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QSAR Study on N- Substituted Sulphonamide Derivatives as Anti-Bacterial Agents

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Abstract

Sulfonamides exert their anti-bacterial action by competiting with of p-aminobenzoic acid in the sequencial pathway of folate synthesis in bacteria. In the QSAR study the predictive model of forty one N-substituted sulfonamides has been buildup with the help of molecular property descriptors, heat of formation; molecular weight; total energy; eigen value of higest occupied molecular orbital; eigen value of lowest unoccupied molecular orbital; absolute hardness and electronegativity. For QSAR prediction, the 3D modeling and geometry optimization of all the derivatives have been done with the help of PCMODEL software using the semiempirical PM3 Hamiltonian. The first QSAR model has been made for eighteen N-substituted sulfonamides include the molecular weight; total energy; eigen value of highest occupied molecular orbital and eigen value of lowest unoccupied molecular orbital as best descriptors as the model has cross validation coefficient and correlation coefficient 0.795181 and 0.854468 respectively. The second QSAR model has been made for twenty-three N-phenyl substituted sulfonamides include the heat of formation, molecular weight, eigen value of highest occupied molecular orbital and eigen value of lowest unoccupied molecular orbital as best descriptors as the model has cross validation coefficient and correlation coefficient 0.74232 and 0.856631respectively. The predicted activity of the N-substituted sulfonamides as calculated from first and second models has also correlated with observed activity and correlation result is also good. On the basis of statistical quality of result it is clear that one can use these equations to predict the antibacterial activity of a hypothetical compound of similar series.

Keywords: QSAR, Sulfonamides, molecular descriptors, PM3.

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