ATINARY
ENABLING SELF-DRIVING LABORATORIES

Maximizing Yield and Conversion in Chemical Synthesis with IBM Research Europe

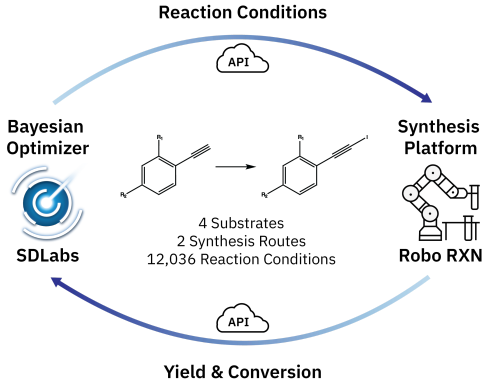
Sector
Molecular Discovery & Green Chemistry

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.

Challenges
Traditional methods for optimizing chemical reactions are often slow and resource-intensive. Researchers typically rely on trial and error, which can lead to inconsistent results and extended timelines. For complex chemical reactions like the iodination of terminal alkynes, these issues are even more pronounced, making it difficult to achieve reliable outcomes quickly.

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,

Platform Integration
The exploration of the optimal iodination of terminal alkyne was achieved through the seamless integration of Atinary and IBM Research Europe's two cloud-based solutions: Atinary's SDLabs platform and IBM's RoboRXN robotic platform. A smooth workflow was established by creating a backend application that enabled communication between the SDLabs and RoboRXN using a

JSON-based protocol to transfer reaction parameters and results.. Researchers could input experimental parameters into the SDLabs platform and receive optimized conditions within minutes, significantly speeding up the workflow and improving result accuracy. In addition, Atinary's analytics module provided diverse visualization techniques to follow the performance of the Bayesian optimizer as a function of the parameter space and the seen experiments.

Results

This study focused on the iodination of terminal alkynes, which holds significant importance in synthesizing complex organic molecules while preserving the alkyl group and introducing an iodide group. By exploring two different iodination routes, one involving chloramine salts and the other utilizing N-iodosuccinimide (NIS) as the iodinating agent, Atinary's SDLabs platform guided the optimization of the most effective reaction conditions. From a search space covering a total of 12 036 possible combinations, we have successfully optimized four different terminal alkynes and two reaction routes using IBM's automation platform combined with Atinary's proprietary machine learning optimization algorithms.

- 12,036 possible combination
- 8 parameters
- 2 reaction routes
- Over 80% conversion for all four reactants within a minimal number of just 25 distinct reactions, covering only ca. 0.2% of the total number of possible combinations.

These results were recently published in the Chemical Science Journal from the Royal Society of Chemistry, demonstrating the power of integrating Atinary SDLabs, our no-code AI Platform and Self-Driving Labs technology, with IBM's RoboRXN automated retrosynthesis platform for chemistry to revolutionize chemical reaction optimization.

Benefits

- **Accelerated Innovation:** AI and robotics integration speeds up the discovery and optimization of chemical reactions, leading to faster innovation.
- **Cost Efficiency:** Significant cost savings through reduced experimentation time and resource utilization.
- **Enhanced Accuracy:** High success rates in identifying optimal conditions reduce the need for repeated experiments.
- **Scalability:** The AI platform can be applied across various chemical reactions and industries, including pharmaceuticals and materials science.

Conclusion

The collaboration between Atinary Technologies and IBM Research Europe highlights the practical benefits of AI in chemical research. By combining machine learning algorithms with robotic platforms, Atinary's SDLabs platform delivers efficiency, cost savings, and accelerated innovation for R&D. This use case demonstrates how AI and robotics can drive significant advancements in chemical research.

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