DiGiTAL TOTAL

Beitrag ID: **134** Beitragskennung: **85**   Typ: **Poster**

Predicting multiple conformations of flexible proteins

We developed a pipeline for predicting multiple conformations of flexible proteins. A range of conformations is first generated using the deep learning model AlphaFold2 (AF2), which are then filtered using distance constraints and solvent-accessibility data from crosslinking mass spectrometry (XL-MS), using two scoring functions we developed: the crosslink and monolink probability scores (XLP, MP). The scoring functions were first benchmarked on 200 proteins (each with 300 structural decoys) using simulated XL-MS data, before being tested on an experimental test dataset. We showed that AF2 alone can only identify two out of six conformations in the test dataset, while a combination of AF2 and XLP/MP was able to identify four of six conformations, highlighting the complementarity between AF2 and XL-MS.

Find me @ my poster

2,4

Keywords

protein structure prediction
computational modeling

Autor: MANALASTAS-CANTOS, Karen (Center for Data and Computing in Natural Science, Universität Hamburg)

Co-Autoren: Dr. ADONI, Kish (Institute of Structural and Molecular Biology, Division of Biosciences, University College London); Dr. PFEIFER, Matthias (Leibniz-Institut für Virologie (LIV), Centre for Structural Systems Biology (CSSB), Hamburg, Germany); MÄRTENS, Birgit (Leibniz-Institut für Virologie (LIV), Centre for Structural Systems Biology (CSSB), Hamburg, Germany); Prof. GRÜNEWALD, Kay (Leibniz-Institut für Virologie (LIV), Centre for Structural Systems Biology (CSSB), Hamburg, Germany); Prof. THALASSINOS, Konstantinos (Institute of Structural and Molecular Biology, Division of Biosciences, University College London); Prof. TOPF, Maya (Leibniz-Institut für Virologie (LIV), Centre for Structural Systems Biology (CSSB), Hamburg, Germany)