Tan Thanh Mai

Curriculum Vitae

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Research summary

My research explores innovative approaches to address unmet medical needs. To accelerate the discovery of new therapeutics, I leverage computational methodologies, including QSAR modeling, pharmacophore modeling, molecular docking, and molecular dynamics simulations. My work focuses on developing drug candidates for inflammatory and autoimmune disorders, metabolic disorders, cancer, and infectious diseases.

Education

University of Medicine and Pharmacy at Ho Chi Minh City
Ph.D. Pharmaceutical Chemistry, 2024.
Advisor: Khac-Minh Thai. Thesis: *In silico and in vitro screening of small molecules interacting with interleukin-33 and the ST2 receptor.*

University of Medicine and Pharmacy at Ho Chi Minh City
M.S. Industrial Pharmacy and Pharmaceutics, 2016.
Advisor: Khac-Minh Thai. Thesis: *Design of small-molecule inhibitors for interleukin-33.*

University of Medicine and Pharmacy at Ho Chi Minh City
B.S. Pharmacy, 2013.
Advisor: Khac-Minh Thai. Thesis: *Virtual screening models for antimalarial compounds.*

Employment

Regulatory Reviewer of Drug Technical Dossiers, UMP STC – University of Medicine and Pharmacy at Ho Chi Minh City, assigned by the Drug Administration of Vietnam.
July 2025 – current

Lecturer in Pharmaceutical Chemistry, Deparment of Pharmaceutical Chemistry, School of Pharmacy, University of Medicine and Pharmacy at Ho Chi Minh City.
September 2017 – current

Lecturer in Medicinal Chemistry, Faculty of Pharmacy, Nguyen Tat Thanh University.
February 2017 – September 2017

Lecturer in Medicinal Chemistry and Pharmacology, Faculty of Medicine and Pharmacy, Dong Nam A College.
November 2013 – May 2016

Awards and Honors

PhD Scholarship Programme of Vingroup Innovation Foundation (VINIF), Vingroup Big Data Institute (VINBIGDATA), code VINIF.2019.TS.59 and VINIF.2020.TS.128.

Outstanding Presentation, The 19th National Young Scientists Conference of Medical and Pharmaceutical Universities in Vietnam, 2018.

The Creative Youth Badge awarded by The Ho Chi Minh Communist Youth Union Central Committee, 2018.

Third Prize Presentation, The 14th Student Scientific Research Award – Euréka, organized by The Ho Chi Minh City Youth Union, 2012.

Peer-Reviewed Publications

Journal Publications

Tan Thanh Mai, Nghia Vo-Trong Lai, Thua-Phong Lam, Lam Nguyen-Ngoc Truong, My Ngoc Nguyen, Nghi Van-Tuong Nguyen, Minh-Hoang Phan, Lam-Truong Tuong, and Khac-Minh Thai. Validated virtual screening models for identifying allosteric inhibitors of ATP-citrate lyase: the role of docking scores and protein–ligand interaction similarity in hit selection. *Molecular Diversity.* 2026.

Nham-Linh Nguyen, Thi Trang Nguyen, Thanh Tan Mai, Minh Hao Hoang, Thi Anh Tuyet Nguyen, Nguyen Kim Tuyen Pham, and Thi Nga Vo. A new triterpenoid pentaglycoside from Olax imbricata: isolation and *in vitro*, *in silico* studies on α-glucosidase. *Natural Product Research.* 2025; 1-11.

The-Huan Tran, Thai-Son Tran, Minh-Hieu Nguyen, Thi-Trang Pham, Thanh-Tan Mai, Thanh-Dao Tran. Carbamoyl flavonoids as dual inhibitors of acetylcholinesterase and monoacylglycerol lipase: synthesis, *in vitro* evaluation, and computational studies. *Medicinal Chemistry Research.* 2025; 34:1544-1556.

The-Huan Tran, Thi-My-Hanh Nguyen, Thi-Cam-Nhung Cao, Thai-Son Tran, Thanh-Tan Mai, and Thanh-Dao Tran. Integrating synthesis, enzyme inhibition and *in silico* studies: Carbamoyl luteolin derivatives targeting Alzheimer's disease. *Journal of the Chinese Chemical Society.* 2025; 72(6):739.

Thi-Anh-Truc Phan, Kim-Khanh-Huy Ngo, Thi-Cam-Thu Nguyen, Thanh-Tan Mai, Hai-Dang Nguyen, Thu-Trang Duong, Le-Phu Tran, Thanh-Tuyen Duong, Thi-Kim-Chi Huynh, Elena V. Koroleva, Zhanna V. Ignatovich, Anastasiya L. Ermolinskaya, Hoang-Phuc Nguyen, Thi-Hong-An Nguyen, Anh-Khoa Ton, Tuong-Ha Do, and Thi-Kim-Dung Hoang. 2-Amino-4,6-diarylpyrimidines as potential chronic myeloid leukemia cell inhibitors targeting anti-ABL1 kinase: microwave-assisted synthesis, biological evaluation, molecular docking, and dynamics studies. *RSC Advances.* 2025; 15:4458-4471.

Khac-Minh Thai, Cuong Quoc Duong, Tan Thanh Mai, Minh-Tri Le, Van-Thanh Tran, Phuoc-Vinh Nguyen, and Lam-Truong Tuong. Achievements and Approaches in the Search for Small-Molecule Dengue NS2B/NS3 Inhibitors. *Current Medicinal Chemistry.* 2025; 33(14):2697-2733.

Quoc-Thai Nguyen, Tan Thanh Mai, Lam-Truong Tuong, Thi-Thao-Nhung Nguyen, Thanh-Phuong Vo, Dac-Nhan Nguyen, Cong-Thanh Phan-Van, Dieu-Thuong Thi Trinh, Van-Thanh Tran, and Khac-Minh Thai. Binding ability of Delta and Omicron towards the angiotensin-converting enzyme 2 receptor and antibodies: a computational study. *Journal of Biomolecular Structure and Dynamics*. 2025; 43(18):10785-10797.

Hoang Minh Phan, Tan Thanh Mai, Thinh Nguyen Quang Don, Dat Thanh Do, Khac Minh Thai, Thanh Dao Tran, Phuong Truong, and Phuong Nguyen Hoai Huynh. Synthesis and Evaluation of Antibacterial and Antifungal Activities *In vitro* and *In silico* of Novel Morpholinoalkoxychalcones. *Medicinal Chemistry*. 2025; 21(1):61-68.

Tan Thanh Mai, Thua-Phong Lam, Long-Hung Dinh Pham, Kim-Hung Nguyen, Quoc-Thai Nguyen, Minh-Tri Le, and Khac-Minh Thai. Toward Unveiling Putative Binding Sites of Interleukin-33: Insights from Mixed-Solvent Molecular Dynamics Simulations of the Interleukin-1 Family. *The Journal of Physical Chemistry B*. 2024; 128(35): 8362-8375.

The-Huan Tran, Thanh-Tan Mai, Thi-Thu-Trang Ho, Thi-Ngoc-Dung Le, Thi-Cam-Nhung Cao, Khac-Minh Thai, and Thai-Son Tran. Inhibition of Pancreatic Lipase by Flavonoid Derivatives: *In Vitro* and *In Silico* Investigations. *Advances in Pharmacological and Pharmaceutical Sciences*. 2024; 2024:6655996.

Thua-Phong Lam, Ngoc-Vi Nguyen Tran, Long-Hung Dinh Pham, Nghia Vo-Trong Lai, Bao-Tran Ngoc Dang, Ngoc-Lam Nguyen Truong, Song-Ky Nguyen-Vo, Thuy-Linh Hoang, Tan Thanh Mai, and Thanh-Dao Tran. Flavonoids as dual-target inhibitors against α-glucosidase and α-amylase: a systematic review of *in vitro* studies. *Natural Products and Bioprospecting*. 2024; 14(1):4.

Tan Thanh Mai, Minh-Hoang Phan, Thao Thi Thai, Thua-Phong Lam, Nghia Vo-Trong Lai, Thanh-Thao Nguyen, Thuy-Viet-Phuong Nguyen, Cam-Van Thi Vo, Khac-Minh Thai, and Thanh-Dao Tran. Discovery of novel flavonoid derivatives as potential dual inhibitors against α-glucosidase and α-amylase: virtual screening, synthesis, and biological evaluation. *Molecular Diversity*. 2024; 28:1629-1650.

Linh Thuy Khanh Nguyen, Phu Quynh Dinh Nguyen, Chau Bao Hoai Nguyen, Hoai Thi Nguyen, Thi Van Anh Tran, Thanh-Tan Mai, Thai-Son Tran, and Duc Viet Ho. Sesquiterpenoids from the rhizomes of *Homalomena pendula* (Blume) Bakh.f showing acetylcholinesterase inhibitory activity: *in vitro* and *in silico* studies. *Chemical Papers*. 2023; 77(3):1573-1581.

Thua-Phong Lam, Viet-Hung Tran, Tan Thanh Mai, Nghia Vo-Trong Lai, Bao-Tran Ngoc Dang, Minh-Tri Le, Thanh-Dao Tran, Dieu-Thuong Thi Trinh, and Khac-Minh Thai. Identification of Diosmin and Flavin Adenine Dinucleotide as Repurposing Treatments for Monkeypox Virus: A Computational Study. *International Journal of Molecular Sciences*. 2022; 23(19):11570.

Thua-Phong Lam, Dac-Nhan Nguyen, Tan Thanh Mai, Thanh-Dao Tran, Minh-Tri Le, Phuong Nguyen Hoai Huynh, Duc-Tuan Nguyen, Viet-Hung Tran, Dieu-Thuong Thi Trinh, Phuong Truong, Cam-Van T. Vo, and Khac-Minh Thai. Exploration of chalcones as

3-chymotrypsin-like protease ($3CL^{pro}$) inhibitors of SARS-CoV-2 using computational approaches. *Structural Chemistry*. 2022; 33(5):1707-1725.

Que-Huong Tran, Quoc-Thai Nguyen, Nguyen-Quynh-Huong Vo, Tan Thanh Mai, Thi-Thuy-Nga Tran, Thanh-Dao Tran, Minh-Tri Le, Dieu-Thuong Thi Trinh, and Khac-Minh Thai. Structure-based 3D-pharmacophore modeling to discover novel Interleukin 6 inhibitors: an *in silico* screening, molecular dynamics simulations and binding free energy calculations. *PLOS One*. 2022; 17(4):e0266632.

Minh-Tri Le, Dieu-Thuong Thi Trinh, Trieu-Du Ngo, Viet-Khoa Tran-Nguyen, Dac-Nhan Nguyen, Tung Hoang, Hoang-Minh Nguyen, Tran-Giang-Son Do, Thanh-Tan Mai, Thanh-Dao Tran, and Khac-Minh Thai. Chalcone derivatives as potential inhibitors of P-glycoprotein and NorA: an *in silico* and *in vitro* study. *BioMed Research International*. 2022; 2022:9982453.

Tan Thanh Mai, Phuc Gia Nguyen, Minh-Tri Le, Thanh-Dao Tran, Phuong Nguyen Hoai Huynh, Dieu-Thuong Thi Trinh, Quoc-Thai Nguyen, and Khac-Minh Thai. Discovery of small molecular inhibitors for interleukin-33/ST2 protein–protein interaction: a virtual screening, molecular dynamics simulations and binding free energy calculations. *Molecular Diversity*. 2022; 26(5):2659-2678.

Minh-Tri Le, Tan Thanh Mai, Phuong Huynh Nguyen Hoai, Thanh-Dao Tran, Khac-Minh Thai, and Quoc-Thai Nguyen. Structure-based discovery of interleukin-33 inhibitors: a pharmacophore modelling, molecular docking, and molecular dynamics simulations approach. *SAR and QSAR in Environmental Research*. 2020; 31(12):883-904.

Thai-Son Tran, Thanh-Dao Tran, The-Huan Tran, Thanh-Tan Mai, Ngoc-Le Nguyen, Khac-Minh Thai, and Minh-Tri Le. Synthesis, *In Silico* and *In Vitro* Evaluation of Some Flavone Derivatives for Acetylcholinesterase and BACE-1 Inhibitory Activity. *Molecules*. 2020; 25(18):4064.

Khac-Minh Thai, Nghia-Tin Huynh, Trieu-Du Ngo, Thanh-Tan Mai, Trong-Hiep Nguyen, and Thanh-Dao Tran. Three- and four-class classification models for P-glycoprotein inhibitors using counter-propagation neural networks. *SAR and QSAR in Environmental Research*. 2015; 26(2):139-163.

Conference Presentations

Minh Nhat Le, Nhu Huynh Tam Mai, Nhi Thi Hanh Nguyen, and Tan Thanh Mai. Three-dimensional shape similarity approach for the discovery of IL-1R1 receptor inhibitors. *The 1st International Electronic Conference on Medicinal Chemistry and Pharmaceutics*, November 1-30, 2025, Online on Sciforum.

Tan Thanh Mai, Song-Ky Nguyen-Vo, Thua-Phong Lam, and Khac-Minh Thai. Large-Scale Virtual Screening of Inhibitors Targeting the ST2 Receptor Based on a Novel Allosteric Pocket Identified through Mixed-Solvent Molecular Dynamics Simulations. *The 4th ASEAN PharmNET 2024 & The 2024 US-Thai Pharmacy Consortium Conference: The 30th Anniversary Commemoration*, June 12-14, 2024, Bangkok, Thailand.

Tan Thanh Mai, Thua-Phong Lam, Long-Hung Dinh Pham, Kim-Hung Nguyen, and Khac-Minh Thai. Identification of Putative Orthosteric and Allosteric Binding Sites of Interleukin-

33 using Extensive Molecular Dynamics Simulations. *The 9th International Electronic Conference on Medicinal Chemistry*, November 1-30, 2023, Online on Sciforum.

Tan Thanh Mai, Thua-Phong Lam, Trong-Nghia Vo Lai, Bao-Tran Ngoc Dang, Son-Thach Mai, Lan-Anh Nguyen, Khac-Minh Thai. Identification of novel inhibitors of interleukin-33 using 3D shape-based similarity approach. *Asian Federation for Pharmaceutical Sciences Conference 2023*, November 8-10, 2023 in Hanoi, Vietnam.

Tan Thanh Mai, Bao-Tran Ngoc Dang, Lan-Anh Nguyen, Son-Thach Mai, Khac-Minh Thai. Identification of a potential binding site on the ST2 receptor using blind-docking and automated cavity-detection approach. *Asian Federation for Pharmaceutical Sciences Conference 2023*, November 8-10, 2023 in Hanoi, Vietnam.

Tan Thanh Mai, Quoc-Thai Nguyen, Khac-Minh Thai. Discovery of Interleukin-33 receptor inhibitors for the treatment of cytokine storm in COVID-19 patients. *Rencontres de Quy Nhon - Biology Conference 2021*, Session 2 - Fundamental and Clinical Research during the COVID-19 pandemic, December 13-15, 2021, ICISE Quy Nhon, Vietnam.

Tan Thanh Mai, Phong Thua Lam, Thao Thi Thai, Thanh-Dao Tran, Khac-Minh Thai. Exploration of chalcones as SARS-CoV-2 papain-like protease inhibitors using computational approaches. *Rencontres de Quy Nhon - Biology Conference 2021*, Session 2 - Fundamental and Clinical Research during the COVID-19 pandemic, ICISE Quy Nhon, December 13-15, 2021.

Phuong Thi-Kim Nguyen, Hai Quang Luong, Diem Thi-Thuy Dao, Tan Thanh Mai. 2D-QSAR models for prediction of Hepatis C virus NS3/4A protease inhibitors. *The 4th Pan-Asian Biomedical Science Conference*, Medical Device and High Throughput Data session, December 6-7, 2018, Da Nang, Vietnam.

Thanh-Tan Mai, Thi-Thu-Ha Nguyen, Thanh-Dao Tran, Minh-Tri Le, Khac-Minh Thai. Design of small molecular inhibitors for interleukin-33. *The 2nd International Conference On Pharmacy Education and Research Network of ASEAN 2017 (ASEAN PharmNET 2017)*, November 21-22, 2017, Kuala Lumpur, Malaysia.

Mai Thanh Tan, Do Trong Nhat, Dong Quoc Hiep, Nguyen Duc Khanh Tho, Le Thanh Man, Thai Khac Minh. *In silico* modeling for antimalarial compounds. *Proceeding of The Eighth Indochina Conference on Pharmaceuticals Sciences*, 2013, ISBN 604660159-2, pp. 503-509.

Book Chapters

Khac-Minh Thai, Thai-Son Tran, The-Huan Tran, Thi-Cam-Nhung Cao, Hoang-Nhan Ho, Phuong Nguyen Hoai Huynh, Tan Thanh Mai, Thanh-Dao Tran, Minh-Tri Le, and Van-Thanh Tran. Chapter 8: Recent Advances in Computational Modeling of Multi-targeting Inhibitors as Anti-Alzheimer Agents, in Computational Modeling of Drugs Against Alzheimer's Disease. *Neuromethods*, 2023; 203:231-278.

Grants

"Synthesis and evaluation of *in vitro* and *in silico* DENV-2 inhibitory activities of morpholinoalkoxychalcone derivatives," UMP Institutional-Level Research Project, #209/2024/HĐ-ĐHYD, 22/8/2024 to 22/8/2026 (Key Researcher).

"Development of virtual screening models to identify allosteric ATP-citrate lyase inhibitors for the treatment of dyslipidemia and cancer," UMP Institutional-Level Research Project, #172/2023/HĐ-ĐHYD, 09/15/2023 to 09/15/2025 (PI).

"Screening for inhibitors of the ST2-Interleukin-33 signaling pathway using *in silico* and *in vitro* methods", UMP Institutional-Level Research Project, #224/2022/HĐ-ĐHYD, 09/19/2022 to 09/19/2024 (Key Researcher).

"Evaluation of the therapeutic effectiveness of Sam Thao Can Khuong decoction for COVID-19: *in silico* pharmacological studies, toxicity assessment, clinical trials on mild and moderate COVID-19 patients, and scaling up production batch size", Department-Level Project (Ho Chi Minh City Department of Science and Technology), #24/2021/HĐ-QKHCN,10/01/2021 to 10/01/2022 (Key Researcher).

"Design, screening, and synthesis of chalcone derivatives with inhibitory effects on α-amylase and α-glucosidase," UMP Institutional-Level Research Project, #162/2019/HĐ-ĐHYD, 04/15/2020 to 04/15/2023 (Key Researcher).

"Investigation of the binding potential of some candidate compounds to interleukin-33 uing molecular dynamics simulations," UMP Institutional-Level Research Project, #101/2018/HĐ-NCKH, 07/01/2018 to 07/01/2019 (PI).

Teaching

Pharmaceutical Chemistry 1 & 2
Pharmaceutical Chemistry Practice 1 & 2
Cheminformatics
Drug Discovery and Development
Synthesis of Essential Drugs
Fundamentals of Technology in Medicinal Chemistry

Professional Activities

Journal Reviews

BMC Chemistry
Discover Chemistry
International Journal of Biological Macromolecules
Journal of Biological Engineering
Journal of Diabetes & Metabolic Disorders
Medical Oncology
Medicinal Chemistry Research
MesPharmRes
Molecular Diversity

Scientific Reports

Conference Reviews

Scientific and Technical Conference on Pharmacy, University of Medicine and Pharmacy at Ho Chi Minh City

Grant Proposal Review Panels

Institutional-level Scientific Research Project, University of Medicine and Pharmacy at Ho Chi Minh City

MEF Project Joint Research Program

Vietnam National University, Ho Chi Minh City Level Scientific Research Project

Service

University Service

Academic Advisor, Bachelor of Pharmacy Class of 2020 *(2020–2025)*

Academic Advisor, Bachelor of Pharmaceutical Chemistry Class of 2025 *(2025–present)*

Departmental Service

Coordinator of E-learning Courses, Department of Pharmaceutical Chemistry, School of Pharmacy *(2021–present)*