INTERNATIONAL INSTITUTE OF INFORMATION TECHNOLOGY
HYDERABAD

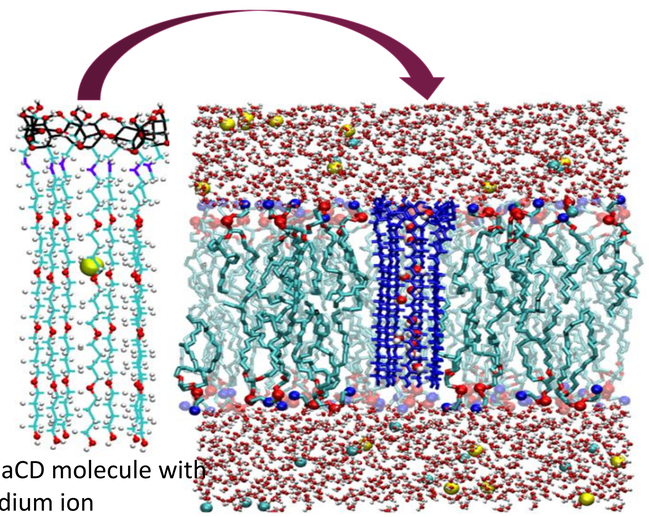
R&D SHOWCASE 2021

Modeling Ion Permeation Activity in Cyclodextrin Based Synthetic Ion Channels

ABSTRACTS

The natural channels possess controllable ion transportation ability. The gating caused by the stimulus from the environment, like, membrane potential, mechanical force, and chemical signals. The anion/cation selectivity is a critical property of ion channels and underpins their physiological function. Modelling of artificial ion channels may improve our understanding of natural ion channels. This open up possible applications in materials and biological sciences. The properties like high thermal or chemical stability, mechanical stability, high aspect ratio, high flexibility, of synthetic ion channel can lead to use in place of natural ion channel. Moreover, the congenital or acquired channelopathic diseases can be treated by synthetic ion channels. This study focuses on the ion passage through the synthetic cyclodextrin based ion channels which are considered ideal candidates for molecular tubes because of their diameter being closer to natural ion channels.

SYSTEMS

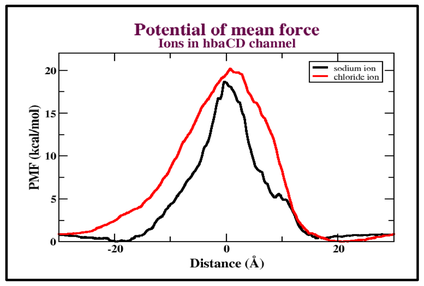


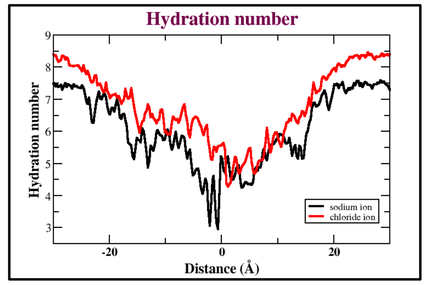
hbaCD molecule with sodium ion

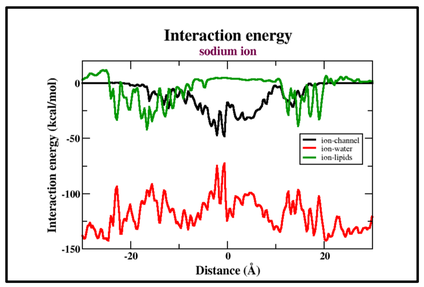
OBJECTIVE

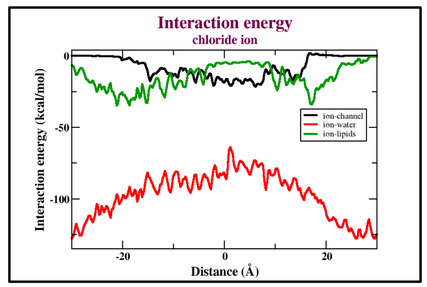
- hbaCD channel compatibility in the membrane
- Study ion permeation and ion selectivity of hbaCD channel using molecular dynamics free energy calculations

RESULTS



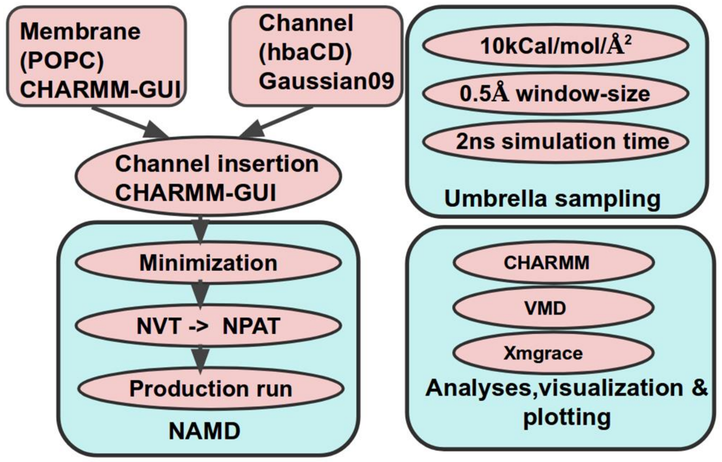






- The space in the channel is well covered by umbrella sampling (figure not shown)
  The magnitude energy barrier for both the ions is almost same
- Both ions experiences the unfavourable conditions as they enter from side of the channel
- Lowering the hydration number in the middle of the channel depicts the partial dewetting of the ions
- Ions are only interacting with the channel in the middle region
- Hydrophilic head groups of lipid bilayer trying interact with the ions where the hydrophobic tail part doesn't show favourability

METHODS



INFERENCES

- The hydrophobicity of a pore contributes to the dewetting effect
- Favourable movements of ion found near terminals of the channel
- Increasing simulation period makes water passage through middle of the channel by losing ion-channel interaction
- Hydration number reduction at the middle of the channel indicates the partial dehydration of the sodium ion
- Well sampling distribution of the channel

FUTURE PLAN

- To see the selectivity among the anions, planning to transport the halide anions through the channel

REFERENCES

1. Madhavan, Nandita, Erin C. Robert, and Mary S. Gin. "A Highly Active Anion-Selective Aminocyclodextrin Ion Channel." *Angewandte Chemie International Edition* 44.46 (2005): 7584-7587.
2. Madhavan, Nandita, and Mary S. Gin. "Increasing pH Causes Faster Anion-and Cation-Transport Rates through a Synthetic Ion Channel." *ChemBioChem* 8.15 (2007): 1834-1840.

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