

Supporting information

For

Reaction of Silylallenes with Triplet Molecular Oxygen

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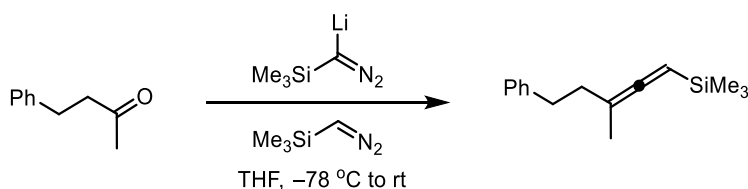
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General Information


Reactions were carried out in oven or flame-dried glassware unless otherwise noted. Compounds were purchased from Aldrich or Acros or TCI America or Oakwood or GFS or Strem chemicals unless otherwise noted. Dichloromethane (DCM) were distilled over calcium hydride (CaH₂) under nitrogen atmosphere. Flash chromatography was performed using silica gel 60 Å (32–63 mesh) purchased from Silicycle Inc. Analytical thin layer chromatography (TLC) was performed on 0.25 mm E. Merck precoated silica gel 60 (particle size 0.040–0.063 mm). Yields refer to chromatographically and spectroscopically pure compounds unless otherwise stated. ¹H NMR and ¹³C NMR spectra were recorded on a Bruker DRX-500 spectrometer. Multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), qn (quintet), sext (sextet), m (multiplet), b (broad), and app (apparent). ¹H NMR signals that fall within a ca. 0.3 ppm range are generally reported as a multiplet, with a single chemical shift value corresponding to the 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 in the University of Illinois at Urbana-Champaign. Electron impact (EI) mass spectra and Chemical Ionization (CI) mass spectra were obtained using a Micromass 70-VSE in the University of Illinois at Urbana-Champaign.

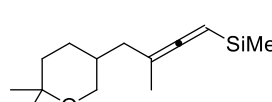
Experimental Details and Characterization Data

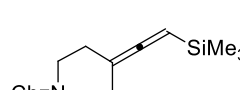
General procedure for preparation of silyllallenes



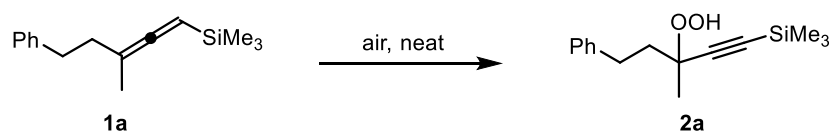
Silyllallenes **1a**, **1b**, **1d–1f**, and **3a–3j** were prepared by published three component coupling involving ketones, lithiated trimethylsilyl diazomethane and trimethylsilyl diazomethane.^{1–4} The characterization data of compounds **1a**, **1b**, **1d**, **1f**, **3a**, **3b** and **3d–3j** were found in reference 1–4. Other allenes **1c**, **1g**, **1h**, and **3e'** were synthesized according to reported procedures in reference 2–4. The characterization data of compounds **1g**, **1h**, and **3e'** were found in reference 2 and 4.

 **1b**: ¹H NMR (501 MHz, CDCl₃) δ 7.43 (d, $J = 7.4$ Hz, 2H), 7.38 (t, $J = 7.7$ Hz, 2H), 7.22 (t, $J = 7.2$ Hz, 1H), 5.40 (dd, $J = 7.0, 3.4$ Hz, 1H), 2.14 (d, $J = 3.4$ Hz, 3H), 0.24 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 210.5, 137.7, 128.4, 125.7, 125.1, 93.7, 85.5, 16.1, -0.5.

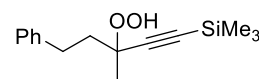
 **1e**: ¹H NMR (501 MHz, CDCl₃) δ 4.81 (m, 1H), 3.68 (m, 1H) 3.29 (m, 1H) 1.86-1.62 (m), 1.53-1.41 (m), 1.33-1.26 (m), 1.20 (s, 3H), 1.18 (s, 3H), 0.06 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 209.0, 209.0, 89.2, 81.9, 81.8, 71.1, 66.8, 66.7, 36.5, 36.4, 36.1, 35.9, 33.9, 33.9, 31.6, 30.5, 30.2, 22.7, 22.5, 22.3, 18.2, 18.1, 14.1, -0.7.; HRMS (ESI) calcd for C₄₉H₅₀NO₂SSi₂[M+H]⁺: 772.3101, found 772.3089.

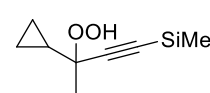
 **3c**: ¹H NMR (501 MHz, CDCl₃) δ 7.37-7.30 (m, 5H), 5.14 (s, 2H), 4.92-4.90 (m, 1H), 3.68-3.66 (m, 2H), 3.42-3.37 (m, 2H), 0.09 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 205.7, 155.2, 136.9, 128.5, 127.9, 90.8, 82.7, 67.1, 45.3, 30.0, 30.0, -0.8; HRMS (ESI) calcd for C₁₈H₂₅NO₂SiNa [M+Na]⁺: 338.1552, found 338.1552.

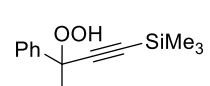
General procedure for autooxidation of silyllallenes

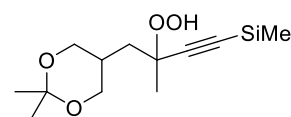


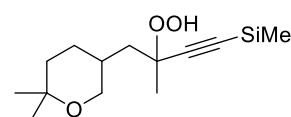
Silyllallene **1a** (23 mg, 0.1 mmol) under air was stirred for 48 h (monitored by TLC and ^1H NMR). After the starting material disappearance, the crude material was purified by silica gel column chromatography (Hexanes/EtOAc = 98 : 2) to provide peroxide **2a** (26.9 mg, > 98 % yield).

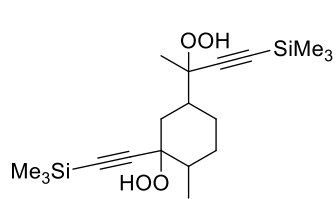
 **2a:** ^1H NMR (501 MHz, CDCl_3) δ 7.93 (br, HOO-, 1H), 7.31 (t, $J = 7.5$ Hz, 2H), 2.81 (t, $J = 8.8$ Hz, 2H), 2.16-2.01 (m, 2H), 1.56 (s, 3H), 0.24 (s, 9H); ^{13}C NMR (126 MHz, CDCl_3) δ 141.8, 128.5, 128.4, 126.0, 105.3, 90.7, 80.9, 40.8, 30.7, 24.5, 0.0; HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{22}\text{O}_2\text{SiNa}[\text{M}+\text{Na}]^+$: 285.1287, found 285.1283.

 **2b:** ^1H NMR (501 MHz, CDCl_3) δ 7.75 (s, HOO-, 1H), 1.04 (m, 1H), 0.88 (m, 1H), 0.07 (m, 1H), 0.41 (m, 1H), 0.17 (s, 9H); ^{13}C NMR (126 MHz, CDCl_3) δ 102.2, 91.0, 83.8, 29.7, 25.4, 17.2, 2.9, 1.5, -0.01; HRMS (ESI) calcd for $\text{C}_{10}\text{H}_{18}\text{O}_2\text{SiNa} [\text{M}+\text{Na}]^+$: 221.0974, found 221.0979.

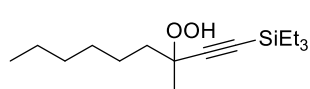
 **2c:** ^1H NMR (501 MHz, CDCl_3) δ 8.03 (br, HOO-, 1H), 7.66 (d, $J = 7.3$ Hz, 2H), 7.41 (t, $J = 7.4$ Hz, 2H), 7.36 (t, $J = 7.1$, 1H), 1.76 (s, 3H), 0.28 (s, 9H); ^{13}C NMR (126 MHz, CDCl_3) δ 141.0, 128.5, 128.4, 128.3, 127.7, 126.0, 125.0, 104.4, 92.5, 83.0, 33.4, 28.7, 0.0; HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{18}\text{O}_2\text{SiNa} [\text{M}+\text{Na}]^+$: 257.0974, found 257.0979.

 **2d:** ^1H NMR (501 MHz, CDCl_3) δ 8.19 (s, HOO-, 1H), 3.99 (m, 2H), 3.70-3.62 (m, 2H), 2.10 (m, 1H), 1.78-1.64 (m, 2H), 1.51 (s, 3H), 1.42 (s, 3H), 1.41 (s, 3H), 0.18 (s, 9H); ^{13}C NMR (126 MHz, CDCl_3) δ 104.9, 97.9, 90.8, 80.3, 65.1, 65.1, 37.5, 31.1, 25.9, 25.1, 22.1, -0.1; HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{27}\text{O}_4\text{Si}[\text{M}+\text{H}]^+$: 287.1679, found 287.1688.

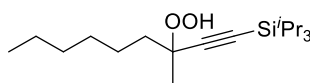
 **2e:** (mixture of two diastereomers) ^1H NMR (501 MHz, CDCl_3) δ 8.26 (s, HOO-, 1H), 8.15 (s, HOO-, 1H), 3.79-3.73 (m, 1H), 3.37-3.33 (m, 1H), 1.85-1.79 (m, 2H), 1.69-1.35 (m, 8H), 1.20 (s, 3H), 1.17 (s, 3H), 0.17 (s, 9H); ^{13}C NMR (126 MHz, CDCl_3) δ 105.7, 105.5, 90.4, 90.2, 80.6, 80.6, 71.1, 66.7, 41.0, 40.9, 35.7, 32.1, 32.1, 29.7, 27.6, 27.5, 25.2, 25.0, 22.9, 22.9, -0.1; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{27}\text{O}_3\text{Si}[\text{M}-\text{H}]^+$: 307.1729, found 307.1719.



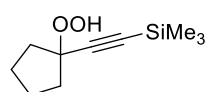
2f: (mixture of four diastereomers) $^1\text{H NMR}$ (501 MHz, CDCl_3) δ 7.78 (s, HOO-, 1H), 7.73 (s, HOO-, 1H), 7.72 (s, HOO-, 1H), 7.70 (s, HOO-, 1H), 7.68 (s, HOO-, 1H), 7.67 (s, HOO-, 1H), 7.62 (s, HOO-, 1H), 2.75-2.54 (m), 2.29-1.56 (m), 1.48 (s, 3H), 1.40 (s, 3H), 1.41 (s, 3H), 1.43-1.13 (m), 1.08-1.06 (m), 0.99-0.97 (m), 0.19 (s), 0.18 (s) $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 105.8, 105.0, 104.6, 104.5, 104.4, 102.5, 94.1, 94.0, 91.6, 91.5, 91.4, 91.0, 90.0, 86.2, 86.2, 83.5, 83.4, 83.4, 83.2, 82.2, 82.2, 42.6, 42.4, 40.8, 40.7, 38.9, 38.6, 38.3, 37.2, 37.0, 35.5, 34.9, 31.8, 29.0, 28.9, 27.1, 26.7, 26.7, 26.2, 22.3, 22.1, 21.5, 21.0, 16.0, 0.2, 0.0, -0.2; **HRMS** (ESI) calcd for $\text{C}_{19}\text{H}_{35}\text{O}_4\text{Si}_2[\text{M}+\text{H}]^+$: 383.2074, found 383.2070.



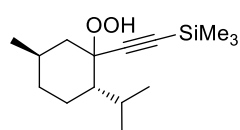
2g: $^1\text{H NMR}$ (501 MHz, CDCl_3) δ 7.71 (s, 1H), 1.79-1.73 (m, 1H), 1.69-1.62 (m, 1H), 1.52-1.41 (m, 5H), 1.35-1.25 (m, 6H), 0.99 (t, $J = 7.9$, 7.9 Hz, 9H), 0.88 (t, $J = 6.8$, 6.8 Hz, 3H), 0.61 (q, $J = 7.9$, 7.9, 7.9 Hz, 6H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 107.0, 87.5, 81.5, 38.8, 31.7, 29.4, 24.5, 24.3, 22.5, 14.1, 7.5, 4.4; **HRMS** (ESI) calcd for $\text{C}_{18}\text{H}_{32}\text{O}_2\text{SiNa} [\text{M}+\text{Na}]^+$: 331.2069, found 331.2066.



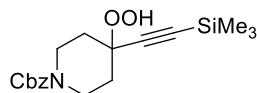
2h: $^1\text{H NMR}$ (501 MHz, CDCl_3) δ 7.70 (s, 1H), 1.80-1.74 (m, 1H), 1.69-1.62 (m, 1H), 1.53-1.42 (m, 5H), 1.36-1.24 (m, 6H), 1.11-1.02 (m, 21H), 0.88 (t, $J = 6.9$, 6.9 Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 107.7, 86.5, 81.6, 38.9, 31.7, 29.4, 24.6, 24.4, 22.5, 18.6, 4.1, 11.1; **HRMS** (ESI) calcd for $\text{C}_{19}\text{H}_{38}\text{O}_2\text{SiNa} [\text{M}+\text{Na}]^+$: 349.2539, found 349.2533.



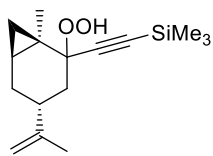
4a: $^1\text{H NMR}$ (501 MHz, CDCl_3) δ 7.99 (s, HOO-, 1H) 2.16-2.11 (m, 2H), 1.92-1.88 (m, 2H), 1.73-1.71 (m, 4H), 0.18 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 105.8, 89.6, 87.9, 38.1, 24.1, 0.0; **HRMS** (EI) calcd for $\text{C}_{10}\text{H}_{18}\text{O}_2\text{Si}[\text{M}]^+$: 198.1076, found 198.1076.



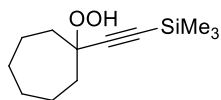
4b: $^1\text{H NMR}$ (501 MHz, CDCl_3) δ 7.58 (s, HOO-, 1H), 2.34-2.32 (m, 1H), 2.11 (m, 1H), 1.73-1.67 (m, 3H), 1.43-1.16 (m, 4H), 0.95-0.90 (m, 10H), 0.18 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 104.4, 93.8, 84.9, 49.5, 45.6, 34.7, 30.1, 26.3, 24.3, 23.7, 22.0, 18.2, -0.1; **HRMS** (EI) calcd for $\text{C}_{15}\text{H}_{28}\text{O}_2\text{Si} [\text{M}]^+$: 252.1910, found 252.1890.



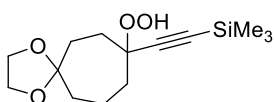
4c: $^1\text{H NMR}$ (501 MHz, CDCl_3) δ 8.01 (s, HOO-, 1H), 7.38-7.26 (m, 5H), 5.13 (s, 2H), 3.81 (br, 2H), 3.40-3.35 (m, 2H), 1.96 (s, 2H), 1.81 (s, 2H) 0.19 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 155.1, 136.7, 128.5, 128.1, 127.9, 103.7, 92.3, 79.3, 67.3, 40.6, 34.3, -0.1; **HRMS** (ESI) calcd for $\text{C}_{18}\text{H}_{25}\text{NO}_4\text{SiNa} [\text{M}+\text{Na}]^+$: 307.1451, found 307.1444.



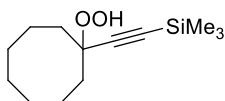
4d: $^1\text{H NMR}$ (501 MHz, CDCl_3) δ 7.83 (s, HOO-), 4.69 (d, $J = 11.2$ Hz, 2H), 2.13 (d, $J = 14.5$ Hz, 1H), 1.95-1.80 (m, 2H), 1.68 (s, 3H), 1.64-1.59 (m, 1H), 1.39 (dd, $J = 14.4, 12.4$ Hz, 1H), 1.28 (s, 3H), 1.08-0.98 (m, 1H), 0.85 (t, $J = 5.6$ Hz, 1H), 0.44-0.41 (m, 1H), 0.19 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 148.4, 109.3, 105.5, 91.6, 83.3, 38.7, 33.1, 28.8, 26.4, 21.6, 21.0, 20.3, 13.0 -0.1; **HRMS** (ESI) calcd for $\text{C}_{16}\text{H}_{26}\text{O}_2\text{SiNa}$ $[\text{M}+\text{Na}]^+$: 301.1600, found 301.1597.



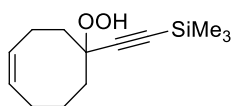
4e: $^1\text{H NMR}$ (501 MHz, CDCl_3) δ 7.87 (s, HOO-, 1H), 2.03-1.98 (m, 2H), 1.88-1.84 (m, 2H), 1.67-1.53 (m, 8H), 0.17 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 106.8, 90.1, 85.0, 37.4, 28.7, 22.5, 0.0; **HRMS** (ESI) calcd for $\text{C}_{12}\text{H}_{22}\text{O}_2\text{SiNa}$ $[\text{M}+\text{Na}]^+$: 249.1287, found 249.1298.



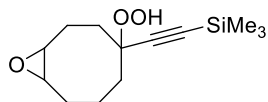
4f: $^1\text{H NMR}$ (501 MHz, CDCl_3) δ ; 7.85 (s, HOO-, 1H), 3.91 (m, 4H), 2.07-2.01 (m, 6H), 0.18 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 111.6, 106.3, 90.2, 84.1, 64.2, 39.4, 38.2, 31.5, 30.4, 18.1, 0.0; **HRMS** (ESI) calcd for $\text{C}_{14}\text{H}_{24}\text{NO}_4\text{Si}$: 307.1342, found 307.1338



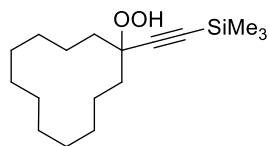
4g: $^1\text{H NMR}$ (501 MHz, CDCl_3) δ 7.71 (s, HOO-, 1H), 2.00 (m, 2H), 1.90 (m, 2H), 1.48-1.47 (m, 10H), 0.18 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 106.2, 90.3, 84.9, 32.7, 27.9, 24.9, 22.1, 0.0; **HRMS** (ESI) calcd for $\text{C}_{49}\text{H}_{50}\text{NO}_2\text{SSi}_2$ $[\text{M}+\text{H}]^+$: 772.3101, found 772.3105



4h: $^1\text{H NMR}$ (501 MHz, CDCl_3) δ 7.71 (s, HOO-, 1H), 5.80-5.75 (m, 1H), 5.57-5.51 (m, 1H), 2.49-2.31 (m, 2H), 2.22-2.15 (m, 2H), 2.03 (m, 1H), 1.84 (m, 3H), 1.68 (m, 1H), 1.56 (m, 1H), 0.21 (s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 131.1, 128.4, 104.2, 93.0, 85.9, 37.2, 31.6, 24.0, 23.8, 22.8, -0.1; **HRMS** (ESI) calcd for $\text{C}_{13}\text{H}_{22}\text{NO}_2\text{SiNa}$ $[\text{M}+\text{Na}]^+$: 261.1287, found 261.1294.



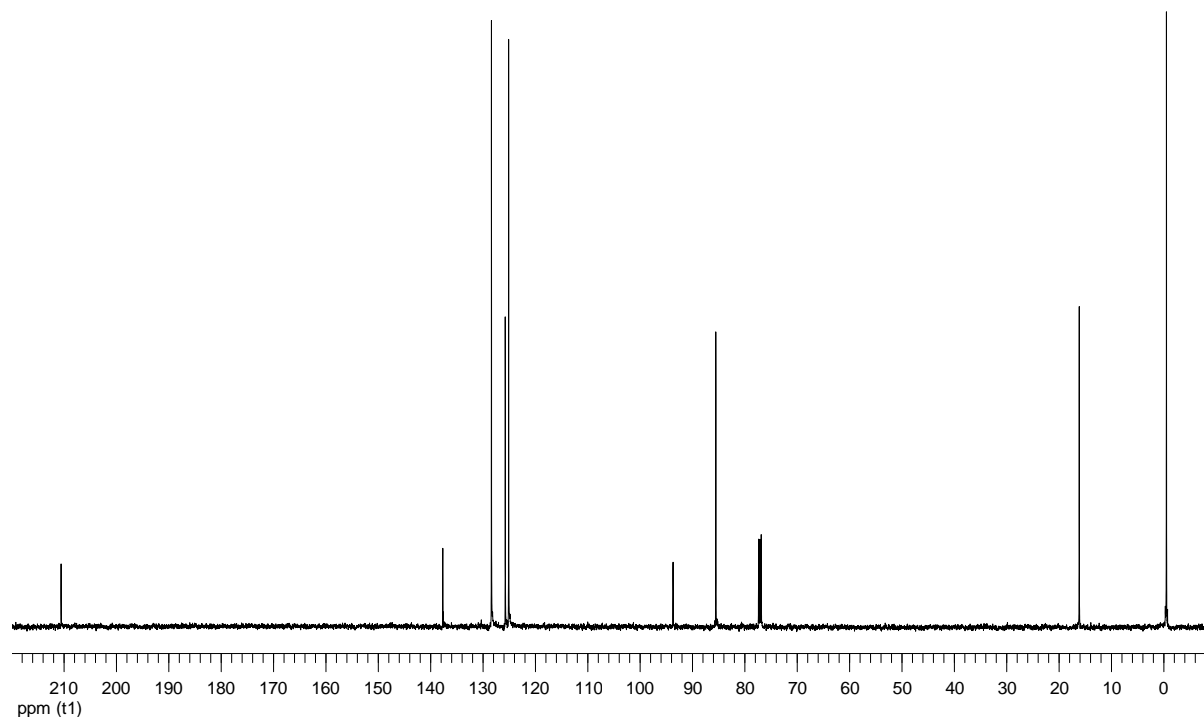
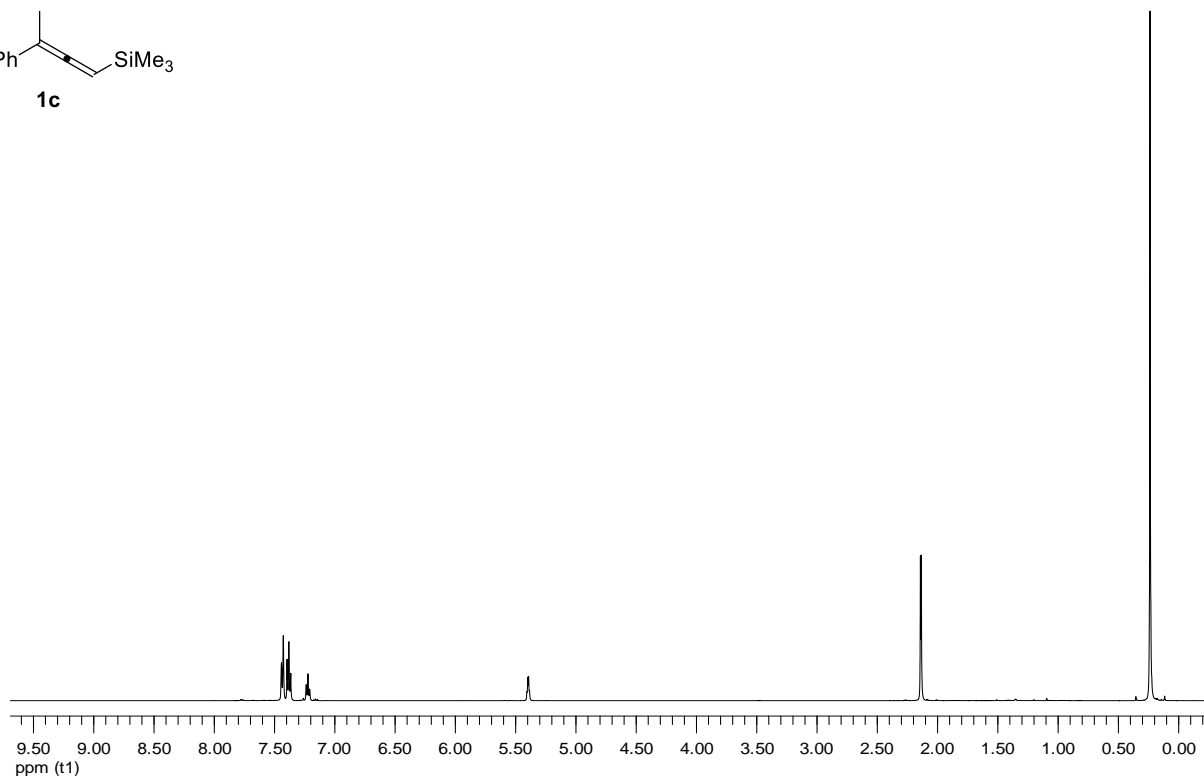
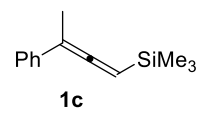
4i: $^1\text{H NMR}$ (501 MHz, CDCl_3) (mixture of diastereomers) δ 7.97 (s, HOO-, 1H), 3.08-2.92 (m, 1H), 2.92-2.87 (m, 1H), 2.30-2.00 (m, 5H), 1.94-1.41 (m, 5H), 0.18 (2s, 9H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 110.0, 105.0, 102.3, 93.8, 93.5, 85.3, 84.9, 56.9, 55.9, 55.1, 54.9, 35.2, 34.6, 34.3, 33.2, 28.3, 24.2, 23.6, 22.9, 21.9, 21.8, -0.2; **HRMS** (ESI) calcd for $\text{C}_{13}\text{H}_{23}\text{O}_3\text{Si}_2$ $[\text{M}+\text{H}]^+$: 255.1416, found 255.1412.

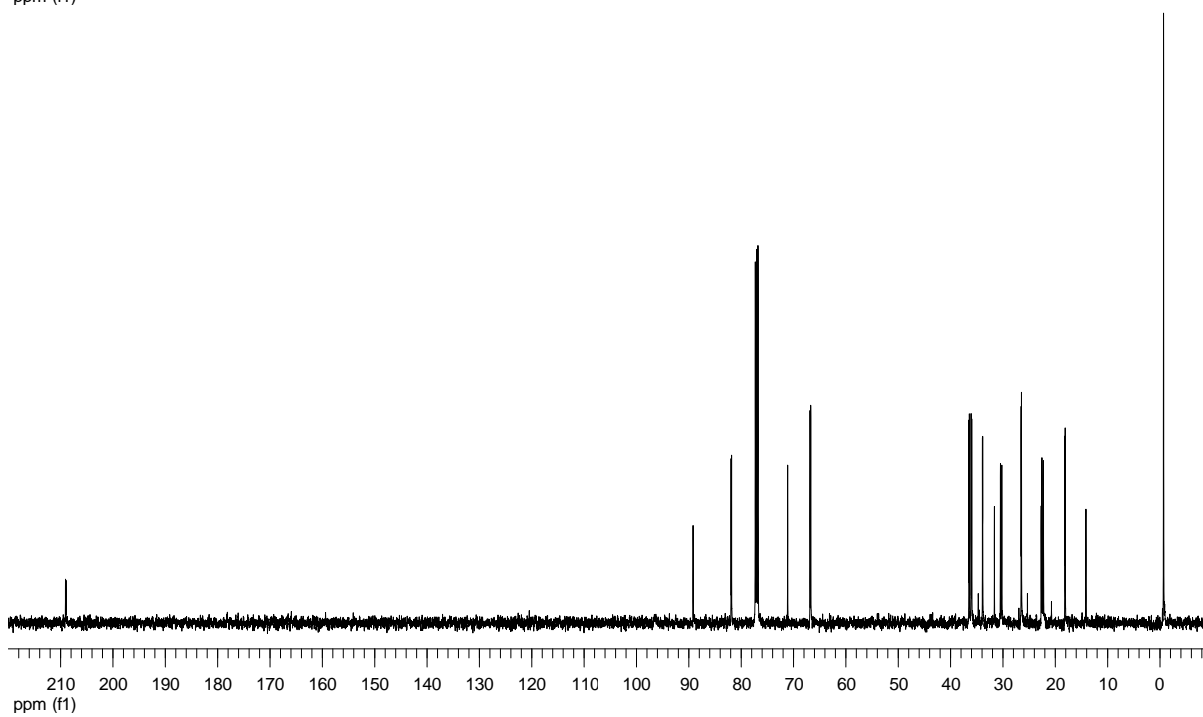
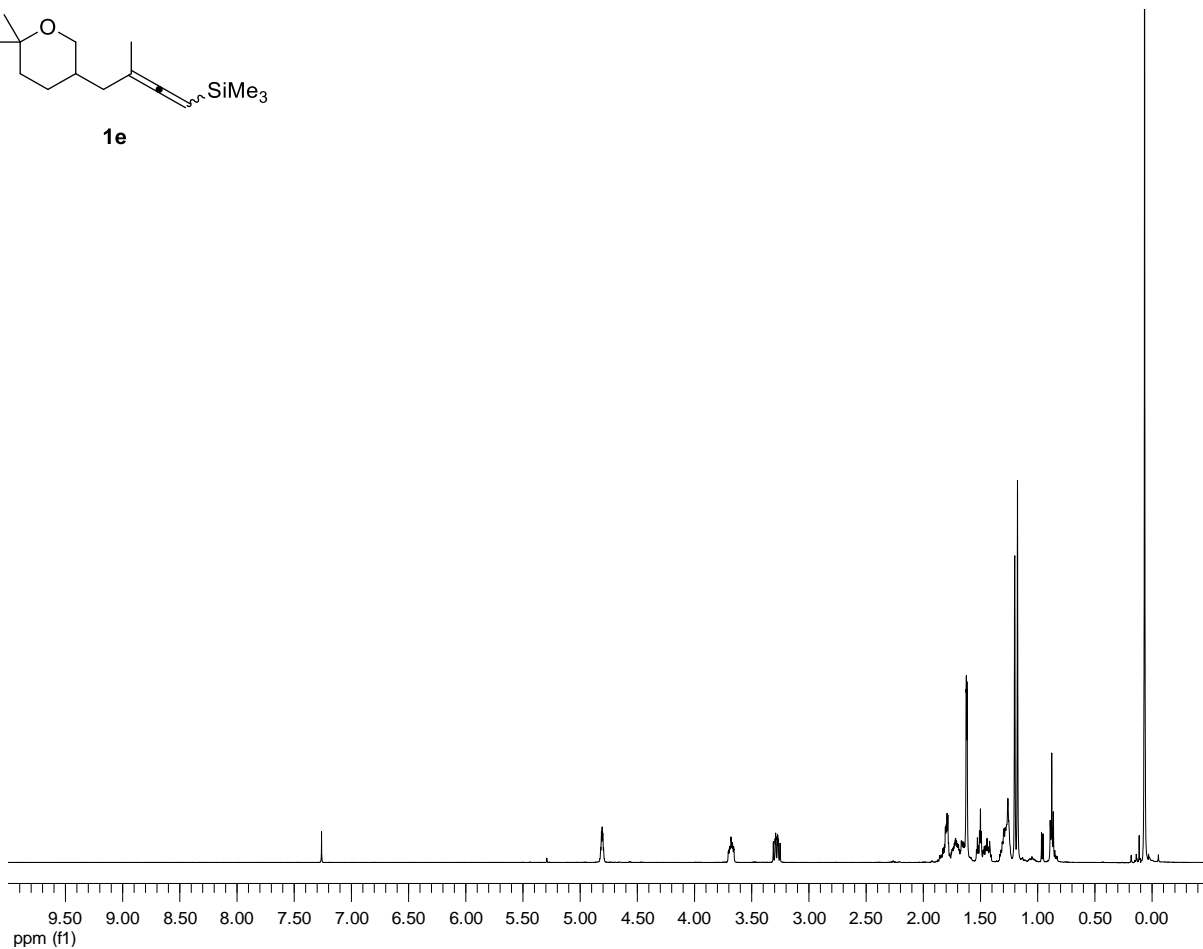
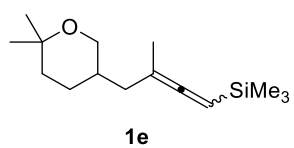


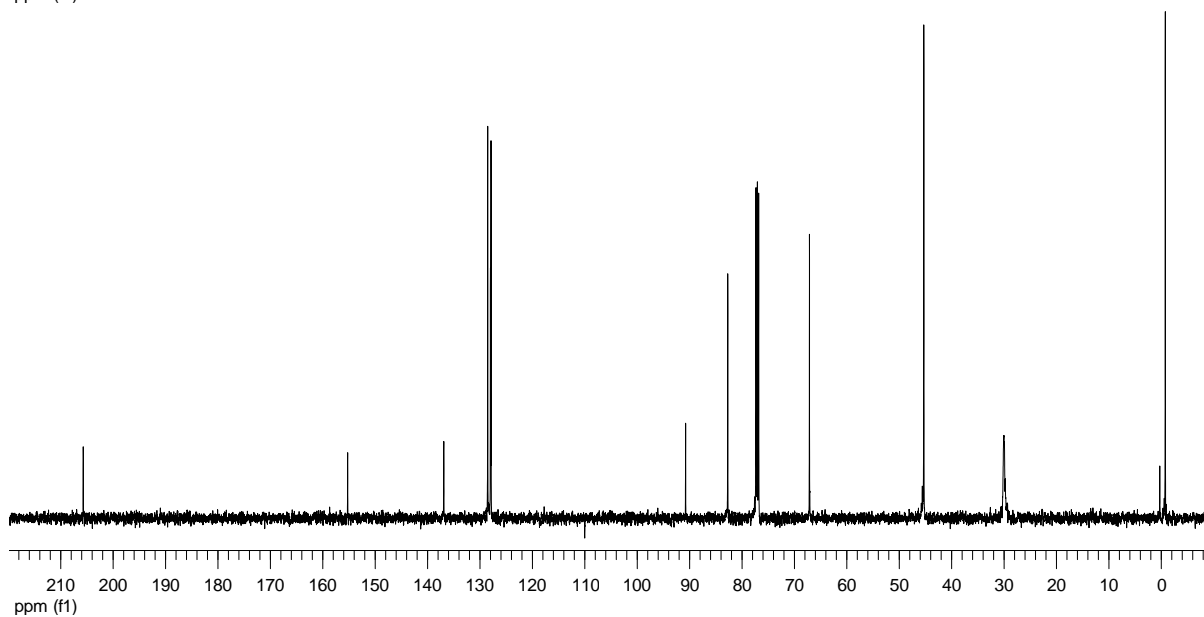
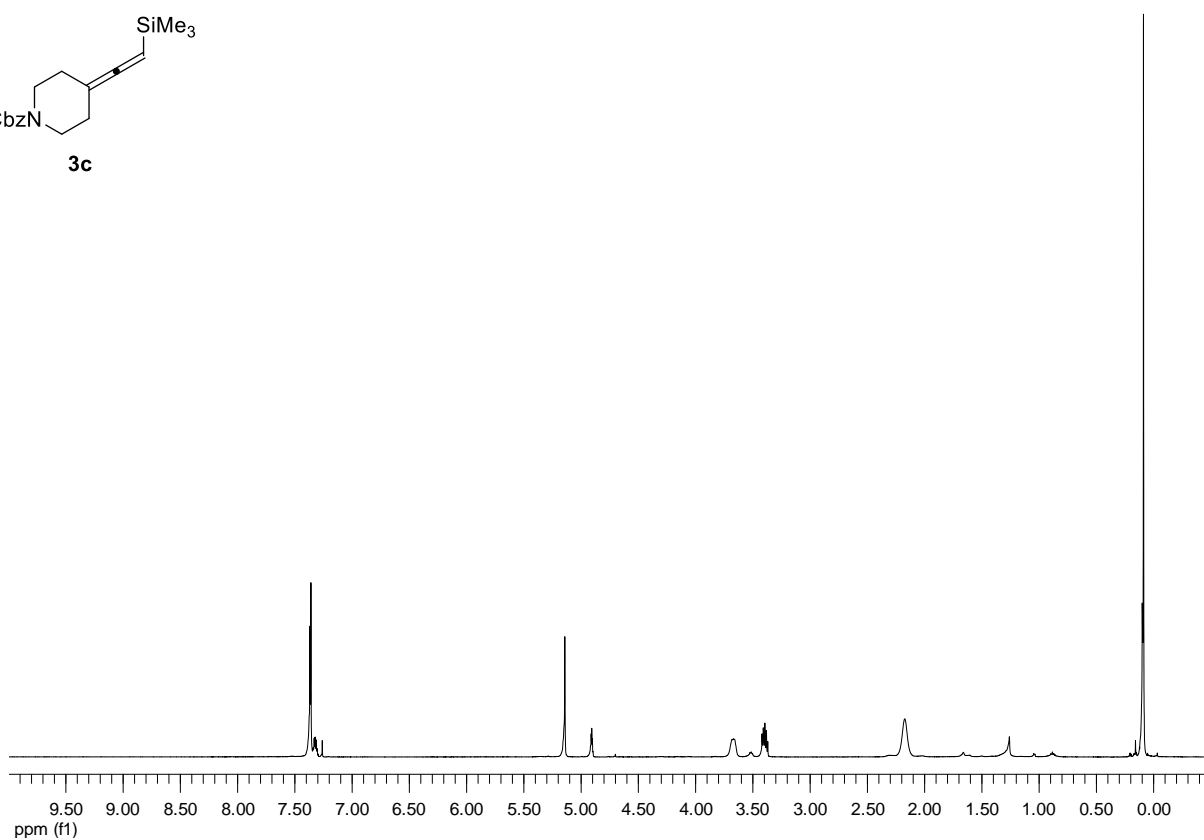
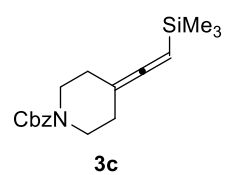
4j: $^1\text{H NMR}$ (501 MHz, CDCl_3) δ 7.74 (s, HOO-, 1H), 2.17 (s, 4H), 1.90-1.84 (m, 2H), 1.66-1.60 (m, 3H), 1.51-1.49 (m, 3H), 1.35 (m, 12H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 106.1, 90.3, 84.2, 31.0, 26.0, 22.4, 22.1, 19.3, 0.0; **HRMS** (ESI) calcd for $\text{C}_{17}\text{H}_{32}\text{O}_2\text{SiNa}[\text{M}+\text{Na}]^+$: 319.2069, found 319.2081.

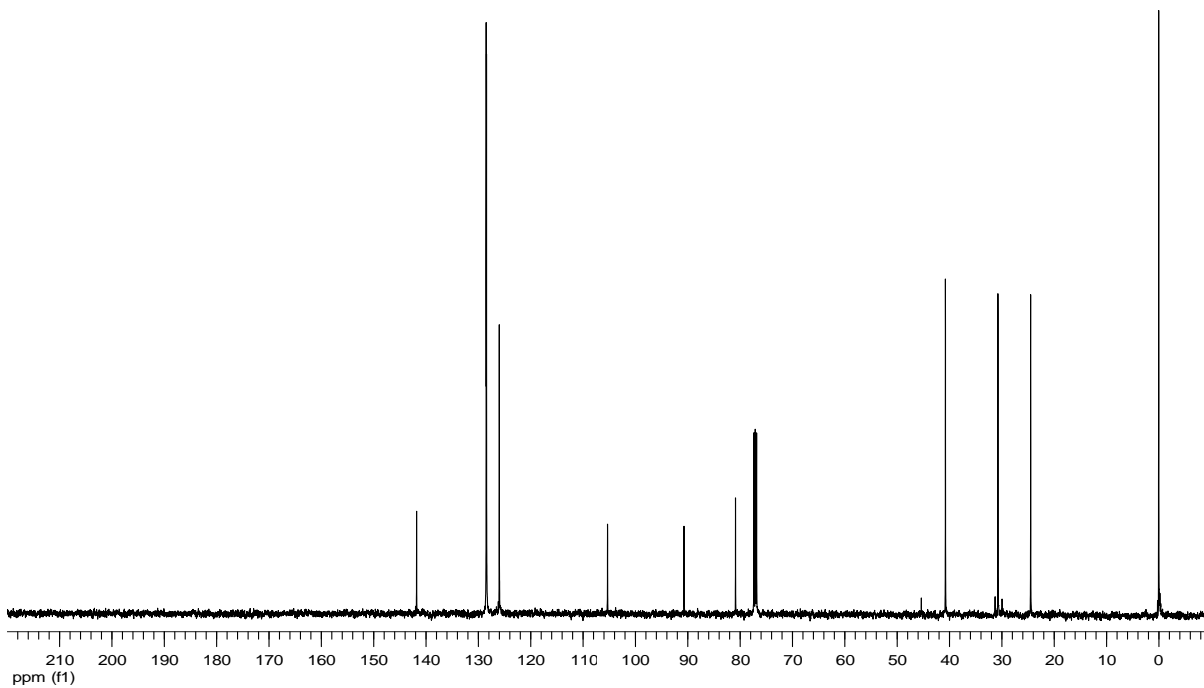
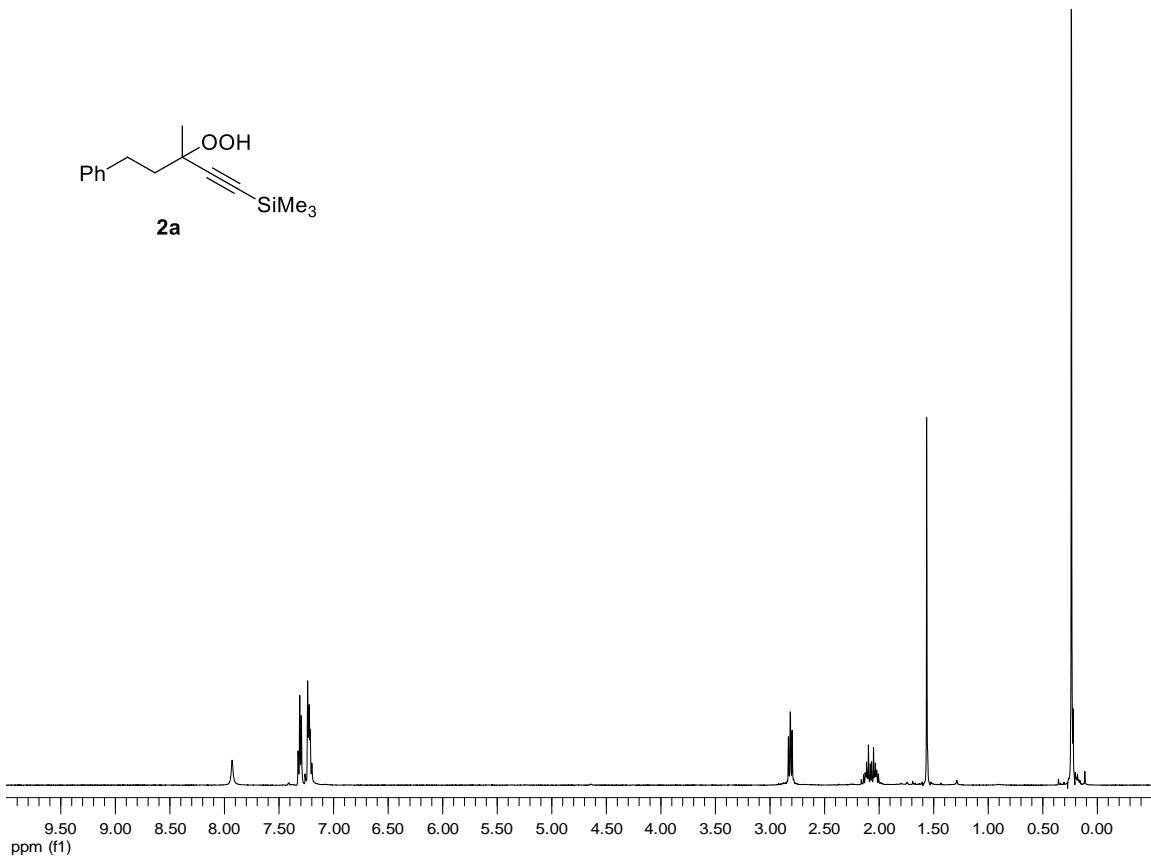
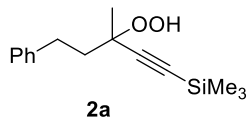
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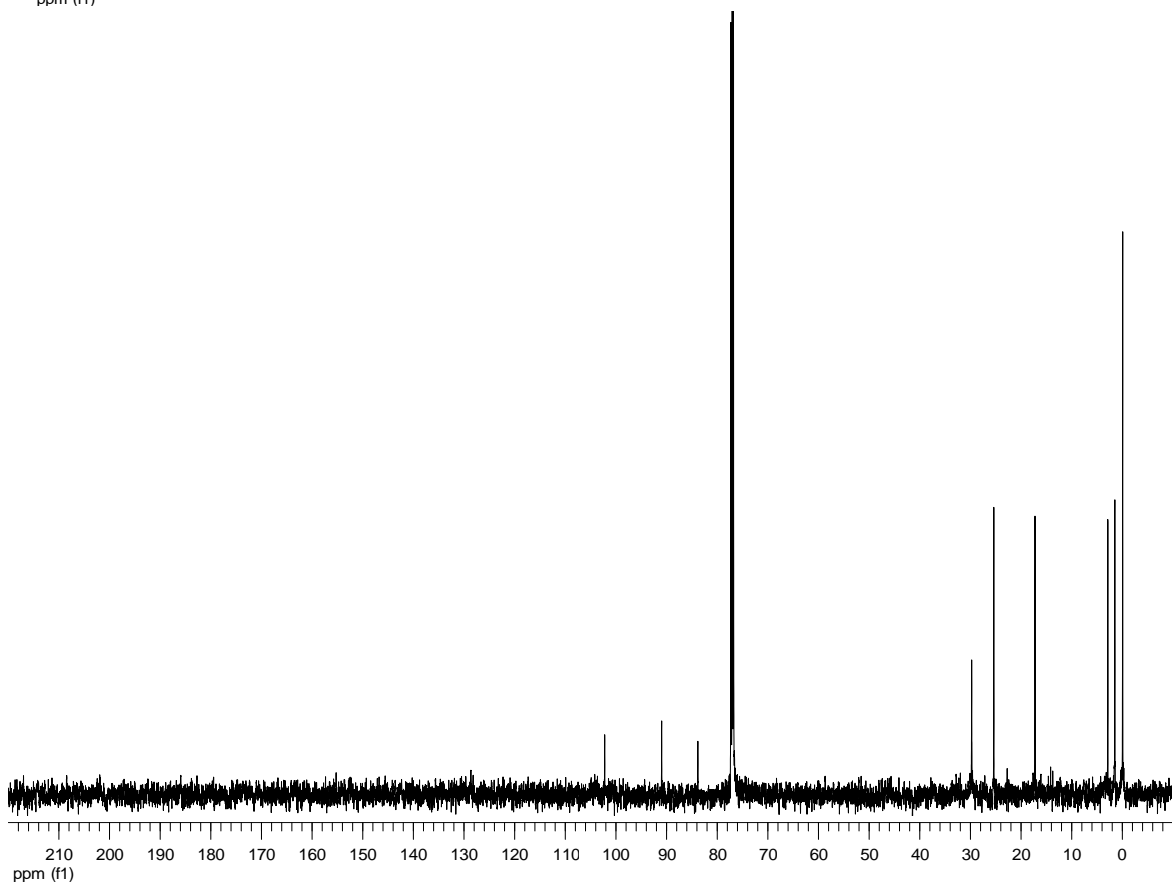
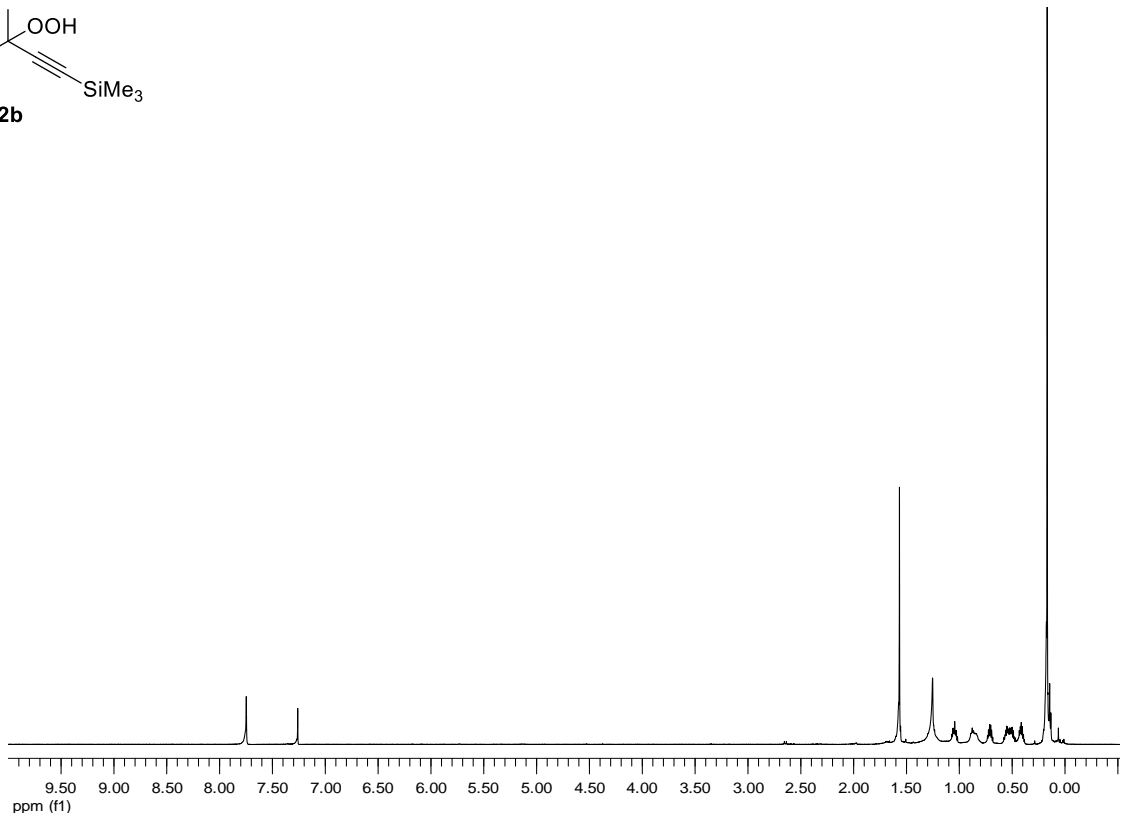
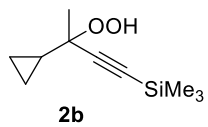
- (1) Zheng, J.-C.; Yun, S. Y.; Sun, C.; Lee, N.-K.; Lee, D. *J. Org. Chem.* **2011**, *76*, 1086.
- (2) Sabbasani, V. R.; Lee, D. *Org. Lett.* **2013**, *15*, 3954.
- (3) Sabbasani, V. R.; Lee, D. *Org. Lett.* **2015**, *17*, 4878.
- (4) Sabasani, V. R.; Huang, G.; Xia, Y.; Lee, D. *Chem. Eur. J.* **2015**, *21*, 17210.

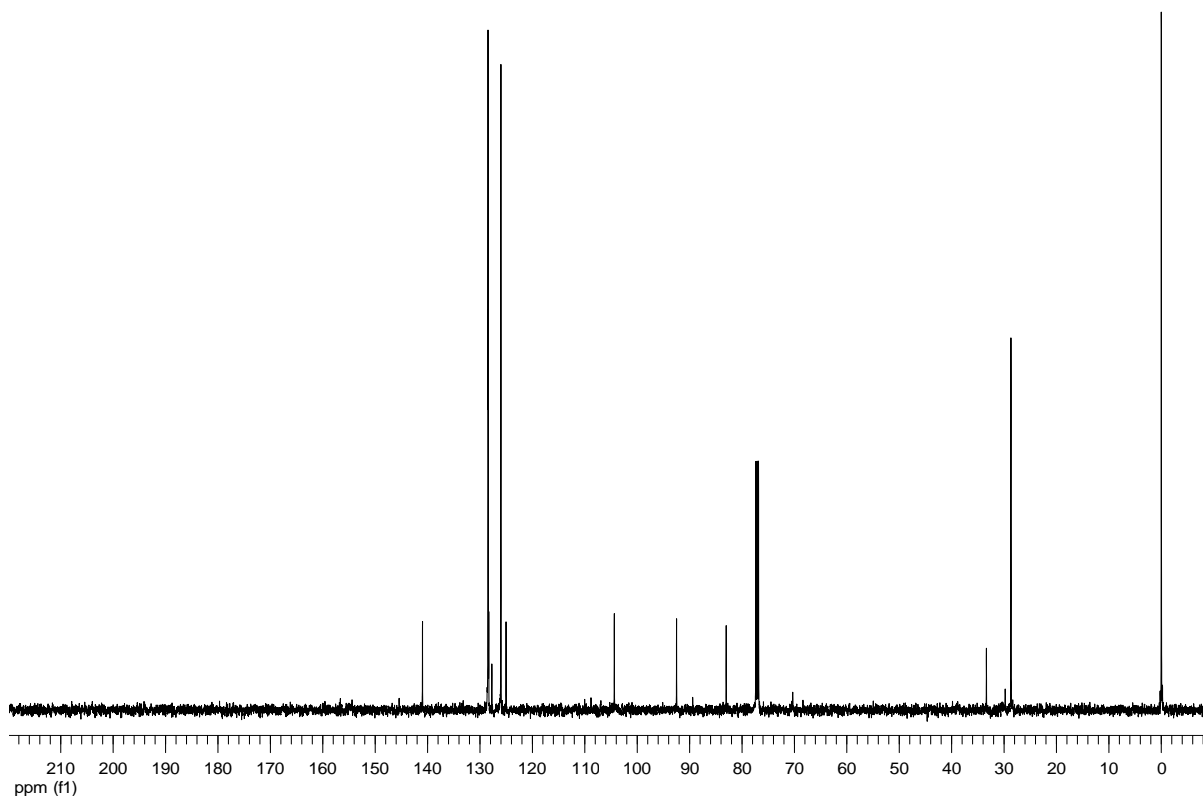
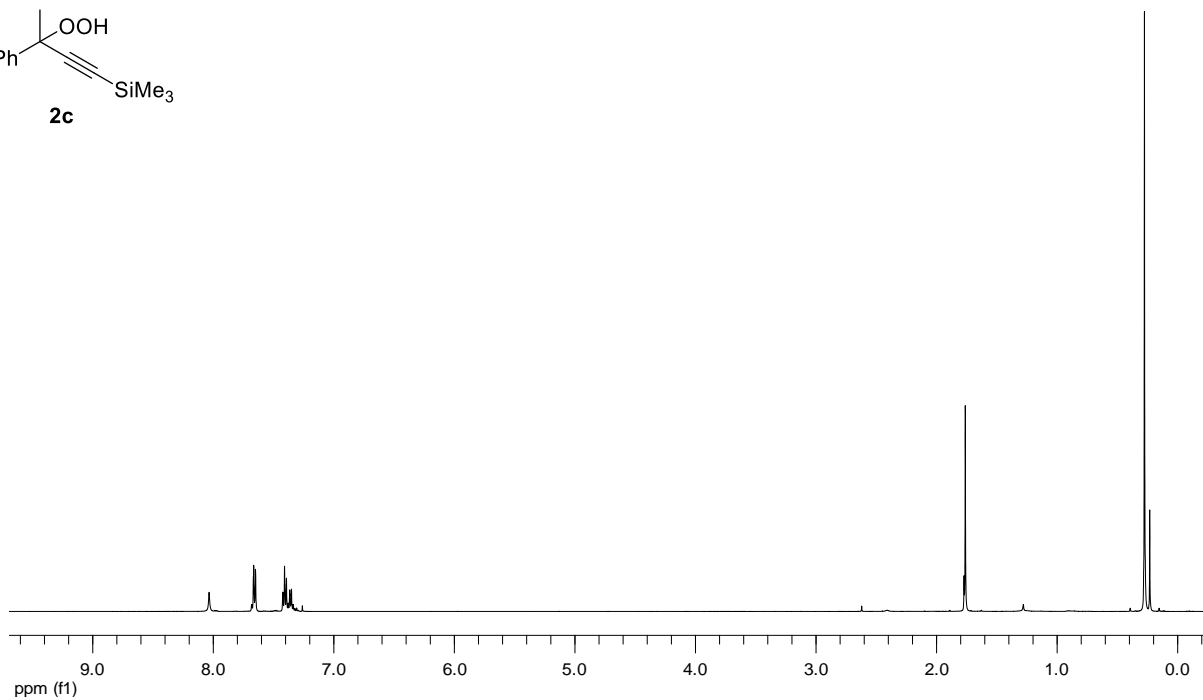
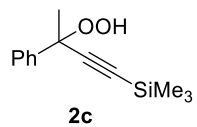


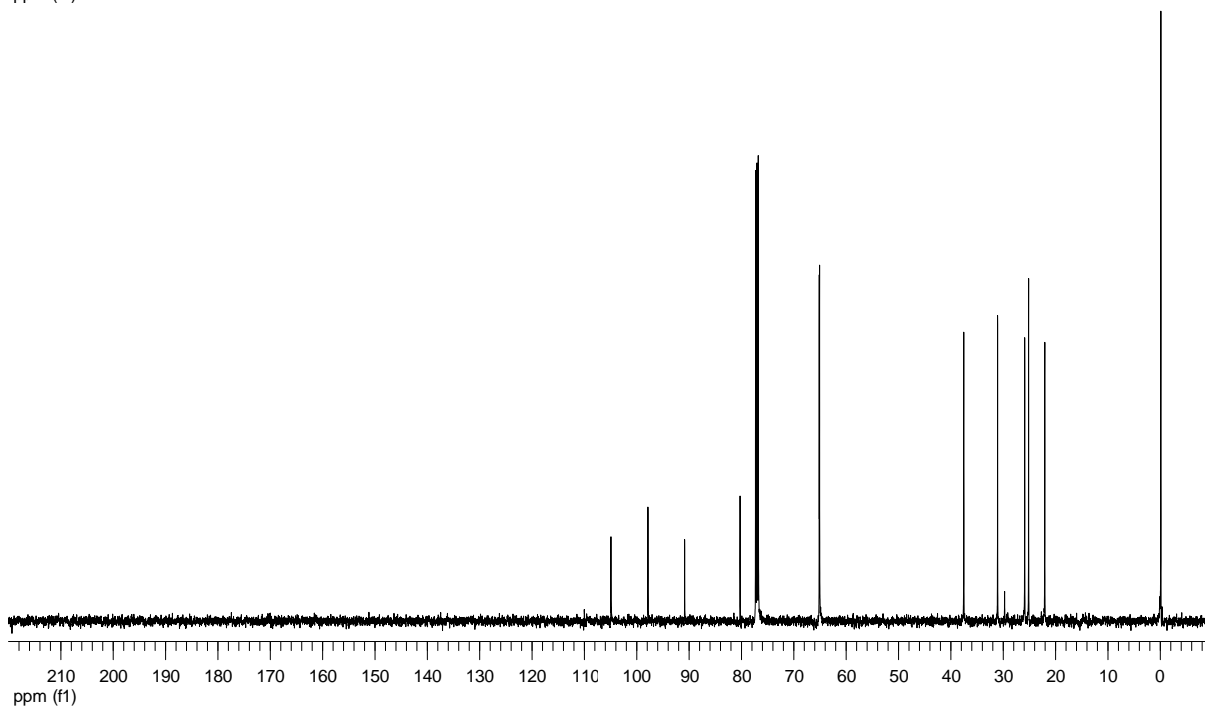
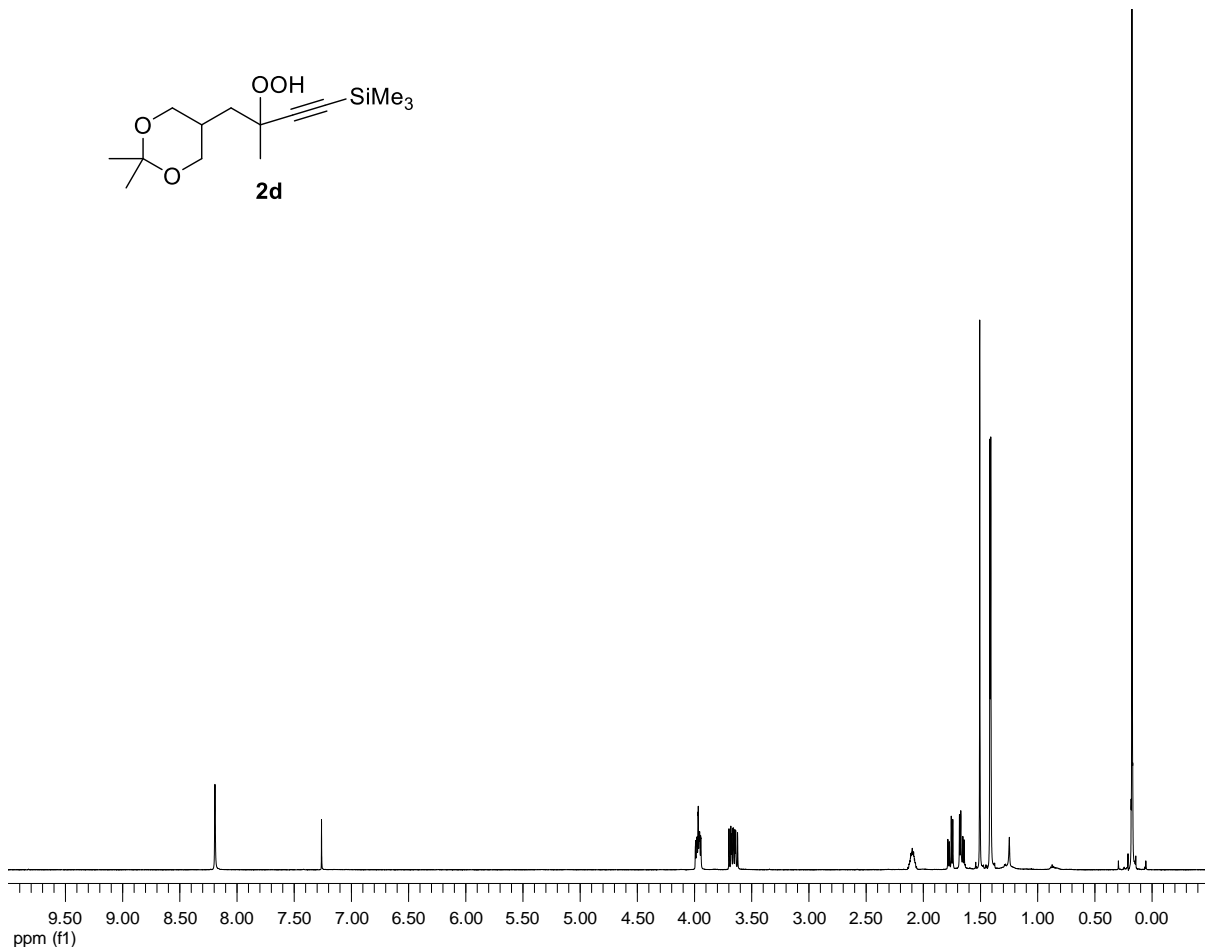
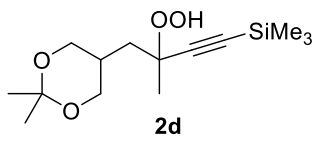


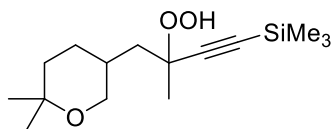




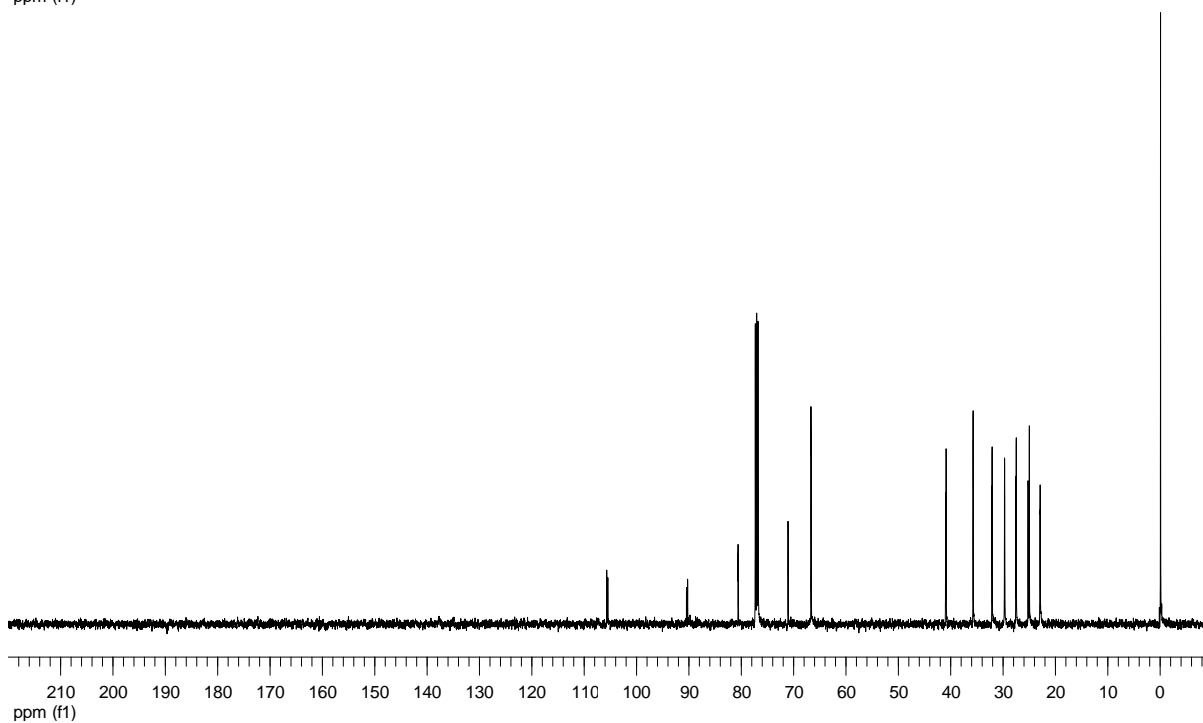
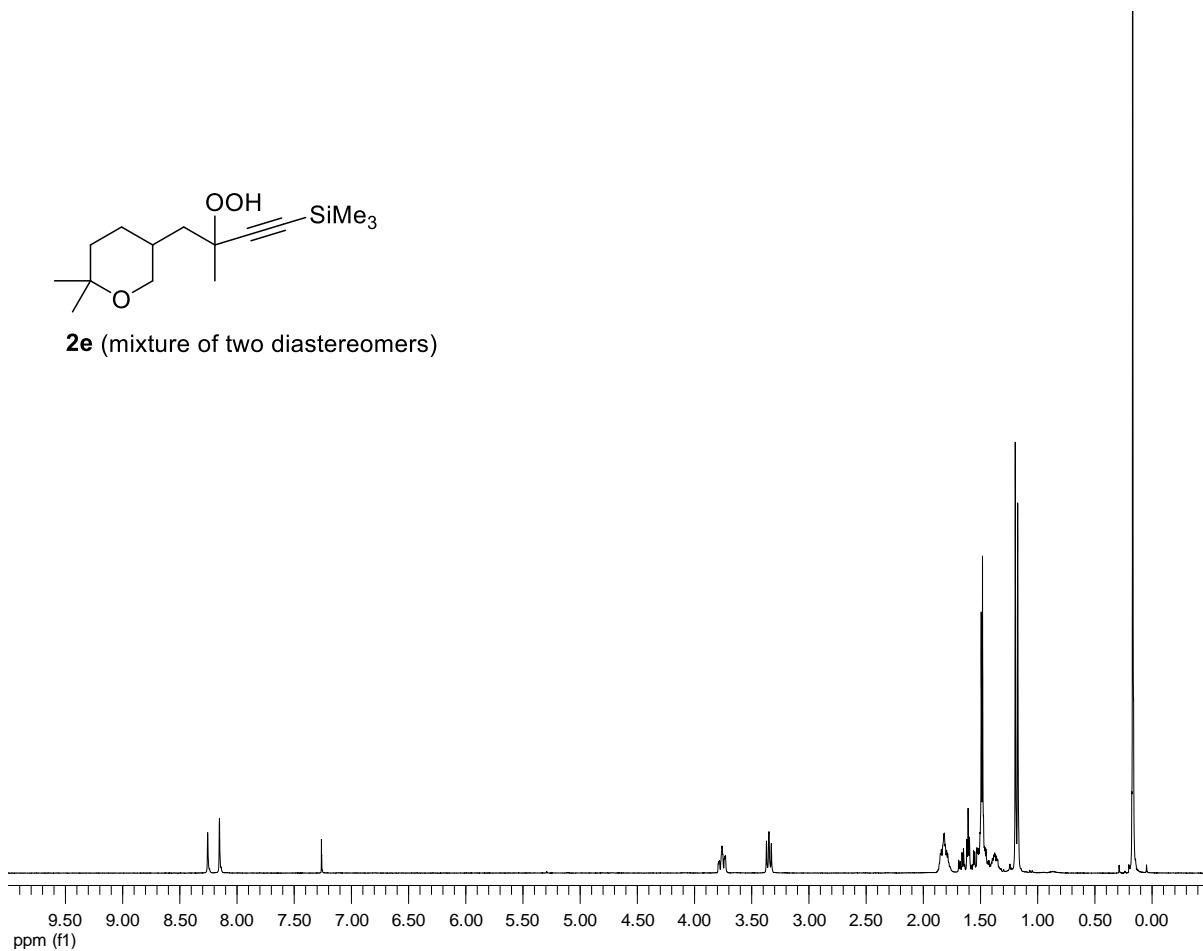


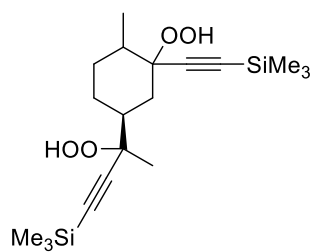




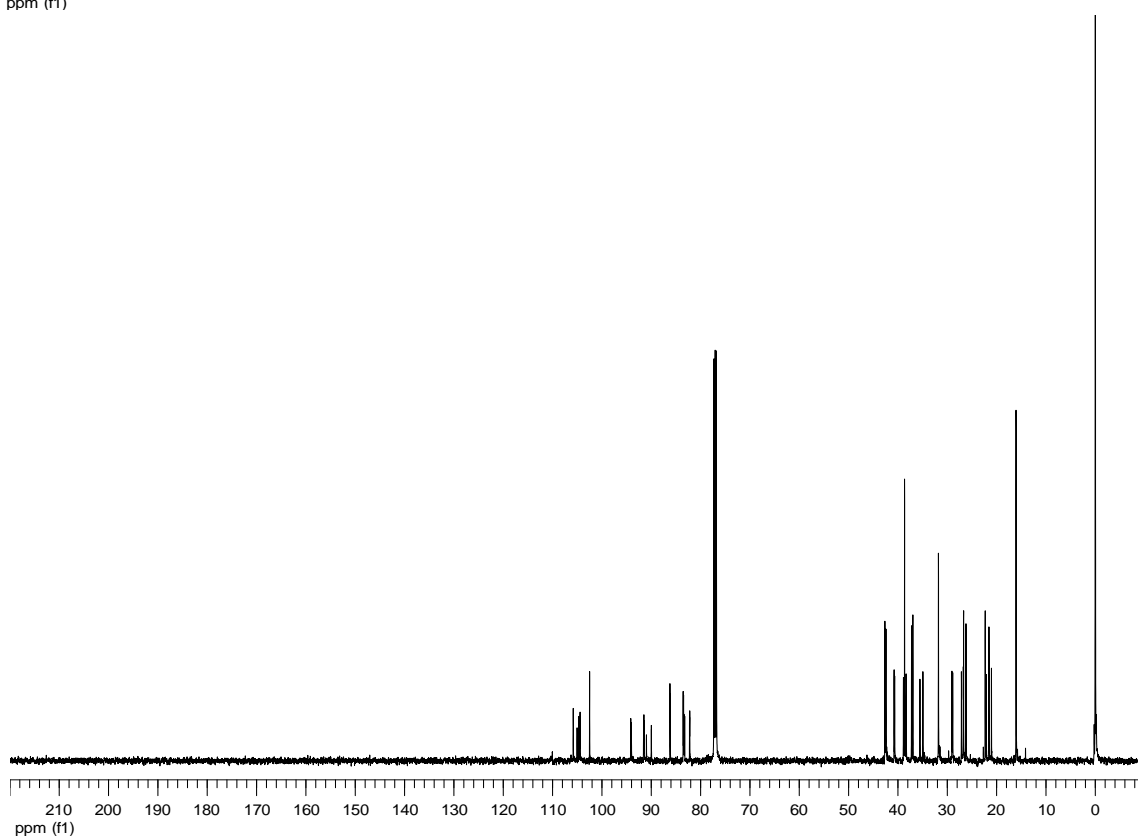
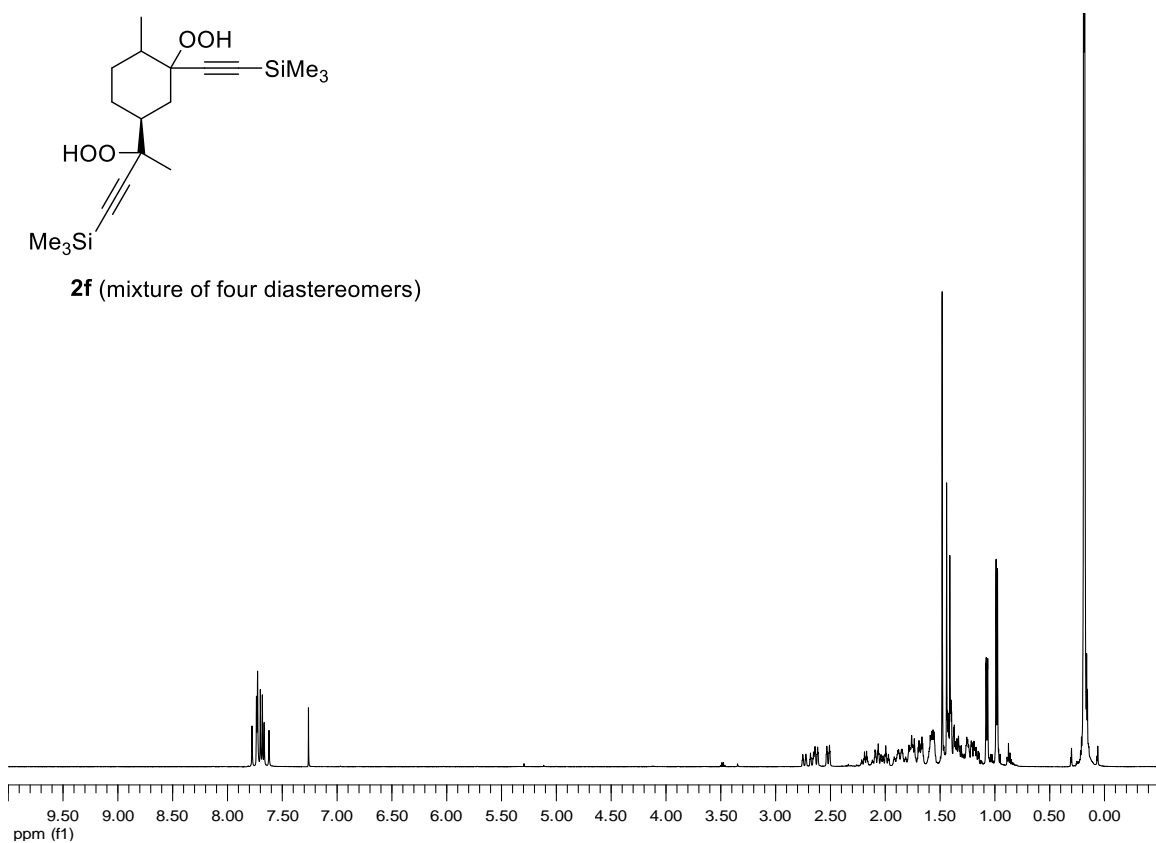


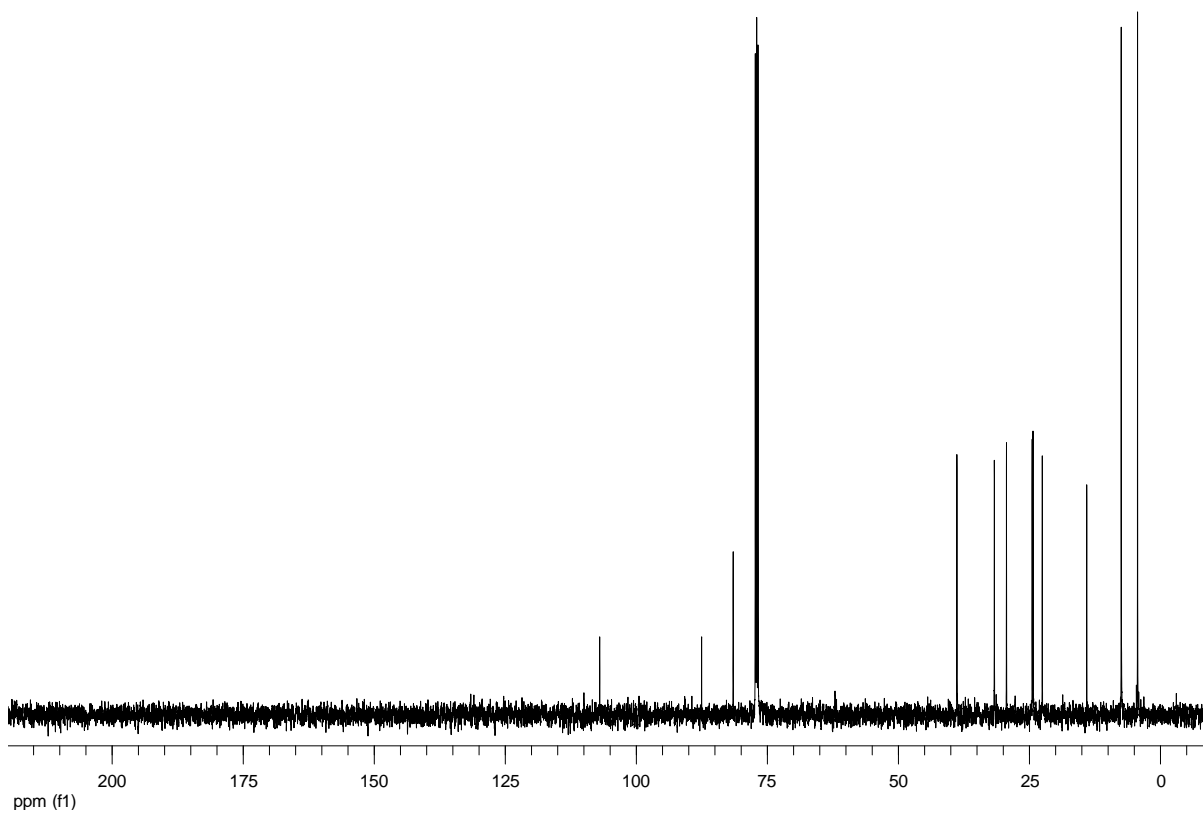
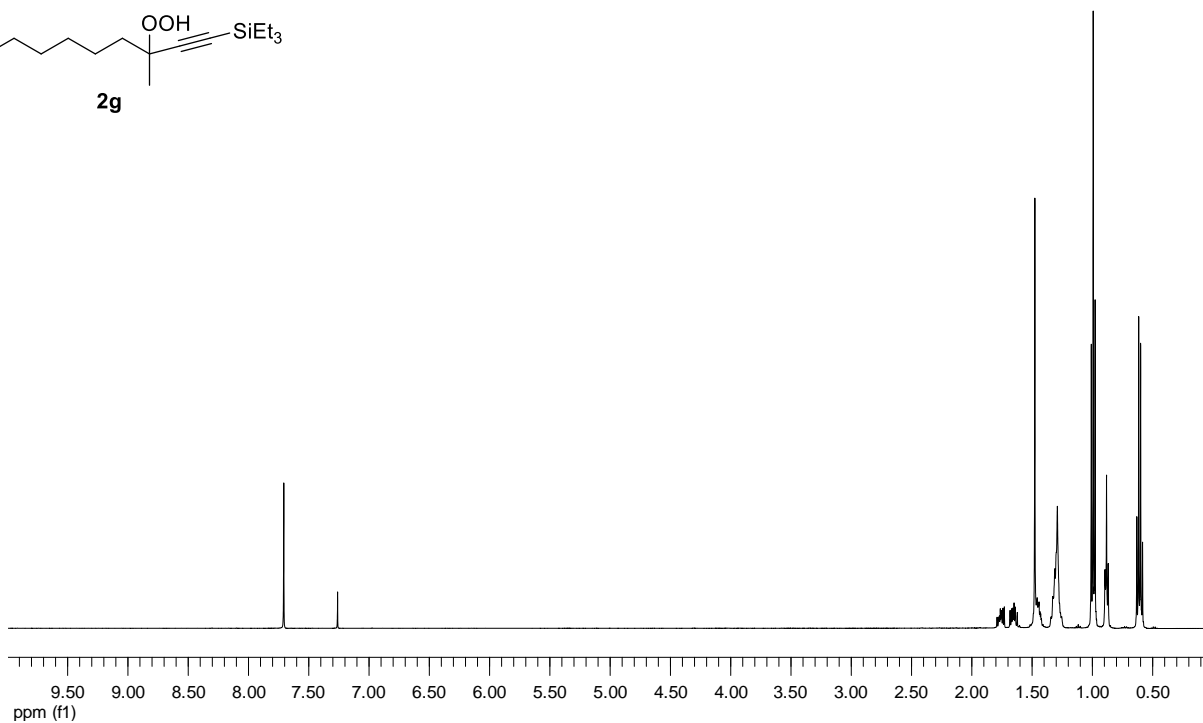
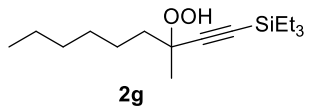
2e (mixture of two diastereomers)



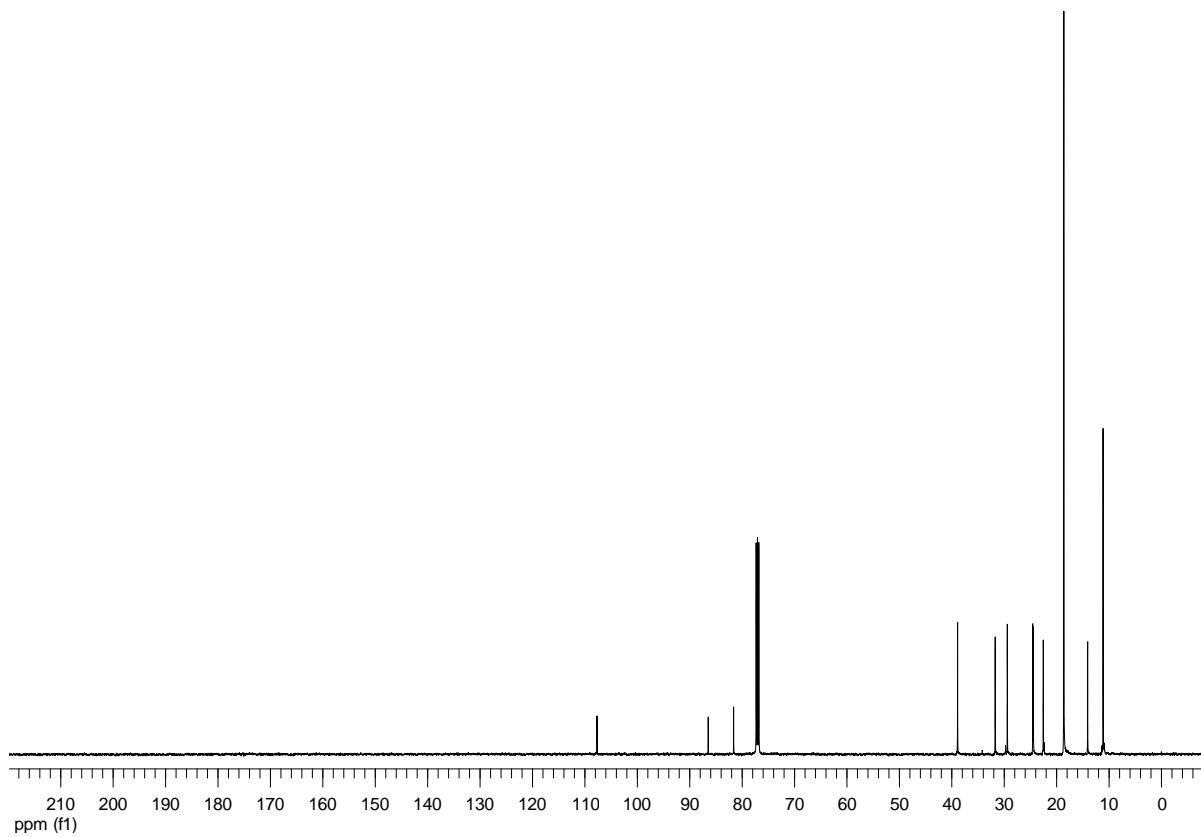
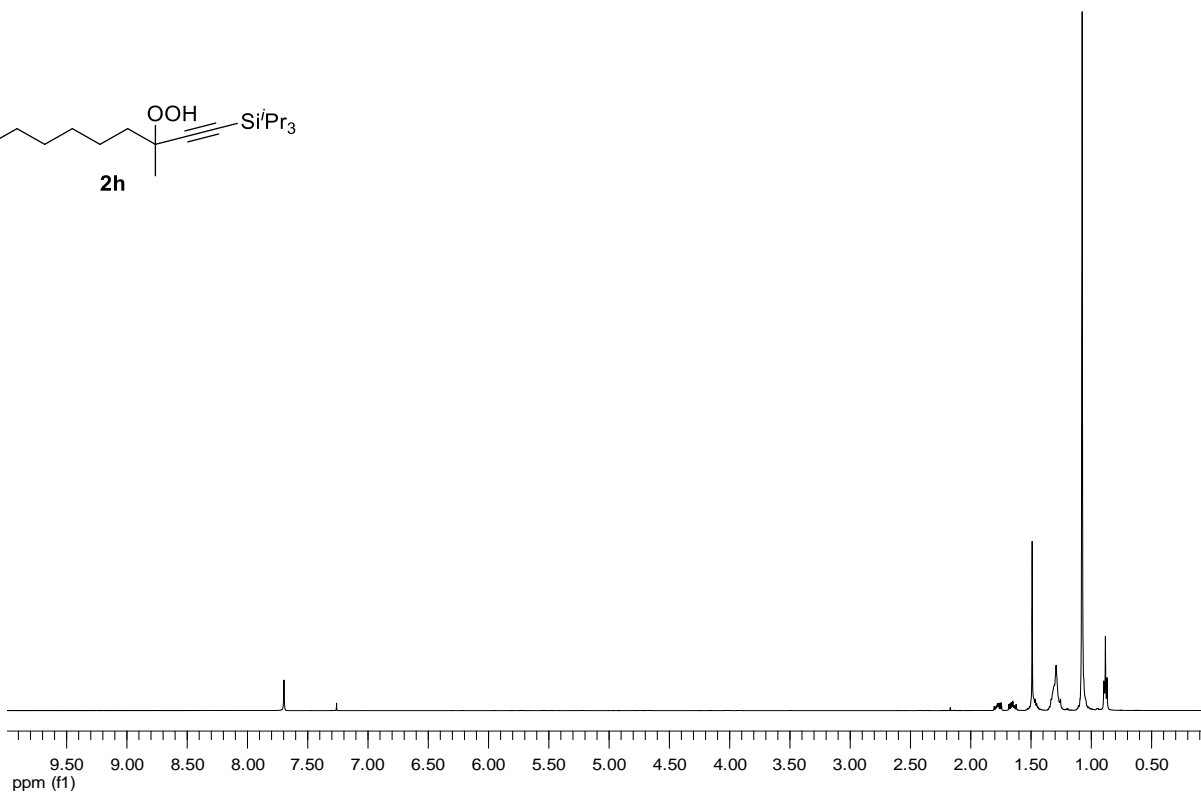
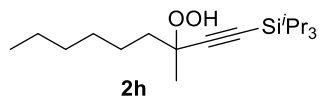


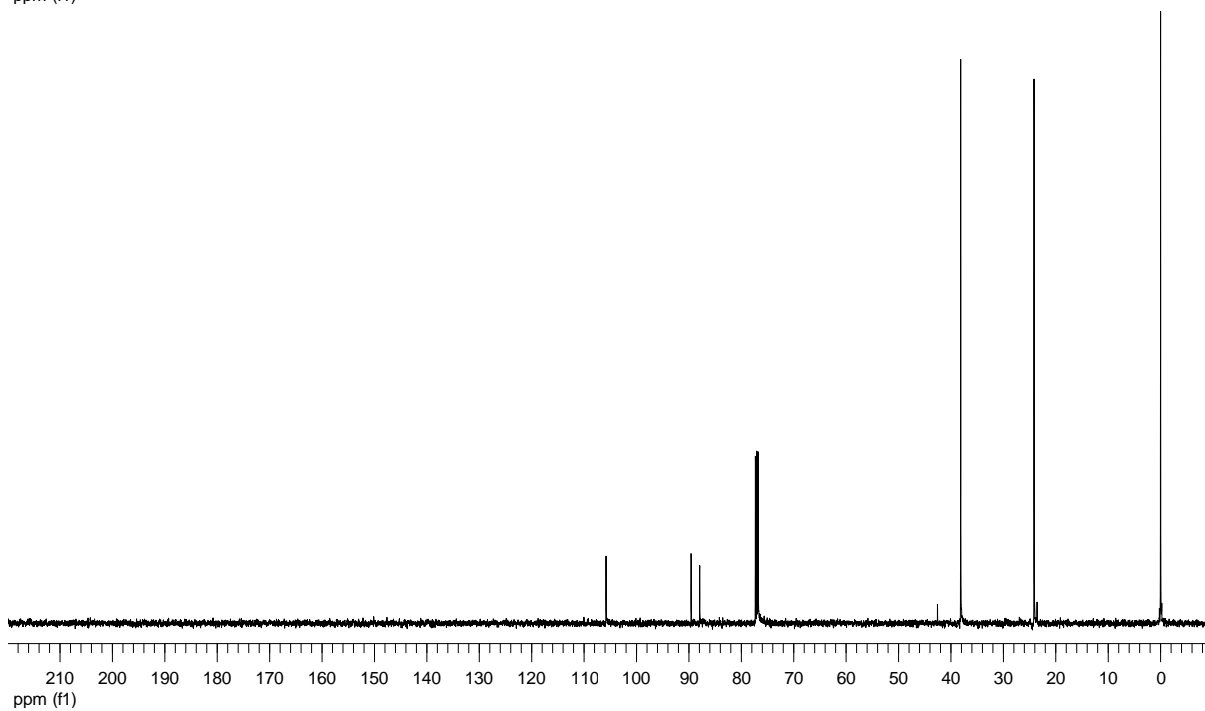
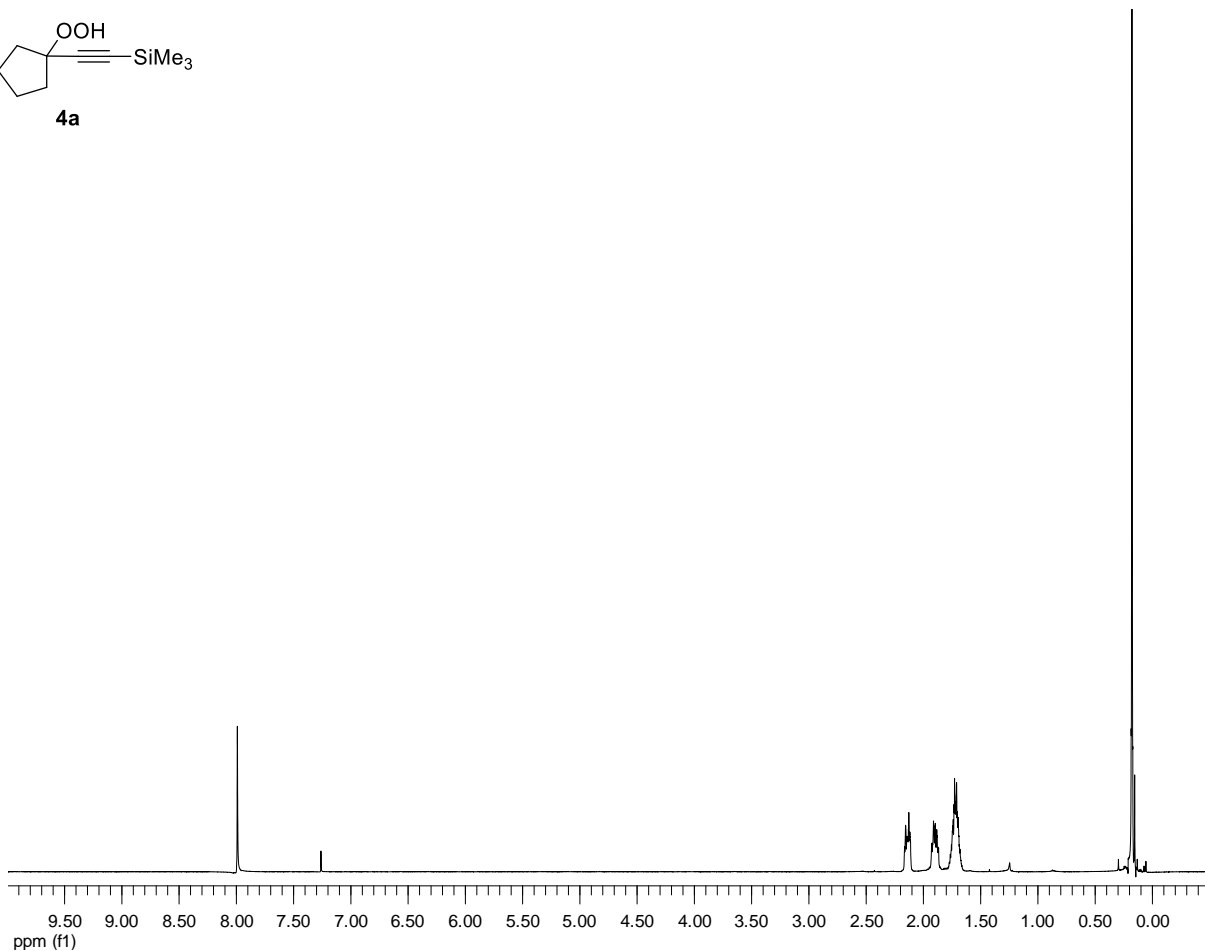
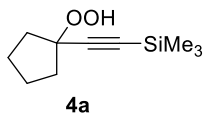
2f (mixture of four diastereomers)

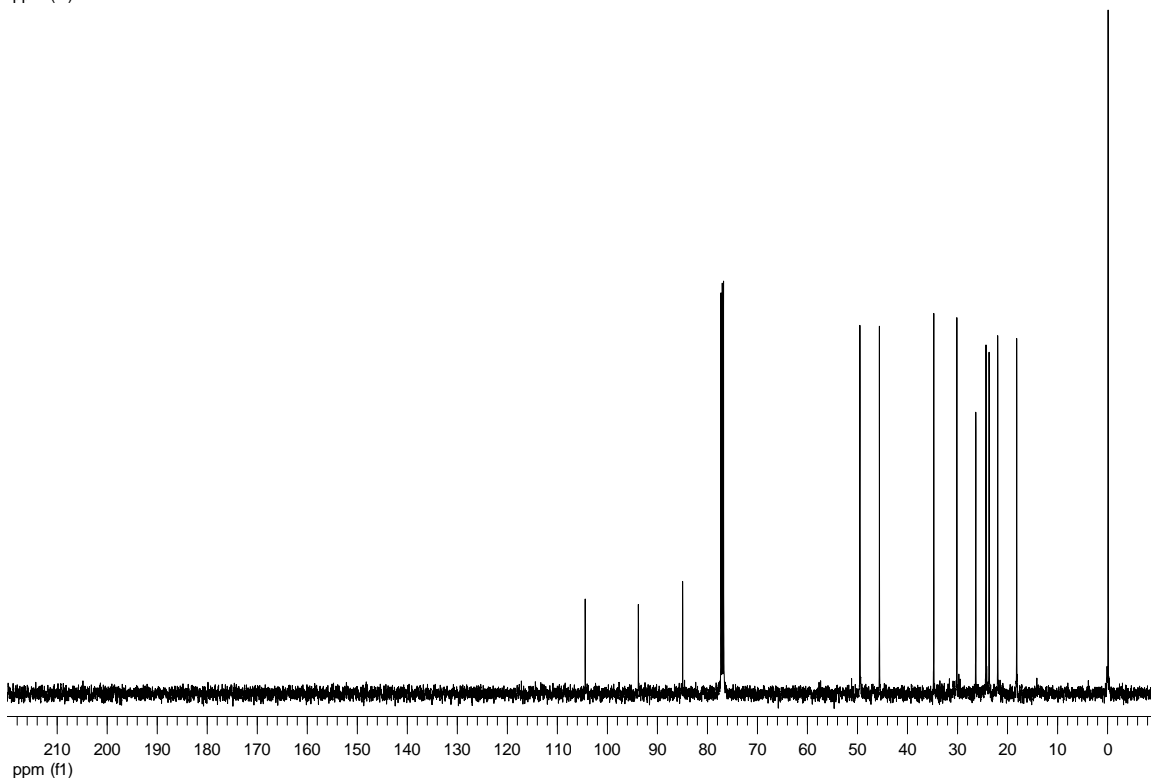
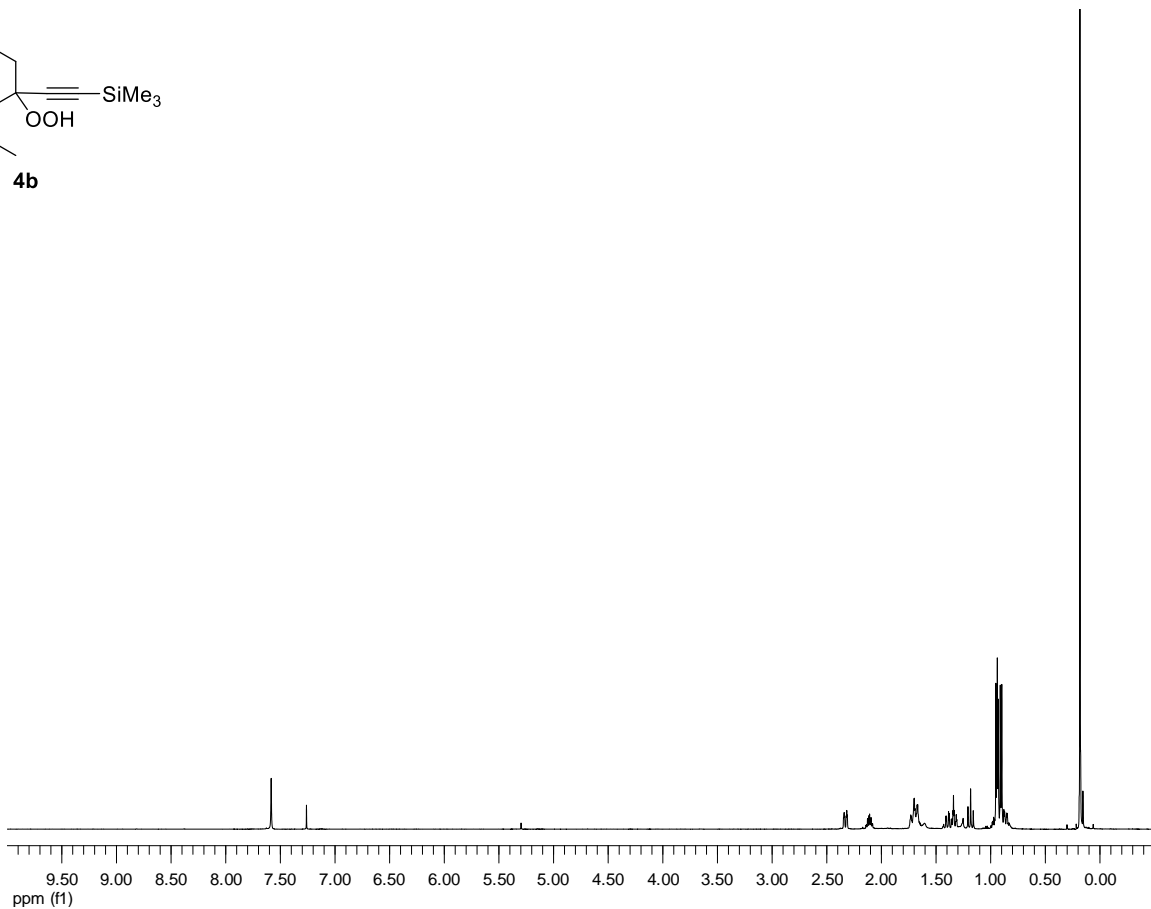
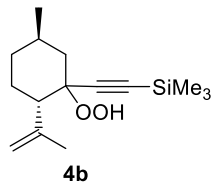


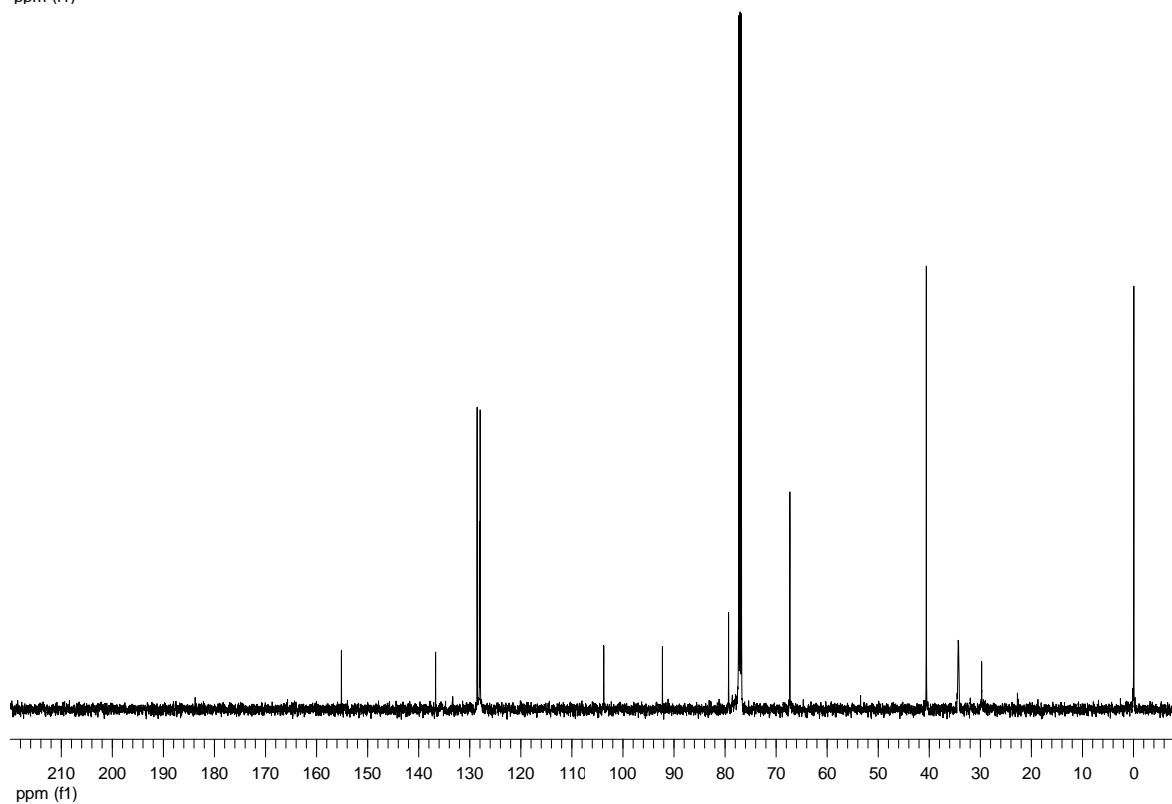
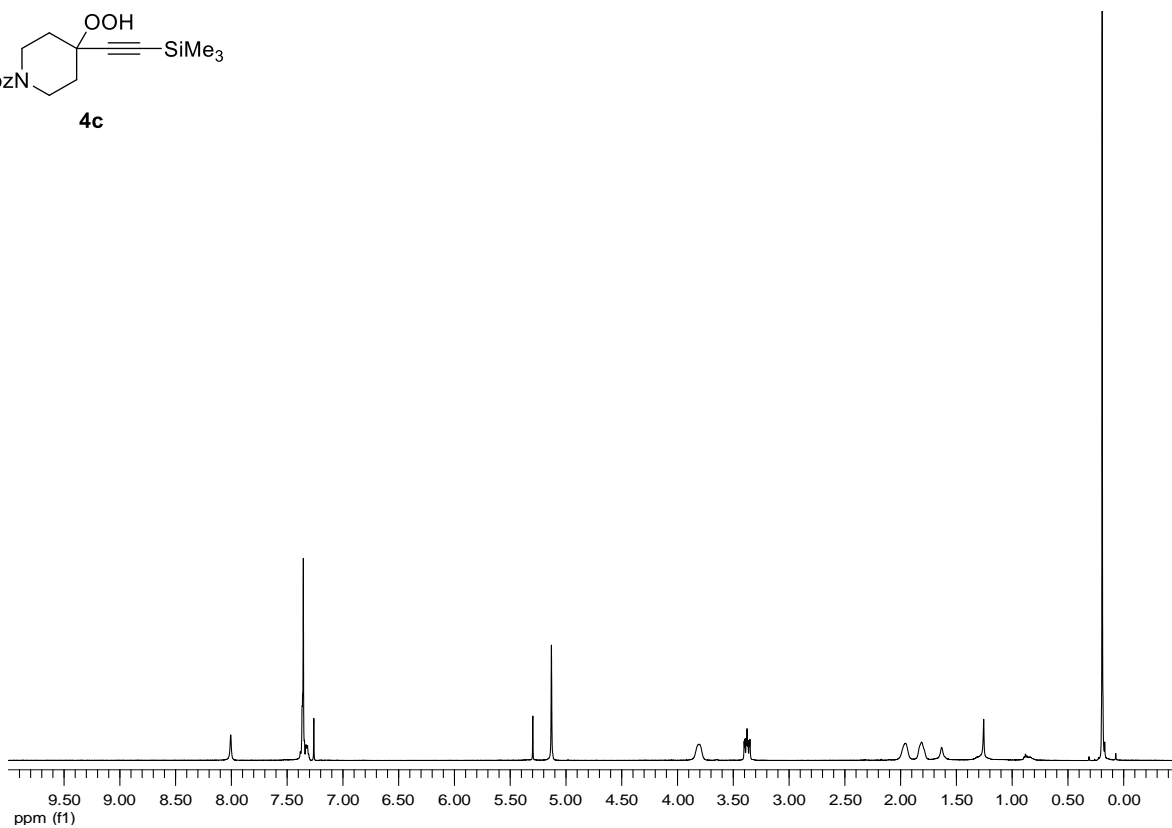
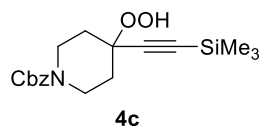


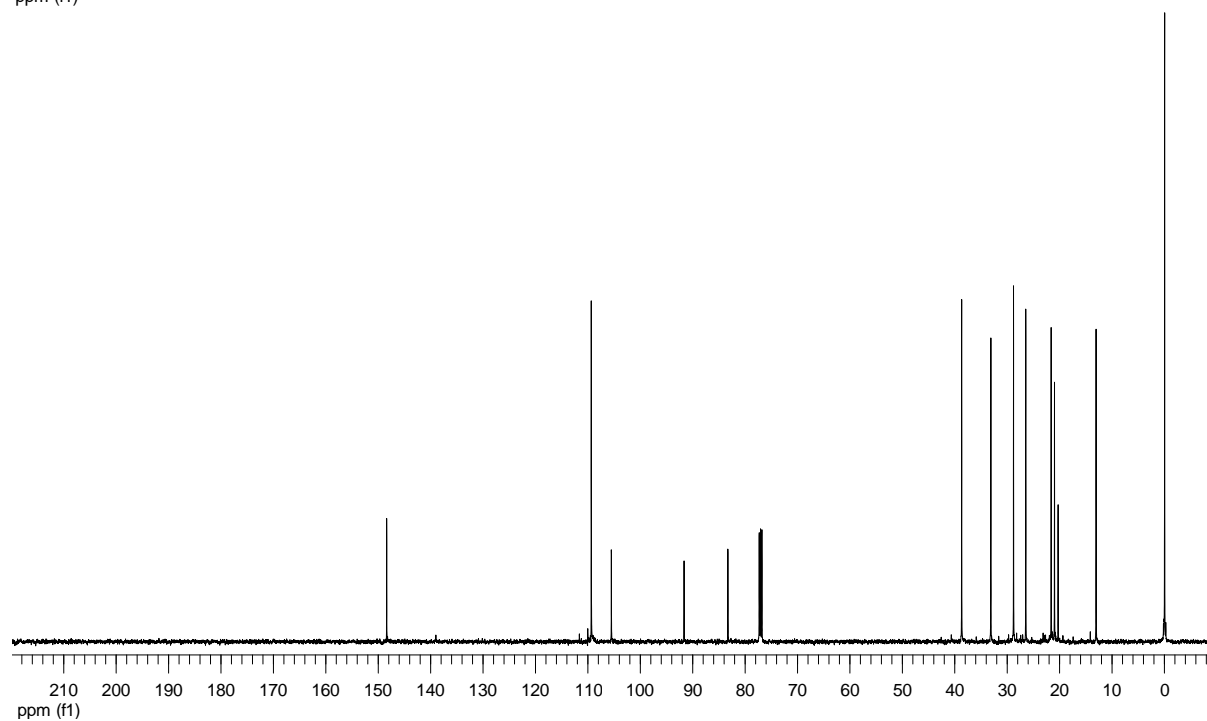
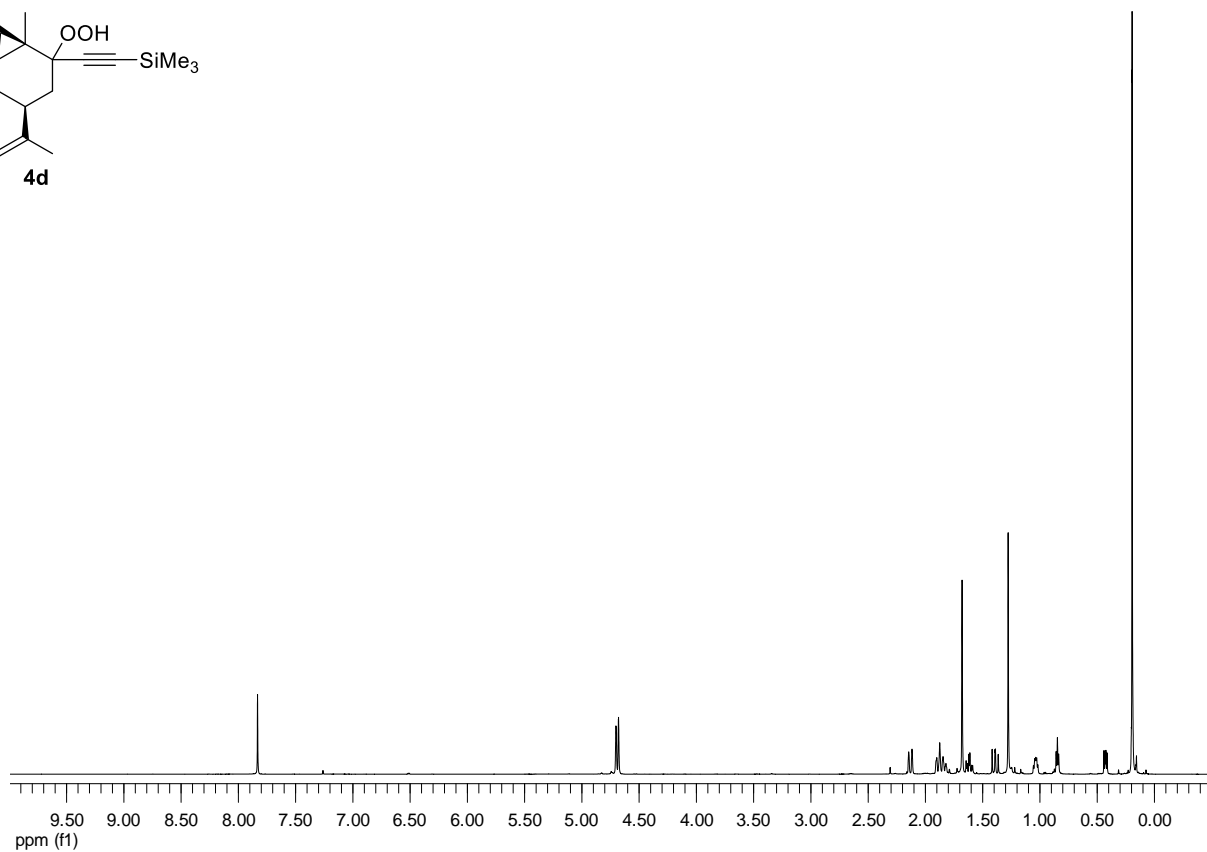
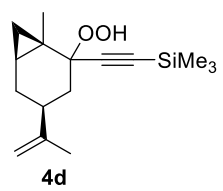
S16

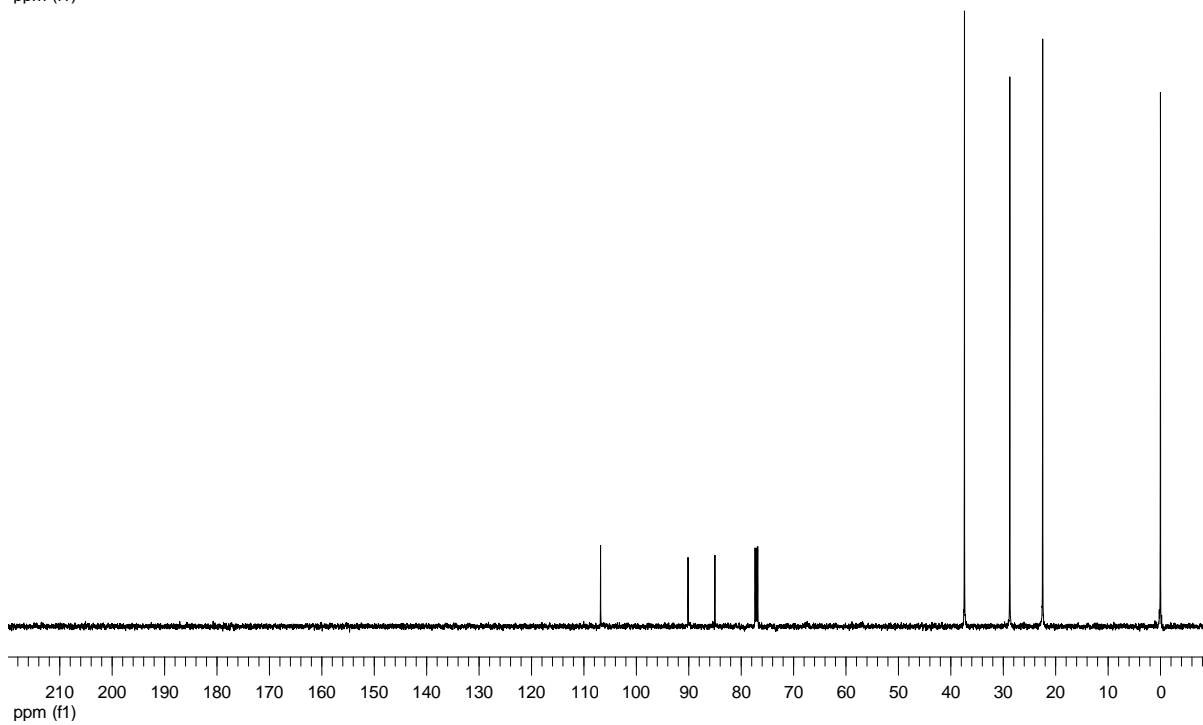
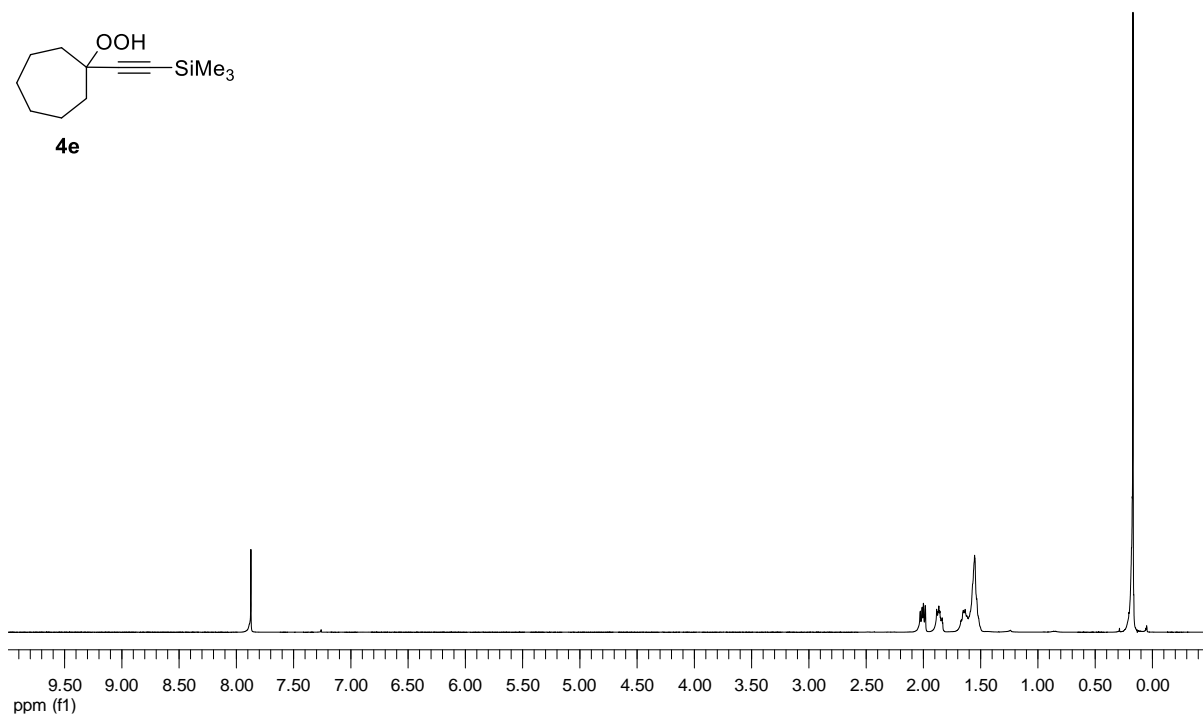
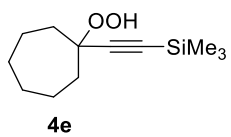


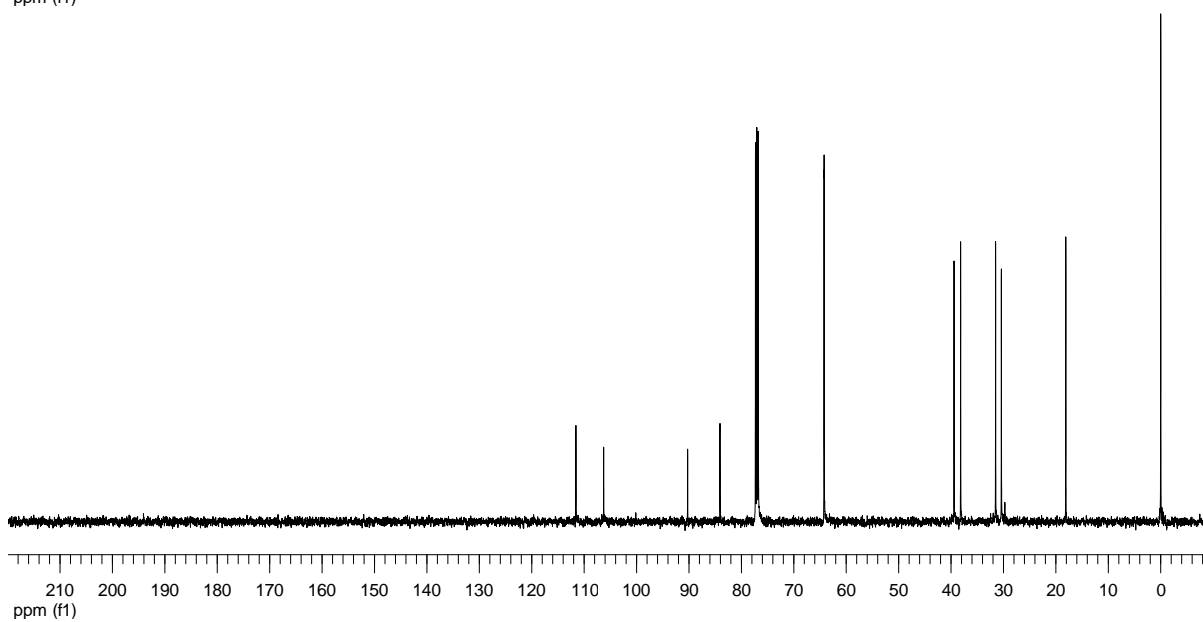
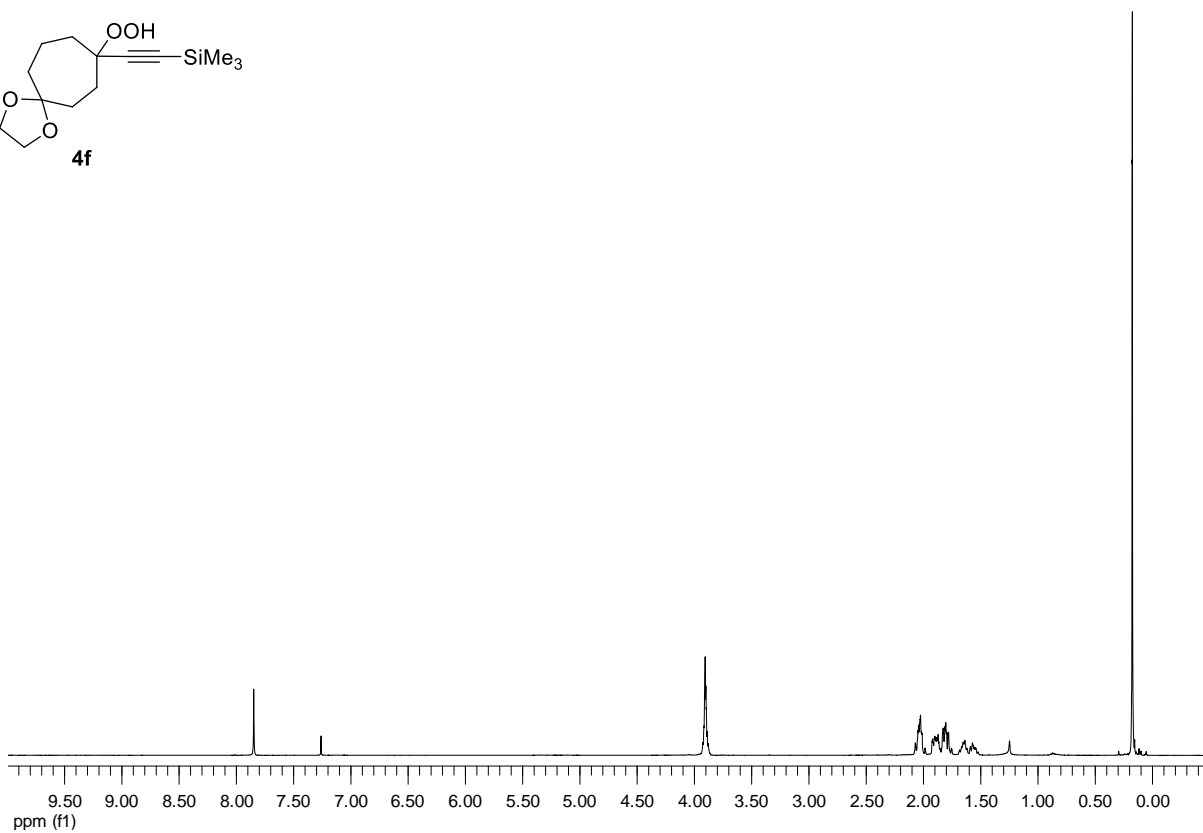
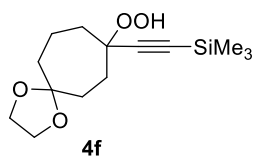


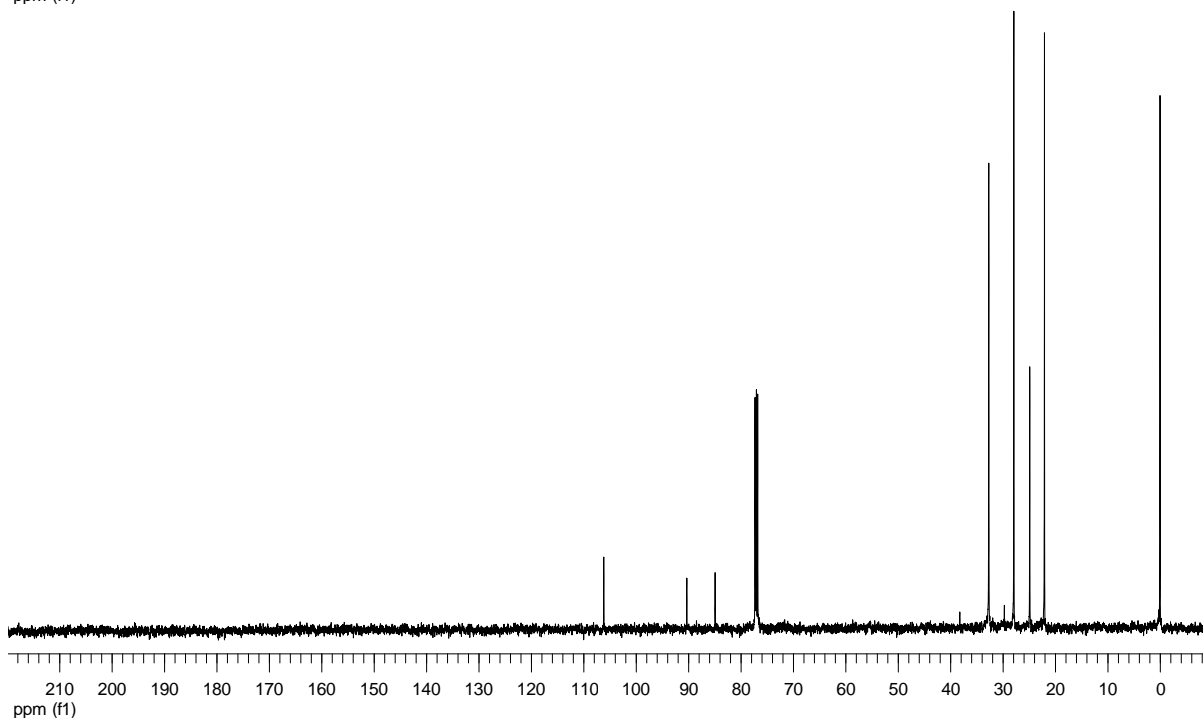
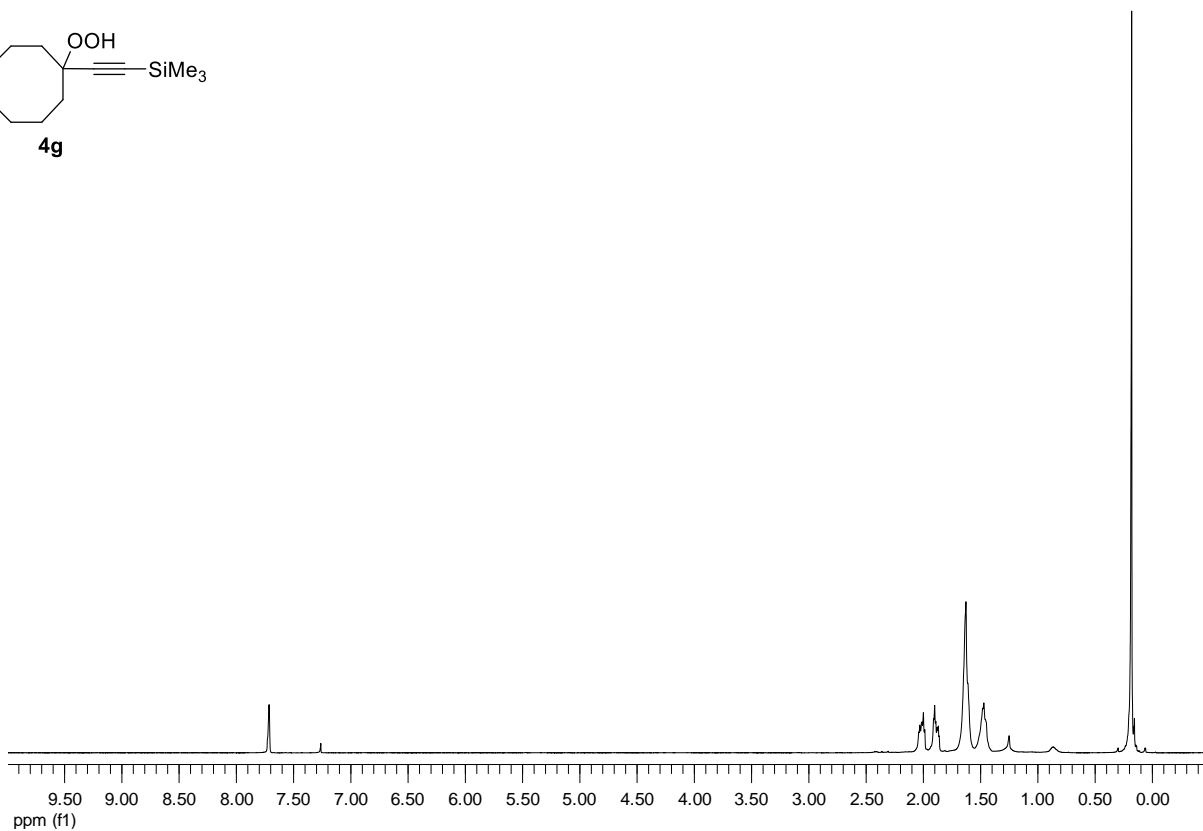
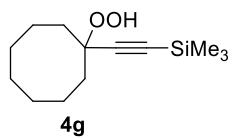


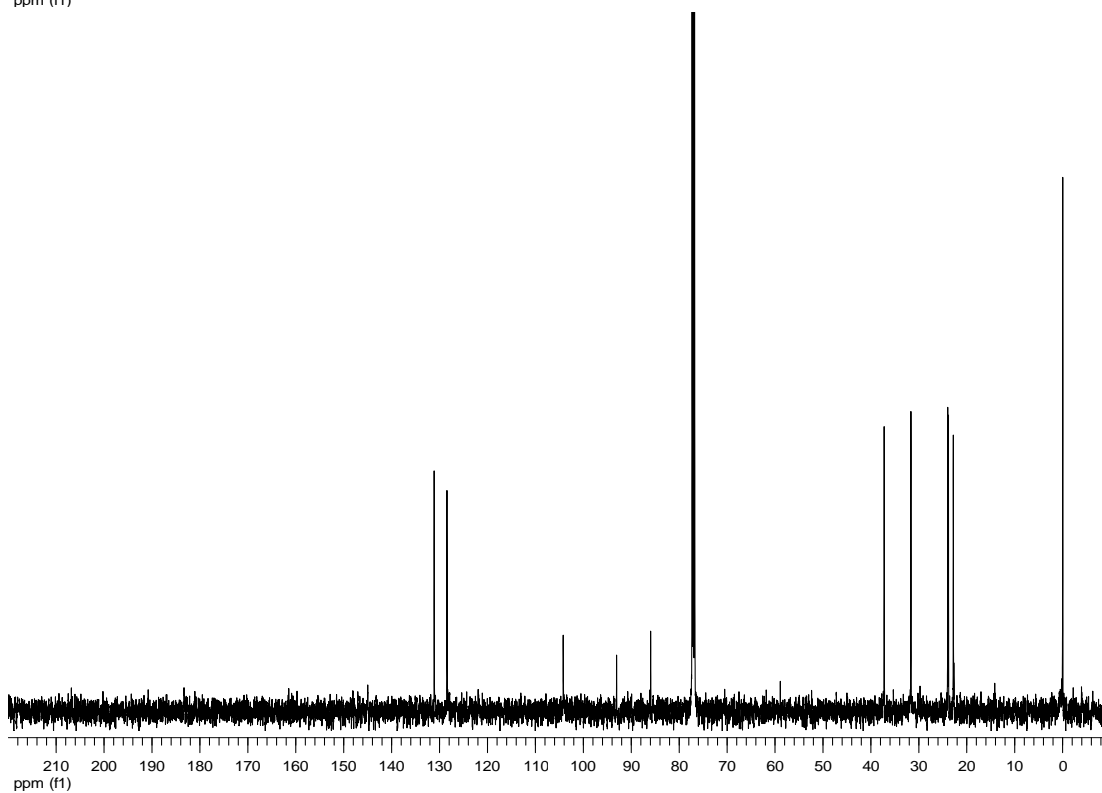
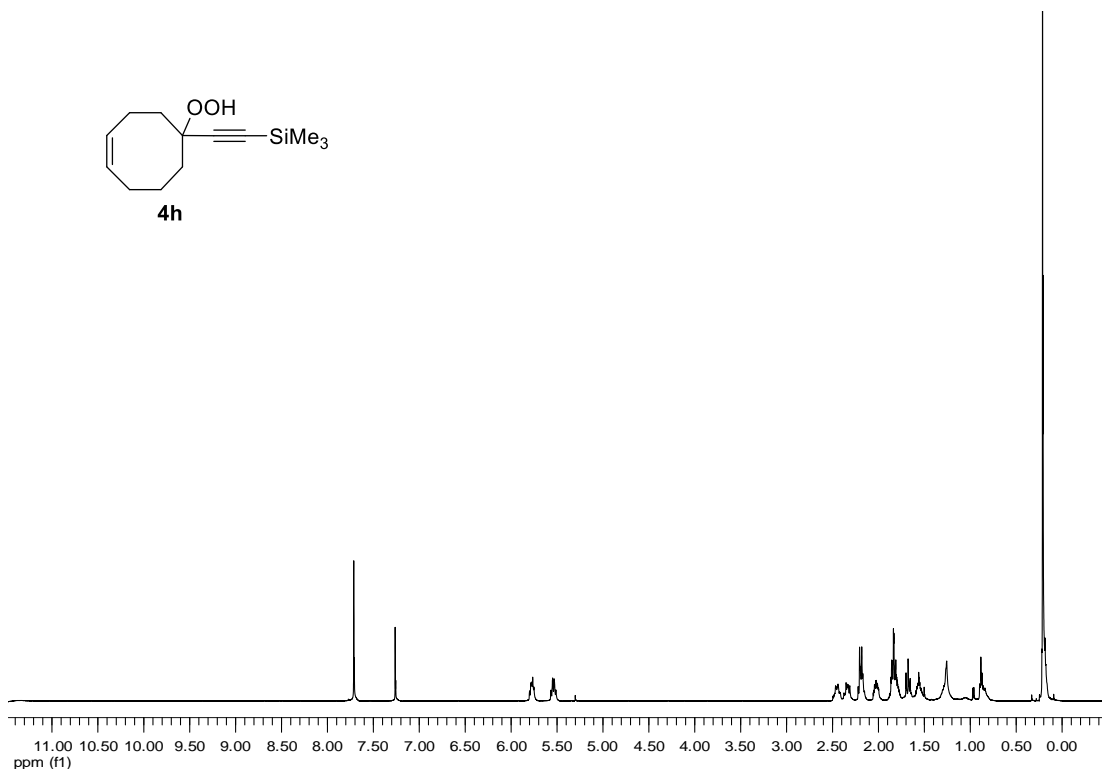
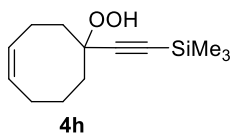


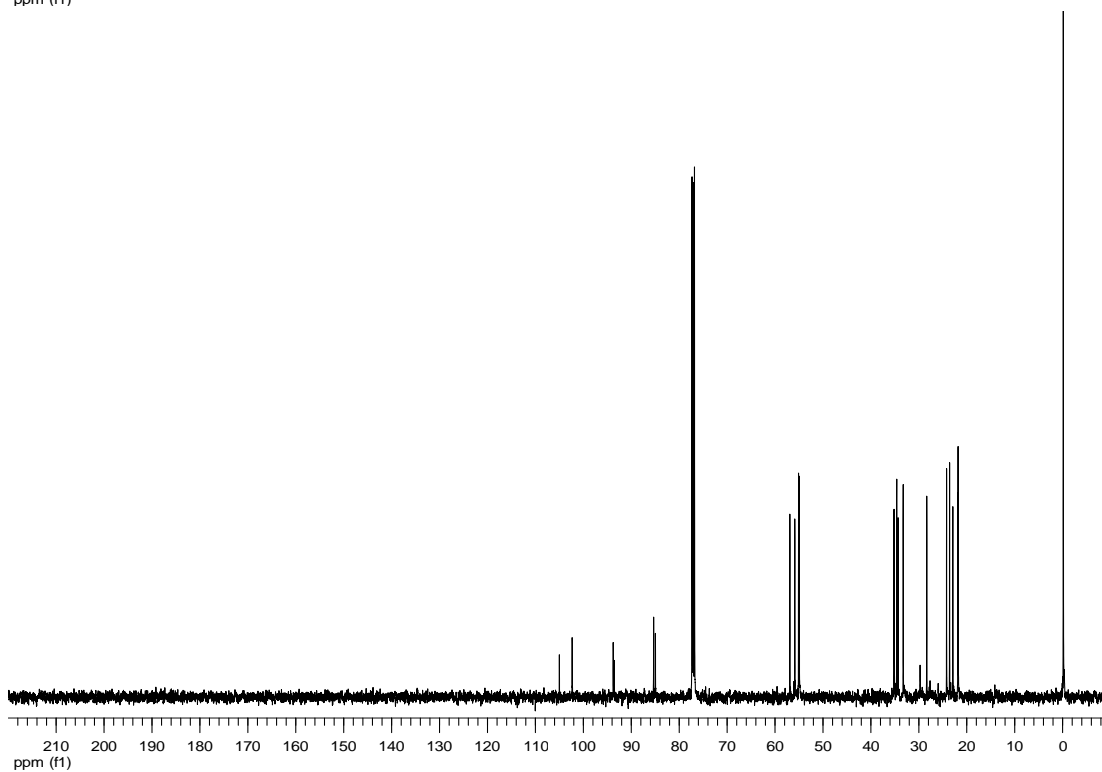
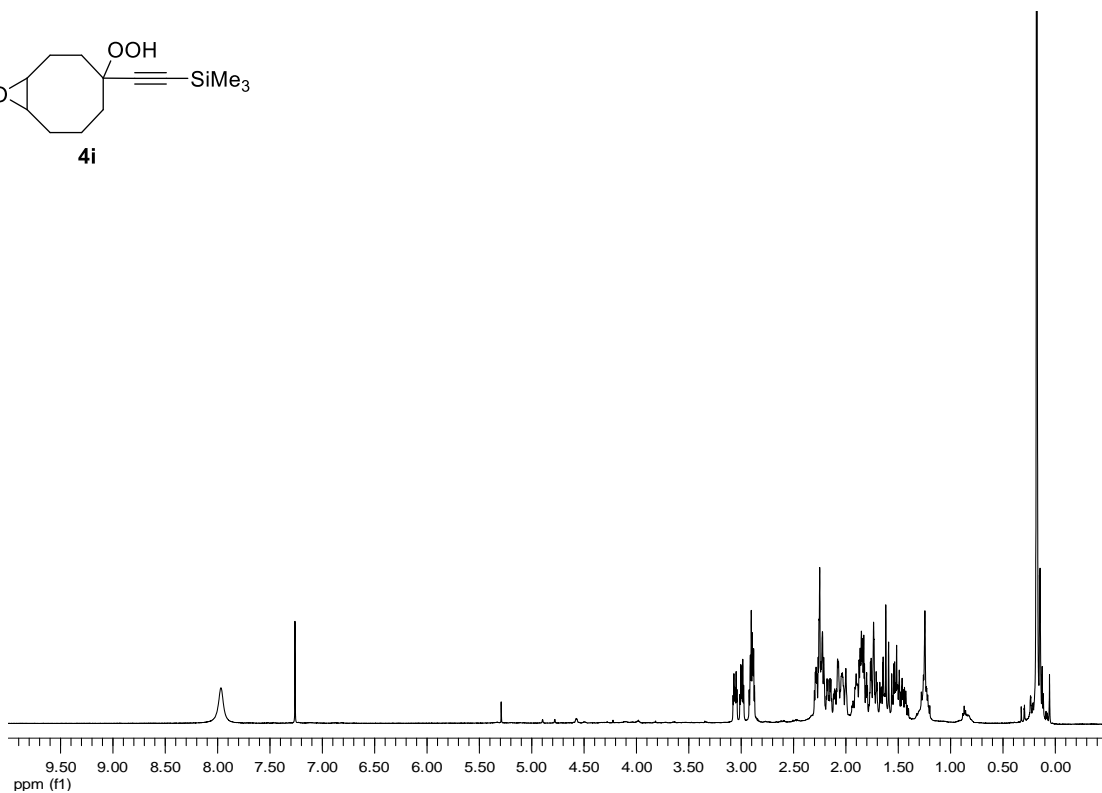
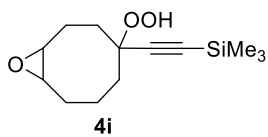


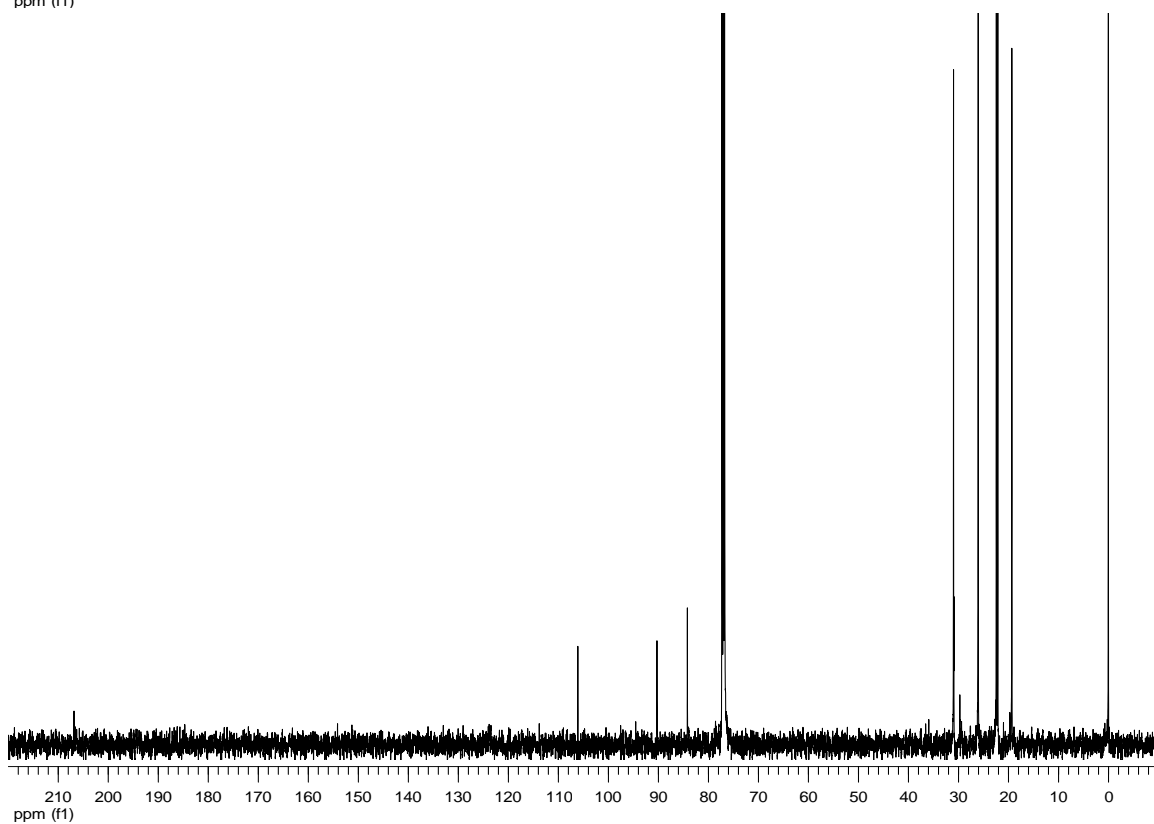
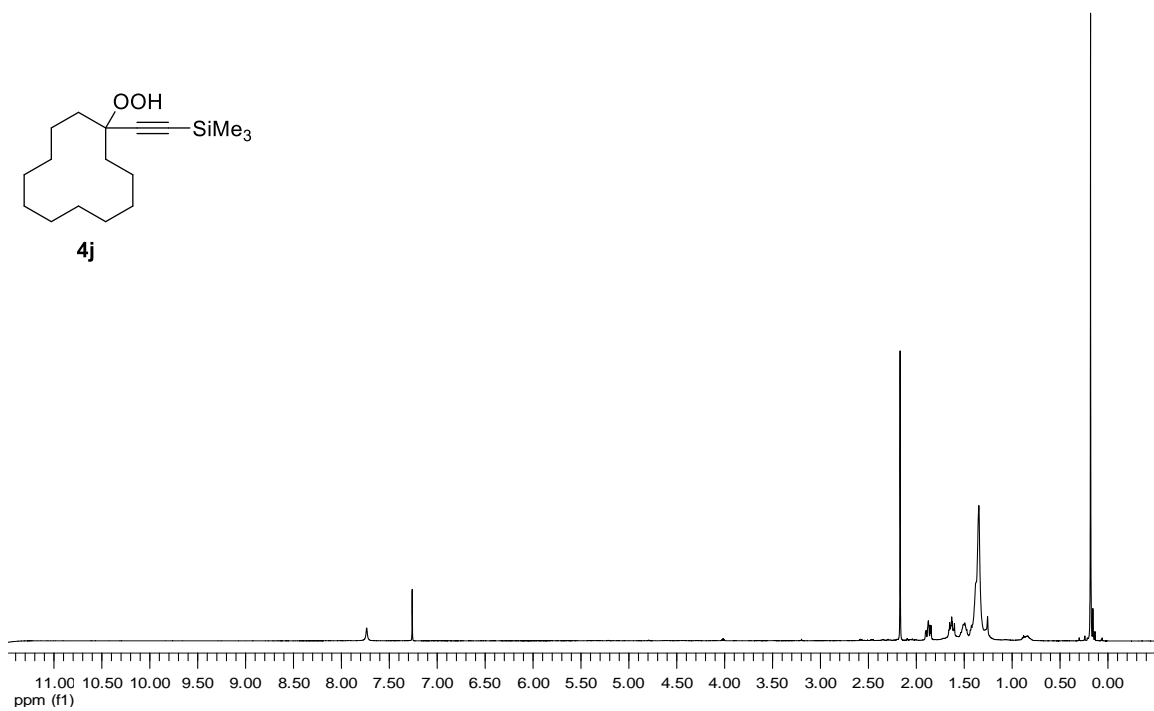
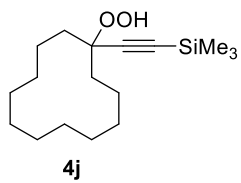




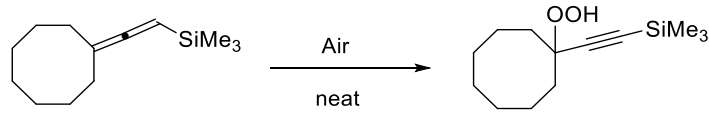






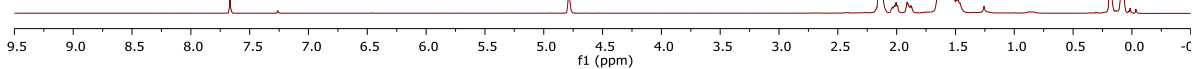


Monitoring the Reaction of 3g to 4g by ^1H NMR



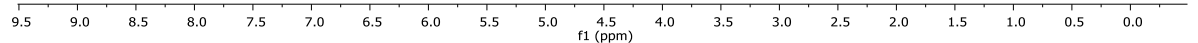
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3 Comment	H1 standard parameters, BBO probe.
4 Origin	Bruker BioSpin GmbH
5 Owner	sgupta97
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.2
11 Pulse Sequence	zg
12 Experiment	1D
13 Probe	5 mm BBO BB-1H Z8007/ 0099
14 Number of Scans	8
15 Receiver Gain	45.3
16 Relaxation Delay	1.0000
17 Pulse Width	3.5000
18 Presaturation Frequency	
19 Acquisition Time	2.7263
20 Acquisition Date	2018-07-07T22:52:58
21 Modification Date	2018-07-09T15:31:55
22 Class	
23 Spectrometer Frequency	500.64
24 Spectral Width	6009.6
25 Lowest Frequency	-264.0
26 Nucleus	^1H
27 Acquired Size	16384
28 Spectral Size	65536

~ 30 % conv, this initial conversion had already occurred while taking first NMR of the allene which indicates conversion already occurred during rotavap or in the process of preparing NMR sample.



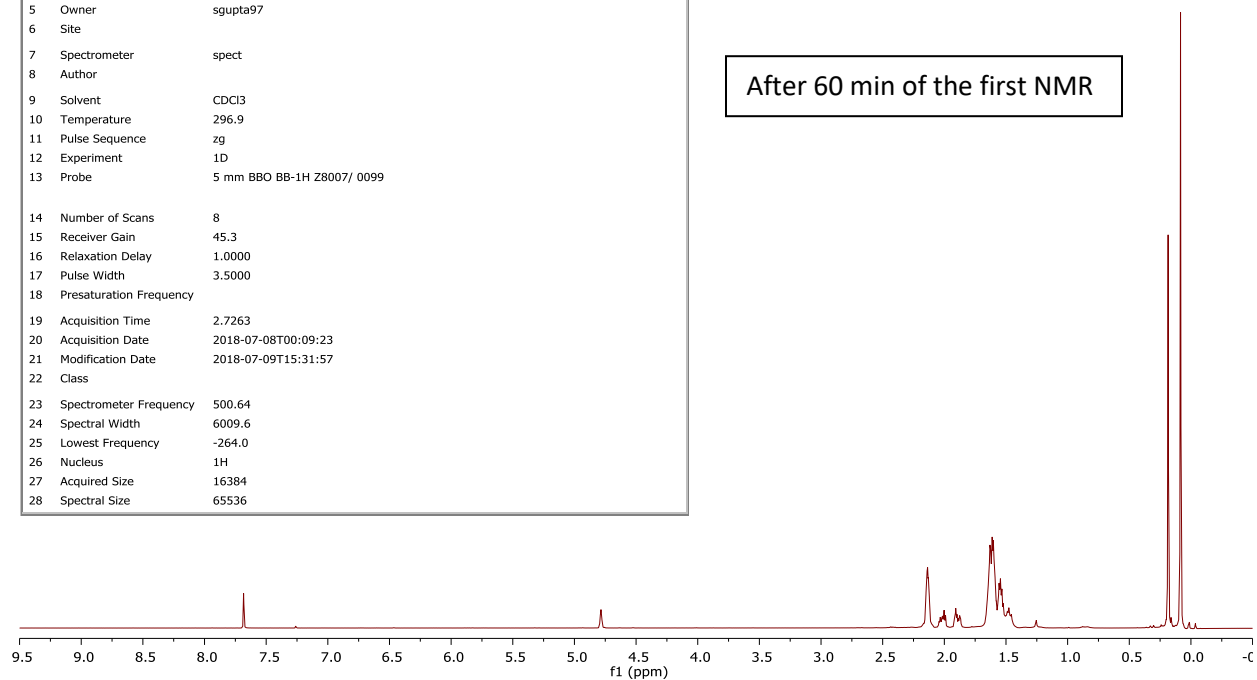
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4 Origin	Bruker BioSpin GmbH
5 Owner	sgupta97
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.0
11 Pulse Sequence	zg
12 Experiment	1D
13 Probe	5 mm BBO BB-1H Z8007/ 0099
14 Number of Scans	8
15 Receiver Gain	45.3
16 Relaxation Delay	1.0000
17 Pulse Width	3.5000
18 Presaturation Frequency	
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21 Modification Date	2018-07-09T15:31:57
22 Class	
23 Spectrometer Frequency	500.64
24 Spectral Width	6009.6
25 Lowest Frequency	-264.0
26 Nucleus	^1H
27 Acquired Size	16384
28 Spectral Size	65536

After 40 min of the first NMR



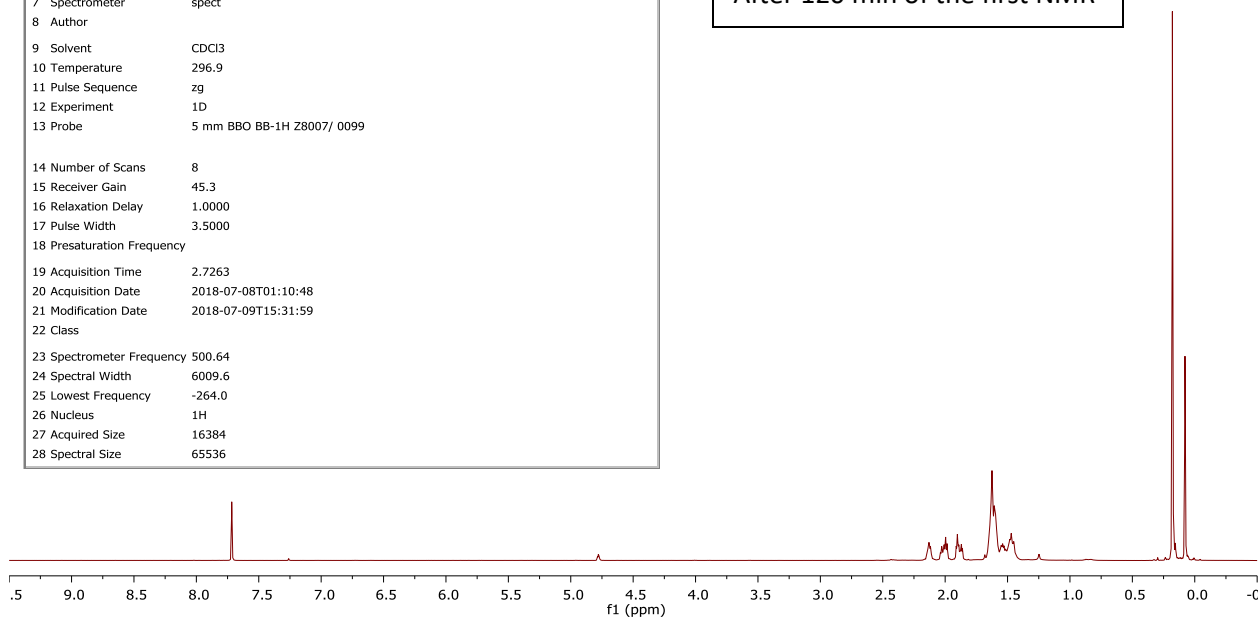
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5 Owner	sgupta97
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.9
11 Pulse Sequence	zg
12 Experiment	1D
13 Probe	5 mm BBO BB-1H Z8007/ 0099
14 Number of Scans	8
15 Receiver Gain	45.3
16 Relaxation Delay	1.0000
17 Pulse Width	3.5000
18 Presaturation Frequency	
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21 Modification Date	2018-07-09T15:31:57
22 Class	
23 Spectrometer Frequency	500.64
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25 Lowest Frequency	-264.0
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536

After 60 min of the first NMR



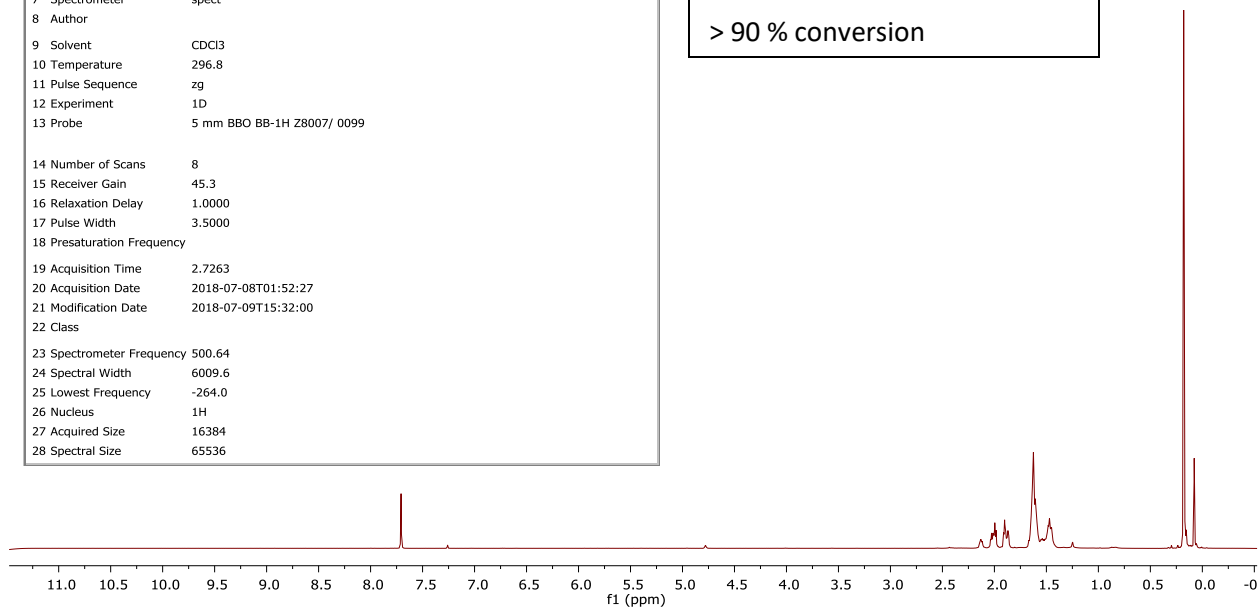
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6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.9
11 Pulse Sequence	zg
12 Experiment	1D
13 Probe	5 mm BBO BB-1H Z8007/ 0099
14 Number of Scans	8
15 Receiver Gain	45.3
16 Relaxation Delay	1.0000
17 Pulse Width	3.5000
18 Presaturation Frequency	
19 Acquisition Time	2.7263
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21 Modification Date	2018-07-09T15:31:59
22 Class	
23 Spectrometer Frequency	500.64
24 Spectral Width	6009.6
25 Lowest Frequency	-264.0
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536

After 120 min of the first NMR



Parameter	Value
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3 Comment	H1 standard parameters, BBO probe.
4 Origin	Bruker BioSpin GmbH
5 Owner	sgupta97
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.8
11 Pulse Sequence	zg
12 Experiment	1D
13 Probe	5 mm BBO BB-1H Z8007/ 0099
14 Number of Scans	8
15 Receiver Gain	45.3
16 Relaxation Delay	1.0000
17 Pulse Width	3.5000
18 Presaturation Frequency	
19 Acquisition Time	2.7263
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21 Modification Date	2018-07-09T15:32:00
22 Class	
23 Spectrometer Frequency	500.64
24 Spectral Width	6009.6
25 Lowest Frequency	-264.0
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536

After 160 min of the first NMR
> 90 % conversion



1. Computational Details

All calculations were carried out with the Gaussian 09 suite of computational programs.¹ The geometries for all species were optimized using the M062X hybrid functional² at the basis set level of 6-31+G(d). Frequencies were analytically computed at the same level of theory. The bond dissociation energies (BDE) refer to the enthalpy changes at 0 K for reaction $R-H \rightarrow R\cdot + H\cdot$.

2. Originally Calculated Energy Values

Species	Enthalpies (in a.u.)
H_a (radical)	-0.494305
1m'	-547.268718
1m'-radical	-546.635423
1m	-798.67353
1m-radical	-798.04992
G1a	-720.161094
G1a-radical	-719.536141
G2a	-525.006698
G2a-radical	-524.377852
G2b	-564.272011
G2b-radical	-563.645586
G2c	-721.32973
G2c-radical	-720.704229
G3a	-755.888323
G3a-radical	-755.269559
1c	-795.154225
1c-radical	-794.535948
G3b	-986.767331
G3b-radical	-986.15132

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

² (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157.

3. Cartesian Coordinates

H_a (radical)

H	0.04964500	1.91489400	0.00000000
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1m'

C	-2.23058800	-1.03005900	0.12409200
C	-1.95026100	-2.27735100	-0.16531900
H	-2.77688500	-2.97257700	-0.33633300
C	-0.44964300	-4.05563500	0.68608600
H	0.52837500	-4.54273400	0.59219200
H	-0.56771900	-3.71401900	1.72018100
H	-1.22231300	-4.80724500	0.48590400
C	0.52326600	-1.84558000	0.02684600
H	0.45818000	-0.98418500	-0.64772400
H	0.42240100	-1.47779700	1.05425000
H	1.51760400	-2.29344300	-0.08230900
C	-0.38057300	-3.39062900	-1.72872400
H	0.59522200	-3.87761500	-1.84464200
H	-1.15638600	-4.12261500	-1.98273900
H	-0.44344300	-2.56599000	-2.44706900
C	-2.52658500	0.21464300	0.41962000
C	-2.67007400	1.24870200	-0.68695000
C	-2.74719100	0.63195500	1.86243800
C	-1.37888600	1.98041300	-1.12832300
H	-3.41999700	1.99524800	-0.38732800
H	-3.07433900	0.73510100	-1.56539500
H	-2.46532300	-0.20337400	2.51338300
H	-3.82025300	0.81276800	2.01887400
C	-1.95983500	1.89111000	2.25547700
C	-0.95839300	3.21083000	-0.30656200
H	-0.55635000	1.25362500	-1.18135900
H	-1.55275200	2.31686700	-2.15755000
C	-0.48045600	1.82041100	1.83234900
H	-2.43948500	2.76657800	1.80169400
H	-2.05146800	2.03355000	3.33798200
C	-0.04350300	2.95508200	0.90049600
H	-0.43136900	3.90844700	-0.96925500
H	-1.86522800	3.74324000	0.01002100
H	-0.30186800	0.86529400	1.32316000
H	0.17219200	1.81788200	2.71288000
H	0.96815000	2.73248200	0.53556000
H	0.03537000	3.89041900	1.47139900
C	-0.55855300	-2.87664800	-0.29244900

1m'-radical

C	-1.79093500	-0.64400500	0.12437000
C	-1.46009300	-1.80726700	-0.07703500
C	-1.48562500	-4.06357600	0.89238400
H	-1.19554900	-5.10740100	0.72444500
H	-1.00072600	-3.71063200	1.80801000
H	-2.56942500	-4.02280500	1.03907200
C	0.46143100	-3.28517600	-0.49313100
H	0.78331400	-2.68181300	-1.34767300
H	0.97702500	-2.92032400	0.40072600
H	0.76104700	-4.32532000	-0.66849300
C	-1.75909700	-3.72628300	-1.58398400
H	-1.46629600	-4.76678400	-1.76810500
H	-2.84747100	-3.68459400	-1.47661700
H	-1.47605300	-3.12615300	-2.45435700
C	-2.16281300	0.67730100	0.34749100
C	-2.07423300	1.65894200	-0.78913100
C	-2.56613300	1.13095600	1.72445500
C	-0.65866300	2.22357100	-1.08030500
H	-2.75830700	2.49946800	-0.60395900
H	-2.42529800	1.15687800	-1.69893400
H	-2.45905600	0.29118900	2.41996900
H	-3.63038000	1.41441100	1.72696200
C	-1.72727500	2.32428800	2.22004300
C	-0.22614500	3.42400800	-0.22257500
H	0.07563600	1.40940000	-1.00644400
H	-0.65632300	2.54473900	-2.12882100
C	-0.21470600	2.09494700	2.02603400
H	-2.04327700	3.22724600	1.68404300
H	-1.96645900	2.50559600	3.27377600
C	0.46958900	3.12127900	1.11335600
H	0.46766900	4.03801400	-0.81031400
H	-1.10325800	4.06348100	-0.05432700
H	-0.05626000	1.09235600	1.60809700
H	0.29965700	2.09956700	2.99397100
H	1.48907900	2.76901200	0.90704000
H	0.57867100	4.07130500	1.65432900
C	-1.06534000	-3.20609600	-0.31318300

1m

C	-0.87174500	-0.44498800	0.10214500
C	-0.48094700	-1.68480800	-0.07272000
H	-1.10162300	-2.35077100	-0.67784900

Si	1.12349100	-2.30047700	0.69357200	C	2.69998400	-1.92787500	2.10254600
C	0.75845200	-3.76543300	1.82119200	H	3.37131800	-1.12043000	1.79228800
H	1.68314000	-4.16977500	2.24906400	H	2.30549400	-1.67578700	3.09253300
H	0.10299400	-3.47074200	2.64782600	H	3.29189500	-2.84598300	2.19615100
H	0.26296800	-4.57447800	1.27291200	C	2.00700300	-2.56705000	-0.83476400
C	1.87960700	-0.88798300	1.67692500	H	2.59008300	-3.49463800	-0.80171800
H	2.08514300	-0.02587500	1.03243100	H	1.20689700	-2.69532600	-1.57119700
H	1.20045000	-0.55425600	2.46942500	H	2.66463500	-1.76597200	-1.18838100
H	2.82191300	-1.19594600	2.14408900	C	-1.01022700	1.63687500	0.58380200
C	2.29378800	-2.85032700	-0.67708800	C	-0.80483700	2.57001100	-0.57935300
H	3.23218400	-3.23708900	-0.26315800	C	-2.04447100	1.93457600	1.63605700
H	1.84473500	-3.64421100	-1.28465000	C	-2.11903500	2.88972100	-1.31614900
H	2.53600000	-2.01529400	-1.34320100	H	-0.09125700	2.11691300	-1.27598600
C	-1.19302300	0.80874400	0.32513600	H	-0.35286300	3.50843300	-0.22236200
C	-0.69218300	1.90536600	-0.59675400	H	-2.20434800	3.02017300	1.69758700
C	-2.07219000	1.16522300	1.51314400	H	-1.64242100	1.61469400	2.60453500
C	-1.80926600	2.83760100	-1.09154700	C	-3.41675600	1.23596900	1.44320900
H	-0.18939200	1.44091000	-1.45269400	C	-2.93346200	1.61964300	-1.63325800
H	0.06488400	2.49832900	-0.06324200	H	-2.71469400	3.57678800	-0.70328800
H	-1.80198900	2.16954800	1.87044400	H	-1.87731900	3.44164600	-2.23100700
H	-1.83059700	0.47085000	2.32554200	C	-4.40500700	1.94061100	0.49984900
C	-3.60172600	1.10291700	1.28628200	H	-3.24952500	0.19737900	1.12579800
C	-3.03260800	2.06810500	-1.62307800	H	-3.88222300	1.18182200	2.43448500
H	-2.10964300	3.49759100	-0.26888800	C	-4.32690900	1.58605200	-0.99316600
H	-1.39461000	3.49706400	-1.86206700	H	-3.05019900	1.50139200	-2.71662200
C	-4.26111400	2.34031100	0.65414600	H	-2.37020600	0.73959600	-1.29735200
H	-3.83998100	0.20099100	0.70583800	H	-4.30232900	3.02563500	0.63623100
H	-4.05516400	0.95797400	2.27429900	H	-5.42481600	1.70556600	0.82897700
C	-4.33630900	2.38133400	-0.87935800	H	-4.99048400	2.27438900	-1.53437400
H	-3.18196000	2.27291200	-2.68933800	H	-4.74624700	0.58166500	-1.13821200
H	-2.83594200	0.99118300	-1.54818000				
H	-3.75320100	3.23735800	1.03310900				
H	-5.29001500	2.41430400	1.02762900				
H	-4.69331100	3.37797800	-1.17305400				
H	-5.10383600	1.67077600	-1.21404000				

G1a

1m-radical

C	-0.29406300	0.45538700	0.66766600	C	-1.17354200	-0.34143200	-1.68467400
C	0.34229300	-0.60079200	0.73996000	C	-1.81186600	-1.11473900	-2.53014900
Si	1.30468300	-2.16208300	0.86158400	H	-2.34834600	-1.98468000	-2.14246800
C	0.15952000	-3.53794300	1.43902900	Si	-1.80364200	-0.73929100	-4.37306100
H	0.70860100	-4.48172000	1.53686700	C	-0.93524600	-2.13625400	-5.29420900
H	-0.28164500	-3.30025500	2.41275100	H	-0.93479600	-1.95354800	-6.37504100
H	-0.65806400	-3.69340000	0.72737900	H	0.10531800	-2.23342900	-4.96612000
				H	-1.43283200	-3.09647200	-5.11781700
				C	-0.89232800	0.88381400	-4.63825000
				H	-1.39493000	1.70431300	-4.11366100
				H	0.13326300	0.82498200	-4.25667000
				H	-0.84581800	1.13856600	-5.70299400

C	-3.58054800	-0.60421100	-4.98636300
H	-3.61051000	-0.40426700	-6.06370500
H	-4.13239600	-1.53331500	-4.80419500
H	-4.11213900	0.20638600	-4.47648800
C	-0.51460500	0.46830200	-0.89148300
C	-1.14367800	1.70555300	-0.28447300
C	0.95202400	0.27082200	-0.56657200
C	-0.32354400	2.95031300	-0.65269600
H	-1.15329700	1.59771900	0.81114000
H	-2.18247300	1.80703800	-0.61334200
C	1.75045600	1.53142700	-0.92794800
H	1.05356500	0.08431300	0.51372100
H	1.34490400	-0.60704600	-1.08857800
C	1.14806700	2.77531900	-0.26926900
H	-0.74505700	3.83416900	-0.15926200
H	-0.39812700	3.11763900	-1.73629000
H	2.79769800	1.40872200	-0.62686700
H	1.74043200	1.65924200	-2.01937300
H	1.72089200	3.66664500	-0.55018000
H	1.22726700	2.67913600	0.82391300

G1a-radical

C	-0.58846100	0.38506800	-2.34312900
C	-1.04518800	-0.01989700	-3.41807600
Si	-1.72515600	-0.64234900	-5.00730300
C	-1.47600700	-2.50590900	-5.09097300
H	-1.87083600	-2.90644200	-6.03204700
H	-0.41307700	-2.76257800	-5.03234900
H	-1.98974500	-3.00913300	-4.26526500
C	-0.81293900	0.18703600	-6.42873100
H	-0.93727200	1.27439000	-6.39591300
H	0.25932500	-0.03133900	-6.38608900
H	-1.19390700	-0.17085400	-7.39232500
C	-3.55889300	-0.23243000	-5.08080500
H	-3.99640200	-0.59198800	-6.01933400
H	-4.09940600	-0.70275000	-4.25267100
H	-3.72390700	0.84839600	-5.02091000
C	-0.08412900	0.83667500	-1.14186700
C	-0.98635600	1.26576200	-0.01749500
C	1.39464000	0.90362500	-0.87481200
C	-0.56607400	2.64308900	0.52238800
H	-0.90517200	0.53193100	0.80226700
H	-2.03020400	1.27165200	-0.34399100
C	1.78746100	2.28474800	-0.32341700

H	1.65269100	0.14271400	-0.11852100
H	1.95966300	0.66394500	-1.78007900
C	0.92173700	2.66266000	0.88051000
H	-1.17514200	2.89919700	1.39694900
H	-0.76527600	3.40309200	-0.24517200
H	2.84868800	2.28412200	-0.04891400
H	1.65775100	3.03539500	-1.11454600
H	1.20721700	3.65290300	1.25388900
H	1.10688800	1.94968700	1.69777200

G2a

C	-1.33159000	0.13008800	0.08634000
C	-0.23088800	0.34170800	-0.58795000
H	0.04875800	-0.38316500	-1.35591500
C	-2.42649600	-0.04221900	0.78483800
H	-2.41614300	-0.60555300	1.71355900
H	-3.37570600	0.36458200	0.44766000
Si	0.85460600	1.84641100	-0.26352300
C	0.09284300	2.84695800	1.13128400
H	0.69140000	3.74111500	1.33857400
H	-0.92270900	3.16955900	0.87764000
H	0.03335400	2.25786300	2.05288600
C	0.95425000	2.87239100	-1.83975200
H	1.58774700	3.75493600	-1.69285900
H	1.38044900	2.28987200	-2.66427800
H	-0.03823000	3.21613500	-2.14989800
C	2.57986100	1.25642100	0.20773300
H	3.02418200	0.65427200	-0.59277800
H	3.24682300	2.10589100	0.39509300
H	2.55256000	0.64182000	1.11377900

G2a-radical

C	-1.61743300	0.22293600	0.00048600
C	-0.64679100	0.98817900	-0.02727600
C	-2.69551200	-0.62778200	0.03132500
H	-3.08513100	-0.99635200	0.97296900
H	-3.17685500	-0.94724300	-0.88564600
Si	0.80684700	2.11982400	-0.06875900
C	0.72667300	3.25047600	1.43083700
H	1.58417700	3.93312700	1.44375900
H	-0.18714300	3.85336600	1.42262800
H	0.74040300	2.67116100	2.35987300
C	0.73789800	3.12369500	-1.65623400
H	1.59612800	3.80266500	-1.71922500

H	0.75566100	2.47172100	-2.53563600	H	0.09855300	3.79367400	-1.84009100
H	-0.17530500	3.72608400	-1.70108300	C	2.29737300	0.99016300	0.06106300
C	2.37325700	1.07984600	-0.01874800	H	2.28052500	0.25528900	-0.75058000
H	2.42497500	0.40561500	-0.87991600	H	3.25298900	1.52551000	0.01536400
H	3.26166800	1.72170000	-0.03522500	H	2.25849800	0.44521700	1.01000000
H	2.41123700	0.47032300	0.88997100	C	-3.59050700	-0.52422300	1.40272300
				H	-4.58417400	-0.07186100	1.51619400
G2b				H	-3.73215500	-1.61188500	1.42997500
C	-1.58214500	0.40675800	-0.10471300	H	-2.97991000	-0.23255400	2.25990700
C	-0.39759800	0.46616500	-0.66156100				
H	-0.10734600	-0.33480200	-1.34611300	G2c			
C	-2.75229600	0.38647300	0.48569800	C	-1.20639800	0.05436600	0.33794700
H	-3.59048100	0.86944900	-0.01610300	C	0.09269200	0.05222200	0.51745100
Si	0.78931800	1.88116300	-0.29986600	H	0.58411400	-0.88767100	0.78203400
C	-0.01406000	3.02833300	0.95298600	C	-2.50334700	0.12389800	0.14869100
H	0.65154700	3.86284900	1.20072700	Si	1.09248200	1.63415000	0.32727100
H	-0.94937000	3.44417400	0.56304500	C	2.05516800	1.95163200	1.91581700
H	-0.24974900	2.49488500	1.88049200	H	2.66257700	2.86038400	1.83320100
C	1.15666300	2.80333700	-1.90119500	H	1.37759400	2.07368800	2.76778300
H	1.87546800	3.61318000	-1.73137500	H	2.73046100	1.11871200	2.14198500
H	1.58311800	2.13095400	-2.65407900	C	-0.10396900	3.04531800	-0.00747700
H	0.24458800	3.24103400	-2.32079900	H	0.43198500	3.98665400	-0.17272400
C	2.39345100	1.16870500	0.38632900	H	-0.71489300	2.84026700	-0.89395300
H	2.84035700	0.45686800	-0.31690300	H	-0.78528700	3.18688700	0.83902500
H	3.12783800	1.96130500	0.57033100	C	2.30631300	1.44400400	-1.10163600
H	2.21941700	0.64209600	1.33074000	H	1.77989300	1.26628500	-2.04548100
C	-3.01824100	-0.26855000	1.81852000	H	2.91738200	2.34666800	-1.21838700
H	-3.39857100	0.46241400	2.54053300	H	2.98532200	0.60065200	-0.93258800
H	-3.77203700	-1.05751300	1.72146400	C	-3.44329600	0.44536200	1.29300400
H	-2.10523900	-0.71152600	2.22385800	H	-4.16973100	-0.37450900	1.40078300
				H	-2.87405600	0.49311900	2.22858800
G2b-radical				C	-3.11264100	-0.09222500	-1.21860500
C	-1.77556400	0.61004700	0.05336000	H	-3.92841000	-0.82370500	-1.16112600
C	-0.71812200	1.24787400	-0.00299600	H	-3.53566500	0.84004600	-1.61121700
C	-2.95368300	-0.09981100	0.11602100	H	-2.36963800	-0.45595400	-1.93193300
H	-3.44844600	-0.35918700	-0.81632000	C	-4.20395200	1.76083600	1.09187500
Si	0.85856700	2.19267200	-0.08708800	H	-3.47995800	2.56895900	0.91498500
C	0.89637200	3.42152600	1.33556600	H	-4.82825700	1.69849700	0.18994200
H	1.83058000	3.99481100	1.32747500	C	-5.08829100	2.11629500	2.28602300
H	0.06352200	4.12907500	1.26731100	H	-4.46672800	2.18073200	3.18911100
H	0.82285600	2.90728300	2.29959500	H	-5.80427500	1.30187700	2.46127500
C	0.93217900	3.09145100	-1.73611300	C	-5.84135400	3.42979500	2.08520000
H	1.86675400	3.65747800	-1.82439700	H	-6.46591200	3.67292000	2.95043700
H	0.88391800	2.38461900	-2.57103200	H	-5.14239200	4.25976500	1.93169000

H	-6.49228300	3.37717800	1.20516000	C	0.06167500	2.75589500	1.15757400
				H	0.68094100	3.60975800	1.45407200
G2c-radical				H	-0.93322400	3.13272100	0.89665600
C	-1.50852600	1.04092800	0.01792100	H	-0.05162300	2.09895800	2.02752100
C	-0.34369200	1.44491200	-0.06566300	C	0.94096800	2.92956400	-1.81114400
C	-2.80867600	0.58362400	0.11624600	H	1.56209400	3.81162400	-1.61685200
Si	1.38276300	2.05979500	-0.20286300	H	1.38379900	2.38922700	-2.65527500
C	1.76982400	3.11382000	1.30637400	H	-0.05178100	3.27596500	-2.11714900
H	2.79563300	3.49702900	1.25573300	C	2.55829900	1.21994000	0.17104500
H	1.09070200	3.97019200	1.37283100	H	3.00135100	0.63810600	-0.64493100
H	1.67068600	2.53240800	2.22904800	H	3.22960500	2.05976600	0.38462200
C	1.53045800	3.08826000	-1.77063600	H	2.52517400	0.58082200	1.06014300
H	2.55276500	3.46424200	-1.89339300	C	-2.36081000	-0.83390700	2.07422500
H	1.27889200	2.49403900	-2.65534300	C	-3.55325400	-1.00295400	2.78734900
H	0.85360500	3.94847800	-1.73967000	C	-1.17973100	-1.37182800	2.60538600
C	2.55743800	0.59213200	-0.28126000	C	-3.56891400	-1.69151200	3.99851100
H	2.33295200	-0.04503800	-1.14308600	H	-4.47620300	-0.59007500	2.38663800
H	3.59540700	0.93334400	-0.37136200	C	-1.19554400	-2.05939700	3.81324700
H	2.47900600	-0.02254000	0.62156600	H	-0.24656500	-1.24753200	2.06032400
C	-3.50593000	0.54081800	1.44758300	C	-2.39048200	-2.22344400	4.51693700
H	-3.96771200	-0.44985100	1.58030000	H	-4.50524000	-1.81228300	4.53606400
H	-2.77407600	0.66890100	2.25272200	H	-0.27101900	-2.47003700	4.20949100
C	-3.58388600	0.21576400	-1.11598700	H	-2.40067400	-2.76183200	5.45997900
H	-4.21323600	-0.66282600	-0.92711400				
H	-4.25461900	1.03193300	-1.42096000	G3a-radical			
H	-2.92010300	0.00136600	-1.95682100	C	-1.52726200	0.14753000	0.06370500
C	-4.60087600	1.61201900	1.57900700	C	-0.58360000	0.93405400	-0.00136200
H	-4.15105300	2.60225700	1.42468200	C	-2.59345300	-0.74170900	0.14704400
H	-5.34593100	1.47714000	0.78270900	H	-2.99684800	-1.14122600	-0.78001800
C	-5.30123500	1.56990600	2.93605300	Si	0.83664300	2.10732700	-0.08268700
H	-4.55487400	1.69980000	3.73085300	C	0.81586700	3.16091000	1.47455700
H	-5.74201400	0.57493900	3.08440600	H	1.65158200	3.87012400	1.47195100
C	-6.38478900	2.63823900	3.06765700	H	-0.11484700	3.73286700	1.54899900
H	-6.87614500	2.59364900	4.04464500	H	0.90286800	2.53887500	2.37172600
H	-5.95995000	3.64132900	2.95033900	C	0.63998200	3.18272300	-1.61046400
H	-7.15486400	2.51098700	2.29853600	H	1.47049100	3.89368700	-1.68980400
				H	0.62677300	2.57421300	-2.52063400
G3a				H	-0.29340600	3.75374000	-1.57287200
C	-1.32180400	0.09864400	0.03321400	C	2.42916400	1.11295400	-0.18033400
C	-0.24349000	0.33416400	-0.66545200	H	2.44651100	0.48633700	-1.07796000
H	0.03587800	-0.36792400	-1.45529900	H	3.29883100	1.77936500	-0.21362300
C	-2.37620900	-0.09317400	0.79744700	H	2.53642100	0.45732600	0.69010000
H	-3.33153300	0.32080600	0.47669600	C	-3.18948700	-1.16370100	1.38357900
Si	0.83723600	1.83490200	-0.28301500	C	-4.26544900	-2.07754100	1.36811500

C	-2.73042800	-0.69080200	2.63274100
C	-4.85575500	-2.50095300	2.55026300
H	-4.62896700	-2.44912600	0.41300500
C	-3.32570800	-1.11833600	3.81029700
H	-1.90282300	0.01312300	2.65654600
C	-4.38965000	-2.02461300	3.77836300
H	-5.68286000	-3.20433600	2.51833800
H	-2.96059600	-0.74523400	4.76289500
H	-4.85155900	-2.35698200	4.70322500

1c

C	-1.34695000	0.07961500	0.01722600
C	-0.25223000	0.29630200	-0.66374500
H	0.03546000	-0.40961400	-1.44733700
C	-2.42941200	-0.06233100	0.75622600
Si	0.82095900	1.79596600	-0.26200300
C	0.01016700	2.71248400	1.16349700
H	0.61115300	3.57688000	1.46709100
H	-0.98600800	3.07293800	0.88337700
H	-0.10873400	2.05685800	2.03372900
C	0.94971500	2.89785500	-1.78370000
H	1.56194800	3.78249400	-1.57344700
H	1.41176400	2.36383000	-2.62150100
H	-0.03872300	3.24046900	-2.10770600
C	2.53860700	1.19512600	0.22480000
H	3.00215600	0.61964200	-0.58427900
H	3.19813300	2.04036800	0.45324800
H	2.49443600	0.55313700	1.11137300
C	-2.38667100	-0.80466200	2.04371900
C	-3.55180600	-0.99099100	2.79768200
C	-1.18349700	-1.32739500	2.54562500
C	-3.51779600	-1.67685400	4.01209700
H	-4.49988800	-0.60059900	2.44105300
C	-1.15010100	-2.01070000	3.75431600
H	-0.26763700	-1.19420300	1.97461900
C	-2.31919300	-2.19012500	4.49706600
H	-4.43638900	-1.80814300	4.57729100
H	-0.20677800	-2.40580700	4.12106300
H	-2.29228700	-2.72491600	5.44187400
C	-3.73543100	0.54787600	0.29580400
H	-4.50115100	-0.22246200	0.14857400
H	-4.11522200	1.25999100	1.03788000
H	-3.59718800	1.07583900	-0.64980200

1c-radical

C	-1.72481900	0.52754000	0.00538700
C	-0.68428000	1.18308700	-0.00897700
C	-2.90822000	-0.21248200	0.02830800
Si	0.86778500	2.17352000	-0.07215300
C	0.74600700	3.56652900	1.18386200
H	1.65689900	4.17603000	1.17433200
H	-0.10375700	4.22099800	0.96369900
H	0.61363300	3.17066900	2.19615900
C	1.04566300	2.86601100	-1.81122900
H	1.95196000	3.47716200	-1.89304400
H	1.11365900	2.06008100	-2.54968700
H	0.18814700	3.49423600	-2.07397800
C	2.32053100	1.05234000	0.33870300
H	2.39862800	0.23001300	-0.37989300
H	3.26068400	1.61556200	0.31428200
H	2.21136800	0.61746900	1.33761800
C	-3.40292400	-0.73870100	1.34789400
H	-4.40104000	-0.34580300	1.58056100
H	-3.47795300	-1.83360800	1.33433200
H	-2.72609000	-0.45196300	2.15416000
C	-3.64077900	-0.46027900	-1.19536300
C	-4.84286500	-1.20026300	-1.18532300
C	-3.17846100	0.03191600	-2.43669000
C	-5.54685900	-1.43336900	-2.36067500
H	-5.22843200	-1.59455900	-0.25016100
C	-3.88583400	-0.20530400	-3.60540400
H	-2.25592800	0.60485500	-2.46412200
C	-5.07533400	-0.93889700	-3.57723100
H	-6.46943600	-2.00596300	-2.32789600
H	-3.51018700	0.18353600	-4.54761600
H	-5.62700600	-1.12367700	-4.49410800

G3b

C	-1.41604600	-0.03853800	0.05470600
C	-0.34581200	0.10848600	-0.67891500
H	-0.10986500	-0.64035500	-1.43930800
C	-2.47342500	-0.08340500	0.84536100
Si	0.75018300	1.62614100	-0.42211700
C	-0.11576400	2.75436600	0.80404900
H	0.46072200	3.67243900	0.96472900
H	-1.10995500	3.03614400	0.43907600
H	-0.24906900	2.26548600	1.77570900
C	0.97711600	2.48586000	-2.08143300

H	1.63320000	3.35854600	-1.98496800	H	2.35391100	0.53405100	-0.74667800
H	1.42575300	1.81086600	-2.81888100	H	3.10620100	1.93908700	0.03227000
H	0.01567800	2.82796000	-2.47909700	H	2.31346900	0.69555900	1.01601100
C	2.42301300	1.07056400	0.24208500	C	-3.20227800	-1.25223000	1.33438500
H	2.91246900	0.37492900	-0.44855800	C	-4.53479700	-1.66409100	1.53365400
H	3.09221000	1.92673600	0.38574600	C	-2.32205300	-1.30168200	2.43268700
H	2.31302400	0.56281700	1.20664800	C	-4.95879300	-2.12528200	2.77458200
C	-2.39627200	-0.75798800	2.17234600	H	-5.24599600	-1.58839100	0.71651800
C	-3.52931800	-1.36599100	2.72769700	C	-2.74863900	-1.77077300	3.66864100
C	-1.18745500	-0.82441400	2.87712000	H	-1.29421100	-0.97696100	2.29677600
C	-3.45325100	-2.02575100	3.95199900	C	-4.06824000	-2.18909000	3.84660800
H	-4.47333200	-1.32782800	2.19066600	H	-5.99384500	-2.42681400	2.90846700
C	-1.11102400	-1.48554700	4.09903100	H	-2.04836400	-1.81195300	4.49805700
H	-0.30210600	-0.35298300	2.45652500	H	-4.40208400	-2.55314900	4.81371200
C	-2.24474900	-2.08862100	4.64342900	C	-3.34185500	-1.13121300	-1.23253800
H	-4.34203900	-2.49517400	4.36426800	C	-3.93513400	-2.39751100	-1.40537200
H	-0.16469300	-1.52462400	4.63131000	C	-3.28696100	-0.26755900	-2.34369600
H	-2.18609300	-2.60110300	5.59923400	C	-4.46865800	-2.77161600	-2.63308700
C	-3.74189700	0.56275200	0.39906600	H	-3.94434700	-3.10074000	-0.57801200
C	-4.16640200	0.47004900	-0.93104000	C	-3.82898000	-0.64301300	-3.56629400
C	-4.50889900	1.31235200	1.30078200	H	-2.82241100	0.70793900	-2.22852300
C	-5.32552400	1.11655200	-1.35369600	C	-4.42684900	-1.89534400	-3.71786400
H	-3.58125300	-0.12038500	-1.63152700	H	-4.91025200	-3.75756300	-2.74715300
C	-5.66792900	1.95763100	0.87824400	H	-3.78632600	0.04454300	-4.40623400
H	-4.18639800	1.39397200	2.33584500	H	-4.84740300	-2.18942400	-4.67502700
C	-6.08133300	1.86197600	-0.45040000				
H	-5.64281800	1.03088800	-2.38920500				
H	-6.24831500	2.54013600	1.58830900				
H	-6.98786600	2.36275300	-0.77785000				

G3b-radical

C	-1.68548400	0.18269300	0.02773100
C	-0.75747400	0.98704900	0.00829300
C	-2.74587500	-0.73471900	0.04417000
Si	0.63338000	2.19654700	-0.04938000
C	0.45737900	3.38526600	1.39501700
H	1.27326100	4.11735400	1.39381600
H	-0.49006700	3.93132800	1.34179200
H	0.48384800	2.85002700	2.34996400
C	0.53156300	3.11725800	-1.68466900
H	1.34699200	3.84428400	-1.77266200
H	0.60304700	2.42369300	-2.52914200
H	-0.41609300	3.65920100	-1.77142300
C	2.25366700	1.25133600	0.07439000