KEMIJSKI INŠTITUT

Vabilo na Preglov kolokvij / Invitation to the Pregl colloquium

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Velika predavalnica Kemijskega inštituta /
Great Lecture Hall
National Institute of Chemistry
Hajdrihova 19, Ljubljana, Slovenia

The Protein Dance – from Experiments to AI Predictions

Why can we not design efficient enzymes or highly selective drugs to date? While one can solve high resolution structures of ground states experimentally, and even now predict them with Alphafold; for biological function proteins need to traverse the entire energy landscape from the lowest energy state over the transition states into higher energy states. I will share novel experimental approaches to visualize the structures of transition-state ensembles and high-energy states of proteins. Since conformational substates and interconversion between them are essential for biological function, we developed a novel powerful method (AF-cluster) to predict multiple protein conformations using AI. Next, I will highlight how we developed a large curated NMR data set to train a new dynamics model (Dyna-1) using machine learning. Dyna-1 has predictive power for us-ms protein dynamics, with the strongest predictive power for motions directly linked to biological function. Finally, visions (and success) for putting protein dynamics at the heart of drug design are discussed.

Info: Prof. Dr. Franci Merzel franci.merzel@ki.si

Vljudno vabljeni / Kindly invited