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Machine Learning Meets Sustainable Reaction Engineering: Selecting Greener Reaction Conditions for Pharmaceutical Syntheses

Aim

The aim of this master thesis is to apply machine learning algorithms to evaluate the sustainability of chemical reactions and recommend greener reaction conditions.

Justification

Bringing a new drug to the market takes on average 15 years, costs over 1 billion euro, and has an enormous environmental impact. The pharmaceutical sector has the lowest sustainability score among the whole chemical industry with more than 25 kg of waste produced per kg of product, compared to the energy sector, which produces less than 0.1 kg of waste per kg of product. A crucial step in the pathway towards green pharmaceuticals is the implementation of continuous reactors instead of traditional batch reactors. Pharmaceutical syntheses usually consist of several reaction steps that are performed in series. In the case of a batch process, the product is filtered and isolated after each reaction step and the conditions of the next reaction step is independent of the previous step. However, in a continuous process the reactors are coupled and side-products that are performed in the previous reactor will hamper the effectiveness of the next reactor. Moreover, all reactions are ideally performed in the same solvent, since it is infeasible to extract solvents between reactors. Eventually, regulatory instances have added another layer of complexity by phasing out or banning a large number of common solvents because of environmental, hazard, or safety reasons.

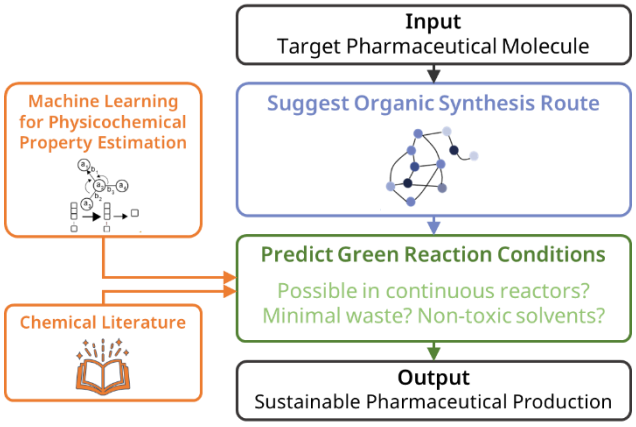

Figure 1: Overview of approach for developing greener pharmaceutical production pathways

In the past years, researchers have developed various machine learning tools to support synthetic chemists. These methods facilitate the design of synthetic procedures and the prediction of physicochemical properties of chemical compounds. A fundamental challenge remains: at which reaction conditions (solvent, reagents, temperature, …) should a reaction be performed to maximize the yield and to minimize the footprint?

Program

- Literature survey on computational approaches for reaction yield estimation
- Extension and application of existing machine learning tools for computer-aided synthesis planning
- Development of a new green chemistry metric to evaluate the sustainability of a chemical reaction
- Sanity check: evaluation of machine learning results and comparison with chemical rules

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Funded by the European Union