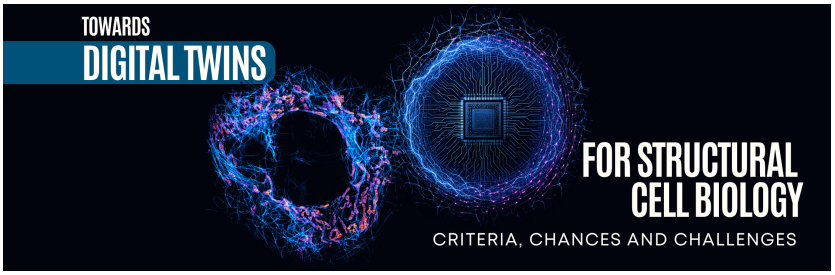

Contribution ID: **62** Type: **not specified**

Understanding STIM1 by combining advanced simulations and experiments

We used the AI for Molecular Mechanism Discovery to simulate and understand the activation cascade of the Ca(2+)-sensing stromal interaction molecule 1 (STIM1) dimer. The detailed atomistic insight into the dimerization pathways enabled us to shed light on the experimentally observed changes in dimerization propensities for four different mutants and to reconcile previous experimental results. This work highlights the potential of combining advanced simulations with experimental measurements to further our understanding of biomolecular processes.

Presenter: Dr JUNG, Hendrik (Goethe University Frankfurt)

Session Classification: POSTER SESSION