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# Merck to deploy Insilico Medicine's Chemistry42 AI platform for generative chemistry

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**Insilico Medicine announces the first deployment of its flagship generative chemistry AI platform for de novo molecular design, Chemistry42™ on Merck KGaA, Darmstadt, Germany's high-performance computing infrastructure**


Following the release of Chemistry42 to a select group of key experts in the pharmaceutical industry in Q3 2020, Insilico Medicine announced that Merck KGaA, Darmstadt, Germany will be the first launch partner for its flagship generative chemistry artificial intelligence (AI) platform - Chemistry42. Merck KGaA, Darmstadt, Germany will integrate Chemistry42™ into their discovery pipeline to facilitate rapid and effective drug design. Chemistry42 v1.0 will be customized and deployed on state-of-the-art high-performance computing (HPC) infrastructure at Merck KGaA, Darmstadt, Germany.

Since the publication of Ian Goodfellow's original paper on generative adversarial networks (GANs) in 2014, Insilico Medicine has been developing generative chemistry and generative biology algorithms. In 2016, Insilico Medicine published the first peer-reviewed publication describing the application of GANs to small molecule discovery in oncology. Between 2016 and 2020 Insilico Medicine authored over 40 papers and has been granted several patents in this field. Insilico Medicine has conducted several proof of concept validation experiments that demonstrate that generative models can successfully identify novel targets, and design molecules with desired properties that can be synthesized and tested *in vitro* and *in vivo*.

Chemistry42™ is a core part of Insilico's Pharma.ai drug discovery suite. It is a flexible, user-friendly software platform that bridges artificial intelligence (AI) and machine learning methods with domain expertise in the fields of medicinal and computational chemistry, for the design of novel small molecules with desirable physicochemical properties. The platform is a scalable distributed web application, capable of running multiple tasks in parallel in a matter of hours. Container orchestration and workflow management allow for predictable hardware-agnostic resource allocation, and for the implementation on either cloud or local HPC infrastructures.

"Chemistry42 v1.0 is the result of years of comprehensive research in generative chemistry, close collaboration between computational and medicinal chemistry scientists, and best high-performance computing engineering practices. We are excited to work closely with Merck KGaA, Darmstadt, Germany and look forward to demonstrating the impact of our collaboration on their drug discovery programs," said Alex Zhebrak, PhD, CTO of Insilico Medicine.