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Research article

Quantitative structure pharmacokinetic relationship modeling of Cephalosporins: Elimination half-life

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Abstract

Quantitative structure-property and relationships, often simply known as QSPR, is an analytical application that can be used to interpret the quantitative relationship between the pharmacokinetic property of a particular molecule and its structure. It is considered a major method of chemical researching all over the world today and is frequently used in various fields like agricultural, biological, environmental, and more commonly in pharmaceutical industry. Drug half-life ($t_{1/2}$) is one of the key pharmacokinetic parameters for establishment of dosing regimen. Surprisingly, the relationship between the chemical structure and $t_{1/2}$ is still poorly explored. The aim of the present study was to derive quantitative structure – pharmacokinetic relationships for $t_{1/2}$ of cephalosporins. Molecular descriptors describing molecular size, shape and solubility were calculated from the 3D molecular structure of each cephalosporin. The final predictive models showed significant correlations with literature values of $t_{1/2}$. Electrostatic and constitutional descriptors were shown to play important roles in determining drug $t_{1/2}$. This novel combination of theoretical and experimental data for pharmacokinetic modeling may lead to further progress in drug development.

Key words: Cephalosporins, ADME, QSPR.

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