



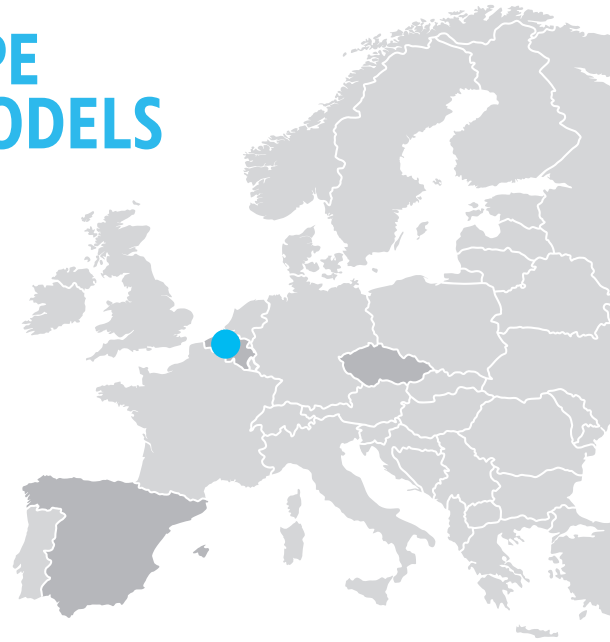
FORTISSIMO  
PLUS

## FFPLUS SUCCESS STORY: INNOVATION STUDY

# ACCELERATING STRUCTUREGUIDED EPITOPE MAPPING VIA HYBRID AI MODELS

## ORGANIZATIONS

**PUXANO** is a Belgian SME specialising in AI-driven protein design and cryo-electron microscopy services for pharmaceutical, biotechnology and agricultural clients. **CSIC**, Spain's national research council, contributed advanced computational methods for cryo-EM structure reconstruction. **IT4I**, the Czech national supercomputing centre, provided access to the Karolina supercomputer and expert HPC support.



## THE CHALLENGE

Drug discovery is slow, costly and uncertain, with R&D investment often exceeding US\$2.6 billion per programme. While structure-guided design can accelerate early research, current AI protein prediction tools lack accuracy to replace labour-intensive experiments. Integrating AI with sparse cryo-EM constraints promised faster, reliable structures, but no scalable datasets or workflows existed to combine these methods during large-scale training.



**Technology used:** HPC, GenAI, Diffusion Models, Cryo-EM  
**Industry Sector:** Biotechnology

## THE SOLUTION

HARMONY is a hybrid model that combines AI-based protein structure prediction with sparse cryo-electron microscopy data to deliver accurate structures at 10–15× lower cost than standard cryo-EM. An AI-generated draft structure is refined using cryo-EM images to correct errors. Optimised alignment algorithms accelerated training by around 100×. Using the EuroHPC Karolina supercomputer, the team processed terabytes of data and completed 200,000 GPU hours of training to enable de novo prediction.

## THE IMPACT

HARMONY strengthens PUXANO's position as a platform-based contract research organisation by enabling faster, more reliable protein structure determination at a fraction of traditional cryo-EM costs. Large-scale HPC access enabled a proprietary hybrid AI model that blends prediction with experimental evidence, creating a differentiated and scalable service that supports revenue growth and market expansion across pharmaceutical, biotechnology and agricultural sectors.

For clients, faster and more accurate structures improve early-stage drug development decisions. More antibody variants, vaccine candidates or small molecules can be screened within the same budget, reducing risk and increasing success rates. Social impact arises from the potential acceleration of new therapeutics, benefiting patient groups with limited treatment options.

Environmental benefits include reduced reliance on repeated wet-lab experiments and energy-intensive cryo-EM sessions. Shorter experimental cycles lowered material use and energy consumption, supporting more sustainable results.

## BENEFITS

- 20× faster alignment reduces per-iteration time from 30 s to 1.5 s, enabling large-scale AI training.
- Hybrid AI cryo-EM workflows cut structure determination costs by 10–15× for clients. Screening capacity increases from 1–3 to 12–24 variants per session.
- New HPC and data-processing expertise strengthens PUXANO's long-term AI platform.



**EuroHPC**  
Joint Undertaking