

Talent on Demand: Sourcing an Expert Computational Chemist to Accelerate Discovery Pipelines

OVERVIEW

Facing an impending patent cliff for several major revenue-generating therapies, a global biopharmaceutical company sought to proactively close its future revenue gap and strengthen its early-stage pipeline. To do this, they aimed to transition away from traditional, labor-intensive trial-and-error experimentation and embrace a prediction-first R&D model. Their strategy centered on forming high-value AI partnerships capable of accurately predicting on- and off-target molecule safety and accelerating the design-make-test-analyze (DMTA) cycle far beyond what physical laboratories could achieve alone.



Given our ability to rapidly source niche scientific expertise, the company partnered with Kalleid to provide a senior-level Computational Chemistry Consultant to work within its multidisciplinary research teams. The expert supported several high-stakes drug discovery programs, helping the organization operate and implement advanced computer methods and drive faster, more informed decision-making across its drug discovery pipeline.

BUSINESS CASE

In the biopharmaceutical industry, securing highly specialized talent in computational science, machine learning, and advanced *in silico* molecular design is increasingly difficult. The company needed an immediate, flexible staffing solution to strengthen its internal teams without increasing permanent headcount.

The key business and scientific drivers behind this contingent staffing engagement included:

- **Specialized Talent Gap:**

Modern drug discovery sits at the intersection of advanced computational chemistry methodologies/tools (AI, free energy, cheminformatics, and multi-modality design). Scientists who can operate across these domains are exceptionally rare and cannot be sourced quickly through traditional HR pipelines.

- **Fluctuating Pipeline Demands:**

The organization was advancing multiple parallel discovery programs across small molecules, PROTACs, RNA inhibitors, and peptides. This required a resource capable of shifting seamlessly between diverse modalities and project needs.

- **Immediate Operational Impact:**

The organization could not afford a lengthy onboarding or training ramp-up phase. They needed a plug-and-play expert who could immediately guide molecular design decisions, improve potency/selectivity, and optimize ADMET properties with minimal ramp-up time.

SERVICES PROVIDED

The Kalleid consultant provided **comprehensive end-to-end computational chemistry support** while working directly alongside the client's internal R&D teams.

Computational Strategy & Design

- Independently designed, developed, and executed high-level computational research initiatives across multiple drug discovery programs.
- Provided key technical knowledge and input to guide project-team decision making.
- Developed computational strategies to prioritize molecular designs, improve potency/selectivity, and optimize ADMET endpoints.

Advanced Methodology Implementation

- Built, validated, and deployed advanced computational tools, including large-scale virtual screening, ligandability analyses, homology modeling, quantum mechanics, pharmacophore elucidation, and machine learning models.
- Contributed to the development and deployment of next-generation design and AI platforms to accelerate drug discovery.

Data Analysis & Scientific Reporting

- Executed intensive data-mining and advanced analytical workflows to extract actionable insights.
- Delivered regular scientific presentations to internal stakeholders, communicating critical findings and design recommendations with clarity and impact.

Cross-Functional Leadership

- Collaborated seamlessly with cross-functional partners – including medicinal chemists, structural biologists, data scientists, and biologists – across multiple global sites.
- Led high-value computational chemistry initiatives such as holo structure prediction, ligandability analyses, and automated virtual screening pipelines.



RESULTS DELIVERED

Partnering with a **domain-aware staffing firm** enabled the company to offload recruitment, screening, and onboarding of a highly specialized resource. This approach reduced the financial risk associated with long-term hiring while ensuring rapid access to the specialized expertise required to keep critical R&D programs on schedule.

Kalleid delivered a **highly qualified Computational Chemistry Consultant** who functioned as a seamless extension of the internal research organization, contributing a full 40-hour work week. The strategic consulting collaboration met all milestone timelines and financial constraints while providing exceptional technical depth, operational agility, and strategic value to the client's discovery teams.

- **Rapid Time-to-Productivity:** The consultant achieved rapid operational impact, completing a thorough review of all active initiatives and aligning with internal Subject Matter Experts (SMEs) within the first month. This accelerated onboarding and enabled the team to hit its critical milestones without delay.
- **Continuous High-Value Output:** Throughout the engagement, the consultant delivered continuous, uninterrupted computational strategies, modeling, and data-analysis support. This ensured that active drug design pipelines remained optimized for potency, selectivity, and safety, directly supporting faster and more informed decision-making.
- **100% Resource Utilization & Budget Predictability:** The consultant fully delivered the contracted allocation of specialized scientific support. The project concluded exactly at the capped budget, with zero unauthorized pass-through or out-of-pocket expenses, giving the company complete financial predictability and cost containment.

The company was highly satisfied with the results of the engagement and plans to further expand its use of **Kalleid's staff augmentation services** moving forward. Ultimately, this engagement demonstrates how biopharmaceutical organizations can bypass lengthy hiring cycles and rapidly inject high-impact domain-specific expertise into active therapeutic pipelines accelerating discovery efforts while maintaining cost containment and operational flexibility.



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