



Q-Scientist: A Tailored AI Ecosystem for Life Science R&D

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Booth #244

Quantori is an AI-first Informatics Service Provider, Focusing on the Life Science Industry



10 of the 12

Largest pharmaceutical companies served

30+

peer-reviewed scientific articles
(2020 – present)

Recognized as a Leader

in the Everest Group PEAK Matrix

Global Scale

Capabilities across the US and Europe,
Armenia, Portugal, the UK, and North
America

700+ Experts

AI/ML Scientists, HCLS-fluent Cloud,
Software, and QA Engineers

NEBIUS



Google Cloud
Partner



databricks



Challenges

Open-Source	Commercial
Generic and not optimized for life sciences R&D	
Scalability & Performance Optimization	Technology Lock-In
Enterprise-Grade Capabilities	Expensive & Resource-Intensive
Data Security & Compliance	Restrictive Data Policies

Lack of built-in support for bioinformatics, molecular modeling, lab workflows, and regulatory auditability

Q-Scientist can be deployed as a dedicated SaaS or within the clients' infrastructure under their control and ownership

Key Benefits

- Boost operational efficiency
- Elevate enterprise value
- Slash deployment costs
- Seamlessly integrate your own models and data sources

- Chats
- Workflows
- R&D
- Health Care
- Commercial
- SSBO
- Datasets
- Agents
- AI Models
- Knowledge
- Workspace
- RAGs
- Applications
- Marketplace
- Monitoring
- Search

- Recent
- Perfect Square Divisors
Today
- Drug Discovery Analysis
Yesterday
- Genomic Sequencing
2 days ago



R&D Workflows

AI-powered research and development workflows for life sciences

Powered by Bio-LLMs, deep learning models, and AI frameworks

Filter by Category:

Drug DiscoveryGenomicsImmunologyStructural BiologyComputer VisionGraph AnalyticsData Science

Create New Workflow



Advanced

Small Molecule Optimization

AI-powered drug discovery and molecular property optimization using advanced ML models

CATEGORY

Drug Discovery

MODELS

ChemBERTaMolBERT+1 more

Configure & Run >



Intermediate

Biomarker Identification

Discover and validate biomarkers using multi-omics data integration and AI analysis

CATEGORY

Genomics

MODELS

DNABERTGenSLMs+1 more

Configure & Run >



Advanced

Antibody Design & Engineering

Design therapeutic antibodies with optimized binding affinity and reduced immunogenicity

CATEGORY

Immunology

MODELS

AntiBERTyIgLM+1 more

Configure & Run >



Advanced

Protein Engineering

Engineer proteins with enhanced stability, activity, and desired functional properties

CATEGORY

Structural Biology

MODELS

ESMProtTrans+1 more

Configure & Run >



Intermediate

Target Identification & Validation

Identify and validate novel therapeutic targets using AI-driven pathway analysis

CATEGORY

Drug Discovery

MODELS

ChemBERTaBioGPT+1 more

Configure & Run >



Advanced

Single-Cell Analysis & Cell State Prediction

Analyze single-cell data to predict cell states, trajectories, and gene expression patterns

CATEGORY

Genomics

MODELS

scGPTscBERT+1 more

Configure & Run >

Pre-configured Customizable Workflows



- ✓ **Deep Life Sciences and Healthcare-specific**
- ✓ **Combination of bioinformatics, cloud-native platforms, and AI/ML**
- ✓ **Modular, orchestrated agents**
- ✓ **Seamless cloud deployment (GCP, AWS, Azure, or on-prem)**
- ✓ **Tailored for every stage of scientific discovery and development**

Agent System	Description	Use Cases
Drug Repurposing	Identifies new uses for existing compounds using semantic and data-driven reasoning	Drug Discovery, Repurposing Pipelines
Ideation to Innovation	Generates novel research hypotheses by synthesizing multi-source data	Scientific Co-Pilots, Hypothesis Generation
Drug Target Discovery	Automates target identification from fragmented data	Target Discovery & Validation, Competitive Intelligence
Drug Optimization	Enhances PK/PD modeling and dosing strategies to improve clinical success	PK/PD Modeling, Simulation & Refinement
Biomarker Discovery	Integrates clinical, molecular, and genomic data to identify biomarkers	Multomics, Bioinformatics Pipelines
Scientific Context Search	Contextualized retrieval across literature and databases for rapid insights	Competitive Intelligence, Literature Mining
Rare Disease Diagnosis	Combines structured and unstructured patient data for rare disease identification	Diagnostics, RWE
Platform for PK/PD	Orchestrates EDA, modeling, and reporting agents for data-driven PK/PD	PK/PD Modeling, Simulation, Regulatory Insights

AI-Driven Innovation Across HCLS Organizations

A Life Science LLM Library



Genomics & DNA Sequence Modeling

Models: DNABERT, GenSLMs, HyenaDNA

Downstream tasks:

- Synthetic promoter design
- Mutation effect prediction
- Functional annotation

Single-Cell Analysis

Models: scGPT, scBERT, Geneformer, etc.

Downstream tasks:

- Cell type annotation
- Trajectory inference
- Gene expression modeling

Antibodies & Immune Repertoire Modeling

Models: AntiBERTy, IgLM, AbLang, etc.

Downstream tasks:

- Antibody sequence generation
- Binding affinity prediction

TCR (T-Cell Receptor) Modeling

Models: TCR-BERT, TITAN, DeepTCR

Downstream tasks:

- TCR-epitope interaction prediction
- Immune repertoire analysis
- TCR antigen specificity modeling

Drug Discovery & Target Identification

Models: ChemBERTa, MolBERT, etc.

Downstream Tasks:

- Drug-target interaction prediction
- Molecular property prediction
- Compound screening & optimization

Proteins & Peptide Modeling

Models: ESM, ProtTrans, AlphaFold2

Downstream tasks:

- Protein structure prediction
- Protein function annotation
- Protein-protein and protein-ligand interaction modeling

R&D workflows that can utilize Bio-LLMs:

- Small molecule optimization
- Biomarker identification
- Antibody design
- Protein engineering
- Target identification and validation
- Multi-omics data integration (genomics, transcriptomics, proteomics, metabolomics)
- Drug-target interaction prediction
- RNA structure modeling and design
- Single-cell analysis and cell state prediction
- TCR and immune repertoire profiling
- De novo drug design and molecular generation

Integration with Public Datasets

Attraction Points:

- Large-scale genomic, proteomic, clinical, and biomedical datasets are readily available, eliminating the need for data acquisition or storage management.
- Seamless integration with scalable multi-omics data processing, AI/ML model training, and bioinformatics workflows.
- No upfront costs for storing massive datasets; pay only for computation and usage.
- Centralized cloud-hosted data simplifies cross-team and multi-site research.
- Standardized datasets enhance benchmarking, validation, and regulatory transparency.
- Secure & compliant environment.

Data sources

Genomics & Transcriptomics

- The Cancer Genome Atlas Program (TCGA)
- Cancer Cell Line Encyclopedia (CCLE)
- ClinVar

Chemical Databases

- ChEMBL
- PubChem
- BindingDB

Single-Cell Datasets

- TCGA Single-Cell Data
- Single Cell Portal (Broad)
- CelIXGene Discover

Proteomics & Metabolomics

- PRIDE (Proteomics Identification Database)
- PeptideAtlas & SWATHAtlas
- Metabolomics Workbench

Multi-Agent Flow Builder

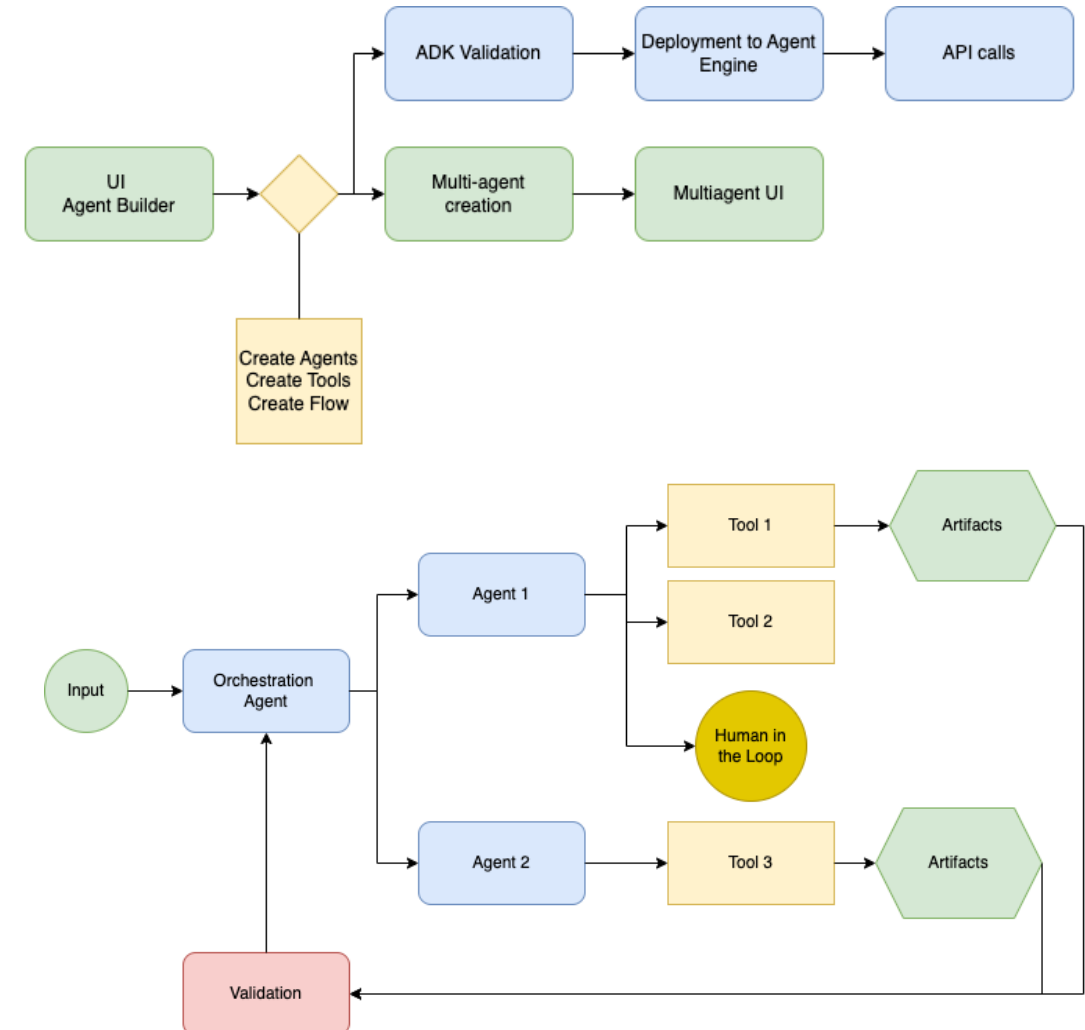


Flow Builder For Creating Agent-based Workflows

- Drag-and-drop interface for node-based workflow design
- Support for multiple node types:
 - Agents (LLM-powered)
 - Tools (custom functions)
 - Human-in-the-Loop interactions
 - Parallel processing
 - Conditional branching
 - Error handling and retries

Deployment to Google Cloud Vertex AI using ADK

- Automatic conversion of visual workflows to ADK-compatible agents
- Containerized deployment with standardized interfaces
- Managed endpoints for production deployment
- Integrated monitoring and logging



Input

PRE-DEFINED

UPLOAD

Choose Structure

Reference Structure *

Sample Molecule 1 4

Numbers of Molecules to generate

1 4 60

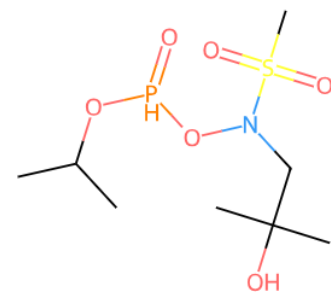
Variance in Number of Atoms

1 2 5

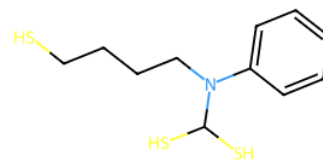
GENERATE

Output

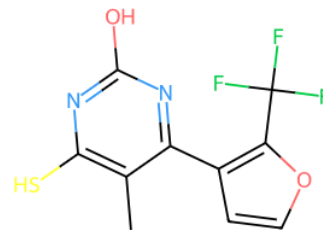
DOWNLOAD .SDF



0.6769868731



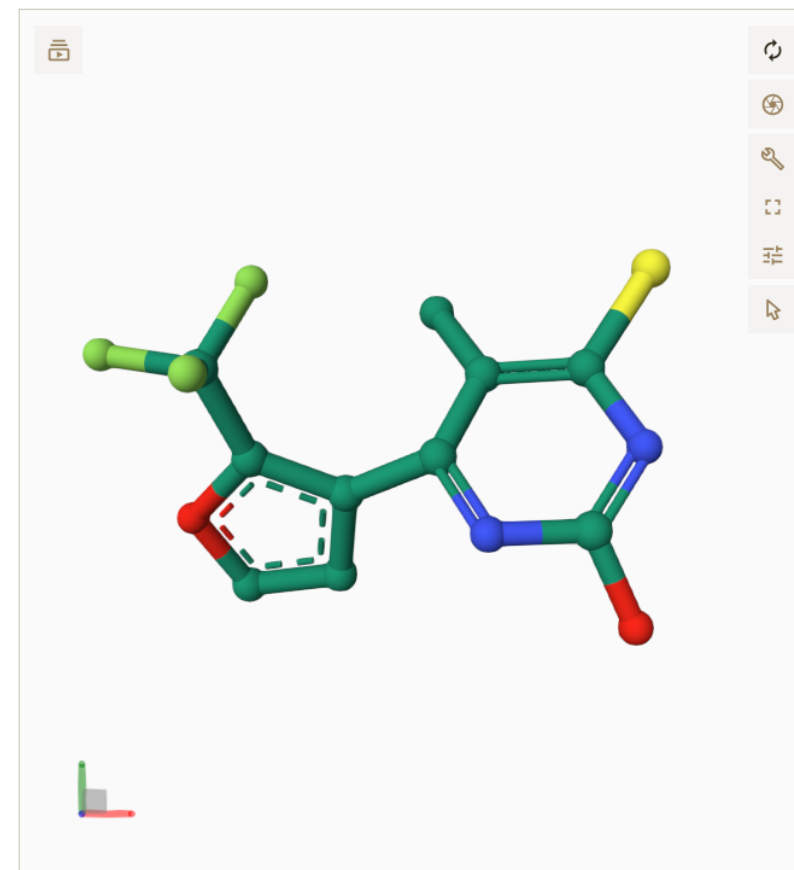
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Preview

DOWNLOAD .MOL

CLOSE



Life Sciences Applications



Q-Scientist

Intelligent AI assistant for HCLS

A

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load a file and create 3 molecules https://github.com/Membrizard/ml_conformer_generator/blob/main/assets/demo_files/ceyyag.mol

Molecule Conformer Generator v0_4



load a file and create 3 molecules

https://github.com/Membrizard/ml_conformer_generator/blob/main/assets/demo_files/ceyyag.mol



Here is the comprehensive table summarizing all generated molecules, including their images, SMILES, similarity scores, SA Scores, synthesis feasibility, PoseBusters scores, pose quality, and test results:

Image	SMILES	Shape Similarity	Chemical Similarity	Average Similarity	SA Score	Synthesis Feasibility	PoseBusters Score	Pose Quality	Passed/Total Tests
	<chem>CN(CC(=O)O)C(=O)C@@H1CCCC1</chem>	0.584	0.036	0.310	3.08	Easy to synthesize	1.0	Excellent	8/8

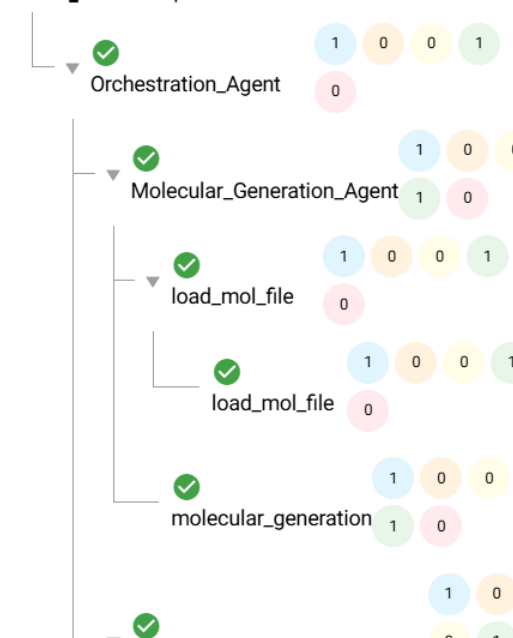
How can I help you?



Code review



State Graph



Healthcare and Life Sciences Applications



**Q-Scientist**
Intelligent AI assistant for HCLS

> Pathology-viewer

+



 Demo User

 User

AI Models

Knowledge

Workspace

RAGs

Applications

Marketplace

Monitoring

Search

Recent

Perfect Square Divisors
Today

Drug Discovery Analysis
Yesterday

Genomic Sequencing
2 days ago

Mathematical Proofs
1 week ago

Pathology WSI Viewer

Whole Slide Image Analysis with AI-powered Risk Prediction

Data Selection

Search by Case ID

Select Study

BLCA - Bladder Urothelial Carcinoma

Select Patient

TCGA-E7-A677-01Z-00-DX1

Viewing Modes

Curtain Side by Side Overlay

Model Type

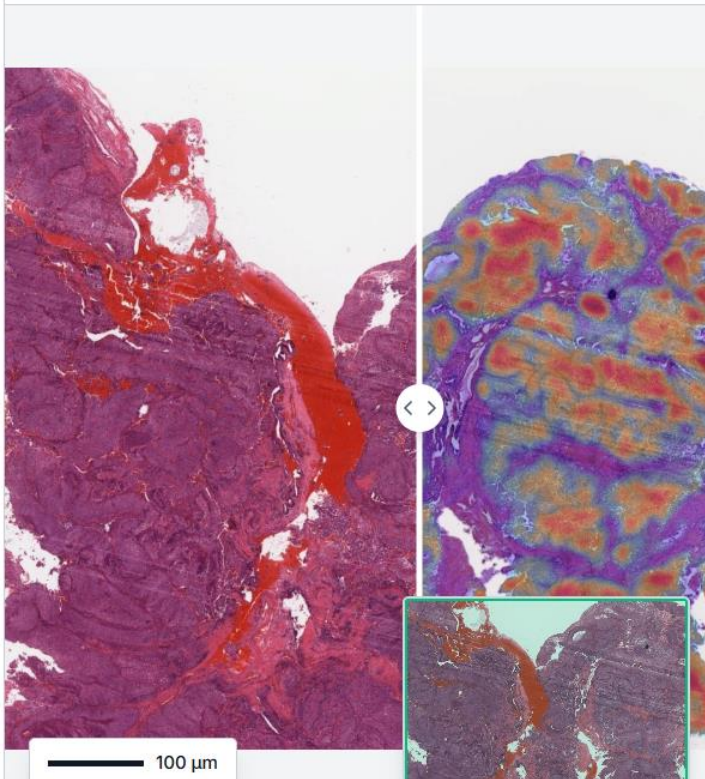
Unimodal ☒ Multimodal

Case Information

100%

Reset

Multimodal Model



Close Chat

AI Assistant

AI

Hello! I'm your AI pathology assistant. You're viewing case TCGA-E7-A677 (BLCA) in Curtain mode: H&E on the left, risk heatmap on the right. Use Capture Snapshot to mark regions of interest and I'll comment on them.

Model summary (Multimodal): Risk score 0.72 → High. Dataset lists survival 24 months, censoring status True. This is a prognostic model and does not replace a pathology report.

Capture Snapshot

Ask about the pathology images...

Press Enter to send, Shift+Enter for new line

Git

Prompts

Running

Statistics

Q-Scientist: The AI Backbone for Life-Science R&D

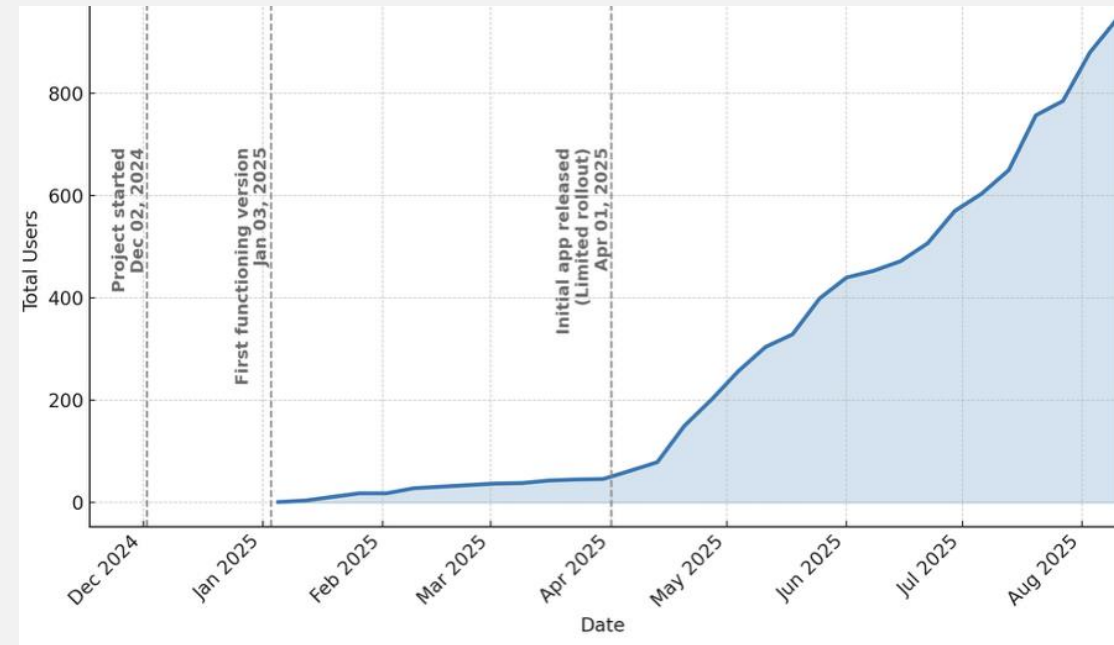


Comprehensive, modular, agentic AI platform designed specifically for life sciences

Delivers a unified, intuitive user experience across modules

Overcomes the limitations of generic AI tools

Platform offered as a Service



Contact Information



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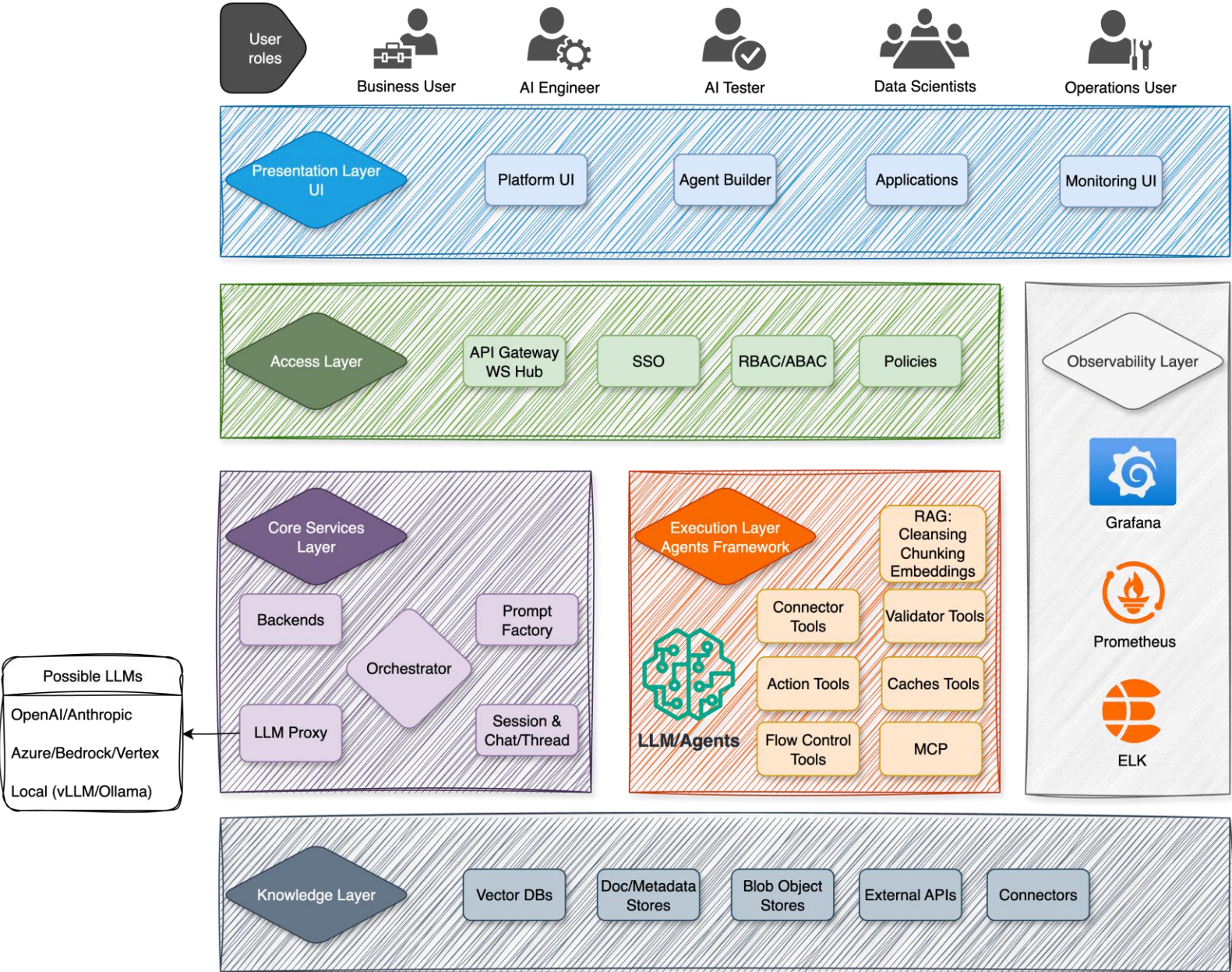
artem.terentyuk@quantori.com

+972 55 285 3689

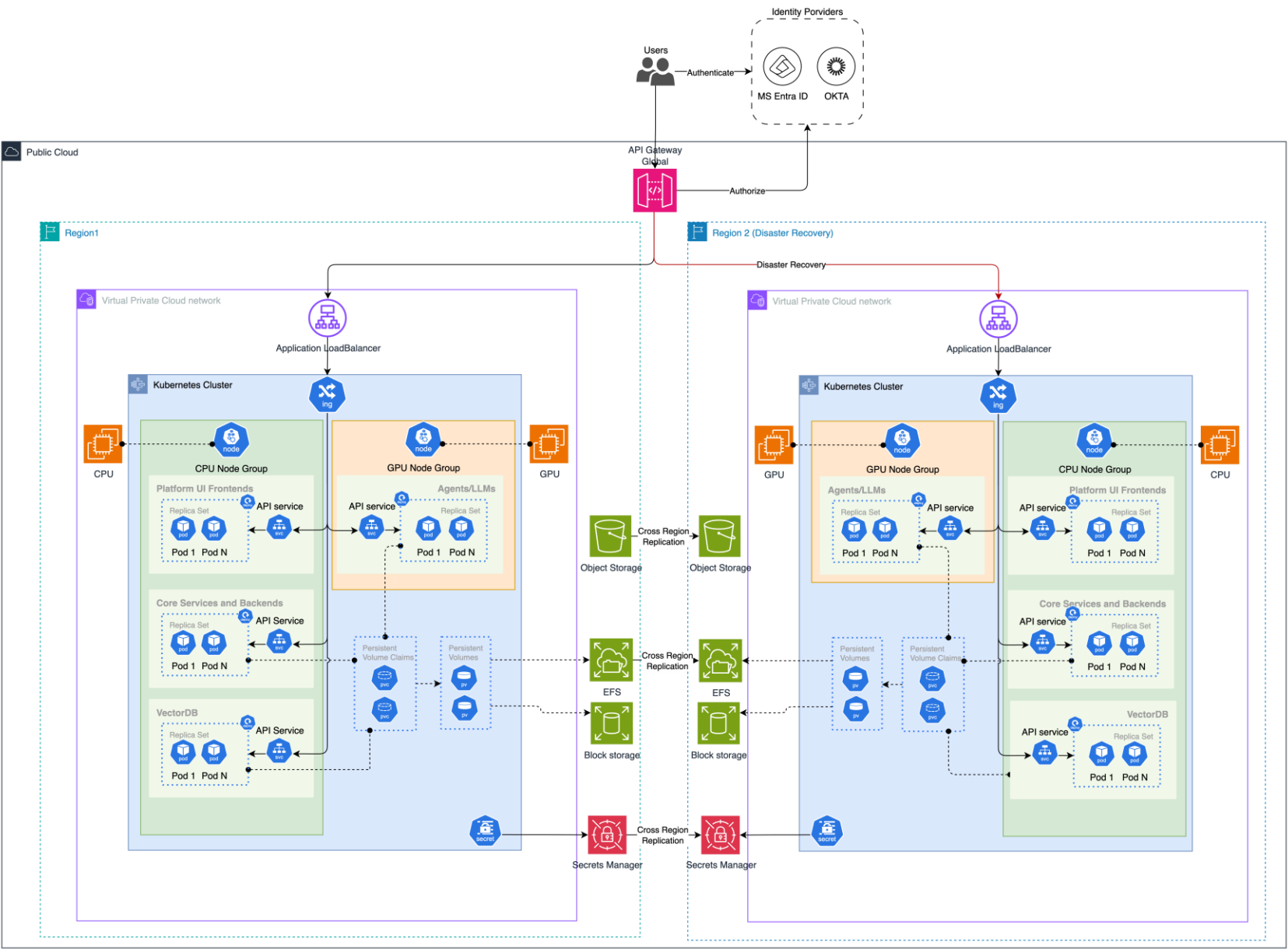
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Appendix

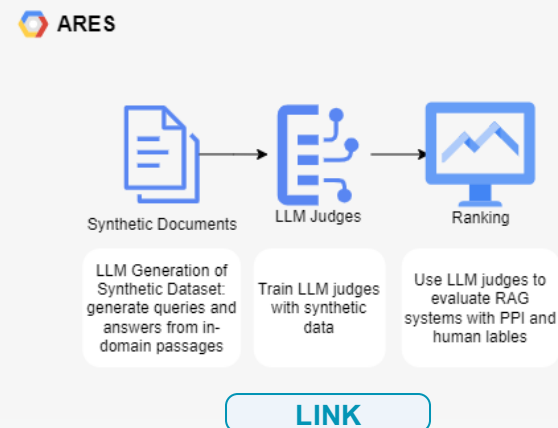
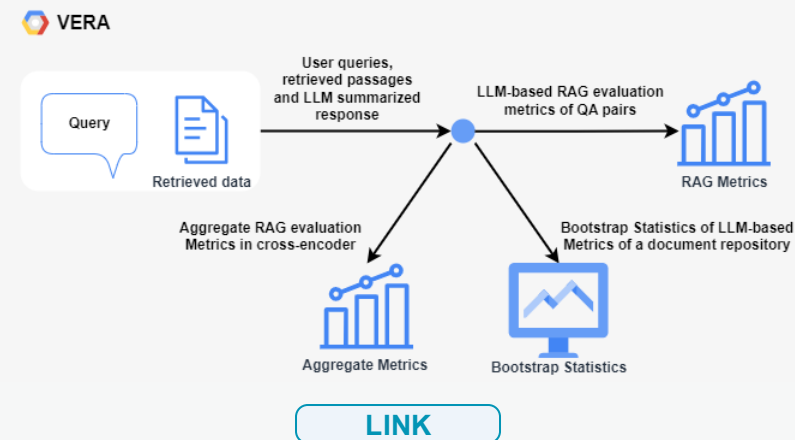
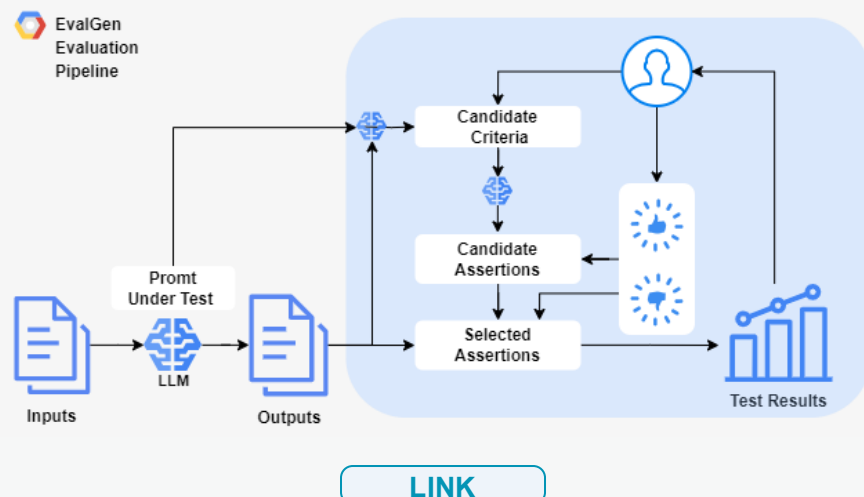
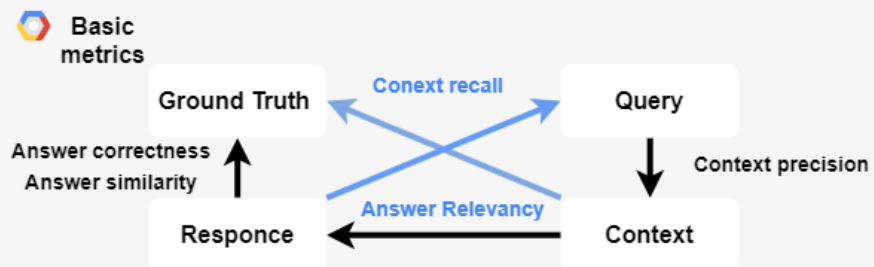
Solution Architecture



Solution Architecture



AI Agents Validation Frameworks



Depending on the use case, it is possible to integrate specific automatic validation scenarios into a multi-agent workflow.