OFFICIAL ABSTRACT and CERTIFICATION

Potential Pitfalls in the Protein Structure Determination via Protein Crystallography

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The influx of protein structures added to the PDB is correlated to the decreased level of difficulty to crystallize a protein. Due to this vast volume of structures, there are bound to be issues with the process, as honest errors can be made at every point. The aim of this project was to address the potential pitfalls associated with macromolecular crystallogenesis and structural resolution. Pitfalls can occur at any step along the meticulous process, including during crystallization, during data collection, and during data and model refinement. Throughout the crystallization and analysis of bovine thyroglobulin and human insulin structures, the pitfalls in each step were recorded and discussed. These errors included (1) errors during crystallization, such as using a scaffold and the crystallogenesis of salt, (2) errors during data collection, such as an electron density that doesn ' t match a known structure and (3) errors during data refinement, such as using the wrong sequence to analyze the structure. However, along the way, these pitfalls can be prevented by checking log files along the way and the R free and R factor values in CCP4i. These problems can also be completely circumvented through the use of other structural resolution techniques, such as Small Angle X-Ray Scattering, Cryo EM, and NMR Spectroscopy.

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