Enamine and SyntheticGestalt to Collaborate on the Creation of AI-Based Model to Facilitate Drug Discovery

KYIV, UKRAINE , January 11, 2024 /EINPresswire.com/ -- □□□□□□□□□□□□□□□□□ □□□□□ □□□□□□□□ □ □□□□-□□□□□□□□ □□ □□□□□□ □□ □□□□□□□□□ □□□□□□□□□□□□□□ □□□□□-□□□□□ □□□□ □□□□□□□□□□□. □□□□□ □□□□□□ □□□□□ □□□□□□□□ 38 □□□□□□□□ □□□□□□□□□□ □□□□□ □□□□□□□□ □□□□□ □□□□□□□□□ □□ □ □□□□□□□□ □□□□ □□□□-□□□□□□□□□.

SyntheticGestalt, a research and development company specializing in the application of AI to the life sciences domain, and Enamine, the world's leading provider of chemical building blocks, screening compounds, and integrated drug discovery services, have announced the start of a joint effort to create a suite of AI models that will enable the generation of synthetically accessible biologically active compounds with optimized physicochemical and ADME/ Tox properties. The models will be applicable to the compound discovery initiatives of SyntheticGestalt, as well as its service for both academic users and pharmaceutical companies.

Enamine will provide access to its largest enumerated database of make-on-demand compounds, Enamine REAL database, which has 38 billion molecules in its current edition. SyntheticGestalt will add the REAL database to its Drug Discovery Service, which uses proprietary AI models to provide predictions on physicochemical and ADME/ Tox properties of compounds. For compounds with issues, the service proposes improved alternative compounds instantaneously.
Enamine will synthesize the selected compounds within just 3-4 weeks and provide quality pharmacological □□ □□□□□ profiling data through the in-house tests to streamline and shorten the discovery cycle.

Furthermore, SyntheticGestalt will enhance its pre-trained AI model using the data provided by Enamine. It is expected to become the largest pre-trained model in the world based on the 3D

structures of the compounds, to improve the predictive accuracy of SyntheticGestalt's machine learning models. The resulting models will be offered on a joint research basis to certain interested parties. The pre-trained AI model and its performance will be presented at NVIDIA's annual event, NVIDIA GTC Japan AI Day, in March of 2024.

[illegible], [illegible] at [illegible] commented: "[illegible]

[illegible], [illegible] at [illegible] commented: "[illegible]

[illegible]

[illegible]
SyntheticGestalt is an artificial intelligence research and development company specialising in AI drug discovery and other life science fields. Its research and development are focused on the discovery of useful substances using its independently developed artificial intelligence technology. The AI platform used in this research has a cloud-based, scalable structure and can make predictions on large libraries, making it possible to predict physicochemical and ADME/ Tox properties and early toxicity, as well as enzyme functions. SyntheticGestalt welcomes open innovation through joint research with public institutions and private companies. For more information visit: https://syntheticgestalt.com

[illegible]
SyntheticGestalt offers a web service specifically aimed at proposing solutions to ADME/ Tox and physicochemical problems of Hit ~ Lead compounds, based on its proprietary machine learning models. The service is available for trial from the following link:
https://drugdiscovery.syntheticgestalt.com/

[illegible]
Enamine is a scientifically driven integrated discovery Contract Research Organisation with

unique partnering opportunities in exploring new chemical space. The company combines access to the in-house produced screening compounds (4M in stock) and building blocks (300K in stock) with a comprehensive platform of integrated discovery services to advance and accelerate the efforts in Drug Discovery. For more information visit: https://enamine.net

□□□□□ □□□□□□□ □□□□ □□□□□□□□

Enamine REAL® Database (□□adily □ccesib□e) is a collection of over 38 billion enumerated molecules that can be synthesized at Enamine extremely fast (3-4 weeks), with high feasibility (over 80%), and inexpensive. The REAL compounds are created by parallel chemistry through the compilation of 137,000 building blocks via 167 different synthesis protocols, underlying Enamine's approach to design make-on-demand compounds to maximize synthesis success rate.

Iaroslava Kos
Enamine Ltd.
info@enamine.net
