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Protein crystallization by mutational surface engineering

Protein crystallization constitutes a major bottleneck in the high-resolution structural characterization of proteins and their complexes. It is estimated that the probability of obtaining single crystals as a result of screening ranges from less than 1% to 25%, depending on the source and biophysical properties of the target protein or complex. A further complication arises if the crystals lack diffraction quality, impeding high-resolution data collection. Nearly two decades ago we proposed a new approach to protein crystallization based on rational surface engineering to generate surface patches with an enhanced propensity to form crystal contacts. The method relies on the mutational replacement of surface residues with high conformational entropy, such as Lys and Glu/Gln with Ala or other small amino acids. The design of variants with enhanced crystallization propensity is possible using a dedicated server (<http://services.mbi.ucla.edu/SER/>). This methodology, known as Surface Entropy Reduction (SER), has been successfully used in hundreds of studies, not only to obtain crystals of otherwise intractable proteins or complexes, but also to generate new crystal forms with improved diffraction quality allowing to collect X-ray data to much higher resolution than that recorded for the wild-type crystals. In addition, the database of protein crystal structures determined with the help of SER provides interesting insights into the mechanistic aspects of protein crystallization.

Biography

Zygmunt Derewenda obtained PhD and DSc degrees from the University of Lodz in Poland. His Postdoctoral studies were conducted at the University of York, UK. Prior to joining the faculty of the University of Virginia, where he is currently a Harrison Distinguished Professor of Molecular Physiology and Biological Physics, he was an Associate Professor at the University of Alberta in Edmonton, Canada. He has published more than 150 papers on a range of subjects in structural biology, which were cited over 11,000 times (H-factor 58).

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