Czech Society for Structural Biology

15th Structural Biology Club of the Czech Society for Structural Biology

online on

26 April 2023, 13:00

with the following scientific talks kindly delivered by our guests

JumpCount: Calculation of uncertainties in biomolecular simulations

Presented by **Vojtěch Spiwok, Department of Biochemistry and Microbiology, University of Chemistry and Technology, Prague**

Assessment of the accuracy of biomolecular simulations is crucial for their applications in ligand design, protein engineering, and other fields. Inaccuracies may originate from systematic errors (e.g., from force field inaccuracies) and from random errors (uncertainties). We proposed a very easy method to calculate uncertainties in simulations, simply from the count of transitions between states of the system (e.g., protein folding and unfolding, ligand binding and unbinding and other events). Our results show that the uncertainties are surprisingly low. If we observe one unfolding and one folding (or one unbinding and one binding, etc.) at 300 K, the standard error of folding/binding/… Delta G is 4.53 kJ/mol (1.09 kcal/mol), and the 95 % confidence interval is Delta G ± 9.14 kJ/mol (2.19 kcal/mol). Standard error lower than 1 kcal/mol requires two foldings and two unfoldings. We will present our recent efforts to extend this method to parallel tempering and metadynamics as well as to systems with non-Markovian transitions.

G-quadruplexes: Mutations for function

Presented by **Pavel Srb, Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague**

G-quadruplexes are non-canonical nucleic acid structures formed by stacked guanine tetrads. They are important scaffolds in biotechnology and play widespread biological roles. Their remarkable functional and structural diversity highlights the importance of better understanding the relationship among G-quadruplex primary sequence, structure and biochemical function. We are exploring this question in the context of 496 variants of a monomeric reference G-quadruplex, whose structure we solved previously. We have also characterized each sequence functionally (GTP binding, peroxidase reaction promotion, intrinsic fluorescence generation and oligomerization) and structurally (NMR spectroscopy, IONEX). Current level of our understanding the structure-function relationship will be discussed.

Moderator: **Richard Hrabal**, University of Chemistry and Technology, Prague

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Please, join us on this Zoom link (join 5-10 minutes before the beginning)
https://cesnet.zoom.us/j/98867419047?pwd=WEF6THZuU01YQVpmMmxsV1hFaWZjQT09
Meeting ID: 988 6741 9047
Passcode: 726237

Richard Hrabal and Jan Dohnálek
on behalf of the Czech Society for Structural Biology

https://cssb.structbio.org