

Xiang Zhang

Departments of Chemistry and Pharmacology & Toxicology, University of Louisville
Louisville, KY 40292

Phone: 502-852-8878

Email: xiang.zhang@louisville.edu

RESEARCH INTEREST

I am interested in molecular systems biology, by exploiting high-throughput technologies for analyses of complex mixtures to promote health and wellness. We develop high-throughput multi-dimensional chromatography mass spectrometry-based bioanalytical platforms for metabolomics, lipidomics and epitranscriptomics, using two-dimensional liquid chromatography-mass spectrometry (2DLC-MS) and comprehensive two-dimensional gas chromatography mass spectrometry (GC×GC-MS). Using the high information content data generated from these bioanalytical platforms, we further develop advanced bioinformatics algorithms and data analysis platforms to uncover the biological information from the massive instrument data. The developed bioanalytical and bioinformatics platforms are then integrated and employed to discover molecular biomarkers and to understand the mechanisms of molecular regulation changes in a biological system.

EDUCATION

Ph.D. in Analytical Chemistry, 2001

Department of Chemistry, Purdue University, West Lafayette, Indiana, USA

Advisor: Prof. Fred E. Regnier

M.S. in Nuclear Physics, 1994

Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou, CHINA

Advisor: Prof. Wenxin Li

B.S. in Radiochemistry, 1989

Department of Modern Physics, Lanzhou University, Lanzhou, CHINA

Advisor: Prof. Daren Ling

POSITIONS AND PROFESSIONAL ACTIVITIES

06/2018 – present President, Chinese American Chromatography Association

06/2016 – 05/2018 President Elect, Chinese American Chromatography Association

12/2013 – present Professor of Pharmacology & Toxicology, University of Louisville School of Medicine, Louisville, KY.

10/2013 – present Director, Center for Regulatory and Environmental Analytical Metabolomics, University of Louisville, Louisville, KY.

06/2012 – 05/2016 Secretary, Chinese American Chromatography Association

07/2011 – present Professor of Chemistry, University of Louisville School of Arts & Sciences, Louisville, KY.

01/2008 – 06/2011 Associate Professor of Chemistry, University of Louisville School of Arts & Sciences, Louisville, KY.

04/2004 – 12/2007 Research Assistant Professor, Bindley Bioscience Center, Purdue University, West Lafayette, IN.

06/2001 – 03/2004 Senior Scientist, Beyond Genomics Medicine, Waltham, MA.

08/1996 – 05/2001 Research Assistant, Department of Chemistry, Purdue University, West Lafayette, IN.

08/1994 – 07/1996 Research Associate, Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou, China.

07/1989 – 07/1991 Patent Agent, Institute of Science & Technology Information of Gansu Province, Lanzhou, China.

AWARDS AND RECOGNITION

1. 2019 Distinguished Faculty Award, University of Louisville
2. 2019 Career Achievement Award, College of Arts and Sciences, University of Louisville
3. 2017 University Scholar, University of Louisville
4. 2014 University Scholar, University of Louisville
5. 2007 Seed for Success Award, Purdue University
6. 2007 Bioinformatics Platform Dissemination Award, Canary Foundation
7. 2005 Seed for Success Award, Purdue University
8. 2005 Professional Development Award, Purdue University
9. 2004 Seed for Success Award, Purdue University
10. 2004 Patent Agent, the United State Patent and Trademark Office, US
11. 2000 Jon and Ruthanna Amy Travel Award, Purdue University
12. 1992 Patent Agent, the Patent and Trademark Office, China

RESEARCH GRANTS

Active Research Support

9. NIH/NCI 1R21CA245560-01 K. Yaddanapudi (PI) \$368,445 12/07/19-11/30/21
Overcoming resistance to cancer immunotherapy by targeting MDSC-derived adenosine
The objective of this study is to test the anti-tumor efficacy of a novel cancer immunotherapy involving systemic administration of adenosine deaminase (ADA)—an enzyme that irreversibly converts adenosine into inosine, a non-immunosuppressive nucleoside.
Role: Co-I
8. NIH/NCI 1R01CA227874-01 D. Guo (PI) \$1,248,000 07/01/19-06/30/24
Defining the molecular mechanisms regulating the hexosamine-N-glycosylation pathway in glioblastoma
The objective of this study is to better understand glioblastoma (GBM) pathogenesis in order to provide the foundation for identifying new effective approaches to target GBM.
Role: Sub-PI
7. NIH/NCI 1R01CA213990-01 J. Yan (PI) \$1,761,375 02/06/17-01/31/22
Transcriptional Regulation of Immunosuppressive Macrophages by c-Maf in Cancer
The objective of this study is to investigate the mechanisms of transcriptional regulation of immunosuppressive macrophages induced by transcription factor c-Maf in cancer.
Role: Co-I
6. NIH/NIGMS 1P20GM113226-01 C. McClain (Director) \$11,530,145 06/10/16-03/31/21
The Hepatobiology and Toxicology COBRE
The overarching theme of this grant is to maximize our capability for deciphering the mechanisms and therapy for liver injury, nutrition and gut:liver interactions, and liver:environment/toxin/drug interactions.
Role: Omics Core Director
5. NIH/NIAAA 1P50AA024337-01 C. McClain (Director) \$7,662,403 05/15/16-04/30/21
The Role of Nutrition in the Development/Progression of Alcohol-induced Organ Injury
The overarching theme of this center is to examine the role of nutrition in the development and progression of alcohol-induced organ injury.
Role: Omics Core Director
4. NIH/NIEHS 2T32ES011564-11 G. Arteel (PI) \$2,311,776 04/01/16-03/31/21
UofL Environmental Health Sciences Training Program
The objectives of this study are to establish a substantially improved pre-doctoral and postdoctoral training program that serves as an umbrella for interdisciplinary and integrated approaches to environmental health sciences.
Role: Mentor

3. NIH/NIAAA 1R01AR067188-01 W. Feng (PI) \$1,226,000 09/15/15-08/31/20
Mechanisms of Probiotics in Alcoholic Liver Disease
The objectives of this study are to elucidate mechanisms of gut barrier dysfunction in experimental alcoholic liver disease (ALD) and to define specific mechanisms of action of *Lactobacillus rhamnosus* Gorbach-Goldin (LGG)/ LGG supernatant (LGGs) in the treatment of experimental ALD.
Role: Co-I
2. NIH/NIAMS 1R01AR067188-01 M. Kosiewicz (PI) \$2,094,514 09/01/15-08/31/20
Interplay of Androgens, Microbiota and Immunoregulation in Lupus
The objective of this study is to understand the independent and interdependent effect of the microbiota and androgens on the immune response.
Role: Co-I
1. Industry Research Gift X. Zhang (PI) \$90,000 No time limit
Mass Informatics of Differential Metabolomics
The goal of this project is to support the bioinformatics projects to study metabolite regulation.
Role: PI

Completed Research Support

21. UofL/EVPRI X. Zhu, X. Zhang (PI) \$9,800 01/01/19-12/31/19
Statistical algorithms to analyze metabolomic data for peak detection
This interdisciplinary project will develop a LC-MS peak deconvolution method using a mixed-effect skew-t mixture model, and further apply the developed method for metabolomics studies.
Role: Co-PI
20. Lupus Research Institute M. Kosiewicz (PI) \$565,358 02/01/15-01/31/19
Sex and Microbiota Influence on Immunoregulation and Disease in BWF1Mice
The objective of this study is to identify of protective metabolites in male microbiota from lupus-prone mice using both LC-MS and GC×GC-MS.
Role: Co-I
19. NIH/NHLBI 3R01HL122581-02S1 S. Baba, X. Zhang (PIs) \$149,934 09/15/15-04/30/17
Cardiac Pathophysiology of Histidyl Dipeptides
This study uses a combination of global metabolomic analysis and stable isotope labeling assisted untargeted metabolomics (SIAM) approach to determine derangements in the global metabolome of the myocardium and the appearance of metabolites in the perfusate of hearts subjected to low flow I/R ex vivo, and further to determine the role of histidyl dipeptides in preventing I/R injury.
Role: Co-PI
18. NSF DMS-1312603 S. Kim (PI) \$180,000 09/01/13-02/28/17
Bayesian Ensemble Metabolomic Network Construction
The goal of this project is to infer metabolic networks from the measurements of metabolites using this high-throughput comprehensive GC×GC-MS.
Role: Co-Investigator
17. NIH/OD 1S10OD020106-01 X. Zhang (PI) \$600,000 02/27/15-02/26/16
Ultra Performance Liquid Chromatography High Resolution High Mass Accuracy Mass Spectrometer
The objective of this study is to acquire a UPLC system with capability of two dimensional separation and a high resolution, high mass accuracy mass spectrometer for metabolomics.
Role: PI
16. NIH/NIDDK 3R01DK091338-02S1 L. Cai, X. Zhang (PIs) \$150,000 09/10/14-08/31/15
Metabolomics Study on the Preventive Mechanisms for LDR on Diabetic Nephropathy

The objective of this study is to apply low-dose radiation (LDR) as a new and non-invasive tool to prevent and treat diabetic nephropathy through stimulation of renal multiple protective mechanisms against oxidative damage and inflammation.

- | | | | | |
|--|------------------------|-----------------|-------------|-------------------|
| 15. | KSEF-13-RDE-017 | W. Feng (PI) | \$30,000 | 07/01/14-06/30/15 |
| Identification of Active Ingredients in Probiotic Culture Supernatant for Alcohol-induced Intestinal Barrier Dysfunction
The goal of this project is to identify a list of bioactive molecules in the LGGs, which will form the basis for probiotic-based drug development for liver disease.
Role: Co-I | | | | |
| 14. | NIH/NIEHS 1R21ES021311 | W. Watson (PI) | \$450,000 | 04/01/12-03/30/15 |
| Effect of Dietary Fat on the Hepatotoxicity of Environmental Arsenic
In this project, we will test the hypothesis that arsenic exposure facilitates the progression from simple steatosis to steatohepatitis by altering metabolic pathways related to inflammation. We will use a combination of metabolomics and proteomics to identify pathways that are dysregulated in our novel animal model of environment-diet interactions.
Role: Co-I | | | | |
| 13. | NIH/NIGMS 1R01GM087735 | X. Zhang (PI) | \$1,405,380 | 05/01/09-04/30/14 |
| Mass Informatics of Two Dimensional Gas Chromatography Time-of-flight Mass Spectrometry
This project will develop informatics tools to analyze metabolomics data generated from comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry experiments to enable comparative metabolite profiling with high precision and high volume.
Role: PI | | | | |
| 12. | Industry Grant | X. Zhang (PI) | \$71,939 | 04/01/12-03/31/13 |
| Development of Peak Alignment Methods for High-resolution Gas Chromatography Mass Spectrometry
This project will develop software package to align peak lists generated by both one-dimensional and two-dimensional gas chromatography mass spectrometry.
Role: PI | | | | |
| 11. | NIH/NIAAA 1RC2AA019385 | C. McClain (PI) | \$1,616,440 | 10/01/09-09/30/12 |
| Biomarkers for Steatohepatitis
This project will discover metabolite and protein biomarkers for steatohepatitis using high-information-throughput technologies and advanced bioinformatics methods.
Role: Co-I | | | | |
| 10. | UofL/MRG | M. Yu (PI) | \$10,000 | 06/01/11-05/31/12 |
| Quantum Mechanics Simulation-based Metabolite Identification
This project will create an in-silico MS/MS database based on quantum mechanics simulation. A bioinformatics system will be further developed for metabolite identification using the in-silico MS/MS database.
Role: Co-I | | | | |
| 9. | MMRF | M. Wang (PI) | \$750,000 | 08/01/08-07/31/11 |
| Biomarker Discovery and Validation in Multiple Myeloma Cells Using Multiple Proteomics Platforms
The goal of this project is to employ cutting-edge proteomic technologies to analyze myeloma patient tissue samples and identify biomarkers that are responsible for the disease's onset and progression, as well as patients' response to treatments.
Role: Co-I | | | | |
| 8. | NIH/NCI 1U24CA126480 | F. Regnier (PI) | \$6,986,506 | 10/01/06-09/30/11 |
| APT: the Analytical Proteomics Team | | | | |

The major goal of this proposal is to develop robust protocols and standards for biomarker discovery in MS based proteomics. High specificity immunologic reagents will be developed for precise detection and quantification of biomarkers of relevance for breast and prostate cancer.

Role: Co-I

7. UofL/CEG 54079 X. Zhang (PI) \$14,500 02/01/09–01/31/10
Development of Two Dimensional Gas Chromatography Time-of-flight Mass Spectrometry
This one year project will assess the technical capability of comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry for differential metabolomics.
Role: PI
6. UofL/MRG X. Fu (PI) \$10,000 01/01/10–12/31/10
A Microdevice System for Direct Analysis of Volatile Metabolites in Biological Samples for Differential Metabolomics
This project will develop an integrated microGC system coupled with an MS instrument for rapid and sensitive analysis of biosamples such as body fluids and tissue samples for metabolite identification and quantification.
Role: Co-I
5. NIH/STTR 1R41RR024306-A1 X. Zhang (PI) \$149,711 02/01/08–07/30/09
Accurate Protein Identification using Peptide Separation Information and Tandem MS Algorithms
This project will develop algorithms aimed at predicting peptide separation profiles for two-dimensional ion mobility spectrometry. The developed algorithms will be used to assist protein identification.
Role: PI
4. NIH/NIGMS U24GM077905 B. Wanner (PI) \$1,077,550 06/01/06–05/30/09
Development of the www.Ecoli-Community.org Information Resource
The overall goal of this project is to develop an information resource for E. coli community.
Role: Collaborator
3. Canary Foundation X. Zhang, Y. Chen (PIs) \$20,000 06/01/07–05/30/08
CAPS Bioinformatics Platform Dissemination
The major goal of this project is to develop bioinformatics system for meta data management for the computational proteomics analysis system.
Role: Co-PI
2. NIH/NIDDK R33DK070290 F. Regnier (PI) \$4,719,117 10/01/04–09/30/07
Tools for Differential Metabolomics
The major goal of this project is to develop a new set of tools for characterizing and recognizing temporal changes in the metabolome of model organisms.
Role: Co-I
1. Showalter Trust SPS0IK44 S. Mohammed (PI) \$65,000 07/01/06–06/30/07
Use of Proteomics to Determine Pathways of Metastasis
The major goal of this proposal is to identify biomarkers that distinguish metastatic mammary tumors in lymph and also evaluate the predictive value of the biomarkers.
Role: Co-I

REVIEWER OF RESEARCH PROPOSALS

1. National Institute of Health, US
 - a. Instrumentation and Systems Development (ISD) Study Section (2011, 2012)
 - b. Special Emphasis Panel (2013, 2015, 2016)
 - c. R15 (2013, 2014)
 - d. EMNR-V55 (2016)
 - e. Common Fund Metabolomics Program (R03) (2017)
 - f. Innovative Technologies for Cancer-Relevant Biospecimen Science (R21) (2017)

- g. Advanced Development and Validation of Emerging Technologies for Cancer-Relevant Biospecimen Science (R33) (2017)
- 2. National Science Foundation, US
 - a. Division of Chemistry (2009)
 - b. Chemical Measurements & Imaging (CMI) program (2013)
- 3. The Agence Nationale de la Recherche, France
 - a. Programme de Recherche Translationnelle en Santé (2013)
- 4. Others: Palph E. Powe Junior Faculty Enhancement Award Program (2010), CEGIB Pilot Project Program (2010), CFRTC Pilot and Feasibility Application (2016)

REVIEWER OF FOLLOWING SCIENTIFIC JOURNALS

1. Analytical Chemistry
2. Bioinformatics
3. Scientific Reports
4. Journal of Proteome Research
5. Analytica Chimica Acta
6. Analytical Methods
7. PeerJ Analytical Chemistry
8. Food & Function
9. Drug Metabolism Reviews
10. Journal of Chromatography A
11. Journal of Chromatography B
12. Journal of Separation Science
13. Proteomics – Clinical Applications
14. Toxicological Sciences
15. Computer Science and Systems Biology
16. PloS ONE
17. Journal of Psychiatric Research
18. The Crop Journal
19. Current Metabolomics
20. Molecules
21. Microchemical Journal
22. Rapid Communications in Mass Spectrometry
23. IEEE Transactions on Computational Biology and Bioinformatics
24. FEMS Microbiology Letters
25. Statistics and Its Interface
26. Journal of Bioinformatics and Computational Biology
27. Electrophoresis
28. Methods of Enzymology
29. BMC Medical Genomics
30. Cancer Letters
31. Central European Journal of Biology
32. Cancer Chemotherapy and Pharmacology
33. Briefings in Functional Genomics and Proteomics
34. Proteomics
35. The ISME Journal
36. Protein Science
37. IEEE Transactions on Information Technology in Biomedicine

CONSULTANTSHIPS

1. 2008 – 2015 LECO Corporation, St. Joseph, MI
2. 2011 – 2014 Menssana Research, Inc. Newark, NJ
3. 2013 – 2014 David H. Murdock Research Institute, NC
4. 2010 – 2012 MaiHealth Inc., Columbus, IN

5. 2007 – 2009 Predictive Physiology and Medicine, Inc., Bloomington, IN
6. 2004 – 2005 Beyond Genomics Medicine, MA

MEMBER OF PROGRAM COMMITTEE

1. Program Committee Member, *14th Annual Conference of the Metabolomics Society*, Seattle, WA. June. 24-28, 2018.
2. Program Committee Member, *International Conference on Intelligent Computing (ICIC'17)*, Liverpool, UK. Aug. 7-10, 2017.
3. Session Chair, Bioinformatics: metabolite identification and quantification. *Pittcon 2017*, Chicago, IL. March 6-8, 2017.
4. Session Chair, Bioinformatics: metabolite identification and quantification. *Pittcon 2016*, Atlanta, GA. March 6-10, 2016.
5. Session Chair, Bioinformatics: metabolite identification and quantification. *Pittcon 2015*, New Orleans, LA. March 8-12, 2015.
6. Session Chair, Bioinformatics: metabolite identification and quantification. *Pittcon 2014*, Chicago, IL. March 2-6, 2014.
7. Workshop co-Chair, CACA: How to be successful in your career. *Pittcon 2014*, Chicago, IL. March 2-6, 2014.
8. Publicity co-Chairs, *9th International Conference on Intelligent Computing (ICIC'13)*, Nanning, Guangxi, China. July 28-31, 2013.
9. Publicity co-Chairs, *8th International Conference on Intelligent Computing (ICIC'12)*, Huangshan, Hunan, China. July 25-29, 2012.
10. Publicity co-Chairs, *7th International Conference on Intelligent Computing (ICIC'11)*, Zhengzhou, Henan, China. Aug 11-14, 2011.
11. Session Chair, *35th International Symposium on Capillary Chromatography (ISCC)*, San Diego, CA. May 1-5, 2011.
12. Special Session/Workshop Chair, *6th International Conference on Intelligent Computing (ICIC'10)*, Changsha, Hunan, China. Aug. 18-21, 2010.
13. Program Committee member, *7th International Workshop on Data Mining in Bioinformatics*, San Jose, California. Aug. 12, 2007.

TEACHING EXPERIENCE

University of Louisville

1. CHEM 622, Separation Sciences, S09, F10, F12, F14, F16, F18
2. CHEM 625, Advanced Analytical Chemistry, F08, S16, S19
3. CHEM 425, Instrumental and Statistical Analysis, F16, F17
4. CHEM 208, An Introduction to Chemical Analysis II, S13, F13, S14, S15, S18, S19
5. CHEM 207, An Introduction to Chemical Analysis I, S10
6. CHEM 210, An Introduction to Chemical Analysis IV, F09, F11, S12, S20
7. CHEM 209, An Introduction to Chemical Analysis III, F08, F09, F11, F13, S16, S20
8. CHEM 209H, An Introduction to Chemical Analysis III, S16

Purdue University

1. Workshop, Protein Identification in Mass Spectrometry-based Proteomics, April, 2006
2. CHEM 696D, Computational Proteomics and Metabolomics, Guest lecturer, Spring 2005, Spring 2006, Spring 2007

STUDENTS AND POSTDOCTORAL FELLOWS MENTORED

Research Faculty

Dr. Liqing He, Research Assistant Professor (09/2019–present), Dr. Xiaoli Wei, Research Assistant Professor (07/2014–12/2018), Dr. Imhoi Koo, Research Assistant Professor (07/2014–06/2016)

Postdoctoral Associates

Dr. Liqing He (08/2016–09/2019), Dr. Xiaoli Wei (01/2010 – 06/2014), Dr. Imhoi Koo (07/2010–06/2014), Dr. Jun Zhang (08/2009–07/2011), Dr. Bing Wang (08/2008–07/2011), Dr. Cheolhwan Oh (06/2005–12/2007)

Lab Technologists

Xipeng Ma (03/2018 – present), Xinmin Yin (06/2008–present), Biyun Shi (08/2014–05/2018)

Graduate Students

Md Touhidul Islam (PhD, 08/2019–present), Raobo Xu (PhD, 08/2019–present), Yuan Fang (PhD, 08/2016–present), Md Aminul Islam Prodhan (PhD, 01/2015–12/2019), Xue Shi (PhD, 08/2009–12/2014), Yuan Zhang (MS, 08/2010–05/2013), Aiqin Fang (MS, 08/2008–05/2011)

Undergraduate Students

Ryan P. Crowe (Spring 2019), Connor Smith (Summer 2014), Brent Hukill (Summer 2013), Jiayang Zhang (Summer 2012, 2013), Nathan R. Millson (F2019, S2020)

Visiting Scholars

Prof. Hsiao-yu Yang (2019), Bernat M. Pérez (2019), Shuting Yu (2019), Ting Linghu (2019), Prof. Yinmao Wei (2017), Zijun Wang (2013–2014), JiaYuan Zhang (2011–2013), Shiwen Wu (2011–2012), Yaping Zhao (2010–2011), Wenlong Sun (2010–2011), Hyeyoung Cho (2006–2007), Qi Ouyang (Programmer, 2006)

ACADEMIC SERVICE

University Service

Director, Center for Regulatory and Environmental Analytical Metabolomics (2013–present)
Research Computing Governance Council (2010–present)
Service Center Committee (2014–present)
Faculty Search Committee (JBCC 2014)

Department Service

Faculty Search Committee (2019), Staff Search Committee (2018), Lab Fee Committee (2016–present), Department Seminar Coordinator (2015), Faculty Search Committee, Chemistry (2015), Personal Committee (2012–2015, 2017–2019), Director of Graduate Admissions Committee (2010–2012), Graduate Admissions Committee (2009–2010), Undergraduate Advisor Committee (2008–2011)

Students' Original Research Proposal Committees

Tirtha Raj Sibakoti (2019), Anthony Ewurum (2019), Shengzong Liang (2015), Mumiye A. Ogunwale (2015), Sadakatali Shokatali Gori (2014), Yuan Zhang (2013), Xue Shi (2012), Sarah E Milliner (2011), Sebastien Laulhe (2011), Weibo Wang (2010), Juan Chen (2010), Richard T Woofter (2009), Rami Mahdi (2008)

Students' Dissertation Committees

Md Aminul Prodhan (2019), Tirtha Raj Sibakoti (2019), Shengzong Liang (2017), Mumiye A. Ogunwale (2017), Sadakatali Shokatali Gori (PhD, 2016), James Harder (PhD, 2015), Samantha M. Carlisles (MS, 2015), Xue Shi (PhD, 2014), Yuan Zhang (MS, 2013), Rafael Masitas (PhD, 2013), Stephanie Mattingly (PhD, 2013), Ruiqui Liu (MS, 2013), Sebastien Laulhe (PhD, 2013), Xuan Huang (PhD, 2012), Richard T Woofter (PhD, 2011), Weibo Wang (PhD, 2011), Yang Yang (MS, 2011), Rami Mahdi (PhD, 2010), Marybeth Miskovic (PhD, 2010), Lukasz Sztaberek (PhD, 2009), Weibo Wang (MS, 2009), Yang Han (MS, 2008), Catherine P. Riley (MS, 2008)

BOOKS

2010 De-Shuang Huang, Xiang Zhang, Carlos Alberto Reyes Garcia (Eds.): Advanced Intelligent Computing Theories and Applications, 6th International Conference on Intelligent Computing, ICIC 2010, Changsha, China, August 18–21, 2010, Proceedings. Lecture Notes in Computer Science. 6216 Springer 2010, ISBN 978-3-642-14931-3.

PUBLICATIONS

Submitted

173. Yuan, F.; Kim, S.; Yin, X.; Zhang, X.; Kato, I. Integrating two-dimensional gas and liquid chromatography mass spectrometry for untargeted colorectal cancer metabolomics: a proof of principle study. *J. Chromatogr. Sci.* **2019**, submitted.

172. Ren, D.; Quan, N.; Zhang, J.; Xuan Li, X.; He, L.; Zhang, X.; Li, J. Aged-related Sestrin2 modulates Pyruvate Dehydrogenase activity leading to a critical adaptive metabolic response during ischemia/reperfusion stress. *Circ. Res.* **2019**, submitted.
171. Zhao, J.; Conklin, D.; Guo, Y.; Zhang, X.; Obal, D.; Guo, L.; Jagatheesan, G.; Katragadda, K.; He, L.; Yin, X.; Prodhon, A. M.; Shah, J.; Hoetker, D.; Kumar, A.; Kumar, V.; Wempe, M.; Bhatnagar, A.; Baba, S. Cardiospecific overexpression of ATP5D1 increases histidine dipeptide levels and prevents myocardial ischemia-reperfusion injury. *J. Am. Heart Assoc.* **2019**, under revision.
170. Warner, D.R.; Warner, J.B.; Hardesty, J.E.; Song, Y.L.; King, T.N.; Kang, J.X.; Chen, C.; Xie, S.; Yuan, F.; Yin, X.; Ma, X.; Zhang, X.; Rouchka, E.C.; Whitlock, J.; Li, E.C.; Wang, G.P.; McClain, C.J.; Kirpich, I.A. Beneficial effects of decreased omega-6:omega-3 PUFA ratio on intestinal homeostasis and microbiota are linked to the improvement of liver injury associated with ethanol and LPS administration in mice. *PLoS ONE* **2019**, under revision.
169. Li, Z.; Kim, S.; Zhong, S.; Zhong, Z.; Kato, I.; Zhang, X. Coherent point drift peak alignment algorithms using distance and similarity measures for analysis of comprehensive two-dimensional gas chromatography mass spectrometry data. *Chemometrics* **2019**, under revision.
168. Liu, M.; Tong, Z.; Ding, C.; Luo, F.; Wu, S.; Albeituni, S.; He, L.; Hu, X.; Tieri, D.; Rouchka, E.C.; Hamada, M.; Takahashi, S.; Gibb, A.G.; Kloecker, G.; Zhang, H.; Bousamra II, M.; Hill, B.G.; Zhang, X.; Yan, J. Transcription Factor c-Maf Is A Molecular Checkpoint that Controls Immune Suppression by Programming Macrophages in Lung Cancer. *J. Clin. Invest.* **2019**, submitted.
167. Reynolds, L.; Dougherty, S.; Kruer, T.; Metcalf, S.; Lorkiewicz, P.; He, L.; Yin, X.; Zhang, X.; Arumugam, S.; Young, L.; Sun, R.; Clem, B. Loss of Rb1 enhances glycolytic metabolism in Kras-driven lung tumors in vivo. *Cancers* **2019**, submitted.

2020

166. Liu, Y.; Chen, K.; Li, F.; Gu, Z.; Liu, Q.; He, L.; Shao, T.; Song, Q.; Zhu, F.; Zhang, L.; Jiang, M.; Zhou, Y.; Barve, S.; Zhang, X.; McClain, C.J.; Feng, W. Probiotic LGG prevents liver fibrosis through inhibiting hepatic bile acid synthesis and enhancing bile acid excretion in mice. *Hepatology*. **2020**, in press.
165. Yuan, F.; Harder, J.; Yin, X.; Zhang, X.; Kosiewicz, M.M. Effects of androgen depletion in mouse feces analyzed using multiple metabolic platforms. *J. Proteome Res.* **2020**, in press.
164. Warner, D.R.; Warner, J.B.; Hardesty, J.E.; Song, Y.L.; King, T.N.; Kang, J.X.; Chen, C.; Xie, S.; Yuan, F.; Prodhon, A.; Ma, X.; Zhang, X.; Rouchka, E.C.; Whitlock, J.; Li, E.C.; Wang, G.P.; McClain, C.J.; Kirpich, I.A. Decreased $\omega 6/\omega 3$ PUFA ratio attenuates ethanol-induced alterations in intestinal homeostasis, microbiota and liver injury. *J. Lipid Res.* **2020**, in press. (PMID: 31586017)
163. Liu, Q.; Liu, Y.; Li, F.; Gu, Z.; Liu, M.; Shao, T.; Zhang, L.; Zhou, G.; Pan, C.; He, L.; Cai, J.; Zhang, X.; Barve, S.; McClain, C.J.; Chen, Y.; Feng, W. Probiotic culture supernatant improves metabolic function through FGF21-adiponectin pathway in mice. *J. Nutr. Biochem.* **2020**, 75, 108256. (PMID: 31760308)

2019

162. Sundaram, K.; Miller, D.P.; Kumar, A.; Teng, Y.; Sayed, M.; Mu, J.; Lei, C.; Sriwastva, M.K.; Zhang, L.; Jun, Y.; Merchant, M.L.; He, L.; Yuan, F.; Zhang, X.; Park, J.W.; Lamont, R.J.; Zhang, H. Plant-derived exosomal nanoparticles inhibit pathogenicity of *Porphyromonas gingivalis*. *iScience* **2019**, 21, 308-327. (PMID: 31678913; PMCID: PMC6838522)
161. Lorkiewicz1, P.K.; Gibb, A.A.; Rood, B.R.; He, L.; Zheng, Y.; Clem, B.F.; Zhang, X.; Hill, B.G. Integration of flux measurements and pharmacological controls to optimize stable isotope-resolved metabolomics workflows and interpretation. *Sci. Rep-UK* **2019**, 9:13750. (PMID: 31548575; PMCID: PMC6757038)
160. Young, J. L.; Yan, X.; Xu, J.; Yin, X.; Zhang, X.; Arteel, G.E.; Barnes, G.N.; States, C.J.; Watson, W.; Kong, M.; Cai, L.; Freedman, J.H. Cadmium and high-fat diet disrupt renal, cardiac and hepatic essential metals. *Sci. Rep-UK.* **2019**, 9:14675. (PMID: 31604971; PMCID: PMC6789035)

159. He, L.; Li, F.; Yin, X.; Bohman, P.; Kim, S.; McClain, C.J.; Feng, W.; Zhang, X. Profiling of Polar Metabolites in Mouse Feces Using Four Analytical Platforms to Study the Effects Of Cathelicidin-Related Antimicrobial Peptide in Alcoholic Liver Disease. *J. Proteome. Res.* **2019**, 18, 7, 2875-2884. (PMID: 31188604; PMCID: N/A)
158. Prodhan, A.I.; Shi, B.; Song, M.; He, L.; Yuan, F.; Yin, X.; Bohman, P.; McClain, C.J.; Zhang, X. Integrating comprehensive two-dimensional gas chromatography mass spectrometry and two-dimensional liquid chromatography mass spectrometry for untargeted metabolomics. *Analyst* **2019**, 144, 4331-4341. (PMID: 31192319; PMCID: PMC6677244)
157. He, L.; Wei, X.; Ma, X.; Yin, X.; Song, M.; Donninger, H.; Yaddanapudi, K.; McClain, C.J.; Zhang, X. Simultaneous quantification of nucleosides and nucleotides from biological samples. *J. Am. Soc. Mass Spectrom.* **2019**, 30(6), 987-1000. (PMID: 30847833; PMCID: PMC6520184)
156. Chakravarty, S.; Mandal, R. K.; Duff, M. L.; Yuan, F.; Zhang, X.; Schmidt, N. W. 14. *PLoS ONE* **2019**, 14(2):e0214449. (PMID: 30917184; PMCID: PMC6436795)
155. Kim, S.; Yin, X.; Prodhan, A.I.; Zhang, X.; Zhong, Z.; Kato, I. Global plasma profiling for colorectal cancer associated volatile organic compounds: a proof of principle study. *J. Chromatogr. Sci.* **2019**, 57, 385-396. (PMID: 30796770; PMCID: PMC6478127)
154. Roumani, A.; Madkour, A.; Ouzzani, M.; McGrew, T.; Omran, E.; Zhang, X. BioNetApp: an interactive visual data analysis platform for molecular expressions. *PLoS ONE* **2019**, 14(2):e0211277. (PMID: 30794548; PMCID: PMC6386483)
153. Shahrajoohaghghi, A.; Hichem, F.; Zhang, X.; Wei, X.; Shi, B.; McClain, C.J. Ensemble feature selectin for biomarker discovery in mass spectrometry-based metabolomics. *Proceedings of the 34th ACM/SIGAPP Symposium on Applied Computing (SAC'19)*. Page 19-24. April 8-12, **2019**. Limassol, Cyprus. <https://dl.acm.org/citation.cfm?id=3297283> [Peer-reviewed conference paper]
152. Trabelsi, A.; Shi, B.; Wei, X.; Frigui, H.; Zhang, X.; McClain, C.J.; Shahrajoohaghghi, A. Molecule specific normalization for protein and metabolite biomarker discovery. *Proceedings of the 34th ACM/SIGAPP Symposium on Applied Computing (SAC'19)*. Pages 25-31. April 8-12, **2019**. Limassol, Cyprus. <https://dl.acm.org/citation.cfm?id=3297284> [Peer-reviewed conference paper]
151. Prodhan, A.I.; McClain, C.J.; Zhang, X. Comprehensive two-dimensional gas chromatography mass spectrometry-based metabolomics. *Cancer Metabolomics: Technology and Applications*. Springer. Editor, Shen Hu. To be published in Fall **2019** [Book Chapter]

2018

150. Shao, T.; Zhao, C.; Li, F.; Gu, Z.; Liu, L.; Zhang, L.; Wang, Y.; He, L.; Liu, Y.; Liu, Q.; Chen, Y.; Donde, H.; Wang, R.; Jala, R.J.; Barve, S.; Chen, S-Y.; Zhang, X.; Chen, Y.; McClain, C.J.; Feng, W. Intestinal HIF-1 α deletion exacerbates alcoholic liver disease through inducing intestinal dysbiosis and barrier dysfunction. *J. Hepatol.* **2018**, 69(4), 886-895. (PMID: 29803899; PMCID: PMC6615474)
149. Prodhan, A.I.; Yin, X.; Kim, S.; McClain, C.J.; Zhang, X. Surface fitting for calculating the second dimension retention index in comprehensive two-dimensional gas chromatography mass spectrometry. *J. Chromatogr. A.* **2018**, 1539, 62-70. (PMID: 29395161; PMCID: PMC5826898)
148. Warner, D.R.; Liu, H.; Dastidar, S.G.; Warner, J.B.; Prodhan, A.I.; Yin, X.; Zhang, X.; Feldstein, A.E.; Gao, B.; Prough, R.A.; McClain, C.J.; Kirpich, I.A. Ethanol and unsaturated dietary fat induce unique patterns of hepatic ω -6 and ω -3 PUFA oxylipins in a mouse model of alcoholic liver disease. *PLoS ONE* **2018**, 13(9): e0204119. (PMID: 30256818; PMCID: PMC6157879)
147. Song, M.; Li, X.; Zhang, X.; Shi, H.; Vos, M.; Wei, X.; Wang, Y.; Gao, H.; Rouchka, E.C.; Yin, X.; Zhou, Z.; Prough, R.; Cave, M.; McClain, C.J. Dietary copper-fructose interactions alter gut microbial activity in male rats. *Am. J. Physiol. –Gastr. L.* **2018**, 314, G119-G130. (PMID: 29025734; PMCID: PMC5866377)
146. He, L.; Prodhan, A.I.; Yuan, F.; Yin, X.; Lorkiewicz, P.K.; Wei, X.; Feng, W.; McClain, C.; Zhang, X. Simultaneous quantification of straight-chain and branched-chain short fatty acids by

- gas chromatography mass spectrometry. *J. Chromatogr. B.* **2018**, 1092, 359-367. (PMID: 29936372; PMCID: PMC6190712)
145. Prodhan, A.I.; Sleman, A.A.; Kim, S.; McClain, C.J.; Zhang, X. Generalization of reference system for calculating the second dimension retention index in GC×GC-MS. *J. Anal. Test.* **2018**, 2018, 3, 263-273.
 144. Gao, Y.; Gao, L.; Tian, J.; Qin, X.; Zhang, X. A network pharmacology approach to decipher the mechanisms of anti-depression of Xiaoyaosan formula. *World J. Tradit. Chin. Med.* **2018**, 4, 147-162.
 143. Zhao, F.; Chang, Y.; Gao, L.; Qin, X.; Du, G.; Zhang, X.; Zhou, Y. Protective effects of *Scutellaria baicalensis* Georgi extract on D-galactose induced aging rats. *Metab. Brain Dis.* **2018**, 33(5), 1401-1412 (PMID: 29855978; PMCID: N/A)
 142. Gao, X.; Liang, M.; Fang, Y.; Zhao, F.; Tian, J.; Zhang, X.; Qin, X. Deciphering the differential effective and toxic responses of *Bupleuri Radix* following the induction of chronic unpredictable mild stress and in healthy rats based on serum metabolic profiles. *Front. Pharmacol.* **2018**, 8:995. (PMID: 29379441; PMCID: PMC5775221)

2017

141. Wei, X.; Shi, B.; Koo, I.; Yin, X.; Lorkiewicz, P.; Suhail, H.; Rattan, R.; Giri, S.; McClain, C.J.; Zhang, X. Analysis of stable isotope assisted metabolomics data acquired by GC-MS. *Analytica Chimica Acta* **2017**, 980, 25-32. (PMID: 28622800; PMCID: PMC5541907).
140. Kim, S.; Jang, H.; Koo, I.; Lee, J.; Zhang, X. Normal-Gamma-Bernoulli peak detection for analysis of comprehensive two-dimensional gas chromatography mass spectrometry data. *Comput. Stat. Data Anal.* **2017**, 105, 96-111. (PMID: 27667882; PMCID: PMC5029791)
139. Wei, X.; Lorkiewicz, P.; Salabei, J.K.; Shi, B.; Hill, B.G.; Kim, S.; McClain, C.J.; Zhang, X. Analysis of stable isotope assisted metabolomics data acquired by high resolution mass spectrometry. *Anal. Methods* **2017**, 9, 2275-2283. (PMID: 28622800; PMCID: PMC5541907)
138. Gibb, A.A.; Lorkiewicz, P.K.; Zheng, Y.; Zhang, X.; Epstein, P.N.; Jones, S.P.; Bhatnagar, A.; Hill, B.G. Integration of flux measurements to resolve changes in anabolic and catabolic metabolism in cardiac myocytes. *Biochem. J.* **2017**, 474(16), 2785-2801. (PMID: 28706006; PMCID: PMC554592)
137. Zhou, Y.; Zhao, F.; Gao, L.; Du, G.; Zhang, X.; Qin, X. Licorice extract attenuates brain aging of D-galactose induced rats through inhibition of oxidative stress and attenuation of neuronal apoptosis. *RSC Advances* **2017**, 7, 47758-47766.
136. Zhou, Y.; Yan, M.; Gao, L.; Zhang, Q.; Qin, X.; Zhang, X.; Du, G. Metabonomics approach to assessing the metabolism variation and gender gap of *Drosophila melanogaster* in aging process. *Experimental Gerontology* **2017**, 98, 110-119. (PMID: 28811139)
135. Li, J.; Gao, W.; Gao, J.; Li, H.; Zhang, X.; Qin, X.; Li, Z. Metabolomics reveal the protective effect of *Farfarae Flos* against asthma using an OVA-induced rat model. *RSC Adv.* **2017**, 7 (63), 39929-39939.
134. Ma, K.; Miao, Y.; Li, X.; Zhou, Y.; Gao, X.; Zhang, X.; Chao, J.; Qin, X. Discovery of 1,3-diyne compounds as novel and potent antidepressant agents: synthesis, cell-based assay and behavioral studies. *RSC Adv.* **2017**, 7, 16005-16014.
133. Zhou, Y.; Li, X.; Gong, W.; Tian, J.; Gao, X.; Gao, L.; Zhang, X.; Du, G.; Qin, X. Protective effect of isoliquiritin against corticosterone-induced neurotoxicity in PC12 cells. *Food & Function*, **2017**, 8, 1235-1244. (PMID: 28229156)
132. Ma, K.; Miao, Y.; Gao, X.; Chao, J.; Zhang, X.; Qin, X. Total syntheses of bupleurynol and its analog. *Chin. Chem. Lett.* **2017**, 28(5), 1035-1038.
131. Shahrjooiaghghi, A.; Frigui, H.; Zhang, X.; Wei, X.; Shi, B.; Trabelsi, A. An ensemble feature selection method for biomarker discovery. *IEEE International Symposium on Signal Processing and Information Technology*. University of Deusto – Auditorio Icaza. Dec. 18-20, **2017**. Bilbao,

2016

130. Deng, B.; Kim, S.; Li, H.; Heath, E.; Zhang, X. Global peak alignment for comprehensive two-dimensional gas chromatography mass spectrometry using point matching algorithms. *J. Bioinf. Comput. Biol.* **2106**, 9:1650032. (PMID: 27650662; PMCID: PMC5226864)
129. Tian, J.; Xia, X.; Wu, Y.; Zhao, L.; Xiang, H.; Du, G.; Zhang, X.; Qin, X. Discovery, screening and evaluation of a plasma biomarker panel for subjects with psychological suboptimal health state using ¹H-NMR-based metabolomics profiles. *Sci. Rep-UK* **2016**, 21, 6:33820. (PMID: 27650680; PMCID: PMC5030673)
128. Salabei, J.K.; Lorkiewicz, P.K.; Mehra, P.; Gibb, A.A.; Haberzettl, P.; Hong, K.U.; Wei, X.; Zhang, X.; Li, Q.; Wysoczynski, M.; Bolli, R.; Bhatnagar, A.; Hill, B.G. Type 2 diabetes dysregulates glucose metabolism in cardiac progenitor cells. *J. Biol. Chem.* **2016**, 26, 13634-13648. (PMID: 27151219; PMCID: PMC4919448)
127. Carlisle, S.M.; Trainor, P.J.; Yin, X.; Doll, M.A.; States, J.C.; Zhang, X.; Hein, D.W. Untargeted polar metabolomics of transformed MDA-MB-231 breast cancer cells expressing varying levels of human arylamine *N*-acetyltransferase 1. *Metabolomics* **2106**, 12:111. (PMID: 27872580; PMCID: PMC5115175)
126. Wang, S.; Luo, M.; Zhang, Z.; Gu, J.; Chen, J.; Payne, K.M.; Tan, Y.; Wang, Y.; Yin, X.; Zhang, X.; Liu, G.C.; Wintergerst, K.; Liu, Q.; Zheng, Y.; Cai, L. Zinc deficiency exacerbates while zinc supplement attenuates cardiac hypertrophy in high-fat diet-induced obese mice through modulating p38 MAPK-dependent signaling. *Toxicol Lett.* **2016**, 258:134-46. (PMID: 27346292; PMCID: N/A)
125. Liu, R.; Wu, D.; Zhang, X.; Kim, S. Compound identification using penalized linear regression in metabolomics. *J. Mod. Appl. Stat. Meth.* **2016**, 15(1), 373-388. (PMID: 27212894; PMCID: PMC4871161)
124. Koo, I.; Kim, S.; Shi, B.; Lorkiewicz, P.; Song, M.; McClain, C.J.; Zhang, X. Elder: a compound identification tool for gas chromatography-mass spectrometry data. *J. Chromatogr. A* **2016**, 1448, 107-114. (PMID: 27131963)
123. Chung, D.; Golden, J.E.; Adcock, R.S.; Chu, Y.; Sotsky, J.B.; Cramer, D.E.; Chilton, P.M.; Song, C.; Anantpadma, M.; Schroeder, C.E.; Prophan, A.I.; Yin, X.; Zhang, X. Discovery of a broad-spectrum antiviral compound that inhibits pyrimidine biosynthesis and establishes a type 1 interferon-independent antiviral state. *Antimicrob. Agents Chemother.* **2106**, 60(8), 4552-4562. (PMID: 27185801; PMCID: PMC4958224)
122. Luo, M.; Luo, P.; Zhang, Z.; Payne, K.; Watson, S.; Wu, H.; Tan, Y.; Ding, Y.; Sun, W.; Yin, X.; Zhang, X.; Liu, G.; Wintergerst, K.; Miao, L.; Cai, L. Zinc delays the progression of obesity-related glomerulopathy in mice via down-regulating P38 MAPK-mediated inflammation. *Obesity*, **2016**, 24(6), 1244-1256. (PMID: 27028368)
121. Kirpich, I.A.; Petrosino, J.; Ajami, N.; Feng, W.; Wang, Y.; Liu, Y.; Beier, J.I.; Barve, S.S.; Yin, X.; Wei, X.; Zhang, X.; McClain, C.J. Saturated and unsaturated dietary fats differentially modulate ethanol-induced changes in gut microbiome and metabolome in a mouse model of alcoholic liver disease. *Am. J. Pathol.* **2016**, 186(4), 765-776. (PMID: 27012191; PMCID: PMC5808146)
120. Zhang, J.; Xia, Y.; Zheng, H.; Wang, B.; Zhang, X.; Chen, P. Combine multiple mass spectral similarity measures for compound identification. *Int. J. Data Mining and Bioinformatics* **2016**, 15(1), 84-100.

2015

119. Wei, X.; Song, M.; Yin, X.; Schuschke, D.A.; McClain, C.J.; Zhang, X. Effects of dietary different doses of copper and high fructose feeding on rat fecal metabolome. *J. Proteome Res.* **2015**, 14(9), 4050-4058. (PMID: 26216400; PMCID: PMC6545594)
118. Shi, X.; Wei, X.; Yin, X.; Wang, Y.; Zhang, M.; Zhao, C.; Zhao, H.; McClain, C.J.; Feng, W.; Zhang, X. Hepatic and fecal metabolomic analysis of the effects of *Lactobacillus rhamnosus* GG on alcoholic fatty liver disease in mice. *J. Proteome Res.* **2015**, 14, 1174-1182. (PMID: 25592873; PMCID: PMC6469358)
117. Winnike, J.; Wei, X.; Knagge, K.J.; Colman, S.D.; Gregory, S.G.; Zhang, X. Comparison of GC-MS and GC×GC-MS in the analysis of human serum samples for biomarker discovery. *J. Proteome Res.* **2015**, 14, 1810-1817. (PMID: 25735966; PMCID: PMC4849136)
116. Zhong, W.; Li, Q.; Sun, Q.; Zhang, W.; Zhang, J.; Sun, X.; Yin, X.; Zhang, X.; Zhou, Z. Preventing gut leakiness and endotoxemia contributes to the protective effect of zinc on alcohol-induced steatohepatitis in rats. *J. Nutr.* **2015**, 145(12), 2690-2698. (PMID: 26468492; PMCID: PMC4656905)
115. Song, M.; Schuschke, D.A.; Zhou, Z.; Zhong, W.; Zhang, J.; Zhang, X.; Wang, Y.; McClain, C.J. Kupffer cell depletion protects against the steatosis, but not the liver damage, induced by marginal copper, high fructose diet in male rats. *Am. J. Physiol. –Gastr. L.* **2015**, 308(11), 934-945. (PMID: 25813056; PMCID: PMC4451322)
114. Kim, S.; Zhang, X. Discovery of false identification using similarity difference in GC-MS based metabolomics. *J. Chemometrics.* **2015**, 29(2), 80-86. (PMID: 25937705; PMCID: PMC4414261)
113. Miskovic, F.M.; Couetil, L.; Riley, C.; Zhang, X.; Adamec, J.; Raskin, R. Secretoglobulin and transferrin expression in bronchoalveolar lavage fluid of horses with chronic respiratory disease. *J. Vet. Intern. Med.* **2015**, 29(6), 1692-1699. (PMID: 26332291; PMCID: PMC4895674)
112. Phillips, M.; Cataneo, R.; Chaturvedi, A.; Kaplan, P.; Libardoni, M.; Mundada, M.; Patel, U.; Thrall, K.; Zhang, X. Breath biomarkers of whole-body gamma irradiation in the Göttingen minipig. *Health Phys.* **2015**, 108(5), 538-546. (PMID: 25811151)
111. Tian, J.; Liu, C.; Xiang, H.; Zheng, X.; Guo-jiang Peng, G.; Xiang Zhang, X.; Du, G.; Qin, X. Investigation on the antidepressant effect of sea buckthorn seed oil through the GC-MS-based metabolomics approach coupled with multivariate analysis. *Food Funct.* **2015**, 6, 3585-3592. (PMID: 26328874)
110. Kim, S.; Lee, J.; Jang, H.; Zhang, X. Metabolic network construction using ensemble algorithms. *The First International Workshop on Bioinformatics*. Dec. 3-5, **2015**. New York City, NY, USA. [Conference paper].

2014

109. Wei, X.; Shi, X.; Kim, S.; S, K.; Patrick, J.S.; Binkley, J.; Kong, M.; McClain, C.J.; Zhang, X. Data dependent chromatographic peak model-based spectrum deconvolution for analysis of LC-MS data. *Anal. Chem.* **2014**, 86, 2156–2165. (PMID: 24533635; PMCID: PMC3982975)
108. Shi, X.; Wei, X.; Koo, I.; Schmidt, R.H.; Yin, X.; Vaughn, A.; Kim, S.H.; McClain, C.J.; Arteel, G.E.; Zhang, X.; Watson, W.H. Metabolomic analysis of the effects of chronic arsenic exposure in a mouse model of diet-induced fatty liver disease. *J. Proteome Res.* **2014**, 13, 547–554. (PMID: 24328084; PMCID: PMC3946282)
107. Wei, X.; Koo, I.; Kim, S.; Zhang, X. Compound identification in GC-MS by simultaneously evaluating mass spectrum and retention index. *Analyst* **2014**, 139 (10), 2507 - 2514. (PMID: 24665464; PubMed Central PMCID: PMC4308046)
106. Kim, S.; Ouyang, M.; Shen, C.; Zhang, X. A new method of peak detection for analysis of comprehensive two-dimensional gas chromatography mass spectrometry data. *Ann. Appl. Stat.* **2014**, 8, 1209-1231. (PMID: 25264474; PMCID: PMC4175529)

105. Koo, I.; Yao, S.; Zhang, X.; Kim, S. Comparative analysis of false discovery rate in constructing metabolic association networks. *J. Bioinformatics Computational Biology* **2014**, 12(4), 1450018. (PMID: 25152043; PMCID: PMC4144070)
104. Koo, I.; Wei, X.; Shi, X.; Zhou, Z.; Kim, S.; Zhang, X. Constructing metabolic association networks using high-dimensional mass spectrometry data. *Chemometri. Intell. Lab.* **2014**, 138, 193-202. (PMID: 25414536; PMCID: PMC4233464)
103. Sun, Q.; Li, Q.; Zhong, W.; Zhang, J.; Yin, X.; Sun, X.; Tan, X.; Sun, X.; Zhang, X.; Zhou, X. Dysregulation of hepatic zinc transporters in a mouse model of alcoholic liver disease. *Am. J. Physiol. –Gastr. L.* **2014**, 307(3), 313-322. (PMID: 24924749; PMCID: PMC4121635)
102. Li, X.; Li, Y.; States, V.A.; Li, S.; Zhang, X.; Martin, R.C. The effect of black raspberry extracts on MnSOD activity in protection against Concanavalin A induced liver injury. *Nutri. Cancer*, **2014**, 9:1-8. (PMID: 24911141; PMCID: PMC4559274)
101. Koo, I.; Shi, X.; Kim, S.; Zhang, X. iMatch2: compound identification using retention index for analysis of GC-MS data. *J. Chromatogr. A* **2014**, 1337, 202-210. (PMID: 24630063; PMCID: PMC4106036)
100. Li, Y.; Shi, X.; Zhang, J.; Zhang, X.; Martin, R. Hepatic protection and anticancer activity of curcuma: A potential chemopreventive strategy against hepatocellular carcinoma. *Int. J. Oncol.* **2014**, 44, 505-513. (PMID: 24270742; PMCID: PMC3898719)
099. Koo, I.; Wei, X.; Zhang, X. Analysis of metabolic profiling data acquired on GC-MS, *Methods in Enzymology*, Vol 543: *Cell-wide metabolic alterations associated with malignancy*, Edited by Lorenzo Galluzzi and Guido Kramer, UK Burlington: Academic Press, **2014**, pp. 315-324. (PMID: 24924140) [Book Chapter]
098. Shi, X.; Yin, X.; Zhang, X. Analysis of mouse liver metabolites on GC×GC-TOF MS. *Mass Spectrometry Methods in Metabolomics*, Edited by Daniel Raftery, **2014**, pp. 99-105. [Book Chapter]

2013

097. Wei, X.; Shi, X.; Koo, I.; Kim, S.; Schmidt, R.H.; Arteel, G.E.; Watson, W.H.; McClain, C. J.; Zhang, X. MetPP: A computational platform for comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry-based metabolomics. *Bioinformatics* **2013**, 29, 1786-1792. (PMID: 23665844; PMCID: PMC3702250)
096. Koo, I.; Kim, S.; Zhang, X. Comparative analysis of mass spectral matching-based compound identification in gas chromatography mass spectrometry. *J. Chromatogr. A* **2013**, 1298, 132-138. (PMID: 23726352; PMCID: PMC3686837)
095. Wei, X.; Shi, X.; Merrick, M.; Willis, P.; Alonso, D.; Zhang, X. A method of aligning peak lists generated by gas chromatography high-resolution mass spectrometry. *Analyst* **2013**, 138, 5453-5460. (PMID: 23885350; PMCID: PMC3933976)
094. Laulhé, S.; Geers, T.E.; Shi, X.; Zhang, X.; Nantz, M.H. Electron ionization–induced release of coded isotopic reporter ions in an *m/z* zone of minimal interference for quantifiable, multiplexed GC-MS analyses. *Analytical Methods* **2013**, 5 (18), 4701 - 4706. (PMID: 24235976; PMCID: PMC3822575)
093. Phillips, M.; Cataneo, R.N.; Chaturvedi, A.; Kaplan, P.D.; Libardoni, M.; Mundada, M.; Patel, U.; Zhang, X. Detection of an extended human volatome with comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry. *PLoS ONE* **2013**, 8(9):e75274. (PMID: 24086492; PMCID: PMC3783494)
092. Kim, S.; Zhang, X. Comparative analysis of mass spectral similarity measures on peak alignment for two-dimensional gas chromatography mass spectrometry. *Computational and Mathematical Methods in Medicine*. **2013**, 509761. (PMID: 24151524; PMCID: PMC3787630)
091. Schmidt, R.H.; Jokinen, J.D.; Massey, V.L.; Falkner, K.C.; Shi, X.; Yin, X.; Zhang, X.; Beier, J.I.; Arteel, G.E. Olanzapine activates hepatic mammalian target of rapamycin (mTOR): new

- mechanistic insight into metabolic dysregulation with a typical antipsychotic drugs. *J. Pharmacol. Exp. Ther.* **2013**, 347, 126-135. (PMID: 23926289; PMCID: PMC3781405)
090. Phillips, M.; Byrnes, R.; Cataneo, R.N.; Chaturvedi, A.; Kaplan, P.; Libardoni, M.; Mehta, V.; Mundada, M.; Patel, U.; Ramakrishna, N.; Schiff, P.; Zhang, X. Detection of volatile biomarkers of therapeutic radiation in breath. *J. Breath Res.* **2013**, 7:036002. (PMID: 23793046)
 089. Song, M.; Schuschke, D.A.; Zhou, Z.; Chen, T.; Shi, X.; Zhang, J.; Zhang, X.; Pierce, W.M.; Johnson, T.W.; Vos, M.B.; McClain, C.J. Modest fructose beverage intake causes liver injury and fat accumulation in marginal copper deficient rats. *Obesity* **2013**, 21(8), 1669-1675. (PMID: 23512597; PMCID: PMC3695073)
 088. Wei, X.; Shi, X.; Tang, Y.; Sun, W.; Yin, X.; Sun, X.; Bogdanov, B.; Kim, S.; McClain, C.; Zhou, Z.; Zhang, X. Chronic alcohol exposure disturbs lipid homeostasis at the adipose-liver axis: analysis of triacylglycerols using high-resolution mass spectrometry in combination with *in vivo* metabolite deuterium labeling. *PloS ONE* **2013**, 8(2):e55382. (PMID: 23405143; PMCID: PMC3566154)
 087. Jeong, J.; Zhang, X.; Shi, X.; Kim, S.; Shen, C. An efficient post-hoc integration method improving peak alignment of metabolomics data from GC×GC/TOF-MS. *BMC Bioinformatics* **2013**, 14:123. (PMID: 23575005; PMCID: PMC3637833)

2012

086. Wei, X.; Shi, X.; Kim, S. H.; Zhang, L.; Patrick, J. S.; Binkley, J.; McClain, C.J.; Zhang, X. Data preprocessing method for liquid chromatography mass spectrometry-based metabolomics. *Anal. Chem.* **2012**, 84, 7963–7971. (PMID: 22931487; PMCID: PMC3471364)
085. Kim, S.; Koo, I.; Jeong, J.; Wu, S.; Shi, X.; Zhang, X. Compound identification using partial and semi-partial correlations for gas chromatography mass spectrometry data. *Anal. Chem.* **2012**, 84, 6477–6487. (PMID: 22794294; PMCID: PMC3418476)
084. Kim, S.; Koo, I.; Wei, X.; Zhang, X. A method of finding optimal Weight factors for compound identification in gas chromatography–mass spectrometry. *Bioinformatics* **2012**, 28(8), 1158–1163. (PMID: 22333245; PMCID: PMC3324511)
083. Shi, X.; Wahlang, B.; Wei, X.; Yin, X.; Falkner, K.; Prough, R.; Kim, S.; McClain, C.J.; Cave, M.; Zhang, X. Metabolomic analysis of the effects of polychlorinated biphenyls in non-alcoholic fatty liver disease. *J. Proteome Res.* **2012**, 11, 3805–3815. (PMID: 22686559; PMCID: PMC3391350)
082. Zhong, W.; Zhao, Y.; Sun, X.; Wei, X.; Shi, X.; Sun, W.; Yin, X.; Sun, X.; Kim, S.; McClain, C.J.; Zhang, X.; Zhou, Z. Chronic alcohol exposure stimulates adipose tissue lipolysis in mice: Role of reverse triglyceride transport in the pathogenesis of alcoholic steatosis. *Am. J. Pathol.* **2012**, 180, 998–1007. (PMID: 22234172; PMCID: PMC3349880)
081. Zhang, C.; Lu, X.; Tan, Y.; Li, B.; Miao, X.; Jin, L.; Shi, X.; Zhang, X.; Miao, L.; Li, X.; Cai, L. Diabetes-induced hepatic pathogenic damage, inflammation, oxidative stress, and insulin resistance was exacerbated in zinc deficient mouse model. *PloS ONE* **2012**, 7(12):e49257. (PMID: 23251339; PMCID: PMC3520990)
080. Koo, I.; Zhao, Y.; Zhang, J.; Kim, S.; Zhang, X. A method of calculating the second dimension hold-up time for comprehensive two-dimensional gas chromatography. *J. Chromatogr. A* **2012**, 1260, 193–199. (PMID: 22964052; PMCID: PMC3459176)
079. Zhang, J.; Koo, I.; Wang, B.; Gao, Q.; Zheng, C.; Zhang, X. A large scale test dataset to determine optimal retention index threshold based on three mass spectral similarity measures. *J. Chromatogr. A* **2012**, 1251, 188–193. (PMID: 22771253; PMCID: PMC3430127)
078. Laulhe, S.; Bogdanov, B.; Johannes, L.M.; Gutierrez, O.; Harrison, J.G.; Tantillo, D.J.; Zhang, X.; Nantz, M.H. Fragmentation of oxime and silyl oxime ether odd-electron positive ions by the McLafferty rearrangement: new insights on structural factors that promote α,β -fragmentation. *J. Mass Spectrom.* **2012**, 47(6), 676–686. (PMID: 22678949; PMCID: PMC3396437)
077. Jeong, J.; Shi, X.; Zhang, X.; Kim, S.; Shen, C. Model-based peak alignment of metabolomics

- profiling from comprehensive two-dimensional gas chromatography mass spectrometry. *BMC Bioinformatics* **2012**, 13:27. (PMID: 22316124; PMCID: PMC3323827)
076. Feutz, M.M.; Riley, P.C.; Zhang, X.; Adamec, J.; Thompson, C.; Couetil, L.L. Proteomic analysis of bronchoalveolar lavage fluid in an equine model of asthma during a natural antigen exposure trial. *J. Integrated Omics* **2012**, 2, 123-131.
 075. Kim, S.; Ouyang, M.; Zhang, X. Compute Spearman correlation coefficient with Matlab/CUDA. *IEEE International Symposium on Signal Processing and Information Technology*, Dec. 12-15, **2012**. Ho Chi Minh City, Vietnam. [Conference paper]
 074. Koo, I.; Zhang, X.; Kim, S. Reconstruction of metabolic association networks using high-throughput mass spectrometry data. *2012 International Conference on Intelligent Computing*, July 25-29, **2012**. Huangsan, Hunan, China. [Conference paper]
 073. Wei, X.; Shi, X.; Kim, S.; McClain, C.J.; Zhang, X. A novel two-stage alignment method for liquid chromatography mass spectrometry-based metabolomics. *2012 International Conference on Intelligent Computing*, July 25-29, **2012**. Huangsan, Hunan, China. [Conference paper]

2011

072. Wei, X.; Sun, W.; Shi, X.; Koo, I.; Wang, B.; Yin, X.; Tang, Y.; Bogdanov, B.; Kim, S.; Zhou, Z., McClain, C.J.; Zhang, X. MetSign: A computational platform for high-resolution mass spectrometry-based metabolomics. *Anal. Chem.* **2011**, 83, 7668–7675. (PMID: 21932828; PMCID: PMC3196362)
071. Koo, I.; Zhang, X.; Kim, S. Wavelet- and Fourier-Transforms-based spectrum similarity approaches to compound identification in gas chromatography/mass spectrometry. *Anal. Chem.* **2011**, 83, 5631–5638. (PMID: 21651237; PMCID: PMC3136582)
070. Kim, S.; Fang, A.; Wang, B.; Jeong, J.; Zhang, X. An optimal peak alignment for comprehensive two-dimensional gas chromatography mass spectrometry using mixture similarity measure. *Bioinformatics* **2011**, 27, 1660–1666. (PMID: 21493650; PMCID: PMC3106184)
069. Zhang, J.; Fang, A.; Wang, B.; Bogdanov, B.; Kim, S. H.; Zhou, Z.; McClain, C.J.; Zhang, X. iMatch, A retention index tool for analysis of gas chromatography mass spectrometry data. *J. Chromatogr. A* **2011**, 1218, 6522–6530. (PMID: 21813131; PMCID: PMC3163042)
068. Zhao, Y.; Zhang, J.; Wang, B.; Kim, S.; Fang, A.; Bogdanov, B.; Zhou, Z.; McClain, C.J.; Zhang, X. A method of calculating the second dimension retention index in comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry. *J. Chromatogr. A* **2011**, 1218, 2577–2583. (PMID: 21429495; PMCID: PMC3078172)
067. Jeong, J.; Shi, X.; Zhang, X.; Kim, S.; Shen, C. An empirical Bayes model using a competition score for metabolite identification in gas chromatography mass spectrometry. *BMC Bioinformatics* **2011**, 12:392. (PMID: 21985394; PMCID: PMC3228553)
066. Kim, S.; Koo, I.; Fang, A.; Zhang, X. Smith-Waterman peak alignment for comprehensive two-dimensional gas chromatography mass spectrometry. *BMC Bioinformatics* **2011**, 12:235. (PMID: 21676240; PMCID: PMC3133553)
065. Riley, C.P.; Zhang, X.; Nakshatri, H.; Schneider, B.; Regnier, F.E.; Adamec, J.; Buck, C. A large, consistent plasma proteomics data set from prospectively collected breast cancer patient and healthy volunteer samples. *J. Transl. Med.* **2011**, 9:80. (PMID: 21619653; PMCID: PMC3120690)
064. Zhao, Y.; Tan, Y.; Dai, J.; Li, B.; Guo, L.; Cui, J.; Wang, G.; Shi, X.; Zhang, X.; Mellen, N.; Li, W.; Cai, L. Exacerbation of diabetes-induced testicular apoptosis by zinc deficiency is most likely associated with oxidative stress; p38 MAPK activation; and p53 activation in mice. *Toxicol. Lett.* **2011**, 200, 100–106. (PMID: 21078376)
063. Wang, B.; Fang, A.; Shi, X.; Kim, S.; Zhang, X. A comprehensive peak alignment algorithm for two-dimensional gas chromatography time-of-flight mass spectrometry. *2011 International Conference on Intelligent Computing*, Aug 11-14, **2011**. Zhengzhou, Henan, China. [Conference paper]

062. Koo, I.; Zhang, X.; Kim, S. Comparison of spectral similarity measures for compound identification. *The 5th International Conference on Bioinformatics and Biomedical Engineering*, May 10-12, **2011**. Wuhan, Hubei, China. [Conference paper]
061. Chen, Y.T.; Zhang, J.; Zhang, X.; Kim, S. Statistical analysis of gas chromatography retention index database. *The 5th International Conference Bioinformatics and Biomedical Engineering*, May 10-12, **2011**. Wuhan, Hubei, China. [Conference paper]
060. Zhang, X. Review on the book “Proteome Bioinformatics” (ISBN 978-1-60761-443-2). *Briefings in Bioinformatics* **2011**, 12, 80-81.

2010

059. Wang, B.; Fang, A.; Heim, J.; Bogdanov, B.; Pugh, S.; Libardoni, M.; Zhang, X. DISCO: distance and spectrum correlation optimization alignment for two dimensional gas chromatography time-of-flight mass spectrometry - based metabolomics. *Anal. Chem.* **2010**, 82, 5069–5081. (PMID: 20476746; PMCID: PMC2891529)
058. Wang, B.; Valentine, S.; Plasencia, M.; Raghuraman, S.; Zhang, X. Artificial neural networks for the prediction of peptide drift time in ion mobility mass spectrometry. *BMC Bioinformatics* **2010**, 11:182. (PMID: 20380738; PMCID: PMC2874804)
057. Zhang, X.; Fang, A.; Riley, C.P.; Wang, M.; Regnier, F.E. Buck, C. Multi-dimensional liquid chromatography in quantitative proteomics. *Anal. Chimica Acta* **2010**, 664, 101–113. (PMID: 20363391; PMCID: PMC2852180)
056. Riley, P.C.; Gough, S.E.; He, J.; Jandhyala, S.S.; Kennedy, B.; Orcun, S.; Ouzzani, M.; Buck, C.; Roumani, A.M.; Zhang, X. The Proteome Discovery Pipeline – A data analysis pipeline for mass spectrometry-based differential proteomics discovery. *The Open Proteomics Journal* **2010**, 3, 8–19.
055. Wang, B.; Valentine, S.; Plasencia, M.; Zhang, X. Prediction of drift time in ion mobility-mass spectrometry based on peptide molecular Weight. *Protein Pept. Lett.* **2010**, 17(9), 1143–1147. (PMID: 20509855)
054. Wang, B.; Chen, P.; Zhang, J.; Zhao G.; Zhang, X. Inferring protein-protein interactions using a hybrid GA/SVM method. *Protein Pept. Lett.* **2010**, 17(9), 1079–1084. (PMID: 20509854)
053. Wang, B.; Chen, P.; Wang, P.; Zhao, G.; Zhang, X. Radial basis function neural network ensemble for predicting protein-protein interaction sites in heterocomplexes. *Protein Pept. Lett.* 2010, 17(9), 1111–1116. (PMID: 20509853).
052. Wang, B.; Zhang, X. Evolutionary computation applications in current bioinformatics. *New Achievement in Evolutionary Computation* Edited by Peter Korosec, **2010**, 173–180. [Book Chapter]
051. Zhang, J.; Wang, B.; Zhang, X. Optimal selection of support vector regression parameters and molecular descriptors for retention indices prediction. *Advanced Intelligent Computing Theories and Applications with Aspects of Artificial Intelligence*. Aug. 18–21, **2010**, Changsha, Hunan, China. [Conference paper]
050. Wang, B.; Zhang, J.; Zhang, X. Multiple linear regression for peptides drift time prediction. *The 2010 International Conference on Bioinformatics, Computational Biology, Genomics and Chemoinformatics*, July 12–14, **2010**. Orlando, FL. [Conference paper]

2009

049. Zhang, X.; Oh, C.; Riley, C.P.; Buck, C.; Cho, H. Computational approaches to peptide retention time prediction for proteomics. *Biological Data Mining* Edited by Jake Y. Chen, Stefano Lonardi, **2009**, 337–349. [Book Chapter]
048. Zhang, X.; Orcun S.; Ouzzani, M.; Oh, C. Mass informatics in differential proteomics. *Encyclopedia of Data Warehousing and Mining - 2nd Edition*, Edited by John Wang, **2008**, 1176–1181. [Book Chapter]

2008

- 047. Oh, C.; Huang, X.; Buck, C.; Regnier, E.F.; Zhang, X. Comprehensive two-dimensional gas chromatography/time-of-flight mass spectrometry peak sorting algorithm. *J. Chromatogr. A* **2008**, 1179, 205–215. (PMID: 18093607; PMCID: PMC3933977)
- 046. Zhang, M.; Ouyang, Q.; Stephenson, A.; Kane, M.D.; Salt, D.E.; Prabhakar, S.; Burger, J.; Buck, C.; Zhang, X. Interactive analysis of 'omics molecular expression data. *BMC Systems Biology* **2008**, 2:23. (PMID: 18312669; PMCID: PMC2294108)
- 045. Shen, C.; Wang, Z.; Shankar, G.; Zhang, X.; Li, L. A hierarchical statistical model to assess the confidence of peptide and protein identifications made by tandem mass spectrometry. *Bioinformatics* **2008**, 24, 202–208. (PMID: 18024968; PMCID: N/A)
- 044. Saha, S.; Harrison, S.H.; Shen, C.; Tang, H.; Radivojac, P.; Arnold, R. J.; Zhang, X.; Chen, J.Y. HIP2: an online database of human plasma proteins from healthy individuals. *BMC Medical Genomics* **2008**, 1:12. (PMID: 18439290; PMCID: PMC2396660)
- 043. Culbertson, A.W.; Williams, W.B.; Mckee, A.G.; Zhang, X.; March, K.L.; Naylor, S.; Valentine, S.J. Inside the personalized medicine toolbox: GC×GC-mass spectrometry for high throughput profiling of the human plasma metabolome. *LC/GC* **2008**, 26(6), 560–569.
- 042. Ralston-Hooper, K.; Baker, S.; Hopf, A.; Oh, C.; Zhang, X.; Adamec, J.; Sepúlveda, M.S. Development of GC-GC/TOF-MS metabolomics for use in ecotoxicological studies with invertebrates. *Aquatic Toxicology* **2008**, 88, 48–52. (PMID: 18423646)

2007

- 041. Oh, C.; Zak, S.H.; Mirzaei, H.; Regnier, F.E.; Zhang, X. Neural network prediction of peptide behavior in strong anion exchange chromatography. *Bioinformatics* **2007**, 23, 114–118. (PMID: 17092987)
- 040. Zhang, X.; Oh, C.; Riley, C.P.; Buck, C. Current status of computational approaches for protein identification using tandem mass spectra. *Current Proteomics* **2007**, 4, 121–130.
- 039. Zhao, Y.; Fleet, C. J.; Adamec, J.; Terry, D. E.; Zhang, X.; Kemeh, S.; Davisson, J.V.; Weaver, M.C. Effects of hindlimb unloading and bisphosphonates on the serum proteome of rats. *Bone* **2007**, 41, 646–658. (PMID: 17627911)
- 038. Qiu, R.; Zhang, X.; Regnier, F.E. A method for the identification of glycoproteins from human serum by a combination of lectin affinity chromatography along with anion exchange and Cu-IMAC selection of tryptic peptides. *J. Chromatogr. B* **2007**, 845, 143–150. (PMID: 16945596)
- 037. Fedulova, I.; Ouyang, Z.; Buck, C.; Zhang, X. PepTiger: search engine for error-tolerant protein identification from *de novo* sequence tags. *The Open Spectroscopy Journal* **2007**, 1, 1–8.
- 036. Zhang, M.; Zhang, X.; Zhang, X.; Prabhakar, S. Tracing lineage beyond relational operators. *VLDB'07 Proceedings of the 33rd International Conference on Very Large Databases* **2007**, 1116–1127. [Conference paper]

2006

- 035. Pevtsov, S.; Fedulova, I.; Mirzaei, H.; Buck, C.; Zhang, X. Performance evaluation of existing *de novo* sequencing algorithms. *J. Proteome Res.* **2006**, 5, 3018–3028. (PMID: 17081053)
- 034. Asara, J.M.; Zhang, X.; Zheng, B.; Christofk, H.H.; Wu, N.; Cantley, L.C. In-gel stable isotope labeling: a strategy for mass spectrometry based relative quantification. *J. Proteome Res.* **2006**, 5, 155–163. (PMID: 16396506)
- 033. Asara, J.M.; Zhang, X.; Zheng, B.; Christofk, H.H.; Wu, N.; Cantley, L.C. In-gel stable isotope labeling for relative quantification using mass spectrometry. *Nature Protocols* **2006**, 1, 46–51. (PMID: 17406210)

2005

- 032. Zhang, X.; Asara, J.M.; Adamec, J.; Ouzzani, M.; Elmagarmid, A.K. Data preprocessing in liquid chromatography mass spectrometry based proteomics. *Bioinformatics* **2005**, 21, 4054–4059. (PMID: 16150809)
- 031. Zhang, X.; Hines, W.; Adamec, J.; Asara, J.; Naylor, S.; Regnier, F.E. An automated method for the analysis of stable isotope labeling data for proteomics. *J. Am. Soc. Mass Spectrom.* **2005**, 16, 1181–1191. (PMID: 15922621)
- 030. Ouzzani, M.; Aref, W.G.; Bertino, E.; Christine, A.C.; Clifton, C.W.; Hon, W.; Elmagarmid, A.K.; Ghafoor, A.; Hambruch, S.E.; Prabhakar, S.; Vitter, J.; Zhang, X. The Indiana Center for Database Systems at Purdue University. *SIGMOD Record* **2005**, 34, 53–58.

2004

- 029. Davidov, E.; Clish, C. B.; Oresic, M.; Meys, M.; Stochaj, W.; Snell, P.; Lavine, G.; Londo, T.R.; Adourian, A.; Zhang, X.; Johnston, M.; Morel, N.; Marple, E.W.; Plasterer, T.N.; Neumann, E.; Verheij, E.; Vogels, J, T.W.E.; Havekes, L.M.; Greef, J.; Naylor, S. Methods for the differential integrative omics analysis of plasma from a transgenic disease animal model. *Omics: A Journal of Integrative Biology* **2004**, 8, 267–288. (PMID: 15703476)
- 028. Clish, C.B.; Davidov, E.; Oresic, M.; Plasterer, T.; Lavine, G.; Londo, T.R.; Meys, M.; Snell, P.; Stochaj, W.; Adourian, A.; Zhang, X.; Morel, N.; Neumann, E.; Verheij, E.; Vogels, J, T.W.E.; Havekes, L.M.; Afeyan, N.; Regnier, F.E.; Greef, J.; Naylor, S. Integrative biological analysis of the APOE*3 Leiden transgenic mouse. *Omics: A Journal of Integrative Biology* **2004**, 8, 3–13. (PMID: 15107233)

2002

- 027. Wang, S.; Zhang, X.; Regnier, F.E. Quantitative proteomics strategy involving the selection of peptides containing both cysteine and histidine from tryptic digests of cell lysates. *J. Chromatogr. A* **2002**, 949, 153–162. (PMID: 11999731)

2001

- 026. He, B.; Burke, J.; B.; Zhang, X.; Zhang, R.; Regnier, F.E. A picoliter volume mixer for microfluidic analytical systems. *Anal. Chem.* **2001**, 73, 1942–1947. (PMID: 11354474)
- 025. Geng, M.; Zhang, X.; Bina, M.; Regnier, F.E. Proteomics of glycoproteins based on affinity selection of glycopeptides from tryptic digests. *J. Chromatogr. B* **2001**, 752, 293–306. (PMID: 11270868)
- 024. Regnier, F.E.; Amini, A.; Chakraborty, A.; Geng, M.; Ji, J.; Riggs, L.; Sioma, C.; Wang, S.; Zhang, X. Multidimensional chromatography and the signature peptide approach to proteomics. *LC/GC* **2001**, 19, 200–213.
- 023. Wang, X.; Tian, J.; Yin, X.; Zhang, X.; Qin, Z.; Li, Z.; Wang, Q.; Li, S. Distribution of trace elements in normal and tumor-bearing mice using the multitracers technique. *Biological Trace Element Research* **2001**, 81, 177–183. (PMID: 11554398)

2000

- 022. Zhang, X.; Regnier, F.E. Analysis of channel effects on separation efficiency in rectangular-capillary electrochromatography columns. *J. Chromatogr. A* **2000**, 869, 319–328. (PMID: 10720247)
- 021. Ji, J.; Chakraborty, A.; Geng, M.; Zhang, X.; Amini, A.; Bina, M.; Regnier, F.E. Strategy for qualitative and quantitative analysis in proteomics based on signature peptides. *J. Chromatogr. B* **2000**, 745, 197–210. (PMID: 10997715)
- 020. Wang, X.; Tian, J.; Yin, X.; Zhang, X.; Wang, Q. The excretion of biotrace elements using the

- multitracer technique in tumor-bearing mice. *Applied Radiation and Isotopes* **2000**, 53, 969–974. (PMID: 11077959)
019. Li, W.; Yin, X.; Zhang, X.; Sun, T.; Qin, Z.; Ambe, S.; Ohkubo, Y.; Ambe, F. Projectile-mass dependence of the linear momentum transfer in central collisions. *J. Radioanal. Nucl. Chem.* **2000**, 243, 797–801.
- Before 2000**
018. Wang, X.; Yin, X.; Zhang, X.; Li, Z.; Tian J.; Wu, M.; Sheng, X. Excretion of biotrace elements using the multitracer technique in mice. *J. Radioanal. Nucl. Chem.* **1999**, 240, 963–967.
017. Yin, X.; Wang, X.; Zhang, X.; Li, W.; Tao, Z.; Du, J. Preparation of a radioactive multitracer solution from the reaction of selenium with 25 MeV/nucleon ^{40}Ar ions. *J. Radioanal. Nucl. Chem.* **1997**, 221, 225–226.
016. Yin, X.; Zhang, X.; Sun, T.; Qin, Z.; Zhao, L. Preparation of multitracer from the interaction of selenium with 25 MeV/A ^{40}Ar ions. *J. Nucl. Tech.* **1997**, 20, 382–384.
015. Du, J.; Yin, X.; Wang, X.; Dai, X.; Zhang, X.; Sun, T.; Tao, Z. Adsorption study of 47 elements on alumine and bentonite using a multitracer technique. *Adsorption Science and Technology* **1997**, 15, 341–347.
014. Sun, T.; Li, W.; Wu, D.; Yin, X.; Zhao, L.; Zhang, X.; Qin, Z.; Zheng, J.; Liu, G.; Jing, G. Target residues from interaction of ^{197}Au with 8~24 MeV/nucleon ^{40}Ar ions. *J. Nucl. Radiochem.* **1997**, 19, 49–54.
013. Zhang, X.; Yin, X.; Li, W.; Sun T.; Qin, Z.; Zhao L.; Wu D. Production of hafnium nuclides in the reactions of 6.3~24.5 MeV/nucleon ^{40}Ar ions with nature tungsten. *Radiochem. Acta* **1996**, 75, 7–10.
012. Yin, X.; Du, J.; Zhang, X.; Wang, X.; Dai, X.; Sun, T.; Tao, Z. Preparation of multitracer nuclides from $\text{UO}_2(\text{NO}_3)_2$ irradiated by ^{40}Ar ion beam. *J. Radioanal. Nucl. Chem.* **1996**, 214, 89–94.
011. Qin, Z.; Li, W.; Yin, X.; Zhang, X. , Sun, T.; Zhao, L.; Wang, X. Multitracer technique and prospects of its application. *TREND in Nucl. Phys.* **1996**, 13, 31–34.
010. Zhang, X.; Li, W.; Sun, T.; Yin, X.; Qin, Z.; Zhao, L.; Wu, D.; Zheng, J.; Liu, G. Production of hafnium isotopes from interaction of ^{nat}W with 6.3~24.6 MeV/u ^{40}Ar ions. *J. High Energy Phys. Nucl. Phys.* **1996**, 20, 21–25.
009. Qin, Z.; Li, W.; Sun, T.; Zhao, L.; Zhang, X.; Yin, X.; Wu, D.; Zhen, J.; Liu, G.; Zhao, Z. Target residues from the interaction of natural uranium target with 20 MeV/nucleon ^{40}Ar ions. *J. Nucl. Radiochem.* **1996**, 18, 229–233.
008. Li, W.; Sun, T.; Wu, D.; Sun, R.; Zhao, L.; Yin, X.; Zhang, X.; Luo, Q.; Zhang, F.; Jin, G. Target residues from the interaction of copper with 20~46 MeV/nucleon ^{12}C ions. *Radiochim. Acta* **1996**, 72, 109–119.
007. Liu, G.; Cheng, K.; Yu, X.; Zheng, J.; Jin, W.; Sun T.; Wu, D.; Zhao, L.; Zhang, X.; Yin, X.; Qin, Z. Fragment angular distributions for $^{40}\text{Ar} + ^{197}\text{Au}$ reaction. *Chin. J. Nucl. Phys.* **1995**, 17, 21–23.
006. Zhang, X.; Li, W.; Yin, X.; Wen, W.; Sun, T.; Jin, G.; Luo, Q. Mass yield distribution in intermediate energy heavy ion reactions. *Chinese J. Nucl. Phys.* **1995**, 17, 247–249.
005. Zhang, X.; Li, W.; Yin, X.; Sun, T.; Ambe, S.; Ohkubo, Y.; Iwamoto, M.; Kobayashi, Y.; Maeda, H.; Ambe, F. Isotopic distributions of Hf from the interaction of heavy ions with W. *J. Nucl. Radiochem.* **1995**, 17, 193–197.
004. Yang, W.; Yuan, S.; Mou, W.; Zhang, X.; Li, Z.; Yu, X.; Gan, Z.; Liu, H.; Guo, Y.; Zhang, J.; Lei, X.; Guo, J.; Du, Y.; Zhao, L.; Zhang, X. A new heavy neutron-rich isotope ^{239}Pa . *J. High Energy Phys. Nucl. Phys.* **1995**, 19, 479–480.
003. Zhang, X.; Yin, X.; Li, W.; Qin, Z.; Zhao, L.; Wu, D.; Sun, T. Study on the adsorption behavior of fission products on mud and sand in Yellow River using multitracer. *J. Nucl. Radiochem.* **1995**, 17, 60–64.

002. Yin, X.; Li, W.; Zhang, X.; Sun, T.; Ambe, S.; Ohkubo, Y.; Iwamoto, M.; Kobayashi, Y.; Maeda, H.; Ambe, F. Target residues from the interaction of copper with 40 MeV/u ^{40}Ar ions. *J. High - Energy Phys. Nucl. Phys.* **1995**, 19, 991–997.
001. Liu, G.; Cheng, K.; Yu, X.; Zheng, J.; Jin, W.; Sun T.; Wu, D.; Zhao, L.; Zhang, X.; Yin, X.; Qin, Z. Fragment angular distributions of the 600 MeV $^{40}\text{Ar} + ^{197}\text{Au}$ reaction. *J. High Energy Phys. Nucl. Phys.* **1995**, 19, 305–309.

INVITED TALKS

85. Development of Mass Spectrometry-based Metabolomics. Department Seminar, Department of Chemistry, Southern Illinois University, Carbondale, IL. Sept. 26-27, 2019.
84. Mass Spectrometry-based Metabolomics. College of Agriculture, Shandong Agriculture University, Taian, China. Aug. 8, 2019.
83. High Resolution Mass Spectrometry, Operation and Data Analysis. College of Agriculture, Shandong Agriculture University, Taian, China. Aug. 8, 2019.
82. Sample Preparation in Metabolomics. College of Agriculture, Shandong Agriculture University, Taian, China. Aug. 7, 2019.
81. GC-MS and LC-MS for Analysis of Small Molecules. College of Agriculture, Shandong Agriculture University, Taian, China. Aug. 7, 2019.
80. Integrated Parallel Two-dimensional Liquid Chromatography Mass Spectrometry and Comprehensive Two-dimensional Gas Chromatography Mass Spectrometry for Metabolomics. *iCC2018*. Sept.13, 2018.
79. Integrated Parallel Two-dimensional Liquid Chromatography Mass Spectrometry and Comprehensive Two-dimensional Gas Chromatography Mass Spectrometry for Metabolomics. *47th International Symposium on High Performance Liquid Phase Separations and Related Techniques*. Washington, DC. July 28 – Aug. 2, 2018.
78. Mass Spectrometry-based Epitranscriptomics. Modern Research Center for Traditional Chinese Medicine, Shanxi University, TaiYuan, China. June 27, 2018.
77. Comprehensive Metabolomics for Accurate Metabolite Biomarker Discovery. Modern Research Center for Traditional Chinese Medicine, Shanxi University, TaiYuan, China. June 27, 2018.
76. Calculating the Second Dimension Retention Index in GC×GC-MS. Modern Research Center for Traditional Chinese Medicine, Shanxi University, TaiYuan, China. June 27, 2018.
75. Mass spectrometry-based metabolomics in CREAM. James Graham Brown Cancer Center Seminar Series, University of Louisville, Louisville, KY. May 9, 2018.
74. Development of mass spectrometry-based metabolomics. Center for Urban Responses to Environmental Stressors (CURES), School of Medicine, Wayne State University, Detroit, MI. March 22, 2018.
73. Mass Spectrometry-based Metabolomics. *Spring Meeting, Kentucky Chapter of American Statistical Association*, University of Louisville, March 2, 2018.
72. Bioinformatics for Proteomics and Metabolomics. College of Computer Science and Information Technology, Shanxi University, TaiYuan, China. Jan. 9, 2018.
71. Mass Spectrometry-based Epitranscriptomics. Modern Research Center for Traditional Chinese Medicine, Shanxi University, TaiYuan, China. Jan. 5, 2018.
70. Stable Isotope Assisted Metabolomics. Modern Research Center for Traditional Chinese Medicine, Shanxi University, TaiYuan, China. Jan. 5, 2018.
69. Development of Mass Spectrometry-based Metabolomics. College of Agriculture, Shandong Agriculture University, Taian, China. Dec. 11, 2017.
68. Bioinformatics of Stable Isotope Assisted Metabolomics. *SCIX 2017*, Grand Sierra Resort, Reno, NV. Oct. 8-13, 2017.
67. Mass Informatics of Stable Isotope Assisted Metabolomics. *Pittcon 2017*, Chicago, IL. March 5-9, 2017.
66. Development of mass spectrometry-based metabolomics. Division of Pharmaceutics and Pharmaceutical Chemistry, College of Pharmacy, Ohio State University, Columbus, Ohio. Dec. 19, 2016.

65. Walking in the woods of metabolites with mass spectrometry. Department of Chemistry, Ohio University, Athens, Ohio. Nov. 28, 2016.
64. How to Present Your Work via Oral Presentation – personal opinion. Shanxi University, TaiYuan, China. July 26-July 26, 2016.
63. How to Present Your Work via Research Papers – personal opinion. Shanxi University, TaiYuan, China. July 26-July 26, 2016.
62. Integrative LCxLC-MS and GCxGC-MS Platform for Quantitative Metabolomics. Xi'an Jiao Tong University, Xi'an, Shaanxi, China. July 11-12, 2016.
61. Mass Informatics of Quantitative Metabolomics by Integrating LCxLC-MS and GCxGC-MS Data. *Pittcon 2016*, Atlanta, GA. March 6-10, 2016.
60. Effects of Different Dietary Doses of Copper and High Fructose Feeding on Rat Fecal and Liver Metabolome. *2016*, Atlanta, GA. March 6-10, 2016.
59. Toward elucidation of disease mechanism using mass spectrometry-based metabolomics. Xi'an Jiao Tong University, Xi'an, Shaanxi, China. Nov. 9, 2015.
58. Development of mass spectrometry-based metabolomics. Northwest Agriculture and Forest University, Yanling, Shaanxi, China. Nov. 7, 2015.
57. Toward deciphering of disease mechanism via mass spectrometry-based metabolomics. Dalian Institute of Chemical Physics, Chinese Academy of Science, Dalian, Liaoning, China. Nov. 3, 2015.
56. Unlocking the Power of Metabolomics. *International Workshop of Metabolomics*, Chung Gang University of Science and Technology, Taipei, Taiwan. Oct. 24-25, 2015.
55. Deciphering disease mechanisms using mass spectrometry-based metabolomics. *Department of Pediatrics Research Meeting*, Department of Pediatrics, University of Louisville, KY. Sept. 28, 2015
54. Unlocking the Power of Metabolomics. *Department of Seminar*, Department of Chemistry, West Virginia University, WV. Sept. 16, 2015
53. Walking in the Woods of Metabolites with Mass Spectrometry. Clariant Co, Louisville, KY. June 8, 2015.
52. Walking in the Woods of Metabolites with Mass Spectrometry. Barbara Ann Karmanos Cancer Institute, Wayne State University, MI. April 9, 2015.
51. Effects of dietary different doses of copper and high fructose feeding on rat fecal metabolome. *Pittcon 2015*, New Orleans, LA. March 8-12, 2015.
50. Stable Isotope Labeling Analysis for High Resolution Mass Spectrometry-based Metabolomics. *Pittcon 2015*, New Orleans, LA. March 8-12, 2015.
49. Bioinformatics of Mass Spectrometry-Based Stable Isotope Assisted Metabolomics. *Pittcon 2015*, New Orleans, LA. March 8-12, 2015.
48. Accurate Deconvolution of GC-MS Data Using Gaussian Model-based Curve Fitting of Selected Ion Chromatogram. *Pittcon 2015*, New Orleans, LA. March 8-12, 2015.
47. Metabolomics Study Reveals High Fructose Feeding Inducing Copper Deficiency. *Pittcon 2015*, New Orleans, LA. March 8-12, 2015.
46. Walking in the woods of metabolites with mass spectrometry. Department of Applied Chemistry, Northwestern Polytechnical University, Xi'an, China. Dec. 26, 2014.
45. Walking in the woods of metabolites with mass spectrometry. College of Life Sciences, Xi'an Jiaotong University, Xi'an, China. Dec. 21, 2014.
44. Metabolomics program at the CREAM Center. *Department seminar*, Department of Oral Immunology and Infectious Diseases, Dental School, University of Louisville, KY. Oct. 17, 2014.
43. Impact of chronic ethanol consumption on metabolic profiles of mouse liver: a time course study. *Pittcon 2014*, Chicago, IL. March 2-6, 2014.
42. A computation platform for GCxGC-TOF MS based metabolomics. *Pittcon 2014*, Chicago, IL. March 2-6, 2014.
41. Development of GCxGC-TOF MS based metabolomics for biomarker discovery. *Departmental Seminar*, Department of Genetics, Texas Biomedical Research Institute, TX. Dec. 17, 2013.
40. Development of MS based metabolomics. *Seminar*, Brown Cancer Center, University of Louisville, Louisville, KY. Nov. 21, 2013.

39. Development of mass spectrometry-based metabolomics for biomarker discovery. *International Workshop of Metabolomics*, Shanxi University, TaiYuan, China. Oct. 14-17, 2013.
38. A practical analytical workflow of GC-MS based metabolomics. *International Workshop of Metabolomics*, Shanxi University, TaiYuan, China. Oct. 14-17, 2013.
37. A computational platform for high resolution mass spectrometry-based and liquid chromatography mass spectrometry-based metabolomics. *Pittcon 2013*, Philadelphia, PA. March 17–21, 2013.
36. Metabolomics for study of nutritional interactions. *Pittcon 2013*, Philadelphia, PA. March 17–21, 2013.
35. Working in a small biotech company, personal experience. *Pittcon 2013*, Philadelphia, PA. March 17–21, 2013.
34. Walking in the forest of metabolites. Beijing Institute of Technology, Beijing, China. Jan. 12, 2013.
33. Story of metabolomics as an analytical approach to radiation research. Beijing Atomic Energy Institute, Beijing, China. Jan. 10, 2013.
32. Development of mass spectrometry based metabolomics. Shandong Agriculture University, Tiaan, Shangdong, China. Jan. 6th, 2013.
31. Metabolomics analysis reveals reverse fatty acid transport in alcohol induced fatty liver. *Center Seminar*, Birth Defects Center, Louisville, KY. Jan. 10, 2012.
30. Development of comprehensive two-dimensional gas chromatography mass spectrometry for differential metabolomics. *35th International Symposium on Capillary Chromatography*. San Diego, CA. May 1-5, 2011.
29. Metabolomics as a key to deciphering molecular regulation in liver injury. *IMD3 Symposium 2011*. Louisville, KY. March 8th, 2011.
28. Mass informatics for differential metabolomics. *Department Seminar*, Department of Physics, University of Louisville, Louisville, KY. Oct. 29, 2010.
27. Optimal selection of support vector regression parameters and molecular descriptors for retention indices prediction. *2010 International Conference on Intelligent Computing (ICIC'10)*, Changsha, Hunan, China. Aug 18-21, 2010.
26. Multiple linear regression for peptide drift time prediction. *2010 International Conference on Bioinformatics and Computational Biology*, Orlando, FL, July 12-15, 2010.
25. Development of two dimensional gas chromatography-mass spectrometry for disease biomarker discovery. *Biophysical and Structural Biology Seminar*, Brown Cancer Center, Louisville, KY, June 8, 2010.
24. Development of Metabolic Profiling Pipeline for Disease Biomarker Discovery. *UT-ORNL-KBRIN Bioinformatics Summit 2010*. Cadiz, KY, March 19 – 21, 2010.
23. Experimental bioinformatics for molecular systems biology. Department of Computer Science and Computer Engineer, University of Louisville, KY. Sept. 4, 2009.
22. Current development of mass informatics for Pegasus-based differential metabolomics. LECO Corporation, St. Joseph, MI. Aug. 27, 2009.
21. Molecular systems biology for cancer biomarker discovery. College of Life Science and Technology, Beijing Institute of Technology, Beijing, China. July 23, 2009.
20. Bioinformatics for cancer biomarker discovery. Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou, China. July 17, 2009.
19. Molecular systems biology. College of Agronomy, Shandong Agriculture University, Taian, China. July 3, 2009.
18. Two dimensional gas chromatography time-of-flight mass spectrometry based metabolomics. Department of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indianapolis, IN. March 9, 2009.
17. Mass informatics for comparative proteomics. Department of Bioinformatics and Biostatistics, University of Louisville, KY. Oct. 24, 2008.
16. Comparative proteomics for molecular cancer biomarker discovery. *Cancer Prevention & Control Seminar*. James Graham Brown Cancer Center, University of Louisville, KY. Oct. 14, 2008.
15. Mass informatics of mass spectrometry-based protein biomarker discovery. *Biomarker Discovery Summit 2008*. Philadelphia, PA. Sept. 29 – Oct. 1, 2008.

14. Proteome discovery pipeline for mass spectrometry-based proteomics. *UT-ORNL-KBRIN Bioinformatics Summit 2008*. Cadiz, KY, March 28 – 30, 2008.
13. Integrated omics for cancer biology. *Methodist Research Institute*. Indianapolis, IN, Feb. 8, 2008.
12. Bioinformatics in proteomics. *The Veterinary Comparative Respiratory Society (VCRS) 25th Symposium*. Lafayette, IN, Oct. 11-13, 2007.
11. Mass informatics for molecular profiling study at Bindley Bioscience Center. *Indiana Roundtable on Computational Proteomics*. Indianapolis, IN, Jan 26, 2007
10. The systems biology approach for biomarker discovery. Radiochemical Institute, China Institute of Atomic Energy, Beijing, China, July 3, 2006.
09. Comparative proteomics. Shanghai Institute of Applied Physics, the Chinese Academy of Sciences, Shanghai, China, June 29, 2006.
08. Bioinformatics of proteomics for biomarker discovery. Department of Pharmacology, Zhongshan University, China. June 8, 2006.
07. Neural network prediction of peptide behavior in strong anion exchange. *Third Annual Indiana Bioinformatics Conference*. Indianapolis, IN. May 19-20, 2006.
06. Bioinformatics of mass spectrometry based proteomics for biomarker discovery. *Department of Statistics, Purdue University*. Jan. 13, 2006.
05. Tools for differential metabolomics. *230th ACS Fall National Meeting*, Washington, DC. Aug. 28, 2005.
04. Biomarker Discovery. Agilent Customer Meeting, *53th ASMS Conference on Mass Spectrometry and Allied Topics*, San Antonio, TA, June, 2005.
03. Multidimensional binary elution chromatography (mBEC): a new approach to proteomics mapping, *18th International Symposium on Microscale Bioseparation*, New Orleans, Feb. 12, 2005.
02. Biomarker discovery based on global internal standard technology (GIST), Beyond Genomics Inc.; Waltham, MA, May, 2003.
01. Bioinformatics of signature peptide approach to proteomics, Indiana Mass Spectrometry Discussion Meeting, Purdue University, IN, Nov. 1999.

CONFERENCE PRESENTATION

114. Song, M.; Fang, Y.; Li, X.; Rouchka, E. C.; Zhang, X.; McClain, C. J. Dietary copper-fructose interactions alter gut microbiome in a sex-differential manner likely contributes to the sex differences in the metabolic phenotype. *Experimental Biology 2020*, San Diego, California, USA. April 4-7, 2020
113. Fulghum, K.; Lorkiewicz, P.; Rood, B.; Vargas, L.; McNally, L.; Zhang, X.; Jones, S.; Hill, B. Stable isotope-resolved metabolomics to assess cardiac metabolism in vivo. *The 26th Annual Conference of the Society for Redox Biology and Medicine (SfRBM)*, Planet Hollywood Resort & Casino, Las Vegas, NV, Nov 20-23, 2019
112. Miller, H.; Lynch, C.; Yin, X.; Hu, X.; Zhang, X.; Yan, J.; Miller, D.; Berkel, V.; Frieboes, H. Metabolic profiling of NSCLC patient tissue biopsies for personalized classification. *Research!Louisville*, University of Louisville, Louisville, KY, Sept. 10-12, 2019
111. Fulghum, K.; Lorkiewicz, P.; Rood, B.; Vargas, L.; McNally, L.; Zhang, X.; Jones, S.; Hill, B. Stable isotope-resolved metabolomics to assess cardiac metabolism in vivo. *Research!Louisville*, University of Louisville, Louisville, KY, Sept. 10-12, 2019
110. He, L.; Wei, X.; Ma, X.; Yin, X.; Song, M.; Donninger, H.; Yaddanapudi, K.; McClain, C.; Zhang, X. Simultaneous Quantification of Nucleosides and Nucleotides from Biological Samples. *Research!Louisville*, University of Louisville, Louisville, KY, Sept. 10, 2019
109. Harder, J.; Ma, J.; Chhabra, A.; Alard, P.; Zhang, X.; Yuan, F.; Ferrill, R.; Hua, Y.; Kosiewicz, M. Androgens may influence lupus development via an effect on the composition and metabolic activities of intestinal microbiota in BWF1 mice. *Research!Louisville*, University of Louisville, Louisville, KY, Sept. 10-12, 2019
108. He, L.; Vatsalya, V.; Ma, X.; Zhang, J.; Yin, X.; McClain, C.; Zhang, X. Metabolic profiling of bile acids from human urine by solid phase extraction liquid chromatography mass spectrometry. *Research!Louisville*, University of Louisville, Louisville, KY, Sept. 10-12, 2019

107. Prodhan, A.; Sleman, A.A.; Kim, S.; McClain, C.J.; Zhang, X. A method of calculating retention index of the second dimension separation in comprehensive two-dimensional gas chromatography mass spectrometry. *67th Conference on Mass Spectrometry & Allied Topics*, Georgia World Congress Center, Atlanta, GA. June 2 - 6, 2019.
106. Lorkiewicz, P.K.; Gibb, A.A.; Rood, B.R.; He, L.; Zheng, Y.; Zhang, X.; Hill, B.G. Stable isotope-resolved metabolomics under pharmacologically controlled metabolic states. *67th Conference on Mass Spectrometry & Allied Topics*, Georgia World Congress Center, Atlanta, GA. June 2 - 6, 2019.
105. Warner, D.R.; Warner, J.B.; Song, Y.; Whitlock, J.; Li, E.C.; Wang, G.; Rouchka, E.; Yuan, F.; Yin, X.; Zhang, X.; McClain, C.J.; Kirpich, I.A. Complementary Responses of the Intestinal Mucosa and Microbiota to Ethanol and LPS Challenge: Role of Modulation of Tissue $\omega 6:\omega 3$ PUFA Ratio. *The Digestive Disease Week 2019*, Walter San Diego Convention Center, San Diego, CA, May 18-21, 2019.
104. Prodhan, A.; Shi, B.; Yin, X.; Feng, W.; McClain, C.J.; Zhang, X. Integrating comprehensive two-dimensional gas chromatography mass spectrometry and two-dimensional liquid chromatography mass spectrometry for metabolomics. *Pittcon 2019*, Philadelphia, PA, March 17-21, 2019
103. He, L.; Li, F.; Yuan, F.; Yin, X.; Prodhan, A.; McClain, C.J.; Feng, W.; Zhang, X. Relative quantification of metabolites in fecal samples using three analytical platforms and the role of cathelicidin-related antimicrobial peptide in alcoholic liver disease. *Pittcon 2019*, Philadelphia, PA, March 17-21, 2019.
102. Reynolds, R.; Dougherty, S.; Kruer, T.; He, L.; Shi, B.; Zhang, X.; Clem, B. Retinoblastoma protein regulates metabolic reprogramming in lung cancer. *Research!Louisville*, University of Louisville, Louisville, KY, Oct. 12, 2018
101. Prodhan, A.; Sleman, A.A.; Kim, S.; McClain, C.J.; Zhang, X. Universal reference system for calculating the second dimension retention index in GC $\times$ GC-MS. *Research!Louisville*, University of Louisville, Louisville, KY, Oct. 12, 2018
100. He, L.; Li, F.; Yuan, F.; Yin, X.; Prodhan, A.; McClain, C.J.; Feng, W.; Zhang, X. Relative quantification of metabolites in fecal samples using three analytical platforms and the role of cathelicidin-related antimicrobial peptide in alcoholic liver disease. *Research!Louisville*, University of Louisville, Louisville, KY, Oct. 12, 2018
99. Young, J.L.; Yan, X.; Xu, J.; Yin, X.; Zhang, X.; Arteel, G.E.; Barnes, G.N.; States, C.J.; Watson, W.; Kong, M.; Cai, L.; Freedman, J.H. Cadmium and High-Fat Diet Disrupt Renal, Cardiac and Hepatic Essential Metals. *Research!Louisville*, University of Louisville, Louisville, KY, Oct. 12, 2018
98. Yuan, F.; Howard, R.; Zhang, X.; Mellen, N. Preliminary mechanism exploration for preferential delivery of 6 β -naltrexol into fetal mouse central nervous system. *Research!Louisville 2018*, University of Louisville, Louisville, KY, Oct. 12, 2018
97. Gibb, A.A.; Lorkiewicz, P.K.; Rood, B.; Zheng, Y.; He, L.; Zhang, X.; Hill, B.G. Stable isotope metabolomics under controlled metabolic states. *16th Annual Meeting of the SHVM*, Charleston, SC, USA, Sept. 30 – Oct. 3, 2018.
96. Prodhan, A.; Shi, B.; Yin, X.; Feng, W.; McClain, C.J.; Zhang, X. Integrated parallel two-dimensional liquid chromatography mass spectrometry and comprehensive two-dimensional gas chromatography mass spectrometry for metabolomics. *HPLC 2018*, Washington, DC, July 29-Aug. 2, 2018 (Oral by Xiang)
95. Shrestha, B.; Olivos, H.; Liu, Q.; Yin, X.; Feng, K.; Zhang, X. Integrated MALDI imaging and LC/MS workflow for spatial lipidome analysis of liver tissues. *14th Annual Conference of the Metabolomics Society*, Seattle, WA, June 24 – 28, 2018.
94. Shrestha, B.; Olivos, H.; Liu, Q.; Yin, X.; Feng, K.; Zhang, X. Integrated MALDI imaging and LC/MS workflow for spatial lipidome analysis of liver tissues. *66th ASMS Conference on Mass Spectrometry and Allied Topics*, San Diego, CA, June 3 – 7, 2018.
93. Li, Z.; Zhong, Z.; Kato, I.; Zhang, X.; Kim, S. Coherent point drift peak alignment algorithms using distance and similarity measures for mass spectrometry data. *Lipids@Wayne 2018*, Wayne State University, May 2, 2018

92. Surface Fitting for Calculating the Second Dimension Retention Index in GC×GC-MS. *Midwestern Universities Analytical Chemistry Conference (MUACC)*, Ohio University, Athens, OH. October 19-21, 2017. (Oral by Aminul Prodhon)
91. Song M, Zhang X, Wang Y, Vos M, Mendoza M, Prough R, Cave M, and McClain C.J. Dietary Copper-Fructose Interactions Alter Gut Microbial Activity Concurrent with the Development of Hepatic Steatosis in Male Rats. *The 56rd Annual Meeting of the Society of Toxicology 2017*, Baltimore, Maryland, March 12-16, 2017.
90. Song, M.; Zhang, X.; Wang, Y.; Vos M.; Prough R.A.; Cave M.C.; McClain C.J. Endotoxemia is not Required for Dietary Copper-Fructose Interactions Induced Hepatic Steatosis in Male Rats. *Gastroenterology*. 2017; 152(5) S1117.
89. Song M, Zhang X, Wang Y, Vos MB, Prough RA, Cave MC, and McClain CJ. Dietary High and Low Copper-Fructose Interactions Induce Hepatic Steatosis Associated with Distinct Alterations of Gut Microbial Activity in Male Rats. *Experimental Biology 2017*, Chicago, IL, April 22-26, 2017.
88. Song M, Zhang X, Wang Y, Vos MB, Prough RA, Cave MC, and McClain CJ. Endotoxemia is not Required for Dietary Copper-Fructose Interactions Induced Hepatic Steatosis in Male Rats. *Digestive Disease Week 2017*, Chicago, IL, May 6-9, 2017.
87. Alonso, D.; Zhang, X.; Binkley, J. Untargeted investigation of non-alcoholic fatty liver disease using effective multiplatform GC-MS instrumentation. *65th ASMS Conference on Mass Spectrometry and Allied Topics*, Indianapolis, IN, June 4 – 8, 2017.
86. Li, Z.; Zhong, Z.; Kato, I.; Zhang, X.; Kim, S. Point matching peak alignment algorithms using retention time distance and mass spectral similarity in metabolomics. 2017 Lipids@Wayne Symposium, Detroit, MI, May 10, 2017.
85. Carlisle, S.M.; Trainor, P.J.; Zhang, X.; Yin, X.; Doll, M.A.; States, J.C.; Hein, D.W. Untargeted polar metabolomics reveals differences in palmitoleic acid between transformed MDA-MB-231 breast cancer cells expressing varying levels of human arylamine *N*-acetyltransferase 1. *Kentucky Academy of Science Annual Meeting*, Louisville, KY. Nov. 4 – 5, 2016.
84. Carlisle, S.M.; Trainor, P.J.; Yin, X.; Doll, M.A.; States, J.C.; Zhang, X.; Hein, D.W. Untargeted metabolomics of transformed MDA-MB-231 breast cancer cells expressing varying levels of human arylamine *N*-acetyltransferase. *The 7th International Workshop on N-Acetyltransferases*, University Trier, Germany. June, 18 – 20, 2016.
83. Wei, X.; Koo, I.; Shi, B.; Lorkiewicz, P.; Suhail, H.; Rattan, R.; Giri, S.; Zhang, X. A computational platform for analysis of stable isotope assisted metabolomics data acquired on GC-MS. *64th ASMS Conference on Mass Spectrometry and Allied Topics*, San Antonio, TX, June 5 – 9, 2016
82. Wei, X.; Lorkiewicz, P.; Salabei, J.K.; Shi, B.; Hill, B.G.; Kim, S.; McClain, C.J.; Zhang, X. Analysis of Stable Isotope Assisted Metabolomics Data Acquired by High Resolution Mass Spectrometry. *64th ASMS Conference on Mass Spectrometry and Allied Topics*, San Antonio, TX, June 5 – 9, 2016
81. Shi, B.; Song, M.; Wei, X.; Yin, X.; Schuschke, D.A.; Koo, I.; McClain, C.J.; Zhang, X. Effects of Dietary Different Doses of Copper and High Fructose Feeding on Rat Fecal Metabolome. *64th ASMS Conference on Mass Spectrometry and Allied Topics*, San Antonio, TX, June 5 – 9, 2016
80. Global peak alignment for comprehensive two-dimensional gas chromatography mass spectrometry using point matching algorithms. *The GLBIO/CCBC Great Lakes Bioinformatics and the Canadian Computational Biology Conference 2016*, the University of Toronto, Canada. May 16 – 19, 2016.
79. Carlisle, S.M.; Trainor, P.J.; Yin, X.; Doll, M.A.; States, J.C.; Zhang, X.; Hein, D.W. Metabolomics of Transformed MDA-MB-231 Breast Cancer Cells Expressing Varying Levels of Human Arylamine *N*-Acetyltransferase 1 (NAT1). *UT-KBRIN Bioinformatics Summit 2016*, Lake Barkley State Resort Park in Cadiz, KY, April 8 – 10, 2016
78. Kosiewicz, M.; Alard, P.; Zhang, X.; Fausnaught, T.; Jala, V.; Bodduluri, H.; Chhabra, A. Investigating pathway changes associated with varying levels of human arylamine *N*-acetyltransferase 1 (NAT1) activity in MDA-MB-231 breast cancer cells. *Research!Louisville 2015*. University of Louisville, Louisville, KY, Oct. 27 – 30, 2015.

77. Carlisle, S.M.; Trainor, P.J.; Zhang, X.; Yin, X.; Doll, M.A.; States, J.C.; Hein, D.W. Investigating pathway changes associated with varying levels of human arylamine N- acetyltransferase 1 (NAT1) activity in MDA-MB-231 breast cancer cells. *Research!Louisville 2015*. University of Louisville, Louisville, KY, Oct. 27 – 30, 2015.
76. Shi, B.; Zheng, S.; Wei, X.; Yin, X.; Cao, A.; Zhang, X.; Cai, L. Effects of low-dose γ -irradiation on kidney of mice with type 1 diabetes. *NIH Common Fund Metabolomics Annual Meeting*, University of Kentucky, Lexington, KY, Sept. 26 – 27, 2015.
75. Winnike, J.; Wei, X.; Gregory, S.; Zhang, X. The advantages of comprehensive two-dimensional GC-MS in the analysis of serum samples for metabolomics. *11th International Conference of the Metabolomics Society*, Burlingame, San Francisco Bay, CA, June 29 – July 2, 2015.
74. Kirpich, I. A.; Petrosino, J.; Ajami, N.; Feng, W.; Beier, J. I.; Barve, S. S.; Yin, X.; Wei, X.; Zhang, X.; McClain, C. J. Alterations of gut microbiome and metabolome caused by ethanol and unsaturated fat diet were prevented by dietary saturated fat in a mouse model of alcoholic liver disease. *The AASLD Liver Meeting*, San Francisco, CA, Nov, 13 – 17, 2015.
73. Song, M.; Wei, X.; Yin, X.; Schuschke, D. A.; Koo, I.; McClain, C. J.; Zhang, X. Effects of dietary different doses of copper and high fructose feeding on rat fecal metabolome. *The AASLD Liver Meeting*, San Francisco, CA, Nov, 13 – 17, 2015.
72. Tran, T.; Li, H.; Zhang, X.; Kim, S. Global peak alignment for comprehensive two-Dimensional gas chromatography coupled with mass spectrometry (GC $\times$ GC-MS). *International Society for Computational Biology*, Purdue University, West Lafayette, Indiana, May 18 – 20, 2015.
71. Yin, X.; Wei, X.; Song, M.; McClain, C. High fructose feeding induces copper deficiency: a fecal metabolomics study. *PITTCON Conference & Expo 2015*. New Orleans, LA, March 8 – 12, 2015.
70. Jala, V.R.; Bodduluri, S.; Kumar, S.; Vemula, P.K.; Vadhanam, M.; Annamalai, L.; Zhanga, X.; Burlison, J.A.; Trent, J.O.; Haribabu, B. Urolithin A, microbial metabolite modulate the gut microbiota and colonic inflammation: It's role in preventing colitis and colon tumorigenesis. *Brown Cancer Center Retreat*, Louisville, KY, Oct. 17, 2014.
69. Song, M.; Yin, X.; Wei, X.; Zhang, X.; McClain, C. High fructose feeding induces copper deficiency: a metabolomics study. *Brown Cancer Center Retreat*, Louisville, KY, Oct. 17, 2014.
68. Shi, B.; Yin, X.; Wei, X.; Chhabra, A. Y.; Alard, P.; Zhang, X.; Kosiewicz, M. M. Differential production of metabolites by microbiota from lupus-prone female and male mice correlates with disease susceptibility. *Brown Cancer Center Retreat*, Louisville, KY, Oct. 17, 2014.
67. Carlisle, M.S.; Trainor, P. J.; Zahng, X.; Yin, X.; Doll, M. A.; States, J. C.; Hein, D. W. Metabolomics of transformed MDA-MB-231 cell lines expressing different levels of human arylamine N-Acetyltransferase 1 (NAT1). *Research!Louisville*, Louisville, KY, Sept. 16-19, 2014.
66. Kim, S.; Shen, C.; Zhang, X. Hierarchical peak detection algorithms for comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry data. *JSM 2014*. Boston, MA, August 4, 2014.
65. Winnike, J.H.; Wei, X.; Gregory, S.G.; Zhang, X. Examination of human serum samples from subjects with and without a chronic neurodegenerative disorder. *62th ASMS Conference on Mass Spectrometry and Allied Topics*, Baltimore, MD, June 14 – 19, 2014.
64. Shi, X.; Wei, X.; Yin, X.; Watson, W.H.; Arteel, E.G.; Kim, S.; Zhang, X. Metabolomic analysis of the effects of chronic arsenic exposure in a mouse model of diet-induced fatty liver disease. *2013 AASLD Annual Meeting*, Washington DC, Nov. 1 – 5, 2013.
63. Song, M.; ???; Zhang, X.; McClain, C. Kupffer cell derived MCP-1 induces hepatic steatosis by up-regulation of SREBP1 in high fructose and marginal copper deficient diet fed rats. *2013 AASLD Annual Meeting*, Washington DC, Nov. 1 – 5, 2013.
62. Shi, X.; Wei, X.; Yin, X.; Watson, W.H.; Arteel, E.G.; Kim, S.; Zhang, X. Metabolomic analysis of the effects of arsenic in non-alcoholic fatty liver disease. *Pittcon 2013*, Philadelphia, PA. March 17–21, 2013.
61. Wei, X.; Shi, X.; Koo, I.; Kim, S.; Zhang, X. A computational platform for comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry-based metabolomics profiling. *Pittcon 2013*, Philadelphia, PA. March 17–21, 2013.
60. Laulhé, S.; Geers, T.E., Shi, X.; Zhang, X.; Nantz, M.H. Quantifiable Multiplexed GC-MS Analysis of Carbonyl and Amine Metabolites Using the Electron-Induced Cleavage of an Isotopic

- Reporter tag. *IMD3 Symposium*, 03, 12, 2013.
59. Wei, X.; Sun, W.; Shi, X.; Koo, I.; Kim, S.; Zhou, Z.; McClain, C.; Zhang, X. MetSign: a Computational Platform for High Resolution Mass Spectrometry-based Metabolomics. *IMD3 Symposium*, 03, 12, 2013.
 58. Shi, X.; Wei, X.; Sun, W.; Yin, X.; Zhang, X. Metabolomics Analysis of Alcohol on Mice Fed with Unsaturated Fat Diet Using GC×GC-MS. *IMD3 Symposium*, 03, 12, 2013.
 57. Laulhé, S.; Geers, T.E.; Shi, X.; Zhang, X.; Nantz, M.H. Multiplexed Metabolite Quantitation Using an Isotope Coding Strategy for GC-MS Analysis. *SERMACS*, Raleigh, NC; November 16, 2012.
 56. Laulhé, S.; Johannes, L.M.; Geers, T.E.; Zhang, Y.; Shi, X.; Zhang, X.; Nantz, M.H. Strategy for Relative Quantification of Metabolites via Multiplexed GC-MS Analysis. *244th ACS National Meeting and Exposition*, Philadelphia, PA; August 19, 2012.
 55. Philips, M.; Cataneo, R.; Kaplan, P.; Mundada, M.; Zhang, X.; Libardoni, M.; Schiff, P.; Ramakrishna, N.; Mehta, V.; Byrnes, R. Breath test for biomarkers of radiation exposure. *58th Annual Meeting of the Radiation Research Society*, San Juan, Puerto Rico, Sept 30–Oct. 3, 2012.
 54. Song M.; Schuschke, D. A.; Zhou, Z.; Chen, T.; Shi, X.; Zhang, J.; Zhang, X.; Pierce, W. M.; Johnson, W. T.; McClain, C. Low fructose beverage consumption impairs copper status and causes liver injury and fat accumulation in marginal copper deficient rats. *63rd Annual Meeting of the American Association for the Study of Liver Diseases*, Boston, MA, Nov. 9–13, 2012.
 53. Song M.; Schuschke, D. A.; Zhou, Z.; Shi, X.; Zhang, X.; Pierce, W. M.; McClain, C. Kupffer cells depletion eliminates high fructose induced fatty liver in marginal copper deficient rats. *63rd Annual Meeting of the American Association for the Study of Liver Diseases*, Boston, MA, Nov. 9–13, 2012.
 52. Patrick, J. S. ; Siek, K.; Zhang, L.; Binkley, J.; Shi, X.; Wei, X.; Zhang, X. Identification of biomarkers for alcoholic liver disease from mice fed with unsaturated fat diets by gas chromatography-high resolution time-of-flight mass spectrometry. *Metabolomics 2012*, Washington, DC. June 25–28, 2012.
 51. Patrick, J. S. ; Siek, K.; Zhang, L.; Binkley, J.; Shi, X.; Wei, X.; Koo, I.; Kim, S.; Feng, W.; McClain, C.; Zhang, X. Repeatability of LECO LC-HRT-MS in analysis of metabolite extract from mouse liver. *Metabolomics 2012*, Washington, DC. June 25–28, 2012.
 50. Shi, X.; Zhang, L.; Slek, K.; Wahlang, B.; Wei, X.; Koo, I.; Patrick, J.; Binkley, J.; Kim, S.; McClain, C.; Cave, M.; Zhang, X. A Comprehensive Approach to Disease Biomarker Discovery. *60th ASMS Conference on Mass Spectrometry and Allied Topics*, Vancouver, BC, CA. May 20–24, 2012.
 49. Shi, X.; Zhang, L.; Alonso, D.; Siek, K.; Wei, X.; Kirpich, I.; Koo, I.; Patrick, J.; Binkley, J.; Kim, S.; Feng, W.; McClain, C.; Zhang, X. Identification of biomarkers from mouse liver by gas chromatography-high resolution time of flight mass spectrometry. *PITTCON Conference & Expo 2012*, Orlando, FL. March 15–15, 2012.
 48. Shi, X.; Zhang, L.; Siek, K.; Wei, X.; Kirpich, I.; Koo, I.; Patrick, J.; Binkley, J.; Kim, S.; Feng, W.; McClain, C.; Zhang, X. Robustness of HILIC-TOF-MS in the analysis of lipids and other metabolite extracts from mouse liver. *PITTCON Conference & Expo 2012*, Orlando, FL. March 15–15, 2012.
 47. Wahlang, B.; Shi, X.; Zhang, X.; Falkner, K.C.; McClain, C.J.; Prough, R.; Cave, M. The metabolic effects of Pcb 153 depend on nutrient interactions in obesity/nonalcoholic fatty liver disease. *Digestive Disease Week 2012*. San Diego, CA. May 19–22, 2012.
 46. Laulhé, S.; Johannes, L.; Geers, T.; Zhang, Y.; Zhang, X.; Nantz, M.H. A Strategy for Relative Quantification of Metabolites via Multiplexed GC-MS Analysis. Poster No. 7, Annual IMD3 Symposium, Louisville, KY; March 13, 2012.
 45. Laulhé, S.; Johannes, L.; Geers, T.; Zhang, Y.; Zhang, X.; Nantz, M.H. A ‘Click-Chemistry’ Reagent for High Throughput Carbonyl Profiling. Poster No. 49, Research! Louisville, Louisville, KY; October 11, 2011.
 44. Zhong, W.; Zhao, Y.; Tang, Y.; Wei, X.; Shi, X.; Sun, W.; Sun, X.; Yin, X.; Sun, X.; Kim, S.; McClain, C J.; Zhang, X.; Zhou, Z. Chronic alcohol exposure causes adipose fat overflux to the

- liver in mice: A mechanistic link between lipodystrophy and steatosis. *The 62nd Annual Meeting of the American Association for the Study of Liver Disease*. San Francisco, CA. Nov. 4–8, 2011.
43. Shi, X.; Wang, B.; Zhang, J.; Wei, X.; Kim, S.; Kirpich, I.; Feng, W.; McClain, C.; Zhang, X. Metabolomics analysis of alcohol on mice fed with unsaturated fat diet using GC×GC-MS. *59th ASMS Conference on Mass Spectrometry and Allied Topics*, Denver, CO. June 5–9, 2011.
 42. Wei, X.; Shi, X.; Tang, Y.; Sun, W.; Yin, X.; Sun, X.; Bogdanov, B.; Kim, S.; McClain, C.; Zhou, Z.; Zhang, X. Metabolomics analysis reveals reverse fatty acid transport in alcoholic fatty liver. *59th ASMS Conference on Mass Spectrometry and Allied Topics*, Denver, CO. June 5–9, 2011.
 41. Wei, X.; Sun, W.; Xue, S.; Koo, I.; Yin, X.; Wang, B.; Bogdan, B.; Kim, S.; Zhou, Z.; McClain, C.; Zhang, X. MetSign: a computational platform for high resolution mass spectrometry-based metabolomics. *59th ASMS Conference on Mass Spectrometry and Allied Topics*, Denver, CO. June 5–9, 2011.
 40. Zhang, J.; Fang, A.; Wang, B.; Kim, S.; Bogdan, B.; Zhou, Z.; McClain, C.; Zhang, X. iMatch: A retention index tool for analysis of gas chromatography-mass spectrometry data. *59th ASMS Conference on Mass Spectrometry and Allied Topics*, Denver, CO. June 5–9, 2011.
 39. Koo, I.; Zhang, X.; Kim, S. Improved compound identification using mass spectral similarity measures based on Wavelet/Fourier transforms. *59th ASMS Conference on Mass Spectrometry and Allied Topics*, Denver, CO. June 5–9, 2011.
 38. Fang, A.; Zhang, X. Reproducibility of comprehensive two-dimensional gas chromatography mass spectrometry. *59th ASMS Conference on Mass Spectrometry and Allied Topics*, Denver, CO. June 5–9, 2011.
 37. Kim, H. S.; Wang, B.; Zhang, X. A peak alignment algorithm for two-dimensional gas chromatography/time-of-flight mass spectrometry based metabolomics. *35th International Symposium on Capillary Chromatography (ISCC)*, San Diego, CA. May 1–5, 2011.
 36. Roumani, A. M.; Gough, E. S.; McGrow, T.; Riley, C. P.; Buck, C.; Zhang, X. Mass Spectrometry-based Differential Proteomics Using The Omics Discovery Pipeline. *Third Annual Breast Cancer Discovery Group Retreat*, Purdue University, IN, USA, May 12, 2011.
 35. Roumani, A. M.; Riley, C. P.; Gough, E. S.; Buck, C.; Zhang, X. The Proteome Discovery Pipeline: A Data Analysis Pipeline for Mass Spectrometry Based Differential Proteomics. *Chronic Disease Research Session*, Purdue University, IN, USA, Apr. 27, 2011.
 34. Roumani, A.M.; Riley, C. P.; Gough, E. S.; Buck, C.; Zhang, X. The Omics Discovery Pipeline: A Data Analysis Pipeline for Mass Spectrometry Based Differential Proteomics and Metabolomics Discovery. *CI Days at Purdue*, IN, USA, Dec. 8–9, 2010.
 33. Johannes, L.M.; Laulhé, S.; Shi, X.; Zhang, X.; Nantz, M.H. McLafferty Rearrangement: Structural Factors that Promote α,β -Fragmentation. Poster, Summer Research Opportunities for Undergraduates, University of Louisville, Louisville, KY; August 4, 2010.
 32. Wang, B.; Heim, J.; Libardoni, M.; Zhang, X. MetPP: a bioinformatics platform for two dimensional gas chromatography-mass spectrometry based metabolomics. *57th ASMS Conference on Mass Spectrometry and Allied Topics*, Philadelphia, PA. May 31–June 4, 2009.
 31. Wang, B.; Valentine, S.; Raghuraman, S.; Plasencia, M.; Zhang, X. Predicting peptide drift time in ion mobility-mass spectrometry using an artificial neural network regression model. *UT-ORNL-KBRIN Bioinformatics Summit 2009*. Pikeville, KY, March 20–22, 2009.
 30. Jannasch, A.; Perera, R.; Riley, C.; Zhang, X.; Yoder, J. L.; Sedlak, M.; Adamec, J.; Kuhn, R. J. A lipidomics approach to study effects of dengue virus on human liver cells using LC/ESI-MS. *Sanibel Conference on Mass Spectrometry*. St. Petersburg Beach, FL. Jan. 23–26, 2009.
 29. Wang, B.; Riley, C. P.; Chen, J.; Buck, C.; Regnier, F. E.; Zhang, X. Comparative study of peptide profile variation in label-free proteomics. *Clinical Proteomic Technologies Initiative for Cancer Annual Meeting*. Boston, MA. Oct. 28–29, 2008.
 28. Saha, S.; Harrison, S. H.; Shen, C.; Tang, H.; Radivojac, P.; Arnold, R. J.; Zhang, X.; Chen, J. Y. HIP2 : An online Database of Human Plasma Proteins from Healthy Individuals and its Analysis. *Clinical Proteomic Technologies Initiative for Cancer Annual Meeting*. Boston, MA. Oct. 28–29, 2008.
 27. Perera, R.; Hopf-Jannasch, A.; Edwards, T.J.; Owston, M.; Yoder, J. L.; Zhang, X.; Adamec, J.; Kuhn, R. J. Early events in flavivirus infection: a lipidomics approach. *15th International*

- Symposium on Hepatitis C Virus and Related Viruses*. San Antonio, Texas. Oct. 5–9, 2008.
26. Huang, X.; Oh, C.; Xu, Z.; Madian, A.; Alloosh, M.; Sturek, M.; Buck, C. R.; Regnier, F. E.; Zhang, X. Differential metabolomics analysis of serum from metabolic syndrome obese swine by stable isotope labeling and pattern recognition. *56th ASMS Conference on Mass Spectrometry and Allied Topics*, Denver, CO. June 1–5, 2008.
 25. Cho, H.; Oh, C.; Huang, X.; Buck, C. R.; Zhang, X. Comparative study of data imputation methods for metabolomics data from two dimensional gas chromatography time-of-flight mass spectrometry. *56th ASMS Conference on Mass Spectrometry and Allied Topics*, Denver, CO. June 1–5, 2008.
 24. Gough, E.; Oh, C.; He, J.; Riley, C. P.; Buck, C. R.; Zhang, X. Proteome discovery pipeline for mass spectrometry-based proteomics. *UT-ORNL-KBRIN Bioinformatics Summit 2008*. Cadiz, KY, March 28–30, 2008.
 23. Harrison, S.; Saha, S.; Zhang, X.; Chen, J. Proteomics pipeline infrastructure at IUPUI for the CPTAC Purdue University Research Team. *Clinical Proteomic Technologies Initiative for Cancer Annual Meeting*. Washington DC. Oct. 24–25, 2007.
 22. Harrison, S.; Hussey, P.; Saha, S.; Rudnick, P.; Zhang, X.; Chen, J. A data model for managing experimental metadata for mass spectrometry based clinical proteomics. *Clinical Proteomic Technologies Initiative for Cancer Annual Meeting*. Washington DC. Oct. 24–25, 2007.
 21. Miskovic, M.; Riley, C. P.; Couetil, L. L.; Zhang, X.; Adamec, J. Protein expression patterns in bronchoalveolar lavage fluid of horse with recurrent airway obstruction. *The Veterinary Comparative Respiratory Society (VCRS) 25th Symposium*. Lafayette, IN, Oct. 11–13, 2007.
 20. Zhang, M.; Kane, M.; Salt, D.; Prabhakar, S.; Buck, C.; Regnier, F. E.; Zhang, X. Interactive Visualization of ‘Omics Molecular Expression Networks. *55th ASMS Conference on Mass Spectrometry and Allied Topics*, Indianapolis, IN, June, 2007.
 19. Riley, C.; Adamec, J.; Zhang, X.; Walls, E.; Buck, C.; Mohammed, S. Proteomic profile of lymph in metastatic breast cancer. *55th ASMS Conference on Mass Spectrometry and Allied Topics*, Indianapolis, IN, June, 2007.
 18. Ralston-hooper, K. J.; Baker, S.; Hopf, A.; Adamec, J.; Zhang, X.; Sepulveda, M. The Use of GCxGC-MS for Biomarker Identification in Vertebrate and Invertebrate Species Exposed to Various Environmental Stressors. *55th ASMS Conference on Mass Spectrometry and Allied Topics*, Indianapolis, IN, June, 2007.
 17. Oh, C.; Huang, X.; Buck, C.; Zhang, X. Comprehensive GCxGC-MS data alignment for metabolomics. *55th ASMS Conference on Mass Spectrometry and Allied Topics*, Indianapolis, IN, June, 2007.
 16. Oh, C.; Liu, F.; Valentine, S.; Williams, B.; Buck, C.; Clemmer, D.; Naylor, S.; Regnier, F.; Zhang, X. Artificial neural network prediction of peptide separation in strong cation exchange chromatography. *HUPO 5th Annual World Congress*, Long Beach, CA, Oct. 28–Nov. 1, 2006.
 15. Oh, C.; Mirzaei, H.; Regnier, F. E.; Zhang, X. Assessment of tandem mass spectra quality using intelligent algorithms. *54th ASMS Conference on Mass Spectrometry and Allied Topics*, Seattle, WA, May, 2006.
 14. Fedulova, I.; Mirzaei, H.; Pevtsov, S.; Ouyang, Z.; Zhang, X. PepTiger: search engine for error-tolerant protein identification from de novo sequences. *54th ASMS Conference on Mass Spectrometry and Allied Topics*, Seattle, WA, May, 2006.
 13. Zhang, X.; Orcun, S.; Jandhyala, S.; Ouzzan, M.; Baxter, I.; Salt, D.; Regnier, F. E.; Elmagarmid, A.; Davisson, V. J.; Pekny, J. A bioinformatics infrastructure for mass spectrometry-based proteomics. *54th ASMS Conference on Mass Spectrometry and Allied Topics*, Seattle, WA, May, 2006.
 12. Asara, M. J.; Zhang, X.; Zheng, B.; Matsuo, M.; Li, Q. T.; Cantley, C. L. InGel stable isotope labeling an alternative approach, *53th ASMS Conference on Mass Spectrometry and Allied Topics*, San Antonio, TX, June, 2005.
 11. Fedulova, I.; Pevtsov, S.; Zhang, M.; Ouyang, Z.; Prabhakar, S.; Zhang, X. InProID: an Integrated Protein Identification System, *53th ASMS Conference on Mass Spectrometry and Allied Topics*, San Antonio, TX, June, 2005.
 10. Ouzzani, M.; Zhang, X.; Eltabakh, M.; Elmeleegy, H.; Zhang, M.; Elmagarmid, A.; Prabhakar,

- S.; Aref, W. G. Online data system for comparative proteomics, *2nd Midwest Database Research Symposium*, Chicago, IL, April 16, 2005.
09. Zhang, X.; Asara, M. J.; Adamec, J.; Ouzzani, M. Data preprocessing in LC/MS based proteomics, *USHUPO 2005 Symposium*, Washington D. C. March, 2005.
 08. Zhang, X.; Adamec, J.; Nalyor, S.; Davisson, V. J.; Regnier, F. E. A binary elution chromatography approach for high throughput proteomics, *Indiana Proteomics Symposium*, Bloomington, IN, Oct. 2004.
 07. Zhang, X.; Adamec, J.; Davisson, V. J. Systems biology approach for drug discovery, *Bionano Technology Symposium*, West Lafayette, IN, July 2004.
 06. Corbo, A. J.; Finch, W. J.; Dourdeville, T.; Zhang, X.; Meys M. Quantitative LC/MS proteomic analysis of biological samples using a novel nano flow LC system. *52th ASMS Conference on Mass Spectrometry and Allied Topics*, Nashville, TN, May, 2004.
 05. Zhang, X.; Hines, W.; Adamec, J.; Asara, M. J.; Naylor, S.; Regnier E. F. An automated method for the analysis of stable isotope labeling data in proteomics. *52th ASMS Conference on Mass Spectrometry and Allied Topics*, Nashville, TN, May, 2004.
 04. Asara, J.; Adamec, J.; Zhang, X.; Hines, W.; London, T.; Hincapie, M.; Naylor, S. Quantitative protein profiling of serum and plasma using Global Internal Standard Technology (GIST), *ABRF 2003*. Denver, CO, Feb. 2003.
 03. Regnier, F.; Clemmer, D.; Naylor, S.; Zhang, X.; Adamec, J.; Ren, D.; Penner, N. The peak capacity issue in proteomics. *The 13th Annual Frederick Conference on Capillary Electrophoresis*, National Cancer Institute at Frederick, Maryland, USA, 2002.
 02. Johnston, M.; Moss, D.; Adamec, J.; Wayne S.; Zhang, X.; Meys, M. Automation: Robotic in-solution digestion of complex protein mixture and analysis by MALDI-TOF mass spectrometry. *HPLC 2002*, Montreal, Canada, June 2002.
 01. Lavine, G.; Valentine, S.; London, T.; Zhang, X.; Naylor, S. Using ion mobility / time of flight mass spectrometry in the "omics" revolution, *50th ASMS Conference on Mass Spectrometry and Allied Topics*, Orlando, FL, June 2002.