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ENABLING SELF-DRIVING LABORATORIES

Optimizing HPLC method development to maximize peak resolution

Sector
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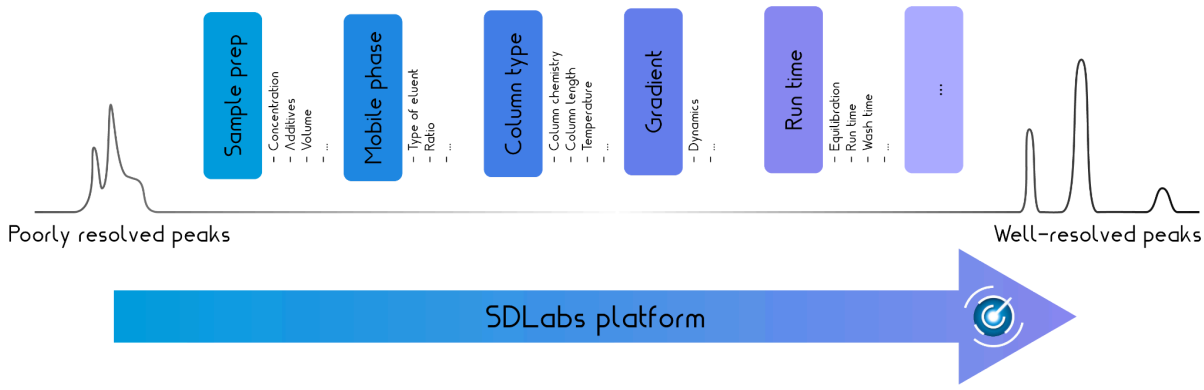
Impact
Process Optimization in Analytical Chemistry

Overview
High-Performance Liquid Chromatography (HPLC) method development is a critical process in analytical chemistry, aimed at optimizing the separation of components in a mixture. The method involves selecting appropriate mobile phases, column types, flow rates, and temperature conditions to achieve optimal peak resolution, which is essential for accurately identifying and quantifying each compound in a sample.

Challenges
Factors such as the choice of solvent, gradient profile, and column type significantly influence peak separation, with small adjustments potentially leading to sharper peaks and better resolution, ensuring reliable and reproducible results in complex mixtures. Typically, it is cumbersome to investigate all possible parameters as the instrumentation requires downtime to change parts (i.e. eluent or column) and needs time to equilibrate.

Use Case
The goal was to develop an HPLC method that includes eluent composition, column, running conditions, etc. to separate a complex mixture of chemicals. Maximizing the resolution throughout the chromatogram and reducing the runtime are the two primary objectives. Achieving these goals requires finding the sweet spot in all process variables, while minimizing the number of runs.



Schematic diagram highlighting the use of Atinary's SDLabs platform in integrating multiple parameters and multi-objective optimization in HPLC method development. With a complex interplay of variables, AI can significantly accelerate the time and HPLC processes of complex chemical mixtures that yield sharp and well-resolved peaks.

Benefits

Atinary's no-code AI platform, SDLabs, offers advanced optimization capabilities that allow for multiparameter and multi-objective optimization in HPLC method development. In SDLabs, researchers can add various **constraints**, such as conditional exclusion, to account for **incompatibilities** between column types and eluents, or **equality** constraints, where the sum of different constituents in the eluent must equal a specific value. Additionally, SDLabs handles **batch-constrained** optimization, streamlining the experimental workflow by grouping similar conditions together. This comprehensive approach ensures that every aspect of the method is optimized globally, leading to more precise, quicker and reliable analytical outcomes.