



CAS BIOFINDER®

**What if your discovery team
could predict success before
investing millions?**

CAS 
A division of the
American Chemical Society



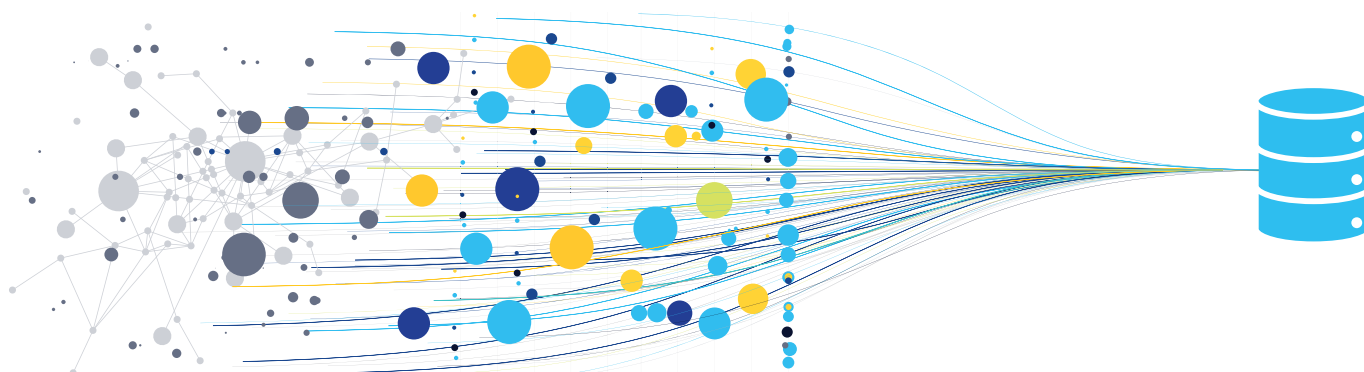
Advance pipeline priorities and reduce costly failures

CAS BioFinder empowers drug discovery teams to make confident decisions early that reduce risk and accelerate progress across the entire preclinical workflow. Unlike niche solutions and generic AI tools, CAS BioFinder connects the world's most trusted human-curated biology and chemistry data with AI-driven analytical and predictive models to help R&D leaders prioritize investments and streamline collaboration.

With CAS BioFinder, you can:

- Align modality investments with disease biology, accessibility, and development timelines.
- Prioritize the targets and drug candidates most likely to succeed, minimizing investment risk.
- Explore repurposing opportunities and competitive intelligence to stay at the forefront of discovery.

Powered by the trusted **CAS Content Collection™** and enhanced by the **CAS Newton™** AI research assistant, CAS BioFinder delivers actionable insights through intuitive visualizations and predictive analytics. Whether you're leading a portfolio strategy or guiding scientific decisions, CAS BioFinder helps you uncover hidden connections and move promising candidates forward with confidence.



Scientific data landscape:
Countless sources of unstructured data

CAS BioFinder:
A single, integrated source of drug discovery data

"CAS BioFinder is an all-in-one platform for looking at your target or your ligands. What's already been done, what's predicted for it, what the landscape of that looks like. You can follow your lead in whatever direction you like."



Chemical and molecular biologist
CAS BioFinder development partner

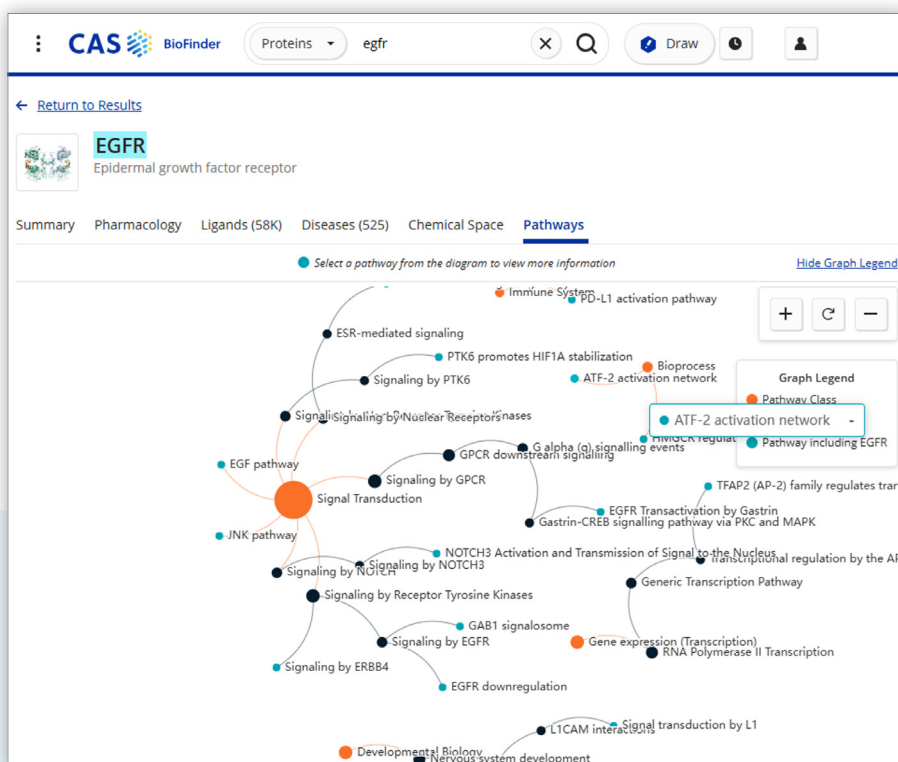
"CAS BioFinder... enables rapid in silico prediction of pharmacological activity and bioactivity by modeling protein–ligand interactions based on data extracted from the scientific literature. ...The AI-driven target prediction (CAS BioFinder) successfully narrowed down the candidate search for in vitro testing."

P. Natho et al.,
Angew. Chem. Int. Ed. 2025,
doi: anie.202521633¹

Predict your success with confidence

- **Cross-functional decisions:** Align teams quickly on modality selection with integrated target accessibility, pathway context, and ligand selectivity data.
- **Biology teams:** Identify and validate targets using biomarker summaries, interconnected protein information, and pathway visualizations. Explore antibody and peptide visualizations to aid in the design of ADCs and PDCs.
- **Chemistry workflows:** Optimize SAR and predict safety with pharmacology tables, chemical space visualizations, and ADMET profiles. Compare the effect of structural changes with matched molecular pairs analysis. Screen novel and known candidates against target panels with AI-powered predictive models to flag safety risks early.

Explore binding sites, scaffold hop, predict ligand activity, and assess synthetic feasibility, all within a single platform. AI-driven summaries and substantiated predictive models accelerate discovery by narrowing candidate lists and revealing safety risks early in the process.





CAS connects the world's scientific knowledge to accelerate breakthroughs that improve lives. We empower global innovators to efficiently navigate today's complex data landscape and make confident decisions in each phase of the innovation journey. As a specialist in scientific knowledge management, our team builds the largest authoritative collection of human-curated scientific data in the world and provides essential information solutions, services, and expertise. Scientists, patent professionals, and business leaders across industries rely on CAS to help them uncover opportunities, mitigate risks, and unlock shared knowledge so they can get from inspiration to innovation faster. CAS is a division of the American Chemical Society.

Connect with us at cas.org

1. P. Natho, A. Vicenti, F. Mastrodorito, F. De Franco, L. Walsh-Benn, M. Colella, E. Mesto, E. Schingaro, O. Nicolotti, A. Gioiello, R. Luisi, *Angewandte Chemie International Edition*. 2025, e21633. <https://doi.org/10.1002/anie.202521633>