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The use of quantum chemistry in the prediction of ADME-Tox properties

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ADME-Tox properties are very important in pharmaceutical research, determining the fate of many molecules in the drug design sequence. Knowledge of ADME-Tox properties in the earliest stages of drug design is therefore highly desirable. The aim of this investigation is to construct low throughput in silico QSAR models in which ADME-Tox properties of single compounds are predicted with high accuracy based on Quantum Chemical information [1].

The possible role of quantum chemical information in chemoinformatics is discussed, with a closer look to the advantages, disadvantages and capabilities of quantum chemical descriptors in QSAR environments.

The use of quantum chemical information is explained by a worked-out example concerning the distribution of medicinal active molecules through the blood-brain barrier [2].

References

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