

## AI-driven and self-driving labs technologies to accelerate R&D

Loïc Roch

Atinary Technologies, Route de la Corniche 4, 1066 Epalinges, Switzerland  
*loic@atinary.com*

In this talk, I will introduce Atinary's AI platform and self-driving labs technology solutions – SDLabs<sup>[1]</sup> – and will cover various use-case demonstrating how one can significantly accelerate and enhance R&D with a data-driven approach. Uses-case will span catalysis, reaction screening and process optimization.<sup>[2;3;4]</sup>

Scientists and operators can connect to SDLabs in the cloud and seamlessly integrate lab equipment and off-the-shelf robotic platforms into their workflows after just a few hours of onboarding. This allows companies and R&D labs to deploy AI and machine learning solutions seamlessly, without requiring coding or ML expertise, starting with simulations or directly within their existing wet lab workflows, with or without robots.

Atinary's AI solutions enable users to tackle complex optimization and discovery challenges that current methods cannot handle, including multi-objective and multi-parameter optimizations, categorical variables, and physicochemical descriptors.<sup>[5]</sup> We also provide algorithms for various constrained optimizations.

[1] <https://www.atinary.com>

[2] A. Ramirez, E. Lam, D. Pacheco Gutierrez, Y. Hou, H. Tribukait, L. M. Roch, C. Copéret, P. Laveille, *Chem. Catalysis*, **2024**, *4*, 100888

[3] O. Schilter, D. Pacheco Gutierrez, L. M. Folkmann, A. Castrogiovanni, A. García-Durán, F. Zipoli, L. M. Roch and T. Laino, *Chem. Sci.*, **2024**, *15*, 7732-7741

[4] <https://atinary.com/use-cases/>

[5] D. Pacheco Gutierrez, L. M. Folkmann, H. Tribukait and L. M. Roch, *Chimia* **2023**, *77*, 7