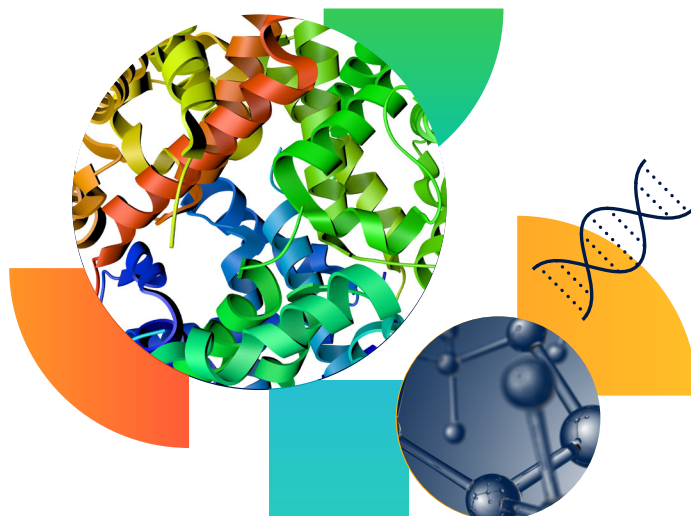


Case Study

Accelerating in silico discovery from plasmid to structure



Schrödinger uses the Sapio laboratory informatics platform to augment and extend its proprietary computational platform for in silico discovery of high-quality, novel molecules and to accelerate drug discovery efficiently.



About the Project

Founded in
1990

Location
New York, New York

Products
Sapio LIMS & Sapio ELN

Website
www.schrodinger.com

The Customer

[Schrödinger](#), founded in 1990, has approximately 900 employees globally and is a leader in computational chemistry, leveraging its physics-based platform to discover high-quality, novel molecules for [materials science](#) and drug development. Schrödinger's material science group has achieved breakthroughs in areas like organic light-emitting diodes (OLEDs), and its [life science](#) group is a multidisciplinary team of platform experts and scientists advancing proprietary programs in drug discovery and development and collaborating on programs in multiple disease areas. The company maintains its [proprietary drug discovery](#) pipeline, alongside collaborations with major biopharmaceutical companies, including Bristol Myers Squibb and Novartis.

The Challenge

Schrödinger, which historically focused on computational methods and utilized external CROs for lab work, decided to establish its internal wet lab to accelerate drug discovery. The CRO it acquired in 2021 utilized paper-based processes, which lacked the digitization, scalability, traceability, and efficiency needed to meet Schrödinger's ambitious goals. In 2022, Rajesh Kumar, Ph.D, joined Schrödinger as senior director of drug discovery. Specific challenges he faced included:

- Collecting, storing, and managing massive datasets, including complex images, in a searchable format.
- Establishing an end-to-end audit trail for lab processes.
- Ensuring adaptability for future technological and process needs.
- Demonstrating incremental value to secure continued leadership buy-in.

Dr. Kumar had previous experience with an ELN (Electronic Laboratory Notebook), which was good for documentation, and he knew a LIMS (Laboratory Information Management System) could be used to search large amounts of data. At Schrödinger, he wanted to "find a platform that would master both."

The Solution

From the 6 to 8 vendors it evaluated, Schrödinger selected the [Sapio Platform](#), which integrates the [Sapio ELN](#) and [Sapio LIMS](#) in one seamless environment. The decision was based on:

1. **Unified Functionality:** Seamless integration of ELN and LIMS to address Schrödinger's present and future informatics needs.
2. **Advanced Search and Traceability:** Comprehensive data capture and audit trails for regulatory and operational insights.
3. **Customization Capabilities:** Tailored workflows to support specialized lab functions, developed collaboratively with the [Sapio Consulting](#) team.

Implementation

Dr. Kumar executed a strategy to improve laboratory operations and simultaneously demonstrate the value of the improvements to Schrödinger's leadership group through an iterative, multi-phase process:

- **Customized Workflows:** Unique workflows for plasmid expression, protein purification, binding studies, and structural biology were developed iteratively with Sapio, and weekly feedback sessions ensured alignment with lab needs.
- **Automated Calculations:** Features protein sequence automated calculations, accessed through webhooks, boosting efficiency.
- **Instrument Integration:** Initial deployment focused on plate readers, and future phases will integrate more instruments, aligning with Schrödinger's "future-proof" vision.

The platform was tested for a month, refined, and fully deployed, with Sapio and Schrödinger teams maintaining close communication throughout.

Results and Added Value

1. Improved Operational Efficiency

- Unified visibility across the entire drug discovery process (plasmid to structure) for all 25 lab team members.

- Automated tracking of resource consumption, such as media costs (\$40 to \$350 per liter depending on cell type), enabling real-time cost analysis and decision-making.

2. Enhanced Traceability and Reporting

- Comprehensive documentation of lab activities accelerates new drug filings and simplifies audit readiness.
- Leadership gains detailed insights into lab performance, justifying ongoing investments in lab expansion.

3. Strategic Insights for Resource Allocation

- Historical data enables predictive planning and budgeting for new projects.
- Metrics like resource consumption and project timelines are benchmarked for continuous improvement.

4. Long-Term Knowledge Retention

- Archival data supports future projects, ensuring scientists can easily access historical insights for decades to come.

Conclusion

Schrödinger transformed its wet lab into a model of efficiency, adaptability, and value creation. This iterative, multiphase approach enhances current drug discovery workflows and establishes a robust foundation for future advancements, ensuring that Schrödinger remains at the forefront of innovation.

The value of the Sapio Informatics Platform to Schrödinger is end-to-end lab performance to automatically capture the cost of media, consumables, and other resources across multiple projects in their pipeline. They can determine which project is consuming the most resources and why. And they can quickly search and capture key metrics weekly, monthly, quarterly, and annually to create a constantly expanding timeline of key performance information.

This transparency and traceability efficiently and effectively help Schrödinger progress from plasmid to the target structure and accelerate the drug discovery process to create value now. In addition, 5, 10, or even 20 years from now, scientists at Schrödinger can quickly and easily find key end-to-end archival data to understand past laboratory experiments and inform their own.