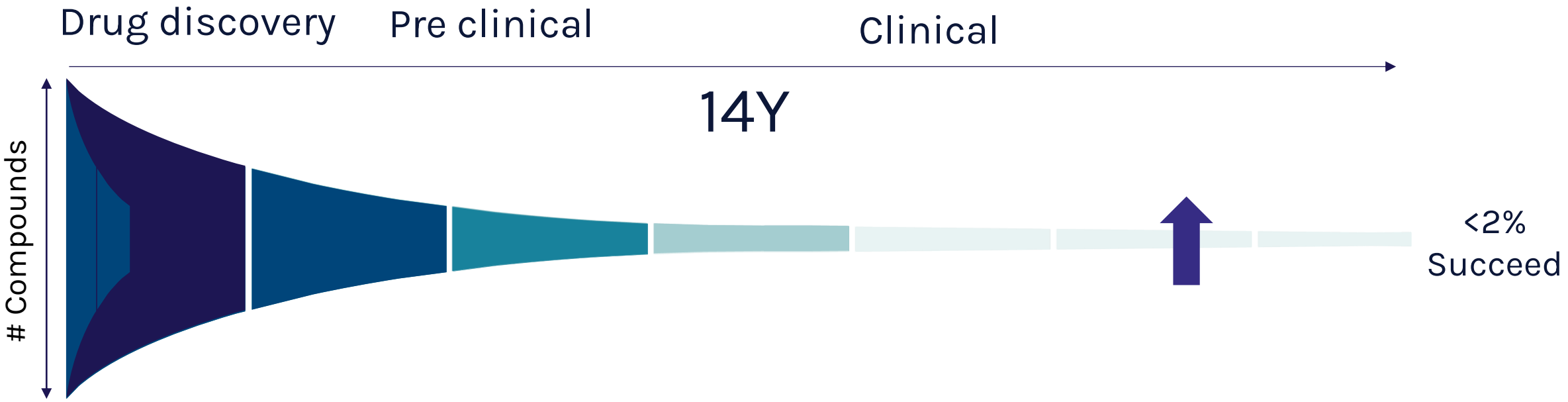
Tomorrow's drug discovery

Problem



- Biologic activity
- Target – drug complementarity

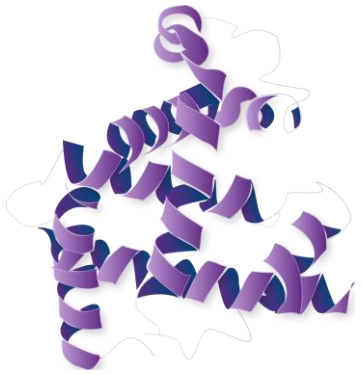
Solution

i-TripleD: Ai Powered, Patent Pending, Ultra-fast, Disease Agnostic, Target Based, Small-molecular Drug Designer

INPUT:

Target Protein

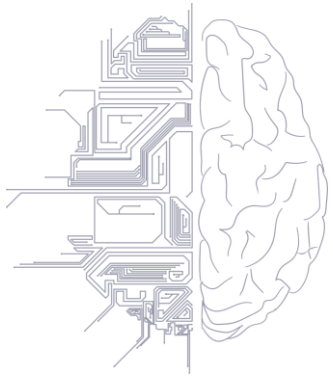
Indicator for disease (.pdb file)



Preferably a crystal structure including a co-crystalized ligand.

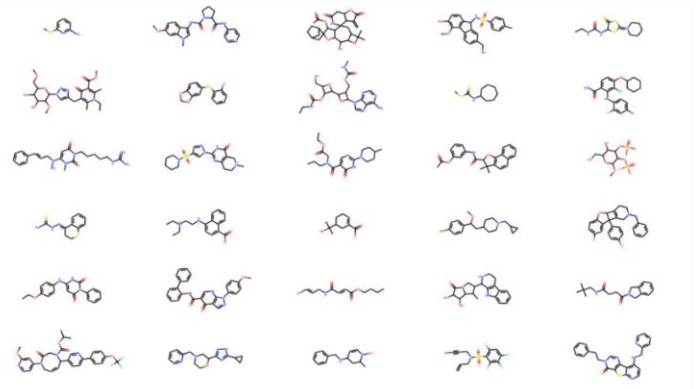
Process

~50 x 1-dimensional generative AI and ML models optimized for speed and accuracy



OUTPUT:

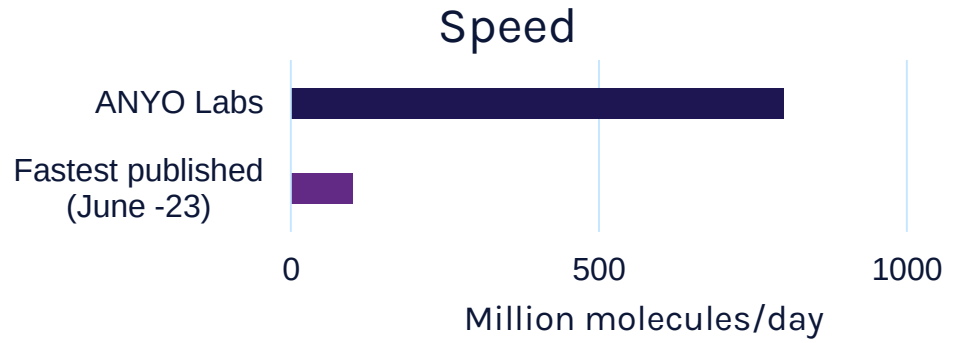
Novel potential drug compounds



Results ranked according to predicted binding affinity as well as the properties listed below.

Synthetic-Score	Caco2	ClogD	Solubility	BBB	PPBR	CYP1A2	CYP2C9	CYP2C19	CYP2D6	CYP3A4	Half_Life	AMES	hERG_central_inhib

Ultra-fast and accurate drug discovery



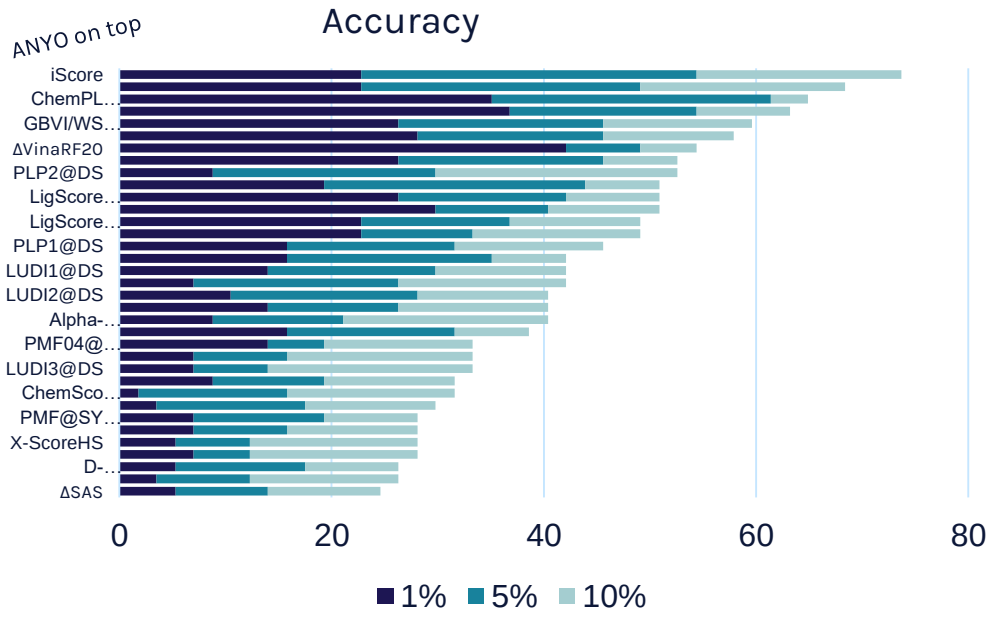


*Chart recreated for marketing purposes. Based on benchmark performance

Services

HIT IDENTIFICATION

- Target validation

  For every target we perform protein assessment and if necessary, homology modelling and dynamics to ensure highest possible accuracy downstream.

- *De novo* Drug Discovery

  Expanding on the chemical space, allowing our algorithms to tailor make the best possible compounds for selected binding pockets optimizing ADMET parameters and selectivity.

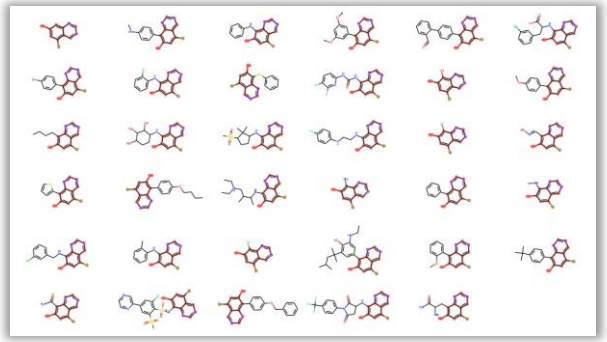
- Database screening

  Current speeds allow us to filter through the Enamines REAL library (6.7 billion) in under 2 days. Selecting synthesizable compounds based on predicted binding affinity, ADMET parameters and selectivity

LEAD OPTIMIZATION

- Scaffold Optimization

  Once hit compounds exist, we deploy multiparameter optimization on >2000 new analogues per second to fast-track medicinal chemistry of confirmed hits.

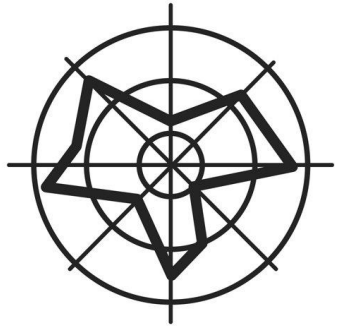


PRECLINICAL

IND/CTA

- Scaffold Optimization + ADMET

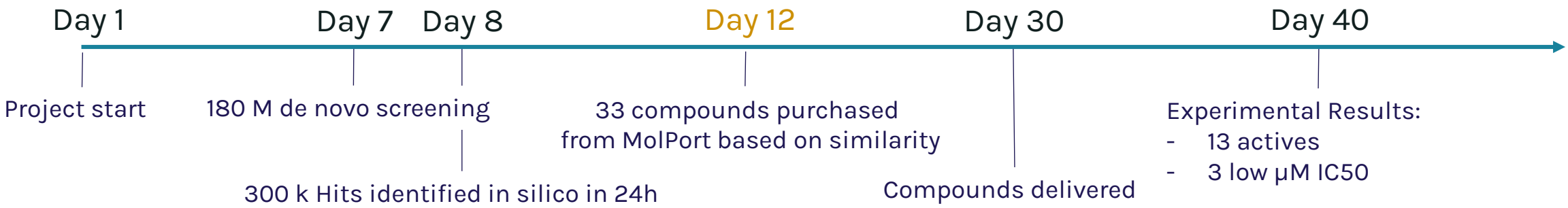
  Keep iterating and explore SAR relationships based on experimental findings. Expedite decision-making and take data-driven decisions on what to make/test next.

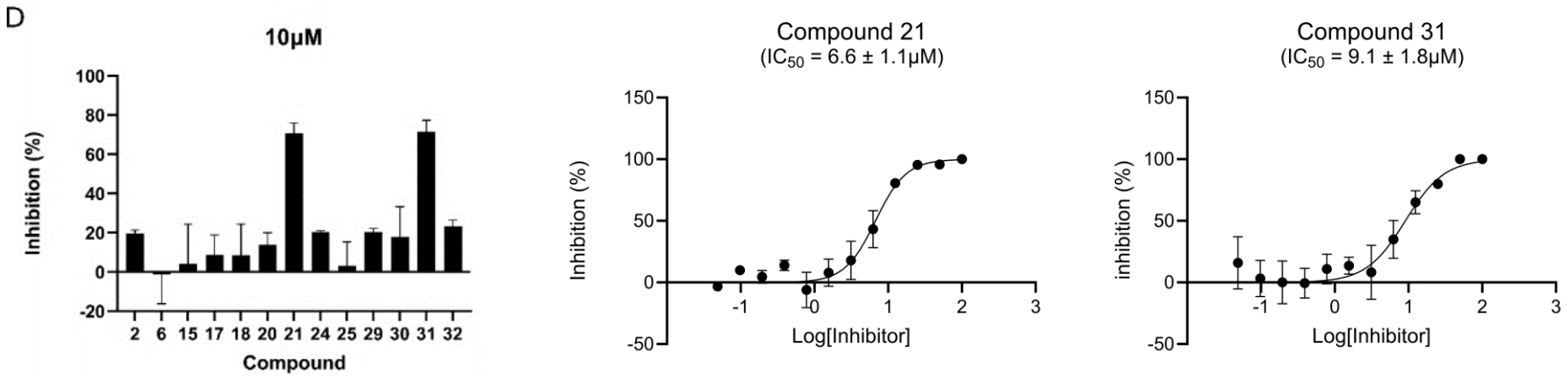


Used case

DENGUE VIRUS *DE NOVO* SCREENING & SIMILARITY SEARCH POC

“ANYO Labs novel in silico AI-driven screening program allows for rapid and cost-efficient exploration of an extremely large portion of chemical space, which cannot be matched by any other in silico drug discovery tool.”
- Prof. Johan Lennerstrand, Uppsala University





Strong & Diverse Founding Team

Prof. Leif A. Eriksson

PI & Chairman

Co-founder of 4 spin-off companies
PI, Theoretical biochemistry group
>300 publications
3 patents (drug compounds)

Dr. S. Jalil Mahdizadeh, PhD

Researcher

Ph.D, Theo. & Comp. Chemistry
Researcher, Theo.
Biochemistry, drug discovery and ML
37 publications

Albin Boman

CEO

BSc. Mechanical Engineering
MSc. Entrepreneurship & Business Design

Marek Szczygiel, MD

CMO

MD & 6 years of clinical experience
MSc. Entrepreneurship & Business Design

André Stadelmann

CTO

BSc. Development engineering
MSc. Entrepreneurship & Business Design

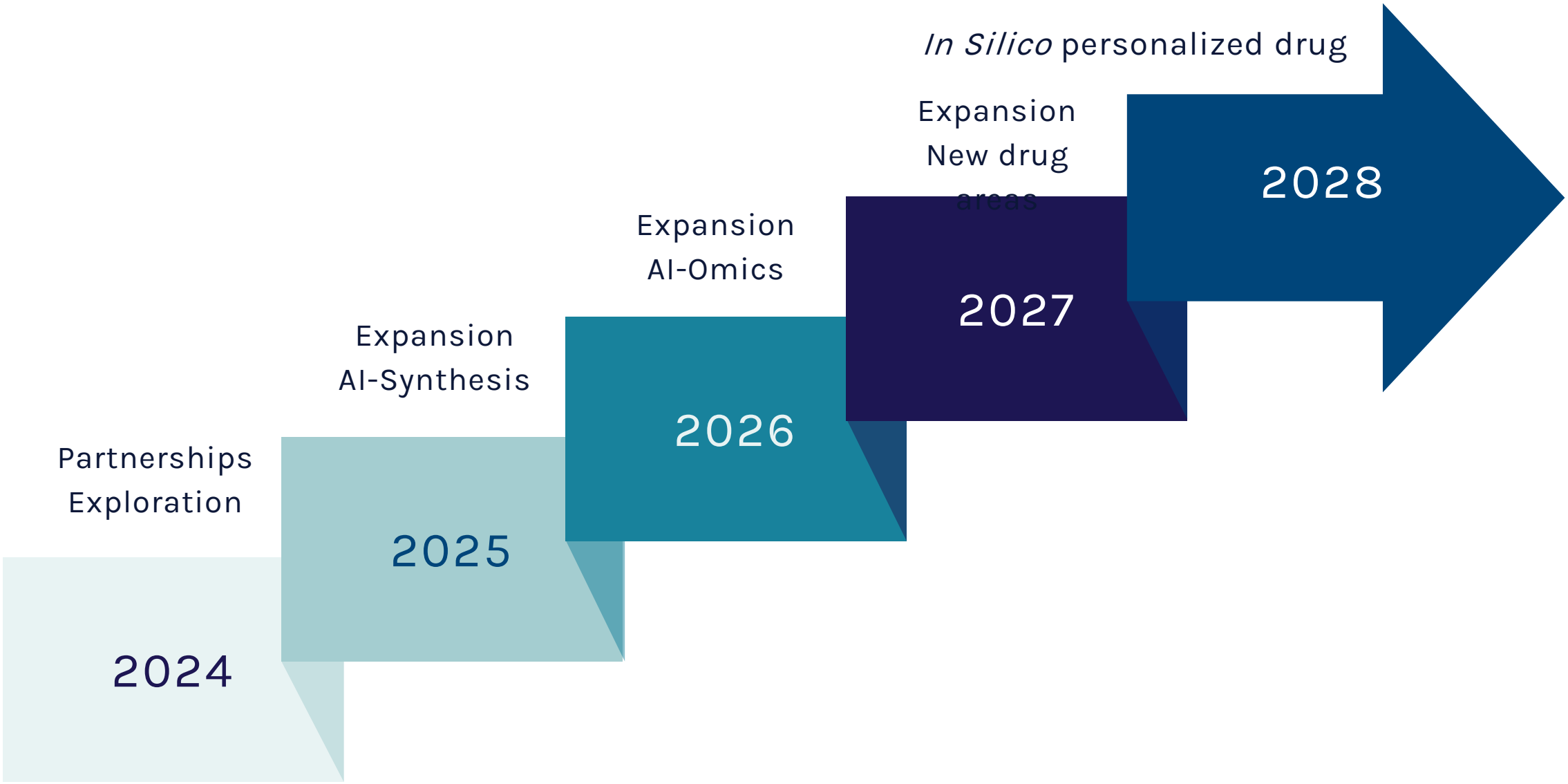
Partners:

UNIVERSITY OF GOTHENBURG

CHALMERS VENTURES what if

NVIDIA

CGit


2024
Partnerships
Exploration
2025
Expansion
AI-Synthesis
2026
Expansion
AI-Omics
2027
Expansion
New drug
areas
2028
In Silico personalized drug

Tomorrow’s drug discovery

Book a meeting or contact us

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