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Japan verifies use of AI for retrosynthetic analysis in pharma applications

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A retrosynthetic analysis model would provide tremendous benefit in exploring various synthetic routes and reducing development times



Japan-based Elix, Inc., an AI drug discovery company, has commenced joint research on the retrosynthetic analysis module Elix Synthesize with Shionogi & Co., for the purpose of verifying retrosynthetic analysis using chemical reaction data from Shionogi.

In the Pharmaceutical industry, artificial intelligence (AI) is being used for activity and property prediction as well as molecular design with desired properties. Moreover, there is an increased attention being given to the purpose of utilizing AI for retrosynthetic analysis.

Elix Synthesize features peerless high-speed processing using parallel computation and it can efficiently explore various synthetic routes by processing large amounts of data at high speed. It can propose a more optimized synthetic route, considering multiple factors, such as yield, cost, and available reagents. In addition to the aforementioned variables, Elix Synthesize is highly customizable, making it possible to consider custom variables that are inline with the client's objectives when proposing a route.

In this joint research, Elix Synthesize will be customized to match Shionogi's proprietary data to validate a highly accurate, high-speed, practical retrosynthetic analysis model for drug discovery research.

Shinya Yuki, CEO of Elix, Inc. said: "In recent years, we have seen numerous examples of molecular design using AI, but those models have not been able to take into account the synthesizability. This is why retrosynthetic analysis models have been attracting attention. In reality, however, they are yet to see commercialization due to two major limitations: (1) the complexity of the algorithms and (2) the lack of data sets. We look forward to collaborating with Shionogi by leveraging our different strengths; Elix's knowledge of algorithms and Shionogi's data set and understanding of the field's needs".