

Supplementary Information

Polarized Fluorescence of a Crystal having Uniaxially Oriented Molecules by a Carbazole-diyl-bridged Macrocage

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1. Experimental Procedure

All reactions were conducted under an argon atmosphere. The chemical shifts of ^1H and ^{13}C NMR spectra are based on the residual solvent resonances, except for ^{29}Si NMR, in which the chemical shifts were referenced to external tetramethylsilane. HRMS analyses were carried out by electrospray ionization (ESI) using a FT-ICR-MS system. The sample solutions for HRMS were prepared in a mixture of chloroform/methanol with a small amount of NaI. Preparatory GPC was carried out using a recycling preparative chromatograph; chloroform stabilized with ethanol was used as the eluent. Fluorescence studies in solution were carried out with samples thoroughly degassed by several freeze–pump–thaw sequences. Solid state ^2H NMR were recorded using quadrupolar echo pulse sequences. Commercially available reagents were used without further purification.

Synthesis of 9-Methyl-2,7-bis(trimethylsilyl)carbazole (TMSCar) A solution of 9-Methyl-2,7-dibromocarbazole (0.85 g, 2.51 mmol) dissolved in tetrahydrofuran (50 mL) was prepared. Subsequently, *n*-BuLi solution (1.6 M in hexane, 3.5 mL, 2.2 equiv.) was added slowly at $-78\text{ }^\circ\text{C}$ with stirring for 10 min. Trimethylchlorosilane (0.70 g, 23.6 mmol) was then added as the temperature of the reaction was slowly *raised* to room temperature, and stirred for 18h. The mixture was extracted with hexane and volatile materials were removed *in vacuo*. After column chromatography purification of crude products, the pure compound, **TMSCar** (0.60 g, 1.84 mmol), was obtained as colorless crystals with 73% yield. **TMSCar**: mp 117-118 $^\circ\text{C}$; a white solid; ^1H NMR (CDCl_3 , 500 MHz) δ 0.37 (s, 18H, Si- $(\text{CH}_3)_3$), 3.90 (s, 3H, N- CH_3), 7.37 (d, $J = 8.0$ Hz, 2H, Cz-*H*), 7.54 (s, 2H, Cz-*H*), 8.08 (d, $J = 8.0$ Hz, 2H, Cz-*H*); ^{13}C NMR (CDCl_3 , 126 MHz) δ -0.7 (6C), 29.0 (1C), 113.1 (2C), 119.7 (2C), 123.2 (2C), 123.5 (2C), 137.8 (2C), 140.7 (2C); ^{29}Si NMR(CDCl_3 , 99 MHz) δ -3.2; HRMS (ESI positive) calcd for $\text{C}_{19}\text{H}_{27}\text{NSi}_2\text{Na}$: 348.15742 (M+Na $^+$), found: 348.15744 (M+Na $^+$).

Synthesis of 9-Methyl-2,7-bis(tri-9-decenylsilyl)carbazole (2) The same procedure in the synthesis of **TMSCar** from 9-Methyl-2,7-dibromocarbazole (3.33 g, 9.82 mmol), tetrahydrofuran

(60 mL), *n*-BuLi solution (1.6 M in hexane, 13.5 mL, 2.2 equiv.), and tris(9-decenyl)chlorosilane (9.50 g, 23.6 mmol) was performed for the production of 2,7-Bis(tri-9-decenylsilyl)-9-methylcarbazole. The product (3.50 g, 3.27 mmol) was obtained as a colorless oil in 30% yield. **2**: a colorless oil; ¹H NMR (CDCl₃, 500 MHz) δ 0.85-0.95 (m, 12H), 1.30-1.38 (m, 72H), 2.06 (q, *J* = 7.0 Hz, 12H), 3.92 (s, 3H), 4.95 (d, *J* = 10.0 Hz, 6H), 5.01 (d, *J* = 17.0 Hz, 6H), 5.83 (ddt, *J* = 17.0, 10.0, 7.0 Hz, 6H), 7.37 (d, *J* = 7.5 Hz, 2H, *Cz-H*), 7.53 (s, 2H, *Cz-H*), 8.10 (d, 7.5 Hz, 2H, *Cz-H*); ¹³C NMR (CDCl₃, 126 MHz) δ 12.7 (6C), 23.9 (6C), 28.9 (6C), 28.9 (1C), 29.2 (6C), 29.2 (6C), 29.3 (6C), 29.4 (6C), 33.8 (6C), 114.1 (6C), 116.1 (2C), 119.6 (2C), 123.7 (2C), 124.8 (2C), 135.7 (2C), 139.2 (6C), 139.3 (2C); ²⁹Si NMR (CDCl₃, 99 MHz) δ -1.2; HRMS (ESI positive) calcd for C₇₃H₁₂₃NSi₂Na: 1092.90863 (M+Na⁺), found: 1092.90874 (M+Na⁺).

Synthesis of Molecular Gyrotop C18Car and its isomer C18iCar A solution of 2,7-(tri-7-octenylsilyl)-9-methylcarbazole (**2**) (0.960 g, 0.90 mmol) in dichloromethane (200 mL) was added to a dichloromethane (700 mL) solution of first-generation Grubbs' catalyst (0.05 g, 0.06 mmol) dropwise while stirring for 12 h. The mixture was further stirred for another 12 h. The volatile materials were removed *in vacuo*, and the catalyst was removed from the toluene-soluble fraction by column chromatography. The reaction mixture was then added with toluene (15 mL) and placed in an autoclave together with 10% Pd/C (0.030 g). Subsequently, hydrogen gas (3 atm) was introduced. The mixture was left for 72 h, and then filtered to remove the Pd/C. The fractions containing **C18Car** and **C18iCar** were collected separately by GPC (chloroform), and the solvents were evaporated. The pure compound **C18Car** (0.030 g, 0.033 mmol, 3.0% yield) was obtained as colorless crystals by recrystallization from THF/methanol (4:1). Pure compound **C18iCar** (0.340 g, 0.34 mmol, 34% yield) was obtained without further purification. **C18Car**: colorless crystals; mp 220-221 °C; ¹H NMR (CDCl₃, 500 MHz) δ 0.81-0.84 (m, 12H), 1.16-1.34 (m, 96H), 3.91(s, 3H, N-CH₃), 7.34 (d, *J* = 7.5 Hz, 2H, *Cz-H*), 7.53 (s, 2H, *Cz-H*), 8.05 (d, *J* = 7.5 Hz, 2H, *Cz-H*); ¹³C NMR (CDCl₃, 126 MHz) δ 13.0 (6C), 23.3 (6C), 28.2 (6C), 28.6 (6C), 28.7 (1C), 29.4 (6C), 29.5 (6C), 29.9 (6C), 29.9(6C) 32.8 (6C), 116.7 (2C), 119.5 (2C), 123.6 (2C), 125.2 (2C), 135.3 (2C), 139.2 (2C); ²⁹Si NMR (CDCl₃, 99 MHz) δ -0.7; HRMS (ESI positive) calcd for C₆₇H₁₁₇NSi₂Na:

1014.86168 (M+Na⁺), found: 1014.86160 (M+Na⁺). **C18iCar**: a colorless oil; ¹H NMR (CDCl₃, 500 MHz) δ 0.70-0.76 (m, 4H), 0.80-1.00 (m, 8H) 1.15-1.25 (m, 32H), 1.26-1.46 (m, 64H), 3.91(s, 3H, N-CH₃), 7.33 (d, J = 7.5 Hz, 2H, Cz-H), 7.50 (s, 2H, Cz-H), 8.07 (d, J = 7.5 Hz, 2H, Cz-H); ¹³C NMR (CDCl₃, 126 MHz) δ 12.1, 13.8, 23.5, 23.6, 27.3, 27.6, 28.1, 28.2, 28.5, 28.5, 28.9, 28.9, 29.0, 29.0, 29.4, 29.5, 29.6, 33.3, 33.6, 113.8 (2C), 119.6 (2C), 123.1 (2C), 124.3 (2C), 135.5 (2C), 140.7 (2C); ²⁹Si NMR (CDCl₃, 99 MHz) δ -0.6; HRMS (ESI positive) calcd for C₆₇H₁₁₇NSi₂Na: 1014.86168 (M+Na⁺), found: 1014.86171 (M+Na⁺).

Synthesis of Deuterated Molecular Gyrotop C18Car-d₆ Deuterated molecular gyrotop **C18Car-d₆** was synthesized using the same procedure as **C18Car**. **C18Car-d₆**: colorless crystals; mp 221-222 °C; ¹H NMR (CDCl₃, 500 MHz) δ 0.75-0.85 (m, 12H), 1.10-1.38 (m, 96H), 7.98 (s, 1H, N-H); ¹³C NMR (CDCl₃, 126 MHz) δ 13.1 (6C), 23.3 (6C), 28.3 (6C), 28.7 (6C), 29.4 (6C), 29.5 (6C), 29.9 (6C), 29.9 (6C), 32.9 (6C), 116.3 (t, J = 23.5 Hz, 2C), 119.2 (t, J = 23.5 Hz, 2C), 123.5 (s, 2C), 124.8 (t, J = 23.5 Hz, 2C), 135.0 (s, 2C), 139.2 (s, 2C); ²⁹Si NMR (CDCl₃, 99 MHz) δ -0.7; HRMS (ESI positive) calcd for C₆₇H₁₁₁D₆NSi₂Na: 1020.89934 (M+Na⁺), found: 1020.89960 (M+Na⁺)

2. Copies of NMR and HRMS Spectra for New Compounds

a. Spectra of TMSCar

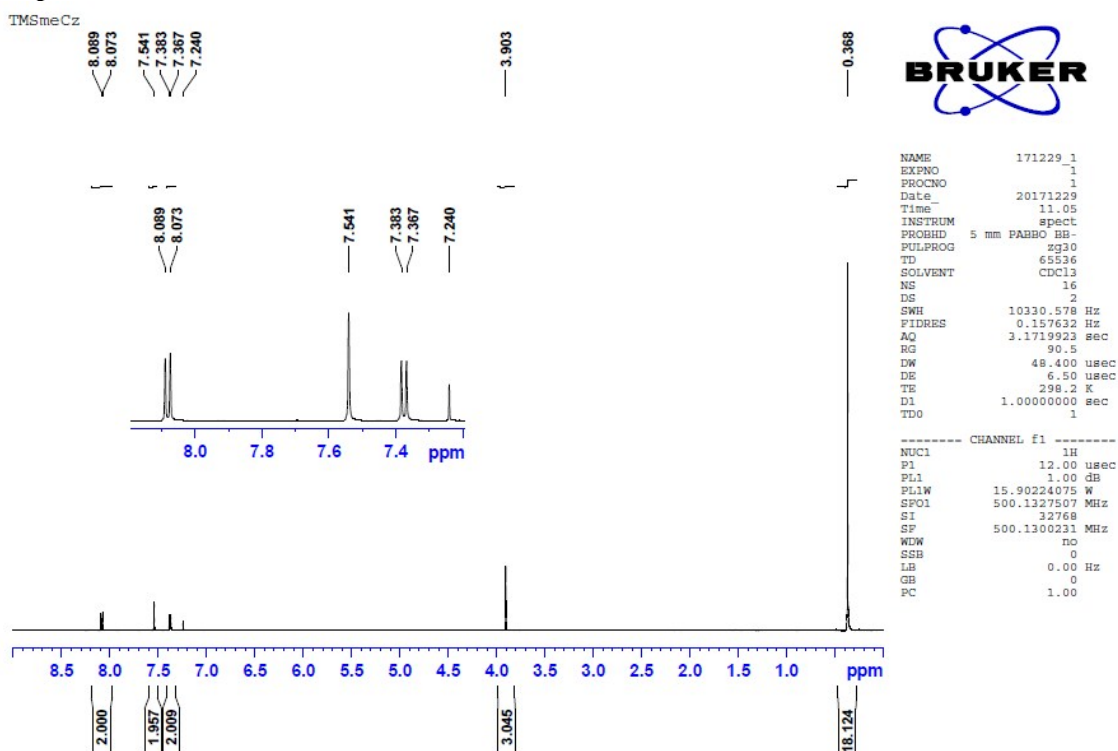


Fig. S1. ¹H NMR spectrum of TMSCar in CDCl₃.

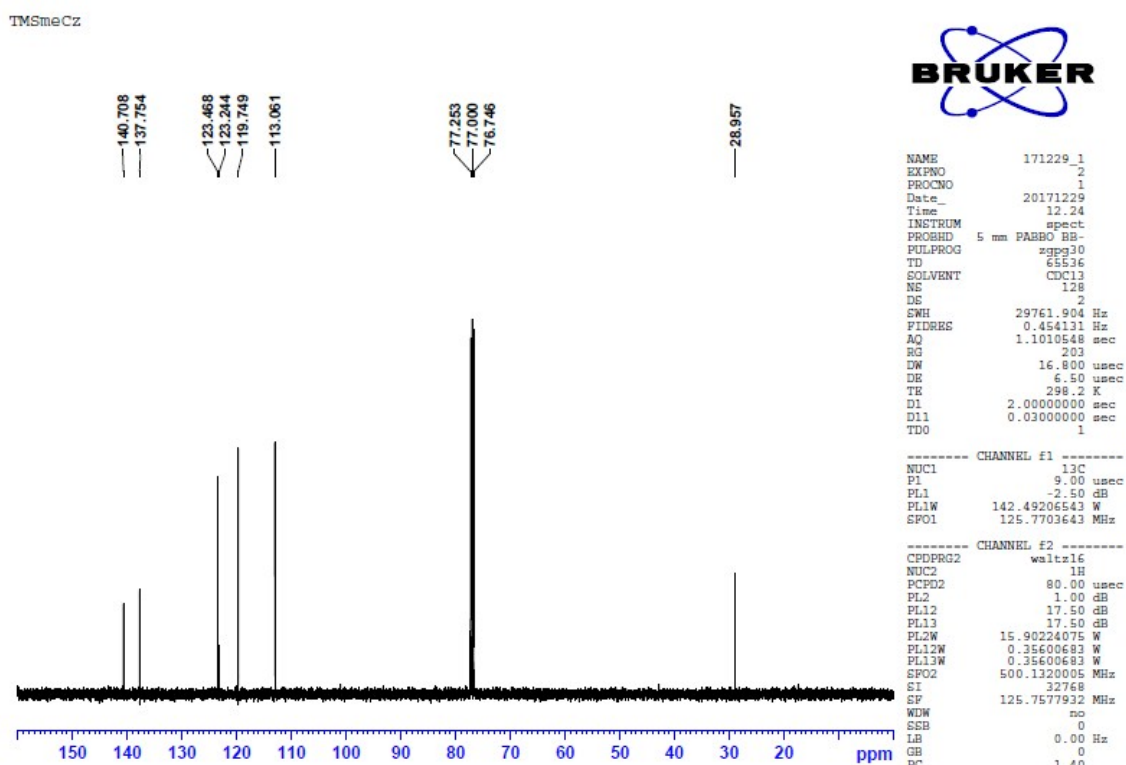


Fig. S2. ¹³C NMR spectrum of TMSCar in CDCl₃.

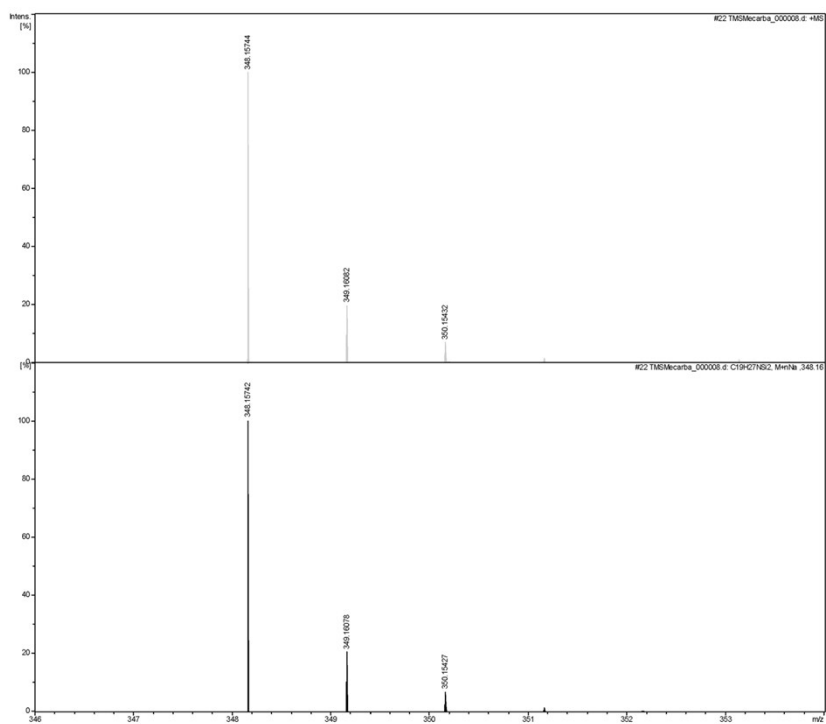


Fig. S3. HRMS spectrum of TMSCar (ESI, positive). Top: obsd. Bottom: sim.

b. Spectra of 2

C10-N-methylcarbazole-C10

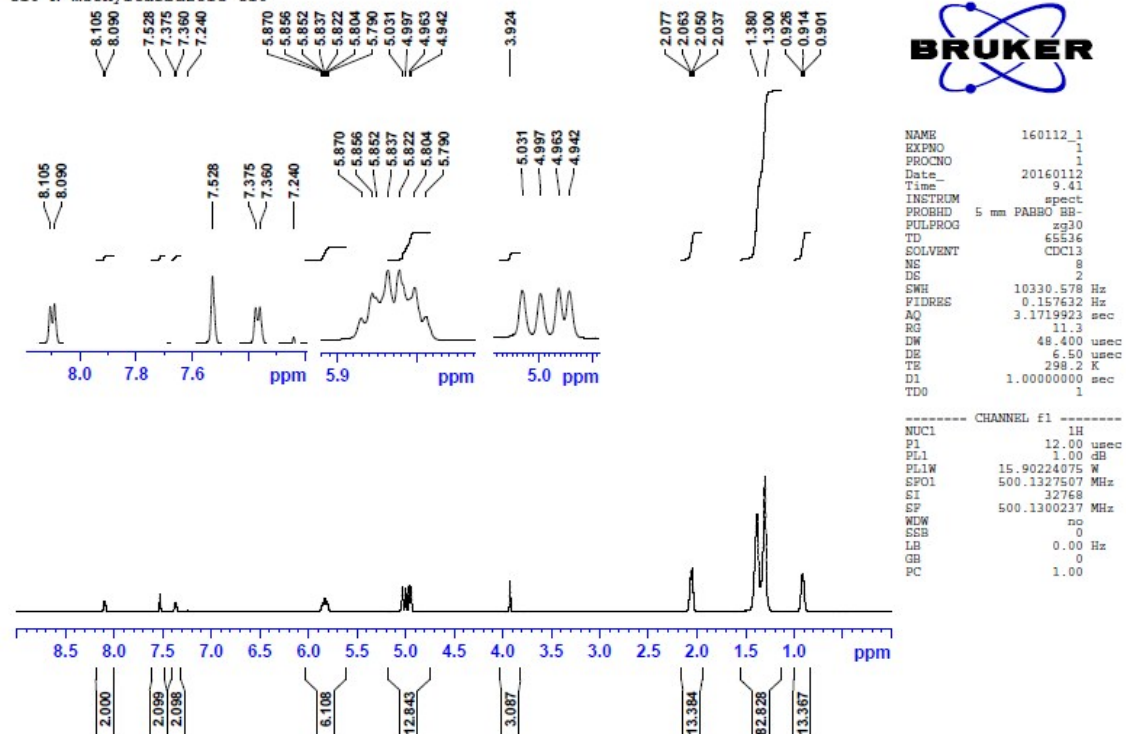


Fig. S4. ^1H NMR spectrum of **2** in CDCl_3 .

C10-N-methylcarbazole-C10

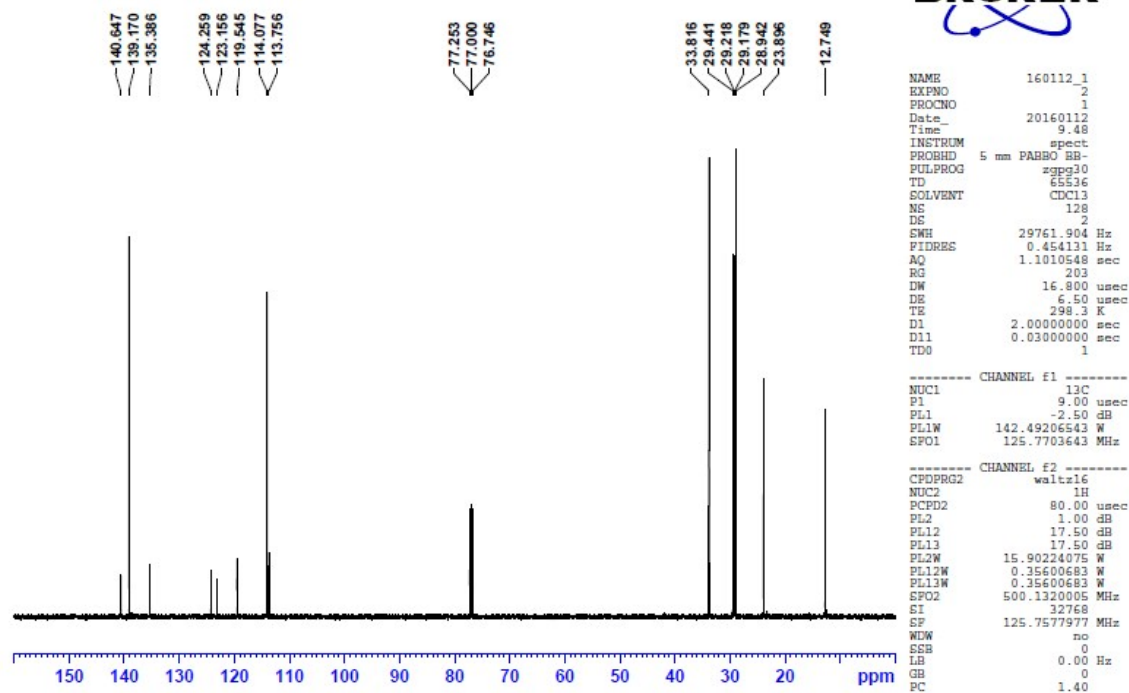


Fig. S5. ^{13}C NMR spectrum of **2** in CDCl_3 .

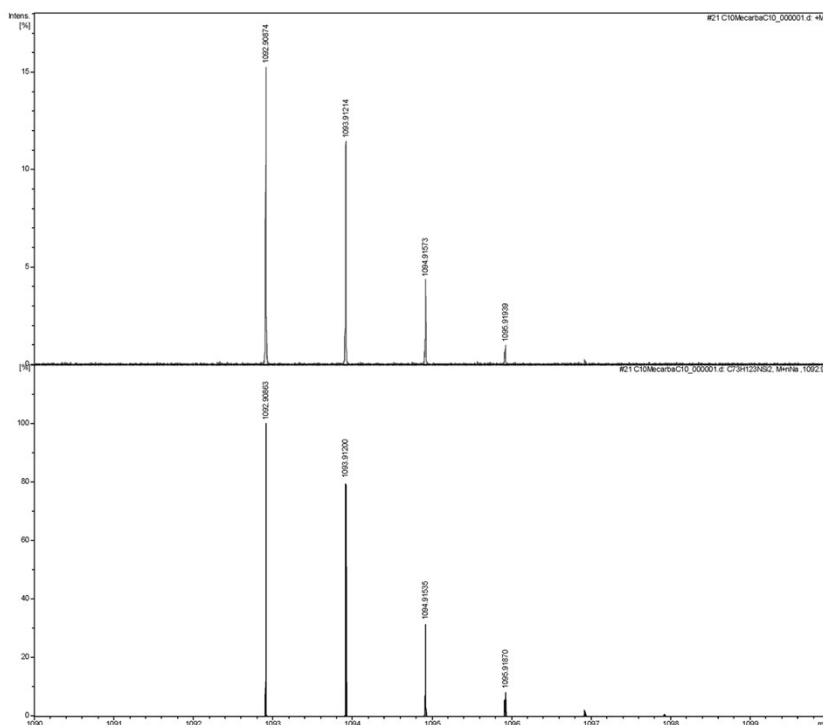


Fig. S6. HRMS spectrum of **2** (ESI, positive). Top: obsd. Bottom: sim.

c. Spectra of C18Car

C18 N-methylcarbazole sat.cage

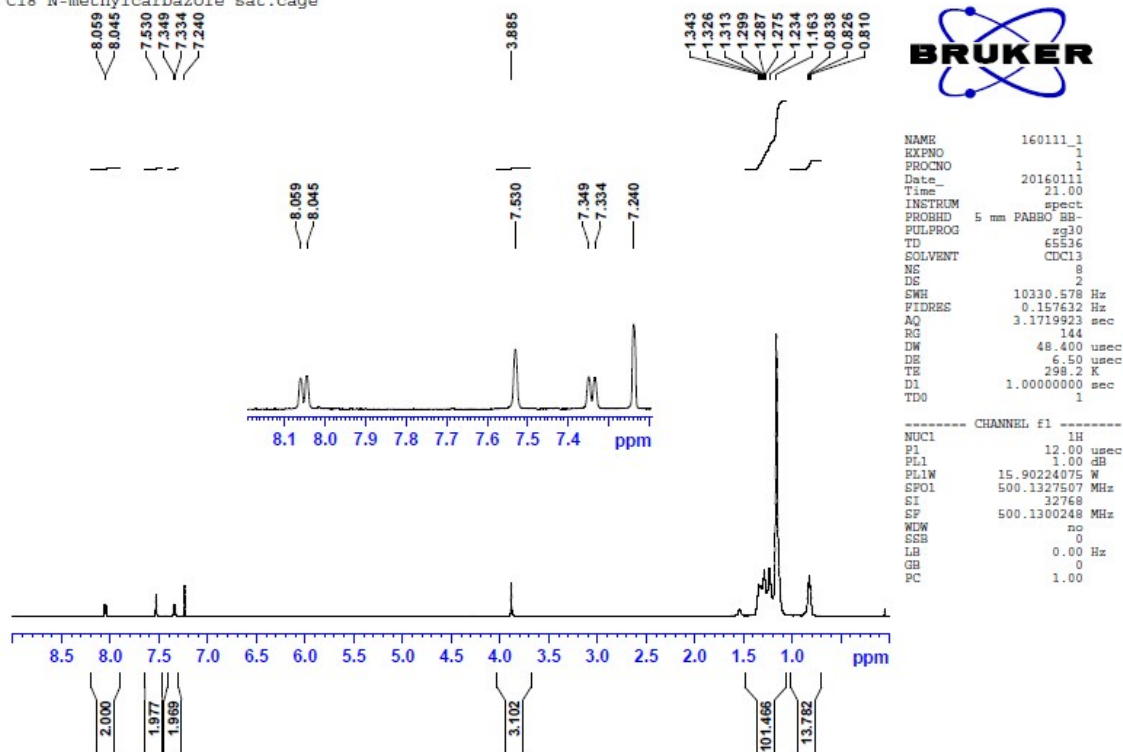


Fig. S7. ¹H NMR spectrum of C18Car in CDCl₃.

C18 N-methylcarbazole sat.cage

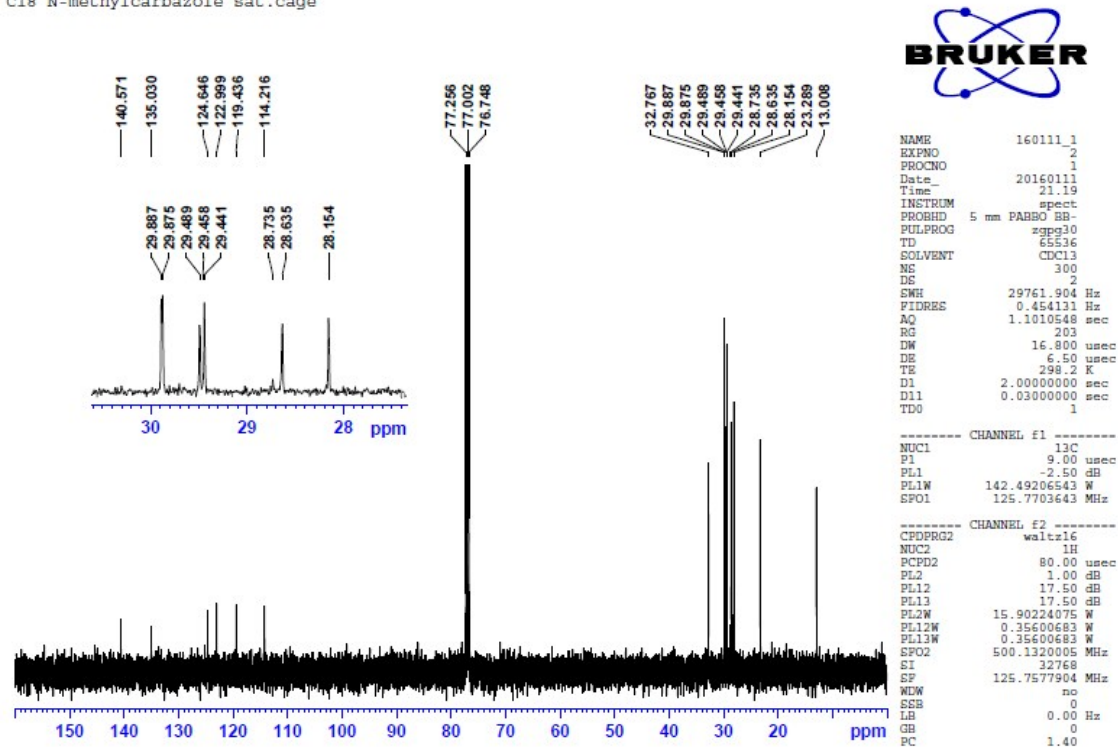


Fig. S8. ¹³C NMR spectrum of C18Car in CDCl₃.

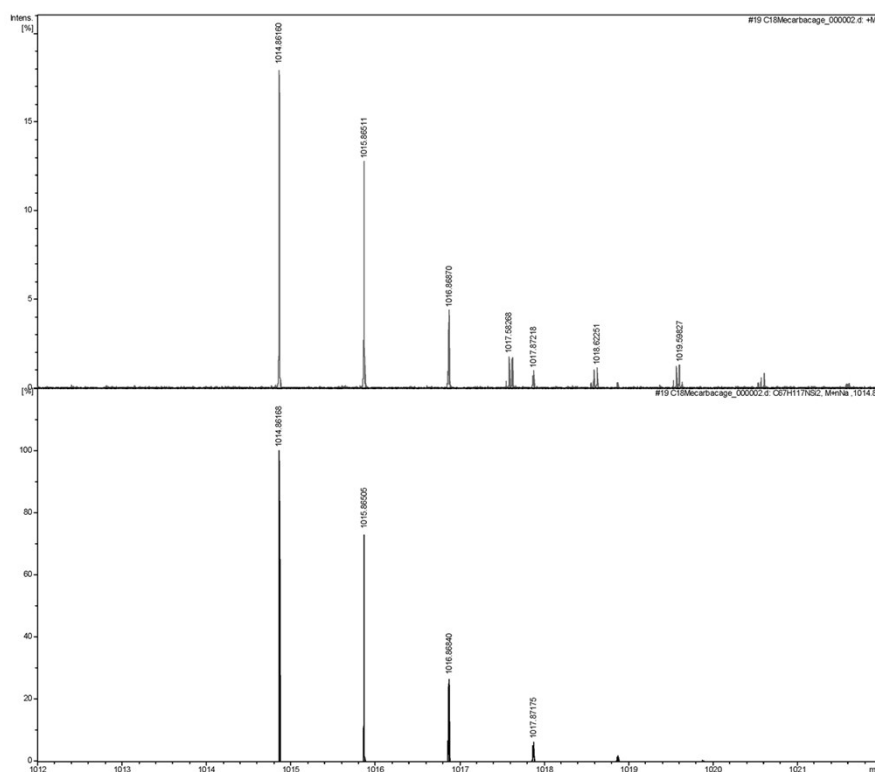


Fig. S9. HRMS spectrum of C18Car (ESI, positive). Top: obsd. Bottom: sim.

d. Spectra of C18Cari

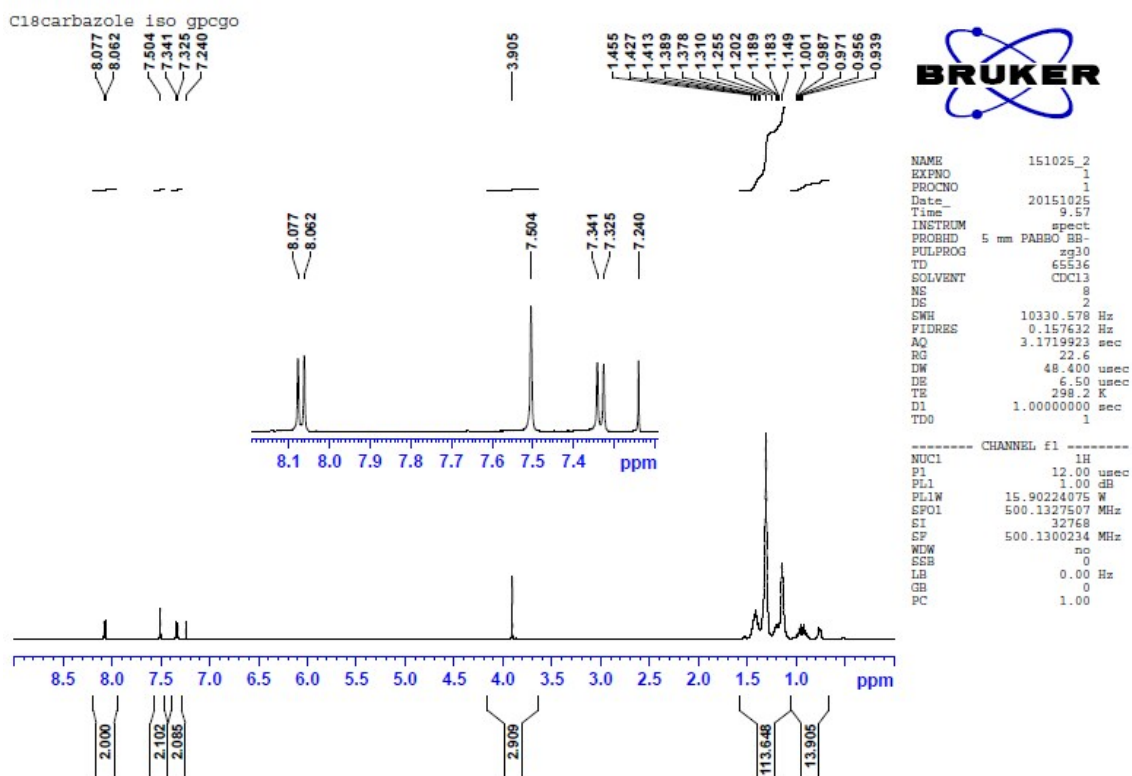


Fig. S10. ¹H NMR spectrum of C18Cari in CDCl₃.

C18carbazole iso gpcgo

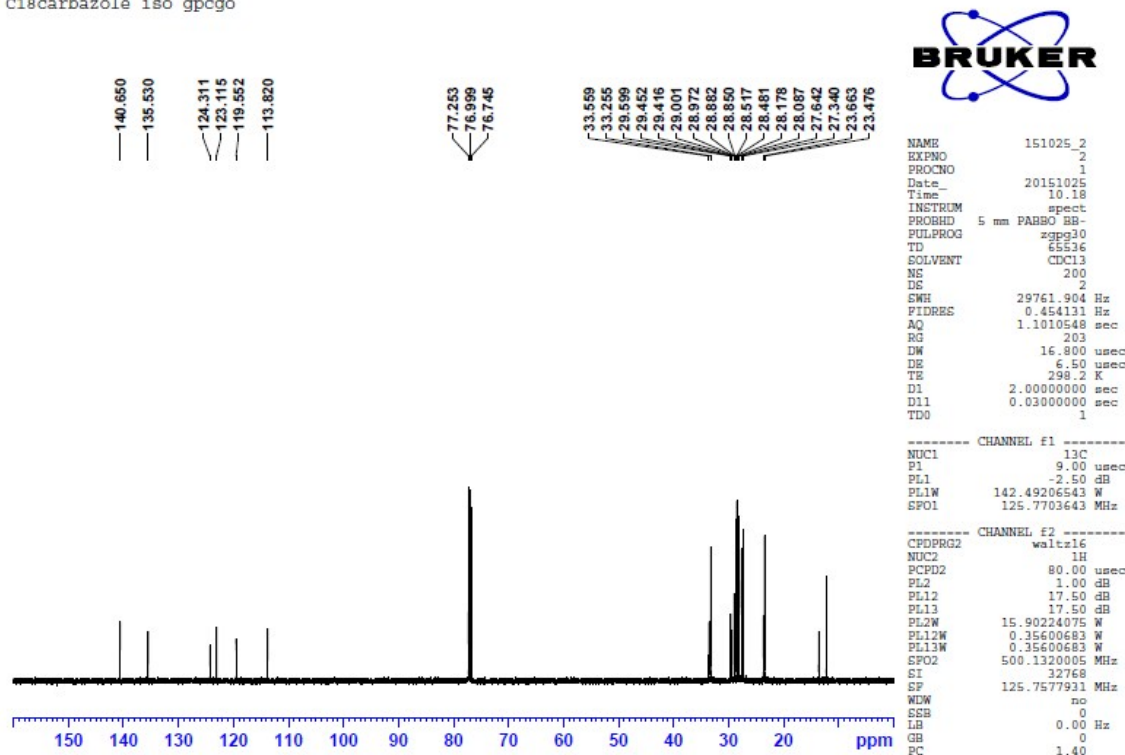


Fig. S11. ¹³C NMR spectrum of C18Cari in CDCl₃.

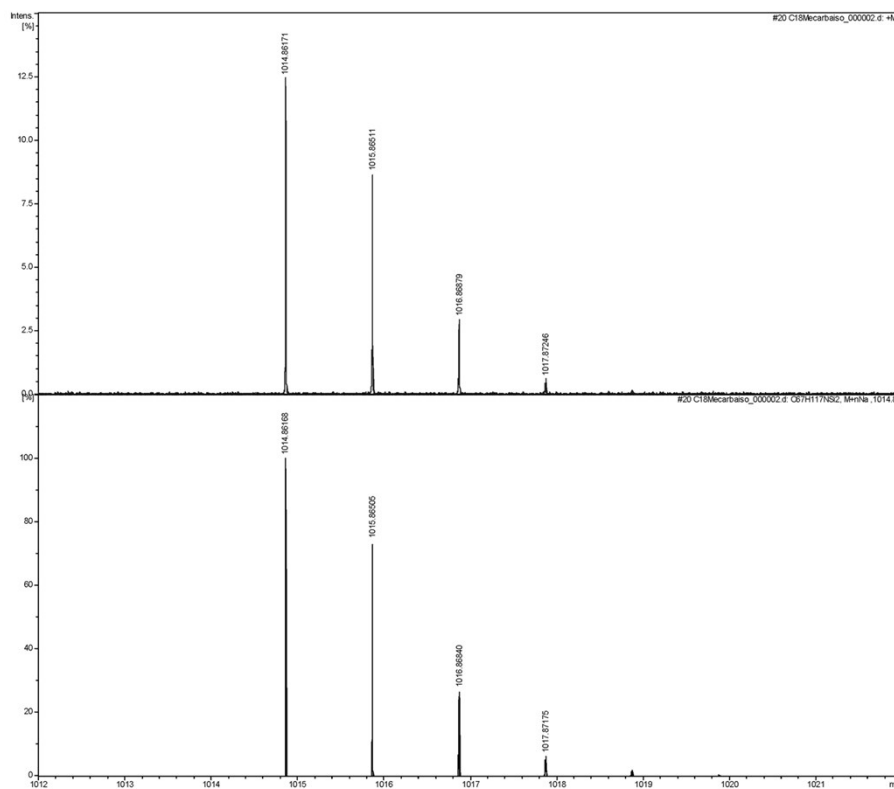
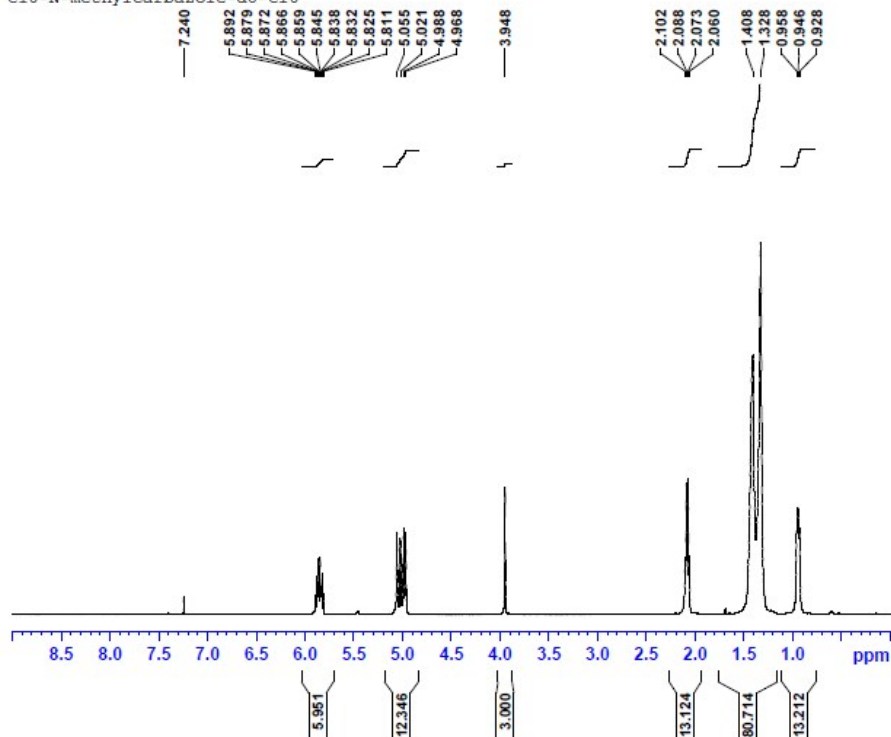


Fig. S12. HRMS spectrum of C18Cari (ESI, positive). Top: obsd. Bottom: sim.

e. Spectra of C18Car-*d*₆

C10-N-methylcarbazole-*d*₆-C10



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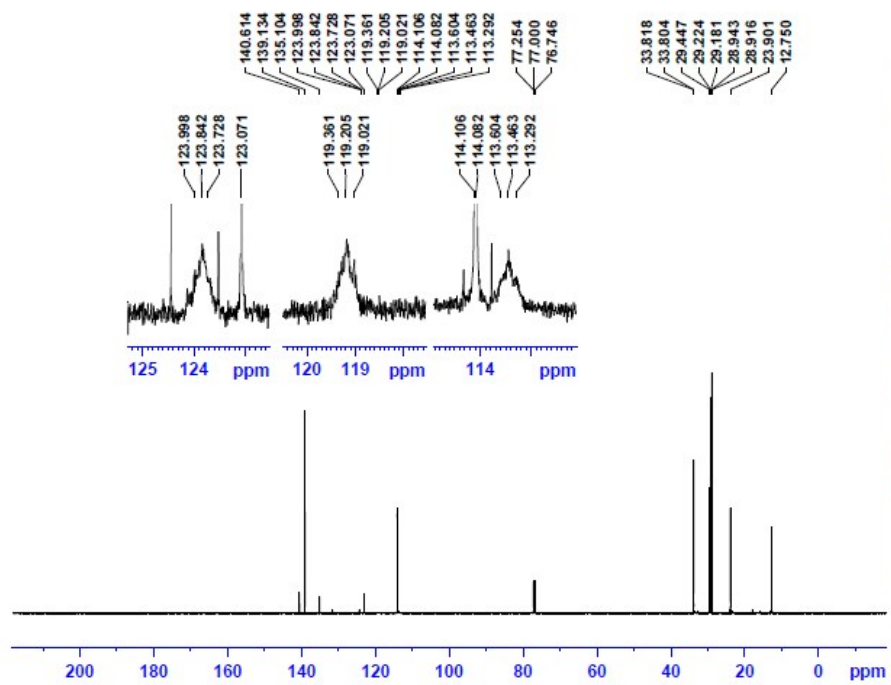
NAME          160617_1
EXPNO         1
PROCNO        1
Date_         20160617
Time          11.32
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           10330.578 Hz
FIDRES        0.157632 Hz
AQ            3.1719923 sec
RG            11.3
DW            48.400 usec
DE            6.50 usec
TE            298.2 K
D1            1.00000000 sec
TDO           1
  
```

```

----- CHANNEL f1 -----
NUC1          1H
P1            12.00 usec
PL1           1.00 dB
PL1W          15.90224075 W
SFO1          500.1327507 MHz
SI            32768
SF            500.1300231 MHz
WDW           no
SSB           0
LB            0.0 Hz
GB            0
PC            1.00
  
```

Fig. S13. ¹H NMR spectrum of C18Car-*d*₆ in CDCl₃.

C10-N-methylcarbazole-*d*₆-C10



```

NAME          160617_1
EXPNO         2
PROCNO        1
Date_         20160617
Time          12.35
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            1151
DS            2
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG            203
DW            16.800 usec
DE            6.50 usec
TE            298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TDO           1
  
```

```

----- CHANNEL f1 -----
NUC1          13C
P1            9.00 usec
PL1           2.50 dB
PL1W          142.49206543 W
SFO1          125.7703643 MHz
  
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----- CHANNEL f2 -----
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           1.00 dB
PL12          17.50 dB
PL13          17.50 dB
PL2W          15.90224075 W
PL12W         0.35600683 W
PL13W         0.35600683 W
SFO2          500.1320005 MHz
SI            32768
SF            125.7578013 MHz
WDW           no
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
  
```

Fig. S14. ¹³C NMR spectrum of C18Car-*d*₆ in CDCl₃.

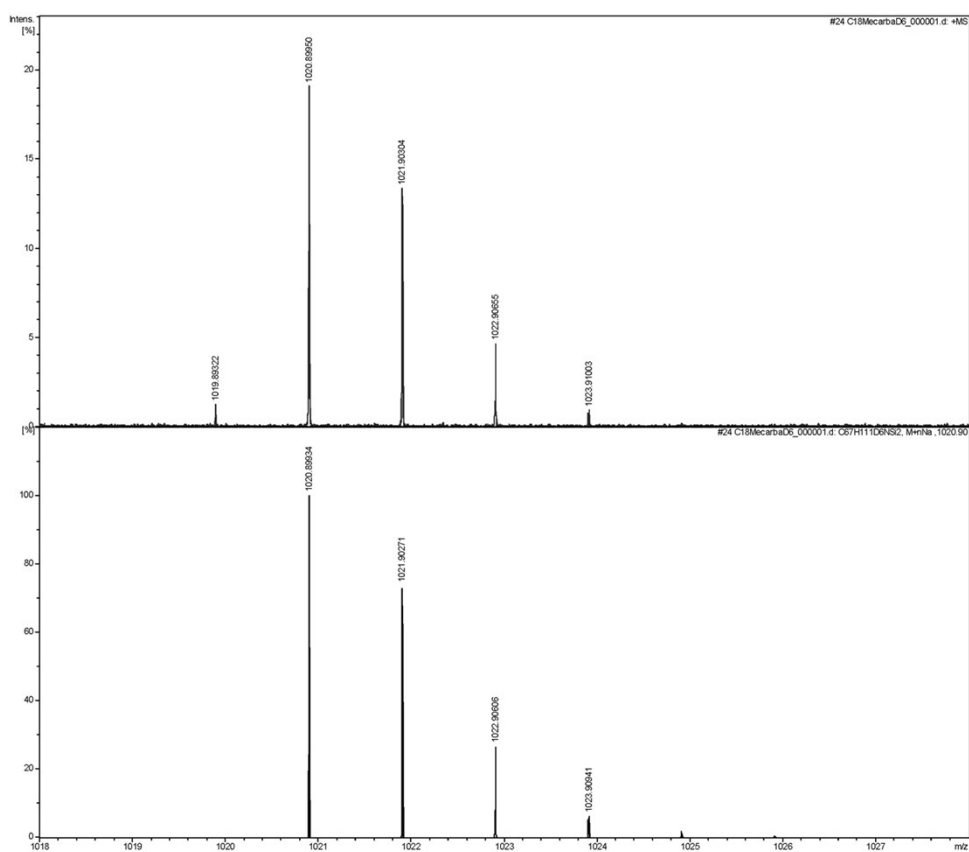


Fig. S15. HRMS spectrum of bromosilylthiophene **C18Car-d₆** (ESI, positive). Top: obsd. Bottom: sim.

3. Details of X-ray Crystallography

3-1. Crystal Data

Table S1. Crystal Data

Sample	C18Car	TMSCar	
CCDC #	1825557	1825558	
Empirical formula	C ₆₇ H ₁₁₇ N Si ₂	C ₁₉ H ₂₇ N Si ₂	
Crystal shape	prism	prism	
Crystal color	colorless	colorless	
Crystal size	0.40 x 0.40 x 0.20 mm ³	0.27 x 0.22 x 0.19 mm ³	
Formula weight / g mol ⁻¹	992.79	325.59	
Crystal system	Monoclinic	Monoclinic	
Space group	<i>C</i> ₂ / <i>c</i>	<i>P</i> ₂ / <i>1</i> / <i>n</i>	
Z	4	4	
Calculated density	1.017 Mg/m ³	1.093 Mg/m ³	
Cell parameter	<i>a</i>	34.673(6) Å	15.104(7) Å
	<i>b</i>	12.090(2) Å	6.317(4) Å
	<i>c</i>	17.728(3) Å	20.8662(10) Å
	α	90°	90°
	β	119.214(2)°	96.345(11)°
	γ	90°	90°
	<i>V</i>	6486.4(19) Å ³	1978.7(16) Å ³
F(000)	2216	704	
Absorption coefficient	0.091 mm ⁻¹	0.177 mm ⁻¹	
θ range for collection (deg)	1.346 to 27.369°	3.105 to 27.516°	
Index ranges	-32 ≤ <i>h</i> ≤ 43, -14 ≤ <i>k</i> ≤ 14, -21 ≤ <i>l</i> ≤ 19	-19 ≤ <i>h</i> ≤ 19, -5 ≤ <i>k</i> ≤ 8, -27 ≤ <i>l</i> ≤ 27	
Reflections collected	16192	18281	
Independent reflections	6658 [R(int) = 0.0342]	4510 [R(int) = 0.0974]	
Completeness	99.9 %	99.5 %	
Goodness-of-fit on F ²	1.291	0.889	
Final R indices [I > 2σ(I)]	R1 = 0.1083, wR2 = 0.3444	R1 = 0.0487, wR2 = 0.1114	
R indices (all data)	R1 = 0.1726, wR2 = 0.3993	R1 = 0.0605, wR2 = 0.1140	
Largest diff. peak and hole	1.050 and -0.349 e.Å ⁻³	0.263 and -0.322 e.Å ⁻³	

3-2. Disorder of Carbazole Moieties in C18Car

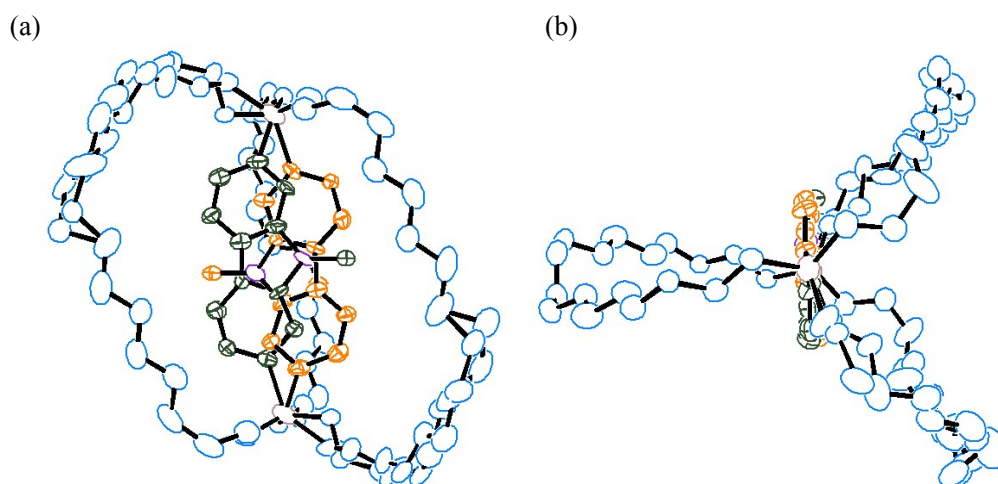


Fig. S16. Disorder in C18Car: (a) equatorial view; (b) axial view.

4. Details of Solid-state ^2H NMR Study of $\text{C18Car-}d_6$

Solid-state ^2H NMR was employed to observe dynamics of the carbazole moiety in a crystalline state of $\text{C18Car-}d_6$. In this spectra, the molecular motion of the deuterated moieties can be observed selectively. Fig. S17 shows temperature dependent solid-state ^2H NMR spectra of the powdered samples. Broad signals due to quadrupole coupling, called a Pake doublet, were observed, indicating the rotor was almost static.

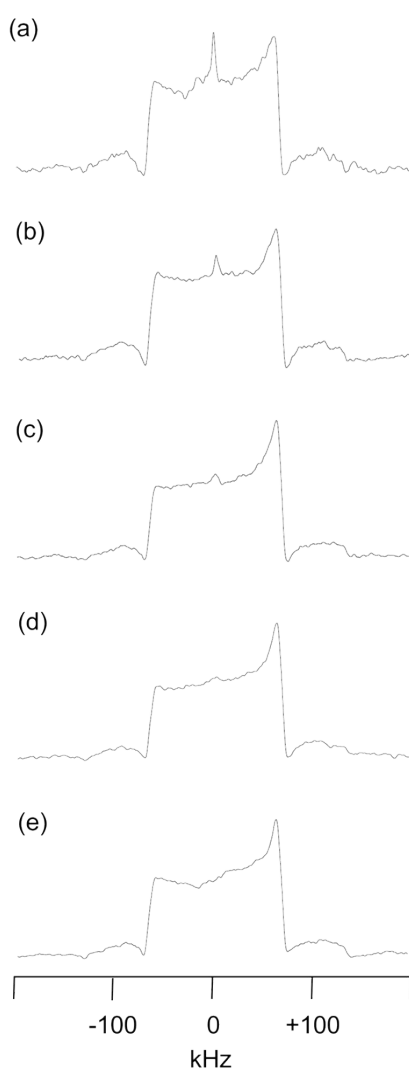


Fig. S17. Temperature dependent solid-state ^2H NMR spectra of $\text{C18Car-}d_6$: (a) 330 K, (b) 320 K, (c) 310 K, (d) 300 K, (e) 290 K.

5. Details of Fluorescence Study

4-1. Fluorescence Parameters

Table S2. Fluorescence Parameters of Silylcarbazoles

compound	λ_{abs} / nm	λ_{emi} / nm	Storks Shift $\Delta\lambda$ / nm	Quantumn	Lifetime τ / ns	
				Yield Φ_f		
Solution	TMSCar	354	360	6	0.76	15.05
	C18Car	354	361	7	0.65	15.40
Solid state	TMSCar	370	386	16	0.28	10.53
	C18Car	364	381	17	0.08	6.61

4-2. Details of Solid-State Fluorescence Studies

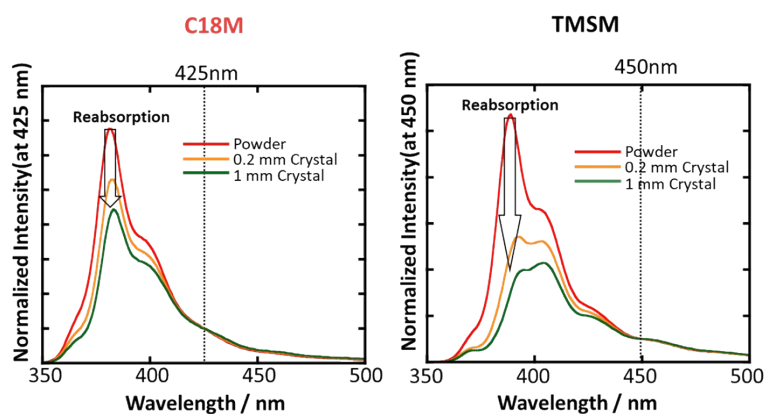


Fig. S18. Thickness dependent fluorescence spectra from a single crystal: **C18Car** (left), **TMSCar** (right).

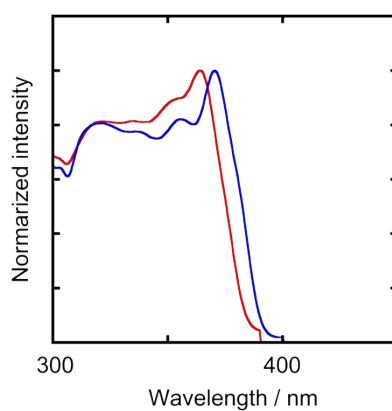


Fig. S19. Excitation spectra for powdered fluorescence: **C18Car** (red line, $\lambda_{abs} = 364$ nm), **TMSCar** (blue line, $\lambda_{abs} = 370$ nm).

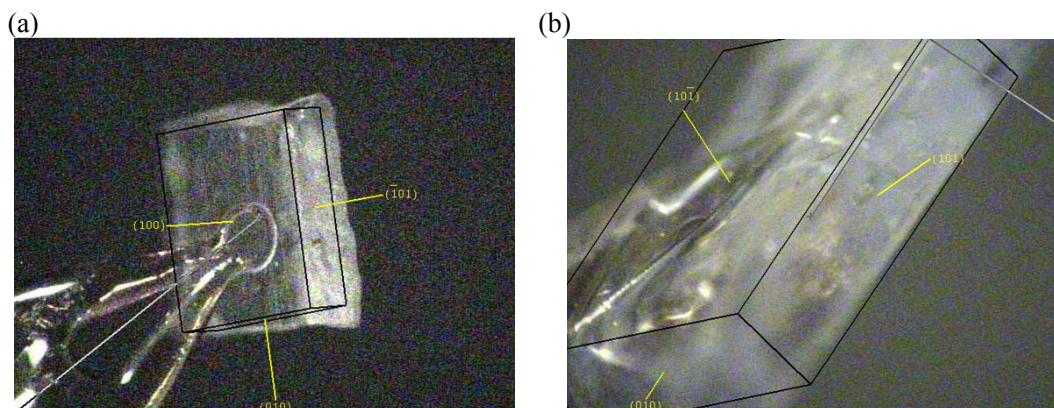


Fig. S20. Orientation mapping of the single crystal determined by X-ray diffraction: (a) **C18Car**, (b) **TMSCar**.

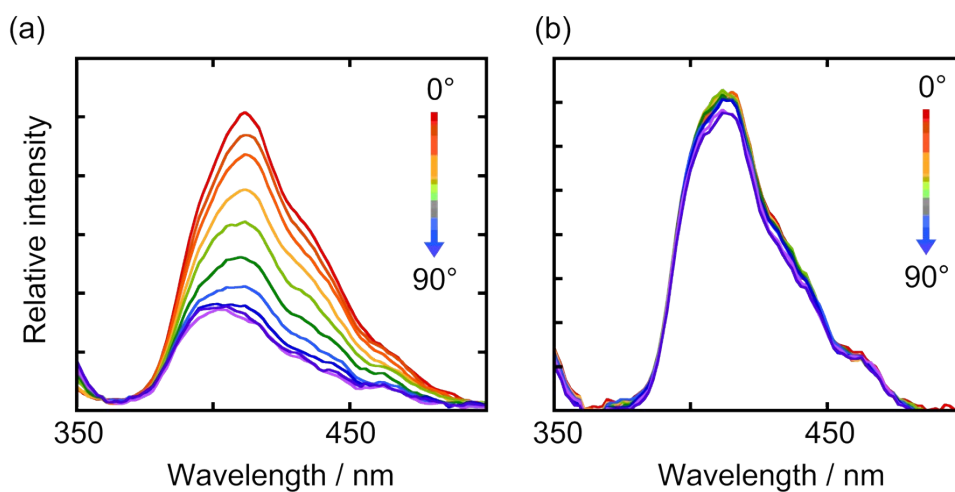


Fig. S21. Polarized fluorescence spectra from a single crystal of (a) **C18Car** and (b) **TMSCar**. Values of the angles were stated in the caption of Fig. 3. [Note: These spectra include optical properties of the polarizer, such as the wavelength dependence of extinction ratios. Thus, a discussion on the spectral shapes is futile. However, the intensities of fluorescence that depend on the angles at certain wavelengths reflect the magnitudes of their polarity.]

5. Details of DFT Calculations

a. Optimized Structure, Total Energy, Excitation energies, and Direction of Transition Moment of 2,7-trimethylsilyl-9-methylcarbazole

All calculation were carried out using Gaussian 16 (Revision A.03) program packages^{S1} on Fujitsu PRIMERGY CX400 supercomputer at Nagoya University ICTS and the Research Center for Computational Science, Okazaki, Japan

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.

b. Optimized Structure, Total Energy, Excitation energies, and Direction of Transition Moment of 2,7-trimethylsilyl-9-methylcarbazole at B3LYP/6-31G(d,p) level

Table S3. Optimized Structural Coordinate and its Total Energy at B3LYP/6-31G(d,p) level
total energy: = -1374.1768645 hartree (NImag = 0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	6.109633	-0.787396	-1.389467
2	6	0	-6.101979	-0.774386	-1.444270
3	6	0	-5.544346	2.070938	-0.378127
4	6	0	5.548690	2.058929	-0.327735
5	6	0	3.036465	-1.528112	0.319611
6	6	0	3.455853	-0.194243	0.083977
7	6	0	1.693464	-1.881744	0.381447
8	6	0	2.480572	0.798921	-0.089151
9	6	0	0.003356	2.670150	-0.426835
10	6	0	-3.460214	-0.186717	0.052769
11	6	0	-3.045879	-1.521493	0.292174
12	6	0	-2.481257	0.804321	-0.111553
13	6	0	0.719211	-0.891786	0.208690
14	6	0	1.128826	0.448277	-0.019240
15	6	0	-1.704263	-1.878032	0.366122
16	6	0	-0.726342	-0.890194	0.202167
17	6	0	-1.130953	0.450766	-0.029444
18	6	0	6.120605	-0.243300	1.651304
19	6	0	-6.139002	-0.229598	1.596171
20	1	0	5.678911	-0.527846	-2.362329
21	1	0	-5.662010	-0.515976	-2.413290
22	1	0	-5.091793	2.376462	-1.327699
23	1	0	7.187822	-0.597150	-1.438784
24	1	0	-7.179268	-0.581810	-1.503266
25	1	0	5.969935	-1.864048	-1.244855
26	1	0	5.105396	2.365619	-1.281290
27	1	0	-6.611884	2.311479	-0.432858
28	1	0	-5.965924	-1.851309	-1.298211
29	1	0	0.009836	2.880035	-1.504240
30	1	0	6.617198	2.297163	-0.372771
31	1	0	-5.110714	2.689122	0.415370

32	1	0	3.783597	-2.306767	0.454380
33	1	0	1.403684	-2.913903	0.559005
34	1	0	2.771438	1.827244	-0.281673
35	1	0	-3.795888	-2.298519	0.420191
36	1	0	-0.881269	3.135075	0.014473
37	1	0	-2.768174	1.833256	-0.306707
38	1	0	-1.418330	-2.910813	0.546279
39	1	0	5.109246	2.677898	0.461944
40	1	0	0.883641	3.133474	0.024773
41	1	0	-7.216665	-0.033707	1.558975
42	1	0	7.198993	-0.049817	1.623786
43	1	0	5.980578	-1.302957	1.890330
44	1	0	-6.003490	-1.289519	1.836622
45	1	0	-5.721411	0.351462	2.425232
46	1	0	5.696917	0.338550	2.476709
47	7	0	0.000365	1.252045	-0.143071
48	14	0	-5.305655	0.222358	-0.043931
49	14	0	5.302977	0.210809	0.003902

Table S4. Ground to excited state transition electric dipole moments (Au) at B3LYP/6-31G(d,p) level

state	X	Y	Z	Dip. S.	Osc.
1	-0.0001	-0.5713	0.0005	0.3263	0.0309
2	-1.9193	0.0000	0.0000	3.6838	0.3913
3	2.1976	-0.0000	-0.0000	4.8293	0.6112
4	-2.0115	0.0001	0.0000	4.0463	0.5170
5	-0.0001	-0.3904	0.0104	0.1525	0.0198

Table S5. Excitation energies and oscillator strengths at B3LYP/6-31G(d,p) level

Excited State 1:	Singlet-A	3.8635 eV	320.91 nm	f=0.0309	<S**2>=0.000
87 -> 90	-0.16765				
	HOMO(88) -> LUMO(89)	0.68236			
Excited State 2:	Singlet-A	4.3356 eV	285.97 nm	f=0.3913	<S**2>=0.000
87 -> 89	0.63561				
88 -> 90	0.28873				
Excited State 3:	Singlet-A	5.1658 eV	240.01 nm	f=0.6112	<S**2>=0.000
85 -> 90	-0.10104				
86 -> 89	0.25968				
87 -> 89	-0.17004				
87 -> 91	-0.25071				
88 -> 90	0.52120				
88 -> 92	-0.21507				
Excited State 4:	Singlet-A	5.2148 eV	237.75 nm	f=0.5170	<S**2>=0.000
86 -> 89	0.53904				
87 -> 89	0.21513				
87 -> 91	-0.25168				
88 -> 90	-0.29784				
Excited State 5:	Singlet-A	5.2996 eV	233.95 nm	f=0.0198	<S**2>=0.000
86 -> 92	0.10078				
87 -> 90	0.56127				
87 -> 92	-0.13577				
88 -> 89	0.11681				
88 -> 91	0.35557				