



Bacteriochlorin–Styrylnaphthalimide Conjugates for Simultaneous Photodynamic Therapy and Fluorescence Imaging

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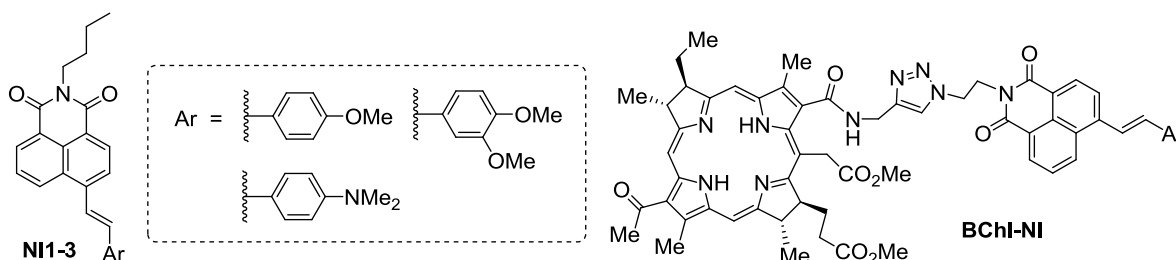
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1,8-Naphthalimide derivatives are famous organic fluorophores which generally exhibit high thermo and photostability and are known to act as fluorescent brighteners and dyes for polymer fibers, laser active media, electroluminescent materials and optical memory devices. Because of its intense fluorescence, large Stokes shifts along with the relative ease of synthetic operations for targeted modification of the molecular structure, this type of compounds has found application in the construction of fluorescent chemosensors for biologically relevant cations and anions, labels or probes for proteins, cells, lysosomes and other acidic organelles. However, the emission bands of most naphthalimides are in blue and green-yellow regions. This limits their application as fluorescent probes and imaging agents in life sciences. Although it is well-known that electron-donating groups at the C-4,5-positions of naphthalene ring usually increase the fluorescence quantum yield of the compounds and cause the red shift in the spectra, the reports on 1,8-naphthalimide derivatives with emission wavelengths longer than 600 nm are very few.



In the present work, we focused on the spectroscopical investigation of styryl-1,8-naphthalimides **NI1–3** as promising long wavelength imaging units in bifunctional conjugates for simultaneous fluorescence diagnostics and photodynamic therapy of cancer. Firstly, steady-state and time resolved photophysical properties of these compounds were studied in protic and aprotic solvents of different polarity. We have found very interesting behavior related to the interplay between fluorescence, formation of TICT states and *E,Z*-isomerization¹. The observed spectral effects have been rationalized using quantum-chemical calculations, X-ray data and NMR spectroscopy. At the second step, conjugates (**BChl-NI**) of styryl naphthalimides with propargyl-15²,17³-dimethoxy-13¹-amide of bacteriochlorin *e* known as a highly effective natural photosensitizer (PS) in PDT have been prepared². The idea was to combine the modalities of PS and fluorescent probe in one molecule where the excitation of the naphthalimide fragment is expected to produce the strong emission signal, which could be used to monitor tumor responses to treatment. Further excitation by an other light wavelength corresponding to the absorption maxima of PS would lead to formation of singlet oxygen responsible for cancer cell damage. In this work, the details of our study of optical characteristics as well as evaluation of photosensitizing activity of **BChl-NI** in solution and in living cells are presented.

Bibliography

¹ P. A. Panchenko, *et al.*, Controlling photophysics of styrylnaphthalimides through TICT, fluorescence and *E,Z*-photoisomerization interplay. *Phys. Chem. Chem. Phys.*, 2017, 19, 1244–1256.

² P. A. Panchenko, *et al.*, A novel bacteriochlorin–styrylnaphthalimide conjugate for simultaneous photodynamic therapy and fluorescence imaging. *Phys. Chem. Chem. Phys.*, 2017, 19, 30195–30206.

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