# Techniques for improving optimization performance of molecular generators

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Over the last few years, deep neural networks became an indispensable tool in de-novo computational drug design via molecular generators. A wide range of architectures and optimization algorithms have already been tested with promising results. In addition to that, there are other features that can potentially improve generator performance. Two of those promising features are Transfer learning and Initial population. Both were already used in various setups, however a multi-generator comparison aimed to evaluate the contribution of these features to optimization enhancement under standardized conditions is still missing. In this work, we performed such a comparison using several deep neural networks-based generators and a set of standardized benchmarks from GuacaMol benchmarking platform. We report that Transfer learning significantly enhanced the optimization results across all tested generators and majority of benchmarks both with regard to achieved results and also the amount of time necessary to achieve those results. Use of Initial population also led to optimization improvement in some cases, however to a much lesser extent.