



CAS CUSTOM SERVICES<sup>SM</sup>

# CUSTOM API SOLUTIONS HELP ACCELERATE DRUG DISCOVERY

Solution success story

## The challenge: Disparate data and fragmented workflows slow a high-impact drug discovery pipeline

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 many diseases and modalities.

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

Calibr-Skaggs faced several challenges slowing these critical processes across its drug discovery pipeline, including inefficient manual processes, limited access to integrated contextual information for promising compounds, and fragmented workflows. These challenges hampered data-driven decision-making and led to higher risk, reduced confidence, and slowed innovation.

Recognizing the need for automation and richer data context, Calibr-Skaggs partnered with CAS to deliver an integrated solution that could accelerate confident decision-making and boost efficiency across its discovery pipeline.

**CAS**

A division of the  
American Chemical Society



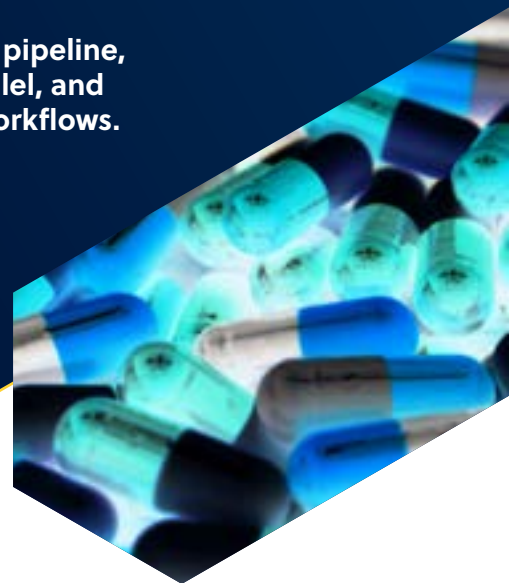
## The solution: A tailored CAS API solution streamlines critical parts of the drug discovery workflow

In collaboration with Calibr-Skaggs' team, CAS Custom Services<sup>SM</sup> designed an API solution to streamline and support early stages of the team's pipeline, from hit discovery through candidate selection.

The 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. 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.

**The solution also helped Calibr-Skaggs streamline its cross-functional pipeline, allowing the team's medicinal chemists and biologists to work in parallel, and eliminating delays caused by sequential validation steps and siloed workflows.**

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. This added consistency and real-time collaboration across workflows to accelerate drug discovery.



**"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](https://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>