Introduction

• The development of alternative methods relies on the availability of in silico, in vitro, and in vivo data. While these methods are useful in predicting skin sensitization risk, they are limited in their predictive accuracy due to the complexity of skin sensitization.

Study Design

• The National Toxicology Program’s Center for the Evaluation of Alternative Methods (NTP) and the Intramural Research Program of the National Institute of Environmental Health Sciences (NIEHS) have been working to develop and validate alternative methods for predicting skin sensitization hazards.

Analysis of Variable Importance

• A database of 96 substances was used to test the models. The models were trained using a variety of feature selection and classification algorithms, including logistic regression (LR), support vector machines (SVM), and decision trees.

Model Building

• The models used in this study included several non-animal methods, such as the binary in silico predictions of skin sensitization hazard produced using a machine learning approach, and the inclusion of chemical descriptors such as the log octanol-water partition coefficient (log P).

Results

• Comparison of the Machine Learning Models vs Other Approaches

- The models were compared to other approaches, such as the skin sensitization prediction software provided by the Organization for Economic Co-operation and Development (OECD), to determine their performance.

Performance Statistics for the Machine Learning Models

• The model accuracies were calculated using the Receiver Operating Characteristic (ROC) curve, which plots the true positive rate against the false positive rate.

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References

• The references for this study include a variety of sources, such as scientific journals and conference proceedings. These sources provide the necessary background knowledge and the latest advancements in the field of skin sensitization prediction.

Machine Learning Approaches for Predicting Sensitization to Chemicals

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