NUVISAN
The Science CRO

Interested in structural biology support tailored to your project neaeds?
Have a look at our established and ready-to-go crystallization systems

Structural Biology Platform at Nuvisan ICB

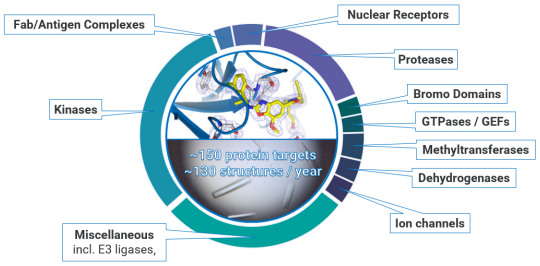
Protein Structure Determination, Cryo-electron Microscopy, HT X-ray, NMR Spectroscopy

NUVISAN ICB GmbH, Muellerstr. 178, 13353 Berlin, Germany

Protein Structure Determination

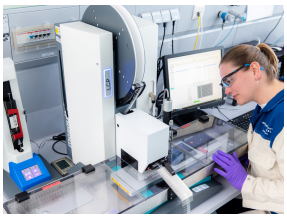
The NUVISAN **structural biology team** supports **industrial drug discovery programs**, identifying and implementing the optimal strategy to deliver **timely and high-quality 3D-structural data**

- >20 years experience **enabling** the entire **gene-to-structure** process for a **broad range** of **target classes**:



Tailored structural biology services enable structure-based drug discovery:

- ***De-novo*** structure determination, **optimization** of literature targets for industrial crystallography and our own proprietary **Xrays2Go**
- **Close interaction with design teams** to maximize learning from the structural data and to guide the **rational molecule design** of improved molecules



Our state-of-the-art crystallization platform includes:

- Liquid-handling systems for **crystallization screen preparation** of **broad panel of proprietary and vendor screens**
- Nanoliter liquid-handling machines (including **humidity control box**) for **accurate drop setting** for protein samples including specialized **membrane protein liquid cubic phase (LCP) platform**
- **Automated imaging systems** (visible and UV) at 4°C and 20°C for plate inspection.
- **Bi-weekly access to third-generation high-brilliance synchrotron sources**, complemented with our in-house automated crystal screening sample changer and two X-ray sources.

NMR Spectroscopy

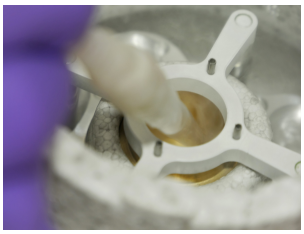
NMR is a highly versatile technique that can support a range of drug-discovery activities. We offer:

- **Protein-observed NMR**, as a robust and information-rich NMR method to validate and characterize compound binding.
- **Ligand-observed NMR**, as a method of choice for target engagement studies with larger targets and/or targets for which no labeling scheme is available.
- NMR-based **fragment-screening** as a powerful method in the field of fragment-based drug discovery, for hit identification or characterization of more advanced fragment analogs.

Cryo-Electron Microscopy

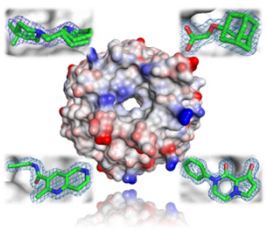
We offer a range of cryo-EM solutions **tailored to fit your needs**, including:

- stand-alone EM packages, such as **negative-staining EM**, to confirm sample quality.
- adaption of literature-described cryo-EM structure-determination methods to deliver **target-ligand complex structures**.
- complete gene-to-high-resolution-structure determination for new targets.
- Typical cryo-EM targets include **membrane proteins**, protein-protein & nucleic-acid protein complexes, Fab-antigen complexes.



HT X-ray Platform

HTX fragment screening is a powerful technique for detecting and elucidating the **binding mode of very weak binders**. Our HTX workflow is fully integrated into our internal structural biology platform and allows for fast and efficient screening of **up to 1,000 fragments**.



- **Echo Acoustic Liquid Handler** for soaking large number of HTX fragments into crystals
- **Crystal Shifter** used for freezing crystals for data collection.
- Visual Basic scripts allow for **reliable data tracking** throughout the complete workflow.
- **Fast and reliable crystallographic data collection** through continuous access to high-brilliance synchrotron sources.
- In-house **proprietary data analysis pipeline**, including **PanDDA**, enables quick identification of datasets with a high likelihood of fragment binding.

Selected literature

Roehrig, S. et al. Design and Preclinical Characterization Program toward Asundexian (BAY 2433334), an Oral Factor XIa Inhibitor for the Prevention and Treatment of Thromboembolic Disorders. J. Med. Chem. 66, 12203–12224 (2023).

Günther, J. et al. BAY-069, a Novel (Trifluoromethyl)pyrimidinedione-Based BCAT1/2 Inhibitor and Chemical Probe. J. Med. Chem. 65, 14366–14390 (2022).

Orsi, D. L. et al. Discovery and Structure-Based Design of Potent Covalent PPARγ Inverse-Agonists BAY-4931 and BAY-0069. Journal of Medicinal Chemistry 65, 14843–14863 (2022).

Hillig, RC., et al., Discovery of potent SOS1 inhibitors that block RAS activation via disruption of the RAS-SOS1 interaction. PNAS (2019).

Schaefer, M., et al., Allosteric Inhibition as a New Mode of Action for BAY 1213790, a Neutralizing Antibody Targeting the Activated Form of Coagulation Factor XI. JMB (2019).