

## Whelton A. Miller III

Assistant Professor  
Department of Medicine  
Health Sciences Division  
Loyola University Medical Center  
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### (a) Professional Preparation

Institution	Major/Concentration	Degree & Year
University of Delaware, Newark, DE	Biochemistry	B.S., 2001
University of the Sciences (Saint Joseph's University), Philadelphia, PA	Theoretical/Computational Physical Organic Chemistry	Ph.D., 2012
University of Pennsylvania, Philadelphia, PA	Bioengineering	Postdoc, 2012-2015

**Thesis Title:** "Computational Study of Substituent effects on Organometallic and Inorganic Compounds: A Novel Class of Paramagnetic Chemical Exchange Saturation Transfer Agents, and Cyclic Phosphazenes"

### (b) Graduate and Postdoctoral Advisors:

Advisor	Name	Present Affiliation
Ph.D.	Dr. Preston B. Moore	Department of Chemistry, University of the Sciences, Philadelphia, PA
Postdoc	Dr. Ravi Radhakrishnan	Department of Bioengineering, University of Pennsylvania, Philadelphia, PA

### (c) Research Areas

Bioengineering, Bioinformatics, Biomedical Engineering, Biomolecular Engineering, Biophysics, Computational Biology, Computational Chemistry, Computer Aided Drug Design, Computational Science, Computational Resource Management, Electronic Structure Methods, Materials Science, Molecular Dynamics Simulations, Organometallic Compounds, Quantum Mechanics, Reaction Modeling, STEM Education

### (d) Highlighted Skills

Linux/Unix systems, Windows systems, Apple OS X, Python, R, C and C++ Programming, Good Verbal and Written Communication Skills, Synthetic Organic Chemistry, NMR Spectroscopy, IR, HPLC, LC/MS, and Reverse Phase Chromatography, Ab Initio Computational and Semi-Empirical Quantum Chemistry Methods, Computer Systems Repair Administration and Networking

### **(e) Research Summary**

Understanding fundamental relationships ranging from the quantum level can be essential to understanding the overall system. From graduate school onward, the focus of my research has been using computational chemistry techniques, such as Density Functional Theory (DFT) and Molecular Dynamics (MD), for theoretical design and study of small molecular (organic) compounds, organometallic and inorganic compounds, protein ligand interactions, polymer design and characterization, and drug design. My goal is to employ several computational techniques to understand, as well as predict molecular interactions, e.g., protein-ligand interactions and protein-protein interactions. Some examples of projects I'm working on are, Magnetic Resonance Imaging (MRI) contrast agents, and small molecular inhibitors of Anaplastic Lymphoma Kinase (ALK).

### **(f) Appointments**

#### Current Appointments:

Dates	Position
2019-	Assistant Professor (primary), Department of Medicine, Loyola University Medical Center, Loyola University Chicago, Chicago, IL
2022-	Director, Center for Biophysical Simulations (CBS), Department of Medicine, Loyola University Medical Center, Loyola University Chicago, Chicago, IL
2023-	Director, Institute for Racial Justice SSOM Annex, Department of Medicine, Loyola University Medical Center, Loyola University Chicago, Chicago, IL
2021-	Faculty Affiliate, Institute for Racial Justice, Loyola University of Chicago, Maywood, IL
2020-	Assistant Professor (secondary), Department of Molecular Pharmacology & Neuroscience, Loyola University Medical Center, Loyola University of Chicago, Maywood, IL
2020-	Assistant Professor (secondary), Bioinformatics Program, Loyola University Chicago, Chicago, IL
2018-	Adjunct Professor, Department of Biomedical Engineering, University of Ghana, Accra, GH
2018	Adjunct Assistant Professor, School of Engineering & Applied Science, Department of Chemical & Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA

#### Past Appointments:

Dates	Position
2015- 2019	Assistant Professor of Chemistry, Department of Chemistry, Physics, & Engineering Lincoln University, Lincoln University, PA
2015- 2019	Director, Center for Informatics and Molecular Modeling (CIMM), Department of Chemistry, Physics, & Engineering, Lincoln University, Lincoln University, PA
2018- 2019	Affiliate Assistant Professor, Loyola University Medical Center, Loyola University of Chicago, Maywood, IL

- 2015- 2018 Visiting Assistant Professor, School of Engineering & Applied Science, Department of Chemical & Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA
- 2017- 2018 Visiting Faculty, University of New Mexico, Albuquerque, NM
- 2012- 2015 Postdoctoral Research Associate, School of Engineering & Applied Science, Department of Bioengineering, University of Pennsylvania, Philadelphia, PA
- 2012- 2015 NRSA Postdoctoral Fellow, Perelman School of Medicine, Penn-PORT program (NIH-IRACDA), University of Pennsylvania, Philadelphia, PA
- 2015- 2015 Adjunct Professor, Department of Chemistry, Rutgers State University of New Jersey, Camden, NJ
- 2013- 2015 Adjunct Professor, Department of Chemistry & Physics, College of Science and Technology, Lincoln University, Lincoln University, PA
- 2001- 2004 Associate Scientist (Synthetic Organic Chemist), AstraZeneca Pharmaceuticals LP, Wilmington, DE.
- 2007- 2012 Linux Systems Administrator, West Center for Computational Chemistry and Drug Design, Department of Chemistry & Biochemistry, University of the Sciences, Philadelphia, PA.
- 1999- 1999 Research Assistant, U.S. Army Research Laboratory (ARL), Aberdeen Proving Ground, Aberdeen, MD.

**(g) Publications:**

1. Miller III, W.A. and Moore, P.B., (2014). A Quantum Mechanical Study of Structural and Electronic Dilution Effects in Paramagnetic Chemical Exchange Saturation Transfer Agents. *Journal of Organic and Biomolecular Simulations*, 1(1), p.1-13. <http://doi.org/10.3844/jobsp.2014.1.13>
2. Miller III, W.A. and Moore, P.B., (2014). Computational Study of Intramolecular Heterocyclic Ring Formation with Cyclic Phosphazenes. *International Journal of Engineering Research & Technology (Ahmedabad)*, 3(8), p.1575-1582
3. Singh, A.K., Rajendran, V., Singh, S., Kumar, P., Kumar, Y., Singh, A., Miller, W., Potemkin, V., Grishina, M., Gupta, N. and Kempaiah, P., (2018). Antiplasmodial activity of hydroxyethylamine analogs: synthesis, biological activity and structure activity relationship of plasmepsin inhibitors. *Bioorganic & Medicinal Chemistry*, 26(13), pp.3837-3844. <https://doi.org/10.1016/j.bmc.2018.06.037>
4. Kwofie, S.K., Dankwa, B., Odame, E.A., Agamah, F.E., Doe, L., Teye, J., Agyapong, O., Miller, W.A., Mosi, L. and Wilson, M.D., (2018). In silico screening of isocitrate lyase for novel anti-buruli ulcer natural products originating from Africa. *Molecules*, 23(7), p.1550. <https://doi.org/10.3390/molecules23071550>
5. Miller, I.I.I., Whelton, A., Teye, J., Achieng, A.O., Mogire, R.M., Akala, H., Ong'echa, J.M., Rathi, B., Durvasula, R., Kempaiah, P. and Kwofie, S.K., (2018). Antimalarials: Review of Plasmepsins as Drug Targets and HIV Protease Inhibitors Interactions. *Current Topics in Medicinal Chemistry*, 18(23), pp.2022-2028.
6. Kwofie, S.K., Enniful, K.S., Yussif, J.A., Asante, L.A., Adjei, M., Kan-Dapaah, K., Tiburu, E.K., Mensah, W.A., Miller, W.A., Mosi, L. and Wilson, M.D., (2019). Molecular informatics studies of the iron-dependent

- regulator (ideR) reveal potential novel anti-mycobacterium ulcerans natural product-derived compounds. *Molecules*, 24(12), p.2299. <https://doi.org/10.3390/molecules24122299>
7. Kwofie, S.K., Broni, E., Teye, J., Quansah, E., Issah, I., Wilson, M.D., Miller III, W.A., Tiburu, E.K. and Bonney, J.H., (2019). Pharmacoinformatics-based identification of potential bioactive compounds against Ebola virus protein VP24. *Computers in Biology and Medicine*, 113, p.103414.
  8. Gupta, Y., Miller III, W. A., Kwofi, S. K., Rathi, B., Durvasula, R., & Kempaiah, P. (2019, January). A Bioinformatics Pipeline to Repurpose Approved Drugs as Anti-Parasitic Leads. In *American Journal of Tropical Medicine and Hygiene* (Vol. 101, Pp. 284-284). 8000 Westpark Dr, Ste 130, Mclean, VA 22101 USA: Amer Soc Trop Med & Hygiene.
  9. Simpson, J., Gupta, Y., Goicoechea, S., Miller III, W. A., Rathi, B., Durvasula, R., & Kempaiah, P. (2019, January). Dual Pronged Attack on Malaria: Drugs with Antiparasitic And Immunomodulatory Properties. In *American Journal of Tropical Medicine and Hygiene* (Vol. 101, Pp. 478-478). 8000 Westpark Dr, Ste 130, Mclean, VA 22101 USA: Amer Soc Trop Med & Hygiene.
  10. Goicoechea, S., Gupta, Y., Simpson, J., Miller III, W. A., Rathi, B., Durvasula, R., & Kempaiah, P. (2019, January). Repurposing Fda Approved Drugs to Treat Malaria: Understanding the Mechanism of Action. In *American Journal of Tropical Medicine and Hygiene* (Vol. 101, Pp. 284-284). 8000 Westpark Dr, Ste 130, Mclean, VA 22101 USA: Amer Soc Trop Med & Hygiene.
  11. Kwofie, S.K., Broni, E., Dankwa, B., Enniful, K.S., Kwarko, G.B., Darko, L., Durvasula, R., Kempaiah, P., Rathi, B., Miller Iii, W.A. and Yaya, A., (2020). Outwitting an Old Neglected Nemesis: A Review on Leveraging Integrated Data-Driven Approaches to Aid in Unraveling of Leishmanicides of Therapeutic Potential. *Current Topics in Medicinal Chemistry*, 20(5), pp.349-366.
  12. Kwofie, S. K., Adobor, C., Quansah, E., Bentil, J., Ampadu, M., Miller III, W. A., & Wilson, M. D. (2020). Molecular docking and dynamics simulations studies of OmpATb identifies four potential novel natural product-derived anti-Mycobacterium tuberculosis compounds. *Computers in Biology and Medicine*, 103811.
  13. Kwofie, S.K., Broni, E., Dankwa, B., Enniful, K.S., Teye, J., Davidson, C.R., Nimely, J.B., Chioma Orizu, J., Kempaiah, P., Rathi, B. and Miller, W.A., 2020. Review of Atypical Organometallic Compounds as Antimalarial Drugs. *Journal of Chemistry*, 2020.
  14. Witek, G. M., Miller, W., Slochower, D., Berko, E., Mossé, Y., Lemmon, M., & Radhakrishnan, R. (2020). 4558 Investigating the functional consequences of anaplastic lymphoma kinase (ALK) mutations arising upon Lorlatinib treatment. *Journal of Clinical and Translational Science*, 4(s1), 9-10.
  15. Kwofie, S. K., Broni, E., Yunus, F. U., Nsoh, J., Adoboe, D., Miller III, W. A., & Wilson, M. D. (2021). Molecular Docking Simulation Studies Identifies Potential Natural Product Derived-Antiwoibachial Compounds as Filaricides against Onchocerciasis. *Biomedicines*, 9(11), 1682.

16. Kwofie, S. K., Dolling, N. N., Donkoh, E., Laryea, G. M., Mosi, L., Miller, W. A., ... & Wilson, M. D. (2021). Pharmacophore-Guided Identification of Natural Products as Potential Inhibitors of Mycobacterium ulcerans Cystathionine  $\gamma$ -Synthase MetB. *Computation*, 9(3), 32.
17. Sakyi, P.O., Amewu, R.K., Devine, R.N.O.A., Bienibuor, A. K., Miller III, W. A., Kwofie, S. K. "Unravelling the myth surrounding sterol biosynthesis as plausible target for drug design against leishmaniasis." *J Parasit Dis* (2021). <https://doi.org/10.1007/s12639-021-01390-1>
18. Kwofie, S. K., Agyenkwa-Mawuli, K., Broni, E., Miller III, W. A., & Wilson, M. D. (2021). Prediction of antischistosomal small molecules using machine learning in the era of big data. *Molecular Diversity*, 1-11.
19. Agyapong, O., Asiedu, S. O., Kwofie, S. K., Miller, W. A., Parry, C. S., Sowah, R. A., & Wilson, M. D. (2021). Molecular modelling and de novo fragment-based design of potential inhibitors of beta-tubulin gene of *Necator americanus* from natural products. *Informatics in Medicine Unlocked*, 100734.
20. Broni, E., Kwofie, S. K., Asiedu, S. O., Miller, W. A., & Wilson, M. D. (2021). A Molecular Modeling Approach to Identify Potential Antileishmanial Compounds Against the Cell Division Cycle (cdc)-2-Related Kinase 12 (CRK12) Receptor of *Leishmania donovani*. *Biomolecules*, 11(3), 458.
21. Agyapong, O., Miller, W. A., Wilson, M. D., & Kwofie, S. K. (2021). Development of a proteochemometric-based support vector machine model for predicting bioactive molecules of tubulin receptors. *Molecular Diversity*, 1-12.
22. Sakyi, P. O., Amewu, R. K., Devine, R. N., Ismaila, E., Miller, W. A., & Kwofie, S. K. (2021). The Search for Putative Hits in Combating Leishmaniasis: The Contributions of Natural Products Over the Last Decade. *Natural Products and Bioprospecting*, 11(5), 489-544.
23. Sakyi, P. O., Broni, E., Amewu, R. K., Miller III, W. A., Wilson, M. D., & Kwofie, S. K. (2022). Homology Modeling, de Novo Design of Ligands, and Molecular Docking Identify Potential Inhibitors of *Leishmania donovani* 24-Sterol Methyltransferase. *Frontiers in Cellular and Infection Microbiology*, 657.
24. Kwofie, S. K., Asiedu, S. O., Koranteng, R., Quarshie, E., Tiburu, E. K., Miller III, W. A., ... & Wilson, M. D. (2022). Computer-aided identification of potential inhibitors against *Necator americanus* glutathione S-transferase 3. *Informatics in Medicine Unlocked*, 30, 100957.
25. Agyapong, O., Miller, W. A., Wilson, M. D., & Kwofie, S. K. (2022). Development of a proteochemometric-based support vector machine model for predicting bioactive molecules of tubulin receptors. *Molecular Diversity*, 26(4), 2231-2242.
26. Kwofie, S. K., Agyenkwa-Mawuli, K., Broni, E., Miller III, W. A., & Wilson, M. D. (2022). Prediction of antischistosomal small molecules using machine learning in the era of big data. *Molecular Diversity*, 26(3), 1597-1607.
27. Sakyi, P.O., Kwofie, S.K., Tuekpe, J.K., Gwira, T.M., Broni, E., Miller III, W.A., Wilson, M.D. and Amewu, R.K., (2023). Inhibiting *Leishmania donovani* Sterol Methyltransferase to Identify Lead Compounds Using Molecular Modelling. *Pharmaceuticals*, 16(3), 330.

28. Broni, E., & Miller III, W. A. (2023). Computational Analysis Predicts Correlations among Amino Acids in SARS-CoV-2 Proteomes. *Biomedicines*, 11(2), 512.
29. Sakyi, P. O., Broni, E., Amewu, R. K., Miller III, W. A., Wilson, M. D., & Kwofie, S. K. (2023). Targeting Leishmania donovani sterol methyltransferase for leads using pharmacophore modeling and computational molecular mechanics studies. *Informatics in Medicine Unlocked*, 101162.
30. Broni, E., Ashley, C., Adams, J., Manu, H., Aikins, E., Okom, M., Miller III, W.A., Wilson, M.D. and Kwofie, S.K. (2023). Cheminformatics-Based Study Identifies Potential Ebola VP40 Inhibitors. *International Journal of Molecular Sciences*, 24(7), 6298.
31. Broni, E., Striegel, A., Ashley, C., Sakyi, P.O., Peracha, S., Velazquez, M., Bebla, K., Sodhi, M., Kwofie, S.K., Ademokunwa, A. and Khan, S. and Miller III, W. A. (2023). Molecular Docking and Dynamics Simulation Studies Predict Potential Anti-ADAR2 Inhibitors: Implications for the Treatment of Cancer, Neurological, Immunological and Infectious Diseases. *International Journal of Molecular Sciences*, 24(7), p.6795.

**Mentions:**

1. Clark, C. J., J. Wu, H. J. Pletsch, Lucas Guillemot, B. Allen, C. Aulbert, C. Beer et al. "The Einstein@ Home gamma-ray pulsar survey. I. Search methods, sensitivity, and discovery of new young gamma-ray pulsars." *The Astrophysical Journal* 834, no. 2 (2017): 106.

**(h) Presentations:**

1. “Lead Identification with Molecular Docking and Biomolecular Simulations”

- (i) Department of Chemistry, Claflin University, Orangeburg, SC, Fall 2018 (Oral)
- (ii) Department of Medicine, Loyola University, Maywood, IL, Spring 2019 (Oral)
- (iii) 1<sup>st</sup> International Conference on Integrative Chemistry, Biology & Translational Medicine, Feb 25-26 2019 (Oral)
- (iv) Department of Molecular Pharmacology and Neuroscience, Loyola University, Maywood, IL, Spring 2019 (Oral)

2. “Computational Modeling Workshop: Understanding Structure and Function and its Application to Computer Aided Drug Design (CADD)”

- (i) University of Ghana Computing Systems (UGCS), University of Ghana, Accra, Ghana, Spring 2017 (Oral)
- (ii) University of Ghana Computing Systems (UGCS), University of Ghana, Accra, Ghana, Spring 2018 (Oral)

3. “Molecular Docking-Intro & Tutorial”

- (i) 10th Annual Q-bio Summer, University of New Mexico, Albuquerque, NM, Summer 2016 (Oral)
- (ii) 11th Annual Q-bio Summer, Colorado State University, Fort Collins, CO, Summer 2017 (Oral)

4. “Structural and Electronic Relationships in the Anomeric Effect”

- (i) Lincoln University 9th Annual Science Conference, Spring 2015 (Oral, Student)
- (ii) Louis Stokes Alliance for Minority Participation (LSAMP), Spring 2015 (Poster)

5. “IRACDA Collaboration Network (ICN): Development of a Collaboration Network for Current and Past IRACDA Fellows”

- (i) Institutional Research and Academic Career Development Awards (IRACDA) Conference, San Diego, CA, June 2015 (Poster)

6. “Computational Study of Interaction of Small Drug Molecules and Anaplastic Lymphoma Kinase (ALK) Mutations”

- (i) Philadelphia Section ACS YCC Poster Session, April 2014 (Poster)

7. “Using Molecular Simulation to Elucidate the Structure, Function, Dynamics, and Energetics of Complex Molecular Systems”

- (i) Institutional Research and Academic Career Development Awards (IRACDA) Conference, New Mexico, June 2014 (Poster)
- (ii) Lincoln University 19th Annual Science Fair, October 2014 (Poster)

8. “Computational Study of Substituent effects on Organometallic and Inorganic Compounds: A Novel Class of Paramagnetic Chemical Exchange Saturation Transfer Agents, and Cyclic Phosphazenes”

- (i) Sandia National Laboratory, June 2014 (Oral)
- (ii) Los Alamos National Laboratory, June 2014 (Oral)

9. “Computational Study of Structural Modifications to a Novel Class of Paramagnetic Chemical Exchange Saturation Transfer Agents”

- (i) USP Scholarly Day 2007, April 2007 (Poster)
- (ii) ACS Mid-Atlantic Regional Meeting (MARM), May 2007 (Poster)
- (iii) Philadelphia Section ACS-8th Annual Graduate Student & 3rd Annual Undergraduate Poster Sessions, January 2008 (Poster)
- (iv) 235<sup>th</sup> ACS National Meeting New Orleans, LA, April 2008 (Poster)
- (v) USP Research Day 2008, April 2008 (Poster)
- (vi) 2008 NBCR Summer Institute, August 2008 (Poster)
- (vii) International Interdisciplinary Scientific Research Congress (IX CIC) Santo Domingo, Dominican Republic, June 2013 (Oral)

(viii) 249<sup>th</sup> ACS National Meeting Denver, CO, March 2015 (Oral)

10. “Computational Study of the Electronic Structure and Function of a Novel Class of Cyclic Phosphazenes”

- (i) USP Research Day 2009, April 2009 (Poster)
- (ii) 2009 NBCR Summer Institute, August 2009 (Poster)
- (iii) ACS Mid-Atlantic Regional Meeting (MARM), May 2010 (Poster)
- (iv) 244<sup>th</sup> ACS National Meeting Philadelphia, PA, August 2012 (Oral)

11. “Computational Method of Calculating the Surface area of Nanostructures”

- (i) USP Research Day 2009, April 2009 (Poster)

**(i) Synergistic Activities:**

- 1. Professional member, American Chemical Society (ACS), 2001-present,
- 2. Professional member, Biophysical Society, 2013-present,
- 3. Professional member, National Organization of Black Chemist and Chemical Engineers (NOBCChE), 2001-2005, 2013-present
- 4. University of Pennsylvania, Institute for Translational Medicine and Therapeutics (ITMAT), Associate Member, 2013-present
- 5. University of Pennsylvania, Penn Institute for Computational Science (PICS), Member, 2013-present
- 6. Chair, Engineering Postdoc Association (EPoD), February 2013 – July 2015. University of Pennsylvania, School of Engineering and Applied Science, Philadelphia, PA
- 7. Biomedical Postdoctoral Council (BPC), October 2012 – August 2015. University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA
- 8. Educational Journal Club, November 2012 – July 2015. University of Pennsylvania, Philadelphia, PA
- 9. Graduate Ambassador, September 2011-October 2012. University of the Sciences in Philadelphia, College of Graduate Studies, Philadelphia, PA
- 10. President, May 2008-September 2009. University of the Sciences in Philadelphia, Graduate Student Organization (GSO), Philadelphia, PA
- 11. Chemistry Representative, August 2007 – May 2008. University of the Sciences in Philadelphia, Graduate Student Organization, Philadelphia, PA
- 12. Co-Chair, July 2002 – July 2003. AstraZeneca Core Diversity Challenge Team Wilmington, DE.

**(j) Professional Committees & Service:**

- 1. Faculty Member, Stritch School of Medicine (SSOM) Admissions, Executive Admissions Committee, Loyola University Chicago, Summer 2022 – present



2. Faculty Member, Stritch School of Medicine (SSOM) Admissions, Executive Admissions Committee, Diversity Equity & Inclusion (DEI) subcommittee, Loyola University Chicago, Summer 2022 - present
3. Faculty Member, Stritch School of Medicine (SSOM) Student Appeal Board (SAB), Loyola University Chicago, Spring 2022 - present
4. Faculty Member, Stritch School of Medicine (SSOM) Awards Committee, Loyola University Chicago, Spring 2022 - present
5. Faculty Member, Stritch School of Medicine (SSOM) Admissions, Selection Committee, Loyola University Chicago, Fall 2021 – present
6. Reviewer, Ford Foundation, 2021 - present
7. Visiting Faculty Panelist, Department of Energy (DOE) - National Organization of Black Chemist and Chemical Engineers (NOBCChE) Conference 2022, Orlando Florida
8. Institute for Racial Justice, Strategic Planning Committee, Loyola University Chicago: nominated November 2020
9. University of Florida, Broadening Participation: 2020 MPS Workshop, November 2020: Top Mock Proposal (Panel PO2DMR)
10. ABRCMS Abstract Reviewer August 2020
11. BioRender Abstract Reviewer June 2020
12. IRACDA Conference 2018: Poster Session Judge
13. IRACDA Conference 2017: Partner School Faculty Panel
14. Graduate Student Research Day, University of the Sciences, 2017: Poster Session Judge
15. Faculty Member, Committee for General Education, Lincoln University, Fall 2017 - 2019
16. Faculty Member, Judicial Review Board, Lincoln University, Fall 2016 - 2019
17. Faculty Advisor, Prostate Cancer Research Summer Training Program, University of Iowa and Lincoln University, 2017 - 2019
18. Ad Hoc Reviewer, National Sciences Foundation
19. Ad Hoc Reviewer, Online Journal of Biological Sciences, ISSN: 1608 - 4217 (OJBS)
20. Editorial Board Member, International Journal of Computational and Theoretical Chemistry, ISSN: 2376 - 7286 (IJCTC Print), ISSN: 2376 - 7308 (IJCTC Online)
21. Ad Hoc Reviewer, International Journal of Engineering Research and Technology, ISSN: 2278 - 0181 (IJERT)
22. Seminar Speaker, NIH-NIGMS, Training, Workforce Development, & Diversity (TWD) Available Spring 2016-2017
23. Book Reviewer, “Strategies for Increasing Diversity in Engineering Majors and Careers”
24. NIH, Biochemistry and Biophysics of Membranes Study Section (BBM), Biological Chemistry and Macromolecular Biophysics Integrated Review Group, February 2021

## **(k) Grants & Awards**

1. Department of Energy (DOE) Visiting Faculty Panelist, National Organization of Black Chemist and Chemical Engineers (NOBCCChE) Conference, *Awarded* (Travel, ~\$1,500), September 2022, Role: Awardee
2. Loyola University Chicago, Faculty Center for Ignatian Pedagogy, Scholarship of Teaching and Learning (SOTL) Faculty Fellowship, *Awarded*, (\$2,000), 2021 – 2023, Role: Fellow
3. National Science Foundation (NSF) BPC-DP: Community Outreach Opportunities with Research in Data Science (COORDS), *Awarded, October 2022* (\$299,985), 10/1/22-09/30/24, Role: PI
4. National Science Foundation (NSF-2051118), REU Site: Computational Biology & Informatics Research Experience for Undergraduates (Compute REU), *Pending August 2022* (\$389,982), 9/1/23-08/31/26, Role: PI
5. National Science Foundation (NSF-2040988), NSF INCLUDES (Planning Grant): Underrepresented Student Education for STEM Informatics Research (USESIR), *Pending Resubmission* (\$99,965), Role: PI
6. National Research Mentoring Network (NRMN) *Awarded* (Travel, ~\$1,500), 09/1/20-08/31/23, Role: Awardee
7. National Institutes of Health (NIH-3U01CA227550-02S1), A Plasticity and Reprogramming Paradigm for Therapy Resistance at The Single Cell Level, *Awarded* (\$331,707), 09/1/19-08/31/24, Role: Awardee
8. National Science Foundation (NSF-1912104), Targeted Infusion Project: Lincoln University Bioinformatics Program (LUBi), *Awarded* (\$400,000), 7/1/19-06/30/22, Role: PI (former)
9. LEAPS-T: Research Component, Lincoln University 2018, *Awarded* (\$2,500), 08/31/18-05/31/19, Role: PI
10. Faculty Development Award, 2018 Lincoln University, *Awarded* (\$3,500), 06/1/18, Role: PI
11. National Science Foundation (NSF-1818693), Targeted Infusion Project: Implementation of an HBCU Undergraduate Bioinformatics Program - Lincoln University (LUBi) – Planning Grant, *Awarded* (\$179,846), 06/1/18-01/31/20, Role: PI (former)
12. LEAPS-T: Research Component, Lincoln University 2017, *Awarded* \$2,500, 08/31/17-05/31/17, Role: PI
13. National Science Foundation (NSF-1400399), 2017 Greater Philadelphia Louis Stokes Alliance For Minority Participation (LSAMP), *Awarded* (\$38,000), Summer 2017, Role: PI
14. Department of Energy (DOE), 2017 Visiting Faculty Program (VFP) Fellowship, Los Alamos National Laboratory, Los Alamos, NM., *Awarded* (\$15,000), Summer 2017, Role: co-PI
15. Undergraduate Research Council, Research Grant, Lincoln University, *Awarded* (\$6,000), Spring 2017, Role: PI
16. Department of Energy (DOE), 2016 Visiting Faculty Program (VFP) Fellowship, Los Alamos National Laboratory, Los Alamos, NM., *Awarded* (\$15,000), Summer 2016, Role: co-PI
17. Computational Equipment & Hardware, 2015 Idaho National Laboratory (INL) Education and Research Transfer Program (ERTP): *Estimated Equipment Value Awarded* (\$105,921.21), Role: PI
18. LEAPS-Forward Mach, Lincoln University 2013, *Awarded* (\$3,000), 08/31/13-05/31/14, Role: PI
19. National Institutes of Health (NIH), National Institute of General Medical Sciences (NIGMS) (NIH K12 GM081259), Institutional Research and Academic Career Development Award, 10/1/12-08/31/15, PI: Yvonne J. Paterson, Role: Project Participant/Awardee

20. Postdoc Bootcamp, University of California-San Francisco (UCSF) 2009, Travel & Attendance, *Awarded* (~\$3,000), 6/2009, Role: Awardee
21. National Biomedical Computation Resource (NBCR) Summer Institute, University of California-San Diego (UCSD) 2009, Travel & Attendance, *Awarded* (~\$3,000), 6/2009, Role: Awardee
22. Future Faculty Workshop: Diverse Leaders of Tomorrow, Massachusetts Institute of Technology (MIT) 2008, Travel & Attendance, *Awarded* (~\$2,000), 6/2008, Role: Awardee
23. Graduate Student Poster Award, William Penn Foundation 2008, Philadelphia, PA., *Awarded* (\$100), Role: Best Poster
24. National Biomedical Computation Resource (NBCR) Summer Institute, University of California-San Diego (UCSD) 2008, Travel & Attendance, *Awarded* (~\$3,000), 06/2008 Role: Awardee

### **(I) Representative Collaborators**

Name	Present Affiliation
Dr. George Acquaaah-Mensah,	Professor, Department of Pharmaceutical Science, School of Pharmacy Massachusetts College of Pharmacy & Health Sciences (MCPHS University) Worcester, MA
Dr. Terrick Andey,	Assistant Professor, Department of Pharmaceutical Science, School of Pharmacy Massachusetts College of Pharmacy & Health Sciences (MCPHS University) Worcester, MA
Dr. Karen Baskerville	Professor, Department of Biology, Lincoln University, Lincoln University, PA
Dr. William S. Hlavacek	Scientist, Theoretical Biology and Biophysics, Los Alamos National Laboratory, Los Alamos, NM
Dr. Samuel Kojo Kwofie	Lecturer, Biomedical Engineering Department, University of Ghana
Dr. Zhiwei Liu	Assistant Professor, Department of Chemistry & Biochemistry, University of the Sciences, Philadelphia, PA
Dr. Preston B. Moore	Professor, Department of Chemistry & Biochemistry, University of the Sciences, Philadelphia, PA
Dr. Brian Munsky	Assistant Professor, Department of Chemical & Biological Engineering, Colorado State University, Fort Collins, Co
Dr. Kenny Nguyen	Scientist, Center for Applied Genomics, Children's Hospital of Philadelphia
Dr. Vojislava Pophristic	Dean, College of Science & Mathematics, Professor, Department of Chemistry & Biochemistry, University of the Sciences, Philadelphia, PA
Dr. D. Vladimir Perez	Professor, Universidad Autonoma De Santo Domingo
Dr. Ravi Radhakrishnan	Professor, Department of Bioengineering, University of Pennsylvania, Philadelphia, PA

Dr. Brijesh Rathi	Assistant Professor, Department of Chemistry, Hansraj College University Enclave, University of Delhi, Delhi-110007 India
Dr. Monsheel Sodhi	Assistant Professor, Department of Molecular Pharmacology & Neuroscience, Loyola University Medical Center, Loyola University Chicago, Maywood, IL
Dr. Derrick Swinton	Professor, Associate Dean, New Jersey Center for Science, Technology, and Mathematics, Kean University, Union, NJ
Dr. Andrey Semichaevsky	Associate Professor, Department of Chemistry and Physics, Lincoln University, Lincoln University, PA
Dr. Elvis Tiburu	Chair & Lecturer, Biomedical Engineering Department, University of Ghana
Dr. Mary Watson	Associate Professor, Department of Chemistry & Biochemistry, University of Delaware, Newark, DE

**(m) Continuing Education:**

Statistical Analysis for Research in Medical Education I; Loyola University Chicago, Spring 2021, Deacon Dr. James M. Sinacore

Statistical Analysis for Research in Medical Education II; Loyola University Chicago, Spring 2021, Deacon Dr. James M. Sinacore

School on Molecular Dynamics and Enhanced Sampling Methods; Temple University, Summer 2015, Dr. Christopher M. MacDermaid

Translational Therapeutics; University of Pennsylvania, Spring 2014, Drs. Steven Siegel, Tomas Isakowitz

Postdoc Teaching Seminar; University of Pennsylvania, Spring 2013, Dr. Marybeth Gasman

Toxicology; Lehigh University, Spring 2006, Dr. Ned Heindel

Advanced Organic Chemistry; Lehigh University, Fall 2005, Dr. Ned Heindel

ACS short course in Synthetic Organic Chemistry; ACS National Meeting, March 2004, Dr. Paul Helquist

Advanza Institute Short-Course in HPLC; April 2003, Mr. C. David Carr

Practical NMR Spectroscopy; University of Delaware, Fall 2001, Dr. Steve Bai

**(n) Teaching Experience**

Loyola University Chicago, Stritch School of Medicine (SSOM), Maywood, IL

*Assistant Professor (Department of Medicine), July 2019-*

*Assistant Professor (Department of Molecular Pharmacology & Neuroscience), July 2019-*

*Assistant Professor (Department of Bioinformatics), July 2019-*

Principles of Pharmacology (Pharm 409), January 27<sup>th</sup> Lecture, Spring 2021

Pharmacokinetics Small Group I, Fall 2021

Principles of Pharmacology (Pharm 409), January 5<sup>th</sup> Lecture, Spring 2022

Lincoln University, Lincoln, PA

*Assistant Professor (Department of Chemistry & Physics), September 2015- May 2019*

Organic Chemistry I & II

Physical Chemistry I, II, & III

Physical Science I & II

Undergraduate Research Physics & Chemistry

Rutgers University, Camden, NJ

*Adjunct Professor (Department of Chemistry), January 2015 – May 2015*

Heterocyclic Chemistry (graduate)

Lincoln University, Lincoln, PA

*Visiting/Adjunct Professor (Department of Chemistry & Physics), September 2013 – August 2015*

Organic Chemistry I & II

Physical Chemistry I, II, & III

Physics II

Advanced Inorganic Chemistry

Undergraduate Research Physics & Chemistry

Lincoln University, Lincoln, PA

*Research Mentor (Department of Mathematics and Computer Science), September 2013 – August 2019*

Lincoln University, Lincoln, PA

*Graduate Curriculum Design (Graduate Program in Chemistry), April 2013*

Lincoln University, Lincoln, PA

*Guest Lecturer (Organic Chemistry), March 2013*

University of the Sciences in Philadelphia, Student Academic Support Services, Philadelphia, PA *Supplemental Instructor (Organic Chemistry), January 2008 – December 2012.*

University of the Sciences in Philadelphia, Student Academic Support Services, Philadelphia, PA *Supplemental Instructor (General Chemistry), January 2012-December 2012*

University of the Sciences in Philadelphia, Dept. of Chemistry & Biochemistry, Philadelphia, PA  
*Graduate Student Instructor, January 2007 – August 2011.*

University of the Sciences in Philadelphia, Student Academic Support Services, Philadelphia, PA  
*Tutor (General Chemistry), September 2007 – January 2008.*

The Abdus Salam International Centre for Theoretical Physics Advanced School in High Performance and GRID  
Computing, Trieste, Italy  
*Teaching Assistant, November 2008*

**(o) Student Mentoring Experience (Summer):**

1. University of Pennsylvania/University of the Sciences in Philadelphia/STEM-PREP Project, Physician Scientist Training Program, Philadelphia, PA, Summer Student Mentor, June - August 2013, June – August 2014.
2. Lincoln University, Summer Enrichment Program, Lincoln, PA, Undergraduate Research Student Co-Mentor, June 2016 – August 2016.
3. Visiting Faculty Program (VFP) Internship Los Alamos National Laboratory, Los Alamos, NM., June 2017 – August 2017
4. Lincoln University Bioinformatics Program (LUBi) Supplemental Internship, (NSF-1818693), June 2019 – August 2019.
5. Lincoln University Bioinformatics Program (LUBi) Supplemental Internship, (NSF-1818693), June 2021 – August 2021.
6. Lincoln University Bioinformatics Program (LUBi) Supplemental Internship, (NSF-1912104), June 2022 – August 2022.
7. Loyola University-MAPSCorps Internship Program (Pilot), June 2022 – August 2022.
8. Lincoln University Bioinformatics Program (LUBi) Supplemental Internship, (NSF-1912104), June 2023 – August 2023.

*Undergraduate Research Advisees (currently enrolled):*

Ezra McGuire (Loyola University Chicago, undergraduate student)  
Adesanya A. Ademokunwa (Loyola University Chicago, undergraduate student)  
Sufia Khan (Loyola University Chicago, undergraduate student)

*Undergraduate Research Advisees (graduated):*

Josephine Nimely (National Institutes of Health, post-bachelorette student)  
Eunice Obi (student-employee, applying for medical school)  
Cedar Davidson (student-employee, applying for medical school)  
J. Chioma Orizu (University of Michigan, pharmacy student)  
Bria Garia (University of Delaware, graduate student)  
William C. Bell (University of Pittsburgh, graduate student)  
Covahna O. Bollar (Univ. of Delaware, graduate student)  
Kasey Campbell (Lehigh University, graduate student)  
Nonye Ibik (Penn State University, medical student)  
Mydirah V. Littlepage-Saunders (Univ. of Iowa, Post-bachelorette program, applying for medical school)  
Sarai McCoy (applying for medical school)

*Graduate & Professional Research Advisees:*

Carolyn Ashley (Loyola University Chicago, PhD student)  
Saqib Peracha (Loyola University Chicago, medical student)  
Sana Iqbal (Loyola University Chicago, rotating graduate student)  
Emily Krueger (Loyola University Chicago, rotating PhD student)  
Sana Iqbal (Loyola University Chicago, rotating PhD student)  
Olivia Seale (Loyola University Chicago, MS/MBA student)  
Kyndall Wallace (Loyola University Chicago, MS/MBA student)  
Miriam Velázquez (Loyola University Chicago, MS/MBA student)

*Graduate Dissertation/Qualifying Committee Service:*

Tris Buck (Loyola University Chicago, PhD student)  
F.O. Okunlola, Thesis Examiner (University of KwaZulu-Natal, PhD student)