

英科智能 Insilico Medicine

insilico.com

Next-generation Artificial Intelligence for
Health and Longevity

F R O S T  S U L L I V A N

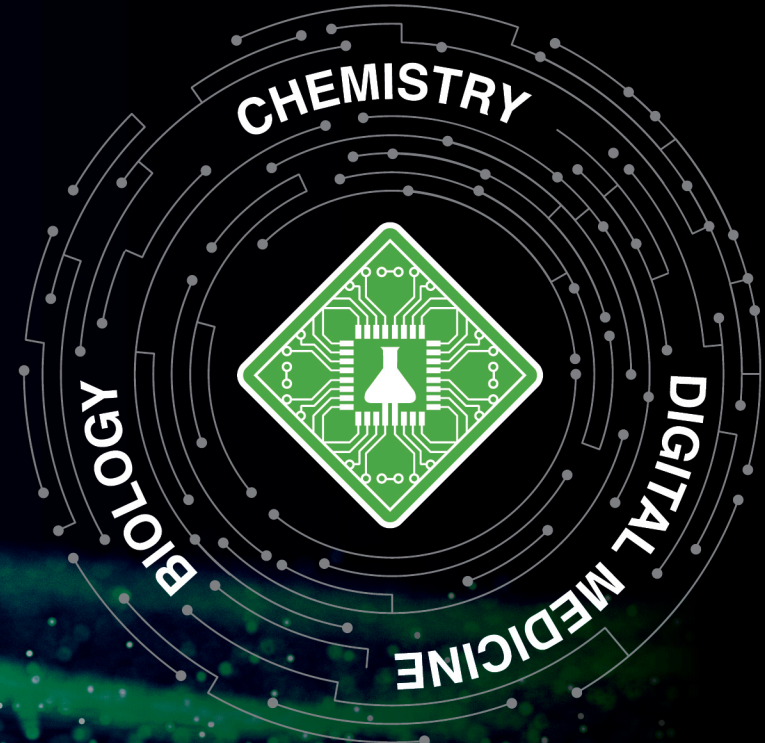
2018 North American Artificial Intelligence for Aging
Research and Drug Development Award



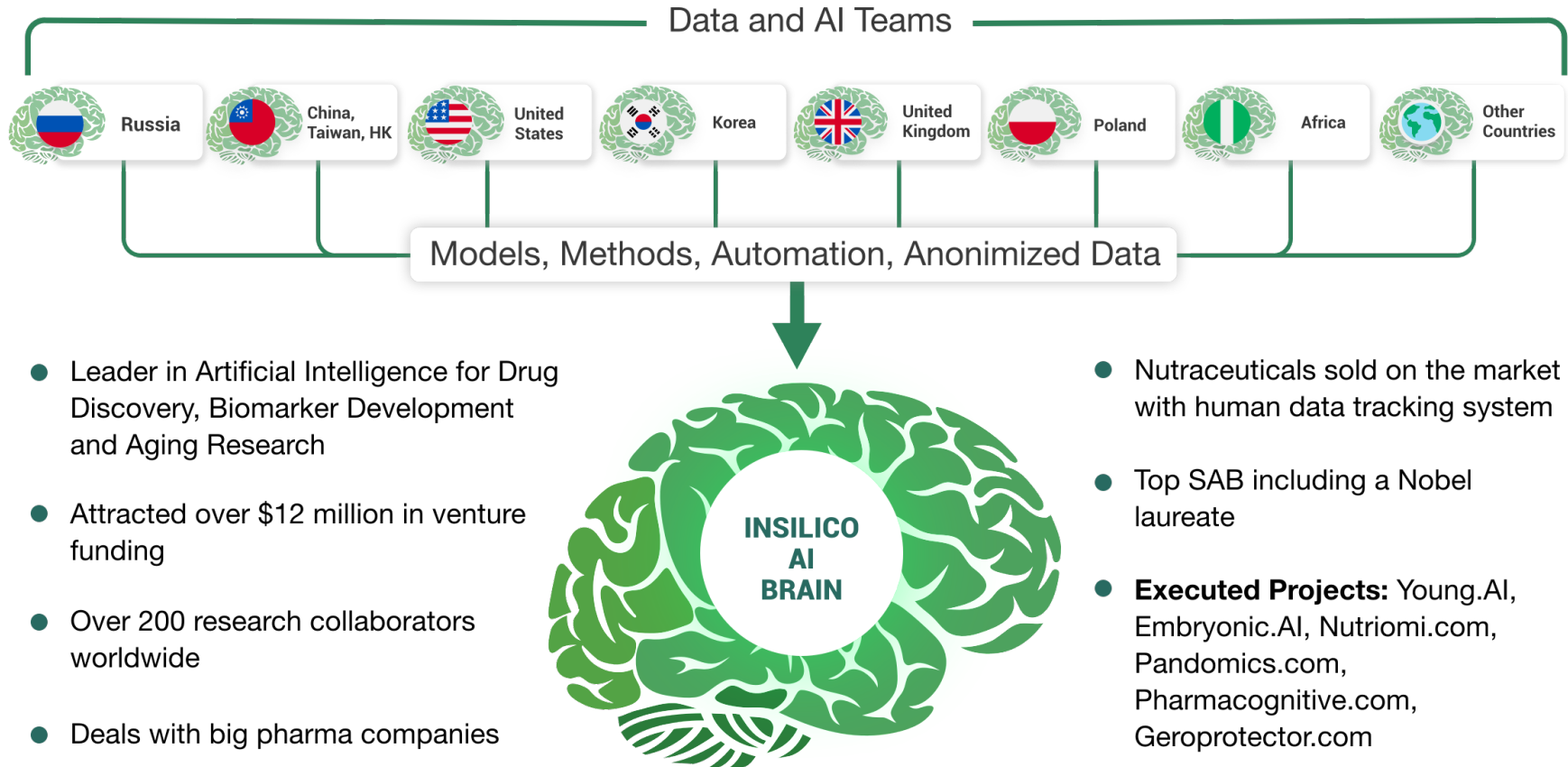
Insilico AI Engine is a Unique Blend of Scientific Disciplines



- In the pharmaceutical companies human domain experts in biology, chemistry and digital medicine are disconnected.
- While most other AI startups focus on specific verticals and applications in a disconnected manner, Insilico AI engine aims to bridge biology, chemistry and digital modules into one seamless learning pipeline enabling our AI scientists to take on previously impossible chemistry and biology tasks.



Global sourcing of talent, data and innovation



Market Opportunity — Pharmaceuticals



The current drug development process is expensive and inefficient. Most of the failures are due to the wrong disease-target association. **Using AI, we can bring effective drugs to market faster.**

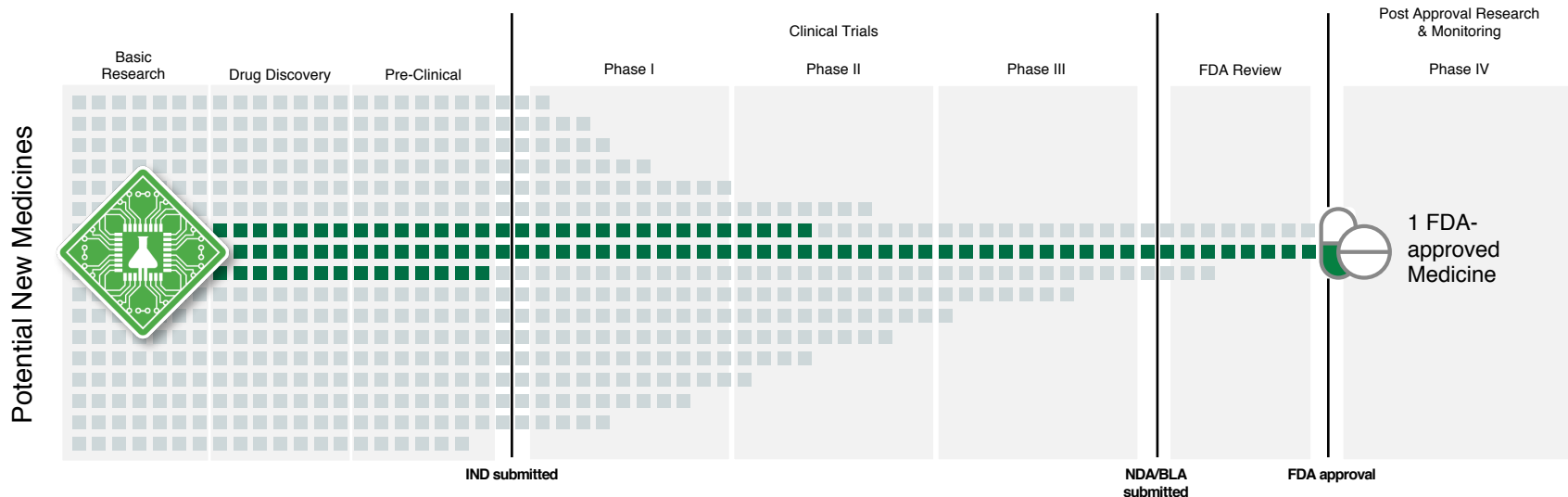
> \$2.63B

to develop one drug

92%

failure rate after
years of development

Current State of Drug Discovery and the Potential of AI

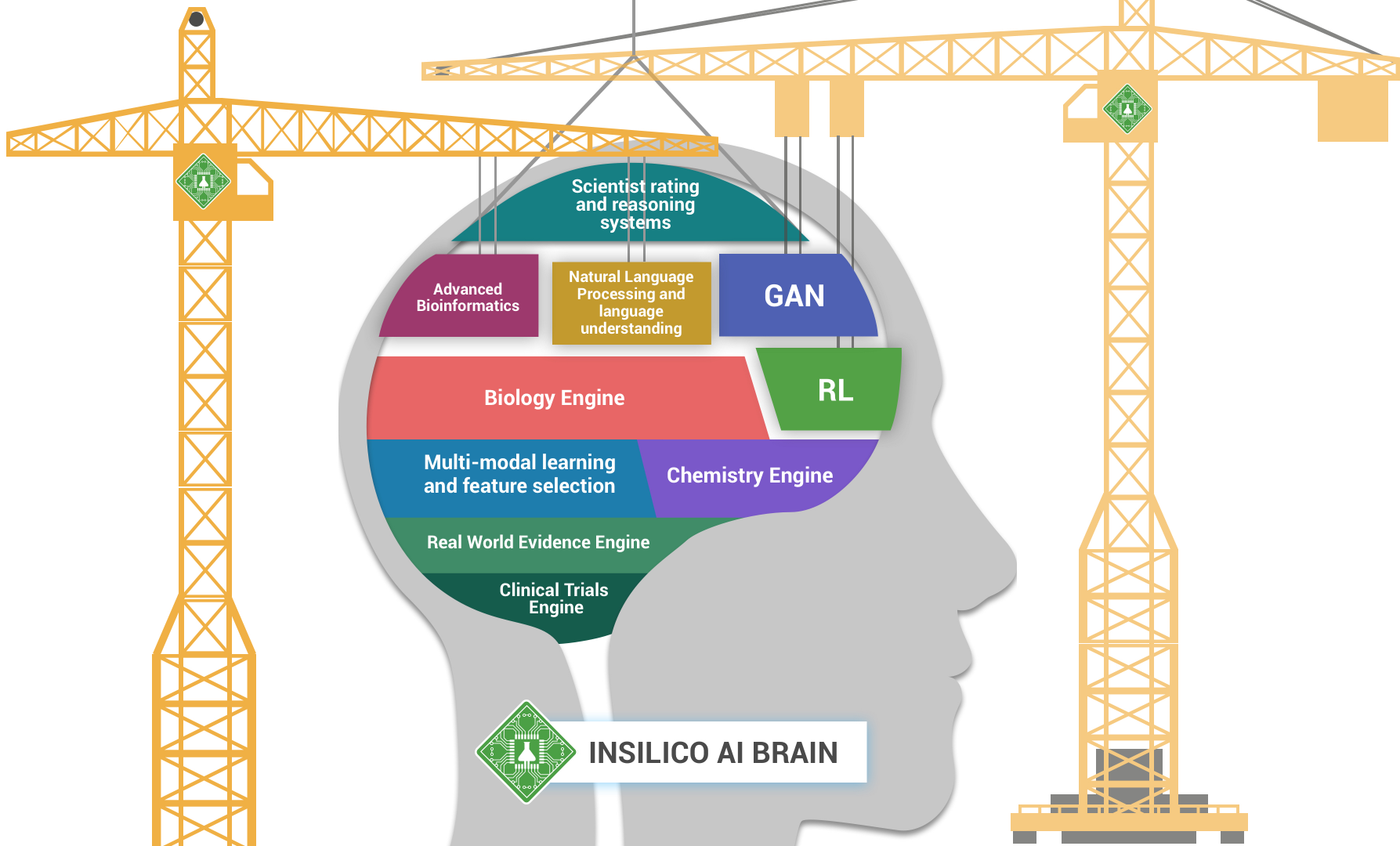


The potential to reduce failures and deliver cures is at the **preclinical** stage.

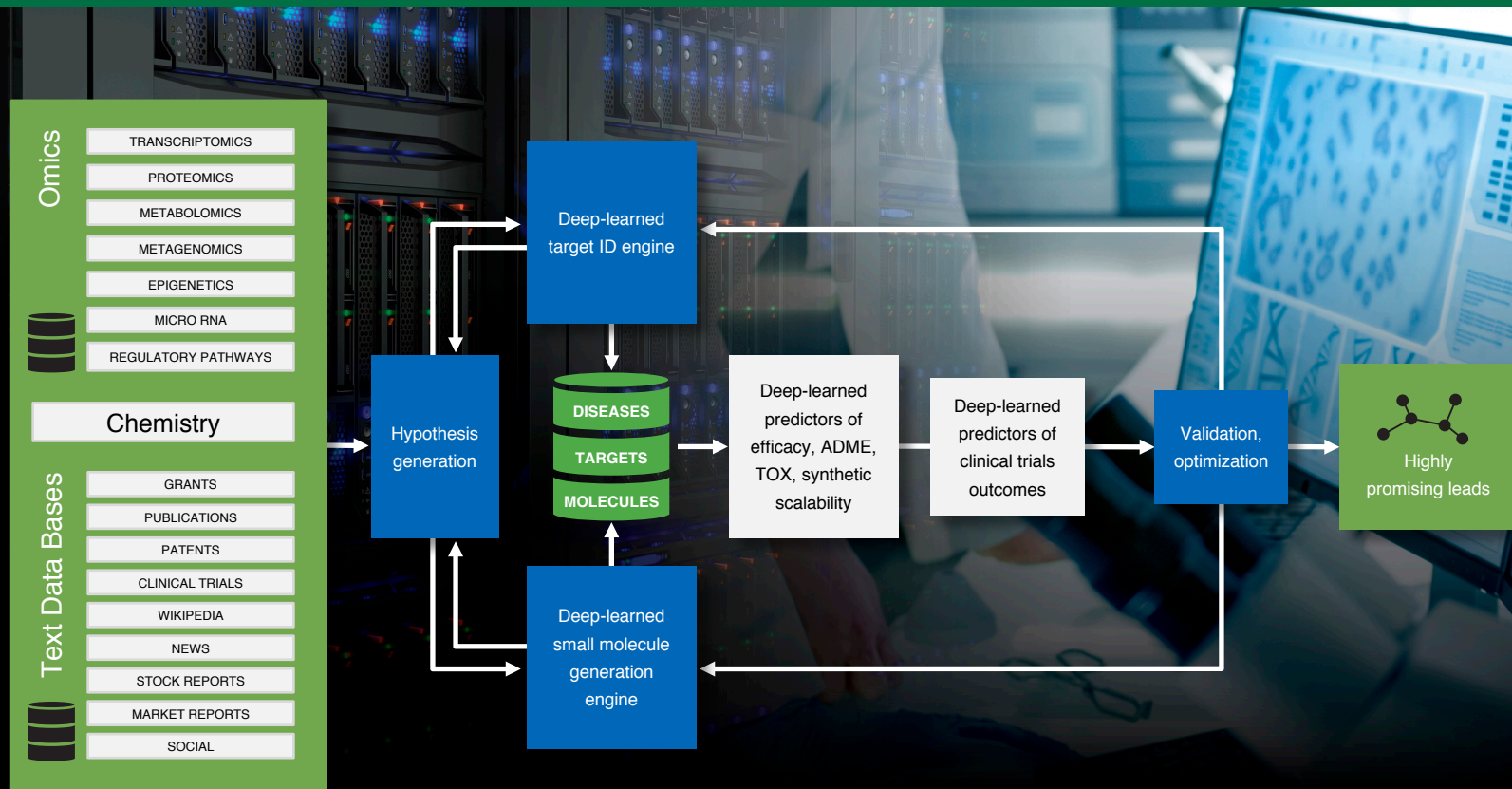
AI cannot shorten the clinical trials cycle but it can **deliver real cures to the right patients and reduce the failure rate.**

Once several drugs designed by AI reach the market the regulators are likely to **shorten the clinical trials time.**

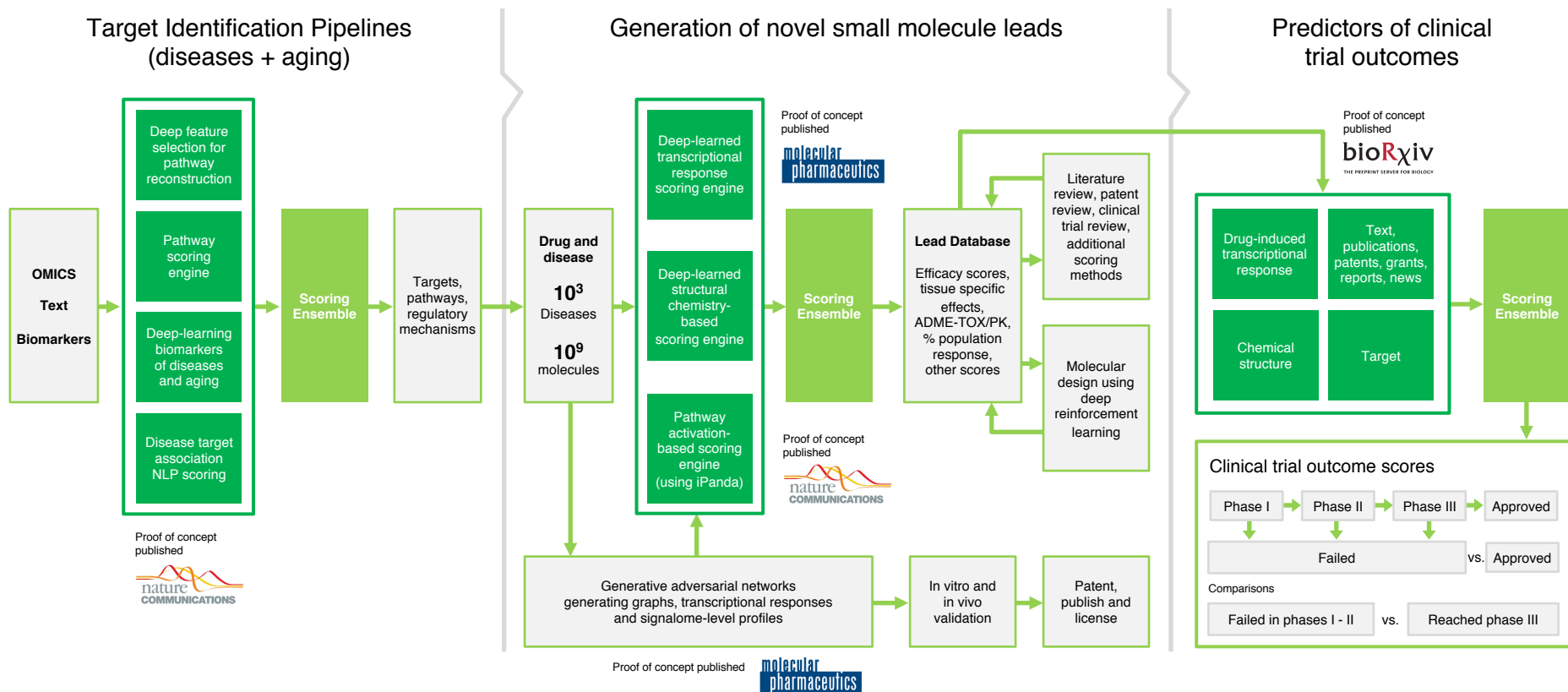
The goal of AI is to shorten the research, discovery and preclinical stage from 3-4 years to a matter of months. This will save valuable time and financial resources in the development stage while providing stronger drug candidates for approval.



The Industry's Most Advanced End-to-End Drug Discovery AI



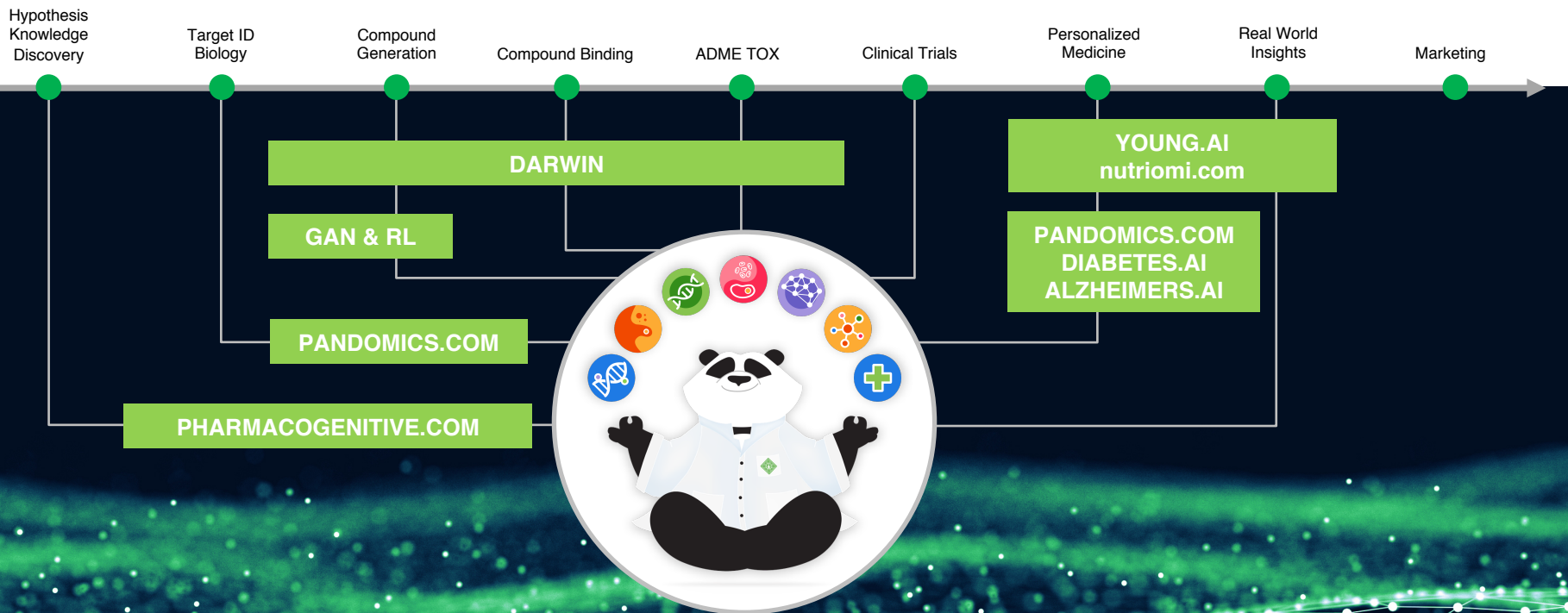
The Industry's Most Advanced End-to-End Drug Discovery AI



Panda.AI Integrated Deep Learning Framework and Library



Applicable to every step of pharmaceutical drug discovery and development



Proof of Concept Publications: PUBMED: “Insilico + Medicine”

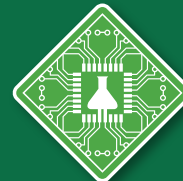


Type	Title
GAN-RL for Med. Chemistry	Entangled Conditional Adversarial Autoencoder for de Novo Drug Discovery. <i>ACS Mol. Pharm</i> , 2018
GAN-RL for Med. Chemistry	Reinforced Adversarial Neural Computer for De Novo Molecular Design. <i>ACS Chem. Informatics</i> , 2018
GAN-RL for Med. Chemistry	Adversarial Threshold Neural Computer for Molecular De Novo Design. <i>ACS Mol. Pharm</i> , 2018
DNNs for Target ID	Machine Learning on Human Muscle Transcriptomic Data for Biomarker Discovery and Tissue-Specific Drug Target Identification, <i>F. Gen.</i> 2018
3D Representation of Molecules	3D Molecular Representations Based on the Wave Transform for Convolutional Neural Networks. <i>ACS Mol. Pharm</i> , 2018
DNNs for Age Prediction	Population specific biomarkers of human aging: a big data study using South Korean, Canadian and Eastern European patient populations. <i>Journal of Gerontology Section A</i> , 2018
GANs for Med. Chemistry	druGAN: An Advanced Generative Adversarial Autoencoder Model for de Novo Generation of New Molecules with Desired Molecular. <i>Properties In Silico. ACS Mol. Pharm.</i> , 2017
DNNs for Side Effects	Towards natural mimetics of metformin and rapamycin. <i>Aging</i> , 2017
DNNs for Target ID	Use of deep neural network ensembles to identify embryonic-fetal transition markers: repression of COX7A in embryonic and cancer cells. <i>Oncotarget</i> , 2017
GANs for Medicinal Chemistry	The cornucopia of meaningful leads: Applying deep adversarial autoencoders for new molecule development in oncology. <i>Oncotarget</i> , 2016
Dimensionality Reduction Algorithm	In silico Pathway Activation Network Decomposition Analysis (iPANDA) as a method for biomarker development. <i>Nature Communications</i> , 2016
DNNs for Classification of Molecules	Deep Learning Applications for Predicting Pharmacological Properties of Drugs and Drug Repurposing Using Transcriptomic Data. <i>ACS Molecular Pharmaceutics</i> , 2016
DNNs for Age Prediction	Deep biomarkers of human aging: Application of deep neural networks to biomarker development. <i>Aging</i> , 2016
DL Review	Applications of Deep Learning in Biomedicine. <i>ACS Molecular Pharmaceutics</i> , 2016

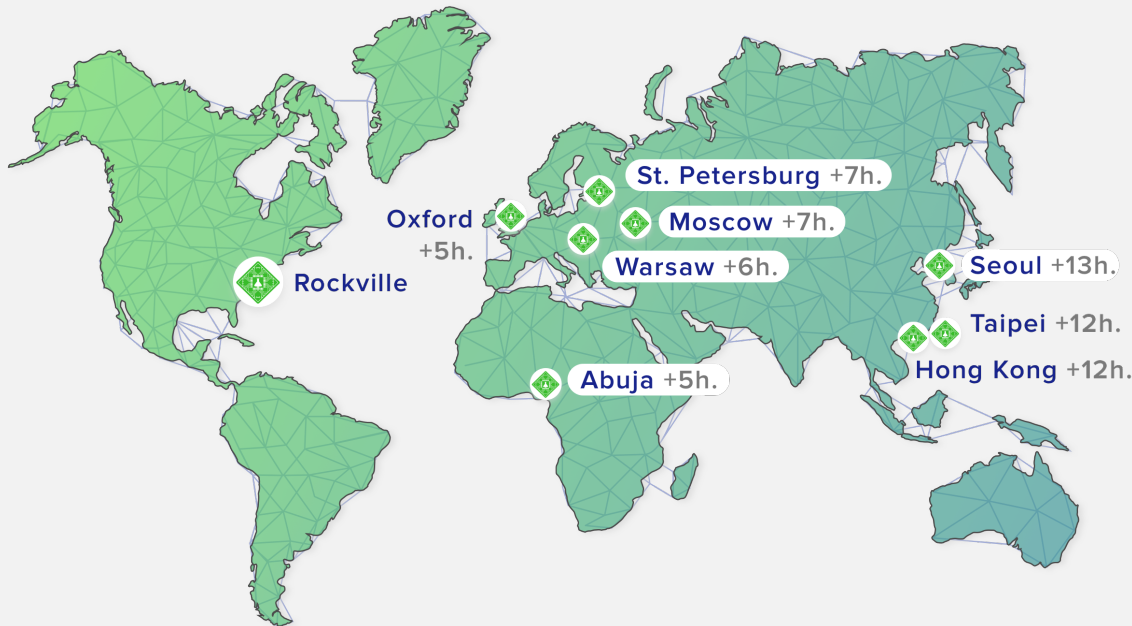
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