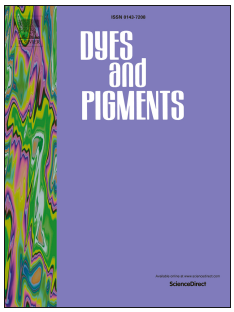


Influence of the chemical structure and solvent polarity on the fluorescence of 3-aryl-7-benzoyl-pyrrolo [1,2-c]pyrimidines

Eleonora-Mihaela Ungureanu, Marian-Laurentiu Tatu, Emilian Georgescu, Cristian Boscornea, Marcel-Mirel Popa, Gabriela Stanciu

PII: S0143-7208(19)31400-7

DOI: https://doi.org/10.1016/j.dyepig.2019.108023

Reference: DYPI 108023

To appear in: *Dyes and Pigments*

Received Date: 15 June 2019

Revised Date: 8 October 2019

Accepted Date: 4 November 2019

Please cite this article as: Ungureanu E-M, Tatu M-L, Georgescu E, Boscornea C, Popa M-M, Stanciu G, Influence of the chemical structure and solvent polarity on the fluorescence of 3-aryl-7-benzoyl-pyrrolo [1,2-c]pyrimidines, *Dyes and Pigments* (2019), doi: https://doi.org/10.1016/j.dyepig.2019.108023.

Influence of the chemical structure and solvent polarity on the fluorescence of 3-aryl-7-benzoyl-pyrrolo[1,2-c]pyrimidines

Eleonora-Mihaela Ungureanu[a], Marian-Laurentiu Tatu[a,b], Emilian Georgescu[c], Cristian Boscornea[d], Marcel-Mirel Popa[e], Gabriela Stanciu[f*]

[a]*Department of Inorganic Chemistry, Physical Chemistry and Electrochemistry, University "Politehnica" of Bucharest, Gh. Polizu 1-7, 011061, Bucharest, Romania*
[b]*Research-Development Institute for Non-Ferrous and Rare Metals (IMNR), 102 Biruintei Blvd, 077145, Pantelimon, Romania*
[c]*Chimcomplex Research Center, Uzinei Street 1, 240050, Ramnicu Valcea, Romania*
[d]*Department of Bioresources and Polymer Science University "Politehnica" of Bucharest, Gh. Polizu 1-7, 011061, Bucharest, Romania*
[e]*Center of Organic Chemistry "C. D. Nenitzescu", Romanian Academy, Spl. Independentei, 202 B, 060023, Bucharest, Romania*
[f]*Department of Chemistry and Chemical Engineering, Ovidius University, Constanta, 124 Mamaia Blvd, 900527, Romania*

[*]Corresponding authors. E-mail: *gstanciu66@yahoo.com*, Tel. +40 724936673

Abstract

Structure-fluorescence properties of new synthesized 3-aryl-7-benzoyl-pyrrolo[1,2-c]pyrimidines were measured in order to correlate the nature of the substituents with the absorption and emission features (absorption intensity, fluorescence quantum yield, Stokes shifts, fluorescence quenching in presence of inhibitors). The influence of the solvent on the fluorescence of the title compounds was investigated by multiple linear regressions, connecting the polarity of different solvents with the luminescent properties. Some of the new pyrrolo[1,2-c]pyrimidines show strong fluorescence in the blue region of the visible spectrum, making them potential candidates for OLED technology or advanced materials.

Keywords: pyrrolo[1,2-c]pyrimidines, fluorescence, quantum yield, Stokes shift, solvent polarity functions

1. Introduction

Fluorescence is an important property [1] of organic molecules, very useful in designing advanced materials for practical applications such as OLEDs [2], dye-sensitized solar cells [3,4], bioimaging [5], chemical sensors [6] or even for the study of supramolecular structures by fluorescence resonance energy transfer [7]. Small nitrogen containing molecules from the class of *N*-bridgehead heterocycles are promising candidates for important fluorescence applications [8-10]. In this class, pyrrolo[1,2-*c*]pyrimidines have shown interesting biological activity [11,12], the same heterocyclic moiety being found in the structures of several natural compounds [13,14]. However, the literature is rather scarce in what concerns the photophysical properties of these compounds, even if the interest in their synthetic strategies is permanent [15-20]. Among the synthetic methods of the pyrrolo[1,2-*c*]pyrimidines, the 1,3-dipolar cycloaddition of the corresponding *N*-ylides has been found especially advantageous [21-24].

The effect of the solvent on excitation and emission properties of organic compounds is also a current subject of interest [25]. When the photon excites a molecule, a redistribution of charges occurs. This can lead to the change of the dipole moment in the excited state, which offers information about the molecule electronic structure and geometry. The method used

for calculation of the dipole moment is based on the spectral shifts [26,27]. The position, shape and intensity of the bands in excitation and emission spectra of a molecule change in solvents with different polarity. This phenomenon can be attributed to the solvent – solute interactions, which can be non-specific (electrostatic interaction) or specific (hydrogen bonding) [28-31].

Organic molecules which have the property to change their colour in presence of solvents with different polarity are potential candidates as environment-sensitive fluorescent probes [1,2]. If the fluorophores possess photo-switching ability, they can be used as molecular probes for super-resolution fluorescence microscopes [32,33].

Several electrochemical and fluorescence measurements [34-36] have been conducted in our group as part of the general interest in finding and describing the applicative properties of pyrrolopyrimidines. A series of 3-aryl-7-benzoyl-pyrrolo[1,2-c]pyrimidines in which the 3-aryl ring is substituted with methoxy groups (which were proved to have high enhancing effect on the photophysical features of pyrrolo[1,2-*c*]pyrimidines [35]) have been synthesized and investigated. The compounds described in this paper have additional structural changes given by substitution of the benzoyl moiety in C-7 [37,38]. The structural effect of substitution was quantified by fluorescence properties (quantum yield, Stokes shifts and fluorescence quenching). The correlation between substituents and excitation/fluorescence spectra of the studied compounds are discussed herein. The influence of the solvent polarity was also investigated.

2. Materials and methods

2.1. Equipment, materials and methods

Melting points were determined on Boëtius hot plate microscope. Elemental analysis was carried out on COSTECH Instruments EAS32 apparatus. IR spectra were recorded in KBr pellets on Bruker Vertex 70 ATR or Nicolet Impact 410 spectrometers. NMR spectra were recorded on Varian Gemini 300 BB, operating at 300 MHz for ^{1}H-NMR and 75 MHz for ^{13}C-NMR or on Bruker Advance III 400 instrument, operating at 400 MHz for ^{1}H-NMR and 100 MHz for ^{13}C-NMR. JASCO V550 spectrophotometer has been used to record UV-Vis spectra. Quartz cuvettes with 1 cm optical path length where used for the measurements performed in solution. Jasco FP6500 spectrofluorometer was used to measure excitation and emission spectra applying a reading angle of 90º. Refractive indices were measured at 25^{o}C using Abbe refractometer (from CETI Belgium). Quantum yields were calculated using quinine sulphate as standard [36]. The spectra were recorded in chloroform ($CHCl_3$), dichloromethane (CH_2Cl_2), acetonitrile (CH_3CN) or dimethyl sulfoxide (DMSO) of spectrophotometric quality. High resolution MS spectra have been recorded on Bruker Maxis II QTOF spectrometer with electrospray ionization (ESI) in the positive mode.

2.2. Main characteristics of the new 3-aryl-7-benzoyl-pyrrolo[1,2-*c*]pyrimidines

The new pyrrolo[1,2-c]pyrimidines have been synthesized by a previously reported general synthetic procedure based on the 1,3-dipolar cycloaddition reactions of *N*-heterocyclic ylides, generated *in situ* from the corresponding *N*-heterocycle quaternary salts in the presence of epoxides as acid scavengers and reaction medium, with activated acetylenes [39,40]. All reactions have been performed in the presence of 1,2-epoxybutane at reflux temperature starting from 2.5 mmol of pyrimidinium quaternary salts [21,23,24]. Their main characteristics are given below.

Ethyl 3-(2,4-dimethoxyphenyl)-7-(4-methylbenzoyl)pyrrolo[1,2-c]pyrimidine-5-carboxylate **3a**: yellow crystals; 0.53 g (48 %). IR (ν, cm^{-1}): 2985, 1686, 1612, 1572, 1523, 1472, 1408, 1349, 1327, 1299, 1257, 1206, 1087. ^{1}H NMR (δ, 300 MHz, $CDCl_3$):1.44 (t, 3H, *J* = 7.1 Hz, CH_3); 2.46 (s, 3H, CH_3); 3.87, 3.97 (2s, 6H, 2MeO); 4.40 (q, 2H, *J* = 7.1 Hz, CH_2); 6.57 (d, 1H, *J* = 2.5 Hz, H-3'); 6.64 (dd, 1H, *J* = 8.2, 2.5 Hz, H-5'); 7.33 (d, 2H, *J* = 8.8 Hz, H-2", H-6"); 7.76 (d, 2H, *J* = 8.2 Hz, H-3", H-5"); 7.83 (s, 1H, H-6); 8.22 (d, 1H, *J* = 8.8 Hz, H-6'); 8.90 (d, 1H, *J* = 1.5 Hz, H-4); 10.52 (d, 1H, *J* = 1.5 Hz, H-1). ^{13}C NMR (δ, 75 MHz, $CDCl_3$): 14.7 (CH_3); 21.7 (CH_3); 55.6, 55.7 (2MeO); 60.4 (CH_2); 99.0 (C-3'); 105.3 (C-5'); 106.6 (C-5); 112.2 (C-4); 118.8 (C-1'); 122.2 (C-7); 129.5 (C-6, C-3", C-5"); 130.1 (C-2", C-6"); 132.3 (C-6'); 140.3 (C-1); 136.6, 140.6, 142.6, (C-4a, C-1", C-4"); 147.5 (C-3);159.4, 162.2 (C-2', C-4'); 163.9 (COO);185.0 (COAr). HRMS-ESI (*m*/*z*): $[M+H]^+$ for $C_{26}H_{24}N_2O_5$, calcd. 445.17580, found 445.17590; Elem. anal.: calcd. for $C_{26}H_{24}N_2O_5$ (444,48): C 70.26, H 5.44, N 6.30; found C 70.37, H 5.53, N 6.22.

Ethyl 3-(3,4-dimethoxylphenyl)-7-(4-fluorobenzoyl)pyrrolo[1,2-c]pyrimidine-5-carboxylate **3b**: yellow crystals; 0.56 g (50 %). IR (ν, cm^{-1}): 2949, 1697, 1618, 1597, 1505, 1476, 1411, 1330, 1270, 1229, 1197, 1151,1084. ^{1}H NMR (δ, 300 MHz, $CDCl_3$): 1.43 (t, 3H, *J* = 7.1 Hz, Me); 3.95, 4.01 (2s, 6H, 2MeO); 4.41 (q, 2H, *J* = 7.1 Hz, CH_2); 6.96 (d, 1H, *J* = 8.4 Hz, H-5'); 7.21 (t, 2H, *J* = 8.5 Hz, H-3", H-5"); 7.70 (d, 1H, *J* = 2.1 Hz, H-2'); 7.73-7.76 (m, 3H, H-6', H-6); 7.85-7.90 (m, 2H, H-2", H-6"); 8.50 (d, 1H, *J* = 1.5 Hz, H-4); 10.49 (d, 1H, *J* = 1.5 Hz, H-1); ^{13}C NMR (δ, 75 MHz, $CDCl_3$): 14.6 (Me); 56.1 (2MeO); 60.6 (CH_2); 106.7 (C-5); 107.4 (C-4); 109.8 (C-2'); 111.3 (C-5'); 115.7 (*J*= 22.0 Hz, C-3", C-5"); 119.9 (C-6'): 122.0 (C-7); 129.4 (C-1'); 129.9 (C-6);131.5 (*J*= 8.1 Hz, C-2", C-6") 140.7 (C-1);135.3, 141.2, 149.4, 149.8, 151.1 (C-3, C-4a, C-3', C-4', C-1"); 165.1 (*J* = 251.9 Hz, C-4"); 163.7 (CO_2Et); 183.7 (COAr). HRMS-ESI (*m*/*z*): $[M+H]^+$ for $C_{25}H_{21}FN_2O_5$, calcd. 449.15073, found 449.15095; Elem. anal.: calcd. for $C_{25}H_{21}FN_2O_5$(448.44): C 66.96, H 4,72, N 6.25; found C 66.89, H 4.67, N 6.31.

Ethyl 3-(3,4-dimethoxylphenyl)-7-(2,4-dimethoxybenzoyl)pyrrolo[1,2-c]pyrimidine-5-carboxylate **3d**: yellow crystals; 0.57 g (47 %). IR (ν, cm^{-1}): 1692, 1619, 1599, 1476, 1329, 1266, 1200.^{1}H NMR (δ, 300 MHz, $CDCl_3$): 1.42 (t, 3H, *J* = 7.1 Hz, Me); 3.84, 3.96, 4.00, 4.03 (4s, 12H, 4MeO); 4.40 (q, 2H, *J* = 7.1 Hz, CH_2);6.57 (s, 1H, H-3"); 6.99 (d, 1H, *J* = 8.4 Hz, H-5'); 7.73 (d, 1H, *J* = 2.1 Hz, H-2'); 7.76-7.79 (m, 3H, H-6', H-5", H-6"); 7.53 (s, 1H, H-6); 8.46 (d, 1H, *J* = 1.5 Hz, H-4); 10.52 (d, 1H, *J* = 1.5 Hz, H-1); ^{13}C NMR (δ, 75 MHz, $CDCl_3$): 14.5 (Me); 56.0, 56.1, 56.2, 56.4 (4MeO); 60.4 (CH_2); 96.7 (C-3"); 106.6 (C-5); 107.4 (C-4); 109.8 (C-2'); 111.2 (C-5'); 119.9 (C-6'):122.5 (C-7); 130.2, 133.7 (C-6, C-5", C-6");140.7 (C-1);101.9, 129.4, 141.0, 149.3, 149.8, 150.9, 158.1, 158.6 (C-3, C-4a, C-1', C-3', C-4', C-1", C-2", C-4"); 163.7 (CO_2Et); 182.5 (COAr). HRMS-ESI (*m*/*z*): $[M+H]^+$ for $C_{27}H_{26}N_2O_7$, calcd. 491.181278, found 491.05077; Elem. anal.: calcd. for $C_{27}H_{26}N_2O_7$ (490.50): C 66.11, H 5.34, N 5.71; found C 66.20, H 5.39, N 5.60.

Dimethyl 3-(2-methoxyphenyl)-7-benzoyl-pyrrolo[1,2-c]pyrimidine-5,6-dicarboxylate **3e**: yellow crystals; 0.43 g (39%). IR (ν, cm^{-1}): 2945, 1746, 1697, 1626, 1518, 1490, 1448, 1382, 1344, 1303, 1265, 1202, 1167, 1108.^{1}H NMR (δ, 300 MHz, $CDCl_3$): 3.34, 3.91, 3.99 (3s, 6H, 3MeO); 7.06 (dd, 1H, *J* = 8.3, 1.1 Hz, H-3'); 7.13 (td, 1H, *J* = 7.8, 1.1 Hz, H-5');7.41-7.61 (2m, 4H, H-4', H-3", H-4", H-5"); 7.71-7.74 (m, 2H, H-2", H-6"); 8.18 (dd, 1H, *J* = 7.8, 1.8 Hz, H-6'); 8.95 (d, 1H, *J* = 1.5 Hz, H-4); 10.30 (d, 1H, *J* = 1.5 Hz, H-1). ^{13}C NMR (δ, 75 MHz, $CDCl_3$): 51.7, 52.3, 55.6 (3MeO); 104.7 (C-5); 111.5 (C-3'); 113.5 (C-4); 120.2 (C-7); 121.1, 130.9, 131.0 (C-4', C-5', C-6'); 128.1, 128.6, 132.1 (C-2", C-3", C-4", C-5", C-6"); 125.5, 132.8, 138.9, 139.0 (C-4a, C-6, C-1', C-1"); 139.7 (C-1); 147.9 (C-3); 157.9 (C-2'); 162.9, 164.5 (2COO); 186.3 (COAr). HRMS-ESI (*m*/*z*): $[M+H]^+$ for $C_{25}H_{20}N_2O_6$, calcd. 445.13941, found 445.13861; Elem. anal.: calcd. for $C_{25}H_{20}N_2O_6$ (444.44): C 67.56, H 4.54, N 6.30; found C 67.63, H 4.61, N 6.22.

Diethyl 3-(3-methoxyphenyl)-7-(3-nitrobenzoyl)pyrrolo[1,2-c]pyrimidine-5,6-carboxylate **3f**: yellow crystals; 0.66 g (51%). IR (ν, cm^{-1}): 2986, 1732, 1707, 1619, 1530, 1493, 1439, 1340, 1224, 1197, 1118. ^{1}H NMR (δ, 400 MHz, $CDCl_3$): 1.09, 1.40 (2t, 6H, *J* = 7.1 Hz, $2CH_3$); 3.92 (s, 3H, MeO); 3.71, 4.37 (2q, 4H, *J* = 7.1 Hz, $2CH_2$); 7.03-7.06 (m, 1H, H-4'); 7.44 (t, 1H, *J* = 7.8 Hz, H-5'); 7.66-7.75 (m, 3H, H-2', H-6', H-5");8.04-8.07 (m, 1H, H-6"); 8.42-8.45 (m, 1H, H-4"); 8.57 (t, 1H, *J* = 1.8 Hz, H-2"); 8.65 (d, 1H, *J* = 1.5 Hz, H-4); 10.37 (d, 1H, *J* = 1.5 Hz, H-1). ^{13}C NMR (δ, 100 MHz MHz, $CDCl_3$): 13.5, 14.3 (2Me); 55.5 (MeO);61.0, 62.3 ($2CH_2$), 105.7 (C-5); 108.9 (C-4); 112.5, 116.5 (C-2', C-4'), 123.6 (C-4"); 126.4, 129.5 134.3 (C-2", C-5", C-6"); 119.3, 130.1 (C-5', C-6'); 119.1, 133.8, 137.4, 140.1, 140.2, 150.6 (C-4a, C-6, C-7, C-1', C-1", C-3");140.3 (C-1);147.7 (C-3);160.2 (C-3'); 162.2, 164.0 (2COO); 183.5 (COAr); HRMS-ESI (*m*/*z*): $[M+Na]^+$ for $C_{27}H_{23}N_3O_8$, calcd. 540.13774, found 540.13834; Elem. anal.: calcd. for $C_{27}H_{23}N_3O_8$ (517.49): C 62.66, H 4.48, N 8.12; found C 62.74, H 4.52, N 8.03.

Dimethyl 3-(2,4-dimethoxyphenyl)-7-(4-bromobenzoyl)pyrrolo[1,2-c]pyrimidine-5,6-dicarboxylate **3g:** yellow crystals;0.57 g (41%). IR (ν, cm^{-1}): 2945, 1739, 1704, 1605, 1502, 1446, 1386, 1292, 1261, 1201, 1177, 1106.^{1}H NMR (δ, 400 MHz, $CDCl_3$): 3.41, 3.89, 3.90, 3.98 (2s, 6H, 2MeO); 6.58 (d, 1H, *J* = 2.5 Hz, H-3'); 6.66 (dd, 1H, *J* = 8.2, 2.5 Hz, H-5');7.57 (d, 2H, *J* = 8.8 Hz, H-2", H-6"); 7.62 (d, 2H, *J* = 8.8 Hz, H-3", H-5"); 8.24 (d, 1H, *J* = 8.8 Hz, H-6'); 8.93 (d, 1H, *J* = 1.5 Hz, H-4); 10.25 (d, 1H, *J* = 1.5 Hz, H-1); ^{13}C NMR (δ, 100 MHz MHz, $CDCl_3$): 51.8, 52.5 (2Me); 55.5, 55.6 (MeO); 98.92 (C-4") 104.5 (C-5); 105.3 (C-4); 130.1, 132.2 (C-2", C-3", C-5", C-6"); 112.1, 133.1 (C-5', C-6'); 118.1, 119.6, 127.0, 137.7, 139.6 (C-4a, C-6, C-7, C-1', C-1"); 139.7 (C-1);148.1 (C-3); 159.4 (C-2'); 162.4 (C-4'); 162.9, 164.6 (2COO); 184.9 (COAr);); HRMS-ESI (*m*/*z*): $[M+H]^+$ for $C_{26}H_{21}BrN_2O_7$, calcd. 553.06049; 555.05888, found 553.06020; 555.05848; Elem. anal.: calcd. for $C_{26}H_{21}BrN_2O_7$ (553.36): C 56.43, H 3.82, N 5.06; found C 56.38, H 3.76, N 5.11.

Diethyl 3-(3,4-dimethoxylphenyl)-7-(3-nitrobenzoyl)pyrrolo[1,2-c]pyrimidine-5,6-dicarboxylate **3h**: yellow crystals; 0.57 g (43 %). (ν, cm^{-1}): 2991, 1731, 1689, 1617, 1531, 1504, 1435, 1401, 1384, 1348, 1331, 1256, 1222, 1200. ^{1}H NMR (δ, 400 MHz, $CDCl_3$): 1.08, 1.39 (2t, 6H, *J* = 7.1 Hz, $2CH_3$); 3.98, 4.03 (2s, 6H, 2MeO); 3.70, 4.38 (2q, 4H, *J* = 7.1 Hz, $2CH_2$); 7.00 (d, 1H, *J* = 8.4 Hz, H-5'); 7.69 (t, 1H, *J* = 8.00 Hz, H-5"); 7.74-7.77 (m, 2H, , H-2', H-6'); 8.03-8.05, 8.42-8.44 (2m, 2H, H-4", H-6"); 8.55 (t, 1H, *J* = 1.1 Hz, H-2"); 8.58 (d, 1H, *J* = 1.5 Hz, H-4); 10.35 (d, 1H, *J* = 1.5 Hz, H-1); ^{13}C NMR (δ, 100 MHz MHz, $CDCl_3$): 13.5, 14.2 (2Me); 56.0 (MeO);61.0, 62.2 ($2CH_2$), 105.1 (C-5); 107.4 (C-4); 109.8, 111.3, 120.1 (C-2' C-5', C-6'); 123.6 (C-4"); 126.3, 129.5 134.3 (C-2", C-5", C-6"); 119.0, 128.8, 133.9, 140.3, 140.5, 149.4 (C-4a, C-6, C-7, C-1', C-1", C-3");140.3 (C-1);147.6 (C-3);150.3,151.3 (C-3', C-4'); 162.3, 164.0 (2COO); 183.4 (COAr); HRMS-ESI (*m*/*z*): $[M+H]^+$ for $C_{28}H_{25}N_3O_9$, calcd. 548.16636, found 548.16741; Elem. anal.: calcd. for $C_{28}H_{25}N_3O_8$ (531.51): C 63.27, H 4.74, N 7.91; found C 63.38, H 4.68, N 7.82.

Dimethyl 3-(3,4-dimethoxylphenyl)-7-(2,4-dimethoxybenzoyl)pyrrolo[1,2-c]pyrimidine-5,6-dicarboxylate **3i**: yellow crystals; IR (ν, cm^{-1}): 1701, 1610, 1504, 1475, 1329, 1267, 1199. ^{1}H NMR (δ, 300 MHz, $CDCl_3$): 3.47, 3.81, 3.89, 3.98, 3.99, 4.04 (6s, 18H, 6MeO); 6.49 (s, 1H, H-3"); 7.01 (d, 1H, *J* = 8.4 Hz, H-5'); 7.73 (d, 1H, *J* = 2.1 Hz, H-2'); 7.76-7.79 (m, 3H, H-6', H-5", H-6"); 8.52 (d, 1H, *J* = 1.5 Hz, H-4); 10.49 (d, 1H, *J* = 1.5 Hz, H-1); ^{13}C NMR (δ, 75 MHz, $CDCl_3$): 51.9, 52.6, 56.0 (2C) 56.1, 56.4 (6MeO); 96.0 (C-3"); 107.3 (C-4); 109.8 (C-2'); 111.1 (C-5'); 120.0 (C-6'): 122.8 (C-7); 133.2, 133.4 (C-5", C-6"); 139.8 (C-1); 101.2, 104.2, 120.6, 129.0, 140.5, 149.3, 150.3, 151.0, 158.7, 158.8 (C-3, C-4a, C-5, C-6, C-1', C-3', C-4', C-1", C-2", C-4");162.9, 164.6 ($2CO_2Me$);182.8 (COAr). Elem. anal.: calcd. for $C_{26}H_{24}N_2O_5$: C 70.26, H 5.44, N 6.30; found C 70.42, H 5.65, N 6.17.

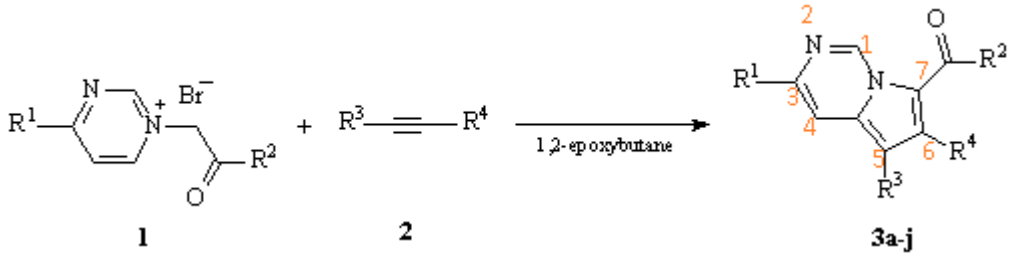
Dimethyl 3-(3-methylphenyl)-7-(3-nitrobenzoyl)pyrrolo[1,2-c]pyrimidine-5,6-dicarboxylate **3j**: yellow crystals; 0.52 g (44 %). IR (ν, cm^{-1}): 2955, 1747, 1709, 1620, 1600, 1530, 1496,

1447, 1424, 1387, 1339, 1248, 1209, 1119. ^{1}H NMR (δ, 300 MHz, $CDCl_3$): 2.47 (s, 3H, Me); 3.92 (s, 6H, 2MeO); 7.31-7.33 (m, 1H, H-4'); 7.42 (t, 1H, *J* = 7.6 Hz, H-5'); 7.70 (t, 1H, *J* = 8.0 Hz, H-3");7.95-7.99 (m, 3H, H-2', H-6');8.03-8.06 (m, 1H, H-6"); 8.43-8.46 (m, 1H, H-4");8.56 (t, 1H, *J* = 1.8 Hz, H-2"); 8.61 (d, 1H, *J* = 1.5 Hz, H-4); 10.38 (d, 1H, *J* = 1.5 Hz, H-1).^{13}C NMR (δ, 75 MHz, $CDCl_3$): 21.5 (Me); 52.0, 52.5 (2MeO); 105.3 (C-5); 108.6 (C-4); 123.5, 124.2 (C-4', C-4"); 126.4, 131.1, 134.2 (C-2", C-5", C-6"); 127.7, 129.0, 129.5 (C-2', C-5', C-6'); 119.1, 133.6, 136.0, 138.9, 140.2, 140.3, 151.3 (C-4a, C-6, C-7, C-1', C-1", C-3', C-3");140.1 (C-1);147.7 (C-3);162.6, 164.3 (2COO); 183.4 (COAr). HRMS-ESI (*m*/*z*): $[M+H]^+$ for $C_{25}H_{19}N_3O_7$, calcd. 474.12958, found 474.13102; Elem. anal.: calcd. for $C_{25}H_{19}N_3O_7$ (473.43): C 63.42, H 4.05, N 8.87; found C 63.35, H 4.13, N 8.76.

3. Results and Discussion

3.1. Synthesis of pyrrolo[1,2-c]pyrimidines

The pyrrolo[1,2-c]pyrimidines **3a-j** have been synthesized (Scheme 1) starting from the pyrimidinium bromides **1** by 1,3-dipolar cycloaddition with the alkyne dipolarophiles **2** in 1,2-epoxybutane as reaction medium and acid scavenger [21,23,24]. Their structures are presented in Table 1. In view of future exploitation of these compounds in the field of bio-imaging investigations a study of their photophysical properties has been undertaken.



1 **2** **3a-j**

Scheme 1. Synthesis of the pyrrolo[1,2-*c*]pyrimidines **3a-j**

Table 1. Substituents of the pyrrolo[1,2-c]pyrimidines and their melting points

Compound	R^1	R^2	R^3	R^4	m.p.(°C)
3a	2,4-diMeO-C_6H_3	4-Me-C_6H_4	CO_2Et	H	197-199
3b	3,4-diMeO-C_6H_3	4-F-C_6H_4	CO_2Et	H	223-225
3c	3,4-diMeO-C_6H_3	4-Me-C_6H_4	CO_2Et	H	193-195*
3d	3,4-diMeO-C_6H_3	2,4-diMeO-C_6H_3	CO_2Et	H	238-241
3e	2-MeO-C_6H_4	C_6H_5	CO_2Me	CO_2Me	166-168
3f	3-MeO-C_6H_4	3-NO_2-C_6H_4	CO_2Et	CO_2Et	180-182
3g	2,4-diMeO-C_6H_3	4-Br-C_6H_4	CO_2Me	CO_2Me	209-211
3h	3,4-diMeO-C_6H_3	3-NO_2-C_6H_4	CO_2Et	CO_2Et	221-223
3i	3,4-diMeO-C_6H_3	2,4-diMeO-C_6H_3	CO_2Me	CO_2Me	201-203
3j	3-Me-C_6H_4	3-NO_2-C_6H_4	CO_2Me	CO_2Me	230-231

***reference [24]

3.2. UV-Vis and fluorescence spectra

The photophysical properties of compounds **3a-j** have been studied in different solvents. Figures 1 and 2 show their absorption and emission spectra, respectively, in chloroform, and Table 2 gives their spectral parameters. The spectra of the compounds were initially measured in chloroform. Compounds **3a-d** (group (a) in Table 2) have clearly shown higher fluorescence than compounds **3e-j** (group (b) in Table 2) (Figure 1). Consequently, the studied compounds were divided into two groups (Table 2): (a) and (b), according to the substituent R^4 at C-6 of the pyrrolo[1,2-c]pyrimidine framework: R^4 = -H for group (a) and

R^4 = -COOMe(or -COOEt) for group (b). This division agrees with the entire range of fluorescence properties, as it will be shown below.

The absorption spectra of compounds **3a-j** (Figure 1) display two main domains. In the first domain, the maximum wavelength λ_{abs1} varies in the range 242-275 nm and corresponds to conformers with a lower conjugation, by not-involving the R^1 group in the conjugation due to the rotation outside the plane related to the pyrrolo[1,2-c]pyrimidine cycle.

In the second one, , the maximum wavelength λ_{abs2} varies between 386 and 405 nm and corresponds to compounds with a larger conjugation chain, in which the substituent R^1 also participates. The ratio of the two types of conformers varies in both groups depending of the structure of R^1 and also of R^3.

The values of the extinction coefficient (ε) for each compound at the main wavelengths (ε_1 at λ_{max1} and ε_2 at λ_{max2}) are given in Table 2. The extinction coefficients were calculated using the slopes of linear absorbance - concentration dependences.

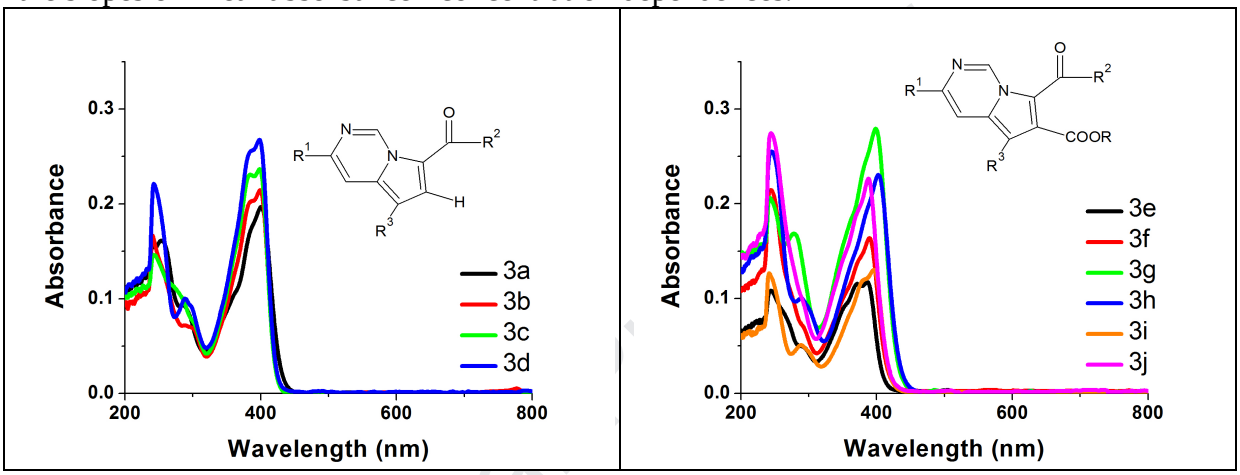


Figure 1. Absorption spectra of chloroform solutions (5μmol/L) for compounds **3a-j** unsubstituted at C-6 (group (a)) and with an ester COOR attached to C-6 (group (b))

The emission spectra, recorded in chloroform for the compounds **3a-j** are shown in Figure 2. The emission spectra were obtained by exciting the molecules at λ_{abs2} at which a higher intensity of the fluorescence was obtained (as shown in Figure 2 inset for compound **3c** : fluorescence(λ_{abs2}) > fluorescence(λ_{abs1}).

A main emission band can be seen in the region 437–463 nm, corresponding to the blue region of the visible spectrum. The spectroscopic features for fluorescence of **3a-j** are summarized in Table 2 together with the wavelengths for the main UV-Vis bands (λ_{abs1}, λ_{abs2}) and extinction coefficients (ε_1, ε_2).

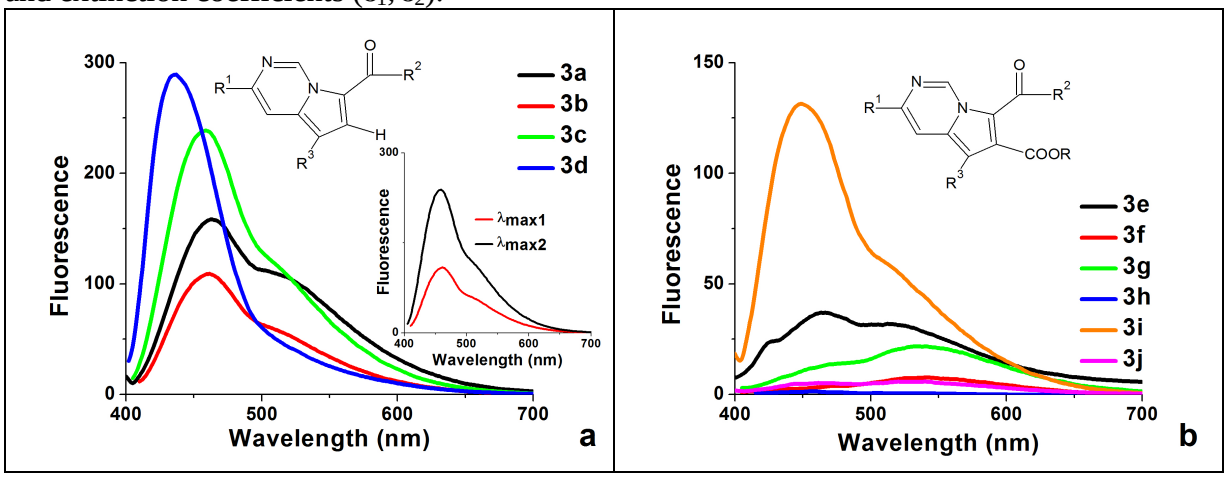


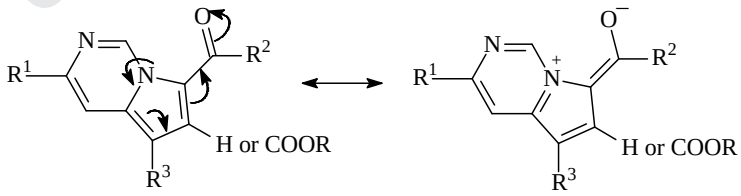
Figure 2. Emission spectra in chloroform solutions (1μmol/L) of compounds **3a-j** with (a) R^4 = H (group (a)) and (b) R^4 = COOR (group (b)); Figure 2a inset: fluorescence emission for different absorption wavelengths: λ_{abs1} = 275 nm (red) and λ_{abs2} = 397 nm (black) for compound **3c**.

Table 2 Absorption and fluorescence parameters for compounds **3a-j** in chloroform solutions (10^{-6} M)*. Compounds of type **a** and **b** are on pink and blue backgrounds, respectively

Cpd	R^4	λ_{abs1} (nm)	ε_1*	λ_{abs2} (nm)	ε_2*	λ_{em} (nm)	$\Delta\tilde{\nu}_1$ (cm^{-1})	$\Delta\tilde{\nu}_2$ (cm^{-1})	Emission intensity	
3a	H	268	23300	396	39100	462	15668	3608	158.12	**a**
3b	H	265	25200	400	36800	462	16091	3355	109.10	
3c	H	275	29090	397	47900	458	14530	3355	238.75	
3d	H	258	42300	405	53800	437	15876	1808	289.58	
3e	CO_2Me	261	44620	386	46960	463	16716	6786	36.83	**b**
3f	CO_2Et	252	39520	390	50630	539	21130	7088	7.72	
3g	CO_2Me	242	42770	392	57930	440	18595	6957	21.78	
3h	CO_2Et	250	61060	395	65910	456	18070	3387	1.84	
3i	CO_2Me	242	25600	396	27850	450	19100	3030	131.40	
3j	CO_2Me	268	56200	388	47200	535	18622	7116	5.83	

* Extinction coefficient (in L/mol/cm calculated from the linear correlation between absorbance and concentration)

Table 2 shows the absorption and emission spectra parameters in chloroform for the compounds **3a-j**. An important change of the emission spectra of compounds **3a-j** was noticed upon the variation of the substituent R^4 (Table 2). The presence of an ester group attached to the pyrrolo[1,2-c]pyrimidine framework at C-6 (R^4) dramatically decreases the emission intensity in all compounds from group b (Figure 2b), compared to the unsubstituted ones (Figure 2a), as it can be seen also from Table 2. This behaviour is similar in all studied solvents (Table 4). The 7-benzoyl-pyrrolo[1,2-*c*]pyrimidine could present a zwitterionic structure in which the opposite charges are in close contact, and in which there is a clear coplanarity (due to the exocyclic double bond) between the pyrrolo[1,2-c]pyrimidine framework and the benzoyl at C-7 (Scheme 2).



Scheme 2. Proposed zwitterionic structure of the 3-aryl-7-benzoyl-pyrrolo[1,2-c]pyrimidine framework

The decrease of quantum yield (QY) in case of compounds **3e-j** from group (b) with respect to compounds **3a-d** from group (a) could be caused by the electronic withdrawing effect of the supplementary ester group, which tends to affect the charge distribution within the pyrrolopyrimidine fluorophore, and by the steric effects which should be accounted, such as the influence on conjugation degree between the pyrrolo[1,2-c]pyrimidine framework and the benzoyl core attached to C-7.

3.3 Influence of substituents on the absorption spectra

Influence of R^1 on the absorption spectra

When the substituent attached to C-3 (R^1) varied, important changes in UV-Vis spectra were observed (Table 2). For instance, comparing compounds **3a** and **3c**, which differ by the positions of the methoxy groups, the extinction coefficient increased from 23300 to 29090 for λ_{max1}, and from 39100 to 47900 for λ_{max2}. Also, this comparison indicates a shift of λ_{max1} from 268 to 275 nm, while for $\lambda_{max2,}$ of only 1 nm (from 396 to 397). The increase of the extinction coefficient value for **3c** with respect to **3a** may be attributed to the decrease in the steric constraints in case of *meta* (in **3c**) substitution vs *ortho* (in **3a**). Also, compound **3h** has ε_1 and ε_2 values greater than **3f** (61060> 39520; 65910> 50630). These values may be explained by the substitution pattern, an MeO group in *ortho* position may influence the electron distribution within the fluorophore pyrrolo[1,2-cpyrmidine] (oxygen in MeO possesses a lone pair of electrons) and thus causing a loss in fluorescence by non-radiative effects.

Influence of R^2 on the absorption spectra

Changing the benzoyl moiety on C-7 yields important absorbance variations, as it results from the comparison between compounds **3b** and **3c** (with the same R^1, R^3 and R^4 substituents, but with 4-F and 4-CH_3, respectively). The extinction coefficients increase from 25200 to 29090 for λ_{max1}, and from 36800 to 47900 for λ_{max2}. Also, shifts of λ_{max1} from 265 to 275 nm, and λ_{max2} from 400 to 397 nm occur. The increase of extinction coefficient values for **3c** relatively to **3b** can be explained by the opposite electronic effects of substituent at the aromatic ring (electron donor for 4-Me and electron withdrawing for 4-F).

Based on similar electronic effect consideration, the conjugation in the zwitterionic structure would be easily extended to the phenyl ring of the benzoyl moiety, when a mild electron donor such as a methyl group is present, but it would be more difficult to achieve such conjugation, when a strong electron withdrawing substituent, such as a fluorine atom, is in the 4- position of the aromatic ring of R^2.

Influence of R^4 on the absorption spectra

By comparing the compounds **3d** and **3i**, which have the same substituents R^1 and R^2, it is found that the introduction of an ester group CO_2Me (R^4) determines the decrease in the values of the extinction coefficient from 42300 to 25600 for λ_{max1}, and from 53800 to 27850 for λ_{max2}. Also, shifts of λ_{max1} from 258 to 242 nm, and of λ_{max2} from 405 to 396 nm occur. The other values in Table 2 are difficult to be attributed to the effects of substituents, due to the complexity of the structures and of the electronic effects involved.

3.4 Influence of substituents on fluorescence spectra

QY values were compared for similar structures to assess the influence of R^1, R^2, R^3 and R^4 on the fluorescence of the pyrolo[1,2-c]pyrimidines. For the scope of investigation, the structures of the compounds were virtually assigned as pyrrolo[1,2-c]pyrimidine fluorophore connected to two other fluorophore entities (**F1** and **F2**), as depicted in Figure 3. The first fluorophore entity (**F1**) is a phenyl ring substituted with methoxy groups, and the second one is a substituted benzoyl moiety (**F2**).

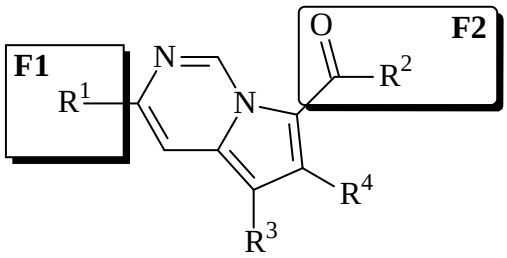


Figure 3. Schematic representation of fluorophore entities of pyrrolo[1,2-c]pyrimidines

Table 3 Fluorescence yield (QY) and KSV values of quenching for compounds **3a-j** in chloroform solutions (10^{-6} M)

Cpd	R^1	R^2	R^4	λ_{em} (nm)	QY[*a] (%)	K_{SV}[*b]	
3a	2,4-diMeO-C_6H_3	4-Me-C_6H_4	H	462	51.77	928	**(a)**
3b	3,4-diMeO-C_6H_3	4-F-C_6H_4	H	462	38.26	367	
3c	3,4-diMeO-C_6H_3	4-Me-C_6H_4	H	458	61.35	638	
3d	3,4-diMeO-C_6H_3	2,4-diMeO-C_6H_3	H	437	42.40	885	
3e	2-MeO-C_6H_4	C_6H_5	CO_2Me	463	11.04	307	**(b)**
3f	3-MeO-C_6H_4	3-NO_2-C_6H_4	CO_2Et	539	2.64	160	
3g	2,4-diMeO-C_6H_3	4-Br-C_6H_4	CO_2Me	440	6.63	287	
3h	3,4-diMeO-C_6H_3	3-NO_2-C_6H_4	CO_2Et	456	2.99	79	
3i	3,4-diMeO-C_6H_3	2,4-diMeO-C_6H_3	CO_2Me	450	27.46	644	
3j	3-Me-C_6H_4	3-NO_2-C_6H_4	CO_2Me	535	3.24	242	

[*a] quinine sulphate standard; [*b] calculated from the quenching experiments in presence of benzoquinone

Influence of R^1 on the fluorescence spectra

Important variations of the QY are produced by changing the position of substituent R^1 on the phenyl ring (**F1**) attached to C-3 (see Table 2, 3). By comparing the quantum yields of compounds **3a** (2.4-diMeO substituted) and **3c** (3,4-diMeO substituted), it was found that the relative position of the two methoxy groups influences the emission spectra. The QY value for **3a** (51.77%) is smaller than for **3c** (61.35%), due to the steric hindrance that diminishes the conjugation in the structure of **F1** (see above).

Comparing the compounds **3f** and **3h**, which have the same substituents R^2, R^3, R^4, the quantum yield was found to slightly increase (2.99%) in compound **3h**, due to the presence of an additional MeO- group attached to the C-3 phenyl ring (**F1**), while for compound **3f** was of 2.64%.

Influence of R^2 on the fluorescence spectra

The QY values for compounds **3b** and **3c** were compared, in order to evaluate this influence of the R^2 substituent on fluorescence. These compounds have the same R^1, R^3 and R^4 substituents, but different R^2 substituents, 4-F-C_6H_4- and 4-Me-C_6H_4- , respectively. When the fluorine atom is replaced by Me group, the value of the QY significantly increases (from 38% to 61%). This indicates the growth of conjugation inside the pyrrolo[1,2-c]pyrimidine fragment due to the donor effect of the methyl group. Conversely, that of F decreases the conjugation (due to its electron withdrawing effect).

The confirmation of the contribution of the substituted benzoyl moiety (**F2**) to fluorescence has been done because the presence of two electron donating methoxy groups in compound **3d** lead to higher QY than that of **3b**.

The QY value for **3i** (27.46%) increases more than 10 times, compared to that for **3h** (2.99%), due to the different electronic effects of the two dimethoxy (electron donor) groups from **3i** and nitro (electron withdrawing) group from **3h**. In the same time, the nitro group induces a shift toward lower wavelengths (hypsochromic effect), while the methoxy groups induce a shift toward higher wavelengths (bathochromic effect).

It was also noticed that the presence of the Br atom on the benzoyl fragment (in compound **3g**) decreases the fluorescence intensity of the compound **3g** to 6.63%. The unsubstituted aromatic ring on **F2** (R^2 = -C_6H_5) would be expected to have QY > 11.04% (value corresponding to the compound **3e**), as in the case of comparison between compound **3f** and **3h** (where an additional group on **F1** leads to the increase in QY value: QY = 2.64% for **3f**,

and QY = 2.99% for **3h**). In case of compound **3g**, the decrease of QY compared to a hypothetical parent compound with R^2 = 4-Br-C_6H_4 (with the same **F1**) is explained by the internal effect of fluorescence quenching by heavy atoms (Br).

Influence of R^3 on the fluorescence spectra

The R^3 substituent varies slightly along the series of compounds (-COOMe or -COOEt). Upon comparing compounds **3f** and **3j**, which have the same **F2**, and **F1** substituted in *meta*-position (thus expecting a weak influence on conjugation), both having $R^4 \neq H$, it can be noticed that the quantum yields are similar. It can be concluded that the presence of a carboetoxy or carbomethoxy group (R^3) does not have a major influence on the emission intensity and absorption wavelength.

Influence of R^4 on the fluorescence spectra

The introduction of a substituent in position 6 of the pyrrolo[1,2-c]pyrimidine ring determines the decrease in quantum yield, as seen in Table 3 for all studied compounds. Compounds **3a-d**, unsubstituted in position 6, have all without exception quantum yields greater than compounds **3e-j**, substituted in this position, regardless the nature of the other substituents (R^1, R^2, R^3). Comparing the compound **3d**, unsubstituted in position 6, with compound **3i**, substituted in 6, with the same substituents R^1 and R^2, a decrease in quantum yield from 42.4% to 27.46% is observed. This decrease may be determined by the electron withdrawing effect of the ester group and also by its steric effect, which influences the degree of conjugation between pyrrolo[1,2-c]pyrimidine and the benzoyl attached to C-7.

3.5. Fluorescence quenching

Fluorescence quenching is a property that can be linked to important applications, such as investigation of supramolecular assemblies [41]. The fluorescence quenching of the new synthesized compounds has been examined using 1,4-benzoquinone (BQ) as inhibitor. In the presence of BQ, a decrease of fluorescence intensity occurs, as shown for the compound **3d** (Figure 4a-inset). The quenching (F_0/F) was calculated as the ratio of the solution fluorescence without BQ (F_0) and in presence of BQ (F), for increasing concentrations of BQ. F_0/F *vs* [BQ] plots obtained for all the compounds **3a-j** (Figure 4) are liniar. These plots predict the occurrence of collisional quenching of fluorescence [42].

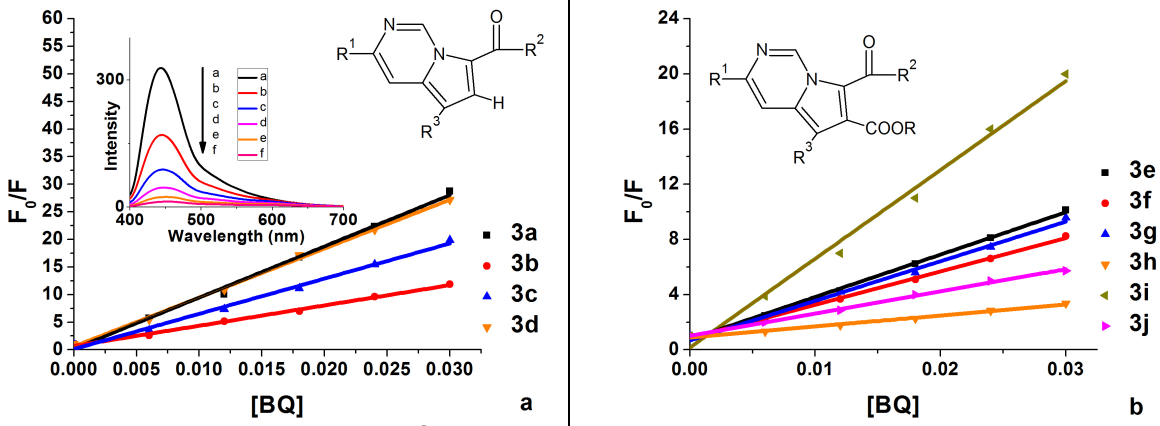


Figure 4. F_0/F *vs* [BQ] plot in 10^{-6} mol/L $CHCl_3$ solutions of compounds **3a-d** with R_4 = H (a) and **3e-j** with R_4 = COOR (b)**;** Figure 4a inset: fluorescence quenching spectra of **3d**

The spectroscopic features for the fluorescence of **3a-j** compounds with the substituent R^4 attached to C-6 of the pyrrolo[1,2-c]pyrimidine framework can be summarized from Table 2 and 3:

- The wavelengths for the main fluorescence (λ_{em}) are smaller for compounds of the group (a) with R^4 = H than those substituted with R^4 = COOMe or COOEt from the group (b), being situated in the blue region;
- Stokes shifts are smaller for compounds of the group (a) than those of the group (b), $\Delta\nu_2$ being at least 3 times smaller than $\Delta\nu_1$;
- Quantum yield (QY) is at least 2 times bigger for compounds of group (a) than those of group (b); QY varies between 42% and 61% for compounds **3a-d**, and between 2% and 27% for compounds **3e-j**.
- Stern-Volmer constant (K_{SV}) is generally bigger for compounds of group (a) than those of group (b).
- Important changes of QY and K_{SV} occur when F1 and F2 structures vary.
- The study of each substituent's effects on the spectral properties allows the prediction of the functional groups that will lead to the best values for quantum yields and K_{SV}.

3.6. Influence of solvent on photophysical properties

The photoluminescence of organic fluorophores in solutions is influenced by solvent polarity [43]. To evaluate this influence, the UV-Vis and fluorescence spectra of the new synthesized compounds were recorded in solvents with various dielectric constant (ε) and refractive index (n). To identify the link between the solvent properties and the spectral characteristics, the spectra have been recorded in different solvents: chloroform ($CHCl_3$), dichloromethane (CH_2Cl_2), acetonitrile (CH_3CN), and dimethyl sulfoxide (DMSO). The data obtained in chloroform are given in Table 2, and the data obtained in dichloromethane, acetonitrile and dimethyl sulfoxide are resumed in Table 4. For instance, the influence of solvent on absorption and emission spectra, in case of compound **3g,** is depicted in Figure 5.

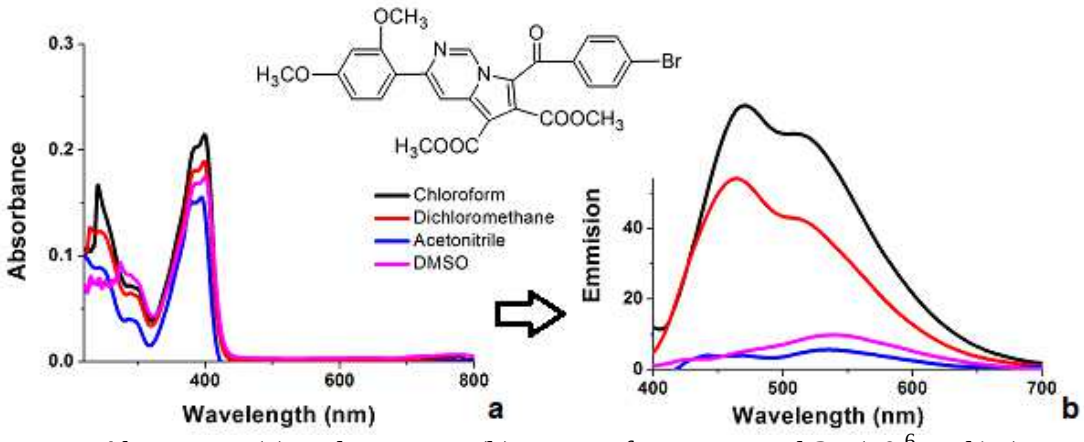


Figure 5. Absorption (a) and emission (b) spectra for compound **3g** (10^{-6} mol/ L) in solvents with different polarity: chloroform, dichloromethane, acetonitrile, DMSO

The change of the solvent leads to important variations of absorption and fluorescence maximum wavelength and intensity. This compound has the biggest red shift of the emission wavelength from 440 nm (in $CHCl_3$) to 557 nm (in DMSO). A bathochromic shift of the emission peaks can be seen when passing from $CHCl_3$ to CH_2Cl_2, CH_3CN, DMSO (Tables 2-4). This suggests the implication of photo-induced intramolecular charge transfer (ICT) in the singlet excited state with larger dipole moment, as expected [44].

Table 4. Several photophysical parameters for compounds **3a-j** in solutions (10^{-6} M) with different solvents (S)

Solvent	Dichloromethane					Acetonitrile					Dimethyl sulfoxide				
Compound	λ_{abs} nm	ε L/mol/cm	λ_{em} nm	$\Delta\tilde{\nu}$ (cm^{-1})	QY (%)	λ_{abs} (nm)	ε L/mol/cm	λ_{em} (nm)	$\Delta\tilde{\nu}$ (cm^{-1})	QY (%)	λ_{abs} (nm)	ε L/mol/cm	λ_{em} (nm)	$\Delta\tilde{\nu}$ (cm^{-1})	QY (%)
3a	246 397	24300 43000	466	19191 3729	25.98	270 390	43400 29700	468	15669 4273	29.80	289 395	15500 31800	468	13234 3948	51.51
3b	244 398	122800 197100	466	19524 3666	5.67	244 395	17600 27600	469	19661 3994	10.7	290 390	14000 31600	470	20390 4364	21.74
3c	266 397	89000 148600	468	16226 3821	20.99	266 393	20900 39600	481	16226 4077	52.60	292 390	25000 49300	492	12833 4227	87.26
3d	240 402	34100 44100	438	18835 2284	17.90	252 400	44300 83100	439	16903 2666	3.89	295 395	13200 40300	467	11476 3219	40.16
3e	242 394	36900 39200	470	19392 3007	0.80	248 375	21500 24800	525	21347 7691	2.88	291 378	15600 25000	457	12482 4573	4.66
3f	246 386	22900 17700	437	17767 3023	0.84	246 380	81600 59500	428	17285 2951	1.74	290 390	19600 25500	435	11494 2652	0.80
3g	245 388	21000 29800	459	19029 3986	10.07	277 391	64100 85600	555	18083 7557	0.50	290 395	18400 22400	557	16529 7363	5.64
3h	245 394	40100 37400	460	18886 3007	0.14	244 390	47300 38600	465	20019 4352	2.29	290 388	26400 44900	455	19688 34672	0.60
3i	245 394	27800 32500	460	19927 3836	12.33	240 391	44000 38700	468	20299 4207	8.84	270 396	46300 49700	470	15760 3513	6.80
3j	245 387	50300 42100	457	18934 3957	1.29	245 382	43200 33600	520	21585 6947	1.64	290 385	23400 27600	536	15826 7317	2.03

The comparison of spectral parameters (Tables 2 - 4) shows that the investigated pyrrolo[1,2-*c*]pyrimidines **3a-j** have fluorescence quantum yields with significant variations (from 0 to about 90 %), which are very much dependent on solvent.

The common behaviour of the new synthesized compounds is a shift of the emission peaks to lower wavelengths (hypsochochromic shift) with the increase of solvent polarity, from 6 nm in case of compound **3a**, to 117 nm for compound **3g**. This is a typical tendency found for these compounds, when ICT occurs upon excitation (solvatochromic behaviour) and leads to a charge-separated (highly polar) emitting state, which can be stabilized by polar solvents. The emission wavelength increases with the solvent polarity (red shift). This behaviour leads to the conclusion that ICT is polar for the excited state, with a large dipole moment. This state is understandably very stable when the solvent is polar.

Figure 5 shows that the change of the solvent has no major impact on the absorption spectra, but it has a significant effect on fluorescence intensity and wavelength. The values from Table 2 -4 confirm this behaviour for all compounds.

To rationalize the obtained results for the influence of solvent on fluorescent properties of the studied compounds (Stokes shifts, etc.), solvent polarity function (Δf) expressed by Lippert-Mataga equation (1) [45] has been examined. The solvent polarity values have been calculated using equation (2).

$$\Delta\bar{\nu}_{st} = \frac{2(\mu_e - \mu_g)^2}{hca^3}\Delta f + Const. \qquad (1)$$

$$\Delta f = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1} \qquad (2)$$

where $^{\Delta\bar{\nu}_{st}}$ is the Stokes shift (cm^{-1}), h is Planck's constant, c is the vacuum light speed, a is the radius of Onsager cavity, ε and n are, respectively, the dielectric constant and refractive index of the solvent. μ_e and μ_g are the compound dipole moment in excited and ground states, respectively, while Δf is the solvent orientation polarizability. Δf reflects the electron mobility and dipole moment of the solvent molecule. The changes in the dipole moment ($\Delta\mu = \mu_e - \mu_g$) were calculated using Lippert-Mataga method [46].

Bakhshiev's (Eq. 3) and Kawski-Chamma-Viallet's (Eq. 6) equations [47] were used to calculate the dipole moments in the fundamental and excited states for each compound **3a-j**. By plotting Stokes shift (ν_{abs} - ν_{em}) *vs* solvent polarity function F_1 (Figure 7a), S_1 has been calculated using equation (3). Plotting the average sum of the absorption-emission maxima *vs* F_2 [48] (Figure 7b), allowed the calculation of S_2 using equation (8).

$$\nu_{abs} - \nu_{em} = S_1 \cdot F_1(D, n) + const. \quad (3)$$

In (3), ν_{abs} and ν_{em} are the wave numbers (cm^{-1}) for excitation and emission maxima, respectively, F_1 (orientation solvent polarity function), and S_1 being defined as in equations (4) and (5):

$$F_1(\varepsilon, n) = \frac{2n^2+1}{n^2+2}\left[\frac{\varepsilon-1}{\varepsilon+2} - \frac{n^2-1}{n^2+2}\right] \quad (4)$$

$$S_1 = \frac{2\left(\mu_e - \mu_g\right)^2}{hca^3} \quad (5)$$

$$(\nu_{abs} + \nu_{em})/2 = -S_2 \cdot F_2(\varepsilon, n) + const. \quad (6)$$

F_2 and S_2 were defined as in equations (7) and (8):

$$F_2(\varepsilon, n) = \frac{1}{2}F_1(\varepsilon, n) + \frac{3}{2}\left(\frac{n^4-1}{(n^2+2)^2}\right) \quad (7)$$

$$S_2 = \frac{2\left(\mu_e^2 - \mu_g^2\right)}{hca^3} \quad (8)$$

Looking at the differences between the dipole moments Δμ, given in Table 5 (calculated for all studied compounds), the compound **3c** has the smallest value of the difference between the μ_g, and μ_e. That is why, this compound has been selected to estimate the solvent influence on fluorescence properties for the studied compounds, through the dependence of Stokes shifts on solvent polarity (Figure 6). The R^2 value (0.973) from Figure 6 for the linear dependence of Δυ *vs* Δf shows a good correlation.

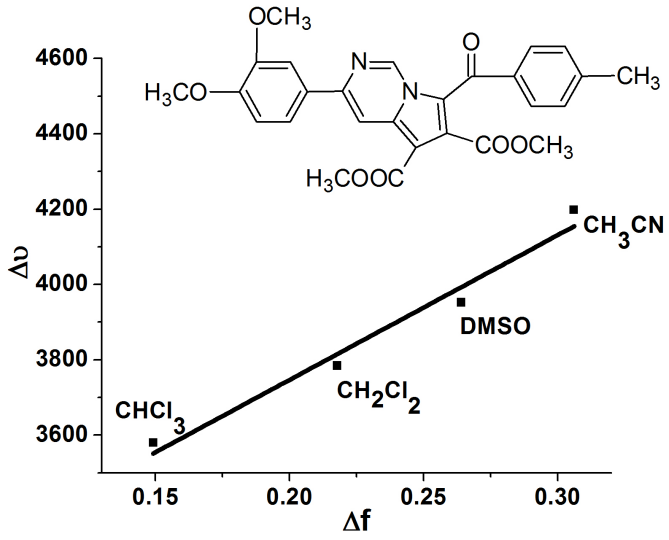


Figure 6. Dependence of Stokes shift values (Δυ) on orientation solvent polarity (Δf) in different solvents for compound **3c**

Table 5. Calculated values for Δμ (Δμ = μ_e- μ_g) between the ground (μ_g) and excited (μ_e) dipole moments for the compounds using equations (1), (2), (3) and (6)

Group	Compound	Δμ (D)	μ_g (D)	μ_e (D)
(a)	**3a**	3.64	2.83	6.47
	3b	5.21	2.42	7.64
	3c	0.38	4.32	4.7
	3d	2.08	3.11	5.16
(b)	**3e**	10.24	3	13.24
	3f	0.82	4.06	4.89
	3g	11.84	4.35	16.17
	3h	5.32	4.15	9.48
	3i	9.27	0.2	9.68
	3j	4.88	2.63	7.52

In Figure 7, the variation of Stokes shift Δυ with *F1* (a), and of the average value between absorption - emission maximum wavelength shifts with *F2* (b) are shown, respectively, for compound **3c.** Figure 7b shows the dependence of the average value between absorption – emission maximum wavelength shifts Δυ *vs* the solvent polarity (F_2), for the compound **3c**, used to evaluate *S2* for the compound **3c**. The correlation coefficient obtained has a small value (R^2 = 0.422) attributed to the specific interaction between solute and solvent [49]. The more polar solvent, acetonitrile, stabilizes better the excited state of a compound, when the dipole moment of the solute in the excited state is bigger than that in the ground state.

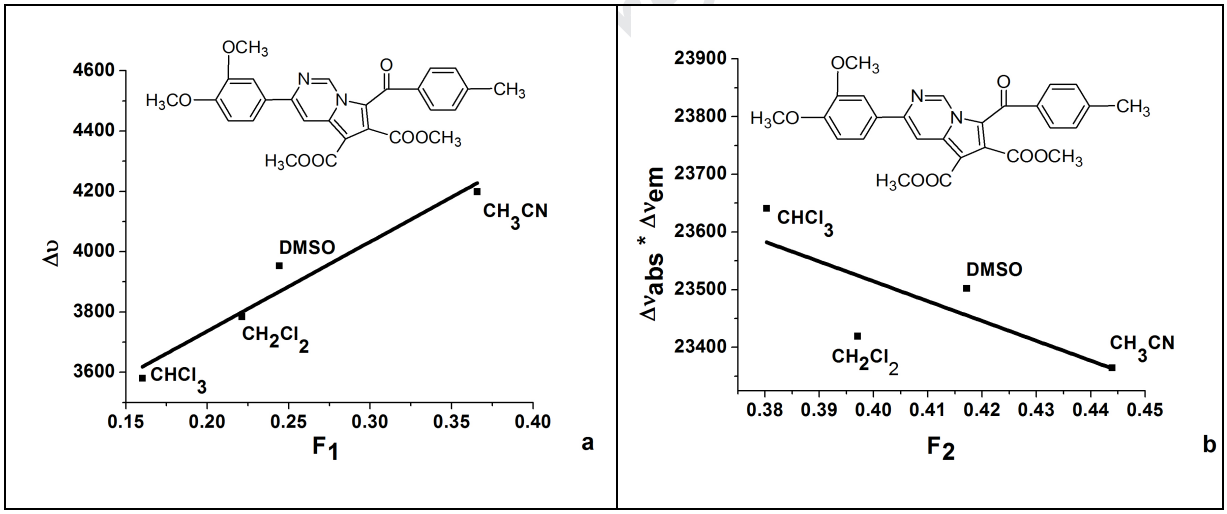


Figure 7. Stokes shift variation with *F1* (a) and the average value between absorption and emission maximum wavelength shifts with *F2* (b), respectively, for compound **3c**

The calculated properties (*F1*, *F2*, etc.) for all the pyrrolo[1,2-*c*]pirimidines were examined in correlation with the experimental values, to describe the solvent influence on fluorescence properties of the investigated compounds. The overall effects of the solvent on optical properties (absorption and emission) were analyzed by Kamlet-Taft solvatochromic equation (Eq. 9) [50]. In (9), π* is the solvent polarizability, β is the hydrogen bond acceptor (HBA) ability, α is the hydrogen bond donor ability (HBD). The coefficients *s*, *b*, and *a* are constants characteristic for the solute. Their absolute value and sign reflect the contribution of the corresponding solvent-solute interactions on the investigated property (such as electronic transition energy). ν and ν_0 represent the solvent-dependent property under study, for instance λ_{max} value in the UV-Vis spectrum.

$$\nu = \nu_0 + s \cdot \pi^* + b \cdot \beta + a \cdot \alpha \qquad (9)$$

The solvents parameters π*, α, and β, are given in Table 6 [44].

Table 6. Solvent polarity parameters [44]

Solvent	Δf	π*	β	α
Chloroform	0.15	0.69	0.10	0.20
Dichloromethane	0.21	0.73	0.10	0.13
DMSO	0.26	1.00	0.76	0.00
Acetonitrile	0.30	0.66	0.19	0.40

The data obtained after the calculation using equation (9) by multiple linear regression analysis, for solvatochromic parameters for all compounds **3a-j**, are presented in Tables 7 and 8. The multiple linear regression in Figure 8 shows a good correlation between the calculated and experimental data. The values of *a* and *b* coefficients present smaller values than *s* coefficients, which indicates that the ability of the solvent to donate or accept hydrogen bonds is weaker than the solute-solvent dipole-dipole interactions.

For the compounds with positive values of *s* and *a* coefficients (Table 7), it is expected a bathochromic shift of the emission wavelength with the solvent polarity increase. This is seen in Table 4, for compound **3d** (which has positive *s* and *a* coefficients, *s* = 10.72 and *a* = 4.55). It shows a positive solvatochromic behaviour (λ_{em} (nm) is 438, 439, and 467 in DCM, CH_3CN and DMSO, respectively). A stabilization of the electronic excited state relatively to the ground state occurs in this case. If the coefficient *b* is negative, a hypsochromic shift occurs, that indicates the stabilization of the ground state, relatively to the electronic excited state.

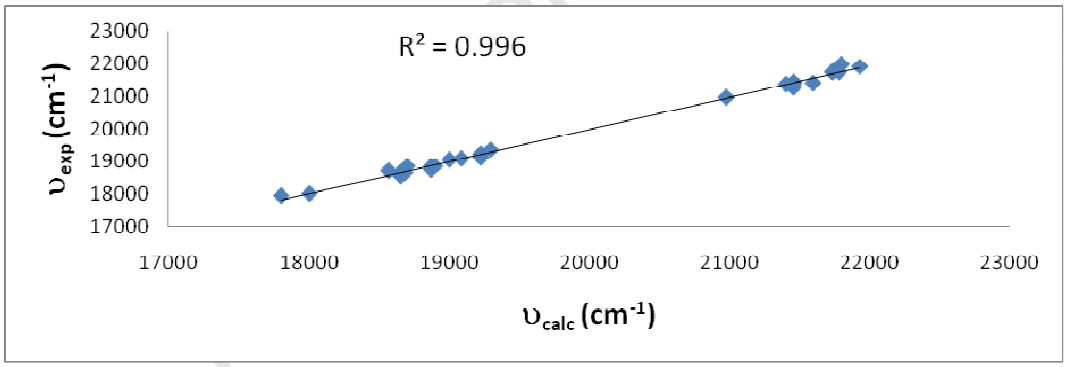


Figure 8. Experimental (υ_{exp}) *vs.* calculated (υ_{calc}) values of Stokes shifts for compounds **3a-j** from Eq. (9)

Table 7. Coefficients of solvatochromic parameters for compounds **3a-j** calculated by multiple linear regression using equation (9)

Group	Compound	υ_0 (cm^{-1})	s (10^3)	b (10^3)	a (10^3)
(a)	**3a**	32410	-14630	4720	-5710
	3b	31640	-13620	4290	-5130
	3c	44870	-34410	10660	-13280
	3d	11180	10720	-3660	4550
(b)	**3e**	11180	10720	-3660	4550
	3f	14950	5380	-2050	1560
	3g	1650	29070	-12370	6930
	3h	19660	3120	-2390	1780
	3i	47410	-34480	11580	-12800
	3j	19010	-500	470	-290

Table 8. Contribution of solvatochromic parameters coefficients from equation (9)

Group	Compound	P_{π^*}	P_{β}	P_{α}
(a)	**3a**	0.58	0.19	0.23
	3b	0.59	0.19	0.22
	3c	0.59	0.18	0.23
	3d	0.61	0.21	0.18
(b)	**3e**	0.57	0.19	0.24
	3f	0.60	0.23	0.17
	3g	0.60	0.26	0.14
	3h	0.43	0.32	0.24
	3i	0.40	0.37	0.23
	3j	0.59	0.20	0.22

The solvatochromic parameters contributions of the new compounds are presented in Table 8. The obtained values indicate that the solvatochromic behaviour of investigated [1,2-c]pyrimidines is mainly influenced by the solvent polarizability (P_{π^*}). The hydrogen bond acceptor ability, or hydrogen bond donor ability of the solvents, have smaller influence on the solvatochromic properties of compounds **3a-j.** However, for compound **3i**, $\mathbf{P_{\pi^*}}$ and $\mathbf{P_{\beta}}$ have close values. These values could be correlated to the other values of the parameters: **QY** values decrease with the increasing of the solvent polarity (Table 4).

4. Conclusions

The new synthesized [1,2-c]pyrimidines present blue fluorescence, some of them showing high quantum yields. The substituent effects on absorption and fluorescence parameters of these derivatives were discussed. It was shown that the presence and position of the methoxy or methyl groups on the phenyl ring in position 3, or on the benzoyl group in position 7, have a strong influence on the fluorescence of compounds. The presence of an ester group grafted on C-6 atom of the pyrrolopyrimidine dramatically reduces the fluorescence. The examination of UV-Vis and fluorescence spectra of the new compounds, in close connection with the substituent nature (halogen, methyl, methoxy and nitro), has revealed that these spectra are also function of solvent properties. The interaction of these compounds with solvents having different polarity (chloroform, dichloromethane, acetonitrile or dimethyl sulfoxide) has been investigated through correlation of the absorption and fluorescence features with solvent polarity functions. Solvent parameters (polarity, basicity, and acidity) contribution onto solvent-solute interactions has been evaluated. Solvent polarity has been found to be the most important parameter which influences the emission spectra of these compounds - potential candidates for OLED technology and fluorescent probes. Further studies directed to the electrochemical properties of all these compounds are in progress for practical applications (e.g. chemical sensors).

Acknowledgement

Access to research infrastructure developed in the “Petru Poni” Institute of Macromolecular Chemistry through the European Social Fund for Regional Development, Competitiveness Operational Programme Axis 1, Project InoMatPol (ID P_36_570, Contract 142/10.10.2016, cod MySMIS: 107464) is gratefully acknowledged.

References

[1]. Valeur B. Molecular Fluorescence: Principles and Applications. Wiley-VCH, Weinheim GE. 2000

[2]. Chen D, Su SJ, Cao Y. Nitrogen heterocycle-containing materials for highly efficient phosphorescent OLEDs with low operating voltage. J Mater Chem. 2014; C2: 9565-9578. doi: 10.1039/C4TC01941E

[3]. Yen YS, Ni JS, Lin TY, Hung WI, Lin JT. Imidazole-Based Sensitizers Containing Double Anchors for Dye-Sensitized Solar Cells. Eur J Org Chem. 2015; 33: 7367-7377. doi: https://doi.org/10.1002/ejoc.201501131

[4]. Ooyama Y, Uenaka K, Ohshita J. Development of D–π–A Fluorescent Dyes with a 3-Pyridyl Group as Electron-Withdrawing Anchoring Group for Dye-Sensitized Solar Cells. Eur J Org Chem. 2015; 17: 3713-3720. doi: https://doi.org/10.1002/ejoc.201500341

[5]. Firmino ADG, Goncalves MST. Bifunctionalised long-wavelength fluorescent probes for biological applications. Tetrahedron Lett. 2012; 53:4946-4950. doi: 10.1016/j.tetlet.2012.07.004

[6]. Zhang Y, Yan Y, Chen S, Gao Z, Xu H. 'Naked-eye' quinoline-based 'reactive' sensor for recognition of Hg^{2+} ion in aqueous solution. Bioorg Med Chem Lett. 2014; 24: 5373-5376. doi: https://doi.org/10.1016/j.bmcl.2014.10.052

[7]. Suresh M, Mandal AK, Suresh E, Das A. First demonstration of two-step FRET in a synthetic supramolecular assembly. Chem Sci. 2013; 4: 2380-2386. doi: 10.1039/C3SC50282A

[8]. Ying W, Yang J, Wielopolski M, Moehl T. Moser JE, Comte P, Hua J, Zakeeruddin, SM, Tian H, Gratzel M. New pyrido[3,4-*b*]pyrazine-based sensitizers for efficient and stable dye-sensitized solar cells. Chem Sci. 2014; 5: 206-214. doi: 10.1039/C3SC51844B

[9]. Huckaba AJ, Giordano F, McNamara LE, Dreux KM, Hammer NI, Tschumper GS, Zakeeruddin SM, Gratzel M, Nazeeruddin MK, Delcamp JH. Indolizine-based donors as organic sensitizer components for dye-sensitized solar cells. Adv Energ Mater. 2014; 5:1401629. doi: https://doi.org/10.1002/aenm.201401629

[10]. Dumitrascu F, Vasilescu M, Draghici C, Caproiu MT, Barbu L, Dumitrescu DG. New fluorescent indolizines and bisindolizinylethylenes. Arkivoc. 2011; (x): 338-350. doi: 10.3998/ark.5550190.0012.a28

[11]. Kristafor S, Kraljevic TG, Ametamey SM, Cetinac M, Ratkajd I, Haceke RT, Pavelic SK, Malic, SR. Syntheses and Antitumor Evaluation of C(6)-Isobutyl- and C(6)-Isobutenyl-Substituted Pyrimidines, and Dihydropyrrolo[1,2-*c*]pyrimidine-1,3-diones. Chem Biodivers. 2011; 8: 1455-1469. doi: https://doi.org/10.1002/cbdv.201000202

[12]. Kim JT, Hamilton AD, Bailey CM, Domoal RA, Wang L, Anderson KS, Jorgensen WL. FEP-guided selection of bicyclic heterocycles in lead optimization for non-nucleoside inhibitors of HIV-1 reverse transcriptase. J Am Chem Soc. 2006; 128: 15372-15373. doi: 10.1021/ja066472g

[13]. Bondu S, Genta-Jouve G, Leiros M, Vale C, Guigonis JM, Botana LM, Thomas OP. Additional bioactive guanidine alkaloids from the Mediterranean sponge Crambecrambe. RSC Adv. 2012; 2: 2828-2835. doi: 10.1039/C2RA00045H

[14]. Perry NB, Ettouati L, Litaudon M, Blunt JW, Munro MHG, Parkin S, Hope H. Alkaloids from the antarctic sponge Kirkpatrickiavarialosa.: Part 1: Variolin b, a new antitumour and antiviral compound. Tetrahedron. 1994; 50: 3987-3992. doi: https://doi.org/10.1016/S0040-4020(01)89673-3

[15]. Alvarez M, Fernandez D, Joule JA. Synthesis of 1,2-dihydropyrrolo[1,2-*c*]pyrimidin-1-ones. J Chem Soc Perkin Trans. 1999; 3: 249-256. doi: 10.1039/A809280J

[16]. Weidner H, Michaels FM, Beltman DJ, Montgomery CJ, Wadsworth DH, Briggs BT, L. Picone M. Indolizines. 5. Preparation and structural assignments of azaindolizinols. J Org Chem. 1991; 56: 5594-5598. doi: 10.1021/jo00019a024

[17]. Copar A, Stanovnik B, Tisler M. A new approach for the synthesis of fused pyrroles. The synthesis of acyl substituted pyrrolo[1,2-x]azines. J Heterocycl Chem. 1993; 30: 1577-1579. doi: https://doi.org/10.1002/jhet.5570300621

[18]. Baumann M, Rodriguez-Garcia AM, Baxendale IR. Flow synthesis of ethyl isocyanoacetate enabling the telescoped synthesis of 1,2,4-triazoles and pyrrolo[1,2-*c*]pyrimidines. Org Biomol Chem. 2015; 13: 4231-4239. doi: 10.1039/C5OB00245A

[19]. Minguez Ortega JM, Vaquero Lopez JJ, Garcia-Navio JL, Alvarez-Builla J. Improved synthesis of pyrrolo[1,2-*c*]pyrimidine and derivatives. Tetrahedron Lett. 1996; 37: 4263-4266. doi: https://doi.org/10.1016/0040-4039(96)00812-X

[20]. Romashin YN, Liu MTH, Nijjar SS, Attanasi OA. Arylchlorocarbenes in the synthesis of heterocycles containing two nitrogen atoms. Chem Commun. 2000; 1147-1148. doi: 10.1039/B002940H

[21]. Iuhas PC, Georgescu F, Georgescu E, Draghici C, Caproiu MT. Regiochemistry of the 1,3-dipolar cycloaddition of some N-heterocyclic cycloimmoniumylides to unsymmetrical alkynes. Rev Roum Chim. 2002; 47: 333-338.

[22]. Mangalagiu GC, Mangalagiu II, Olariu RI, Petrovanu MG. 4-Methylpyrimidinium ylides II: Selective reactions of pyrimidinium ylides with activated alkynes. Synthesis. 2000; 14: 2047-2050. doi: 10.1055/s-2000-8731

[23]. Georgescu E, Georgescu F, Draghici C, Cristian L, Popa MM, Dumitrascu F. Fast and green one-pot multicomponent synthesis of a library of pyrrolo [1,2-c]pyrimidines under microwave irradiation. Comb Chem High T Scr. 2013; 16: 851-857. doi: 10.2174/13862073113169990050

[24]. Georgescu E, Georgescu F, Popa MM, Draghici C, Tarko L, Dumitrascu F. Efficient one-pot, three-component synthesis of a library of pyrrolo[1,2-*c*]pyrimidine derivatives. ACS Comb Sci. 2012; 14: 101-107. doi: 10.1021/co2002125

[25]. Bhavya P, Melavanki R, Manjunatha MN, Koppal V, Patil NR, Muttannavar VT. Solvent effects on the photophysical properties of coumarin dye. AIP Conference Proceedings 1953, 080022 (2018). doi: https://doi.org/10.1063/1.5032828

[26]. Melavanki RM, Patil HD, Umapathy S, Kadadevaramath JS. Solvatochromic Effect on the Photophysical Properties of Two Coumarins. J. Fluoresc., 2012; 22, 137-144. doi: https://doi.org/10.1007/s10895-011-0939-7

[27]. Yang S, Liang X, Zhao Y, Fan J. Solvent effect on the absorption and fluorescence of ergone: Determination of ground and excited state dipole moments. Spectrochim. Acta A, 2013; 102, 194-199. doi: 10.1016/j.saa.2012.10.013

[28]. Nagachandra KH, Mannekutla JR, Amarayya SM, Inamdar SR. Solvent effect on the spectral properties of dipolar laser dyes: Evaluation of ground and excited state dipole moments. Eur. J. Chem., 2012;3 (2), 163-171. doi: 10.5155/eurjchem.3.2.163-171.538

[29]. Deepa HR, Thipperudrappa J, Suresh Kumar HM. Effect of solvents on the spectroscopic properties of LD-489 & LD-473: estimation of ground and excited state dipole moments by solvatochromic shift method. Spectrochim. Acta A, 2013; 108, 288-294. doi: 10.1016/j.saa.2013.01.084

[30]. Mostafa S, El-Sadek M, Alla EA. Spectrophotometric determination of ciprofloxacin and pefloxacin through charge transfer complexation. J. Pharmacol. Biomed. Anal., 2002; 27, 133-142. doi: https://doi.org/10.1016/S0731-7085(01)00524-6

[31]. Subhani MS, Bhatti NK, Mohammed M, Khan Turk AY. Spectroscopic Studies of Charge-Transfer Complexes of 2,3-Dichloro-5,6-Dicyano-P-Benzo-Quinone. J. Chem., 2000; 24, 223-230.

[32]. Yang J, Cao Y, He JH, Yang T, Kim X, Peng X, Kim JS. Macro-/micro-environment-sensitive chemosensing and biological imaging. Chem Soc Rev., 2014; 43, 4563-4601. doi: 10.1039/C4CS00051J

[33]. Klymchenko AS. Solvatochromic and fluorogenic dyes as environment-sensitive probes: design and biological applications. Acc Chem Res, 2017; 50, 366-375. doi: 10.1021/acs.accounts.6b00517
[34]. Tatu L, Georgescu E, Boscornea C, Ungureanu EM. Synthesis and fluorescence of 1-[7-(4-nitrobenzoyl)-3-(biphenyl-4-yl)pyrrolo[1,2-*c*]pyrimidin-5-yl]ethanone. UPB Bull Sci. 2015; 77: 49-58.
[35]. Tatu ML, Georgescu E, Boscornea C, Popa MM, Ungureanu EM. Synthesis and fluorescence of new 3-biphenylpyrrolo[1,2-c]pyrimidines. Arab J Chem. 2016; 10: 643-652. doi: https://doi.org/10.1016/j.arabjc.2016.09.013
[36]. Tatu ML, Harja F, Ungureanu EM, Georgescu E, Popa MM. Electrochemical characterization of some pyrrolo[1,2-*c*]pyrimidine derivatives. Rev Chim (Buc). 2018; 69: 499-506.
[37]. Tatu ML, Spectral and electrochemical studies of several pyrrolopyrimidines. Universitatea Politehnica Bucuresti. 2017, PhD Thesis
[38]. Zugravescu I, Georgescu F, Chiraleu F, Filip P I, Georgescu E. Pyrimidinium-ylides. I. The synthesis and the stability of some 4-phenylpyrimidinium-ylides. Rev Chim (Buc) vol. 31, 1980, p 11-13.
[39]. Georgescu E, Druta I, Petrovanu M. Dipolar derivatives in the quinazoline series. I. The synthesis of pyrrolo[1,2-*c*]quinazolines. Rev. Roum. Chim. vol. 26, 1981, p 109-116
[40]. Georgescu F, Chiraleu F, Georgescu E, Zugravescu I. Pyrimidinium-ylides. II. The reactions of several carbanion-monosubstituted 4-phenylpyriminium-ylides with activated acetylenes. Rev. Roum. Chim. vol. 26, 1981, p 879-885
[41]. Wang C, Huang J, Ye J. Binding of aromatic anion amphiphile to phospholipid vesicles: a fluorescence study. Colloids Surf A. 2002; 204: 125-129. doi: https://doi.org/10.1016/S0927-7757(01)01133-5
[42]. Lakowicz JR. Principles of Fluorescence Spectroscopy. Springer-Verlag US. 2006; 277-290.
[43]. Raikar US, Renuka CG, Nadaf YF, Mulimani BG, Karguppikar AM Soudagar MK. Solvent effects on the absorption and fluorescence spectra of coumarins 6 and 7 molecules: determination of ground and excited state dipole moment, Spectrochim. Acta A. 2006; 65: 673-677. doi: https://doi.org/10.1016/j.saa.2005.12.028
[44]. Ziołek M, Filipczak K, Maciejewski A. Spectroscopic and photophysical properties of salicylaldehyde azine (SAA) as a photochromic Schiff base suitable for heterogeneous studies. Chem Phys Lett. 2008; 464: 181-186. doi: https://doi.org/10.1016/j.cplett.2008.09.030
[45]. Abboud JM, Kamlet MJ, Taft RW, (1977) Regarding a generalized scale of solvent polarities. J Am Chem Soc. 1977; 99: 8325-8327. doi: 10.1021/ja00467a039
[46]. Zakerhamidia MS, Ghanadzadeha A, Tajalli H, Moghadamb M, Jassas M. Hosseininiaa R. Substituent and solvent effects on the photo-physical properties of some coumarin dyes. Spectrochimica Acta A. 2010; 77: 337-334. doi: https://doi.org/10.1016/j.saa.2009.12.060
[47]. Kawski A. On the Estimation of Excited-State Dipole Moments from Solvatochromic Shifts of Absorption and Fluorescence Spectra. Z Naturforsch. 2002; 57: 255-262. doi: https://doi.org/10.1515/zna-2002-0509
[48]. Pannipara M, Asiri AM, Alamry KA, Salem IA, El-Daly SA. Spectral behavior and photophysical parameters of (2Z)-3-[4-(dimethylamino) phenyl]-2-(4-fluorophenyl) prop-2-ene-nitrile (DPF) in different media. J Luminesc. 2015; 157: 163-171. DOI: https://doi.org/10.1016/j.jlumin.2014.08.053
[49]. Liu L, Sun Y, Wei S, Hu X, Zhao Y, Fan J. Solvent effect on the absorption and fluorescence of ergone: Determination of ground and excited state dipole moments. Spectrochim Acta A. 2012; 86: 120-123. DOI: https://doi.org/10.1016/j.saa.2011.10.016

728 [50]. Kamlet MJ, Taft RW. The solvatochromic comparison method. I. The beta-scale of
729 solvent hydrogen-bond acceptor (HBA) basicities. J Am Chem Soc. 1976; 98: 377-383. doi:
730 10.1021/ja00418a009

Highlights

- New 3-arylpyrrolo[1,2-*c*]pyrimidines substituted at C3 and C7 were synthesized. 79
- Their absorption spectra display two main absorption domains, and blue fluorescence appeared.95
- The excitation and emission spectra were recorded in different solvents.74
- The dipole moments have been calculated using the solvent polarity functions. 79
- The fluorescence is influenced by substituents (halogen, methyl, methoxy and NO_2). 85