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G-Quadruplexes Spontaneously Bind Small Molecules

Guanosine-rich tracts of nucleic acids self-assemble into stacks of stable square planar guanine quartets, having specific regulatory roles on their own function. The meaning is, possible stable aggregates of biomolecules control storage and transfer of information potentially involved in complete cell life cycles. [1] Smaller molecules are the human means to interfere with these cycles with medicinal or other purposes. [2] We assumed the stacking mode of association of ligands and G-quadruplexes as the one to provide certain selectivity requisites to expected effect on chosen biological systems. [3, 4, 5] Stabilization of stacked ligand – G-quadruplex aggregates depending on their affinity has the potential of defining quantitative relationships with potentially useful therapeutic propeties.[6] This research has been funded by the Bulgarian National Research Fund via grant KP-06-N59/1 of 15.11.2021; and sponsored by grant D01-325/01.12.2023 and Consortium Petascale Supercomputer-Bulgaria and EuroHPC supercomputer.

Primary author(s) : KANETI, Jose (Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria); Prof. BAKALOVA, Snezhana M. (Institute of Organic Chemistry with Centre of Phytochemistry)

Presenter(s) : KANETI, Jose (Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria)