

MOLECULAR QUANTUM SIMILARITY IN QSAR AND DRUG DESIGN%0A

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Particularities and limitations of QSAR models based on quantum similarity measures are outlined in this chapter. Chapters 4 to 7 show different possible approximations to the QSAR problem using quantum similarity measures and provide several application examples. The first approach (chapter 4) uses the entire quantum similarity matrix to derive the descriptors. The convenient pretreatment is discussed in full, including dimensionality reduction and variable selection. Three application

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The molecular quantum similarity framework is used to present a new set of Quantum Quantitative Structure-Properties Relationship (QQSPR) procedures. The theoretical basis consists of the so

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The authors introduce the concept of Molecular Quantum Similarity, developed in their laboratory, in a didactic form. The basis of the concept combines quantum theoretical calculations with molecular structure and properties even for large molecules. They give definitions and procedures to compute similarities molecules and provide graphical tools for visualization of sets of molecules as n-dimensional point charts.

Molecular quantum similarity measures as an alternative to ...

Abstract. A new molecular descriptor of hydrophobicity based on molecular quantum similarity measures (MQSM), which can be used to replace the log P parameter in QSAR studies, is proposed.

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Molecular Quantum Similarity and the Fundamentals of QSAR

A general overview on quantum similarity and applications to QSAR is presented. The concepts regarding quantum similarity from its theoretical foundation and consecutive development, involving mathematical formulation and similarity measures, are presented and complemented with application examples.

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This volume highlights some of the advances in molecular similarity. Molecular similarity research is a dynamic field where the rapid transfer of ideas and methodologies from the theoretical, quantum chemical and mathematical chemistry disciplines

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Full molecular quantum similarity matrices as QSAR ...

In this chapter, a scheme of the application of molecular quantum similarity matrices to describe a molecular property of interest is exposed. Quantum similarity matrices need to be conveniently transformed when employed as descriptor source in QSAR procedures. In order to describe the usual transformations, dimensionality reduction and variable selection techniques will be discussed. Combination of different quantum similarity matrices, constituting the Tuned QSAR model, is also discussed

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