Supporting Information (SI)

Linear and Nonlinear Optical Properties of Quadrupolar Bithiophenes and Cyclopentadithiophenes as Fluorescent Oxygen Photosensitizers

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1. ^{1}H / $^{13}C\{^{1}H\}$/ $^{19}F\{^{1}H\}$ NMR spectra for the new compounds 1a,b 2a, b and 9

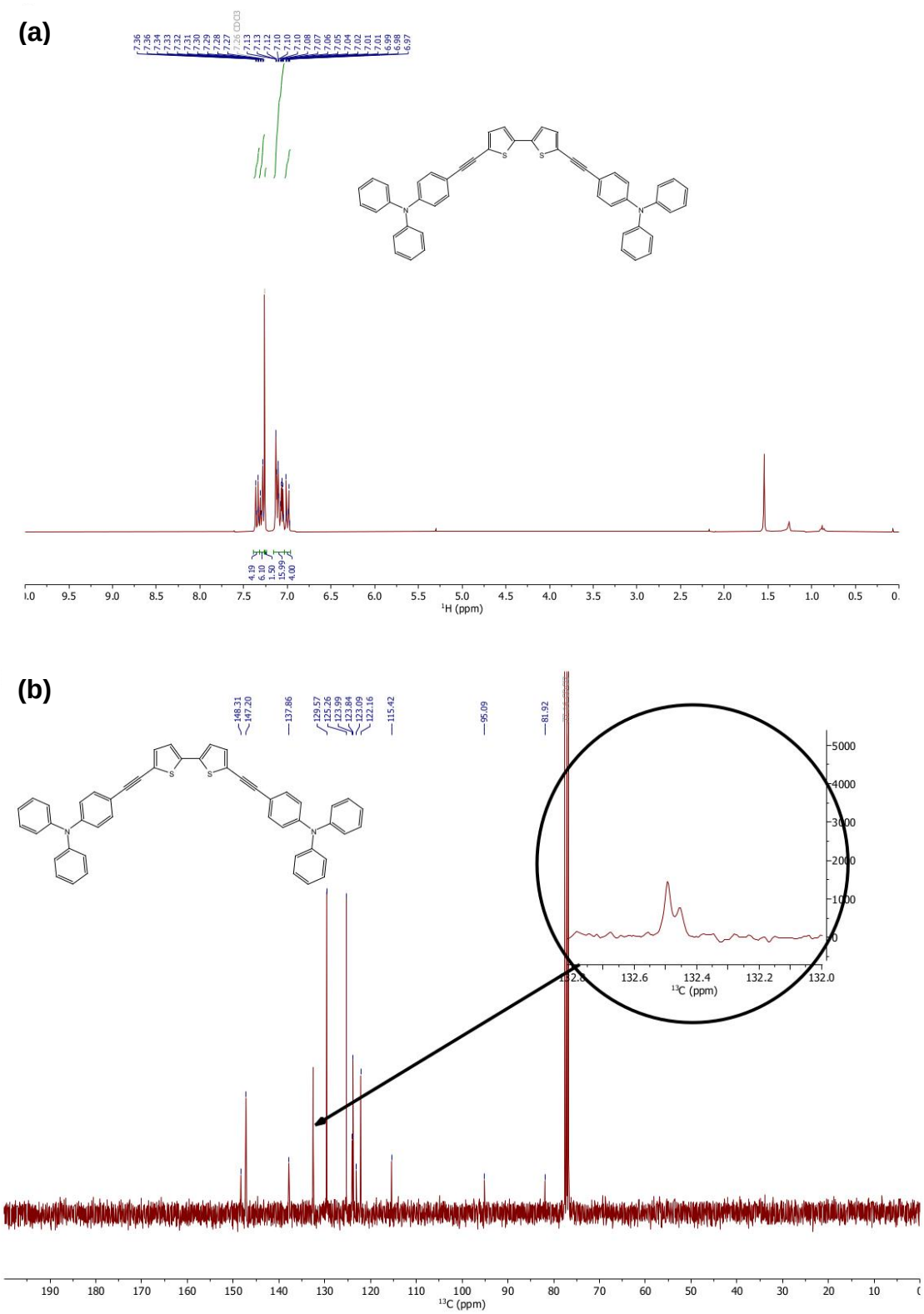


Figure S1. ^{1}H (a) and $^{13}C\{^{1}H\}$ (b) NMR spectra at 300 and 75 MHz, respectively, for **1a** in $CDCl_3$.

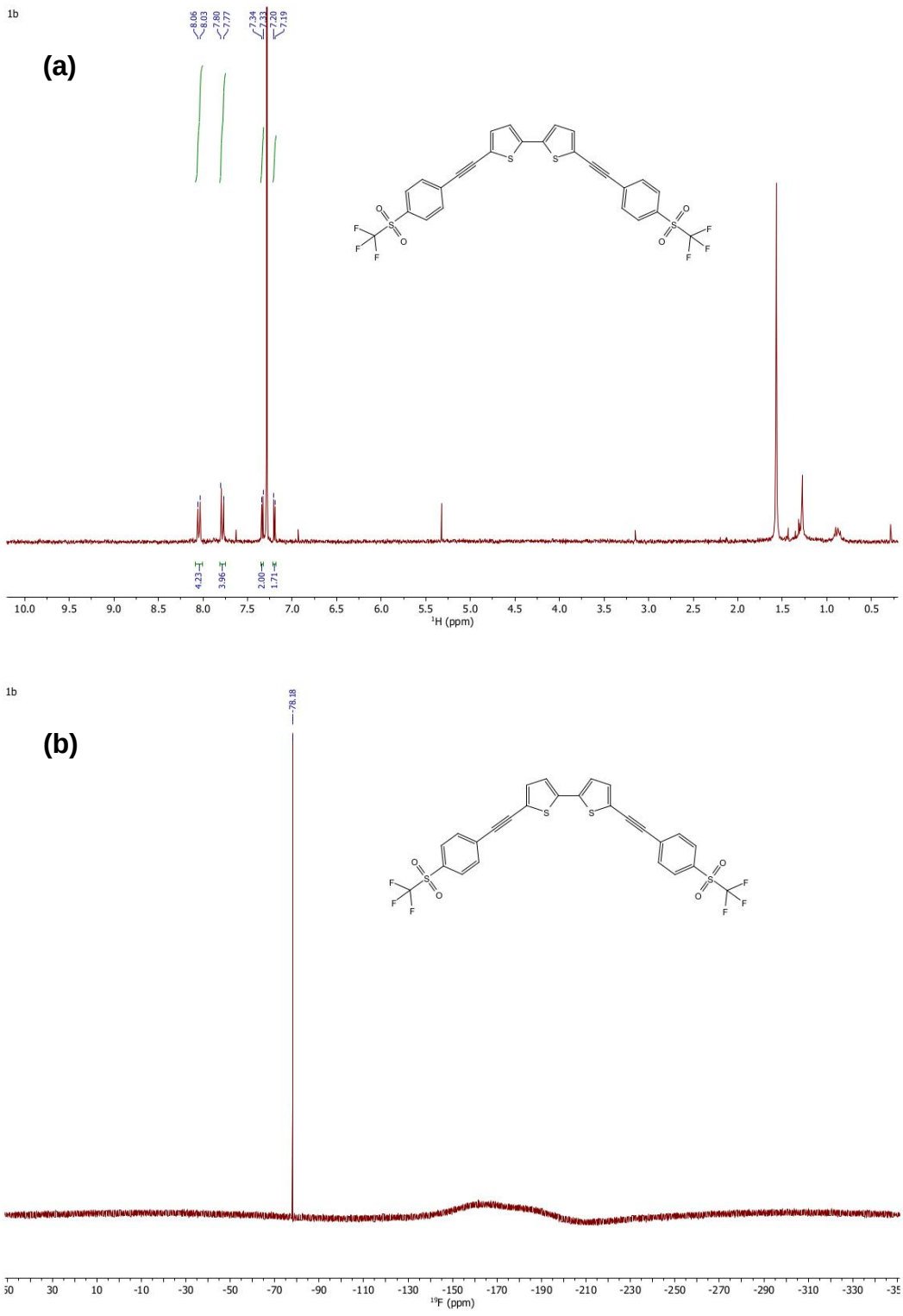


Figure S2. ^{1}H (a) and $^{19}F\{^{1}H\}$ (b) NMR spectra at 300 and 282 MHz, respectively, for **1b** in $CDCl_3$.

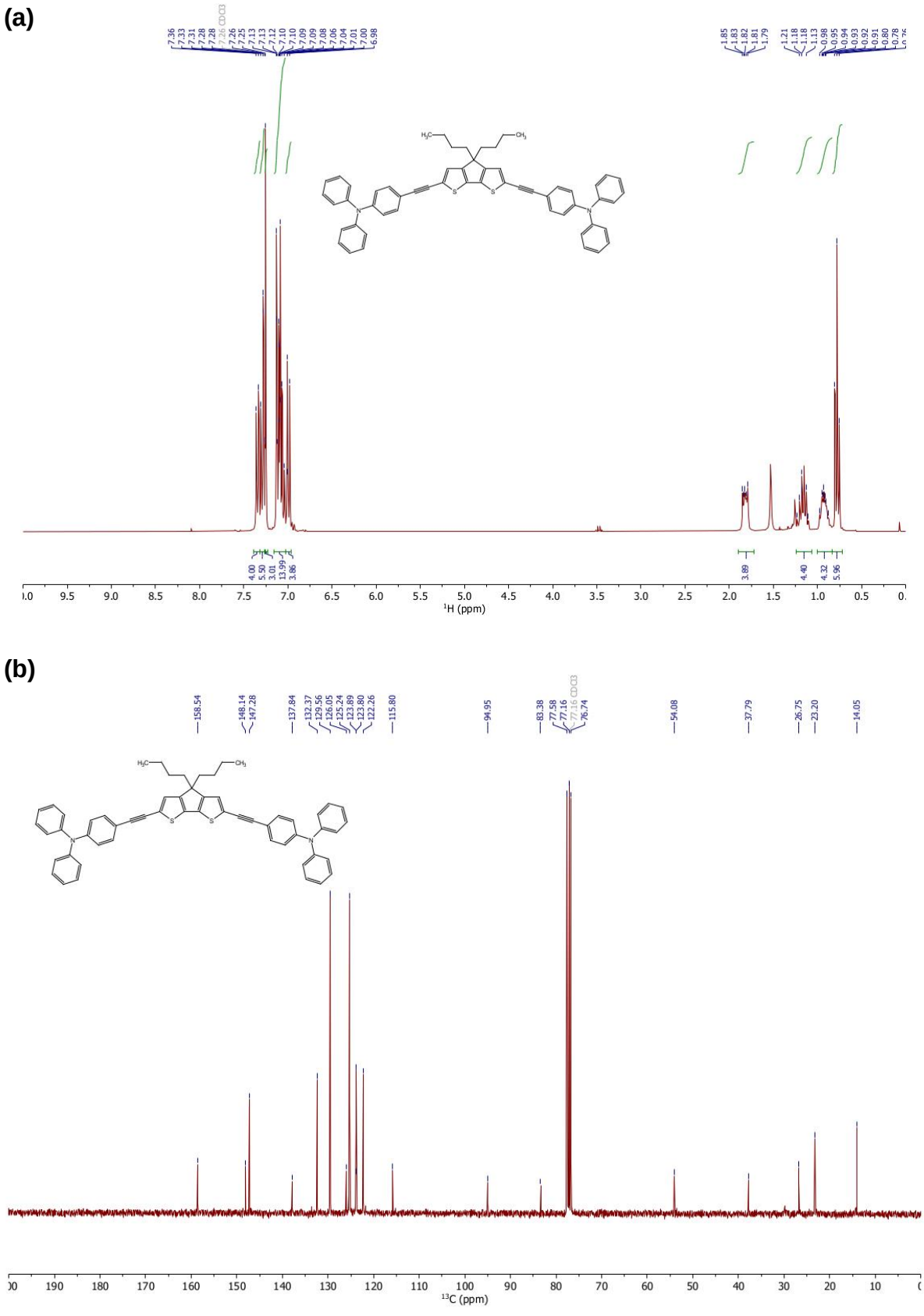


Figure S3. ^{1}H (a) and $^{13}C\{^{1}H\}$ (b) NMR spectra at 300 and 75 MHz, respectively, for **2a** in $CDCl_3$.

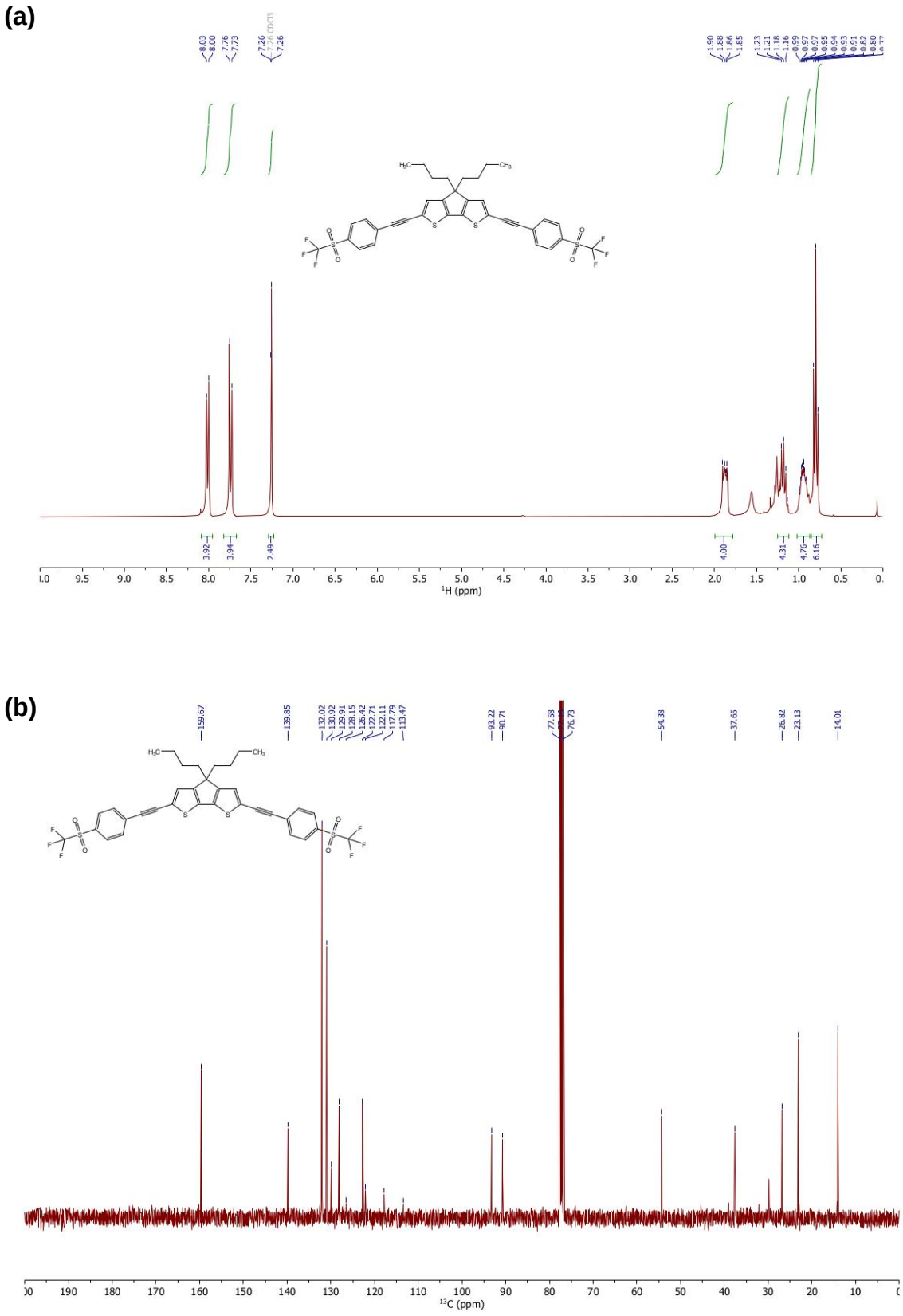


Figure S4. ^{1}H (a) and $^{13}C\{^{1}H\}$ (b) NMR spectra at 300 and 75 MHz, respectively, for **2b** in $CDCl_3$.

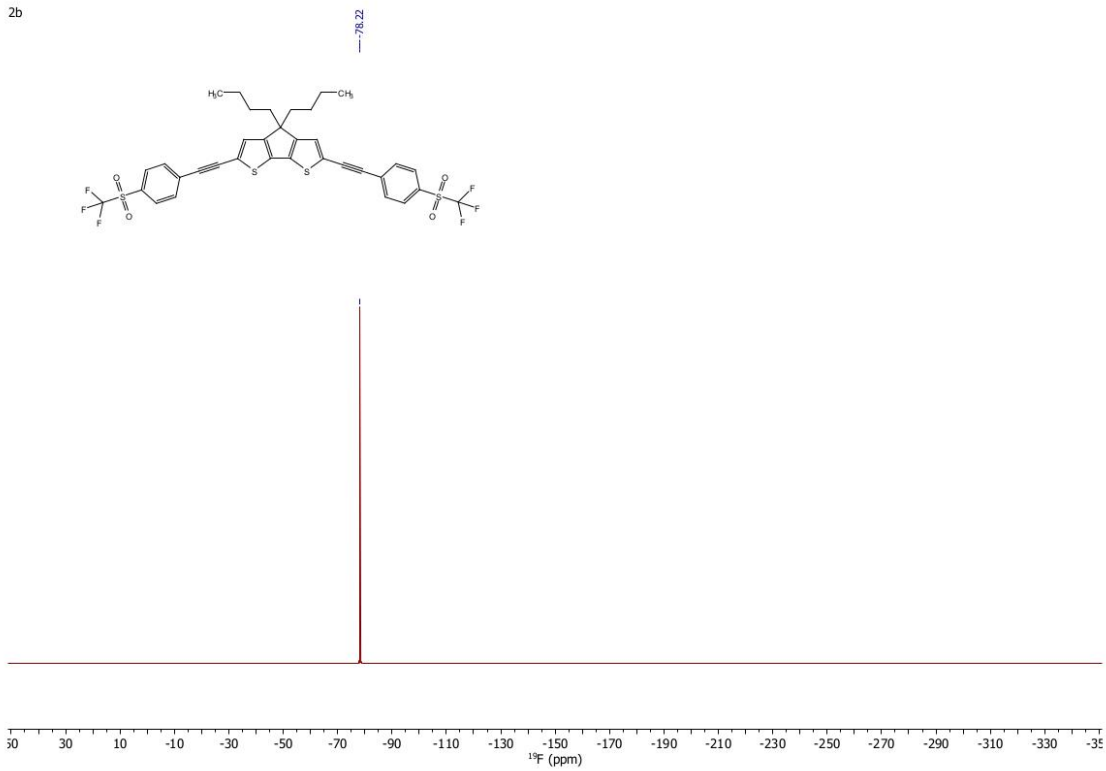


Figure S5. ^{19}F NMR spectrum at 282 MHz for **2b** in $CDCl_3$.

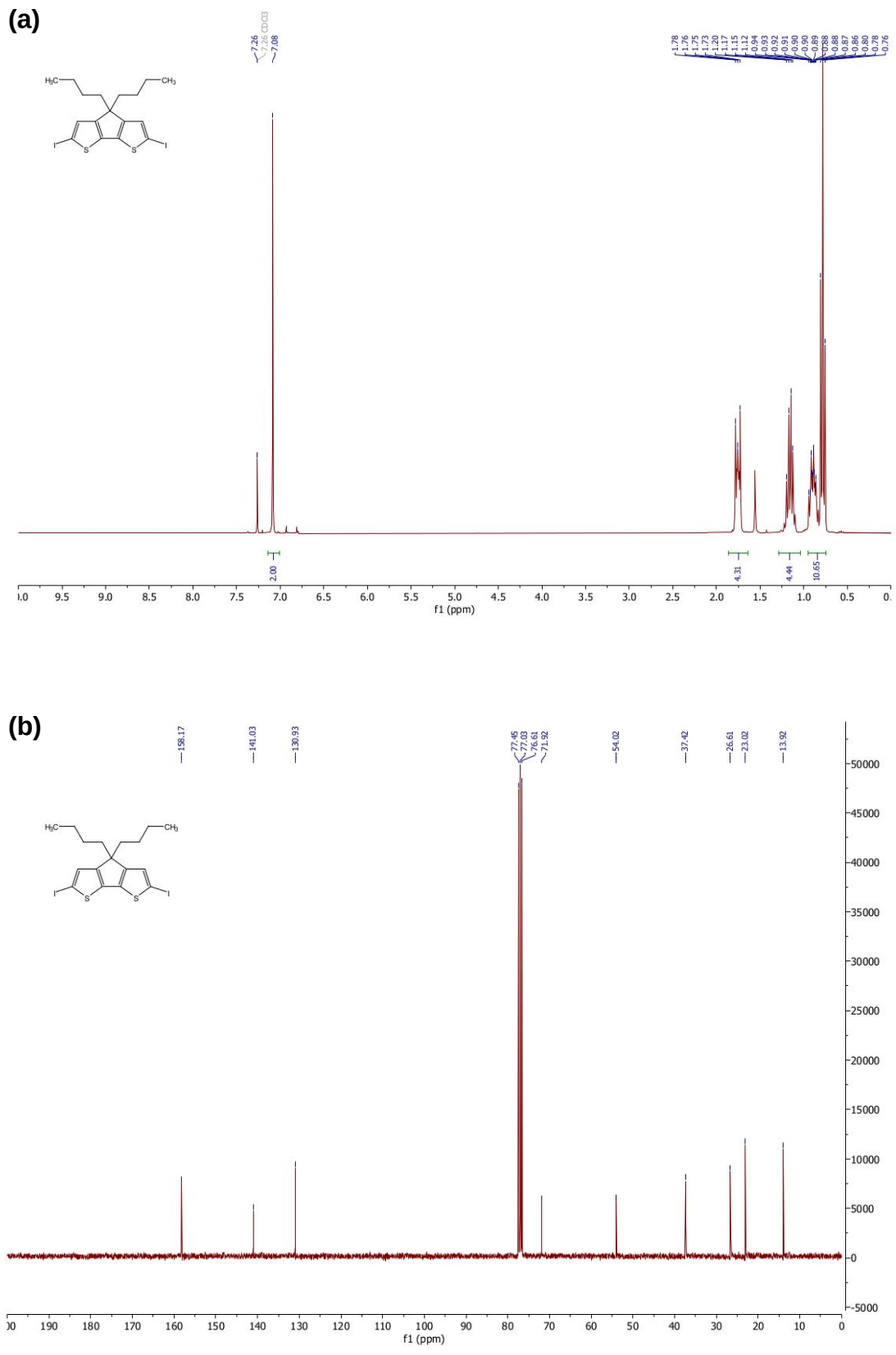


Figure S6. ^{1}H (a) and $^{13}C\{^{1}H\}$ (b) NMR spectra at 300 and 75 MHz, respectively, for **9** in $CDCl_3$

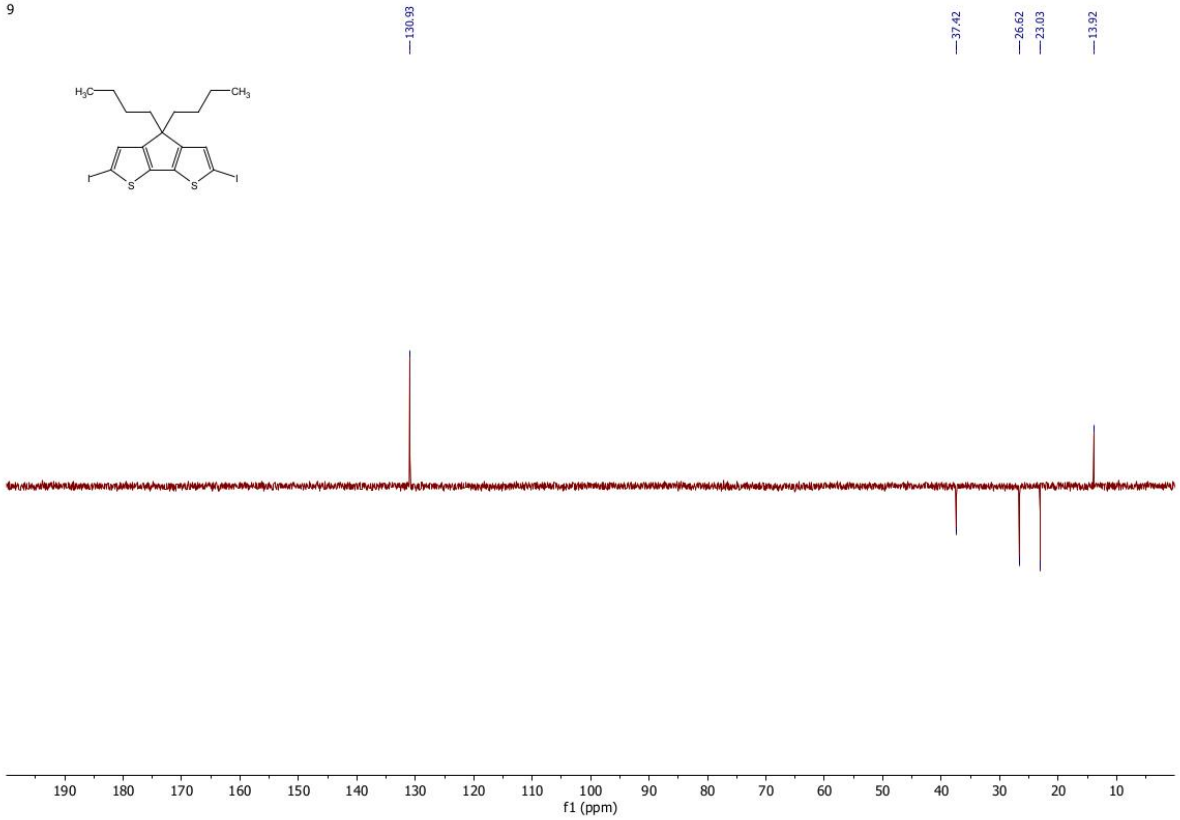


Figure S7. $^{13}C\{^{1}H\}$ DEPT NMR spectrum at 75 MHz for **9** in $CDCl_3$

2. Two-photon excited fluorescence (2PEF) data for 1a,b and 2a,b

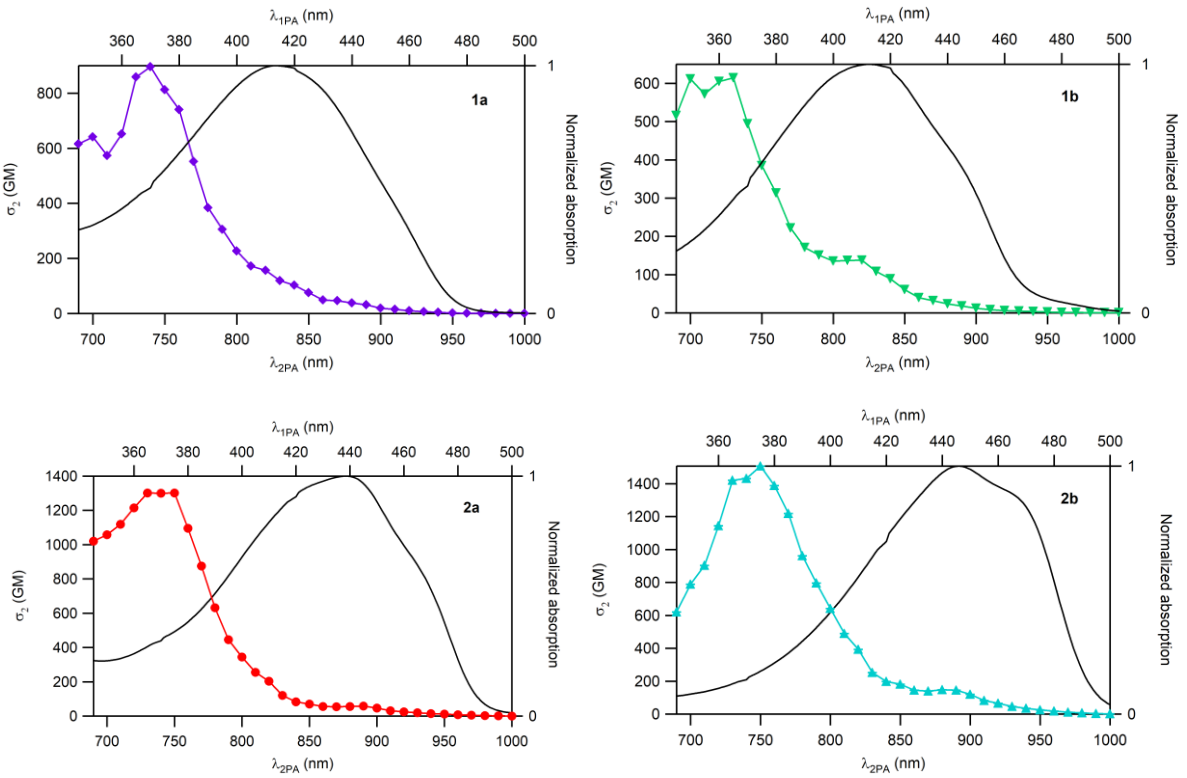


Figure S8. Overlay of one- and two-photon absorption spectra for **1a,b** and **2a,b** in toluene (25 °C).

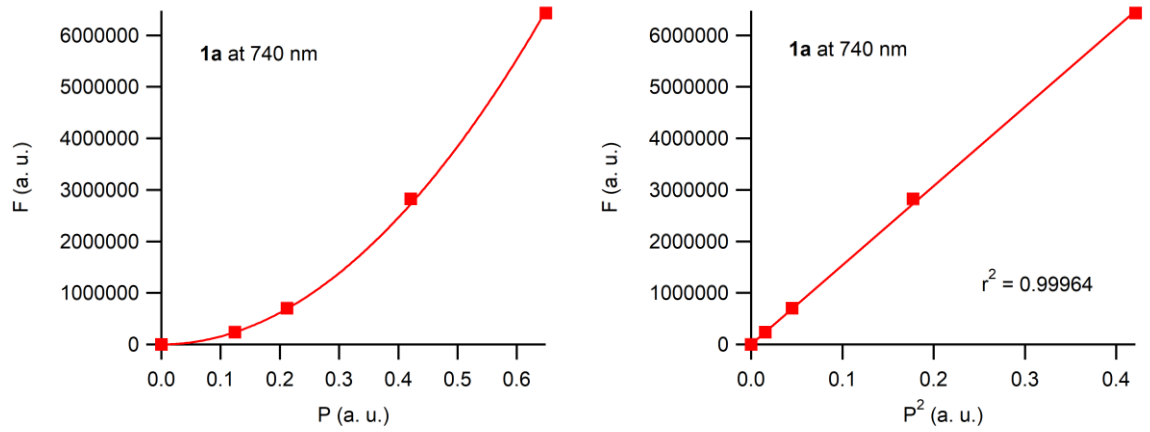


Figure S9. Left: quadratic dependence of the emission intensity (F) on laser excitation power (P) for **1a,b** and **2a,b** at their maxima nm in toluene (25 °C). Right: dependence of F on P^2.

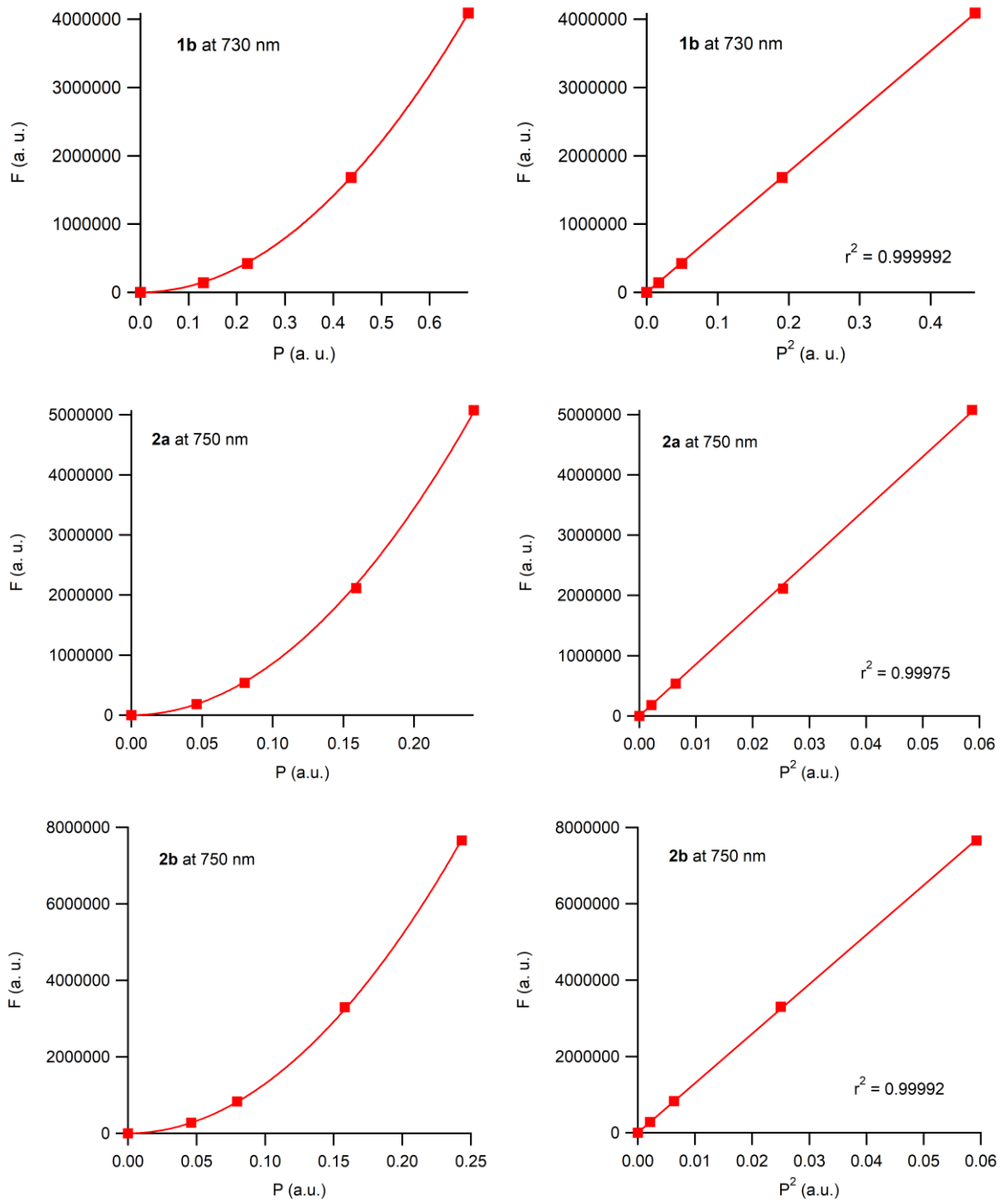
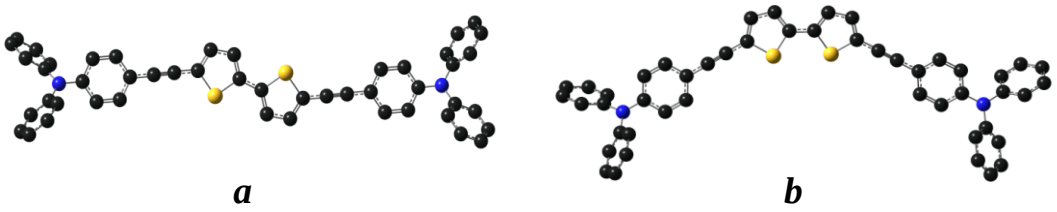


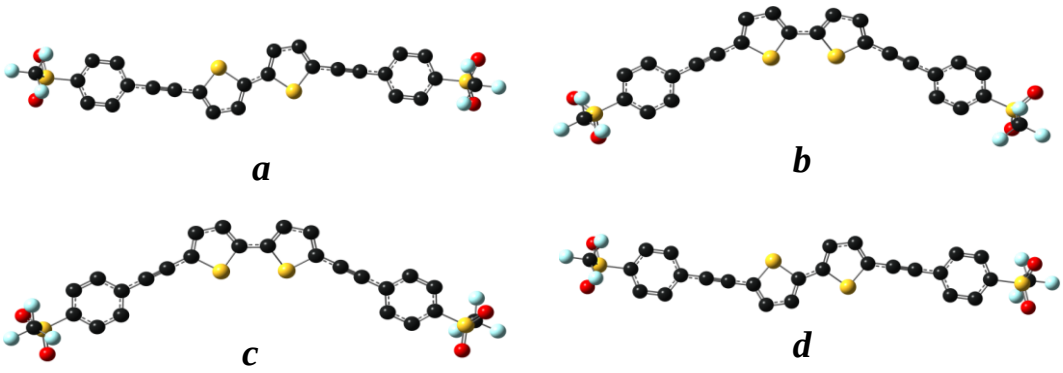
Figure S9 (continued). Left: quadratic dependence of the emission intensity (F) on laser excitation power (P) for **1a,b** and **2a,b** at their maxima nm in toluene (25 °C). Right: dependence of F on P^2.

3. Conformers and conformational freedom at the PBE0/6-31+G(d) level of theory for 1a,b and 2a,b

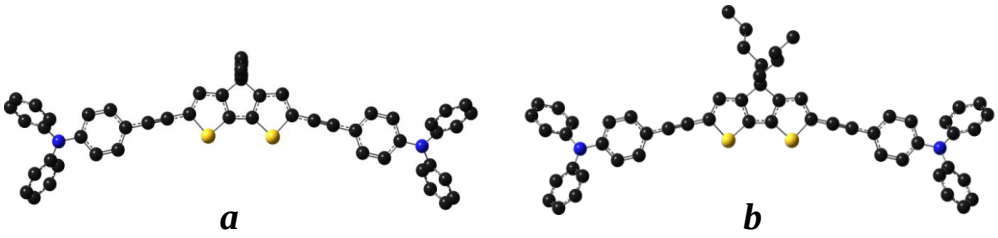
Molecule **1a**



Molecule **1b**



Molecule **2a**



Molecule **2b**

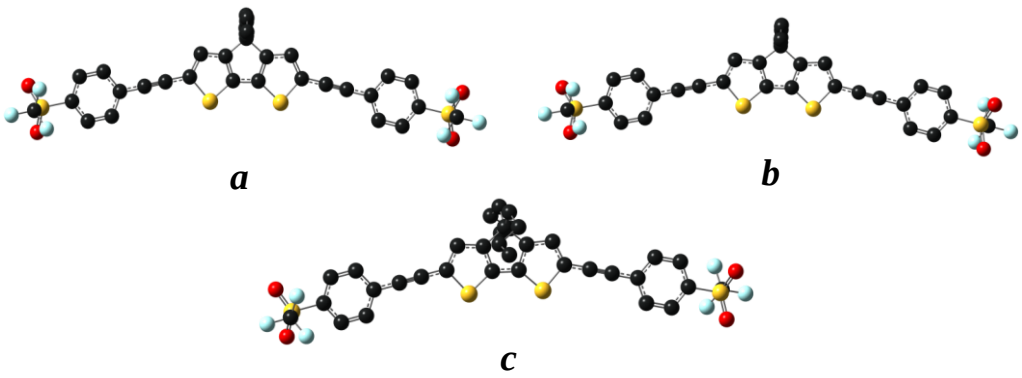
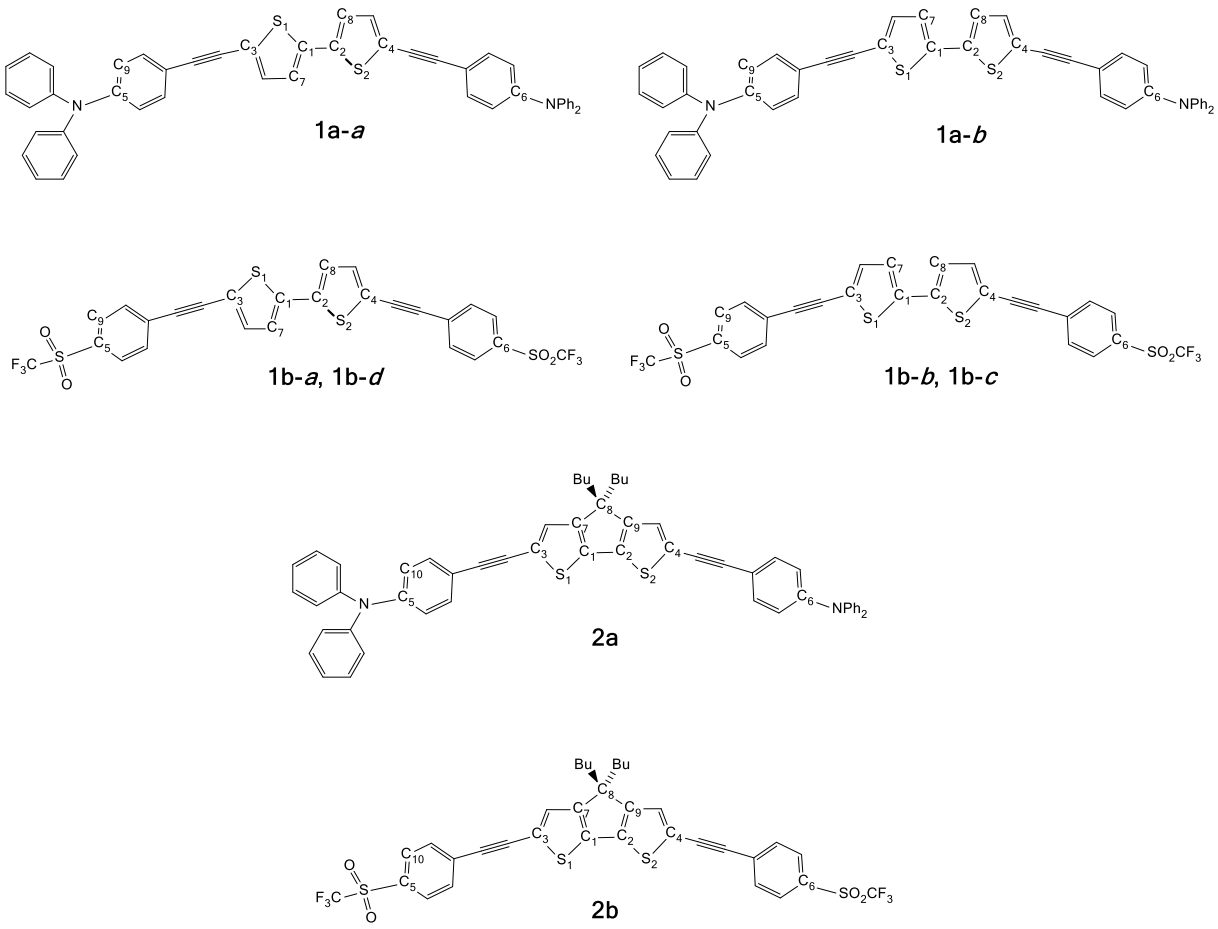


Figure S10. PBE0/6-31+G(d)-optimized geometries, using the PCM solvation model in toluene, involving the different configurations of **1a**,**b,** and **2a**,**b**. (S, yellow; C, black; H, white; O, red; N, blue; and F, sky blue).

Table S1. PBE0/6-31+G(d) relative energies (ΔE, kcal.mol^{-1}) of the conformers relative to the most stable optimized conformer in level, in toluene.											
Compound	**1a**		**2a**		**1b**				**2b**		
Form	***a***	***b***	***a***	***b***	***a***	***b***	***c***	***d***	***a***	***b***	***c***
ΔE	0.00	0.80	0.00	0.80	0.00	0.00	0.70	0.70	0.00	0.10	4.30

In the most stable configuration (form ***a***) of **2a** and **2b**, the two butyl groups are perpendicular to the plane of the molecule. In the case of **1a** and **1b**, a *trans* arrangement is adopted at the bithiophene units**.** For **2b**, forms ***a*** and ***b*** are very close in energy, differing in the orientation of the triflate (SO_2CF_3) terminal group. In all of these conformers, the peripheral *para*-substituted phenyleneethynylene arms are coplanar with the bithiophene core. Given their energy differences, all these conformers (apart, perhaps, for isomer ***c*** of **2b**) should coexist in solution, This is certainly the case for the *cis* and *trans* conformers of **1a** and **1b**.



Scheme S1. Atom numbering in the **1a,b** and **2a,b** series of compounds. Hydrogen atoms omitted for clarity.

Pertinent calculated important geometrical parameters are presented (below) in Table S2. The data shows that the bond lengths and bond angles remain unchanged in the different conformers of a given compound. Trigonal planar sulfur atoms are observed in all compounds. The bond

angle at the sulfur is around 93°, the C-C-S angle is around 109° and the other two carbons show a bond angle around 114°. The C-C bonds of the carbons adjacent to the sulfur are about 1.34 Å, the C-S bond length is around 1.70 Å, and the other C-C bond is about 1.41 Å. Different types of dihedral angles are considered to describe the geometry of the considered bi-thiophene derivatives (Scheme S1). These dihedral angles do not vary significantly from a *trans* form to a *cis* form of the thiophene rings.

Table S2. Pertinent computed bond lengths (Å), bond angles (°), and dihedral angles (°) for compounds **1a**-**2b**. See Scheme S1 for the atom numbering.

2b Bond lengths	$S_{0toluene}$		
	a	***b***	***c***
S_1-C_1 (Or S_2-C_2)	1.712	1.711	1.711
C_1-C_2	1.434	1.432	1.432
S_1-C_3 (Or S_2-C_4)	1.756	1.756	1.757
S-C_5 (Or S-C_6)	1.765	1.765	1.765
Bond angles			
C_1-S_1-C_3 (Or C_2-S_2-C_4)	90.6	90.6	90.5
C_5-S-C (Or C_6-S-C)	103.2	103.2	130.2
C_7-C_8-C_9	100.2	100.2	100.3
Dihedral angles			
S_1-C_1-C_2-C_9 (Or S_2-C_2-C_1-C_7)	0.02	0.12	0.5
C_3-S_1-C_1-C_2 (Or C_4-S_2-C_2-C_1)	0.05	0.07	0.9
C_{10}-C_5-S-C	90.1	90.2	90.2

1b Bond lengths	$S_{0toluene}$			
	a	***b***	***c***	***d***
S_1-C_1 (Or S_2-C_2)	1.734	1.734	1.733	1.733
C_1-C_2	1.443	1.443	1.445	1.445
S_1-C_3 (Or S_2-C_4)	1.742	1.742	1.742	1.741
S-C_5 (Or S-C_6)	1.766	1.766	1.766	1.766
Bond angles				
C_1-S_1-C_3 (Or C_2-S_2-C_4)	92.0	92.0	91.9	92.0
C_5-S-C (Or C_6-S-C)	103.1	103.2	103.1	103.1
Dihedral angles				
S_1-C_1-C_2-S_2	14	-	-	17.1
S_1-C_1-C_2-C_8 (Or S_2-C_2-C_1-C_7)	-	22.2	20.8	-

C_3-S_1-C_1-C_2 (Or C_4-S_2-C_2-C_1)	0.4	0.1	0.1	0.6
C_9-C_5-S-C	89.9	90	90	90
1a		$S_{0toluene}$		
Bond lengths		***a***	***b***	
S_1-C_1 (Or S_2-C_2)		1.738	1.737	
C_1-C_2		1.443	1.445	
S_1-C_3 (Or S_2-C_4)		1.744	1.743	
C_5-N (Or C_6-N)		1.404	1.404	
Bond angles				
C_1-S_1-C_3 (Or C_2-S_2-C_4)		92.2	92.2	
C_5-N-C (Or C_6-N-C)		120.4	120.4	
Dihedral angles				
S_1-C_1-C_2-S_2		16	-	
S_1-C_1-C_2-C_8 (Or S_2-C_2-C_1-C_7)		-	23.2	
C_3-S_1-C_1-C_2 (Or C_4-S_2-C_2-C_1)		0.5	0.3	
C_9-C_5-N-C		35	35	
2a		$S_{0toluene}$		
Bond lengths		***a***	***b***	
S_1-C_1 (Or S_2-C_2)		1.714	1.714	
C_1-C_2		1.434	1.431	
S_1-C_3 (Or S_2-C_4)		1.758	1.757	
C_5-N (Or C_6-N)		1.405	1.405	
Bond angles				
C_1-S_1-C_3 (Or C_2-S_2-C_4)		90.8	90.7	
C_7-C_8-C_9		100.3	100.1	
C_5-N-C		120.3	120.4	
Dihedral angles				
C_3- S_1-C_1-C_2 (Or C_4- S_2-C_2-C_1)		0.1	3.0	
S_1-C_1-C_2-C_8 (Or S_2-C_2-C_1-C_7)		0.1	2.4	
C_9-C_5-N-C		36.2	36	

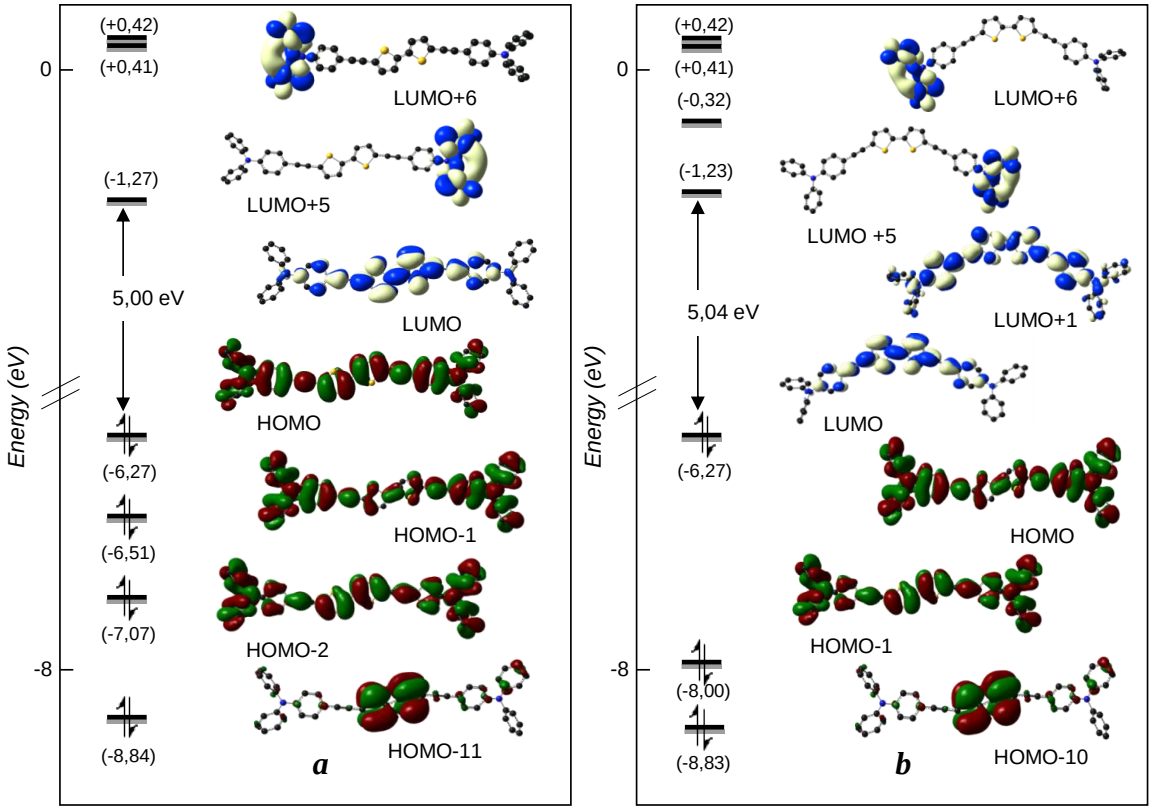


Figure S11. Frontier molecular orbital (MO) diagram of **1a** in toluene. Contour isodensity values are ± 0.02 $(e/bohr^3)^{1/2}$.

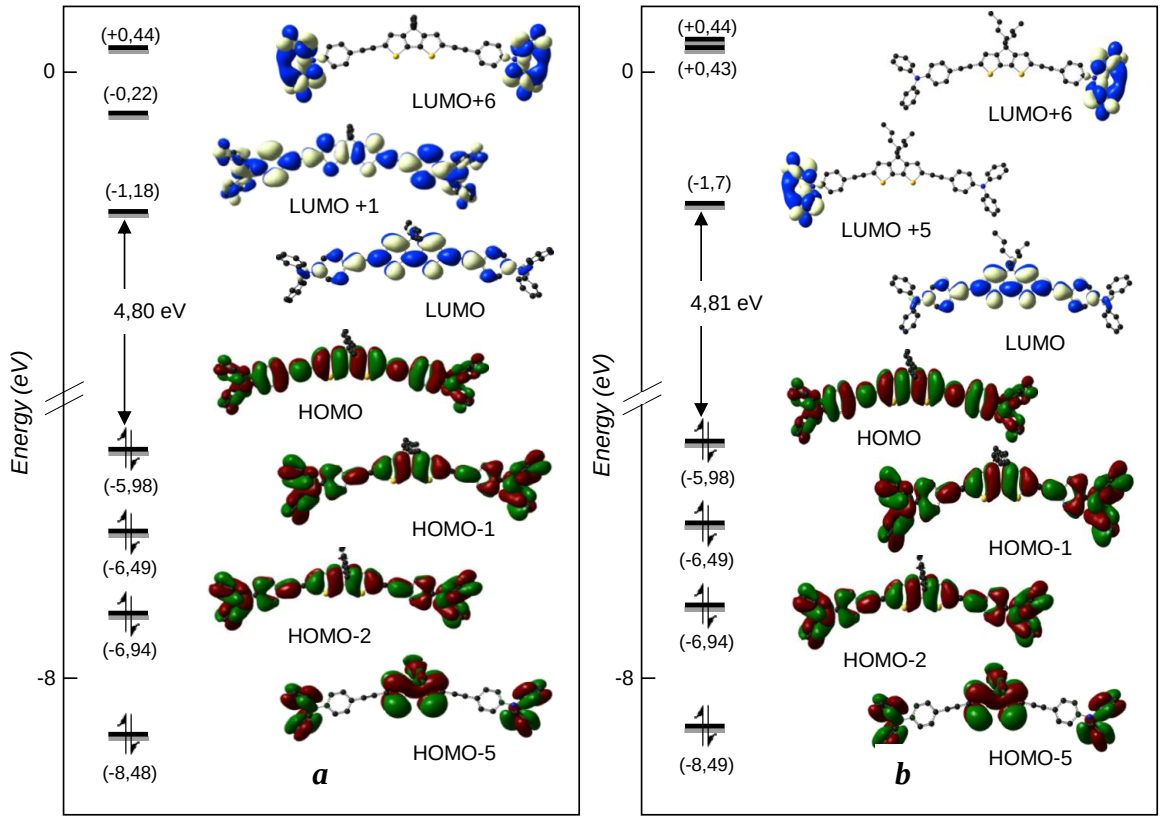


Figure S12. Frontier molecular orbital (MO) diagram of **2a** in toluene. Contour isodensity values are ± 0.02 $(e/bohr^3)^{1/2}$.

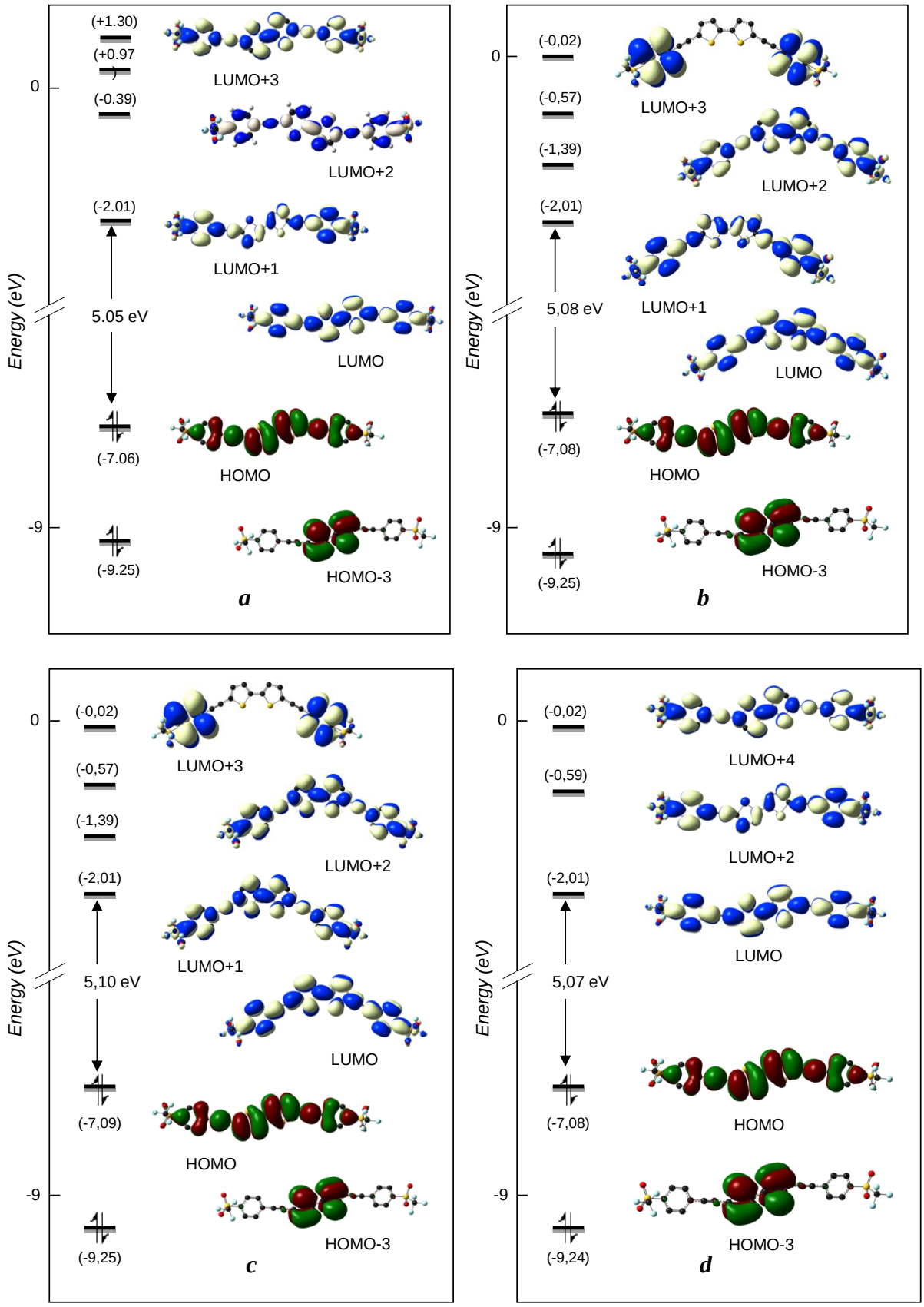


Figure S13. Frontier molecular orbital (MO) diagram of **1b** in toluene. Contour isodensity values are ± 0.02 $(e/bohr^3)^{1/2}$.

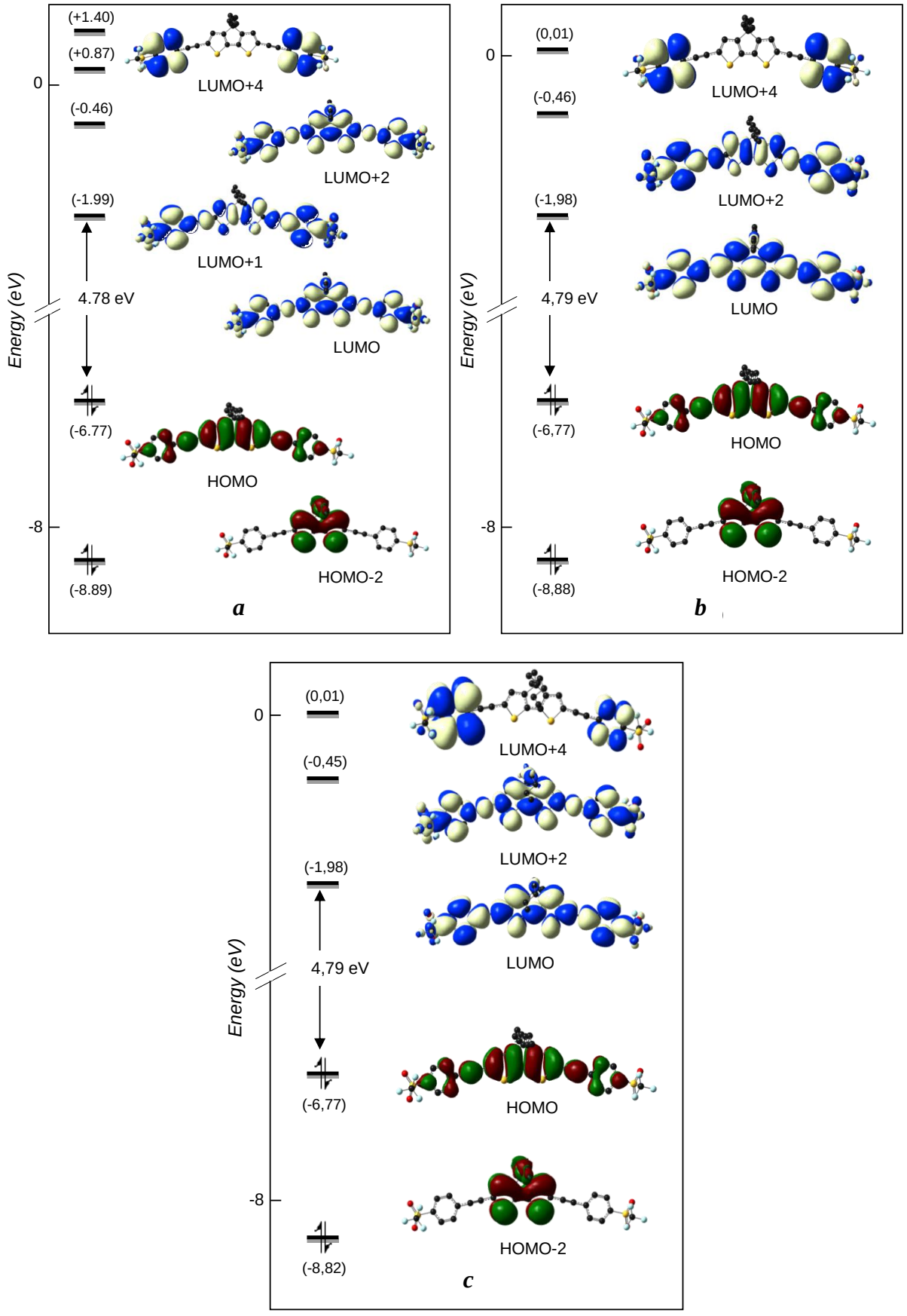


Figure S14. Frontier molecular orbital (MO) diagram of **2b** in toluene. Contour isodensity values are ± 0.02 $(e/bohr^3)^{1/2}$.

4. TD-DFT calculations for 1a,b and 2a,b

Table S3. Experimental and theoretical UV-vis absorption maxima (λ_{max} (nm)) for the most stable form (*a*) of compounds **1a-2b** in toluene.

Compound	λ_{max}^{abs} (nm)		
	PBE0	CAM-B3LYP	Exp
1a	500	433	414
1b	477	426	413
2a	520	454	438
2b	525	455	446

Table S4. CAM-B3LYP calculations for the four lowest-energy electronic transitions of **1a,b,** and **2a,b** in toluene (PCM approach). S_n is the excited state number, E_{0n} is the transition energy (in eV), λ_{calc} is the wavelength (in nm) and f_{0n} is the oscillator strength of the absorption transition.

Molecule	S_n	E_{0n}	λ_{calc}	f_{0n}	Main MO transition percentage
Complex 2b					
a	1	2.86	455	2.40	HOMO → LUMO (90%)
	2	3.64	340	0.11	HOMO → LUMO+1 (72 %)
	3	4.42	281	0.37	HOMO → LUMO+2 (73 %)
	6	4.77	260	0.22	HOMO-2 → LUMO (77 %)
	18	5.42	229	0.22	HOMO → LUMO+4(47 %)
					HOMO-6 → LUMO+1 (28 %)
b	1	2.72	455	2.40	HOMO → LUMO (90%)
	3	4.42	281	0.37	HOMO → LUMO+2 (73 %)
	6	4.77	260	0.22	HOMO-2 → LUMO (77 %)
	18	5.42	229	0.22	HOMO → LUMO+3 (48 %)
c	1	2.73	454	2.38	HOMO → LUMO (90%)
	3	4.41	281	0.38	HOMO → LUMO+2 (72 %)
	6	4.74	262	0.20	HOMO-2 → LUMO (80 %)
	18	5.42	229	0.22	HOMO → LUMO+4 (40 %)
Complex 1b					
a	1	2.74	426	2.44	HOMO → LUMO (89%)
	2	3.74	331	0.003	HOMO → LUMO+1 (65 %)
	4	4.48	277	0.38	HOMO → LUMO+2 (58 %)
	10	4.97	250	0.23	HOMO-1 → LUMO+1 (21 %)
					HOMO-3 → LUMO (33 %)
	18	5.55	223	0.26	HOMO → LUMO+3 (53 %)

	1	2.95	420	2.17	HOMO → LUMO (89%)
	2	3.77	330	0.45	HOMO → LUMO+1 (63 %)
b	4	4.50	275	0.20	HOMO→ LUMO+2 (56 %)
	11	4.98	250	0.21	HOMO-3 → LUMO (73 %)
	18	5.56	222	0.20	HOMO → LUMO+3 (27 %)
	1	2.96	418	2.17	HOMO → LUMO (89%)
	2	3.77	329	0.44	HOMO→ LUMO+1 (63 %)
c	4	4.51	275	0.20	HOMO→ LUMO+2 (55 %)
	11	4.99	249	0.20	HOMO-3 → LUMO (73 %)
	18	5.57	223	0.19	HOMO → LUMO+3 (52 %)
	1	2.93	423	2.44	HOMO → LUMO (89%)
	4	4.49	276	0.37	HOMO → LUMO+2 (58 %)
d	10	4.98	250	0.23	HOMO-3 → LUMO (66 %)
	18	5.56	223	0.26	HOMO → LUMO+4 (40 %)
Complex 1a					
	1	2.88	433	2.89	HOMO → LUMO (79%)
	2	3.50	354	0.008	HOMO-1 → LUMO (48 %)
a	3	3.97	313	0.37	HOMO-2 → LUMO (48 %)
	8	4.33	286	0.54	HOMO-1 → LUMO+6 (26 %)
					HOMO→ LUMO+5 (17 %)
	27	5.26	236	0.23	HOMO-11 → LUMO (42 %)
	1	2.89	429	2.54	HOMO → LUMO (79%)
	2	3.51	352	0.55	HOMO-1 → LUMO (49 %)
					HOMO → LUMO+1 (34 %)
b	8	4.33	286	0.44	HOMO→ LUMO+6 (26 %)
					HOMO-1 → LUMO+5 (22 %)
					HOMO-1 → LUMO+6 (21 %)
	23	5.15	241	0.14	HOMO-10→ LUMO (48 %)
Complex 2a					
	1	2.73	454	2.80	HOMO → LUMO (85%)
	2	3.51	353	0.13	HOMO-1 → LUMO (46 %)
a	3	3.95	314	0.43	HOMO-2 → LUMO (40 %)
	8				HOMO-1 → LUMO+1 (28 %)
		4.31	288	0.55	HOMO-1 → LUMO+6 (42 %)
	20	5.02	248	0.24	HOMO-5→ LUMO (58 %)
	1	2.75	450	2.83	HOMO → LUMO (85%)
b	3	3.96	313	0.40	HOMO-2 → LUMO (40 %)
	8	4.31	288	0.55	HOMO-1 → LUMO+5 (24 %)
					HOMO-1 → LUMO+6(18 %)
	20	5.01	247	0.25	HOMO-5→ LUMO (45 %)

Table S5. Experimental and CAM-B3LYP/6-31+G(d) computed fluorescence wavelengths (λ^{em}, nm) of **1a,b and 2a,b** in toluene.			
Compound	λ^{em} Exp.	Form	$\lambda^{em\text{-}elec}$ Theo.
1a	475 (2.61); 507 (2.45)	***a***	530 (2.34)
		b	535 (2.32)
1b	467 (2.66); 496 (2.50)	***a***	520 (2.38)
		b	520 (2.38)
		c	524 (2.37)
		d	524 (2.37)
2a	485 (2.56); 517 (2.40)	***a***	543 (2.28)
		b	548 (2.26)
2b	496 (2.50); 520 (2.38)	***a***	542 (2.29)
		b	542 (2.29)
		c	540 (2.30)

Table S6. CAM-B3LYP/6-31+G(d) photo-physical properties of the molecules **1a**,**b** and **2a**,**b**, including experimental and computed absorption wavelength (λ^{abs}, nm), fluorescence (vibronic OPE and electronic) wavelengths (λ^{em}, nm), quantum yield (Φ_F), lifetime (τ, ns), and $\Delta\omega$ is the Stokes shift ($\Delta\omega$, cm^{-1}) in toluene.

Cmpd	**Experimental**[a]					**Theoretical**[b]					
	λ_{max}^{abs}	λ_{max}^{em}	$\Delta\omega$	Φ_F	τ	Form	λ_{max}^{abs}	$\lambda_{max}^{em-elec}$	$\lambda_{max}^{em-vibro}$	$\Delta\omega$	τ
1a	414	475, 507	3102	0.35	0.29	***a***	433	530	475, 512	2042	1.54
						b	429	535	478, 515	2389	1.54
1b	413	467, 496	2800	0.28	0.27	***a***	426	520	473, 510	2446	1.68
						b	423	520	470, 498	2364	1.90
						c	418	524	470, 498	2646	1.91
						d	420	524	468, 504	2442	1.69
2a	438	485, 517	2212	0.34	0.56	***a***	454	543	488, 526	1534	1.64
						b	450	548	485, 523	1603	1.60
2b	446	496, 520	2261	0.39	0.80	***a***	455	542	493, 532	1694	1.81
						b	455	542	493, 532	1694	1.82
						c	454	540	501, 541	2066	1.82

[a]Experimental absorption and fluorescence. [b]Theoretical absorption and fluorescence maxima from wavelengths obtained by using CAM-B3LYP/6-31+G(d) calculations in toluene.

5. Vibronic calculations for emissions of 1a,b and 2a,b

As suggested by the structured emissions observed for all compounds, some vibrational modes appear to contribute to the fluorescence decay more than others. The so-called AH approach was used (*vide infra*) to learn more about these particular modes. Note that in order to reach a sufficient spectrum convergence (>90%), normal modes smaller than 100 cm^{-1} were excluded from the vibronic calculations. These are modes that involve deformations of the two thiophene and phenyl rings, appearing at 1466 and 1502 cm^{-1} for **2b**, 726 and 1522 cm^{-1} for **1b**, 1081 and 1529 cm^{-1} for **1a**, and 1464 and 1500 cm^{-1} for **2a** in the S_1 excited state (Figure S15). According to our simulations, a normal mode with such characteristics occurs at ca. 1500 cm^{-1} with a moderate shift vector. It corresponds to a mixture of C-C stretching and C-H bending localized on the bithiophene and phenyl rings, consistent with structural changes in the lowest excited state being mostly located on the thiophene rings in **1a**,**b** and **2a**,**b**, in line with its assignment as a $\pi \rightarrow \pi^*$ transition.

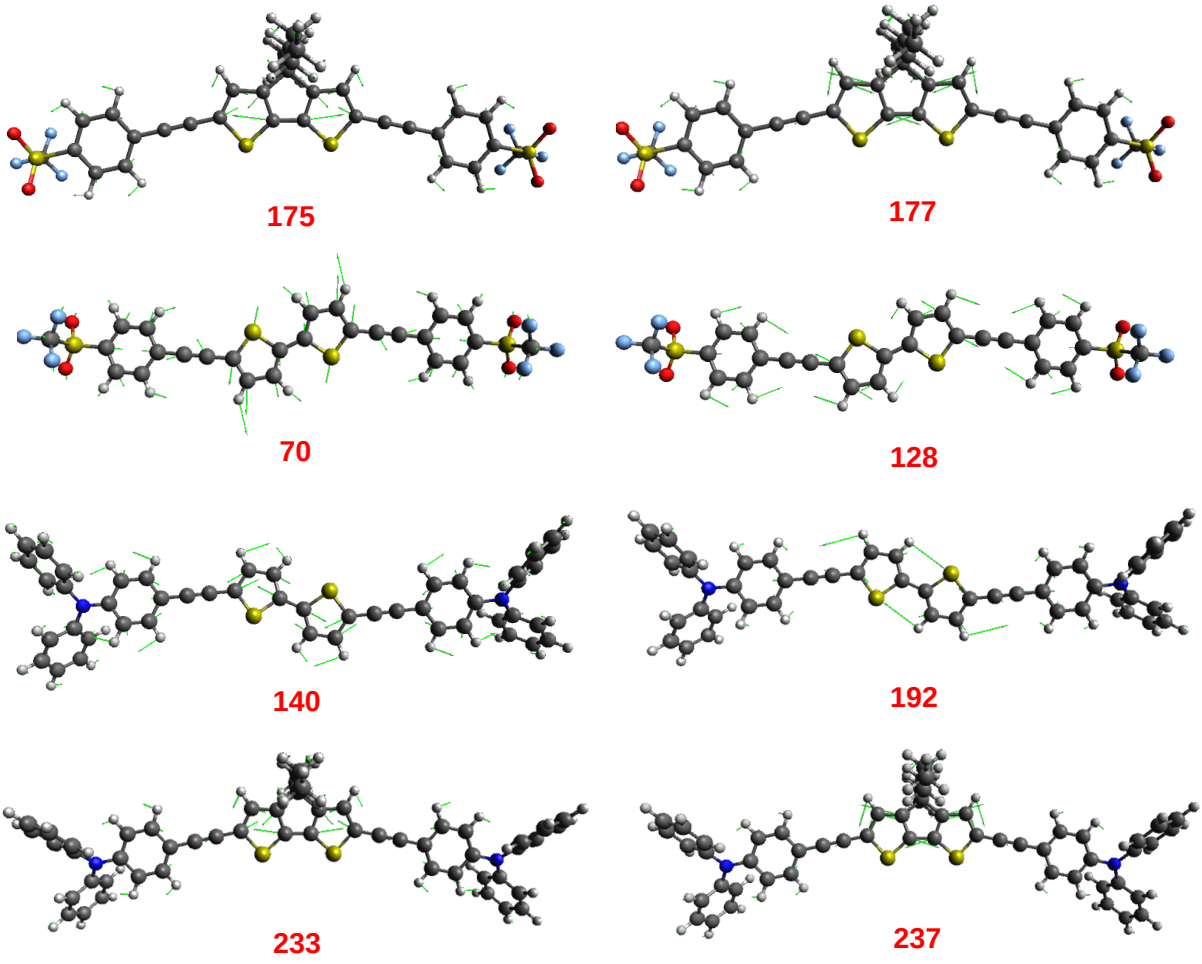


Figure S15. Representation of the normal mode eigenvectors with the largest shift-vectors for **2b, 1b, 1a** and **2a** during the S_1-S_0 transition in toluene, computed at the CAM-B3LYP/6-31+G(d) level in toluene.

6. Calculated spin density in the first triplet (T_1) excited state of 1a,b and 2a,b

The spin distribution was computed for **1a**,**b** and **2a**,**b** to map the localization of unpaired electrons in the T_1 triplet states (Figure S16). For all these molecules, the positive spin density accumulates around the central C=C-S units, adopting a z-shaped distribution in the *trans*-disposed-bithiophene conformers **1a-b** and a u-shaped distribution in **2a**,**b**, while the negative spin density alternates with positive spin density on the π-manifolds of the peripheral phenylethynyl arms. Interestingly, there is no localization of spin density on the butyl groups, the triflate groups, or the diphenylamino-substituted peripheral phenyls. Calculations indicate that within each family (**1a**,**b** or **2a**,**b**), proceeding from the triflate to the diphenylamino-substituted derivative slightly increases the spin density in the π-manifold of the central bithiophene unit and that, for a given terminal substituent, proceeding from a bithiophene-cored to a fused cyclopentadithiophene-cored compound has the same effect. Thus, the maximal spin density in the T_1 state is found for **2b** and decreases in the order: **2b** > **2a** ≈ **1b** > **1a**, while the spin density on the sulfur atom is slightly lower in **2a**,**b** than in **1a**,**b** and is independent of the peripheral substituent.

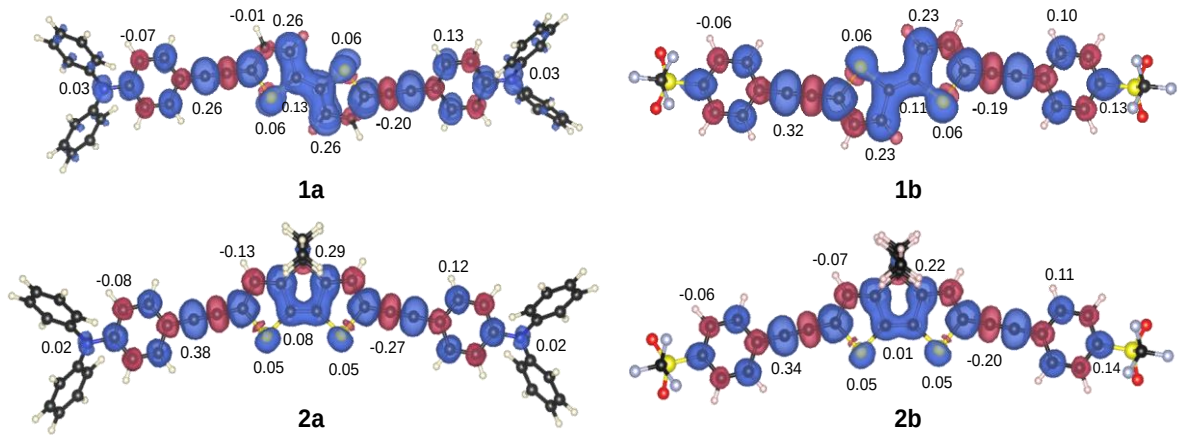


Figure S16. 3D map of the spin density, for structures **1a**,**b** and **2a**,**b** in their first triplet state computed at the CAM-B3LYP/6-31+G(d) level in toluene**.** An iso-surface value of 8×10^{-3} electron.Å^{-2} was used for this plot. The positive and negative electron spin are represented in blue and pink, respectively. The graphics were created using VESTA software.[1]

[1] Momma, K.; Izumi, F., Ref. AB. *J Appl.Cryst.*, **2008**,*41*, 653-658.

7. Calculated one-photon and two-photon absorption using SOAP functionals for 1a,b and 2a,b

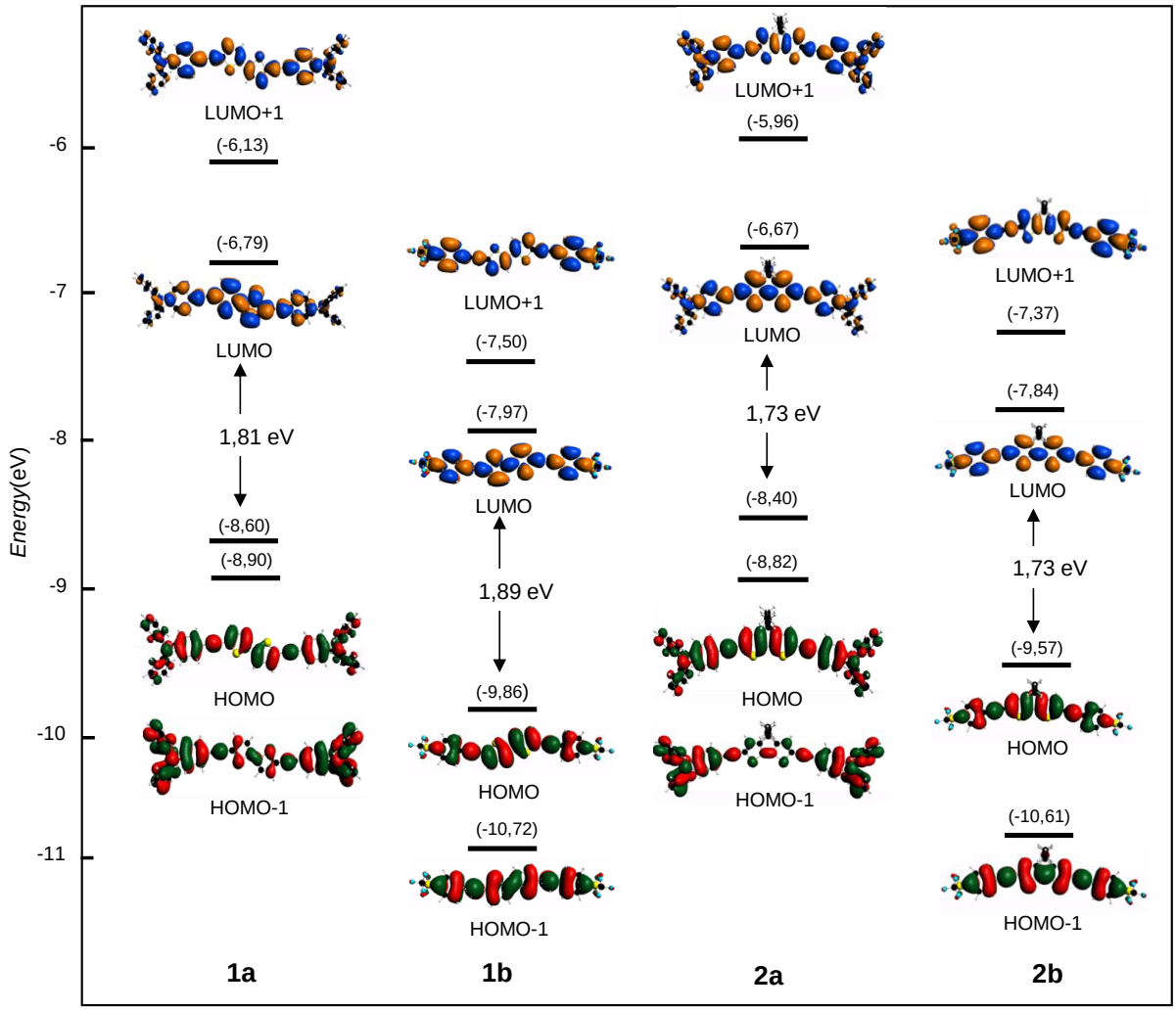


Figure S17. SAOP/DZP frontier MO diagrams for **1a**,**b** and **2a**,**b**. Contour isodensity values: ± 0.02 $(e/bohr^3)^{1/2}$. Hydrogen atoms are omitted for clarity.

Table S7. Theoretical results of OPA wavelenghts (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **1a** (conformer ***a***).

S_n	1	2	3	4	5	6	7	8	9	10
ω^{OPA}	2.07	2.22	2.75	2.78	2.87	2.89	2.90	3.02	3.03	3.22
λ^{OPA}	599	559	451	446	432	429	428	410	409	385
f_{0n}	1.690	$0.350\ 10^{-3}$	0.968	$0.327\ 10^{-2}$	0.175	$0.120\ 10^{-2}$	$0.124\ 10^{-2}$	$0.124\ 10^{-1}$	$0.124\ 10^{-1}$	$0.714\ 10^{-2}$

Main MO transition percentage

S_1 : HOMO → LUMO (92%)

S_2 : HOMO-1 → LUMO (85%)

Table S8. TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **1a** (conformer ***a***) calculated at the SAOP/DZP level of theory.

ω^{TPA}	0.97	1.00	1.03	1.1	1.12	1.18	1.24	1.3	1.4	1.5	1.61	1.68	1.72	1.77
λ^{TPA}	1278	1240	1204	1127	1107	1051	1000	954	886	827	770	740	720	700
σ_2	793	1362	2557	12514	13168	5222	2470	1624	1438	1275	2198	7623	14514	9920

Table S9. Theoretical results of OPA wavelenghts (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **1b** (conformer ***a***).

S_n	1	2	3	4	5	6	7	8	9	10
ω^{OPA}	2.32	2.55	3.28	3.32	3.43	3.45	3.45	3.49	3.62	3.84
λ^{OPA}	534	486	378	446	362	359	359	355	343	323
f_{0n}	1.826	$0.174\ 10^{-3}$	0.439	$0.884\ 10^{-3}$	0.166	$0.698\ 10^{-5}$	$0.893\ 10^{-3}$	$0.785\ 10^{-3}$	$0.142\ 10^{-1}$	$0.259\ 10^{-2}$

Main MO transition percentage

S_1 : HOMO → LUMO (95%)

S_2 : HOMO → LUMO+1 (73%)

Table S10. TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **1b** (conformer ***a***). calculated at the SAOP/DZP level of theory.

ω^{TPA}	1.10	1.12	1.16	1.20	1.24	1.26	1.28	1.30	1.32	1.34	1.37	1.46	1.55	1.67	1.77
λ^{TPA}	1127	1107	1069	1033	1000	984	969	954	939	925	905	850	800	743	700
σ_2	248	334	66	1407	3651	5567	6288	5575	3942	2758	1688	664	412	459	353

Table S11. Theoretical results of OPA wavelenghts (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **2a** (conformer ***a***).

S_n	1	2	3	4	5	6	7	8	9	10
ω^{OPA}	2.07	2.25	2.68	2.76	2.76	2.78	2.88	2.89	2.94	3.28
λ^{OPA}	599	551	463	449	449	446	430	429	422	378
f_{0n}	2.09	$0.41\ 10^{-2}$	0.57	$0.311\ 10^{-4}$	$0.201\ 10^{-2}$	$0.603\ 10^{-1}$	$0.336\ 10^{-1}$	$0.250\ 10^{-1}$	0.178	$0.543\ 10^{-2}$

Main MO transition percentage

S_1 : HOMO → LUMO (91%)

S_2 : HOMO-1 → LUMO (82%)

Table S12. TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **2a** (conformer ***a***) calculated at the SAOP/DZP level of theory.

ω^{TPA}	0.95	0.99	1,03	1,08	1.13	1.18	1,24	1,34	1.45	1.64	1.77
λ^{TPA}	1305	1250	1204	1148	1097	1051	1000	925	855	756	700
σ_2	512	568	1994	6273	15241	7978	3357	2050	1633	5852	14052

Table S13. Theoretical results of OPA wavelenghts (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **2b** (conformer ***a***).

S_n	1	2	3	4	5	6	7	8	9	10
ω^{OPA}	2.21	2.49	3.22	3.27	3.27	3.29	3.39	3.42	3.51	3.81
λ^{OPA}	561	498	385	379	379	377	366	363	353	325
f_{0n}	2.012	$0.124\ 10^{-1}$	0.234	$0.168\ 10^{-2}$	$0.133\ 10^{-3}$	$0.192\ 10^{-1}$	$0.687\ 10^{-1}$	$0.129\ 10^{-1}$	$0.848\ 10^{-1}$	$0.176\ 10^{-2}$

Main MO transition percentage

S_1 : HOMO → LUMO (96%)

S_2 : HOMO → LUMO+1 (77%)

Table S14. TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **2b** (conformer ***a***) calculated at the SAOP/DZP level of theory.

ω^{TPA}	0.99	1.03	1.08	1.1	1.18	1.21	1.24	1.28	1.3	1.37	1.46	1.5	1,63	1.7
λ^{TPA}	1253	1204	1150	1127	1050	1025	1000	969	954	905	849	827	761	729
σ_2	101	159	315	478	1882	3795	6579	4275	2984	1041	480	391	715	855

8. Optimized Cartesian coordinates for 1a,b and 2a,b using PBE1PBE/6-31+G(d) in toluene

1. **Table S15: 1a**

a				***b***			
atom	*x*	*y*	*z*	atom	*x*	*y*	*z*
C	9.112427	0.974545	-0.377462	C	-7.971081	-1.169301	-0.074322
C	7.735439	0.822653	-0.372311	C	-6.756373	-0.514584	0.047974
C	7.138616	-0.355469	0.114241	C	-6.695079	0.889178	0.128818
C	7.980912	-1.372435	0.601270	C	-7.904168	1.608319	0.087828
C	9.357414	-1.216226	0.606918	C	-9.119917	0.953354	-0.022585
C	9.948541	-0.040990	0.114830	C	-9.175570	-0.447531	-0.108532
H	9.551463	1.887408	-0.769311	H	-7.992977	-2.252656	-0.147920
H	7.105270	1.617019	-0.762438	H	-5.834958	-1.089857	0.067003
H	7.541708	-2.286423	0.991178	H	-7.881809	2.692169	0.159086
H	9.987314	-2.009402	0.999014	H	-10.041061	1.528506	-0.039190
C	5.729440	-0.513208	0.113198	C	-5.450740	1.558594	0.248250
C	4.517973	-0.656616	0.115198	C	-4.383279	2.140123	0.350535
C	3.123802	-0.808495	0.112360	C	-3.149279	2.795651	0.471195
S	2.087389	0.440284	-0.525913	S	-1.661318	1.894339	0.581115
C	0.984011	-1.689255	0.401529	C	-1.524032	4.461413	0.633110
C	0.654887	-0.483497	-0.188519	C	-0.710650	3.344555	0.674839
C	-0.979984	1.079520	-1.358259	C	1.548369	4.300098	1.311090
C	-0.651815	0.032010	-0.518421	C	0.728672	3.312636	0.797557
S	-2.085428	-0.670123	0.167897	S	1.670747	1.954938	0.263827
C	-3.120922	0.438126	-0.692670	C	3.163606	2.714179	0.746970
C	-4.515427	0.373633	-0.558593	C	4.393601	2.062046	0.577116
C	-5.727189	0.309395	-0.433052	C	5.457800	1.485908	0.423313
C	-7.136631	0.241283	-0.293784	C	6.698921	0.822810	0.248055
C	-7.978220	1.116119	-1.005954	C	7.908536	1.439406	0.618790
C	-9.355472	1.045594	-0.874328	C	9.120467	0.789194	0.452531
C	-9.947502	0.105065	-0.015226	C	9.173385	-0.499886	-0.102742
C	-9.111405	-0.766218	0.702362	C	7.969316	-1.117076	-0.479722
H	-9.549840	-1.494849	1.377942	C	7.990443	-2.110497	-0.918190
C	-7.734749	-0.703272	0.561175	C	6.756612	-0.471281	-0.302259
H	-9.985393	1.722501	-1.444041	H	10.040249	1.279499	0.757846
H	-7.539197	1.846541	-1.679782	H	7.887322	2.434057	1.055287
H	-7.104458	-1.381871	1.129132	H	5.836261	-0.962714	-0.605179
C	2.371075	-1.873739	0.572134	C	-2.895275	4.154652	0.523319
H	2.821770	-2.757980	1.008842	H	-3.685708	4.894988	0.468101
C	-2.367133	1.309919	-1.457211	C	2.917557	3.967318	1.279177
H	-2.817112	2.081301	-2.072180	H	3.712097	4.608524	1.644523
N	11.343960	0.115051	0.115064	N	-10.407132	-1.111283	-0.225475
N	-11.342782	0.037275	0.123065	N	10.402026	-1.156750	-0.276729
C	12.188209	-0.996115	-0.125397	C	-11.467937	-0.529125	-0.961119
C	11.893182	-1.903657	-1.150479	C	-11.226807	0.069114	-2.204273
C	13.334291	-1.194178	0.654415	C	-12.773869	-0.555091	-0.456499
C	12.725685	-2.994956	-1.380514	C	-12.274074	0.640345	-2.921147
H	11.009949	-1.748947	-1.764393	H	-10.216565	0.083355	-2.604461
C	14.170721	-2.278837	0.406808	C	-13.818312	0.003522	-1.187555
H	13.565919	-0.493324	1.451887	H	-12.964788	-1.016783	0.508496
C	13.870431	-3.188077	-0.607256	C	-13.575667	0.608478	-2.420595

H	12.483552	-3.690668	-2.180142	H	-12.071254	1.100699	-3.884993
H	15.056946	-2.419377	1.020739	H	-14.826925	-0.024449	-0.782619
H	14.522121	-4.037365	-0.793877	H	-14.392210	1.049196	-2.986142
C	-11.983252	-1.209728	0.324610	C	10.494149	-2.559729	-0.107464
C	-13.005162	-1.332348	1.273977	C	11.227676	-3.333427	-1.015248
C	-11.611077	-2.330290	-0.428488	C	9.862567	-3.188350	0.972988
C	-13.645032	-2.554346	1.460092	C	11.329866	-4.710352	-0.839176
H	-13.295602	-0.465597	1.861521	H	11.717736	-2.849752	-1.855894
C	-12.244315	-3.552720	-0.224236	C	9.955744	-4.567814	1.132347
H	-10.824833	-2.237777	-1.172946	H	9.299702	-2.591034	1.685256
C	-13.266588	-3.672428	0.717217	C	10.691789	-5.336954	0.231070
H	-14.436794	-2.633939	2.200920	H	11.902784	-5.297720	-1.552482
H	-11.944604	-4.413640	-0.816717	H	9.460028	-5.041380	1.976167
H	-13.763708	-4.626659	0.869309	H	10.768098	-6.412968	0.362145
C	-12.127467	1.214607	0.061106	C	11.563156	-0.424082	-0.623357
C	-13.322528	1.228102	-0.668510	C	12.783668	-0.696362	0.006756
C	-11.724757	2.374035	0.735621	C	11.508029	0.572757	-1.605600
C	-14.100983	2.380974	-0.716091	C	13.927605	0.013896	-0.345804
H	-13.637830	0.331019	-1.194474	H	12.830325	-1.467803	0.770625
C	-12.500384	3.527730	0.668989	C	12.652865	1.289993	-1.940133
H	-10.802896	2.365685	1.310986	H	10.565273	0.781231	-2.104281
C	-13.693801	3.538440	-0.053040	C	13.869577	1.013774	-1.316415
H	-15.026409	2.375940	-1.286707	H	14.867944	-0.209059	0.152303
H	-12.174767	4.419910	1.198177	H	12.594319	2.060537	-2.704926
H	-14.300504	4.438868	-0.097274	H	14.763056	1.570885	-1.585004
C	11.922167	1.384909	0.356400	C	-10.603566	-2.370844	0.391403
C	11.432318	2.205815	1.379966	C	-10.159160	-2.598895	1.699798
C	12.998340	1.830049	-0.421133	C	-11.255114	-3.400329	-0.298789
C	12.003718	3.453687	1.610680	C	-10.354635	-3.839662	2.299204
H	10.603307	1.861016	1.992160	H	-9.661022	-1.800179	2.242795
C	13.575032	3.072273	-0.172755	C	-11.461620	-4.632876	0.313998
H	13.380309	1.197055	-1.217504	H	-11.599859	-3.227876	-1.314773
C	13.079718	3.893670	0.839769	C	-11.009369	-4.862605	1.613203
H	11.612446	4.079433	2.409050	H	-10.004137	-4.001520	3.315567
H	14.409979	3.404110	-0.784965	H	-11.969016	-5.422501	-0.234711
H	13.527996	4.865686	1.026958	H	-11.166350	-5.828050	2.086581
H	0.241691	-2.428531	0.685960	H	-1.133026	5.473134	0.654998
H	-0.236748	1.653679	-1.902692	H	1.163145	5.226870	1.722961

2. **Table S16: 1b**

a				***b***			
atom	*x*	*y*	*z*	atom*x*	*y*	*z*	
C	9.093841	-1.044371	-0.574695	C	8.012712	-1.358645	-0.886167
C	7.716321	-0.913160	-0.496435	C	6.787662	-0.729096	-0.731178
C	7.129650	0.358020	-0.339994	C	6.720860	0.585821	-0.230143
C	7.953347	1.498532	-0.267003	C	7.910125	1.260884	0.108381
C	9.331491	1.373769	-0.344836	C	9.138110	0.636985	-0.045013
C	9.887176	0.101827	-0.495746	C	9.175596	-0.668560	-0.538584
H	9.552594	-2.019337	-0.707571	H	8.072703	-2.367605	-1.282516

H	7.081234	-1.791016	-0.561044	H	5.872091	-1.246191	-1.000393
H	7.500877	2.478746	-0.154954	H	7.859429	2.277234	0.485911
H	9.972017	2.249322	-0.301959	H	10.059488	1.155491	0.201828
C	5.720772	0.488651	-0.263140	C	5.466958	1.227062	-0.073197
C	4.509620	0.608585	-0.195673	C	4.392328	1.785054	0.066666
C	3.116319	0.733347	-0.121514	C	3.152163	2.417796	0.221729
C	2.366885	1.885890	0.037169	C	2.892798	3.683466	0.718896
S	2.082461	-0.663656	-0.234493	S	1.672297	1.620964	-0.232838
C	0.981567	1.642088	0.075950	C	1.521380	3.996834	0.745461
C	0.654522	0.303744	-0.052954	C	0.716872	2.979166	0.263652
C	-0.654521	-0.303800	-0.053123	C	-1.548270	4.098733	0.094894
C	-3.116324	-0.733355	-0.121905	C	-0.723535	2.988776	0.148123
C	-4.509618	-0.608503	-0.196006	S	-1.652037	1.527166	0.074459
C	-5.720763	-0.488471	-0.263442	C	-2.913525	3.774564	-0.008653
C	-7.129633	-0.357719	-0.340226	C	-3.147829	2.410624	-0.042579
C	-7.716216	0.913593	-0.495902	C	-4.375123	1.744071	-0.151748
C	-9.093732	1.044948	-0.574065	C	-5.437824	1.154540	-0.245911
C	-9.887143	-0.101242	-0.495824	C	-6.677362	0.476799	-0.356858
C	-9.331543	-1.373317	-0.345698	C	-7.881054	1.205533	-0.424523
H	-9.972112	-2.248865	-0.303380	C	-9.094655	0.545489	-0.535791
C	-7.953411	-1.498220	-0.267921	C	-9.103160	-0.849991	-0.579281
H	-9.552432	2.020022	-0.706322	C	-7.924753	-1.596378	-0.518312
H	-7.081071	1.791446	-0.559984	H	-7.959817	-2.680241	-0.570177
H	-7.501007	-2.478531	-0.156456	C	-6.714265	-0.930587	-0.406776
S	11.642953	-0.061139	-0.596595	H	-10.025344	1.100668	-0.600996
O	11.983879	-1.322539	-1.244855	H	-7.852018	2.290094	-0.394540
O	12.232571	1.209223	-1.004171	H	-5.786350	-1.491975	-0.363146
O	-11.983697	1.324105	-1.243435	S	10.738687	-1.467609	-0.732061
O	-12.232594	-1.207916	-1.005664	O	10.617192	-2.561895	-1.688766
S	-11.642905	0.061936	-0.596601	O	11.795595	-0.466396	-0.822608
C	-12.153541	0.280678	1.194490	O	-11.654442	-0.789376	-1.266471
C	12.153473	-0.281909	1.194287	O	-10.430147	-3.032383	-1.259909
F	-13.472205	0.417469	1.246734	S	-10.648035	-1.694144	-0.722141
F	-11.576267	1.364938	1.706884	C	-11.153290	-1.964845	1.063376
F	-11.791088	-0.782511	1.908359	C	10.999698	-2.299847	0.928145
F	11.576303	-1.366852	1.705358	F	-12.317885	-2.600240	1.083165
F	11.790816	0.780388	1.909372	F	-11.277176	-0.796071	1.687887
F	13.472151	-0.418586	1.246487	F	-10.238826	-2.698657	1.693076
H	2.819520	2.866845	0.128225	F	10.017830	-3.165870	1.167062
H	0.239129	2.422220	0.210798	F	11.021803	-1.390080	1.899393
S	-2.082460	0.663714	-0.234066	F	12.159070	-2.944499	0.902273
C	-0.981571	-1.642217	0.074983	H	-3.713728	4.503576	-0.071016
C	-2.366889	-1.885997	0.036071	H	3.679910	4.346085	1.061007
H	-0.239133	-2.422430	0.209359	H	1.123484	4.929691	1.129793
H	-2.819521	-2.867006	0.126558	H	-1.169045	5.114780	0.104195

c				***d***			
atom	*x*	*y*	*z*	atom	*x*	*y*	*z*
C	7.976411	-1.657948	0.255427	C	-9.097330	-1.070243	-0.532264
C	6.758647	-0.997891	0.206255	C	-7.718666	-0.930734	-0.505072
C	6.684423	0.381448	0.482820	C	-7.133666	0.347977	-0.420745
C	7.857713	1.086976	0.814750	C	-7.960351	1.487417	-0.367129
C	9.078307	0.432450	0.865923	C	-9.339658	1.354403	-0.394385

C	9.124442	-0.933936	0.582860	C	-9.893488	0.075233	-0.474458
H	8.039689	-2.723095	0.055024	H	-9.555269	-2.051562	-0.609561
H	5.853439	-1.543300	-0.041241	H	-7.081616	-1.808158	-0.554218
H	7.799394	2.147896	1.036332	H	-7.509480	2.473112	-0.310341
H	9.984770	0.966757	1.133344	H	-9.982792	2.228668	-0.366608
C	5.437501	1.052982	0.433153	C	-5.723637	0.486892	-0.397009
C	4.368558	1.637257	0.392186	C	-4.511517	0.614090	-0.378321
C	3.134497	2.298444	0.340967	C	-3.117103	0.747335	-0.356806
C	2.868851	3.636133	0.578260	C	-2.369249	1.909380	-0.282096
S	1.672453	1.443810	-0.063742	S	-2.079930	-0.650110	-0.424669
C	1.505546	3.960360	0.450056	C	-0.981801	1.674036	-0.290752
C	0.714554	2.877962	0.107709	C	-0.652227	0.332733	-0.371468
C	-1.505590	3.960574	-0.449397	C	0.659767	-0.267852	-0.410432
C	-0.714588	2.878013	-0.107592	C	3.115083	-0.713680	-0.267926
S	-1.672465	1.443749	0.063062	C	4.499239	-0.615203	-0.075617
C	-2.868907	3.636417	-0.577673	C	5.702377	-0.521107	0.095766
C	-3.134569	2.298642	-0.340896	C	7.102602	-0.421295	0.289242
C	-4.368646	1.637493	-0.392218	C	7.669576	0.777218	0.765210
C	-5.437608	1.053257	-0.433248	C	9.038701	0.877300	0.956196
C	-6.684532	0.381725	-0.482884	C	9.843279	-0.227119	0.669414
C	-7.857891	1.087328	-0.814403	C	9.306778	-1.428268	0.201574
C	-9.078485	0.432796	-0.865554	H	9.954728	-2.276285	0.002103
C	-9.124544	-0.933678	-0.582910	S	7.937042	-1.522061	0.012295
C	-7.976441	-1.657765	-0.255887	H	9.481734	1.793516	1.334374
H	-8.039656	-2.722979	-0.055813	H	7.025741	1.622469	0.986977
C	-6.758686	-0.997696	-0.206705	H	7.498949	-2.448187	-0.346154
H	-9.985007	0.967162	-1.132658	S	-11.650775	-0.098865	-0.510365
H	-7.799630	2.148314	-1.035691	O	-12.260270	1.149587	-0.954794
H	-5.853428	-1.543164	0.040476	O	-12.005396	-1.389403	-1.090361
S	10.678380	-1.771007	0.645548	O	11.880507	0.983090	1.839756
O	10.459979	-3.201077	0.831940	O	12.160139	-1.436181	1.065607
O	11.613903	-1.011388	1.467431	S	11.588447	-0.103153	0.911114
O	-11.614190	-1.010774	-1.466954	C	12.207405	0.500074	-0.753156
O	-10.460109	-3.200735	-0.832710	C	-12.102487	-0.240668	1.304215
S	-10.678479	-1.770752	-0.645618	F	13.526203	0.632508	-0.692971
S	-11.323468	-1.602938	1.107285	F	11.658400	1.675751	-1.048987
F	-12.503608	-2.204254	1.184960	F	11.894349	-0.376633	-1.704380
F	-11.460855	-0.317764	1.424915	F	-11.720257	0.853124	1.959133
F	-10.479434	-2.173791	1.963403	F	-11.505992	-1.300729	1.844291
C	11.323754	-1.602391	-1.107133	F	-13.418397	-0.376905	1.404721
F	11.461349	-0.317083	-1.424115	H	-2.824086	2.892293	-0.232594
F	12.503846	-2.203800	-1.184852	H	-0.238703	2.464479	-0.259873
F	10.479830	-2.172738	-1.963696	S	2.061392	0.629357	0.077147
H	3.644578	4.343911	0.848382	C	1.008065	-1.547596	-0.804357
H	-3.644649	4.344341	-0.847373	C	2.390115	-1.800476	-0.724576
H	-1.101450	4.951134	-0.627656	H	0.284585	-2.274005	-1.160378
H	1.101396	4.950832	0.628781	H	2.858376	-2.739513	-0.997349

3. **Table S17: 2a**

a				***b***			
atom	*x*	*y*	*z*	atom	*x*	*y*	*z*
C	8.945253	1.648760	-0.825534	C	-8.916663	-2.067657	-0.383965
C	7.590234	1.397585	-0.682180	C	-7.565053	-1.771036	-0.314385
C	7.133089	0.203458	-0.093390	C	-7.123423	-0.459271	-0.057876
C	8.093305	-0.724824	0.351471	C	-8.095553	0.540740	0.132957
C	9.448336	-0.468076	0.219206	C	-9.447178	0.241570	0.075987
C	9.898898	0.721884	-0.374726	C	-9.882243	-1.067343	-0.187169
H	9.274643	2.571489	-1.294414	H	-9.234037	-3.084590	-0.595878
H	6.867459	2.124491	-1.042085	H	-6.832844	-2.557499	-0.474636
H	7.764082	-1.648984	0.818264	H	-7.778357	1.558536	0.342332
H	10.171316	-1.193515	0.580884	H	-10.179528	1.027051	0.238745
C	5.746667	-0.057427	0.046761	C	-5.740183	-0.154877	0.005260
C	4.554923	-0.290804	0.170817	C	-4.550708	0.113791	0.059313
C	3.184302	-0.548391	0.305648	C	-3.181600	0.406052	0.118878
S	2.001099	0.613458	-0.278769	S	-1.992472	-0.858423	-0.154750
C	1.165837	-1.571970	0.826426	C	-1.167363	1.550036	0.329683
C	0.716980	-0.399886	0.235109	C	-0.715901	0.263428	0.068510
C	-0.000015	-2.440610	1.265467	C	1.167825	1.535908	0.389501
C	-1.165843	-1.571929	0.826452	C	0.714706	0.254779	0.105040
C	-0.716956	-0.399859	0.235130	S	1.989730	-0.861870	-0.151007
S	-2.001050	0.613558	-0.278671	C	3.180468	0.403497	0.111027
C	-3.184283	-0.548257	0.305750	C	4.549313	0.112756	0.039145
C	-4.554901	-0.290629	0.170948	C	5.738789	-0.152221	-0.030720
C	-5.746644	-0.057216	0.046945	C	7.122205	-0.451713	-0.111221
C	-7.133069	0.203644	-0.093210	C	8.093000	0.550260	0.076126
C	-7.590242	1.397598	-0.682327	C	9.444907	0.256335	0.001281
C	-8.945269	1.648723	-0.825710	C	9.881375	-1.049068	-0.276422
C	-9.898895	0.721966	-0.374609	C	8.917101	-2.051341	-0.469475
C	-9.448305	-0.467821	0.219650	H	9.235607	-3.065562	-0.692434
H	-10.171267	-1.193168	0.581548	C	7.565335	-1.759962	-0.382622
C	-8.093267	-0.724517	0.351950	H	10.176403	1.043172	0.161336
H	-9.274680	2.571309	-1.294856	H	7.774701	1.565360	0.296621
H	-6.867484	2.124399	-1.042482	H	6.834043	-2.547715	-0.540711
H	-7.764021	-1.648546	0.818987	C	-2.571822	1.628560	0.370870
C	-0.000006	-2.676252	2.793633	C	2.572387	1.623054	0.380775
C	0.000050	-1.423184	3.662877	H	3.155948	2.520450	0.554129
H	0.879436	-3.289834	3.037610	N	-11.253117	-1.368991	-0.252321
H	-0.879486	-3.289773	3.037629	N	11.252501	-1.345430	-0.359502
C	0.000020	-1.747077	5.154816	C	-12.163830	-0.437353	-0.805937
H	0.879696	-0.808738	3.426073	C	-11.847684	0.251683	-1.983721
C	0.000096	-0.499854	6.031413	C	-13.396829	-0.200183	-0.185641
H	-0.878955	-2.363307	5.393510	C	-12.746222	1.168286	-2.521656
H	0.878912	-2.363421	5.393520	H	-10.895970	0.064830	-2.473839
H	0.000071	-0.757666	7.096779	C	-14.296806	0.705683	-0.739492
H	0.884923	0.119035	5.837669	H	-13.645488	-0.730786	0.729468
H	-0.884644	0.119153	5.837655	C	-13.976802	1.398881	-1.906726
C	-0.000036	-3.810467	0.548428	H	-12.486316	1.694781	-3.436725
C	-0.000068	-3.766614	-0.975998	H	-15.250073	0.878818	-0.246123
C	-0.000131	-5.159857	-1.600241	H	-14.679056	2.110080	-2.333172
C	-0.000157	-5.125852	-3.124317	C	11.745021	-2.585980	0.111880

H	0.878787	-5.717594	-1.245633	C	12.697120	-3.296432	-0.629812
H	-0.879077	-5.717531	-1.245600	C	11.293098	-3.114198	1.327866
H	-0.000202	-6.136496	-3.548679	C	13.190067	-4.509479	-0.157791
H	-0.884926	-4.602683	-3.507645	H	13.048848	-2.891884	-1.575012
H	0.884639	-4.602749	-3.507675	C	11.778656	-4.335989	1.784351
H	-0.879527	-0.808645	3.426057	H	10.560702	-2.562998	1.911531
H	-0.879640	-3.211324	-1.330152	C	12.731825	-5.039609	1.048122
H	0.879532	-3.211393	-1.330189	H	13.928733	-5.049089	-0.745400
H	-0.879566	-4.370850	0.897470	H	11.417995	-4.732637	2.730221
H	0.879508	-4.370852	0.897430	H	13.113899	-5.990060	1.410701
C	2.567290	-1.659442	0.868138	C	12.153208	-0.407099	-0.918103
H	3.139481	-2.482830	1.282805	C	13.392672	-0.169102	-0.311131
C	-2.567299	-1.659344	0.868204	C	11.820424	0.288086	-2.087672
H	-3.139511	-2.482715	1.282877	C	14.282542	0.743654	-0.869982
N	11.273248	0.978867	-0.514771	H	13.654288	-0.704427	0.597591
N	-11.273249	0.978879	-0.514730	C	12.709001	1.211482	-2.630507
C	12.170927	-0.076638	-0.804733	H	10.863621	0.100685	-2.567567
C	11.844547	-1.043492	-1.764166	C	13.945983	1.442947	-2.028894
C	13.400822	-0.161355	-0.140299	H	15.240997	0.917344	-0.386964
C	12.729774	-2.080645	-2.042710	H	12.436154	1.742713	-3.539049
H	10.895286	-0.977336	-2.288979	H	14.640391	2.159503	-2.459203
C	14.287721	-1.192207	-0.437109	C	-11.735666	-2.608810	0.231252
H	13.657399	0.585200	0.606433	C	-11.268718	-3.128437	1.445253
C	13.957337	-2.160395	-1.385126	C	-12.692843	-3.327033	-0.496262
H	12.462030	-2.823185	-2.790401	C	-11.744605	-4.349511	1.913675
H	15.238727	-1.244264	0.087270	H	-10.532281	-2.571141	2.017947
H	14.649301	-2.967533	-1.609945	C	-13.175986	-4.539317	-0.012294
C	-12.170894	-0.076724	-0.804428	H	-13.056210	-2.929104	-1.439866
C	-13.400826	-0.161275	-0.140045	C	-12.702816	-5.060894	1.191582
C	-11.844432	-1.043849	-1.763560	H	-11.372321	-4.739473	2.857818
C	-14.287684	-1.192231	-0.436613	H	-13.918764	-5.085069	-0.588941
H	-13.657466	0.585493	0.606453	H	-13.077248	-6.010768	1.563528
C	-12.729617	-2.081103	-2.041858	C	0.000760	2.499351	0.562800
H	-10.895141	-0.977823	-2.288334	C	0.097143	3.598986	-0.522264
C	-13.957220	-2.160688	-1.384329	C	-1.011631	4.646244	-0.529226
H	-15.238721	-1.244156	0.087722	H	0.129489	3.099896	-1.500218
H	-12.461810	-2.823853	-2.789318	H	1.066134	4.104344	-0.408968
H	-14.649153	-2.967907	-1.608958	C	-0.818133	5.682742	-1.634167
C	-11.772912	2.295076	-0.367332	H	-1.986172	4.158575	-0.666753
C	-12.740037	2.787333	-1.252600	H	-1.054529	5.163542	0.439780
C	-11.313303	3.117784	0.668930	C	-1.918754	6.737075	-1.659123
C	-13.239883	4.077047	-1.097445	H	0.157767	6.172391	-1.504623
H	-13.098003	2.153661	-2.059508	H	-0.776421	5.171186	-2.606129
C	-11.805891	4.412100	0.806632	H	-1.755702	7.467842	-2.459476
H	-10.569350	2.737834	1.363957	H	-2.901994	6.278612	-1.822259
C	-12.773851	4.899190	-0.071675	H	-1.962810	7.286464	-0.710375
H	-13.990265	4.444753	-1.793007	C	-0.094826	3.064079	2.000724
H	-11.438989	5.038324	1.616141	C	1.015292	4.017225	2.431068
H	-13.161283	5.907968	0.042634	H	-0.127758	2.211212	2.692137
C	11.772889	2.295027	-0.366986	H	-1.063452	3.572729	2.102297
C	11.313175	3.117471	0.669439	C	0.824552	4.515992	3.862002
C	12.740073	2.787526	-1.252055	H	1.989206	3.514725	2.357130
C	11.805719	4.411765	0.807498	H	1.058165	4.883474	1.755656
H	10.569173	2.737335	1.364310	C	1.926512	5.468849	4.310704
C	13.239878	4.077212	-1.096540	H	-0.150930	5.016619	3.944108

H	13.098113	2.154066	-2.059096	H	0.783600	3.653981	4.542733
C	12.773741	4.899094	-0.070608	H	1.765649	5.811894	5.339108
H	11.438733	5.037782	1.617128	H	2.909434	4.983143	4.271776
H	13.990306	4.445107	-1.791953	H	1.969762	6.356032	3.666553
H	13.161137	5.907854	0.043980	H	-3.153778	2.519898	0.577683

4. Table S18: 2b

a				**b**			
atom	*x*	*y*	*z*	atom	*x*	*y*	*z*
C	8.915369	-1.626435	-1.326036	C	-8.891497	-2.078442	-0.554665
C	7.560929	-1.372107	-1.181509	C	-7.540661	-1.782168	-0.467845
C	7.120075	-0.217028	-0.504755	C	-7.104203	-0.442205	-0.443699
C	8.069481	0.682200	0.021288	C	-8.054027	0.596890	-0.512612
C	9.425118	0.433146	-0.120085	C	-9.406046	0.306762	-0.599972
C	9.834444	-0.721203	-0.791119	C	-9.811385	-1.029554	-0.617963
H	9.261356	-2.508171	-1.856657	H	-9.233416	-3.108430	-0.585672
H	6.830844	-2.060851	-1.594685	H	-6.809620	-2.583282	-0.423338
H	7.731270	1.576457	0.535129	H	-7.718392	1.629038	-0.502451
H	10.161593	1.127423	0.272762	H	-10.141797	1.102422	-0.665842
C	5.735680	0.040670	-0.359598	C	-5.723290	-0.142835	-0.357455
C	4.544322	0.269898	-0.229812	C	-4.534663	0.122608	-0.283783
C	3.175597	0.520297	-0.087673	C	-3.168845	0.411965	-0.198962
C	2.563005	1.604497	0.532382	C	-2.558468	1.661529	-0.161838
S	1.994395	-0.607448	-0.733814	S	-1.989067	-0.886975	-0.124056
C	1.164109	1.522677	0.484943	C	-1.162013	1.568061	-0.074331
C	0.716286	0.380905	-0.168715	C	-0.714724	0.252598	-0.045249
C	0.000039	2.368442	0.968585	C	0.000014	2.542397	-0.000090
C	-1.164043	1.522567	0.485166	C	1.162045	1.568074	0.074269
C	-0.716243	0.380857	-0.168615	C	0.714757	0.252606	0.045436
S	-1.994374	-0.607511	-0.733651	S	1.989104	-0.886950	0.124425
C	-2.562935	1.604250	0.532892	C	2.558501	1.661562	0.161731
C	-3.175552	0.520078	-0.087182	C	3.168880	0.412005	0.199085
C	-4.544289	0.269396	-0.228709	C	4.534701	0.122668	0.283925
C	-5.735719	0.040494	-0.358424	C	5.723332	-0.142763	0.357565
C	-7.120103	-0.217014	-0.504032	C	7.104249	-0.442125	0.443765
C	-8.069541	0.682061	0.022218	C	8.054077	0.596979	0.512483
C	-9.425169	0.433094	-0.119389	C	9.406100	0.306862	0.599812
C	-9.834454	-0.721017	-0.790857	C	9.811438	-1.029453	0.617974
C	-8.915346	-1.626090	-1.325987	C	8.891545	-2.078349	0.554880
H	-9.261302	-2.507650	-1.856923	H	9.233464	-3.108332	0.586025
C	-7.560915	-1.371850	-1.181227	C	7.540705	-1.782086	0.468092
H	-10.161669	1.127244	0.273638	H	10.141858	1.102527	0.665523
H	-7.731357	1.576102	0.536453	H	7.718442	1.629126	0.502192
H	-6.830803	-2.060498	-1.594514	H	6.809658	-2.583203	0.423747
S	11.560467	-1.043330	-0.968547	S	-11.532914	-1.402477	-0.727487
O	11.779887	-1.960561	-2.081413	O	-11.712705	-2.759685	-1.231102
O	12.311264	0.199000	-0.823079	O	-12.249914	-0.262209	-1.287787
O	-12.311273	0.199199	-0.822600	O	12.250005	-0.262006	1.287541

O	-11.779822	-1.959864	-2.081757	O	11.712800	-2.759490	1.231264
S	-11.560467	-1.043074	-0.968515	S	11.532974	-1.402359	0.727453
C	-11.969222	-2.038201	0.567351	C	12.069337	-1.476882	-1.067827
F	11.969137	-2.037855	0.567729	F	13.365607	-1.757007	-1.113141
F	-13.260870	-2.341548	0.546495	F	11.849822	-0.306068	-1.661846
F	-11.700465	-1.326913	1.659952	F	11.390324	-2.423654	-1.711244
C	-11.252821	-3.159592	0.592944	C	-0.081804	3.441311	1.255924
C	11.252647	-3.159181	0.593779	C	-0.166125	2.715719	2.594761
H	11.700434	-1.326097	1.660037	H	-0.956611	4.097129	1.139798
H	13.260761	-2.341311	0.546996	H	0.797880	4.100715	1.252052
C	-0.000111	3.773255	0.321419	C	-0.244377	3.679709	3.776149
H	-0.000326	3.808365	-1.203362	H	-1.046740	2.058453	2.606097
C	0.879180	4.314504	0.699258	C	-0.328546	2.963946	5.119374
H	-0.879341	4.314432	0.699501	H	0.635161	4.339468	3.766135
H	-0.000486	5.232684	-1.753190	H	-1.118868	4.334888	3.653659
H	0.879302	3.273173	-1.587292	H	-0.383721	3.676263	5.950387
H	-0.000730	5.278828	-3.276839	H	-1.216789	2.322215	5.170525
H	-0.879291	5.770595	-1.369335	H	0.549393	2.327070	5.283741
C	0.878383	5.770687	-1.369610	C	0.081814	3.441263	-1.256103
C	-0.000833	6.310454	-3.646649	C	0.166023	2.715602	-2.594915
C	0.884114	4.777260	-3.687743	C	0.244218	3.679513	-3.776367
C	-0.885660	4.777183	-3.687461	C	0.328286	2.963661	-5.119551
H	0.000191	2.524139	2.507499	H	-0.635305	4.339291	-3.766339
H	0.000413	1.228233	3.311768	H	1.118730	4.334682	-3.653977
H	0.000502	1.477075	4.818149	H	0.383412	3.675923	-5.950614
H	0.000751	0.187496	5.630997	H	1.216517	2.321915	-5.170721
H	0.879238	2.080766	5.087143	H	-0.549673	2.326785	-5.283815
H	-0.878360	2.080518	5.087286	H	0.708898	2.062668	2.719011
H	0.000806	0.392303	6.707607	H	1.046618	2.058308	-2.606266
H	-0.884072	-0.421139	5.407295	H	-0.709027	2.062565	-2.719060
H	0.885715	-0.420883	5.407156	H	0.956660	4.097044	-1.140055
H	-0.880003	3.273076	-1.587044	H	-0.797835	4.100713	-1.252217
C	-0.879179	0.625788	3.045367	C	-12.069379	-1.476730	1.067773
F	0.880113	0.626006	3.045228	F	-11.849916	-0.305820	1.661623
F	-0.879069	3.124585	2.781865	F	-13.365646	-1.756871	1.113058
F	0.879387	3.124765	2.781676	F	-11.390388	-2.423391	1.711377
H	-3.136959	2.403023	0.990537	H	-3.132995	2.581197	-0.198539
H	3.137046	2.403403	0.989772	H	3.133026	2.581238	0.198259

c

atom	*x*	*y*	*z*
C	-8.888470	1.956333	0.584058
C	-7.538165	1.659564	0.490894
C	-7.102463	0.319449	0.463073
C	-8.052408	-0.719321	0.534771
C	-9.403902	-0.428716	0.628484
C	-9.808512	0.907762	0.650093
H	-9.229822	2.986422	0.617837
H	-6.806949	2.460395	0.444219
H	-7.717258	-1.751592	0.521760
H	-10.139714	-1.224135	0.696487

C	-5.722045	0.019522	0.370592
C	-4.533882	-0.246469	0.292495
C	-3.168392	-0.536334	0.202497
C	-1.988596	0.763122	0.125404
S	-1.162022	-1.692193	0.072181
C	-0.714112	-0.376596	0.051132
C	-0.000034	-2.664732	-0.002729
C	1.161960	-1.692024	-0.075268
C	0.714068	-0.376478	-0.050924
C	1.988564	0.763403	-0.122425
S	3.168337	-0.535873	-0.202846
C	4.533815	-0.245792	-0.292342
C	5.721959	0.020394	-0.370069
C	7.102338	0.320626	-0.462122
C	8.052293	-0.717891	-0.537297
C	9.403742	-0.426953	-0.630682
C	9.808293	0.909598	-0.648443
C	8.888238	1.957931	-0.578894
C	9.229536	2.988129	-0.609730
C	7.537983	1.660834	-0.486097
H	10.139561	-1.222133	-0.701356
C	7.717187	-1.750209	-0.527247
H	6.806753	2.461492	-0.436741
H	-11.529400	1.281403	0.766946
H	-11.706497	2.638197	1.272644
S	-12.244788	0.140944	1.328904
O	12.244317	0.144850	-1.330455
O	11.705968	2.641911	-1.266722
O	11.529119	1.283648	-0.764895
O	12.073344	1.354937	1.028147
S	13.369591	1.635948	1.068340
C	11.857305	0.182783	1.620769
F	11.396470	2.299914	1.676426
F	-0.051952	-3.584382	-1.252792
F	0.078742	-2.951717	-2.640252
C	-0.985275	-4.162983	-1.201866
C	0.761604	-4.313012	-1.131554
H	-1.130622	-2.173200	-3.156324
H	0.969708	-2.309300	-2.674783
C	-0.966407	-1.760958	-4.615324
H	-2.032765	-2.792911	-3.048640
C	-1.299235	-1.279208	-2.545284
H	-1.837631	-1.201018	-4.973684
H	-0.083557	-1.123242	-4.748544
H	-0.842069	-2.637027	-5.264278
H	0.051901	-3.587453	1.245065
H	-0.078686	-2.958207	2.634092
C	1.130736	-2.181009	3.152018
C	0.966646	-1.772418	4.612058
C	2.032861	-2.800463	3.042709
C	1.299315	-1.285492	2.543208
H	1.837907	-1.213387	4.971746
H	0.083816	-1.135025	4.746947
H	0.842351	-2.650106	5.258829
H	0.277363	-3.772742	-3.344698

H	-0.969629	-2.315851	2.670267
H	-0.277286	-3.780966	3.336517
H	0.985195	-4.165972	1.192667
H	-0.761695	-4.315745	1.122082
H	-12.072898	1.357884	-1.026101
H	-11.856624	0.187450	-1.622029
C	-13.369128	1.639018	-1.066005
F	-11.395755	2.304730	-1.671364
F	-2.558363	-1.785371	0.164919
F	-3.132994	-2.704980	0.200516
H	2.558291	-1.784989	-0.168354
H	3.132902	-2.704517	-0.206323