THUA-PHONG LAM

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Website | GitHub | Google Scholar

I obtained my pharmacy degree in 2022 and completed a Master's in Pharmaceutical Modeling in 2025 at Uppsala University. My research interests lie in applying computational techniques, particularly molecular modeling and machine learning predictive models, to support and accelerate the drug discovery process. I am highly motivated, responsible, and collaborative, with a strong commitment to continuous learning and a long-term goal of pursuing a career in academia.

EDUCATION

Transcripts

Uppsala University, Uppsala, Sweden **2023 - 2025**

- **Master** of Pharmaceutical Science | **Major:** Pharmaceutical modeling | **Grade**: VGs in all taken courses
- **Thesis:** Synthon-based docking and machine learning to accelerate structure-based drug discovery in ultralarge libraries
- **Principal subjects/skills covered:**
  - Train, validate, and deploy machine learning and deep-learning models based on biochemical data.
  - 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)

WORK EXPERIENCE

Uppsala University, Uppsala, Sweden

Master's Thesis Student, Carlsson's Lab, Department of Cell and Molecular Biology (ICM) **11/2024 – 06/2025**

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

Synthon-Based Docking and Machine Learning to Accelerate Structure-Based Drug Discovery in Ultralarge Libraries: The project aims to investigate the impact of the conformal predictor framework on top of the fragment-based method in discovery potential starting point in vast chemical space containing multi-billion compounds.

Summer Intern, Carlsson's Lab, Department of Cell and Molecular Biology (ICM) **06/2024 – 11/2024**

Advisors: Dr. Szymon Pach | Dr. Israel Cabeza de Vaca

MolSanitizer (https://carlssonlabtools.icm.uu.se/molsani): Main contributor of MolSanitizer, a rule-based, open-source Python pipeline that supports protonation, tautomerization, filtering, and conformational sampling of small molecules for structure-based drug discovery.

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. 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 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-α-glucosidase and α-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.

HONOURS AND AWARDS

- **Hill scholarship (2025):** a scholarship awarded by Uppsala University for highly merit pharmacy students.
- **Wasenius scholarship (2025):** a scholarship awarded by Uppsala University for exceptionally talented students.
- **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.
- **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 students.
- **OPC Scholarship (2020):** full tuition scholarship for 10 excellent students in the academy, awarded by OPC 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 α-glucosidase and α-amylase: a systematic review of in vitro studies. *Nat. prod. bioprospect*. 14(4). [Link]
3. Mai TT, Phan MH, Thao TT, **Lam TP**, … & Tran TD. (2023). Discovery of novel flavonoid derivatives as potential dual inhibitors against α-glucosidase and α-amylase: virtual screening, synthesis, and biological evaluation. Mol. Divs. [Link]
4. **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]
5. **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.

REFERENCES

Prof. Jens Carlsson,
Master's thesis supervisor
Professor at ICM
Uppsala University, Sweden
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Dr. Szymon Pach,
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Prof. Khac-Minh Thai
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