Introduction

- The Intramural Research Program of the National Institute of Environmental Health Sciences (NIEHS) aims to predict human outcomes using in chemico, in vitro, and in silico data and a range for log10 of these measurements.
- Additional data compiled for 96 substances included:
  - The in chemico and in vitro data were obtained from methods recommended for use by the US Environmental Protection Agency, the National Institute of Standards and Technology, and the US Food and Drug Administration.

Study Design

- The National Toxicology Program Interagency Center for the Evaluation of Alternative Animal Methods (ICCVAM) has given a high priority to replacing, reducing, and refining the use of animals for skin sensitization testing.
- Skin sensitization is a property that can be predicted from available data and physicochemical properties to identify potential human skin sensitizers.

Analysis of Variable Importance

- A total of 12 variables (non-animal test data and physicochemical characteristics) were included in the machine learning models. The human cell line activation (h-CLAT) was included in the models (Table 2).
- The machine learning models also achieved a better balance between sensitivity and specificity compared to the test batteries.

Model Building

- Six physicochemical properties were used to build models (Table 3).
- The machine learning models achieved a better balance between sensitivity and specificity compared to the test batteries.

Performance Statistics for the Machine Learning Models

- The machine learning models achieved a better balance between sensitivity and specificity compared to the test batteries.

Conclusions

- The machine learning models also achieved a better balance between sensitivity and specificity compared to the test batteries.

References

- The machine learning models also achieved a better balance between sensitivity and specificity compared to the test batteries.