Special Issue

State-of-the-Art Protein X-Ray Crystallography

Message from the Guest Editors

X-ray crystallography stands as the main technique for detailed protein structural determination. A bottleneck of this procedure is the construction of a protein density map from X-ray diffraction data, the so-called phase problem. A promising avenue to overcome these challenges involves the application of iterative projection algorithms and deep learning methods to direct phasing. This has led to a significant breakthrough in the last decade. Trial calculations utilizing hybrid input–output and difference-map iterative algorithms have demonstrated the feasibility of obtaining high-resolution structures starting from a random electron density. This implies that ab initio phasing, devoid of any model bias, is attainable for a notable fraction of protein crystals. This Special Issue aims to present an overview of the progress made in the field of direct phasing for protein crystals. Contributions from researchers will explore new ground. Through the exchange of ideas, it is hoped that this Special Issue will promote general knowledge and stimulate further growth of this new and important area of research in protein crystallography.

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