Perylene-(cyanine dye) dyad as NIR agent for theranostics

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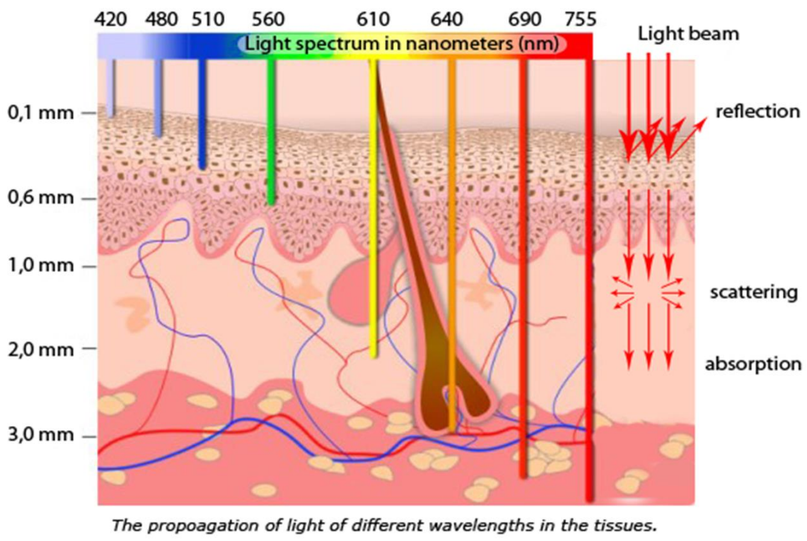
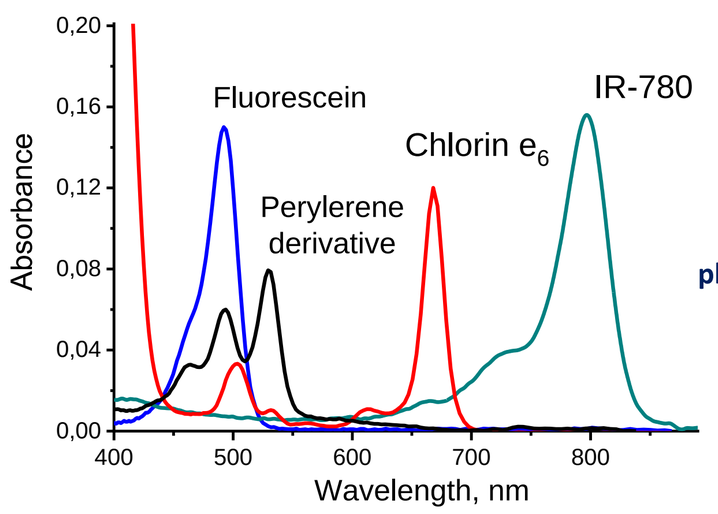
Application of near infrared light (NIR) in biomedicine



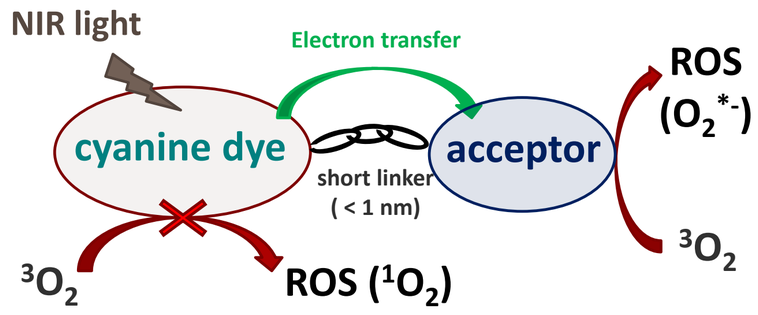
The propoagation of light of different wavelengths in the tissues.



NIR light (700-950 nm) has the deepest penetration into the living tissues and highly attractive to diagnostics and therapy applications.

In addition to diagnostics, combination of NIR dyes with an organic acceptor allows to create effective type I type photosensitizers for PDT based on donor-acceptor (D-A) dyads

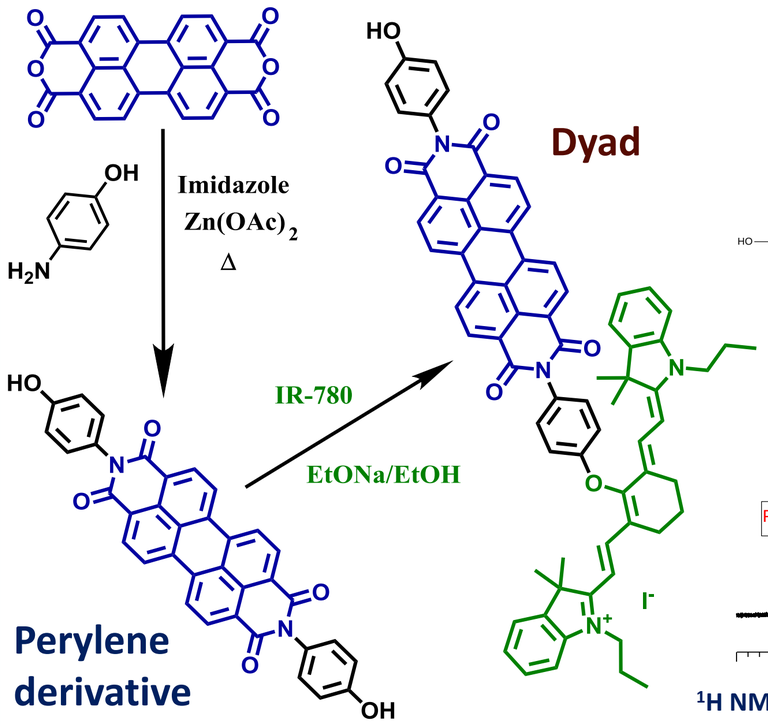
D-A dyads as NIR Type I photosensitizers for PDT

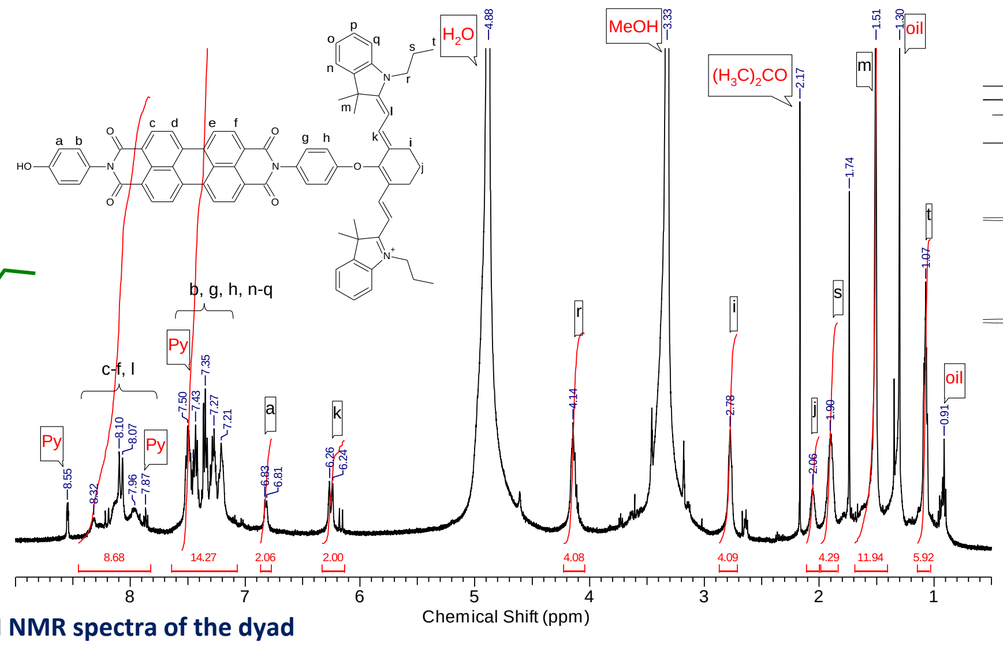


Such type I photosensitizers have two major advantages compared to the traditional (type II, based on the singlet oxygen generation) photosensitizers:

- Donor (dye) does not require to have a high quantum yield to the triplet state;
- Type I phototoxicity is also more effective against solid hypoxic tumors.

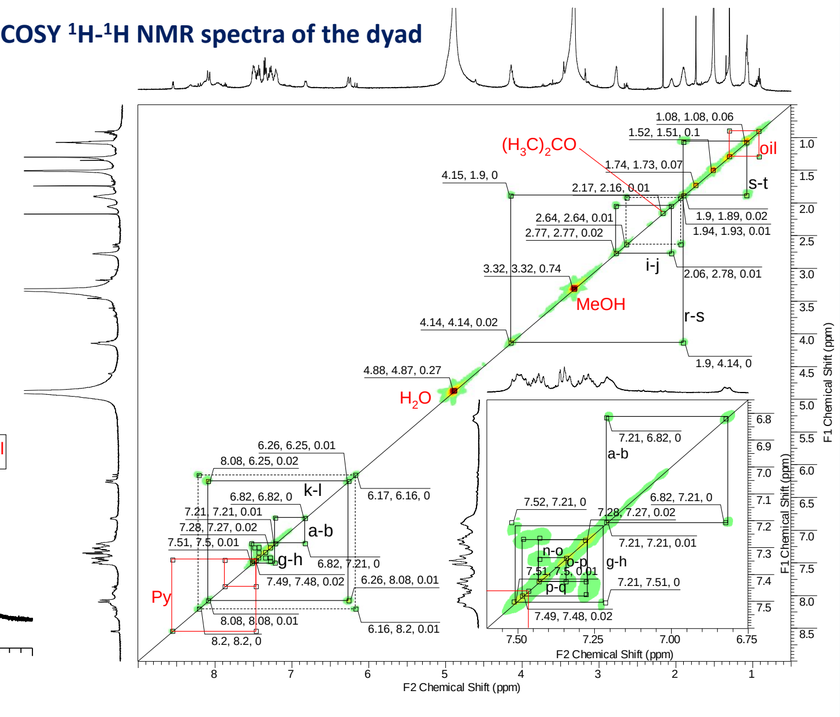
Synthesis of perylene-cyanine dyad



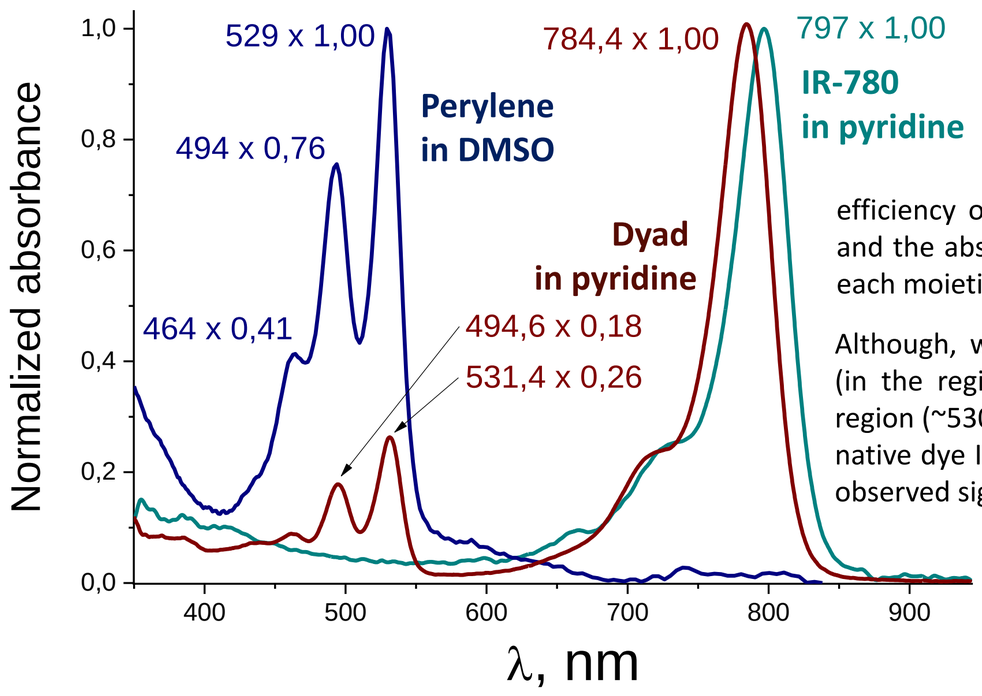


1H NMR spectra of the dyad

COSY 1H-1H NMR spectra of the dyad

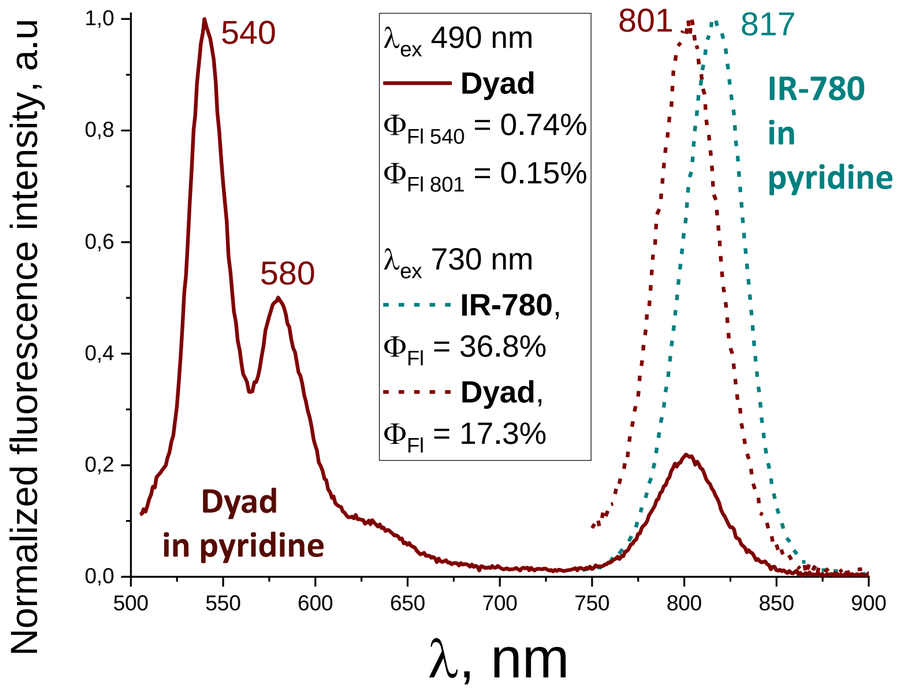


Photophysical properties



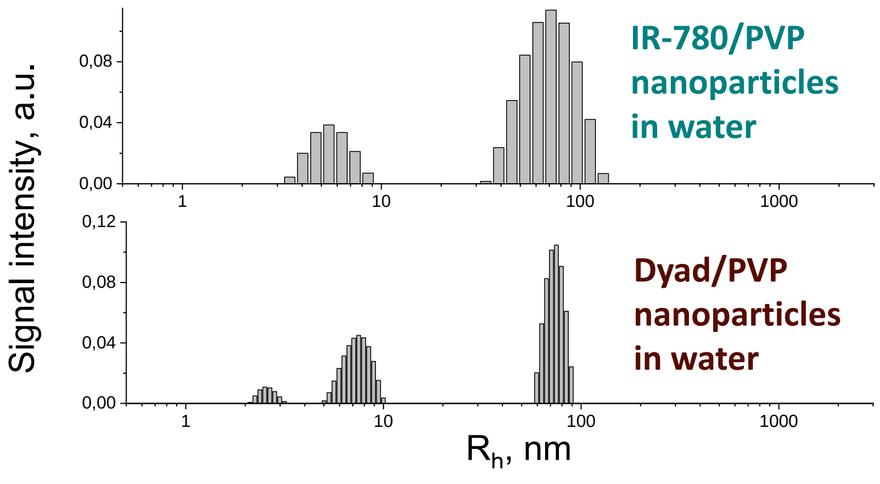
It was shown that the dye and acceptor in the obtained structure have small influence on each other, which is expressed in the low efficiency of fluorescence quenching of the dye moiety and the absence of changes in the absorption spectra of each moieties of the dyad.

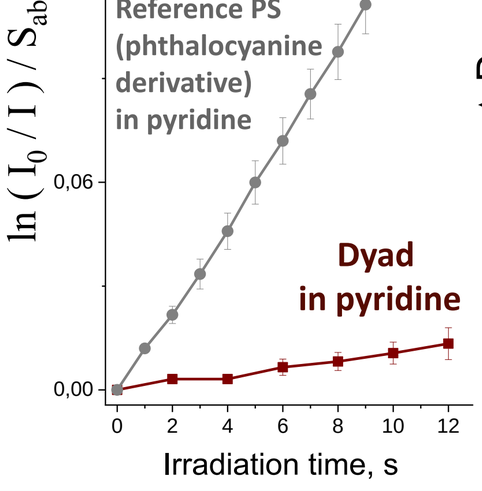
Although, we observed fluorescence signal from IR780 (in the region >780 nm) upon excitation in the green region (~530 nm), while no fluorescence detected for the native dye IR780 in the same conditions. We believe the observed signal caused by the Förster energy transfer mechanism from the photoexcited perylene derivative to IR780 moieties.

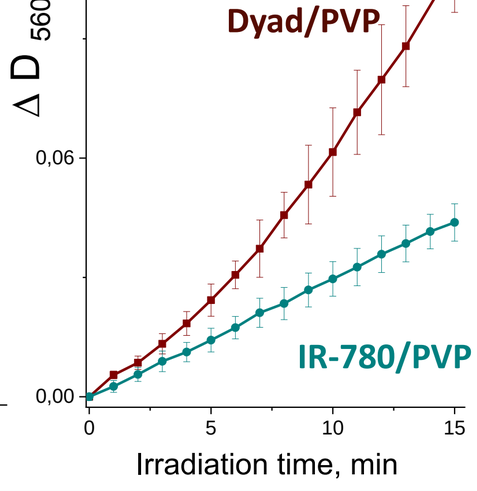


ROS generation under NIR light irradiation

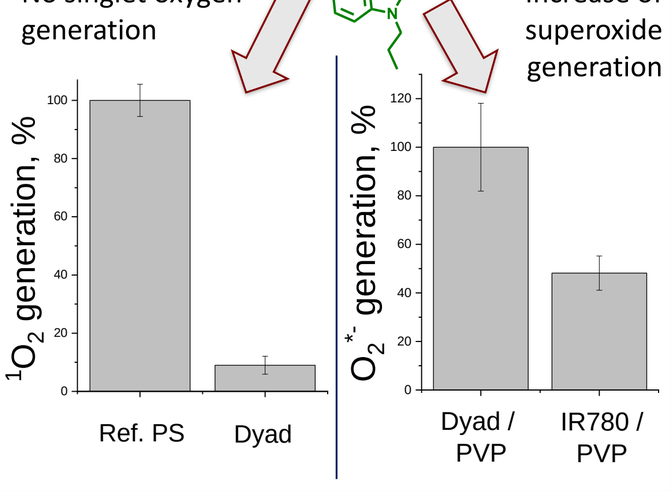
In order to evaluate superoxide generation efficiency we prepared PVP-based nanoparticles from IR-780 and the dyad and measured their size by DLS method.







ROS generation by the dyad



Summary

In our previous works we have shown high efficiency of fullerene-dye dyads as type I photosensitizers for photodynamic therapy [1-3]. In the present work, we synthesized covalently-linked dyad of a non-fullerene acceptor – perylenediimide with cyanine dye IR-780. The obtained dyad has high absorbance in the NIR region, high fluorescence quantum yield and could generate superoxide under NIR light irradiation.

Thus, obtained results show promising potential of such perylene-(cyanine dye) dyads as agents for theranostics and other biomedical applications.

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1. A.V. Kozlov, A.Yu. Rybkin, A.Yu. Belik, E.A. Kostina, N.S. Goryachev, I.V. Sulimenkov, V.I. Kozlovskiy, O.I. Istakova, D.V. Konev, A.I. Kotelnikov. Synthesis and photophysical properties of heptamethine cyanine-fullerene C60 dyads with non-quenched fluorescence // Mendeleev Communications, 2021, Vol. 31, P. 807–809 (**DOI:** 10.1016/j.mencom.2021.11.012)
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3. Kozlov A.V., Rybkin A.Yu., Belik A.Yu., Taziev K.R., Tarakanov P.A., Goryachev N.S. et al. Synthesis by the Hummelen-Wudl Method and Physicochemical Study of Pyropheophorbide-Fullerene Dyad. Macroheterocycles 2020;13:147–55 (**DOI:** 10.6060/mhc200500r)