Digital Chemistry at Syngenta
From academic labs to industrial applications

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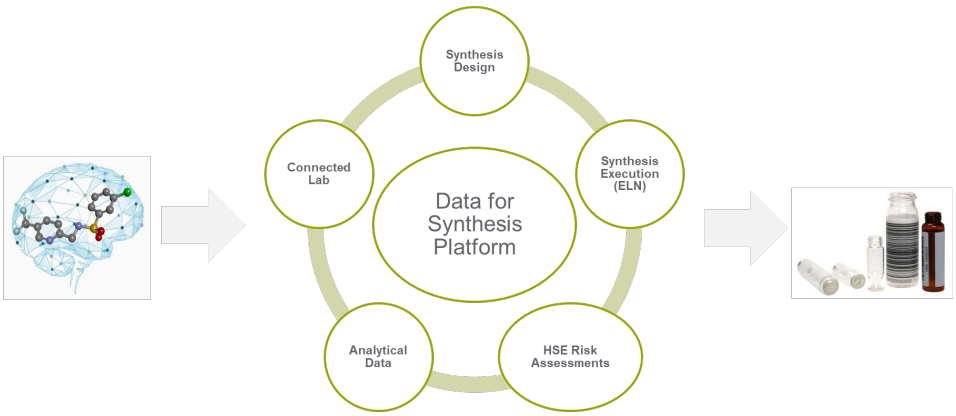
Modern agrochemicals must strike the right balance across a large panel of target properties from biological efficacy, resistance management, environmental impact, and cost of goods. This is arguably one of the more complex optimization tasks mankind undertakes. The introduction of the concept of inverse design and breakthroughs in generative chemistry enable to rethink this optimization approach.[1,2]

The linchpin to such approaches is the ability to select with high confidence molecules that can be readily synthesized. This requires reliable chemical reactivity models which need to be built on relevant high quality reaction data. Unfortunately, current electronic lab notebook technologies were not designed with data science applications in mind and do not enable to fully exploit the information contained in them.

To overcome this and as part of its digital transformation, Syngenta Crop Protection Research Chemistry has initiated an ambitious program to overhaul the whole software infrastructure that supports chemical synthesis from idea to physical sample.



In this presentation we will describe the main concepts and philosophy that went into the design of this platform and how this enables to integrate recent cutting-edge technology in a production environment that will ultimately serve hundreds of chemists worldwide.

References:

(1) Vanhaelen, Q.; Lin, Y.-C.; Zhavoronkov, A. The Advent of Generative Chemistry. *ACS Med. Chem. Lett.* **2020**, *11* (8), 1496–1505. https://doi.org/10.1021/acsmedchemlett.0c00088

(2) Sanchez-Lengeling, B.; Aspuru-Guzik, A. Inverse Molecular Design Using Machine Learning: Generative Models for Matter Engineering. *Science (80).* **2018**, *361* (6400), 360–365. https://doi.org/10.1126/science.aat2663