

**NUVISAN**



*DRUG DISCOVERY*

# **Digital Life Sciences**

[www.nuvisan.com](http://www.nuvisan.com)

# DIGITAL LIFE SCIENCE EXPERTISE



## Bioinformatics

- *In silico* target prediction
- Omics Data analysis & interpretation

## 10X GENOMICS CERTIFIED SERVICE PROVIDER



Single Cell Gene Expression & Single Cell Immune Profiling



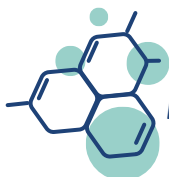
## MOLECULAR MODELING

support from early druggability to lead optimization campaigns



## STATE-OF-THE-ART

Data Science Technology under *FAIR Data Principles*



**3 million compound library with 1 billion *in vitro* / *vivo* data points**

High throughput screening, virtual screening & data mining

## QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP (QSAR) & MACHINE LEARNING (ML)

MODEL DEVELOPMENT FOR ACTIVITY, DMPK & PHYSCHEM PROPERTY PREDICTION



## Our Digital Science For Drug Discovery

At NUVISAN, we believe that data is at the very core of the drug discovery process. Our team of digital experts works closely with our clients to implement the most suitable strategy for a new target identification, hit finding, or lead optimization program. With decades of pharma expertise, NUVISAN uses computer-aided drug design approaches to deliver the next blockbuster drugs by leveraging the latest digital technologies together with the in-house Life Science Database to accelerate and guide scientific decisions. We offer:

- A **highly multidisciplinary team** collaborating across the functions, using state-of-the-art digital technologies, committed to the FAIR data principles
- Experienced partner for the **omics data analysis and interpretation**, as well as bioinformatics expertise for *in silico* target and indication space evaluation
- Our Life Science Database contains **3 million well-characterized compounds** associated with ~1 billion *in vitro* and *in vivo* data points
- We apply molecular modeling to support projects **from early druggability analysis and hit finding**, to hit-to-lead and lead optimization campaigns
- Fine analysis of chemical matters, including **QSAR and ML/AI model development** for different ADME endpoints is supported by our cheminformatics team

BIOINFORMATICS



CHEMINFORMATICS  
& MACHINE LEARNING



LIFE SCIENCE  
DATABASE



MOLECULAR  
MODELING





# From Target Identification to Novel Chemical Matter



## Bioinformatics

We facilitate integrated design, implementation, and data analysis for target validation or biomarker discovery by employing state-of-the-art data science methods including data mining, multivariate statistics, data visualization, and machine learning. Application fields include:

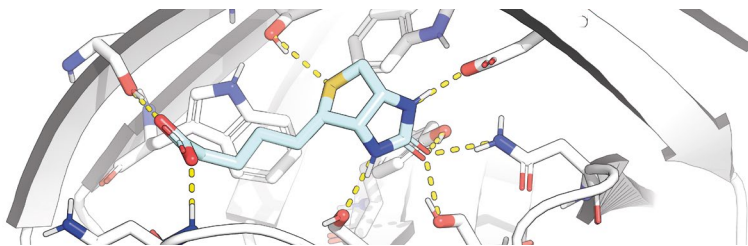
- Transcriptomics, genomics, and epigenomics
- High-content cellular assays
- *In silico* target and indication space evaluation



## Cheminformatics & Machine Learning

Our data platform enables efficient screening, prediction of efficacy and safety, and design/optimization of new chemical series. Get ahead of competition with cutting-edge approaches for:

- Mining Life Science Database
- QSAR modeling
- ML physchem and DMPK endpoint prediction
- AI-powered de novo generative molecular design



# Data Driven Molecule Generation



## Life Science Database (LSDB)

NUVISAN'S proprietary LSDB is built on decades of pharma research and contains 3 million unique molecules associated with ~1 billion experimental data points covering biological activity, physchem, DMPK endpoints and more. We rely on LSDB for:

- Analyzing data for hits identified through high-throughput screens
- Data mining and virtual screening approaches



## Molecular Modeling

Accelerate projects from hit finding to lead optimization by predicting the behavior of potential drug candidates & optimize their properties before synthesis & testing with cutting-edge computer-aided drug design techniques:

- Binding pocket identification and druggability assessment
- Ligand- and structure-based virtual screening
- Docking and molecular dynamics simulations
- Multi-parameter optimization in Design-Make-Test-Analyze (DMTA) cycles

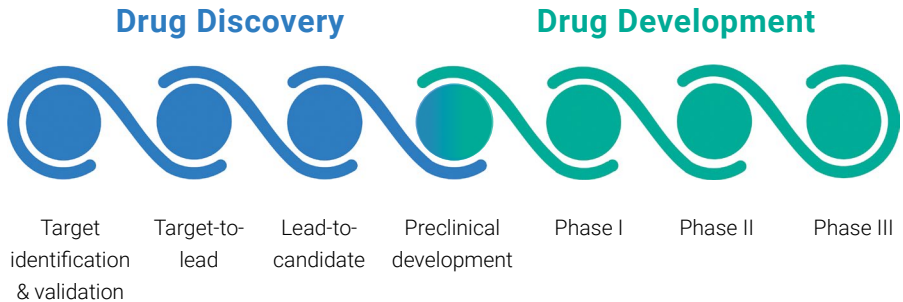


## The Science CRO - From Target to Patient

The NUVISAN group is a contract research and development and manufacturing organization (CRO/CDMO) with six sites in Germany and France as well as local experts situated in Latin America.

We offer unique, high-quality, and tailored integrated solutions along the drug discovery and development value chain to our biotech startup, pharma, non-profit, and venture capital clients – from target identification to the patient.

Thanks to more than 40 years of experience and about 1,000 employees (incl. > 70 % industry experienced scientists and lab professionals), we know how to discover, develop, and bring the next generation medicines to market. At the same time, our scientists understand that every project is different. With a flexible and innovative approach and transparent communication, our teams are passionate about closely collaborating with you to adapt to your individual needs.



### Contact us



**Dr. Dusan Petrovic**  
**Head of Digital Life Sciences**  
dusan.petrovic@nuvisan.com

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



**Christoph Sachse**  
**VP Business Development**  
christoph.sachse@nuvisan.com

Web: [www.nuvisan.com](http://www.nuvisan.com)  
Email: [hello@nuvisan.com](mailto:hello@nuvisan.com)  
LinkedIn: [company/nuvisan](https://www.linkedin.com/company/nuvisan)