

Artificial Intelligence and Organic Chemistry  
for Drug Discovery and Materials design

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Who we are

# AI + Organic chemistry + Synthesis

AITENEA Biotech is an R&D spin-off combining artificial intelligence and deep chemical expertise to accelerate the design, optimization and synthesis of molecules and materials.

We are a multidisciplinary team of 10+ researchers bringing together expertise in data science, organic chemistry and computational chemistry, based at the Madrid Science Park.



## AI and Machine Learning

Predictive and Generative AI · Bayesian Optimization · QSAR Modeling



## Computational Chemistry

De Novo Molecular Design · Molecular Descriptors · Virtual Screening



## Organic Synthesis

State-of-the-Art In-House Laboratory  
Synthesis · Purification · Characterization



## Data & Analytics

Data Curation · Visual Analytics · Interactive Data Tools

Why

# AITENEA Biotech?



We help industry partners to do speed their R&D programs by combining deep learning models and Organic and Medicinal Chemistry knowledge.



We cut candidate screening time from months to weeks

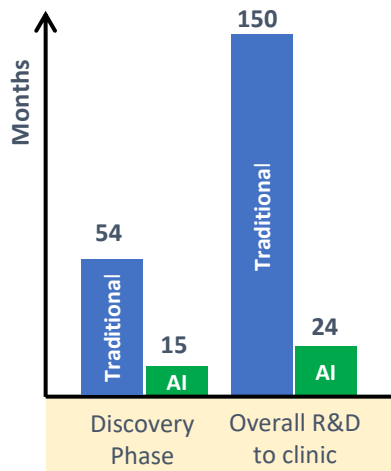


Clients get a tool they can run in-house after the project



We are not a CRO, we don't give just a report. Clients get a validated R&D Project and new IP.

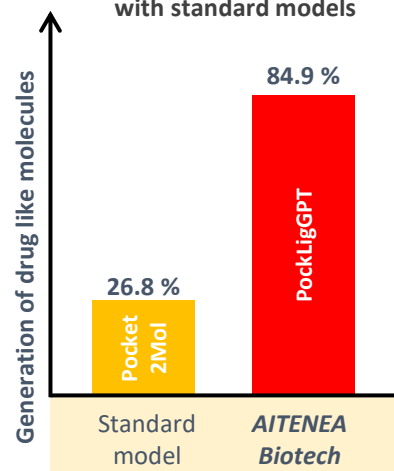
Research Timeline (Industry Averages)\*:  
Traditional vs AI-accelerated  
**6x fold acceleration**



## AITENEA METRIX

- 3.2 fold increase in drug like molecule generation comparing with standard models J. Chem. Inf. Model. 2026 doi.org/10.1021/acs.jcim.6c01980
- Models are productive even with small datasets
- Pre-trained models ready to use in 2 weeks

Success rate in Pharmaceutical generation:  
**Our models present 3.2 fold increase in druglike molecules generation comparing with standard models**



\* Industry averages: sources Insilico Medicine, Exscientia case study.

## SECTORS

# Cross-Industry Impact



### Pharmaceuticals

Drug Discovery · Lead Optimization · Risk Mitigation · Candidate Synthesis

**AI in drug development**  
**Ames Mutagenicity Prediction**  
**Nontoxic DYRK1A Inhibitors**  
**MolOrgGPT**  
**PockLigGPT**

*Molecular Diversity* 2021, 25, 1461–1479  
*J. Chem. Inf. Model.* 2022, 62, 6342–6351  
*J Med Chem.* 2025, 3, 68, 10346–10364  
*J Chem Inf Model.* 2026, 7, 910–922  
*J. Chem. Inf. Model.* 2026, x, xxx



### Industry

New Molecular Entities · Catalysis · Functional and Advanced Materials · Polymers

**New Dispersants**  
**Novel Fuel additives**  
**Novel polymer additive**

*Patent EP23382811.0*  
*Patent application filed*  
*Patent application filed*



### R&D

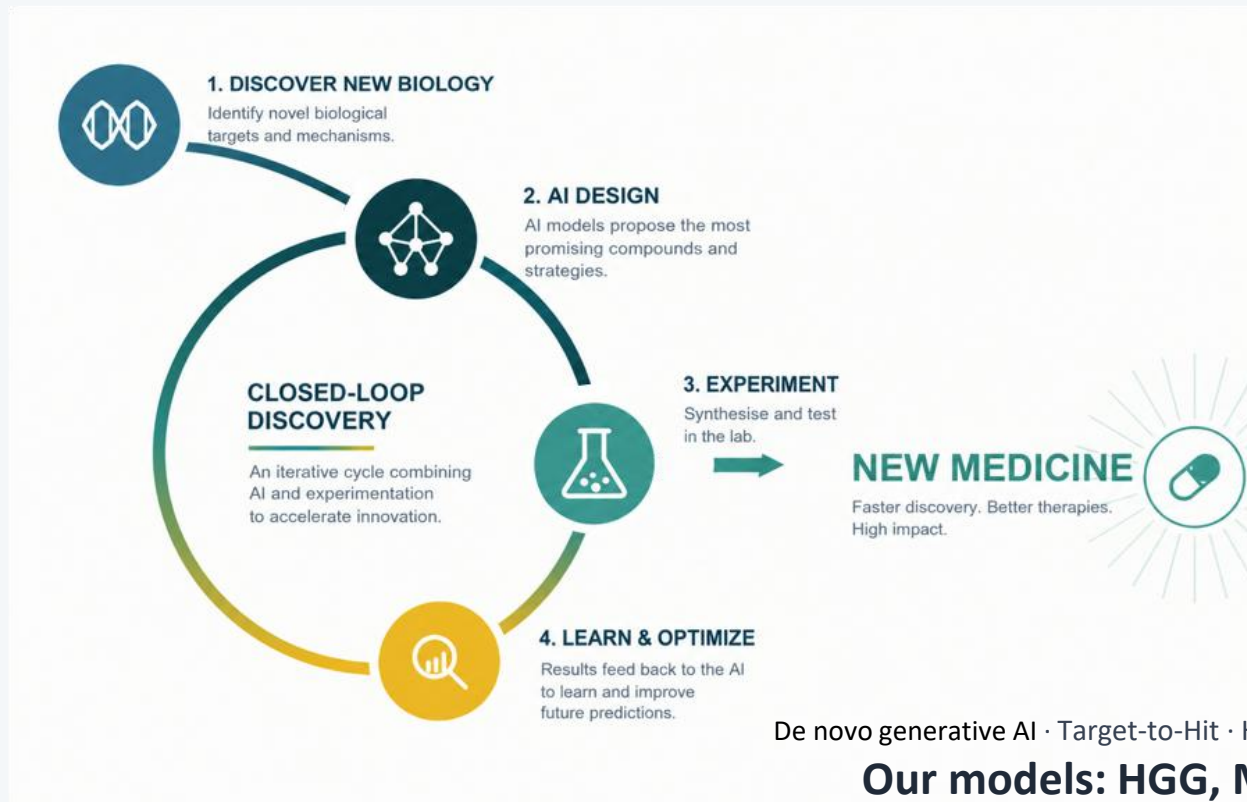
From Complex Challenges to Innovative Solutions

**CDTI NEOTEC**  
**Regioselectivity in Cu-catalyses**  
**New Dispersants**  
**Winners III Challenge of open innovation**

*2023 SNEO-20222073*  
*ACS Catal.* 2025, 15, 20230–20242  
*Polymers* 2023, 15, 1324–1342  
*2026 Digital twin with BASF*



# Drug discovery



Protein modeling



Allosteric sites detection



Generative model



ADME predictions



Toxicity filter

De novo generative AI · Target-to-Hit · Hit-to-Lead · Drug Repurposing · Custom QSA

**Our models: HGG, MolOrgGPT, PockLigGPT..**

Capabilities

# Artificial intelligence



## ADMET predictions

Absorption, Distribution, Metabolism, Excretion and Toxicity: LogP, solubility, permeability, CYP enzymes.



## Regio- and enantioselectivity

Selectivity of catalytic reactions and asymmetric transformations.



## GHS Classification

Prediction of Hazard and labelling of substances for regulatory compliance.



## Allosteric sites

Detection of orthosteric and allosteric binding pockets in targets.



## Protein modeling

AlphaFold / homology structures, target preparation and analysis.



## ASO strands in oligonucleotides

Design and prediction of antisense oligonucleotides (RNA therapies).

**De novo generative AI** · Target-to-Hit · Hit-to-Lead · Drug Repurposing · Custom QSAR

**Our models: HGG, MolOrgGPT, PockLigGPT..**

Capabilities

# Organic Synthesis

We close the loop! We design molecules and hypothesis, and we validate our design in the laboratory.



## Complex molecules

Clarifiers, Dispersants, Polymers and Organometallic catalysts (Cu, Pd and Ni Catalysis).



## Drug Discovery & Medicinal Chemistry

Small molecules and new modalities:  
Oligonucleotides & Nucleotides, Peptides, Macrocycles



## Novel technologies

Flow-Photochemistry, with emerging capabilities and enzyme-based synthesis.



## Purification and Characterization

HPLC, LC-MS, GC-MS, CD, GPC, NMR, NP and RP FCC, XRF, ICP-MS, Elemental analysis.  
Certified laboratories.

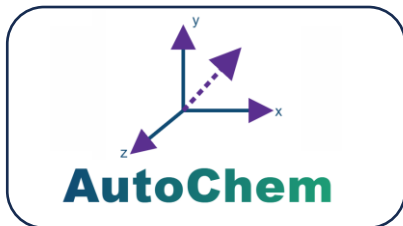




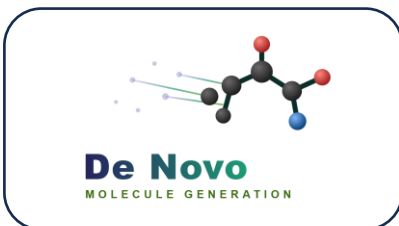
# AITENEA Platform – in development

Web platform: Our tools to support drug discovery programs. To request a Demo contact [nuria.campillo@aitenea.es](mailto:nuria.campillo@aitenea.es)

SaaS product



**Autochem** generates molecular descriptors.



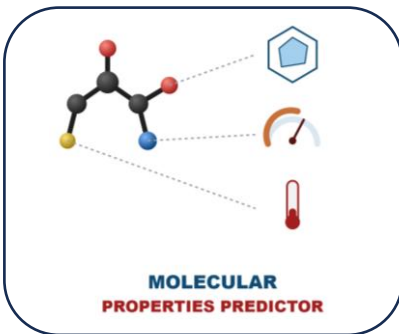
**De Novo** contains genetic and GPT algorithms for molecule generation



**DOE - Bayesian Optimization**  
Intelligently selects the next experiments, accelerating multiparameter process optimization with fewer experiments.



**Toxicity predictor** for unknown molecules



**Molecular predictor** for Physical properties



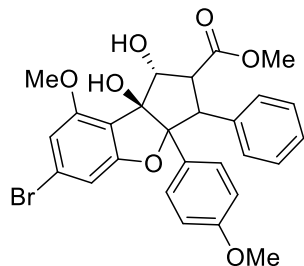
**Label printer** predicts the GHS classification of novel entities



# Case Study: Label printer

SaaS product

- The model was provided with the SMILES structure of a molecule that was not included in the training dataset.
- The model correctly predicted GHS08 (Health Hazard), which is applicable to this class of compounds due to their activity against eIF4A.



*J. Med. Chem.* 2024, 67, 289–321

Reported as Pan-antiviral Agents against  
Hepatitis E Virus and Emerging Viruses



**Label Printer**

Label printer predicts the toxicity and  
GHS classification of novel entities

## GHS Hazard Classification

Enter a SMILES string to predict GHS hazard pictograms and hazard categories for a molecule.

O[C@@]12C(C(C3=CC=CC=C3)C(C(OC)=O)[C@H]2O)(C4=CC=C(C(OC)=C4)OC5=CC(Br)=CC(OC)=C51

Predict

Reset

2 GHS hazards identified O[C@@]12C(C(C3=CC=CC=C3)C(C(OC)=O)[C@H]2O)(C4=CC=C(C(OC)=C4)OC5=CC(Br)=CC(OC)=C51

Download PDF

### GHS Pictograms



GHS01  
Explosive



GHS02  
Flammable



GHS03  
Oxidizing



GHS04  
Corrosive



GHS05  
Toxic



GHS06  
Harmful / Irritant



GHS07  
Health Hazard



GHS08  
Environment

## Summary

Security report:

GHS label(s): GHS07 GHS08

Categories and phrases:

STOT SE 3

H335: May cause respiratory irritation

H336: May cause drowsiness or dizziness

Repr. 2

H361: Suspected of damaging fertility or the unborn child

H361f: Suspected of damaging fertility

H361d: Suspected of damaging the unborn child

H361fd: Suspected of damaging fertility; Suspected of damaging the unborn child

STOT RE 1

H372: Causes damage to organs through prolonged or repeated exposure

Asp. Tox. 1

H304: May be fatal if swallowed and enters airways

# Case Study: polymer chemistry

*A major international oil company commissioned the development of innovative polymers.*

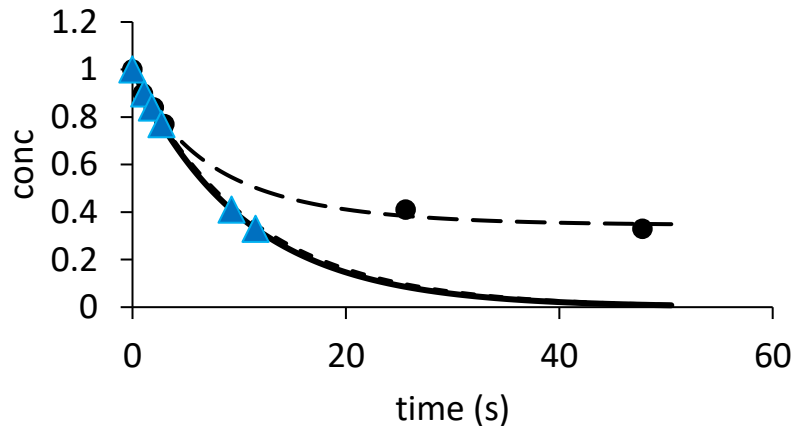
## AITENEA's solution

- Designed and synthesized a library of 82 novel polymers candidates through **deep mechanistical and kinetic understanding** during the initial discovery campaign.
- Selected one high-performing candidate and optimized its synthetic route to enable further scale-up and production.

## Results

- Lead candidate successfully identified in 9 months.
- Optimized synthesis on 200 g scale.
- Route was handed to CDMO for scale-up.
- A **patent application has been filed.**

Model vs Experimental Data



- conc 1 fit initial times    — conc 1 fit  
— conc 1 fit corrected    ● conc 1  
▲ conc 1 time corrected

# Case study: AI-Driven Design of Next-Generation Dispersants

*A major international company commissioned the discovery of high-performance lubricant dispersants to reduce experimental screening and development costs.*

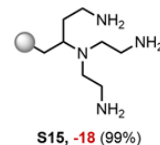
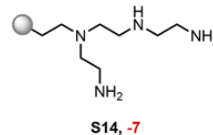
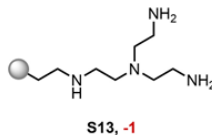
## AITENEA's solution

- Developed an AI platform combining machine learning, Bayesian modeling, structural similarity analysis, and interactive data visualization.
- Integrated chemical expert knowledge into the AI workflow to improve decision-making.
- Predicted dispersancy performance from molecular structure and performed virtual screening and optimization

## Results

- Novel predictive AI model** for dispersancy efficiency.
- Successfully screened and prioritized novel dispersant candidates in a **small-data environment** and reduced trial-and-error experimentation.
- The novel developed technology was **patented (Patent EP23382811.0)**.

### Successful AI-to-Experimental Validation

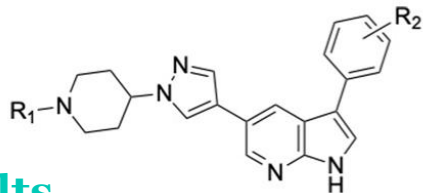


# Case study: AI-Guided Discovery of Novel DYRK1A Inhibitors

Develop novel, drug-like DYRK1A inhibitors despite **limited experimental data** using an AI-driven drug discovery workflow.

## AITENEA's solution

- Designed an integrated AI platform combining generative AI, QSAR modeling, toxicity prediction, and molecular docking.
- Generated and prioritized novel chemical entities for synthesis.
- Synthesized lead compounds and analogues.
- Experimentally validated biological activity through in vitro assays.

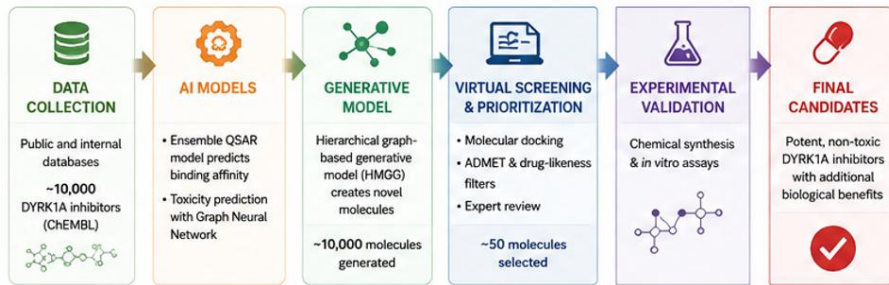


## Results

- Identified a novel nanomolar DYRK1A inhibitor.
- Discovered a new family of pyrazolyl pyrrolopyridine derivatives.
- Confirmed enzyme inhibition, anti-inflammatory, and antioxidant properties with nanomolar activities.

## OUR AI-POWERED PIPELINE

Integration of artificial intelligence and experimental validation



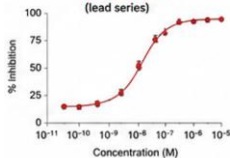
## BIOLOGICAL RESULTS (EXPERIMENTAL)



### ENZYMATIC INHIBITION

Potent DYRK1A inhibition

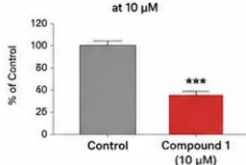
IC<sub>50</sub> (DYRK1A)  
**1 – 50 nM**  
(lead series)



### ANTI-INFLAMMATORY ACTIVITY

Reduces pro-inflammatory mediators

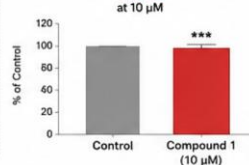
Example: TNF- $\alpha$  reduction  
**~70%**  
at 10  $\mu$ M



### ANTIOXIDANT CAPACITY

Protects against oxidative stress

DPPH radical scavenging  
**~80%**  
at 10  $\mu$ M



# Types of collaboration



## Internal IP generation – Aitenea Biotech

Drug Discovery · Generation and advancement of new models



## R&D Partnership

Collaborations · Consortium – **Shared IP**



## Service – Full R&D project

We develop the Project from ideation to practise  
AI + Computational + Synthesis



## Service – Consulting

AI · Computational chemistry · Catalysis



## Service – Partial R&D project only AI only computational or only synthesis

ISO 27001 certification in progress



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From computational design to real synthesis



[aitenea.com](https://aitenea.com)



Let's talk about your project



[nuria.campillo@aitenea.com](mailto:nuria.campillo@aitenea.com)



Meet the team