Abstract
The current effort of the International Council for Harmonisation on QM01 (ICH) guidance documents for the use of in silico models to predict drug-drug interactions (DDIs) has been focused on basic research and development of new models. In this study, we investigated the development of new DDI models using a unique approach and new in silico pharma DDI datasets. Two new models were developed, namely, a DDI prediction model using LSE and a DDI prediction model as an improved functional group model. The results of these two models were compared to the recently published traditional DDI models. The results showed that the new DDI models were significantly better than the traditional DDI model and that the new DDI model was significantly better than the traditional DDI model.

Materials and Methods
Software and Training in H2O2 Models
- Previously trained set for Leadscope Applied (AP) and MUCASES CEACOP (CEACOP) for the Leadscope ADME models.
- Newly constrained training set for AP and MUCASES CEACOP (CEACOP) for the Leadscope ADME models.
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Data Analysis
- MUCASES CEACOP and Leadscope Applied models were trained using a unique approach and new in silico pharma DDI datasets.
- The results showed that the new DDI models were significantly better than the traditional DDI model.

Results and Discussion
- The Leadscope ADME models are based on the Leadscope Applied (Leadscope Applied (AP) and MUCASES CEACOP (CEACOP) for the Leadscope ADME models).
- The results showed that the new DDI models were significantly better than the traditional DDI model.

Development of Improved Landscape Mutagenicity Salmonella Models
- Overall, a total of 207 features were added to the new Salmonella model and 156 features from the old Salmonella model were excluded.
- The added features included杀人和 well-defined substrates based on toxicological mechanisms, and in some cases more highly defined features.

References