G-Quadruplex - Characterization of functions and potential therapeutic uses of non-canonical DNA structures

Aims & Scope:

Personalized drug design is a challenging area of research because it fuses complex screening of therapeutics with individuals’ susceptibility and genetics. Thanks to advances in high-throughput sequencing and its affordable cost, wide genetic sequencing of populations is feasible, and this opens up new opportunities for generating large amount of data that allow studying gene-based therapeutics.

Characterizing the 2-dimensional and 3-dimensional structures of the human coding genes is not an easy task and we are getting more aware about the importance of the non-coding portions of the DNA. G-Quadruplexes (G4s) are particularly interesting DNA structures, alternative to the standard double helix fold. G4s are usually found in telomeric regions and exhibit oncogenic properties, but are also present in other portions of organisms’ genomes with less clear functions. G4s can be seen as ‘molecular devices’ with two relevant properties: (i) their cylindrical-shaped structure is an ideal container for drugs; and (ii) they can be used to inhibit genes potentially related to pathologies. Drug delivery in cells is hard because of the lipid barrier, so having a molecular device to be used as a transporter inside cells can be groundbreaking in a number of treatments, from cancer to infectious diseases. Recent studies have shown that G4s can be wrapped to HIV inhibitors and help passing cell membranes, e.g. into brain.

It is important to study G4 both in terms of their functions with respect to gene regulation and disease onset, as well as potential uses as a containers and transporters of novel therapeutic agents. G4 research is currently an understudied field, yet of utter importance for medicine and medicinal chemistry. Further, development of computational tools for G4 characterization can become a resource for scientists working on drug design.

Keywords: G-quadruplexes, drug design, drug transporters, machine learning, computational drug design, gene regulation

Sub topics:

- Prediction of G4 structures
- Gene regulation and transcription
- Drug design

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