VABILO NA INŠITUTSKO PREDAVANJE / INVITATION TO THE INSTITUTE LECTURE

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Tracking conformational change in membrane proteins: Monte Carlo normal mode following

Important features of the slow conformational changes in protein structure that govern the functioning of pumps, channels and other enzymes can be reliably studied by coupling theory with high-resolution atomic level structures. New methods for tracking proteins’ low frequency deformational modes are applied to provide insight into structural change in channels and transporters. Details of gating transitions for two ion channels, gramicidin and KcsA, are elucidated. In both the lowest frequency normal mode (NM) is the crucial mode that initiates transition between open and closed states. Tracking these NMs reveals their gating mechanism. Gramicidin dissociates via relative opposed monomer rotation and simultaneous lateral displacement. WT KcsA does not open. When its cytoplasmic glutamates are protonated KcsA opens via a complex set of motions initiated near the smoke hole of the “tepee” and propagating to the “glycine hinge,” ultimately adopting a structure reminiscent of MthK. In both systems NM structure changes as the system evolves; the gating mechanisms are not simple, exhibiting complex backbone realignments and side chain reorganizations. Preliminary analysis of the leucine transporter and lactose permease suggest similar qualitative features: conformational change involves complex global rearrangements.

References

Vljudno vabljeni! / Kindly invited!

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