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BioSim Talk #7

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4.00 – 5.30 pm

Institute for Protein Research
Osaka U. (Suita Campus)
4th floor conference room

Studying Viral–Host Protein Interactions with AlphaFold and Molecular Dynamics

AlphaFold offers powerful tools for predicting protein complexes, but distinguishing plausible interactions from prediction artefacts remains challenging. We developed a top-down modelling pipeline that combines repeated AlphaFold predictions, systematic assessment of confidence metrics (pLDDT and PAE), and targeted refinement of candidate binding regions. We further assess selected models using molecular dynamics simulations to examine interface stability.

We illustrate this approach with two hepatitis E virus (HEV) proteins. For the capsid protein ORF2i, we identified an interface with human integrin $\beta 1$, which experiments later supported (Fu et al., 2025). For the largely disordered ORF3 protein, initially poor predictions improved substantially when modelling focused on a candidate interaction site with a human host protein.

These examples show how iterative modelling can reveal candidate interfaces missed by initial full-length predictions and help prioritize viral–host interactions for experimental investigation.

Link/QR code for online participation via Zoom:

Meeting ID: 872 6700 2213

Passcode: 431824

Please inform us if you will be participating online or joining our Slack channel

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