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How Polymorphism and Ligand Binding modulate G-quadruplex Fast Dynamics

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G-quadruplexes (G4s) formed by the human telomeric sequence AG3(TTAG3)3 (Tel22) play a key role in cancer and ageing. G4 structures are known to display a variety of topologies, which are determined by several factors, resulting in structural polymorphism. Neutron Scattering techniques are a valuable tool to investigate how G4 structural polymorphism and ligand binding affect their sub-nanosecond dynamics. Within this context, we combined FTIR spectroscopy to monitor the Tel22 conformation and EINS to assess the corresponding dynamical properties. K+ and Na+ stabilized G4s were found to be in the parallel and mixed parallel-antiparallel topologies, respectively, with the latter resulting to be dynamically more stable. This result is compatible with the presence of ordered hydration-water structures in the antiparallel conformation. Complexation with the model ligand BRACO19 (BR19) resulted in an overall increase of Tel22 mobility. Such a dynamical enhancement, which is uncorrelated to the G4 topology, can be ascribed to a preferential binding of water molecules to Tel22 rather than to BR19.

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