Sakda Khoomrung, PhD

13/01/2025

- Siriraj Center of Research Excellence for Metabolomics and Systems Biology (SiCORE-MSB),
- Department of Biochemistry, Siriraj Hospital
- Siriraj Metabolomics and Phenomics Center (SiMPC), Siriraj Hospital

10th fl, Sri Savarindira Building, Faculty of Medicine, Siriraj Hospital Mahidol University

2 Prannok Road, Bangkok 10700, Thailand Email: <u>sakda.kho@mahidol.edu</u> https://metsysbio.com/

Personal information

Place of birth: Chumphon, Thailand Citizenship: Thai, Swedish ORCID ID: 0000-0001-9461-8597

SUMMARY

I hold an MSc in Chemistry from Prince of Songkla University, Thailand (2006), and a PhD in Chemistry from Karl-Franzens University, Austria (2011). Following postdoctoral (2011-2012) and project leadership roles in metabolomics at Chalmers University of Technology (2013-2017), I co-founded and co-directed the Chalmers Metabolomics Centre (now the Chalmers Mass Spectrometry Infrastructure), providing services nationally and internationally (<u>https://www.chalmers.se/en/infrastructure/cmsi/</u>).

Since joining Siriraj Hospital, Mahidol University in 2017 (Associate Professor, 2019), I have led a research team of over 20 people, establishing a thriving metabolomics and systems biology program and directing the SiCORE-MSB (https://metsysbio.com/). My research focuses on developing innovative approaches to understand cellular metabolism and disease, integrating advanced wet-lab techniques (mass spectrometry, ion mobility mass spectrometry, mass spectrometry imaging) with cutting-edge bioinformatic tools. This work addresses a wide range of biological and medical questions, including research in chronic kidney disease, aging, cancers, skin diseases, precision medicine, and natural products. My contributions include over 50 publications (1800+ citations, h-index 20), mentorship of numerous postdoctoral researchers and graduate students, and numerous national and international awards and grants. I serve as an Associate Editor for a computational and structural biotechnology journal and review for several others. In my free time, I also co-founded and serve as Secretary of the Thailand Metabolomics Society (https://thailand-metabolomics.org/).

Educations & trainings

2017-2020:

2019 (Jan -Fab):

2011 – 2012:	Post Doc; Systems and Synthetic Biology, Chalmers University of Technology, Sweden (Supervisor: Prof. Jens Nielsen)
2007 - 2011:	Dr. rer. nat. (Ph.D.) in Chemistry; Karl-Franzens University, Austria (Supervisor: UniProf. Kevin A. Francesconi)
2003 - 2006:	M. Sc. in Analytical Chemistry; Prince of Songkla University, Thailand
2004:	Diploma (Environmental Analysis); Technical University of Denmark, Denmark
1997 - 2001:	B.Sc. in education (Chemistry); Prince of Songkla University, Thailand
Positions	
2023-	Director: SiCORE-MSB
2019-	Assoc. Prof.: Department of Biochemistry, Siriraj Hospital, Thailand
2018-	Instructor; Department of Biochemistry, Siriraj Hospital, Thailand

Visiting researcher: Chalmers University of Technology, Sweden

Visiting researcher; Department of Biomedical Informatics, University of

	Arkansas for Medical Sciences, USA	
2017- 2018:	Instructor; Center of Applied Thai Traditional Medicine, Siriraj Hospital, Thailand	
2013-2017:	Project leader; Systems and Synthetic Biology, Chalmers University of Technology, Sweden	
2016:	Visiting scholar; Center of Applied Thai Traditional Medicine, Siriraj Hospital	
2013- 2015:	Co-founder and co-director; Chalmers Metabolomics Centre (later became Chalmers Ma	
	Spectrometry Infrastructure), Gothenburg, Sweden	
2011 2013:	Post Doc; Systems and Synthetic Biology, Chalmers University of Technology, Sweden	
2007-2011:	PhD student; Institute of Chemistry, Karl-Franzens University of Graz, Austria	
2006-2007:	Research assistant; Pilot Plant Development and Training Institute, King Mongkut's	
	University of Technology Thonburi, Bangkok, Thailand	
2001-2003:	Research assistant; King Mongkut's Institute of Technology Ladkrabang, Thailand	

Awards/Honors

2023:	Best poster presentation from PMU-B Brainpower Congress 2023: Frontier Research to Future	
	Industries by I conNEXT with U", Hua Hin, Thailand	
2023:	Research excellent award (pre-clinic) from Faculty of Medicine Siriraj Hospital (รับพระราชทานรางวัลจากสมเด็จ	
	พระกนิษฐาราชเจ้า กรมสมเด็จพระเทพรัตนราชสุดาฯ สยามบรมราชกุมารี)	
2019:	Young research Grant from the Thailand Research Fund (ทุนสงเสริมนักวิจัยรุ่นใหม่จาก สกว)	
2016:	Visiting scholar at Faculty of Medicine Siriraj Hospital, Mahidol University	
2015:	Wallenberg foundation: Travel grant for the metabolomics workshop, Imperial College London, UK	
2014:	Wallenberg foundation: Travel grant for the 10 th metabolomics annual meeting, Tsuruoka, Japan	
2014:	Wallenberg foundation: Travel grant for the AMBC2014, Bangkok, Thailand	
2013:	Wallenberg foundation: Travel grant for the 9th metabolomics annual meeting, Glasgow, Scotland	
2012:	Wallenberg foundations: travel grant for the LipidMaps annual meeting CA, USA	
2007 - 2010:	ÖAD Austrian exchange service program, fellowship for doctoral study, Austria	
2003 - 2005:	Postgraduate Education and Research Program in Chemistry (master degree),	
	Thailand	
2004:	ASEM-DUO-Denmark fellowship program (scholarship for exchange student program),	
	Denmark	

Position of Trust

Scientific Organizing Committee for the 20 th Annual Conference of the Metabolomics Society 16-20
June, 2024, Osaka, Japan.
Founding member and Secretary of Thailand Metabolomics Society, Thailand
International committee member of the 16 th Annual Conference of the metabolomics Society 2020,
Shanghai, China
Member of the American Chemical Society, USA

Key Grants

- 2025-2026The Development of Low FODMAP diets for irritable bowel syndrome patients (3.892 MTHB)
PI: Dr. Waraporn Sorndech, Dr. Sakda Khoomrung (Co-investigator)
Funder: Thailand Institute of Scientific and Technology Research (TISTR)
- 2025-2026 Development of IM-MS and GCxGC-TOFMS lipidomics for early detection of patients with diabetic kidney disease (3,000,000 MTHB) PI: Dr. Sakda Khoomrung

	Funder: Mahidol University (Fundamental Fund: fiscal year 2023 by National Science Research and Innovation Fund (NSRF).
2024-2026	The Metabolomics of Aging in Thai population (1.5 mTHB)
2021 2020	PI: Dr. Sakda Khoomrung
	Funder: Faculty of Medicine Siriraj Hospital, Mahidol University
2024-2026	Scholarship for Ph.D. 2566 (2023) (0.6 mTHB)
	PI: Dr. Sakda Khoomrung
	Funder: Mahidol University
2024-2027	Searching for pharmacologically active compounds for drug development (3 years, 7.5 mTHB);
	Main-PI: Prof. Dr. Prasat Kittakoop
	Sub-Project 4: Cutting-edge mass spectrometry to deepen the metabolomics study of Mitragyna
	speciosa (3 years, 1.8 mTHB), Sub-PI: Dr. Sakda Khoomrung
	Funder: National Research Council of Thailand (NRCT)
2024-2027	Mulitomics tracking Biosynthetic Pathways of Mallotus spodocarpus Cyclic Peptides (3 years:
	4.9 mTHB)
	PI: Dr. Sakda Khoomrung
	Funder: PERCH-CIC
2024-2025	Siriraj Center of Research Excellence in Metabolomics and Systems Biology (1 m THB)
	PI: Dr Sakda Khoomrung
	Funder: Faculty of Medicine Siriraj Hospital, Mahidol University
2023-2024	National Higher Education Science Research and Innovation Policy Council (NXPO), 5 mTHB);
	Program Management Unit for Human Resources & Institutional Development, Research and
	Innovation (PMU-B)
	PI: Development of Ion mobility-mass spectrometry and artificial intelligence for medical
	metabolomics to aid precision medicine in patients with kidney diseases
2022-2023	Mahidol University (Fundamental Fund: fiscal year 2023 by National Science Research and
	Innovation Fund (NSRF): 1.34 mTHB
	PI: Development of deep learning for metabolomics data analysis of patients with chronic kidney
	disease
2022-2025	National Higher Education Science Research and Innovation Policy Council (NXPO), 3.29
	mTHB); Program Management Unit for Human Resources & Institutional Development, Research
	and Innovation (PMU-B)
	PI: The use of three-dimensional convolutional neural network (3DCNN) in combination with quantum
	chemistry and IM-MS for accurate compound identifications and properties predictions of isomeric
	lipids
2022-2024	Ministry of Higher Education, Science, Research and Innovation (MHESI),
	2.4 million THB
2021 2024	PI: The study of foot-skin microbiome and metabolomics of Thai naval cadets with pitted keratolysis
2021-2024	Center of Excellent for Innovation in Chemistry (PERCH-CIC), 3.55 mTHB
	PI: Metabolomics and systems biology to identify novel bioactive metabolites and the study
2021 2024	biosynthesis of pyranonaphthoquinone metabolites in Ventilago harmandiana
2021-2024	PMUB Organizational Bridging Found: S&T 2564, program 16, 45 mTHB
	Co-investigator: High-Quality Manpower and Institutional Development through Collaboration on
	Innovative Bioresources in Biorefinery, Metabolomics of Natural Products, and Materials for
2020 2022	Sustainability Feasity of Medicine Sirinei Hegnitel, Mehidel University (0.40 mTHP)
2020-2022	Faculty of Medicine Siriraj Hospital, Mahidol University (0.49 mTHB) PI: Integrated Metabolomics and Transcriptomics of Lingzhi (<i>Ganoderma lucidum</i>)
2020-2021	Center of Excellent for Innovation in Chemistry (2.7 mTHB)
2020-2021	PI: Development of comprehensive MS- and NMR-based metabolomics platform for biomarker
	discovery of disease: A case study for the diagnosis of various types of CKD
2020-2023	Faculty of Medicine Siriraj Hospital, Mahidol University (2.7 mTHB)
	PI: The study of foot-skin microbiome and metabolomics of Thai naval cadets with pitted keratolysis
2019-2022	Mahidol University (3.34 mTHB/year)
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PI: Development of a comprehensive MS- and NMR-based metabolomics platform to support the development of precision medicine: The first example for the diagnosis of various types of CKD 2019-2021 **CPF Food Research and Development Center (3.9 mTHB)** PI: Metabolomics and microbiome in human affected by Asiatic juice and fiber added Asiatic juice 2019-2021 Thailand research fund: Young research Grant (0.6 mTHB) PI: Development of a comprehensive MS- and NMR-based metabolomics platform for the diagnosis of various types of CKD Center of Excellent for Innovation in Chemistry (PERCH-CIC), 4.02 mTHB 2018-2021 PI: Genome-wide association studies with metabolomics of Ventilago harmandiana BioVacSafe, Innovative Medicines Initiative, EU grant 726 KEUR (27 mTHB) 2012-2020 Co-PI for WP5: Metabolomics of fluad and stamaril Co-PI for WP7: Data management

PI = Principal Investigator

Editorial Activities:

Editor roles

Associate Editor 2023: Computational and Structural Biotechnology Journal, Since November 2023-Review Editor: Frontiers in Chemistry (organic chemistry), 2021-

Reviewer

- Analytical Chemistry
- Scientific Reports
- Briefing in bioinformatics
- Journal of food composition and analysis
- Metabolomics
- Frontiers in nutrition
- Frontiers in pharmacology
- Frontiers in plan science
- Frontiers in Nutrition
- Journal of proteome research
- Frontier Oncology
- iScience
- Nature Communications
- Advanced Science
- Npj Biofilms and Microbiomes
- Artificial Intelligence in Medicine
- Computational and Structural Biotechnology Journal
- Npj Science of Food

Publication/ conference presentations

Google scholar ID: <u>Sakda Khoomrung Google citations</u>

Research papers in international journals with peer-reviewed, H-index of 20 (Scopus)

- 48 : Research articles in peer reviewed journal
- 6 : Review articles in peer reviewed journal
- 1. Indrati N, Phonsatta N, Poungsombat P, **Khoomrung S**, Sumpavapol P, Atikorn P. (2025). *Investigation on Volatile and non-volatile metabolite profiles related to deterioration of Southern Thailand sweet pickle mango*. Submitted.

- Mathema V.B., Jariyasopit N, Phochmak T, Wanichthanarak K, Werayachankul T, Sathirapongsasuti N, ChagKitiyakara C, Sirivatanauksorn Y, Khoomrung S* (2025) CRISP II: Leveraging Deep Learning for Multiclass Phenotyping in GC×GC-TOFMS of End-Stage Renal Disease Patients. Submitted.
- Kurilung A, Limjiasahapong S, Wanichthanarak K, Manokasemsan W, Khwanta Kaewnarin, Duangkumpha K, Manocheewa S, Tansawat R, Chaiteerakij R, Nookaew N, Sirivatanauksorn Y, Khoomrung S^{*} (2025) QTOF-MS^E for Simultaneous Metabolite Quantification and Profiling in Human Urine. Submitted.
- Jariyasopit N, Phochmak T, Manocheewa S, Wanichthanarak K, Limjiasahapong S, Kleebkomut N, Sirivatanauksorn Y, Sirivatanauksorn V, Phrommintikul A, Chattipakorn N, Chattipakorn S*, Khoomrung S* (2025). Plasma Kynurenine to Tryptophan for the Prediction of Mild Cognitive Impairment in Treated Metabolic Syndrome Patients. Submitted.
- 5. Saxena K, Andersson R, **Khoomrung S**, Hanzén S, Widlund O.P., Nielsen J, Nyström T. (2025) *Pertubations in L-serine metabolism regulates protein quality control through sensor of retrograde response pathway Rtg2 in S.cerevisae.* revision in Journal of Biological Chemistry.
- Yabueng N[#], Sansupa[#] C, Noirungsee N, Kraisitnitikul P, Chansuebsri S, Janta R, Khoomrung S, Terd Disayathanoowat T^{*}, Chantara S^{*} (2025) *Characterization of Airborne Microbial Communities in Northern Thailand: Impacts ofSmoke Haze Versus Non-Haze Conditions.* Environ. Pollut. 364: 125302.
- Wisanpitayakorn P, Jariyasopit N, Duangkumpha K, GOH-J X, Palmer ME, Sirivatanauksorn Y, Khoomrung S*. (2024) Multi-Pass Arrival Time Correction in Cyclic Ion Mobility Mass Spectrometry for Imaging and Shotgun lipidomics. Accepted in ACS Measurement Science Au. (Selected and the front cover)
- Sureram S, Chutiwitoonchai N, Pooprasert T, Sangsopha W, Limjiasahapong S, Jariyasopit N, Yongyut Sirivatanauksorn Y, Khoomrung S, Mahidol C, Ruchirawat S, Kittakoop P. (2024). Discovery of procyanidin condensed tannins of (-)-epicatechin from Kratom, Mitragyna speciosa, as virucidal agents against SARS-CoV-2[†]. Int. J. Biol. Macromol. 273: 133059.
- Manokasemsan W, Jariyasopit N, Poungsombat P, Kaewnarin K, Kwanjeera Wanichthanarak K, Kurilung A, Duangkumpha K, Limjiasahapong S, Pomyen Y, Chaiteerakij R, Tansawat R, Srisawat C, Sirivatanaukson Y, Sirivatanauksorn V, Khoomrung S*. (2024) *Quantifying fecal and plasma short-chain fatty acids in healthy Thai individuals*. Comput. Struct Biotechnol. 23: 2163–2172.
- Kurilung A, Kaewnarin K, Wisanpitayakorn P, Jariyasopit N, Wanichthanarak K, Sartyoungkul S, Chee Wong S-C, Limjiasahapong S, Sathirapongsasuti N, Kitiyakara C, Sirivatanauksorn Y, Khoomrung S*. (2024) *Measurement of Very Low-Molecular Weight Metabolites by Traveling Wave Ion Mobility and Its Use in Human Urine Samples.* J. Pharm. Anal. 14(5): 100921.
- Wisanpitayakorn P, Sartyoungkul S, Kurilung A, Sirivatanauksorn Y, Visessanguan W, Sathirapongsasuti N, Khoomrung S* (2024) Accurate Prediction of Ion Mobility Collision Cross Section using Ion's Polarizability and Molecular Mass with Limited Data. J. Chem. Inf. Model. 64 (5), 1533-1542. (Selected as the front cover).
- 12. Wanichthanarak K, In-on A, Fan S, Fiehn O, Wangwiwatsin A*, **Khoomrung S***. (2024) *Data processing* solutions to render metabolomics more quantitative: case studies in food and clinical metabolomics using *Metabox 2.0*. GigaScience 13, 1-14.
- Thongkongkaew T, Jariyasopit N, Khoomrung S, Siritutsoontorn S, Jitrapakdee S, Kittakoop P, Somsak Ruchirawat S. (2023) Anti-Xanthine Oxidase Inhibitors, 5'-Hydroxyhericenes A-D, from the Edible Mushroom Hericium erinaceus and Structure Revision of 3-[2,3-Dihydroxy-4-(hydroxymethyl)tetrahydrofuran-1-yl]pyridine-4,5-diol. ACS Omega 8 (48): 46284–46291.
- Suta S, Ophakas S, Manosan T, Honwichit O, Suvimol Charoensiddhi, Apinya Surawit, Pongkunakorn T, Pumeiam S, Mongkolsucharitkul P, Pinsawas B, Sutheeworapong S, Puangsombat P, Khoomrung S, Mayurasakorn K. (2023) Influence of Prolonged Whole Egg Supplementation on Insulin-like Growth Factor 1 and Short-Chain Fatty Acids Product: Implications for Human Health and Gut Microbiota. Nutrients. (15): 4804.
- 15. Suta S, Surawit A, Mongkolsucharitkul P, Pinsawas B, Manosan T, Ophakas S, Pongkunakorn T, Pumeiam S, Sranacharoenpong K, Sutheeworapong S, Poungsombat P, **Khoomrung S**, Akarasereenont P, Thaipisuttikul I

, Suktitipat B, Mayurasakorn K. (2023) *Prolonged Egg Supplement Advances Growing Child's Growth and Gut Microbiota*. Nutrients. 24;15(5):1143. doi: 10.3390/nu15051143.

- 16. Wanichthanarak K, Nookaew I, Pasookhush P, Wongsurawat T, Jenjaroenpun P, Leeratsuwan N, Wattanachaisaereekul S, Visessanguan W, Sirivatanauksorn Y, Nuntasaen N, Kuhakarn C, Reutrakul V, Ajawatanawong P*, Khoomrung S*. (2023) Revisiting Chloroplast Genomic Landscape and Annotation towards Comparative Chloroplast Genomes of Rhamnaceae. BMC Plant Biology 23(1) 1-22.
- 17. Jariyasopit N, Limjiasahapong S, Kurilung A, Sartyoungkul S, Wisanpitayakorn P, Nuntasaen N, Kuhakarn C, Reutrakul V, Kittakoop P, Sirivatanauksorn Y, Khoomrung S*. (2022) *Travelling Wave Ion Mobility-derived Collision Cross Section Database for Plant Specialized Metabolites: An Application to Ventilago harmandiana* Pierre. J. Proteome Res. 21(10): 2481. (Selected as the front Cover).
- Duangkumpha K, Jariyasopit N, Wanichthanarak K, Dhakal E, Wisanpitayakorn P, Thotsiri S, Sirivatanauksorn Y, Kitiyakara C, Sathirapongsasuti N, Khoomrung S*. (2022) GC×GC-TOFMS metabolomics analysis identifies elevated levels of plasma sugars and sugar alcohols in diabetic mellitus patients with kidney failure. J. Biol. Chem. 298 (10): 102445.
- Indrati N, Sumpavapol P, Phonsatta N, Poungsombat P, Khoomrung S, and Panya A. (2022). Metabolic profiles alteration of Southern Thailand traditional sweet pickled mango during the production process. Frontiers in Nutrition. doi: 10.3389/fnut.2022.934842
- Indrati N, Sumpavapol P, Samakradhamrongthai RS, Phonsatta N, Poungsombat P, Khoomrung S, Panya A. (2022) Volatile and non-volatile compound profile of commercial sweet pickled mango (Ma-Muang Bao Chae Im) and its correlation with consumer acceptance. J. Food Sci. Technol. 57: 37603770.
- Mathema VB, Duangkumpha K, Wanichthanarak K, Jariyasopit N, Dhakal E, Sathirapongsasuti N, Kitiyakara C, Sirivatanauksorn Y, Khoomrung S^{*}. (2022) CRISP: A Deep Learning Architecture for GC×GC-TOFMS Contour ROI Identification, Simulation, and Analysis in Imaging Metabolomics. Brief. Bioinform. 23(2): 1-7. Selected as research excellent award in 2023 by Siriraj Hospital
- 22. Anekthanakul K, Manocheewa M, Chienwichai K, Poungsombat P, Limjiasahapong S, Wanichthanarak K, Jariyasopit N, Mathema VB, Kuhakarn C, Reutrakul V, Phetcharaburanin J, Panya A, Phonsatta N, Visessanguan W, Pomyen Y, Sirivatanauksorn Y, Worawichawong S, Sathirapongsasuti N, Kitiyakara C*, Khoomrung S*. (2021) Predicting of Lupus Membranous Nephritis using Reduced Picolinic Acid to Tryptophan Ratio as a Urinary Biomarker. iScience. 24(11): 103355
- Kaewnarin K, Limjiasahapong S, Jariyasopit N, Anekthanakul K, Kurilung A, Chee Wong S-C, Sirivatanauksorn Y, Visessanguan W, Khoomrung S*. (2021) *High-Resolution QTOF-MRM for Highly Accurate Identification and Quantification of Trace Levels of Triterpenoids in Ganoderma lucidum* Mycelium. J. Am. Soc. Mass Spectrom Chem. 32:2451-2462. (Selected as the front cover).
- Jariyasopit N, Khamsaeng S, Panya A, Vinaisuratern P, Metem P, Asawalertpanich W, Visessanguan W, Sirivatanauksorn V, Khoomrung S*. (2021) *Quantitative Analysis Nutrient Metabolite Compositions of Retail Cow's Milk and Milk Alternatives in Thailand*. J. Food Compos. Anal. 97: 103785.
- 25. Limjiasahapong S, Kaewnarin K, Jariyasopit N, Hongthong S, Nuntasaene N, Robinson JL, Nookaew I, Sirivatanauksorn Y, Kuhakarn C, Reutrakul V, **Khoomrung S*.** (2021) UPLC-ESI-MRM for absolute quantification and MS/MS structural elucidation of six specialized pyranonaphthoquinone metabolites from Ventilago harmandiana. Front. Plant Sci. 11, 2038.
- 26. Kenneth H, Jiradej M, Robinson JL, **Khoomrung S**, Trairak P. (2020) *Deep Proteomic Deconvolution of Interferon and Hepatitis B Effects on a Hepatoblastoma Cell Line*. ACS Omega. 16:16796-16781.
- 27. Liu Y, Liu Q, Krivoruchko A, **Khoomrung S**, Nielsen J. (2020) *Engineering yeast phospholipid metabolism for de novo oleoylethanolamide production*. Nat Chem Biol. 16:197-205.
- 28. **Khoomrung S***, Nookaew I, Sen P, Olafsdottir TA, Persson J, Moritz T, Andersen P, Harandi A, Nielsen J. (2019) *Metabolic profiling and compound-class identification reveal alterations in serum triglyceride levels in*

mice immunized with human vaccine adjuvant Alum. J. Proteome Res. 19: 269-278. (Selected as the front cover)

- 29. Jariyasopit N, Tung P, Su K, Halappanavar S, Evans GJ, Su Y, **Khoomrung S**, Harner T. (2019) *Polycyclic Aromatic Compounds in Urban Air and Associated Inhalation Cancer Risks: A Case Study Targeting Distinct Source Sectors.* Environ. Pollut. 252: 1882-1891.
- Jeennor S, Anantayanon J, Panchanawaporn S, Khoomrung S, Chutrakul C, Laoteng K. (2019) Reengineering Aspergillus oryzae to enhance dihomo-gamma linolenic acid production using integrative approach. Gene. 706: 106-114.
- 31. Wanichthanarak K, Jeamsripong S, Pornputtapong N, **Khoomrung S*.** (2019) *Accounting for biological variation with linear mixed-effects modelling improving quality of clinical metabolomics data*. Comput. Struct Biotechnol. J. 17: 611-618.
- 32. Guo Z, **Khoomrung S**, Nielsen J, Olsson L. (2018) *Changes in lipid metabolism convey acid tolerance in Saccharomyces cerevisiae*. Biotechnol Biofuels. 11 (1):297.
- 33. Rodriguez A, Chen Y, **Khoomrung S**, Özdemir E, Borodina I, Nielsen J. (2017) *Comparison of the metabolic response to over-production of p-coumaric acid in two yeast strains*. Metab. Eng. 44: 265-272.
- 34. Fletcher E, Feizi A, Bisschops MMM, Hallström BM, **Khoomrung S**, Siewers V, Nielsen J. (2017) *Evolutionary engineering reveals divergent paths when yeast is adapted to different acidic environments*. Metab. Eng. 39: 19-28.
- 35. Olafsdottir TA, Lindqvist M, Nookaew I, Andersen PL, Maertzdorf J, Persson J, Weiner J, Zhang Y, Anderson J, Khoomrung S, Sen P, Agger EM, Coler R, Carter D, Meinke A, Kaufmann SHE, Reed SG, Harandi AM. (2016) Comparative Systems Biology Analysis Reveals Molecular Signature of Three Clinically Tested Vaccine Adjuvants. Sci. Rep. 6:39097.
- 36. Tippmann S, Nielsen J, **Khoomrung S*.** (2016) Improved quantification of farnesene during microbial production from S. cerevisiae in two-liquid-phase fermentations. Talanta. 146: 100-106.
- Khoomrung S*, Martinez JL, Tippmann, S, Jansa-Ard S, Buffing M, Nicastro R, Nielsen J. (2015) Expanded metabolite coverage of Saccharomyces cerevisiase extract through improved chloroform/methanol extraction and t-BDMS derivatization. Anal. Chem Res. 6:9-16.
- Qin J. G., Zhou Y. J., Krivoruchko A, Huang M, Liu L, Khoomrung S, Siewers S, Jiang B, Nielsen J. (2015) Modular pathway rewiring of Saccharomyces cerevisiae enables high-level production of L-ornithine. Nat Commun 6: 8224.
- Nicastro R, Tripodi F, Guzzi C, Reghellin V, Khoomrung S, Airoldi C, Nielsen J, Alberghina L, Coccetti P. (2015) *Enhanced amino acid utilization sustains growth of cells lacking Snf1/AMPK*. BBA- Mol Cell Res. 1853: 1615-1625.
- 40. **Khoomrung S**^{*}, Raber G, Laoteng K, Francesconi KA. (2014) *Identification and characterization of fish oil supplements based on fatty acid analysis combined with a hierarchical clustering algorithm.* Eur Lipid Sci Tech. 116:795-804.
- 41. Knuf C, Nookaew I, Remmers I, **Khoomrung S**, Brown S, Berry A, Nielsen J. (2014) *Physiological Characterization of the High Malic Acid-Producing Aspergillus oryzae Strain 2103a-68*. Appl Microbiol Biotechnol 98(8): 3517-3527.
- Hussain A, Olausson H, Nilsson S, Nookaew I, Khoomrung S, Andersson L, Koskela A, Tuukkanen J, Ohlsson C, Holmag A. (2013) *Maternal beef and postweaning herring diets increase bone mineral density and strength in mouse offspring*. Exp Biol Med (Maywood). 238:1362-1369.
- 43. Hussain A, Nookaew I. **Khoomrung S**, Andersson L, Larsson I, Hulthen L, Jansson N. Jakubowicz R, Nilsson S, Sandberg AS, Nielsen J, Holmang A. (2013) *A maternal diet of fatty fish reduces body fat of offspring compared with a maternal diet of beef and a post-weaning diet of fish improves insulin sensitivity and lipid profile in adult C57BL/6 male mice*. Acta Physiol. 209: 220-234.

- 44. **Khoomrung S**, Chumnanpuen P, Jansa-Ard S, Ståhlman M, Nookaew I, Boren J, Nielsen J. (2013) *Rapid quantification of yeast lipid using microwave-assisted total lipid extraction and HPLC-CAD*. Anal Chem. 85: 4912-4919.
- 45. **Khoomrung S**, Chumnanpuen P, Jansa-ard S, Nookaew I, Nielsen J. (2012) *Fast and accurate preparation fatty acid methyl esters by microwave-assisted derivatization in the yeast Saccharomyces cerevisiae*. Appl Microbiol Biotechnol, 94: 1637-1646.
- 46. Shi S, Valle-Rodríguez JO, **Khoomrung S**, Siewers V, Nielsen J. (2012) Functional expression of five wax ester synthases in Saccharomyces cerevisiae and their utility for biodiesel production. Biotechnol Biofuels, 5:7.
- 47. Raber G, **Khoomrung S**, Taleshi MS, Edmonds JS, Francesconi KA. (2009) *Identification of arsenolipids with GC/MS*. Talanta. 78: 1215-1218.
- 48. **Khoomrung S**, Laoteng K, Jitsue S, Cheevadhanarak S. (2008) *Significance of fatty acid supplementation on profile of cell growth, fatty acid and gene expression of three desaturases in Mucor rouxii*. Appl Microbiol Biotechnol. 80: 499 -506.

Review articles

- 1. Jariyasopit N, Khoomrung S*. (2023) Mass Spectrometry-based Analysis of Gut Microbial Metabolites of Aromatic Amino Acids. Comput. Struct Biotechnol. 21:4777-4789.
- Mathema VB, Sen P, Lamichhane S, Orešič M, Khoomrung S*. (2023) Deep learning facilitates multi-data type analysis and predictive biomarker discovery in cancer precision medicine. Comput. Struct Biotechnol. 21:1372-1382.
- **3.** Pomyen Y, Wanichthanarak K, Poungsombat P, Fahrmann J, Grapov D, **Khoomrung S*** (2020) Deep Metabolome: Applications of deep learning in metabolomics. Comput. Struct Biotechnol. 18: (2818-2825).
- 4. Sen P, Lamichhane S, Mathema VB, McGlinchey A, Dickens AM, Khoomrung S, Orešič M. (2021) Deep learning meets metabolomics: A methodological perspective. Briefings in Bioinformatics. 00:1-12.
- **5.** Grapov D, Fahrmann F, Wanichthanarak K, **Khoomrung S**. (2018) *Rise of deep learning for genomic, proteomic and metabolomic data integration in precision medicine*. OMICS. 10: 630-636.
- 6. Khoomrung S^{*}, Wanichthanarak K, Nookaew I. Thamsermsang O, Seubnooch P, Laohapand T, <u>Akarasereenont P^{*}. (2017)</u> Metabolomics and integrative omics for the development of Thai traditional medicine. Front. Pharmacol 8: 474.
 - * =Corresponding author

Selected invited Lectures/Talks

- 1. Enhancing Mass spectrometry and Bioinformatics for Chronic Kidney Disease Metabolite Biomakrers Discovery. The 18th International Conference on Data and Text Mining in Biomedical Informatics (DTMBIO) December 16-19, 2024. Queen Sirikit National Convention Center, Bangkok, Thailand.
- 2. Advances in Natural product research and Its application in human health. Empowering Connectivity in Chemistry Tai-Thailand Bilateral Symposium, August 11-15, 2024, Kaohsiung, Taiwan (Invited Speaker)
- 3. Natural product research and its application to host-microbe interactions. The 20th National Research & innovation conference, King Narasuan the Great Exhibition & Convention Center, July 11, 2024 (Invited Speaker)
- 4. Scratching the Surface of personalized Nutrition in Thailand. e-ASIA Workshop for the 13th Joint Call Proposal Discovering Synergies: Connecting People Across Asian Research Frontiers Jan 16, 2024 (Online)
- 5. **Metabolomics and Chronic Kidney Disease**. KMUTT Biotechnology Seminar, Salocha Meeting Room, Pilot Plant Development and Training Institute, KMUTT Bangkhuntien, 13-12-2023.

- 6. Advances in Mass-Spectrometry-Based Metabolomics for Kidney Precision Medicine: The 30th FAOBMB and BMB Conference, Bangkok, 22-25 November 2023. (International Conference).
- 7. Insights for the Development of Siriraj Metabolomics and Phenomics Center, and Thailand Metabolomics Society: Special lecture at Faculty of Medicine, Prince of Songkhla University, 21 November, 2023.
- 8. **MS-based metabolomics standards in clinical research**: The 23rd Annual Meeting, August 7-11, 2023 Bangkok, Thailand, Genomic Standards for Precision Medicine, Agriculture, Comparative Genomics, and Metabolomics: Presentation title: (International conference)
- 9. Advances in MS-based metabolomics for natural product frontiers research: Thailand-Taiwan Bilateral Symposium July 23-26, 2023 Classic Hotel Kameo & Serviced, Ayutthaya, Thailand. (International conference)
- Advances in Mass Spectrometry-Based Metabolomics for Precision Medicine in Kidney Disease: The 4th Materials Research Society of Thailand International Conference (MRS-Thailand 2023) 28 February – 4 March 2023, Ubon Ratchathani, Thailand (International Conference).
- Metabolomics for the Development of human Vaccine. The 44th on Science and Technology of Thailand; Science and Technology in the Disruptive Era October 29th-31st 2018, Bangkok Internaltional Trade & Exhibition Centre (BITEC), Bangkok, Thailand.
- 12. **Metabolomics of Alum Adjuvant**: The 2nd CU FPhS-RIKEN CDB Symposium and 34th International Annual Meeting in Pharmaceutical Sciences, with the theme of "*Advances in Cellular and Molecular Biology*, March 8-9, (2018) Bangkok, Thailand.
- 13. **Metabolomics research in Thailand:** The 1st Asian Oceania Metabolomics Forum (nine countries including Australia, New Zealand, Korea, Indonesia, Japan, Singapore, Malaysia, China and Thailand), September 6, (2017) Bangkok, Thailand.
- 14. **Metabolomics at SiMPC**: Seminar on Metabolomics and Phenomics Study at Faculty of Medicine Siriraj Hospital, Mahidol University July 7, (2017) Bangkok Thailand.
- 15. Metabolomics of Fluad and Stamaril: The 5th BiovacSafe Annual meeting, 8-10 June, (2017) Reykjavik, Iceland.
- 16. **Rapid quantification of yeast lipid using microwave-assisted total lipid extraction and HPLC-CAD:** Swedish Mass Spectrometry Society, Annual Symposium, 5-7 (2014) October, Sweden.
- 17. Metabolomics: A tool for understanding biological complexity: Advanced course in Lipid-Protein Interactions: Understanding their Importance and Modulation in Cell Physiology, 18-21 August (2014) Cuernavaca, Morelos, Mexico.
- 18. **Metabolomics: Analytics method driving progress in biological research:** The 1st Regional Undergraduate Conference on Agricultural Sciences and Technology; RUCA I. "Challenging Sustainable and Green Agriculture toward AEC", 3-5 April (2014) Silpakorn University (Petchaburi Campus), Thailand.
- 19. Metabolomics: Analytics Method Driving Progress in Cell Factories: The 1st ASEAN Microbial Biotechnology Conference 2014 (AMBC2014) 19 21 February (2014), BIOTEC, Bangkok Thailand.
- 20. Analytical platform for characterization and identification of high-value chemicals in microbial cells: Mini-symposium "Agilent in Metabolomics Nordic Tour" at Chalmers University of Technology, November 14 (2012) Gothenburg, Sweden.
- 21. Determination of arsenic containing-fatty acids in cod liver oil by GC/MS: The 16th Young Investigators' Seminar on Analytical Chemistry, June 26 July 2 (2009) Graz, Austria
- 22. Preliminary attempts to determine arsenic-containing fatty acids by GC/MS: The 15th Young Investigators' Seminar on Analytical Chemistry, July 2 5 (2008) Ljubljana, Slovenia

Poster presentation

 Khoomrung S, Nookaew I, Sen P, Olafsdottir TA, Persson J, Moritz T, Andersen PL, Harand AM, Nielsen J. *Metabolomics of Alum Adjuvant*. The 14th Annual Metabolomics 2018 Conference. June 24-28 (2018) Seattle WA, USA.

- Akarasereenont P, Wattanarangsan J, Wanichthanarak K, Manocheewa S, Limsuvan S, Boonrak R, Vannabhum M, Khoomrung S. Absolute Quantification of Phenolic Compounds in Thai Herbal Medicines by LC-MS/MS. The 14th Annual Metabolomics 2018 Conference. June 24-28 (2018) Seattle WA, USA.
- **3.** Khoomrung S, Sen P, Nookaew I, Moritz T, Nielsen J. *Metabolomics for biomarkers of vaccine immunosafety*. 3rd Advance & Application in Human Disease Conference, May 25-26, (2016) Boston, USA.
- 4. Khoomrung S, Martinez JL, Jansa-Ard S, Nielsen J. Improved Chemical Derivatization of Tertbutyldimethylsilylation for Quantitative Analysis of Amino/Non-amino Acids by GC-MS in Saccharomyces cerevisiae. Annual Metabolomics Meeting, 26-27 March, (2015) Uppsala, Sweden.
- **5.** Khoomrung S, Nielsen J. *Rapid quantification of yeast lipid using microwave-assisted extraction total lipid extraction and HPLC-CAD*. The 4th European lipidomics meeting, September 22-24, (2014) Graz, Austria.
- Khoomrung S, Jansa-ard S, Martinez JL, Nookaew I, Moritz T, Nielsen J. Analytical Plattform for metabolome analysis of microbial cell factory. The 10th International Conference of the Metabolomics Society, 23-26 June, (2014) Tsuruoka, Japan.
- Khoomrung S, Jansa-ard S, Martinez JL, Nookaew I, Moritz T, Nielsen J. Analytical platform for metabolome analysis of microbial cell factory. The 9th International Conference of the Metabolomics Society, 1-4 July, (2013) Glasgow, Scotland.
- 8. Khoomrung S, Chumnanpuen P, Nookaew I, Nielsen J. Microwave-assisted: *Fast and accurate sample preparation technique for hight-hrouput lipidomics*. LIPID MAPS Annual Meeting 2012: Lipidomics impact on cell biology, metabolomics and translational medicine, May 7-8, (2012) La Jolla, CA USA.
- **9.** Khoomrung S, Nookaew I, Chumnanpuen P, Nielsen J. *Optimization of mouse lipidomic analysis: a fast and accurate method*. Metabolomeeting. September 25-28, (2011) Helsinki Finland.
- **10. Khoomrung S,** Laoteng K, Tanticharoen M, and Cheevadhanarak, S. *Lipid classification of Mucor rouxii under different growth environments.* The 8th Annual Meeting of the Thai Society for Biotechnology, 2-3, November (2006) Bangkok, Thailand

Computer software and Web application development

- 1. Metabox 2.0: <u>https://metsysbio.com/tools_protocols/metabox-2-0/</u>
- 2. Linear mixed-effects modelling for normalization of clinical metabolomics data by using subject metada. http://metsysbio.com/tools.html

Teaching and Mentoring experience

Course lectures

Faculty of Medicine Siriraj hospital, Mahidol University 2017-present: Graduate:

-Metabolomics approach for precision medicine

-Microbiome and disease related

-Metabolomics and Systems Biology in Stem Cell research

-Introductory to medical metabolomics

-Metabolomics data analysis

-Omics and Systems Biology in Biomedical Research

-Big data and Biomedical Sciences

-Metabolomics & its applications

-Mass Spectrometry

-Uni and multi variate analysis

Undergraduate

-Introduction to medical metabolomics -Introduction to clinical metabolomics

Faculty of Science, Mahidol University Graduate:

-Metabolomics & its applications -Mass spectrometry-based metabolomics

Mentoring activities (Current)

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Prince Mahidol Award Youth Program (อาจารย์ที่ปรึกษาโครงการเขาวชนทุนเจ้าฟ้ามหิดล)

- นพ. ฐิติพัฒน์ พัฒนาประทีป (2567)
- นพ.ปุญญภัทร มาประโพธิ์ (2561)

Alumni (Faculty of Medicine Siriraj Hospital, Mahidol University)

Postdoc

I UL		
1.	Dr. Wilailak Kaewsri	2023-2024
2.	Dr. Kassaporn Duangkumpha	2020-2024
3.	Dr. Fredrick Nwude Eze	2022-2023
4.	Dr. Alongkorn Kurilung	2020-2022
5.	Dr. Oyenike Olufunmi Olatunji	2022-2022
6.	Dr. Sitanan Sartyoungkul	2020-2022
7.	Dr. Krittima Anekthanakul	2019-2022
8.	Dr. Khwanta Kaewnarin	2019-2021
9.	Dr. Apiwat Sangphukieo	Jan- May 2020
10.	Dr. Sakchai Hongtong	2018-2019
Res	search Assistant	
1.	Kittiphat Pitchayametathun (B/Sc.)	2020-2022
2.	Suphitcha Limjiasahapong (M.Sc.)	2018-2020
3.	Chalita Phutthasimma (M.Sc.)	2019-2020
4.	Santikorn Chaimanee (M.Sc.)	2019-2020
Ph	D student	
1.	Weerawon Manokasemsan	2018-2024
Ma	ster Student	
1.	Nichapa Kleekomut	2021-2024

2.	Thiwat Phochmak	2020-2023
3.	Kajol Thapa	2020-2022
4.	Esha Dhakal	2018-2022

Internship

1.	Louis Lim Li Jie, PhD Student, NTU, Singapore	2024
2.	Nicha Tongdee (class of 2026 Choate Rosemary Hall) USA	2024
3.	Lew Yen Jun Renee (PhD student) NUS, Singapore	2024
4.	Na Minyoung (Phd Student) NTU, Singapore	2024
5.	Rungwalee Saibuakham, (B.Sc.) KMUTT, Thailand	2023
6.	Dylan Koh Hong Zheng (Phd student), NTU, Singapore	2023
7.	Praj Chirathivat (Choate Rosemary Hall, Wallingford, CT), USA	2021
8.	Ruthairatch Poonsornsiri (Deerfield Academy, Massachusetts), USA	2020
9.	Prattakorn Metem (Chulalongkorn University), Thailand	2019
10.	Punvinai Vinaisuratern (Chulalongkorn University), Thailand	2019
11.	Wichaya Asawalertpanich (Chulalongkorn University), Thailand	2019

Chalmer University of Technology, Sweden Master student

1. Marieke F Buffing

2011-2011

Phd Thesis examiner

- 1. Dr. Nureesun Mahamud: NEUROPROTECTIVE EFFECTS AND METABOLOMIC STUDIES OF OXYRESVERATROL IN ROTENONE-INDUCED NEUROBLASTOMA SH-SY5Y CYTOTOXICITY FOR A PREVENTIVE APPROACH TO PARKINSON'S DISEASE, Chulalongkorn University (June 9, 2023)
- 2. Dr. Thanikarn Suk-aram: Analysis of VOCs from exhaled breath for the diagnosis of hepatocellular carcinoma, Chulalongkorn University (June 9, 2023).
- 3. Dr. Niken Indrati: *Ma-Muang Bao Chae-Im*, an Osmotic Dehydrated Mango: Metabolomics analysis and its related microbial diversity during Production and Storage, Prince of Songkla University (April 28, 2022).
- 4. Dr Kassporn Duangkumpha: A peptidomic approach for discovery of cholangiocarcinoma risk biomarkers in serum and urine of subject with periductal fibrosis in an opisthorchiasis endemic area of Thailand, Khon Kaen University (December 12, 2018).