Electronic Supplementary Material (ESI) for ChemComm.


Supplementary Information

# Simultaneous Synthesis and Characterization of *in/out*-Isomers of Disilabicyclo[14.14.14]alkanes

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## 1. Details of Synthetic Studies

**General.** All synthetic reactions were carried out in anhydrous conditions under an argon atmosphere unless otherwise noted. The chemical shifts in the $^{1}H$ and $^{13}C$ NMR spectra were based on the residual solvent resonances, while those in $^{29}Si$ and $^{19}F$ NMR spectra were referenced to external standard samples. HRMS analyses were carried out using a time-of-flight mass spectrometry (TOF-MS) system with atmospheric pressure chemical ionization (APCI) or electrospray ionization (ESI).

**Materials** Commercially available reagents were used without further purification unless otherwise noted.

**Synthesis of hexa-7-octenyldisiloxane (C8OC8).** To a 50-mL round bottomed flask with a magnetic stirrer, tri-7-octenylsilane[S1] (1.47 g, 4.00 mmol), $InBr_3$ (177 mg, 0.130 mmol), and dry oxygen-saturated dimethoxyethane (20 mL) was added and was stirred for 23 h. The solvents were distilled off and the residue was treated with column chromatography (silica gel, eluent: a hexane and $CH_2Cl_2$ mixture). The desired **C8OC8** was obtained as a colorless oil (1.03 g, 1.39 mmol, 70%).

**C8OC8:** a colorless oil; $^{1}H$ NMR ($CDCl_3$, 500 MHz): $\delta$ 5.80 (ddt, $J$ = 17, 10, 6 Hz, 6H), 4.98 (d, $J$ = 17 Hz, 6H), 4.92 (d, $J$ = 10.0 Hz, 6H, $H_2C$=CH-), 2.04 (q, $J$ = 6 Hz, 12H), 1.2-1.4 (br, 48H), 0.32-0.45 (br, 12H); $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz): $\delta$ 139.2, 114.1, 33.9, 33.6, 28.9 (duplicated), 23.2, 15.8; $^{29}Si\{^{1}H\}$ NMR ($CDCl_3$, 99 MHz): $\delta$ −6.1; HRMS (APCI) $m/z$: $[M+H]^+$ Calcd for $C_{48}H_{91}Si_2O$ 739.6603; Found: 739.6630.

S1: W. Setaka and K. Yamaguchi, *Proc. Natl. Acad. Sci. U.S.A.*, 2012, **109**, 9271–9275.

**Synthesis of siloxane cage C14O.** To a 500-mL three-necked flask with a magnetic stirrer, condenser, glass stopper, and dropping funnel, siloxane **C8OC8** (1.64 g, 2.22 mmol) and $CH_2Cl_2$ (500 mL) was added. Then, 1st generation Grubbs catalyst (90 mg) was added to the flask, and the solution was stirred under reflux. After 40h, the reaction mixture was cooled to room temperature, and the solvent was distilled off. The residue was treated with column chromatography (silica gel, eluent: hexane) to remove metal complexes. The crude products (0.85 g), toluene (15 mL), and Pd/C catalyst (ca. 50 mg) were added to an autoclave. The vessel was heated to 60 °C and stirred for 72 h under a hydrogen atmosphere (3 atm). The reaction mixture was filtered, and volatile materials were removed in vacuo. The desired siloxane cage **C14O** (883 mg, 1.34 mmol, 60%) was obtained as colorless crystals.

**C14O**: colorless crystals; mp 68.3–72.2 °C; $^{1}H$ NMR ($CDCl_3$, 500 MHz): $\delta$ 1.25-1.40 (br, 72H), 0.46-0.54 (br, 12H); $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz): $\delta$ 32.8, 27.3, 27.0 (duplicated), 26.1, 22.7, 15.6; $^{29}Si\{^{1}H\}$ NMR ($CDCl_3$, 99 MHz): $\delta$ 6.0; HRMS (APCI) $m/z$: $[M+H]^+$ Calcd for $C_{42}H_{85}Si_2O$ 661.6133; Found: 661.6127.

**Synthesis of diphenyldisilabicyclo[14.14.14]tetratetracontanes BCAs.** To a 30-mL two-necked flask with a magnetic stirrer, a condenser, and a septum, siloxane cage **C14O** (483 mg, 0.730 mmol), $BF_3$ diethylether complex (465 mg, 3.28 mmol), and $CHCl_3$ (3 mL) was added. Then, the solution was stirred at 50 °C. After 19 h, the reaction mixture was cooled to room temperature. The volatile materials were removed in vacuo, and then the flask was filled with argon gas. By measuring NMR the small amount of the mixture, formation of fluorosilanes could be confirmed (Two isomers, of which structures could not be determined, were included. Isomer A ($\delta^{29}Si$ = 31.8, $^{1}J_{Si\text{-}F}$ = 287 Hz, $\delta^{19}F$ = −171), isomer B ($\delta^{29}Si$ = 32.2, $^{1}J_{Si\text{-}F}$ = 289 Hz, $\delta^{19}F$ = −170)). To the mixture was dropwised 2.0 M PhLi dibuthylether solution (7.3 mL, 14.6 mmol) at 0 °C, then the mixture was raised to room temperature with stirring. After 26 h, the mixture was quenched with a dilute aqueous $NH_4Cl$ solution and extracted with hexane. The organic layer was washed several times and dried over anhydrous $Na_2SO_4$ and filtered, and the volatile materials were removed in vacuo. After flash column chromatography, crude mixtures of BCAs (758 mg) were obtained. The crude products were treated with gel permeation chromatography, pure ***out,out*-BCA** (310 mg, 0.388 mmol, 53% yield, retention time: 45.7 min.) and ***twist-out,out*-BCA** (58 mg, 0.073 mmol, 10% yield, retention time: 46.5 min.) were obtained after evaporation of the solvents of the fractions.

***out,out*-BCA:** colorless crystals; mp 67.8–69.0 °C; $^{1}H$ NMR ($CDCl_3$, 500 MHz): $\delta$ 7.51-7.56 (br, 4H), 7.35-7.40 (br, 6H), 1.32-1.46 (br, 72H), 0.83-0.90 (br, 12H); $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz): $\delta$ 138.4, 134.0, 128.6, 127.6, 33.4, 29.5 (duplicated), 29.2, 28.9, 23.6, 12.5; $^{29}Si\{^{1}H\}$ NMR ($CDCl_3$, 99 MHz): $\delta$ −2.2; HRMS (ESI) $m/z$: $[M+Na]^+$ Calcd for $C_{54}H_{94}Si_2Na$ 821.6786; Found: 821.6792.

***twist-out,out*-BCA:** colorless crystals; mp 55.6–61.5 °C; $^{1}H$ NMR ($CDCl_3$, 500 MHz): $\delta$ 7.45-7.52 (br, 4H), 7.31-7.35 (br, 6H), 1.20-1.40 (br, 72H), 0.77-0.82 (br, 12H); $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz): $\delta$ 138.5, 134.0, 128.6, 127.6, 32.8, 29.0 (duplicated), 28.7, 28.5, 23.4, 12.3; $^{29}Si\{^{1}H\}$ NMR ($CDCl_3$, 99 MHz): $\delta$ −1.7; HRMS (ESI) $m/z$: $[M+Na]^+$ Calcd for $C_{54}H_{94}Si_2Na$ 821.6786; Found: 821.6768.

## 2. Copies of $^{1}H$, $^{13}C$, $^{29}Si$ NMR, and HRMS Spectra for All New Compounds

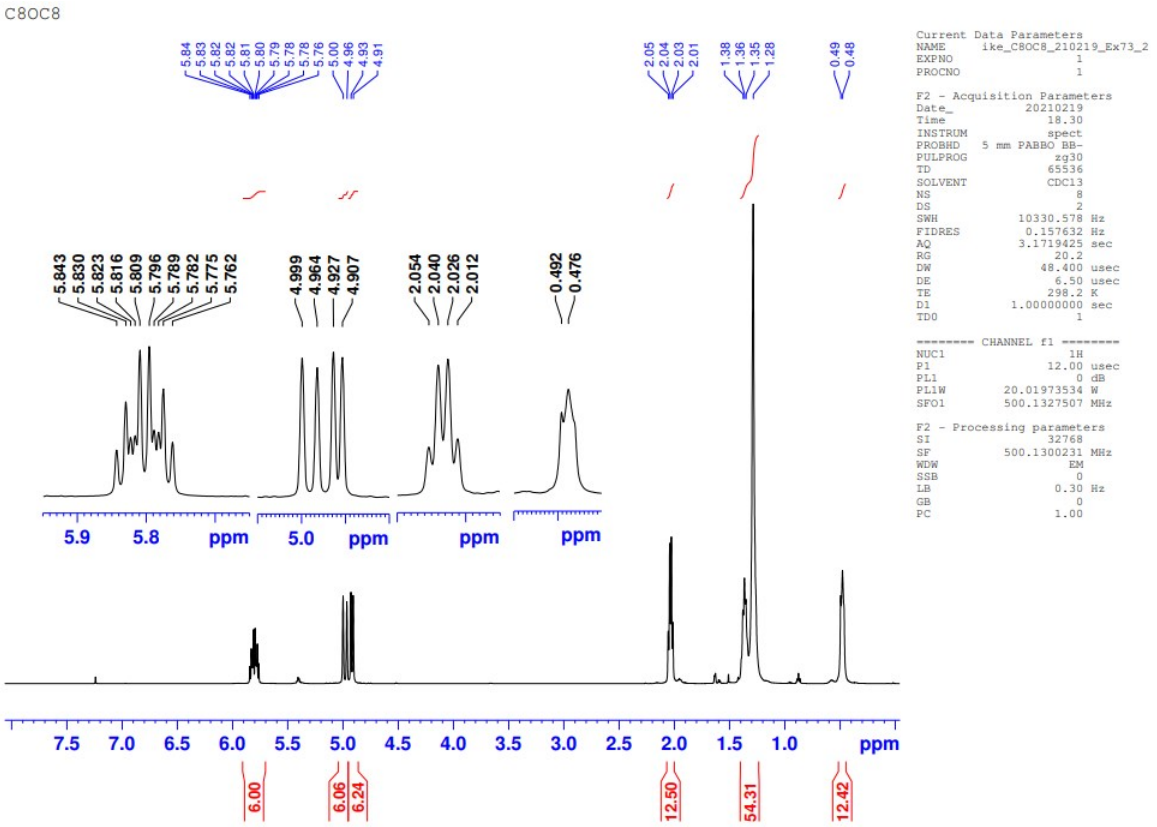


**Fig. S1.** $^{1}H$ NMR spectrum of hexa-7-octenyldisiloxane (**C8OC8**) in $CDCl_3$.

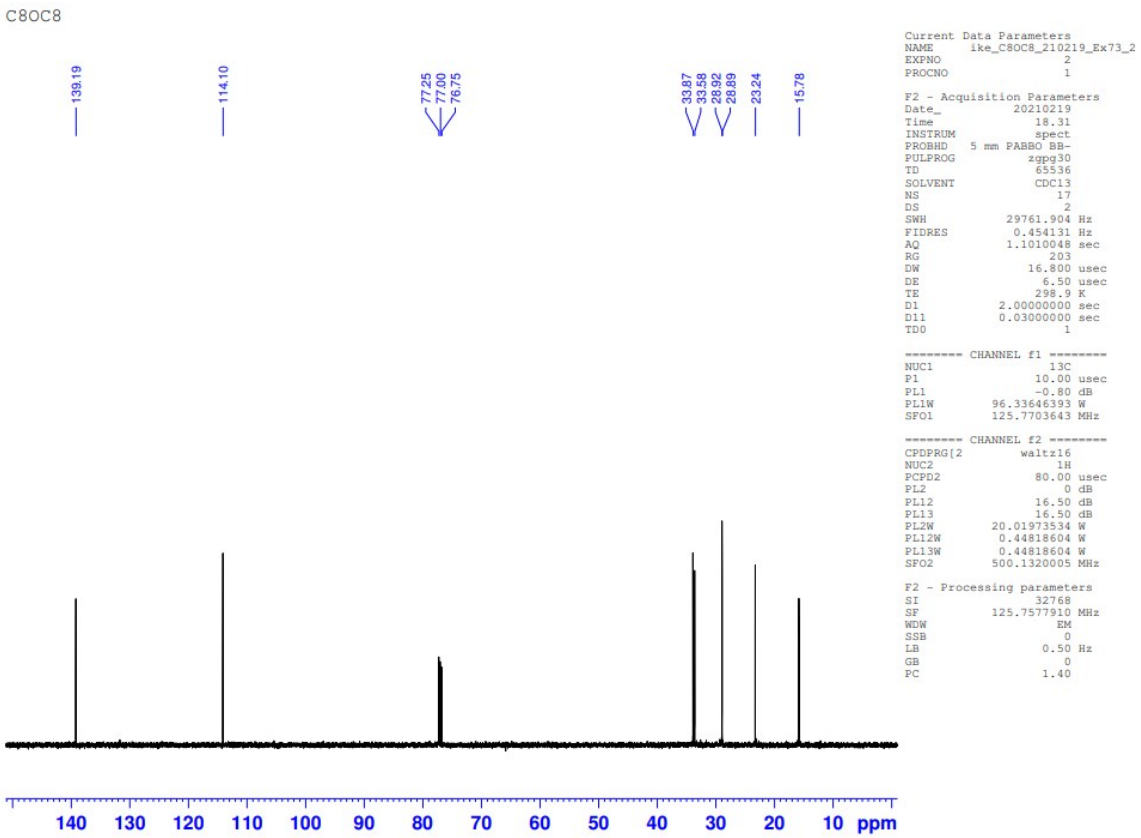


**Fig. S2.** $^{13}C$ NMR spectrum of hexa-7-octenyldisiloxane (**C8OC8**) in $CDCl_3$

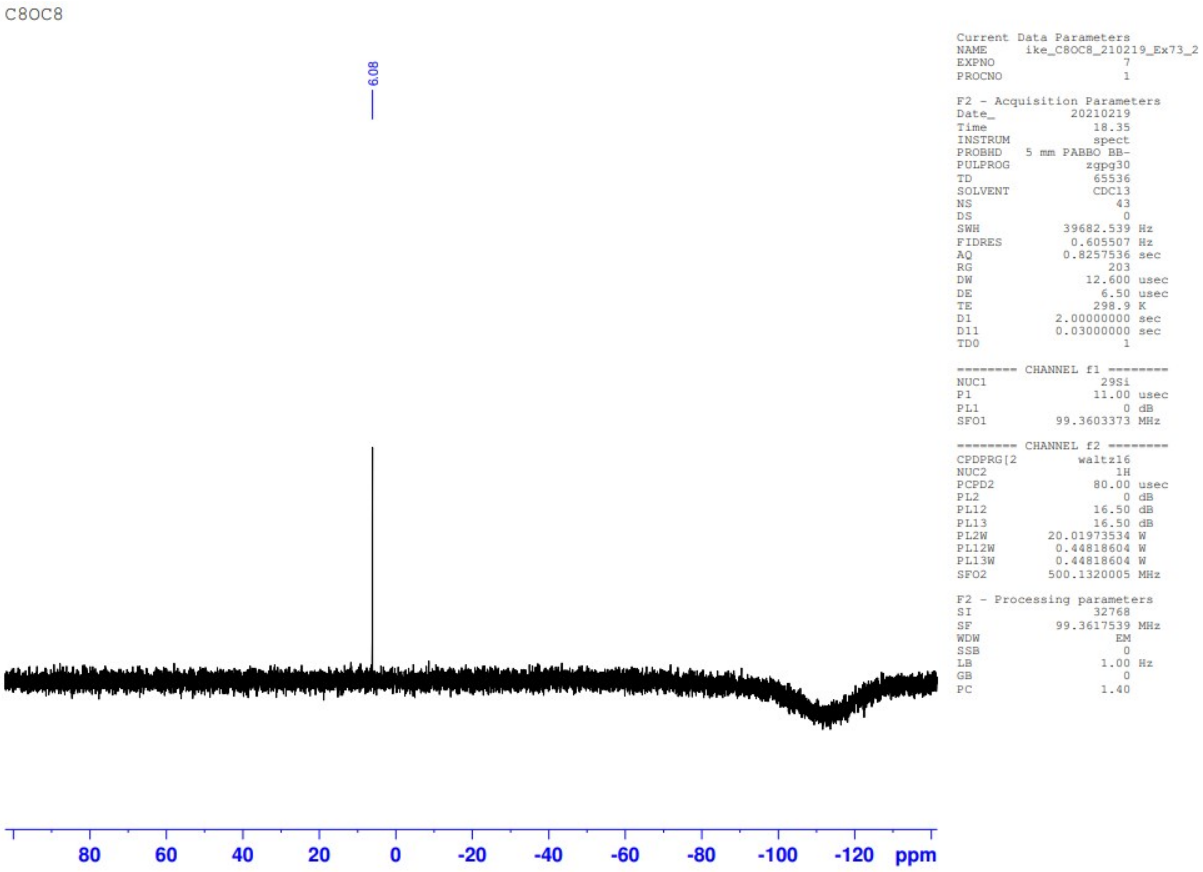


**Fig. S3.** $^{29}$Si NMR spectrum of hexa-7-octenyldisiloxane (**C8OC8**) in $CDCl_3$.

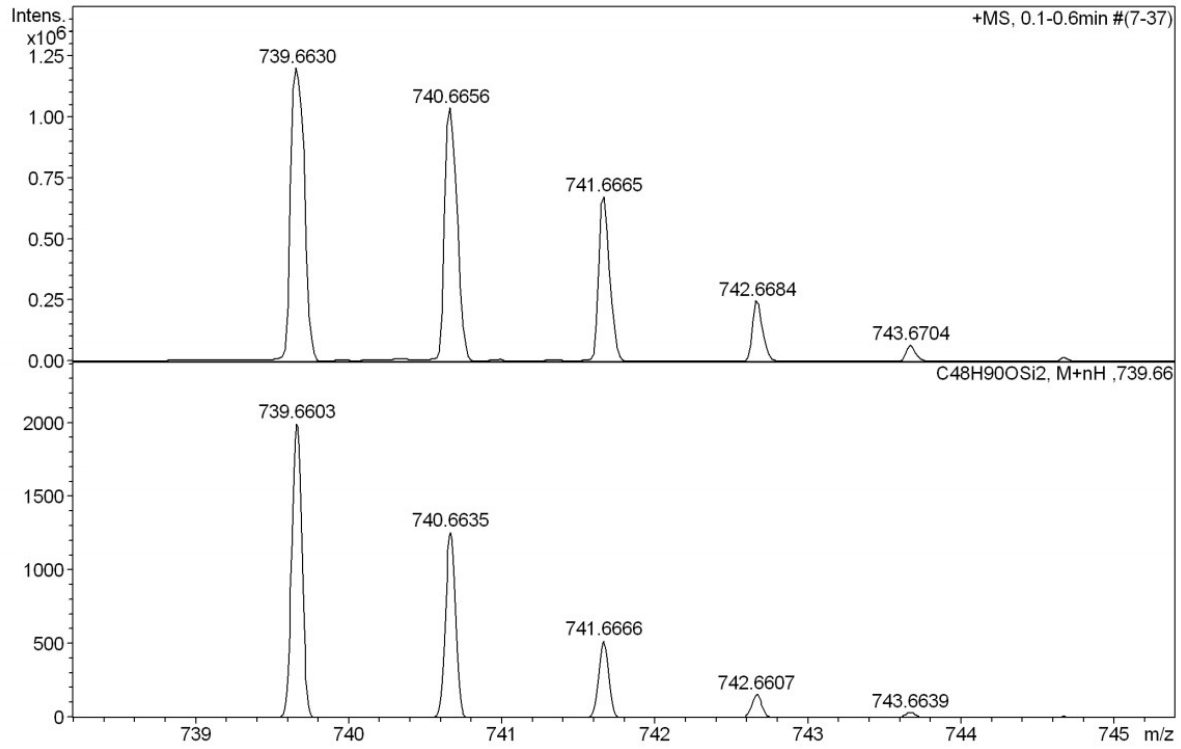


**Fig. S4.** HRMS spectrum of hexa-7-octenyldisiloxane (**C8OC8**) (APCI, positive). Top: obsd. Bottom: sim.

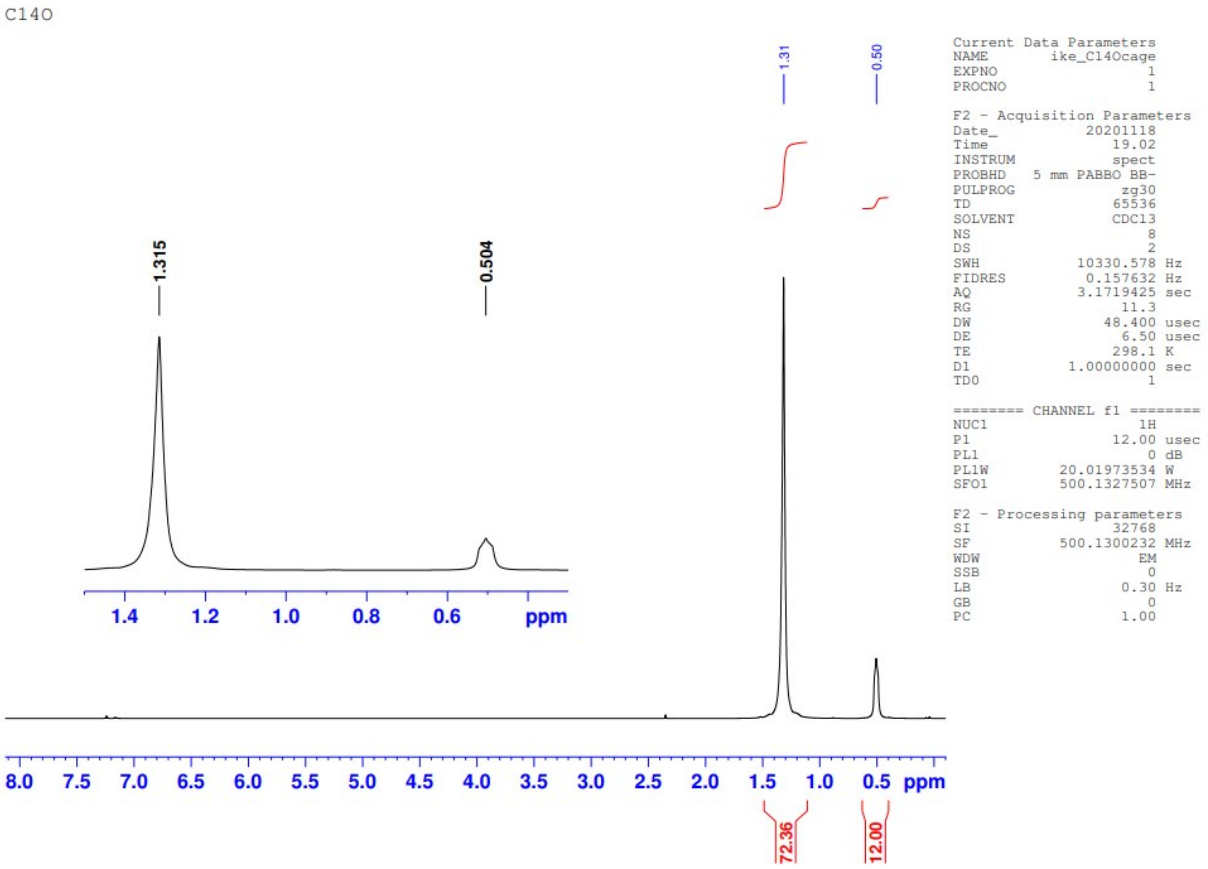


**Fig. S5.** $^{1}$H NMR spectrum of siloxane cage **C14O** in $CDCl_3$.

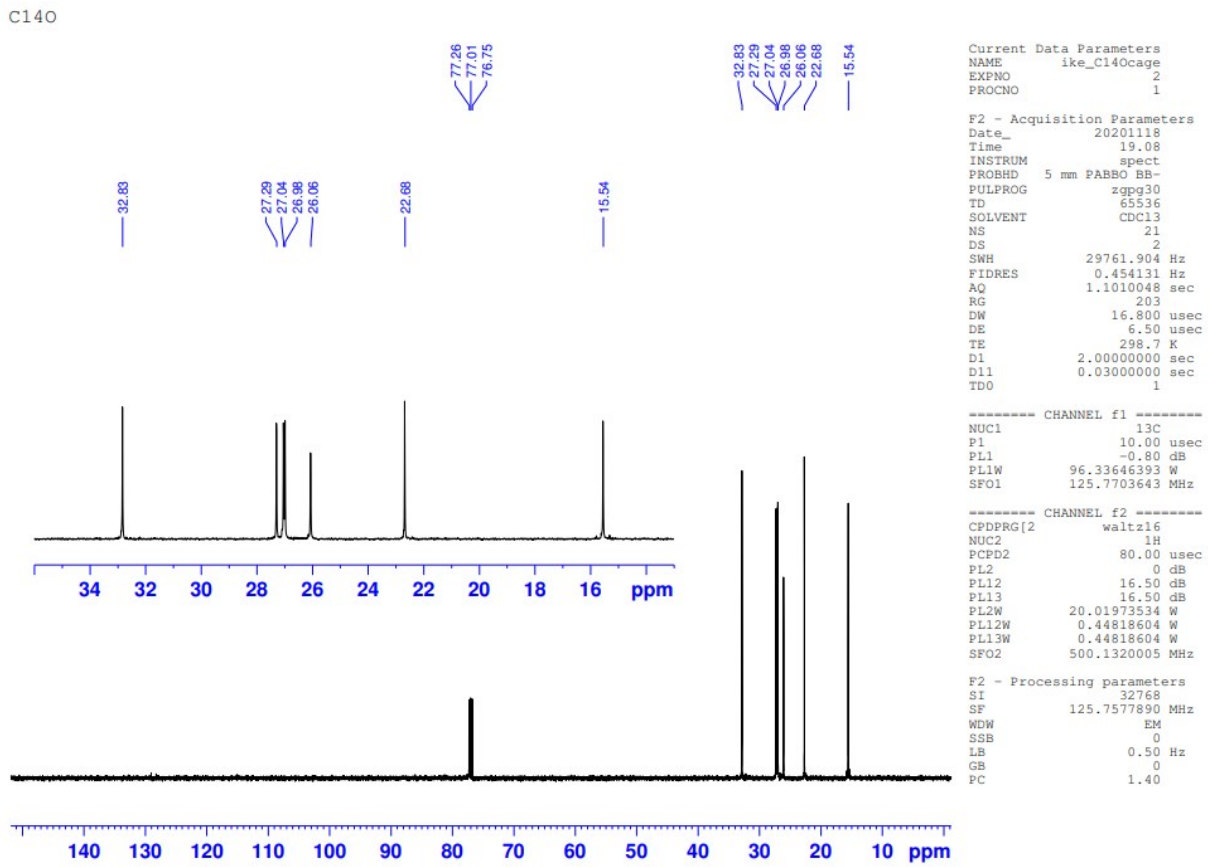


**Fig. S6.** $^{13}$C NMR spectrum of siloxane cage **C14O** in $CDCl_3$.

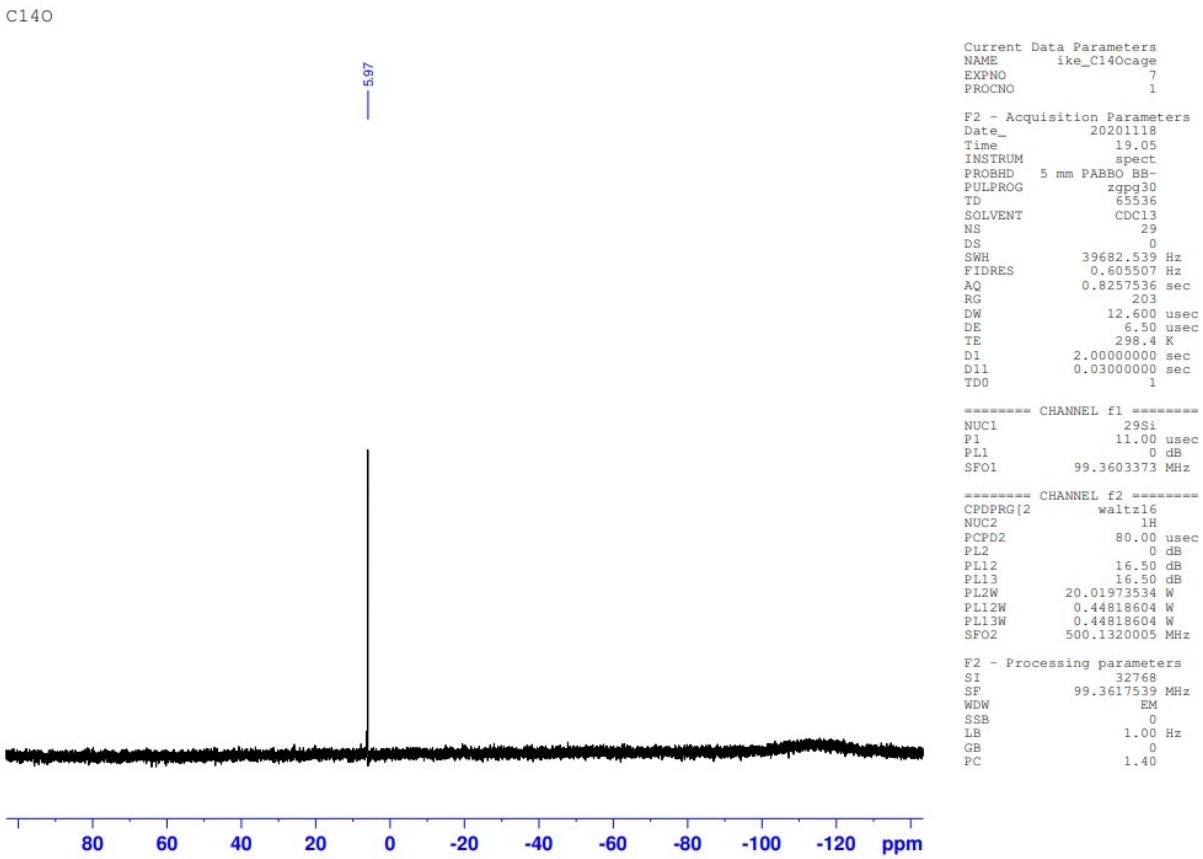


**Fig. S7.** $^{29}$Si NMR spectrum of siloxane cage **C14O** in $CDCl_3$.

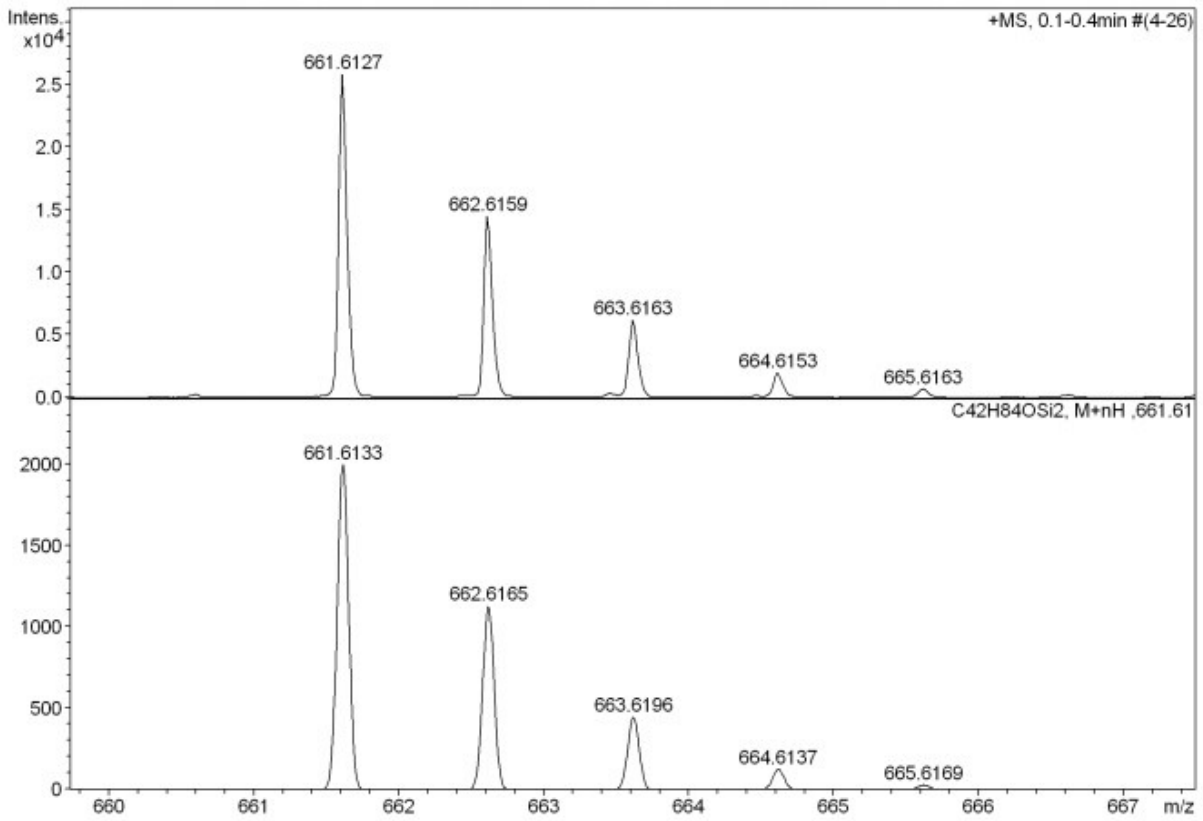


**Fig. S8.** HRMS spectrum of siloxane cage **C14O** (APCI, positive). Top: obsd. Bottom: sim.

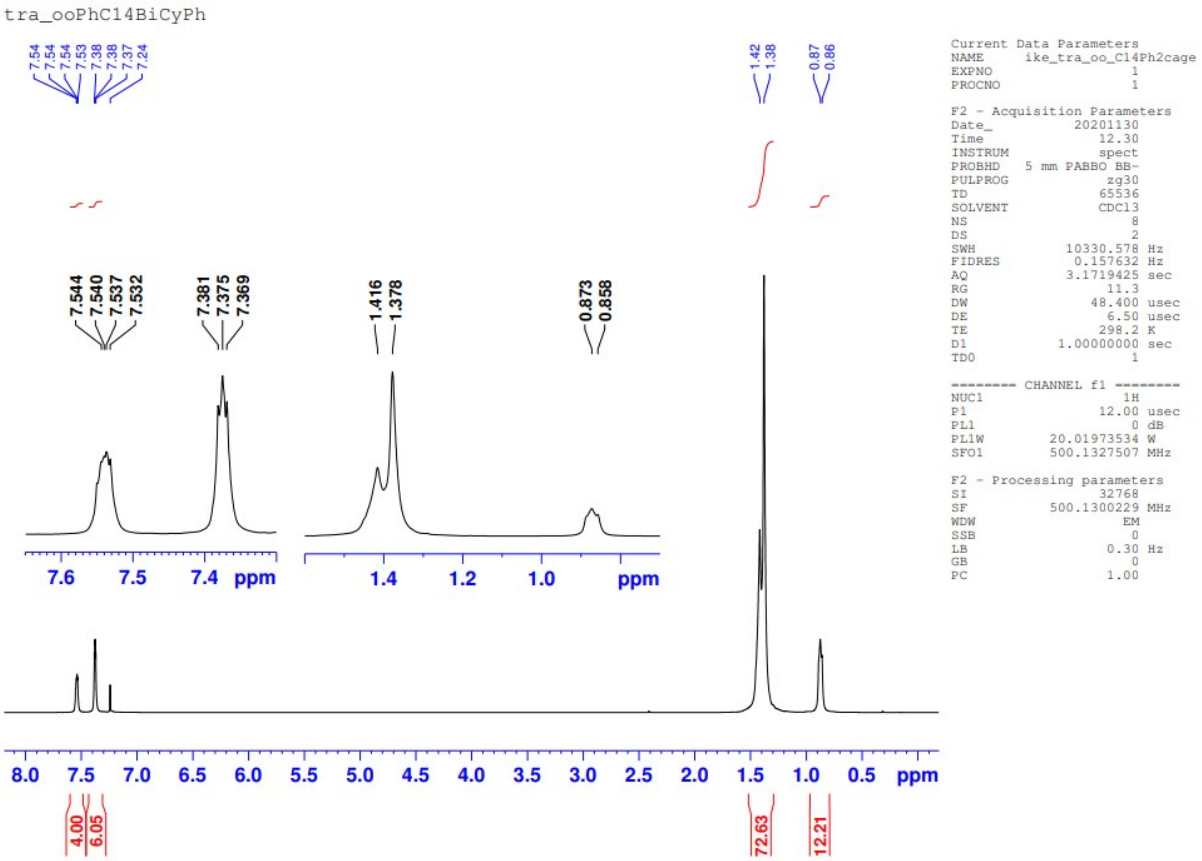


**Fig. S9.** $^{1}$H NMR spectrum of Diphenyldisilaicycloalkane ***out,out*-BCA** in $CDCl_3$.

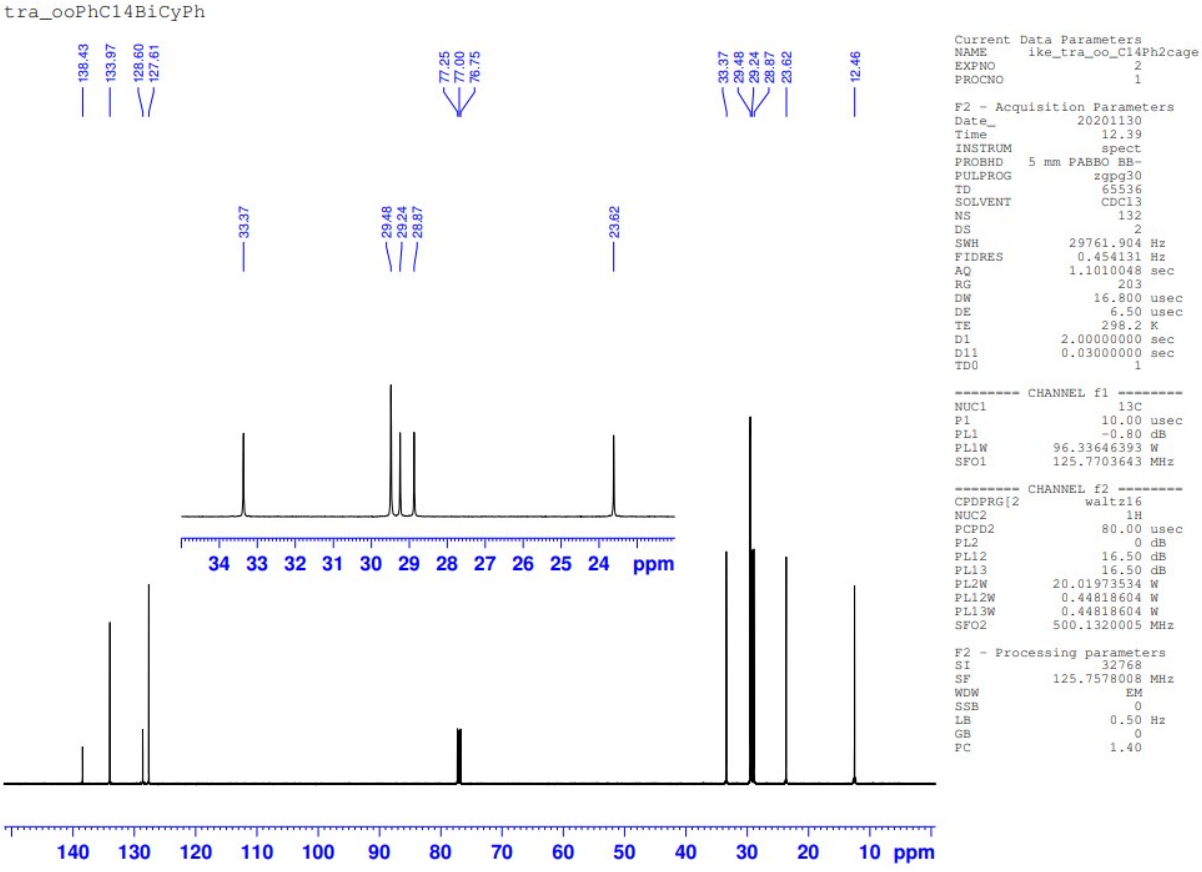


**Fig. S10.** $^{13}$C NMR spectrum of Diphenyldisilaicycloalkane ***out,out*-BCA** in $CDCl_3$.

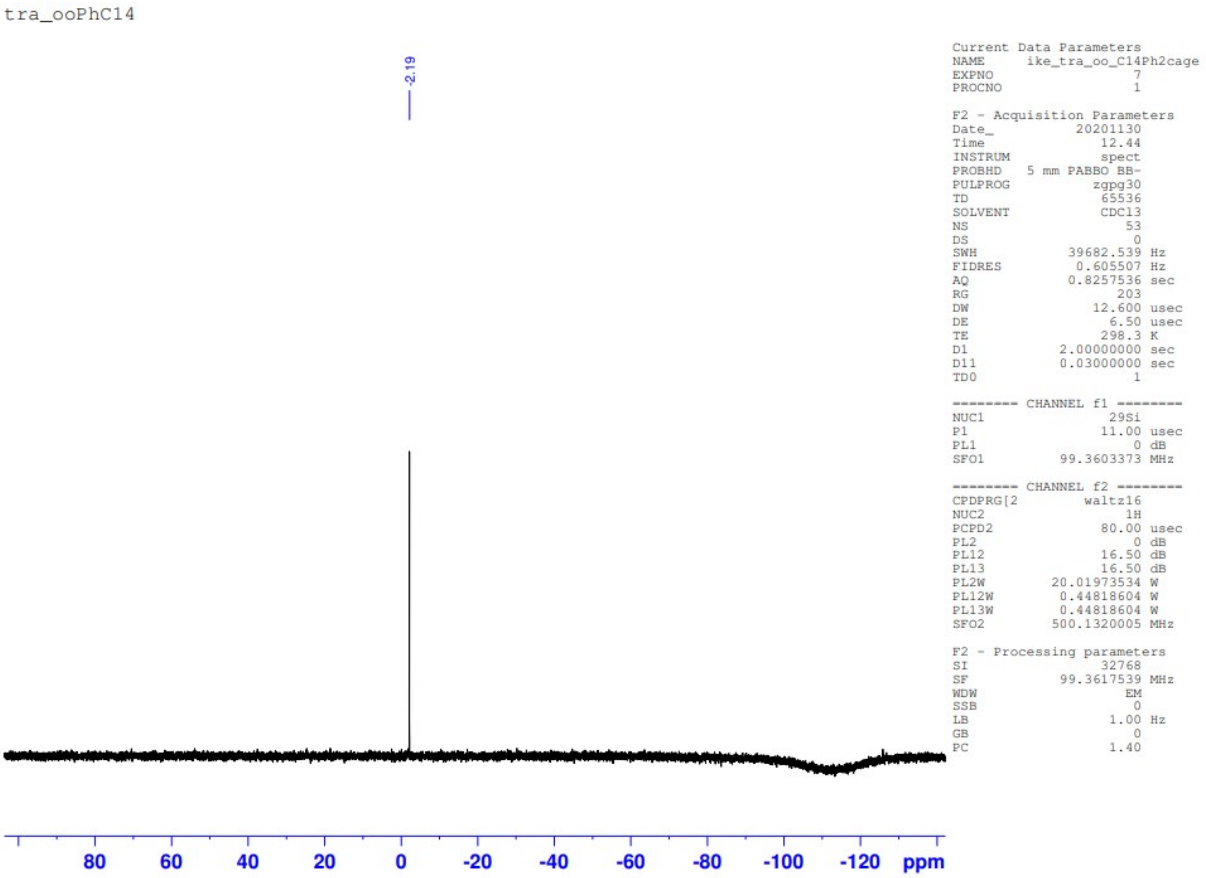


**Fig. S11.** $^{29}$Si NMR spectrum of Diphenyldisilaicycloalkane ***out,out*-BCA** in $CDCl_3$.

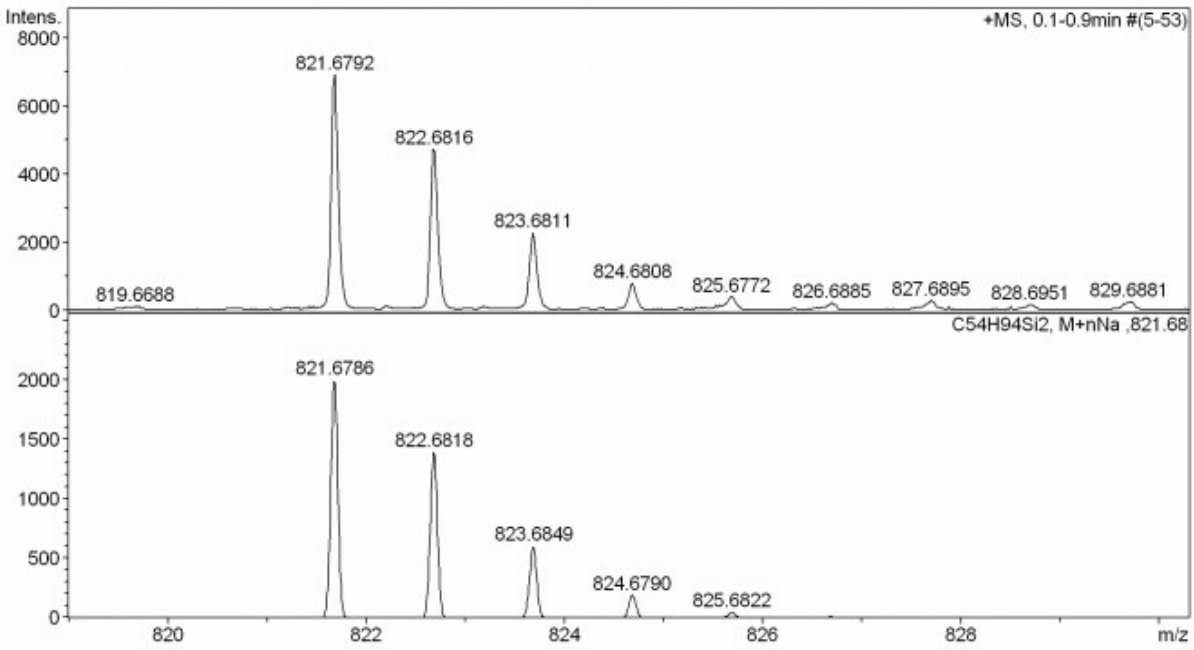


**Fig. S12.** HRMS spectrum of Diphenyldisilaicycloalkane ***out,out*-BCA** (APCI, positive). Top: obsd. Bottom: sim.

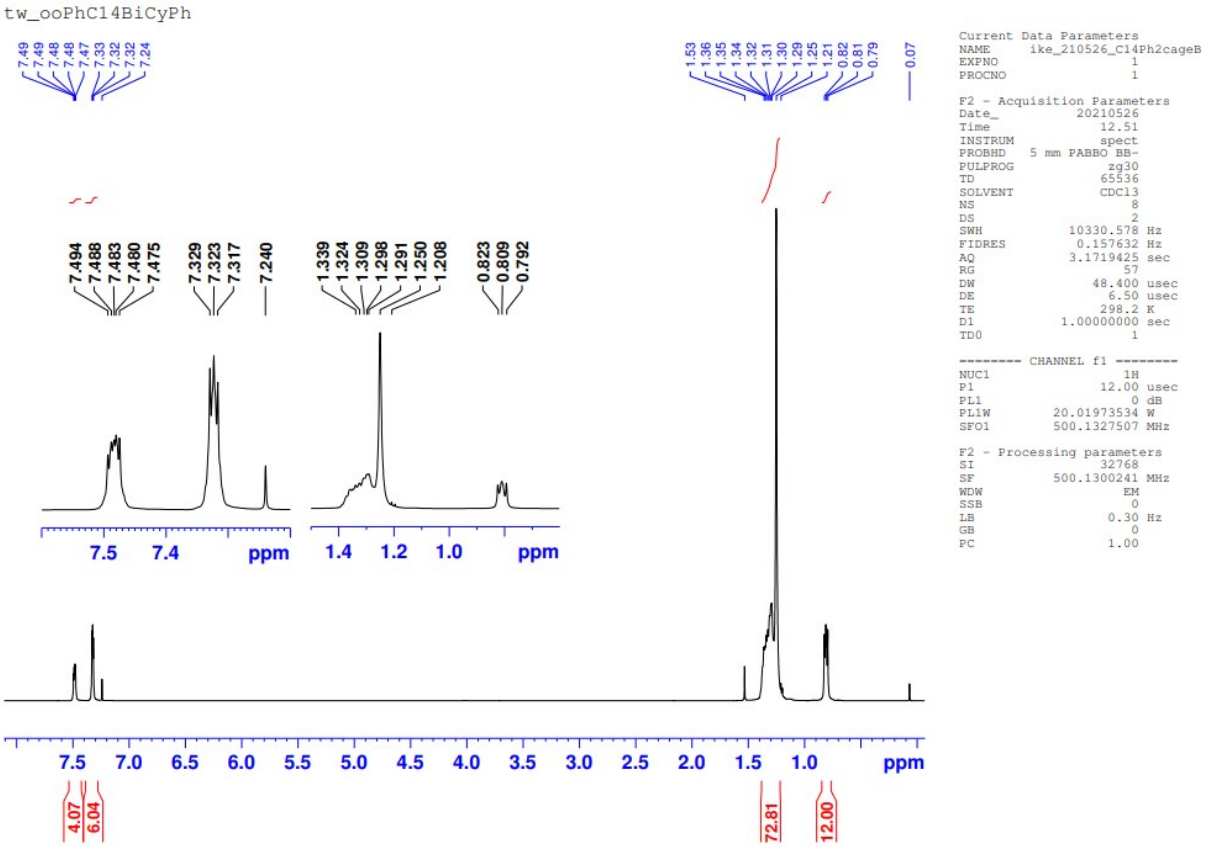


**Fig. S13.** $^{1}$H NMR spectrum of Diphenyldisilaicycloalkane ***twist-out,out*-BCA** in $CDCl_3$.

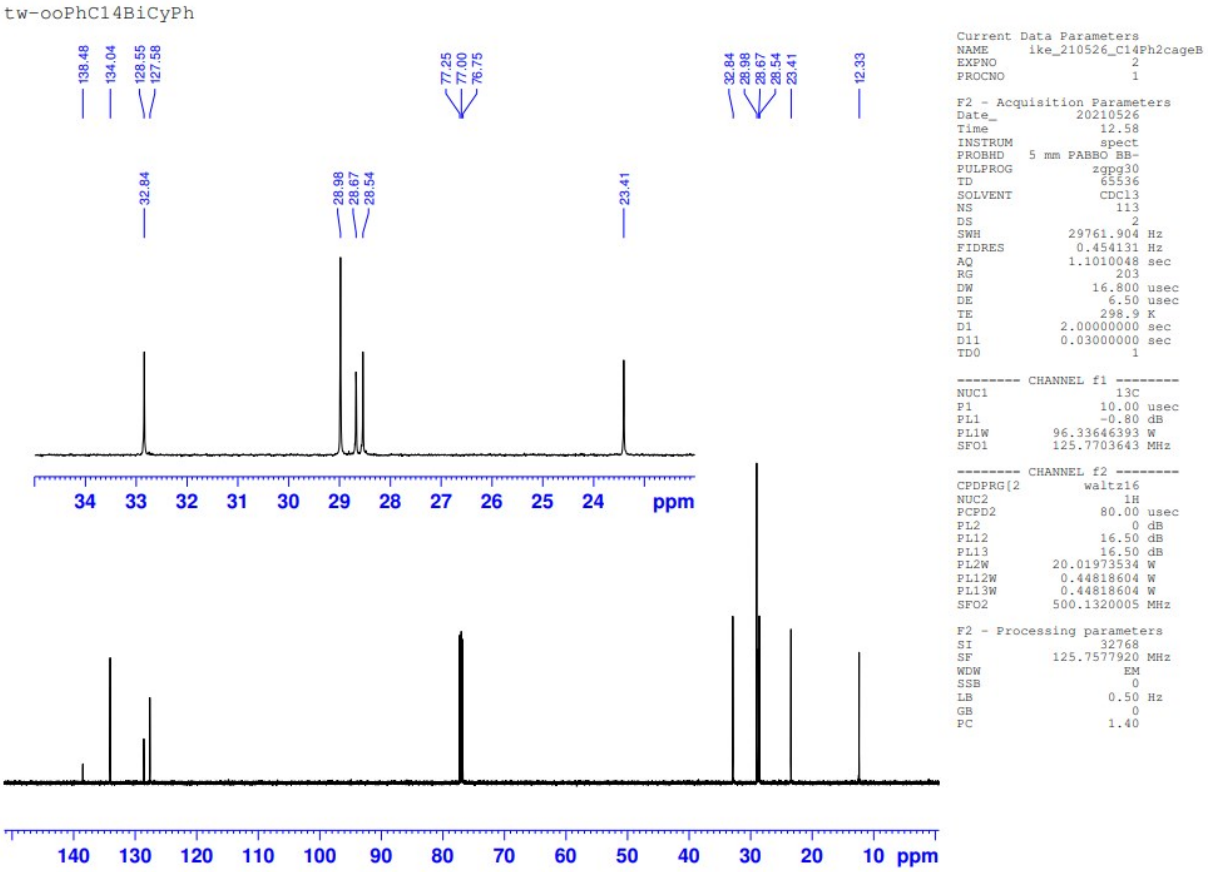


**Fig. S14.** $^{13}$C NMR spectrum of Diphenyldisilaicycloalkane ***twist-out,out*-BCA** in $CDCl_3$.

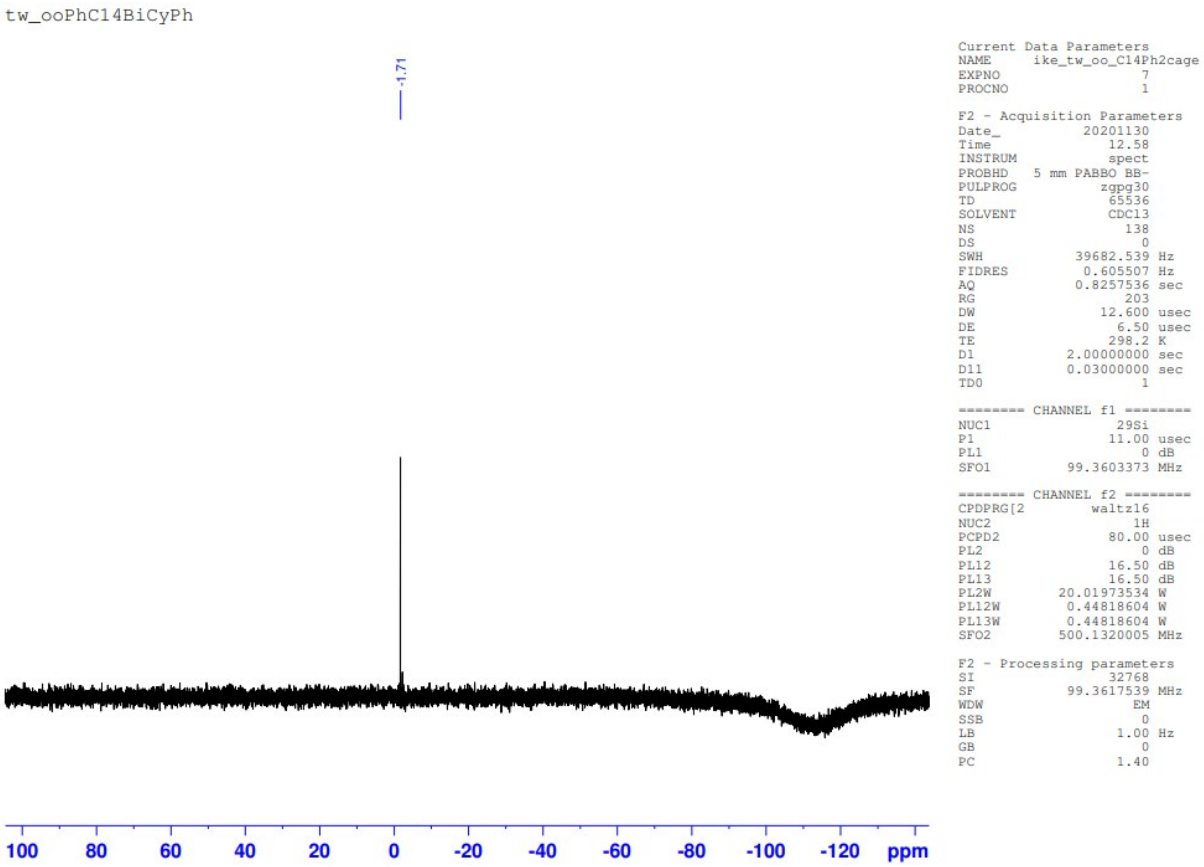


**Fig. S15.** $^{29}$Si NMR spectrum of Diphenyldisilaicycloalkane ***twist-out,out*-BCA** in $CDCl_3$.

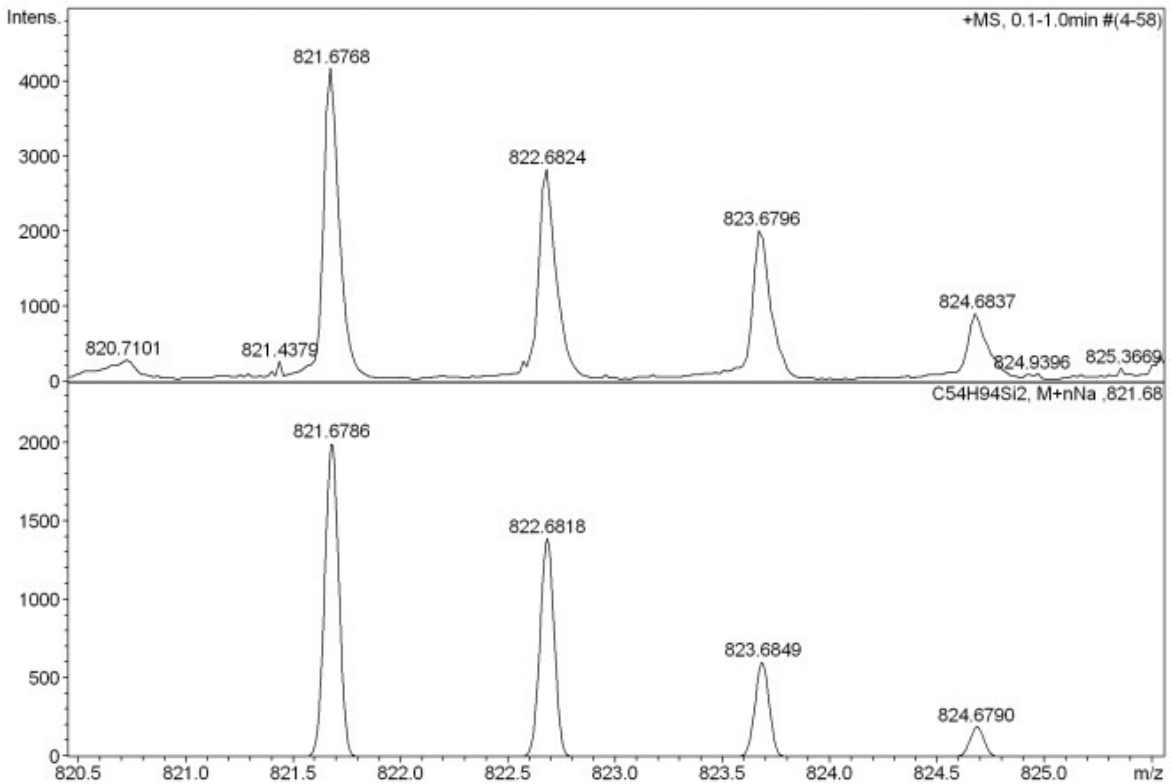


**Fig. S16.** HRMS spectrum of Diphenyldisilaicycloalkane ***twist-out,out*-BCA** (APCI, positive). Top: obsd. Bottom: sim.

### 3. Observation of C14F2 Intermediate

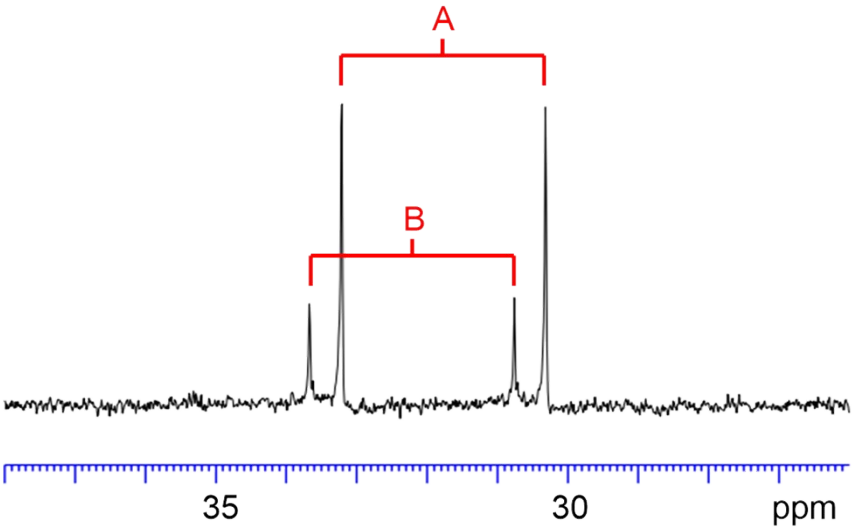


**Fig. S17.** $^{29}$Si NMR spectrum of a diastereomers mixture of **C14F2**.

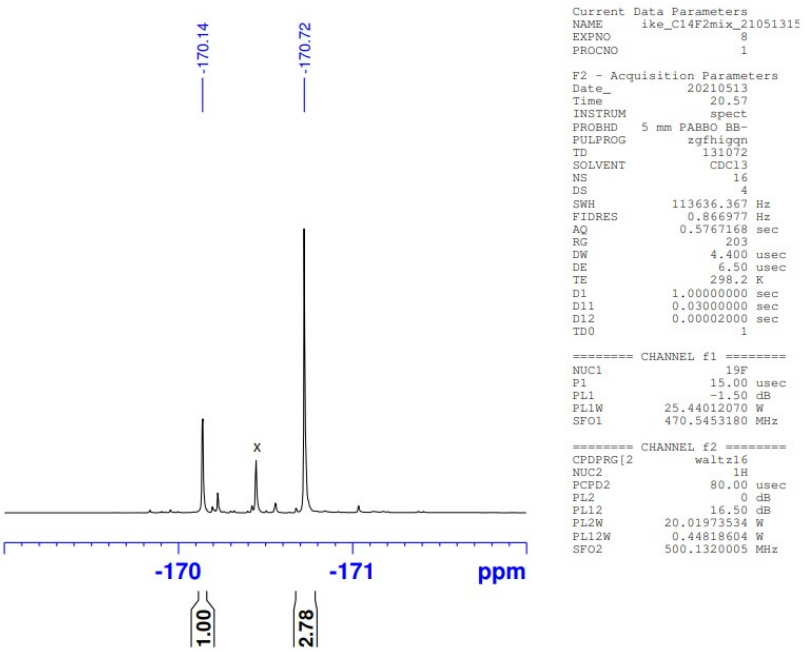


**Fig. S18.** $^{19}$F NMR spectrum of a reaction mixture of Difluorodisilabicyclo[14.14.14]alkane **C14F2**. The signal indicated by symbol x was due to the impurity.

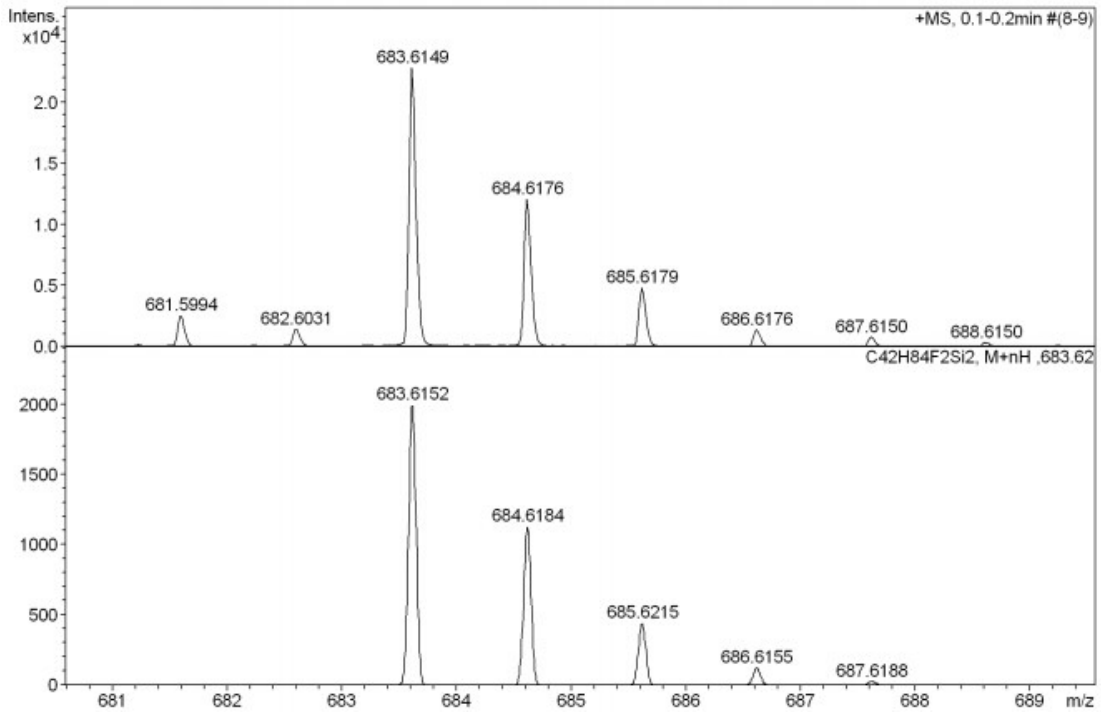


**Fig. S19.** HRMS spectrum of a reaction mixture of Difluorodisilabicyclo[14.14.14]alkane **C14F2** (APCI, positive). Top: obsd. Bottom: sim. (HRMS (APCI) *m*/*z*: $[M+H]^+$ Calcd for $C_{42}H_{85}F_2Si_2$ 683.6152; Found: 683.6149)

## 4. Details of DFT Calculations

All calculations were carried out using Gaussian 16 (Revision C.01) program packages[S1] at the Research Center for Computational Science, Okazaki and the Nagoya University ICTS, Japan. Geometry optimizations were carried out at the B3LYP/6-31G(d) level in the gas phase using default size of the grid.

S1: Gaussian 16, Revision C.01,
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, 2019.

**Table S1.** Calculated Energies for Diphenyldisilabicyclo[14.14.14]alkanes

| Energy | *out,out*-BCA | *in,in*-BCA | *in,out*-BCA | *twist-out,out*-BCA |
|---|---|---|---|---|
| Total energy *E* / hartree | -2693.4929594 | -2693.4777654 | -2693.4802905 | -2693.4856754 |
| Relative energy Δ*E* / kcal mol$^{-1}$ | 0.0 | +9.5 | +7.9 | +4.6 |
| ZPE[a] / hartree | 1.382716 | 1.384471 | 1.383723 | 1.383193 |
| (*E*+ZPE) / hartree | -2692.110244 | -2692.093295 | -2692.096568 | -2692.102483 |
| Relative energy Δ(*E*+ZPE) / kcal mol$^{-1}$ | 0.0 | +10.6 | +8.6 | +4.9 |
| *E*+*G* [b] / hartree | -2692.223342 | -2692.200392 | -2692.207460 | -2692.213294 |
| Relative energy Δ(E+*G*) / kcal mol$^{-1}$ | 0.0 | +14.4 | +10.0 | +6.3 |

a. Zero-point correction. b. Sum of electronic and thermal Free Energies at 298 K.

**Table S2.** Optimized Structural Coordinate and its Total Energy for ***out,out*-BCA** at B3LYP/6-31G(d) level

total energy: = `-2693.4929594 hartree` (NImag = 0)

| Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 7.0141084794 | -1.9929345065 | -0.5216515284 |
| Si | -7.0311379453 | 1.8073284124 | 0.7999179177 |
| C | 5.6184458211 | -1.2201730434 | -5.1285178602 |
| C | 7.0943072597 | -0.9974652423 | -4.743918525 |
| C | 3.1630882368 | -0.4920519764 | -4.8289154344 |
| C | 4.6393628682 | -0.2153522554 | -4.5068090402 |
| C | 7.379863561 | -0.9203640423 | -3.2294035173 |
| C | 0.7200757946 | 0.0257189597 | -4.1423048751 |
| C | 2.2129869702 | 0.3178463999 | -3.9373448967 |
| C | 6.9227803337 | -2.1499883685 | -2.4200861073 |
| C | -1.6530750164 | 0.418481447 | -3.1790100462 |
| C | -0.1419840654 | 0.6400271083 | -3.0320802137 |
| C | -3.9495425369 | 0.8163558363 | -2.0490114795 |
| C | -2.4215096068 | 0.8718290217 | -1.9306631447 |
| C | 2.5846706152 | -5.1475272594 | 0.3101293493 |
| C | 4.1001030293 | -4.9935381934 | 0.5322683053 |
| C | 4.6894000443 | -3.6766316087 | 0.0008503225 |
| C | -6.1768134988 | 1.3302568017 | -0.8342050412 |
| C | 6.2067682673 | -3.5425288768 | 0.2416096291 |
| C | 6.0650409458 | -0.4227519602 | -0.0067161165 |
| C | -4.6463436917 | 1.1908750694 | -0.7317971402 |
| C | 0.2100508026 | -4.3917531348 | 0.9196425823 |
| C | -6.0528653072 | 4.5661167758 | 0.526363157 |
| C | 1.7098588044 | -4.2785500542 | 1.2262256872 |
| C | -5.4231233707 | 5.8323945475 | 1.1438200594 |

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C,0,-2.167196774,-3.6328870499,1.5301407973
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H,0,6.9044887381,-0.0157670341,-2.8283149156
H,0,7.4955609925,-3.0349986334,-2.7348044624
H,0,2.4680534045,0.1089658719,-2.8871530887
H,0,-1.8559318713,-0.6464175212,-3.3659646915
H,0,0.0567017996,1.7205034998,-2.9713948305
H,0,-4.2795837468,1.5007306662,-2.844389923
H,0,2.3503790671,-4.9219585013,-0.7413445585
H,0,4.6203655373,-5.8276578455,0.0404345507
H,0,4.4723828031,-3.6118630755,-1.0753970414
H,0,-6.4197051668,2.0852234585,-1.5963114396
H,0,-4.2676261647,-0.1897924632,-2.3596983658
H,0,2.3060880569,-6.2000810654,0.460721649
H,0,0.1857371055,0.2228356003,-2.0679124122
H,0,-2.12449972,1.9015033043,-1.6808599623
H,0,6.7133313133,-4.4324250146,-0.1625665002
H,0,5.0994680353,-0.4436065519,-0.5323504749
H,0,6.5903433336,0.458023255,-0.4060154569
H,0,-6.608295318,0.388086132,-1.2030982459
H,0,0.0227412256,-4.0216085519,-0.0994484744
H,0,-5.4244517714,4.223750064,-0.3062748313
H,0,-2.8037178583,5.5655072762,0.1226934577
H,0,-5.2870419157,6.5745394643,0.3436017709
H,0,-7.0133607112,4.8488626372,0.0744245758
H,0,-0.0830625206,-5.4522396337,0.9140344605
H,0,-2.1027488653,0.2541101037,-1.0773309667
H,0,-0.4473665222,4.31941181,0.0558507306
H,0,-4.2177755006,2.1365768034,-0.3714196499
H,0,1.7203327193,2.8514788831,0.0935907938
H,0,4.1709152138,-2.826518657,0.4637182323
H,0,4.3244691508,-5.0876766366,1.6053247631
H,0,3.766912369,1.3008457476,0.1991005801
H,0,-2.2909025534,-3.1243252234,0.5622133273
H,0,2.0093809392,-3.2240264857,1.1470366368
H,0,-3.3138721313,3.9881779457,0.6983275696
H,0,6.4063818077,-3.5562357349,1.3229115886
H,0,-4.3883207823,0.4389930908,0.0282662855
H,0,-2.5029807655,-4.6685756576,1.3721020706

H,0,-1.1184931012,2.9239184893,0.8828412025
H,0,-1.2009242674,5.7860308937,1.9897385049
H,0,1.8924127803,-4.5677289572,2.2721289689
H,0,-6.138297325,6.2762997693,1.8510981822
H,0,-6.6168554285,-1.274546893,0.7905311436
H,0,1.2308257927,4.6465045493,1.8392788093
H,0,5.7212847251,1.9307510231,1.57904429
H,0,1.0094620429,1.659596149,1.1684213209
H,0,3.5195479777,3.3325996642,1.7246302893
H,0,-3.7334516587,6.6097821026,2.2351385983
H,0,3.1261955799,0.2975633439,1.4910033607
H,0,-4.5795745191,-2.2206431966,1.2291751187
H,0,5.259276349,-1.0843580915,1.8978951233
H,0,-4.9182593329,-3.8295772147,1.8457699907
H,0,6.8017805141,-0.258829671,2.0263744123
H,0,-0.3321927755,-2.588557006,1.988292452
H,0,-5.3155458947,3.1242457038,1.976605517
H,0,-8.2189554343,-1.0009655537,1.4406252712
H,0,-6.9062925756,3.747044858,2.3481936817
H,0,-0.5576219916,-4.0645148204,2.9135284797
H,0,-4.2454257553,5.0247083133,2.7771182795
H,0,-1.8570990993,4.3616044819,2.7813125369
H,0,0.4731237178,3.416673986,2.839828525
H,0,2.7692745318,2.2888226344,2.9225317632
H,0,5.0405234966,1.1227254485,2.9834473556
H,0,-5.6883725898,0.4797092782,2.3776481456
H,0,-7.318435562,-3.0048241432,2.4560081993
H,0,-2.6791014903,-1.9614374063,2.8056830488
H,0,-3.0158202963,-3.5318739412,3.5163036427
H,0,-7.2939897206,0.7335832448,3.0228899112
H,0,-5.0231901398,-1.2933850182,3.5688560833
H,0,-7.4968062364,-1.7638554082,3.6869565292
H,0,-5.4256425979,-2.9132923021,4.0974415009
C,0,8.816646782,-1.8766092601,0.0598416074
C,0,9.5162422364,-0.6545888715,0.0294692795
C,0,10.8514331085,-0.5654038452,0.4266600381
C,0,11.5254622289,-1.7046522619,0.8697999265
C,0,10.8557296945,-2.9282901954,0.9126009513
C,0,9.520259771,-3.0083238776,0.513148432
H,0,9.0122074983,0.2490365187,-0.3071275734
H,0,11.3644867966,0.3926854844,0.3930028884
H,0,12.5647697334,-1.638591028,1.1816422287
H,0,11.3720596913,-3.8201081767,1.2595356147
H,0,9.0198105211,-3.9729625684,0.5603891216
C,0,-8.887849942,2.0483891476,0.4947152083
C,0,-9.4827055523,1.8315223401,-0.7614367935
C,0,-10.8535758474,2.010419294,-0.9617293276
C,0,-11.6674900354,2.4130083025,0.0973157695
C,0,-11.1032564538,2.6350490182,1.3554780896
C,0,-9.7332649464,2.4541889885,1.5460568481
H,0,-8.8695281186,1.5175049191,-1.6028207939
H,0,-11.2849081585,1.8356063978,-1.9444163445
H,0,-12.734608607,2.5533773476,-0.0554576351
H,0,-11.7305906861,2.9491920145,2.1861593372
H,0,-9.3173633119,2.6343961839,2.5362092018

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**Table S3.** Optimized Structural Coordinate and its Total Energy for ***in,in*-BCA** at B3LYP/6-31G(d) level

total energy: = -2693.4777654 hartree (NImag = 0)

| Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Si | 3.9290987728 | -1.9636977641 | -1.5305964694 |
| Si | -3.4917439929 | 0.6712411269 | 1.1302179685 |
| C | 6.4178722497 | -2.1245224697 | 0.1211614117 |
| C | 5.8172208915 | -2.2248352856 | -1.2982457186 |

C,0,6.8373683503,-0.7372701186,2.2228724411
C,0,6.3230437176,-0.739754981,0.7760278317
C,0,6.892747566,0.647386106,2.8919517642
C,0,3.9590205278,2.2123583399,-2.7420249657
C,0,4.3302653083,3.5863801125,-2.1487616765
C,0,3.2444587937,-3.3324513346,-2.6761898028
C,0,3.5853399476,-0.2965856657,-2.3913890202
C,0,4.0774414375,1.0250070786,-1.7680741662
C,0,1.1334413419,-4.516406875,-3.5830538111
C,0,5.5559390755,1.4014797764,3.008872072
C,0,1.7113608619,-3.2984882664,-2.8462823762
C,0,3.2705215285,4.218697468,-1.2253560393
C,0,-0.3990238744,-4.5022477068,-3.7359797979
C,0,4.4677593997,0.6803486732,3.8182923661
C,0,2.0095882794,4.7084835571,-1.955636221
C,0,-1.1791133397,-4.5637882354,-2.4123371981
C,0,3.2256166371,1.5523932293,4.0501713336
C,0,0.9096427702,5.2229680272,-1.0143211483
C,0,-2.6945855579,-4.7221102265,-2.6028560792
C,0,2.0725465455,0.8254668299,4.7560982505
C,0,-0.4358471232,5.4615518429,-1.7163454945
C,0,-3.4783115978,-4.7919576942,-1.2833079924
C,0,0.8774904106,1.7445275899,5.0496086467
C,0,-1.5925478428,5.75638219,-0.7491592708
C,0,-4.9824573047,-5.0340315293,-1.4826196281
C,0,-0.3490038738,1.043269424,5.6629086249
C,0,-1.1318215465,0.0979375583,4.7305513528
C,0,-1.7543135489,0.7927288158,3.5076581662
C,0,-2.9700023872,5.7327563882,-1.4296431978
C,0,-2.724145479,-0.0992599928,2.7052263124
C,0,-5.7864138233,-5.2271568967,-0.1824482683
C,0,-4.9539145808,-0.3969023589,0.5367643554
C,0,-4.010716565,2.4701153059,1.511320578
C,0,-5.945844109,-3.9860305329,0.7164504108
C,0,-4.193227434,3.4086808959,0.2999043368
C,0,-6.8039608746,-2.8712597881,0.0987017826
C,0,-4.1768577207,5.8894828372,-0.4819543919
C,0,-4.2355812478,4.8950365955,0.6944257898
C,0,-5.9123855064,-0.9376034147,1.6139972727
C,0,-7.1262241055,-1.7005660458,1.0458351972
H,0,7.4767698495,-2.4207166429,0.0828735925
H,0,5.929040407,-2.8542464284,0.7791574464
H,0,6.0570215189,-3.2163960754,-1.7088529257
H,0,6.3312545207,-1.5100704245,-1.9587651917
H,0,7.8490787016,-1.1680179626,2.2419091498
H,0,6.2126982113,-1.4144611389,2.8217501944
H,0,6.8949795548,-0.0125555327,0.1792845981
H,0,5.2798413023,-0.3993149706,0.7595910563
H,0,7.6009233578,1.2797474886,2.3369213218
H,0,7.3186723546,0.5291518657,3.8988609571
H,0,4.6129283874,2.0106121612,-3.6022580625
H,0,2.9394535625,2.2460298801,-3.1515804628
H,0,5.275377852,3.4868220581,-1.5962303665
H,0,4.5352907108,4.285936903,-2.9715772298
H,0,3.7377760974,-3.2849083467,-3.6588666777
H,0,3.5375448714,-4.3021968967,-2.2445330361
H,0,4.0427303609,-0.405445974,-3.3887782602
H,0,2.5050967991,-0.2248421114,-2.5822710191
H,0,5.1274814498,0.9333111114,-1.4588694444
H,0,3.5127896496,1.2310499565,-0.8486513455
H,0,1.5908486758,-4.585211149,-4.5806181887
H,0,1.4315545573,-5.4313165169,-3.0489905002
H,0,5.7559426295,2.3771978682,3.4751753624
H,0,5.1659818372,1.6263354051,2.0060930833
H,0,1.4177335495,-2.3853883349,-3.3846714834
H,0,1.2452482929,-3.2254610201,-1.8566154237
H,0,3.7237874838,5.0648532726,-0.6903019769
H,0,2.981564699,3.4973036003,-0.4466173401
H,0,-0.6954539842,-5.3576377122,-4.3602615881
H,0,-0.7014721143,-3.6027919117,-4.2936363859

H,0,4.8795622126,0.3695272276,4.7905495239
H,0,4.1674026602,-0.242289942,3.3036730247
H,0,2.2862001867,5.4959120847,-2.6720080628
H,0,1.5929876988,3.889997731,-2.5586142136
H,0,-0.8033380847,-5.4068643407,-1.812867356
H,0,-0.9854280905,-3.6593537477,-1.8204205559
H,0,3.5112300595,2.4408033847,4.6336107539
H,0,2.8662407424,1.9311832385,3.0813374871
H,0,1.2452206328,6.1420909067,-0.5123741589
H,0,0.7566091101,4.4836871754,-0.2137728153
H,0,-2.8918917914,-5.6334958515,-3.1871336606
H,0,-3.0765006269,-3.8870384877,-3.2095410829
H,0,1.7583654752,-0.0224462751,4.1336433296
H,0,2.4330106069,0.3924813755,5.7014534014
H,0,-0.3393165952,6.2753470528,-2.4498160532
H,0,-0.688756338,4.5598489619,-2.2928432098
H,0,-3.065597953,-5.6013394489,-0.6622491734
H,0,-3.3136310231,-3.8637070742,-0.7178233769
H,0,0.5837560732,2.2649649706,4.1270696801
H,0,1.2064934804,2.534174348,5.7400447496
H,0,-1.5687831159,5.0010957059,0.0477525713
H,0,-1.435215131,6.7257471167,-0.253183116
H,0,-5.1082000299,-5.9366110259,-2.0976694976
H,0,-5.4114803087,-4.2118349704,-2.0726565193
H,0,-0.0279214656,0.4792793246,6.5504777916
H,0,-1.0437682322,1.8125587941,6.0300193173
H,0,-0.4866331414,-0.7255044116,4.3934586892
H,0,-1.9358616256,-0.3722968763,5.3145865912
H,0,-0.9514833861,1.1536191122,2.8514505465
H,0,-2.2865000474,1.6903709794,3.8523700685
H,0,-3.0663986803,4.791292897,-1.9874546591
H,0,-3.0151813634,6.5296135204,-2.1855220518
H,0,-2.2167396702,-1.0314273796,2.4142941861
H,0,-3.5468633763,-0.4082887036,3.36695165
H,0,-5.3126409354,-6.0285740652,0.4025219907
H,0,-6.7892764705,-5.5958573917,-0.4421718418
H,0,-4.536196954,-1.2479696279,-0.0172566349
H,0,-5.5235569719,0.1840559145,-0.205097293
H,0,-3.2256987909,2.8927468905,2.1558054243
H,0,-4.9183398795,2.4660108166,2.1334792875
H,0,-4.9559181621,-3.5944569016,0.9866054749
H,0,-6.4094652413,-4.3031613106,1.662012818
H,0,-3.3646073365,3.2486449078,-0.3985996875
H,0,-5.1064173728,3.1452920991,-0.2532356874
H,0,-6.3170626502,-2.4836217036,-0.8054268729
H,0,-7.754840209,-3.3073244098,-0.2403431211
H,0,-4.1813410409,6.9084731417,-0.0691320499
H,0,-5.0961855445,5.8018471515,-1.0785105909
H,0,-3.3971344432,5.0966302505,1.3756473685
H,0,-5.1444679608,5.092925324,1.2801395491
H,0,-5.3577514034,-1.5945311744,2.2964608524
H,0,-6.2898033341,-0.1127512072,2.2349190918
H,0,-7.7681623222,-0.9883735291,0.507599131
H,0,-7.7267271286,-2.076742828,1.8869973424
C,0,2.9798433141,-2.1696420834,0.100307514
C,0,1.9668958269,-1.2804709597,0.4993149456
C,0,1.1940378807,-1.5175278474,1.6387837656
C,0,1.4235941267,-2.6521804219,2.4180291615
C,0,2.4244174311,-3.5520148299,2.0455104864
C,0,3.1837242477,-3.312965629,0.8996980734
H,0,1.7531646002,-0.3970030572,-0.0960116286
H,0,0.4070242023,-0.8187593429,1.908228584
H,0,0.8218094709,-2.8395339858,3.3038766662
H,0,2.606740731,-4.4427853065,2.6417568011
H,0,3.941245219,-4.0423807852,0.6190872376
C,0,-2.2157236473,0.712867934,-0.283788433
C,0,-2.4320135263,0.0405319506,-1.5015291976
C,0,-1.5168421713,0.1081824128,-2.5545066712
C,0,-0.3485273358,0.8565408112,-2.4161901049
C,0,-0.1033642915,1.5307337398,-1.2175331276

```
 C,0,-1.0267188262,1.4605605169,-0.1726724796
 H,0,-3.3369552226,-0.5428322602,-1.6453127837
 H,0,-1.7208287121,-0.4188454933,-3.4832868889
 H,0,0.362775233,0.920418297,-3.2354768305
 H,0,0.8031774035,2.1168289773,-1.0989977935
 H,0,-0.8165337876,2.0133576367,0.7406539697
---------------------------------------------------------------------
```

**Table S4.** Optimized Structural Coordinate and its Total Energy for ***in,out*-BCA** at B3LYP/6-31G(d) level

total energy: = `-2693.4802905 hartree` (NImag = 0)

```
---------------------------------------------------------------------
   Atomic                Coordinates (Angstroms)
    Type                 X           Y           Z
---------------------------------------------------------------------
Si,0,-7.3995353653,-1.2717843078,0.3661065774
 C,0,-5.5117923107,-1.4793652478,0.4604625233
 C,0,-4.7847787338,-1.1837705515,1.6294493649
 C,0,-4.7744024846,-1.8877095683,-0.6669382491
 C,0,-7.7468983288,0.4985172457,-0.2567360464
 C,0,-7.0665726023,1.6032305842,0.5762511384
 C,0,-7.127932115,3.0041449725,-0.048429105
 C,0,-6.366040116,4.0534948491,0.773745933
 C,0,-6.3386199934,5.4420716465,0.1228283869
 C,0,-5.6395682591,6.5289176711,0.9584068506
 C,0,-4.1349514767,6.3275144605,1.2218168752
 C,0,-8.0594490151,-2.5346169404,-0.898923679
 C,0,-7.8334188625,-4.0204224429,-0.5312901349
 C,0,-7.8237186948,-5.0008097776,-1.7189775789
 C,0,-6.6034190738,-4.8468054831,-2.6410249305
 C,0,-6.4408431262,-6.0014390378,-3.6395451272
 C,0,-5.3127957706,-5.8061172302,-4.6665656271
 C,0,-3.1531228718,-4.7452080401,5.763830985
 C,0,-4.1868804811,-4.6024713569,6.8921499019
 C,0,-5.6522479474,-4.8028766388,6.4690070208
 C,0,-6.2060297386,-3.6956460349,5.5619658121
 C,0,-7.6963671932,-3.8615466792,5.2268817278
 C,0,-8.2678288097,-2.7310549901,4.3523217181
 C,0,-7.7506524905,-2.7337825475,2.9045757711
 C,0,-8.1618087942,-1.4841529618,2.1007131175
 Si,0,1.6671940418,-0.7865451229,0.6873828127
 C,0,-2.6910067378,-1.7144961236,0.5440290182
 C,0,-3.3844413306,-2.0040692791,-0.6316176874
 C,0,-3.3942171997,-1.3002604861,1.6762350282
 C,0,1.5131161621,1.0575266146,1.1782941487
 C,0,0.2494650587,1.7987839774,0.6927312624
 C,0,0.1606181197,3.2469838598,1.2007093764
 C,0,-0.9233434594,4.0870710193,0.5076193179
 C,0,-1.0165997944,5.5179478667,1.0628305101
 C,0,-1.7775195228,6.5152208645,0.1712098271
 C,0,-3.2769016502,6.2495270469,-0.0523601724
 C,0,0.8912935117,-1.8359602865,2.0783523845
 C,0,0.8004937831,-3.3609707842,1.8523374964
 C,0,0.675463678,-4.1972280845,3.1385846611
 C,0,-0.5568853069,-3.9164793107,4.0109102229
 C,0,-0.6116931515,-4.845895605,5.2340911208
 C,0,-1.7142628899,-4.539259237,6.2602642766
 C,0,-3.9002396628,-5.6666657558,-4.0761477845
 C,0,-2.8203085939,-5.5923061508,-5.1651279202
 C,0,-1.3790711976,-5.3929240021,-4.665828734
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C,0,-1.11861746,-4.0489619459,-3.9631592723
C,0,0.3715286619,-3.6757517931,-3.9019339299
C,0,0.6546723605,-2.3260793003,-3.212796391
C,0,0.8380443339,-2.3971257069,-1.6861901825
C,0,0.8828836752,-0.9972107994,-1.0381555314
C,0,3.5097015689,-1.2445013799,0.5598887485
C,0,4.2048992547,-1.8596391512,1.6179091169
C,0,4.2496007938,-0.9428710504,-0.600276726
C,0,6.2738564552,-1.8453455929,0.3658315216
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H,0,3.7585751112,-0.4693665171,-1.4479748815
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H,0,6.152295354,-0.990042667,-1.6105681064
H,0,6.073216352,-2.6335871183,2.3628267261
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**Table S5.** Optimized Structural Coordinate and its Total Energy for ***twist-out,out*-BCA** at B3LYP/6-31G(d) level

total energy: = -2693.4856754 hartree (NImag = 0)

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| Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|

---

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C,0,-3.1169995668,-1.1468282293,-3.2466758651
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