MM-ChemAgent: A Multi-modal and Agentic LLM for Chemical Discovery

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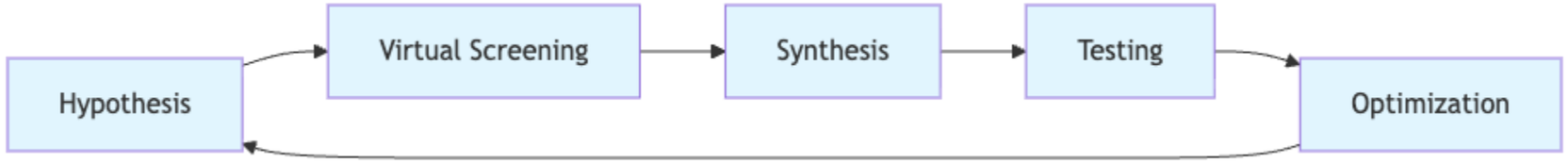
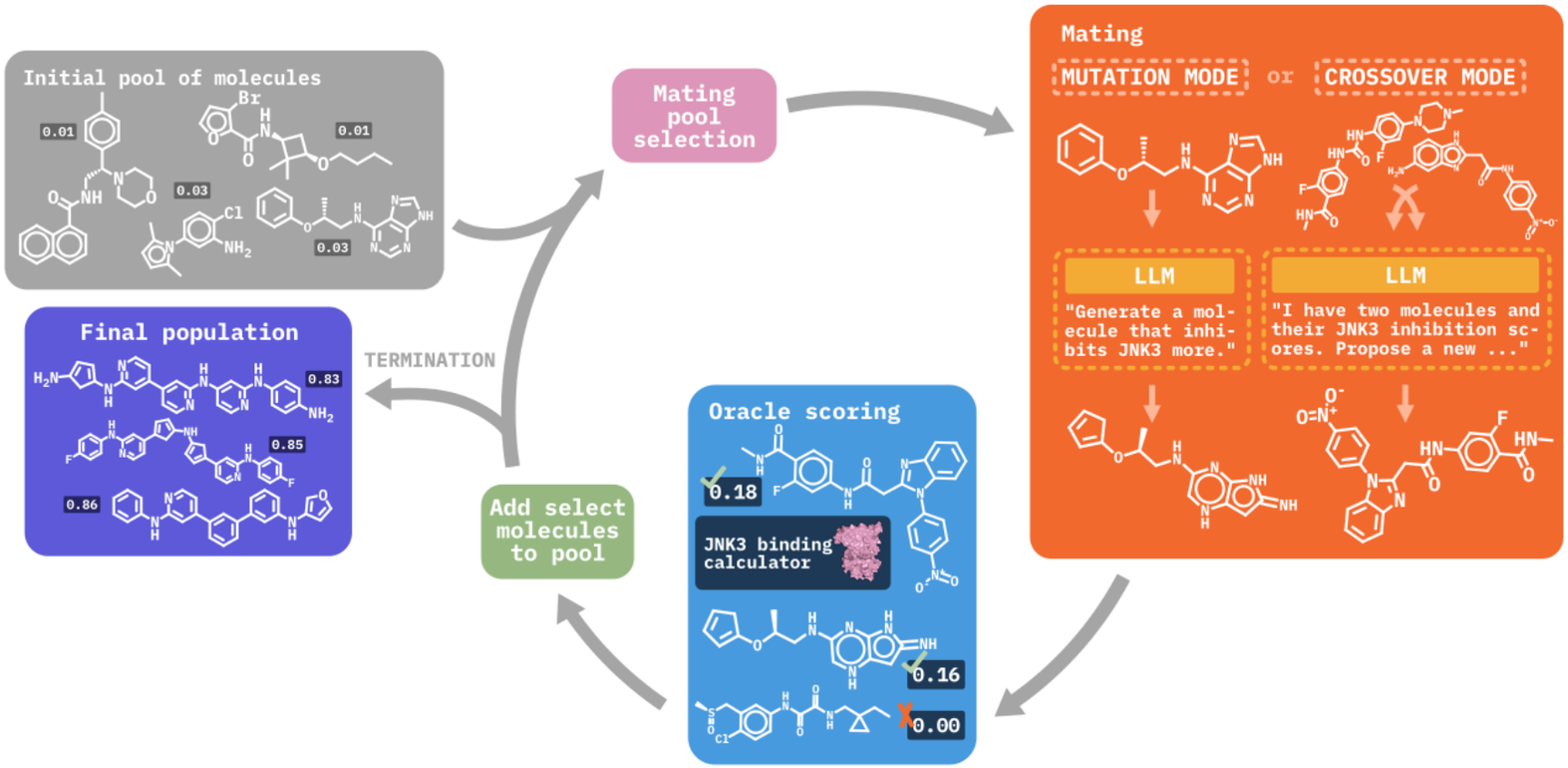
The Challenge: Molecular Discovery is Costly and Slow

- Chemical space: ~10^{60} possible molecules vs. ~10^{8} discovered
- Traditional discovery is slow, expensive, and manual
- Most AI-designed molecules cannot be synthesized



Our Prior Work: LLMs for Molecular Optimization

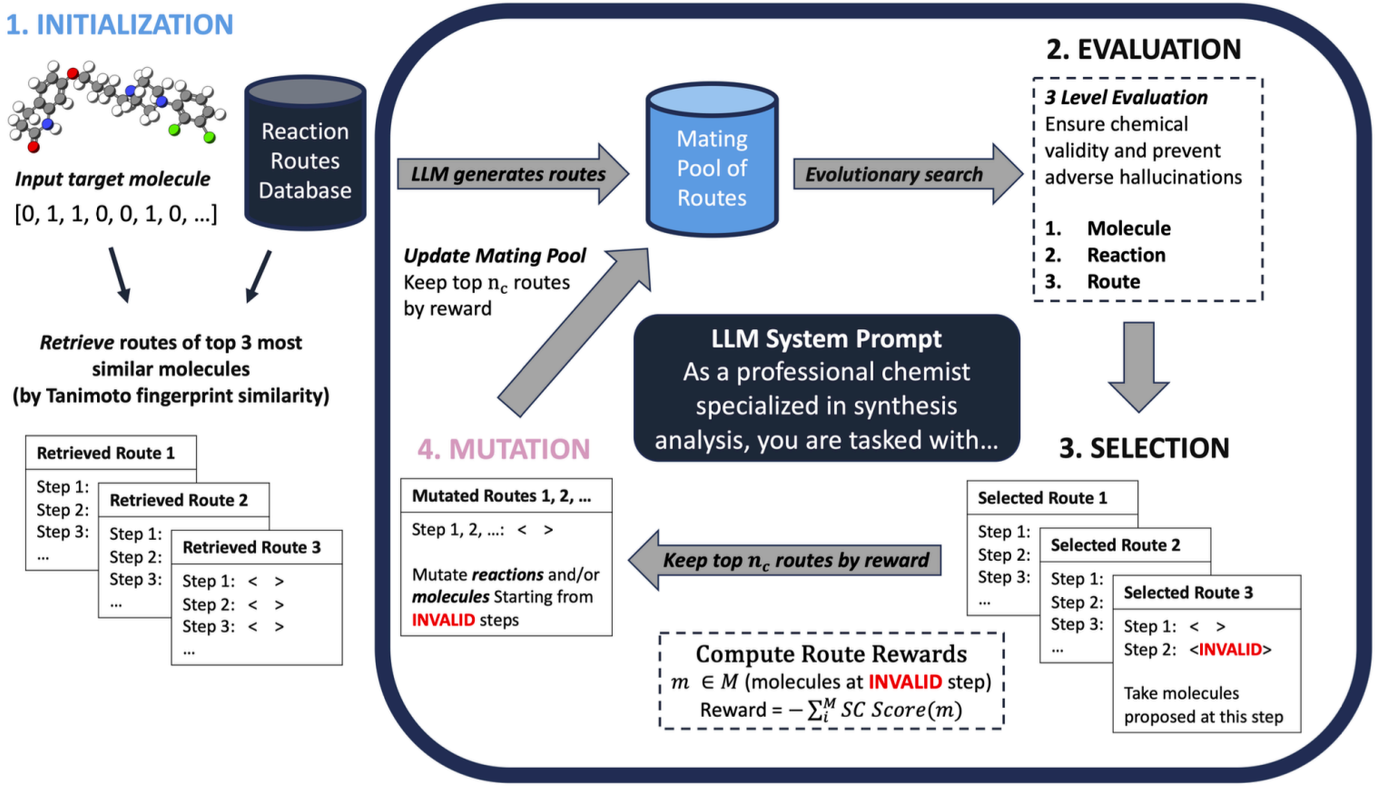
- LLM-guided evolutionary search for new molecular structures
- LLM acts as intelligent mutation and crossover operator



MOLLEO: Efficient Evolutionary Search Over Chemical Space with Large Language Models, Wang et. al., ICLR 2025

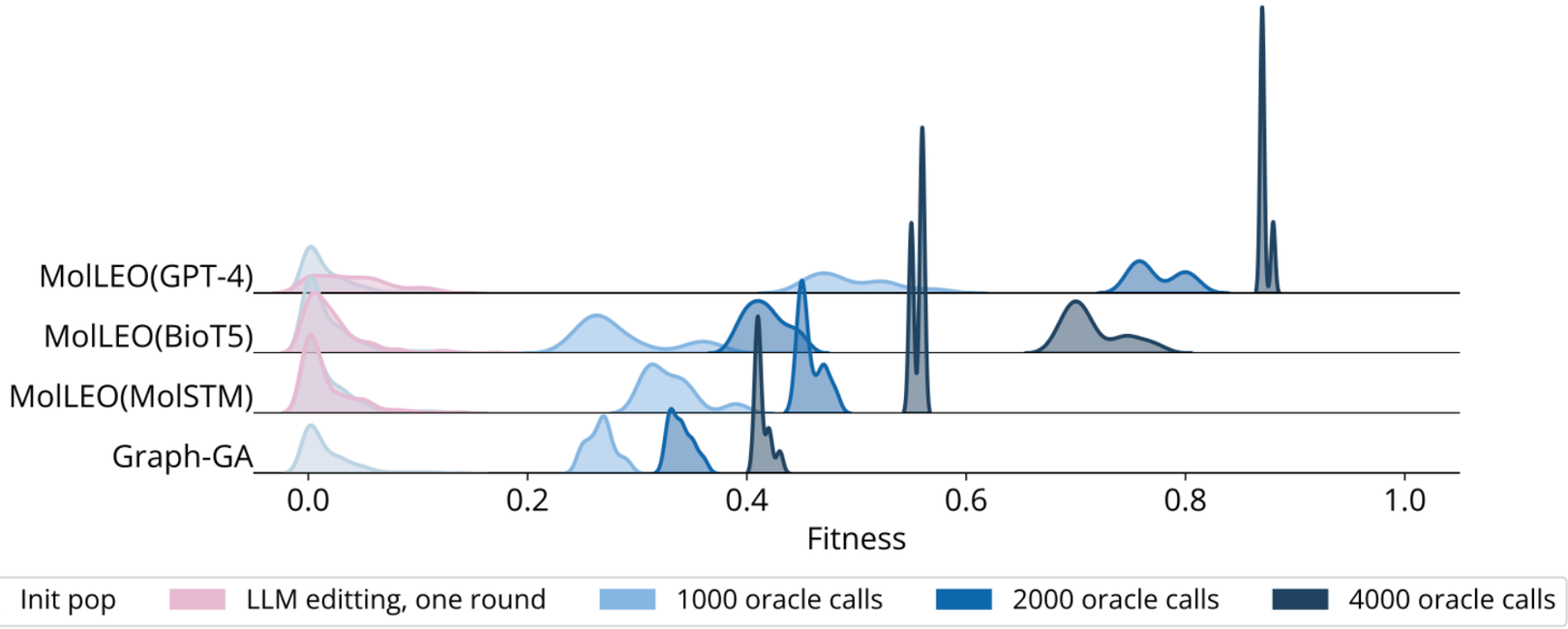
Our Prior Work: LLMs for Retrosynthesis Planning

- LLM-based evolutionary search for whole-route optimization
- Uses chemical feasibility scores to guide route refinement



LLM-Augmented Chemical Synthesis and Design Decision Programs, Wang et. al., ICML 2025

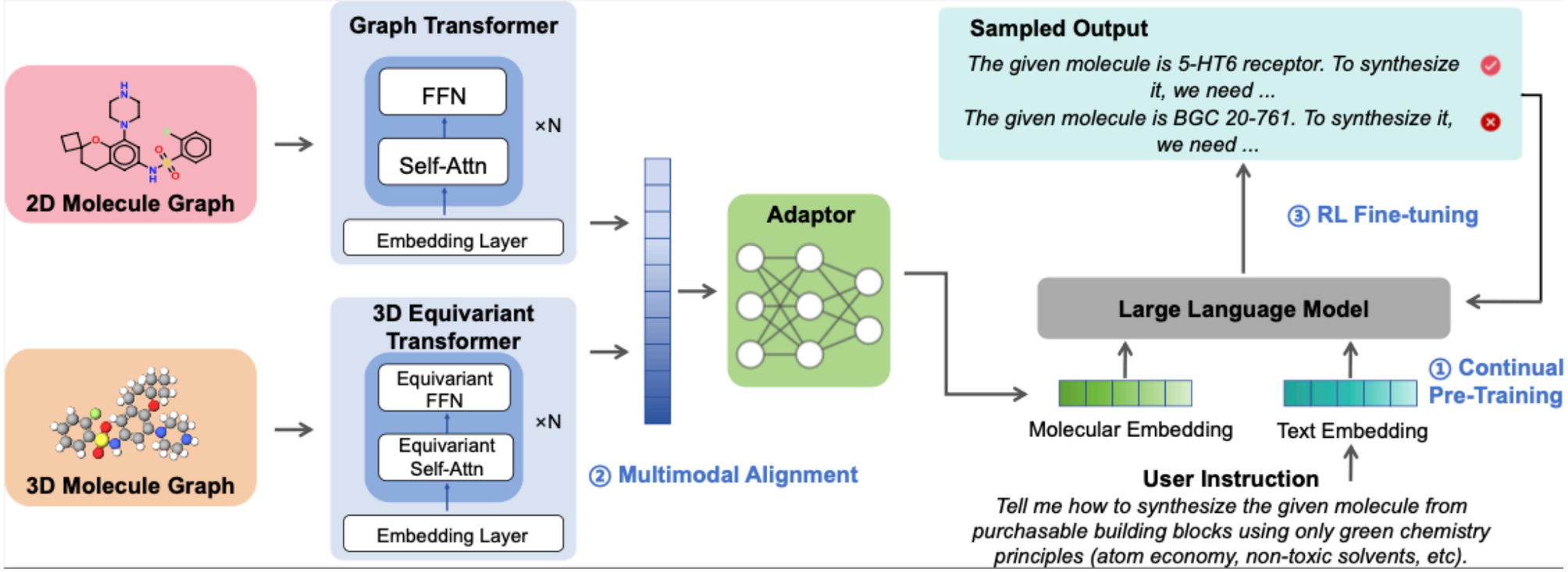
Results: How do LLM agents perform for molecule optimization?



- Outperforms traditional baselines on 15+ optimization benchmarks
- Demonstrated multi-objective improvements across different properties
- Near-100% solve rates on USPTO benchmarks with synthesizable routes

But can we do better with multimodal + RL fine-tuning?

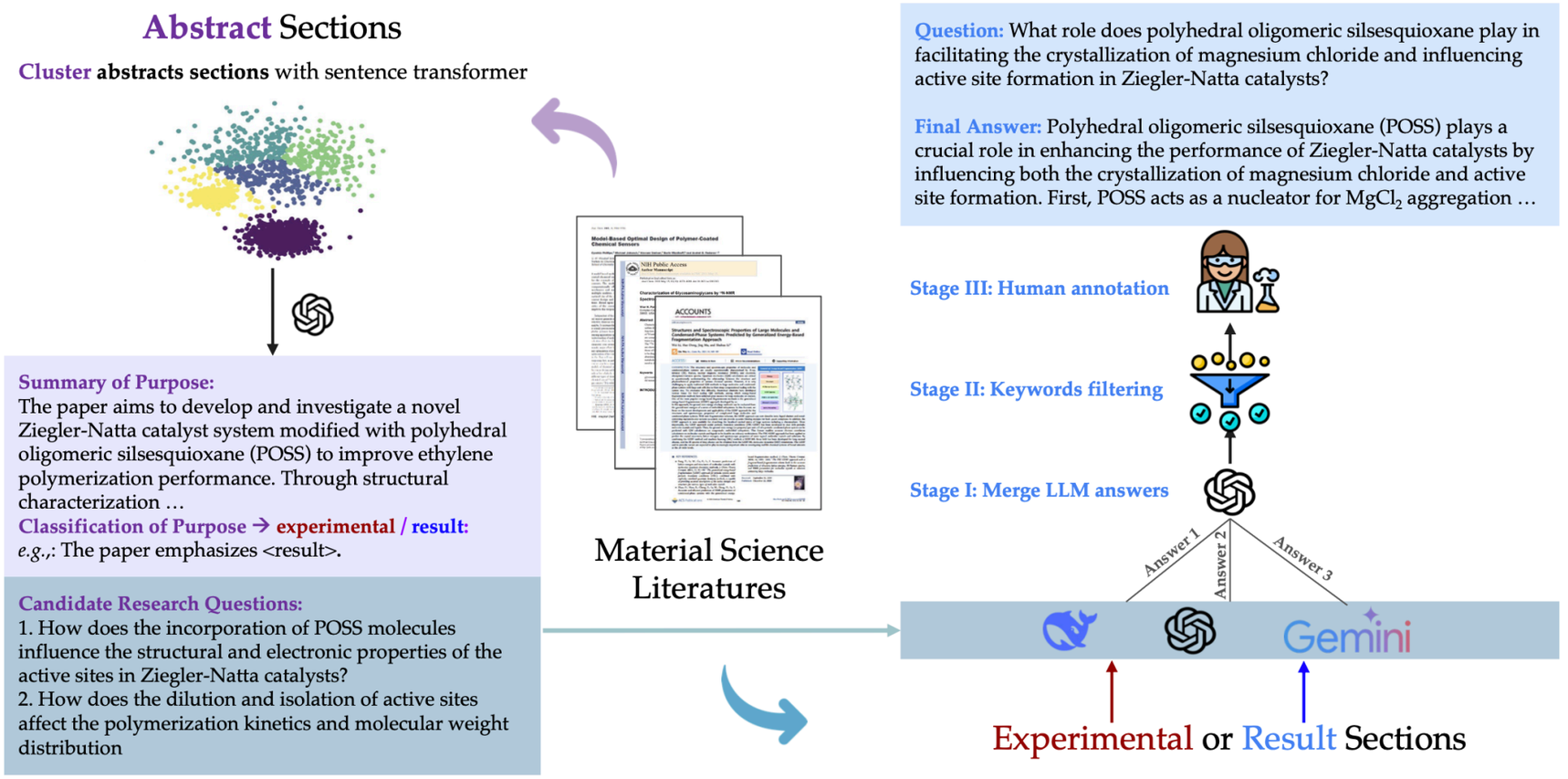
This Project: Multimodal and Agentic LLM for Chemical Discovery



Core Innovation: Multimodal (Text & Molecules) + RL fine-tuning

- Multi-modal alignment (text ↔ molecular representations)
- RL fine-tuning for better agentic capabilities (plan, use tools, adapt through trial and outcomes)

Data & Tools



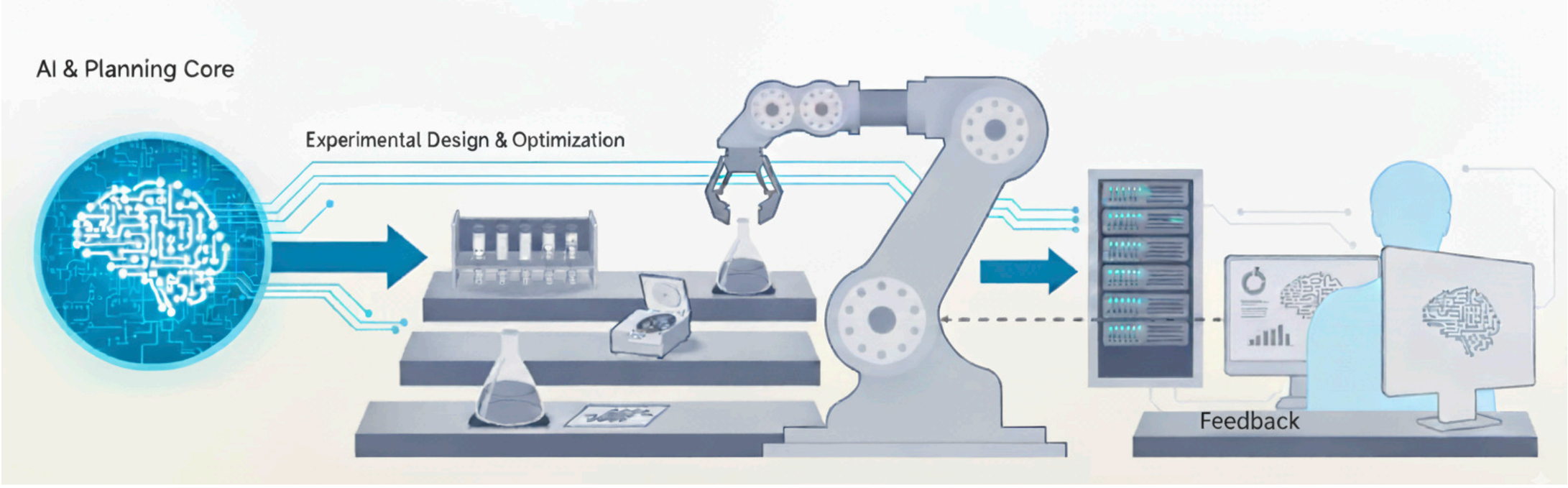
- **Tasks:** Molecular optimization, synthesis planning, property prediction
- **Tools:** Web search, chemical databases, property APIs, simulation tools
- **Feedback**: Chemoinformatics (e.g., RDKit), ML predictors, simulation

Applications & Impact

Target Impact: Faster and better molecular discovery, open-source

- Benchmarks: molecule optimization (e.g., TDC); Recyclable polymer design
- Metrics: molecular properties, synthesizability, cost

Future Vision: Self-driving labs powered by multimodal agents for autonomous discovery



Thank You

Thank you to GT-IDEAS and Microsoft for this support!

Link to resources:

- MOLLEO: Efficient Evolutionary Search Over Chemical Space with Large Language Models
- May the Force be with You: Unified Force-Centric Pre-Training for 3D Molecular Conformations

Q&A?