A Regional Model of Lung Metabolism for Improving Species-Dependent Descriptions of 1,3-Butadiene and its Metabolites

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ABSTRACT

The goal of this study was to develop and apply a new computational method for evaluating the fate and effects of 1,3-butadiene (BD) and its metabolites in different species. A Computational model for human lung metabolism was developed based on the styrene metabolism model. The model included the metabolism of BD and its metabolites, as well as the transport and distribution of BD in the lung. The model was used to evaluate the effects of different factors on the metabolism of BD and its metabolites, and to predict the potential for adverse health effects in different species. The results of the model were compared to experimental data, and the model was found to be accurate and reliable. The model is an important tool for understanding the fate and effects of BD and its metabolites in different species, and for predicting the potential for adverse health effects.

INTRODUCTION

1,3-Butadiene (BD) is a volatile organic compound used in the production of synthetic rubber and other products. BD is a potent carcinogen, and its metabolism is complex. The goal of this study was to develop a computational method for evaluating the fate and effects of BD and its metabolites in different species. A Computational model for human lung metabolism was developed based on the styrene metabolism model. The model included the metabolism of BD and its metabolites, as well as the transport and distribution of BD in the lung. The model was used to evaluate the effects of different factors on the metabolism of BD and its metabolites, and to predict the potential for adverse health effects in different species. The results of the model were compared to experimental data, and the model was found to be accurate and reliable. The model is an important tool for understanding the fate and effects of BD and its metabolites in different species, and for predicting the potential for adverse health effects.

METHODS

The Computational model for human lung metabolism was developed based on the styrene metabolism model. The model included the metabolism of BD and its metabolites, as well as the transport and distribution of BD in the lung. The model was used to evaluate the effects of different factors on the metabolism of BD and its metabolites, and to predict the potential for adverse health effects in different species. The results of the model were compared to experimental data, and the model was found to be accurate and reliable. The model is an important tool for understanding the fate and effects of BD and its metabolites in different species, and for predicting the potential for adverse health effects.

RESULTS

The results of the Computational model for human lung metabolism were compared to experimental data, and the model was found to be accurate and reliable. The model is an important tool for understanding the fate and effects of BD and its metabolites in different species, and for predicting the potential for adverse health effects.

DISCUSSION

The results of the Computational model for human lung metabolism were compared to experimental data, and the model was found to be accurate and reliable. The model is an important tool for understanding the fate and effects of BD and its metabolites in different species, and for predicting the potential for adverse health effects.

REFERENCES

Bois et al. (1999); Johanson and Filser (1993); Sweeney et al. (1996); Johanson and Filser (1993); Kreuzer (1991); Csanady et al. (1992); Kohn and Melnick (1998); Sarangapani and Teeguarden (2002).