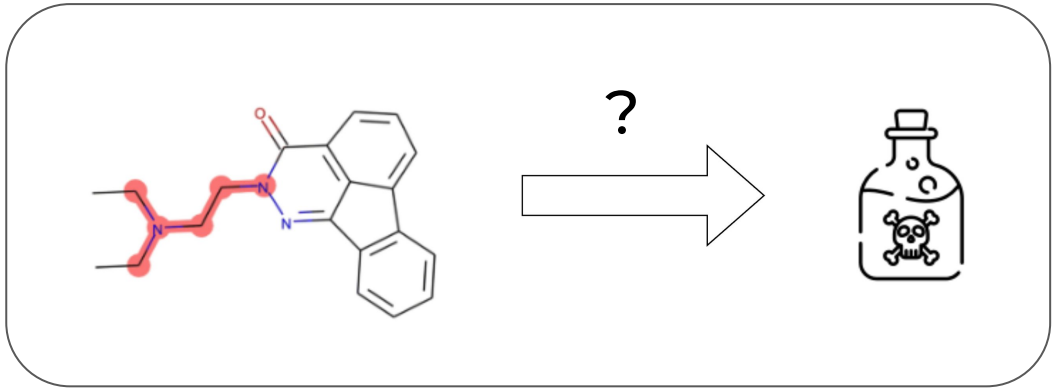
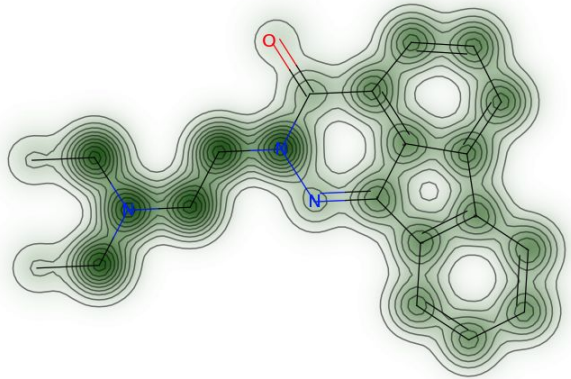
Cytotoxicity Maps





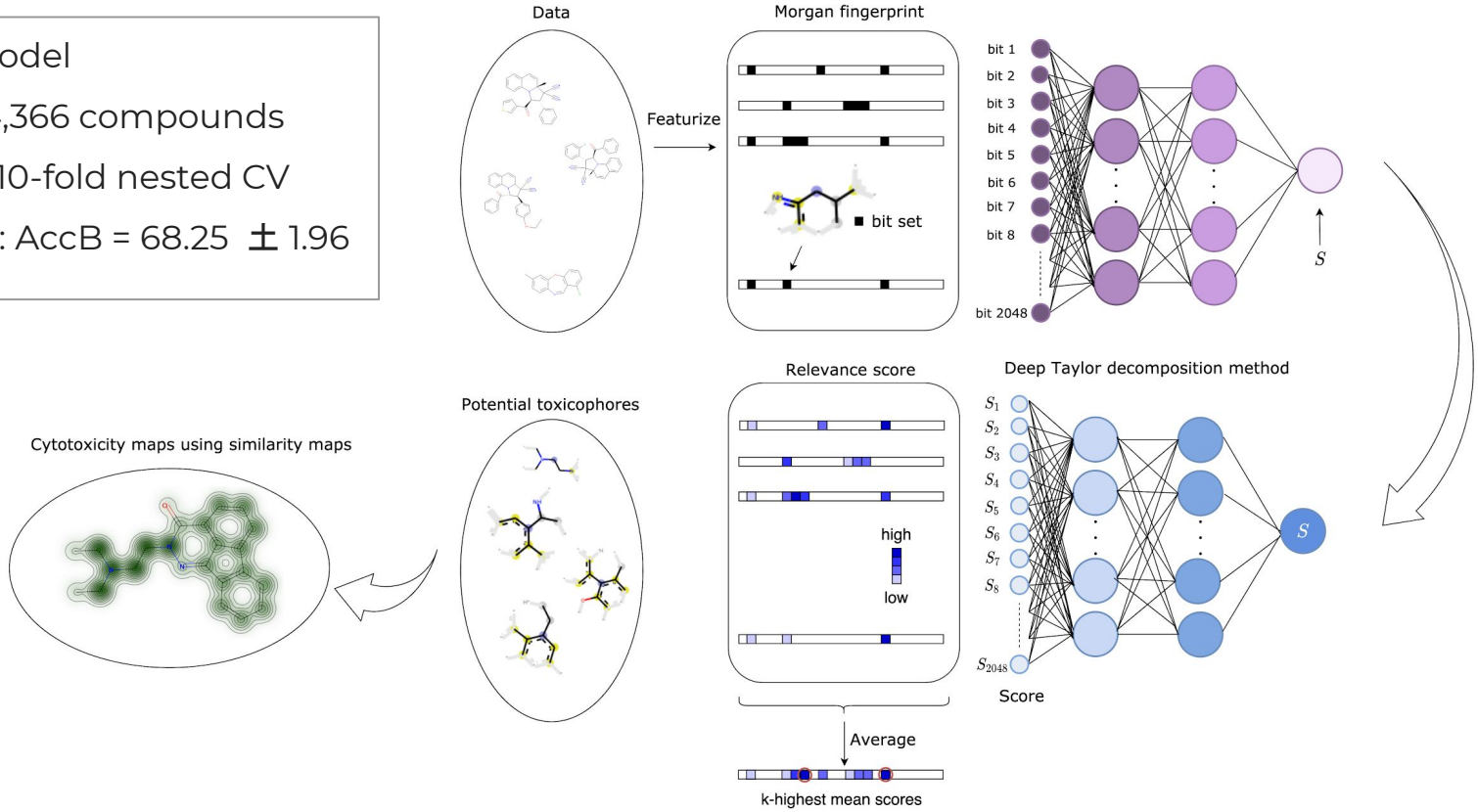
Drug Discovery Pipeline

Target Discovery → Lead Generation → Lead Optimization → Preclinical Development → Clinical Phases → Drug to Market

Workflow

Our cytotoxicity model

- FMP data: 34,366 compounds
- Model: FNN, 10-fold nested CV
- Results (test): AccB = 68.25 ± 1.96



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Reference

Webel, H.E., Kimber, T.B. et al. Revealing cytotoxic substructures in molecules using deep learning. *J Comput Aided Mol Des* 34, 731–746 (2020). https://doi.org/10.1007/s10822-020-00310-4