DYNAMICA

Compute first.
Experiment smarter.



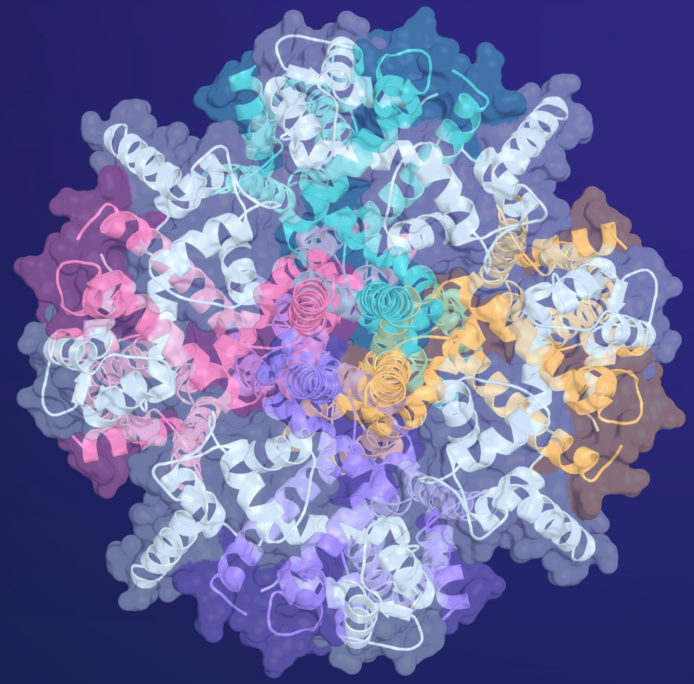
Computational modelling as a service for life science R&D

Inter-university spin-off of UNIVPM and the University of Rome Tor Vergata, Italy

DYNAMICA

WHY WE EXIST

The problem



Every code covers one scale: binding, transport or response. DYNAMICA links them, so a result at the molecule reaches the system.

We build software in-house and combine it with existing tools to run multiphysics and multiscale simulations.

Expertise

Molecular simulation needs significant expertise to give usable results, which are hard to validate and to reproduce across codes.

LiveCoMS, 2018

Tools alone fall short

Docking on 296 proteins with AlphaFold structures scored an average auROC of 0.48, close to chance. Machine-learning rescoring raised it to 0.63.

Wong et al., Mol Syst Biol, 2022

Skills are scarce

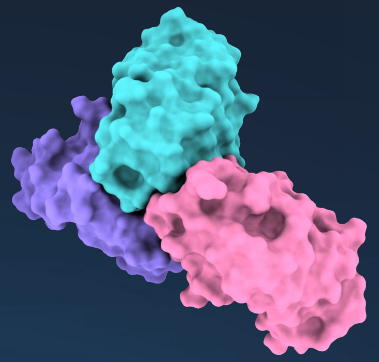
Computational chemistry has been a top priority skills gap in four consecutive surveys of UK pharma.

ABPI, 2023

In a consortium, this is the gap a modelling partner fills.

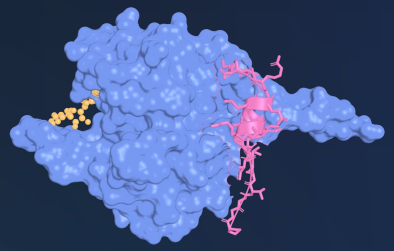
SERVICES

What we do



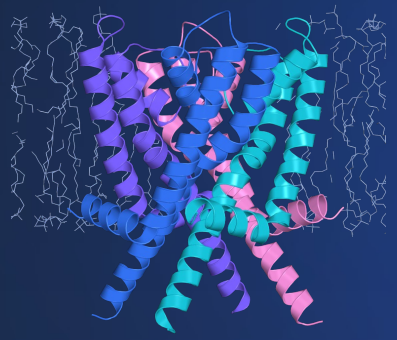
Protein-protein interaction

How two proteins recognise and bind each other, for example an antibody and its target



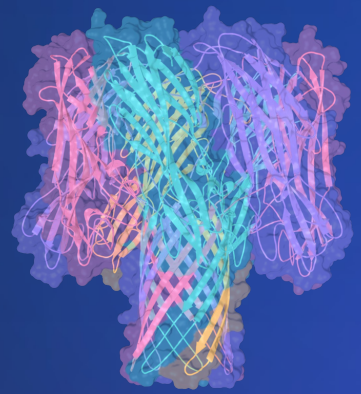
Antibody, peptide and small-molecule design and screening

From virtual screening and de novo design to a ranked list of candidates



Membrane proteins and variants

Channels, receptors and transporters: how a variant changes the protein and where a drug can act



Nanopore and biosensor modelling

Design of sensors that detect biomarkers in complex fluids



Big data analysis

Genomics, proteomics, structural and affinity analyses

MULTISCALE

From atoms to systems

One team covers the whole chain, and each level feeds the next.

ATOMS

0.1 to 10 nm

METHODS

Molecular dynamics, docking, enhanced sampling

ANSWERS

How a drug binds, and how a variant changes a protein

Ion-channel variants: PNAS 2024

MOLECULAR ASSEMBLIES

10 nm to 1 µm

METHODS

Coarse-grained molecular dynamics

ANSWERS

How large complexes, membranes and pores behave

Nanopores: ACS Nano 2022, JACS 2025

TRANSPORT AND FLOW

1 µm to 1 mm

METHODS

Continuum fluid and electrohydrodynamic models, Brownian dynamics

ANSWERS

How ions and molecules move through a channel or a sensor

Electroosmosis: Flow 2025, Advanced Materials 2024

SYSTEM AND PROCESS

1 mm to metres

METHODS

Multiphysics and transport phenomena

ANSWERS

How a device or a bioreactor behaves, and what to change

Atomistic results set the parameters of the larger models, so we follow a candidate from the first screen to the working system.

AI across all scales: it learns from simulations and experiments to speed up screening and to point to the next experiment.

HORIZON TOPIC TOOL-04

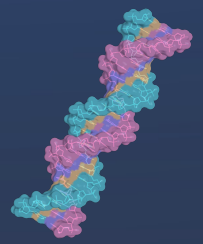
Potential application: virtual human twin

We supply the molecular and subcellular layer of the twin.

DYNAMICA + CLINIC

A patient variant

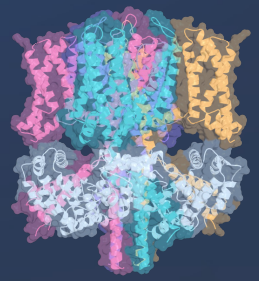
A variant of unknown effect in a protein of the patient. We can analyse the genomic data.



DYNAMICA

Atomistic model

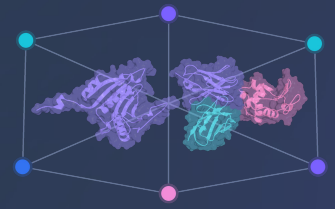
How the variant changes the protein, its dynamics and its response to a drug.



DYNAMICA

Cell pathways equilibrium

Systems biology, transport models and interactomics to model the change in cell equilibrium and homeostasis.



TWIN PARTNER

Organ model

The twin uses these inputs to simulate the patient.

CLINICAL PARTNER

Check on patient data

Predictions are compared with measurements. Differences feed back to the models.

Each comparison with patient data refines the models.

APPROACH

Lab and simulation, in a loop

Each side checks the other, so predictions come with a measured accuracy.

Laboratory data

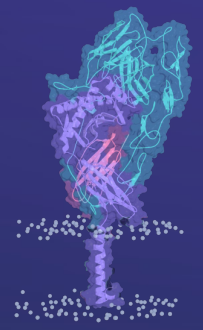
Assays, structures and published results. The failures too.

Calibrate and validate

Test and update

In silico data

Simulations, screening and models, at every scale.



1

Start

Start from your data. What must the model reproduce?

2

Validate

Run the models on cases with a known outcome and report how often they are right.

3

Predict

Apply the validated pipeline to new candidates or conditions.

4

Test and update

Your lab tests the top of the list. Every result goes back into the models.

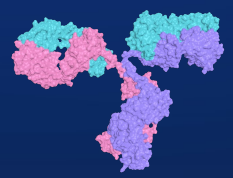
Then repeat: we measure accuracy at every cycle.

POTENTIAL APPLICATION: ANTIBODY DESIGN

A work package in practice

We characterize candidates, we rank them, and we learn from the experimental outputs.

THE OPTIMIZATION CYCLE



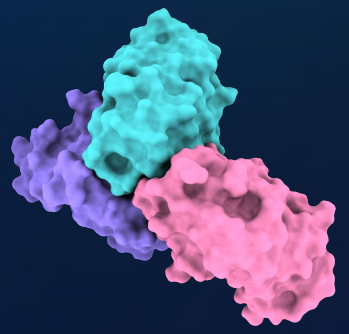
Candidates

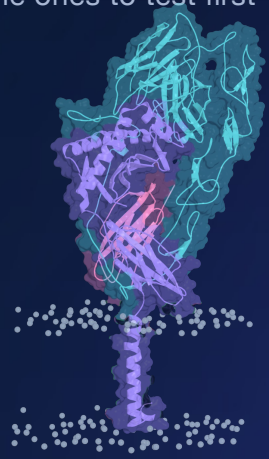
Molecular dynamics

WHAT WE CHECK

pose
contacts
chemical liabilities
colloidal behaviour
CDR

A short list
the ones to test first





Your bench
results, the failures too

TYPICAL TIMINGS FOR ONE CANDIDATE

4 weeks

Modelling and developability

Chemical liabilities and aggregation propensity of the candidates.

8 weeks

Binding mechanism

One complex with the antigen, its cofactors and cross-reactants.

12 weeks

CDR optimization and de novo design

Up to 15 variants in total, optimized or new.

Each stage includes the previous one.

WHAT WE ADD

Why DYNAMICA

A company's speed, with academic rigour.

One team across scales

From genomics to atomistic models to the whole system.

Software that fits the problem

We build software in-house and combine it with existing tools, instead of adapting the question to the tool.

Reliable results

Laboratory and in silico data check each other, and we measure accuracy at every cycle.

European computing resources

We rely on European computing resources: CINECA HPC, EuroHPC and CSCS.

WHO WE ARE

Team and network



Giovanni Di Muccio

Nanopores, multiscale modelling, supercomputing



Agnese Roscioni

Ion channels, molecular dynamics, drug targets



Beatrice Campanelli

Computational chemistry, drug design



Francesco Pignotti

Virtual screening, AI models, peptide design

Prof. Emiliano Trucchi
UNIVPM. Bioinformatics and evolutionary genetics

Prof. Mauro Chinappi
Tor Vergata. Nanofluidics and biosensing

Two research fellows
Antibody and oligonucleotide modelling

ACADEMIC AND CLINICAL COLLABORATORS

UNIVERSITÀ POLITECNICA DELLE MARCHE · TOR VERGATA UNIVERSITÀ DEGLI STUDI DI ROMA · iit ISTITUTO ITALIANO DI TECNOLOGIA · FONDAZIONE IRCCS ISTITUTO NAZIONALE DEI TUMORI · I.R.C.C.S. Ospedale San Raffaele · UNIVERSITÀ DEGLI STUDI DI NAPOLI FEDERICO II · UBC · university of groningen

HORIZON EUROPE HEALTH 2027

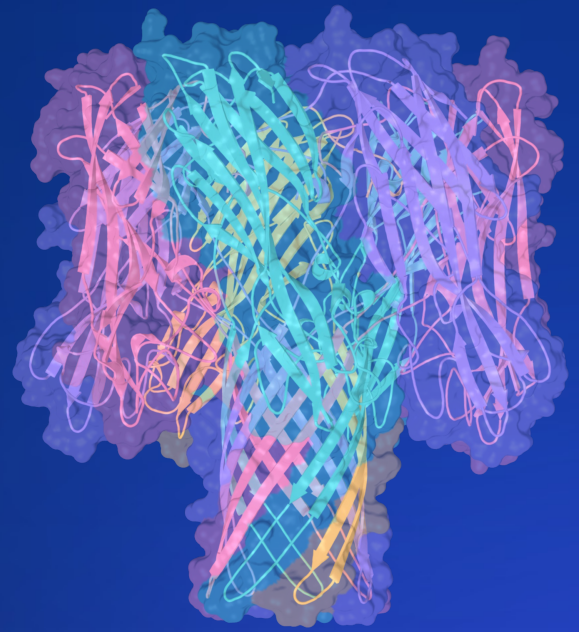
Expertise on the call topics

CALL TOPIC	WHAT WE BRING	EVIDENCE
Adverse drug reactions from multiple medications HORIZON-HLTH-2027-01-CARE-02	Molecular models of how gene variants change drug binding	Clinical variants of ion channels: PNAS 2024, Nature Communications 2025
Virtual human twins HORIZON-HLTH-2027-03-TOOL-04	Atomistic models of proteins and their clinical variants	PNAS 2024, Nature Communications 2025
Monoclonal antibodies HORIZON-HLTH-2027-01-DISEASE-06	Atomistic model of antibody and target: binding mechanism, orientation and affinity	Ongoing work with Istituto Nazionale dei Tumori and San Raffaele Hospital. Papers in preparation
Antimicrobials against resistant pathogens HORIZON-HLTH-2027-01-DISEASE-08	Design and screening of peptides and small molecules, plus membrane and poration modelling	Published for cancer targets (eIF4E, USP14): Cancer Drug Resistance 2025
Antivirals for pathogens with epidemic potential HORIZON-HLTH-2027-01-DISEASE-05	Design and screening of peptides and small molecules	Published for cancer targets (eIF4E, USP14): Cancer Drug Resistance 2025
AI-based predictive biomarkers HORIZON-HLTH-2027-02-TOOL-01	Nanopore sensors and de novo receptor design for biomarker detection	JACS 2025, ACS Nano 2026

Peer-reviewed work from the team in Nature Communications, PNAS, JACS, ACS Nano, Advanced Materials and Light: Science & Applications.

LET'S TALK

Let's compute first.



THREE QUESTIONS WE WOULD LIKE TO ASK YOU

1. **Which step of your project is still a guess?**
2. **Where do you lack someone who can model?**
3. **What data do you already have that nobody has analysed?**

We would like to meet coordinators who need a modelling work package, experimental labs that test our predictions, and groups with data to analyse.

Meet us at the brokerage event
24 and 25 November 2026

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