

# THUA-PHONG LAM

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[Website](#) | [GitHub](#) | [Google Scholar](#)

I obtained my pharmacist degree in 2022 and I am currently pursuing a Master's degree in Pharmaceutical Science, majoring in Pharmaceutical modeling at Uppsala University, Sweden. My research interest involves employing computational techniques, especially molecular modeling methods and machine learning predictive models to advance the drug discovery process. I am a person who is always willing to learn and share, have a sense of responsibility, and pursue a career in academia.

## EDUCATION

[Transcripts](#)

**Uppsala University**, Uppsala, Sweden

2023 - 2025

- **Master** of Pharmaceutical Science | **Major:** Pharmaceutical modeling
- **Principal subjects/skills covered:**
  - Train, validate, and deploy machine learning and deep-learning models based on biochemical data.
  - Set up, perform, and evaluate different virtual screening methods.
  - Account for how a molecular mechanics forcefield is constructed.
  - Account for and set up molecular dynamics simulations and free energy calculation.

**University of Medicine and Pharmacy at Ho Chi Minh City**, Ho Chi Minh City, Vietnam

2017 - 2022

- **Bachelor** of Pharmacy (5-year program) | **Major:** Medicinal chemistry | Computer-aided drug design
- **Thesis:** In silico virtual screening and binding affinity evaluation of potential interleukin-33 inhibitors.
- **GPA:** 3.59/4.00 (rank 2/368) – **Thesis:** 9.9/10 (rank 1/30)

**Additional courses – Selected:**

[Training certificates](#)

- **Deep Learning Specialization (DeepLearning.AI):** certified by Coursera (2024)
- **Data Scientist with Python:** certified by Datacamp (2023)
- **Machine Learning Specialization (Stanford University & DeepLearning.AI):** certified by Coursera (2023)
- **VinUni-Illinois Smart Health Center Workshop:** a fully funded program for 40 students across Vietnam about the applications of AI/ML in healthcare devices in VinUniversity campus, Hanoi, Vietnam (2022).

## WORK EXPERIENCE

**Uppsala University**, Uppsala, Sweden

**Summer Intern, Carlsson's Lab, Department of Cell and Molecular Biology**

06/2024 – 09/2024

**Advisors:** Dr. Israel Cabeza de Vaca Lopez | Prof. Dr. Jens Carlsson

**Conformal Predictor for Ultra-Large Chemical Libraries:** Contributed to a project employing the conformal predictor framework to predict docking scores of ultra-large compound libraries. Applied active learning methods to enhance compound diversity and improve hit rates in drug discovery efforts.

**MolSanitizer:** Developed MolSanitizer, a tool for preparing and filtering SMILES databases by removing salts, enumerating stereoisomers, applying protonation, and eliminating undesirable substructures (e.g., PAINS, reactive functional groups). The package also generated drug-like conformations of small molecules for drug discovery projects.

**University of Medicine and Pharmacy at Ho Chi Minh City**, Ho Chi Minh City, Vietnam

**Research Assistant, Department of Medicinal Chemistry**

05/2019 – 12/2023

**Advisors:** Dr. Tan Thanh Mai | Prof. Dr. Khac-Minh Thai

**IL-33/ST2 inhibitors project (2021-2023):** The project aimed to apply *in-silico* approaches and *in-vitro* methods to discover the small molecule inhibitors of the Interleukin-33 (IL-33) / ST2 axis.

My responsibilities:

- Conducted different virtual screening stages including homology modeling, 3D-pharmacophore, molecular docking, molecular dynamics simulation, and binding free energy calculation for identifying putative IL-33 inhibitors.
- Applied conventional machine learning methods (Linear Regression, SVM, RandomForest, XGBoost) and deep learning techniques (MLP, GNN) to build a classification model for ST2 inhibitors.
- Applied cosolvent dynamics simulation methods (MixMD) to find putative binding sites on IL-33 and ST2.
- Adapted and applied an *in-vitro* protocol for binding properties characterization using fluorescent spectroscopy.

**Flavonoids as anti- $\alpha$ -glucosidase and  $\alpha$ -amylase dual-target inhibitors (2022-2023):** The project aimed to evaluate the inhibitory activity of synthetic and natural flavonoids against anti-diabetic targets.

**Computational antiviral projects (2021-2022):** The projects' goals were to evaluate the inhibitory activity of in-house chalcones and commercial drugs against emerging viral pandemics such as COVID-19 and Monkeypox.

*Research Assistant, Department of Clinical Pharmacy*

08/2022 – 02/2023

**Prediction of antibiotic resistance in hospitalized patients using machine learning algorithms from medical record data:**

The study aims to develop machine learning models to predict the susceptibility of bacteria against a set of empirical antibiotics used in current treatment guidelines. My main responsibilities included developing machine learning models using different resampling methods to handle the imbalanced dataset.

## HONOURS AND AWARDS

- **Anders Wall Scholarships (2024):** a tuition fee scholarship awarded by Uppsala University.
- **Graduate Student Merit Award for Top-ranking graduates (2022):** awarded to the top 1% of students.
- **Certificate of outstanding contribution to the faculty's extracurricular activities (2022).**
- **UMP Scholarship for excellent students (2017-2022):** full tuition fee scholarship for the top 10% of best students.
- **Third prize in Summer Research Scholarship (2020):** a student scientific research program for 5 outstanding students.
- **OPC Scholarship (2020):** full tuition scholarship for 10 excellent students in the academy, awarded by OPC Company.
- **Homtamin scholarship (2019):** for outstanding students in the academy and social activities, awarded by Korea United Pharm Company

## PUBLICATIONS Selected articles

[Full list of publications and conference attendances](#)

1. Mai TT, Lam TP, Pham L-HD, ... & Thai KM. (2024). Toward Unveiling Putative Binding Sites of Interleukin-33: Insights from Mixed-Solvent Molecular Dynamics Simulations of the Interleukin-1 Family. *J. Phys. Chem. B.*, 128(35). [\[Link\]](#)
2. Lam TP, Tran N-VN, Pham L-HD, ... & Tran TD. (2024). Flavonoids as dual-target inhibitors against  $\alpha$ -glucosidase and  $\alpha$ -amylase: a systematic review of in vitro studies. *Nat. prod. bioprospect.* 14(4). [\[Link\]](#)
3. Lam TP, Tran VH, Mai TT, Lai NVT, Dang BTN., Le MT, ... & Thai KM. (2022). Identification of Diosmin and Flavin Adenine Dinucleotide as Repurposing Treatments for Monkeypox Virus: A Computational Study. *Int. J. Mol. Sci.*, 23(19). [\[Link\]](#)
4. Lam TP, Nguyen DN, Mai TT, Tran TD, Le MT,... & Thai KM. (2022). Exploration of chalcones as 3-chymotrypsin-like protease (3CLpro) inhibitors of SARS-CoV-2 using computational approaches. *Struct. Chem.*, 33(5). [\[Link\]](#)

## SOFT SKILLS

**Languages:** Vietnamese (native), English (full professional proficiency)

### Technical skills:

- **Programming languages:** Python, R, Bash.
- **Operating systems:** Windows, Linux, MacOS, HPC operating using SLURM.
- **Molecular modeling techniques and software:**
  - Structure prediction: AlphaFold, MODELLER, RoseTTAFold.
  - Virtual screening: molecular docking, 3D-pharmacophore, 2D/3D-QSAR, shape screening.
  - Molecular dynamics simulation: AMBER, GROMACS, NAMD.
  - Molecular visualization: Pymol, Maestro, VMD, ChimeraX.
- **Machine learning and chemoinformatics:** Rdkit, Sci-kit Learn, TensorFlow, and PyTorch.
- **Laboratory:** fluorescent and UV-Vis spectroscopy; enzyme-based assays.

### Leadership skills:

- Good communication skills gained through five years of working in the faculty's academic club and two years working in the faculty's student association.
- Good organizational skills gained through organizing at least 14 research-oriented seminars and 6 student scientific research programs for young pharmacy students.
- Leadership (worked as the academic club president leading 30 club members for 2 years).
- Mentoring (mentored two junior research groups participating in student research programs in 2022).

## SOCIAL ACTIVITIES

**2023:** Contributor of [Sweden Mentor](#), an AI chatbot based on a large language model to provide information for new students.

**2019 – 2021:** Member of the committee of the Faculty's Student Association.

**2017 - 2022:** Member/President/Mentor of Pharmacy Academic Club.

## REFERENCES

**Prof. Khac-Minh Thai,**

Head of the Department of Medicinal Chemistry  
Faculty of Pharmacy,  
University of Medicine and Pharmacy at Ho Chi Minh City  
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