0.19477100
H	-5.40719300	-1.81614100	1.18960900
C	-3.56030200	-2.06171300	2.31006600
H	-2.64833000	-2.67056400	2.24424200
H	-4.04470400	-2.34027800	3.25373300
C	-3.18815800	-0.57640400	2.32208100
H	-2.51684900	-0.34515000	3.15658500
H	-2.68056500	-0.28450500	1.39426800
H	-4.07819000	0.05614700	2.42611400
Si	-9.01748100	-7.80958800	-1.09314600
Si	-8.65963500	-2.79938400	4.94358000
C	-9.78387000	-1.30937800	5.29724800
H	-9.87686200	-1.15538200	6.37991000
H	-9.35133500	-0.39626900	4.87131400
H	-10.79421600	-1.41358300	4.88844300
C	-9.30970800	-4.35589000	5.81092700
H	-9.41331900	-4.17031300	6.88764200
H	-10.28057700	-4.69572900	5.43654800
H	-8.60243700	-5.18292300	5.68328500
C	-6.93187200	-2.41906500	5.61065600
H	-6.23983500	-3.23608300	5.37486100
H	-6.52811200	-1.49826300	5.17119600
H	-6.94341500	-2.28652800	6.69937100
C	-10.84116300	-7.81946400	-0.57130100
H	-11.26869000	-6.81905900	-0.69927200

H	-11.40979400	-8.50860300	-1.20865700
H	-11.00488200	-8.11660100	0.46981100
C	-8.90738300	-7.14875300	-2.86024000
H	-7.87607000	-7.17373300	-3.23345800
H	-9.52178500	-7.74321300	-3.54735500
H	-9.25695000	-6.11088200	-2.89997600
C	-8.29195700	-9.56431200	-1.05834100
H	-8.25071900	-10.00396000	-0.05682500
H	-8.88993400	-10.23182900	-1.69194100
H	-7.27036800	-9.56147700	-1.45670400

TS4-1a

C	-5.95729900	-5.27680500	5.89074500
O	-5.07050800	-5.89579700	6.46418900
C	-7.03467300	-5.82789300	5.00475800
C	-7.10007000	-7.13450500	4.63104900
C	-7.32844200	-8.38205800	5.00517000
H	-7.02732500	-9.21136900	4.36956500
C	-7.92026500	-4.73198900	4.59605700
C	-9.07216500	-4.91977200	3.89386200
H	-9.25788800	-5.96692000	3.64473900
C	-8.47619600	-7.45529900	1.26348300
C	-7.27640800	-6.75273400	1.76543100
C	-7.11546700	-5.46494100	1.02330400
O	-6.22363900	-4.63800900	1.14044900
C	-6.32633100	-7.17148200	2.64970000
C	-5.04407300	-7.51174400	2.71668200
H	-4.61363500	-7.76573200	1.74220800

C	-8.88308700	-8.68427600	1.67580000
H	-8.24866500	-9.10217700	2.45959700
C	-8.24120200	-5.42909900	0.05111900
C	-8.51237800	-4.44816800	-0.89847500
C	-9.04142700	-6.57659200	0.19947500
C	-9.62803800	-4.61045800	-1.72029300
H	-7.85731100	-3.58562300	-0.98250500
C	-10.15946900	-6.72668000	-0.62662000
C	-10.44304400	-5.74171200	-1.57756600
H	-9.86854200	-3.86332600	-2.47155800
H	-10.81010700	-7.58828200	-0.54465600
H	-11.31267100	-5.85888700	-2.21885600
C	-6.20366900	-3.81671300	5.94998800
C	-7.33322800	-3.48960100	5.17681400
C	-5.45929800	-2.85788100	6.63055600
C	-7.71116600	-2.14967800	5.07696900
C	-5.85015800	-1.52300400	6.52911300
H	-4.59593300	-3.16049900	7.21601000
C	-6.96512600	-1.17916900	5.75373000
H	-8.55914800	-1.84484300	4.47734700
H	-5.28973900	-0.74741400	7.04341700
H	-7.25638600	-0.13539600	5.67048300
C	-8.00475300	-8.74319600	6.31044200
H	-7.30240900	-9.34994000	6.90198800
H	-8.19969900	-7.83354400	6.88903700
C	-9.30991800	-9.53654500	6.12062600
H	-9.10524700	-10.43306500	5.51883300
H	-10.01588700	-8.92875300	5.53946900

C	-9.94787700	-9.94664100	7.45181400
H	-10.87576100	-10.50697600	7.29149000
H	-9.27118900	-10.58116200	8.03704500
H	-10.18926800	-9.06839700	8.06258000
C	-4.08240100	-7.63800500	3.86304100
H	-4.56659500	-7.44070600	4.82004600
H	-3.71244700	-8.67508400	3.89360700
C	-2.87481900	-6.69247500	3.69392500
H	-3.24180400	-5.66090200	3.62630900
H	-2.36975800	-6.90251300	2.74048000
C	-1.88143800	-6.81471500	4.85288300
H	-2.36504500	-6.55996700	5.80229600
H	-1.49002100	-7.83660400	4.93625900
H	-1.02771800	-6.14144100	4.71381200
Si	-10.52709500	-3.79307900	3.44528700
Si	-10.25256500	-9.88333300	1.17688700
C	-11.25481700	-3.01044100	5.01493900
H	-12.10621500	-2.36745300	4.75784700
H	-11.62287800	-3.78838000	5.69434200
H	-10.53360400	-2.40363300	5.57110900
C	-10.09668800	-2.46166900	2.16577500
H	-9.26313000	-1.81616300	2.45986200
H	-9.82659900	-2.92678100	1.21151900
H	-10.96956600	-1.82025500	1.98843000
C	-11.84673100	-4.92376200	2.69507300
H	-11.49328500	-5.39122500	1.76898300
H	-12.13102400	-5.72492700	3.38801700
H	-12.75489300	-4.35706000	2.45573100

C	-11.98726300	-9.20476300	1.54388700
H	-12.75017600	-9.94646500	1.27520900
H	-12.09461800	-8.99394900	2.61458600
H	-12.21930000	-8.27971600	1.00606300
C	-9.98886000	-11.42124900	2.25187100
H	-10.73780500	-12.19128400	2.03088100
H	-9.00064900	-11.86484000	2.07923800
H	-10.06510300	-11.18391600	3.31981500
C	-10.10320200	-10.41846900	-0.63814300
H	-9.13852100	-10.91108700	-0.80819500
H	-10.89116300	-11.14022200	-0.88824200
H	-10.17444800	-9.58813000	-1.34765000

IN2-1a

C	-9.87540800	-2.96827400	-0.33535800
O	-9.60398600	-2.96741900	-1.53440400
C	-8.94339300	-3.00765100	0.81922600
C	-7.50388900	-3.09586600	0.70806800
C	-6.80317600	-2.41480900	-0.24447900
H	-5.75277000	-2.68210000	-0.35684300
C	-9.70690700	-3.00340900	2.03488100
C	-9.14687000	-2.95037600	3.29401500
H	-8.06450300	-2.83858800	3.28953800
C	-8.36483300	-6.00887300	1.61862900
C	-7.40404500	-5.15118600	2.25270800
C	-7.24458400	-5.56929600	3.66808700
O	-6.52441900	-5.07453900	4.53298700
C	-6.73061900	-4.02075100	1.65157500

C	-5.43035000	-3.71540900	1.93110500
H	-5.06897000	-2.75365300	1.56799400
C	-8.68904000	-5.94299800	0.27956300
H	-8.09491900	-5.22609700	-0.28349800
C	-11.24674300	-2.95383900	0.24706600
C	-12.46341700	-2.90889300	-0.41947600
C	-11.15493800	-3.00941400	1.64777900
C	-13.63733200	-2.93215800	0.34231700
H	-12.48572300	-2.85733000	-1.50450200
C	-12.32615400	-3.03847000	2.39893000
C	-13.56234200	-3.00186000	1.73572100
H	-14.60691100	-2.89834200	-0.14674500
H	-12.30592100	-3.09551800	3.47963900
H	-14.47751800	-3.02778100	2.32138300
C	-7.22863700	-1.26449400	-1.10524100
H	-7.27408000	-1.60026100	-2.15129200
H	-8.23479400	-0.92397000	-0.85174600
C	-6.23781300	-0.08522900	-1.00419200
H	-5.22847400	-0.43278200	-1.26616100
H	-6.18436700	0.25540900	0.03867100
C	-6.62862700	1.08612300	-1.91034100
H	-7.61956100	1.47594400	-1.64831100
H	-5.91201800	1.91074300	-1.82457000
H	-6.66216500	0.77836700	-2.96250100
C	-8.16847300	-6.72214000	3.85994800
C	-8.37920900	-7.47243300	5.00857500
C	-8.85998600	-6.96535200	2.66158800
C	-9.32688400	-8.50138100	4.96322900

H	-7.81474500	-7.25285300	5.91057000
C	-9.80531800	-7.98620300	2.62519900
C	-10.03253000	-8.74658900	3.78257100
H	-9.51704500	-9.10853800	5.84390400
H	-10.37408600	-8.20204400	1.72997400
H	-10.77284600	-9.54183500	3.75558100
C	-4.37006900	-4.55034000	2.58241600
H	-4.12490500	-4.11382200	3.56139700
H	-4.72340600	-5.56416600	2.78245500
C	-3.08645900	-4.60467200	1.72677400
H	-2.73562100	-3.58177800	1.52957100
H	-3.32131000	-5.04300700	0.74743800
C	-1.96990400	-5.40941000	2.39870700
H	-1.06854800	-5.43499200	1.77595200
H	-1.69657900	-4.97378000	3.36739000
H	-2.28140100	-6.44540200	2.57834700
Si	-9.77931200	-6.97910300	-0.88061900
Si	-9.83655200	-2.78604900	5.05634400
C	-10.87282800	-1.20070300	5.21077300
H	-11.24452700	-1.09532900	6.23816600
H	-10.25643200	-0.32063900	4.99255300
H	-11.73523200	-1.17309100	4.53782500
C	-10.83362400	-4.30061500	5.61107900
H	-11.71005000	-4.50863400	4.98923200
H	-10.20516500	-5.19774600	5.60028300
H	-11.18376800	-4.15246800	6.64071600
C	-8.32155800	-2.61706100	6.17276000
H	-7.64401200	-3.46938600	6.05044000

H	-7.75513300	-1.70727200	5.93830600
H	-8.61496000	-2.55910500	7.22822000
C	-11.62425300	-6.87501600	-0.45624300
H	-12.19954900	-7.49274300	-1.15771300
H	-11.86786800	-7.20902800	0.55715700
H	-11.98126400	-5.84382200	-0.55269600
C	-9.51383000	-6.25286900	-2.60423500
H	-8.47161100	-6.36669300	-2.92726500
H	-10.14481900	-6.75890700	-3.34530300
H	-9.75109500	-5.18342800	-2.62363100
C	-9.18635700	-8.78472000	-0.89752800
H	-9.80398700	-9.37491900	-1.58673100
H	-8.15134500	-8.84010200	-1.25518000
H	-9.22165700	-9.26946100	0.08294900

TS-IN2-1a

C	-9.88835800	-2.70557300	-0.37282100
O	-9.62335600	-2.65993600	-1.56771000
C	-8.95163600	-2.72018900	0.78663000
C	-7.50911800	-2.85310500	0.68412800
C	-6.78714000	-2.22046400	-0.28182200
H	-5.75665000	-2.54159200	-0.42463000
C	-9.68789400	-2.90296300	1.96281600
C	-9.05938600	-3.04954100	3.22330900
H	-8.06497500	-2.60950800	3.25453500
C	-8.48892400	-5.79835100	1.73357400
C	-7.62032900	-4.80370400	2.36908600
C	-7.32000500	-5.27093400	3.75398100
O	-6.55293500	-4.77225000	4.57166100

C	-6.81190300	-3.81794500	1.64094900
C	-5.47095900	-3.71263300	1.82156300
H	-4.98933200	-2.84860900	1.36502500
C	-8.75007600	-5.83740300	0.39505800
H	-8.23856300	-5.06359800	-0.17601900
C	-11.25764900	-2.83828600	0.20895600
C	-12.47552600	-2.84956900	-0.44793000
C	-11.14151100	-3.00205900	1.60061000
C	-13.63857900	-3.04202100	0.31368700
H	-12.51299200	-2.71739100	-1.52575900
C	-12.29699900	-3.20125700	2.34846200
C	-13.54118500	-3.22082800	1.69252600
H	-14.61169300	-3.05679800	-0.16902500
H	-12.26660900	-3.34903800	3.41951300
H	-14.44256600	-3.37920500	2.27869600
C	-7.17769400	-1.05054900	-1.13450600
H	-7.24415200	-1.37273100	-2.18347300
H	-8.16839100	-0.67584800	-0.86635700
C	-6.14534600	0.09264300	-1.03164800
H	-5.15102400	-0.28774200	-1.30529100
H	-6.07100800	0.42103800	0.01381000
C	-6.50176500	1.28542100	-1.92398800
H	-7.47644600	1.70704400	-1.65035800
H	-5.75617600	2.08389800	-1.83690900
H	-6.55440900	0.98897300	-2.97865800
C	-8.15285100	-6.48515200	3.96689900
C	-8.24504100	-7.26759400	5.11236000
C	-8.87996000	-6.76904100	2.79868300

C	-9.11462300	-8.36089300	5.09893200
H	-7.64867500	-7.01997900	5.98616100
C	-9.75812500	-7.85254800	2.79902700
C	-9.86884700	-8.63854100	3.95281700
H	-9.21125200	-8.99444000	5.97621800
H	-10.35742200	-8.09483300	1.93023600
H	-10.55298000	-9.48308500	3.95427700
C	-4.49933100	-4.65404300	2.47395200
H	-4.17492400	-4.23227000	3.43604300
H	-4.96233000	-5.61611100	2.70694400
C	-3.26054300	-4.88712700	1.58542200
H	-2.78598100	-3.92130800	1.36107000
H	-3.57887000	-5.30356500	0.62000600
C	-2.23731400	-5.82130700	2.23795300
H	-1.36561100	-5.97040600	1.59076700
H	-1.88117600	-5.41383300	3.19197100
H	-2.67378600	-6.80650600	2.44226300
Si	-9.72782700	-6.98403800	-0.75417300
Si	-9.82632400	-3.00004400	4.97704000
C	-10.87591500	-1.41471100	5.07350200
H	-11.29453400	-1.31603900	6.08376400
H	-10.24694500	-0.53458100	4.89419900
H	-11.70434500	-1.37838200	4.36074800
C	-10.85338900	-4.52335900	5.44701900
H	-11.46553400	-4.91864200	4.63093800
H	-10.19822900	-5.33510600	5.77750100
H	-11.52290200	-4.27771400	6.28117600
C	-8.43175500	-2.78387800	6.23185500

H	-7.73360100	-3.62511700	6.23064300
H	-7.85247900	-1.87520400	6.02718800
H	-8.85480400	-2.68217500	7.23963200
C	-11.59018900	-6.94277800	-0.39581700
H	-12.12157700	-7.59160400	-1.10378100
H	-11.85534600	-7.26852700	0.61534000
H	-11.97855300	-5.92565800	-0.52123200
C	-9.44207000	-6.29070800	-2.49045100
H	-8.38581000	-6.35989400	-2.77831600
H	-10.02439800	-6.84106600	-3.23944300
H	-9.72949600	-5.23418300	-2.54760200
C	-9.06073100	-8.76021100	-0.69052200
H	-9.62033500	-9.39958000	-1.38510700
H	-8.00849100	-8.78216300	-0.99777900
H	-9.12244700	-9.21244700	0.30426900

2a

C	-9.44702400	-1.94075200	-0.89778700
O	-8.99394000	-1.50927600	-1.94381700
C	-8.72658900	-2.23782000	0.37897800
C	-7.28788400	-2.29074500	0.64966000
C	-6.38595900	-1.32892000	0.36298700
H	-5.35745000	-1.51178000	0.67457300
C	-9.60701800	-2.71357100	1.30463300
C	-9.03152400	-3.07361500	2.66241800
H	-8.47515900	-2.16994400	2.96751700
C	-8.38265100	-5.54646300	2.18533900
C	-7.84054800	-4.11447700	2.41372900

C	-7.05698600	-4.22681400	3.74549100
O	-6.39984100	-3.34048300	4.25821200
C	-6.90000800	-3.58492200	1.30507200
C	-5.78803400	-4.21552300	0.88263800
H	-5.25302300	-3.73885700	0.06108800
C	-8.96151400	-5.94731100	1.03337900
H	-8.98710800	-5.16571600	0.27085200
C	-10.87550700	-2.31165300	-0.63031900
C	-11.95588900	-2.25522500	-1.48668500
C	-10.97234900	-2.79392400	0.69314100
C	-13.20267700	-2.70869100	-1.01889300
H	-11.82967400	-1.87625100	-2.49721000
C	-12.20495300	-3.24992000	1.14511600
C	-13.31454100	-3.20178500	0.27700300
H	-14.07278300	-2.68039000	-1.66850000
H	-12.33788200	-3.64401300	2.14389100
H	-14.27633100	-3.55943700	0.63521500
C	-6.62897500	0.00207500	-0.28645400
H	-6.08640100	0.03338100	-1.24461300
H	-7.68530000	0.12992000	-0.53807600
C	-6.14625400	1.17753200	0.58654900
H	-5.08835500	1.02861300	0.84473600
H	-6.69544200	1.16752400	1.53746100
C	-6.32132000	2.53521400	-0.10052400
H	-7.37418300	2.72423700	-0.34309500
H	-5.97402900	3.35409200	0.53989700
H	-5.75401700	2.58031400	-1.03835300
C	-7.29495300	-5.57968800	4.29286000

C	-6.83408400	-6.09229800	5.50653900
C	-8.09992400	-6.32487500	3.41279200
C	-7.20414600	-7.38588400	5.86142300
H	-6.20685100	-5.47725100	6.14550600
C	-8.47605500	-7.62263400	3.78985400
C	-8.02580700	-8.13754300	5.00521400
H	-6.86634000	-7.81615700	6.79990800
H	-9.11494600	-8.22722600	3.15880300
H	-8.31877800	-9.14310000	5.29570100
C	-5.15075400	-5.49136900	1.35605300
H	-4.18934900	-5.24412200	1.83509800
H	-5.74977300	-5.99034000	2.12229900
C	-4.87983300	-6.47638100	0.20289900
H	-4.28209000	-5.97266100	-0.56949200
H	-5.83471700	-6.73832300	-0.27157300
C	-4.16031300	-7.74785800	0.66215000
H	-3.97483700	-8.42685100	-0.17798300
H	-3.19165300	-7.51153700	1.11988800
H	-4.75337900	-8.29308100	1.40664200
Si	-9.72198900	-7.55043900	0.37620900
Si	-10.21803900	-3.22861700	4.19067900
C	-11.33456500	-1.69289300	4.13358600
H	-12.00200200	-1.69495800	5.00487500
H	-10.72122400	-0.78549200	4.20157000
H	-11.95489800	-1.60381000	3.23835800
C	-11.22647800	-4.83486600	4.29744800
H	-11.56296600	-5.21404700	3.32828900
H	-10.62829000	-5.62637100	4.76150100

H	-12.11222500	-4.68204000	4.92711400
C	-9.25237400	-3.04736800	5.81260700
H	-8.72916000	-3.95961900	6.11131500
H	-8.51275800	-2.24136000	5.76484300
H	-9.96541000	-2.80108600	6.61026400
C	-11.31130900	-8.01840700	1.30366400
H	-11.74535300	-8.93175600	0.87743900
H	-11.16608500	-8.18955300	2.37557100
H	-12.05639900	-7.22064100	1.19846700
C	-10.18887600	-7.17491000	-1.41947300
H	-9.30821100	-6.90432500	-2.01445900
H	-10.65690600	-8.04339300	-1.89846400
H	-10.89780300	-6.34048700	-1.48163300
C	-8.48304900	-8.98800100	0.37907900
H	-8.94828200	-9.89269100	-0.03230500
H	-7.62077700	-8.74460400	-0.25301600
H	-8.09839400	-9.23500600	1.37371200

1a

C	-3.23989400	1.27293800	-0.20961200
C	-1.84374600	1.21423800	-0.19797500
C	-1.10942900	2.38227900	-0.02308400
C	-1.74057100	3.62035000	0.16364400
C	-3.15624100	3.68844400	0.12999500
C	-3.88496500	2.49506400	-0.05909900
H	-3.82618400	0.36828200	-0.34552500
H	-1.33263700	0.26416000	-0.32486300
H	-0.02471200	2.36252200	-0.02022700

H	-4.96808700	2.55296600	-0.09635400
C	-0.82477700	4.79088400	0.37900200
C	-3.90403400	4.90455600	0.19126300
C	-4.64618100	5.87465000	0.17245800
C	-1.23889700	5.85487500	1.26864000
C	-1.44295800	6.72424300	2.09050700
C	-1.69160200	7.78151200	3.06523600
H	-2.77278800	7.96551700	3.13507900
H	-1.38099800	7.42301200	4.05768100
O	0.29804400	4.80016600	-0.11482900
C	-0.95638800	9.10064200	2.74298700
H	0.12003000	8.90072300	2.66969800
H	-1.27325200	9.45335700	1.75282700
C	-1.21866900	10.18719200	3.79225600
H	-2.30056000	10.36728500	3.86686700
H	-0.90106600	9.82267700	4.77957600
C	-0.50146300	11.50385300	3.47798600
H	-0.70580300	12.26070900	4.24348400
H	0.58492100	11.36193000	3.43020000
H	-0.82486700	11.91023600	2.51201500
Si	-5.76747600	7.33014100	0.06620900
C	-7.54771700	6.73477500	0.28933600
H	-8.24999100	7.57497000	0.22171400
H	-7.82392200	6.00600000	-0.48108200
H	-7.68950300	6.25833800	1.26607700
C	-5.54828500	8.13542200	-1.62915200
H	-6.19968900	9.01236700	-1.73162600
H	-4.51440500	8.46544800	-1.78047500

H	-5.79635700	7.43741100	-2.43658400
C	-5.32762700	8.56551200	1.42944900
H	-5.99889300	9.43268900	1.39746200
H	-5.41630400	8.11110000	2.42297200
H	-4.30172500	8.93322100	1.31409300

TS5-1a

C	-4.40398500	1.52662500	5.82870800
O	-4.34034700	2.73570100	5.59742300
C	-3.54588900	0.44807400	5.31839900
C	-2.51370000	0.61063700	4.42317600
C	-1.19211100	0.52649000	4.31464200
H	-0.72545800	0.54239200	3.33369400
C	-4.04512700	-0.85210300	5.80974200
C	-3.52415300	-2.05795400	5.45885700
H	-2.67754900	-1.97162900	4.77141700
C	-3.21390200	-0.12193700	2.02581800
C	-3.20381900	0.97927100	2.61555800
C	-5.39878300	0.86343500	6.71421300
C	-5.19187500	-0.52855100	6.70542000
C	-6.40623900	1.46109500	7.46448100
C	-6.02198600	-1.33798700	7.48390900
C	-7.23466900	0.64289400	8.23342500
H	-6.52822000	2.54028200	7.43916300
C	-7.03808600	-0.74440400	8.23984300
H	-5.89414300	-2.41309000	7.51649500
H	-8.03177000	1.07751400	8.83059400
H	-7.68579300	-1.37374700	8.84486000

C	-3.37101300	-1.39919100	1.45397100
C	-2.32153100	-2.14838100	0.83737300
C	-4.67701700	-1.95192900	1.46419400
C	-2.61682000	-3.40350000	0.28527600
C	-4.93868100	-3.19367700	0.90512200
H	-5.47183500	-1.37985700	1.93137300
C	-3.90354400	-3.93054600	0.31537600
H	-1.81199700	-3.96663500	-0.17591100
H	-5.94910300	-3.59230500	0.92949800
H	-4.10192700	-4.90548500	-0.11983100
C	-0.93305800	-1.61669000	0.76623800
O	-0.60289900	-0.53810700	1.25361700
C	0.06073500	-2.42211900	0.07420700
C	0.95057500	-3.02969900	-0.48473300
C	2.04363600	-3.72907900	-1.15622400
H	1.66191300	-4.21153700	-2.06737000
H	2.39315100	-4.54570300	-0.50788300
C	3.23088500	-2.80833000	-1.51275600
H	2.87078500	-1.99552600	-2.15616300
H	3.60292800	-2.33553600	-0.59510100
C	4.36726800	-3.56392700	-2.21137300
H	3.97948300	-4.04390500	-3.12127000
H	4.71562900	-4.37894400	-1.56099400
C	5.54860500	-2.65870200	-2.57441800
H	6.34518800	-3.22519700	-3.06929000
H	5.23859100	-1.85556000	-3.25364400
H	5.97793700	-2.18975500	-1.68095600
C	-0.26709600	0.43294700	5.50536700

H	0.35640500	1.33973600	5.53734400
H	-0.84737400	0.41338900	6.43432200
C	0.65606900	-0.79790900	5.42712400
H	1.19209400	-0.78873800	4.46848600
H	0.03937900	-1.70616600	5.42598900
C	1.66034900	-0.85426900	6.58244300
H	2.30166400	-1.73999100	6.50836600
H	2.31057300	0.02924500	6.58626900
H	1.14860500	-0.89296200	7.55178000
Si	-3.93235200	-3.85233700	5.84465300
C	-3.67609700	-4.28291500	7.67714700
H	-3.90020500	-5.34205900	7.85786200
H	-2.63108200	-4.11330600	7.96295500
H	-4.29815400	-3.69064300	8.35617300
C	-5.68211700	-4.33136900	5.28150700
H	-6.46805900	-3.72867500	5.74791800
H	-5.77347200	-4.20540200	4.19595900
H	-5.88617800	-5.38477000	5.51201900
C	-2.69997800	-4.88151700	4.83619300
H	-2.80132700	-4.68683400	3.76164900
H	-1.66449100	-4.65383700	5.11792600
H	-2.85572200	-5.95558300	4.99512200
Si	-3.39094800	2.81265800	2.17275100
C	-2.21615800	3.86690300	3.19511700
H	-2.28546100	4.91630200	2.88117000
H	-2.48562100	3.80326900	4.25308200
H	-1.17419800	3.54949500	3.07497700
C	-5.18783200	3.33625100	2.40960000

H	-5.45409700	3.32673600	3.47022300
H	-5.33377200	4.35537100	2.02876000
H	-5.87494900	2.67689200	1.86663100
C	-2.92842300	2.89939200	0.33805900
H	-1.91900600	2.50865800	0.16823000
H	-3.62114100	2.31308000	-0.27675900
H	-2.95681500	3.93623500	-0.02063900

IN3-1a

C	-4.64432700	1.41534200	5.46789300
O	-4.69009000	2.54483200	4.96307700
C	-3.70648100	0.33683900	5.18350500
C	-2.67968600	0.40973200	4.20222400
C	-1.36653700	0.09555700	4.31596100
H	-0.76637800	0.08784400	3.40846700
C	-4.08547700	-0.85192700	5.94902000
C	-3.52817900	-2.08993700	5.80408200
H	-2.74335900	-2.11620100	5.04342400
C	-3.14720500	-0.18988200	1.95912700
C	-3.13452100	0.82771000	2.73073900
C	-5.55728300	0.90362900	6.52552300
C	-5.22177100	-0.42890500	6.82462100
C	-6.58819500	1.57371900	7.17317900
C	-5.93946800	-1.10054500	7.81316500
C	-7.30651200	0.89129000	8.15817900
H	-6.81328200	2.60300100	6.90835600
C	-6.97891800	-0.43244700	8.47311200
H	-5.70740400	-2.12255000	8.08643600

H	-8.11793000	1.38629700	8.68509900
H	-7.53844500	-0.95374600	9.24565000
C	-3.34133900	-1.31837500	1.17456900
C	-2.30811100	-1.99364100	0.43532300
C	-4.67542500	-1.81726400	1.07885400
C	-2.65158300	-3.10672100	-0.34123200
C	-4.97611200	-2.91909300	0.29907600
H	-5.45240200	-1.30717500	1.63889500
C	-3.96103200	-3.57272100	-0.41654800
H	-1.86569500	-3.61137900	-0.89393500
H	-5.99998900	-3.27821300	0.24604500
H	-4.19326100	-4.43976200	-1.02767400
C	-0.90183200	-1.52392900	0.48781600
O	-0.54405800	-0.56958400	1.17881800
C	0.07520400	-2.22986800	-0.32344800
C	0.95012800	-2.76774000	-0.97069100
C	2.02693000	-3.38757300	-1.73948500
H	1.67664400	-3.58138800	-2.76354700
H	2.25002800	-4.37398000	-1.30731000
C	3.31626400	-2.53902700	-1.78317700
H	3.08290900	-1.55844600	-2.21705100
H	3.65409400	-2.35135700	-0.75620000
C	4.43290500	-3.21484600	-2.58733000
H	4.07834400	-3.40939900	-3.60960200
H	4.65328600	-4.19821100	-2.14801500
C	5.71596800	-2.37951300	-2.64111900
H	6.49600600	-2.88617700	-3.22007800
H	5.53429300	-1.40386700	-3.10766300

H	6.11214700	-2.19688200	-1.63497900
C	-0.62466300	-0.12804500	5.60352200
H	-0.01348900	0.76735500	5.80437100
H	-1.32156500	-0.22558100	6.44192900
C	0.31829400	-1.34496600	5.54818700
H	0.99804100	-1.23880100	4.69178200
H	-0.27209600	-2.25129700	5.35997400
C	1.13046400	-1.51764500	6.83519400
H	1.79307800	-2.38852300	6.77376100
H	1.75411700	-0.63686400	7.03197300
H	0.47370700	-1.65796300	7.70248300
Si	-3.81766500	-3.78313200	6.56737300
C	-3.39868300	-3.83153300	8.42021100
H	-3.55512800	-4.84053900	8.82280300
H	-2.34439600	-3.57354000	8.57732200
H	-3.99518000	-3.13741100	9.02130100
C	-5.57560800	-4.43741200	6.26566000
H	-6.35650100	-3.78957800	6.67614900
H	-5.76342300	-4.53554000	5.18974300
H	-5.69455000	-5.43184900	6.71466700
C	-2.61498200	-4.95024200	5.67946900
H	-2.80738900	-4.97776300	4.59997400
H	-1.57325000	-4.63744400	5.82199400
H	-2.70516200	-5.97594300	6.05732400
Si	-3.24993600	2.64559000	2.09072700
C	-2.23452500	3.75775300	3.22130500
H	-2.21065700	4.77839700	2.81844100
H	-2.67550500	3.78750700	4.22043200

H	-1.19863900	3.40789200	3.29995300
C	-5.04194000	3.20087700	1.88989800
H	-5.53749700	3.27301300	2.86041300
H	-5.07496800	4.18396500	1.40232900
H	-5.60304400	2.50223600	1.25749200
C	-2.44165000	2.58140100	0.37692200
H	-1.43684500	2.14805000	0.42801000
H	-3.02958400	1.97202800	-0.32034300
H	-2.35965200	3.58828500	-0.05205900

1f

C	-3.23989400	1.27293800	-0.20961200
C	-1.84374600	1.21423800	-0.19797500
C	-1.10942900	2.38227900	-0.02308400
C	-1.74057100	3.62035000	0.16364400
C	-3.15624100	3.68844400	0.12999500
C	-3.88496500	2.49506400	-0.05909900
H	-3.82618400	0.36828200	-0.34552500
H	-1.33263700	0.26416000	-0.32486300
H	-0.02471200	2.36252200	-0.02022700
H	-4.96808700	2.55296600	-0.09635400
C	-0.82477700	4.79088400	0.37900200
C	-3.90403400	4.90455600	0.19126300
C	-4.64618100	5.87465000	0.17245800
C	-1.23889700	5.85487500	1.26864000
C	-1.44295800	6.72424300	2.09050700
C	-1.69160200	7.78151200	3.06523600
H	-2.77278800	7.96551700	3.13507900

H	-1.38099800	7.42301200	4.05768100
O	0.29804400	4.80016600	-0.11482900
C	-0.95638800	9.10064200	2.74298700
H	0.12003000	8.90072300	2.66969800
H	-1.27325200	9.45335700	1.75282700
C	-1.21866900	10.18719200	3.79225600
H	-2.30056000	10.36728500	3.86686700
H	-0.90106600	9.82267700	4.77957600
C	-0.50146300	11.50385300	3.47798600
H	-0.70580300	12.26070900	4.24348400
H	0.58492100	11.36193000	3.43020000
H	-0.82486700	11.91023600	2.51201500
Si	-5.76747600	7.33014100	0.06620900
C	-7.54771700	6.73477500	0.28933600
H	-8.24999100	7.57497000	0.22171400
H	-7.82392200	6.00600000	-0.48108200
H	-7.68950300	6.25833800	1.26607700
C	-5.54828500	8.13542200	-1.62915200
H	-6.19968900	9.01236700	-1.73162600
H	-4.51440500	8.46544800	-1.78047500
H	-5.79635700	7.43741100	-2.43658400
C	-5.32762700	8.56551200	1.42944900
H	-5.99889300	9.43268900	1.39746200
H	-5.41630400	8.11110000	2.42297200
H	-4.30172500	8.93322100	1.31409300

TS0-1f

C	-3.67428500	1.87919200	-0.38423600

C	-2.36741900	1.38818400	-0.23495600
C	-1.32043400	2.26503500	0.03285400
C	-1.59661300	3.62837300	0.14852300
C	-2.89734500	4.12689800	0.00142400
C	-3.94913900	3.24041200	-0.26854000
H	-4.48634300	1.18778100	-0.59333400
H	-2.17757700	0.32273400	-0.32928900
H	-0.29803800	1.91952300	0.15403000
H	-4.96072600	3.61740400	-0.38413200
C	-0.59190800	4.67626000	0.42973100
C	-3.05353300	5.57532200	0.14695600
C	-3.96442100	6.44662800	0.10705000
C	-1.25361400	5.99937000	0.48066500
C	-1.03610000	7.23372200	0.66121900
O	0.60248900	4.48814700	0.59631600
C	-5.21750900	7.11106900	-0.01427800
C	-6.03915800	7.31847200	1.11776700
C	-5.67244300	7.57370100	-1.27078100
C	-7.26987200	7.95488200	0.98946200
H	-5.69899800	6.96904900	2.08789500
C	-6.90524000	8.20906000	-1.38452100
H	-5.04911700	7.42152000	-2.14674000
C	-7.71024300	8.40433500	-0.25868700
H	-7.89020000	8.10071400	1.86985800
H	-7.24062400	8.55349900	-2.35925800
H	-8.67108500	8.90216700	-0.35308900
C	-1.81544100	8.43513400	0.68310700
C	-1.90667800	9.13959800	2.05557200

C	-1.51951200	9.43937700	-0.45380700
H	-2.85305000	7.96334000	0.46579300
C	-2.93270400	10.28262900	2.02501800
H	-0.91523000	9.53702000	2.31127200
H	-2.16460900	8.40641900	2.82812700
C	-2.55065700	10.57824500	-0.46630900
H	-0.51217300	9.85081300	-0.30434100
H	-1.50922100	8.91339900	-1.41512800
C	-2.63578700	11.28205900	0.89648100
H	-2.94030900	10.79455500	2.99552200
H	-3.93915300	9.86324800	1.88332700
H	-2.29158500	11.29900100	-1.25201900
H	-3.53768300	10.16996200	-0.72718200
H	-3.40547500	12.06347800	0.87117100
H	-1.68102700	11.78839100	1.10253700

IN1-1f

C	-3.93471900	2.23873500	-0.40833000
C	-2.63984100	1.81720500	-0.06848500
C	-1.68759700	2.75387100	0.32426800
C	-2.06019000	4.09525200	0.38203700
C	-3.36473200	4.53221600	0.07325200
C	-4.30750400	3.58172100	-0.34347800
H	-4.66636500	1.50341000	-0.73336000
H	-2.38264100	0.76309000	-0.12436400
H	-0.66899800	2.47022900	0.57309100
H	-5.31215600	3.87373100	-0.62392600
C	-1.18504100	5.24908300	0.70051700

C	-3.44253400	6.00900100	0.18935000
C	-4.46407600	6.87727600	0.00554900
C	-2.06174300	6.46399200	0.53694800
C	-1.62555700	7.69759400	0.70012500
O	-0.00742900	5.21286400	1.01438200
C	-5.90083900	6.64429000	-0.20924200
C	-6.63714900	5.70069400	0.53048000
C	-6.59857100	7.45740700	-1.12222700
C	-8.00950800	5.55140500	0.33603700
H	-6.12974900	5.10075400	1.27981600
C	-7.96850500	7.30277500	-1.32292000
H	-6.05131900	8.20992200	-1.68503700
C	-8.68044500	6.34542400	-0.59668400
H	-8.55846800	4.82061600	0.92432400
H	-8.48233900	7.93412100	-2.04311400
H	-9.75028600	6.22851300	-0.74645900
C	-1.14843700	8.90255800	0.86352600
C	-1.16839000	9.61757100	2.20684000
C	-0.56292600	9.71160600	-0.28491400
H	-4.18266100	7.93109800	0.02975900
C	-1.84580400	10.99623800	2.08111300
H	-0.12714400	9.75770400	2.53505200
H	-1.66454000	9.00292300	2.96388900
C	-1.24661900	11.08874000	-0.38694400
H	0.51020200	9.85729900	-0.08822000
H	-0.64551000	9.16032000	-1.22642100
C	-1.21934500	11.83434700	0.95616700
H	-1.77513400	11.52764600	3.03845800

H	-2.91586600	10.85171800	1.87669600
H	-0.75547500	11.68543500	-1.16584500
H	-2.28916500	10.94774200	-0.70491100
H	-1.74312600	12.79411800	0.86521900
H	-0.17724700	12.07086400	1.21803700

TS1-1f

C	-3.04787700	1.98385700	0.18616300
C	-1.71449900	1.98825800	0.61496800
C	-1.07523500	3.20084700	0.86987800
C	-1.79966100	4.37729600	0.70516700
C	-3.14987900	4.39042500	0.30273300
C	-3.77154600	3.16957200	0.02267600
H	-3.53670200	1.03655800	-0.02676000
H	-1.18115000	1.04972500	0.73748500
H	-0.03583500	3.24893100	1.18183500
H	-4.79747400	3.12408400	-0.31976900
C	-1.30628600	5.76383000	0.86211400
C	-3.60722600	5.80511600	0.16305200
C	-4.78536000	6.32332100	-0.29031200
C	-2.46686800	6.64979600	0.50496800
C	-2.36566800	8.00476300	0.57716900
O	-0.17885300	6.11196800	1.18639100
C	-6.05435800	5.64649800	-0.58610800
C	-6.61590200	4.68459400	0.27495700
C	-6.78247400	6.02031700	-1.73149500
C	-7.83724200	4.08548600	-0.02778800
H	-6.10531400	4.44205000	1.20187900

C	-7.99769200	5.41277700	-2.03826400
H	-6.37740100	6.78476100	-2.39007300
C	-8.52734800	4.43731600	-1.19033100
H	-8.25750300	3.35024300	0.65356400
H	-8.53509900	5.70486400	-2.93666600
H	-9.47844800	3.96699500	-1.42523200
C	-1.67463000	9.04934000	0.13746600
C	-1.45062100	10.37634000	0.83162500
C	-0.93377100	8.90298300	-1.19400500
H	-4.77455100	7.38803300	-0.51294900
C	-1.57828900	11.59235400	-0.10875400
H	-0.42443500	10.35941400	1.23223100
H	-2.11940800	10.47527000	1.68919000
C	-1.11361200	10.12456700	-2.11088300
H	0.13593600	8.79145400	-0.95776900
H	-1.24375800	7.98477300	-1.70007200
C	-0.74555300	11.42558100	-1.38683300
H	-1.27211600	12.49530000	0.43395900
H	-2.63088500	11.74045000	-0.38453800
H	-0.49886000	9.99650400	-3.01081300
H	-2.15909600	10.17583900	-2.44784900
H	-0.89325400	12.28757800	-2.04937300
H	0.32385500	11.40654100	-1.12902400
C	-7.18586100	8.83931700	1.38248900
C	-7.23158400	7.72780000	2.24531000
C	-8.42237600	7.08833900	2.57813500
C	-9.60796400	7.56294600	2.02090400
C	-9.57621700	8.64873000	1.13473400

C	-8.37971500	9.29106600	0.80743000
C	-4.95447100	8.36395300	2.03768000
C	-5.86048900	7.35516200	2.67287100
H	-8.40330500	6.23618200	3.25131800
H	-10.55559400	7.08841000	2.26069900
H	-10.50288100	9.00073100	0.68846800
H	-8.39150800	10.12170400	0.11260000
O	-5.55326500	6.44002800	3.42558500
C	-3.64199200	8.42189800	2.39242200
C	-2.87395000	8.42156300	3.48325600
C	-3.48857200	8.93845100	4.78530100
C	-1.43582400	7.97793800	3.63145700
C	-2.60736300	9.98750600	5.48687800
H	-3.59846100	8.06591200	5.44740400
H	-4.49212100	9.33166700	4.60591200
C	-0.56517900	9.02814600	4.35462300
H	-1.44442400	7.06125800	4.24275200
H	-0.98684500	7.71138600	2.67586000
C	-1.17708900	9.47172200	5.68878500
H	-3.06134600	10.25560900	6.44941800
H	-2.58505700	10.90565700	4.88251400
H	0.43697200	8.61001000	4.50901100
H	-0.44142300	9.90608300	3.70594900
H	-0.55453600	10.24619000	6.15474000
H	-1.19305000	8.62005800	6.38500300
C	-5.77299800	9.28060300	1.21645300
C	-5.24808700	10.28034400	0.46322700
H	-4.16390700	10.28943200	0.39529000

C	-5.91286400	11.36226700	-0.28247900
C	-5.46847700	11.68827900	-1.57824900
C	-6.92057400	12.16130300	0.28885400
C	-6.03393500	12.74524100	-2.28919700
H	-4.68094100	11.09153300	-2.03224100
C	-7.48217400	13.22253300	-0.41960000
H	-7.24636100	11.95583100	1.30415300
C	-7.04612600	13.51623900	-1.71369300
H	-5.68209300	12.96888900	-3.29299900
H	-8.25516200	13.82906900	0.04529900
H	-7.48357500	14.34470000	-2.26412900

2f-1

C	-3.32915500	2.02949400	-0.62320400
C	-2.01973300	1.76367500	-0.23666600
C	-1.21648000	2.80315700	0.26677000
C	-1.77042000	4.06153000	0.37879100
C	-3.10758800	4.34101300	0.01919700
C	-3.88785500	3.31845000	-0.50617700
H	-3.94236000	1.22849800	-1.02812700
H	-1.61532500	0.76011200	-0.33420700
H	-0.18245400	2.63570100	0.55588600
H	-4.90632200	3.48791900	-0.83048100
C	-1.11287100	5.34116100	0.80301900
C	-3.33452900	5.80013400	0.26266800
C	-4.51977100	6.72331700	0.07908800
C	-2.17057000	6.38731800	0.64557900
C	-2.14444400	7.82246100	0.95891200

O	0.03602400	5.48307800	1.18485300
C	-5.82643100	6.11977600	-0.41884500
C	-6.49039300	5.07032600	0.23698500
C	-6.40461500	6.63592800	-1.58671300
C	-7.68797700	4.55826500	-0.26351300
H	-6.06522300	4.64233500	1.13873800
C	-7.60295200	6.12720000	-2.08994400
H	-5.90938400	7.45106900	-2.10861700
C	-8.24993000	5.08399000	-1.42851800
H	-8.18176100	3.74432100	0.26089200
H	-8.02677800	6.54575700	-2.99900400
H	-9.18230200	4.68261800	-1.81663500
C	-1.27497100	8.70184600	0.40113300
C	-1.31755400	10.19561600	0.64281000
C	-0.17325200	8.27793000	-0.55006600
H	-4.19914900	7.43204700	-0.69639800
C	-1.32133100	11.00421000	-0.67267500
H	-0.42337400	10.48575800	1.21821000
H	-2.18286800	10.46630200	1.25218700
C	-0.19395900	9.08728600	-1.86314600
H	0.79627200	8.44336400	-0.05432700
H	-0.22225200	7.21058900	-0.76968100
C	-0.16854300	10.59713300	-1.59763200
H	-1.27259000	12.07558600	-0.44057900
H	-2.27592900	10.84183100	-1.19456200
H	0.65798200	8.79107100	-2.48806300
H	-1.10259100	8.83283000	-2.42809100
H	-0.22143800	11.15409500	-2.54205300

H	0.78873600	10.86776900	-1.12736000
C	-6.95910700	8.48783600	1.68828900
C	-6.80894700	7.37154400	2.53173600
C	-7.86531800	6.84405500	3.27447200
C	-9.11877100	7.43453900	3.15161900
C	-9.29524800	8.52540900	2.28423100
C	-8.23436100	9.05860300	1.55381200
C	-4.67529800	7.67649700	1.37891200
C	-5.42608700	6.85647300	2.45901200
H	-7.69341500	5.98578800	3.91776100
H	-9.96511800	7.04923100	3.71336900
H	-10.28346800	8.96544800	2.17749300
H	-8.40575300	9.89613800	0.88864900
O	-4.96390700	5.92315800	3.08979000
C	-3.28656300	8.16159100	1.87635000
C	-3.08304100	8.69275900	3.10612800
C	-4.17852200	9.05794000	4.08951200
C	-1.70298600	8.90691700	3.70677900
C	-3.99117400	10.48040100	4.66138200
H	-4.15784000	8.33808400	4.92297600
H	-5.17276500	8.99269900	3.64814600
C	-1.50085800	10.31525200	4.30143700
H	-1.60489600	8.18059400	4.53104000
H	-0.91235900	8.66841400	2.99457100
C	-2.61045900	10.66353500	5.30083600
H	-4.78419900	10.68191600	5.39283600
H	-4.11720300	11.21035000	3.84887200
H	-0.51737400	10.36807700	4.78569800

H	-1.49369100	11.05985000	3.49413100
H	-2.49104300	11.69214900	5.66497600
H	-2.52885200	10.00694800	6.17984800
C	-5.66914700	8.80953700	1.04288800
C	-5.30679700	9.85029400	0.26294900
H	-4.30731000	9.78923200	-0.16850500
C	-6.02831200	11.08766000	-0.09060700
C	-5.93957000	11.58239600	-1.40461100
C	-6.72972500	11.85284200	0.85817200
C	-6.56532500	12.77311100	-1.76882900
H	-5.37891900	11.01831600	-2.14645500
C	-7.34935300	13.04806600	0.49647000
H	-6.76973900	11.51399900	1.88895900
C	-7.27672900	13.51004000	-0.81969000
H	-6.49234400	13.12914900	-2.79309000
H	-7.88055700	13.62629600	1.24804300
H	-7.75894700	14.44255600	-1.09988500

TS3-1f

C	-3.09657800	1.45606400	-0.30416600
C	-1.81263900	1.39801400	0.26611600
C	-1.17017500	2.56916000	0.65422200
C	-1.82610700	3.78718200	0.45850600
C	-3.10356800	3.85345600	-0.11129400
C	-3.75053600	2.67082200	-0.49489600
H	-3.58980400	0.53427500	-0.60184300
H	-1.32618800	0.43642500	0.40294800
H	-0.18013500	2.55960000	1.10028400

H	-4.74395300	2.71609900	-0.92975700
C	-1.30489500	5.11860400	0.81122400
C	-3.63668600	5.20391300	-0.21589300
C	-4.72759300	5.77238700	-0.58291200
C	-2.30960800	6.18208700	0.38735400
C	-2.21995300	7.44073700	0.37076600
O	-0.23639100	5.36091200	1.33966500
C	-5.13536700	7.11404000	-0.70182900
C	-6.18595600	7.66715000	0.07522900
C	-4.38732400	7.98165200	-1.54112300
C	-6.46437600	9.02245300	0.01736800
H	-6.75905500	7.01045300	0.72270900
C	-4.69939200	9.34331600	-1.60996500
H	-3.61338200	7.56131100	-2.17390100
C	-5.72309200	9.86875500	-0.82655400
H	-7.26490100	9.43472800	0.62605700
H	-4.13981600	9.99020600	-2.28115200
H	-5.96301700	10.92733200	-0.87828300
C	-1.76941600	8.81401700	0.55524800
C	-1.02302000	8.94659500	1.91591000
C	-0.85629500	9.26708400	-0.61536300
H	-2.63999100	9.48966700	0.58042100
C	-0.49338800	10.37432100	2.11775200
H	-0.19873400	8.22293000	1.93286000
H	-1.70328500	8.67014700	2.72940100
C	-0.33081200	10.69246600	-0.39136500
H	-0.01398400	8.56699900	-0.69166300
H	-1.41070800	9.20474300	-1.55869600

C	0.40013000	10.82318300	0.95263300
H	0.05838100	10.42754100	3.06463100
H	-1.34301200	11.06694800	2.21158500
H	0.33533400	10.97078600	-1.21765500
H	-1.17403500	11.39852500	-0.41819300
H	0.73101800	11.85824200	1.10482500
H	1.30780000	10.20260100	0.93281500

IN2-1f

C	-2.62637200	1.72339000	-0.40124100
C	-1.34224500	1.88886900	0.14728200
C	-0.90769000	3.14770400	0.55969200
C	-1.77378700	4.22882300	0.40443300
C	-3.05859700	4.06972900	-0.14994300
C	-3.49604300	2.80326700	-0.54990100
H	-2.94747000	0.73229900	-0.71142800
H	-0.68958300	1.02657400	0.25179900
H	0.07738000	3.30035400	0.99124600
H	-4.49298700	2.66895400	-0.95959100
C	-1.52560900	5.65362400	0.76006600
C	-3.74435000	5.35758200	-0.14131800
C	-4.98156400	5.78030900	-0.41158400
C	-2.75203600	6.40159200	0.31078000
C	-2.93400000	7.69754700	-0.03131300
O	-0.49421600	6.08263700	1.26256000
C	-5.33608700	7.09440700	-0.44170800
C	-6.49546600	7.63591300	0.19739500
C	-4.23687200	8.02535800	-0.91849700

C	-6.70513100	8.98361000	0.24348600
H	-7.20252700	6.94005700	0.64006500
C	-4.66263600	9.45990100	-0.99761800
H	-3.87870900	7.73454400	-1.92039200
C	-5.80301300	9.89690800	-0.41933000
H	-7.58537600	9.38222200	0.74039900
H	-4.06353800	10.14049900	-1.59673300
H	-6.08630600	10.94370800	-0.49599700
C	-1.96393100	8.84167400	0.18909600
C	-1.60926000	9.03767400	1.68469600
C	-0.68191100	8.72712500	-0.67433000
H	-2.47309400	9.76137100	-0.12473700
C	-0.68857400	10.25391400	1.87367400
H	-1.11287800	8.13514400	2.05250100
H	-2.53215500	9.16811300	2.26373400
C	0.23250700	9.94501300	-0.46746800
H	-0.14436200	7.81431900	-0.39891200
H	-0.95503500	8.63726600	-1.73449900
C	0.57997400	10.14512500	1.01512300
H	-0.42240000	10.34995300	2.93415300
H	-1.23138100	11.17326700	1.60502100
H	1.14749400	9.82405000	-1.06145700
H	-0.26935400	10.84819900	-0.84721400
H	1.20198100	11.04081300	1.14061400
H	1.17900700	9.29182700	1.36302600

2f-2

C	-2.75123500	1.72954900	0.02969900

C	-1.38371500	1.89198100	0.28811600
C	-0.83763100	3.17277900	0.41415900
C	-1.68767000	4.26333600	0.27636700
C	-3.05733400	4.10880900	0.01761700
C	-3.60207500	2.83281700	-0.10839600
H	-3.16039900	0.72712400	-0.06539300
H	-0.74846700	1.01671100	0.39052000
H	0.21874500	3.32753500	0.61446300
H	-4.66010000	2.68583300	-0.30833100
C	-1.35796500	5.71521600	0.36745300
C	-3.66801500	5.44817900	-0.06910300
C	-4.96906700	5.78429700	-0.30399400
C	-2.65929300	6.45206800	0.14149800
C	-2.95786500	7.81036400	0.11794400
O	-0.23739400	6.15498800	0.58346600
C	-5.33760500	7.15704000	-0.34364300
C	-6.68631800	7.51808900	-0.58819100
C	-4.34370900	8.17830400	-0.13584800
C	-7.07689200	8.83769700	-0.63426300
H	-7.41231400	6.72298000	-0.74022400
C	-4.79621300	9.52683700	-0.19440800
C	-6.11654400	9.84940800	-0.43510200
H	-8.11473100	9.09822400	-0.82277000
H	-4.09909100	10.34191000	-0.04915000
H	-6.41450400	10.89363200	-0.47068800
C	-1.91250100	8.89700900	0.34700000
C	-1.29949800	8.86386600	1.76974900
C	-0.82004100	8.93953200	-0.75101200

H	-2.41769900	9.86344300	0.28043600
C	-0.32580200	10.03521300	1.97381300
H	-0.76868900	7.92099600	1.92135800
H	-2.10672700	8.91115800	2.51239500
C	0.14727100	10.11050300	-0.51508300
H	-0.26087600	8.00082000	-0.75177900
H	-1.29914800	9.03878400	-1.73392000
C	0.76345200	10.06178500	0.89107100
H	0.12931400	9.96660700	2.97032500
H	-0.88141000	10.98549700	1.95075100
H	0.93634200	10.09611500	-1.27794500
H	-0.39000900	11.06330400	-0.64099400
H	1.42902400	10.92140500	1.04363000
H	1.38401500	9.15925600	0.98147300
H	-5.73335900	5.02727300	-0.46231500

1h

C	-3.37134400	1.12348900	-0.34464400
C	-1.98679700	0.94608100	-0.26526100
C	-1.17196600	2.03554800	0.01881800
C	-1.70601600	3.31349600	0.24251900
C	-3.10982900	3.50172500	0.14345900
C	-3.92165900	2.38395100	-0.15014700
H	-4.02126800	0.28089400	-0.56467500
H	-1.54862200	-0.03541300	-0.42217900
H	-0.09469900	1.92540200	0.08105400
H	-4.99342400	2.53409900	-0.23220400
C	-0.70349600	4.38091800	0.57539500

C	-3.75974700	4.76325300	0.26604700
C	-4.42017300	5.78395300	0.30843300
C	-1.11072400	5.55136600	1.31737100
C	-1.29786500	6.53161600	2.01210400
O	0.48158500	4.23245300	0.28495300
C	-5.12085000	7.02218600	0.37378400
C	-6.51999600	7.05256600	0.53970700
C	-4.41967500	8.24160800	0.27023800
C	-7.19475500	8.26865100	0.60299300
H	-7.06362300	6.11608600	0.61859300
C	-5.10374900	9.45248100	0.33426400
H	-3.34279500	8.21970500	0.13596700
C	-6.49110700	9.47146200	0.50111300
H	-8.27374800	8.27845100	0.73141600
H	-4.55317100	10.38565300	0.24985400
H	-7.02144100	10.41858800	0.54912400
C	-1.55875500	7.68075300	2.82444600
C	-0.55056800	8.09240700	3.89651800
C	-0.69547500	8.93248000	2.66921500
H	-2.60626500	7.85154800	3.06371200
H	0.33776400	7.47728800	3.99696600
H	-0.96231400	8.45736300	4.83287400
H	-1.20838500	9.88676300	2.74665800
H	0.09382800	8.89635500	1.92526100

TS0-1h

C	-3.02373700	1.56895100	-0.10989400
C	-1.61894000	1.57960400	-0.05919000

C	-0.93075500	2.78851100	-0.08460400
C	-1.66489500	3.97416900	-0.16587900
C	-3.06445100	3.97154800	-0.21965900
C	-3.75456300	2.75216900	-0.18648700
H	-3.55110800	0.61871100	-0.08830600
H	-1.07415200	0.64171600	0.00083900
H	0.15353000	2.83215800	-0.04374300
H	-4.83940800	2.74521300	-0.21945400
C	-1.10781200	5.33726500	-0.20725700
C	-3.66143900	5.29754900	-0.27377000
C	-4.82740000	5.82677900	-0.24190200
C	-2.23256600	6.34397800	-0.34258700
C	-2.20694500	7.59434400	-0.51217800
O	0.07280000	5.63631800	-0.17659400
C	-5.34024700	7.13421400	-0.34626600
C	-6.09907700	7.74207200	0.68642100
C	-4.98929400	7.91630500	-1.47775100
C	-6.48110900	9.06993100	0.58913900
H	-6.36693800	7.15014800	1.55633700
C	-5.40043700	9.24954900	-1.57104900
H	-4.44653200	7.44952800	-2.29215100
C	-6.13502500	9.83087200	-0.54110000
H	-7.05605300	9.52562600	1.39103100
H	-5.14711700	9.82910600	-2.45518600
H	-6.45437500	10.86696900	-0.61489100
C	-1.82813800	8.95442600	-0.69580800
C	-0.33018700	9.29387600	-0.60351000
C	-1.01513900	9.34145100	-1.93073700

H	-2.51617200	9.71269400	-0.32574800
H	0.33441100	8.45922800	-0.40311300
H	-0.07718000	10.22636900	-0.10669900
H	-1.24095100	10.30904900	-2.37001600
H	-0.79675700	8.55490200	-2.64626100

IN1-1h

C	-2.87017000	1.54743400	-0.32259300
C	-1.48055000	1.65568700	-0.13725700
C	-0.88812200	2.90438900	0.04686700
C	-1.70663900	4.03221700	0.03208500
C	-3.09763000	3.93020900	-0.15950200
C	-3.69030800	2.67521000	-0.33051100
H	-3.31283400	0.56390000	-0.45806100
H	-0.86927300	0.75743000	-0.13436300
H	0.18205300	3.01402100	0.19738600
H	-4.76543100	2.58727100	-0.45790600
C	-1.29799900	5.45604600	0.20187700
C	-3.69096000	5.26153100	-0.08791600
C	-4.93679500	5.74485100	-0.11431100
C	-2.56270600	6.25706200	0.01468700
C	-2.75972600	7.52278400	-0.41668200
O	-0.15489500	5.83775800	0.40425700
C	-5.22271800	7.07384700	-0.20342900
C	-6.20976400	7.74300000	0.58785300
C	-4.21039000	7.88508400	-0.99214000
C	-6.33918600	9.10029700	0.55011000
H	-6.85181200	7.13319700	1.21709100

C	-4.53564300	9.34704700	-1.07000700
H	-4.12486900	7.51499900	-2.02871300
C	-5.51887300	9.90196700	-0.32950900
H	-7.08877900	9.59370200	1.16290500
H	-3.98790700	9.95062300	-1.78812400
H	-5.73284300	10.96426400	-0.41611700
C	-1.75492700	8.60240600	-0.58430600
C	-1.69299700	9.73335700	0.44190400
C	-0.53773300	8.78388900	0.28127500
H	-1.66233700	8.94242700	-1.61720300
H	-2.31011400	9.63101000	1.32996000
H	-1.60644400	10.75078600	0.07019200
H	0.36343100	9.14281800	-0.20846200
H	-0.35403300	8.04953600	1.05439900

2h-2

C	-2.85373200	1.59167300	0.08565300
C	-1.47557900	1.67920200	-0.14987500
C	-0.87089700	2.92543500	-0.34123200
C	-1.67156600	4.05935100	-0.28642900
C	-3.05514800	3.97921500	-0.05222200
C	-3.65734000	2.73713700	0.13575800
H	-3.30899300	0.61554200	0.23146800
H	-0.87758300	0.77283900	-0.18397500
H	0.19498600	3.02086900	-0.52838700
H	-4.72509800	2.64870500	0.31790200
C	-1.27607300	5.49076600	-0.46262800
C	-3.61356800	5.34587800	-0.06451500

C	-4.90436800	5.77189500	0.08035800
C	-2.54627900	6.28194900	-0.27887100
C	-2.76454400	7.64636300	-0.32124700
O	-0.15465000	5.88894000	-0.73271100
C	-5.19521100	7.16451800	-0.00957400
C	-6.52890600	7.63419300	0.09089000
C	-4.13153000	8.10796000	-0.21943900
C	-6.82285400	8.97572300	-0.02819400
H	-7.32287200	6.90969600	0.25606100
C	-4.47499200	9.48011500	-0.34329500
C	-5.78517800	9.90482200	-0.25461500
H	-7.85132600	9.31833100	0.04705500
H	-3.68734600	10.20261500	-0.51946100
H	-6.01912200	10.96077100	-0.35913200
C	-1.64106500	8.62452400	-0.50553800
C	-1.37516500	9.73455500	0.49921700
C	-0.40866900	8.59144400	0.35897800
H	-1.46580500	8.89460900	-1.54732700
H	-1.99277100	9.76735600	1.39302100
H	-1.09593600	10.71327200	0.11662600
H	0.54827800	8.75891000	-0.12462100
H	-0.37442800	7.85821100	1.15795200
H	-5.72084000	5.07233200	0.24397700

TS1-1h

C	-3.37028100	1.51430000	-0.31941800
C	-1.98509500	1.34718600	-0.16226700
C	-1.17123800	2.45116100	0.07818000

C	-1.76201400	3.71217300	0.15793400
C	-3.13950900	3.88568600	0.00287200
C	-3.95778000	2.77620500	-0.23911600
H	-3.99693600	0.64633500	-0.50690500
H	-1.55168900	0.35325100	-0.22930800
H	-0.09659500	2.35771800	0.20428000
H	-5.02940500	2.90216400	-0.36104300
C	-1.05834500	4.98999500	0.40524500
C	-3.60070500	5.28164700	0.11640400
C	-4.73519100	5.83922200	0.04120300
C	-2.05078700	6.09558700	0.41431400
C	-2.04556400	7.36677300	0.57145200
O	0.14260000	5.12013100	0.57476800
C	-6.09178000	6.20921800	-0.08616500
C	-6.94500600	6.24030100	1.04542500
C	-6.63983300	6.53047300	-1.35339600
C	-8.28723000	6.57228300	0.90606200
H	-6.53461800	5.99824000	2.02093200
C	-7.98421800	6.86026100	-1.47601300
H	-5.99421200	6.51205700	-2.22601600
C	-8.81503800	6.88456700	-0.35104200
H	-8.92824700	6.58768700	1.78347900
H	-8.38890500	7.10024800	-2.45560400
H	-9.86476600	7.14448300	-0.45309300
C	-3.07210600	8.34206800	0.56084200
C	-3.11812600	9.56471900	1.46679700
C	-2.93015100	9.74710800	-0.00799900
H	-4.04327300	7.80902500	0.37137000

H	-2.26779400	9.72200200	2.12228000
H	-4.08279200	9.81444800	1.89917500
H	-3.76532900	10.12239700	-0.59240400
H	-1.94953600	10.03123700	-0.37562200

IN2-1h

C	-3.83211800	1.93818200	-0.23602900
C	-2.48691100	1.70500300	0.08834600
C	-1.65380900	2.77635500	0.39976000
C	-2.19413000	4.06037300	0.39455100
C	-3.55067500	4.30942300	0.10168700
C	-4.37251100	3.22488800	-0.23486100
H	-4.47061100	1.09830700	-0.49784000
H	-2.09792100	0.69056400	0.08367900
H	-0.60195500	2.63896600	0.63347000
H	-5.41219300	3.37031200	-0.50155000
C	-1.46818700	5.33285200	0.62523800
C	-3.81454800	5.76943900	0.14254300
C	-4.94130700	6.49202400	-0.06153900
C	-2.49937000	6.41025100	0.42978500
C	-2.22259500	7.69886000	0.53068700
O	-0.28804600	5.46662500	0.90265500
C	-6.34065200	6.07109600	-0.22911000
C	-6.93955100	5.08047500	0.57071600
C	-7.15091400	6.74688900	-1.16123000
C	-8.28579400	4.75308800	0.41608400
H	-6.34746800	4.58619000	1.33482500
C	-8.49412200	6.41432800	-1.32167000

H	-6.71165800	7.53322400	-1.77050800
C	-9.06726500	5.41206600	-0.53569600
H	-8.72881600	3.98945200	1.05015500
H	-9.09607500	6.94160700	-2.05712800
H	-10.11667300	5.15635400	-0.65418000
C	-1.92413900	8.94354900	0.63234800
C	-1.74798000	10.14750900	1.48493700
C	-1.43393600	10.19503700	-0.00089100
H	-4.79544000	7.57230500	-0.10085600
H	-0.92000600	10.14422600	2.19110300
H	-2.64423800	10.65327100	1.83938700
H	-2.11689200	10.73364600	-0.65534600
H	-0.39129000	10.22442000	-0.31111900

TS1-1h(endo)

C	-2.86703800	1.89079000	-0.13098300
C	-1.53467800	1.92053800	0.30002000
C	-0.92438600	3.14330400	0.57838600
C	-1.67545200	4.30515700	0.43234300
C	-3.02530200	4.29058100	0.02849500
C	-3.61876600	3.06174600	-0.27396100
H	-3.33202000	0.93575500	-0.36182100
H	-0.97883600	0.99313300	0.40635000
H	0.11302500	3.20922400	0.89380500
H	-4.64398000	3.00018700	-0.61722600
C	-1.21710400	5.70322100	0.61557000
C	-3.52007500	5.69480600	-0.08285300
C	-4.73023600	6.19415200	-0.47086300

C	-2.39366000	6.55623000	0.24358100
C	-2.35062000	7.91224800	0.37173400
O	-0.11173800	6.07740000	0.98127500
C	-5.99913500	5.49390100	-0.70223300
C	-6.48617900	4.50746200	0.17658700
C	-6.80338000	5.86795400	-1.79554000
C	-7.71156500	3.88720800	-0.06001300
H	-5.91428400	4.26176900	1.06615000
C	-8.02233400	5.23885800	-2.03664600
H	-6.45514700	6.64962000	-2.46631200
C	-8.47890700	4.24077000	-1.17263800
H	-8.07396200	3.13356900	0.63432600
H	-8.61978400	5.53164100	-2.89605200
H	-9.43303100	3.75388500	-1.35584700
H	-4.75517300	7.26263400	-0.67596300
C	-7.05479500	8.71646700	1.45800100
C	-7.05223600	7.56971600	2.27540800
C	-8.22127900	6.90385200	2.63138000
C	-9.43416000	7.38583900	2.14256400
C	-9.45098100	8.50527300	1.29931100
C	-8.27562500	9.17508300	0.94993900
C	-4.79507600	8.21536600	1.96248400
C	-5.65909600	7.18810400	2.61917100
H	-8.16556100	6.02520000	3.26740300
H	-10.36577600	6.89021900	2.40161200
H	-10.39875600	8.86180200	0.90391800
H	-8.32417600	10.03033400	0.28705600
O	-5.30853000	6.24245000	3.31242900

C	-3.44691700	8.21678300	2.16094400
C	-5.65428800	9.17961500	1.25082100
C	-5.16043400	10.24150100	0.56153000
H	-4.07794300	10.26319300	0.46968500
C	-5.83877100	11.37966600	-0.07577100
C	-5.36043800	11.85848600	-1.31108200
C	-6.88778800	12.08645400	0.54182400
C	-5.93447900	12.96888700	-1.92598500
H	-4.53723100	11.33815700	-1.79551000
C	-7.45781500	13.20187500	-0.06968900
H	-7.23705000	11.76957000	1.51963400
C	-6.98999200	13.64439200	-1.30918400
H	-5.55539000	13.31002200	-2.88585100
H	-8.26236300	13.73510200	0.43021400
H	-7.43507000	14.51469000	-1.78366300
C	-1.76077800	9.02064100	0.01786900
C	-1.34001100	10.40612800	0.27272500
C	-0.92475300	9.68456400	-1.01082500
H	-0.58678300	10.57598600	1.04091000
H	-2.07113700	11.20909800	0.18651300
H	-1.39537100	9.99675600	-1.94163900
H	0.10549400	9.34968300	-1.11671700
C	-2.50867500	8.13437900	3.07033700
C	-1.12819900	7.85844600	3.48480900
C	-2.13320500	8.45532700	4.46925900
H	-0.33907000	8.50162700	3.09980300
H	-0.82570900	6.81991000	3.59975400
H	-2.54075800	7.81822800	5.25228600

H	-2.02569800	9.50196800	4.74859800

2h-1

C	-3.06379700	2.38929700	-1.76511300
C	-1.79052600	2.01876800	-1.33994600
C	-1.05694300	2.87552800	-0.50059500
C	-1.64032700	4.06530400	-0.11373600
C	-2.93817500	4.44104900	-0.51226800
C	-3.65428400	3.60195800	-1.35984600
H	-3.62156600	1.72973200	-2.42500200
H	-1.36166000	1.07491100	-1.66467700
H	-0.05349300	2.62634200	-0.16645800
H	-4.64562700	3.85803600	-1.71227000
C	-1.06106600	5.17489700	0.70769800
C	-3.22267900	5.78176700	0.08150400
C	-4.45099500	6.64054900	-0.08932300
C	-2.11984300	6.24579000	0.73003200
C	-2.01589400	7.58738800	1.29370700
O	0.03181200	5.17298000	1.24523900
C	-5.73944400	5.88344600	-0.40665000
C	-6.16456000	4.78376400	0.35595400
C	-6.53141100	6.28533400	-1.49020200
C	-7.34788400	4.11483200	0.04324300
H	-5.56185700	4.44179000	1.19076000
C	-7.71570700	5.61678500	-1.80587000
H	-6.21724400	7.13307200	-2.09387600
C	-8.12899000	4.52820100	-1.03764300
H	-7.65590800	3.26353300	0.64458500

H	-8.31167000	5.94724000	-2.65259900
H	-9.04932700	4.00390600	-1.28097500
H	-4.24982900	7.28511800	-0.95826400
C	-6.87594300	8.44434100	1.65135200
C	-6.57746600	7.43882600	2.58873800
C	-7.49801100	6.99962000	3.54096200
C	-8.76703300	7.56856000	3.54469900
C	-9.09584600	8.54569000	2.59036800
C	-8.17078800	8.98814300	1.64631000
C	-4.62345200	7.64295900	1.12956600
C	-5.22665600	6.89606800	2.35460500
H	-7.21270800	6.22061800	4.24208600
H	-9.51013800	7.25120700	4.27087600
H	-10.09806900	8.96663600	2.58416000
H	-8.46271500	9.73426700	0.91771100
O	-4.67996700	6.01344300	2.99053300
C	-3.29833800	8.27820700	1.60673500
C	-5.70661700	8.69069600	0.78515900
C	-5.49613400	9.60728100	-0.18277300
H	-4.55299100	9.50966100	-0.72251700
C	-6.30347100	10.75740000	-0.63309600
C	-6.37331000	11.04188100	-2.00942300
C	-6.93133800	11.64742200	0.25655100
C	-7.08158800	12.14446600	-2.48272300
H	-5.86869800	10.38290600	-2.71232600
C	-7.63252000	12.75635400	-0.21531100
H	-6.85081700	11.47619300	1.32547300
C	-7.71828900	13.00579100	-1.58669300

H	-7.13060200	12.33550100	-3.55148700
H	-8.10389600	13.43388100	0.49192900
H	-8.26467500	13.87069000	-1.95271100
C	-0.81669600	8.18060200	1.42511100
C	-0.03667600	9.39369100	1.69550600
C	0.62686300	8.10352800	1.19832200
H	0.14177600	9.69399900	2.72753700
H	-0.12335600	10.23540200	1.00730300
H	0.99630900	8.06823900	0.17304500
H	1.23032800	7.52811600	1.89668000
C	-3.34966200	9.34763100	2.40582200
C	-2.66369400	10.26886200	3.31688100
C	-4.18603500	10.31186700	3.13541200
H	-2.08415300	11.09468900	2.90653300
H	-2.26135000	9.87287100	4.24936200
H	-4.81779400	9.95758800	3.94953800
H	-4.60211100	11.16206900	2.59563500

IN1-4a

C	-4.82285800	3.32773200	0.40541300
C	-3.68868900	2.51125900	0.54040600
C	-2.41350800	3.07228200	0.49756900
C	-2.30342300	4.44889700	0.32012600
C	-3.43461700	5.27924800	0.18441200
C	-4.71234700	4.70725700	0.22719200
H	-5.81045300	2.87502500	0.44015100
H	-3.80994800	1.44036600	0.67769900
H	-1.51651000	2.46805600	0.59785800

H	-5.59766800	5.32331000	0.12346100
C	-1.06049500	5.25587400	0.24417400
C	-3.01343400	6.67975000	0.01205800
C	-3.76583900	7.80035900	-0.15502200
C	-1.52910800	6.68116100	0.04901300
C	-0.71119100	7.70911800	-0.06217700
O	0.08642600	4.85447800	0.32350000
C	-5.16939400	7.89360800	-0.20120900
C	-6.37743200	8.06065300	-0.25159500
C	-7.78399100	8.26372900	-0.31260100
C	-8.68065800	7.18795700	-0.14482100
C	-8.30753300	9.55343300	-0.54377600
C	-10.05467300	7.39926600	-0.20749000
H	-8.28659300	6.19224700	0.03457500
C	-9.68300300	9.75484200	-0.60502900
H	-7.62227800	10.38536100	-0.67365600
C	-10.56144900	8.68098500	-0.43760800
H	-10.73361600	6.56105300	-0.07630700
H	-10.07208900	10.75350400	-0.78404800
H	-11.63482700	8.84205300	-0.48594600
C	0.12674500	8.70406400	-0.16221200
H	0.48361800	8.98327300	-1.15698600
H	-3.22646700	8.74128700	-0.26770500
C	0.65186000	9.52548500	0.99749600
H	1.74689200	9.42659500	1.02330800
H	0.27460100	9.11515500	1.94087800
C	0.28284500	11.01541200	0.88321600
H	-0.81056900	11.11270900	0.86758500

H	0.63998100	11.40400100	-0.08061500
C	0.86442800	11.85451600	2.02506000
H	1.95956900	11.79684500	2.04241200
H	0.58739000	12.90952100	1.92184700
H	0.49853500	11.50729500	2.99888100

exo-TS1

C	-8.69363500	-2.49457700	-1.02257200
O	-8.02888600	-2.12788900	-1.98378900
C	-8.27564000	-2.52954700	0.41448200
C	-7.04026800	-2.17327600	0.86866700
C	-6.19218700	-1.26122000	1.30001400
H	-5.17121000	-1.54120700	1.53984500
C	-9.35694300	-3.11484200	1.19914600
C	-9.28672800	-3.30230500	2.55263000
H	-8.38003200	-2.95988000	3.04987300
C	-10.25655000	-3.88811100	3.38079000
C	-11.04410800	-4.39440300	4.16533800
C	-6.72332100	-5.97047000	2.14391200
C	-6.08405800	-4.66681000	1.91101600
C	-5.50635900	-4.18567400	3.20068300
O	-4.89951800	-3.14179700	3.41344300
C	-6.02524400	-4.00214700	0.72418200
C	-5.61639800	-4.00224700	-0.53815500
H	-6.06015400	-3.31656300	-1.25863900
C	-7.35923400	-6.69525900	1.17725300
H	-7.41381600	-6.24862500	0.18455600
C	-7.96668300	-7.95422400	1.31168100

C	-8.51340100	-9.04628200	1.33978200
C	-10.08123500	-3.02431500	-1.04190200
C	-10.93265200	-3.16734200	-2.13217700
C	-10.46389500	-3.40254700	0.26121200
C	-12.20388800	-3.70065900	-1.91252200
H	-10.60101400	-2.86556800	-3.12158100
C	-11.73852800	-3.93223900	0.47508200
C	-12.59596200	-4.07638100	-0.62005700
H	-12.89394100	-3.82540300	-2.74238800
H	-12.05854800	-4.22490000	1.46824800
H	-13.58934700	-4.48919600	-0.46434300
C	-6.58466700	0.17599200	1.56445100
H	-5.94997800	0.82686800	0.94436000
H	-7.62023200	0.34853200	1.24958800
C	-6.40644700	0.56407900	3.04390800
H	-5.37899500	0.33686300	3.35678200
H	-7.05760000	-0.07018200	3.65882100
C	-6.71701500	2.04113000	3.30578100
H	-7.75058500	2.28583200	3.03177500
H	-6.58516000	2.29119500	4.36452100
H	-6.05626800	2.69554200	2.72379900
C	-11.95500300	-4.98184900	5.08429300
C	-11.70930200	-4.91345600	6.47243100
C	-13.11610000	-5.64364000	4.63200400
C	-12.59988700	-5.48804800	7.37383000
H	-10.81676200	-4.40630500	6.82532600
C	-14.00036300	-6.21547100	5.54146700
H	-13.30862800	-5.70603800	3.56530700

C	-13.74733700	-6.14001800	6.91380700
H	-12.39898900	-5.42731000	8.44000500
H	-14.89018200	-6.72309600	5.17914600
H	-14.44032100	-6.58748100	7.62095200
C	-9.15219700	-10.31571000	1.36246700
C	-9.24565700	-11.06206200	2.55628900
C	-9.70759500	-10.85408700	0.18174300
C	-9.87364400	-12.30377000	2.56420700
H	-8.82254700	-10.65548100	3.46982300
C	-10.33302400	-12.09679400	0.19970800
H	-9.63925600	-10.28448300	-0.73990700
C	-10.41913500	-12.82650600	1.38857500
H	-9.93810800	-12.86698500	3.49132000
H	-10.75534500	-12.49867700	-0.71736000
H	-10.90820900	-13.79665000	1.39890700
C	-5.79699200	-5.25561300	4.18911200
C	-5.44824300	-5.29760600	5.53516700
C	-6.51062200	-6.29971600	3.56852300
C	-5.82597700	-6.41464300	6.28112500
H	-4.89545900	-4.47312300	5.97639600
C	-6.88450200	-7.41699900	4.32079500
C	-6.53713000	-7.45980400	5.67363500
H	-5.56989200	-6.47901700	7.33513400
H	-7.43385400	-8.23295700	3.86638900
H	-6.82513200	-8.32332400	6.26771300
C	-4.48772200	-4.87205900	-1.04445800
H	-3.64700400	-4.22060200	-1.32782000
H	-4.12705800	-5.52657200	-0.24307900

C	-4.90275500	-5.70556400	-2.27196500
H	-5.30193600	-5.03708100	-3.04645800
H	-5.72464100	-6.37616900	-1.98938600
C	-3.74047800	-6.52401500	-2.84284300
H	-4.06147300	-7.11437600	-3.70830600
H	-2.91909700	-5.87391500	-3.16798900
H	-3.33883100	-7.21882000	-2.09542400

exo-5a-1

C	-9.31786100	-2.09646200	-0.65301500
O	-8.96382200	-1.60750700	-1.71104500
C	-8.47486000	-2.44157400	0.54299500
C	-7.02431000	-2.37879800	0.74460500
C	-6.23203600	-1.32807100	0.43831000
H	-5.18163000	-1.41267800	0.71645500
C	-9.27256600	-3.01232700	1.48397300
C	-8.62556300	-3.43402900	2.78020300
H	-8.21501700	-2.51698300	3.23397400
C	-9.49968200	-4.05791000	3.77361900
C	-10.18082700	-4.55087000	4.64758800
C	-7.68153500	-5.77020300	2.19321700
C	-7.31788300	-4.30457100	2.47191700
C	-6.57357600	-4.37721900	3.83962500
O	-6.05904200	-3.43143300	4.40330800
C	-6.46922900	-3.62117800	1.38150300
C	-5.28974500	-4.10561100	0.94709000
H	-4.82672200	-3.56788800	0.11999200
C	-8.19392300	-6.19120700	1.00942500

H	-8.33282900	-5.44317100	0.23068000
C	-8.55483900	-7.50600800	0.64559500
C	-8.88657200	-8.60857600	0.24284300
C	-10.71324300	-2.50606000	-0.27890800
C	-11.88032800	-2.39726100	-1.00740700
C	-10.68358200	-3.06184400	1.01726600
C	-13.07315600	-2.86256300	-0.42348500
H	-11.86582600	-1.96375400	-2.00367500
C	-11.85978600	-3.52100500	1.59445100
C	-13.05442700	-3.41366500	0.85502700
H	-14.00888000	-2.79287500	-0.97088700
H	-11.86871000	-3.95475000	2.58680800
H	-13.98002800	-3.77236400	1.29752000
C	-6.61525000	-0.01712100	-0.18288700
H	-6.12635900	0.06496800	-1.16673200
H	-7.68874900	0.02988000	-0.38068500
C	-6.18192200	1.18557600	0.67907400
H	-5.10268100	1.12184100	0.87691500
H	-6.67485400	1.12239900	1.65828000
C	-6.50513200	2.53037100	0.02092000
H	-7.58195800	2.63521600	-0.15923800
H	-6.18912500	3.36889400	0.65196900
H	-5.99795100	2.62995100	-0.94669000
C	-10.99970900	-5.13578100	5.66318600
C	-11.97565300	-4.36631000	6.32565400
C	-10.84237600	-6.49018300	6.01547400
C	-12.77360700	-4.94055800	7.31206500
H	-12.09610700	-3.32056200	6.05946500

C	-11.64381900	-7.05495500	7.00431100
H	-10.08857500	-7.08464100	5.50877100
C	-12.61126300	-6.28496200	7.65463800
H	-13.52316500	-4.33637900	7.81599300
H	-11.51333500	-8.10098400	7.26855400
H	-13.23475400	-6.73006700	8.42524400
C	-9.27905000	-9.89039700	-0.23527300
C	-9.03728600	-11.05385900	0.52385900
C	-9.92010300	-10.01586200	-1.48557000
C	-9.42721300	-12.30111500	0.04505900
H	-8.53933700	-10.96605600	1.48478000
C	-10.30705600	-11.26718000	-1.95565400
H	-10.10811900	-9.12326900	-2.07408000
C	-10.06318300	-12.41314700	-1.19410300
H	-9.23402100	-13.18964300	0.64001200
H	-10.80066300	-11.34939300	-2.92014800
H	-10.36623900	-13.38846900	-1.56469600
C	-6.68178100	-5.76451900	4.33142800
C	-6.22859400	-6.27316200	5.54782800
C	-7.34957100	-6.56322700	3.38293700
C	-6.45401200	-7.61895100	5.82543300
H	-5.71841300	-5.61920200	6.24896200
C	-7.57389900	-7.91819900	3.67259900
C	-7.12291500	-8.42736300	4.89060400
H	-6.11603200	-8.04825100	6.76435000
H	-8.08856800	-8.55664800	2.96468000
H	-7.29196900	-9.47620400	5.12128200
C	-4.50139300	-5.29795600	1.40871200

H	-3.52524900	-4.94403800	1.77738600
H	-4.97646200	-5.80405500	2.25321200
C	-4.25441400	-6.31743900	0.27858200
H	-3.77979300	-5.80710700	-0.57100000
H	-5.22137400	-6.68727000	-0.08482800
C	-3.38285300	-7.49503600	0.72534600
H	-3.22355800	-8.20501100	-0.09411300
H	-2.39810700	-7.15347800	1.06795900
H	-3.85071200	-8.04131700	1.55340300

exo-TS2

C	-9.56914800	-1.96872600	-0.49696700
O	-9.30076900	-1.51147300	-1.60711800
C	-8.68060600	-2.42755400	0.57858100
C	-7.22717000	-2.37514200	0.69309100
C	-6.42543200	-1.37757800	0.21706500
H	-5.35557100	-1.47492800	0.40586200
C	-9.45393800	-2.97699300	1.60735800
C	-8.87883800	-3.57104100	2.76644700
C	-9.67114600	-4.16354900	3.79219500
C	-10.27059900	-4.61859100	4.75404900
C	-7.74153900	-5.73840300	2.15414900
C	-7.47911600	-4.25768500	2.51831000
C	-6.78088500	-4.38291200	3.89770000
O	-6.29795500	-3.45283600	4.55997000
C	-6.61903700	-3.52912500	1.45219600
C	-5.39121200	-3.97272500	1.09960700
H	-4.92797100	-3.47097400	0.25089900

C	-8.19539600	-6.12604300	0.93482000
H	-8.36138800	-5.34573300	0.19306300
C	-8.47297800	-7.43716800	0.49943800
C	-8.72633700	-8.53513900	0.03117100
C	-10.96505700	-2.20829800	0.00608100
C	-12.16970400	-1.93983100	-0.61588800
C	-10.89713000	-2.79157800	1.28313200
C	-13.35392200	-2.25048400	0.07263800
H	-12.18356500	-1.49971400	-1.60913500
C	-12.06820900	-3.10952900	1.96206700
C	-13.29786200	-2.82553600	1.34197900
H	-14.31796500	-2.04427900	-0.38487400
H	-12.04304700	-3.56842100	2.94269900
H	-14.22073200	-3.06410000	1.86430700
C	-6.78340400	-0.17140600	-0.61100500
H	-7.85665000	0.02265300	-0.58520300
H	-6.27867700	0.71108600	-0.18556700
C	-6.34431900	-0.31217700	-2.08422700
H	-6.86223700	-1.17859900	-2.50673700
H	-5.26530400	-0.52084000	-2.12681700
C	-6.66514800	0.93697000	-2.90932000
H	-6.16926500	1.82749600	-2.50185900
H	-6.33836300	0.82014700	-3.94919700
H	-7.74466700	1.12635700	-2.91750900
C	-11.00589900	-5.14573500	5.85303500
C	-12.23500300	-4.56887000	6.23850200
C	-10.52456900	-6.25366300	6.58238800
C	-12.95585300	-5.08898800	7.30961200

H	-12.61024500	-3.70901500	5.69153100
C	-11.25020900	-6.76155500	7.65630600
H	-9.58164800	-6.70727600	6.29322000
C	-12.46876300	-6.18586000	8.02495700
H	-13.90147500	-4.63253800	7.59046300
H	-10.86402800	-7.61538700	8.20736500
H	-13.03294500	-6.58735100	8.86222600
C	-9.03115900	-9.80659100	-0.52952600
C	-8.76301200	-10.99651400	0.17806900
C	-9.61115300	-9.89359200	-1.81265700
C	-9.06766500	-12.23297200	-0.38310500
H	-8.31349700	-10.93759500	1.16474200
C	-9.91312700	-11.13453600	-2.36488700
H	-9.82007100	-8.98013900	-2.36059500
C	-9.64351400	-12.30716200	-1.65415100
H	-8.85577700	-13.14245300	0.17241000
H	-10.36072600	-11.18773200	-3.35346100
H	-9.88064200	-13.27423100	-2.08877600
C	-6.84071500	-5.77289200	4.32912600
C	-6.41211200	-6.30867900	5.54757600
C	-7.42586500	-6.56439900	3.31711000
C	-6.58116000	-7.67180000	5.75966000
H	-5.96634500	-5.66196200	6.29729100
C	-7.59517700	-7.93872400	3.54604100
C	-7.17129900	-8.47138900	4.76183500
H	-6.26199800	-8.12496500	6.69358400
H	-8.05144400	-8.57090000	2.79432700
H	-7.30062700	-9.53473700	4.94623100

C	-4.55810300	-5.10597300	1.63250200
H	-3.61136500	-4.69473000	2.02051300
H	-5.03147600	-5.61384800	2.47568300
C	-4.21803300	-6.14396200	0.54300100
H	-3.73477600	-5.63441400	-0.30186800
H	-5.15117900	-6.56931600	0.15409000
C	-3.30985300	-7.26413200	1.05861300
H	-3.08371000	-7.98577000	0.26584200
H	-2.35711900	-6.86643600	1.42982300
H	-3.78464200	-7.81190900	1.88170300
H	-8.53445600	-2.19920800	3.58054000
O	-8.12802800	-1.44092200	4.26284900
H	-7.46391400	-1.99426100	4.74011500
H	-7.53784600	-0.74105900	3.69778200
O	-6.60700700	0.04632000	2.95363600
H	-6.74306300	-0.24125400	2.02437800
H	-5.72298600	-0.35959200	3.17783300
O	-4.47998300	-1.55097400	3.45279800
H	-4.97423700	-2.24130800	3.94094300
H	-4.34191400	-1.96167000	2.58356700

5c-2

C	-9.81962900	-1.17107100	-0.03058400
O	-9.48511600	-0.39029200	-0.91635500
C	-9.00325200	-2.21618000	0.65651500
C	-7.70216200	-2.55607100	0.43000000
C	-6.91386600	-1.84139400	-0.64835600
H	-6.21954900	-2.53518400	-1.13521800

C	-9.84681800	-2.86153100	1.66256900
C	-9.38222700	-3.86273200	2.45705900
C	-10.17519400	-4.48974800	3.44757800
C	-10.81484400	-5.04534200	4.32474700
C	-7.97368900	-5.88935700	2.06634800
C	-7.92518300	-4.36462600	2.30604400
C	-7.29047800	-4.26525900	3.73910400
O	-6.90734200	-3.24514400	4.27024300
C	-7.08000300	-3.59948700	1.26357800
C	-5.75559300	-3.85320900	1.11130700
C	-8.28271100	-6.41849000	0.85642000
H	-8.49818200	-5.72069200	0.04741800
C	-8.34372700	-7.78381000	0.50708200
C	-8.40605300	-8.93974700	0.12254000
C	-11.16537600	-1.24692900	0.59122700
C	-12.28782000	-0.48361000	0.28504200
C	-11.18358100	-2.24327900	1.58834100
C	-13.46499700	-0.72627100	0.99149500
H	-12.22784900	0.27535700	-0.48975100
C	-12.37081600	-2.48421600	2.28942000
C	-13.49842200	-1.72050300	1.98107500
H	-14.36033700	-0.14921800	0.77721200
H	-12.41942400	-3.25126800	3.05170000
H	-14.42419100	-1.90230200	2.52103300
C	-6.14284800	-0.60868000	-0.12576400
H	-6.86573200	0.09312700	0.30769600
H	-5.46525700	-0.90253100	0.68734500
C	-5.35001200	0.09522100	-1.23358800

H	-6.04112800	0.39418900	-2.03324700
H	-4.64472400	-0.61652100	-1.68748000
C	-4.58356100	1.32319800	-0.73157400
H	-3.86379300	1.04989200	0.05007000
H	-4.02719600	1.80608800	-1.54321200
H	-5.26645200	2.06832500	-0.30599400
C	-11.56565600	-5.68804000	5.34906600
C	-12.75735300	-5.11327200	5.83755200
C	-11.12744800	-6.91268400	5.89485900
C	-13.48760500	-5.74848900	6.83757600
H	-13.09490200	-4.16504100	5.43022500
C	-11.86485200	-7.53887900	6.89543800
H	-10.21048900	-7.35926600	5.52385400
C	-13.04598000	-6.96253900	7.36999100
H	-14.40362300	-5.29365600	7.20480700
H	-11.51686000	-8.48245500	7.30734100
H	-13.61813100	-7.45537500	8.15120600
C	-8.47975700	-10.28789900	-0.32755200
C	-8.04752000	-11.34953900	0.49391300
C	-8.98759100	-10.58393100	-1.60973100
C	-8.12331100	-12.66426900	0.04398200
H	-7.65027800	-11.12892700	1.48009800
C	-9.06016900	-11.90188400	-2.05062600
H	-9.32180300	-9.77037100	-2.24601000
C	-8.62955900	-12.94587000	-1.22756800
H	-7.78606600	-13.47273100	0.68693200
H	-9.45417000	-12.11607700	-3.04031600
H	-8.68744300	-13.97345800	-1.57556700

C	-7.25879700	-5.63395400	4.29978800
C	-6.87713100	-6.01425400	5.58490700
C	-7.65350700	-6.57018200	3.32471100
C	-6.90231600	-7.36933800	5.90736600
H	-6.57475000	-5.25838500	6.30374400
C	-7.67371200	-7.93341100	3.65740700
C	-7.29911200	-8.31461300	4.94619000
H	-6.61553600	-7.70012300	6.90158800
H	-7.97910400	-8.67505300	2.92903200
H	-7.31282400	-9.36858800	5.21212200
C	-4.85475300	-4.83299200	1.80044700
H	-4.12930100	-4.26521900	2.40521000
H	-5.38805600	-5.48336600	2.49544900
C	-4.07437200	-5.70445600	0.79365800
H	-3.53046200	-5.05297000	0.09564400
H	-4.78945000	-6.27678800	0.18904700
C	-3.09283600	-6.65956700	1.47915600
H	-2.55020000	-7.26401900	0.74375100
H	-2.35219400	-6.10966100	2.07268600
H	-3.61590500	-7.34684000	2.15492800
H	-5.22684800	-3.26100700	0.37023500
H	-7.61263700	-1.49498300	-1.41173100

endo-TS1

C	-6.37171500	-5.21420300	5.87095200
O	-5.46229500	-5.80296700	6.43572700
C	-7.38256700	-5.80102600	4.92121500
C	-7.34324700	-7.10141700	4.53420700

C	-7.45393200	-8.38134400	4.84070900
H	-6.99280100	-9.13560100	4.20675300
C	-8.23338900	-4.72736600	4.43331500
C	-9.24619100	-4.91972200	3.53312100
H	-9.43089100	-5.94137900	3.20711700
C	-10.09875300	-3.94460500	2.98978300
C	-10.87589100	-3.16365200	2.46343500
C	-8.35384400	-7.32376900	1.08724000
C	-7.19853400	-6.60461500	1.63564000
C	-7.05385600	-5.30600900	0.89055200
O	-6.17932900	-4.46331700	1.02193700
C	-6.34372700	-6.92130400	2.64117400
C	-5.07438000	-6.99162800	3.02381300
H	-4.80502500	-6.85309400	4.06956400
C	-8.75522200	-8.56771700	1.48479200
H	-8.17225400	-9.04813900	2.26649900
C	-9.84322400	-9.31574200	1.00137500
C	-10.76303400	-10.03532000	0.64361100
C	-11.78220700	-2.26733900	1.83432500
C	-12.51035200	-2.67859000	0.69754200
C	-11.97156500	-0.95959200	2.32765700
C	-13.39859800	-1.80433400	0.07877400
H	-12.35849500	-3.68099000	0.30982000
C	-12.86373300	-0.09381500	1.70251000
H	-11.41652000	-0.63782700	3.20359600
C	-13.57996800	-0.51140700	0.57760400
H	-13.95251700	-2.13185100	-0.79691900
H	-13.00159500	0.91055100	2.09363300

H	-14.27564200	0.16745300	0.09208700
C	-11.83299900	-10.87534400	0.23028000
C	-11.99848100	-12.15356200	0.80530600
C	-12.74800800	-10.45342200	-0.75727300
C	-13.04499800	-12.97755800	0.40296900
H	-11.29742700	-12.48438200	1.56536300
C	-13.79135400	-11.28469400	-1.15314700
H	-12.62908000	-9.47151100	-1.20519400
C	-13.94486100	-12.54820000	-0.57627500
H	-13.15958800	-13.95927800	0.85453700
H	-14.48836500	-10.94616400	-1.91500400
H	-14.76079200	-13.19433500	-0.88800700
C	-8.17547300	-5.28263100	-0.08388000
C	-8.48859700	-4.28970000	-1.00568200
C	-8.93416300	-6.46300400	0.03300300
C	-9.59528800	-4.48171600	-1.83380400
H	-7.87660500	-3.39436900	-1.06417400
C	-10.03902300	-6.65197600	-0.80314300
C	-10.35771500	-5.65432000	-1.72889900
H	-9.86821900	-3.72484300	-2.56398800
H	-10.63735100	-7.55285900	-0.73710100
H	-11.21369700	-5.79362800	-2.38454300
C	-6.70328300	-3.76985100	5.95233300
C	-7.78437200	-3.48242700	5.09537700
C	-6.08129700	-2.78616900	6.71347200
C	-8.25441800	-2.17084400	5.00154800
C	-6.55611700	-1.47718700	6.61589500
H	-5.24808800	-3.04678000	7.35974600

C	-7.63049500	-1.18007800	5.76605400
H	-9.08007000	-1.92266800	4.34510400
H	-6.09246200	-0.68406400	7.19577300
H	-7.98614000	-0.15532400	5.69670400
C	-8.23175600	-8.89121500	6.03393700
H	-7.53945700	-9.45522900	6.67715000
H	-8.59797200	-8.04574200	6.62658900
C	-9.40498300	-9.80628600	5.63653800
H	-9.02559900	-10.63736700	5.02570500
H	-10.09582500	-9.24454500	4.99490100
C	-10.15469900	-10.36151200	6.85140500
H	-10.98475300	-11.00702500	6.54348800
H	-9.49001800	-10.95383800	7.49223300
H	-10.57073200	-9.55238300	7.46372300
C	-3.93929400	-7.28211800	2.07021800
H	-3.37288700	-8.15342600	2.43171300
H	-4.33573500	-7.53887900	1.08177400
C	-2.99154200	-6.06929000	1.95576700
H	-2.61577800	-5.80739000	2.95424000
H	-3.57536500	-5.21129700	1.60427300
C	-1.81347500	-6.33810400	1.01467900
H	-1.20546400	-7.18236600	1.36330000
H	-2.16109100	-6.57416900	0.00153500
H	-1.15901500	-5.46191000	0.94541700

IN2-4a

C	-6.79867400	-5.59782500	6.13057200
O	-6.03621300	-6.27616200	6.80412200

C	-7.55235900	-6.02440900	4.90922200
C	-7.26568200	-7.24973800	4.19165600
C	-7.25842700	-8.49600900	4.70243100
H	-6.84721700	-9.29050400	4.07740100
C	-8.31216100	-4.93691800	4.44816100
C	-9.19836000	-5.03388700	3.36789500
H	-9.49201300	-6.03199500	3.06438100
C	-9.86877600	-3.98153400	2.74505400
C	-10.47000600	-3.11471900	2.12335300
C	-8.58091800	-7.34023600	1.15614100
C	-7.45961200	-6.60422700	1.69661500
C	-7.24024800	-5.39740400	0.84740100
O	-6.35938100	-4.55034700	0.94925000
C	-6.63369600	-6.93284200	2.82769200
C	-5.27436500	-6.86342900	2.85773400
H	-4.80642600	-6.99809700	3.83338600
C	-9.01137800	-8.56615700	1.61213400
H	-8.46510800	-9.00850700	2.43999600
C	-10.08622300	-9.32513600	1.13229600
C	-11.00134400	-10.05901300	0.78526000
C	-11.17520200	-2.11901300	1.40291500
C	-12.09354900	-2.48740000	0.39445500
C	-10.97463500	-0.74805400	1.67571700
C	-12.78890000	-1.51086100	-0.31052400
H	-12.24025500	-3.54005200	0.17517500
C	-11.67654800	0.21956000	0.96502000
H	-10.26314300	-0.45967800	2.44328700
C	-12.58577000	-0.15672800	-0.02805000

H	-13.49294700	-1.80500200	-1.08412500
H	-11.51410400	1.27132000	1.18383600
H	-13.13221400	0.60238700	-0.58087100
C	-12.06379700	-10.91120000	0.38588200
C	-12.28780600	-12.13352100	1.05677400
C	-12.91570200	-10.55848800	-0.68316100
C	-13.32980300	-12.96925600	0.66862600
H	-11.63571400	-12.41033200	1.87933300
C	-13.95403900	-11.40201100	-1.06441000
H	-12.75032400	-9.62111700	-1.20547900
C	-14.16620900	-12.60867300	-0.39167900
H	-13.49081700	-13.90650100	1.19428500
H	-14.60164300	-11.11810600	-1.88948500
H	-14.97861700	-13.26444300	-0.69219300
C	-8.32577000	-5.41310500	-0.16935400
C	-8.58463700	-4.48413700	-1.16853600
C	-9.12032200	-6.55840100	0.01284800
C	-9.67480700	-4.70989800	-2.01372600
H	-7.94714600	-3.61129700	-1.27517100
C	-10.20629600	-6.78245200	-0.83357800
C	-10.47240500	-5.84821600	-1.84298900
H	-9.90544500	-4.00349800	-2.80643000
H	-10.83479100	-7.65704600	-0.71546200
H	-11.31564700	-6.01387900	-2.50889900
C	-7.15426500	-4.16341600	6.34188200
C	-8.03875000	-3.76043100	5.32476200
C	-6.73567000	-3.29733000	7.33969400
C	-8.52122700	-2.45691300	5.30757000

C	-7.21436200	-1.98046600	7.31628600
H	-6.05386400	-3.64343700	8.11142800
C	-8.09451500	-1.57234000	6.31155200
H	-9.20927100	-2.12441900	4.53887100
H	-6.90198100	-1.27429500	8.08054000
H	-8.45953400	-0.54855400	6.30459500
C	-7.79276300	-8.93020300	6.03691300
H	-6.95578100	-9.30162100	6.64688500
H	-8.20962300	-8.07500600	6.57883600
C	-8.85335600	-10.04243400	5.91844900
H	-8.43135200	-10.88836100	5.35722000
H	-9.69870800	-9.67124900	5.32372300
C	-9.35322300	-10.53016800	7.28153000
H	-10.10827500	-11.31680500	7.17101800
H	-8.53093500	-10.93741500	7.88251100
H	-9.80595200	-9.71111500	7.85343600
C	-4.31681000	-6.72498100	1.71500300
H	-3.72204000	-7.65215200	1.66085400
H	-4.84549100	-6.62944100	0.76360800
C	-3.35205900	-5.53673100	1.90242900
H	-2.83697600	-5.63424300	2.86844300
H	-3.94874200	-4.62025300	1.94588200
C	-2.32016200	-5.44029100	0.77505000
H	-1.70504000	-6.34715600	0.71474900
H	-2.81048300	-5.30377400	-0.19619500
H	-1.64645300	-4.58976800	0.92938400

endo-5a-1

C	-9.17052000	-2.05593400	-0.29599100
O	-8.68858300	-1.48959700	-1.26074700
C	-8.46854300	-2.56658400	0.93042800
C	-7.04053900	-2.64459300	1.24931400
C	-6.13631200	-1.65242900	1.09883700
H	-5.11788400	-1.86586900	1.42532400
C	-9.38492700	-3.16010900	1.73781800
C	-8.89022300	-3.73127700	3.04561700
H	-8.47702600	-2.87976500	3.60898500
C	-9.89107400	-4.36614900	3.90389500
C	-10.68691200	-4.87671500	4.66325600
C	-7.00110700	-5.04946300	4.12889000
C	-7.61988500	-4.66909800	2.77586600
C	-8.16406200	-6.02643100	2.24094900
O	-8.64762100	-6.21060200	1.14144900
C	-6.64888200	-3.98998500	1.79162800
C	-5.52349300	-4.57285400	1.33717500
H	-4.96809200	-4.01652800	0.58257100
C	-6.26661600	-4.17460900	4.86043700
H	-6.10685400	-3.18305600	4.43587900
C	-5.65191200	-4.39731900	6.11042300
C	-5.08420000	-4.50512600	7.18463100
C	-10.61697600	-2.39983400	-0.08867800
C	-11.70053200	-2.14407700	-0.90404500
C	-10.74516300	-3.06819300	1.14652800
C	-12.97002500	-2.57315600	-0.47493600
H	-11.56379200	-1.62749200	-1.85010400
C	-11.99725500	-3.49065800	1.57163900

C	-13.10714300	-3.23451300	0.74262900
H	-13.84325900	-2.39050200	-1.09481300
H	-12.12807600	-4.01040500	2.51276300
H	-14.09107300	-3.56517000	1.06493100
C	-6.35572600	-0.26011400	0.58319600
H	-5.79575300	-0.13714000	-0.35722200
H	-7.40497800	-0.09490600	0.32684100
C	-5.87770000	0.81474800	1.57959800
H	-4.82534000	0.62979200	1.83834300
H	-6.44396500	0.71480700	2.51559800
C	-6.02904000	2.23743500	1.03261800
H	-7.07593300	2.46083700	0.79404000
H	-5.68537700	2.98299600	1.75880800
H	-5.44577000	2.37176200	0.11338600
C	-11.64391800	-5.47491000	5.54093200
C	-12.65130800	-4.69149700	6.13657200
C	-11.59532300	-6.85423500	5.82090400
C	-13.58596600	-5.27611500	6.98748500
H	-12.68908800	-3.62713400	5.92522100
C	-12.53363600	-7.42931400	6.67432000
H	-10.81961300	-7.46090800	5.36425900
C	-13.53093200	-6.64513900	7.25917700
H	-14.35886200	-4.66118400	7.44058800
H	-12.48709400	-8.49476500	6.88323600
H	-14.26128100	-7.09853100	7.92379900
C	-4.41889200	-4.62453700	8.43711200
C	-4.33312800	-5.86772800	9.09711900
C	-3.82914800	-3.49353400	9.03946400

C	-3.67802800	-5.97207800	10.32053800
H	-4.78045300	-6.74392600	8.63764500
C	-3.17688200	-3.60752800	10.26340400
H	-3.89203900	-2.53404900	8.53555700
C	-3.09834900	-4.84471500	10.90830500
H	-3.61865100	-6.93645600	10.81770100
H	-2.72749000	-2.72801700	10.71637000
H	-2.58763400	-4.92996600	11.86344800
C	-8.00946200	-7.02109900	3.32316800
C	-8.43147000	-8.34981200	3.32210300
C	-7.34747400	-6.44391500	4.42377600
C	-8.19106300	-9.11914100	4.45880000
H	-8.93371400	-8.75539400	2.44856700
C	-7.11104300	-7.22549200	5.56457200
C	-7.53818200	-8.55280300	5.56729000
H	-8.50495600	-10.15875100	4.49226300
H	-6.61112400	-6.80467500	6.42866400
H	-7.36072200	-9.16474500	6.44794200
C	-4.93062200	-5.91476800	1.66117900
H	-3.89533200	-5.76792500	2.00743100
H	-5.45523400	-6.40882500	2.48346400
C	-4.90925600	-6.85042500	0.43404200
H	-4.38098400	-6.35215800	-0.39048600
H	-5.93906900	-7.00569000	0.08941000
C	-4.24705000	-8.19892800	0.73198100
H	-4.24561300	-8.84467100	-0.15350900
H	-3.20569300	-8.06962200	1.05259900
H	-4.77621200	-8.73162600	1.53171000

4a

C	-3.31045800	1.31046900	-0.45935900
C	-1.93773000	1.14289200	-0.25366800
C	-1.16364600	2.23176600	0.12944200
C	-1.72722800	3.50056600	0.32888700
C	-3.11913100	3.67794500	0.10709600
C	-3.88997000	2.56086800	-0.28768700
H	-3.92832400	0.46830300	-0.75862100
H	-1.47686200	0.16888400	-0.39068300
H	-0.09584300	2.12936100	0.28956900
H	-4.95135500	2.70366300	-0.46300600
C	-0.76866900	4.57203500	0.76745700
C	-3.80263700	4.92122400	0.20801900
C	-4.52118200	5.90934700	0.21998000
C	-1.27083800	5.76518200	1.41035500
C	-1.58793900	6.77184500	2.00882500
C	-2.01256500	7.98450200	2.70020000
H	-2.99326200	8.29083800	2.30881600
H	-2.17244300	7.74642000	3.76208700
O	0.44128200	4.41306500	0.63155600
C	-1.00794400	9.15045500	2.57975200
H	-0.03413200	8.82483300	2.96713500
H	-0.85667800	9.38341800	1.51792900
C	-1.47699400	10.40369500	3.32775500
H	-2.45824800	10.71261300	2.94021300
H	-1.63215800	10.15674100	4.38773600
C	-0.49058600	11.57016000	3.21364800

H	-0.85090200	12.45053100	3.75750200
H	0.48989600	11.30158000	3.62509500
H	-0.34125000	11.86216100	2.16707200
C	-5.27873800	7.03684700	0.24864300
C	-5.95999500	8.05127800	0.27357400
C	-6.75237900	9.23175000	0.29795000
C	-8.07693300	9.19542800	0.78087800
C	-6.22561400	10.45723500	-0.16044500
C	-8.84748400	10.35415300	0.80341700
H	-8.48545300	8.25370400	1.13388700
C	-7.00540900	11.60969000	-0.13453400
H	-5.20733000	10.48805100	-0.53547700
C	-8.31635200	11.56329800	0.34689300
H	-9.86667100	10.31397600	1.17785100
H	-6.58937400	12.54770800	-0.49181100
H	-8.92165900	12.46532700	0.36539900

TS3-IN1

C	-8.44365700	-2.71045100	0.19111200
O	-8.41706800	-2.16197100	-0.89974300
C	-7.78391100	-2.28371300	1.46012800
C	-6.84875300	-1.28300100	1.57491800
C	-6.65704000	0.02624900	1.58427100
H	-5.64939900	0.43484400	1.55999400
C	-8.05510300	-3.25925900	2.47821400
C	-7.52954900	-3.16511900	3.74781000
H	-7.03998300	-2.22771000	4.00379900
C	-7.63589100	-4.10510200	4.78749300

C	-7.65404000	-4.87906400	5.73316500
C	-4.20733800	-1.54951600	0.75876000
O	-3.60725500	-0.51414800	0.99593900
C	-5.05780800	-2.16714200	1.82592900
C	-4.85630400	-2.97474600	2.75469200
C	-4.36711000	-3.93430600	3.74160900
H	-4.86192300	-3.77267900	4.70888200
H	-3.29824100	-3.72654100	3.91341700
C	-7.69353700	-5.77831200	6.83468000
C	-7.21332600	-5.37944100	8.10045100
C	-8.21172100	-7.08234000	6.68628600
C	-7.25275200	-6.25876800	9.17813200
H	-6.81601100	-4.37640700	8.22209600
C	-8.24844400	-7.95369400	7.77067900
H	-8.58041600	-7.39827000	5.71506800
C	-7.77008800	-7.54722200	9.01918700
H	-6.88028400	-5.93752800	10.14705000
H	-8.65127500	-8.95464900	7.64185100
H	-7.80020100	-8.23059500	9.86324200
C	-4.12169400	-2.25677900	-0.54949900
C	-4.84269700	-3.43829900	-0.76963000
C	-3.30899600	-1.73418900	-1.59576100
C	-4.78213300	-4.10983800	-1.98650500
H	-5.46027100	-3.82892000	0.03075800
C	-3.25794400	-2.43280900	-2.82075900
C	-3.98374300	-3.60226300	-3.01413200
H	-5.35732400	-5.01890600	-2.13333000
H	-2.63756600	-2.03310400	-3.61634100

H	-3.92794500	-4.11647800	-3.96961900
C	-9.16137900	-3.97803000	0.53401600
C	-8.91338000	-4.31062100	1.87962800
C	-9.95748700	-4.76868700	-0.28300000
C	-9.48304100	-5.46195500	2.42279500
C	-10.52077700	-5.92756900	0.26188400
H	-10.12865700	-4.48049900	-1.31645600
C	-10.28363300	-6.26418000	1.59962100
H	-9.31574800	-5.73080100	3.45991000
H	-11.14735500	-6.56897700	-0.35192600
H	-10.73178900	-7.16529600	2.01042400
C	-7.78877000	1.02582500	1.66095500
H	-7.75028300	1.65613700	0.75980800
H	-8.75116300	0.50271900	1.64183700
C	-7.69774300	1.92750900	2.90561000
H	-6.71659000	2.42135600	2.92472300
H	-7.74365400	1.30033300	3.80575500
C	-8.80760000	2.98240800	2.95054700
H	-8.72305800	3.60951200	3.84525900
H	-8.76388700	3.64175700	2.07503200
H	-9.79953300	2.51452500	2.96332400
C	-4.54920700	-5.40724700	3.31756800
H	-5.61749200	-5.60067300	3.16602500
H	-4.05593200	-5.56516100	2.34948800
C	-3.98431400	-6.38346300	4.35611600
H	-2.91700500	-6.17226000	4.51382200
H	-4.48016900	-6.20964500	5.32081200
C	-4.16048000	-7.84949700	3.94855300

H	-5.22081400	-8.09941000	3.82283300
H	-3.65406200	-8.06204200	2.99904800
H	-3.74656500	-8.52455100	4.70585400
C	-2.53805400	-0.54657200	-1.49392000
C	-1.82370900	0.44148600	-1.58095000
C	-1.04349800	1.55069800	-1.63415400
C	-0.34135800	2.54969000	-1.68535200
C	0.46829900	3.71690200	-1.72816100
C	0.53932200	4.57790300	-0.61290400
C	1.21170900	4.03434000	-2.88401200
C	1.33131600	5.72123700	-0.65824700
H	-0.03190900	4.33571300	0.27776400
C	2.00093000	5.18009200	-2.91867500
H	1.15876700	3.37384100	-3.74386900
C	2.06377300	6.02648700	-1.80859100
H	1.37787100	6.37718900	0.20678400
H	2.56903600	5.41436200	-3.81483200
H	2.68087800	6.92025100	-1.83985400

IN5-4a

C	-9.91539100	-2.40952500	1.52042300
O	-10.35855800	-2.12330000	0.42320700
C	-8.50626800	-2.22920200	2.04386600
C	-7.34510700	-1.60735900	1.40825900
C	-7.36196900	-0.62917500	0.46722300
H	-6.38964200	-0.27674100	0.12455200
C	-8.42916200	-2.87139500	3.24114800
C	-7.14030400	-3.02415500	4.01154800

H	-7.16129200	-2.30624300	4.85443200
C	-7.02386100	-4.36948400	4.60568400
C	-6.92292600	-5.47583700	5.09276400
C	-4.79589600	-1.69847900	1.16973200
O	-4.03100400	-0.83363100	1.57083400
C	-6.03928000	-2.05497400	1.96797000
C	-5.90635500	-2.67116100	3.16312200
C	-4.56338900	-3.00582700	3.78811100
H	-4.70123000	-3.11941800	4.87078600
H	-3.88415100	-2.16028400	3.64323300
C	-6.81477100	-6.78555200	5.65662800
C	-6.44902600	-6.95778600	7.00554000
C	-7.07484200	-7.92436800	4.87001700
C	-6.34691600	-8.23586400	7.54900100
H	-6.24662200	-6.08258100	7.61544200
C	-6.97106400	-9.19879800	5.42147900
H	-7.35819300	-7.79499000	3.83003000
C	-6.60720700	-9.35931800	6.76065100
H	-6.06295800	-8.35566900	8.59100100
H	-7.17471100	-10.06956300	4.80420500
H	-6.52654000	-10.35511500	7.18779600
C	-4.54223300	-2.43125000	-0.11150200
C	-5.30697700	-3.55869500	-0.44636300
C	-3.51109400	-2.01052700	-0.99822500
C	-5.07871800	-4.27241700	-1.61889800
H	-6.08664000	-3.88254300	0.23458400
C	-3.29944800	-2.74233800	-2.18680600
C	-4.07065900	-3.85713400	-2.49288500

H	-5.68382300	-5.14389500	-1.85074900
H	-2.51576700	-2.41417700	-2.86204500
H	-3.88455800	-4.40271800	-3.41392700
C	-10.66665200	-3.09880500	2.61676900
C	-9.76277400	-3.37746400	3.65655900
C	-12.00362300	-3.43828300	2.68968100
C	-10.21220600	-4.00127000	4.81330500
C	-12.46133900	-4.07001400	3.85953200
H	-12.67332300	-3.21445300	1.86396800
C	-11.57559500	-4.34011100	4.90144600
H	-9.53718600	-4.23608300	5.62880400
H	-13.50757500	-4.34692900	3.95289400
H	-11.94066000	-4.82740800	5.80162200
C	-8.50600100	0.13129100	-0.13873700
H	-8.74766000	-0.29625900	-1.12421100
H	-9.41651800	0.02504600	0.45398100
C	-8.16499100	1.62328500	-0.31495300
H	-7.25455900	1.72018700	-0.92291200
H	-7.92470700	2.05835200	0.66454800
C	-9.30351800	2.41383900	-0.96602600
H	-9.03807500	3.47068700	-1.08278500
H	-9.54323700	2.01692000	-1.96017300
H	-10.21775000	2.36374900	-0.36208500
C	-3.89290800	-4.28650900	3.24652700
H	-4.58241500	-5.13285700	3.35312500
H	-3.70346000	-4.17189800	2.17117400
C	-2.57421900	-4.60291500	3.96255200
H	-1.89405200	-3.74499400	3.86599200

H	-2.76689200	-4.72157100	5.03837500
C	-1.88830700	-5.86330500	3.42542400
H	-2.53123700	-6.74453700	3.54168200
H	-1.65357000	-5.76247100	2.35865000
H	-0.94972300	-6.06376600	3.95487200
C	-2.67594700	-0.88344300	-0.77621300
C	-1.87911000	0.04351800	-0.76097700
C	-1.00948000	1.08395300	-0.70459900
C	-0.22288400	2.01816700	-0.65798100
C	0.68680800	3.10799900	-0.59050100
C	0.60627700	4.04198100	0.46367600
C	1.68435200	3.27298600	-1.57395100
C	1.49928000	5.10740000	0.52703300
H	-0.16022800	3.91696600	1.22202300
C	2.57329200	4.34122600	-1.50035700
H	1.74860800	2.55591500	-2.38643900
C	2.48449200	5.26102400	-0.45208800
H	1.42744300	5.82065800	1.34361000
H	3.33802000	4.45745400	-2.26353300
H	3.18012400	6.09398000	-0.39848200

TS-4a

C	-3.90921400	2.10112400	-0.00636700
C	-2.63784700	1.50436300	-0.03879300
C	-1.49576100	2.29820400	-0.09511500
C	-1.64490300	3.68515500	-0.11847500
C	-2.90830400	4.28819100	-0.08625800
C	-4.05681300	3.48610700	-0.02951600
H	-4.79469100	1.47256000	0.03744600

H	-2.55019800	0.42180500	-0.01982400
H	-0.49818600	1.86994800	-0.12150600
H	-5.04014700	3.94533900	-0.00452900
C	-0.54603300	4.66920000	-0.17729700
C	-2.90484500	5.75122800	-0.11646700
C	-3.80122300	6.65358400	-0.09946800
C	-1.12089400	6.04519400	-0.18752400
C	-0.72890500	7.25160200	-0.23635700
O	0.64471600	4.41301400	-0.21160500
C	-4.85938800	7.47805300	-0.06472900
C	-5.84305900	8.21680200	-0.02707900
C	-6.97380100	9.06616400	0.01792900
C	-7.49699100	9.50175000	1.25644200
C	-7.59935600	9.49710800	-1.17379100
C	-8.60628900	10.33974700	1.29456900
H	-7.02165200	9.17343000	2.17550200
C	-8.70821800	10.33502500	-1.12140600
H	-7.20273400	9.16568700	-2.12837700
C	-9.21646000	10.76029600	0.10934000
H	-8.99783200	10.66704500	2.25392500
H	-9.17917200	10.65878500	-2.04561100
H	-10.08266000	11.41499700	0.14461600
C	-1.32059100	8.56403600	-0.24088400
H	-1.12153000	9.09539800	-1.18215800
H	-2.42750600	8.31631500	-0.24321800
C	-0.99958800	9.46826600	0.96542100
H	0.07232100	9.70321500	0.96197400
H	-1.19543000	8.91112200	1.89029700

C	-1.81990500	10.76372300	0.95228900
H	-2.89008600	10.51486000	0.94354400
H	-1.62462600	11.30704300	0.01678300
C	-1.51318800	11.67352000	2.14590500
H	-0.45543300	11.96326000	2.16306500
H	-2.10989000	12.59180000	2.10901400
H	-1.73405800	11.17045800	3.09517900

4. Figures for DFT calculations

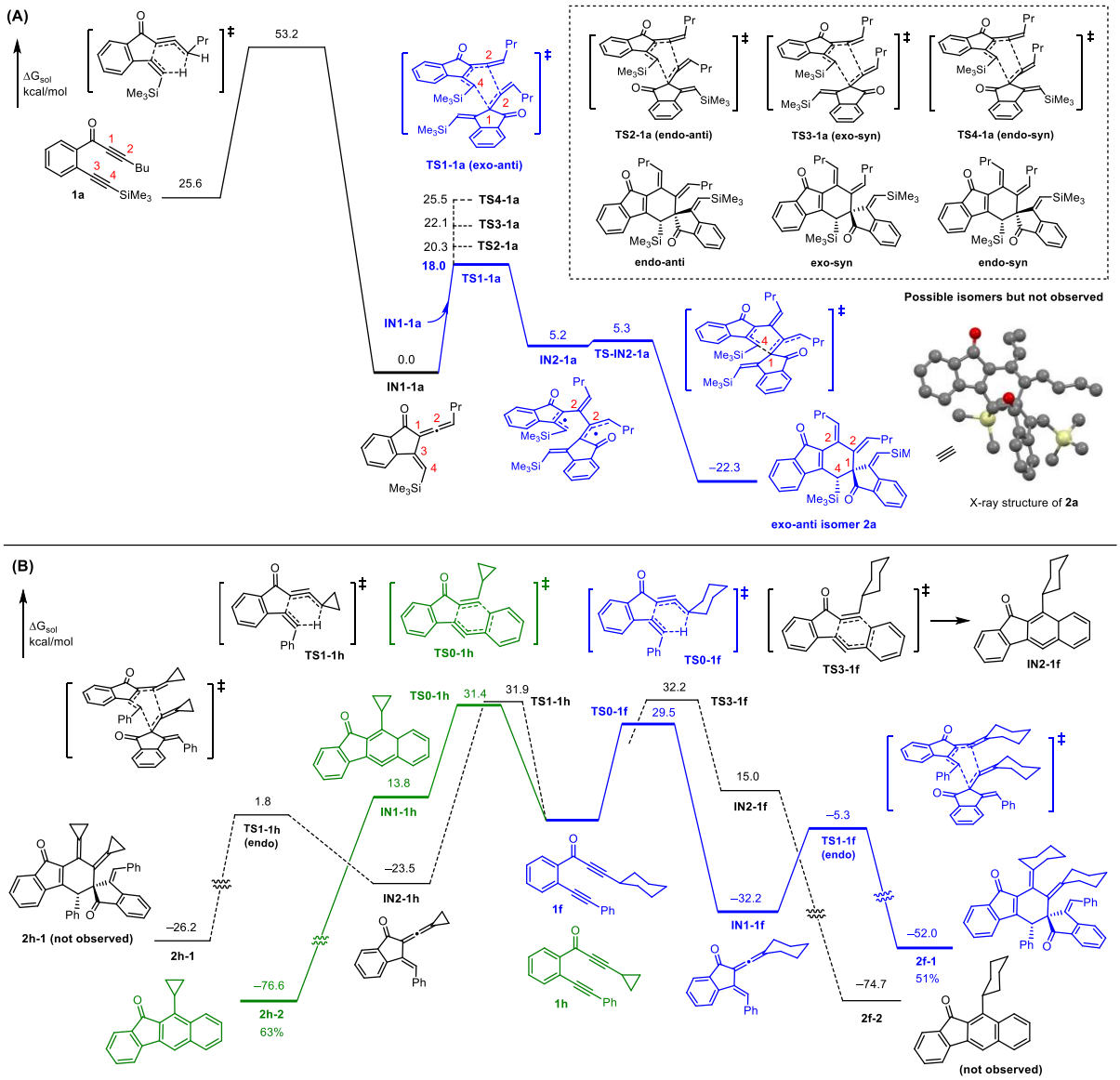


Figure 1. (A) DFT calculations for chemo-, regio-, and stereoselectivity in the Diels-Alder reaction of ene-allene **IN1-1a**, and (B) mode selectivity of alkynyl ketones **1f/1h** (Optimization: B3LYP/6-31G(d); Solvation: M06/6-311+G(d,p))

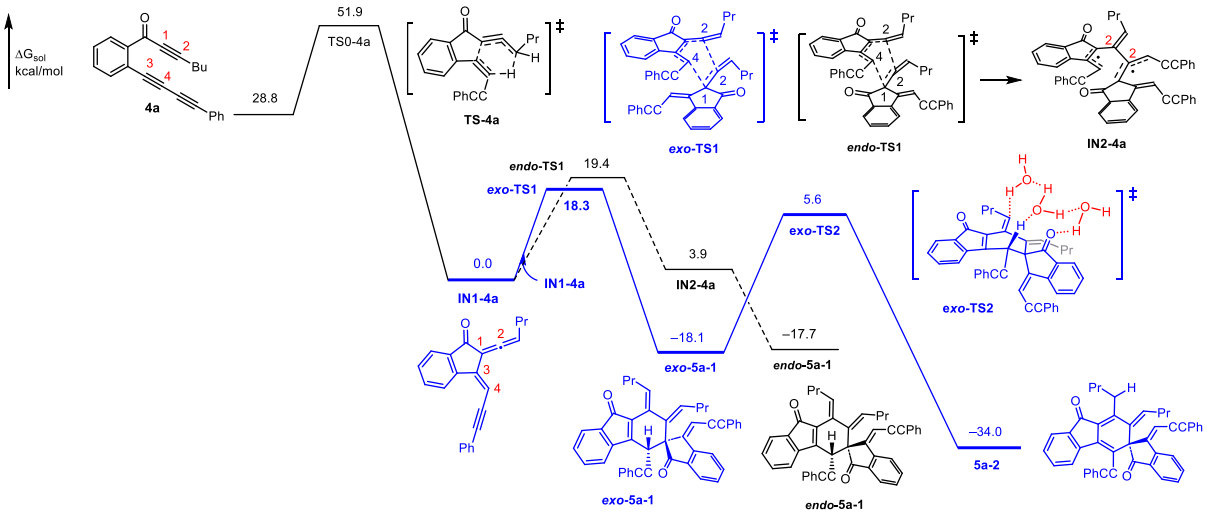


Figure 2. DFT calculations for chemoselectivity and regioselectivity in the Diels-Alder reaction of enyne-allene **IN1-4a** and 1,5-H shift (Optimization: B3LYP/6-31G(d); Solvation: M06/6-311+G(d,p))