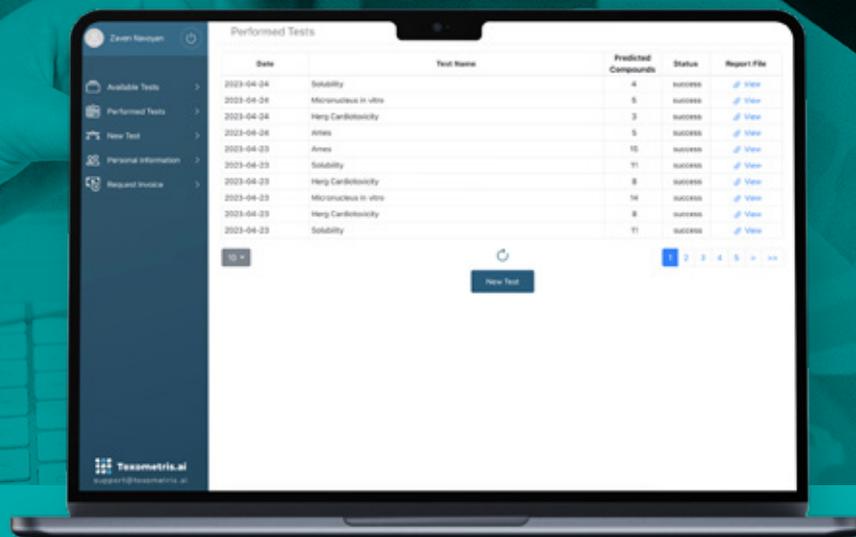


Toxometris.ai Integrates with eLabNext to Accelerate Toxicity Predictions and Drug Design



BOSTON, MA (October 2023) – Today, eLabNext, an Eppendorf Group Company offering a flexible, AI-powered Digital Laboratory Platform equipped with a Laboratory Inventory Management System (LIMS) and Electronic Lab Notebook (ELN), announced the inclusion of Toxometris.ai, an artificial intelligence (AI) tool that performs precise in silico toxicity and ADME property predictions of chemicals and substances, in eLabNext’s add-on library, the eLabMarketplace.

The integration of the Toxometris.ai platform enables eLabNext users to access a powerful report on a chemical compounds’ physicochemical, biological, and toxic activity in just a few clicks, reducing researchers’ reliance on expensive and time-consuming wet lab testing in the early stages of pre-clinical drug development.

“Our vision has always been to replace experimental in vivo safety assessment methods

experimental in vivo safety assessment methods with hybrid models that combine in silico and in vitro technologies to minimize the usage of animals for testing,” says Zaven Navoyan, CEO of Toxometris.ai. “Making the Toxometris.ai platform available in the eLabNext software furthers this goal and enables researchers to easily prioritize their leads for further testing, derisk drug candidates, and ultimately, advance the safest and most effective drug products.”



“Many eLabNext users are deeply entrenched in the pharmaceutical R&D, so we are always looking for techniques and technologies that make their jobs easier and more efficient,” comments Zareh Zurabyan, Head of eLabNext, Americas. “As a platform that has long fostered laboratory digitalization, eLabNext has also been excited to adopt powerful AI tools that help users overcome global barriers, like the high failure rate and cost of small molecule drug development. Toxometris’ shared interest in this issue has created a productive partnership with eLabNext, allowing us to offer our users a new technology for advancing promising drug candidates.”

Currently, the Toxometris.ai add-on supports the following prediction endpoints: Genotoxicity, including AMES, in vitro micronucleus and in vivo micronucleus testing, aqueous solubility, hERG cardiotoxicity, rodent carcinogenicity, and hepatotoxicity predictions. The number of endpoints is constantly increasing and will eventually cover almost all absorption, distribution, metabolism, and excretion (ADME), and toxicity tests.

About Toxometris.ai

Toxometris.ai is a company that combines expertise from academic research labs focusing on in vitro and in vivo assessment of chemicals and an IT company specializing in different AI applications. Within the company, biologists and machine learning specialists work together to create cutting-edge AI models that predict the outcomes of toxicity assessment tests. Leveraging their collective experience, the team can develop highly accurate prediction models that help ensure the safety of chemicals and substances.

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Toxometris.ai

Compound SMILES: C1=CC=CC=C2C(=C1)N=CN=C2

Applicability domain status: In

Mutagenic activity: Non-Mutagenic

Rule-based prediction: Non-Mutagenic

Value type: Experimental

Individual model statistics: Prediction of mutagenic/non-mutagenic activity of the target compound according to models utilizing molecular description, fingerprints and graph based is reported along with the models predictive performance.

	Prediction value	Prediction confidence
Statistical model using descriptors	Non-Mutagenic	0.9
Statistical model using fingerprints	Non-Mutagenic	0.92
Graph neural network model 1	Non-Mutagenic	0.98
Graph neural network model 2	Non-Mutagenic	1.0
Large language model	Non-Mutagenic	0.81

Top 6 positive alerts: Structural alerts (SA) associated with mutagenic activity (positive SA) found in the target compound, ranked according to their likelihood ratio (LR) are reported. Higher LR values indicate the more predictive accuracy for a specific alert. Rule-based prediction is based on the SA highlighted in red.

No alert found					
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Top 6 negative alerts: Structural alerts (SA) associated with non-mutagenic activity (negative SA) found in the target compound, ranked according to their likelihood ratio (LR) are reported. Higher LR values indicate the more predictive accuracy for a specific alert. Rule-based prediction is based on the SA highlighted in red.

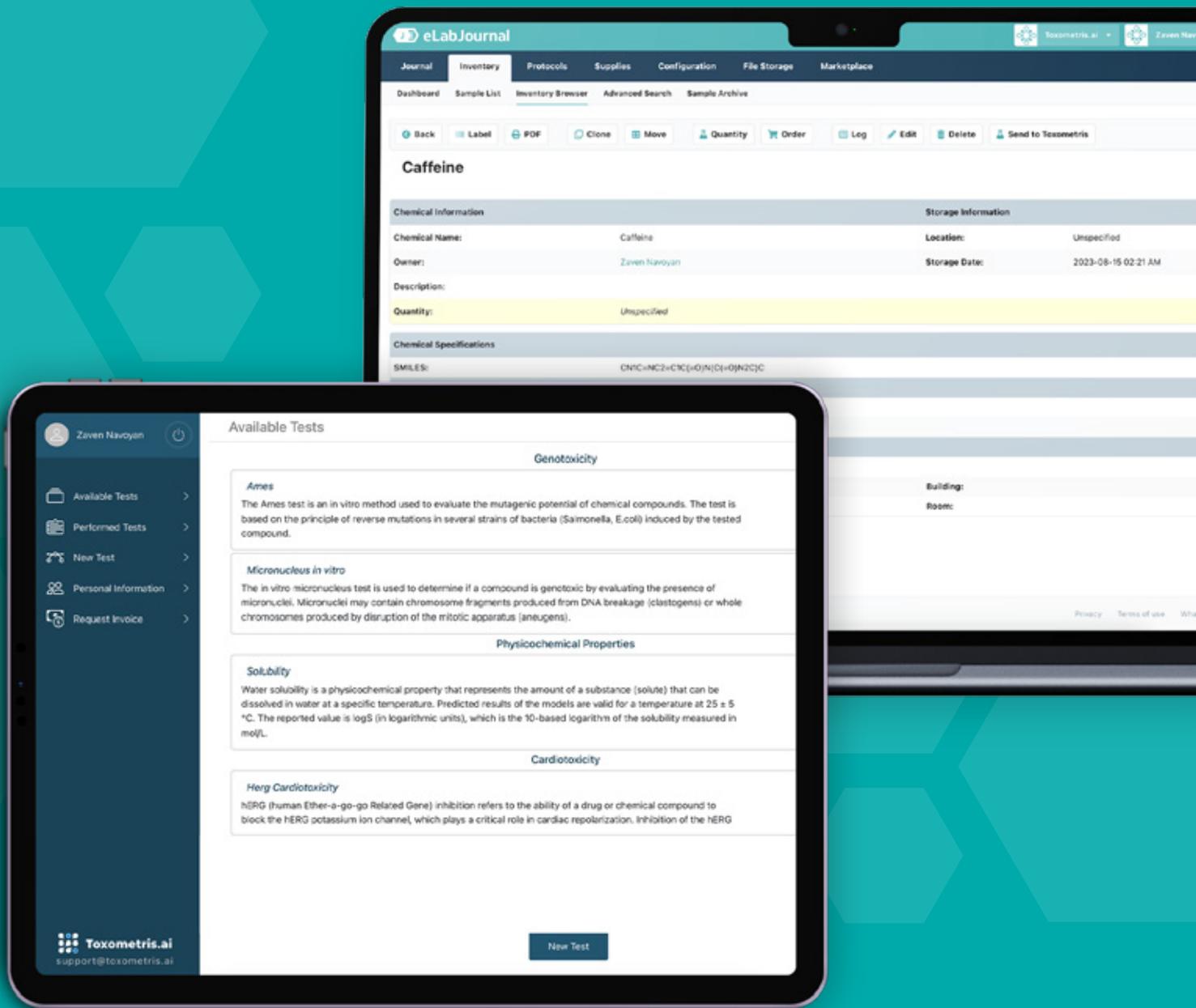
	No alert found				
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LC: 14.99

Read-across study: Experimental values of 3 nearest neighbors from the training set are shown. The threshold for compounds similarity is defined as follows: 1 >= index > 0.85 strongly similar; index <= 0.85 low similar compounds.

SMILES: <chem>C1=CC=C(C=C1)N</chem> Activity: Non-Mutagenic Similarity: 0.98	SMILES: <chem>C1=CC=C(C=C1)N</chem> Activity: Non-Mutagenic Similarity: 0.98	SMILES: <chem>C1=CC=C(C=C1)N</chem> Activity: Mutagenic Similarity: 0.8





About eLabNext

eLabNext is an all-in-one Digital Lab Platform that offers an intuitive and flexible solution to collect, manage, and analyze laboratory information. The software includes modules for an electronic lab notebook, sample tracking, inventory management, and protocol management, as well as a wide range of marketplace add-ons to extend functionality. eLabNext enhances productivity by streamlining the processes of documenting, organizing, searching, and archiving data, samples, and protocols. The data is accessible through cloud-hosted ISO-certified data centers. The software is most suitable for industry R&D labs, ranging from start-up companies to mid-size pharma and biotech companies and academic research groups and institutes.

