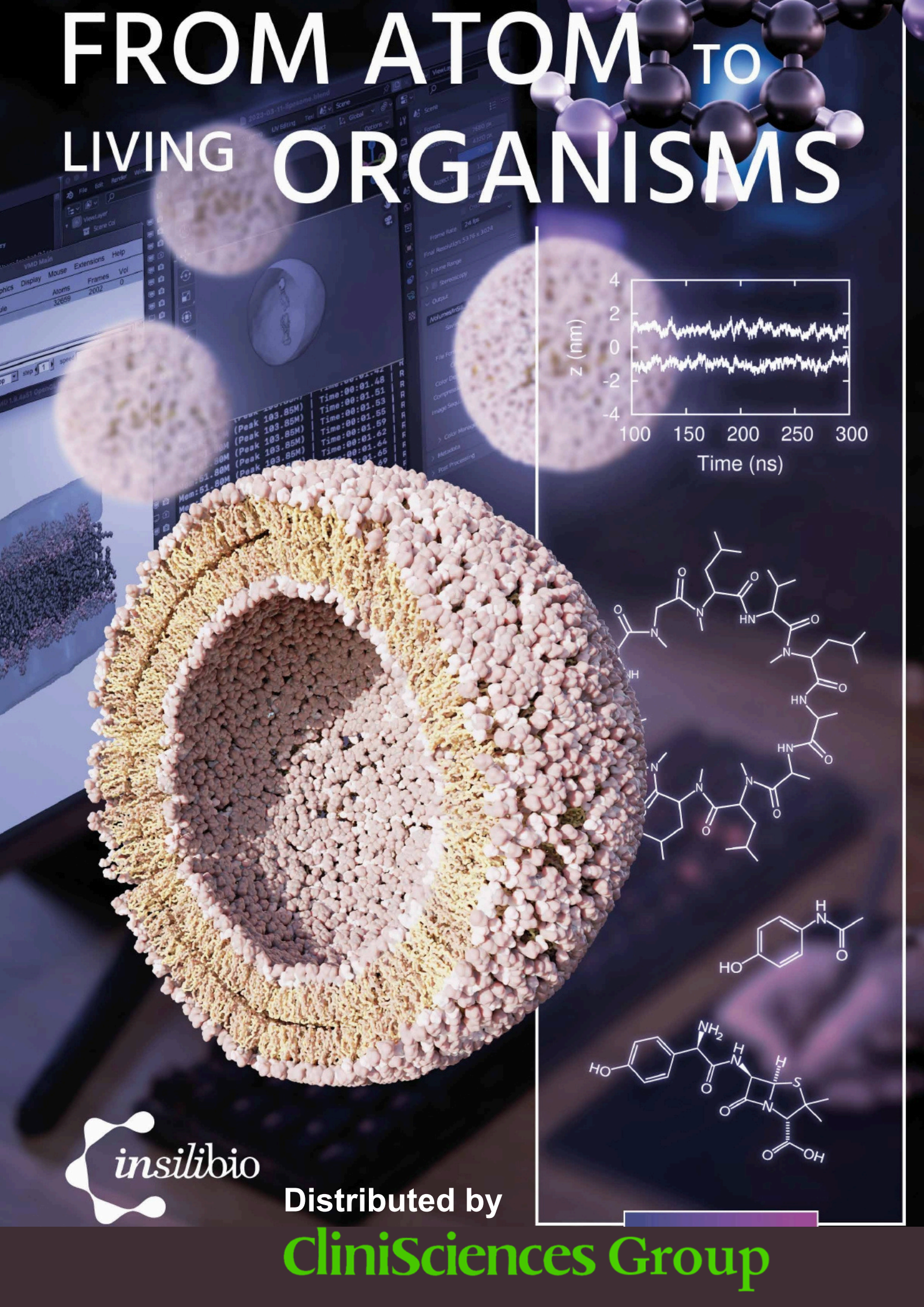
# FROM ATOM TO LIVING ORGANISMS

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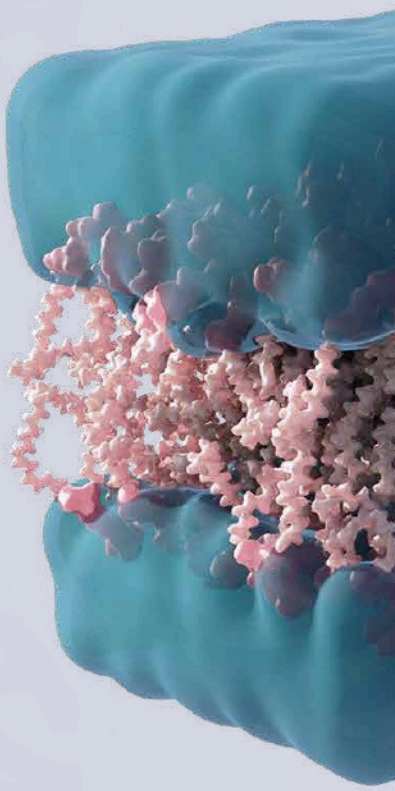
# InSiliBio, molecular modeling for your R&D...

InSiliBio is a wonderful toolbox of **innovative digital techniques** for performing molecular modeling simulations. We support the R&D of our partners and customers by **understanding mechanisms of action** related to biological activities, and by highlighting key processes at the molecular level.

InSiliBio gathers experts in **molecular modeling**. **Reliable methods** and methodologies are employed to study:

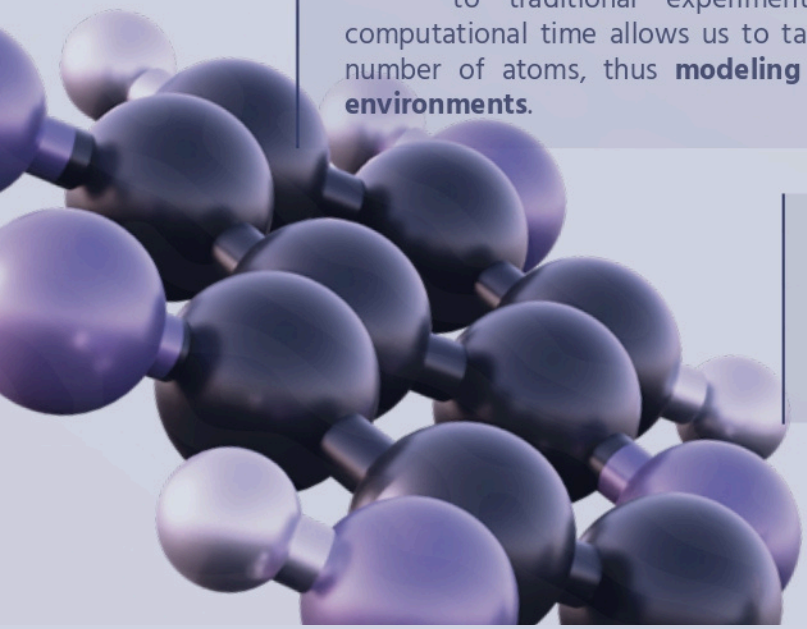
- Molecule - membrane interactions
- Drug carriers
- Intermolecular interactions
- Protein - ligand interactions



InSiliBio calculates highly **reliable physical chemical descriptors** of a wide range of drugs. InSiliBio's experience is based on more than 20 years of academic research, developed with the systematic aim of **correlating theoretical data with experiments**. The atomic resolution of our data is virtually impossible to reach experimentally.

InSiliBio's solutions are less expensive than most experiments. The use of high-performance computing avoids the need for large laboratory infrastructures. The optimization and automation of our methodologies of molecular simulations are an endless way to **reduce costs**, while maintaining and even **improving, data accuracy**.

InSiliBio's solutions are **faster than** most of **experiments**. By using our own computing power and optimized methodologies, we can save time with respect to traditional experiments. Moreover, this continuous optimization of computational time allows us to tackle molecular systems with a greater and greater number of atoms, thus **modeling** biological systems closer and closer to **realistic environments**.



InSiliBio's methods are free from any ethical constraints and can even drastically **reduce animal experimentation**. By acting upstream of experiments, InSiliBio supports R&D by better **focusing** on key steps of **development**.

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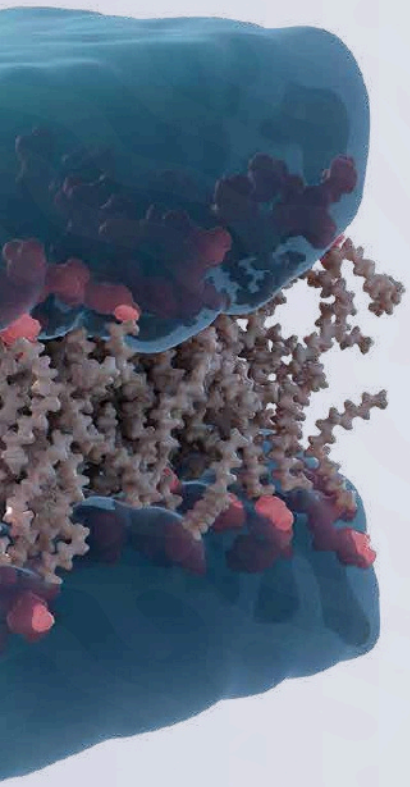
# Technology and capabilities

## Molecule-membrane interactions



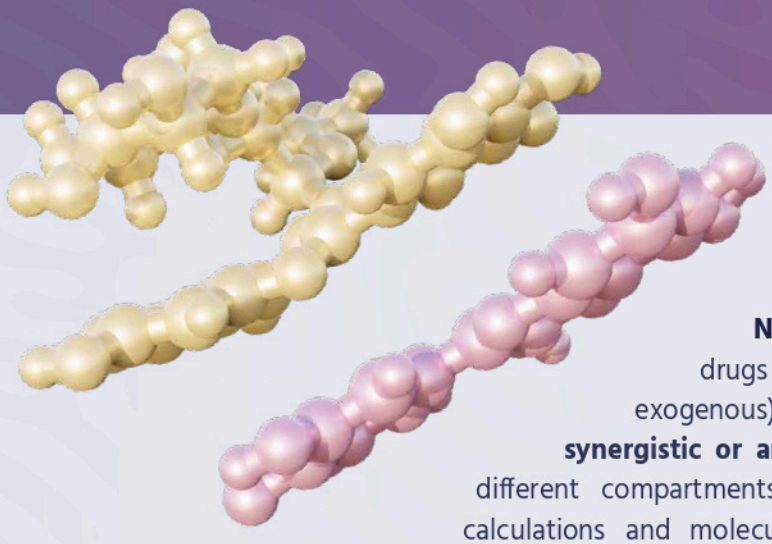
Membranes are important compartments of cells and organelles. They consist of **lipids arranged in bilayers** with embedded proteins, cholesterol, carbohydrates and various other specific ingredients. Membranes are **highly dynamic**, diverse in composition and diverse in physical-chemical properties. Molecule-membrane interactions and crossing events are **key steps in drug pharmacokinetics**. Based on in silico methods, InSiliBio creates and simulates the dynamics of molecular membrane models with **customized lipid compositions** and environmental conditions, specific to different organisms, organs, and organelles.

Molecular dynamic simulations performed at InSiliBio evaluate **insertion, diffusion and membrane crossing** of molecules. Several related parameters can be calculated including **molecule position** and **orientation** of drugs, and impact on the surrounding membrane (*e.g.*, thickness, **order parameter**, area per lipid, and hydration). These simulations shed light on the mechanisms underlying drug-membrane interactions and crossing events at an atomic resolution. The use of **artificial intelligence** tools can enhance data analysis and help uncover hidden information.

## Drug carriers

Drug carriers are a matter of intense development in pharmaceutical formulation. They allow better control of **drug** stability, **delivery** and bioavailability. They are key to improving treatment efficacy and acceptance, especially through better control of dosage.

By using quantum chemistry calculations and molecular dynamic simulations, InSiliBio simulates the conformational and dynamic behavior of **peptides, liposomes, nanoparticles** and various other drug carriers. The drug delivery process can also be rationalized by studying the interactions between biological membrane models and the drug carriers. The **mechanism** of **drug release** can also be elucidated at this stage. The structure-property relationships that can be established provide chemical recommendations to improve drug transport and delivery.



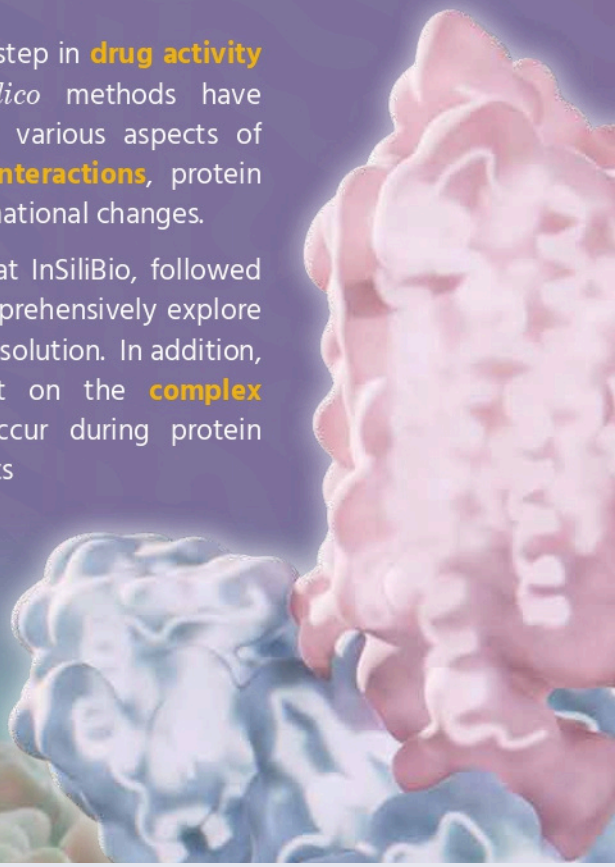
## Intermolecular interactions

**Non-covalent intermolecular interactions** between drugs or between drugs and other (endogenous / exogenous) compounds can drive biological actions, in particular **synergistic or antagonistic effects**. Such interactions can occur in different compartments, more or less hydrophilic. Quantum chemistry calculations and molecular dynamic simulations provide highly accurate descriptions of physical-chemical properties of drugs and help to gain insight into such intermolecular interactions. The **driving forces** of these interactions are often crucial **to rationalize biological properties**.

## Protein-ligand interactions

Protein-ligand interaction is a key step in **drug activity** and **pharmacodynamics**. *In silico* methods have become highly efficient to study various aspects of protein activity, **ligand-protein interactions**, protein **polymorphisms**, and large conformational changes.

Molecular simulations performed at InSiliBio, followed by in-depth analyses, help to comprehensively explore these different aspects at atomic resolution. In addition, *in silico* simulations shed light on the **complex conformational changes** that occur during protein binding / unbinding. This supports the development of more effective drugs and therapies that target specific proteins and related functions.



# ... from questions to conclusions

## Problematic

We start by meeting with our experts in physical-chemistry and molecular modeling to discuss your problem. Together, we **propose solutions** to unravel the molecular interactions that give rise to the biological action of your active compounds.

## Conceptualization

The **feasibility** and milestones of the project are established. The size of the molecular systems and the **achievable goals** are discussed with you at an early stage. This is followed by a detailed proposal... at an atomic scale!

## 3D modeling & parameterization

This is a crucial step aimed at **defining accurate parameters** (molecular flexibility, atomic properties, T and p, molecular environment...) to mimic as closely as possible the experimental **realistic conditions**. Any drawbacks will be discussed with you.

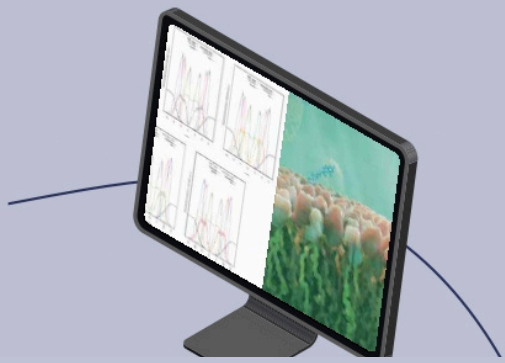
## Our computing power at your service

The calculations are achieved on **our supercomputers**. The simulation time depends on the size of the molecular system and the time-scale of the chemical and biological processes under investigation.
The **behavior** of the molecular assemblies is **monitored daily**, to optimize the simulation time and further data mining.

## Scientific & commercial deliveries

A thorough analysis of the data (sampling of numerous molecular events) **unravels your scientific problem** and InSiliBio delivers:

- **Scientific reports** & oral presentations
- Fascinating **3D visualizations** (images and videos)
- **Virtual reality** experience



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