

Cellworks Presents Novel Mechanistic Approach to Predicting Drug-Drug Interaction Risk in Oncology at AACR 2026

Study suggests biologically grounded predictions could reduce safety-related failures in combination therapies in drug development and clinical care settings



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[Cellworks Group](#) Inc., the leader in Personalized Therapy Solutions across the Drug Development and Clinical Care Lifecycle, today announced results from a new study demonstrating a mechanistically-based approach to predicting drug-drug interaction (DDI) risk in oncology. The findings highlight the potential of integrating FDA drug label data with gene-level mechanistic insights to identify and classify clinically relevant DDIs in cancer combination therapies.

[Results from this study](#) were presented at the AACR 2026 Annual Meeting in San Diego, California, as poster #1475, titled "An evidence-based tool to systematically identify potential adverse drug-drug interactions."

Combination therapies are widely used in oncology but are often associated with adverse drug-drug interactions that can impact both safety and efficacy. While machine learning approaches have been applied to this challenge, they frequently lack biological interpretability. In this study, Cellworks developed a DDI risk assessment tool that integrates mechanistic biology, shared gene interactions, and clinical evidence to provide an explainable framework for identifying potential risks.

"The toxicity of many drug combinations is unknown," said [James Wingrove](#), PhD, Chief Development Officer at Cellworks and co-author of the study. "This study demonstrates the importance of understanding drug interactions at a mechanistic, biological level in addition to what has been published by the FDA. By linking drug behavior to shared gene pathways and mechanistic impact, clinicians and drug developers can better anticipate toxicity risks and make more informed decisions when selecting and designing novel combination therapies."

Key Findings

- **High Predictive Accuracy:** The DDI tool achieved 100% accuracy when evaluated against a curated dataset of known DDI-positive and DDI-negative drug pairs.
- **Mechanistic Identification of Risk:** Among 544 drug pairs predicted to have efficacy, 6.8% were identified as DDI-positive, with most showing shared gene mechanisms and clear victim-perpetrator relationships. Close to 80% of the DDI-positive positive were identified solely by mechanistic means.
- **Clinical Relevance of Predictions:** Nearly 19% of predicted DDI-positive pairs had documented clinical trial failures due to toxicity, supporting the tool's real-world relevance.
- **Clear Differentiation of Low-Risk Combinations:** The majority (93%) of DDI-negative pairs lacked shared gene pathways or mechanistic relationships, reinforcing the model's specificity.

"What's particularly compelling about this work is the ability to combine multiple layers of evidence - mechanistic biology, regulatory data, and clinical outcomes - into a single, coherent framework," said Ansu Kumar, Senior Director of Research and Distinguished Scientist at Cellworks. "This allows us to move beyond black-box predictions and instead deliver actionable insights grounded in biological rationale. Ultimately, this type of approach can help reduce unexpected toxicities and improve the success rate of combination therapies in clinical development."

Study Design

Researchers developed a drug-drug interaction (DDI) assessment tool using a curated dataset from FDA drug labels, capturing drug-gene and drug-drug interactions across 338 approved therapies. The approach evaluates shared gene mechanisms, mechanistic impact, and supporting clinical evidence to classify potential DDIs. Performance was assessed using both a curated validation dataset and a larger set of mechanistically predicted drug combinations. By integrating regulatory data with mechanistic insights and clinical evidence, this method provides a structured and explainable framework for evaluating DDI risk in oncology.

The Cellworks Platform

The Cellworks Platform applies mechanistic AI to perform computational biosimulation of protein-protein interactions, enabling in silico modeling of tumor behavior using genomic data from next-generation sequencing (NGS). This approach allows clinicians to evaluate how personalized treatment strategies interact with a patient's unique tumor network. At the core of the platform is the Cellworks Computational Biology Model (CBM), a mechanistic network encompassing more than 6,000 human genes, 30,000 molecular species, and 600,000 molecular interactions. The CBM and its drug models biosimulate how specific compounds or combinations affect disease pathways, producing a therapy response prediction that can guide treatment selection. The CBM has been validated across multiple clinical datasets, with findings featured in more than 125 peer-reviewed presentations and publications in collaboration with global partners.

About Cellworks Group

Cellworks Group, Inc. is dedicated to improving patient outcomes by harnessing the power of computational science to deliver Personalized Therapy Solutions across the Drug Development and Clinical Care Lifecycle. The Cellworks Platform predicts patient-specific therapy response for oncology and other complex diseases using a mechanistic Computational Biology Model (CBM), AI and biosimulation technology. Cellworks is backed by Artiman Ventures, Bering Capital, Sequoia Capital, UnitedHealth Group and Agilent Ventures. Headquartered in South San Francisco, the company also operates a CLIA-certified computational lab in Franklin, Tennessee. Learn more at www.cellworks.life.

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