Investigating the influence of polyamines on G-Quadruplex structures: Insights from Molecular Dynamics

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The DNA G-quadruplexes are complex secondary structures that form in the guanine-rich regions of the genome by stacking guanine bases through H-bonds. These complex structures have attracted considerable attention in biological and pharmaceutical research due to their potential roles in regulating gene expression and genomic stability. Given the crucial function of DNA G-quadruplexes, it becomes imperative to extensively investigate their interactions with other biological entities, in particular polyamines, as these molecules are known to play an important role in regulating cell growth and stabilizing canonical DNA (configurations). Spermidine3+(SPD3+), a naturally occurring polyamine, is known for its role in promoting cell longevity and regeneration, while diminazine2+(DA2+), a synthetic polyamine, is used in the treatment of some parasitic diseases and has remarkable pharmacological properties. Both polyamines exhibit interesting interactions with the G-quadruplex of DNA. This study shows that fluctuations in polyamine concentration and temperature can alter the interaction of polyamine with DNA structures, providing new insights into molecular understanding and, eventually, the design of new therapeutic approaches.

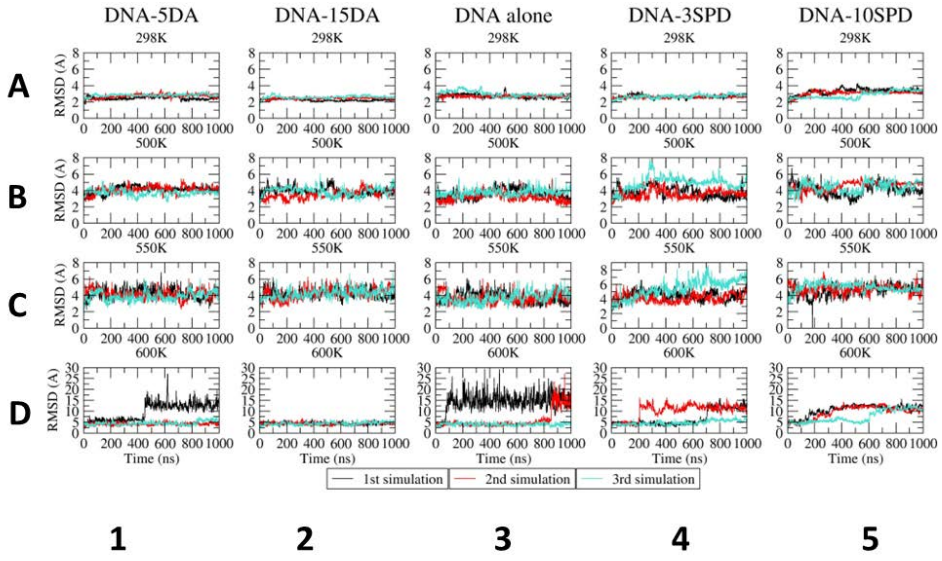

Fig 1. RMSD calculated on all heavy atoms of the G4 at 298K (row A), 500K (row B), 550K (row C), 600K (row D) in the system G4-5DA (col 1), G4-15DA (col 2), G4 (col 3), G4-3SPD (col 4), G4-10SPD (col 5).