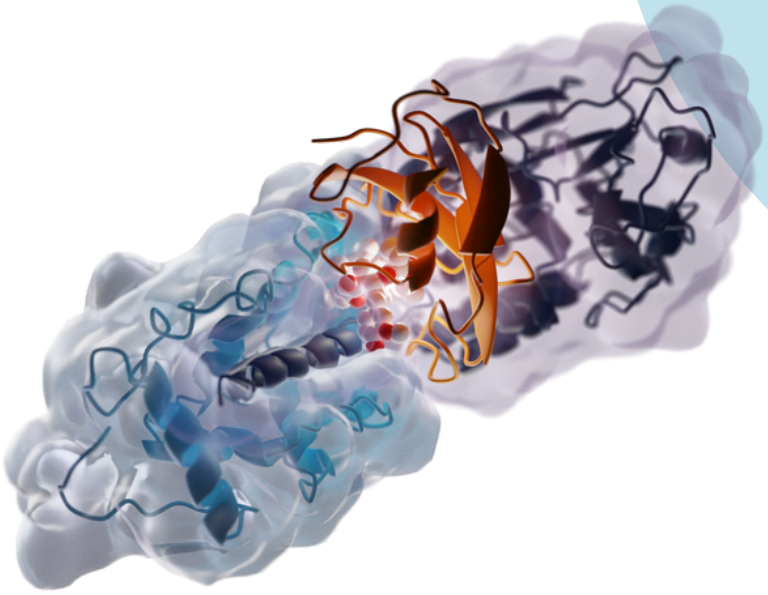
Structural Biology Services

Fast Track Your Discovery Pipeline with Atomic-Level Insight

In today's biotech landscape, early-stage drug developers face relentless pressure to achieve more with less: tighter timelines, reduced funding, cautious investors, and an increasing demand for robust, early proof-of-concept data to unlock the next round of support. Structural biology and biophysics, expertly applied, can deliver the deep mechanistic insights and high-quality data needed to make faster, smarter decisions, reducing risk, building confidence, and delivering value at every stage of the discovery critical path.



Unlock the Power of Structural Biology in Drug Discovery

Structural biology provides the molecular-level understanding necessary to de-risk and accelerate your drug discovery programs. By elucidating the 3D structure of your target proteins and their complexes with ligands, we enable informed decision-making across hit identification, lead optimization, and candidate selection.

At the Oncodesign Services-ZoBio Group, we partner with you to turn complex biology into clear, actionable answers, helping you move forward with certainty, even in uncertain times.

Why Incorporate Structural Biology and Biophysics into Your Program?

- **Structure-Based Drug Design (SBDD): Guide medicinal chemistry through detailed atomic interactions.**
- **Target and Mechanism Validation: Confirm ligandability and binding modes.**
- **Risk Reduction: Minimize late-stage failures due to unexpected binding or poor selectivity.**
- **Efficiency: Prioritize the most promising chemical series early, reducing costs and timelines.**

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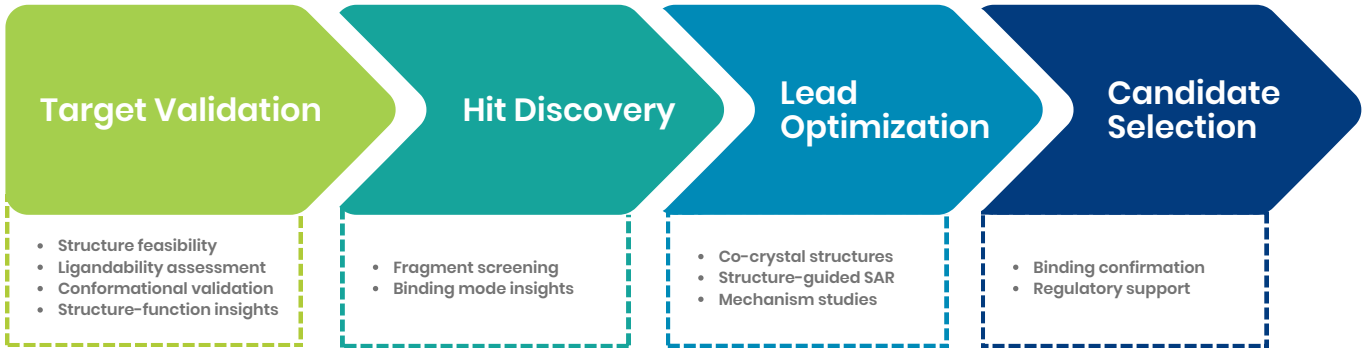
The Role of Structural Biology in the Drug Discovery Pipeline

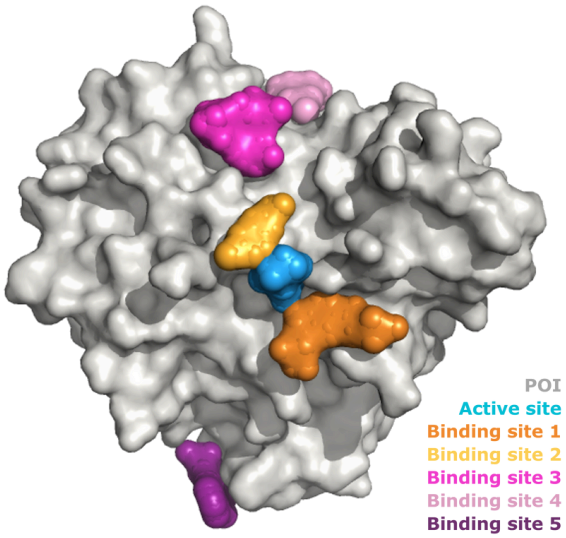


Our Structural Biology Capabilities

We offer a comprehensive suite of services, fully tailorable to your research objectives and challenges:

- X-ray Crystallography
- Cryo-Electron Microscopy (Cryo-EM)
- NMR-based Structure Determination and Structural Analysis
- Computational Modeling and Molecular Dynamics
- Protein-Ligand Interaction Characterization

Our structural biologists support a diverse spectrum of small molecule drug discovery projects, including work with challenging and 'undruggable' targets, and well-profiled targets requiring a novel approach.



Above: *A crystallography-enabled fragment screening campaign identified chemically diverse hits and uncovered multiple binding pockets, opening the door to developing active site inhibitors and exploring alternative routes such as targeted protein degradation.*

Our Technologies: Key Advantages for Drug Discovery

Technology	Key Advantages
X-ray Crystallography	High-resolution, atomic-level structural insights to support hit discovery, lead optimization, and mechanistic understanding.
Cryo-Electron Microscopy	Ideal for large dynamic targets or complexes, enabling structure determination without the need for crystals.
NMR Spectroscopy	Provides dynamic, structural and interaction data in solution.
Biophysical Assays	Rapid assessment of binding kinetics, affinities, and mechanism of action in real time.
Computational Modeling	Integrates experimental data to predict structures, binding modes, and guide compound design.

Validating Structural Insights with Biophysics

Determining a protein structure is only part of the journey.

To confidently prepare for and progress medicinal chemistry, structural findings must be validated through robust, quantitative biophysical data. We integrate biophysics into our structural biology workflows to confirm binding interactions, explore mode of action, and strengthen the link between structure and activity.

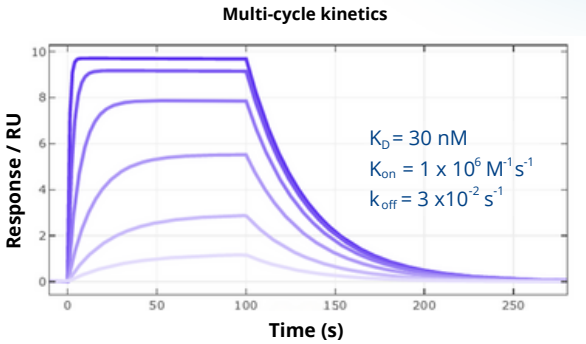
Biophysical assays provide essential confirmation of:

- **Binding events** to verify ligand engagement and affinity
- **Mechanistic insights** to clarify how molecules interact with targets
- **Structure-function relationships** to validate that the structure reflects biologically relevant states
- **Compound prioritization** by combining structural and kinetic data for SAR

Techniques such as Surface Plasmon Resonance (SPR), Nuclear Magnetic Resonance (NMR), Fluorescence-based assays (e.g., TR-FRET or FP), and Thermal Shift assays (TSA) are applied strategically to generate orthogonal evidence and reduce ambiguity.

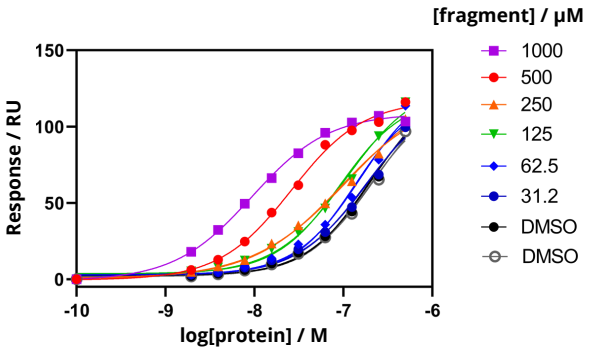
By combining high-resolution structure with validated activity, we help you make informed Medicinal Chemistry decisions, increasing the efficiency of your workflow and lowering risk.

Binding Events



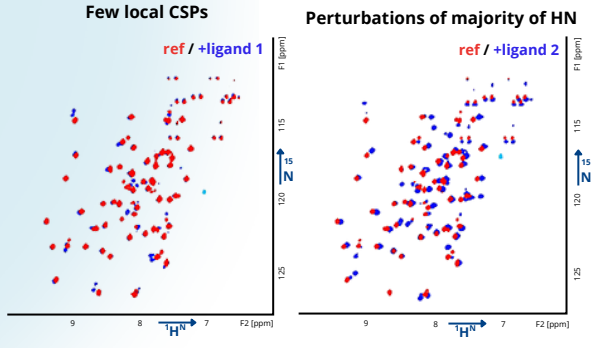
Binding Events Example Readout: *An example of a typical SPR sensorgram. Binding is observed here using multi-cycle kinetics through the injection of an analyte (small molecule) at increasing concentrations ranging from 4 nM to 1 µM, with full dissociation monitored for 150 seconds after each injection. Combining high sensitivity with high throughput, SPR is a leading technique, not only to confirm binding events but also to obtain kinetic and affinity information throughout a drug discovery campaign.*

Mechanistic Insights



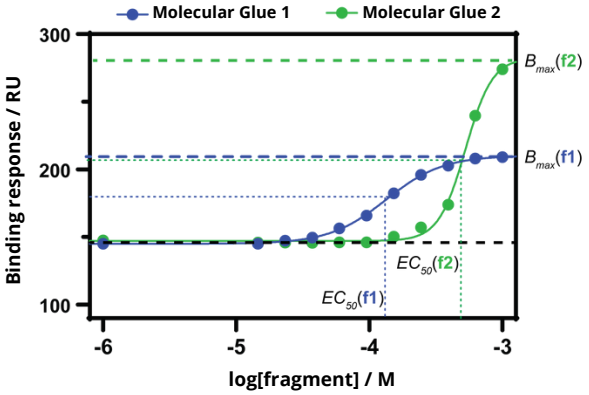
Mechanistic Insights Example Readout: *2D SPR titration to characterize ternary complex formation. Here, one protein is immobilized, and each curve represents titration of a partner protein at a fixed concentration of a fragment. Increasing the concentration of the fragment shifts the affinity for the partner protein to the left, a hallmark of molecular glues. Combining this type of assay with mathematical models provides biophysical insights into underlying molecular interaction mechanisms, such as cooperativity.*

Structure-Function Relationships



Structure-Function Relationships Example Readout: *2D NMR spectra of covalent ligand-protein complexes. The spectrum of apo protein (red) is overlayed with the spectrum of protein conjugated to covalent ligands (blue). Ligand 1 shows only a few peaks shift between the two spectra indicating a minimal interaction of the compound with the protein. Ligand 2's large number of peaks shift shows a good interaction between compound and protein. These information-rich experiments confirm the presence of non-covalent interactions but can also detect heterogeneity in the ligand and non-druglike interactions, supporting structure-function studies for rational compound optimization.*

Compound Prioritization



Compound Prioritization Example Readout: *Dose response curves of two molecular glues to determine potency (EC_{50}) and the change in maximal amount of protein-protein complex induced by the glue (B_{max}). While glue 1 (blue) has stronger potency, glue 2 (green) results in greater concentration of the complex when binding of the compound is saturated. Biophysical readouts of this nature enable quantitative compound ranking and prioritization for hit-to-lead and lead optimization efforts.*

The Importance of High-Quality, Integrated Protein Science

Successful drug discovery depends on more than having access to protein – it requires high-quality, fit-for-purpose protein science, integrated with your project's needs from the outset. Poorly characterized or unstable proteins waste time, mislead decision-making, and put programs at risk.

We deliver tailored, expert solutions to produce, characterize, and supply the right form of protein for your assays, biophysics, or structural studies. From challenging targets to routine supply for DMTA cycles, we ensure consistency, stability, and compatibility. Our protein sciences team works with you to design a tailored strategy, from choosing the optimal expression host to delivering targeted QC, ensuring the right protein is paired with the right assay to facilitate the best results.

What sets us apart:

- **Scientific partnership mindset** underpinned by transparency, flexibility, and clear communication
- **Creative, problem-solving approach** to complex targets
- **Detailed QC and reporting** to build trust and reduce downstream risks

Our knowledge and experience in protein science delivers not just material, but confidence, providing a solid foundation for both your studies and your discovery decisions.

The Foundation of Fit-for-Purpose Protein

One of the critical factors that determines the success of your downstream assays, structural studies, and screening campaigns is choosing the right expression system to produce the protein target. We evaluate each target's complexity, functional requirements, and end-use to recommend the optimal host (whether E. coli or mammalian) ensuring your protein is best fit for purpose.

Key Deliverables and Their Value

Our structural biology services deliver actionable insights at every stage of your project. Deliverables are aligned to your program's milestones, ensuring relevance and impact for decision-making and funding rounds.

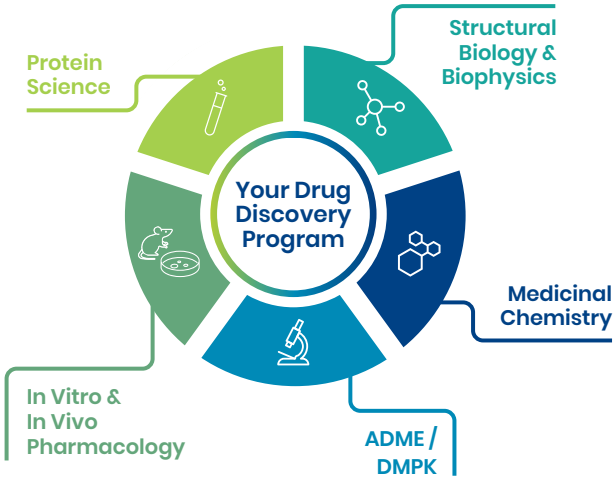
Deliverable	Value to Your Program
High-quality protein and protein-ligand structures	• Support ligandability assessment and visualize key binding interactions, de-risking chemistry by providing insights into targets and driving structure-based drug design (SBDD).
Molecular modeling reports	• Accelerate hypothesis generation and compound design, supporting speed into lead optimization. • Virtual exploration, reducing wet lab iterations to conserve chemistry resources and experimental lead time.
Protein-Ligand interaction characterization	• Mechanistic insights, characterization of binding kinetics and affinities, strengthening the link between structure and activity.
Expert interpretation & recommendations	• Translate data into next-step strategies.

Why Partner with the Oncodesign Services-ZoBio Group?

In a space crowded with generic offerings, real innovation and quality science demands more. We aim to be the partner who doesn't just deliver data, but helps drive decisions and confidence with deep scientific insight, tailored strategy, and seamless integration into your program.

We're not aiming to be the biggest CRO you work with. Our goal is to be the most **collaborative**, **responsive**, and **scientifically precise** partner at the earliest and most critical stages of your pipeline:

- **Integrated Expertise:** From protein production to structure elucidation and data-driven project guidance.
- **Track Record of Success:** Trusted by leading pharma and biotech companies globally.
- **State-of-the-Art Platforms:** Access cutting-edge technologies, including cryo-EM, synchrotron sources, advanced biophysics and virtual screening.
- **Seamless Integration:** Structural biology fully embedded within a comprehensive drug discovery platform, including medicinal chemistry, ADME/DMPK, *in vitro* / *in vivo* pharmacology, and more.
- **Creativity and Flexibility:** Tailored program design and resource allocation to meet unique scientific challenges, timelines, and budgets.
- **Agility and Responsiveness:** We offer the flexibility and pace needed in biotech programs, backed by the depth of experience and scientific discipline trusted by big pharma.
- **Collaboration Without Compromise:** Our partnership-oriented ethos ensures transparency, scientific alignment, and respect for your autonomy.



Next steps

When you're ready to learn more, you can request an informal conversation with our team, in which we'll learn a little more about your objectives, answer any questions you might have, and provide you with the information you need to decide whether to move forward.

Reach out to your relationship manager or contact us at:

- **oncodesign-services.com**
- **contact@oncodesign-services.com**

More information

Oncodesign Services is a leading CRO specializing in drug discovery and preclinical services. In 2024, it acquired ZoBio, a boutique CRO with gene-to-lead expertise in small molecules. The Oncodesign-ZoBio Group contributes to the development of innovative therapies from target to preclinical candidates through stand-alone and integrated capabilities in medicinal chemistry, computer-assisted drug design, protein production, biophysics, structural biology, ADME/DMPK, in vitro / in vivo pharmacology, and in vivo pharmaco-imaging.

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