

nostrum
biodiscovery

ONE STEP AHEAD IN MOLECULAR DESIGN

THE ORIGINS OF NOSTRUM

BORN FROM WORLD-CLASS RESEARCH

An in silico company that has pioneered an industry-leading suite of **AI-enhanced molecular modeling** and computational tools to design and optimize **next-generation therapies** and biotech products





nostrum biodiscovery

CO-FOUNDER

President

Prof. Modesto Orozco

CO-FOUNDER

CSO

Prof. Victor Guallar

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OUR TECHNOLOGY:

Discover

Targets & **assets**

Combine AI speed with physics-based accuracy for unmatched screening efficiency

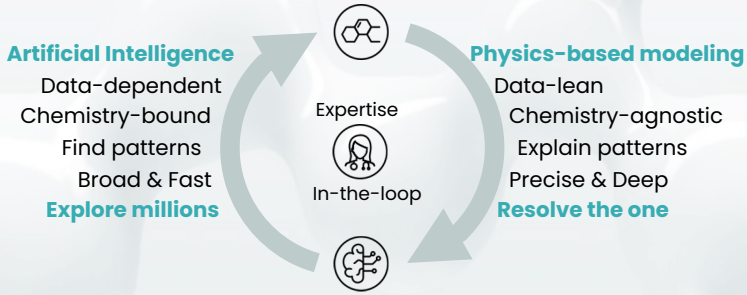
Design

Ultra-large libraries screening, fragment growing,

Tailor-made proteins, ligands or nucleic acids

Optimize

Accelerate multi-parameter optimization — activity, specificity, ADMET, and beyond



Physics-grounded. AI-accelerated. Human-guided.

WHAT WE DO

ONE-STEP AHEAD IN MOLECULAR DESIGN

Physics meets AI. We combine and tailor proprietary AI algorithms with **physics-based molecular modeling** to validate every result and to rationalize and understand our outcomes for an unprecedented success level for our partners' challenges

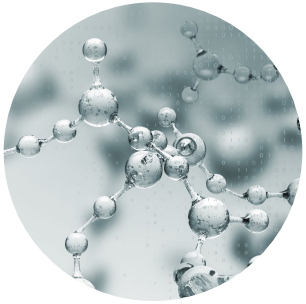
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OUR SPECIALTY AREAS



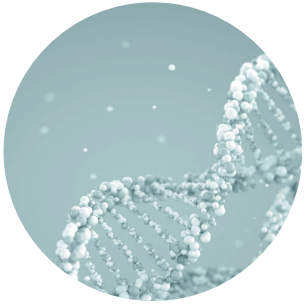
SMALL MOLECULES

Screen, design and optimize small molecules, macrocycles, molecular glues and degraders (TPD) for complex targets



PROTEIN ENGINEERING

Bioprospecting, design and engineering of enzymes, peptides, vaccines, antibodies and protein binders



NUCLEIC ACIDS

RNA/DNA design and chemically modified NAs: ASOs, siRNAs, aptamers and RNA vaccines

Our Flagship Platforms

Proximity inducers
PELEGLUE™ PELETAC™

Polypharmacology
POLYPLAT™

Bi-active enzymes
Plurizymes™

Protein binders & vaccines
NostrumBiologics

RNA software
XNAhub™

Language models
ChaRNAbert

130
targets modelled
across oncology, immunology and infectious disease

45
protein families
from kinases and GPCRs to antibodies

18
peer-reviewed papers
from our AI department

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COMMERCIAL VALIDATION FROM GLOBAL DRUG DEVELOPERS

Our scientific excellence is **proven by the clients who trust us**

220+
Projects delivered

98
Total clients

29
Active clients

90%
Success rate

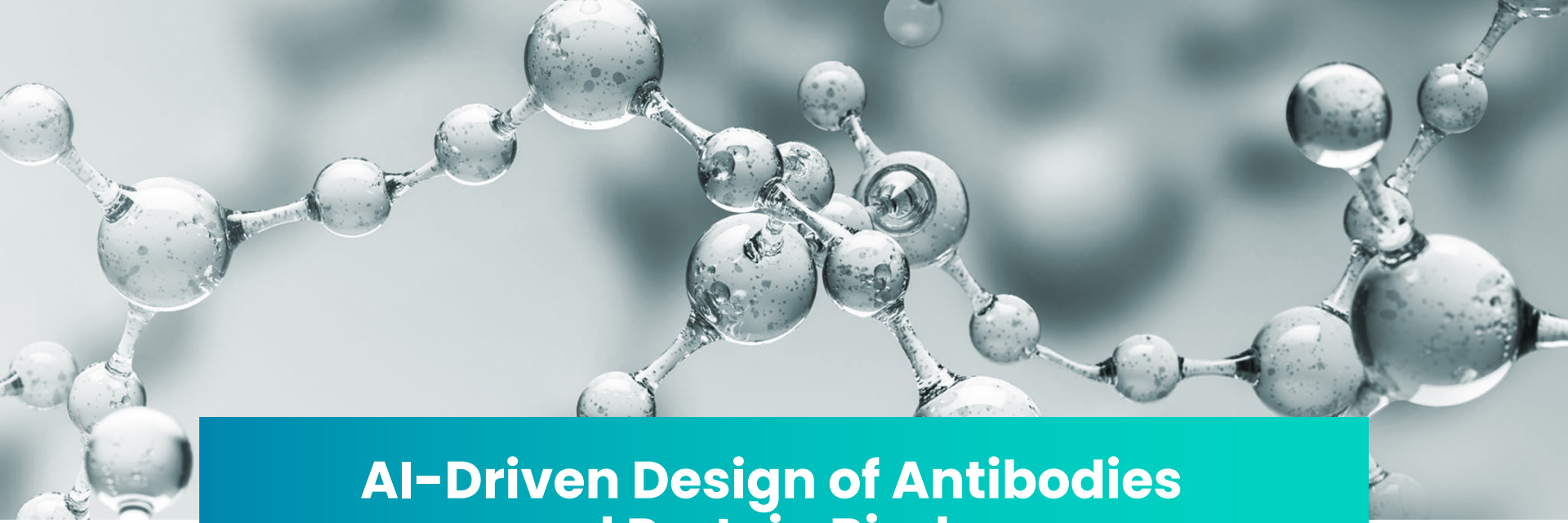
5 top-10 big pharma



Barcelona HQ & Boston office

NOVARTIS · janssen · AMGEN · sanofi · ENSEM THERAPEUTICS · senolytx · GSK · Superluminal MEDICINES · werfen · P&G · Chiesi · Navigo Proteins PURE PRECISION · AstraZeneca · almirall feel the science

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AI-Driven Design of Antibodies and Protein Binders

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END-TO-END ANTIBODY DISCOVERY

We cover the full pipeline: **from target discovery to antibody design, de-risking and ranking**

STEP 1

Target discovery

In-house tools rank human genes with knowledge graphs to uncover new targets for specific diseases

STEP 2

De novo design / affinity maturation

Generative AI designs new binders and matures existing ones for the proposed targets

Abs, VHHs, VNARs, bispecifics and any protein binder

STEP 3

Design de-risking

Predictive tools flag aggregation, toxicity, off-target reactivity and immunogenicity in every sequence, so we de-risk our designs early

STEP 4

Validation & ranking

With physics-based simulations, we can rationalize how each candidate interacts with its target, so we can rank and prioritize the best ones



<40 sequences

are all our clients need to reach an optimal antibody candidate

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STEP 1 STEP 2 STEP 3 STEP 4

TARGET DISCOVERY WITH YGGDRASIL

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Yggdrasil, our in-house tool, organises biological knowledge as a graph of **13 node types and 28 relationship types**: transcripts, genes, proteins, gene ontology terms, tissues, variants, phenotypes, pathways and molecules.

It uses this graph to **uncover meaningful paths between diseases, compounds and targets**.

THE GRAPH CONTAINS

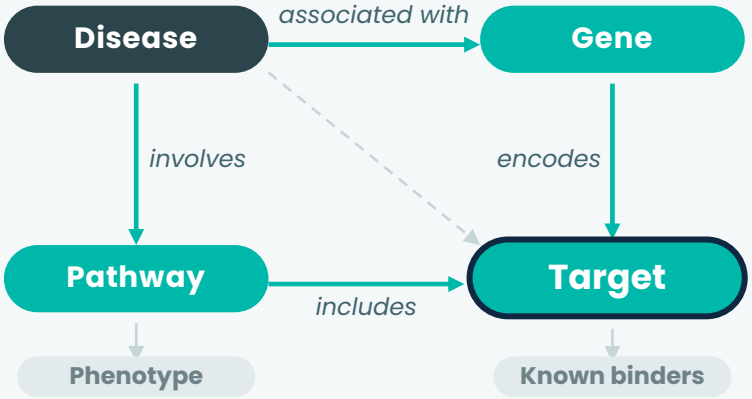
2.47 M

Entities: diseases · targets · compounds

56.82 M

biological and chemical relationships

EXAMPLE PATH FOUND BY YGGDRASIL



Yggdrasil scores every disease-to-protein path and **ranks the strongest candidate targets**

Graph contents

ChEMBL · PubChem · OpenTargets · BindingDB · ChEBI · Mondo

Biological question

Start from a disease or therapeutic context

Yggdrasil search

Explore paths and score candidates

WHAT YOU GET

Ranked outputs

Prioritised targets with reviewable evidence

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DE NOVO DESIGN & AFFINITY MATURATION

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With generative AI we design new binders for your target, using **proprietary and 3rd-party models**

WHAT THE MODELS PRODUCE

Backbones docked on the target epitope, and the amino-acid sequences that fold into them and bind

OUR MODEL TOOLKIT

Antibody Language Models

Proprietary & 3rd party software

Learn antibody language to generate and refine natural-like sequences

AntiBERTy · AbLang · ESM3

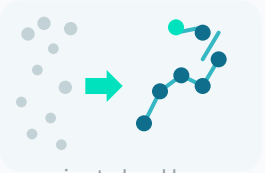


Diffusion Models

3rd party software

Generate new backbones directly on the target epitope

RFDiffusion · RFAntibody

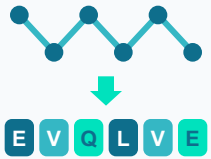


Inverse Folding Design

3rd party software (own weights)

Design the sequences that fold into each generated backbone

proteinMPNN · AntiFold · NostrumAbMPNN



Integrated Pipelines

3rd party software

Co-design the binder's structure and sequence in a single run

BoltzGen · AnewOmni



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DESIGN DE-RISKING

Predictive tools flag **aggregation, toxicity, off-target reactivity and immunogenicity** before synthesis

SEQUENCE LIABILITIES
Aggregation and CDR-loop flexibility scored per design

IMMUNE RISK
Germline distance and T-cell epitope hotspots

Aggregation prediction
In-house tool
Scores how likely each design is to aggregate, straight from the H and L chain sequence

Output: **Aggregate / Not aggregate**

Immunogenicity prediction
In-house tool
Measures how close each heavy-light pair sits to the human germline V-gene (FR1-FR3)

Output: **Low / High risk**

Flexibility prediction
In-house tool
Predicts CDR-loop flexibility, both for the loop alone and with its flanking residues

Output: **Rigid / Flexible**

T-cell epitope prediction
In-house tool (PredIG)
Predicts peptide binding to MHC and flags the T-cell epitope hotspots in a design

Output: **Epitope hotspots**

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VALIDATION & RANKING

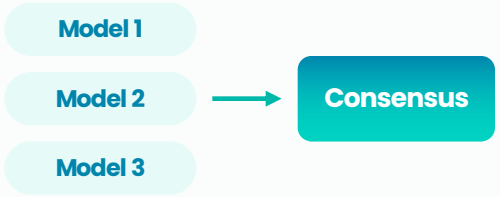
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Physics-based simulations show **how each candidate binds its target**, so we can rank and prioritize

1 Ab-Ag structure prediction

AI co-folding models

Every antibody-antigen complex is predicted with more than one AI model, and the consensus structure carries its confidence metrics

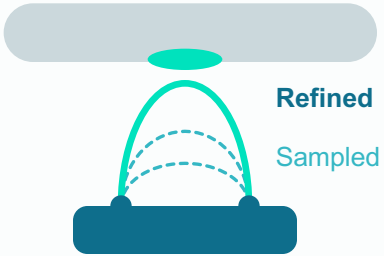


Output: **Consensus Ab-Ag structure**

2 PELE with Loop Closure

Proprietary software

Enhanced conformational exploration of the flexible CDR loops on the predicted complex

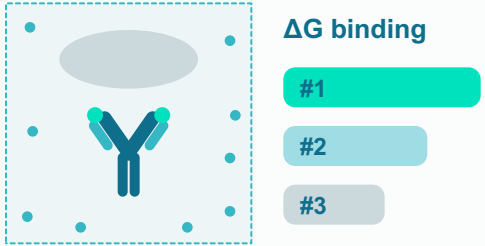


Output: **Refined CDR conformations**

3 Molecular Dynamics

3rd party software

We run several analyses of the interaction: RMSD of ligand, target and complex, and the associated free binding energies



Output: **Ranked binding energies**

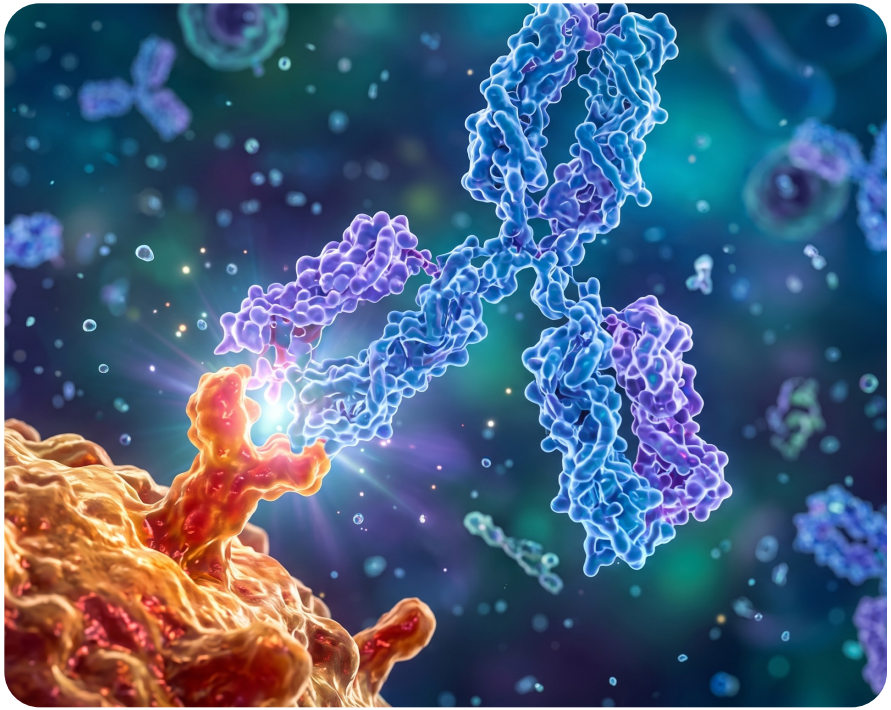
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WHAT YOU GET

Our clients reach at least one promising candidate by testing **fewer than 40 sequences in the wet lab**

<40 **sequences**
tested in the wet lab to reach at least one promising candidate

- **Ranked candidate panel**
  Designs ordered by predicted affinity, with their binding mode
- **De-risked before the wet lab**
  Every sequence screened for developability, toxicity and immunogenicity
- **Full data package**
  Structures, simulations, risk flags and scores for every design



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APPLICATIONS IN YOUR PIPELINE

Four project types our partners run with us, **from finding a first binder to designing a vaccine**



De novo design

A target, no binder yet: we generate and rank new binders against the epitope you choose



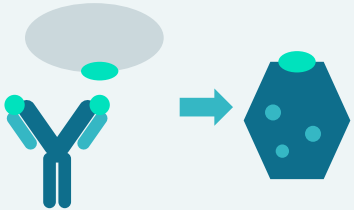
Affinity maturation

An existing antibody: we redesign its CDRs to raise affinity and keep specificity



Epitope characterization

We map where and how a binder engages its antigen: hot spots, mechanism of action and competing epitopes



Vaccine design

From a known neutralizing antibody, we design immunogens that keep its epitope in native conformation

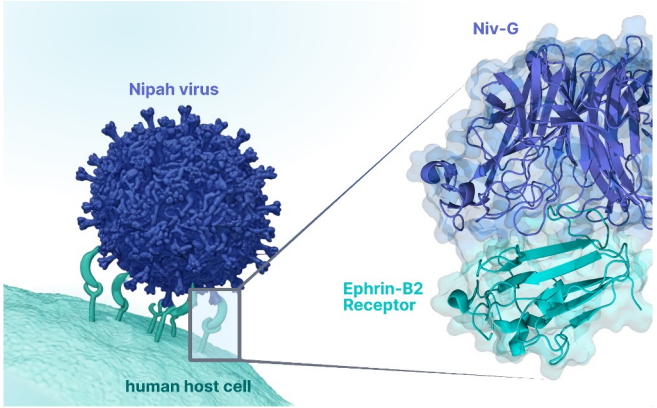
These are our standard projects. **We adapt to the specific needs of each partner**, and our scientific experience lets us build the workflow your programme requires

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CASE STUDY 1

DE NOVO BINDERS AGAINST NIPAH VIRUS

The challenge: neutralize Nipah virus, a pathogen with 75% fatality and no approved treatment or vaccine, by binding its glycoprotein G.



Our protocols competed in the Adaptyv Bio Nipah Binder Competition for de novo Nipah virus binders. Selected entries were produced and tested in the lab, and **a Nostrum design ranked in the Top 10**

HOW WE RANKED

2nd	BEST IN SILICO DESIGN (ipSAE 0.880)
39th	OVERALL GLOBAL RANKING
Verified	HIGH EXPERIMENTAL EXPRESSION

680 protein designers competing › **10,000+** designs submitted › **1,200** proteins tested in the lab › **Top 10** our design's global rank

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CASE STUDY 2

DE NOVO SCAFFOLD DESIGN

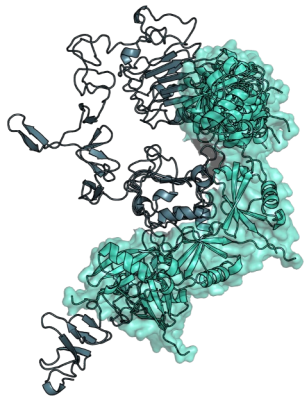
Nostrum AI-MM pipeline **matched massive physical screening libraries at a fraction of time and cost**

We designed a binder against the client's target **in parallel with their traditional phage display campaign**. Both approaches yielded high-affinity binders, translating into two patents for our partner.

3x
Faster to high-affinity hits

99.5%
Less sequence screening volume

Traditional Phage Display	**Nostrum** AI+MM Pipeline
Timeline	
6 Months	2 Months
Sequences Screened in the wet-lab	
~ 10,000	12
Hit Rate (<100 nM)	
4 Hits	2 Hits



Designed binder on its target

2 client-secured patents

Navigo Proteins PURE PRECISION

Diaz-Rovira A. et al., Int. J. Mol. Sci. 2025, 26(10), 4683

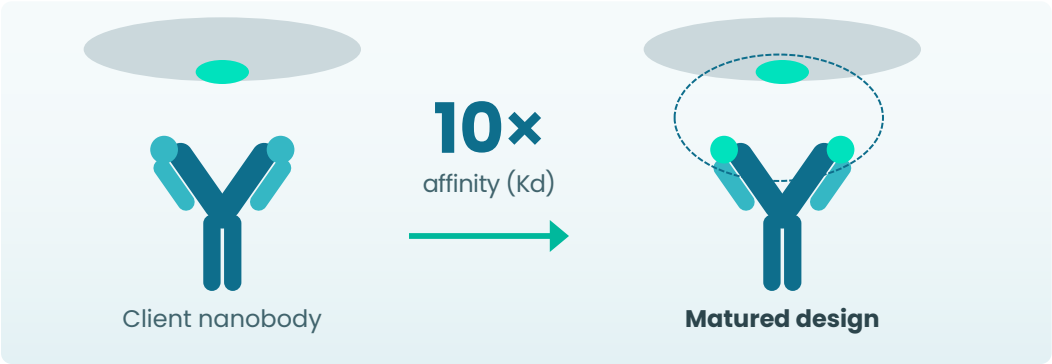
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CASE STUDY 3

AFFINITY MATURATION

One month of redesign on the client's nanobody gave **an order-of-magnitude affinity gain**

WHAT WE REDESIGNED



We characterised the epitope first, then let the models rebuild only the CDR positions that drive binding.

HOW IT RAN

1 month

brief to lab-ready sequences

- Nanobody (VHH) format
- NostrumAbMPNN + RFAntibody
- Epitope mapped before design

~120 variants screened in silico › **10** sequences made in the lab › **9** expressed › **1** **order-of-magnitude gain**

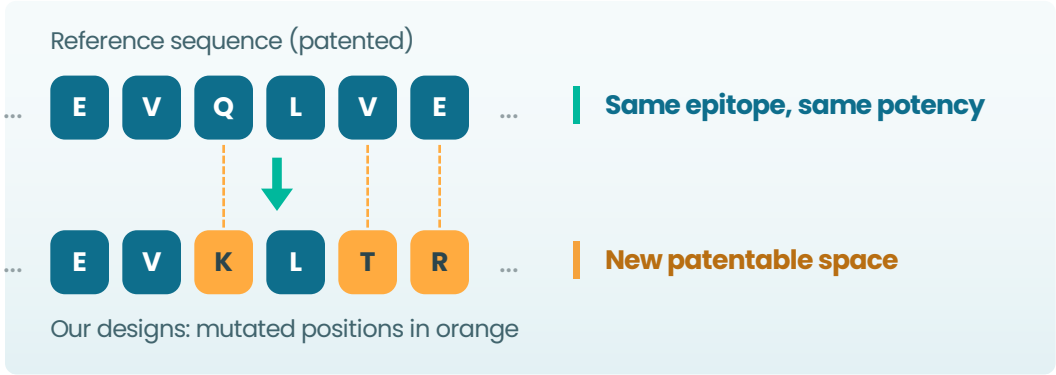
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CASE STUDY 4

IP EXPANSION

From a patented reference sequence we designed binders with **the same potency and enough sequence distance to expand the IP**

SAME BINDING, NEW SEQUENCE



Illustrative example: real sequences and positions stay with the client.

HOW IT RAN

1 month

reference sequence to leads

- Starts from the client's patent
- NostrumAbMPNN + AbLang
- Kd < 10 nM confirmed in vitro

~150 variants screened in silico › **24** sequences made in the lab › **7** expressed › **2** **nM-affinity leads**

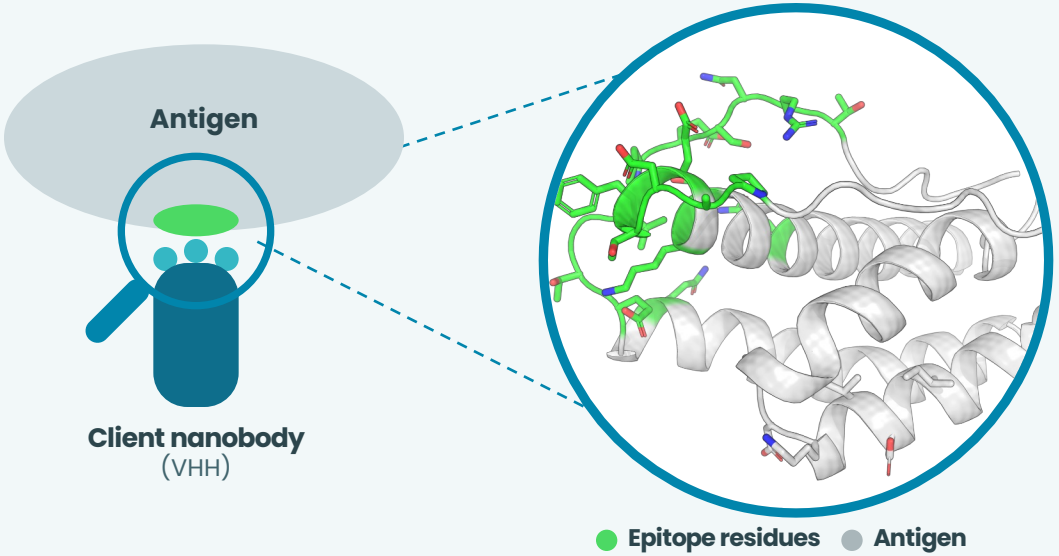
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CASE STUDY 5

EPITOPE CHARACTERIZATION

We mapped how the client's nanobody binds its antigen and **the residues their patent rests on**

FROM BINDING TO RESIDUES



WHAT THE CLIENT GOT

1. **Binding mode**
   How the nanobody sits on its antigen, at atomic level

2. **Key residues**
   The epitope amino acids that drive binding

3. **Patent support**
   Our report backed the client's patent filing

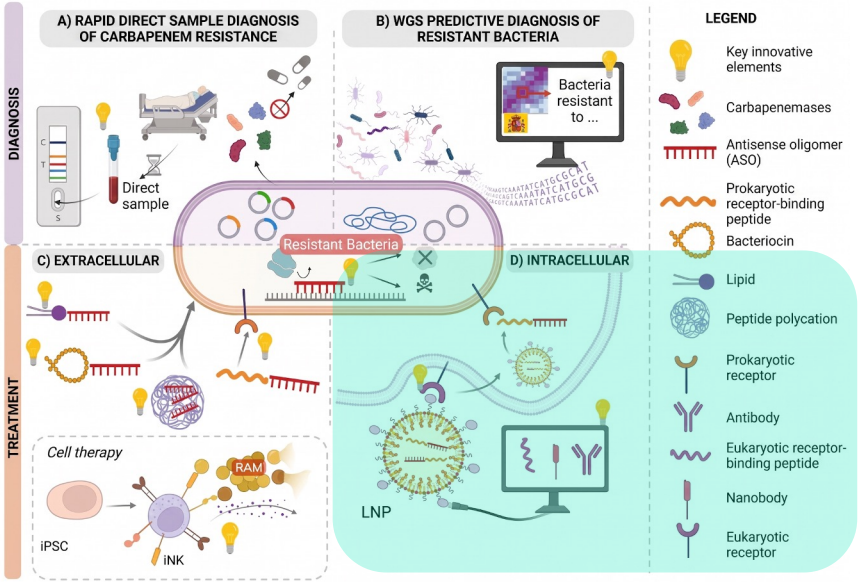
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CASE STUDY 6

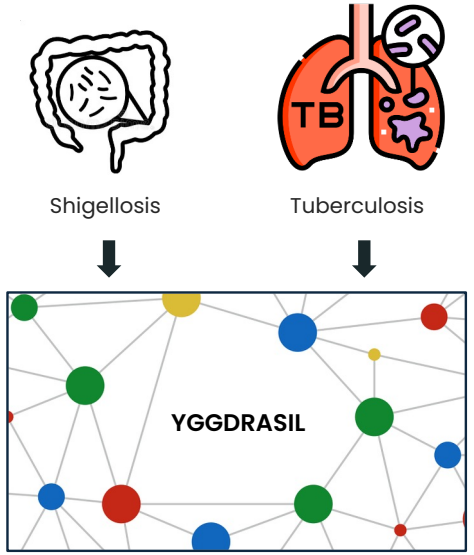
TARGETS FOR BACTERIAL VACCINES

We are partner of a Spanish national consortium END-RAM, where we ranked targets for shigellosis and tuberculosis, and found **6 shared by both diseases**

THE END-RAM CONSORTIUM



OUR ROLE: TARGET DISCOVERY



Human genes ranked according to their connection with the disease

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CASE STUDY 6

PEPTIDE BINDERS FOR ONE SHARED TARGET

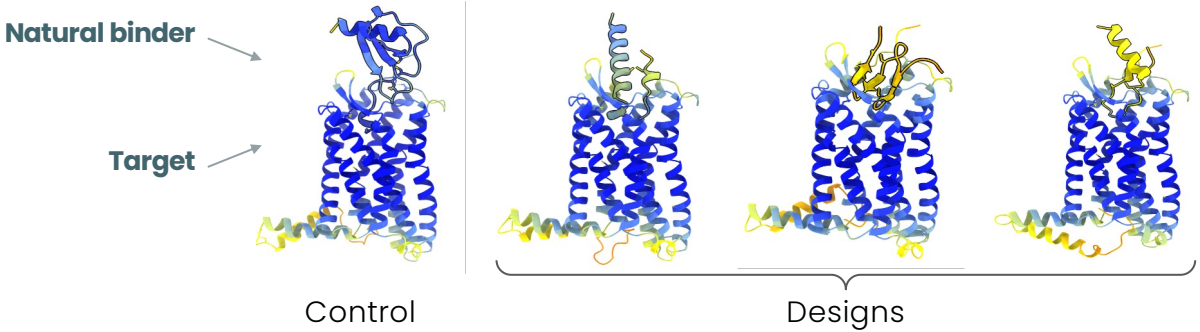
We designed peptide binders for one of the six shared targets, **scored end to end by our simulation stack**

OUR SIMULATION STACK

PELE → BOLTZ-2 → AF2 → MD

	PELE	BOLTZ-2	AF2	MD
CALCULATED METRICS	Avg energy	Confidence score (i)pTM pLDDT PDE	ipTM pLDDT	ΔE MMPBSA ΔE MMGBSA RMSDs

DESIGNED BINDERS ON THE TARGET



RANKED DESIGNS

Binder	Score	Sequence length
Control	3.21	71
$Design_1$	3.71	30
$Design_2$	3.60	30
$Design_3$	3.44	30
$Design_4$	3.30	30
$Design_5$	3.19	36
$Design_6$	3.09	35
$Design_7$	2.94	35
$Design_8$	2.83	30
$Design_9$	2.75	30
$Design_{10}$	2.68	30
$Design_{NC}$	1.51	30

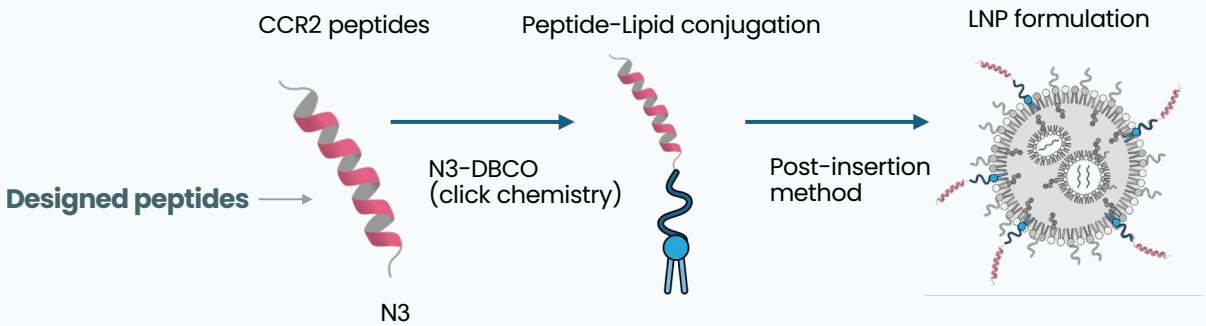
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CASE STUDY 6

FROM BINDER TO TARGETED LNP VACCINE

The designed binders are conjugated to the LNP lipids, so the vaccine **reaches the right cells**

FROM PEPTIDE TO LNP



EXPECTED IN VIVO RESULT



In collaboration with certest

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Design better.
Fail less.
Move faster.

Working on a difficult molecular design challenge?

Partner with **nostrum** to build the computational system that problem actually requires.

Proposed next step

A scoped pilot, structured to demonstrate speed, mechanistic depth, and capital efficiency vs. your current approach.

A model that fits your project

Let's meet to discuss your needs. We adapt the collaboration model to each project:

Fee for service · Partnership · FTE

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ONE STEP AHEAD IN MOLECULAR DESIGN