# Maximizing Yield and Conversion in Chemical Synthesis with IBM Research Europe

**Sector**
Molecular Discovery & Green Chemistry

**Impact**
Accelerated Reaction Optimization

**Overview**
Atinary Technologies and IBM Research Europe collaborated to enhance chemical reaction optimization, addressing the inefficiencies of traditional methods that rely on time-consuming trial and error. By combining Atinary's no-code AI platform, SDLabs, and Self-Driving Labs technology with IBM's RoboRXN (Chemspeed robotics), this partnership creates an autonomous workflow that efficiently navigates the large parameter space that is composed of more than 12,000 combinations, accelerating the optimization of chemical synthesis, specifically in the iodination of terminal alkynes.

**Challenge**
Establish an integrated and autonomous workflow (robotic automation and Bayesian Optimization techniques) for a desired chemical transformation - the iodination of terminal alkynes.

**Use Case**
IBM Research Europe used Atinary's SDLabs platform for a fully integrated AI, machine learning, and robotics workflow to close the loop in the optimization of iodination of terminal alkynes. This reaction, known for its complexity, was previously a bottleneck due to the extensive experimentation required — a chemical reaction with 2 synthesis routes and multiple optimization parameters to reach the objectives of maximum yield and high conversion rate. By combining their platforms, Atinary and IBM Research Europe demonstrated the power of integrating AI, automation, and robotics to run a data-driven approach that accelerates the speed and efficiency of chemical reaction optimization, produces high yield, and maximizes conversion rates.
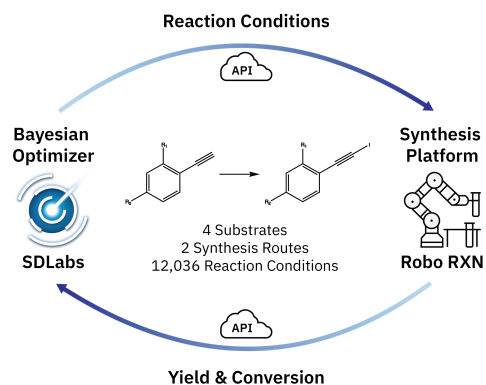


>80% Conversion reached for all 4 substrates in 25 experiments

Graphical abstract from Schilter et al. illustrating the integration of Atinary's AI platform and Self-driving labs technology, SDLabs, with IBM's RoboRXN robot.

**By the numbers**



| 8 | 2 | 12K |
|---|---|---|
| parameters | routes | possible combinations |

**Outcome**

Maximized product yield and achieved a conversion rate of over 80% for all four substrates in just 23 experiments, covering ca. 0.2% of the combinatorial space.

The integration of ML-driven experiment planning, automated equipment, and interpretability tools demonstrate the potential for expedited reaction condition optimization, allowing for a cleaner and more sustainable industry.

**Resources**

- Link to Atinary-IBM Research Europe Partnership Press Release:
- Link to Publication: Schilter et al. Combining Bayesian optimization and automation to simultaneously optimize reaction conditions and routes. *Chem Sci.* 2024 https://doi.org/10.1039/D3SC05607D
- Link to Atinary Webinar
- More about IBM Research Europe in Zurich

> *"The widespread use of AI and cloud technology will alter the way chemistry is conducted on a global scale and put chemists on the fast track to discovering new materials.*
>
> *Atinary's SDLabs and IBM'S RoboRXN are two pioneering technologies with the goal of embodying chemistry in the cloud and conducting real-world impactful research anywhere there is an internet connection.*
>
> *The synergy of the two complementary capabilities will demonstrate what two innovative groups can do with new technological paradigms."*
>
> — **Dr. Teodoro Laino**, Distinguished Research Scientist of IBM Research