

References:

- [1] Hašek, J. (2011). *J. Synchrotron Radiation*, 18, 50-52.
- [2] Hašek, J. (2006). *Zeitschrift für Kristallogr.* 23, 613-619.
- [3] Nanev, C.N. et al (2017). *Scientific Reports*, 7, 35821-35828.

Keywords: protein crystallization, principle of dominant adhesion mode, porous materials

MS40-P04

Crystallization of the quadruplex (GGGGTTTTGGGG)₂ with BRACO19

Rositsa Nikolova¹, Hristina Sbirikova-Dimitrova¹, Rusi Rusev¹, Louiza Dimova¹, Boris Shivachev¹

1. Institute of Mineralogy and Crystallography, Sofia, Bulgaria

email: rosica.pn@clmc.bas.bg

One of the approaches for to development of new anti-cancer compounds focuses on the design and screening of compounds, small molecules that interact selectively with cancers cells. As telomeres are G-rich noncoding regions located at the end of chromosomes. The telomere shortens with each cell division. When it reaches a critical length it triggers DNA damage response which leads to cell death. Cancer cells have active telomerase (responsible for the maintenance of telomeres) that maintain a shorten but not critical telomere length, provoking those cells to unlimited cell division. G-rich telomeres are in practice forming G-quadruplex structures *in vivo*. Ligands that selectively bind and stabilize G-quadruplex, are interfering with telomerase activity: maintenance and elongation of telomere. We report on the interaction of the (GGGGTTTTGGGG)₂ sequence with the small molecule BRACO-19. In addition, single crystal of the DNA complex with BRACO19 were grown (Figure 1). The initial crystallization conditions included KCl, K₂CO₃ pH7.5, MgCl₂, Spermine and MPD. The crystals were brownish in color and diffracted up to 2.5 Å resolution. In order to solve the crystal structure, currently diffraction limit and crystal quality are optimized through modification of the crystallization conditions.

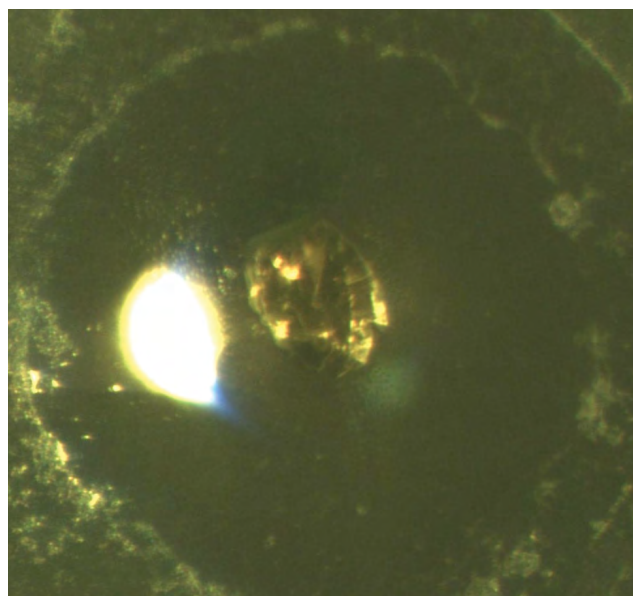


Figure 1. Observed crystals of (GGGGTTTTGGGG)₂ with BRACO19

References:

The authors are grateful to the Bulgarian national Science fund grant T02/14 for the financial support.

Keywords: G-4, quadruplex, BRACO19