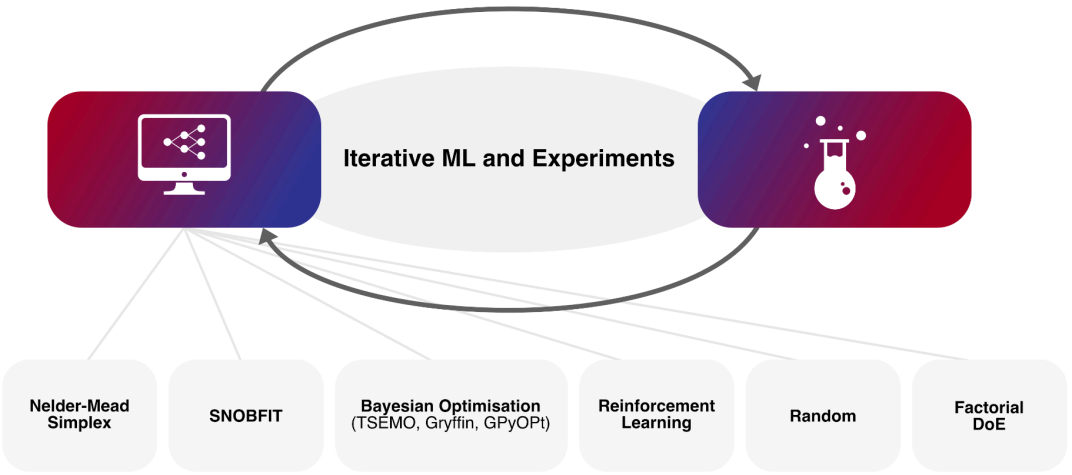
Summit

Summit is the first package to enable rigorous comparison of various machine learning algorithms for optimizing chemical reactions. It has two main features:

- Benchmarks: Simulations of reactions that can be used as virtual experiments
- Strategies: Machine-learning driven optimization algorithms



In this tutorial, I will demonstrate how to use Summit to optimize both single and multiobjective problems and, time-permitting, how to create your own benchmarks.