



**Ural Branch
of the Russian Academy
of Sciences**

MedChem

Russia 2019

4th Russian Conference
on Medicinal Chemistry
with international participants

June 10-14, 2019
Ekaterinburg, Russia

Abstract book

© Ural Branch of the Russian Academy of Sciences. All rights reserved
© Authors, 2019

**4th Russian Conference on Medicinal Chemistry with international participants.
MedChem Russia 2019
Abstract book – Ekaterinburg : Ural Branch of the Russian Academy of Sciences,
2019. – 512 p.
ISBN 978-5-7691-2521-8**

**Abstract book includes abstracts of plenary lectures, oral and poster presentations, and
correspondent presentations of the Conference**

Conformationally fixed tricarbocyanines modified with β -alanine, as the basis for the vector delivery of biogenic molecules

Doroshenko I.A.^{1,2}, Mestergazi M.G.^{1,2}, Podrugina T.A.^{1,3}, Radchenko E.V.^{1,3}, Pavlova A.S.¹, Kostyukov A.A.², Kuzmin V.A.²

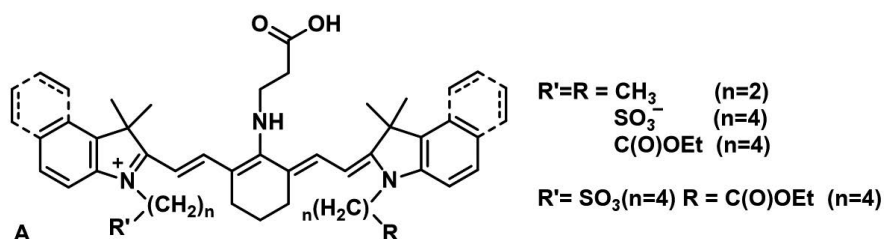
¹Department of Chemistry, Lomonosov Moscow State University,
119991, Russia, Moscow, Leninskie Gory, 1/3

²Emanuel Institute of Biochemical Physics RAS, 119334, Russia, Moscow, Kosygina st., 4

³Institute of Physiologically Active Substances RAS,
142432, Russia, Moscow region, Noginsk District, Chernogolovka, North Passage, 1

The effective fluorescence of tricarbocyanine dyes in the near infrared region allows their use in medicine and biology. The formation of complexes with transport proteins of the blood (for example, serum albumin HSA) is another key factor due to which they can be used in angiography [1].

As reagents that effectively participate in the modification of conformationally fixed tricarbocyanines at the meso-position, ω -amino acids, for example, β -alanine, have been described [2]. In the framework of this study, a series of symmetric conformationally fixed tricarbocyanines based on indolenin and benzindolenin was synthesized and a meso-position was modified by β -alanine. The molecular docking method was used to evaluate the possibility of binding the previously described modified dyes **A** with HSA and it was shown that the interaction of the ligand with the protein is possible at three binding sites of IIA, IIIA and IIB. The optical properties of the dye-albumin complexes were studied using spectrofluorimetry and time-resolved fluorimetry (TCSPC). The binding constants of modified tricarbocyanines **A** with BSA are determined.



References

- [1] M.V. Proskurnina, T.A. Podrugina, V.A. Kuzmin, T.D. Nekipelova, N.S. Zefirov, Fluorophores with indolenin scaffold and their use in biomedical purposes. Ufa: Hilem, Bashk. encycl., **2016**.
- [2] K. Kiyose, S. Aizawa, E. Sasaki, H. Kojima, K. Hanaoka, T. Terai, Y. Urano, T. Nagano, Chem. Eur. J. **2009**, 15, 9191 – 9200.