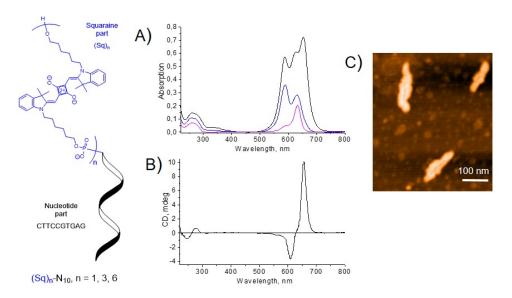
Aggregation of a squaraine-modified oligonucleotide in aqueous solution

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Squaraine-based compounds are promising chromophores for the creation of new materials for biomedical or diagnostic applications through the methods of supramolecular chemistry. Squaraine dyes exhibit a molar absorptivity of up to 260 000 M⁻¹cm⁻¹. They absorb and emit light in the long-wavelength region of the visible spectrum. Furthermore, they tend to form well-ordered aggregates in organic and aqueous solutions.

In this work, we study the aggregation properties of oligomers which consist of squaraines (1, 3, or 6 molecules) and nucleotides (10 units). Their aggregation properties are studied by spectroscopic (UV-Vis and CD) and microscopic (AFM and TEM) methods in water/ethanol solutions (see Figure below).



A) UV-Vis spectra of the oligomers: $(\mathbf{Sq})_1-\mathbf{N}_{10}$ (magenta, no aggregation), $(\mathbf{Sq})_3-\mathbf{N}_{10}$ (blue, Haggregation), and $(\mathbf{Sq})_6-\mathbf{N}_{10}$ (black, oblique aggregation) B) CD spectrum and C) AFM image of the $(\mathbf{Sq})_6-\mathbf{N}_{10}$ oblique aggregates

Based on UV/vis spectroscopy, oligomer $(\mathbf{Sq})_1$ - \mathbf{N}_{10} with one squaraine molecule shows no well-defined type of aggregation. Oligomer $(\mathbf{Sq})_3$ - \mathbf{N}_{10} containing three squaraine units, however, reveals stacking of the chromophores in H-type fashion (blue shifted absorption band). Finally, oligomer $(\mathbf{Sq})_6$ - \mathbf{N}_{10} can form both H-type and oblique (splitting of the absorption band) aggregates depending on the conditions of preparation. The oblique aggregates of the $(\mathbf{Sq})_6$ - \mathbf{N}_{10} exhibit the signs of the supramolecular polymers, in which the squaraine-nucleotide oligomers are arranged in a helical fashion.