

عنوان مقاله:

Binding Mechanism of Glycosaminoglycans to Glycosylated Interleukin 1 Receptor Type I

محل انتشار:

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خلاصه مقاله:

Interleukin 1 family of cytokines are the key players in establishing inflammatory and immune responses [1]. Among the 11 known family members, interleukin 1β (IL-1β) is involved in the chronic inflammatory and autoimmune conditions [1, 2]. Thus, inhibition of IL-1β is of great pharmacological importance [3]. IL-1β activates its target cells by binding to the glycosylated IL-1 transmembrane receptor type I (IL-1RI) with high affinity [4]. Previous biochemical studies have suggested that upon the immune responses, IL-1ß is retained on the target cells by interacting with the glycosaminoglycans of the extracellular matrix (GAGs) [5]. 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

کلمات کلیدی:

Interleukin 1β, Interleukin 1 Receptor Type I, Glycosaminoglycans, Glycosylation, Molecular Dynamics simulation

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