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Improved Analysis of the Hydrophilic Dimensions of Membrane Proteins from X-ray Crystallographic Data

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Modern life science is inconceivable without radiation studies such as X-ray diffraction or electron microscopy. Radiation research methods have made a particularly significant contribution to structural biology - the study of a variety of biological macromolecules. One important area of structural biology is the study of membrane proteins and their structures.

Membrane proteins (MPs) are key to how cells work and interact with their environment, acting as transporters, receptors, and so on. Getting the structures of membrane proteins is super important and essential for understanding their functions and how they interact with ligands, including drugs. For a long time, X-ray diffraction (XRD) was the most popular method for obtaining the structures of membrane proteins. This method requires the crystallization of membrane proteins. There are two most common methods of MP crystallization: in meso (in lipid cubic phases) and in surfo (in detergent micelles). The problems with these methods are finding the optimal conditions, detergents, and their concentrations for in surfo crystallization and the size of water channels in lipid cubic phases in the in meso method, which imposes restrictions on the size of crystallized proteins.

If the structure of a membrane protein is obtained using X-ray diffraction, the resulting PDB file may contain several proteins or parts thereof in the unit cell. Therefore, when calculating the hydrophilic size from the PDB file, the calculations may be incorrect, if the parts of the neighbors in the unit cell were incorrectly interpreted as a part of the protein under study. We proposed an algorithm for the unambiguous separation of the hydrophilic part of a protein from extraneous elements and more accurate calculation of its size. The resulting algorithm was used to construct a more accurate distribution of the resolution of membrane protein structures depending on the size of the hydrophilic part. The similar distribution we plotted in the previous work [1] showed, without the application of the refinement algorithm, that some proteins crystallized in meso had a hydrophilic size exceeding 100
$mathringA$, which cannot be achieved with the existing methods. This highlights the need for a corrective algorithm for accurate statistical analysis of membrane protein structures.

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1. Zhuravlev S.A. [et al.]. Comparative Analysis of High-Resolution Structures of Membrane Proteins // Biochem. (Mosc.) Suppl. Ser. A Membr. Cell Biol. 2025. V. 19. P. 145-149.

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