

# THANK YOU EVERYONE FOR YOUR PARTICIPATION!



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SERIES 92  
&  
CMBRI Seminar Series FY2024-02  
Dr. Arjun Ray  
2024-06-17

## Series – 92

Date & Time : 17 June 2024 (15:30 JST | 12:00 IST)

Venue : Zoom

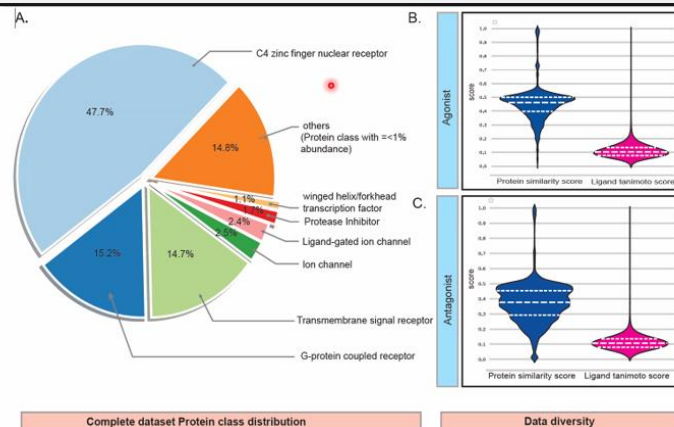
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## Peering inside the unexplored world of protein cavities

Internal cavities in proteins are of critical functional importance. They can serve as ligand-binding sites, paths for movement of biomolecules and even mediate domain conformations occurring during structural transitions. Yet, there is a paucity of computational tools that can accurately characterize these inner cavities of the proteins. We have developed a method, CICLOP, that can identify these regions at an atomistic resolution. CICLOP builds on a novel algorithm that imparts it unprecedented accuracy, and reproducibility, allowing it to outperform its predecessors. It can detect all internal cavities, including channels, pores and voids. The method can detect residues lining the inner cavity, the diameter/volume occupied by the cavity, physico-chemical properties and conservation scores of residues lining the cavity, allowing for a thorough functional characterization of the cavity. We showcase the usage and practicality of these analytical modules for biological inferences. We also demonstrate the accuracy, precision, and sensitivity of our method through in-silico validation. Lastly, the talk shall highlight how utilizing machine learning techniques along with shape descriptors can unravel a wondrous world of protein engineering.



## > 35 participants

