





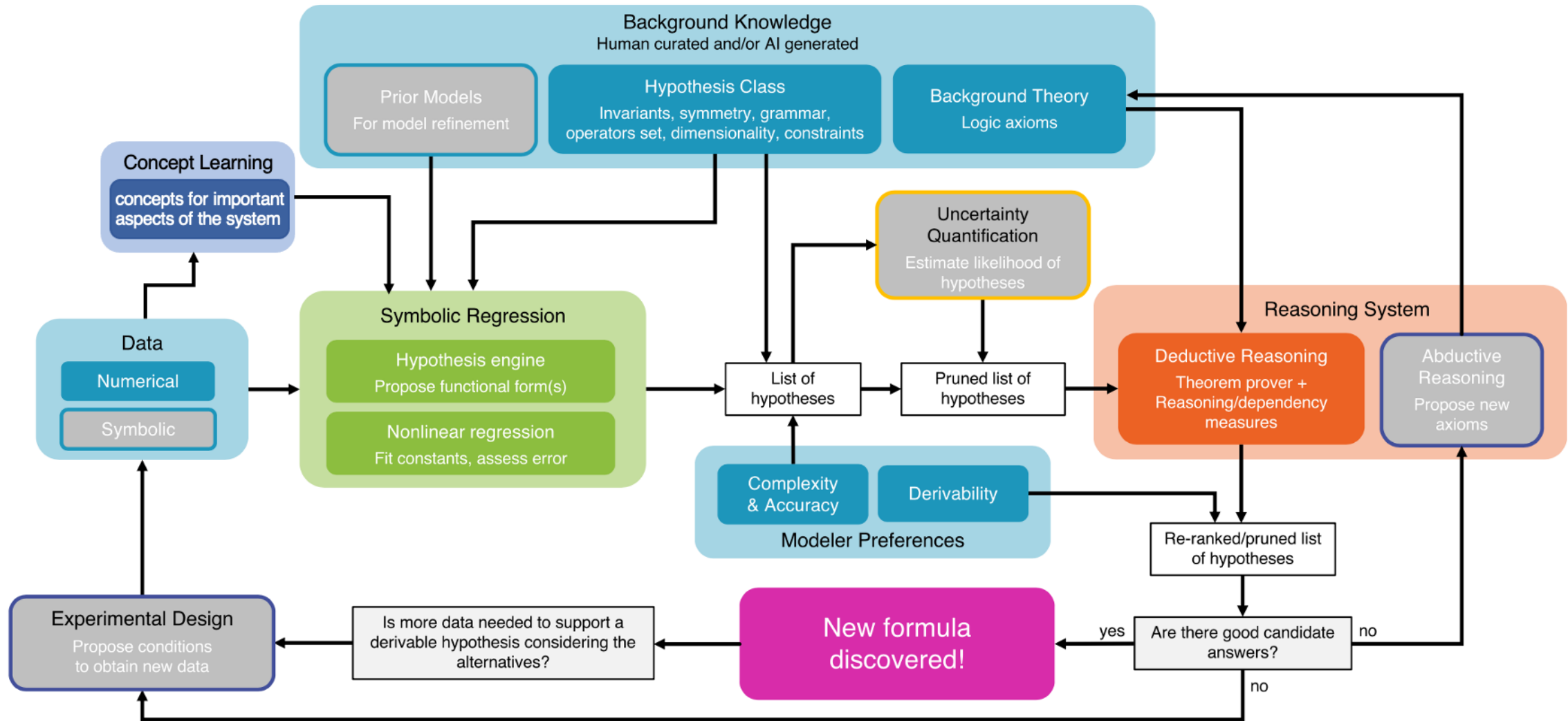
# Outline

-  AI agent for scientific research
-  AI agent for Engineering
-  How to learn a new discipline in one week
-  Turning LLMs into scalable scientific productivity

# | AI agent for scientific research



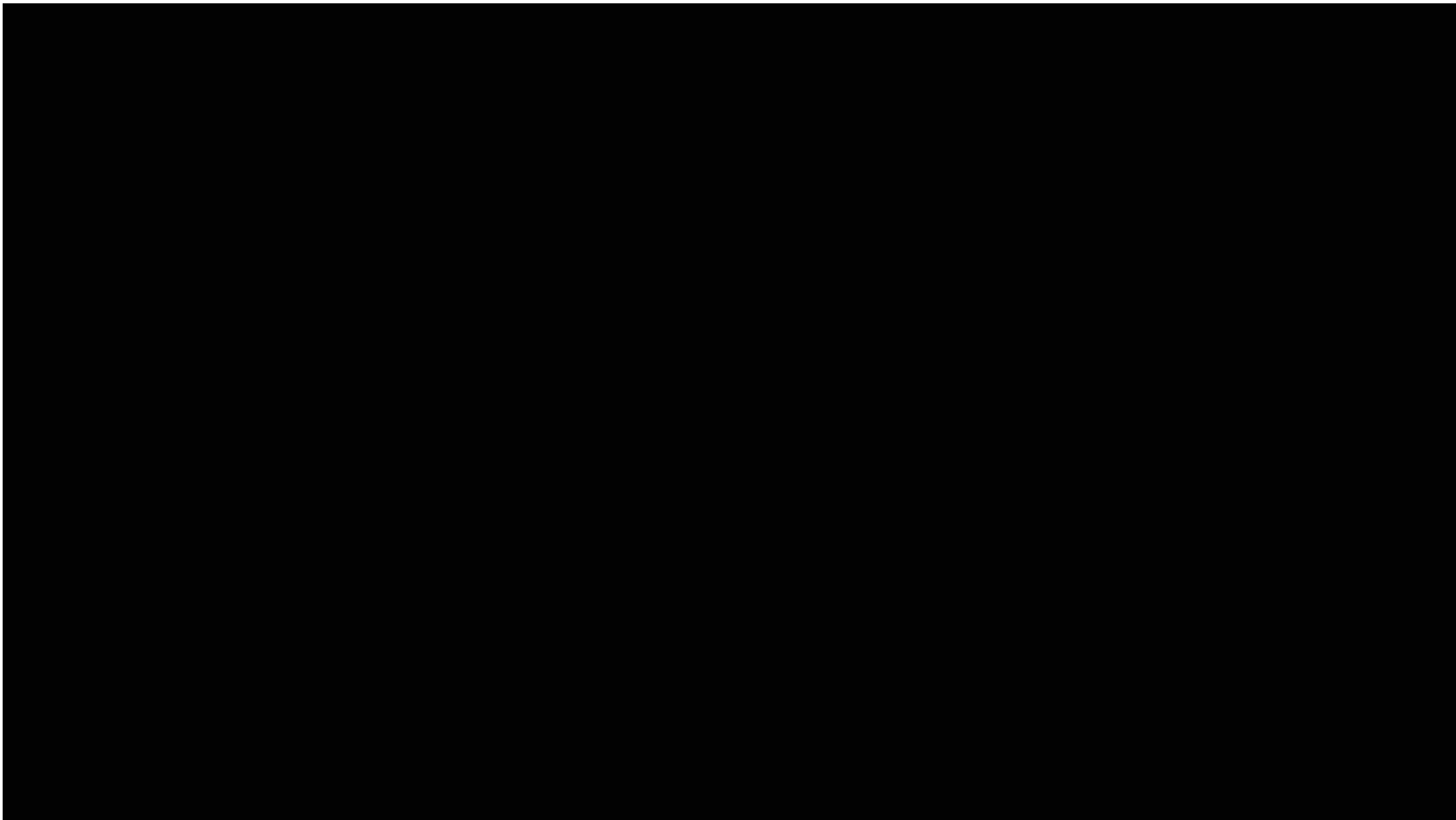
# What is an ultimate AI Scientist?



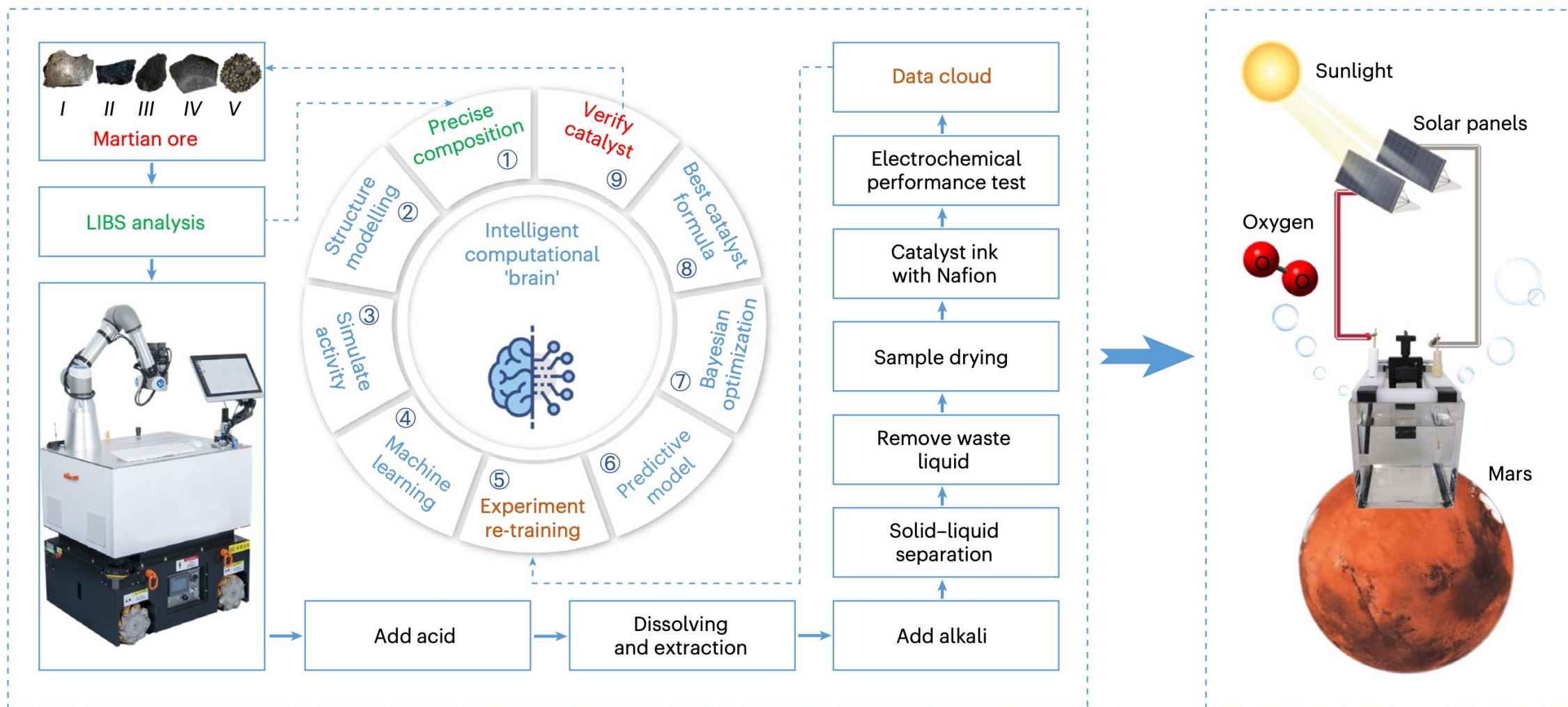
Cornelio, Cristina, et al. "Combining data and theory for derivable scientific discovery with AI-Descartes." *Nature Communications* 14.1 (2023): 1777.



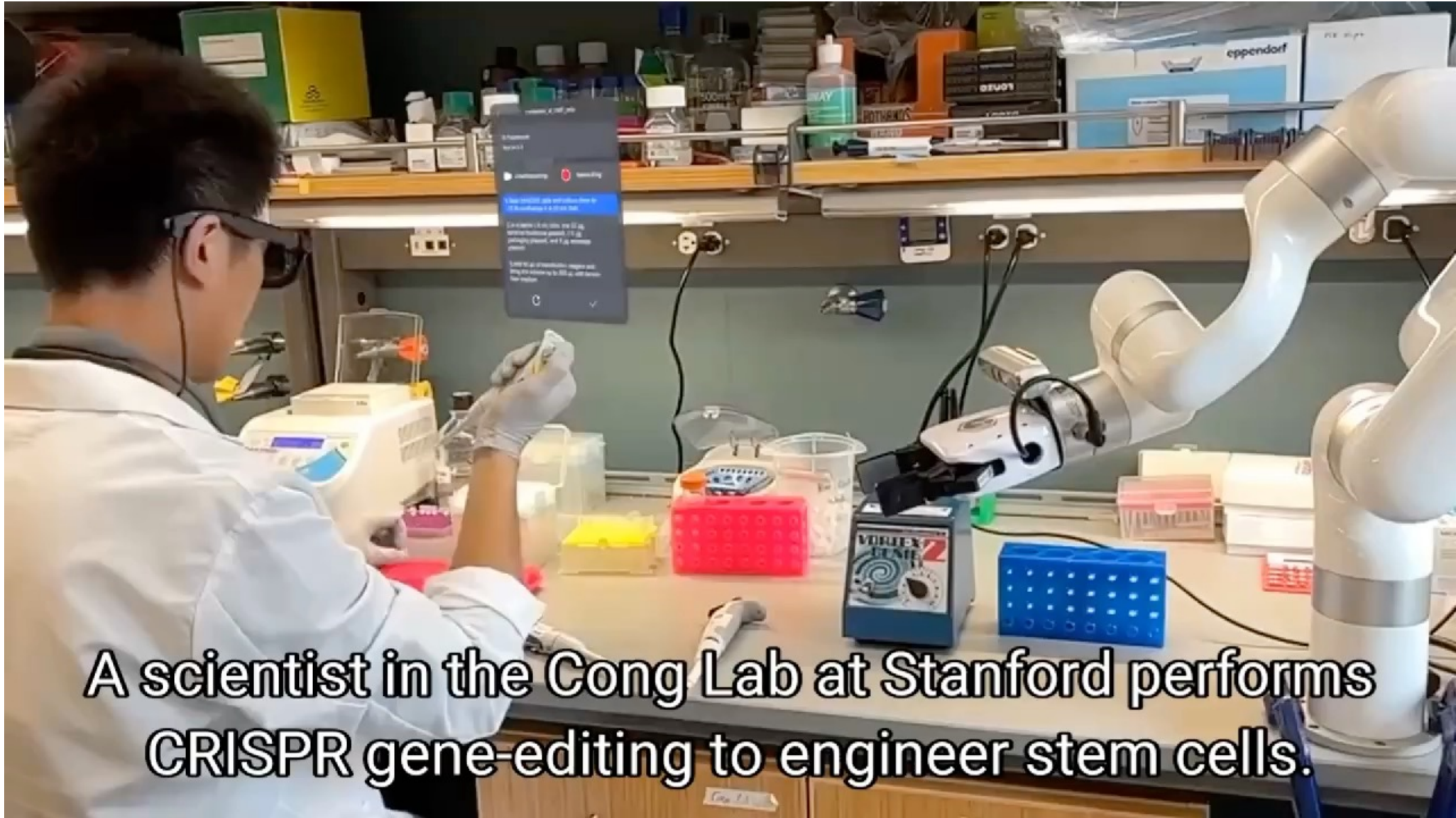
# Work 1: Synthesize catalysts from Martian meteorites



# Work 1: Synthesize catalysts from Martian meteorites



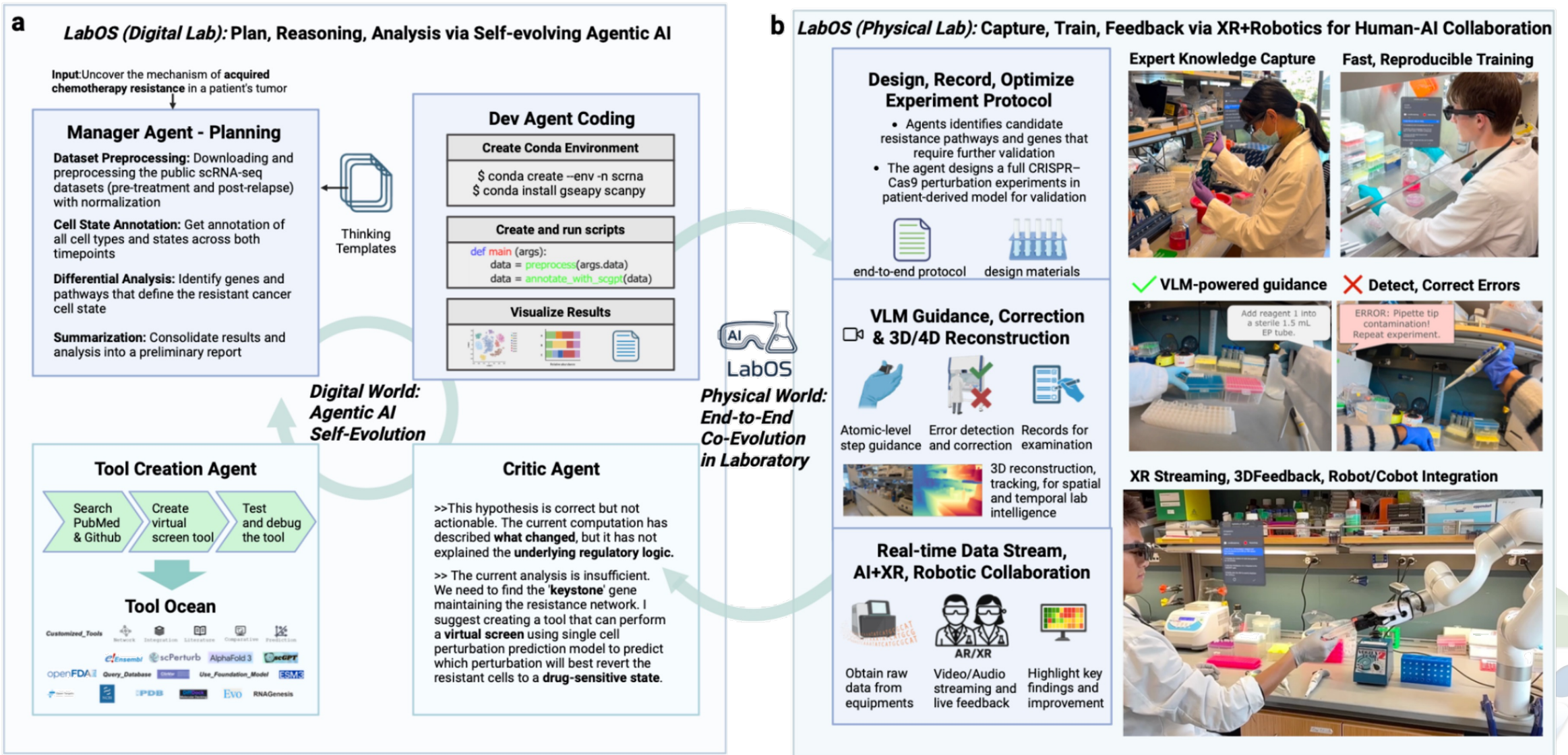
Dai, Tianwei, et al. "Autonomous mobile robots for exploratory synthetic chemistry." *Nature* (2024): 1-8.



**A scientist in the Cong Lab at Stanford performs CRISPR gene-editing to engineer stem cells.**



# Work 2: LabOS: The AI-XR Co-Scientist



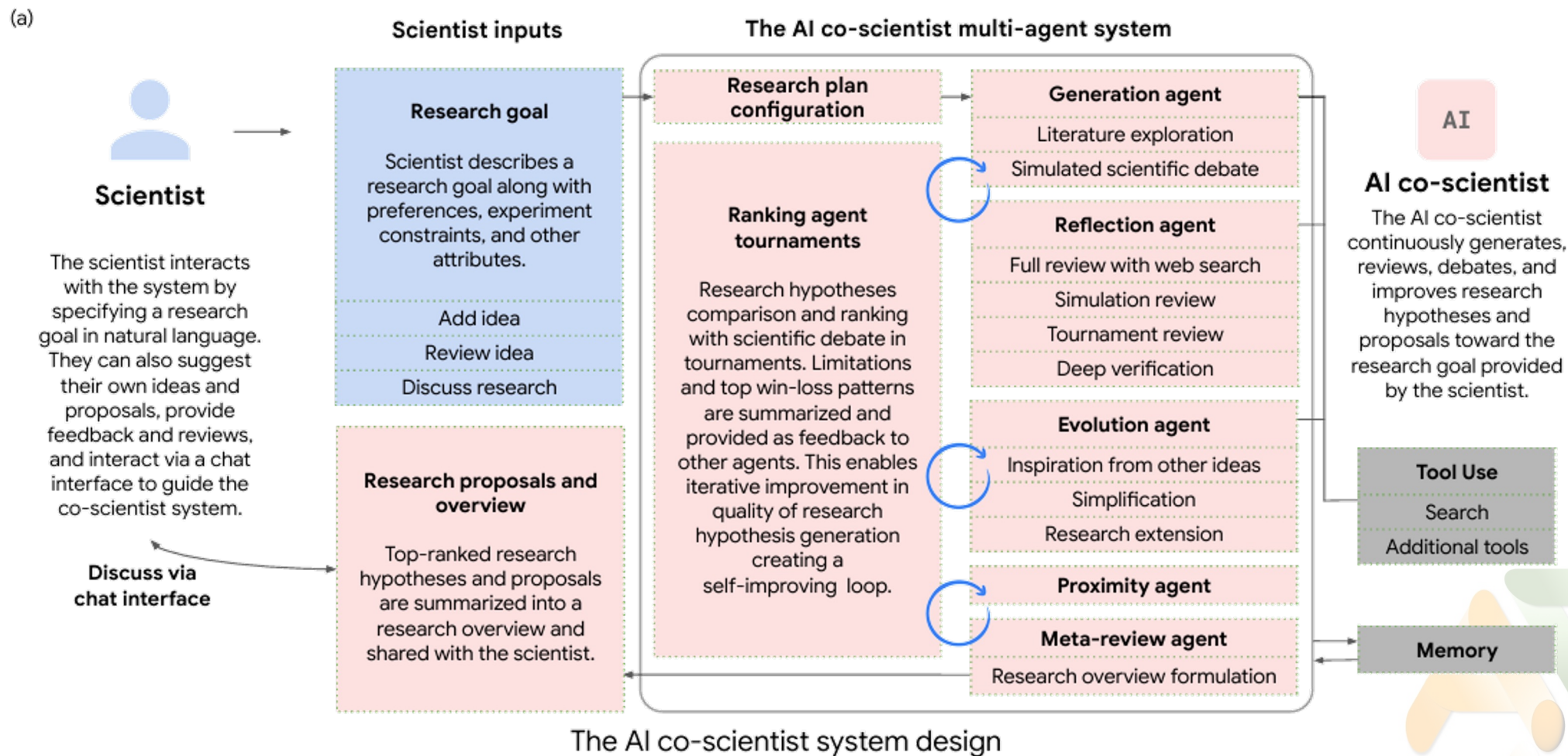
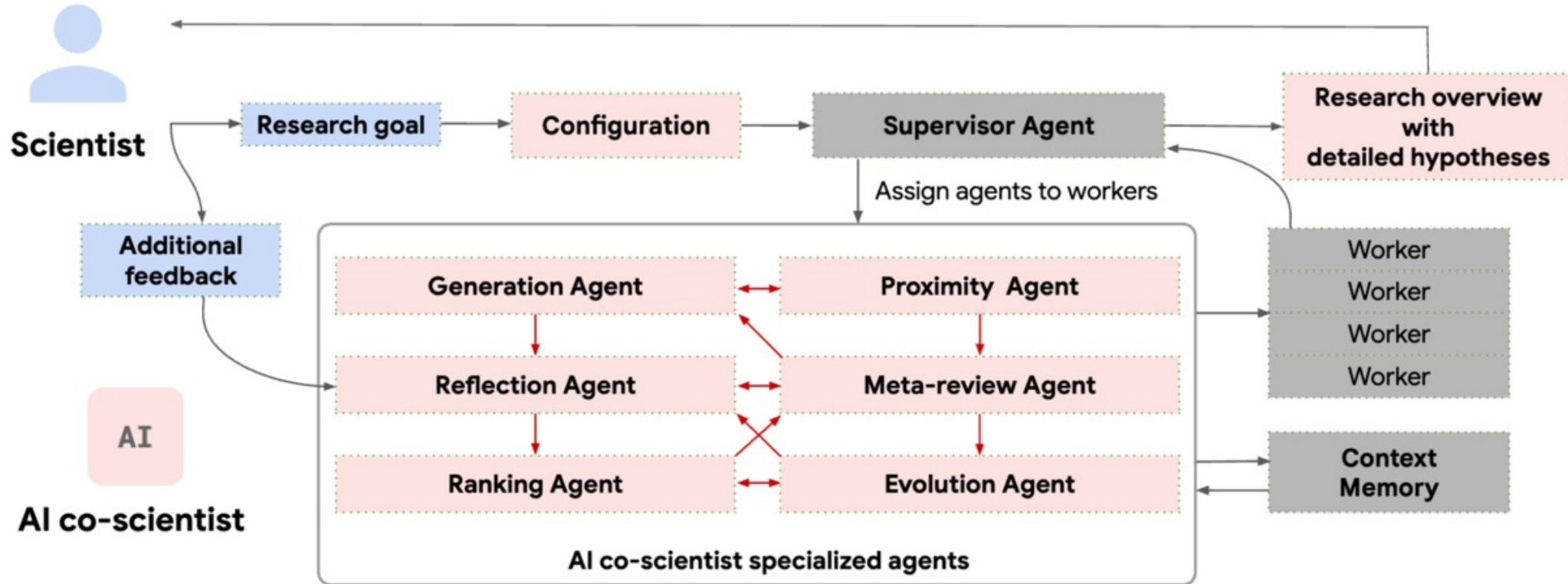


Illustration of the different components in the AI co-scientist multi-agent system and the interaction paradigm between the system and the scientist.



# Work 3: Google AI Co-Scientist



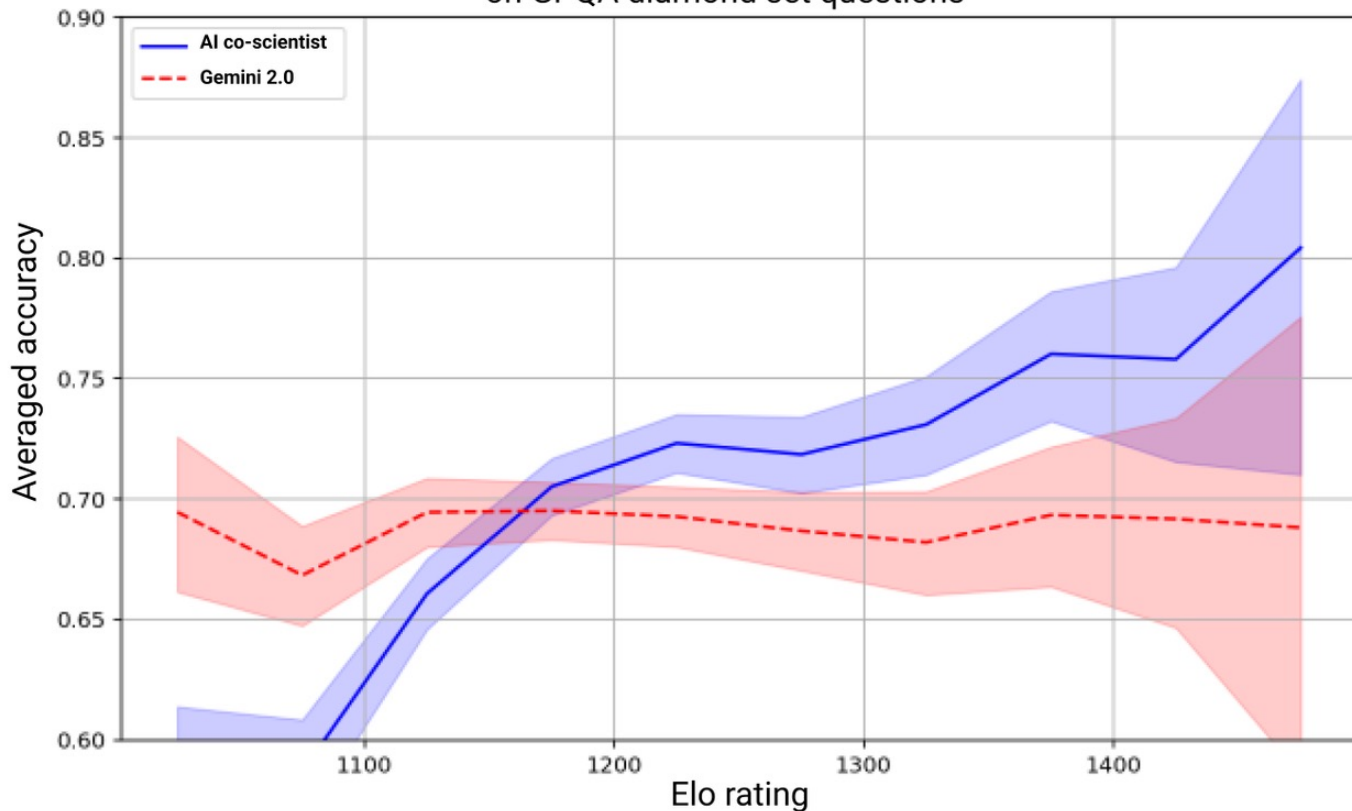
AI co-scientist system overview:

- Specialized agents (**red boxes**, with unique roles and logic)
- Scientist input and feedback (**blue boxes**)
- System information flow (**dark gray arrows**)
- Inter-agent feedback (**red arrows** within the agent section).





Concordance of the Elo rating with AI co-scientist performance on GPQA diamond set questions



$$E_A = \frac{1}{1 + 10^{\frac{R_B - R_A}{400}}}$$
$$R'_A = R_A + K(S_A - E_A)$$
$$R'_B = R_B + K(S_B - E_B)$$

$R_A$  : Current rating of Player A

$R_B$  : Current rating of Player B

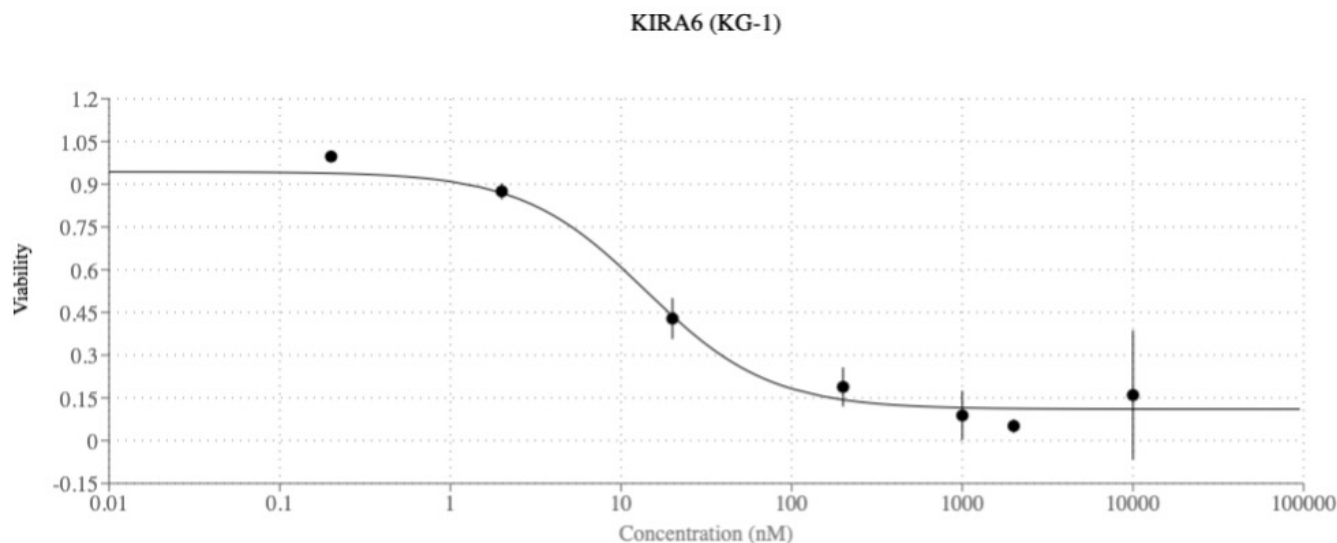
$S_A$  : 1 for a win, 0.5 for a draw, 0 for a loss

$E_A$  : The probability of Player A winning

$K$  : K-factor, defining the maximum possible rating change

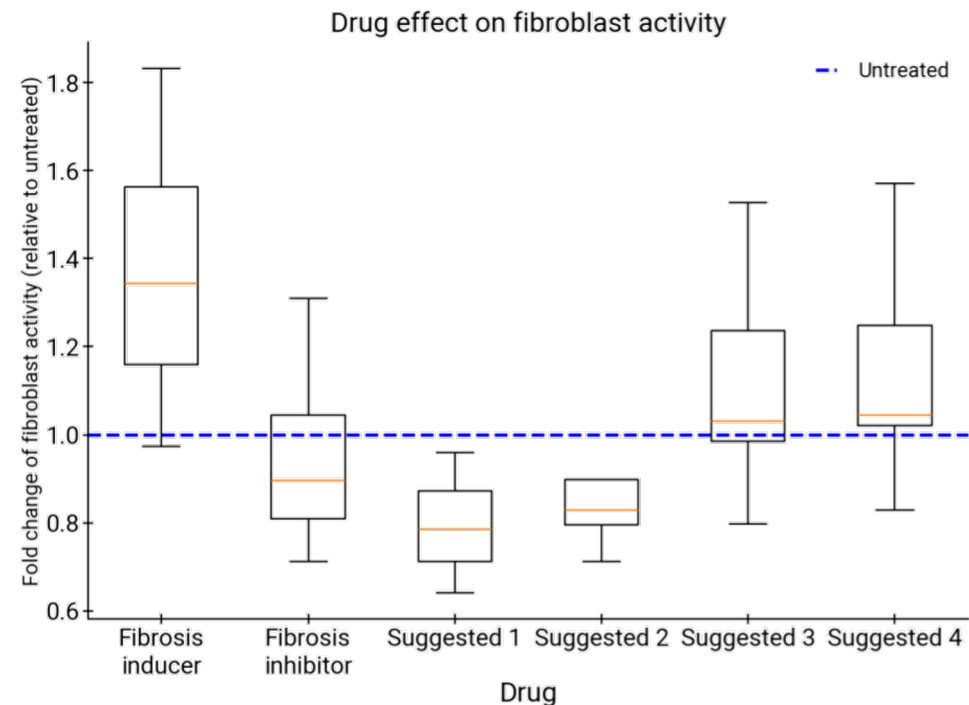
Average accuracy of the AI co-scientist (blue line) and reference Gemini 2.0 (red line) responses.

**GPQA diamond:** A challenging multiple-choice question set in biology, chemistry, and physics.



## Drug repurposing for ALM (药物再利用用于急性髓系白血病)

- Assist with the prediction of **drug repurposing opportunities** and validated predictions through computational biology, expert clinician feedback, and *in vitro* experiments.
- Experiments confirmed that the suggested drugs **inhibit tumor viability** in multiple AML cell lines.

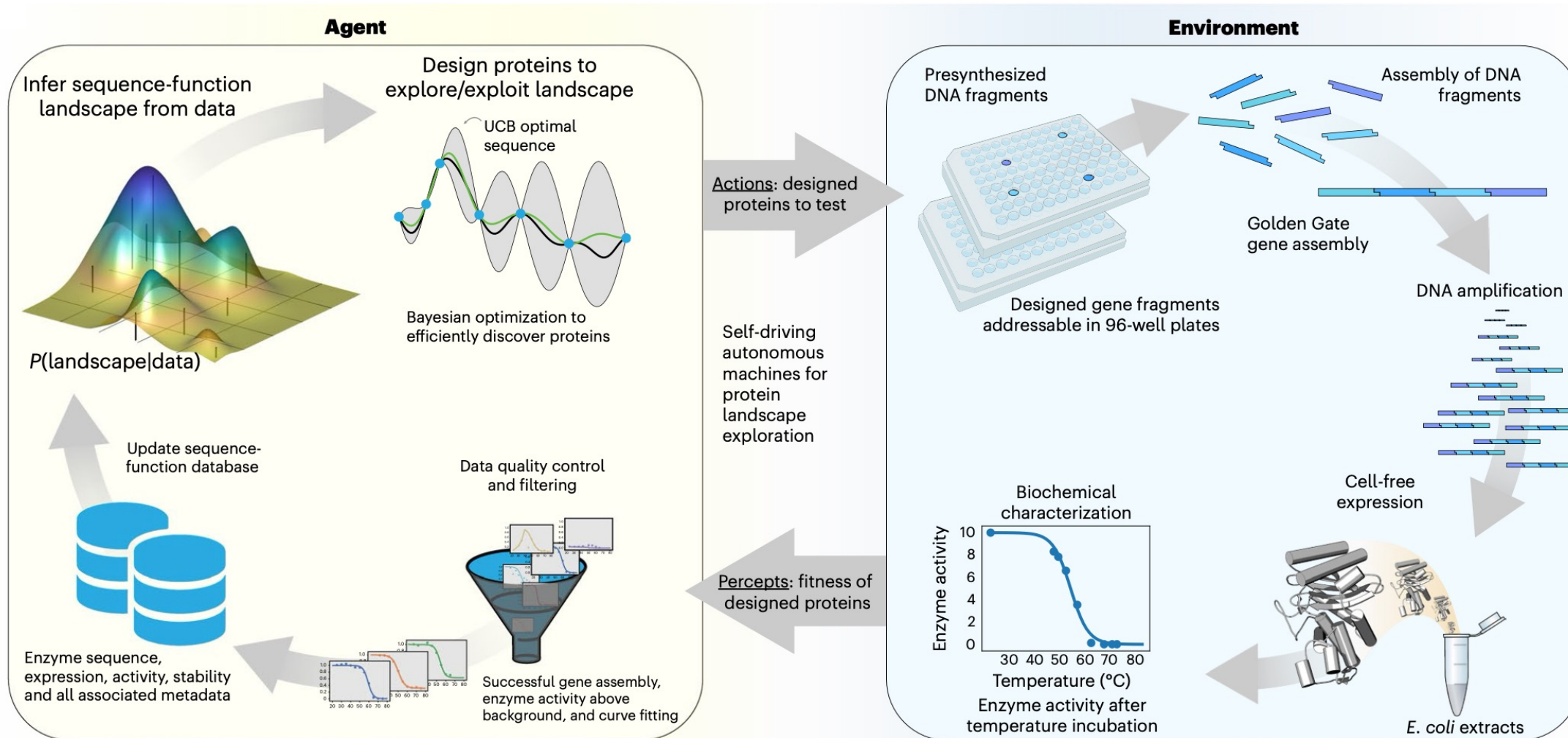


## Target discovery for liver fibrosis (肝纤维化靶点发现)

- Propose, rank, and generate hypotheses and experimental protocols for target discovery.
- Identified epigenetic targets grounded in preclinical evidence with significant **anti-fibrotic** activity in human hepatic

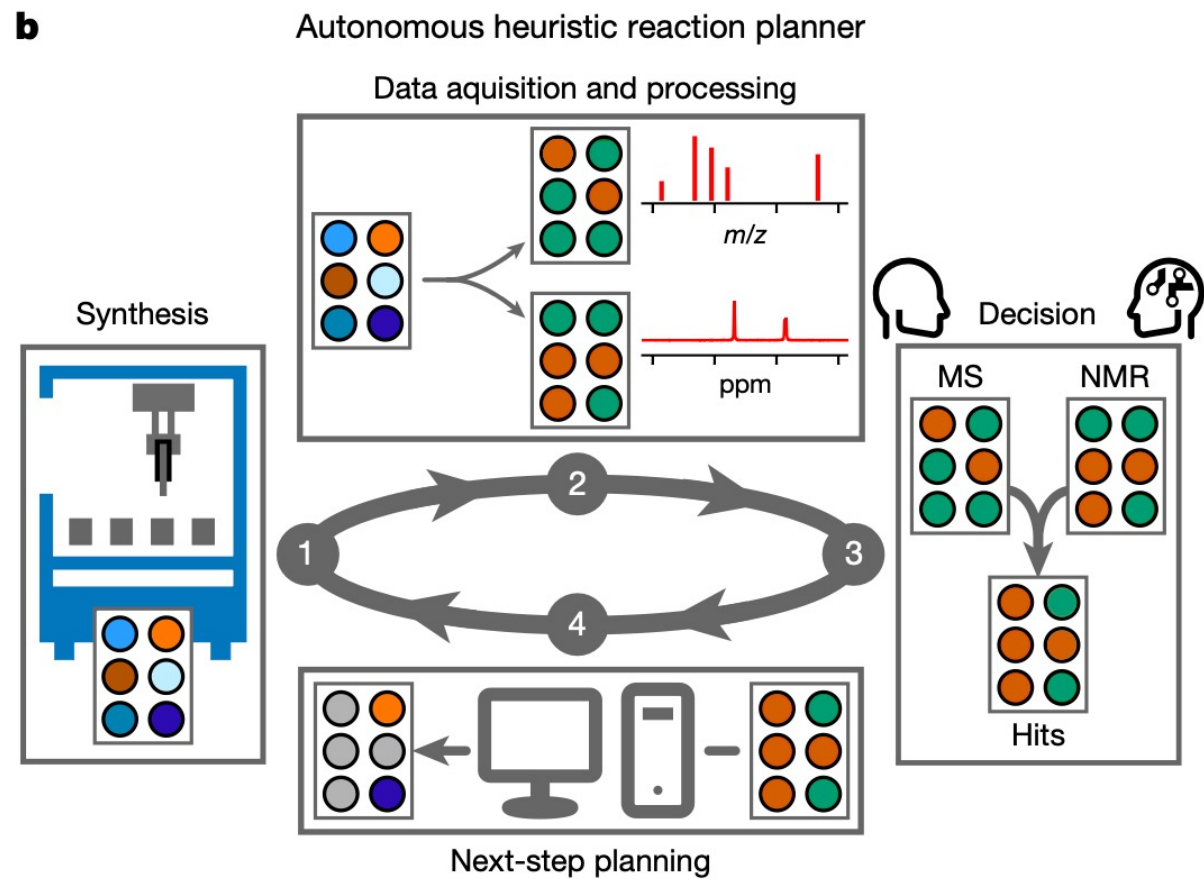
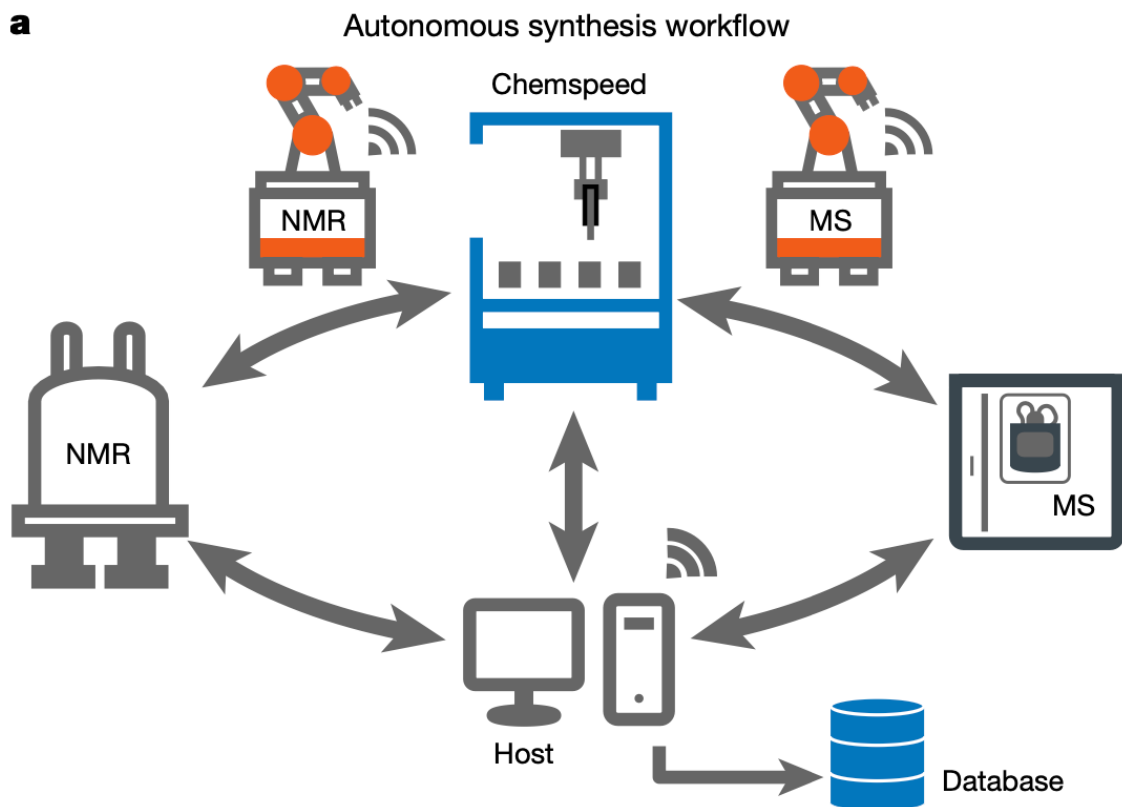


# Work 4: Autonomous lab for exploring protein fitness landscape

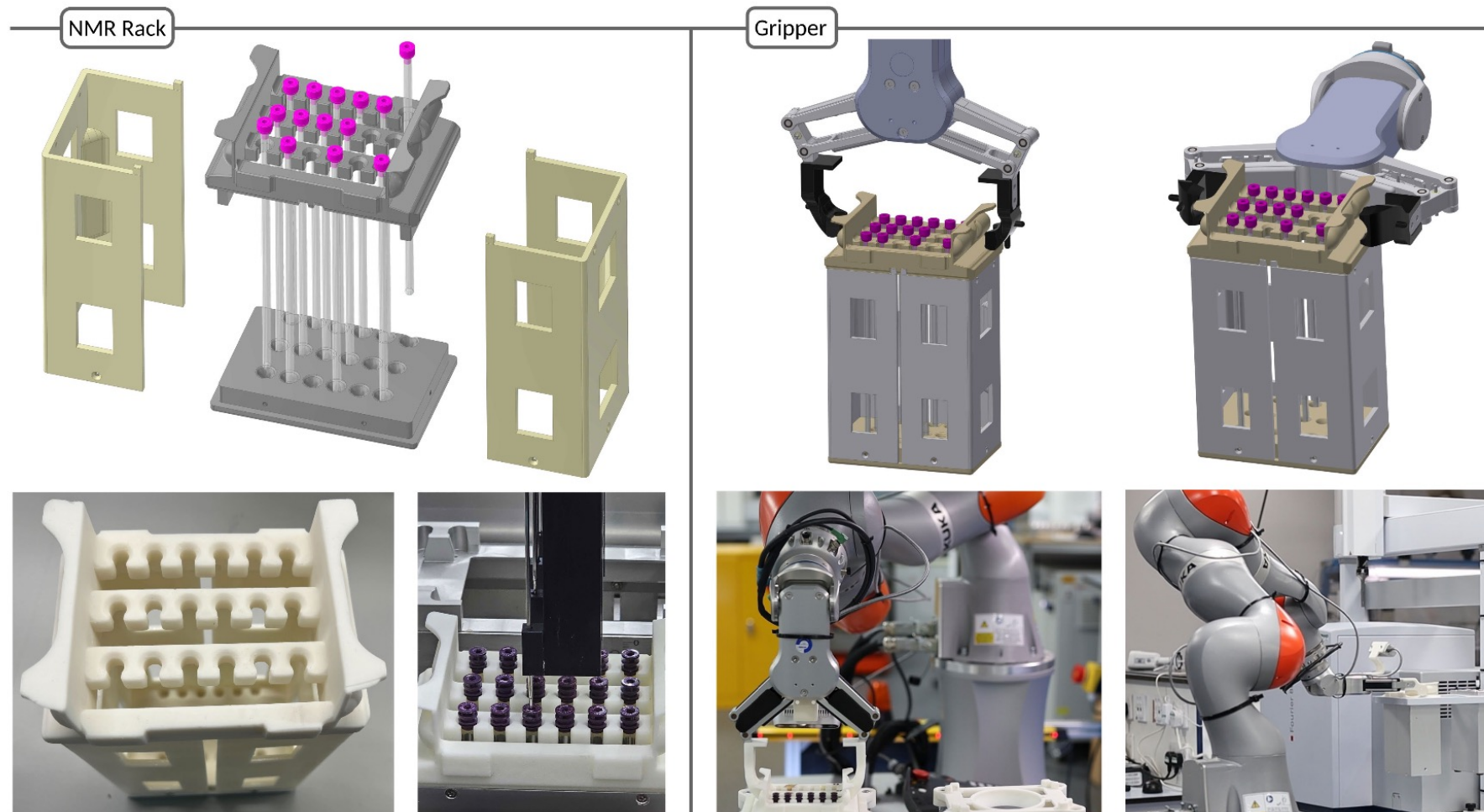


Rapp, Jacob T., et al. "Self-driving laboratories to autonomously navigate the protein fitness landscape." *Nature chemical engineering* 1.1 (2024): 97-107.

Pipeline:

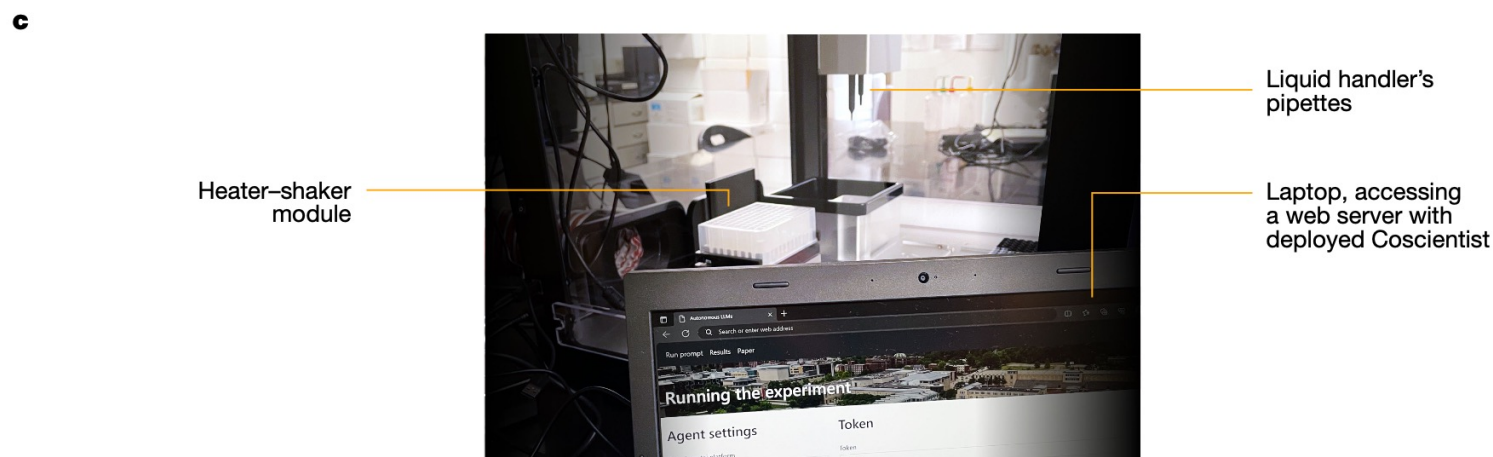
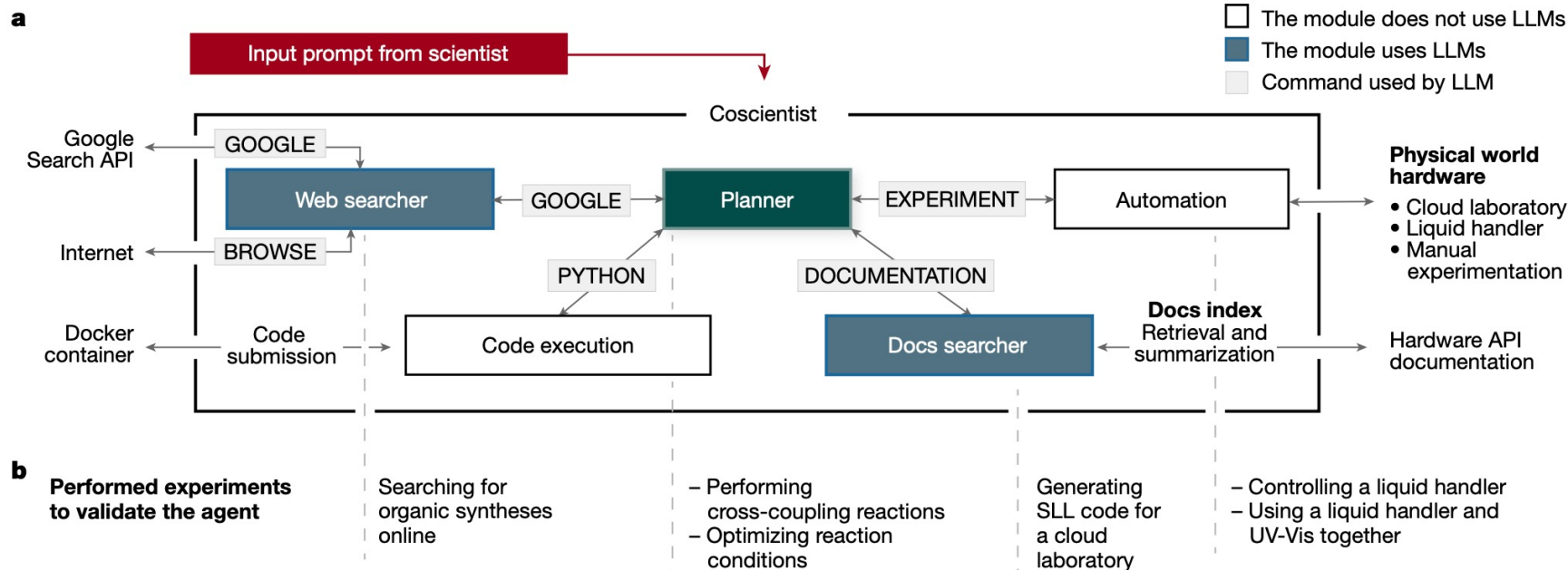


Involving mobile robots:



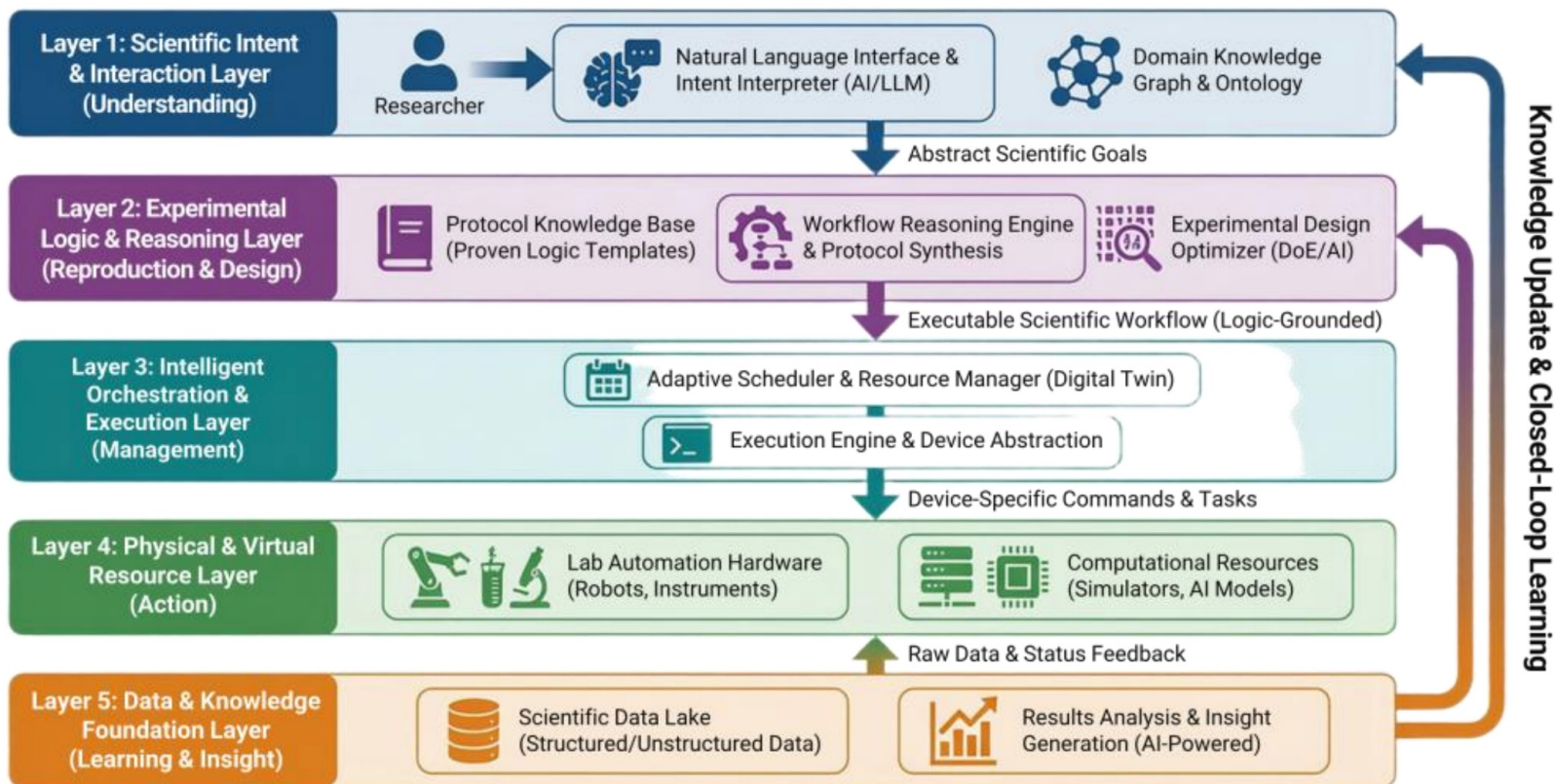
Dai, Tianwei, et al. "Autonomous mobile robots for exploratory synthetic chemistry." *Nature* (2024): 1-8.

# Work 7: LLM for autonomous chemical research



Boiko *et al.* "Autonomous chemical research with large language models." *Nature* 624.7992 (2023): 570-578.

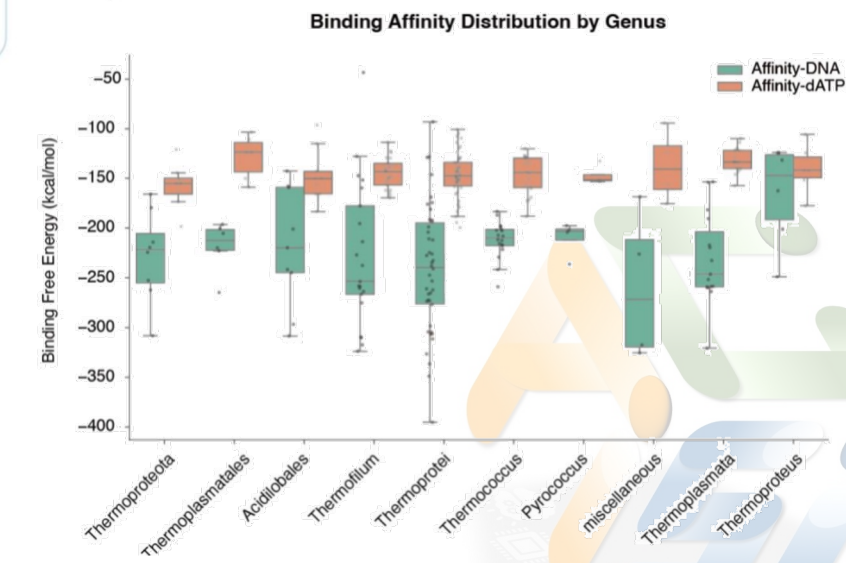
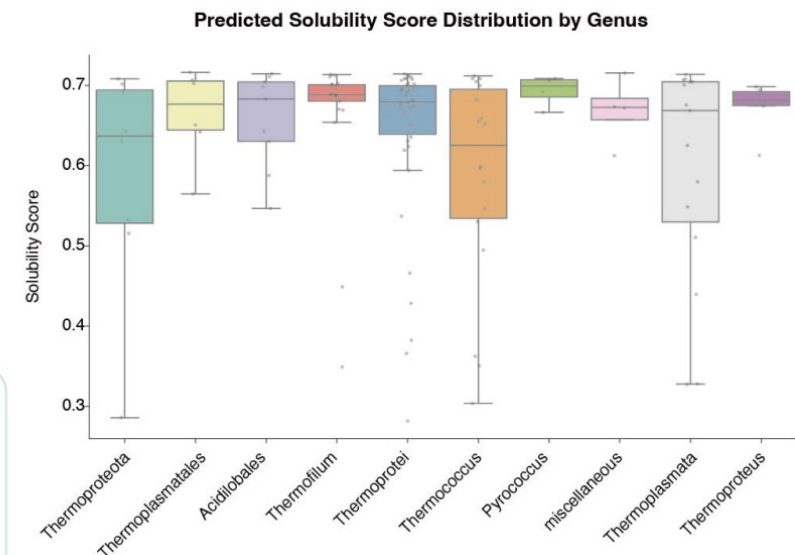
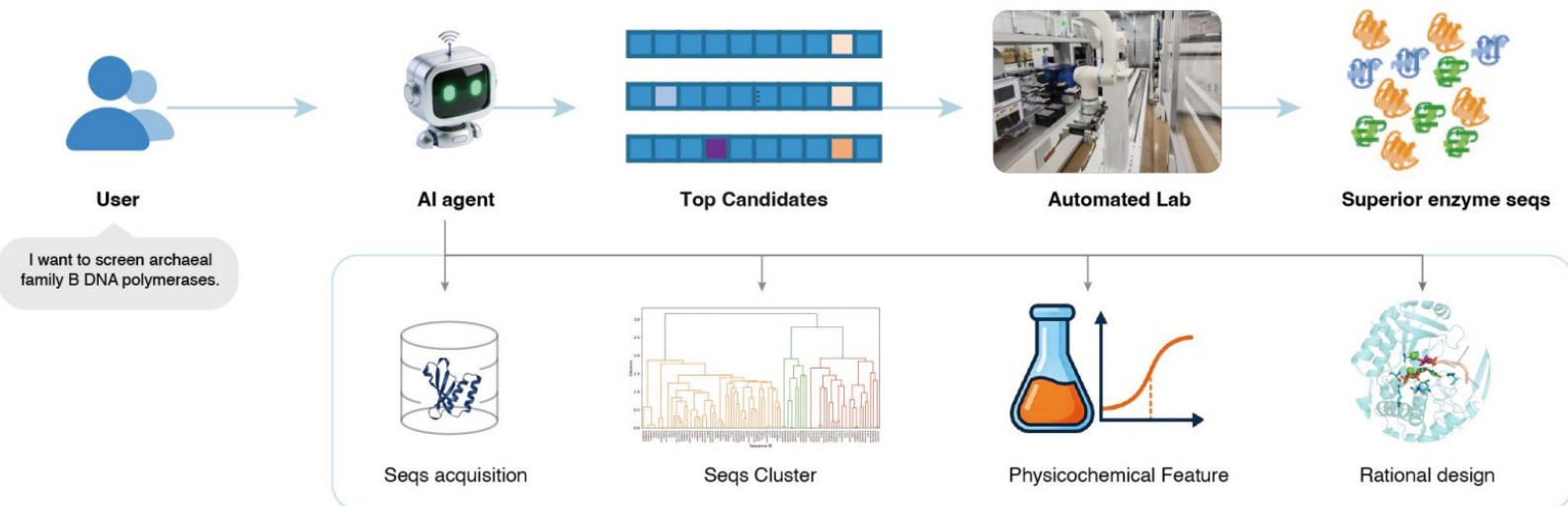
## AI-Native Automated Laboratory Execution Management System



1. Scientific intent interpretation
2. Experimental logic synthesis
3. Intelligent orchestration
4. Physical/virtual resource execution
5. Foundational data-driven knowledge

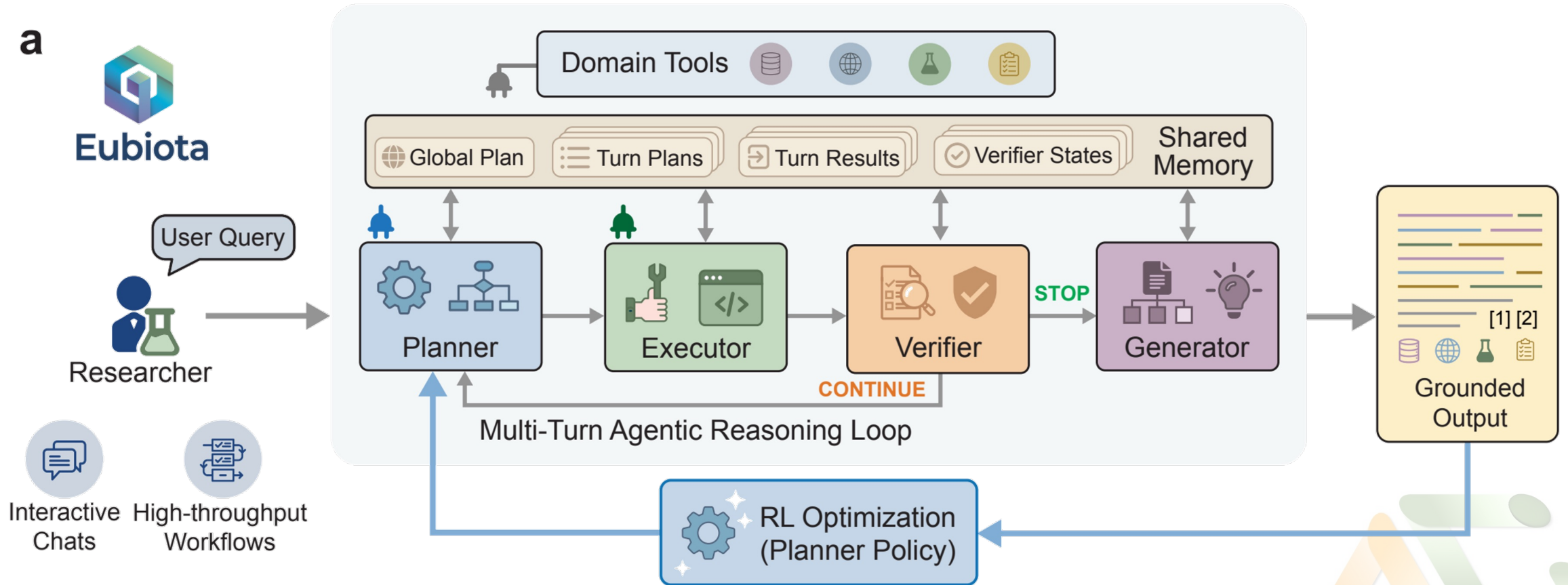


# Work 9: AI-Native Biofoundry



Task: discovering novel thermostable DNA polymerases.

- Distribution of predicted **solubility scores** (SoluProt) across candidates.
- Molecular Dynamics (MD)-based **binding free energy** for the top candidates.

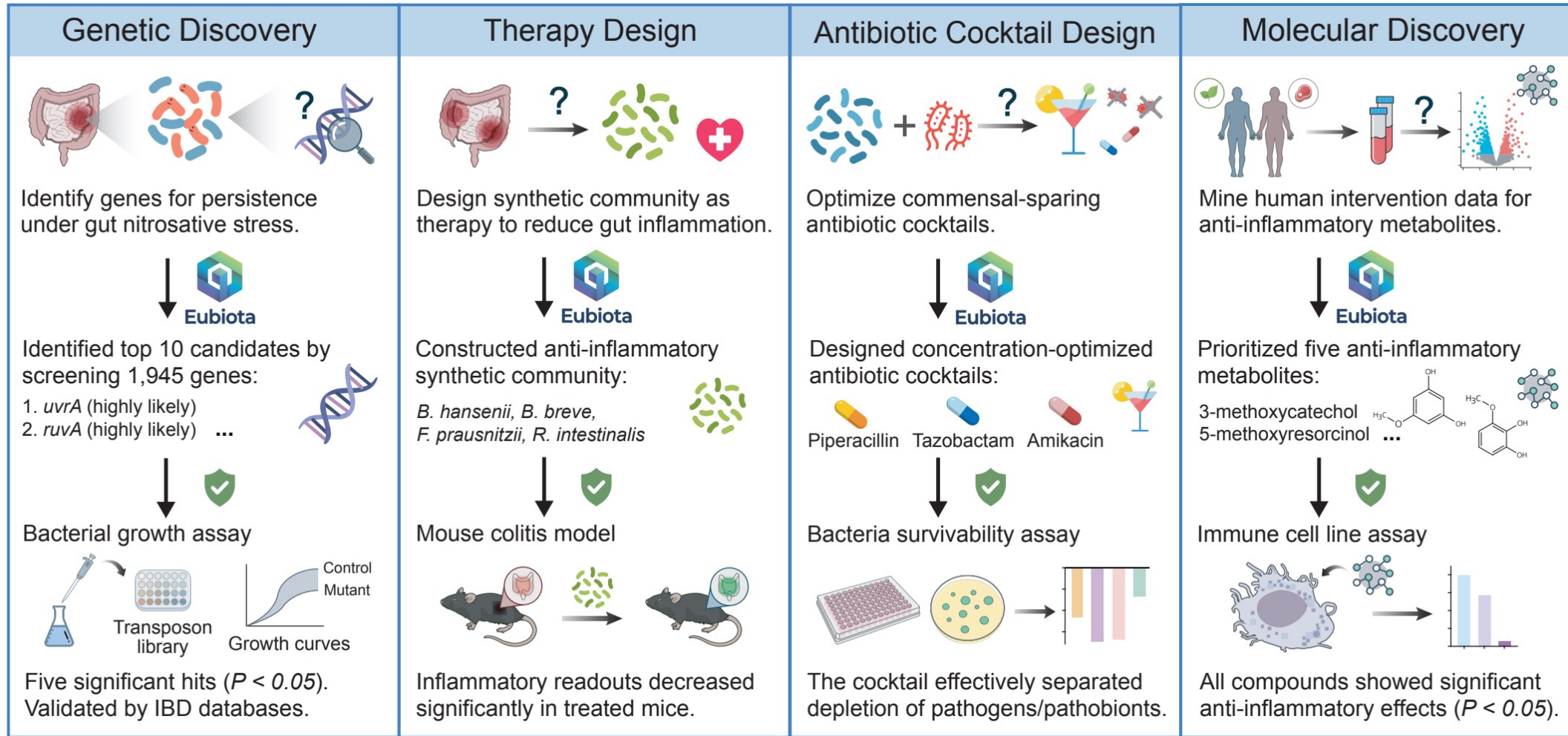


Schematic of the Eubiota framework:

A multi-turn agentic reasoning loop orchestrated by specialized agents (Planner, Executor, Verifier, and Generator), shared Memory, domain tools, and outcome driven reinforcement learning.



# Work 11: Eubiota



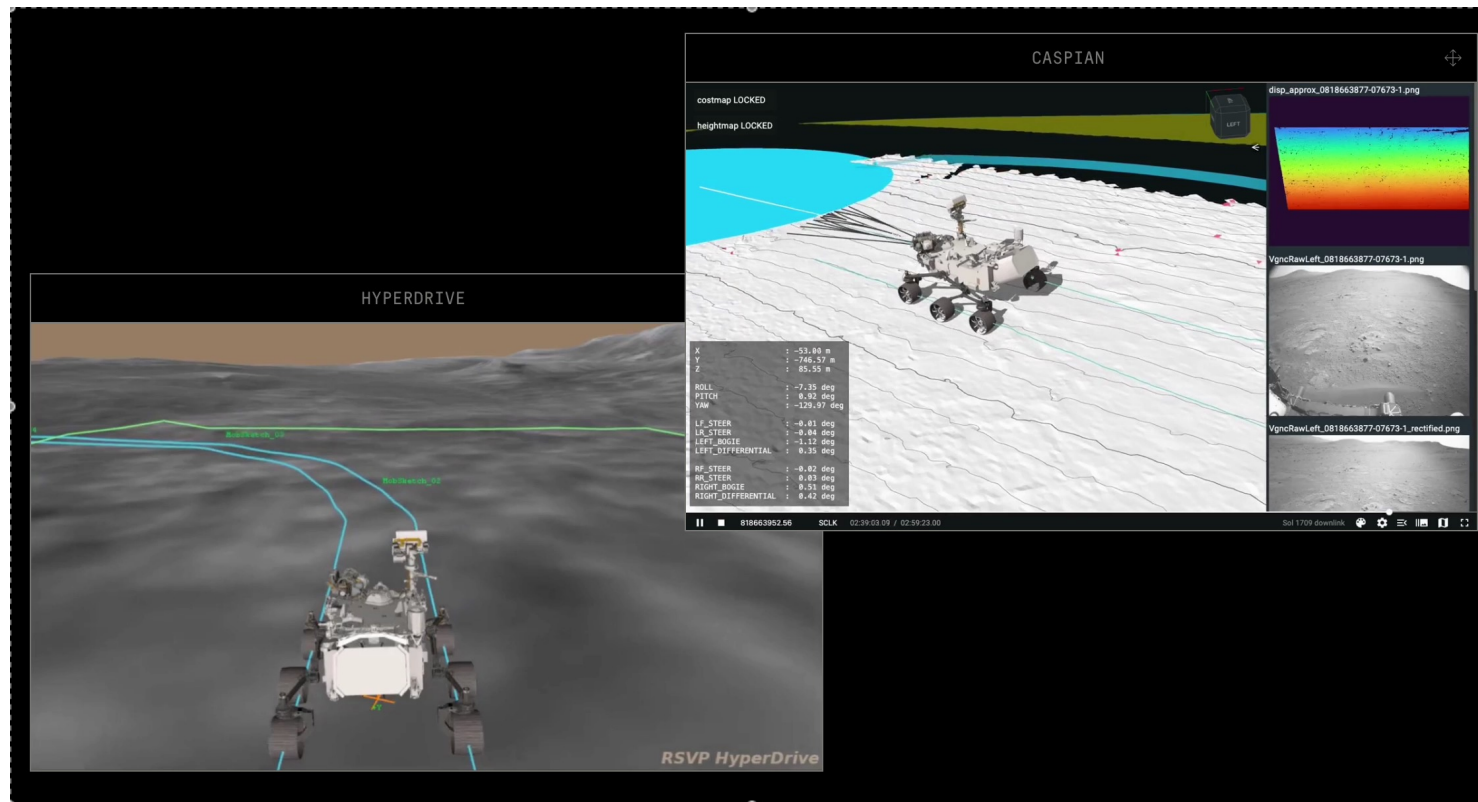
## End-to-end biological discovery and design tasks

||

AI agent for  
Engineering

## Agent planned Mars rover drives:

LLM agent planned waypoint routes for Perseverance: first AI-planned drives on another planet

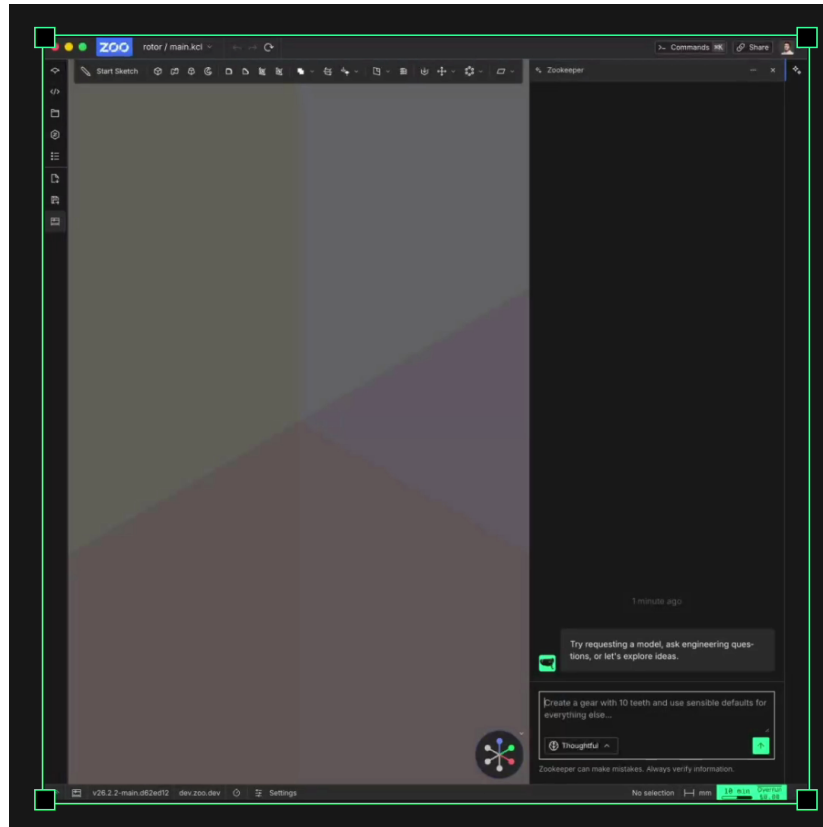


Anthropic. "Claude AI Powers NASA's First AI-Planned Mars Rover Drive."  
Anthropic, 2026. [anthropic.com/features/claude-on-mars](https://anthropic.com/features/claude-on-mars).

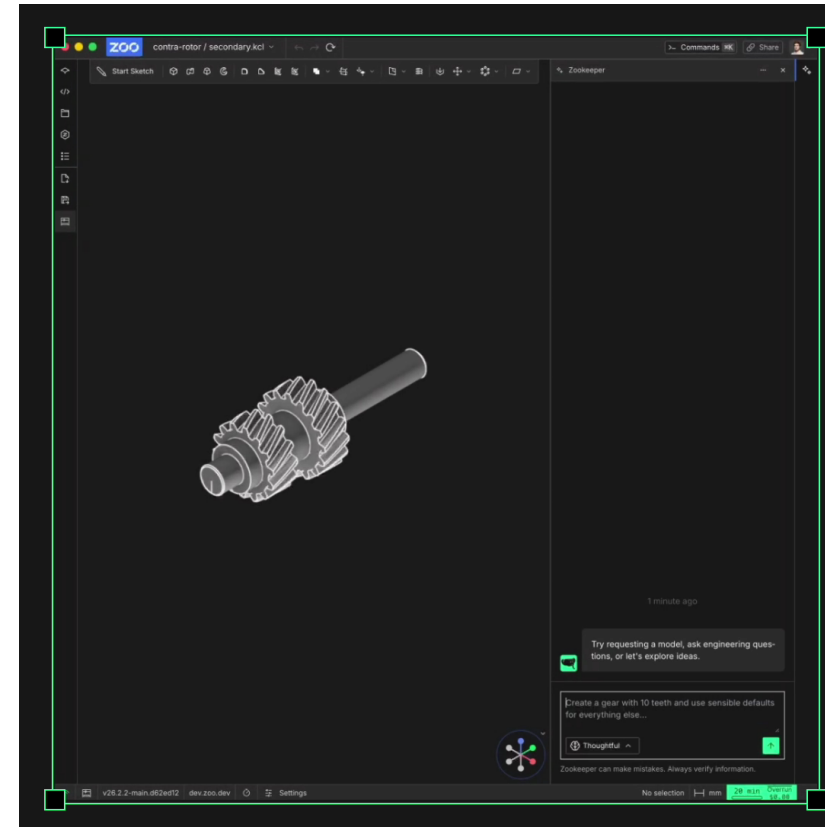


## Text-to-CAD:

## Conversational agents in CAD modeling software



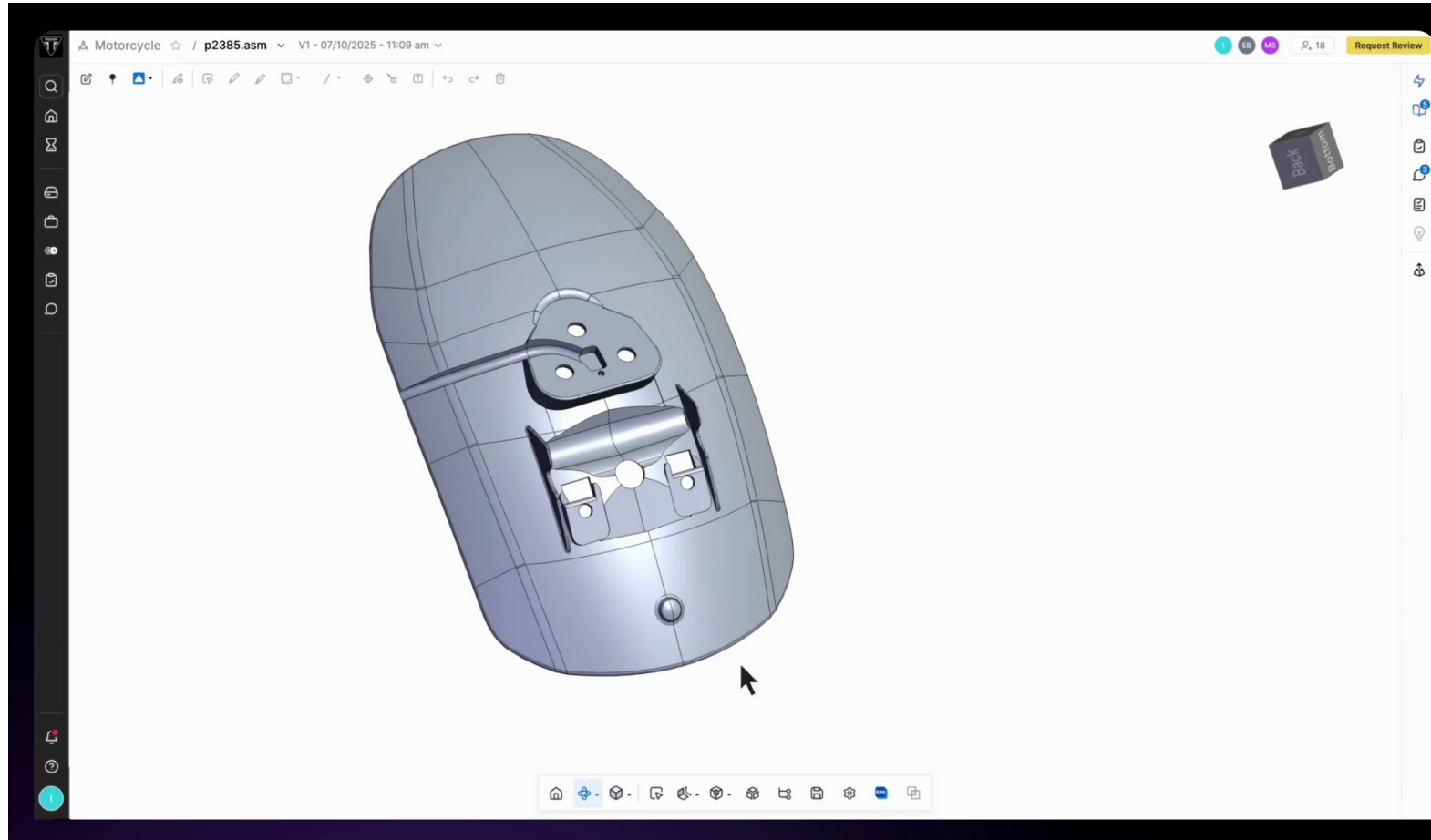
Designs around your prompts



Researches and reasons as it iterates

## Automatic CAD models review:

Conversational agents for auto-review analyzes 3D models and drawings,



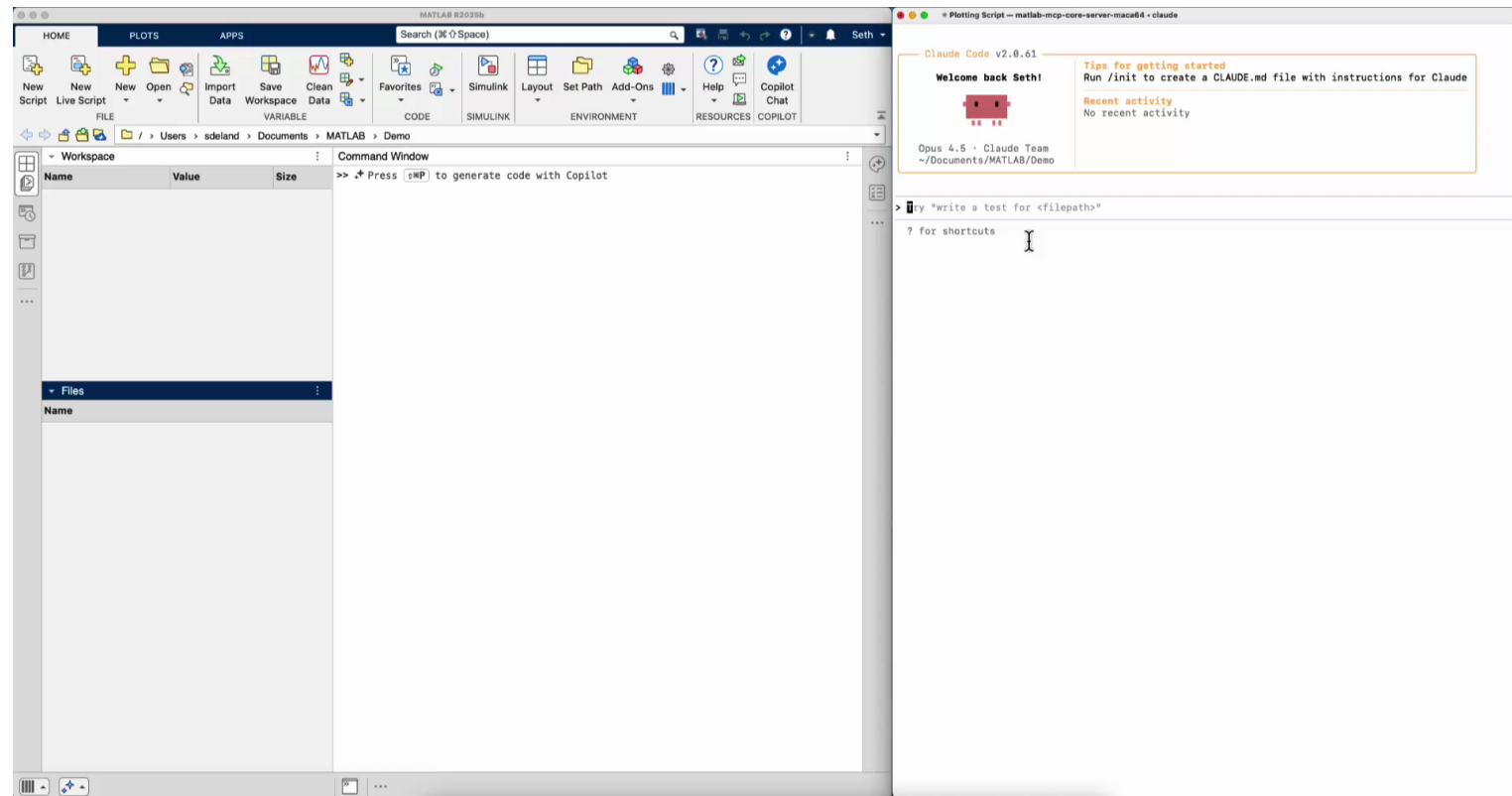
CoLab Software. "AutoReview." [colabsoftware.com/product/autoreview](https://colabsoftware.com/product/autoreview) (2025).



## MATLAB agentic AI Integration:

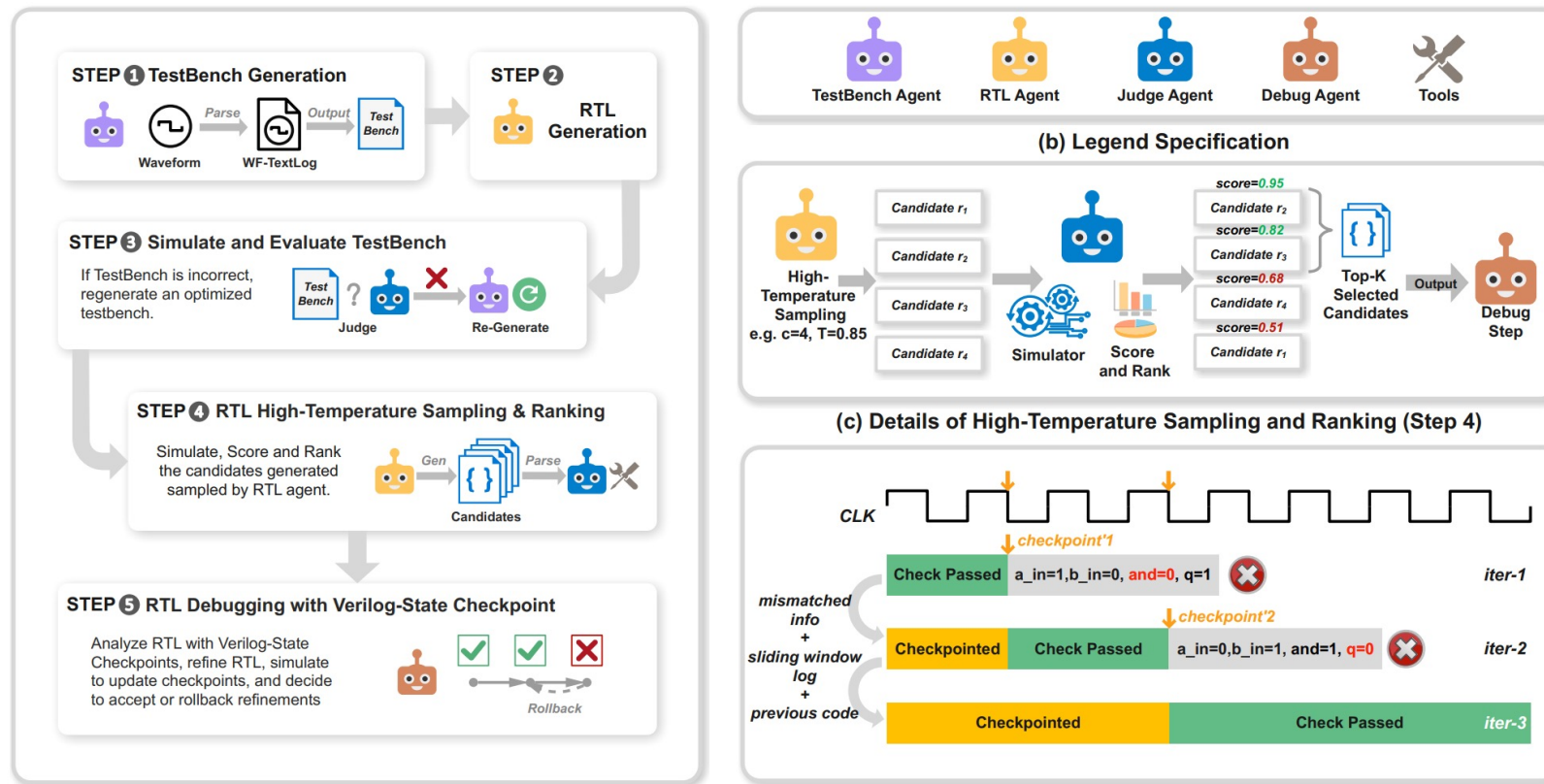
MATLAB MCP Core Server standardizes connections between agentic AI apps and MATLAB, enabling code execution, debugging, and automation.

Claude Code operating  
on MATLAB



## Agent for EDA (Electronic Design Automation):

Multi-agent system for automated Integrated Circuits (IC) design in Register-Transfer Level (RTL) codes



Zhao, Yujie, et al. "MAGE: A Multi-Agent Engine for Automated RTL Code Generation." Proceedings of the 62nd ACM/IEEE Design Automation Conference (DAC), 2025.

III

# AI agent Frameworks



## Famous frameworks:

- [AutoGen](#) by Microsoft
- [MetaGPT](#) by Meta
- [Swarm](#) by OpenAI

## Course:

- [Advanced Large Language Model Agents](#) by UC Berkeley
- Lecture: [LLM Agents](#) by UC Berkeley





## AI co-scientist:

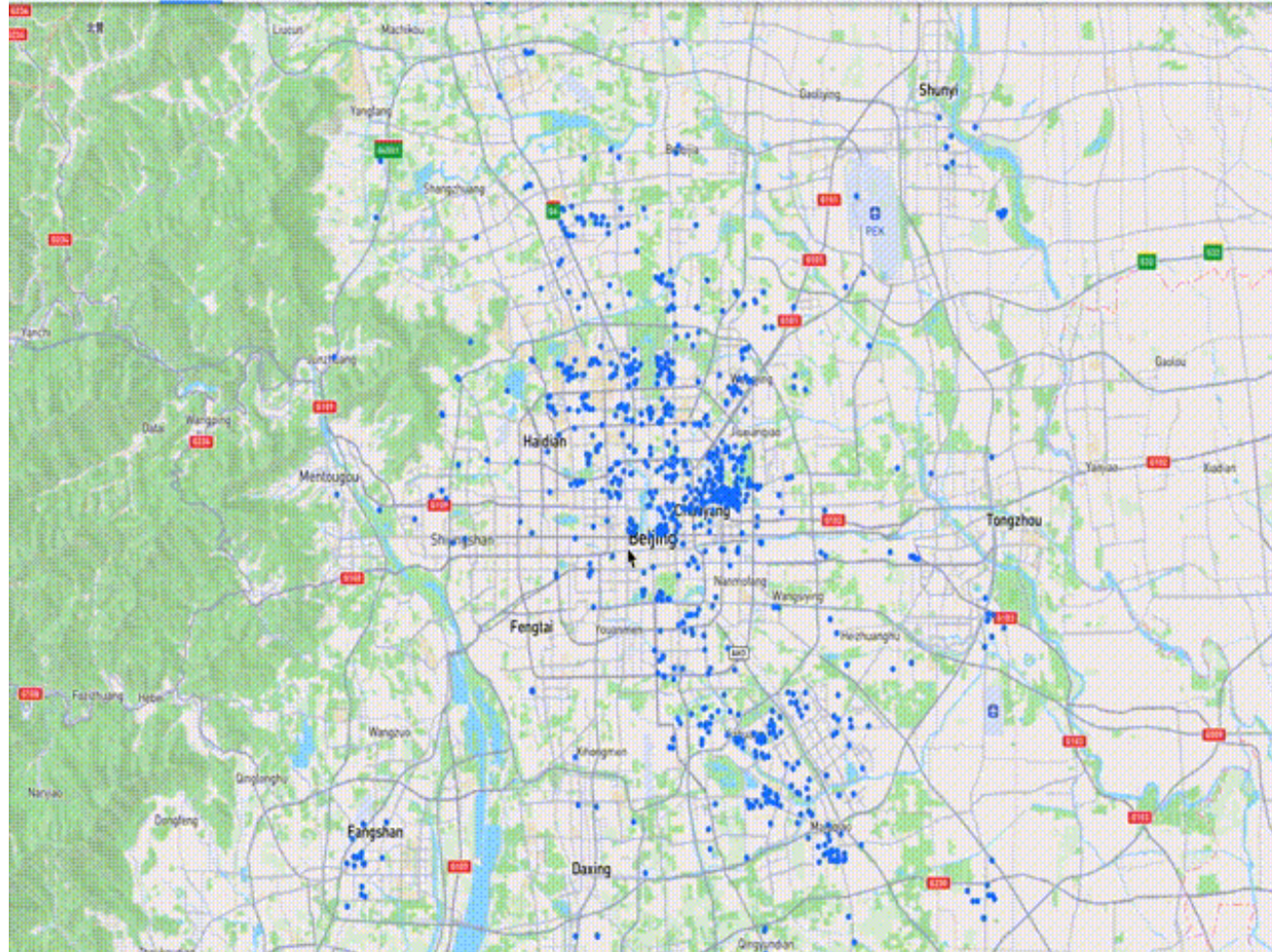
A virtual scientific collaborator to help scientists generate novel hypotheses and research proposals. Video:





Agent society:

Building (>10,000) agents in urban simulation environments



Project Sid:

A glimpse at the first AI agent civilization (in future 100 billion agents)

