

Abstract

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Mutagenicity analysis based on Rough Set theory and Formal Concept Analysis

Most of the current Machine Learning applications in cheminformatics are black box applications. Support vector machine and neural networks are the most used classification techniques in prediction of the mutagenic activity of compounds. The problem of these techniques is that the rules/reasons of prediction are unknown. The rules could show the most important features/descriptors of the compounds and the relations among them. This article proposes a model for generating the rules that governs prediction through the rough set theory. These rules, which based on two levels of ion for the highly discriminating power features, are visualized by lattice generated using the formal concept analysis approach. That is, better understanding of the reasons that leads to the mutagenic activity can be obtained. The resulted lattice shows that lipophilicity, number of nitrogen atoms, and electronegativity are the most important parameters in mutagenicity detection. Moreover, experimental results are compared against previous researches for validating the proposed model.