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Predicting drug solubility through digital models: towards pharmaceutical industry 5.0

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In the pharmaceutical industry, drug solubility is a critical quality attribute. For example, drug solubility in organic solvents mixtures is usually screened in drug development to select the best solvent system for crystallization in such a way as to design the manufacturing process. Solubility is also important in the final product because it has a direct impact on the way the drug is absorbed by the patient. Despite the different challenges posed by different application domains, we propose digital models to predict solubility both in organic solvent mixtures for crystallization process development and in gastrointestinal fluids for oral drug absorption.
The first machine-learning model predicts the solubility of drugs in mixtures of organic solvents commonly used in crystallization processes. The new proposed method identifies solvents using molecular descriptors based on UNIFAC subgroups. Solubility prediction is achieved as a function of temperature, solvent functional subgroups, and mixture composition employing Partial Least-Squares (PLS) regression.
The second approach addresses the challenge of predicting drug solubility in the human gastrointestinal tract, a key factor influencing bioavailability for evaluating its therapeutic efficacy. A hybrid model incorporating Gaussian Process Regression (GPR) in existing physiological models is proposed to guarantee prediction accuracy, physiological insight, and improved interpretability by elucidating the relationship between intestinal components and drug solubility.
The predictive accuracy of the proposed methodologies is tested in different industrial case studies and are further validated for literature benchmarks, paving the way of personalized pharmaceutical industry 5.0 through digital models.

Type of presentation

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