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

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

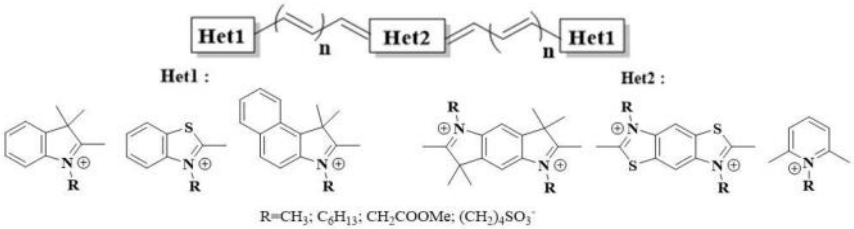
New structural types of carbocyanines with two chromophore groups: synthesis and properties

Shmykova A.M.[1], Kriveleva A.S.[1,2], Mestergazi M.G.[1,2], Kostyukov A.A.[2], Kuzmin V.A.[2], Shtil A.A.[3], Podrugina T.A.[1,2]

[1]Department of Chemistry, Lomonosov Moscow State University, Lenin Hills 1,Moscow, 119991, Russia.
[2]Emanuel Institute of Biochemical Physics RAS, Kosygin st., 4, Moscow, 119334, Russia.
[3]N. N. Blokhin Russian Cancer Scientific Center, the Ministry of Healthcare of the Russian Federation, 23 Kashirskoe shosse, 115478, Moscow, Russia.

Due to their highly effective fluorescent properties, carbocyanine dyes are successfully used in biology and medicine to investigate the mechanisms of action of drugs, as well as a means of early diagnosis and as therapeutic agents. The carbocyanines containing two chromophore fragments are the least studied in this area [1]. The structure of the dye containing four heterocyclic cores allows to significantly expand the combinatorial possibilities for the directed design of the structures in order to optimize the photophysical and pharmacophoric properties.

In the present investigation, the synthesis of a series of new biscarbocyanine dyes based on a combination of heterocycles of different structural types and hydrophilic and lipophilic substituents at nitrogen atoms was performed. It has been shown that the photophysical properties (absorption maximum, extinction coefficient, fluorescence quantum yield, etc.) depend both on the replacement of the heterocyclic system and on the variation of functional groups in the substituent at the nitrogen atom. For example, it was shown on the HCT116 cell line that dyes containing hydrophobic alkyl groups have pronounced cytotoxicity, and the introduction of hydrophilic sulfo groups into a substituent at the nitrogen atom leads to sharp decrease of the cytotoxicity.



References

[1] O.P. Klochko, I.A. Fedyunyayeva, S.U. Khabuseva, O.M. Semenova, E.A. Terpetschnig, L.D. Patsenker, *Dyes and Pigments*. **2010**, *85*, 7–15.

This work was supported by the Russian Science Foundation, project № 18-13-00463.