

**AOMSc2025 PRE-EVENT**

# **YOUNG SCIENTIST FORUM**

**June 21-22, 2025**

**Ishigaki Island**

**Okinawa, Japan**

**YSF Networking Meeting**

**@ Ohama Nobumoto Memorial Hall**

**•Date & Time:** Saturday, June 21, 2025

- Networking Meeting: 16:00–19:00 (JST)
- Dinner: 19:15–21:00 (JST)

**Young Scientist Forum**

**@ ANA International Ishigaki Resort**

**•Date & Time:** Sunday, June 22, 2025

- Registration: 8:30–9:00 (JST)
- Session 1: 9:00–11:30 (JST)
- Session 2 (Public Session): 11:30–12:00 (JST)



YSF Program ~Session 1~  
@ ANA International Ishigaki Resort  
•Date & Time: Sunday, June 22, 2025

Important

- Each presentation is limited to 9 minutes, including the Q&A.
- Speakers must submit their presentation file on a USB flash drive to the staff no later than 9:00 a.m.
- \*is under consideration for the YSF Best Presentation Award.

Speaker	Title
Mengze Sun*	Investigation of Extraction-Ionization Process of t-SPESI by Current Measurement
Tomohiko Ikeda*	Structural analysis of recombinant adeno-associated virus capsids using hydrogen/deuterium exchange mass spectrometry
Arisa Suto*	Development and Application of Cysteine-specific modification for LC-MS analysis
Keitaro Miyoshi*	Analysis of serine-related lipid changes in Niemann-Pick disease type C model mice using an improved analytical method
Masahiro Watanabe*	Fundamental study of LC/MS/MS analytical conditions for tryptophan-derived metabolites in Niemann-Pick Disease Type C model cells
Rui QIAN*	BIOSP-Based Multi-Scale Proteomics Decodes the Adipose-Brain Axis in Obesity
Thomas Ka Yam LAM*	Single Tissue Multimodal Imaging for Cellular-level Spatial Metabolomics and Transcriptomics Analysis
Laura Choong	Interrogation of the subcellular location of ceramides utilising targeted mass spectrometry
Daiyu MIAO*	Thiol Profiling Based on Live-Cell Derivatization
Niqesha Lau Yi-Sha	Mitigating Sample Loss in Mass Spectrometry: Acoustic Levitation as an Alternative to Low-Protein-Binding Containers
Ning-En Chang*	Mass spectrometry reveals the stoichiometric regulation and phosphorylation for early stage activation of NLRP3 inflammasome
Huan-Chi Chiu*	MiProChip: Microfluidic Device for Multiplexed Isotopic labeling-based Streamlined Single-cell Profiling
Wei-Chen Wang*	Flavors in a Teacup
Lai Thi Khanh Ly	Mass Analysis of Ultra-High Molecular Weight Polystyrene: a Comparison of Copper and Silver Salts Using MALDI LIT-MS
Anna Mae Vorwerk*	Using an online GC-EI-TOF-MS for the source apportionment of an air pollution episode in March 2023 at a suburban site in Hong Kong

# YSF Program ~Session 2 YSF Public Session~

Co-hosted by MSSJ-KSMS Young Researcher

## Invited Speaker 1 Dr. Young Beom Kwak (Inje University)

### **Molecular Networking as a Tool for Understanding Drug Metabolism and Its Applications in Preclinical and Forensic Science**

Molecular networking plays a crucial role in the interpretation of mass spectrometry data, visually representing the interactions of complex compounds and elucidating relationships between compounds in multidimensional data. This approach allows for the identification of hidden patterns and similarities that may not be detected with conventional single-mass data, particularly in non-targeted analysis. Molecular networking has become an essential tool in various research fields, including metabolomics, compound structure analysis, and the discovery of novel biomarkers. In this study, we explored the application of molecular networking in the field of drug metabolism, with a focus on preclinical research and forensic science. Molecular networking serves as a powerful tool for analyzing metabolomics data and visualizing interactions within complex physiological systems, facilitating the tracking of drug metabolism pathways and metabolic changes. This technique enables a more accurate understanding of drug metabolism and excretion pathways, providing crucial information on drug efficacy, safety, and interactions. Additionally, in forensic science, molecular networking can be utilized to identify metabolic profiles related to toxic substances or the illicit use of drugs. Such technological approaches play a significant role in assessing the physiological impact of drugs in preclinical experiments and in providing legal evidence.

## Invited Speaker 2 Dr. Jong-Min Park (Hallym University)

### **Development of rapid MRSA screening software based on MALDI-TOF mass spectrometry and machine learning**

Rapid detection of methicillin-resistant *Staphylococcus aureus* (MRSA) is essential to prevent healthcare-associated infections such as bacteremia, pneumonia, and surgical wound infections, and prompt treatment of antimicrobials against MRSA improves treatment outcomes. However, traditional MRSA screening tests based on molecular diagnostics are time-consuming, labor-intensive, and costly. The objective of this study was to develop and evaluate the rapid MRSA screening software based on MALDI-TOF MS with machine learning. AMRQuest software was developed to be able to compare MALDI-TOF mass spectra of *S. aureus* with a database by working on machine learning techniques and was successfully used to screen MRSA and identify the bacterial species simultaneously. From the test, the sensitivity, specificity, percent agreement, and Cohen's kappa value were calculated to determine the accuracy of the AMRQuest software. The *SCCmecA* gene was detected to compare the discrepancy between the cefoxitin disk diffusion test and the results of AMRQuest MRSA screening. Using the results from the AMRQuest software, MRSA and MSSA were successfully distinguished statistically, and the PPV and NPV were estimated to be 97.4% and 99.3%, respectively. In conclusion, the clinical performance of AMRQuest software for MRSA screening was evaluated to determine if it would be sufficient for use in laboratories.



# YSF Networking Meeting

@ Ohama Nobumoto Memorial Hall

•Date & Time: Saturday, June 21, 2025



16:00–16:30: Registration for YSF

16:30–19:00: Poster Presentations

- Participants will be divided into groups; each group will hold self-introductions and poster presentations.

19:15–21:00: Dinner

- 3,000 JPY (Cash only).

