Myrnel **Fortuna**

9002 RS(5G1) Gen. Malvar Str Araneta Center Cubao, Quezon City, Philippines

(+639)49 434 8520 | myrnelalmoradie@outlook.com | myrnelaf.github.io

Experience

SCIENCE RESEARCH SPECIALIST II

España Manila

UNIVERSITY OF SANTO TOMAS, RESEARCH CENTER FOR THE NATURAL AND APPLIED SCIENCES — *Jun 2024 - Aug 2024*

- Project: GAGAMBA (Gamot mula sa Gagamba at Mananaliksik ng Bayan): An Omics-guided Bioprospecting of Philippine Spiders (DOST-PCHRD-funded)
- good ViBEs (Virtual Biochemical Explorations) laboratory manager
- I initiated the computational arm of the project.
- I wrote SOPs for standardizing *in silico* practices in the lab.
- I did academic research daily where I model peptides for peptide-protein interaction analyses.
- I conducted undergraduate and graduate student training on computational methods.
- I performed miscellaneous admin duties such as grant writing, group financials, and general up-keep of laboratory premises and databases.

SCIENCE RESEARCH SPECIALIST II

Diliman Quezon City

UNIVERSITY OF THE PHILIPPINES DILIMAN — *Jul 2023 - May 2024*

- Project: Technical Battle Against COVID: Design and Synthesis of SARS-COV2, ACE2, SARS- COV2:ACE2 Destabilizing Compounds. (DOST-PCHRD-funded)
- good ViBEs (Virtual Biochemical Explorations) laboratory manager, Principal Investigator: Dr. Ricky B. Nellas, Specialization: Drug Design and Discovery, Biophysics, Protein Engineering
- I did academic research daily, designing drugs and performing biophysical analysis in support of the COVID-19 drug-discovery effort of DOST under their Technical program against COVID-19. I designed a library of 10,000 compounds with drug-like properties against COVID-19 spike protein. 27 were found to have activity against the virus and will be patented after assay tests at the National Institute of Molecular Biology and Biotechnology (UPD-NIMBB, c/o Dr. Pia Bagamasbad collaboration).
- I wrote proposal grants for laboratory funding. I headed the writing process of a six-project program proposal for DOST-GIA of several institutes across the Philippines which was recently approved.
- I conducted undergraduate and graduate student training on computational drug design, drug safety (ADMETox), and big data handling (Machine learning techniques in drug discovery).
- I wrote SOPs for analysis protocols for standardization of scientific analysis in our laboratory.
- I handled several datasets and was responsible for upkeep of the group's data management.
- I wrote and reviewed scientific manuscripts for journal publication.
- I created scientific illustrations for the laboratory. My recent published illustration is the journal cover of the American Society of Chemistry (ACS) Omega for their Volume 8, Issue 48 (Published December 05, 2023). This accompanied the paper 'Cheng, R. L., Quirante, J. C., Vargas, L. E. Z., Gatchalian, A. F., and Nellas, R. B. (2023). Complementary Pocket and Network-Based Approach to Search for Spike Protein Allosteric Pocket Sites. *ACS omega*, 8(48), 45313-45325.', the review of which I participated in.

GRADUATE STUDENT INTERN, INTERNATIONAL INTERNSHIP PILOT PROGRAM - TAIWAN

Taipei, Taiwan

ACADEMIA SINICA — *March - April 2024*

- Project: Neural Network Potential (NNP) applications in Chemistry, Adviser: Dr. Jer-Lai Kuo
- I am training to apply machine learning techniques in studying peptides at the atomic scale. This will be used for peptide drug optimization and development.

SCIENCE RESEARCH SPECIALIST I

Diliman Quezon City

UNIVERSITY OF THE PHILIPPINES DILIMAN — *Aug 2021 - Jun 2023*

- Project:Synthesis and Derivatization of Disease-specific Bioactive Hits and Lead Compounds (Phase II) Project 6. Computer-Aided Drug Design of Natural Products-Based, and Synthetic Antidiabetic, Antifungal, and Anticancer Lead Compounds and Derivatives (DOST-PCHRD-funded)
- I did academic research daily, designing drugs and performing biophysical analysis in support of the drug-discovery efforts of DOST against cancer. I designed a library of 3,000 compounds against breast and prostate cancer.
- I conducted undergraduate student training on computational drug design and principles of drug safety (ADMETox).
- I reviewed scientific manuscripts for journal publication.

GMP QUALITY ASSURANCE ASSOCIATE *Salcedo St. Legazpi Village, Makati*

NOVARTIS HEALTHCARE PHILIPPINES INC. *Aug 2017 - Aug 2018*

- I inspected products before their commercial and clinical trial distribution.
- I prepared the necessary documents and requirements for product release.
- I managed the department's databases, including data entry, monitoring, and quality control, for product out-flow into commercial and clinical trial site distribution.

CLINICAL RESEARCH INTERN *Bonifacio Global City, Taguig*

ASTRAZENECA PHARMACEUTICALS PHILIPPINES INC. *Aug 2016 - Sep 2016*

- I helped clinical research associates in clinical trial rounds and database managament.

RESEARCH ASSISTANT *Ermita, Manila*

NATIONAL INTEGRATED RESEARCH PROGRAM ON MEDICINAL PLANTS (UP-NIRPROMP) *Feb 2016 - Aug 2016*

- Project: Preformulation Studies on Powdered *Cassia fistula L.* leaves (NIRPROMP-funded)
- I performed stability and compatibility studies on *Cassia fistula* tablets.

Skills

Programming Languages Mathematica (working), Python (working), Bash, Latex

Pharmaceutical Industry GCP, QA, SOP writing, Product formulation, Drug design and development, Statistical analysis

General Research Grant writing, Protocol development, Technical writing, Data analysis, Mentorship and training, GitHub website creati

Publications

December 5, 2023, Supplementary cover art of ACS Omega Volume 8, Issue 48 Created the supplementary cover art that accompanies the journal article 'Cheng, R. L., Quirante, J. C., Vargas, L. E. Z., Gatchalian, A. F., and Nellas, R. B. (2023). Complementary Pocket and Network-Based Approach to Search for Spike Protein Allosteric Pocket Sites. *ACS omega*, 8(48), 45313-45325.'

Published online December 2024 Cabanding, J. M. G., Yu, S. S. F., Lin, Z. H., ***Fortuna, M. A.***, Elatico, A. J. J., and Nellas, R. B. (2024). The importance of helical structures to the overall activity and structural stability of a lipase from *Pseudomonas aeruginosa* PAO1 in n-hexane. *Archives of Biochemistry and Biophysics*, 110226.

Accepted for publication in Computational and Structural Biotechnology Reports Computational Reverse Protein Engineering of a Lipase from *Pseudomonas Aeruginosa* in n-Hexane

Under peer review in Scientific Reports Exploring the Effects of N234 and N343-linked glycans to pocket accessibility using Gaussian Accelerated Molecular Dynamics Simulations

Final draft to be submitted to ACS Omega *In Vitro* and *In Silico* Analysis of Naringenin Derivatives on their Inhibitory Activities to SARS-CoV-2 Spike Protein:ACE2 Protein-Protein Interaction

Training and Mentorship

Exploring point mutations in lipase T6 from *Geobacillus steothermophillus*: A computational biophysical study through molecular dynamics simulations 2023 - 2024; Thesis mentor to Raphael Angelo H. Guevarra

***In silico* design of lipase T6 from *Geobacillus steothermophillus* in methanol** 2023 - 2024; Thesis mentor to Kritza Mae L. Arquisola

Virtual Design of benzyliosoquinonline alkaloid derivatives as potential therapeutic in PCOS insulin resistance 2023 - 2024; Thesis mentor and reader to Anatalia Marie M. Bisquera and Rineia Kirsten M. Santos

2023 good ViBEs Laboratory Undergraduate Internship Program Mentor

***In silico* molecular simulation studies and computational retrosynthesis of potential agonists of ADIPOR1 and ADIPOR2** 2022 - 2023; Thesis mentor to Crystal Anne A. Mallari, Aldrin V. Abraham, and Ashley Jud Chris A. Robosa; Won - 3rd Place Best Poster for Central Luzon Health Research and Development Consortium

2022 good ViBEs Laboratory Undergraduate Internship Program Mentor

University of the Philippines Manila, College of Pharmacy Career Mentorship Program Graduate Student Mentee under Dr. Francis R. Capule

Conferences and Relevant Training

Two-Day Program: *In Silico* Techniques for Designing Antibiotics from Natural Compounds for Fish Bacterial Infections — *University of the Philippines Diliman*

Organizer and Lecturer — *September 6-7 2024*

I organized the lecture manual and curricula of the course, and also served as the lecturer for ADMETox.

10th Annual CCPBioSim and MGMS 2024 Conference: Molecular modelling in structure-based drug design — *Newcastle University, Tyne, England/ Hybrid*

Graduate Student Participant — *April 19-20 2024*

I attended the online lectures and enganged in fora.

Hybrid Hünfeld Workshop: Computer Simulation and Theory of Macromolecules 2024 - Max Planck Institute for Multidisciplinary Sciences — *Max-Planck-Gesellschaft/ Hybrid*

Graduate Student Participant — *July 1-4 2024*

I attended the plenaries on drug design, protein engineering, and biophysics.

2023 UNHAN Quantum and Qiskit Workshop — *Jakarta, Indonesia*

Philippines Representative — *December 15 2023*

I attended the Quantum Computing Workshop hosted by IBM to discuss the future direction of quantum computing in drug design as well as some hands-on activities on their server.

3rd EU-ASEAN High Performance Computing (HPC) School — *Bogor, Indonesia*

Philippines Representative — *December 10-16 2023*

I attended the Life Science Track wherein I interacted with some of the leading scientists in drug discovery from the EU and SEA. I learned new computational techniques in drug safety and drug design.

37th Philippine Chemistry (PCC) Congress — *Bacolod City, Negros Occidental, Philippines*

Presenter for <Molecular Docking Simulations of Deguelin-Derived Compounds Against Small-Molecule Binding Conformations of the K-Ras GTPase> — *July 26-28 2023*

I manned a five-day poster booth on the cancer-inhibitory compounds my team designed.

36th Philippine Chemistry (PCC) Congress — *Online Conference*

Presenter for <A shape-based ligand modification algorithm in tandem with target fishing to design target-specific analogs of two candidate anti-cancer compounds> — *2022*

I presented the findings of my study on reformulation and repurposing of commercially available and investigatory drugs.

36th Philippine Chemistry (PCC) Congress — *Online Conference*

Presenter for <A network pharmacology approach to investigate cancer targets of deguelin and rotenone> — *2022*

I presented the findings of my studies on finding the mechanism of action of the cancer compounds I designed for DOST-DDHP.

Hybrid Hünfeld Workshop: Computer Simulation and Theory of Macromolecules 2022 - Max Planck Institute for Multidisciplinary Sciences — *Max-Planck-Gesellschaft/ Hybrid*

Graduate Student participant — *April 08-09 2022*

I attended and participated in the plenaries on drug design and protein engineering.

35th Philippine Chemistry (PCC) Congress — *Online Conference*

Presenter for <Druggability studies targeting the allosteric sites of Q61R NRas GTPase> — *2021*

I presented the findings of my study on discovering new binding sites for drug-like compounds in the cancer target NRas.

Good Clinical Practice (GCP) Training Course — *Bonifacio Global City, Taguig*

Participant — *2016*

I attended the certificate course as a requirement for the culmination of the clinical trial monitoring internship program.

26th Federation of Asian Pharmaceutical Associations (FAPA) Congress — *Bangkok, Thailand*

Presenter for <An Exploratory Study on the Application of Design of Experiments (DOE) in the Assessment of the Stability of Amoxicillin Capsules> — *November 09-13 2016*

I, together with my thesis group mate, attended the conference to keep up to date with the pharmaceutical industry in SEA and to present the findings of our undergraduate study.

Scholarships

2019 **Graduate Scholarship Program**, DOST - ASTHRDP (Accelerated Science and Technology Human Resource Development

Program) *DOST*

Education

University of the Philippines Diliman *Diliman, Quezon City*

Master of Science in Chemistry *Sep 2019 - Q2 2025*

- Courses: Medicinal chemistry, biochemistry, computational chemistry, drug design.

University of the Philippines Diliman *Diliman, Quezon City*

Non-Degree Program *Sep 2018 - Jul 2019*

- Courses: Medicinal chemistry, Biochemistry, physical chemistry, inorganic chemistry, and organic chemistry.

University of the Philippines Manila *Ermita, Manila*

Bachelor of Science in Industrial Pharmacy *Jun 2010 - Jun 2016*

- Courses: Clinical and hospital pharmacy, pharmacology, drug and cosmetics formulation.