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"Crystallization propensity of protein chains"

Structural genomics is a word-wide initiative aimed at producing a comprehensive mapping of protein structure space. The resulting knowledge of the protein structures will be vitally important for understanding and manipulating their biochemical and cellular functions. One of the main challenges this initiative faces it that only about 2-10% of pursued protein targets yield high-resolution protein structures. A significant bottleneck in acquiring the structures is the ability to obtain diffraction-quality crystals. The application of current protocols yields crystals for approximately 30% of the input proteins and well-diffracting crystals for even a smaller fraction. This motivated the development of models that can be used to either support or directly predict protein crystallization. Several in-silico methods, including SECRET (*Proteins* 62:343-55, 2006), OB-score (*FEBS Lett*. 580:4005-9, 2006), CRYSTALP (*BBRC* 355:764-9, 2007), and ParCrys (*Bioinformatics* 24:901-7, 2008), which predict crystallization propensity using the protein sequence as the input have recently been proposed. These methods account only for intra-molecular factors that are encoded in the protein chain, while ignoring inter-molecular factors such as protein-protein, protein-ligand, and/or protein-precipitant interactions, buffer composition, precipitant diffusion method, gravity, etc. In spite of this significant limitation the above methods were shown to succeed in providing useful predictions. In this talk, we will overview the current state-of-the-art in sequence-based prediction of protein crystallization propensity. We will describe our current findings that support the claim that the crystallization propensity can be predicted directly from the protein chain and we will also introduce our new predictor, CRYSTALP2.