An approach towards catalytic DNA nanostructures

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In the last years, DNA nanotechnology has inspired researchers from a wide range of disciplines to develop novel technologies. The possibility to design objects in the nanoscale facilitated very promising applications as e.g. therapeutics and catalytic compartments [1,2]. In the highly ambitious H2020 FETopen project MARA, we are refining such applications and are developing DNA nanostructures that comprise catalytic sites of proteins [3]. For the design of such structures, the new software tool ADENTIA was developed. It is implemented in the SAMSON Connect framework that enables the atomic-based modelling and simulation of nanosystems using a GUI and personal computer. An outstanding feature is that PDB-files from e.g. proteins can be imported and modified in our DNA nanostructure editor (Fig, 1). The tool can load Cadnano designs and has implemented the Daedalus algorithm for the design of wireframe structures. In addition to a new multiscale visualisation concept (incl. 1D, 2D, 3D) that facilitates the inspection and modification of DNA nanostructures [4], a data model was developed that can be exported for oxDNA simulations. Thus, we are convinced that our tool should be useful for many researchers working with DNA and DNA nanostructures (Fig 1).

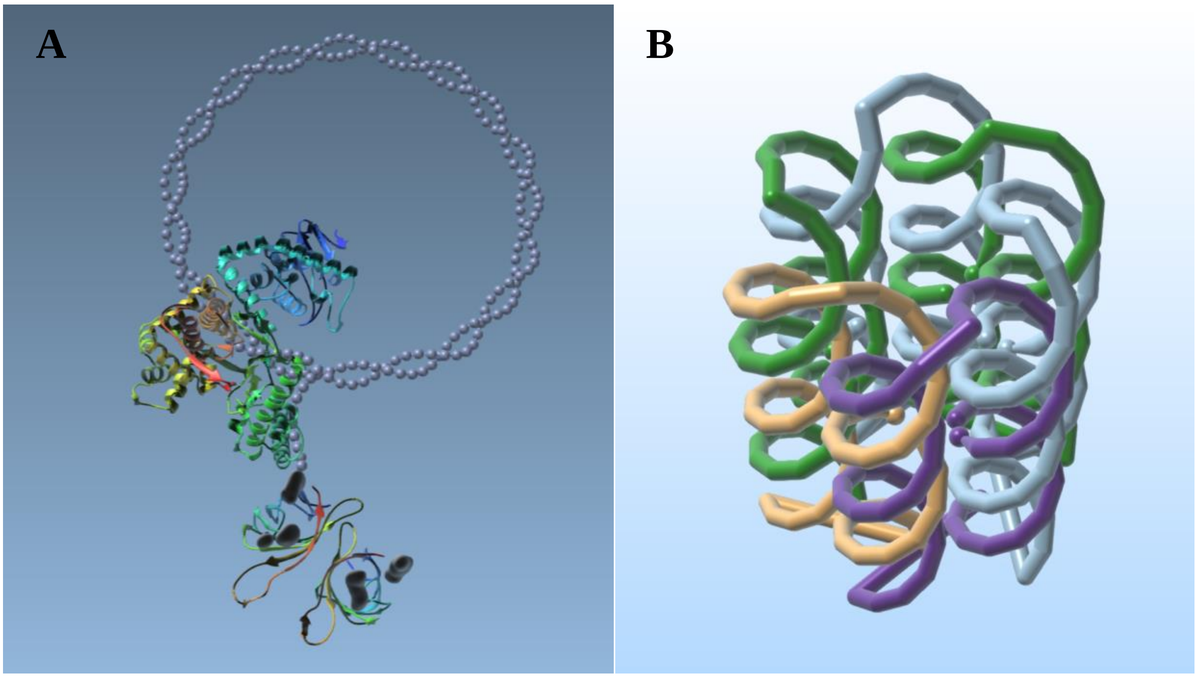

Figure 1: Adenita screenshots illustrating a (A) biosensor surface with neutravidin, an oligonucleotide, DNA polymerase and circularised padlock probe and (B) a DNA pore.

In addition to Adenita, we will present in our talk the first designs of DNA nanostructures comprising the catalytic site of the FlaI motor protein of the archaeallum and preliminary results concerning enzymatic activity of these structures.

References

[1] S. Li et al., Nature Nanotech. 2018, **36**, 258-264.
[2] Z. Zhao et al., Nature Commun. 2018, **36**, 258-264.
[3] www.maraproject.eu
[4] H. Miao et al. IEEE Tran Vis Comput Graph. 2018, 24(1), 1014-1024