

SyntheticGestalt presents the world's largest molecule-specific 'large-scale pre-trained model' at NVIDIA GTC

The presentation will cover the utility of the model in making predictions on data that is far removed from the training data in the Drug Discovery domain

TOKYO, JAPAN, March 15, 2024

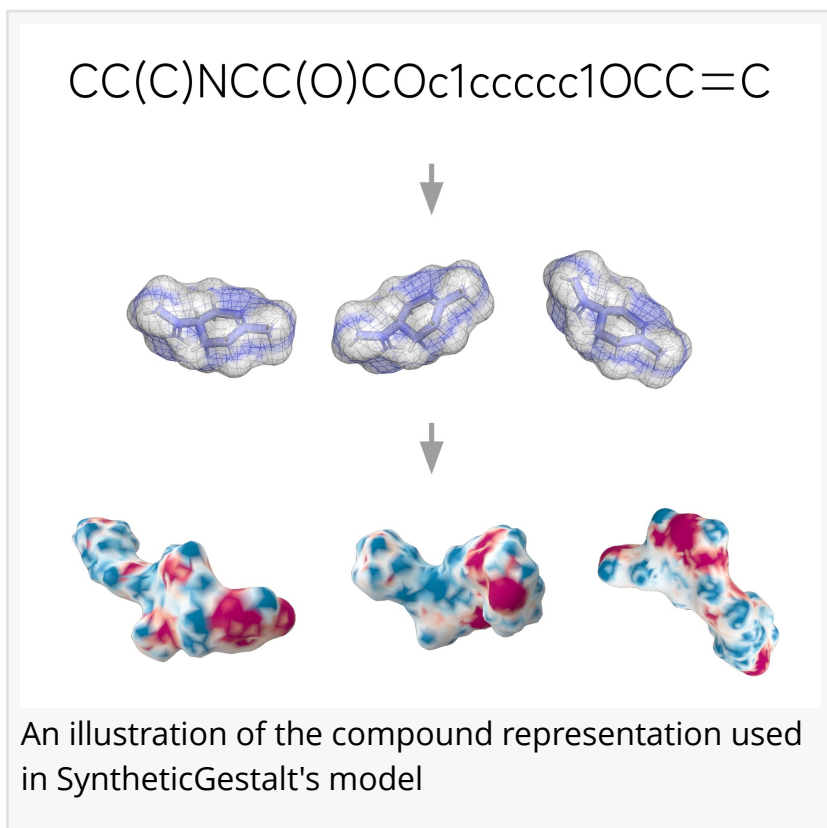
/EINPresswire.com/ -- SyntheticGestalt is pleased to announce that on 22 March 2024 (Friday) at 16:00 JST, the Company will be presenting the results of its research, a large-scale pre-trained model specialising in small molecules. The presentation will take place online at GTC, a global artificial intelligence conference for developers, hosted by NVIDIA.

The presentation title is as follows (English with Japanese Subtitles) :

One billion compounds to empower next-gen AI drug discovery: a case study in the use of large-scale pre-training [SE62873]

Our presentation proposes a solution to one of the biggest challenges in AI drug discovery, namely that AI cannot make good predictions on data that is far from the trained data. We report achieving a significant improvement in accuracy by using a large-scale training data set of one billion compounds. Although other companies have developed large-scale pre-trained models specialising in molecules, this is the largest model in the world in terms of both the volume of training data and the complexity of the compound features used in the training.

Dr Souradip Mookerjee, our Research Engineer, will present the utility of our large-scale pre-trained model in making predictions on data that is far removed from the training data, based on the prediction accuracy against actual experimentally measured values (initial toxicity and pharmacokinetic parameters).



The presentation will also show that the model's ability to significantly improve prediction accuracy can be used in various other molecular discovery projects, and that it can also be used to build more accurate models for specific purposes.

How to watch:

Please [register with NVIDIA GTC Day](#) to watch the following seminar on 22 Mar from 16:00-16:25 JST:

[Seminar link](#)

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