

News Release

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MilliporeSigma Launches First Ever AI Solution to Integrate Drug Discovery and Synthesis

- **Combines generative AI, machine learning and computer-aided drug-design to increase the success rate of new drugs and therapies**
- **Virtually screens compounds from a universe of >60 billion chemical targets and evaluates synthesis routes for safer, cost-effective, higher-yield drug manufacturing**
- **Recommends chemicals, reagents and building blocks for synthesis**

Burlington, MA, December 5, 2023 – MilliporeSigma, the U.S. and Canada Life Science business of Merck KGaA, Darmstadt Germany, a leading science and technology company, today launched its [AIDDISON™ drug discovery software](#), the first software-as-a-service platform that bridges the gap between virtual molecule design and real-world manufacturability through [Synthia™ retrosynthesis software](#) application programming interface (API) integration.

It combines generative AI, machine learning and computer-aided drug-design to speed up drug development. Trained on more than two decades of experimentally validated datasets from pharmaceutical R&D, AIDDISON™ software identifies compounds from over 60 billion possibilities that have key properties of a successful drug, such as non-toxicity, solubility, and stability in the body. The platform then proposes ways to best synthesize these drugs.



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“With millions of people waiting for the approval of new medicines, bringing a drug to market, still takes on average, more than 10 years and costs over US\$2 billion¹” said Karen Madden, Chief Technology Officer, Life Science business sector of Merck. “Our platform enables any laboratory to count on generative AI to identify the most suitable drug-like candidates in a vast chemical space. This helps ensure the optimal chemical synthesis route for development of a target molecule in the most sustainable way possible.”

Discovering drugs is a long, iterative process. Only about 10% of drug candidates evaluated in Phase I made it to market². To find the most suitable chemical compound from a universe of more than 10⁶⁰ molecules³ requires significant time, resources, and expertise. Artificial Intelligence (AI) and machine learning models like AIDDISON™ software can extract hidden insights from huge datasets, thus increasing the success rate of delivering new therapies to patients. AI has the potential to offer more than US\$70 billion in savings for the drug discovery process by 2028, and to save up to 70% time and costs for drug discovery in pharmaceutical companies⁴.

Merck is a globally diversified science and technology company with leading positions in life science, healthcare, and electronics, leveraging key synergies to fuel future-forward innovation. By combining expertise in small molecules, biologics, and new modalities with AI and other digital tools, Merck helps to redefine how drugs are discovered, developed, and made. Aligning the right bioconvergent technologies, knowledge, and partners to leverage AI, automation and other digital tools will help bring better therapies to patients faster.

¹ <https://pubmed.ncbi.nlm.nih.gov/32270704/>

² <https://www.sciencedirect.com/science/article/pii/S2211383522000521>

³ <https://pubs.acs.org/doi/10.1021/ar500432k>

⁴ <https://bekryl.com/industry-trends/ai-artificial-intelligence-in-drug-discoverymarket-size-analysis>

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About the Life Science business of Merck KGaA, Darmstadt, Germany

The Life Science business of Merck KGaA, Darmstadt, Germany, which operates as MilliporeSigma in the U.S. and Canada, has more than 28,000 employees and more than 55 total manufacturing and testing sites worldwide, with a portfolio of more than 300,000 products focused on scientific discovery, biomanufacturing and testing services. Merck KGaA, Darmstadt, Germany, a leading science and technology company, operates across healthcare, life science and electronics.

More than 64,000 employees work to make a positive difference to millions of people's lives every day by creating more joyful and sustainable ways to live. From providing products and services that accelerate drug development and manufacturing as well as discovering unique ways to treat the most challenging diseases to enabling the intelligence of devices – the company is everywhere. In 2022, Merck KGaA, Darmstadt, Germany, generated sales of € 22.2 billion in 66 countries.