BIOGRAPHICAL SKETCH

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NAME: Deredge, Daniel Joseph

eRA COMMONS USER NAME (credential, e.g., agency login): deredge

POSITION TITLE: Assistant Professor

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable. Add/delete rows as necessary.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	Completion Date MM/YYYY	FIELD OF STUDY
Louisiana State University	B.S	05/2003	Biochemistry
Louisiana State University	Ph.D.	12/2009	Biochemistry
Case Western Reserve University	Postdoctoral	01/2012	Biophysics/Biochemistry
University of Maryland, School of Pharmacy	Postdoctoral	11/2018	Biophysics/Mass spectrometry

A. Personal Statement

I have a background in biochemistry and biophysics with specific training in macromolecular interactions and protein structural dynamics. My expertise centers on the structural characterization of complex protein systems using various experimental approaches with a particular emphasis on mass spectrometry-based approaches such as Hydrogen/Deuterium exchange coupled with Mass Spectrometry (HDX-MS). HDX-MS is an isotopic labeling method that is ideally suited for the characterization of large tertiary/quaternary structural changes in solution as well as sensitive enough to detect subtle perturbations in a solution conformational ensemble. As a result, it is uniquely equipped to answer wide ranging biophysical questions from the identification and characterization of the binding mode of ligands to the characterization of protein-protein interactions (PPI) or to the delineation of long-range structural dynamics consequences of perturbations which are often invisible to other structural approaches. I have successfully applied this expertise to take part in multiple efforts or grant applications that have yielded multiple peer reviewed publications. In these studies, I have applied HDX-MS to various proteins that bind therapeutic ligands or engage in PPI with the potential to be targets for the development of therapeutic compounds. In the context of drug discovery, these works have laid the basis for the determination of the conformational mechanism for allosteric effects and inhibition, the classification of drugs based on their HDX signatures, or the identification of potential allosterically targetable sites. More recently, my work has focused on integrating HDX-MS data with in-silico modeling and molecular dynamics simulations. Such integration has helped improve the conformational characterization of macromolecular complexes such as EndoS2, an endoglycosidase that specifically deglycosylates IgG antibodies, together with Dr. MacKerell's group, but has also successfully helped reveal cryptic drug binding sites for drug development in ongoing effort to be published in the near future.

As part of my research program, I aim to implement such integrative workflow to aid in the development of a therapeutic program targeting viral polymerases and in particular, the Non Structural 5 protein (NS5), the RNA-dependent RNA polymerase from dengue virus. DNA and RNA polymerases are responsible for the synthesis of nucleic acids and genetic material. Thus, they are critical proteins in the proliferation of all forms of life and understanding how these proteins function is therefore essential. Consequently,

polymerases constitute one of the most extensively studied classes of proteins and are among some of the most widely used biotechnological tools. In addition, polymerases from pathogens have also constituted choice targets in the development of antimicrobials, especially antivirals. The biophysical characterization of various polymerases has been a recurring theme in my research, spanning from basic characterization of DNA binding properties of DNA polymerase I from *E.coli* and *T.aquaticus* (Taq polymerase) to the biophysical characterization of inhibition of HIV reverse transcriptase or HCV RNA dependent RNA polymerase (NS5b) by small molecule inhibitors currently available or in development. Towards this application centered on dengue virus NS5, we demonstrate through preliminary data our ability to express and purify various constructs of NS5 and perform various biophysical approaches, including cryoEM, to monitor its structural properties and RNA binding properties.

Ongoing and completed research support

Janssen R&D, PI 05/01/2020-05/01/2024
Research Agreement for HDX-MS

NIH 2R44GM130198 Co-I (PI: MacKerell) 08/2021 - 08/2023 (NCE)
Computational methods for accelerating biologics formulation
Investigate the effects of various excipients and formulations on various biologics including IgGs using hydrogen/deuterium exchange-mass spectrometry (HDX-MS) together with computational approaches.

NIH R01 AI132766 Co-I (PI: Sundberg) 08/2021 – 06/2023
Molecular mechanisms of IL-33 cytokine signaling
Investigate the structural basis of cytokine signaling through the IL1 receptor accessory protein.

NSF 2016515 Co-PI (PI: Fondufe-Mittendorf) 08/15/2020-07/31/2023
Role of poly(ADP-ribose) polymerase 1 in regulating RNA polymerase II elongation and mRNA splicing
Investigate the structural and functional role of PARP1, a chromatin binding enzyme, within the larger perspective of Alternative Splicing using a variety of techniques including hydrogen/deuterium exchange using mass spectrometry (HDX-MS).

Particularly relevant citations include:

1. **Deredge, D.J.**, Baker, J.T., Datta K. & Licata V.J. (2010) The glutamate effect on DNA binding by pol I DNA polymerases: osmotic stress and the effective reversal of salt linkage. *J Mol Biol*., 401(2), 223-38
2. **Deredge, D.**, Li, J., Johnson, K.A. & Wintrode, P.L. (2016) Hydrogen/deuterium exchange kinetics demonstrate long range allosteric effects of thumb site 2 inhibitors of Hepatitis C Viral RNA-dependent RNA polymerase. *J Biol Chem*, 291(19), 10078-88
3. Obi, J.O., Gutiérrez-Barbosa, H., **Chua, J.V.**, **Deredge D.J**. (2021) Current Trends and Limitations in Dengue Antiviral Research. *Trop Med Infect Dis.*, 30;6(4).

B. Positions, Scientific Appointments, and Honors

Positions and Scientific Appointments

Sep 2021	Assistant Professor, University of Maryland, School of Pharmacy
Nov 2018	Research Assistant Professor, University of Maryland, School of Pharmacy
Jan 2012	Postdoctoral research fellow, University of Maryland School of Pharmacy
Feb 2010	Postdoctoral research fellow, Case Western Reserve University School of Medicine

Professional memberships and other experience

2023	Organizer, annual Frontiers at the Chemistry Biology Interface Symposium
2023-	Member, Committee on Inclusion and Diversity, Biophysical Society
2021-	Advisor, UMB Biophysical Society Student Chapter

2021 Member, American Association of Immunologists.
2019 Member, American Association of Colleges of Pharmacy
2019 Member, Rho Chi Society
2019 Member, International Society for HDX-MS
2018 Organizer, Biophysic's week symposium, Mass spectrometry: an expanding tool for the Biophysicist, University of Maryland, Baltimore
2017 Panel Member, Chemistry-Biology Interface
2014 Member, American Society for Mass Spectrometry
2005 Member, Biophysical Society

Honors

2019 Best Poster Award, International Conference on HDX-MS
2019 Nominated and inducted to Rho Chi Society, an academic honor society in pharmacy
2015 Best Poster Award, Annual FCBI Symposium

Ad hoc manuscript reviewer for Biophysical Journal, BBA – Protein and Proteomics, Protein Science, Protein: Structure, Function and Bioinformatics, Rapid Communications in Mass Spectrometry, Analytical and Bioanalytical Chemistry, Biophysical Journal, Frontiers in Molecular Bioscience, Journal of the American Society for Mass Spectrometry, Nature Communications.

Ad hoc grant reviewer for University of Maryland MPOWER COVIS seed grant.

Invited talks

2024 University of Maryland, School of Medicine, Baltimore, MD
2024 4th International Conference on HDX-MS, Monterey, CA
2023 Computer-Aided Drug Design Center symposium, UMB, Baltimore, MD
2022 Annual Biophysical Society meeting, San Francisco, CA
2021 Annual ASMS conference, Philadelphia, PA
2021 University of Maryland, School of Pharmacy, Baltimore, MD
2019 Frontiers in Metals in Medicine, Baltimore, MD
2019 Emory University, Atlanta, GA
2018 Biophysics week symposium, Baltimore, MD
2017 UMB-JHU Joint symposium on drug discover, UMB, Baltimore, MD
2016 Waters HDX seminar, Emory University, Atlanta, GA
2016 Waters HDX seminar, UMB, Baltimore, MD
2015 Frontiers in Chemistry and Biology Interface Symposium, UMBC, Baltimore, MD

C. Contributions to Science

1. In addition to the contributions described above, my recent efforts have focused on developing a quantitative platform to leverage HDX-MS data against various in-silico modeling, computational and Molecular Dynamics (MD) approaches. The nature of the structural dynamics information obtained by HDX-MS is uniquely advantageous for quantitative integration with MD simulations and the development of such platform will aid in attaining an enhanced conformational understanding of the native ensemble of a given system or characterize interactions of proteins with other macromolecules or small molecule ligands. Applying such approach, I have participated in the successful characterization of LeuT, a bacterial membrane protein homologous to the Neurotransmitter:Sodium Symporter (NSS) family of proteins and the macromolecular assembly of EndoS2, an endoglycosidase that specifically deglycosylates IgGs. More particularly, I have also applied such platform to characterize the structural and conformational consequences of heme binding to PhuS, a bacterial protein involved in heme uptake in P. aeruginosa. In initial studies, HDX-MS revealed that heme binding induces large conformational

changes in C-terminal proximal helices that form part of the binding pocket. MD simulations revealed that the crystallographic conformations do not adequately capture the complexity of the conformational landscape of these local structural motifs in solution, potentially biasing any structure-based drug design. In follow up studies, the ensemble structure of these local structural motifs was modeled using a post hoc ensemble reweighting approach called Hydrogen-Deuterium Exchange ensemble reweighting (HDXer) which was developed and optimized in separate studies. Ongoing efforts center on the continued development of HDXer and the expansion of the application of HDXer to various biological systems with both mechanistic and therapeutic perspectives.

a. Adhikary, S., **Deredge, D.J**., Nagarajan, A., Forrest, L.R., Wintrode, P.L. & Singh, S.K. (2017) Conformational dynamics of a neurotransmitter:sodium symporter in a lipid bilayer. *Proc Natl Acad Sci U.S.A.*,114(10) E1786-E1795Rep, 6,30832
b. Aytenfisu, A.H., **Deredge, D.**, Klontz, E.H., Du, J., Sundberg, E.J., **MacKerell, A.D. Jr.** (2021) Insights into substrate recognition and specificity for IgG by Endoglycosidase S2. *PLoS Comput Biol.* 17(7)
c. Kihn, K.C., Wilson, T., Smith, A.K., Bradshaw, R.T., Wintrode, P.L., Forrest, L.R., Wilks, A., **Deredge, D.J.** (2021) Modeling the native ensemble of PhuS using enhanced sampling MD and HDX-ensemble reweighting. *Biophys J.* 120(23):5141-5157.
d. Lee, P.S., Bradshaw, R., Kihn, K., Smith, A., Wintrode, P.L., **Deredge, D.J.**, Faraldo-Gómez, J.D., Forrest, L.R. (2022) Interpreting Hydrogen-Deuterium Exchange Experiments with Molecular Simulations: Tutorials and Applications of the HDXer Ensemble Reweighting Software [Article v1.0]. *Living Journal of Computational Molecular Science*, 3(1):1521.

2. With collaborators with varying expertise including all co-investigators in this proposal, I directly participated in the detailed structural and dynamic characterization of complex systems such as membrane proteins or large multi-subunit protein complexes with HDX-MS in an effort to complement high resolution structural information. The use of HDX-MS aims to provide solution conformational detail which builds upon or complements biochemical data or high-resolution crystallographic data to establish a mechanistic link between structure and function. The work performed in such studies have yielded information beyond that obtained from crystal structures alone on the protein/protein interfaces, subtle conformational changes induced by polymorphism, the conformational and kinetic basis of shared protein co-receptors or the interactions of small molecules inhibitors with target proteins.

    a. Klontz, E.H., Tomich, A.D., Günther, S., Lemkul, J.A., **Deredge, D.**, Silverstein, Z., Shaw, J.F., McElheny, C., Doi, Y., Wintrode, P., **MacKerell, A.D**. Jr, Sluis-Cremer, N. & Sundberg, E.J. (2017) Structure and dynamics of FosA-mediated fosfomycin resistance in Klebsiella pneumoniae and Escherichia coli. Antimicrob Agents Chemother. pii:AAC.01572-17
    b. Centola, G., **Deredge, D.J**., Hom, K., Ai, Y., Dent, A.T., **Xue, F.**, & Wilks, A. (2020) Gallium(III)-Salophen as a Dual Inhibitor of Pseudomonas aeruginosa Heme Sensing and Iron Acquisition. *ACS Infect Dis.*, 6(8), 2073-2085
    c. Fields, J.K., Kihn, K., Birkedal, G.S., Klontz, E.H., Sjöström, K., Günther, S., Beadenkopf, R., Forsberg, G., Liberg, D., **Snyder, G.A.**, **Deredge, D.**, Sundberg, E.J. (2021) Molecular Basis of Selective Cytokine Signaling Inhibition by Antibodies Targeting a Shared Receptor. *Front Immunol.* 12:779100
    d. Klontz E., Obi, J.O., Wang, Y., Glendening, G., Carr, J., Tsibouris, C., Buddula, S., Nallar, S., Soares, A.S, Beckett, D., Redzic, J.S., Eisenmesser, E., Palm, C., Schmidt, K., Scudder, A.H., Obiorah, T., Essuman, K., Milbrandt, J., Diantonio, A., Ray, K., Snyder, M.L.D., **Deredge, D.**, **Snyder, G.A.** (2023) The structure of NAD+ consuming protein Acinetobacter baumannii TIR domain shows unique kinetics and conformations *J. Biol. Chem.* 299(11):105290

Complete List of Published Work in MyBibliography:

https://www.ncbi.nlm.nih.gov/myncbi/1xqHvpvivejkg/bibliography/public/

STUDENT BIOGRAPHICAL INFORMATION FORM

NAME Juliet Obi. DEPT. Pharmaceutical Sciences YEAR OF GRAD STUDY Fifth

MENTOR(S) Daniel Deredge (PhD) SOURCE(S) OF SUPPORT **Graduate Research Assistantship** (September 2022 – date)

EDUCATION:

INSTITUTION	DEGREE	YEAR	MAJOR
Kwame Nkrumah University of Science and Technology (KNUST), Ghana	BPharm	Aug 2009 – June 2013	Pharmacy (Bachelor of Pharmacy)
Albany College of Pharmacy and Health Sciences (ACPHS)	MS	August 2017 – July 2019	Pharmaceutical Sciences
University of Maryland, Baltimore (UMB)	Ph.D.	August 2019 - Present	Pharmaceutical Sciences

HONORS:

Graduated from Bachelor of Pharmacy program with second class honors (upper division) - June 2013
Member, Rho Chi Honor Society, UMB School of Pharmacy (SOP) Omicron Chapter

Awards:
Outstanding poster award at the 2024 Frontiers in Chemistry and Biology Interface Symposium (FCBIS)
UMB Initiative for Maximizing Student Development (IMSD) 2024 Student Travel Award
UMB Department of Pharmaceutical Sciences Fellowship Award (Sep 2023 – Aug 2024)
Student Research Achievement Award (SRAA) at the Biophysical Society 2023 Conference.
Nico conference scholarship award by Nicoya Lifesciences to attend the Experimental Biology (EB) 2022 conference.
Graduate student travel award for the EB 2022 conference, through American Society for Biochemistry and Molecular Biology (ASBMB)
Graduate student travel award for the annual Biophysical Society (BPS) 2022 conference
Nigeria Association of Pharmacists and Pharmaceutical Scientists in the Americas (NAPPSA) scholarship award (2021)
Graduate Teaching Assistantship award in partnership with the UMB's Faculty Center for Teaching and Learning (2020-2022)
Graduate student travel award for the American Society for Biochemistry and Molecular Biology (ASBMB) 2019 conference
ACPHS travel scholarship award for the AAPS Northeast Regional Discussion Group (NERDG) 2019 annual meeting
ACPHS Graduate Research Assistantship award (Jan 2018 – July 2019)

Journal Cover Artwork Accepted:
Journal Cover Artwork by Parikh, S.J. Publication: Parikh, S.J.; Evans, C.M.; **Obi, J.O.**; Zhang, Q.; Maekawa, K.; Glass, K.C.; Shah, M.B. Structure of Cytochrome P450 2C9*2 in Complex with Losartan: Insights into the Effects of Genetic Polymorphism. *Molecular Pharmacology*. 2020, 98, 529-539.

Positions:
President, Biophysical Society UMB Student Chapter Executive Board (2022-2023)
Vice President and co-founding officer, Biophysical Society UMB Student Chapter Executive Board (2020-2022)
Vice President of Graduate Affairs, Rho Chi Honor Society, UMB SOP Omicron Chapter Executive Board (2021-2022)
Secretary, AAPS UMB Student Chapter Executive Board (2020-2022)
Mentor, UMB Continuing Umbrella of Research Experiences (CURE) Scholars Program (2019 to date)
Biologics Focus Group Chair to the New Medicines Special Interest Group, International Pharmaceutical Federation (2019 to date)

Professional Memberships:
Sigma Xi, The Scientific Research Honor Society, Full Member (2023 to date)
Nigeria Association of Pharmacists and Pharmaceutical Scientists in the Americas, NAPPSA (2021 to date)
International Society for HDX-MS (May 2021 to date)
Biophysical Society, BPS (Jan 2021 to date)
American Society for Mass Spectrometry, ASMS (2020 to date)
American Association of Pharmaceutical Scientists, AAPS (2020 to date)
American Society for Biochemistry and Molecular Biology, ASBMB (Jan 2019 to date)
International Pharmaceutical Federation, FIP (2015 to date)

TEACHING EXPERIENCE:

Teaching Assistant (Fall 2020 to Spring 2022) – Master's in Medical Cannabis Science and Therapeutics – UMB School of Pharmacy
Teaching Assistant (Spring 2020) – Immunology – UMB School of Pharmacy
Teaching Assistant (Fall 2019) – Abilities lab – UMB School of Pharmacy
Teaching Assistant (Spring 2019) – Biochemistry - ACPHS

RESEARCH EXPERIENCE (prior to entering program):

Jan 2018 to July 2019 – Graduate research assistant, MS in Pharmaceutical Sciences program, ACPHS

CURRENT RESEARCH ACTIVITIES (brief description)

***Dissertation Topic*:** Insights into the structure and dynamics of the dengue virus nonstructural 5 (NS5) protein

Flaviviruses are positive-sense, single-stranded RNA viruses which give rise to many of the mosquito-borne and tick-borne viral infections worldwide. Among them, dengue virus is the most prevalent mosquito-borne virus, with up to 400 million people getting infected with the virus annually. Dengue virus has four serotypes (DENV1-4) and humans who have been infected with one serotype, can be re-infected with another serotype leading to the more severe dengue hemorrhagic fever (DHF) and dengue shock syndrome (DSS). DHF and DSS are life-threatening conditions, characterized by vascular leakage, thrombocytopenia and systemic shock, which can be deadly. To date, there are no antiviral drugs approved for the treatment of dengue infection, and there is no effective vaccine available to protect people from getting infected.

The non-structural protein 5 (NS5) is the largest and most conserved protein encoded by flaviviruses. It is a key component of the RC with multiple enzymatic and biological functions and is a major target for antivirals due to its critical functions. The dengue virus NS5 contains an N-terminal methyltransferase (MTase) domain, responsible for synthesis of the 5' RNA cap and methylation, and a C-terminal RNA-dependent RNA polymerase (RdRp) domain, responsible for *de novo* RNA synthesis. Structure-function studies which have been carried out on NS5, show interdomain interactions between the MTase and RdRp domains, and the interactions of NS5 with different RNA structures. Crystal structures of the dengue NS5 have also shown that crucial interactions between the two NS5 domains can be maintained within a monomer or through intermolecular interactions within a dimer, suggesting that NS5 can adopt multiple conformations in carrying out its viral replication functions. However, whether these multiple conformations are essential for all or some of its complex functions remains an unanswered question. The crystal structures currently available are not sufficient to fully elucidate this, and there is no RNA-bound structure of the dengue NS5 available to date.

Hydrogen deuterium exchange coupled to mass spectrometry (HDX-MS) has proven to be a powerful biophysical approach, used to study protein structure and dynamics. We employed solution HDX-MS analysis to probe solvent accessibility and assess the conformational landscape of the DENV2 NS5 protein. We have characterized regions with high deuterium uptake in the DENV2 NS5 apo structure and identified regions with EX1 kinetics suggestive of significant conformational changes. We aim to probe these regions further by corroborating our findings with molecular dynamics (MD) simulations. The results obtained from this combined biophysical approach will enable us to identify solvent accessible regions in the DENV2 NS5 protein, which will be further explored with the aim of identifying novel binding site(s) for small molecule inhibitors against the dengue virus.

COURSES TAKEN

2021	Molecular Biophysics	B+	2018	Pharmacology and Molecular Genetics of Cancer	A
2021	Issues at the CBI (Spring and Fall)	Pass	2017	Foundations of Pharmaceutical Sciences	B+
2021	Journal Club (Spring and Fall)	Pass	2017	Research Rotation	A
2020	Issues at the CBI (Fall)	Pass			
2020	Principles of Virology	A-	2017	Macromolecular Structure	B+
2020	Principles of Drug Development	A	2017	Experimental Design/Data Analysis	A+
2020	Spectrometric Methods	A	2022	Issues at the CBI (Spring and Fall)	Pass
2020	Drug Design	A	2023	Issues at the CBI (Spring and Fall)	Pass
2020	Journal Club (Spring and Fall)	Pass			
2019	Principles of Drug Discovery	A			
2019	Introduction to Lab Research	A			
2019	Ethics and Biostatistics	A			
2019	Bioanalytical Pharmacological Methods	A			
2018	Systems Biology in Drug Discovery	A			

2018	Pharmacological Regulation of Signal Transduction	A
2018	Neural System Pharmacology	A

APPLICATION(S) FOR PRE-DOCTORAL FUNDING: N/A

APPLICATION(S) FOR POST-DOCTORAL FUNDING: N/A

APPLICATION(S) FOR POST-DOCTORAL OR POST GRADUATE EMPLOYMENT: N/A

CROSS DISCIPLINARY TRAINING COMPONENT:

Our research is primarily focused on the use of biophysical techniques to characterize the structure and dynamics of the dengue virus NS5 protein. We aim to characterize the multiple conformations it can adopt in its apo form, and in its RNA-bound form. To this end, we will use hydrogen-deuterium exchange mass spectrometry (HDX-MS), in correlation with atomic resolution molecular dynamics (MD) simulations to probe the dynamics of the dengue NS5. We will leverage the data obtained from these studies against a structure-based drug design approach for the development of novel lead compounds against dengue. Our studies will shed light on multiple regions on the protein which may be biophysically relevant to its multiple and complex functions. This will lead to the assessment of the clinical relevance of our results, and whether our biophysical studies are translatable, and can be expanded to pre-clinical studies. To this end, my cross disciplinary training project will be with the laboratory of Dr. Joel Chua at the Institute of Human Virology (IHV), University of Maryland, Baltimore School of Medicine. We plan to perform viral infectivity assays on humanized mouse models to understand how the rate of viral infection is affected by different strains and/or serotypes of the dengue virus. Mouse models of dengue virus infection are increasingly being developed, especially to identify vaccine candidates for clinical trials. However, the development of these models will also allow us to study the pathogenesis of dengue virus infection in a strain and serotype-specific manner, and for the testing of novel therapeutics against dengue. Additionally, in collaboration with Dr. Greg Synder at the IHV, we will perform CryoEM single particle analysis to characterize the structure(s) of dengue NS5 with various RNA substrates at the Institute for Bioscience and Biotechnology Research (IBBR).

PUBLICATIONS (this graduate program):

Fields, J.K; Gyllenbäck, E.J.; Bogacz, M.; **Obi, J.O.**; Birkedal, G.S.; Sjöström, K.; Maravillas, K.; Grönberg, C.; Rattik, S.; Kihn, K.; Flowers, M.; Smith, A.K.; Hansen, N.; Floretos, T.; Huyhn, C.; Liberg, D.; Deredge, D.; Sundberg, E.J. Antibodies targeting the shared cytokine IL-1 receptor accessory protein invoke distinct mechanisms to block all cytokine signaling. *Cell Reports* **2024**, 114099.

Klontz, E.; **Obi, J.O.**; Wang, Y.; Glendening, G.; Carr, J.; Tsibouris, C.; Buddula, S.; Nallar, S.; Soares, A.S.; Beckett, D.; Redzic, J.S.; Eisenmesser, E.; Palm, C. et al. The structure of NAD+ consuming protein *Acinetobacter baumannii* TIR domain shows unique kinetics and conformations. *Journal of Biological Chemistry.* **2023**, 299(11).

Chun, H.; Kurasawa, J.H.; Olivares, P.; Marakasova, E.S.; Shestopal, S.A.; Hassink, G.U.; Karnaukhova, E.; Migliorini, M.; **Obi, J.O**.; Smith, A.K.; Wintrode, P.L. et al. Characterization of interaction between blood coagulation factor VIII and LRP1 suggests dynamic binding by alternating complex contacts. *Journal of Thrombosis and Haemostasis.* **2022**, 20(10), 2255-2269.

Sestok, A.E.; Brown, J.B.; **Obi, J.O.**; O'Sullivan, S.M.; Garcin, E.D.; Deredge, D.J.; Smith, A.T. A fusion of the *Bacteroides fragilis* ferrous iron import proteins reveal a role for FeoA in stabilizing GTP-bound FeoB. *Journal of Biological Chemistry.* **2022**, 298(4), 101808.

Obi, J.O.; Gutierrez-Barbosa, H.; Chua, J.V.; Deredge, D.J. Current Trends and Limitations in Dengue Antiviral Research. *Tropical Medicine and Infectious Disease*. **2021**, 6(4), 180.

PUBLICATIONS (Master's program):

Parikh, S.J.; Evans, C.M.; **Obi, J.O.**; Zhang, Q.; Maekawa, K.; Glass, K.C.; Shah, M.B. Structure of Cytochrome P450 2C9*2 in Complex with Losartan: Insights into the Effects of Genetic Polymorphism. *Molecular Pharmacology.* **2020**, 98, 529-539.

Obi, J.O.; Lubula, M.Y.; Cornilescu, G.; Henrickson, A.; McGuire, K.; Evans, C.M.; Phillips, M.; Boyson, S.P.; Demeler, B.; Markley, J.L.; Glass, K.C. The BRPF1 bromodomain is a molecular reader of di-acetyllysine. *Current Research in Structural Biology.* **2020**, 2, 104-115.

PRESENTATIONS: (this graduate program)

First Author Presentations:

Obi, J.O.; McQueen, L.; Deredge, D. *A Structural and Dynamic Basis for the Interactions of the Dengue Virus Nonstructural 5 (NS5) Protein with Stem Loop A (SLA).* Frontiers at the Chemistry-Biology Interface Symposium 2024. (Oral Talk and Poster)

Obi, J.O.; McQueen, L.; Deredge, D. *A Structural and Dynamic Basis for the Interactions of the Dengue Virus Nonstructural 5 (NS5) Protein with Stem Loop A (SLA).* University of Maryland, Baltimore (UMB) Graduate Research Conference (GRC) 2024. (Oral Talk)

Obi, J.O.; Smith, A.K.; Kihn, K.C.; McQueen, L.; Deredge, D. *A Structural and Dynamic Basis for the Interactions of the Dengue Virus Nonstructural 5 (NS5) Protein with Stem Loop A (SLA).* Biophysical Society Annual Meeting 2024. (Flash Talk and Poster)

Obi, J.O.; McQueen, L.; Deredge, D. *A Structure-Based Drug Design Approach for Targeting the Dengue Virus Nonstructural 5 (NS5) Protein).* Computer-Aided Drug Design Symposium 2023. (Poster)

Obi, J.O.; McQueen, L.; Deredge, D. *Inter-domain Coordination Essential for Dengue Virus Nonstructural 5 (NS5) Interaction with Stem Loop A (SLA).* Frontiers at the Chemistry-Biology Interface Symposium 2023. (Poster)

Obi, J.O.; McQueen, L.; Deredge, D. *Inter-domain Coordination Essential for Dengue Virus Nonstructural 5 (NS5) Interaction with Stem Loop A (SLA).* Biophysical Society Annual Meeting 2023. (Poster)

Obi, J.O.; Fields, J.K.; McQueen, L.; Deredge, D. *Insights into the Binding of the Dengue Virus Nonstructural 5 (NS5) Protein to Stem Loop A (SLA).* American Society for Biochemistry and Molecular Biology (ASBMB) Annual Meeting, EB 2022. (Poster)

Obi, J.O.; Kihn, K.C.; Deredge, D. *Insights into the Structural Dynamics and RNA Binding of the Dengue Nonstructural 5 (NS5) Protein.* Biophysical Society Annual Meeting 2022. (Poster)

Obi, J.O.; Smith, A.K.; Deredge, D.J. *Structural and Dynamic Insights into the Dengue Nonstructural 5 (NS5) Protein.* American Society for Mass Spectrometry Annual Meeting 2021. (Poster)

Obi, J.O.; Kihn, K.C.; Deredge, D. *A Solution HDX-MS Approach in Probing the Structure and Dynamics of the Dengue Nonstructural 5 (NS5) Protein.* Virtual Biophysical Society Annual Meeting 2021. (Poster)

Obi, J.O.; Smith, A.K.; Deredge, D. *Structural Dynamics of the Dengue Virus Nonstructural 5 (NS5) Protein.* Annual ASMS Conference on Mass Spectrometry and Allied Topics 2021. (Poster)

Mentored Presentations: N/A

PRESENTATIONS: (Master's program)

First Author Presentations:

Obi, J.O.; Lubula, M.Y.; Cornilescu, G.; Henrickson, A.; McGuire, K.; Evans, C.M.; Demeler, B.; Markley, J.L.; Glass, K.C. *Molecular Insights into Di-acetyllysine Histone Recognition by the BRPF1 Bromodomain*. American Society of Biochemistry and Molecular Biology Annual Meeting, Orlando, Florida, 2019. (Poster)

Obi, J.O.; Lubula, M.Y.; Cornilescu, G.; Henrickson, A.; McGuire, K.; Evans, C.M.; Demeler, B.; Markley, J.L.; Glass, K.C. *Molecular Insights into Di-acetyllysine Histone Recognition by the BRPF1 Bromodomain.* AAPS Northeast Regional Discussion Group (NERDG) 2019 annual meeting. (Poster)