Supporting Information

Dielectric Relaxation of Powdered Molecular Gyrotops Having a Thiophene Dioxide-diyl as a Dipolar Rotor

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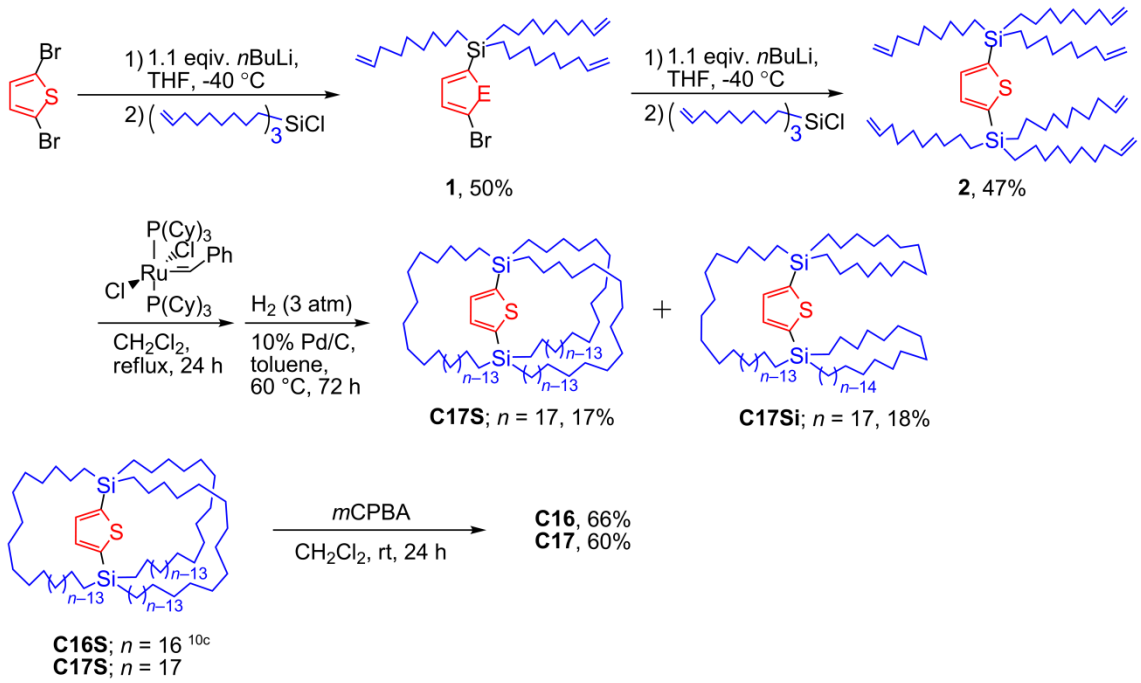
1. Synthetic Procedure

General

All reactions were performed under anhydrous conditions using argon, unless otherwise noted. The chemical shifts of ^{1}H and ^{13}C NMR spectra are based on residual solvent resonances. NMR signals were assigned using 1D and 2D NMR techniques (^{1}H, ^{13}C, HSQC, and HMBC).

Materials

Commercially available reagents were used as received without further purification.



Scheme S1. Synthesis of molecular gyrotops **C16** and **C17**.

Synthesis of 2-Bromo-5-tri(8-nonenyl)silylthiophene (1)

2,5-Dibromothiophene (2.7 g, 11.4 mmol) was dissolved in dry tetrahydrofuran (80 mL). An *n*-BuLi solution (1.6 M in hexane, 7.2 mL, 11.2 mmol) was added dropwise to the mixture for 10 min at −55 °C. After the reaction mixture was then stirred for 40 min at −55 °C, chlorotri(8-nonenyl)silane (4.9 g, 11.2 mmol) was added. Then the mixture was warmed to room temperature, and stirred for 16 h. The mixture was hydrolyzed with dilute HCl (aq) solution and extracted with hexane. The organic layer was washed with saturated $NaHCO_3$ (aq) solution and dried over anhydrous Na_2SO_4. Silica gel column chromatography (hexane and toluene = 4 : 1 as an eluent) of the concentrated residue afforded crude product as a colorless oil. Pure compound **1** (3.4 g, 6.0 mmol, 50% yield) was obtained as a colorless oil after GPC purification (chloroform).

1: a colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$, 7.24 ppm) δ 0.73 (t, *J* = 5.0, 6H, Si-C*H*$_2$-), 1.26-1.36 (m, 30H), 2.02 (q, *J* = 7.0 Hz, 6H, H_2C=CH-C*H*$_2$-), 4.91 (d, *J* = 10.5 Hz, 3H, *H*$_2$C=CH-), 4.97 (d, *J* = 18.0 Hz, 3H, *H*$_2$C=CH-), 5.79 (ddt, *J* = 18.0, 10.5, 7.0 Hz, 3H, H_2C=C*H*-), 6.93 (d, *J* = 3.3 Hz, 1H, thiophene), 7.06 (d, *J* = 3.3 Hz, 1H, thiophene); ^{13}C NMR (126 MHz, $CDCl_3$,

77.0 ppm) δ 13.20, 23.63, 28.90, 29.01, 33.52, 33.78, 114.10 (-CH=*C*H_2), 116.54 (Br*C*), 130.98, 134.89 (thiophene, *C*H), 139.03 (-*C*H=CH_2), 140.52 (Si*C*); ^{29}Si NMR (99 MHz, $CDCl_3$) δ −3.5; HRMS (APCI, positive) calcd for $C_{31}H53BrSSi$, 564.2815; (M^+) found, 564.2816 (M^+).

Synthesis of 2-tri(9-decenyl)silyl-5-tri(8-nonenyl)silylthiophene (2)

2-Bromo-5-tri(8-nonenyl)silylthiophene (**1**, 2.8 g, 4.9 mmol) was dissolved in dry tetrahydrofuran (120mL). An *n*-BuLi solution (1.6 M in hexane, 3.4 mL, 5.4 mmol) was added dropwise to the mixture for 10 min at −55 °C. After the reaction mixture was then stirred for 40 min at −55 °C, chlorotri(9-decenyl)silane (2.6 g, 5.4 mmol) was added. Then the mixture was warmed to room temperature, and stirred for 16 h. The mixture was hydrolyzed with dilute HCl (aq) solution and extracted with hexane. The organic layer was washed with saturated $NaHCO_3$ (aq) solution and dried over anhydrous Na_2SO_4. Silica gel column chromatography (hexane and toluene = 4 : 1 as an eluent) of the concentrated residue afforded crude product as a colorless oil. Pure compound **2** (2.2 g, 2.4 mmol, 47% yield) was obtained as a colorless oil after GPC purification (chloroform).

2: a colorless oil; ^{1}H NMR ($CDCl_3$, 500 MHz, 7.24 ppm): δ 0.79 (t, *J* = 7.5 Hz, 12H, Si-C*H*$_2$-), 1.27-1.40 (m, 66H), 2.03 (q, *J* = 7.4 Hz, 12H, H_2C=CH-C*H*$_2$-), 4.92 (d, *J* = 10.5 Hz, 6H, *H*$_2$C=CH-), 4.97 (d, *J* = 17.5 Hz, 6H, *H*$_2$C=CH-), 5.81 (ddt, *J* = 17.5, 10.5, 7.4 Hz, 6H, H_2C=C*H*-), 7.28 (s, 2H, thiophene), ^{13}C NMR (126 MHz, $CDCl_3$, 77.0 ppm) δ 13.59, 13.60, 23.77, 28.96, 29.07, 29.19, 29.44, 33.60, 33.66, 33.82, 33.84, 114.10 (-CH=*C*H_2), 135.25, (thiophene, *C*H), 139.17 (-*C*H=CH_2), 142.96, 143.02 (thiophene, Si*C*); ^{29}Si NMR (99 MHz, $CDCl_3$) δ −4.3; HRMS (ESI, positive) calcd for $C_{61}H_{110}SSi_2Na$, 953.7759; ($M+Na^+$) found, 953.7759 ($M+Na^+$).

Procedure for Synthesis of molecular gyrotop C17S and Non-cage Isomer C17Si

To a solution of first-generation Grubbs' catalyst (ca. 0.05 g, ca. 0.06 mmol) in dichloromethane (750 mL), precursor **2** (1000 mg, 1.1 mmol) in dichloromethane (250 mL) was added dropwise while stirring over 10 h, and the mixture was further stirred for 24 h. The volatile materials were removed *in vacuo*, and the metal catalyst was removed from the toluene-soluble fraction by flash column chromatography (silica gel, toluene).

To the reaction mixture solution of toluene (10 mL) under the presence of 10% Pd/C (ca. 0.03 g) in an autoclave hydrogen gas (3 atm) was introduced. The mixture was stirred for 72 h at 60°C. After the excess H_2 gas was released, the mixture was filtered to remove the Pd/C. The volatile materials were removed *in vacuo*. The fractions containing cage and non-cage isomer were collected separately by GPC (chloroform), and the solvents were evaporated. Pure compound **C17S** (160 mg, 0.19 mmol in 17% yield) was obtained as colorless crystals by recrystallization from ethanol solution. Pure compound **C17Si** (174 mg, 0.20 mmol in 18% yield) was obtained without further purification.

C17S: a colorless oil, ^{1}H NMR ($CDCl_3$, 500 MHz, 7.24 ppm): δ 0.74-0.78 (m, 12H, Si-C*H*$_2$-), 1.23-1.37 (m, 90H), 7.31 (s, 2H, thiophene), ^{13}C NMR (126 MHz, $CDCl_3$, 77.0 ppm) δ 13.68, 23.40, 28.16, 28.38, 28.40, 28.41, 28.57, 28.73, 33.16, 135.22, (thiophene, *C*H), 142.90 (Si*C*); ^{29}Si NMR (99 MHz, $CDCl_3$) δ −4.0; HRMS (ESI, positive) calcd for $C_{55}H_{104}SSi_2Na$, 875.7290; ($M+Na^+$) found, 875.7289 ($M+Na^+$).

C17Si: a colorless oil, ^{1}H NMR ($CDCl_3$, 500 MHz, 7.24 ppm): δ 0.73-0.75 (m, 4H, Si-C*H*$_2$-), 0.78-0.88 (m, 8H), 1.23-1.37 (m, 78H), 7.29 (s, 2H, thiophene), ^{13}C NMR (126 MHz, $CDCl_3$, 77.0 ppm) δ 13.31, 13.36, 13.99, 14.03, 23.06, 23.34, 23.44, 27.13, 27.40, 27.61, 27.64, 27.70, 27.76, 27.94, 27.99, 28.05, 28.08, 28.12, 28.16, 28.18, 28.29, 28.31, 28.33, 28.39, 28.43, 28.55, 28.59, 28.64, 28.67, 32.40, 32.98, 33.19, 135.24 (thiophene, *C*H), 143.20, 143.21 (Si*C*); ^{29}Si NMR (99 MHz, $CDCl_3$) δ −4.0; HRMS (ESI, positive) calcd for $C_{55}H_{104}SSi_2Na$, 875.7290; ($M+Na^+$) found, 875.7290 ($M+Na^+$).

Procedure for Synthesis of Thiophene-dioxide Bridged Macrocages

Macrocage and *m*-chloroperoxybenzoic acid (*m*CPBA) were dissolved in dry CH_2Cl_2 (50 mL). The reaction mixture was then stirred for 24 h at rt. The mixture was quenched with dilute aqueous $NaHCO_3$ solution and extracted with dichloromethane. The organic layer was washed 10 times with dilute aqueous $NaHCO_3$ solution to remove chlorobenzoic acid completely. The mixture was dried over anhydrous Na_2SO_4, the solution was filtered, and the volatile materials were removed in vacuo. The crude residue was fractionated by GPC (chloroform). Pure compound was obtained as a colorless oil after recrystallization from ethanol solution.

a. Synthesis of C16

The title compound (**C16**: 170 mg, 0.20 mmol in 66% yield) was synthesized from **C16S** (250 mg, 0.31 mmol) and *m*CPBA (211 mg, 1.24 mmol).

C16: colorless crystals, mp 133-134 ºC, ^{1}H NMR ($CDCl_3$, 500 MHz, 7.24 ppm): δ 0.78-0.81 (m, 12H, Si-C*H*$_2$-), 1.22-1.37 (m, 90H); ^{13}C NMR (126 MHz, $CDCl_3$, 77.0 ppm) δ 11.88, 23.01, 28.32, 28.41, 28.49, 28.79, 28.86, 33.02, 136.29, 149.45; ^{29}Si NMR (99 MHz, $CDCl_3$) δ −2.2; HRMS (ESI, positive) calcd for $C_{52}H_{98}O_2SSi_2Na$, 865.6718; ($M+Na^+$) found, 865.6718 ($M+Na^+$).

b. Synthesis of C17

The title compound (**C17**: 132 mg, 0.15 mmol in 60% yield) was synthesized from **C17S** (220 mg, 0.26 mmol) and *m*CPBA (176 mg, 1.00 mmol).

C17: colorless crystals, mp 89.9-91.6 ºC, ^{1}H NMR ($CDCl_3$, 500 MHz, 7.24 ppm): δ 0.78-0.81 (m, 12H, Si-C*H*$_2$-), 1.22-1.37 (m, 90H), 6.72 (s, 2H, thiophene), ^{13}C NMR (126 MHz, $CDCl_3$, 77.0 ppm) δ 11.88, 23.01, 28.32, 28.41, 28.49, 28.79, 28.86, 33.02, 136.29 (thiophene, *C*H), 149.45 (Si*C*); ^{29}Si NMR (99 MHz, $CDCl_3$) δ −2.7; HRMS (ESI, positive) calcd for $C_{55}H_{104}O_2SSi_2Na$, 909.7188; ($M+Na^+$) found, 907.7187 ($M+Na^+$).

c. Synthesis of C16-*d*$_2$

The title compound was synthesized from **C16S-*d*$_2$**.

C16-*d*$_2$: colorless crystals, mp 133-136 ºC, ^{1}H NMR ($CDCl_3$, 500 MHz, 7.24 ppm): δ 0.76-0.80 (m, 12H, Si-C*H*$_2$-), 1.24-1.38 (m, 84H) , ^{13}C NMR (126 MHz, $CDCl_3$, 77.0 ppm) δ 11.68, 22.80, 27.68, 28.13, 28.25, 28.73, 28.75, 32.70, 135.86 (t, *J* = 25.8, thiophene, *C*H), 149.66; ^{29}Si NMR (99 MHz, $CDCl_3$) δ −2.2; HRMS (ESI, positive) calcd for $C_{52}H_{96}D_2O_2SSi_2Na$, 867.6844 ($M+Na^+$) found, 867.6844 ($M+Na^+$).

d. Synthesis of C17

The title compound was synthesized from **C17S-*d*$_2$**.

C17-*d*$_2$: colorless crystals, mp 90.6-92.3 ºC, ^{1}H NMR ($CDCl_3$, 500 MHz, 7.24 ppm): δ 0.77-0.80 (m, 12H, Si-C*H*$_2$-), 1.24-1.34 (m, 90H), ^{13}C NMR (126 MHz, $CDCl_3$, 77.0 ppm) δ 11.88, 23.02, 28.33, 28.42, 28.50, 28.80, 28.86, 33.04, 135.95 (t, *J* = 23.8, thiophene, *C*H), 149.39 (Si*C*); ^{29}Si NMR (99 MHz, $CDCl_3$) δ −2.7; HRMS (ESI, positive) calcd for $C_{55}H_{102}D_2O_2SSi_2Na$, 909.7313; ($M+Na^+$) found, 909.7312 ($M+Na^+$).

2. Copies of NMR and HRMS Spectra for New Compounds

a. Spectra of 1

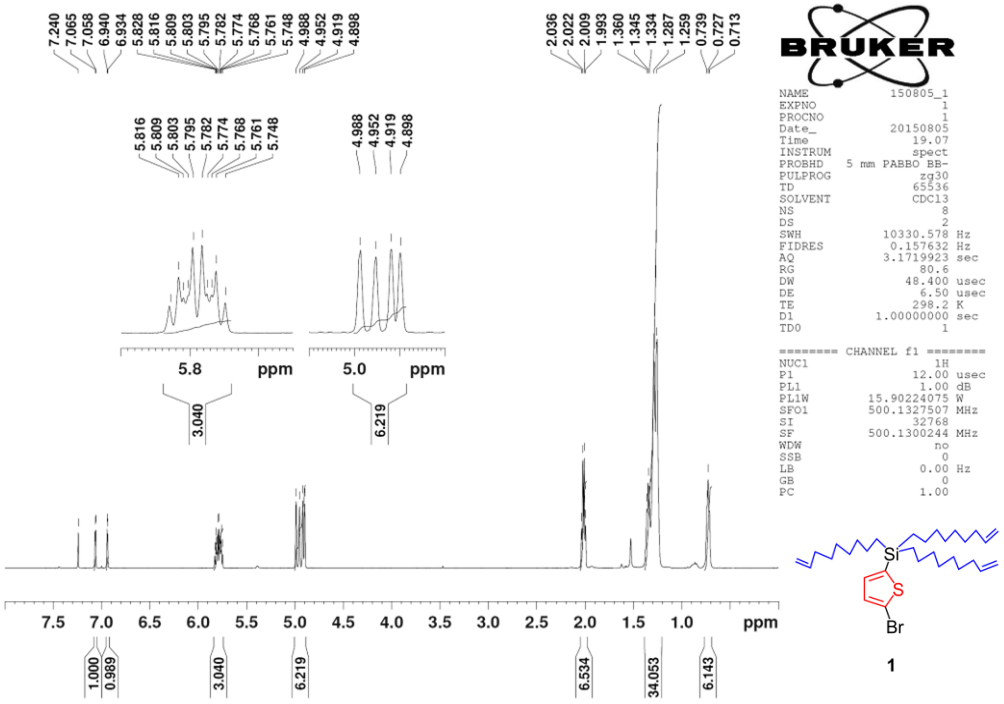


Figure S1. ^{1}H NMR spectrum of bromosilylthiophene **1** in $CDCl_3$.

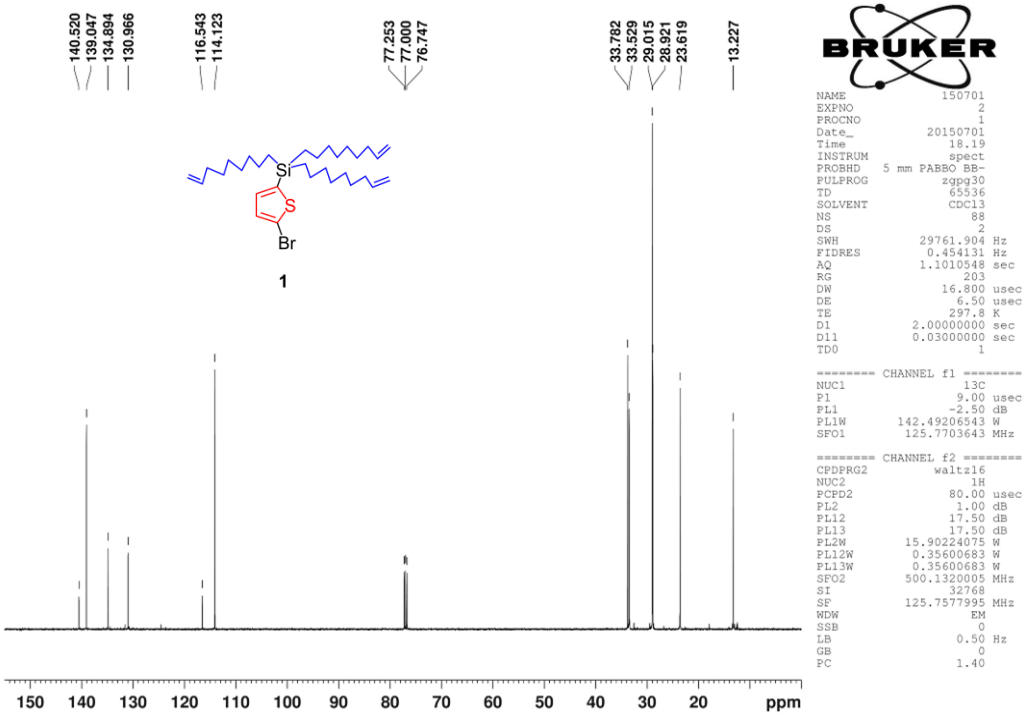


Figure S2. ^{13}C NMR spectrum of bromosilylthiophene **1** in $CDCl_3$.

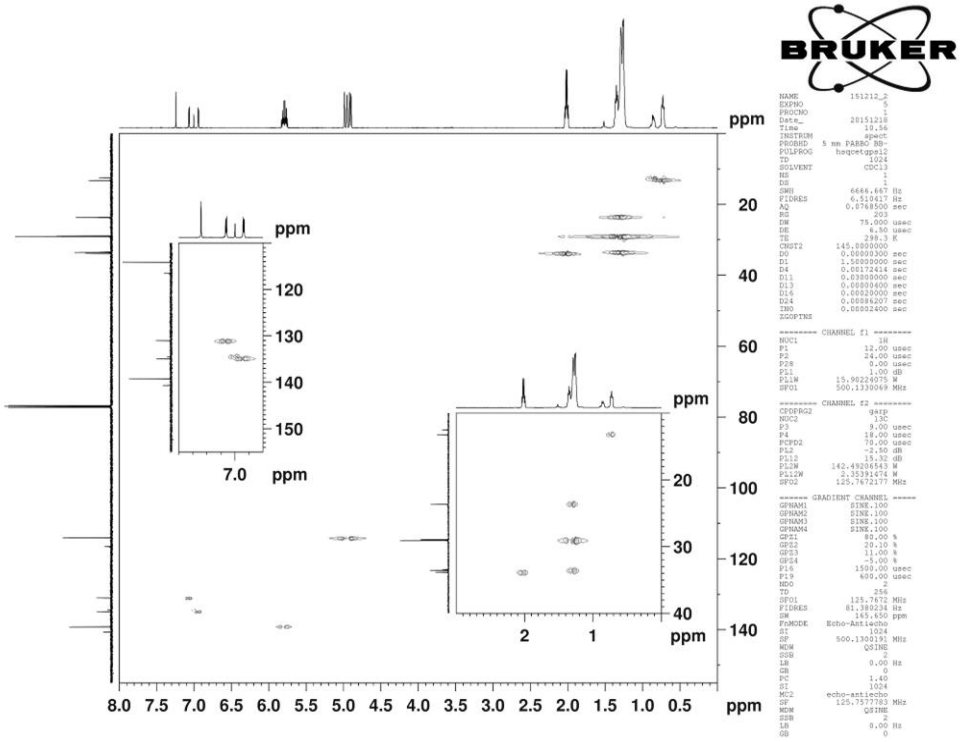


Figure S3. ^{1}H -^{13}C hsqc spectrum of bromosilylthiophene **1** in $CDCl_3$.

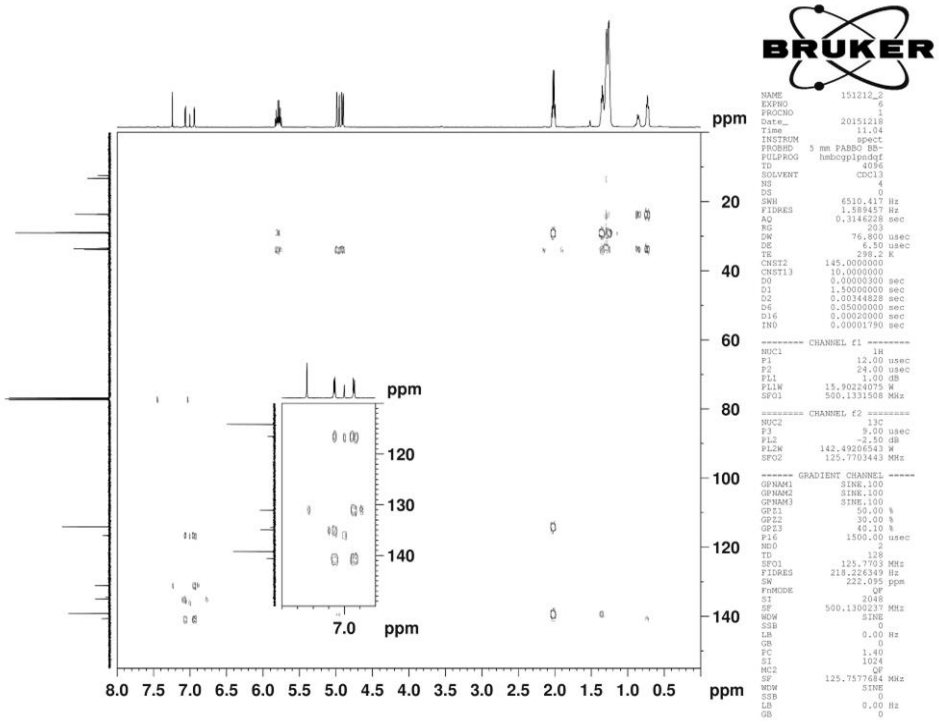


Figure S4. ^{1}H -^{13}C hmbc spectrum of bromosilylthiophene **1** in $CDCl_3$.

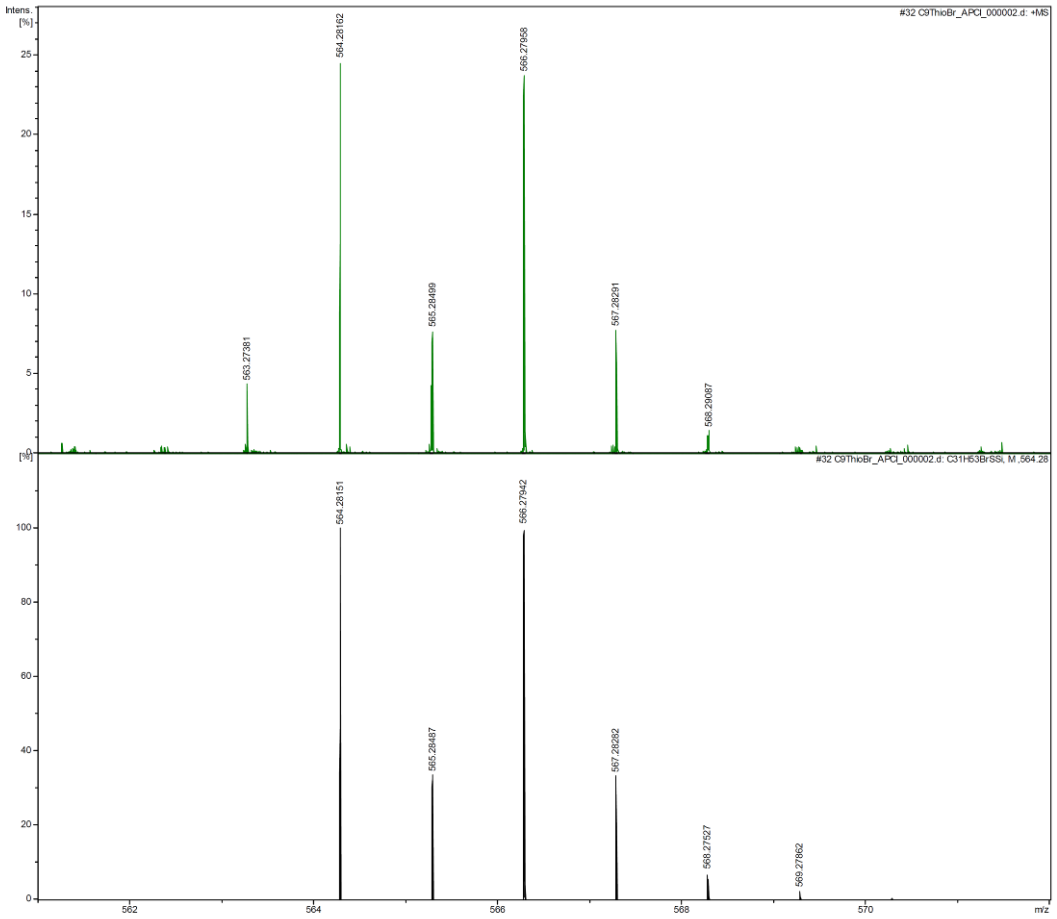


Figure S5. HRMS spectrum of bromosilylthiophene **1** (ESI, positive). Top: obsd. Bottom: sim.

b. Spectra of 2

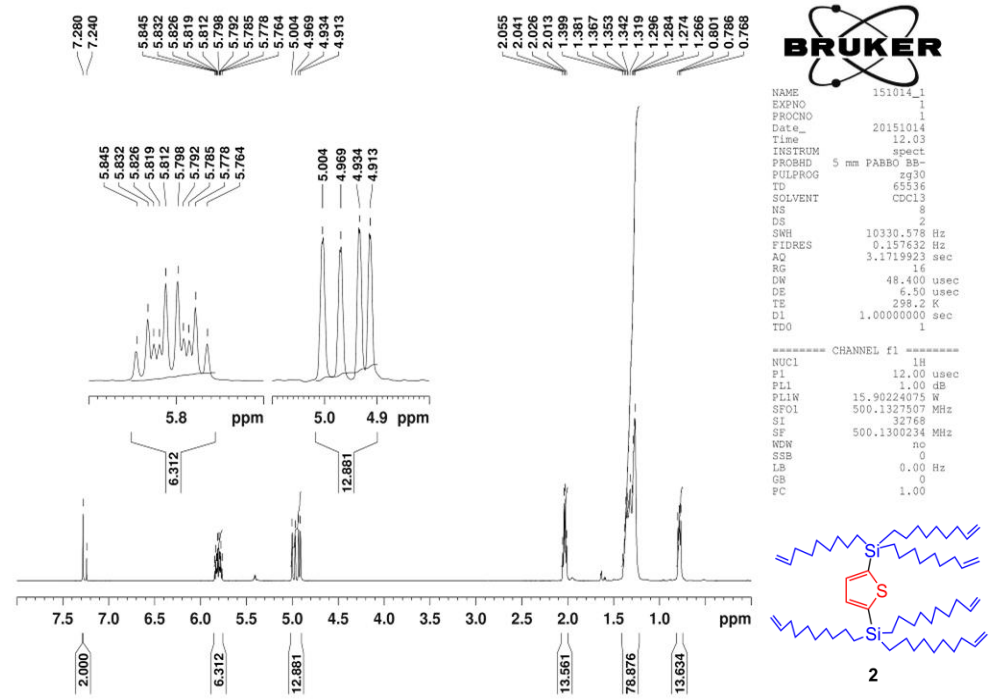


Figure S6. ^{1}H NMR spectrum of bissilylthiophene **2** in $CDCl_3$.

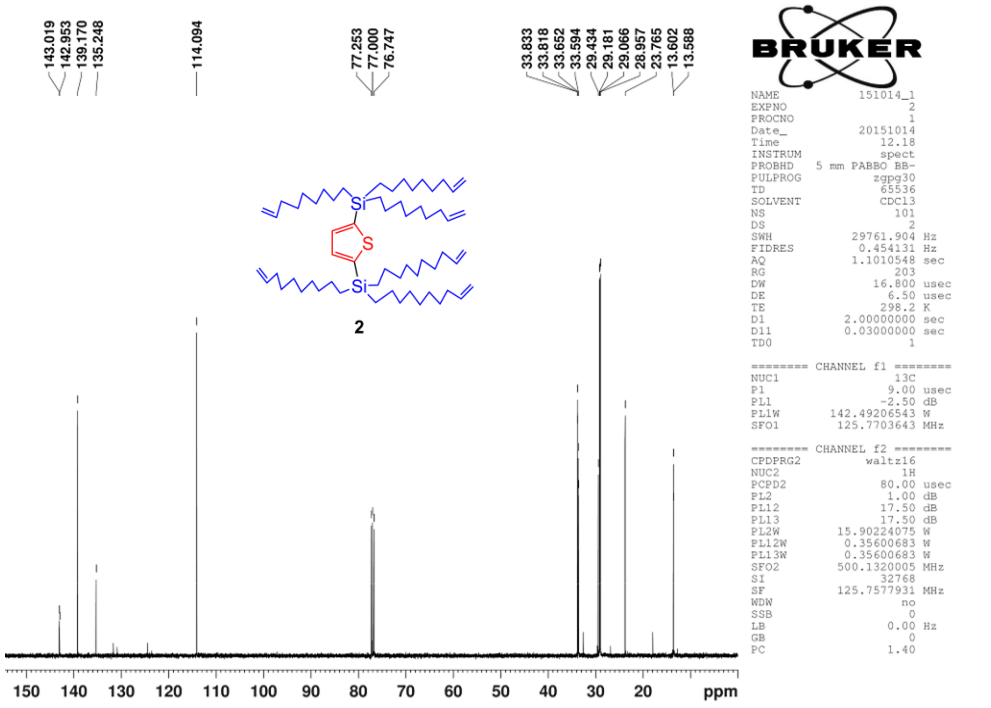


Figure S7. ^{13}C NMR spectrum of bissilylthiophene **2** in $CDCl_3$

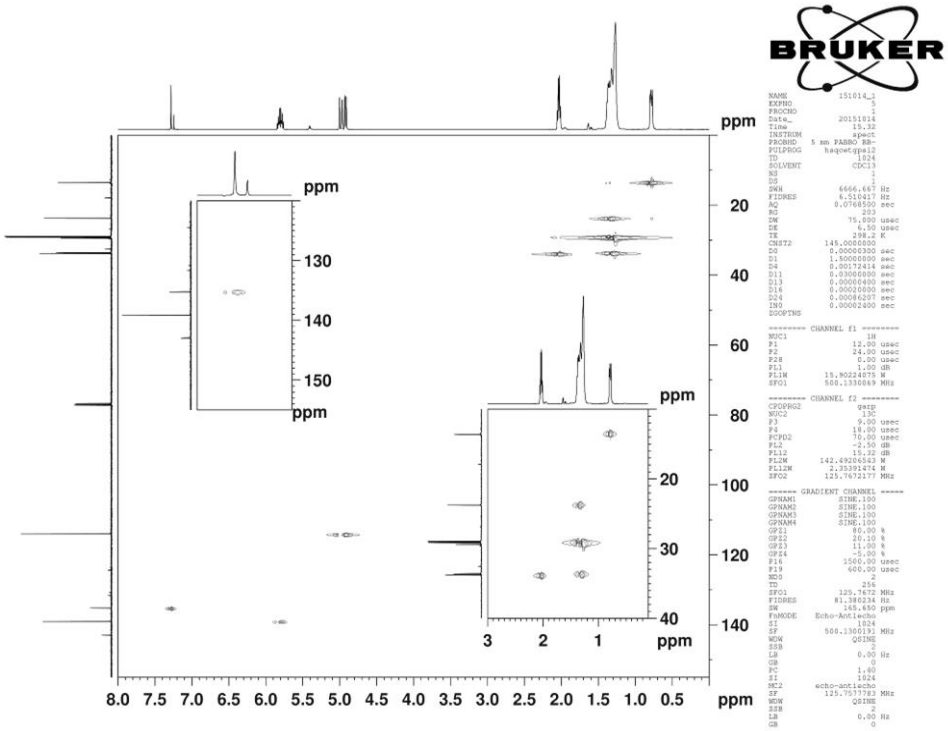


Figure S8. ^{1}H -^{13}C hsqc spectrum of bissilylthiophene **2** in $CDCl_3$.

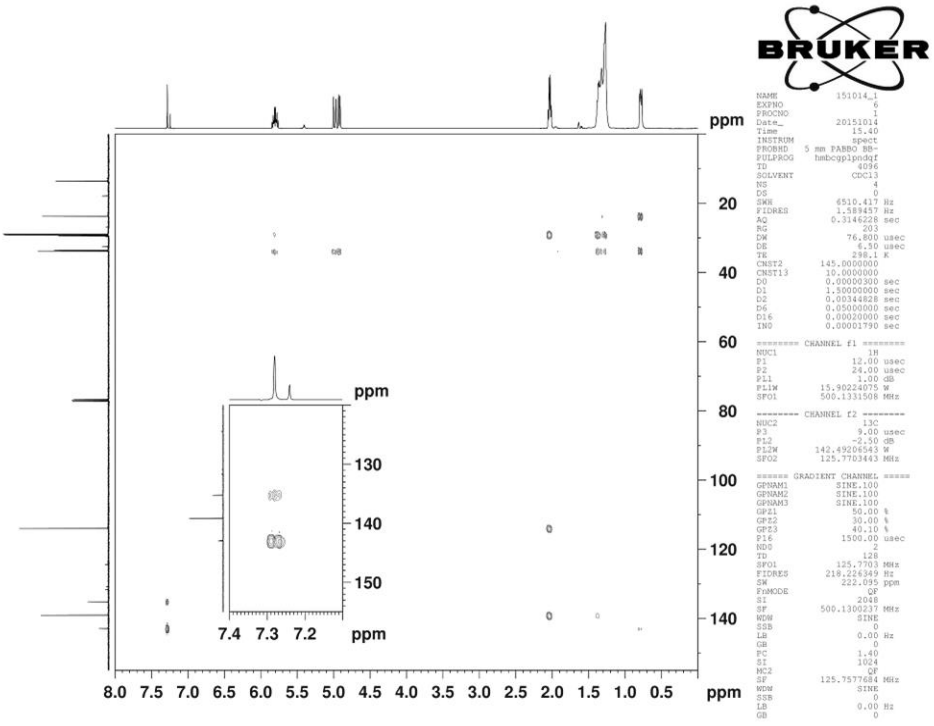


Figure S9. ^{1}H -^{13}C hmbc spectrum of bissilylthiophene **2** in $CDCl_3$.

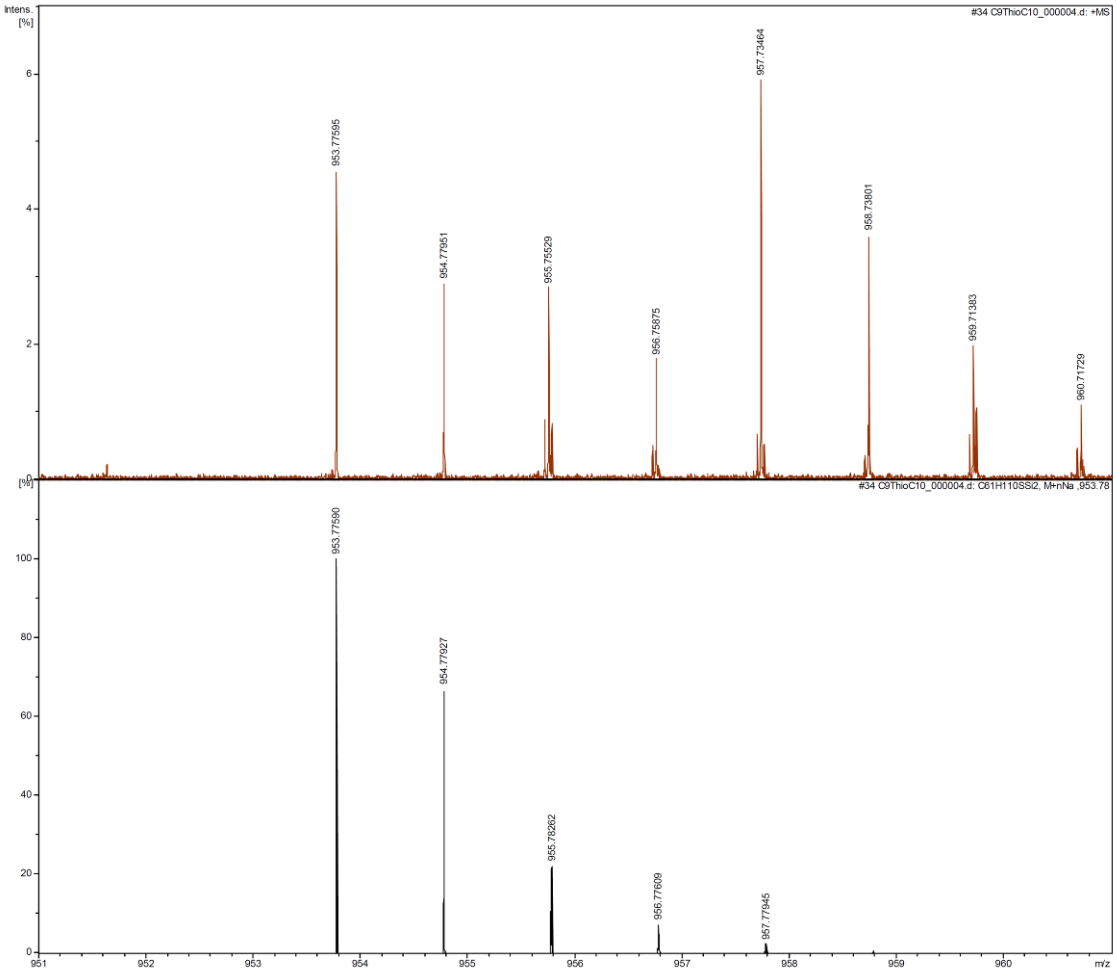


Figure S10. HRMS spectrum of bissilylthiophene **2** (ESI, positive). Top: obsd. Bottom: sim.

c. Spectra of C17S

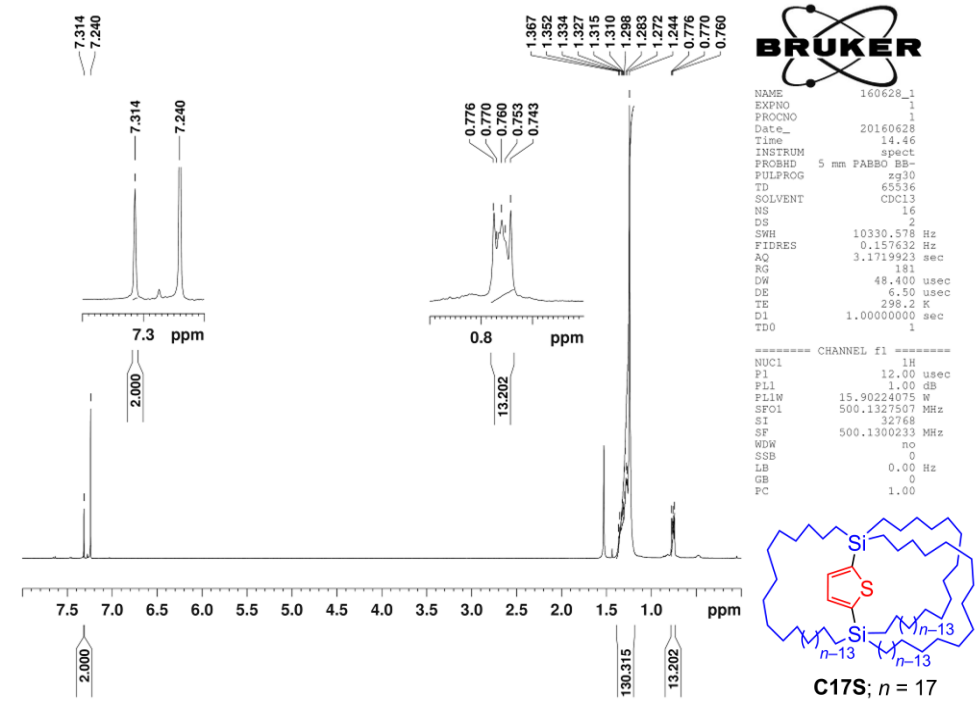


Figure S11. ^{1}H NMR spectrum of gyrotop **C17S** in $CDCl_3$.

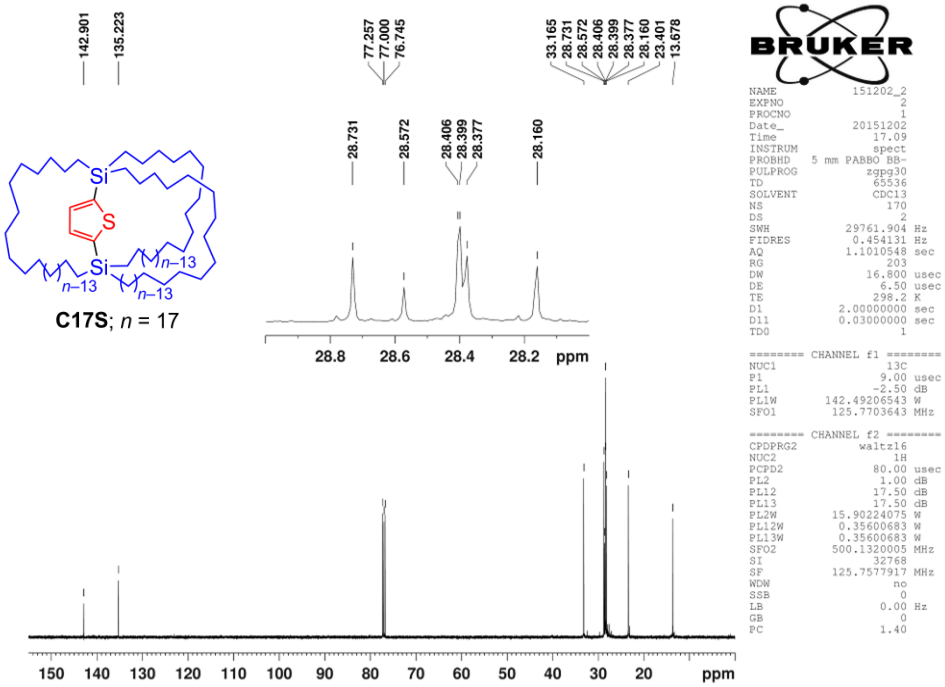


Figure S12. ^{13}C NMR spectrum of gyrotop **C17S** in $CDCl_3$.

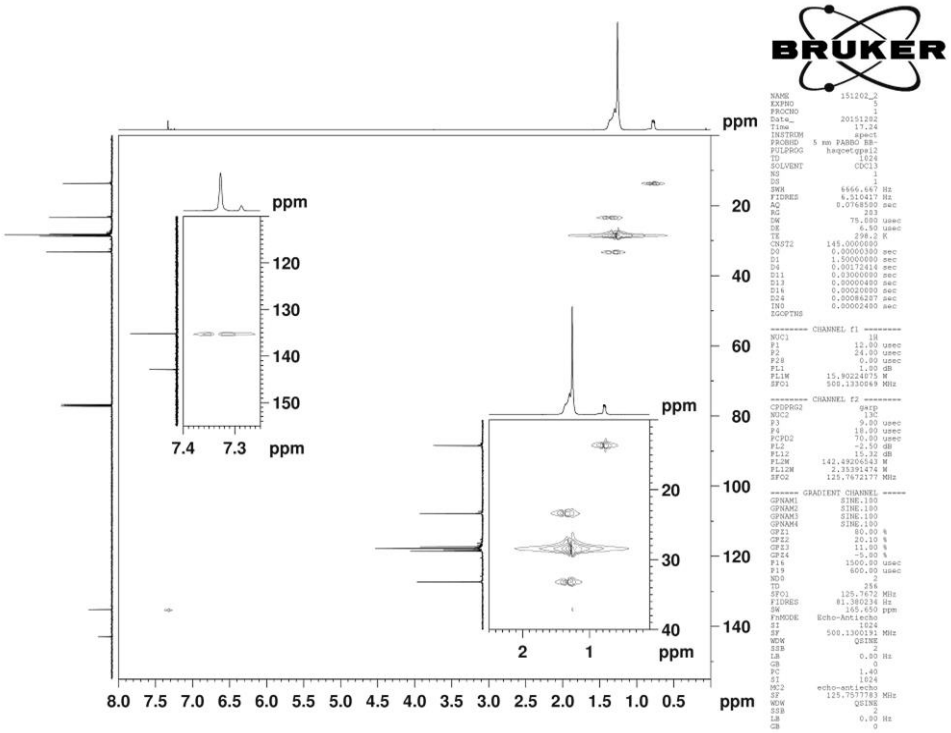


Figure S13. ^{1}H -^{13}C hsqc spectrum of gyrotop **C17S** in $CDCl_3$.

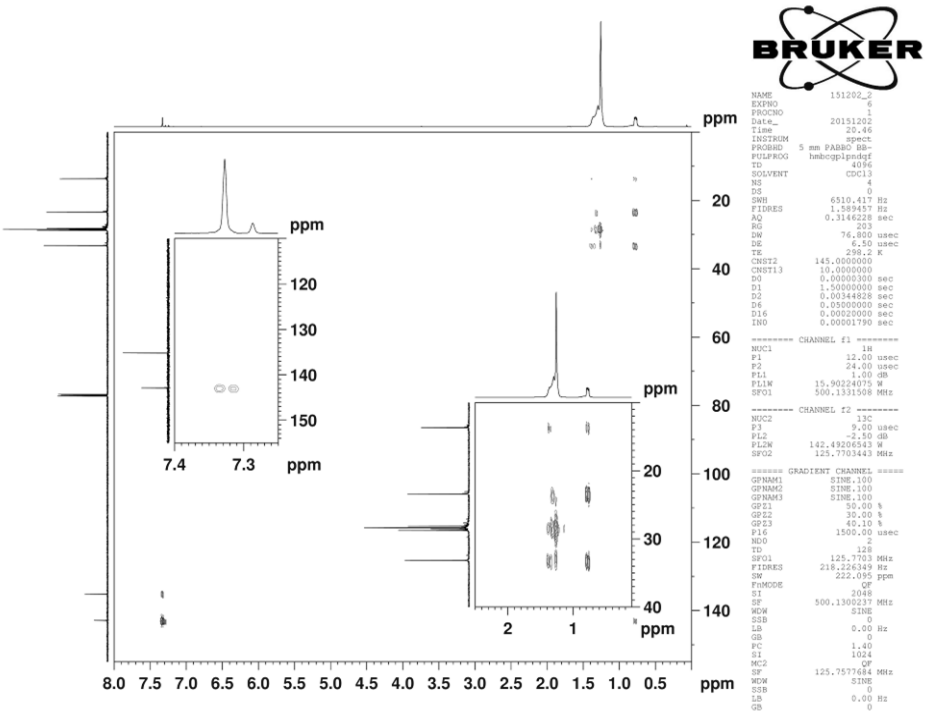


Figure S14. ^{1}H -^{13}C hmbc spectrum of gyrotop **C17S** in $CDCl_3$.

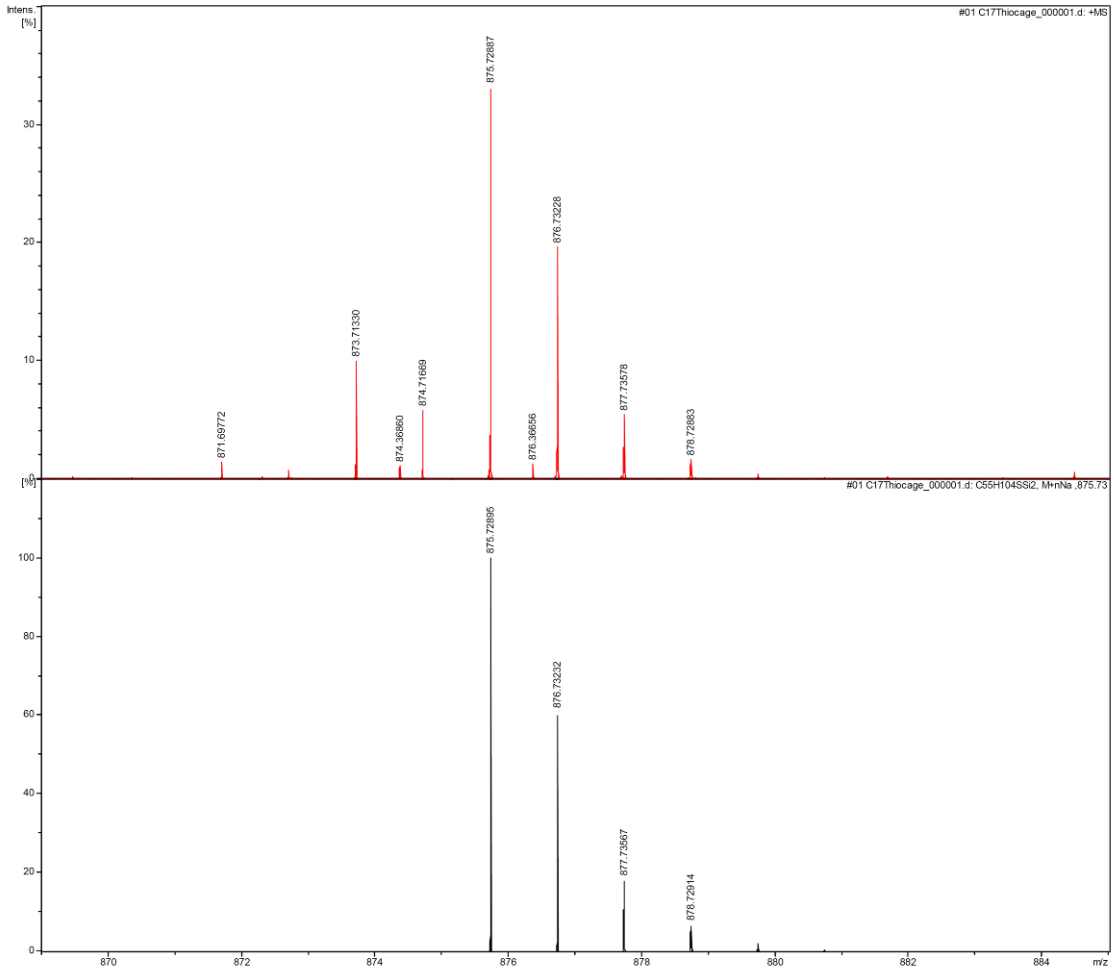


Figure S15. HRMS spectrum of gyrotop **C17S** (ESI, positive). Top: obsd. Bottom: sim.

d. Spectra of C17Si

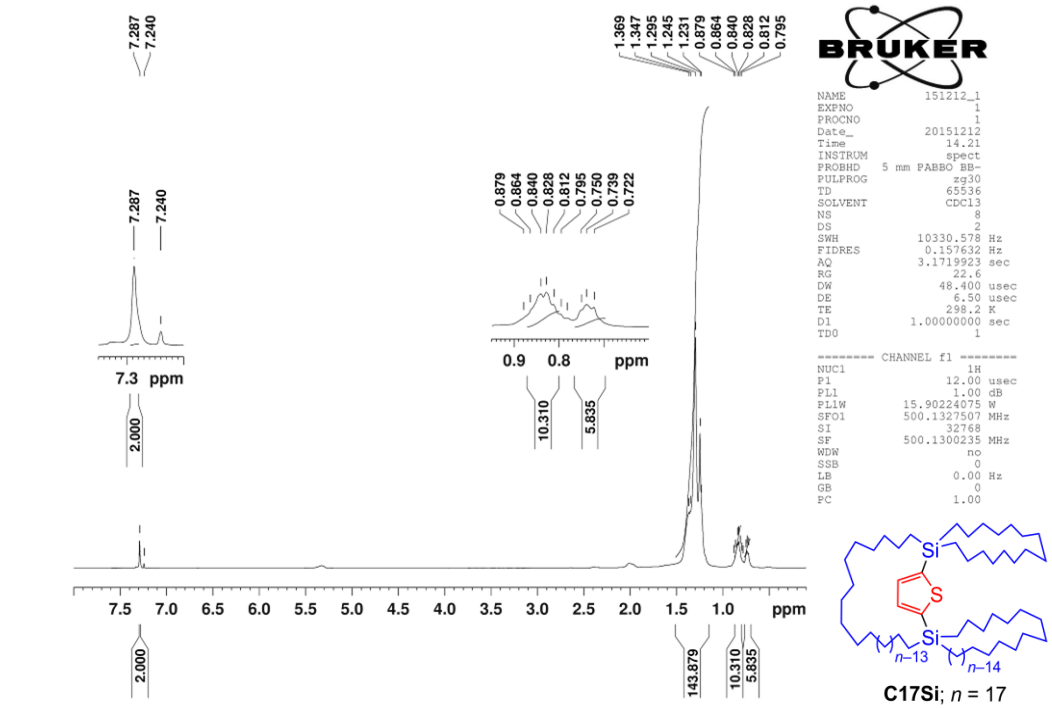


Figure S16. ^{1}H NMR spectrum of gyrotop isomer **C17Si** in $CDCl_3$.

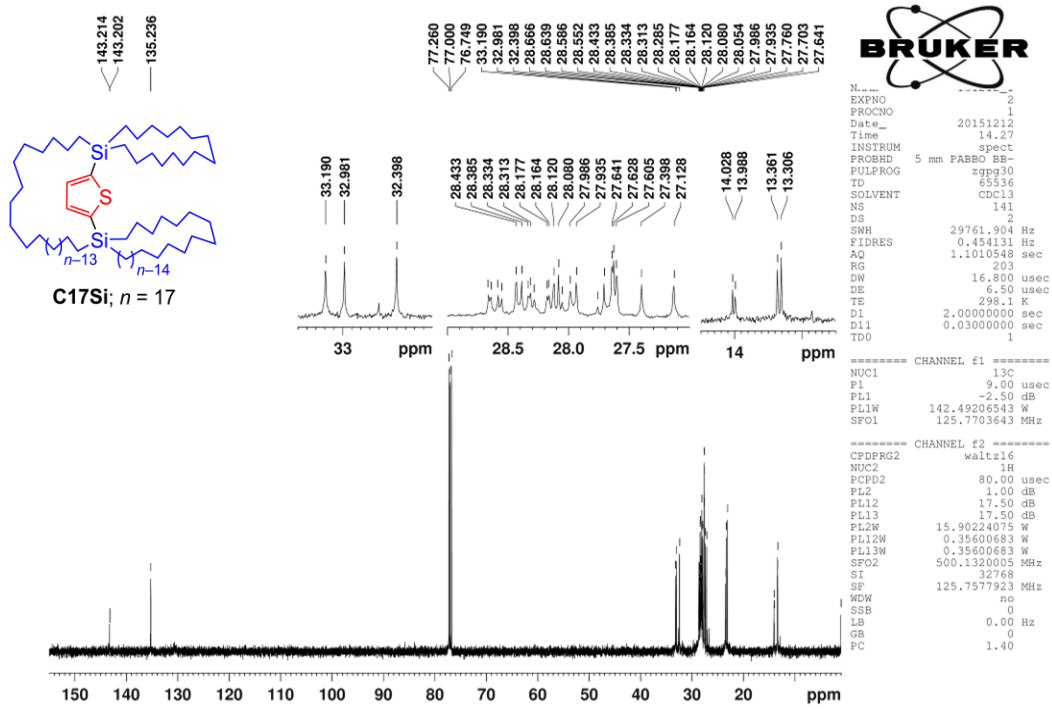


Figure S17. ^{13}C NMR spectrum of gyrotop isomer **C17Si** in $CDCl_3$.

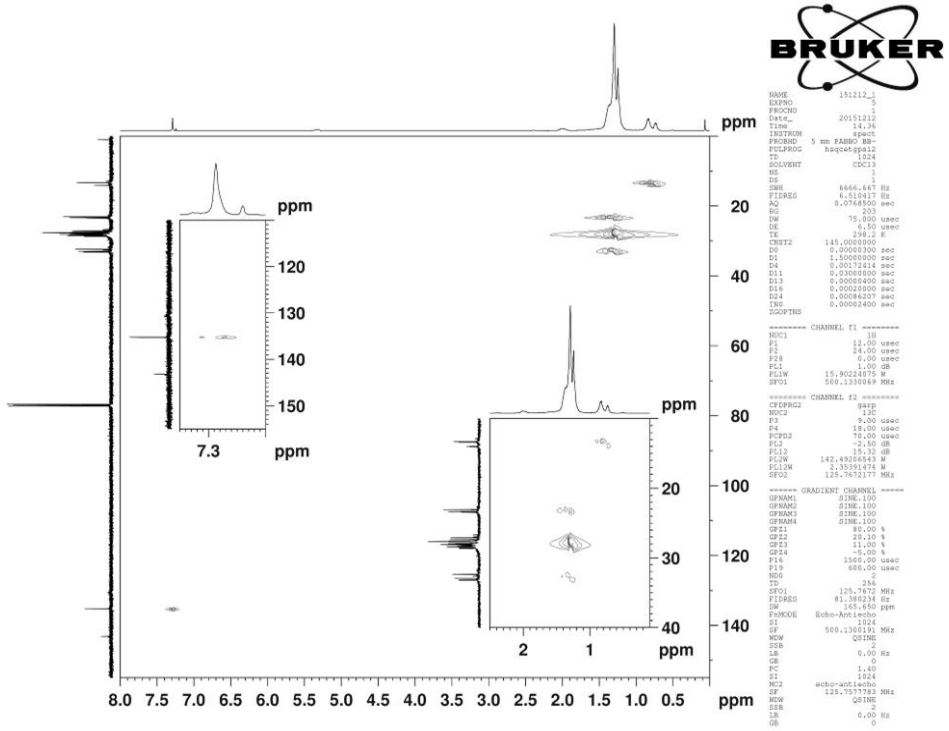


Figure S18. ^{1}H -^{13}C hsqc spectrum of gyrotop isomer **C17Si** in $CDCl_3$.

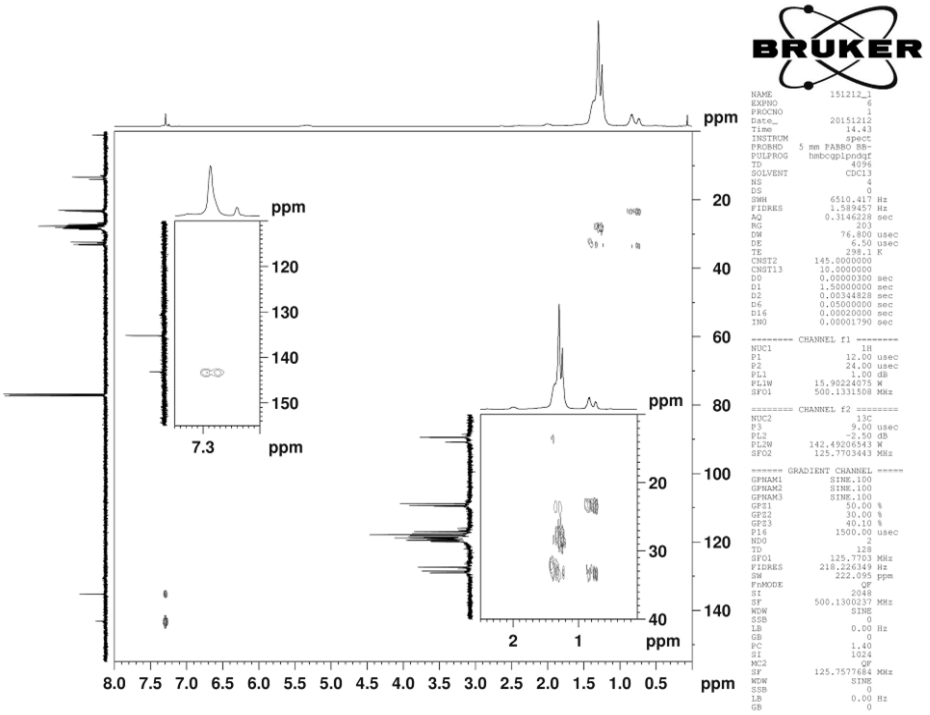


Figure S19. ^{1}H -^{13}C hmbc spectrum of gyrotop isomer **C17Si** in $CDCl_3$.

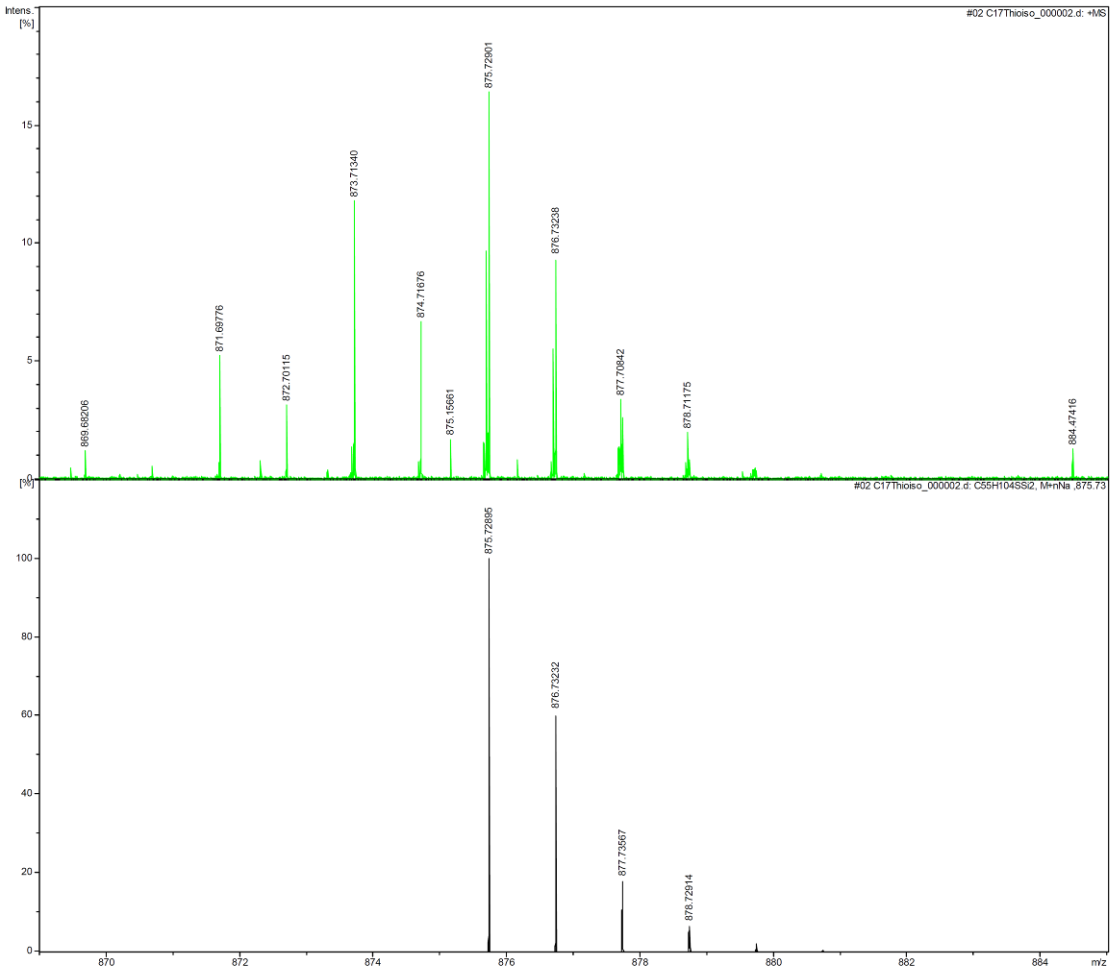


Figure S20. HRMS spectrum of gyrotop isomer **C17Si** (ESI, positive). Top: obsd. Bottom: sim.

e. Spectra of C16

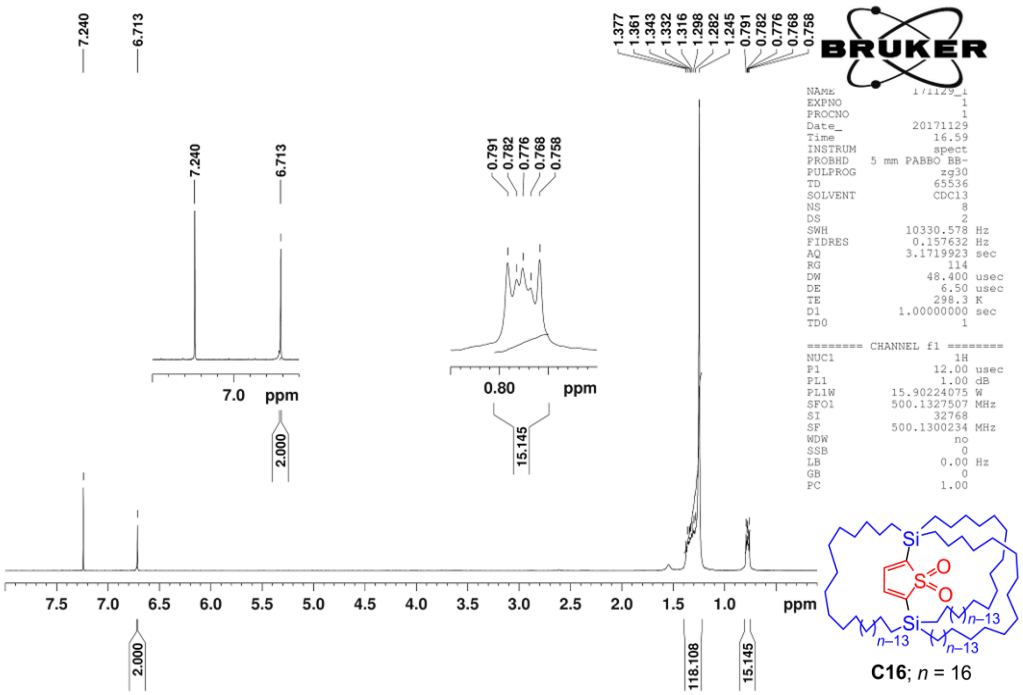


Figure S21. ^{1}H NMR spectrum of gyrotop **C16** in $CDCl_3$.

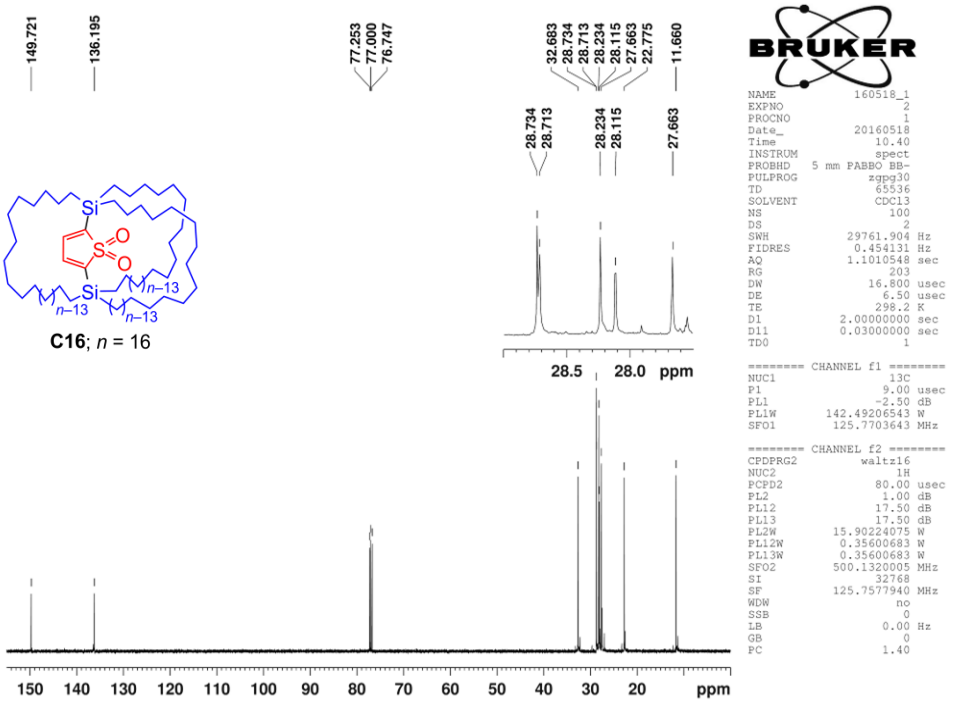


Figure S22. ^{13}C NMR spectrum of gyrotop **C16** in $CDCl_3$.

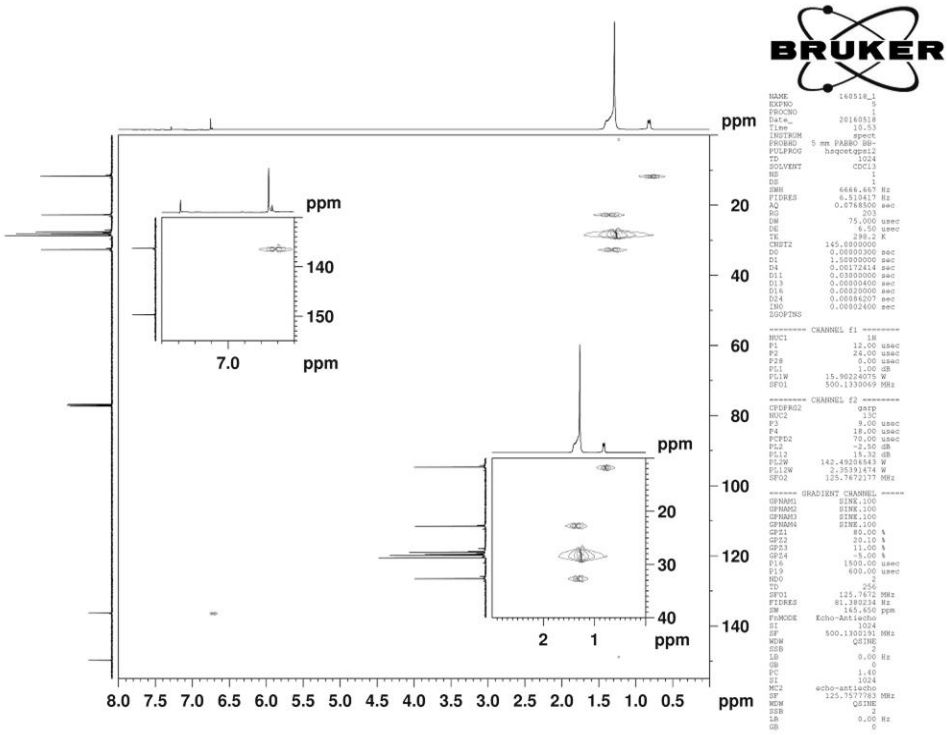


Figure S23. ^{1}H -^{13}C hsqc spectrum of gyrotop **C16** in $CDCl_3$.

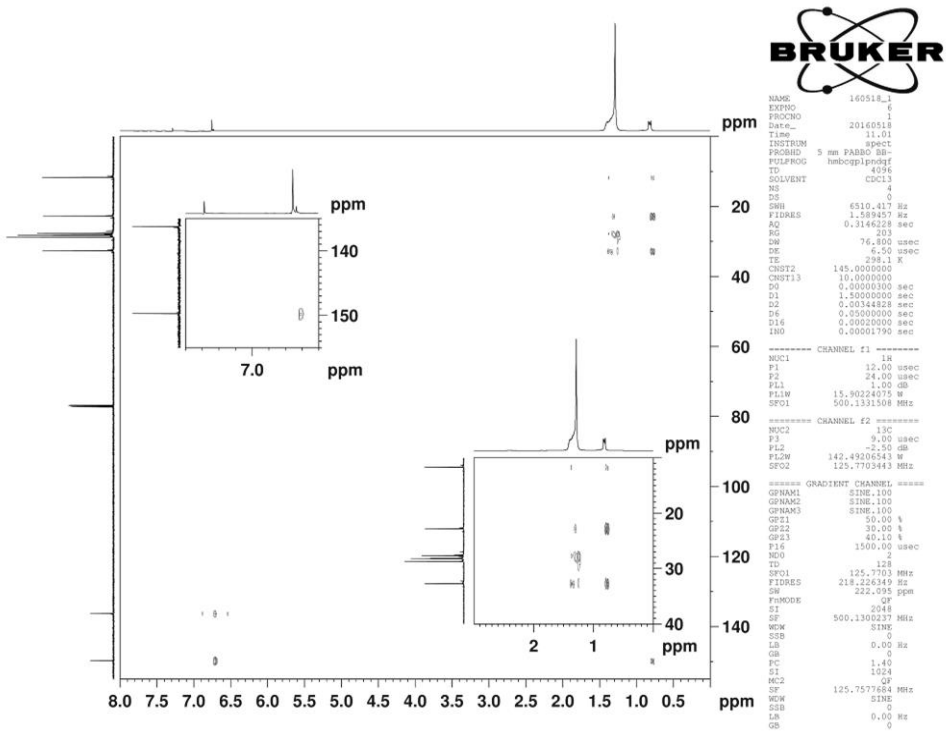


Figure S24. ^{1}H -^{13}C hmbc spectrum of gyrotop **C16** in $CDCl_3$.

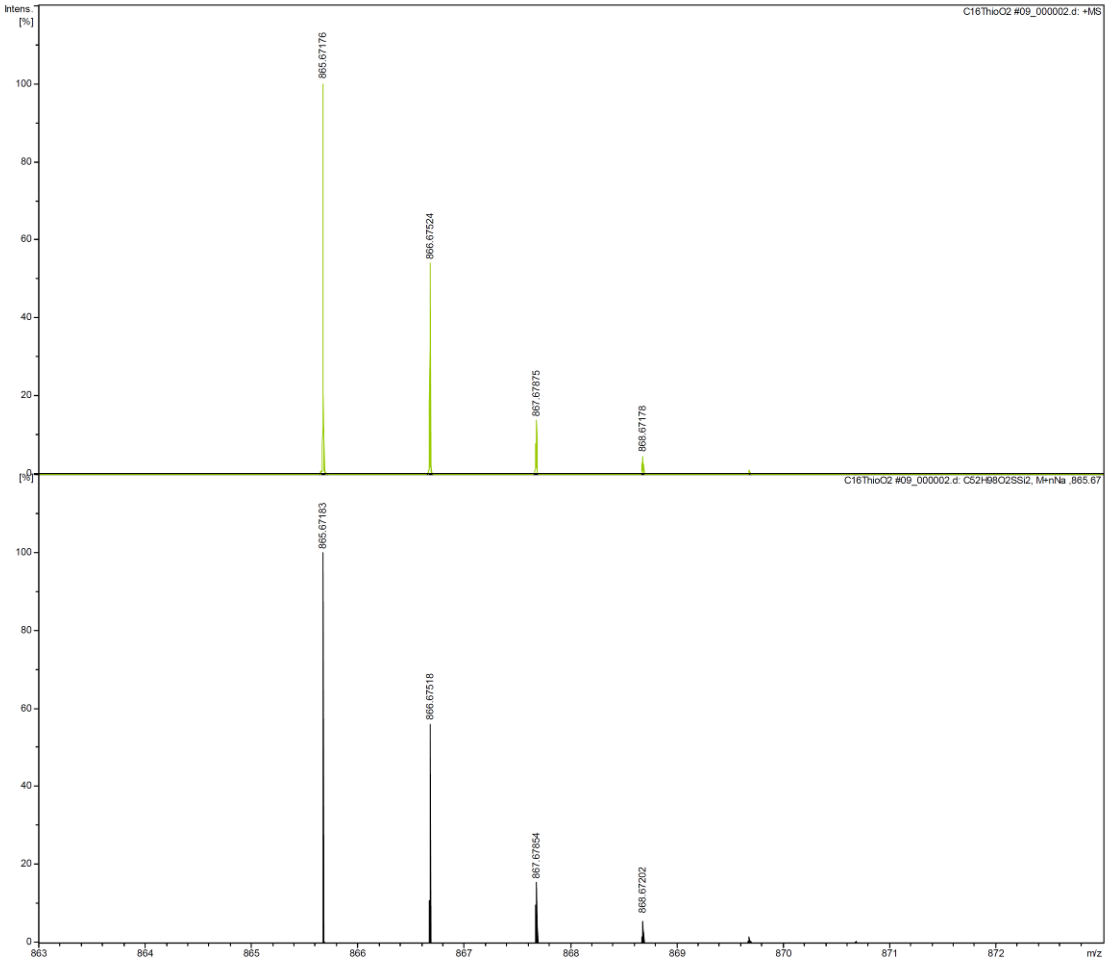


Figure S25. HRMS spectrum of gyrotop **C16** (ESI, positive). Top: obsd. Bottom: sim.

f. Spectra of C17

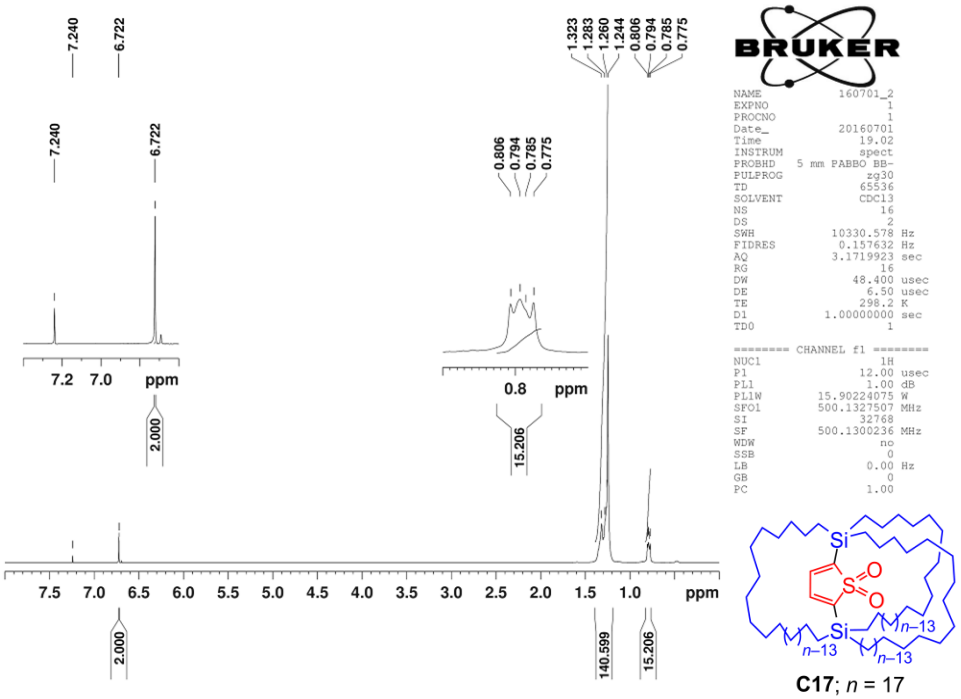


Figure S26. [1]H NMR spectrum of gyrotop **C17** in $CDCl_3$.

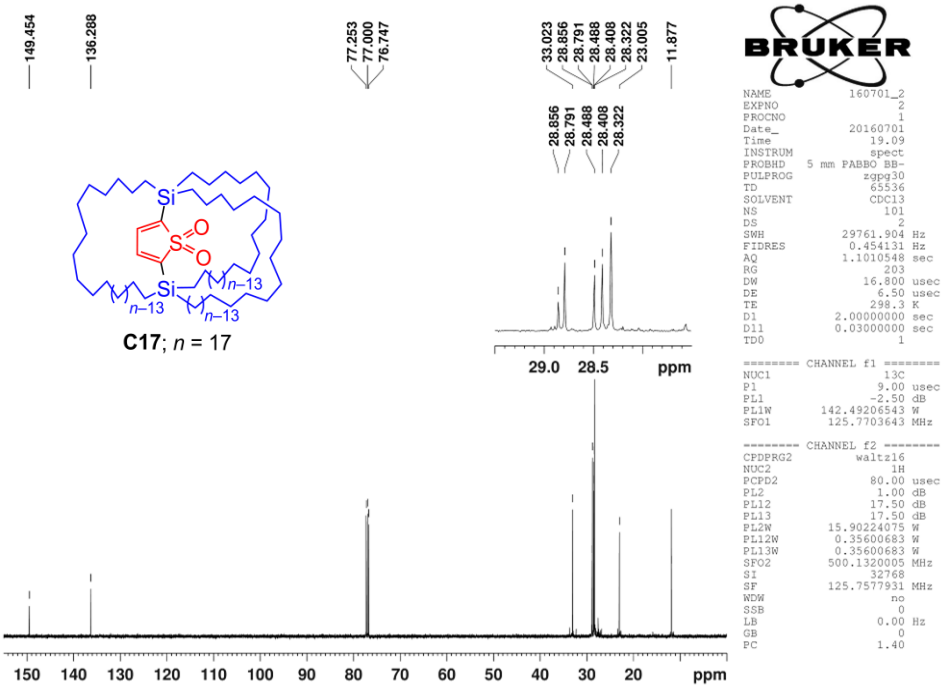


Figure S27. [13]C NMR spectrum of gyrotop **C17** in $CDCl_3$.

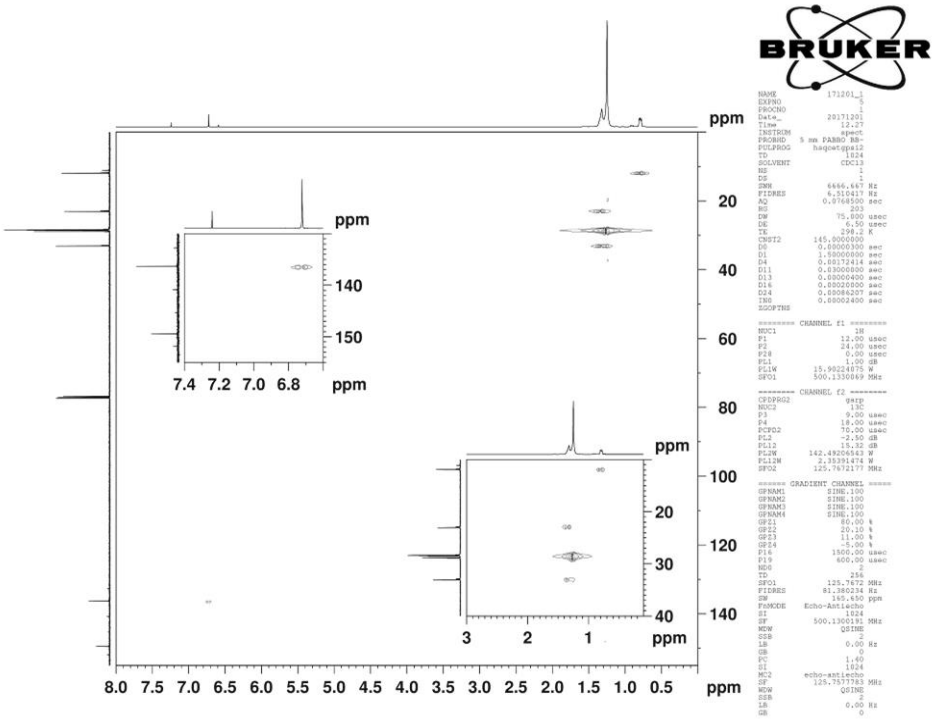


Figure S28. ^{1}H -^{13}C hsqc spectrum of gyrotop **C17** in $CDCl_3$.

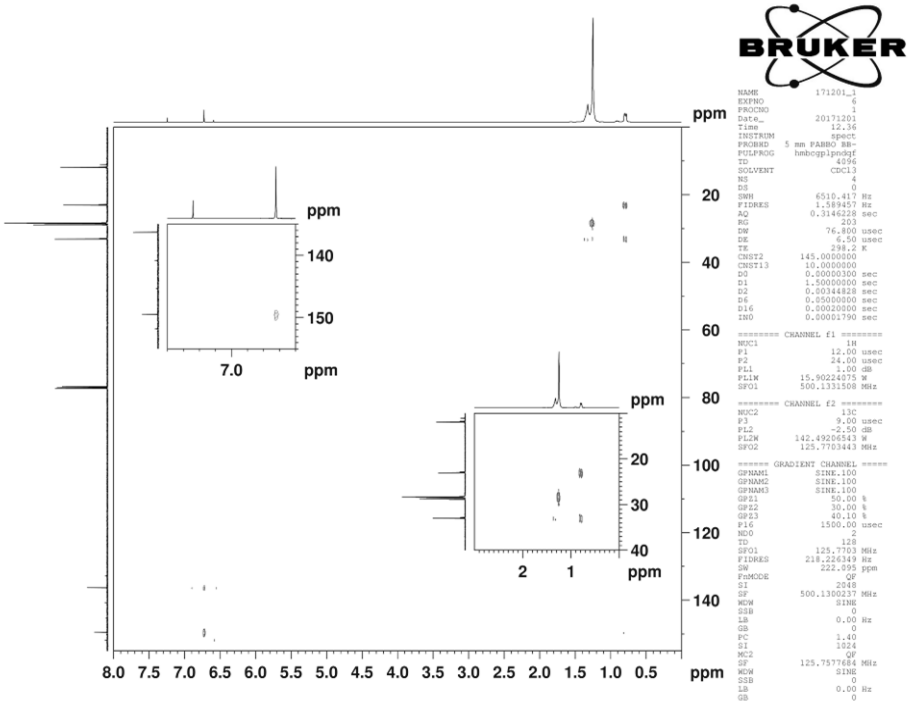


Figure S29. ^{1}H -^{13}C hmbc spectrum of gyrotop **C17** in $CDCl_3$.

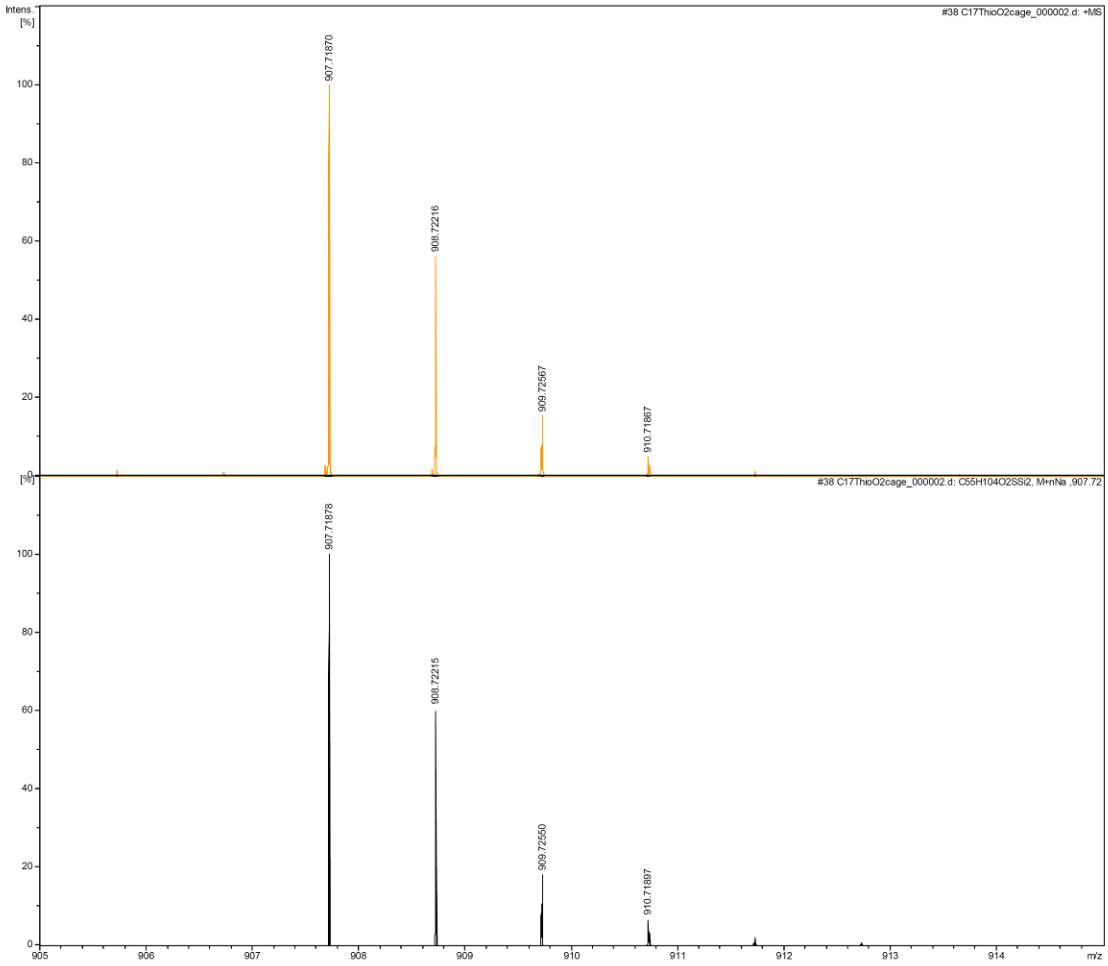


Figure S30. HRMS spectrum of gyrotop **C17** (ESI, positive). Top: obsd. Bottom: sim.

g. Spectra of C16-d_2

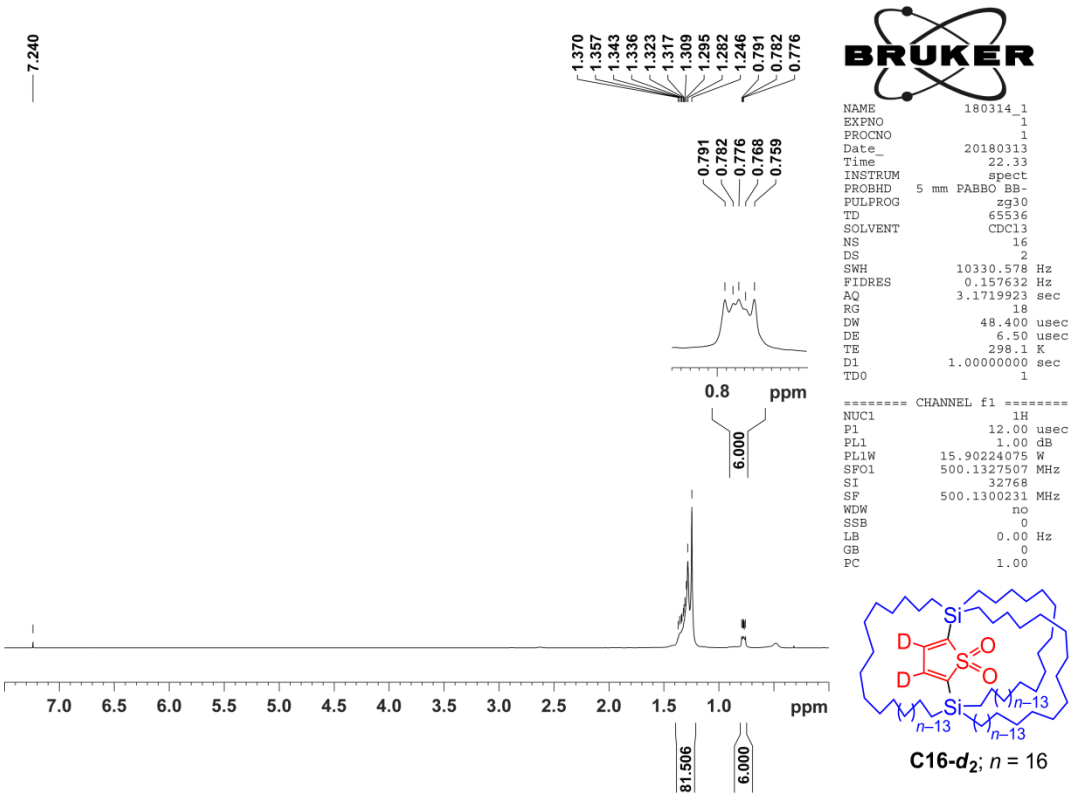


Figure S31. ^{1}H NMR spectrum of gyrotop **C16-d_2** in $CDCl_3$.

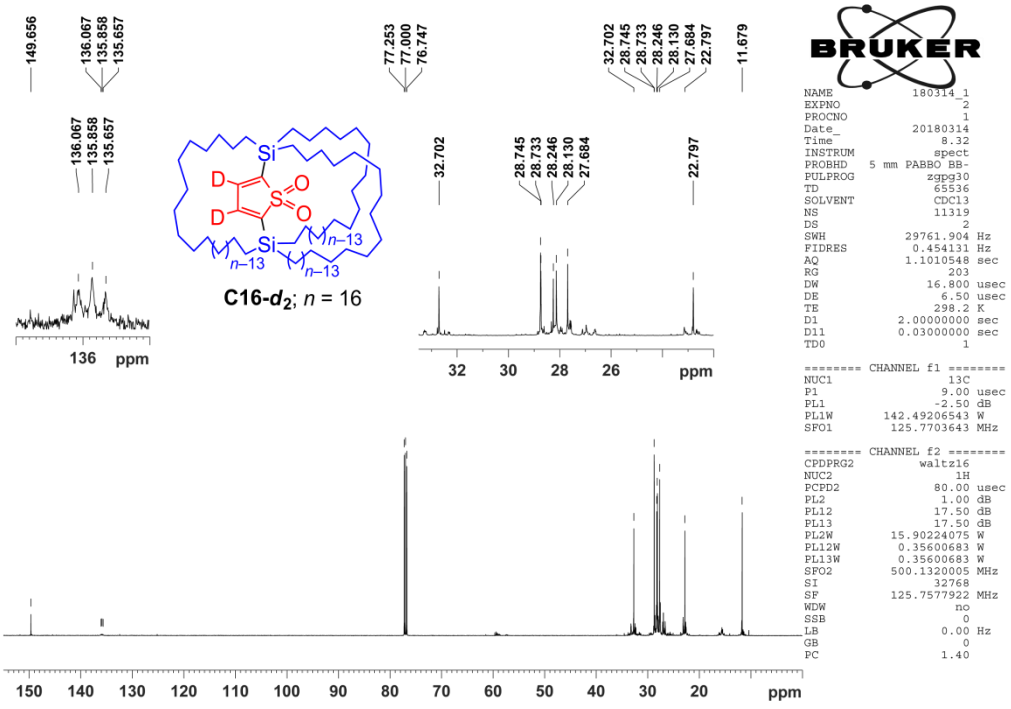


Figure S32. ^{1}H NMR spectrum of gyrotop **C16-d_2** in $CDCl_3$.

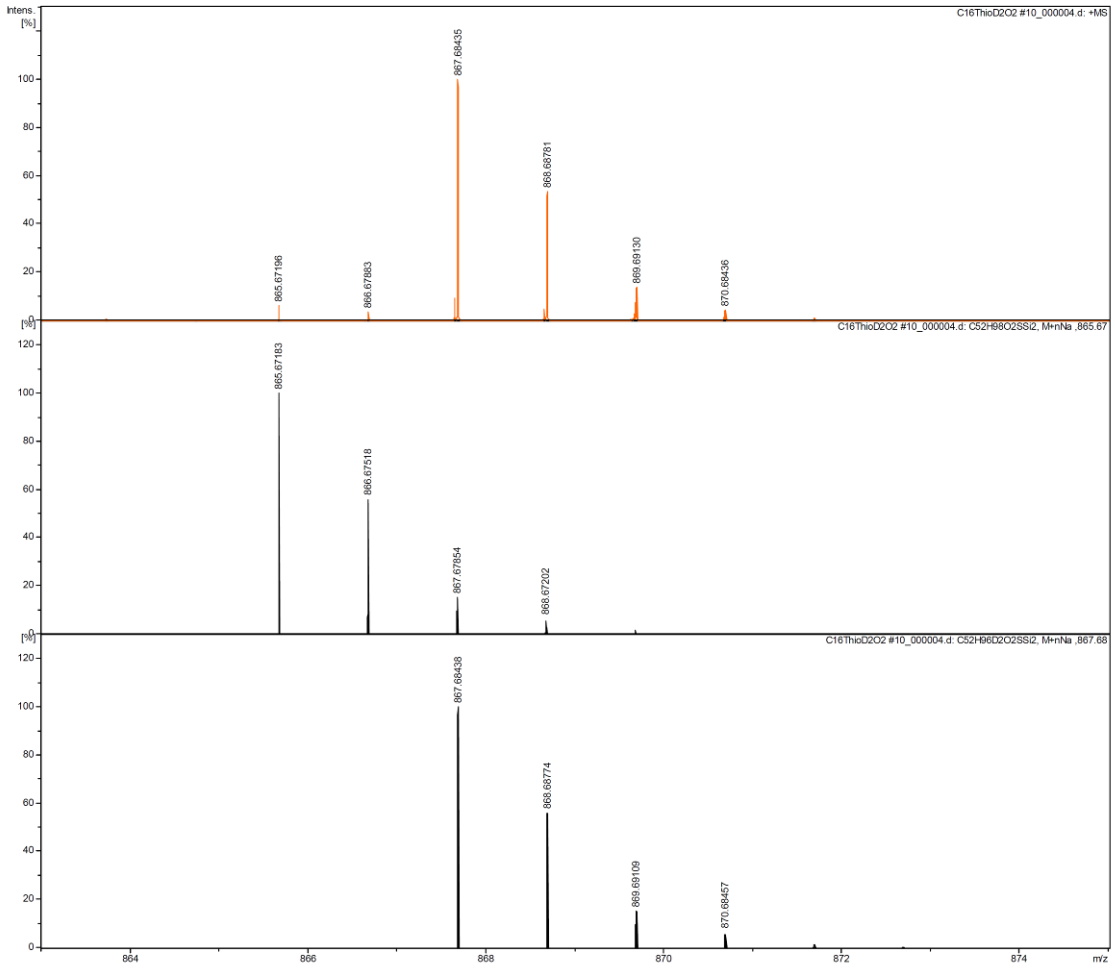


Figure S33. HRMS spectrum of gyrotop **C16-*d*$_2$** (ESI, positive). Top: obsd. Bottom: sim.

h. Spectra of C17-d_2

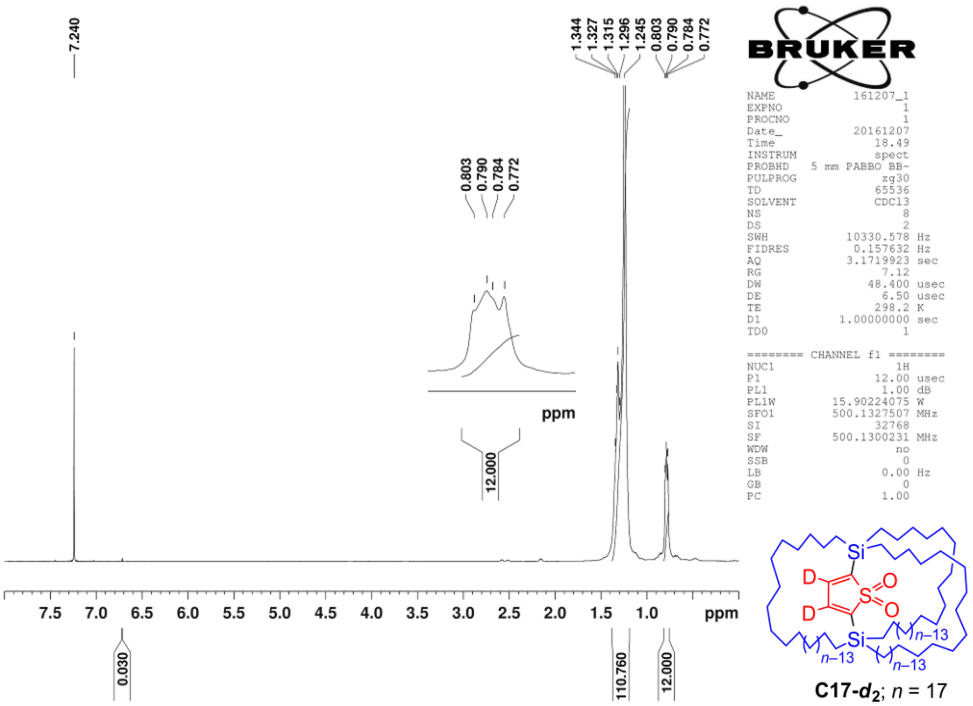


Figure S34. ^{1}H NMR spectrum of gyrotop **C17-d_2** in $CDCl_3$.

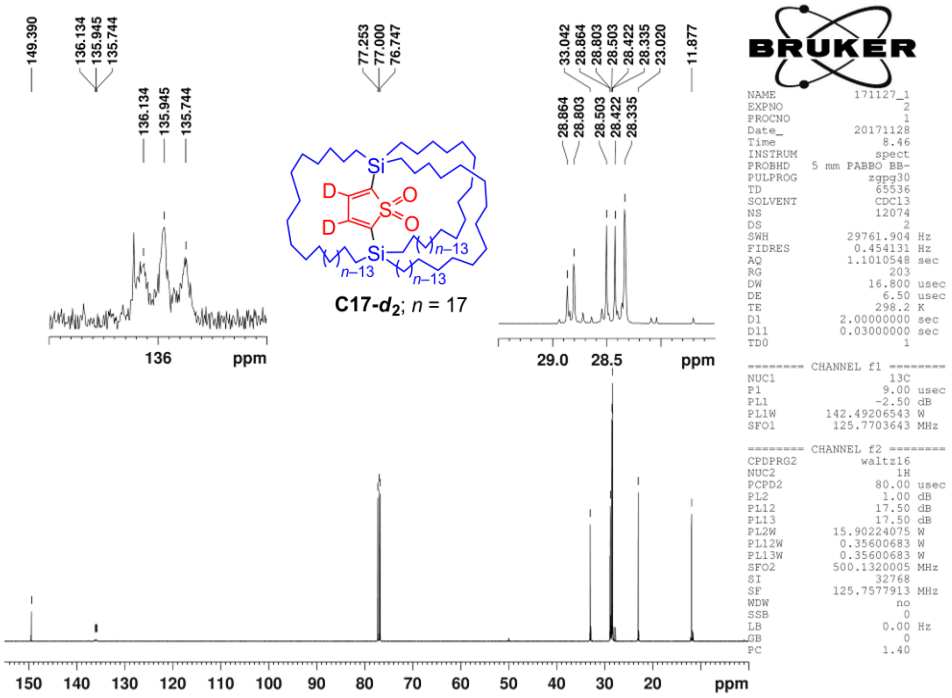


Figure S35. ^{13}C NMR spectrum of gyrotop **C17-d_2** in $CDCl_3$.

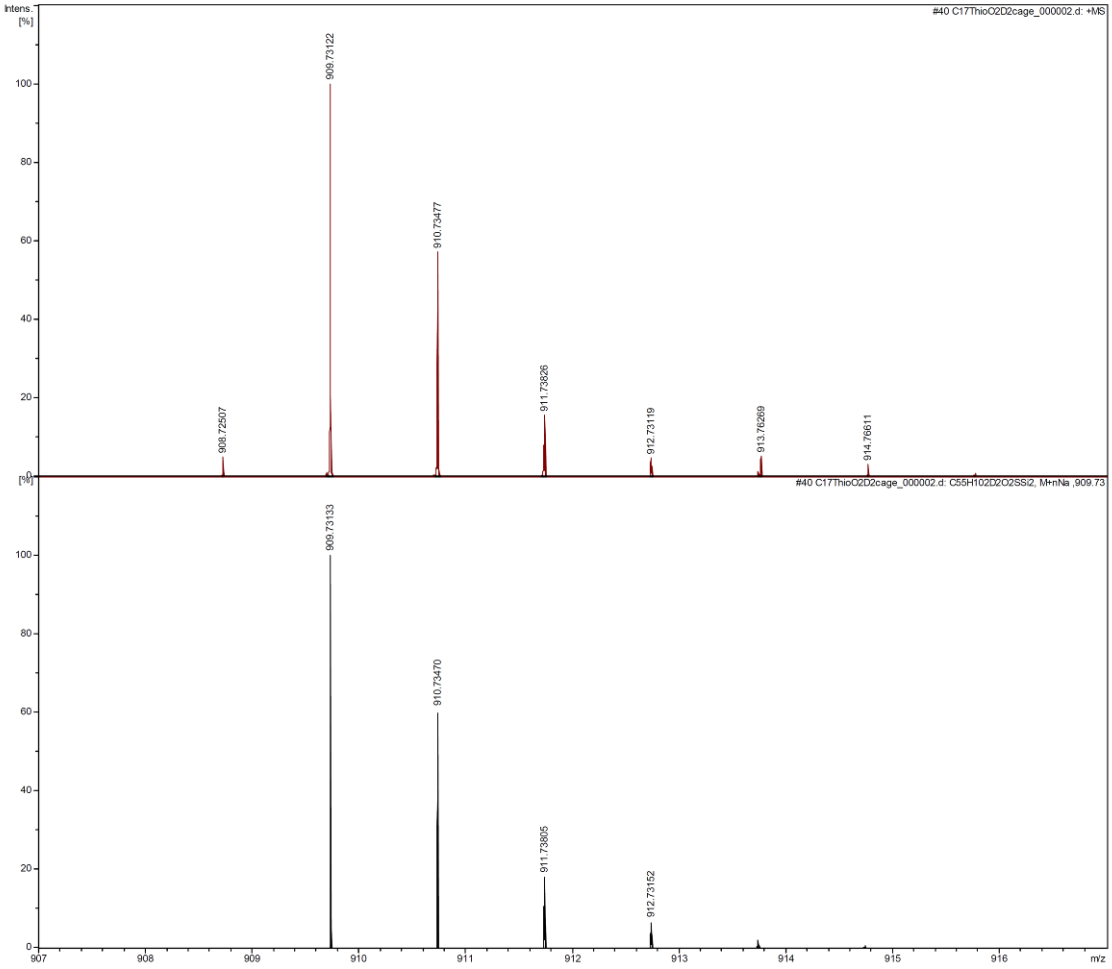


Figure S36. HRMS spectrum of gyrotop **C17-*d*$_2$** (ESI, positive). Top: obsd. Bottom: sim.

3. Details of X-ray Crystallography

3-1. summary

Table S1. Crystal Data

Compound		C16SO2	C17SO2●EtOH (α)	C17SO2●EtOH (β)
CCDC #		1829637	1829638	1829639
Temperature		190 K	173 K	253 K
Empirical formula		C52 H98 O2 S Si2	C57 H110 O3 S Si2	C57 H110 O3 S Si2
Crystal shape		prism	prism	prism
Crystal color		colorless	colorless	colorless
Crystal size		0.400 x 0.400 x 0.050 mm^3	0.300 x 0.200 x 0.200 mm^3	0.300 x 0.200 x 0.200 mm^3
Formula weight / g mol^{-1}		843.54	931.68	931.68
Crystal system		Monoclinic	Trigonal	Trigonal
Space group		*C*2/*c*	$P\,3_1$	$P\,3_1$
Z		12	3	3
Calculated density		1.036 Mg/m^3	1.023 Mg/m^3	1.023 Mg/m^3
Cell parameter	*a*	33.246 (4) Å	14.4449(4) Å	14.4570(6) Å
	b	12.053(2) Å	14.4449(4) Å	14. 4570(6) Å
	c	40.775(5) Å	25.1101(9) Å	25.7526(12) Å
	α	90°	90°	90°
	β	96.848(2)°	90°	90°
	γ	90°	120°.	120°.
	V	16223(4) $Å^3$	4537.4(3) $Å^3$	4661.3(4) $Å^3$
F(000)		5640	1560	1560
Absorption coefficient		0.139 mm^{-1}	1.125 mm^{-1}	1.095 mm^{-1}
□ range for collection (deg)		1.234 to 27.407°.	3.520 to 66.879°	3.432 to 42.541°
Index ranges		-41<=h<=42, -14<=k<=8, -51<=l<=52	-17<=h<=17, -17<=k<=17, -27<=l<=29	-12<=h<=12, -12<=k<=12, -22<=l<=22
Reflections collected		40046	41877	13553
Independent reflections		16513 [R(int) = 0.0755]	10063 [R(int) = 0.0607]	4356 [R(int) = 0.0475]
Completeness		99.2 %	99.9 %	100.0 %
Goodness-of-fit on F^2		1.236	1.028	1.909
Final R indices [I>2sigma(I)]		R1 = 0.1395, wR2 = 0.2635	R1 = 0.0545, wR2 = 0.1382	R1 = 0.1786, wR2 = 0.4245
R indices (all data)		R1 = 0.3685, wR2 = 0.4480	R1 = 0.0616, wR2 = 0.1480	R1 = 0.1941, wR2 = 0.4426
Largest diff. peak and hole		1.175 and -0.406 e.$Å^{-3}$	0.294 and -0.196 e.$Å^{-3}$	0.684 and -0.581 e.$Å^{-3}$

3-2. Details for X-ray structural Analysis of C16SO2

Two crystallographically independent molecules were observed in a unit cell.

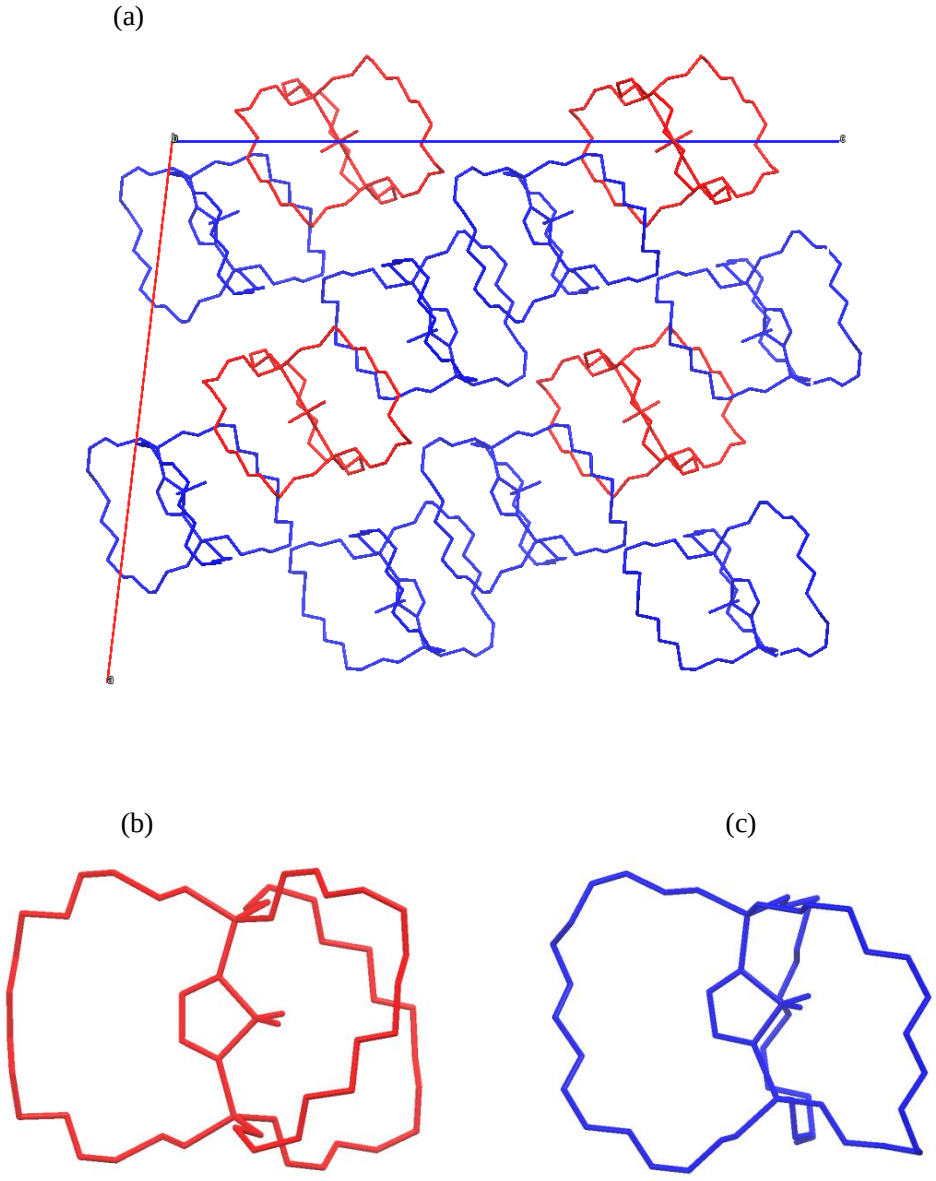


Figure S37. (a) crystal paking structure of **C16**, (b) molecular structure possessing C_2-symmetry, and (c) molecular structure possessing C_1-symmetry.

3-3. Axial View of the Structures of Molecular Gyrotops

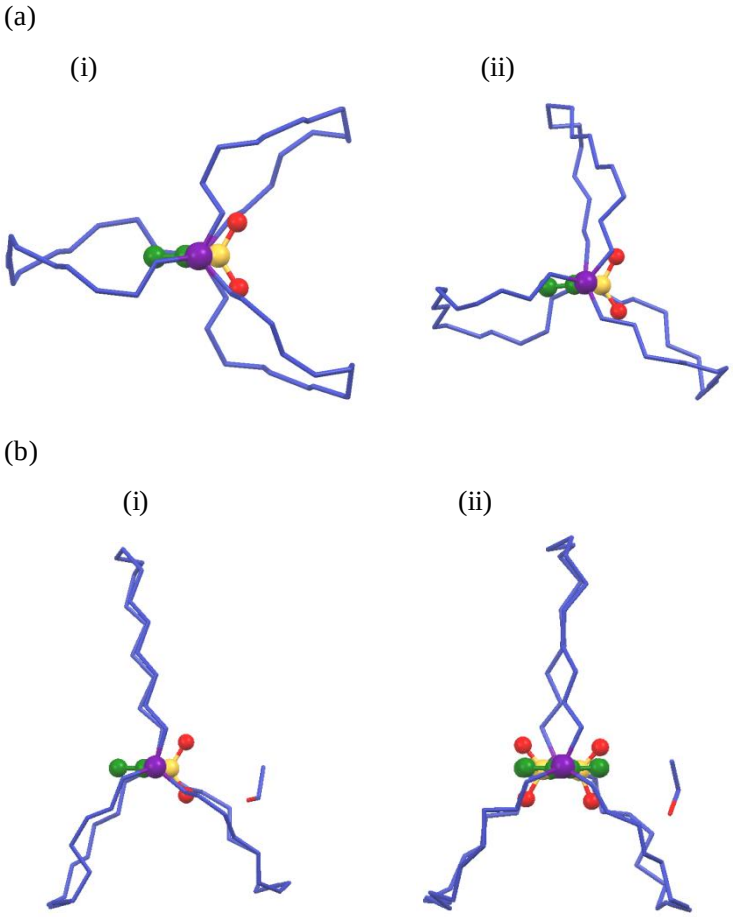


Figure S38. Axial view of the molecular structures of molecular gyrotops: (a-i) **C16** (C_2-symmetry); (a-i) **C16** (C_1-symmetry); (b-i) **C17** with EtOH at 175 K; (b-ii) **C17** with EtOH at 250 K.

4. Details of ^{2}H NMR Study

4-1. ^{2}H NMR spectra

a. Temperature Dependent Solid state ^{2}H NMR spectra of C16-d_2.

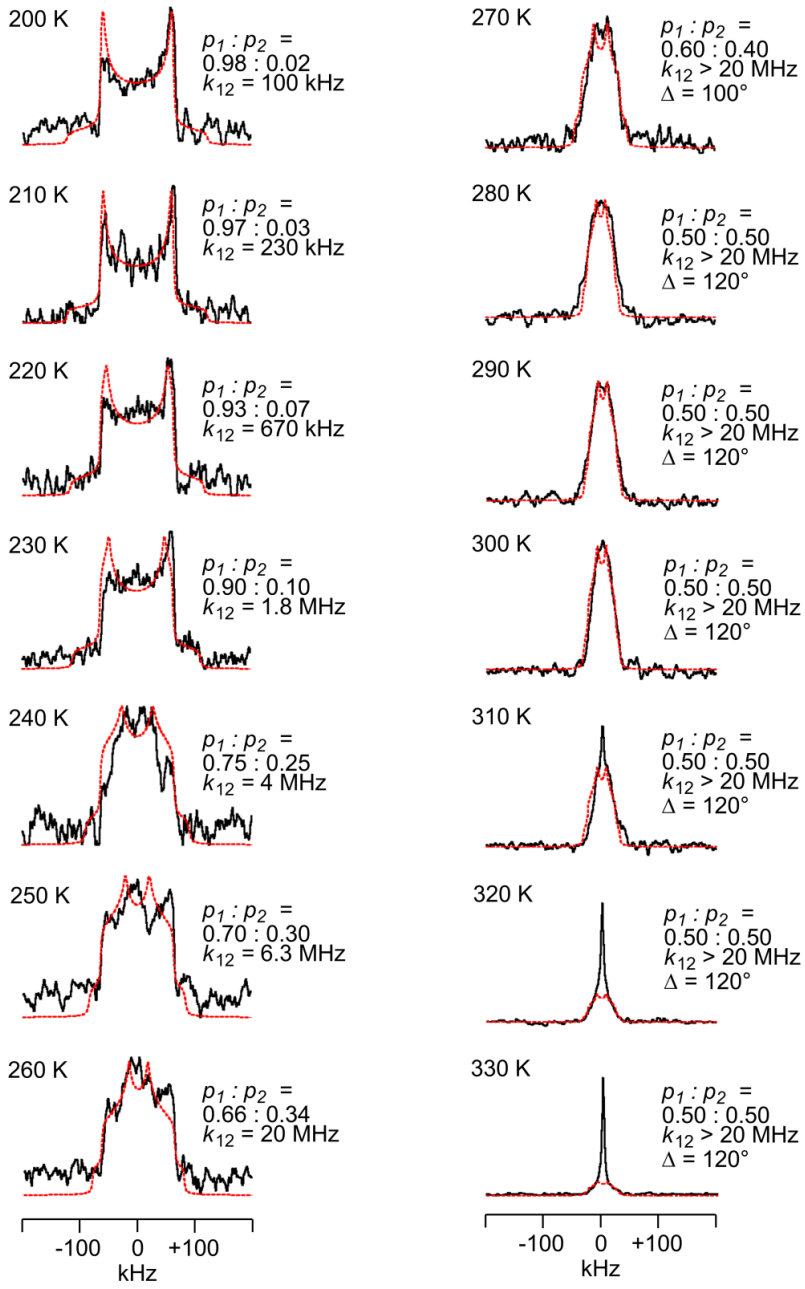


Figure S39. Temperature dependence of solid-state ^{2}H NMR spectra of **C16**-d_2 [solid black line: observed spectra; dotted red line: spectra simulated by assuming 180º flipping with designated exchange rate constants, k, and population ratio between two saites, $p1$:$p2$, and degree of angular displacement (Δ).].

b. Temperature Dependent Solid state ^{2}H NMR spectra of C17-d_2.

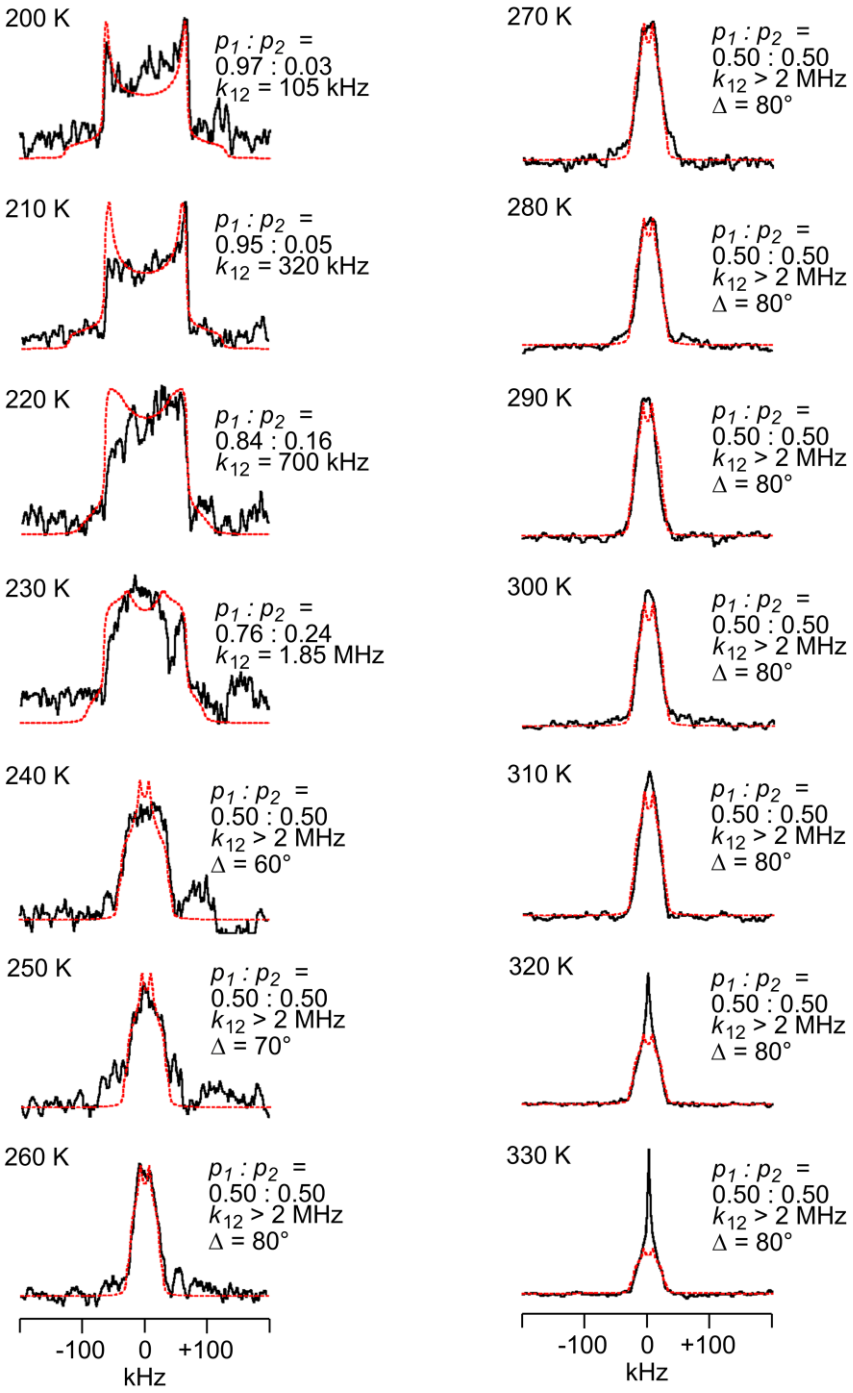


Figure S40. Temperature dependence of solid-state ^{2}H NMR spectra of **C17**-d_2 [solid black line: observed spectra; dotted red line: spectra simulated by assuming 180º flipping with designated exchange rate constants, *k*, and population ratio between two sites, *p*1:*p*2, and degree of angular displacement (Δ).].

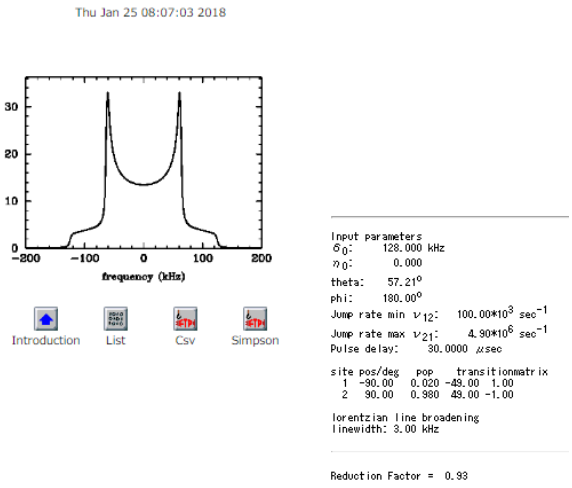
4-2. Simulation of ^{2}H NMR spectra

Spectral simulations were carried out on NMR-WEBLAB 4.5 given by V. Macho, L. Brombacher, R. Graf and H.W. Spiess at MPI for Polymer Research Mainz (reference #16).

(http://weblab.mpip-mainz.mpg.de/weblab/)

A representative simulation was shown below:

(a)



(b)

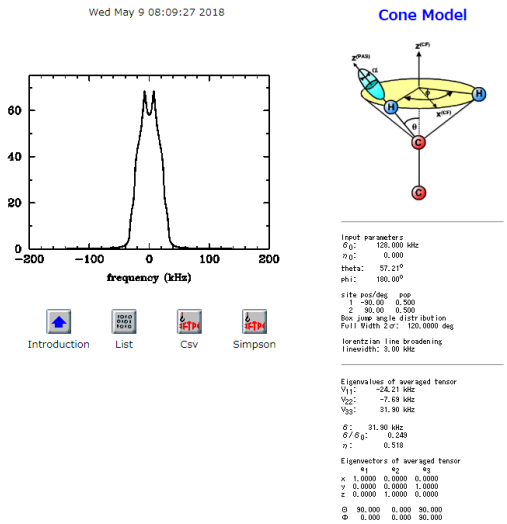


Figure S41. Representative displays of ^{2}H NMR spectral simulation: (a) an example for 2-site exchange at certain rate (**C16-*d*$_2$** at 200 K); (b) an example for 2-site exchange at fast rate limit (**C16-*d*$_2$** at 280 K).

a. Simulation parameters for C16-d_2.

Table S2. Simulation Parameters for ^{2}H NMR spectra of **C16-d_2**

Temp.	δ_0/kHz	η_0	theta	phi	*Pulsedelay*	$\nu_{1\leftarrow2}$	*p*1	*p*2	*Δ/deg*
200 K	128	0.0	57.2	180.0	30 µs	100 kHz	0.020	0.980	--
210 K	128	0.0	57.2	180.0	30 µs	230 kHz	0.030	0.970	--
220 K	128	0.0	57.2	180.0	30 µs	670 kHz	0.070	0.990	--
230 K	128	0.0	57.2	180.0	30 µs	1.8 MHz	0.100	0.900	--
240 K	128	0.0	57.2	180.0	30 µs	4.0 MHz	0.250	0.750	--
250 K	128	0.0	57.2	180.0	30 µs	6.3 MHz	0.300	0.700	--
260 K	128	0.0	57.2	180.0	30 µs	20 MHz	0.340	0.660	--
270 K	128	0.0	57.2	180.0	30 µs	fast limit	0.400	0.600	100
280 K	128	0.0	57.2	180.0	30 µs	fast limit	0.500	0.500	120
290 K	128	0.0	57.2	180.0	30 µs	fast limit	0.500	0.500	120
300 K	128	0.0	57.2	180.0	30 µs	fast limit	0.500	0.500	120
310 K	128	0.0	57.2	180.0	30 µs	fast limit	0.500	0.500	120
320 K	128	0.0	57.2	180.0	30 µs	fast limit	0.500	0.500	120
330 K	128	0.0	57.2	180.0	30 µs	fast limit	0.500	0.500	120

c. Simulation parameters for C17-d_2.

Table S3. Simulation Parameters for ^{2}H NMR spectra of **C17-d_2**

Temp.	δ_0/kHz	η_0	theta	phi	*Pulsedelay*	$\nu_{1\leftarrow2}$	*p*1	*p*2	*Δ/deg*
200 K	133	0.0	56.9	180.0	30 µs	105 kHz	0.030	0.970	--
210 K	133	0.0	56.9	180.0	30 µs	320 kHz	0.050	0.950	--
220 K	133	0.0	56.9	180.0	30 µs	700 kHz	0.160	0.840	--
230 K	133	0.0	56.9	180.0	30 µs	1.85 MHz	0.240	0.760	--
240 K	133	0.0	56.9	180.0	30 µs	fast limit	0.500	0.500	60
250 K	133	0.0	56.9	180.0	30 µs	fast limit	0.500	0.500	70
260 K	133	0.0	56.9	180.0	30 µs	fast limit	0.500	0.500	80
270 K	133	0.0	56.9	180.0	30 µs	fast limit	0.500	0.500	80
280 K	133	0.0	56.9	180.0	30 µs	fast limit	0.500	0.500	80
290 K	133	0.0	56.9	180.0	30 µs	fast limit	0.500	0.500	80
300 K	133	0.0	56.9	180.0	30 µs	fast limit	0.500	0.500	80
310 K	133	0.0	56.9	180.0	30 µs	fast limit	0.500	0.500	80
320 K	133	0.0	56.9	180.0	30 µs	fast limit	0.500	0.500	80
330 K	133	0.0	56.9	180.0	30 µs	fast limit	0.500	0.500	80

4-3. Analysis of Activation Energy *E*a for the Ring Flipping

a. C16

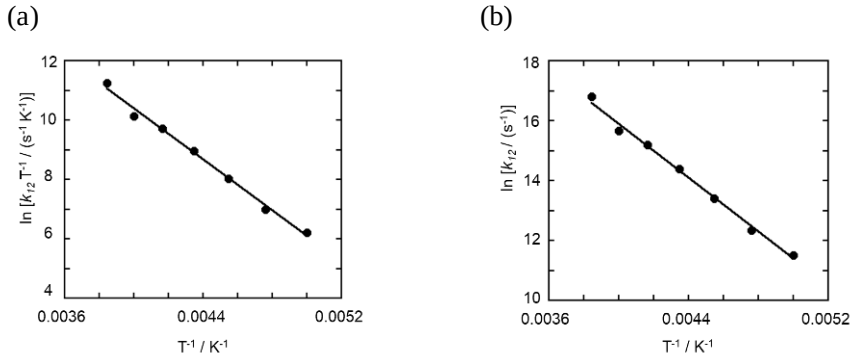


Figure S42. (a) Eyring and (b) Arrhenius plots of the ring flipping in **C16** determined from VT- ^{2}H NMR spectroscopy.

The Eyring and Arrhenius plots are shown above. From the plots, the following parameters were determined:

$\Delta H^{\ddagger}$ = 8.53 kcal mol^{-1}, $\Delta S^{\ddagger}$ = 7.56 cal mol^{-1} K^{-1}

E_a = 8.99 kcal mol^{-1}, A = 5.80 × 10^{14} s^{-1}

5. Details of Dielectric Study

5-1. Functions for dielectric simulation

Based on the Debye-relaxation model, the relationship of real (ε') and imaginary (ε") permittivities versus field frequency (ω) is expressed as follows:

$$\varepsilon'(\omega) = C_1 \frac{1}{1 + \omega^2\tau^2} \qquad (1)$$

$$\varepsilon''(\omega) = C_2 \frac{\omega\tau}{1 + \omega^2\tau^2} \qquad (2)$$

, where C_1 and C_2 are constants, and τ is the relaxation time.

τ is expressed as a function of temperature (T) by Arrhenius equation:

$$\frac{1}{\tau} = A \exp\left(-\frac{Ea}{RT}\right) \qquad (3)$$

, where Ea is the activation energy, A is the frequency factor, and R is the gas constant.

5-2. Simulation parameters for ttheoretical curves shown in Figure 4

a. C16

Table S4. Line-fitting Parameters for Temperature Depedence of Real Permittivity ε' (Figure 4a)

f [a.]	$C_1 = \varepsilon'(0) - \varepsilon'(\infty)$	A	Ea / kcal·mol^{-1}
50 kHz	4.27 − 3.78	3.0 x 10^{14}	9.1
100 kHz	4.27 − 3.78	4.5 x 10^{14}	9.1
500 kHz	4.27 − 3.78	7.0 x 10^{14}	9.1

a. $f = \omega/2\pi$

Table S5. Line-fitting Parameters for Temperature Depedence of Real Permittivity ε' (Figure 4a)

f [a.]	C_2	A	Ea / kcal·mol^{-1}
50 kHz	0.24	3.0 x 10^{14}	9.1
100 kHz	0.23	4.5 x 10^{14}	9.1
500 kHz	0.32	7.0 x 10^{14}	9.1

a. $f = \omega/2\pi$

b. C17•EtOH

Table S6. Line-fitting Parameters for Temperature Depedence of ImaginaryPermittivity ε" (Figure 4b)

f [a.]	$C_1 = \varepsilon'(0) - \varepsilon'(\infty)$	A	Ea / kcal·mol^{-1}
50 kHz	4.4 − 4.0	8.0 x 10^{13}	8.3
100 kHz	4.4 − 4.0	1.0 x 10^{14}	8.3
500 kHz	4.4 − 4.0	1.1 x 10^{14}	8.3

a. $f = \omega/2\pi$

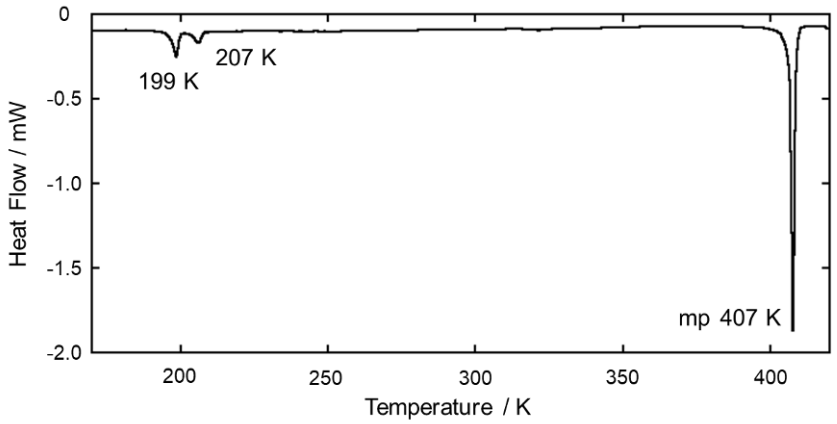
Table S7. Line-fitting Parameters for Temperature Depedence of ImaginaryPermittivity ε" (Figure 4b)

f [a.]	C_2	A	Ea / kcal·mol^{-1}
50 kHz	0.24	8.0 x 10^{13}	8.3
100 kHz	0.24	1.0 x 10^{14}	8.3
500 kHz	0.33	1.1 x 10^{14}	8.3

a. $f = \omega/2\pi$

6. Details of DSC Study

6-1. DSC chart



199 K ΔH = 0.61 kcal mol^{-1}, ΔS = 3.09 cal mol^{-1} K^{-1}, *degree of freedom* ; 5

207 K $\Delta H'$ = 0.25 kcal mol^{-1}, $\Delta S'$ = 1.19 cal mol^{-1} K^{-1}, *degree of freedom* ; 2

Mp 407 K $\Delta H'$ = 5.09 kcal mol^{-1}, ΔS = 12.50 cal mol^{-1} K^{-1}, *degree of freedom* ; 539

Figure S43. Differential scanning calorimetry (DSC) of powdered molecular gyrotop **C16** (temperature ramp of +10 °C/min)

7. Details of DFT Study

7-1. General

All calcularion were carried out using Gaussian 16 (Revision A.03) program packages[S1] on Fujitsu PRIMERGY CX400 supercomputer.

S1: Gaussian 16, Revision A.03,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

7-2. Optimized structure and dipole moment of C16 (C_1-symmetry) calculated at B3LYP/6-31G(d) level

Total energy: -3168.2329343 hartree (NImag = 0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.064742	-2.165421	1.267282
2	14	0	0.305452	3.192685	-2.175326
3	6	0	-0.426577	-2.129531	3.134281
4	6	0	-1.912359	7.320739	0.735982
5	6	0	-1.992099	6.478754	-0.552412
6	6	0	-2.133841	6.522803	2.036025
7	6	0	-0.832941	5.483844	-0.732040
8	6	0	-1.018729	4.539895	-1.937418
9	6	0	4.575795	3.818901	-2.262770
10	6	0	5.792309	3.040055	-2.790729
11	6	0	-3.590408	6.045904	2.247837
12	6	0	2.032481	3.962304	-1.994942
13	6	0	3.227583	3.107116	-2.458210
14	6	0	0.104937	2.310635	-3.840008
15	6	0	-1.309236	0.699195	-5.248997
16	6	0	-2.679907	0.054729	-5.519432
17	6	0	-1.292382	1.707317	-4.090820
18	6	0	7.311492	0.984250	-2.543059
19	6	0	6.008235	1.677592	-2.117525
20	6	0	-3.708152	4.636199	2.849215
21	6	0	-3.116120	4.465939	4.255388
22	6	0	-3.287723	-0.655634	-4.299856
23	6	0	7.421635	-0.477449	-2.076881
24	6	0	-4.484465	-1.555671	-4.633251
25	6	0	7.423086	-0.669054	-0.553944
26	6	0	-3.068100	2.996447	4.694362
27	6	0	-5.186976	-2.095855	-3.380034
28	6	0	-6.278792	-3.132451	-3.678397
29	6	0	-2.508155	2.775070	6.106646
30	6	0	7.401391	-2.143026	-0.128744
31	6	0	-7.164454	-3.487968	-2.470394

32	6	0	-2.290314	1.292859	6.463074
33	6	0	7.318351	-2.328729	1.392403
34	6	0	-6.432289	-4.026141	-1.228205
35	6	0	-1.071067	0.656530	5.777409
36	6	0	-5.699787	-5.359245	-1.441748
37	6	0	7.190474	-3.789479	1.860296
38	6	0	1.664763	-2.854859	0.895129
39	6	0	-1.454084	-3.076363	0.334779
40	6	0	0.609414	-1.386031	4.001218
41	6	0	-0.941838	-0.850557	6.038661
42	6	0	5.949709	-4.547943	1.353274
43	6	0	4.605066	-3.904824	1.723238
44	6	0	0.363465	-1.478951	5.519867
45	6	0	-5.120259	-5.965722	-0.150017
46	6	0	3.401017	-4.745355	1.277281
47	6	0	-2.630578	-5.295239	-0.306617
48	6	0	2.027143	-4.155254	1.646138
49	6	0	-3.943071	-5.202443	0.486359
50	6	0	-1.426453	-4.618012	0.376914
51	1	0	-2.018447	7.151200	-1.421118
52	1	0	-2.654433	8.129741	0.682875
53	1	0	-0.930175	7.812542	0.777624
54	1	0	-2.943080	5.927192	-0.575584
55	1	0	4.537728	4.799710	-2.759333
56	1	0	-1.046364	5.133572	-2.864178
57	1	0	0.106358	6.043594	-0.840060
58	1	0	-1.817140	7.136427	2.888490
59	1	0	2.016159	4.908005	-2.560490
60	1	0	6.692086	3.656999	-2.651440
61	1	0	5.689714	2.895547	-3.876861
62	1	0	0.375206	3.002253	-4.651746
63	1	0	-4.126764	6.765760	2.881460
64	1	0	-4.121089	6.045144	1.286691
65	1	0	-0.952210	1.189565	-6.166257
66	1	0	3.109636	2.853072	-3.521709
67	1	0	-1.461352	5.654115	2.039681
68	1	0	-2.003325	4.053615	-1.877485
69	1	0	-3.385886	0.816317	-5.883462
70	1	0	-0.716524	4.891999	0.184586
71	1	0	4.717174	4.026001	-1.191246
72	1	0	-2.017439	2.511442	-4.285658
73	1	0	2.173603	4.253135	-0.943825
74	1	0	7.385331	1.006268	-3.640055
75	1	0	-2.567328	-0.669216	-6.339449
76	1	0	8.171992	1.559913	-2.170117
77	1	0	0.850609	1.504333	-3.871834
78	1	0	-0.583865	-0.093428	-5.018067
79	1	0	3.227471	2.157586	-1.911812
80	1	0	-3.207196	3.929598	2.168130
81	1	0	-4.765115	4.334838	2.867885
82	1	0	5.998165	1.816343	-1.027661
83	1	0	-2.097613	4.877610	4.284778
84	1	0	-5.211533	-0.998222	-5.242768
85	1	0	5.162485	1.014220	-2.343387
86	1	0	-3.704085	5.054347	4.975211
87	1	0	-1.631685	1.196423	-3.182902
88	1	0	8.335287	-0.922576	-2.496494
89	1	0	-3.603699	0.092823	-3.560012
90	1	0	-4.145213	-2.394761	-5.258793
91	1	0	6.582435	-1.045844	-2.505036
92	1	0	-2.511118	-1.256611	-3.804251
93	1	0	8.302181	-0.168263	-0.120544
94	1	0	-6.929345	-2.747808	-4.477026

95	1	0	-5.626674	-1.251554	-2.827172
96	1	0	6.544616	-0.173077	-0.120443
97	1	0	-2.460300	2.441004	3.965289
98	1	0	-1.555370	3.315010	6.213034
99	1	0	-3.195670	3.227822	6.834355
100	1	0	-4.077503	2.562211	4.637092
101	1	0	-5.812789	-4.040741	-4.085439
102	1	0	-7.727716	-2.590342	-2.176697
103	1	0	-4.433517	-2.533891	-2.710210
104	1	0	8.293537	-2.658758	-0.515114
105	1	0	-7.915069	-4.226242	-2.787776
106	1	0	6.539707	-2.627246	-0.608488
107	1	0	8.213565	-1.890524	1.856301
108	1	0	6.469869	-1.745489	1.776400
109	1	0	-1.119160	0.836176	4.695143
110	1	0	-2.170037	1.194618	7.550824
111	1	0	-0.160394	1.166543	6.126185
112	1	0	-3.196041	0.722582	6.206892
113	1	0	-4.902351	-5.237128	-2.186767
114	1	0	-5.729559	-3.266487	-0.861921
115	1	0	1.738258	-3.023188	-0.189386
116	1	0	-6.406721	-6.081167	-1.875788
117	1	0	0.655621	-0.332628	3.696417
118	1	0	-2.407366	-2.700511	0.734312
119	1	0	-7.172251	-4.160325	-0.425561
120	1	0	8.088366	-4.344623	1.552688
121	1	0	2.398555	-2.068801	1.112880
122	1	0	-1.418248	-2.743073	-0.712041
123	1	0	4.539551	-2.905250	1.275819
124	1	0	6.002973	-4.662283	0.261770
125	1	0	-1.428918	-1.703045	3.284618
126	1	0	7.187759	-3.803535	2.959835
127	1	0	-2.757962	-4.865251	-1.309937
128	1	0	3.445753	-4.896481	0.188454
129	1	0	1.209831	-1.002926	6.036085
130	1	0	1.609236	-1.792723	3.799239
131	1	0	-4.220834	-4.151116	0.638685
132	1	0	-1.807867	-1.369036	5.603208
133	1	0	-1.001777	-1.030566	7.121550
134	1	0	-4.796317	-6.996495	-0.353729
135	1	0	4.559348	-3.757225	2.813534
136	1	0	5.980033	-5.568987	1.760270
137	1	0	-5.930910	-6.044356	0.588652
138	1	0	1.264297	-4.919098	1.448435
139	1	0	-1.369058	-4.973122	1.416745
140	1	0	-0.505068	-3.174286	3.472724
141	1	0	-2.395005	-6.358790	-0.458354
142	1	0	0.385016	-2.538054	5.814444
143	1	0	1.999527	-3.978043	2.731053
144	1	0	-0.508310	-4.966338	-0.113221
145	1	0	3.483197	-5.745834	1.726720
146	1	0	-3.766946	-5.614473	1.490694
147	16	0	0.732448	0.205560	-0.834446
148	8	0	2.183371	0.282809	-0.569460
149	8	0	0.276722	-0.560579	-2.013766
150	6	0	-0.148600	-0.369231	0.643509
151	6	0	-0.901397	0.667991	1.053399
152	6	0	-0.824516	1.900525	0.237022
153	6	0	-0.003706	1.872415	-0.830405
154	1	0	-1.553442	0.626085	1.922034
155	1	0	-1.424739	2.766079	0.501386

Dipole moment (field-independent basis, Debye):

X= -2.8299 Y= 1.6919 Z= 2.7095 Tot= 4.2676

7-3. Optimized structure and dipole moment of C16 (C_2-symmetry) calculated at B3LYP/6-31G(d) level

Total energy: -3168.234998 hartree (NImag = 0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	2.371820	-0.189644	2.127034
2	14	0	-2.371819	-0.189646	-2.127034
3	6	0	1.526704	0.463728	3.696798
4	6	0	-5.406914	2.835667	-1.706472
5	6	0	-7.107864	3.667964	0.050545
6	6	0	-4.991628	-3.630971	-1.728058
7	6	0	-4.603234	1.649994	-2.271583
8	6	0	-4.246876	-4.813186	-2.375583
9	6	0	-6.216378	2.513550	-0.442679
10	6	0	-6.369580	4.966195	0.432313
11	6	0	-3.359657	-1.768237	-2.522987
12	6	0	-4.133031	-2.406384	-1.352219
13	6	0	0.093012	0.027453	-5.670488
14	6	0	-2.430824	-6.621830	-2.137842
15	6	0	-1.526704	0.463726	-3.696799
16	6	0	-3.034840	-5.319673	-1.581732
17	6	0	-3.462785	1.156259	-1.355867
18	6	0	0.790135	1.398161	-5.643610
19	6	0	-0.471151	-0.466812	-4.324769
20	6	0	-5.285933	4.823926	1.515242
21	6	0	-5.814702	4.426182	2.901912
22	6	0	-0.973201	-6.864550	-1.709065
23	6	0	1.985131	1.491811	-4.684777
24	6	0	2.753620	2.814158	-4.811096
25	6	0	-4.712647	4.238977	3.959771
26	6	0	-3.883656	2.958219	3.784156
27	6	0	3.883655	2.958217	-3.784159
28	6	0	4.712646	4.238975	-3.959774
29	6	0	-2.753620	2.814161	4.811093
30	6	0	5.814700	4.426182	-2.901913
31	6	0	-1.985131	1.491813	4.684775
32	6	0	5.285929	4.823928	-1.515245
33	6	0	2.430829	-6.621828	2.137845
34	6	0	3.034844	-5.319671	1.581735
35	6	0	-0.790135	1.398163	5.643607
36	6	0	0.471151	-0.466810	4.324768
37	6	0	3.462785	1.156261	1.355867
38	6	0	-0.093014	0.027455	5.670486
39	6	0	6.369575	4.966201	-0.432315
40	6	0	4.133033	-2.406381	1.352221
41	6	0	3.359658	-1.768234	2.522988
42	6	0	6.216375	2.513557	0.442682
43	6	0	4.246879	-4.813183	2.375586
44	6	0	7.107861	3.667972	-0.050544
45	6	0	4.991631	-3.630967	1.728061
46	6	0	4.603229	1.650003	2.271585
47	6	0	5.406909	2.835676	1.706472
48	6	0	0.973206	-6.864549	1.709068
49	6	0	0.743148	-6.947621	0.193090
50	6	0	-0.743143	-6.947621	-0.193087
51	1	0	-6.096113	3.195064	-2.485156
52	1	0	-7.842167	3.908161	-0.731973
53	1	0	-5.792989	-3.309352	-2.408413

54	1	0	-4.961797	-5.637331	-2.509716
55	1	0	-5.294198	0.820717	-2.484853
56	1	0	-4.187383	1.953625	-3.242138
57	1	0	-4.713348	3.664026	-1.507012
58	1	0	-4.064816	-1.503895	-3.326466
59	1	0	-7.692896	3.313791	0.909719
60	1	0	-3.916912	-4.538606	-3.387319
61	1	0	-5.910455	5.397376	-0.467203
62	1	0	-7.115728	5.701316	0.767147
63	1	0	-5.492359	-3.986182	-0.815718
64	1	0	-6.858601	1.644041	-0.647205
65	1	0	-0.724784	0.062143	-6.405176
66	1	0	-2.316837	0.677670	-4.433312
67	1	0	-4.797764	-1.655902	-0.903766
68	1	0	-2.463516	-6.590455	-3.236172
69	1	0	-3.060044	-7.473089	-1.840926
70	1	0	1.129031	1.628910	-6.664012
71	1	0	-2.676122	-2.501708	-2.973009
72	1	0	-5.539289	2.203091	0.363254
73	1	0	0.062014	2.180892	-5.388334
74	1	0	-0.905694	-1.463122	-4.489660
75	1	0	0.804710	-0.724075	-6.042895
76	1	0	-3.318434	-5.457088	-0.529241
77	1	0	-3.866995	0.780199	-0.407168
78	1	0	-3.431924	-2.686547	-0.555792
79	1	0	-1.072043	1.432132	-3.450301
80	1	0	-4.758811	5.784265	1.608402
81	1	0	-2.815811	2.000998	-1.079368
82	1	0	-6.516699	5.201130	3.242223
83	1	0	-2.255783	-4.543073	-1.585268
84	1	0	-6.399423	3.497852	2.833022
85	1	0	-4.528973	4.102374	1.182347
86	1	0	2.052974	3.654439	-4.694307
87	1	0	3.165762	2.901924	-5.827958
88	1	0	-0.602050	-7.783123	-2.184645
89	1	0	0.350548	-0.609822	-3.612304
90	1	0	2.673997	0.655045	-4.878786
91	1	0	-1.239513	-7.842049	0.211311
92	1	0	1.644705	1.375136	-3.647411
93	1	0	-1.223093	-6.089142	0.296866
94	1	0	-3.448049	2.921466	2.776627
95	1	0	-5.171991	4.224592	4.958468
96	1	0	5.171991	4.224589	-4.958470
97	1	0	4.044865	5.113586	-3.946382
98	1	0	-4.044866	5.113588	3.946377
99	1	0	3.448048	2.921465	-2.776630
100	1	0	4.554670	2.088633	-3.857731
101	1	0	1.239519	-7.842048	-0.211308
102	1	0	1.223097	-6.089141	-0.296863
103	1	0	0.356677	-6.046677	2.112971
104	1	0	-2.673998	0.655047	4.878784
105	1	0	-3.165762	2.901928	5.827955
106	1	0	6.516697	5.201129	-3.242225
107	1	0	-2.052974	3.654442	4.694303
108	1	0	6.399421	3.497852	-2.833021
109	1	0	4.758806	5.784266	-1.608408
110	1	0	-0.350548	-0.609821	3.612302
111	1	0	4.528970	4.102375	-1.182349
112	1	0	2.255787	-4.543071	1.585270
113	1	0	3.318438	-5.457086	0.529244
114	1	0	2.815810	2.000998	1.079362
115	1	0	3.060049	-7.473086	1.840929
116	1	0	1.072043	1.432134	3.450300

117	1	0	3.431927	-2.686545	0.555793
118	1	0	3.866999	0.780200	0.407170
119	1	0	-0.804712	-0.724073	6.042893
120	1	0	2.463521	-6.590453	3.236175
121	1	0	-0.062014	2.180894	5.388332
122	1	0	5.539289	2.203095	-0.363252
123	1	0	-1.129032	1.628913	6.664010
124	1	0	0.905694	-1.463120	4.489659
125	1	0	7.115722	5.701322	-0.767150
126	1	0	2.676124	-2.501705	2.973010
127	1	0	5.910448	5.397383	0.467199
128	1	0	7.692894	3.313797	-0.909716
129	1	0	4.797766	-1.655899	0.903767
130	1	0	6.858599	1.644049	0.647211
131	1	0	2.316836	0.677672	4.433312
132	1	0	0.724782	0.062144	6.405175
133	1	0	5.492362	-3.986178	0.815721
134	1	0	3.916914	-4.538603	3.387321
135	1	0	4.961801	-5.637327	2.509720
136	1	0	4.713342	3.664033	1.507008
137	1	0	4.064817	-1.503891	3.326467
138	1	0	4.187374	1.953636	3.242137
139	1	0	5.294195	0.820728	2.484860
140	1	0	7.842162	3.908171	0.731974
141	1	0	5.792991	-3.309347	2.408416
142	1	0	6.096105	3.195076	2.485157
143	1	0	0.602056	-7.783123	2.184647
144	1	0	-4.554671	2.088635	3.857729
145	1	0	-1.644706	1.375138	3.647408
146	1	0	-0.356672	-6.046677	-2.112968
147	16	0	-0.000000	0.575155	0.000000
148	8	0	-0.810289	1.334176	0.974873
149	8	0	0.810287	1.334178	-0.974872
150	6	0	-1.019365	-0.650469	-0.872375
151	6	0	-0.559634	-1.854284	-0.483845
152	6	0	0.559638	-1.854283	0.483843
153	6	0	1.019366	-0.650468	0.872375
154	1	0	-0.968447	-2.792613	-0.846918
155	1	0	0.968454	-2.792612	0.846915

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= -4.3850 Z= -0.0000 Tot= 4.3850