

2024 NCTR SOT Presentations – March 11, 2024

NCTR Divisions

Division of Bioinformatics and Biostatistics (DBB)
Division of Biochemical Toxicology (DBT)
Division of Genetic and Molecular Toxicology (DGMT)
Division of Microbiology (DM)
Division of Neurotoxicology (DNT)
Division of Systems Biology (DSB)
Office of Scientific Coordination (OSC)

9:15 AM - 11:15 AM (ToxExpo, Exhibit Hall C, Salt Palace Convention Center)

POSTER SESSION: Skin

1. Luísa Camacho (DBT). **Abstract ID:** 3188, **Poster Board Number:** P297.
Title: "Permeation of Select Dermatological Product Ingredients Through Diverse Skin Types In Vitro"
Additional Comments: Presenter: Luísa Camacho. Authors and Affiliations: A. T. Salminen, R. P. Felton, N. C. Twaddle, K. J. Davis, L. Elkins, F. A. Beland, N. An, Y. Zang, J. Srinivasan, L. M. Katz, P. Manga, and L. Camacho.

POSTER SESSION: Medical Devices

1. Shelby Skoog (FDA/CDRH). **Abstract ID:** 3360, **Poster Board Number:** P485.
Title: "Evaluation of the Ability of the In Vitro Reconstructed Human Epidermis (RhE) Irritation Assay to Predict the Irritation Potential of Medical Devices Compared with the In Vivo Intracutaneous Reactivity Assay per ISO 10993-23"
Additional Comments: Presenter: Shelby Skoog. Authors and Affiliations: S. Skoog¹, C. Silva², T. Kudlyk², N. Twaddle², C. Ghosh¹, L. Camacho², and P. Goering¹. ¹Center for Devices and Radiological Health (US FDA), Silver Spring, MD; and ²National Center for Toxicological Research (US FDA), Jefferson, AR.

10:20 AM - 10:50 AM (Grand Ballroom F, Salt Palace Convention Center)

SYMPOSIUM SESSION: Looking through the Haze: Is the Picture Any Clearer on the Effects of Cannabis and Cannabis-Related Products on Reproduction and Development?

1. Si Chen (DBT). **Abstract Number:** 1035.
Title: "Cannabidiol and Its Main Metabolites Induced Toxicity in Mouse and Human Sertoli Cells"

11:45 AM - 1:45 PM (ToxExpo, Exhibit Hall C, Salt Palace Convention Center)

POSTER SESSION: Epigenetics

1. Marta Pogribny (DBT). **Abstract Number:** 3125, **Poster Board Number:** P230.
Title: "Effect of food-grade titanium dioxide exposure on epigenetic outlook in human cells"



POSTER SESSION: Genotoxicity/DNA Repair

1. Xiaoqing Guo (DGMT). **Abstract Number:** 3094, **Poster Board Number:** P198.
Title: "In vitro mutagenicity assessment of *N*-nitrosodimethylamine in 2D and 3D HepaRG cell cultures using High-Fidelity sequencing"
2. Jaime Miranda-Colon (DGMT). **Abstract Number:** 3095, **Poster Board Number:** P199.
Title: "Assessment of In Vivo Chemical Mutagenesis by HiFi Sequencing"
3. Xilin Li (DGMT). **Abstract Number:** 3090, **Poster Board Number:** P194.
Title: "Mutagenicity and Genotoxicity of Twelve Nitrosamine Drug Substance-Related Impurities in Human TK6 Cells: Correlation with Enhanced Ames Test"
4. Mason Pearce (DGMT). **Abstract Number:** 3096, **Poster Board Number:** P200.
Title: "Effects of Cisplatin on Erythrocyte PIG-A Mutation Frequencies of Cancer Patients"
5. Javier Revollo (DGMT). **Abstract Number:** 3097, **Poster Board Number:** P201.
Title: "Determination of the Background Mutation Frequencies of TK6 and L5178Y Cell Cultures by Clone Sequencing"
6. Tao Chen (DGMT). **Abstract Number:** 3091, **Poster Board Number:** P195.
Title: "Application of Duplex Sequencing to Evaluate Mutagenicity of Aristolochic Acid and Methapyrilene in Fisher 344 Rats"



2024 NCTR SOT Presentations – March 12, 2024

NCTR Divisions

Division of Bioinformatics and Biostatistics (DBB)
Division of Biochemical Toxicology (DBT)
Division of Genetic and Molecular Toxicology (DGMT)
Division of Microbiology (DM)
Division of Neurotoxicology (DNT)
Division of Systems Biology (DSB)
Office of Scientific Coordination (OSC)

9:15 AM - 11:15 AM (ToxExpo, Exhibit Hall C, Salt Palace Convention Center)

POSTER SESSION: Evaluation of Reproductive, Developmental, and Genetic Toxicities of Eugenol using *Caenorhabditis elegans* Model

1. Tao Chen (DGMT). **Abstract Number:** 3759. **Poster Board Number:** P247

9:45 AM - 10:00 AM (Grand Ballroom J, Salt Palace Convention Center)

ORAL PRESENTATION: Advances in Mechanisms of Drug- and Diet-Induced Liver Injury

1. Rose Willett (DBT). **Abstract Number:** 2033.
Title: "Development of severe NASH-like liver injury by chronic administration of a high-fat and high-sucrose diet in mice"

11:45 AM - 1:45 PM (ToxExpo, Exhibit Hall C, Salt Palace Convention Center)

POSTER SESSION: Respiratory Toxicology I

1. Elysia Masters (DSB). **Abstract Number:** 4255. **Poster Board Number:** P829.
Title: "SARS-CoV-2 614G, Delta and BA.1 Induce Distinct Organ-Specific Pathology in K18-hACE2 Transgenic Mice"
2. Yuxi Li (DBT). **Abstract Number:** 3871. **Poster Board Number:** P379.
Title: "Induction of apoptosis by cannabidiol and its main metabolites in human Leydig cells"

POSTER SESSION: Immunotoxicity II

1. Brandon Canup (DBT). **Abstract Number:** 4156. **Poster Board Number:** P694.
Title: "Survey of Sex-Based Immune Differences following Food-Grade Titanium Dioxide Exposure in Human Peripheral Blood Mononuclear Cells and Plasma"

POSTER SESSION: Developmental and Juvenile Toxicology

1. John Talpos (DNT). **Abstract Number:** 3840. **Poster Board Number:** P343.
Title: "The effects of early life exposure to the chemotherapeutics cisplatin or methotrexate on adult measures of motivation, reversal learning, and attention in the rat"



POSTER SESSION: Liver: In Vivo

1. Volodymyr Tryndyak (DBT). **Abstract Number:** 3724. **Poster Board Number:** P211.
Title: "Transcriptomic alterations associated with the progression of nonalcoholic fatty liver disease in CC042 Collaborative Cross mice."

2:15 PM - 4:15 PM (ToxExpo, Exhibit Hall C, Salt Palace Convention Center)

POSTER SESSION: New Approach Methods: In Vitro I

1. Qiang Shi (DSB). **Abstract Number:** 4174. **Poster Board Number:** P723.
Title: "Donor-dependent responses to acetaminophen in human primary liver cells cultured in a liver microphysiological system"

POSTER SESSION: Neurotoxicity: General

1. Qiang Gu (DNT). **Abstract Number:** 3781. **Poster Board Number:** P274.
Title: "Combined tissue-clearing and Fluoro-Gold for brain vasculature labeling"
2. Kelly Mercer (DSB). **Abstract Number:** 3791. **Poster Board Number:** P284.
Title: "SARS-Co V-2 614G induced marked neurodegeneration and microglial activation in K18-hACE2 mice compared to more recent variants"

2:15 PM - 2:30 PM (Room 250 D, Salt Palace Convention Center)

ORAL PRESENTATION: Advancements in Cardiotoxicity Assessment

1. Huixiao Hong (DBB). **Abstract Number:** 2042.
Title: "Developing Machine Learning and Deep Learning Models for Predicting hERG Blockade of Compounds to Assist Drug Safety Assessment"

5:10 PM - 5:30 PM (Grand Ballroom A, Salt Palace Convention Center)

ORAL PRESENTATION: Nitrosamines: mechanistic evidence to support subclasses with varying mutagenic potency

1. Robert Heflich (DGMT). **Abstract Number:** 1210.
Title: "FDA *N*-nitrosamine drug impurity project" (Also participating in panel discussion after presentations: Carcinogenic potency assessment and other hot topics for regulation of *N*-nitrosamines: a panel discussion)



2024 NCTR SOT Presentations – March 13, 2024

NCTR Divisions

Division of Bioinformatics and Biostatistics (DBB)
Division of Biochemical Toxicology (DBT)
Division of Genetic and Molecular Toxicology (DGMT)
Division of Microbiology (DM)
Division of Neurotoxicology (DNT)
Division of Systems Biology (DSB)
Office of Scientific Coordination (OSC)

9:15 AM - 11:15 AM (ToxExpo, Exhibit Hall C, Salt Palace Convention Center)

POSTER SESSION: Cardiovascular Toxicology/Hemodynamics

1. Prathyusha Bagam (DSB). **Abstract Number:** 4660. **Poster Board Number:** P547.
Title: "Investigating the protective role of dexrazoxane against doxorubicin induced cardiotoxicity using human-induced pluripotent stem cell-derived cardiomyocytes."

POSTER SESSION: Natural Products

1. Nan Mei (DGMT). **Abstract Number:** 4531. **Poster Board Number:** P363.
Title: "Luteolin-Induced Cytotoxicity and Genotoxicity in Human Lymphoblastoid TK6 Cells"

POSTER SESSION: Stem Cell Biology and Toxicology

1. Li Pang (DSB). **Abstract Number:** 4610. **Poster Board Number:** P447.
Title: "Predicting Oncology Drug-Induced Cardiotoxicity with Donor-Specific iPSC-CMs - A Proof-of-Concept Study with Doxorubicin"

11:45 AM - 1:45 PM (ToxExpo, Exhibit Hall C, Salt Palace Convention Center)

POSTER SESSION: Computational Toxicology I

1. Kiara Fairman (DBT). **Abstract Number:** 4361. **Poster Board Number:** P146.
Title: "Using PBPK Modeling to Identify the Cause of Pharmacokinetic Differences between Sexes"
2. Minjun Chen (DBB). **Abstract Number:** 4358. **Poster Board Number:** P143.
Title: "Drug Interaction with UGT Enzymes Is an Important Predictor of Drug-Induced Liver Injury"
3. Jie Liu (DBB). **Abstract Number:** 4377. **Poster Board Number:** P162.
Title: "Developing a machine learning model to repurpose FDA approved drugs for the treatment of COVID-19"
4. Leihong Wu (DBB). **Abstract Number:** 4371. **Poster Board Number:** P156.
Title: "A framework enabling LLMs into regulatory environment for transparency and trustworthy: A case study on drug labeling document"



5. Dongying Li (DBB). **Abstract Number:** 4373. **Poster Board Number:** P158.
Title: "DICTrank: The largest Dataset of Comprehensive Annotation for Drug-Induced Cardiotoxicity Using FDA Labeling Documents"
6. Dong Wang (DBB). **Abstract Number:** 4374. **Poster Board Number:** P159.
Title: "Optimize in vitro assay based prediction models for drug toxicity by combining adverse outcome pathway (AOP) networks and the topological properties of Bayesian networks"

POSTER SESSION: Neurotoxicity: Developmental II

1. Cheng Wang (DNT). **Abstract Number:** 4452. **Poster Board Number:** P256.
Title: "Assessing the Developmental Effects of Fentanyl Using Neural Stem Cell Models"
2. Chengzhong Cai (DSB). **Abstract Number:** 4461. **Poster Board Number:** P265.
Title: "Investigation of the Developmental Neurotoxicity of Opioids using Human Induced Pluripotent Stem Cells (hiPSCs)"

2:15 PM - 4:15 PM (ToxExpo, Exhibit Hall C, Salt Palace Convention Center)

POSTER SESSION: New Approach Methods: Computational

1. Xi Chen (DBT). **Abstract Number:** 4318. **Poster Board Number:** P102.
Title: "Comparing Conventional Machine Learning Models with Generative AI in Predictive Toxicology"

POSTER SESSION: Bioinformatics

1. Fan Dong (DBB). **Abstract Number:** 4440. **Poster Board Number:** P229.
Title: "Development of a BERT-Based Language Model for Extracting Adverse Events from Social Media Data"
2. Taylor Ingle (OSC). **Abstract Number:** 4438. **Poster Board Number:** P227.
Title: "Exploring Adverse Event Profiling in FDA Approved Monoclonal Antibody Drug Product by Using FDALabel"
3. Wenjing Guo (DBB). **Abstract Number:** 4442. **Poster Board Number:** P231.
Title: "Assessing Quality of Drug Nomenclatures in RxNorm to Enhance Drug Safety Surveillance using Unstructured Data"
4. Ting Li (DSB). **Abstract Number:** 4439. **Poster Board Number:** P228.
Title: "TransORGAN: An Artificial Intelligence Mapping of Rat Transcriptomic Profiles between Organs, Ages, and Sexes"



2024 NCTR SOT Presentations – March 14, 2024

NCTR Divisions

Division of Bioinformatics and Biostatistics (DBB)
Division of Biochemical Toxicology (DBT)
Division of Genetic and Molecular Toxicology (DGMT)
Division of Microbiology (DM)
Division of Neurotoxicology (DNT)
Division of Systems Biology (DSB)
Office of Scientific Coordination (OSC)

8:30 AM - 11:30 AM (ToxExpo, Exhibit Hall C, Salt Palace Convention Center)

POSTER SESSION: Late-Breaking 1

1. Gregory Pellar (DBT). **Abstract Number:** 5008. **Poster Board Number:** P109.
Title: " Pharmacokinetic Analysis of Nicotine and its Metabolites (Cotinine and trans-3'-Hydroxycotinine) in Male Sprague-Dawley Rats Following Nose-Only Inhalation Exposure, Oral Gavage, and Intravenous Injection of Nicotine"
2. Joshua Xu (DBB). **Abstract Number:** 5010. **Poster Board Number:** P111.
Title: "The Landscape of Fusion Transcripts in Reference Samples Characterized by Targeted RNA Sequencing"
3. Daniel Yeisley (DSB). **Abstract Number:** 5029. **Poster Board Number:** P130.
Title: "Disruption of Primary Human Hepatocyte Functions by 6PPD-Quinone, the Transformation Product of a Ubiquitous Vehicle Tire Rubber Additive"

POSTER SESSION: Late-Breaking 2

1. Yiyang Wang (DGMT). **Abstract Number:** 5070. **Poster Board Number:** P171.
Title: "Integration of RNA Expression to Evaluate the Developmental Toxicity of Busulfan in Human Embryonic Stem Cells"
2. Yiyang Wang (DGMT). **Abstract Number:** 5067. **Poster Board Number:** P168.
Title: "Evaluation of the Developmental Toxicity of Busulfan in an in vitro Human Placental Barrier-embryo Co-culture System" (Presenting Author: Ying Chen – DGMT)

POSTER SESSION: Late-Breaking 3

1. Richard Beger (DSB). **Abstract Number:** 5085. **Poster Board Number:** P186.
Title: "Comparison of miRNA and Proteomics Profiles in COVID-19 Patients with Mild, Moderate, and Severe Symptoms" (Presenting: Qiang Shi – DSB)
2. Chandra Mohan Reddy Muthumula (DM). **Abstract Number:** 5087. **Poster Board Number:** P188.
Title: "Reshaping the gut microbial ecosystem: Impact of gestational antiretrovirals exposure on short chain fatty acid producers in aged rat offspring"



POSTER SESSION: Late-Breaking 4

1. Yueyi Sun (DGMT). **Abstract Number:** 5129. **Poster Board Number:** P230.
Title: "Comparison of the Inhalation Toxicity of Ortho-Phthalaldehyde in a Human Air-Liquid Interface Airway Model using Two Aerosol Exposure Systems"

POSTER SESSION: Late-Breaking 6

1. Fang Liu (DNT). **Abstract Number:** 5205. **Poster Board Number:** P306.
Title: " Assessing the Effects of Methadone, Buprenorphine, and Nicotine on Human Neural Stem Cells"

POSTER SESSION: Late-Breaking 7

1. Yuan Le (DMGT). **Abstract Number:** 5213. **Poster Board Number:** P315.
Title: "Evaluation of the Genotoxicity of Ortho-Phthalaldehyde in a Human In Vitro Organotypic Airway Tissue Model and Human Lymphoblastoid TK6 Cells"



Satellite Meeting at the SOT 63rd Annual Meeting

Title: AI at FDA-National Center for Toxicological Research

Type: Workshop

Host: Dr. Weida Tong , US FDA/National Center for Toxicological Research

Description:

The Division of Bioinformatics and Biostatistics at the FDA's National Center for Toxicological Research has been at the forefront of harnessing AI and machine learning technologies since its inception. This workshop is designed to highlight the Division's latest advancements, placing particular emphasis on predictive toxicology. The discussions will delve into pivotal topics such as the application of AI as a viable alternative to traditional animal studies, addressing challenges related to the opioid crisis, exploring insights into endocrine disruptors, and delving into the intricacies of drug-induced toxicity. This comprehensive showcase promises to offer invaluable insights into the innovative strides made by the division in advancing the field of toxicological research through cutting-edge AI and machine learning methodologies.

Time: Thursday, March 14, 2024 (1:00 PM – 3:15 PM)

Location: Salt Palace Convention Center, Room 355A

Schedule: (all speakers' affiliation is FDA-National Center for Toxicological Research)

- 01:00 PM - 01:15 PM Dr. Dongying Li, "DICTrank: The Largest Drug-Induced Cardiotoxicity Reference Dataset to Facilitate the Development of NAMs"
- 01:15 PM – 01:30 PM Dr. Wenjing Guo, "Unraveling Drug Nomenclature Chaos: A Comprehensive Quality Assessment of RxNorm for Enhanced Drug Safety Surveillance"
- 01:30 PM – 01:45 PM Dr. Xi Chen, "A Comparative Analysis of GAN-based and Conventional Machine Learning Models for Predicting Compound-Induced Responses in Rat Serum Liver Enzymes"
- 01:45 PM – 02:00 PM Dr. Ting Li, "TransOrGAN: An Artificial Intelligence Mapping of Rat Transcriptomic Profiles among Organs"
- 02:00 PM – 02:15 PM **Break**
- 02:15 PM – 02:30 PM Dr. Binsheng Gong, "An Introduction to the SEQC2 Manually Reviewed Benchmarking Indel Set and Its Potential Use in AI-based Variant Calling Models"
- 02:30 PM – 02:45 PM Dr. Fan Dong, "BERT-based Language Model for Accurate Drug Adverse Event Extraction from Social Media: Implementation, Evaluation, and Contributions to Pharmacovigilance Practices"
- 02:45 PM – 03:00 PM Dr. Leihong Wu, "A Framework Enabling LLMs into Regulatory Environment for Transparency and Trustworthiness: A Case Study with Drug Labeling Document"
- 03:00 PM – 03:15 PM Dr. Joshua Xu, "Elevating Pharmacovigilance with Advanced AI: A Study on LLM-Based Literature Screening"

