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Molecular Descriptors in QSAR/QSPR | Wiley. Molecular descriptors are mathematical values that describe the structure or shape of molecules, helping predict the activity and properties of molecules in complex experiments. This book describes the equations known as QSAR (quantitative structure-activity relationships) and QSPR (quantitative structure-property relationships), showing how they can be used productively in a wide range of industries.

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Molecular descriptors have become the most significant features used in QSAR/QSPR modeling. The information encoded by descriptors generally depends on the kind of molecular representation and the defined algorithm for its calculation. Some of these include: topological indices, and geometrical, constitutional and physicochemical descriptors.

Descriptors and their selection methods in QSAR analysis ...

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Principal steps of QSAR/QSPR including (i) Selection of Data set and extraction of structural/empirical descriptors (ii) variable selection, (iii) model construction and (iv) validation evaluation. * SAR and the SAR paradox. The basic assumption for all molecule based hypotheses is that similar molecules have similar activities.

Quantitative structure-activity relationship - Wikipedia

Molecular descriptors play a fundamental role in QSAR and other in silico models since they formally are the numerical representation of a molecular structure. Molecular descriptors can be...

(PDF) Molecular Descriptors - ResearchGate

A molecular descriptor is a structural or physicochemical property of a molecule or part of a molecule. A QSAR model for predictive toxicology is a mathematical relationship between a chemical's quantitative molecular descriptors and its toxicological endpoint [9,44].

Molecular Descriptor - an overview | ScienceDirect Topics

These molecular descriptors can be used in QSPR and QSAR models to predict different chemical parameters using the structure of the compounds, and are utilized in drug design. The published database, COMMODE, includes more than 25 million compounds and about 2.500 computed descriptors.

[COMMODE] a large-scale database of molecular descriptors ...

QSAR+ has predefined sets of default descriptors relevant to QSAR, Combichem, and QSPR. These sets are accessible from the study table by going to the Preferences/Defaults Setmenu item and selecting the QSAR, COMBICHEM, QSPR, or, if an external set of descriptors is required, Othersubmenu.

QSAR - Working with descriptors

The most important step in QSAR/QSPR is to quantify the molecular structures so as to build a correlation model between the chemical structures of various chemical compounds and the corresponding...

Molecular descriptors in QSAR/QSPR | Request PDF

This handbook and ready reference presents a combination of statistical, information-theoretic, and data analysis methods to meet the challenge of designing empirical models involving molecular descriptors within bioinformatics. The topics range from investigating information processing in chemical and biological networks to studying statistical and information-theoretic techniques for analyzing chemical structures to employing data analysis and machine learning techniques for QSAR/QSPR.

Statistical Modelling of Molecular Descriptors in QSAR/QSPR

Molecular descriptors and fingerprints have been routinely used in QSAR/SAR analysis, virtual drug screening, compound search/ranking, drug ADME/T prediction and other drug discovery processes.

ChemDes: an integrated web-based platform for molecular ...

Molecular descriptors are mathematical values that describe the structure or shape of molecules, helping predict the activity and properties of molecules in complex experiments. This book describes the equations known as QSAR (quantitative structure-activity relationships) and QSPR (quantitative structure-property relationships), showing how they can be used productively in a wide range of industries.

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Molecular descriptors play a fundamental role in chemistry, pharmaceutical sciences, environmental protection policy, and health researches, as well as in quality control, being the way molecules, thought of as real bodies, are transformed into numbers, allowing some mathematical treatment of the chemical information contained in the molecule.This was defined by Todeschini and Consonni as:

Molecular descriptor - Wikipedia

Investigate and research topological in-dices as molecular descriptors that operate on graph-based representations of molecules and provide QSAR/QSPR model review. Specialist in Entropy Advanced Computational Statistical Analysis.