

Curriculum Vitae - Thanet Pitakbut, Dr. rer. nat.

Education

2022 Dr.rer.nat., Technical University of Dortmund

Grade: *Magna cum laude*

Thesis: “Diversity and beneficial mechanisms of endophytic maytansine in *Gymnosporia heterophylla* defense and studies on biological activities of 20-hydroxymaytenin and related natural products.”

Supervisor: Prof. Oliver Kayser

Scholarship: The German Academic Exchange Service (DAAD)

2016 M.Pharm. (Pharmaceutical Sciences), Prince of Songkla University

Grade: 3.85/4.00 GPA with ‘Excellent’ thesis grade

Thesis: “Phytochemical investigation and alpha-glucosidase inhibitory activity of *Borassus flabellifer* L.”

Supervisor: Prof. Sukanya Dejadisai

2011 B.Sc.(Thai Traditional Medicine), Prince of Songkla University

Grade: 3.48/4.00 GPA, a second-class honor

Project: “Effects of Kaysorn-Tung-Haa recipe on heart rate and blood pressure in healthy volunteers.”

Supervisor Prof. Sanan Subhadhirasakul

Advanced training and online course

2024 Intro to programming (Python), Kaggle

2023 Linux Fundamentals, Coursera

2022 The EU-ASEAN High-Performance Computing School, Bangkok, Thailand

Research and teaching positions

01/04/2025 – Now

Postdoctoral researcher; University of Amsterdam

I held a research position with teaching duties. I conducted a project entitled “Establishment of an insect database for odorant–olfactory receptor interaction” with Prof. Astrid Groot.

01/04/2022 – 30/03/2025

Postdoctoral researcher; University of Erlangen-Nuremberg

I held a research position with teaching duties. I conducted a project entitled “Artificial Intelligence (AI) and molecular simulation to determine synergistic bioactive molecule combination against beta-lactamase, a bacterial resistance Mechanism” with Prof. Gregor Fuhrmann. I was also responsible for teaching the undergraduate practical course.

01/07/2016–30/06/2017

Research assistant, Prince of Songkla University

I held a research assistant position. I assisted in a project entitled “Flavonoids isolation from *Caesalpinia pulcherrima* (L.) Sw. leaves extract” with Prof. Sukanya Dejadisai.

Publication metric (Google Scholar, November 2025)

H-index: 10
Publication: 22 peer-reviewed articles (3 co-corresponding, 5 first, and 14 co-authors)
Citation: 317

Research expertise

Drug discovery, Ligand-protein interaction, phytochemicals, molecular simulation, and AI application.

Grants and scholarships

- 2023 Research grant from Dr. Hertha and Helmut Schmauser Foundation, Faculty of Natural Sciences, FAU Erlangen, Germany. **Project:** “Artificial Intelligence (AI) and molecular simulation to determine synergistic bioactive molecule combination against Beta-Lactamase, a bacterial resistance Mechanism
- 2023 Research visiting grant from the Gustav-Adolf and Erika Dornhecker Foundation from the Department of Chemistry and Pharmacy, FAU Erlangen, Germany. **Host:** *Prof. Dr. Florence Tama at RIKEN Center for Computational Science, Japan.*
- 2023 Research visiting grant from the Bavarian University Center for China (BayCHINA). **Host:** *Prof. Dr. Yanjie Wei at Shenzhen Key Laboratory of Intelligent Bioinformatics and Center for High-Performance Computing, Chinese Academy of Science, Shenzhen, China*
- 2017 Doctoral scholarship awarded by the German Academic Exchange Service (DAAD). **Supervisor:** *Prof. Dr. Kayser, Oliver, Technical Biochemistry, Technical University of Dortmund, Germany*
- 2016 Visiting scholarship awarded by the Austrian Agency for International Cooperation in Education and Research (OeAD). **Host:** *Prof. Dr. Brantner, Adelheid (retired) at the Department of Pharmacognosy, Institute for Pharmaceutical Sciences, University of Graz, Austria*

Teaching and mentorship experience

- 2025 Co-supervisor B.Sc. thesis on “Data-driven profiling of odorant–olfactory receptor interactions in insects using graph- and convolutional neural networks”, Mr. Michael Herzog
- 2024 Co-supervisor B.Sc. thesis on “Investigations on the antimicrobial activity of the semi-synthetic cardenolide derivatives: Studies on uptake and synergistic effects in *Bacillus subtilis*”, Ms. Theresa Kiessling
- 2024 Invited keynote speaker at the 2nd International Seminar on Health, Sports Science and Exercise (2024-ISHSSE) at the Faculty of Health and Sports Science, Thaksin University
- 2022-2025 Teaching undergraduate pharmacy practical course, Pharmaceutical Biology I at the University of Erlangen-Nuremberg
- 2021-2019 Supervising exchange pharmacy student trainee (bachelor's degree) at the Technical University of Dortmund, Ms. Jittida Pookchara and Ms. Piraya Noochan

Academic service

I am an active reviewer for international scientific journals, including *Scientific Reports*, *Chemical Papers*, *Heliyon*, *International Journal of Molecular Sciences*, *Biomolecules*, *Molecules*, *Plants*, *ScienceAsia*, and *Trends in Sciences*. Verification of these reviews can be found on my ORCID webpage (<https://orcid.org/0000-0002-1159-3361>).

Oral presentations

- 2025 Oral presentation on “Benefit of Leveraging AI Technology in Virtual Bio-Based Drug Discovery: A Case Study”, The Association of Thai Professionals in the European Region (ATPER), Belgium
- 2021 Oral presentation on “Antiviral Mechanisms of Cannabinoids Against SARS-CoV-2 Infection: A Screening Study” at Vanguard of Natural Product Research, American Pharmacognosy Society (APS), online conference, USA
- 2020 Oral presentation on "Anti-SARS-CoV-2 mechanisms of three major phytocannabinoids, namely THC, CBD, and CBN", presented at the 8th Health Challenge Thailand (HCT), UK
- 2019 Oral presentation on "A critical step in applying a computational approach for drug discovery under the new outbreak situation", presented at the 9th Thai Student Academic Conference (TSAC), Germany

Presentation award

- 2020 Winner of the research Presentation in Biochemistry and Molecular Biology the 8th Health Challenge Thailand (HCT)
- 2019 Best Paper and Presentation Award at the 9th Thai Student Academic Conference (TSAC)

Scientific publications

As the first and co-corresponding author (8 publications)

- 2025 **Pitakbut, T.** and Kayser, O., 2025. Anti-Infective Screening of Selected Nine Cannabinoids Against *Clostridium perfringens* and Influenza A (H5N1) Neuraminidases, and SARS-CoV-2 Main Protease and Spike Protein Interactions. *Current Issues in Molecular Biology*, 47(3), p.185. [**Co-corresponding author**]
- 2025 **Pitakbut, T.**, Munkert, J., Xi, W., Wei, Y. and Fuhrmann, G., 2025. A dataset for machine learning-based QSAR models establishment to screen beta-lactamase inhibitors using the FARM-BIOMOL chemical library. *BMC Research Notes*, 18(1), p.91. [**Co-corresponding author**]
- 2024 **Pitakbut, T.**, Munkert, J., Xi, W., Wei, Y. and Fuhrmann, G., 2024. Utilizing machine learning-based QSAR model to overcome standalone consensus docking limitation in beta-lactamase inhibitors screening: a proof-of-concept study. *BMC Chemistry*, 18(1), p.249.
- 2022 **Pitakbut, T.**, Spittler, M. and Kayser, O., 2022. Genome mining and gene expression reveal maytansine biosynthetic genes from endophytic communities living inside *Gymnosporia heterophylla* (Eckl. and Zeyh.) Loes. and the relationship with the plant biosynthetic gene, friedelin synthase. *Plants*, 11(3), p.321.

- 2021 **Pitakbut, T.**, Nguyen, G. N. and Kayser, O., 2021. Activity of THC, CBD, and CBN on human ACE2 and SARS-CoV1/2 main proteases to understand antiviral defense mechanism. *Planta Medica*. 88(12), pp.1047-1059.
- 2021 **Pitakbut, T.**, Spitteller, M. and Kayser, O., 2021. In Vitro Production and Exudation of 20-Hydroxymaytenin from *Gymnosporia heterophylla* (Eckl. and Zeyh.) Loes. *Cell Culture. Plants*, 10(8), p. 1493.
- 2020 **Pitakbut, T.** 2020. The Antiviral Activity of andrographolide, the Active Metabolite from *Andrographis paniculata* (Burm. f.) Wall. ex Nees. against SARS-CoV-2 by using bio- and chemoinformatic tools. *Walailak Journal of Science and Technology (WJST)*, 17(8), p. 851–866. **[Corresponding author]**
- 2019 **Pitakbut, T.**, Kusari, S., Kayser, O. and Spitteller, M., 2019. Isolation, purification and identification of 20–hydroxymaytenin as a bioactive metabolite from *Maytenus heterophylla* liquid cell culture. *Planta Medica*, 85(18), p. P180.

As the co-author (15 publications)

- 2025 Sangkanu, S., **Pitakbut, T.**, Phoopha, S., Khanansuk, J., Chandarajoti, K. and Dej-adisai, S., 2025. Insights into Thai and Foreign Hemp Seed Oil and Extracts' GC/MS Data Re-Analysis Through Learning Algorithms and Anti-Aging Properties. *Foods*, 14(21), p.3739.
- 2025 Sangkanu, S., Heemman, A., Phoopha, S., **Pitakbut, T.**, Udomuksorn, W. and Dej-adisai, S., 2025. Antidiabetic Potential of *Senna siamea*: α -Glucosidase Inhibition, Postprandial Blood Glucose Reduction, Toxicity Evaluation, and Molecular Docking. *Scientifica*, 1, p.6650349.
- 2024 Classen, N., **Pitakbut, T.**, Schöfbänker, M., Kühn, J., Hrinčius, E. R., Ludwig, S., ... & Kayser, O. 2024. Cannabigerol and Cannabicyclol Block SARS-CoV-2 Cell Fusion. *Planta Medica*.
- 2023 Sangkanu, S., **Pitakbut, T.**, Phoopha, S., Khanansuk, J., Chandarajoti, K., & Dej-Adisai, S. 2023. A comparative study of chemical profiling and bioactivities between Thai and foreign hemp seed species (*Cannabis sativa* L.) plus an in-silico investigation. *Foods*, 13(1), 55.
- 2023 Parndaeng, K., **Pitakbut, T.**, Wattanapiromsakul, C., Hwang, J.S., Udomuksorn, W. and Dej-adisai, S., 2023. Chemical Constituents from *Streblus taxoides* Wood with Their Antibacterial and Antityrosinase Activities Plus in Silico Study. *Antibiotics*, 12(2), p.319.
- 2023 Dej-adisai, S., Koyphokaisawan, N., Wattanapiromsakul, C., Nuankaew, W., Kang, T.H. and **Pitakbut, T.**, 2023. In Vitro, In Vivo, and In Silico Analyses of Molecular Anti-Pigmentation Mechanisms of Selected Thai Rejuvenating Remedy and Bioactive Metabolites. *Molecules*, 28(3), p.958.
- 2022 Dej-adisai, S., Sakulkeo, O., Wattanapiromsakul, C. and **Pitakbut, T.**, 2022. Flavonoid Constituents and Alpha-Glucosidase Inhibition of *Solanum stramonifolium* Jacq. Inflorescence with In Vitro and In Silico Studies. *Molecules*, 27(23), p.8189.
- 2022 Sakulkeo, O., Wattanapiromsakul, **Pitakbut, T.**, and Dej-adisai, S. 2022. Alpha-glucosidase inhibition and molecular docking of isolated compounds from traditional Thai medicinal plant, *Neuropeltis racemosa* Wall. *Molecules*, 27(3), p.639.
- 2022 Dej-adisai, S., Rais, I.R., Wattanapiromsakul, and **Pitakbut, T.** 2021. Phytochemical investigation of *Bauhinia winitii* based on alpha-glucosidase inhibitory effect and molecular docking affirmation. *Pharmacognosy Magazine*, 17(76), p.666.
- 2021 Hussain, T., Jeena, G., **Pitakbut, T.**, Vasilev, N., Kayser, O., 2021. *Cannabis sativa*

- research trends, challenges and new-age perspectives. ISCIENCE. p.103391.
- 2021 Dej-adisai, S., Rais, I.R., Wattanapiromsakul, C. and **Pitakbut, T.**, 2021. Alpha-glucosidase inhibitory assay-screened isolation and molecular docking model from *Bauhinia pulla* active compounds. *Molecules*, 26(19), p. 5970.
- 2020 Phoopha, S., Wattanapiromsakul, C., **Pitakbut, T.** and Dej-Adisai, S., 2020. A new stilbene derivative and isolated compounds from *Bauhinia pottsii* var. *pottsii* with their anti-alpha-glucosidase activity. *Pharmacognosy Magazine*, 16(68), p. 161.
- 2020 Phoopha, S., Wattanapiromsakul, C., **Pitakbut, T.** and Dej-Adisai, S., 2020. Chemical constituents of *Litsea elliptica* and their alpha-glucosidase inhibition with molecular docking. *Pharmacognosy Magazine*, 16(70), p. 327.
- 2017 Dej-adisai, S., **Pitakbut, T.** and Wattanapiromsakul, C., 2017. Alpha-glucosidase inhibitory activity and phytochemical investigation of *Borassus flabellifer* Linn. *African Journal of Pharmacy and Pharmacology*, 11(3), p.45-52.
- 2015 Dej-Adisai, S. and **Pitakbut, T.**, 2015. Determination of a-glucosidase inhibitory activity from selected Fabaceae plants. *Pakistan Journal of Pharmaceutical Sciences*, 28(5). p. 1679 - 1683.

Data sharing practice

GitHub repositories <https://github.com/ThanetPi/pyTecanEx> (Python application)
<https://github.com/ThanetPi/ML-QSAR-Docking-Proof-of-Concept>
 (Dataset and Python script to develop a machine learning QSAR model)
<https://github.com/ThanetPi/ML-GC-MS-Hemp-Cultivars>
 (Dataset and Python script for a machine learning discriminative model)

Zendo repository <https://zenodo.org/records/13378955> (Dataset and Python script for machine learning QSAR)
<https://zenodo.org/records/17505720> (Dataset and Python script for a machine learning discriminative model for GC/MS Hemp cultivars)

Website development experience

Biography <https://thanetpi.github.io/biography/> (Private website)
 FARM-BIOMOL <https://pharmbio-fau-erlangen.github.io/FARM-BIOMOL/>
 (Project website)

References

Prof. Gregor Fuhrmann, University of Erlangen-Nuremberg. gregor.fuhrmann@fau.de
 PD. Dr. Jennifer Munkert, University of Erlangen-Nuremberg. jennifer.munkert@fau.de
 Prof. Oliver Kayser, Technical University of Dortmund. oliver.kayser@tu-dortmund.de
 Assoc. Prof. Sukanya Dejadisai, Prince of Songkla University. sukanya.d@psu.ac.th