Biopolymers Research

Letter To Editor Open Access

Protein Structure: dynamics and conformational ensembles

Zaidul Islam Sarker*

Department of Pharmaceutical Technology, International Islamic University Malaysia, Bangladesh

Letter To Editor

Protein Structure

Protein structure is the three-dimensional arrangement of tittles in an amino acid- chain patch. Proteins are polymers- specifically polypeptides- formed from sequences of amino acids, the monomers of the polymer. A single amino acid monomer may also be called a residue indicating a repeating unit of a polymer. Proteins form by amino acids witnessing condensation responses, in which the amino acids lose one water patch per response in order to attach to one another with a peptide bond [1]. By convention, a chain under 30 amino acids is frequently linked as a peptide, rather than a protein. To be suitable to perform their natural function, proteins fold into one or further specific spatial conformations driven by a number of non-covalent relations similar as hydrogen cling, ionic relations, Van der Waals forces, and hydrophobic quilting. To understand the functions of proteins at a molecular position, it's frequently necessary to determine their three-dimensional structure. This is the content of the scientific field of structural biology, which employs ways similar as X-ray crystallography, NMR spectroscopy, cryo electron microscopy (cryo-EM) and binary polarisation interferometry to determine the structure of proteins.

Protein dynamics and conformational ensembles

Proteins are not static objects, but rather populate ensembles of conformational states. Transitions between these states typically occur on nanoscales, and have been linked to functionally relevant phenomena such as allosteric signaling and enzyme catalysis [2]. Protein dynamics and conformational changes allow proteins to function as nanoscale biological machines within cells, often in the form of multi-protein complexes Examples include motor proteins, such as myosin, which is responsible for muscle contraction, kinesin, which moves cargo inside cells away from the nucleus along microtubules, and dynein, which moves cargo inside cells towards the nucleus and produces the axonemal beating of motile cilia and flagella. "In effect, the [motile cilium] is a nano machine composed of perhaps over 600 proteins in molecular complexes, many of which also function independently as nano machines. Flexible linkers allow the mobile protein domains connected by them to recruit their binding partners and induce long-range allostery via protein domain dynamics. "

Proteins are often thought of as relatively stable tertiary structures that experience conformational changes after being affected by interactions with other proteins or as a part of enzymatic activity [3]. However, proteins may have varying degrees of stability, and some of the less stable variants are intrinsically disordered proteins. These proteins exist and function in a relatively 'disordered' state lacking a stable tertiary structure. As a result, they are difficult to describe by a single fixed tertiary structure. Conformational ensembles have been devised as a way to provide a more accurate and 'dynamic' representation of the conformational state of intrinsically disordered proteins.

Protein ensemble files are a representation of a protein that can be considered to have a flexible structure. Creating these files requires determining which of the various theoretically possible protein conformations actually exist. One approach is to apply computational algorithms to the protein data in order to try to determine the most likely set of conformations for an ensemble file [4]. There are multiple methods for preparing data for the Protein Ensemble Database that fall into two general methodologies – pool and molecular dynamics (MD) approaches. The pool based approach uses the protein's amino acid sequence to create a massive pool of random conformations. This pool is then subjected to more computational processing that creates a set of theoretical parameters for each conformation based on the structure. Conformational subsets from this pool whose average theoretical parameters closely match known experimental data for this protein are selected. The alternative molecular dynamics approach takes multiple random conformations at a time and subjects all of them to experimental data. Here the experimental data is serving as limitations to be placed on the conformations (e.g. known distances between atoms). Only conformations that manage to remain within the limits set by the experimental data are accepted [5]. This approach often applies large amounts of experimental data to the conformations which is a very computationally demanding task.

The conformational ensembles were generated for a number of highly dynamic and partially unfolded proteins, such as Sic1/Cdc4, p15 PAF, MKK7, Beta-synuclein and P27

Acknowledgement

I would like to thank my Professor for his support and encouragement.

Conflict of Interest

The authors declare that they are no conflict of interest.

References

1. Hodge EA, Benhaim MA, Lee KK (2020) Bridging protein structure, dynamics, and function using hydrogen/deuterium-exchange mass spectrometry. Protein Sci 29:843-855.

2. Nakagawa H, Kataoka M (2020) Rigidity of protein structure revealed by incoherent neutron scattering .Biochim Biophys Acta Gen Subj 1864:129536-129539.

3. Benhaim M, Lee KK, Guttman M (2019) Tracking Higher Order Protein Structure by Hydrogen-Deuterium Exchange Mass Spectrometry. Protein Pept Lett 26:16-26.

***Corresponding author:** Zaidul Islam Sarker, Department of Pharmaceutical Technology, International Islamic University Malaysia, Bangladesh, E-mail: Zaidul@gmail.com

Received: 1-Apr-2022, Manuscript No bsh-22-60143, **Editor assigned:** 4-Apr -2022, Pre QC No bsh-22-60143 (PQ), **Reviewed:** 8-Apr-2022, QC No: bsh-22-60143, **Revised:** 13-Apr-2022, Manuscript No: bsh-22-60143 (R), **Published:** 20-Apr-2022, DOI: 10.4172/bsh.1000111

Citation: Sarker ZI (2022) Protein Structure: dynamics and conformational ensembles. Biopolymers Res 6: 111.

4. Alam FF, Shehu A (2021) Unsupervised multi-instance learning for protein structure determination. J Bioinform Comput Biol 19:2140002-2140005.

5. Tuncbag N, Gursoy A, Keskin O (2011) Prediction of protein-protein interactions: unifying evolution and structure at protein interfaces. Phys Biol 8:035006-035008.