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MICROWAVE ASSISTED SYNTHESIS, ABSORPTION AND FLUORESCENCE OF FUROPYRROLINONE PIGMENTS

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Furopyrrolinone pigments were synthesized using solvent-free conditions and microwave heating. Soluble derivatives were prepared by N-butylation of pigment precursors. Absorption and fluorescence spectra were studied in DMSO both experimentally and theoretically, using time-dependent density functional theory. N-butylated derivatives show solid-state fluorescence.

Introduction

Diketopyrrolopyrroles (DPP) and their derivatives represent a class of brilliant red and strongly fluorescent high performance pigments that have prominent light-,

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weather- and solvent-resistance [1-6]. DPP pigments are known for being poorly soluble in common organic solvents due to their tendency to form strong π-π stacking and hydrogen bonding of adjacent molecules in solid-state and many efforts have been carried out on their functionalization to improve their solubility [7]. As a consequence, during the last few years, several studies have been reported in the literature on the use of these soluble DPP derivatives in modern application fields, as light-emitting diodes [8], field-effect transistors [9] and organic solar cells [10,11]. The symmetrical DPPs are produced by a base catalyzed condensation of 2 mole equivalent of (substituted) benzonitrile and 1 mole equivalent of succinic diester [12]. The synthesis of asymmetrical DPPs is also possible by base catalyzed condensation of aromatic nitrile and pyrrolinone ester [13,14]. Some DPP heteroanalogues, containing either one (furopyrrolinones, DPF) or two (diketofuranofuranones, DFF) oxygens instead of nitrogen, were also described [15,16].

Ethyl 4,5-dihydro-5-oxo-2-aryle(1*H*)pyrrole-3-carboxylate (pyrrolinone ester) has become an interesting intermediate in the color chemistry in recent years and the key for asymmetric synthesis of different analogues of DPP pigments. Methylene carbon in position 4 is activated by carbonyl and ester groups and a condensation with aldehydes [13,17], esters [16], a reaction with aromatic nitriles [5,14], reactions with diazonium salts [18,19] and catalytic oxidation using air oxygen [20] can be carried out.

In this work, we will discuss the synthesis and spectral properties of asymmetrical furopyrrolinone pigments and their alkylated derivatives, which are soluble in most organic solvents. The synthesis of these DPF pigments is based on the condensation reaction of pyrrolinone ester (PES) and different aromatic ester under strongly basic conditions forming aroylated pyrrolinone ester as an intermediate for DPFs formation as shown in Scheme 1.

Experimental and Theoretical Procedures

Materials and Equipment

2-Naphthoic acid (98%), 2-methyl-butan-2-ol (99%), ethyl bromoacetate (98%), 1,2-dimethoxy ethane (99%) and 1-bromobutane (99%) were purchased from Sigma-Aldrich. Dry solvents for synthesis and spectroscopic measurements (spectroscopic grade) were purchased from Fluka.

The absorption spectra were recorded at room temperature in DMSO using a Perkin-Elmer Lambda 35 spectrophotometer with 1 cm path length quartz cuvettes. A Perkin-Elmer (P.-E.) LS55 was used for measuring fluorescence spectra.

An EA 1108 FISONS instrument was used for elemental analysis. Melting

points of compounds were checked on a Büchi 510 melting point apparatus. Thin-layer chromatography (TLC) was performed by a Kieselgel 60 F254 (Merck, Darmstadt, Germany), for observation of reaction progress and to determine the purity of the prepared intermediates and dyes.

Positive-ion and negative-ion atmospheric pressure chemical ionization (APCI) mass spectra were measured on an ion trap analyzer Esquire 3000 (Bruker Daltonics, Bremen, Germany) in the range *m*/*z* 50-1000. The samples were dissolved in acetonitrile and analyzed by direct infusion at the flow rate of 100 μl min^{-1}. The selected precursor ions were further analyzed by MS/MS analysis under the following conditions: the isolation width *m*/*z* = 4, the collision amplitude in the range 0.7-1.0 V depending on the precursor ion stability, the temperature of drying gas was 330 °C, the APCI temperature was 400 °C, the tuning parameter compound stability was 100 %, the flow rate and the pressure of nitrogen were 4 ml min^{-1} and 45 psi, respectively.

The ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Advance II 400 spectrometer at 400.13 MHz and 100.62 MHz, respectively. The samples were dissolved in hexadeuteriodimethyl sulfoxide. The ^{1}H and ^{13}C NMR chemical shifts were referenced to the central signal of the solvent (δ = 2.55 and 39.6, respectively).

Synthesis and Analytics

Ethyl 5-oxo-2-phenyl-4,5-dihydro-1*H*-pyrrole-3-carboxylate and ethyl 5-oxo-2(2-naphthyl)-4,5-dihydro-1*H*-pyrrole-3-carboxylate were prepared by the same method as described in literature [13,21].

Symmetrical pigment **2a** was prepared by the same procedure as described in Ref. [16].

Ethyl 4-[hydroxy(naphthalen-2-yl)methylidene]-5-oxo-2-phenyl-4,5-dihydro-1*H*-pyrrole-3-carboxylate (1b)

To a three-necked 250 ml round flask connected with thermometer and nitrogen inlet, ethyl 5-oxo-2-phenyl-4,5-dihydro-1*H*-pyrrole-3-carboxylate (5.03 g, 21.8 mmol) and ethyl 2-naphthoate (4.37 g, 21.8 mmol) were added successively at 25 °C to a solution of sodium *t*-amyloxide, prepared from sodium (1.50 g, 65.2 mmol) and *t*-amyl alcohol (40 ml), and the mixture was then heated to reflux for 5.5 h under nitrogen. The resulting dark solution was cooled and added to an ice-cooled mixture of methanol (10 ml) and water (50 ml), then acidified dropwise with concentrated hydrochloric acid (3 ml) and extracted with tetrahydrofuran/diethyl ether; the extract was dried and concentrated, to give brownish dark colour

precipitate (3.6 g, yield 43 %), mp 171-173 °C (recrystallized from ethanol–water).

^{1}H-NMR (4 MHz, DMSO-d6, δ, ppm): 0.91 (3H, t, ^{3}J(H, H) = 7.2 Hz, CH_3), 3.91 (2H, q, ^{3}J(H, H) = 7.2 Hz, CH_2), 7.32-8.96 (12H, m, aromatic), 9.72 (1H,s, OH) and 11.24 (1H, s, NH pyrrolinone).

^{13}C-NMR (100 MHz, DMSO-d6, δ, ppm): 12.91 (1×CH_3), 59.67 (1×CH_2), 104.04, 124.59, 125.93, 126.77, 127.33, 127.60, 127.69, 127.98, 128.03, 128.33, 128.70, 128.89, 132,134,163.77 (COO), 169.08 (C=O pyrrolinone).

MS analysis M = 385.40 g mol^{-1}**,** Positive-ion MS: m/z 386 $[M+H]^+$, negative-ion MS: m/z 384 $[M+H]^-$ 100%; m/z 340 $[M+H–C_2H_5OH]^+$.

Elemental analysis; Calculated ($C_{24}H_{19}NO_4$): C (74.79 %), H (4.97 %), N (3.63 %), Found: C (74.81 %), H (4.99 %), N (3.65 %).

3-(Naphthalen-2-yl)-6-phenyl-1*H*-furo[3,4-*c*]pyrrole-1,4(5*H*)-dione (2b)

Ethyl 5-oxo-2(2-naphthyl)-4,5-dihydro-1*H*-pyrrole-3-carboxylate (800 mg, 2 mmol) was irradiated in a microwave reactor (800 W) at 200 °C for 30 min. The crude product was then allowed to cool, methanol was added, and the mixture was stirred at room temperature for 15 min and the precipitate was filtrated off and washed with 200 ml methanol. **2b** (520 mg, 76 %) was separated and dried at 90 °C.

^{1}H-NMR (400 MHz, DMSO-d6, δ, ppm): 7.29-7.69 (5H, m), 8.05 (1H,d), 8.17 (2H,d), 8.40 (2H,d), 8.54 (1H,d), 8.78 (1H,s) and 12.04 (1H, s, NH).

^{13}C-NMR was not observed due to low solubility of the pigment in DMSO.

MS analysis M = 339.3 g mol^{-1}**,** Negative-ion MS: m/z 338 $[M+H]^-$ 100 %.

Elemental analysis; Calculated ($C_{22}H_{13}NO_3$): C (77.87 %), H (3.86 %), N (4.13 %), Found: C (77.91 %), H (3.89 %), N (4.15 %).

5-Butyl-3,6-diphenyl-1*H*-furo[3,4-*c*]pyrrole-1,4(5*H*)-dione (3a)

To a three-necked 100 ml round flask 3,6-diphenyl-1*H*-furo[3,4-*c*]pyrrole-1,4(5*H*)-dione (1.5 g, 5.2 ×10^{-3} mol), anhydrous potassium carbonate (1.45 g, 0.0104 mol) and 40 ml *N*-methyl pyrrolidone were added, the mixture was stirred at 50 °C for 30 minutes. Then butyl bromide (1.43 g, 0.0104 mol) dissolved in 10 ml *N*-methyl pyrrolidone was dropwise added to the mixture during 1 h. The mixture was stirred at this temperature for 24 h, then cooled at room temperature (22 °C) and poured to 200 g water and ice. The precipitate was separated by using centrifugation (6000 rpm) for 20 min. The ppt was dried and the alkylated compound was separated by column chromatography (chloroform was used as eluent), (500 mg, 28% yield), mp 116-119 °C.

^{1}H-NMR (400 MHz, DMSO-d6, δ, ppm): 0.81 (3H, t, CH_3), 1.22 (2H, m,

CH_2), 1.50 (2H, m, CH_2), 3.88 (2H, t, CH_2), 7.68-8.35 (10H, m, aromatic).

^{13}C-NMR (100 MHz, DMSO-d6, δ, ppm): 13.38 (1×CH_3), 19.29 (1×CH_2), 30.49 (1×CH_2), 41.38 (1×CH_2), 103.43, 113.71, 126.39, 127.00, 128.77, 129.29, 129.56, 131.98, 133.37, 150.45, 154.01, 158.85, 160.79.

MS analysis M = 345.4 g mol^{-1}, Negative-ion MS: m/z 344 $[M+H]^-$ 100 %.

Elemental analysis; Calculated ($C_{22}H_{19}NO_3$): C (76.50 %), H (5.54 %), N (4.06 %), Found: C (76.55 %), H (5.59 %), N (4.10 %).

5-Butyl-3-(naphthalen-2-yl)-6-phenyl-1*H*-furo[3,4-*c*]pyrrole-1,4(5*H*)-dione (3b)

To a three-necked 100 ml round flask, 3-(naphthalen-2-yl)-6-phenyl-1*H*-furo[3,4-*c*]pyrrole-1,4(5*H*)-dione (**2b**, 300 mg, 0.88 mmol), anhydrous potassium carbonate (244 mg, 1.76 mmol) and 40 ml *N*-methyl pyrrolidone were added, the mixture was stirred at 50 °C for 30 min. Then (240 mg, 1.76 mmol) butyl bromide in 10 ml *N*-methyl pyrrolidone was added to the mixture dropwise during 1 h. The mixture was stirred at this temperature for 24 h, then cooled at room temperature (22 °C) and poured to 100 g water and ice. The precipitate was filtrated off and washed with water. Then it was dried, and the alkylated compound was separated by column chromatography (chloroform was used as eluent), (100 mg, 29% yield), mp 126-129 °C.

^{1}H-NMR (400 MHz, DMSO-d6, δ, ppm): 0.86 (3H, t, CH_3), 1.25 (2H, m, CH_2), 1.55 (2H, m, CH_2), 3.89 (2H, t, CH_2), 7.25-8.89 (12H, m, aromatic).

^{13}C-NMR (100 MHz, DMSO-d6, δ, ppm): 13.41 (1×CH_3), 19.39 (1×CH_2), 30.72 (1×CH_2), 41.39 (1×CH_2), 104.43, 118.71, 124.81, 125.42, 126.32, 126.59, 127.10, 127.38, 127.81, 128.87, 129.39, 129.59, 132.98, 133.1, 133.37, 144.2, 150.45, 154.11, 158.89, 160.89.

MS analysis M = 395.4 g mol^{-1}, Negative-ion MS: m/z 394 $[M+H]^-$ 100 %.

Elemental analysis; Calculated ($C_{22}H_{19}NO_3$): C (78.97 %), H (5.35 %), N (3.54 %), Found: C (79.05 %), H (5.39 %), N (3.60 %).

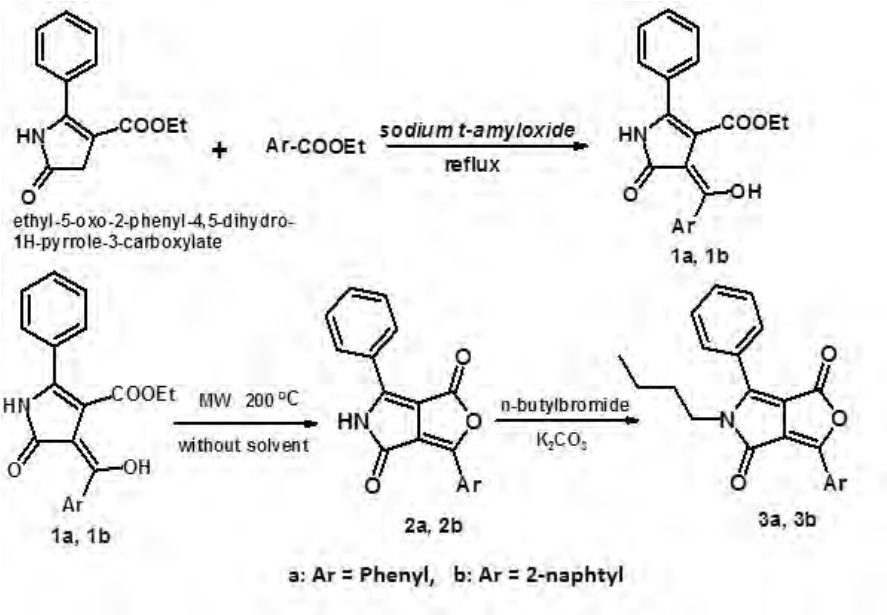
Quantum Chemical Calculations

The theoretical calculations based on density functional theory (DFT) were carried out. The ground state geometry was optimized using B3LYP functional in the combination with 6-311G(d,p) basis set. Time-dependent (TD) DFT calculations of the excitation energies of the lowest six transitions were carried out with the same xc functional and the broader basis set 6-311+G(2d,p). Solvent effect of dimethyl sulfoxide was taken into account through non-equilibrium polarized continuum model (PCM). All calculation codes came from Gaussian09W program suite [22].

Results and Discussion

Synthesis

The preparation of furopyrrolinone pigments **2a** and **2b** was based on the condensation of phenyl pyrrolinone esters with ethyl benzoate (**1a**) or ethyl-2-naphthoate (**1b**) at strongly basic condition (sodium *t*-amyloxide), which form a beige-coloured intermediates (**1a**,**b**) with moderate yields (Scheme 1). ^{1}H NMR shows four sets of signals, corresponding to ethylester group, the main one at δ = 0.91 (methyl) and δ = 3.91 (methylene) and minor ones at δ = 0.58, 0.66 and 0.82 (CH_3) and at δ = 3.80, 3.84 and 4.03 (CH_2), reflecting keto/enol and *E*/*Z* equilibria, as shown in Scheme 2.

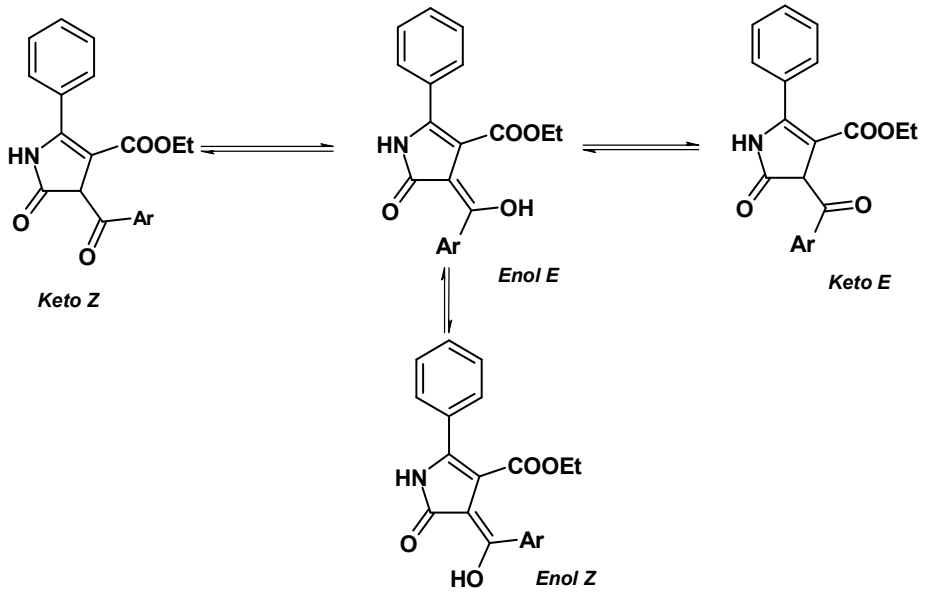


Scheme 1 Synthetic route for **2a**, **2b** pigments and their alkylated derivatives **3a**,**3b**

The solvent free cyclization of aroylated pyrrolinone ester in a microwave oven at 200 °C formed DPFs in a yield always over 70 % (Scheme 1). The *N*-alkylated **3a** and **3b** were prepared by direct alkylation using butyl bromide. The reaction yield was less that 50 % in both cases that goes probably on account of partial opening of a lacton ring at the conditions of *N*-butylation.

Absorption and Emission Spectra

The absorption spectra of all the prepared compounds were measured in DMSO and the spectral data were summarized in Table I. The absorption spectra of **2a** and



Scheme 2 Isomerization / tautomerization of aroylated pyrrolinone ester intermediates (**1a**, **b**)

its asymmetrical analogue **2b** show two long-wavelength vibronic bands with an absolute maximum corresponding to 0-0 transition, as in the case of basic non-alkylated DPP and DFF [23] and also 2-naphtyl substituted DPP [21]. A bathochromic shift of 14 nm, when going from **2a** to **2b**, reflects the effect of conjugation extension. The main visible absorption band of **2a** is of HOMO → LUMO character and its maximum lies between the corresponding maxima of its DPP and DFF heteroanalogues, as predicted by theory (Table II). The second absorption band of **2a** corresponds to HOMO-1 → LUMO and is detectable in the spectrum on the contrary to the symmetrical DPP and DFF analogues. This is quite an illustrative example of a change in symmetry forbidden transition to partially allowed, due to the symmetry perturbation.

Table I Spectral properties in DMSO

Compound	Absorbance λ_{max} nm	Fluorescence λ_{max} nm	Fluorescence in solid state λ_{max} nm	ε mol l^{-1} cm^{-1}
2a	453. 484	498. 5	-	29200
2b	468. 500	514. 56	-	31000
3a	454	520. 55	593	18000
3b	461	528. 55	596	19200

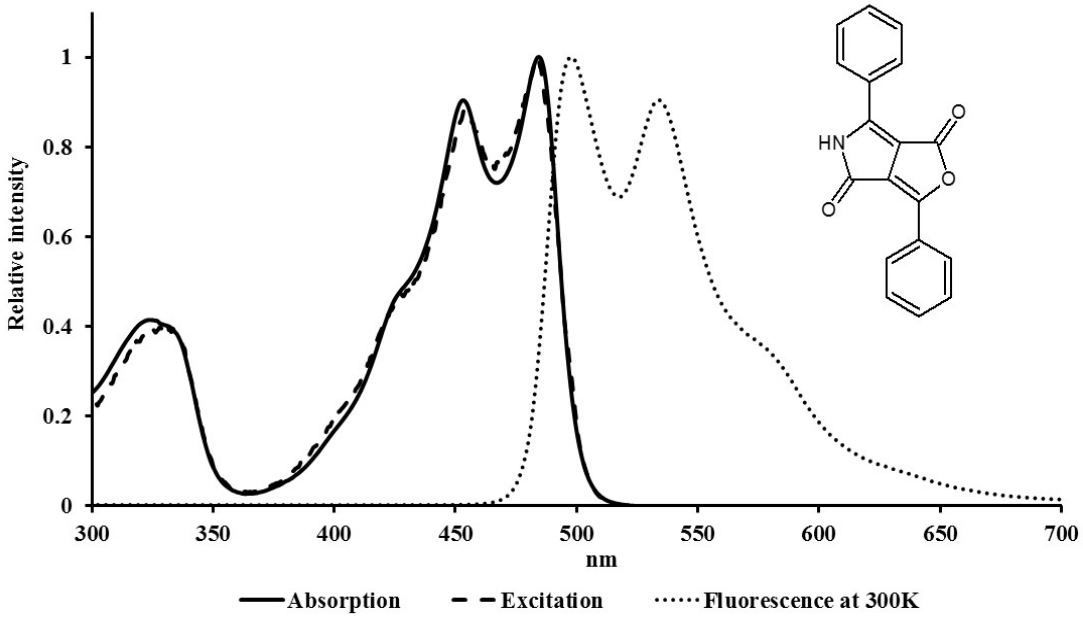


Fig. 1 Absorption and emission spectra of **2a**

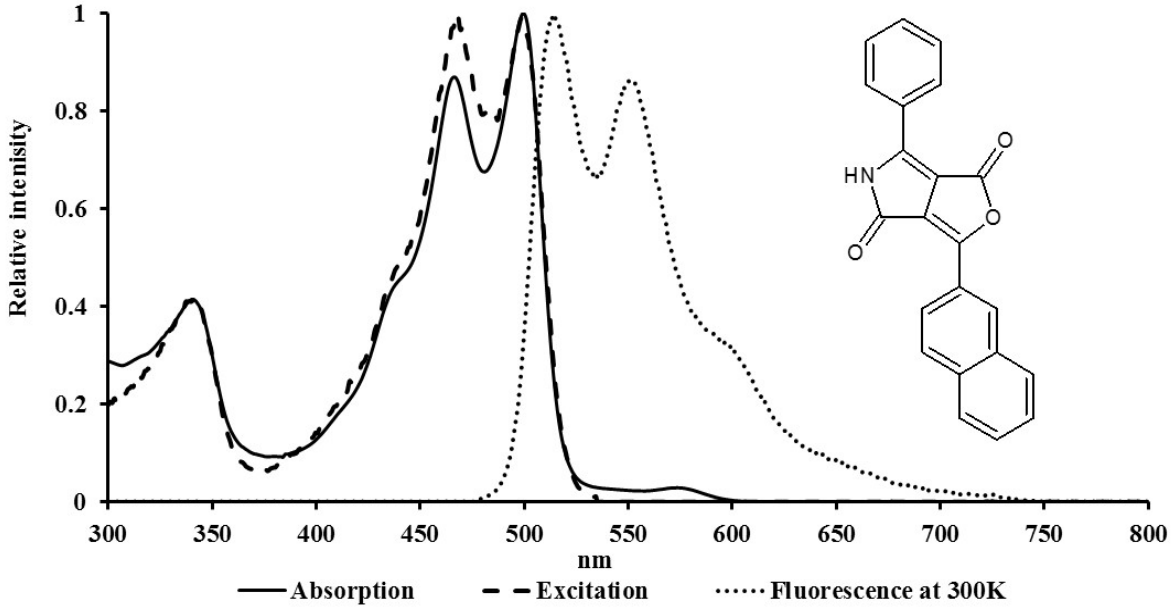
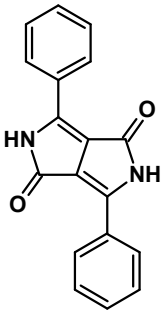


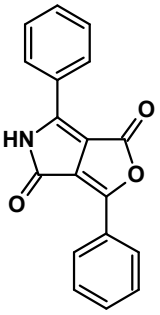
Fig. 2 Absorption and emission spectra of **2b**

N-Butylation causes the hypsochromic and hypochromic shift of the absolute maxima, redistribution of the vibronic bands' intensities in favour of 0-1 transition and overall loss of a sharp vibronic structure (Fig. 3). These are typical manifestations of a chromophore non-planarity [24]. The spectrum of *N*-butylated **2a** resembles more the spectrum of mono *N*-butylated DPP (2-butyl-3,6-diphenyl-

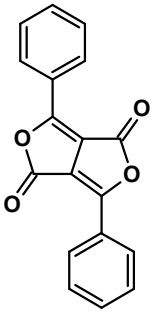
Table II PCM TD DFT computed excitation energies (converted to λ_{max} [nm]) and oscillator strengths (in parenthesis) in DMSO



DPP
Diketopyrrolopyrrol



DPF (2a)
Diketopyrrolofuran



DFF
Diketofurofuran

Compound (Symmetry)	Transition type	Theoretical λ_{max} (f_{osc})	Experimental λ_{max}
DFF	$S_0 \rightarrow S_1$ (HOMO→LUMO)	464 (0.879)	459 [231]
C_{2h})	$S_0 \rightarrow S_2$ (HOMO→LUMO+1)	341 (0.000)	
	$S_0 \rightarrow S_3$ (HOMO-1→LUMO)	338 (0.000)	
	$S_0 \rightarrow S_4$ (HOMO-2→LUMO)	337 (0.028)	
	$S_0 \rightarrow S_5$ (HOMO-3→LUMO)	303 (0.000)	
	$S_0 \rightarrow S_6$ ($n\pi^*$)	292(0.000)	
2a	$S_0 \rightarrow S_1$ (HOMO→LUMO)	479 (0.729)	484
(C_s)	$S_0 \rightarrow S_2$ (HOMO-1→LUMO)	335 (0.042)	324
	$S_0 \rightarrow S_3$ (HOMO→LUMO+1)	332 (0.004)	
	$S_0 \rightarrow S_4$ (HOMO-2→LUMO)	329 (0.036)	
	$S_0 \rightarrow S_5$ ($n\pi^*$)	321 (0.000)	
	$S_0 \rightarrow S_6$ (HOMO-4→LUMO)	315 (0.224)	
DPP	$S_0 \rightarrow S_1$ (HOMO→LUMO)	494 (0.640)	507 [24]
(C_{2h})	$S_0 \rightarrow S_2$ (HOMO-1→LUMO)	358 (0.000)	
	$S_0 \rightarrow S_3$ ($n\pi^*$)	336 (0.000)	
	$S_0 \rightarrow S_4$ (HOMO→LUMO+1)	327 (0.000)	
	$S_0 \rightarrow S_5$ (HOMO-2→LUMO)	322 (0.025)	
	$S_0 \rightarrow S_6$ (mix)	319 (0.000)	

2,5-dihydropyrrolo[3,4-*c*]pyrrole-1,4-dione) with only one phenyl ring rotated out-of-DPP plane, than the spectrum of *N*,*N*´-dibutylated DPP (2,5-dibutyl-3,6-diphenyl-2,5-dihydropyrrolo[3,4-*c*]pyrrole-1,4-dione) with both rings rotated out [24]. Really, the DFT calculations of **3a** predict the phenyl on lactam ring rotated by 29^0, while that one on lacton ring is almost coplanar (2°) with DPF core.

The fluorescence spectra of **2a** and **2b** show small Stokes shift (14 nm) and almost mirror-symmetry between absorption and fluorescence, as a consequence of a small excited state relaxation. On the other hand, considerably higher Stokes of both *N*-butylated derivatives (66- 67 nm) indicates a considerable change of an excited-state geometry of these non-planar molecules. As in the case of DPPs [25], *N*-alkylation enables to observe solid-state fluorescence as the quenching π-π stacking interaction is limited due to the chromophore non-planarity.

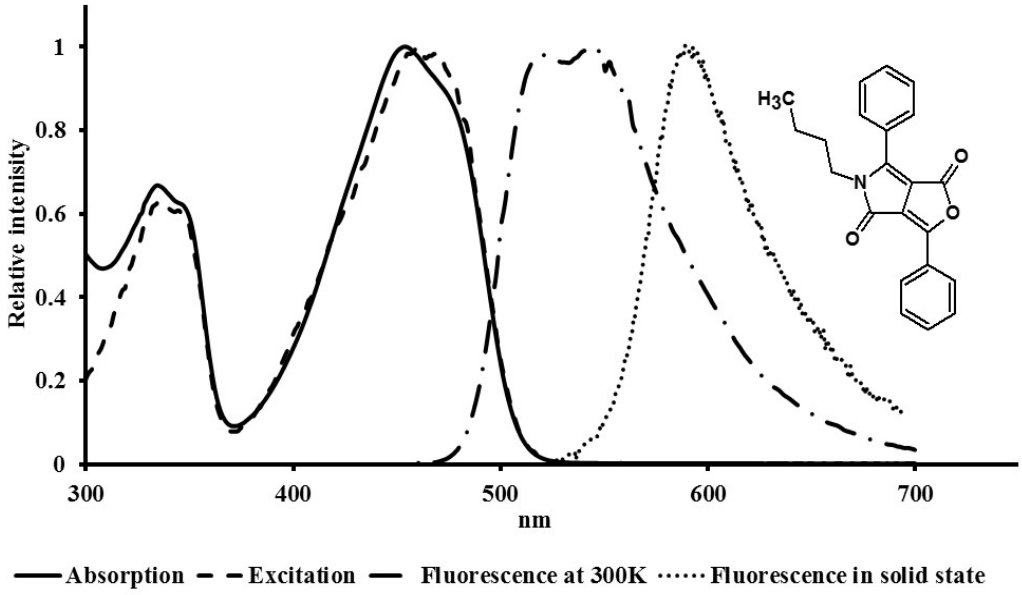


Fig. 3 Absorption and emission spectra of **3a**

Conclusion

New furopyrrolinone pigments were prepared by cyclization of aroylated pyrrolinone ester in a microwave reactor without solvent in very good yield (over 70 %). The soluble derivatives were prepared by *N*-butylation of pigment precursors. DPF pigments fluoresce only in solution, while their *N*-butylated derivatives show also relatively strong solid-state fluorescence, observable by naked-eye under UV illumination.

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