سمینار هفتگي ماده چگال نرم

عنوان سمینار

GAG Positioning on IL-1RI; a Mechanism Regulated by Dual Effects of Surface Charge and Glycosylation

ارائه دهنده

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چکیده

Interleukin 1 family of cytokines are the key players in establishing inflammatory and immune responses. Among the 11 known family members, interleukin 1β (IL-1β) is involved in the chronic inflammatory and autoimmune conditions. Thus, inhibition of IL-1β is of great pharmacological importance. IL-1β activates its target cells by binding to the glycosylated IL-1 transmembrane receptor type I (IL-1RI) with high affinity. Previous biochemical studies have suggested that upon the immune responses, IL-1β is retained on the target cells by interacting with the glycosaminoglycans of the extracellular matrix (GAGs). Herein, molecular dynamics simulations of the glycosylated and unglycosylated IL-1RI have shown that the receptor adopts two conformational states of "Extended" and "Rotated" in its dynamical pattern. Furthermore, it was shown that glycosylation plays a crucial role in the binding mechanism of the GAG to IL-1RI by increasing solvent exposure of the positively charged residues in the receptor that facilitates positing of the GAG in its binding site.

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