Contribution ID: **66** Type: **Poster**

Using machine learning to optimize the crystal volume of protein crystals

Tuesday 9 April 2024 18:30 (20 minutes)

Modern chemical industry companies now routinely use machine learning to optimize protein-enzymes with respect to their yield in their enzymatic reactions. Those reactions can lead to the synthesis of complex drugs which would have to be produced in a more cost-intensive way without protein-enzymes as catalysts. Also, these optimized enzymes help to reduce the production of unwanted side products in these synthesis routes. The variation parameters are the amino acid sequence and the buffer conditions. The data base which the machine learning algorithm is based on is often produced by try and error methods in wet labs or relies on published structures found in the protein data base. In this contribution I propose to use these approaches to modify the outer surface of proteins in order to optimize their crystallization behavior to yield large volume crystals. Those crystals are needed for neutron diffraction. The resulting neutron structures resulting from this technique will lead to a better understanding of the enzymatic mechanisms of the respective enzymes. It will also elucidate the optimization process of the machine learning algorithms mentioned above. I propose to use alpha-fold to predict the fold of these newly designed proteins and I discuss the use of the protein data base as input for the optimization of the surfaces of these proteins for an optimal crystal growth.

Primary author: SCHRADER, Tobias

Presenter: SCHRADER, Tobias

Session Classification: Posters

Track Classification: MLC