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Crystallographic tools towards understanding of macromolecular structure-function relationships

Wladek Minor[1], Przemyslaw Porebski[1], Ivan Shabalin[1], Heping Zheng[1]
[1]*University Of Virginia, Charlottesville, United States*
E-mail: wladek@iwonka.med.virginia.edu

Experimental reproducibility is the cornerstone of scientific research, upon which all progress rests. In contrast to many other areas of biomedical research, macromolecular crystallography has always been at the forefront of 'reproducible research'.

The availability of purified and active protein is the starting point for the majority of in vitro biomedical, biochemical, and drug discovery experiments. The use of overexpressed protein has resulted in great increases of protein production. However, the use of polyhistidine affinity tags, the choice of buffer composition, and contamination of the sample during purification from natural sources may perturb the conformational stability of a protein and/or its activity and may therefore alter the functional characterization and results of the screening methods. In many studies, it is critical to adjust the experimental conditions for each protein or family of proteins, and investigate the influence of these factors on protein activity and structure. Adjustment of experimental conditions can influence the reproducibility and can therefore have a significant "ripple effect" on subsequent studies.

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