OLUBIYI, Olujide O.

CONTACT

Biosciences Research Education and Advisory Centre

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CURRENT POSITION

- **Adjunct Researcher** - Bioscience Research Education and Advisory Centre, Yola, Nigeria (05/2014 – till date)

CONCURRENT POSITION

- **Senior Lecturer** – Department of Pharmacology and Therapeutics, College of Medicine & Health Sciences, Afe Babalola University, Ado-Ekiti, Nigeria

ACADEMIC BACKGROUND

1) Postdoctoral research fellowship, April 2013 — Nov. 2013: Institute of Complex Systems 6, Forschungszentrum Jülich, Germany.

2) PhD in Alzheimer's drug design (*Sehr gut*), March 2011—March 2013:RWTH University Aachen, Germany. *Funding*- German Research School of Simulation Sciences, Jülich, Germany

3) Visiting scientist, Jun. 2011: Prof Paul Axelsen's research laboratory. University of Pennsylvania, Philadelphia, United State of America.

4) Guest researcher appointment, Nov. 2010 — Jan. 2011: Institute of Structural Biochemistry, Forschungszentrum Jülich, Germany.

5) MSc in Drug Discovery (Distinction), Sept. 2009 —Oct. 2010:Dept. of Biological and Pharmaceutical Chemistry. London School of Pharmacy *now* School of Pharmacy, University College London. *Funding*: The DfiD Commonwealth Shared Scholarships Scheme.

6) B.Pharm, Pharmacy (Distinction), June 2000 — Nov 2006:Faculty of Pharmacy, Obafemi Awolowo University, Ile-Ife, Nigeria.

RESEARCH INTEREST

- Molecular basis of drug action
- Drug discovery and structure-based drug design
- Mechanism of drug-receptor interactions and computer-aided drug design
- Ethnopharmacology and drug repurposing

RESEARCH PUBLICATIONS

Selected articles published between 2011&2014

1) Conformational polymorphism in the autophagy-related protein GATE-16. Ma P, Schillinger O, Hartmann R, Stoldt M, Mohrlüder J, Schwarten M, Olubiyi O, Strodel B, Willbold D, and Weiergräber OH. *Biochemistry,* 2015. {*in press*}

2) Early Amyloid B-Protein Aggregation Precedes Conformational Change. Barz B, Olubiyi OO and Strodel B. *Chemical Communications,* 2014.

3) Amyloid Aggregation Inhibitory Mechanism of Arginine-Rich D-Peptides. Olubiyi OO , Frenzel D, Bartnik D, Glück JM, Brener O, Nagel-Steger L, Funke SA, Willbold D, Strodel B. *Current Medicinal Chemistry*, 2014

4) A Predictive Model for Ethnomedicinal Discovery Research- A Nigerian Case Study. Olubiyi OO and Akintayo CO. *Journal of Biomedical and Pharmaceutical Research,* 3, 6, 1-8, 2014.

5) Determination of Binding Affinities of Some Approved Drugs to *Ascaris suum* Mitochondrial Rhodoquinol-Fumarate Reductase By *in silico* Molecular Docking. Uzochukwu IC, Olubiyi OO, Akpojotor CO. *Journal of Pharmaceutical and Allied Sciences,* 2014.

6) Presented paper: Introduction to drug discovery and computer-aided drug design. Workshop on molecular docking and drug design. 4th July 2014, NAFDAC Laboratories/Faculty of Pharmacy, Nnamdi Azikwe University Agulu, Anambra State.

7) Presented paper: Molecular dynamics simulation-From Newton's classical mechanics to pharmacological mechanisms. Workshop on molecular docking and drug design. 4th July 2014, NAFDAC Laboratories/Faculty of Pharmacy, Nnamdi Azikwe University Agulu, Anambra State.

8) Presented paper: Setting up molecular dynamics simulations for test pharmological systems. Workshop on molecular docking and drug design. 4th July 2014, NAFDAC Laboratories/Faculty of Pharmacy, Nnamdi Azikwe University Agulu, Anambra State.

9) Structures of the Amyloid β-Peptides Aβ(1-40) and Aβ (1-42) as Influenced by pH and a D-Peptide. Olubiyi OO and Strodel B. *Journal of Physical Chemistry B*, 116, 3280-3291, 2012.

10) Molecular Dynamics of HIV1-Integrase in Complex with 93del – A Structural Perspective on the Mechanism of Inhibition.Sgobba M, Olubiyi OO, Ke S, Haider S. *Journal of Biomolecular Structure and Dynamics*. 29:863-877, 2012.

11) Molecular Modeling of Human Alkaline Sphingomyelinase. Suresh PS, Olubiyi O, Thirunavukkarasu C, Strodel B, Kumar MS. *Bioinformation*, 6, 78-82, 2011.

12) Book Chapter: From Computational Biophysics to Systems Biology (CBSB11). Olubiyi OO and Strodel B. Jülich,Germany. ISBN 978-3-89336-748-1. 2012

13) Book: Investigation of the interaction between Alzheimer's abeta peptide and aggregation inhibitors using molecular simulations. Olubiyi OO. RWTH Aachen University, Germany. 2013 (Published doctoral thesis available online).

Selected conferences attended between 2011 & 2013:

1) Biophysical Society 57th Annual Meeting. Feb. 2 - 6, 2013,Philadelphia,United States of America.

2) The ABC of Life Science Informatics: Mini-Symposium of Bioinformatics and Chemoinformatics Research Groups fromthe Aachen-Bonn-Cologne Region. Dec. 14, 2012, Bonn, Germany.

3) Challenges in Biomolecular modeling-From QM to Coarse-graining. Jun. 1 - 20, 2012. Stockholm, Sweden

4) CECAM Workshop on: Anchoring simulations to experiments: challenges for understanding and treating Alzheimer'sdisease. May 21 - 23, 2012. Paris, France.

5) Frontiers in Biomolecular Simulation. Jan. 22 - 25, 2012. Physikzentrum Bad-Honnef, Germany.

6) The Brain: Young Researchers Transatlantic Academy 2011. Jun. 12 – 16, 2011. University of Pennsylvania, Philadelphia,United States of America.

7) Computer Simulation and Theory of Macromolecules 2011. Apr. 15 -16, 2011, Hünfeld, Germany.

8) 10th International Conference AD/PD 2011. Mar. 9 -13, 2011,Barcelona, Spain.

Talks delivered at conferences attended between 2011& 2013:

1) Molecular simulation investigation of the inhibitory mechanism of D-peptides against Alzheimer's disease amyloid beta peptide.*Presented at the Lead Generation and Compound Realisation Structure Design & Informatics.* Jul 30, 2013. Centre de recherché Sanofi R&D, Vitry-sur-Seine, France.
2) Alzheimer's disease: modelling the inhibition of the β-amyloid aggregation using D-peptides. *Doctoral Seminar: German Research School for Simulation Sciences.* Nov. 5th, 2012. Jülich, Germany.
3) Modeling the interaction of D3 peptide with Aβ pentamer.*ICS-6 Retreat 2012*, Aug. 15-172012, Hennef, Germany.
4) How abeta 'folds': the effect of pH and a D-peptide on the structural propensities of the Alzheimer's amyloid peptide.*Frontiers in Biomolecular Simulation.* 495 Wilhelm und Else Heraeus-Seminar. Jan. 22-25, 2012, Bad Honnef, Germany.
5) Computational Study of Alzheimer's Disease Abeta Peptide Aggregation Inhibition by a D-Peptide . *Doctoral Seminar: German Research School for Simulation Sciences.* Oct. 27, 2011 Aachen, Germany.
6) Molecular simulation studies on the prevention of amyloid aggregation of Alzheimer's Aβ peptide by D-peptides.*Young Researchers Transatlantic Academy 2011: "The Brain".* Jun 17- 24, University of Pennsylvania, Philadelphia, United States of America.
7) Effects of an amyloid-inhibiting D-peptide on the conformation of Alzheimer's abeta peptide. *Computer Simulation and Theory of Macromolecules 2011*.April 15-17, 2011.Hünfeld, Germany.
8) Effects of an amyloid-inhibiting D-peptide on the conformation of Alzheimer's abeta peptide.*25th Molecular Modelling Workshop 2011.* April 4 ¯ 6, 2011. Erlangen, Germany.

Posters presented at conferences between 2011 & 2013:

1) Olubiyi OO& Strodel B. Modelling the inhibition of amyloid-beta aggregation causing Alzheimer's disease using D-peptides.*Biophysical Society 57th Annual Meeting.* Feb. 2-6 2013, Philadelphia, United States of America.
2) Olubiyi OO& Strodel B. Alzheimer's disease: modelling the inhibition of β-amyloid aggregation using D-peptides. *BioScience 2012 - Frontiers in Biomolecular Sciences: From Molecules to Cells.* Nov. 7-9 2012, Jülich, Germany.

3) Olubiyi OO& Strodel B. Alzheimer's disease: modelling the inhibition of β-amyloid aggregation using D-peptides. *Challenges in biomolecular modeling- from QM to coarse-graining. Långholmen.* Jun. 17-20, 2012. Stockholm, Sweden.

4) Olubiyi OO& Strodel B. How abeta 'folds': the effect of pH and a D-peptide on the structural propensities of the Alzheimer's amyloid peptide.495. *Wilhelm und Else Heraeus-Seminar "Frontiers in Biomolecular Simulation".* Jan. 22-25 2012, Bad Honnef, Germany.

5) Olubiyi OO& Strodel B. Computational investigation of abeta peptide folding: effect of pH and an amyloid-inhibiting D-peptide on the structural propensities of Aβ. *Amyloid Fibrils, Prions and Precursors: Molecules for Targeted Intervention.* Aug. 25-28 2011, Halle (Saale), Germany.

6) Olubiyi OO& Strodel B. Molecular simulation studies on the prevention of amyloid aggregation of Alzheimer's Aβ peptide by D-peptides. *Young Researchers Transatlantic Academy 2011 with the theme "The Brain".* Jun. 17- 24, University of Pennsylvania, Philadelphia, USA.

7) Olubiyi OO& Strodel B. Computational study of Alzheimer's disease abeta peptide aggregation inhibition by a D-peptide. *Computer Simulation and Theory of Macromolecules 2011.* Apr. 15-17, 2011. Hünfeld, Germany.

8) Olubiyi OO& Strodel B. Computational study of Alzheimer's disease abeta peptide aggregation inhibition by a D-peptide. *The 10th International Conference on Alzheimer's and Parkinson's Diseases.* Mar.9-13 2011, Barcelona, Spain.