Partner Search Form
Horizon Europe
Health

Date 02. 07. 2026 Deadline … …

CONTACT

Organisation	Cytocast	**Department**	N/A
Contact person	Istvan BAGYI	**Email**	business@cytocast.com
City	Budapest	**Website**	https://www.cytocast.com/
Country	Hungary		

Organisation type

Research organisation type	☐ Research Organisation ☐ University ☒ Company ☐ Other	**Is your company a Small and Medium Sized Enterprise (SME*)?** **Number of employees:**	☒ YES ☐ NO 17

Your enterprise is an SME if:
- it is engaged in **economic activity**
- it has **less than 250 employees**
- it has either an **annual turnover not exceeding €50M**, **or an balance sheet total not exceeding €43M**
- it is **autonomous**

For the definition of SMEs, look at: http://ec.europa.eu/growth/smes/business-friendly-environment/sme-definition_en

Short introduction of key areas of institute's research: AI- and simulation-powered platform to predict clinically relevant side effects through a multi-layer modelling pipeline.

Former participation in an FP European project?	☐ YES ☒ NO
Project title / Acronym:	
Activities performed:	

Expertise / Commitment offered

Description of your expertise:	AI- and simulation-powered platform to predict clinically relevant side effects through a multi-layer modelling pipeline. Mechanistically grounded prediction rather than chemistry-only similarity; Whole-cell, multi-tissue simulation for system-level biological context; tiered prediction stratification; decision-relevant insight into safety risks. see one-pager

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Keywords specifying your expertise:	Bioinformatics, Drug discovery, Pharmacogenomics, Side-effects, Cell Simulation, Systems biology, Toxicology, Personalised medicine, Scientific computing, Digital Twin
Commitment offered:	☒ Research ☐ Demonstration ☐ Training ☒ Technology ☐ Dissemination ☐ Other:

Interested in participation in project types:			
	☒ Research & Innovation Action	☒ Innovation Action	☒ EIC Pathfinder

Work Programme research areas: indicate your interest

- Horizon Europe Cluster 1 Health
- 2026 Horizon Europe calls to support the EU Mission on cancer
- EIC Pathfinder - Challenge
- IHI call 13

Call topic(s):

1. **HORIZON-HLTH-2027-01-CARE-02:** Personalised approaches to reduce risks from Adverse Drug Reactions due to administration of multiple medications
2. **HORIZON-HLTH-2027-03-TOOL-04:** Virtual Human Twins (VHTs) for integrated clinical decision support in prevention and diagnosis
3. **HORIZON-MISS-2026-02-CANCER-01:** Virtual Human Twin (VHT) Models for Cancer Research
4. **EIC Pathfinder - Challenge** : Biotechnology for Healthy Ageing
5. **EIC Pathfinder - Challenge** : Biomarker-based tools to guide deployment of ageing interventions
6. **EIC Pathfinder – Challenge** : New approach methodologies (NAMs) that replace animal models for preclinical testing of ageing interventions
7. **IHI Call 13** An AI foundation toxicology model and framework to support waiving a second species in drug safety studies

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Do you have other partners for this topic (which partners/country)?	-

Profile of partner sought

Role	☒ technology development	☒ research	☐ training
	☐ dissemination	☐ demonstration	☐ other _____
Country /region	☐		
Expertise required			

I agree with the publication of my contact data: ☒ YES ☐ NO

CYTOCAST DIGITAL TWIN Platform™

Reveal the risks. Understand mechanisms. Advance the best.

AI- and simulation-powered platform integrating systems biology, machine learning, and high-performance computing to predict clinically relevant side effects early in drug development with interpretable, mechanism-linked outputs.

>7,700	15	>1,000	0.70
proteins modeled	tissue types	MedDRA PT side effects	median accuracy, Gold-tier*

How the platform works

The Cytocast platform **predicts clinically relevant side effects through a multi-layer modeling pipeline**. Starting from compound structure (SMILES string), AI models identify potential on- and off-target interactions.

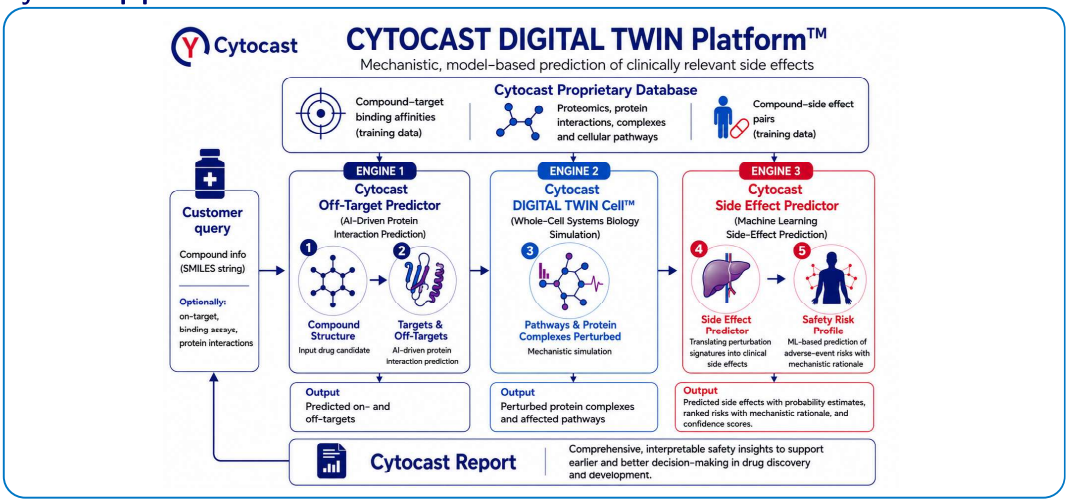
Perturbations propagate through protein complexes[1] and signaling pathways using the CYTOCAST DIGITAL TWIN Cell™ simulation, after which system perturbations are mapped to clinical phenotypes using machine learning models. This mechanistic chain works in both directions: it supports not only prediction of side effects, but also mechanistic interpretation at pathway and off-target level.[2]

Core output

Interpretable safety reports linking predicted adverse-event risks to molecular interactions, perturbed protein complexes, affected pathways, and confidence-ranked side-effect profiles.

The scalable architecture of the platform supports secure integration into pharmaceutical R&D workflows.

Cytocast pipeline



Where Cytocast fits in R&D

DISCOVERY / VIRTUAL SCREENING
Cytocast Screener™
High-throughput triage of hundreds to thousands of compounds during early discovery.

→

LEAD OPTIMIZATION
Cytocast Optimizer™
Comparative safety reasoning to guide compound optimization and series prioritization.

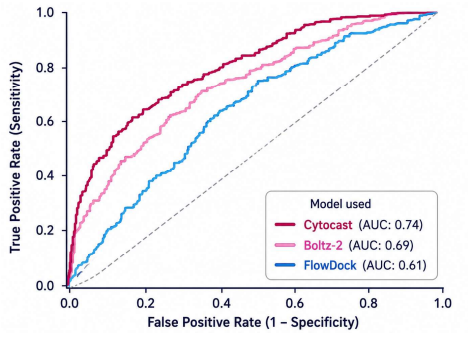
→

CANDIDATE NOMINATION
Cytocast Nominator™
Mechanistic safety reports supporting preclinical development and preparation for first-in-human clinical studies.

Validation and predictive performance

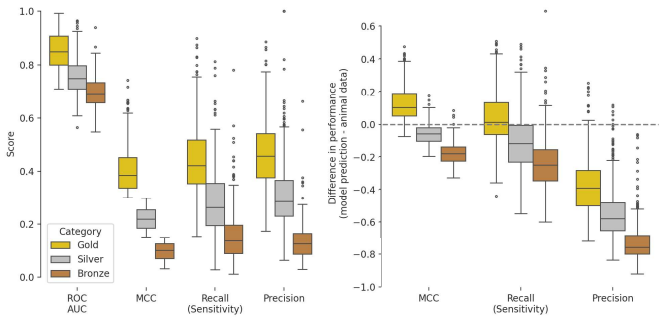
Cytocast validation evaluates: **(i)** compound–protein interaction prediction, **(ii)** clinically observed side-effect ranking, and **(iii)** translational performance relative to animal-to-human toxicity benchmarks. *Gold-tier metrics represent the current decision-grade operating range.

Off-target prediction benchmarking (ROC)



ROC benchmarking shows Cytocast achieving the highest discriminative performance, with an **AUC of 0.74** compared with **0.69 for Boltz-2** and **0.61 for FlowDock**.

Performance relative to animal-to-human translation



Cytocast Gold-tier predictions outperform published animal-to-human toxicity benchmarks (*Clark & Steger-Hartmann, 2018*), demonstrating **improved predictive performance and enhanced detection of clinically relevant safety risks.**

Side-effect prediction performance

- **567 predicted side-effect categories**, stratified into Gold, Silver and Bronze reliability tiers, with **113 clinically relevant side effects in the Gold tier.**
- Most reliable predictions: median balanced accuracy ~**0.70** (IQR 0.68–0.76), median specificity ~**0.85**, and median sensitivity ~**0.58**.

Interpretability

- Predictions are linked to **targets, off-targets, complexes, and pathways**, supporting hypothesis generation and mechanistically grounded safety assessment.

Platform Coverage

- **7,700+ proteins modeled**
- **15 tissue types simulated**
- Predicts **1,000+ MedDRA PT side effects**, compared with approximately **283** commonly assessed in animal toxicology.

Rare-event prediction robustness

- **Rare-event prediction:** balanced accuracy around **0.70** across major organ systems, accounting for class imbalance inherent in rare-event side-effect prediction.

Platform strengths

- **Mechanistically grounded** prediction rather than chemistry-only similarity.
- **Whole-cell, multi-tissue simulation** for system-level biological context.
- **Transparent reliability** via tiered prediction stratification.
- **High-confidence predictions** provide decision-relevant insight into safety risks.
- Enables **large-scale safety assessment** across compound portfolios **at a fraction of the time and cost of traditional animal studies.**
- **Continuous improvement** with documented performance gains.
- **Clinically framed output** using observed side effects.
- Designed to **support earlier go/no-go and prioritization decisions.**
- **Aligned with model-informed drug development frameworks (FDA/EMA MIDD).**

Relevant publications

1. Computational tools to predict context-specific protein complexes. *Current Opinion in Systems Biology*.
2. Digital twin approaches for interpretable side effect prediction in drug discovery. *Drug Discovery Today*.

cytocast.com
info@cytocast.com