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Data Article

Data on diverse roles of helix perturbations in membrane proteins

Ashish Shelar, Manju Bansal *

Molecular Biophysics Unit, Indian Institute of Science, Bangalore 560012, Karnataka, India

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ABSTRACT

The various structural variations observed in TM helices of membrane proteins have been deconstructed into 9 distinct types of helix perturbations. These perturbations are defined by the deviation of TM helices from the predominantly observed linear α-helical conformation, to form 3_{10}- and π-helices, as well as adopting curved and kinked geometries. The data presented here supplements the article 'Helix perturbations in Membrane Proteins Assist in Inter-helical Interactions and Optimal Helix Positioning in the Bilayer' (A. Shelar, M. Bansal, 2016) [1]. This data provides strong evidence for the role of various helix perturbations in influencing backbone torsion angles of helices, mediating inter-helical interactions, oligomer formation and accommodation of hydrophobic residues within the bilayer. The methodology used for creation of various datasets of membrane protein families (Sodium/Calcium exchanger and Heme Copper Oxidase) has also been mentioned.

Specifications Table

Subject area	*Biology*
More specific subject area	*Membrane protein structure and folding, Bioinformatics*

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* Corresponding author.
E-mail address: mb@mbu.iisc.ernet.in (M. Bansal).

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Type of data	*Tables and figures*
How data was acquired	*Data was retrieved from public databases*
Data format	*Analyzed data*
Experimental factors	*Protein structures were retrieved from OPM database and analyzed. Sequence and structural alignments of proteins were performed using Clustal Ω and MAPSCI respectively*
Experimental features	*This work uses X-ray crystal structure data of membrane proteins that has been deposited in the Protein Data Bank (PDB)*
Data source location	*Bangalore, India*
Data accessibility	*Data is within this article. Membrane protein structures aligned along the Z-axis can be readily retrieved from the OPM database* (http://opm.phar.umich.edu/download.php).

Value of the data

- The data on different types of helices shows that, apart from the commonly observed α-helices, 3_{10} and π-helices are also present within the bilayer and have varying lengths as well as distinct sequence signatures. This data provides experimentalists with options to model new 3_{10}- and π-helices in the bilayer and reorient the locations of active sites in TM helices.
- The data on backbone torsion angle variation in perturbed helices indicates that in these regions the disrupted hydrogen bonds lead to free NH– and C=O groups that mediate inter-helical interactions. This information can be used by the scientific community to engineer the desired inter-helical interactions at appropriate locations in TM helices.
- The data showing conservation of a kink in proteins from the Sodium/Calcium exchanger family highlight its crucial functional role in this family. This data can be used for homology modeling of proteins within this family by computational biologists.

1. Data

The data used in this analysis has been generated after a detailed structural examination of membrane proteins. This structural data provides solid evidence for the utility and various roles of perturbed helices in membrane proteins. See Figs. 1–17 and Tables 1–5.

2. Experimental design, materials and methods

Structural analysis of membrane protein structures was performed after they were downloaded from the Orientation of Proteins in Membrane (OPM) database [9]. The identification of secondary structures was carried out using Assignment of Secondary Structures in Proteins (ASSP) [10] and non-bonded interactions were identified using MolBridge [11]. Next, we identified geometries of helical fragments using Helanal-Plus [2] and computed the backbone torsion angles (φ–ψ). Multiple sequence alignment of protein sequences was carried out using ClustalΩ [12].

We prepared datasets of proteins belonging to Sodium Calcium family of transporters as mentioned in [1] to examine conservation of kinks in functionally important helices. A dataset of proteins belonging to Heme Copper Oxidase (HCO) superfamily was created to gain insights about the presence of the π-helix in each protein (Table 3). To understand the variation if any in the π-helix within different types of HCOs, we analyzed two crystal structures from the A-type, one from B-type and