

# Reinforcement learning prioritizes general applicable reaction optimization

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## Abstract

Reaction conditions that are generally applicable to a wide variety of substrates are highly desired. While many approaches exist to evaluate the general applicability of developed conditions, a universal approach to efficiently discover such conditions during optimizations de novo is rare. In this work, we report the design, implementation, and application of reinforcement learning bandit optimization models to identify generally applicable conditions in a variety of chemical transformations. Performance benchmarking on existing datasets statistically showed high accuracies for identifying general conditions. A palladium-catalyzed imidazole C–H arylation reaction and an aniline amide coupling reaction were investigated experimentally to demonstrate utilities of our learning model in practice.

## Main

Chemists have long sought robust synthetic methods that can be applied to a wide variety of substrates<sup>1–3</sup>. However, methodologies are generally developed and optimized with only one or a few model substrates to circumvent synthetic and analytical constraints. These “optimized” conditions are subsequently applied to a substrate scope, usually with higher yielding substrates preferentially reported. Evidently, reaction conditions optimized for a single substrate are not guaranteed to be applicable to other molecules with distinct structural features. Despite the increased efficiency of reaction optimization enabled by automated reaction systems<sup>4–10</sup> and optimization algorithms<sup>11–20</sup>, this phenomenon still significantly hampers the adoption of newly developed methodologies in synthetic chemistry<sup>21,22</sup>. Further optimization for different target substrates is typically required, and pharmaceutically relevant molecules with high structural complexity might not even be compatible with existing conditions at all<sup>23</sup>. Most work to date has focused on retroactively evaluating the general applicability of developed methodologies via substrate scope design. One approach is to cluster commercial substrates into groups with unsupervised learning models, from which a representative substrate scope can be constructed by sampling from all groups<sup>24</sup>. Another approach involves expert-designed scopes intended to test substrate compatibility relevant in pharmaceutical synthesis<sup>25</sup>. Additive screening is also a

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