

Supporting Information

Development of asymmetrical near infrared squaraines with large Stokes shift

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1. General Information

Materials Used

All chemicals, otherwise stated, were purchased from Sigma Aldrich and used without further purifications.

Liquid Chromatography-Mass Spectrum (LC/MS)

Shimadzu 2020 Liquid chromatography – Mass Spectroscopy (LC/MS) was used for analyzing reaction mixture. Sonoma C18 Column, 4.6mm x 50mm, 5 μ 100 \AA particle size columns was used. Analytical method is gradient 5% - 95% ACN over 6 minutes at a flow rate of 1mL/min.

The mobile phases used for LC/MS are 0.05% FA in ACN and 0.05% FA in MilliQ-H₂O.

HRMS was determined using microOTOF-Q II with APCI source in positive ion polarity.

Nuclear Magnetic Resonance Spectroscopy

Proton nuclear magnetic resonance (¹H NMR) and carbon nuclear magnetic resonance (¹³C NMR) spectroscopy were performed on 400 MHz and 300MHz NMR spectrometers. Chemical shifts are reported as δ in units of parts per million (ppm) downfield from tetramethylsilane (δ 0.00), using the residual solvent signal as an internal standard: chloroform-d, CDCl₃, (¹H NMR, δ 7.26, singlet; ¹³C NMR, δ 77.04, triplet). Multiplicities are given as: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplets). The number of protons (n) for a given resonance is indicated by nH.

Cyclic Voltammetry (CV) Measurement

CV measurement was conducted in a three electrode cell consisting of reference electrode (Ag/AgCl), working electrode (Pt) and counter electrode. The working electrode was filled with electrolyte solution (non aqueous c(LiCl) 2mol/L in ethanol) from Fluka Analytical. 0.1M tetrabutylammonium hexafluorophosphate ($(\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2)_4\text{N}(\text{PF}_6)$) from Fluka Analytical in dichloromethane was prepared. The calibration graph for (Fc/Fc^+) was measured by dissolving Ferrocene from Sigma Aldrich in the 0.1M $(\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2)_4\text{N}(\text{PF}_6)$ solution. The same procedure was repeated by dissolving various squaraine dyes to obtain the CV measurement for various squaraine dyes. The E_{ox} and E_{red} values were determined from the CV curve and λ_{ons} from the UV-Abs curve. The HOMO and LUMO energy level were then estimated from the following empirical formulae, $E_{\text{HOMO}}^{\text{opt}} = -5.23\text{eV} - eE_{\text{ox}} + 1/2(E_{\text{cv}}^{\text{sol}} - E_{\text{g}})$, $E_{\text{LUMO}}^{\text{opt}} = -5.23\text{eV} - eE_{\text{red}} - 1/2(E_{\text{cv}}^{\text{sol}} - E_{\text{g}})$, $E_{\text{cv}}^{\text{sol}} = E_{\text{ox}} - E_{\text{red}}$, $E_{\text{g}} = 1240/\lambda_{\text{ons}}$.

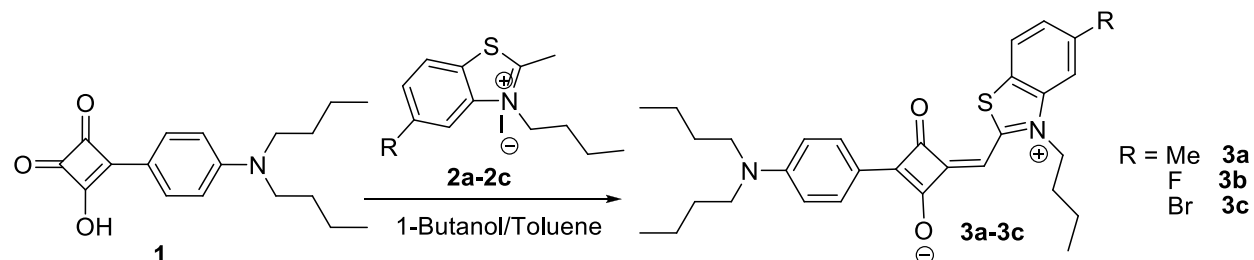
Absorbance and Fluorescence Measurement

UV-Abs characterization was measured in 3 different solvents by UV spectrophotometer (UV-1800) from Shimadzu. Fluorescence measurements were performed in DMSO by an Infinite® 200 PRO multimode reader (Tecan Group Ltd., Männedorf, Switzerland).

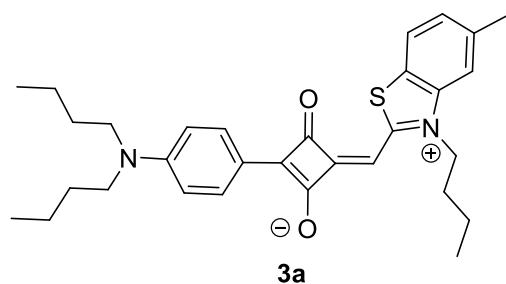
2. Materials Synthesis Scheme and Characterization

The synthesis of compound **1** ^[1] and **4** ^[2] are followed by reported literatures.

General procedures for synthesis of **3a-3c**



To a 50 mL round bottle flask was added 1 mmol of **1** and 1 mmol of **2a-2c** followed by 1:1 BuOH/toluene mixture (20 ml: 20 ml) and set to reflux overnight. Upon completion of reaction, the solvent was then removed under reduced pressure and purified by column chromatography (silica gel, hexane/ EtOAc 10:1) to achieve compound **3a-3c** in a moderate yield.

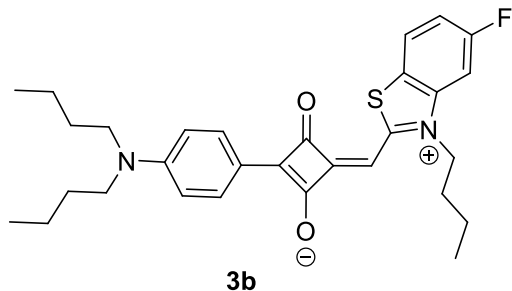


3a, 48% yield, blue paste.

¹H NMR (400 MHz, CDCl₃, ppm) δ 8.08-8.05 (d, 2H, *J* = 9.2 Hz), 7.57-7.55 (d, 1H, *J* = 8.0 Hz), 7.17-7.15 (d, 1H, *J* = 8.0 Hz), 7.11 (s, 1H), 6.64-6.62 (d, 2H, *J* = 2H), 6.26 (s, 1H), 4.27-4.24 (m, 2H), 3.35-3.31 (m, 4H), 2.44 (s, 1H), 1.83-1.80 (m, 2H), 1.60-1.46 (m, 6H), 1.38-1.31 (m, 4H), 1.01-1.00 (m, 9H).

¹³C NMR (100 MHz, CDCl₃, ppm) δ 207.1, 185.2, 183.4, 181.8, 173.8, 168.2, 165.4, 150.1, 140.7, 138.8, 130.0, 127.3, 126.4, 122.4, 119.2, 113.3, 111.5, 89.2, 50.8, 47.2, 40.0, 30.0, 29.5, 21.8, 21.1, 20.3, 20.2, 14.0, 13.8.

HRMS-APCI MS(*m/z*) for C₃₁H₃₉N₂O₂S: 503.2720 (calculated); 503.2727 (measured)

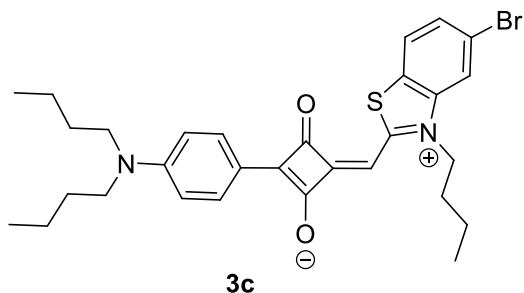


3b, 55% yield, blue paste.

^1H NMR (400 MHz, CDCl_3 , ppm) δ 8.13- 8.11 (d, 2H, $J = 6.0$ Hz), 7.70-7.68 (m, 1H), 7.47-7.45 (m, 1H), 7.34-7.32 (m, 2H), 6.65-6.63 (d, 2H, $J = 6.6$ Hz), 6.21 (s, 1H).

^{13}C NMR (100 MHz, CDCl_3 , ppm) δ 186.6, 183.1, 181.8, 170.1, 165.0, 150.3, 140.5, 130.2, 129.4, 127.9, 126.3, 125.8, 122.8, 122.5, 120.9, 119.3, 122.9, 111.5, 88.7, 50.8, 47.1, 30.0, 29.7, 29.6, 21.5, 20.3, 20.2, 20.1, 14.0, 13.7.

ESI-APCI MS(m/z) for $\text{C}_{30}\text{H}_{35}\text{FN}_2\text{O}_2\text{S}$: 506.68 (calculated); 507.45 (measured).



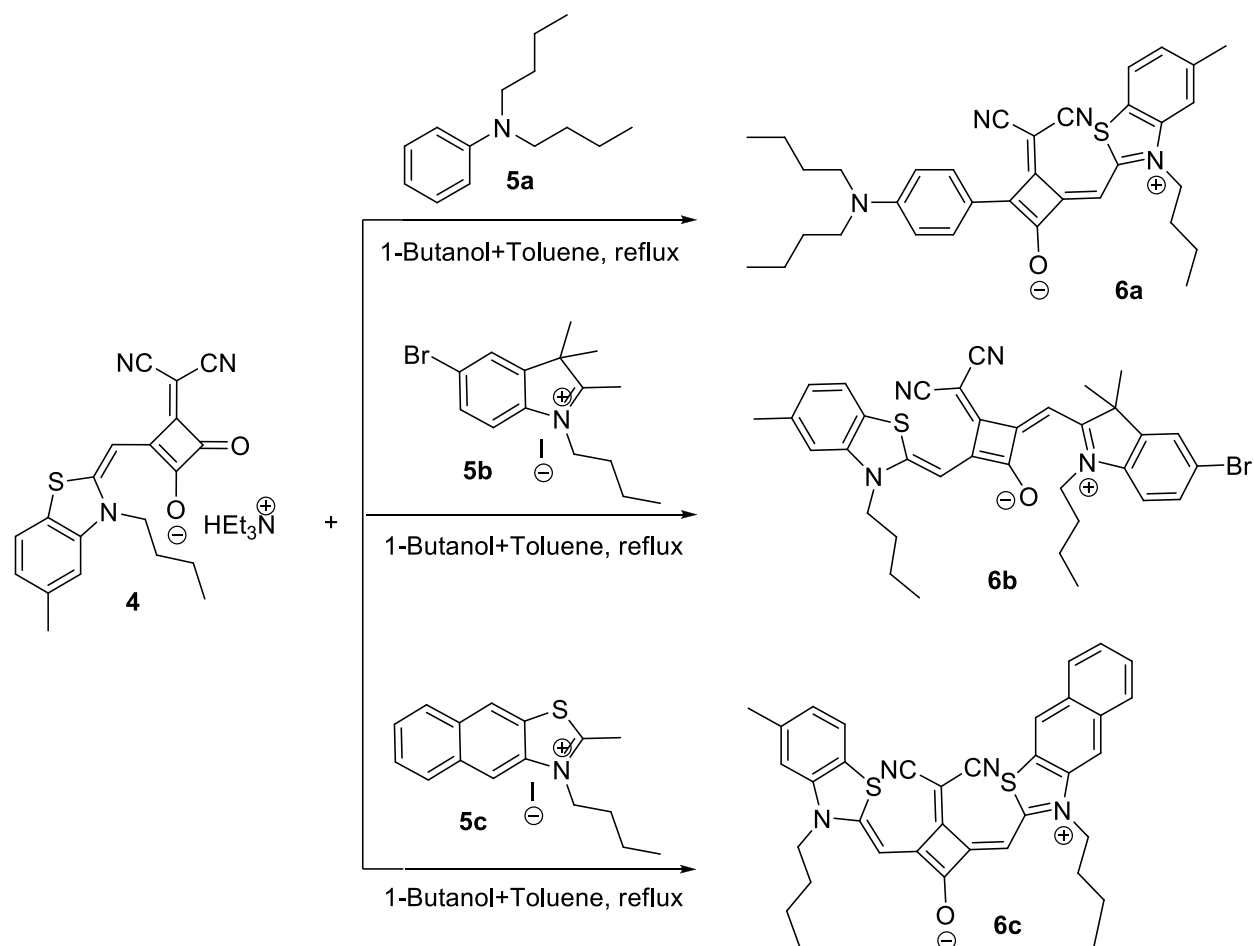
3c, 55% yield, blue paste.

^1H NMR (400 MHz, CDCl_3 , ppm) δ 8.26-8.24 (d, 2H, $J = 8$ Hz), 7.50 (s, 1H), 7.47-7.44 (m, 1H), 6.98-6.96 (d, 1H, $J = 8.1$ Hz), 6.68-6.66 (d, 2H, $J = 8.0$ Hz), 6.13 (s, 1H), 4.09-4.06 (m, 2H), 3.40-3.36 (m, 4H), 1.81-1.75 (m, 8H), 1.65-1.57 (m, 4H), 1.47-1.25 (m, 6H), 1.00-0.97 (m, 9H).

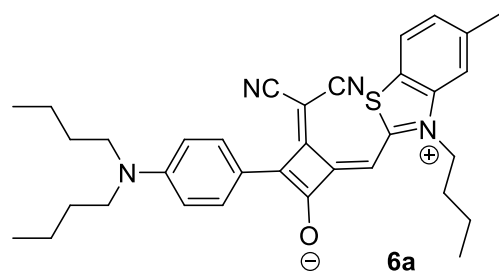
^{13}C NMR (100 MHz, CDCl_3 , ppm) δ 188.1, 176.6, 173.4, 151.7, 144.7, 140.9, 131.5, 131.1, 131.0, 125.9, 125.5, 122.5, 119.0, 118.3, 111.9, 111.8, 111.7, 110.8, 89.1, 89.0, 50.9, 50.8, 50.5, 50.3, 44.2, 29.5, 29.4, 29.3, 29.2, 26.7, 26.5, 20.5, 13.9, 13.8.

ESI-APCI MS(m/z) for $\text{C}_{30}\text{H}_{35}\text{BrN}_2\text{O}_2\text{S}$: 567.59 (calculated); 566.84 (measured).

General procedures for synthesis of **6a-6c**



To a 50 mL round bottle flask was added 1 mmol of **1** and 1 mmol of **5a**, **5b** or **5c** followed by 1:1 BuOH/toluene mixture (20 ml: 20 ml) and set to reflux overnight. Upon completion of reaction, the solvent was then removed under reduced pressure and purified by column chromatography to achieve compound **6a**, **6b** or **6c** in a moderate yield.

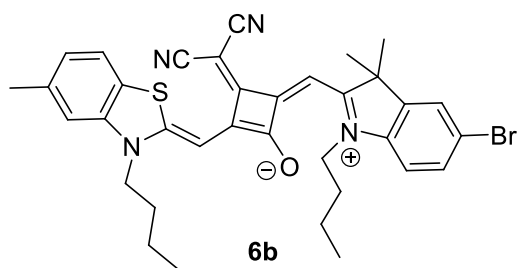


6a, 8 % yield, dark solid.

^1H NMR (CDCl_3 , 400 MHz, ppm) δ 8.30-8.28 (d, 2H, $J = 9.2$ Hz), 7.72-7.70 (d, 1H, $J = 8.2$ Hz), 7.58 (m, 1H), 7.35-7.34 (m, 1H), 7.02 (s, 1H), 6.74-6.72 (d, 2H, $J = 9.3$ Hz), 4.40-4.48 (m, 2H), 3.41-3.37 (m, 4H), 2.59 (s, 3H), 1.26-1.25 (m, 6H), 1.18-1.14 (m, 6H), 1.09-1.08 (m, 9H).

^{13}C NMR (100 MHz, CDCl_3 , ppm) δ 176.7, 170.7, 165.9, 163.9, 160.5, 150.5, 140.6, 139.5, 132.1, 128.2, 126.5, 122.6, 119.6, 117.9, 113.8, 111.7, 91.5, 50.9, 48.1, 43.1, 32.0, 30.3, 29.7, 29.5, 29.4, 22.7, 21.9, 20.3, 20.2, 14.2, 14.0, 13.8.

HRMS-APCI MS (m/z) for $\text{C}_{34}\text{H}_{39}\text{N}_4\text{OS}$: 551.2830 (calculated); 551.2839 (measured).

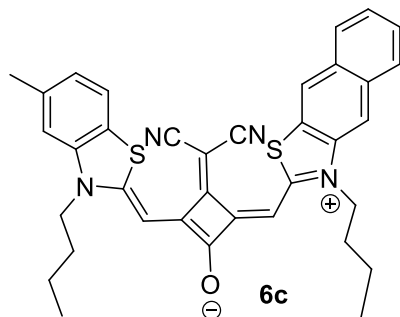


6b, 45% yield, dark solid.

^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.59-7.57 (d, 1H, $J = 8.0$ Hz), 7.45-7.42 (m, 2H), 7.24-7.22 (d, 1H, $J = 8.0$ Hz), 7.18 (s, 1H), 6.86-6.84 (m, 1H), 6.65 (s, 1H), 6.30 (s, 1H), 4.29-4.25 (t, 2H, $J = 7.6$ Hz), 3.90 (m, 2H), 2.56 (s, 1H), 1.90 (m, 2H), 1.79-1.77 (m, 8H), 1.56-1.48 (m, 4H), 1.08-1.02 (m, 6H).

^{13}C NMR (100 MHz, CDCl_3 , ppm) δ 173.8, 167.6, 166.7, 165.3, 163.3, 161.7, 143.8, 141.7, 140.8, 138.9, 130.7, 127.8, 127.2, 125.9, 125.5, 122.2, 119.0, 118.6, 115.9, 114.0, 113.2, 110.4, 88.8, 88.0, 48.5, 47.3, 43.8, 41.1, 29.9, 29.1, 27.1, 21.9, 20.2, 14.0, 13.8.

HRMS-APCI MS (m/z) for $\text{C}_{35}\text{H}_{36}\text{BrN}_4\text{OS}$: 639.1796 (calculated); 639.1788 (measured).



6c, 19 % yield, dark solid.

^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.93-7.86 (m, 3H), 7.50-7.37 (m, 4H), 7.07-7.05 (d, 1H, $J = 8.0$ Hz), 6.97 (s, 1H), 6.26 (s, 1H), 6.10 (s, 1H), 4.24-4.21 (m, 2H), 4.03-4.00 (m, 2H), 2.48 (s, 3H), 1.86-1.77 (m, 4H), 1.55-1.48 (m, 4H), 1.03-1.00 (m, 6H);

^{13}C NMR (100 MHz, CDCl_3 , ppm) 174.3, 163.1, 162.8, 162.3, 160.1, 141.2, 138.5, 137.9, 130.4, 128.9, 129.0, 128.1, 127.3, 126.2, 125.2, 124.8, 123.5, 121.8, 112.2, 111.4, 86.9, 86.5, 77.4, 77.3, 77.1, 76.7, 47.1, 46.5, 29.9, 29.7, 29.5, 21.8, 20.2, 20.2, 14.2, 13.9, 13.9.

HRMS-APCI MS (m/z) for $\text{C}_{36}\text{H}_{33}\text{N}_4\text{OS}_2$: 601.2103 (calculated); 601.2090 (measured).

3. UV/vis/NIR absorption spectrum

10 μM dye solutions in UV measurements were prepared by diluting 1000 times from 10 mM stock dye solution in DMSO.

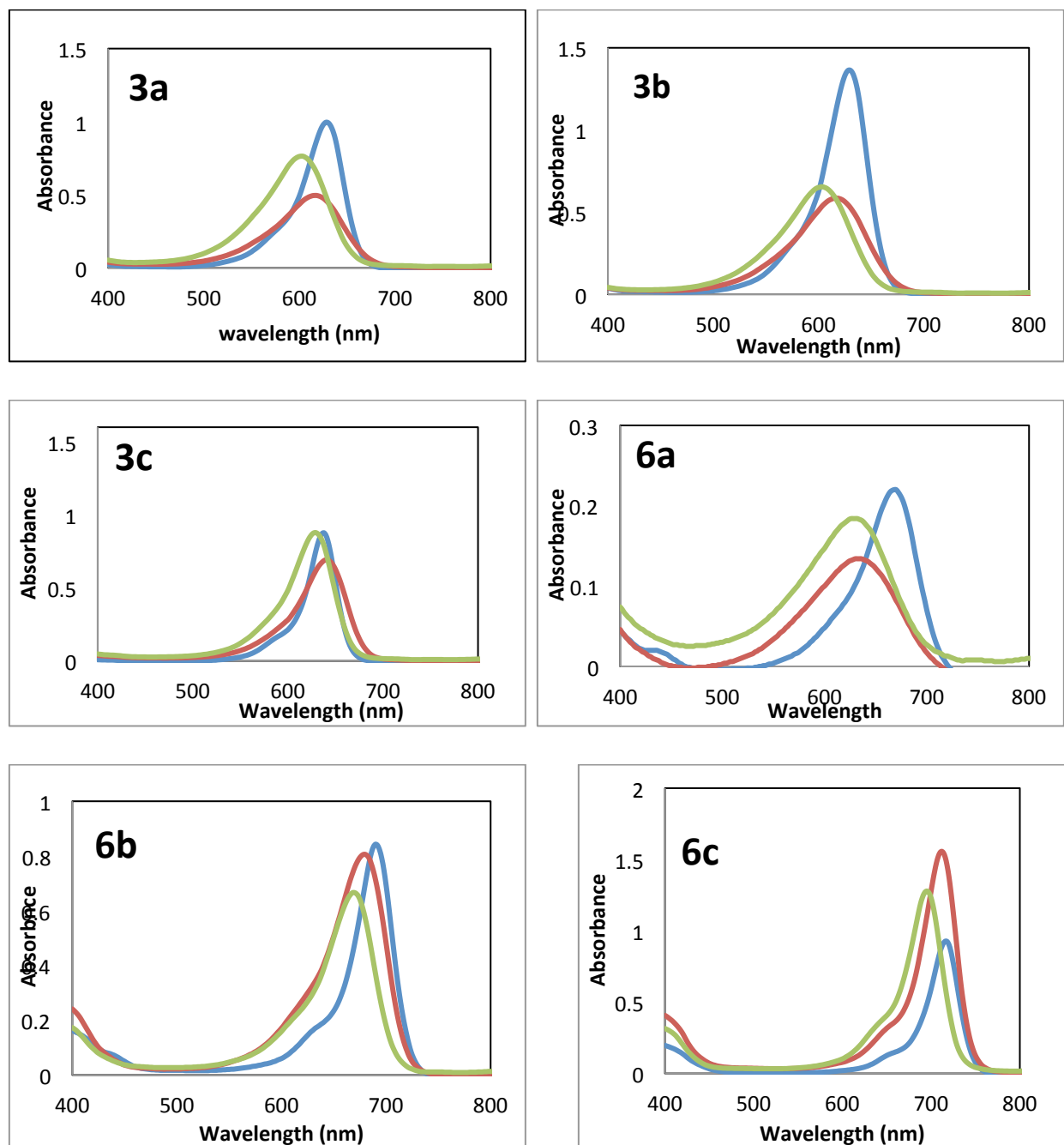


Figure S1: UV spectrum for 10 μM 3a-3c, 6a-6c in different solvents: CHCl_3 (blue line); DMSO (red line); MeOH (green line)

4. Cyclic voltammetry

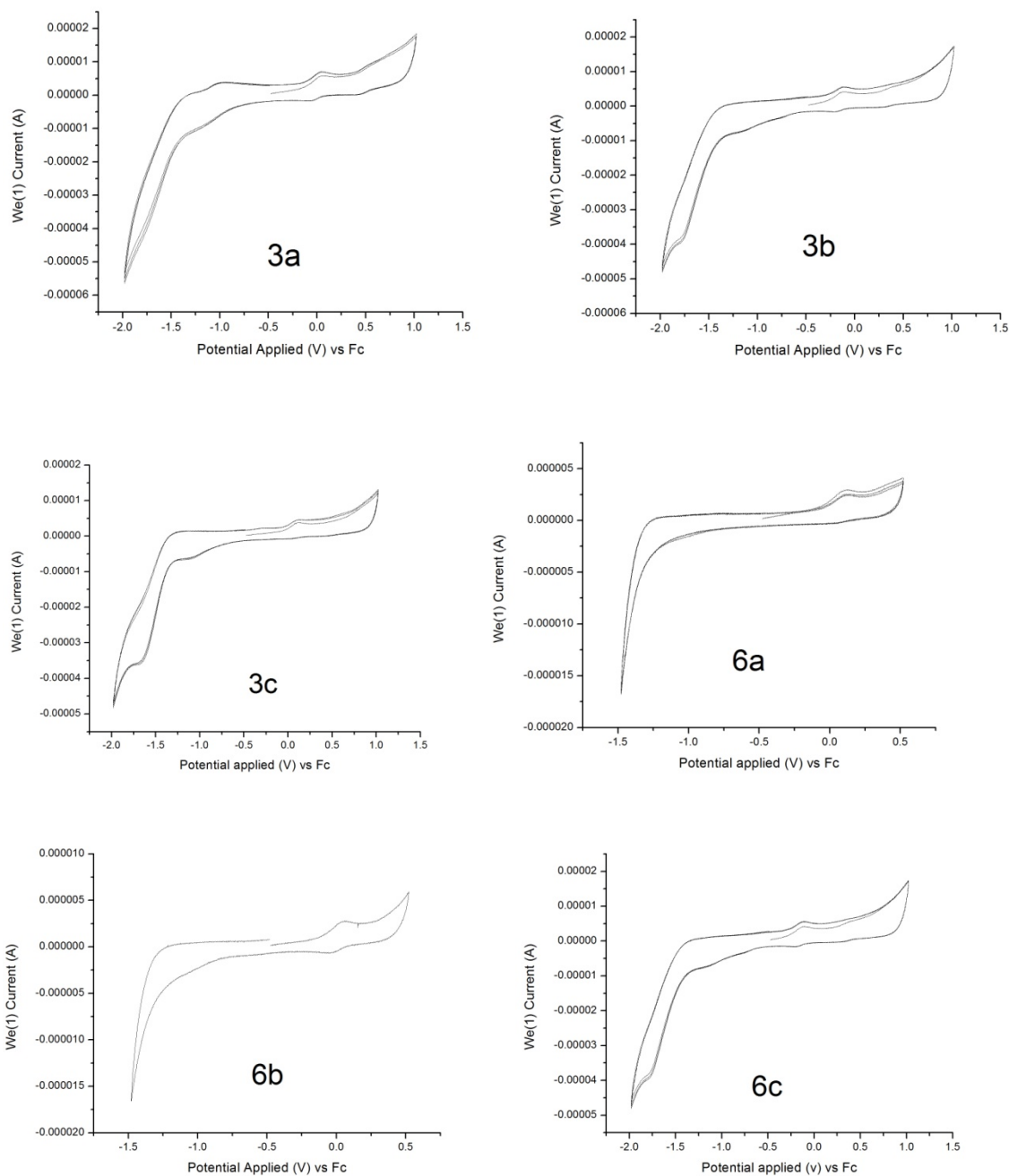


Figure S2: Cyclic voltammograms of **3a-3c**, **6a-6c** in 0.1 M TBAHF DCM solutions at a scan rate of 100 mV/s. Ferrocene is used as the internal standard.

The HOMO and LUMO levels were obtained according to equations (1) and (2), respectively.^[3] And all the results were summarized in the Table 1.

$$E_{\text{HOMO}}^{\text{opt}} = -5.23\text{eV} - eE_{\text{ox}} + 1/2(E_{\text{cv}}^{\text{sol}} - E_{\text{g}}) \quad (1)$$

$$E_{\text{LUMO}}^{\text{opt}} = -5.23\text{eV} - eE_{\text{red}} - 1/2(E_{\text{cv}}^{\text{sol}} - E_{\text{g}}) \quad (2)$$

Table S1. Electrochemical properties of squaraine dyes in CH₂Cl₂.

Dye ^[a]	$\lambda_{\text{max}}(\text{nm})$	$\lambda_{\text{ons}}(\text{nm})$	E_{g} (eV)	E_{ox} (eV)	$E_{\text{red}}(\text{eV})$	$E_{\text{cv}}^{\text{sol}}$ (eV)	$E_{\text{HOMO}}^{\text{opt}}$ (eV)	$E_{\text{LUMO}}^{\text{opt}}$ (eV)
3a	623	673	1.84	-0.15	-1.36	1.21	-5.39	-3.56
3b	625	675	1.83	-0.13	-1.42	1.29	-5.37	-3.54
3c	638	676	1.83	-0.05	-1.36	1.31	-5.44	-3.61
6a	660	718	1.73	-0.08	-1.30	1.22	-5.40	-3.67
6b	690	727	1.71	-0.14	-1.23	1.09	-5.40	-3.69
6c	718	750	1.65	-0.28	-1.43	1.15	-5.20	-3.55

[a] CV measurement was conducted in a three electrode cell consisting of reference electrode (Ag/AgCl), working electrode (Pt) and counter electrode

5. Emission Spectrum for 10uM dyes in DMSO

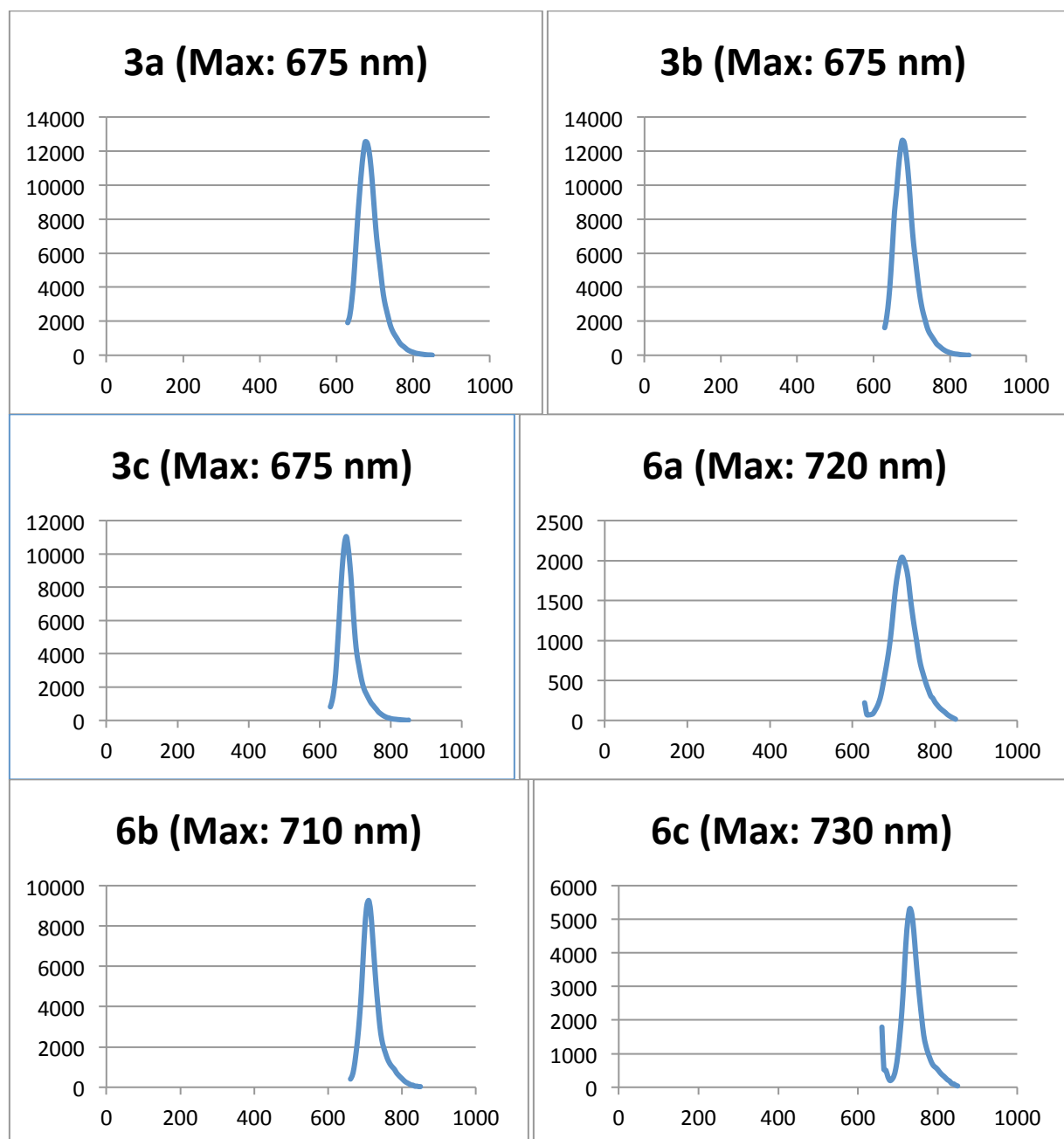


Figure S3: Emission spectra of **3a-3c**, **6a-6c** in DMSO (10 mM).

6. References:

- [1] a) L-H. Liu, K. Nakatani, R. Pansu, J-J. Vachon, P. Tauc and E. Ishow, *Adv. Mater.*, **2007**, 19, 433-436. b) V. Ramalingam, M. E. Domaradzki, S. Jang and R. S. Muthyala, *Org. Lett.*, **2008**, 15, 3315.
- [2] a) U. mayerhoffer, M. Gsanger, M. Stolte, B. Fimmel and F. Wurthner, *Chem. Eur. J.*, **2013**, 19, 218-232. b) S. Kim, G. K. Mor, M. Paulose, O. K. Varghese, C. Baik and C. A. Grimes, *Langmuir*, **2010**, 26, 13486-13492.
- [3] L. Beverina, M. Drees, A. Facchetti, M. Salamone, R. Ruffo and G. A. Pagani, *Eur. J. Org. Chem.* 2011, 5555-5563.

7. TDDFT Benchmark Studies

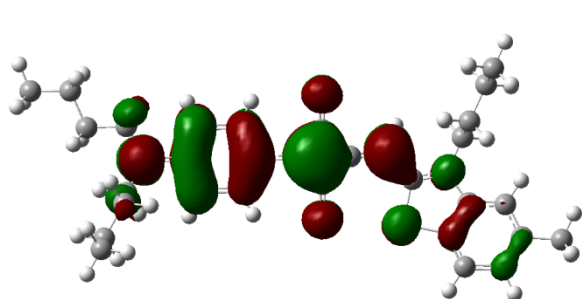
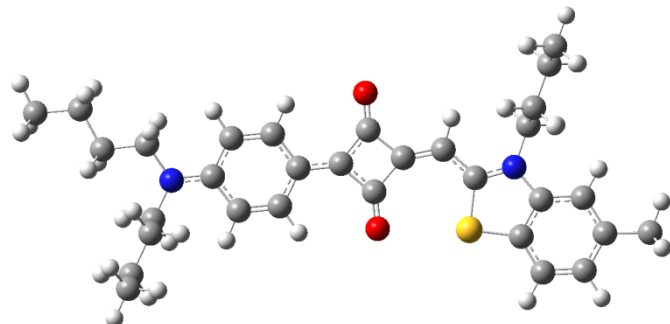
Table S2. Benchmark TDDFT studies of 3a, 6a-c in DMSO.

Dye	TDDFT Method	Structure optimized Method	DMSO Solvation Method	$\lambda_{\text{abs}}(\text{nm})$	$\lambda_{\text{em}}(\text{nm})$	$\Delta\lambda(\text{nm})$
3a	CAM-B3LYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	520.44	597.56	77.12
	CAM-B3LYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	PCM	518.97	581.94	62.97
	ω B97x-D /6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	510.58	596.43	85.85
	LC-BLYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	480.4	600.64	120.24
	B3LYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	572.1	605.68	33.58
	PBE0/6-31+G(d)	ω B97x-D/6-31G(d)	SMD	559.68	598.27	38.59
	CAM-B3LYP/6-311+G(d,p)	PBE0/6-31+G(d)	SMD	544.08	583.49	39.41
	PBE0/6-311+G(d,p)	PBE0/6-31+G(d)	SMD	569.81	594.41	24.6
	CAM-B3LYP/6-311+G(d,p)	CAM-B3LYP/6-31+G(d)	PCM	520.75	580.27	59.52
6a	CAM-B3LYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	519.91	609.05	89.14
	CAM-B3LYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	PCM	527.74	606.28	78.54
	ω B97x-D /6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	507.28	606.91	99.63
	LC-BLYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	464.47	598.91	134.44
	B3LYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	594.78	632.07	37.29
	PBE0/6-31+G(d)	ω B97x-D/6-31G(d)	SMD	579.15	622.53	43.38
	CAM-B3LYP/6-311+G(d,p)	PBE0/6-31+G(d)	SMD	588.95	619.79	30.84
	PBE0/6-311+G(d,p)	PBE0/6-31+G(d)	SMD	545.55	608.43	62.88
	CAM-B3LYP/6-311+G(d,p)	CAM-B3LYP/6-31+G(d)	PCM	531.1	605.83	74.73

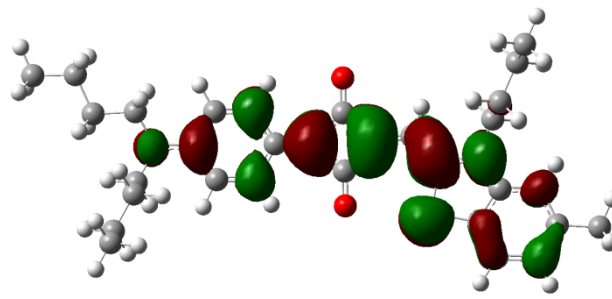
6b	CAM-B3LYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	575.53	614.43	38.9
	CAM-B3LYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	PCM	578.44	615.74	37.3
	ω B97x-D /6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	571.93	613.23	41.3
	B3LYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	604.12	634.43	30.31
	PBE0/6-31+G(d)	ω B97x-D/6-31G(d)	SMD	593.35	623.96	30.61
	CAM-B3LYP/6-311+G(d,p)	CAM-B3LYP/6-31+G(d)	PCM	578.66	615.17	36.51
6c	CAM-B3LYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	595.68	630.96	35.28
	CAM-B3LYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	PCM	599.06	632.42	33.36
	ω B97x-D /6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	591.13	627.7	36.57
	B3LYP/6-311+G(d,p)	ω B97x-D/6-31G(d)	SMD	622.27	651.01	28.74
	PBE0/6-31+G(d)	ω B97x-D/6-31G(d)	SMD	611.05	639.81	28.76
	CAM-B3LYP/6-311+G(d,p)	CAM-B3LYP/6-31+G(d)	PCM	600.75	632.47	31.72

8. 3a, 6a-c HOMO and LUMO of Ground and Excited state

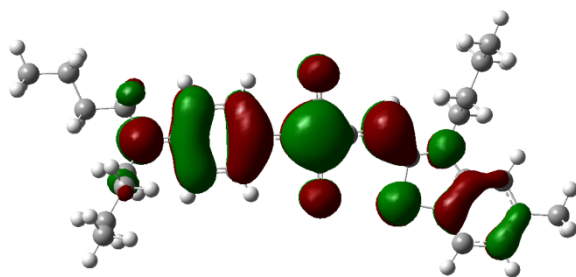
3a



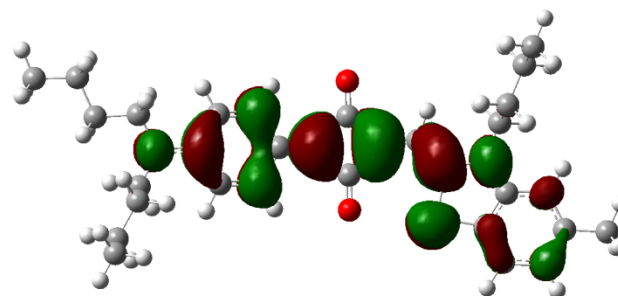
3a S₀ HOMO



3a S₀ LUMO



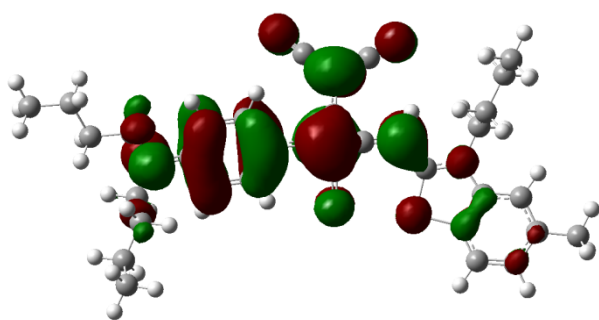
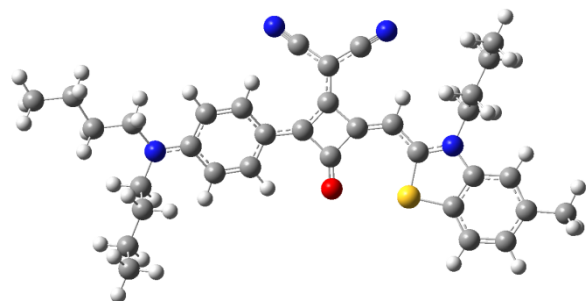
3a S₁ HOMO



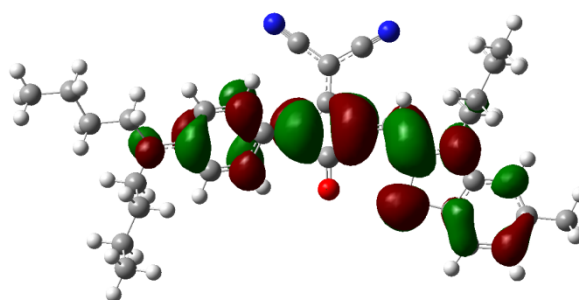
3a S₁ LUMO

Figure S4. 3a HOMO and LUMO of S₀ and S₁.

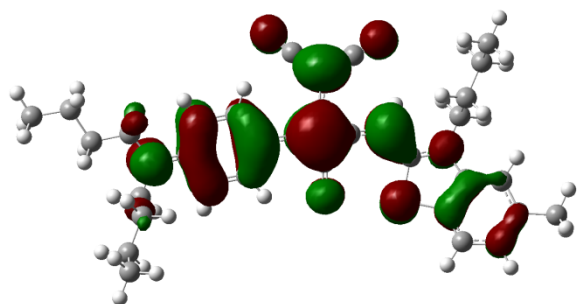
6a



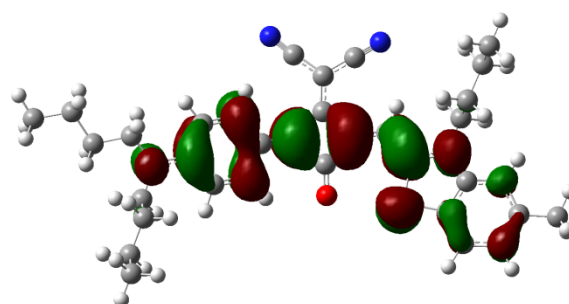
6a S_0 HOMO



6a S_0 LUMO



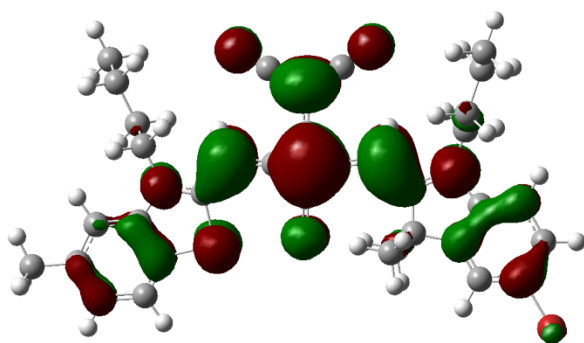
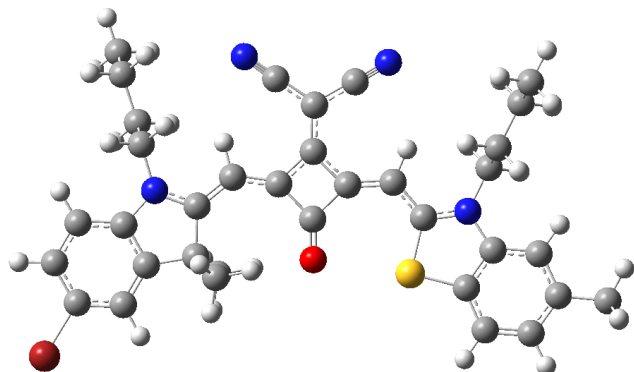
6a S_1 HOMO



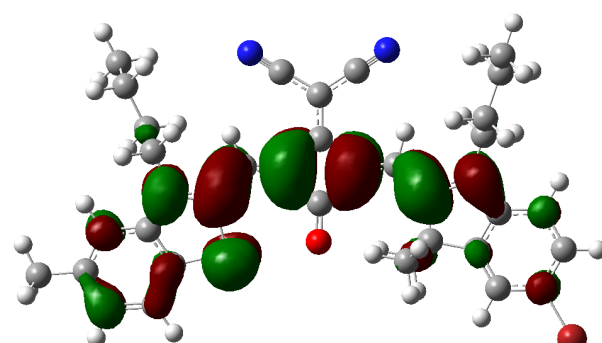
6a S_1 LUMO

Figure S5. 6a HOMO and LUMO of S_0 and S_1

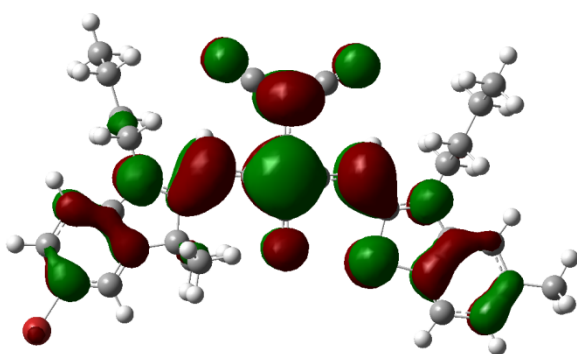
6b



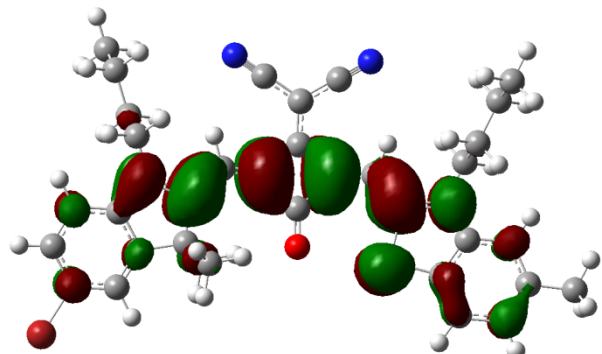
6b S₀ HOMO



6b S₀ LUMO



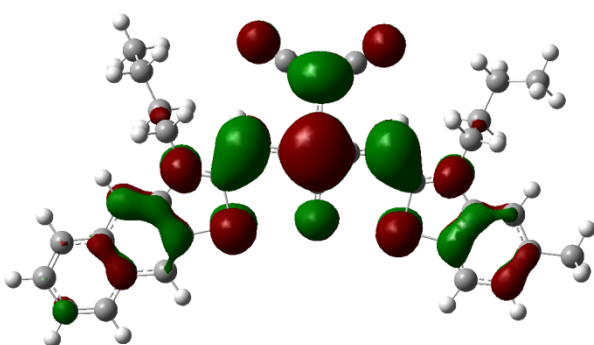
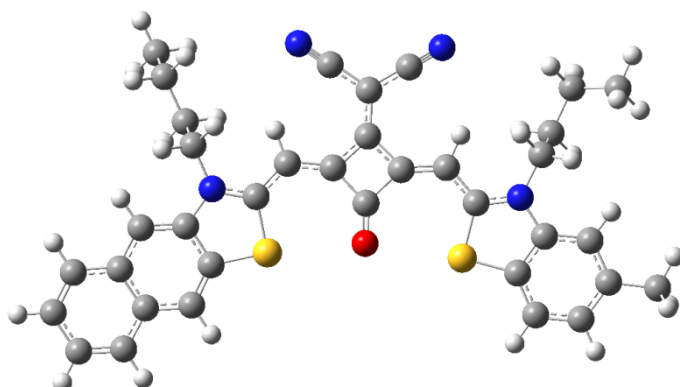
6b S₁ HOMO



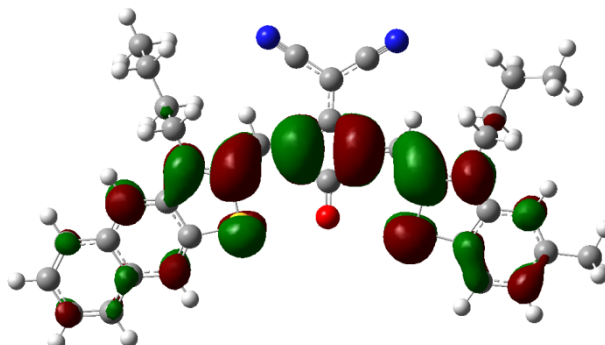
6b S₁ LUMO

Figure S6. 6b HOMO and LUMO of S₀ and S₁

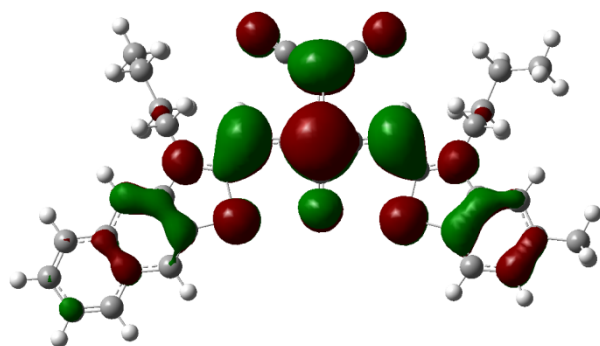
6c



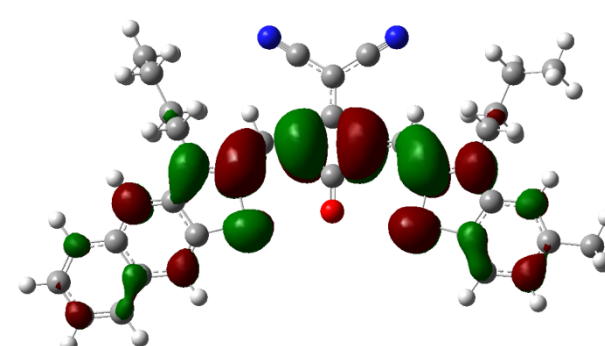
6c S₀ HOMO



6c S₀ LUMO



6c S₁ HOMO



6c S₁ LUMO

Figure S7. 6c HOMO and LUMO of S₀ and S₁

9. 3a, 6a-c Reduced Density Gradient isosurface plot

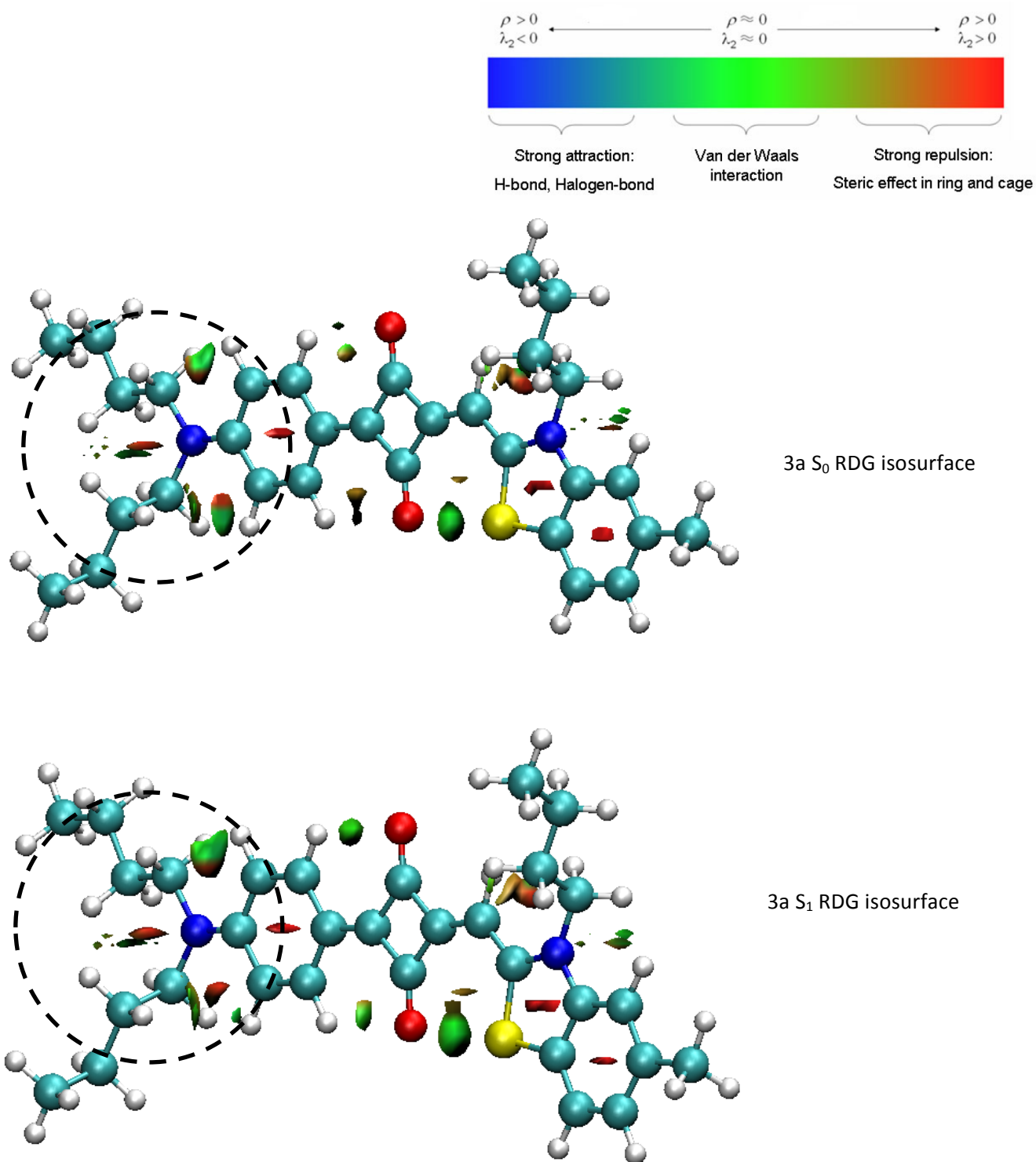


Figure S8. 3a S_0 and S_1 RDG analysis where the increase in red isosurface signifying steric repulsion increases

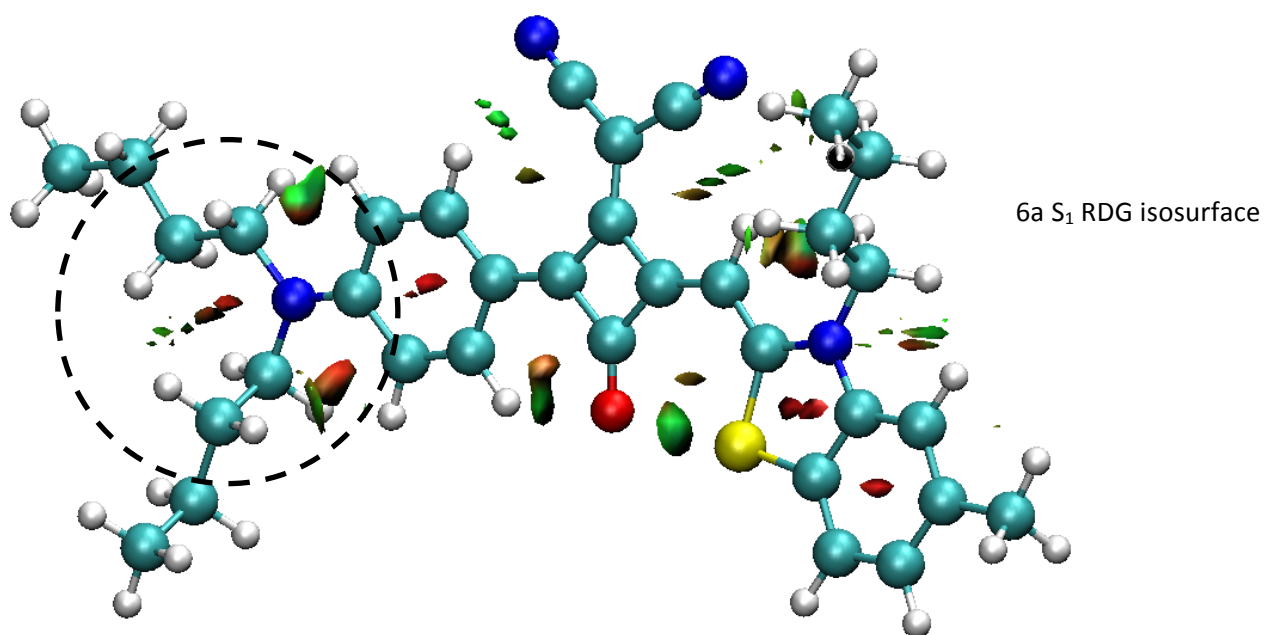
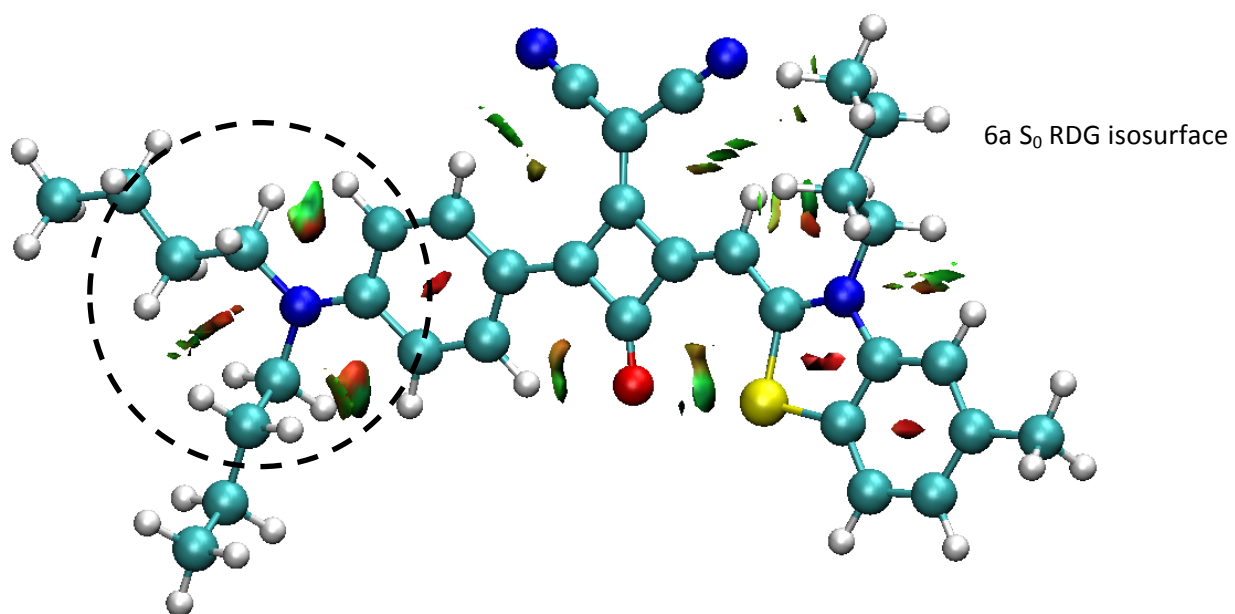
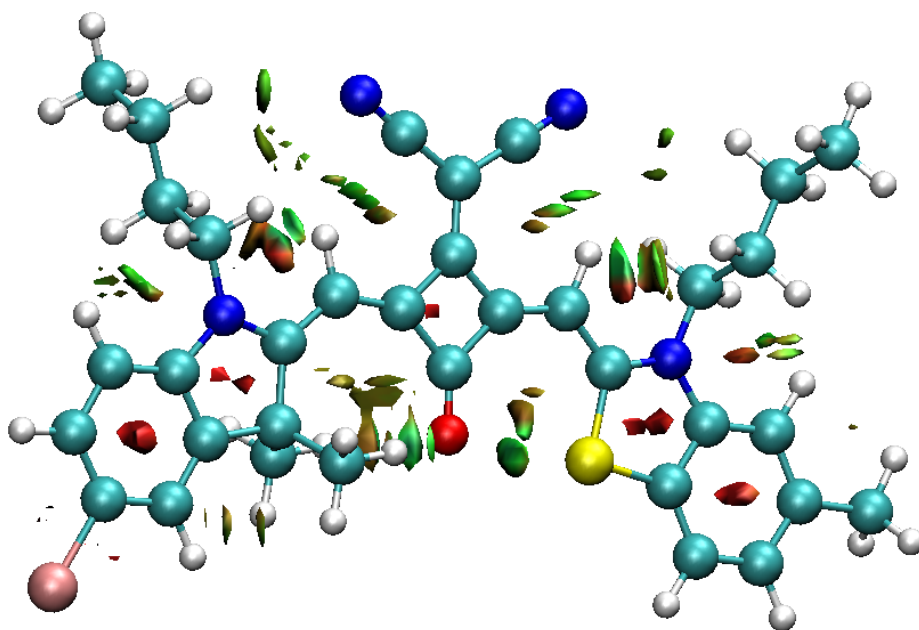
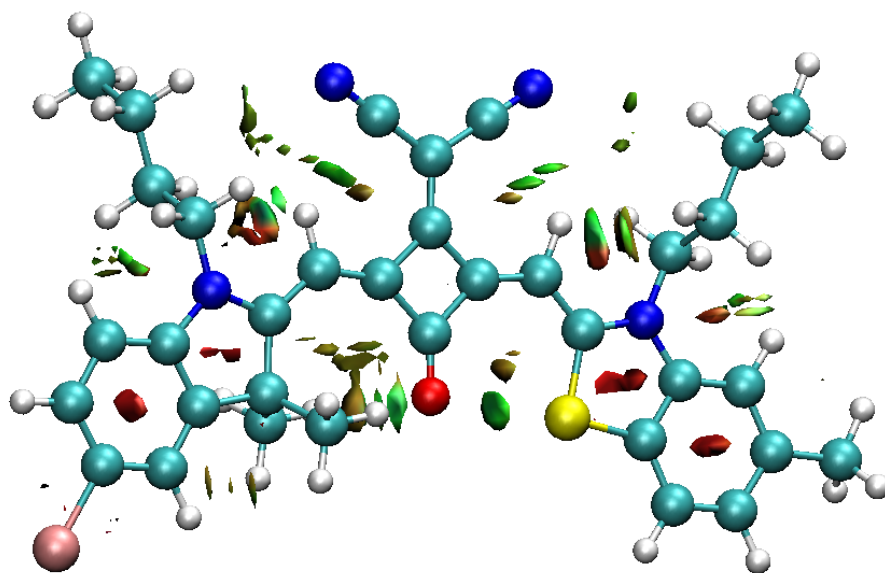


Figure S9. 6a S_0 and S_1 RDG analysis where the increase in red isosurface signifying an increase steric repulsion



6b S_0 RDG isosurface



6b S_1 RDG isosurface

Figure S10. 6b S_0 and S_1 RDG analysis

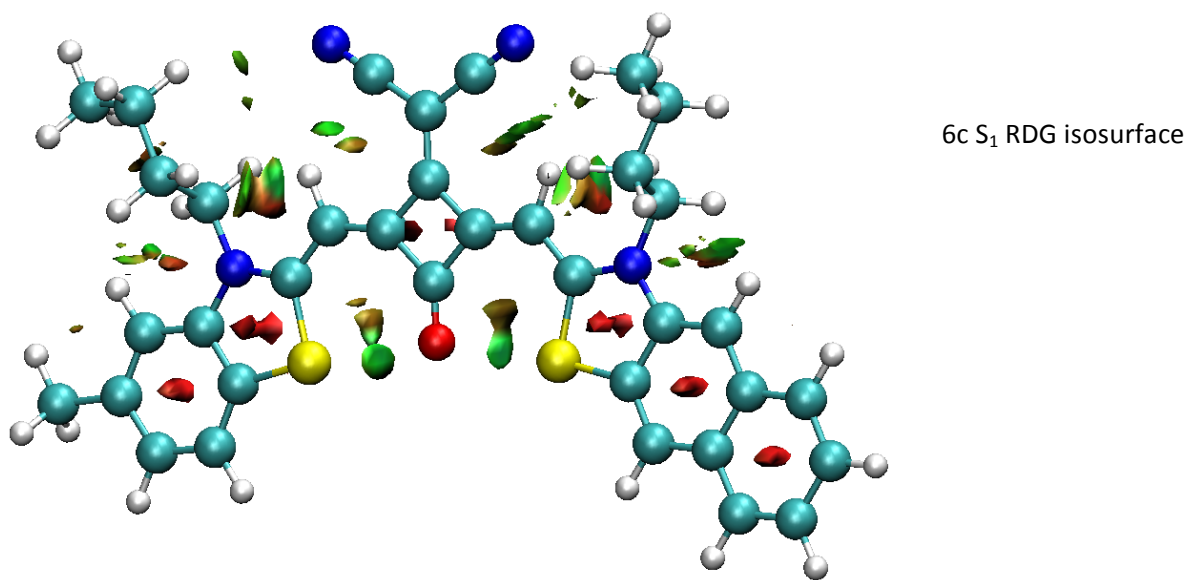
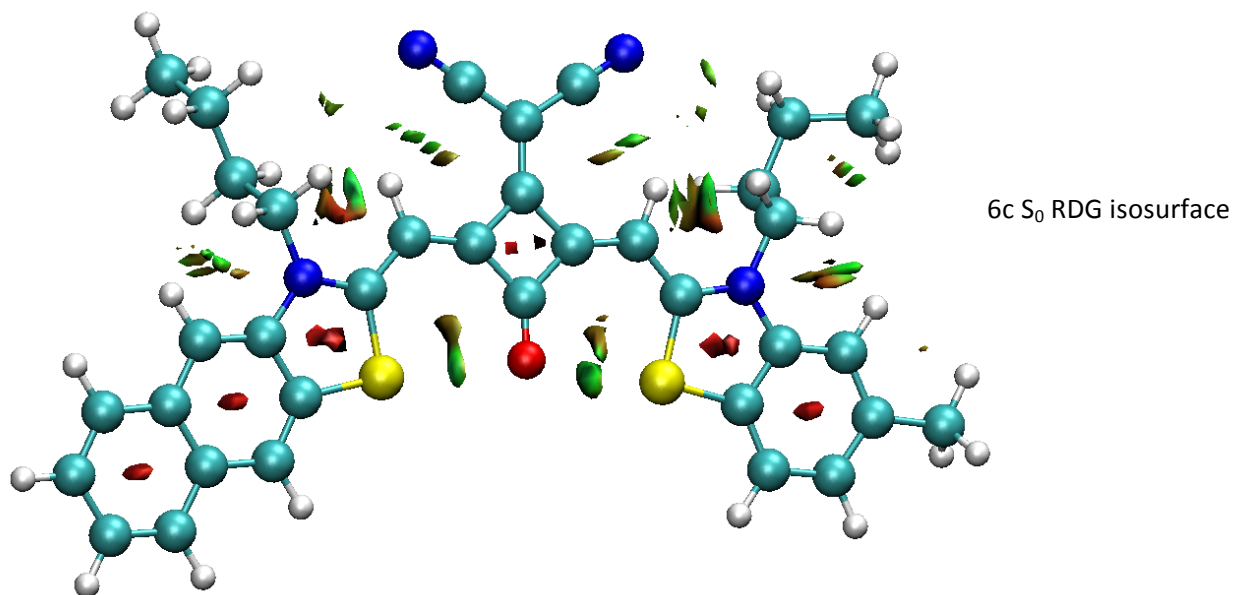
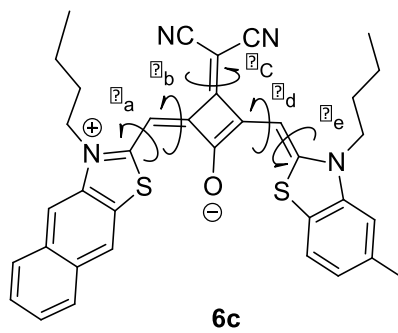
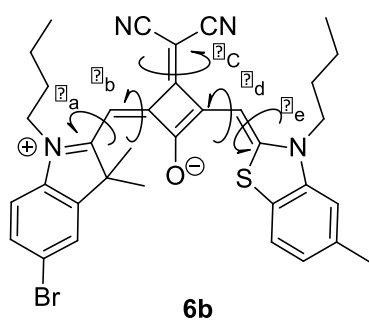
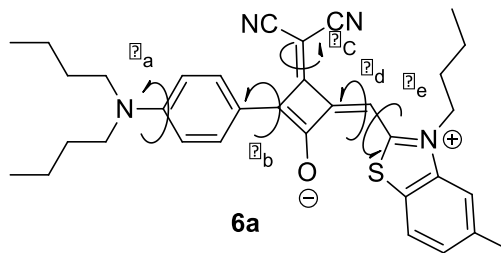
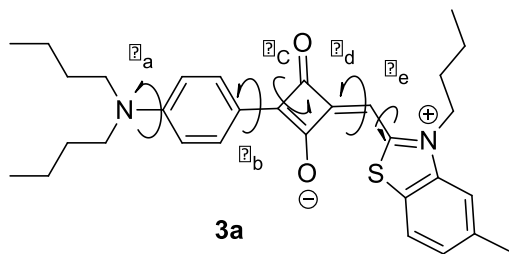


Figure S11. 6c S₀ and S₁ RDG analysis

10. 3a, 6a-c S₀ and S₁ dihedral angle deviation from planarity

Substrate	$\Delta r/\text{\AA}$	θ_a	θ_{a2}	θ_b	θ_c	θ_d	θ_e
3a S₀	3.14	6.3	14.5	0.6	0.3	0.7	2.7
		C44-N43-C40-C38	C50-N43-C40-C36	C35-C33-C16-C14	C33-C16-C14-O70	C14-C13-C11-C10	C13-C11-C10-N30
3a S₁	2.70	3.6	7.8	0.2	0.7	0.7	1.3
		C44-N43-C40-C38	C50-N43-C40-C36	C35-C33-C16-C14	C33-C16-C14-O70	C14-C13-C11-C10	C13-C11-C10-N30
6a S₀	3.31	5.9	13.0	17.7	7.0	1.3	2.9
		C49-N48-C45-C43	C55-N48-C45-C41	C40-C38-C16-C14	C16-C14-C18-C19	C14-C13-C11-C10	C13-C11-C10-N33
6a S₁	1.48	3.9	5.7	5.6	2.3	1.2	1.2
		C49-N48-C45-C43	C55-N48-C45-C41	C40-C38-C16-C14	C16-C14-C18-C19	C14-C13-C11-C10	C13-C11-C10-N33
6b S₀	1.30	1.6	----	0.4	0.8	0.5	2.8
		N58-C32-C30-C29		C32-C30-C29-C27	C29-C27-C43-C44	C27-C26-C24-C23	C26-C24-C23-N59
6b S₁	0.65	1.2	----	0.2	0.3	0.6	1.5
		N58-C32-C30-C29		C32-C30-C29-C27	C29-C27-C43-C44	C27-C26-C24-C23	C26-C24-C23-N59
6c S₀	0.83	2.4	----	2.3	0.4	1.3	2.4
		N58-C22-C23-C25		C22-C23-C25-C26	C25-C26-C42-C41	C26-C28-C29-C31	C28-C29-C31-N57
6b S₁	0.74	1.8	----	1.1	0.2	0.8	1.4
		N58-C22-C23-C25		C22-C23-C25-C26	C25-C26-C42-C41	C26-C28-C29-C31	C28-C29-C31-N57

θ is calculated as the dihedral angle deviation from planarity where the values are taken from the modulus the difference of dihedral angle from 180° or 0° (i.e. 180°-|x| if x > 90° or |x|-0 if x < =90°), whichever is nearer to attaining a planar structure. The dihedral angles taken are shown in the figure below and also listed by its atomic label below its value in Table S2.



11. 3a, 6a-c S₀ and S₁ Cartesian coordinates

3a S₀ CAMB3LYP/6-31+G(d) PCM Optimized Structure in DMSO

0 1			
C	6.09406200	-0.69229200	-0.32204500
C	7.48847100	-0.63060600	-0.31663600
H	8.00935600	0.31999600	-0.30933300
C	8.21728000	-1.81467700	-0.31115500
C	7.53607600	-3.04554300	-0.30954600
H	8.11056700	-3.96728000	-0.30526900
C	6.15230500	-3.11206200	-0.30930100
H	5.64101800	-4.06883900	-0.30483200
C	5.43512500	-1.91849400	-0.31293000
C	3.89815700	0.03136600	-0.30945200
C	2.83684400	0.96702600	-0.27365100
H	3.10591800	2.01528400	-0.20520200
C	1.49817700	0.69894100	-0.29665800
C	0.33588300	1.61782500	-0.24900300
C	0.53397500	-0.43308000	-0.37992300
C	-0.57002900	0.49856200	-0.32766000
C	5.66577900	1.77800300	-0.36373100
H	4.95668500	2.36163900	-0.95167900
H	6.60453700	1.78742500	-0.91936900
C	5.84976800	2.36355300	1.03397300
H	6.55227700	1.73867400	1.59841200
H	4.89454800	2.33087800	1.57150400
C	6.36430200	3.80123800	0.97779000
H	7.31634300	3.82516600	0.43222200
H	5.66069200	4.41674100	0.40292800
C	6.55573000	4.40549600	2.36690500
H	6.92672200	5.43334700	2.30236300
H	7.27693000	3.82492800	2.95319100
H	5.61125400	4.42444300	2.92218800
N	5.19822600	0.38432300	-0.33717000
O	0.65029900	-1.66126000	-0.46378300
S	3.70142800	-1.69557500	-0.30235900
C	-1.99415300	0.35649800	-0.35535700
C	-2.60445200	-0.90962600	-0.44032300
C	-2.84335600	1.47490500	-0.28851300
C	-3.97728800	-1.05139800	-0.46755200
H	-1.97779400	-1.79517800	-0.48066500
C	-4.21964300	1.34405300	-0.31608000
H	-2.40669300	2.46556200	-0.20639400
C	-4.84014900	0.07395000	-0.42597100
H	-4.38186600	-2.05321400	-0.52178500
H	-4.81560700	2.24347800	-0.24484000
N	-6.21013800	-0.05546000	-0.50380300
C	-7.03234500	1.14685300	-0.32976400
H	-6.90606600	1.54876300	0.68805500
H	-6.65679000	1.91009600	-1.01814600

C	-8.52044400	0.97440000	-0.61507900
H	-8.66116300	0.53945800	-1.61266800
H	-8.98047400	0.28760500	0.10485300
C	-6.82895700	-1.36463800	-0.31426400
H	-7.83058300	-1.33162100	-0.74329700
H	-6.28777900	-2.10341400	-0.91036200
C	-6.90970700	-1.81677500	1.14572700
H	-5.90274000	-1.83207600	1.58135000
H	-7.48674700	-1.07884400	1.71890400
C	-7.55281600	-3.19499800	1.29046500
H	-8.55627200	-3.17630700	0.84477200
H	-6.97294800	-3.92721200	0.71289600
C	-7.64936400	-3.65447500	2.74368300
H	-8.25259300	-2.95814400	3.33758900
H	-8.11073100	-4.64475200	2.81919700
H	-6.65668900	-3.71155900	3.20498400
C	-9.24925400	2.31746900	-0.54491700
H	-8.81543900	3.00612300	-1.28129500
H	-9.08113100	2.77150400	0.44042100
C	-10.74978100	2.18354600	-0.79371200
H	-11.21608700	1.52730200	-0.04989700
H	-11.24912700	3.15655300	-0.74056900
H	-10.94923400	1.75907000	-1.78439500
O	0.24116700	2.84926500	-0.17295200
C	9.72367100	-1.78825200	-0.30483500
H	10.10468400	-0.76406600	-0.29992900
H	10.12093200	-2.30269600	0.57639900
H	10.12768300	-2.29632100	-1.18677500

3a S₁ CAMB3LYP/6-31+G(d) PCM Optimized Structure in DMSO

0	1		
C	6.12089400	-0.69114000	-0.30456700
C	7.51996800	-0.64799000	-0.27293700
H	8.04809200	0.29878500	-0.26300500
C	8.24159800	-1.83700500	-0.24304100
C	7.55646300	-3.06481100	-0.24035000
H	8.12451800	-3.99034400	-0.21629700
C	6.16927500	-3.11822500	-0.26266300
H	5.65165000	-4.07211800	-0.25633100
C	5.45610600	-1.92525500	-0.29219800
C	3.91356300	0.03610800	-0.33453600
C	2.86175300	0.94744800	-0.31602700
H	3.12844100	2.00003600	-0.27901000
C	1.49369800	0.69578200	-0.32327400
C	0.34912600	1.62230700	-0.29101200
C	0.53449100	-0.42905800	-0.39000900
C	-0.60792000	0.50192300	-0.35246100
C	5.71561300	1.76730400	-0.38552800
H	5.01841500	2.34437300	-0.99696200

H	6.66903100	1.77924900	-0.91824300
C	5.86727800	2.38393000	1.00474400
H	6.56593600	1.77673000	1.59331300
H	4.90243900	2.34898600	1.52494000
C	6.36661100	3.82603900	0.93497200
H	7.32676700	3.85254400	0.40349500
H	5.66563000	4.42473900	0.33919600
C	6.53013300	4.45558700	2.31655600
H	6.88959400	5.48697200	2.24163400
H	7.24927800	3.89331700	2.92300300
H	5.57729000	4.47147100	2.85762400
N	5.25127800	0.38194300	-0.35180100
O	0.63494000	-1.65693900	-0.45474400
S	3.72064100	-1.70744200	-0.31988100
C	-1.99656900	0.37050200	-0.36076400
C	-2.62939000	-0.90891300	-0.41577700
C	-2.85876900	1.50649100	-0.30468600
C	-3.99176500	-1.04085300	-0.42418000
H	-2.00473800	-1.79591900	-0.44574600
C	-4.22339100	1.37978100	-0.31661800
H	-2.41371000	2.49476600	-0.24687800
C	-4.85485300	0.09939300	-0.39077900
H	-4.40653000	-2.03926800	-0.45299800
H	-4.82026200	2.27953400	-0.25985300
N	-6.20921200	-0.02218200	-0.43108800
C	-7.03629000	1.19036900	-0.31630000
H	-6.87186200	1.64329100	0.67192400
H	-6.68007400	1.90969300	-1.06030700
C	-8.53324400	1.00368300	-0.53338000
H	-8.72016700	0.56031100	-1.51887200
H	-8.95616200	0.32489700	0.21588800
C	-6.84142900	-1.33798200	-0.34031000
H	-7.83503600	-1.26813600	-0.78015000
H	-6.29161100	-2.03969700	-0.97137900
C	-6.94505000	-1.86904300	1.09189200
H	-5.94484700	-1.91057800	1.54043900
H	-7.52928300	-1.16223100	1.69510100
C	-7.59306300	-3.25147400	1.14589900
H	-8.58955900	-3.20411500	0.68739000
H	-7.00553600	-3.95090100	0.53679700
C	-7.71167600	-3.79087300	2.56969500
H	-8.32097700	-3.12666900	3.19325400
H	-8.17794200	-4.78152300	2.58145800
H	-6.72605300	-3.87909900	3.04074200
C	-9.26036200	2.34725800	-0.44568700
H	-8.85190700	3.03274100	-1.19912400
H	-9.06163800	2.80565800	0.53157800
C	-10.76754900	2.20800200	-0.64609900
H	-11.20805100	1.55326000	0.11443600
H	-11.26667600	3.18017000	-0.57992100
H	-10.99729500	1.78018200	-1.62862800
O	0.24636200	2.85055100	-0.23564900

C	9.74801400	-1.81585000	-0.20956300
H	10.13284900	-0.79292200	-0.20731100
H	10.12830400	-2.32339800	0.68330400
H	10.16695900	-2.33353100	-1.07910200

6a S₀ CAMB3LYP/6-31+G(d) PCM Optimized Structure in DMSO

0 1			
C	5.91266400	-1.20921600	-0.17816800
C	7.30440300	-1.26999600	-0.08074900
H	7.90619300	-0.36908500	-0.05021600
C	7.92059900	-2.51331400	-0.01243500
C	7.13194200	-3.67947800	-0.04250800
H	7.62061100	-4.64792400	0.01104700
C	5.75190100	-3.62491100	-0.13456400
H	5.15818700	-4.53258800	-0.15391400
C	5.14703700	-2.37114500	-0.19925700
C	3.79654500	-0.29690100	-0.32077700
C	2.83169200	0.74974600	-0.36286500
H	3.21890400	1.75504700	-0.27361200
C	1.48211800	0.61350100	-0.47610600
C	0.37548400	1.57659700	-0.50322000
C	0.46207800	-0.47090600	-0.60258000
C	-0.59122600	0.53420300	-0.52700300
C	1.61142500	3.69399300	-0.43413500
C	0.39266500	2.97758200	-0.53691400
C	-0.75500900	3.77500300	-0.76060200
C	5.71452700	1.28761400	-0.26563600
H	5.10798100	1.92709100	-0.90726200
H	6.68629300	1.20030100	-0.75277400
C	5.85403800	1.86803600	1.13929300
H	6.45346600	1.18630800	1.75439400
H	4.86495100	1.93087200	1.60857900
C	6.50350400	3.25096200	1.11339400
H	7.48823600	3.18121900	0.63393500
H	5.90008300	3.92356500	0.49120300
C	6.65607600	3.84679800	2.51092900
H	7.12474300	4.83511700	2.46881100
H	7.27868200	3.20721400	3.14669800
H	5.68201500	3.95864800	3.00018500
N	5.11840600	-0.05883000	-0.26348900
N	2.60426400	4.29431100	-0.34587700
O	0.51352800	-1.68824400	-0.72755600
S	3.44634500	-1.99421800	-0.30973300
N	-1.67159500	4.46330100	-0.95883500
C	-2.01772500	0.37802900	-0.47693600
C	-2.58441900	-0.86337200	-0.83467400
C	-2.90456800	1.37023500	-0.02501900
C	-3.94418600	-1.08667600	-0.78487200
H	-1.93141500	-1.66647300	-1.15931600

C	-4.26788900	1.15534100	0.03772400
H	-2.52476300	2.32797400	0.30812900
C	-4.84632600	-0.07480000	-0.36630800
H	-4.30656200	-2.06439000	-1.07246200
H	-4.88675900	1.95588200	0.41842800
N	-6.20684700	-0.26866200	-0.35632600
C	-7.05706800	0.78573400	0.20913900
H	-6.84555800	0.90440200	1.28329200
H	-6.78297600	1.72920000	-0.27252800
C	-8.55813400	0.59817100	0.01719300
H	-8.78387100	0.44858700	-1.04606400
H	-8.91291000	-0.29054300	0.55177600
C	-6.75405800	-1.61471100	-0.50716800
H	-7.79109100	-1.52499200	-0.83048100
H	-6.24018100	-2.11648800	-1.33065700
C	-6.68227200	-2.46600500	0.76261100
H	-5.63980300	-2.53783300	1.09754500
H	-7.23400200	-1.95989500	1.56594500
C	-7.25285800	-3.86746300	0.55275300
H	-8.29267800	-3.78847700	0.20849500
H	-6.69883600	-4.36695100	-0.25313600
C	-7.19816800	-4.72448700	1.81556200
H	-7.77096300	-4.26416500	2.62887100
H	-7.61234700	-5.72256400	1.63815900
H	-6.16610300	-4.84751900	2.16351500
C	-9.32840100	1.81720600	0.52797500
H	-9.00151100	2.71035100	-0.01976400
H	-9.07635300	1.99080400	1.58224500
C	-10.84014200	1.65630000	0.38596700
H	-11.19973800	0.79009100	0.95314400
H	-11.36952200	2.54071700	0.75529700
H	-11.12458600	1.50972300	-0.66234000
C	9.41905800	-2.62374300	0.09345800
H	9.89032600	-1.63884000	0.13721200
H	9.70790300	-3.17937400	0.99158300
H	9.83276500	-3.15997600	-0.76711900

6a S₁ CAMB3LYP/6-31+G(d) PCM Optimized Structure in DMSO

0	1		
C	5.92468400	-1.24389600	-0.23472500
C	7.31963400	-1.33661300	-0.17087500
H	7.93742700	-0.44571800	-0.16531200
C	7.91950400	-2.59003700	-0.10211000
C	7.11602100	-3.74388200	-0.09418600
H	7.58906500	-4.72013300	-0.03908500
C	5.73146200	-3.66171600	-0.15006300
H	5.12255100	-4.56008100	-0.13979700
C	5.14131300	-2.40446800	-0.21709500
C	3.80073800	-0.30006100	-0.32462300
C	2.86213900	0.72735700	-0.32760200

H	3.26543500	1.73091700	-0.28247900
C	1.47129000	0.62888100	-0.35445600
C	0.39580500	1.60676100	-0.33742900
C	0.44683800	-0.43472500	-0.47978300
C	-0.63618400	0.58186800	-0.41215800
C	1.68349900	3.68384900	-0.23888600
C	0.44045500	2.99946300	-0.31554000
C	-0.68791300	3.85244100	-0.41718500
C	5.77085900	1.23962600	-0.37511700
H	5.14949400	1.87027500	-1.01478700
H	6.72949200	1.13833400	-0.88839500
C	5.96245600	1.87246300	1.00282500
H	6.58738700	1.21335300	1.61790600
H	4.99165300	1.94812600	1.50746800
C	6.60477300	3.25519100	0.90697500
H	7.57149600	3.17212400	0.39356700
H	5.97613400	3.90405100	0.28421700
C	6.80734800	3.90159400	2.27544500
H	7.26976900	4.88951600	2.18185300
H	7.45584700	3.28677800	2.90995200
H	5.85170300	4.02736900	2.79691800
N	5.16534200	-0.09010400	-0.31980900
N	2.69311100	4.25510200	-0.17350800
O	0.47392700	-1.65175700	-0.59942000
S	3.43736400	-2.01675300	-0.29514100
N	-1.57706200	4.59455900	-0.50842500
C	-2.02918200	0.42433000	-0.37063600
C	-2.57845700	-0.88006200	-0.58653600
C	-2.97162700	1.45756200	-0.09434900
C	-3.92462300	-1.11943100	-0.56715200
H	-1.89704100	-1.70259200	-0.77252600
C	-4.32217400	1.22400700	-0.07068900
H	-2.62533500	2.45935100	0.11880100
C	-4.86706500	-0.07094400	-0.32853900
H	-4.26298800	-2.13314800	-0.73317400
H	-4.97501600	2.05395300	0.16163800
N	-6.20695600	-0.28756300	-0.34281500
C	-7.11155700	0.82375200	-0.00109200
H	-6.92642600	1.12333700	1.03996200
H	-6.84574500	1.67792200	-0.63178500
C	-8.60126100	0.55786400	-0.18166500
H	-8.81436400	0.28071600	-1.22097400
H	-8.93016900	-0.27314200	0.45251600
C	-6.74242900	-1.64181800	-0.48268400
H	-7.75200700	-1.56696500	-0.88371400
H	-6.16418300	-2.17334800	-1.24178400
C	-6.76250900	-2.43152200	0.82883900
H	-5.74611100	-2.49002900	1.23732400
H	-7.36548700	-1.88758700	1.56702300
C	-7.32561100	-3.83899800	0.63985200
H	-8.34076400	-3.77155500	0.22715900
H	-6.72334700	-4.37341200	-0.10649600

C	-7.35526100	-4.63999900	1.93972500
H	-7.97629700	-4.14379100	2.69425500
H	-7.76268100	-5.64342700	1.77841800
H	-6.34799500	-4.75073800	2.35716300
C	-9.41492400	1.80332700	0.17713100
H	-9.09686000	2.64136500	-0.45603700
H	-9.19614500	2.09526500	1.21219000
C	-10.91707000	1.58273200	0.01578400
H	-11.26840700	0.77102800	0.66296100
H	-11.47952300	2.48521200	0.27602700
H	-11.16814100	1.31811400	-1.01769000
C	9.41934100	-2.71806600	-0.03474100
H	9.90340200	-1.73857000	-0.00615600
H	9.72654600	-3.27487600	0.85674100
H	9.80549200	-3.26084500	-0.90430900

6b S₀ CAMB3LYP/6-31+G(d) PCM Optimized Structure in DMSO

0 1			
C	4.22479500	2.63245000	-0.45243600
H	5.13690500	2.75533000	-1.04177600
H	3.42007200	3.08183700	-1.03864300
C	4.36822100	3.32613800	0.90200400
H	5.17034500	2.83995300	1.47126000
H	3.44502100	3.19164400	1.47855900
C	4.67036900	4.81550800	0.74825000
H	3.86514800	5.28844700	0.17263700
H	5.59001700	4.94009000	0.16169700
C	4.82250000	5.52399100	2.09245600
H	5.03919500	6.58862600	1.95708100
H	5.63955400	5.08765400	2.67842500
H	3.90509700	5.44218600	2.68641000
C	-5.97782500	-1.66203500	0.40288900
C	-7.34632400	-1.91453700	0.51176000
H	-8.06345900	-1.10417500	0.57597200
C	-7.79270800	-3.23181000	0.52650300
C	-6.85894200	-4.27881300	0.43076200
H	-7.21285200	-5.30559600	0.44271000
C	-5.49963100	-4.03318300	0.31734700
H	-4.79117800	-4.85132200	0.24122300
C	-5.06780700	-2.71000900	0.30164900
C	-4.00254700	-0.46169000	0.23585300
C	-3.20230900	0.69485000	0.14593600
H	-3.72975400	1.63875800	0.13879200
C	-1.83089800	0.76184500	0.04961500
C	-0.90991600	1.87101300	-0.05717000
C	-0.67155800	-0.15929500	0.01685700
C	0.23231000	1.00534400	-0.08614200
C	1.59366700	1.35256400	-0.17452700
H	1.74580300	2.42334300	-0.21581300

C	2.75244500	0.60085100	-0.21523900
C	5.01209000	0.25926900	-0.31324600
C	6.38184800	0.47084200	-0.38438500
H	6.81407900	1.46228000	-0.45455700
C	7.21339800	-0.64911300	-0.35609300
H	8.28859000	-0.52044400	-0.40889800
C	6.66605700	-1.92227600	-0.25825100
C	5.28875000	-2.12786700	-0.17904900
H	4.88454000	-3.13148300	-0.10011000
C	4.46893700	-1.01645800	-0.20505600
C	-2.39194100	3.83169100	-0.05173700
C	-1.09839400	3.25868500	-0.11013700
C	-0.02255700	4.17076600	-0.23322400
C	-6.11260500	0.83588400	0.49013900
H	-5.50667800	1.56093800	1.03481800
H	-6.97619100	0.62466300	1.12265100
C	-6.55043000	1.38013400	-0.86737900
H	-7.13814300	0.61583700	-1.39006900
H	-5.66544700	1.57590500	-1.48463500
C	-7.37469100	2.65857800	-0.72279200
H	-8.25195800	2.45611700	-0.09499300
H	-6.78118700	3.41512200	-0.19439000
C	-7.82823400	3.21434900	-2.07069600
H	-8.41702400	4.12828000	-1.94281300
H	-8.44870900	2.48807800	-2.60785200
H	-6.96909700	3.45556900	-2.70663300
N	3.97338900	1.20077300	-0.33770500
N	-5.34646700	-0.41297300	0.38074900
N	-3.45064100	4.31282600	-0.00379500
O	-0.55815300	-1.37757100	0.06239500
S	-3.43257200	-2.10677500	0.15957300
N	0.84743800	4.93683800	-0.33717400
C	-9.26250800	-3.54299500	0.64135800
H	-9.86104200	-2.63027500	0.69493600
H	-9.60826200	-4.12547900	-0.21902100
H	-9.46823300	-4.13631800	1.53853400
C	2.96101100	-0.91473600	-0.13882200
C	2.44892100	-1.48790400	1.19504200
H	1.36380200	-1.41210800	1.25869900
H	2.71950300	-2.54643200	1.26179100
H	2.90241300	-0.96621100	2.04323700
C	2.32774200	-1.62771800	-1.34821100
H	2.58889400	-2.69035300	-1.31945700
H	1.24134800	-1.54561400	-1.32140800
H	2.70315100	-1.20980200	-2.28719700
Br	7.82453400	-3.42754800	-0.22288600

6b S₁ CAMB3LYP/6-31+G(d) PCM Optimized Structure in DMSO

0 1			
C	-4.24166000	2.62352400	0.45845400
H	-5.15073000	2.74989000	1.05129700
H	-3.43315300	3.07478500	1.03766500
C	-4.39163800	3.31043500	-0.90015300
H	-5.19750700	2.82277300	-1.46238500
H	-3.47143000	3.17222200	-1.48034000
C	-4.69094500	4.80080400	-0.74962900
H	-3.88170200	5.27490200	-0.18077800
H	-5.60707100	4.92881400	-0.15853100
C	-4.84982800	5.50315900	-2.09629600
H	-5.06413200	6.56861200	-1.96390800
H	-5.67106500	5.06556200	-2.67532100
H	-3.93605400	5.41751100	-2.69520900
C	6.01853900	-1.64536100	-0.40431600
C	7.38996000	-1.91216600	-0.49011900
H	8.11289600	-1.10562100	-0.53708800
C	7.83016300	-3.23157100	-0.50276200
C	6.89237700	-4.27668100	-0.42603300
H	7.24186000	-5.30506600	-0.43574600
C	5.53129100	-4.02193400	-0.33331200
H	4.81788000	-4.83734700	-0.27094700
C	5.10123100	-2.69960200	-0.32031500
C	4.03298000	-0.44512500	-0.26027700
C	3.23078500	0.69118700	-0.17169100
H	3.75472400	1.63928900	-0.17423700
C	1.84412700	0.76911700	-0.06723000
C	0.91928500	1.87381000	0.04026100
C	0.68348500	-0.15566000	-0.03699200
C	-0.25066400	1.00776700	0.07190600
C	-1.60006300	1.33901000	0.17464900
H	-1.76279600	2.40873700	0.23043300
C	-2.77147100	0.58116600	0.21585700
C	-5.02822700	0.26029900	0.32584100
C	-6.40190700	0.47521000	0.40904000
H	-6.83125500	1.46711400	0.48820300
C	-7.23398300	-0.64063500	0.38014000
H	-8.30852100	-0.51014300	0.44170400
C	-6.69124000	-1.91755100	0.27042800
C	-5.31474800	-2.12826000	0.17965700
H	-4.91569900	-3.13321700	0.09230200
C	-4.48965400	-1.02182800	0.20589200
C	2.38734100	3.83515600	0.04294000
C	1.09426700	3.25226300	0.09637300
C	0.00549800	4.15466300	0.21529800
C	6.16754200	0.84063700	-0.48026400
H	5.57050700	1.56806500	-1.03418000
H	7.04733000	0.63990400	-1.09526200
C	6.57824300	1.38949700	0.88552300

H	7.16763100	0.63093700	1.41503600
H	5.68125800	1.57148600	1.48968800
C	7.38777600	2.67900200	0.75890100
H	8.27710000	2.49066000	0.14362300
H	6.79263200	3.42981300	0.22386700
C	7.81370400	3.23644300	2.11521300
H	8.39130600	4.15925800	1.99994300
H	8.43630800	2.51693300	2.65905100
H	6.94182000	3.46271200	2.73930700
N	-3.99366100	1.19064200	0.34698700
N	5.40538400	-0.40474400	-0.39172200
N	3.44655800	4.31089300	-0.00111900
O	0.56849500	-1.37066500	-0.08412300
S	3.46199900	-2.10195800	-0.20620400
N	-0.88004300	4.90057600	0.31405800
C	9.30075600	-3.54704000	-0.59411500
H	9.90327600	-2.63606400	-0.63237000
H	9.63024400	-4.13582800	0.26852100
H	9.52025000	-4.13625800	-1.49091600
C	-2.98255900	-0.92709400	0.13155200
C	-2.47426100	-1.49996800	-1.20637300
H	-1.39026500	-1.41264800	-1.27758200
H	-2.73355300	-2.56174600	-1.26854600
H	-2.93796700	-0.98434400	-2.05242800
C	-2.34155400	-1.65476300	1.33096400
H	-2.59329800	-2.71931900	1.28646100
H	-1.25580100	-1.56255600	1.30375600
H	-2.71819500	-1.25320200	2.27628200
Br	-7.85554600	-3.41540000	0.23484000

6c S₀ CAMB3LYP/6-31+G(d) PCM Optimized Structure in DMSO

0 1			
C	-5.90179600	0.92831600	-0.38030000
H	-5.33931800	1.57908900	-1.05177500
H	-6.82238200	0.67227600	-0.90470800
C	-6.18653700	1.61780700	0.95380500
H	-5.23593400	1.79832800	1.46799300
H	-6.76673700	0.93982200	1.59187400
C	-6.93618700	2.94291400	0.78960200
H	-6.34865000	3.61516400	0.15140100
H	-6.98885800	3.42394800	1.77283900
C	-8.35050800	2.79970600	0.22679500
H	-8.86193100	3.76752800	0.21458500
H	-8.94877400	2.11365500	0.83764300
H	-8.35066800	2.42003800	-0.80029400
C	5.08432600	-0.43608900	-0.23446200
C	6.45591000	-0.38753700	-0.24302200
H	6.99476400	0.54395600	-0.37430600
C	7.19179300	-1.58634600	-0.06517900

C	6.50654600	-2.82333600	0.12284300
C	5.08843600	-2.83830500	0.13318400
H	4.56232900	-3.77671100	0.27966600
C	4.40760400	-1.66527100	-0.03925900
C	2.87468300	0.30087500	-0.30989400
C	1.84902500	1.23422500	-0.38479300
H	2.14559800	2.27176400	-0.46089800
C	0.47343000	0.99701800	-0.34549000
C	-0.65231100	1.88273900	-0.37104000
C	-0.44870300	-0.15235600	-0.29635500
C	-1.59348400	0.79058200	-0.30227500
C	-2.97354100	0.75228100	-0.27858100
H	-3.47874100	1.70774400	-0.31990900
C	-3.79534600	-0.38311800	-0.18379600
C	-5.79416100	-1.55218800	-0.05493400
C	-7.16972500	-1.78516100	-0.01705700
H	-7.87947400	-0.96993800	-0.09986200
C	-7.63311200	-3.08769200	0.14089400
C	-6.70880900	-4.13982900	0.26041200
H	-7.07522800	-5.15482700	0.38373700
C	-5.34130600	-3.91296900	0.22896900
H	-4.63901100	-4.73421300	0.32615700
C	-4.89262100	-2.60524000	0.07267900
C	0.32491000	4.13763100	-0.49913500
C	-0.79594000	3.27574300	-0.44160600
C	-2.06924800	3.89264700	-0.46207000
C	4.67199100	1.99118800	-0.64921800
H	3.95557900	2.49112500	-1.30332900
H	5.59868900	1.90776500	-1.22101400
C	4.89676800	2.78358000	0.63678600
H	5.60492700	2.24143400	1.27518100
H	3.95450600	2.84766100	1.19427200
C	5.42640900	4.18856800	0.35370500
H	6.36553000	4.11630200	-0.20995700
H	4.71644500	4.72105700	-0.29175400
C	5.65830600	4.99266400	1.63082100
H	6.03624100	5.99479700	1.40422000
H	6.38896700	4.49792000	2.28081000
H	4.72818700	5.10600500	2.19916500
N	-5.14830300	-0.32109400	-0.21491500
N	4.19393600	0.62813900	-0.40513700
N	1.24234100	4.85246000	-0.54680200
O	-0.32943900	-1.37066300	-0.28054200
S	2.66811400	-1.42567400	-0.05587400
S	-3.24244500	-2.02709900	0.00807800
N	-3.11292100	4.40786300	-0.48064000
C	-9.11153400	-3.37551900	0.18639400
H	-9.38674200	-3.86730800	1.12525900
H	-9.69969400	-2.45860800	0.09934200
H	-9.40555600	-4.04510100	-0.62881400
C	7.26400400	-4.01221000	0.29973200
H	6.73576500	-4.95093200	0.44252000

C	8.63434800	-3.97899700	0.29113400
H	9.20260900	-4.89402500	0.42702300
C	9.31621600	-2.75082800	0.10554300
H	10.40186600	-2.73555100	0.10087100
C	8.61345100	-1.58675100	-0.06755300
H	9.13542200	-0.64450600	-0.21011300

6c S₁ CAMB3LYP/6-31+G(d) PCM Optimized Structure in DMSO

0 1			
C	-5.94607700	0.92001500	-0.37925700
H	-5.39261900	1.57170400	-1.05902300
H	-6.87447300	0.66573200	-0.89192300
C	-6.21738700	1.61888200	0.95429600
H	-5.26162600	1.79449000	1.46073800
H	-6.79737500	0.94704100	1.59924700
C	-6.95915600	2.94846700	0.79123000
H	-6.37228400	3.61415000	0.14532100
H	-7.00117100	3.43458300	1.77264700
C	-8.37875400	2.81264500	0.23983500
H	-8.88368500	3.78391100	0.22576900
H	-8.97716700	2.13425000	0.85908500
H	-8.38898500	2.42668000	-0.78483400
C	5.10188800	-0.42424800	-0.23726000
C	6.48008800	-0.38907900	-0.23993700
H	7.02617100	0.53959500	-0.36019500
C	7.20413700	-1.59274100	-0.07037200
C	6.50966800	-2.82928300	0.10611700
C	5.09204000	-2.83488500	0.11353200
H	4.55950900	-3.77098300	0.25153700
C	4.41654600	-1.65652600	-0.05203000
C	2.89563900	0.31039800	-0.31344100
C	1.86141200	1.24552900	-0.38595300
H	2.16554700	2.28181200	-0.47239900
C	0.49220700	1.01975800	-0.34335500
C	-0.65971000	1.90066800	-0.38879400
C	-0.44951000	-0.13029700	-0.26508300
C	-1.60438900	0.80573500	-0.30696000
C	-2.99445100	0.75079900	-0.29475200
H	-3.50335200	1.70511000	-0.35927000
C	-3.81459700	-0.37314900	-0.19546300
C	-5.81342000	-1.54869000	-0.05341900
C	-7.18929800	-1.80076700	-0.00334400
H	-7.90765600	-0.99243100	-0.07992500
C	-7.63922100	-3.10688200	0.15922900
C	-6.70639800	-4.15293000	0.27438200
H	-7.06346200	-5.17080700	0.40172300
C	-5.34038400	-3.91189100	0.23370500
H	-4.63026000	-4.72704400	0.32805600
C	-4.90056400	-2.60272300	0.07140600

C	0.32658900	4.13951800	-0.54710900
C	-0.80053500	3.28015500	-0.48004500
C	-2.07765200	3.89767300	-0.51096600
C	4.70995100	2.00169800	-0.62318400
H	3.99982300	2.51335900	-1.27552700
H	5.64157700	1.92629400	-1.18846100
C	4.92546800	2.77663000	0.67597800
H	5.62854500	2.22528400	1.31198600
H	3.97866100	2.83324700	1.22662300
C	5.45752800	4.18513500	0.41601300
H	6.40122700	4.12033100	-0.14082600
H	4.75294100	4.72653000	-0.22797500
C	5.67906800	4.97178400	1.70580600
H	6.05908400	5.97672600	1.49570700
H	6.40430800	4.46812000	2.35498200
H	4.74437800	5.07783300	2.26802000
N	-5.19082800	-0.32340400	-0.22091200
N	4.22813100	0.63759900	-0.40210800
N	1.25248700	4.83943900	-0.60154500
O	-0.32277400	-1.34411400	-0.20036500
S	2.68204400	-1.41232300	-0.07595100
S	-3.25334900	-2.02201900	-0.00843400
N	-3.12494600	4.40032300	-0.53665800
C	-9.11482400	-3.40655600	0.21579600
H	-9.37940200	-3.89960800	1.15718100
H	-9.71126100	-2.49467800	0.13163300
H	-9.40923600	-4.07999100	-0.59624400
C	7.25842000	-4.02412500	0.27458900
H	6.72298600	-4.96016900	0.40818300
C	8.62945800	-4.00126300	0.26967100
H	9.19080400	-4.92144400	0.39925200
C	9.32024200	-2.77594900	0.09607600
H	10.40603700	-2.76839800	0.09410100
C	8.62683500	-1.60527100	-0.06882800
H	9.15642900	-0.66594800	-0.20223700