

## Interactions between Artificial Channel Protein, Water Molecules, and Ions Based on Theoretical Approaches

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### Streszczenie

Contemporary techniques of molecular modeling allow for rational design of several specific classes of artificial proteins. Transmembrane channels are among these classes. A recent successful synthesis of self-assembling, highly symmetrical 12- or 16-helix channels by David Baker's group prompted us to study interactions between one of these proteins, TMHC6, and low-molecular-weight components of the environment: water molecules and ions. To examine protein stability in a polar environment, molecular dynamics (MD) with classical force fields of the AMBER family was employed. Further characteristics of the chosen interactions were obtained using interaction energy calculations with usage of partially polarizable GFN-FF force field of Spicher and Grimme, symmetry-adapted perturbation theory (SAPT) and atoms in molecules (AIM) approaches for models of residues from the channel entry, crucial for interactions with water molecules and ions. The comparison of the interaction energy values between the gas phase and solvent reaction field gives the quantitative estimation of the strength of the interactions. The energy decomposition via the SAPT method showed that the electrostatics forces play a dominant role in the substructure stabilization. An application of the AIM theory enabled a description of the intermolecular hydrogen bonds and other noncovalent interactions.

### Słowa kluczowe

artificial channel protein, channel transport, hydrogen bond, molecular dynamics, interaction energy, SAPT

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