

Supporting information for:

Solvatofluorochromic, non-centrosymmetric π -expanded diketopyrrolopyrrole

Marek Grzybowski, Artur Jeżewski, Irena Deperasińska, Daniel H. Friese, Marzena Banasiewicz,
Vincent Hugues, Bolesław Kozankiewicz, Mireille Blanchard-Desce and Daniel T. Gryko

Table of Contents

1. Crystallographic data	S1-S2
2. Optical data	S3
2. NMR data	S4-S9

1. Crystallographic data

X-ray structure determining of 5-(tert-butyl)-9-(3,4-dimethoxyphenyl)-10-(3,3-dimethyl-2-oxobutyl)-2,3-dimethoxy-8H-pyrrolo[3',4':3,4]pyrrolo[2,1-a]isoquinoline-8,11(10H)-dione (3)

Crystal data and measurement conditions are given in Table S-1. The structure was solved by the SHELXL-1997 (Sheldrick, 1997) program.

Table S-1. Crystal data and measurement conditions for 5-(tert-butyl)-9-(3,4-dimethoxyphenyl)-10-(3,3-dimethyl-2-oxobutyl)-2,3-dimethoxy-8H-pyrrolo[3',4':3,4]pyrrolo [2,1-a]isoquinoline-8,11(10H)-dione (3)

Formula	C ₆₉ H ₇₈ Cl ₂ N ₄ O ₁₄
Molecular weight g/mol	1258.25
Crystal system	tetragonal
<i>a</i> [Å]	16.4941(7)
<i>b</i> [Å]	16.4941(7)
<i>c</i> [Å]	24.5221(9)
<i>V</i> [Å ³]	6671.4(5)
Molecular multiplicity	Z=8
Calculated density [g/cm ³]	1.253
Space group	<i>P</i> -4 <i>b</i> 2
Radiation (mirror monochromated)	Cu K α
Wavelength [Å]	1.54184
Absorption coefficient [mm ⁻¹]	1.420
F(000)	2664
Crystal size [mm]	0.17 x 0.15 x 0.03
Temperature [K]	100.0(1)
Scan range (2 θ) [deg]	3.60-72.03
Number of collected data:	
total measured	5854
unique [with <i>I</i> > 2 σ (<i>I</i>)]	3215
<i>R</i> _{<i>I</i>} [<i>I</i> > 2 σ (<i>I</i>)]	0.0749

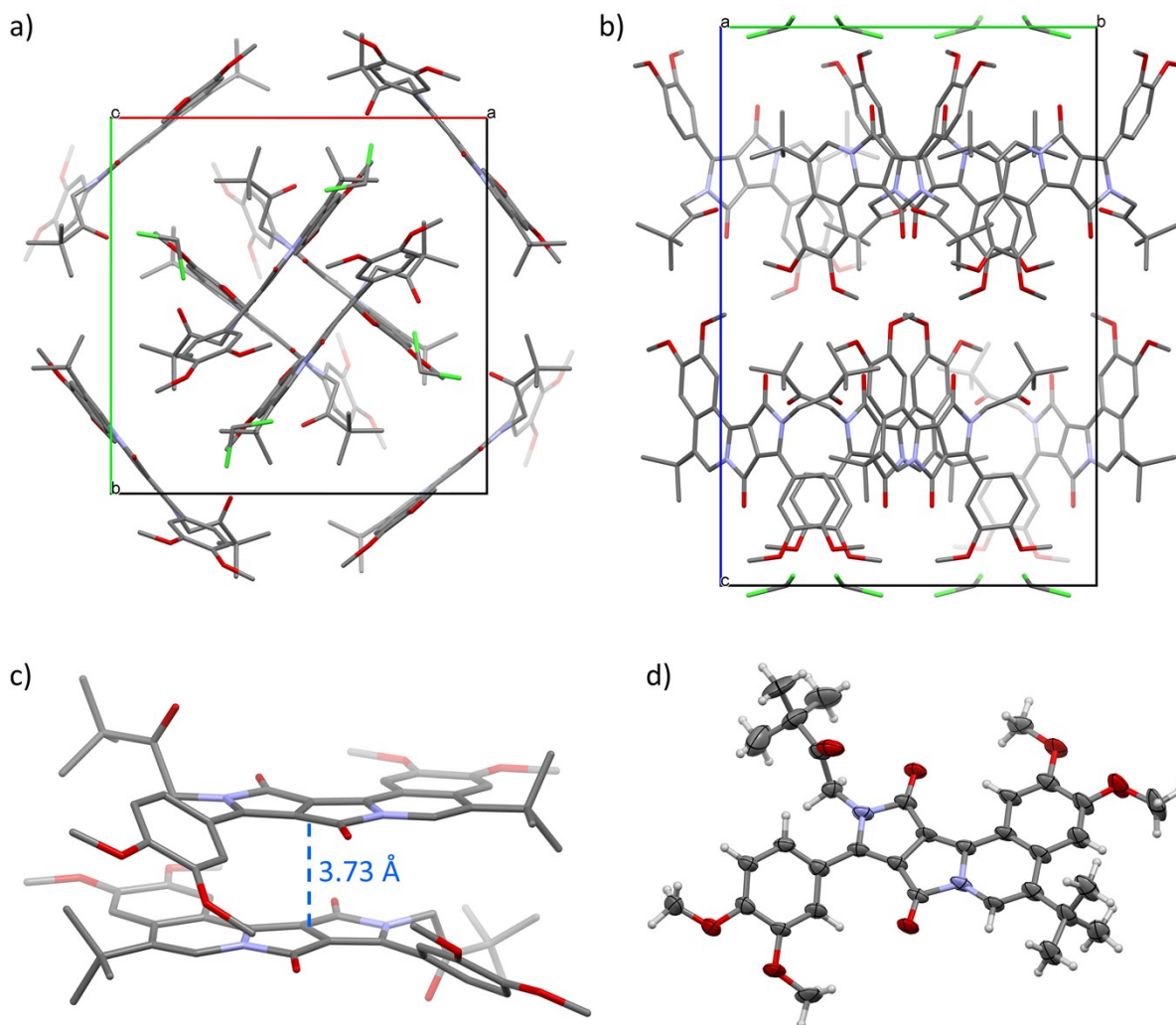


Figure S1. Crystal structure of compound **3**: a), b) Packing of the molecules in the crystal unit cell along crystal *c* and *b* axis respectively; c) Dimer of molecules connected by π - π interactions; d) Thermal ellipsoid plot of compound **3** with the ellipsoids drawn at 50 % probability level. On a), b) c) hydrogen atoms were omitted for clarity.

2. Optical data.

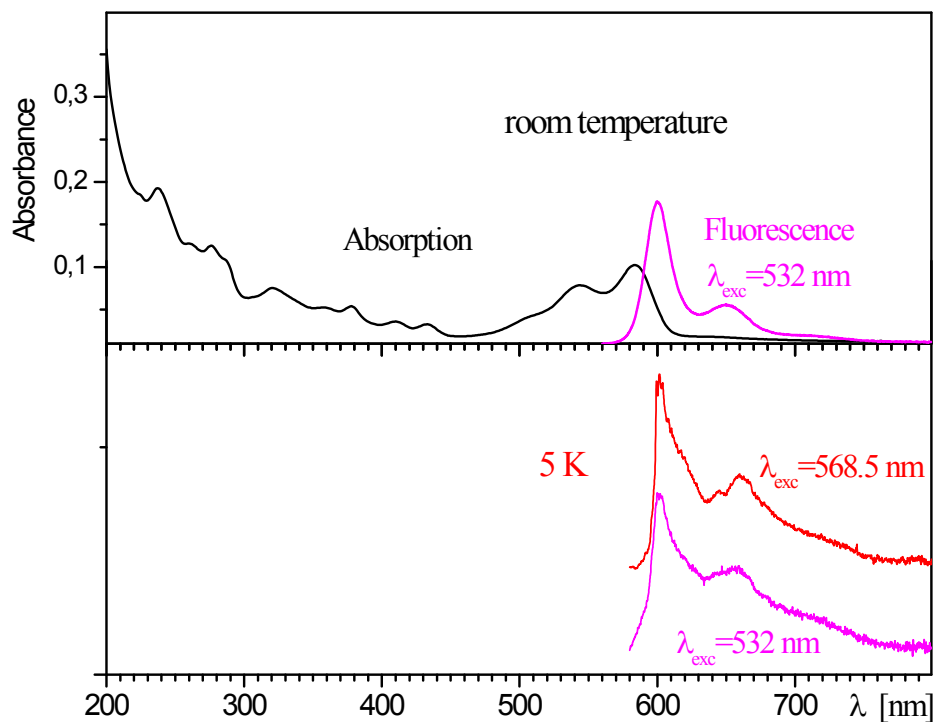


Figure S2. Absorption (solid black line) and emission (magenta and red lines) spectra of compound **3** in *n*-hexane at room temperature and at 5 K.

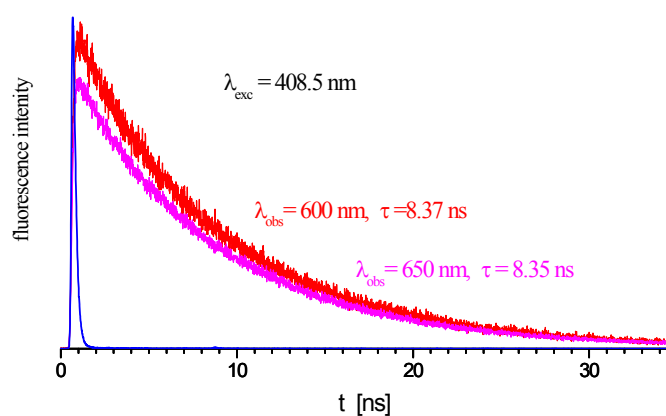


Figure S3. Fluorescence decay curves of compound **3** in *n*-hexane at room temperature.

3. Spectral data

