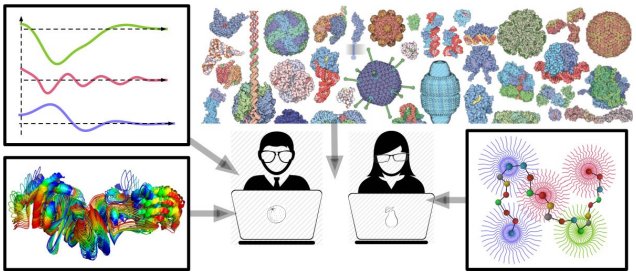

Contribution ID: **25** Type: **Talk**

High-throughput prediction of ATP synthase rotor ring stoichiometries

Friday, 16 February 2024 09:30 (30 minutes)

Rotary ATP synthases are large enzyme complexes present in every living cell. They consist of a transmembrane and a soluble domain, each comprising multiple subunits. The transmembrane part contains an oligomeric rotor ring (*c*-ring), whose stoichiometry defines the ratio between the number of synthesized ATP molecules and the number of ions transported through the membrane. Here, we present an easy-to-use high-throughput computational approach based on AlphaFold that allows us to estimate the stoichiometry of all homooligomeric *c*-rings, whose sequences are present in genomic databases. We validate the approach on the available experimental data, obtaining the correlation of 0.96 for the reference set of *c*-rings with stoichiometry from 8 to 15, and use it to predict the existence of *c*-rings with stoichiometry varying from 8 to 27. We then conduct molecular dynamics simulations of selected *c*-rings to corroborate the machine learning-based predictions. Our work highlights the usability of AlphaFold-based approaches for modeling homooligomeric proteins.

Submitting to:

8th CAPRI assessment meeting

Primary authors: OSIPOV, Stepan D.; ZINOVEV, Egor V.; ANUCHINA, Arina A.; KUZMIN, Alexander S.; MINAEVA, Andronika V.; RYZHYKAU, Yury L.; VLASOV, Alexey V.; GUSHCHIN, Ivan (Moscow Institute of Physics and Technology)

Presenter: GUSHCHIN, Ivan (Moscow Institute of Physics and Technology)

Session Classification: CAPRI