Contribution ID : **144** Type : **Poster Presentation**

EuCompChem - Smart Solvent Selection: Combining In-Silico Insights with High-Throughput Experimentation - oral

In the pharmaceutical industry, process design is the business process tasked with defining reagents, solvents and unit operations needed to develop a chemical route into a chemical process that meets cost of goods, throughput, quality and sustainability goals. Process design is a complex multi-objective, multi-parameter task, which requires careful planning and prioritisation to make the best of limited human and time resources. Planning the sequence of unit operations involved in a process and selecting appropriate solvents is possible, if the right physical property data is available. When experimental data is not available, predicted data can be generated in-silico with the help of quantum-mechanics based methods. Here, we present an overview of in-silico guided solvent design in the pharmaceutical industry. Specifically, we will cover how in-silico prediction may be coupled with high-throughput experimentations to guide solvent selection. We demonstrate innovative in-silico-guided methodologies for optimizing (1) aqueous extraction processes and (2) crystallization procedures. Finally, we present a fully automated data pipeline generating, harvesting and storing physical properties predictions in an online database, to be later consulted by process chemists.

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