G.N. Ramachandran's contribution to crystallography

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Some interesting facts about proteins beyond conventional wisdom

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Abstract:

The talk will focus on some universalities in protein structures identified in our lab. which are yet to be captured in text books. These include the margin of life, the hyper Ramachandran maps - a precursor to alphafold, the new chemical logic of amino acids and so on.

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Enabling the responsible sharing of BIOLOGICAL DATA: Indian Framework

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Abstract:

The exchange of biological data fosters transparency, reproducibility, and accountability in research, improving the overall quality and trustworthiness of scientific results. Acknowledging the importance of data-sharing and exchange, the Biotech-PRIDE (Promotion of Research and Innovation through Data Exchange) Guidelines were issued by the Government in July 2021. Biotech-PRIDE Guidelines were established to promote and support the sharing and dissemination of biological knowledge, information, and data produced from research conducted domestically, particularly regarding high-throughput and high-volume data. These guidelines establish a facilitative process for sharing and exchanging information and knowledge produced/generated/submitted by the Data Producer/Generator/Submitter in accordance with applicable existing laws, rules, regulations, and guidelines of the Government of India (GoI).

Following the extensive Expert and Inter-ministerial deliberations, the Government released the "Framework for Exchange of Data (FeED) Protocols, 2025" for implementation of the Biotech-PRIDE Guidelines. These protocols describe the methods for collecting and distributing biological data, considering data privacy, security, and appropriate attribution. Adhering to these standardized protocols enables researchers to enhance the smooth exchange of biological data, foster scientific discoveries, and expedite advancements in diverse areas of biosciences. The FeED Protocols establish guidelines for researchers, institutions, and policymakers to emphasize ethical data sharing practices, achieving a balance between transparency and data security to maintain the integrity and longevity of data-driven research initiatives. The Biotech-PRIDE Guidelines and the FeEd Protocols collectively provide a foundational framework that boosts data sharing, increases efficiency, and promotes innovation throughout different areas of Biological Sciences.

Effectiveness of Machine Learned Collective Variable Projection in Bio-molecular Energy Landscapes

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Abstract:

Capturing biomolecular behaviour with physical-based simulation is beset with several challenges, primary amongst which are delineation of the most important degrees of freedom (DOF) of many-body system. Simplistic collective variables (CVs), while physically intuitive, may not be orthogonal, and moreover, may not capture the essential bio-physical dynamics. Part amelioration of this problem has been achieved by leveraging the latent space of artificial neural networks (ANNs), though these methods challenge physical interpretability. Our recent efforts towards capturing the essential DOFs in bio-molecular simulations will be presented in this seminar. Our work, incorporating dihedral principal component analysis (dPCA), structural biology based efforts coupled with statistical correlations, as well as latent space elucidation, has been applied to a range of bio-molecules, including an intrinsically disordered protein (IDP), the Abelson Tyrosine Kinase (Abl), and fragments of bacteriorhodopsin (bR) embedded in a biological membrane bilayer. Further integrative efforts on the way will be discussed.

Reference:

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Towards AI Bacteria

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Abstract:

Performing cellular computations with engineered bacteria has enormous importance in biocomputer technology development at the micron scale, where microprocessor-based computers have limitations due to energy, cost, and technological constraints. Here, we designed and built artificial neural networks with genetically engineered bacteria that can identify prime numbers, vowels, and even determine the maximum number of pieces of pizza or pie that can be obtained from a given number of straight cuts. In addition, the 'intelligent' bacteria can answer mathematical questions such as whether a number n's factorial is divisible by $n \times (n + 1)/2$ OR whether a number n's square can be expressed as the sum of three factorials. All those problems are classic abstract computational problems and are solved by a computer by writing codes in Python or C. Introducing such abstract computational capability in living cells, will be a step forward in biocomputer technology development and may help understanding the biochemical nature of 'intelligence'.

Structural Bioinformatics of RNA

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Abstract:

It has been observed that about 97% of the RNA present within cell are not the common messenger RNA (mRNA). While mRNA are short-lived and generally unstructured the other forms of RNA adopt stable three-dimensional structures to perform various catalytic and regulatory roles. Over sixteen thousand three-dimensional structures of RNA, determined by different experimental methods, are now available in public domain, which can be analyzed for obtaining information about them to eventually predict structure and function of an unknown RNA. We have looked at different features like base pairing, stacking between base pairs, double helix formation, etc. on these available structures. Huge number of base pairs have been found in these RNA structures which are not canonical Watson-Crick type and are called non-canonical base pairs. We have analyzed these from all aspects to confirm their importance in structure formation as well as molecular recognition. The lecture would concentrate on these aspects of RNA structures.

Phytochemicals as polypharmacological compounds in AD therapeutics

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Abstract:

Alzheimer's disease (AD) is characterized by extracellular plaques consisting of aggregated amyloid beta peptide (Aβ), and intracellular tangles composed of the hyperphosphorylated tau protein. Due to the multifactorial nature of the disease, the exact cause of the disease still remains elusive. The "one disease–one target–one drug" approach for diseases with complex etiology is largely symptom-based and not mechanism-based. Interaction of a molecule with multiple targets in the network results in its cumulative efficacy at all individual targets thus achieving synergy and dose reduction. This concept of a molecule interacting with two or more targets simultaneously, termed polypharmacology, is being adopted as a ground plan for efficient drug development in recent years, especially in multifaceted neurodegenerative diseases.

According to the amyloid cascade hypothesis, accumulation of aggregated Aβ peptide leads to neurotoxicity and eventually to neuronal death. Production of Aβ occurs by the sequential proteolysis of amyloid precursor protein, by β-secretase (BACE1) followed by γ-secretase. BACE1 and aggregated Aβ therefore have been prominent therapeutic targets although no effective drug has been discovered yet. We aimed to identify compounds with activity for both BACE1 inhibition and anti-amyloidogenic properties. 105 flavonoids and 75 flavonoid derivatives were predicted as potent BACE1 inhibitors using two different approaches - a BACE1-QSAR model for the flavonoids and docking followed by pharmacophore modelling for the flavonoid derivatives. Subsequently, BACE1 activity, Thioflavin-T and Aβ-GFP assays led to the identification of four compounds - genistein, syringetin, tamarixetin, and ZINC53276039 as dual inhibitors with activities that could be effective in reducing the amyloid load in brains of patients suffering from the disease. Another QSAR model to predict the antioxidant property of the compounds was also implemented and further tested *in vitro* since oxidative stress is widely accepted to play a critical role in the pathogenesis of Alzheimer's disease. Adoption of multiple strategies for the prediction of regulation of multiple targets resulted in the identification of potent multi-target-directed ligands (MTDLs) that could be implicated in AD therapeutics.