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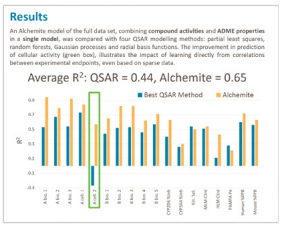
Benedict Irwin, Julian Levell, Thomas Whitehead, Matthew Segall, Gareth Conduit

We have previously described a novel deep learning method for data imputation, Alchemite™ (Whitehead et al J Chem Inf Model (2019) 59 pp 1197-1204). This accepts both molecular descriptors and sparse experimental data as inputs, to exploit the correlations between experimentally measured endpoints, as well as structure activity relationships (SAR). It has been demonstrated to outperform quantitative SAR (QSAR) models, including multi-target deep learning methods, on a challenging benchmark data set of compound bioactivities. Here we will describe the application and validation of this method on drug discovery data covering two projects and diverse endpoints, including activities in both biochemical and cellular assays and absorption, distribution, metabolism and elimination (ADME) endpoints.



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