Hunter N. B. Moseley, Associate Professor

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Broad Research Interests

Develop computational methods, tools, and models for analyzing and interpreting many types of biological and biophysical data that enable new understanding of biological systems and related disease processes.

Research Experience

Head of a Biophysical Informatics & Systems Biochemistry Lab, University of Kentucky
2013-present Associate Professor, Department of Molecular & Cellular Biochemistry, University of Kentucky
2008-2013 Assistant Professor, Department of Chemistry, University of Louisville
1998-2008 Postdoc to Research Assistant Prof, Bioinformaticist, Ctr. Adv. Biotechnology & Medicine, Rutgers Univ.

Education

1992-1998 Ph.D. Biochemistry and Molecular Genetics, N. Rama Krishna (advisor)
University of Alabama at Birmingham, Birmingham, AL

1988-1992 B.A. Chemistry, Computer Science, and Mathematics triple major; Biology minor
Huntingdon College, Montgomery, AL

Major Research Projects

- Metabolomics data analysis and moiety modeling using SIRM data, Univ. of Kentucky.
- Method and System for Identification of Metabolites, U.S. patent app. 15/642,143, Univ. of Kentucky
- Automated protein resonance assignments of NMR data, Univ of Kentucky.
- AutoAssign package for automated protein NMR resonance assignments, Rutgers Univ.
- CORCEMA - NOESY and TrNOESY analysis program, U.S. patent 5,668,734, UAB

Professional Activities

- Co-authored 42 publications with an "h" index of 19.
- Informatics Core Director, Resource Ctr for Stable Isotope-Resolved Metabolomics,Univ.of Kentucky
- Informatics Director, Center for Environmental and Systems Biochemistry, Univ. of Kentucky
- Associate Director, Institute for Biomedical Informatics, Univ. of Kentucky
- Co-Director, Biomedical Informatics Core,Ctr for Clinical & Translational Sciences, Univ. of Kentucky
- Associate Member, Northeast Structural Genomics Consortium
- Review Editor, *Frontiers in Molecular Sciences - Metabolomics*
- Program Committee, UT-KBRIN Bioinformatics Summit
- Peer-reviewed grant proposals for NSF and manuscripts for *J Biomol NMR*, *J Mag Reson, PNAS*, *Protein Sci, Bioinformatics, J Struct Funct Genomics, CEJB, RECOMB, Rap Com MS, Anal Chem*
- Given 37 oral presentations at various conferences, workshops, and universities.

Teaching Experience

2015-present Instructor for biochemistry course BCH-401G-Honors, University of Kentucky
2009-2013 Instructor for biochemistry courses (CHEM 445, CHEM 547, CHEM 647), University of Louisville
2008-2013 Coordinator of Chemistry Dept Graduate Seminar Program (CHEM 695), University of Louisville
2007-2008 Coordinator for CABM Summer Undergraduate Internship Program, Rutgers Univ.

Honors and Awards

2015 UK College of Education Teacher Who Made A Difference Honoree
2013 NSF CAREER Award
2012 Kentucky Academy of Science Outstanding Early Career Award
2011 UofL Faculty Favorite Award (nominated by students for excellence in teaching)
2010 Kentuckiana Metroversity Award for Instructional Development (regional multi-university award)
2008 University of Louisville Faculty Learning Community on Critical Thinking
1999-2001 NSF Postdoctoral Research Fellowship in Biological Informatics
1998 UAB Samuel B. Barker Annual Award for Excellence in Graduate Studies, Doctoral Level, (top university doctoral award; awarded to only one student per year)
1996 UAB Department of Biochemistry & Molecular Genetics McKibben Award (top dept. doctoral award)
1988-1992 4-Year Full Tuition Bellingraph Scholarship, Huntingdon College

Current Research Support

- NIH: 1U24DK097215-01A1; Duration: 09/11/2013 to 08/31/2018; Role: PI ($881,220)
- NSF:1252893 (*CAREER)*; Duration: 07/01/2013 to 6/30/2018; Role: PI ($760,657)
- NIH: 1P01CA163223-01A1; Duration: 03/01/2013 to 2/28/2018; Role: Co-I ($553,602)
- NIH: 1R21CA205778-01; Duration: 08/01/2016 to 07/31/2018; Role: PI ($128,200)

Activities

1994-2013 Certified Moniteur Fencing Instructor, Louisville Fencing Center, Bucks County Acad. of Fencing, & BFC
1998 President and co-founder of the Birmingham Fencing Club (BFC), Birmingham, Alabama.

Personal Statement

My formal education spans multiple disciplines including chemistry, mathematics, computer science, and biochemistry. I have over 20 years of experience in bioinformatics research, particularly in the development of automated analyses of NMR and mass spectrometry data. This includes extensive expertise in algorithm development, mathematical modeling, and systems biochemistry. I also have unique educational and research experiences that allow me to work across computational, mathematical, and biological fields, facilitating and leading collaborations between computational, statistical, and biological scientists. I have been actively developing informatics techniques for metabolomics, and I am the Informatics Core Director within the NIH Common Fund-supported Resource Center for Stable Isotope Resolved Metabolomics (RC-SIRM) at the University of Kentucky (UK). We are actively developing methods to integrate metabolomics data with other omics-level datasets for systems-level analyses that can extract mechanistic information on specific human diseases which will translate into clinical practice.

Contributions to Science

1. Systems Biochemical Tools for Large-Scale Stable-Isotope Resolved Metabolomics (SIRM) Applications. I have worked with Drs. Teresa Fan, Andrew Lane, and Rick Higashi to develop a very fruitful collaboration under the auspices of the University of Kentucky Resource Center for Stable Isotope-Resolved Metabolomics. My lab provides needed bioinformatics expertise into a breadth of metabolomics expertises ranging across sample generation from cells/tissue/animals, sample handling, NMR analytical, mass spec analytical, and human metabolism. Our first goal is to develop a combination of bioinformatic, biostatistical, and systems biochemical tools implemented in an integrated data analysis pipeline that will allow broad application of SIRM from the discovery of specific metabolic phenotypes representing biological and disease states of interest to a mechanism-based understanding of a wide range of specific human disease processes with particular metabolic phenotypes. Our new tools are already providing novel metabolic pathway-specific analyses of complex SIRM datasets. For example, Figure 1 shows a moiety model analysis of SIRM mass spectrometer data, where the relative importance of specific metabolic pathways is determined for the biosynthesis of UDP-GlcNAc in prostate cancer cell culture. Subsequent analyses determined which pathways were impacted by potential cancer therapeutics. As we implement a complete SIRM-based data analysis pipeline, our ultimate goal is to integrate metabolomics datasets with other major omics datasets including epigenomics, genomics, transcriptomics, and proteomics datasets in full systems biochemical analyses that can determine which gene-regulatory, signaling, and metabolic pathways are mechanistically involved in specific human diseases.

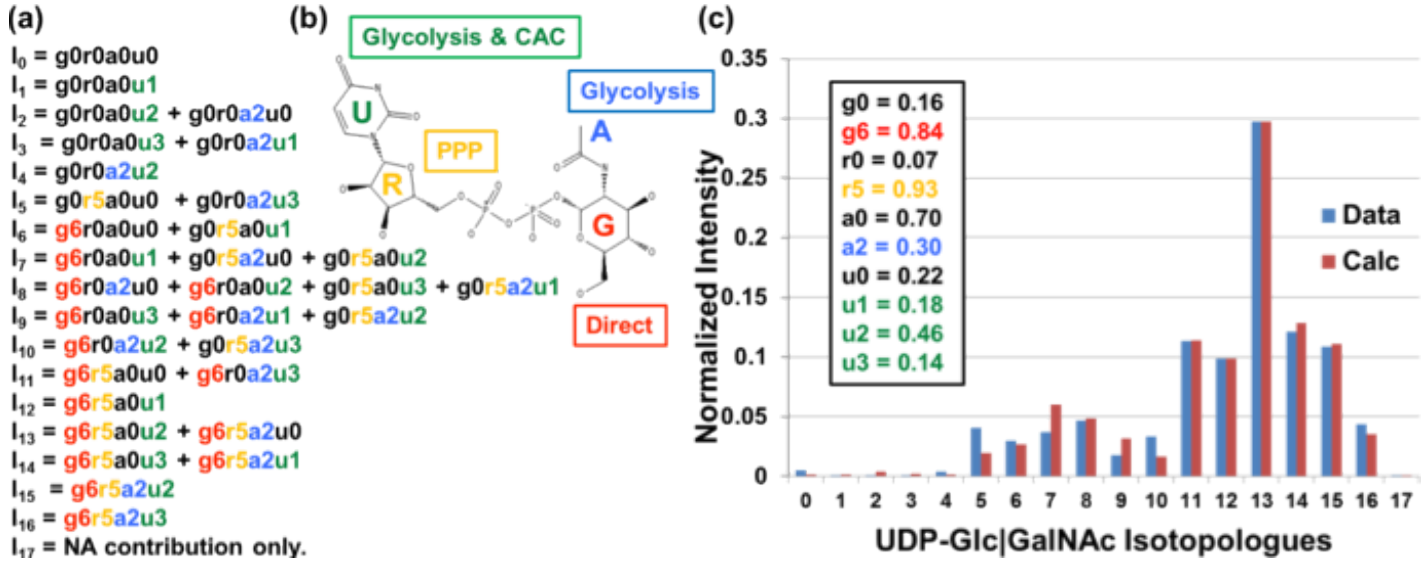
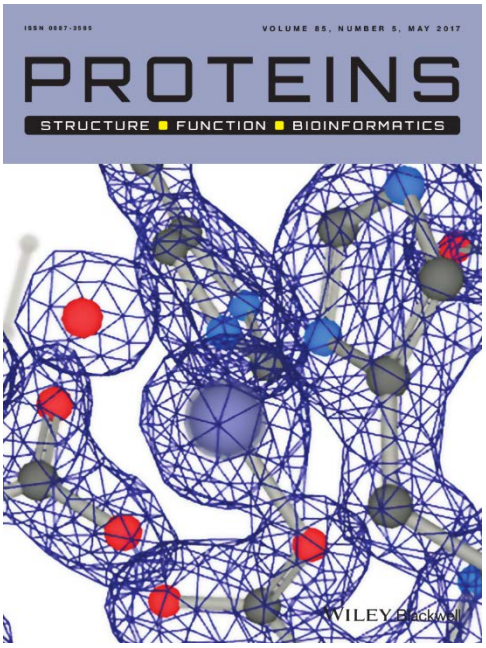


Figure 1: (a) Chemical substructure model representing the possible number of ^{13}C incorporation from $^{13}C_6$-Glc tracer into UDP-GlcNAc, accounting for the observed FT-ICR-MS isotopologue peaks. (b) Structure of UDP-GlcNAc annotated by its chemical substructures and their biosynthetic pathways from $^{13}C_6$-Glc, as in Fig. 2. **U** = uracil, **R** = ribose, **A**_= acetyl, **G**=glucose. NAc-Glucose utilizes Gln as the nitrogen donor. (c) Fit of optimized chemical substructure model parameters to FT-ICR-MS isotopologue data of UDP-GlcNAc extracted from a LN3 prostate cancer cell culture after 48 hours of growth in $^{13}C_6$-Glc.

a) Moseley HNB. Correcting for the Effects of Natural Abundance in Stable Isotope Resolved Metabolomics Experiments Involving Ultra-High Resolution Mass Spectrometry. *BMC Bioinformatics* 11:139, 2010. Citations: 32 (Google Scholar). PMCID: PMC2848236
b) Moseley HNB, Lane AN, Belshoff AC, Higashi RM and Fan TW. A novel deconvolution method for modeling UDP-N-acetyl-D-glucosamine biosynthetic pathways based on (13)C mass isotopologue profiles under non-steady-state conditions. *BMC Biol* 9:37, 2011. Citations: 34 (Google Scholar). PMCID: PMC3126751.
c) Moseley HNB. Error Analysis and Propagation in Metabolomics Data Analysis. *Comput Struct Biotechnol J* 4:2013. Citations: 12 (Google Scholar). PMCID: PMC3647477.
d) Mitchell JM, Fan TW, Lane AN, and Moseley HNB. Development and in silico evaluation of large-scale metabolite identification methos using functional group detection for metabolomics *Frontiers in Genetics* 5:237, 2014. Citations: 12 (Google Scholar). PMCID: PMC4112935

2. Structural Bioinformatics of Metalloproteins. Structural bioinformatics of metalloproteins has historically been hampered by significant numbers of aberrant coordination geometries that prevented systematic classification. My lab has developed combined functional and structural analyses of metalloproteins that have identified aberrant clusters of coordination geometries (CG) of metal ion ligation in the top 5 most abundant metalloproteins. Most of these aberrant CGs are due to multidentate ligands that create compressed ligand-metal-ligand angles below 60°. These angles cause serious deviations from canonical CG models and greatly hamper the ability to characterize metalloproteins both structurally and functionally. Our methods detect coordinating ligands without expectations based on canonical CGs and in a statistically robust manner, producing estimated false positive and false negative rates of ~0.11% and ~1.2%, respectively. Also, our improved analyses of bond-length distributions have revealed bond-length modes specific to chemical functional groups involved in multidentation. By recognizing aberrant CGs in our clustering analyses, high correlations above 0.9 are achieved between structural and functional descriptions of metal ion coordination. This work has been impactful to the field by highlighting the unexpected presence of significant numbers of non-canonical CGs and in characterizing their structural, functional, and chemical characteristics. Our recent publications made the cover of the May 2017 issue of *Proteins*.



a) Yao S, Flight RM, Rouchka EC, Moseley HNB. A less biased analysis of metalloproteins reveals novel zinc coordination geometries. *Proteins* 83:1470, 2015. Citations: 12 (Google Scholar). PMCID: PMC4539273
b) Yao S, Flight RM, Rouchka EC, Moseley HNB. Aberrant coordination geometries discovered in the most abundant metalloproteins. *Proteins* 85:885, 2017. doi:10.1002/prot.25257
c) Yao S, Flight RM, Rouchka EC, Moseley HNB. Perspectives and expectations in structural bioinformatics of metalloproteins. *Proteins* 85:938, 2017. doi:10.1002/prot.25263
d) Yao S, Flight RM, Rouchka EC, Moseley HNB. Cover of May 2017 Issue. *Proteins* 85:cover, 2017. doi:10.1002/prot.25126

3. Automated NMR Protein Resonance Assignments. While at Rutgers University, I developed and maintained the AutoAssign software package for automated protein resonance assignments of solution NMR data, especially for the Northeast Structural Genomics Consortium NMR structure determination pipeline. Figure 2 shows the NMR solution structure of PefI protein (Plasmid-encoded fimbriae; regulatory) from Salmonella typhimurium. This 77 amino acid protein structure determination took only 17 days from the start of data collection to deposition in the PDB (PDB 2JT1) using the NESG NMR structure determination analysis pipeline and conventional triple-resonance NMR experiments. Nearly 300 academic (free) and commercial labs have licensed AutoAssign and the program is cited in

Figure 2: Solution NMR structure of PefI protein from *Salmonella typhimurium*.

twice as many Protein Data Bank and Biological Magnetic Resonance Data Bank (BMRB) entries as all other automated assignment programs combined. We also developed the Assignment Validation Suite (AVS) for validating protein resonance assignments. AVS was the first outside assignment validation tool adopted by the Biological Magnetic Resonance Bank (BMRB), which they use on all submitted entries. I still maintain AVS for the BMRB, to help ensure that only high-quality datasets are deposited in the BMRB.

a) Moseley HNB and Montelione GT. Automated analysis of NMR assignments and structures for proteins. *Curr Opin Struct Biol* 9:635-42, 1999. Citations: 194 (Google Scholar)
b) Moseley HNB, Monleon D and Montelione GT. Automatic determination of protein backbone resonance assignments from triple resonance nuclear magnetic resonance data. *Methods Enzymol* 339:91-108, 2001. Citations: 167 (Google Scholar).
c) Moseley HNB, Riaz N, Aramini JM, Szyperski T and Montelione GT. A generalized approach to automated NMR peak list editing: application to reduced dimensionality triple resonance spectra. *J Magn Reson* 170:263-77, 2004. Citations: 44 (Google Scholar).
d) Moseley HNB, Sahota G and Montelione GT. Assignment validation software suite for the evaluation and presentation of protein resonance assignment data. *J Biomol NMR* 28:341-55, 2004. Citations: 93 (Google Scholar).

4. Complete Relaxation and Conformational Exchange Matrix Analysis (CORCEMA). At the University of Alabama at Birmingham, we developed and I implemented Complete Relaxation and Conformational Exchange Matrix (CORCEMA) methodology for the analysis of 2D-NOESY spectral data of interacting systems undergoing multistate conformational exchange. The current theory is based on generalized rate matrices for relaxation and conformational exchange. The CORCEMA algorithm explicitly incorporates intermolecular dipolar cross-relaxation between the molecules when they are complexed. It permits an analysis of NOESY intensities for both intra- and intermolecular contacts between interacting molecules under a variety of binding conditions. CORCEMA allows for proper quantitative interpretation of specific hydrogen-hydrogen distances from NOESY peak intensities under conditions of exchange and spin-diffusion that would lead to an erroneous interpretation using less sophisticated methods. We demonstrated this in multiple examples involving analysis of both simulated and experimental transferred NOESY datasets.

a) Moseley HNB, Curto EV and Krishna NR. Complete relaxation and conformational exchange matrix (CORCEMA) analysis of NOESY spectra of interacting systems; two-dimensional transferred NOESY. *J Magn Reson B* 108:243-61, 1995. Citations: 100 (Google Scholar).
b) Jackson PL, Moseley HNB, and Krishna NR. Relative Effects of Protein Mediated and Ligand Mediated Spin Diffusion Pathways on Transferred NOESY, and Implications on the Accuracy of the Bound Ligand Conformation. *J Magn Reson B* 107:289-92, 1995. Citations: 22 (ISI)
c) Moseley HNB, Lee W, Arrowsmith CH, and Krishna NR. Quantitative Determination of Conformational, Dynamic, and Kinetic Parameters of a Ligand Protein/DNA Complex from a CORCEMA Analysis of Intermolecular Transferred NOESY. *Biochemistry* 36:5293-99, 1997. Citations: 28 (Google Scholar).
d) Curto EV, Moseley HNB, and Krishna NR. CORCEMA evaluation of the potential role of intermolecular transferred NOESY in the characterization of ligand receptor complexes. *J Comp Aided Molec Design* 10:361-71, 1996. Citations: 17 (Google Scholar).

5. Transdisciplinary Mentoring, Science Education, and Open Software Development. There is a well-documented high demand for transdisciplinary-trained bioinformaticians and data scientists in both academia and industry. Our lab actively recruits postdoctoral fellows, as well as graduate, undergraduate and high school students and trains them in translational bioinformatics and systems biology by actively mentoring them in research projects. Over the last 9 years, the lab has included 4 postdoctoral fellows (including 2 women), 11 graduate students (including 4 women), 50 undergraduate students (including 11 women, 1 LGBT), and 15 high school students (including 3 woman) from a wide range of disciplines including agricultural biotechnology, animal sciences, chemistry, biochemistry, biology, mathematics, statistics, physics, computer science, computer engineering, chemical engineering, and biomedical engineering. One result of this training is that the students and staff in our lab have developed several high-quality and well-documented open software packages that are maintained for high reusability by the broader scientific community on GitHub under the MoseleyBioinformaticsLab organizational account. Other open software projects developed by the lab are maintained on FigShare and the lab website for scientific reproducibility.

I have personally advised many students at graduate, undergraduate, and high school starting points on transdisciplinary, informatics-oriented educational trajectories. One undergraduate lab assistant Tamas Nagy received an NSF Graduate Fellowship in 2015 and is now a graduate student in the Integrative Program in Quantitative Biology at UCSF.
I also developed an undergraduate biochemistry course, CHEM 445-Survey of Biochemistry at the Univ. of Louisville, which won the 2010 Metroversity Award for Instructional Development (regional multi-university award). While creating the Metroversity application, I discovered a lack of publications on explicit revision in content rich courses, including sciences courses. This is in sharp contrast to the use of explicit revision steps in writing courses. I was granted exempted IRB approval at both the Univ. of Louisville and the Univ. of Kentucky to analyze for statistically significant effects of scaffolded explicit revision on biochemistry courses.

a) Webb S, Nagy T, Moseley HNB, Fried M, Dutch RE. Hendra virus fusion protein transmembrane domain contributes to pre-fusion protein stability. *J Biol Chem* accepted 2017.
b) Smelter A, Astra, M, Moseley HNB. A Fast and Efficient Python Library for Interfacing with the Biological Magnetic Resonance Data Bank. *BMC Bioinformatics* accepted 2017.
c) Mitchell JM, Fan TW, Lane AN, and Moseley HNB. Development and in silico evaluation of large-scale metabolite identification methods using functional group detection for metabolomics *Frontiers in Genetics* 5:237, 2014. Citations: 11 (Google Scholar). PMCID: PMC4112935
d) Moseley HNB. MoseleyBioinformaticsLab GitHub Repositories. In: GitHub. 2016. Available from: https://github.com/MoseleyBioinformaticsLab.

Publications

- Current "h" index is 19 as per J. E. Hirsch's definition for quantifying an individual's scientific research output (physics/0508025 v5 09/29/2005).

42) Dries Verdegem, Hunter N.B. Moseley, Wesley Vermaelen, Abel Acosta Sanchez, and Bart Ghesquière. "MAIMS: A software tool for sensitive metabolic tracer analysis through the deconvolution of 13C mass isotopologue profiles of large composite metabolites" *Metabolomics* 13, 123 (2017).

41) Andrey Smelter, Eric C. Rouchka, and Hunter N.B. Moseley. "Detecting and accounting for multiple sources of positional variance in peak list registration analysis and spin system grouping" *J Biomol NMR* 68, 281 (2017).

40) Andrey Smelter, Morgan Astra, Hunter N.B. Moseley. "A Fast and Efficient Python Library for Interfacing with the Biological Magnetic Resonance Data Bank" *BMC Bioinformatics* 18, 175 (2017).

39) Stacy Webb, Tamas Nagy, Hunter N.B. Moseley, Michael Fried, Rebecca E. Dutch. "Hendra virus fusion protein transmembrane domain contributes to pre-fusion protein stability" *Journal of Biological Chemistry* 292, 5685 (2017).

38) Sen Yao, Robert M. Flight, Eric C. Rouchka, Hunter N.B. Moseley. "Perspectives and Expectations in Structural Bioinformatics of Metalloproteins" *Proteins: Structure, Function, and Bioinformatics* 85, 938 (2017).

37) Sen Yao, Robert M. Flight, Eric C. Rouchka, Hunter N.B. Moseley. "Aberrant coordination geometries discovered in the most abundant metalloproteins" *Proteins: Structure, Function, and Bioinformatics* 85, 885 (2017).

37b) Sen Yao, Robert M. Flight, Eric C. Rouchka, Hunter N.B. Moseley. "Cover Image of Volume 85, Issue 5" *Proteins: Structure, Function, and Bioinformatics* 85(5), cover (2017).

36) Narasimharao Nalabothula, Taha Al-jumaily, Robert M. Flight, Abdallah N. Eteleeb, Shao Xiaorong, Eric C. Rouchka, Hunter N.B. Moseley, and Yvonne Fondufe-Mittendorf. "Genome-wide profiling of PARP1 reveals an interplay with gene regulatory regions and DNA methylation" *PLoS ONE* 10, e0135410 (2015). Citations: 6 (Google Scholar)

35) Sen Yao, Robert M. Flight, Eric C. Rouchka, and Hunter N.B. Moseley. "A less biased analysis of metalloproteins reveals novel zinc coordination geometries" *Proteins: Structure, Function, and Bioinformatics* 83, 1470-1487 (2015). Citations: 12 (Google Scholar)

34) Sen Yao, Robert M. Flight, Eric C. Rouchka, and Hunter N.B. Moseley. "A less biased analysis of metalloproteins reveals novel zinc coordination geometries" *BCB '15 Proceedings of the 6th ACM Conference on Bioinformatics, Computational Biology and Health Informatics* pp493-494. doi:10.1145/2808719.2811424 (2015).

33) Andrew N. Lane, Sengodagounder Arumugam, Pawel K. Lorkiewicz, Richard M. Higashi, Sébastien Laulhé, Michael H. Nantz, Hunter N.B. Moseley, and Teresa W.-M. Fan. "Chemoselective detection and discrimination of carbonyl-containing compounds in metabolite mixtures by 1H-detected 15N NMR" *Magnetic Resonance in Chemistry* 53, 337 (2015). Citations: 10 (Google Scholar)

32) Abdallah M. Eteleeb, Hunter N.B. Moseley, and Eric C. Rouchka. "A Comparison of Combined P-value Methods for Gene Differential Expression Using RNA-Seq Data" *BCB'14: Proceedings of the 5th ACM Conference on Bioinformatics, Computational Biology and Health Informatics,* pp417-425. doi:10.1145/2649387.2649421 (2014).

31) Joshua M. Mitchell, Teresa W-.M. Fan, Andrew N. Lane, and Hunter N.B. Moseley. "Development and in silico evaluation of large-scale metabolite identification methos using functional group detection for metabolomics" *Frontiers in Genetics*, 5, 237 (2014). Citations: 10 (Google Scholar)

30) Richard M. Higashi, Teresa W-M. Fan, Pawel K. Lorkiewicz, Hunter N.B. Moseley, Andrew N. Lane. "Stable Isotope Labeled Tracers for Metabolic Pathway Elucidation by GC-MS and FT-MS" *Mass Spectrometry in Metabolomics: Methods in Molecular Biology*, vol 1198, 147, editor D. Raftery. Humana Press (2014). Citations: 7 (Google Scholar)

29) William J. Carreer, Robert M. Flight, and Hunter N.B. Moseley. "A computational framework for high-throughput isotopic natural abundance correction of omics-level ultra-high resolution FT-MS datasets" *Metabolites*, 3, 853-866 (2013). Citations: 6 (Google Scholar)

28) Hunter N.B. Moseley. "Error Analysis and Propagation in Metabolomics Data Analysis" *Comp Struct Biotech J*, 4, e201301006 (2013). Citations: 12 (Google Scholar)

27) Eric C. Rouchka, Robert M. Flight, and Hunter N.B. Moseley. "Proceedings of the Eleventh Annual UT-ORNL-KBRIN Bioinformatics Summit 2012" *BMC Bioinformatics*, 13, A1 (2012).

26) Teresa W-M. Fan, Pawel Lorkiewicz, Katherine Sellers, Hunter N.B. Moseley, Richard M. Higashi, and Andrew N. Lane. "Stable isotope-resolved metabolomics and applications to drug development" *Pharmacology & Therapeutics,* 133, 366 (2012). Citations: 76 (Google Scholar)

25) Hunter N.B. Moseley, Andrew N. Lane, Alex C. Belshoff, Richard M. Higashi, and Teresa W-M. Fan. "A novel method for deconvoluting metabolic subunits from mass isotopologues in stable isotope resolved metabolomic experiments under non steady-state conditions: application to the biosynthesis of UDP-GlcNAc" *BMC Biology*, 9, 37 (2011). Citations: 34 (Google Scholar)

24) Hunter N.B. Moseley, Richard M. Higashi, Teresa W-M. Fan, and Andrew N. Lane. "Metabolic Modeling of Converging Metabolic Pathways: Analysis of Non-Steady State Stable Isotope-Resolve Metabolism of UDP-GlcNAc and UDP-GalNAc" *BIOINFORMATICS 2011 – Proceedings of the International Conference on Bioinformatics Models, Methods and Algorithms*. Ed. Marco Pellegrini, Ana Fred, Joaquim Filipe, and Hugo Gamboa. SciTePress, Portugal, 108-115 (2011). Citations: 3 (Google Scholar)

23) Hunter N.B. Moseley, Lindsay J. Sperling, and Chad M. Rienstra. "Automated Protein Resonance Assignments of Magic Angle Spinning Solid-State NMR Spectra of β1 Immunoglobulin Binding Domain of Protein G (GB1)" *J Biomol NMR*, 48, 123-128 (2010). Citations: 16 (Google Scholar)

22) Hunter N.B. Moseley. "Correcting for the Effects of Natural Abundance in Stable Isotope Resolved Metabolomics Experiments Involving Ultra-High Resolution Mass Spectrometry." *BMC Bioinformatics* 11, 139-144 (2010). Citations: 32 (Google Scholar)

21) Andrew N. Lane, Teresa W-M. Fan, Zhengzhi Xie, Hunter N.B. Moseley, and Richard M. Higashi. "Isotopomer analysis of lipid biosynthesis by high resolution mass spectrometry and NMR." *Anal. Chim. Acta*. 651, 201-208 (2009). Citations: 40 (Google Scholar)

20) Gregory J. Kornhaber, David Snyder, Hunter N.B. Moseley, and Gaetano T. Montelione. "Identification of Zinc-Ligated Cysteine Residues Based on ^{13}Ca and ^{13}Cb Chemical Shift Data." *J Biomol NMR,* 34, 259-269 (2006). Citations: 57 (Google Scholar)

19) Michael Baran, Hunter N.B. Moseley, James M. Aramini, Marvin J. Bayro, Daniel Monleon, Jessica Lau, and Gaetano T. Montelione. "SPINS: A Laboratory Information Management System for Organizing and Archiving Intermediate and

Final Results from NMR Protein Structure Determinations." *Proteins: Struct Funct Bioinformatics,* 62,843-851 (2006). Citations: 13 (Google Scholar)

18) Yuanpeng J. Huang, Hunter N.B. Moseley, Michael C. Baran, Cheryl Arrowsmith, Robert Powers, Roberto Tejero, Thomas Szyperski, and Gaetano T. Montelione. "An integrated platform for automated analysis of protein NMR structures." *Meth Enzymology* 394, 111-141 (2005). Citations: 65 (Google Scholar)

17) Michael C. Baran, Janet Y. Huang, Hunter N.B. Moseley, and Gaetano T. Montelione. "Automated Analysis of Protein NMR Assignments and Structures." *Chemical Reviews* 104, 3541-3556 (2004). Citations: 94 (Google Scholar)

16) Hunter N.B. Moseley, Nadeem Riaz, James M. Aramini, Thomas Szyperski, and Gaetano T. Montelione. "A Generalized Approach to Automated NMR Peak List Editing: Application to Reduced Dimensionality Triple Resonance Spectra." *J Magn Reson* 170, 263-277 (2004). Citations: 44 (Google Scholar)

15) Hunter N.B. Moseley, Gurmukh Sahota, and Gaetano T. Montelione, "Assignment Validation Software Suite for the Evaluation and Presentation of Protein Resonance Assignment Data." *J Biomol NMR* 28, 341-355 (2004). Citations: 93 (Google Scholar)

14) Deyou Zheng, Yuanpeng J. Huang, Hunter N.B. Moseley, Rong Xiao, James Aramini, G.V.T. Swapna, and Gaetano T. Montelione, "Automated protein fold determination using a minimal NMR constraint strategy." *Protein Science* 12, 1232-1246 (2003). Citations: 58 (Google Scholar)

13) Michael Baran, Hunter N.B. Moseley, Gurmukh Sahota, and Gaetano T. Montelione, "SPINS: Standardized ProteIn NMR Storage. A data dictionary and object-oriented relational database for archiving protein NMR spectra." *J Biomol NMR* 24, 113-121 (2002). Citations: 20 (Google Scholar)

12) Daniel Monleon, Kimberly Colson, Hunter N.B. Moseley, Clemens Anklin, Robert Oswald, Thomas A. Szyperski, and Gaetano T. Montelione, "Rapid Analysis of Protein Backbone Resonance Assignments Using Cryogenic Probes, Distributed Linux-based Computing, and Automated Spectral Analysis." *J Struct Func Genomics* 2, 93-101 (2002). Citations: 33 (Google Scholar)

11) Thomas Szyperski, Deok C. Yeh, Dinesh K. Sukumaran, Hunter N.B. Moseley, and Gaetano T. Montelione. "Reduced-dimensionality NMR Spectroscopy for High-Throughput Protein Resonance Assignment: Implementation and Automated Analysis." *Proc Natl Acad Sci USA* 99, 8009-8014 (2002). Citations: 177 (Google Scholar)

10) Hunter N.B. Moseley, Daniel Monleon, and Gaetano T. Montelione, "Automatic Determination of Protein Backbone Resonance Assignments from Triple Resonance NMR Data." *Meth Enzymology* 339, 91 (2001). Citations: 167 (Google Scholar)

9) Hunter N.B. Moseley and Gaetano T. Montelione. "Automated analysis of NMR assignments and structures for proteins." *Curr Opin Struct Biol* 9, 635-642 (1999). Citations: 194 (Google Scholar)

8) N. Rama Krishna and Hunter N.B. Moseley. "Complete Relaxation and Conformational Exchange Matrix Analysis of NOESY Spectra of Reversibly Forming Ligand-Receptor Complexes: Application to Transferred NOESY," in "Structure Computation and Dynamics in Protein NMR." *Biological Mag Resonan* Vol 17, editors: N. R. Krishna and L.J. Berliner, Plenum Press, New York (1999). Citations: 3 (Google Scholar)

7) Hunter N.B. Moseley. "Implementation and Application of Complete Relaxation and Conformational Exchange Matrix Analysis of NOESY Spectra." dissertation (1998). Citations: 1 (Google Scholar)

6) Hunter N.B. Moseley, Weontae Lee, Cheryl H. Arrowsmith, and N. Rama Krishna. "Quantitative Determination of Conformational, Dynamic, and Kinetic Parameters of a Ligand-Protein/DNA Complex from a CORCEMA Analysis of Intermolecular Transferred NOESY." *Biochemistry* 36, 5293 (1997). Citations: 28 (Google Scholar)

5) Ernest V. Curto, Hunter N.B. Moseley, and N. Rama Krishna. "CORCEMA evaluation of the potential role of intermolecular transferred NOESY in the characterization of ligand-receptor complexes." *J Comp-Aided Molec Design* 10, 361 (1996). Citations: 17 (Google Scholar)

4) Hunter N.B. Moseley, Ernest V. Curto, and N. Rama Krishna. "Complete Relaxation and Conformational Exchange Matrix (CORCEMA) Analysis of NOESY Spectra of Interacting Systems: Two-dimensional Transferred NOESY." *J Magn Reson* B108, 243 (1995). Citations: 100 (Google Scholar)

3) Patricia L. Jackson, Hunter N.B. Moseley, and N. Rama Krishna. "Relative Effects of Protein-Mediated and Ligand-Mediated Spin-Diffusion Pathways on Transferred NOESY, and Implications on the Accuracy of the Bound Ligand Conformation." *J Magn Reson* B107, 289 (1995). Citations: 22 (ISI)

2) Curtis C. Maier, Hunter N.B. Moseley, Shan-Ren Zhou, John N. Whitaker, and J. Edwin Blalock. "Identification of Interactive Determinants on Idiotypic-Anti-idiotypic Antibodies through Comparison of Their Hydropathic Profiles." *Immunomethods* 5, 107 (1994). Citations: 27 (Google Scholar)

1) Rick L. Davies and Hunter N.B. Moseley. "Student Roots: Square root algorithm in Forth." *Forth Dimensions* 8, 8-9 (1987). Citations: 0 (unknown)

Oral Presentations

37) "Structural and Functional Characterization of Expected and Aberrant Metal Ion Coordination in Proteins", Mathematics Dept Seminar, Lexington, KY (2016).

36) "Structural and Functional Characterization of Expected and Aberrant Metal Ion Coordination in Proteins", Toxicology & Cancer Biology Dept Seminar, Lexington, KY (2016).

35) "Metadata Capture & DRCC Deposition", RCSIRM Workshop, Lexington, KY (2016).

34) "Advanced Data Analysis", RCSIRM Workshop, Lexington, KY (2016).

33) "Teaching Critical Thinking in STEM Disciplines", STEM Teaching Enhancement Workshop & Forum, Lexington, KY (2015).

32) "Biomedical Informatics at the University of Kentucky", 10th Annual CCTS Spring Conference, Lexington, KY (2015).

31) "Resource Center for Stable Isotope Resolved Metabolomics:Tracing Networks & Pools," NIH Common Fund Annual Meeting – Metabolomics, Triangle, NH (2014).

30) "Natural Abundance Correction and Moeity Modeling in FTMS Data", RCSIRM Workshop, Lexington, KY (2014).

29) "Development of Large-Scale Metabolite Identification Methods for Metabolomics", UT-KBRIN Bioinformatics Summit, Cadiz, KY (2014).

28) "An Informatics and Modeling Platform for Stable Isotope-Resolved Metabolomics." 55th Experimental Nuclear Magnetic Resonance Conference, Boston, MA (2014).

27) "Defining and Cultivating Critical Thinking Among Your Students." University of Kentucky, Lexington, KY (2014).

26) "What is Critical Thinking?" University of Kentucky, Lexington, KY (2013).

25) "Applications of Stable Isotope-Resolved Metabolomics: From Bench to Bedside." University of Kentucky, Lexington, KY (2013).

24) "Scaffolded Explicit Revision as a Practical Framework to Promote Effective Student Effort in Content-Rich Courses." 2013 I2A Institute: Sharing the Impact of Critical Thinking, Louisville, KY (2013).

23) "Scaffolded Explicit Revision as a Practical Framework to Promote Effective Student Effort." 2013 Kentucky Innovations Conference, Lexington, KY (2013).

22) "Scaffolded Explicit Revision as a Practical Framework to Promote Effective Student Effort in Content-Rich Courses." 2013 Celebration of Teaching & Learning: Teaching in Harmony with the Brain: Applying Learning Science in Today's Classroom and Beyond, Louisville, KY (2013).

21) "Metabolic Modeling of Converging Metabolic Pathways. Analysis of Non-Steady State Stable Isotope-Resolved Metabolomics of UDP-GlcNAc and UDP-GalNAc." IUPUI, Indianapolis, IN (2012).

20) "Scaffolded Explicit Revision as a Practical Framework to Promote Effective Student Effort in Content-Rich Science Courses." 2012 Ideas to Action (I2A) Institute: Critical Thinking Innovation, Louisville, KY (2012).

19) "Metabolic Modeling of Converging Metabolic Pathways. Analysis of Non-Steady State Stable Isotope-Resolved Metabolomics of UDP-GlcNAc and UDP-GalNAc." The 25th Anniversary CABM Symposium, Ctr. Adv. Biotech & Med., Rutgers University & UMDNJ., Piscataway, NJ (2011).

18) "Metabolic Modeling of Converging Metabolic Pathways. Analysis of Non-Steady State Stable Isotope-Resolved Metabolomics of UDP-GlcNAc and UDP-GalNAc." BIOINFORMATICS 2011, Rome, Italy (2011).

17) "Metabolic Modeling of Converging Metabolic Pathways. Analysis of Non-Steady State Stable Isotope-Resolved Metabolomics of UDP-GlcNAc and UDP-GalNAc." Metabolomics Network Annual Meeting, NIH Campus, Bethesda, MD (2010).

16) "Metabolic Modeling of Converging Metabolic Pathways. Analysis of Non-Steady State Stable Isotope-Resolved Metabolomics of UDP-GlcNAc and UDP-GalNAc." Huntingdon College, Montgomery, AL (2010).

15) "Stable isotope-resolved metabolomics analysis of UDP-GlcNAc & UDP-GalNAc: Computational resolution and modeling of their converging biosynthetic pathways." 239th American Chemical Society National Meeting and Exposition, San Francisco, CA (2010).

14) "Stable Isotope Resolved Metabolomics (SIRM) of UDP-GlcNAc and UDP-GalNAc Metabolism in Prostate Cancer." 5th Annual Metabolomics Society International Conference, Edmonton, Alberta. Canada (2009).

13) "Automated Analysis of RD and GFT NMR data with Pattern Picker." Protein Structure Initiative NMR Workshop, Rutgers University (2008).

12) "Automated NMR Analysis for Structural Genomics: From FIDS to Resonance Assignments and then to Structure." Huntingdon College, Montgomery, AL (2008).

11) "Automated Analysis from FIDs to Resonance Assignments Using GFT Data," CCPN-NESG Workshop on Automated and Interactive NMR Data Analysis, Rutgers University (2007).

10) "Automated Analysis from FIDs to Resonance Assignments Using GFT Data," ESF Exploratory Workshop: Experimental and Computational Aspects of High-Throughput Protein NMR, European Science Foundation, Goteburg University, Sweden (2006).

9) "NMR Automation: From FIDs to Resonance Assignments and then to Structure," Biomolecular NMR Workshop, BioMagRes Databank, University of Wisconsin-Madison, Madison, WI (2006).

8) "Automation of the NMR Structure Determination Process for Structural Genomics," University of Copenhagen, Denmark (2005).

7) "Current Methods in NMR Structure Determination", DIMACS Working Group on New Algorithms for Inferring Molecular Structure from Distance Restraints, Rutgers University (2004).

6) "Automation of the NMR Structure Determination Process for Structural Genomics," NJ ACS NMR Topical Group, Woodbridge, NJ (2003).

5) "Automated Protein Assignments and Structure Determination," BioNMR Workshop, University of Alabama at Huntsville, Huntsville, AL (2003).

4) "Automatic Determination of Protein NMR Assignments using AutoAssign and AutoPeak," Biomolecular NMR Workshop, BioMagRes Databank, University of Wisconsin-Madison, Madison, WI (2002).

3) "Current Methods in Automated Assignment and Automated Structure Determination," Workshop 2000: NMR Methods for Biomolecular Structures, National Laboratory of Protein Engineering and Plant Genetic Engineering, Peking University, Beijing, China (2000).

2) "Automated Analysis of Protein NMR Spectra: Development for Structural Genomics and Structure-Based Drug Design," Cambridge Healthtech Institute's 2nd International Conference on NMR Technologies (1999).

1) "Automated Analysis of Protein NMR Spectra: Development for Structural Genomics," Intersections of Structural Biology & Genomics Symposium, Cornell Theory Center (1999).

Poster Presentations

116) Smita Joshi*, Meenakshi Banerjee*, Zhen Qi, Penghui Lin, Marc O. Warmoes, Qiushi Sun, Joshua M. Mitchell, Ye Yang, Teresa W.-M. Fan, Richard M. Higashi, Andrew N. Lane, Hunter N. B. Moseley, Sidney W. Whiteheart, and Qingjun Wang. "Platelet metabolism is critical for modulating normal hemostasis and controlling pathogenic thrombosis - Is it a key to platelet hyper-reactivity in metabolic syndrome?" 7th Annual Barnstable Obesity and Diabetes Research Day, Lexington, KY (2017).

115) Yekaterina Y. Zaytseva, Piotr Rychahou, Anh-Thu Le, Robert M. Flight, Timothy Scott, Jennifer Harris, Sally Hodges, Brent Hallahan, Dana Napier, Jinpeng Liu, Chi Wang, Andrew Morris, Ji Tae Kim, Sivakumaran Theru Arumugam, Andrew Lane, Teresa Fan, Hunter N.B. Moseley, Tianyan Gao, Heidi Weiss, Eun Lee, Timothy Heuer George Kemble, and B. Mark Evers. "Activation of Akt pathway and autophagy promotes resistance to FASN inhibition in colorectal cancer patient-derived xenograft models", Markey Cancer Center Research Day, Lexington, KY (2017).

114) Eugene W. Hinderer III and Hunter N.B. Moseley. "GOcats: A tool for categorizing GO into subgraphs of user-defined emergent concepts", Markey Cancer Center Research Day, Lexington, KY (2017).

113) Sen Yao, Robert M. Flight, Eric C. Rouchka, and Hunter N.B. Moseley. "Aberrant coordination geometries discovered in the most abundant metalloproteins", Markey Cancer Center Research Day, Lexington, KY (2017).

112) Joshua M. Mitchell, Robert M. Flight, Qingjun Wang, Andrew N. Lane, Hunter N.B. Moseley. "Detection and Handling of Spectral Artefacts in Fourier Transform Mass Spectra from Metabolomics Experiments", Markey Cancer Center Research Day, Lexington, KY (2017).

111) Jinpeng Liu*, Thilakam Murali*, Chunming Liu, Tianxin Yu, Sivakumaran Theru Arumugam, Hunter Moseley, Igor Jouline, Heidi L. Weiss, Eric Durbin, Sally Ellingson, Jinze Liu, Brent J. Hallahan, Craig Horbinski, Dave Fardo, Chi Wang, Susanne M. Arnold. "Cancer Pathway Analyses Based on Alterations in Squamous Cell Lung Cancer in Appalachian Kentucky", Markey Cancer Center Research Day, Lexington, KY (2017).

110) Yu Zhong, Kabhilan Mohan, Jinpeng Liu, Ahmad Al-Attar, Robert M. Flight, Eugene Hinderer, Joshua Mitchell, Zhen Qi, Qiushi Sun, Marc O. Warmoes, Rahul R. Deshpande, Huijuan Liu, Kyung Sik Jung, Jacob Roney, Mihail I. Mitov, Nianwei Lin, D. Allan Butterfield, Shuyan Lu, Jinze Liu, Hunter N. B. Moseley, Andrew N. Lane, Teresa W. M. Fan, Mark E. Kleinman, and Qingjun Wang. "Loss of juvenile neuronal ceroid lipofuscinosis disease gene CLN3 in retinal pigment epithelium leads to metabolic impairment and autophagy induction", Markey Cancer Center Research Day, Lexington, KY (2017).

109) Sen Yao, Robert M. Flight, Eric C. Rouchka, and Hunter N.B. Moseley. "Aberrant coordination geometries discovered in the most abundant metalloproteins", 6th Bluegrass Molecular Biophysics Symposium, Lexington, KY (2017).

108) Eugene W. Hinderer III and Hunter N.B. Moseley. "GOcats: A tool for categorizing GO into subgraphs of user-defined emergent concepts", 6th Bluegrass Molecular Biophysics Symposium, Lexington, KY (2017).

107) Sen Yao, Robert M. Flight, Eric C. Rouchka, and Hunter N.B. Moseley. "Aberrant coordination geometries discovered in the most abundant metalloproteins", 16th Annual UT/KBRIN Bioinformatics Summit, Montgomery Bell State Park, TN (2017).

106) Andrey Smelter, Xi Chen, Eric C. Rouchka, and Hunter N.B. Moseley. "Registration and grouping algorithms in protein NMR derived peak lists and their application in protein NMR reference correction", 16th Annual UT/KBRIN Bioinformatics Summit, Montgomery Bell State Park, TN (2017).

105) Andrey Smelter, Morgan Astra, and Hunter N.B. Moseley. "A Fast and Efficient Python Library for Interfacing with the Biological Magnetic Resonance Data Bank", 16th Annual UT/KBRIN Bioinformatics Summit, Montgomery Bell State Park, TN (2017).

104) Jinpeng Liu*, Thilakam Murali*, Chunming Liu, Tianxin Yu, Sivakumaran Theru Arumugam, Hunter Moseley, Igor Jouline, Heidi L. Weiss, Eric Durbin, Sally Ellingson, Jinze Liu, Brent J. Hallahan, Craig Horbinski, Dave Fardo, Chi Wang, Susanne M. Arnold. "Cancer Pathway Analyses Based on Alterations in Squamous Cell Lung Cancer in Appalachian Kentucky", 16th Annual UT/KBRIN Bioinformatics Summit, Montgomery Bell State Park, TN (2017).

103) Eugene W. Hinderer III and Hunter N.B. Moseley. "GOcats: A tool for categorizing GO into subgraphs of user-defined emergent concepts", 16th Annual UT/KBRIN Bioinformatics Summit, Montgomery Bell State Park, TN (2017).

102) Joshua M. Mitchell, Robert M. Flight, Qingjun Wang, Andrew N. Lane, Hunter N.B. Moseley. "Detection and Handling of Spectral Artefacts in Fourier Transform Mass Spectra from Metabolomics Experiments", 16th Annual UT/KBRIN Bioinformatics Summit, Montgomery Bell State Park, TN (2017).

101) Xi Chen, Andrey Smelter, and Hunter N.B. Moseley. "Protein NMR reference correction: a statistical solution to an analytical problem", 16th Annual UT/KBRIN Bioinformatics Summit, Montgomery Bell State Park, TN (2017).

100) Andrey Smelter, Xi Chen, Eric C. Rouchka, and Hunter N.B. Moseley. "Registration and grouping algorithms in protein NMR derived peak lists and their application in protein NMR reference correction", 61st Annual Biophysical Society Meeting, New Orleans, LA (2017).

99) Jinpeng Liu*, Thilakam Murali*, Chunming Liu, Tianxin Yu, Sivakumaran Theru Arumugam, Hunter Moseley, Igor Jouline, Heidi L. Weiss, Eric Durbin, Sally Ellingson, Jinze Liu, Brent J. Hallahan, Craig Horbinski, Dave Fardo, Chi Wang, Susanne M. Arnold. "Cancer Pathway Analyses Based on Alterations in Squamous Cell Lung Cancer in Appalachian Kentucky", CCTS Spring Conference, Lexington, Kentucky (2017).

98) Joshua M. Mitchell, Robert M. Flight, Qingjun Wang, Andrew N. Lane, Hunter N.B. Moseley. "Detection and Handling of Spectral Artefacts in Fourier Transform Mass Spectra from Metabolomics Experiments", CCTS Spring Conference, Lexington, Kentucky (2017).

97) Yu Zhong, Kabhilan Mohan, Jinpeng Liu, Ahmad Al-Attar, Robert Flight, Yung Sil Jung, Mihail Mitov, D. Allan Butterfield, Hunter Moseley, Jinze Liu, Teresa Fan, Mark Kleinman, and Qingjun Wang. "Loss of Juvenile Neuronal Ceroid Lipofuscinosis (JNCL) disease gene CLN3 in retinal pigment epithelium leads to metabolic impairment and autophagy induction", Keystone Symposium: Autophagy Network Integration in Health and Disease (B2), Copper Mountain, CO (2017).

96) Xi Chen and Hunter N.B. Moseley. "Protein NMR Reference Correction: A statistical approach for an old problem", MidWest SAS Users Group 27th Annual Conference, Cincinnati, OH (2016).

95) Joshua M. Mitchell, Robert M. Flight, and Hunter N. B. Moseley. "Detection and Handling of Spectral Artefacts in Fourier Transform Mass Spectra of Metabolomics Experiments" 2016 NIH common Fund Metabolomics Program Annual Meeting, Bethesda, MD (2016).

94) Sen Yao, Robert M. Flight, Eric C. Rouchka, and Hunter N.B. Moseley. "Aberrant coordination geometries models discovered in top abundant metalloproteins" Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2016).

93) Xi Chen and Hunter N.B. Moseley. "Protein NMR Reference Correction: A statistical approach for an old problem", Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2016).

92) Robert M Flight and Hunter NB Moseley. "Visualizing the effects of data transformations on errors" Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2016).

91) David R. Henderson and Hunter N.B. Moseley. "1H-NMR Metabolite Assignment through Deduction and Induction Cycles (MADIC)" Markey Cancer Center Research Day, Lexington, KY (2016).

90) Thilakam Murali, Joshua M. Mitchell, William A. McCollam, and Hunter N.B. Moseley. "Graph database implementation of atom-resolved, KEGG-derived metabolic networks" Markey Cancer Center Research Day, Lexington, KY (2016).

89) Joshua M. Mitchell and Hunter N. B. Moseley. "Biochemically Aware Substructure Search (BASS) - an algorithm for finding biochemically relevant chemical subgraphs" Markey Cancer Center Research Day, Lexington, KY (2016).

88) David R. Henderson and Hunter N.B. Moseley. “1H-NMR Metabolite Assignment through Deduction and Induction Cycles (MADIC)” 5th Annual Bluegrass Biophysical Symposium, Lexington, KY (2016).

87) Xi Chen and Hunter N.B. Moseley. “Protein NMR Reference Correction: A statistical approach for an old problem”, 5th Annual Bluegrass Biophysical Symposium, Lexington, KY (2016).

86) Joshua M. Mitchell and Hunter N. B. Moseley. “Biochemically Aware Substructure Search (BASS) - an algorithm for finding biochemically relevant chemical subgraphs” AOA Groves Memorial Research Day, Lexington, KY (2016).

85) Robert M Flight and Hunter NB Moseley. “Visualizing the effects of data transformations on errors” 15th Annual UT-KBRIN Bioinformatics Summit, Cadiz, KY (2016).

84) Sen Yao, Robert M. Flight, Eric C. Rouchka, Hunter N.B. Moseley. “Aberrant coordination geometries models discovered in top abundant metalloproteins” 15th Annual UT-KBRIN Bioinformatics Summit, Cadiz, KY (2016).

83) David R. Henderson and Hunter N.B. Moseley. “1H-NMR Metabolite Assignment through Deduction and Induction Cycles (MADIC)” 15th Annual UT-KBRIN Bioinformatics Summit, Cadiz, KY (2016).

82) Joshua M. Mitchell and Hunter N. B. Moseley. “Biochemically Aware Substructure Search (BASS) - an algorithm for finding biochemically relevant chemical subgraphs” 15th Annual UT-KBRIN Bioinformatics Summit, Cadiz, KY (2016).

81) Eugene W. Hinderer and Hunter N.B. Moseley. “GOcats: A tool for the automatic categorization of Gene Ontology terms into sub-graphs representing user-defined emergent concepts” 15th Annual UT-KBRIN Bioinformatics Summit, Cadiz, KY (2016).

80) Andrey Smelter, Eric C. Rouchka, and Hunter N.B. Moseley. “Automated Assignment of Magic-Angle-Spinning Solid-State Protein NMR Spectra” 15th Annual UT-KBRIN Bioinformatics Summit, Cadiz, KY (2016).

79) Thilakam Murali, Joshua M. Mitchell, William A. McCollam, and Hunter N.B. Moseley. “Graph database implementation of atom-resolved, KEGG-derived metabolic networks” 15th Annual UT-KBRIN Bioinformatics Summit, Cadiz, KY (2016).

78) Richard M. Higashi, Andrew N. Lane, Sadakatali Gori, Pawel K. Lorkiewicz, Sébastien Laulhé, Michael H. Nantz, Hunter N.B. Moseley, Sengodagounder Arumugam, and Teresa W.-M. Fan. “Analysis of chemoselective derivatives of carbonyl and thiol metabolites in complex mixtures by HRMS and NMR” Pacifichem, Honolulu, Hawaii (Dec 2015).

77) Timothy Fahrenholz, Richard Higashi, Hunter Moseley, Robert Flight, Maria Bruno, Rahul Deshpande, Ye Yang, Yan Zhang, Franceska Mehmeti, Andrew Lane, Teresa Fan. “Using Exosome Lipid Profiles from Early Stage Lung Cancer Patients Before and After Surgery to Evaluate Response”, Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2015).

76) Xi Chen and Hunter N.B. Moseley. “Breaking the Chicken-Egg Dilemma in Validating Protein NMR Referencing”, Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2015).

75) Eugene W. Hinderer and Hunter N.B. Moseley. “Extracting subcellular localization from Gene Ontology”, Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2015).

74) Joshua M. Mitchell and Hunter N.B. Moseley. “Biochemically Aware Substructure Search (BASS) - an algorithm for finding biochemically relevant chemical subgraphs”, Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2015).

73) Robert M. Flight and Hunter N.B. Moseley. “Characterization and Visualization of Error in Omics Technologies”, Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2015).

72) William A. McCollam, Joshua M. Mitchell, and Hunter N.B. Moseley. “A graph database atom-resolved implementation of KEGG metabolic pathways”, Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2015).

71) Teresa W.-M. Fan, Andrew N. Lane, Sengodagounder Arumugam, Pawel Lorkiewicz, Sadakatali S. Gori, Sebastien Laulhe, Michael Nantz, Hunter N.B. Moseley, Richard Higashi. “Chemoselective detection of carbonyl and thiol metabolite enable their analysis in complex mixtures by HRMS and NMR”, Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2015).

70) Xi Chen and Hunter N.B. Moseley. “Breaking the Chicken-Egg Dilemma in Validating Protein NMR Referencing”, 4th Annual Bluegrass Biophysical Symposium, Lexington, KY (2015).

69) David R. Henderson and Hunter N.B. Moseley. “Assignment of Metabolites via 1H-NMR Spectral Peak Lists”, 4th Annual Bluegrass Biophysical Symposium, Lexington, KY (2015).

68) Eugene W. Hinderer and Hunter N.B. Moseley. “Extracting subcellular localization from Gene Ontology”, 4th Annual Bluegrass Biophysical Symposium, Lexington, KY (2015).

67) Joshua M. Mitchell and Hunter N.B. Moseley. “Biochemically Aware Substructure Search (BASS) - an algorithm for finding biochemically relevant chemical subgraphs”, Bluegrass Biophysical Symposium, Lexington, KY (2015).

66) Robert M. Flight and Hunter N.B. Moseley. “categoryCompare v2.0: Easier, More Versatile Annotation-Based Meta-Analysis”, Markey Cancer Center Research Day, Lexington, KY (2015).

65) Robert M. Flight and Hunter N.B. Moseley. “Characterization and Visualization of Error in Omics Technologies”, Markey Cancer Center Research Day, Lexington, KY (2015).

64) William A. McCollam, Joshua M. Mitchell, and Hunter N.B. Moseley. “A graph database atom-resolved implementation of KEGG metabolic pathways”, Markey Cancer Center Research Day, Lexington, KY (2015).

63) Joshua M. Mitchell and Hunter N.B. Moseley. “Biochemically Aware Substructure Search (BASS) - an algorithm for finding biochemically relevant chemical subgraphs”, Markey Cancer Center Research Day, Lexington, KY (2015).

62) William A. McCollam, Joshua M. Mitchell, and Hunter N.B. Moseley. “A graph database atom-resolved implementation of KEGG metabolic pathways”, 11th International Conference of the Metabolomics Society, San Francisco, CA (2015).

61) Yvonne M. Johnson, Thilakam Murali, and Hunter N.B. Moseley. “Merging Protein-Protein Interaction Networks with Atom-Resolved Metabolic Networks”, KY-WV LSAMP Alliance-Wide Conference, Lexington, KY (2015).

60) Sen Yao, Robert M. Flight, Eric C. Rouchka, Hunter N.B. Moseley. “A less biased analysis of metalloproteins reveals novel zinc coordination geometries”, The Hitchhiker's Guide to the Protein Galaxy, West Lafayette, IN (2015).

59) Tamas L. Nagy, Stacy R. Webb, Rebecca E. Dutch, Hunter Moseley. “Characterization of the Structural Constraints of Viral Type I Fusion Proteins”, 14th Annual UT-KBRIN Bioinformatics Summit, Paris Landing, TN (2015).

58) Sen Yao, Robert M. Flight, Eric C. Rouchka, Hunter N.B. Moseley. “A less biased analysis of metalloproteins reveals novel zinc coordination geometries”, 14th Annual UT-KBRIN Bioinformatics Summit, Paris Landing, TN (2015).

57) Andrey Smelter, Indraneel Reddy, Eric C. Rouchka, and Hunter N.B. Moseley. “Automated Assignment of Magic-Angle-Spinning Solid-State Protein NMR Spectra”, 14th Annual UT-KBRIN Bioinformatics Summit, Paris Landing, TN (2015).

56) Eugene W. Hinderer and Hunter N.B. Moseley. “Extracting subcellular localization from Gene Ontology”, 14th Annual UT-KBRIN Bioinformatics Summit, Paris Landing, TN (2015).

55) David R Henderson and Hunter N.B. Moseley. “Automated, iterative and scored assignment of metabolites via [1H]-NMR Spectral Peak Lists”, 14th Annual UT-KBRIN Bioinformatics Summit, Paris Landing, TN (2015).

54) William A. McCollam, Joshua M. Mitchell, and Hunter N.B. Moseley. “A graph database atom-resolved implementation of KEGG metabolic pathways”, 14th Annual UT-KBRIN Bioinformatics Summit, Paris Landing, TN (2015).

53) Joshua M. Mitchell, Teresa W.-M. Fan, Andrew N. Lane, and Hunter N.B. Moseley. “Development and in silico Evaluation of Large-Scale Metabolite Identification Methods Using Functional Group Detection for Metabolomics”, 249th American Chemical Society National Meeting & Exposition, Denver, Colorado (2015).

52) Joshua M. Mitchell, Teresa W.-M. Fan, Andrew N. Lane, and Hunter N.B. Moseley. “Development and in silico Evaluation of Large-Scale Metabolite Identification Methods Using Functional Group Detection for Metabolomics”, Experimental Biology 2015, Boston, Massachusetts (2015).

51) Joshua M. Mitchell, Teresa W.-M. Fan, Andrew N. Lane, and Hunter N.B. Moseley. “Development and in silico Evaluation of Large-Scale Metabolite Identification Methods Using Functional Group Detection for Metabolomics”, American Society for Biochemistry and Molecular Biology Annual Meeting, Boston, Massachusetts (2015).

50) Stacy R. Webb, Tamas Nagy, Hunter N.B. Moseley, Mike Fried, & Rebecca E. Dutch. “Fusion protein TM-TM interactions: Modulators of pre-fusion protein stability”, Physical Virology Gordon Research Conference, Ventura, California (2015).

49) Joshua M. Mitchell, Teresa W-.M. Fan, Andrew N. Lane, Richard M. Higashi, and Hunter N.B. Moseley. “Development of Large-Scale Metabolite Identification Methods for Metabolomics”, NIH Common Fund Annual Meeting – Metabolomics, Triangle, NH (2014).

48) Joshua M. Mitchell, Teresa W-.M. Fan, Andrew N. Lane, Richard M. Higashi, and Hunter N.B. Moseley. “Development of Large-Scale Metabolite Identification Methods for Metabolomics”, International Conference of the Metabolomics Society, Tsuruoka, Japan (2014).

47) Andrew N. Lane, Sengodagounder Arumugam, Pawel Lorkiewicz, Richard Higashi, Sebastien Laulhe, Michael Nantz, Hunter N.B. Moseley, Teresa W.-M. Fan. “Chemoselective detection of carbonyl compounds in metabolite mixtures by NMR”, Markey Cancer Center Research Day, Lexington, KY (2014).

46) Joshua M. Mitchell, Teresa W-.M. Fan, Andrew N. Lane, Richard M. Higashi, and Hunter N.B. Moseley. “Development of Large-Scale Metabolite Identification Methods for Metabolomics”, Markey Cancer Center Research Day, Lexington, KY (2014).

45) Joshua M. Mitchell, Teresa W-.M. Fan, Andrew N. Lane, Richard M. Higashi, and Hunter N.B. Moseley. “Development of Large-Scale Metabolite Identification Methods for Metabolomics”, Bluegrass Biophysical Symposium, Lexington, KY (2014).

44) Tamas L. Nagy, Rebecca E. Dutch, Hunter Moseley. “Investigating the Expanding Role of Transmembrane Domains in Enveloped Virus Entry.” 13th Annual UT-KBRIN Bioinformatics Summit, Cadiz, KY (2014).

43) Sen Yao, Robert M. Flight, Hunter N.B. Moseley. “Coordination Characterization of Zinc Metalloproteins.” 13th Annual UT-KBRIN Bioinformatics Summit, Cadiz, KY (2014).

42) Joshua M. Mitchell, Teresa W-.M. Fan, Andrew N. Lane, Richard M. Higashi, and Hunter N.B. Moseley. “Development of Large-Scale Metabolite Identification Methods for Metabolomics.” 13th Annual UT-KBRIN Bioinformatics Summit, Cadiz, KY (2014).

41) Tamas Nagy, Rebecca E. Dutch, and Hunter N.B. Moseley. “Investigating the Expanding Role of Transmembrane Domains in Enveloped Virus Entry.” National Conference on Undergraduate Research, Lexington, KY (2014).

40) Hunter N.B. Moseley. “Scaffolded Explicit Revision as a Practical Framework to Promote Effective Student Effort in Content-Rich Courses.” 2013 I2A Institute: Sharing the Impact of Critical Thinking, Louisville, KY (2013).

39) Sen Yao, Tim D. Cook, and Hunter N.B. Moseley. “Coordination Characterization of Zinc Metalloproteins”, UT-ORNL-KBRIN Bioinformatics Summit, Buchanan, TN (2013).

38) Joshua M. Mitchell and Hunter N.B. Moseley. “Computational Tools for the Identification of Detectable Uncharacterized Derivatized Metabolites within the Context of Known Metabolic Networks”, UT-ORNL-KBRIN Bioinformatics Summit, Buchanan, TN (2013).

37) Pawel K. Lorkiewicz, Richard M. Higashi, Stephanie J. Mattingly, Michael H. Nantz, Hunter N. B. Moseley, Andrew N. Lane, Teresa W-M. Fan. “Chemoselective capture of carbonyl-containing metabolites for stable isotope resolved metabolomic analysis of crude cell extracts by FTICR-MS”, The Institute for Molecular Diversity & Drug Design (IMD^3) 15th Annual Symposium, Louisville, KY (2013).

36) Andrew N. Lane, Sengodagounder Arumugam, Pawel Lorkiewicz, Richard M. Higashi, Sebastien Laulhe, Michael Nantz, Hunter N.B. Moseley, and Teresa W-M. Fan. “Chemoselective detection of carbonyl compounds in metabolite mixtures by NMR”, Keystone Symposium: Frontiers of NMR in Biology, Snowbird, UT (2013).

35) Joshua M. Mitchell and Hunter N.B. Moseley. “Computational tools for the identification of detectable uncharacterized derivatized metabolites within the context of known metabolic networks”, James Graham Brown Cancer Center 11th Annual Retreat, Louisville, Kentucky (2012).

34) Andrew N. Lane, Sengodagounder Arumugam, Pawel Lorkiewicz, Richard M. Higashi, Sebastien Laulhe, Michael Nantz, Hunter N.B. Moseley, and Teresa W-M. Fan. "Chemoselective detection of carbonyl compounds in metabolite mixtures by NMR", James Graham Brown Cancer Center 11th Annual Retreat, Louisville, KY (2012).

33) Alex Belshoff, Michael Bousamra, Teresa W-M. Fan, Richard M. Higashi, Andrew N. Lane, and Hunter N.B. Moseley. "Sodium Selenite alters metabolic pathways involved in UDP-GlcNAc synthesis in human lung cancer models", James Graham Brown Cancer Center 11th Annual Retreat, Louisville, KY (2012).

32) Eugene W. Hinderer and Hunter N.B. Moseley. "Retrieval of Enzyme Category and Subcellular Localization for Use in Metabolic Network Analysis", Kentucky Academy of Science Annual Meeting, Richmond, Kentucky (2012). 1st place undergraduate poster award.

31) Alex Belshoff, Michael Bousamra, Teresa W-M. Fan, Richard M. Higashi, Andrew N. Lane, and Hunter N.B. Moseley. "Sodium Selenite alters metabolic pathways involved in UDP-GlcNAc synthesis in human lung cancer models", Research Louisville, Louisville, KY (2012).

30) Joshua M. Mitchell and Hunter N.B. Moseley. "Developing computational tools for metabolite identification in ultra-high resolution mass spectrometry data," Research Louisville, Louisville, Kentucky (2012). 2nd place undergraduate poster award.

29) Joshua M. Mitchell and Hunter N.B. Moseley. "Developing computational tools for metabolite identification in ultra-high resolution mass spectrometry data," University of Louisville Undergraduate Research Symposium, Louisville, Kentucky (2012).

28) Sen Yao, Timothy D. Cook, Hunter N.B. Moseley. "Coordination characterization and function annotation trends of zinc metalloproteins," 11th Annual UT-ORNL-KBRIN Bioinformatics Summit, Louisville, Kentucky (2012).

27) Joshua M. Mitchell and Hunter N.B. Moseley. "Developing computational tools for metabolite identification in ultra-high resolution mass spectrometry data," 11th Annual UT-ORNL-KBRIN Bioinformatics Summit, Louisville, Kentucky (2012).

26) William J. Carreer and Hunter N.B. Moseley. "Correcting for the effects of natural abundance in stable isotope resolved metabolomics experiments involving multiple simultaneous isotopic labels and ultra-high resolution mass spectrometry," 11th Annual UT-ORNL-KBRIN Bioinformatics Summit, Louisville, Kentucky (2012).

25) Joshua M. Mitchell, Rima R. Patel, Rodney Folz Jr, Andrew McCollam, and Hunter N.B. Moseley. "Developing Computational Tools for Molecular Comparison and Metabolic Placement of Detectable Uncharacterized Metabolites," James Graham Brown Cancer Center 10th Annual Retreat, Louisville,KY (2011).

24) Anne Le, Max Hamaker, Joseph Barbi, Haixia Zhang, Lisa J. Zimmerman, Daniel C. Liebler, Robbert J.C. Slebos, Hunter Moseley, Richard M. Higashi, Andrew Lane, Teresa W. M. Fan and Chi V. Dang. "Myc induction of hypoxic glutamine metabolism and a glucose-independent TCA cycle in human B lymphocytes," AACR Metabolism and Cancer Conference, Baltimore, MD (2011)

23) Alex Belshoff, Andrew N. Lane, Hunter N.B. Moseley, Michael Bousamra, Richard M. Higashi, and Teresa W-M. Fan. "An Investigation of UDP-GlcNAc Synthesis in Human Lung Cancer with Perturbations by Selenium Compound Treatment", Research Louisville, Louisville, KY (2011).

22) Hunter N. B. Moseley, Lindsay J. Sperling, and Chad M. Rienstra. "Development of automated protein resonance assignment methods for magic angle spinning solid-state NMR," Gordon Research Conference: Computational Aspects of Biomolecular NMR, Lucca, Italy (2011).

21) Hunter N. B. Moseley, Lindsay J. Sperling, and Chad M. Rienstra. "Development of automated protein resonance assignment methods for magic angle spinning solid-state NMR," 10th Annual UT-ORNL-KBRIN Bioinformatics Summit, Memphis, Tennessee (2011).

20) Patrick Mullaney, Abigail Hoskins, and Hunter N.B. Moseley. "A Faster, More Efficient Library for Interfacing with the BMRB," 10th Annual UT-ORNL-KBRIN Bioinformatics Summit, Memphis, Tennessee (2011).

19) Tim D. Cook, Yao Sen, and Hunter N.B. Moseley. "Developing Computational Tools to Study Zinc's Functional Role in Proteins," Posters-at-the-Capitol, Lexington, Kentucky (2011).

18) Joshua M. Mitchell, Rima R. Patel, Rodney Folz Jr., and Hunter N.B. Moseley. “Developing Computational tools for Metabolite Molecular Comparison and Search,” Posters-at-the-Capitol, Lexington, Kentucky (2011).

17) Hunter N.M. Moseley, Alex C. Belshoff, Richard M. Higashi, Teresa W-M. Fan, Andrew N. Lane. “Stable Isotope Resolved Metabolomics (SIRM) of UDP-GlcNAc and UDP-GalNAc Metabolism in Prostate Cancer,” James Graham Brown Cancer Center 9th Annual Retreat, Louisville,KY (2010).

16) Hunter N.B. Moseley, N. Riaz, J.M. Aramini, T.A. Szyperski, and G.T. Montelione. “NMR Automation: From FIDS to Resonance Assignments using Peak Pattern Recognition of GFT NMR Data,” Gordon Research Conference: Computational Aspects of Biomolecular NMR, Aussois, France (2006).

15) Hunter N.B. Moseley, Y.J. Huang, M.C. Baran, G. Sahota, D.A. Snyder, N. Riaz, D. Monleon, M. Bayro, J.M. Aramini, G.V.T. Swapna, T.A. Szyperski, and G.T. Montelione. “From Spectra to Resonance Assignments to Structure: Efforts in Automation of Protein NMR Data Analysis,” Intl. Conf. on Structural Genomics, Washington, DC (2004).

14) Hunter N.B. Moseley, N. Riaz, J.M. Aramini, T.A. Szyperski, and G.T. Montelione. “A Generalized Approach to Automated NMR Peak List Editing: Application to Reduced Dimensionality Triple Resonance Spectra,” Gordon Research Conference: Computational Aspects of Biomolecular NMR, Ventura, CA (2004).

13) Hunter N.B. Moseley, G. Sahota, M. Kiriyeva, G.V.T. Swapna, T.A. Szyperski, and G.T. Montelione. "AutoPeak/AutoAssign: An Expert System for Automated Analysis of Protein Resonance Assignments,” Keystone Conference: Frontiers of NMR in Molecular Biology VIII, 130, Taos, NM (2003).

12) Hunter N.B. Moseley, G. Sahota, M. Kiriyeva, G.V.T. Swapna, T.A. Szyperski, and G.T. Montelione. "AutoAssign: An Expert System for Automated Analysis of Protein Resonance Assignments,” 43rd Exp. NMR Conf., Asilomar, CA (2002).

11) Hunter N.B. Moseley, G. Sahota, M. Kiriyeva, G.V.T. Swapna, T.A. Szyperski, and G.T. Montelione. "AutoAssign: An Expert System for Automated Analysis of Protein Resonance Assignments,” Keystone Conference: Structural Genomics: From Gene Sequence to Function, Breckenridge, Colorado (2002).

10) Hunter N.B. Moseley, G. Sahota, M. Kiriyeva, G.V.T. Swapna, T.A. Szyperski, and G.T. Montelione. "AutoAssign: An Expert System for Automated Analysis of Protein Resonance Assignments,” Gordon Research Conference: Computational Aspects of Biomolecular NMR, Lucca, Italy (2001).

9) Hunter N.B. Moseley, G. Sahota, M. Kiriyeva, G.V.T. Swapna, T.A. Szyperski, and G.T. Montelione. "AutoAssign: An Expert System for Automated Analysis of Protein Resonance Assignments," Keystone Symposium: Frontiers of NMR in Molecular Biology VII (2001).

8) Hunter N.B. Moseley, D.E. Zimmerman, G. Sahota, M. Kiriyeva, C.A. Kulikowski, G. Armhold, and G.T. Montelione. "AutoAssign: An Expert System for Automated Analysis of Protein Resonance Assignments," 41st Exp. NMR Conf., Asilomar, CA (2000).

7) Hunter N.B. Moseley, D.E. Zimmerman, C.A. Kulikowski, G. Armhold, and G.T. Montelione. “AutoAssign: An Expert System for Automated Analysis of Protein Resonance Assignments,” 40th Exp. NMR Conf., Asilomar, CA (1999).

6) Hunter N.B. Moseley, K. Scheffler, N.R. Krishna, and T. Peters. 6th Annual F. L. Suddath Memorial Symposium, Atlanta, GA (1998). 1st place graduate student poster award.

5) Hunter N.B. Moseley, W. Lee, C.H. Arrowsmith, and N.R. Krishna. 38th Exp. NMR Conf., Orlando, FL (1997).

4) Hunter N.B. Moseley and N.R. Krishna. 4th Annual F L. Suddath Memorial Symposium, Atlanta, GA (1996). 2nd place graduate student poster award.

3) Hunter N.B. Moseley, E.V. Curto, and N.R. Krishna. "Complete Relaxation and Conformational Exchange Matrix (CORCEMA) Analysis of NOESY Spectra: Applications to Transferred NOESY and Protein Folding Studies," *Biophysical Journal* 68, A421 (1995).

2) Hunter N.B. Moseley, E.V. Curto, and N.R. Krishna. An International Symposium: NMR as a Structural Tool for Macromolecules, Indianapolis, IN (1994).

1) Hunter N.B. Moseley, E.V. Curto, and N.R. Krishna. 35th Exp. NMR Conf., Asilomar, CA (1994).

Research Support

Current Support

NIH: 1P01CA163223-01A1 Fan/Lane/Yan(PIs) 03/01/2013 to 02/28/2018
Systems Biochemistry in Lung Cancer: toward a mechanistic understanding of NSCLC
Goals: The program comprises three project areas utilizing stable isotope resolved metabolomics to gain a mechanistic understanding of NSCLC in situ. The projects combine cell culture, animal models and human subjects to define the influence of the tumor microenvironment on cancer progression.
Role: Co-I ($553,602 direct)

NSF 1252893 Moseley(PI) 07/01/2013 to 06/30/2018
CAREER:Developing Biochemoinformatics Tools for Large Scale Metabolomics Applications
Goals: Develop a web-based data analysis platform for stable isotope-resolved metabolomics datasets and omics integration. Develop and test scaffolded explicit revision methodologies that promote effective student effort in content-rich science courses.
Role: PI ($760,657 direct)

NIH: 1U24DK097215-01A1 Higashi/Fan/Lane/Moseley(PIs) 09/11/2013 to 08/31/2018
Resource Center for Stable Isotope-Resolved Metabolomics
Goals: To conduct ring trials which will ultimately lead to the establishment of a set of common standards for the entire metabolomic process, from sample acquisition and storage through metabolite extraction to data recording, reduction and analysis.
Role: PI ($881,220 direct)

NIH: 1R21CA205778-01 Wang/Moseley(PIs) 08/01/2016 to 07/31/2018
Statistical Detection and Biochemical Classification of Cancer Driver Mutation Patterns in Biological Networks
Goals: Develop and combine advance sequence variation analyses with complementary biological network analyses into a highly novel systems biology approach that will: i) detect sets of related mutations in driver regulatory/signaling pathways, ii) classify these pathways as stimulated, inhibited, or mixed with respect to their role in the tumor development process, and iii) predict direct metabolic outcomes of these perturbed pathways.
Role: PI ($128,200 direct)

NSF: ACI1626364 Zhang/Griffioen/Moseley/Payne(PIs) 07/01/2016 to 06/30/2019
MRI: Acquisition of the Kentucky Research Informatics Cloud (KyRIC)
Goals: Build a high memory node HPC resource for research.
Role: PI ($2,800,000 direct support is for instrumentation)

U54 TR001998-01 Kern(PI) 08/15/16 to 05/31/20
Kentucky Center for Clinical and Translational Science
Goals: The Biomedical Informatics Core of the University of Kentucky Center for Clinical and Translational Science (CCTS) will enhance the CCTS Enterprise Data Trust, operationalize and deploy informatics tools to augment translational research, promote data--supported team science locally and nationally, and train the clinical and translational research workforce. The BMI will adopt, customize and develop new tools and methods that will improve user experience and visualization of data through sophisticated approaches for complex data capture, integration, querying and analyses.
Role: Co-Director, Educational Programs (10% effort)

NIH P20 GM121327 (MPI: St. Clair, D.; Zhou, B.) 12/01/16 to 11/30/21
"University of Kentucky Center for Cancer and Metabolism"
Goals: To strengthen UK's cancer research enterprise by providing a thematically focused multidisciplinary infrastructure dedicated to defining the contribution of metabolism in the development and treatment of cancer.
Role: Co-Investigator for bioinformatics support (5% effort)

1P30ES026529 (PI: Shi, X) 04/01/17 to 03/31/22

"Center for Appalachian Research in Environmental Sciences"
Goals: The overarching goal of the Analytical Core is to improve the capacity, quality, efficiency and cost-effectiveness of environmental disease research at the University of Kentucky by providing researchers in the UK Center for Appalachian Research in Environmental Science with premium access to expert advice, consultation and technical support to develop and validate analytical methods using state-of- the-art technologies for studies spanning the range of environmental disease research interest areas represented in the center.
Role: Co-Leader, Analytical Core (10% effort)

Completed Research Support

NIH 1R03CA211835-01 Wang, Flight (MPI) 09/14/16 to 08/31/17
Differential Abundance Methods for Large Heterogeneous-Featured Metabolomics Datasets
Goals: New large metabolomics datasets have a variety of issues related to ambiguity in metabolite assignment, correspondence of measurements across samples, and redundancy of information. We are developing new computational methods to address these issues.
Role: Co-I ($40,000 direct)

NIH: 1R01ES022191-01 Fan/Higashi/Moseley/Nantz(PIs) 09/26/2012 to 06/30/2017
Integrated Chemoselective and Informatics Platform for Large-Scale Metabolomics
Goals: This project designs and synthesizes chemoselective reagents for targeting metabolites bearing specific functional groups, incorporating a permanent positive change and a stable isotope for increasing sensitivity and identification and quantification of classes of metabolites by mass spectrometry and NMR.
Role: PI ($324,298 direct)

DOE: DE-EM0000197 Kalbflesch/Rouchka (PIs) 01/01/2010 to 12/31/2011
DOE Grant to U of L for Bioinformatics and Computational Biology: $679,789 (direct)
Role: Co-I ($82,564 direct)

NIH: P20 RR016481S1 Cooper (PI) 09/17/2009 to 09/16/2011
Development of a Systems Biology Team: $675,676 (direct)
Role: Co-I ($40,164 direct)

NSF: 9974200 Moseley (PI) 10/01/99 to 09/30/01
NSF Postdoctoral Fellowship in Biological Informatics: $100,000 (direct)
Automatic Analysis of Protein NMR Spectra for High-Throughput NMR Structure Determination: A New Technique for the Human Proteome Project
Role: PI ($100,000 direct)