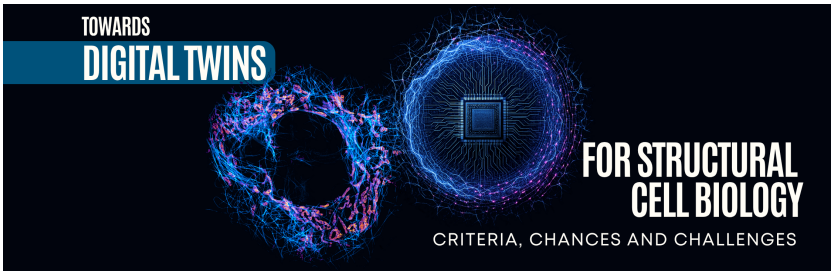

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In Situ and In Silico Structure and Dynamics of a C. elegans Stomatin–Gap Junction Complex

Here, we investigate Caenorhabditis elegans gap junctions (GJs) using an integrative approach combining electron cryo-tomography and molecular dynamics (MD) simulations. Cryo-tomographic analysis of primary embryonic cells revealed hexagonally packed arrays of GJs at cell–cell junctions. Notably, we identified a previously uncharacterized cap-like cytosolic density occluding the channel pore. We propose that this density corresponds to a multimeric assembly of the stomatin protein UNC-1, which is known to interact with the innexin UNC-9. To test this hypothesis, we generated AlphaFold 3 models of multimeric UNC-1 and compared them with experimentally observed GFP-tagged UNC-1 assemblies. Coarse-grained MD simulations were used to probe the stability, conformational dynamics, and lipid interactions of the proposed UNC-1 cap complex. In addition, atomistic MD simulations of palmitoylated UNC-1 dimers demonstrate a stabilizing role for palmitoyl anchors in mediating membrane association and positioning relative to the gap junction pore. Together, our results suggest a structural and dynamic basis for stomatin-mediated regulation of gap junctions and illustrate how the integration of in situ structural data with multiscale simulations can elucidate complex regulatory mechanisms in membrane protein assemblies.

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