
CAS BIOFINDER®
Use cases for biologists and chemists
Updated 27 January 2026
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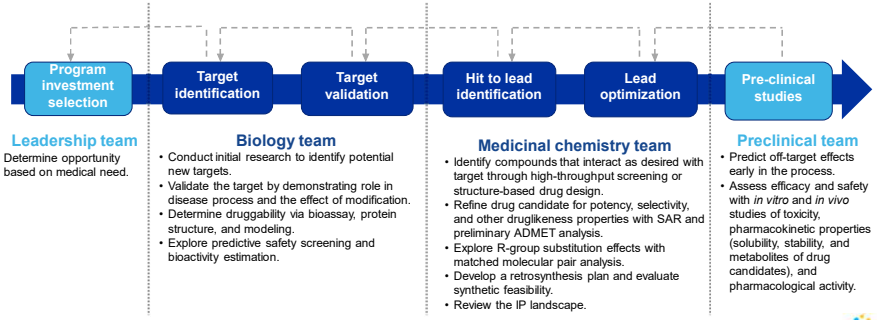
How to use this deck

DO NOT USE THIS SLIDE IN YOUR PRESENTATION

- These slides cover the identified research questions and use cases for CAS BioFinder for biology and chemistry teams as of December 2025. Most slides have light and dark versions available.
- Use cases are best suited for scientists and team leads (Seths and Roberts), **not** procurement specialists or executives (Lucys or Christophers).
- **Choose only the slides that are relevant to your audience!**
- The notes section includes the research steps in CAS BioFinder to support each use case.
- **Recommendation:** Customize the example use cases and screenshots based on your account's pipeline and research priorities.
- Be sure to include the ® symbol on the first use of CAS BioFinder, and always include "CAS" in the solution name.

Drug discovery is a complex process with multiple decision points and hand-offs

You need a solution that helps everyone work together with confidence



Leadership team

Determine opportunity based on medical need.

Biology team

- Conduct initial research to identify potential new targets.
- Validate the target by demonstrating role in disease process and the effect of modification.
- Determine druggability via bioassay, protein structure, and modeling.
- Explore predictive safety screening and bioactivity estimation.

Medicinal chemistry team

- Identify compounds that interact as desired with target through high-throughput screening or structure-based drug design.
- Refine drug candidate for potency, selectivity, and other druglikeness properties with SAR and preliminary ADMET analysis.
- Explore R-group substitution effects with matched molecular pair analysis.
- Develop a retrosynthesis plan and evaluate synthetic feasibility.
- Review the IP landscape.

Preclinical team

- Predict off-target effects early in the process.
- Assess efficacy and safety with *in vitro* and *in vivo* studies of toxicity, pharmacokinetic properties (solubility, stability, and metabolites of drug candidates), and pharmacological activity.

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Answer critical drug discovery questions

Make confident, informed decisions about where to invest your time and money

Cross-functional teams

- Invest in the most effective modality for the validated target.
- Find new targets and indications to repurpose drugs.
- Maintain visibility into other research on your disease, protein, or drug candidate.

Discovery biology teams

- Inform research paths with an understanding of the disease's mechanisms and pathogenesis.
- Uncover potential new targets for disease treatment.
- Identify early signals of therapeutic potential.
- Confirm a target's therapeutic relevance before passing to the chemistry team.
- Design the best possible delivery mechanism for the proposed therapy.

Chemistry teams

- Identify the most promising location on the target to bind with a therapeutic drug.
- Identify ligands that interact in a specific way with a target.
- Connect ligand activity to therapeutic potential.
- Maximize potency and minimize off-target risks.
- Optimize leads for potency, safety, synthetic feasibility, and druglikeness.

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CAS Newton℠ in CAS BioFinder

Ask a complex question, get a thorough answer.

Any CAS BioFinder user can ask a complex research question and receive a detailed summary report based on data from the CAS Content Collection ™.

The CAS Newton deep research AI assistant in CAS BioFinder allows you to ask precise scientific questions in your preferred language and receive a detailed and well-cited response.

- Establish a starting point for future research with a landscape view.
- Facilitate cross-functional collaboration by establishing a baseline of knowledge about other scientific areas.
- Test theories early with rapid literature searches.

Establish a quick starting point

Scientists use the AI assistant to quickly summarize data and develop a starting point for further research. For example, they may know how to use the traditional CAS BioFinder interface to filter and prioritize the most potent JAK-1 inhibitors and how to delve into ligand details to learn the indications for each one. But the AI assistant can provide a sample of this data very quickly with linked sources for additional research. Through follow-up questions, the user can redefine the question or redirect the results in a way that's most helpful for their research.

Facilitate cross-functional collaboration

Early research indicates that many CAS BioFinder users also use the AI assistant to establish a baseline of knowledge about other scientific areas that impact their own work. For example, a medicinal chemist seeking to understand why the biology team recommended a particular protein target discovers that it has a broad binding profile that makes it ideal for a variety of drug candidates. In this way, the AI assistant helps to create a common ground for cross-disciplinary conversations.

Test theories early

The rich, well-sourced hyperlinked data in CAS BioFinder's traditional interface helps scientists draw connections

they may not have expected. They can use the AI assistant to easily explore their new theories and direct their further research paths. For example, a scientist who notices similarities in proteins and pathways involved in both Parkinson's disease and hypoxia asks the AI assistant for a summary of research associations between the two diseases. They then follow up with questions about potential treatments to understand the market landscape.


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RESEARCH OUTCOMES FOR CROSS-FUNCTIONAL TEAMS
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CAS BioFinder for cross-functional teams

Invest in the most effective therapeutic modality for the validated target

Question: How can we determine the best modality for our disease-target combination?

Why it matters: Align modality investments with disease biology, accessibility, and development timelines.

Use cases: **The biologist** validates the accessibility of LRRK2 and its biological context by understanding the effect of existing treatments and binding affinity to minimize off-target effects.

The cheminformaticist analyzes binding pockets and physicochemical properties to determine if the target is suitable for small-molecule inhibition.

Pathway details show you the biological role of a protein in the body. This example shows LRKK2 interactions, including phosphorylation and out molecules.

Research steps in CAS BioFinder

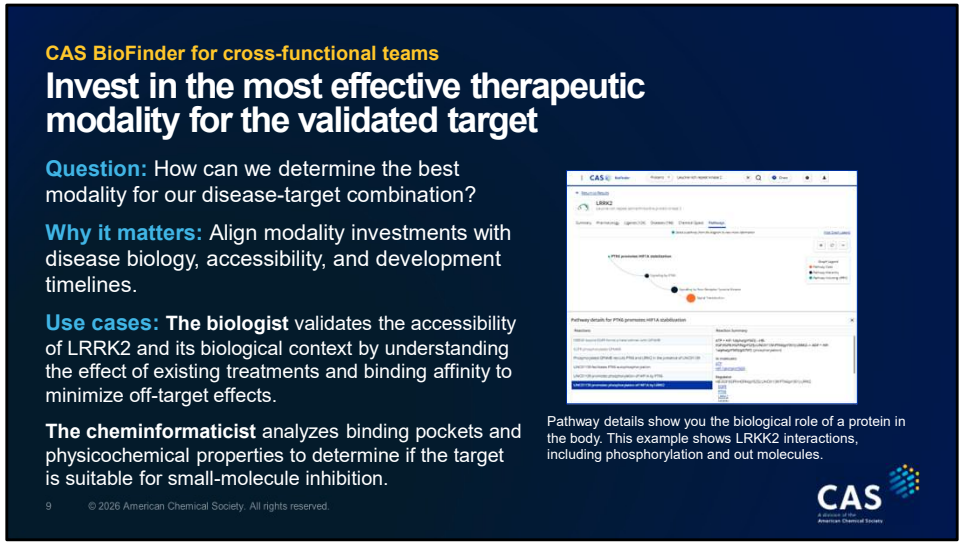
Review the selectivity of existing therapies.

--Explore target details, such as the structure, sequence, and related pathways to understand the accessibility and biological role of the target protein.

--Conduct a BLAST search to confirm novelty and to identify homologs that could indicate potential for cross-activity.

--Review existing large and small molecules that are associated with the target, identifying ligands with a higher risk of binding to multiple targets, therefore causing off-target effects, using pValue.

--Review the biological role of the target via pathways and the anticipated function of a new therapeutic to determine if the candidate will need to cross the blood-brain barrier. Explore ligands associated with a target filtered to sizes below 600 Da to begin design considerations.



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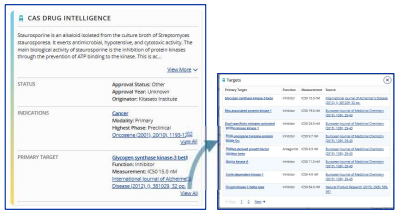
CAS BioFinder for cross-functional teams

Find new targets and indications to repurpose drugs

Question: How can we explore the untapped therapeutic potential of an approved drug?

Why it matters: Offer senior leadership a potential new therapy for a new market with minimal time and cost investment.

Use case: **The biologist** seeks patentable new uses for the cancer drug staurosporine by exploring less common protein interactions.



Learn about approved drugs at a glance to identify primary targets and indications. Easily view all primary targets to understand typical or approved mechanisms.

Research steps in CAS BioFinder

Explore all proteins and diseases associated with a drug.

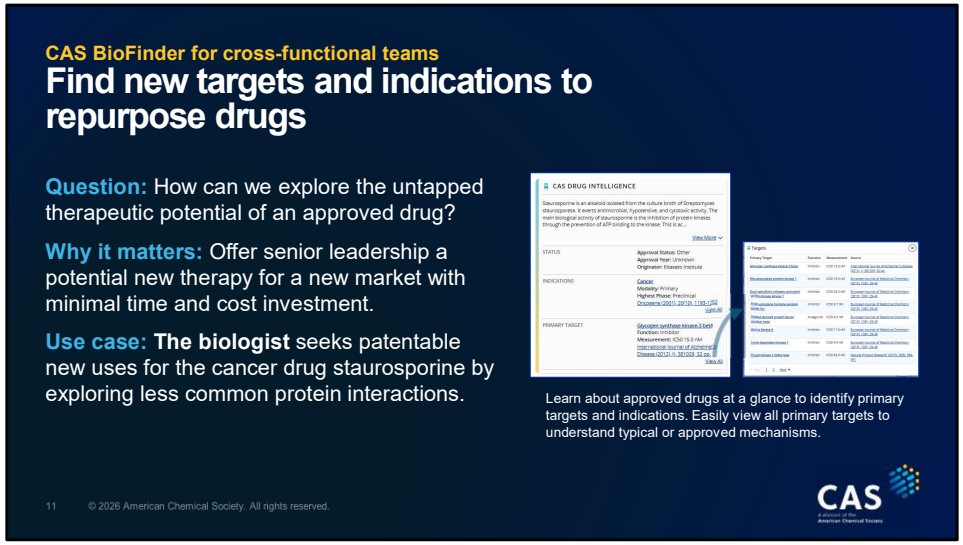
--Review drug intelligence summaries to learn about current research into functions, indications, and limitations. View primary target and indications and links to drug labels as well as clinical trial data.

--Review other proteins and diseases the drug is associated with, including function and relevant measurements, to identify potentially valuable activities. Dive into less common targets and their disease relationships with assay details to fully understand the mechanism of action.

--Review drugs already associated with the disease and their status in the market, including those that have been withdrawn. Explore detailed information about the drugs' primary targets and indications to identify repurposing opportunities and gaps in current therapeutic approaches.

--Filter by cell lines and compare assay results to better understand experimental conditions.

--Predict ligand activity against other targets of interest to identify new research areas.



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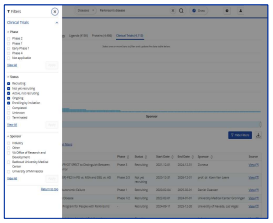
CAS BioFinder for cross-functional teams

Maintain visibility into other research on your diseases, proteins, or drug candidates

Question: How can we stay aware of competitive challenges?

Why it matters: Avoid investing in a research path that is already being pursued by another organization.

Use case: **A chemist or biologist** working on a novel treatment for Parkinson's disease regularly reviews clinical trial data, patents, and publications to understand the competitive market, identify potential PTO issues, and learn from new research.



Clinical trial data helps you keep up to date on active research on your disease of interest. This example displays data from more than 4,000 clinical trials related to Parkinson's disease, filtered for actively recruiting and ongoing trials.

Research steps in CAS BioFinder

Monitor clinical trials associated with your disease of interest and filter by phase, status, and sponsor to set your research path and detect safety issues.

CAS BioFinder for cross-functional teams

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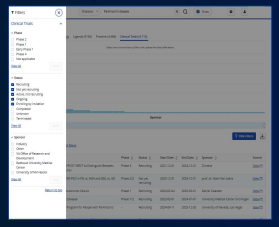

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RESEARCH OUTCOMES FOR DISCOVERY BIOLOGY TEAMS
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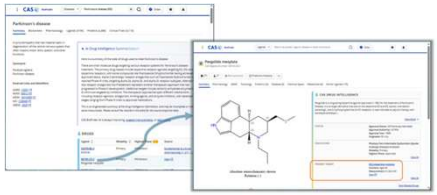
CAS BioFinder for biologists

Inform research paths with an understanding of the disease's mechanisms and pathogenesis

Question: How can I better understand the mechanisms of a specific disease?

Why it matters: Confidently direct the team's target research to save time and resources.

Use case: **The discovery biologist** seeks genetic associations for Parkinson's disease.



Delve into drug information to clarify which proteins are (and are not) involved in a disease.

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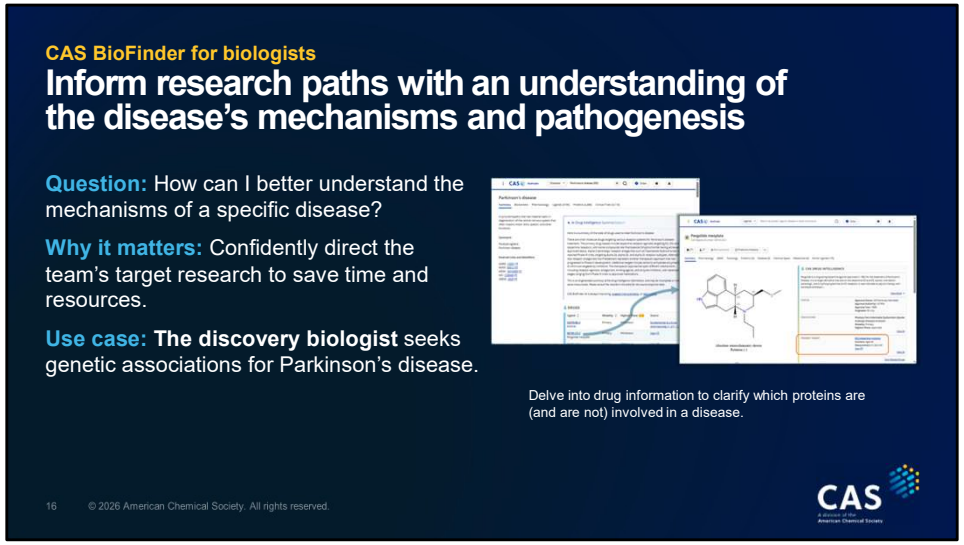
Research steps in CAS BioFinder

Explore disease details.

- Better understand the disease with a description, synonyms, and links to external identifiers, such as NCI, MESH, and EFO, which help you align research and ensure consistency when connecting your results with public data or collaborators.
- Review drugs already associated with the disease and their status in the market, including those that have been withdrawn. Explore detailed information about the drugs' primary targets and indications to better understand how the disease interacts with the therapies.
- Use disease-related biomarkers to identify molecular changes involved in diagnosing, monitoring, and treating the disease. Focus on the most relevant biomarkers with filters for categories, parameters, organism, biochemical agent, specimen, and treatment. Review assay details for each measurement to better understand its context.



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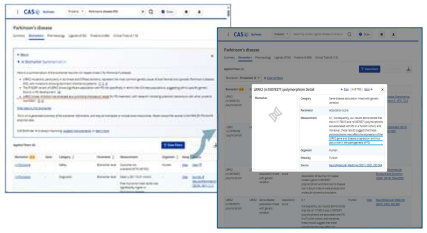
CAS BioFinder for biologists

Uncover potential new targets for disease treatment

Question: How can I identify the most biologically and clinically relevant targets for my disease of interest?

Why it matters: Reduce uncertainty before committing the team's resources.

Use case: With an understanding of genetic markers of Parkinson's disease, **the discovery biologist** seeks potential targets for treatment.



Biomarker summaries help you quickly see how specific biomarkers are involved in a disease. In this example, a gene association reveals a potential target for treating Parkinson's disease by inhibiting LRRK2. The table provides additional data, including assay details and source material.

Research steps in CAS BioFinder

On the disease detail page:

- Browse proteins associated with the disease. Filter by organism, parameter, function, and experiment type to narrow the list.
- Use the AI summaries on the biomarker tab to identify genes associated with the disease that may provide therapeutic opportunities. Explore detailed biomarker data to better understand the effect of the protein on the disease and provide recommendations for tracking the effectiveness of potential therapeutics.
- Review measurement data for the protein as a biomarker of your disease of interest to quickly understand current research on the protein-disease relationship. View assay details for each measurement and follow links to the source material for further research.
- Use detailed biomarker data to compare expression patterns across diseases or conditions and identify potential diagnostic or prognostic indicators, along with AI-generated summaries to help you understand and

prioritize the most relevant data

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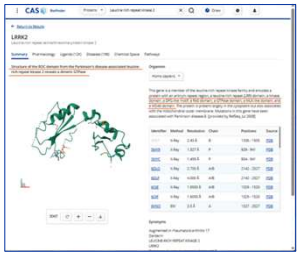
CAS BioFinder for biologists

Identify early signals of therapeutic potential

Question: How does my target protein function in the body?

Why it matters: Invest only in targets that have the desired effects.

Use case: Following a lead gleaned from biomarker information, **the discovery biologist** seeks to understand the effect of inhibiting leucine-rich repeat serine/threonine-protein kinase 2 (LRRK2) mutations.



Protein summaries provide information that can inspire future research directions.

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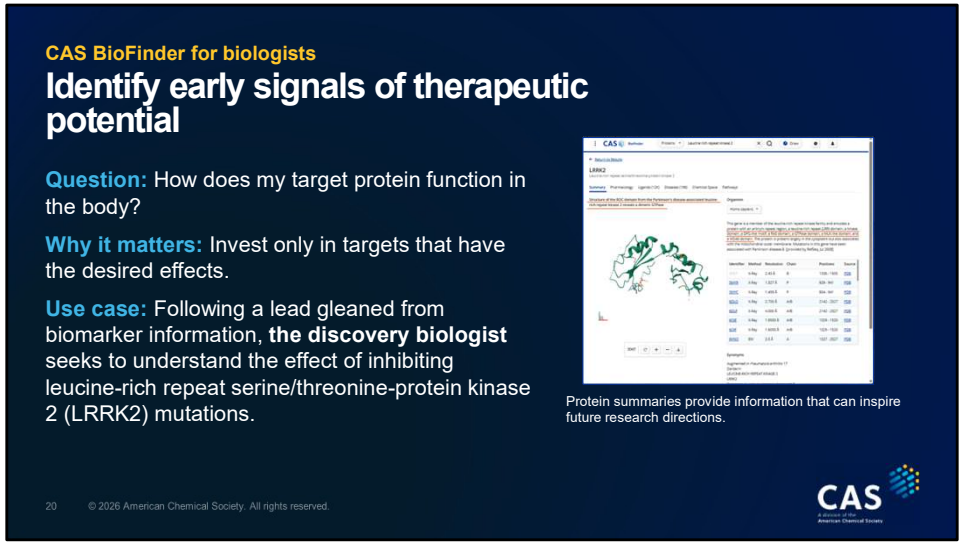
Research steps in CAS BioFinder

Explore detailed protein information.

- Review basic information about the protein at a glance to understand its standard binding affinity and normal function in the body.
- Cross-reference data and simplify collaboration across platforms and teams with synonyms and linked external identifiers, such as NCBI, UniProt, and PDB.
- Interact with 3D crystal structures of proteins, highlighting ligand and sugar binding sites, as well as visualizing the waters of crystallization, in order to analyze drug-ability and binding interactions in a structural context.
- Explore biological pathways to see the upstream and downstream effects of modifying a protein and to understand what biological processes it’s involved in. Follow links to source material and related proteins for further research.



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CAS BioFinder for biologists

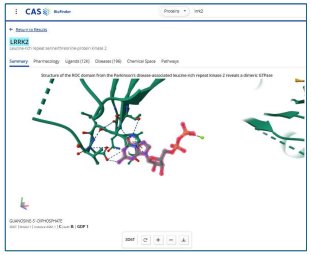
Confirm a target's therapeutic relevance

Question: How can I confidently validate my recommended target before passing it to the chemistry team?

Why it matters: Ensure that the recommended target will not waste the chemistry team's time and resources.

Use case: **The discovery biologist** determines whether LRRK2 is an effective and safe protein to target when treating Parkinson's disease.

The computational biologist supports the LRRK2 recommendation by exploring its modes of action.



Interactive, 3D protein models allow you to explore potential binding sites. In this example, LRRK2 is shown with the molecule guanosine-5'-diphosphate.

Research steps in CAS BioFinder

Explore the target's novelty and interactions with ligands.

- Explore structural insights and potential binding sites with 3D models of targets binding to ligands highlighting hydrogen bonding, pi stacking, and the presence of salts, metals, and waters of hydration.
- Download and copy sequences, filtered by organism, to focus research on species-relevant data to support in vitro, in vivo, or translational research. Run a BLAST search to confirm the novelty of a target or to determine how a ligand interacts with similar proteins with similar modes of action.
- Reduce the trial-and-error cycle by finding ligands with strong target interactions and exploring their druglikeness, selectivity, and potential safety risks, as well as the toxicity of their predicted and known metabolites.
- View related ligands and their metabolites with pharmacology data to explore how the protein reacts to them to assess ligand potency and predict metabolic profiles.
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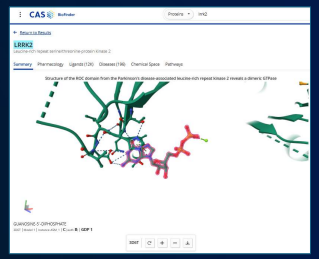

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CAS BioFinder for biologists

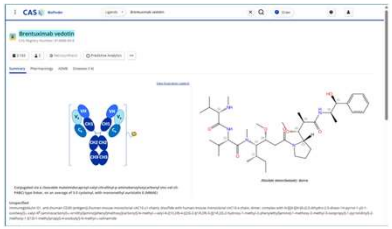
Design the best possible delivery mechanism for the proposed therapy

Question: How can I design an antibody or peptide for my target that delivers the drug the chemistry team designs?

Why it matters: Balance innovation with manufacturability and ensure that the modality aligns with the company's therapeutics strategy, safety requirements, and development timelines.

Use cases: **The peptide engineer** seeks to design a short sequence for improved tissue penetration or receptor targeting on LRKK2.

The antibody engineer designs or selects antibodies for delivery into LRKK2.



Explore the structure of existing antibodies and, when available, the full details of an ADC. By reviewing molecules known to interact with a target, you can select an existing antibody (or peptide) to deliver a drug or innovate a new antibody based on past successes.

Research steps in CAS BioFinder

Explore existing antibodies and peptides.

- Explore all known antibodies or protein/peptides associated with a protein target. Review structure and sequence information to understand binding properties and options for modifying or innovating on the design.
- Quickly move between detailed and structured information on disease, targets, ligands, pharmacology data, antibody structure, sequences, and references to make well-informed recommendations.

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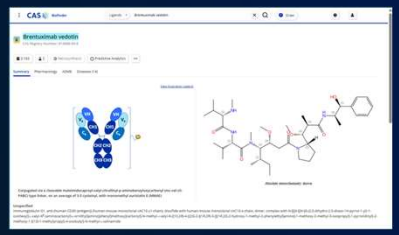

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FOR CHEMISTRY TEAMS
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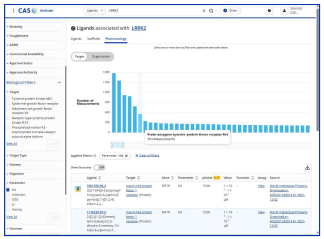
CAS BioFinder for chemists

Identify the most promising location on the target to bind with a therapeutic drug

Question: How do I select the most effective binding site for our chosen modality?

Why it matters: Confirm that the recommended binding site maximizes therapeutic effects while minimizing risk and cost.

Use case: **The computational chemist** uses structural biology data, ligand-binding information, and predictive modeling to identify druggable pockets on the target protein provided by the biology team, LRRK2.



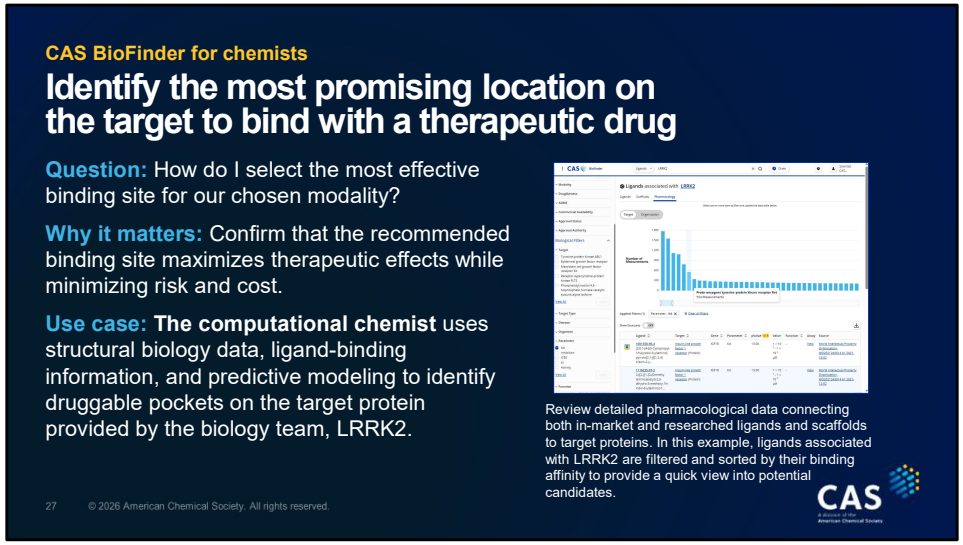
Review detailed pharmacological data connecting both in-market and researched ligands and scaffolds to target proteins. In this example, ligands associated with LRRK2 are filtered and sorted by their binding affinity to provide a quick view into potential candidates.

Research steps in CAS BioFinder

The computational chemist must provide evidence and rank binding sites based on their affinity, selectivity, and off-target effects to assist the chemistry team with informed design decisions.

Explore protein details and ligand interactions.

- View the 3D crystal structure for the target protein. Adjust resolution and organism filters for maximum relevance.
- Analyze known ligands for the target protein and similar kinases. Filter pharmacological data to focus on binding affinity (Kd).
- Predict binding sites by exporting relevant structural data for in-house computational chemistry tools, such as docking software, to rank the druggable pockets.
- Quickly assess the safety and druglikeness of candidate ligands prior to high-throughput screening by exploring their physicochemical properties and ADMET profiles. Dig deeper into metabolites to identify toxicology risks.



Research steps in CAS BioFinder

The computational chemist must provide evidence and rank binding sites based on their affinity, selectivity, and off-target effects to assist the chemistry team with informed design decisions.

Explore protein details and ligand interactions.

- View the 3D crystal structure for the target protein. Adjust resolution and organism filters for maximum relevance.
- Analyze known ligands for the target protein and similar kinases. Filter pharmacological data to focus on binding affinity (Kd).
- Predict binding sites by exporting relevant structural data for in-house computational chemistry tools, such as docking software, to rank the druggable pockets.
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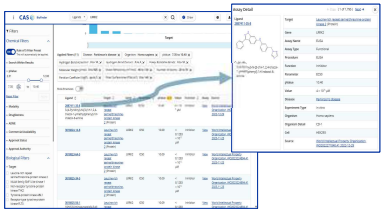
CAS BioFinder for chemists

Identify ligands that interact in a specific way with a specific target

Question: How do I uncover molecule-target pairs with strong potential for therapeutic development?

Why it matters: Reduce the time and resources required to develop an initial list of ligands.

Use case: Using the Parkinson's disease target LRRK2 provided by the biology team, **the medicinal chemist** explores known and predicted inhibitors and their potency.

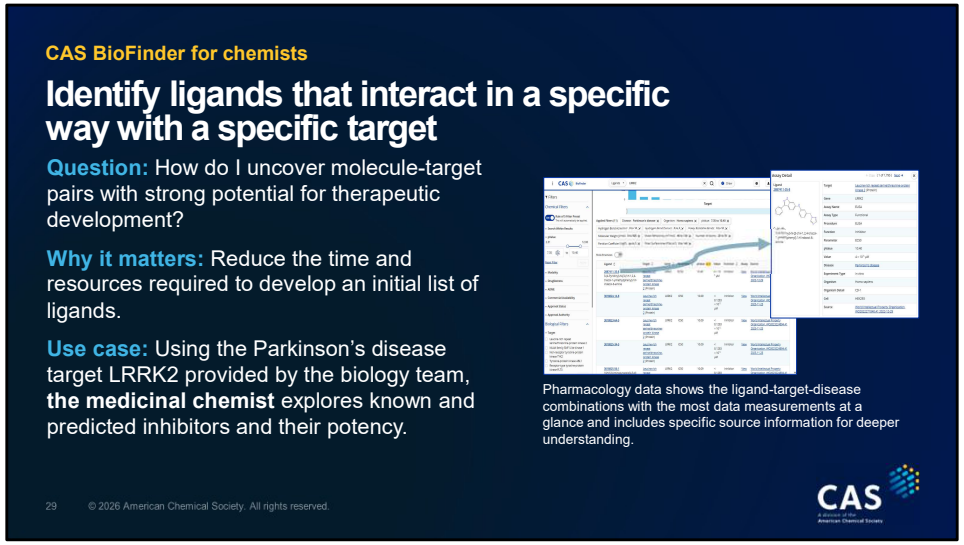


Pharmacology data shows the ligand-target-disease combinations with the most data measurements at a glance and includes specific source information for deeper understanding.

Research steps in CAS BioFinder

Explore scaffolds and approved drugs expected to treat a disease via a specific target.

- Explore the multi-faceted relationship between targets, diseases, and ligands to better identify drug candidates. View all ligands associated with a disease-target-organism combination, then filter by druglikeness properties, function, approval status, and more.
- Choose a drug to explore its primary target, research stage, and mechanism of action to direct your future research path.
- Explore scaffolds of ligands associated with your protein-disease combination with the same filters to understand binding options at a glance. Use this information to begin novel analog design.
- Dig deeper into the pharmacology data tables, with source material and assay detail associated with each measurement and assess ADMET profiles early in the pipeline.
- Review and select the most relevant biomarkers to indicate the effectiveness of the candidate drugs.



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CAS BioFinder for chemists

Connect ligand activity to therapeutic potential

Question: How do I optimize top therapeutic candidates from my ligand set?

Why it matters: Focus the team's resources on candidates most likely to be best-in-class therapeutics.

Use case: With a viable list of a few hundred ligands associated with LRRK2 and Parkinson's disease, **the medicinal chemist** begins focusing on what they can learn from existing research to create a novel molecule.

Judge the effect of small modifications on pActivity with matched molecular pairs analysis. In this example, a medicinal chemist seeks ways to improve a promising candidate that previously failed in mouse trials.

Research steps in CAS BioFinder

Research molecules already associated with your target and disease and look for ways to improve.

- Explore scaffolds and ligands similar to those that already failed in in vitro or in vivo trials to identify modifications that would potentially improve performance.
- Delve into pharmacology details on non-approved drugs to further understand assay conditions, safety concerns, mechanisms of action, and potency.
- Explore the nearby chemical space by mapping measurements of similar ligands on 2D and 3D graphs to identify analogs and structure-activity trends. Map similar compounds along key characteristics to scaffold hop away from scaffolds with IP or white space issues.
- Experiment with R-group substitutions on through matched molecular pairs analysis to see the effect of small changes and identify activity cliffs.
- Flag potential off-target effects or safety concerns before advancing a candidate.

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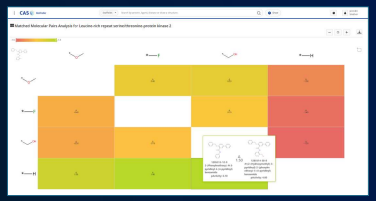

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CAS BioFinder for chemists

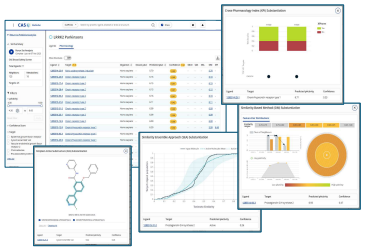
Maximize potency and minimize off-target risks

Question: How can I confidently assess the balance of potency and safety?

Why it matters: Prioritize the most attractive candidates earlier in development.

Use cases: With a short list of available and novel molecules to consider as potent LRRK2 inhibitors, **the medicinal chemist** seeks to identify the compound with the best combination of activity, safety, and druglikeness.

The toxicologist explores all potential on- and off-target interactions as well as other adverse effects.

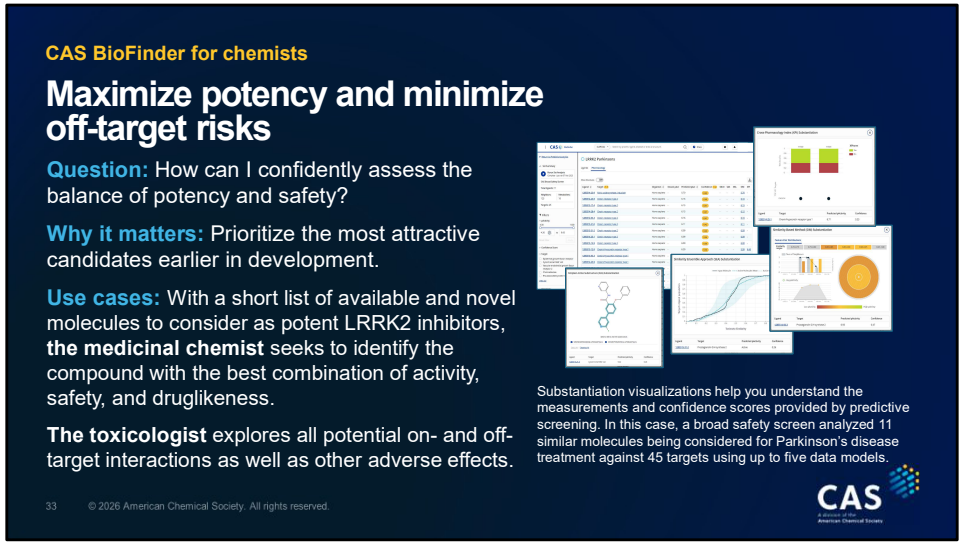


Substantiation visualizations help you understand the measurements and confidence scores provided by predictive screening. In this case, a broad safety screen analyzed 11 similar molecules being considered for Parkinson's disease treatment against 45 targets using up to five data models.

Research steps in CAS BioFinder

Conduct predictive screenings and review safety data.

- Screen your list of novel and known high-priority ligands against all targets, a pre-set safety panel, or a disease-specific panel of targets to estimate how active and selective your ligand is for binding at the desired site of action.
- Delve into predictive substantiation visualizations to better understand the measurements that go into each predicted measurement and the related confidence scores.
- Recognize potential safety risks early to flag likely failures before investing in synthesis and clinical trials, and redirect research efforts.
- Review adverse event data for drugs similar to your potential candidates to flag potential safety issues.
- Explore protein pathways and connections for potential upstream and downstream effects of modifying your target.



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CAS BioFinder for chemists

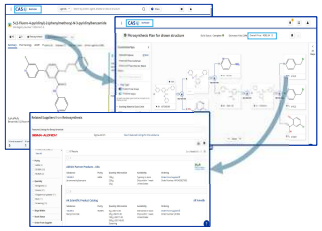
Optimize leads for potency, safety, synthetic feasibility, and druglikeness

Question: How can I evaluate our ability to synthesize the proposed candidate?

Why it matters: Advance only the drug candidates most likely to succeed without derailing timelines or budgets with synthetic complexity.

Use cases: After predicting safety risks, **the medicinal chemist** selects the most promising drug candidate and delivers the design to the synthetic chemist.

The synthetic chemist reviews the proposed candidate and intended target to prepare a retrosynthesis plan that considers route complexity, availability of starting materials, and potential bottlenecks.



Seamlessly jump from CAS BioFinder to CAS SciFinder® to continue the drug development process. In this example, the medicinal chemist has identified a known molecule for consideration, 1285515-21-0, and the synthetic chemist has developed a plan and pricing estimate for creating it in-house.

Research steps in CAS BioFinder

Evaluate a molecule's synthetic feasibility.

- Explore known ligands with similar structures to evaluate potential metabolites and estimate druglikeness features, such as log p.
- Jump into CAS SciFinder to create a retrosynthesis plan so you can begin in vivo testing with your molecule.
- Draw a structure of a novel molecule in CAS SciFinder's retrosynthesis tool to predict the best synthesis plan.
- Locate chemical suppliers and estimate pricing, shipping time, and inventory status to judge synthetic feasibility.

CAS BioFinder for chemists

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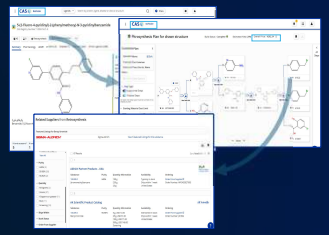

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Thank you

Presenter's name
Presenter's title
Presenter's contact info

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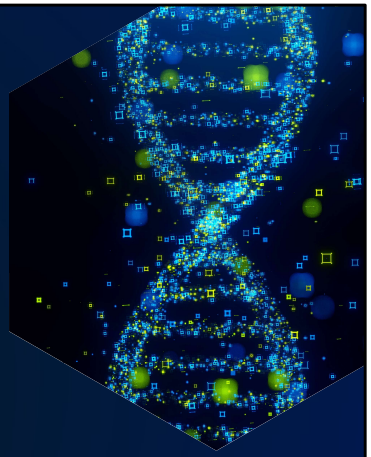

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