Calculating Binding Free Energies of Variants of hIFN-γ and their Extracellular Receptor

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Cytokines play an important role in cellular communication and in modulation of the cellular immune responses. A computational protocol is presented that allows the prediction and analysis of the effect of particular mutations in the cytokine molecules on the interactions with their receptors. It is based on the theory developed by B. Jayaram and D. L. Beverige [1] and relies on collecting statistical data from molecular dynamics simulations. The protocol was first tested on a native cytokine receptor complexes against experimental data such as association/dissociation constants or binding free energies on a particular cytokine receptor system, namely the human interferon gamma (hIFNγ) human interferon gamma receptor (hIFNγR) complex.

References

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