

# National Center for Toxicological Research (NCTR)

## 2023 NCTR SOT Presentations – March 20, 2023

### *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)

### **9:00am-10:45am (ToxExpo, Hall C, Music City Center)**

#### **POSTER SESSION: ALTERNATIVES TO MAMMALIAN MODELS I**

1. Qiang Shi (DSB). **Abstract Number** 3005, **Poster Board Number** P106. **Poster Title:** *Lessons Learned in Establishing a Reliable and Low-Cost Assay for Urea Production in Human Primary Hepatocytes Cultured in a Liver Chip for the Study of Drug Hepatotoxicity*
2. Xi Chen (DBB). **Abstract Number** 3026, **Poster Board Number** P127. **Poster Title:** *AnimalGAN: A Generative AI Alternative to Animal Clinical Pathology Testing*
3. Prathyusha Bagam (DSB). **Abstract Number** 3027, **Poster Board Number** P128. **Poster Title:** *Cardiotoxicity Assessment of HESI Reference Compounds Using Human iPSC-CMs*
4. Xiaoqing Guo (DGMT). **Abstract Number** 3029, **Poster Board Number** P130. **Poster Title:** *Performance of the Three-Dimensional HepaRG Micronucleus Assay for In Vitro Genotoxicity Testing*

#### **POSTER SESSION: EPIDEMIOLOGY AND PUBLIC HEALTH**

1. Huyen Le (DBB). **Abstract Number** 3190, **Poster Board Number** P306. **Poster Title:** *A Systematic Analysis and Data Mining of Opioid-Related Adverse Events Submitted to the FAERS Database*
2. Paul Rogers (DBB). **Abstract Number** 3191, **Poster Board Number** P307. **Poster Title:** *Assessment of Modified Sandwich Estimator for Generalized Estimating Equations with Application to Opioid Poisoning in MIMIC-IV ICU Patients*
3. Wen Zou (DBB). **Abstract Number** 3192, **Poster Board Number** P308. **Poster Title:** *RxNorm for Drug Name Normalization: A Case Study of Prescription Opioids in the US FDA Adverse Events Reporting System*

#### **POSTER SESSION: REPRODUCTIVE AND DEVELOPMENTAL TOXICOLOGY I**

Yiyang Wang (DGMT). **Abstract Number** 3542, **Poster Board Number** P667. **Poster Title:** *Assessing the Developmental Toxicity of Busulfan in an In Vitro Human Placental Barrier-Embryo Co-culture System*

#### **POSTER SESSION: CARCINOGENICITY**

Rose Willett (DBT). **Abstract Number** 3598, **Poster Board Number** P726. **Poster Title:** *DNA Methylation and Transcriptomic Alterations Induced by Extended Treatment of Normal Human MCF10A Mammary Gland Epithelial Cells with Non-cytotoxic Doses of Lorcaserin*

### **9:15am-9:30am Session Room: Music City Center, Room 209**

#### **PLATFORM SESSION: EXPLORING TIME AND CELL DIVERSITY IN TOXICOGENOMICS SPACE**

Carlos Wells (DBT). **Abstract Number:** 2000, **Oral Presentation Title:** *Effect of Food-Grade Titanium Dioxide on DNA Methylation in Human Cells*

## National Center for Toxicological Research (NCTR)

### **9:45am-10:05am Session Room: Music City Center, Room 207B**

#### **WORKSHOP SESSION: UNDERSTANDING THE CONCEPT OF SIMILARITY AND ITS APPLICATIONS TO TOXICOLOGICAL RESEARCH AND RISK ASSESSMENT**

Huixiao Hong (DBB). **Abstract Number:** 1054, **Oral Presentation Title:** *Structure similarity based on chemical descriptors, fingerprints, and structural alerts*

### **10:45am-12:30pm (ToxExpo, Hall C, Music City Center)**

#### **POSTER SESSION: DNA DAMAGE AND REPAIR**

1. Nan Mei (DGMT). **Abstract Number** 3226, **Poster Board Number** P343. **Poster Title:** *Evaluation of Newly Developed 14 Human TK6-Derived Cell Lines That Individually Express a Human Cytochrome P450 for Toxicity Studies*
2. Xilin Li (DGMT). **Abstract Number** 3228, **Poster Board Number** P345. **Poster Title:** *Nitrosamine Drug Impurities Induce Genotoxicity in Human Lymphoblastoid TK6 Cells*
3. Yuan Le (DGMT). **Abstract Number** 3229, **Poster Board Number** P346. **Poster Title:** *Actein Contributes to Black Cohosh Extract-Induced Genotoxicity in Human TK6 Cells*
4. Ji-Eun Seo (DGMT). **Abstract Number** 3252, **Poster Board Number** P369. **Poster Title:** *Assessment of DNA Damage-Induced by 10 Nitrosamine Impurities Using 2D and 3D HepaRG Models*
5. Javier Revollo (DGMT). **Abstract Number** 3253, **Poster Board Number** P370. **Poster Title:** *Evaluation of the DNA Mutagenicity of N-hydroxycytidine in Mouse Lymphoma Cells by HiFi and Clone Sequencing*
6. Vasily Dobrovolsky (DGMT). **Abstract Number** 3254, **Poster Board Number** P371. **Poster Title:** *HiFi Sequencing for Detecting In Vivo Somatic Mutation*
7. Jaime Miranda (DGMT). **Abstract Number** 3255, **Poster Board Number** P372. **Poster Title:** *HiFi Sequencing Detects the On- and Off-Target Effects of a Cytosine-to-Thymine Base Editor in E. coli*

#### **POSTER SESSION: BIOTRANSFORMATION/CYTOCHROME P450**

Si Chen (DBT). **Abstract Number** 3267, **Poster Board Number** P386. **Poster Title:** *Study of the Roles of Cytochrome P450 (CYPs) in the Metabolism and Cytotoxicity of Perhexiline*

### **2:30pm-4:15pm (ToxExpo, Hall C, Music City Center)**

#### **POSTER SESSION: COMPUTATIONAL TOXICOLOGY I**

1. Leihong Wu (DBB). **Abstract Number** 3060, **Poster Board Number** P162. **Poster Title:** *Using Language Model to Facilitate COVID-19-Associated Neurological Disorder Literature Analysis: A BERTox Research*
2. Liang Xu (DBB). **Abstract Number** 3061, **Poster Board Number** P166. **Poster Title:** *Development of Random Forest Model for Predicting SARS-CoV-2 Main Protease Binders as Potential Candidates for Repurposing to COVID-19 Treatment*
3. Fan Dong (DBB). **Abstract Number** 3062, **Poster Board Number** P167. **Poster Title:** *Opioid Agonist/Antagonist Database (OADB): A Database to Facilitate Opioid Drug Development*
4. Jie Liu (DBB). **Abstract Number** 3063, **Poster Board Number** P168. **Poster Title:** *Machine Learning Models for Rat Multigeneration Reproductive Toxicity Prediction*

# National Center for Toxicological Research (NCTR)

## 2023 NCTR SOT Presentations – March 21, 2023

### *NCTR Divisions*

Division of Bioinformatics and Biostatistics (DBB)  
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Division of Genetic and Molecular Toxicology (DGMT)  
Division of Microbiology (DM)  
Division of Neurotoxicology (DNT)  
Division of Systems Biology (DSB)

### **9:00am-10:45am (ToxExpo, Hall C, Music City Center)**

#### **POSTER SESSION: COMPUTATIONAL TOXICOLOGY II**

Minjun Chen (DBB). **Abstract Number** 3705, **Poster Board Number** P190. **Poster Title:** *Machine Learning for Predicting Risk of Drug-Induced Autoimmune Diseases by Structural Alerts and Daily Dose*

#### **POSTER SESSION: SYSTEMS BIOLOGY**

Luisa Camacho (DBT). **Abstract Number** 4119, **Poster Board Number** P617. **Poster Title:** *Assessment of the Toxicity of Cannabidiol (CBD) in Rats upon Oral Developmental Exposure*

#### **POSTER SESSION: REPRODUCTIVE AND DEVELOPMENTAL TOXICOLOGY III**

1. Yuxi Li (DBT). **Abstract Number** 4165, **Poster Board Number** P664. **Poster Title:** *Cannabidiol-Induced Transcriptomic Changes and Cellular Senescence in Human Sertoli Cells*
2. Mallikarjun Bidarimath (DSB). **Abstract Number** 4191, **Poster Board Number** P690. **Poster Title:** *COVID-19 Effects on Pregnancy, Prenatal, and Postnatal Development*

### **10:45am-12:30pm (ToxExpo, Hall C, Music City Center)**

#### **POSTER SESSION: SAFETY ASSESSMENT: PHARMACEUTICAL-DRUG DEVELOPMENT II**

Dong Wang (DBB). **Abstract Number** 3867, **Poster Board Number** P357. **Poster Title:** *Obtain Drug Safety Rankings through Meta-analysis of Clinical Trial Data Using Penalized Bayesian Model*

#### **POSTER SESSION: BIOMARKERS**

Syed Imam (DNT). **Abstract Number** 3725, **Poster Board Number** P211. **Poster Title:** *T2-MRI Mapping as a Minimally Invasive Correlate of Central Nervous System (CNS) Toxicity in a Cuprizone Model: A Biomarker Study*

#### **POSTER SESSION: EPIGENETICS**

Ira Roudachevski (DBT). **Abstract Number** 4145, **Poster Board Number** P643. **Poster Title:** *Effect of the Weight-Loss Drug Lorcaserin on DNA Methylation in Mammary Glands of Sprague Dawley Rats*

### **1:45pm-2:00pm Session Room: Music City Center, Room 201**

#### **PLATFORM SESSION: ENHANCING TOXICOLOGY WITH MACHINE LEARNING**

Joshua Xu (DBB). **Abstract Number:** 2032, **Oral Presentation Title:** *PathologAI - a deep learning framework for whole slide classification in preclinical pathology*

## National Center for Toxicological Research (NCTR)

### **2:30pm-4:15pm (ToxExpo, Hall C, Music City Center)**

#### **POSTER SESSION: ALTERNATIVES TO MAMMALIAN MODELS II**

**Chair:** Qiang Shi (DSB)

Tao Chen (DGMT). **Abstract Number** 3619, **Poster Board Number** P101. **Poster Title:** *Whole Genome Sequencing Analysis of Mutagenicity of N-Nitrosodiethylamine Using Caenorhabditis elegans Models*

#### **POSTER SESSION: BIOINFORMATICS**

1. Meng Song (DBB). **Abstract Number** 3727, **Poster Board Number** P213. **Poster Title:** *Deep Learning-Based Genotype Imputation for Enhancing Toxicogenomic Data*
2. Zhiyuan Lu (DBB). **Abstract Number** 3729, **Poster Board Number** P215. **Poster Title:** *Statistical Methods for Exploring Spontaneous Adverse Event Reporting Databases for Drug-Host Factor Interactions*
3. Skylar Connor (DBB),. **Abstract Number** 3732, **Poster Board Number** P218. **Poster Title:** *Development of a Large List of Drugs for the Study of Nephrotoxicity in Drug Discovery*
4. Zoe Li (DBB). **Abstract Number** 3733, **Poster Board Number** P219. **Poster Title:** *Random Forest Model for Predicting  $\mu$  Opioid Receptor Binding Activity for Assisting Development of Opioid Drugs*
5. Ting Li (DBB). **Abstract Number** 3737, **Poster Board Number** P223. **Poster Title:** *DeepAmes: Deep Learning-Powered Ames Test Prediction Using Model-Level Representation*

#### **POSTER SESSION: RISK ASSESSMENT II**

Winjing Guo (DBB). **Abstract Number** 3841, **Poster Board Number** P331. **Poster Title:** *Informing Selection of Drugs for COVID-19 Treatment through Analysis of Adverse Events*

#### **POSTER SESSION: NEUROTOXICITY: DEVELOPMENTAL I**

1. Jacqueline Yeary (DNT). **Number** 3968, **Poster Board Number** P462. **Poster Title:** *Cytokine-Mediated Chemotherapy-Induced Cognitive Impairment in Cisplatin and Methotrexate Treated Sprague Dawley Rats*
2. Wesley Gill (DNT). **Abstract Number** 3975, **Poster Board Number** P469. **Poster Title:** *Examining Immune Modulatory Effects of Perinatal Cannabidiol Exposure in Sprague Dawley Rats*
3. John Talpos (DNT). **Abstract Number** 3979, **Poster Board Number** P473. **Poster Title:** *The Neurotoxic Potential of a Single Dose of Ketamine in Adolescent and Adult Rats*

#### **POSTER SESSION: NEUROTOXICITY: DEVLEOPMENTAL II**

1. Timothy Flanigan (DNT). **Abstract Number** 3985, **Poster Board Number** P479. **Poster Title:** *Behavioral Effects of Cisplatin and Methotrexate Treatment in Juvenile Sprague Dawley Rats*
2. Chengzhong Cai (DSB). **Abstract Number** 3987, **Poster Board Number** P481. **Poster Title:** *Investigation of the Developmental Neurotoxicity of Opioids Using Human-Induced Pluripotent Stem Cells*

#### **POSTER SESSION: NEUROTOXICITY: GENERAL**

Qiang Gu (DNT). **Abstract Number** 4029, **Poster Board Number** P524. **Poster Title:** *A Modified Approach of Fluoro-Jade C Labeling for Neurotoxicity Assessments*

#### **POSTER SESSION: IMMUNOTOXICITY I**

Brandon Canup (DBT). **Abstract Number** 4054, **Poster Board Number** P551. **Poster Title:** *Sex-Based Differences in Inflammatory Responses to Silver Nanoparticles*

# National Center for Toxicological Research (NCTR)

## 2023 NCTR SOT Presentations – March 22-23, 2023

### *NCTR Divisions*

- Division of Bioinformatics and Biostatistics (DBB)
- Division of Biochemical Toxicology (DBT)
- Division of Genetic and Molecular Toxicology (DGMT)
- Division of Microbiology (DM)
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### **March 22, 2023**

#### **8:00am-10:45am Session Room: Karl Dean Ballroom C1, Music City Center**

##### **WORKSHOP SESSION 1195: MOVING STEM CELL-DERIVED NEW APPROACH METHODS TOWARD REGULATORY ACCEPTANCE**

**Chair:** Li Pang (DSB)

Li Pang (DSB). **Abstract Number** 1200, **Oral Presentation Title:** *Predicting Interindividual Variability of Doxorubicin Cardiotoxicity with Induced Pluripotent Stem Cell-Derived Cardiomyocytes*

#### **9:00am-10:45am (ToxExpo, Hall C, Music City Center)**

##### **POSTER SESSION: BIOLOGICAL MODELING**

1. Miao Li (DBT). **Abstract Number** 4323, **Poster Board Number** P188. **Poster Title:** *A Multiscale Physiologically Based Pharmacokinetic (PBPK) Model to Predict the Plasma Concentration and the Tissue Distribution of Doxorubicin*
2. Kiara Fairman (DBT). **Abstract Number** 4333, **Poster Board Number** P198. **Poster Title:** *Using Various Machine-Learning Algorithms to Determine the Best Method for Predicting Population Physiologically Based Pharmacokinetic Model Plasma Profiles*

#### **10:45am-12:30pm (ToxExpo, Hall C, Music City Center)**

##### **POSTER SESSION: KIDNEY**

Elysia Masters (DSB). **Abstract Number** 4310, **Poster Board Number** P174. **Poster Title:** *Evaluating Renal Pathology in Post-COVID-19 Human Autopsy Tissues*

##### **POSTER SESSION: SKIN AND DERMAL TOXICITY**

Alec Salminen (DBT). **Abstract Number** 4449, **Poster Board Number** P322. **Poster Title:** *Parallel Evaluation of Alternative Skin Barrier Models and Excised Human Skin for Dermal Absorption Studies In Vitro*

#### **2:30pm-4:15pm (ToxExpo, Hall C, Music City Center)**

##### **POSTER SESSION: LIVER I: IN VIVO**

**Chair:** Si Chen (DBT)

Volodymyr Tryndyak (DBT). **Abstract Number** 4247, **Poster Board Number** P109. **Poster Title:** *Gene Expression Changes Predict the Severity of NAFLD-Like Liver Injury in Male Collaborative Cross Mice*

## National Center for Toxicological Research (NCTR)

### POSTER SESSION: LIVER II: IN VIVO

1. Dongying Li (DBB). **Abstract Number** 4275, **Poster Board Number** P138. **Poster Title:** *hnRNP-Q and hnRNP-L Influence Drug Metabolism and Toxicity by Regulating mRNA Processing of Drug Metabolizing Enzymes and Nuclear Receptors in HepaRG Cells*

### POSTER SESSION: RESPIRATORY TOXICOLOGY I

- Yueyi Sun (DGMT). **Abstract Number** 4602, **Poster Board Number** P492. **Poster Title:** *Establishing a Continuous Aerosol Exposure Method for Evaluating the Respiratory Toxicity of Ortho-Phthalaldehyde*

**March 23, 2023**

**8:30am-11:30am (Hall A1, Music City Center)**

### POSTER SESSION: LATE-BREAKING 2-4

1. Kumari Karn (DM). **Abstract Number** 5037, **Poster Board Number** P138. **Poster Title:** *Potential Link of High-Fat Diet on the Expression of Alzheimer's Disease-Related Genes in the Ileal Mucosa of Alzheimer's Disease Model of Rats*
2. Leah Latham (DNT). **Abstract Number** 5072, **Poster Board Number** P173. **Poster Title:** *The Effects of Cannabidiol and Its Main Metabolites on Human Neural Stem Cells*
3. Fang Liu (DNT). **Abstract Number** 5081, **Poster Board Number** P182. **Poster Title:** *Comparison of the Effects of Delta-9 Tetrahydrocannabinol and Cannabidiol on Human Neural Stem Cells*
4. Andrew Shen (DNT). **Abstract Number** 5084, **Poster Board Number** P185. **Poster Title:** *Assessment of Potential Developmental Neurotoxicity of Purified Cannabidiol in Sprague Dawley Rats*