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Fast-tracking Pharmaceutical Process Development with Small Data and Machine Learning

Pharmaceutical process design and optimization is a time-consuming and complex task. Data-driven machine learning (ML) can accelerate the process by predicting behavioral trends, variable effects, and optimal conditions. However, conventional ML algorithms often require extensive datasets, posing a resource-intensive challenge in experimental data collection.

To address this bottleneck, we introduce an enhanced Bayesian optimization (BO) approach, enabling a reaction-agnostic pathway for designing and implementing intelligent experimental campaigns. SuntheticsML is an accessible online ML platform tailored for researchers without coding or ML expertise. The pivotal in-lab validation of this approach demonstrates compelling returns on material and experimental efficiency, as well as performance gains against a competitive baseline.

SuntheticsML is a versatile technology that allows numeric, discrete, and mixed-integer optimization problems with up to 20 input parameters, further facilitating bounded-target, multi-objective, and constrained-input optimizations. Case studies of SuntheticsML with industrial partners showcase accelerated formulation optimization, process characterizations, and process development efforts in chemocatalytic reactions, biocatalytic cascades, crystallizations, tablet formulations, in-vitro mRNA transcription processes, and more.

The in-lab validation of SuntheticsML convincingly demonstrates impressive returns on material efficiency, with up to a 75% reduction in the use of expensive or complex reagents. Experimental efficiencies enabling 9-12% increases in previously-optimized yields with a 2-32X reduction in optimization experiments.

The talk will showcase SuntheticsML as a platform available to researchers in industry and academia who are redefining the landscape of reaction engineering, process development, and optimization, with easy, accessible, and powerful AI.