Supplementary Information (SI) for Organic Chemistry Frontiers.

Intermediate diradical character and cis-trans isomerization of near-infrared absorbing thionated squaraine dyes

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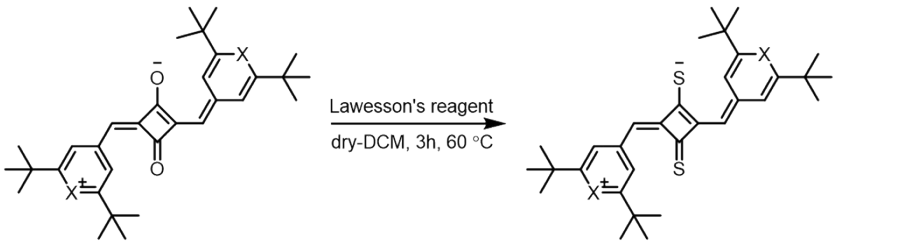
1. Experimental Section

1-1. Materials and Instruments

^{1}H-NMR spectra were obtained using JEOL ECX-400 spectrometers operating at 400 MHz. Variable-temperature ESR spectra were recorded with a JEOL JES-TE-200 X-band spectrometer with a JEOL DVT2 variable-temperature unit. The electrospray ionization mass spectra (ESI-MS) were recorded on a JEOL JMS-T100CS spectrometer using methanol-dichloromethane (1/1, v/v) as eluents. The absorption spectra were measured in a 1.0 or 0.10 cm quartz cell on a Shimadzu UV-3600 spectrophotometer.

All solvents and reagents were purchased from commercial sources and used as received without further purification. Silica gel (SiO_2, spherically-shaped, neutral) for the flash chromatography was purchased from Kanto chemical (Tokyo, Japan). Spectroscopic-grade solvents were purchased from Wako Pure Chemicals (Osaka, Japan) and used immediately after opening for all spectroscopic measurements. **SQ1a** and **SQ1b** and were prepared according to our priviously literature.[1]

1-2. Synthesis and characterization



SQ1 X = O (**SQ1a**)
S (**SQ1b**)

SQ2 X = O (**SQ2a**) (77%)
S (**SQ2b**) (74%)

Preparation of SQ2a

SQ1a (0.049 g, 0.1 mmol) and 2,4-bis(4-methoxyphenyl)-1,3-dithia-2,4-diphosphetane 2,4-disulfide (Lawesson's Reagent) (0.081 g, 0.2 mmol) were dissolved in dry dichloromethane (20 mL) under an atmosphere of nitrogen. The solution was heated at 60 °C or 3 hours. After cooling, the solvent was removed on a rotary evaporator, and the residue was purified by silica gel column chromatography (eluent: $CHCl_3$) to give **SQ2a** (0.042 g, 0.077 mmol) as a black solid in 77% yield.; ^{1}H NMR (400 MHz, $CDCl_3$, 213K): δ 9.17 (s, 1.8H, Ar-H in the trans isomer), 8.95 (s, 0.2H, Ar-H in the cis isomer), 6.51 (s, 1.8H, Ar-H in the trans isomer), 6.49 (s, 0.2H, Ar-H in the cis isomer), 6.12 (s, 2H, Ar-H),1.38 (s, 18H, CH), 1.30 (s, 18H, CH_3). UV/Vis/NIR (DMSO): λ_{max} (ε) = 754 (167000 $mol^{-1}L^3cm^{-1}$). HRMS (ESI): *m/z* calcd for $[C_{32}H_{42}O_2S_2+H^+]^-$: 523.2704, found 523.2709. Elemental analysis calcd (%) for $C_{32}H_{42}O_2S_2$: C 73.52, H 8.10; found: C 73.42, H 8.20.

Preparation of SQ2b

SQ1b (0.052 g, 0.1 mmol) and 2,4-Bis(4-methoxyphenyl)-1,3-dithia-2,4-diphosphetane 2,4-Disulfide (Lawesson's Reagent) (0.081 g, 0.2 mmol) were dissolved in dry dichloromethane (20 mL) under an atmosphere of nitrogen. The solution was heated at 60 °C for 3 hours. After cooling, the solvent was removed on a rotary evaporator, and the residue was purified by silica gel column chromatography (eluent: $CHCl_3$) to give **SQ2b** (0.041 g, 0.074 mmol) as a black solid in 74% yield.; ^{1}H NMR (400 MHz, $CDCl_3$, 213K): δ 9.68 (s, 1.8H, Ar-H in the trans isomer), 9.41 (s, 0.2H, Ar-H in the cis isomer), 7.24 (s, 2H, Ar-H), 6.35 (s, 0.2H, Ar-H in the cis isomer), 6.32 (s, 1.8H, Ar-H in the trans isomer),1.49 (s, 18H, CH), 1.38 (s, 18H, CH_3). UV/Vis/NIR (DMSO): λ_{max} (ε) = 849 (192000 $mol^{-1}L^3cm^{-1}$). HRMS (ESI): *m/z* calcd for $C_{32}H_{42}S_4$: 554.2169, found 554.2170. Elemental analysis calcd (%) for $C_{32}H_{42}S_4$: C 66.26, H 7.63; found: C 66.41, H 7.58.

2. Evaluation of stability

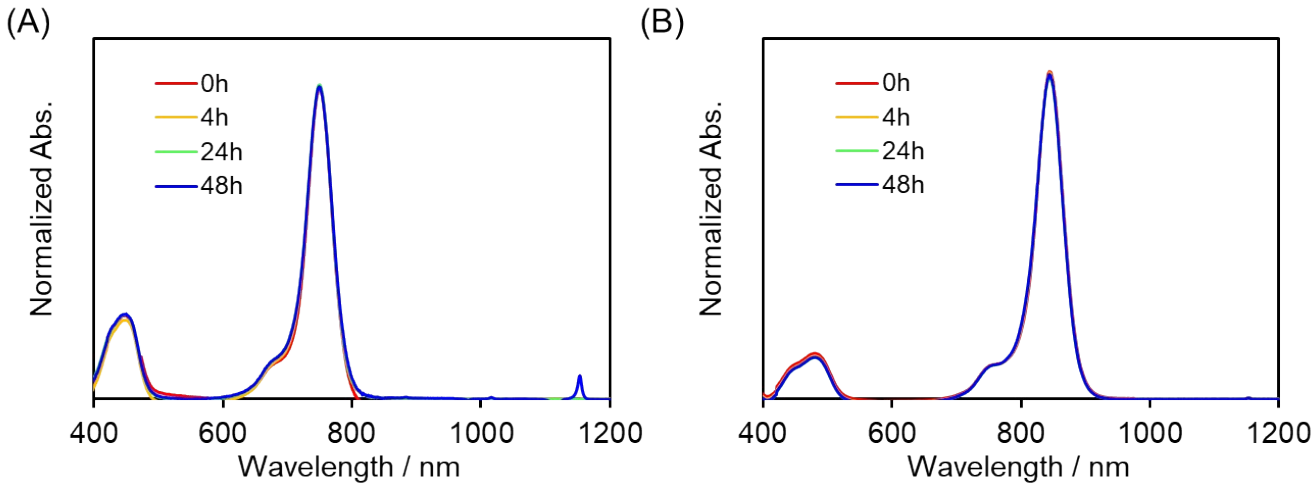


Fig. S1. Time dependent UV-vis-NIR absorption spectra (50 μM, $CHCl_3$) of **SQ2a** (A), and **SQ2b** (B) measured in a 1-mm-cuvette under dark and ambient air condition. No change in spectra were observed for each compound within 48 h.

3. X-ray crystallographic analysis

Single crystals of **SQ2a**, **SQ2b** were obtained by the slow diffusion of hexane into its chloroform solution. A metallic purple plate-like crystal of **SQ2a** having approximate dimensions of 0.400 x 0.250 x 0.050 mm, a bronze crystal of **SQ2b** having approximate dimensions of 0.200 x 0.100 x 0.050 mm. Each crystal was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB Synergy diffractometer multi-layer mirror monochromated Cu-Kα radiation (λ = 1.54187 Å) at 100 K. The structure was solved by a direct methods using the SIR2004 program.[2] All the calculations were performed using the CrystalStructure 4.3 software package of the Molecular Structure Corporation.[3]

A summary of the crystallographic data and structure refinement for these two compounds is given in Table S1. Full crystallographic details excluding structure factors have been deposited at the Cambridge Crystallographic Data Centre (CCDC). CCDC- 2382744 for **SQ2a** and CCDC- 2382745 for **SQ2b** contains the supplementary crystallographic data for this paper. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystallographic data for **SQ2a** and **SQ2b** at 173 K.

	SQ2a	**SQ2b**
Empirical Formula	$C_{32}H_{42}O_4S_2$	$C_{32}H_{42}S_4$
Formula Weight	522.80	554.92
T / K	100	100
Color, habit	metallic purple, plate	bronze, platelet
Size, mm	0.400 × 0.250 × 0.050	0.200 × 0.100 × 0.050
Crystal system	Triclinic	Triclinic
Lattice Type	Primitive	Primitive
Space group	P-1 (#2)	P-1 (#2)
a / Å	6.04154(17)	9.0667(8)
b / Å	14.0513(4)	9.3465(7)
c / Å	17.6572(5)	9.5913(8)
α / °	80.969(3)	80.584(7)
β / °	86.619(2)	72.219(8)
γ / °	88.252(2)	79.365(7)
V/ Å^3	1477.44(7)	755.65(11)
Z	2	1
*D*calc / g cm^{-3}	1.175	1.219
F_{000}	564	298
μ / cm^{-1}	CuKα, 18.207	CuKα, 30.136
2*ϑ*max / º	162.8	158.1
Total reflections	16877	7825
Unique reflections	6073	3076
Reflection/Parameter Ratio	14.05	13.49
R (*I* > 3.00σ(*I*)[a]	0.0894	0.0641
*R*w (*I* > 3.00σ(*I*)[b]	0.0750	0.0685
Goodness of Fit Indicator	1.025	0.979

[a]R = Σ ||*F*o| - |*F*c|| / Σ |*F*o|, [b]*R*w = [Σ w (|*F*o| - |*F*c|)^2 / Σ w *F*o^2]$^{1/2}$

Fig. S2 displays ORTEP drawing and molecular packing of **SQ2a**-**b**. In the crystal of **SQ2a**, two crystallographically independent molecules exist with a nearest distance of 3.447 Å and 3.517 Å. On the other hand, **SQ2b** overlapped in the shorter distance of 3.418 Å, indicating π-π interactions.

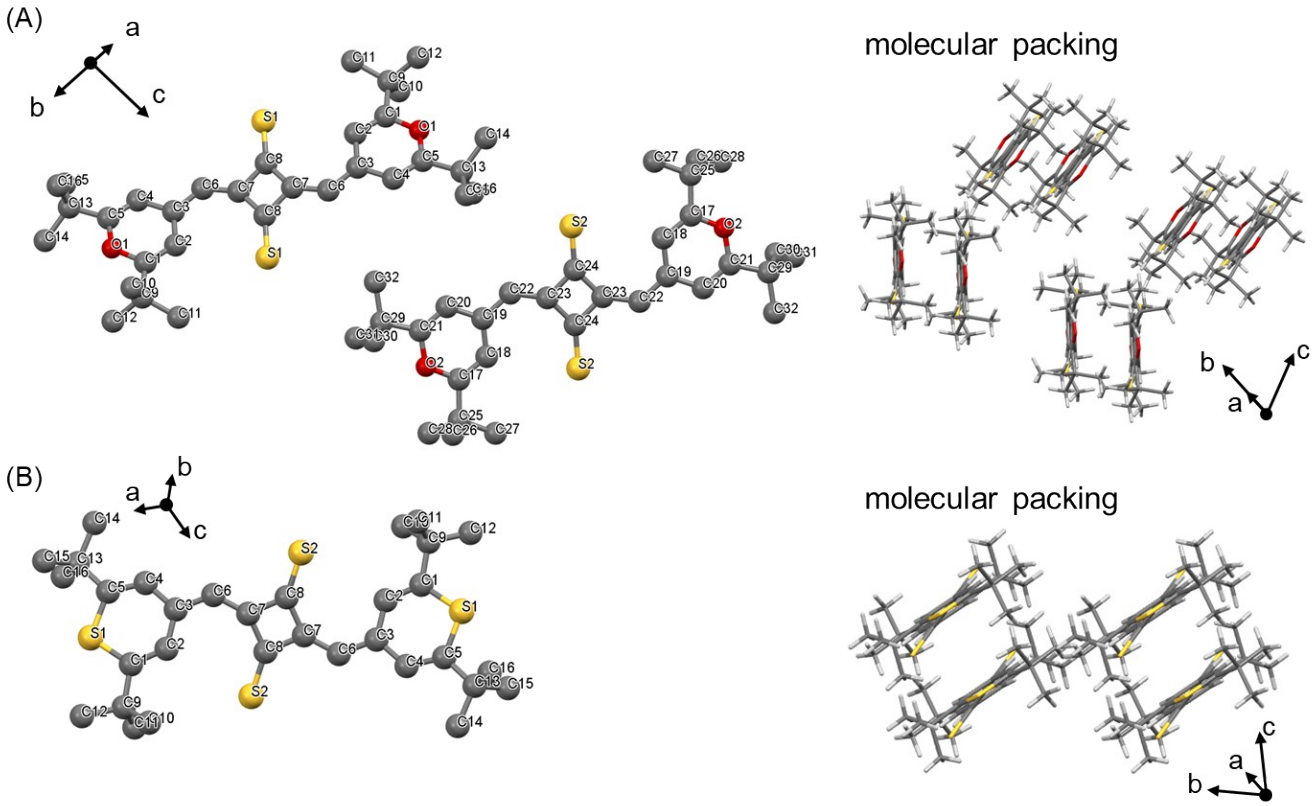


Fig. S2. Oak Ridge thermal ellipsoid program (ORTEP) drawing and molecular packing of **SQ2a** (A) and **SQ2b** (B).

Table S2. Representative C-C bond lengths of the single crystal of **SQ2a** and **SQ2b** at 100 K.

SQ2a		**SQ2a**		**SQ2b**	
bond	length (Å)	bond	length (Å)	bond	length (Å)
O1-C1	1.371	O2-C17	1.366	S1-C1	1.737
O1-C5	1.358	O17-C21	1.366	S1-C5	1.735
C1-C2	1.349	C17-C18	1.355	C1-C2	1.356
C2-C3	1.430	C18-C19	1.430	C2-C3	1.434
C3-C4	1.441	C19-C20	1.434	C3-C4	1.429
C4-C5	1.347	C20-C21	1.349	C4-C5	1.356
C3-C6	1.398	C19-C22	1.394	C3-C6	1.405
C6-C7	1.391	C22-C23	1.396	C6-C7	1.381
C7-C8	1.467	C23-C24	1.467	C7-C8	1.470
C8-S1	1.661	C24-S2	1.656	C8-S2	1.659

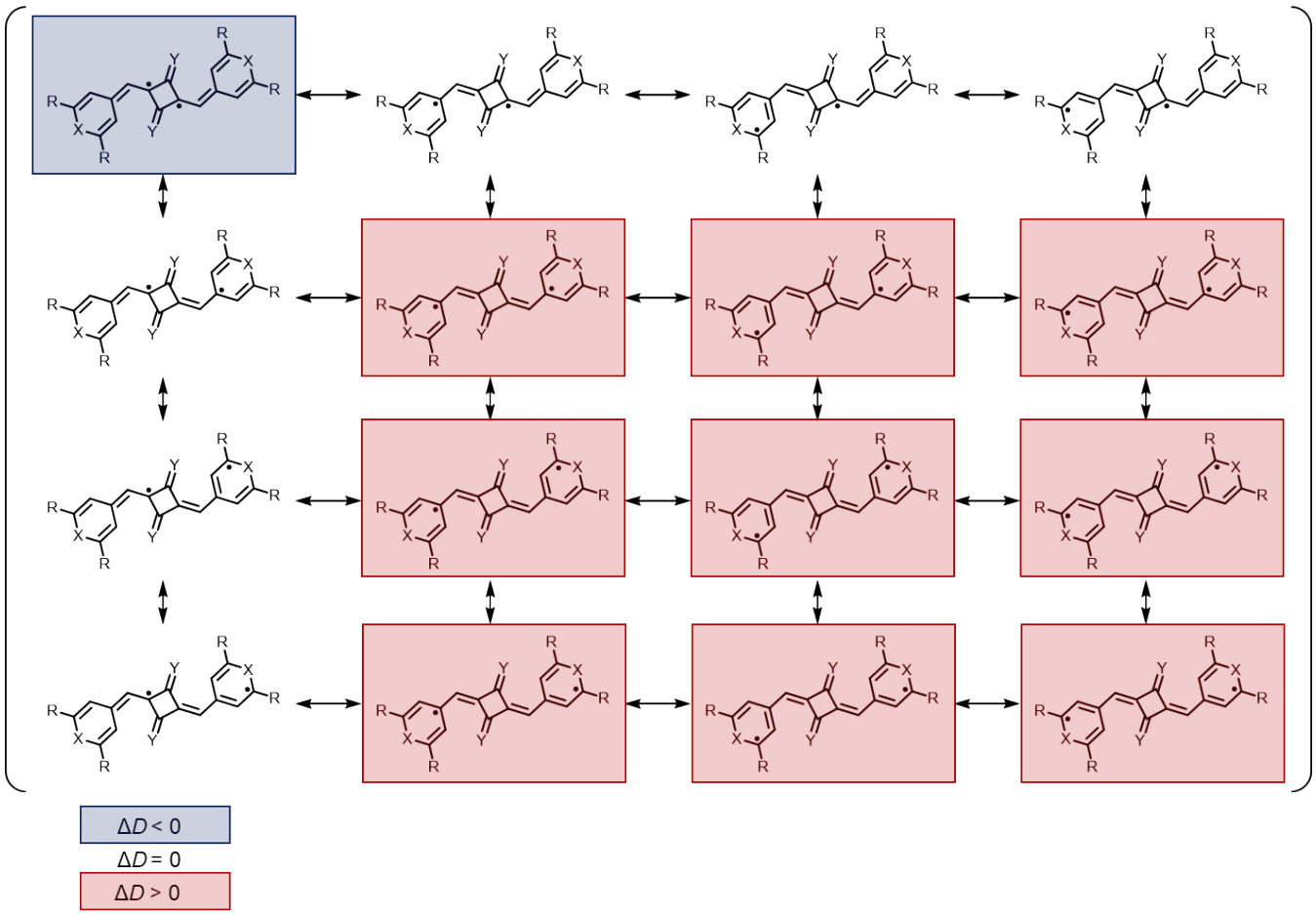


Fig. S3. Resonance structures for thionated squaraine dyes bearing chalcogenopyrylium components. Glay and red backgrounds indicate resonance forms with $\Delta D < 0$ and $\Delta D > 0$, respectively. ΔD is defined in the main text as following equation: ΔD = ave. (g, p) – ave. (h, q).

4. Electron spin resonance (ESR) spectra

ESR spectroscopy helps to detect triplet species in both **SQ2a** and **SQ2b** (Fig. S4). In the solid state, both dyes exhibited broad ESR signals at g = 2.006, indicating the presence of these diradical species. These provide experimental evidence of thermally populated triplet species in these dyes. **SQ2b** with the thiopyrylium component displayed distinct temperature dependence in its ESR intensity, unlike **SQ2a** with a pyrylium component. The product of ESR intensity (I_{ESR}) and temperature (T) for **SQ2b** is shown in Fig. S4C. Although we attempted to estimate the singlet–triplet energy gap ($\Delta E_{S\text{-}T}$) using $I_{ESR}T$ vs. T plots and the Bleaney–Bowers equation, accurate curve fitting to determine $\Delta E_{S\text{-}T}$ was likely hindered by intermolecular interactions in the solid state.

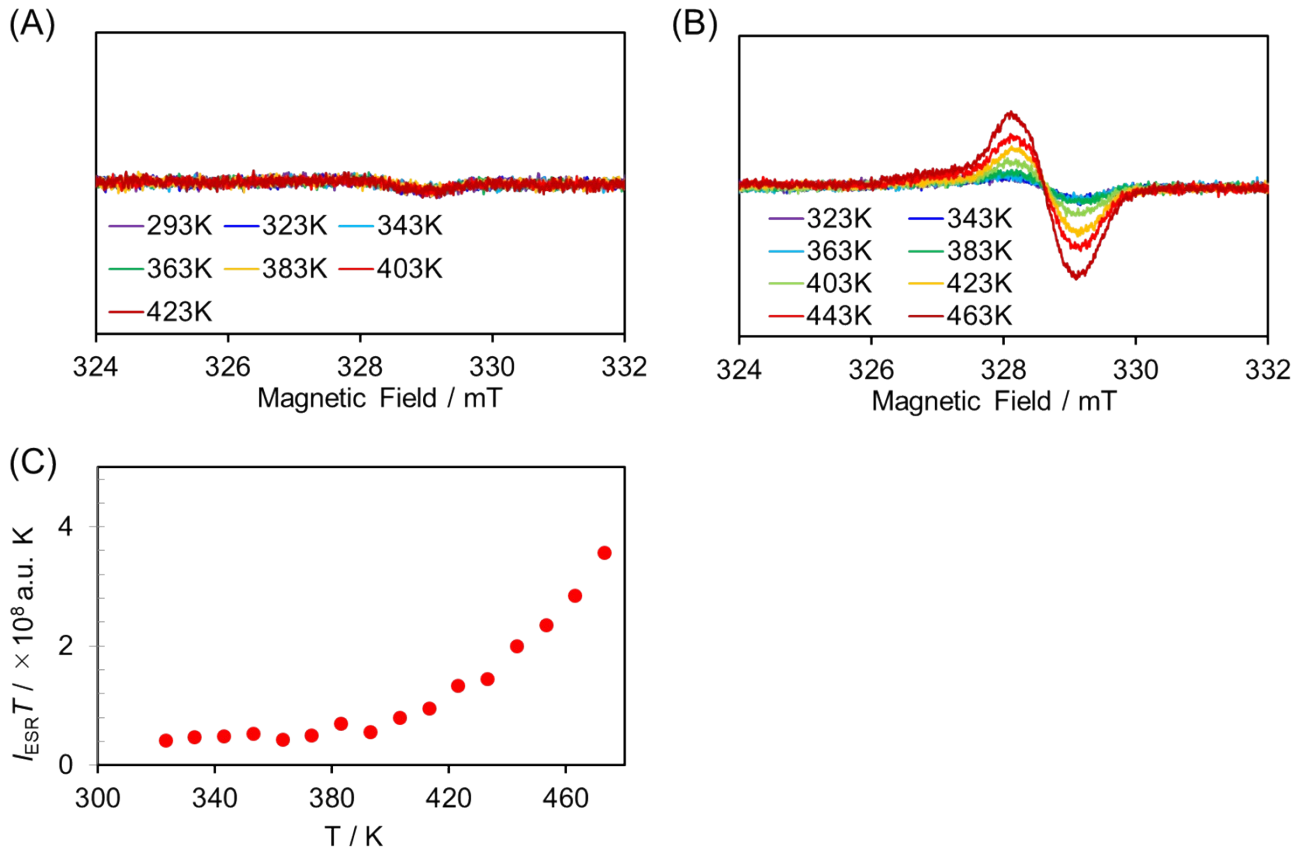


Fig. S4 ESR spectra of **SQ2a** (A) and **SQ2b** (B) and $I_{ESR}T/T$ plots of **SQ2b** (C).

5. DFT calculations

All geometry optimizations have been performed in the gas phase within DFT using the UB3PW91 functional in combination with the cc-pVDZ basis set (Fig. S5, Fig. S6). TD-DFT calculations were performed at the same level (Table S3, Table S4). The solvation effect of DMSO was accounted for in all TD-DFT calculations using the polarizable continuum model (PCM). All these calculations have been carried out using the Gaussian 09 package. The coordinates are summarized in Table S7-S14 at the end of this document.[4]

Diradical index y_0

The singlet diradical character in all molecules has been estimated using the diradical index (y_0) in equation (1).[5]

$$y_0 = 1 - \frac{2T}{1+T^2} \quad (T = \frac{n_{HOMO} - n_{LUMO}}{2}) \quad \cdots (1)$$

The diradical character y_0, where $y_0 = 0$ and $y_0 = 1$ indicate a closed-shell and an open-shell electronic structure, respectively, is commonly used to express the degree of contribution of the diradical form in singlet diradicaloids. We estimated y_0 values for **SQ2a** and **SQ2b** using the spin-projected unrestricted Hartree-Fock (PUHF) theory using the 6-31G(d,p) basis set. The optimized structures of *trans* isomers obtained at the B3PW91/cc-pVDZ level were used for the calculation.[6-7] The y_0 values for **SQ2a** and **SQ2b** were estimated to be 0.24 and 0.37, respectively (Table S3). Thus, the thiopyrylium skeleton is expected to increase the contribution of the diradical form. Under the calculation condition we used, **SQ2a**-**b** showed lower y_0 values compared to **SQ1a** (y_0 = 0.37) and **SQ1b** (y_0 = 0.47), which have the previously reported cyclobutenedione skeleton (Table S4).

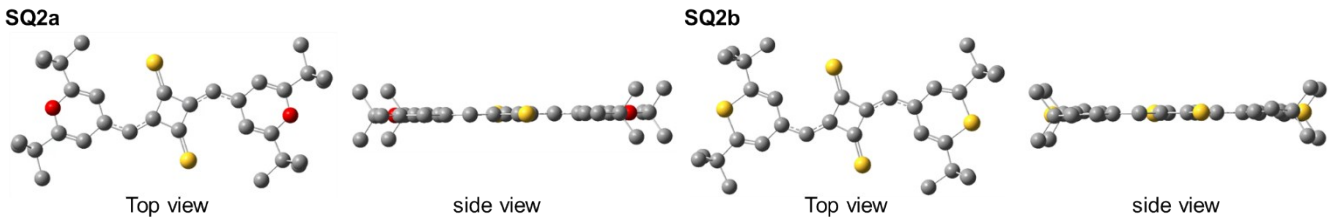


Fig. S5. Optimized structures of **SQ2a** and **SQ2b** at the B3PW91/cc-pVDZ level.

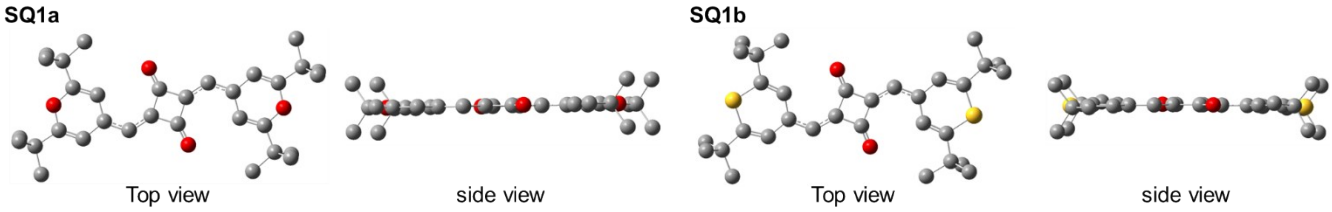


Fig. S6. Optimized structures of **SQ1a** and **SQ1b** at the B3PW91/cc-pVDZ level.

Table S3. Molecular properties of **SQ2a** and **SQ2b** calculated at the B3PW91/cc-pVDZ level.

	SQ2a		**SQ2b**	
	cis	*trans*	*cis*	*trans*
LUMO (eV)	−2.761	−2.738	−3.019	−2.999
HOMO (eV)	−4.573	−4.562	−4.613	−4.602
λ_{Abs} (nm)	659.2	655.19	737.75	733.46
Oscillator strength (*f*)	0.9784	1.0552	1.1157	1.2053
Composition[a]	H⟶L (96%)	H⟶L (96%)	H⟶L (95%)	H⟶L (95%)
Total Energy (A.U.)	−2190.96762854	−2190.96868060	−2836.88344082	−2836.88457024
y_0	0.242	0.239	0.372	0.37

[a] H: highest occupied molecular orbital (HOMO), L: Lowest unoccupied molecular orbital (LUMO).

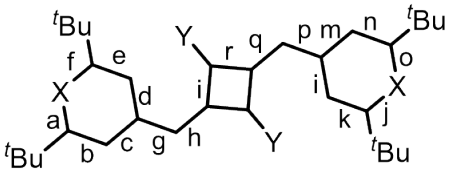
Table S4. Molecular properties of **SQ1a** and **SQ1b** calculated at the B3PW91/cc-pVDZ level.

	SQ1a		**SQ1b**	
	cis	*trans*	*cis*	*trans*
LUMO (eV)	−2.542	−2.576	−2.863	−2.832
HOMO (eV)	−4.461	−4.489	−4.537	−4.508
λ_{Abs} (nm)	625.14	621.99	704.58	699.27
Oscillator strength (*f*)	1.3576	1.6116	1.4439	1.7187
Composition[a]	H⟶L (97%)	H⟶L (97%)	H⟶L (96%)	H⟶L (96%)
Total Energy (A.U.)	−1545.06743007	−1545.06794792	−2190.98519638	−2190.98619453
y_0	0.377	0.373	0.473	0.470

[a] H: highest occupied molecular orbital (HOMO), L: Lowest unoccupied molecular orbital (LUMO).

The DFT calculations supported the result of the bond length analysis (BLA) focused on ΔD (Å) values (Table S6). We calculated the bond length difference ΔD of optimised structures for the closed-shell singlet state and the open-shell triplet state using the B3PW91/cc-pVDZ level and the UB3PW91/cc-pVDZ level, respectively. For thiopyrylium-based dyes (**SQ1b**, **SQ2b**), the experimental ΔD values from the X-ray structures was found to be between those for the DFT-optimized structures of the closed-shell singlet states and the open-shell triplet states (Table S6). The ΔD values in the crystal structures of the pyrylium-based dyes (**SQ2a** and **SQ1a**) were close to those of the closed-shell singlet state but fell roughly between the closed-shell singlet and open-shell triplet states. These results supported the substantial contribution of diradical resonance forms δ of these dyes.

Table S5. Bond length difference ΔD for singlet and triplet states of present squaraine dyes.



	ΔD (Å) = ave(g, p) – ave(h, q)		
Dye	Singlet [a]	XRD	Triplet [a]
SQ2a (X = O, Y = S)	0.004	0.002 / 0.005	0.03
SQ2b (X = S, Y = S)	0.011	0.024	0.039
SQ1a (X = O, Y = O)	0.000	0.003	0.041
SQ1b (X = S, Y = O)	0.009	0.019 / 0.012	0.051

[a] Optimized structures at the UB3PW91/cc-pVDZ level.

6. Variable temperature ^{1}H-NMR spectra

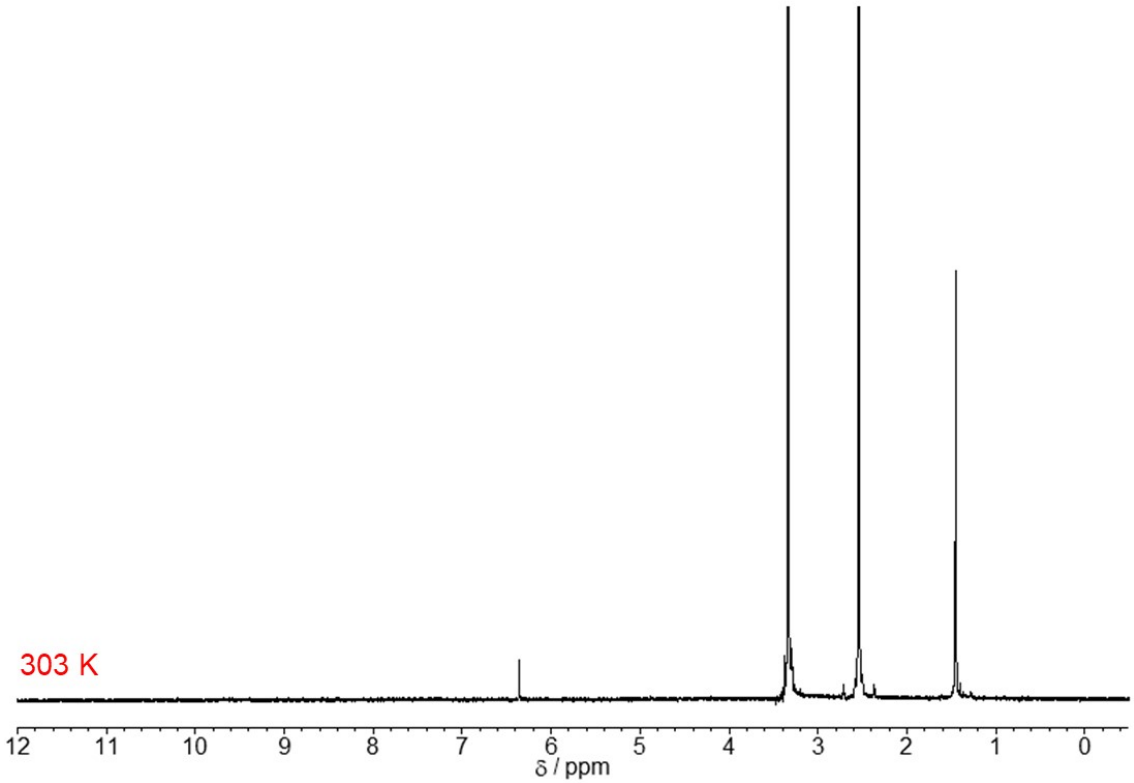


Fig. S7. ^{1}H-NMR spectra (DMSO-d_6, 303 K) of **SQ2b**.

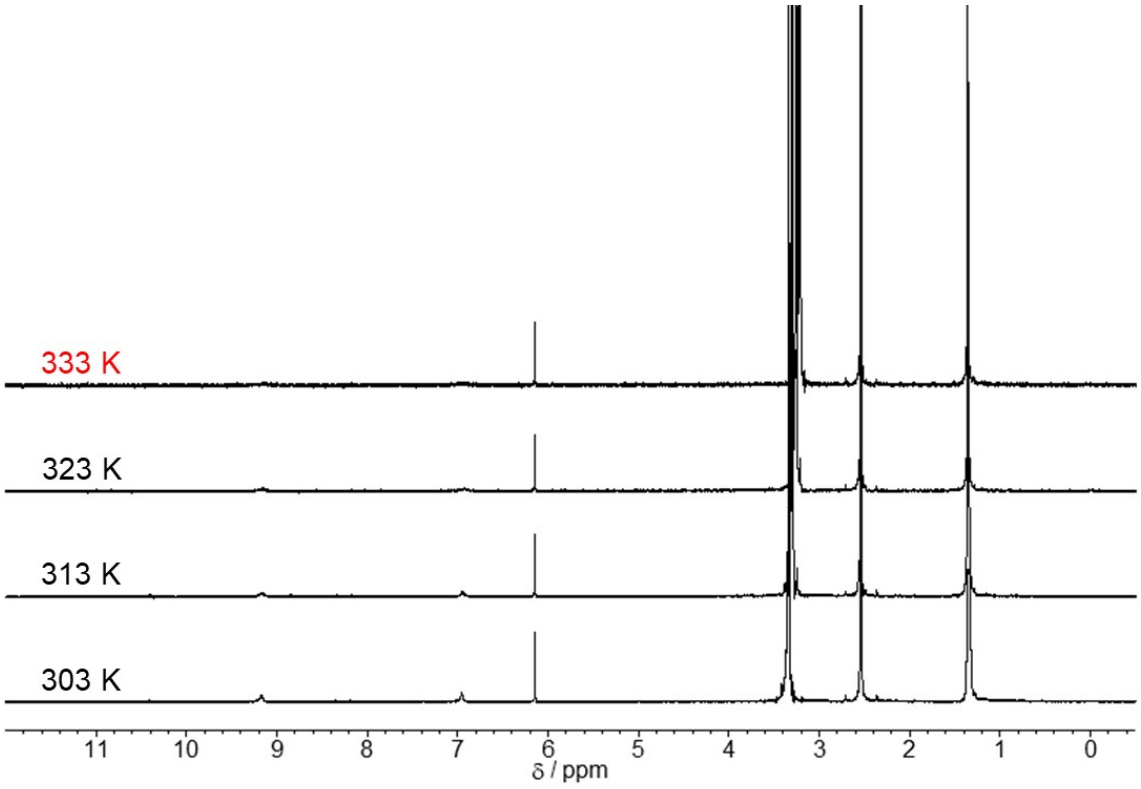


Fig. S8. Valiable-temperature ^{1}H-NMR spectra (DMSO-d_6, 303-333 K) of **SQ2a**.

7. Dynamic NMR method for cis-trans isomerization.

Using $CDCl_3$ as the solvent, we estimated the Gibbs free energy of activation (Δ*G*‡) for the *cis-trans* isomerization. The Δ*G*‡ was calculated using the equation below.[9]

$$\Delta G \ddagger\ (cal/mol) = 4.57 T_c\,(10.32 + log\,(\frac{T_c}{k_c}) \quad \cdots (1)$$

Where k_c is the rotational velocity and T_c is the peak fusion temperature (K).

$$k_C = \frac{\pi \times \Delta\nu}{\sqrt{2}} \quad \cdots (2)$$

Δ*v* is expressed as the product of the NMR resonance frequency (MHz) and the width of the splitting peak (ppm). The signal at 213 K were used for the splitting peak analysis. Peak coalescence was observed for **SQ1b**, **SQ2a**, and **SQ2b** at H^a, but not for **SQ1a**. In contrast, peak coalescence was noted at H^c for **SQ1a**.

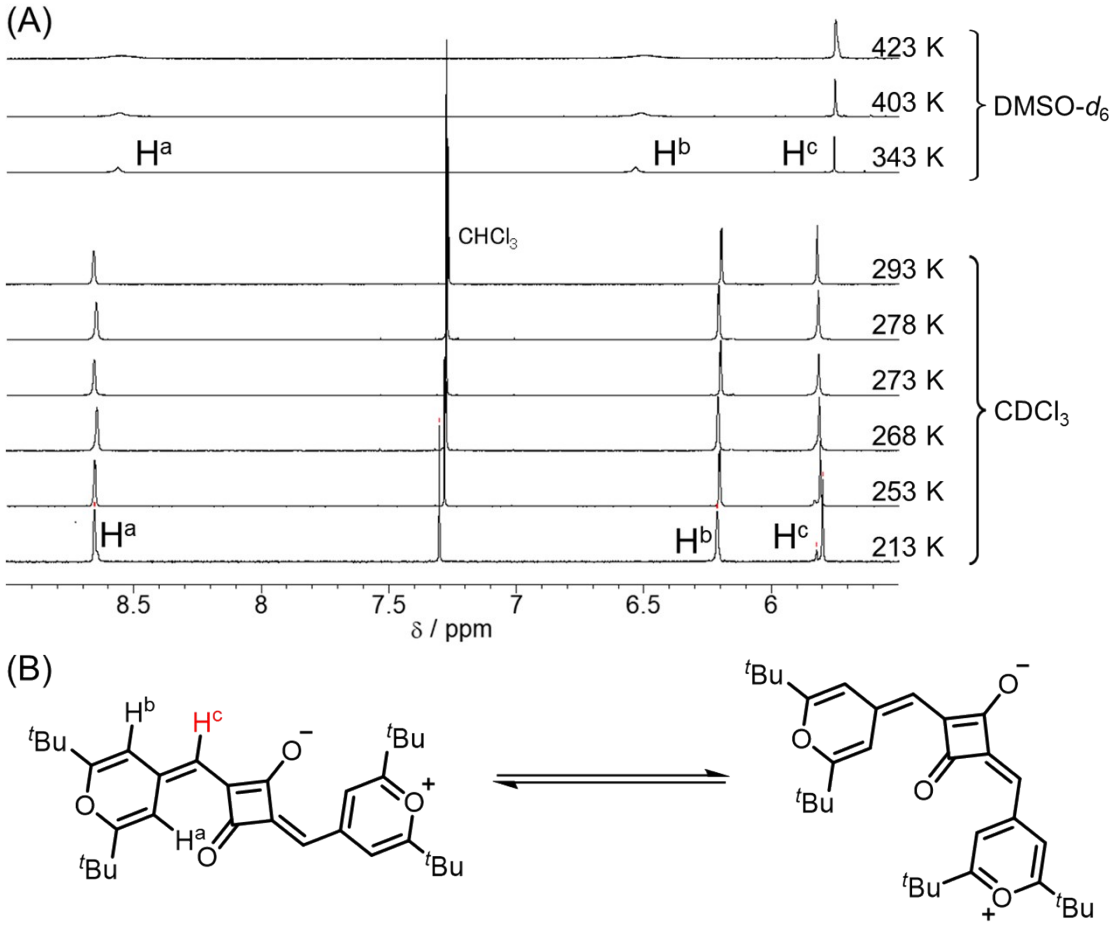


Fig. S9. Variable-temperature ^{1}H-NMR spectra ($CDCl_3$: 213 K-293 K, DMSO-d_6: 343-423K) of **SQ1a**.

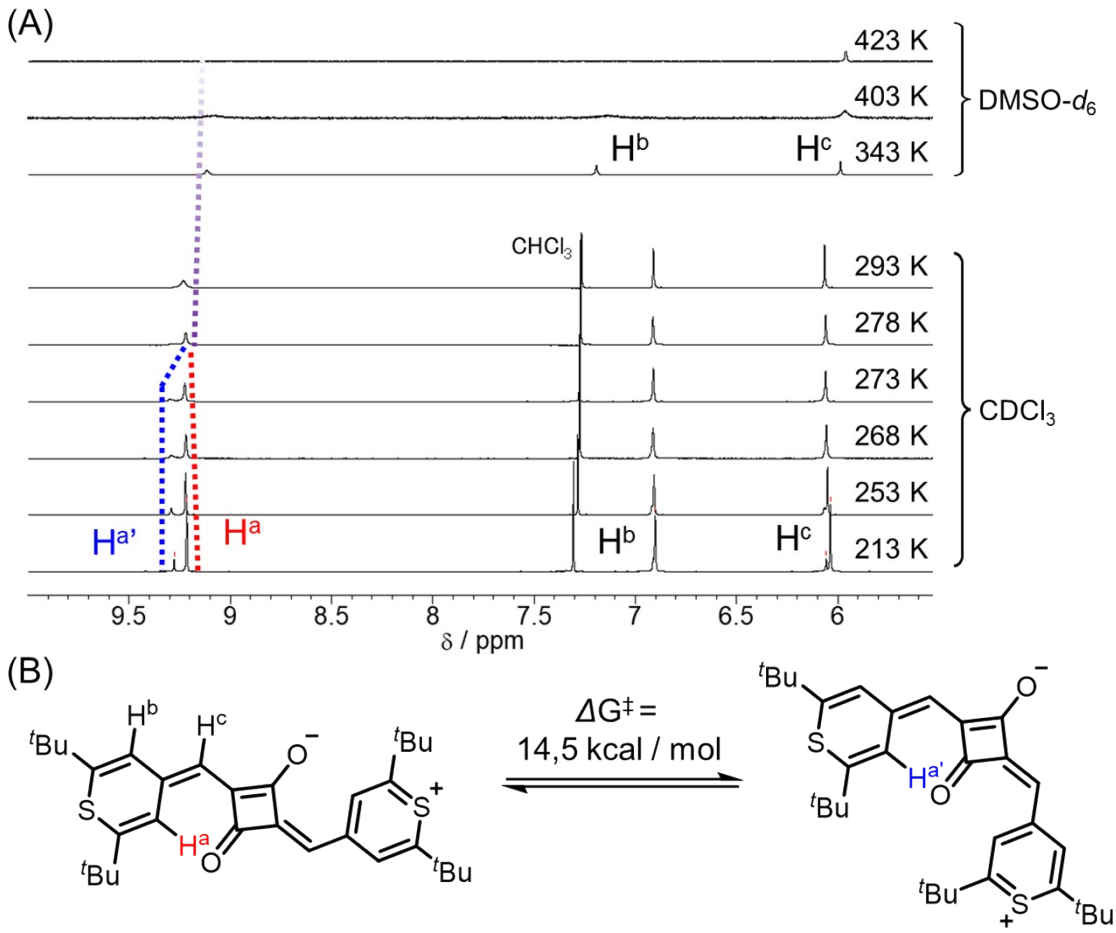


Fig. S10. Variable-temperature ^{1}H-NMR spectra ($CDCl_3$: 213 K-293 K, DMSO-d_6: 343-423K) of **SQ1b**.

Table S6. Summary of T_c, splitting peak, Δv, $\Delta G^{\ddagger}$ value

	T_c [a] (K)	splitting peak [b] (ppm)	Δv [c] (Hz)	k_c [d] (s^{-1})	$\Delta G^{\ddagger}$ [e] (kJ/mol)
SQ2a	278	0.227	90.6	201	13.7
SQ2b	273	0.262	105	233	13.4
SQ1b	278	0.063	25.0	55.6	14.5

[a] Coreless temperature of H^a and $H^{a'}$. [b] Peak difference between H^a and $H^{a'}$ at 213 K. [c] Calculated for the splitting peak. [d] Calculated using equation (2) [e] Calculated using equation (1)

8. FT-IR measurements

Simulated IR spectra were calculated by quantum chemical calculations (B3PW91 cc-pVDZ Level Solvent: Chloroform). The absorption near 1550 cm^{-1} was identified as the vibration of the methine carbon. IR spectroscopy measured in $CHCl_3$ sandwiched between KBr plates. Based on comparison with experimental values, the sharp absorption observed at 1478 - 1487 cm^{-1} is inferred to correspond to the vibration of the methine carbon. In Fig. S11-14 , the calculation results were shifted by approximately 65 cm^{-1} to correct for the difference between the calculated and experimental values. This peak is indicated by the red arrow.

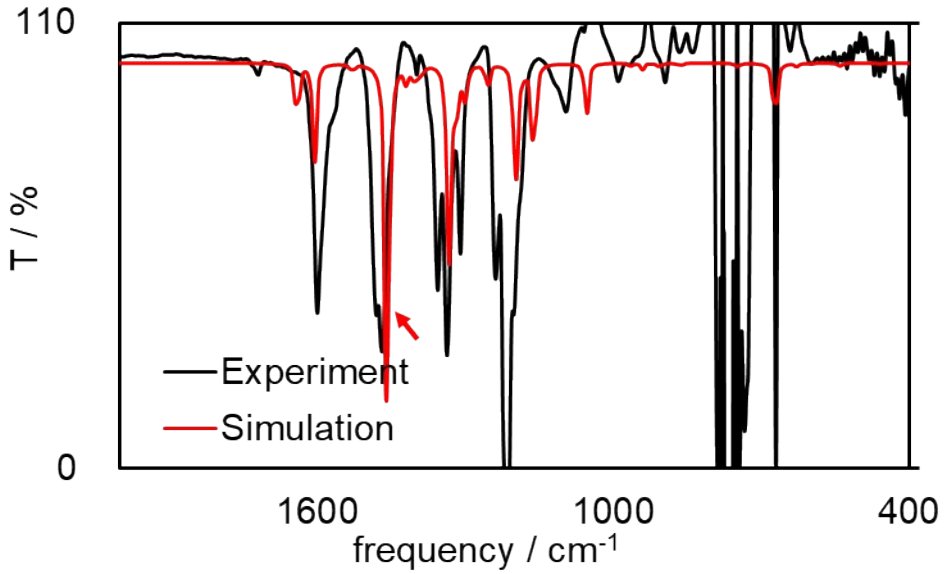


Fig. S11 Simulated and measured IR spectra of **SQ2a**.

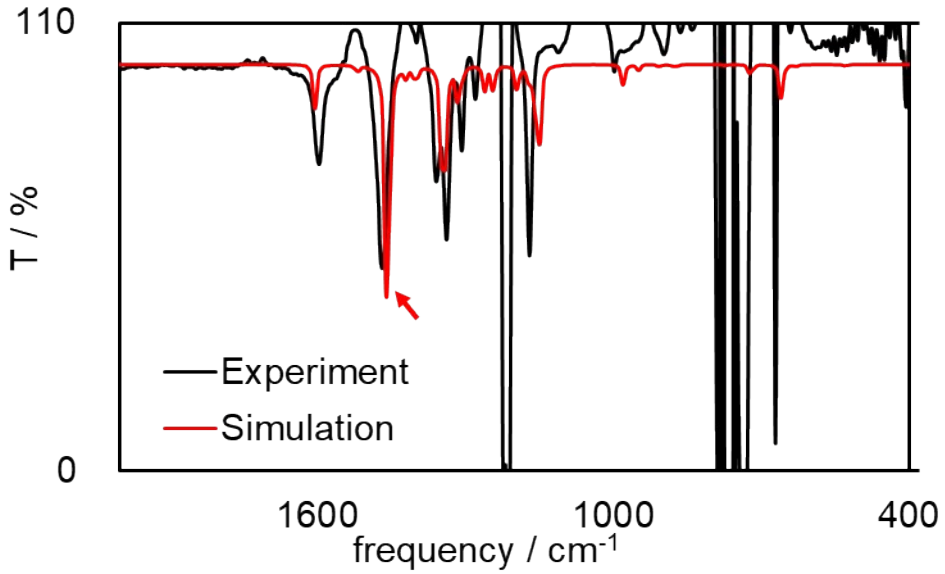


Fig. S12 Simulated and measured IR spectra of **SQ2b**.

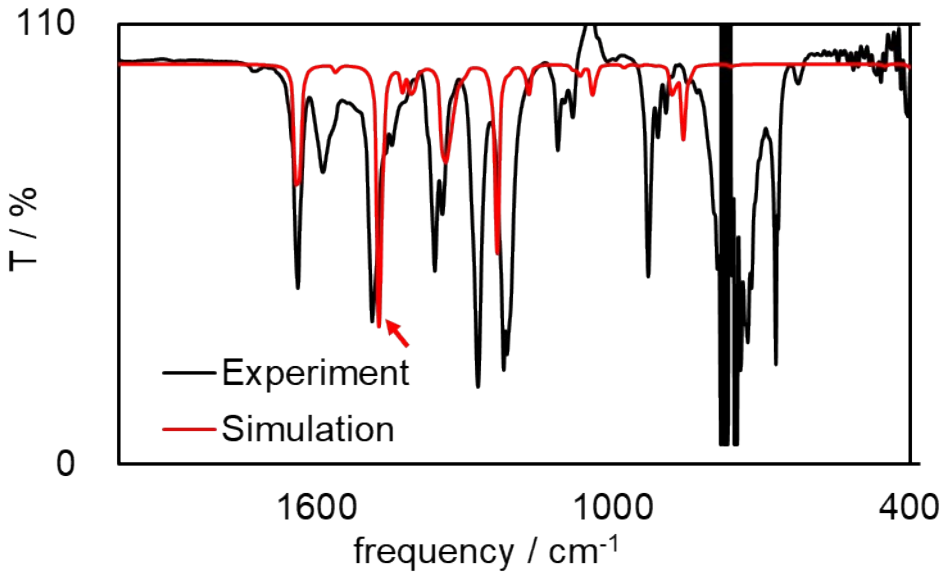


Fig. S13 Simulated and measured IR spectra of **SQ1a**.

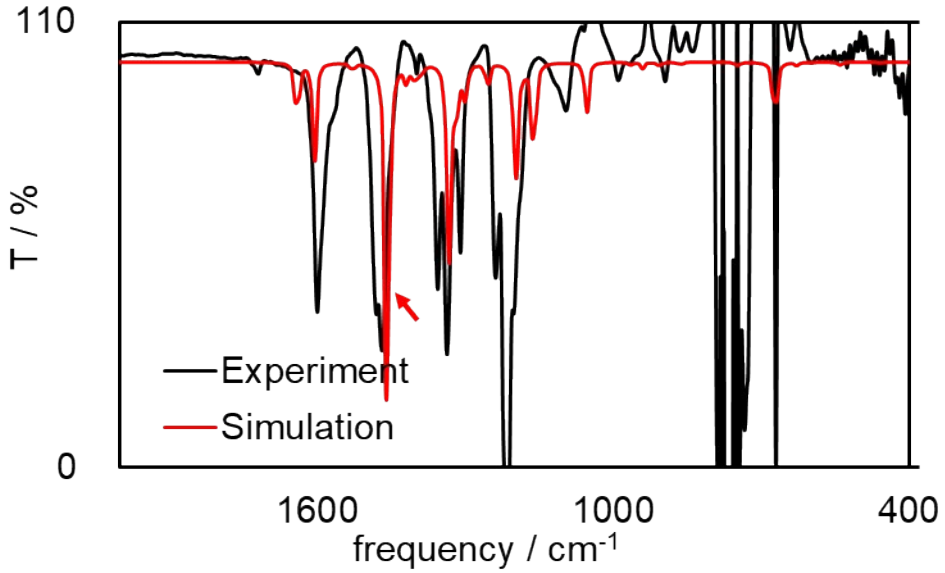


Fig. S14 Simulated and measured IR spectra of **SQ1b**.

9. Variable temperature electronic absorption spectra

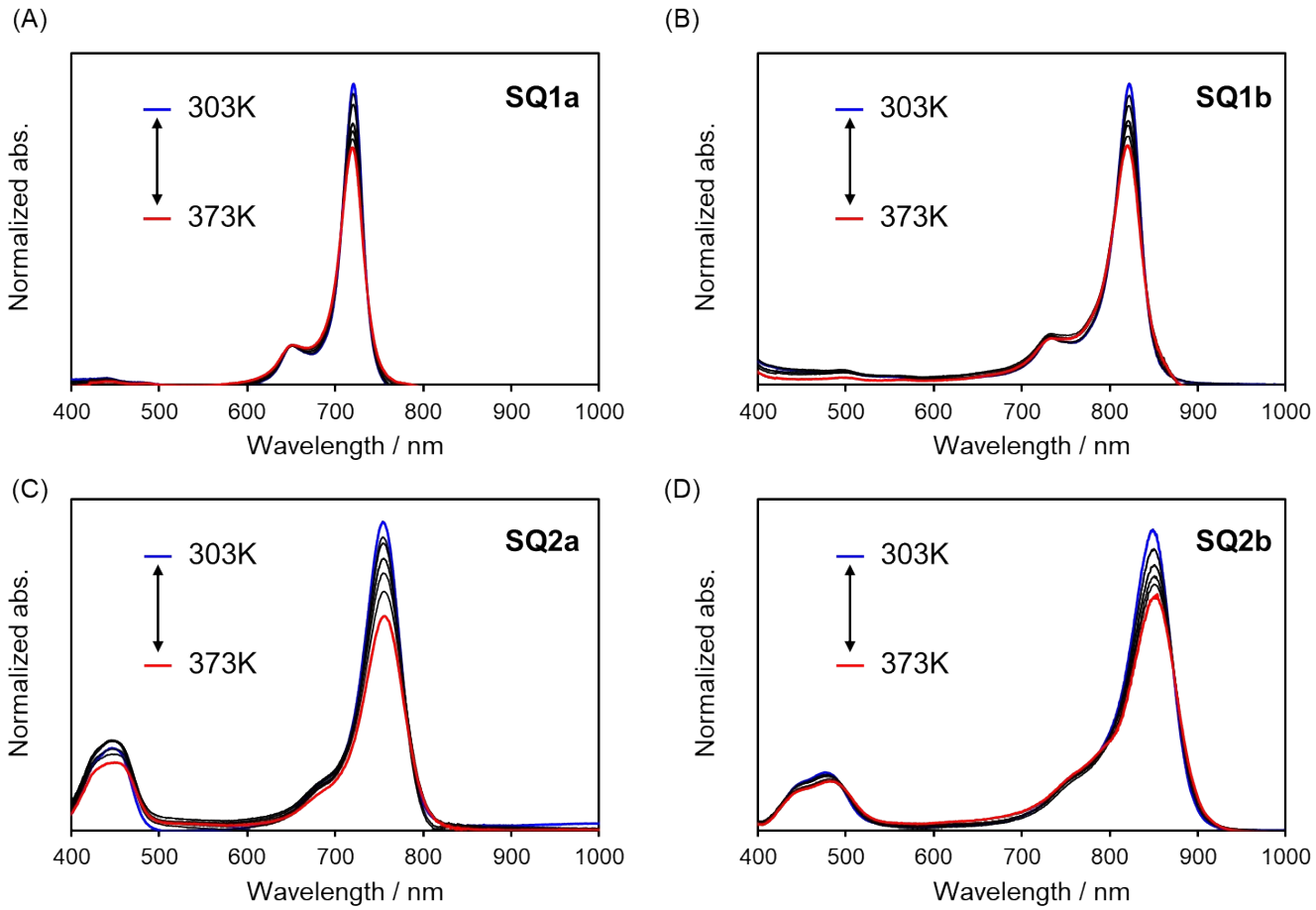


Fig. S15 Variable-temperature absorption spectra of **SQ1a** (A), **SQ1b** (B), **SQ2a** (C) and **SQ2b** (D) in DMSO (5 μM).

10. NMR and MS spectra

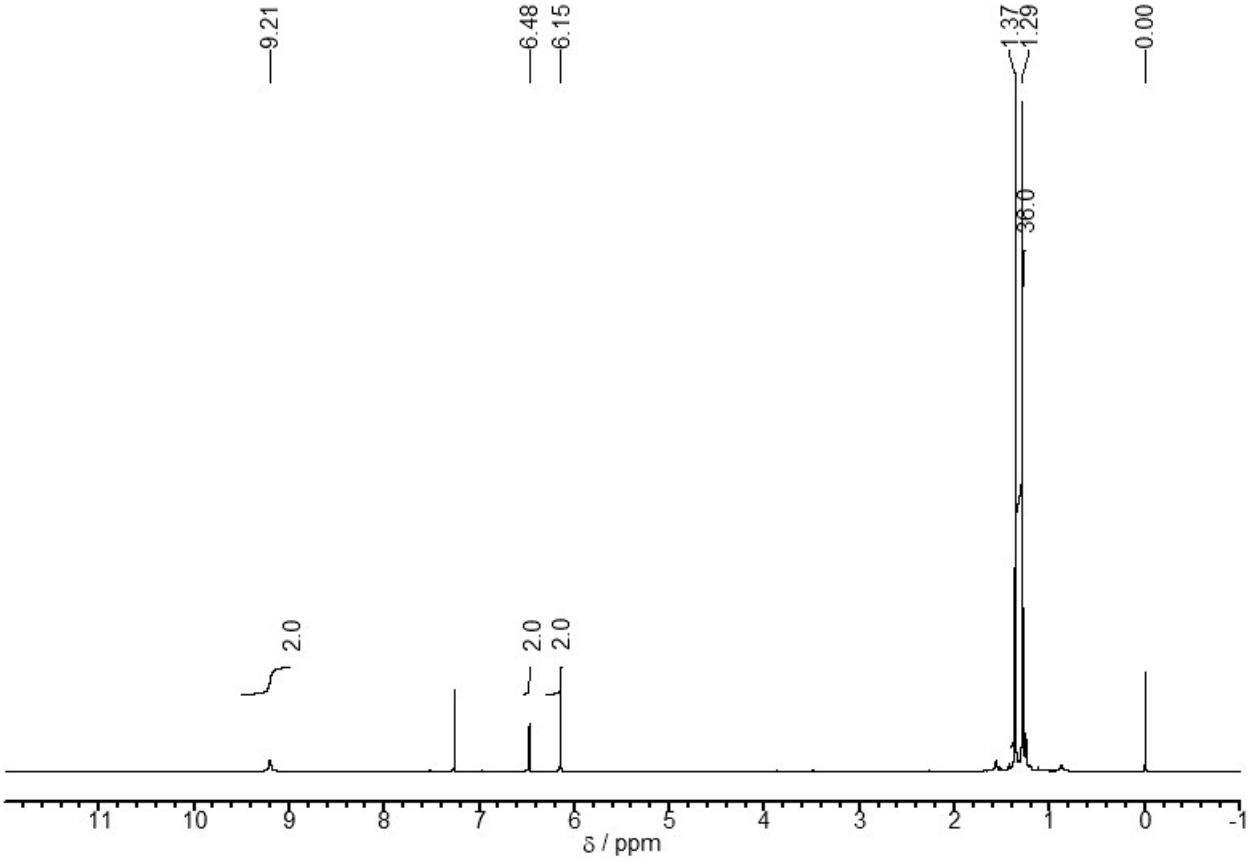


Fig. S16 A ^{1}H NMR spectrum ($CDCl_3$, 298K) of **SQ2a**.

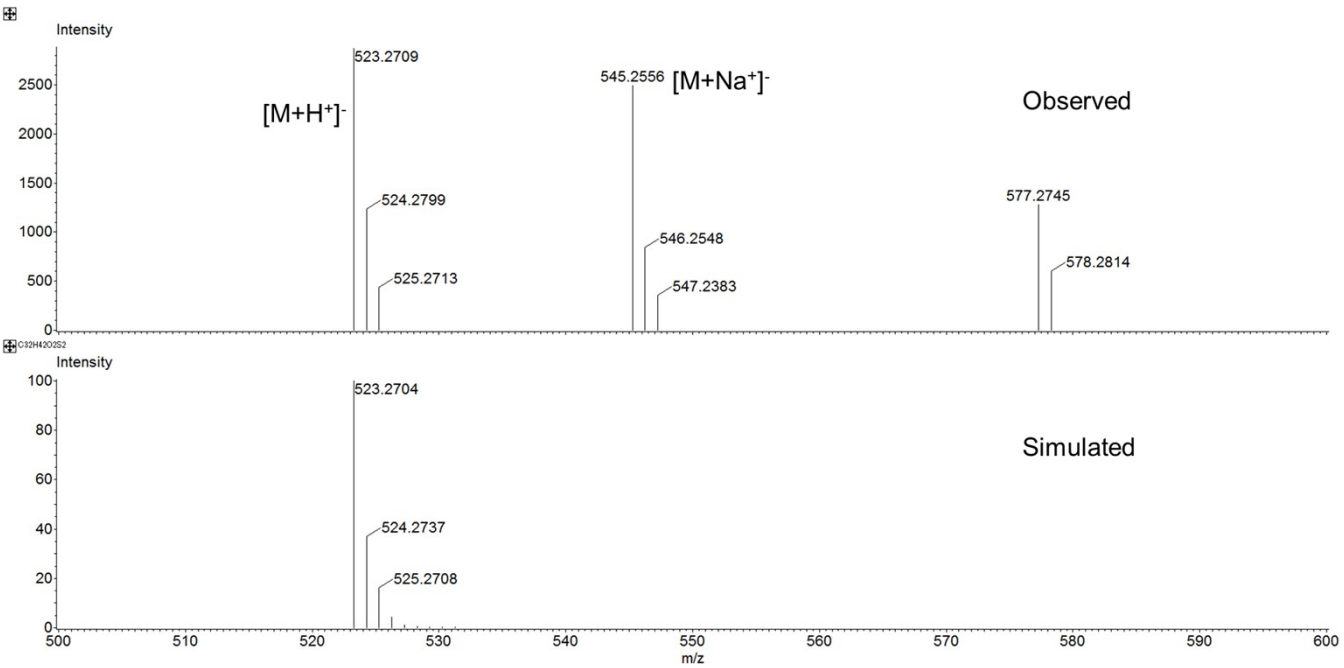


Fig. S17 ESI-MS (eluent: CH_2Cl_2/CH_3OH, 1/1, v/v) spectrum of **SQ2a** (Top) and its simulated spectrum (Bottom).

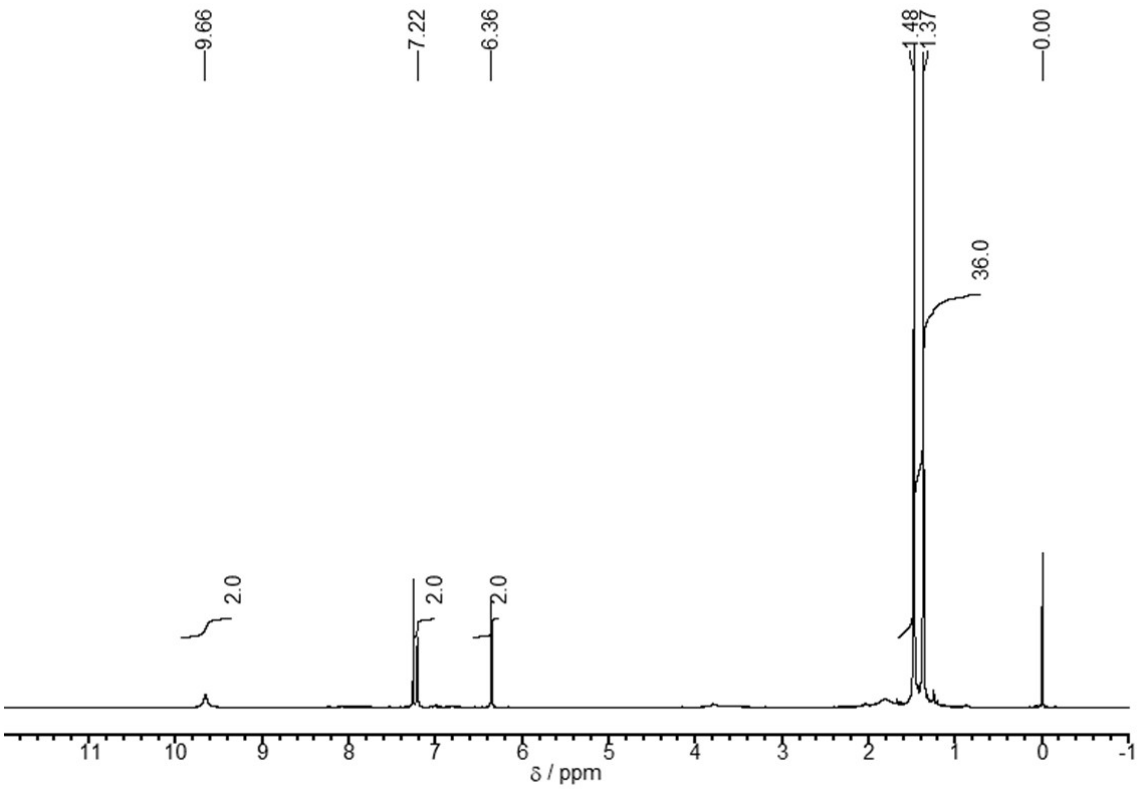


Fig. S18 A ^{1}H NMR spectrum ($CDCl_3$, 298K) of **SQ2b**.

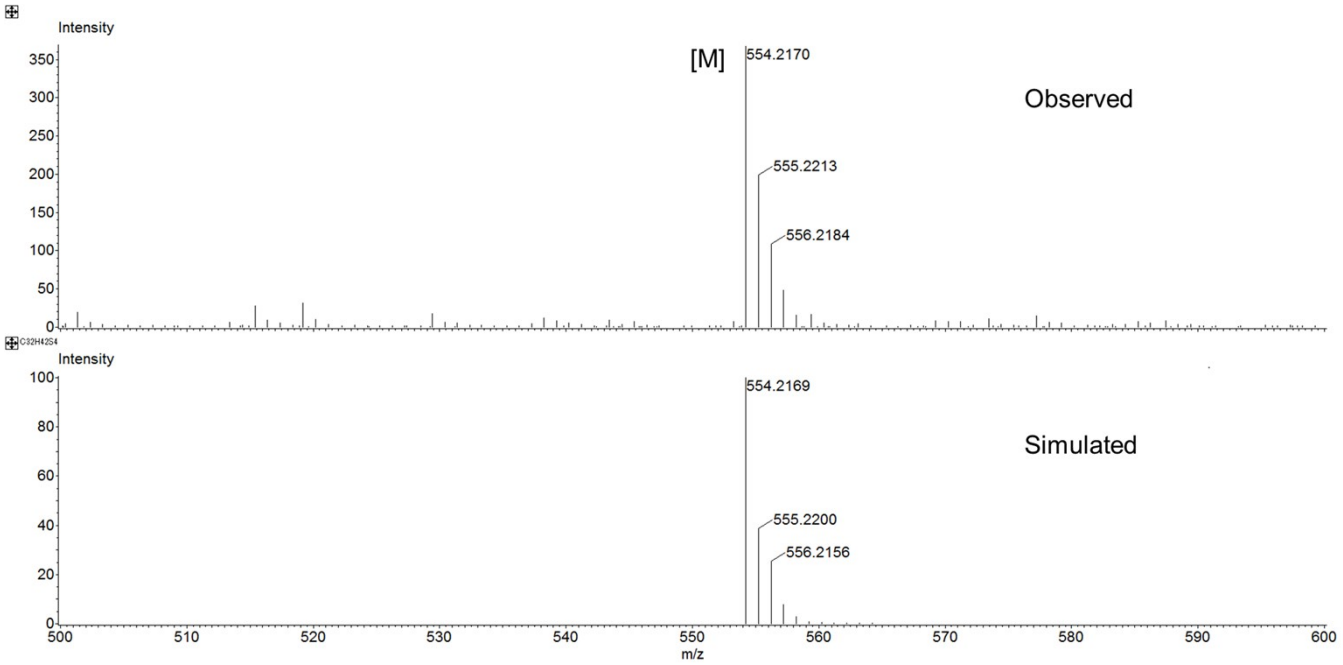


Fig. S19 ESI-MS (eluent: CH_2Cl_2/CH_3OH, 1/1, v/v) spectrum of **SQ2b** (Top) and its simulated spectrum (Bottom).

11. Cartesian Coordinates of quantum chemical calculations

Table S7 Optimized Cartesian coordinate of **SQ1a** (*trans*) UB3PW91/ccpVDZ Singlet

O	6.0679187	0.2560881	0.0000354	C	7.9308951	-1.5176005	-1.2597801
C	5.8311589	-1.0844387	-0.0000059	H	8.1652359	-0.4440333	-1.2895912
C	4.5619781	-1.5647522	-0.0000327	H	8.8805812	-2.0752166	-1.2691123
C	3.4262079	-0.6832200	-0.0000116	H	7.3753537	-1.7733578	-2.1754865
C	3.7388606	0.7208964	0.0000247	C	6.8378207	-3.3873483	0.0001098
C	5.0258791	1.1460712	0.0000534	H	6.2744197	-3.6986971	0.8930658
C	7.1211708	-1.8815737	-0.0000778	H	6.2741950	-3.6988858	-0.8926389
C	5.5174644	2.5793951	0.0000618	H	7.7909144	-3.9377408	0.0000378
C	2.1255707	-1.1909530	-0.0000280	C	7.9312330	-1.5173644	1.2593348
C	0.9351431	-0.4620069	0.0000455	H	7.3759290	-1.7729216	2.1752423
C	-0.4598665	-0.9396092	0.0000593	H	8.8809017	-2.0750110	1.2685322
H	4.4000076	-2.6412798	-0.0000524	H	8.1656135	-0.4438000	1.2888721
H	2.9186056	1.4459964	-0.0000009	C	-4.3367035	-3.5557003	0.0000943
H	2.0067683	-2.2798849	-0.0000701	H	-3.6982457	-3.4297303	-0.8862371
O	-6.0679198	-0.2560849	0.0000193	H	-3.6983061	-3.4297195	0.8864672
C	-5.8311555	1.0844411	-0.0000313	H	-4.7192388	-4.5878917	0.0000861
C	-4.5619731	1.5647506	-0.0000577	C	-6.3742140	-2.8146219	-1.2593106
C	-3.4262052	0.6832153	-0.0000347	H	-6.7485243	-3.8504733	-1.2687143
C	-3.7388627	-0.7209002	-0.0000042	H	-7.2422226	-2.1400324	-1.2919666
C	-5.0258825	-1.1460713	0.0000298	H	-5.7819408	-2.6587744	-2.1744366
C	-7.1211642	1.8815806	-0.0000746	C	-6.3742048	-2.8145661	1.2594592
C	-5.5174729	-2.5793931	0.0000632	H	-7.2422173	-2.1399819	1.2920985
C	-2.1255663	1.1909438	-0.0000406	H	-6.7485061	-3.8504204	1.2689093
C	-0.9351402	0.4619946	0.0000375	H	-5.7819204	-2.6586773	2.1745707
C	0.4598693	0.9395964	0.0000624	C	-7.9311441	1.5174515	1.2594156
H	-4.3999995	2.6412778	-0.0000848	H	-8.8808240	2.0750786	1.2686250
H	-2.9186108	-1.4460038	-0.0000355	H	-8.1654992	0.4438840	1.2890444
H	-2.0067597	2.2798753	-0.0000782	H	-7.3757890	1.7730890	2.1752693
C	6.3741019	2.8146309	-1.2593812	C	-7.9309775	1.5175309	-1.2596977
H	6.7484258	3.8504775	-1.2688042	H	-8.1653438	0.4439671	-1.2894167
H	7.2420999	2.1400309	-1.2921171	H	-8.8806510	2.0751687	-1.2690096
H	5.7817501	2.6588016	-2.1744595	H	-7.3754925	1.7732092	-2.1754608
C	4.3366912	3.5556971	0.0001981	C	-6.8378090	3.3873535	-0.0000060
H	3.6981514	3.4297290	-0.8860742	H	-6.2743193	3.6987558	0.8928759
H	3.6983776	3.4297077	0.8866304	H	-6.2742698	3.6988341	-0.8928287
H	4.7192215	4.5878903	0.0001594	H	-7.7909004	3.9377502	-0.0000105
C	6.3742992	2.8145695	1.2593872	O	0.9743324	2.0569144	0.0000840
H	7.2423233	2.1399974	1.2919507	O	-0.9743295	-2.0569271	0.0000761
H	6.7485852	3.8504294	1.2688117				
H	5.7820947	2.6586678	2.1745485				

Table S8. Optimized Cartesian coordinate of **SQ1a** (*cis*) UB3PW91/ccpVDZ Singlet

C	5.7405432	-0.6300250	-0.0000412	H	7.5896387	0.9370652	-1.2892707
C	4.7936409	-1.6014524	0.0001468	H	8.9220126	-0.2447726	-1.2733379
C	3.3908319	-1.2853008	0.0002401	H	7.4265607	-0.6000510	-2.1763417
C	3.0802733	0.1193578	0.0001988	C	7.6259654	-2.2913633	0.0007028
C	4.0667678	1.0491817	0.0000919	H	7.2470947	-2.8110920	0.8940010
C	7.2463979	-0.8069676	-0.0005664	H	7.2463990	-2.8128491	-0.8912729
C	3.9068256	2.5561867	0.0002606	H	8.7223209	-2.3876170	0.0003358
C	2.4332364	-2.3006388	0.0003659	C	7.8275764	-0.1335784	1.2579719
C	1.0430160	-2.1741930	0.0004818	H	7.4287967	-0.5954303	2.1745864
C	0.0000177	-3.2239133	0.0005447	H	8.9234477	-0.2426844	1.2692935
H	5.1021410	-2.6455496	0.0002171	H	7.5915740	0.9397055	1.2840523
H	2.0307644	0.4282548	0.0002967	C	-2.4244555	2.9430525	0.0014795
H	2.7979609	-3.3337252	0.0003846	H	-1.9004318	2.5598840	0.8891783
C	-5.7405377	-0.6300307	-0.0001251	H	-1.8984897	2.5593556	-0.8848343
C	-4.7936266	-1.6014481	0.0000976	H	-2.3358519	4.0403659	0.0012467
C	-3.3908167	-1.2852890	0.0003462	C	-4.5852782	3.1317948	1.2584375
C	-3.0802704	0.1193683	0.0004676	H	-4.4816803	4.2282931	1.2709682
C	-4.0667729	1.0491862	0.0002286	H	-5.6579665	2.8914825	1.2851360
C	-7.2463906	-0.8069849	-0.0004705	H	-4.1202506	2.7351164	2.1743282
C	-3.9068395	2.5561948	0.0000435	C	-4.5826598	3.1309830	-1.2601447
C	-2.4332349	-2.3006414	0.0004332	H	-5.6551773	2.8901633	-1.2891552
C	-1.0430113	-2.1742214	0.0005392	H	-4.4795184	4.2275222	-1.2729352
C	-0.0000129	-1.1305055	0.0005041	H	-4.1153617	2.7340721	-2.1747754
H	-5.1021231	-2.6455465	0.0000679	C	-7.8265051	-0.1350570	-1.2602988
H	-2.0307664	0.4282768	0.0007085	H	-8.9223891	-0.2439759	-1.2723409
H	-2.7979926	-3.3337151	0.0003707	H	-7.5902757	0.9381520	-1.2875109
C	4.5843333	3.1316244	-1.2587156	H	-7.4270836	-0.5981186	-2.1760218
H	4.4808668	4.2281351	-1.2712456	C	-7.8271832	-0.1346416	1.2588164
H	5.6569683	2.8911642	-1.2862402	H	-7.5909891	0.9385789	1.2858054
H	4.1185201	2.7349308	-2.1741998	H	-8.9230702	-0.2435812	1.2703064
C	2.4244350	2.9430183	-0.0001272	H	-7.4282459	-0.5973904	2.1749089
H	1.8997429	2.5597469	-0.8873840	C	-7.6259400	-2.2913852	-0.0003196
H	1.8991512	2.5594062	0.8866301	H	-7.2464850	-2.8121439	-0.8927685
H	2.3358125	4.0403306	0.0000603	H	-7.2469434	-2.8118314	0.8925063
C	4.5835607	3.1311516	1.2598724	H	-8.7222944	-2.3876523	-0.0005906
H	5.6561377	2.8905033	1.2880629	O	-0.0000149	0.1085202	0.0004947
H	4.4802643	4.2276762	1.2726628	O	0.0000402	-4.4444708	0.0005778
H	4.1170512	2.7342464	2.1749089	O	5.3875780	0.6855340	-0.0000640
C	7.8261082	-0.1360689	-1.2611404	O	-5.3875790	0.6855339	-0.0000996

Table S9. Optimized Cartesian coordinate of **SQ1b** (*trans*) UB3PW91/ccpVDZ Singlet

C	-5.8977233	1.1724809	0.0382542	H	8.4326601	-1.0184211	-1.1307864
C	-4.5754855	1.4869216	0.0044121	C	6.0942434	3.3344571	-1.2409766
C	-3.4734546	0.5642535	-0.0401548	H	6.2411520	4.4258725	-1.2605204
C	-3.7236465	-0.8524035	-0.0627599	H	7.0883824	2.8657691	-1.1763423
C	-4.9502863	-1.4394287	-0.0423434	H	5.6380255	3.0340444	-2.1969931
C	-7.0368929	2.1965676	0.1038843	C	3.8634391	3.7151306	-0.1876830
C	-5.1882560	-2.9541584	-0.0530105	H	3.3378809	3.4677039	-1.1211692
C	-2.1751411	1.0937348	-0.0558760	H	3.1718414	3.5043017	0.6395993
C	-0.9589082	0.4146642	-0.0762410	H	4.0710943	4.7964047	-0.1911068
C	0.4124840	0.9608510	-0.0788756	C	5.8660809	3.3713443	1.2679208
H	-4.3069945	2.5443350	0.0178824	H	6.8441805	2.8843557	1.4045314
H	-2.8415422	-1.5023592	-0.0949221	H	6.0296656	4.4607706	1.2755182
H	-2.0832916	2.1857999	-0.0439527	H	5.2339343	3.1143336	2.1318568
C	5.8978151	-1.1724332	0.0382143	C	-6.4938068	3.6311576	0.0904139
C	4.5755886	-1.4869507	0.0045630	H	-5.8473545	3.8352014	0.9573846
C	3.4735129	-0.5643496	-0.0402911	H	-5.9254588	3.8474592	-0.8269470
C	3.7236219	0.8523131	-0.0630308	H	-7.3370159	4.3372453	0.1331307
C	4.9502364	1.4393976	-0.0428584	C	-7.9688180	2.0157929	-1.1110482
C	7.0370490	-2.1964397	0.1040548	H	-8.4329334	1.0180567	-1.1300066
C	5.1880524	2.9541524	-0.0530112	H	-8.7786739	2.7615327	-1.0753697
C	2.1752231	-1.0938927	-0.0560459	H	-7.4186134	2.1506348	-2.0552125
C	0.9589837	-0.4148480	-0.0763760	C	-7.8371481	1.9885126	1.4054031
C	-0.4124209	-0.9610368	-0.0792551	H	-8.6522247	2.7270417	1.4674931
H	4.3071494	-2.5443712	0.0184809	H	-8.2879050	0.9857327	1.4549946
H	2.8414811	1.5022298	-0.0949613	H	-7.1922170	2.1132130	2.2890762
H	2.0834225	-2.1859625	-0.0441935	C	-5.8684297	-3.3716657	1.2667057
S	6.4365036	0.4968908	0.0165806	H	-6.8467508	-2.8847296	1.4018916
S	-6.4365003	-0.4968247	0.0173092	H	-6.0320580	-4.4610860	1.2737521
C	6.4940245	-3.6310605	0.0914022	H	-5.2377032	-3.1149132	2.1317583
H	5.8476032	-3.8346348	0.9585080	C	-6.0926336	-3.3339752	-1.2425270
H	5.9256662	-3.8479091	-0.8258209	H	-6.2397769	-4.4253518	-1.2625898
H	7.3372648	-4.3370895	0.1344839	H	-7.0867327	-2.8650117	-1.1792667
C	7.8376582	-1.9877530	1.4052499	H	-5.6348323	-3.0334006	-2.1977308
H	8.6527602	-2.7262431	1.4674680	C	-3.8635335	-3.7152833	-0.1857709
H	8.2884214	-0.9849472	1.4542479	H	-3.3365139	-3.4679766	-1.1184516
H	7.1929812	-2.1120476	2.2891659	H	-3.1731896	-3.5044874	0.6425762
C	7.9686203	-2.0161825	-1.1112272	H	-4.0713061	-4.7965371	-0.1894419
H	8.7785384	-2.7618504	-1.0754295	O	-0.8718332	-2.1007152	-0.0795782
H	7.4181474	-2.1515050	-2.0551668	O	0.8718947	2.1005297	-0.0787154

Table S10. Optimized Cartesian coordinate of **SQ1b** (*cis*) UB3PW91/ccpVDZ Singlet

C	5.9038401	-0.8145884	0.0054850	H	8.1317648	0.2699139	-1.2793820
C	4.7999948	-1.6078462	0.0000990	H	9.1230704	-1.2062181	-1.2343283
C	3.4286425	-1.1739820	-0.0150890	H	7.5927784	-1.1851315	-2.1511654
C	3.1213423	0.2315401	-0.0358280	C	7.3933330	-2.8600637	0.0387734
C	4.0334925	1.2404794	-0.0364403	H	6.9035351	-3.2778897	0.9313937
C	7.3486513	-1.3267029	0.0235198	H	6.9199964	-3.2951468	-0.8544780
C	3.6804491	2.7325388	-0.0392038	H	8.4433508	-3.1898820	0.0515262
C	2.4313597	-2.1591785	-0.0086015	C	8.0651491	-0.8043783	1.2850276
C	1.0450505	-2.0177954	-0.0053492	H	7.5519673	-1.1411721	2.1990893
C	0.0000107	-3.0674656	0.0008979	H	9.0992632	-1.1829644	1.3120189
H	4.9541765	-2.6878346	0.0104434	H	8.1099870	0.2950497	1.3081300
H	2.0580616	0.4951219	-0.0482772	C	-2.1656742	2.9351666	0.1599921
H	2.7693443	-3.2019143	-0.0011344	H	-1.7679803	2.5074818	1.0916190
C	-5.9038283	-0.8146405	-0.0066283	H	-1.6147261	2.4767004	-0.6728135
C	-4.7999409	-1.6078227	-0.0005407	H	-1.9473069	4.0143862	0.1601687
C	-3.4286061	-1.1739120	0.0154197	C	-4.3632878	3.4329826	1.2312198
C	-3.1213493	0.2316257	0.0363836	H	-4.0880120	4.4994322	1.2422569
C	-4.0334901	1.2405602	0.0364621	H	-5.4612886	3.3738359	1.1781461
C	-7.3486120	-1.3268192	-0.0246255	H	-4.0449859	2.9872796	2.1863953
C	-3.6805059	2.7326207	0.0395583	C	-4.1623949	3.3708720	-1.2792630
C	-2.4313173	-2.1590996	0.0094805	H	-5.2534259	3.2904716	-1.4034876
C	-1.0449894	-2.0177678	0.0068755	H	-3.9003727	4.4408864	-1.2944927
C	0.0000419	-0.9747397	0.0007909	H	-3.6851951	2.8886057	-2.1463413
H	-4.9540670	-2.6878193	-0.0109680	C	-8.0663919	-0.8021574	-1.2843992
H	-2.0580792	0.4952233	0.0494588	H	-9.1004302	-1.1809531	-1.3111633
H	-2.7693202	-3.2018282	0.0018875	H	-8.1116029	0.2972983	-1.3053153
C	4.3627124	3.4331287	-1.2310240	H	-7.5540013	-1.1369781	-2.1996316
H	4.0873414	4.4995554	-1.2417971	C	-8.0868938	-0.8314283	1.2352436
H	5.4607398	3.3740766	-1.1783904	H	-8.1302558	0.2672860	1.2821558
H	4.0440826	2.9875370	-2.1861425	H	-9.1218821	-1.2086288	1.2351374
C	2.1655621	2.9350452	-0.1589789	H	-7.5907049	-1.1895899	2.1505599
H	1.7674922	2.5074471	-1.0904837	C	-7.3931985	-2.8601526	-0.0428334
H	1.6149762	2.4764828	0.6740157	H	-6.9034004	-3.2761860	-0.9362944
H	1.9471544	4.0142558	-0.1589443	H	-6.9198077	-3.2969676	0.8495404
C	4.1628535	3.3705796	1.2795322	H	-8.4431948	-3.1900199	-0.0560659
H	5.2539322	3.2901493	1.4033167	S	5.7666197	0.9346643	-0.0115029
H	3.9008470	4.4405937	1.2950410	S	-5.7667035	0.9347112	0.0102797
H	3.6859813	2.8881724	2.1467123	O	0.0000790	0.2626571	0.0007499
C	8.0881373	-0.8288798	-1.2346512	O	0.0000067	-4.2872120	0.0009782

Table S11. Optimized Cartesian coordinate of **SQ2a** (*trans*) UB3PW91/ccpVDZ Singlet

C	-5.8977233	1.1724809	0.0382542	H	8.4326601	-1.0184211	-1.1307864
C	-4.5754855	1.4869216	0.0044121	C	6.0942434	3.3344571	-1.2409766
C	-3.4734546	0.5642535	-0.0401548	H	6.2411520	4.4258725	-1.2605204
C	-3.7236465	-0.8524035	-0.0627599	H	7.0883824	2.8657691	-1.1763423
C	-4.9502863	-1.4394287	-0.0423434	H	5.6380255	3.0340444	-2.1969931
C	-7.0368929	2.1965676	0.1038843	C	3.8634391	3.7151306	-0.1876830
C	-5.1882560	-2.9541584	-0.0530105	H	3.3378809	3.4677039	-1.1211692
C	-2.1751411	1.0937348	-0.0558760	H	3.1718414	3.5043017	0.6395993
C	-0.9589082	0.4146642	-0.0762410	H	4.0710943	4.7964047	-0.1911068
C	0.4124840	0.9608510	-0.0788756	C	5.8660809	3.3713443	1.2679208
H	-4.3069945	2.5443350	0.0178824	H	6.8441805	2.8843557	1.4045314
H	-2.8415422	-1.5023592	-0.0949221	H	6.0296656	4.4607706	1.2755182
H	-2.0832916	2.1857999	-0.0439527	H	5.2339343	3.1143336	2.1318568
C	5.8978151	-1.1724332	0.0382143	C	-6.4938068	3.6311576	0.0904139
C	4.5755886	-1.4869507	0.0045630	H	-5.8473545	3.8352014	0.9573846
C	3.4735129	-0.5643496	-0.0402911	H	-5.9254588	3.8474592	-0.8269470
C	3.7236219	0.8523131	-0.0630308	H	-7.3370159	4.3372453	0.1331307
C	4.9502364	1.4393976	-0.0428584	C	-7.9688180	2.0157929	-1.1110482
C	7.0370490	-2.1964397	0.1040548	H	-8.4329334	1.0180567	-1.1300066
C	5.1880524	2.9541524	-0.0530112	H	-8.7786739	2.7615327	-1.0753697
C	2.1752231	-1.0938927	-0.0560459	H	-7.4186134	2.1506348	-2.0552125
C	0.9589837	-0.4148480	-0.0763760	C	-7.8371481	1.9885126	1.4054031
C	-0.4124209	-0.9610368	-0.0792551	H	-8.6522247	2.7270417	1.4674931
H	4.3071494	-2.5443712	0.0184809	H	-8.2879050	0.9857327	1.4549946
H	2.8414811	1.5022298	-0.0949613	H	-7.1922170	2.1132130	2.2890762
H	2.0834225	-2.1859625	-0.0441935	C	-5.8684297	-3.3716657	1.2667057
S	6.4365036	0.4968908	0.0165806	H	-6.8467508	-2.8847296	1.4018916
S	-6.4365003	-0.4968247	0.0173092	H	-6.0320580	-4.4610860	1.2737521
C	6.4940245	-3.6310605	0.0914022	H	-5.2377032	-3.1149132	2.1317583
H	5.8476032	-3.8346348	0.9585080	C	-6.0926336	-3.3339752	-1.2425270
H	5.9256662	-3.8479091	-0.8258209	H	-6.2397769	-4.4253518	-1.2625898
H	7.3372648	-4.3370895	0.1344839	H	-7.0867327	-2.8650117	-1.1792667
C	7.8376582	-1.9877530	1.4052499	H	-5.6348323	-3.0334006	-2.1977308
H	8.6527602	-2.7262431	1.4674680	C	-3.8635335	-3.7152833	-0.1857709
H	8.2884214	-0.9849472	1.4542479	H	-3.3365139	-3.4679766	-1.1184516
H	7.1929812	-2.1120476	2.2891659	H	-3.1731896	-3.5044874	0.6425762
C	7.9686203	-2.0161825	-1.1112272	H	-4.0713061	-4.7965371	-0.1894419
H	8.7785384	-2.7618504	-1.0754295	O	-0.8718332	-2.1007152	-0.0795782
H	7.4181474	-2.1515050	-2.0551668	O	0.8718947	2.1005297	-0.0787154

Table S12. Optimized Cartesian coordinate of **SQ2a** (*cis*) UB3PW91/ccpVDZ Singlet

C	5.9038401	-0.8145884	0.0054850	H	8.1317648	0.2699139	-1.2793820
C	4.7999948	-1.6078462	0.0000990	H	9.1230704	-1.2062181	-1.2343283
C	3.4286425	-1.1739820	-0.0150890	H	7.5927784	-1.1851315	-2.1511654
C	3.1213423	0.2315401	-0.0358280	C	7.3933330	-2.8600637	0.0387734
C	4.0334925	1.2404794	-0.0364403	H	6.9035351	-3.2778897	0.9313937
C	7.3486513	-1.3267029	0.0235198	H	6.9199964	-3.2951468	-0.8544780
C	3.6804491	2.7325388	-0.0392038	H	8.4433508	-3.1898820	0.0515262
C	2.4313597	-2.1591785	-0.0086015	C	8.0651491	-0.8043783	1.2850276
C	1.0450505	-2.0177954	-0.0053492	H	7.5519673	-1.1411721	2.1990893
C	0.0000107	-3.0674656	0.0008979	H	9.0992632	-1.1829644	1.3120189
H	4.9541765	-2.6878346	0.0104434	H	8.1099870	0.2950497	1.3081300
H	2.0580616	0.4951219	-0.0482772	C	-2.1656742	2.9351666	0.1599921
H	2.7693443	-3.2019143	-0.0011344	H	-1.7679803	2.5074818	1.0916190
C	-5.9038283	-0.8146405	-0.0066283	H	-1.6147261	2.4767004	-0.6728135
C	-4.7999409	-1.6078227	-0.0005407	H	-1.9473069	4.0143862	0.1601687
C	-3.4286061	-1.1739120	0.0154197	C	-4.3632878	3.4329826	1.2312198
C	-3.1213493	0.2316257	0.0363836	H	-4.0880120	4.4994322	1.2422569
C	-4.0334901	1.2405602	0.0364621	H	-5.4612886	3.3738359	1.1781461
C	-7.3486120	-1.3268192	-0.0246255	H	-4.0449859	2.9872796	2.1863953
C	-3.6805059	2.7326207	0.0395583	C	-4.1623949	3.3708720	-1.2792630
C	-2.4313173	-2.1590996	0.0094805	H	-5.2534259	3.2904716	-1.4034876
C	-1.0449894	-2.0177678	0.0068755	H	-3.9003727	4.4408864	-1.2944927
C	0.0000419	-0.9747397	0.0007909	H	-3.6851951	2.8886057	-2.1463413
H	-4.9540670	-2.6878193	-0.0109680	C	-8.0663919	-0.8021574	-1.2843992
H	-2.0580792	0.4952233	0.0494588	H	-9.1004302	-1.1809531	-1.3111633
H	-2.7693202	-3.2018282	0.0018875	H	-8.1116029	0.2972983	-1.3053153
C	4.3627124	3.4331287	-1.2310240	H	-7.5540013	-1.1369781	-2.1996316
H	4.0873414	4.4995554	-1.2417971	C	-8.0868938	-0.8314283	1.2352436
H	5.4607398	3.3740766	-1.1783904	H	-8.1302558	0.2672860	1.2821558
H	4.0440826	2.9875370	-2.1861425	H	-9.1218821	-1.2086288	1.2351374
C	2.1655621	2.9350452	-0.1589789	H	-7.5907049	-1.1895899	2.1505599
H	1.7674922	2.5074471	-1.0904837	C	-7.3931985	-2.8601526	-0.0428334
H	1.6149762	2.4764828	0.6740157	H	-6.9034004	-3.2761860	-0.9362944
H	1.9471544	4.0142558	-0.1589443	H	-6.9198077	-3.2969676	0.8495404
C	4.1628535	3.3705796	1.2795322	H	-8.4431948	-3.1900199	-0.0560659
H	5.2539322	3.2901493	1.4033167	S	5.7666197	0.9346643	-0.0115029
H	3.9008470	4.4405937	1.2950410	S	-5.7667035	0.9347112	0.0102797
H	3.6859813	2.8881724	2.1467123	O	0.0000790	0.2626571	0.0007499
C	8.0881373	-0.8288798	-1.2346512	O	0.0000067	-4.2872120	0.0009782

Table S13. Optimized Cartesian coordinate of **SQ2b** (*trans*) UB3PW91/ccpVDZ Singlet

C	-5.9160464	1.2551193	0.0322132	H	8.6464886	-3.0432826	-1.1499984
C	-4.5743245	1.4720829	0.0152143	H	7.3092039	-2.3370652	-2.0960748
C	-3.5361324	0.4756848	-0.0155211	H	8.4238519	-1.2796024	-1.1968756
C	-3.8851675	-0.9188397	-0.0419558	C	6.4450613	3.2041882	-1.2478064
C	-5.1551732	-1.4135911	-0.0354556	H	6.6789819	4.2801346	-1.2724555
C	-6.9795186	2.3588180	0.0718955	H	7.3992289	2.6581259	-1.1889547
C	-5.5195466	-2.9039978	-0.0510936	H	5.9587277	2.9387213	-2.1992471
C	-2.2184954	0.9584250	-0.0187993	C	4.2657314	3.7751879	-0.1776180
C	-0.9791836	0.3238383	-0.0282984	H	3.7079414	3.5644708	-1.1015794
C	0.3294594	0.9878786	-0.0286131	H	3.5723244	3.6336631	0.6631872
H	-4.2314572	2.5074195	0.0289983	H	4.5658515	4.8343623	-0.1960121
H	-3.0509448	-1.6305557	-0.0665585	C	6.2410434	3.2641493	1.2635996
H	-2.1092293	2.0497758	-0.0078964	H	7.1796442	2.7026366	1.3894562
C	5.9160490	-1.2551195	0.0320638	H	6.4884672	4.3375043	1.2691197
C	4.5743330	-1.4720952	0.0146532	H	5.5996544	3.0564773	2.1338785
C	3.5361398	-0.4756959	-0.0159649	C	-6.3346072	3.7504459	0.0728120
C	3.8851758	0.9188321	-0.0423222	H	-5.6937874	3.9080555	0.9534997
C	5.1551732	1.4135939	-0.0355415	H	-5.7332621	3.9265352	-0.8319324
C	6.9795176	-2.3588156	0.0719652	H	-7.1262192	4.5146985	0.0985277
C	5.5195517	2.9039929	-0.0511716	C	-7.8902212	2.2424487	-1.1668075
C	2.2185018	-0.9584301	-0.0192577	H	-8.4230942	1.2800105	-1.1981535
C	0.9791892	-0.3238406	-0.0285233	H	-8.6457294	3.0436817	-1.1509072
C	-0.3294541	-0.9878805	-0.0286943	H	-7.3078640	2.3377124	-2.0963501
H	4.2314756	-2.5074396	0.0280769	C	-7.8252688	2.2094020	1.3525843
H	3.0509552	1.6305475	-0.0670621	H	-8.5832171	3.0074585	1.3954573
H	2.1092322	-2.0497825	-0.0084890	H	-8.3524291	1.2438882	1.3880195
S	0.7518579	2.5931873	-0.0247078	H	-7.1957804	2.2847143	2.2527646
S	-0.7518558	-2.5931886	-0.0248734	C	-6.2411705	-3.2641021	1.2636357
S	6.5675635	0.3685183	0.0101720	H	-7.1797090	-2.7024769	1.3894185
S	-6.5675652	-0.3685131	0.0098351	H	-6.4887030	-4.3374325	1.2691266
C	6.3346278	-3.7504548	0.0720380	H	-5.5998037	-3.0565020	2.1339485
H	5.6933843	-3.9084337	0.9523514	C	-6.4449642	-3.2042179	-1.2477833
H	5.7337223	-3.9261860	-0.8330684	H	-6.6788067	-4.2801806	-1.2724871
H	7.1262392	-4.5147054	0.0978297	H	-7.3991859	-2.6582426	-1.1889651
C	7.8244764	-2.2097760	1.3532216	H	-5.9586240	-2.9386817	-2.1992038
H	8.5824276	-3.0078190	1.3963269	C	-4.2657160	-3.7751969	-0.1773969
H	8.3515825	-1.2442541	1.3892842	H	-3.7078301	-3.5644795	-1.1012937
H	7.1944258	-2.2853789	2.2529840	H	-3.5724263	-3.6336404	0.6634994
C	7.8909781	-2.2420583	-1.1661408	H	-4.5658288	-4.8343714	-0.1957911

Table S14. Optimized Cartesian coordinate of **SQ2b** (*cis*) UB3PW91/ccpVDZ Singlet

C	-6.0330463	0.9185630	0.0004194	H	-4.6764570	-3.1137293	2.1746753
C	-4.8097244	1.5107638	0.0002936	C	-8.1722793	1.2975368	-1.2590622
C	-3.5284121	0.8548685	-0.0003182	H	-8.4066776	0.2227007	-1.2928916
C	-3.4631376	-0.5809777	-0.0007652	H	-9.1256090	1.8490276	-1.2720415
C	-4.5375488	-1.4195834	-0.0008332	H	-7.6157044	1.5520937	-2.1742727
C	-7.3676272	1.6739702	0.0011268	C	-7.1444179	3.1915387	0.0018428
C	-4.4578638	-2.9514815	-0.0007207	H	-6.5959514	3.5275517	0.8948250
C	-2.4072166	1.6987240	-0.0004201	H	-6.5963039	3.5284416	-0.8910245
C	-1.0318880	1.4747161	-0.0005593	H	-8.1208232	3.6993532	0.0022747
C	0.0000208	2.5139236	-0.0007056	C	-8.1716850	1.2962772	1.2613290
H	-4.7789868	2.6008966	0.0007838	H	-7.6147023	1.5500058	2.1765198
H	-2.4585491	-1.0206634	-0.0010013	H	-9.1250368	1.8477015	1.2752514
H	-2.6271737	2.7733710	-0.0003093	H	-8.4059894	0.2213948	1.2942366
C	6.0330859	0.9185807	0.0001272	C	3.0008304	-3.4252235	0.0019742
C	4.8097668	1.5107673	-0.0002370	H	2.4525906	-3.0758823	0.8885399
C	3.5284361	0.8548879	-0.0001492	H	2.4508776	-3.0759909	-0.8835626
C	3.4631261	-0.5809586	0.0002561	H	2.9819375	-4.5261270	0.0020459
C	4.5374969	-1.4196074	0.0005994	C	5.1552935	-3.5046179	1.2601888
C	7.3676819	1.6739443	0.0000337	H	5.0757221	-4.6031341	1.2756550
C	4.4577597	-2.9515040	0.0006111	H	6.2250685	-3.2466097	1.2923960
C	2.4072589	1.6987537	-0.0004951	H	4.6833041	-3.1147586	2.1752508
C	1.0319282	1.4747090	-0.0005635	C	5.1528774	-3.5041758	-1.2605151
C	0.0000273	0.4319907	-0.0004598	H	6.2225071	-3.2458388	-1.2947661
H	4.7790296	2.6009009	-0.0006148	H	5.0735285	-4.6027091	-1.2761042
H	2.4585302	-1.0206226	0.0002311	H	4.6789347	-3.1141732	-2.1745018
H	2.6271955	2.7734017	-0.0007351	C	8.1720165	1.2966580	-1.2601048
S	0.0000215	4.1642011	-0.0009858	H	9.1253901	1.8480587	-1.2736425
S	-0.0000017	-1.2371357	-0.0003798	H	8.4062985	0.2217780	-1.2933122
C	-5.1568378	-3.5048680	-1.2593741	H	7.6152517	1.5506965	-2.1753440
H	-5.0771449	-4.6033760	-1.2747540	C	8.1720356	1.2970452	1.2602824
H	-6.2266967	-3.2470419	-1.2903603	H	8.4063523	0.2221840	1.2938157
H	-4.6860114	-3.1151126	-2.1750818	H	9.1253942	1.8484729	1.2736310
C	-3.0009456	-3.4252197	-0.0036515	H	7.6152733	1.5513495	2.1754477
H	-2.4536939	-3.0758714	-0.8908298	C	7.1445296	3.1915232	-0.0001816
H	-2.4500031	-3.0760131	0.8812750	H	6.5962467	3.5278753	-0.8931520
H	-2.9820716	-4.5261234	-0.0037563	H	6.5962539	3.5281230	0.8926973
C	-5.1515676	-3.5038259	1.2613365	H	8.1209520	3.6993052	-0.0002714
H	-6.2211022	-3.2452710	1.2967976	S	-6.1914369	-0.8241044	-0.0005618
H	-5.0723823	-4.6023692	1.2770292	S	6.1914540	-0.8241771	0.0007475

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