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BioSim Talk #6

Thibault Tubiana, PhD.

Postdoctoral Researcher,
Institute for Integrative Biology of the Cell (I2BC),
CEA/CNRS & Université Paris-Saclay, France

September 27th 2024 (Fri)
4.30 – 6.00 pm
Institute for Protein Research
Osaka U. (Suita Campus)
2nd floor conference room (#202)

Deciphering viral protein-protein interactions using AlphaFold

AlphaFold (AF) has shown remarkable proficiency in forecasting the interactions between different proteins. However, the AF database is lacking in viral proteins. By augmenting the database independently, we have recently used AF to study the domain decomposition and structural organization of Hepatitis E ORF1p protein (Fieulaine et al. 2023). Since then, we have extended our research to investigate the interactions between the HepE capsid protein (ORF2i) and various cellular partners. We have employed a methodical "Top-Down" approach in our modelling. This process starts with the modelling of entire systems to pinpoint potential interactions. After identifying these interactions, we refine our models to concentrate on key areas where these interactions occur. Thus, we were able to identify a potential novel dimerization area in the HepC NS5A protein. This discovery was further studied and validated through MD simulations and experiments including Isothermal Titration Calorimetry (ITC), differential scanning fluorimetry (nanoDSF) and nuclear magnetic resonance (NMR).

Link for online participation via Zoom:
Meeting ID: 892 1891 3516
Passcode: 657022
Please inform us if you will be participating online or joining our slack
sandhyatiwari@protein.osaka-u.ac.jp, shinobu.ai.prime@osaka-u.ac.jp