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Dilshana Shanavas Rasheeda (COMPBC): Can We Use AI to Provide Quantitative Predictions for Chemical Bioactivity and Toxicity?

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Abstract: "Understanding and predicting chemical bioactivity is central to drug development, chemical safety, and environmental risk assessment. However, large numbers of unlabelled compounds remain unexplored due to the cost and scale of experimental testing. In this work, we investigate the potential of artificial intelligence (AI) to provide accurate, structure-based predictions for chemical toxicity and related properties.

We focus on cytotoxicity data from invitroDB and calculated lipophilicity as representative endpoints. Using molecular fingerprints and graph-based representations of chemical structures, we develop regression models with deepFPlearn (a feedforward neural network framework) and Graph Neural Networks (GNNs). Our automated workflow covers data preprocessing, model training, and prediction on unseen compounds.

The models show strong predictive performance and generalization cross datasets. The workflow is scalable, interpretable, and adaptable to other physicochemical or biological endpoints. By combining cheminformatics with deep learning, this work demonstrates a practical and extensible pipeline for predictive toxicology, supporting more efficient, data-driven chemical screening."

Session Classification: Session II: Data science and modelling , Chair: tbd