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Thermodynamics of Ligand – Receptor Interaction

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Biomolecules! The associations between them, is a variable, upon which are the structure and functions of living cells critically dependent. For the last few decades, researchers have been working on the dramatic advancement of understanding the non-covalent interactions of macromolecules and its role in the biological systems. Ligand-receptor interactions have become one of the most exciting and innovative research subjects in the most recent years.

Receptors are referred to as the "molecular machinery" in which the ligand binds to activate or deactivate the machinery. The relationship between thermodynamics and kinetics of binding depends on the strength of binding and is related to the kinetics of ligand-receptor association and dissociation: how fast the ligand binds and how fast it dissociates [1].

Using X-ray and NMR techniques, which are important tools in explaining the molecular architecture, researchers have understood the ligand-receptor system which is of crucial importance for understanding how the ligand–protein or protein–protein interaction functions in the molecular machinery [2]. Moreover, simulation studies and various other techniques like atomic force microscopy, transducers, and biomembrane probes are also involved in analyzing and obtaining experimental information of ligand-receptor interactions [3].

The main advances achieved in ligand-receptor interactions are the recent years are:

i)Structure-function relationship, involving the ligand-receptor complexes (interactions through equilibrium and kinetic constants, location of the atoms and solvent molecules and the conformation of free and bound molecules.

ii)Dynamic experimental methods producing quantitative information of biomolecules and its interaction with the bonds. The use of site directed mutagenesis to analyze the effectiveness of binding affinity and specificity of amino acids to protein receptors.

iii)Computer simulation approach to analyze the study interactions of macromolecules in aqueous nature [4].

Furthermore, the future developments and applications expected in ligand-receptor interactions are improved quantitative models for analysis of bond life, strength and kinetic association, and the behavior of adhesion receptors [5]. Advanced computer simulation procedures need to be developed with adequate prediction properties for drug designing, mimicking intermolecular forces. Use of algorithms to estimate interaction energies for estimation of bond lifetime and binding forces should involve stringent tests for analyzing the validity of the ligand-receptor interactions [6]. Analytical formulas for determining the association and dissociation of ligand-receptor is of great importance as its very significant in testing the reliability of computational methods, decreasing the computational load and thereby increasing the wide range of applications of simulation procedures [7]. Lastly, and most importantly, the approximate analytical formulas can be used for better understanding the significance of numerical data.

As researchers we should try to develop advanced techniques and applications like cell function analysis, computer simulation processes to exploit it for improved rational drug design. Our future research and studies may be hoped that the continuous lines of research will lead us to this goal in the near future.

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