



ARTIFICIAL INTELLIGENCE FOR NEW DRUG DESIGN



IKTOS

Facts and figures

Company



2016



1M€ financing



10 people



Proprietary technology for MPO

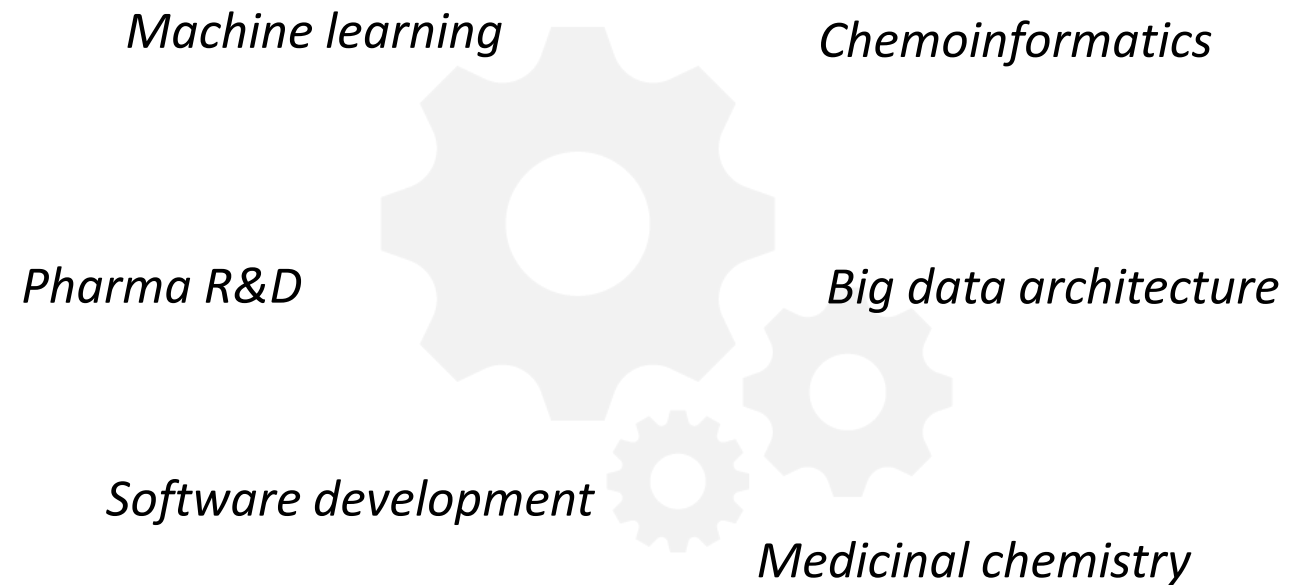


4 PoC in progress

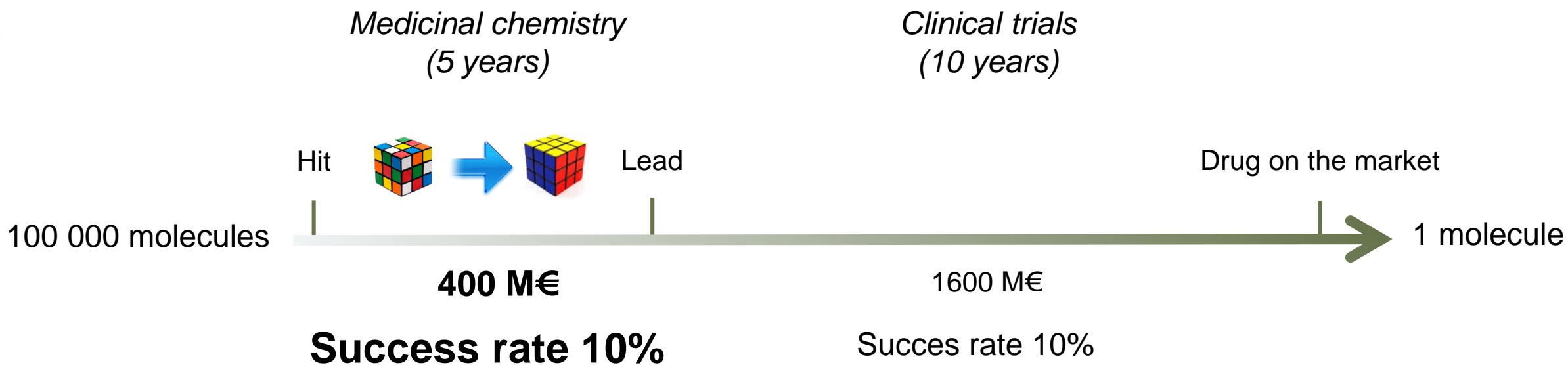


Software release June 2018

Skills



R&D life cycle and spending



***Less than 1% chance to find a new drug...
Our objective: reduce costs and risks!***

Medicinal chemistry a hard job!



Activity



Specificity



Solubility



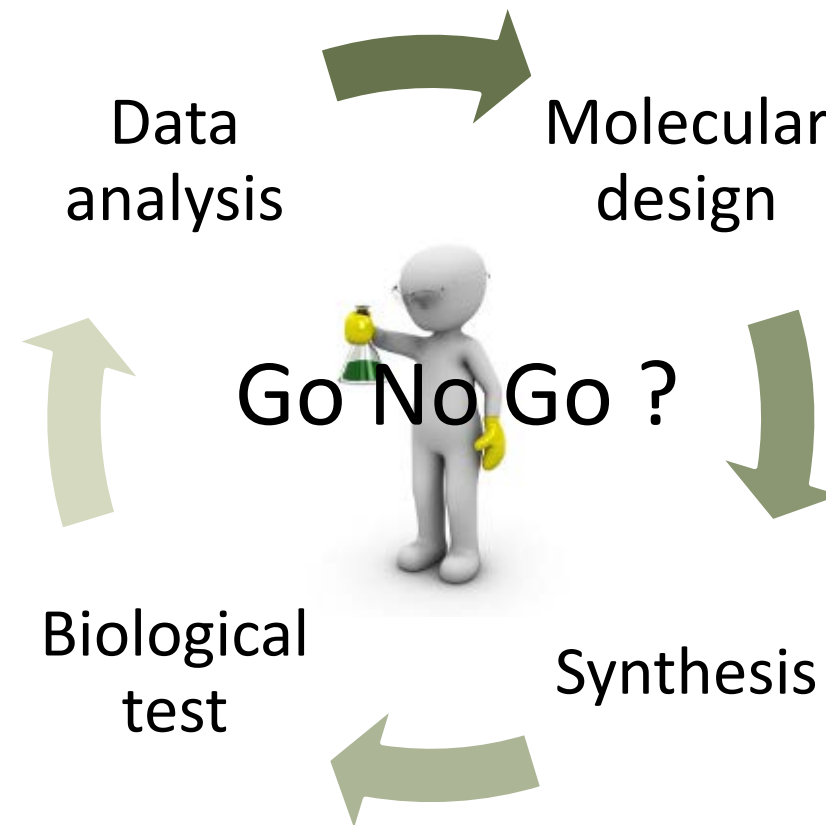
Permeability



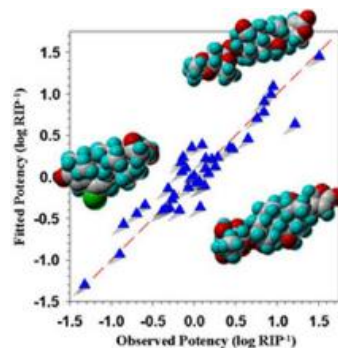
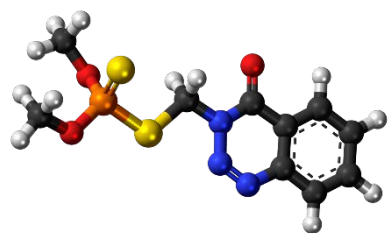
Stability



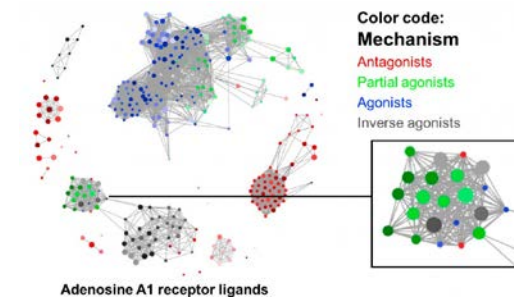
...



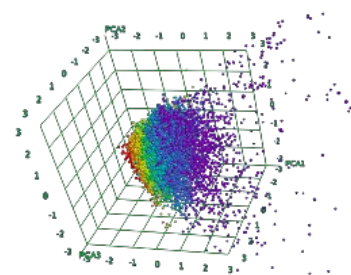
Classic technologies can only predict...



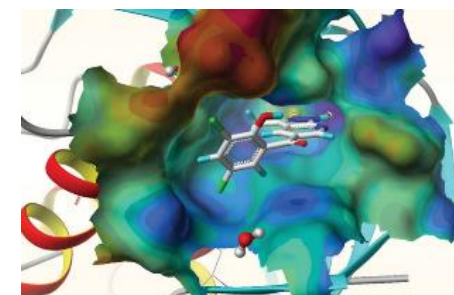
QSAR



Data visualization



Clustering models



Docking

They cannot tell you what to do!

State of the art Deep Neuronal Network perform outstanding tricks



Automatic colorization of black and white images



"girl in pink dress is jumping in air."

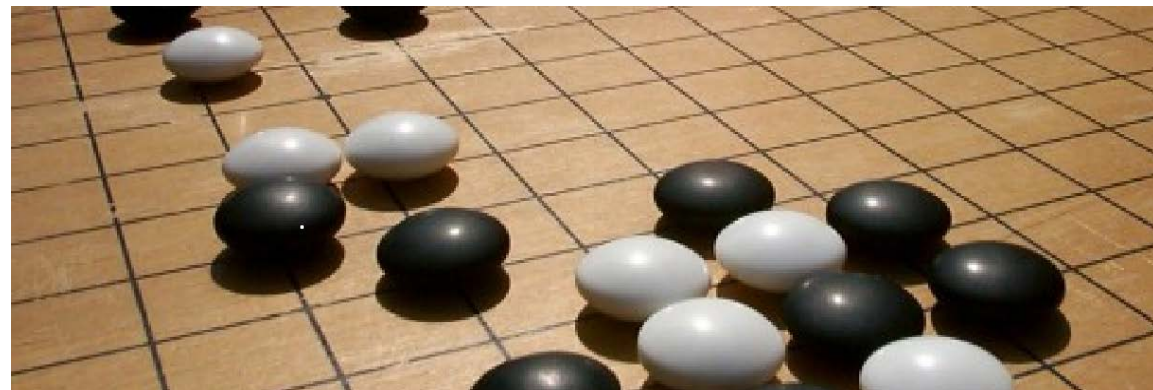


"black and white dog jumps over bar."



"young girl in pink shirt is swinging on swing."

Automatic image caption generation



Automatic game playing



Automatic picture generation

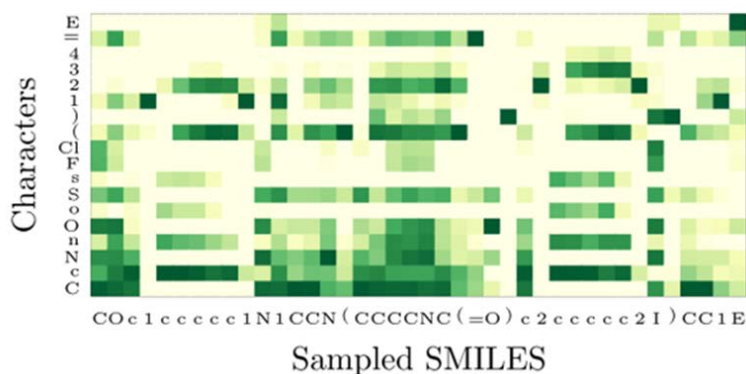
Our plan: apply those new concepts to medicinal chemistry!

Generative models

Sequence based

Long Short Term Memory

- LSTM (Characters or Grammar)
- LSTM with Reinforcement learning



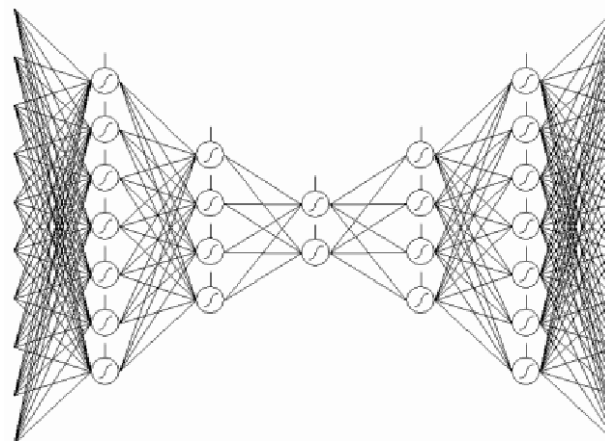
AstraZeneca 2017

High Valid smiles rate
No latent space

Latent space

Variational Auto-Encoder

- CVAE, GVAE, SD-VAE



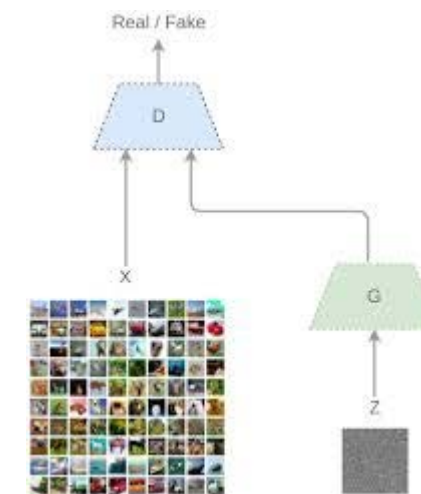
Toronto
Cambridge 2016

Latent space
Low valid smiles rate

GAN

Generative Adversarial Network

- ORGAN

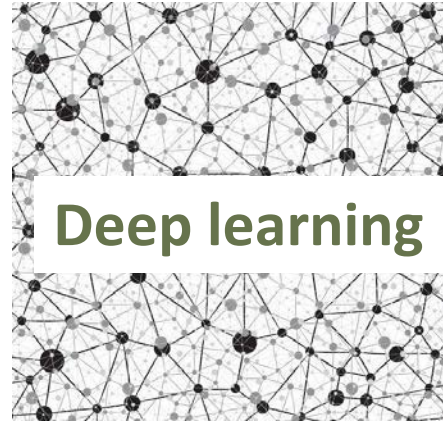
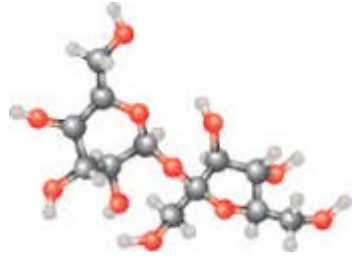


Harvard 2017

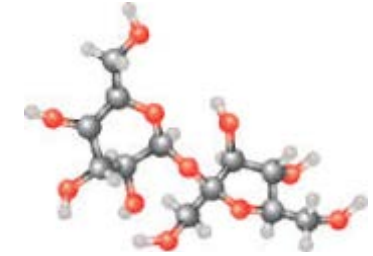
Hard to converge
Low valid smiles rate

Iktos asset

Molecule
(86 million)




Molecule
(86 million)

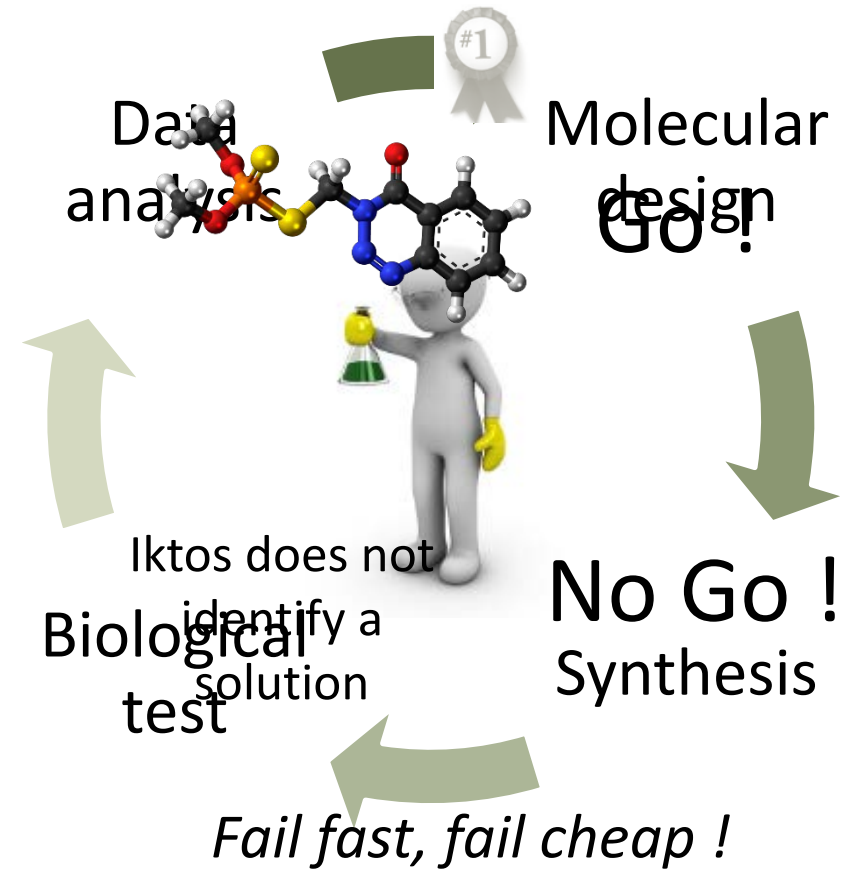


- ⊕ **Fully functional molecule generator enabling in silico De novo design**
 - ↪ Compatible with all types of predictors (2D : MorganFP, 3D : USRCAT (in progress)) and requirements (similarity/dissimilarity, sub-structures...)
 - ↪ Reinforcement learning converging to optimal solutions : Multi-Parameter Optimization (MPO) & diversity
- ⊕ **Proprietary high performance scalable technical architecture (GPU parallel processing)**
 - ↪ Online learning (streaming)
 - ↪ Few hours to solve a multi parametric optimization issue

Iktos goal: Acceleration and costs reduction



Activity	✓
Specificity	✗
Solubility	✗
Permeability	✗
Stability	✗
...	✗



A unique value proposition

What does Iktos need?

- Iktos needs the project's dataset: the molecules and the experimental data (Activity, Potency, ADME...)

What does Iktos deliver?

- Iktos propose a short listing of the most promising molecules which simultaneously fit all the objective of the project.

Why is Iktos unique ?

- Iktos is not a virtual screening approach, Iktos is not based on combinatorial concepts, Iktos doesn't filter databases... Iktos can explore the chemical space better than any other solution.

Iktos automatically extracts the project's SAR to design optimal and original molecules in a matter of hours.

A well differentiated market positioning

CADD Technology providers



Traditional approaches: combinatorial, 3D...

AI players

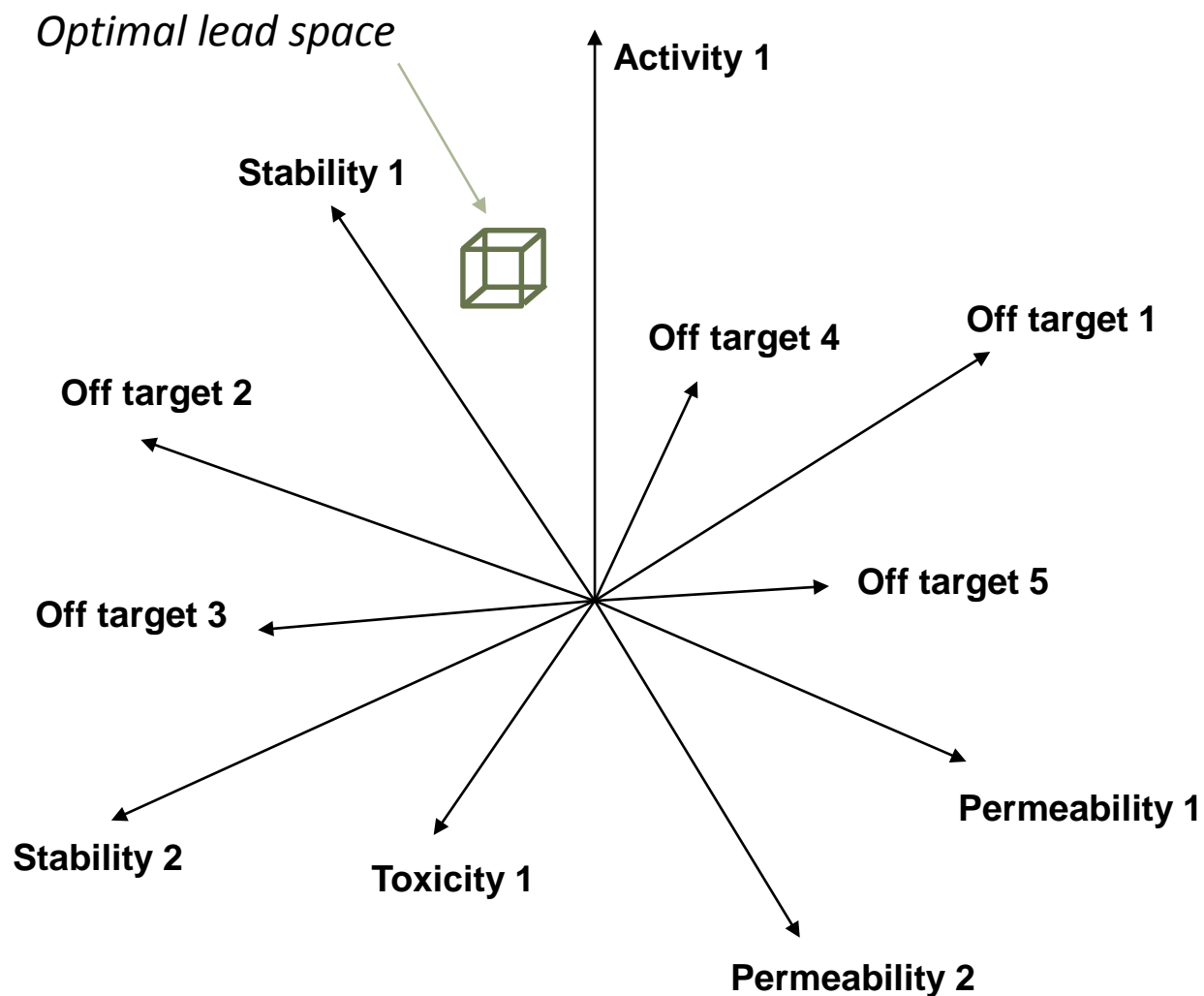


*Different business models (drug discovery)
Proprietary technologies for their own use*



**Deep learning powered ligand-based de novo drug design technology provider,
focusing on Multi-Parameter Optimization**

Client success story



Client facts and figures

11 objectives
600 molecules
+10 years of research
+5 chemists on the project

No molecule meeting simultaneously the 11 objectives of the blueprint...



Iktos work

120 optimal virtual molecules generated
20 molecules selected to be synthesized
11 molecules synthesized and tested
8 molecules matching 9/11 objectives
3 molecules matching 10/11 objectives
1 molecule matching 11 objectives

Iktos business model(s)

MedChem Services: we use our technology to provide solutions to bottlenecks in our clients' research programs

Software: Iktos technology for use by end-users

- ***Corporate licenses***
- ***Freemium access: SaaS, pay per use...***

Chemical data hub Platform: Data sharing platform that will leverage the power of the technology for subscribers through Federated Learning



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