

Imputation of Assay Bioactivity Data using Deep Learning

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Abstract

We describe a novel deep learning neural network method and its application to impute assay pIC₅₀ values. Unlike conventional machine learning approaches, this method is trained on sparse bioactivity data as input, typical of that found in public and commercial databases, enabling it to learn directly from correlations between activities measured in different assays.

In two case studies on public domain data sets we show that the neural network method outperforms traditional quantitative structure-activity relationship (QSAR) models and other leading approaches. Furthermore, by focussing on only the most confident predictions the accuracy is increased to $R^2 > 0.9$ using our method, as compared to $R^2 = 0.44$ when reporting all predictions.

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