PaDEL-descriptor: An open source software to calculate

Dec 17, 2010 · There are currently a large number of molecular descriptors, which can be classified into three broad categories: 1- , 2- , and 3D descriptors that encode chemical composition, topology, and 3D shape and functionality, respectively. 2 A descriptor can be simple, like molecular volume, which encode only one feature of a compound, or can be complex

Molecular Descriptor - an overview | ScienceDirect Topics

A molecular descriptor is a structural or physicochemical property of a molecule or part of a molecule. A QSAR model for prediction toxicology is a mathematical relationship between a chemical’s quantitative molecular descriptors and its toxicological endpoint [9,44]. Molecular descriptors derived from atomic or molecular properties that translate physicochemical, topological, and surface

Computational and Structural Biotechnology Journal

Molecular docking was used for analyzing two binding clusters of ligand and receptor. The results confirmed that the key amino acids interacting with the ligand were Asp335, Tyr383, and Gln384. On the basis of molecular dynamics, inhibitors 1 and 2 were noted to interact at a distance of 3.5 Å from Asp335, Tyr383, Leu408 and

Tyr466, and Asp335

Machine-learning-assisted materials discovery using failed
Open-source platform to benchmark fingerprints for ligand-based virtual screening. J. Cheminform. 5

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molecular descriptors for chemoinformatics volume
The Ro5 predicts that compounds are more likely to have poor absorption or permeation when two or more of the following parameters are exceeded: molecular mass >500 Dalton, calculated octanol