



Exploring Intricate Interactions: A Comprehensive Study of Novel *Bis-Acridine Orange* Dyes with Double-Stranded DNA

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Understanding DNA interactions with small or large molecules is crucial for fundamental and applied research. The conformational space these molecules explore depends on the environment, especially when confined in grooves or pockets of large molecular systems [1]. This confinement can alter favored conformations, impacting properties like chemical, mechanical, and optical characteristics. Such variations can be harnessed for diverse biochemical applications. For instance, the binding of small organic molecules to specific DNA structures influences fluorescence, enabling double-stranded DNA detection. Molecular modeling aids in comprehending atomic-level interactions, facilitating the rational design of molecules with various applications.

In this talk, I'll present results from our recent study [2] on the interplay between dsDNA and a novel series of dyes (BAO), designed with two acridine orange (AO) units connected by different linkers. Biochemical assays reveal superior performance compared to the widely used dye, Eva Green (EG), in qPCR analysis. Molecular dynamics simulations show how the dyes adopt different conformations in DNA grooves, impacting fluorescence properties based on linker differences.

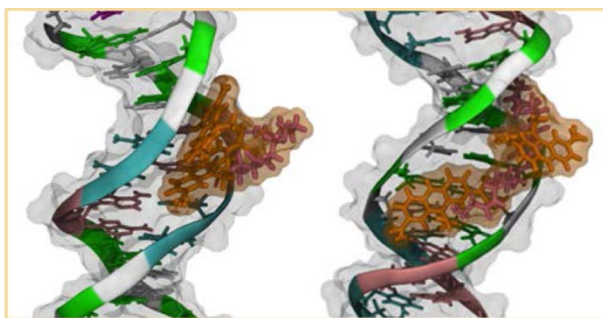


Fig 1. Representative conformations of EG (left) and a BAO dye (right). Color code: guanine in green, cytosine in white, thymine in cyan and adenine in pink. The AO moieties of the dye are orange and the linkers purple.

References:

1. T. Vasiliu, F. Mocci, A. Laaksonen, L.D. Engelbrecht, S. Perepelytsya, *Front. Chem.* (2022), **10**, 836994
2. O. Kulyk et al., R. Svoiakov, O. Kolosova, I. Prylutska, T. Vasiliu, R. Puf, F. Mocci, A. Laaksonen, S. Perepelytsya, A. Krivoshey, D. Kobzev, Z. Tkachuk, A. Tatarets, *manuscript in preparation*.