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**Imputation of Assay Bioactivity Data Using Deep Learning**
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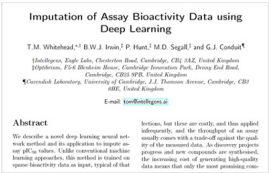
## Abstract

We describe a novel deep learning neural network method and its application to impute assay $pIC_{50}$ 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.


Imputation of Assay Bioactivity Data using Deep Learning

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Abstract

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lections, but these are costly, and thus applied infrequently, and the throughput of an assay usually comes with a trade-off against the quality of the measured data. As discovery projects progress and new compounds are synthesized, the increasing cost of generating high-quality data means that only the most promising com-

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