

1           **Advancements in Organic Fluorescent Materials: Unveiling the Potential of**  
2           **Peripheral Group Modification in dithienyl-diketopyrrolopyrrole derivatives for**  
3           **One- and Two-Photon Bioimaging**  
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## Support information

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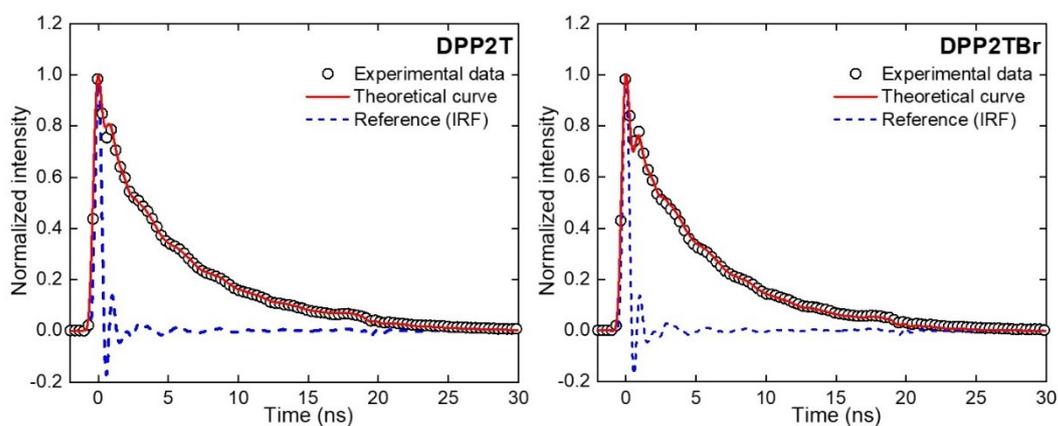
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### 42 1. Time-resolved fluorescence technique

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44 The fluorescence lifetime of the dyes was obtained using the time-domain  
45 fluorescence technique. The samples were excited with a  $190\text{ fs}$  laser pulse at  $515\text{ nm}$   
46 (2nd harmonic of the  $1030\text{ nm}$ ) operating with a repetition rate of  $300\text{ Hz}$ , delivered by  
47 a laser system (Light Conversion, model Pharos-PH1). The fluorescence signal was  
48 collected perpendicularly to the excitation beam by a multimode optical fiber. The optical  
49 fiber directs the fluorescence signal to a silicon photodetector with a temporal resolution  
50 of approximately  $700\text{ ps}$ . The electronic signal generated by the photodetector is acquired  
51 by a  $1\text{ GHz}$  oscilloscope<sup>1</sup>. The signal convolution method was used to obtain an accurate  
52 representation of the dyes lifetime, where a theoretical function is convoluted with the  
53 temporal instrument response function (IRF)<sup>1,2</sup>. **Figure SII** shows the experimental  
54 curves of fluorescence intensity as a function of time for both compounds.

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57 **Figure SII** - Dithienyl-diketopyrrolopyrrole derivatives fluorescence emission lifetimes, deconvoluted  
58 fluorescence signal, and instrument response function.

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### 60 2. Quantum chemical calculations details

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62 **Table SII** – Optimized structures of dithienyl-diketopyrrolopyrrole derivatives obtained through PCM-  
63 B3LYP calculations in chloroform medium. Basis set:  $6-311G(d,p)$  for H, C, N and O atoms;  $cc-pVDZ$   
64 for S and Br atoms.

	DPP2T			DPP2TBr			
N	-1.640341	1.004437	0.732580	N	-1.639660	1.017670	0.739790
C	-0.646879	2.038698	0.773240	C	-0.639630	2.045510	0.768750

C	0.525295	1.424230	0.195192	C	0.526510	1.419000	0.191100
C	0.194962	0.089911	-0.162585	C	0.187720	0.085100	-0.155340
C	-1.136010	-0.163686	0.166163	C	-1.143980	-0.157130	0.180530
N	2.360414	0.509908	-0.700547	N	2.353770	0.486520	-0.704430
C	1.856152	1.677974	-0.133973	C	1.858150	1.661280	-0.145060
C	1.367014	-0.524421	-0.741030	C	1.353760	-0.541360	-0.733260
O	-0.881171	3.150172	1.227229	O	-0.863130	3.162210	1.214650
O	1.601268	-1.635863	-1.195119	O	1.577210	-1.658030	-1.179270
C	3.702284	0.206216	-1.192721	C	3.694160	0.170760	-1.194380
C	4.659134	-0.293987	-0.102764	C	4.649890	-0.323230	-0.100620
C	6.046828	-0.624953	-0.661878	C	6.035950	-0.664480	-0.657860
C	7.015227	-1.159755	0.399112	C	7.002610	-1.193580	0.407610
C	8.405189	-1.495525	-0.153194	C	8.390820	-1.539660	-0.142750
C	9.366107	-2.030010	0.912571	C	9.350080	-2.068390	0.927320
C	-2.982267	1.308191	1.224563	C	-2.980080	1.333600	1.229600
C	-3.939018	1.808450	0.134568	C	-3.935530	1.827820	0.135720
C	-5.326825	2.139096	0.693554	C	-5.321580	2.169460	0.692760
C	-6.295053	2.674282	-0.367409	C	-6.287990	2.698700	-0.372880
C	-7.685172	3.009640	0.184738	C	-7.676110	3.045330	0.177320
C	-8.645923	3.544469	-0.881007	C	-8.635150	3.574130	-0.892930
C	2.563668	2.918248	0.066131	C	2.570760	2.898850	0.042580
C	2.011357	4.059501	0.625419	C	2.027480	4.045940	0.598090
C	2.913553	5.144083	0.714214	C	2.925370	5.134040	0.678350
C	4.157889	4.850175	0.228349	C	4.161940	4.825360	0.184320
S	4.253760	3.222857	-0.354499	S	4.262410	3.189300	-0.395150
C	-1.843580	-1.403904	-0.034056	Br	5.664020	5.963000	0.087360
C	-1.291187	-2.545291	-0.592968	C	-1.856640	-1.394640	-0.007260
C	-2.193530	-3.629733	-0.682069	C	-1.313340	-2.541880	-0.562420
C	-3.438041	-3.335572	-0.196813	C	-2.211390	-3.629850	-0.642920
S	-3.533897	-1.708174	0.385858	C	-3.448110	-3.320900	-0.149470
H	3.563943	-0.580786	-1.936452	S	-3.548540	-1.684770	0.429840
H	4.104681	1.076531	-1.713340	Br	-4.950410	-4.458300	-0.053010
H	4.219720	-1.187122	0.353048	H	3.551110	-0.622230	-1.930770
H	4.748079	0.457569	0.688600	H	4.100070	1.033030	-1.726440
H	6.477938	0.272402	-1.124504	H	4.207240	-1.210480	0.363400
H	5.946597	-1.365390	-1.465598	H	4.742550	0.434160	0.684900
H	6.584112	-2.056512	0.862000	H	6.470580	0.226840	-1.128660
H	7.115274	-0.420375	1.204111	H	5.932060	-1.411660	-1.454780
H	8.835547	-0.599251	-0.616355	H	6.568190	-2.084450	0.878700
H	8.304419	-2.234265	-0.957453	H	7.106220	-0.447260	1.205650

H	9.514458	-1.299212	1.713756	H	8.824330	-0.649160	-0.613870
H	10.346863	-2.259706	0.487293	H	8.286590	-2.285130	-0.940330
H	8.979565	-2.946304	1.369531	H	9.501920	-1.330960	1.721680
H	-3.384735	0.437866	1.745130	H	10.329550	-2.305650	0.503400
H	-2.843985	2.095163	1.968341	H	8.960300	-2.979090	1.392630
H	-4.027756	1.057010	-0.656936	H	-3.386210	0.471300	1.761440
H	-3.499680	2.701716	-0.321058	H	-2.837020	2.126470	1.966100
H	-5.226821	2.879202	1.497610	H	-4.028280	1.070430	-0.649800
H	-5.757968	1.241515	1.155711	H	-3.492600	2.714950	-0.328260
H	-6.394831	1.935260	-1.172770	H	-5.217610	2.916670	1.489630
H	-5.863925	3.571298	-0.829781	H	-5.756490	1.278280	1.163570
H	-7.584671	3.748044	0.989340	H	-6.391780	1.952280	-1.170800
H	-8.115525	2.113115	0.647418	H	-5.853230	3.589340	-0.844080
H	-8.259385	4.461001	-1.337494	H	-7.571700	3.790950	0.974730
H	-9.626798	3.773873	-0.455846	H	-8.109940	2.155090	0.648620
H	-8.794015	2.813992	-1.682532	H	-8.245060	4.484610	-1.358410
H	0.981028	4.093456	0.958271	H	-9.614580	3.811780	-0.469120
H	2.648899	6.109089	1.125365	H	-8.787160	2.836570	-1.687140
H	5.028979	5.484932	0.173201	H	0.999040	4.086300	0.937860
H	-0.260732	-2.579455	-0.925410	H	2.670530	6.102880	1.083790
H	-1.928836	-4.594828	-1.092991	H	-0.284780	-2.582430	-0.901820
H	-4.309249	-3.970191	-0.141951	H	-1.956500	-4.598790	-1.048110

65

66 Using the compounds optimized structures (see **Table SI1**), QOCs concerning the  
67 one-photon absorption (1PA) and two-photon absorption (2PA) processes were  
68 performed. **Tables SI2** and **SI3** summarize the results obtained, including transition  
69 energy, oscillator strength, 2PA probability, and 2PA cross-section ( $\sigma^{2PA}$ ).

70 The computed 1PA spectrum of the compounds in molar absorptivity was  
71 obtained using the oscillator strength and transition energy values, as provided in **Table**  
72 **SI2**, and utilizing the equation described in<sup>3</sup>. It is important to note that the line widths  
73 used were estimated from the decomposition of the experimental 1PA spectrum into three  
74 absorption bands and its fitting using Gaussian curves (the average FWHM linewidth  
75 values for the three bands are: 0.4 eV, 0.4 eV, and 0.3 eV), and that although 20 transitions  
76 were computed using the TD-DFT method, only those within the experimental spectral  
77 range were used to computed the 1PA spectrum<sup>3,4</sup>.

78 As described in the manuscript, the two highest-energy electronic bands observed  
79 in the 1PA spectrum are ascribed to some electronic transitions. For greater accuracy, it

80 was observed that for the **DPP2T** molecule, the second band is related with three  
 81 electronic transitions, labeled as 4, 5, and 7 (see **Table SI2**). On the other hand, the third  
 82 band is ascribed to a single transition, labeled as 10. Conversely, for the **DPP2TBr**  
 83 molecule, the second band comprises two electronic transitions (4 and 5), and the third  
 84 band comprises 4 transitions (9, 10, 12, and 14). However, transitions 10 and 14 have a  
 85 negligible contribution, given the low values of their oscillator strength, and TD-DFT  
 86 calculations are likely overestimating these values, a typical behavior of DFT theory<sup>5</sup>.

87 To obtain a computed 2PA spectrum in terms of  $\sigma^{2PA}$ , the properties summarized  
 88 in **Table SI3** were utilized, along with the equation described in<sup>4</sup>. The spectrum was  
 89 obtained considering only the second electronic excited-state (electronic transition 2, see  
 90 **Table SI3**), while states 3 and 6 were not included as they lie in a spectral region where  
 91 the resonant enhancement effect due to 1PA occurs.

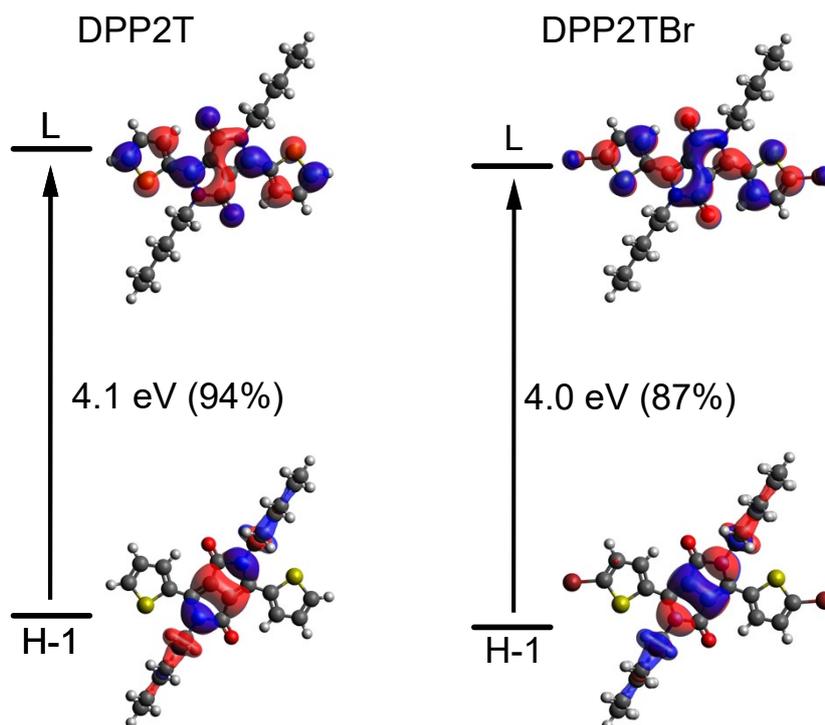
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93 **Table SI2** – Theoretical one-photon absorption properties of dithienyl-diketopyrrolopyrrole samples  
 94 obtained by TD-PCM-B3LYP calculations in chloroform medium. Basis set: *6-311++G(d,p)* for H, C, N  
 95 and O atoms; *aug-cc-pVDZ* for S and Br atoms.

States number	DPP2T			DPP2TBr		
	<i>E</i> (eV)	Wavelength (nm)	<i>f</i>	<i>E</i> (eV)	Wavelength (nm)	<i>f</i>
1	2.264	548	0.5080	2.177	570	0.6270
2	3.139	395	0.0000	3.096	400	0.0000
3	3.409	364	0.0000	3.266	380	0.0000
4	3.663	338	0.0490	3.522	352	0.3490
5	3.739	332	0.2540	3.632	341	0.0160
6	3.896	318	0.0000	3.680	337	0.0000
7	3.942	315	0.0310	3.977	312	0.0000
8	3.993	310	0.0000	4.004	310	0.0000
9	4.024	308	0.0000	4.034	307	0.0210
10	4.377	283	0.2430	4.038	307	0.0050
11	4.526	274	0.0000	4.040	307	0.0000
12	4.656	266	0.0000	4.204	295	0.2390
13	4.796	259	0.0000	4.529	274	0.0000
14	4.862	255	0.0000	4.535	273	0.0010
15	4.906	253	0.0190	4.651	267	0.0000
16	4.915	252	0.0870	4.749	261	0.0000
17	4.997	248	0.0000	4.776	260	0.0800
18	5.037	246	0.0000	4.913	252	0.0540
19	5.114	242	0.0210	4.915	252	0.0090
20	5.171	240	0.0000	4.942	251	0.0010

97 **Table SI3** – Theoretical two-photon absorption properties of dithienyl-diketopyrrolopyrrole samples  
 98 obtained by QRF-PCM-B3LYP calculations in chloroform medium. Basis set: *6-311++G(d,p)* for H, C, N  
 99 and O atoms; *aug-cc-pVDZ* for S and Br atoms.

<b>DPP2T</b>					
<b>States number</b>	$E_{2P}$ (eV)	<b>Two-photons Wavelength (nm)</b>	<b>2PA prob. (<math>\times 10^3</math> a.u.)</b>	$\Gamma_{FWHM}$ (eV)	$\sigma_{theor}^{2PA}$ (GM)
1	4.520	1097	0.00	---	---
2	6.280	790	8.61	0.50	12.4
3	6.820	727	127.00	---	---
4	7.320	677	0.00	---	---
5	7.480	663	0.00	---	---
6	7.800	636	50.10	---	---
<b>DPP2TBr</b>					
<b>States number</b>	$E_{2P}$ (eV)	<b>Two-photons Wavelength (nm)</b>	<b>2PA prob. (<math>\times 10^3</math> a.u.)</b>	$\Gamma_{FWHM}$ (eV)	$\sigma_{theor}^{2PA}$ (GM)
1	4.360	1137	0.0	---	---
2	6.200	800	25.8	0.50	36.4
3	6.540	758	250.0	---	---
4	7.040	704	0.0	---	---
5	7.260	683	0.0	---	---
6	7.360	674	119.0	---	---



101

102 **Figure S12** – Representation of the MOs (H: HOMO, L: LUMO) involved in the lowest-energy allowed  
 103 2PA transition of dithienyl-diketopyrrolopyrrole derivatives, along with the respective percentage  
 104 contributions of the excitations. Results obtained from QRF-PCM-B3LYP calculations.

105

### 106 3. Two-photon absorption measurements

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108 To determine the two-photon absorption cross-section ( $\sigma^{2PA}$ ) of dithienyl-  
 109 diketopyrrolopyrrole derivatives in chloroform, solutions with a concentration of *ca.*  
 110  $10^{-2}$  mol/L were prepared and placed in quartz cells with optical paths of 2 mm lengths.

111 The  $\sigma^{2PA}$  was measured from 790 nm to 1000 nm by the open-aperture Z-Scan  
 112 technique using a 150 – 180 fs laser-like pulse delivered by a tunable optical parametric  
 113 amplifier (OPA) (Light Conversion, model ORPHEUS). OPA was pumped by a 190 fs  
 114 pulse from a laser system (Light Conversion, model Pharos-PH1) centered at 1030 nm  
 115 operating at a repetition rate of 750 Hz.

116 The open-aperture Z-Scan technique consists in determining the change in light  
 117 transmittance when the sample is scanned along the focus of a Gaussian laser pulse (Z-  
 118 axis)<sup>6</sup>. In this process, the sample is subjected to different excitation intensities according  
 119 to the Z-position. In order to remove linear effects from the measurement, the transmitted  
 120 power at a given Z-position is divided by the transmitted power when the sample is far  
 121 away from the pulse focus, and nonlinear optical effects are not present, thus obtaining

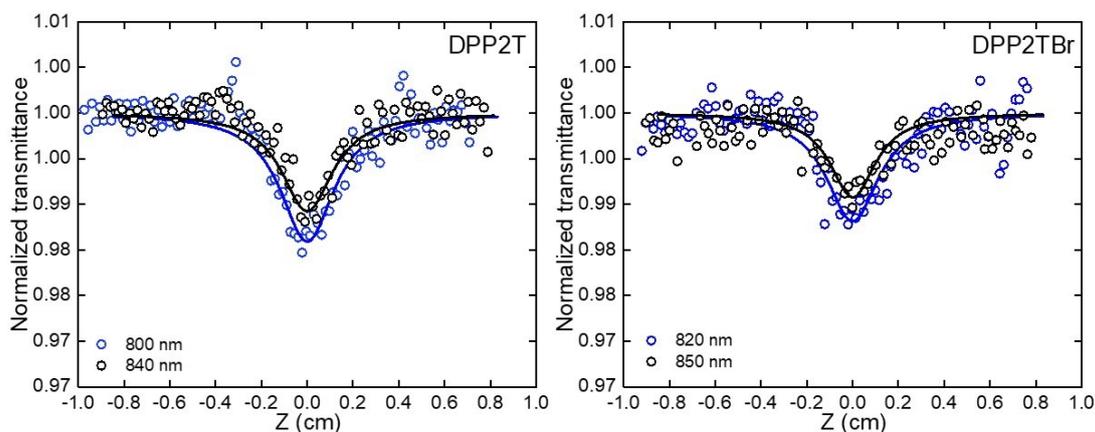
122 the normalized transmittance (NT)<sup>7</sup>. The nonlinear absorption coefficient ( $\beta$ ) is obtained  
 123 from the NT curve fit using the equation,

$$T(z) = \frac{1}{\sqrt{\pi}q_0(z,0)} \int_{-\infty}^{\infty} \ln[1 + q_0(z,0)e^{-t^2}] dt \quad (1)$$

125

126 in this  $q_0(z,0) = \beta I_0 L (1 + (z^2/z_0^2))^{-1}$ ,  $L$  is the sample length (2 mm quartz sample  
 127 cell),  $z_0$  the Rayleigh length,  $z$  the sample position and  $I_0$  is the laser-like pulse intensity  
 128 at the focus. Finally, the 2PA cross-section is determined from the  $\sigma_{2PA} = (\hbar\omega\beta)/N$ ,  
 129 where  $\hbar\omega$  is the photon energy and  $N$  is the number of molecules per cubic centimeter<sup>7</sup>.  
 130 The  $\sigma_{2PA}$  is expressed in Goppert-Mayer ( $GM$ ) units, where  
 131  $1 GM = 1 \cdot 10^{-50} \cdot cm^4 \cdot s \cdot photon^{-1}$ . **Figure SI3** shows some typical open-aperture  
 132 Z-scan curves, with the respective adjustment curves.

133



134

135 **Figure SI3** – Open-aperture z-scan curves of **DPP2T** and **DPP2TBr** compounds, where circles represent  
 136 experimental data and lines correspond to curves obtained through fitting.

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#### 138 4. Measurements of fluorescence excited by 2PA

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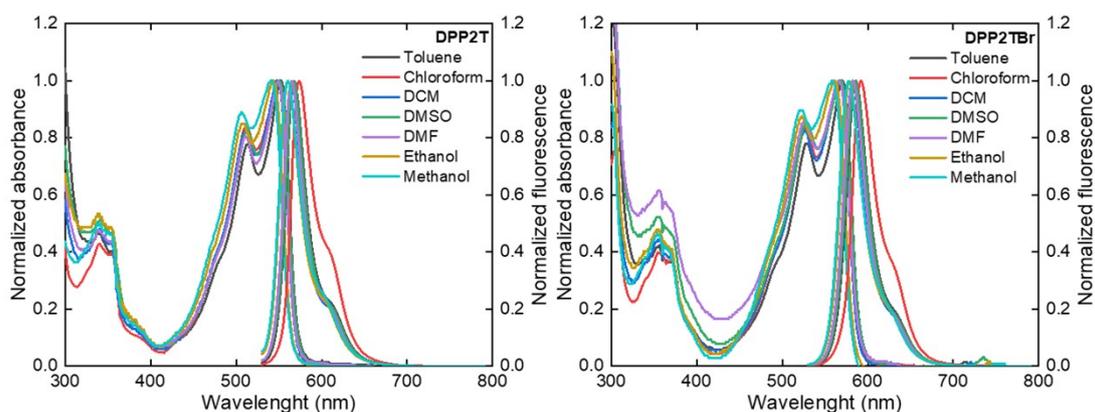
140 Fluorescence emission induced by two-photon absorption measurements, excited  
 141 in 850 nm and 900 nm, were performed using the same laser system operated at a  
 142 repetition rate of 1.5 kHz. The fluorescence signal was collected through an optical fiber  
 143 connected to a spectrophotometer (Ocean Optics, model HR-2000++). The excitation  
 144 laser power was controlled by means of a rotating polarizer, which allowed monitoring

145 of the fluorescence emission induced by 2PA as a function of the laser intensity for  
 146 different pulse energies. The fluorescence spectra are the results of an average of 5 s of  
 147 spectrophotometer data acquisition<sup>7-9</sup>.

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## 149 5. Solvatochromism measurement

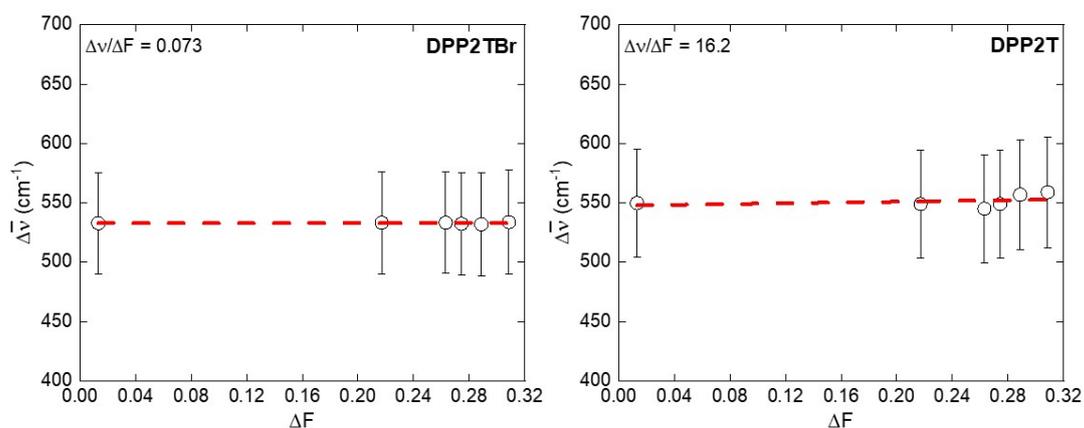
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151

152 **Figure SI4** - Spectrum of absorption and fluorescence normalized for the compounds in different solvents.

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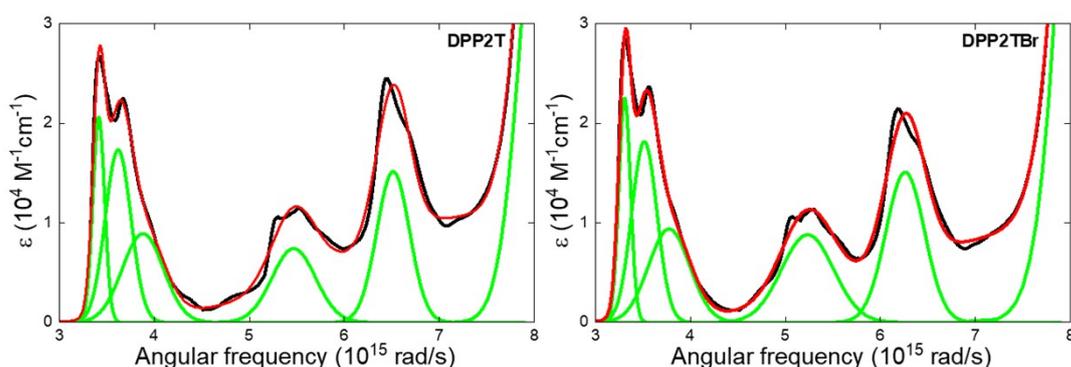
155 **Figure SI5** - Stokes shift (black circles) as a function of the Lippert-Mataga polarity functions. The red  
 156 dashed lines are the linear fit to determine the slope  $\frac{\Delta\nu}{\Delta F}$ .

157

## 158 6. Transition dipole moment

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160 **Figure SI6** shows the one-photon absorption spectra of dithienyl-  
 161 diketopyrrolopyrrole derivatives, which were decomposed into some Gaussian curves to  
 162 determine the transition dipole moment of the electronics bands. The equation used is  
 163 described in<sup>3</sup>.



165

166 **Figure S16** – One-photon absorption spectrum of dithienyl-diketopyrrolopyrrole derivatives (black lines)  
 167 decomposed with three Gaussian curves (green lines). The red lines are sum of overlap Gaussian curves.

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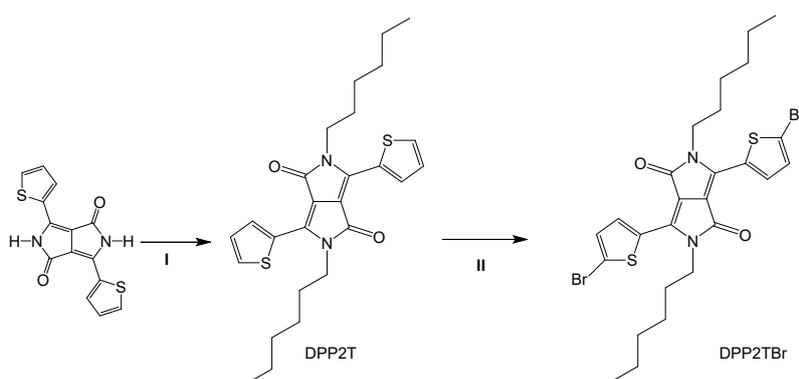
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## 170 7. Synthesis of the diketopyrrolopyrroles derivatives.

171 The solvents and reagents were purchased from Sigma-Aldrich and used as  
 172 received. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded using a Bruker Avance III HD  
 173 500 MHz spectrometer at room temperature. The total nitrogen, carbon, hydrogen, and  
 174 sulfur are determined using a CHNS analyzer (Fison Instrument model EA 1108).

175 The DPP2T and DPP2TBr (Scheme 1) were synthesized following the procedure  
 176 reported by Scalon *et al.*<sup>10</sup>, described briefly following:

177



178

179 Scheme S1. Synthetic procedures for the synthesis of DPP derivatives. (I): bromohexane,  
 180  $\text{K}_2\text{CO}_3$ , DMF, 130 °C. (II): NBS,  $\text{CHCl}_3$ , 0 °C.

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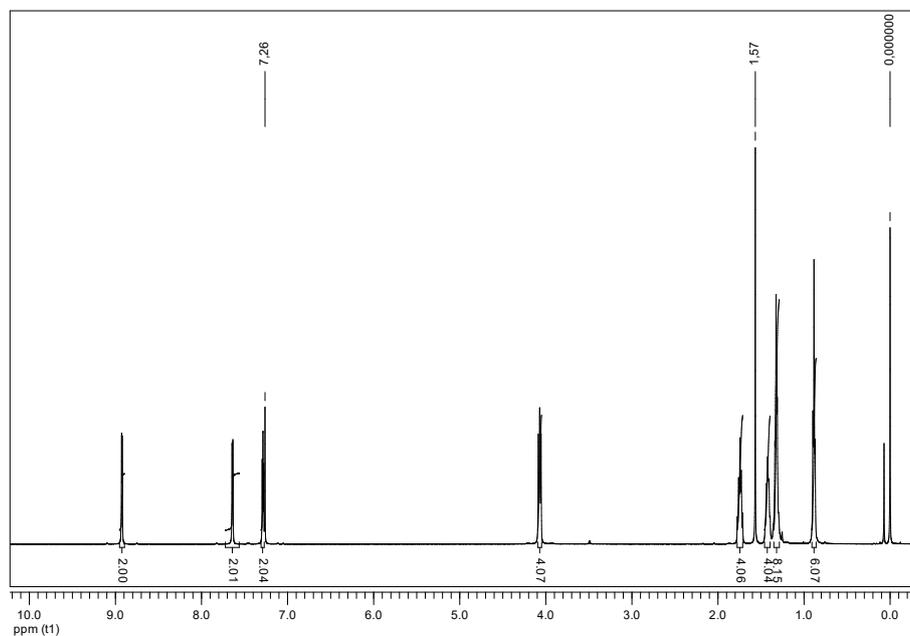
182 **DPP2T**: In a round-bottom flask 3,6-di(thiophen-2-yl)pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-  
 183 dione (1.7 mmol), potassium carbonate (5.8 mmol), and 20 mL of anhydrous  
 184 dimethylformamide were added under argon atmosphere. After a stirring at 90 °C for one  
 185 hour, 1-bromohexane (43 mmol) was added dropwise, and the reaction was stirred at

186 130 °C overnight. In sequence, the solution was cooled down to room temperature,  
187 poured in 22.0 mL of deionized water, and stirred for 1 h. The reaction product was  
188 extracted with chloroform and dried over anhydrous sodium sulphate. After solvent  
189 evaporation, the product was purified using chromatography column (chloroform as  
190 eluent) and recrystallized with methanol.

191  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$ (ppm): 8.92 (d,  $J = 3.2$  Hz, 2H), 7.64 (d,  $J = 4.3$  Hz, 2H),  
192 7.28 (dd,  $J = 8.7, 4.0$  Hz, 2H), 4.09 – 4.05 (m, 4H), 1.78 – 1.71 (m, 4H), 1.41 (dd,  $J =$   
193 14.5, 7.0 Hz, 4H), 1.32 (dd,  $J = 8.8, 5.3$  Hz, 8H), 0.88 (t,  $J = 6.9$  Hz, 6H).

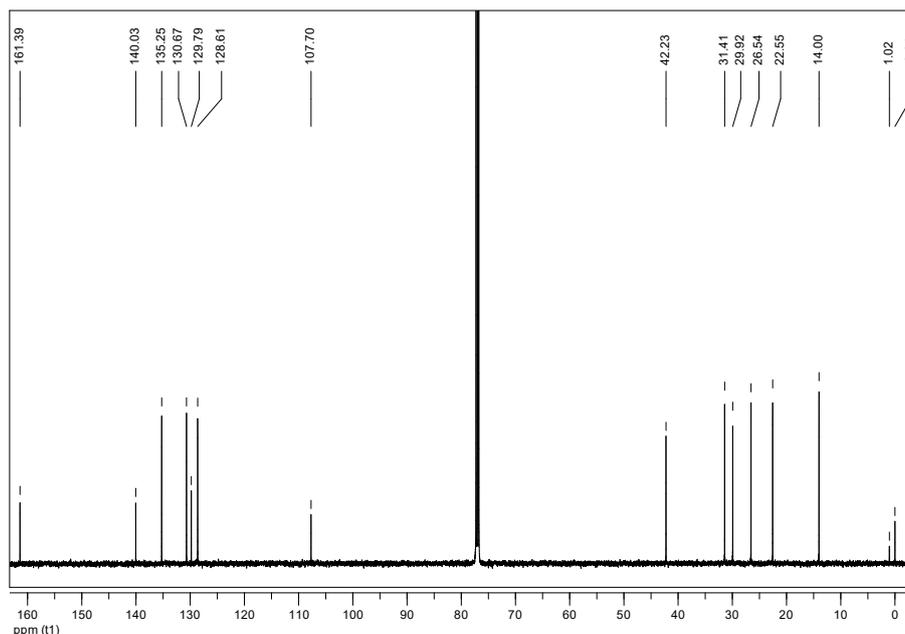
194  $^{13}\text{C}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$ (ppm): 161.39, 140.03, 135.25, 130.67, 129.79, 128.61,  
195 107.70, 42.23, 31.41, 29.92, 26.54, 22.55, 14.00.

196 Elemental Analysis: Calcd for  $\text{C}_{26}\text{H}_{32}\text{N}_2\text{O}_2\text{S}_2$ : C 66.63; H 6.88; N 5.98; S 13.68. Found:  
197 C 65.64; H 6.16; N 5.88; S 13.69.



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201 Figure SI7 -  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the DPP2T.

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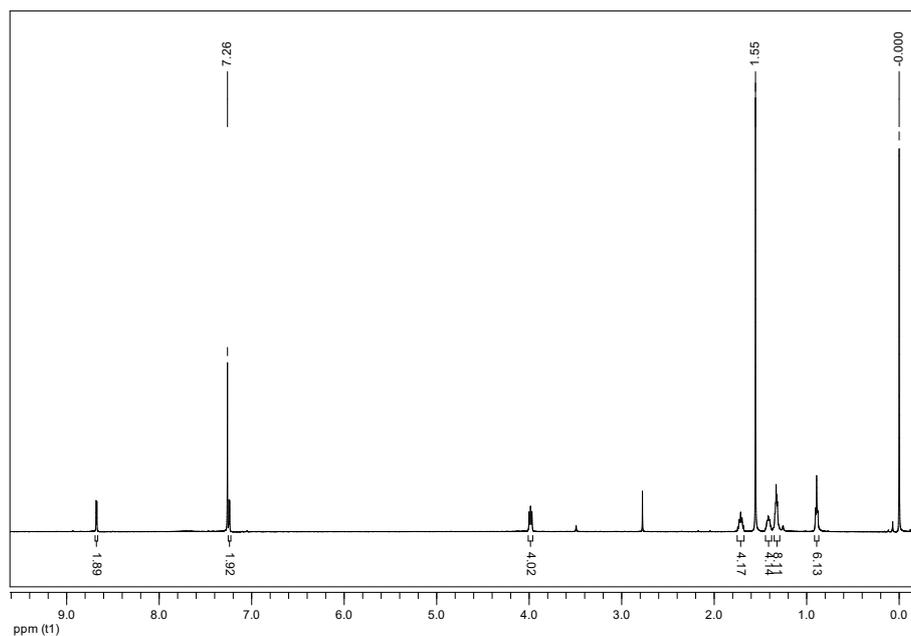
203 **DPP2TBr**: In a round-bottom flask DPP2T (1.3 mmol), *N*-bromosuccinimide (NBS)  
 204 (3.0 mmol), and 30 mL of anhydrous chloroform were added, and the reaction was stirred  
 205 overnight at 0 °C protect from light. The solvent was rotaevaporated and the crude solid  
 206 was recrystallized with methanol.

207  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 8.68 (d,  $J = 4.2$  Hz, 2H), 7.24 (d,  $J = 4.2$  Hz, 2H),  
 208 4.01 – 3.96 (m, 2H), 1.75 – 1.68 (m, 4H), 1.42 (s, 2H), 1.35 – 1.29 (m, 8H), 0.89 (t,  $J =$   
 209 6.9 Hz, 6H).

210  $^{13}\text{C}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  161.06, 139.01, 135.36, 131.66, 131.12, 119.16, 107.82,  
 211 42.29, 31.36, 29.95, 26.51, 22.52, 14.00.

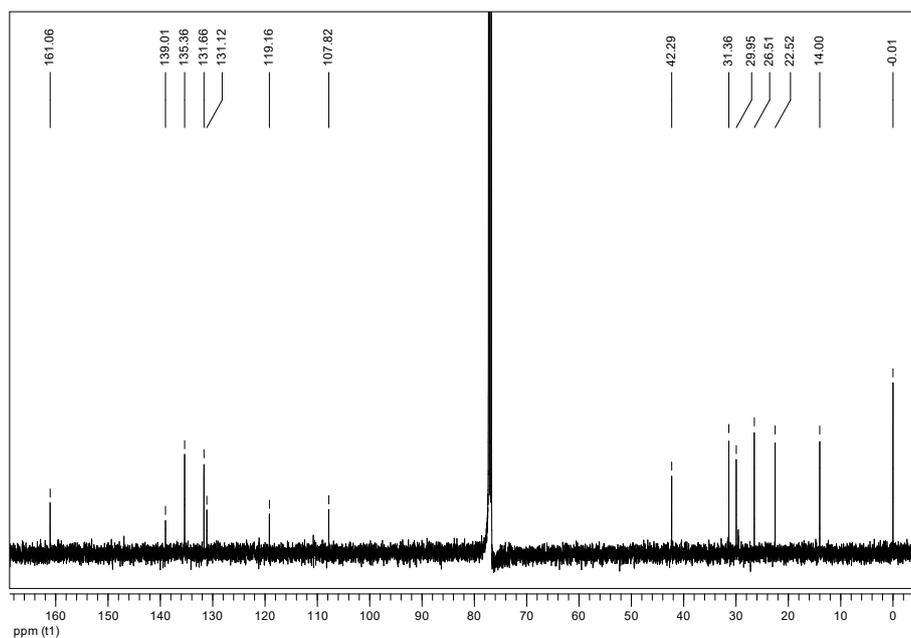
212 Elemental Analysis: Calcd for  $\text{C}_{26}\text{H}_{30}\text{Br}_2\text{N}_2\text{O}_2\text{S}_2$ : C 49.85; H 4.83; N 4.47; S 10.24.  
 213 Found: C 49.78; H 4.92; N 4.43; S 10.20.

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218 Figure SI8 -  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the DPP2TBr.

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## 223 8. References

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