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Comparison of the bacterial mutagenicity of the chemicals with the QSAR Data

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QSAR (Quantitative Structure Activity Relationship) is a computer based predictive system used for evaluation of the biological activity of the chemicals. One of the important application fields of QSAR is to predict the toxicological effects of a chemical because this prediction system is able to reduce the cost and the time for toxicity testing using animals, Actually, the QSAR data is accepted by regulatory agencies and authorities in Europe and North America. This study is performed to validate the mutagenicity data of QSAR. The Ames assay results of 42 chemicals, evaluated for the past 5 years, were compared with the QSAR data. As the results, overall accordance rate was 88.1%. Although the prediction accuracy for positive was relatively low (54.5%), the accuracy for negative prediction was high (100 %). Therefore, the QSAR data will be applicable to select a candidate for toxicity testing.

Keyword : genetic toxicity, Ames assay, QSAR