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Protein interaction modeling

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We use this protocol and it's working

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Abstract

Protein interaction modeling using Alphafold 2.0 Multimer

1 **Structure Prediction in AlphaFold 2.0 Multimer** - Use full-length mouse Ezrin (UniProt ID: Q4KML7) and Atg7 (UniProt ID: Q9D906) for structure prediction. - Predict the structure of Ezrin in the open conformation: - Independently predict Ezrin N- and C-termini. - Thread them onto an open ERM hinge structure using PyMOL2 molecular visualization software.

2 **Modeling Ezrin:Atg7 Interaction** - Predict the structures of Ezrin and the Atg7 homodimer using AlphaFold 2.0 Multimer. - Dock the predicted structures to model the Ezrin:Atg7 interaction and associated conformational changes.

3 **Assess Conformational Changes** - Use CABS-flex 2.0 (REF: https://doi.org/10.1093/nar/gky356) and PyMOL2 to assess conformational changes in the Ezrin:Atg7 protein complex.

4 **Select High-Confidence Structures** - For all predicted structure models, select the highest-confidence structures based on the predicted local distance difference test (pLDDT).

5 **Energy Minimization** - Subject the highest-confidence structures to energy minimization via AMBER relaxation.

6 **Import and Visualize Minimized Structures** - Import the minimized structures into PyMOL2. - Use PyMOL2 to produce representative models of the structures.