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Protein localization and folding mechanisms revealed by molecular dynamics simulations

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<p>Many nascent proteins, including nearly all membrane and secreted proteins, must traverse a membrane-bound protein-conducting channel prior to their full maturation. This channel, the Sec translocon, is found in all domains of life and possesses the novel ability to direct nascent proteins to the membrane or to the extracellular space, depending on their sequences, often concomitant with their synthesis by the ribosome. By combining atomic structures with cryo-electron microscopy data using the molecular dynamics flexible fitting method, we have developed some of the first views of inactive and active translocons in complex with the ribosome. These views reveal a conserved mode of interaction between translocon and ribosome as well as the roles of specific elements of both in protein localization. We also carried out two-dimensional potential-of-mean-force calculations to explore the structure of the nascent peptide within the translocon environment. The calculations revealed that the translocon exerts a small bias on the peptide towards a helical state. This bias can serve to facilitate, e.g., the insertion of nascent membrane proteins into the otherwise inhospitable lipid bilayer.

Level (Hons, MSc,
   PhD, other)?

PhD

Consider for a student
   award (Yes / No)?

no

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

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