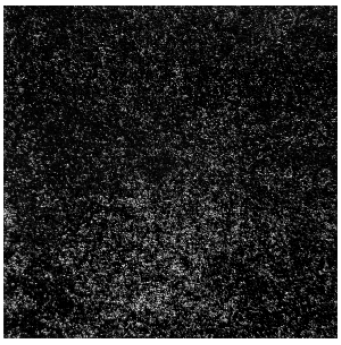
SyntheticGestalt to pioneer Enamine' B-REAL Space of 38 billion compounds leveraging AI to deliver lead compounds faster

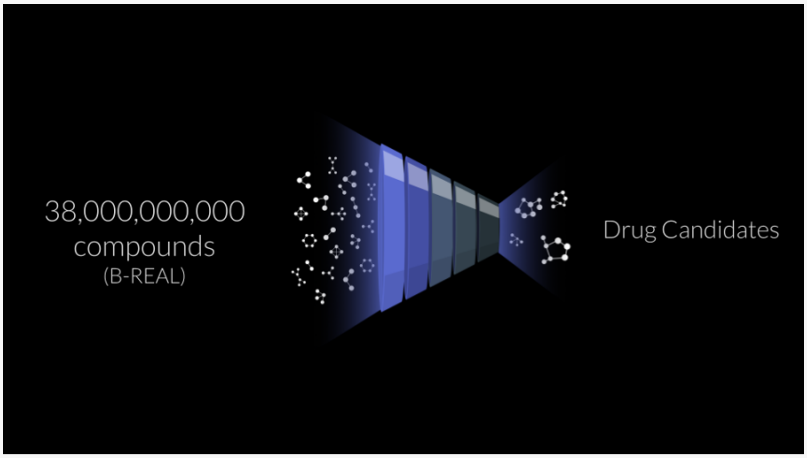
KYIV, UKRAINE, June 21, 2024 /EINPresswire.com/ -- SyntheticGestalt, an AI company specializing in the life sciences domain, and Enamine, a pioneer in the creation of ultra-large chemical spaces of highly feasible compounds, announced today a new research program involving the application of AI for novel drug discovery, followed by biological tests of REAL compounds directly at Enamine (B-REAL).



At the beginning of 2024, the partners started collaborating on generating synthetically accessible biologically active compounds with optimized physicochemical and ADME/ Tox properties.

SyntheticGestalt has developed the world's largest molecular-specific AI model using Enamine's REAL Space of 38 billion compounds. In this program, SyntheticGestalt will predict the activity against selected targets with simultaneous optimization of ADME/ Tox parameters, to search for favourable lead compounds from the REAL space of 38 billion compounds.

In the longer term, the company aims to solve the long-standing problem of AI drug discovery of "high performance on training data but low performance in empirical research." SyntheticGestalt's efforts were presented at this year's NVIDIA annual conference (see: https://www.nvidia.com/en-us/on-demand/session/gtc24-se62873/).



The developed AI model significantly reduces the drug discovery cycle, and while relying on Enamine's REAL Space, it offers another immense benefit. With ever-increasing complications in chemical compound logistics and customs formalities, shipping research samples has significantly contributed to drug discovery's sluggish speed and exorbitant cost. Typical collaboration projects involve multiple CROs, which all must be repeatedly served with chemical compounds to work on. The discovery collaborations are suffocated by compounds stuck at customs or delayed by logistics and compound management teams. The compounds synthesized using the B-REAL platform will be immediately subjected to a broad panel of ADME/ Tox, PK and activity tests directly at Enamine in Bienta biology labs. The data will be provided in a time that is shorter than required for shipping compounds alone. Thus, the overall synthesis and test turnaround time will be reduced to 4-6 weeks.

Dr Petro Borysko, Head of Enamine's biology department Bienta, commented: "We are delighted to contribute our expertise to the largest-ever compound search initiative in Japan. Our biology labs receive compounds from chemistry colleagues within only one day after short registration in our database. There is no need for our partners to deal with unnecessary compound logistics. The early biological data can guide further research quicker."

Dr Iaroslava Kos, Director of Business Development at Enamine, added: "While our partners are discovering new drug candidates from among 38 billion compounds, Enamine's B-REAL platform converts virtual hits into tangible results. Within weeks, novel and promising compounds are synthesized and rigorously tested in vitro. This represents the pinnacle of efficiency and reliability in discovery chemistry and our commitment to advancing drug development and reshaping the landscape of pharmaceutical research."

Kotaro Kamiya, CTO at SyntheticGestalt, commented: "The immense scale of this AI drug discovery initiative, combining SyntheticGestalt's world-largest model with Enamine's colossal REAL Space, presents a significant challenge for us. We are deeply grateful for the various support we have received, which has enabled us to embark on this ambitious endeavour. We are confident that the success of this project will pave the way for new possibilities in AI-driven drug research, opening doors to groundbreaking advancements in the field."

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