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Wladek Minor

University of Virginia, USA

The impact of reproducibility on structure based drug discovery

The drug discovery process depends on the veracity of every decision point on the path from initial experiments to FDA approval, and erroneous data collected along the path can waste valuable time and resources. The presentation will discuss the sources of uncertainty that affect the drug discovery process, focusing on factors that impact structure based drug design the most. The selection of structures used as the basis of computations or data mining will be discussed in detail. All aspects of procedures essential for structural validation and best practices for data management of all experimental steps will be also discussed.

Recent Publications

1. Handing K B, Niedzialkowska E, Shabalin I G, Kuhn M L, Zheng H and Minor W (2018) Characterizing metal-binding sites in proteins with x-ray crystallography. Nature Protocols 13(5):1062-1090.
2. Zheng H, Cooper D R, Porebski P J, Shabalin I G, Handing K B, Minor W (2017) CheckMyMetal: a macromolecular metal-binding validation tool. Acta Crystallographica Section D 73:223-233.
3. Rupp B, Wlodawer A, Minor W, Helliwell J R and Jaskolski M (2016) Correcting the record of structural publications requires joint effort of the community and journal editors. FEBS Journal 283:4452-4457.
4. Grabowski M, Langner K M, Cymborowski M, Porebski P J, Sroka P, Zheng H, Cooper D R, Zimmerman M D, Elsliger M A, Burley S K and Minor W (2016) A public database of macromolecular diffraction experiments. Acta Crystallographica Section D 72:1181-1193.
5. Niedzialkowska E, Gasiorowska O, Handing K B, Majorek K A, Porebski P J, Shabalin I G, Zasadzinska E, Cymborowski M and Minor W (2016) Protein purification and crystallization artifacts: The tale usually not told. Protein Science 25:720-33.

Biography

Wladek Minor is a Harrison Distinguished Professor of Molecular Physiology and Biological Physics at University of Virginia. He is an expert in structural biology and data mining. He is an author of over 190 papers that attracted over 41,000 of citations. His relative citations ratio is above 600. He has trained over 90 scientists that currently pursue career in academia, government and industry.