



**Weida Tong, PhD**

# AI: Revolutionizing Chemical Safety

## *AI Model Redefines Testing Methods for Enhanced Efficiency*

Dr. Tong is a distinguished scientist heading the National Center for Toxicological Research (NCTR) Division of Bioinformatics and Biostatistics within the U.S. Food and Drug Administration. He is widely recognized for his work predicting the safety of chemicals and drugs using computer-based AI (Artificial Intelligence) models, applying existing chemical property data to predict potential toxicity.

The goal is to replace animal testing with AI models that can accurately and quickly predict the safety of a chemical. This summary focuses on Dr. Tong's efforts to develop virtual animal models.

## **The Challenge**

Testing products using animals can be time-consuming, costly, and has ethical concerns. Additionally, the results of animal testing may not always translate well to human health. Scientists are in search of more accurate and efficient methods to test product safety. Regulatory agencies and companies also have an interest in ensuring that products are safe and effective before they are available to the public.

Computer-based models have been used in the past, but at the time were not accurate enough to replace animal testing entirely, often lacking the ability to predict toxicity across a broad range of chemicals. Previous models were also not reliable enough to meet regulatory requirements.



## **The Solution**

Dr. Tong and his team have developed the AI model AnimalGAN that can predict the toxicity of chemicals with remarkable accuracy, decreasing reliance on animal testing to effectively determine chemical safety. The potential uses for the AnimalGAN model are vast. It could be used to refine animal studies that assess the safety of a wide range of products, from cosmetics to industrial chemicals and pharmaceuticals.

By accurately predicting toxicity, the model may also help to identify potentially harmful chemicals earlier in product development. AnimalGAN may not only reduce animal testing but also reduce the likelihood of adverse effects on human health and the environment.

## Methods & Data

Dr. Tong and his team used computer programs called deep learning algorithms to create the AnimalGAN model, which then “learned” to predict chemical toxicity. They trained the model using a large existing database of toxic chemicals and then tested the model on chemicals that were not in the database to determine if toxicity was accurately predicted. The model was able to generate accurate results for many different types of chemicals, making it a very useful tool for evaluating the safety of new products.

## Next Milestones

The team’s next goal is to refine the AnimalGAN model to further enhance its accuracy, resilience, and regulatory application. More chemicals with a wider range of toxicity levels will be included to ensure that the predictive ability of the model is current and reliable, and to further validate the model using established toxicity guidelines. By improving the accuracy and efficiency of toxicity testing, Dr. Tong and his team hope to reduce the need for animal studies and promote more effective methods for product safety evaluation.

Furthermore, the team is developing a new framework called “TRIAL” for the effective and efficient use of AI and machine learning technologies at the FDA. This framework is based on five key principles: Transparency, Reliability, Interpretability, Applicability, and Liability. By adhering to these principles, the team hopes to ensure that AI is used effectively and uniformly in the regulatory space, setting new standards for safety assessments.

## Contact & Additional Information



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