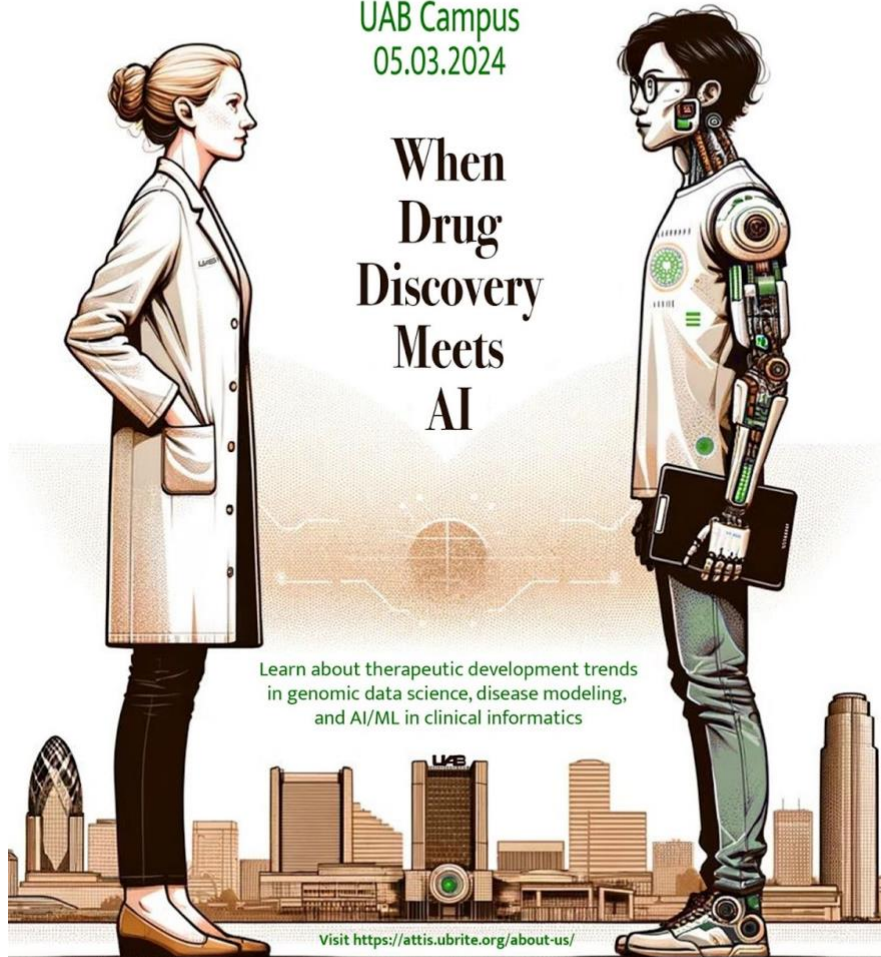


The 2024 Annual Translational and
Transformative Informatics Symposium (ATTIS '24)

UAB Campus
05.03.2024

When
Drug
Discovery
Meets
AI



Learn about therapeutic development trends
in genomic data science, disease modeling,
and AI/ML in clinical informatics

Visit <https://attis.uabrite.org/about-us/>



Margaret Cameron Spain Auditorium
620 19th Street South, Birmingham, AL 35233

8:00 AM – 5:15 PM CST
Friday, May 3rd, 2024

8:00 AM – 8:20 AM **Seating**

8:20 AM - 8:30 AM **Introduction**

[Jake Y. Chen, Ph.D.](#)

Founding Director, Systems Pharmacology AI Research Center (SPARC), Triton Endowed Professor of Bioinformatics and Data Science, Adjunct Professor of Genetics, Computer Science, and Biomedical Engineering, University of Alabama at Birmingham Chair – ATTIS 2024

8:30 AM - 9:30 AM **Keynote Speaker Talk**

[Alex Zhavoronkov, Ph.D.](#)

Founder and CEO, Insilico Medicine

“Generative AI in Drug Discovery: Case Studies of Discoveries That Progressed Into Human Clinical Trials”

9:30 AM - 9:45 AM **Break**

- ***Coffee and water to be provided on-site***

9:45 AM – 11:00 AM **Research Session**

Moderator: [Jin Chen, Ph.D., FAMIA](#)

Associate Professor of Medicine, Nephrology, Associate Director for Education, Department of Biomedical Informatics and Data Science, University of Alabama at Birmingham

- [Stephen Barnes, Ph.D.](#), Distinguished Professor of Pharmacology and Toxicology, University of Alabama at Birmingham, ***“SCIEX ZenoTOF 7600”***
- [Aik Choon Tan, Ph.D.](#), Senior Director of Data Science at the Huntsman Cancer Institute, University of Utah, ***“Computational Strategies for Drug Repurposing and Drug Combination Prediction”***
- [Keshav Singh, Ph.D.](#), Professor of Genetics, Pathology and Environmental Health, University of Alabama at Birmingham, ***“Skin/Hair Loss Restoration Research and Finishing Off with a Thriving Commercial Story”***
- [Christopher Willey, M.D., Ph.D.](#), Hale-Stephens ROAR Endowed Professor, Associate Vice Chair for Translational Research in Radiation Oncology, Kinome Core Director, Department of Radiation Oncology, University of Alabama at Birmingham, ***“Pharmacokinomic Testing in Glioblastoma”***

11:00 AM – 12:00 PM

Flash Talks Session

Moderator: Chindo Hicks, Ph.D.

Professor and Program Director, Department of Genetics, Louisiana State University Health Sciences Center

- *Rahul Sharma, Ph.D*, Informatics Architect, UAB, **“Enhancing Drug Discovery with *drug-smile-fet*: A User-Friendly Tool for SMILES Feature Extraction”**
- *Brittany Lasseigne, Assistant Professor, Cell, Developmental and Integrative Biology (CDIB) University of Alabama at Birmingham*, **“Adverse Events are Associated with Sex- and Tissue-biased Drug Target and Metabolism Gene Expression and Gene-regulatory Network Properties**
- *Ehsan Saghapour, Ph.D*, Postdoctoral Fellow, Department of Biomedical Informatics and Data Science, University of Alabama at Birmingham, **“From Static to Dynamic: Temporal Visualization of Gene Expression in Cancer Cell Line”**
- *Ilana Chefetz Menaker, Ph.D.*, Associate Professor, Mercer School of Medicine, Mercer University, **“Dual Inhibition of ALDH1A and MEK1/2 Causes Synergistic Cell Death in High-grade Serous Ovarian Cancer Triggered b Enhanced DNA Damage and Diminished DNA Repair”**
- *Kevin Song, Ph.D. student, Biomedical Engineering, University of Alabama at Birmingham*, **“PharmAlchemy: A Comprehensive Knowledge Base for Mining Gene-Drug-Disease Relationships”**

12:00 PM – 1:00 PM

Poster Session (over Lunch)

Moderator: Amy Wang, M.D., MBI

Associate Professor of Medicine and Family and Community Medicine, UAB Department of Biomedical Informatics and Data Science, University of Alabama at Birmingham

1. **“Artificial Intelligence in Drug Metabolism Prediction and in Vitro-in Vivo Extrapolations (IVIVE)”**, University of Alabama at Birmingham
2. **“PharmAlchemy: A Comprehensive Knowledge Base for Mining Gene-Drug-Disease Relationships”**, University of Alabama at Birmingham
3. **“Digital Twin of Pre-Clinical Trial: An Advanced Approach for Personalized Oncology Drug Screening,”** University of Alabama at Birmingham
4. **“Untargeted Metabolomics Mass Spectroscopy Tools for Data Processing: MS-DIAL, ADAP-BIG, and Asari”**, University of Alabama at Birmingham
5. **“Structural Definition of Polyspecific Compensatory Ligand Recognition by P-glycoprotein,”** University of Alabama at Birmingham
6. **“BioComputeHub: An On-demand, User-Friendly Computation Platform for Biomedical Informatics and Data Science,”** University of Alabama at Birmingham
7. **“Exploring SERPINEs as Precision Medicine Biomarkers for Targeted Therapies in Aggressive Prostate Cancer: Insights from Integrated Multi-Omics Pan-Cancer Analysis”**, Auburn University

8. ***“UAB Biological Data Sciences (U-BDS) Core Provides Comprehensive Computational Biology Support to the UAB Research Community”***, University of Alabama at Birmingham
9. ***“Unraveling Endocrinology’s Future: A Comprehensive Exploration of Artificial Intelligence Applications”***, Mercer University
10. ***“Early Warnings - Leveraging Cell-Painting to Predict Pharmaceutical Toxicity”***, University of Alabama at Birmingham
11. ***“Mondrian Map - Piet Mondrian’s Abstraction for Effective Drug Target Search”***, University of Alabama at Birmingham
12. ***“Unveiling Pancreatic Cancer Gene Interactions: A PAGER Case Study for Drug Discovery Progress,”*** University of Alabama at Birmingham

1:00 PM – 2:30 PM

Computational Drug Discovery Workshop

Moderator: [Lurong Pan, Ph.D.](#)

Senior Scientist, SPARC, Department of Biomedical Informatics and Data Science, University of Alabama at Birmingham

- Teresa Wilborn, Pharm.D., Ph.D., Professor and Interim Chair, Department of Pharmacology and Toxicology, University of Alabama at Birmingham, ***“A Guide to Drug Discovery and Development”***
- Lurong Pan, Ph.D., Senior Scientist, SPARC, Department of Biomedical Informatics and Data Science, University of Alabama at Birmingham, ***“Unleashing the Power of AI in Preclinical Studies: Translational Medicine, Target Modeling, and Drug Design”***
- Edward Acosta, Pharm.D., Professor, Department of Pharmacology and Toxicology, University of Alabama at Birmingham, ***“Navigating Clinical Pharmacology: Pharmacokinetics and Pharmacodynamics in Phase I/II Studies”***
- Jake Chen, Ph.D., Founding Director, Systems Pharmacology AI Research Center (SPARC), Triton Endowed Professor of Bioinformatics and Data Science, Adjunct Professor of Genetics, Computer Science, and Biomedical Engineering, University of Alabama at Birmingham, ***“Envisioning the Future: AI’s Transformative Role in Drug Discovery”***

2:30 PM – 2:45 PM

Break

2:45 PM – 3:45 PM

Panel Discussion

“AI in Drug Discovery: Hope or Hype?”

Moderator: [Jake Y. Chen, Ph.D.](#),

Founding Director, Systems Pharmacology AI Research Center (SPARC), Triton Endowed Professor of Bioinformatics and Data Science, Adjunct Professor of Genetics, Computer Science, and Biomedical Engineering, University of Alabama at Birmingham

Panelists:

- [Robert D. “Rusty” Arnold, Ph.D.](#), Professor and Director of Research Development & Support at Auburn University Harrison College of Pharmacy
- [Aik Choon Tan, Ph.D.](#), Senior Director of Data Science at the Huntsman Cancer Institute, University of Utah
- [Joel H. Dobbs, Pharm.D., MPH](#), Executive in Residence and Senior Instructor, Collat School of Business, University of Alabama at Birmingham
- [Mark M. Banaszak Holl, Ph.D.](#), Professor and Associate Dean for Research, School of Engineering, University of Alabama at Birmingham
- [Sixue Zhang, Ph.D.](#), Head of Computer-Aided Drug Discovery, Southern Research

3:45 PM – 5:00 PM

Technical Session

Moderator: [Christopher Willey, M.D., Ph.D.](#)

Professor, Department of Radiation Oncology, University of Alabama at Birmingham

- [Bin Chen, Ph.D.](#), Associate Professor of Pediatrics & Human Development, Pharmacology & Toxicology, Michigan State University, **“Transcriptomics-based Drug Discovery”**
- [Zhongming Zhao, Ph.D.](#), Chair Professor and Director of Center for Precision Health, University of Texas Health Science Center at Houston (UTHealth), **“Deep Generative Neural Network for Accurate Drug Response Prediction”**
- [Amit Mitra, Ph.D.](#), Assistant Professor, Division of Pharmacology, Auburn University, **“Drug Discovery Using Omics/Data Science/AI”**
- [Robert Reynolds, Ph.D.](#), Professor, Division of Hematology and Oncology, University of Alabama at Birmingham, **“An Overview of Targeted Degradation Technology”**

5:00 PM – 5:15 PM

Poster Awards/Closing Remarks

[Jake Y. Chen, Ph.D.](#)

Founding Director, Systems Pharmacology AI Research Center (SPARC), Triton Endowed Professor of Bioinformatics and Data Science, Adjunct Professor of Genetics, Computer Science, and Biomedical Engineering, University of Alabama at Birmingham

[Amy Wang, M.D., MBI](#)

Associate Professor of Medicine and Family and Community Medicine, UAB Department of Biomedical Informatics and Data Science

5:15 PM – 6:00 PM

Social Networking Event