S5.4 Molecular architecture of the elongator catalytic sub-complex and its tRNA interaction

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The highly conserved eukaryotic Elongator complex performs specific chemical modifications on wobble base uridines of tRNAs, which are essential for proteome stability and homeostasis (Nedialkova, 2015). Elongator is of fundamental clinical relevance, as mutations affecting its integrity and activity are related to the onset of neurodegenerative diseases, cancer and intellectual disabilities. The Elongator is formed by two copies of each of its six individual subunits (Elp1-6) that are all important for its tRNA modification activity (Huang, 2005). Although the overall architecture of the Elongator has been proposed using an integrative approach (Dauden, 2017), high resolution information of both the Elp123 catalytic sub-complex and the Elongator is still missing. Moreover, the detailed chemistry of the Elongator modification reaction is insufficiently described. Here we show the Elp123 structure at 3.3 Å resolution solved by cryo-electron microscopy, revealing novel structured parts that may be implicated in tRNA binding. We prove that Elp123 sub-complex is able to bind tRNA in the absence of the Elp456 sub-complex. Finally, we characterize this interaction in molecular detail solving the structure of the Elp123-tRNA complex also by cryo-EM. These structures provide the structural framework to understand the tRNA binding and modification in molecular detail.

S5.5 Theoretical description of ssDNA adsorption on carbon nanotubes

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A series of experimental studies show, that single-stranded DNAs (ssDNA) form a stable complex with Single-walled carbon nanotubes (SWCNT) which uses successfully for dispersion and structure-based sorting of SWCNTs into an aqueous solution. Inspired by these experiments we investigated the ssDNA/SWCNT complex formation theoretically. It is shown, that thermodynamics and kinetics of CNT –DNA nanohybrid formation can be addressed in terms of models similar to those, describing the helix-coil transition in biopolymers. To address the assembly and disassembly of DNA/SWCNT we applied an approach developed earlier for the description of conformational transition in two-strand polynucleotides and polypeptides. The approach is formulated in terms of GMPC, which is the Potts-like model with multi-particle interaction. We adopted the analytical model to describe the adsorption of the ssDNA and dsDNA molecules on the surface of substantially one – dimensional SWCNT. The results were compared with experimental data. It is shown that the proposed theoretical model can be developed for the account of the effect of stacking-interaction, single-strand rigidity, energy of adsorption, sequence heterogeneity, etc. Theoretical results obtained for the homogeneous sequences are in good agreement with experiment.