From LLMs to Multi-Agent Systems: Advancing AI-Powered R&D in Pharma and Biotech

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Unlocking the Power of AI in R&D

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Pharmaceutical and biotech R&D teams are generating and analyzing more data than ever before. However, extracting actionable insights from unstructured text, molecular data, and clinical research remains a challenge.

Large language models (LLMs) have evolved from isolated AI tools to orchestrated multi-agent systems that can **integrate biomedical data, generate hypotheses, and streamline research workflows**.

In this session, we will explore:

How LLMs are **transforming R&D operations** in pharma and biotech.

The **shift from standalone LLMs to multi-agent systems** for drug target identification, biomarker discovery, and competitive intelligence.

Real-world applications demonstrating how AI-powered platforms are enhancing decision-making in scientific research.

What it takes to make AI successful.

By leveraging advanced **retrieval-augmented generation (RAG), knowledge graphs, and AI orchestration**, we can **unlock insights from unstructured biomedical data** at an unprecedented scale.

The R&D Challenge:
Pharma R&D Teams Face a Data Storm

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Fragmented, Siloed Data

- Scientific knowledge is trapped in PDFs, ELNs, omics, clinical data, patents, and publications
- Data silos block integration and insight generation

Unstructured & Multimodal Complexity

- Data spans text, images, molecular structures, and time-series
- Traditional analytics fall short across these formats

Manual, Time-Consuming Workflows

- Scientists spend hours curating, extracting, and searching
- Valuable time lost on repetitive tasks, not real discovery

Limited AI Adoption

- Rule-based tools lack reasoning and flexibility
- AI models have struggled with complex scientific questions

Compliance & Validation Pressures

- AI must meet stringent governance, security, and regulatory standards
- Bias, provenance, and explainability remain key barriers

What Does Utilizing LLM's Mean for a Scientist?

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Significant time savings for researchers, allowing them to focus on actual research by automating routine tasks (e.g., LLM assistants for ELNs, literature reviews, etc.).

Enhancing drug discovery by generating draft hypotheses for scientists to assess and prioritize.

Faster scientific knowledge extraction and potential integration with omics and clinical data, dramatically accelerating key R&D processes such as:

- Target identification & validation
- Understanding drug resistance mechanisms
- Finding biomarkers
- Drug repurposing & repositioning
- Pharmacovigilance & detection of adverse drug events (ADEs)

The Evolution of LLMs in Pharma and Biotech

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Phase 1: Early Adoption

2017

- First transformer NLP models used for **literature mining and text extraction**
- Basic **chatbots and search engines** for retrieving biomedical information
- AI-driven data curation, but **limited contextual understanding**

Challenges: Minimal contextual understanding, no domain adaptation, limited integration into research workflows

Phase 2: Single LLM Implementation

2022-2023

- **Introduction of LLMs** (GTP, and domain specific LLM's. E.g. BioBERT) for **summarization, entity extraction, and search augmentation**
- Used in **drug discovery, clinical trial analysis,** and **advanced analytics**

Challenges: Hallucinations, lack of domain-specific knowledge, limited reasoning capabilities, and low context. Limited prompt control

The Evolution of LLMs in Pharma and Biotech

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Phase 3: Advanced Retrieval-Augmented Generation (RAG)

2023-2024

- RAG-based approaches **combine structured and unstructured data sources** (PubMed, patents, clinical trials)
- Fine-tuned LLMs for **target identification, biomarker discovery, and therapeutic landscape assessment**
- Integration of **vector databases** (e.g., pgvector, FAISS) **for semantic search**

Challenges: Complex pipeline architecture, dependency on retrieval quality, prompt tuning and response evaluation bottlenecks, maintaining accurate context across sources

Phase 4: Multi-Agent AI Systems & Autonomous Research Assistants

2024-Present

- **Multi-agent architectures** enable **collaborative AI-driven research workflows**
- **Specialized agents for molecular data, omics analysis, and pathway interpretation**
- AI systems are **orchestrated to provide real-time scientific insights, hypothesis generation,** and **decision support**

Challenges: Defining clear agent roles and coordination protocols, orchestration complexity and potential agent overlap, governance, monitoring, and validation at scale

Real World Successes: Case Studies

Target Identification Platform (Major Pharma Company)

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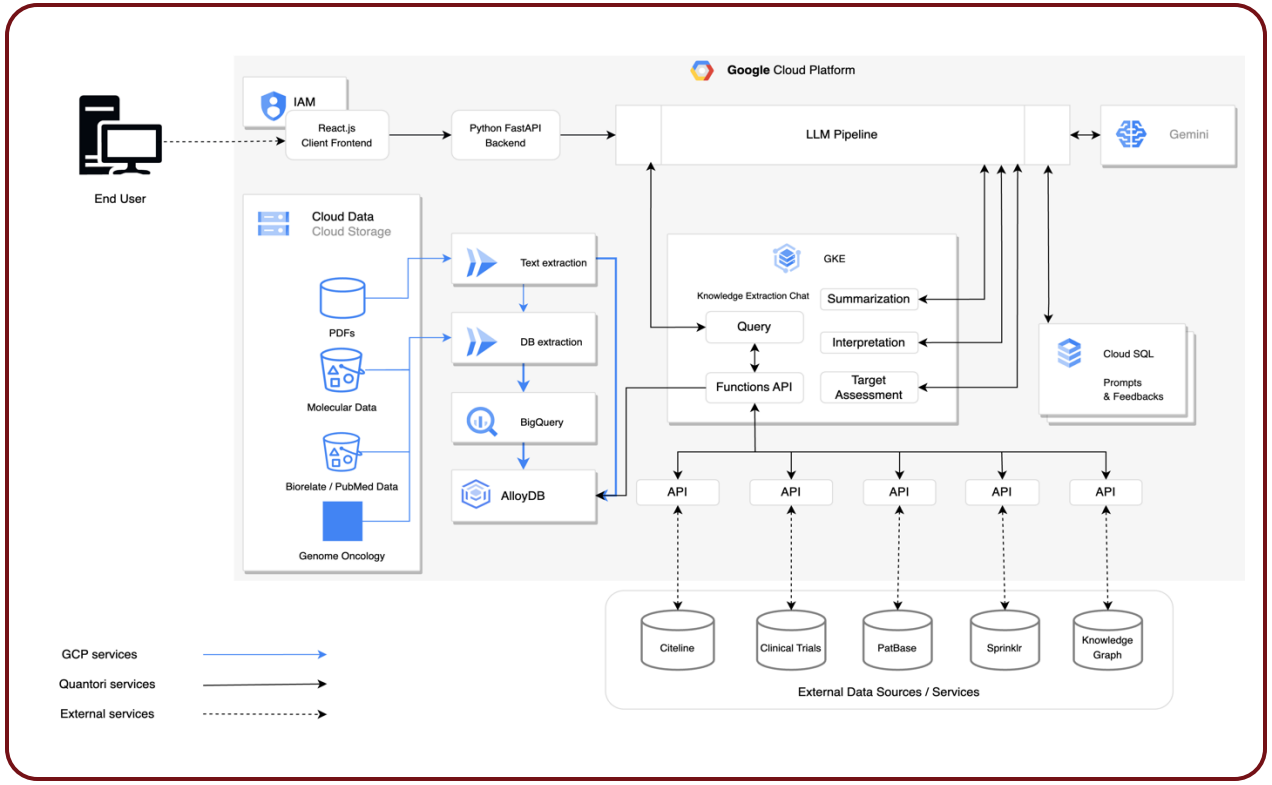
Challenge

- Scientists and stakeholders struggled to search, retrieve, and analyze diverse data types (PDFs, tables, APIs).
- High latency in data gathering and analysis for drug target identification.
- Many users lacked the technical skills to operate existing tools for data ingestion and analysis.

Solution

- Created an AI-powered internal platform to enable drug target identification and discovery.
- Built a GPT-style frontend with customized functions for non-technical users.
- Focused on supporting multiple use cases and flexible configurations.



Target Identification Platform (Major Pharma Company)

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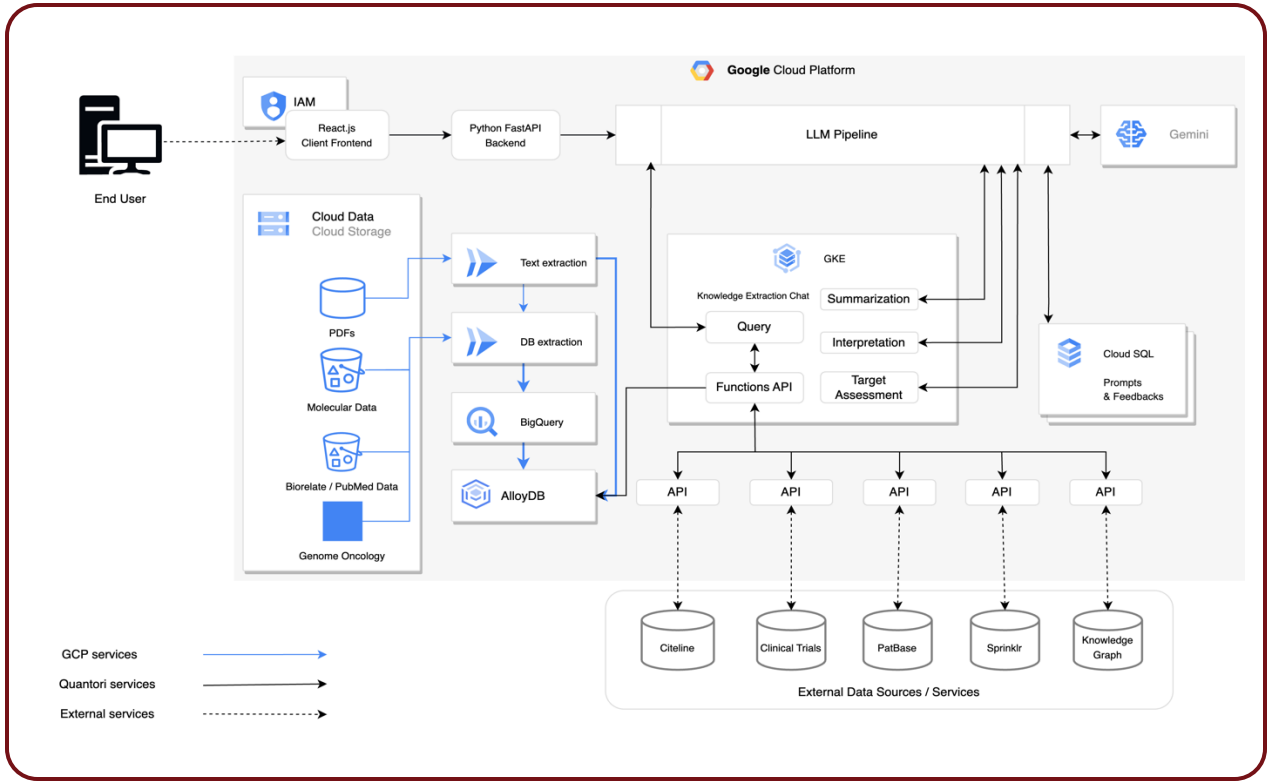
Results

- Reduced time-to-insight for scientists.
- Self-service tool used in Oncology
- Enabled faster, more accurate decision-making for drug discovery.

Key Takeaways

- Accelerated go-to-market speed for R&D insights.
- Improved data integration and decision-making.
- Reduced scientists' burden with simplified access to diverse internal data.
- Demonstrated the value of using an internal, secure LLM platform for scientific search.



Scalable LLM Deployment (Major Pharma Company)

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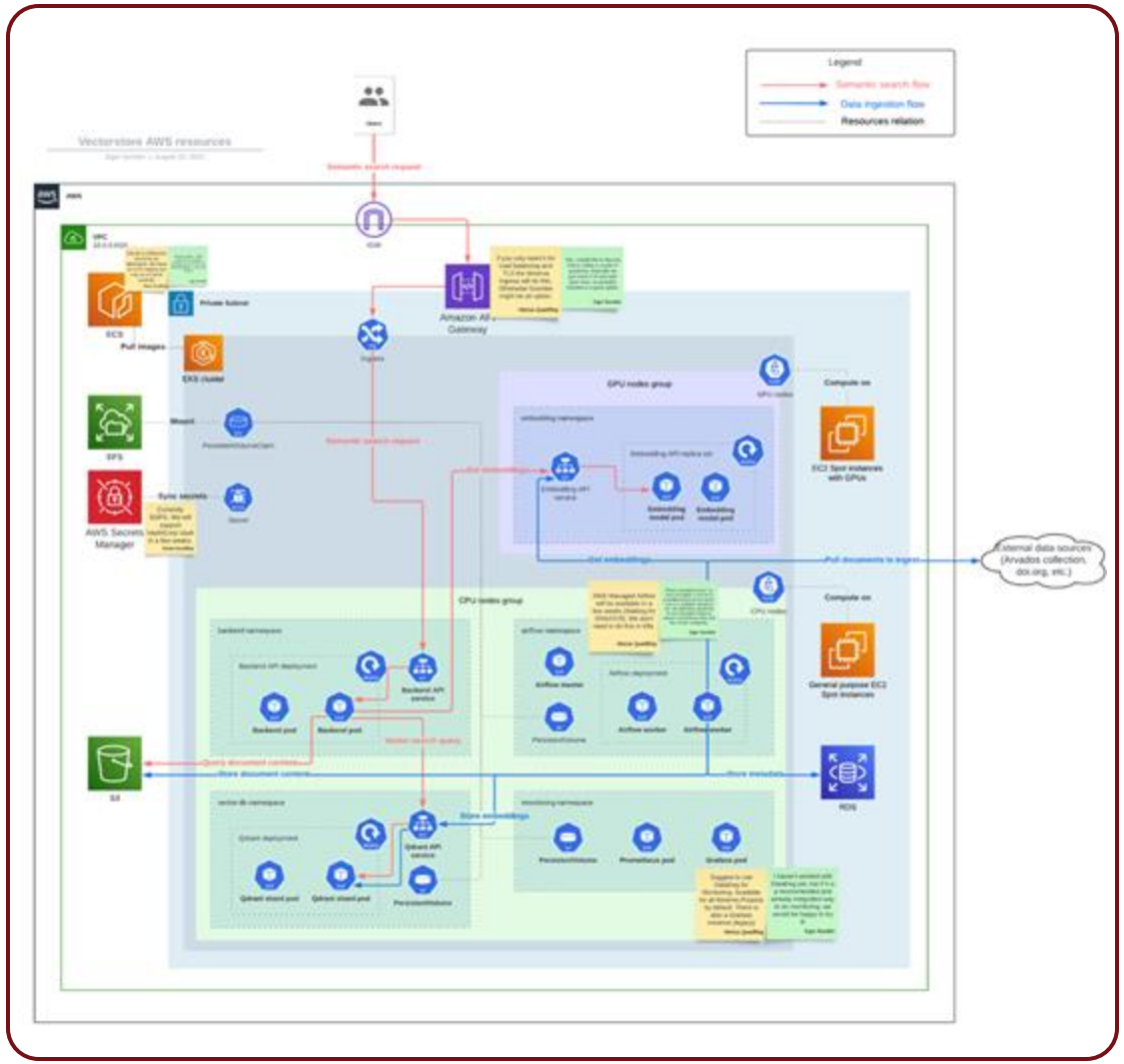
Challenge

- Need to support over 20,000 unique users within a large enterprise.
- Required low-latency, highly scalable, and cost-efficient system.
- System needed to be secure and integrated with internal data.

Solution

- Deployed chatbot system on AWS with scalable backend.
- Created separate pipelines for CPU-heavy and GPU-heavy tasks.
- Segmented workloads to allow elastic scaling of components as needed.



Scalable LLM Deployment (Major Pharma Company)

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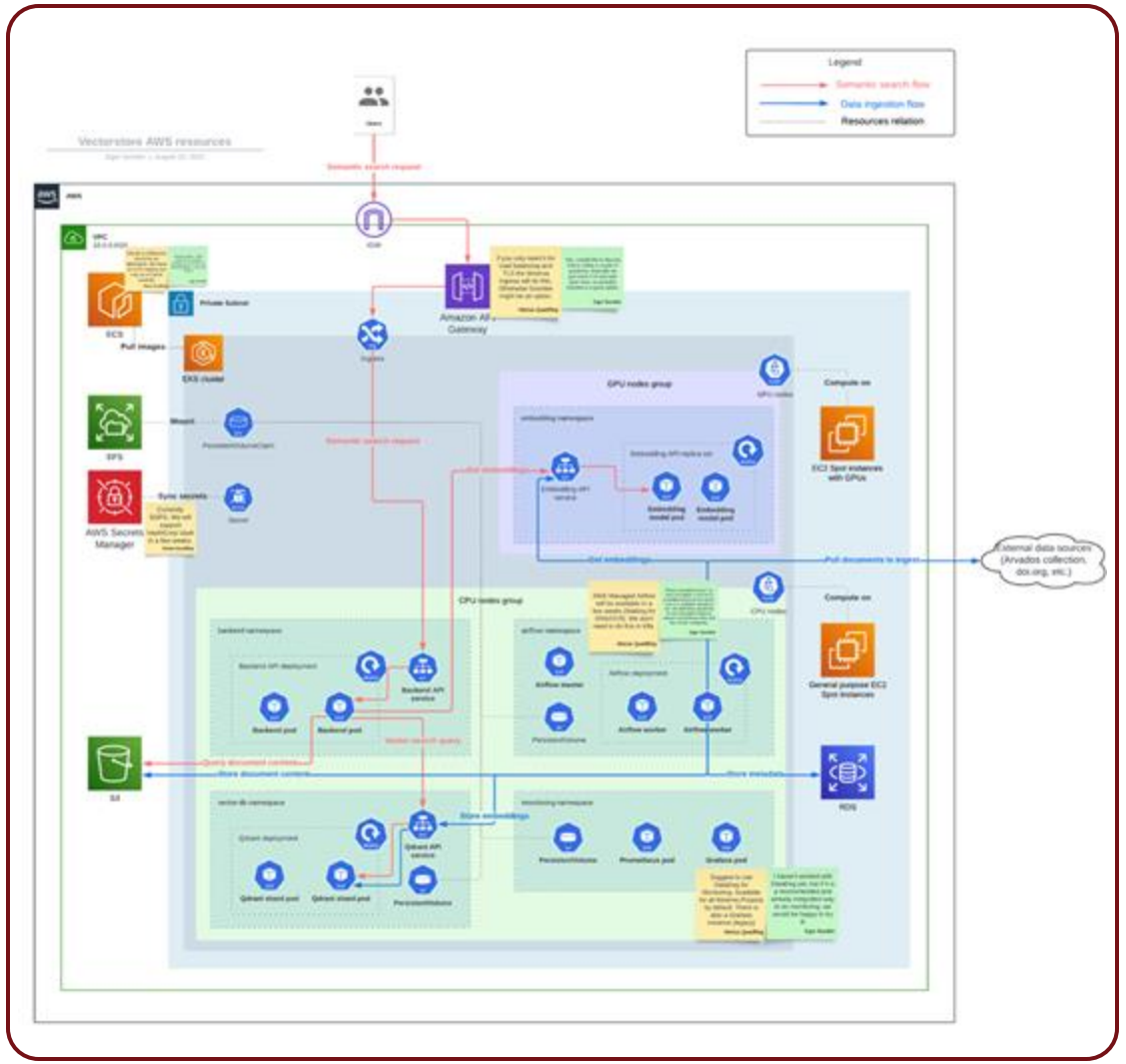
Results

- Reliable, low-latency performance for thousands of users.
- Efficient backend scaling and significant cost reduction through spot instances.
- High availability and stability across all workloads.

Key Takeaways

- Achieved enterprise-scale chatbot deployment.
- Balanced performance, reliability, and cost.
- Illustrates best practices in scaling AI solutions within an enterprise.
- System shows how infrastructure matters when rolling out LLMs at scale.



Multi-Agent Platform (Major Pharma Company)

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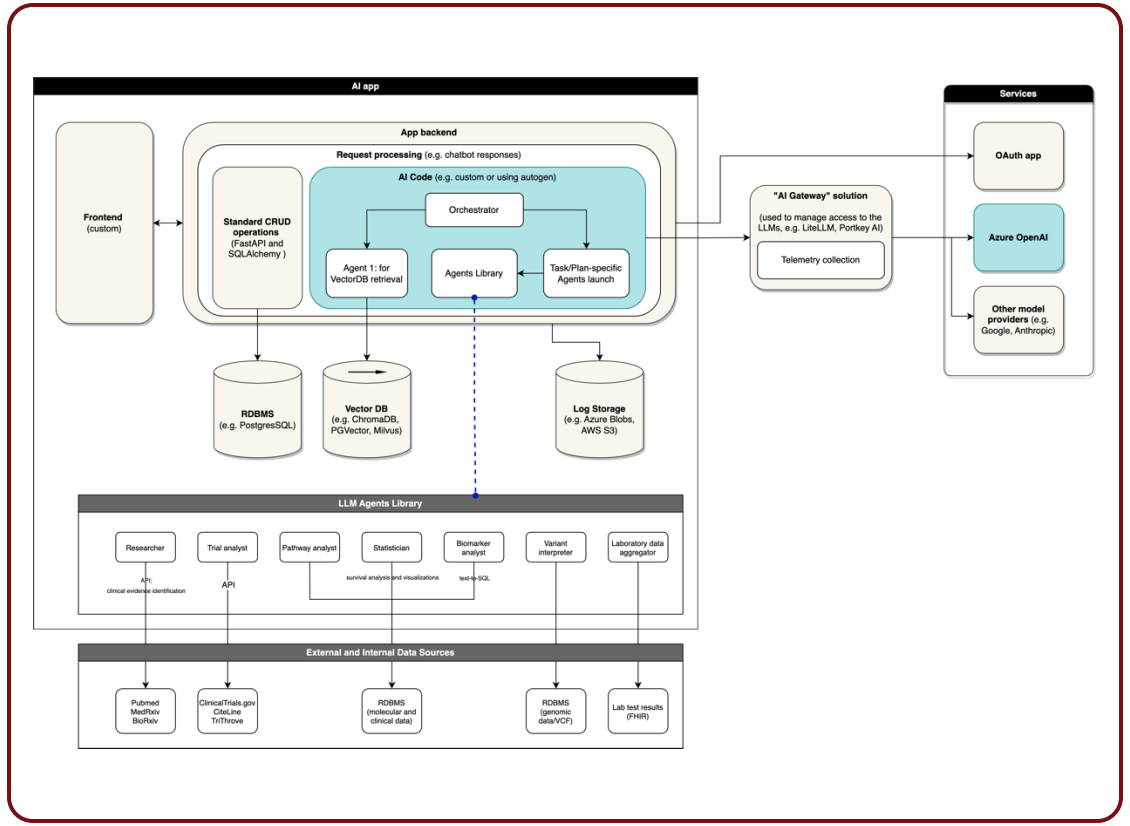
Challenge

- Needed a scalable, modular platform to support biomarker discovery.
- Diverse data sources and tools needed to be orchestrated.
- The system had to support various AI models running in parallel.

Solution

- Built a **multi-agent architecture** for modular AI processing.
- Each agent performed specialized tasks (e.g., data retrieval, tool usage).
- Enabled system expansion without redesigning the full pipeline.



Multi-Agent Platform (Major Pharma Company)

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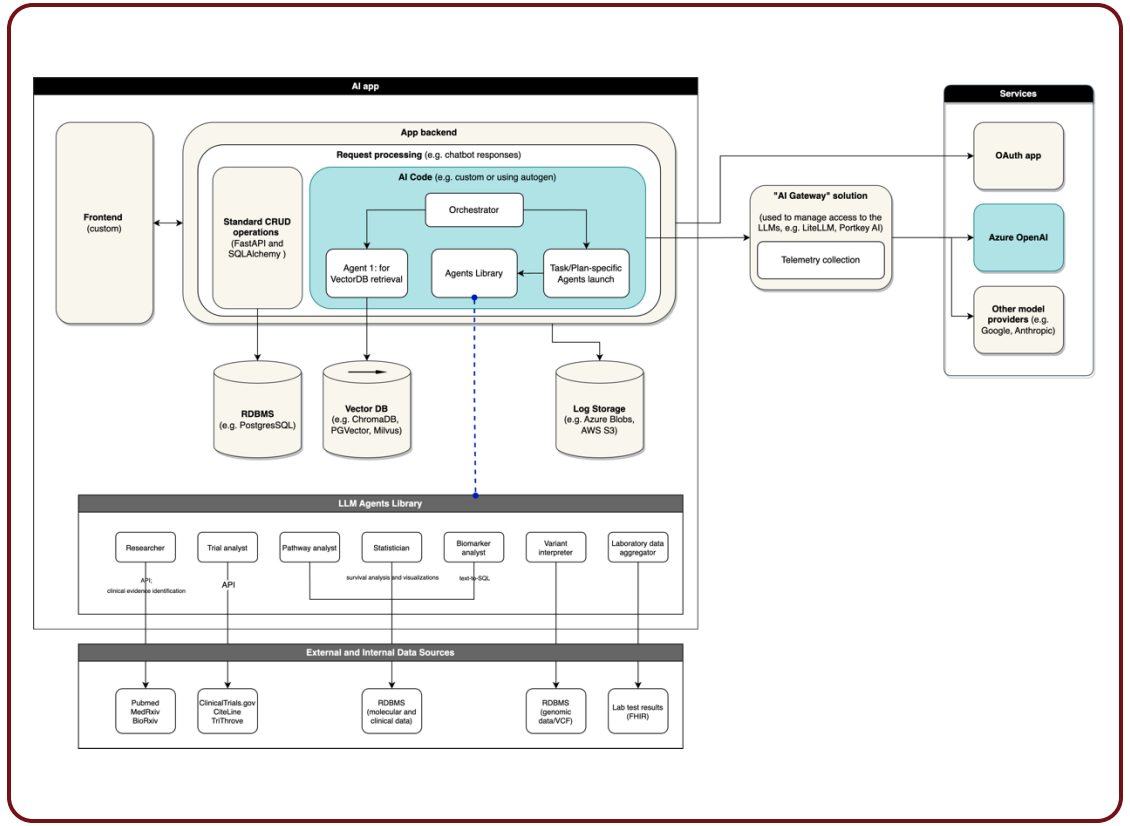
Results

- Delivered a scalable, robust platform for biomarker discovery.
- Easier QA, debugging, and validation at the agent level.
- System ready for future enhancements without major rework.

Key Takeaways

- Multi-agent systems represent the future of complex AI applications.
- Increased system flexibility, observability, and modularity.
- Easier validation, better traceability, and enterprise readiness.
- Strong foundation for regulated environments and clinical-grade use cases.



Multi-Agent Platform Solution

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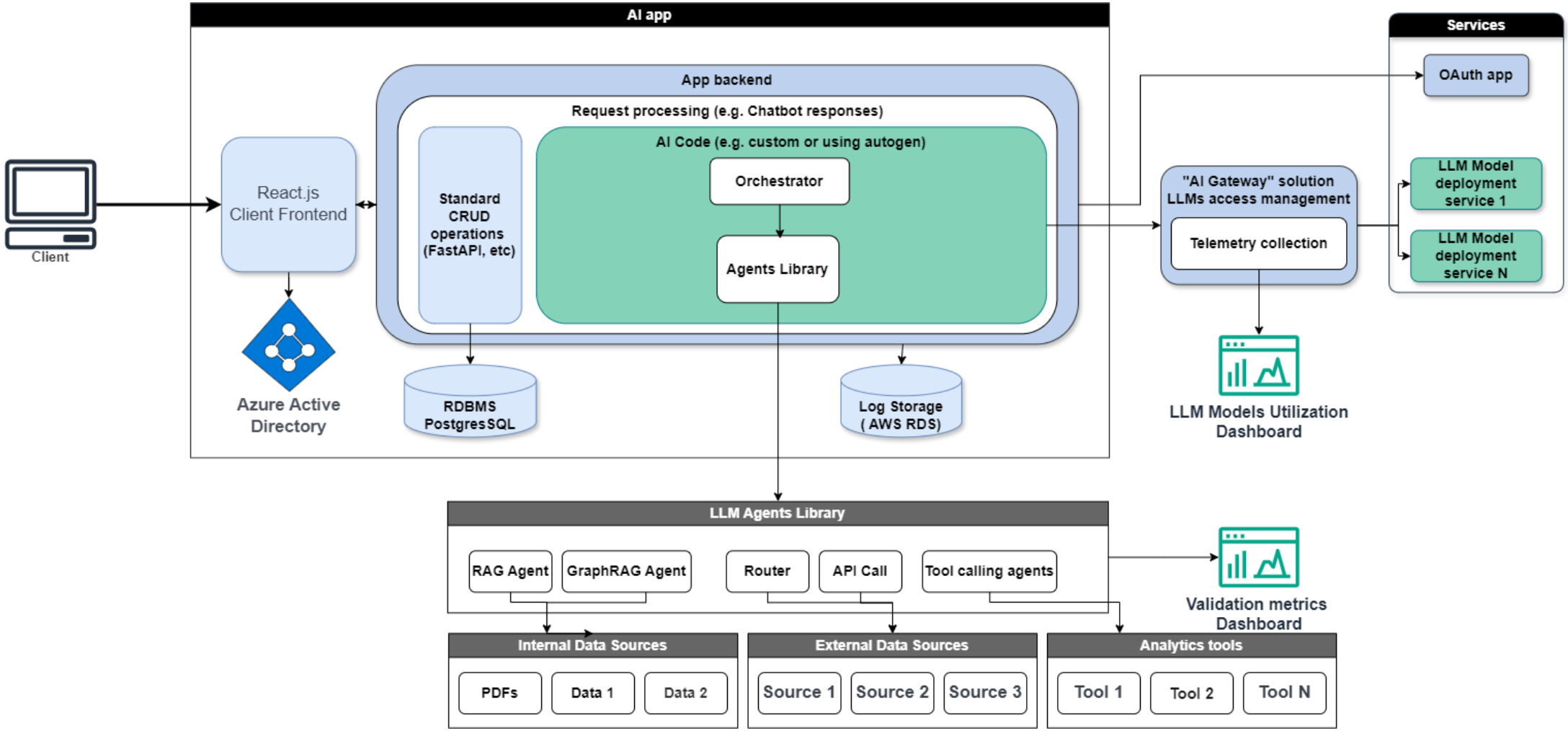

5 Critical Success Factors for Enterprise AI in Pharma

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1 Data Quality & Governance

- Accurate, consistent, and well-structured data remains the foundation of effective AI.
- Clear governance frameworks ensure compliance, privacy, and trust in enterprise AI.

2 Iterative Prototyping for RAG Apps

- Start with small-scale pilots to validate retrieval strategies and refine prompt engineering.
- Use real-world feedback loops to continuously improve relevance, accuracy, and response times.

3 Multi-Agent Orchestration & Collaboration

- Clearly define agent roles and communication protocols to avoid overlap or conflicting decisions.
- Centralized orchestration frameworks help manage complexity and enable scalable solutions.

4 Robust Monitoring & Maintenance

- Implement logging, performance monitoring, and alerting for real-time issue detection.
- Plan for indexing updates, and agent behavior refinement to maintain long-term effectiveness.

5 Cross-Functional Alignment & Stakeholder Buy-In

- Early and ongoing collaboration with business, IT, and compliance teams ensures strategic alignment.
- Fully understand business goals and process before optimizing.
- Communicate ROI and technical feasibility to secure executive sponsorship and continuous support.

Future Directions for LLMs & Multi-Agent Systems in Pharma R&D

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Self-Learning AI Models

Continuously adapt and improve by learning from real-world biomedical and clinical data.

High level of process optimization

Simplify complex technical and scientific processes

Specialized Multi-Agent Ecosystems

Deploy collaborative AI agents focused on tasks such as molecular modeling, literature mining, and predictive analytics.

Autonomous AI Research Teams

Enable multi-agent systems to independently generate, test, and refine hypotheses — paving the way for always-on, AI-powered research labs.

AI-Driven Decision Support for Clinical Trials

Use LLMs to optimize trial design, enhance patient recruitment strategies, and streamline regulatory documentation.

Preparing for the Future: What Pharma Should Do Now

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To capitalize on next-generation AI capabilities, pharmaceutical companies should focus on six critical readiness areas:

1

Data Foundation

Catalog all data assets (structured and unstructured), implement FAIR data principles and build secure data lakes designed for AI integration.

2

Technical Infrastructure

Invest in scalable cloud infrastructure with vector database capabilities, flexible APIs, and specialized cybersecurity frameworks for AI systems accessing sensitive data.

3

Talent Ecosystem

Develop multidisciplinary teams blending domain scientists with AI specialists, build company-wide AI literacy, and establish ethics committees to guide implementation.

Preparing for the Future: What Pharma Should Do Now

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To capitalize on next-generation AI capabilities, pharmaceutical companies should focus on six critical readiness areas:

4

Strategic Experimentation

Launch targeted high-ROI pilot projects, create sandboxed "AI labs" for safe experimentation, and form strategic partnerships with AI startups, consulting companies and academic institutions.

5

Focus on Business Problems

Design scientist-centered AI-integrated workflows and establish continuous feedback mechanisms to refine tools based on real-world use.

6

AI Industrialization Strategy

- Transition from isolated AI projects to a scalable platform approach.
- Standardize MLOps pipelines for continuous model improvement.
- Establish center-of-excellence teams to scale AI proofs-of-concept into enterprise solutions.
- Implement monitoring frameworks to track AI performance and impact.
- Develop modular AI components for diverse scientific applications.

How Quantori Helps You Leverage AI in Pharma R&D: Our Capabilities

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Why Partner with Quantori?

At Quantori, we bring together PhD scientists, AI and machine learning engineers, full-stack developers, data engineers, and cloud infrastructure architects to deliver AI projects at scale.

AI Solutions for Life Sciences That Drive Impact

- **Deep expertise in LLM-powered** analytics and multi-agent systems
- From target ID to clinical trials — **full-spectrum AI support across R&D**

Breaking Down Silos, Aligning Teams

- Translate scientific needs into **actionable data science & IT specs**
- **Foster collaboration** across science, data, and tech teams.

Infrastructure Built for AI Scale

- **Scalable** MLOps, DevOps, and data pipelines
- **Robust architecture** for industrializing AI, not just POCs

Making Data Work for You

- Turn fragmented, **unstructured data into insights**
- **Master R&D data management** for better decision-making

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Let’s discuss how Quantori can accelerate your AI-driven research initiatives!

Or visit us in the Exhibition Hall at Booth 403