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Modern agrochemicals must strike the right balance across a large panel of target properties from biological efficacy, environmental impact, resistance management, and cost of goods. This is arguably one of the most complex optimization tasks in the chemical industry. Recent breakthroughs in inverse design and generative chemistry enable to rethink this optimization approach.1,2 Successful adoption of inverse design as research strategy, requires high quality data to build accurate models for relevant target properties. Most importantly, compounds need to be designed that can be readily synthesized. To address these challenges, 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.

References: