



**CAS CUSTOM SERVICES<sup>SM</sup>**

# HOW CAS CUSTOM API SOLUTIONS HELP CALIBR-SKAGGS ACCELERATE DRUG DISCOVERY

## Case Study

### About Calibr-Skaggs

Calibr-Skaggs Institute for Innovative Medicines is a leading nonprofit translational research center focused on advancing drug discovery from early-stage compound screening to human proof-of-concept studies across a wide range of diseases and modalities.

**Its mission:** To tackle urgent and complex healthcare challenges by pursuing novel therapeutic approaches that not only treat but have the potential to cure.

### Organization

Calibr-Skaggs Institute for Innovative Medicines, a division of Scripps Research

### Industry

Nonprofit translational research

### Focus

Preclinical drug discovery and early-stage clinical research

**CAS**

A division of the  
American Chemical Society



For drug discovery organizations like Calibr-Skaggs, the ability to quickly determine which compounds to prioritize for development is crucial. This decision-making process directly impacts research efficiency, resource allocation, and ultimately, the speed at which potentially life-saving treatments reach patients.

## Three challenges slowing Calibr-Skaggs' high-impact drug discovery pipeline

### 1. Inefficient manual processes hamper early 'go/no-go' discovery decisions

Despite access to CAS SciFinder® under Scripps Research, Calibr-Skaggs lacked an integrated solution to efficiently verify compounds' novelty and identify potential IP (intellectual property) conflicts early in the drug discovery process.

Without an automated way to retrieve compound information, Calibr-Skaggs' chemists had to manually browse for CAS REGISTRY® entry dates—used as a proxy to assess IP risk and compliance limits.

#### IMPACT ACROSS DRUG DISCOVERY PIPELINES

Often applied to as many as 1,000 compounds per day, this manual approach placed a heavy burden on Calibr-Skaggs' team and significantly reduced efficiency across their workflows.

**The result:** Slower decision-making, delayed “go/no-go” calls, and a higher risk of prioritizing the wrong compounds or wasting time on molecules already covered by existing patents. In all cases, collaboration between the IP and R&D teams remains essential for successful outcomes. However, the specific focus areas and strategies may vary depending on the nature of the therapeutic development, the IP landscape, and the regulatory considerations associated with discovering new therapeutics versus developing generics.

### 2. Limited metadata access restricts confident compound prioritization

To prioritize the most promising compounds, Calibr-Skaggs needs access to more than basic match results. They need easy access to comprehensive contextual information, including:

- **Chemical metadata**, such as Tanimoto chemical structure similarity scores and CAS Registry Numbers®.
- **Biological metadata**, including bioactivity indicators.
- **Scientific literature metadata**, including both document and patent identifiers.

#### IMPACT ACROSS DRUG DISCOVERY PIPELINES

Without the ability to retrieve and analyze enriched metadata, research teams cannot fully contextualize compounds within the broader chemical and IP landscape to make informed decisions at scale.

**The result:** Longer evaluation cycles, slower data-driven decision-making, and reduced confidence in lead prioritization.





### 3. Workflow fragmentation impedes concurrent efforts

Spanning biology and medicinal chemistry, Calibr-Skaggs' departments must collaborate in real time to drive drug discovery forward efficiently. Yet, the lack of advanced workflow integration and seamless data exchange between tools forced discovery teams to operate in silos.

#### IMPACT ACROSS DRUG DISCOVERY PIPELINES

Workflow fragmentation creates communication gaps at the most critical early stages of the discovery pipeline, impacting the rapid feedback loops needed to identify and evaluate compounds effectively.

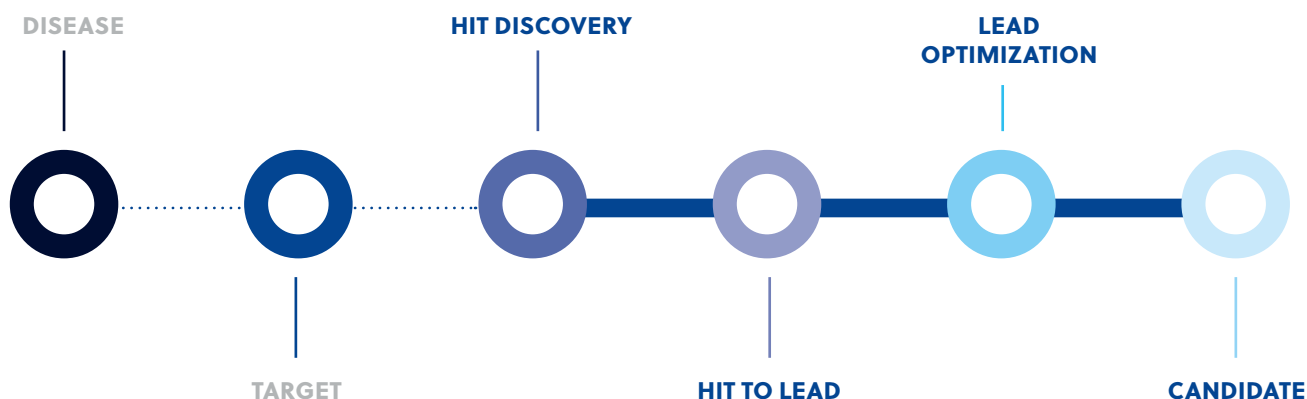
**The result:** Slower iteration cycles, delayed decision-making, potential miscommunications leading to delayed or wasted resources for synthesizing, and reduced efficiency in advancing high-potential compounds through life-changing pipelines.

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Recognizing the need for automation and richer data context, Calibr-Skaggs sought a trusted partner to deliver an integrated solution that could accelerate confident decision-making across its discovery pipeline. With the world's largest curated collection of chemical compounds and unparalleled expertise in scientific literature curation, CAS emerged as the clear choice.

## A unique solution tailored to Calibr-Skaggs' discovery goals

In collaboration with Calibr-Skaggs team, CAS Custom Services<sup>SM</sup> designed a tailored API solution to streamline critical parts of their drug discovery workflow.



*CAS API integration supports critical early stages of Calibr-Skaggs' pipeline, from hit discovery through candidate selection.*



### How CAS API helps Calibr-Skaggs fast-track "go/no-go" discovery decisions

The CAS tailored API solution automatically generates reports on candidate compounds through structure similarity queries, allowing Calibr-Skaggs' researchers to run real-time compound similarity searches and in silico screening directly within their system.

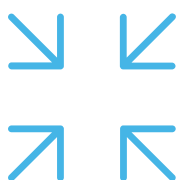
**If an exact match is found**, the API automatically populates reports with key substance metadata, including:

- Compound name
- CAS Registry Number®
- CAS REGISTRY® entry date
- Tanimoto similarity score
- Structure data
- Bioactivity indicators

**If no identical match is found**, the API automatically retrieves information from the nearest substance based on Tanimoto similarity scores to ensure relevant comparisons surface.

This automation delivers enriched metadata and faster insights at scale, reducing time spent on manual research for better informed "go/no-go" decisions earlier in Calibr-Skaggs' pipeline.





## How CAS API helps Calibr-Skaggs streamline its cross-functional pipeline

### Workflow integration



The API allows **Calibr-Skaggs' medicinal chemists and biologists to work in parallel**, eliminating delays caused by sequential validation steps and siloed workflows.

### Process standardization



The API enables Calibr-Skaggs' researchers to **apply the same structure search and metadata standards across teams**, improving reproducibility and reducing human error.

Beyond individual tasks, the CAS API-driven solution contributes to bringing consistency and real-time collaboration across workflows to accelerate drug discovery.

Through its partnership with CAS, Calibr-Skaggs seamlessly integrated CAS-quality insights into its internal processes, empowering researchers to evaluate and prioritize compounds with speed and confidence.

“The team immediately adopted it as they no longer had to manually check if a compound design was known and could find nearest neighbors in the CAS database in real-time, [saving our chemists] valuable time.”

Associate Director, Computational Chemistry  
Calibr-Skaggs Institute for Innovative Medicines, Scripps Research





## CAS Custom Services: Tailored solutions for immediate impact

At CAS, we design custom solutions that integrate smoothly into existing systems to help your teams leverage enhanced, high-impact workflows from day one—without disrupting your pipeline.

Find out how **CAS Custom Services** can help you streamline your workflows and accelerate high-impact pipelines. Learn more at **cas.org**.



Calibr-Skaggs is part of Scripps Research, ranked the most influential research institution in the world, according to the journal Nature.

Nature Index 2017 Innovation supplement: <https://www.nature.com/nature-index/supplements/nature-index-2017-innovation/index>

