

A Canonical Framework for Multi-Dimensional Retrosynthetic Scoring

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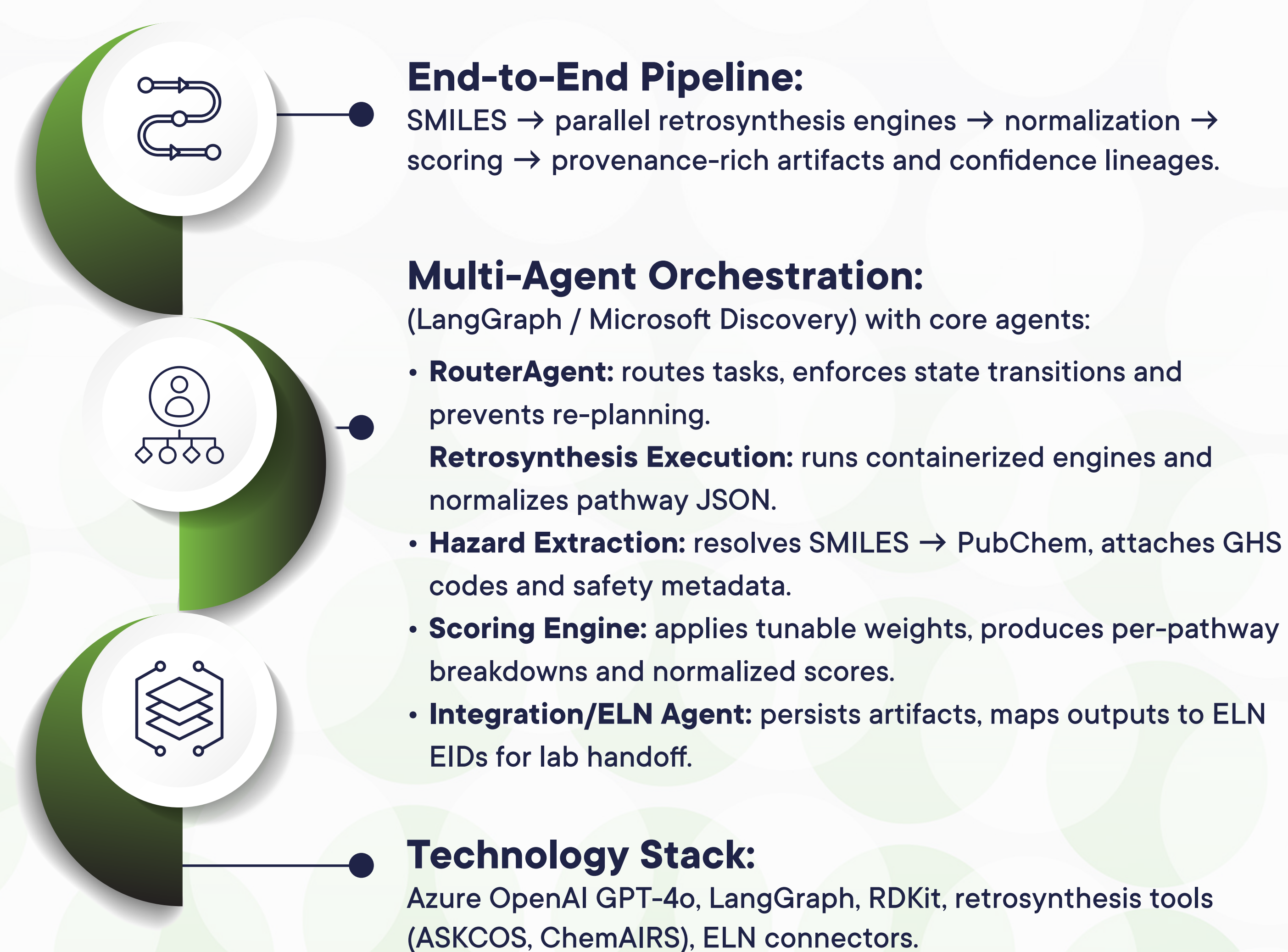
Problem Statement

- Selecting an optimal Route of Synthesis (ROS) for an API is a high-stakes, time-sensitive decision that remains manual, fragmented, and error-prone.
- Chemists and legal teams must stitch together patents, literature, commercial databases and tribal expertise across disconnected tools, creating patent complexity, information overload, tool fragmentation, limited predictive insight (impurity/scale-up risk), and systemic human bias.
- These gaps drive higher production cost, regulatory burden, impurity and safety risks, potential IP infringement, and lengthy time-to-market.
- The result: critical ROS choices are slow, non-reproducible, and poorly traceable necessitating an automated, auditable, multi-engine pipeline to deliver fast, evidence-backed route selection.

Objectives

- Automate ROS selection to deliver breadth, rigor, and traceability; run complementary retrosynthesis engines in parallel; normalize outputs into a canonical pathway model; apply configurable, reproducible scoring.
- Automate generation, evaluation, and prioritization of ROS candidates.
- Produce reproducible, auditable shortlists with provenance for FTO and lab validation.

Methodology / System Architecture



Outcomes (Key Capabilities)



Conclusions & Implications



Converts ROS into a fast, objective, auditable pipeline that accelerates decision-making without sacrificing technical rigor or traceability.

Future Enhancements



Patent intelligence.



Org-specific retrosynthesis.



Compound-preference ranking.

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