Merck launches first ever AI solution to integrate drug discovery and synthesis

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Combines generative AI, machine learning and computer-aided drug-design to increase the success rate of new drugs and therapies

Merck, a leading science and technology company, has 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 ^{TM} retrosynthesis software application programing 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.

Discovering drugs is a long, iterative process. Only about 10% of drug candidates evaluated in Phase I made it to market. To find the most suitable chemical compound from a universe of more than 10^{60} molecules 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 $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 companies.