

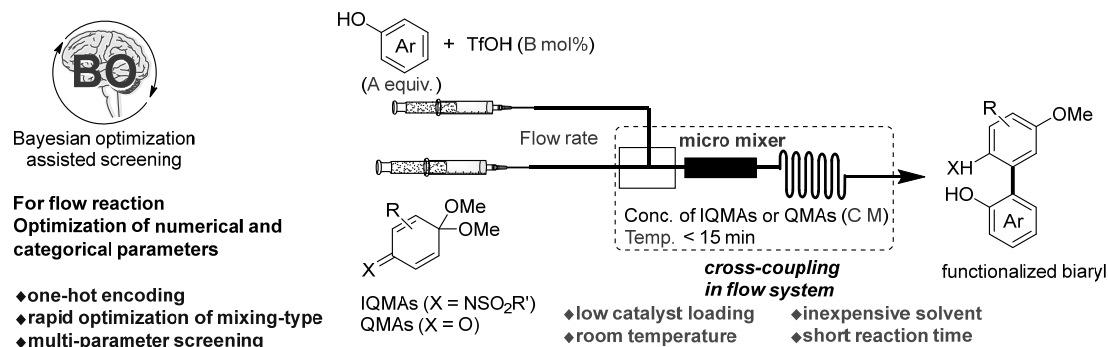
ベイズ最適化による精密有機合成反応条件の探索

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 Bayesian optimization-assisted screening of multiple parameters for fine chemical synthesis
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Traditional optimization methods using one variable at a time approach waste time and chemicals and assume that different parameters are independent from one another. Hence, a simpler, more practical, and rapid process for predicting reaction conditions that can be applied to several manufacturing environmentally sustainable processes is highly desirable. In this study, biaryl compounds were synthesized efficiently using an organic Brønsted acid catalyst in a flow system. Bayesian optimization (BO)-assisted multi-parameter screening, which employs one-hot encoding and appropriate acquisition function, rapidly predicted the suitable conditions for the synthesis of 2-amino-2'-hydroxy-biaryls (up to 96% yield). In this presentation, we will also report BO-assisted screening on the electrochemical synthetic conditions of ketimines.

Keywords : Bayesian Optimization; Organocatalysis; Flow Synthesis; Domino Reaction; Electrochemical Synthesis

効率的かつ高収率にて目的有機化合物を合成するためには、反応条件を網羅的に探索し最適化する必要がある。しかしながら、反応パラメータが多くなるとその探索数は指数関数的に増加し、熟練者の経験に基づく逐次網羅的スクリーニングでも多大なコストを要する。本講演では、最近、我々が展開しているガウス過程回帰¹及び、ベイズ最適化による多次元パラレル探索を基軸とする最少実験試行数での反応条件最適化について、『アミンの電解酸化によるケチミン合成』²及び、『有機酸触媒によるビアリール化合物のフロー合成』³の研究を例に紹介する。



- 1) M. Kondo, H. D. P. Wathsala, M. Sako, Y. Hanatani, K. Ishikawa, S. Hara, T. Takaai, T. Washio, S. Takizawa, H. Sasai, *Chem. Commun.* **2020**, 56, 1259.
- 2) M. Kondo, A. Sugizaki, Md. I. Khalid, H. D. P. Wathsala, K. Ishikawa, S. Hara, T. Takaai, T. Washio, S. Takizawa, H. Sasai, *Green Chem.* **2021**, 23, 5825.
- 3) M. Kondo, H. D. P. Wathsala, M. S. H. Salem, H. Ishikawa, S. Hara, T. Takaai, T. Washio, H. Sasai, S. Takizawa, *Commun. Chem.* **2022**, 5, 148.