

PHYO PHYO KYAW ZIN

Cheminformatician, Data Scientist & Software Developer

k.z.phyophyo.re@gmail.com | 919.771.5803 | Raleigh NC, 27606 | [in phyophyokyawzin](#) | [z inph](#) | [z inph](#)

EXPERIENCE

Cheminformatics Intern

Collaborations Pharmaceuticals Inc., Raleigh, NC.
June 2019 – July 2019

- Mined, curated macrolactones with bioactivity information from public repositories and constructed **MacrolactoneDB**, a web application with options to subset chemical space based on chemical property related filters.
- Developed new molecular descriptors to better characterize macrolactones.
- Built QSAR regressors for three protein targets with high frequency across MacrolactoneDB using 7 ML methods and 7 descriptor sets to predict biological endpoints of macrolides.

Graduate Research Assistant (Cheminformatics)

North Carolina State University, Raleigh, NC.
August 2016 – May 2020

- Implemented RF and DNN QSAR regressors using hybrid 2D, 3D, 4D (MD; molecular dynamics) descriptors on Imatinib derivatives to estimate highly accurate drug activities.
- Extracted SARs (structure-activity relationships) from docking studies, QSAR modeling and cheminformatics analysis of large chemical data.
- Developed cheminformatics biosynthetic engineering-based algorithms, software (PKS Enumerator & SIME) to generate *in-silico* chemical libraries with multiple user constraints.

SKILLS

Python, R, Keras, Tensorflow, Linux, RDKit	5/5
Machine Learning, Deep Learning	5/5
Multi-GPU computing, Big Data Analysis	4/5
Chemical Data Mining, Curation & Data Visualization	5/5
Virtual Chemical Manipulation & Library Design	5/5
Algorithm, Software Development	5/5
Web Development, PHP, HTML, CSS	3.5/5
Technical Writing & Presentations	5/5

FELLOWSHIPS

- AAUW International Doctoral Fellowship (\$20k), 2019-2020
- Olive Ruth Russell Fellowship (\$6k) (2016, 2017, 2019)
- 4-year tuition scholarship (\$130k) at Berea College, 2012-2016
- Scholarship (\$3.5k) at Pre-Collegiate Program of Yangon, 2011

EDUCATION

PhD in Chemistry

North Carolina State University, Raleigh, NC
Adviser: Denis Fourches
August 2016 – May 2020

B.A. in Computer Science and Chemistry

Berea College, Berea, KY
August 2012 – May 2016 (Dean's List)

Publications can be found on [Google Scholar](#).

ACHIEVEMENTS & AWARDS

- Best Use of Google Cloud Platform at PackHacks2019 (Apr 19)
- Second-Best Overall Project at DiamondHacks2019 (Mar 19)
- Best Use of AI/ML at PearlHacks2019 (Feb 19)
- CINF Scholarship for Scientific Excellence at ACS (Aug 17)
- Storytelling prize at ETHDenver (Feb 18)
- Class of 1958 Chemistry Award at Berea (Apr 16)
- 2nd place in poster presentation at TRIWiC, Ohio (Feb 16)
- Pugsley Award for Excellence in Mathematics at Berea (Dec 12)

PROJECTS

PKS Enumerator (PhD Thesis): Developed Structural Motif (SM) based enumeration algorithm to generate *in-silico* chemical libraries of macrolide scaffolds with multiple user constraints.

SIME (PhD Thesis): Developed scaffold-based enumeration method that integrates SMs and sugars of interest at specified places to create virtual libraries of fully assembled macrolides.

MacrolactoneDB (PhD Thesis): See Cheminformatics Intern at Collaborations Pharmaceuticals Inc. in **Experience**.

CryptoChem (PhD Thesis): Developed a novel cheminformatics-based encryption system to securely store and transfer information with chemicals. (funded by DARPA)

Imatinib DLNN (PhD Thesis): Implemented rigorously validated and highly predictive QSAR regression models using 2D/3D/4D (time-series based) descriptors for Imatinib analogues.

Virtual Bio-profiling of PFAS Derivatives: Conducted cheminformatics analysis and generated chemical network visualizations of PFAS derivatives from EPA database.

River Blindness: Identified new potent Closantel analogues via drug repositioning, cheminformatics analysis, QSAR modeling and structure activity-based docking.

Sustainability Dashboard Management System: Developed an integrated platform for displaying sustainability data in meaningful graphs, along with an administrative backend to effectively store, organize and manipulate large data.

GhostWriter: Devised an intelligent system that adaptively co-authors movie scripts with images and creates audiobooks.

RecipeGenie: Designed an AI-based software to suggest dishes along with recipes by taking a snap of food in the pantry/fridge.

ChemX: Developed a program that takes a molecule and generates its analogues by replacing its fragments with the building blocks sharing similar chemical properties.

MyPueblo: Built an AI system that predicts real-estate property values, classifies bank transaction data into relevant finance categories & visualizes total cost breakdown for each category.