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Supporting Information

Toward Helical-shaped Diradicaloids: Cyclobutenyl *o*-Quinodimethane-bridged Indeno[1,2-*b*]fluorenes

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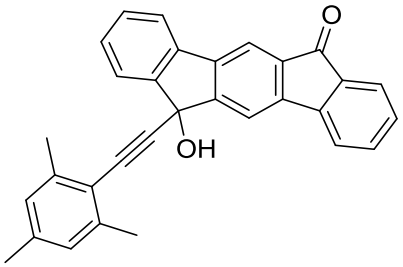
1. General information

Solvents were purified and dried by standard methods prior to use. All commercially available reagents were used without further purification unless otherwise noted. Column chromatography was generally performed on silica gel (200 - 300 mesh) and reactions were monitored by thin layer chromatography (TLC) using silica gel GF254 plates with UV light to visualize the course of reaction. The ^{1}H and ^{13}C NMR data were recorded on a 400 MHz spectrometer using $CDCl_3$ as solvent at room temperature. All chemical shifts are quoted in ppm, relative to tetramethylsilane, using residual solvent peak as a reference standard. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, m = multiplet. Atmospheric pressure chemical ionization mass spectrometry (APCI MS) measurements were performed on a Finnigan TSQ 7000 triple stage quadrupole mass spectrometer operating in a MALDI-TOF mode. UV-*vis*-NIR absorption spectra were recorded on a Shimadzu UV-3600 plus. Cyclic voltammetry (CV) was performed on a Chenhua 650D electrochemical using a three-electrode cell with a glassy carbon working electrode, a platinum wire counter electrode and a Ag/AgCl reference electrode in anhydrous dichloromethane containing recrystallized tetra-*n*-butyl-ammoniumhexafluorophosphate ($TBAPF_6$, 0.1 M) as supporting electrolyte at 298 K. The potential was externally calibrated by the ferrocene/ferrocenium couple. Continuous wave X-band ESR spectra were recorded on a JES-FA200 spectrometer.

2. Preparation of starting materials

Compound 2

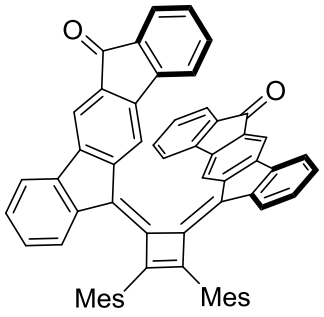


A solution of 2-ethynyl-1,3,5-trimethylbenzene (0.23 g, 1.56 mmol) in THF (20 mL) was cooled to -78 ℃, and then *n*-BuLi (0.63 mL, 1.56 mmol, 2.5 M in hexane) was added dropwise under N_2 atmosphere. To complete formation of organic lithium acetylide, the mixture was kept stirring at

-78 ℃ for 1 h. To a solution of indeno[1,2-b]fluorene-6,12-dione (0.40 g, 1.42 mmol) in THF (200 mL) at 0 ℃, the above pre-prepared lithium acetylide was slowly added. The mixture was then warmed up to the room temperature and stirred for another 1 h. Upon completion of reaction, the solution was diluted with water (50 mL) and dichloromethane (50 mL). The organic layer was dried by anhydrous $MgSO_4$. After filtration, the organic solvents were evaporated to dryness. The residue was purified by column chromatography on silica gel (petroleum ether/CH_2Cl_2 = 1:1) to afford compound **2** (0.41 g, 67%) as an orange solid compound. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (s, 2H), 7.78 (d, *J* = 7.2 Hz, 1H), 7.67 (s, 2H), 7.52 - 7.56 (m, 2H), 7.47 - 7.38 (m, 2H), 7.32 (d, *J* = 7.1 Hz, 1H), 6.82 (s, 2H), 2.76 (s, 1H), 2.35 (s, 6H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 206.64, 154.13, 153.75, 147.46, 147.29, 145.36, 144.27, 140.74, 138.43, 137.87, 135.73, 134.98, 134.49, 130.02, 129.14, 129.08, 127.61, 124.41, 124.18, 120.53, 120.30, 116.45, 116.29, 99.98, 95.36, 82.24, 75.15, 21.34, 20.90. HRMS (MALDI-TOF, *m/z*): calcd for $C_{31}H_{22}O_2$ $[M]^+$, 426.1620; found, 426.1613 (error = - 1.6 ppm).

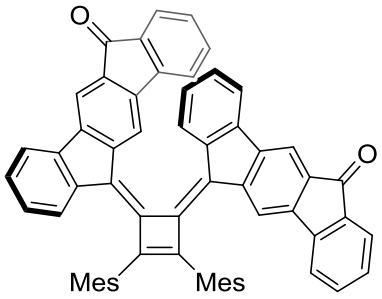
Isomer 3a/3b

To a solution of compound **2** (270 mg, 0.62 mmol) in dry DCM (50 mL), anhydrous $SnCl_2$ (580 mg, 3.06 mmol) was added under N_2 atmosphere. The resulting mixture was kept stirring overnight at room temperature. The reaction was monitored by TLC to confirm consumption of the starting material. Upon completion, the mixture was evaporated to dryness. The residue was purified by the column chromatography on silica gel (petroleum ether/CH_2Cl_2 = 1:2) to afford **3a** (58 mg, 23%) and **3b** (89 mg, 35%), respectively.



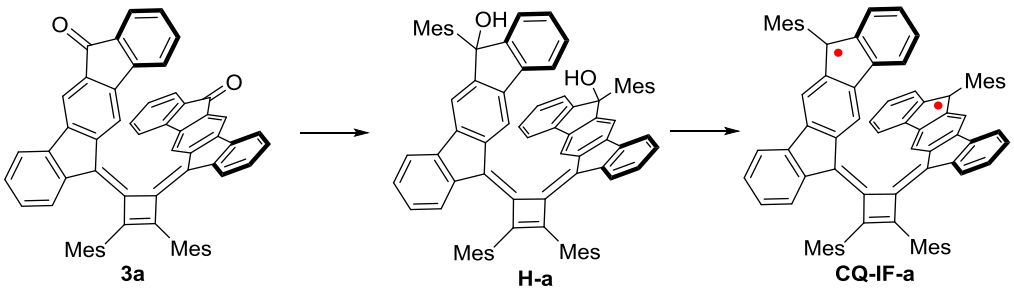
3a was obtained as an orange solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (s, 2H), 7.82 (s, 2H), 7.76 (d, *J* = 7.7 Hz, 2H), 7.45 (d, *J* = 7.2 Hz, 2H), 7.30 (d, *J* = 7.6 Hz, 2H), 7.16 (t, *J* = 7.6 Hz, 2H), 7.08 (t, *J* = 7.6 Hz, 2H), 6.96 (s, 2H), 6.87 - 6.79 (m, 4H), 6.69 - 6.61 (m, 4H), 2.33 (s, 6H), 2.31

(s, 6H), 2.00 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 193.41, 162.72, 148.63, 144.37, 143.08, 142.32, 140.88, 139.15, 138.81, 138.14, 136.28, 135.69, 134.66, 134.60, 133.23, 130.56, 129.12, 128.74, 128.50, 127.75, 126.96, 125.56, 124.60, 123.89, 120.38, 119.59, 119.39, 115.32, 21.21, 20.97, 20.48. HRMS (APCI, *m*/*z*): $[M+H]^+$ calcd for $C_{62}H_{42}O_2$, 819.3258; found, 819.3263 (error = + 0.7 ppm).



3b was obtained as an orange solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.05 (s, 1H), 7.95 (s, 1H), 7.76 - 7.60 (m, 5H), 7.51 (d, *J* = 7.2 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.25 - 7.06 (m, 6H), 6.98 (s, 1H), 6.89 - 6.79 (m, 5H), 6.73 (d, *J* = 7.5 Hz, 1H), 6.65 (d, *J* = 8.0 Hz, 1H), 6.56 (d, *J* = 7.3 Hz, 1H), 2.42 (s, 3H), 2.37 (s, 6H), 2.34 (s, 3H), 2.07 (s, 3H), 1.98 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 193.67, 193.60, 162.71, 161.59, 148.43, 148.17, 144.86, 144.53, 144.30, 143.17, 142.87, 142.22, 140.97, 140.62, 139.48, 139.19, 139.04, 138.92, 138.10, 137.55, 136.82, 136.30, 136.23, 135.68, 135.01, 134.73, 134.55, 134.37, 133.29, 133.06, 131.04, 130.43, 129.42, 129.12, 128.79, 128.74, 128.49, 128.37, 128.08, 127.74, 126.90, 125.32, 125.17, 124.58, 124.01, 123.81, 120.47, 119.93, 119.57, 119.36, 116.66, 115.50, 115.24, 21.21, 21.16, 21.12, 20.98, 20.52, 20.40. HRMS (APCI, *m*/*z*): $[M+H]^+$ calcd for $C_{62}H_{42}O_2$, 819.3258; found, 819.3259 (error = + 0.1 ppm).

Synthesis of compound CQ-IF-a

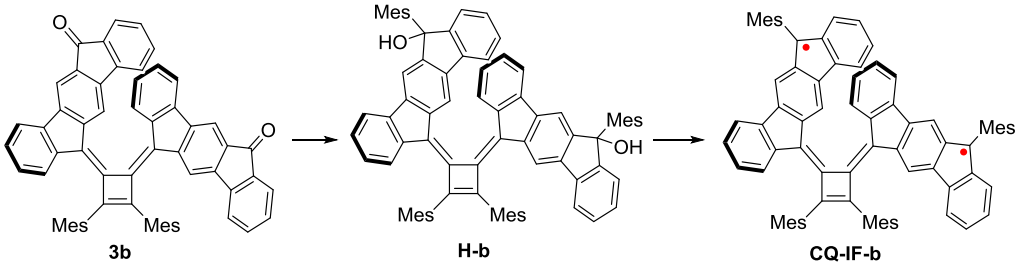


To a solution of **3a** (82 mg, 0.10 mmol) in dry THF (30 mL) at 0 ℃, mesitylmagnesium bromide

(2 mL, 2.00 mmol, 1 M in THF) was added dropwise under N_2 atmosphere. The mixture was warmed up to room temperature and stringing overnight. Upon completion, the solution was diluted with water (50 mL) and dichloromethane (50 mL). The organic layer was dried by anhydrous $MgSO_4$. After filtration, the organic solvents were evaporated to dryness. The residue was purified by flash column chromatography on silica gel (petroleum ether/dichloromethane = 1:1) to afford the alcohol precursor **H-a**. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, *J* = 7.9 Hz, 2H), 7.61 (s, 2H), 7.57 (d, *J* = 7.4 Hz, 2H), 7.24 (d, *J* = 7.0 Hz, 4H), 7.17 - 7.08 (m, 6H), 7.00 (d, *J* = 12.4 Hz, 4H), 6.86 (d, *J* = 7.6 Hz, 2H), 6.79 (t, *J* = 7.6 Hz, 2H), 6.66 (s, 2H), 6.63 (s, 2H), 3.00 (s, 6H), 2.46 (s, 6H), 2.26 (s, 12H), 2.14 (s, 2H), 1.96 (s, 6H), 1.23 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.02, 150.77, 150.69, 146.40, 140.66, 139.71, 139.66, 139.09, 139.02, 138.85, 138.05, 137.90, 136.83, 136.23, 136.07, 135.44, 132.32, 131.41, 130.84, 129.08, 128.70, 128.55, 128.43, 127.90, 127.11, 126.31, 125.62, 123.91, 120.20, 119.25, 117.02, 114.97, 85.90, 25.78, 21.25, 21.14, 20.54, 20.49. MS (MALDI-TOF, *m/z*): $[M]^+$ 1058.77; Anal. calcd for $C_{80}H_{66}O_2$, C, 90.70; H, 6.28; found C, 90.62; H, 6.23.

To a solution of the alcohol precursor in dry DCM (5 mL), anhydrous $SnCl_2$ (189 mg, 1.00 mmol) was added in the glove box under an argon atmosphere. The reaction was monitored by TLC to confirm consumption of starting material. Upon completion, the mixture was evaporated to dryness. The residue was purified by a short length of neutral aluminium oxide (hexane/CH_2Cl_2 = 2:1) under N_2 atmosphere to afford **CQ-IF-a** (91 mg, 89%) as a red solid. There is only rather broad NMR peaks recorded in solution due to the strong paramagnetic response. HRMS (APCI, *m/z*): $[M+H]^+$ calcd for $C_{80}H_{64}$, 1025.5081, found, 1025.5073 (error = - 0.8 ppm); Anal. calcd for $C_{80}H_{64}$, C, 93.71; H, 6.29; found C, 93.58; H, 6.33.

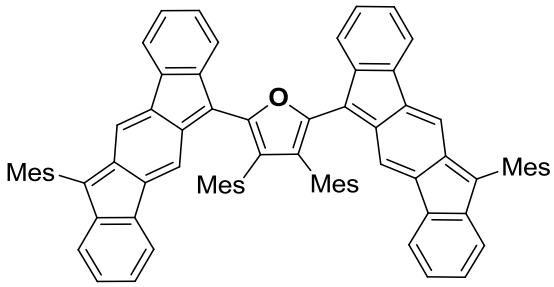
Synthesis of compound CQ-IF-b



CQ-IF-b was synthesized similarly as described for that of **CQ-IF-a**. The alcohol precursor

H-b: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, *J* = 8.0 Hz, 1H), 7.72 - 7.56 (m, 5H), 7.27 - 7.23 (m, 4H), 7.21 - 7.04 (m, 7H), 7.02 - 7.01 (m, 4H), 6.89 (d, *J* = 6.7 Hz, 1H), 6.85 (d, *J* = 6.6 Hz, 1H), 6.79 (t, *J* = 7.7 Hz, 2H), 6.68 (s, 1H), 6.64 (d, *J* = 5.1 Hz, 2H), 3.01 (s, 6H), 2.48 (s, 3H), 2.47 (s, 3H), 2.39 (s, 3H), 2.33 (s, 1H), 2.28 (s, 9H), 2.16 (s, 1H), 2.08 (s, 3H), 1.95 (s, 3H), 1.33 (s, 3H), 1.23 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.17, 160.09, 151.10, 150.70, 150.68, 150.09, 146.47, 146.31, 140.77, 140.65, 139.88, 139.72, 139.63, 139.32, 139.15, 139.04, 138.85, 138.06, 138.02, 137.98, 137.90, 136.86, 136.74, 136.28, 136.25, 136.08, 135.42, 135.20, 132.33, 132.31, 131.66, 131.36, 130.82, 129.27, 129.10, 128.75, 128.68, 128.59, 128.56, 128.49, 127.91, 127.12, 127.08, 126.21, 125.37, 125.27, 123.90, 123.85, 120.21, 120.10, 119.17, 119.12, 117.03, 116.79, 115.00, 114.94, 85.94, 85.89, 25.84, 25.78, 21.72, 21.27, 21.22, 21.18, 21.15, 20.59, 20.54, 20.44. MS (MALDI-TOF, *m/z*): $[M]^+$ 1058.74; Anal. calcd for $C_{80}H_{66}O_2$, C, 90.70; H, 6.28; found C, 90.73; H, 6.31. **CQ-IF-b** was obtained in 84% yield as a red solid. There is only rather broad NMR peaks recorded in solution due to the strong paramagnetic response. HRMS (APCI, *m*/*z*): $[M+H]^+$ calcd for $C_{80}H_{64}$, 1025.5081, found, 1025.5073 (error = - 0.8 ppm); Anal. calcd for $C_{80}H_{64}$, C, 93.71; H, 6.29; found C, 93.76; H, 6.37.

Compound 4



Compound **4** was afforded in about 56% isolated yield as a blue solid, when solution of **CQ-IF-a** or **CQ-IF-b** in DCM or toluene exposed to air during the process of growing single crystals at room temperature. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 (d, *J* = 7.6 Hz, 2H), 7.30 (d, *J* = 7.7 Hz, 2H), 7.00 (s, 6H), 6.85 - 6.95 (m, 12H), 6.81 (s, 2H), 6.76 (s, 2H), 6.60 (d, *J* = 7.4 Hz, 2H), 2.38 (s, 6H), 2.26 (s, 6H), 2.15 (s, 12H), 2.11 (s, 12H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.81, 146.14, 143.80, 141.50, 139.20, 139.15, 138.36, 138.20, 137.93, 137.68, 137.52, 137.05, 134.64, 133.01, 131.25, 130.02, 130.00, 129.38, 129.23, 128.19, 127.76, 127.31, 127.15, 127.02, 124.70, 122.02, 120.60, 120.12, 119.62, 118.75, 21.22, 21.17, 20.82, 20.40. HRMS (APCI, *m*/*z*): $[M+H]^+$ calcd for

$C_{80}H_{64}O$, 1041.5030; found, 1041.5039 (error = + 0.9 ppm).

3. ESR spectra

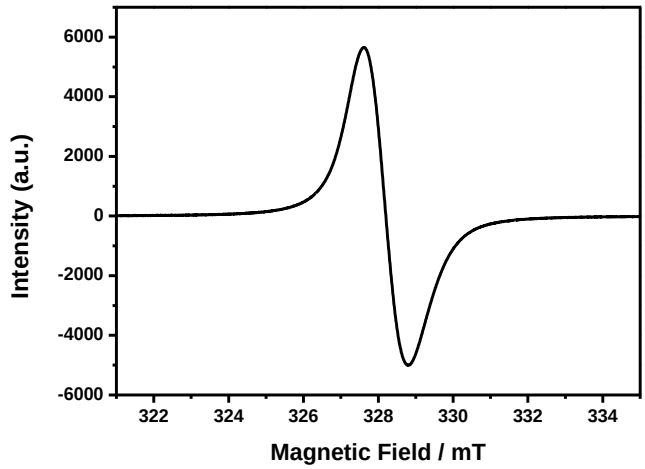


Fig. S1. ESR spectrum of **CQ-IF-a** recorded in toluene at 298 K.

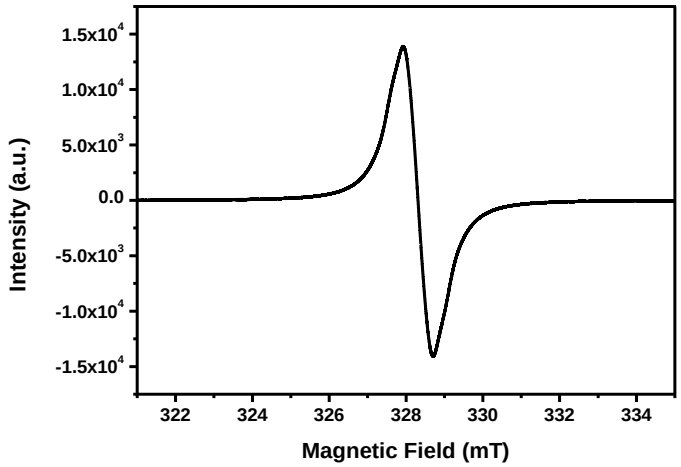


Fig. S2. ESR spectrum of **CQ-IF-b** recorded in toluene at 298 K.

4. Photophysical and electrochemical properties

4.1 UV spectra

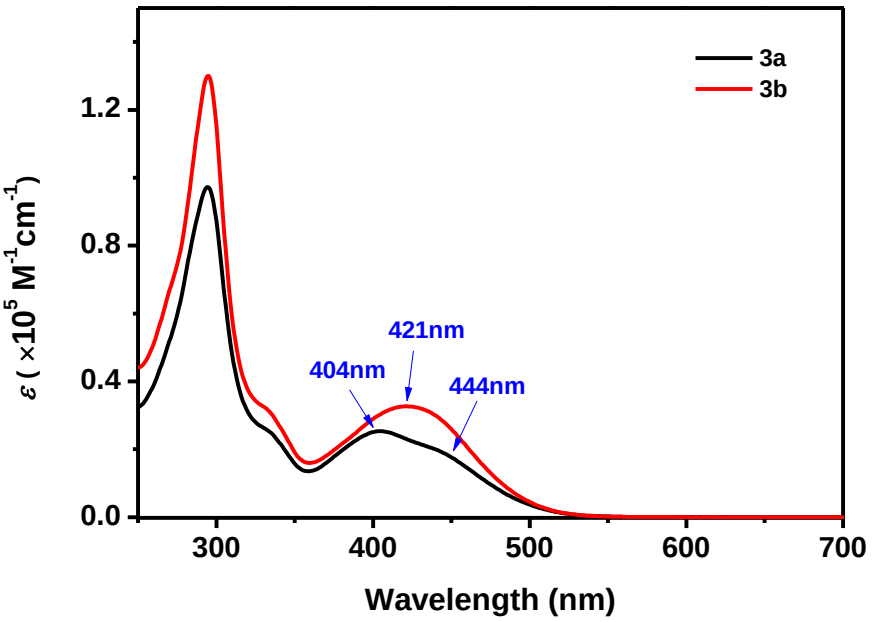


Fig. S3. UV-*vis* absorption spectra of compounds **3a** and **3b** recorded in CH_2Cl_2.

4.2 Electrochemical properties

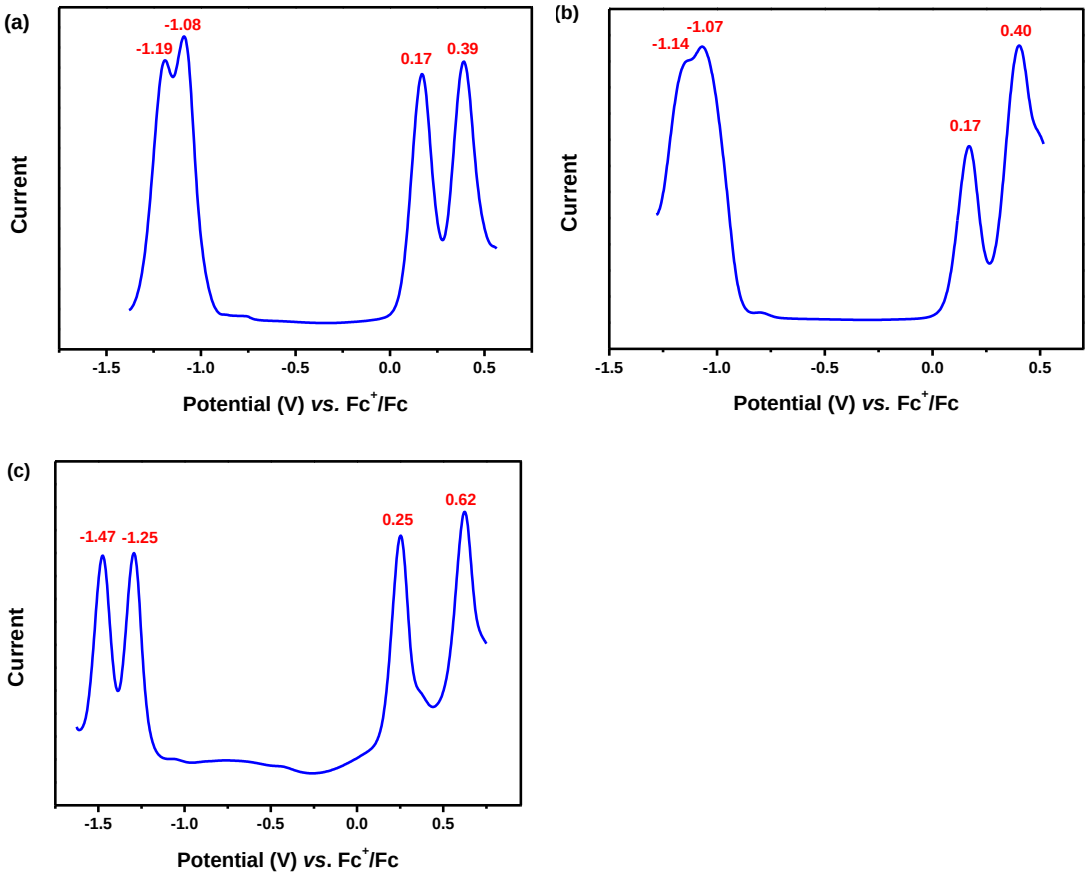


Fig. S4. Differential pulse voltammograms of 1.0 mM solution **CQ-IF-a** (a), **CQ-IF-b** (b) and **4** (c) in DCM: redox potentials were determined by using 0.10 M *n*-$Bu_4N^+PF_6^-$ as the supporting electrolyte; the electrode potential was externally calibrated by the

ferrocene/ferrocenium redox couple.

5. Theoretical calculations

Theoretical calculations were performed with the Gaussian09 program suite.[S1] All calculations were carried out using the density functional theory (DFT) method with Becke's three-parameter hybrid exchange functionals and the Lee-Yang-Parr correlation functional (B3LYP) employing the 6-31G(d,p) basis set for all atoms.[S2] Natural orbital occupation number (NOON) calculations were done by spin unrestricted UCAM-B3LYP/ 6-31G(d,p) method and the diradical character (y_0) was calculated according to Yamaguchi's scheme: $y_0 = 1 - (2T/(1 + T^2))$, and $T = (n_{HOMO} - n_{LUMO})/2$ (n_{HOMO} is the occupation number of the HOMO, n_{LUMO} is the occupation number of the LUMO).[S3]

Table S1 Calculated natural orbital occupation numbers (NOON)) and the diradical character (y_0).

Compound	**CQ-IF-a**	**CQ-IF-b**
n_{HOMO}	1.00647	1.03091
n_{LOMO}	0.99353	0.96909
y_0	0.99	0.94

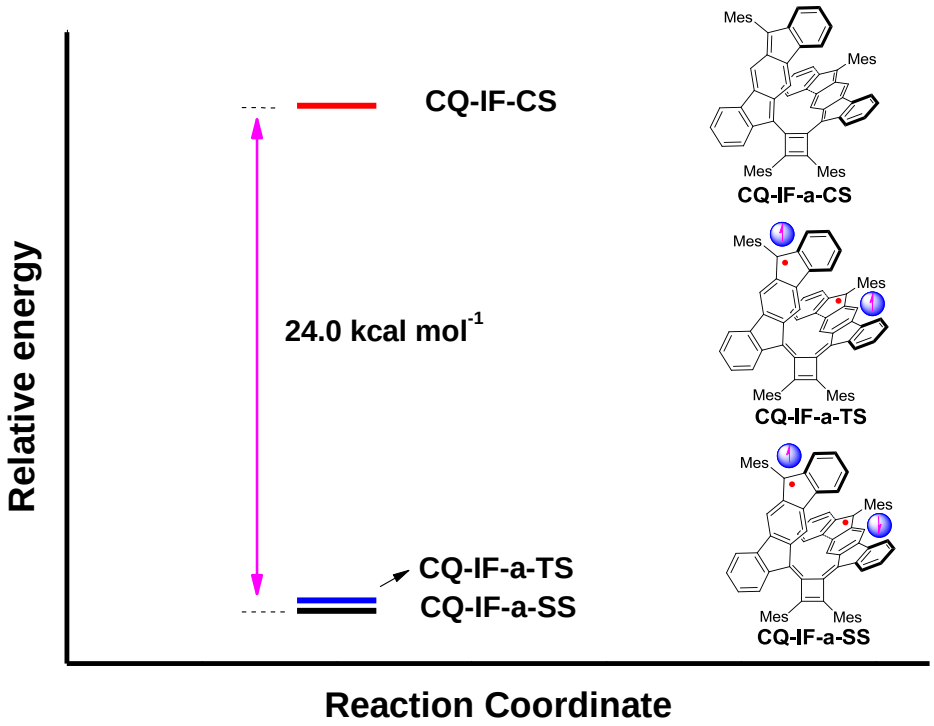


Fig. S5. Lowest energy states of **CQ-IF-a** obtained from DFT calculations at the (U)CAM-B3LYP/6-31G(d, p) level, where "CS', "TS" and "SS" represent close-shell singlet state, open-shell triplet state and singlet state, respectively.

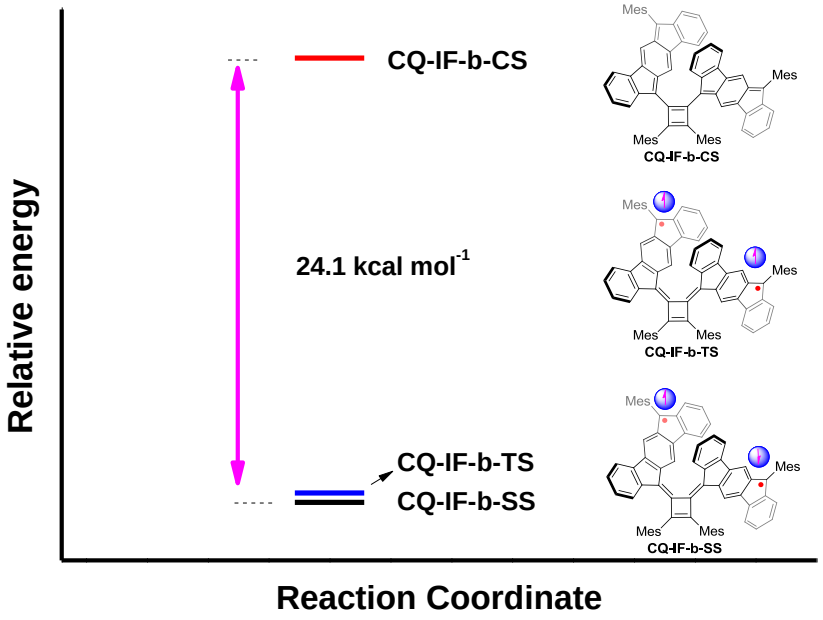


Fig. S6. Lowest energy states of **CQ-IF-b** obtained from DFT calculations at the (U)CAM-B3LYP/6-31G(d, p) level, where "CS', "TS" and "SS" represent close-shell singlet state, open-shell triplet state and singlet state, respectively.

6. X-ray crystallographic data

6.1 X-ray crystallographic data of 3a $CHCl_3$ (CCDC: 1855030)

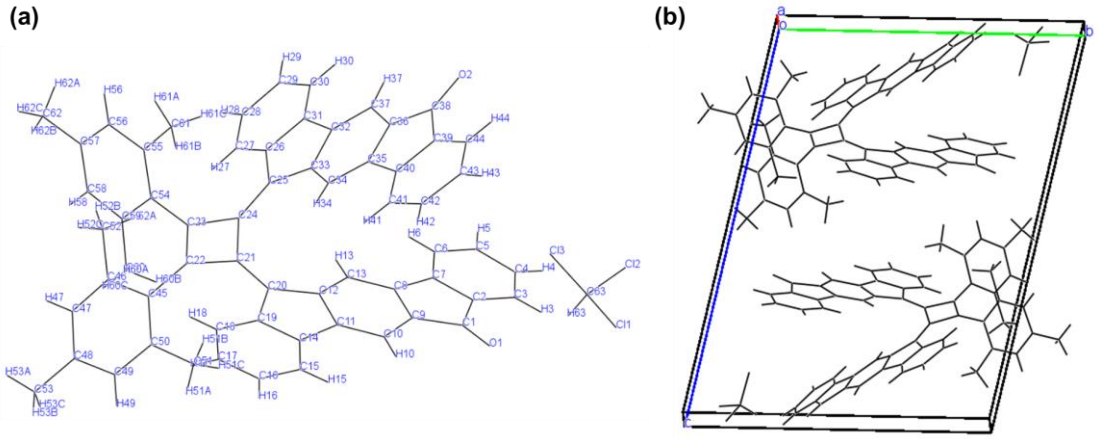


Fig. S7. (a) Crystallographic structure of **3a** $\cdot CHCl_3$ and (b) its racemic structures in the cell.

Table S2. Crystal data and structure refinement for **3a** $\cdot CHCl_3$.

Identification code	3a $CHCl_3$
Empirical formula	C_{63} H_{43} Cl_3 O_2
Formula weight	938.32
Temperature	293(2) K
Wavelength	1.54178 Å
Crystal system	Triclinic
Space group	P -1

Unit cell dimensions	a = 8.1774(6) Å	α= 100.693(4) °.
	b = 15.6087(10) Å	β= 99.580(4) °.
	c = 20.2266(15) Å	γ = 104.108(4) °.
Volume	2398.9(3) $Å^3$	
Z	2	
Density (calculated)	1.299 Mg/m^3	
Absorption coefficient	2.086 mm^{-1}	
F(000)	976	
Crystal size	0.170 x 0.100 x 0.040 mm^3	
Theta range for data collection	2.280 to 64.997 °.	
Index ranges	-9<=h<=7, -18<=k<=18, -23<=l<=23	
Reflections collected	20303	
Independent reflections	7808 [R(int) = 0.0768]	
Completeness to theta = 67.679 °	89.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5611	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7808 / 0 / 620	
Goodness-of-fit on F^2	0.980	
Final R indices [I>2sigma(I)]	R1 = 0.0779, wR2 = 0.2120	
R indices (all data)	R1 = 0.1219, wR2 = 0.2467	
Extinction coefficient	0.0018(4)	
Largest diff. peak and hole	0.352 and -0.429 $e.Å^{-3}$	

Table S3. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **3a CHCl$_3$**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Cl1	6481(3)	8646.0(15)	23.9(10)	145.8(8)
Cl2	10127(3)	9045(2)	526.5(17)	215.9(15)
Cl3	7810(3)	8288.1(16)	1316.5(10)	140.8(8)
O1	7569(4)	6068(2)	220.3(17)	80.5(10)
O2	12469(4)	8353(2)	3933(2)	87.5(11)
C1	8493(5)	5735(3)	569(2)	56.5(10)
C2	10414(5)	5955(3)	712(2)	56.9(10)
C3	11569(6)	6527(3)	441(2)	67.3(12)
C4	13310(6)	6608(3)	646(3)	76.1(13)
C5	13869(6)	6159(3)	1117(3)	73.8(13)
C6	12720(5)	5583(3)	1386(2)	65.0(12)

C7	10970(5)	5477(3)	1175(2)	50.7(9)
C8	9441(5)	4900(2)	1337(2)	47.5(9)
C9	7949(5)	5052(3)	966(2)	49.9(9)
C10	6310(5)	4573(3)	973(2)	51(1)
C11	6141(4)	3956(2)	1388.9(19)	45.6(9)
C12	7629(4)	3830(2)	1794.9(18)	43.3(9)
C13	9280(4)	4281(2)	1744.8(19)	47.0(9)
C14	4607(5)	3336(2)	1477.3(19)	47.3(9)
C15	2879(5)	3227(3)	1212(2)	56.8(11)
C16	1640(5)	2588(3)	1382(2)	67.2(13)
C17	2128(6)	2071(3)	1817(3)	72.4(13)
C18	3853(5)	2174(3)	2101(2)	61.7(11)
C19	5113(5)	2807(2)	1924.3(19)	46.6(9)
C20	7016(5)	3120(2)	2162.6(19)	45.9(9)
C21	8001(4)	2802(2)	2628.7(19)	45.4(9)
C22	7777(5)	1933(2)	2843.6(19)	47.3(9)
C23	9421(5)	2215(2)	3254.7(19)	45.4(9)
C24	9788(4)	3126(2)	3092.7(19)	44.9(9)
C25	11077(5)	3919(2)	3350.2(19)	45.3(9)
C26	12901(5)	4013(2)	3677(2)	47.6(9)
C27	13802(5)	3376(3)	3748(2)	56.4(10)
C28	15555(5)	3676(3)	4060(2)	68.0(12)
C29	16413(5)	4592(3)	4281(2)	65.4(12)
C30	15547(5)	5231(3)	4192(2)	59.4(11)
C31	13801(5)	4947(2)	3890(2)	50.4(10)
C32	12599(5)	5463(2)	3716(2)	48.1(9)
C33	10959(5)	4850(2)	3395.8(19)	44.5(9)
C34	9513(5)	5167(2)	3233.2(18)	47.2(9)
C35	9786(5)	6091(2)	3347.1(19)	46.8(9)
C36	11445(5)	6703(2)	3642(2)	51.4(10)
C37	12844(5)	6397(2)	3849(2)	55.5(10)
C38	11301(6)	7647(3)	3694(2)	60.9(11)
C39	9456(5)	7552(3)	3392(2)	55.3(10)
C40	8559(5)	6629(3)	3194(2)	51.1(10)
C41	6801(5)	6359(3)	2924(2)	61.3(11)
C42	5980(6)	7029(3)	2847(2)	68.5(12)
C43	6881(6)	7948(3)	3025(3)	75.6(14)
C44	8642(6)	8209(3)	3307(2)	67.8(12)
C45	6444(5)	1049(2)	2660(2)	47.9(9)
C46	5747(5)	681(2)	3166(2)	48.1(9)

C47	4554(5)	-167(3)	2971(2)	56.5(11)
C48	4016(5)	-675(3)	2303(3)	61.1(12)
C49	4720(5)	-305(3)	1804(2)	64.9(12)
C50	5930(5)	539(3)	1967(2)	54.8(10)
C51	6687(6)	889(3)	1400(2)	73.0(13)
C52	6179(6)	1196(3)	3910(2)	63.3(11)
C53	2704(6)	-1599(3)	2110(3)	87.7(16)
C54	10343(4)	1805(2)	3743.3(19)	45.7(9)
C55	10806(5)	2249(2)	4456(2)	50.5(10)
C56	11663(5)	1855(3)	4915(2)	58.9(11)
C57	12067(5)	1051(3)	4707(2)	58.4(11)
C58	11555(5)	619(3)	4009(2)	54.3(10)
C59	10687(5)	979(2)	3527(2)	48.8(9)
C60	10184(6)	448(3)	2779(2)	60.8(11)
C61	10340(5)	3096(3)	4726(2)	61.5(11)
C62	12983(7)	628(4)	5211(3)	85.5(16)
C63	8118(8)	8337(5)	497(3)	108(2)

Table S4. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **3a CHCl$_3$**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Cl1	164.0(18)	146.8(18)	119.2(15)	3.0(12)	-12.8(12)	81.4(15)
Cl2	127.7(19)	250(3)	261(3)	142(3)	19.8(19)	-8.3(19)
Cl3	115.6(14)	176(2)	105.6(14)	12.2(13)	8(1)	23.0(13)
O1	70(2)	91(2)	86(2)	56(2)	2.4(16)	15.3(17)
O2	68(2)	42.2(16)	143(3)	23.6(18)	7.7(19)	9.5(14)
C1	56(2)	59(2)	53(2)	21(2)	5.0(18)	12.5(18)
C2	60(3)	54(2)	55(3)	15(2)	11.2(19)	10.4(19)
C3	66(3)	73(3)	62(3)	22(2)	17(2)	11(2)
C4	69(3)	77(3)	80(4)	20(3)	31(3)	7(2)
C5	52(3)	74(3)	91(4)	14(3)	21(2)	11(2)
C6	53(3)	61(3)	80(3)	15(2)	12(2)	16.0(19)
C7	50(2)	46(2)	53(2)	10.0(18)	8.6(17)	11.9(16)
C8	47(2)	43.5(19)	53(2)	12.7(17)	7.9(16)	15.9(15)
C9	50(2)	51(2)	52(2)	20.6(18)	9.0(17)	15.9(17)
C10	44(2)	56(2)	58(2)	23.3(19)	5.6(17)	18.9(17)
C11	40(2)	45.2(19)	55(2)	17.4(17)	7.2(16)	16.3(15)
C12	46(2)	43.9(19)	45(2)	13.6(16)	8.9(15)	19.6(15)
C13	41(2)	49(2)	53(2)	14.3(17)	3.3(15)	19.9(16)
C14	45(2)	49(2)	51(2)	18.3(17)	6.7(16)	18.4(16)

C15	48(2)	63(2)	64(3)	27(2)	5.1(18)	19.3(18)
C16	44(2)	79(3)	84(3)	38(3)	8(2)	18(2)
C17	48(3)	83(3)	100(4)	48(3)	22(2)	20(2)
C18	55(3)	69(3)	74(3)	39(2)	15(2)	25(2)
C19	45(2)	46(2)	51(2)	15.2(17)	6.8(16)	16.7(16)
C20	45(2)	43.9(19)	52(2)	14.3(17)	7.1(16)	19.3(15)
C21	45(2)	39.8(18)	52(2)	14.3(16)	5.4(16)	15.7(15)
C22	49(2)	50(2)	46(2)	16.6(17)	6.6(16)	19.3(16)
C23	50(2)	38.3(18)	49(2)	9.5(16)	5.8(16)	19.4(15)
C24	47(2)	40.6(18)	50(2)	14.2(16)	6.8(16)	18.2(15)
C25	47(2)	41.4(19)	49(2)	12.2(16)	6.2(16)	17.3(15)
C26	43(2)	43.8(19)	58(2)	15.5(17)	6.9(16)	16.8(15)
C27	49(2)	50(2)	73(3)	16(2)	11.2(19)	19.9(17)
C28	57(3)	60(3)	93(3)	21(2)	9(2)	30(2)
C29	37(2)	69(3)	87(3)	16(2)	5(2)	17.9(18)
C30	50(2)	50(2)	72(3)	16(2)	0.6(19)	10.6(17)
C31	48(2)	45(2)	59(2)	15.2(18)	6.3(17)	16.0(16)
C32	45(2)	42.8(19)	57(2)	14.3(17)	9.7(16)	12.9(15)
C33	47(2)	39.9(18)	48(2)	14.0(16)	7.8(16)	15.1(15)
C34	46(2)	45(2)	51(2)	10.1(17)	6.7(16)	16.3(15)
C35	51(2)	44.2(19)	51(2)	16.6(17)	11.3(16)	19.4(16)
C36	56(2)	39.9(19)	59(3)	12.4(18)	10.8(18)	15.5(16)
C37	43(2)	44(2)	74(3)	12.9(19)	6.6(18)	8.3(16)
C38	63(3)	43(2)	81(3)	19(2)	19(2)	16.2(19)
C39	63(3)	49(2)	65(3)	21.9(19)	19(2)	25.5(18)
C40	57(2)	48(2)	53(2)	15.5(18)	11.1(18)	23.7(17)
C41	59(3)	54(2)	70(3)	14(2)	2(2)	22.5(19)
C42	66(3)	64(3)	74(3)	13(2)	0(2)	28(2)
C43	84(3)	64(3)	87(4)	23(3)	7(3)	40(2)
C44	73(3)	51(2)	85(3)	24(2)	13(2)	24(2)
C45	45(2)	40.1(18)	58(2)	14.6(17)	1.0(17)	14.9(15)
C46	48(2)	36.5(18)	64(3)	17.5(17)	8.7(17)	18.1(15)
C47	47(2)	44(2)	82(3)	19(2)	15(2)	16.5(17)
C48	45(2)	47(2)	86(3)	12(2)	6(2)	11.9(17)
C49	49(2)	56(2)	78(3)	-2(2)	-1(2)	15.2(19)
C50	47(2)	50(2)	65(3)	14(2)	4.5(18)	14.1(17)
C51	70(3)	75(3)	64(3)	6(2)	5(2)	15(2)
C52	73(3)	51(2)	67(3)	19(2)	16(2)	17(2)
C53	69(3)	59(3)	112(4)	7(3)	6(3)	-3(2)
C54	40.8(19)	37.9(18)	56(2)	15.6(16)	0.9(16)	11.0(14)

C55	43(2)	49(2)	60(3)	18.5(19)	4.1(17)	16.3(16)
C56	60(3)	65(3)	53(3)	19(2)	-0.5(18)	24.6(19)
C57	49(2)	66(3)	71(3)	32(2)	8.3(19)	26.4(19)
C58	50(2)	45(2)	76(3)	26(2)	10.3(19)	22.4(17)
C59	46(2)	40.9(19)	61(3)	15.5(17)	8.1(17)	14.0(15)
C60	78(3)	45(2)	61(3)	13.8(19)	11(2)	24(2)
C61	64(3)	60(2)	59(3)	10(2)	2.3(19)	27(2)
C62	90(4)	97(4)	84(4)	40(3)	2(3)	49(3)
C63	108(5)	107(5)	103(5)	20(4)	13(4)	31(4)

Table S5. Bond Lengths for **3a** $CHCl_3$.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Cl1	C63	1.732(6)	C26	C31	1.412(5)
Cl2	C63	1.727(7)	C27	C28	1.391(5)
Cl3	C63	1.730(7)	C28	C29	1.380(6)
O1	C1	1.220(5)	C29	C30	1.377(5)
O2	C38	1.224(5)	C30	C31	1.382(5)
C1	C9	1.477(5)	C31	C32	1.453(5)
C1	C2	1.489(6)	C32	C37	1.390(5)
C2	C7	1.387(5)	C32	C33	1.410(5)
C2	C3	1.390(6)	C33	C34	1.404(5)
C3	C4	1.382(6)	C34	C35	1.373(5)
C4	C5	1.367(7)	C35	C36	1.413(5)
C5	C6	1.387(6)	C35	C40	1.486(5)
C6	C7	1.383(5)	C36	C37	1.376(5)
C7	C8	1.476(5)	C36	C38	1.492(5)
C8	C13	1.379(5)	C38	C39	1.491(6)
C8	C9	1.418(5)	C39	C44	1.373(5)
C9	C10	1.370(5)	C39	C40	1.395(5)
C10	C11	1.390(5)	C40	C41	1.379(5)
C11	C12	1.427(4)	C41	C42	1.391(5)
C11	C14	1.446(5)	C42	C43	1.391(6)
C12	C13	1.392(5)	C43	C44	1.385(6)
C12	C20	1.481(5)	C45	C46	1.398(5)
C14	C15	1.383(5)	C45	C50	1.414(6)
C14	C19	1.410(5)	C46	C47	1.381(5)
C15	C16	1.374(6)	C46	C52	1.508(6)
C16	C17	1.374(6)	C47	C48	1.371(6)
C17	C18	1.390(5)	C48	C49	1.389(6)
C18	C19	1.387(5)	C48	C53	1.510(6)

C19	C20	1.478(5)	C49	C50	1.385(6)
C20	C21	1.378(5)	C50	C51	1.518(6)
C21	C22	1.479(5)	C54	C59	1.394(5)
C21	C24	1.509(4)	C54	C55	1.422(5)
C22	C23	1.377(5)	C55	C56	1.392(5)
C22	C45	1.473(5)	C55	C61	1.495(5)
C23	C54	1.475(4)	C56	C57	1.384(6)
C23	C24	1.489(5)	C57	C58	1.391(6)
C24	C25	1.362(5)	C57	C62	1.507(5)
C25	C33	1.467(5)	C58	C59	1.392(5)
C25	C26	1.488(4)	C59	C60	1.518(5)
C26	C27	1.388(5)			

Table S6. Bond Angles for **3a**·$CHCl_3$.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O1	C1	C9	127.3(4)	C30	C31	C26	120.6(3)
O1	C1	C2	127.6(4)	C30	C31	C32	130.9(4)
C9	C1	C2	105.0(3)	C26	C31	C32	108.4(3)
C7	C2	C3	121.7(4)	C37	C32	C33	121.0(3)
C7	C2	C1	109.5(3)	C37	C32	C31	130.1(3)
C3	C2	C1	128.7(4)	C33	C32	C31	108.8(3)
C4	C3	C2	117.9(4)	C34	C33	C32	120.7(3)
C5	C4	C3	120.6(5)	C34	C33	C25	130.2(3)
C4	C5	C6	121.6(4)	C32	C33	C25	108.8(3)
C7	C6	C5	118.6(4)	C35	C34	C33	117.5(3)
C6	C7	C2	119.5(4)	C34	C35	C36	121.5(3)
C6	C7	C8	131.9(4)	C34	C35	C40	130.3(3)
C2	C7	C8	108.6(3)	C36	C35	C40	108.2(3)
C13	C8	C9	120.3(3)	C37	C36	C35	121.2(3)
C13	C8	C7	131.8(3)	C37	C36	C38	130.6(4)
C9	C8	C7	107.8(3)	C35	C36	C38	108.1(3)
C10	C9	C8	122.1(3)	C36	C37	C32	117.8(3)
C10	C9	C1	128.9(3)	O2	C38	C39	127.2(4)
C8	C9	C1	109.0(3)	O2	C38	C36	126.7(4)
C9	C10	C11	117.7(3)	C39	C38	C36	106.1(3)
C10	C11	C12	120.9(3)	C44	C39	C40	121.7(4)
C10	C11	C14	130.0(3)	C44	C39	C38	129.9(4)
C12	C11	C14	109.1(3)	C40	C39	C38	108.4(3)
C13	C12	C11	120.3(3)	C41	C40	C39	119.9(3)
C13	C12	C20	131.8(3)	C41	C40	C35	131.0(4)

C11	C12	C20	107.5(3)	C39	C40	C35	109.0(3)
C8	C13	C12	118.4(3)	C40	C41	C42	118.1(4)
C15	C14	C19	120.9(4)	C43	C42	C41	122.0(4)
C15	C14	C11	130.4(3)	C44	C43	C42	119.2(4)
C19	C14	C11	108.7(3)	C39	C44	C43	119.0(4)
C16	C15	C14	119.4(4)	C46	C45	C50	119.2(3)
C17	C16	C15	119.9(4)	C46	C45	C22	121.1(3)
C16	C17	C18	122.1(4)	C50	C45	C22	119.7(4)
C19	C18	C17	118.4(4)	C47	C46	C45	118.9(4)
C18	C19	C14	119.3(3)	C47	C46	C52	118.7(4)
C18	C19	C20	131.9(3)	C45	C46	C52	122.3(3)
C14	C19	C20	108.6(3)	C48	C47	C46	123.4(4)
C21	C20	C19	126.4(3)	C47	C48	C49	117.4(4)
C21	C20	C12	127.6(3)	C47	C48	C53	121.8(5)
C19	C20	C12	106.0(3)	C49	C48	C53	120.8(4)
C20	C21	C22	134.4(3)	C50	C49	C48	122.0(4)
C20	C21	C24	137.4(3)	C49	C50	C45	119.2(4)
C22	C21	C24	88.0(3)	C49	C50	C51	119.2(4)
C23	C22	C45	131.1(3)	C45	C50	C51	121.6(4)
C23	C22	C21	92.4(3)	C59	C54	C55	119.9(3)
C45	C22	C21	136.2(3)	C59	C54	C23	121.6(3)
C22	C23	C54	132.6(3)	C55	C54	C23	118.4(3)
C22	C23	C24	92.7(3)	C56	C55	C54	118.1(3)
C54	C23	C24	134.2(3)	C56	C55	C61	119.6(4)
C25	C24	C23	134.3(3)	C54	C55	C61	122.2(3)
C25	C24	C21	138.0(3)	C57	C56	C55	122.8(4)
C23	C24	C21	86.9(3)	C56	C57	C58	117.7(3)
C24	C25	C33	128.0(3)	C56	C57	C62	122.2(4)
C24	C25	C26	126.3(3)	C58	C57	C62	120.1(4)
C33	C25	C26	105.6(3)	C57	C58	C59	122.1(3)
C27	C26	C31	119.4(3)	C58	C59	C54	119.3(4)
C27	C26	C25	132.1(3)	C58	C59	C60	117.6(3)
C31	C26	C25	108.3(3)	C54	C59	C60	123.1(3)
C26	C27	C28	119.0(4)	Cl2	C63	Cl3	111.4(4)
C29	C28	C27	121.1(4)	Cl2	C63	Cl1	111.4(4)
C30	C29	C28	120.5(4)	Cl3	C63	Cl1	111.8(4)
C29	C30	C31	119.4(4)				

Table S7. Hydrogen Bonds for **3a**·$CHCl_3$.

D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/ °**

C63	H63	O1	0.98	2.50	3.385(8)	150.3
C63	H63	O1	0.98	2.50	3.385(8)	150.3

Table S8. Torsion Angles for **3a**·$CHCl_3$.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
O1	C1	C2	C7	175.3(5)	C28	C29	C30	C31	1.0(7)
C9	C1	C2	C7	-2.3(5)	C29	C30	C31	C26	0.4(7)
O1	C1	C2	C3	-5.7(8)	C29	C30	C31	C32	-177.7(4)
C9	C1	C2	C3	176.6(4)	C27	C26	C31	C30	-2.6(7)
C7	C2	C3	C4	0.1(7)	C25	C26	C31	C30	-177.9(4)
C1	C2	C3	C4	-178.7(4)	C27	C26	C31	C32	176.0(4)
C2	C3	C4	C5	-2.0(7)	C25	C26	C31	C32	0.6(5)
C3	C4	C5	C6	2.5(8)	C30	C31	C32	C37	-5.1(8)
C4	C5	C6	C7	-0.9(7)	C26	C31	C32	C37	176.5(4)
C5	C6	C7	C2	-1.0(6)	C30	C31	C32	C33	178.3(4)
C5	C6	C7	C8	177.1(4)	C26	C31	C32	C33	0.0(5)
C3	C2	C7	C6	1.4(6)	C37	C32	C33	C34	-3.0(6)
C1	C2	C7	C6	-179.6(4)	C31	C32	C33	C34	173.9(4)
C3	C2	C7	C8	-177.1(4)	C37	C32	C33	C25	-177.5(4)
C1	C2	C7	C8	2.0(5)	C31	C32	C33	C25	-0.6(5)
C6	C7	C8	C13	-0.5(8)	C24	C25	C33	C34	4.5(7)
C2	C7	C8	C13	177.7(4)	C26	C25	C33	C34	-172.8(4)
C6	C7	C8	C9	-179.0(4)	C24	C25	C33	C32	178.3(4)
C2	C7	C8	C9	-0.8(5)	C26	C25	C33	C32	0.9(4)
C13	C8	C9	C10	-2.7(6)	C32	C33	C34	C35	5.0(6)
C7	C8	C9	C10	175.9(4)	C25	C33	C34	C35	178.2(4)
C13	C8	C9	C1	-179.4(4)	C33	C34	C35	C36	-2.4(6)
C7	C8	C9	C1	-0.7(4)	C33	C34	C35	C40	176.2(4)
O1	C1	C9	C10	7.8(8)	C34	C35	C36	C37	-2.4(6)
C2	C1	C9	C10	-174.5(4)	C40	C35	C36	C37	178.7(4)
O1	C1	C9	C8	-175.8(4)	C34	C35	C36	C38	179.9(4)
C2	C1	C9	C8	1.8(4)	C40	C35	C36	C38	1.0(5)
C8	C9	C10	C11	3.3(6)	C35	C36	C37	C32	4.5(7)
C1	C9	C10	C11	179.3(4)	C38	C36	C37	C32	-178.4(4)
C9	C10	C11	C12	0.2(6)	C33	C32	C37	C36	-1.8(6)
C9	C10	C11	C14	-177.0(4)	C31	C32	C37	C36	-178.0(4)
C10	C11	C12	C13	-4.4(6)	C37	C36	C38	O2	1.3(8)
C14	C11	C12	C13	173.3(3)	C35	C36	C38	O2	178.7(5)
C10	C11	C12	C20	-178.8(3)	C37	C36	C38	C39	-179.0(5)
C14	C11	C12	C20	-1.1(4)	C35	C36	C38	C39	-1.6(5)

C9	C8	C13	C12	-1.5(6)	O2	C38	C39	C44	0.4(9)
C7	C8	C13	C12	-179.8(4)	C36	C38	C39	C44	-179.3(5)
C11	C12	C13	C8	4.9(5)	O2	C38	C39	C40	-178.7(5)
C20	C12	C13	C8	177.8(4)	C36	C38	C39	C40	1.7(5)
C10	C11	C14	C15	-5.1(7)	C44	C39	C40	C41	-1.8(7)
C12	C11	C14	C15	177.5(4)	C38	C39	C40	C41	177.3(4)
C10	C11	C14	C19	176.3(4)	C44	C39	C40	C35	179.7(4)
C12	C11	C14	C19	-1.1(4)	C38	C39	C40	C35	-1.1(5)
C19	C14	C15	C16	-0.7(6)	C34	C35	C40	C41	3.1(8)
C11	C14	C15	C16	-179.1(4)	C36	C35	C40	C41	-178.1(4)
C14	C15	C16	C17	0.7(7)	C34	C35	C40	C39	-178.7(4)
C15	C16	C17	C18	0.3(8)	C36	C35	C40	C39	0.1(5)
C16	C17	C18	C19	-1.3(8)	C39	C40	C41	C42	1.1(7)
C17	C18	C19	C14	1.3(6)	C35	C40	C41	C42	179.1(4)
C17	C18	C19	C20	175.6(4)	C40	C41	C42	C43	0.7(7)
C15	C14	C19	C18	-0.3(6)	C41	C42	C43	C44	-1.8(8)
C11	C14	C19	C18	178.4(4)	C40	C39	C44	C43	0.7(7)
C15	C14	C19	C20	-175.8(4)	C38	C39	C44	C43	-178.3(5)
C11	C14	C19	C20	2.9(4)	C42	C43	C44	C39	1.0(8)
C18	C19	C20	C21	2.2(7)	C23	C22	C45	C46	61.7(6)
C14	C19	C20	C21	176.9(4)	C21	C22	C45	C46	-126.1(5)
C18	C19	C20	C12	-178.2(4)	C23	C22	C45	C50	-114.6(5)
C14	C19	C20	C12	-3.5(4)	C21	C22	C45	C50	57.6(6)
C13	C12	C20	C21	8.8(7)	C50	C45	C46	C47	-1.0(5)
C11	C12	C20	C21	-177.7(4)	C22	C45	C46	C47	-177.3(3)
C13	C12	C20	C19	-170.7(4)	C50	C45	C46	C52	-177.6(3)
C11	C12	C20	C19	2.8(4)	C22	C45	C46	C52	6.0(5)
C19	C20	C21	C22	26.4(7)	C45	C46	C47	C48	0.4(6)
C12	C20	C21	C22	-153.0(4)	C52	C46	C47	C48	177.2(3)
C19	C20	C21	C24	-160.0(4)	C46	C47	C48	C49	-0.1(6)
C12	C20	C21	C24	20.6(7)	C46	C47	C48	C53	-179.9(4)
C20	C21	C22	C23	174.3(4)	C47	C48	C49	C50	0.5(6)
C24	C21	C22	C23	-1.4(3)	C53	C48	C49	C50	-179.8(4)
C20	C21	C22	C45	0.1(8)	C48	C49	C50	C45	-1.1(6)
C24	C21	C22	C45	-175.6(5)	C48	C49	C50	C51	178.1(4)
C45	C22	C23	C54	-11.6(8)	C46	C45	C50	C49	1.3(5)
C21	C22	C23	C54	173.8(4)	C22	C45	C50	C49	177.7(3)
C45	C22	C23	C24	176.1(4)	C46	C45	C50	C51	-177.9(3)
C21	C22	C23	C24	1.4(3)	C22	C45	C50	C51	-1.5(5)
C22	C23	C24	C25	169.8(5)	C22	C23	C54	C59	62.9(6)

C54	C23	C24	C25	-2.4(8)	C24	C23	C54	C59	-127.8(4)
C22	C23	C24	C21	-1.4(3)	C22	C23	C54	C55	-113.9(5)
C54	C23	C24	C21	-173.6(4)	C24	C23	C54	C55	55.4(6)
C20	C21	C24	C25	15.3(9)	C59	C54	C55	C56	2.7(6)
C22	C21	C24	C25	-169.2(5)	C23	C54	C55	C56	179.5(4)
C20	C21	C24	C23	-174.1(5)	C59	C54	C55	C61	-174.9(4)
C22	C21	C24	C23	1.3(3)	C23	C54	C55	C61	2.0(6)
C23	C24	C25	C33	-148.5(4)	C54	C55	C56	C57	-0.6(6)
C21	C24	C25	C33	18.3(8)	C61	C55	C56	C57	177.0(4)
C23	C24	C25	C26	28.4(7)	C55	C56	C57	C58	-1.2(7)
C21	C24	C25	C26	-164.9(4)	C55	C56	C57	C62	-179.5(4)
C24	C25	C26	C27	7.1(7)	C56	C57	C58	C59	0.9(6)
C33	C25	C26	C27	-175.5(4)	C62	C57	C58	C59	179.2(4)
C24	C25	C26	C31	-178.4(4)	C57	C58	C59	C54	1.2(6)
C33	C25	C26	C31	-0.9(4)	C57	C58	C59	C60	-179.8(4)
C31	C26	C27	C28	3.2(7)	C55	C54	C59	C58	-3.0(6)
C25	C26	C27	C28	177.3(4)	C23	C54	C59	C58	-179.7(4)
C26	C27	C28	C29	-1.9(7)	C55	C54	C59	C60	178.0(4)
C27	C28	C29	C30	-0.3(8)	C23	C54	C59	C60	1.3(6)

Table S9. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **3a**·$CHCl_3$.

Atom	***x***	***y***	***z***	**U(eq)**
H3	11182	6846	132	81
H4	14107	6971	461	91
H5	15049	6241	1261	89
H6	13118	5276	1701	78
H10	5344	4659	709	61
H13	10252	4167	1981	56
H15	2557	3583	921	68
H16	475	2505	1202	81
H17	1276	1639	1926	87
H18	4156	1827	2403	74
H27	13241	2757	3589	68
H28	16159	3252	4122	82
H29	17584	4779	4490	79
H30	16132	5847	4334	71
H34	8412	4767	3055	57
H37	13917	6802	4072	67
H41	6181	5747	2798	74

H42	4792	6857	2670	82
H43	6308	8381	2957	91
H44	9263	8821	3437	81
H47	4091	-406	3310	68
H49	4369	-635	1347	78
H51A	6459	395	1004	109
H51B	7913	1152	1562	109
H51C	6168	1342	1274	109
H52A	6196	1818	3932	95
H52B	7294	1172	4132	95
H52C	5322	926	4139	95
H53A	2754	-1868	2501	131
H53B	2958	-1982	1735	131
H53C	1567	-1535	1973	131
H56	11979	2145	5381	71
H58	11800	73	3860	65
H60A	11118	221	2666	91
H60B	9943	840	2485	91
H60C	9172	-52	2713	91
H61A	10353	3160	5208	92
H61B	9205	3058	4479	92
H61C	11163	3612	4663	92
H62A	13973	1083	5510	128
H62B	13351	150	4963	128
H62C	12209	383	5482	128
H63	8080	7724	258	130

6.2 X-ray crystallographic data of 3b (CCDC: 1855032)

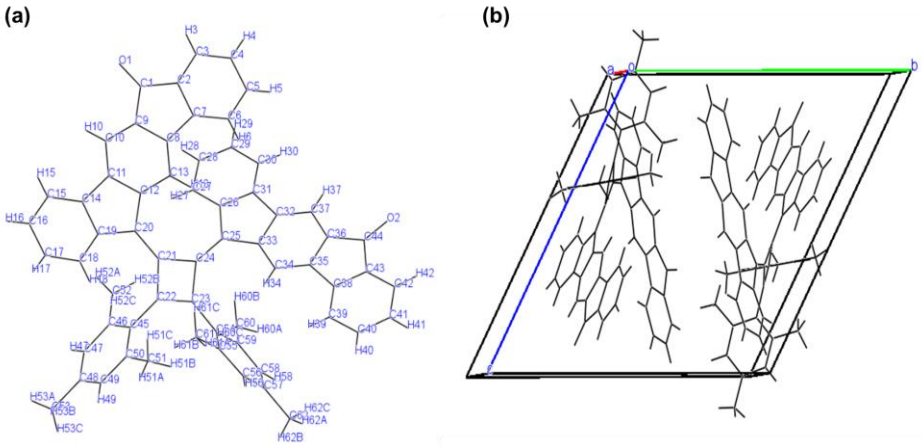


Fig. S8. (a) Crystallographic structure of **3b** and (b) its racemic structures in the cell.

Table S10. Crystal data and structure refinement for **3b**.

Identification code	3b	
Empirical formula	C_{62} H_{42} O_2	
Formula weight	818.95	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.7002(4) Å	α= 116.4440(10) °.
	b = 16.2234(6) Å	β= 98.0640(10) °.
	c = 16.3308(6) Å	γ = 105.7650(10) °.
Volume	2762.93(17) $Å^3$	
Z	2	
Density (calculated)	0.984 Mg/m^3	
Absorption coefficient	0.058 mm^{-1}	
F(000)	860	
Crystal size	0.180 x 0.150 x 0.100 mm^3	
Theta range for data collection	1.461 to 24.999 °.	
Index ranges	-15<=h<=15, -19<=k<=19, -19<=l<=19	
Reflections collected	44560	
Independent reflections	9703 [R(int) = 0.0594]	
Completeness to theta = 25.242 °	97.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6961	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9703 / 0 / 584	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0811, wR2 = 0.2329	
R indices (all data)	R1 = 0.1189, wR2 = 0.2639	
Extinction coefficient	0.039(4)	
Largest diff. peak and hole	0.571 and -0.286 e.$Å^{-3}$	

Table S11. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **3b**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
O1	10066.2(18)	5689.4(18)	6458.2(17)	94.5(7)
O2	1968(3)	2759(3)	9057.0(18)	125.7(10)
C1	9131(2)	5271(2)	6483(2)	67.2(8)
C2	8707(2)	5561(2)	7331(2)	67.3(7)
C3	9252(3)	6333(3)	8264(2)	89.8(10)

C4	8657(4)	6424(3)	8924(3)	102.9(12)
C5	7551(3)	5772(3)	8666(2)	96.5(11)
C6	7005(3)	4995(3)	7726(2)	79.4(9)
C7	7585(2)	4895(2)	7053.6(19)	62.2(7)
C8	7241(2)	4161(2)	6017.3(18)	55.8(6)
C9	8170(2)	4388(2)	5673(2)	58.7(7)
C10	8098(2)	3836(2)	4719(2)	62.3(7)
C11	7082(2)	3034(2)	4119.3(18)	59.2(7)
C12	6155(2)	2783(2)	4466.7(18)	58.4(7)
C13	6233(2)	3373(2)	5425.3(18)	57.9(7)
C14	6733(2)	2326(3)	3083(2)	71.2(8)
C15	7348(3)	2216(3)	2436(2)	97.1(12)
C16	6864(4)	1411(5)	1528(3)	138(2)
C17	5759(4)	690(5)	1256(3)	151(2)
C18	5115(3)	833(4)	1895(2)	116.8(15)
C19	5606(3)	1660(3)	2804(2)	77.9(9)
C20	5178(2)	1948(2)	3649.2(19)	65.1(7)
C21	4072(2)	1579(2)	3646.8(18)	60.9(7)
C22	2927(2)	1180(2)	2945.1(18)	61.8(7)
C23	2392(2)	1302.4(19)	3636.7(18)	56.5(6)
C24	3481(2)	1627.4(19)	4381.3(18)	55.3(6)
C25	3763(2)	1740.7(19)	5268.6(18)	55.6(7)
C26	4750(2)	1597(2)	5708.8(19)	59.3(7)
C27	5587(2)	1289(2)	5346(2)	71.5(8)
C28	6359(3)	1136(3)	5901(3)	90.6(10)
C29	6288(3)	1258(3)	6776(3)	107.1(13)
C30	5447(3)	1527(3)	7124(3)	99.7(12)
C31	4678(2)	1709(2)	6598(2)	70.5(8)
C32	3690(2)	1962(2)	6777.5(19)	63.8(7)
C33	3118(2)	1963.8(19)	5972.0(17)	54.7(6)
C34	2174(2)	2248.1(19)	5980.0(18)	58.4(7)
C35	1787(2)	2486(2)	6773.4(19)	62.1(7)
C36	2347(3)	2444(2)	7552(2)	71.2(8)
C37	3297(3)	2195(3)	7568(2)	78.2(9)
C38	822(3)	2790(2)	6987(2)	67.7(8)
C39	2(3)	2892(3)	6439(3)	82.3(9)
C40	-844(3)	3166(3)	6834(3)	100.6(12)
C41	-858(4)	3339(3)	7733(4)	115.2(14)
C42	-32(4)	3226(3)	8280(3)	103.5(12)
C43	795(3)	2937(2)	7894(2)	80.9(9)

C44	1745(3)	2729(3)	8295(2)	86.5(10)
C45	2514(2)	889(2)	1924(2)	68.3(8)
C46	2857(3)	1599(3)	1648(2)	82.6(9)
C47	2436(3)	1321(4)	686(3)	100.9(12)
C48	1697(4)	362(4)	0(3)	100.6(13)
C49	1368(3)	-326(3)	286(2)	91.6(11)
C50	1761(3)	-77(3)	1237(2)	76.0(9)
C51	1373(4)	-876(3)	1493(3)	103.0(12)
C52	3650(3)	2650(3)	2352(3)	106.7(12)
C53	1257(5)	94(5)	-1038(3)	155(2)
C54	1186(2)	1123(2)	3645.3(18)	55.1(6)
C55	649(2)	1738(2)	3536(2)	63.6(7)
C56	-458(2)	1575(2)	3588(2)	72.7(8)
C57	-1071(2)	822(2)	3716(2)	71.6(8)
C58	-529(2)	221(2)	3804(2)	67.7(7)
C59	589(2)	363(2)	3786.5(19)	60.5(7)
C60	1125(3)	-303(2)	3921(2)	75.1(8)
C61	1256(3)	2559(3)	3372(3)	102.5(12)
C62	-2292(3)	673(3)	3747(3)	107.4(13)

Table S12. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **3b**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	61.3(13)	108.9(18)	90.6(16)	47.3(14)	26.4(11)	4.5(12)
O2	138(2)	193(3)	64.6(16)	67.0(18)	46.1(16)	78(2)
C1	51.5(16)	76.0(19)	70.1(19)	40.1(16)	18.2(14)	13.3(15)
C2	63.2(17)	70.8(18)	59.5(17)	32.1(15)	16.5(14)	16.1(15)
C3	76(2)	84(2)	70(2)	27.2(18)	11.5(17)	2.3(18)
C4	106(3)	96(3)	57(2)	17.4(18)	16(2)	11(2)
C5	91(3)	106(3)	56(2)	22.8(19)	28.1(18)	16(2)
C6	69.3(19)	91(2)	59.2(18)	28.3(17)	24.5(15)	18.8(17)
C7	61.0(17)	69.0(18)	51.4(15)	29.8(14)	19.2(13)	17.4(14)
C8	49.4(14)	66.2(17)	52.6(15)	31.8(13)	16.7(12)	19.6(13)
C9	50.6(15)	73.1(18)	62.3(17)	41.8(15)	21.1(13)	21.8(14)
C10	54.0(16)	85(2)	62.7(17)	44.9(16)	27.2(13)	28.9(15)
C11	52.0(15)	80.8(19)	52.6(15)	35.4(14)	21.3(12)	30.3(15)
C12	49.2(14)	72.9(17)	50.5(15)	27.8(13)	18.1(12)	23.9(13)
C13	50.7(15)	69.5(17)	52.9(15)	30.2(14)	21.6(12)	19.9(14)
C14	57.8(17)	111(2)	53.3(16)	40.3(16)	24.6(13)	42.3(17)
C15	78(2)	166(4)	60(2)	54(2)	36.4(17)	63(2)

C16	90(3)	247(6)	62(2)	52(3)	35(2)	84(4)
C17	115(4)	231(6)	51(2)	16(3)	22(2)	86(4)
C18	78(2)	163(4)	54(2)	11(2)	16.8(17)	46(3)
C19	62.1(18)	108(2)	46.5(16)	22.4(16)	13.5(13)	38.3(18)
C20	53.0(16)	84(2)	47.6(15)	23.5(14)	18.3(12)	27.3(15)
C21	48.6(15)	74.1(18)	48.1(15)	22.1(13)	11.3(12)	23.9(14)
C22	52.9(15)	72.4(18)	48.2(15)	24.7(13)	11.1(12)	19.4(14)
C23	51.5(14)	58.8(16)	52.1(15)	25.3(12)	8.5(12)	19.6(12)
C24	46.9(14)	60.4(16)	53.9(15)	25.0(13)	13.4(11)	21.4(12)
C25	46.3(14)	62.3(16)	53.1(16)	26.2(13)	12.6(11)	20.1(12)
C26	44.2(14)	65.4(17)	59.0(16)	28.2(13)	6.4(12)	18.2(13)
C27	58.8(17)	81(2)	79(2)	42.0(17)	19.4(15)	32.1(16)
C28	62.8(19)	110(3)	112(3)	61(2)	21.4(18)	45(2)
C29	85(2)	163(4)	110(3)	86(3)	25(2)	71(3)
C30	77(2)	157(4)	85(2)	75(3)	19.4(19)	51(2)
C31	55.6(16)	89(2)	64.2(18)	38.8(16)	8.4(13)	28.2(16)
C32	56.7(16)	82.5(19)	51.8(16)	34.3(14)	13.4(13)	26.6(15)
C33	46.9(14)	60.6(16)	48.6(14)	24.4(12)	10.7(11)	17.0(12)
C34	58.8(16)	62.7(16)	50.9(15)	27.1(13)	15.8(12)	22.4(13)
C35	58.4(16)	65.1(17)	55.5(16)	26.7(13)	15.7(13)	20.6(14)
C36	73.7(19)	84(2)	51.6(16)	31.0(15)	21.7(14)	27.8(17)
C37	70.6(19)	109(3)	57.6(18)	43.3(17)	14.2(15)	38.8(19)
C38	66.4(17)	63.6(17)	69.5(19)	27.9(15)	26.9(15)	26.7(15)
C39	80(2)	90(2)	98(2)	53(2)	40.8(19)	45.7(19)
C40	93(3)	111(3)	134(4)	71(3)	53(2)	62(2)
C41	119(3)	138(4)	136(4)	76(3)	82(3)	80(3)
C42	109(3)	121(3)	96(3)	49(2)	57(2)	62(3)
C43	84(2)	81(2)	73(2)	30.6(17)	35.8(17)	34.0(18)
C44	85(2)	107(3)	59(2)	35.0(18)	26.1(17)	34(2)
C45	55.1(16)	93(2)	53.0(16)	32.5(16)	16.4(13)	30.8(16)
C46	79(2)	110(3)	68(2)	50(2)	28.0(17)	36(2)
C47	100(3)	151(4)	84(3)	71(3)	42(2)	65(3)
C48	99(3)	160(4)	58(2)	52(3)	28(2)	73(3)
C49	82(2)	118(3)	51.4(18)	23.1(19)	4.7(16)	48(2)
C50	66.0(18)	92(2)	52.9(17)	23.0(16)	7.2(14)	34.6(18)
C51	111(3)	85(3)	76(2)	27(2)	1(2)	24(2)
C52	99(3)	117(3)	108(3)	71(3)	34(2)	22(2)
C53	166(4)	259(7)	62(2)	75(3)	32(3)	123(5)
C54	46.2(14)	65.4(16)	48.5(14)	27.2(13)	9.1(11)	19.2(13)
C55	55.8(16)	74.6(18)	67.1(17)	39.9(15)	15.5(13)	28.3(14)

C56	62.6(18)	90(2)	80(2)	49.2(18)	19.9(15)	39.5(17)
C57	53.9(16)	94(2)	73.0(19)	42.2(17)	22.1(14)	34.4(17)
C58	56.7(16)	72.0(18)	71.0(19)	36.4(15)	20.0(14)	19.1(15)
C59	55.1(16)	68.1(17)	54.9(16)	28.9(14)	12.1(12)	24.9(14)
C60	66.3(18)	77(2)	89(2)	46.4(18)	21.1(16)	28.8(16)
C61	92(2)	119(3)	147(4)	97(3)	47(2)	53(2)
C62	68(2)	134(3)	146(4)	81(3)	51(2)	47(2)

Table S13. Bond Lengths for **3b**.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O1	C1	1.214(3)	C27	C28	1.388(4)
O2	C44	1.212(4)	C28	C29	1.372(5)
C1	C2	1.481(4)	C29	C30	1.363(5)
C1	C9	1.483(4)	C30	C31	1.389(4)
C2	C3	1.380(4)	C31	C32	1.450(4)
C2	C7	1.396(4)	C32	C37	1.381(4)
C3	C4	1.379(5)	C32	C33	1.412(4)
C4	C5	1.379(5)	C33	C34	1.397(3)
C5	C6	1.389(4)	C34	C35	1.380(4)
C6	C7	1.381(4)	C35	C36	1.406(4)
C7	C8	1.479(4)	C35	C38	1.470(4)
C8	C13	1.368(4)	C36	C37	1.373(4)
C8	C9	1.406(3)	C36	C44	1.491(4)
C9	C10	1.382(4)	C38	C39	1.370(4)
C10	C11	1.384(4)	C38	C43	1.398(4)
C11	C12	1.417(3)	C39	C40	1.403(4)
C11	C14	1.470(4)	C40	C41	1.369(6)
C12	C13	1.395(3)	C41	C42	1.386(6)
C12	C20	1.472(4)	C42	C43	1.383(4)
C14	C15	1.378(4)	C43	C44	1.482(5)
C14	C19	1.400(4)	C45	C50	1.396(4)
C15	C16	1.366(6)	C45	C46	1.402(5)
C16	C17	1.416(7)	C46	C47	1.400(5)
C17	C18	1.392(5)	C46	C52	1.497(5)
C18	C19	1.381(4)	C47	C48	1.384(6)
C19	C20	1.481(4)	C48	C49	1.380(6)
C20	C21	1.368(4)	C48	C53	1.523(5)
C21	C22	1.486(4)	C49	C50	1.392(4)
C21	C24	1.486(4)	C50	C51	1.514(5)
C22	C23	1.365(4)	C54	C59	1.394(4)

C22	C45	1.482(4)	C54	C55	1.409(4)
C23	C54	1.483(3)	C55	C56	1.381(4)
C23	C24	1.493(3)	C55	C61	1.501(4)
C24	C25	1.358(3)	C56	C57	1.378(4)
C25	C33	1.475(3)	C57	C58	1.381(4)
C25	C26	1.482(4)	C57	C62	1.515(4)
C26	C27	1.391(4)	C58	C59	1.381(4)
C26	C31	1.400(4)	C59	C60	1.500(4)

Table S14. Bond Angles for **3b**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O1	C1	C2	126.6(3)	C30	C29	C28	120.8(3)
O1	C1	C9	127.4(3)	C29	C30	C31	119.3(3)
C2	C1	C9	106.0(2)	C30	C31	C26	120.4(3)
C3	C2	C7	121.5(3)	C30	C31	C32	130.6(3)
C3	C2	C1	129.9(3)	C26	C31	C32	108.9(2)
C7	C2	C1	108.6(2)	C37	C32	C33	120.8(3)
C4	C3	C2	117.9(3)	C37	C32	C31	130.7(3)
C3	C4	C5	121.5(3)	C33	C32	C31	108.4(2)
C4	C5	C6	120.4(3)	C34	C33	C32	120.4(2)
C7	C6	C5	118.8(3)	C34	C33	C25	130.6(2)
C6	C7	C2	119.8(3)	C32	C33	C25	108.6(2)
C6	C7	C8	131.4(3)	C35	C34	C33	118.6(2)
C2	C7	C8	108.8(2)	C34	C35	C36	119.9(3)
C13	C8	C9	121.4(2)	C34	C35	C38	131.4(3)
C13	C8	C7	130.4(2)	C36	C35	C38	108.7(2)
C9	C8	C7	108.2(2)	C37	C36	C35	122.3(3)
C10	C9	C8	121.5(2)	C37	C36	C44	129.5(3)
C10	C9	C1	130.0(2)	C35	C36	C44	108.2(3)
C8	C9	C1	108.5(2)	C36	C37	C32	118.0(3)
C9	C10	C11	117.3(2)	C39	C38	C43	120.9(3)
C10	C11	C12	121.5(2)	C39	C38	C35	130.4(3)
C10	C11	C14	130.4(2)	C43	C38	C35	108.6(3)
C12	C11	C14	108.1(2)	C38	C39	C40	117.2(3)
C13	C12	C11	120.1(2)	C41	C40	C39	122.3(4)
C13	C12	C20	130.9(2)	C40	C41	C42	120.2(3)
C11	C12	C20	108.5(2)	C43	C42	C41	118.2(4)
C8	C13	C12	118.1(2)	C42	C43	C38	121.1(3)
C15	C14	C19	120.9(3)	C42	C43	C44	129.9(3)
C15	C14	C11	130.4(3)	C38	C43	C44	108.9(3)

C19	C14	C11	108.6(2)	O2	C44	C43	127.2(3)
C16	C15	C14	118.8(4)	O2	C44	C36	127.3(3)
C15	C16	C17	120.9(3)	C43	C44	C36	105.5(3)
C18	C17	C16	120.0(4)	C50	C45	C46	119.4(3)
C19	C18	C17	118.3(4)	C50	C45	C22	120.8(3)
C18	C19	C14	120.8(3)	C46	C45	C22	119.7(3)
C18	C19	C20	130.1(3)	C47	C46	C45	119.1(4)
C14	C19	C20	108.8(2)	C47	C46	C52	118.9(4)
C21	C20	C12	127.2(2)	C45	C46	C52	122.0(3)
C21	C20	C19	126.7(3)	C48	C47	C46	121.7(4)
C12	C20	C19	105.8(2)	C49	C48	C47	118.4(3)
C20	C21	C22	134.2(3)	C49	C48	C53	121.8(5)
C20	C21	C24	136.1(2)	C47	C48	C53	119.8(5)
C22	C21	C24	88.07(19)	C48	C49	C50	121.7(4)
C23	C22	C45	132.6(2)	C49	C50	C45	119.7(3)
C23	C22	C21	92.0(2)	C49	C50	C51	118.6(3)
C45	C22	C21	134.9(2)	C45	C50	C51	121.7(3)
C22	C23	C54	134.4(2)	C59	C54	C55	119.7(2)
C22	C23	C24	92.4(2)	C59	C54	C23	120.2(2)
C54	C23	C24	133.1(2)	C55	C54	C23	120.1(2)
C25	C24	C21	136.3(2)	C56	C55	C54	118.4(3)
C25	C24	C23	135.7(2)	C56	C55	C61	120.0(3)
C21	C24	C23	87.1(2)	C54	C55	C61	121.5(2)
C24	C25	C33	127.7(2)	C57	C56	C55	122.9(3)
C24	C25	C26	126.9(2)	C56	C57	C58	117.3(3)
C33	C25	C26	105.3(2)	C56	C57	C62	120.1(3)
C27	C26	C31	119.8(2)	C58	C57	C62	122.6(3)
C27	C26	C25	131.2(3)	C57	C58	C59	122.6(3)
C31	C26	C25	108.7(2)	C58	C59	C54	119.0(2)
C28	C27	C26	118.4(3)	C58	C59	C60	119.1(3)
C29	C28	C27	121.4(3)	C54	C59	C60	121.9(2)

Table S15. Torsion Angles for **3b**.

A	**B**	**C**	**D**	**Angle/**°	**A**	**B**	**C**	**D**	**Angle/**°
O1	C1	C2	C3	-1.2(6)	C28	C29	C30	C31	-2.1(7)
C9	C1	C2	C3	-179.7(3)	C29	C30	C31	C26	1.4(6)
O1	C1	C2	C7	179.2(3)	C29	C30	C31	C32	177.2(3)
C9	C1	C2	C7	0.7(3)	C27	C26	C31	C30	0.8(5)
C7	C2	C3	C4	0.7(5)	C25	C26	C31	C30	174.5(3)
C1	C2	C3	C4	-178.9(3)	C27	C26	C31	C32	-175.8(3)

C2	C3	C4	C5	-0.4(6)	C25	C26	C31	C32	-2.2(3)
C3	C4	C5	C6	0.5(7)	C30	C31	C32	C37	7.5(6)
C4	C5	C6	C7	-0.8(6)	C26	C31	C32	C37	-176.3(3)
C5	C6	C7	C2	1.1(5)	C30	C31	C32	C33	-173.6(4)
C5	C6	C7	C8	-179.9(3)	C26	C31	C32	C33	2.5(3)
C3	C2	C7	C6	-1.1(5)	C37	C32	C33	C34	3.1(4)
C1	C2	C7	C6	178.6(3)	C31	C32	C33	C34	-175.9(2)
C3	C2	C7	C8	179.8(3)	C37	C32	C33	C25	177.1(3)
C1	C2	C7	C8	-0.6(3)	C31	C32	C33	C25	-1.9(3)
C6	C7	C8	C13	1.0(5)	C24	C25	C33	C34	-10.1(5)
C2	C7	C8	C13	-179.9(3)	C26	C25	C33	C34	173.7(3)
C6	C7	C8	C9	-178.8(3)	C24	C25	C33	C32	176.8(3)
C2	C7	C8	C9	0.2(3)	C26	C25	C33	C32	0.6(3)
C13	C8	C9	C10	1.2(4)	C32	C33	C34	C35	-2.7(4)
C7	C8	C9	C10	-179.0(2)	C25	C33	C34	C35	-175.1(3)
C13	C8	C9	C1	-179.6(2)	C33	C34	C35	C36	0.4(4)
C7	C8	C9	C1	0.2(3)	C33	C34	C35	C38	-178.8(3)
O1	C1	C9	C10	0.1(5)	C34	C35	C36	C37	1.6(5)
C2	C1	C9	C10	178.5(3)	C38	C35	C36	C37	-179.1(3)
O1	C1	C9	C8	-179.0(3)	C34	C35	C36	C44	-179.6(3)
C2	C1	C9	C8	-0.6(3)	C38	C35	C36	C44	-0.2(3)
C8	C9	C10	C11	-1.6(4)	C35	C36	C37	C32	-1.2(5)
C1	C9	C10	C11	179.4(3)	C44	C36	C37	C32	-179.7(3)
C9	C10	C11	C12	-0.3(4)	C33	C32	C37	C36	-1.2(5)
C9	C10	C11	C14	178.5(3)	C31	C32	C37	C36	177.5(3)
C10	C11	C12	C13	2.6(4)	C34	C35	C38	C39	2.4(5)
C14	C11	C12	C13	-176.5(2)	C36	C35	C38	C39	-176.8(3)
C10	C11	C12	C20	175.9(3)	C34	C35	C38	C43	179.5(3)
C14	C11	C12	C20	-3.2(3)	C36	C35	C38	C43	0.2(3)
C9	C8	C13	C12	1.2(4)	C43	C38	C39	C40	1.1(5)
C7	C8	C13	C12	-178.7(3)	C35	C38	C39	C40	177.9(3)
C11	C12	C13	C8	-3.0(4)	C38	C39	C40	C41	0.7(6)
C20	C12	C13	C8	-174.6(3)	C39	C40	C41	C42	-1.3(7)
C10	C11	C14	C15	5.8(6)	C40	C41	C42	C43	0.0(7)
C12	C11	C14	C15	-175.3(3)	C41	C42	C43	C38	1.8(6)
C10	C11	C14	C19	-178.5(3)	C41	C42	C43	C44	-177.8(4)
C12	C11	C14	C19	0.4(3)	C39	C38	C43	C42	-2.4(5)
C19	C14	C15	C16	-3.7(6)	C35	C38	C43	C42	-179.9(3)
C11	C14	C15	C16	171.5(4)	C39	C38	C43	C44	177.2(3)
C14	C15	C16	C17	-1.1(7)	C35	C38	C43	C44	-0.2(4)

C15	C16	C17	C18	4.8(8)	C42	C43	C44	O2	1.4(7)
C16	C17	C18	C19	-3.4(8)	C38	C43	C44	O2	-178.2(4)
C17	C18	C19	C14	-1.4(6)	C42	C43	C44	C36	179.7(4)
C17	C18	C19	C20	-173.4(4)	C38	C43	C44	C36	0.0(4)
C15	C14	C19	C18	5.1(5)	C37	C36	C44	O2	-2.9(6)
C11	C14	C19	C18	-171.1(3)	C35	C36	C44	O2	178.4(4)
C15	C14	C19	C20	178.6(3)	C37	C36	C44	C43	178.8(3)
C11	C14	C19	C20	2.5(4)	C35	C36	C44	C43	0.1(4)
C13	C12	C20	C21	2.9(5)	C23	C22	C45	C50	-69.3(4)
C11	C12	C20	C21	-169.4(3)	C21	C22	C45	C50	120.9(4)
C13	C12	C20	C19	176.9(3)	C23	C22	C45	C46	108.9(4)
C11	C12	C20	C19	4.5(3)	C21	C22	C45	C46	-60.9(4)
C18	C19	C20	C21	-17.5(6)	C50	C45	C46	C47	0.0(4)
C14	C19	C20	C21	169.7(3)	C22	C45	C46	C47	-178.3(3)
C18	C19	C20	C12	168.5(4)	C50	C45	C46	C52	179.2(3)
C14	C19	C20	C12	-4.3(3)	C22	C45	C46	C52	1.0(4)
C12	C20	C21	C22	142.3(3)	C45	C46	C47	C48	-0.5(5)
C19	C20	C21	C22	-30.5(5)	C52	C46	C47	C48	-179.8(3)
C12	C20	C21	C24	-18.8(6)	C46	C47	C48	C49	0.6(5)
C19	C20	C21	C24	168.4(3)	C46	C47	C48	C53	179.8(3)
C20	C21	C22	C23	-162.2(3)	C47	C48	C49	C50	-0.2(5)
C24	C21	C22	C23	4.8(2)	C53	C48	C49	C50	-179.4(3)
C20	C21	C22	C45	10.3(6)	C48	C49	C50	C45	-0.4(5)
C24	C21	C22	C45	177.3(3)	C48	C49	C50	C51	-179.3(3)
C45	C22	C23	C54	5.9(6)	C46	C45	C50	C49	0.5(4)
C21	C22	C23	C54	178.7(3)	C22	C45	C50	C49	178.7(3)
C45	C22	C23	C24	-177.6(3)	C46	C45	C50	C51	179.3(3)
C21	C22	C23	C24	-4.8(2)	C22	C45	C50	C51	-2.5(4)
C20	C21	C24	C25	-28.1(6)	C22	C23	C54	C59	110.7(4)
C22	C21	C24	C25	165.4(3)	C24	C23	C54	C59	-64.5(4)
C20	C21	C24	C23	162.2(4)	C22	C23	C54	C55	-71.0(4)
C22	C21	C24	C23	-4.4(2)	C24	C23	C54	C55	113.8(3)
C22	C23	C24	C25	-165.1(3)	C59	C54	C55	C56	1.0(4)
C54	C23	C24	C25	11.5(5)	C23	C54	C55	C56	-177.3(2)
C22	C23	C24	C21	4.8(2)	C59	C54	C55	C61	-179.3(3)
C54	C23	C24	C21	-178.7(3)	C23	C54	C55	C61	2.4(4)
C21	C24	C25	C33	167.0(3)	C54	C55	C56	C57	-1.8(5)
C23	C24	C25	C33	-27.7(5)	C61	C55	C56	C57	178.5(3)
C21	C24	C25	C26	-17.6(5)	C55	C56	C57	C58	0.7(5)
C23	C24	C25	C26	147.7(3)	C55	C56	C57	C62	-178.8(3)

C24	C25	C26	C27	-2.6(5)	C56	C57	C58	C59	1.2(5)
C33	C25	C26	C27	173.7(3)	C62	C57	C58	C59	-179.3(3)
C24	C25	C26	C31	-175.3(3)	C57	C58	C59	C54	-2.0(4)
C33	C25	C26	C31	1.0(3)	C57	C58	C59	C60	177.9(3)
C31	C26	C27	C28	-2.3(4)	C55	C54	C59	C58	0.8(4)
C25	C26	C27	C28	-174.3(3)	C23	C54	C59	C58	179.1(2)
C26	C27	C28	C29	1.6(5)	C55	C54	C59	C60	-179.1(3)
C27	C28	C29	C30	0.6(6)	C23	C54	C59	C60	-0.8(4)

Table S16. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **3b**.

Atom	***x***	***y***	***z***	**U(eq)**
H3	9997	6778	8443	108
H4	9011	6937	9558	123
H5	7167	5853	9124	116
H6	6262	4549	7552	95
H10	8706	3997	4490	75
H13	5617	3234	5655	70
H15	8079	2681	2615	116
H16	7266	1335	1082	166
H17	5464	121	651	181
H18	4372	383	1713	140
H27	5630	1188	4747	86
H28	6936	946	5676	109
H29	6820	1157	7136	128
H30	5388	1588	7708	120
H34	1813	2277	5462	70
H37	3664	2183	8095	94
H39	6	2784	5831	99
H40	-1416	3233	6473	121
H41	-1424	3534	7976	138
H42	-34	3341	8891	124
H47	2658	1793	502	121
H49	870	-972	-168	110
H51A	946	-1505	918	155
H51B	895	-718	1900	155
H51C	2032	-910	1825	155
H52A	4406	2743	2287	160
H52B	3674	2789	2992	160
H52C	3377	3094	2229	160

H53A	1821	-47	-1356	233
H53B	1119	641	-1052	233
H53C	555	-482	-1360	233
H56	-805	1993	3534	87
H58	-932	-300	3878	81
H60A	692	-630	4201	113
H60B	1900	86	4338	113
H60C	1128	-792	3310	113
H61A	858	3007	3497	154
H61B	1268	2281	2719	154
H61C	2029	2913	3796	154
H62A	-2593	120	3838	161
H62B	-2758	542	3154	161
H62C	-2300	1262	4269	161

6.3 X-ray crystallographic data of 4 (CCDC: 1855033)

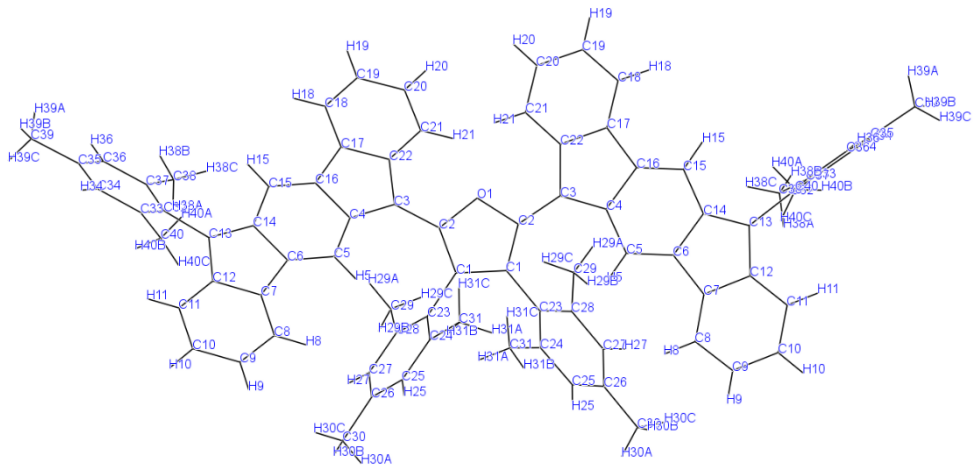


Fig. S9. Crystallographic structure of **4**

Table S17. Crystal data and structure refinement for **4**.

Identification code	4	
Empirical formula	C_{80} H_{64} O	
Formula weight	1041.31	
Temperature	170 K	
Wavelength	1.34139 Å	
Crystal system	Orthorhombic	
Space group	Pbcn	
Unit cell dimensions	a = 18.9589(5) Å	α= 90 °.
	b = 17.5568(4) Å	β= 90 °.
	c = 20.8566(5) Å	γ = 90 °.
Volume	6942.3(3) $Å^3$	

Z	4
Density (calculated)	0.996 Mg/m^3
Absorption coefficient	0.280 mm^{-1}
F(000)	2208
Crystal size	0.2 x 0.12 x 0.08 mm^3
Theta range for data collection	3.508 to 54.982 °.
Index ranges	-23<=h<=23, -21<=k<=21, -18<=l<=25
Reflections collected	71781
Independent reflections	6602 [R(int) = 0.0540]
Completeness to theta = 53.594 °	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7508 and 0.5314
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6602 / 0 / 373
Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 = 0.0565, wR2 = 0.1496
R indices (all data)	R1 = 0.0673, wR2 = 0.1562
Extinction coefficient	0.00144(14)
Largest diff. peak and hole	0.202 and -0.188 $e.Å^{-3}$

Table S18. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **4**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
O1	5000	2829.1(10)	2500	39.7(4)
C1	4873.2(9)	4038.7(10)	2824.3(8)	34.7(4)
C2	4802.2(10)	3287.2(11)	3006.3(9)	37.7(4)
C3	4618.9(10)	2862.6(11)	3573.7(9)	37.3(4)
C4	4219.1(10)	3082.1(10)	4104.5(8)	37.8(4)
C5	3828.2(9)	3761.8(11)	4248.5(9)	37.2(4)
C6	3481.6(10)	3805.5(11)	4817.2(9)	39.6(4)
C7	3048.1(10)	4412.9(11)	5100.1(9)	41.7(4)
C8	2865.8(11)	5132.1(12)	4889.3(11)	48.8(5)
C9	2448.6(13)	5588.5(14)	5282.4(11)	58.9(6)
C10	2224.1(13)	5331.7(15)	5878.8(12)	63.3(6)
C11	2398.5(12)	4608.4(14)	6092.4(11)	55.5(6)
C12	2812.5(10)	4146.9(12)	5706(1)	46.4(5)
C13	3085.4(11)	3378.4(12)	5807.1(9)	45.0(5)
C14	3486(1)	3183.5(11)	5277.8(9)	41.6(4)
C15	3857.3(11)	2498.9(11)	5132.6(9)	43.7(5)

C16	4204.2(10)	2456.6(11)	4564.0(9)	41.1(4)
C17	4610.4(11)	1832.9(11)	4286.2(9)	45.8(5)
C18	4754.7(14)	1113.8(13)	4521.7(12)	63.1(6)
C19	5162.2(16)	626.5(14)	4157.4(12)	70.3(7)
C20	5428.3(14)	855.4(13)	3568.8(12)	59.8(6)
C21	5281.3(11)	1573.0(12)	3328.4(10)	47.6(5)
C22	4863.5(10)	2070.0(11)	3683.0(9)	41.1(4)
C23	4724.6(9)	4723.6(10)	3224.3(8)	35.2(4)
C24	4170.6(10)	5217.6(11)	3050.9(9)	39.5(4)
C25	4033.3(11)	5848.9(11)	3436(1)	46.3(5)
C26	4415.5(12)	6004.4(11)	3989.3(10)	48.1(5)
C27	4942.7(12)	5499.4(11)	4156.2(9)	45.9(5)
C28	5112.9(10)	4865.5(11)	3786.4(9)	38.3(4)
C29	5694.7(11)	4349.0(13)	4007.9(10)	47.7(5)
C30	4247.5(16)	6699.0(13)	4388.4(12)	68.7(7)
C31	3699.7(11)	5075.6(14)	2482.7(10)	51.0(5)
C32	2930.5(11)	2897.6(12)	6375.7(10)	48.1(5)
C33	3438.1(13)	2780.2(13)	6855.6(10)	53.3(5)
C34	3243.9(15)	2358.6(15)	7392.7(11)	66.3(7)
C35	2577.1(17)	2042.2(16)	7456.5(13)	73.1(8)
C36	2099.2(15)	2143.5(15)	6970.4(13)	71.6(8)
C37	2257.6(12)	2563.8(14)	6424.2(11)	57.5(6)
C38	1730.2(14)	2637.6(16)	5882.8(13)	71.4(7)
C39	2385(2)	1594(2)	8056.7(15)	108.2(12)
C40	4175.8(13)	3090.8(15)	6795.6(12)	63.3(6)

Table S19. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **4**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	51.6(11)	37.4(9)	30.2(9)	0	4.8(8)	0
C1	34.6(9)	39.8(9)	29.8(9)	1.3(7)	-0.1(7)	-0.9(8)
C2	41.5(10)	41.8(10)	29.7(9)	-3.0(8)	2.2(8)	0.3(8)
C3	42.1(10)	40(1)	29.9(9)	0.8(8)	-2.3(8)	-3.2(8)
C4	42.6(10)	39.9(10)	30.9(9)	1.6(8)	-0.4(8)	-7.2(8)
C5	39.4(10)	41.3(10)	31.0(9)	0.0(8)	0.6(8)	-6.5(8)
C6	38.6(10)	45.2(10)	35(1)	-1.5(8)	0.3(8)	-7.4(8)
C7	36.8(10)	48.8(11)	39.5(11)	-3.5(9)	2.6(8)	-7.0(8)
C8	46.8(11)	53.3(12)	46.5(12)	-3.4(10)	4.9(9)	-1.9(9)
C9	57.0(13)	59.1(14)	60.7(14)	-5.5(11)	6.8(11)	8.8(11)
C10	59.1(14)	69.1(16)	61.8(15)	-12.3(12)	15.5(12)	3.9(12)

C11	52.6(13)	67.2(15)	46.6(12)	-7.8(11)	12.6(10)	-2.9(11)
C12	42.7(11)	56.6(12)	39.9(11)	-6.3(9)	5.7(9)	-9.1(9)
C13	44.8(11)	53.8(12)	36.5(10)	-1.7(9)	6.0(9)	-11.9(9)
C14	42.7(10)	49.0(11)	33.2(10)	0.6(8)	2.8(8)	-10.5(9)
C15	52.9(12)	43.2(10)	35(1)	5.6(8)	2.3(9)	-7.5(9)
C16	47.0(11)	41.8(10)	34.4(10)	3.1(8)	-0.3(8)	-3.6(8)
C17	57.3(12)	43.5(11)	36.5(10)	4.0(8)	-0.9(9)	-3.4(9)
C18	86.9(18)	49.0(13)	53.5(14)	13.6(11)	7.5(13)	6.5(12)
C19	104(2)	48.5(13)	58.1(15)	12.3(11)	7.5(14)	16.9(13)
C20	75.8(16)	48.5(13)	55.0(14)	1.3(10)	1.7(12)	13.8(11)
C21	58.7(12)	45.3(11)	38.9(11)	1.2(9)	0.6(9)	3.8(9)
C22	48.4(11)	39.6(10)	35.4(10)	2.3(8)	-2.9(8)	-1.2(8)
C23	38.6(10)	37.9(9)	29.0(9)	1.0(7)	5.3(7)	-2.5(8)
C24	43.2(10)	41.2(10)	34.2(10)	1.7(8)	6.5(8)	-0.9(8)
C25	53.0(12)	44.6(11)	41.2(11)	3.6(9)	10.8(9)	7.7(9)
C26	64.4(13)	39.8(11)	40.1(11)	-4.4(9)	13.5(10)	-7.8(10)
C27	57.2(12)	49.8(11)	30.6(10)	-4.4(8)	4.8(9)	-13.6(10)
C28	40.5(10)	41.6(10)	32.7(10)	0.8(8)	4.1(8)	-8.4(8)
C29	47.0(11)	58.1(12)	37.9(11)	0.8(9)	-5.5(9)	-4.3(9)
C30	101(2)	49.9(13)	55.1(14)	-14.5(11)	14.2(14)	-2.2(13)
C31	45.4(11)	64.3(13)	43.3(11)	-0.3(10)	-2.4(9)	10.1(10)
C32	55.5(12)	51.2(12)	37.5(11)	-3.6(9)	13.3(9)	-11.1(10)
C33	65.8(14)	55.3(13)	38.9(11)	1.2(10)	11.1(10)	-10.3(11)
C34	86.9(18)	68.8(15)	43.2(13)	6.9(11)	12.6(12)	-6.2(14)
C35	91(2)	70.4(16)	57.7(15)	9.4(13)	29.5(15)	-17.3(15)
C36	73.7(17)	72.0(17)	69.0(17)	4.3(13)	27.9(14)	-22.8(14)
C37	59.1(14)	58.0(13)	55.3(13)	-5.6(11)	19.0(11)	-14.9(11)
C38	57.7(14)	77.5(17)	79.2(18)	-7.9(14)	5.2(13)	-20.1(13)
C39	147(3)	105(3)	73(2)	28.9(18)	42(2)	-25(2)
C40	64.2(15)	77.3(16)	48.3(13)	8.6(12)	-1.9(11)	-13.0(13)

Table S20. Bond Lengths for **4**.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O1	C2	1.379(2)	C17	C18	1.382(3)
O1	C2[1]	1.379(2)	C17	C22	1.409(3)
C1	C1[1]	1.436(4)	C18	C19	1.381(3)
C1	C2	1.380(3)	C19	C20	1.387(3)
C1	C23	1.490(2)	C20	C21	1.384(3)
C2	C3	1.441(3)	C21	C22	1.391(3)
C3	C4	1.396(3)	C23	C24	1.409(3)

C3	C22	1.484(3)	C23	C28	1.407(3)
C4	C5	1.437(3)	C24	C25	1.393(3)
C4	C16	1.458(3)	C24	C31	1.504(3)
C5	C6	1.358(3)	C25	C26	1.390(3)
C6	C7	1.470(3)	C26	C27	1.381(3)
C6	C14	1.454(3)	C26	C30	1.510(3)
C7	C8	1.381(3)	C27	C28	1.392(3)
C7	C12	1.419(3)	C28	C29	1.501(3)
C8	C9	1.393(3)	C32	C33	1.404(3)
C9	C10	1.390(3)	C32	C37	1.408(3)
C10	C11	1.386(3)	C33	C34	1.392(3)
C11	C12	1.386(3)	C33	C40	1.506(3)
C12	C13	1.460(3)	C34	C35	1.387(4)
C13	C14	1.383(3)	C35	C36	1.371(4)
C13	C32	1.485(3)	C35	C39	1.522(4)
C14	C15	1.426(3)	C36	C37	1.390(3)
C15	C16	1.358(3)	C37	C38	1.514(4)
C16	C17	1.459(3)			

Table S21. Bond Angles for **4**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C2	O1	$C2^1$	108.66(19)	C18	C17	C22	121.3(2)
$C1^1$	C1	C23	126.21(9)	C22	C17	C16	108.22(17)
C2	C1	$C1^1$	106.97(10)	C19	C18	C17	118.8(2)
C2	C1	C23	126.82(16)	C18	C19	C20	120.7(2)
O1	C2	C1	108.70(16)	C21	C20	C19	120.7(2)
O1	C2	C3	113.12(16)	C20	C21	C22	119.5(2)
C1	C2	C3	138.08(17)	C17	C22	C3	107.91(17)
C2	C3	C22	122.38(17)	C21	C22	C3	133.18(18)
C4	C3	C2	129.75(17)	C21	C22	C17	118.88(18)
C4	C3	C22	107.86(16)	C24	C23	C1	119.59(16)
C3	C4	C5	132.47(17)	C28	C23	C1	120.69(16)
C3	C4	C16	108.90(17)	C28	C23	C24	119.67(17)
C5	C4	C16	118.58(16)	C23	C24	C31	122.85(17)
C6	C5	C4	118.62(17)	C25	C24	C23	118.73(18)
C5	C6	C7	131.45(18)	C25	C24	C31	118.36(18)
C5	C6	C14	122.12(18)	C26	C25	C24	122.52(19)
C14	C6	C7	106.43(16)	C25	C26	C30	120.4(2)
C8	C7	C6	132.49(18)	C27	C26	C25	117.43(18)
C8	C7	C12	120.37(19)	C27	C26	C30	122.2(2)

C12	C7	C6	107.13(17)	C26	C27	C28	122.79(19)
C7	C8	C9	118.7(2)	C23	C28	C29	122.29(17)
C10	C9	C8	120.9(2)	C27	C28	C23	118.82(18)
C11	C10	C9	120.8(2)	C27	C28	C29	118.88(18)
C10	C11	C12	118.9(2)	C33	C32	C13	121.16(18)
C7	C12	C13	108.73(17)	C33	C32	C37	120.6(2)
C11	C12	C7	120.2(2)	C37	C32	C13	118.2(2)
C11	C12	C13	131.0(2)	C32	C33	C40	121.61(19)
C12	C13	C32	124.78(18)	C34	C33	C32	118.1(2)
C14	C13	C12	107.92(17)	C34	C33	C40	120.3(2)
C14	C13	C32	127.3(2)	C35	C34	C33	122.1(3)
C13	C14	C6	109.78(18)	C34	C35	C39	120.2(3)
C13	C14	C15	130.49(19)	C36	C35	C34	118.6(2)
C15	C14	C6	119.71(17)	C36	C35	C39	121.1(3)
C16	C15	C14	118.08(18)	C35	C36	C37	122.1(2)
C4	C16	C17	107.10(16)	C32	C37	C38	120.6(2)
C15	C16	C4	122.84(18)	C36	C37	C32	118.4(2)
C15	C16	C17	130.06(18)	C36	C37	C38	120.9(2)
C18	C17	C16	130.5(2)				

Table S22. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **4**.

Atom	***x***	***y***	***z***	**U(eq)**
H5	3812.44	4172.28	3952.05	45
H8	3021.93	5312.17	4483.91	59
H9	2315.5	6082.3	5140.84	71
H10	1947.86	5655.97	6143.19	76
H11	2236.94	4431.68	6497.09	67
H15	3862.1	2084.24	5425.25	52
H18	4576.85	957.71	4926.7	76
H19	5261.36	128.73	4311.62	84
H20	5714.76	516.03	3327.82	72
H21	5464.38	1724.98	2924.23	57
H25	3664.31	6185.91	3315.79	56
H27	5200.24	5588.42	4539.66	55
H29A	5492.53	3917.6	4242.63	72
H29B	6014.35	4631.84	4290.14	72
H29C	5957.11	4160.43	3635.49	72
H30A	4121.27	7123.28	4105.4	103
H30B	4661.27	6838.66	4644.3	103

H30C	3850.96	6585.81	4674.33	103
H31A	3930.03	5263.35	2092.85	77
H31B	3251.03	5343.15	2543.72	77
H31C	3611.3	4527.84	2441.38	77
H34	3578.65	2285.22	7725.96	80
H36	1645.04	1919.26	7008.11	86
H38A	1552.22	3161.31	5866.67	107
H38B	1336.44	2286.48	5955.87	107
H38C	1960.37	2512.76	5475.46	107
H39A	2639.57	1108.43	8057.5	162
H39B	1876.15	1497.31	8061.43	162
H39C	2516.24	1888.96	8437.61	162
H40A	4471.95	2722.25	6567.39	95
H40B	4370.92	3181.09	7224	95
H40C	4164.41	3571.01	6556.33	95

7. ^{1}H and ^{13}C NMR spectra of all compounds

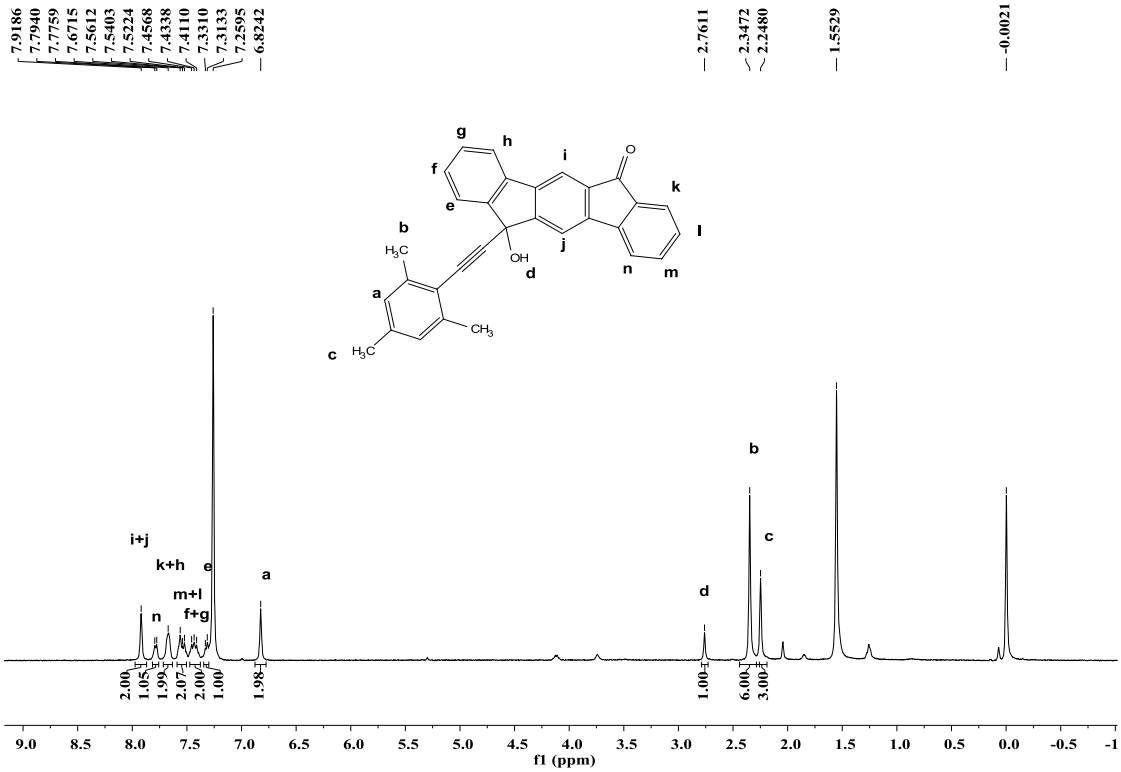


Fig. S10. ^{1}H NMR spectrum (400 M) of compound **2** in $CDCl_3$ at 298 K.

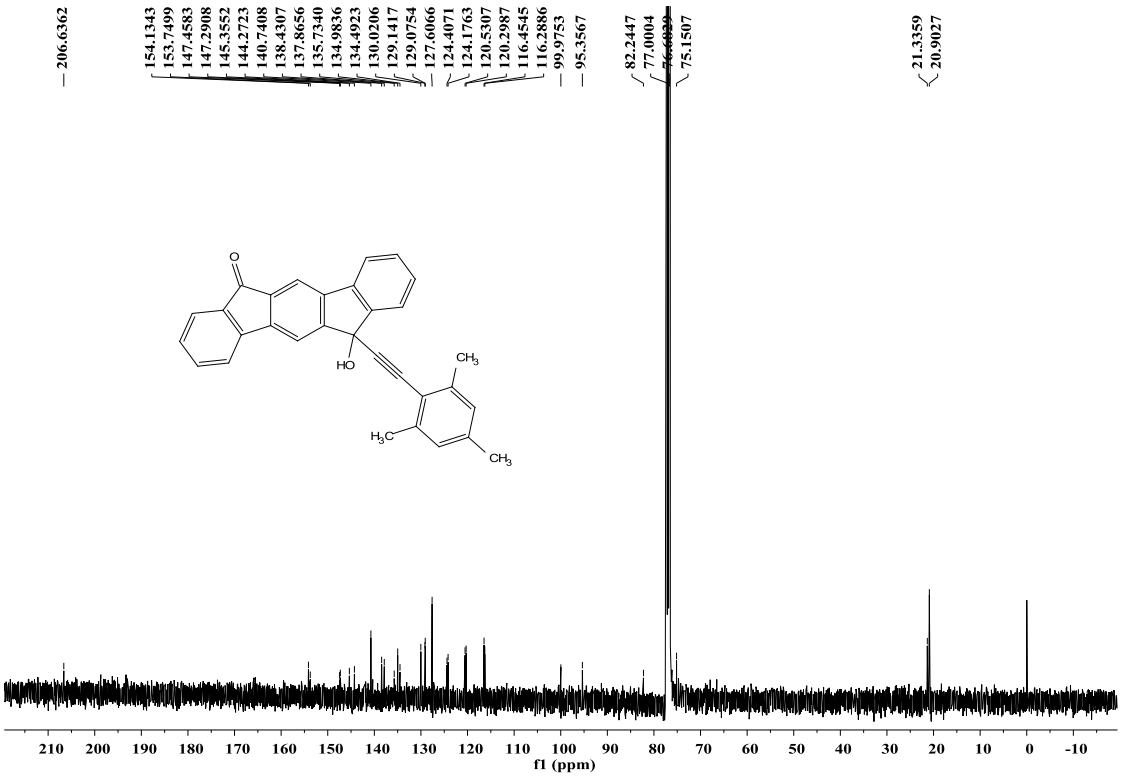


Fig. S11. ^{13}C NMR (100 M) spectrum of compound **2** in $CDCl_3$ at 298 K.

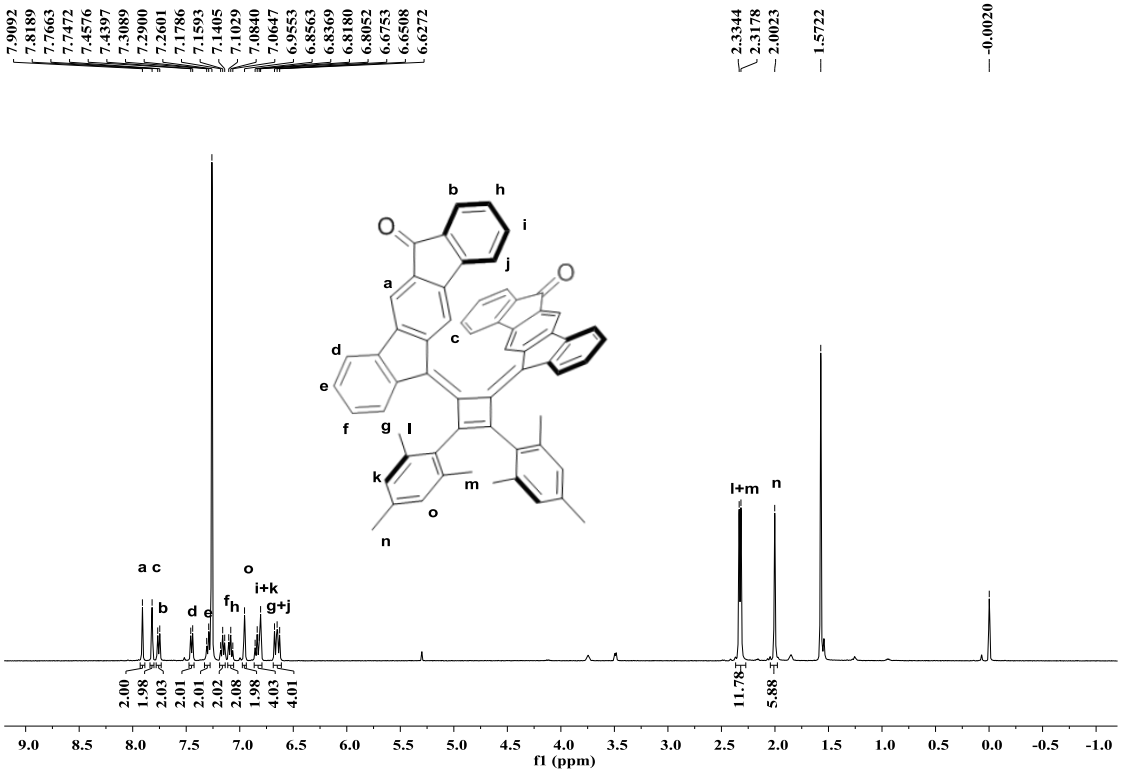


Fig. S12. ^{1}H NMR (400 M) spectrum of compound **3a** in $CDCl_3$ at 298 K.

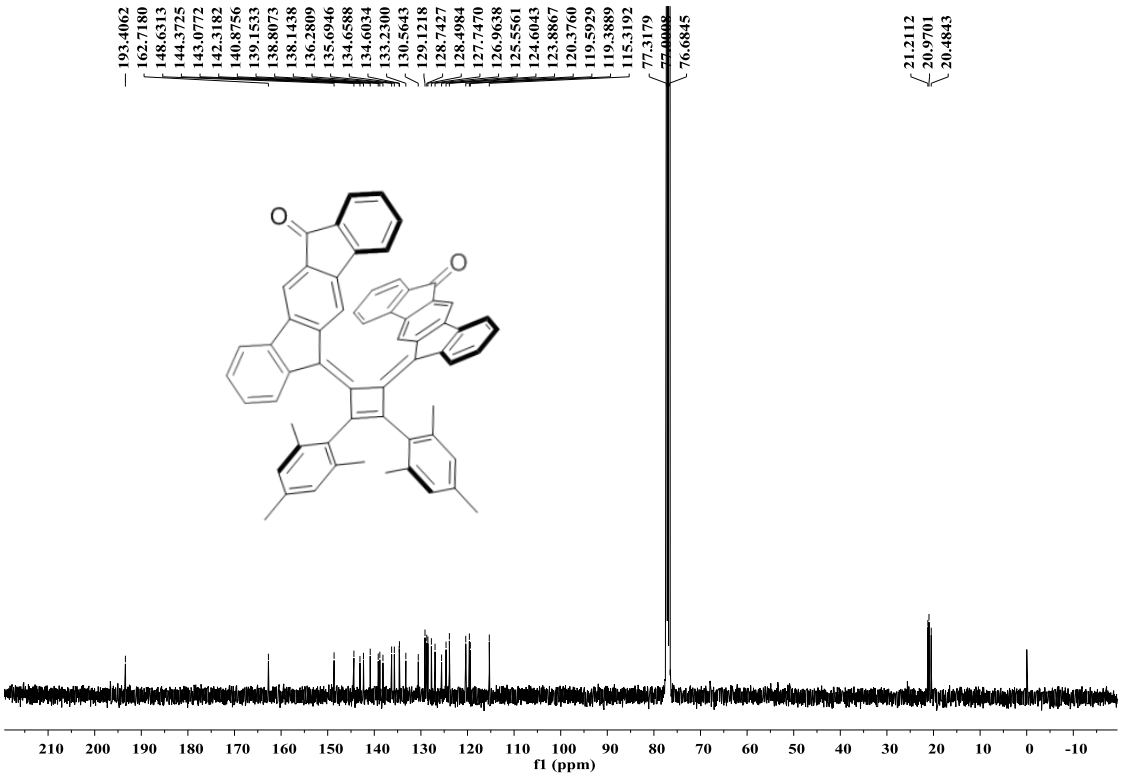


Fig. S13. ^{13}C NMR (100 M) spectrum of compound **3a** in $CDCl_3$ at 298 K.

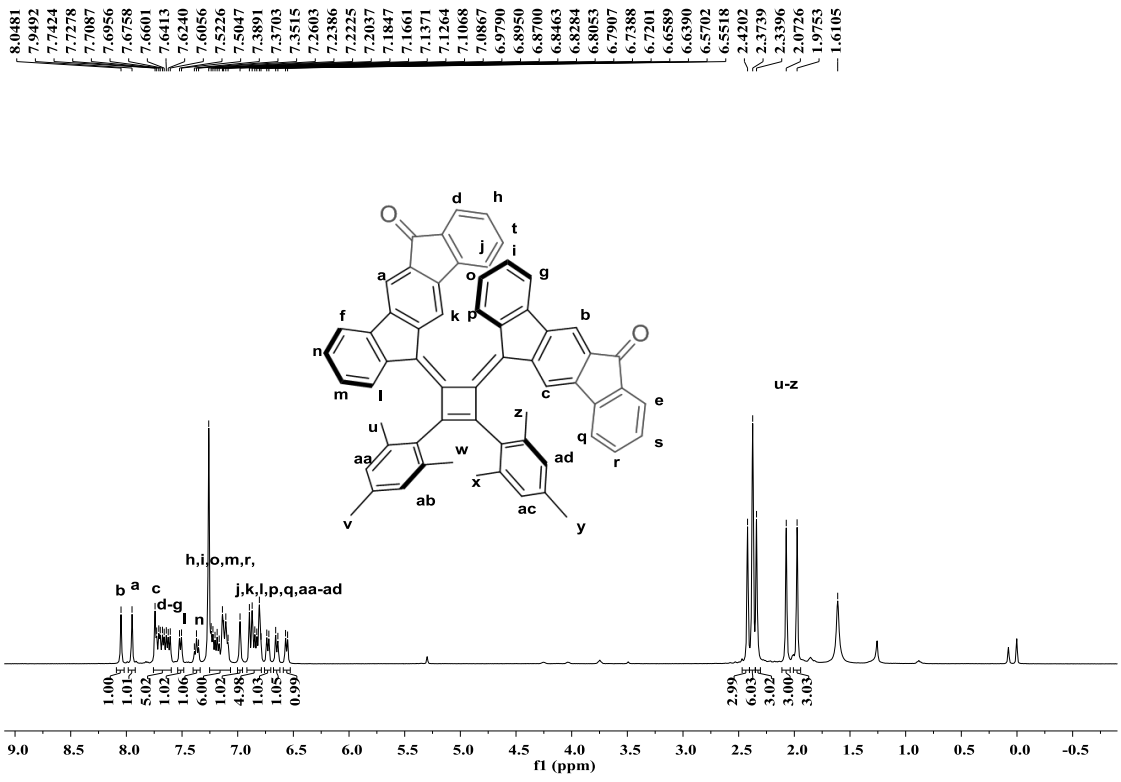


Fig. S14. ^{1}H NMR (400 M) spectrum of compound **3b** in $CDCl_3$ at 298 K.

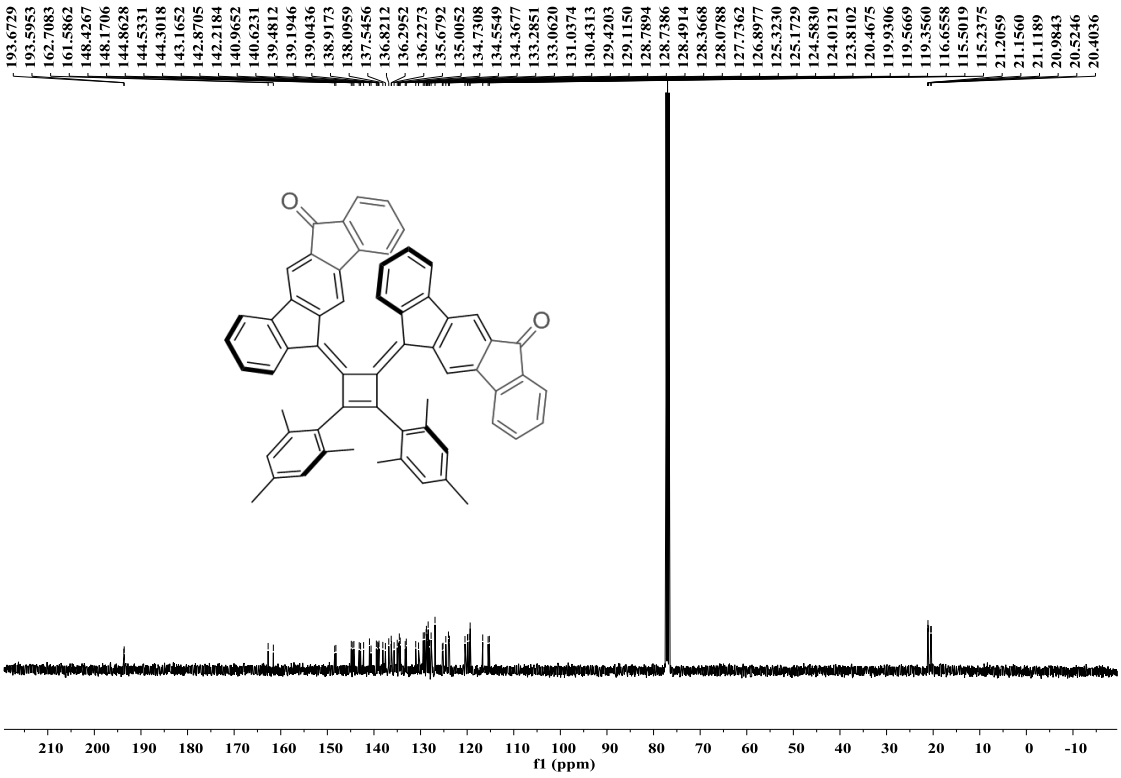


Fig. S15. ^{1}H NMR (400 M) spectrum of compound **3b** in $CDCl_3$ at 298 K.

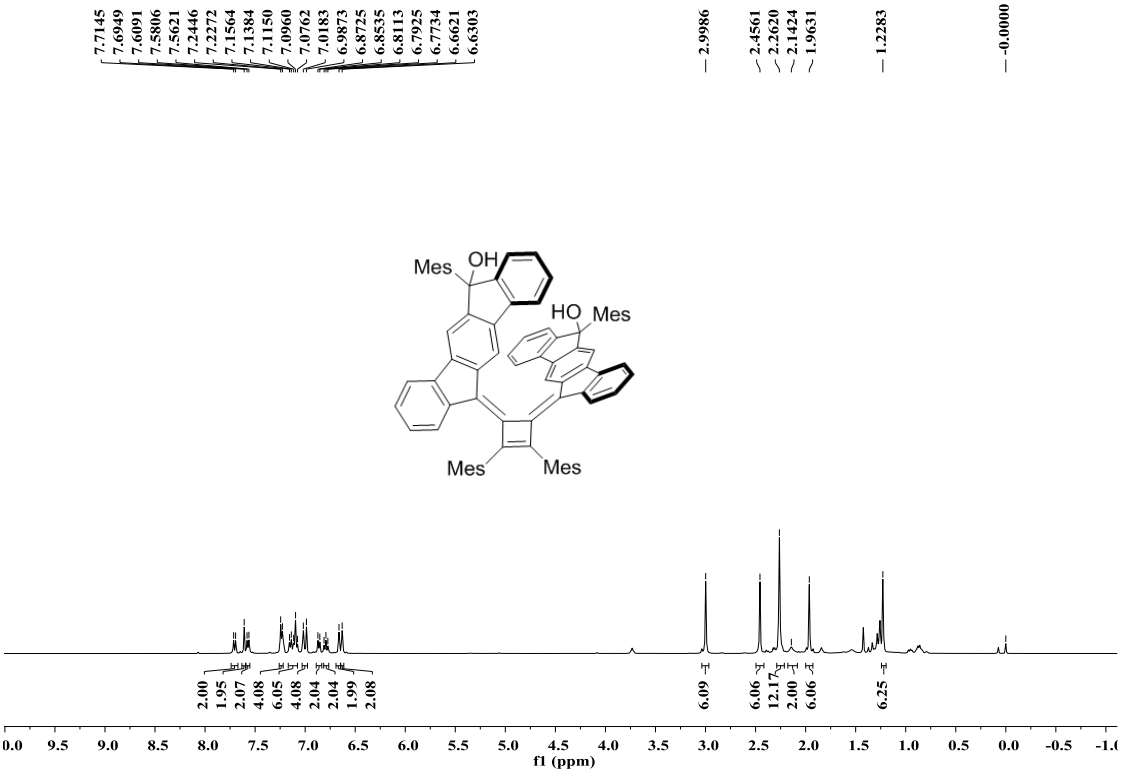


Fig. S16. ^{1}H NMR (400 M) spectrum of the alcohol precursor **H-a** in $CDCl_3$ at 298 K.

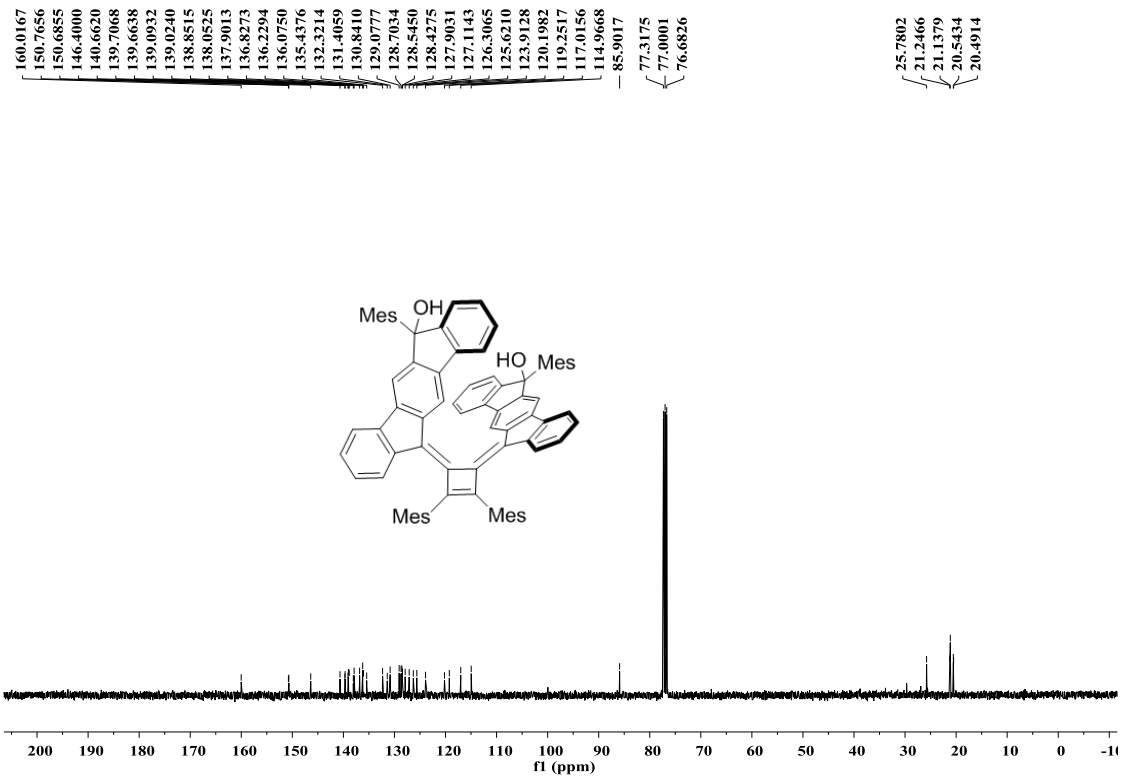


Fig. S17. ^{13}C NMR (100 M) spectrum of the alcohol precursor **H-a** in $CDCl_3$ at 298 K.

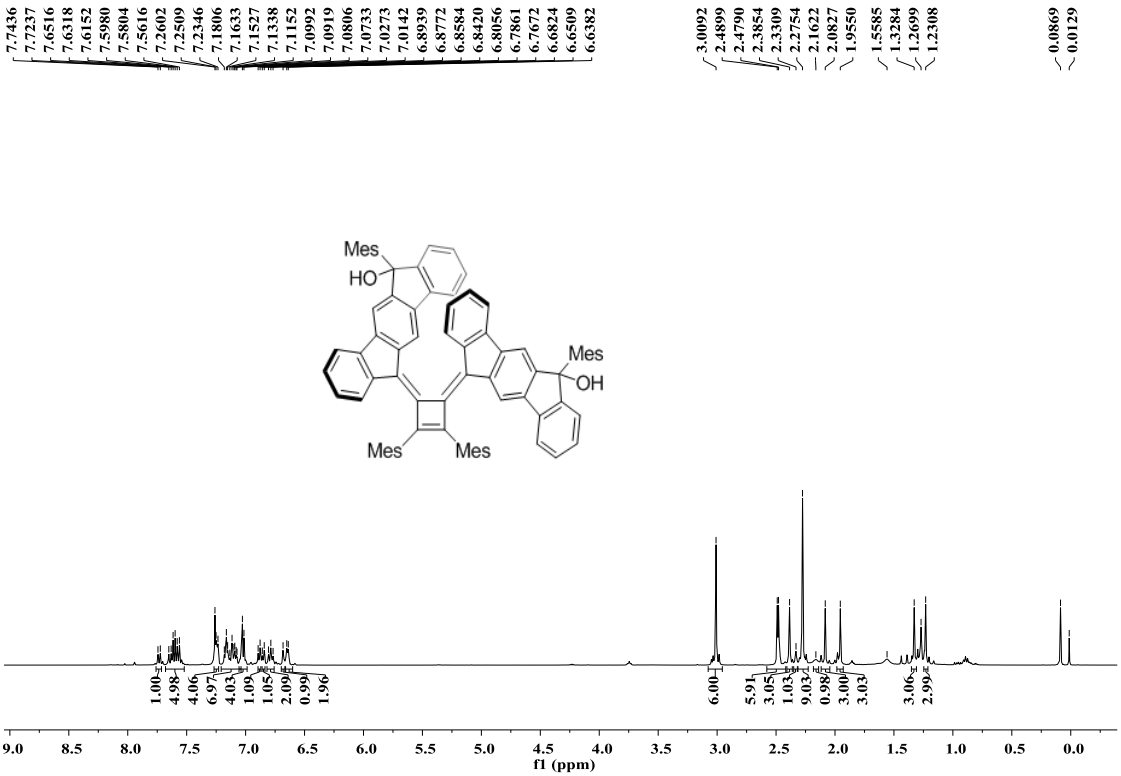


Fig. S18. ^{1}H NMR (400 M) spectrum of the alcohol precursor **H-b** in $CDCl_3$ at 298 K.

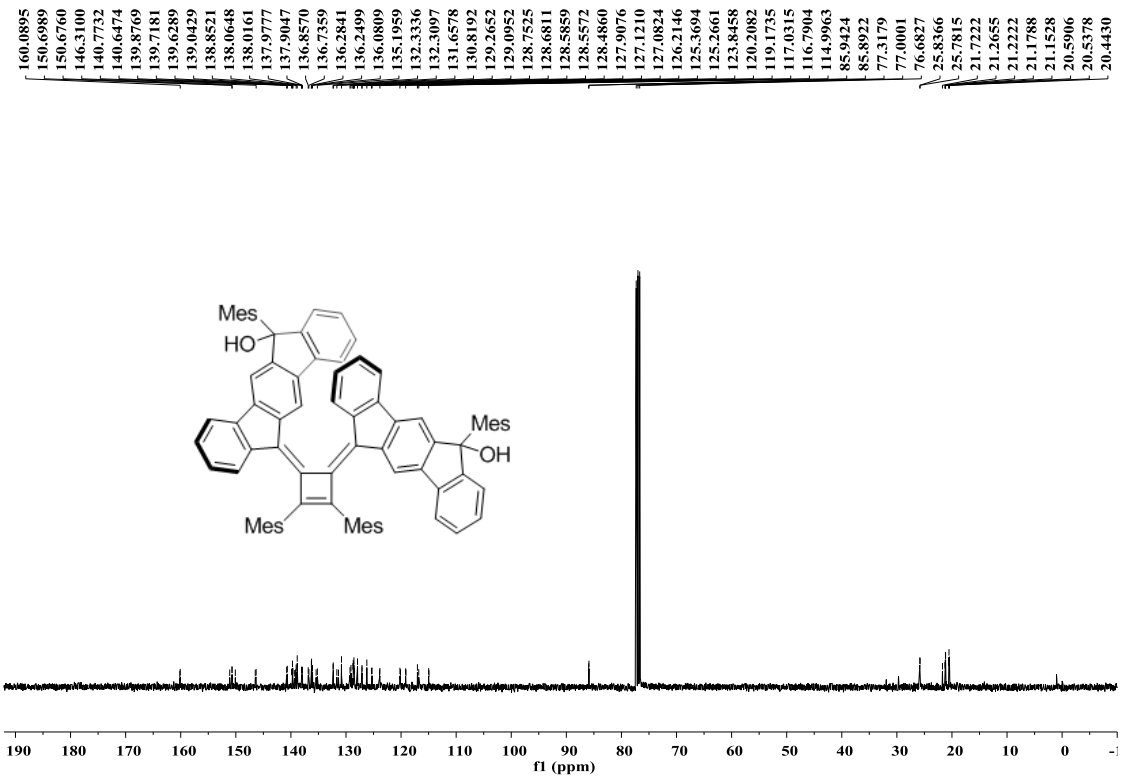


Fig. S19. ^{13}C NMR (100 M) spectrum of the alcohol precursor **H-b** in $CDCl_3$ at 298 K.

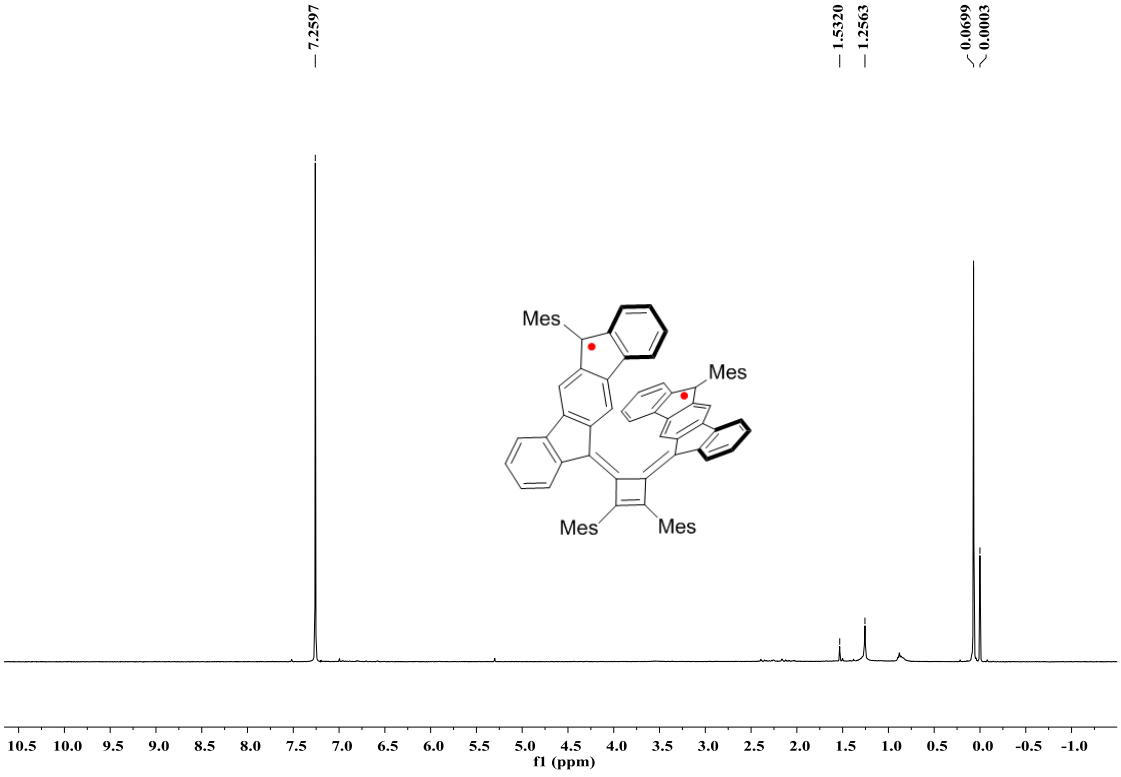


Fig. S20. ^{1}H NMR (400 M) spectrum of compound **CQ-IF-a** in $CDCl_3$ at 213 K.

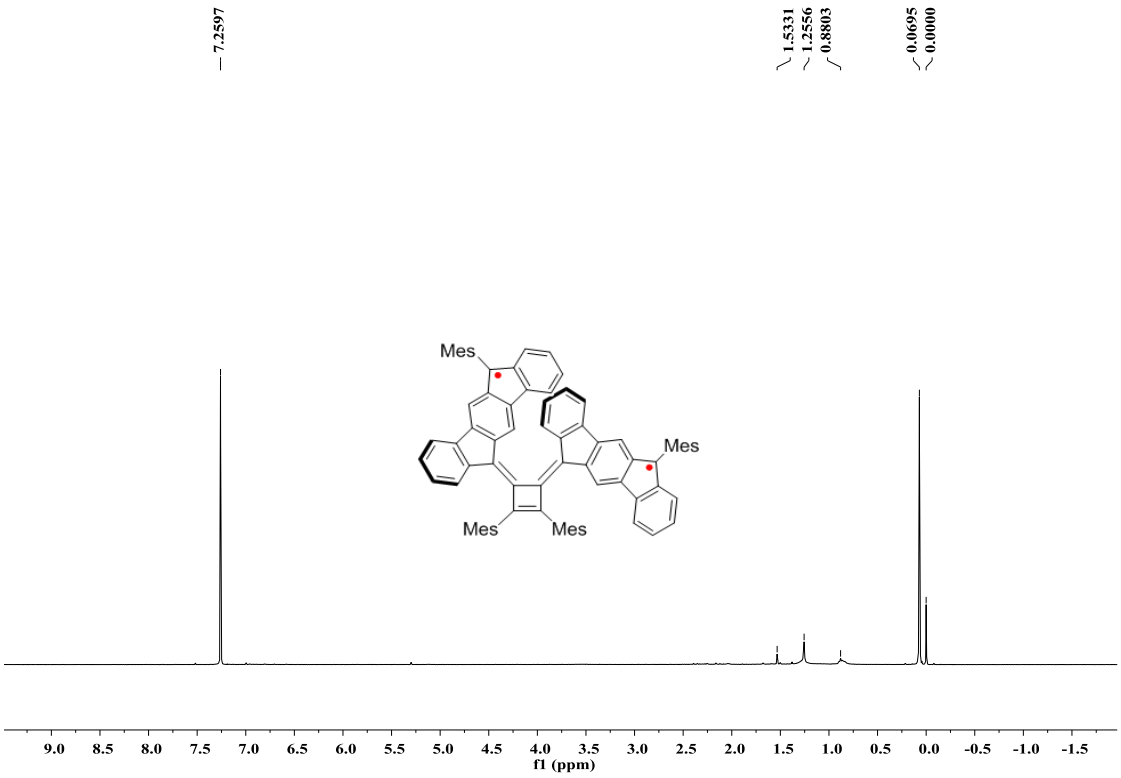


Fig. S21. ^{1}H NMR (400 M) spectrum of compound **CQ-IF-b** in $CDCl_3$ at 213 K.

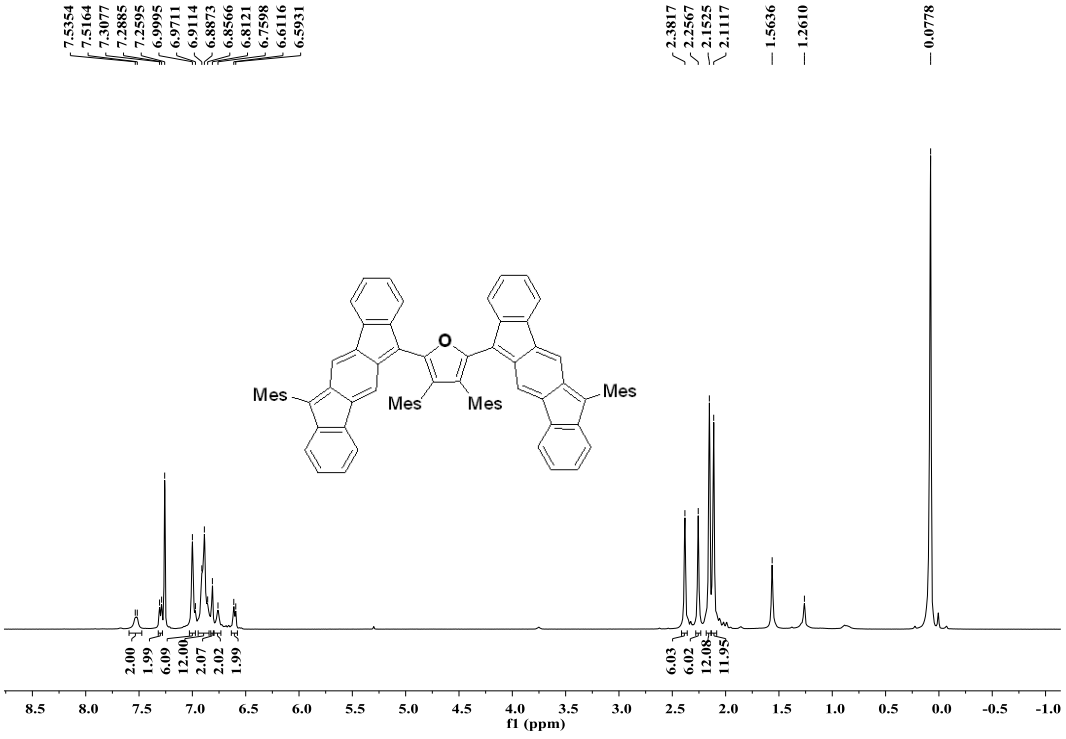


Fig. S22. ^{1}H NMR (400 M) spectrum of compound **4** in $CDCl_3$ at 298 K.

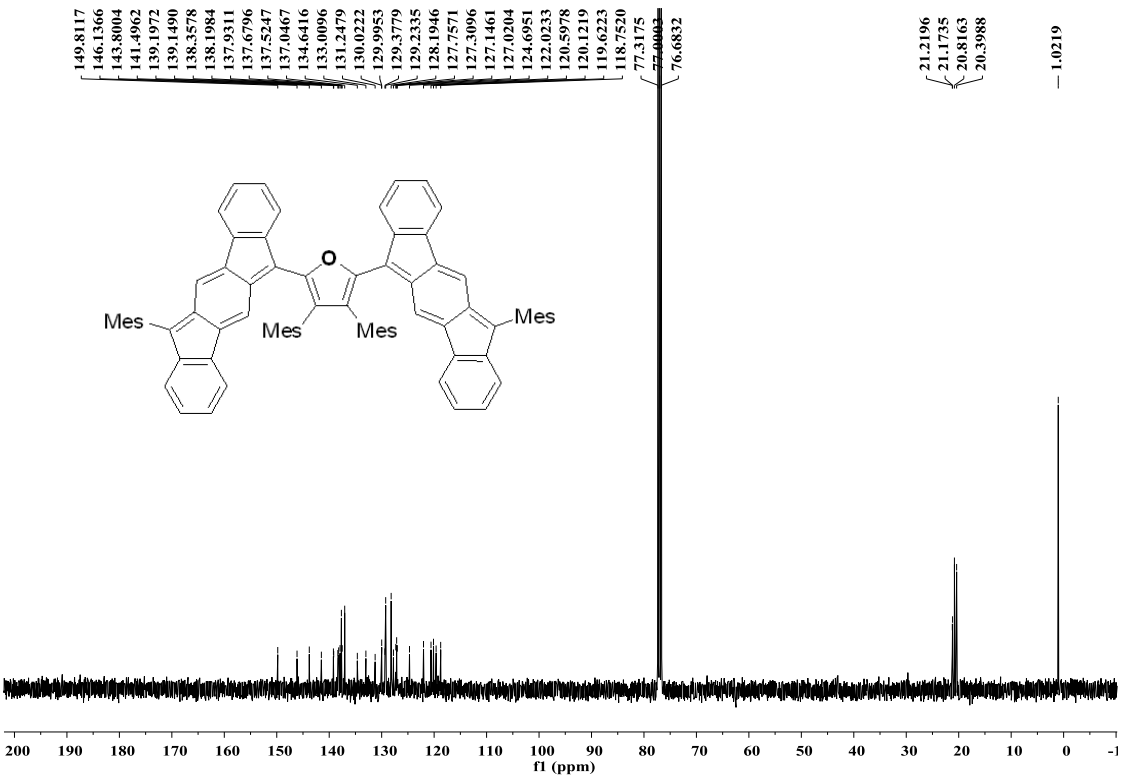


Fig. S23. ^{13}C NMR (100 M) spectrum of compound **4** in $CDCl_3$ at 298 K.

8. Mass spectra of all compounds

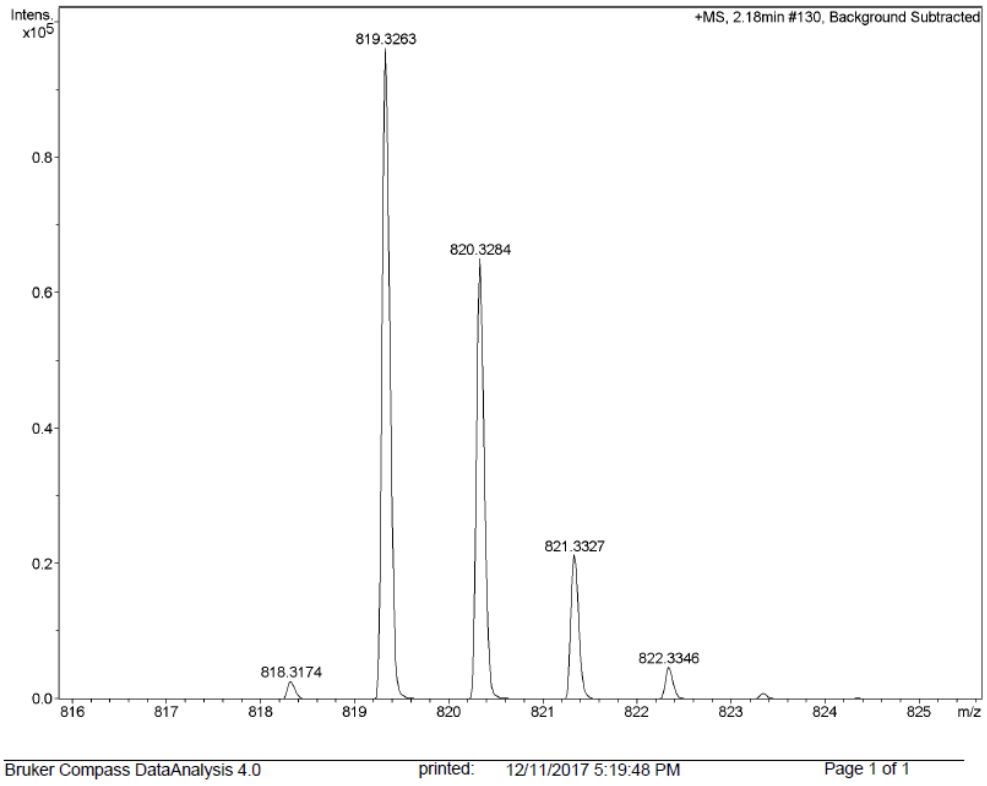


Fig. S24. HR mass spectrum (APCI) of compound **3a**

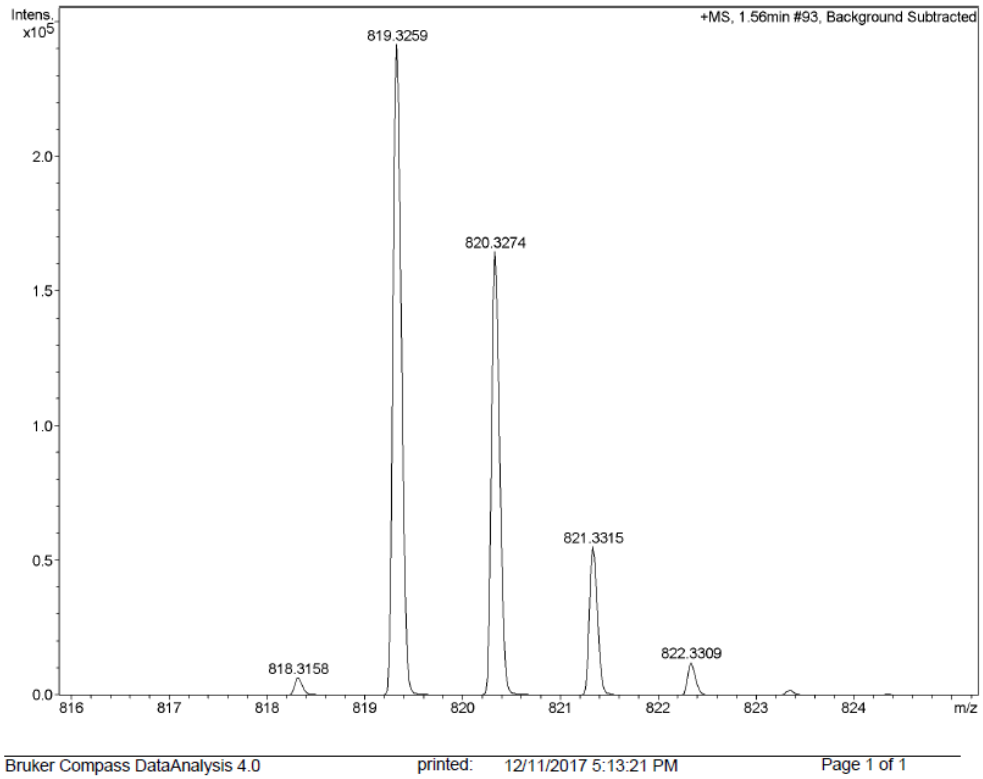


Fig. S25. HR mass spectrum (APCI) of compound **3b**

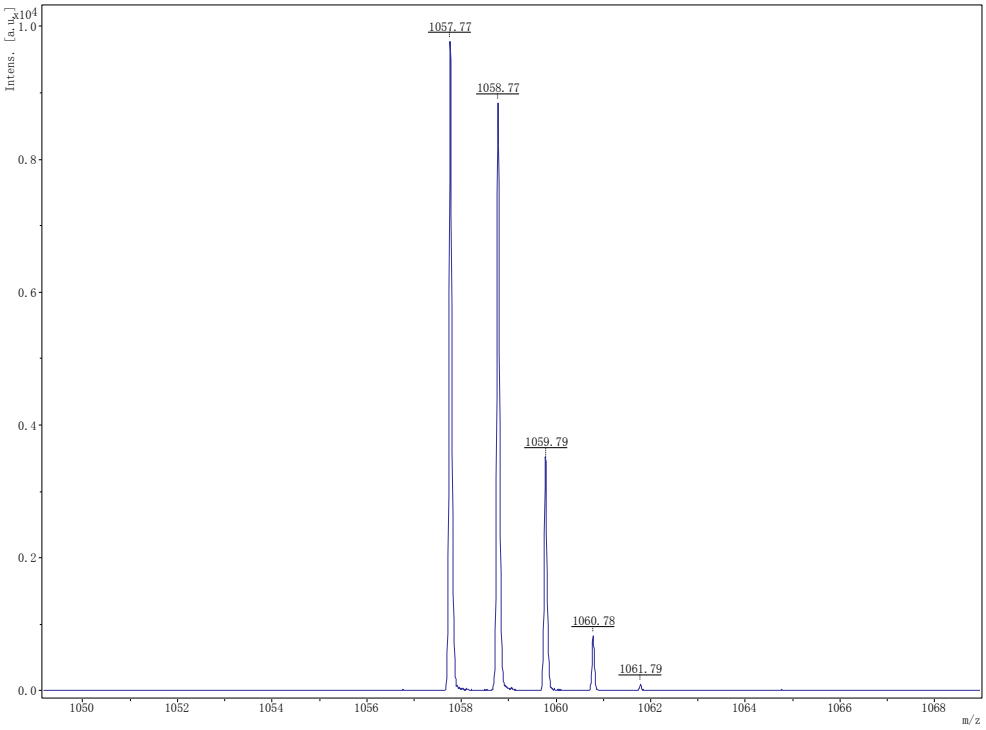


Fig. S26. Mass spectrum (MALDI-TOF) of the alcohol precursor **H-a**

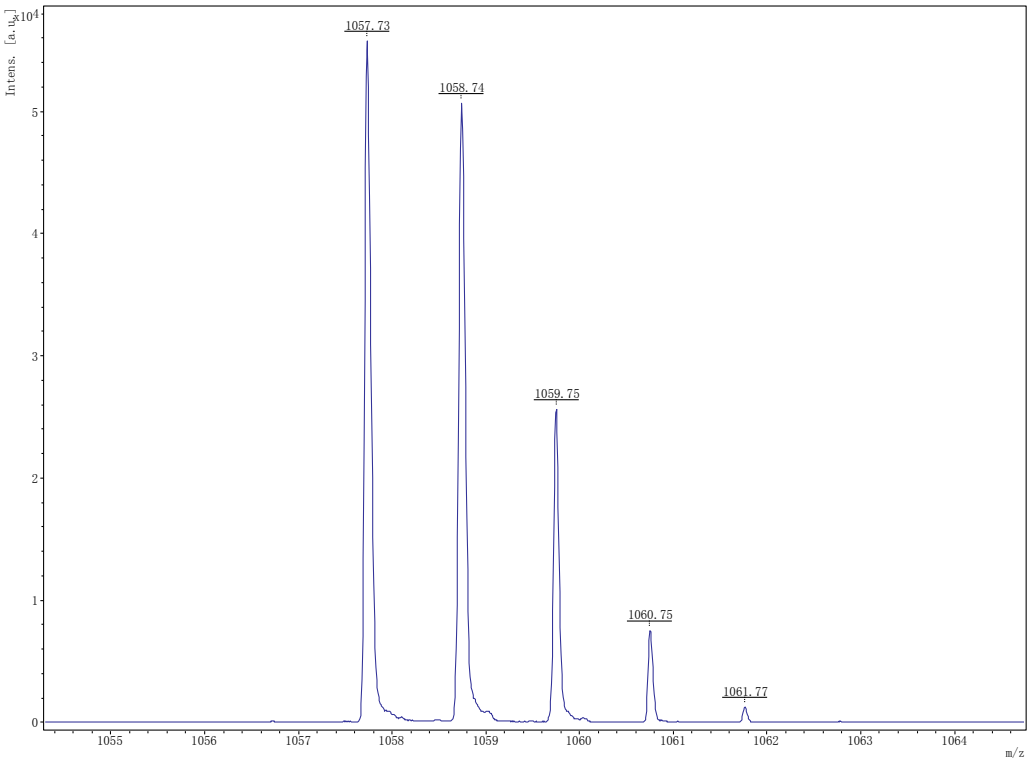


Fig. S27. Mass spectrum (MALDI-TOF) of the alcohol precursor of **H-b**

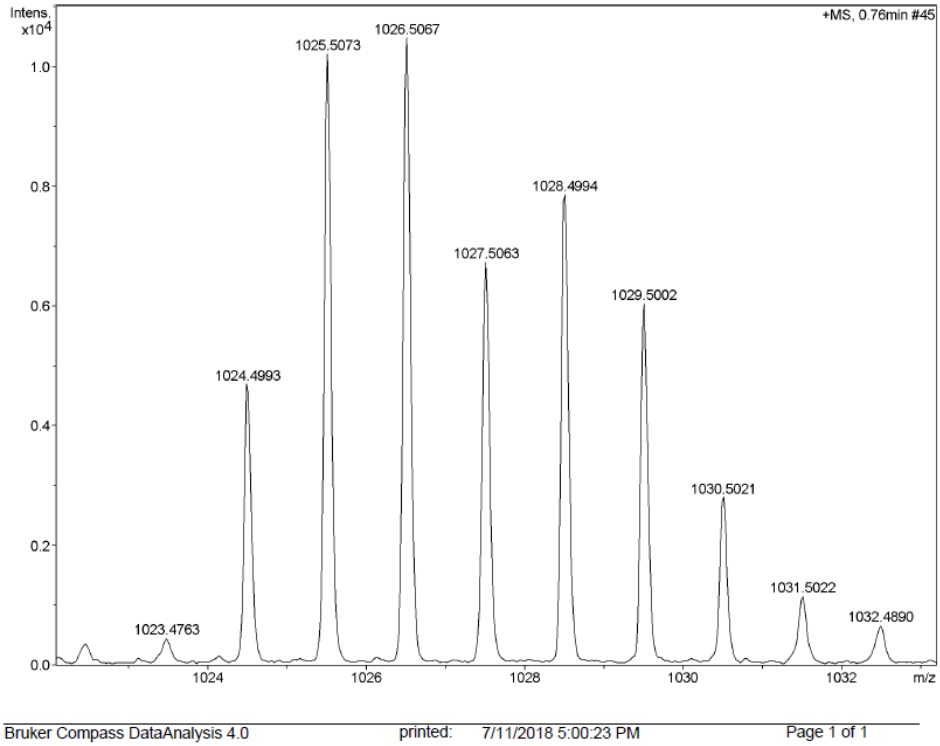


Fig. S28. Mass spectrum (MALDI-TOF) of compound **CQ-IF-a**

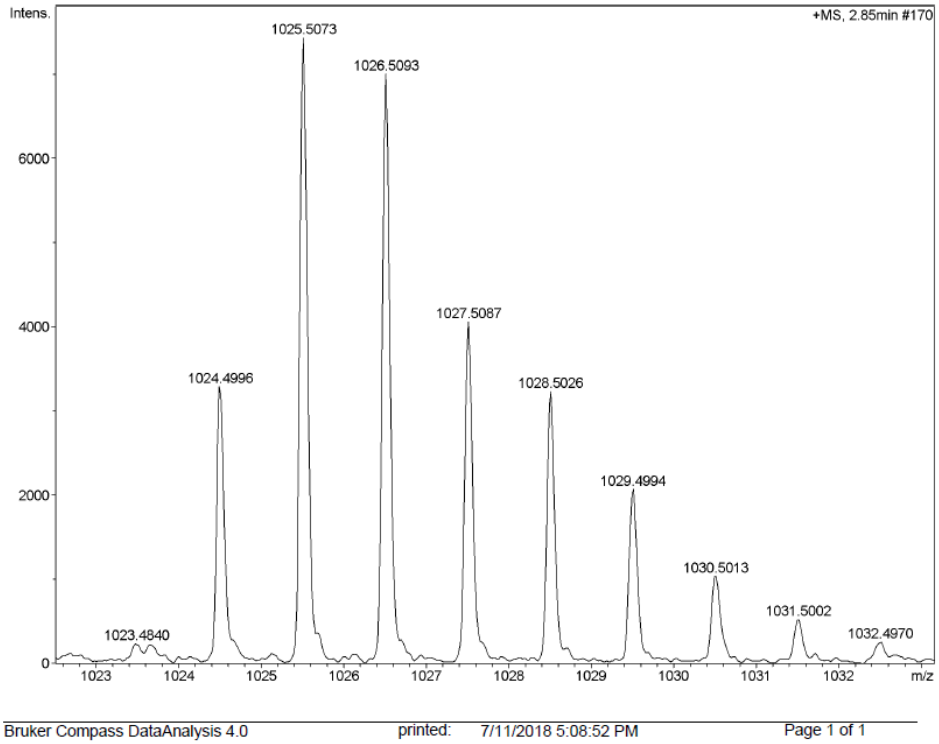


Fig. S29. Mass spectrum (MALDI-TOF) of compound **CQ-IF-b**

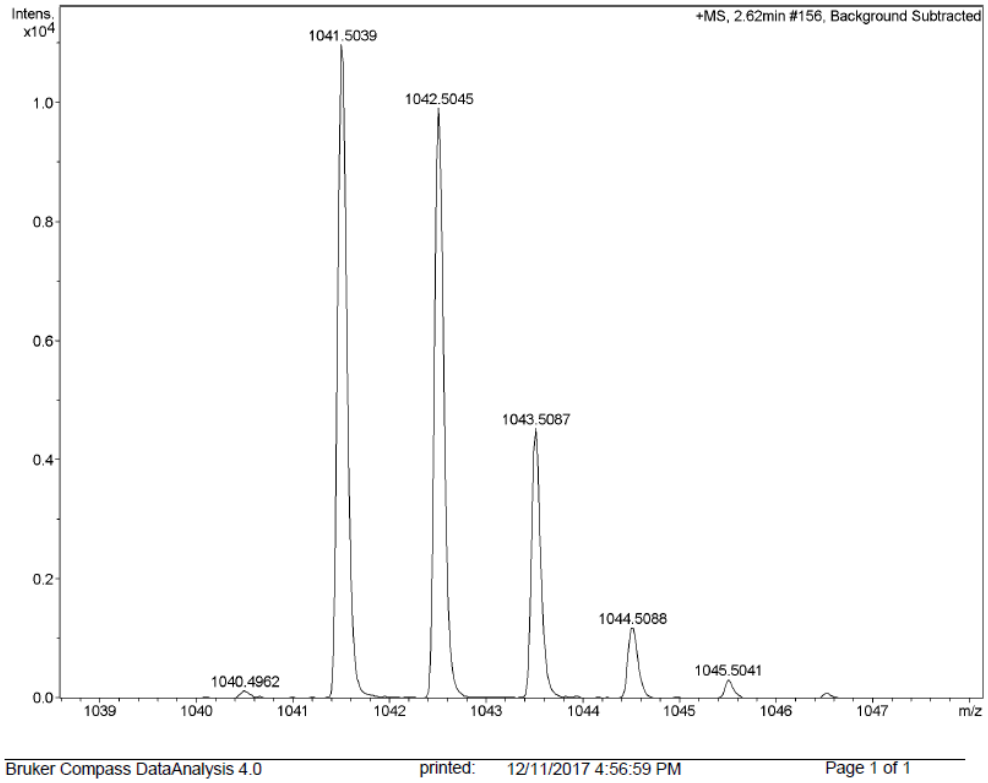


Fig. S30. HR mass spectrum (APCI) of compound **4**

9. HPLC curves of the targets

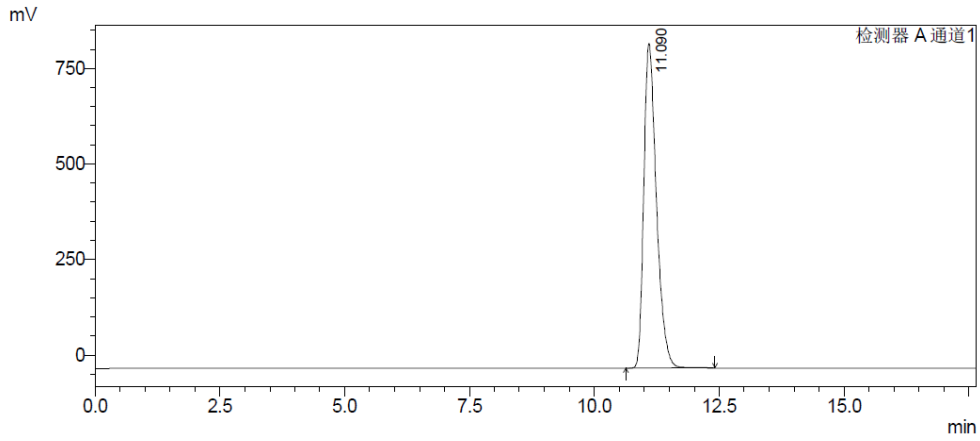


Fig. S31 Representative HPLC curve of compound **CQ-IF-a**. Inertsil PREP-SIL column (10 × 250 mm), hexane/DCM = 50/50 as eluent, flow rate 3 mL min^{-1}, and detection wavelength is 530 nm.

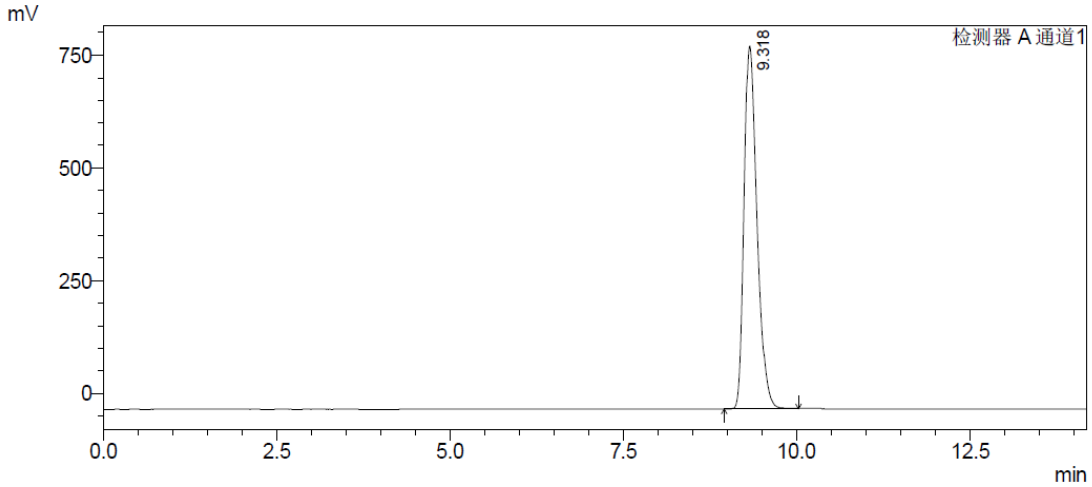


Fig. S32 Representative HPLC curve of compound **CQ-IF-b**. Inertsil PREP-SIL column (10 × 250 mm), hexane/DCM = 50/50 as eluent, flow rate 3 mL min^{-1}, and detection wavelength is 530 nm.

10. References

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11. Cartesian coordinates for all atoms of optimized geometries

CQ-IF-a (Singlet, UCAM-B3LYP/6-31G(d,p))

C	-1.89754800	0.17569200	-0.08976500
C	-1.54707200	-1.27071000	-0.05693700
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CQ-IF-a (Triplet, UCAM-B3LYP/6-31G(d,p))

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C	-4.35989700	0.36917400	-1.08695900
C	0.16667200	1.58137900	0.41873400
C	0.35830500	2.91715600	0.82794600
C	-0.95141500	3.52768900	1.06215500
C	-1.94520100	2.56086300	0.76988000
C	-4.42401100	1.70021500	-1.71032700
C	-5.76174000	1.96949800	-2.09219200
C	-6.57836300	0.80854100	-1.73373500
C	-5.74215800	-0.17124800	-1.15991100
C	-7.94388700	0.59941700	-1.86188000
C	-8.48718700	-0.59699300	-1.40573900
C	-7.67232200	-1.55646600	-0.81045300
C	-6.30311100	-1.34615000	-0.66966500
C	-3.39880800	2.59010400	-2.05433600

C	-3.74412600	3.77460800	-2.66954600
C	-5.10197100	4.07773700	-2.98989900
C	-6.11667600	3.14993000	-2.72260500
C	1.26956200	0.81008400	0.06633100
C	2.54570600	1.35498900	0.18168400
C	2.72858400	2.66573700	0.61454000
C	1.63110500	3.45962900	0.93048600
C	-1.27732500	4.79405400	1.51708300
C	-2.63360800	5.09419500	1.69664500
C	-3.62930700	4.09631000	1.47154700
C	-3.29354700	2.83307700	1.03281800
C	-0.35409200	-2.05231100	0.32379900
C	-3.43160500	-2.97129000	-0.63642100
C	-3.81200400	-3.32846100	-1.94500800
C	-4.36142800	-4.58764700	-2.16676900
C	-4.56100700	-5.49963400	-1.13524900
C	-4.19223400	-5.12099100	0.15104100
C	-3.62516200	-3.87814200	0.42048000
C	0.31398700	-2.85050100	-0.62212000
C	1.42915700	-3.58197100	-0.22357600
C	1.89634200	-3.55910300	1.08654600
C	1.22254500	-2.76227500	2.00597800
C	0.11160400	-2.00184200	1.65190300
C	-2.93140000	4.91833400	-3.09476700
C	-3.81255700	5.87947800	-3.65750000
C	-5.16143600	5.37019700	-3.59716300
C	-1.57499200	5.17415800	-3.01142000
C	-1.08865600	6.39082400	-3.49755100
C	-1.95071400	7.33849800	-4.05159200
C	-3.31784600	7.09443600	-4.13283500
C	-3.26951900	6.30127100	2.12307500
C	-4.68953500	6.04735500	2.16450300
C	-4.92950600	4.70437300	1.77016900
C	-5.75597800	6.88666900	2.48877000
C	-7.04998800	6.37985800	2.42667800
C	-7.28073100	5.05894200	2.03942600
C	-6.22031100	4.21253200	1.70452200
C	-2.60036800	7.58125300	2.43622400
C	-6.38142000	6.06981200	-4.05226100
C	-7.23354500	6.67631900	-3.11301700
C	-8.37800600	7.32909600	-3.56318800
C	-8.70128800	7.39983000	-4.91498200
C	-7.84590700	6.79014900	-5.82770300
C	-6.69053100	6.12827200	-5.42142000

C	-2.12593400	8.39795200	1.39481000
C	-1.49767600	9.59914800	1.71251400
C	-1.32673700	10.01474700	3.02967800
C	-1.80018100	9.18979100	4.04533700
C	-2.43622300	7.98175400	3.77289300
C	-2.30348900	7.99874600	-0.04770900
C	-2.91790700	7.11027400	4.90456000
C	-0.67167100	11.33364700	3.34522000
C	-5.80063800	5.46565000	-6.44176800
C	-6.91465400	6.64144600	-1.64034000
C	-9.92843800	8.13956900	-5.37869700
H	-8.58018500	1.36011300	-2.30350400
H	-9.55306900	-0.77742300	-1.50106900
H	-8.10803800	-2.47949200	-0.44215400
H	-5.69591200	-2.09672900	-0.18181300
H	-2.36497000	2.35788000	-1.83423900
H	-7.14305100	3.35502300	-3.01192600
H	1.15323300	-0.20262200	-0.29526300
H	3.40711500	0.74852500	-0.07840000
H	3.73105500	3.07410300	0.69230400
H	1.76898100	4.48964300	1.24456000
H	-0.51383500	5.53425500	1.73707700
H	-4.05207500	2.07532300	0.88584400
H	-4.64802700	-4.85960600	-3.17938800
H	-4.35024300	-5.81230900	0.97453100
H	1.94822500	-4.18693800	-0.96235600
H	1.57416600	-2.72354200	3.03370400
H	-0.89590600	4.45078000	-2.57036500
H	-0.02580400	6.60242100	-3.44059400
H	-1.54891800	8.27685700	-4.42008100
H	-3.99255500	7.83373700	-4.55347200
H	-5.57377600	7.91676000	2.77949200
H	-7.89049800	7.01825300	2.67911500
H	-8.29815500	4.68409400	1.99456900
H	-6.41398300	3.19094800	1.39173000
H	-9.03377100	7.79872900	-2.83436700
H	-8.08561600	6.82555600	-6.88744300
H	-1.13423900	10.22954100	0.90484400
H	-1.66729200	9.49115900	5.08131500
H	-1.73128800	7.10135700	-0.29844500
H	-3.34967500	7.77226900	-0.27276800
H	-1.97990600	8.79788000	-0.71738100
H	-2.63755600	7.53563000	5.87040200
H	-2.49313700	6.10438700	4.83924900

H	-4.00537900	6.99451900	4.88878000
H	0.08274400	11.59311300	2.59837100
H	-0.18753500	11.31462100	4.32464000
H	-1.40711000	12.14540000	3.36044100
H	-6.22519800	5.55206900	-7.44409300
H	-4.80283300	5.91333300	-6.45688700
H	-5.66572200	4.40305200	-6.21973200
H	-7.62665600	7.24236200	-1.07139100
H	-5.91115400	7.02883800	-1.44143100
H	-6.94017300	5.62473400	-1.23895300
H	-10.72718300	8.09351000	-4.63430300
H	-9.70774300	9.19812900	-5.55417000
H	-10.31285700	7.72782200	-6.31507500
C	3.08147500	-4.38949200	1.50130300
H	2.76721500	-5.38754300	1.82526400
H	3.78402700	-4.52195200	0.67500300
H	3.61838800	-3.93018100	2.33461500
C	-0.13125100	-2.91097500	-2.05987500
H	-1.05668300	-3.48325800	-2.16629000
H	-0.31669400	-1.91289300	-2.46596400
H	0.63020500	-3.38998400	-2.67865900
C	-5.13829800	-6.86269700	-1.40893400
H	-4.35696000	-7.56504600	-1.71869200
H	-5.61755300	-7.27863800	-0.51969500
H	-5.88009100	-6.82788400	-2.21064700
C	-3.66174500	-2.38193500	-3.10799100
H	-4.49777600	-1.67778900	-3.14647300
H	-2.74599900	-1.79196400	-3.04379600
H	-3.64755600	-2.93265100	-4.05097900
C	-3.26003000	-3.52749200	1.83919400
H	-2.17599800	-3.51980800	1.98066300
H	-3.63232200	-2.53788300	2.11787300
H	-3.68239300	-4.25427600	2.53600400
C	-0.54241900	-1.13382900	2.69570600
H	-0.19321900	-0.10038200	2.61606700
H	-1.62884000	-1.11586900	2.59487700
H	-0.29856900	-1.49071800	3.69861700

CQ-IF-b (Singlet, UCAM-B3LYP/6-31G(d,p))

C	-1.86692200	0.57487500	-0.25292800
C	-1.57624100	-0.88714600	-0.19671900
C	-2.90750700	-1.20882700	-0.13541900
C	-3.32281100	0.21433000	-0.29287800
C	-1.12745400	1.70545900	-0.08910200

C	-4.49434900	0.83511400	-0.59940100
C	-1.57983800	3.00352200	0.46945100
C	-0.47757000	3.87716500	0.53735300
C	0.69764300	3.18740700	0.00312200
C	0.31100500	1.86832600	-0.35367500
C	-4.67824800	2.07950000	-1.35873500
C	-6.06791000	2.31488200	-1.52559100
C	-6.79719000	1.24709400	-0.83988700
C	-5.86164300	0.34234100	-0.29981500
C	-8.15975600	1.06193900	-0.65704400
C	-8.59590700	-0.03198600	0.08345800
C	-7.67553300	-0.91123900	0.64860100
C	-6.30691800	-0.72389900	0.47452600
C	-3.74211200	2.89730800	-2.00699900
C	-4.20770600	3.96507000	-2.74379100
C	-5.60638200	4.22378500	-2.87949200
C	-6.54420500	3.37633900	-2.27397000
C	-2.79689700	3.39152200	1.01956600
C	-2.91776900	4.66317800	1.57084900
C	-1.83384200	5.53775400	1.59782800
C	-0.60050400	5.14367400	1.09086300
C	1.99043600	3.64474500	-0.17937700
C	2.92442100	2.76420700	-0.74266100
C	2.53034500	1.44673400	-1.12716400
C	1.23417500	1.00513600	-0.95985900
C	-0.34442200	-1.69496200	-0.10014000
C	-3.61269600	-2.50564100	-0.09615300
C	-4.34288500	-2.93797700	-1.21924200
C	-4.98256500	-4.17413500	-1.17217800
C	-4.93543200	-4.98864800	-0.04661600
C	-4.21875400	-4.53632300	1.05725900
C	-3.55049800	-3.31606000	1.05247600
C	0.01867200	-2.56964000	-1.14047100
C	1.20422600	-3.29192800	-1.03437700
C	2.03981700	-3.18023900	0.07331900
C	1.65080000	-2.32727800	1.10023300
C	0.48096000	-1.57543600	1.03437100
C	-3.49986200	4.99443600	-3.51186100
C	-4.48103700	5.83813200	-4.09592900
C	-5.79137100	5.36988100	-3.70991800
C	-2.15436900	5.23927800	-3.71446400
C	-1.78052700	6.32586700	-4.50926200
C	-2.74116000	7.15705600	-5.08634100
C	-4.09742900	6.92434100	-4.88247300

C	4.31039700	2.94241700	-1.03736000
C	4.79034500	1.70738400	-1.61181500
C	3.71627000	0.78127100	-1.67626800
C	6.05685900	1.34912600	-2.07423600
C	6.24560200	0.06984700	-2.58680500
C	5.18860000	-0.83973200	-2.64071400
C	3.91463700	-0.48936800	-2.18540600
C	5.11026000	4.16232900	-0.79676100
C	-7.08346100	5.96995200	-4.10495000
C	-7.80626200	6.75181800	-3.18806800
C	-9.02051700	7.30798200	-3.58133600
C	-9.53900400	7.11271800	-4.85775600
C	-8.81034100	6.33139200	-5.74962300
C	-7.59156800	5.75813200	-5.39802900
C	5.99519700	4.21831700	0.29352600
C	6.73576100	5.37764500	0.50628100
C	6.62777100	6.48244200	-0.33299800
C	5.74423300	6.40809100	-1.40546000
C	4.98388800	5.26860700	-1.65378000
C	6.12933600	3.05266600	1.23964200
C	4.05220300	5.22781000	-2.83820100
C	7.46304900	7.71413500	-0.10251300
C	-6.84605900	4.90215400	-6.38972100
C	-7.27571300	7.00436000	-1.79994500
C	-10.83916300	7.75032700	-5.27132000
H	-8.87466300	1.76403900	-1.07480100
H	-9.65850500	-0.19192900	0.23538300
H	-8.02591300	-1.75017200	1.24090400
H	-5.60979700	-1.40582900	0.94303000
H	-2.68189800	2.69182700	-1.93688400
H	-7.60856100	3.54311300	-2.41096400
H	-3.64298500	2.71748200	1.02796700
H	-3.86991500	4.97333900	1.98853600
H	-1.94829900	6.52553300	2.03235000
H	0.25399800	5.81139200	1.14134600
H	2.28034600	4.65359100	0.09910100
H	0.94604600	0.01481000	-1.28569600
H	-5.54007800	-4.50500100	-2.04458300
H	-4.17667300	-5.15161900	1.95219700
H	1.48275400	-3.96086000	-1.84459800
H	2.28246400	-2.23219200	1.97954600
H	-1.39724700	4.60703700	-3.26068300
H	-0.72758400	6.52793800	-4.67687800
H	-2.42530200	7.99678600	-5.69685700

H	-4.84733000	7.57514000	-5.32171000
H	6.87647900	2.06006100	-2.03444800
H	7.22482100	-0.22498100	-2.94987700
H	5.35748200	-1.83237400	-3.04598500
H	3.10005200	-1.20613600	-2.22817200
H	-9.57493700	7.91408300	-2.86927600
H	-9.20352500	6.15708300	-6.74803200
H	7.41221100	5.41987700	1.35614500
H	5.64447700	7.26083700	-2.07224900
H	5.15888500	2.76545900	1.65458700
H	6.53051900	2.16909300	0.73507100
H	6.79454900	3.29910100	2.06974100
H	4.15586100	6.12956000	-3.44509900
H	3.00677900	5.14824300	-2.52660500
H	4.25824400	4.36287900	-3.47514800
H	7.69240900	7.84794800	0.95746600
H	6.95336400	8.61379100	-0.45593400
H	8.41710800	7.64890100	-0.63685900
H	-7.41938800	4.78506300	-7.31161500
H	-5.87571100	5.33606500	-6.64698000
H	-6.64783000	3.90617000	-5.98319700
H	-7.91342000	7.70903600	-1.26225100
H	-6.26302100	7.41631900	-1.83142300
H	-7.22211600	6.08192500	-1.21476900
H	-11.50531600	7.88899900	-4.41632400
H	-10.67020800	8.73682500	-5.71662200
H	-11.36231900	7.14359600	-6.01456100
C	-5.61727800	-6.33066800	-0.02909300
H	-4.92442600	-7.12686800	-0.32204500
H	-5.98958200	-6.57551800	0.96876900
H	-6.46034300	-6.35906400	-0.72322900
C	-2.79757800	-2.88316900	2.28336400
H	-1.71675400	-2.93605400	2.12698700
H	-3.03624300	-1.85285700	2.56111500
H	-3.04357400	-3.52598900	3.13099700
C	-4.47109600	-2.09977600	-2.46519800
H	-5.29589000	-1.38747400	-2.37075300
H	-3.56806800	-1.52300500	-2.66984700
H	-4.67647300	-2.73142700	-3.33234100
C	3.34445200	-3.92750700	0.13920300
H	3.30070100	-4.86109600	-0.42684200
H	4.15539600	-3.32323100	-0.28215800
H	3.61701300	-4.16584300	1.17006100
C	-0.82862800	-2.72242300	-2.37653300

H	-1.75858700	-3.25417100	-2.15901300
H	-1.10064500	-1.75175300	-2.80039600
H	-0.29285600	-3.28546500	-3.14337800
C	0.15281500	-0.63877900	2.16853900
H	0.53097700	0.36675700	1.96227500
H	-0.92159600	-0.55160400	2.33528800
H	0.61619500	-0.98290800	3.09585300

CQ-IF-b (Triplet, UCAM-B3LYP/6-31G(d,p))

C	-1.86610300	0.58293300	-0.26018800
C	-1.57824600	-0.88016900	-0.20520200
C	-2.90621900	-1.20067700	-0.13246600
C	-3.32544100	0.22172300	-0.29237100
C	-1.12664400	1.70971700	-0.09575200
C	-4.49538600	0.83880600	-0.59781300
C	-1.57563600	3.00913300	0.46289800
C	-0.47029600	3.87844800	0.53534600
C	0.70416300	3.18645900	0.00247600
C	0.31613200	1.87033200	-0.35801200
C	-4.68222000	2.08673000	-1.35793400
C	-6.07100400	2.31654400	-1.52751300
C	-6.79880000	1.24664600	-0.84370400
C	-5.86288700	0.34352500	-0.30184900
C	-8.16162100	1.05907900	-0.66394600
C	-8.59763800	-0.03521500	0.07579900
C	-7.67691600	-0.91240800	0.64366500
C	-6.30830900	-0.72262800	0.47260400
C	-3.74832200	2.90637600	-2.00452600
C	-4.21653700	3.97279500	-2.74331600
C	-5.61469700	4.22599800	-2.88175300
C	-6.55006200	3.37663500	-2.27821400
C	-2.79221600	3.40055800	1.01178500
C	-2.90962200	4.67148000	1.56538100
C	-1.82257600	5.54209100	1.59636700
C	-0.58977000	5.14438300	1.09129300
C	1.99925800	3.64200300	-0.17675300
C	2.93104300	2.76179800	-0.74096200
C	2.53519100	1.44768500	-1.13054800
C	1.23699100	1.00804400	-0.96620400
C	-0.34690200	-1.69011800	-0.11585800
C	-3.60971600	-2.49844500	-0.08387600
C	-4.34205700	-2.93764000	-1.20286100
C	-4.97921300	-4.17479900	-1.14774500
C	-4.92792100	-4.98333700	-0.01810500

C	-4.20961200	-4.52384900	1.08172500
C	-3.54346800	-3.30249800	1.06886700
C	0.01063200	-2.56298600	-1.15946100
C	1.19510300	-3.28790300	-1.05925300
C	2.03475200	-3.18054600	0.04577500
C	1.65132000	-2.32878600	1.07576600
C	0.48297000	-1.57414500	1.01573500
C	-3.51052300	5.00397100	-3.51059500
C	-4.49324400	5.84426100	-4.09795800
C	-5.80201100	5.37302900	-3.71502100
C	-2.16537700	5.25288100	-3.71023200
C	-1.79291500	6.33996900	-4.50507400
C	-2.75474600	7.16785500	-5.08533500
C	-4.11060900	6.93126200	-4.88466000
C	4.32064600	2.93766400	-1.03316100
C	4.79717500	1.70429500	-1.61080600
C	3.72021800	0.78128300	-1.68037600
C	6.06355700	1.34365700	-2.07305500
C	6.24910900	0.06599600	-2.59023800
C	5.18926200	-0.84023600	-2.64921100
C	3.91566400	-0.48783900	-2.19431100
C	5.12265900	4.15451700	-0.78530700
C	-7.09562200	5.96761000	-4.11277300
C	-7.82449200	6.74503300	-3.19684300
C	-9.04047300	7.29571400	-3.59243000
C	-9.55497900	7.09923100	-4.87027500
C	-8.82042600	6.32231800	-5.76115500
C	-7.59972200	5.75459700	-5.40725600
C	6.00631900	4.20315100	0.30639800
C	6.74856100	5.36007900	0.52632900
C	6.64348200	6.46958300	-0.30706500
C	5.76115800	6.40252500	-1.38103500
C	4.99922200	5.26570700	-1.63644100
C	6.13728200	3.03223100	1.24644100
C	4.06920400	5.23263500	-2.82239500
C	7.48043600	7.69866800	-0.06888500
C	-6.84796500	4.90306300	-6.39807700
C	-7.29823700	6.99900500	-1.80736900
C	-10.85725500	7.73089500	-5.28630000
H	-8.87667800	1.76001600	-1.08338500
H	-9.66029700	-0.19693000	0.22541600
H	-8.02704300	-1.75147400	1.23593600
H	-5.61121000	-1.40259900	0.94390300
H	-2.68755500	2.70474400	-1.93269800

H	-7.61478800	3.53906700	-2.41742200
H	-3.64064200	2.72950000	1.01766700
H	-3.86150300	4.98418000	1.98178000
H	-1.93429100	6.52938300	2.03271300
H	0.26719300	5.80867900	1.14508400
H	2.29057000	4.64944900	0.10525600
H	0.94730700	0.01968400	-1.29650800
H	-5.53837700	-4.51111700	-2.01701200
H	-4.16431400	-5.13429300	1.97981100
H	1.46929500	-3.95555400	-1.87198900
H	2.28652200	-2.23662200	1.95284000
H	-1.40739900	4.62343300	-3.25401000
H	-0.74018700	6.54516500	-4.67021200
H	-2.43984600	8.00802100	-5.69574200
H	-4.86138400	7.57947600	-5.32621700
H	6.88520600	2.05202100	-2.02949600
H	7.22789500	-0.23045100	-2.95315000
H	5.35571000	-1.83174300	-3.05826000
H	3.09901200	-1.20198800	-2.24125800
H	-9.59951000	7.89841100	-2.88108800
H	-9.21046400	6.14699700	-6.76062300
H	7.42395200	5.39661900	1.37729500
H	5.66363800	7.25901300	-2.04335500
H	5.16548300	2.74286800	1.65669900
H	6.53999200	2.15140000	0.73830400
H	6.79988800	3.27393300	2.08002100
H	4.17395400	6.13812600	-3.42350300
H	3.02332800	5.15132300	-2.51278000
H	4.27599400	4.37164600	-3.46443200
H	7.71076500	7.82502300	0.99179100
H	6.97157300	8.60132000	-0.41580900
H	8.43398800	7.63592200	-0.60443300
H	-7.41985200	4.78203200	-7.32036100
H	-5.88022700	5.34304200	-6.65483800
H	-6.64368300	3.90848900	-5.99110700
H	-7.94158800	7.69861100	-1.26978000
H	-6.28827100	7.41780100	-1.83644200
H	-7.23947700	6.07605100	-1.22351800
H	-11.52610400	7.86548300	-4.43275400
H	-10.69207200	8.71864100	-5.73025100
H	-11.37567700	7.12233900	-6.03136300
C	-5.60719600	-6.32651300	0.00798900
H	-4.91396800	-7.12267600	-0.28416700
H	-5.97516600	-6.56764600	1.00835100

H	-6.45287800	-6.35955200	-0.68275200
C	-2.78794100	-2.86218600	2.29545100
H	-1.70751000	-2.91781500	2.13732800
H	-3.02466800	-1.82972000	2.56666600
H	-3.03324900	-3.49893700	3.14784300
C	-4.47700100	-2.10585100	-2.45245000
H	-5.31006600	-1.40270300	-2.36199800
H	-3.58039600	-1.51967700	-2.65800900
H	-4.67389400	-2.74324900	-3.31738500
C	3.33793600	-3.93086000	0.10564000
H	3.29091500	-4.86206000	-0.46404500
H	4.14918900	-3.32654200	-0.31506000
H	3.61231700	-4.17389300	1.13491500
C	-0.84160400	-2.71181900	-2.39256700
H	-1.76967100	-3.24609100	-2.17315400
H	-1.11701800	-1.73992700	-2.81132100
H	-0.30823700	-3.27088700	-3.16398100
C	0.16273200	-0.63766000	2.15233300
H	0.54954600	0.36497500	1.94796900
H	-0.91069600	-0.54158100	2.31989100
H	0.62368400	-0.98783500	3.07861500

CQ-IF-a (Close-shell, RCAM-B3LYP/6-31G(d,p))

C	-2.80786200	-0.77115300	-0.18528900
C	-4.16721800	-0.74734800	-0.17786500
C	-4.16717800	0.74731700	0.17801700
C	-2.80782500	0.77103400	0.18548500
C	-1.80241100	-1.76124200	-0.38315300
C	-1.80231400	1.76104300	0.38346600
C	-1.89095800	-2.89323300	-1.33206800
C	-0.68172300	-3.61770000	-1.27860800
C	0.18321000	-2.96572700	-0.29418500
C	-0.56062800	-1.82958100	0.23724200
C	-0.56055600	1.82939600	-0.23695800
C	0.18341900	2.96535200	0.29469400
C	-0.68140800	3.61717700	1.27930800
C	-1.89072900	2.89284100	1.33261600
C	-0.47591200	4.71855600	2.09459000
C	-1.48704600	5.10033100	2.97338400
C	-2.67671900	4.37893100	3.03877000
C	-2.88648700	3.26679300	2.22658500
C	0.01969600	1.02244900	-1.27276900
C	1.28261800	1.29853500	-1.67282100
C	2.04433900	2.40817000	-1.10441800

C	1.44167800	3.25330100	-0.11504500
C	-2.88675100	-3.26725700	-2.22596700
C	-2.67711800	-4.37960400	-3.03790300
C	-1.48754100	-5.10114400	-2.97234200
C	-0.47636200	-4.71929100	-2.09363400
C	1.44148000	-3.25368200	0.11552400
C	2.04434500	-2.40829700	1.10455100
C	1.28273100	-1.29852400	1.67280200
C	0.01976500	-1.02248200	1.27285100
C	-5.23893600	-1.73816800	-0.34039700
C	-5.23883500	1.73820500	0.34054100
C	-5.29805600	2.87577000	-0.48774100
C	-6.34007500	3.78361400	-0.31173500
C	-7.31798000	3.60905200	0.66045900
C	-7.23355900	2.48550800	1.47920100
C	-6.22049100	1.54533200	1.33436300
C	-6.22054200	-1.54525800	-1.33427600
C	-7.23364800	-2.48537600	-1.47914200
C	-7.31816400	-3.60890900	-0.66037900
C	-6.34032500	-3.78349900	0.31186300
C	-5.29825900	-2.87570100	0.48790300
C	2.16282700	0.64834200	-2.64697100
C	3.38757300	1.35518600	-2.63725300
C	3.29298400	2.45270200	-1.67038900
C	1.99472600	-0.45605300	-3.46498400
C	3.05416300	-0.85155600	-4.28314200
C	4.26225200	-0.15618700	-4.27429900
C	4.44127700	0.95142300	-3.44764000
C	3.29311600	-2.45267700	1.67029500
C	3.38788500	-1.35486000	2.63681500
C	2.16312500	-0.64805000	2.64659300
C	4.44181600	-0.95066600	3.44670000
C	4.26296100	0.15723500	4.27299800
C	3.05482200	0.85251900	4.28195500
C	1.99518800	0.45665100	3.46423700
C	4.37804600	-3.41287700	1.36293700
C	4.37794800	3.41291400	-1.36308400
C	5.12299800	3.27968300	-0.17921200
C	6.13929800	4.19538200	0.08445400
C	6.43857100	5.23546400	-0.78932900
C	5.68659500	5.35062700	-1.95500500
C	4.66397400	4.45716100	-2.25937300
C	5.12125800	-3.28126900	0.17770900
C	6.13761200	-4.19691200	-0.08596400

C	6.43871000	-5.23541000	0.78906700
C	5.68851500	-5.34902300	1.95604300
C	4.66592800	-4.45555300	2.26049300
C	4.84610400	-2.16596400	-0.79860900
C	3.86478800	-4.62887200	3.52533700
C	7.56285500	-6.19410000	0.49688600
C	3.86084700	4.63200900	-3.52273800
C	4.84976800	2.16253700	0.79552900
C	7.56267800	6.19423400	-0.49724700
H	0.45644900	5.27344000	2.05420300
H	-1.34400100	5.96247200	3.61669500
H	-3.45178000	4.68402700	3.73429000
H	-3.81353300	2.71134600	2.29361600
H	-0.54450700	0.20618500	-1.70753700
H	1.99809600	4.09636000	0.28441900
H	-3.81372200	-2.71170600	-2.29314300
H	-3.45221200	-4.68475400	-3.73336200
H	-1.34460200	-5.96345200	-3.61545400
H	0.45593300	-5.27427800	-2.05311900
H	1.99775800	-4.09693300	-0.28372800
H	-0.54435100	-0.20611700	1.70753500
H	-6.38465800	4.65654800	-0.95753800
H	-7.97599200	2.33870300	2.25951100
H	-7.97603800	-2.33854400	-2.25948800
H	-6.38499100	-4.65641300	0.95768600
H	1.06217500	-1.01233000	-3.46894500
H	2.93623600	-1.71326700	-4.93210100
H	5.07339400	-0.48338200	-4.91686100
H	5.38498400	1.48804500	-3.43172400
H	5.38559400	-1.48716100	3.43064600
H	5.07428500	0.48474500	4.91517000
H	2.93703000	1.71446700	4.93062200
H	1.06261900	1.01290000	3.46821400
H	6.71577000	4.08826300	0.99980400
H	5.89800100	6.16239600	-2.64650600
H	6.71267900	-4.09099200	-1.00233800
H	5.90129900	-6.15959600	2.64852200
H	3.88586900	-2.28970200	-1.30729000
H	4.80784600	-1.19643600	-0.29485900
H	5.62202100	-2.11914100	-1.56501800
H	4.19208400	-5.51328200	4.07572400
H	2.79858100	-4.73854700	3.30694700
H	3.96288400	-3.76278300	4.18596200
H	7.73614000	-6.29027700	-0.57764900

H	7.35278900	-7.18903500	0.89744400
H	8.50010900	-5.85248600	0.94952900
H	4.18844400	5.51608100	-4.07348700
H	3.95647200	3.76591800	-4.18372000
H	2.79519000	4.74322900	-3.30241000
H	5.62527800	2.11650300	1.56239400
H	4.81423300	1.19358400	0.29042700
H	3.88887600	2.28335600	1.30364300
H	7.73813400	6.28800700	0.57714700
H	8.49921500	5.85432500	-0.95264900
H	7.35111100	7.18996600	-0.89503000
C	-8.44789800	-4.59180600	-0.81340500
H	-9.34649500	-4.24211400	-0.29372200
H	-8.71533000	-4.73096100	-1.86406100
H	-8.18703700	-5.56735300	-0.39704800
C	-6.15995600	-0.36868600	-2.27440600
H	-6.41767500	0.56582700	-1.76947100
H	-5.15665600	-0.24424200	-2.69288100
H	-6.85677300	-0.50228800	-3.10437300
C	-8.44769300	4.59199200	0.81335800
H	-9.34565100	4.24325800	0.29192300
H	-8.71653000	4.72970900	1.86383800
H	-8.18604600	5.56807100	0.39873300
C	-4.27407600	3.13683200	-1.56106900
H	-3.34471600	3.52809800	-1.13732300
H	-4.01605800	2.22601700	-2.10604000
H	-4.64822000	3.87192300	-2.27674900
C	-6.16003100	0.36873000	2.27446400
H	-6.41795100	-0.56572800	1.76952700
H	-5.15672200	0.24410200	2.69285900
H	-6.85676200	0.50243100	3.10448700
C	-4.27434100	-3.13680100	1.56128000
H	-3.34501200	-3.52819700	1.13758400
H	-4.01624100	-2.22597900	2.10619700
H	-4.64858400	-3.87180600	2.27699700

CQ-IF-b (Close-shell, RCAM-B3LYP/6-31G(d,p))

C	-0.17623900	1.88868500	0.72335600
C	-0.76416400	3.26535000	0.26606600
C	0.47655700	3.77265300	0.15098700
C	1.09112500	2.39704700	0.56392500
C	-0.73904000	0.65906600	1.15866900
C	2.41498000	1.87935000	0.59687500
C	-0.14387300	-0.24589900	2.16869500

C	-0.97754200	-1.37272300	2.30895800
C	-2.11262900	-1.20289500	1.40002300
C	-1.93546500	0.08223500	0.73480200
C	2.82029200	0.59460900	0.24886400
C	4.26184000	0.47865700	0.42161200
C	4.73830900	1.77753900	0.90251600
C	3.62178000	2.63553700	0.99478700
C	6.00303000	2.21847600	1.25590700
C	6.15579200	3.52854200	1.70520900
C	5.05444700	4.37460400	1.80756500
C	3.77841200	3.93483300	1.46158900
C	2.07456900	-0.50487700	-0.28582900
C	2.73272300	-1.65424500	-0.56399100
C	4.17260300	-1.78479600	-0.35567800
C	4.92620300	-0.66759300	0.13508200
C	0.97737000	-0.10433700	2.97586300
C	1.27764000	-1.11147700	3.88957100
C	0.46626900	-2.23755500	4.00618800
C	-0.67539200	-2.37180600	3.21994300
C	-3.16946900	-2.00912400	1.13665600
C	-4.14257400	-1.56510000	0.18139500
C	-3.97122100	-0.27367800	-0.47903100
C	-2.89962800	0.51757500	-0.23298900
C	-2.12984800	3.75815400	0.04911000
C	1.03261100	5.07394800	-0.24599700
C	1.89675300	5.15522300	-1.35760100
C	2.41070100	6.39215300	-1.72888600
C	2.10657200	7.55706700	-1.02964800
C	1.25865000	7.45708900	0.06719000
C	0.71063100	6.24163800	0.47147200
C	-2.54397000	4.19493900	-1.22491600
C	-3.86761100	4.58839900	-1.40588900
C	-4.79440400	4.56707000	-0.36767000
C	-4.35830200	4.16176400	0.88998000
C	-3.04864600	3.75278300	1.11811100
C	2.26952300	-2.94056600	-1.09034700
C	3.40199200	-3.78115600	-1.18861100
C	4.58088100	-3.04157100	-0.72856600
C	1.01575000	-3.40442600	-1.44723500
C	0.89413400	-4.71436300	-1.91447100
C	2.00928300	-5.54375800	-2.01376000
C	3.27379500	-5.08567400	-1.64755900
C	-5.29047000	-2.16750500	-0.27009600
C	-5.91799200	-1.26861800	-1.24233300

C	-5.11913900	-0.10912000	-1.37384500
C	-7.08608400	-1.40704700	-1.98185000
C	-7.45766900	-0.37695700	-2.84347700
C	-6.67425000	0.76954800	-2.96425000
C	-5.49624600	0.91228000	-2.22916800
C	-5.81937200	-3.49284400	0.12669700
C	5.95620000	-3.58856400	-0.67935100
C	6.50974800	-3.99352400	0.54650500
C	7.80073200	-4.51574600	0.56595400
C	8.55756500	-4.64891200	-0.59370400
C	7.99216800	-4.23747500	-1.79723800
C	6.70479400	-3.71279500	-1.86238200
C	-6.89939700	-3.57859900	1.02157200
C	-7.38387800	-4.83293000	1.38128300
C	-6.83231000	-6.00614300	0.87502700
C	-5.76277200	-5.89991500	-0.00837900
C	-5.24599900	-4.66527200	-0.39302400
C	-7.51436800	-2.33496600	1.61030800
C	-4.09076400	-4.60418800	-1.36016100
C	-7.39486500	-7.35132700	1.25176500
C	6.13940700	-3.26255700	-3.18482900
C	5.72613000	-3.88100600	1.82970600
C	9.93916500	-5.24669200	-0.55329800
H	6.86142200	1.55701700	1.18843800
H	7.14020300	3.89039400	1.98367500
H	5.18894000	5.39015700	2.16532800
H	2.93097700	4.60367400	1.55346300
H	1.00955400	-0.40532100	-0.46002900
H	6.00234800	-0.75443200	0.25536100
H	1.60835500	0.77267500	2.90220200
H	2.15525100	-1.01444400	4.52025400
H	0.71949200	-3.01130400	4.72363300
H	-1.31923800	-3.23912400	3.32867100
H	-3.29415400	-2.97017000	1.62739500
H	-2.77400800	1.46363600	-0.74495700
H	3.06978000	6.44650800	-2.59164000
H	1.01485000	8.35295700	0.63215800
H	-4.18463900	4.91645300	-2.39259200
H	-5.06018900	4.15717900	1.71966900
H	0.13911200	-2.76948700	-1.36058000
H	-0.08237500	-5.09177900	-2.20039700
H	1.89082000	-6.55980200	-2.37616800
H	4.14189600	-5.73424700	-1.71519700
H	-7.69473300	-2.30125300	-1.88811500

H	-8.36787300	-0.46780800	-3.42750400
H	-6.98278700	1.56009800	-3.64082500
H	-4.89343600	1.81054700	-2.32465600
H	8.22451400	-4.83053000	1.51620400
H	8.57068400	-4.32324100	-2.71358900
H	-8.21361400	-4.89396500	2.08097100
H	-5.31681400	-6.80449600	-0.41408100
H	-6.76566400	-1.73262600	2.13274900
H	-7.94806200	-1.69572600	0.83606000
H	-8.30334300	-2.58936600	2.32096000
H	-3.88111400	-5.59248500	-1.77479700
H	-3.17836100	-4.24229900	-0.87646600
H	-4.30019100	-3.92291100	-2.18927300
H	-7.82010000	-7.33817000	2.25831100
H	-6.62755500	-8.12855600	1.21752300
H	-8.19349100	-7.65106800	0.56448500
H	6.87509300	-3.37940400	-3.98315200
H	5.24889500	-3.83592600	-3.45755900
H	5.83825700	-2.21163300	-3.14954500
H	6.25379600	-4.37264800	2.64964300
H	4.73810300	-4.33972400	1.73524300
H	5.56212700	-2.83738000	2.11329100
H	10.41465500	-5.08797100	0.41757000
H	9.90585200	-6.32762200	-0.72777000
H	10.58386500	-4.81351200	-1.32209600
C	2.66195600	8.88640000	-1.46629400
H	2.08634400	9.29777600	-2.30248000
H	2.63015800	9.61756300	-0.65536000
H	3.69851400	8.79478900	-1.80094000
C	-0.19178400	6.21161000	1.67780500
H	-1.23473700	6.04159400	1.39621500
H	0.08858100	5.41190600	2.36842300
H	-0.14166800	7.15955400	2.21746300
C	2.26514300	3.93283600	-2.15689600
H	3.03522100	3.34527900	-1.64938700
H	1.40626200	3.27581900	-2.31161400
H	2.65697500	4.21620500	-3.13602400
C	-6.23325900	4.93545900	-0.60914600
H	-6.32619000	5.70378100	-1.38072800
H	-6.80306600	4.06197900	-0.94517000
H	-6.70966400	5.30632600	0.30132800
C	-1.60365600	4.21804600	-2.40179500
H	-0.83968000	4.99240300	-2.29277000
H	-1.07909900	3.26525200	-2.51389800

H	-2.15082800	4.41368300	-3.32623700
C	-2.63270100	3.32863200	2.50275100
H	-2.47603600	2.24846000	2.56102400
H	-1.69654600	3.80590200	2.80317100
H	-3.39901700	3.59399900	3.23380600