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Coach	**Supervisor(s)**	**Funding**
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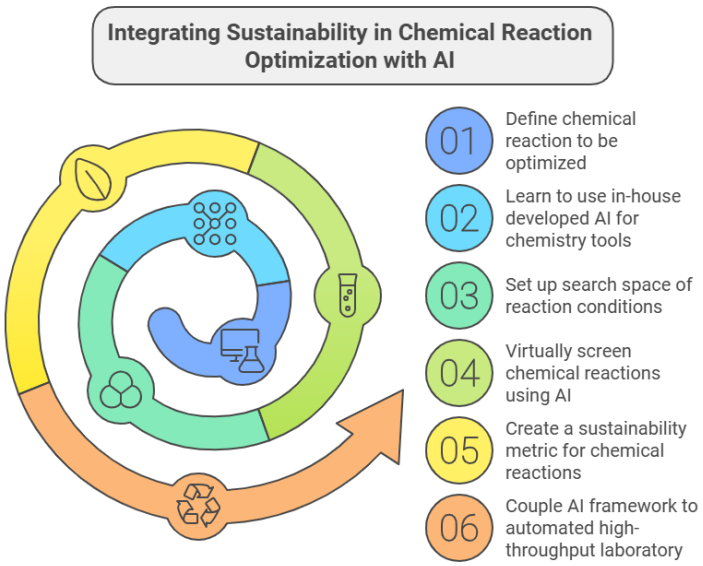
Artificial Intelligence Meets Sustainable Reaction Engineering: Optimizing Reaction Conditions for Greener Chemical Production Processes

Aim

This thesis aims to use machine learning to optimize reaction conditions for producing fine chemicals and pharmaceuticals, focusing on improving multiple objectives, including yield, selectivity, and sustainability.

Justification



For over a century, the ability to create new materials has depended on developing efficient methods to produce chemical compounds. This is particularly true in fields like drug development and agricultural chemistry, where synthesizing a promising new molecule often requires several reaction steps. The optimization of each step is not just crucial, but urgent, for discovering new drugs and materials and enabling chemical production at scale later on.
Artificial intelligence and machine learning offer a promising solution to these challenges. Its ability to handle high-dimensional problems allows it to explore the chemical space efficiently, identifying conditions that optimize multiple objectives, such as yield, selectivity, cost, and productivity. By prioritizing the most promising conditions for experimental testing, machine learning significantly reduces the need for costly and time-consuming trial-and-error experiments. However, much of the current research in this area focuses primarily on goals like maximizing yield or minimizing costs. Environmental factors, which are critical for achieving sustainable production, are often overlooked during the early stages of process design. This oversight can lead to unsustainable methods that require substantial adjustments later.
This thesis aims to address this gap by introducing a sustainability metric into optimizing reaction conditions. The research aims to develop a framework for designing greener and more efficient chemical processes by incorporating this metric alongside traditional objectives like yield and selectivity.

Program

- Literature survey on AI approaches for reaction optimization
- Extension and application of existing machine learning tools for reaction optimization
- Development of a new green chemistry metric to evaluate the sustainability of a set of reaction conditions

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