Supporting information for

Cyclic and Linear Dithienyl-Anthryl Vinylenes: Synthesis, X-ray Crystallography, Spectroscopic Properties, and Photoinduced Mechanical Motions

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Contents

1. Characterization
2. Crystallographic data
3. Photoirradiation to solutions
4. Photoirradiation to free-standing films
5. Density functional calculations
6. Force measurements
7. DSC
8. X-ray diffraction
9. Polarized optical microscopy
10. Cartesian coordinates of the optimized structure

1. Characterization

1-1 Characterization of 1

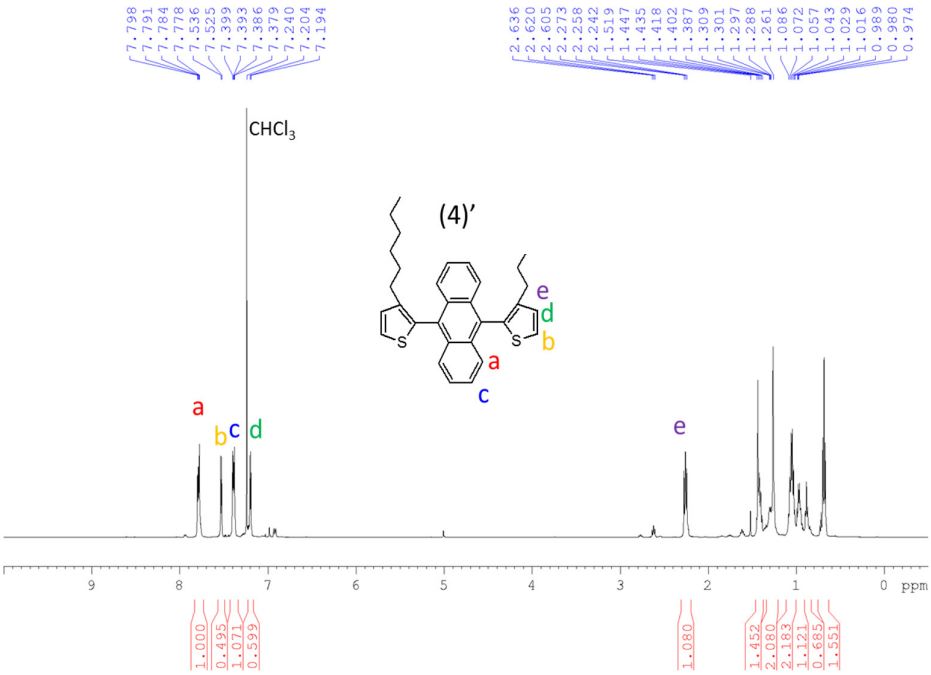


Fig. S1 ^{1}H NMR spectrum (500MHz, $CDCl_3$) of *cis*-conformer.

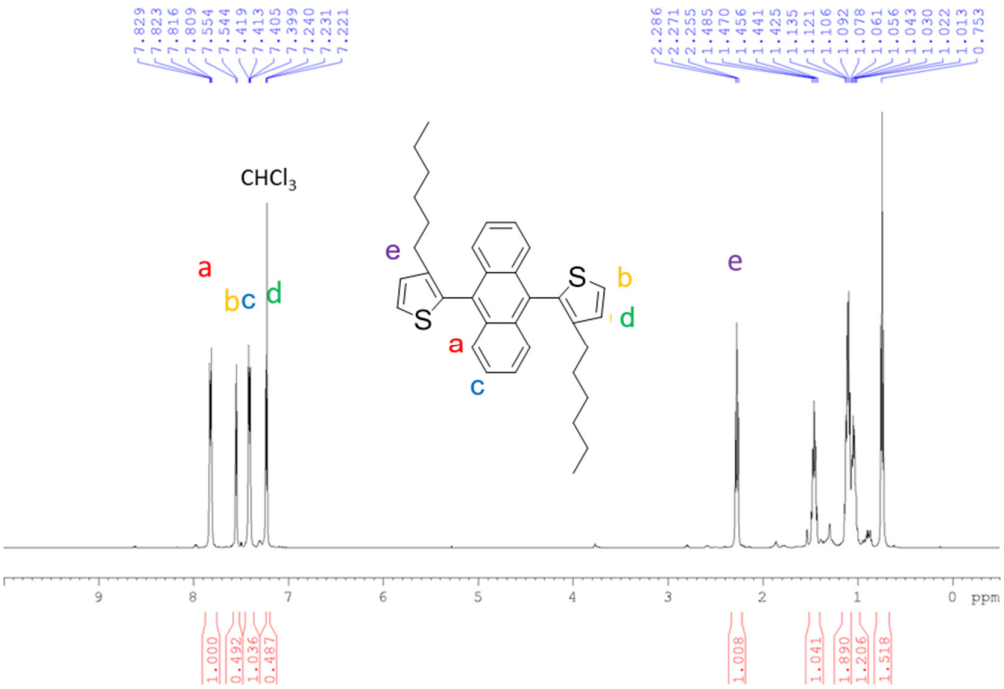
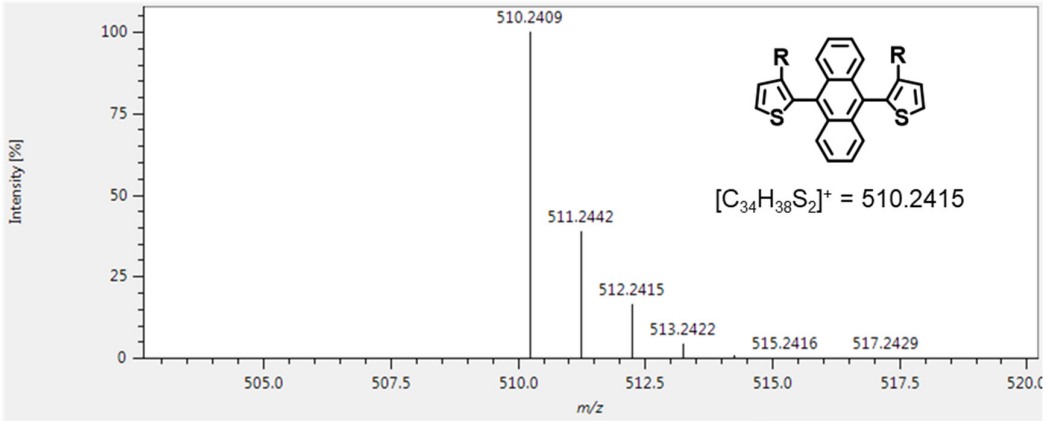


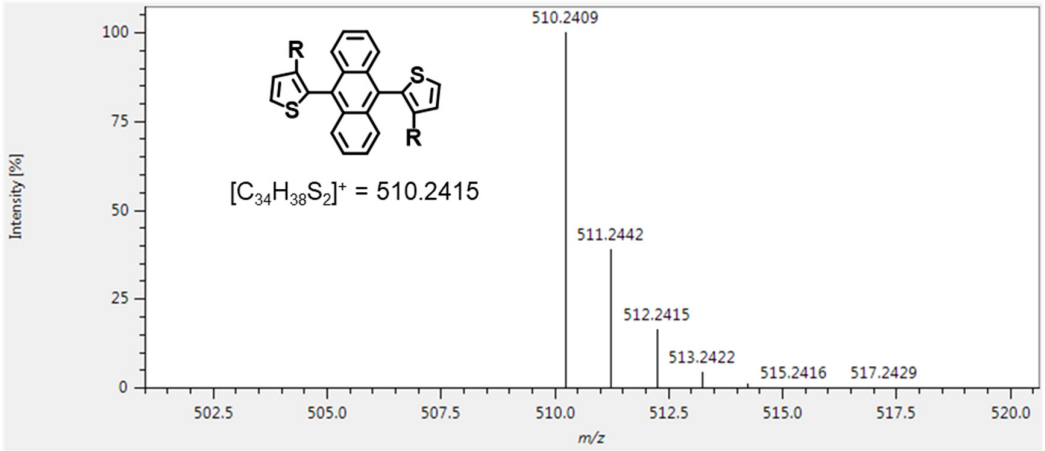
Fig. S2 ^{1}H NMR spectrum (500MHz, $CDCl_3$) of *trans*-conformer.

(a)



Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
510.24070	1688587.00	C34 H38 S2	510.24094	-0.24	-0.48	16.0

(b)



Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
510.24081	826125.63	C34 H38 S2	510.24094	-0.13	-0.26	16.0

Fig. S3 HRFD-MS spectra of (a) *cis*-conformer and (b) *trans*-conformer (R = hexyl).

1-2 Characterization of aa and 2b

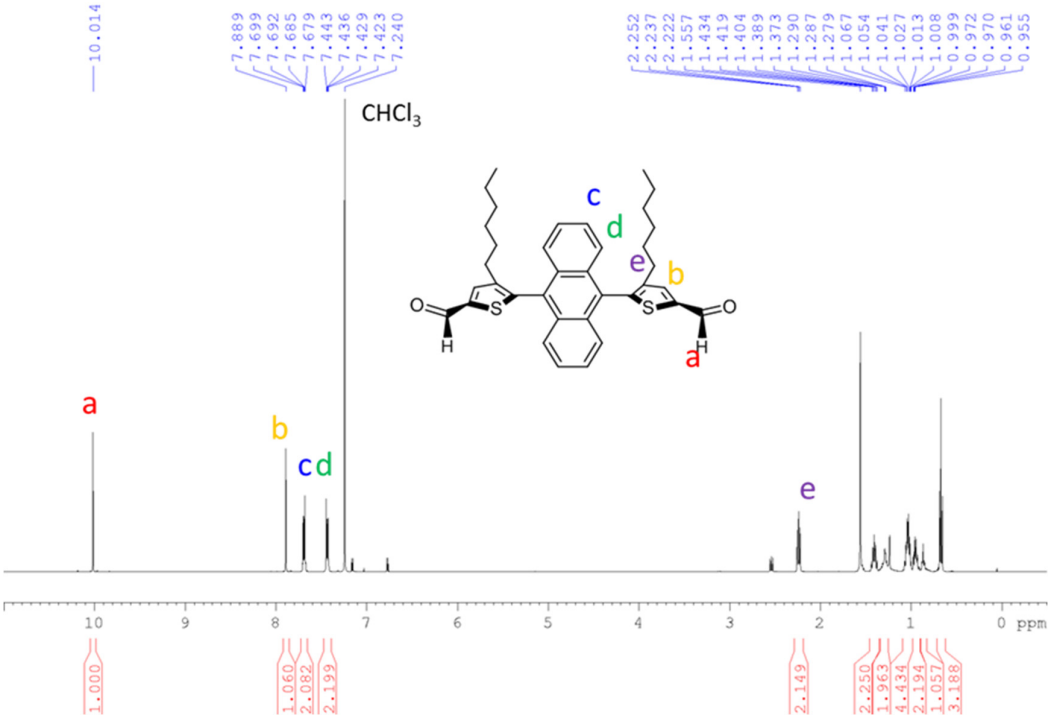


Fig. S4 ^{1}H NMR spectrum (500 MHz, CDCl3) of **2a**.

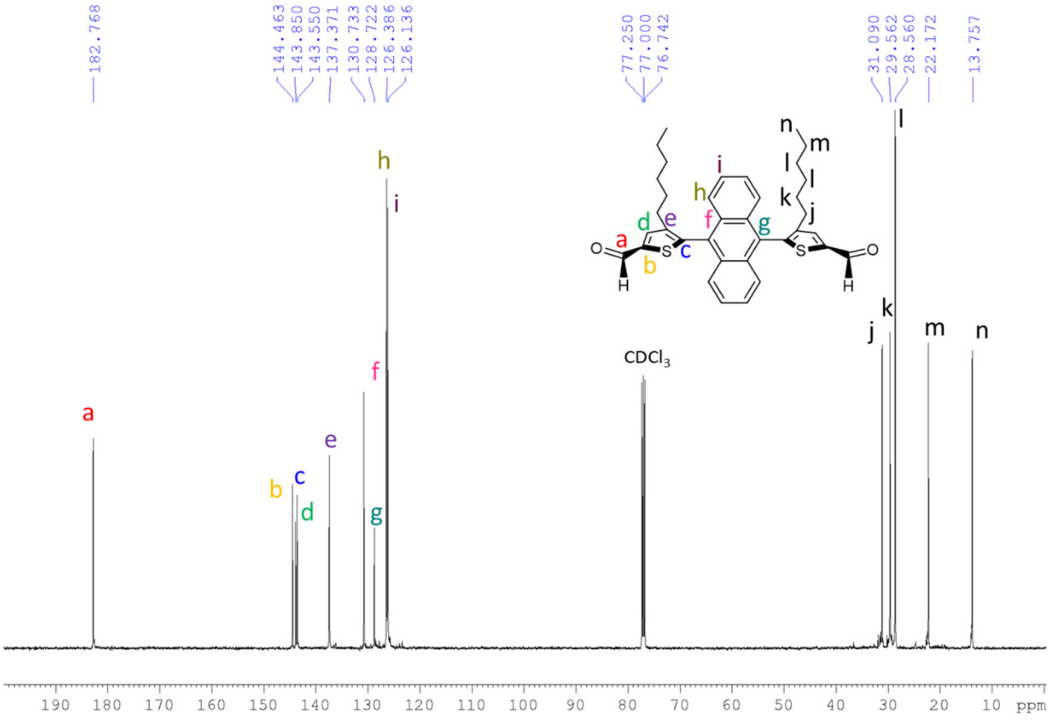


Fig. S5 ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **2a**.

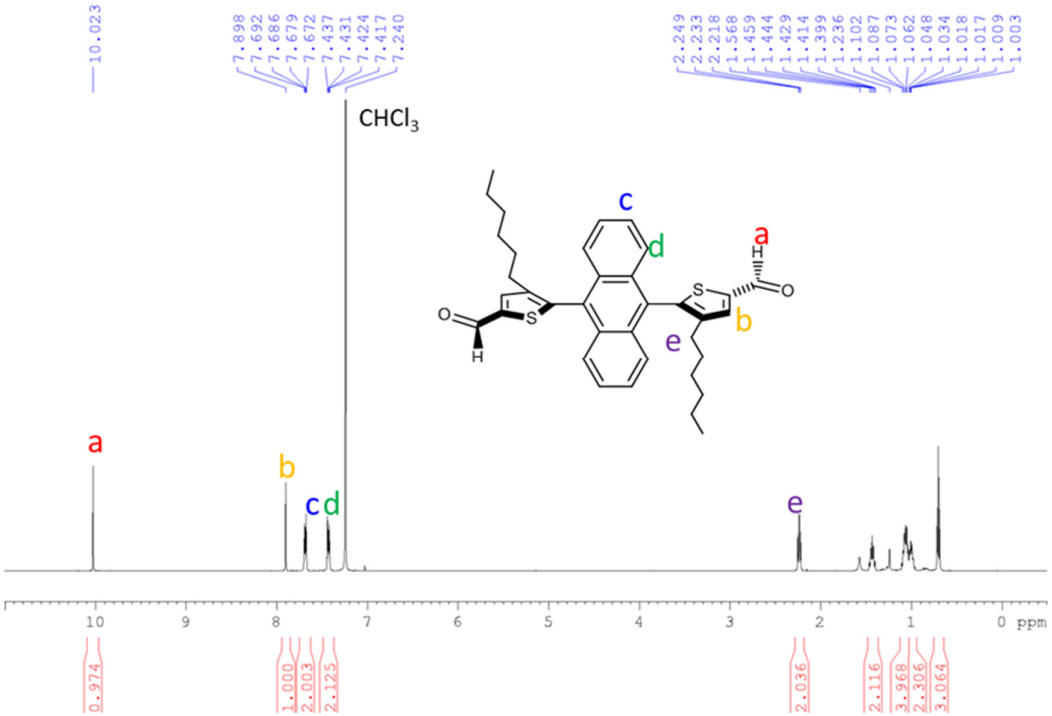


Fig. S6 ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **2b**.

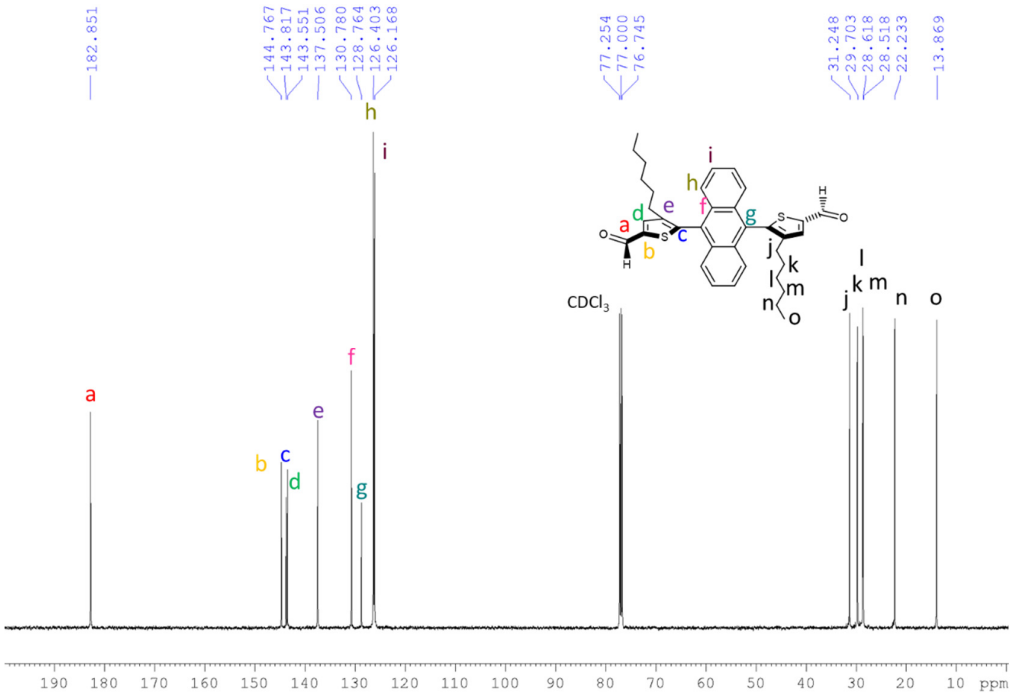


Fig. S7 ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **2b**.

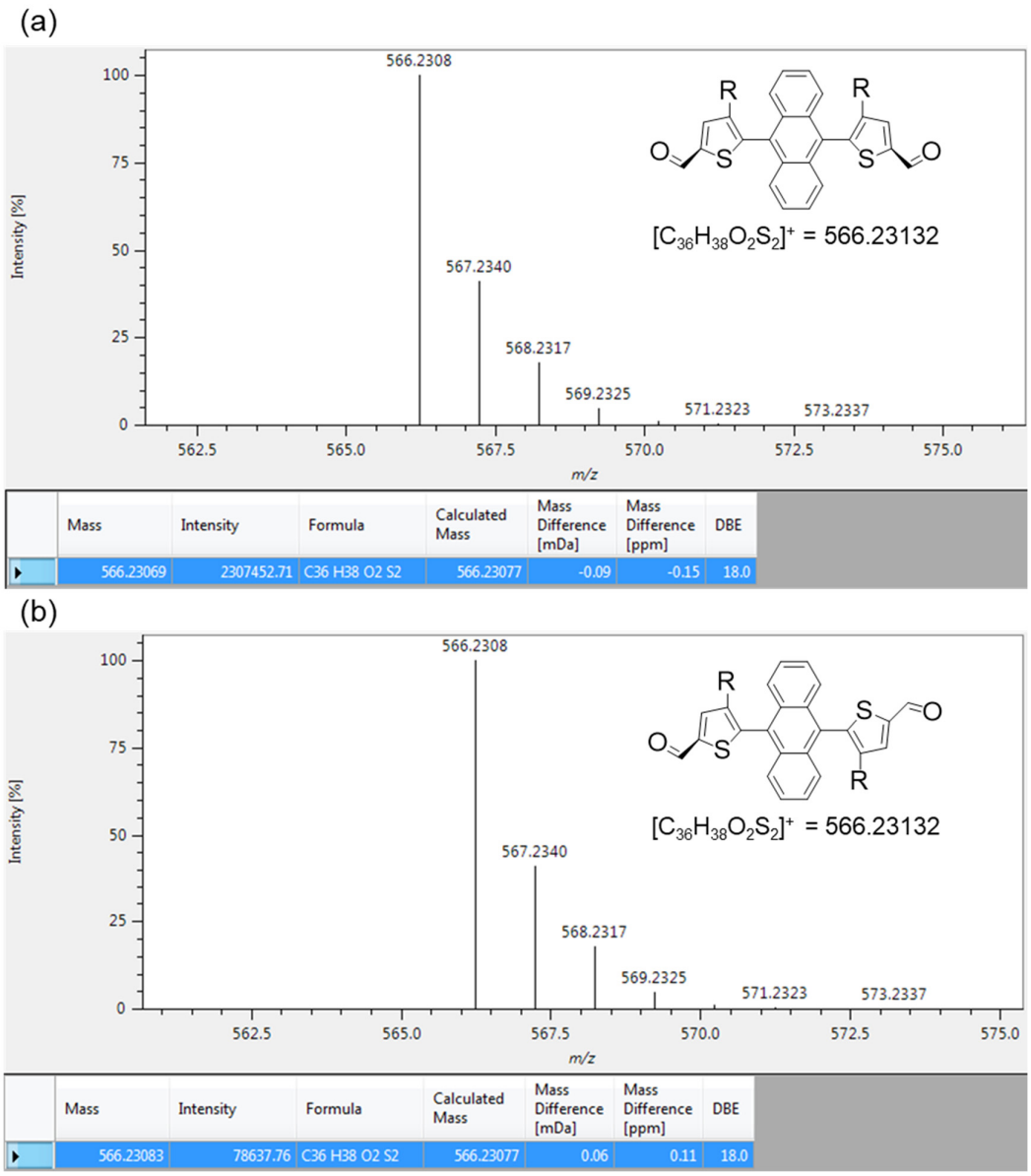


Fig. S8 HRFD-MS spectra of (a) **2a** and (b) **2b** (R= hexyl).

1-3 Characterization of 3 and 4

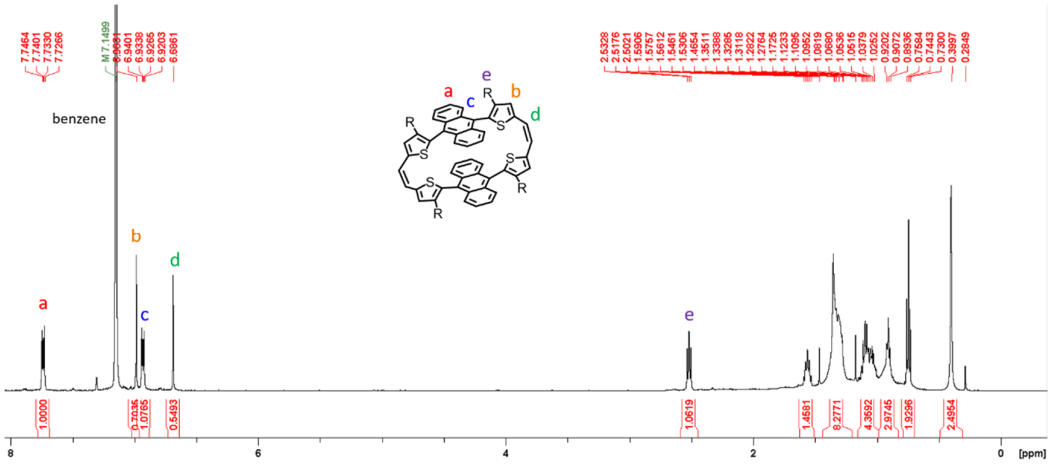


Fig. S9 ^{1}H NMR spectrum (500 MHz, *d*-Benzene) of **3** (R= hexyl).

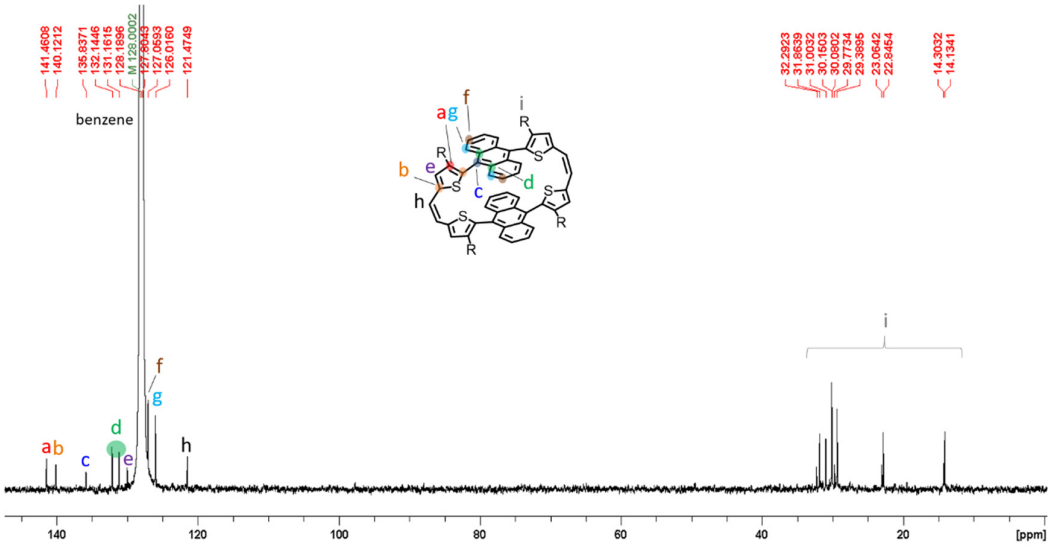


Fig. S9 ^{13}C NMR spectrum (125 MHz, *d*-Benzene) of **3** (R= hexyl).

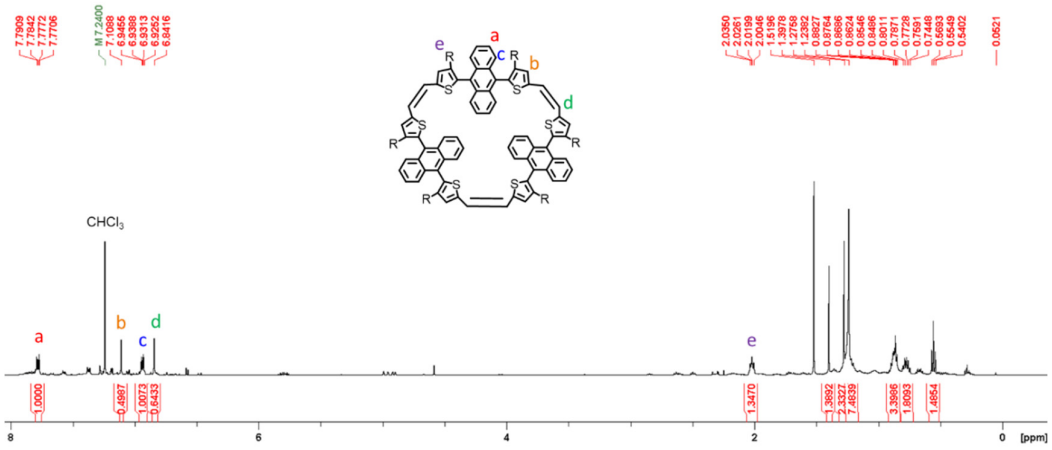


Fig. S10 ^{1}H NMR spectrum (500 MHz, *d*-Benzene) of **4** (R= hexyl).

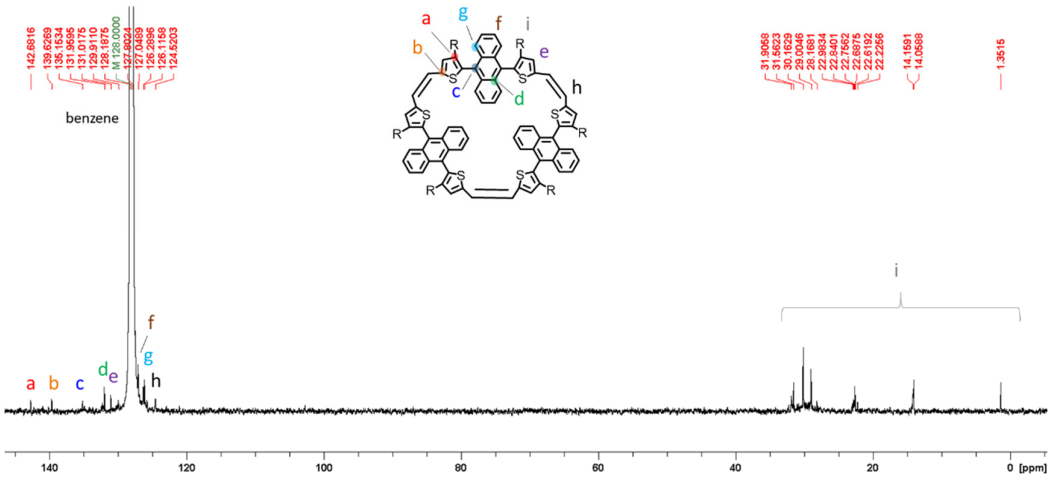
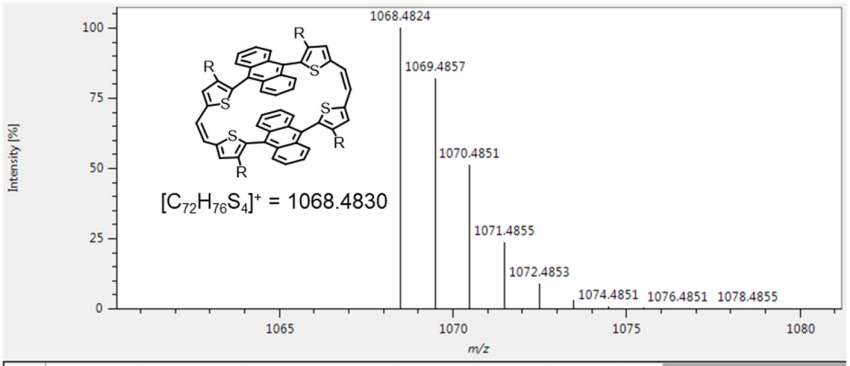


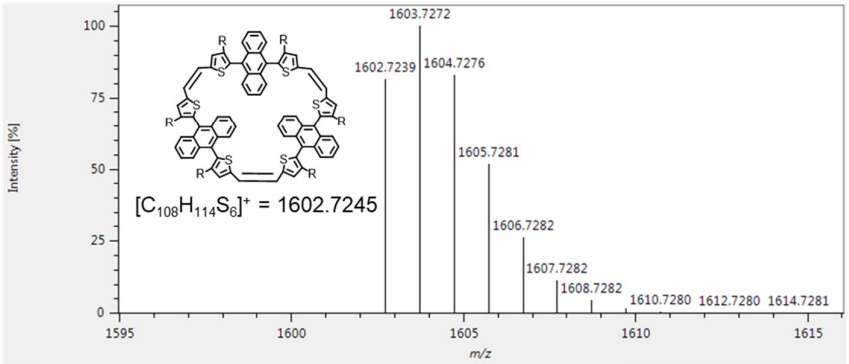
Fig. S11 ^{13}C NMR spectrum (125 MHz, *d*-Benzene) of **4** (R= hexyl).

(a)



Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
1068.48249	76211.45	C72 H76 S4	1068.48244	0.05	0.05	35.0

(b)



Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
1602.72383	255059.00	C108 H114 S6	1602.72393	-0.10	-0.06	52.0

Fig. S12 HRFD-MS spectra of (a) **3** and (b) **4** (R= hexyl).

1-4 Characterization of 5

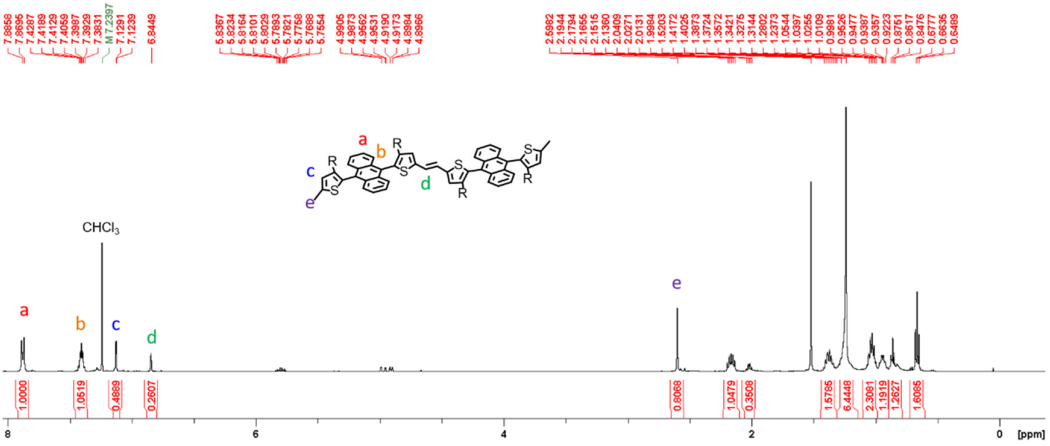
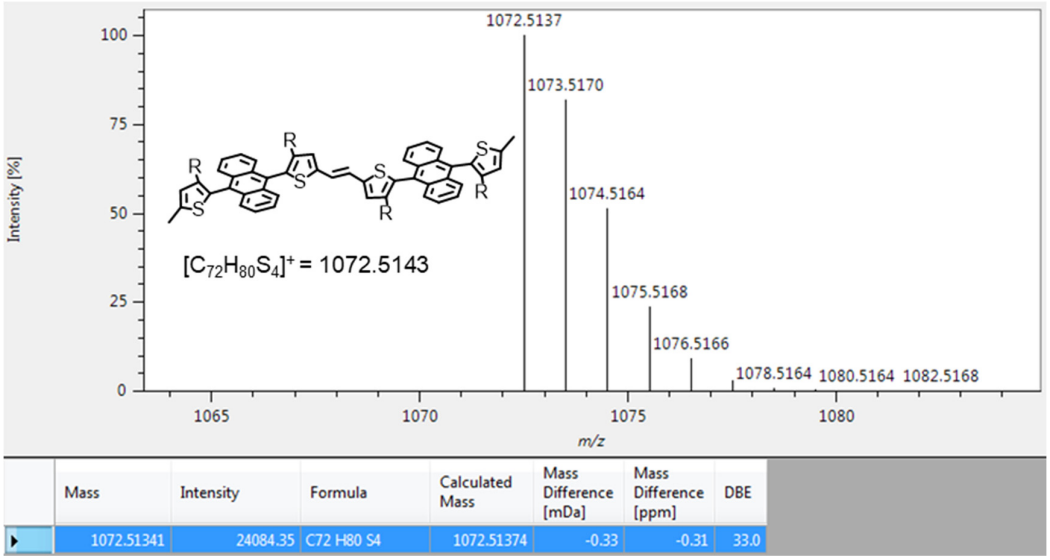


Fig. S13 ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **5** (R= hexyl).



Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
1072.51341	24084.35	C72 H80 S4	1072.51374	-0.33	-0.31	33.0

Fig. S14 HRFD-MS spectra of **5** (R= hexyl).

1-5 Characterization of polymers

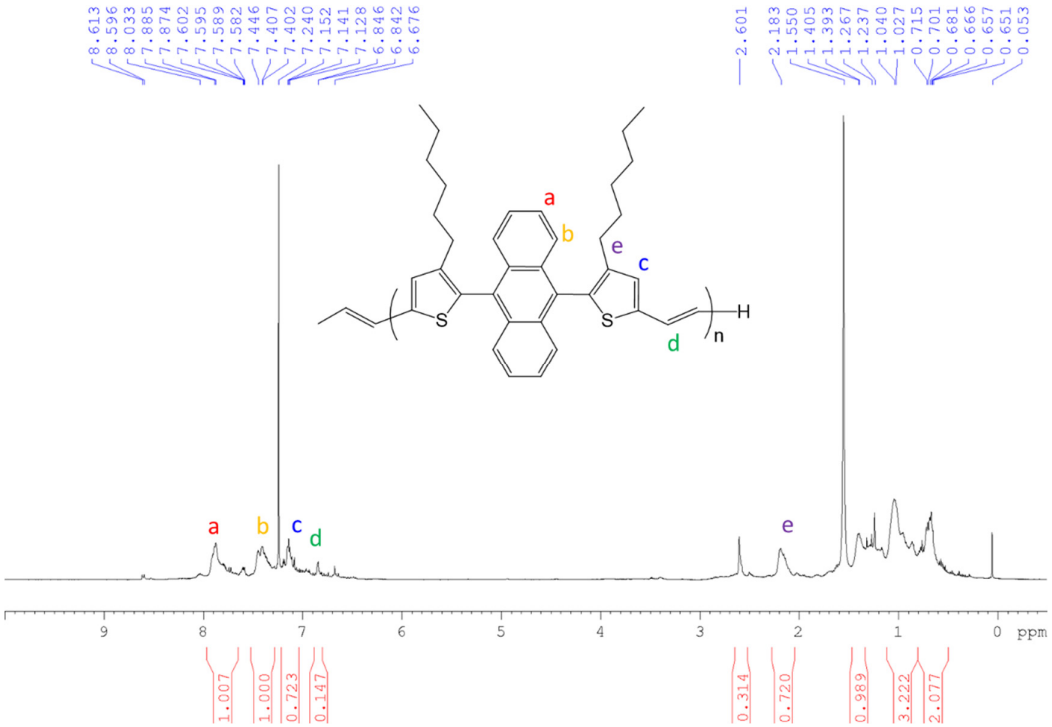
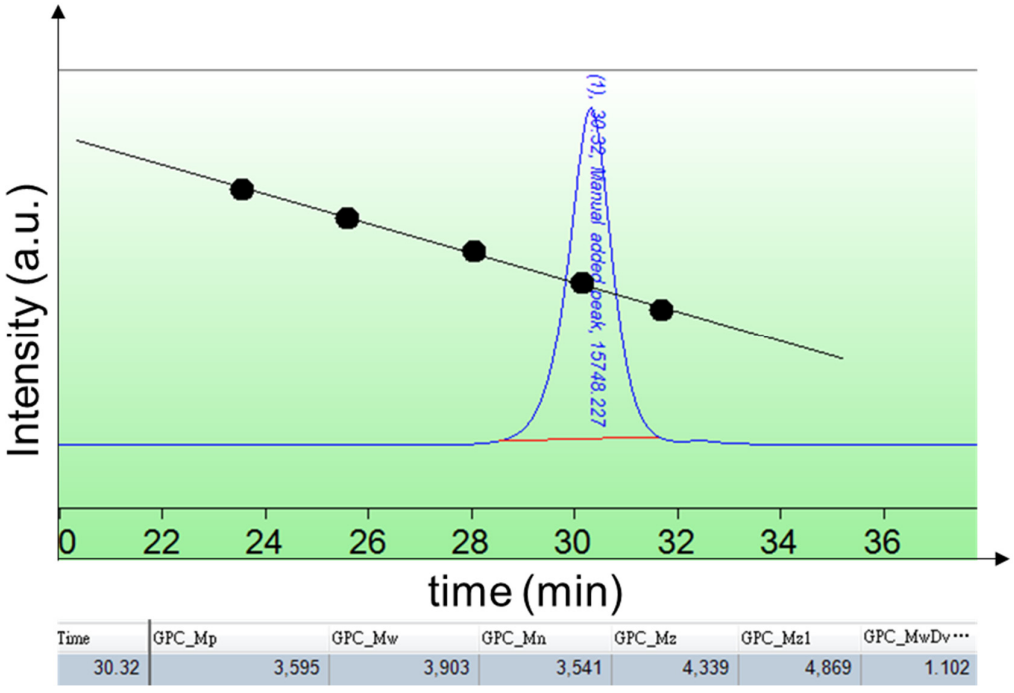


Fig. S15 ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **6**.



Time	GPC_Mp	GPC_Mw	GPC_Mn	GPC_Mz	GPC_Mz1	GPC_MwDv···
30.32	3,595	3,903	3,541	4,339	4,869	1.102

Fig. S16 GPC elution curve of **6**.

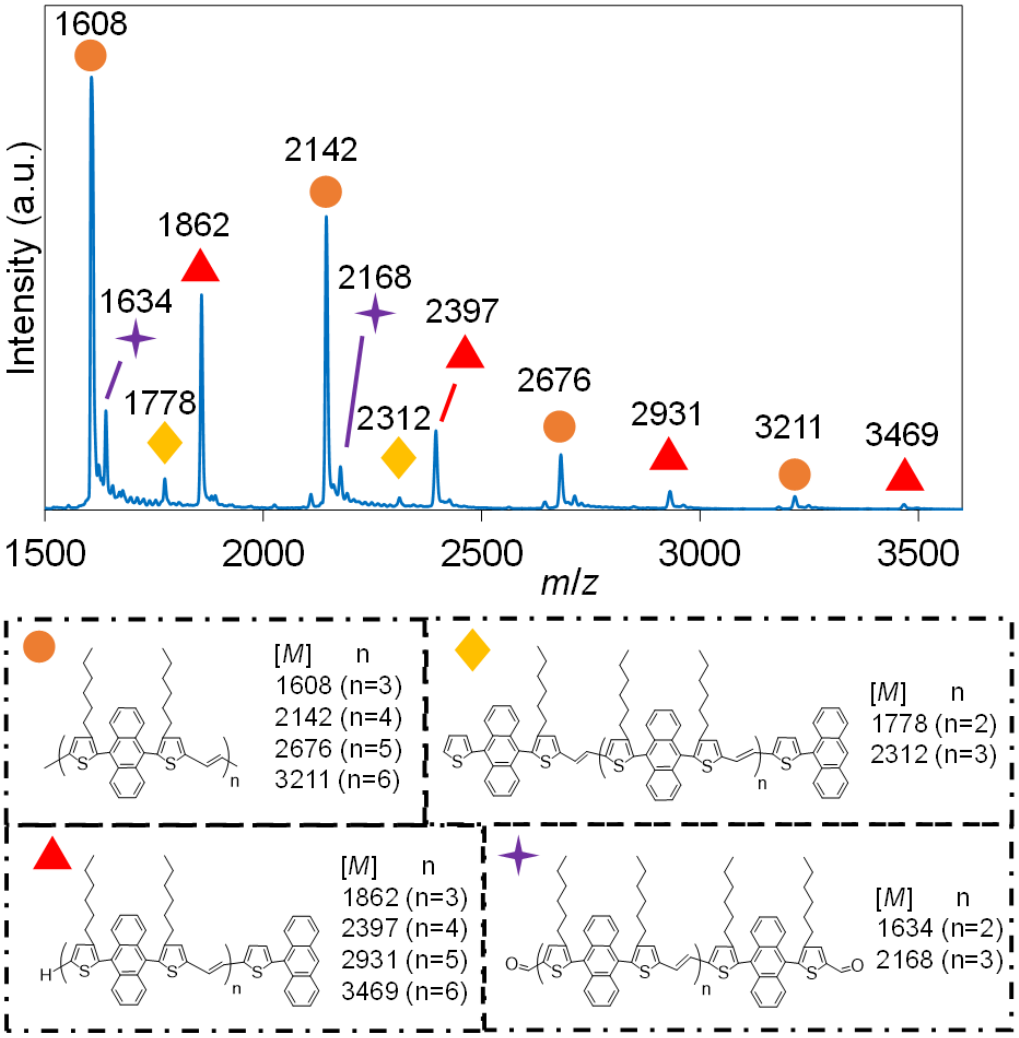


Fig. S17 MALDI-TOF mass spectrum of **6**.

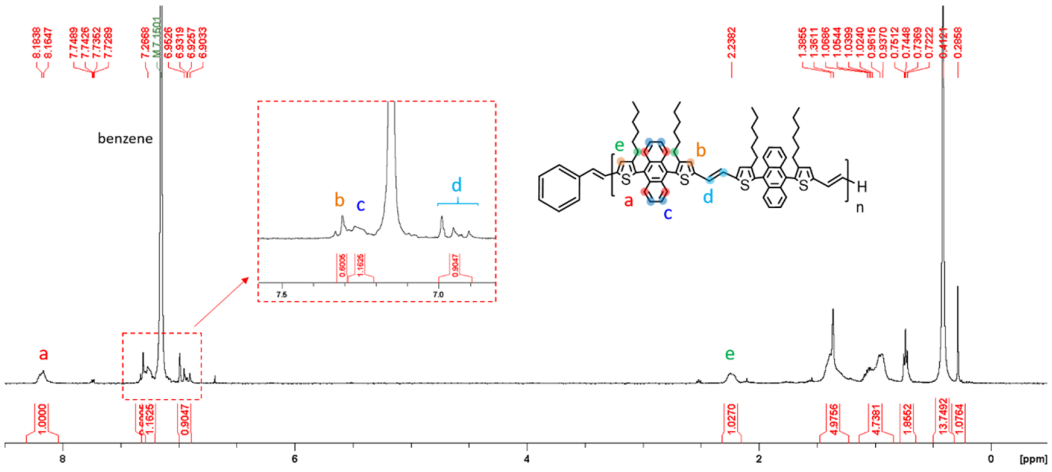
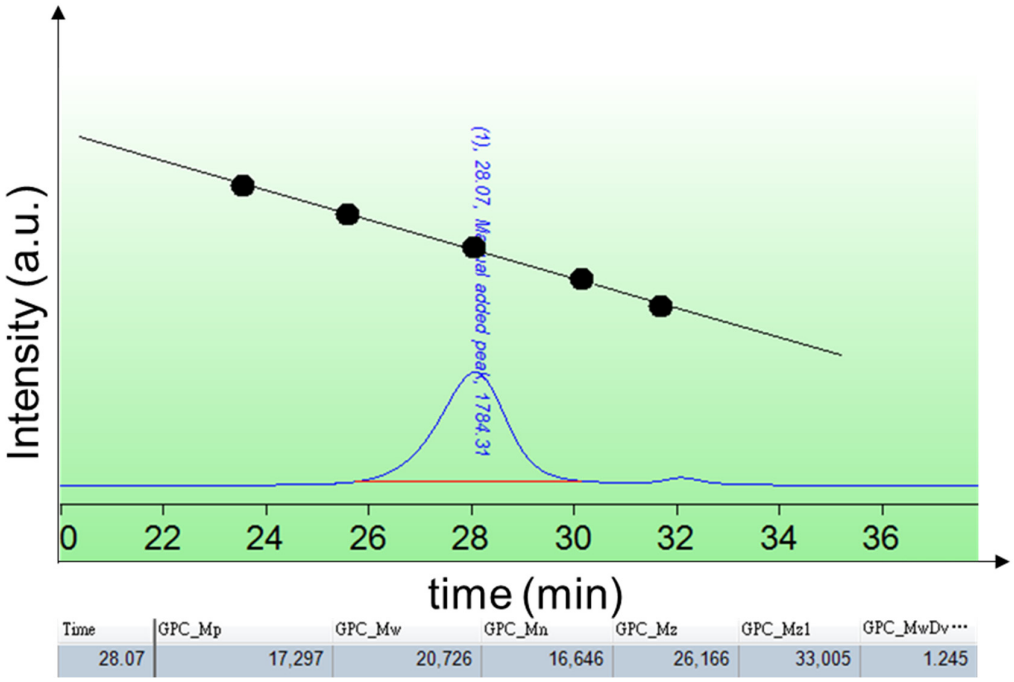


Fig. S18 ^{1}H NMR spectrum (500MHz, *d*-Benzene) of **7** (R= hexyl).



Time	GPC_Mp	GPC_Mw	GPC_Mn	GPC_Mz	GPC_Mz1	GPC_MwDv···
28.07	17,297	20,726	16,646	26,166	33,005	1.245

Fig. S19 GPC elution curve of **7**.

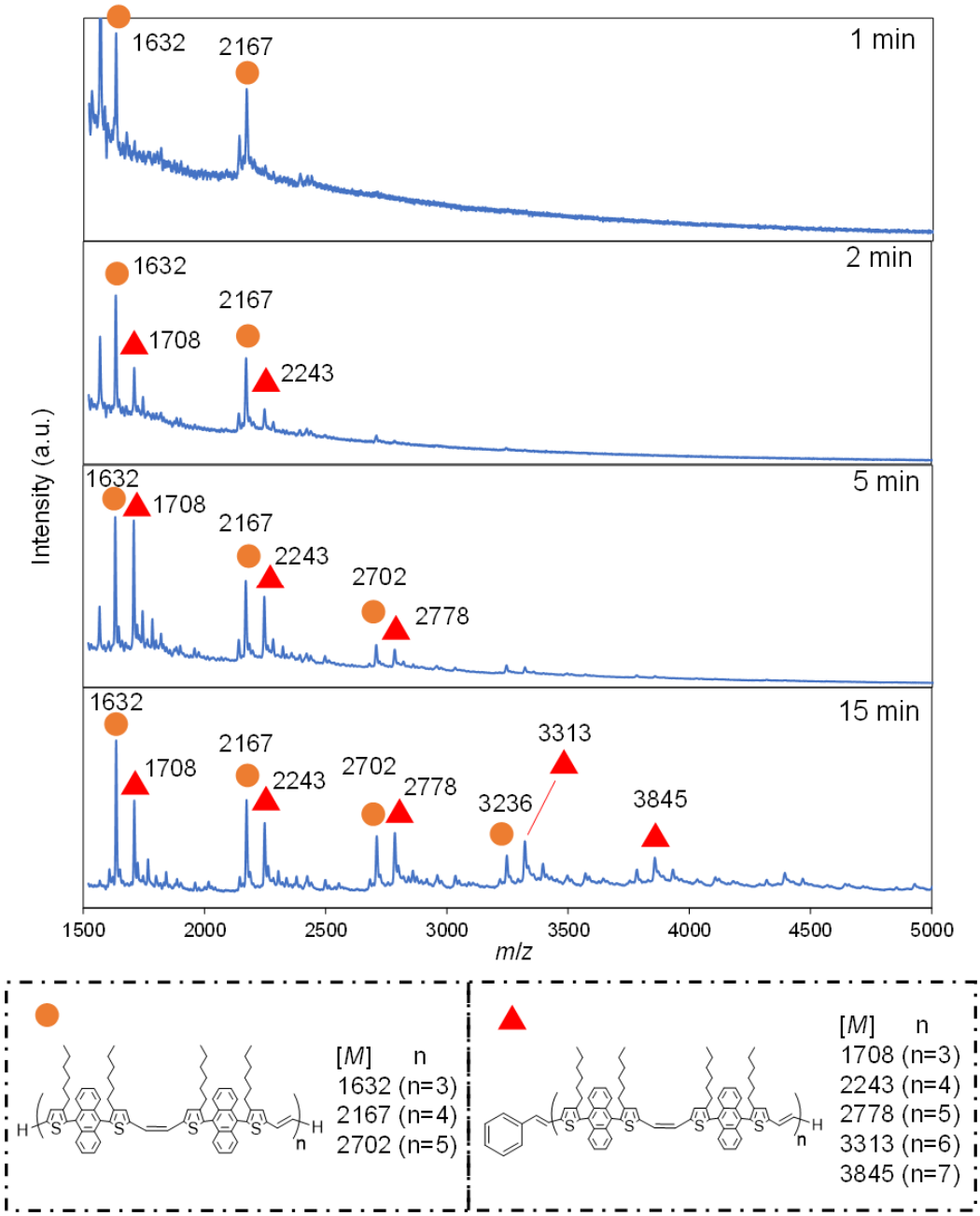


Fig. S20 MALDI-TOF mass spectra of **7**.

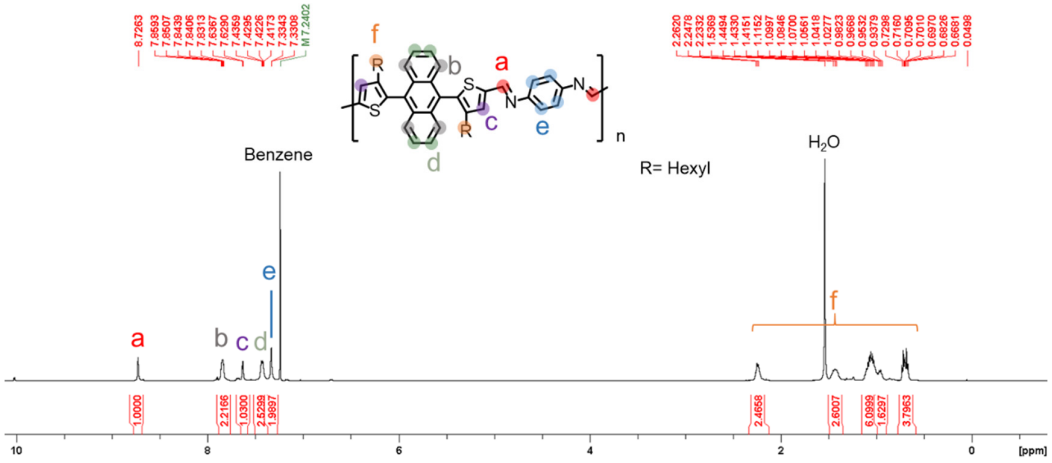
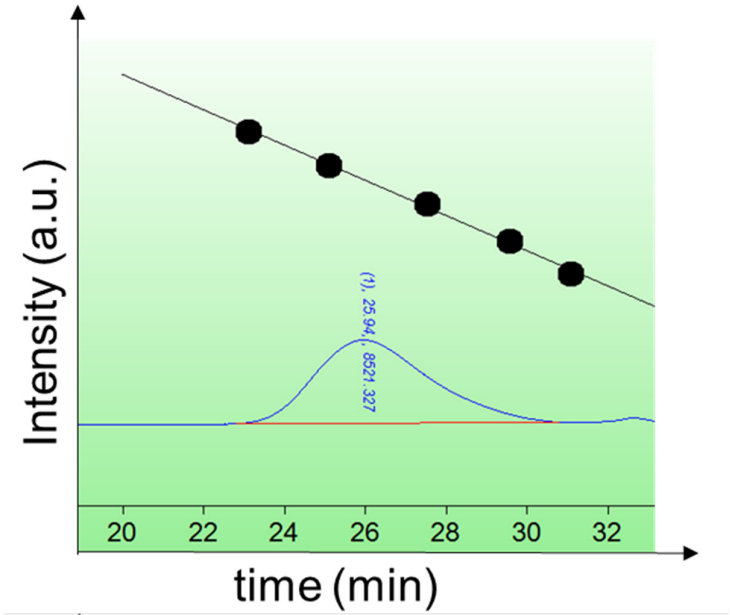


Fig. S21 ^{1}H NMR spectrum (500MHz, *d*-Benzene) of **8** (R= hexyl).



Time	GPC_Mp	GPC_Mw	GPC_Mn	GPC_Mz	GPC_Mz1	GPC_MwDv…
25.94	54,308	60,727	24,652	110,816	164,541	2.463

Fig. S22 GPC elution curve of **8**.

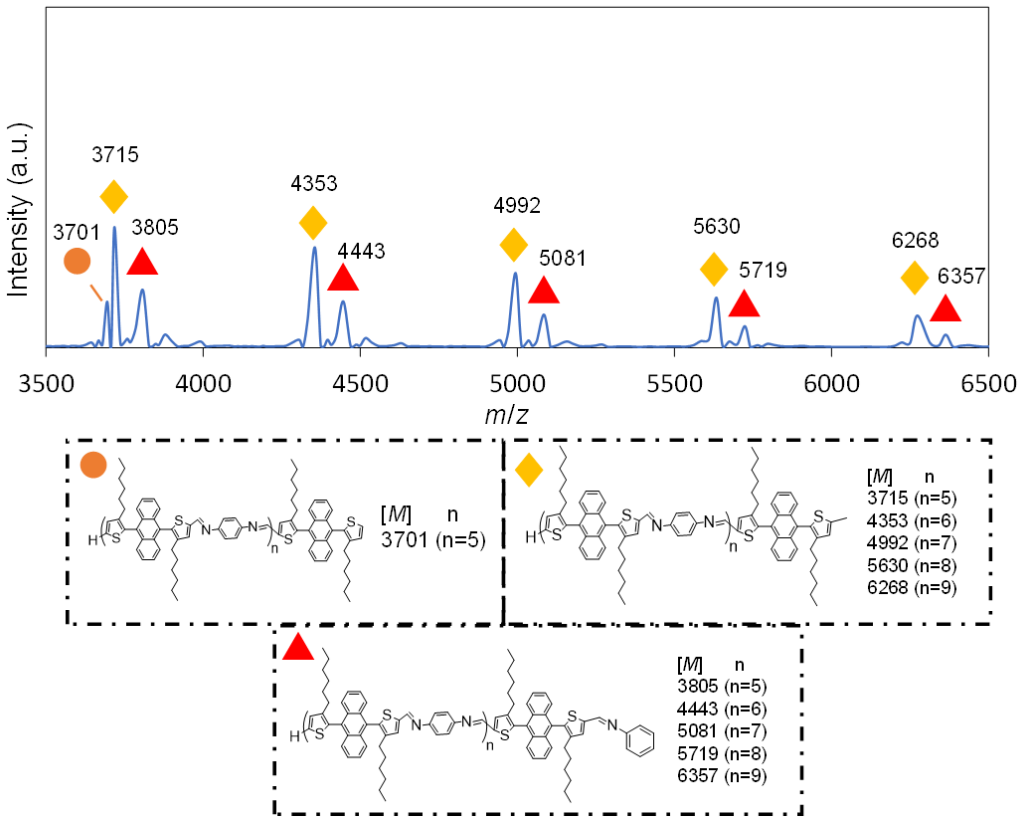


Fig. S23 MALDI-TOF mass spectrum of **8**.

1-6 Comparison of mass spectra of McMurry coupling products of 2a and 2b

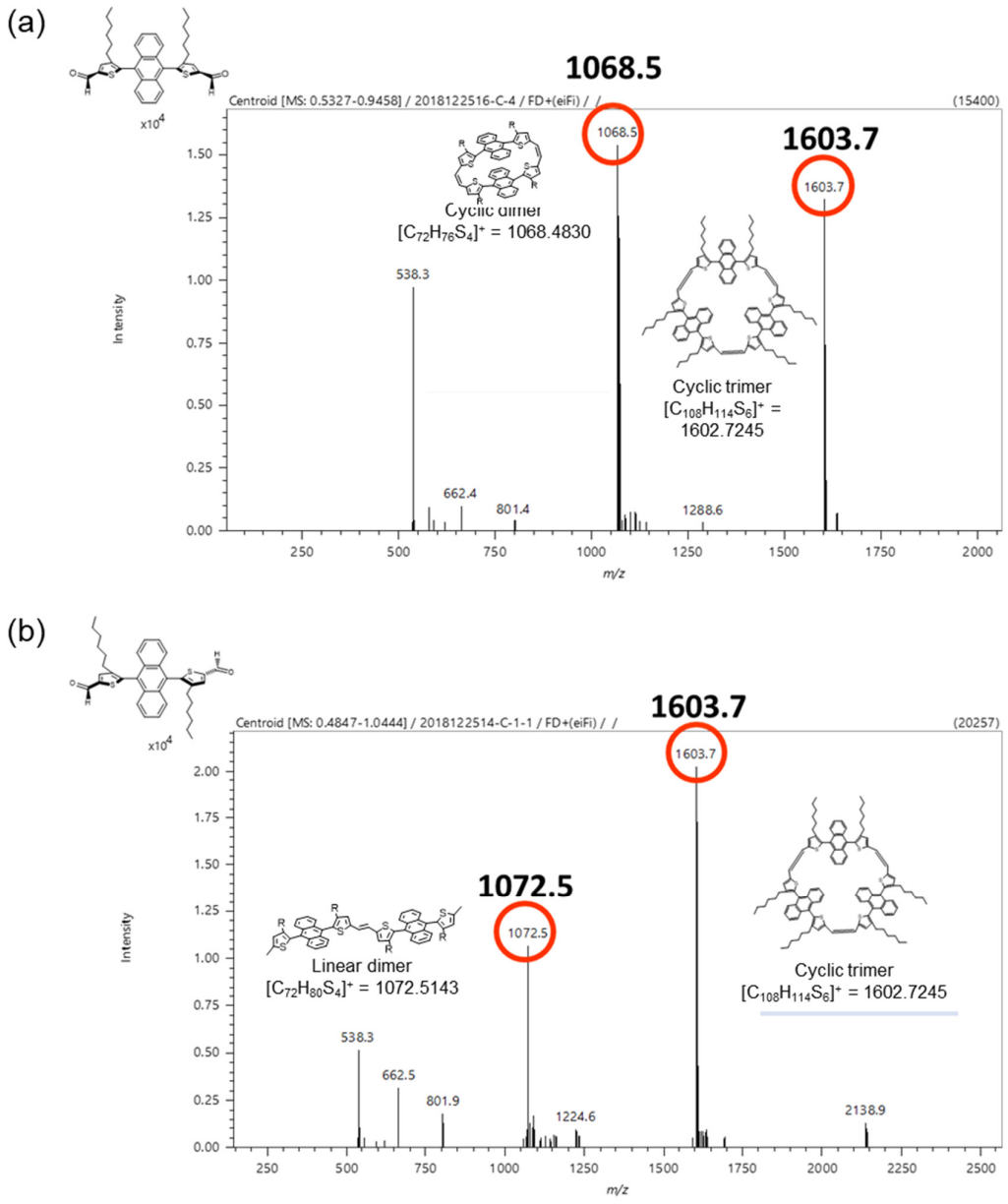


Fig. S24 LRFD mass spectra of McMurry coupling products of (a) **2a** and (b) **2b**. **2a** provided cyclic dimer and trimer, whereas **2b** provided linear dimer and cyclic trimer.

2. Crystallographic data

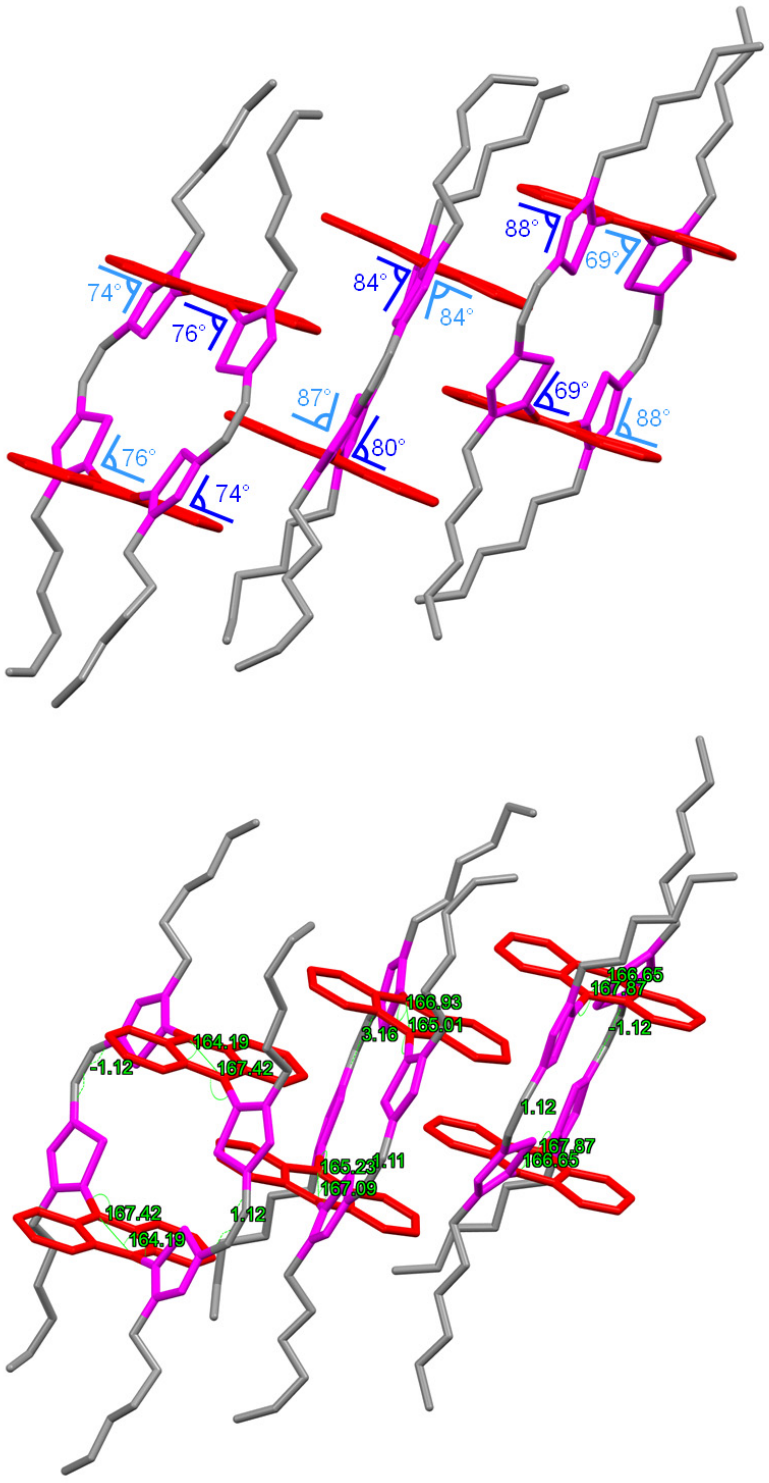


Fig. S26 Molecular structures of **3** with plane and torsion angles.

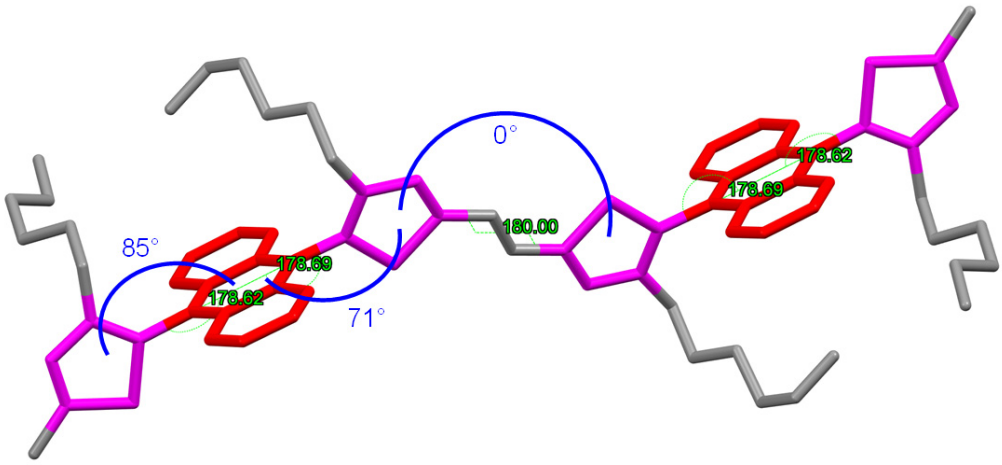


Fig. S27 Molecular structures of **5** with plane and torsion angles.

Table S1 Crystal data and structure refinement for **2a**, **2b**, **3**, and **5**.

	2a	**2b**	**3**	**5**
Formula	$C_{36}H_{38}O_2S_2$	$C_{36}H_{38}O_2S_2$	$C_{144}H_{148}S_8$	$C_{72}H_{80}S_4$
Molecular weight	566.78	566.78	2135.11	1072.514
Crystal system	Monoclinic	Triclinic	Triclinic	Triclinic
Space group	$P2_1/n$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a /Å	9.6891(4)	9.1606(3)	17.9088(9)	9.3240(6)
b /Å	21.8811(9)	10.9813(4)	18.9894(9)	12.8415(9)
c /Å	15.0076(7)	15.2260(5)	19.8159(6)	13.6781(10)
α /deg	90	92.296(1)	86.346(3)	72.939(2)
β /deg	108. 614(1)	91.607(1)	74.574(3)	86.791(2)
γ /deg	90	95.805(1)	64.997(5)	72.114(2)
V /Å^3	3015.3(2)	1521.79(9)	5878.2(5)	1488.95(18)
Z	4	2	2	1
F (000)	1208	604	2280	576
D/g cm^{-3}	1.248	1.237	1.206	1.197
Used	4883	4324	15305	3714
Independent	5508	5390	77438	5210
R	0.0327	0.0625	0.1241	0.0990
R_w	0.0814	0.1763	0.3415	0.1738
GOF	1.015	1.050	1.288	1.178

3. Photoirradiation to solutions

3-1 Compound 3 in benzene solution

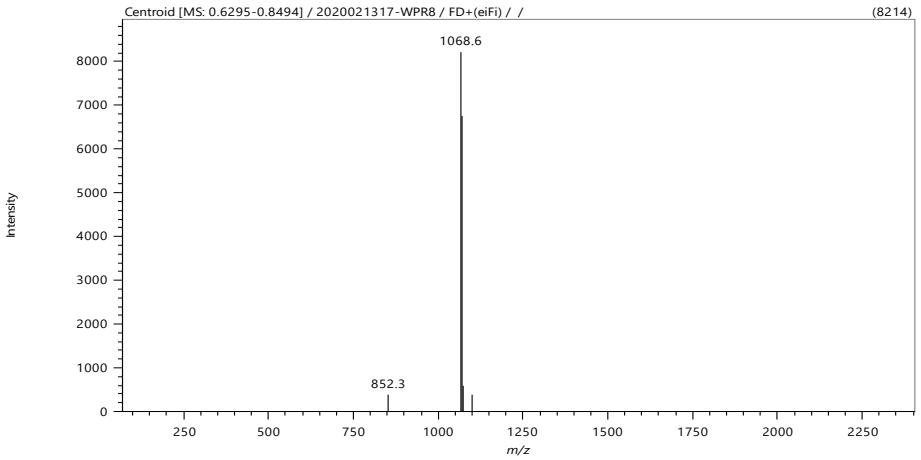


Fig. S28 LRFD of **3** after irradiation to its benzene solution at 365 nm for 1800s. Its molecular mass unchanged.

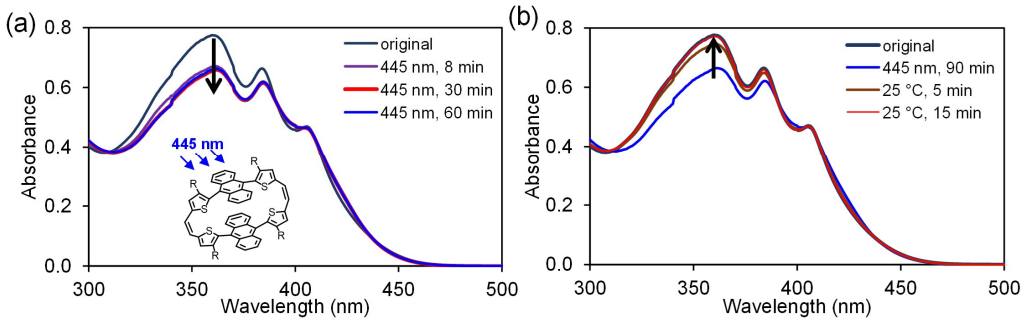


Fig. S29 (a) Time-dependent UV-Vis spectra of **3** in benzene solution during irradiation using 445-nm laser (7.7 mW cm^{-2}). (b) Time-dependent PL spectra of **3** in benzene solution at 25 ℃.

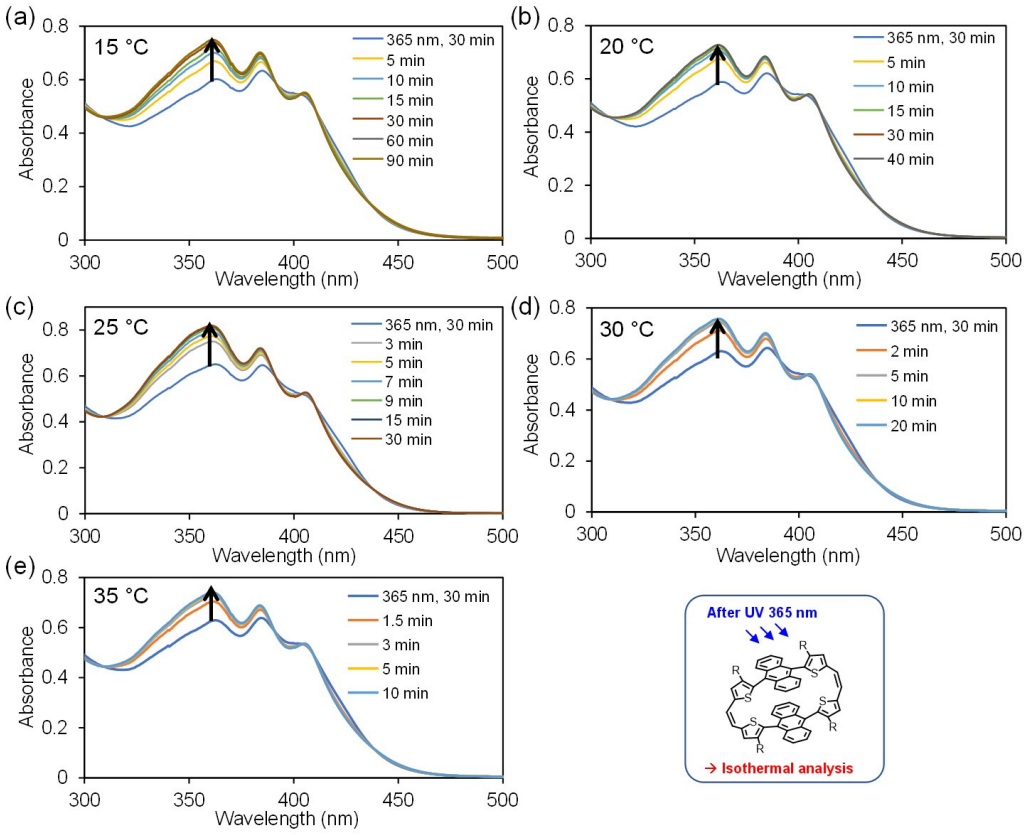


Fig. S30 Time-dependent UV-Vis spectra of **3** at (a) 15 ℃, (b) 20 ℃, (c) 25 ℃, (d) 30 ℃, and (e) 35℃.

3-2 Compound 4 in benzene solution

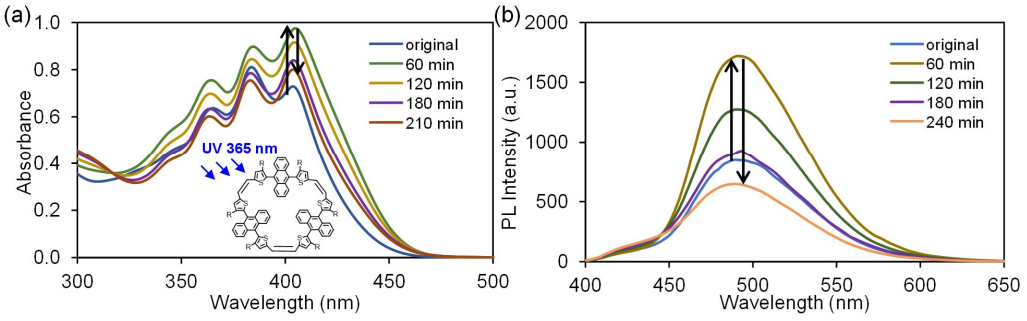


Fig. S31 (a) Time-dependent UV-vis spectra of **4** in benzene solution after irradiation at 365 nm. (b) Time-dependent PL spectra of **4** in benzene solution after irradiation at 365 nm. A mercury UV lamp (365 nm, 4 W cm^{-2}) was used.

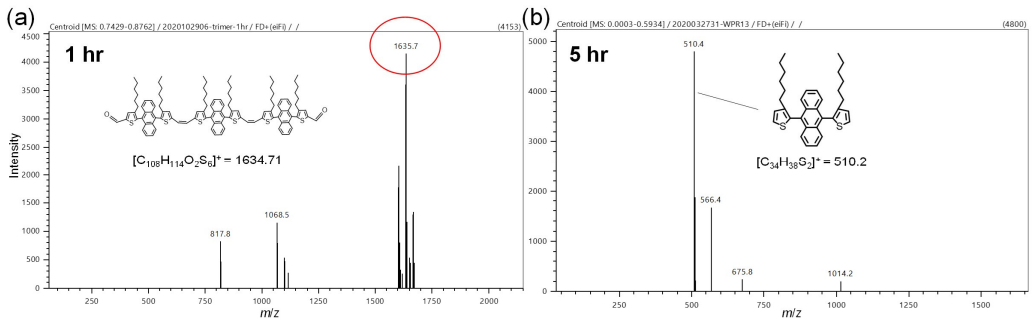


Fig. S32 LRFD of **4** after irradiation to its benzene solution at 365 nm for (a) 1 hour and (b) 5 hours. Fragmentation occurred.

3-3 Compound 5 in benzene solution

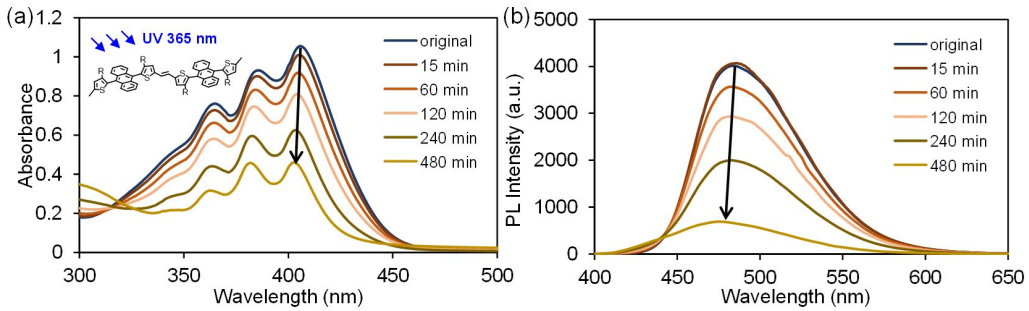


Fig. S33 (a) Time-dependent UV-vis spectra of **5** in benzene solution after irradiation at 365 nm. (b) Time-dependent PL spectra of **5** after irradiation at 365 nm. A mercury UV lamp (365 nm, 4 W cm^{-2}) was used.

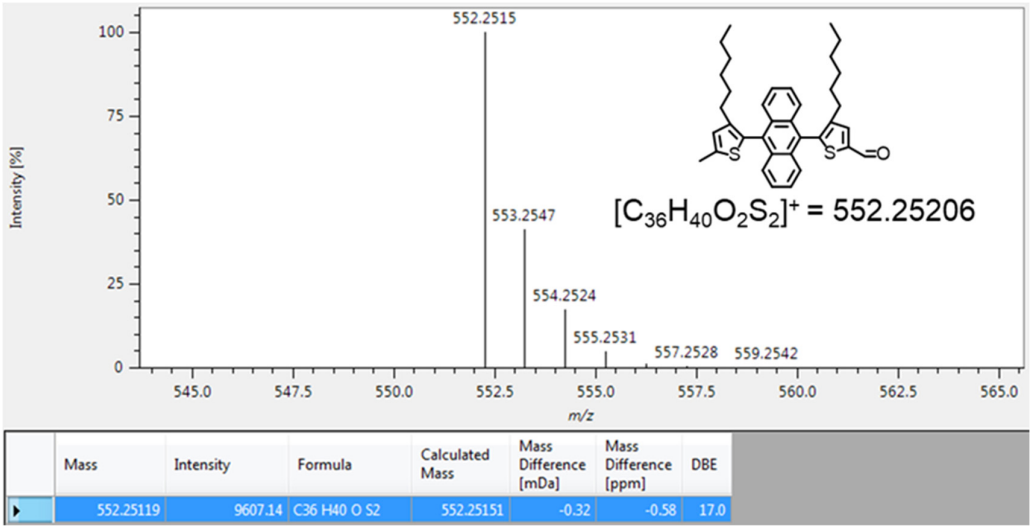


Fig. S34 HRFD of **5** after irradiation to its benzene solution at 365 nm for 8 hours. Fragmentation occurred.

3-4 Compound 6 in benzene solution

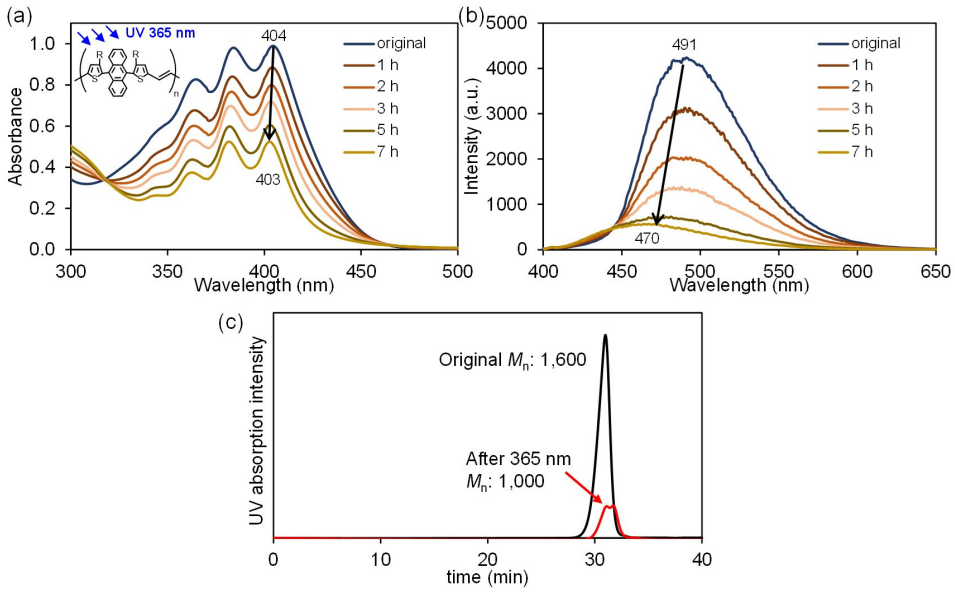


Fig. S35 (a) Time-dependent UV-vis spectra of **6** in benzene solution before and after irradiation at 365 nm. (b) Time-dependent PL spectra of **6** before and after irradiation at 365 nm. A mercury UV lamp (365 nm, 4 W cm^{-2}) was used. (c) GPC curves of **6** before and after photoirradiation. M_n significantly decreased after irradiation.

3-5 Compound 7 in benzene solution

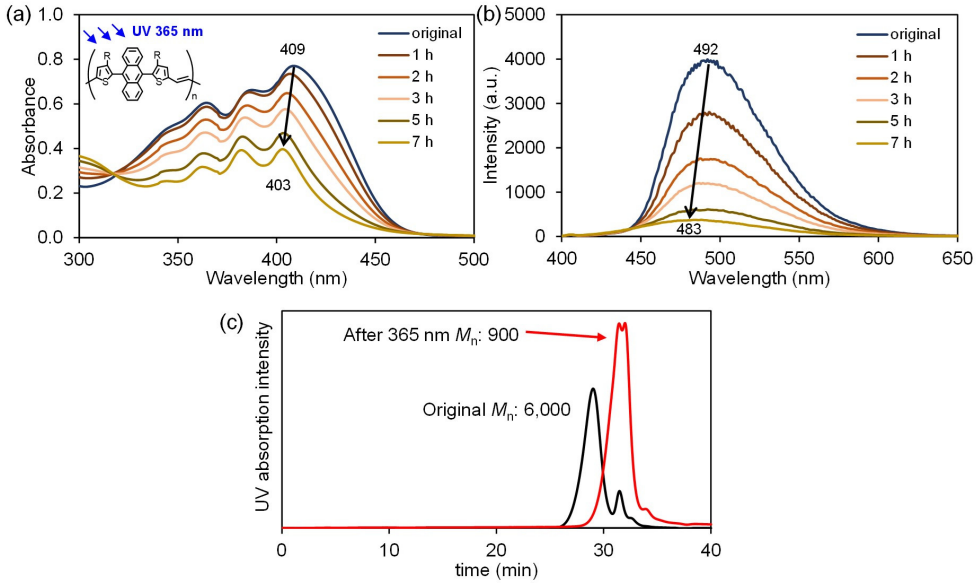


Fig. S36 (a) Time-dependent UV-vis spectra of **7** in benzene solution before and after irradiation at 365 nm. (b) Time-dependent PL spectra of **7** before and after irradiation at 365 nm. A mercury UV lamp (365 nm, 4 W cm^{-2}) was used. (c) GPC curves of **7** before and after photoirradiation. M_n significantly decreased after irradiation.

3-6 Compound 8 in benzene solution

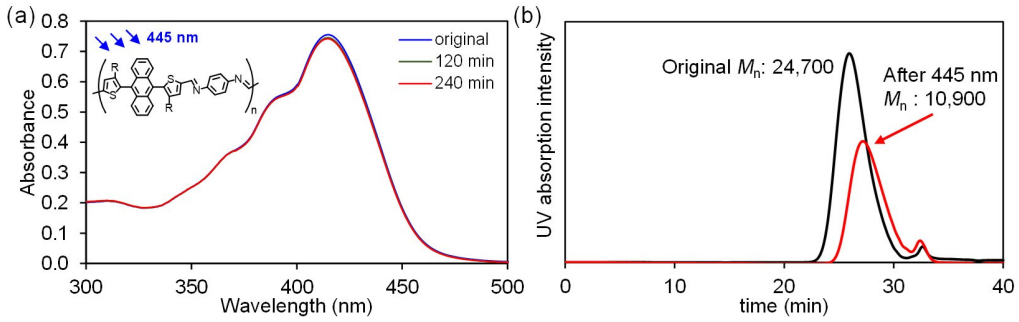


Fig. S37 (a) Time-dependent UV-vis spectra of **8** in benzene solution before and after irradiation at 365 nm. A 445-nm laser (7.7 mW cm^{-2}) was used. (b) GPC curves of **8** before and after photoirradiation. M_n significantly decreased after irradiation.

4. Photoirradiation to free-standing films

4-1 Free-standing film of 8

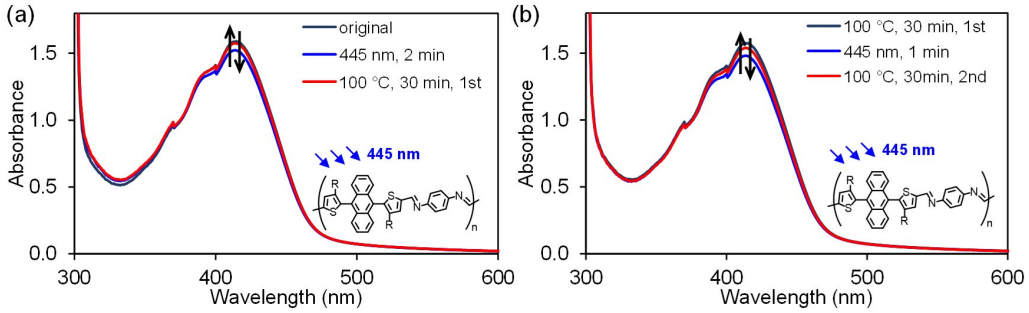


Fig. S38 UV-vis spectra of thin film of **8** after irradiation using a 445-nm laser (0.26 W cm^{-2}) and heating at 100 °C. (a) The first irradiation and heating at 100 °C. (b) The second irradiation and heating at 100 °C. Reversible change at absorption intensity around 420 nm was observed.

4-2 Free-standing film of 7

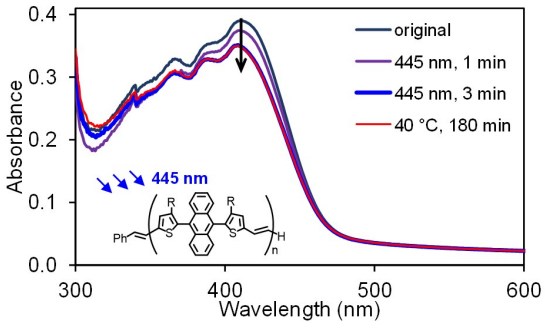


Fig. S39 UV-vis spectra of thin film of **7** after irradiation using a 445- nm laser (0.26 W cm^{-2}) and heating at 40 °C. Absorption intensity around 420 nm decreased.

5. Density functional calculations

5-1 Relative energies of 3

Table S2 Relative energies of conformers of **3** in gas phase. [a]

Compound	ΔH / kJ mol^{-1}	ΔG / kJ mol^{-1}
3a	3.4	3.0
3b	0.0	0.0
3c	3.1	0.6
3d	1.4	5.8
3e	91.1	92.7

[a] Calculated by ORCA 5.0.0 or 5.0.1, r^{2}SCAN-3c

Table S3 Relative energies of conformers of **3** in gas benzene. [a]

Compound	ΔH / kJ mol^{-1}	ΔG / kJ mol^{-1}
3a	0.0	0.0
3b	4.8	5.1
3c	11.5	9.4
3d	10.3	15.1
3e	86.3	88.2

[a] Calculated by ORCA 5.0.0 or 5.0.1, (SMD-)r^{2}SCAN-3c

5-2 Estimated UV–Vis spectra of 3

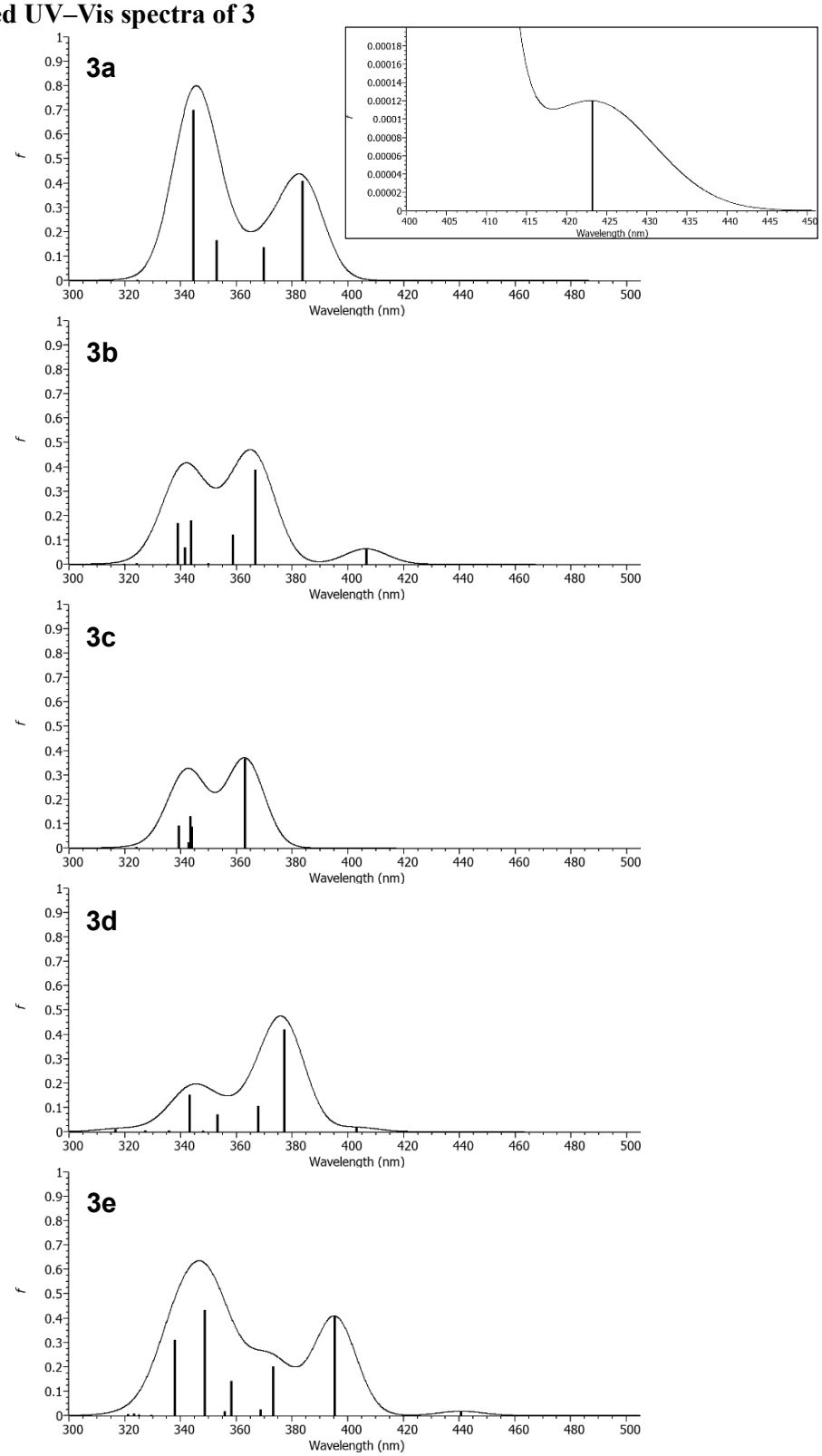


Fig. S40 UV-vis spectra of **3a-3e** calculated by ORCA 5.0.1, TDA-CAMh-B3LYP/def2-TZVP(-f)//r^{2}SCAN-3c. The spectra were broadened by Gaussian function (band width at 1/2 height was set to 18) using ChemCraft version 1.8.

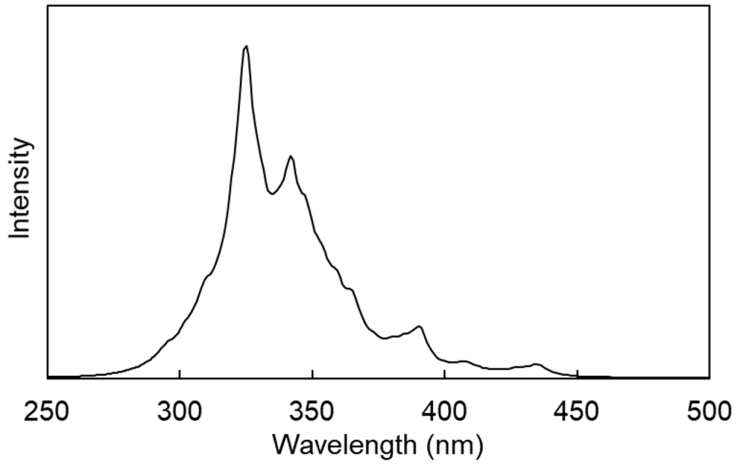


Fig. S41 Vibrational effect corrected UV-vis spectrum of **3a** calculated by VG method with DO approximation implemented in ORCA 5.0.1, TDA-CAMh-B3LYP/def2-SVP //r2SCAN-3c. The spectra were broadened by Voigt function (180 cm^{-1})

5-3 Detailed results of TD-DFT calculations of 3

Table S4 Calculated photophysical properties of **3a** at CAMh-B3LYP/def2-TZVP(−f)//r^{2}SCAN-3c.

State	Wavelength (nm)	Oscillator strength	Assignment			Ratio
1	423	0.00012	HOMO	→	LUMO	0.67
			HOMO−2	→	LUMO+1	0.14
2	384	0.41	HOMO	→	LUMO+1	0.81
			HOMO−2	→	LUMO	0.12
3	370	0.14	HOMO−1	→	LUMO+1	0.89
4	363	0.0000095	HOMO−1	→	LUMO	0.88
5	359	0.00024	HOMO	→	LUMO+3	0.21
			HOMO	→	LUMO	0.18
			HOMO−2	→	LUMO+1	0.15
6	353	0.16	HOMO−2	→	LUMO	0.55
			HOMO−3	→	LUMO+1	0.29
7	345	0.70	HOMO	→	LUMO+2	0.74
			HOMO−1	→	LUMO+3	0.18
8	340	0.00096	HOMO	→	LUMO+3	0.47
			HOMO−2	→	LUMO+1	0.32
9	327	0.00075	HOMO−2	→	LUMO+3	0.35
			HOMO−3	→	LUMO+1	0.26
10	324	0.0028	HOMO−3	→	LUMO	0.52
			HOMO−2	→	LUMO+1	0.11
			HOMO−1	→	LUMO+2	0.13
			HOMO	→	LUMO	0.10
11	322	0.00068	HOMO−2	→	LUMO+4	0.19
			HOMO−5	→	LUMO	0.17
			HOMO	→	LUMO+5	0.15
			HOMO−4	→	LUMO+1	0.13
12	320	0.000010	HOMO−2	→	LUMO+2	0.91

Table S5 Calculated photophysical properties of **3b** at CAMh-B3LYP/def2-TZVP(−f)//r^{2}SCAN-3c.

State	Wavelength (nm)	Oscillator strength	Assignment			Ratio
1	407	0.063	HOMO	→	LUMO	0.72
2	367	0.39	HOMO−1	→	LUMO+1	0.40
			HOMO−1	→	LUMO	0.27
			HOMO	→	LUMO	0.11
3	359	0.12	HOMO−2	→	LUMO	0.87
4	352	0.00085	HOMO	→	LUMO+1	0.68
			HOMO−3	→	LUMO+1	0.13
5	350	0.0048	HOMO−1	→	LUMO	0.44
			HOMO−3	→	LUMO	0.21
6	344	0.18	HOMO	→	LUMO+2	0.25
			HOMO−2	→	LUMO+1	0.50
7	342	0.068	HOMO−3	→	LUMO	0.46
			HOMO−1	→	LUMO+1	0.19
			HOMO−1	→	LUMO	0.18
8	339	0.17	HOMO−2	→	LUMO+1	0.38
			HOMO	→	LUMO+2	0.31
			HOMO−2	→	LUMO+3	0.17
9	336	0.0016	HOMO	→	LUMO+3	0.35
			HOMO−3	→	LUMO	0.20
			HOMO−2	→	LUMO+2	0.16
			HOMO−1	→	LUMO+1	0.12
10	324	0.0032	HOMO−1	→	LUMO+2	0.84
11	320	0.00024	HOMO−1	→	LUMO+3	0.67
			HOMO−3	→	LUMO+1	0.15
12	320	0.0016	HOMO−3	→	LUMO+1	0.29
			HOMO−1	→	LUMO+3	0.22
			HOMO	→	LUMO+3	0.16
			HOMO−3	→	LUMO+3	0.12

Table S6 Calculated photophysical properties of **3c** at CAMh-B3LYP/def2-TZVP(−f)//r^{2}SCAN-3c.

State	Wavelength (nm)	Oscillator strength	Assignment			Ratio
1	384	0.000000001	HOMO	→	LUMO+1	0.43
			HOMO−1	→	LUMO	0.28
			HOMO−2	→	LUMO+3	0.13
			HOMO−3	→	LUMO+2	0.13
2	363	0.37	HOMO	→	LUMO	0.86
3	347	0.00000010	HOMO−1	→	LUMO	0.48
			HOMO	→	LUMO+1	0.43
4	344	0.0000022	HOMO−2	→	LUMO	0.84
5	344	0.089	HOMO−1	→	LUMO+1	0.38
			HOMO−2	→	LUMO+1	0.26
6	344	0.13	HOMO−1	→	LUMO+1	0.38
			HOMO−3	→	LUMO	0.21
			HOMO−2	→	LUMO+2	0.14
			HOMO−3	→	LUMO+3	0.13
7	343	0.024	HOMO−3	→	LUMO	0.60
			HOMO−2	→	LUMO+1	0.17
8	340	0.0000020	HOMO−3	→	LUMO+1	0.84
9	339	0.092	HOMO−2	→	LUMO+1	0.43
			HOMO−2	→	LUMO+2	0.20
			HOMO−3	→	LUMO+3	0.17
10	337	0.00000031	HOMO−3	→	LUMO+2	0.32
			HOMO−2	→	LUMO+3	0.31
			HOMO−1	→	LUMO	0.15
11	326	0.000000002	HOMO	→	LUMO+2	0.92
12	324	0.0048	HOMO	→	LUMO+3	0.92

Table S7 Calculated photophysical properties of **3d** at CAMh-B3LYP/def2-TZVP(−f)//r^{2}SCAN-3c.

State	Wavelength (nm)	Oscillator strength	Assignment			Ratio
1	403	0.018	HOMO−1	→	LUMO	0.54
			HOMO	→	LUMO+1	0.28
2	377	0.42	HOMO	→	LUMO	0.40
			HOMO	→	LUMO+1	0.29
			HOMO−1	→	LUMO	0.25
3	368	0.11	HOMO	→	LUMO	0.56
			HOMO	→	LUMO+1	0.31
4	353	0.071	HOMO−2	→	LUMO	0.75
			HOMO−1	→	LUMO+1	0.10
5	348	0.0032	HOMO−1	→	LUMO+1	0.55
			HOMO−2	→	LUMO+1	0.24
			HOMO−2	→	LUMO	0.11
6	343	0.15	HOMO−1	→	LUMO+2	0.44
			HOMO−2	→	LUMO+2	0.28
7	336	0.0057	HOMO	→	LUMO+2	0.87
8	330	0.00078	HOMO−3	→	LUMO	0.72
9	327	0.0064	HOMO−2	→	LUMO+1	0.52
			HOMO−1	→	LUMO+1	0.25
			HOMO−3	→	LUMO	0.11
10	323	0.00090	HOMO	→	LUMO+5	0.22
			HOMO−8	→	LUMO+1	0.19
			HOMO−4	→	LUMO+1	0.13
			HOMO	→	LUMO+6	0.12
11	321	0.00062	HOMO−9	→	LUMO	0.35
			HOMO−1	→	LUMO+4	0.35
12	317	0.0095	HOMO−2	→	LUMO+2	0.47
			HOMO−1	→	LUMO+2	0.39

Table S8 Calculated photophysical properties of **3e** at CAMh-B3LYP/def2-TZVP(−f)//r^{2}SCAN-3c.

State	Wavelength (nm)	Oscillator strength	Assignment			Ratio
1	441	0.018	HOMO	→	LUMO	0.74
			HOMO−1	→	LUMO+1	0.11
2	395	0.41	HOMO	→	LUMO+1	0.79
3	373	0.2	HOMO−2	→	LUMO	0.84
4	369	0.024	HOMO−2	→	LUMO+1	0.78
			HOMO−1	→	LUMO+1	0.11
5	358	0.14	HOMO−1	→	LUMO	0.41
			HOMO−3	→	LUMO+1	0.18
6	356	0.016	HOMO−3	→	LUMO	0.22
			HOMO−1	→	LUMO	0.19
			HOMO−1	→	LUMO+1	0.12
			HOMO	→	LUMO	0.10
			HOMO	→	LUMO+3	0.10
7	349	0.43	HOMO	→	LUMO+2	0.51
			HOMO−1	→	LUMO+1	0.23
8	338	0.31	HOMO	→	LUMO+3	0.53
			HOMO	→	LUMO+2	0.18
			HOMO−1	→	LUMO+1	0.10
9	330	0.0015	HOMO−3	→	LUMO+1	0.18
			HOMO−1	→	LUMO+3	0.16
			HOMO−3	→	LUMO	0.12
10	325	0.0039	HOMO−1	→	LUMO+4	0.14
			HOMO−7	→	LUMO	0.13
			HOMO	→	LUMO+5	0.12
11	323	0.0082	HOMO−3	→	LUMO	0.29
			HOMO−1	→	LUMO+5	0.11
12	321	0.0056	HOMO−1	→	LUMO+2	0.32
			HOMO−3	→	LUMO	0.14
			HOMO−3	→	LUMO+1	0.12

5-4 Molecular orbitals of 3

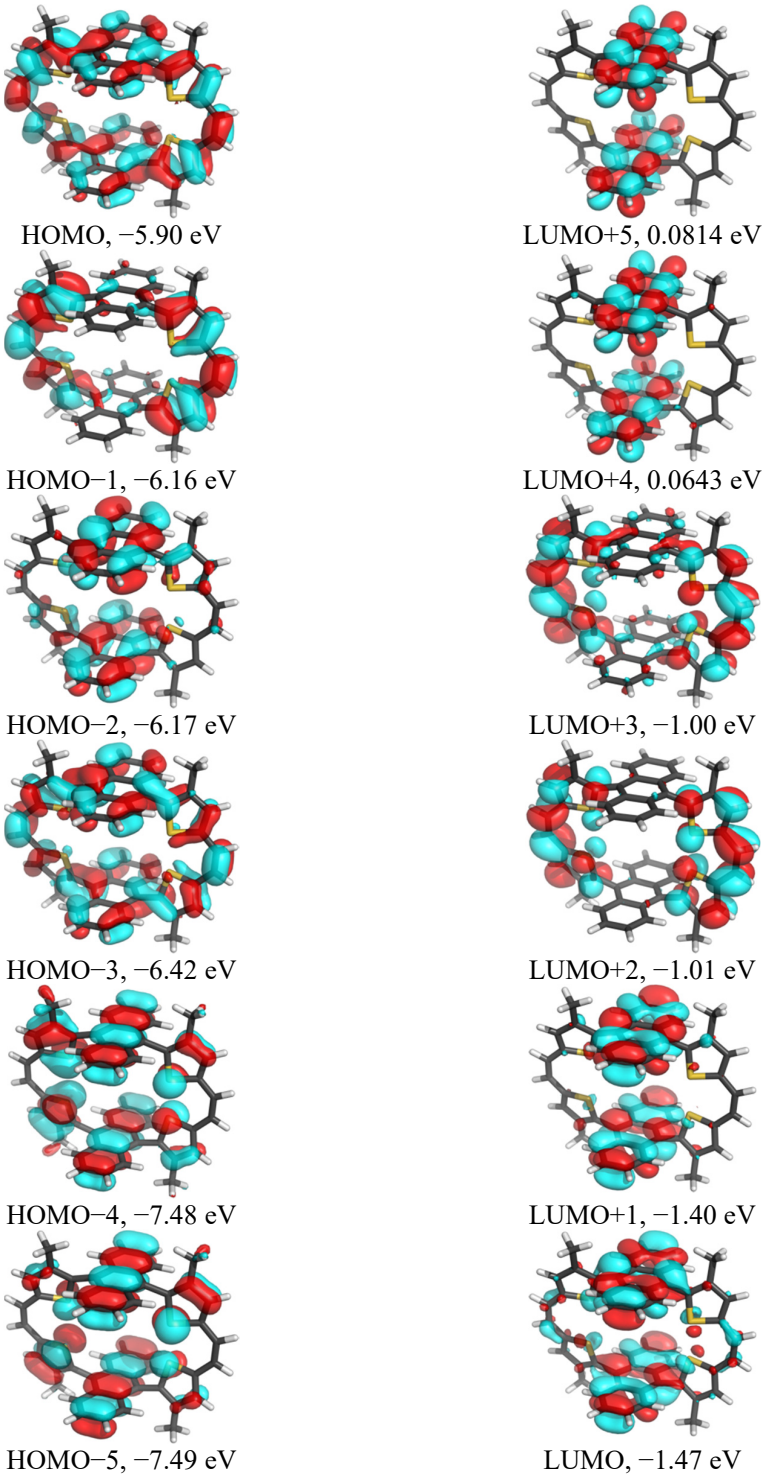


Fig. S42 Molecular orbitals (Kohn–Sham orbitals) of **3a** calculated at CAMh-B3LYP/def2-TZVP(−f)//r^{2}SCAN-3c.

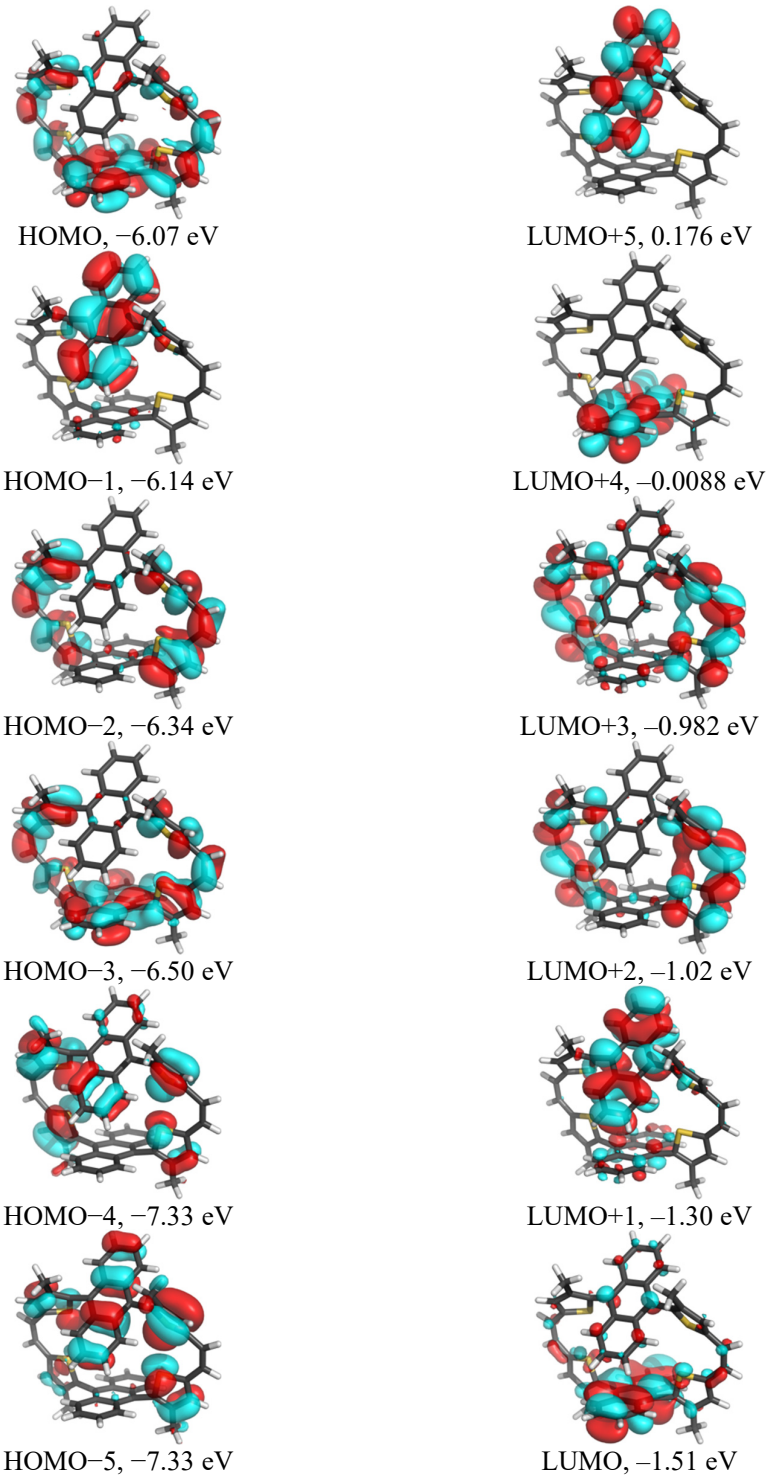


Fig. S43 Molecular orbitals (Kohn–Sham orbitals) of **3b** calculated at CAMh-B3LYP/def2-TZVP(−f)//r^{2}SCAN-3c.

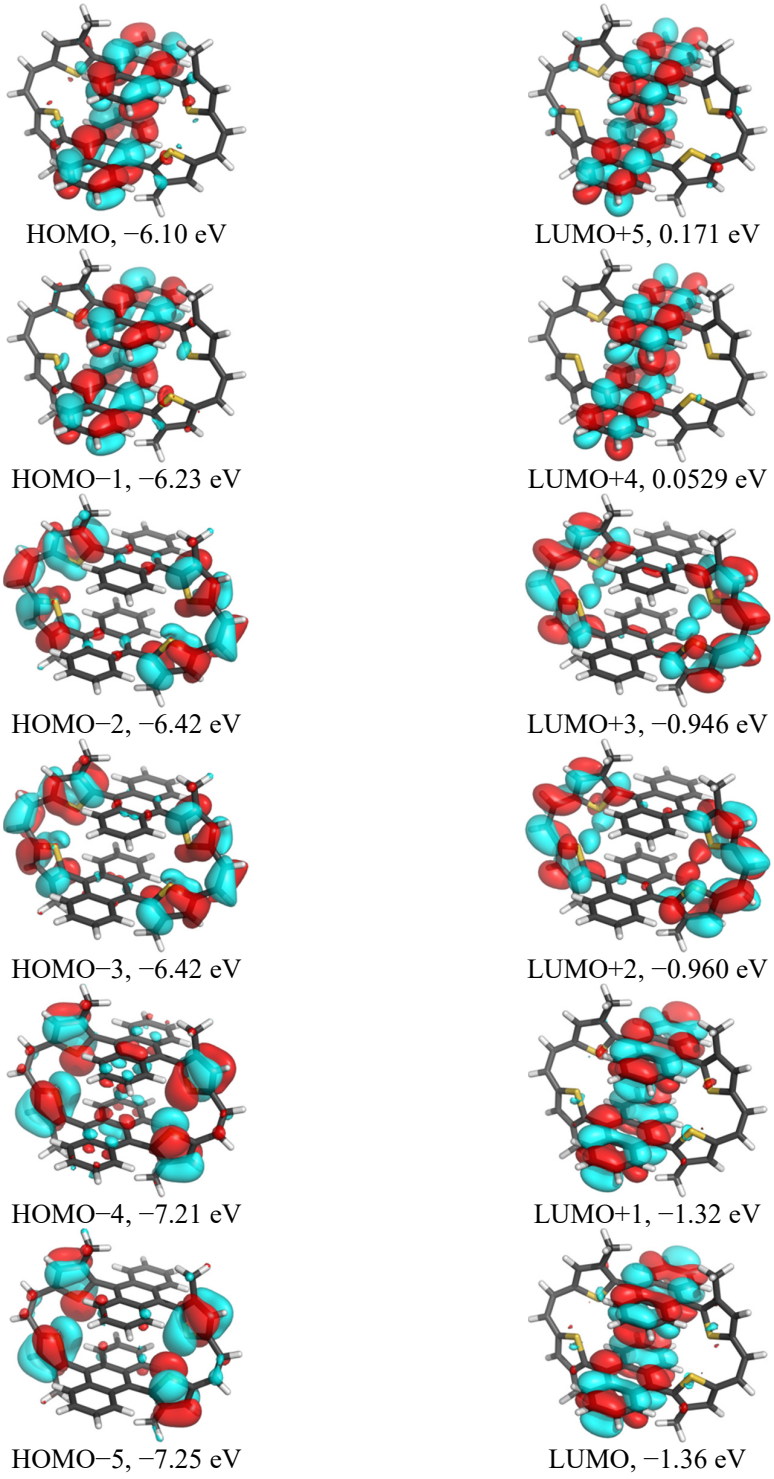


Fig. S44 Molecular orbitals (Kohn–Sham orbitals) of **3c** calculated at CAMh-B3LYP/def2-TZVP(−f)//r^{2}SCAN-3c.

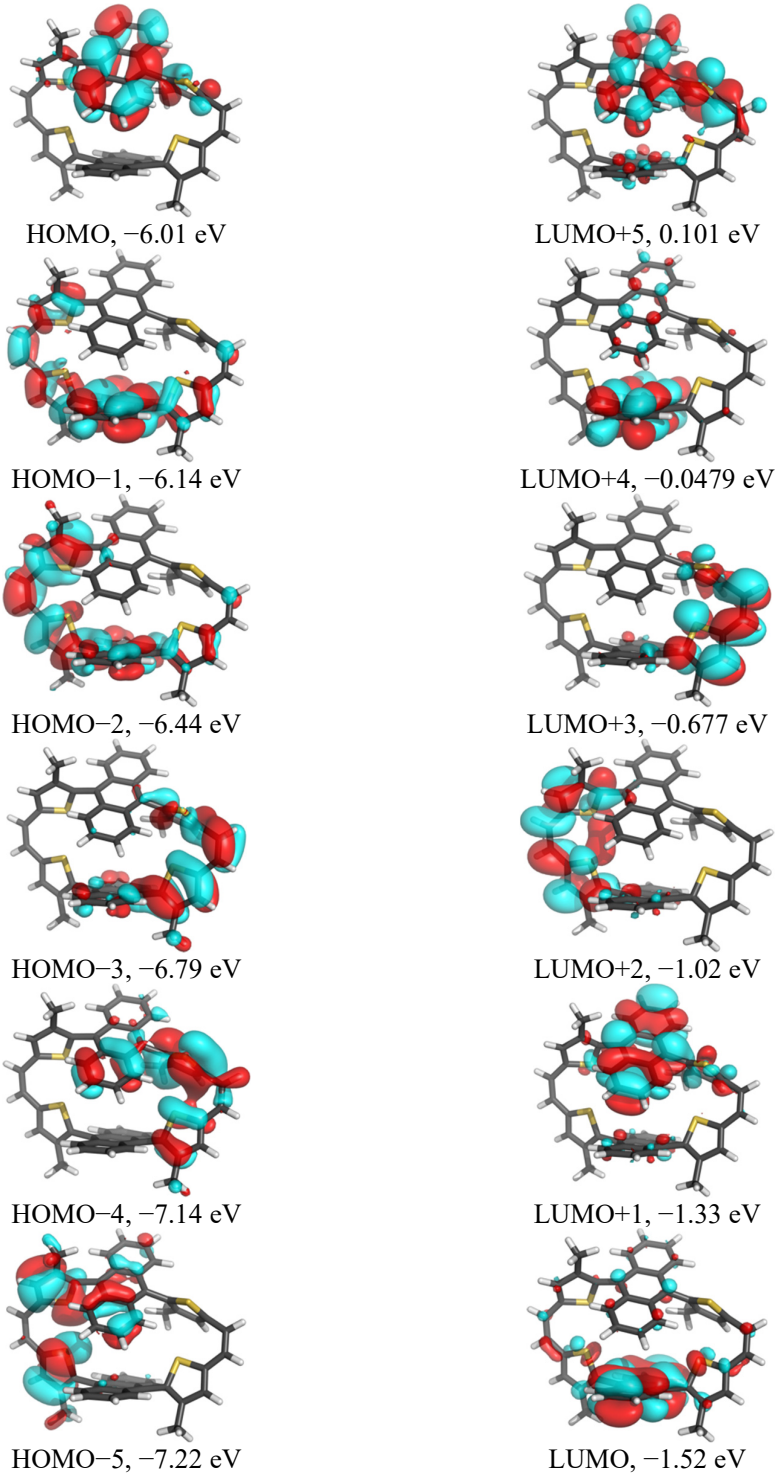
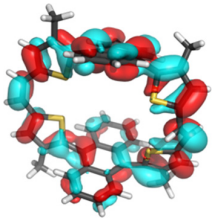
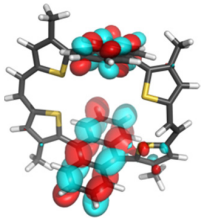


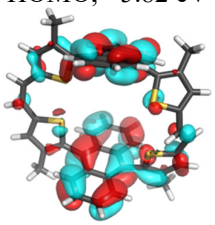
Fig. S45 Molecular orbitals (Kohn–Sham orbitals) of **3d** calculated at CAMh-B3LYP/def2-TZVP(−f)//r^{2}SCAN-3c.



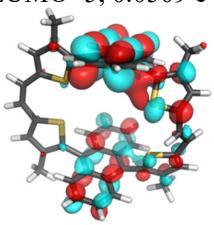
HOMO, −5.82 eV



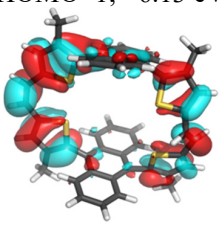
LUMO+5, 0.0509 eV



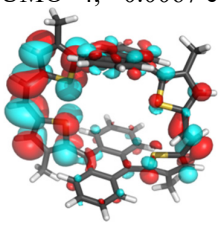
HOMO−1, −6.13 eV



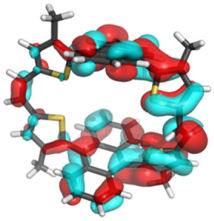
LUMO+4, −0.0067 eV



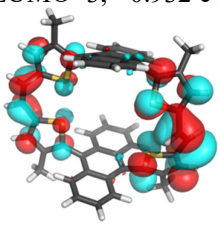
HOMO−2. −6.15 eV



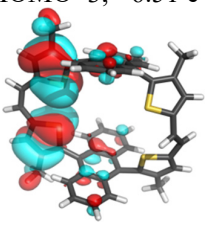
LUMO+3, −0.932 eV



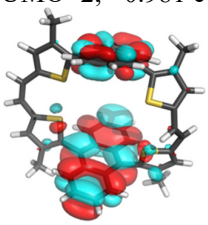
HOMO−3, −6.51 eV



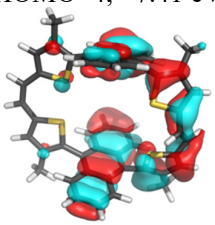
LUMO+2, −0.981 eV



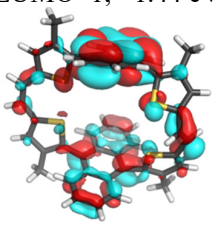
HOMO−4, −7.41 eV



LUMO+1, −1.44 eV



HOMO−5, −7.49 eV



LUMO, −1.51 eV

Fig. S46 Molecular orbitals (Kohn–Sham orbitals) of **3e** calculated at CAMh-B3LYP/def2-TZVP(−f)//r^{2}SCAN-3c.

5-5 Activation energy of 3

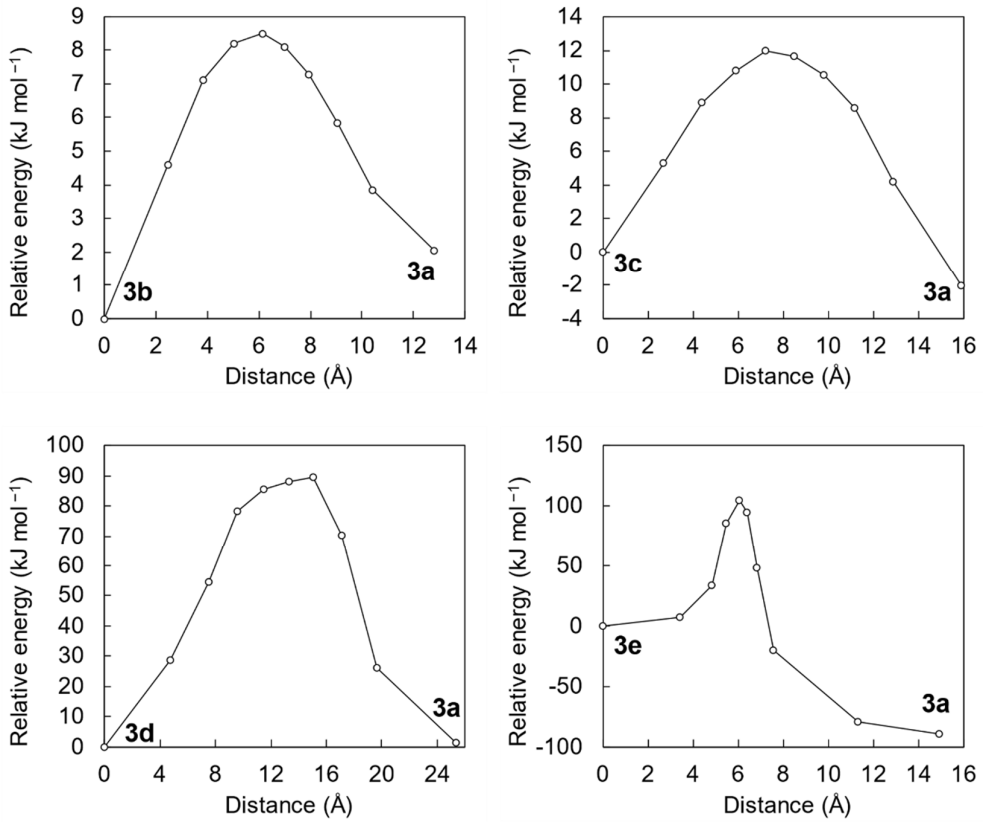


Fig. S47 Activation energies between conformers **3a**-**3e** calculated by EW-CI-NEB method using ORCA 5.0.1 at the r^{2}SCAN-3c for **3a**-**3d** and U-r^{2}SCAN-3c for **3e**.

6. Force measurements

6-1 Single-crystal of 3

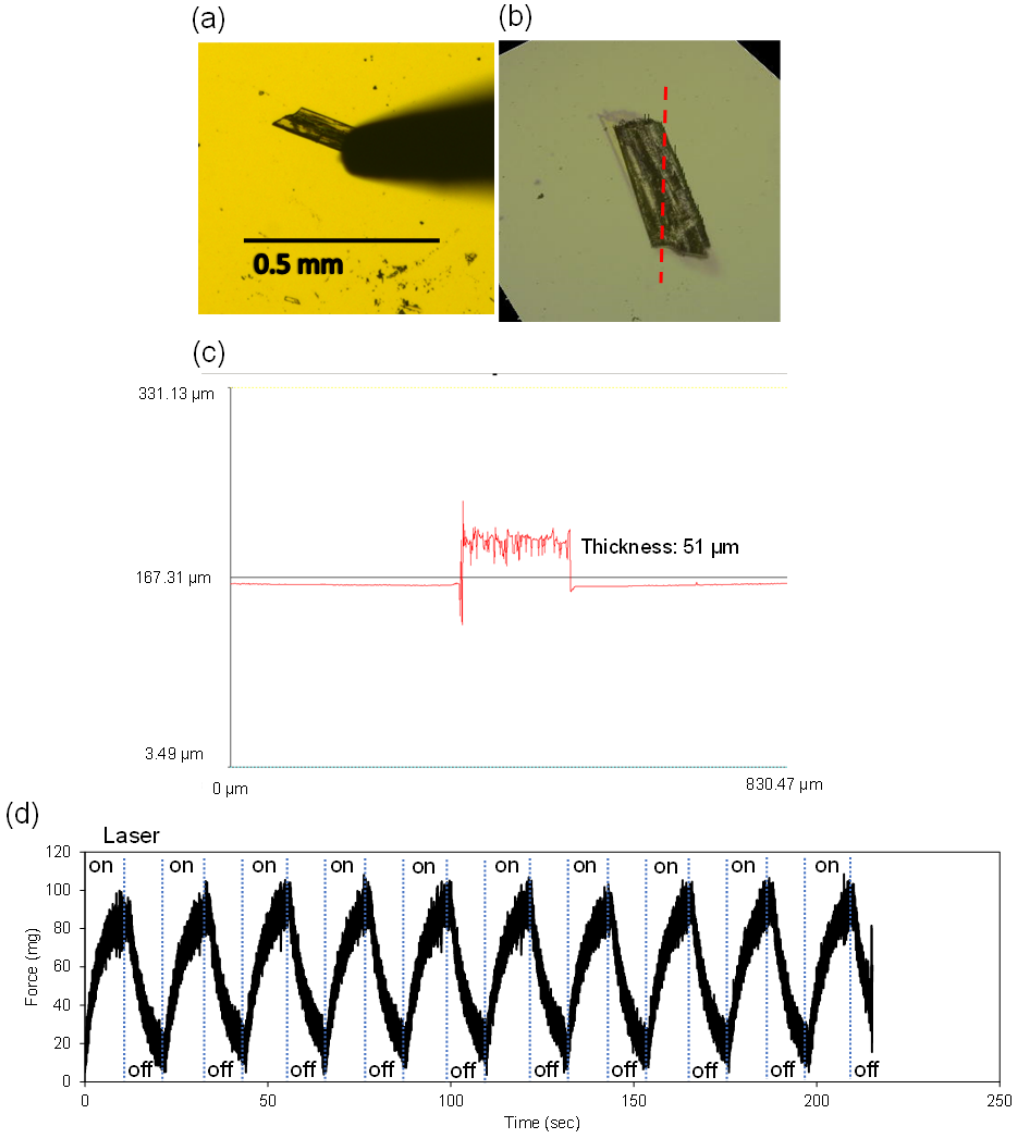


Fig. S48 (a) Optical micrograph of a single-crystal of **3**. (b) Confocal microscopic image and (c) its cross section. (d) Time-dependent force detection produced by the single-crystal of **3** induced by 445-nm laser irradiation (0.18 W cm^{-2}) on/off.

6-2 Free-standing film of 7

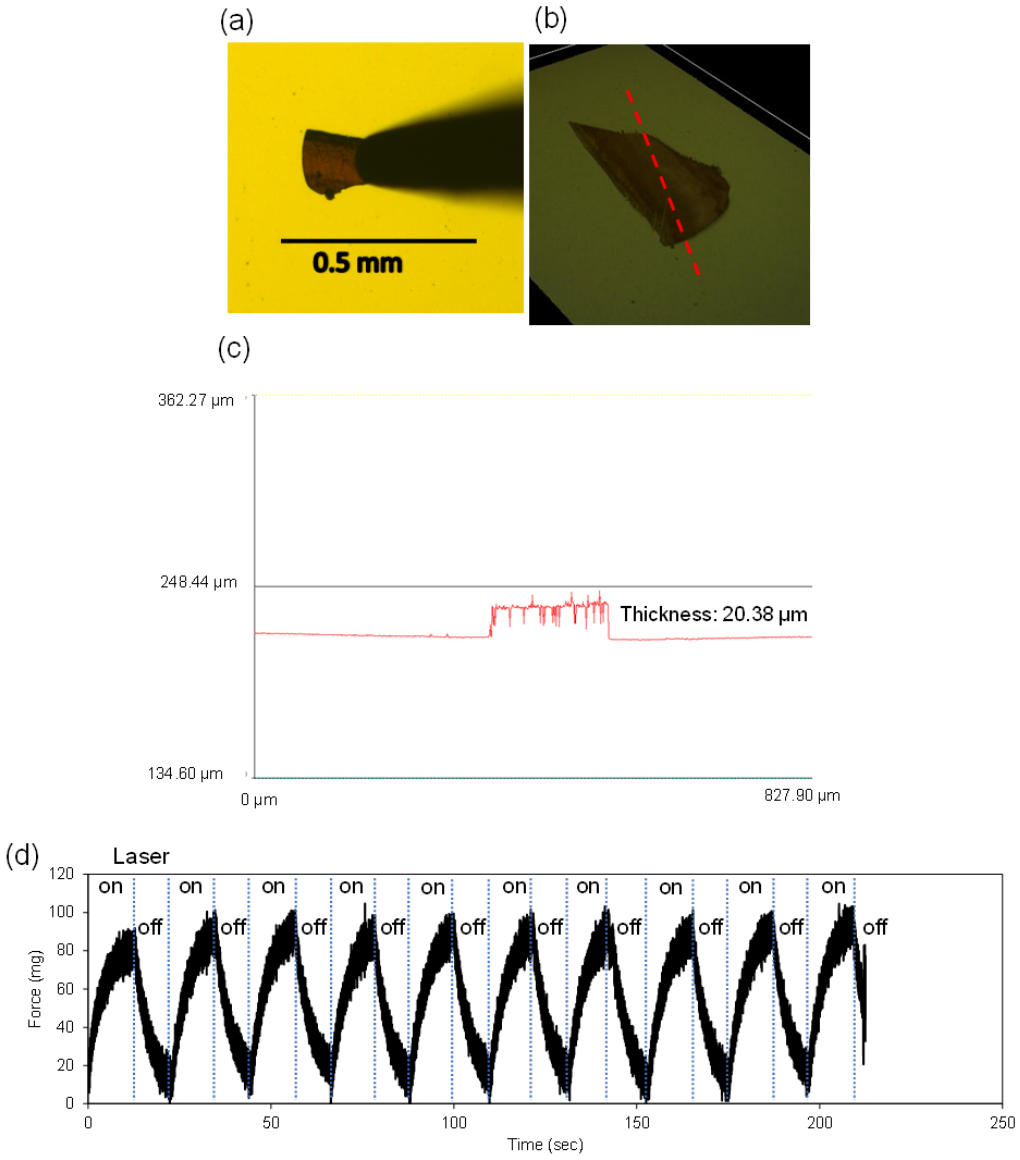


Fig. S49 (a) Optical micrograph of a free-standing film of **7**. (b) Confocal microscopic image and (c) its cross section. (d) Time-dependent force detection produced by the film of **7** induced by 445-nm laser irradiation (0.18 W cm^{-2}) on/off

6-3 Free-standing film of 8

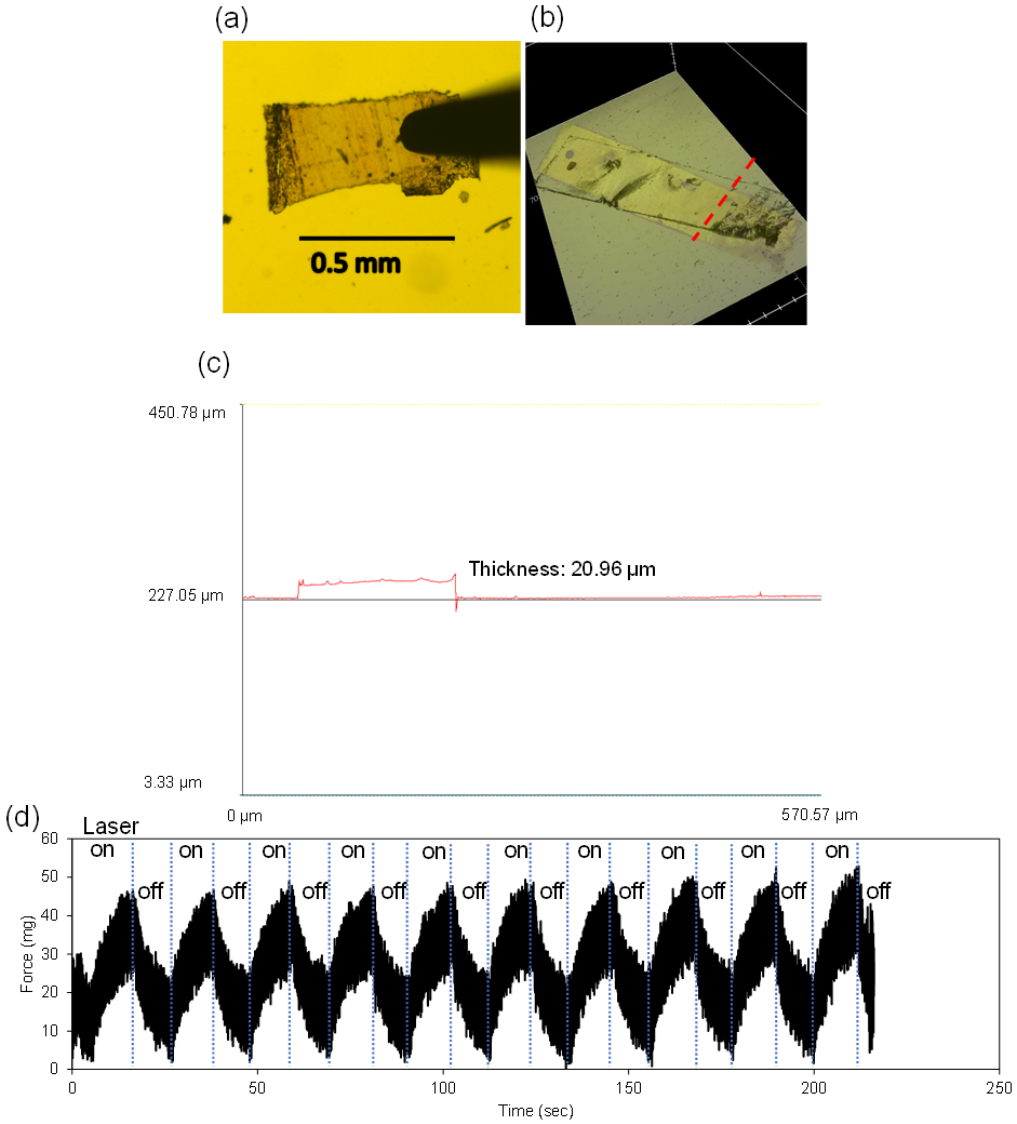


Fig. S50 (a) Optical micrograph of a free-standing film of **8**. (b) Confocal microscopic image and (c) its cross section. (d) Time-dependent force detection produced by the film of **7** induced by 445-nm laser irradiation (0.23 W cm^{-2}) on/off.

7. DSC

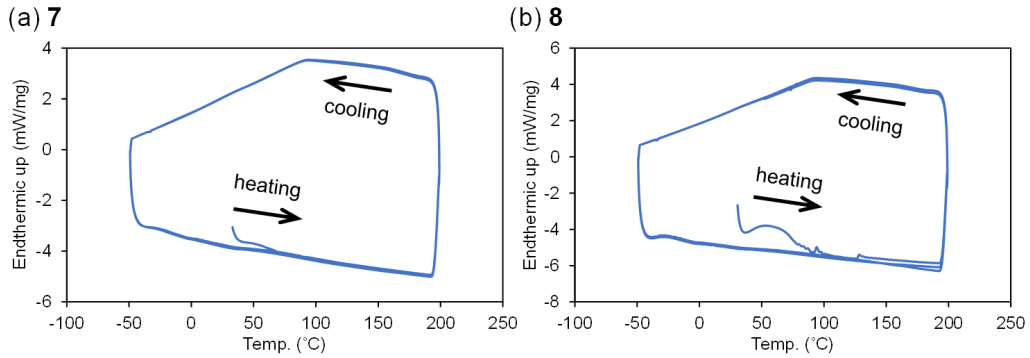


Fig. S51 DSC charts of a piece of a free-standing film of (a) **7** and (b) **8**. An endothermic signal was observed at 47 °C and 51 °C for **7** and **8**, respectively, in the first heating scan.

8. X-ray diffraction

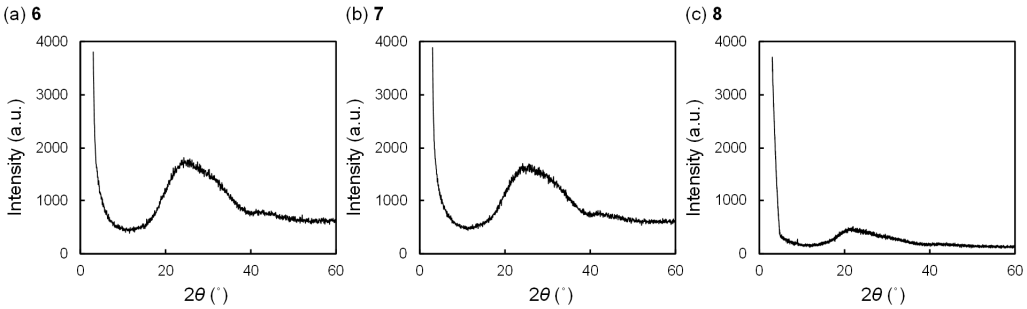


Fig. S52 X-ray diffraction patterns of a drop-casted film of (a) **6**, (b) **7**, and (b) **8** on a glass substrate. A broad and weak peak was observed at 2 theta = 25°, 25°, and 22° for **6**, **7**, and **8**, respectively, suggesting less crystalline or amorphous properties of the polymers.

9. Polarized optical microscopy

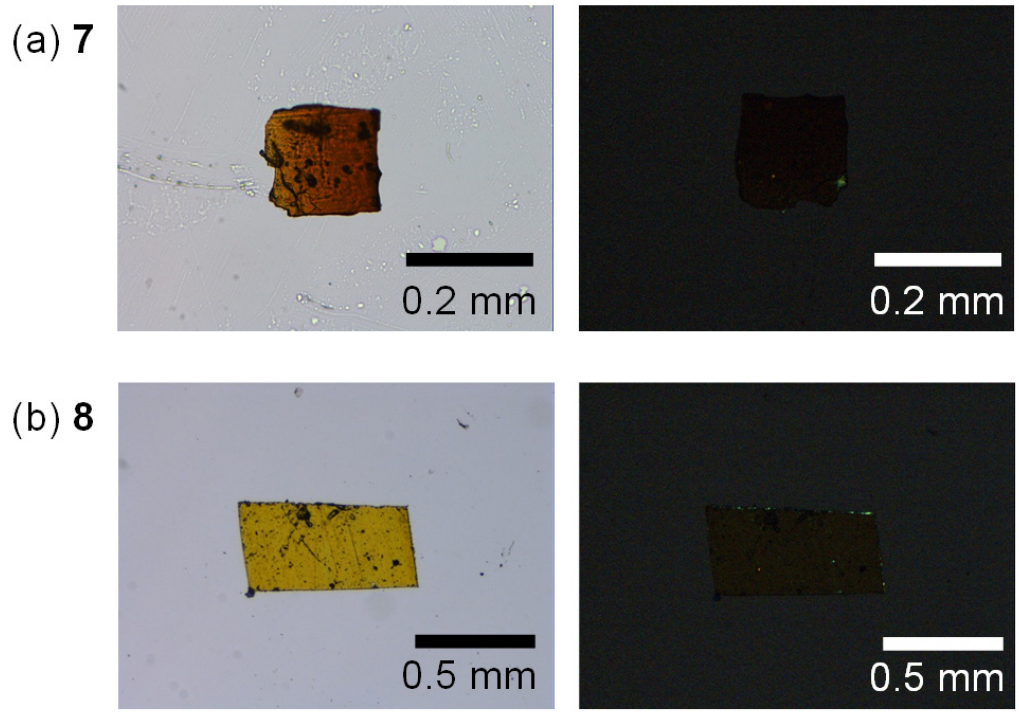


Fig. S53 (a) Optical micrographs of a free-standing film of (a) **7** and (b) **8** without (left) and with polarized light (right). Ordered structures or crystalline domains were not observed in these films.

10. Cartesian coordinate of the optimized structure

3a, r^2SCAN-3c geometry

S	-0.27976393862800	2.97022911680723	-1.91003622721151
S	-2.89737562939444	1.41490801542630	-1.46869210478888
S	2.74367638759501	-1.19467422852963	1.89934527295904
S	0.43251152176716	-3.18667847290998	1.48348790539492
C	-2.20969679671895	-3.16969018322497	-0.58206017776082
C	-2.88620703417636	-2.19690879292228	-1.40218681825661
C	2.93307114811517	2.13615995502162	-1.44150640693311
C	2.23864249477130	3.12092750975889	0.68176960329760
C	3.65082950782522	1.10412892915846	-0.73665830770933
C	1.13833873803243	3.86632872178004	-1.42881152731160
C	-2.99631343567334	-2.03704601145818	1.43257983818828
C	2.99323523873574	2.11491973569629	1.38603816059038
C	2.16947506003803	3.08113111313433	-0.72633108456847
C	1.00098267850787	-4.26629177511147	2.73307995307638
C	-3.05844678870413	-1.88627427850365	2.84734449392883
H	-2.48191013662562	-2.56533424491568	3.46672950587814
C	-2.76660895106282	-2.30552786567469	-2.81711332768275
H	-3.23255735804703	-1.54578480455119	-3.43605452805792
C	-3.57976564148746	-1.13208851878959	-0.79072435489882
C	-1.50815902272164	-4.23065514258288	-1.22310816191687
H	-1.01775300476979	-4.97359863661630	-0.60171104230671
C	-2.20429155061493	-3.03068126367201	0.82082391248012
C	-3.70948443904322	-1.09066558923802	0.61237030504678
C	-1.20831858070114	-3.76529384518163	1.62207091135834
C	2.97096980762945	2.14063411701345	-2.86531977836666
H	2.44647269679345	2.93207686083140	-3.39171807957525
C	-3.96722743737824	0.04202386004872	-1.59400380867393
C	4.04128242479007	-0.14800396415047	1.38358557909415
C	3.62028748413251	1.07319873694831	0.67295844986457
C	-0.05917499599255	-5.03774255857018	3.18162765507404
H	0.06810256835835	-5.79665243862344	3.94839346891569
C	4.31130031754677	0.09887130740435	-1.49926856964349
H	4.81027128325137	-0.70683718518136	-0.97101213024698
C	-1.31069667585982	-4.75186634174410	2.57512605743882
C	-3.75238502151683	2.29328479297638	-2.71274751664300

C	-4.94400527840237	0.25504171027690	-2.53870543485616
C	2.35831107253289	-4.40652884048161	3.19618641751812
H	2.47412619938485	-5.30718953847507	3.79847516775146
C	-1.45854799558874	-4.32395417953673	-2.58586628918891
H	-0.92925205654608	-5.14822065106955	-3.05487647719851
C	4.32297159755993	0.14095211459761	-2.86580959043086
H	4.84109323404162	-0.63143247351108	-3.42683497949295
C	-2.08285794684977	-3.34065430736485	-3.39194528111844
H	-2.01241513024951	-3.40847313111250	-4.47370422029796
C	0.99050757538709	5.20973000219086	-1.68505955022522
C	-1.10261421144891	4.41221297087151	-2.45167403334431
C	3.85203980115495	-2.43439267139982	2.43290164811674
C	-3.45784572825549	3.62314680307600	-3.18290306974141
H	-4.28134101280772	4.01808821127029	-3.77728218600834
C	-4.82414034281094	1.53120737313270	-3.14958244952509
H	-5.51056277065384	1.89009386227836	-3.91122046215054
C	1.52162501965489	4.08554834443652	1.44562484574829
H	0.91180820471263	4.81312525419978	0.92027379914758
C	3.50493566351041	-3.68919517978348	3.05059497042404
H	4.37866550875518	-4.15559778330828	3.50495897466693
C	3.65739855836785	1.18263655213059	-3.55758177878496
H	3.68476268095988	1.21174541372607	-4.64293436798810
C	3.03970869618295	2.16991950672436	2.80851657777217
H	3.62586215487327	1.42229977221666	3.33394896117133
C	2.37494770568408	3.14318783193452	3.50063397496360
H	2.43416436113500	3.17556290430957	4.58462430905035
C	-0.26671942725545	5.50343497199674	-2.27583548055487
H	-0.56588105287973	6.50703737503883	-2.56449289562307
C	-2.41037465288425	4.48135397111947	-3.05268559595490
H	-2.57888426175028	5.45624874309099	-3.50939398146120
C	1.59449327809124	4.10319592827940	2.81086094733346
H	1.04670138517783	4.85435987048101	3.37251906582621
C	-2.59503393836791	-5.43875841219666	2.93199445041035
H	-3.41642157526797	-5.07535419723771	2.30867773404149
H	-2.86068204112595	-5.26284100926824	3.98103327921127
C	2.03456973796605	6.23986569875219	-1.37271130167929
H	2.92408778833186	5.77352650807740	-0.94085435826538
H	1.65825926095324	6.98182649142164	-0.65874598898699

C	-4.49404727720158	-0.08944713411317	1.25312752970443
H	-5.04552023825402	0.60862317536964	0.63096667080165
C	-3.82516119894188	-0.91076220516083	3.42189500788801
H	-3.86489717330445	-0.82040958189235	4.50357574241113
C	-4.56408690646096	-0.01032426322244	2.61584902695996
H	-5.17867609745641	0.75251732732250	3.08482411747654
C	-6.00535285493503	-0.74679773574185	-2.88339168612966
H	-2.51127505669603	-6.52233057895203	2.79291638961914
C	5.15150954683267	-1.99790468783752	2.23030637119032
H	6.00973991720148	-2.60277263001367	2.50892767533753
C	5.26918611034847	-0.71953744821931	1.62367299702779
H	2.33504673278259	6.77976140718982	-2.27763471848858
C	6.57507453858985	-0.06787224307924	1.27881237115972
H	7.14802107454844	-0.67895329415049	0.57166473335710
H	6.41126770952703	0.91334238920172	0.82547786036830
H	7.19462360294825	0.06552026194882	2.17270769835544
H	-7.00538844253595	-0.33283547134274	-2.71235458731650
H	-5.94761422993065	-1.03778800669509	-3.93876148159117
H	-5.89961473710820	-1.64933772135023	-2.27558818844041

3a, CAMh-B3LYP/def2-SVP ground-state geometry

S	-0.32334284000366	3.06733042874322	-1.69232352037000
S	-2.83523346656117	1.31509530342955	-1.59713807201579
S	2.79692157055441	-1.26191007184531	1.69135100346342
S	0.33186461010346	-3.08448614207556	1.65589162325960
C	-2.26886134897836	-3.18220875904943	-0.62256743515280
C	-2.97373105368994	-2.18832832582322	-1.39141842138586
C	3.00393905805486	2.12881258549390	-1.44539600700683
C	2.27914542407425	3.18610892409591	0.63618892930700
C	3.71721843337641	1.13006625580050	-0.69064847853229
C	1.20346049043061	3.87327741754968	-1.52378591433243
C	-3.02396053432278	-2.12024037462762	1.44590413536173
C	2.99506927540951	2.18916944240958	1.39099922822237
C	2.23183266029336	3.10226415451353	-0.77325940777498
C	1.01326368475259	-4.36556813628196	2.60891211897278
C	-3.08540164298394	-2.04483452845249	2.87629199864839
H	-2.53612333621797	-2.78544317896003	3.45835714545034
C	-2.91710773558513	-2.26906281213413	-2.82174746171842

H	-3.43501462775580	-1.50702205791093	-3.40470953647609
C	-3.64211272042184	-1.13213086944132	-0.73252801531802
C	-1.55607300768758	-4.20897842298469	-1.32489450480926
H	-1.01906980427826	-4.95774639456414	-0.74182727296886
C	-2.24022397450671	-3.09340427497307	0.78704763872602
C	-3.73438062162841	-1.13011021109316	0.67715377679499
C	-1.21739580881703	-3.85790822911593	1.55139541180564
C	3.05026384143985	2.06336103788491	-2.87688360901490
H	2.50405186423880	2.81502442738760	-3.44769322092358
C	-4.04634836788935	0.07711320357734	-1.50031914496750
C	4.05334576824983	-0.08476447995038	1.47808917451761
C	3.64639838635012	1.13003106571964	0.72043838388030
C	0.04915534858708	-5.33726813038888	2.81310061392433
H	0.25357948204735	-6.24361737428634	3.38720349653188
C	4.43193673484075	0.11577601950337	-1.40882582132138
H	4.95930933651016	-0.64868951155906	-0.83769830654365
C	-1.22217207751263	-5.06182940135621	2.22002261502921
C	-3.83069277144912	2.34559294180794	-2.57789459213109
C	-5.18331296729212	0.43433384202423	-2.19079540741044
C	2.37315142757328	-4.44461114969287	3.12290831576933
H	2.52031043652789	-5.38466519740786	3.66463114536529
C	-1.55126805504316	-4.26368382367564	-2.69022866496415
H	-1.01139524572493	-5.06239769848415	-3.20377824507191
C	4.46517405497992	0.10194858278167	-2.77488200941059
H	5.02526188378946	-0.67473286527555	-3.30042628786720
C	-2.24061138136034	-3.27631843410998	-3.45054918221663
H	-2.22059232414982	-3.32346957365097	-4.54163781437163
C	1.18274623173358	5.11479164711852	-2.11935751163331
C	-1.03145784502550	4.38780655905450	-2.56906348503750
C	3.83658018516699	-2.35596499824896	2.55000518467543
C	-3.48268313472150	3.65819204596094	-3.10369952476219
H	-4.33348084947327	4.08865644087587	-3.64211232806271
C	-5.04804746228639	1.72367161861549	-2.79263925919596
H	-5.83974263948600	2.19000252977365	-3.38289143049859
C	1.57559727596393	4.20879973637016	1.35357613417162
H	1.02425921355424	4.95610777285289	0.78224869812220
C	3.48025180905872	-3.65741822519550	3.09768724590620
H	4.33797751933753	-4.09719974604752	3.61719315618568

C	3.76463599747110	1.09257685763738	-3.52078575586760
H	3.79507007240168	1.06909757508314	-4.61240606471115
C	2.97057592448038	2.27096984893541	2.82219281195021
H	3.50520684696479	1.51153121470264	3.39357230243216
C	2.30580275187816	3.27711590862966	3.46500116773826
H	2.31070296582859	3.32596936970580	4.55618252199710
C	-0.08989853621210	5.39250160395073	-2.70847704702317
H	-0.31200322691076	6.32497464242027	-3.23189722915350
C	-2.38625681637771	4.46052256715348	-3.09742110349603
H	-2.53809788191187	5.40858316811821	-3.62362234004182
C	1.59655823749292	4.26134782946340	2.71890727184922
H	1.06295739421410	5.05695302146411	3.24373609673358
C	-2.41109188578375	-5.97597830290184	2.32107329481551
H	-3.26866570733070	-5.57727296349745	1.76176870766300
H	-2.72380725817698	-6.11077221348596	3.36916304344343
C	2.34777985587439	6.06398953031509	-2.15115058435902
H	3.21387654647375	5.64879882010653	-1.61754407778514
H	2.09073881103091	7.02799796935284	-1.68370101966083
C	-4.47222612871191	-0.12195614838782	1.38060834682277
H	-5.00348183148841	0.63155700726678	0.79841770867817
C	-3.81719052399202	-1.07756878379691	3.50583713429501
H	-3.85850730750993	-1.04646850022117	4.59692363372601
C	-4.52284799207624	-0.10123337535643	2.74599346412065
H	-5.10056016815856	0.67000085055852	3.26032967544282
C	-6.41541325187731	-0.41868025634275	-2.30639923990129
H	-2.17999414173085	-6.97638196596375	1.92168643417704
C	5.09699421129838	-1.79357505475283	2.65094037821324
H	5.91951059220727	-2.30434424515240	3.15617307244895
C	5.23541231297333	-0.50610876889865	2.04567187460770
H	2.65911150504881	6.27955558693107	-3.18599634391828
C	6.51712078211767	0.27902693005766	2.03086095884247
H	7.30981309080034	-0.25981220613414	1.48707966395961
H	6.38071124197492	1.25588075132314	1.54709035090777
H	6.88887172461853	0.45555149546802	3.05278799656002
H	-7.29933489094593	0.10056642818096	-1.90262932381858
H	-6.63568568636350	-0.66261850101424	-3.35814607824383
H	-6.29900799173774	-1.36364427560021	-1.75841298426923

3a, CAMh-B3LYP/def2-SVP first excited-state geometry

S	-0.30544534582149	3.01884155192584	-2.09079136248664
S	-3.03672679758983	1.56371416135443	-1.42846653887823
S	2.80171290445157	-1.22366286152068	2.08494172262318
S	0.52845771718341	-3.32940878529731	1.47283186184715
C	-2.07887074360043	-3.11891493962201	-0.49389225138763
C	-2.70336892817040	-2.18777779283509	-1.39706689138673
C	2.79068006115168	2.14053835544169	-1.44853663067318
C	2.15238103894548	2.99541040043805	0.77291410507051
C	3.52053499168059	1.05871712388382	-0.83969053828366
C	0.98919302272445	3.86697296360575	-1.27316149565242
C	-2.95966351444769	-1.87134746360780	1.44110801973246
C	2.95667852829048	1.96780233725996	1.38118041838937
C	2.02704603226727	3.04311574086923	-0.64836007316638
C	1.01907412707035	-4.17889588514254	2.91048600274363
C	-3.07203338091482	-1.60822836675702	2.83824219552334
H	-2.46753630386422	-2.18771628785960	3.53265662351109
C	-2.47540352871185	-2.36216572240061	-2.79422049236962
H	-2.84894718760266	-1.60935104785786	-3.48507170534061
C	-3.44801363188127	-1.08916231856974	-0.87219532242228
C	-1.39957592169503	-4.24469627517055	-1.04608358145538
H	-0.98615625742840	-4.98930771053493	-0.36611603347432
C	-2.12224489739010	-2.90289531579450	0.91728562000009
C	-3.65665904427200	-0.99432984926921	0.53629507435651
C	-1.17247815124998	-3.60005478869266	1.78584200789496
C	2.82969106245886	2.26939807314438	-2.86842805406953
H	2.33604569148464	3.12577944264651	-3.32753400750746
C	-3.82289017549032	0.03142629832651	-1.73885228425761
C	4.00635999875903	-0.29503582457310	1.21755703121992
C	3.55263756788885	0.94361624783063	0.58366175276796
C	-0.11166407033459	-4.69617326573157	3.54647663392682
H	-0.03511029484001	-5.30689067494765	4.44858857889380
C	4.11233302439417	0.08961086763888	-1.70215097212660
H	4.57262581105507	-0.79303123241181	-1.26346133577609
C	-1.34395074523147	-4.36310845472243	2.94353085040459
C	-3.68997209295084	2.29040887815623	-2.86779558251771
C	-4.60143115983281	0.10328251792158	-2.89415768594559
C	2.37520113556787	-4.39745045798667	3.33358145483247

H	2.46468722956231	-5.23720805200454	4.03131350462315
C	-1.26474243217732	-4.41573532180426	-2.40351409997792
H	-0.74511528013394	-5.29267823575857	-2.79549504945933
C	4.10189003445633	0.23228733064643	-3.07014835889859
H	4.57520673322966	-0.52535857483329	-3.69870066411986
C	-1.78528481792241	-3.44463042557738	-3.28711004999778
H	-1.63869496513154	-3.55092728862997	-4.36430953519079
C	0.73236510935147	5.23816847949243	-1.23681837478282
C	-1.22319443618896	4.47592853480718	-2.33770494096161
C	3.88004165949530	-2.56957915991914	2.31949663106934
C	-3.46543405813396	3.64573575613561	-3.29947454423510
H	-4.24513047408264	4.00121620499995	-3.98188323721298
C	-4.53524714603577	1.37871484108903	-3.49994749155191
H	-5.09037634771511	1.63921754237463	-4.40361157986313
C	1.44058617006229	3.87963999618622	1.63632980876383
H	0.74360050725259	4.59181766928990	1.19987815861106
C	3.56280001179510	-3.78682132788165	3.01515170683099
H	4.45689948618833	-4.31112423777915	3.36980793993392
C	3.47791195145500	1.35248588270372	-3.66172750321009
H	3.49674418927556	1.48300116566147	-4.74581787856968
C	3.12193575625153	1.98707227636118	2.79739203503366
H	3.78694071524283	1.25460319763789	3.25461635519410
C	2.47595527484508	2.90633925346042	3.59012713485854
H	2.62928029747526	2.90029417379494	4.67138076166243
C	-0.49589527699606	5.56411324669560	-1.85517037318636
H	-0.86419184813068	6.58817675573588	-1.94648318862590
C	-2.49261612365480	4.56711828886362	-3.01114108267221
H	-2.69789846155603	5.57911134742633	-3.37682817972993
C	1.60042817555249	3.84543423043674	3.00197636360657
H	1.04690184692067	4.54587121227635	3.63137006178670
C	-2.67207545341929	-4.84633056240751	3.45893288495216
H	-3.48917072062336	-4.58635891161947	2.77380437646410
H	-2.90890982019153	-4.41366845914129	4.44417912959979
C	1.67167713991766	6.26903217971000	-0.67300928730850
H	2.61977311466458	5.81826980867085	-0.35269723088578
H	1.23441949151413	6.78556378537286	0.19654865626961
C	-4.53686513173506	-0.01495617036019	1.08474963531394
H	-5.11692503729068	0.60497283401379	0.40126263941593

C	-3.90932908956902	-0.63336939724542	3.32824297876984
H	-3.97809753484634	-0.46788855790486	4.40574435381353
C	-4.67543706646473	0.15540677067597	2.44176532766393
H	-5.36377108191757	0.90826487088254	2.83169582777457
C	-5.46554251375844	-1.01391199581303	-3.41174223952283
H	-2.66358364868546	-5.94094426723285	3.58046723555322
C	5.13556610816691	-2.24800244554112	1.79936369725837
H	5.98294708856239	-2.93236560360682	1.87860377429489
C	5.21613461677177	-0.99178461935266	1.16048774325626
H	1.89756373230598	7.03978029080176	-1.42668130396286
C	6.48545161131810	-0.45149645395488	0.56054085038207
H	6.81450595230687	-1.05027122460102	-0.30382694897710
H	6.36257999890781	0.58556920641110	0.22290037525170
H	7.30184461996316	-0.47549398738999	1.29954487118891
H	-6.50754446925524	-0.67596349065157	-3.52648603703215
H	-5.12850625894608	-1.36411254631443	-4.40062416965659
H	-5.45996167030273	-1.87528145442746	-2.73148258416549

3b, r^{2}SCAN-3c geometry

S	0.23505862260602	2.87871259019280	-2.86043166882495
S	-2.44794868294180	1.52566009175261	-1.97630596573543
S	3.40920062051449	-1.84379406931993	1.19718158816848
S	0.53831564765803	-2.91011778605980	1.84078088312475
C	-2.00665101600162	-3.02404083628570	-0.70974238799844
C	-2.66099853875803	-2.05152458379473	-1.54959914442797
C	3.39855513053213	2.43130820962663	-1.08453753732959
C	1.40086259012199	2.27303747405886	0.31254356205450
C	4.05828054629343	1.45496477277174	-0.24888237381112
C	1.28026908592009	3.67066360702873	-1.70779706024466
C	-2.60185209513533	-1.71889501791067	1.26586593292227
C	2.05855911662181	1.30274316740371	1.14577657580475
C	2.07352306126937	2.80541873207668	-0.81002131856373
C	1.18111587270496	-4.41190087750508	2.46498611862364
C	-2.63798653862434	-1.53213534185283	2.67722604086914
H	-2.14898627365579	-2.26928014505218	3.30703564048023
C	-2.63853080402201	-2.25140373721172	-2.95996378404503
H	-3.09963025899615	-1.50413054071892	-3.59658274334082
C	-3.22889979575374	-0.89383821220250	-0.97352558108079

C	-1.36962773782066	-4.13563136258575	-1.33281922530458
H	-0.84537672163621	-4.85019683724973	-0.70775788723118
C	-1.93603821340121	-2.81517902719573	0.68529377477167
C	-3.25661191214821	-0.74731176810455	0.42646671897938
C	-1.00848609918668	-3.63870623540323	1.48335924775902
C	4.11050591282017	2.96914901026800	-2.19431064610264
H	3.60562223894084	3.69878338755069	-2.82127839900560
C	-3.61020637125637	0.22791226873832	-1.85199657495984
C	3.91631958498912	-0.23169508355393	1.63542803887626
C	3.37222886891508	0.88551575537926	0.83548944411175
C	0.19980147062580	-5.38664377507701	2.40490710797911
H	0.37503746468727	-6.39906975585375	2.75800686570570
C	5.39107819840582	1.07182714770053	-0.57243153900724
H	5.87778305043677	0.33152496015819	0.05646902031671
C	-1.03404734402946	-4.96637355827118	1.84162969468297
C	-3.32007449474834	2.27467994672152	-3.29410220330559
C	-4.62674038836801	0.37290613642123	-2.76727887600211
C	2.49613375276867	-4.63222409225767	3.02022239794514
H	2.58895653213249	-5.63807516317543	3.42958149049176
C	-1.40087309828673	-4.30491218008279	-2.68883282999167
H	-0.91130352383654	-5.16360981102203	-3.13895804213653
C	6.04150078918783	1.62193033991717	-1.64154008599241
H	7.05985568559100	1.32151052693410	-1.87075340020243
C	-2.04369134993498	-3.35085634018309	-3.51295359113354
H	-2.04435977925805	-3.48258100041592	-4.59106606633975
C	0.94097448123509	4.99538950470828	-1.56259219834004
C	-0.73889273555112	4.31302128246574	-3.06747671491499
C	3.83869039988688	-2.48016610204219	2.76529393725941
C	-2.97628275708105	3.49922371806317	-3.97833793562899
H	-3.75209979496849	3.78843669962498	-4.68704898647798
C	-4.45903650948799	1.53573290030671	-3.56478378781185
H	-5.16200153250027	1.82858242683171	-4.33965868111794
C	0.05732541660075	2.63527317660173	0.62332942699795
H	-0.44760359043870	3.36449636526872	-0.00084261491236
C	3.59329716429348	-3.85087272898670	3.17583056252040
H	4.40619625191887	-4.29600411121050	3.74835650247153
C	5.39389381955168	2.58189612009999	-2.46175889416086
H	5.92374115823575	3.00627467978937	-3.30969376503137

C	1.33677231039477	0.75077787870166	2.24442879626413
H	1.82480420140187	0.01840199509965	2.87826206711579
C	0.04606919366447	1.11982797756142	2.50163111910110
H	-0.49173614046191	0.67163116304721	3.33151290527325
C	-0.18233773978759	5.35575260096928	-2.35787636312478
H	-0.61924100284019	6.35005401306875	-2.35421486113255
C	-1.93663441543135	4.36464823657156	-3.88708744789235
H	-2.03275877777639	5.27424433201731	-4.47878928369263
C	-0.60156816371364	2.07314080749449	1.68087330519256
H	-1.63129655111200	2.34837546416873	1.88738070558659
C	-2.21346004954344	-5.86910030880596	1.63477350596849
H	-3.05121669472475	-5.32063425489576	1.19613211013924
H	-2.54656971235541	-6.30121977797304	2.58501509107634
C	1.61679600238470	5.92423348682639	-0.60016507101793
H	2.40856047173531	5.40718116879956	-0.05158195782375
H	0.90220627937660	6.32628156736383	0.12710129260632
C	-3.91173077756217	0.35492861323563	1.04630396323911
H	-4.40988397534141	1.08151217703434	0.41143236664505
C	-3.29164626593070	-0.46705487808869	3.23240423639431
H	-3.32546829409814	-0.35399181367849	4.31243736511253
C	-3.93660822720371	0.48773939275770	2.40698548439137
H	-4.45959933264354	1.32475680103027	2.86114030678840
C	-5.76007320361676	-0.59699555249387	-2.92024637287971
H	-1.96445512413763	-6.70146723212036	0.96602229015549
C	4.44647898220118	-1.49420192895503	3.51333478726510
H	4.80747568109276	-1.67430018061820	4.52171381027483
C	4.46770037940749	-0.21302636100317	2.89510806986580
H	2.06503937453724	6.77508214656234	-1.12590846905157
C	4.94165074023551	1.03593739766484	3.57435965377410
H	6.00159889018605	0.95837208863785	3.84216902096385
H	4.81771556807446	1.90423474328033	2.92188247698983
H	4.38131384802452	1.21916721172141	4.49838881981221
H	-6.72275173915489	-0.10664676822471	-2.73675645392095
H	-5.79251667487837	-1.01361533806585	-3.93369155668963
H	-5.65816163804074	-1.42545278656721	-2.21445677517245

3c, r^{2}SCAN-3c geometry

S	-0.21616442741248	2.92127531166065	-2.88115025262044

S	-3.08315187335894	2.09543723649520	-1.54956226469117
S	3.10140112690176	-2.11011255212295	1.51224232438920
S	0.23421876904070	-2.93581256599095	2.84359875448515
C	-0.97260185963895	-2.02004498690981	-0.36855073140408
C	-1.63890775317881	-1.05391715200962	-1.19990421559137
C	2.89623424030212	2.01270870329615	-1.19402920978153
C	0.99070314354012	2.00539398532015	0.33106280092442
C	3.56262731298435	1.03604110244251	-0.36231851774175
C	0.87488560020748	3.47985157073268	-1.63628465234082
C	-2.87823392183101	-2.02761956376003	1.15641190526071
C	1.65700606185480	1.03930517207869	1.16246109578605
C	1.62714540008531	2.49232189701615	-0.83309367190277
C	1.12342706495838	-4.44013232757041	2.83194008388097
C	-3.53902461508786	-2.48108909390223	2.33379310285537
H	-3.03705608995825	-3.22168086585719	2.95010608006245
C	-0.95835497225426	-0.57130521065614	-2.35579362324211
H	-1.45884018010483	0.14441336803470	-2.99667418997235
C	-2.92432680817798	-0.58672586230629	-0.84540181341064
C	0.34076272989920	-2.43504854996610	-0.73432542103465
H	0.84879404166668	-3.16294133846581	-0.11400562225833
C	-1.60909504700151	-2.50713030410328	0.79551210696320
C	-3.54462284271157	-1.05089667480883	0.32475904007766
C	-0.85675801421070	-3.49456918886641	1.59874172914659
C	3.55698279971950	2.46605197892430	-2.37148254128937
H	3.05500989672672	3.20660707799679	-2.98783570635416
C	-3.53278489525609	0.41959471826375	-1.74248788264173
C	3.55086176797456	-0.43421788836642	1.70508123543380
C	2.94237565075397	0.57200964283860	0.80791789217125
C	0.50998180142543	-5.33723598251557	1.98798089907656
H	0.89168093159598	-6.34214125207509	1.83280323530893
C	4.84670376253859	0.56599366581360	-0.76071245554908
H	5.34144183883009	-0.16713770405094	-0.12965698840482
C	-0.59246704269208	-4.80305174179698	1.26445612158087
C	-3.58630079014869	2.48745544252244	-3.17550532085999
C	-4.11703544466164	0.20319920311660	-2.96970803781741
C	2.34254121918919	-4.64588002527336	3.60263458768552
H	2.41754474722258	-5.61098270126766	4.10249345452776
C	0.97237261256135	-1.91774239882278	-1.83062319148788

H	1.98442654406239	-2.23161698528900	-2.07070167643868
C	5.44079799928217	1.02295800338631	-1.90395046508548
H	6.41998234854713	0.65179307416949	-2.19264640669236
C	0.31260055154265	-0.97613908105444	-2.65441155593040
H	0.81851759663405	-0.57314781661756	-3.52736930696405
C	0.61088851829839	4.78840973893931	-1.30206882856861
C	-1.10532972684714	4.42561500423164	-2.86921781641032
C	3.60434721718520	-2.50191788294724	3.13829573881540
C	-3.37141623189024	3.78775630169139	-3.78843350111973
H	-4.15933044675476	4.10362249792855	-4.47142414886151
C	-4.16952488019814	1.38487871201442	-3.76012940300022
H	-4.56145415210247	1.40503456197557	-4.77292007335332
C	-0.32258131884474	2.42057523159479	0.69693318984334
H	-0.83059995334026	3.14846366628930	0.07659639597206
C	3.38938348753841	-3.80213334470568	3.75137446003101
H	4.17723544473509	-4.11792458387296	4.43446976073534
C	4.78889330932531	1.98514305436638	-2.71810269921688
H	5.27669202886339	2.34180096348265	-3.62075106684038
C	0.97653515344039	0.55690841192789	2.31848809977511
H	1.47702966665059	-0.15876097845145	2.95941262907255
C	-0.29435397729116	0.96188850760783	2.61718660187248
H	-0.80021458957336	0.55905126523233	3.49024840146519
C	-0.49160741173885	5.32270308105704	-2.02543658088389
H	-0.87314833955963	6.32766466222010	-1.87024946796079
C	-2.32454031697283	4.63146622045848	-3.63972987784301
H	-2.39956767408180	5.59660712839659	-4.13950966147268
C	-0.95412637565177	1.90345509157313	1.79335706851744
H	-1.96612121008644	2.21746106904500	2.03351206336071
C	-1.30624639062610	-5.54087460326437	0.17240964071705
H	-2.18403778986699	-4.98463245894809	-0.16552980849018
H	-1.63302761069763	-6.52822590909015	0.51592432042717
C	1.32494605610765	5.52616578327111	-0.21015709179234
H	2.20292330096724	4.96998718829544	0.12741490144940
H	0.66789198096117	5.67687167705618	0.65521975044728
C	-4.82873932416087	-0.58093471772617	0.72313215372178
H	-5.32347386640564	0.15223571760021	0.09211922881963
C	-4.77097076119700	-2.00025927085681	2.68039482675706
H	-5.25880062818638	-2.35701769667623	3.58298581307632

C	-5.42287335906563	-1.03802711343867	1.86629775784122
H	-6.40208656168027	-0.66692740626399	2.15497874445329
C	-4.54619608180790	-1.14643107876959	-3.45971187526615
H	-0.64892037748651	-5.69180181402396	-0.69271984476605
C	4.18761551637204	-1.39929800408225	3.72280117936529
H	4.57951893716213	-1.41934785339981	4.73560575801997
C	4.13514865675238	-0.21770247689440	2.93225410385412
H	1.65147051379547	6.51361428661719	-0.55363158511569
C	4.56430553739800	1.13198298472269	3.42211195943295
H	5.62524436847187	1.12997401541142	3.69658079680986
H	4.41177467875170	1.89268102867190	2.65226667778001
H	3.99441664026575	1.42700141419099	4.31097250177258
H	-3.97630669703460	-1.44135887131880	-4.34860154736025
H	-4.39367793481753	-1.90720998894071	-2.68994948419060
H	-5.60713300743707	-1.14438455188096	-3.73418488980211

3d, r^{2}SCAN-3c geometry

S	0.00489588756891	4.14416343952888	-2.18729211413686
S	-2.61636739006840	1.85293412658055	-1.82590438619593
S	2.82872876877131	-0.98698381671290	2.97946107746103
S	0.92307054247260	-3.01014729384223	1.48053730690668
C	-1.47438530881590	-2.78172416453184	-1.01717889591578
C	-2.14138690154447	-1.82639498882736	-1.86831659576813
C	1.64118483544295	1.50079135817457	-0.67362967543379
C	2.21273932540133	3.22429789145239	0.96544312796194
C	2.57550813512598	0.60427533271209	-0.03980422052281
C	0.26738297616889	3.59956237298006	-0.54131557268148
C	-2.42341467220741	-1.70000922347134	0.95359699003624
C	3.10295828210515	2.30281658772449	1.62941349132596
C	1.42574554277147	2.79107242102684	-0.12397006011137
C	1.15638939931777	-4.11067863124421	2.81937167597244
C	-2.56218783622300	-1.55602730657166	2.36485133732338
H	-1.98900204080524	-2.21097784514980	3.01216364293800
C	-1.94075090181338	-1.91855331655320	-3.27501936952788
H	-2.40794720757414	-1.17489171255046	-3.91292454510400
C	-2.92841874041519	-0.80643807395144	-1.29588416140562
C	-0.68431688251768	-3.79832803112054	-1.62597934417448
H	-0.19744303560847	-4.52525591249823	-0.98284349458389

C	-1.58392696531429	-2.68102141745272	0.38310293990566
C	-3.12790592198244	-0.77608560458650	0.10151296866167
C	-0.74104552779560	-3.49852962950966	1.27733466990383
C	0.90982025606284	1.00515380711986	-1.79162873654874
H	0.17472189866274	1.63809372201247	-2.26663634857652
C	-3.40669853691416	0.32518644065968	-2.11129637224458
C	3.88765978986958	-0.08451845208922	1.92254730503433
C	3.23738036907567	0.99356118929704	1.14741808283528
C	-0.00730051336065	-4.82894155877584	3.02852030066501
H	-0.08277982950051	-5.58800610829413	3.80214255535860
C	2.74011913064587	-0.70547029759215	-0.57777818527240
H	3.43170895413330	-1.38414087684286	-0.09182271668448
C	-1.09048446299965	-4.47685588632608	2.18077263620256
C	-3.59187633042494	2.66107104817385	-3.02804416186592
C	-4.37702231553784	0.43340328436882	-3.08279887703428
C	2.37926352136139	-4.30933171274140	3.56742666058399
H	2.33860839051235	-5.21216552629666	4.17670337111930
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