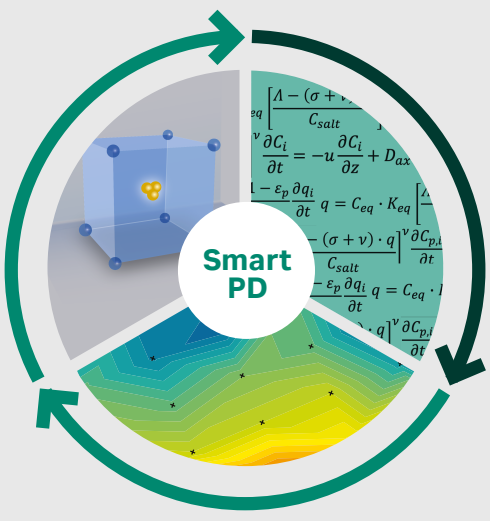
Mechanistic modeling of chromatography

Replace your lab experiments with computer simulations — obtain thousands of results in a few hours

Smart process development approaches

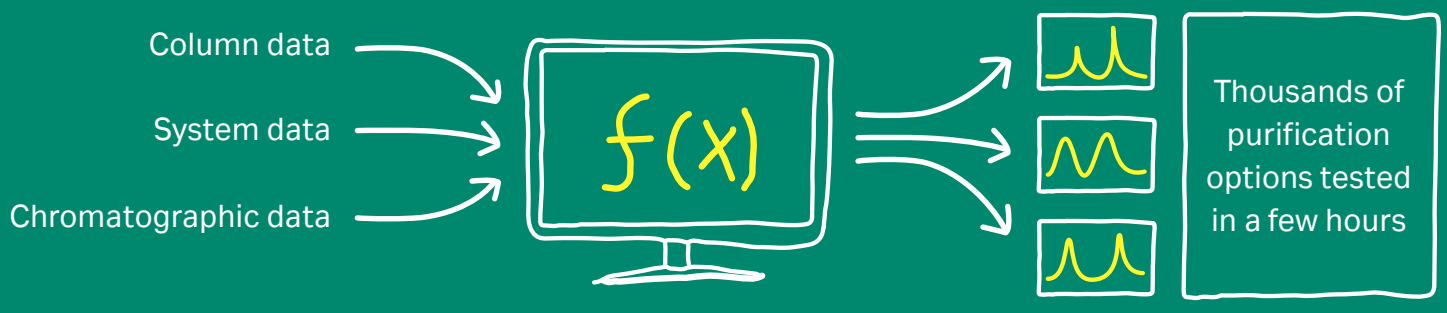


Statistical modeling
Multivariate data analysis such as design of experiments (DoE)

Mechanistic modeling
Computer simulation

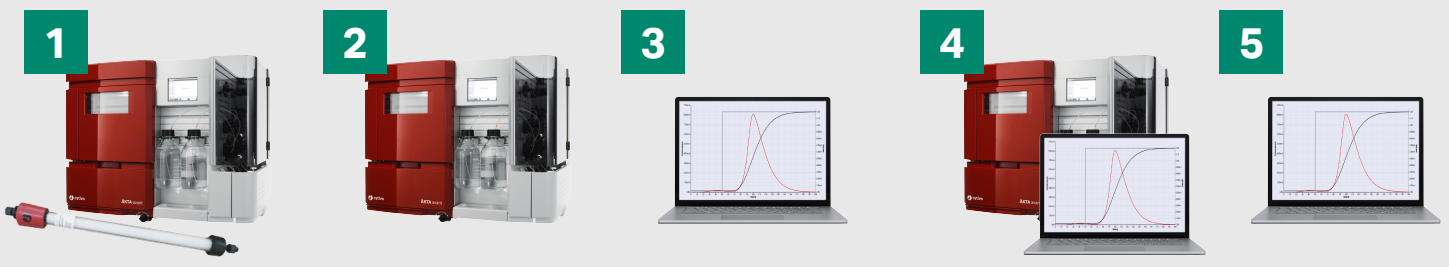
HTPD
Miniaturized and parallelized experiments

Mechanistic modeling = computer simulation of chromatograms



f(x) → Differential equations describe mass transport in the column.
Adsorption isotherms describe interactions with the ligands.

Typical workflow



Benefits of using mechanistic modeling

- Reduces your number of experiments
- Provides easily interpreted model parameter values
- Allows extrapolation beyond the boundaries of your experiments
- Generates process understanding (quality by design, QbD)
- Facilitates tech transfer since the model can be scaled up

→ Accelerated process development and improved processes

What can I use mechanistic modeling for?

- Optimizing wash and elution conditions
- Performing risk assessment
- Studying the influence of process variability (QbD)
- Developing design space and control strategy
- Facilitating tech transfer
- Performing a root cause analysis

How you can use mechanistic modeling throughout the drug development process

Preclinical	Phase I	Phase II	Phase III	Commercial
Accelerate process development for toxicity runs	Reduce number of runs for phase I process	Support scale-up and tech transfer activities	Reduce process characterization wet lab work	Support root cause analysis and release decisions for deviations

Tips to get started

- ✓ Focus on quality of data over quantity
- ✓ Make sure essential analytical support is obtained for fraction analysis
- ✓ Know your column and system parameters
- ✓ Use precalibrated columns
- ✓ Develop your modeling framework to allow for reuse
- ✓ Seek advice from experts if needed

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Learn more from cytiva.com/modeling

- Precalibrated *f*(x) columns
- Insights from modeling experts
- Modeling software