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Merck to use Generative Modelling AI technology

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Generative modelling AI technology enables rapid and cost-effective design of novel drugs



Merck, a leading science and technology company, has announced a collaboration agreement with Iktos, for the use of its generative modelling artificial intelligence (AI) technology, in order to facilitate the rapid and cost-effective discovery and design of promising new compounds.

Iktos' AI technology, which is based on deep generative models, helps bring speed and efficiency to the drug discovery process, by automatically designing virtual novel molecules that have desired activities for treating a given disease. This tackles one of the key challenges in drug design: rapid identification of molecules which simultaneously satisfy multiple drug-like criteria for clinical testing.

The technology is already successfully established in other fields, such as image processing and automatic translation, but has only recently been applied to chemistry.