ci-2022-00779z Cover Page Caption

Supervised Machine learning is typically data-hungry, which is in stark contrast to the limited data for new disease targets. We explore few-shot machine learning which aims to "learn how to learn" from just a few examples. Our proposed architecture makes use of embeddings created through graph convolutional networks, achieving better results than the state-of-the-art on Tox21 data. We classified molecules as active or otherwise, within a previously unseen experimental assay using only 1-10 molecules and a model trained on related assays.