



Gene-to-Drug Hit Discovery

Chris L. Waller, PhD | BioTechX 2026

**Quantori moves
beyond IT services
to build AI-enabled
digital solutions that
solve the most complex
healthcare and life
sciences problems**

With deep domain expertise and end-to-end capabilities in AI, data science, and software engineering, we help biotech, pharmaceutical, and healthcare organizations accelerate research, enhance data-driven decision-making, and improve patient outcomes.

Quantori at a Glance



Trusted by Industry Leaders

Partnering with leading biotech, pharma, and healthcare organizations worldwide to deliver AI and scientific computing solutions



AI-Driven Scientific & Data Platforms

Delivering AI-powered solutions for drug discovery, bioinformatics, scientific data platforms, and advanced analytics



Domain Knowledge

Specializing in pharmaceutical, healthcare, and life sciences, with a strong blend of technology and regulatory knowledge



Agile & Scalable Team

600+ experts worldwide with a flexible, adaptable engagement model, ensuring rapid onboarding and seamless scalability for any project

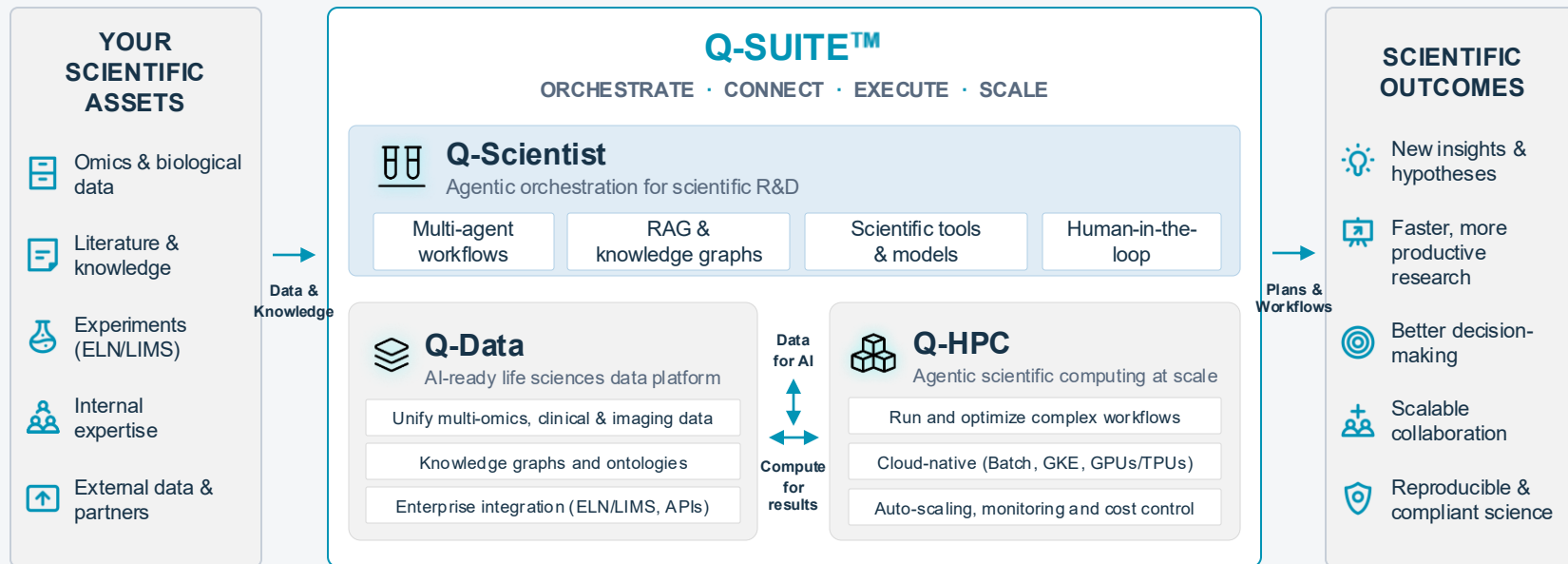
Q-Suite

Zero Gravity Solution Accelerators

Q-SUITE™: Powering Life Sciences R&D



Q-Suite™ is Quantori's scientific solution layer for life sciences R&D: **Q-Data** and **Q-HPC** provide the data and compute foundation, orchestrated through **Q-Scientist** into end-to-end scientific workflows — transforming the way biopharma and healthcare organizations conduct R&D, manage knowledge, and optimize infrastructure.



Accelerate Scientific Discovery

From questions to validated insights faster

Unify Data and Research Workflows

Integrate disparate data into a single AI-ready platform

Scale R&D with Enterprise Infrastructure

Run complex workflows at any scale

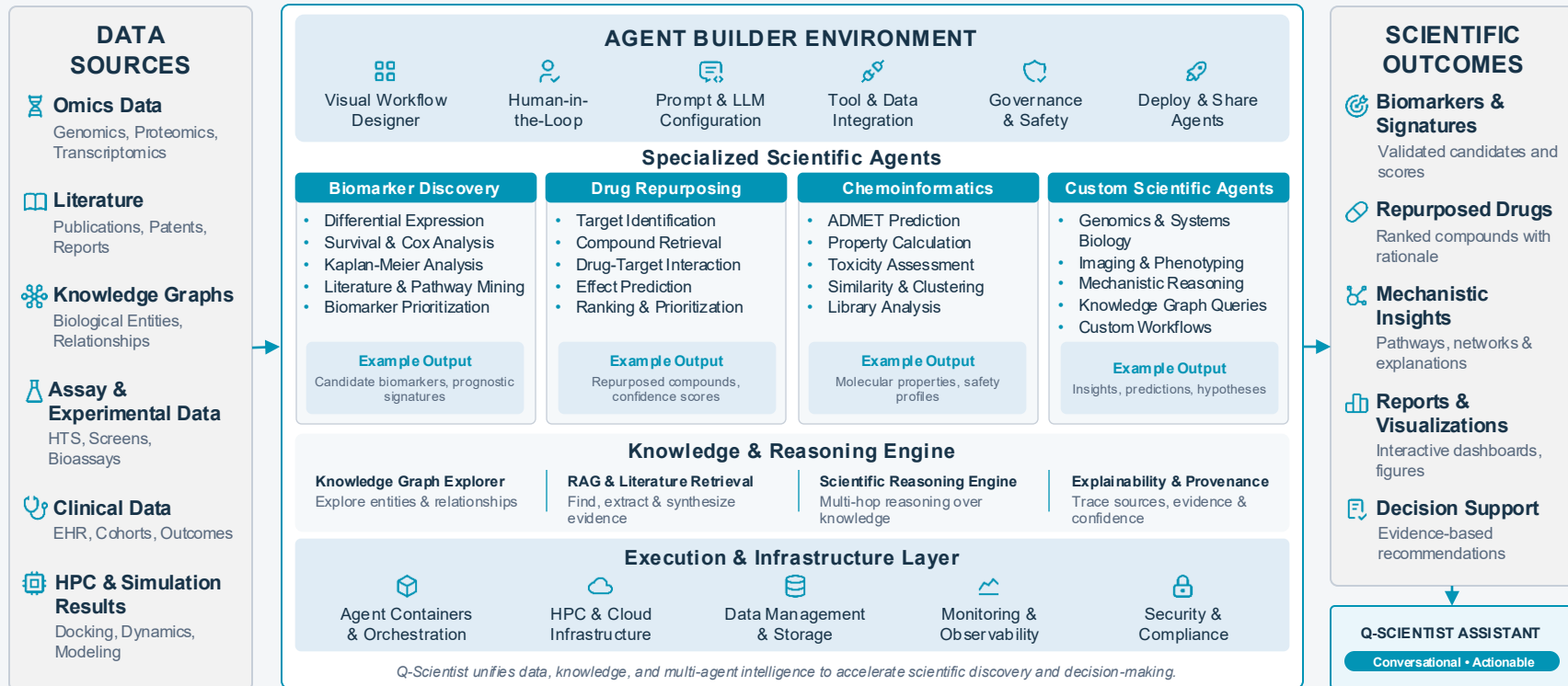
Enable Secure Enterprise AI Adoption

Governed, compliant and reproducible by design

Q-Scientist: Agentic Scientific Discovery and Workflow Orchestration Platform



Q-Scientist is Quantori's agentic AI platform purpose-built for Life Sciences R&D — a unified infrastructure where pharma and biotech organizations deploy cutting-edge AI while maintaining full control over their data, IP, and compliance posture.



Gene-to-Drug Hit Discovery

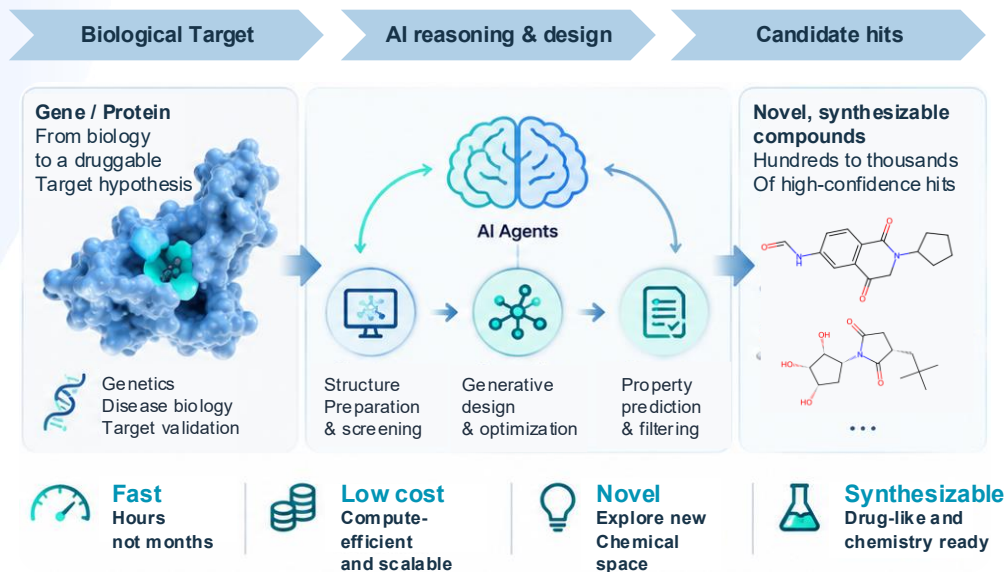
Moonshot: Gene-to-Drug Hit Discovery



Problem statement

A configurable accelerator for cheap, novel, synthesizable hit discovery — built from reusable core technology and adaptable workflow templates.

1. Drug discovery is **slow, fragmented**, and **expensive**, with manual handoffs across target selection, structure preparation, virtual screening, and chemistry follow-up.
2. Early hit discovery must balance novelty, binding quality, synthesizability, and practical access to analogs.
3. Teams need automation at scale while keeping human control over the critical scientific decisions.
4. Moonshot compresses the path from biological hypothesis to prioritized hit series within hours, not weeks.



Fragmented workflows

Human-in-the-loop

Fast hypothesis testing

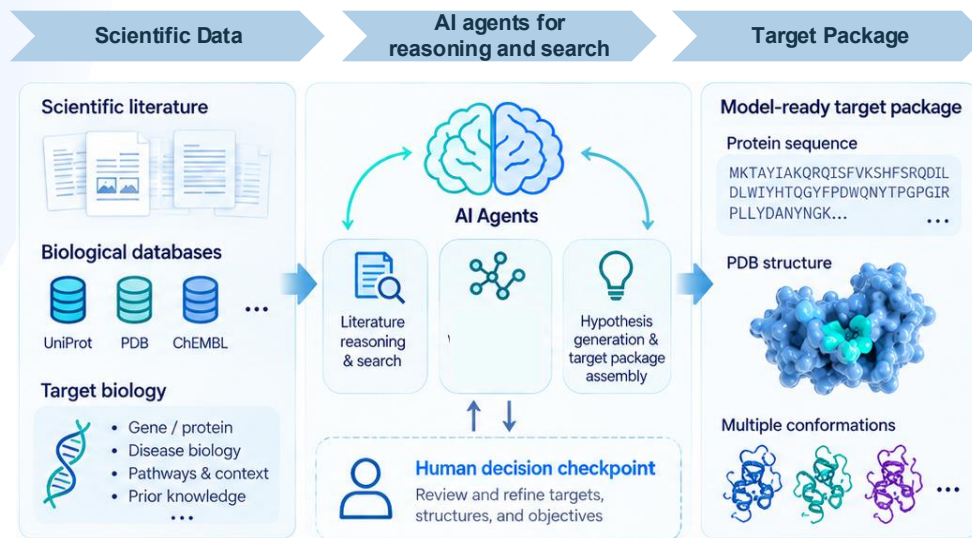
Moonshot: Gene-to-Drug Hit Discovery



Agentic Layer

The agentic front end turns biological hypotheses into model-ready target packages by combining literature reasoning, structural context, and curated knowledge.

1. LLM agents search scientific literature and databases to identify relevant targets, scaffolds, and structure–property relationships.
2. The output is a target package: PDB structure, representative conformations, or protein sequence ready for folding.
3. The package includes references to the databases and resources needed for folding, annotation, and downstream modeling.
4. Human experts remain in control of target selection, structure refinement, and objective definition.



Literature reasoning

Target package

Expert checkpoints

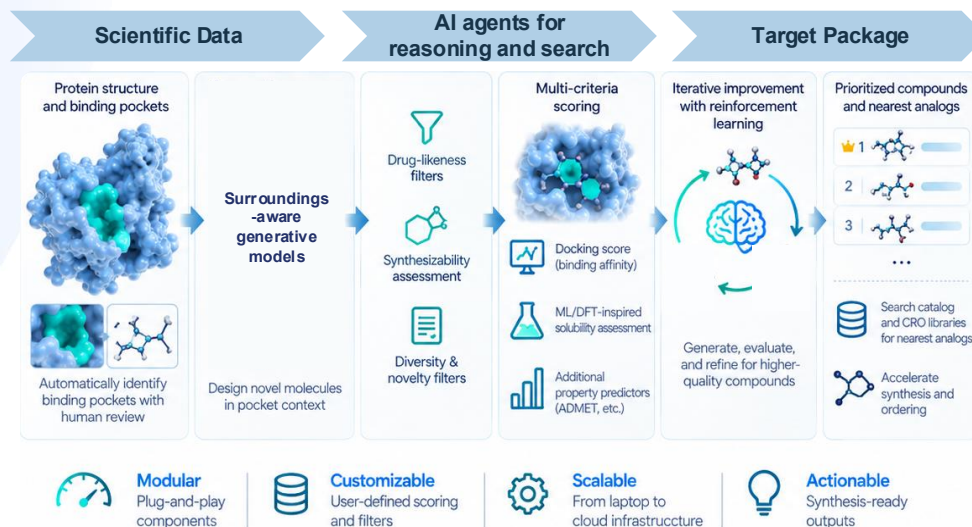
Moonshot: Gene-to-Drug Hit Discovery



Tooling and customizable pipeline

Once the target hypothesis is defined, a modular computational pipeline automates hit generation, evaluation, and prioritization.

1. Potential binding pockets are identified automatically, with human review where needed.
2. Surroundings-aware generative models design molecules while chemical space is constrained for novelty and practicality.
3. Compounds are filtered for synthesizability and scored with user-defined functions such as docking and ML/DFT-inspired solubility.
4. RL-based optimization mines higher-quality compounds, while catalog and CRO-library analogs are surfaced for synthesis follow-up.



Pocket-aware generation

Configurable scoring

Synthesis-ready output

The Pipeline at Work



Some working demos

Full workflow (Long):

[Clipchamp](#)

Fragment-constrained Generation (Short):

[fragment_growth_aws.mp4](#)

De novo generation from a pocket:

[fragment_growth_aws.mp4](#)

Linker Design (Short):

[Clipchamp](#)



LET'S KEEP THE CONVERSATION GOING

Thank You!

Chris L. Waller, Ph.D.

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Come say hi at

Booth #190



October 6-8