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DEVELOPMENT OF NEAR-INFRARED FLUOROPHORES BASED ON SULFUR-CONTAINING HETEROCYCLES FOR BIOIMAGING

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Introduction. The near-infrared region (NIR-II, 700-1700 nm) of the spectrum is valuable for biomedical applications, in particular, bio-imaging because of its high tissue penetrating ability. Among various state-of-the-art bioimaging approaches, one of the greatest challenges in developing novel theranostic probes is to achieve both high resolution and sensitivity. The computer-aided design and synthesis of NIR fluorophores suitable for multimodal imaging is thus emerging as a powerful strategy for acquisition of high-resolution images. NIR fluorophores can convert NIR photons into heat (for photothermal therapy) and/or generate singlet oxygen (for photodynamic therapy) [1,2].

The main part. Using the methods of computational chemistry [3], the following tasks are solved in this work:

1) Optimize and validate quantum chemical calculation methods of molecular geometry and HOMO/LUMO energy values of a number of (thio)pyrylium ions;
2) Select density functional and basis set for calculations of absorption spectra.

Conclusions. PBE0 and B3LYP functionals gave similar trends of HOMO-LUMO energy values of thiopyrylium ions in spite of divergent absolute values. B3LYP functional showed robustness by reproducible HOMO-LUMO energy values compared with literature data.

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