

Description of Additional Supplementary Files

Supplementary Data 1: Dataset and software metadata. This workbook contains the classification and regression-dataset inventories and the software/package versions used in the study.

Supplementary Data 2: Internal and state-of-the-art benchmark results. This workbook contains classification and regression results, aggregator and featurizer win rates, and state-of-the-art benchmark results and win rates

Supplementary Data 3: Generalization and robustness results. This workbook contains AODB, ACNet-Large, out-of-distribution, low-data, k-nearest-neighbour and computational benchmark data.

Supplementary Data 4: Modality robustness and chemical-fidelity results. This workbook contains encoder-replacement, modality-ablation, replacement/ablation win-rate and Complexizer analyses.

Supplementary Data 5: Genomic-stability and statistical results. This workbook contains training compounds, candidate predictions, growth-assay data and exact statistical outputs for benchmark and wet-lab analyses.

Supplementary Data 6: CDI-Generator outputs. This workbook contains generation summaries and generated-molecule records.