

Quantitative structure-activity relationship (QSAR) techniques in Drug Design

QSAR in Drug Design

Compounds + biological activity



New compounds with improved biological activity

Biological Activity = f (Physicochemical properties)

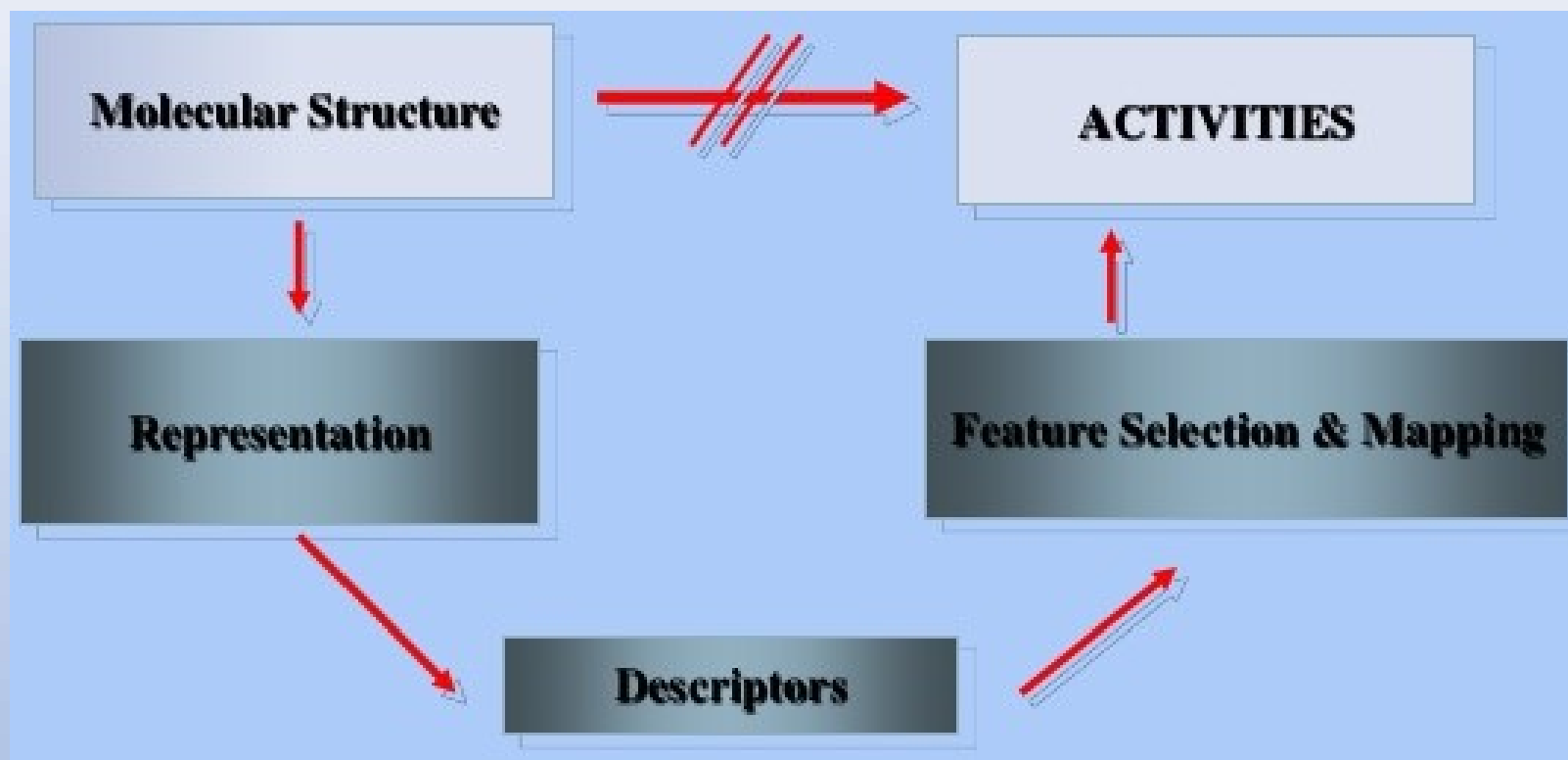
Quantitative Structure Activity Relationships (QSAR)

- QSARs are the mathematical relationships linking chemical structures with biological activity using physicochemical or any other derived property as an interface.

$$\text{Biological Activity} = f(\text{Physicochemical properties})$$

- **The structure of a chemical influences its properties and biological activity.**
- **Similar compounds behave similarly.**
- QSAR correlate within congeneric series of compounds, their chemical or biological activities, either with certain structural features or with atomic, group or molecular descriptors.

QSAR



Mathematical Methods used in QSAR includes various regression and pattern recognition techniques. It establishes an equation of relationship models of properties and activity.

Physicochemical or any other property used for generating QSARs is termed as Descriptors and is treated as independent variable. Biological property is treated as dependent variable.

QSAR in Drug design

Rational drug design methods minimize the time and cost needed in drug designing process in comparison to traditional drug discovery methods.

QSAR studies can be used to design and identify new inhibitors to optimize absorption, distribution, metabolism, excretion and toxicity profile of identified molecules from various sources.

Advances in computational techniques and hardware have eased the application of in silico methods in the designing process.

Drug design can be divided in two groups: Structure based drug design (SBDD) and Ligand based drug design (LBDD).

SBDD is the approach applying the structural information of the drug target to develop its inhibitor.

LBDD is used in the absence of the receptor 3D information and it relies on molecules bind to the biological target of interest.

QSAR in Drug design

QSAR is involved in drug discovery and designing to identify chemical structures with good inhibitory effects on specific targets and with low toxicity levels.

QSAR models are now regarded as a scientifically credible tool for predicting and classifying the biological activities of untested compounds, drug resistance, toxicity prediction and physicochemical properties prediction.

The QSAR methodology is based on the concept that the differences observed in the biological activity of a series of compounds can be quantitatively correlated with differences in their molecular structure.

As a result, all biological activities and functions of molecules relate to specific molecular descriptors and specific regression techniques can be used to estimate the relative roles of those descriptors contributing to the biological effect

QSAR in Drug design

QSAR is one of the widely used approaches in ligand based drug designing processes.

QSAR studies quantitatively correlate the relationships between trends in chemical structure alterations and respective changes in biological endpoint for comprehending which chemical properties are most likely determinants for their biological activities or physicochemical properties

The aim of this method is to optimize the existing leads in order to improve their biological activities and physico-chemical properties.

Also, to predict the biological activities of untested and sometimes yet unavailable compounds.

Thank you!