

Data-driven reaction optimization

About us

Use advanced data-driven optimization for rapidly identifying ideal chemical process parameters without writing even a single line of code. ReactWise reduces the experimental burden by up to 95% by effectively incorporating prior data, compared to full-factorial screening.

Our capabilities



Autonomous experimental design We employ state of the art machine learning algorithms to suggest the most promising experiments to perform next.^{1,2,3}



Multi-objective optimization Our Bayesian optimization algorithm enables multi-objective reaction optimization towards higher yield and reduced cost.4



Transfer-learning optimization The effective use of prior knowledge can reduce experimentation up to 95% compared to exhaustive screening.1



Integration with hardware and software Our platform can interact with commercial automation equipment as well as electronic lab notebook providers.

Our Technology

No-code software for chemical process optimization

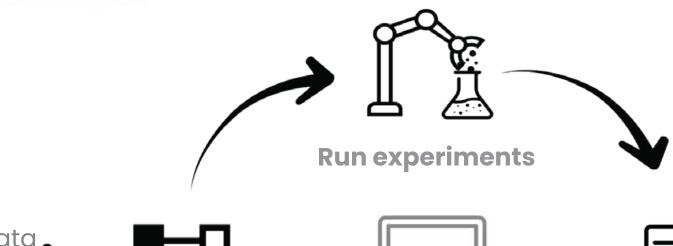


% exp. Saved

Exhaustive Screening

Software-hardware integration We have coupled our algorithmic approaches with commercial equipment to enable fully autonomous chemical reaction optimization.1





Prior Data **Data mining Select experiments**

Use prior Data⁵

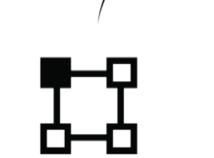
Accelerating workflows

using prior data can

reduce experimentation

up to 95% compared to

exhaustive screening.1







Update dataset

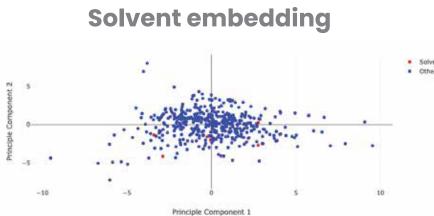




Molecular insights We use explainable AI to allow for traceability of decision making and visualize the impact of

structural elements.^{2,3}





Understand trade-offs We employ Bayesian optimization for multi-objective reaction

optimization increasing yield and sustainability while reducing cost.4

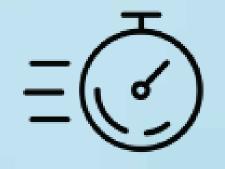
Predict next experiments

Benefits



Accessible machine learning

Data-driven optimization and chemical insights to improve the workflows of process chemists and increase efficiency.



Reduced time-to-market

Reduction of experimentation to identify suitable process parameters for drug synthesis.



Increased sustainability

Mitigation strategies for environmentally unfriendly solvents & reactants within chemical manufacturing.

Partners









conception



Book a demo here



Get in touch



Alexander Pomberger PhD CEO & Co-Founder Chemist & Chemical Engineer

> Alexander has a background in synthetic organic chemistry, laboratory automation and machine learning for chemistry



Daniel Wigh PhD CTO & Co-Founder Chemical Engineer

Daniel is experienced in chemical engineering, machine learning, and data engineering for chemistry.



Prof. Alexei Lapkin Advisor Professor in Chemical Engineering

Alexei's research focuses on sustainable manufacturing and process development by developing machine learning methods and Big Data approaches.

References

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2 Alexander Pomberger et al. React. Chem. Eng., 2022,7, 1368-1379

3 Alexei Lapkin et al Catalysis. Chem. Sci. 2019, 10, 6697–6706t

4 Alexei Lapkin Chem. Eng. Sci. 2022, 247, 116938

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