

Generative Chemistry for Weed Control: A Collaboration Between Syngenta and Insilico Medicine

Chris Baker¹, Suzanna Dale¹, Edward Emmett¹, Adrian Longstaff¹, Christian Noble¹, Steve Wailes¹, Russell Viner¹, Sarah Whalley¹, Bogdan Zagribelnyy², Alex Aliper², Alex Zhavoronkov², Petrina Kamya³, Allen Kao⁴ and Jimmy Lin⁴

¹ Syngenta, Jealott's Hill International Research Centre, Bracknell, Berkshire, UK

² Insilico Medicine, UAE Level 6, Unit 08, Block A, IRENA HQ Building Masdar City, Abu Dhabi, UAE

³ Insilico Medicine Canada Inc., 1250 René-Lévesque Ouest, Suite 3710, Montréal, Québec, Canada H3B 4W8

⁴ Insilico Medicine Taiwan, 110, Taiwan, Taipei City, Xinyi District, Section 1, Keelung Rd

chris.baker@syngenta.com

Generative chemistry has been proposed as a new approach for the design of bioactive small molecules.¹ Employing artificial intelligence (AI) to propose novel chemical structures that meet a pre-defined set of project requirements, it should in principle remove human biases from compound design and enable more efficient exploration of chemical space. But while much has been written in the literature about the potential of generative chemistry, there are, as yet, very few case-studies that describe its application within real-world R&D projects that have been shared outside the companies or organizations where they were performed.²

In February 2021, Syngenta announced a collaboration with the AI company Insilico Medicine,³ in which scientists from both companies would work together to apply Insilico Medicine's state-of-the-art AI platform Chemistry42⁴ within Weed Control chemistry projects within Crop Protection Research at Syngenta. Over the three years of the collaboration, generative chemistry was applied to three Syngenta research projects. In all of these projects, new lead areas were identified using the AI methods, and compounds proposed by generative chemistry showed both *in vitro* and *in vivo* activity. Alongside the novel compounds, the project has also delivered important lessons about the opportunities that a generative chemistry programme can bring. This presentation will share the story of the collaboration between Syngenta and Insilico Medicine: a "real world" deployment of generative chemistry.

[1] D. Mark, L. Friedrich, F. Grisoni, G. Schneider, *Mol Inf.* **2018**, *37*, 1700153.

[2] H. Chen *J. Med. Chem.* **2022**, *65*, 100-102.

[3] <https://www.syngenta.com/en/company/media/syngenta-news/year/2021/syngenta-crop-protection-and-insilico-medicine-harness>

[4] Y. A. Ivanenkov, D. Polykovskiy, D. Bezrukov, B. Zagribelnyy, V. Aladinskiy, P. Kamya, A. Aliper, F. Ren, A. Zhavoronkov, *J. Chem. Inf. Model.* **2023**, *63*, 695-701.