Towards Smarter Drug Discovery

AI-Guided Automation for Faster Optimization of New Potential Drug Candidates

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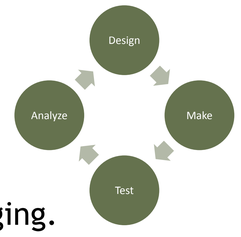
BACKGROUND

- Early drug design & discovery relies on **Design, Make, Test, Analyze (DMTA)** iterative cycle that allows for development & optimization of best drug candidates.
- Inefficiencies in this cycle makes this a **long & expensive** process.
  - Early discovery ➡ clinic timeline ~ 10 years
  - Early discovery ➡ clinic cost ~ $1-2 Billion



- **Druglike chemical space is vast (~10^{60})** and exploration is challenging.
- **Iktos AI tools** guide **compound design** and **synthesis by robots**, maximizing efficiency in chemical space exploration.

TOOLS FOR A NEW APPROACH

- AI is increasingly being recognized as a powerful tool in drug discovery.
- **Iktos is an industry leader** in AI tools for *de novo* drug design & synthesis planning.

makya — *DE NOVO DRUG DESIGN*

spaya.ai — *RETROSYNTHESIS PREDICTION*

- We use our **AI expertise to guide robots** to perform synthesis in a semi-autonomous pipeline in order to **maximize efficiency** and **minimize costs**.

Library Design & Synthesis	
Traditional Approach: *ad hoc* design & synthesis.	**Iktos Approach:** high throughput design & parallelized synthesis.
Limited diversity, high redundancy in the designed molecules.	Multiple exit vectors targeted with high diversity of products.
Robot synthesis protocols and scheduling set up manually by chemists.	Spaya generates synthesis routes and protocols. Ilaka automates robot synthesis planning and scheduling.
Challenging, slow, and costly to impact hit finding and hit to lead phases.	Significant impact in hit finding, hit to lead, and lead optimization due to robotics platform awareness at all stages.

ESTIMATED IMPACT OF IKTOS' APPROACH

1

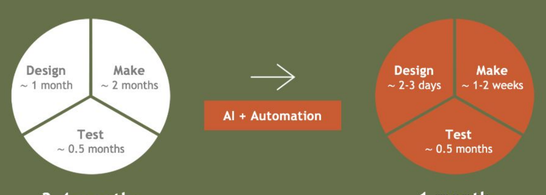
Rapid Convergence

Generate data and use AI to quickly converge on an optimal molecule

2

Shorter DMT Cycle

Build a closed-loop drug candidate discovery platform through the integration of AI, synthesis and automation to drastically impact timelines



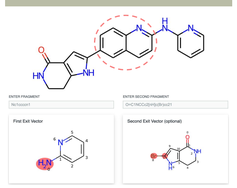
Estimated impact on the timeline of drug discovery process :

Total Duration: 12-18 months (~3x speed-up)

Hit Discovery 3 months → Hit to Lead 3-6 months → Lead Optimization 6-9 months

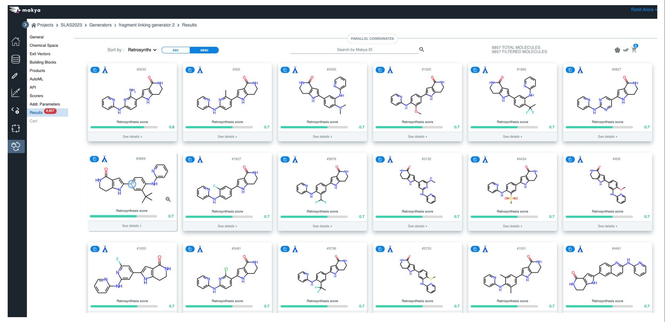
IKTOS ROBOTICS: A SEMI-AUTONOMOUS PIPELINE

FRAGMENT LINKING GENERATOR



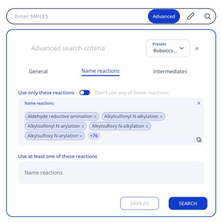
- Generate new ideas for core of reference molecule
- Use commercially available building blocks

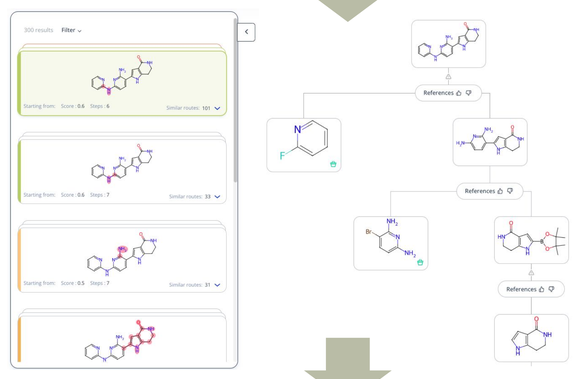
iktosrobotics

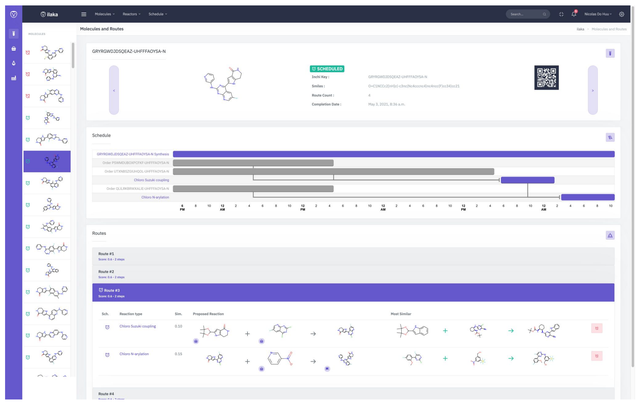


Example output of a Makya generation (t=2 minutes). Generated molecules scored using descriptors, QSAR models, docking, synthetic access, druglikeness, etc.

- >17 partnerships with chemical providers
- >1600 named reactions
- Routes compatible with robots







- Fetches molecules (Makya) &
- synthesis routes (Spaya)
- Selects routes and orgazines reactors to minimize overall synthesis time, and maximize output.
- Other inputs:
  - Number of reactors
  - Reactor specifications
  - Building block availability, cost, and delivery time
  - Reaction conditions

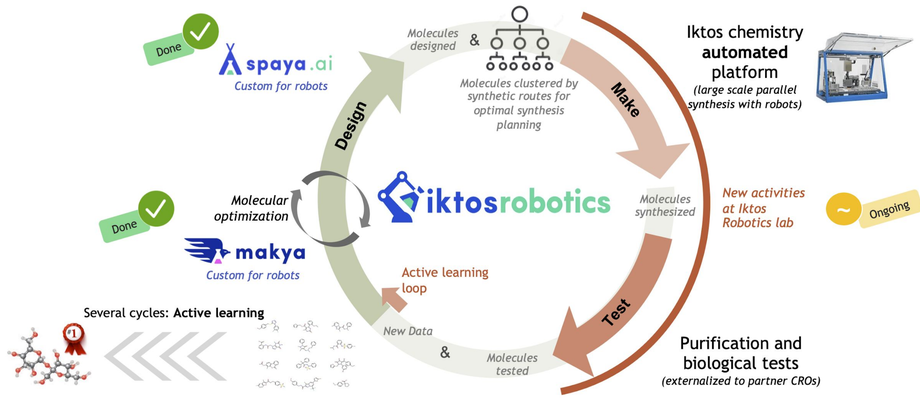
Iktos technology stack

makya — *De novo design using Makya*

spaya.ai — *Retrosynthesis and synthesis planning using Spaya*

ilaka — *Workflow optimization and control with Ilaka*

IKTOS PROVIDES FULLY INTEGRATED DRUG DISCOVERY SERVICES



Robot at Iktos Lab in Paris

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