

# Samuel Kakraba, PhD

## PROFILES

### Institutional/Work (Tulane University)

<https://sph.tulane.edu/bios/samuel-kakraba>

<https://medicine.tulane.edu/departments/tulane-center-aging-tulane-cancer-center/faculty/samuel-kakraba-phd>

### Google Scholar

[https://scholar.google.com/citations?authuser=1&user=S9\\_ha\\_UAAAJ](https://scholar.google.com/citations?authuser=1&user=S9_ha_UAAAJ)

### PubMed

<https://www.ncbi.nlm.nih.gov/myncbi/samuel.kakraba.2/bibliography/public/>

**ORCID** : <https://orcid.org/0000-0002-6362-5126>

### ResearchGate

<https://www.researchgate.net/profile/Samuel-Kakraba>

### LinkedIn

<https://www.linkedin.com/in/kakrabasamuel/>

<b>Address</b>	<b>Phone Number</b>	<b>Email Address</b>
<b><u>Work/Office</u></b> Department of Biostatistics and Data Science/ Tulane School of Public Health and Tropical Medicine/ 1440 Canal Street, Suite 1610H, MB Code #8310/ New Orleans, LA 70112, USA  &  Center for Aging, Tulane University School of Medicine, 1430 Tulane Avenue, New Orleans, LA 70112	<b><u>Office</u></b> +1(504)-988-2475	<b><u>Work/School</u></b> <a href="mailto:Skakraba@tulane.edu">Skakraba@tulane.edu</a>

## PROFESSIONAL SUMMAY AND OBJECTIVE STATEMENT

I am a very passionate data scientist, biostatistician, statistician, applied mathematician, bioinformaticist, inventor and an outstanding university assistant professor of statistics and data science with exceptional intellectual abilities, academic performance, excellent analytical, communication, organizational, and motivational skills for diverse and inclusive students-centered teaching, research and mentoring of graduate and undergraduate students.

My research centers chiefly on the development and implementation of efficient computationally-driven pipelines aided by robust data science, statistical, mathematical and biostatistical predictive modeling machine learning algorithms like neural networks, deep learning, support vector machines, k-nearest neighbors, random forests, Naïve Bayes, and others, in R statistical software, Python, SAS, and others, for estimation, prediction, and inferences into complex high-dimensional relationships in the computational sciences. Through my

collaborative research, I have designed and implemented data science-driven machine learning algorithms in quantitative structure-activity relationship (QSAR) modeling for screening, identification, and characterization of novel small NSAID (non-steroidal anti-inflammatory drug) molecules for treatment of neurodegenerative diseases like Alzheimer's, Parkinson's, Huntington's, and others in drug discovery and design. The conceptual framework of the machine learning pipelines I design and implement through my research is extendable to other fields of study that involve statistical machine learning, biostatistics, and data science-driven projects in public health, among others. Additionally, part of my research involves the application of mathematical graph-theoretic modeling (network graphs) interfaced with statistical and mathematical machine learning, molecular modeling, docking, simulations, and other bioinformatics techniques to address critical questions in complex network and systems biology.

### CURRENT ACADEMIC/WORK POSITION

- **Professor (Assistant) of Biostatistics and Data Science**, Department of Biostatistics and Data Science, School of Public Health and Tropical Medicine, Tulane University, New Orleans, LA, USA, Jan 2024 – present.
- **Professor (Assistant)**, Tulane Center for Aging, Tulane University School of Medicine, Tulane University, New Orleans, LA, USA, Jan 2024 – present.

### EDUCATION AND AFFILIATIONS

<b>University</b>	<b>Degree Awarded</b>	<b>Dissertation Title &amp; Specialty</b>
<b>University of Arkansas at Little Rock (UALR) and University of Arkansas for Medical Sciences (UAMS)</b>   Little Rock, AR, USA	<b>Degree:</b> Ph.D.(Bioinformatics) <b>Duration:</b> 08/2015 – 07/2021 <b>Final Grade Point Average:</b> 4.0/4.0	<b>Dissertation Topic:</b> “Drugs that Protect Against Protein Aggregation in Neurodegenerative Diseases.” <b>Major Advisor:</b> Robert J.S. Reis, Ph.D. <b>Areas of Specialization:</b> Drug Discovery and Design, Applied Statistics, Data Science and Machine Learning, Neuroscience, Biostatistics, Bioinformatics, Computational Biology, Protein Science, and Cheminformatics
<b>East Tennessee State University (ETSU)</b>   Johnson City, TN, USA	<b>Degree:</b> M.S.(Mathematical Sciences) <b>Duration:</b> 08/2013 – 05/2015	<b>Dissertation Topic:</b> “A Hierarchical Graph for Nucleotide Binding Domain 2.” <b>Major Advisor:</b> Debra J. Knisley, Ph.D. <b>Areas of Specialization:</b> Mathematical Predictive Modeling, Computational Biology, Bioinformatics, Applied Statistics, Data Science, Drug Discovery
<b>University of Cape Coast</b>   Cape Coast, Central Region, Ghana,	<b>Degree:</b> B.Ed.(Mathematics) <b>Duration:</b> 08/2007 – 05/2011	<b>Dissertation Topic:</b> “The Relationship Between Students’ Perception of Mathematics and their Mathematics Achievements.” <b>Major Advisor:</b> Benjamin Y. Sokpe, M.Phil. <b>Areas of Specialization:</b> Mathematics, Statistics, Education

## RESEARCH FUNDING SUPPORTS

<b>Grant Title and Grant Number</b>	<b>Source of Funding</b>	<b>Supervisors and Institution</b>	<b>My Role</b>	<b>Direct Cost per Year</b>	<b>Period of Support</b>
Early Events in Alzheimer Pathogenesis ( <b>P01 AG012411-17A1</b> )	National Institute on Aging(NIA)/National Institute on Health (NIH)	<b><u>Supervisors</u></b> Prof. WST Griffin, PI Prof. Robert Reis (Project 3 leader)  <b><u>Institution</u></b> University of Arkansas for Medical Sciences, Little Rock, AR, USA	Doctoral Graduate Research Assistant	\$1.2 – 1.5M	9/30/2016 – 5/31/2021
Analysis and Therapy of Age-Dependent Proteostasis Failure in Neurodegeneration ( <b>I01BX001655</b> )	Veterans Administration Merit Award	<b><u>Supervisor</u></b> Prof. Robert Reis (Principal Investigator)  <b><u>Institution</u></b> University of Arkansas for Medical Sciences, Little Rock, AR, USA	Doctoral Graduate Research Assistant	\$150,000 – 200,000	4/1/2013 – 12/31/2022
P20 GM103429 - Arkansas INBRE program	National Institute of General Medical Sciences (NIGMS), part of the NIH	Donaghey College of Science, Technology, Engineering and Mathematics, University of Arkansas at Little Rock & the University of Arkansas for Medical Sciences, Little Rock, AR 72205, USA	Doctoral Graduate Research Assistant	Covered all tuition, health insurance, conferences, and monthly stipend for 18 months	08/17/2015 - 03/17/2017

## ACADEMIC AWARDS

<b>Award</b>	<b>University/Institution</b>	<b>Year</b>
Outstanding College Doctoral Candidate	Donaghey College of Science, Technology, Engineering and Mathematics, University of Arkansas at Little Rock & the University of Arkansas for Medical Sciences, Little Rock, AR 72205, USA	2020/2021

Outstanding Departmental Doctoral Candidate	Department of Information Sciences, University of Arkansas at Little Rock, Little Rock, AR 72205, USA	2020/2021
Outstanding Oral Presentation (third place)	Drug Discovery & Development Colloquium, University of Arkansas for Medical Sciences, Little Rock, AR 72205, USA	2019/2020
Full-Time Graduate Research Assistantship (full tuition waiver, monthly stipend, and health insurance covered)	Department of Information Science, College of Science, Technology, Engineering and Mathematics, University of Arkansas for Medical Sciences, & the University of Arkansas at Little Rock; and NIH Program Project Grant AG012411-17A1, (Role: Graduate student researcher) Little Rock, AR, USA	2016/2021
Full-time Graduate Research Assistantship (full tuition waiver, monthly stipend, and health insurance covered)	Department of Information Sciences, University of Arkansas at Little Rock, Little Rock, AR 72205, USA	2015/2016
Faculty Award: Outstanding Graduate Student	Department of Mathematics and Statistics, East Tennessee State University, Johnson City, TN 37614, USA	2014/2015
Full-time Graduate Teaching Associateship (full tuition waiver & monthly stipend)	Department of Mathematics and Statistics, East Tennessee State University, Johnson City, TN 37614, USA	2014/2015
Full-time Graduate Teaching Assistantship (full tuition waiver & monthly stipend)	Department of Mathematics and Statistics, East Tennessee State University, Johnson City, TN 37614, USA	2013/2014

### MEDIA SPOTLIGHTS

1. ***UAMS Researchers Receive \$1.8 Million to Study Common Mechanisms Shared by Alzheimer's, Other Diseases***: UAMS College of Medicine”(2018). University of Arkansas for Medical Sciences College of Medicine, Little Rock, AR, USA  
URL: <https://medicine.uams.edu/blog/uams-researchers-receive-1-8-million-to-study-common-mechanisms-shared-by-alzheimers-other-diseases/>
2. ***Where They Are Now***. (2016, August 6). *Illuminated Magazine- East Tennessee State University Graduate School*, 6(1), 12.  
URL: <https://dc.etsu.edu/cgi/viewcontent.cgi?article=1004&context=illuminated>
3. Invited Presentation on “***Effects of Small Molecules on Protein Aggregation and Paralysis in C. elegans Expressing Aβ<sub>1-42</sub> in the Muscle***” and information session on graduate school education at Strengthening Minorities Achievements via Research Training in Mathematics Program Grant with Principal Investigators: Ariel Cintron-Arias and Debra Knisley (Grant # H98230-16-1-0041  
<https://static1.squarespace.com/static/5e9b687d5c9c9e499bb04b9d/t/5ec1606eaa8738407dcaf72c/1589731446009/Report+ETSU+NSA+REU.pdf>

### COMPUTATIONAL PROGRAMMING AND SOFTWARE SKILLS

Statistical & Data Science Software	Molecular Modeling & Simulation	Operating Systems & Typing Programs
• R Statistical Software	• Gromacs	• Linux/Ubuntu

<ul style="list-style-type: none"> <li>• SAS</li> <li>• Python</li> <li>• Graph Pad Prism</li> <li>• Minitab</li> <li>• Hadoop</li> <li>• Apache</li> <li>• Bash scripting</li> <li>• SPSS</li> <li>•</li> </ul>	<ul style="list-style-type: none"> <li>• Discovery Studio</li> <li>• Maestro Schrödinger</li> <li>• AutoDock Vina</li> <li>• Raccoon</li> <li>• Modeler</li> <li>• Chimera</li> <li>• Cystoscape</li> <li>• Sybyl</li> </ul>	<ul style="list-style-type: none"> <li>• Latex</li> <li>• Windows</li> <li>• Android</li> <li>• Microsoft office (word, excel, PowerPoint)</li> </ul>
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### **SELECTED GRADUATE LEVEL COURSEWORK**

<b>Statistics &amp; Data Science &amp; Biostatistics</b>	<b>Computational Biology &amp; Bioinformatics &amp; Drug Discovery &amp; Mathematics</b>
<ul style="list-style-type: none"> <li>➤ Programming in R</li> <li>➤ Programming in Python</li> <li>➤ Introduction to Data Science and Technologies</li> <li>➤ Machine Learning and Applications</li> <li>➤ Deep Learning</li> <li>➤ Data Science and Technologies</li> <li>➤ Big Data and Data Analytics</li> <li>➤ Data Mining and Visualization</li> <li>➤ Predictive Modeling and Analytics</li> <li>➤ Artificial Intelligence</li> <li>➤ Business Analytics and Business Intelligence</li> <li>➤ Data and Information Visualization</li> <li>➤ Data Management and Data Mining</li> <li>➤ Probability and Statistics</li> <li>➤ Regression Analysis</li> <li>➤ Advanced Statistical Analysis</li> <li>➤ Multivariate Statistics</li> <li>➤ Biostatistics I&amp;II</li> <li>➤ Categorical Data Analysis</li> <li>➤ Statistical Methods I &amp;II</li> <li>➤ Statistical Consulting</li> <li>➤ Mathematical Statistics I &amp;II</li> <li>➤ Statistical Inference</li> <li>➤ Probability and Statistics</li> <li>➤ Applied Statistics</li> </ul>	<ul style="list-style-type: none"> <li>➤ Molecular Modeling and Simulation</li> <li>➤ Bioinformatics: Theory and Applications</li> <li>➤ Discrete Models of Proteins</li> <li>➤ Complex Network and Systems Biology</li> <li>➤ Drug Discovery and Design</li> <li>➤ Biology of Aging</li> <li>➤ Molecular Biology</li> <li>➤ Graph Theory I&amp;II</li> <li>➤ Calculus I-III</li> <li>➤ College Algebra</li> <li>➤ Real Analysis</li> <li>➤ Linear Algebra</li> <li>➤ Differential Geometry</li> <li>➤ Complex Analysis</li> <li>➤ Graph-Theoretic Modeling</li> <li>➤ Modern Algebra</li> <li>➤ Ordinary Differential Equations</li> </ul>

### **PREVIOUS FULL-TIME ACADEMIC (WORK) POSITIONS**

<b>Role</b>	<b>Institution</b>	<b>Grade/Level</b>	<b>Duration</b>
Professor (Assistant) of Statistics and Data Science	Department of Mathematics and Statistics, Eastern Kentucky University, Richmond, KY, USA	University	Aug. 1, 2021 to Dec. 31, 2023
Graduate Research Assistant	Department of Information Science, College of Science, Technology, Engineering and Mathematics,	University	Aug.2015 – Jul. 2021

	University of Arkansas for Medical Sciences, & the University of Arkansas at Little Rock; and NIH Program Project Grant AG012411-17A1, (Role: Graduate student researcher) Little Rock, AR, USA		
Graduate Teaching Associate	Department of Mathematics and Statistics, East Tennessee State University, Johnson City, TN 37614, USA	University	2014 - 2015
Graduate Teaching Assistant	Department of Mathematics and Statistics, East Tennessee State University, Johnson City, TN 37614, USA	University	2013 - 2014
Instructor	Wesley Girls' High School, Cape Coast, Central Region, Ghana	Grade 10 - 12	2011 - 2013
Instructor	Wesley Girls' High School, Cape Coast, Central Region, Ghana	Grade 10 - 12	2009 - 2011
Instructor	Montessori Primary School, Pedu, Cape Coast, Central Region, Ghana	Grade 1	2006 - 2007
Instructor	Cherish International School, Pedu, Cape Coast, Central Region, Ghana	Grade 1- 3	2004 - 2006

### UNIVERSITY TEACHING EXPERIENCE

*Key: Graduate(G); Undergraduate(UG); High School (HS); Elementary (E); \* Facilitator*

#### Department of Mathematics & Statistics, Eastern Kentucky University, Richmond, KY, USA

Fall 2021- Fall 2023

Course Prefix & Number	Course Title	Number of Times Taught	Credits Hours	Modality	Level
STA /DSC 780	R and Introductory Data Mining	3	3	In-person	G
STA/DSC 580	R and Introductory Data Mining	3	3	In-person	UG
STA 880/DSC 880	Statistical Machine Learning in R	1	3	Hybrid	G
STA 340	Regression Analysis	3	3	In-person	UG
STA 270	Applied Statistics	4	4	In-person	UG
STA 270L	Applied Statistics Lab	1	2	In-person	UG
STA 215	Introduction to Statistical Reasoning	2	4	E-campus/ Online	UG
STA 215	Introduction to Statistical Reasoning	1	4	In-person	UG
STA 215*	Introduction to Statistical Reasoning	1	4	In-person	UG

STA 840	Applied Multivariate Statistics Analysis	1	4	Online	G
STA 215P	Introduction to Statistical Reasoning- Lab	1	2	E-campus/ Online	UG
STA 215P	Introduction to Statistical Reasoning- Lab	2	2	In-person	UG

## Summary of Eastern Kentucky University teaching evaluation using the Explorance Blue Instrument

My students' ratings "Overall I rate the instructor as..." question on the Eastern Kentucky University Explorance Blue forms.

\* No evaluation reports are generated for courses with low enrollment or with very few students responding to the evaluation survey

Course/CRN	Course Title	Semester	Average or Better
STA/DSC/CSC 580	R and Introductory Data Mining	Fall 2023	<b>100%</b>
STA 215	Introduction to Statistical Reasoning	Fall 2023	<b>90.91%</b>
STA 215P (CRN:13570)	Quantitative Support for STA 215	Fall 2023	<b>88.88%</b>
STA 215P (CRN: 13570)	Quantitative Support for STA 215	Fall 2023	<b>85.72%</b>
STA/DSC/CSC 780	R and Introductory Data Mining	Fall 2023	*
STA 270 (CRN:21335)	Applied Statistics	Spring 2023	<b>100.00%</b>
STA 270 (CRN:24225)	Applied Statistics	Spring 2023	<b>100.00%</b>
STA 840	Applied Multivariate Statistics	Spring 2023	*
STA 215P	Quantitative Support for STA 215	Spring 2023	*
STA 340	Regression Analysis	Fall 2022	<b>100.00%</b>
STA 498W	Seminar/Capstone in Statistics	Fall 2022	<b>100.00%</b>
STA/DSC/CSC 580	R and Introductory Data Mining	Fall 2022	<b>100.00%</b>
STA/DSC/CSC 780	R and Introductory Data Mining	Fall 2022	<b>100.00%</b>
STA 270L	Applied Statistics Lab	Spring 2022	<b>100.00%</b>
STA 340	Regression Analysis	Spring 2022	<b>100.00%</b>
STA 880	Seminar/Special Topic: Statistical Machine Learning in R	Spring 2022	<b>100.00%</b>
STA 270	Applied Statistics	Spring 2022	<b>81.25%</b>
STA 215	Introduction to Statistical Reasoning	Winter 2021/2022	<b>92.85%</b>
STA/DSC/CSC 780	R and Introductory Data Mining	Fall 2021	<b>100.00%</b>

STA/DSC/CSC 580	R and Introductory Data Mining	Fall 2021	<b>100.00%</b>
STA 270	Applied Statistics	Fall 2021	<b>78.78%</b>

**Designed/Developed New Data Science Courses at Eastern Kentucky University, Richmond, KY**

Course Title	Level	Credits	Institution	Modality
Statistical Machine Learning	G	3	Eastern Kentucky University	In-person
Introduction to Data Science	U	3	Eastern Kentucky University	In-person

**Department of Mathematics & Statistics, East Tennessee State University, Johnson City, TN, USA  
(2013-2015)**

Course Prefix & Number	Course Title	Number of Times Taught	Credits Hours	Mode of Teaching	Level
MAT 1330	Probability & Statistics-Non-calculus	3	3	In-person	G
MAT 1530 L	Probability & Statistics -Non-calculus (Learning Support)	3	4	In-person	UG

**OTHER TEACHING EXPERIENCE**

**Department of Mathematics & Statistics, Wesley Girls' High School, Cape Coast, Ghana (2009-2013)**

Course	Course Title	Number of Times Taught	Credits Hours	Mode of Teaching	Level
Elective Mathematics/College Algebra	High School Mathematics for students who intended to study undergraduate science-related programs.	9	14	In-person	HS
Core Mathematics	High School Mathematics for all students	9	9	In-person	HS

**Montessori Junior High School, Pedu, Cape Coast, Central Region, Ghana (2006 -2007)**

Course	Course Title	Number of Times Taught	Credits Hours	Mode of Teaching	Level
All elementary school subjects	Elementary School Subjects (Grade 1-3)	9	28	In-person	E

**Cherish International School, Pedu, Cape Coast, Central Region, Ghana (2004-2006)**

Course	Course Title	Number of Times Taught	Credits Hours	Mode of Teaching	Level
All elementary school subjects	Elementary School Subjects (Grade 1-3)	9	28	In-person	E



## UNIVERSITY RESEARCH EXPERIENCE

### PUBLISHED WORKS (PATENTS, PUBLICATIONS, AND THESIS)

#### Patents (Inventions)

1. Bowroju, K.S., Crooks, P., Penthala N., Ayyadevera, S., Guzman, M., Reis S.J.R., Lopes E., **Kakraba, S.** International Patent Publication WO2021163572A1. World Intellectual Property Organization, Aug. 19, 2021. Accessible link: <https://patents.google.com/patent/WO2021163572A1/en>
2. Bowroju, K.S., Crooks, P., Penthala N., Ayyadevera, S., Guzman, M., Reis S.J.R., Lopes E., **Kakraba, S.** US Patent Number: PCT/US/2021/017970

#### Publications/Peer-Reviewed Journals

1. **Kakraba S**, Ayyadevara S, Mainali N, Balasubramaniam M, Bowroju S, Penthala NR, Atluri R, Barger SW, Griffin ST, Crooks PA, Shmookler Reis RJ. *Thiadiazolidinone (TDZD) Analogs Inhibit Aggregation-Mediated Pathology in Diverse Neurodegeneration Models, and Extend C. elegans Life- and Healthspan*. Pharmaceuticals (Basel). 2023 Oct 20;16(10):1498. doi: 10.3390/ph16101498. PMID: 37895969; PMCID: PMC10610358. Accessible link : <https://doi.org/10.3390/ph16101498>
2. Netsey, E. K., **Kakraba, S.**, Naandam, S. M., & Yadem, A. C. (2021). *A Mathematical Graph-Theoretic Model of Single Point Mutations Associated with Sickle Cell Anemia Disease*. Journal of Advances in Biotechnology, 9, 1–14. Accessible link: <https://doi.org/10.24297/jbt.v9i.9109>
3. Samuel M. Naandam, Gideon K. Gogovi, and **Samuel Kakraba** (2022) *Temperature Effect on the Structural Dynamics of SARS-CoV-2 Nucleocapsid Domain*. Advances in Computer Vision and Computational Biology, Springer Nature - Research Book Series (Accepted, in press)
4. Bowroju, S. K., Mainali, N., Ayyadevara, S., Penthala, N. R., Krishnamachari, S., **Kakraba, S.**, Reis, R. J., & Crooks, P. A. (2020). *Design and synthesis of novel hybrid 8-Hydroxy quinoline-indole derivatives as inhibitors of A $\beta$  self-aggregation and metal chelation-induced A $\beta$  aggregation*. Molecules, 25(16), 3610. Accessible link: <https://doi.org/10.3390/molecules25163610>
5. Balasubramaniam, M., Ayyadevara, S., Ganne, A., **Kakraba, S.**, Penthala, N. R., Du, X., ... Reis, R. J. (2019). *Aggregate Interactome Based on Protein-Crosslinking Interfaces Predicts Drug Targets to Limit Aggregation in Neurodegenerative Diseases*. SSRN Electronic Journal. doi:10.2139/ssrn.3362341. Accessible link: <https://doi.org/10.1016/j.isci.2019.09.026>
6. **Kakraba S.**, Ayyadevara S, Penthala NR, Balasubramaniam M, Ganne A, Liu L, Alla R, Bommagani SB, Barger SW, Griffin WST, Crooks PA, and Shmookler Reis RJ (2019). *A Novel Microtubule-Binding Drug Attenuates and Reverses Protein Aggregation in Animal Models of Alzheimer's Disease*. Front. Mol. Neurosci. 12:310. doi: 10.3389/fnmol.2019.00310. Accessible link: <https://doi.org/10.3389/fnmol.2019.00310>

7. Ayyadevara, S., Balasubramaniam, M., **Kakraba, S.**, Alla, R., Mehta, J. L., & Shmookler Reis, R. J. (2017). *Aspirin-Mediated Acetylation Protects Against Multiple Neurodegenerative Pathologies by Impeding Protein Aggregation*. *Antioxidants & Redox Signaling*, 27(17), 1383-1396. doi:10.1089/ars.2016.6978  
Accessible link: <http://doi.org/10.1089/ars.2016.6978>
8. **Kakraba, S.**, & Knisley, D. (2016). *A graph-theoretic model of single point mutations in the cystic fibrosis transmembrane conductance regulator*. *Journal of Advances in Biotechnology*, 6(1),780-786. doi:10.24297/jbt.v6i1.4013.  
Accessible link: <https://doi.org/10.24297/jbt.v6i1.4013>

### **Published Thesis/Dissertations**

1. **Kakraba, S.** (2021). *Drugs That Protect Against Protein Aggregation in Neurodegenerative Diseases* (Order No. 28648972). Available from ProQuest Dissertations & Theses Global (2569992650).  
<https://www.proquest.com/dissertations-theses/drugs-that-protect-against-protein-aggregation/docview/2569992650/se-2>
2. **Kakraba, Samuel**, *A Hierarchical Graph for Nucleotide Binding Domain 2* (2015). *Electronic Theses and Dissertations*".  
Accessible link: <https://dc.etsu.edu/etd/2517>

### **Manuscripts in preparation**

1. Methods of generating novel molecular descriptors/database for the 20 most essential amino acids.
2. Data science-driven machine learning predictive modeling of amino acids.
3. Data Science-driven image classification and analysis of bioassays- A case study on human neuroblastoma cell lines expressing amyloid aggregates.
4. Designing better DNA polymerase inhibitors for treatment of cancer through data science-driven machine learning predictive modeling.
5. Computer-aided drug discovery for DNA polymerase inhibitors for tumor cells.
6. Machine learning quantitative-structure activity relationship for drug discovery—a case study of the Quinoline family of small molecules.
7. Comparison of performance of machine learning algorithms in quantitative structure-activity relationship predictive modeling for predicting anti-leukemic activity of small molecule library.
8. Interface of graph-theoretic predictive modeling with machine learning for insight into COVID-19 mutations.
9. Insight into mutations associated with Sickle Cell Anemia disease by molecular modeling and simulation.
10. Age difference in associations of alcohol consumption and skin allergy with nonmelanoma skin cancer in US adults.

## SELECTED PROFESSIONAL MEETINGS/CONFERENCES/PRESENTATIONS

1. **Kakraba, S.**, Johnson J., Mainali, N., Penthala, R. N., Crooks A. P., Compadre M. C., Reis, R. J.S., Barger, W. S., and Ayyadevara S. *Computer-aided drug discovery and design to modeling of the inhibition of protein aggregation for treatment of neurodegenerative diseases*. Poster session presented at 15th Annual Midsouth Computational Biology & Bioinformatics Society (MCBIOS) Conference, USA, 2023
2. **Kakraba, S.** *Application of machine learning to drug discovery and design-the case of modeling of anti-leukemia activity of small molecules*. Oral presentation at Coffee Time, Department of Mathematics and Statistics, Eastern Kentucky University, Richmond, KY, USA, Fall 2022  
Accessible link: <https://math.eku.edu/coffee-time>
3. **Kakraba, S.** *Application of machine learning to modeling of the inhibition of protein aggregation as a tool to develop drugs to treat neurodegenerative diseases*. Oral session presented at 14th Annual Midsouth Computational Biology & Bioinformatics Society (MCBIOS) Virtual Conference, USA, 2022
4. Samuel M. Naandam, Gideon K. Gogovi, **Samuel Kakraba**. (July 2022) *Temperature Effect on the Structural Dynamics of SARS-CoV-2 Nucleocapsid Domain*. Oral session presented at the 23rd International Conference on Bioinformatics & Computational Biology (BIOCOMP'22), 2022  
Accessible: <https://american-cse.org/static/CSCE22-book-abstracts-printing.pdf>
5. **Kakraba, S.**, EKU Mathematics and Statistics Colloquium Talk (Spring 2022) on 02/16/2022 titled *A Mathematical Graph-Theoretic Model of Single Point Mutations Associated with Sickle Cell Anemia Disease*.  
Accessible link: <https://math.eku.edu/insidelook/colloquium-dr-samuel-kakraba-0>
6. **Kakraba, S.** *Application of Machine Learning in Drug Design and Discovery*, Colloquium Talk (Fall 2021), Department of Mathematics and Statistics, Eastern Kentucky University, Richmond, KY, USA, 09/2021  
Accessible link: <https://math.eku.edu/archive/202109>
7. **Kakraba, S.**, Ayyadevara, S., Penthala, N. R., Compadre, C., Crooks, A. P., & Shmookler Reis, R. J. (Nov 2019). *Using quantitative structure-activity relationship approach for identifying novel drugs for the treatment of neurodegenerative diseases*. Oral session presented at Southeast Regional IDEa Conference, Galt House Hotel, Louisville, KY, USA.
8. **Kakraba, S.**, Ayyadevara, S., Penthala, N. R., Compadre, C., Crooks, A. P., & Shmookler Reis, R. J. (Nov 2019). *Identification of Novel Drugs for Treatment of Neurodegenerative Diseases by Quantitative Structure-Activity Approach*. Oral session presented at Drug Discovery & Colloquium (DDC), the University of Arkansas at Little Rock, Little Rock, AR, USA.  
Accessible link: [https://ualr.edu/bioinformatics/files/2019/06/DDDC\\_2019\\_Program\\_Fin\\_06\\_12\\_19.pdf](https://ualr.edu/bioinformatics/files/2019/06/DDDC_2019_Program_Fin_06_12_19.pdf)
9. Ayyadevara, S., **Kakraba, S.**, Penthala, N. R., Balasubramaniam, M., Ganne, A., Liu, L., Alla, R., Bommagani, S., Barger, S., Griffin, T. S., Crooks, A. P., & Shmookler Reis, R. J. (June 2019). *A novel microtubule-binding drug attenuates and reverses protein aggregation in animal models of Alzheimer's disease*. Poster session presented at 22nd International C. elegans Conference, Los Angeles, CA, USA.
10. Balasubramaniam, M., Ayyadevara, S., Ganne, A., **Kakraba, S.**, Penthala, N. R., Du, X., ... Reis, R. J. (2019). *Aggregate Interactome Based on Protein-Crosslinking Interfaces Predicts Drug Targets to Limit Aggregation in Neurodegenerative Diseases*. Poster session presented at National Science Foundation (NSF), Chicago, USA
11. **Kakraba, S.**, Ayyadevara, S., Penthala, N. R., Compadre, C., Crooks, A. P., & Shmookler Reis, R. J. (June 2018). *Identifying Novel Drugs for Treatment of Neurodegenerative Diseases by Quantitative Structure-*

- Activity Approach.** Poster session presented at National IDeA Symposium of Biomedical Research Excellence (NISBRE), Washington DC, USA.
12. **Kakraba, S.**, Ayyadevara, S., Penthalala, N. R., Compadre, C., Crooks, A. P., & Shmookler Reis, R. J. (March 2018). *Using quantitative structure-activity relationships in drug discovery to identify potential drugs to treat neurodegenerative diseases*. Poster session presented at 14th Annual MCBIOS: XV, Midsouth Computational Conference, The Mill Conference Center at MSU, Starkville, MS, USA
  13. **Kakraba, S.**, Ayyadevara, S., Penthalala, N. R., Compadre, C., Crooks, A. P., & Shmookler Reis, R. J. (June 2017). *Screening and Characterization of Drugs to Block Protein Aggregation in Neurodegenerative Diseases*. Poster session presented at Southeast Regional IDeA Conference, West Virginia University, West Virginia, USA.
  14. **Kakraba, S.**, Ayyadevara, S., Penthalala, N. R., Compadre, C., Crooks, A. P., & Shmookler Reis, R. J. (June 2017). *Drugs to Block Protein Aggregation in Neurodegenerative Diseases*. Poster session presented at Drug Discovery and Development Colloquium (DDC), the University of Arkansas for Medical Sciences, Little Rock, USA.
  15. Bowroju, K.S., Balasubramaniam, M., **Kakraba, S.**, Penthalala, N. R., Ayyadevara, S., Compadre, C., Crooks, A. P., & Shmookler Reis, R. J. (June 2017). *Design and Synthesis of Cyanoreseveratrol Analogs to Prevent and Treat Age-Related Sarcopenia*. Poster session presented at Drug Discovery and Development Colloquium (DDC), the University of Arkansas for Medical Sciences, Little Rock, USA.
  16. Bowroju, K.S., Balasubramaniam, M., **Kakraba, S.**, Penthalala, N. R., Ayyadevara, S., Compadre, C., Crooks, A. P., & Shmookler Reis, R. J. (May 2017). *P16-Synthesis and Evaluation of Novel Drug Molecules to Prevent and Treat Age-related Sarcopenia*. Poster session presented at MALTO Program Schedule, The University of Louisiana Monroe, Monroe, LA 71209, USA.
  17. **Kakraba, S.**, Ayyadevara, S., Penthalala, N. R., Crooks, A. P., & Shmookler Reis, R. J. (March 2017). *Screening and characterization of small molecules that reduce A $\beta$ 1-42 amyloid aggregation in nematode C. elegans*. Oral session presented at 14th Annual MCBIOS: XIV, Midsouth Computational Conference, Embassy Suites, Little Rock, AR, USA.
  18. **Kakraba, S.**, Ayyadevara, S., Penthalala, N. R., Crooks, A. P., & Shmookler Reis, R. J. (April. 2016). *Effects of small molecules on protein aggregation and paralysis in C. elegans expressing A $\beta$ 1-42 in muscle*. Poster session AR-BIC Second Annual Conference, Little Rock, AR, USA.  
Accessible link: <http://www.arkansasbioinformatics.org/poster-abstracts-2016.htm#Kakraba>
  19. **Kakraba, S.**, Ayyadevara, S., Penthalala, N. R., Crooks, A. P., & Shmookler Reis, R. J. (June 2016). *Effects of small molecules on protein aggregation and paralysis in C. elegans expressing A $\beta$ 1-42 Muscle*. Oral session presented at National (NISBRE), Washington DC, USA.  
Accessible links: <https://na.eventscloud.com/ehome/index.php?eventid=135902&tabid=415648>
  20. **Kakraba, S.** (June 2016). *Drug Design and Discovery*. Visiting speaker for Prof. Debra Knisley and Prof. Ariel Cintron-Arias 2015 Mathematical Association of America's SUMMA Program-Strengthening Underrepresented Minorities in Mathematical Achievement and funded by National Security Agency, East Tennessee State University, Johnson City, TN, USA  
Accessible link: <https://static1.squarespace.com/static/5e9b687d5c9c9e499bb04b9d/t/5ec1606eaa8738407dcaf72c/1589731446009/Report+ETSU+NSA+REU.pdf>

21. **Kakraba, S.**, Knisley, J., D. (Mar 2015). *A graph-theoretic model of nucleotide-binding domain 2 of the cystic fibrosis transmembrane conductance regulator*. Oral session presented at 13th Annual MCBIOS: XIII, Midsouth Computational Biology and Bioinformatics Society Conference, Memphis, TN, USA
22. **Kakraba, S.**, Ke-Sheng Wang (Nov. 2015). *Association of Alcohol Consumption and Skin Allergy with Non-Melanoma Skin Cancer: Findings from the 2012 National Health Interview Survey*. Oral session presented at 2015 Southeast Regional IDeA Meeting, Biloxi, Mississippi  
 Accessible link: <https://seidea15.com/wp-content/uploads/2015/11/SE-IDeA-2015-Abstract-Book.pdf>

### SUPERVISED GRADUATE CAPSTONE/DISSERTATION

Mentee	Department /University	Project Title	Degree	Duration
Stephen D. Mcqueen	Department of Mathematics and Statistics, Eastern Kentucky University, Richmond, KY, USA	Optimization of machine learning models for predicting deposit terms subscription in bank marketing	M.A (Applied Mathematics)	Fall 2023
Kamala Krishna Buddharaju	Department of Mathematics and Statistics, Eastern Kentucky University, Richmond, KY, USA	Modeling drug-induced liver toxicity by machine learning-driven quantitative structure activity relationship (QSAR)	M.A (Applied Mathematics)	Fall 2022
Samuel Christopher (Co-supervised with Dr. Lisa Kay)	Department of Mathematics and Statistics, Eastern Kentucky University, Richmond, KY, USA	Optimizing machine learning algorithms in Shiny App for improved predictions	M.A (Applied Mathematics)	Fall 2022
Edem K. Netsey (Co-supervised with Dr. Samuel M. Naandam)	Department of Mathematics, University of Cape Coast, Cape Coast, Ghana,	A mathematical graph-theoretic model of single point mutations associated with Sickle Cell Anemia Disease <i>(Published in peer-reviewed journal)</i>	MPhil (Mathematics)	2020/2021

### PROFESSIONAL AFFILIATIONS

Organization/Institution	Role/Service	Year
GeroScience, Official Journal of the American Aging Association (AGE), USA	Reviewer	2024
Computational Biology and Bioinformatics Journal	Reviewer	2023 to present
International Society for Computational Biology (ISCB)	Member	2023 to present
American Statistical Association (ASA), USA	Member	2023 to present
American Mathematical Association (AMA), USA	Member	2023 to present.
Midsouth Computational Biology and Bioinformatics Society (MCBIOS), USA	Member	2015 to present
American Association of University Professors, USA	Member	2021 to present
Journal of Advances of Biotechnology	Reviewer	2021- present
University of Arkansas at Little Rock & University of Arkansas for Medical Science Bioinformatics Club - Chapter of the MCBIOS, Little Rock, AR, USA	Vice President	2016/2017
American Mathematical Society, Washington DC, USA	Member	2014/2015
Kappa Mu Epsilon (KME) Tennessee Beta Chapter, TN, USA	Member	2015
ETSU Abstract Algebra Club, Department of Mathematics and Statistics, East Tennessee State University, Johnson City, TN, USA	Member	2014/2015

## INSTITUTIONAL SERVICE

<b>My Role</b>	<b>University/Institution</b>	<b>Service</b>	<b>Date</b>
Member	Doctoral Admission Committee, Department of Biostatistics and Data Science, Tulane School of Public Health and Tropical Medicine, Tulane University, New Orleans, LA 70012	Doctoral application reviews	Spring 2024
Director	Statistical Consulting Center, Eastern Kentucky University, Richmond, KY 40475, USA	Providing research support service that provides free <i>statistical consulting services</i> to faculty and both graduate and undergraduate students.	Aug. 2023 – Dec. 2023
Member	University Academic Integrity Appeals Committee, Eastern Kentucky University	University academic integrity appeals	Aug. 2023 – Dec. 2023
Member (Elected)	College of STEM Research & Faculty Development, Eastern Kentucky University	Research and faculty development	Aug. 2023 – Dec. 2023
Member	Department of Mathematics and Statistics, Eastern Kentucky University	Symposium	2023/2024
Member	Wilson Endowment, Department of Mathematics and Statistics, Eastern Kentucky University	Scholarship application reviews for students applying for the Wilson Endowment	2023/2024
Member	Scholarship Committee, Eastern Kentucky University, Richmond, KY, USA	Scholarship application reviews for students applying for	Fall 2023
Member	Graduate Committee, Eastern Kentucky University, Richmond, KY, USA	Graduate program review, recruitment, retention	Fall 2023
Chair	Eastern Kentucky University, Richmond, KY, USA	The Thirty-Fifth Annual Eastern Kentucky University Symposium in Mathematics and Statistics	Spring 2023
Volunteer	Eastern Kentucky University, Richmond, KY, USA	Workshop to Inspire Statistical Excellence (W.I.S.E)	Spring 2023
Recruiter	Eastern Kentucky University, Richmond, KY, USA	Recruiting at College of STEM Goes Red Event	Spring 2023
Director of the Statistical Consulting Center	Eastern Kentucky University	Providing timely statistical consulting services to faculty, graduate, and undergraduate students at EKU.	Fall 2023- Spring 2024
Member	Eastern Kentucky University, Richmond, KY, USA	Mathematics Faculty Retreat to work on curriculum enrollment and retention issues at College of STEM	Spring 2023
Facilitator	Eastern Kentucky University, Richmond, KY, USA	Workshop for Model School students geared toward recruitment for our program.	Spring 2023

Member	Eastern Kentucky University, Richmond, KY, USA	Ad-hoc Statistics Search Committee (Search for one tenure-track assistant professor of statistics)	Spring 2023
Recruiter	Eastern Kentucky University, Richmond, KY, USA	Recruiting Statistics Club members at Colonel Craze	Spring 2022
Moderator	Eastern Kentucky University, Richmond, KY, USA	The Thirty-Fourth Annual Eastern Kentucky University Symposium in Mathematics and Statistics	Spring 2022
Volunteer	Eastern Kentucky University, Richmond, KY, USA	Big E Welcome Event for first-year students	Fall 2022
Consultant	Eastern Kentucky University, Richmond, KY, USA	Bluegrass DataFest 2022, College of STEM	Spring 2022
Volunteer	Eastern Kentucky University, Richmond, KY, USA	Workshop to Inspire Statistical Excellence (W.I.S.E)	Spring 2022
Volunteer	Eastern Kentucky University, Richmond, KY, USA	Welcome Address, Carter G Academy STEM Day Welcome, College of STEM	Spring 2022
Instructional Designer	Eastern Kentucky University, Richmond, KY, USA	Development of new seminar course “STA 880: Statistical Machine Learning in R” for Spring 2022	Spring 2022
Member	Eastern Kentucky University, Richmond, KY, USA	Ad-hoc Statistics Search Committee (Search for one tenure-track assistant professor of statistics)	Fall 2021 - Spring 2022
Recruiter	Eastern Kentucky University, Richmond, KY, USA	Improving enrollment through local and international recruitment efforts and advising	Fall 2021- Fall 2023
Member	Eastern Kentucky University, Richmond, KY, USA	Graduate Committee, Department of Mathematics and Statistics	Fall 2021- Fall 2023
Member	Eastern Kentucky University, Richmond, KY, USA	Statistics Committee, Department of Mathematics and Statistics	Fall 202- Fall 2023
Member	Eastern Kentucky University, Richmond, KY, USA	Publication, Recruitment, & Alumni Committee, Department of Mathematics and Statistics	Fall 2021- Fall 2023
Member	Eastern Kentucky University, Richmond, KY, USA	Endowment Committee, Department of Mathematics and Statistics	Fall 2021- Fall 2023
Member	Eastern Kentucky University, Richmond, KY, USA	Scholarship Committee, Department of Mathematics and Statistics	Fall 2021- Fall 2023
Chair	Eastern Kentucky University, Richmond, KY, USA	Symposium Committee, Department of Mathematics and Statistics	Fall 2022- Fall 2023
Member	Eastern Kentucky University, Richmond, KY, USA	Statistics Club, Department of Mathematics and Statistics	Fall 202- Fall 2023
Member	Eastern Kentucky University, Richmond, KY, USA	Symposium Committee, Department of Mathematics and Statistics	Fall 2021- Spring 2022
Co-chair	MCBIOS Conference, Memphis, TN, USA	Next Generation Sequence Section	2016/2017
Vice President	University of Arkansas at Little Rock and the University of Arkansas for Medical Sciences, AR, USA	Vice president of the Midsouth Computational Biology and Bioinformatics Society (MCBIOS), Little Rock Chapter, Little Rock, AR	2016/2017

Founder and President	University Practice Senior High School, Cape Coast, Central Region, Ghana	Founded the wildlife conservation club geared toward ecology and conservation, organized workshops, and mentored future leaders for the club, thereby ensuring the sustainability of the club	2002-2004
House Prefect	University Practice Senior High School, Cape Coast, Central Region, Ghana	Pra House Prefect and	2003-2004
Member	University Practice Senior High School, Cape Coast, Central Region, Ghana	Board member of the Students Representative Council	2003-2004
Library Prefect	Tuwohofo Holly International School, Akotokyir, Cape Coast, Central Region, Ghana	Encouraging reading among all students, oversight of all library books and library- related activities	1999-2001
School Prefect (Head Boy)	Tuwohofo Holly International School, Akotokyir, Cape Coast, Central Region, Ghana	Chanell for communication between school authorities and students. Oversight of responsibility allocation to students, ensuring that school rules and regulations are properly followed by students	1998-1999

### **PROFESSIONAL DEVELOPMENT**

1. Junior Faculty Mentorship Program, College of Science, Technology, Engineering, & Mathematics, Eastern Kentucky University, Richmond, KY, USA, 2021-2023
2. Eastern Kentucky University New Faculty Orientation, Richmond, KY, USA, August 2021
3. Attended department PD session on technology for the classroom, Eastern Kentucky University, Richmond, KY, USA, 2021
4. Attended STA 270 workshop, Eastern Kentucky University, Richmond, KY, USA, Fall 2021
5. Attended WebAssign training, Eastern Kentucky University, KY, USA, Fall 2021
6. Attended Junior Faculty Mentoring Program for first-year mentees by Eastern Kentucky University: Orientation (Fall 2021–Spring 2022), Richmond, KY, USA
7. Structure of COS Junior Faculty Mentoring Program, Best Practices on Faculty Mentoring, and Expectations for Mentors and Mentees Legal Issues for Faculty Evaluating Teaching Effectiveness Time Management: Balancing Professional and Personal Life, Eastern Kentucky University, Richmond, KY, USA, 2022
8. Attended workshop hosted by EKU’s Faculty Center for Teaching and Learning: “Integrating Learning Targets into Your Classroom Instruction and Assessment”, Richmond, KY, USA, Fall 2021



## OPEN RESOURCE CERTIFICATIONS

<b>Certification</b>	<b>University/Institution</b>	<b>Platform</b>	<b>Year</b>	<b>Link to certificates</b>
R Programming	Johns Hopkins University, USA	Coursera	2016	<a href="https://coursera.org/share/bdc762aa0c72dc7591c6abcf9659949a">https://coursera.org/share/bdc762aa0c72dc7591c6abcf9659949a</a>
The Data Scientist's Toolbox	Johns Hopkins University, USA	Coursera	2016	<a href="https://coursera.org/share/64c989c07e3923a2fec13946ae895cb0">https://coursera.org/share/64c989c07e3923a2fec13946ae895cb0</a>
Drug Discovery	University of California, San Diego, USA	Coursera	2016	<a href="https://coursera.org/share/1fa7f38b1e807fbb8014774caa50344b">https://coursera.org/share/1fa7f38b1e807fbb8014774caa50344b</a>