Inductive Descriptors

Inductive descriptors

The descriptors were developed by Dr. Artem Cherkasov. These descriptors are calculated based on the previous models of inductive and steric effects, inductive electronegativity and molecular capacitance. These molecular parameters are easily accessible from electronegativities and covalent radii of the constituent atoms and interatomic distances and can reflect a variety of aspects of intra- and intermolecular interactions.

The descriptors are based on the Linear Free Energy Relationships (LFER) equations for inductive and steric substituent constants, were implemented according to Cherkasov. These descriptors were used for modeling of different physicochemical and biological properties

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Cherkasov, A. Inductive QSAR Descriptors. Distinguishing Compounds with Antibacterial Activity by Artificial Neural Networks *Int. J. Mol. Sci.* **2005**, *6*, 63–86.

Cherkasov, A. 'Inductive' Descriptors: 10 Successful Years in QSAR. Curr. Comp. Aid. Drug Des. 2005, 1,2142