# Mirza Ahmed Hammad ul Mubeen Muhammad

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Accomplished Computational Scientist and Biologist with over six years of post-PhD experience. Currently focusing on 1) the newly discovered HEAT Cycle, 2) developing adiposomes/lipid droplets as an efficient drug delivery system, and 3) a new stabilizer term to Van der Waal's equation.

## TECHNICAL SKILLS

- **Computational Techniques:**
  - **Biologics & Systems Modeling:** ***Molecular Dynamics Simulations, Forcefield Generation,*** Protein-Protein Docking, Peptide Modeling, Homology Modeling
  - **Small Molecule Design:** SBDD, LBDD, Virtual Screening, Docking, FEP, Pharmacophore
  - **Machine Learning:** Deep Neural Networks, Support Vector Machines, QSAR Modeling
  - **Software & Tools:** Gaussian, GAMESS, AMBER, GROMACS, CHARMM, OpenEye, NAMD GOLD, AutoDock, Cresset's Forge, Ligandscout, ***Pymol***, VMD
  - **Programming & Scripting:** R, ***Python***, Perl, C++, PHP, JavaScript, Bash/Shell
  - **Databases & Platforms:** PDB, PubChem, ChEMBL, ZINC, ***Linux***/***HPC*** environments
- **Laboratory Techniques:**
  - **Lipid Droplet:** Artificial Lipid Droplet Preparation, Activation of Brown Fat Cells, Cell/Lipid Droplet Size and Counting, TLC
  - **Common Lab Techniques:** RT/qPCR, Western Blotting, Gel Electrophoresis, DNA/RNA Extraction, Plasmid Preparation and Transformation, Tissue Culturing

## ACADEMIC APPOINTMENTS

- **Assistant Professor** | COMSATS University Islamabad - Sahiwal Campus | *Apr-2022 to Current*
  - Conducting advanced research in mitochondrial metabolism and lipid droplet dynamics.
  - Developing novel computational models and forcefields for simulating biological systems.
  - Teaching and developing curriculum for graduate-level courses in Computational Drug Design and Bioinformatics.
  - Mentoring and supervising graduate and undergraduate student research projects.
- **Lecturer (Ph.D.)** | COMSATS University Islamabad, Sahiwal Campus | *Jan-2020 to Apr-2022*
  - Led computational efforts for a biologics program targeting the **Wnt** protein family, using advanced molecular dynamics to elucidate protein dynamics and guide inhibitor design.
  - Co-author of book "**Quick Guideline for Computational Drug Design**" published under Bentham Science Publishers.
  - Taught university-level courses in Computational Drug Design and Bioinformatics.
  - Supervised two graduate students and co-supervised two others.
- **Lecturer** | COMSATS University Islamabad, Sahiwal Campus | *Jan-2015 to Aug-2016*
- **Lecturer** | Punjab Group of Colleges, Shahkot | *Aug-2013 to Aug-2014*

## KEY ACHIEVEMENTS

- Published **12** articles in Q1 peer-reviewed journals.
- Authored a **book** on computational drug design.
- Discovered the **HEAT Cycle** in mitochondrial metabolism using innovative proteomics workflows.
- Developed a **novel forcefield** for triacylglycerol, enabling atomic-scale simulations of lipid droplets for the first time.
- Secured a **patent** application for new research findings.

## INVITED TALKS

- Oral Presentation at 15th Seminar Series at University of Management and Technology, **Lahore**, Pakistan.
- Oral **Presentation** at Department of Chemistry, University of Punjab, Pakistan.
- Oral **Presentation** at Center of Advanced Studies, University of Agriculture, Faisalabad, Pakistan.

## AWARDS & FUNDING

- **Awardee**, CAS-TWAS President's Fellowship Programme 2016.
- **Team Leader,** Deep Space Food Challenge Phase 2, NASA & Methuselah Foundation.
- **Principal Investigator,** Concept Note funded for 'High Performance Server System with GPU Support', COMSATS University (Value: 2 Million PKR).
- **Project Submission (Collaborator),** ANSO project "Identification of HEAT Cycle in Mitochondria of Brown Fat Cells" with PIs from three countries.
- **Poster Presentations (Supervisor)**, Two e-posters submitted by supervised students at the 2022 AAAS Annual Science Meeting. The titles were
  - ***Identification of a New Cycle - HEAT CYCLE in Mitochondria of Mouse Brown Fat Cells***
  - ***Atomistic Simulation of Four-Layer System to Mimic Lipid Droplets with Drug Molecule***

## EDUCATIONAL DETAILS

- **Ph.D. Cell Biology (Sep-2016 to Jan-2020)** | University of Chinese Academy of Sciences, Beijing, China.
  - ***Topic of Research:*** Interaction of Lipid Droplets and Mitochondria and Simulation of Adiposomes
- **M.Phil. Bioinformatics (2011-2013)** | Quaid-i-Azam University, Islamabad, Pakistan.
  - ***Topic of Research:*** Comparative Molecular Dynamics Simulations Studies of Wnt-4 Protein
- **BS (Hons.) Bioinformatics (2007-2011)** | National Institute of Biotechnology and Genetic Engineering (NIBGE), Faisalabad, Pakistan.
  - ***Topic of Research:*** Identification and Cloning of Rust Resistance Genes of NBS-LRR Family and Applying Bioinformatics Tools

## ONLINE PROFILES

- ORCID ID: 0000-0003-4201-9087, Scopus ID: 55243748400, Researcher ID: AAY-3429-2021
- Google Scholar: https://scholar.google.com/citations?user=ZSz4hHAAAAAJ&hl=en&oi=ao
- ResearchGate: https://www.researchgate.net/profile/Hammad_Mubeen2
- CUI Faculty: https://ww2.comsats.edu.pk/faculty/FacultyDetails.aspx?Uid=18855

## SELECTED PUBLICATIONS

1. **Mirza, AH.,** 2022. Study of trioleoylglycerol two-layer and adiposome cross-section mimicking four-layer systems through atomic-level simulations. Structural Dynamics, 9(6), 064701. Doi: https://doi.org/10.1063/4.0000168 (IF=3.67) (**Sole-Author**)
2. **Mirza, AH., Cui, L.,** Zhang, S., Liu, P., 2021. Comparative proteomics reveals that lipid droplet-anchored mitochondria are more sensitive to cold in brown adipocytes. Biochim. Biophys. Acta - Mol. Cell Biol. Lipids 1866, 158992. https://doi.org/10.1016/j.bbalip.2021.158992 (IF=4.698) **(HEAT Cycle**)
3. **Cui L, Mirza AH.,** Zhang S, Liang B, Liu P., 2019. Lipid droplets and mitochondria are anchored during brown adipocyte differentiation. Protein Cell.10(12):921-926. https://10.1007/s13238-019-00661-1 (IF=21.1)
4. Huang, T., Bamigbade, A.T., Xu, S., Deng, Y., Xie, K., Ogunsade, O.O., ***Mirza, AH.,*** Wang, J., Liu, P., Zhang, S., 2021. Identification of noncoding RNA-encoded proteins on lipid droplets. Sci. Bull. 66, 314–318. https://doi.org/10.1016/j.scib.2020.09.022 (IF=18.8)
5. Azam SS, **Mirza AH.,** 2014. Role of thumb index fold in Wnt-4 protein and its dynamics through a molecular dynamics simulation study. J Mol Liq.198:313-321. https://10.1016/j.molliq.2014.07.007 (IF=5.3)

*A complete list of publications is available on my Google Scholar profile.*

## REFERENCES

References available upon request.