



Computer Simulation on Membrane Receptors

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Message from the Guest Editor

Cellular membranes contain membrane receptors which mediate signal transduction for cellular responses to extracellular stimuli. These receptors are transmembrane proteins, and are classified by structure and related function. They are associated with G-proteins, ion channels, and tyrosin–chinase receptors. The domain of the receptor exposed to the external medium often has a binding site for a ligand. The domain exposed to the cytoplasm activates intracellular proteins such as kinases, G-proteins, guanylate cyclase, ion transporters, among a myriad of other functions.

In this Special Issue, we want to focus on various types of simulation aimed at elucidating the structure and the function of these receptors. In addition, studies related to a rational drug design approach with a membrane receptor as target are welcome.

Potential topics include, without being limited to, the following:

- Molecular dynamics simulation of ion channels
- Computer aided drug design targeted at membrane receptors
- Ligand–receptor dynamics
- Function and structure of membrane receptors
- Coarse grained molecular dynamics of receptor association and oligomerization





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