



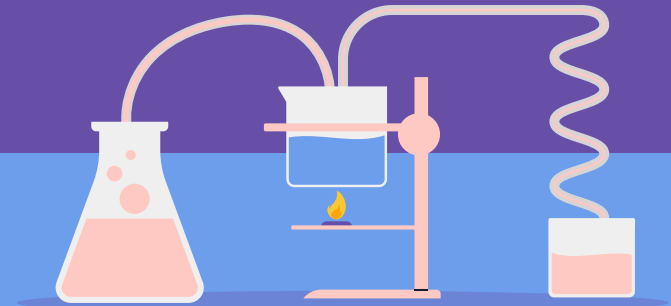
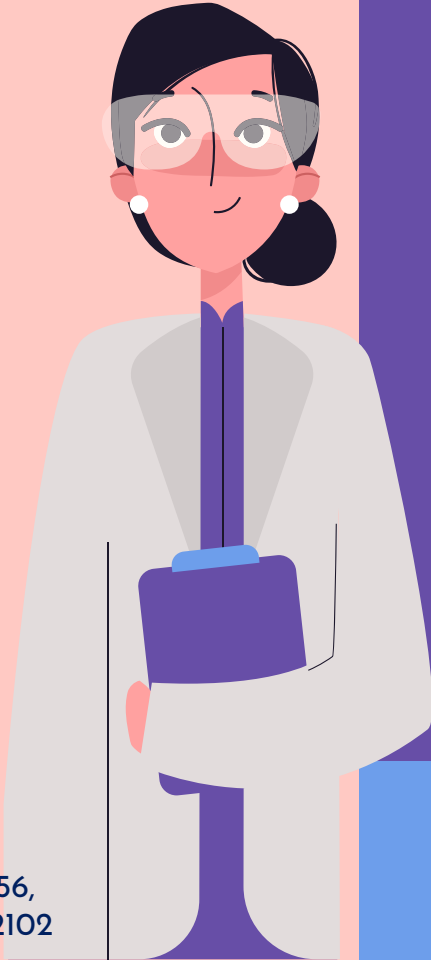
Libyan International Medical University



Faculty of Pharmacy

Second year

Structure Activity Relationship



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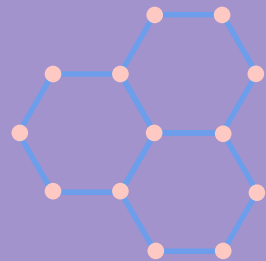
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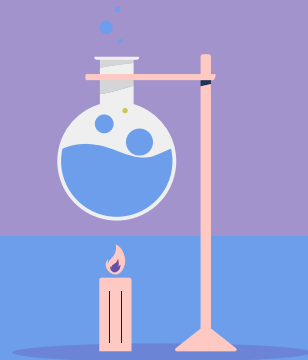
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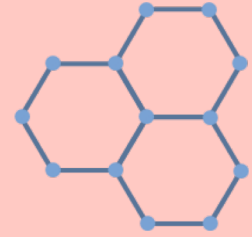
Introduction



The structure-activity relationship (SAR) is the relationship between the chemical structure of a molecule and its biological activity. This idea was first presented by Crum-Brown and Fraser in 1869.



History of SAR study



Early studies of the relationship between chemical structure and biologic activity were conducted by Crum-Brown and Fraser in 1869. Crum-Brown and Fraser therefore concluded that muscle relaxant activity required the presence of a quaternary ammonium group within the structure. This initial hypothesis was later disproven by the discovery of the natural neurotransmitter and activator of muscle contraction, acetylcholine. Even though Crum-Brown and Fraser's initial hypothesis that related chemical structure with action as a muscle relaxant was incorrect, it demonstrated the concept that molecular structure influences the biologic activity of chemical entities and that alterations in structure produce changes in biologic action.

Chemical structure and Biological activity

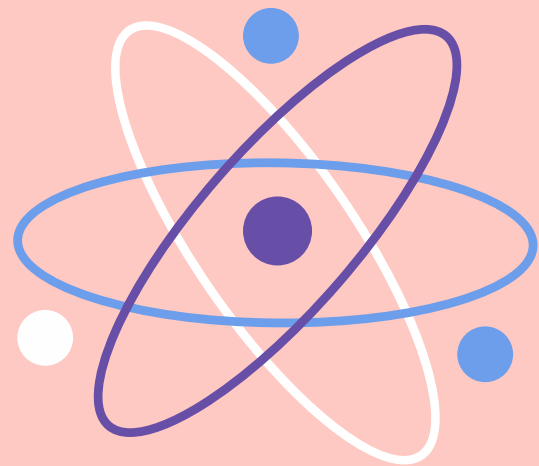
Chemical structure is the arrangement of chemical bonds between atoms in a molecule (or in an ion or radical with multiple atoms), specifically which atoms are chemically bonded to what other atoms with what kind of chemical bond, together with any information on the geometric shape of the molecule needed to uniquely identify the type of molecule.

Biological activity or pharmacological activity describes the beneficial or adverse effects of a drug on living matter.

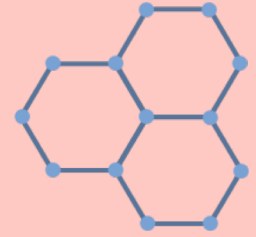
Structure activity relationship and its use

It is basically defined as the relationship between the 3D structure of molecules and their biological activity.

Structure-activity relationship (SAR) is a method used in the detection of the chemical and biological activity relationship of compounds. This concept therefore points to the link between the chemical structures and biological and the biological activities of compounds, which also includes the toxicity. Production of new drugs with a higher potency and limited side effects,



Importance of SAR study

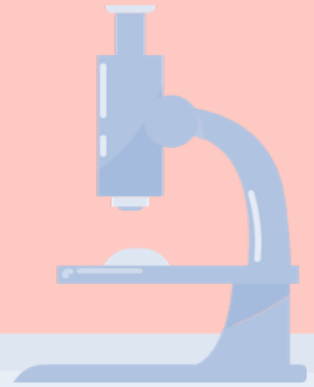


It allows making modification of the effect or the potency of a bioactive compounds like drugs by changing their chemical structures.

To determine pharmacophore, unwanted side effects.

To determine some different activity from an existing drug.

To know the changes in pharmacological properties by performing minor changes in the drug molecule.



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Thank
you!

