# Advancing Evaluation: Recall-Based Metrics for Molecular Generators

Fil Valeriia1, Svozil Daniel1,2

1 Department of Informatics and Chemistry & CZ-OPENSCREEN: National Infrastructure for Chemical Biology, Faculty of Chemical Technology, University of Chemistry and Technology, Technická 5, 16628, Prague, Czech Republic.

2 CZ-OPENSCREEN: National Infrastructure for Chemical Biology, Institute of Molecular Genetics of the Czech Academy of Sciences, Prague, Czech Republic.

Molecular generators enable the systematic exploration of chemical space to identify novel compounds with desirable properties. However, assessing their performance remains challenging due to the structural diversity and volume of the generated molecules. Common evaluation metrics, focused on chemical validity and novelty, do not fully align with the primary goal of molecular generation: the discovery of new biologically active compounds. To address this limitation, we introduce scaffold-based recall metrics that evaluate a generator’s ability to recover biologically relevant scaffolds absent from the input set. Using these metrics, we assessed several molecular generators, including Molpher and DrugEx. The DrugEx Graph Transformer demonstrated the highest scaffold recall and scaffold hopping potential. The proposed recall-based metrics thus provide a more biologically meaningful framework for evaluating molecular generators and optimizing their performance to enhance the design of virtual libraries for drug discovery.