Augmenting Drug Hunters with Generative Chemistry Models

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Small-Molecule Drug discovery is a multi-objective optimization problem in which finding the next drug candidate depends on various characteristics of compounds including efficacy, pharmacokinetics and safety. In the design process of small molecule drugs, medicinal chemistry project teams routinely face this complex multidimensional optimization challenge. Given the massive size of the relevant "chemical space" (estimated to be in the range of up to 10^{60} drug-like molecules), the key question for medicinal chemists is *"What is the best compound to make and test next"*. While humans are extremely good in understanding the bigger picture, computers/algorithms are potentially much better in coming up with and evaluating a large body of complementary solutions – such as the described multidimensional optimization problem.

In this session, the concept of Generative Chemistry and how it approaches the above-mentioned optimization problem will be introduced based on a Novartis in-house initiative. Examples from medicinal chemistry project applications will be provided to highlight how such an *in silico* decision-support system can assists medicinal chemists in multi-objective compound design, selection and prioritization.