

## SUPPORTING INFORMATION

### Push-pull derivatives based on 2,4'-biphenylene linker with quinoxaline, [1,2,5]oxadiazolo[3,4-*b*]pyrazine and [1,2,5]thiadiazolo[3,4-*b*]pyrazine electron withdrawing parts

Egor V. Verbitskiy,<sup>a,b,\*</sup> Pascal le Poul,<sup>c</sup> Filip Bureš,<sup>d,\*</sup> Sylvain Achelle,<sup>c,\*</sup> Alberto Barsella<sup>e</sup>, Yuriy A. Kvashnin<sup>a</sup>, Gennady L. Rusinov<sup>a,b</sup>, Valery N. Charushin<sup>a,b</sup>

<sup>a</sup>*I. Postovsky Institute of Organic Synthesis, Ural Branch of the Russian Academy of Sciences, S. Kovalevskaya Str., 22, Ekaterinburg, 620108, Russia*

<sup>b</sup>*Ural Federal University, Mira St. 19, Ekaterinburg, 620002, Russia*

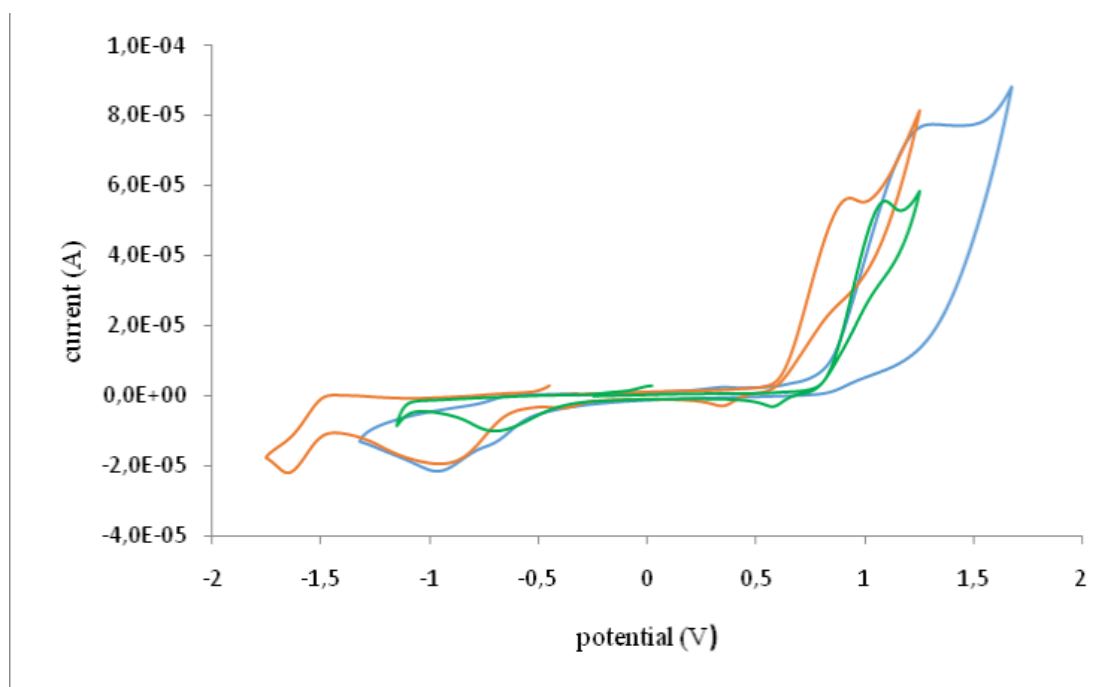
<sup>c</sup>*Univ Rennes, CNRS, Institut des Sciences Chimiques de Rennes – UMR 6226, 35000 Rennes, France*

<sup>d</sup>*Institute of Organic Chemistry and Technology, Faculty of Chemical Technology, University of Pardubice Studenská 573, Pardubice, 53210, Czech Republic*

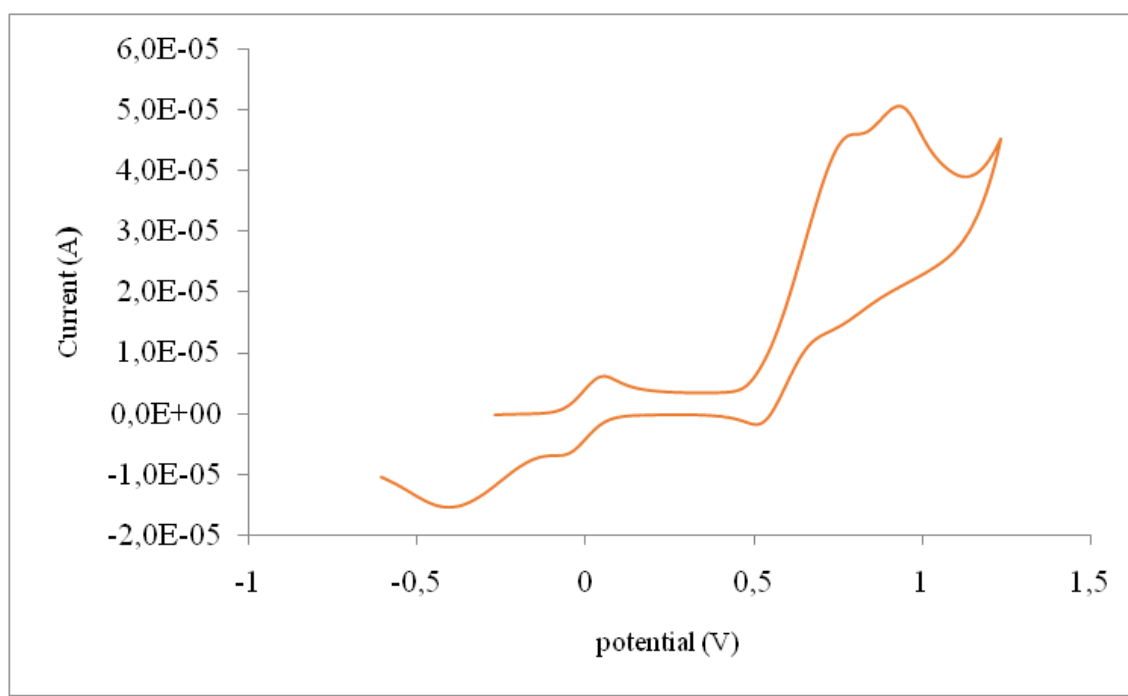
<sup>e</sup>*Département d'Optique ultrarapide et Nanophotonique, IPCMS, UMR CNRS 7504, Université de Strasbourg, 23 rue du Loess, BP 43, 67034 Strasbourg Cedex 2, France*

<b>Figure S1.</b> Oxidation study of compounds <b>9b</b> (green), <b>10b</b> (orange) and <b>11b</b> (blue). .....	3
<b>Figure S2.</b> Oxidation study of compound <b>11a</b> . .....	3
<b>Figure S3:</b> Normalized emission spectra of compound <b>11b</b> in a series of aprotic solvents ( $c \sim 1 \times 10^{-5}$ M). .....	4
<b>Figure S4:</b> Fluorescence color change experienced by <b>11b</b> in various solvents (from left to right: n-heptane, toluene, 1,4-dioxane, CHCl <sub>3</sub> , DCM) The picture was taken in the dark upon irradiation with a handheld UV lamp ( $\lambda_{em} = 366$ nm) .....	4
<b>Figure S5:</b> Emission spectra of compound <b>11b</b> in MeCN/water mixture ( $c = 1.5 \times 10^{-5}$ M, $\lambda_{exc} = 340$ nm). .....	5
<b>Figure S6:</b> Fluorescence color of compound <b>11b</b> in MeCN/water mixture (from left to right: 0% 50%, 80% 97% of water) The picture was taken in the dark upon irradiation with a handheld UV lamp ( $\lambda_{em} = 366$ nm). .....	5
<b>Figure S7:</b> A correlation of the experimental (ELCH) and DFT-calculated HOMO–LUMO gaps of chromophores <b>9–11</b> . .....	6
<b>Figure S8:</b> TD-DFT ( $nstates = 8$ ) B3LYP/6-311+G(2d,f,p) calculated UV-Vis spectra of chromophores <b>1a–9a</b> in CHCl <sub>3</sub> (red curves) along with the experimental spectra (black curves). Red vertical lines represent oscillator strengths ( $f$ ). .....	7

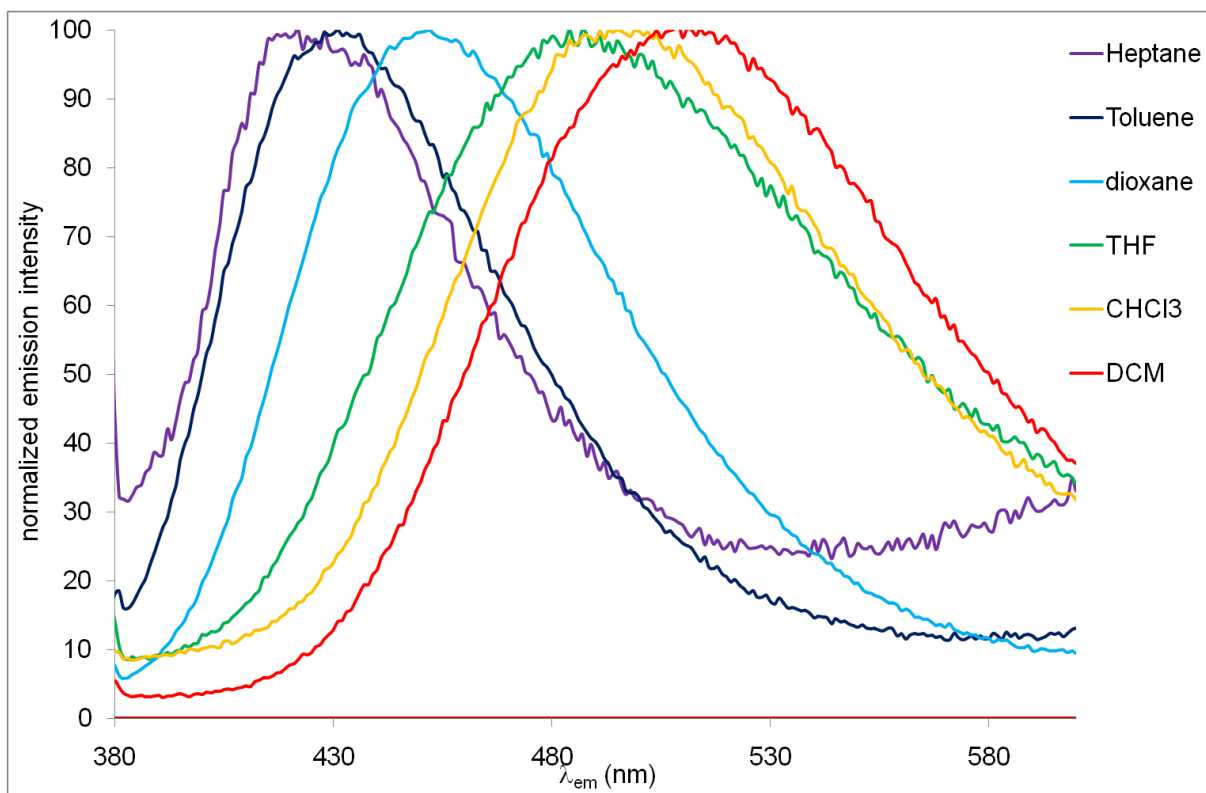
<b>Figure S9:</b> A correlation of the experimental (EXP) and DFT-calculated $\lambda_{\text{max}}$ values of chromophores <b>9–11</b> .	7
<b>Figure S10.</b> $^1\text{H}$ NMR (600 MHz, DMSO- $d_6$ ) spectrum of <b>6</b> .	8
<b>Figure S11.</b> $^{13}\text{C}$ NMR (151 MHz, DMSO- $d_6$ ) spectrum of <b>6</b> .	8
<b>Figure S12.</b> $^1\text{H}$ NMR (600 MHz, DMSO- $d_6$ ) spectrum of <b>9a</b> .	9
<b>Figure S13.</b> $^{13}\text{C}$ NMR (151 MHz, DMSO- $d_6$ ) spectrum of <b>9a</b> .	9
<b>Figure S14.</b> $^1\text{H}$ NMR (600 MHz, DMSO- $d_6$ ) spectrum of <b>9b</b> .	10
<b>Figure S15.</b> $^{13}\text{C}$ NMR (151 MHz, DMSO- $d_6$ ) spectrum of <b>9b</b> .	10
<b>Figure S16.</b> $^1\text{H}$ NMR (600 MHz, DMSO- $d_6$ ) spectrum of <b>10a</b> .	11
<b>Figure S17.</b> $^{13}\text{C}$ NMR (151 MHz, DMSO- $d_6$ ) spectrum of <b>10a</b> .	11
<b>Figure S18.</b> $^1\text{H}$ NMR (600 MHz, DMSO- $d_6$ ) spectrum of <b>10b</b> .	12
<b>Figure S19.</b> $^{13}\text{C}$ NMR (151 MHz, DMSO- $d_6$ ) spectrum of <b>10b</b> .	12
<b>Figure S20.</b> $^1\text{H}$ NMR (600 MHz, DMSO- $d_6$ ) spectrum of <b>11a</b> .	13
<b>Figure S21.</b> $^{13}\text{C}$ NMR (151 MHz, DMSO- $d_6$ ) spectrum of <b>11a</b> .	14
<b>Figure S22.</b> $^1\text{H}$ NMR (600 MHz, DMSO- $d_6$ ) spectrum of <b>11b</b> .	14
<b>Figure S23.</b> $^{13}\text{C}$ NMR (151 MHz, DMSO- $d_6$ ) spectrum of <b>11b</b> .	15
<b>Figure S24.</b> IR spectrum of <b>9a</b> .	15
<b>Figure S25.</b> IR spectrum of <b>9b</b> .	16
<b>Figure S26.</b> IR spectrum of <b>10a</b> .	16
<b>Figure S27.</b> IR spectrum of <b>10b</b> .	17
<b>Figure S28.</b> IR spectrum of <b>11a</b> .	17
<b>Figure S29.</b> IR spectrum of <b>11b</b> .	18
TD-DFT data of chromophore <b>9a</b> .	18
TD-DFT data of chromophore <b>9b</b> .	19
TD-DFT data of chromophore <b>10a</b> .	20
TD-DFT data of chromophore <b>10b</b> .	21
TD-DFT data of chromophore <b>11a</b> .	22
TD-DFT data of chromophore <b>11b</b> .	23



**Figure S1.** Oxidation study of compounds **9b** (*green*), **10b** (*orange*) and **11b** (*blue*).



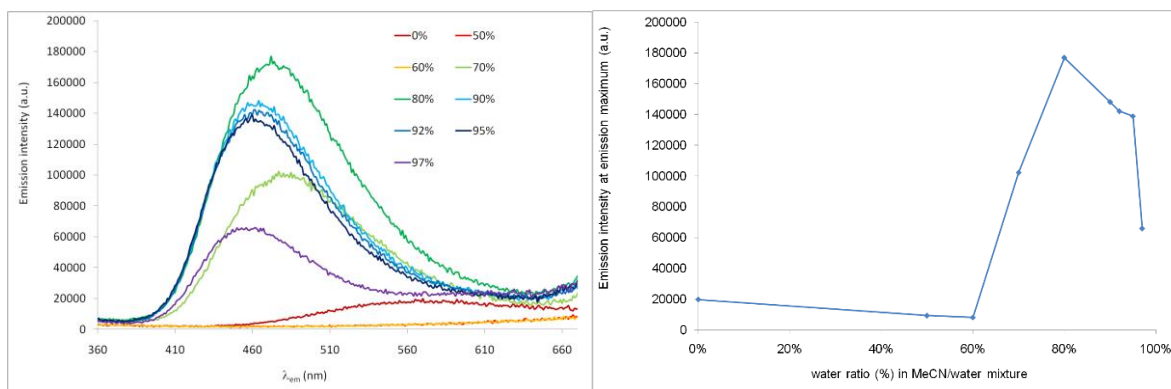
**Figure S2.** Oxidation study of compound **11a**.



**Figure S3:** Normalized emission spectra of compound **11b** in a series of aprotic solvents ( $c \sim 1 \times 10^{-5}$  M).



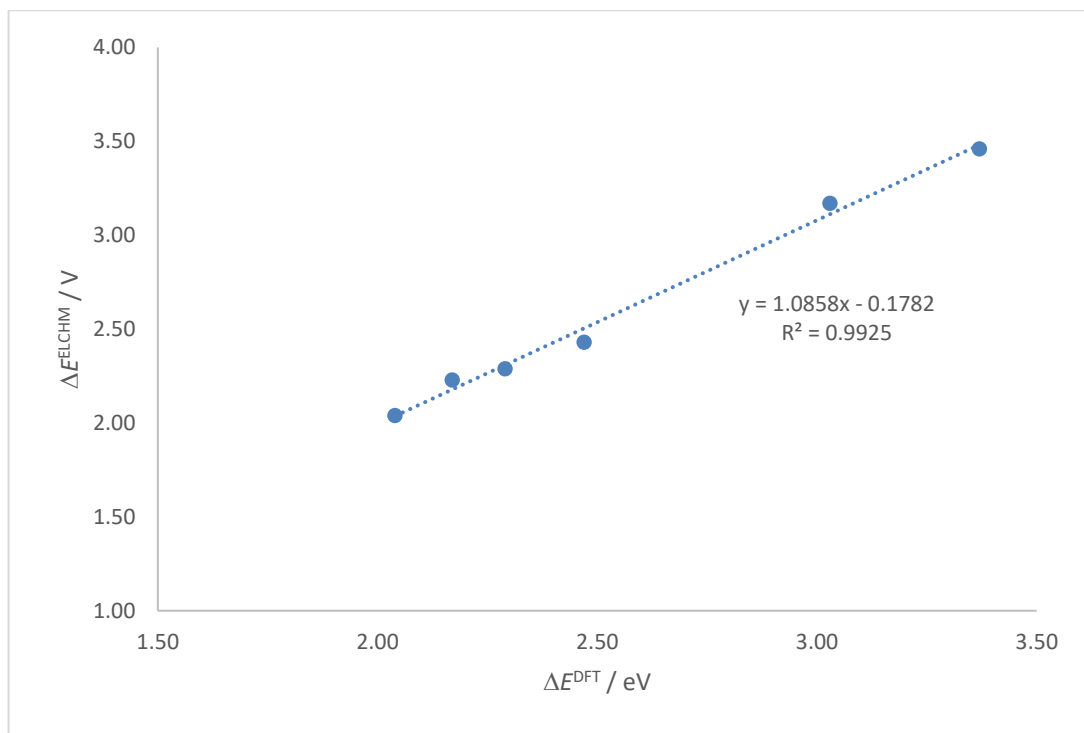
**Figure S4:** Fluorescence color change experienced by **11b** in various solvents (from left to right: n-heptane, toluene, 1,4-dioxane,  $\text{CHCl}_3$ , DCM) The picture was taken in the dark upon irradiation with a handheld UV lamp ( $\lambda_{em} = 366$  nm)



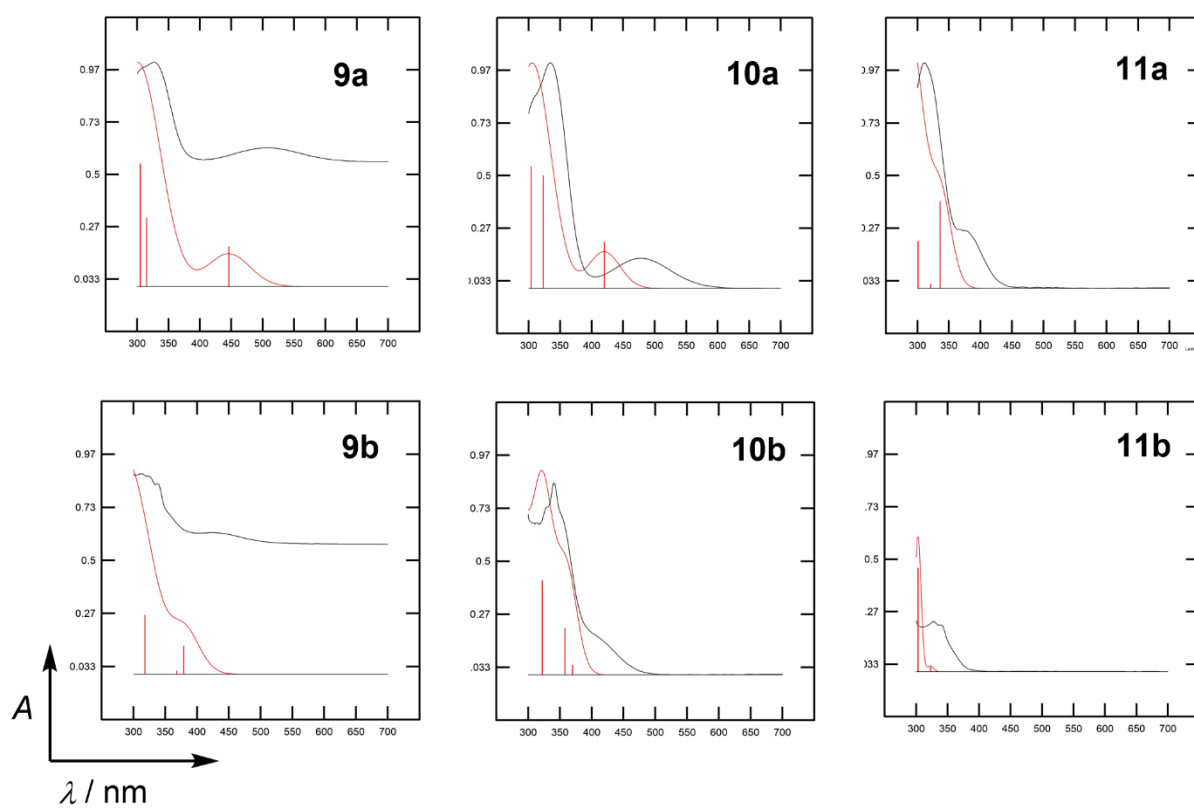
**Figure S5:** Emission spectra of compound **11b** in MeCN/water mixture ( $c = 1.5 \times 10^{-5}$  M,  $\lambda_{exc} = 340$  nm).



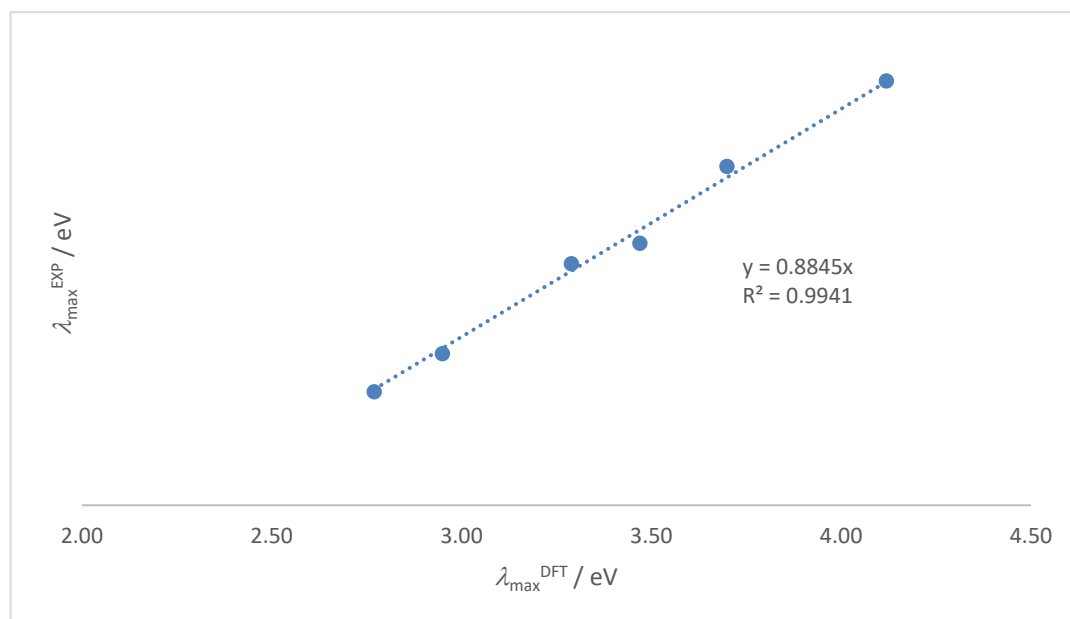
**Figure S6:** Fluorescence color of compound **11b** in MeCN/water mixture (from left to right: 0% 50%, 80% 97% of water) The picture was taken in the dark upon irradiation with a handheld UV lamp ( $\lambda_{em} = 366$  nm).



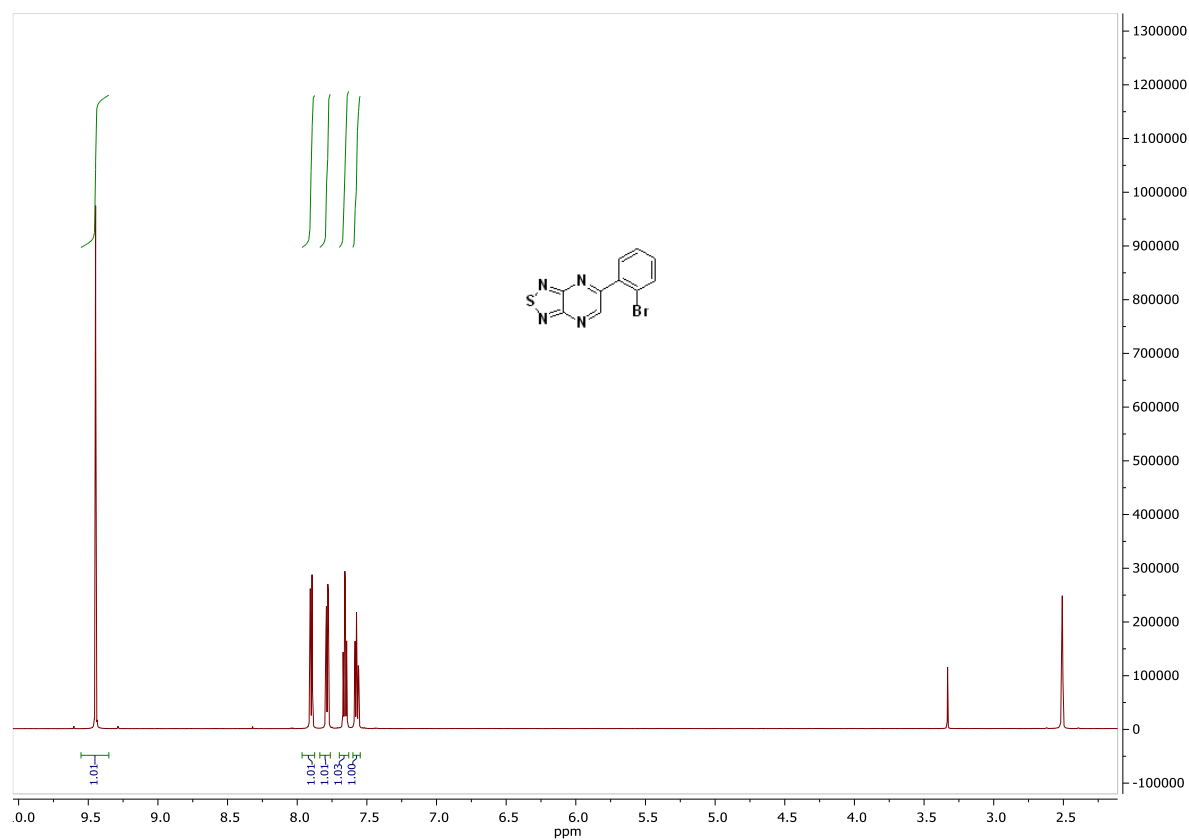
**Figure S7:** A correlation of the experimental (ELCHM) and DFT-calculated HOMO–LUMO gaps of chromophores **9–11**.



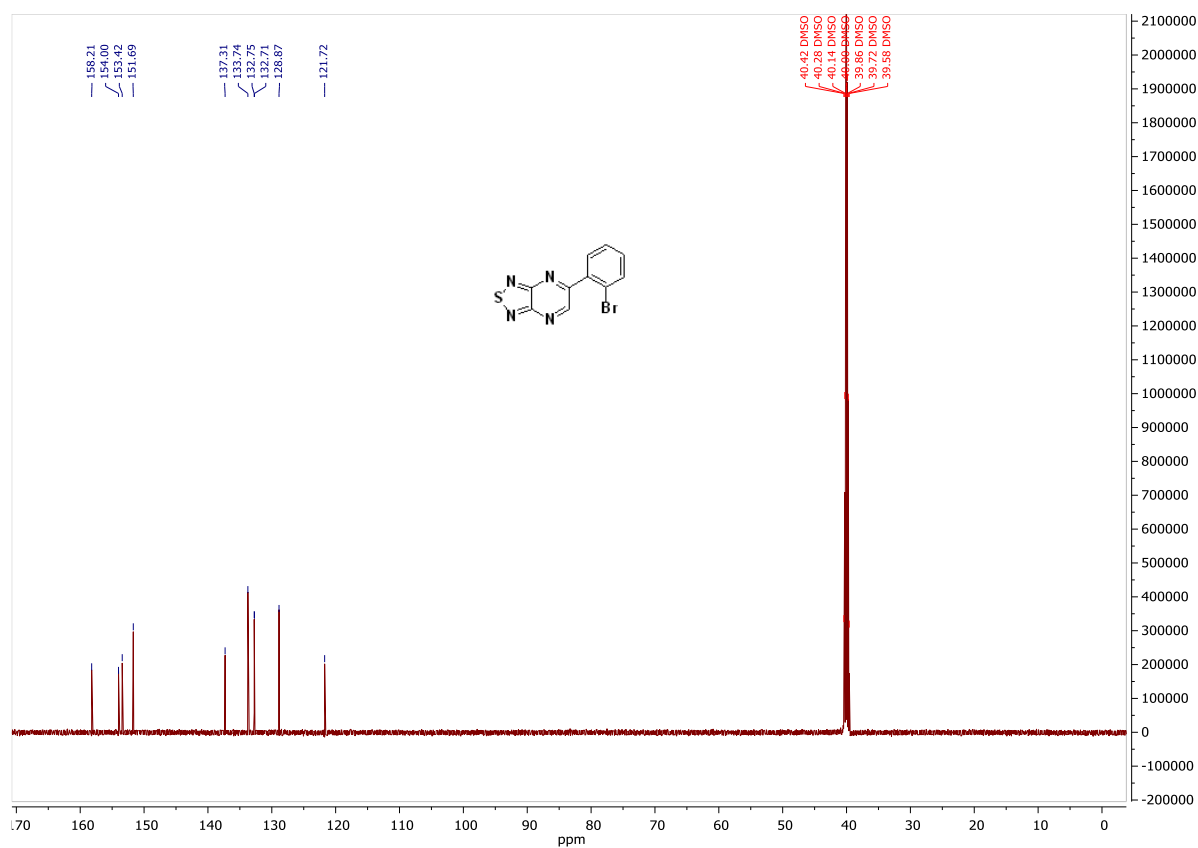
**Figure S8:** TD-DFT ( $n_{\text{states}} = 8$ ) B3LYP/6-311+G(2d,f,p) calculated UV-Vis spectra of chromophores **1a–9a** in  $\text{CHCl}_3$  (red curves) along with the experimental spectra (black curves). Red vertical lines represent oscillator strengths ( $f$ ).



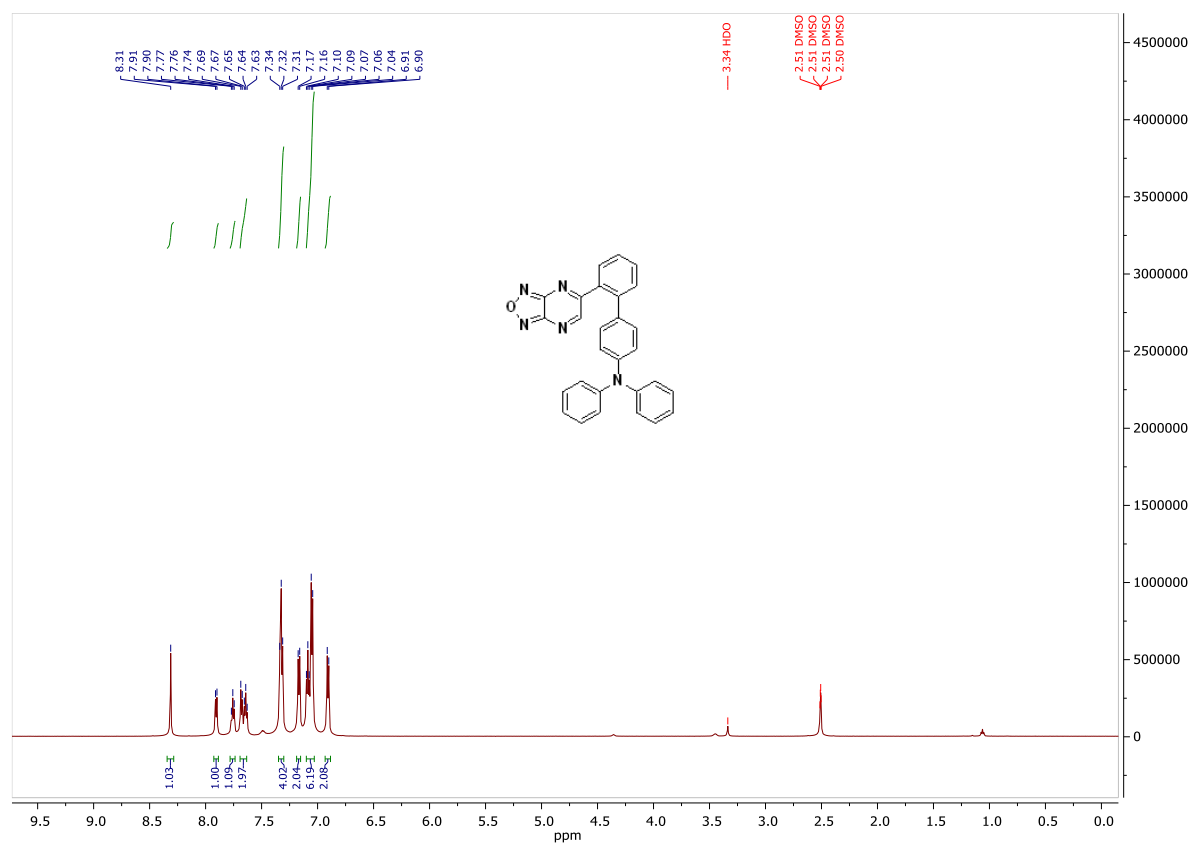
**Figure S9:** A correlation of the experimental (EXP) and DFT-calculated  $\lambda_{\text{max}}$  values of chromophores **9–11**.



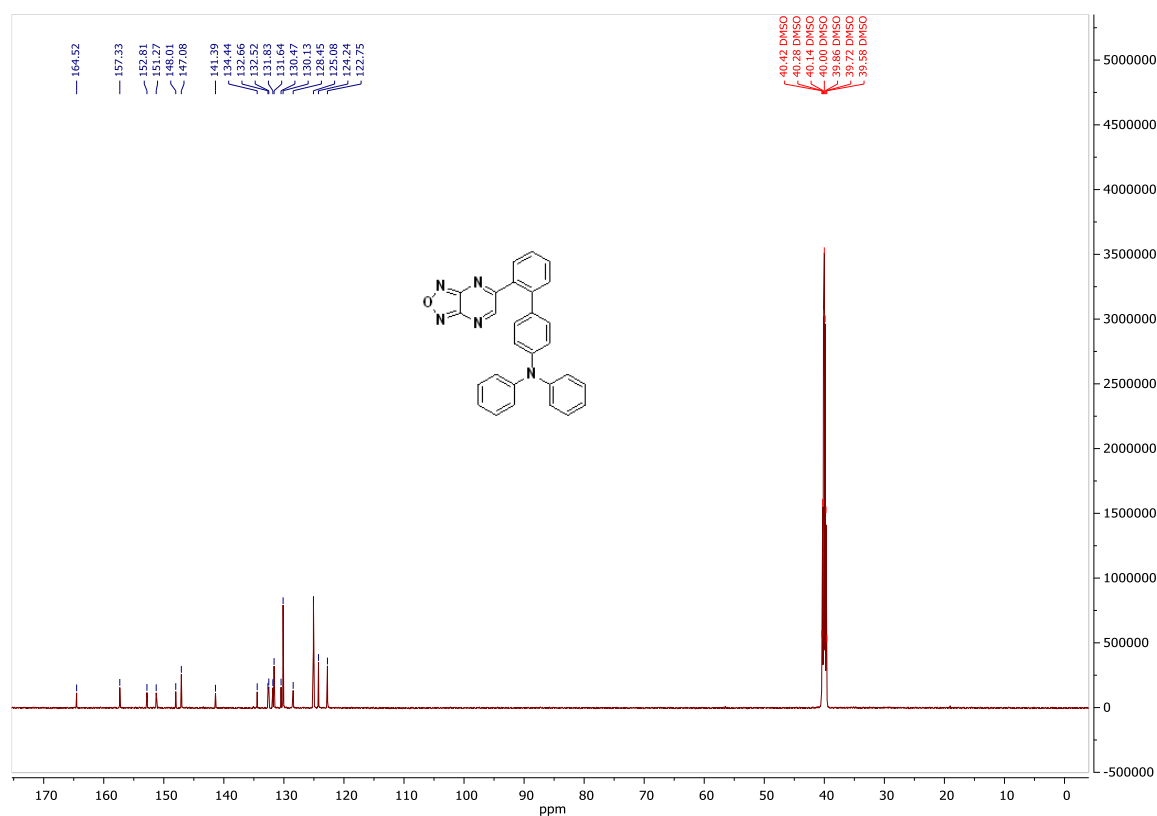
**Figure S10.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **6**.



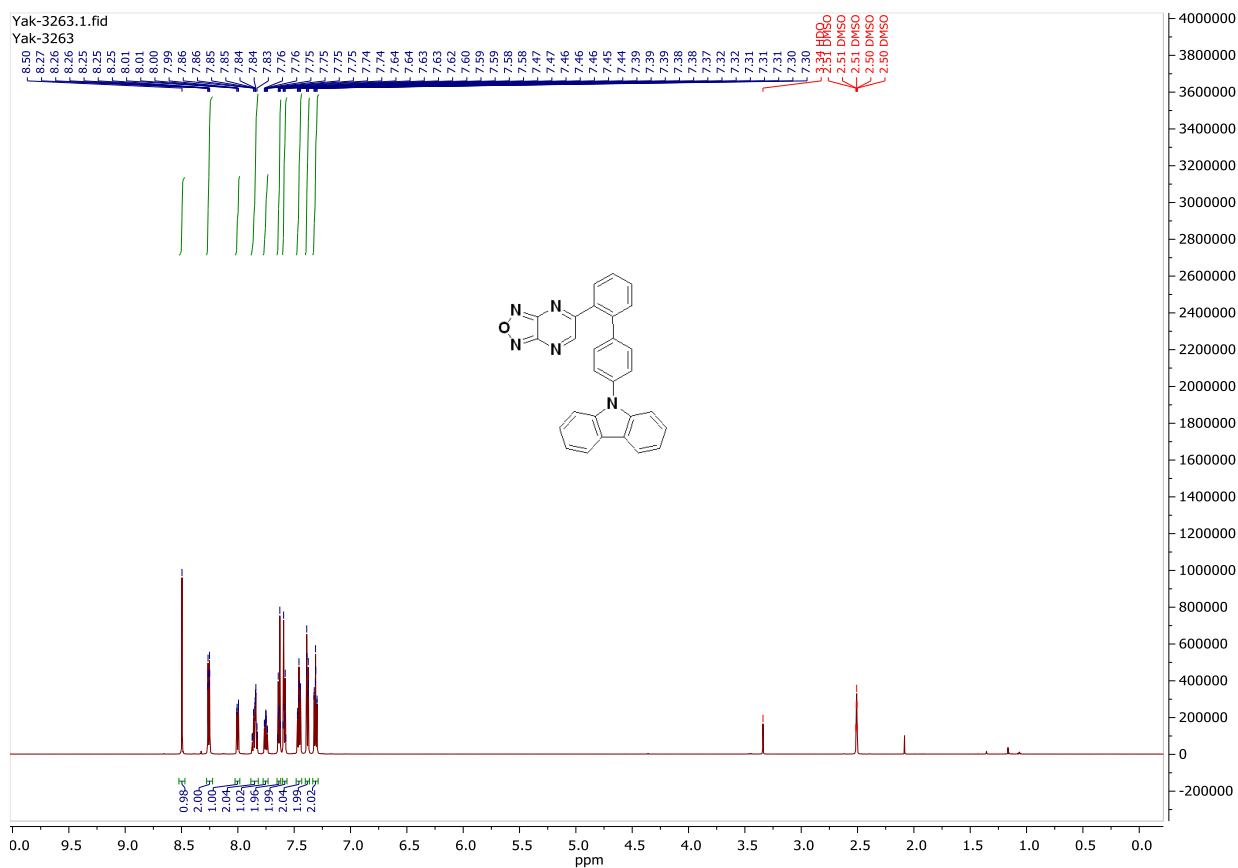
**Figure S11.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of **6**.



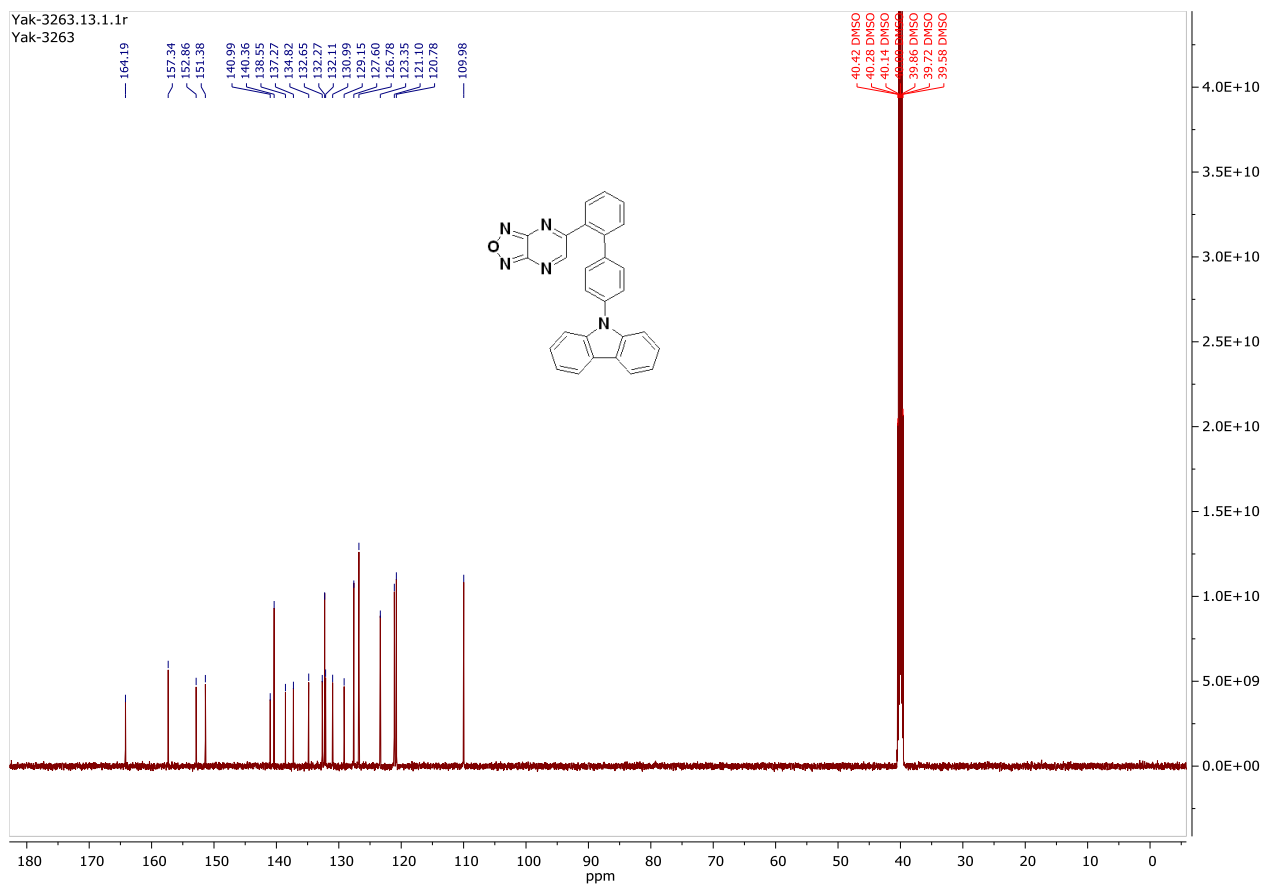
**Figure S12.**  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ ) spectrum of **9a**.



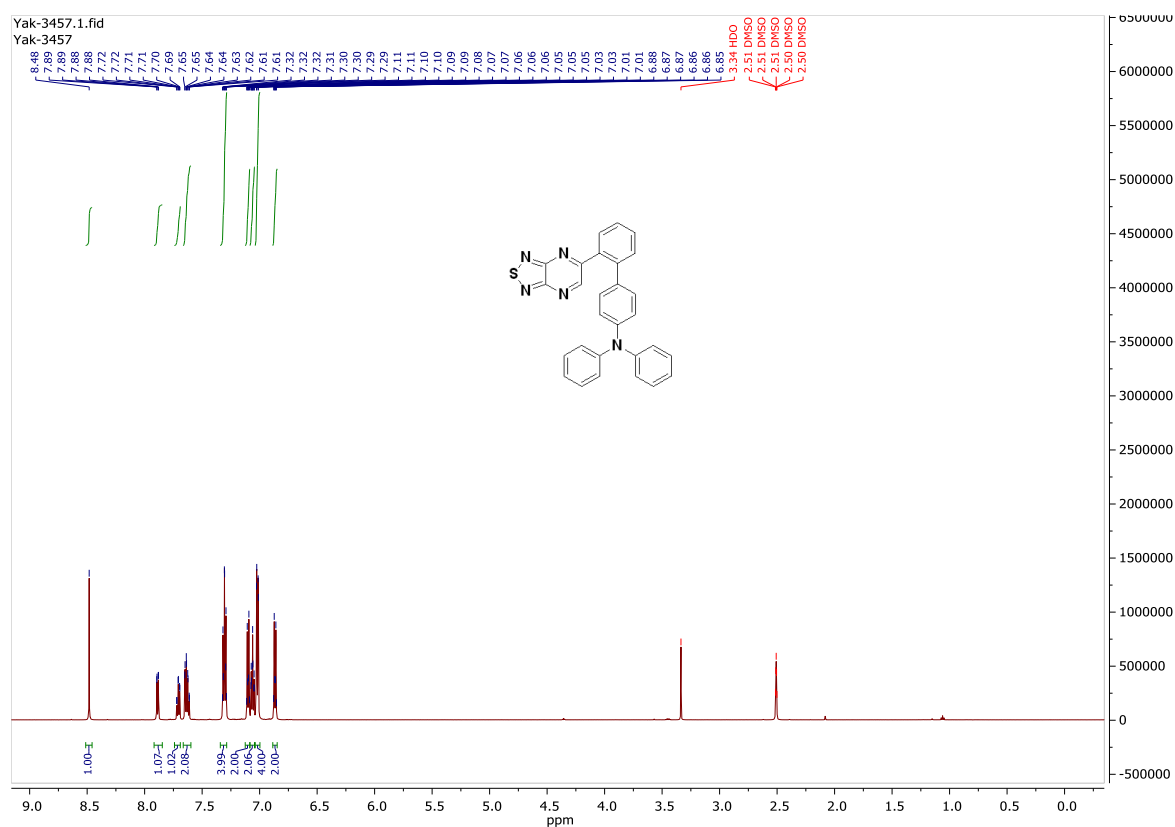
**Figure S13.**  $^{13}\text{C}$  NMR (151 MHz, DMSO- $d_6$ ) spectrum of **9a**.



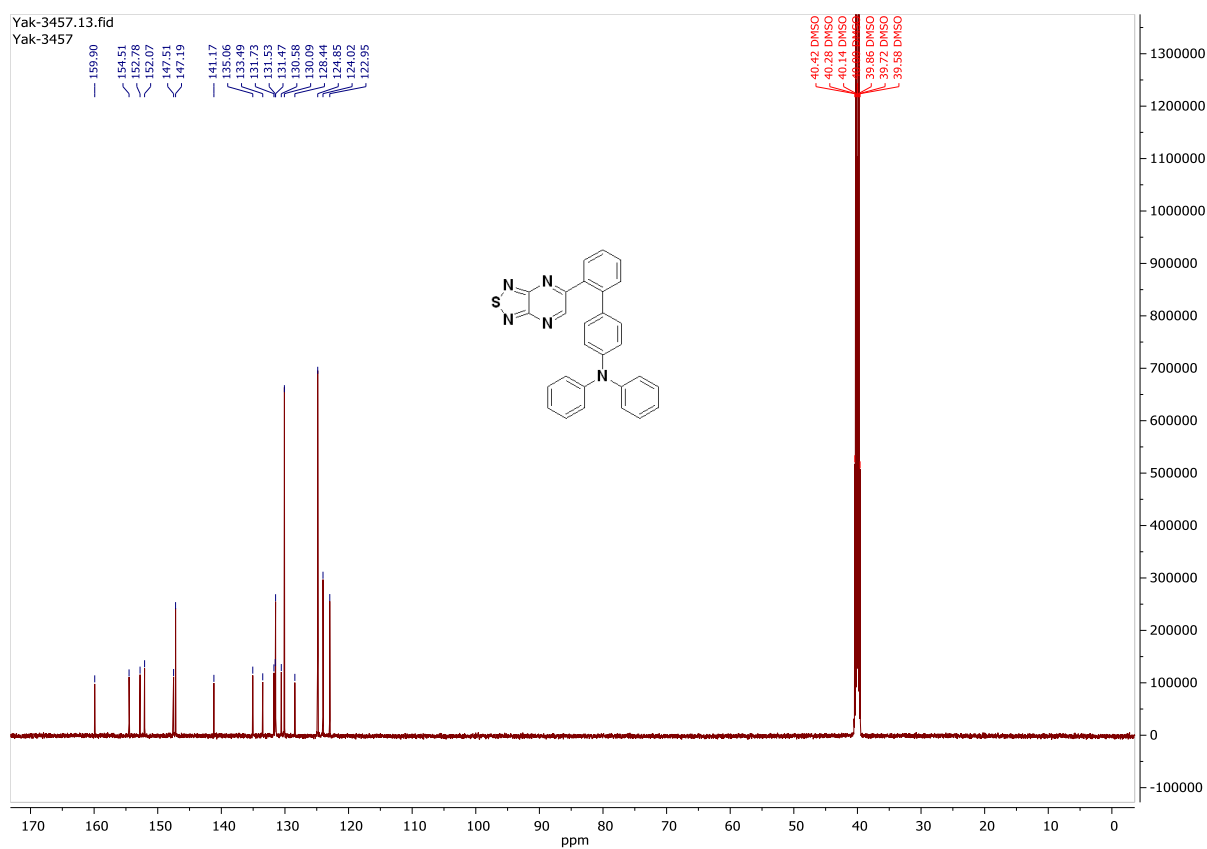
**Figure S14.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **9b**.



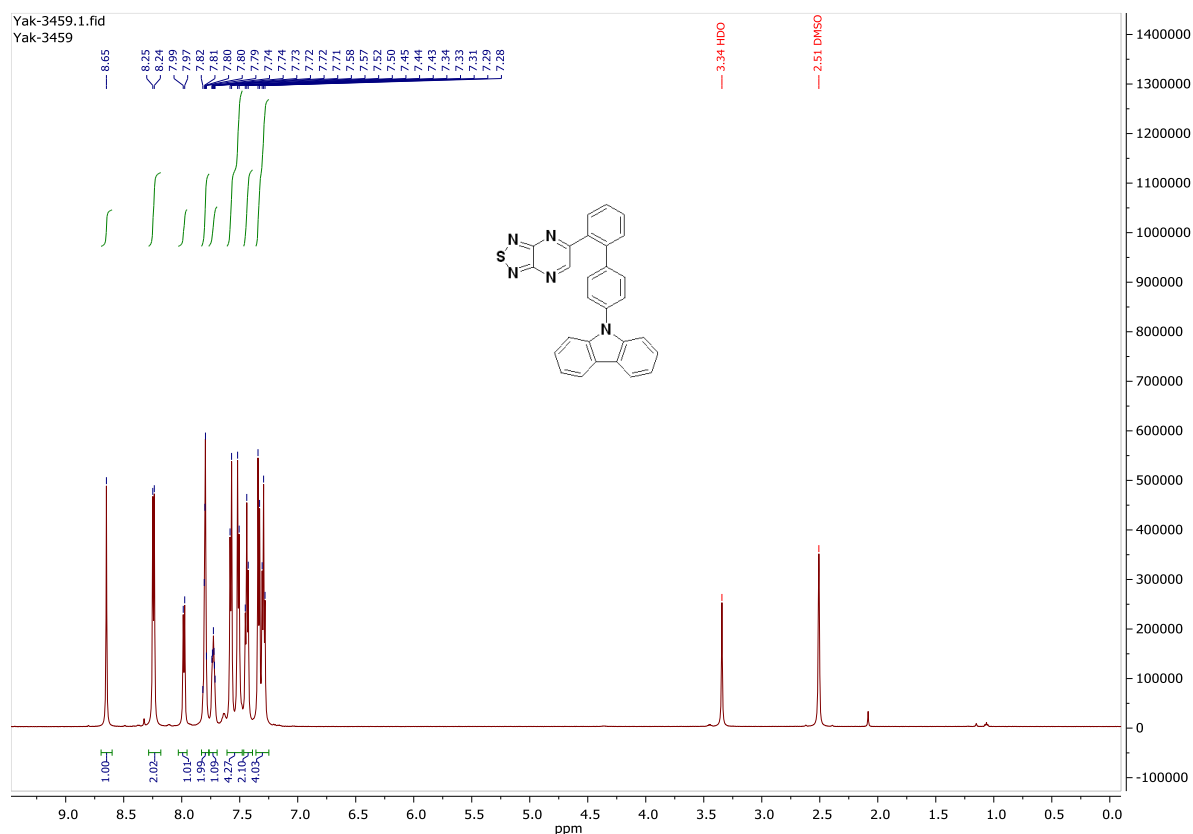
**Figure S15.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of **9b**.



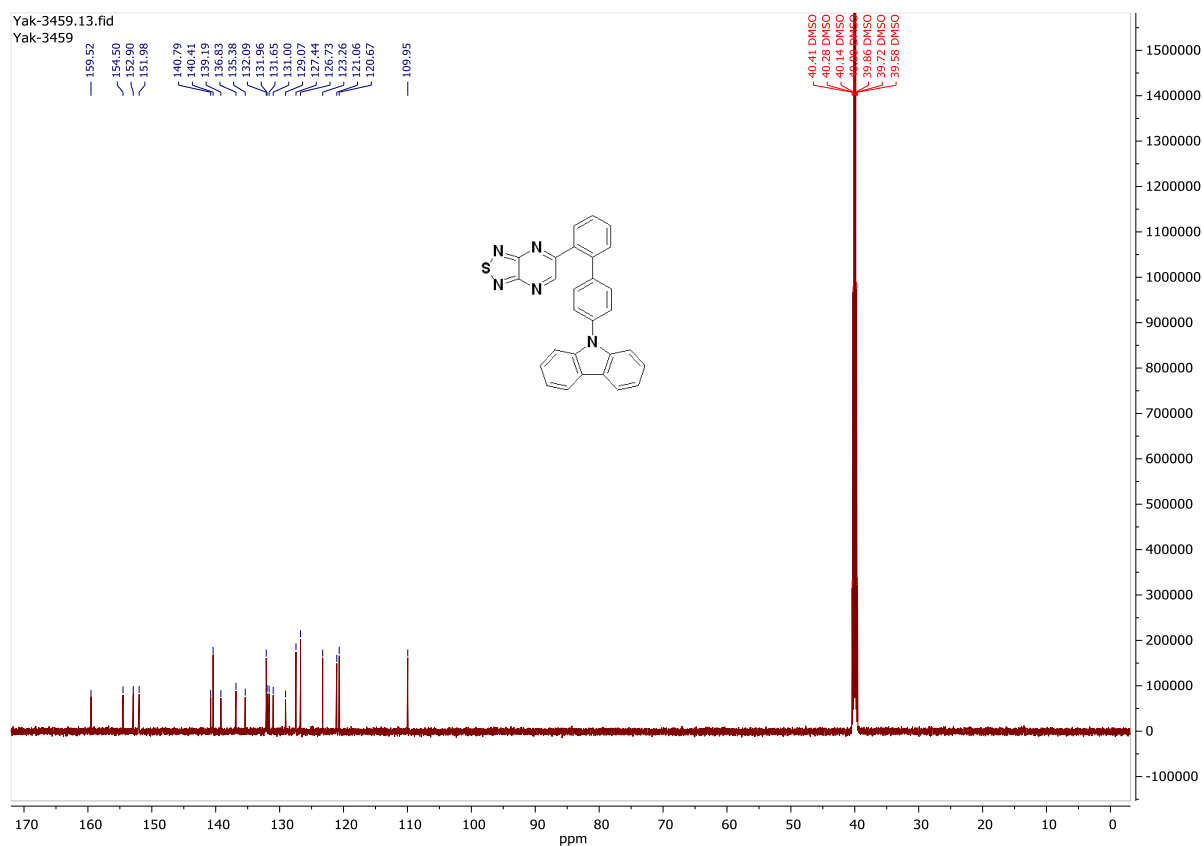
**Figure S16.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **10a**.



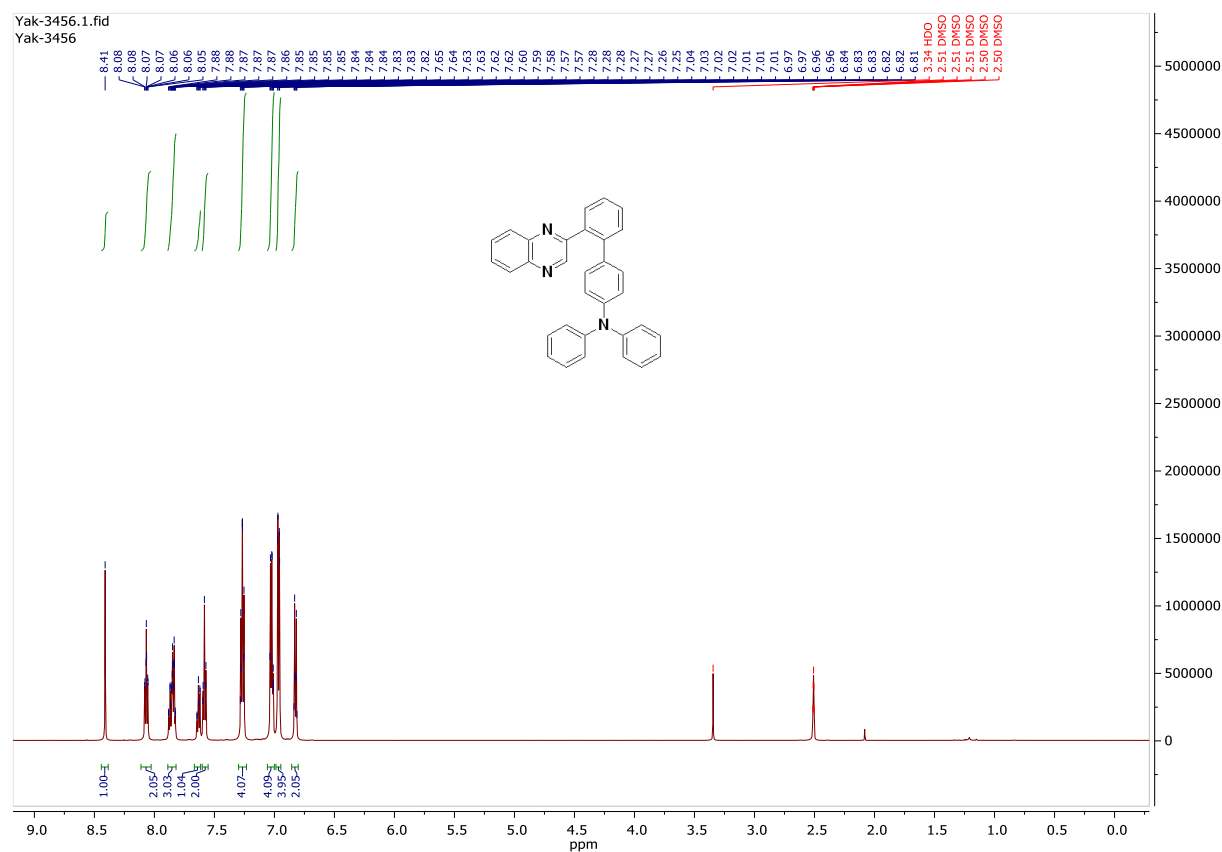
**Figure S17.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of **10a**.



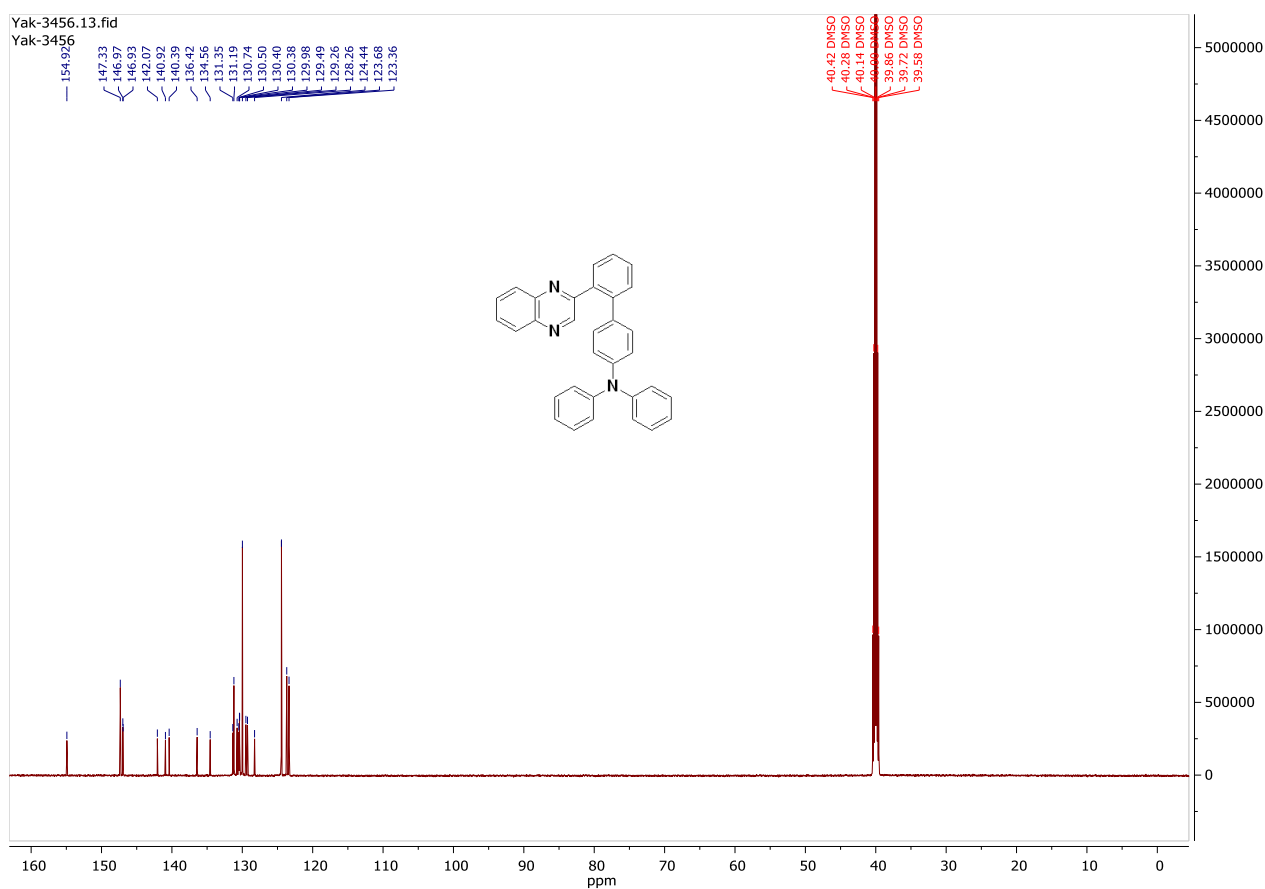
**Figure S18.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **10b**.



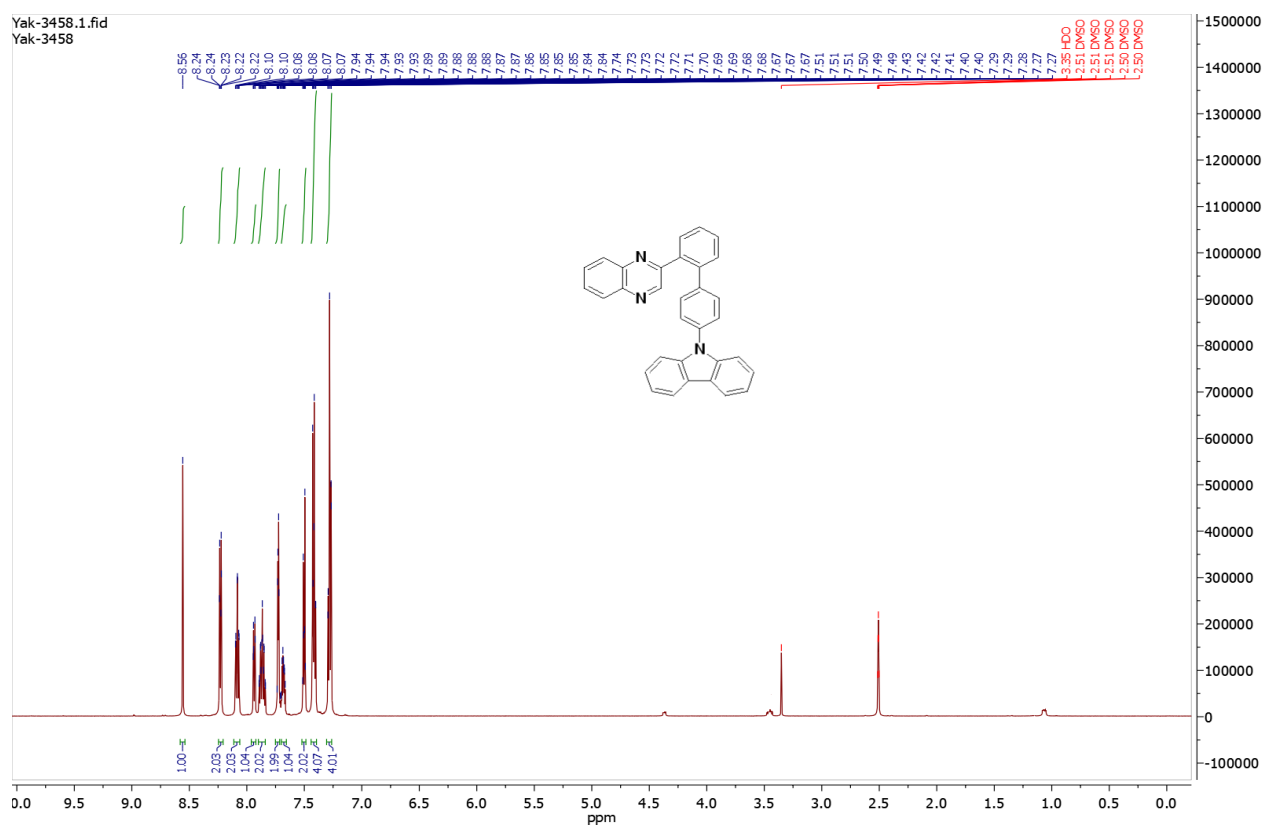
**Figure S19.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of **10b**.



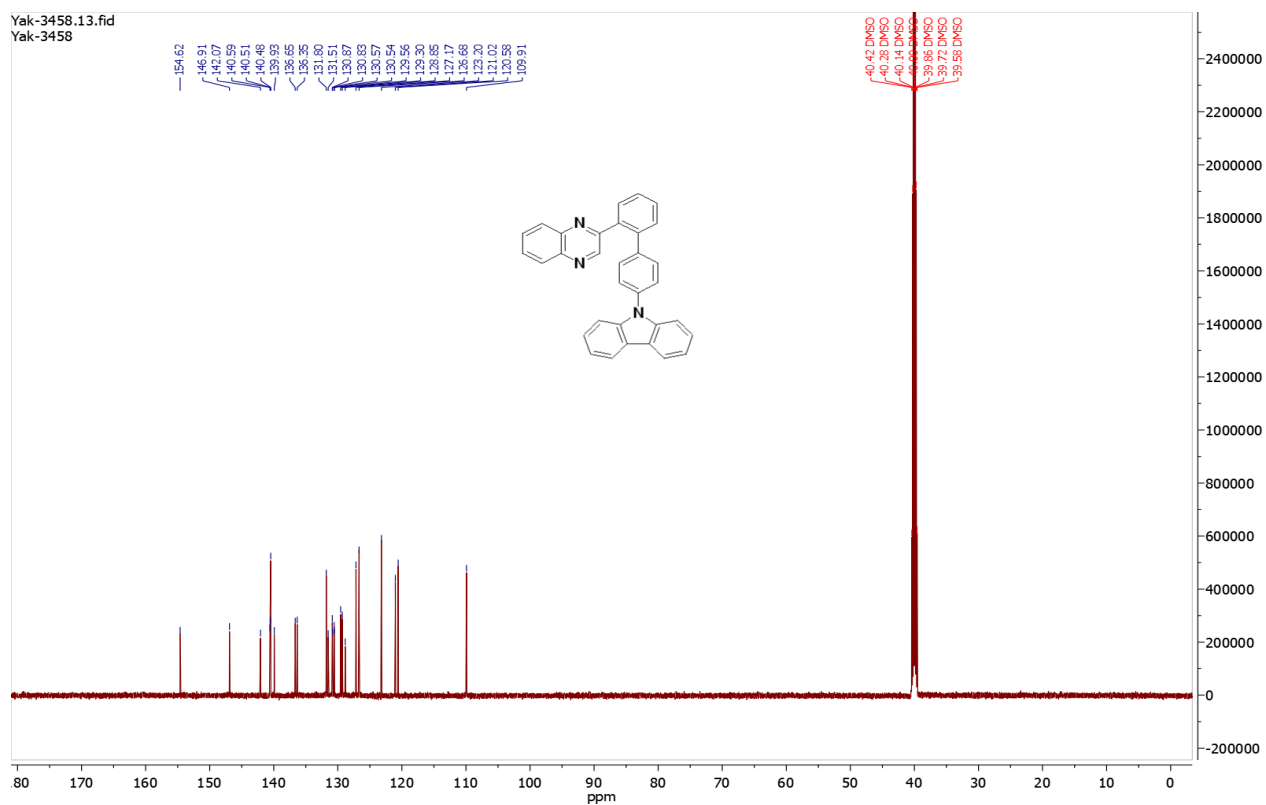
**Figure S20.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of **11a**.



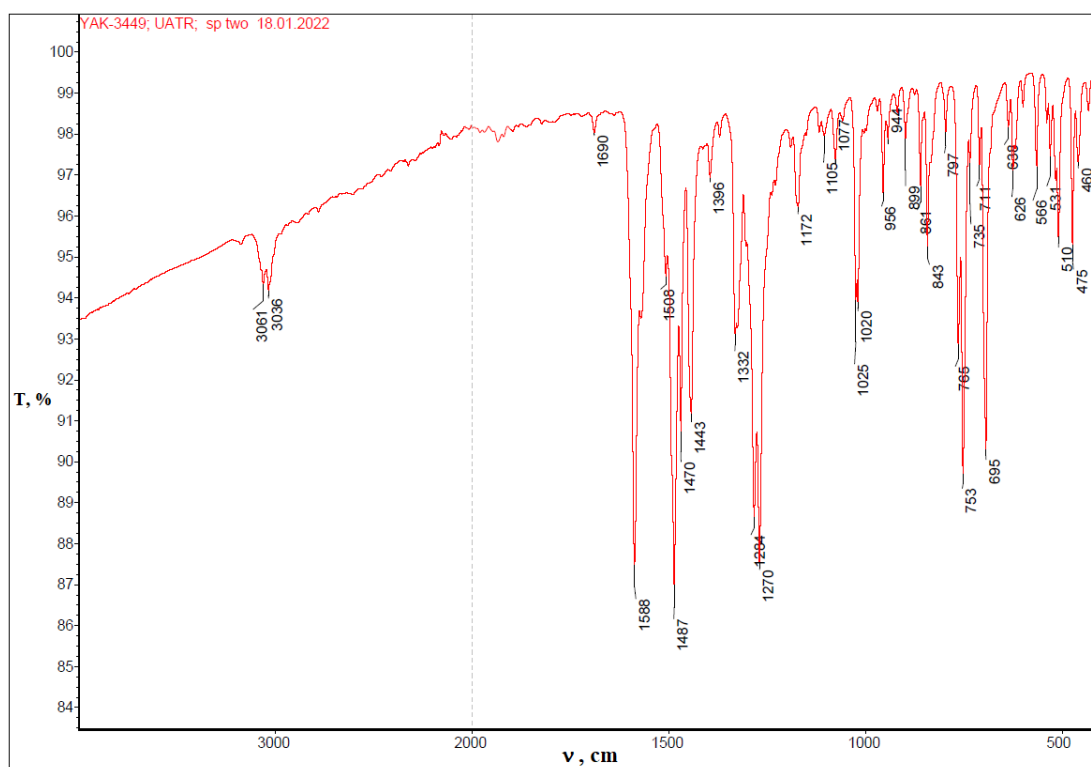
**Figure S21.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **11a**.



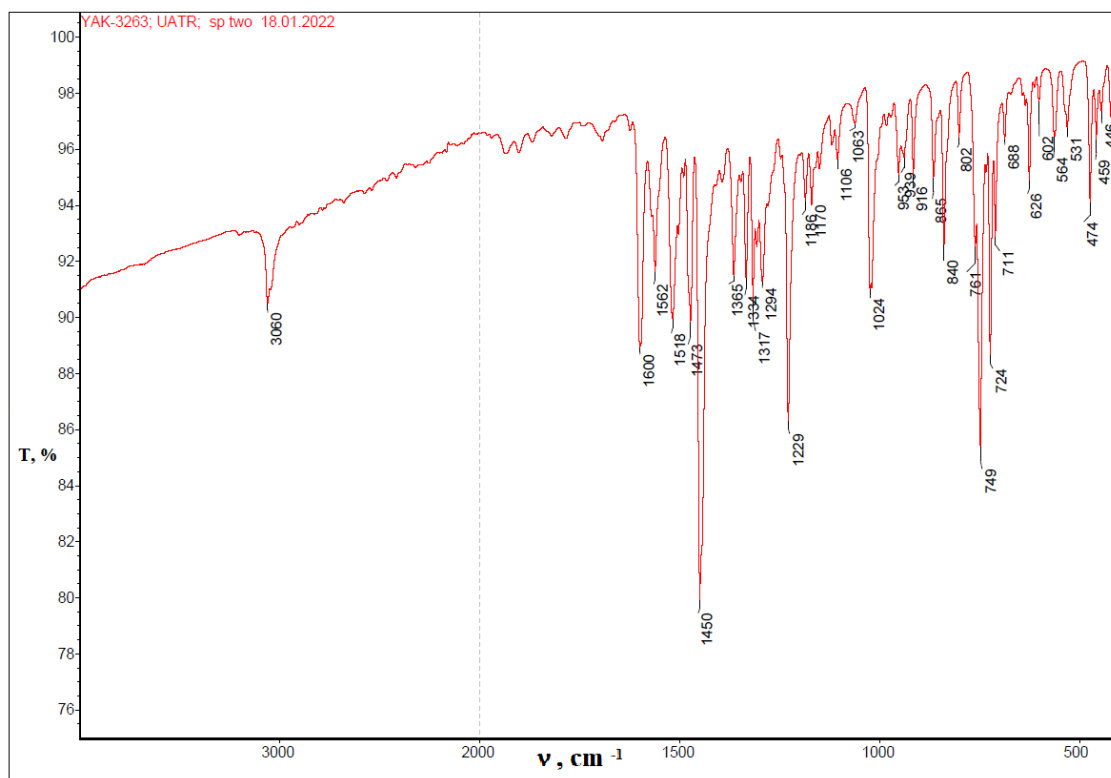
**Figure S22.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of **11b**.



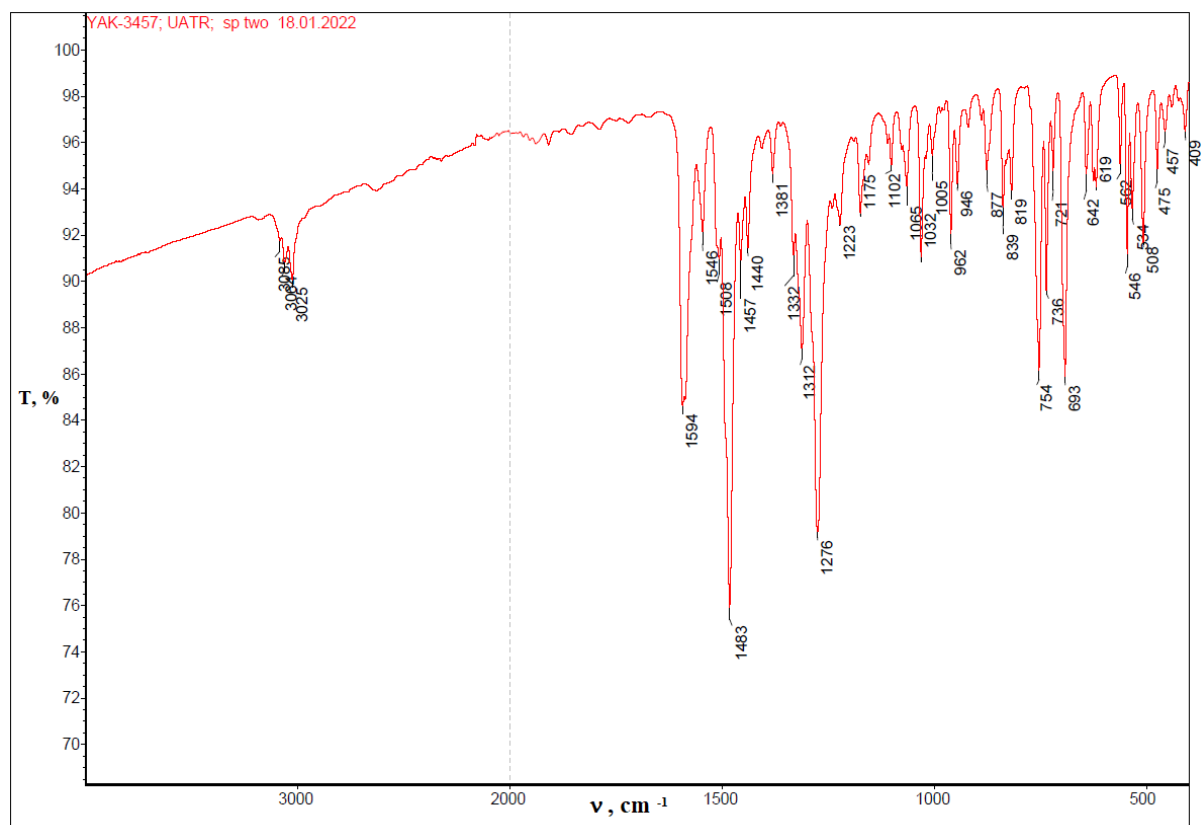
**Figure S23.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **11b**.



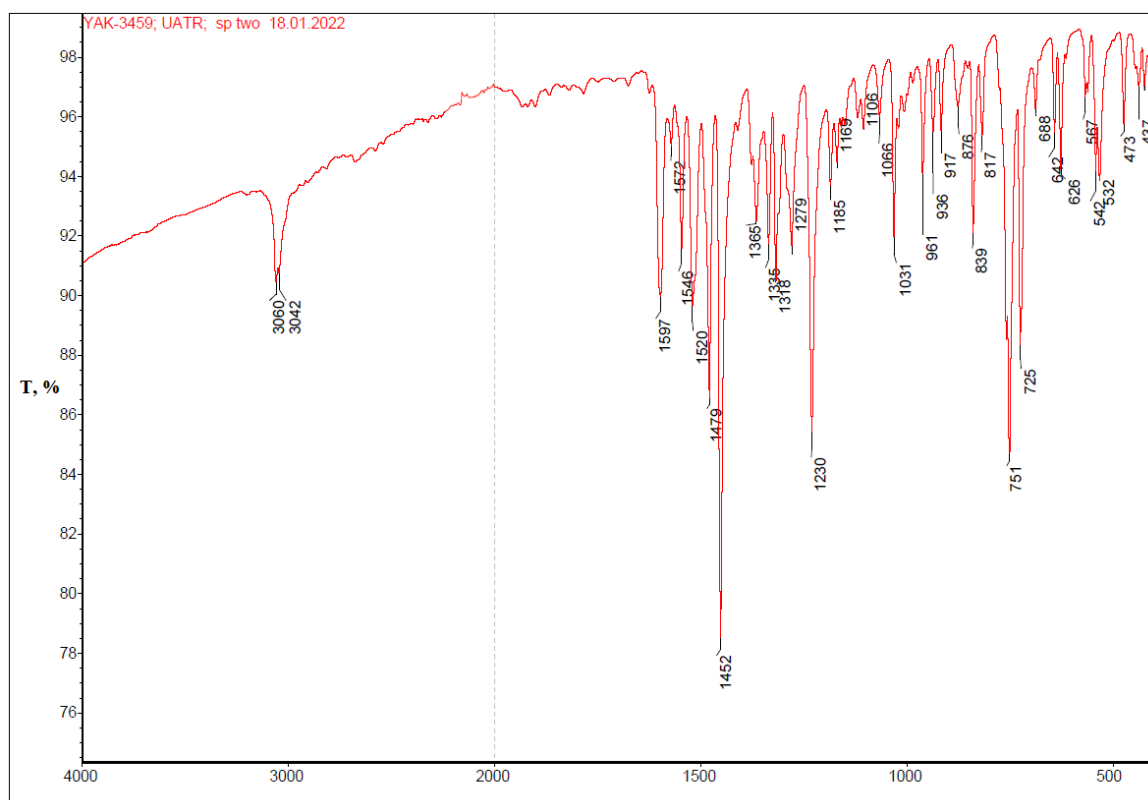
**Figure S24.** IR spectrum of **9a**.



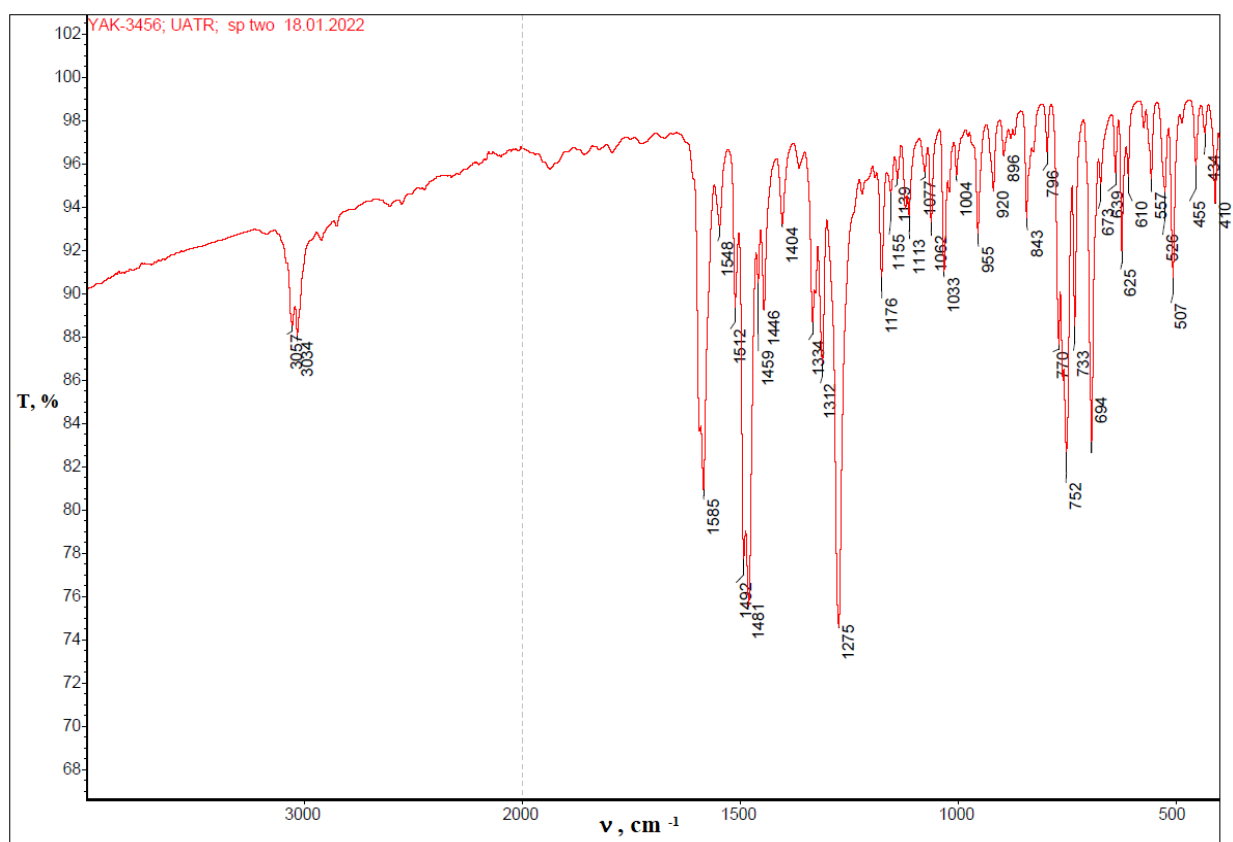
**Figure S25.** IR spectrum of **9b**.



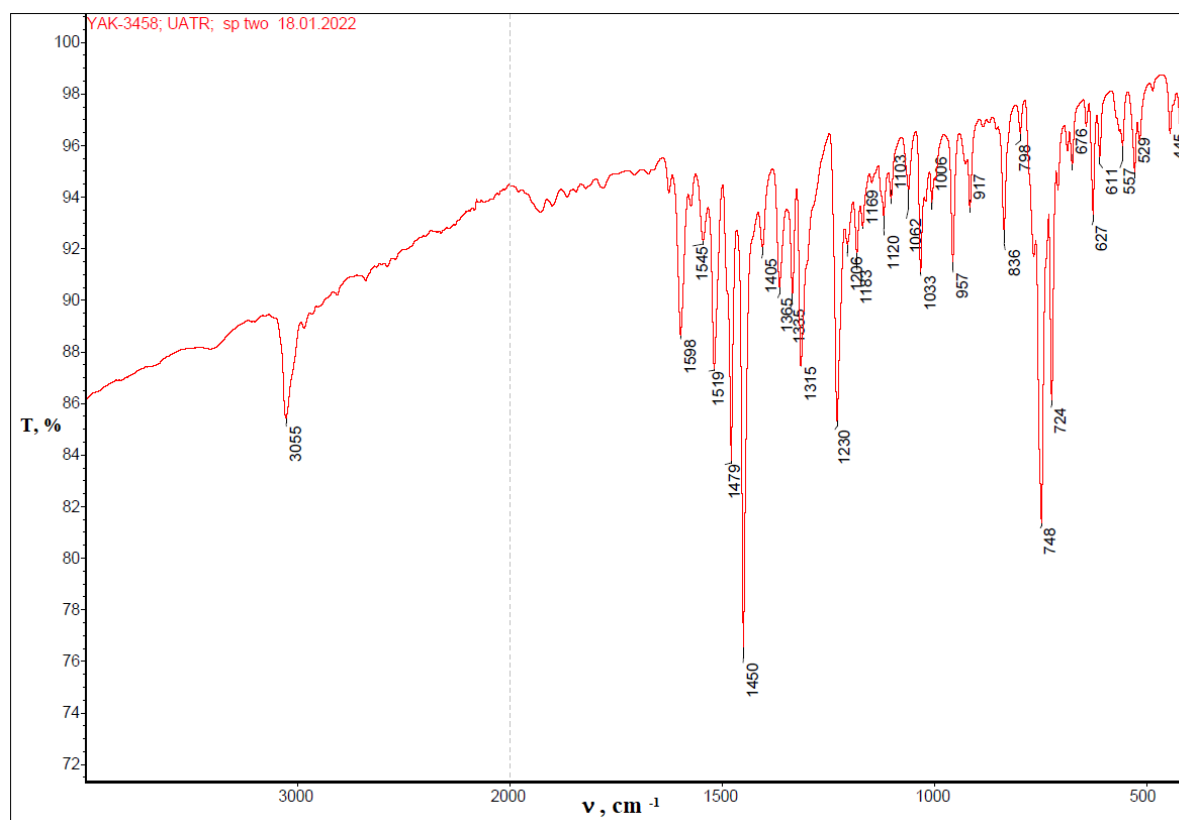
**Figure S26.** IR spectrum of **10a**.



**Figure S27.** IR spectrum of **10b**.



**Figure S28.** IR spectrum of **11a**.



**Figure S29.** IR spectrum of **11b**.

## TD-DFT data of chromophore **9a**

Excitation energies and oscillator strengths

iMO	E(MO)	Type MO
111	-0.32320	HOMO-4
112	-0.31824	HOMO-3
113	-0.31720	HOMO-2
114	-0.30659	HOMO-1
115	-0.24746	HOMO
116	-0.08610	LUMO
117	-0.01380	LUMO+1
118	-0.00078	LUMO+2
119	0.00276	LUMO+3
120	0.00995	LUMO+4

EXCITED STATE 1: SINGLET-A 2.7791 EV 446.12 NM F=0.1775 <S\*\*2>=0.000  
 114 -> 116 -0.15570  
 115 -> 116 0.67889

THIS STATE FOR OPTIMIZATION AND/OR SECOND-ORDER CORRECTION.

TOTAL ENERGY, E(TD-HF/TD-KS) = -1426.88970916

COPYING THE EXCITED STATE DENSITY FOR THIS STATE AS THE 1-PARTICLE RHOCI DENSITY.

EXCITED STATE 2: SINGLET-A 3.3705 EV 367.85 NM F=0.0009 <S\*\*2>=0.000  
 107 -> 116 0.66695  
 108 -> 116 0.14274

EXCITED STATE 3: SINGLET-A 3.9374 EV 314.89 NM F=0.3059 <S\*\*2>=0.000  
 111 -> 116 -0.38269  
 113 -> 116 0.20045  
 114 -> 116 0.42922  
 115 -> 116 0.13038  
 115 -> 117 0.22254

EXCITED STATE 4: SINGLET-A 4.0613 EV 305.28 NM F=0.5466 <S\*\*2>=0.000  
 111 -> 116 0.16971  
 113 -> 116 -0.10625  
 114 -> 116 -0.17415

115 -> 117	0.50776		
115 -> 118	-0.29295		
115 -> 119	-0.12272		
115 -> 125	0.16204		
EXCITED STATE 5: SINGLET-A 4.1883 EV 296.02 NM F=0.0985 <S**2>=0.000			
115 -> 117	0.18267		
115 -> 119	0.60721		
115 -> 122	-0.14500		
EXCITED STATE 6: SINGLET-A 4.2139 EV 294.23 NM F=0.0231 <S**2>=0.000			
108 -> 116	-0.15451		
111 -> 116	0.51864		
114 -> 116	0.37936		
EXCITED STATE 7: SINGLET-A 4.4197 EV 280.53 NM F=0.2841 <S**2>=0.000			
115 -> 120	-0.22000		
115 -> 121	0.61242		
115 -> 122	0.15444		
EXCITED STATE 8: SINGLET-A 4.5013 EV 275.44 NM F=0.0443 <S**2>=0.000			
107 -> 116	-0.10202		
109 -> 116	0.45099		
112 -> 116	0.36153		
113 -> 116	0.29349		

## TD-DFT data of chromophore 9b

Excitation energies and oscillator strengths

iMO	E(MO)	Type MO
110	-0.32615	HOMO-4
111	-0.32148	HOMO-3
112	-0.30854	HOMO-2
113	-0.27624	HOMO-1
114	-0.26169	HOMO
115	-0.08898	LUMO
116	-0.01781	LUMO+1
117	-0.00563	LUMO+2
118	-0.00411	LUMO+3
119	0.00474	LUMO+4

EXCITED STATE 1: SINGLET-A 3.2678 EV 379.41 NM F=0.1231 <S**2>=0.000			
107 -> 115	0.23693		
108 -> 115	0.10678		
112 -> 115	0.26105		
114 -> 115	0.58960		

THIS STATE FOR OPTIMIZATION AND/OR SECOND-ORDER CORRECTION.

TOTAL ENERGY, E(TD-HF/TD-KS) = -1425.69576463

COPYING THE EXCITED STATE DENSITY FOR THIS STATE AS THE 1-PARTICLE RHOCI DENSITY.

EXCITED STATE 2: SINGLET-A 3.3689 EV 368.03 NM F=0.0141 <S**2>=0.000			
107 -> 115	0.56184		
108 -> 115	0.28065		
114 -> 115	-0.28138		

EXCITED STATE 3: SINGLET-A 3.8954 EV 318.28 NM F=0.2590 <S**2>=0.000			
107 -> 115	-0.10193		
110 -> 115	0.32204		
112 -> 115	0.55496		
114 -> 115	-0.22845		

EXCITED STATE 4: SINGLET-A 3.9614 EV 312.98 NM F=0.0006 <S\*\*2>=0.000  
113 -> 115 0.70336

EXCITED STATE 5: SINGLET-A 4.1646 EV 297.71 NM F=0.0736 <S\*\*2>=0.000  
110 -> 115 0.60079  
112 -> 115 -0.29724

EXCITED STATE 6: SINGLET-A 4.2706 EV 290.32 NM F=0.0887 <S\*\*2>=0.000  
113 -> 127 0.17996  
114 -> 117 0.65584

EXCITED STATE 7: SINGLET-A 4.4863 EV 276.36 NM F=0.3571 <S\*\*2>=0.000  
109 -> 115 0.10652  
112 -> 116 0.15322  
114 -> 116 0.56076  
114 -> 118 -0.25256  
114 -> 124 -0.16940

EXCITED STATE 8: SINGLET-A 4.6324 EV 267.65 NM F=0.0310 <S\*\*2>=0.000  
105 -> 115 -0.14259  
107 -> 115 0.12661  
109 -> 115 0.55214  
111 -> 115 -0.19927  
113 -> 117 0.16382  
114 -> 116 -0.10247  
114 -> 119 0.13119

## TD-DFT data of chromophore 10a

Excitation energies and oscillator strengths

iMO	E(MO)	Type MO
115	-0.31742	HOMO-4
116	-0.31633	HOMO-3
117	-0.31324	HOMO-2
118	-0.30109	HOMO-1
119	-0.24543	HOMO
120	-0.08055	LUMO
121	-0.01049	LUMO+1
122	0.00173	LUMO+2
123	0.00445	LUMO+3
124	0.01065	LUMO+4

EXCITED STATE 1: SINGLET-A 2.9515 EV 420.07 NM F=0.2035 <S\*\*2>=0.000  
118 -> 120 -0.17422  
119 -> 120 0.67171

THIS STATE FOR OPTIMIZATION AND/OR SECOND-ORDER CORRECTION.

TOTAL ENERGY, E(TD-HF/TD-KS) = -1749.95757881

COPYING THE EXCITED STATE DENSITY FOR THIS STATE AS THE 1-PARTICLE RHOCI DENSITY.

EXCITED STATE 2: SINGLET-A 3.3779 EV 367.04 NM F=0.0007 <S\*\*2>=0.000  
112 -> 120 0.67003  
113 -> 120 0.10667

EXCITED STATE 3: SINGLET-A 3.8427 EV 322.65 NM F=0.4993 <S\*\*2>=0.000  
110 -> 120 -0.11866  
115 -> 120 -0.15756  
117 -> 120 0.35168  
118 -> 120 0.52165  
119 -> 120 0.14957

EXCITED STATE 4: SINGLET-A 4.0769 EV 304.12 NM F=0.5395 <S\*\*2>=0.000  
119 -> 121 0.51388

119 -> 122 -0.37329  
 119 -> 129 -0.16107  
  
 EXCITED STATE 5: SINGLET-A 4.1751 EV 296.96 NM F=0.1127 <S\*\*2>=0.000  
 119 -> 121 0.23114  
 119 -> 122 0.24181  
 119 -> 123 0.53153  
 119 -> 126 -0.18892  
  
 EXCITED STATE 6: SINGLET-A 4.3669 EV 283.92 NM F=0.0216 <S\*\*2>=0.000  
 111 -> 120 0.15295  
 115 -> 120 0.37980  
 116 -> 120 0.14603  
 117 -> 120 -0.33703  
 118 -> 120 0.32849  
 119 -> 122 0.10257  
  
 EXCITED STATE 7: SINGLET-A 4.3883 EV 282.54 NM F=0.2781 <S\*\*2>=0.000  
 119 -> 124 0.13775  
 119 -> 125 0.62636  
 119 -> 126 -0.16442  
  
 EXCITED STATE 8: SINGLET-A 4.5693 EV 271.34 NM F=0.0482 <S\*\*2>=0.000  
 107 -> 120 0.15314  
 109 -> 120 0.15797  
 110 -> 120 0.42144  
 111 -> 120 0.14595  
 113 -> 120 -0.30210  
 116 -> 120 -0.29070

## TD-DFT data of chromophore 10b

Excitation energies and oscillator strengths

iMO	E(MO)	Type MO
114	-0.32034	HOMO-4
115	-0.31750	HOMO-3
116	-0.30199	HOMO-2
117	-0.27521	HOMO-1
118	-0.26049	HOMO
119	-0.08289	LUMO
120	-0.01419	LUMO+1
121	-0.00473	LUMO+2
122	-0.00082	LUMO+3
123	0.00614	LUMO+4

EXCITED STATE 1: SINGLET-A 3.3535 EV 369.71 NM F=0.0424 <S\*\*2>=0.000  
 112 -> 119 0.61766  
 113 -> 119 0.13219  
 116 -> 119 -0.18512  
 118 -> 119 0.20519

THIS STATE FOR OPTIMIZATION AND/OR SECOND-ORDER CORRECTION.  
 TOTAL ENERGY, E(TD-HF/TD-KS) = -1748.76721752  
 COPYING THE EXCITED STATE DENSITY FOR THIS STATE AS THE 1-PARTICLE RHOCI DENSITY.

EXCITED STATE 2: SINGLET-A 3.4623 EV 358.10 NM F=0.2038 <S\*\*2>=0.000  
 112 -> 119 -0.25383  
 116 -> 119 -0.27643  
 118 -> 119 0.57481

EXCITED STATE 3: SINGLET-A 3.8451 EV 322.45 NM F=0.4142 <S\*\*2>=0.000  
 115 -> 119 -0.34854  
 116 -> 119 0.49742  
 118 -> 119 0.31398

EXCITED STATE 4: SINGLET-A 4.1363 EV 299.75 NM F=0.0002 <S\*\*2>=0.000  
117 -> 119 0.70358

EXCITED STATE 5: SINGLET-A 4.2628 EV 290.85 NM F=0.0921 <S\*\*2>=0.000  
117 -> 131 0.18142  
118 -> 121 0.65707

EXCITED STATE 6: SINGLET-A 4.3050 EV 288.00 NM F=0.0505 <S\*\*2>=0.000  
115 -> 119 0.55984  
115 -> 120 -0.10942  
116 -> 119 0.32081  
118 -> 119 0.11995

EXCITED STATE 7: SINGLET-A 4.5427 EV 272.93 NM F=0.3596 <S\*\*2>=0.000  
113 -> 119 -0.10302  
116 -> 120 -0.15425  
118 -> 120 0.54810  
118 -> 122 0.26779  
118 -> 128 0.11868  
118 -> 129 -0.13155

EXCITED STATE 8: SINGLET-A 4.5917 EV 270.02 NM F=0.0384 <S\*\*2>=0.000  
107 -> 119 -0.35206  
108 -> 119 0.15663  
110 -> 119 0.42417  
111 -> 119 0.17300  
113 -> 119 -0.26048

## TD-DFT data of chromophore 11a

Excitation energies and oscillator strengths

iMO	E(MO)	Type MO
114	-0.31440	HOMO-4
115	-0.31036	HOMO-3
116	-0.30543	HOMO-2
117	-0.29317	HOMO-1
118	-0.24334	HOMO
119	-0.04364	LUMO
120	-0.00627	LUMO+1
121	0.00223	LUMO+2
122	0.00650	LUMO+3
123	0.01275	LUMO+4

EXCITED STATE 1: SINGLET-A 3.6920 EV 335.82 NM F=0.3842 <S\*\*2>=0.000  
112 -> 119 0.11394  
117 -> 119 -0.23894  
118 -> 119 0.58664  
118 -> 120 -0.13530  
118 -> 121 -0.12700  
118 -> 122 -0.13210

THIS STATE FOR OPTIMIZATION AND/OR SECOND-ORDER CORRECTION.

TOTAL ENERGY, E(TD-HF/TD-KS) = -1397.03413784

COPYING THE EXCITED STATE DENSITY FOR THIS STATE AS THE 1-PARTICLE RHOCI DENSITY.

EXCITED STATE 2: SINGLET-A 3.8569 EV 321.46 NM F=0.0181 <S\*\*2>=0.000  
110 -> 119 -0.16819  
112 -> 119 0.61871  
114 -> 119 0.11016  
118 -> 119 -0.12808

EXCITED STATE 3: SINGLET-A 4.1149 EV 301.31 NM F=0.2068 <S\*\*2>=0.000  
118 -> 120 -0.29300

118 -> 121	-0.38593	
118 -> 122	0.42121	
118 -> 123	-0.13358	
EXCITED STATE 4: SINGLET-A 4.2382 EV 292.54 NM F=0.3699 <S**2>=0.000		
115 -> 119	-0.12516	
117 -> 119	0.39336	
118 -> 120	-0.25142	
118 -> 121	-0.21128	
118 -> 122	-0.34557	
EXCITED STATE 5: SINGLET-A 4.3550 EV 284.69 NM F=0.3038 <S**2>=0.000		
118 -> 123	-0.36696	
118 -> 124	0.55994	
EXCITED STATE 6: SINGLET-A 4.3610 EV 284.30 NM F=0.1348 <S**2>=0.000		
109 -> 119	-0.10586	
115 -> 119	-0.12732	
116 -> 119	-0.21380	
117 -> 119	0.38218	
118 -> 119	0.30508	
118 -> 120	0.16452	
118 -> 121	0.12430	
118 -> 122	0.29722	
EXCITED STATE 7: SINGLET-A 4.4986 EV 275.61 NM F=0.0214 <S**2>=0.000		
114 -> 119	0.16724	
115 -> 119	0.46780	
116 -> 119	-0.40366	
117 -> 120	-0.13962	
EXCITED STATE 8: SINGLET-A 4.7860 EV 259.05 NM F=0.0340 <S**2>=0.000		
115 -> 120	-0.10077	
116 -> 119	0.23848	
116 -> 120	-0.11982	
117 -> 120	-0.15133	
117 -> 121	0.14766	
118 -> 120	0.35538	
118 -> 121	-0.32397	
118 -> 131	0.10439	
118 -> 132	0.10261	
118 -> 134	-0.11854	

## TD-DFT data of chromophore 11b

Excitation energies and oscillator strengths

iMO	E(MO)	Type MO
113	-0.31308	HOMO-4
114	-0.30699	HOMO-3
115	-0.29388	HOMO-2
116	-0.27437	HOMO-1
117	-0.25928	HOMO
118	-0.04585	LUMO
119	-0.00891	LUMO+1
120	-0.00397	LUMO+2
121	-0.00064	LUMO+3
122	0.01216	LUMO+4

EXCITED STATE 1: SINGLET-A		3.8350 EV	323.30 NM	F=0.0197	<S**2>=0.000
110 -> 118	-0.18364				
111 -> 118	0.61947				
111 -> 119	0.10067				
112 -> 118	-0.10206				
115 -> 118	-0.13980				

THIS STATE FOR OPTIMIZATION AND/OR SECOND-ORDER CORRECTION.

TOTAL ENERGY, E(TD-HF/TD-KS) = -1395.85385393

COPYING THE EXCITED STATE DENSITY FOR THIS STATE AS THE 1-PARTICLE RHOCI DENSITY.

EXCITED STATE 2: SINGLET-A		4.0901 EV	303.13 NM	F=0.4596	<S**2>=0.000
111 -> 118	0.14283				
113 -> 118	0.14468				
115 -> 118	0.50620				

117 -> 118    -0.37112

EXCITED STATE 3:    SINGLET-A    4.2543 EV   291.43 NM   F=0.0740   <S\*\*2>=0.000

116 -> 130    -0.17385

117 -> 120    0.65565

EXCITED STATE 4:    SINGLET-A    4.4115 EV   281.05 NM   F=0.1756   <S\*\*2>=0.000

113 -> 118    0.10579

114 -> 118    -0.29623

115 -> 118    0.29715

117 -> 118    0.42563

117 -> 119    -0.18403

117 -> 121    0.16683

117 -> 123    -0.10757

EXCITED STATE 5:    SINGLET-A    4.4825 EV   276.60 NM   F=0.0650   <S\*\*2>=0.000

113 -> 118    0.46421

114 -> 118    0.43915

115 -> 119    0.13959

117 -> 119    -0.10070

EXCITED STATE 6:    SINGLET-A    4.6550 EV   266.35 NM   F=0.2920   <S\*\*2>=0.000

116 -> 120    0.63619

117 -> 130    0.16368

EXCITED STATE 7:    SINGLET-A    4.7097 EV   263.25 NM   F=0.1493   <S\*\*2>=0.000

113 -> 118    0.13855

116 -> 120    -0.13782

117 -> 118    0.23605

117 -> 119    0.36895

117 -> 121    -0.35716

117 -> 123    -0.17716

EXCITED STATE 8:    SINGLET-A    4.8878 EV   253.66 NM   F=0.0506   <S\*\*2>=0.000

108 -> 118    0.12308

113 -> 118    -0.26810

113 -> 119    0.16177

114 -> 118    0.33406

114 -> 119    -0.11940

115 -> 118    0.22785

115 -> 119    -0.15178

115 -> 121    -0.17105

115 -> 126    -0.10769

117 -> 118    0.18894

117 -> 123    -0.10077