Hunter N. B. Moseley, 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 Bioinformatics, Computational Biology, & Systems Biochemistry Lab, Univ. of Kentucky
2022-present **Professor, Department of Molecular & Cellular Biochemistry, University of Kentucky**
2013-2022 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 & System for Ident. of Metabolites, U.S. patent 10,607,723B2, Univ. of Kentucky**
- Ontology-driven Annotation Enrichment Analysis, Univ. of Kentucky
- Regional electron density analysis, 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 84 publications, 44 as first/corresponding author, "h" index of 26, and 2800+ citations**
- **ORCID: 0000-0003-3995-5368, https://scholar.google.com/citations?hl=en&user=ctE_FZMAAAAJ**
- **Developed 30+ open-source codebases on GitHub: https://github.com/MoseleyBioinformaticsLab**
- **Associate Director, Institute for Biomedical Informatics, Univ. of Kentucky**
- **Co-Director, Biomedical Informatics Core,Ctr for Clinical & Translational Sciences, Univ. of Kentucky**
- **Member of the University of Kentucky Superfund Research Center**
- **Member of the Markey Cancer Center Molecular Tumor Board**
- Review Editor, *Frontiers in Molecular Sciences - Metabolomics*
- **Member of Editorial Board and Section Editor-in-Chief - *Metabolites***
- **Peer-reviewed grant proposals for both NSF and NIH as ad hoc panel reviewer on 18 sections.**
- **Peer-reviewed 80+ manuscripts for 30+ journals**
- **Given 59 oral presentations at various conferences, workshops, and universities.**

Teaching Experience

2015-present **Instructor for biomedical science courses IBS-611, BMI-633, BCH-401G-Honors, Univ. of Kentucky**
2009-2013 **Instructor for biochemistry courses CHEM 445, CHEM 547, CHEM 647, Univ. of Louisville**
2008-2013 Coordinator of Chemistry Dept Graduate Seminar Program (CHEM 695), Univ. 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

NSF: 2020026; Duration: 08/15/2020 to 7/31/2024; Role: PI ($1,163,869)

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.

Last Updated: 11/01/2023

Personal Statement

My formal education spans multiple disciplines including chemistry, mathematics, computer science, and biochemistry. I have over 25 years of experience in bioinformatics research, particularly in the development of automated analyses of nuclear magnetic resonance (NMR), mass spectrometry (MS), x-ray crystallographic, ontological, and next generation sequencing (NGS) data. This includes extensive expertise in algorithm development, mathematical modeling, and biophysical informatics. 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 am an Associate Director of the Institute for Biomedical Informatics at the University of Kentucky (UK). My lab has a strong history of developing open-source software tools that enable access of public repository data including the Biological Magnetic Resonance Bank (BMRB), worldwide Protein Data Bank (wwPDB), and the Metabolomics Workbench (MWbench). We also develop new methods in functional annotation enrichment and molecular interaction network analyses. 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 biological processes and 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. My lab provides bioinformatics and systems biology expertise for the analysis and interpretation of SIRM experiments. Our 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, we have used a moiety model analysis of SIRM mass spectrometer data to quantitate the relative importance of specific metabolic pathways in 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.

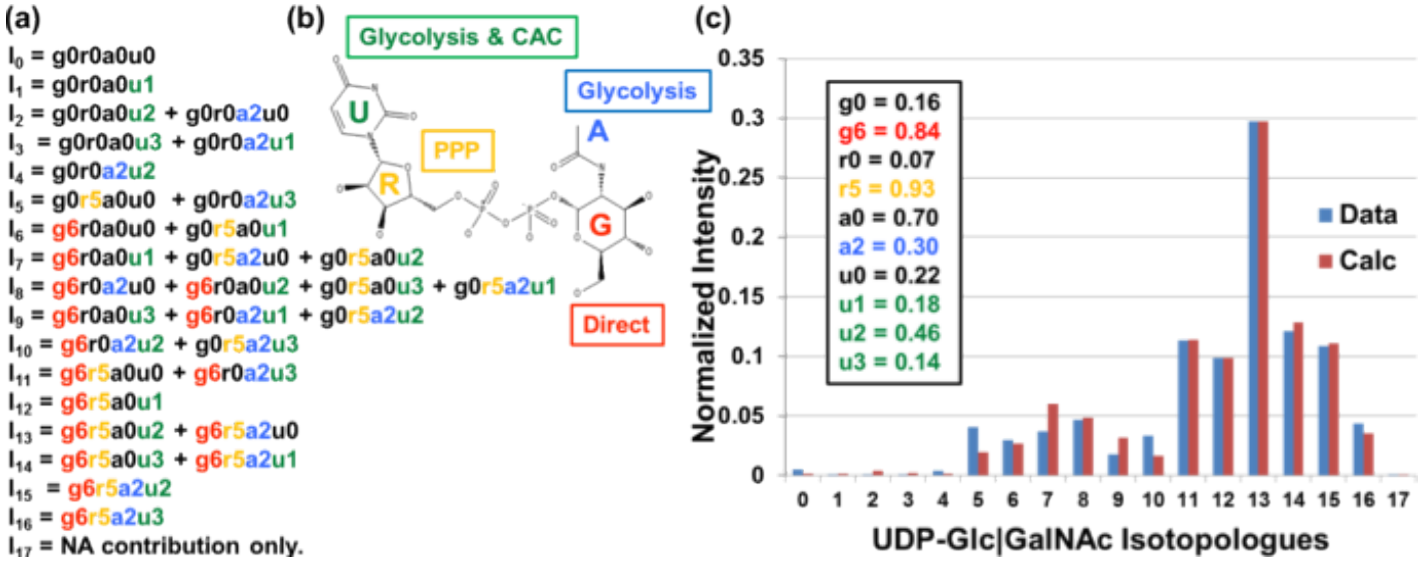


Figure 1: (a) Chemical substructure model representing the possible number of ^{13}C incorporation from $^{13}C_6$-Glc tracer into UDP-GlcNAc, accounting for the observed FT-ICR-MS isotopologue peaks. (b) Structure of UDP-GlcNAc annotated by its chemical substructures and their biosynthetic pathways 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: 112** (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: **74** (Google Scholar). PMCID: PMC3126751.
c) **Moseley HNB**. Error Analysis and Propagation in Metabolomics Data Analysis. ***Comput Struct Biotechnol J*** 4:2013. **Citations: 59** (Google Scholar). PMCID: PMC3647477.
d) 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: 31 (Google Scholar). PMCID: PMC4112935.
e) Mitchell JM, Flight RM, Wang QJ, Higashi RM, Fan TW, Lane AN, and **Moseley HNB**. New methods to identify high peak density artifacts in Fourier transform mass spectra and to mitigate their effects on high-throughput metabolomic data analysis. ***Metabolomics*** 14:125, 2018. Citations: 17 (Google Scholar). PMCID: PMC6153687
f) Jin H and **Moseley HNB**. Moiety Modeling Framework for Deriving Moiety Abundances from Mass Spectrometry Measured Isotopologues. ***BMC Bioinformatics*** 20:524, 2019. Citations: 7 (Google Scholar).
g) Mitchell JM, Flight RM, and **Moseley HNB**. Small Molecule Isotope Resolved Formula Enumeration: a Methodology for Assigning Isotopologues and Metabolites in Fourier Transform Mass Spectra. ***Analytical Chemistry*** 91:8933, 2019. Citations: 10 (Google Scholar). PMID: 31260262 DOI: 10.1021/acs.analchem.9b00748
h) Jin H and **Moseley HNB**. Robust Moiety Model Selection Using Mass Spectrometry Measured Isotopologues. ***Metabolites*** 10, 118 (2020). Citations: 8 (Google Scholar).
i) Christian D. Powell and **Hunter N.B. Moseley**. "The mwtab Python library for RESTful Access and Enhanced Quality Control, Deposition, and Curation of the Metabolomics Workbench Data Repository" ***Metabolites*** 11, 163 (2021). Citations: 10 (Google Scholar).
j) Huan Jin and **Hunter N.B. Moseley**. "Hierarchical Harmonization of Atom-Resolved Metabolic Reactions Across Metabolic Databases" ***Metabolites*** 11, 431 (2021). Citations: 3 (Google Scholar).
k) Robert M. Flight, Joshua M. Mitchell, and **Hunter N.B. Moseley**. "Scan-Centric, Frequency-Based Method for Characterizing Peaks from Direct Injection Fourier transform Mass Spectrometry Experiments" ***Metabolites*** 12, 515 (2022).

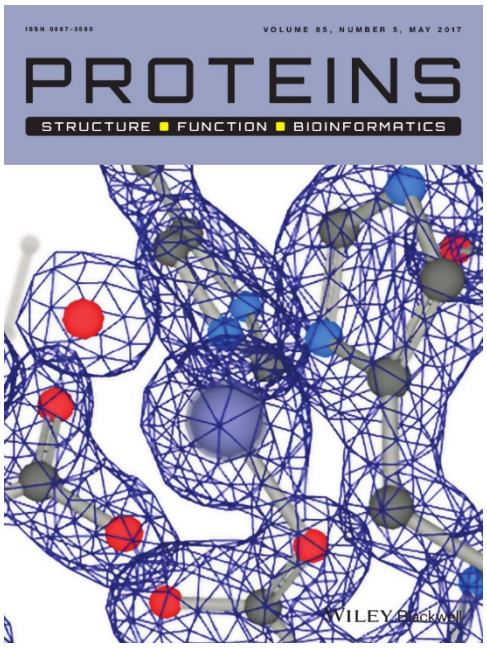
2. FAIR Data Sharing and Open Science. The FAIR (Findable, Accessible, Interoperable, and Reusable) Guiding Principles of Data Stewardship are a major part of Open Science, with the goal to make all research data, products, and knowledge openly accessible by anyone, both promoting collaborative research efforts. Our lab has developed a variety of open-source tools that promote the FAIRness of specific data repositories and knowledgebases. For example, we have developed the open-source mwtab Python library and package for FAIRer access to Metabolomics Workbench as well as the Metabolomics Workbench Validation website that provides weekly evaluations of all datasets made available in the repository with respect to consistency and conformity to repository deposition standards. Also, we have developed the open-source nmrstarlib Python library for FAIRer access of the Biological Magnetic Resonance Data Bank and the open-source kegg_pull Python package for FAIRer access of the Kyoto Encyclopedia of Gene and Genomes (KEGG). Moreover, we have extended and developed new data deposition standards when such standards were lacking or missing. For example, we developed the draft Minimum Information About Geospatial Information System (MIAGIS) standard for facilitating public deposition of geospatial information system (GIS) datasets as well as the open-source miagis Python package that facilitates generation of the MIAGIS deposition format. Recently, we developed the open-source MESSES Python package for comprehensive (meta)data capture, validation, and conversion into mwTab deposition format.

All Python packages are available through the Python Package Index (PyPI) and GitHub with extensive end-user documentation. Similarly, all R packages are available via GitHub and CRAN or Bioconductor with comprehensive end-user documentation vignettes. All GitHub repositories are organized and managed under the Moseley Bioinformatics and Systems Biology Lab organizational account: https://github.com/MoseleyBioinformaticsLab

a) Smelter A, **Astra, M**, **Moseley HNB**. A Fast and Efficient Python Library for Interfacing with the Biological Magnetic Resonance Data Bank. ***BMC Bioinformatics*** 18, 175 (2017). Citations: 13 (Google Scholar).
b) Andrey Smelter and Hunter N.B. Moseley. "A Python library for FAIRer access and deposition to the Metabolomics Workbench Data Repository" ***Metabolomics*** 14, 46 (2018). Citation: 7 (Google Scholar). PMCID: PMC5910482. https://doi.org/10.1007/s11306-018-1356-6

c) Christian D. Powell and **Hunter N.B. Moseley**. "The mwtab Python library for RESTful Access and Enhanced Quality Control, Deposition, and Curation of the Metabolomics Workbench Data Repository" ***Metabolites*** 11, 163 (2021). Citations: 4 (Google Scholar).
d) P. Travis Thompson, Christian D. Powell, and **Hunter N.B. Moseley**. "Academic Tracker: Software for Tracking and Reporting Publications Associated with Authors and Grants" ***PLOS One*** 17, e0277834 (2022). Citations: 1 (Google Scholar). https://doi.org/10.1371/journal.pone.0277834
e) Erik Huckvale and **Hunter N.B. Moseley**. "kegg_pull: a Software Package for the RESTful Access and Pulling from The Kyoto Encyclopedia of Gene and Genomes" ***BMC Bioinformatics*** 24, 78 (2023). Citations 2: (Google Scholar). https://doi.org/10.1186/s12859-023-05208-0
f) P. Travis Thompson, Sweta Ojha, Christian D. Powell, Kelly G. Pennell, and **Hunter N.B. Moseley**. "A proposed FAIR approach for disseminating geospatial information system maps" ***Scientific Data*** 10, 389 (2023). Citations: 1 (Google Scholar). https://doi.org/10.1038/s41597-023-02281-1
g) Rance Nault, Matthew C. Cave, Gabriele Ludewig, **Hunter N.B. Moseley**, Kelly G. Pennell, and Tim Zacharewski. "A case for accelerating standards to achieve the FAIR principles of environmental health research experimental data" ***Environmental Health Perspectives*** 131, 6 (2023). https://doi.org/10.1289/EHP11484
h) P. Travis Thompson and **Hunter N.B. Moseley**. "MESSES: Software for Transforming Messy Research Datasets into Clean Submissions to Metabolomics Workbench for Public Sharing" ***Metabolites*** 13, 842 (2023). https://doi.org/10.3390/metabo13070842
i) Christian D. Powell and **Hunter N.B. Moseley**. "The Metabolomics Workbench File Status Website: A Metadata Repository Promoting FAIR Principles of Metabolomics Data" ***BMC Bioinformatics*** 24, 299 (2023). Citations: 5 (Google Scholar). https://doi.org/10.1186/s12859-023-05423-9

3. 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*.



j) Yao S, Flight RM, Rouchka EC, **Moseley HNB**. A less biased analysis of metalloproteins reveals novel zinc coordination geometries. ***Proteins*** 83:1470, 2015. Citations: 27 (Google Scholar). PMCID: PMC4539273
k) Yao S, Flight RM, Rouchka EC, **Moseley HNB**. Aberrant coordination geometries discovered in the most abundant metalloproteins. ***Proteins*** 85:885, 2017. Citations: 5 (Google Scholar). doi:10.1002/prot.25257
l) Yao S, Flight RM, Rouchka EC, **Moseley HNB**. Perspectives and expectations in structural bioinformatics of metalloproteins. ***Proteins*** 85:938, 2017. Citations: 5 (Google Scholar). doi:10.1002/prot.25263
m) Yao S, **Moseley HNB**. Finding high-quality metal ion-centric regions across the worldwide Protein Data Bank. ***Molecules*** 24:3179, 2019. Citations: 4 (Google Scholar). doi:10.3390/molecules24173179
n) Yao S, **Moseley HNB.** A chemical interpretation of protein electron density maps in the worldwide protein data bank. ***PLOS One*** 15:e0236894, 2020. Citations: 6 (Google Scholar). doi:10.1371/journal.pone.0236894

4. Improved Utilization and Curation of the Gene Ontology. The Gene Ontology (GO) is the largest and best curated ontology in the OBO Foundry and is used extensively to precisely describe the functions, locations, and processes of gene(-product)s through specific annotations stored across many knowledgebases. But there is a fundamental problem with a lack of tools that organize ontology terms into usable domain-specific concepts that biomedical researchers can easily interpret, leverage within statistically rigorous analyses, and integrate with other types of information. Therefore, we have developed the GO Categorization Suite (GOcats), which streamlines the slicing of GO into custom, biologically-meaningful subgraphs representing emergent concepts in GO. GOcats uses a list of user-defined keywords or GO terms that describe a concept, the structure of GO, and relationship properties to automatically generate a subgraph of child terms and a mapping of these child terms to their respective concept-defining term. GOcats enables the utilization of additional GO relationship types in a manner that preserves proper scoping and scaling. Furthermore, we have demonstrated improvements in statistical power via the use of GOcats in annotation enrichment analyses performed by categoryCompare. We have also integrated GOcats driven annotation enrichment analysis with principal component analysis and molecular interaction network analysis (see Figure). Moreover, we have collaborated in the development of advanced curation tools that can help detect missing and erroneous relationships in GO, which are needed due to GO's size (over 40,000 terms) and rate of growth.

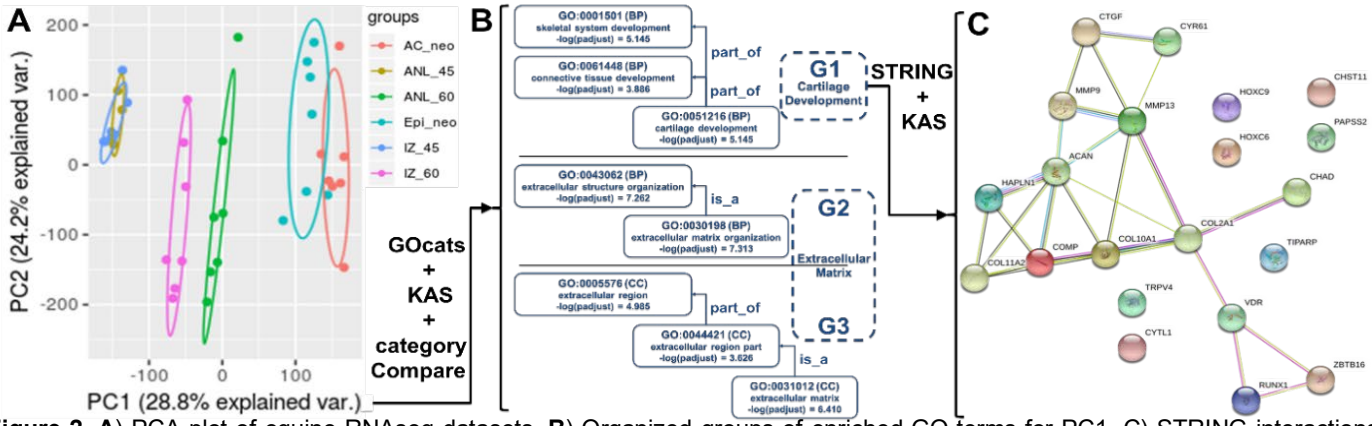


Figure 2. A) PCA plot of equine RNAseq datasets. **B**) Organized groups of enriched GO-terms for PC1. C) STRING interactions between high PC1 loading gene(-product)s annotated with group G1 GO terms (cartilage development).

a) Abeysinghe R, Hinderer III EW, **Moseley HNB**, and Cui L. Auditing Subtype Inconsistencies among Gene Ontology Concepts. ***The 2nd International Workshop on Semantics-Powered Data Analytics (SEPDA 2017) -- Bioinformatics and Biomedicine (BIBM), 2017 IEEE International Conference*** 1242-1245, 2017. Citations: 20 (Google Scholar).

b) Abeysinghe R, Zheng F, Hinderer III EW, **Moseley HNB**, and Cui L. A Lexical Approach to Identifying Subtype Inconsistencies in Biomedical Terminologies. ***Quality Assurance of Biological and Biomedical Ontologies and Terminologies Workshop -- Bioinformatics and Biomedicine (BIBM), 2018 IEEE International Conference*** 1982-1989, 2018. Citations: 16 (Google Scholar).

c) Hinderer III EW, Flight RM, Dubey R, MacLeod JN, and **Moseley HNB**. Advances in Gene Ontology Utilization Improve Statistical Power of Annotation Enrichment. ***PLOS One*** 14:e0220728, 2019. Citations: 13 (Google Scholar).

d) Hinderer III EW and **Moseley HNB**. GOcats: A tool for categorizing Gene Ontology into subgraphs of user-defined concepts. ***PLOS One*** 15:e0233311, 2020. Citations: 8 (Google Scholar).

e) Rashmie Abeysinghe, Eugene W. Hinderer III, **Hunter N.B. Moseley**, and Licong Cui. "SSIF: Subsumption-based Sub-term Inference Framework to Audit Gene Ontology" ***Bioinformatics*** 36, 3207 (2020). Citations: 11 (Google Scholar).

5. 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 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.

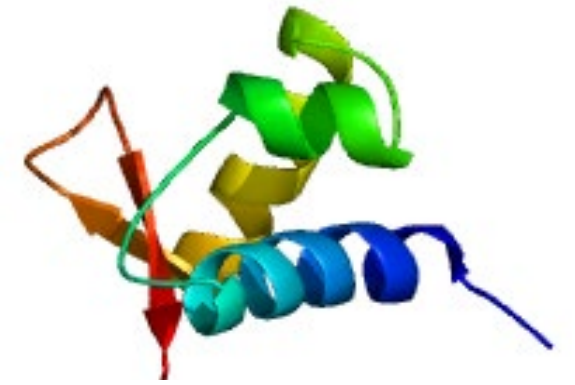


Figure 3: Solution NMR structure of PefI protein from *Salmonella typhimurium*.

a) **Moseley HNB** and Montelione GT. Automated analysis of NMR assignments and structures for proteins. ***Curr Opin Struct Biol*** 9:635-42, 1999. **Citations: 227** (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: 200** (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: 47 (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: 114** (Google Scholar).

6. 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: 129** (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: 23 (Google Scholar)
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: 32 (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: 22 (Google Scholar).

7. Transdisciplinary Mentoring and Science Education. 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 15 years, the PI's lab has included 5 postdoctoral fellows (2 women), 9 graduate students (3 women), 79 undergraduate students (29 women), and 32 high school students (7 women) 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 (https://github.com/MoseleyBioinformaticsLab). 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 (ULA) Joshua Mitchell finished the MD/PhD Program at the University of Kentucky with a computationally-focused Biochemistry PhD and is now a postdoctoral fellow at Los Alamos National Labs. ULA Tamas Nagy received an NSF Graduate Fellowship in 2015 and is now a graduate student in the Integrative Program in Quantitative Biology at UCSF. ULA Kelly Sovacool, entered the Bioinformatics PhD program at the University of Michigan. ULA Christian Powell is now in the Data Science MS Program at UK. 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) **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: 31 (Google Scholar).
b) 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*** 292, 5685 (2017). Citations: 16 (Google Scholar).
c) Smelter A, **Astra, M**, **Moseley HNB**. A Fast and Efficient Python Library for Interfacing with the Biological Magnetic Resonance Data Bank. ***BMC Bioinformatics*** 18, 175 (2017). Citations: 12 (Google Scholar).
d) **Powell CD**, Kirchhoff DC, DeRouchey JE, and **Moseley HNB**. Entropy-Based Analysis of Vertebrate Sperm Protamine Sequences: Evidence of Potential Dityrosine and Cysteine-Tyrosine Cross-Linking in Sperm Protamines. ***BMC Genomics*** 21:277, 2020. Citations: 4 (Google Scholar).

Publications

- **Current "h" index is 26 as per J. E. Hirsch's definition for quantifying an individual's scientific research output (physics/0508025 v5 09/29/2005).**
- **84 publications with 44 as first/corresponding author.**
- **2800+ citations: https://scholar.google.com/citations?hl=en&user=ctE_FZMAAAAJ ;**
- **ORCID: https://orcid.org/0000-0003-3995-5368**

84) Huan Jin and **Hunter N.B. Moseley**. "md_harmonize: a Python package for atom-level harmonization of public metabolic databases" ***Metabolites*** 13, 1199 (2023). https://doi.org/10.3390/metabo13121199

83) Alan Luo and **Hunter N.B. Moseley**. "Electron Density Discrepancy Analysis of Energy Metabolism Coenzymes" ***International Journal of Bioengineering and Life Sciences*** 17, 307 (2023). https://publications.waset.org/10013393/pdf

82) Erik D. Huckvale, Christian D. Powell, Huan Jin, and **Hunter N.B. Moseley**. "Benchmark dataset for training machine learning models to predict the pathway involvement of metabolites" ***Metabolites*** 13, 1120 (2023). https://doi.org/10.3390/metabo13111120

81) Christian D. Powell and **Hunter N.B. Moseley**. "The Metabolomics Workbench File Status Website: A Metadata Repository Promoting FAIR Principles of Metabolomics Data" ***BMC Bioinformatics*** 24, 299 (2023). https://doi.org/10.1186/s12859-023-05423-9

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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: 5 (Google Scholar). https://doi.org/10.1007/0-306-47084-5_7

7) **Hunter N.B. Moseley**. "Implementation and Application of Complete Relaxation and Conformational Exchange Matrix Analysis of NOESY Spectra." **dissertation** (1998). ISBN: 978-0-599-04716-7

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: 31 (Google Scholar). https://doi.org/10.1021/bi970242k

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: 20 (Google Scholar). https://doi.org/10.1007/bf00124470

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: 125 (Google Scholar).** https://doi.org/10.1006/jmrb.1995.1129

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: 25 (Google Scholar). https://doi.org/10.1006/jmrb.1995.1092

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: 28 (Google Scholar). https://doi.org/10.1006/immu.1994.1044

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

Oral Presentations

59) "A Cautionary Tale About Properly Vetting Datasets for Supervised Machine Learning Predicting Metabolic Pathway Involvement" , Metabolomics Association of North America SOftware and DAta Exchange (MANA SODA) Meeting, virtual (2023).

58) "kegg_pull: a Software Package for the RESTful Access and Pulling from The Kyoto Encyclopedia of Gene and Genomes" CTSA Informatics EC Full Membership Meeting, virtual (2023).

57) "A Cautionary Tale About Properly Vetting Datasets for Supervised Machine Learning Predicting Metabolic Pathway Involvement" Commonwealth Computational Summit, Lexington, KY (2023).

56) "Understanding the NIH Data Management & Sharing Policy" CCTS BMI Lunch n Learn Seminar, Lexington, KY (2023).

55) "Finalizing Report on the Isotopologue Working Group" InChI Cambridge Meeting, virtual (2022).

54) "Progress Report on the Isotopologue Working Group" InChI Open Meeting, virtual (2022).

53) "Improving Deposition Quality, FAIRness, and Impact of Metabolomics" NIH Data Sharing and Reuse Seminar Series, virtual (2022).

52) "Improving Deposition Quality and FAIRness of Metabolomics Workbench" Metabolomics Association of North America SOftware and DAta Exchange (MANA SODA) Meeting, virtual (2021).

51) "Improving Deposition Quality and FAIRness of Metabolomics Workbench II" NIH Common Funds Data Ecosystem Seminar, NIH virtual (2021).

50) "Improving Deposition Quality and FAIRness of Metabolomics Workbench" NIH Council of Councils CFDE Working Group, NIH virtual (2021).

49) "Improving Deposition Quality and FAIRness of Metabolomics Workbench" NIH Common Funds Data Ecosystem Seminar, NIH virtual (2021).

48) "Integration and Analysis of SRC-Generated Cardiometabolic Syndrome Data Streams from Animal Models" Superfund Research Program External Use Case Showcase, NIH, virtual, co-presented with Rance Nault (2021).

47) Discussions in sessions and chair of session at **Dagstuhl Seminar 20051**, Wadern, Germany (2020).

46) "Community Update on the Isotopologue InChI Extension" InChI Symposium, San Diego, CA (2019).

45) "Public Deposition of SIRM Datasets" in Workshop 12: EMN Workshop – Stable Isotope-Resolved Metabolomics: An Introduction and Overview, **15th Annual Conference of the Metabolomics Society**, The Hague, Netherlands (2019).

44) "Introduction to Stable Isotope Resolved Metabolomics" in Workshop 12: EMN Workshop – Stable Isotope-Resolved Metabolomics: An Introduction and Overview, **15th Annual Conference of the Metabolomics Society**, The Hague, Netherlands (2019).

43) "Developing Methods for Truly Untargeted Metabolomics Analysis", **14th Annual Conference of the Metabolomics Society**, Seattle, WA (2018).

42) "Proposal for New Isotopologue and Isotopomer Specifications for the IUPAC International Chemical Identifier Standard", **14th Annual Conference of the Metabolomics Society**, Seattle, WA (2018).

41) "Mutational Characterization of Squamous Cell Lung Cancers from Appalachian Kentucky: Moving Closer to Personalized Treatment", **21st Century Cures Southeast Conference**, Knoxville, TN (2018).

40)" Developing Methods for Truly Untargeted Metabolomics Analysis", **Intl. Conference on Molecular Genetics, Metabolomics, & Integrative Biology**, Bangkok, Thailand (2018).

39) "Statistical Analysis Primer", **RCSIRM Workshop**, Lexington, KY (2017).

38) "Small Molecule Isotope Resolved Formula Enumerator (SMIRFE)", **Kentucky Bioinformatics Retreat**, Shaker Village, Kentucky (2017).

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 or Oral Presentations by Lab Members

171) P. Travis Thompson and Hunter N.B. Moseley. “MESSES: Software for Transforming Messy Research Datasets into Clean Submissions to Metabolomics Workbench” 2023 NIH/NIEHS Superfund Research Program Annual Meeting, Albuquerque, NM (2023).

170) Ibrahim Imam, Sally Ellingson, Ralph Zinner, Xiaoqi Liu, Shuling Zhang, Christine Brainson, Hunter N.B. Moseley, and Qing Shao. “In-silico Pipeline to Discover Small Molecules Overcoming Mutation Induced Drug Resistance for EGFR”, TODD Symposium: Therapeutics Outcomes Discovery and Delivery, Lexington, KY (2023).

169) P. Travis Thompson, Sweta Ojha, Christian D. Powell, Kelly G. Pennell, and Hunter N.B. Moseley. “A Draft Minimum Information about Geospatial Information System (MIAGIS) Standard”, 2022 NIH/NIEHS Superfund Research Program Annual Meeting, Raleigh, NC (2022).

168) P. Travis Thompson, Christian D. Powell, and Hunter N.B. Moseley. “Academic Tracker: Tracking and Reporting Publications Associated with Authors and Grants”, 2022 NIH/NIEHS Superfund Research Program Annual Meeting, Raleigh, NC (2022).

167) Christian D. Powell and Hunter N.B. Moseley. “The mwtab Python Library for RESTful Access and Enhanced Quality Control, Deposition, and Curation of the Metabolomics Workbench Data Repository”, NIH/NIEHS Superfund Research Program - Risk e-Learning Webinar Series: Session III - Integrating Omics Data Across Model Organisms and Populations (2021). Oral presentation.

166) Pan Deng, Taylor Valentino, Michael D. Flythe, Hunter N.B. Moseley, Jacqueline R. Leachman, Andrew J. Morris, Bernhard Hennig. “Untargeted stable-isotope probing of the gut microbiota metabolome using 13C-labeled dietary fibers”, 2020 NIH/NIEHS Superfund Research Program Annual Meeting, Virtual Platform (2020).

165) Christian D. Powell and Hunter N.B. Moseley. “The mwtab Python library for RESTful Access and Enhanced Deposition, Quality Control, and Curation of the Metabolomics Workbench Data Repository”, 2020 NIH/NIEHS Superfund Research Program Annual Meeting, Virtual Platform (2020).

164) Huan Jin, Joshua M. Mitchell, and Hunter N.B. Moseley. “Atom Identifiers Generated by a Neighborhood-Specific Graph Coloring Method Enable Compound Harmonization Across Metabolic Databases”, Commonwealth Computational Summit 2020, Lexington, KY (2020).

163) Christian D. Powell and Hunter N.B. Moseley. “The mwtab Python library for RESTful Access and Enhanced Deposition, Quality Control, and Curation of the Metabolomics Workbench Data Repository”, Commonwealth Computational Summit 2020, Lexington, KY (2020).

162) Robert M. Flight and Hunter N.B. Moseley. “High-DensityMass-Spectrometry DataProcessing on theKyRic OpenStackCluster”, Commonwealth Computational Summit 2020, Lexington, KY (2020).

161) Rance Nault, Hunter N.B. Moseley, Kelly Pennel, Matthew Cave, Gabrielle Ludewig, and Timothy R. Zacharewski. “Development of minimum requirements and data management framework for animal toxicology experiments”, 2020 Michigan Regional Chapter of the Society of Toxicology Fall Meeting, Virtual Platform (2020).

160) Tim Zacharewski, Matt Cave, Kelly Pennell, Hunter N.B. Moseley, Norb Kaminski, Sanjay Srivastava, and Bernard Hennig. “Integration and Analysis of SRC-Generated Cardiometabolic Syndrome Data Streams from Animal Models”, 2019 NIEHS Superfund Research Program Annual Meeting, Seattle, WA (2019).

159) Huan Jin and Hunter N.B. Moseley. “Moiety Modeling Framework for Deriving Pathway-Specific Relative Metabolic Flux from Mass Spectrometry Measured Isotopologues”, Metabolomics Association of North America 2019, Atlanta, GA (2019).

158) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. “Untargeted Lipidomics of NSCLC Shows Differentially Abundant Lipid Classes in Cancer vs Non-Cancer Tissue”, Commonwealth Computational Summit 2019, Lexington, KY (2019).

157) Huan Jin and Hunter N.B. Moseley. “Moiety Modeling Framework for Deriving Pathway-Specific Relative Metabolic Flux from Mass Spectrometry Measured Isotopologues”, Commonwealth Computational Summit 2019, Lexington, KY (2019).

156) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. “Untargeted Lipidomics of NSCLC Shows Differentially Abundant Lipid Classes in Cancer vs Non-Cancer Tissue”, University of Kentucky Cancer and Metabolism Symposium, Lexington, KY (2019).

155) Huan Jin and Hunter N.B. Moseley. “Moiety Modeling Framework for Deriving Pathway-Specific Relative Metabolic Flux from Mass Spectrometry Measured Isotopologues”, University of Kentucky Cancer and Metabolism Symposium, Lexington, KY (2019).

154) Andrey Smelter and Hunter N.B. Moseley. “Generation of Isotope-Resolved IUPAC International Chemical Identifiers to Facilitate Deposition and Reuse of NMR-based Metabolomics Datasets”, University of Kentucky Cancer and Metabolism Symposium, Lexington, KY (2019).

153) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. “Untargeted Lipidomics of NSCLC Shows Differentially Abundant Lipid Classes in Cancer vs Non-Cancer Tissue”, 15th Annual Conference of the Metabolomics Society, The Hague, Netherlands (2019).

152) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. “Untargeted lipidomics of NSCLC shows differentially abundant lipid classes in cancer vs non-cancer tissue”, Markey Cancer Center Research Day, Lexington, KY (2019).

151) Huan Jin and Hunter N.B. Moseley. “Moiety Modeling Framework for Deriving Pathway-Specific Relative Metabolic Flux from Mass Spectrometry Measured Isotopologues”, Markey Cancer Center Research Day, Lexington, KY (2019).

150) Reena Kumai, Timothy L. Scott, Ethan Strattan, Katharina Kohler, Chi Wang, Daheng He, Teresa W-M. Fan, Robert M. Flight, Joshua M. Mitchell, Hunter Moseley, Andrew N. Lane, Senthilnathan Palaniyandi, and Gerhard C Hildebrandt. "Lipid profiling of spleen and lung after allogeneic hematopoietic cell transplantation in a murine model of GVHD", Markey Cancer Center Research Day, Lexington, KY (2019).

149) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. "Untargeted lipidomics of NSCLC shows differentially abundant lipid classes in cancer vs non-cancer tissue", CCTS Spring Conference, Lexington, Kentucky (2019).

148) Huan Jin and Hunter N.B. Moseley. "Moiety Modeling Framework for Deriving Pathway-Specific Relative Metabolic Flux from Mass Spectrometry Measured Isotopologues", CCTS Spring Conference, Lexington, Kentucky (2019).

147) Christian D. Powell and Hunter N.B. Moseley. "Evidence for cysteine-tyrosine and dicysteine cross-linking in mammalian sperm protamines", National Conference on Undergraduate Research, Kennesaw, GA (2019). Oral presentation.

146) Andrey Smelter and Hunter N.B. Moseley. "Isotopic Enumerator: a Python package to facilitate isotopically-resolved annotation and deposition of metabolomics data", Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2018).

145) Robert M. Flight, Eugene W. Hinderer III, and Hunter N. B. Moseley. "categoryCompare: A Flexible Framework for Enrichment of Feature Annotations and Their Comparisons", Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2018).

144) Eugene W. Hinderer III, Robert M. Flight, and Hunter N. B. Moseley. "Advances in Gene Ontology Utilization Improve Statistical Power of Annotation Enrichment", Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2018).

143) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. "Small Molecule Isotope Resolved Formula Enumerator (SMIRFE): a tool for assigning isotopologues and metabolites in Fourier transform mass spectra", Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2018).

142) Katherine Thompson, Corrine Elliott, Joshua Lambert, Thilakam Murali, Hunter Moseley, Arnold Stromberg. "Using the Feasible Solutions Algorithm to Identify Combinations of Genetic Factors Associated with Multiple Sclerosis", 7th Biennial National IDeA Symposium of Biomedical Research Excellence (NISBRE), Washington, DC (2018).

141) Robert M. Flight, Eugene W. Hinderer III, and Hunter N. B. Moseley. "categoryCompare: A Flexible Framework for Enrichment of Feature Annotations and Their Comparisons", 8th Annual Barnstable Obesity and Diabetes Research Day, Lexington, KY (2018).

140) Eugene W. Hinderer III, Robert M. Flight, and Hunter N. B. Moseley. "Advances in Gene Ontology Utilization Improve Statistical Power of Annotation Enrichment", 8th Annual Barnstable Obesity and Diabetes Research Day, Lexington, KY (2018).

139) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. "Small Molecule Isotope Resolved Formula Enumerator (SMIRFE): a tool for assigning isotopologues and metabolites in Fourier transform mass spectra", 8th Annual Barnstable Obesity and Diabetes Research Day, Lexington, KY (2018).

138) Eugene W. Hinderer III, Robert M. Flight, and Hunter N. B. Moseley. "Advances in Gene Ontology Utilization Improve Statistical Power of Annotation Enrichment", 7th Bluegrass Molecular Biophysics Symposium, Lexington, KY (2018).

137) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. "Small Molecule Isotope Resolved Formula Enumerator (SMIRFE): a tool for assigning isotopologues and metabolites in Fourier transform mass spectra", 7th Bluegrass Molecular Biophysics Symposium, Lexington, KY (2018).

136) Xi Chen, Andrey Smelter, and Hunter N.B. Moseley. "Automatic 13C Chemical Shift Reference Correction for Unassigned Protein NMR Spectra Using Data Mining and Bayesian Statistical Modeling", 7th Bluegrass Molecular Biophysics Symposium, Lexington, KY (2018).

135) Robert M. Flight, Eugene W. Hinderer III, and Hunter N. B. Moseley. "categoryCompare: A Flexible Framework for Enrichment of Feature Annotations and Their Comparisons", Markey Cancer Center Research Day, Lexington, KY (2018).

134) Eugene W. Hinderer III, Robert M. Flight, and Hunter N. B. Moseley. “Advances in Gene Ontology Utilization Improve Statistical Power of Annotation Enrichment”, Markey Cancer Center Research Day, Lexington, KY (2018).

133) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. “Small Molecule Isotope Resolved Formula Enumerator (SMIRFE): a tool for assigning isotopologues and metabolites in Fourier transform mass spectra”, Markey Cancer Center Research Day, Lexington, KY (2018).

132) Xi Chen, Andrey Smelter, and Hunter N.B. Moseley. “Automatic 13C Chemical Shift Reference Correction for Unassigned Protein NMR Spectra Using Data Mining and Bayesian Statistical Modeling”, SIAM International Conference on Data Mining, San Diego, CA (2018).

131) Kelly L. Sovacool and Hunter N.B. Moseley. “Developing a Global Homology Analysis Framework for Comparative Genomics”, University of Kentucky Undergraduate Research Showcase, Lexington, KY (2018).

130) Eugene W. Hinderer III, Robert M. Flight, and Hunter N. B. Moseley. “Advances in Gene Ontology Utilization Improve Statistical Power of Annotation Enrichment”, CCTS Spring Conference, Lexington, Kentucky (2018).

129) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. “Small Molecule Isotope Resolved Formula Enumerator (SMIRFE): a tool for truly untargeted metabolomics analysis of metabolites represented in Fourier transform mass spectra”, CCTS Spring Conference, Lexington, Kentucky (2018).

128) Robert M. Flight, Eugene W. Hinderer III, and Hunter N. B. Moseley. “categoryCompare: A Flexible Framework for Enrichment of Feature Annotations and Their Comparisons”, CCTS Spring Conference, Lexington, Kentucky (2018).

127) Kelly L. Sovacool and Hunter N.B. Moseley. “Developing a Global Homology Analysis Framework for Comparative Genomics”, National Conference on Undergraduate Research, Edmond, OK (2018).

126) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. “Small Molecule Isotope Resolved Formula Enumerator (SMIRFE): a tool for truly untargeted metabolomics analysis of metabolites represented in Fourier transform mass spectra”, 21st Century Cures Southeast Conference, Knoxville, TN (2018).

125) Robert M. Flight, Joshua M. Mitchell, and Hunter N.B. Moseley. “Between-scan peak correspondence and normalization for direct-injection Fourier transform mass spectrometry data”, 21st Century Cures Southeast Conference, Knoxville, TN (2018).

124) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. “Small Molecule Isotope Resolved Formula Enumerator (SMIRFE): a tool for assigning isotopologues and metabolites in Fourier transform mass spectra” 33rd Asilomar Conference on Mass Spectrometry Impact of Metabolomics in Translational and Clinical Research, Pacific Grove, CA (2017).

123) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. “Small Molecule Isotope Resolved Formula Enumerator (SMIRFE): a tool for assigning isotopologues and metabolites in Fourier transform mass spectra” The Common Fund Metabolomics Consortium Meeting, Davis, CA (2017).

122) Joshua M. Mitchell, Robert M. Flight, Qingjun Wang, Andrew N. Lane, Richard M. Higashi, Teresa W.-M. Fan, and Hunter N.B. Moseley. “Detection and Handling of Spectral Artefacts in Fourier Transform Mass Spectra from Metabolomics Experiments”, The Common Fund Metabolomics Consortium Meeting, Davis, CA (2017).

121) Joshua M. Mitchell, Robert M. Flight, and Hunter N.B. Moseley. “Small Molecule Isotope Resolved Formula Enumerator (SMIRFE): a tool for assigning isotopologues and metabolites in Fourier transform mass spectra” Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2017).

120) Robert M. Flight, Joshua M. Mitchell, and Hunter N.B. Moseley. “Between-scan peak correspondence and normalization for direct-injection Fourier transform mass spectrometry data” Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2017).

119) Joshua M. Mitchell, Robert M. Flight, Qingjun Wang, Andrew N. Lane, Richard M. Higashi, Teresa W.-M. Fan, and Hunter N.B. Moseley. “Detection and handling of spectral artifacts in Fourier transform mass spectra of metabolomics experiments” Resource Center for Stable Isotope-Resolved Metabolomics Metabolomics Symposium, Lexington, KY (2017).

118) Smita Joshi, Meenakshi Banerjee, Penghui Lin, Marc Warmoes, Qiushi Sun, Hunter N. B. Moseley, Richard M. Higashi, Andrew N. Lane, Teresa W.-M. Fan, Sidney W. Whiteheart, Qingjun Wang. “Analysis of Platelet Activation by Stable Isotope-Resolved Metabolomics (SIRM)” International Society on Thrombosis and Haemostasis (ISTH) 2017 Congress, Beling, Germany (2017).

117) 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, Yung Sil 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, Qingjun Wang. “Loss of juvenile neuronal ceroid lipofuscinosis disease gene CLN3 in retinal pigment epithelium leads to metabolic impairment and autophagy induction” FASEB Biology and Chemistry of Vision Conference, Steam Boat Spring, CO (2017).

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

NSF: 2020026 Moseley (PI) 08/15/2020 to 7/31/2024
IIBR Informatics: Comprehensive Metabolism Phenotype Characterization and Interpretation
Goals: Develop new data analysis tools that enable effective analysis, integration, interpretation, and public deposition of large metabolomics analytical datasets collected from new high-end instruments.
Role: PI ($1,163,869 total)

NSF: 2216140 (MPI: Talbert, JC; Bumgardner, V; Griffioen, JN; Moseley, HNB; Risko, C) 08/01/2022-07/31/25
MRI: Acquisition of the Kentucky Research Informatics Composable Cloud (KyRICC)
Goals: Build composable high performance computing resource for research applications
Role: PI

NIH 1R01DA058933-01 (PD: Gipson-Reichardt) 06/15/2023-04/30/2028
"Neurobehavioral Mechanisms Underlying Xylazine and Fentanyl Co-use and Withdrawal"
Goals: 1) Determine how xylazine impacts the effects of fentanyl, 2) Determine viable therapeutic targets to resensitize fentanyl withdrawal following the escalation of xylazine-fentanyl SA, and 3) Determine neural circuits altering the NAcore and ventral tegmental area (VTA) kinomes following the escalation of xylazine-fentanyl SA and if these underlie naloxone resistance.
Role: Co-Investigator

NIH: P30 CA177558 (PI: Evers, BM) 07/08/2013-06/30/2028
"University of Kentucky Markey Cancer Center – Cancer Center Support Grant"
Goals: To support the ongoing research infrastructure, research programs, shared resources, developmental funds, and administration of the Markey Cancer Center to ensure the development of more effective approaches to cancer prevention, diagnosis, and therapy.
Role: Faculty Bioinformatician

NIH: U01 DE031223 (PI: Shaddox, LM) 09/01/2022-8/31/2027
Susceptibility Patterns for Grade C Periodontitis in Young Individual
Goals: Characterization of susceptibility, molecular, and microbial phenotypes of Grade C Periodontitis
Role: co-I

NIH: R01 CA249734 Zaytseva (PI) 04/01/2021-03/31/2026
Targeting Lipid Metabolism in Colorectal Cancer
Goals: To investigate the mechanisms of how lipid metabolism promotes colorectal cancer metastasis.
Role: Bioinformatician

NIH: P42 ES007380 Pennell, K (PI) 12/01/2019-11/30/2024
Nutrition and Superfund Chemical Toxicity
Goals: Address the persistence of halogenated organics at Superfund sites and elsewhere.
Role: Co-Leader of the Data Management and Analysis Core

NIH: U54 TR001998-05A1 Kern (PI) 01/01/2022-12/31/2025
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.) 12/01/2016 to 12/31/2026
"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)

NIH R01 DK112034 Evers, BM (PI) 02/01/2017-06/30/2026
Mechanisms Regulating Neurotensin Secretion and Function
Goals: To determine if FFA-mediated NT release by EE cells, through a cross-talk mechanism involving AMPK activation, mTOR inhibition, and ERK1/2 activation, promotes intestinal absorption of FFAs.
Role: Collaborator

Completed Research Support

NIH: R01CA214638-05 (PI: St. Clair) 12/01/2017-06/30/2023
"A Redox-Mediated Mechanism of UVB-Induced Metabolic Switch in Skin Carcinogenesis"
Goals: Test the hypothesis that O2•- triggers an uncoupling protein (UPC)-dependent metabolic switch. Test the hypothesis that MnSOD is a critically important target of UVB-induced peroxynitrite formation leading to activation of autophagy responses. Test the concept that UVB-induced O2•- and OONO- are critical mediators that promote UV carcinogenesis.
Role: Co-Investigator

NIH: R03 OD030603 Moseley (PI) 09/01/2020-08/31/2022
Improving Deposition Quality and FAIRness of Metabolomics Workbench
Goals: Develop methods and tools that: a) comprehensively capture, validate, and deposit metadata-rich metabolomics data, b) improve the FAIRness of MWbench datasets, especially reuse, c) enable integration of MWbench and GTEx datasets to generate biomedically-relevant human gene-metabolite associations, and d) enable interpretation of gene-metabolite associations within molecular interaction networks.
Role: PI ($302,804 total)

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

NIH: 1U24DK097215-01A1 Higashi/Fan/Lane/Moseley(PIs) 09/11/2013 to 08/31/2018
Resource Center for Stable Isotope-Resolved Metabolomics
Goals: To establish and operate a regional metabolomics center focused on the analysis of stable isotope tracing experiments.
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 1419282 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: 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)

NIH: 1R03CA211835-01 Wang, Flight (MPI) 09/14/2016 to 08/31/2017
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) 10/01/1999 to 09/30/2001
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)