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Synthesis and fluorescence of dihydro-[1,2,4]triazolo[4,3-*a*]pyridin-2-ium-carboxylates: An experimental and TD-DFT comparative study

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PII: S0143-7208(18)31040-4

DOI: [10.1016/j.dyepig.2018.09.005](https://doi.org/10.1016/j.dyepig.2018.09.005)

Reference: DYPI 6987

To appear in: *Dyes and Pigments*

Received Date: 7 May 2018

Revised Date: 31 August 2018

Accepted Date: 3 September 2018

Please cite this article as: Fedorowicz J, Sączewski Jarosław, Drazba Z, Wiśniewska P, Gdaniec M, Wicher B, Suwiński G, Jalińska A, Synthesis and fluorescence of dihydro-[1,2,4]triazolo[4,3-*a*]pyridin-2-ium-carboxylates: An experimental and TD-DFT comparative study, *Dyes and Pigments* (2018), doi: 10.1016/j.dyepig.2018.09.005.

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1 **Synthesis and fluorescence of dihydro-[1,2,4]triazolo[4,3-*a*]pyridin-2-ium-carboxylates: an**  
2 **experimental and TD-DFT comparative study**

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16  
17 **Abstract**

18 A series of inexpensive and water-soluble fluorescent dihydro-[1,2,4]triazolo[4,3-*a*]pyridin-2-  
19 ium-carboxylates (*Safirinium* dyes) have been synthesized and characterized by UV-Vis, IR, <sup>1</sup>H-  
20 and <sup>13</sup>C-NMR spectroscopic techniques as well as by single crystal X-ray analysis. Significantly  
21 lower fluorescence quantum yields were determined in aprotic polar solvent (DMF). The  
22 photophysical properties of zwitterions and hydrochlorides were rationalized theoretically. A  
23 combined experimental and DFT/TD-DFT study of absorption and emission spectra have been  
24 performed. The calculations were carried out within the vertical non-equilibrium approximation  
25 or the state-specific approach using conventional (APFD, B3LYP and PBE0) and long-range-

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