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## A computational study on the nature of DNA G-quadruplex structure

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DOI:  
[10.33612/diss.159767021](https://doi.org/10.33612/diss.159767021)

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*Document Version*  
Publisher's PDF, also known as Version of record

*Publication date:*  
2021

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*Citation for published version (APA):*  
Gholamjani Moghaddam, K. (2021). *A computational study on the nature of DNA G-quadruplex structure*. [Thesis fully internal (DIV), University of Groningen]. University of Groningen.  
<https://doi.org/10.33612/diss.159767021>

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# List of Publications

The papers related to this thesis are highlighted as black.

- **K. G. Moghaddam**, S. Faraji, A. H. de Vries and S. J. Marrink, *On the nature of interactions between the DEAH-box helicase RHAU and G-quadruplex*, **2020**, in preparation.
- **K. G. Moghaddam**, G. Giudetti, W. Sipma and S. Faraji, *Theoretical insights into the effect of size and substitution patterns of azobenzene derivatives on the DNA G-quadruplex*, *Phys. Chem. Chem. Phys.*, **2020**, 22, 26944.
- **K. G. Moghaddam**, A. H. de Vries, S. J. Marrink and S. Faraji, *Binding of quinazolinones to c-KIT G-quadruplex; an interplay between hydrogen bonding and  $\pi$ - $\pi$  stacking*, *Biophys. Chem.*, **2019**, 253, 106220.
- A. Khorsandi-Langol, **K. G. Moghaddam** and S. M. Hashemianzadeh, *Tuning of elastic properties of nanotubes by imposing a transverse electric field: computational approach*, *J. Phys. Chem. C.*, **2016**, 120, 17801.
- S. Hassanzadeh, A. Kiani, **K. G. Moghaddam**, *Nanoparticles: Polymer-Drug Interactions Chapter in Encyclopedia of Biomedical Polymers and Polymeric Biomaterials*, Taylor and Francis, **2015**, 5545.
- **K. G. Moghaddam**, S. M. Hashemianzadeh, *The effect of amino substituents on the interactions of quinazolone derivatives with c-KIT G-quadruplex: insight from molecular dynamics simulation study for rational design of ligands*, *RSC Adv.*, **2015**, 5, 76642.
- M. Eslami, **K. G. Moghaddam**, S. M. Hashemianzadeh, *Computational evidence to design an appropriate candidate for the treatment of Alzheimer's disease through replacement of the heptamethylene linker of bis(7)tacrine with S-allylcysteine*, *RSC Adv.*, **2015**, 5, 66840.