

# The Lab of the Present: Agentic AI in Action

February 19, 2026

# Agenda



- Quantori Intro
- Industry Perspective on AI-driven R&D
- Overview of Expert Systems Models
- Q-Scientist & Q-Models demo
- Q&A

# Speakers



**Chris Waller, PhD**

Chief Strategist



**Tudor Oprea, MD, PhD**

CEO, Expert Systems



**Alisa O. Vershinina, PhD**

Sr Scientist, Business Analyst



# Quantori is an AI-enabled, accelerator-powered technology partner dedicated to the Life Sciences and Healthcare

**10+**

Largest pharmaceutical companies served

**30+**

Innovative startup and mid-market clients

## Global Scale

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

## 500+ Experts (60+ MDs/PhDs)

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



**NEBIUS**



**databricks**

# Quantori Scientific and Domain Expertise



**Quantori brings deep domain expertise in pharmaceuticals, healthcare, and life sciences, with a strong focus on laboratory informatics, analytical data automation, and regulatory compliance.**

## Scientific Informatics

Empowering scientific discovery with innovative computational solutions and advanced informatics platforms.

- CryoEM
- High-Performance Computing (HPC)
- Image analysis
- Chromatography Data Systems (CDS) & HTS
- AI/ML, LLM/GenAI

## Pharmaceutical R&D

Enhancing drug discovery and development with cutting-edge technologies, advanced data analytics, AI/ML, and simulation tools.

- Computational drug discovery
- Cheminformatics
- Bioinformatics
- Regulatory affairs

## Laboratory Informatics

Optimizing laboratory operations through automation, data management, and seamless instrument integration.

- Process automation
- Instruments and equipment integration
- LIMS / ELN development
- High-throughput screening (HTS) solutions

## Clinical Research Informatics

Accelerating clinical research with technology-driven solutions to improve patient recruitment, data quality, and real-time monitoring.

- Study design
- Clinical Trials Management System
- Electronic Data Capture (EDC)
- Patient recruitment & RWE
- Clinical genomics

## Regulatory Compliance

Ensuring compliance with industry regulations through robust quality assurance and validation.

- GxP compliance
- Quality assurance and Computer System Validation (CSV)
- Data integrity and audit readiness
- Compliance with industry regulations (FDA, EMA, HIPAA, GDPR, 21 CFR Part 11)

# The Barriers of the Present – Why R&D Velocity Stalls



## The Wet Lab Reality

- **Data Fragmentation:**  
Research remains trapped in silos (LIMS, ELN, logs), making experimental lineage impossible to trace.
- **Manual Overhead:**  
Scientists spend up to 40% of their time on repetitive tasks and sample setup rather than innovation.
- **Rigid Automation:**  
Existing robotics rely on hard-coded scripts that fail if a single variable (like temperature) deviates.
- **The "Black Box":**  
A lack of metadata and provenance makes results difficult to audit or reproduce.

## The Dry Lab Reality

- **Model Staleness:**  
Predictive models degrade as new data is generated, leading to outdated predictions and failed experiments.
- **Manual Hypothesis Testing:**  
Computational chemists lack the tools to efficiently explore billions of molecules, limiting the design space.
- **The Reality Gap:**  
High-potency in-silico designs often fail in the wet lab due to poor "developability" (toxicity, permeability).
- **Technical Debt:**  
Fragile, isolated pipelines and custom scripts create a "reproducibility tax" on every project.

# Grounding Terminology



## AI Agent

An autonomous system that perceives its environment, makes decisions, plans, and acts to achieve a goal, often using multiple tools

## AI Workflow

A structured, step-by-step process with defined logic, often using APIs or models sequentially

## AI Service (or Tool/Function)

A specific, reusable function or API that performs a distinct task (e.g., search the web, send an email, access a database)

## How They Work Together

**Agents use Services:** An agent might decide to use a search service, then a summarization service, then a writing service.

**Workflows use Services:** A workflow might call a database service, then an email service, then a calendar service in a fixed order.

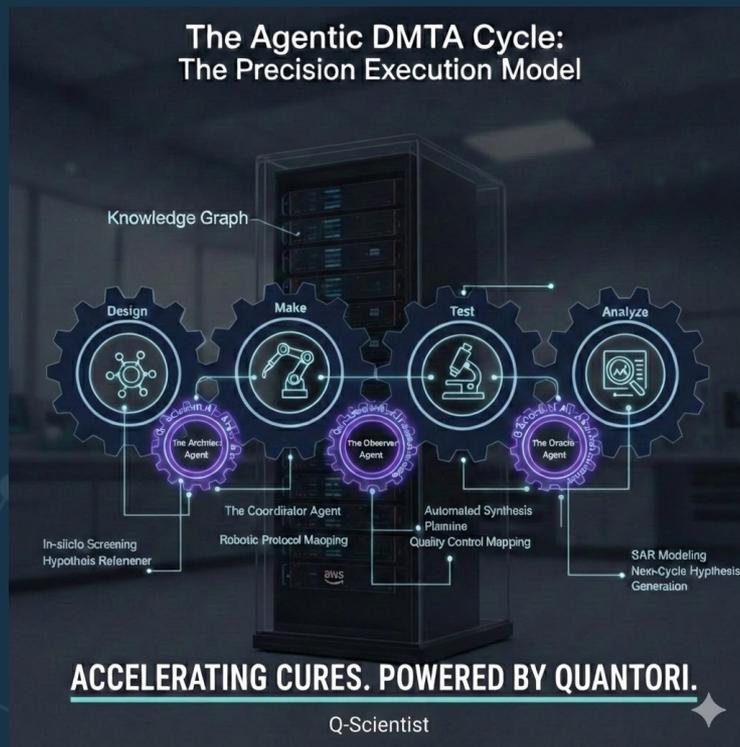
**Agentic Workflows:** Combine both: a structured workflow that incorporates intelligent, agent-like decision points or calls an agent for complex sub-tasks.

# AI Companions in the Lab of the Present



**Design:**  
The Architect

**Make:**  
The Coordinator



**Analyze:**  
The Oracle

**Test:**  
The Observer

# Powering Life Sciences R&D with Q-Suite



**“Zero-Gravity”**: you receive full source code, complete knowledge transfer, and a free, unlimited license. No strings attached

**Fully customizable and extensible**

**Multi-cloud**: leverage hybrid or public cloud infrastructure

**LS Domain-savvy**: designed for security, compliance, and enterprise-grade governance

**Delivered as a Service**: we support customization, integration, and feature development based on your priorities

## Q-Scientist

Accelerate research through agentic AI



## Q-Discover

Support all standard drug discovery workflows



## Q-Models

Provide a single source of truth for collaborative document creation



## Q-HPC

Optimize and simplify on-prem, cloud, & quantum computing ops



## Q-Portal

Secure and controlled access to the world of large language models



## Q-Image

Time-lapse fusion analysis of 3D medical images



## Q-Data

The intelligent data foundation for life sciences



**A comprehensive AI-first platform built to scale research, streamline data operations, and accelerate drug discovery**

# Expert Systems



# Bioactivity Models: Comprehensive Target Coverage



## Extensive Target Coverage

**6,159 total ML models based on targets with defined UniProt IDs, including 2,982 human, 816 mouse, and 813 rat proteins.**

In total, 5,120 proteins are of mammalian origin.

## Quality-Tiered Models

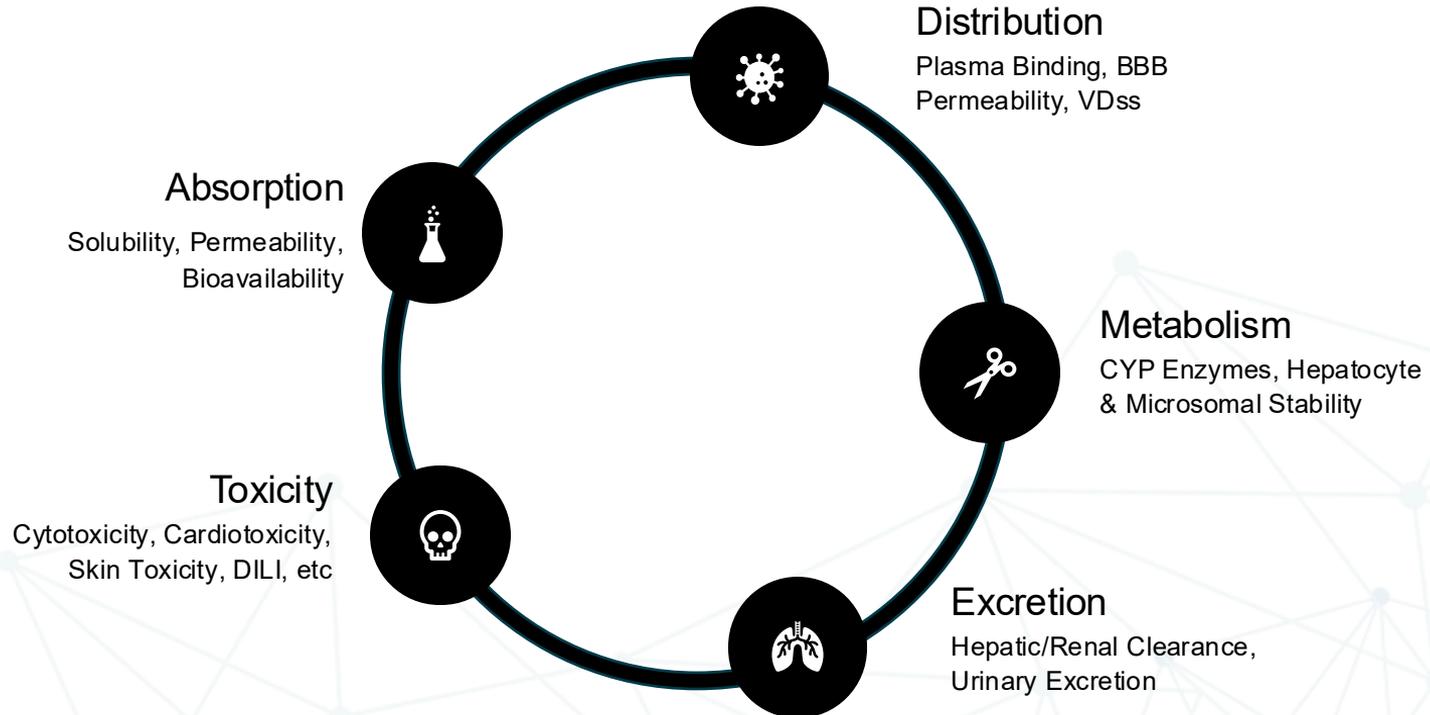
**1,821 high and medium-quality ML models with over 2 log unit spread and 80+ training compounds.**

An additional 1,860 lower-quality and 2,478 similarity-based models for in-depth analyses.

## Cell Line Analysis

**1,240 ML models for cell lines, primarily focused on cancer cell cytotoxicity and viability assays, all with built-in uncertainty quantification for each prediction.**

# ADMET Models: Critical Drug Property Prediction



# Location Models: Tissues, Cells, Compartments



- 134 distinct cell type models for precise cellular response prediction

Cell Type Coverage

- 60 diverse tissue type models for targeted drug development

Tissue Specificity

- Chemical library optimization for increased tissue targeting

Library Design

- High-resolution insights into intracellular compound localization

Subcellular Compartments

**DEMO**





New Chat

Chats

Workflows

R&D

Commercial

SSBO

Agents

AI Models

Chatbots

Data Sources

RAGs

Workspace

Applications

Marketplace

Monitoring

Notes

Search

Expert\_Systems

Temperature



How can I help you?

+ | Code review



Chats

Compare toxicity of these molecules  
Ibuprofen CC(C)CC1=CC=C(C=C1)C(C)C(=O)OC

16 minutes ago | 2 messages

what can you do

21 minutes ago | 2 messages

CC12CCC3C(C1CCC2O)CCC4=CC(=O)CCC34C

22 days ago | 0 messages

Identify drugs that act on pathways or targets implicated in Alzheimer's Disease, but approved for other non-Alzheimer's indications.

about 1 month ago | 2 messages

what can you do

3 months ago | 6 messages

Screenshot

# Q-Suite Accelerators



## Q-Scientist

Accelerate research through agentic AI



## Q-Discover

Support all standard drug discovery workflows



## Q-Models

Provide a single source of truth for collaborative document creation



## Q-HPC

Optimize and simplify on-prem, cloud, & quantum computing ops



## Q-Portal

Secure and controlled access to the world of large language models



## Q-Image

Time-lapse fusion analysis of 3D medical images



## Q-Data

The intelligent data foundation for life sciences



# Q&A



## Upcoming Events



**Lab OF THE Future**  
**USA** March 2<sup>nd</sup> & 3<sup>rd</sup> 2026  
The Sheraton Boston Hotel

Dates: March 2-3, 2026

Booth: #25

Panel Discussion: March 2, 14:05 PM, Automated Lab Track

**Bio·ITWorld**  
**CONFERENCE & EXPO**

Dates: May 19-21, 2026

Booth: #505

Presentation: May 20, 12:40 PM, AI for Drug Discovery & Development Track

# Contact info

[contact@quantori.com](mailto:contact@quantori.com)



[quantori.com](https://quantori.com)

