



سمینار هفتگی ماده چگال نرم

Elucidating the Roles of Interleukin I Receptor type II (IL-1RII) in the Regulation of Human Immune System, Atomistic Molecular Dynamics simulations

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Abstract

Interleukin 1 family of cytokines has critical roles in human immunoregulation and inflammation. They play their roles by binding to their specific receptors on the cell. Interleukin 1 Receptor Type II (IL-1RII) is a decoy receptor of the Interleukin 1 Receptors (IL-1Rs) family. IL-1RII is a ligand-binding receptor. It is homologous to the signaling Interleukin 1 Receptor Type I (IL1RI). Both receptors are able to bind the same cytokines and the same accessory protein. Due to the lack of intracellular Toll Interleukin Receptor (TIR) domain, the IL-1RII is not able to signal and suppress the downstream pathways. IL-1RII is glycosylated in-vivo. Glycosylation has shown to affect the dynamics and ligand binding of receptors. The detailed mechanism of IL-1RII functioning in the presence of glycan at the molecular scales was not clear. In this project all-atom Molecular Dynamic simulations (MD) were carried out to study the dynamics of glycosylated IL-1RII. The results showed that the IL-1RII exists in two states of "extended" and "compact" conformations. IL-1RII seems to be more stable in the extended conformation upon glycosylation. Also, it is necessary for IL-1RII to bind to its ligand to maintain its stable shape on the cell surface. Finally, the competitive reactions between IL-1RI and IL-1RII at the chemical equilibrium condition were compared and it showed that when both systems are glycosylated, the IL-1RII has more chance to bind to the same cytokines. Therefore, a reduction of the immune response is expected as a result.

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مکان (کلاس مجازی آقای دکتر اجتهادی):

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