

POSTER PRESENTATION

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Prediction of the partition coefficient between air and body compartments from the chemical structure

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For PBPK modeling, partition coefficients between tissues and environmental compartments are required. A simple approach starts with the system blood/air, fat/air, and fat/blood. Employing thermodynamic relationships, one of the three coefficients can be calculated from the other two values. With respect to available human and mammal data, modeling efforts focus on the blood/air and fat/air partition coefficient.

Respective data sets from literature have been collected and evaluated. The chemical domain of the sets is presented in terms of chemical structure, complexity, and polarity. Data gaps have been identified.

The blood/air and fat/air partition coefficient data sets have been applied to a validation of literature models, with particular remark on the performance for specific compound classes. A new model for the blood/air partition coefficient and a preliminary new model for the fat/air partition coefficient are presented.

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