CURRICULUM VITAE   Oct. 1, 2025

SHUZHAO LI

ACADEMIC APPOINTMENTS

01/2020 - Present: Associate Professor, The Jackson Laboratory for Genomic Medicine, Farmington, CT

11/2020 - Present: Visiting Associate Professor, Department of Immunology, University of Connecticut School of Medicine

PROFESSIONAL EXPERIENCE

2020 - present: Associate Professor, The Jackson Laboratory for Genomic Medicine Farmington, CT

2014 – 2019:   Assistant Professor of Medicine, Division of Pulmonary, Allergy, Critical Care and Sleep Medicine, Department of Medicine, Emory University, School of Medicine, Atlanta, GA

2014 – 2019:   Associate Director, Clinical Biomarkers Laboratory, Department of Medicine, Emory University, Atlanta, GA

SERVICES

NIH Metabolomics Consortium, Steering Committee, 2018 – 2022
NIH National Exposure Assessment Laboratory Network, Untargeted analysis, 2015 – 2019
Center for Children's Health, the Environment, the Microbiome, and Metabolomics, Emory University, Executive Committee, 2015 – 2019

EDUCATIONAL BACKGROUND

2009 – 2013   Postdoctoral fellow, Emory Vaccine Center, Atlanta, GA
2007 – 2009   Ph.D., University of Southern Mississippi, Hattiesburg, MS
2001 – 2006   M.Sc., Montana State University, Bozeman, MT
1994 – 1998   B.A., Sichuan University, Chengdu, China

PRINT AND ORAL SCHOLARSHIP

PUBLICATIONS: Peer Reviewed Journal Articles
*Indicates corresponding Author

1. Christopher B. Medina, Ewelina Sobierajska, Minghao Gong, Daniel McManus, Maheshwor Thapa, Sejin Im, Jason E. Toombs, Joshua M. Mitchell, Yating Wang, Jenny Carlisle, Gordon J. Freeman, Viraj A. Master, Suresh S. Ramalingam, Haydn T. Kissick, **Shuzhao Li**, Rolf A. Brekken, and Rafi Ahmed. Exposed phosphatidylserine as a non-classical inhibitory molecule during CD8 T cell exhaustion. *Nature.* Accepted.

2. MorPhiC Consortium (2025). Towards functional characterization of human genes: Generating a consistent catalog of molecular phenotypes of null alleles in human cells. *Nature* 638 (8050), 351-359.

3. Banbury Consortium (2025). Integrating Exposomics into the Biomedical Enterprise. *Science* 388 (6745), 356-358.

4. Metz TO, Chang CH, Gautam V, Anjum A, Tian S, Wang F, Colby SM, Nunez JR, Blumer MR, Edison AS, Fiehn O, Jones DP, **Li S**, Morgan ET, Patti GJ, Ross DH, Shapiro MR, Williams AJ, Wishart DS. Introducing 'identification probability' for automated and transferable assessment of metabolite identification confidence in metabolomics and related studies. *Anal. Chem*. 2025, 97, 1, 1–11

5. Cortese M, Hagan T, Rouphael N, Wu SY, Xie X, Kazmin D, Wimmers F, Gupta S, van der Most R, Coccia M, Aranuchalam PS, Nakaya HI, Wang Y, Coyle E, Horiuchi S, Wu H, Bower M, Mehta A, Gunthel C, Bosinger SE, Kotliarov Y, Cheung F, Schwartzberg PL, Germain RN, Tsang J, **Li S**, Albrecht R, Ueno H, Subramaniam S, Mulligan MJ, Khurana S, Golding H, Pulendran B. "System vaccinology analysis of predictors and mechanisms of antibody response durability to multiple vaccines in humans." *Nature Immunology* (2025): 1-15.

6. Joshua M. Mitchell, Yuanye Chi, Shujian Zheng, Maheshwor Thapa, Eric Wang, **Shuzhao Li***. Annotation of Metabolites in Stable Isotope Tracing Untargeted Metabolomics via Khipu-web. *Journal of the American Society for Mass Spectrometry*, 2024. https://doi.org/10.1021/jasms.4c00175

7. Mitchell, J.M., Chi, Y., Thapa, M., Pang, Z., Xia, J. and **Li, S***., 2024. Common data models to streamline metabolomics processing and annotation, and implementation in a Python pipeline. *PLOS Computational Biology*, *20*(6), p.e1011912.

8. Pang Z, Lu Y, Zhou G, Hui F, Xu L, Viau C, Spigelman AF, MacDonald PE, Wishart DS, **Li S**, Xia J. MetaboAnalyst 6.0: towards a unified platform for metabolomics data processing, analysis and interpretation. *Nucleic Acids Research*. 2024. https://doi.org/10.1093/nar/gkae253.

9. **Li, S.***, Siddiqa, A., Thapa, M., Chi, Y. and Zheng, S., 2023. Trackable and scalable LC-MS metabolomics data processing using asari. *Nature Communications*, *14*(1), p.4113.

10. Siddiqa, A., Wang, Y., Thapa, M., Martin, D.E., Cadar, A.N., Bartley, J.M.* and **Li, S.***, 2023. A pilot metabolomic study of drug interaction with the immune response to seasonal influenza vaccination. *npj Vaccines*, *8*(1), p.92.

11. **Li, S.*** and Zheng, S., 2023. Generalized tree structure to annotate untargeted metabolomics and stable isotope tracing data. *Analytical Chemistry*, *95*(15), pp.6212-6217.

12. Lee, C.M., Liu, K.H., Singer, G., Miller, G.W., **Li, S.**, Jones, D.P. and Morgan, E.T., 2022. High-Throughput Production of Diverse Xenobiotic Metabolites with Cytochrome P450–Transduced Huh7 Hepatoma Cell Lines. *Drug Metabolism and Disposition*, *50*(9), pp.1182-1189.

13. Liu, K.H., Lee, C.M., Singer, G., Bais, P., Castellanos, F., Woodworth, M.H., Ziegler, T.R., Kraft, C.S., Miller, G.W., **Li, S**. and Go, Y.M., Morgan E.T., Jones D.P. 2021. "Large scale

enzyme based xenobiotic identification for exposomics." *Nature communications* 12.1 (2021): 1-9.

14. Pang, Z., Chong, J., Zhou, G., de Lima Morais, D.A., Chang, L., Barrette, M., Gauthier, C., Jacques, P.É., **Li, S**. and Xia, J., 2021. MetaboAnalyst 5.0: narrowing the gap between raw spectra and functional insights. *Nucleic acids research*. 2021 Jul 2;49(W1):W388-W396. doi: 10.1093/nar/gkab382.

15. Chang, H.Y., Colby, S.M., Du, X., Gomez, J.D., Helf, M.J., Kechris, K., Kirkpatrick, C.R., **Li, S.**, Patti, G.J., Renslow, R.S. and Subramaniam, S., Verma M, Xia J and Young J.D. 2021. A Practical Guide to Metabolomics Software Development. *Analytical chemistry*, 93(4), pp.1912-1923.

16. Landay A, Bartley JM, Banerjee D, Hargis G, Haynes L, Keshavarzian A, Kuo CL, Kwon OS, Li S, **Li S**, Oh J. Network topology of biological aging and Geroscience-guided approaches to COVID-19. *Frontiers in aging*. 2021 Jul 23;2:695218.

17. Liu Q, Walker D, Uppal K, Liu Z, Ma C, Tran V, **Li S**, Jones DP, Yu T. (2020) Addressing the batch effect issue for LC/MS metabolomics data in data preprocessing. *Sci Rep.* 10(1):13856. PMCID: PMC7431853

18. Goll JB, **Li S**, Edwards JL, Bosinger SE, Jensen TL, Wang Y, Hooper WF, Gelber CE, Sanders KL, Anderson EJ, Rouphael N, Natrajan MS, Johnson RA, Sanz P, Hoft D, Mulligan MJ. (2020) Transcriptomic and Metabolic Responses to a Live-Attenuated Francisella tularensis Vaccine. *Vaccines* (Basel). 8(3). pii: E412. PMCID: PMC7563297

19. Palermo, A., Huan, T., Rinehart, D., Rinschen, M.M., **Li S**, O'Donnell, V.B., Fahy, E., Xue, J., Subramaniam, S., Benton, H.P. and Siuzdak, G. (2020). Cloud-based archived metabolomics data: A resource for in-source fragmentation/annotation, meta-analysis and systems biology. *Analytical Science Advances*, 1(1), pp.70-80.

20. Pang Z, Chong J, **Li S**, Xia J. (2020) MetaboAnalystR 3.0: Toward an Optimized Workflow for Global Metabolomics. *Metabolites*. 10(5). pii: E186. PMID: 32392884, PMCID: PMC7281575

21. Collins JM, Siddiqa A, Jones DP, Liu K, Kempker RR, Nizam A, Shah NS, Ismail N, Ouma SG, Tukvadze N, **Li S**, Day CL, Rengarajan J, Brust JC, Gandhi NR, Ernst JD, Blumberg HM, Ziegler TR. (2020) Tryptophan catabolism reflects disease activity in human tuberculosis. *JCI Insight*. 5(10). pii: 137131. PMCID: PMC7259525

22. Ferranti EP, Frediani JK, Mitchell R, Fernandes J, **Li S**, Jones DP, Corwin E, Dunlop AL. (2020) Early Pregnancy Serum Metabolite Profiles Associated with Hypertensive Disorders of Pregnancy in African American Women: A Pilot Study. *J Pregnancy*. doi:10.1155/2020/1515321. PMCID: PMC7049834

23. Corwin E, Dunlop AL, Fernandes J, **Li S**, Pearce B, Jones DP (2020). Metabolites and Metabolic Pathways Associated with Glucocorticoid Resistance in Pregnant African-American Women. *Compr Psychoneuroendocrinol.* 2020 Feb-May;1-2:100001. doi: 10.1016/j.cpnec.2020.100001. Epub 2020 Mar 30. PMID: 33693436; PMCID: PMC7943062.

24. Hu X, **Li S**, Cirrilo P, Krigbaum N, Tran V, Ishikawa T, La Merrill A, Jones DP, Cohn B. (2020) Metabolome Wide Association Study of serum DDT and DDE in Pregnancy and Early Postpartum. *Reproductive Toxicology*. https://doi.org/10.1016/j.reprotox.2019.05.059. PMID: 31102720

25. Hu X, **Li S**, Cirillo PM, Krigbaum NY, Tran V, Jones DP, Cohn BA. (2020) Metabolome Wide Association Study of Serum Poly and Perfluoroalkyl Substances (PFASs) in Pregnancy and Early Postpartum. *Reprod Toxicol*. 92:120-128. PMID:31923462

26. **Li S***, Cirillo P, Hu X, Tran V, Krigbaum N, Yu S, Jones DP, Cohn B*. (2020) Understanding mixed environmental exposures using metabolomics via a hierarchical community network model in a cohort of California women in 1960's. *Reprod Toxicol*. 92:57-65. PMCID: PMC6949431

27. Ge Y, Gong M, Zadeh M, Li J, Abbott JR, Li W, Morel L, Sonon R, Supekar NT, Azadi P, Wang Y, Jones DP, **Li S**, Mohamadzadeh M. (2020) Regulating colonic dendritic cells by commensal glycosylated large surface layer protein A to sustain gut homeostasis against pathogenic inflammation. *Mucosal Immunol*. Jan; 13(1):34-46. Epub 2019 Oct 16. PMCID: PMC6917853

28. Hagan T, Cortese M, Rouphael N, Boudreau C, Linde C, Maddur MS, Das J, Wang H, Guthmiller J, Zheng NY, Huang M, Uphadhyay AA, Gardinassi L, Petitdemange C, McCullough MP, Johnson SJ, Gill K, Cervasi B, Zou J, Bretin A, Hahn M, Gewirtz AT, Bosinger, SE, Wilson, PC, **Li S**, Alter, Khurana, S, Golding, H, Pulendran, B. (2019) Antibiotics-Driven Gut Microbiome Perturbation Alters Immunity to Vaccines in Humans. *Cell*. 178(6):1313-1328.e13. PMCID: PMC6750738

29. Khadka M, Todor A, Maner-Smith KM, Colucci JK, Tran V, Gaul DA, Anderson EJ, Natrajan MS, Rouphael N, Mulligan MJ, McDonald CE, Suthar M, **Li S**, Ortlund EA. The Effect of Anticoagulants, Temperature, and Time on the Human Plasma Metabolome and Lipidome from Healthy Donors as Determined by Liquid Chromatography-Mass Spectrometry. *Biomolecules*. (2019); 9(5). pii: E200. PMCID: PMC6571950

30. Cordy RJ, Patrapuvich R, Lili LN, Cabrera-Mora M, Chien JT, Tharp GK, Khadka M, Meyer EV, Lapp SA, Joyner CJ, Garcia A, Banton S, Tran V, Luvira V, Rungin S, Saeseu T, Rachaphaew N, Pakala SB, DeBarry JD; MaHPIC Consortium, Kissinger JC, Ortlund EA, Bosinger, SE, Barnwell, JW, Jones, DP, Uppal, Karan, **Li S**, Sattabongkot, J, Moreno, A. (2019) Distinct amino acid and lipid perturbations characterize acute versus chronic malaria. *JCI Insight*. 4(9). pii: 125156. PMCID: PMC6538326

31. Fischer, T, Frederick AB, Tran V, **Li S**, Jones DP, Fridovich-Keil JL. (2019) Metabolic perturbations in classic galactosemia beyond the Leloir pathway: Insights from an untargeted metabolomic study. *J Inherit Metab Dis*. 42(2):254-263. PMCID: PMC6414239

32. Ge Y, Gong M, Colliou N, Zadeh M, Li J, Jones DP, **Li S**, Mohamadzadeh M. (2019) Neonatal intestinal immune regulation by the commensal bacterium, P. UF1. *Mucosal Immunol*. 12(2):434-444. Epub 2019 Jan 15. PMCID: PMC6375783

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33. Chong J, Soufan O, Li C, Caraus I, **Li S**, Bourque G, Wishart DS, Xia J. (2018) MetaboAnalyst 4.0: towards more transparent and integrative metabolomics analysis. *Nucleic Acids Res*. 46(W1):W486-W494. PMCID: PMC6030889

34. Gardinassi LG, Arévalo-Herrera M, Herrera S, Cordy RJ, Tran V, Smith MR, Johnson MS, Chacko B, Liu KH, Darley-Usmar VM, Go YM; MaHPIC Consortium., Jones DP, Galinski MR, **Li S***. (2018) Integrative metabolomics and transcriptomics signatures of clinical tolerance to Plasmodium vivax reveal activation of innate cell immunity and T cell signaling. *Redox Biol.* 17:158-170. PMCID: PMC6007173

35. Sato SE, **Li S**, Long Q. (2018) Integrative analysis of transcriptomic and metabolomic data via sparse canonical correlation analysis with incorporation of biological information. *Biometrics*. Mar;74(1):300-312. doi: 10.1111/biom.12715. Epub 2017 May 8. PMCID: PMC5677597

36. Colliou N, Ge Y, Sahay B, Gong M, Zadeh M, Owen JL, Neu J, Farmerie WG, Alonzo F 3rd, Liu K, Jones DP, **Li S**, Mohamadzadeh M. (2017) Commensal Propionibacterium strain UF1 mitigates intestinal inflammation via Th17 cell regulation. *J Clinical Investigation*. 127(11):3970-3986. PMCID: PMC5663347

37. Gardinassi LG, Cordy RJ, Lacerda MVG, Salinas JL, Monteiro WM, Melo GC, Siqueira AM, Val FF, Tran V, Jones DP, Galinski MR, **Li S***. (2017) Metabolome-wide association study of peripheral parasitemia in Plasmodium vivax malaria. *Int J Med Microbiol*. 307(8):533-541. Epub 2017 Sep 6. PMCID: PMC5698147

38. Sinclair C, Bommakanti G, Gardinassi L, Loebbermann J, Johnson MJ, Hakimpour P, Hagan T, Benitez L, Todor A, Machiah D, Oriss T, Ray A, Bosinger S, Ravindran R, **Li S**, Pulendran B. (2017) mTOR regulates metabolic adaptation of APCs in the lung and controls the outcome of allergic inflammation. *Science*. 357(6355):1014-1021. PMCID: PMC5746055

39. Fischer ST, Lili LN, **Li S**, Tran VT, Stewart KB, Schwartz CE, Jones DP, Sherman SL, Fridovich-Keil JL. (2017) Low-level maternal exposure to nicotine associates with significant metabolic perturbations in second-trimester amniotic fluid. *Environ Int.* 107:227-234. PMCID: PMC5569895

40. Myers OD, Sumner SJ, **Li S,** Barnes S, Du X. (2017) One Step Forward for Reducing False Positive and False Negative Compound Identifications from Mass Spectrometry Metabolomics Data: New Algorithms for Constructing Extracted Ion Chromatograms and Detecting Chromatographic Peaks. *Anal Chem.* 89(17):8696-8703. PMID: 28752754

41. Myers OD, Sumner SJ, **Li S**, Barnes S, Du X. (2017) Detailed Investigation and Comparison of the XCMS and MZmine 2 Chromatogram Construction and Chromatographic Peak Detection Methods for reprocessing Mass Spectrometry Metabolomics Data. *Anal Chem.* 89(17):8689-8695. PMID: 28752757

42. Gardinassi L, Xia J, Safo S, **Li S***. (2017) Bioinformatics tools for the interpretation of metabolomics data. *Current Pharmacology Reports*, 3(6), 374-383.

43. **Li S,** Sullivan NL, Rouphael N, Yu T, Banton S, Maddur MS, McCausland M, Chiu C, Canniff J, Dubey S, Liu K, Tran V, Hagan T, Duraisingham S, Wieland A, Mehta AK, Whitaker JA,

Subramaniam S, Jones DP, Sette A, Vora K, Weinberg A, et al. (2017) Metabolic Phenotypes of Response to Vaccination in Humans. *Cell*. 169(5):862-877. PMCID: PMC5711477

44. Alvarez JA, Chong EY, Walker DI, Chandler JD, Michalski ES, Grossmann RE, Uppal K, **Li S**, Frediani JK, Tirouvanziam R, Tran VT, Tangpricha V, Jones DP, Ziegler TR. (2017) Plasma metabolomics in adults with cystic fibrosis during a pulmonary exacerbation: A pilot randomized study of high-dose vitamin D(3) administration. *Metabolism*. 70:31-41. PMCID: PMC5407388

45. Barnes S, Benton HP, Casazza K, Cooper SJ, Cui X, Du X, Engler J, Kabarowski JH, **Li S**, Pathmasiri W, Prasain JK, Renfrow MB, Tiwari HK. (2016) Training in metabolomics research. II. Processing and statistical analysis of metabolomics data, metabolite identification, pathway analysis, applications of metabolomics and its future. *J Mass Spectrom*. 51(8):535-548. PMCID: PMC5584587

46. Barnes S, Benton HP, Casazza K, Cooper SJ, Cui X, Du X, Engler J, Kabarowski JH, **Li S**, Pathmasiri W, Prasain JK, Renfrow MB, Tiwari HK. (2016) Training in metabolomics research. I. Designing the experiment, collecting and extracting samples and generating metabolomics data. *J Mass Spectrom*. 2016 Jul;51(7):461-75. PMCID: PMC4964969

47. Uppal K, Walker DI, Liu K, **Li S**, Go YM, Jones DP. (2016) Computational Metabolomics: A Framework for the Million Metabolome. *Chem Res Toxicol*. 29(12):1956-1975. Review. PMCID: PMC5376098

48. Chandler JD, Wongtrakool C, Banton SA, **Li S**, Orr ML, Barr DB, Neujahr DC, Sutliff RL, Go YM, Jones DP. (2016) Low-dose oral cadmium increases airway reactivity and lung neuronal gene expression in mice. *Physiological Rep*. 4(13). pii: e12821. Doi: 10.14814/phy2. 12821. PMCID: PMC4945833

49. Ravindran R, Loebbermann J, Nakaya HI, Khan N, Ma H, Gama L, Machiah DK, Lawson B, Hakimpour P, Wang YC, **Li S**, Sharma P, Kaufman RJ, Martinez J, Pulendran B. (2016) The amino acid sensor GCN2 controls gut inflammation by inhibiting inflammasome activation. *Nature*. 531(7595):523-527. PMCID: PMC4854628

50. Jin R, Banton S, Tran VT, Konomi JV, **Li S,** Jones DP, Vos MB. (2016) Amino Acid Metabolism is Altered in Adolescents with Nonalcoholic Fatty Liver Disease-An Untargeted, High Resolution Metabolomics Study. *J Pediatr.* 172:14-19. e5. PMCID: PMC5321134

51. Cribbs SK, Uppal K, **Li S**, Jones DP, Huang L, Tipton L, Fitch A, Greenblatt RM, Kingsley L, Guidot DM, Ghedin E, Morris A. (2016) Correlation of the lung microbiota with metabolic profiles in bronchoalveolar lavage fluid in HIV infection. *Microbiome*. 2016 Jan 20;4:3. PMCID: PMC4721204

52. **Li S***, Todor A and Luo R. (2016). Blood transcriptomics and metabolomics for personalized medicine. *Computational and Structural Biotechnology Journal.* 14:1-7. PMID: 26702339. Review. PMCID: PMC4669660

53. **Li S**, Dunlop AL, Jones DP, Corwin EJ. (2016) High-Resolution Metabolomics: Review of the Field and Implications for Nursing Science and the Study of Preterm Birth. *Biol Res Nurs.* 18(1):12-22. PMCID: PMC4684995

54. Xu X, Araki K, **Li S**, Han JH, Ye L, Tan WG, Konieczny BT, Bruinsma MW, Martinez J, Pearce EL, Green DR, Jones DP, Virgin HW, Ahmed R. (2014) Autophagy is essential for effector CD8(+) T cell survival and memory formation. *Nature Immunology*. 15(12):1152-61. PMCID: PMC4232981

55. Boube I., Lotz J. M., Pozhitkov A. E., **Li S**., Griffitt, R. J. (2014). Identification of Genes Involved in Taura Syndrome Virus Resistance in Litopenaeus Vannamei. *Journal of Aquatic Animal Health*, 26(3), 137-143.

56. Hoffman JM, Soltow QA, **Li S**, Sidik A, Jones DP, Promislow DE. (2014) Effects of age, sex, and genotype on high sensitivity metabolomic profiles in the fruit fly, Drosophila melanogaster. *Aging Cell.* 13(4):596-604. PMCID: PMC4116462

57. **Li, S**, Rouphael N, Duraisingham S, Romero-Steiner S, Presnell S, Davis C, Schmidt DS, Johnson SE, Milton A, Rajam G, Kasturi S, Carlone GM, Quinn C, Chaussabel D, Palucka AK, Mulligan MJ, Ahmed R, Stephens DS, Nakaya HI, Pulendran B. (2014) Molecular signatures of antibody responses derived from a systems biology study of five human vaccines. *Nature Immunology*. 15(2):195-204. PMCID: PMC3946932

58. Ravindran R, Khan N, Nakaya HI, **Li S**, Loebbermann J, Maddur MS, Park Y, Jones DP, Chappert P, Davoust J, Weiss DS, Virgin HW, Ron D, Pulendran B. (2014) Vaccine activation of the nutrient sensor GCN2 in dendritic cells enhances antigen presentation. *Science*. 343(6168):313-317. PMCID: PMC4048998

59. **Li S***, Park Y, Duraisingham S, Strobel FH, Khan N, Soltow QA, Jones DP, Pulendran B. (2013) Predicting network activity from high throughput metabolomics. *PLoS Comput Biol.* 9(7):e1003123. PMCID: PMC3701697

60. **Li S**, Nakaya HI, Kazmin DA, Oh JZ, Pulendran B. (2013) Systems biological approaches to measure and understand vaccine immunity in humans. *Seminars in Immunology*. 25(3):209-18. Review. PMCID: PMC3797847

61. Yu T, Park Y, **Li S**, Jones DP. (2013) Hybrid feature detection and information accumulation using high-resolution LC-MS metabolomics data. *J Proteome Res*. 12(3):1419-27. PMCID: PMC3624888

62. Nakaya, HI, **Li S**, Pulendran, B. (2012) Systems vaccinology: learning to compute the behavior of vaccine induced immunity. *Wiley Interdiscip Rev Syst Biol Med.* 4(2): 193-205. PMCID: PMC3288517

63. Roede JR, Park Y, **Li S**, Strobel FH, Jones DP. (2012). Detailed mitochondrial phenotyping by high resolution metabolomics. *PLoS One*. 7(3):e33020. PMCID: PMC3295783

64. Wilkinson P, Filali-Mouhim A, **Li S**, Ahlers J, Schatzle J, Pulendran B, Sekaly RP, Cameron MJ. An open-ended plea for the development of a global database of HIV vaccine responses. *Curr Opin HIV AIDS*. 2012 Jan;7(1):10-6. PMID: 22156846; PMCID: PMC3253342.

65. Nakaya HI, Wrammert J, Lee EK, Racioppi L, Marie-Kunze S, Haining WN, Means AR, Kasturi SP, Khan N, Li GM, McCausland M, Kanchan V, Kokko KE, **Li S**, Elbein R, Mehta

AK, Aderem A, Subbarao K, Ahmed R, Pulendran B. (2011). Systems biology of vaccination for seasonal influenza in humans. *Nature Immunology*. 12(8):786-95. PMCID: PMC3140559

66. Pulendran B, **Li S**, Nakaya HI. (2010) Systems vaccinology. *Immunity*. 33(4):516-29. PMCID: PMC3001343

67. **Li S***, Pozhitkov A, Ryan RA, Manning CS, Brown-Peterson N, Brouwer M. (2010). Constructing a fish metabolic network model. *Genome Biology*. 11(11):R115. PMCID: PMC3156954

68. **Li S***, Pozhitkov A, Brouwer M. (2010). Linking probe thermodynamics to microarray quantification. *Physical Biology*. 7(4):048001

69. Cornish EJ, Hassan SM, Martin JD, **Li S**, Merzdorf CS. (2009). A microarray screen for direct targets of Zic1 identifies an aquaporin gene, aqp-3b, expressed in the neural folds. *Developmental Dynamics*. 238(5):1179-94

70. **Li S*,** Pozhitkov, A, Brouwser, M. (2008) A competitive hybridization model predicts probe signal intensity on high density DNA microarrays. *Nucleic Acids Research* 36(20): 6585-6591

71. **Li S**, Shin Y, Cho KW, Merzdorf CS. (2006). The Xfeb gene is directly upregulated by Zic1 during early neural development. *Developmental Dynamics*. 235:2817-27.

UNDER REVIEW, REVISION OR IN SUBMISSION:

- Chi, Y., Mitchell, J.M., Zheng, S. and **Li, S***., 2025. Systematic pre-annotation explains the "dark matter" in LC-MS metabolomics. *bioRxiv*. doi: 10.1101/2025.02.04.636472. In submission.

- Chi, Y, Mitchell, JM., Thapa, M, Zheng, S., Frohock, Z., Li, Y., Smirnov, A., Du, X. and **Li, S***. 2025b. Constructing a consensus serum metabolome. *bioRxiv* https://doi.org/10.1101/2025.05.07.652782. In submission.

- **Li, S***. 2025. Circular van Krevelen diagram for visualizing metabolic pathways. *bioRxiv* doi: 10.1101/2025.05.31.657198

- Joshua Mitchell, Jasmine Chong, and **Shuzhao Li*** Metabolomics Data Processing using the Asari Toolkit. Book chapter. Under review.

- Jasmine Chong, Susan McClatchy, Joshua Mitchell and **Shuzhao Li***. Practicing data science in interactive notebooks. Book chapter. Under review.

- Maria van de Lavoir, Yuanye Chi, Ting Zeng, Rani Robeyns, Maria del Mar Delgado Povedano, Leen Jacobs, Celine Gys, Hugo Neels, **Shuzhao Li**, Alexander L.N. van Nuijs, Adrian Covaci. Human Hair Atlas: the metabolome and lipidome landscape across hair lengths. Under review.

- Vanessa A. Leone et al. Sleep restriction alters 24-hour patterns in host and microbially-mediated metabolites detected in human serum. Under revision.

BOOK CHAPTERS:

Karnovsky A and **Li Shuzhao***. (2020) Pathway analysis for targeted and untargeted metabolomics. In *Computational Methods and Data Analysis for Metabolomics* (pp. 387-400, series of *Methods in Molecular Biology*). Humana, New York, NY.

Pittard WS, Villaveces C and **Li Shuzhao***. (2020) A bioinformatics primer to data science, with examples for metabolomics. In *Computational Methods and Data Analysis for Metabolomics* (pp. 245-263). Humana, New York, NY.

Pittard WS, and **Li Shuzhao***. (2020) The essential toolbox of data science: Python, R, Git and Docker. In *Computational Methods and Data Analysis for Metabolomics* (pp. 265-311). Humana, New York, NY.

Zhou, G., **Li Shuzhao.** and Xia, J., 2020. (2020) Network-Based Approaches for Multi-omics Integration. In *Computational Methods and Data Analysis for Metabolomics* (pp. 469-487). Humana, New York, NY.

Li Shuzhao*. (2015) Pathway and network analysis for high-throughput metabolomics. In "Data processing methods in metabolomics". Rudaz S (Ed.). Future Science Group, London, UK. doi: 10.4155/9781910420287. eISBN: 978-1-910420-28-7.

BOOKS:

Li, Shuzhao. (Ed.). (2020) Computational Methods and Data Analysis for Metabolomics (Methods in Molecular Biology). Springer, ISBN-13: 978-1071602386. ISBN-10: 1071602381

Recent Oral Presentations

Invited presentations – National and International

2025   The Exposome Boot Camp, Columbia University, New York. July 18, 2025

2025   Virtual Metabolomic Epidemiology Webinar, Brigham and Women's Hospital, Harvard Medical School. Jan. 27, 2025

2024   The 21st Annual Ohio Mass Spectrometry Symposium, Columbus, Ohio, October 15, 2024.

2024   The Exposome Boot Camp, Columbia University, New York. July 17-19, 2024

2023   NIH ME/CFS Research Roadmap webinar, Oct. 26, 2023

2023   Metabolomics Association of North America, SODA group meeting, Aug. 8, 2023

2022   CASMS Conference, Advancing Biological and Pharmaceutical Mass Spectrometry, Oct. 21, 2022

2022   Cold Spring Harbor Laboratory Metabolomics Course, June 2022

2022   NIH Common Fund Metabolomics Consortium Meeting, May 31, 2022

2021   NIH Common Fund Metabolomics Consortium Meeting, Sept. 28, 2021

2021   NINDS ME/CFS Research Consortium Meeting, Sept. 3, 2021

2021   CASMS Conference, Advancing Biological and Pharmaceutical Mass Spectrometry, August 11, 2021

2021   The Exposome Boot Camp, Columbia University, July 23, 2021

2020   28th annual International Conference on Intelligent Systems for Molecular Biology (ISMB), special session on Systems Immunology, July 13, 2020. Montreal/Virtual.

2020   28th annual International Conference on Intelligent Systems for Molecular Biology (ISMB), COSI track Computational Mass Spectrometry, July 16, 2020. Montreal/Virtual. (Session chair)

2020   Common Fund Metabolomics Consortium, National Institutes of Health, Rockville, MD

2019   Metabolomics and data analysis, week-long workshop taught at ESPOL, Guayaquil, Ecuador.

2019   Atlanta Athens Mass Spectrometry Discussion Group Symposium. Atlanta, GA.

2019   Common Fund Metabolomics Consortium, National Institutes of Health, Rockville, MD. (Joint presentation with Jeff Xia and Gary Siuzdak)

2018   The 6th Annual Workshop on Metabolomics, University of Alabama, Birmingham, AL (NIH sponsored international workshop)

2018   The 2018 ISES-ISEE joint annual meeting. Ottawa, Canada

2018   Common Fund Metabolomics Consortium, National Institutes of Health, Rockville, MD

2018   Children's Health Exposure Analysis Resource Network, New York, NY

2017   Chinese Academy of Science, Shanghai, China

2017   Human Immunology Project Consortium, National Institutes of Health, Potomac, MD

2017   The 5th Annual Workshop on Metabolomics, University of Alabama, Birmingham, AL (NIH sponsored international workshop)

2017   The 3rd Symposium of Metabolism in Infectious Diseases. Fort Collins, CO

2017   NIAID Systems Biology Program Meeting, Chicago, IL

2016   The 4th Annual Research Retreat, Center for Inflammation and Mucosal Immunology, University of Florida, Gainesville, FL

2016   NIAID Systems Biology Centers, New York, NY

2016   The 65th ASTMH Meeting, Atlanta, GA (Deputy symposium chair)

2016   The 4th Annual Workshop on Metabolomics, University of Alabama, Birmingham, AL (NIH sponsored international workshop)

2016   Emory Exposome Summer Course, Atlanta, GA (NIH sponsored international workshop)

2016   The 40th SIAM Southeastern Atlantic Section Conference, Athens, GA

2016   California Breast Cancer Research Program, Berkeley, CA

2016   "Systems biology of Herpes Zoster (Zostavax®) vaccination". National Institute of Health, Rockville, MD.

2016   Mummichog, Metabolomics and Data integration. Department of Chemistry, University of Florida, Gainesville, FL

2016   Small molecules and big data for precision medicine and precision immunology, Kansas State

University, Manhattan, KS

2016 MRC^2 Metabolomics Workshop, University of Michigan, Ann Arbor, MI

2016 Multi-omics modeling for systems medicine, Tulane University, New Orleans, LA

2015 The 3th Annual Workshop on Metabolomics, University of Alabama, Birmingham, AL (NIH sponsored international workshop)

2015 School of Biology seminar, Georgia Institute of Technology

2015 "Metabolomics and systems medicine: What do we learn from big data?" Purdue University

2015 The 28th Lake Louise Tandem Mass Spectrometry Workshop, Lake Louise, Alberta, Canada.

2015 Human Immunology Project Consortium, National Institue of Health, Rockvile, MD.

2015 The 3rd Annual Research Retreat, Center for Inflammation and Mucosal Immunology, University of Florida, Gainesville. Nov. 13, 2015 (Keynote address)

2015 Workshop on Computational Network Biology: Modeling, Analysis, and Control, The 6th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics, Atlanta. Sept. 9, 2015 (Keynote address)

2014 Systems-Scale Metabolism workshop, Georgia Institute of Technology

2013 "Network Modeling Reveals Distinct Transcriptional Signatures of Antibody Responses to Five Different Vaccines in Humans". National Institute of Health, Bethesda, MD. Sept. 10, 2013

2012 "Rapid Functional Analysis for High Throughput Metabolomics". National Institute of Health, Bethesda, MD. July 10, 2012

Conference presentations – National and International (selected from abstracts, since 2015)

2024 The 6th Annual Conference for Metabolomics Association of North America, Tampa FL. Oct. 24, 2024

2019 Metabolomics Association of North America, 1st Annual Conference. Atlanta, GA

2018 The 26th Annual International Conference on Intelligent Systems for Molecular Biology, Chicago, IL

2016 24th Annual International Conference on Intelligent Systems for Molecular Biology, Orlando, FL.

2015 Great Lakes Bioinformatics Conference, West Lafayette, Indiana, May 19, 2015

Invited presentations – Institutional (since 2015)

2025 JAX-GM Scientific Directors Forum seminar, August 27, 2025

2023 University of Connecticut School of Medicine, Nov. 2, 2023

2023 JAX-GM Scientific Directors Forum seminar, July 26, 2023

2022 The Jackson Laboratory Faculty Retreat, Portland, ME. Oct. 12, 2022

2021 Jackson Laboratory 5th Annual Scientific Symposium, Oct. 12

2021 JAX-GM Scientific Directors Forum seminar, May 26, 2021

2021   Jackson Laboratory Metabolism Interest Group, April 20, 2021

2020   Institute for Systems Genomics, University of Connecticut, CT

2020   Metabolomics for precision medicine and precision immunology, The Jackson Laboratory Faculty Retreat, Farmington, CT

2020   The Jackson Laboratory Computational Community Retreat, Farmington, CT

2019   The Tuberculosis Research Units Meeting, Emory University, Atlanta, GA

2019   Emory-QIMR Omics Research Symposium. Emory University, Atlanta, GA

2019   Winship Cancer Center, Emory University, Atlanta, GA

2019   Nutritional metabolomics course, March 25, 2019. Emory University, Atlanta, GA

2017   Center for Clinical and Molecular Nutrition, Emory University School of Medicine, Atlanta, GA

2017   Emory University School of Nursing, Center for Children's Health, the Environment, the Microbiome, and Metabolomics (C-CHEM2), Emory University, Atlanta, GA

2016   Division of Digestive Diseases, visiting professorship, Emory University School of Medicine, Atlanta, GA

2016   Rollins School of Public Health, Emory University, Atlanta, GA

2016   Pulmonary Division Research Seminar, Emory University, Atlanta, GA

2016   Multi-omics modeling for systems medicine Pulmonary Division Research Seminar, Emory University, Atlanta, GA

2016   Multi-omics analysis for Systems Medicine, DOM Research Resource 101, Emory University, Atlanta, GA

2015   Environmental metabolomics workshop, Emory University, Atlanta, GA

Posters and Trainee presentations (peer reviewed, since 2016)

2025   Li, S., An update of the asari suite of tools and an explanation of the metabolomics "dark matter". American Society for Mass Spectrometry 72nd Annual Conference, Baltimore, June 2-6, 2025. Poster.

2025   Shujian Zheng; Joshua Mitchell; Elizabeth Aiken; Shuzhao Li. Exploration of steroid metabolism by Cytochrome P450 Enzymes using isotope labeling. American Society for Mass Spectrometry 72nd Annual Conference, Baltimore, June 2-6, 2025. Poster.

2025   Maheshwor Thapa et al. Biochemical phenotyping of null alleles in hIPSC-derived cell lineages: integrating genetics with metabolomics. American Society for Mass Spectrometry 72nd Annual Conference, Baltimore, June 2-6, 2025. Poster.

2024   Joshua Mitchell. Performant and extensible metabolomics data processing using the Asari suite of tools. The 6th Annual Conference for Metabolomics Association of North America (Oct. 2024). Oral. *Early Career Award winner (one of two annual awards) presentation.*

2024   Minghao Gong[1], Courtney Gunter[1], Fatih Karabacak[1], Lina Kozhaya[1], Suzanne Vernon[2], Lucinda Bateman[2], Derya Unutmaz[1,3,*] and Shuzhao Li[1]. Dysregulation of

immunometabolomics in ME/CFS patients is linked to xenobiotics and predictive of clinical symptoms. The 6th Annual Conference for Metabolomics Association of North America (Oct. 2024). Oral.

2024 Shujian Zheng et al. Enhanced sensitivity and coverage of metabolomics using chemoselective derivatization. The 6th Annual Conference for Metabolomics Association of North America (Oct. 2024). Poster.

2024 Maheshwor Thapa et al. Biochemical phenotyping of null alleles in hIPSC-derived cell lineages: integrating genetics with metabolomics. The 6th Annual Conference for Metabolomics Association of North America (Oct. 2024). Poster.

2024 Minghao Gong[1], Courtney Gunter[1], Fatih Karabacak[1], Lina Kozhaya[1], Suzanne Vernon[2], Lucinda Bateman[2], Derya Unutmaz[1,3,*] and Shuzhao Li[1]. Dysregulation of immunometabolomics in ME/CFS patients is linked to xenobiotics and predictive of clinical symptoms. 28th annual International Conference on Intelligent Systems for Molecular Biology (ISMB), July 2024. Montreal, Canada. Poster.

2024 Minghao Gong, Courtney Gunter, Fatih Karabacak, Suzanne Vernon, Derya Unatmaz, Shuzhao Li. Post-Exertional Malaise: A Manifestation of Post-Exposure Immune Dysregulation?. Symposium on Systems Immunology in Aging and Complex Diseases. June 27-28, 2024. Farmington, CT, USA. Poster.

2024 Joshua M. Mitchell, Yuanye Chi, Maheshwor Thapa and Shuzhao Li. High-performance LC-MS metabolomics data processing using the Asari suite of tools. 20th Annual International Conference of the Metabolomics Society, June 16-20, 2024. Osaka, Japan. Oral.

2024 Yuanye Chi, Joshua M. Mitchell, Shuzhao Li. A consensus serum metabolome by large-scale data mining reveals major gaps in metabolomic measurements and modeling. 20th Annual International Conference of the Metabolomics Society, June 16-20, 2024. Osaka, Japan. Poster.

2024 Minghao Gong, Courtney Gunter, Fatih Karabacak, Suzanne Vernon, Derya Unatmaz, Shuzhao Li. Systematic Association Studies Across Symptomatology, Immune Profiles, Metabolomics and Exposures in a ME/CFS cohort. JAX Research Symposium. May 20-21, Portland, ME. Oral.

2024 Maheshwor Thapa[1], Luca Catalano[2], Joshua Mitchell[1], Julia Tevini[2], Daniela Weber[2], Barbara Kolfer[2], Shuzhao Li[1] Combined therapeutic effects by ketogenic diet and metformin in mouse neuroblastoma models using metabolomics and lipidomics. JAX Research Symposium. May 20-21, Portland, ME. Poster.

2024 Shujian Zheng, et al. Building a Metabolomic Atlas for Human induced Pluripotent Stem Cells and derived Cell Types. JAX Research Symposium. May 20-21, Portland, ME. Poster.

2024 Joshua Mitchell[1], Maheshwor Thapa[1], Shujian Zheng[1], Amnah Siddiqa[1], Quynh-Mai Pham[1], Arti Taggar [1,2], Yuanye Chi[1], Minghao Gong[1], Anahita Amiri[1], Justin McDonough[1], Gang Ning[1], William Skarnes[1,2], Paul Robson[1,2], and Shuzhao Li[1,2] Biochemical phenotyping of null alleles in hIPSC-derived cell lineages: integrating genetics with metabolomics. NIH MorPhiC Consortium Meeting, Jan 31st- Feb 2nd (2024) Coral Gables, FL. Poster.

2023 Joshua M. Mitchell, et al. Biochemical phenotyping of null alleles in human induced pluripotent

stem cell-derived cell lineages: integrating genetics with metabolomics. NIH Morphic Consortium Meeting, June 26 2023 - virtual, oral

2023   Joshua Mitchell, Yuanye Chi and Shuzhao Li. A Python-Centric pipeline for high-fidelity and high-performance LC-MS metabolomics data processing. 5th Annual MANA Conference, October 23-27, 2023, University of Missouri, Columbia, MO, USA. Oral.

2023   Yuanye Chi, Joshua Mitchell, Paul Robson and Shuzhao Li. Building a Metabolomic Atlas for Human Induced Pluripotent Stem Cells and Derived Cell Types. 5th Annual MANA Conference, October 23-27, 2023, University of Missouri, Columbia, MO, USA. Oral.

2023   LC-MS metabolomics dataset of human urines with the software program Asari. 5th Annual MANA Conference, October 23-27, 2023, University of Missouri, Columbia, MO, USA. Poster.

2023   Joshua M. Mitchell, et al. Biochemical phenotyping of null alleles in human induced pluripotent stem cell-derived cell lineages: integrating genetics with metabolomics. NIH Morphic Consortium Meeting, June 26 2023 - virtual, oral

2023   Joshua M. Mitchell, Yuanye Chi, and Shuzhao Li. A Python-centric pipeline for high-fidelity and high-performance LC-MS metabolomics data processing. 19th Annual International Conference of the Metabolomics Society, June 18-22, 2023. Niagara Falls, Ontario, Canada

2023   Minghao Gong, Maheshwor Thapa, Elisabeth Fleming, Julia Oh and Shuzhao Li. Untargeted Metabolomic Profiling of Staphylococcus sp. Bridges the Gap between Metabolic and Genetic Variations. 19th Annual International Conference of the Metabolomics Society, June 18-22, 2023. Niagara Falls, Ontario, Canada. Oral presentation. *Early Career Researcher Travel Award.*

2023   Shuzhao Li, Amnah Siddiqa, Maheshwor Thapa, Shujian Zheng. High-fidelity and high-performance LC-MS metabolomics data processing using asari. 19th Annual International Conference of the Metabolomics Society, June 18-22, 2023. Niagara Falls, Ontario, Canada

2023   Maheshwor Thapa, Shujian Zheng, Nelio Oliveira, Arti Taggar, Amnah Siddiqa, Minghao Gong, Anahita Amiri, Justin McDonough, William Skarnes, Paul Robson, and Shuzhao Li. Biochemical phenotyping of null alleles in human induced pluripotent stem cell-derived cell lineages: integrating genetics with metabolomics. 19th Annual International Conference of the Metabolomics Society, June 18-22, 2023. Niagara Falls, Ontario, Canada

2023   Joshua M. Mitchell, Yuanye Chi, and Shuzhao Li. A Python-centric pipeline for high-fidelity and high-performance LC-MS metabolomics data processing. 19th Annual International Conference of the Metabolomics Society, June 18-22, 2023. Niagara Falls, Ontario, Canada

2023   **Shuzhao Li**, Amnah Siddiqa, Maheshwor Thapa, Shujian Zheng. High-fidelity and high-performance LC-MS metabolomics data processing using asari. American Society for Mass Spectrometry 70th Annual Conference, Houston, TX, June 3-8, 2023

2023   Shujian Zheng, Maheshwor Thapa, Nelio Oliveira, Arti Taggar, Amnah Siddiqa, Minghao Gong, Anahita Amiri, Justin McDonough, William Skarnes, Paul Robson, and Shuzhao Li. Biochemical phenotyping of null alleles in human induced pluripotent stem cell-derived cell

lineages: integrating genetics with metabolomics. American Society for Mass Spectrometry 70th Annual Conference, Houston, TX, June 3-8, 2023

2023   Maheshwor Thapa, Shujian Zheng, Nelio Oliveira, Arti Taggar, Amnah Siddiqa, Minghao Gong, Anahita Amiri, Justin McDonough, William Skarnes, Paul Robson, and Shuzhao Li. Biochemical phenotyping of null alleles in human induced pluripotent stem cell-derived cell lineages: integrating genetics with metabolomics. Jackson Laboratory 7th Annual Scientific Research Symposium, May 2023

2023   Shujian Zheng, Joshua M. Mitchell, Maheshwor Thapa, Arti Taggar, Paul Robson and Shuzhao Li. Enhanced sensitivity and coverage of metabolomics using chemoselective derivatization. Jackson Laboratory 7th Annual Scientific Research Symposium, May 2023

2023   Minghao Gong, Maheshwor Thapa, Elisabeth Fleming, Julia Oh and Shuzhao Li. Untargeted Metabolomic Profiling of Staphylococcus sp. Bridges the Gap between Metabolic and Genetic Variations. Jackson Laboratory 7th Annual Scientific Research Symposium, May 2023

2023   Joshua M. Mitchell, Yuanye Chi, and Shuzhao Li. A Python-centric pipeline for high-fidelity and high-performance LC-MS metabolomics data processing. Jackson Laboratory 7th Annual Scientific Research Symposium, May 2023

2022   Minghao Gong, Courtney Gunter, Shuzhao Li, Derya Unatmaz. ImmunoMetabolomics of ME/CSF. NINDS ME/CFS Research Consortium Meeting, June 13, 2022. National Institutes of Health, Rockville, MD.

2022   Minghao Gong et al. "JMS to bridge genome-scale metabolic models and metabolomics". NIH Common Fund Metabolomics Consortium meeting, June 2022. Oral presentation

2022   Amnah Siddiqa, et al. "Trackable and scalable LC-MS metabolomics data processing using asari". NIH Common Fund Metabolomics Consortium meeting, June 2022. Oral presentation

2022   Maheshwor Thapa, Arti Taggar, Amnah Siddiqa,Minghao Gong, Anahita Amiri, Paul Robson, Shuzhao Li. Simultaneous metabolomic and lipidomic profiling reveals intracellular pathways within the implanting human trophoblast responsive to microenvironmental nutrients. NIH Common Fund Metabolomics Consortium meeting, June 2022. Oral presentation

2022   Amnah Siddiqa, Maheshwor Thapa, Minghao Gong, Shuzhao Li. Processing, Quality Control and Annotation of Large-scale Metabolomics Data. Jackson Laboratory 6th Annual Scientific Research Symposium, May 2022

2022   Minghao Gong, Maheshwor Thapa, Elisabeth Fleming, Julia Oh and Shuzhao Li. Bridging the gap between genome-scale metabolic models and high-resolution metabolomics. Jackson Laboratory 6th Annual Scientific Research Symposium, May 2022

2022   Maheshwor Thapa, Arti Taggar, Amnah Siddiqa,Minghao Gong, Anahita Amiri, Paul Robson, Shuzhao Li. Simultaneous metabolomic and lipidomic profiling reveals intracellular pathways within the implanting human trophoblast responsive to microenvironmental nutrients. Jackson Laboratory 6th Annual Scientific Research Symposium, May 2022

2022   Shujian Zheng and Shuzhao Li. Distinguishing in-source reactions and biochemical reactions in

high-resolution metabolomics data. Jackson Laboratory 6th Annual Scientific Research Symposium, May 2022

2020   Pang et al. OptiLCMS: an R package for efficient and optimized LC-MS spectra processing. Common Fund Metabolomics Consortium, National Institutes of Health, Rockville, MD

2019   Sherman SL, Fischer T, Mateja A, Jones DP, **Li Shuzhao**, Wang Y, Tran V, Stewart K, Schwartz CE, Fridovich-Keil JL. Metabolomic patterns associated with fetal trisomy 21 based second-trimester maternal serum and amniotic fluid. The Gatlinburg Conference on Research and Theory in Intellectual and Developmental Disabilities. San Antonio, TX

2019   **Li Shuzhao**, Pittard S, Siddiaq A. Multi-omics integration via Hierarchical Community Networks. Common Fund Metabolomics Consortium, National Institute of Health, Rockville, MD

2018   Morris CR, Ma C, **Li Shuzhao**, Jones DP, Brown LA, Machado RF, Kato GJ, Zhang Y, Nouraie SM, Gladwin MT. Biomarker Discovery: Novel Insights into Red Blood Cell Metabolomics in Patients with Sickle Cell Disease at Risk for Early Mortality. 12th Annual Symposium of Foundation for Sickle Cell Disease Research. (Blood 130:Suppl 1, 4772)

2018   Gardinassi L, Arévalo-Herrera M, Herrera S, Cordy RJ, Tran V, Smith MR, Johnson MS, Chako B, Darley-Usmar VM, Liu K, Go Y, Jones DP, Galinski M, Li S. Integrative metabolomics and transcriptomics signatures of clinical tolerance to Plasmodium vivax malaria highlight a role for platelets. June 6, 2018. Minas Gerais, Brazil

2018   Wang Y, Gardinassi L, Xiong L and **Li Shuzhao**. Multiscale, multifactorial networks to integrate metabolomics with high-dimensional immunology. The 14th Annual Conference of the Metabolomics Society. Seattle, WA

2018   Xiong L and **Li Shuzhao**. Contextualizing metabolomics for personalized medicine using mummichog. The 26th Annual International Conference on Intelligent Systems for Molecular Biology. Chicago, IL

2018   **Li Shuzhao**, Xiong L, Gardinassi L, Wang Y. Multi-omics, multiscale networks of human immune responses to vaccination and infection. The 26th Annual International Conference on Intelligent Systems for Molecular Biology. Chicago, IL

2017   **Li Shuzhao**, Jones DP, Pulendran B. Blood metabolomics and transcriptomics define metabolic axes of human immune response to herpes zoster vaccine. American Society of Mass Spectrometry meeting, Indianapolis, IN

2017   Gardinassi L, Arévalo-Herrera M, Herrera S, Cordy RJ, Tran V, Jones DP, Galinski M, **Li Shuzhao**. Molecular signatures of clinical tolerance to *Plasmodium vivax* revealed by integrative metabolomics and transcriptomics. The 6th International Conference on *Plasmodium vivax* Research, Manaus, AM, Brazil

2017   Gardinassi L, Cordy RJ, Arévalo-Herrera M, Herrera S, Tran V, Jones DP, Galinski M, **Li Shuzhao**. Multi-omics modeling of different clinical manifestation of Plasmodium vivax infection. 6th Annual Southeastern Immunology Symposium. Nashville, TN

2017 Li S. Industrialization of big data immunology through modular computing. The 5th Annual Immunogenomics Conference. Huntsville, AL

2017 Li S. Ten lessons learned from big data immunology and relevance to cancers. Cold Spring Harbor Asia "Tumor Immunology & Immunotherapy". Suzhou, China

2016 Shuzhao Li, Karan Uppal, ViLinh Tran, Andrei Todor, Dean Jones, Annette Esper. High-resolution metabolomics analysis of sepsis. Keystone Symposium on Systems Immunology: From Molecular Networks to Human Biology. Big Sky, MT, USA.

2016 Bantan S, Todor A, Luo R, Jones DP, Li S. Computational development for omics integration. New Strategies and Challenges in Lung Proteomics and Metabolomics Workshop. National Jewish Health, Denver CO. (winner 2nd place prize)

2016 Sophia Banton, Piera Cirrilo, Douglas Walker, ViLinh Tran, William Hu, Dean P. Jones, Barbara Cohn, Shuzhao Li. Metabolome-wide Association of PCB compounds in humans. California Breast Cancer Research Program Research Symposium, San Francisco, CA.

2016 Joshua Chandler, Andrei Todor, James Wise, Dean P. Jones, Joe Griffitt, Shuzhao Li. Distinct metabolomic axes in Gulf coast minnows after Deepwater Horizon oil spill. The 55th Annual Meeting of the Society of Toxicology, New Orleans, LA

2016 Sophia Banton, Piera Cirrilo, Douglas Walker, ViLinh Tran, William Hu, Dean P. Jones, Barbara Cohn, Shuzhao Li. Metabolome-wide Association of PCB compounds in humans. The 55th Annual Meeting of the Society of Toxicology, New Orleans, LA

2016 K Perry-Walker, DI Walker, JA Alvarez, JE Han, JL Jones, L Hao, S Li, ... Impact of vitamin D status and high-dose vitamin D3 administration on the plasma metabolome in critically ill adults. Federation of American Societies for Experimental Biology meeting. (The FASEB Journal 30 (1 Supplement), 271.3-271.3)

2016 Uppal K, Tran V, Jones D, Li S, Esper A. High-Resolution Metabolomics Reveals Distinct Pathways In Septic Patients That Developed Acute Respiratory Distress Syndrome. American Thoracic Society International Conference. San Francisco, CA (Am J Respir Crit Care Med 193;2016:A4407)

2016 Loukia N. Lili, Michele La Merill, Sophia A. Banton, Tomoko Ishikawa, Piera Cirrilo, Nickilou Krigbaum, Lauren Zimmermann, ViLinh Tran, Dean P. Jones, Barbara Cohn, Shuzhao Li. Metabolome wide association of DDT exposure in humans and mice. 24th Annual International Conference on Intelligent Systems for Molecular Biology, Orlando, FL.

2016 Andrei Todor, Sophia Banton, Luiz Gardinassi, Shuzhao Li. Reanalysis of Snyderome with mummichog and blood transcription modules. 24th Annual International Conference on Intelligent Systems for Molecular Biology, Orlando, FL.

2016 Sophia Banton, Bali Pulendran, Shuzhao Li. Multiscale, multifactorial response network of immunization in humans. 24th Annual International Conference on Intelligent Systems for Molecular Biology, Orlando, FL.

2016 Gardinassi L, Arévalo-Herrera M, Herrera S, Cordy RJ, Tran V, Jones DP, Galinski M, Li S.

Molecular signatures of clinical tolerance to *Plasmodium vivax* revealed by integrative metabolomics and transcriptomics. The 65th ASTMH Meeting, Atlanta, GA

2016   Banton S, Luo R, Joice R, Moreno A, Galinski M, Jones DP, Li S. Pathway group LASSO integration of metabolomics and transcriptomics to characterize malaria infection in Rhesus macaques. The 65th ASTMH Meeting, Atlanta, GA

GRANTS

Pending Grant Applications

1R01LM015162-01 (Li)
NIH/NLM
Repository-scale consensus annotation of metabolomics and exposomics
Role: Principal Investigator
Funding period: 12/01/2025 – 11/30/2029

1R01GM164317-01 (Li)
NIH/NIGMS
Broadly untargeted isotope tracing metabolomics to discover novel molecules and biochemical pathways
Role: Principal Investigator
Funding period: 04/01/2026 – 03/31/2031

Current Research Support

R01 AI149746 (Li)
NIH/NIAID
ImmunoMetabolomics of Zoster vaccines
Role: Principal Investigator
Funding period: 12/01/2019 – 11/30/2025 NCE

UM1 HG012651 (Robson)
NIH/NHGRI
JAX MorPhiC Data Production Center
Role: Co-Investigator
Funding period: 08/2022 - 05/2027

D24AC00345 (Miller)
ADVANCED RESEARCH PROJECTS AGENCY for HEALTH (ARPA-H)
IndiPHARM: Individual Metabolome and Exposome Assessment for Pharmaceutical Optimization
Role: Site PI
Funding period (Phase I): 9/11/2024 to 9/10/2027

U01AI141919 (Weinberg)
NIH/NIAID
Persistence of protection conferred by shingrix against herpes zoster in older adults
Role: Co-Investigator
Funding period: 3/1/2024 to 2/28/2029

R01 HD116631 (Weinberg)
NIH/NIDDK
Developing Interventions for The Protection of HIV-Exposed Uninfected Infants against Severe Infections
Role: Co-Investigator
Funding period: 08/2024 - 07/2029

P30 AG067988 (Kuchel)
NIH/NIA
Claude D. Pepper Older American Independence Centers
Role: Co-Investigator
Funding period: 08/2021 - 06/2026

Completed Research Support

R01 HD107793 (Weinberg)
Eunice Kennedy Shriver National Institute of Child Health and Human Development
Relationship between maternal and fetal immune responses
Role: Co-Investigator
Funding period: 09/2022 - 08/2025

JAX-DIF-2022-Oh-Acidosis (Oh)
The Jackson Laboratory
Microbial modulation of aging-associated kidney acidosis
Role: Co-Investigator
Funding period: 02/2023 - 08/2024

R21 AI155257A (Weinberg)
NIH/ NIAID
Dynamics of m. tuberculosis-specific innate and adaptive immunity during pregnancy and postpartum in women with hiv
Role: Co-Investigator
Funding period: 08/2022 - 07/2024

R01 AI149746-06-05S1 (Li)
NIH
Enhancement of asari software for metabolomics data processing
Role: Principal Investigator
Funding period: 12/1/2023 to 11/30/2024

U01 CA235493 (Li/Xia/Siuzdak)
NIH/NCI
Mummichog 3, aligning mass spectrometry data to biological networks
Role: Lead Principal Investigator
Funding period: 09/06/2018 - 08/31/2023

U2C ES030163 (Jones/Li/Miller/Morgan)
NIH/NIEHS
Mega-scale Identification tools for xenobiotic metabolism
Role: co- Principal Investigator

Funding period: 09/01/2018 - 08/30/2022

U19 AI090023-07 (Pulendran)
NIH/NIAID
HIPC: System Biological Analyses of Innate and Adaptive Responses to Vaccination
Role: Co- Investigator
Funding period: 07/01/2016 – 6/30/2023

R01 GM124061 (Kang, Yu)
NIGMS
Bayesian Network Biomarker Selection in Metabolomics Data
Role: Co- Investigator
Funding period: 09/01/2017 – 08/31/2021

UH2 AI132345 (Li)
NIH/NIAID
Multiscale, multifactorial immune networks as a web service
Role: Principal Investigator
Funding Period: 06/24/2017 – 05/31/2019

P50 ES026071
NIH/NIESH
Center for Children's Health, the Environment, the Microbiome, and Metabolomics (C-CHEM2)
Role: Co-Investigator, co-lead of Project 3
Funding Period: 09/30/2015 – 06/30/2019

83615301
EPA
Center for Children's Health, the Environment, the Microbiome, and Metabolomics
Role: Co-Investigator, co-lead of Project 3
Funding Period: 09/01/2015 – 08/31/2019

P30 ES019776
NIH/NIEHS
HERCULES: Health and Exposome Research Center at Emory
Role: co-Director the IHSFC Core (relinquished due to institutional change)
Funding Period: 05/21/2017-03/31/2022

U2C ES026560
NIH/NIEHS
National Exposure Assessment Laboratory at Emory
Role: Co-Investigator
Funding Period: 09/30/2015 – 08/31/2019

HHSN272201300018I
NIH/NIAID
Vaccine and Treatment Evaluation Units (VTEU), Task Order Request-TASK AREA A. D
Role: Co-Investigator (relinquished due to institutional change)
Funding Period: 09/16/2015 – 09/15/2023

R01 DK107900
NIH/NIDDK
Mechanism, Modification, and Intervention in a Pre-Clinical Model of Galactosemia
Role: Co-Investigator
Funding Period: 12/01/2015 – 11/30/2019

R01 AI121252
NIH/NIAID
Understanding the Survival of Human Bone Marrow Long-lived Plasma Cells
Role: Co-Investigator (relinquished due to institutional change)
Funding Period: 01/01/2016 – 12/31/2020

UFDSP00011230
NIH/University of Florida Sub
Bacterial surface layer-specific immune protection against gut microbial infection
Role: Co- Investigator
Funding Period: 04/01/16 – 3/31/2020

HHSN272201200031C
NIH/NIAID
Systems Biology of Malaria as a Model for Host-Pathogen Interactions
Role: Co-Investigator
Funding Period: 09/30/2012 – 09/29/2017

UG3OD023318
NIH
The Impact of the Intrauterine and Early Childhood Environments on Neurocognitive
Role on Project: Co-Investigator
Funding Period: 09/21/16 – 08/31/2017

21UB-8002
California Breast Cancer Research Program   .
Chemical Safety During Breast Cancer Susceptible Windows
Role: Co-Investigator
Funding Period: 03/01/2015-02/28/2018

R21HD089056
NIH/CHOA Sub
Anti-LPS antibody for Pediatric Nonalcoholic Fatty Liver Disease
Role on Project: Key Personnel
Funding Period: 09/01/2016 – 8/31/2018

W911NF-16-C-0008
DOD/Defense Advanced Research Projects Agency (DARPA)
Immune Resilience in host-pathogen interactions
Role: Co - Investigator
Funding Period: 03/09/2016-03/08/2019

AWARDS AND HONORS:

2005	Montana State University Research Enhancement Travel Award
2004	Gary K. Lynch Memorial Award, Montana State University
2001- 2004	National Science Foundation IGERT Fellowship

Peer Review Activities:

Grants:

National and International:
Israel Science Foundation, 2015
Ad hoc Reviewer, NIH study section ZES1 LAT-D (R1), 2020
Ad hoc Reviewer, NIH study section ZDK1 GRB-T (M2), 2021
Ad hoc Reviewer, NIH study section ZDK1 GRB-7 (O4), 2022
Ad hoc Reviewer, NIDDK study section P30 DDRCC, 2022
European Research Council (ERC-2023-STG), 2023
Ad hoc Reviewer, NIDDK study section P30 DDRCC, 2023
Ad hoc Reviewer, NIAID study section ZAI1 LG-M (J1), 2023
Swiss National Science Foundation, 2024
German Research Foundation (Deutsche Forschungsgemeinschaft), 2024

Institutional
Ad-hoc reviewer for ACTSI KL2 Career development program, 2016
Ad-hoc reviewer for Emory University WHSC Synergy Award, 2017
Ad-hoc reviewer for Emory University HERCULES pilot grants, 2019

Manuscripts (frequency ranked, incomplete list):

Analytical Chemistry, Nature Methods, Nature Communications, Nature Immunology, Nature Metabolism, Nature Medicine, Bioinformatics, Cell Reports, Cell Systems, Scientific Reports, Science Immunology, Metabolites, Journal of Proteome Research, Metabolomics, Aging, American Journal of Medical Sciences, Analytica Chimica Acta, BMC Genomics, BMC Bioinformatics, Cell Reports Medicine, Computer Methods and Programs in Biomedicine, Current Metabolomics, Current Opinions in Biotechnology, Current Pharmacology Reports, Genome Medicine, Human Genomics, IEEE Transactions on Biomedical Engineering, Investigative Ophthalmology & Visual Science, Journal of Clinical Medicine, Journal of the American Geriatrics Society, Journal of Occupational and Environmental Medicine, Mediators of Inflammation, Oncoimmunology, PLoS ONE, Reproductive Health, Science Translational Medicine, Vaccine

Editorships and Editorial Boards:

Editorial board: *Frontiers in Molecular Diagnostics*

Editor for Springer Nature book "*Computational Methods and Data Analysis for Metabolomics*" Part of the series of "*Methods in Molecular Biology*", aimed as the first major book on computational metabolomics. 2020.
ISBN-13: 978-1071602386. ISBN-10: 1071602381
(184K downloads, by Sept. 30, 2025)

Society Memberships:

International Society for Computational Biology
Metabolomics Society
Metabolomics Association of North America
American Society for Mass Spectrometry

GitHub profile:
https://github.com/shuzhao-li
https://github.com/shuzhao-li-lab/

Google Scholar profile:
Citations 18065, h-index 43, i10-index 64 (Sept. 30, 2025)
https://scholar.google.com/citations?user=lNBq0asAAAAJ&hl=en