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AI for Designing Greener Pharmaceuticals and Agrochemicals

Aim

The aim of this master thesis is to apply machine learning algorithms to predict physicochemical properties of molecules and create sustainability-driven selection criteria for these compounds based on these properties.

Justification

Synthetic chemicals play a crucial role in sustaining human life. Active pharmaceutical ingredients can cure life-threatening diseases, and agrochemicals increase crop yield, providing more food per area of land. However, many of these synthetic chemicals are toxic to the environment. Pharmaceuticals are excreted from the body and end up in sewage but cannot be filtered out in wastewater treatment plants, thus ending up in rivers. As an example, over-the-counter drugs such as diclofenac or paracetamol are very harmful to aquatic life, resulting in the death of fish. Agrochemicals, used in fertilizers, herbicides, and insecticides, have a similar effect on aquatic life and enhance the growth of blue-green algae. Consequentially, environmentally harmful synthetic chemicals are being banned or face restrictions despite their usefulness for humans.

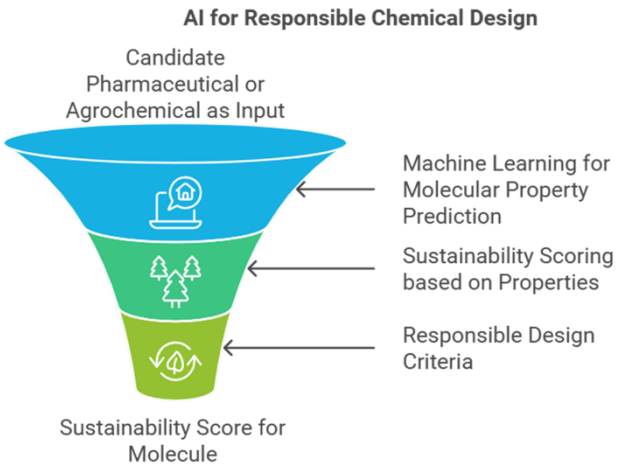

Figure 1: Overview of approach for developing more sustainable chemicals

Environmental effects must be considered from the start of the molecular design phase. However, performing (eco)toxicological tests is extremely time-consuming and is only done when a chemical has already been selected. Artificial intelligence (AI) can speed up this process by predicting a new compound's physicochemical and (eco)toxicological properties. In the past years, a state-of-the-art AI platform for molecular property prediction has been developed at the LCT [1]. However, creating a molecular screening platform building on these properties is still a fundamental challenge. Such a screening platform receives a molecule as input, predicts its properties on the fly, and then calculates scores to represent its suitability as a drug or agrochemical, as well as the corresponding environmental footprint. The goal of this master's thesis is, in the first step, to train AI models for predicting various physicochemical and (eco)toxicological properties. These trained models will subsequently be used as a filter on datasets of approved and banned pharmaceuticals and agrochemicals to calculate sustainability scores. This approach is fundamental to promoting more responsible and sustainable chemical design, balancing human needs and environmental impact.

Program

- Literature survey on AI approaches for molecular design
- Extension and application of existing machine learning tools for molecular property prediction
- Development of a new green chemistry metric to evaluate the sustainability of a chemical

1. Dobbelaere, M.R., et al., *Geometric deep learning for molecular property predictions with chemical accuracy across chemical space.* Journal of Cheminformatics, 2024. **16**(99).

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