Molecular Design oF New Drug

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Over the past decade molecular design using computer modeling technique has provided a powerful tool in the process of discovering new and more effective therapeutic drugs. In order to design a new drug, it is necessary to understand the interaction between enzymes or receptors and ligands. Ligands, in most cases organic molecules, should possess certain properties to interact with enzyme/receptor effectively in order to express any biological and physiological responses. These properties can be measured experimentally sometimes but only when they are available in hand. However, computer modeling technique provides an alternative possibility, a theoretical approach, to estimate these characteristics of organic molecules as well as their shapes and sizes. All these informations about the ligands are usefully utilized in establishing the quantitative structure and biological activity reationship(QSAR) which is our ultimate goal in durg design. Recently, the classic QSAR approach has developed to the 3-dimentional QSAR by incorporating unique features of the modelcules themselves.

In this talk, I would like to discuss how this computer modeling technique, particularly the 3D-QSAR concept, has been employed in designing molecules and in optimizing chemical structures in our research efforts to develop new antihypertensive drugs based on the activation of potassium channel and the competitive antagonism of the angiotensin II receptor.