

In silico prediction of drug-induced liver injury of drug candidates

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The demand for accurate prediction of drug-induced liver injury (DILI) of drug candidates is increasing. DILI is one of challenging hurdles in the early stages of drug development, because DILI accounts for almost 20% of drug withdrawal in the market. Though many DILI prediction models have been developed, for facilitated drug development a highly accurate DILI prediction model is required for practical use. In this study, we developed an ensemble model consisted of sub-models trained by 12 different machine learning algorithms. The ensemble model achieved high predictive performance, with an area under the curve of 0.88, F1-score of 0.81, and accuracy of 0.80. When evaluated on an independent test dataset, the ensemble model showed an accuracy of 0.76 and F1-score of 0.79. The performance of our ensemble model was higher than that of other DILI prediction models. Our model would be of use in drug discovery and facilitate computational drug development.