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Research Field(s)	Molecular dynamics, Computer aided molecular design, Quantum calculation

Academic Career

- 1994 B.Sc. (Chemistry), Chiang Mai University, Chiang Mai, Thailand;
2001 Ph.D. (Physical Chemistry & Pharmaceutical Sciences), University of Missouri-Kansas City, USA;
2002-2003 Post Doctoral Scholarship, Chulalongkorn University, Thailand;
2001-2009, Assistance Professor, Department of Chemistry, Chiang Mai University, Thailand;
2010-Present, Associate Professor, Department of Chemistry, University of Malaya, Malaysia

Selected Publications

1. Chong, W. L., Saparpakorn, P., Sangma, C., Lee, V. S., & Hannongbua, S. (2023). Insight into free energy and dynamic cross-correlations of residue for binding affinity of antibody and receptor binding domain SARS-CoV-2. *Heliyon*, e12667.
2. Tan, X. H., Chong, W. L., Lee, V. S., Abdullah, S., Jasni, K., Suarni, S. Q., ... & Chan, Y. F. (2023). Substitution of Coxsackievirus A16 VP1 BC and EF Loop Altered the Protective Immune Responses in Chimera Enterovirus A71. *Vaccines*, 11(8), 1363
3. Rani, A. N. A., Gaurav, A., Tatt, L. M., Zain, S. M., Lee, V. S., Nasir, N. M., & Patil, V. M. (2023). Investigations on the Gingerols and Shogaols as Potential Selective PDE4B Inhibitors by Molecular Docking Screening. *Current Trends in Biotechnology & Pharmacy*, 17.
4. Juntit, O., Sornsuwan, K., Wisitponchai, T., Lee, V. S., & ... (2023). Dimeric Ankyrin with Inverted Module Promotes Bifunctional Property in Capturing Capsid to Impede HIV-1 Replication. *International Journal of Molecular Sciences*, 24(6), 5266.
5. Chong, W.L., Vao-soongnern, V., Nimmanpipug, P., Tayapiwatana, C., Lin, J.H., Lin, Y.L., Chee, H.Y., Zain, S.M., Abd Rahman, N. and Lee, V.S., 2022. Molecular dynamics simulations and Gaussian network model for designing antibody mimicking protein towards dengue envelope protein. *Journal of Molecular Liquids*, 346, p.118086
6. Al-Nema, M., Gaurav, A., Lee, M. T., Okechukwu, P., Nimmanpipug, P., & Lee, V. S. (2022). Evaluation of the acute oral toxicity and antipsychotic activity of a dual inhibitor of PDE1B and PDE10A in rat model of schizophrenia. *Plos one*, 17(12), e0278216.
7. Al-Nema, M., Gaurav, A., Lee, V.S., Gunasekaran, B., Lee, M.T., Okechukwu, P. and Nimmanpipug, P., 2022. Structure-based discovery and bio-evaluation of a cyclopenta [4, 5] thieno [2, 3-d] pyrimidin-4-one as a phosphodiesterase 10A inhibitor. *RSC Advances*, 12(3), pp.1576-1591.
8. Chong, W.L., Chupradit, K., Chin, S.P., Khoo, M.M., Khor, S.M., Tayapiwatana, C., Nimmanpipug, P., Thongkum, W. and Lee, V.S., 2021. Protein-Protein Interactions: Insight from Molecular Dynamics Simulations and Nanoparticle Tracking Analysis. *Molecules*, 26(18), p.5696.
9. Gautam, V., Chong, W.L., Chin, S.P., Zain, S.M., Rahman, N.A., Vao-soongnern, V. and Lee, V.S., 2019. Loop dynamics behind the affinity of DARPins towards ERK2: Molecular dynamics simulations (MDs) and elastic network model (ENM). *Journal of Molecular Liquids*, 274, pp.612-620.
10. Karim, H.A.A., Rungrotmongkol, T., Zain, S.M., Rahman, N.A., Tayapiwatana, C. and Lee, V.S., 2019. Designed antiviral ankyrin-A computational approach to combat HIV-1 via intracellular pathway by targeting the viral capsid of HIV-1. *Journal of Molecular Liquids*, 277, pp.63-69.

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Research Field(s)	pharmaceutical chemistry, computational chemistry

Academic Career

B.Sc. in Chemistry, University of Indonesia, 1999; Ph.D. in Biotechnology, Universiti Putra Malaysia, 2004; Postdoctorate, University of Kansas, 2005–2008. Dean of Faculty of Applied Sciences, UCSI University Malaysia (2016-2019). He is currently an associate professor at the Department of Chemistry, Universiti Putra Malaysia. His work involves the use of computational and molecular techniques to study the structure and function of biomolecules. Currently he is working on drug design against tuberculosis and dengue.

Selected Publications

1. F.F. Baharuddin, N.M. Nasir, B.A. Tejo, S.P. Koh, S. Ramakrishnan, N.Q.A.A. Nordin, A.N. Adzahar, P. Devakrishman, S.M. Razib. Potent halogenated xanthone derivatives: synthesis, molecular docking and study on antityrosinase activity. *Journal of Asian Natural Products Research* (accepted).
2. Norhayati, J. Ekowati, N.W. Diah, B.A. Tejo, S. Hegazy. Chemoinformatic approach to design and development vanillin analogs as COX-1 inhibitor. *Journal of Public Health in Africa*, 2023; 14(s1):2517.
3. T. El Moudaka, P. Murugan, M.B.A. Rahman, B.A. Tejo. Discovery of Mycobacterium tuberculosis CYP121 new inhibitor via structure-based drug repurposing. *Pertanika Journal of Science and Technology*, 2023; 31(3):1503–1521.
4. A.A.Q. Al-Khdhairawi, S.S. Ng, A. Muhamad, B.A. Tejo. Rational design and characterization of short antifreeze peptides derived from Lolium perenne antifreeze protein. *Cryobiology*, 2021; 103:181.
5. I.A. Nadzirin, A.L.T. Chor, A.B. Salleh, M.B.A. Rahman, B.A. Tejo. Discovery of new inhibitor for the protein arginine deiminase type 4 (PAD4) by rational design of α -enolase-derived peptides. *Computational Biology and Chemistry*, 2021; 92:107487.
6. N.N.N. Maarof, A. Alsalahi, E.A. Malek, S. Fakurazi, B.A. Tejo, M.B.A. Rahman. Efficacy of afatinib in the treatment of patients with non-small cell lung cancer and head and neck squamous cell carcinoma: A systematic review and meta-analysis. *Cancers*, 2021; 13(4):688.
7. B.A. Tejo, A.A. Asmawi, M.B.A. Rahman. Antifreeze proteins: Characteristics and potential applications. *Makara Journal of Science*, 2020; 24(1):58–64.
8. L.F. Kong, A.A.Q. Al-Khdhairawi, B.A. Tejo. Rational design of short antifreeze peptides derived from Rhagium inquisitor antifreeze protein. *Biocatalysis and Agricultural Biotechnology*, 2020; 23:10147.
9. D. Afriza, S.J.A. Ichwan, W.H. Suriyah, F.S. Wahyuni, Yanwirasti, B.A. Tejo. Prediction of binding affinity of nordentatin and quercetin against anti-apoptotic Bcl-2 protein. *Journal of International Dental and Medical Research*, 2018; 11(3):1116–1122.
10. S.S. Ang, A.B. Salleh, L.T. Chor, Y.M. Normi, B.A. Tejo, M.B.A. Rahman, M.-A. Fatima. Biochemical characterization of the cytochrome P450 CYP107CB2 from *Bacillus lehensis* G1. *The Protein Journal*, 2018; 37(2):180–183.

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Social Media Channel	N/A
Research Field(s)	Chemical Glycobiology, Bioorganic Chemistry, Protein Modifications

Academic Career

Academic qualifications: DPhil, University of Oxford, 2005; MSc, Universiti Putra Malaysia, 1998; **Appointments:** Current (primary): Professor, Department of Chemical Sciences, Universiti Kebangsaan Malaysia (UKM), 2012-present; current (secondary): Principal Research Fellow, Institute of Systems Biology, UKM, 2012-present. Research Fellow, Oxford Glycobiology Institute & Postdoctoral Researcher, Department of Chemistry, University of Oxford, 2006-2012; Lecturer, Universiti Pertanian Malaysia, 2005-2006. My research interests represent an intersection between chemistry and the biosciences with particular emphasis on carbohydrates, proteins and natural product/secondary metabolite inhibitors.

Selected Publications

1. Altammar KA et al. Characterization of AnCUT3, a plastic-degrading paucimannose cutinase from *Aspergillus niger* expressed in *Pichia pastoris*. *Int J Biol Macromol.* 2022 Dec 1;222(Pt B):2353-2367
2. Jailani N et al. Cross-linked cyclodextrin glucanotransferase aggregates from *Bacillus lehensis* G1 for cyclodextrin production: Molecular modeling, developmental, physicochemical, kinetic and thermodynamic properties. *Int J Biol Macromol.* 2022;213:516-533.
3. Jaafar NR et al. Structural and functional characterisation of a cold-active yet heat-tolerant dehydroquinase from *Glaciozyma antarctica* PI12. *J Biotechnol.* 2021;329:118-127.
4. Jaafar NR et al. Crystal structure of fuculose aldolase from the Antarctic psychrophilic yeast *Glaciozyma antarctica* PI12. *Acta Crystallogr F Struct Biol Commun.* 2016;72(Pt 11):831-839.
5. Loenarz C. et al. Hydroxylation of the eukaryotic ribosomal decoding center affects translational accuracy. *Proc Natl Acad Sci U S A.* 2014;111(11):4019-4024
6. Ge W et al. Oxygenase-catalyzed ribosome hydroxylation occurs in prokaryotes and humans. *Nat Chem Biol.* 2012;8(12):960-962.
7. Altun M et al. Activity-based chemical proteomics accelerates inhibitor development for deubiquitylating enzymes. *Chem Biol.* 2011;18(11):1401-1412.
8. Scanlan EM et al. Synthesis and solution-phase conformation of the RG-I fragment of the plant polysaccharide pectin reveals a modification-modulated assembly mechanism. *J Am Chem Soc.* 2010;132(21):7238-7239.

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Social Media Channel

Research Field(s)

Natural products, organic chemistry, medicinal chemistry

Academic Career

BSc (Hons)(Chemistry), 1987, Waterloo University, Canada; MSc (Chemistry), 1990, Universiti Malaya (UM); PhD, (Natural Products Chemistry), 1993, Universite Rene Descartes (Paris V).

Selected Publications

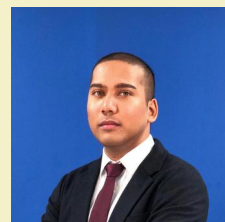
1. Leong, S. T., Liew, S. Y., Khaw, K. Y., Ahmad Hassali, H., Richomme, P., Derbré, S., Lee, V. S., Yahya, R., & Awang, K. (2023). ¹³C NMR-based dereplication using MixONat software to decipher potent anti-cholinesterase compounds in *Mesua lepidota* bark. *Bioorganic chemistry*, 141, 106859.
2. Bihud, NV; Rasol, NE; Imran, S; Awang, K; Ahmad, FB; Mai, CW; Leong, CO; Cordell, GA; Ismail, NH. 2019. Goniolanceolatin A-H, Cytotoxic Bis-styryllactones from *Goniothalamus lanceolatus*, *Journal of Natural Products*. 2019 Sep 27;82(9), pp:2430-2442.
3. Salim, F; Yunus, YM; Anouar, E; Awang, K; Langat, M; Cordell, GA; Ahmad, R. 2019. Absolute Configuration of Alkaloids from *Uncaria longiflora* through Experimental and Computational Approaches, *Journal Natural Products*. 2019(82), pp:2933 2940.
4. El-Seedi, H.R., Azeem, M., Khalil, N.S., Sakr, H.H., Khalifa, S.A.M., Awang, K., Saeed, A., Farag, M.A., AlAjmi, M.F., P Isson, K., Borg-Karlson, A.-K. 2017. Essential oils of aromatic Egyptian plants repel nymphs of the tick *Ixodes ricinus* (Acari: Ixodidae). *Experimental and Applied Acarology* 73(1):139-157
5. Hematpoor, A., Liew, S.Y., Azirun, M.S., Awang, K. 2017. Insecticidal Activity and The Mechanism Of Action Of Three Phenylpropanoids Isolated From The Roots Of *Piper Sarmentosum* Roxb. *Scientific Reports* 7(1): Article number 12576
6. Leong KH, Mahdzir MA, Din MFM, Awang K, Tanaka Y, Kulkeaw K, Ishitani T, Sugiyama D. 2016. Induction of Intrinsic Apoptosis in Leukaemia Stem Cells and in Vivo Zebrafish Model by Betulonic Acid Isolated from *Walsura pinnata* Hassk (Meliaceae). *Phytomedicine* 26(2017) pp: 11-21.
7. Aziz, A.N., Ibrahim, H., Syamsir, D.R., Mohtar, M., Vejayan, J. & Awang, K. 2013. Antimicrobial Compounds From *Alpinia conchigera*. *Journal of Ethnopharmacology* 145(3):798-802.
8. Kassim, N.K, Rahmani, M, Ismail, A, Sukari, M.A, Ee, G.C.L, Nasir, N.M. & Awang, K. 2013. Antioxidant Activity-Guided Separation of Coumarins and Lignan from *Melicope glabra* (Rutaceae). *Food Chemistry* 139(1-4):87-92.
9. Chong, S.L., Awang, K., Martin, M.T., Mokhtar, M.R., Chan, G., Litaudon, M., Gueritte, F. & Mohamad, K. 2012. Malayanines A and B, Two Novel Limonoids from *Chisocheton erythrocarpus* Hiern. *Tetrahedron Letters* 53(40):5355-5359.
10. Sivasothy, Y., Hadi, A.H.A., Mohamad, K., Leong, K.H., Ibrahim, H., Sulaiman, S.F., Ooi, K.L. & Awang, K. 2012. Spectraflavoside A, a New Potent Iron Chelating Dimeric Flavonol Glycoside from The Rhizomes of *Zingiber spectabile* Griff. *Bioorganic & Medicinal Chemistry Letters* 22(11):3831-3836.

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Research Field(s)	Natural Products Chemistry, Medicinal Chemistry

Academic Career

Young Scientist Fellowship Programme, Funded by Mustafa Science and Technology Foundation (MSTF) in collaboration with Comstech and National University of Science and Technology (NUST), 2023

Ph.D., Life Science, Hokkaido University, Japan, 2019

MSc, Chemistry, University of Malaya, 2016

BSc, Pure Chemistry, University of Malaya, 2014

Selected Publications

1. Usman Ahmed, Yasodha Sivasothy, Khalid Mohammed Khan, Naveed Ahmed Khan, Siti Mariam Abdul Wahab, Khalijah Awang, Muhamad Aqmal Othman, Ayaz Anwar. "Malabaricones from the fruit of *Myristica cinnamomea* King as potential agents against *Acanthamoeba castellanii*". *Acta Tropica*, 2023, 248, 107033.
2. Muhamad Aqmal Othman, Yasodha Sivasothy. Acylphenols and Dimeric Acylphenols from the Genus *Myristica*: A Review of Their Phytochemistry and Pharmacology. *Plants*, 2023, 12, 1589.
3. Yasodha Sivasothy, Kok Hoong Leong, Kong Yong Loo, Siti Mariam Abdul Wahab, Muhamad Aqmal Othman and Khalijah Awang. "Giganteone A and Malabaricone C as Potential Pharmacotherapy for Diabetes Mellitus". *Natural Product Research*, 2021, 1–6.
4. Yasodha Sivasothy, Sook Yee Liew, Muhamad Aqmal Othman, Siti Mariam Abdul Wahab, Maywan Hariono, Mohamed Sufian Nawi, Habibah Abdul Wahab, Marc Litaudon and Khalijah Awang. "Natural DENV-2 NS2B/NS3 Protease Inhibitors from *Myristica cinnamomea* King". *Tropical Biomedicine*, 2021
5. Muhamad Aqmal Othman, Kohei Yuyama, Yuta Murai, Yasuyuki Igarashi, Daisuke Mikami, Yasodha Sivasothy, Khalijah Awang, and Kenji Monde. "Malabaricone C as natural sphingomyelin synthase inhibitor against diet-induced obesity and its lipid metabolism in mice" *ACS Med. Chem. Lett.* 2019, 10, 1154-1158
6. Muhamad Aqmal Othman, Yasodha Sivasothy, Chung Yeng Looi, Abdulwali Ablat, Jamaludin Mohamad, Marc Litaudon and Khalijah Awang. "Acylphenols and dimeric acylphenols from *Myristica maxima* Warb". *Fitoterapia*, 2016, 111, 12-17
7. Yasodha Sivasothy, Thiba Krishnan, Kok Gan Chan, Siti Mariam Abdul Wahab, Muhamad Aqmal Othman, Marc Litaudon and Khalijah Awang. "Quorum Sensing Inhibitory Activity of Giganteone A from *Myristica cinnamomea* King against *Escherichia coli* Biosensors". *Molecules*, 2016, 21, 391