

Division of Chemical Toxicology Program



Hyatt Regency	Sunday	8 AM	CRT Young Investigator Award, <i>James Galligan</i>
	Sunday	2 PM	Founders Award, <i>Cynthia Burrows</i>
	Sunday	7 PM	Virtual Poster Session
MCP	Monday	8 AM	Artificial Intelligence in Drug Discovery in Drug Design (w/MEDI)
	Monday	2 PM	Current Approaches to COVID-19 Drug Discovery & Safety Assessment (w/MEDI)
	Monday	7 PM	Sci-Mix
HR	Tuesday	8 AM	Student & Post-Doctoral Scholar Symposium
	Tuesday	2 PM	Chemical Biology on DNA Damage & Repair (w/BIO)
	Tuesday	5 PM	TOXI Keynote, <i>Wei Yang</i>
MCP	Tuesday	7 PM	TOXI in person Poster Session
	Tuesday	8 PM	TOXI Dinner
	Tuesday	9 PM	TOXI Business Meeting & Student Awards
HR	Wednesday	8 AM	Mechanism-Driven Hazard Identification of Chemical Respiratory Allergens
	Wednesday	2 PM	Topics in Chemical Toxicology



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ACS Fall 2022 National Meeting

(Aug 21-25)

Sustainability in a Changing World



Young Investigator

#TOXI



University of Arizona

James Galligan



ACS Technical Division
Chemical Toxicology (TOXI)

Founders Award



University of Utah

Cynthia Burrows

#ACSFall2022

Keynote Speaker



NIH - NIDDK

Wei Yang

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TOXI1 - Sunday 08:00am - 12:00pm		
Chemical Research in Toxicology: Young Investigator Award – James Galligan		
Location: Regency A (Hyatt Regency McCormick Place)		
Time (CST)	Abstract Title	Presenting Author
8:00 AM	New Rules and New Tools for Selective Protein Glycation	Rebecca Sheck
8:33 AM	Reactivity Metabolomics and Retrospective Metabolomics – two Techniques to Elucidate Direct Metabolite Conjugates of potential Biological Relevance	Mogens Johannsen
9:06 AM	Uncovering cancer-associated epigenetic events using novel chemical tools	Yael David
9:39 AM	<i>Intermission</i>	
9:54 AM	Sensitive LC-MS/MS quantification of tissue acyl-CoA pools: Potential implications for non-enzymatic protein N-acylation	Andrew James
10:27 AM	New Insights into Acetylation & Oncometabolism from Chemoproteomics	Jordan Meier
11:00 AM	Introduction	Yingsheng Wang
11:10 AM	Establishing metabolic feedback through non-enzymatic post-translational modifications	James Galligan

TOXI2 - Sunday 02:00pm - 6:00pm		
Chemical Research in Toxicology: Founders Award Lecture & Symposium– Cynthia Burrows		
Location: Regency A (Hyatt Regency McCormick Place)		
Time (CST)	Abstract Title	Presenting Author
2:00 PM	Epigenetic marks of DNA and their role in lung cancer	Natalia Tretyakova
2:40 PM	Nimble NEIL N-glycosylases: Interplay between DNA modification, recognition and repair	Sheila David
3:20 PM	RNA methylation in gene expression regulation	Chuan He
4:00 PM	<i>Intermission</i>	
4:15 PM	Nanopore dwell-time analysis identifies stress-dependent rRNA modifications	Aaron Flemming
4:55 PM	Introductory Remarks	Natalia Tretyakova
5:05 PM	Linking DNA damage and repair to gene expression	Cynthia Burrows

TOXI Virtual Poster Session		
Sunday 7-9pm		
Virtual only		
Control ID	Abstract Title	Presenting Author
3732283	In silico elucidation of physicochemical properties factor on activation of THP-1 cells of TiO ₂ NP	Akiko Ohno
3737086	Effects of the nitro-group on the mutagenicity of nitrated benzo[a]pyrenes	Akiko Ohno
3740843	Pro-inflammatory and pro-fibrogenic effects of TiO ₂ and Ag-TiO ₂ photocatalysts in the murine lung	huang xiaoquan
3750881	Exploring regression-based QSTR models for toxicity prediction of diverse pesticides on multiple avian species	Trina Podder
3754932	In vitro toxicity of amorphous silica nanoforms in multiple cell lines	Premkumari Kumarathan

TOXI3 - Monday 08:00am - 12:00pm		
A Developing Role for Artificial Intelligence in Drug Discovery in Drug Design, Development, & Safety Assessment		
Location: Regency A (Hyatt Regency McCormick Place)		
Time (CST)	Abstract Title	Presenting Author
8:00 AM	<i>Introductions</i>	Presiders
8:05 AM	Challenges and Opportunities for AI in Drug Discovery	Patrick Walters
8:45 AM	GLORYx: Using machine learning to predict metabolites for phase I and phase II metabolism	Christina de Bruyn Kops
9:25 AM	<i>Intermission</i>	
9:40 AM	Using Machine Learning to Understand Structural Alerts and the Bioactivation of Medicines	Joshua Swamidass
10:20 AM	Machine Learning in Predictive Toxicology	Jonathan Goodman
11:00 AM	SafetAI – An AI Framework to Facilitate the CDER IND Review	Zhichao Liu
	Poster Rapid Talks	
11:40 AM	Identification and functional characterizations of recognition proteins for major- and minor-groove DNA damage	Andrew Kellum
11:42 AM	Repurposing the antihypertensive drug hydralazine as an inhibitor of AP Endonuclease-1	Tanhaul Islam
11:44 AM	An ELISA-based method for detecting DNA-protein-crosslinks in mitochondria from human cell cultures	Wenyan Xu
11:46 AM	Methylglyoxal as a regulator of AMPK signaling	Dominique Gaffney
11:48 AM	Comparing bottom-up proteomics and the FIRE methodology for untargeted protein adductomics	Andrew Rajcewski

TOXI4 - Monday 02:00pm - 6:00pm		
Current Approaches to COVID-19 Drug Discovery & Safety Assessment		
Location: Regency A (Hyatt Regency McCormick Place)		
Time (CST)	Abstract Title	Presenting Author
2:00 PM	<i>Introduction</i>	Presiders
2:05 PM	Developing Exosome-CD24 as a cytokine-storm mitigator	Zucaï Suo
2:55 PM	Optimizing antiviral therapy with nucleoside analogs for the treatment of COVID-19	Ashley Brown
3:45 PM	<i>Intermission</i>	
4:00 PM	ADME approaches for the Pfizer oral COVID-19 protease inhibitor program	Amit Kalgutkar
4:50 PM	Pan-ErbB inhibition protects from SARS-CoV-2 replication, inflammation, and lung injury	Shirit Einav
	Poster Rapid Talks	
5:40 PM	Single-nucleotide resolution mapping of Abasic Sites in Mitochondrial DNA	CHAOXING LIU
5:42 PM	Human Serum Albumin (HSA)-Cys34 Adducts as Biomarkers of Oxidative Stress (OS)	Yeunook Bae
5:44 PM	Regulatory Role of the Glyoxalase Cycle in Inflammation	Erin Jennings
5:46 PM	Investigation of Structural Effects of 6-oxo-M1dG Lesion in DNA	Yizhi Fu
5:48 PM	Repair of Cisplatin-Induced DNA-Protein Crosslinks in Human Cells	Luke Erber

Sci-Mix - Monday 08:00pm - 10:00pm		
Location: Hall F2 (McCormick Place Convention Center)		
Control ID	Abstract Title	Presenting Author
3737499	Mechanism of perfluorooctanoic acid driven hyperandrogenism in polycystic ovary syndrome	Andrea Address
3740371	Pol k interact with DDX23 to unwind R-loop structure induced by N2-alkyl-dG lesions	Yinan Wang
3744305	Nornitrogen mustard and mitoxantrone cytotoxicity and DNA damage in MDA-MB-231 human breast cancer cells	Kyle Brandt
3746306	Synthesis and fate of 2' radical precursors of uridine and 2'-O-Me uridine	Mel Fernand Bedi
3750052	Altering e-liquid composition and toxicology through the addition of water	Hanno Erythropel
3751869	Conformational heterogeneity of the fluoroaminofluorene-deoxyguanine adduct (dG-FAF) in epigenetically modified sequence contexts	Alicia Crisalli
3753001	Studies of Biochemical Function and Structure of MCM8/9	David McKinzey
3754497	Investigating the molecular events in response to Glyoxalase1 inhibition in breast and prostate cancer cells	Leticia Reque
3738253	An ELISA-based method for detecting DNA-protein-crosslinks in mitochondria from human cell cultures	Wenyan Xu
3743811	Methylglyoxal as a regulator of AMPK signaling	Dominique Gaffney
3743951	Single-nucleotide resolution mapping of Abasic Sites in Mitochondrial DNA	CHAOXING LIU
3740713	Human Serum Albumin (HSA)-Cys34 Adducts as Biomarkers of Oxidative Stress (OS)	Yeunook Bae
3750091	Regulatory Role of the Glyoxalase Cycle in Inflammation	Erin Jennings
3755054	Investigation of Structural Effects of 6-oxo-M1dG Lesion in DNA	Yizhi Fu
3743834	Repurposing the antihypertensive drug hydralazine as an inhibitor of AP Endonuclease-1	Tanhaul Islam
3742011	Comparing bottom-up proteomics and the FIRE methodology for untargeted protein adductomics	Andrew Rajcewski
3743912	Toxicity Induced by Reduced-Graphene Oxide and Impacts from Protein Corona	Wenwan Zhong
3754348	Efficacy Medical Countermeasure agent and Chemical therapeutic development for repurposing agents against Chemical and Biological threat , and bio-modelling capabilities of the MCMs for CBRNe agents	Salako Olatunji
3747045	Human TDP1, APE1, and TREX1 repair 3'-DNA-peptide/protein cross-links arising from abasic sites in vitro	Kun Yang

TOXI5 - Tuesday 08:00am - 12:00pm		
TOXI Student & Post-Doctoral Scholar Symposium		
Location: Regency A (Hyatt Regency McCormick Place)		
Time (CST)	Abstract Title	Presenting Author
8:00 AM	<i>Introductory Remarks</i>	Presiders
8:05 AM	Controlling Protein Glycation with Spatiotemporal Control	Alexander Hurben
8:20 AM	Montelukast neurotoxicity unveiled by MS multiomics – HPA axis and redoxome dysregulation	Catia Marques
8:35 AM	IN VITRO CYP450 ACTIVATION/INHIBITION BY ORGANOPHOSPHOROUS PESTICIDES AND NERVE AGENT SURROGATES USING FLOUROMETRIC ASSAYS	Pratik Shriwas
8:50 AM	Glyoxalase 1 promotes adipogenesis in 3T3-L1 pre-adipocytes	Marissa Trujillo
9:05 AM	Vitamin E acetate in pulmonary surfactant: Biophysical explanation of the EVALI epidemic	Mitchell DiPasquale
9:20 AM	<i>Intermission</i>	
9:30 AM	Role of nuclear factor erythroid 2-related factor 2 and aldo-keto reductases in the metabolic activation of 1-nitropyrene in human lung cells (A549 and HBEC3-KT)	Anthony Su
9:45 AM	Post-labeling assay for the detection of photo-induced non-adjacent anti cyclobutane pyrimidine dimers that form in G-Quadruplex forming sequences	Natalia Gutierrez-Bayona
10:00 AM	Uncovering the role of glutamate in mitochondrial transcription factor A facilitated AP-DNA cleavage reaction	Wenxin Zhao
10:15 AM	Sequencing Oxidative Guanine Damage in DNA using Click Chemistry	Songjun Xiao
10:30 AM	<i>Intermission</i>	
10:55 AM	Monitoring the Formation and Repair Kinetics of Platinum Drug-Induced DNA-DNA Cross-Links by Comprehensive Ultra Performance Liquid Chromatograph-Selective Ion Monitoring (UPLC-SIM) Assays	Arnold Groehler
11:10 AM	Proximity proteomics profiling the interacting proteome of DNA polymerase η	Feng Tang
11:25 AM	Removal of Lesions in NCPs by BER Enzymes is Dependent on the Initiation Step	Treshaun Sutton
11:40 AM	Correlating the mutational signatures of the aflatoxin B1-Fapy-dG adduct with sequence-dependent DNA repair and adduct structure	Rachana Tomar
11:55 AM	<i>Concluding Remarks</i>	Presiders

TOXI6 - Tuesday 02:00pm - 6:00pm Chemical Biology on DNA Damage & Repair Location: Regency A (Hyatt Regency McCormick Place)		
Time (CST)	Abstract Title	Presenting Author
2:00 PM	Going from bad to worse: interstrand cross-links derived from abasic sites in duplex DNA	Kent Gates
2:30 PM	Exploiting Abasic Sites in Mitochondrial DNA: Mechanistic Insights and Functional Implications	Linlin Zhao
3:00 PM	Role of NEIL1-initiated DNA base excision repair in aflatoxin- and inflammatory-driven mutagenesis	R. Stephen Lloyd
3:30 PM	Intermission	
3:45 PM	Obstacles and opportunities for DNA repair in nucleosome core particles	Sarah Delaney
4:15 PM	DNA-protein crosslinking for residue-specific mapping of oxidatively induced DNA lesions in human cells	Yinsheng Wang
4:45 PM	Intermission	
5:00 PM	Introduction	Michael Trakselis
5:03 PM	DNA Repair and RNA Regulation in Multiple Dimensions	Wei Yang

TOXI Reception and Dinner

Tuesday 7:00-9:00pm

Hall F2 (McCormick Place Convention Center)

Carving stations, a la cart sides, and a cash bar.

20x20 draped off area for TOXI

Must have a green circle sticker on badge for entry!

TOXI OPEN Business Meeting

Tuesday 9:00-10:00pm

W181c (McCormick Place Convention Center)

TOX18 Poster Session - In person**Tuesday 7:00-9:00pm****Location: Hall F2 (McCormick Place Convention Center)**

Control ID	Abstract Title	Presenting Author
3737086	Effects of the nitro-group on the mutagenicity of nitrated benzo[a]pyrenes	Kiyoshi Fukuhara
3732283	In silico elucidation of physicochemical properties factor on activation of THP-1 cells of TiO ₂ NP	Akiko Ohno
3750881	Exploring regression-based QSTR models for toxicity prediction of diverse pesticides on multiple avian species	Trina Podder
3728437	Computational Approach for Respiratory Hazard Identification of Flavor Chemicals in Tobacco Products	Reema Goel
3734490	Products generated by amine-catalyzed strand cleavage at abasic site in duplex DNA	Jay Jha
3736759	A Computational Mechanistic Study of the Degradation of Hydro(chloro)fluoroether Volatile Anesthetics	Daniel Sadowsky
3737499	Mechanism of perfluorooctanoic acid driven hyperandrogenism in polycystic ovary syndrome	Andrea Andress
3737942	Quantitation of acrolein and crotonaldehyde-derived DNA adducts in oral brushings from smokers and nonsmokers using liquid chromatography-nanoelectrospray ionization-high resolution tandem mass spectrometry	Guang Cheng
3738157	Method evaluation and validation of fentanyl and fentanyl analogs by LC-MS/MS	James LaPalme
3740371	Pol k interact with DDX23 to unwind R-loop structure induced by N ² -alkyl-dG lesions	Yinan Wang
3739531	Exploration of potential MIE interactions of neonicotinoid pesticides and relevant metabolites by molecular docking to human nicotinic acetylcholine receptors (nAChRs)	Karin Grillberger
3742987	Effects of rotenone neurotoxicity on dopamine release and uptake in zebrafish	Piyanka Hettiarachchi
3744305	Nornitrogen mustard and mitoxantrone cytotoxicity and DNA damage in MDA-MB-231 human breast cancer cells	Kyle Brandt
3744846	Interstrand DNA cross-links generated by an Endo III-derived base excision repair intermediate	Tanhauil Islam
3746029	Occupational aerosols: Characterization, inhibition of lung surfactant, and cytotoxicity	James Liu
3746306	Synthesis and fate of 2' radical precursors of uridine and 2'-O-Me uridine	Mel Fernand Bedi
3750052	Altering e-liquid composition and toxicology through the addition of water	Hanno Erythropel
3751402	Data science pipeline for using the systemic effect of drugs in the prediction of toxicity	Barbara Füzi
3751869	Conformational heterogeneity of the fluoroaminofluorene-deoxyguanine adduct (dG-FAF) in epigenetically modified sequence contexts	Alicia Crisalli
3752702	New approach methods to determine phthalate and phthalate replacement mixture toxicity.	Jordan Crago
3752960	Preferential binding and cleavage from 5'-ends for human mitochondrial genome maintenance nuclease 1 (MGME1) is conferred by a phosphate group	Kathleen Urrutia
3753001	Studies of Biochemical Function and Structure of MCM8/9	David McKinzey
3744212	Effect of nucleosome occupancy on base excision repair	Giovannia Barbosa
3754497	Investigating the molecular events in response to Glyoxalase1 inhibition in breast and prostate cancer cells	Leticia Reque

3754476	Investigating the ability of metformin to scavenge for methylglyoxal and impact downstream biological effects	Ryan Boggess
3749209	Implications of human microglia neuroinflammatory response due to pesticide exposure	Alec Kramer
3740843	Pro-inflammatory and pro-fibrogenic effects of TiO ₂ and Ag-TiO ₂ photocatalysts in the murine lung	Huang Xiaoquan
3739862	Biochemical characterization of colibactin-DNA interstrand crosslink formation using short oligonucleotides	Erik Carlson
3738253	An ELISA-based method for detecting DNA-protein-crosslinks in mitochondria from human cell cultures	Wenyan Xu
3738952	Identification and functional characterizations of recognition proteins for major- and minor-groove DNA damage	Andrew Kellum
3743811	Methylglyoxal as a regulator of AMPK signaling	Dominique Gaffney
3743951	Single-nucleotide resolution mapping of Abasic Sites in Mitochondrial DNA	CHAOXING LIU
3740713	Human Serum Albumin (HSA)-Cys34 Adducts as Biomarkers of Oxidative Stress (OS)	Yeunook Bae
3745529	Mechanism of lesion verification by the human XPD helicase in nucleotide excision repair	Iwen Fu
3750091	Regulatory Role of the Glyoxalase Cycle in Inflammation	Erin Jennings
3755054	Investigation of Structural Effects of 6-oxo-M1dG Lesion in DNA	Yizhi Fu
3754566	Repair of Cisplatin-Induced DNA-Protein Crosslinks in Human Cells	Luke Erber
3743834	Repurposing the antihypertensive drug hydralazine as an inhibitor of AP Endonuclease-1	Tanhau Islam
3742011	Comparing bottom-up proteomics and the FIRE methodology for untargeted protein adductomics	Andrew Rajcewski
3729600	DNA interstrand cross-links induced by C8-modified adenines	Seongmin Lee
3743912	Toxicity Induced by Reduced-Graphene Oxide and Impacts from Protein Corona	Wenwan Zhong
3751660	Identification of N'-Nitrosornicotine-1N-oxide in the Urine of Cigarette Smokers	Yupeng Li
3754348	Efficacy Medical Countermeasure agent and Chemical therapeutic development for repurposing agents against Chemical and Biological threat , and bio-modelling capabilities of the MCMs for CBRNe agents	Salako Olatunji
3754438	Detection, Investigation and its effective Countermeasure of Cyanides and Cyanogen in Natural Occurring Food Substance and as a Chemical threat to Human, respectively	Salako Olatunji
3742011	Comparing bottom-up proteomics and the FIRE methodology for untargeted protein adductomics	Andrew Rajcewski
3747045	Human TDP1, APE1, and TREX1 repair 3'-DNA-peptide/protein cross-links arising from abasic sites in vitro	Kun Yang
3730469	Toxicological analysis of monoazo dyes for sustainable human hair coloration	Tova Williams
3754932	In vitro toxicity of amorphous silica nanoforms in multiple cell lines	Premkumari Kumarathan
Extra	Correlating the mutational signatures of the aflatoxin B1-Fapy-dG adduct with sequence-dependent DNA repair and adduct structure	Rachana Tomar

TOXI9 - Wednesday 08:00am - 12:00pm		
Mechanism-Driven Hazard Identification of Chemical Respiratory Allergens		
Location: Regency A (Hyatt Regency McCormick Place)		
Time (CST)	Abstract Title	Presenting Author
8:00 AM	<i>Introductory Remarks</i>	Kristie Sullivan
8:05 AM	Adverse Outcome Pathway for Low Molecular Weight Respiratory Sensitizers and Weight of Evidence Approaches	Jessica Ponder
8:35 AM	Peptide Reactivity of Low Molecular Weight Respiratory Sensitizers	Nora Krutz
9:05 AM	Protein Reactivity of Phthalic Anhydride using HRMAS and LC-MS/MS Proteomics	Jean-Pierre Lepoittevin
9:35 AM	Defining structural alerts to identify respiratory sensitizers	Steve Enoch
10:05 AM	<i>Intermission</i>	
10:20 AM	<i>Panel Discussion - Q&A with the panel and questions from the audience regarding refining the standing in vitro and in silico test methods to address regulatory needs for identifying chemical hazards</i>	
11:20 AM	<i>Concluding Remarks</i>	Jessica Ponder

TOXI10 - Wednesday 02:00pm - 6:00pm		
Current Topics in Chemical Toxicology		
Location: Regency A (Hyatt Regency McCormick Place)		
Time (CST)	Abstract Title	Presenting Author
2:00 PM	<i>Introductory remarks</i>	
2:05 PM	Similar in vitro metabolic kinetics for 5F-APINACA between CD-1 mouse and human but involve different cytochromes P450	Grover Miller
2:25 PM	Pyridyloxobutyl DNA adducts formed from tobacco specific nitrosamines yield a unique mutational signature in both cell and animal models	Lisa Peterson
2:45 PM	DNA polymerase K is involved in ribosomal DNA repair after benzo(a)pyrene diol epoxide damage	Thomas Spratt
3:05 PM	Clues to the etiology of Type I diabetes from studies of the streptozocin family of microbial glycotoxins.	Jonathan King
3:25 PM	Mapping and distinguishing endogenous from exogenous DNA adducts using third generation single molecule sequencing.	Gunnar Boysen
3:45 PM	<i>Intermission</i>	
4:15 PM	Safety assessment of potential risks associated with nitrosamine impurities in Human drugs and pharmaceuticals	FARAAT ALI
4:35 PM	Mitochondrial and nuclear DNA damage by the cooked meat carcinogen 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine in human neuroblastoma cell line	Medjda Bellamri
4:55 PM	Biochemical characterization of colibactin-DNA interstrand crosslink formation using short oligonucleotides	Erik Carlson
5:15 PM	Malondialdehyde induces post-translational modifications in hemoglobin of breast cancer patients	Hauh-Jyun Chen
5:35 PM	Two Interaction Sites between XPA and RPA Organize the Pre-incision Complex in Nucleotide Excision Repair	Orlando Scharer
5:55 PM	<i>Concluding remarks</i>	