

# Physics-informed AI agents offered for biophysical and pharmaceutical research under Horizon Europe call HORIZON-CL4-2026-05-DIGITAL-EMERGING-02

## Summary

Profile type

**Research & Development Request Greece**

Company's country

POD reference

**RDRGR20260209003**

Profile status

**PUBLISHED**

Type of partnership

**Research and development  
cooperation agreement**

Targeted countries

**• World**

Contact Person

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Term of validity

**9 Feb 2026  
9 Feb 2027**

Last update

**9 Feb 2026**

## General Information

### Short summary

A Greek university lab and an affiliated Physics and AI Research Centre intend to participate in a Horizon Europe Research and Innovation Action under the call HORIZON-CL4-2026-05-DIGITAL-EMERGING-02. The group develops physics-informed AI methods combining advanced numerical simulations with experimental pharmaceutical validation. The partners seek a project coordinator to integrate their expertise into a large consortium developing autonomous AI agents for real-world scientific applications.

### Full description

The proposed Research and Development Request addresses the need for reliable and interpretable AI agents capable of performing complex scientific tasks in real-world environments, as defined in the Horizon Europe call HORIZON-CL4-2026-05-DIGITAL-EMERGING-02. Current AI-driven discovery workflows often rely on data-intensive approaches that lack physical consistency and limited adaptability when applied to experimental research settings.

The requesting entities consist of a university pharmaceutical laboratory and a physics and artificial intelligence research centre. The collaboration focuses on the integration of physics-informed artificial intelligence with experimental biophysical and pharmaceutical research. The objective is to contribute to the development of autonomous AI agents that can decompose complex scientific problems into structured sub-tasks, operate within known physical laws, and adapt their behaviour based on continuous feedback from simulations and experimental data.

The physics and AI research centre contributes expertise in applied mathematics, numerical modelling and high-fidelity simulations, including fluid, particle and magnetohydrodynamic models originally developed for astrophysical research. These methods are combined with physics-informed neural networks to accelerate simulations and reduce computational cost while preserving physical consistency.

The university pharmaceutical laboratory provides application-driven use cases, experimental workflows and high-quality datasets. Its activities include computational drug design with a focus on G protein-coupled receptors and antimicrobial compounds, molecular dynamics simulations of biomolecular systems, and experimental validation in pharmaceutical and theranostic research. The laboratory enables the validation and benchmarking of AI agent outputs through real experimental feedback.

Within a Horizon Europe Research and Innovation Action, the partners aim to support the design, testing and validation of AI agents that operate across simulation and experimental environments. The consortium is expected to submit a single-stage proposal by the call deadline of 15 April 2026, with an expression of interest deadline of 25 March 2026. The partners are seeking a coordinator to lead the consortium and integrate their contributions into a coherent multi-agent research framework under a research and development cooperation agreement.

### Advantages and innovations

The proposed collaboration offers a combination of methodological and application-driven innovation. A key advantage is the transfer of advanced numerical acceleration and modelling techniques from physics research to biophysical and pharmaceutical applications, enabling faster and more physically consistent simulations than conventional data-driven approaches.

The integration of physics-informed neural networks allows AI agents to operate under explicit physical constraints, improving robustness, interpretability and reliability in scientific discovery tasks. This approach supports scalability to complex biological systems that are otherwise computationally demanding.

An additional innovation is the availability of a closed-loop research environment, where AI agent predictions can be directly tested and refined through experimental validation in a university pharmaceutical laboratory. This enables systematic benchmarking of autonomous agents against real-world experimental outcomes and supports continuous improvement of agent reasoning and decision-making capabilities.

### Technical specification or expertise sought

#### Stage of development

**Under development**

#### Sustainable Development goals

**• Goal 13: Climate Action**

IPR Status

IPR Notes

## Partner Sought

### Expected role of the partner

The Greek collaborating institutions are looking for a Consortium Coordinator (University, Research and Technology Organization (RTO), or an Innovation-driven Large Enterprise) currently forming a proposal for the call: HORIZON-CL4-2026-05-DIGITAL-EMERGING-02.

The ideal coordinator should have a strong background in AI systems, multi-agent frameworks, or large-scale digital transformation and be seeking a high-specialization partner to handle the Scientific and Biophysical application domain.

Required Partnership Type: Research and Development Cooperation Agreement.

Expected Role and Tasks: The Greek collaborators (AI/Physics Research Centre + University Pharma Lab) are prepared to lead or contribute significantly to the following areas:

1. Domain-specific AI agent development (WP Lead/Partner): They will provide the "Physics-Informed" reasoning layer for next-generation AI agents. By utilizing PINNs (Physics-Informed Neural Networks), they aim to move beyond black-box AI, enabling agents to operate within the strict physical constraints required for real-world scientific applications.
2. Autonomous scientific discovery workflows: They can design the "tool-use" protocols for AI agents, allowing them to autonomously utilize MHD (Magnetohydrodynamic) simulations and Molecular dynamics (MD) engines (e.g., GROMACS, NAMD) to achieve specified research goals in drug development and metal catalysis.
3. Numerical Acceleration for Real-Time Adaptation: A key requirement of the call is real-time behaviour adaptation. They offer expertise in accelerating the underlying numerical simulations (using techniques from Astrophysics and Applied Maths) so that the AI agent can receive immediate feedback from its environment/simulation and update its planning accordingly.
4. Validation and Benchmarking (Pharma Sector): They provide the experimental environment to test the "autonomy, robustness, and reliability" of the agents.  
This includes:
  - Testing agents on complex multi-step tasks like GPCR (G Protein-Coupled Receptor) modelling and Protein-Lipid interaction predictions.
  - Benchmarking agent performance in discovering new antimicrobials or Cancer Theragnostics.
  - Providing "Wet-lab" feedback to refine the agent's autonomous planning mechanisms.

Technical Profile of the Coordinator: The coordinator should ideally have the capacity to manage the overarching Multi-agent framework and decentralized coordination protocols.

The Greek collaborators offer the specialized "Agent Brain" and "Environmental Testing Ground" that grounds the project in a high-impact economic sector (Healthcare & Biotechnology and/or Data/Open Science)



Type of partnership

**Research and development cooperation agreement**

Type and size of the partner

- **Big company**
- **R&D Institution**
- **University**

## Call Details

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Framework program

**Horizon Europe**

Call title and identifier

**Next-Generation AI Agents for Real-World Applications in the Apply AI sectors (RIA) (Partnership in AI, Data and Robotics) HORIZON-CL4-2026-05-DIGITAL-EMERGING-02**

Submission and evaluation scheme

**Single Stage Submission**

Anticipated project budget

Coordinator required

**Yes**

Deadline for EoI

**25 Mar 2026**

Deadline of the call

**15 Apr 2026**

Project duration in weeks

Web link to the call

Project title and acronym

## Dissemination

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Technology keywords

Targeted countries

- **World**

Market keywords

- **04005 - Biochemistry / Biophysics**
- **02007016 - Artificial intelligence related software**
- **05005014 - Oncology**
- **05007002 - Pharmaceuticals/fine chemicals**

Sector groups involved

- **Health**
- **Digital**