

# Toward Redox-Active Indenofluorene-Extended Tetrathiafulvalene Oligomers – Synthesis and Studies of Dimeric Scaffolds

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## Supporting Information

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## Regioisomers of dimers **1a** and **1b**

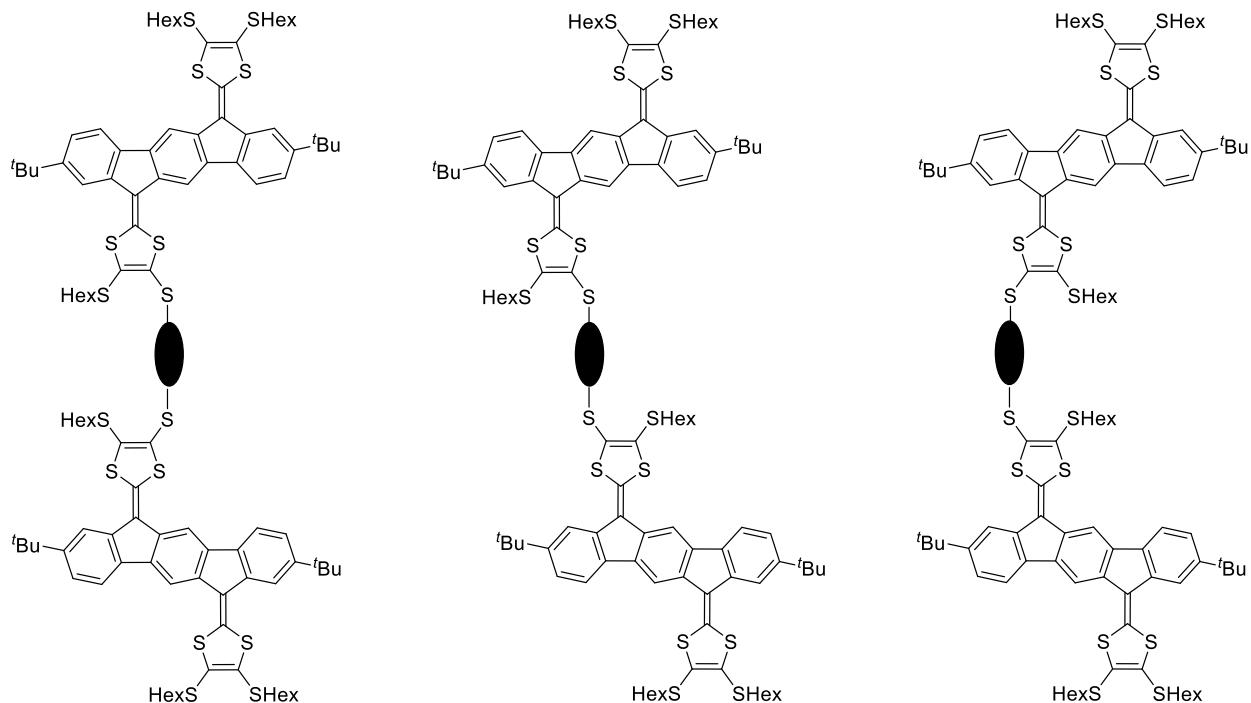


Figure S1: Formed regioisomers of **1a** and **1b** (linkers are shown schematically for clarity).

# NMR spectra ( $^1\text{H}$ and $^{13}\text{C}$ ) of all synthesized compounds

## Compound 1a

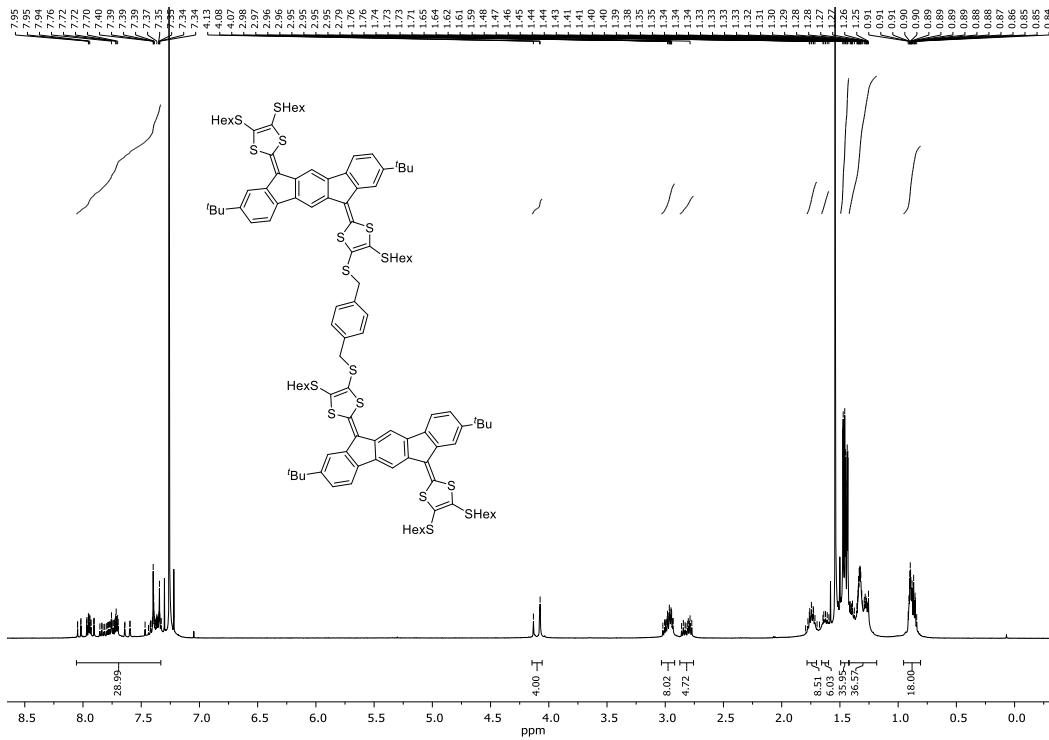


Figure S2:  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 500 MHz) spectrum of **1a**.

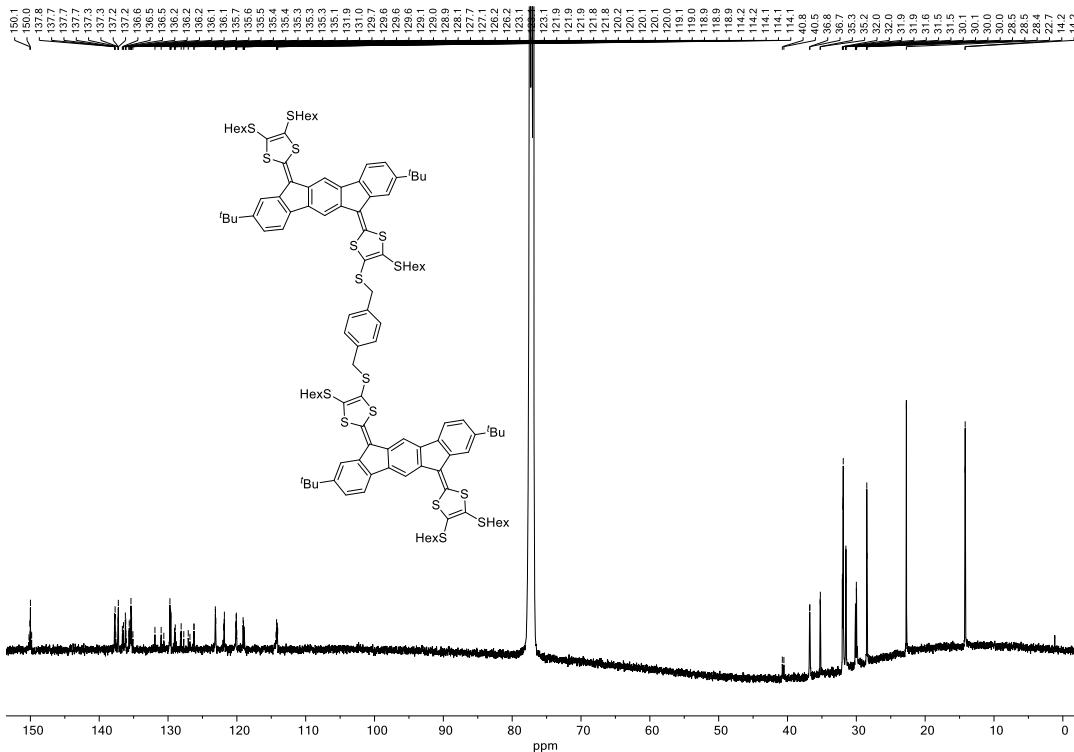


Figure S3:  $^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 126 MHz) spectrum of **1a**.

## Compound 1b

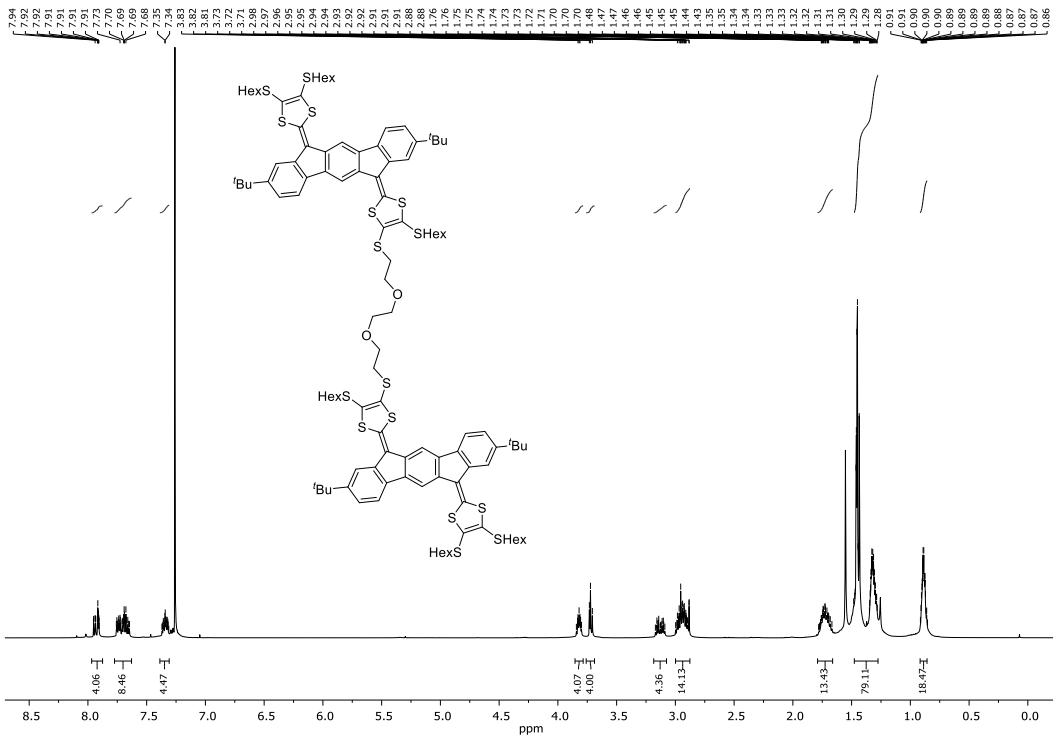


Figure S4:  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 500 MHz) spectrum of **1b**.

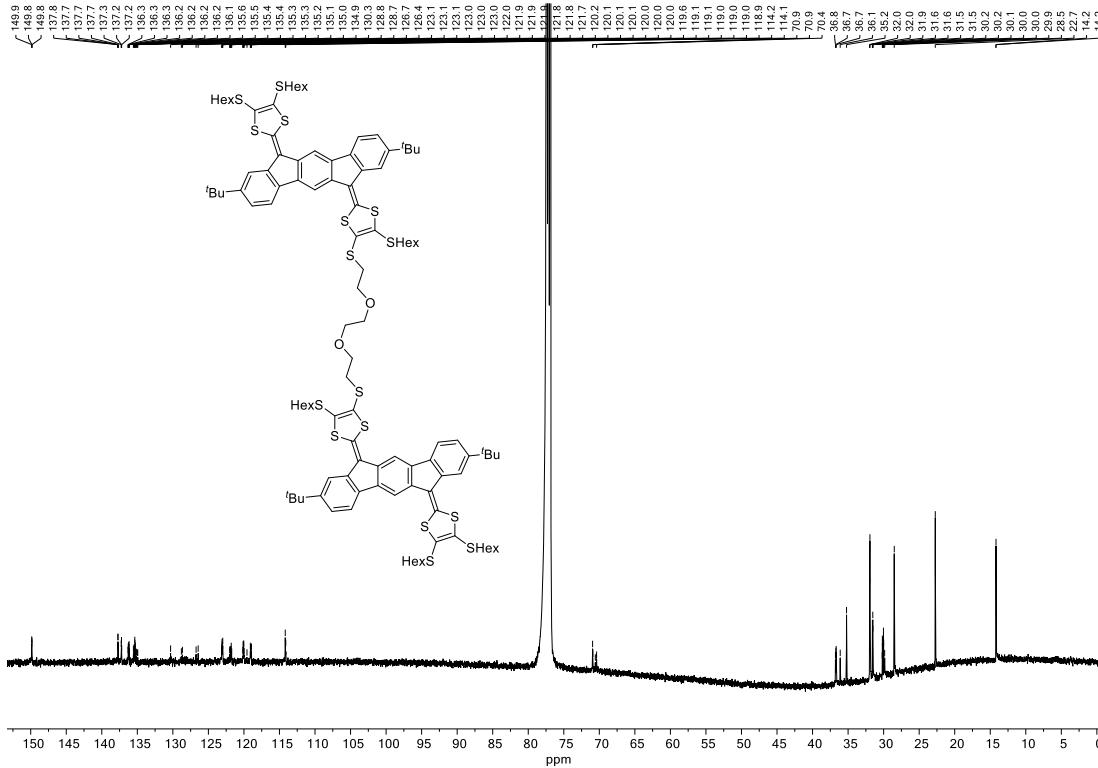


Figure S5:  $^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 126 MHz) spectrum of **1b**.

## Compound 4

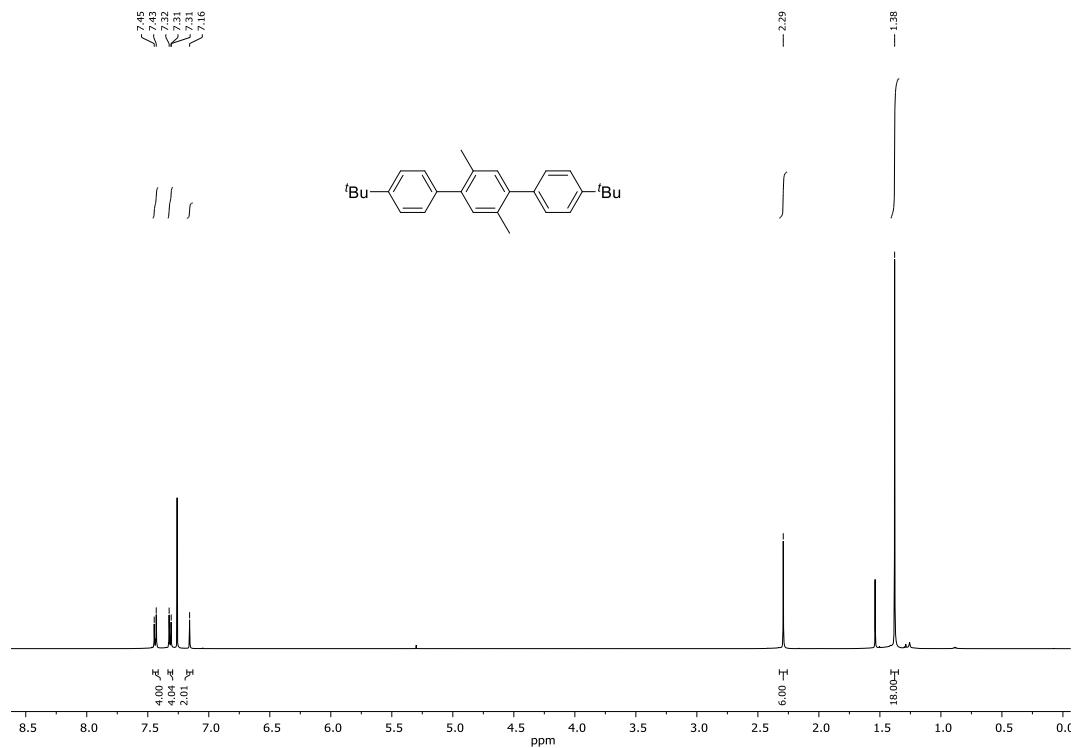


Figure S6: <sup>1</sup>H-NMR ( $\text{CDCl}_3$ , 500 MHz) spectrum of **4**.

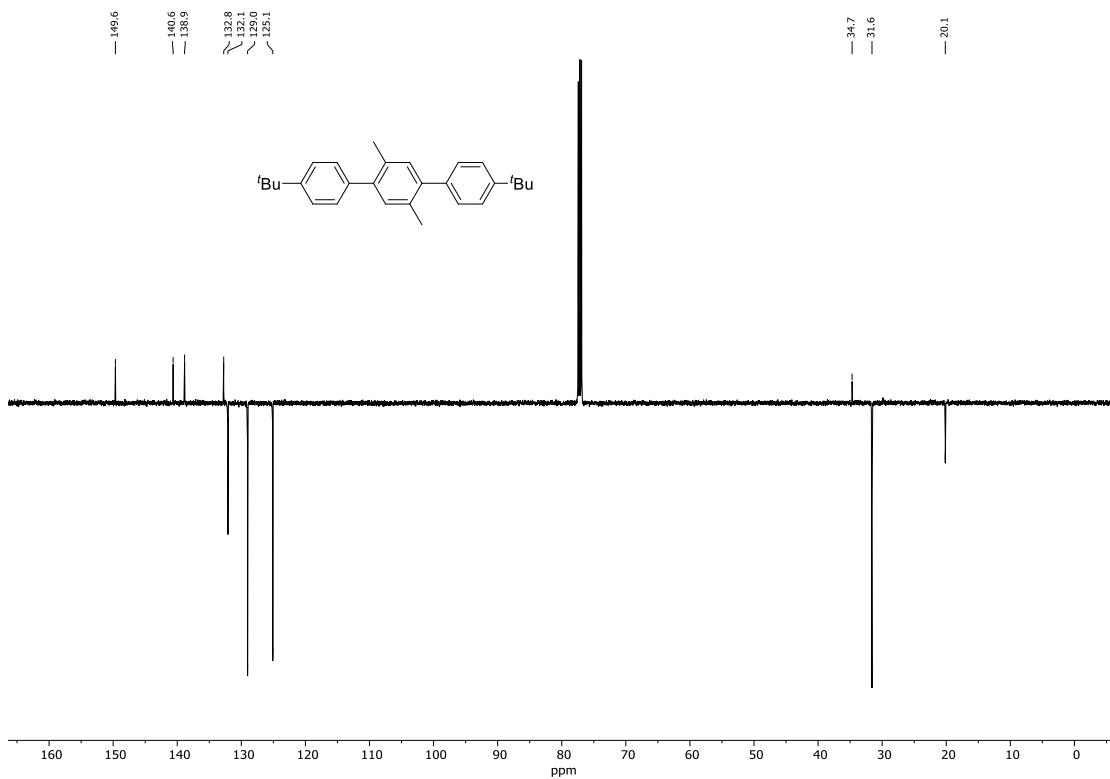


Figure S7: <sup>13</sup>C-APT NMR ( $\text{CDCl}_3$ , 126 MHz) spectrum of **4**.

## Compound 5

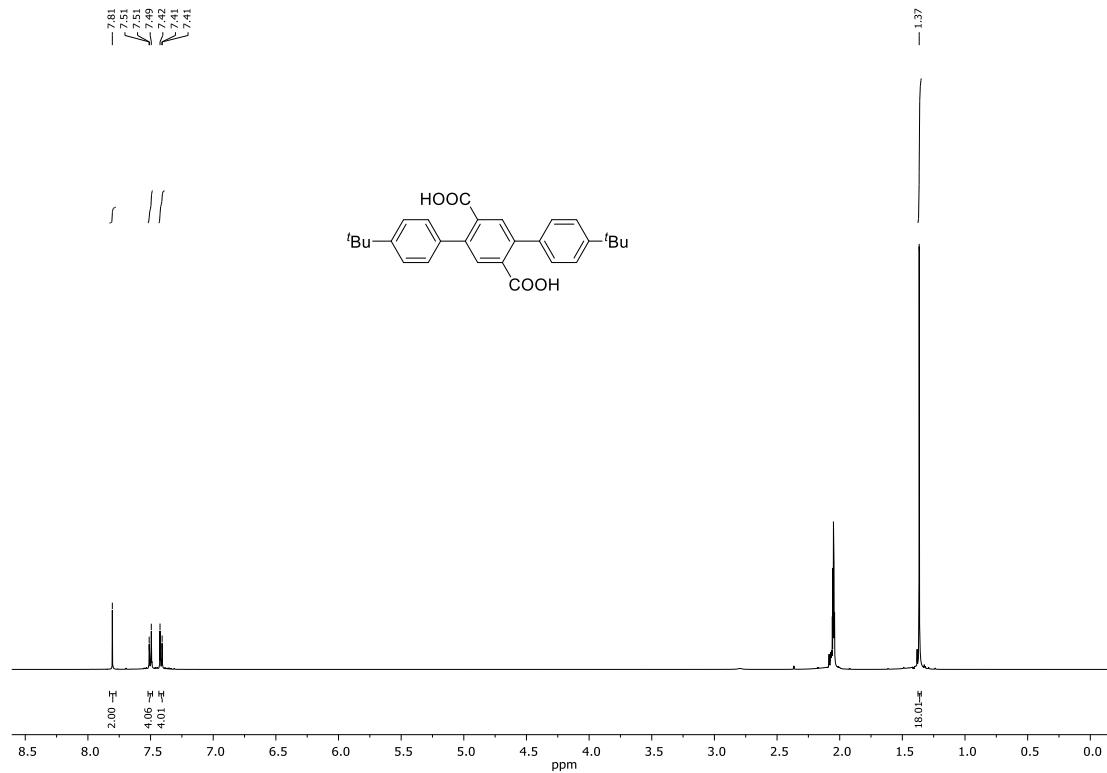


Figure S8:  $^1\text{H}$ -NMR ( $(\text{CD}_3)_2\text{CO}$ , 500 MHz) spectrum of **5**.

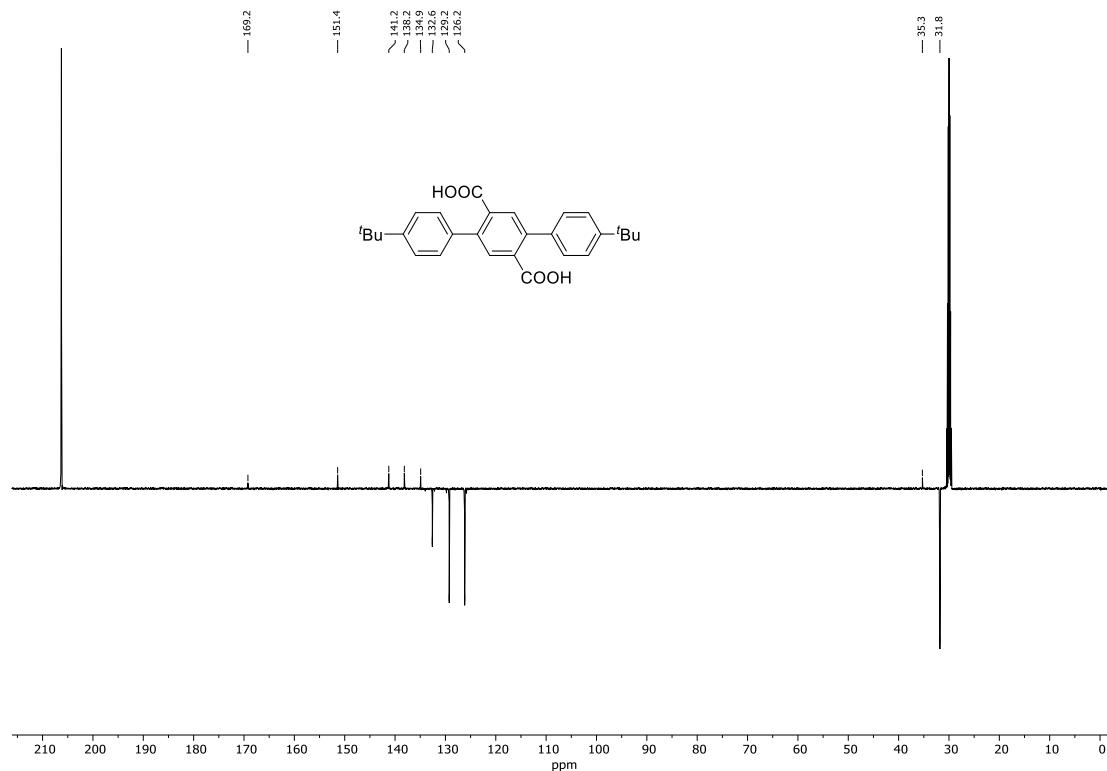
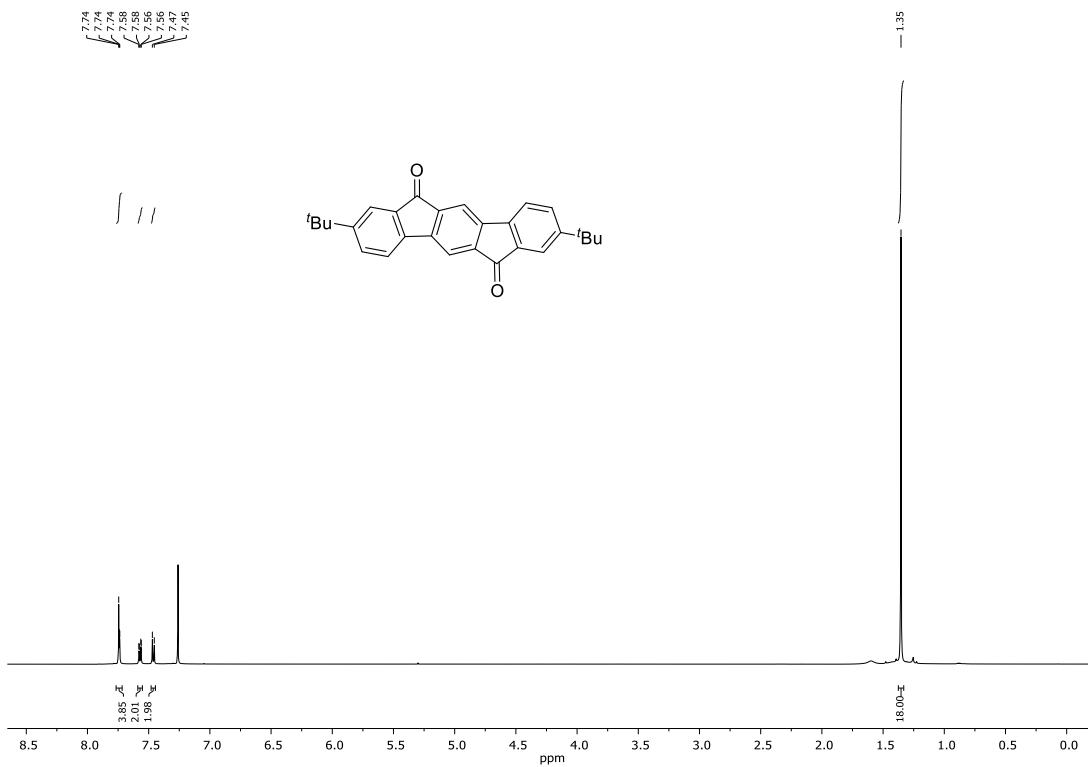


Figure S9:  $^{13}\text{C}$ -APT NMR ( $(\text{CD}_3)_2\text{CO}$ , 126 MHz) spectrum of **5**.

## Compound 6



## Compound 7

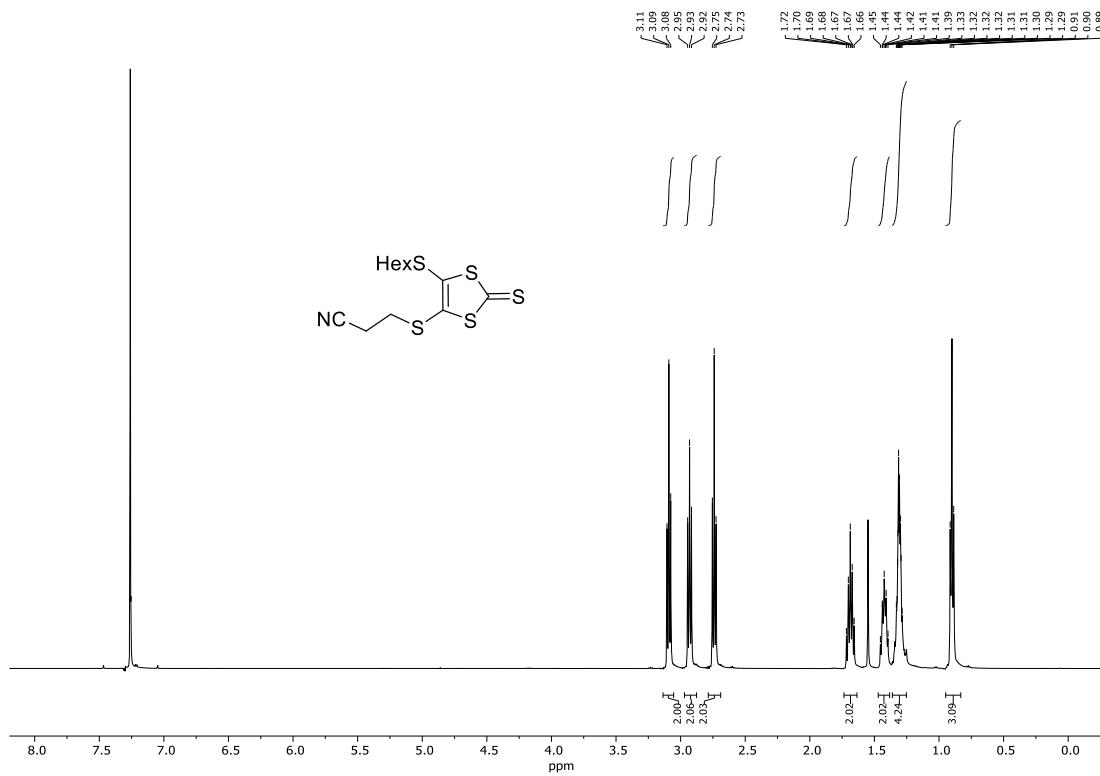


Figure S12: <sup>1</sup>H-NMR (CDCl<sub>3</sub>, 500 MHz) spectrum of **7**.

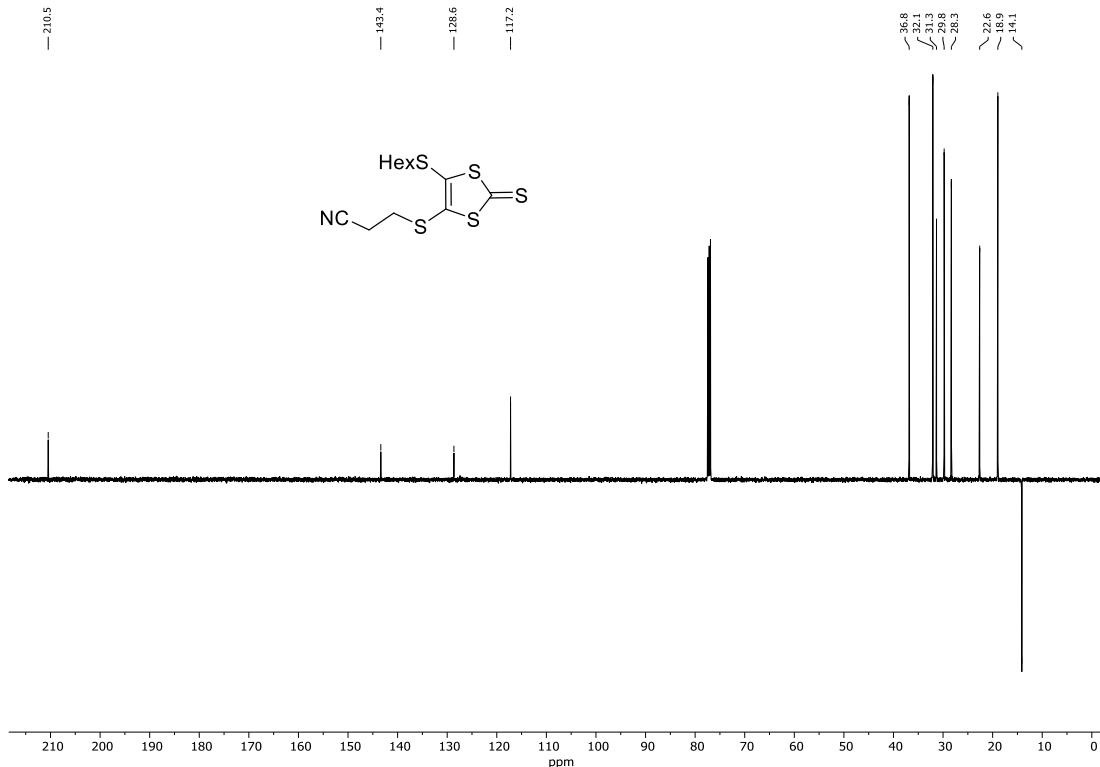


Figure S13: <sup>13</sup>C-APT NMR (CDCl<sub>3</sub>, 126 MHz) spectrum of **7**.

## Compound 8

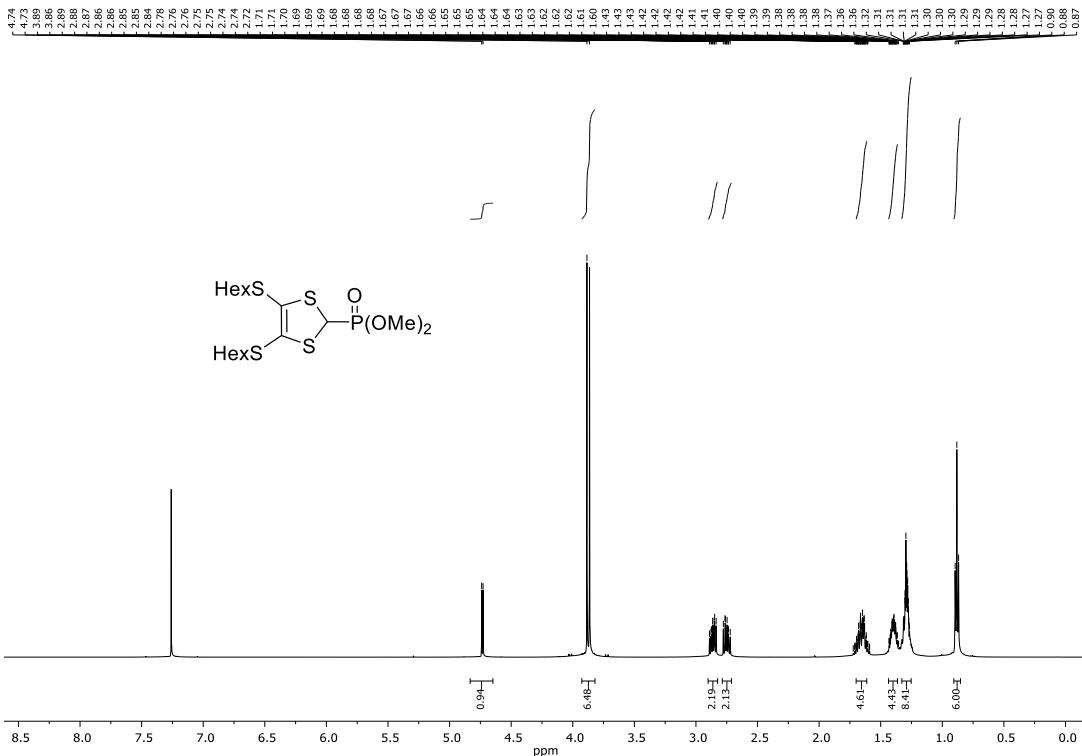


Figure S14:  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 500 MHz) spectrum of **8**.

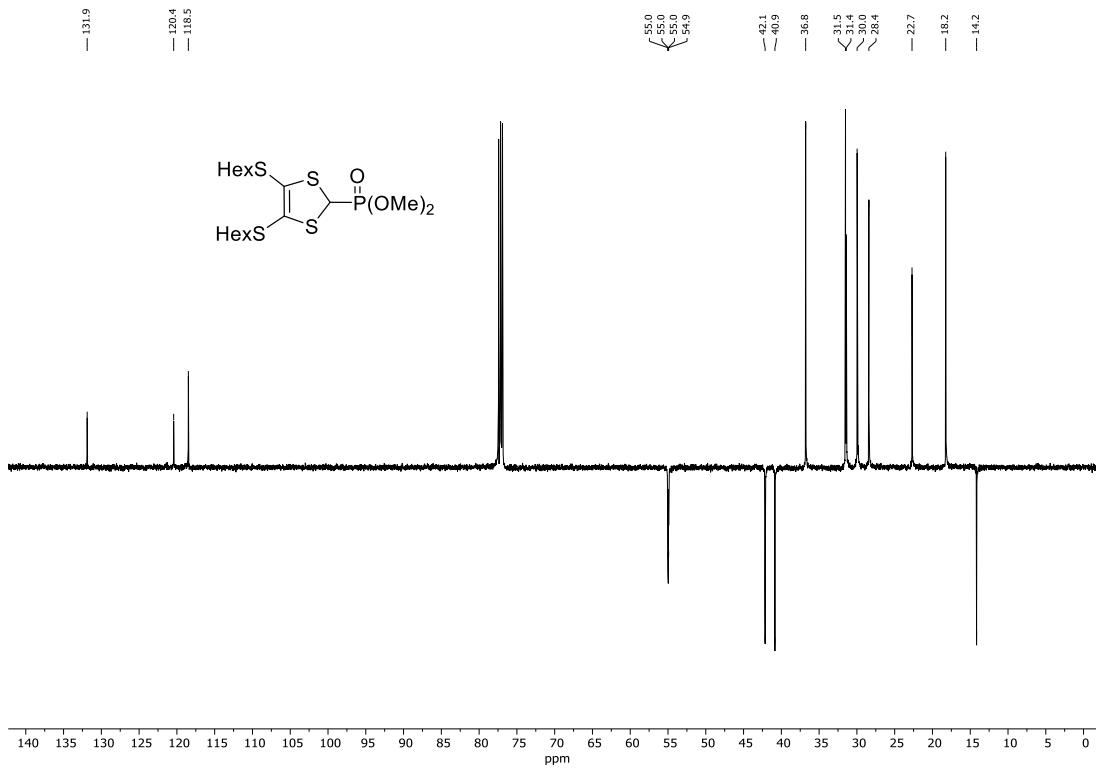


Figure S15:  $^{13}\text{C}$ -APT NMR ( $\text{CDCl}_3$ , 126 MHz) spectrum of **8**.

## Compound 9

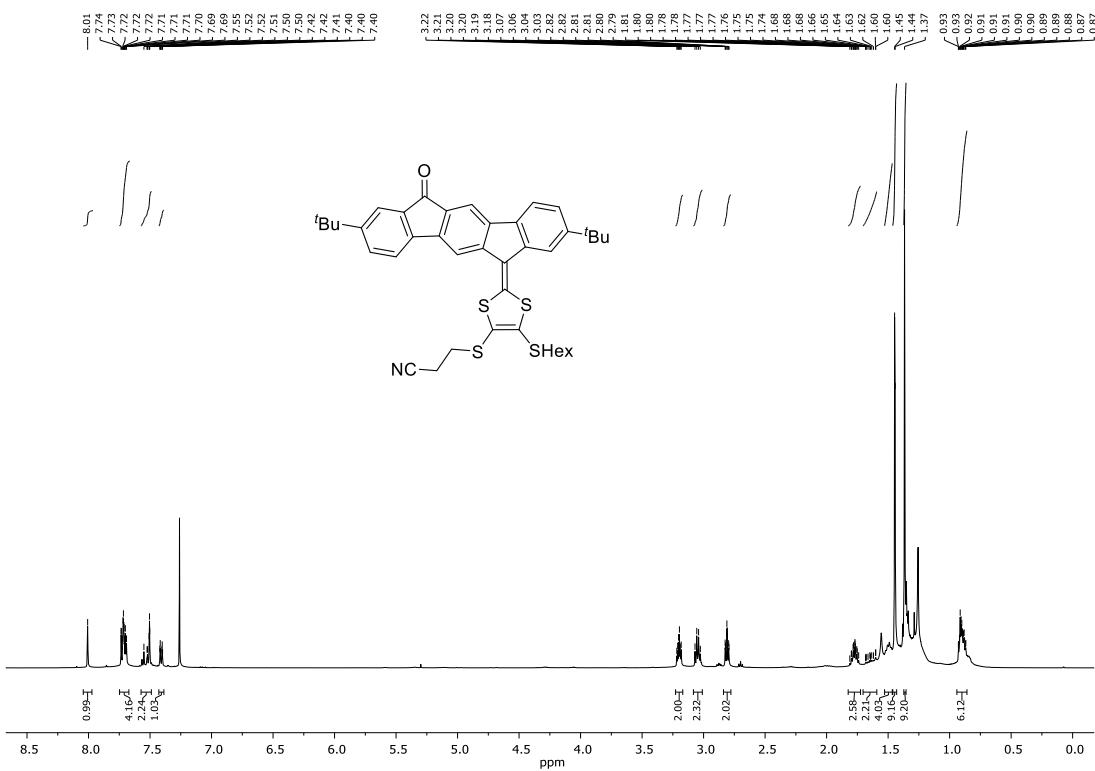


Figure S16:  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 500 MHz) spectrum of **9**.

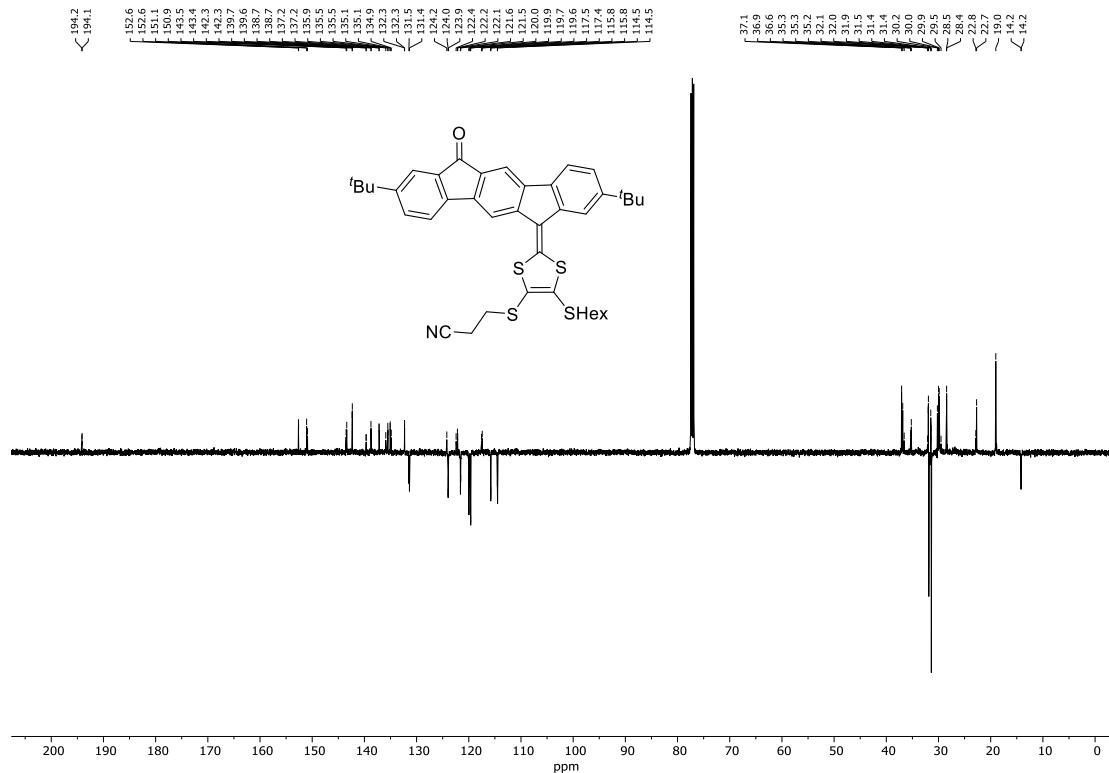


Figure S17:  $^{13}\text{C}$ -APT NMR ( $\text{CDCl}_3$ , 126 MHz) spectrum of **9**.

**Compound 1,2-bis(2-iodoethoxy)ethane**

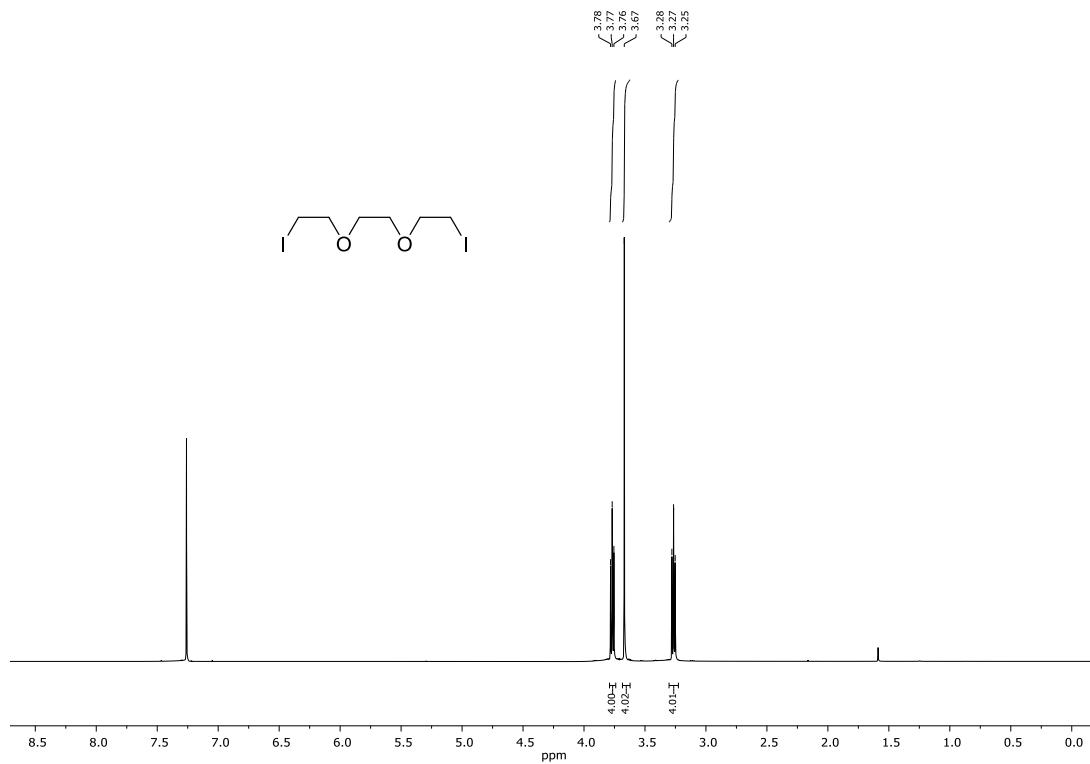


Figure S18: <sup>1</sup>H-NMR (CDCl<sub>3</sub>, 500 MHz) spectrum of 1,2-bis(2-iodoethoxy)ethane.

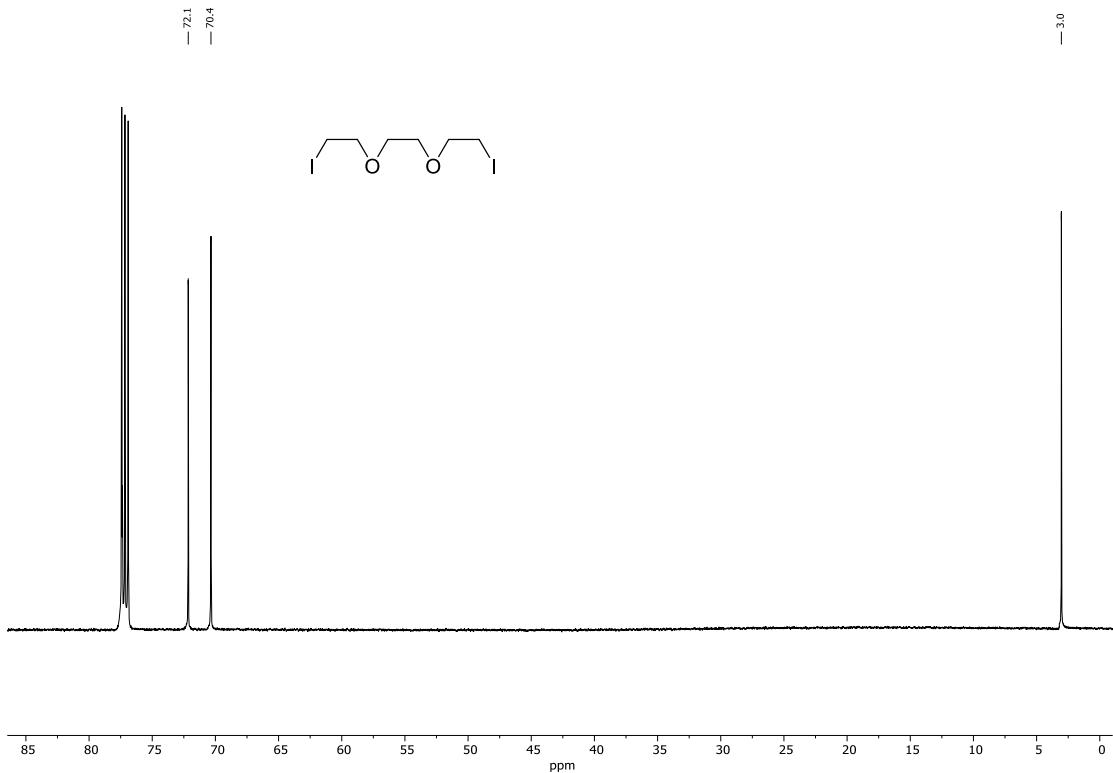


Figure S19: <sup>13</sup>C-NMR (CDCl<sub>3</sub>, 126 MHz) spectrum of 1,2-bis(2-iodoethoxy)ethane.

## Compound 10a

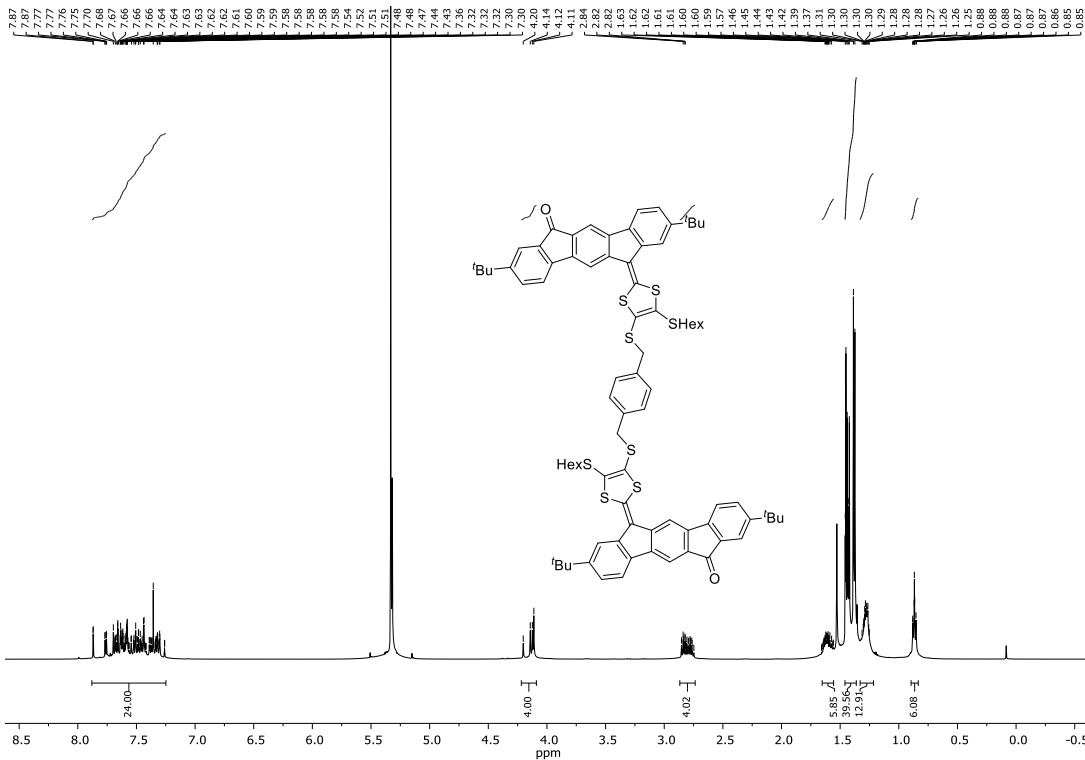


Figure S20:  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 500 MHz) spectrum of **10a**.

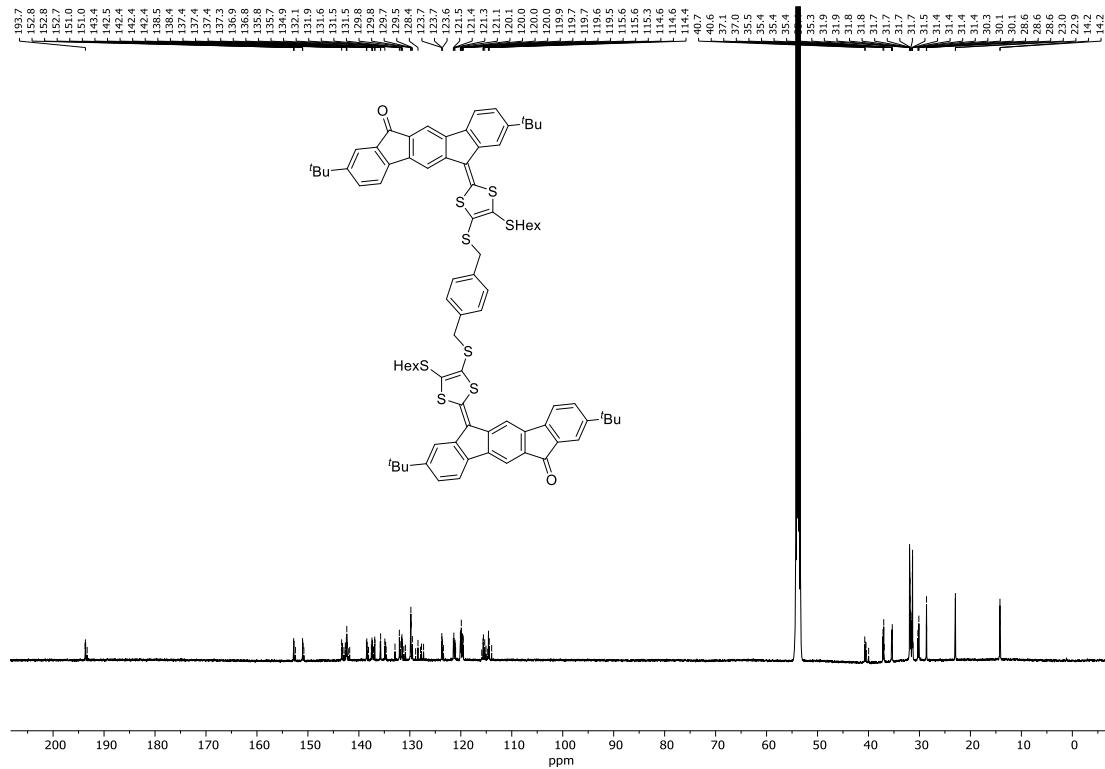


Figure S21:  $^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 126 MHz) spectrum of **10a**.

## **Compound 10b**

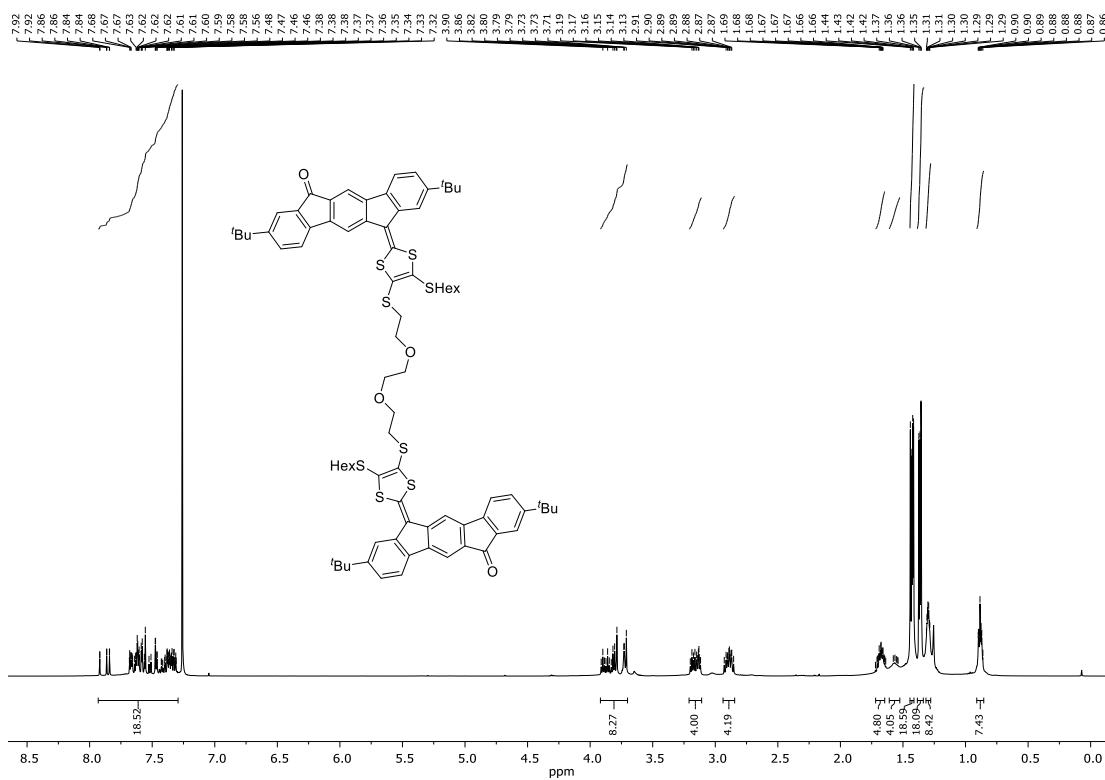


Figure S22:  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 500 MHz) spectrum of **10b**.

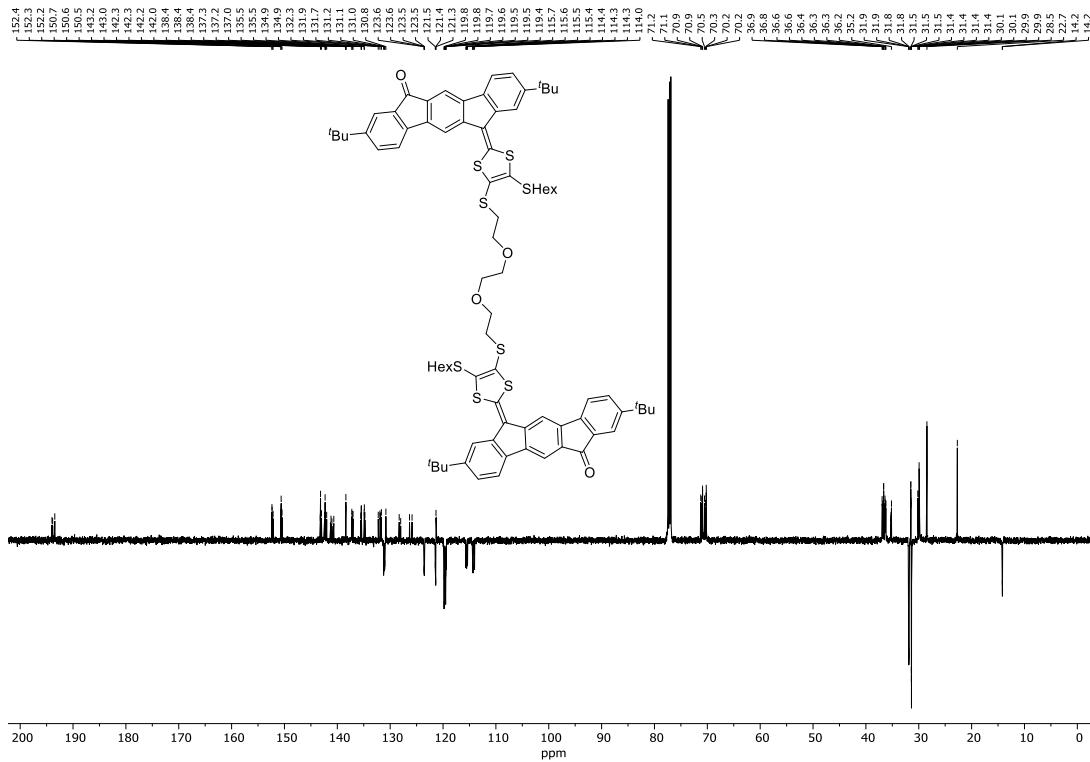


Figure S23:  $^{13}\text{C}$ -APT NMR ( $\text{CDCl}_3$ , 126 MHz) spectrum of **10b**.

## Compound 11

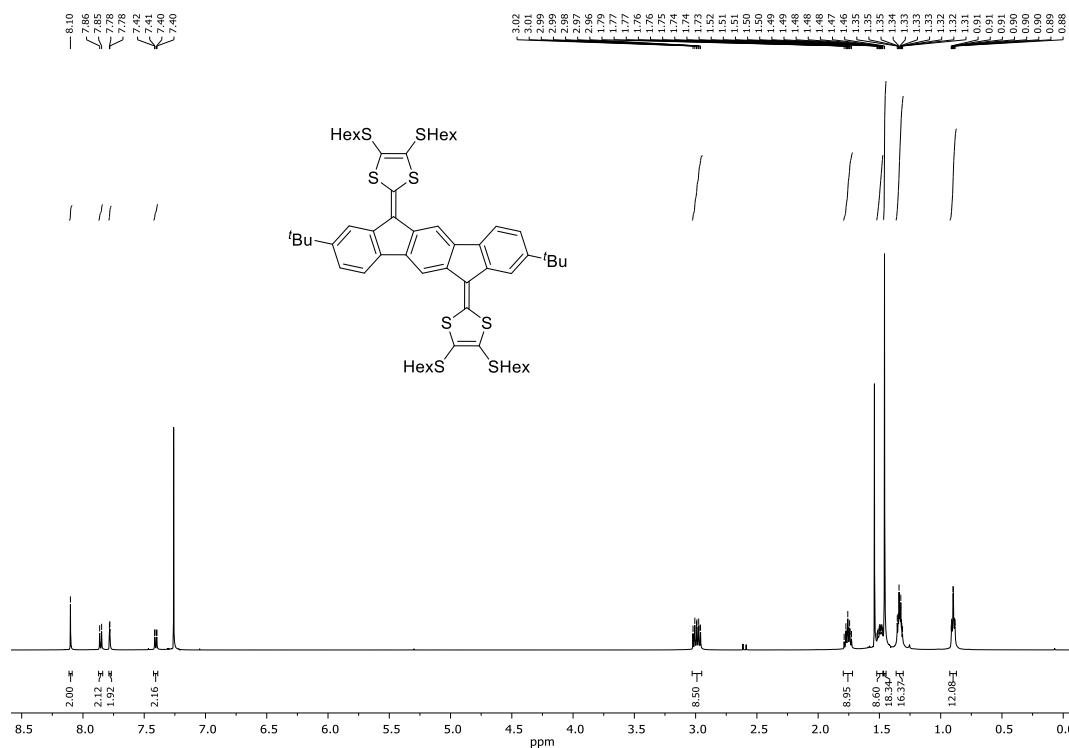


Figure S24: <sup>1</sup>H-NMR (CDCl<sub>3</sub>, 500 MHz) spectrum of **11**.

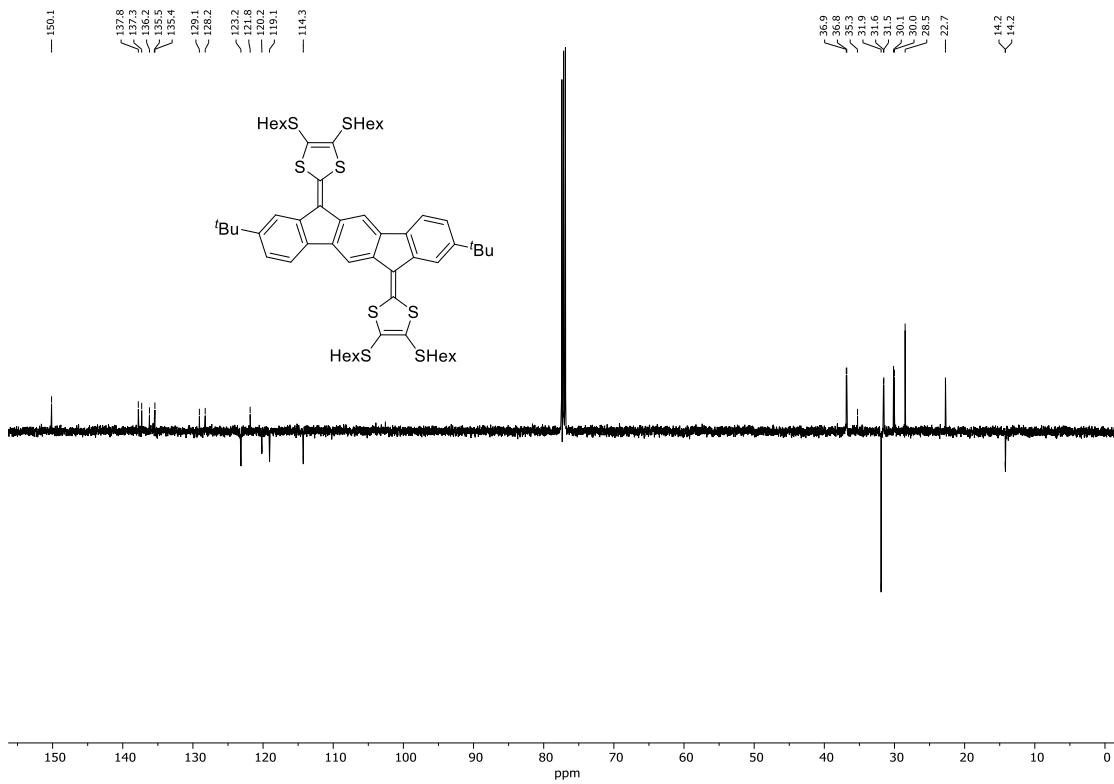


Figure S25: <sup>13</sup>C-APT NMR (CDCl<sub>3</sub>, 126 MHz) spectrum of **11**.

## Cyclic voltammograms of compounds **1a**, **1b**, **10a**, **10b** and **11**

Table S1: Oxidation and reduction potentials (in V vs. Fc/Fc<sup>+</sup>) for compounds **1a**, **1b**, **10a**, **10b** and **11**, determined based on differential pulse voltammograms (recorded in CH<sub>2</sub>Cl<sub>2</sub>, electrolyte: 0.1 M NBu<sub>4</sub>PF<sub>6</sub>, scan rate: 0.1 V/s)

Compound	E <sub>ox,1</sub>	E <sub>ox,2</sub>	E <sub>ox,3</sub>	E <sub>red,1</sub>	E <sub>red,2</sub>	E <sub>red,3</sub>
<b>1a</b>	0.15	0.31	0.46	-2.23*	-2.42*	-
<b>1b</b>	0.12	0.30	0.45	-2.20*	-2.39*	-
<b>10a</b>	0.40	0.53	0.99*	-1.40	-1.76	-2.24
<b>10b</b>	0.44	0.57	0.91*	-1.38	-2.29	-
<b>11</b>	0.27	0.39	-	-2.27	-	-

\* irreversible.

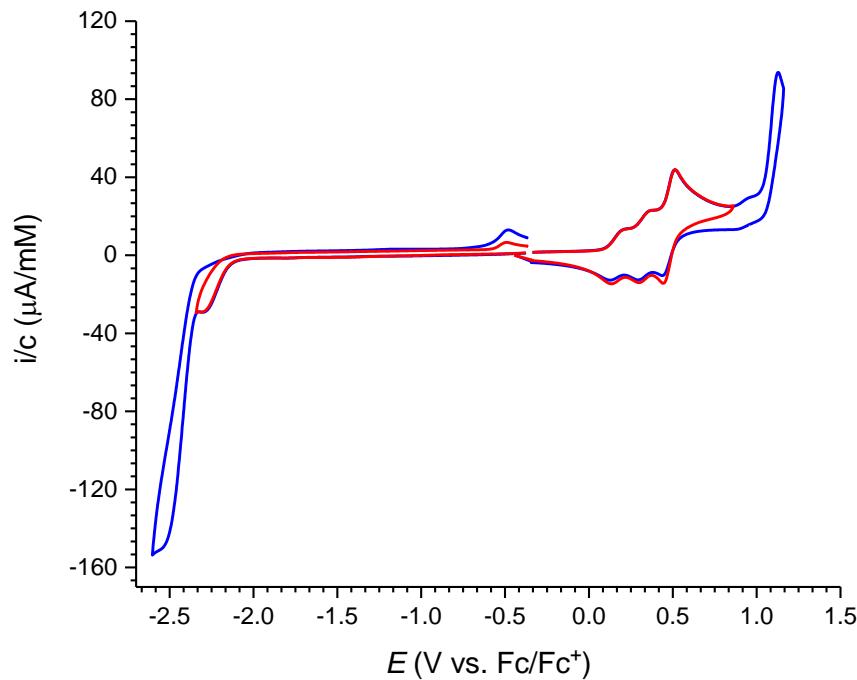


Figure S26: Cyclic voltammogram of **1a** recorded in CH<sub>2</sub>Cl<sub>2</sub>. Electrolyte: 0.1 M NBu<sub>4</sub>PF<sub>6</sub>, scan rate: 0.1 V/s.

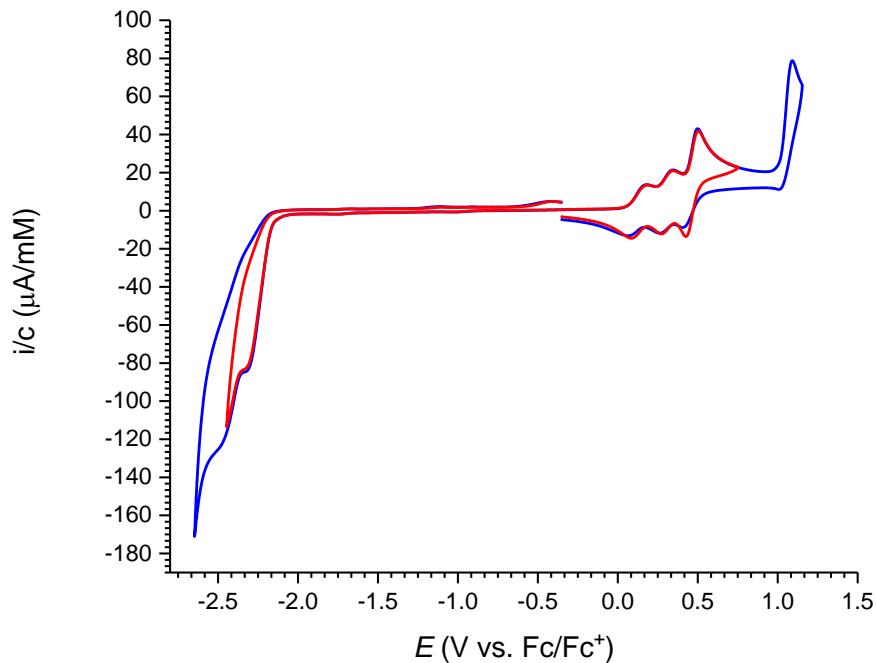


Figure S27: Cyclic voltammogram of **1b** recorded in  $\text{CH}_2\text{Cl}_2$ . Electrolyte: 0.1 M  $\text{NBu}_4\text{PF}_6$ , scan rate: 0.1 V/s.

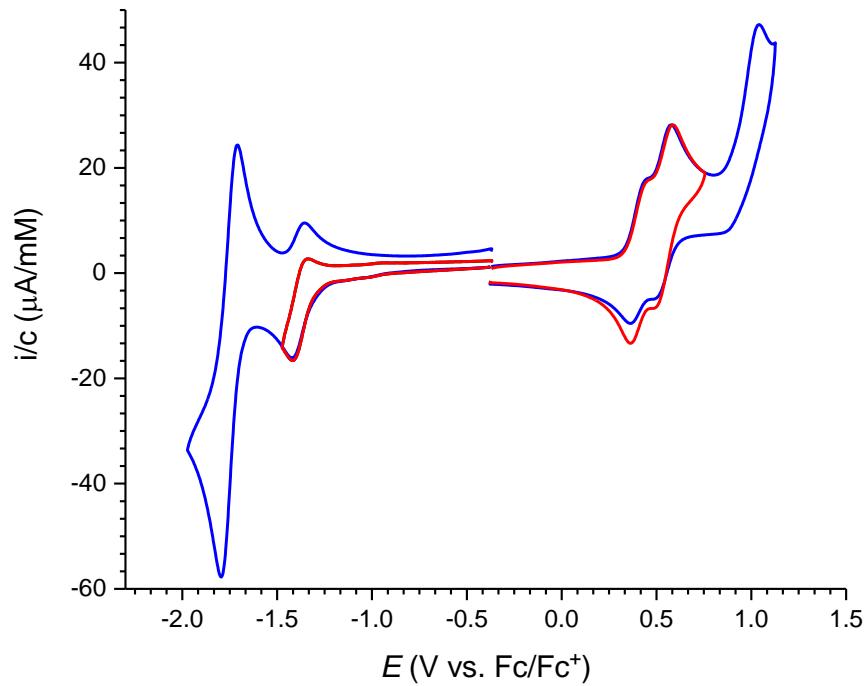


Figure S28: Cyclic voltammogram of **10a** recorded in  $\text{CH}_2\text{Cl}_2$ . Electrolyte: 0.1 M  $\text{NBu}_4\text{PF}_6$ , scan rate: 0.1 V/s.

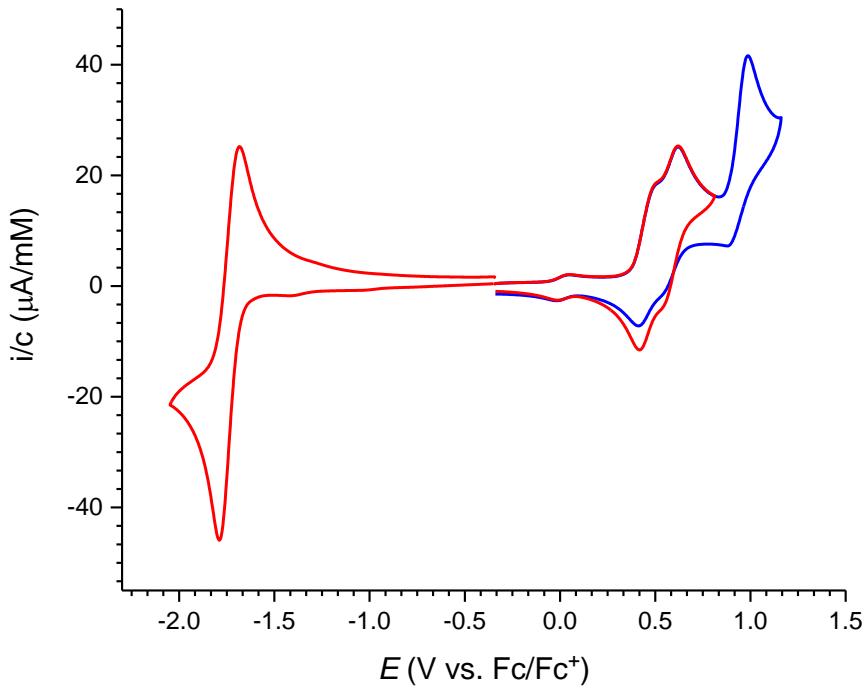


Figure S29: Cyclic voltammogram of **10b** recorded in  $\text{CH}_2\text{Cl}_2$ . Electrolyte: 0.1 M  $\text{NBu}_4\text{PF}_6$ , scan rate: 0.1 V/s.

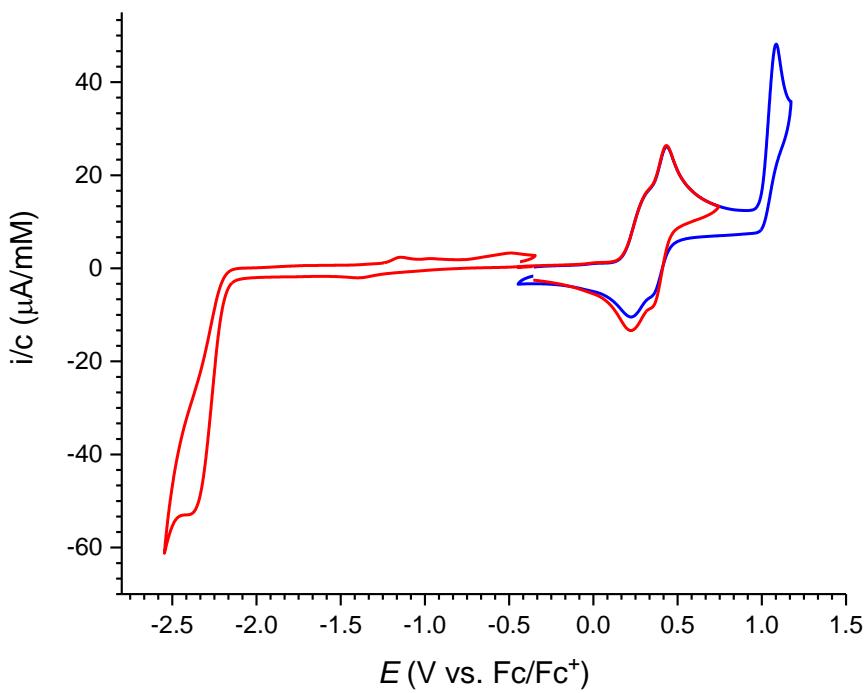


Figure S30: Cyclic voltammogram of **11** recorded in  $\text{CH}_2\text{Cl}_2$ . Electrolyte: 0.1 M  $\text{NBu}_4\text{PF}_6$ , scan rate: 0.1 V/s.

## Study of concentration dependency of differential pulse voltammograms of **1a** and **11**

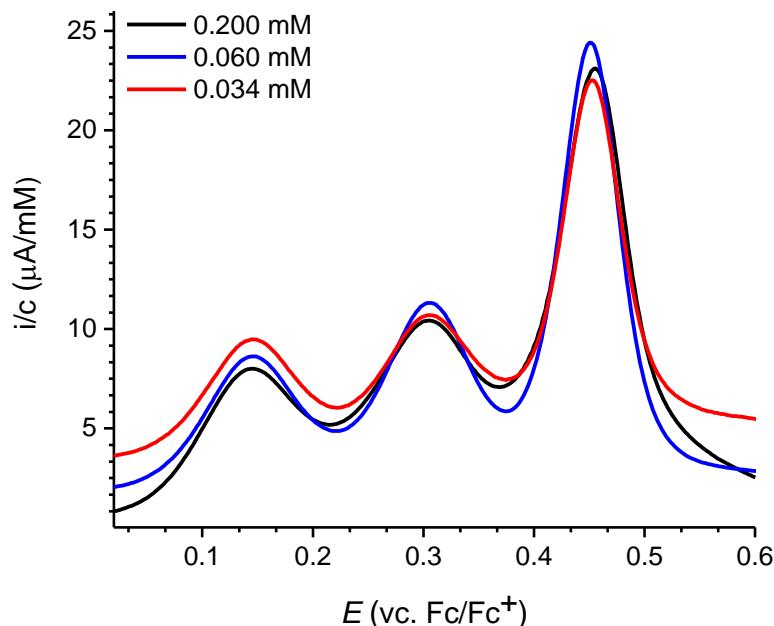


Figure S31: Differential Pulse Voltammograms of **1a** at different concentrations, showing no significant concentration dependency. Potentials referred vs.  $\text{Fc}/\text{Fc}^+$  (solvent:  $\text{CH}_2\text{Cl}_2$ , 0.1 M  $\text{NBu}_4\text{PF}_6$  electrolyte, scan rate: 0.1 V/s).

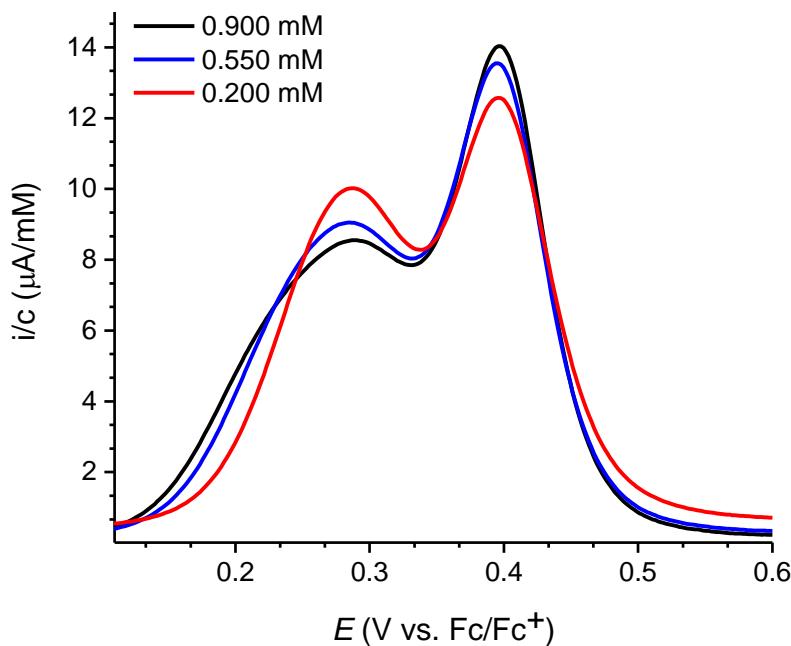


Figure S32: Differential Pulse Voltammograms of **11** at different concentrations, showing only little concentration dependency. Potentials referred vs.  $\text{Fc}/\text{Fc}^+$  (solvent:  $\text{CH}_2\text{Cl}_2$ , 0.1 M  $\text{NBu}_4\text{PF}_6$  electrolyte, scan rate: 0.1 V/s).

## UV-Vis spectra of compounds **10a** and **10b**

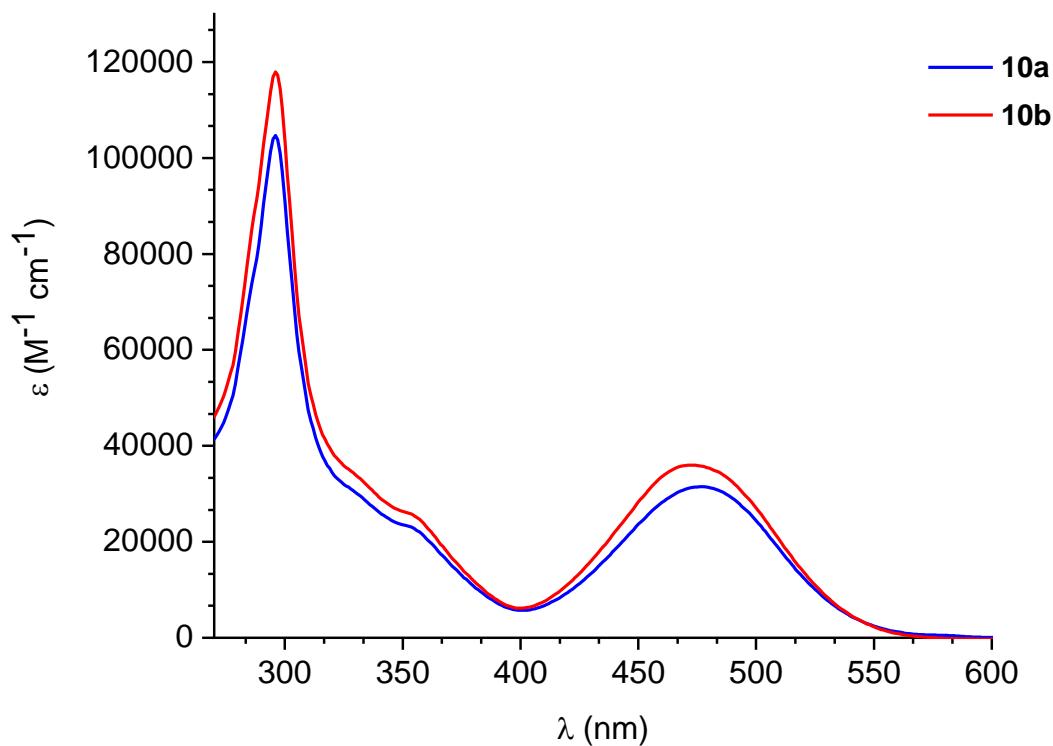


Figure S33: UV/Vis absorption spectra of dimers **10a** and **10b** recorded in  $\text{CH}_2\text{Cl}_2$  at 25 °C.

## Spectroelectrochemistry of **1b** and **11**

**Compound 11:**

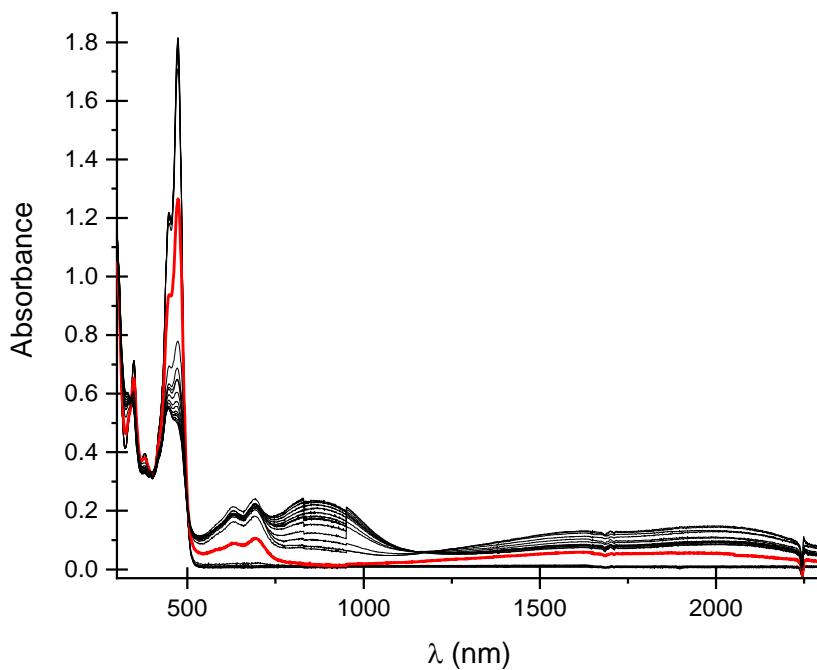


Figure S34: Spectroelectrochemistry of a 1.3 mM solution of **11** in 0.2 M Bu<sub>4</sub>NPF<sub>6</sub> electrolyte in CH<sub>2</sub>Cl<sub>2</sub>. The measurement selected for comparison is marked in red, and is chosen as it is the last measurement before absorbance of the tetracation (750–1000 nm) is detected.

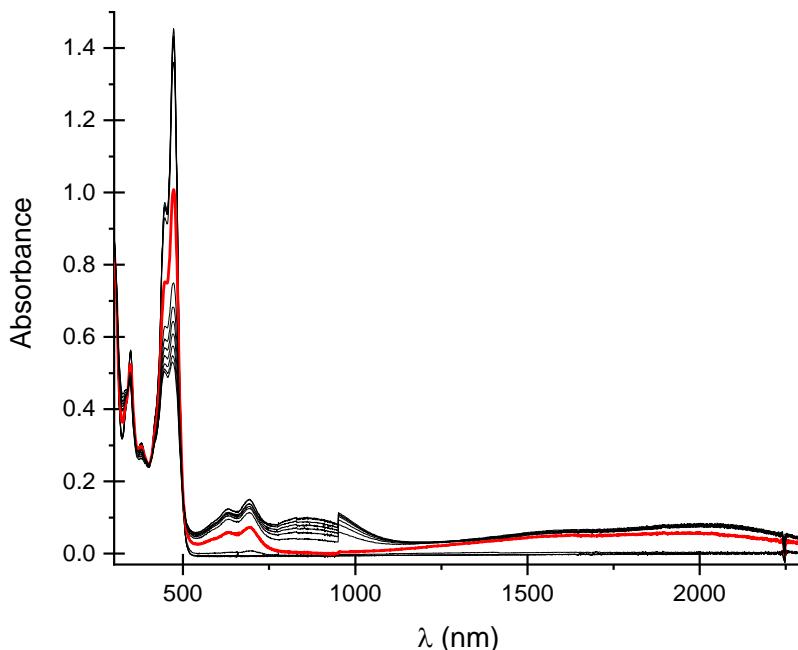


Figure S35: Spectroelectrochemistry of a 1.0 mM solution of **11** in 0.2 M Bu<sub>4</sub>NPF<sub>6</sub> electrolyte in CH<sub>2</sub>Cl<sub>2</sub>. The measurement selected for comparison is marked in red, and is chosen as it is the last measurement before absorbance of the tetracation (750–1000 nm) is detected.

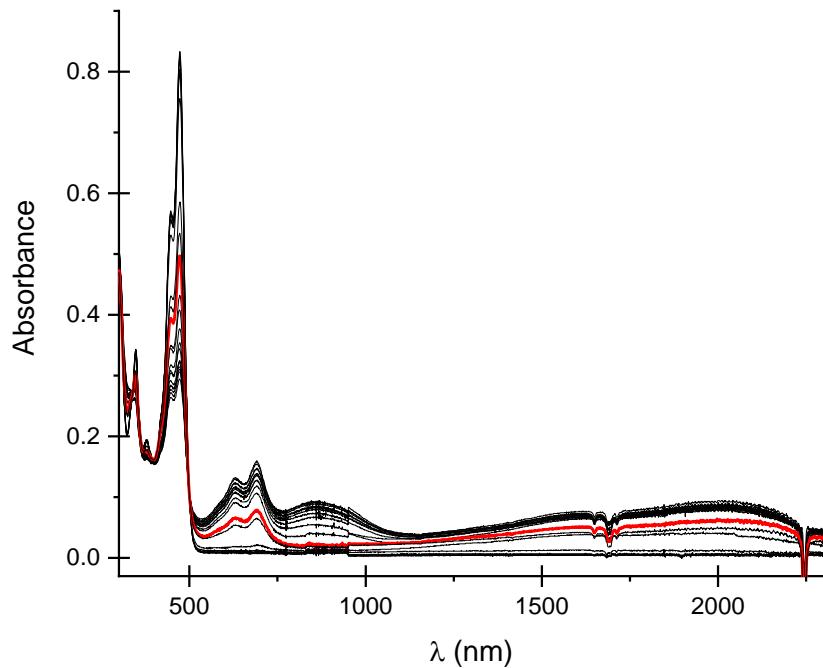


Figure S36: Spectroelectrochemistry of a 0.6 mM solution of **11** in 0.2 M  $\text{Bu}_4\text{NPF}_6$  electrolyte in  $\text{CH}_2\text{Cl}_2$ . The measurement selected for comparison is marked in red, and is chosen as it is the last measurement before absorbance of the tetracation (750-1000 nm) is detected.

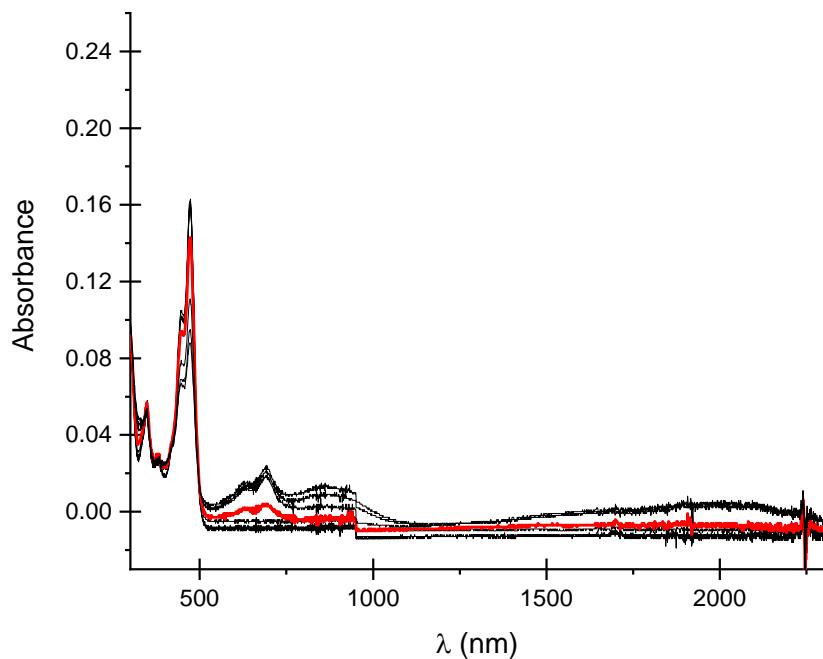


Figure S37: Spectroelectrochemistry of a 0.1 mM solution of **11** in 0.2 M  $\text{Bu}_4\text{NPF}_6$  electrolyte in  $\text{CH}_2\text{Cl}_2$ . The measurement selected for comparison is marked in red, and is chosen as it is the last measurement before absorbance of the tetracation (750-1000 nm) is detected.

**Compound 1b:**

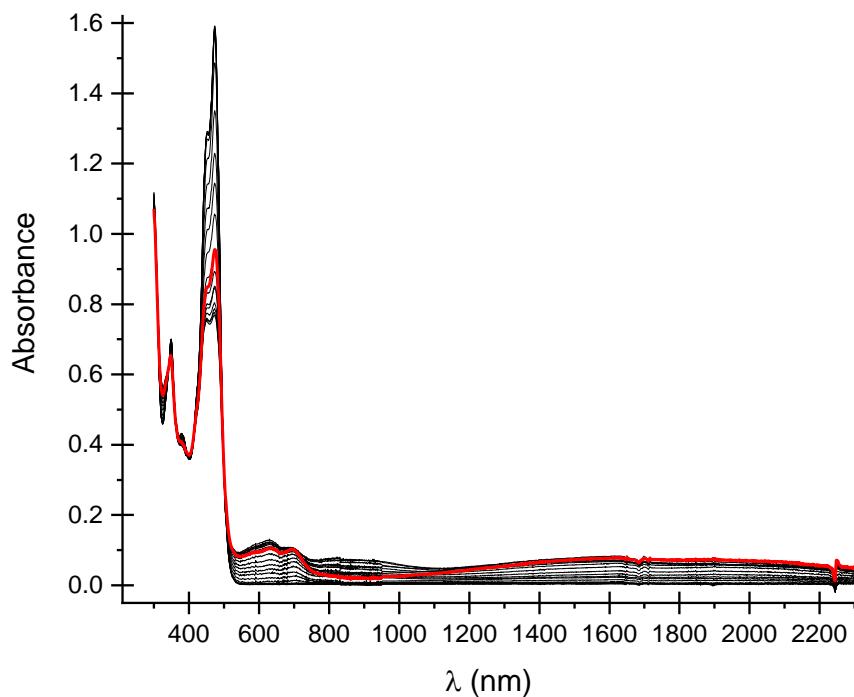


Figure S38: Spectroelectrochemistry of a 0.75 mM solution of **1b** in 0.2 M  $\text{Bu}_4\text{NPF}_6$  electrolyte in  $\text{CH}_2\text{Cl}_2$ . The measurement selected for comparison is marked in red, and is chosen as it is the last measurement before absorbance of the tetracation (750-1000 nm) is detected.

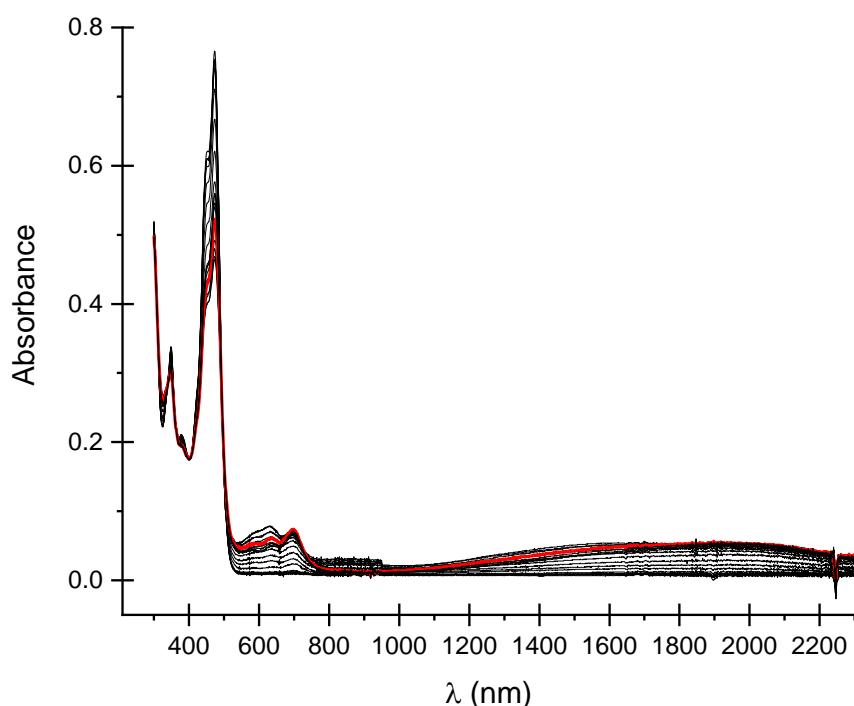


Figure S39: Spectroelectrochemistry of a 0.40 mM solution of **1b** in 0.2 M  $\text{Bu}_4\text{NPF}_6$  electrolyte in  $\text{CH}_2\text{Cl}_2$ . The measurement selected for comparison is marked in red, and is chosen as it is the last measurement before absorbance of the tetracation (750-1000) is detected.

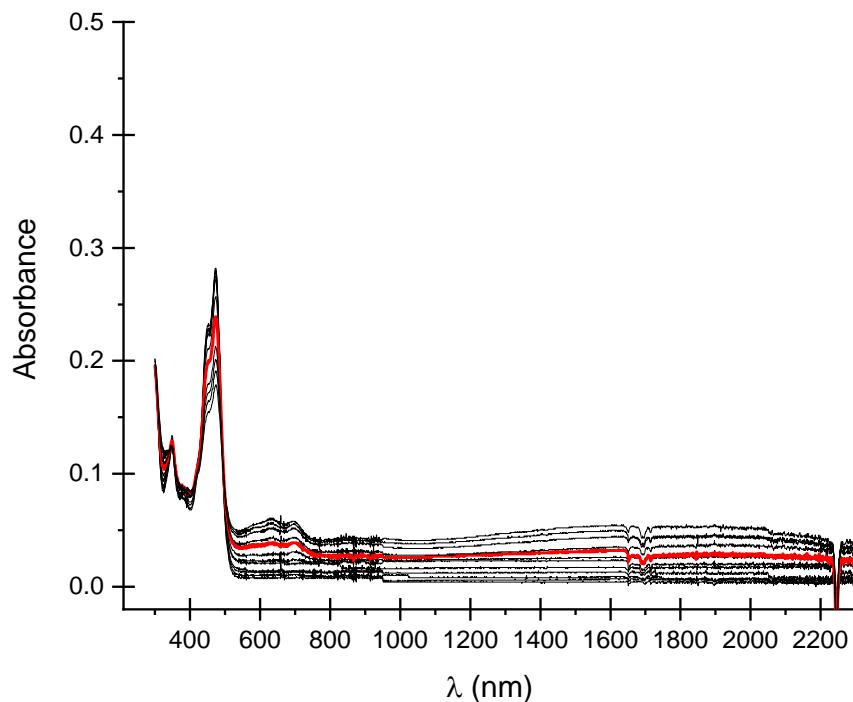
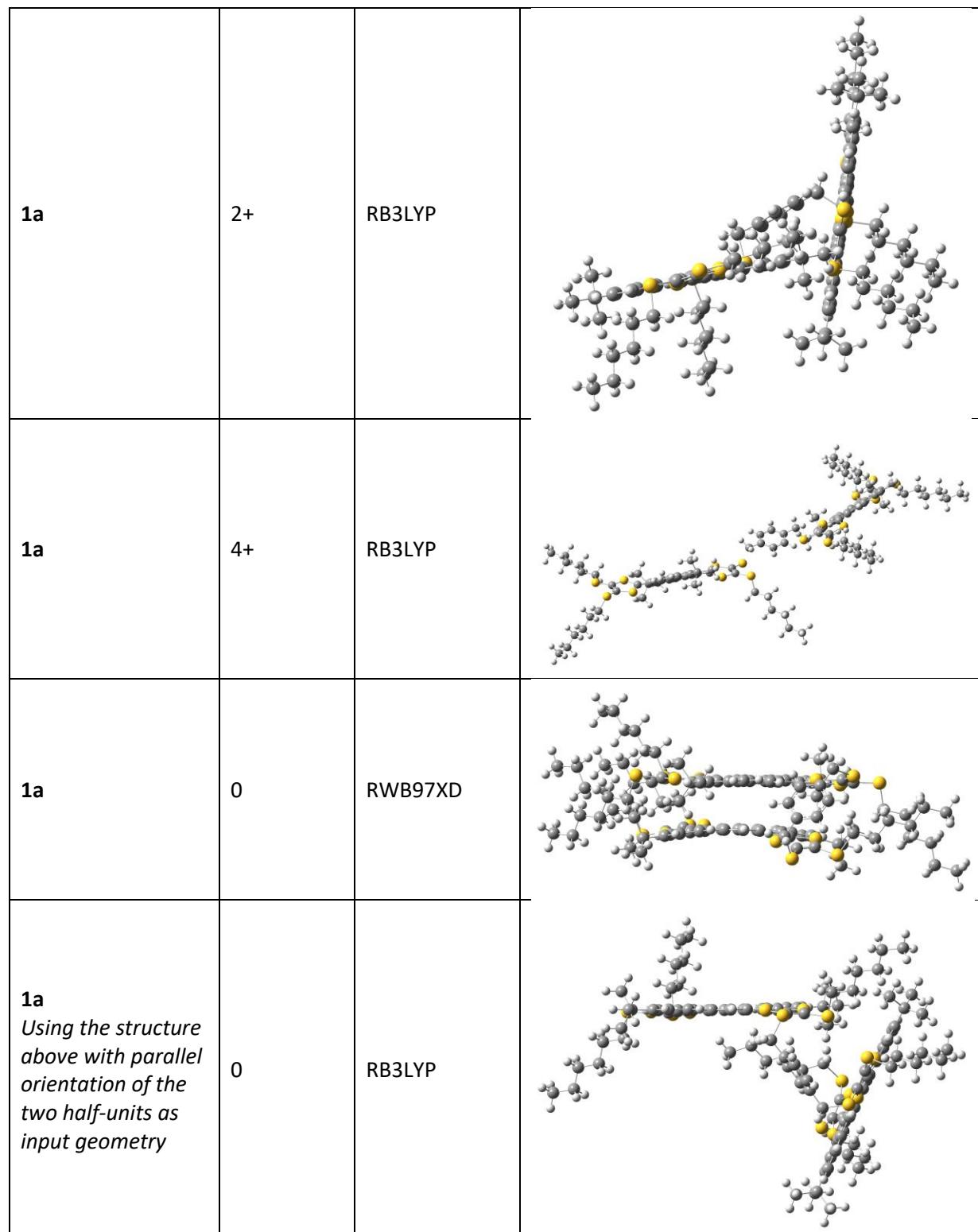


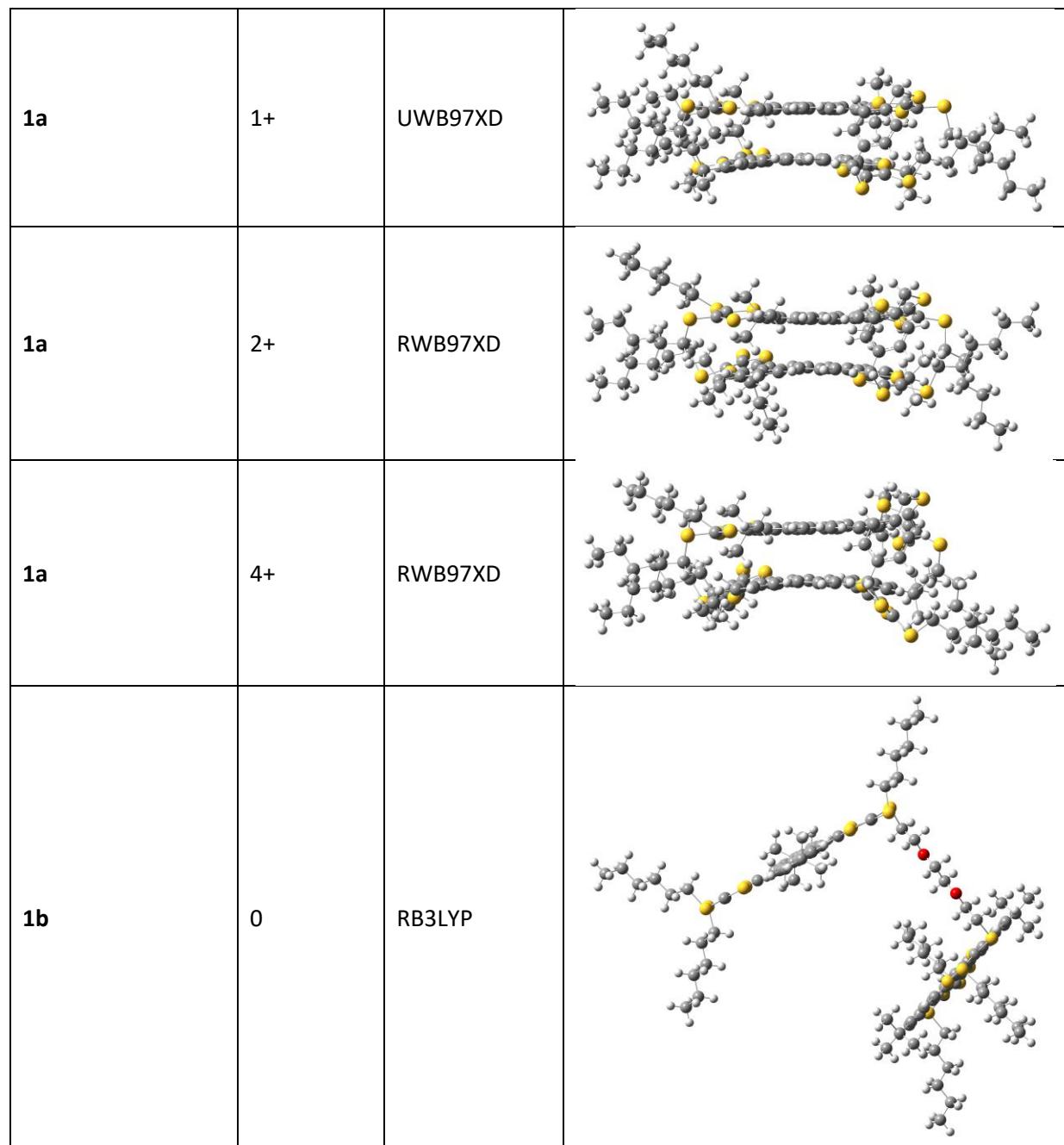
Figure S40: Spectroelectrochemistry of a 0.10 mM solution of **1b** in 0.2 M Bu<sub>4</sub>NPF<sub>6</sub> electrolyte in CH<sub>2</sub>Cl<sub>2</sub>. The measurement selected for comparison is marked in red, and is chosen as it is the last measurement before absorbance of the tetracation (750-1000) is detected.

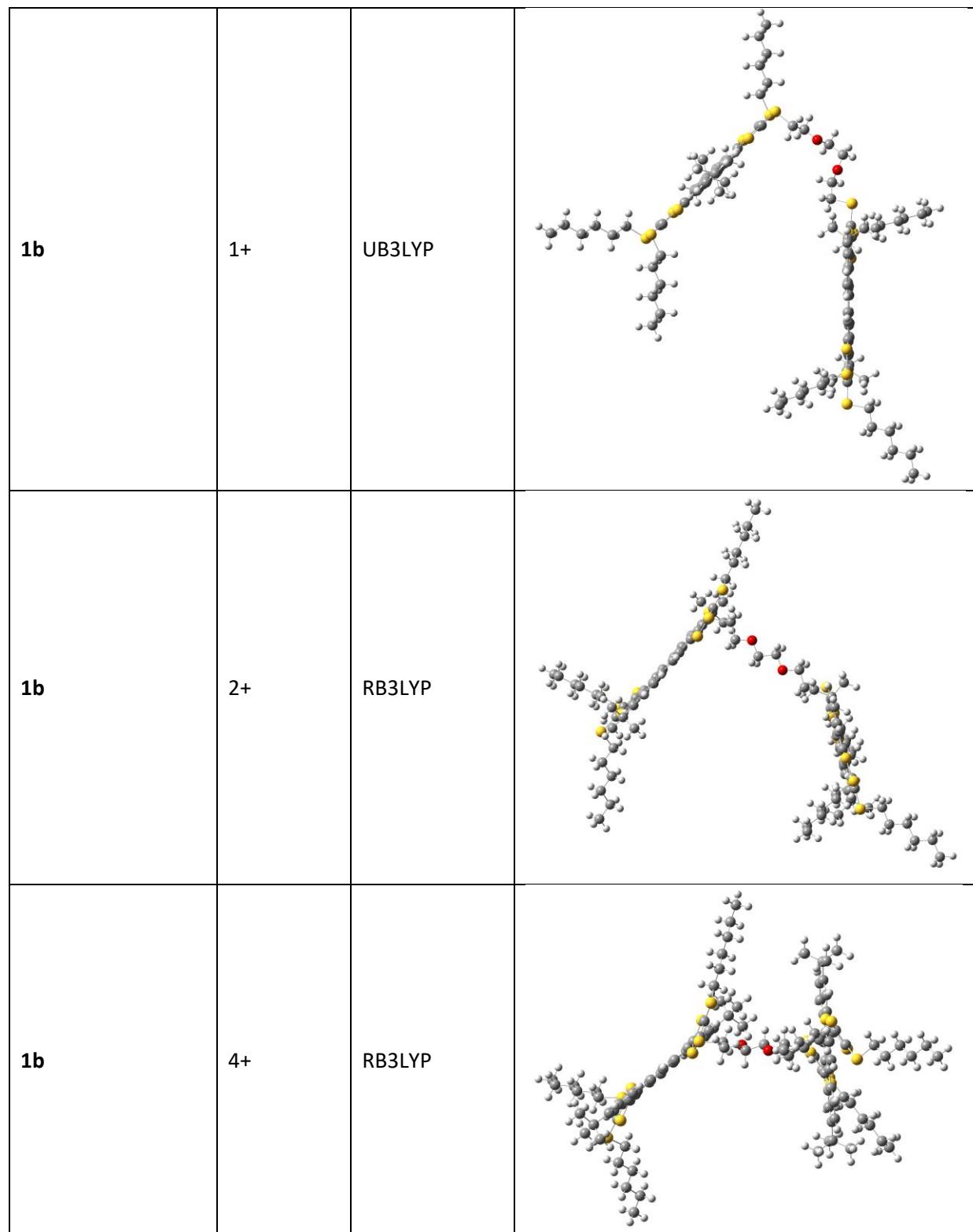
## Computational Studies

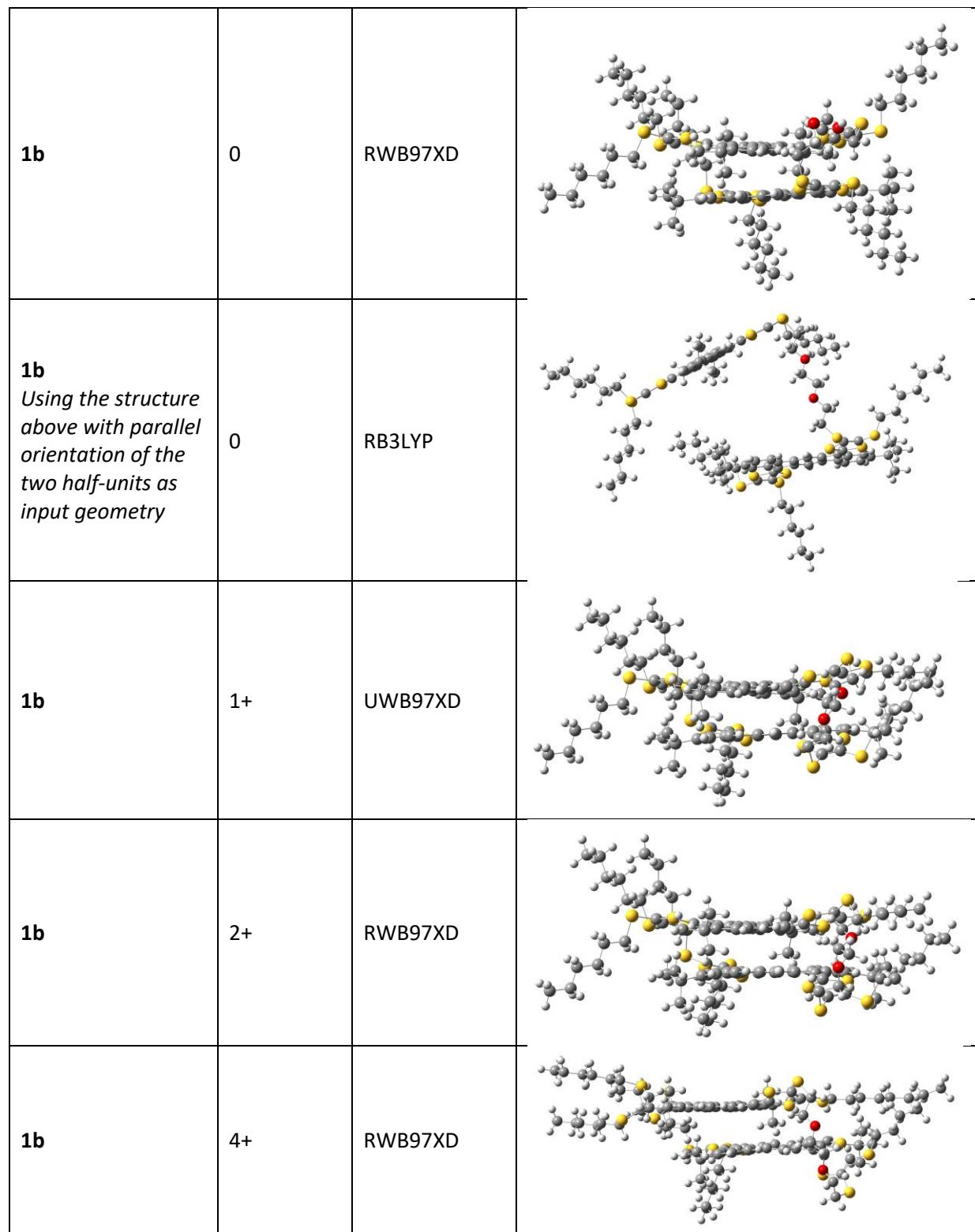
Structures of the IF-TTF dimers resulting from DFT calculations with the cc-pVDZ basis set. The functional is given in the table.

Compound	Oxidation state	Functional	Optimized structure
1a	0	RB3LYP	
1a	1+	UB3LYP	









<p><b>1a</b> without hexyl and t-butyl groups</p> <p><i>Using the structure above with parallel orientation of the two half-units, but without the hexyl and t-butyl groups, as input geometry</i></p>	4+	RWB97XD	
<p><b>1b</b> without hexyl and t-butyl groups</p> <p><i>Using the structure above with parallel orientation of the two half-units, but without the hexyl and t-butyl groups, as input geometry</i></p>	4+	RWB97XD	

## Computational output (geometries and energies)

### **1a 0 SPhSsyn (RB3LYP/cc-pVDZ):**

```
1\1\GINC-NODE226\FOpt\RB3LYP\CC-pVDZ\C112H138S16\HAMMERIC\16-Aug-2019\
0\\# opt=tight freq=noraman rb3lyp/cc-pvdz geom=connectivity\\Line 1a
neutral SPhSsyn\\0,1\C,-11.0141483572,-1.3572487837,-1.5431054988\C,-
9
.8334217161,-2.143420724,-1.6410913287\C,-9.7744943827,-
3.2102945965,-
2.5335231889\C,-10.8838272675,-3.505033804,-3.3345962053\C,-
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2.35308
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8.8712564181,-3.8199943171,-2.6130888475\H,-10.8131807157,-
4.345089130
3,-4.0245052875\H,-13.0241789712,-1.0825630756,-2.2955345215\C,-
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### **1a 0 SPhSsyn (RWB97XD/cc-pVDZ):**

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 [X(C112H138S16)  
 ]\\@

**1a 0 SPhSsyn with RWB97XD/cc-pVDZ (above) as input (B3LYP/cc-pVDZ):**

1\1\GINC-NODE215\FOpt\RB3LYP\CC-pVDZ\C112H138S16\HAMMERIC\10-Oct-2019\  
 0\\# opt=tight freq=noraman rb3lyp/cc-pvdz\\Line 1a neutral with  
 wb97xd

parallel aaa as input\\0,1\C,-5.4149014841,-6.0733356933,-  
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5.6  
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### **1a 1+ SPhSsyn (UWB97XD/cc-pVDZ):**

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$\backslash H, -0.961385649, 1.2225325355, -1.7017962451 \backslash C, -0.2602719459, -$   
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 $531028 \backslash H, -0.0563942924, -3.6620258419, -1.4885708112 \backslash \text{Version=EM64L-}$   
 G09R  
 $\text{evE.01} \backslash \text{State=1-A} \backslash \text{HF=-10722.1557354} \backslash \text{RMSD=5.353e-09} \backslash \text{RMSF=3.792e-}$   
 07 \Dipol  
 $e=0.040049, -1.4770728, -0.5932842 \backslash \text{Quadrupole}=740.5740676, -$   
 342.5541498, -  
 $398.0199178, -4.7094811, 29.0278768, 6.7835242 \backslash \text{PG=C01}$   
 $[\text{X(C112H138S16)}] \backslash \backslash @$

### **1a 2+ SPhSsyn (RWB97XD/cc-pVDZ):**

1\1\GINC-NODE234\FOpt\RwB97XD\CC-pVDZ\C112H138S16(2+)\ROOT\19-Apr-2019  
 $\backslash 0 \backslash \# \text{ opt=tight freq=noraman rwb97xd/cc-pvdz geom=connectivity} \backslash \text{Line}$   
 1  
 $a \text{ dication restricted} \backslash 2, 1 \backslash C, -0.7898157457, -$   
 3.9164267257, 1.1480446845\br/>
 $C, 0.6031258517, -3.7037091986, 1.2019161968 \backslash C, 1.4797124992, -$   
 4.7643332017  
 $, 1.0621335931 \backslash C, 0.9708427243, -6.0511372171, 0.8599594395 \backslash C, -$   
 0.404767016  
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 $5 \backslash C, -1.4594485735, -2.6079543001, 1.3785230295 \backslash C, -0.4552294565, -$   
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### **1a 4+ SPhSsyn (RWB97XD/cc-pVDZ):**

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### **1b 0 (RWB97XD/cc-pVDZ):**

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**1b 0 with RWB97XD/cc-pVDZ (above) as input (B3LYP/cc-pVDZ):**

1\1\GINC-NODE212\FOpt\RB3LYP\CC-pVDZ\C110H142O2S16\HAMMERIC\22-Sep-201  
 9\0\\# opt=tight freq=noraman rb3lyp/cc-pvdz\\Line 1b neutral with  
 par  
 allel as input\\0,1\C, -7.9175975937, -3.8688018155, -0.5852472666\C, -  
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 5.96438888, -1.7796252504\C, -8.6076547321, -4.6075441464, -  
 1.5580372927\C  
 , -8.0216857406, -2.4564176615, -0.1491089484\C, -7.0165601462, -  
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$6, 0.9228250218\text{C}, -6.3469683908, -3.5305142075, 1.1175972358\text{H}, -5.8335434$   
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 $625251, 2.0666535142\text{C}, -6.6481946394, -1.1876355709, 1.7104875376\text{H}, -7.12$   
 $14197131, -0.2127569695, 1.6083946415\text{C}, -5.635370445, -1.3475178538, 2.658$   
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 $775754171\text{C}, -3.6752294739, 1.0892969032, 5.5581056973\text{H}, -4.9390321784, 2.$   
 $737290439, 4.9322657838\text{C}, -8.8746332737, -1.4985958091, -0.6379241298\text{C}, -$   
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 $, -1.9391204364\text{s}, -8.9330958144, 0.1844503472, -0.0502086661\text{C}, -10.732591$   
 $8034, -0.1342520436, -1.9992787873\text{C}, -10.2195803076, 0.7639969467, -1.1238$   
 $119898\text{s}, -10.6635554039, 2.4797226918, -0.9708478646\text{s}, -12.0377848585, 0.$   
 $1496808157, -3.1739592904\text{C}, -11.0869535749, 0.9641149679, -4.5458646652\text{H}$

$, -10.6428584089, 1.8841901316, -4.1374121773 \text{H}, -$   
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 $2.5248191$   
 $293, 6.1404421028 \text{H}, 3.0541041374, -$   
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 $\text{H}, 4.4785499518, -2.6769275031, 9.1607455549 \text{C}, 0.0878177482, -$   
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 $, 2.101879059 \text{H}, -0.3692034064, -5.7148932856, 2.0672488609 \text{H}, -$   
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$\backslash H, -11.9103633279, 4.2974294302, 0.9597704721 \backslash H, -$   
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 $219, -0.5079306513 \backslash C, -13.9737150891, 3.7028261872, 1.2772547274 \backslash H, -$   
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**1b 1+ (UB3LYP/cc-pVDZ):**

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 G09RevE.01\\State=2-A\\HF=-10799.0252859\\S2=0.753411\\S2-  
 1=0.\\S2A=0.75001  
 \\RMSD=1.016e-09\\RMSF=1.538e-07\\Dipole=0.7048312, -  
 0.4285722, 0.424359\\Qu  
 adrupole=141.1165071, 6.9381271, -148.0546342, 32.412537, -0.7974474, -  
 2.08  
 78743\\PG=C01 [X(C110H142O2S16)]\\@

### **1b 1+ (UWB97XD/cc-pVDZ):**

1\\1\\GINC-NODE216\\FOpt\\UWB97XD\\CC-pVDZ\\C110H142O2S16(1+, 2)\\HAMMERIC\\03-  
 Sep-2019\\0\\# opt=tight freq=noram uwb97xd/cc-pvdz\\Line 1b radical  
 cation parallel (restart after node failure)\\1,2\\c,1.6571791186, -  
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**1b 2+ (RB3LYP/cc-pVDZ):**

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### **1a 4+ without the hexyl and t-butyl groups (RWB97XD/cc-pVDZ):**

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893.1552154  
  
\PG=C01 [X(C60H34S16)] \\@

### **1b 4+ without the hexyl and t-butyl groups (RWB97XD/cc-pVDZ):**

1\1\GINC-SLEJPNER\FOpt\RwB97XD\CC-pVDZ\C58H38O2S16(4+)\HAMMERICH\18-Ja  
n-2020\0\#\ opt=tight freq=noraman rwb97xd/cc-pvdz\Line 1b  
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 $, 3.0267664073, -3.8945706248, -1.260723486 \backslash S, 4.1210073598, -$   
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