出國報告（出國類別：其他（視訊會議））

參加第 70 屆 ASMS
美國質譜學會年會視訊報告

服務機關：行政院農業委員會農業藥物毒物試驗所
姓名職稱：施念昊 助理研究員
派赴國家：美國(視訊會議)
出國期間：111 年 6 月 5 日至 111 年 6 月 9 日
報告日期：111 年 8 月 5 日

摘要

美國質譜學會（American Society for Mass Spectrometry, ASMS）為美國公認之國際性非營利性科學團體，每年 6 月舉辦一次年度會議，每年約有 6,500 多名科學家參加，超過 3,000 篇論文以海報和演講的形式呈現。第 70 屆美國質譜學會年會於 2022 年 6 月 5 日至 6 月 9 日在美國明尼亞波里斯舉行，本次會議因疫情關係，同時以實體及線上方式舉辦。因應當時國內疫情仍持續嚴峻，並考量感染風險及後續回台隔離措施，本次會議採遠端參加，遠端會議提供口頭會議之直播和錄影，以及參展壁報論文之閱覽。

會議期間，除第一天為開幕式外，其餘 4 天，每日皆有近百場演講與 500 多篇海報張貼，內容涵蓋最新開發質譜儀器功能介紹、生物、化學、醫學、藥品及食品各領域之研究應用，除此之外還有近百家廠商參展，每年年會皆可讓與會人員更加了解質譜分析及儀器發展之趨勢。

目次

壹、目的

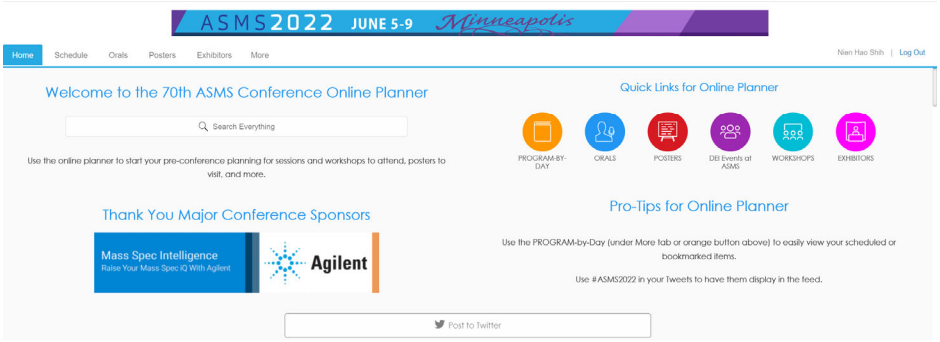
美國質譜年會為推廣質譜相關技術及應用所舉辦之國際會議，每年皆會於美國境內舉辦一次，參加者皆為學界與業界的代表領袖，透過會議交流可獲得最新資訊。會議中除了提供質譜分析技術的最新動態外，也可作為科學分析方法之開發、確效與使用的交流平台。

行政院農業委員會農業藥物毒物試驗所為我國農產品安全之權責檢驗機關，為維護消費者權益及國人健康，須隨時提供具公信力之檢驗數據，供行政管理單位執行公權力之依據，因此派員藉由研習及交流農藥、動物用藥、重金屬或毒物等檢測相關技術，能確保並提昇本所實驗室檢測品質與量能，有助於業務之推展。

貳、過程

本次美國質譜年會於美國明尼蘇達州，明尼亞波里斯希爾頓飯店舉行，會議採實體及遠端混合形式舉辦，參加者可使用美國質譜學會開發之 App 或 Online Planner 遠端參與會議。

ASMS 2022 App 畫面

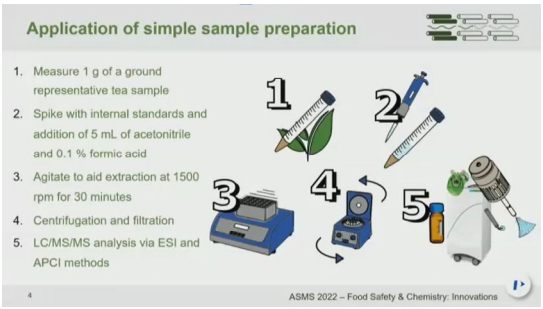


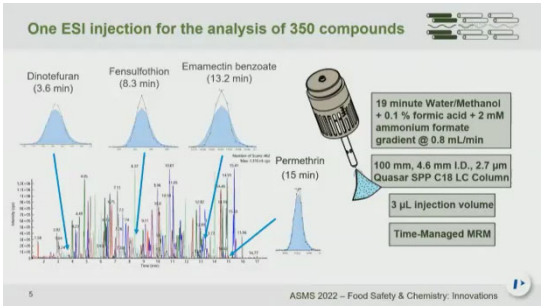
Online Planner 首頁畫面

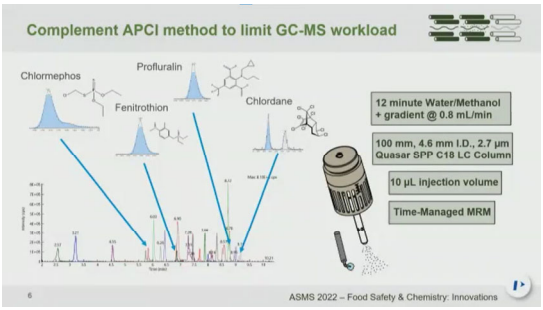
會議期間每日議程大致可分為：1.廠商早餐研討會(corporate breakfast seminar)：由質譜儀相關廠商舉辦，可了解目前最新技術。2.口頭論文發表(oral)：每日可分為上午及下午時段，同時段平行舉辦 8 場不同主題之論文發表，一天即有 16 場，每場約有 6 篇研究內容發表，會期約有 380 篇研究由口頭形式發表。3.壁報發表(poster)：會期壁報約有 140 種主題，近 2 千篇論文發表。4.工作坊(workshop)，針對議題進行討論。會期更有多達 150 家廠商參展，展示質譜儀業界最新及最先進之技術。較可惜的是遠端會議只能參加口頭發表及壁報發表，經由遠端操作與會者可線上觀看口頭發表之錄影及壁報發表之壁報內容及摘要，由於會議內容廣泛，涵蓋核酸、基因體學、蛋白質體學、代謝物、環境汙染及食品安全等，謹就與殘留管制組業務較為相關之重要內容及國際發展趨勢進行分享。

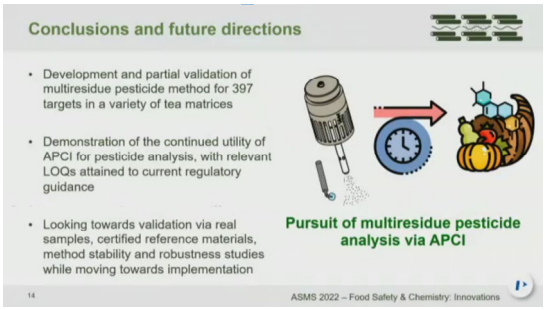
一、口頭論文發表內容

主題一：以 LC/MS/MS 分析茶葉中 400 種農藥：簡單的樣品製備及 APCI 可提高分析物覆蓋率(Analysis of 400 pesticides in tea via LC/MS/MS: Simple sample preparation and APCI to improve analyte coverage)。由珀金埃爾默公司(PerkinElmer)發表演說。現今檢驗方法追求一種方法可用來分析多種基質和目標物，此次研究中以一種簡單的提取方法與 ESI 和 APCI 結合，使用 LC/MS/MS 分析從茶中超過 400 種農藥，高達 93% (371 種)農藥的分析效果出色(回收率 70-120%，RSD < 20%)，包括通常以 GC/MS 分析的農藥，如三福林(trifluralin)、chlorfenson 及 chlormephos 等，此方法將農藥檢驗整合到一台儀器中，使用一台儀器進行農藥分析。試驗步驟：稱取 1 g 磨碎和過篩的茶葉樣品到 15 mL 離心管中，以 5 mL 乙腈和 0.1%甲酸萃取，離心過濾後以 APCI 和 ESI 游離方法在一台儀器上進行分析，儀器為 QSight LX50 UHPLC 和 QSight 420 三重四極桿質譜儀，以正負極切換 MRM 模式進行。所有儀器控制、方法開發和數據處理均使用 Simplicity 3Q 套裝軟體完成。





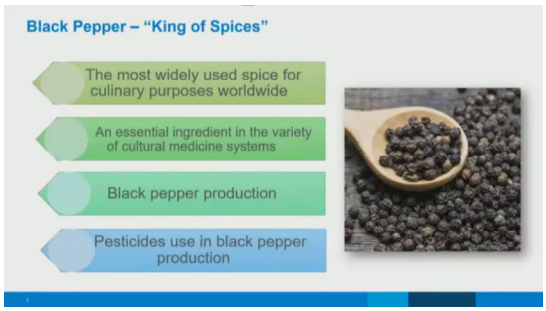


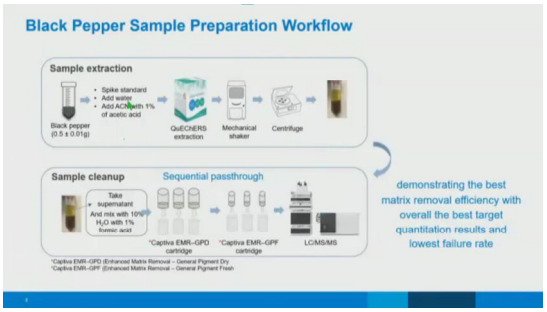


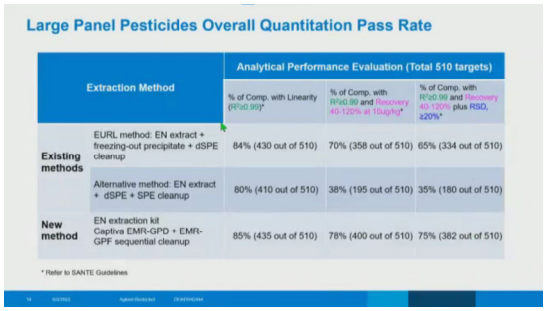
(Alexander Kasperkiewicz et al., 2022)

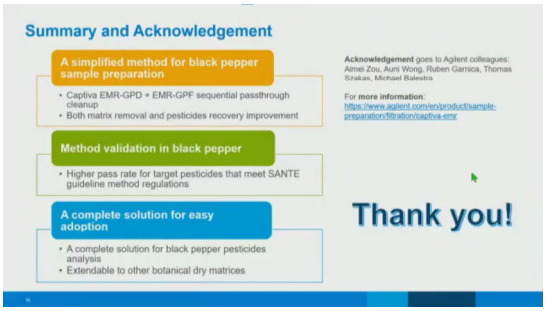
主題二：黑胡椒中 510 種多重農藥殘留分析樣品前處理改進策略(An Improved Sample Preparation Strategy for the Analysis of 510 Multiple Pesticide Residues in Black Pepper)。由安捷倫公司(Agilent)發表演說。黑胡椒是一種高度複雜且難以清理的樣品基質，其天然的複雜性會導致顯著的基質干擾和離子抑制效應，當前的方法採用高稀釋度來降低影響方法的基質效應，或採密集的樣品淨化來獲得乾淨的萃取物，這些方法通常會降低回收率。此項研究使用 QuEChERS 萃取，然後以 Captiva EMR 淨化再以 LC/MS/MS 分析，開發並優化了樣品製備策略。改進的樣品製備方法提供了高效和選擇性的基質淨化，510 種農藥有 80%以上有不錯的回收率。

此方法工作流程簡單、高效、穩健且可靠，適用於黑胡椒中 510 種農藥的定量分析。試驗步驟：依據 SANTE/12682/2019 指南使用 QuEChERS 進行樣品萃取，然後依次使用 EMR-GPD (Captiva Enhanced Matrix Removal General Pigmented Dry)及 EMR-GPF (General Pigmented Fresh)進行淨化。使用 Agilent ZORBAX RRHD Eclipse Plus C18 層析管柱以 Agilent 1290 Infinity II LC 搭配 6470 MS/MS 進行分析。



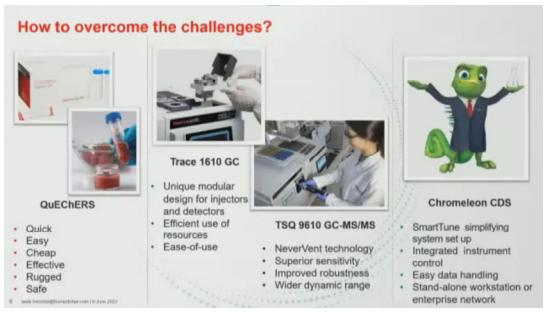


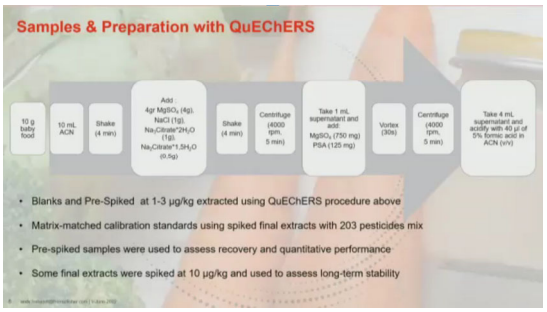


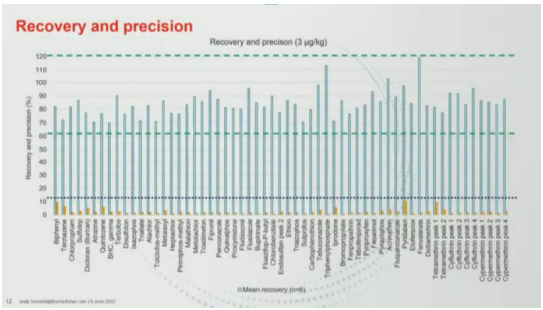


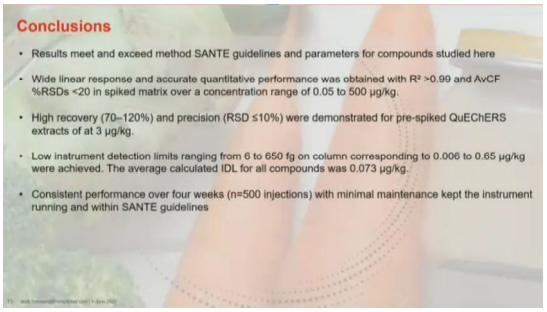
(Ruben Garnica et al., 2022)

主題三：以 GC-MS/MS 分析嬰兒食品中的超微量農藥殘留(Confident analysis of ultra-trace pesticides residues in baby food using triple quadrupole GC)。由賽默飛世爾科技(Thermo Scientific)發表演說。歐盟(EU)已將嬰兒食品中禁用的特定農藥之 LOD 及 MRL 設定在 3－8 μg/kg 之間，實驗室必須滿足此監管限制，以確保嬰兒食品的安全。此研究以 QuEChERS 進行萃取，以 Thermo Scientific Trace 1610 GC 及 TSQ 9610 GC-MS/MS 進行分析，樣品經 TraceGOLD 層析管柱，200 多種農藥均滿足 SANTE MRL 為 10 µg/kg 的標準，並且超過 95%農藥偵測濃度< 1 µg/kg。3 µg/kg 添加回收中，回收率在 70-120%之間，RSD ≤ 10%。可拆式 AEI (Advanced Electron Ionization)無須洩真空拆卸和維護，減少儀器停機時間並提高生產率。





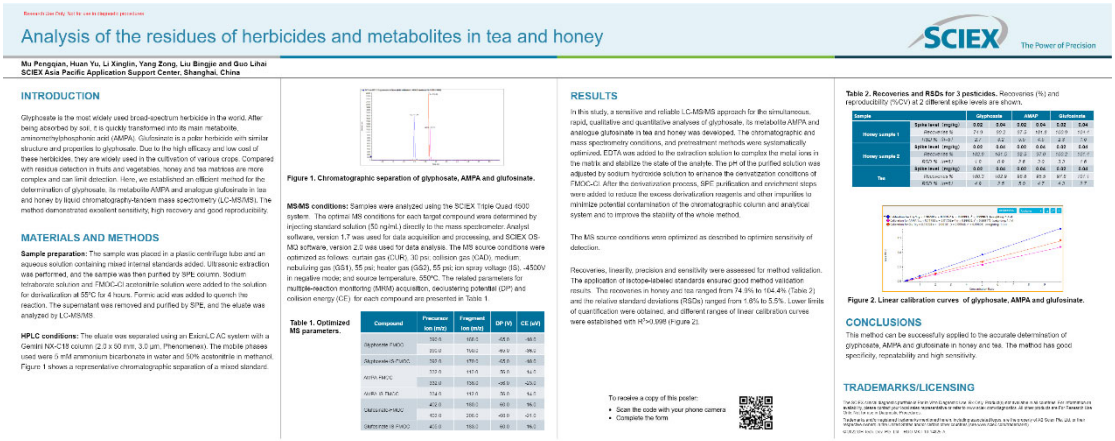




(Andy Fornadel et al., 2022)

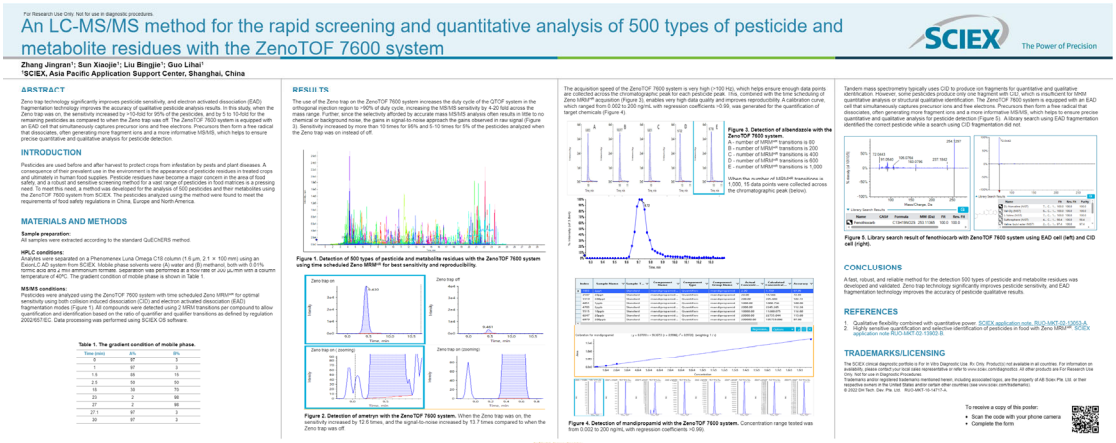
二、壁報展示內容

壁報一：茶葉和蜂蜜中除草劑和代謝物殘留分析(Analysis of the residues of herbicides and metabolites in tea and honey)。由塞爾克斯(Sciex) Mu Pengqian 等人發表。嘉磷塞(glyphosate)是世界上使用最廣泛的除草劑，被土壤吸收後會迅速轉化，主要代謝物為 AMPA (aminomethylphosphonic acid)。固殺草(glufosinate)是一種極性除草劑，其結構和性質與嘉磷塞相似。由於除草劑的高效和低成本，被廣泛用於各種農作物生產過程中。與水果和蔬菜中的殘留檢測相比，蜂蜜和茶的基質更複雜，可能會影響檢測。此研究使用 LC-MS/MS 測定茶和蜂蜜中嘉磷塞、其代謝物 AMPA 和固殺草，具優異的靈敏度、高回收率和良好的重現性。試驗步驟：樣品置於塑膠離心管中，加入含有混合內標的水溶液，然後經過 SPE 管柱純化樣品，萃取液中加入四硼酸鈉溶液和 FMOC-Cl 乙腈溶液在 55℃下衍生 4 小時後，加入甲酸中止反應。上清液以 SPE 管柱純化後，萃取液以 ExionLC 及 SCIEX Triple Quad 4500 分析，層析管柱為 NX-C18 (2.0x50 mm，3.0 µm，Phenomenex)，流動相為 5 mM 碳酸氫銨水溶液和 50%乙腈甲醇溶液。質譜源條件優化如下：氣簾 30 psi，碰撞氣體 Medium，霧化氣體 55 psi，加熱器氣體 55 psi，離子噴霧電壓-4.5 kV，離子源溫度 550℃。蜂蜜和茶的回收率範圍為 74.9%至 104.4%，相對標準偏差(RSD)範圍為 1.6%至 5.5% (每個濃度重複 6 次)。$R^2 > 0.998$。



(Mu Pengqian et al., 2022)

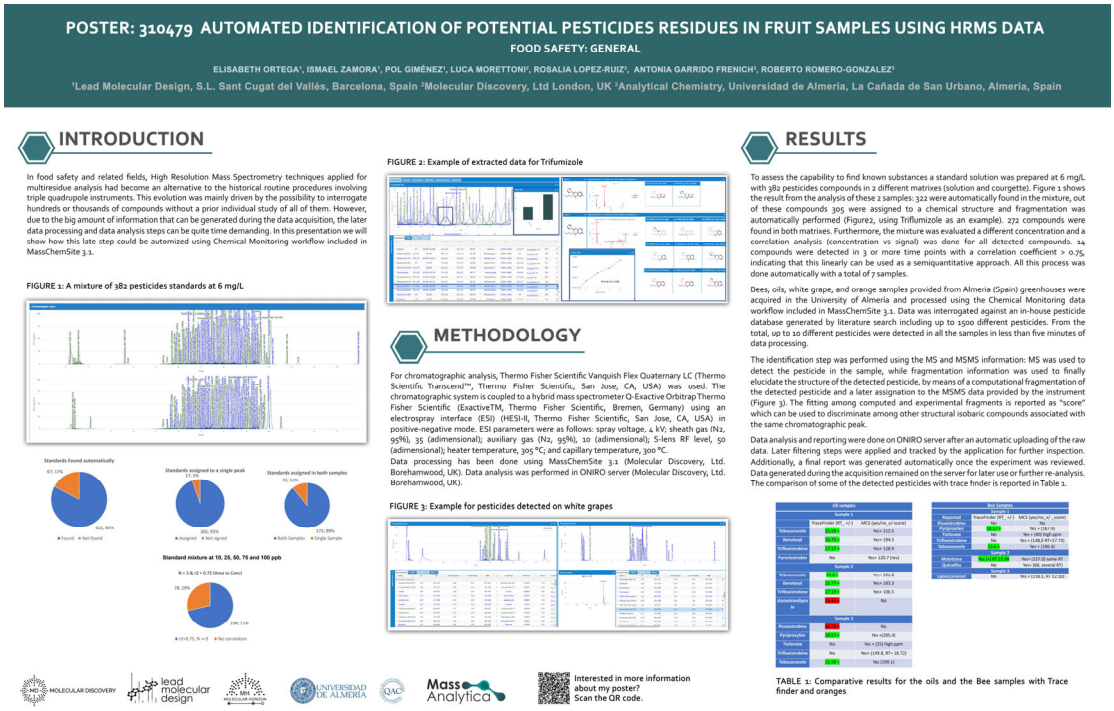
壁報二：以 ZenoTOF 7600 系統對 LC-MS/MS 分析的 500 種農藥和代謝物進行快速篩選和定量(A rapid screening and quantitative LC-MS/MS method of 500 types of pesticide and metabolite residues with the ZenoTOF 7600 system)。由塞爾克斯(Sciex) Jingran Zhang 等人發表。以 SCIEX ZenoTOF 7600 系統分析 500 種農藥及其代謝物，此方法符合中國、歐洲及北美食品安全法規要求。樣品依照 QuEChERS 方法萃取，以 SCIEX ExionLC AD 搭配 Phenomenex Luna Omega C18 管柱進行分析，流動相為水和甲醇(均含 0.01%甲酸和 2 mM 甲酸銨)，流速 300 µL/min，管柱溫度 40℃。再搭配 ZenoTOF 7600 系統使用 CID (collision induced dissociation)及 EAD (electron activated dissociation)碎裂模式可獲得最佳靈敏度，MS/MS 靈敏度提高 4-20 倍，檢量線範圍為 0.002 至 200 ng/mL，回歸係數> 0.99。Zeno trap 技術顯著提高了農藥靈敏度，EAD 碎裂技術提高了農藥定性結果的準確性。



(Jingran Zhang et al., 2022)

壁報三：使用 HRMS 數據自動識別水果樣品中的潛在農藥殘留(Automated identification of potential pesticides residues in fruit samples using HRMS data)。由西班牙 Lead Molecular Design 公司 Elisabeth Ortega 等人發表。在食品安全及相關領域，應用高解析質譜儀(High Resolution Mass Spectrometry, HRMS)來取代三重四極桿儀器已成為一種趨勢，由於 HRMS 在數據蒐集過程中會產生大量信息，因此後期的數據處理和數據分析步驟可能需要相當長的時間，本研究以 MassChemSite 3.1 (Molecular Discovery, Ltd. Borehamwood, UK)進行自動化處理，使用分析儀器為 LC (Thermo Fisher Scientific Vanquish Flex Quaternary LC)串聯高解析質譜儀(Thermo Fisher Scientific Q-Exactive Orbitrap)，ESI 負電荷模式，噴霧電壓 4 kV，sheath gas 及 auxiliary gas 皆為氮氣(95%)，加熱器溫度 305℃，毛細管溫度 300℃。取草莓、白葡萄和橘子為樣品，並使用 MassChemSite 3.1 進行數據處理，可從資料庫中比對多達 1500 種農藥，所有樣品不到五分鐘的數據處理時間內，最後測得 10 種農藥。本技術使用 MS 和 MSMS 信息執行鑑定步驟：MS 用於檢測樣品中農藥，而碎片信息用於最終確定檢測到農藥的結構。碎片信息可與資料庫比對產生“分

數”，用於區分同一色譜峰相似的結構異構物。原始數據自動上傳 ONIRO 伺服器後，數據分析和報告即可完成。



POSTER: 310479 AUTOMATED IDENTIFICATION OF POTENTIAL PESTICIDES RESIDUES IN FRUIT SAMPLES USING HRMS DATA

FOOD SAFETY: GENERAL

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[1]Lead Molecular Design, S.L. Sant Cugat del Vallés, Barcelona, Spain [2]Molecular Discovery, Ltd London, UK [3]Analytical Chemistry, Universidad de Almería, La Cañada de San Urbano, Almería, Spain

INTRODUCTION

In food safety and related fields, High Resolution Mass Spectrometry techniques applied for multiresidue analysis had become an alternative to the historical routine procedures involving triple quadrupole instruments. This evolution was mainly driven by the possibility to interrogate hundreds or thousands of compounds without a prior individual study of all of them. However, due to the big amount of information that can be generated during the data acquisition, the later data processing and data analysis steps can be quite time demanding. In this presentation we will show how this late step could be automized using Chemical Monitoring workflow included in MassChemSite 3.1.

FIGURE 1: A mixture of 382 pesticides standards at 6 mg/L

FIGURE 2: Example of extracted data for Trifumizole

METHODOLOGY

For chromatographic analysis, Thermo Fisher Scientific Vanquish Flex Quaternary LC (Thermo Scientific Transcend™, Thermo Fisher Scientific, San Jose, CA, USA) was used. The chromatographic system is coupled to a hybrid mass spectrometer Q-Exactive Orbitrap Thermo Fisher Scientific (ExactiveTM, Thermo Fisher Scientific, Bremen, Germany) using an electrospray interface (ESI) (HESI-II, Thermo Fisher Scientific, San Jose, CA, USA) in positive-negative mode. ESI parameters were as follows: spray voltage, 4 kV; sheath gas (N2, 95%), 35 (adimensional); auxiliary gas (N2, 95%), 10 (adimensional); S-lens RF level, 50 (adimensional); heater temperature, 305 °C; and capillary temperature, 300 °C.
Data processing has been done using MassChemSite 3.1 (Molecular Discovery, Ltd. Borehamwood, UK). Data analysis was performed in ONIRO server (Molecular Discovery, Ltd. Borehamwood, UK).

FIGURE 3: Example for pesticides detected on white grapes

RESULTS

To assess the capability to find known substances a standard solution was prepared at 6 mg/L with 382 pesticides compounds in 2 different matrixes (solution and courgette). Figure 1 shows the result from the analysis of these 2 samples: 322 were automatically found in the mixture, out of these compounds 305 were assigned to a chemical structure and fragmentation was automatically performed (Figure2, using Trifumizole as an example). 272 compounds were found in both matrixes. Furthermore, the mixture was evaluated a different concentration and a correlation analysis (concentration vs signal) was done for all detected compounds. 24 compounds were detected in 3 or more time points with a correlation coefficient > 0.75, indicating that this linearly can be used as a semiquantitative approach. All this process was done automatically with a total of 7 samples.

Bees, oils, white grape, and orange samples provided from Almeria (Spain) greenhouses were acquired in the University of Almeria and processed using the Chemical Monitoring data workflow included in MassChemSite 3.1. Data was interrogated against an in-house pesticide database generated by literature search including up to 1500 different pesticides. From the total, up to 10 different pesticides were detected in all the samples in less than five minutes of data processing.

The identification step was performed using the MS and MSMS information: MS was used to detect the pesticide in the sample, while fragmentation information was used to finally elucidate the structure of the detected pesticide, by means of a computational fragmentation of the detected pesticide and a later assignation to the MSMS data provided by the instrument (Figure 3). The fitting among computed and experimental fragments is reported as "score" which can be used to discriminate among other structural isobaric compounds associated with the same chromatographic peak.

Data analysis and reporting were done on ONIRO server after an automatic uploading of the raw data. Later filtering steps were applied and tracked by the application for further inspection. Additionally, a final report was generated automatically once the experiment was reviewed. Data generated during the acquisition remained on the server for later use or further re-analysis. The comparison of some of the detected pesticides with trace finder is reported in Table 1.

TABLE 1: Comparative results for the oils and the Bee samples with Trace finder and oranges

Interested in more information about my poster? Scan the QR code.

(Elisabeth Ortega et al., 2022)

參、心得

本次研討會口頭及壁報發表內容之農藥殘留檢驗及自動化運作與本所之重要業務相關，且會議內容主題非常廣泛，期能將此次研討會所帶回之資訊應用於業務上，達成國際接軌之目標。較可惜的是本次研討會因當時疫情嚴峻，且出國返台須檢疫隔離 10 日及自主健康管理 7 日，考量感染風險及後續回台隔離衍生之額外經費，最後選擇參加遠端會議。遠端會議僅能觀看口頭及壁報發表內容，其他會議內容如工作坊討論及廠商展示，皆屬大會最精華之活動，無法現場參與實屬可惜。

四、建議

一、 質譜儀為目前檢驗工作中的最大利器，相關技術發展非常訊速，藉由參與全世界最盛大的質譜會議-美國質譜學會年會，可獲得目前最新質譜技術與研究發展，參與實體會議能與其他國家的專家們直接進行交流，對於拓展研究及國際觀都有相當大的助益，建議能持續參與該國際會議，蒐集國際資訊才能與國際接軌，使國內的技術能與國際同步。

二、 美國質譜學會年會內容涵蓋廣泛，除了食品農藥分析外，還涵蓋大數據分析、自動化、質譜成像及環境污染等議題，其專業包羅萬象，實難一人就

可以完全吸收，建議在經費許可情形下，能派出多位不同領域之人員一同參加學習，透過相互討論將可吸收更多的新知及其運用。

附錄一：大會之議程表

SATURDAY

9:00 AM - 5:00 PM	SHORT COURSES

SUNDAY

9:00 AM - 4:30 PM	SHORT COURSES
10:00 AM - 8:00 PM	ATTENTION: FIRST-TIME GRADUATE STUDENTS AND UNDERGRADUATE STUDENTS **Plan your Strategy: What to See and Do at ASMS,** Hall A
5:00 - 5:45 PM	**TUTORIAL SESSION I,** Hall A **5:00 – 5:45 pm** Mass Spectrometry in Biopharma: From Small Molecules to Multi-Specific Antibodies and Beyond  **Iain D. G. Campuzano** *Amgen Research* **5:45 – 6:30 pm** Machine Learning in Mass Spectrometry  **Randy Julian** *Indigo BioAutomation* **TUTORIAL SESSION II,** Room L100 **5:00 – 5:45 pm** Radical Chemistry for Biomolecular Identification: From Fundamentals to Applications  **Ryan R. Julian** *University of California, Riverside* **5:45 – 6:30 pm** Mass Spectrometry in Natural Product Research  **Laura Sanchez** *University of California, Santa Cruz*
6:45 - 7:45 PM	**CONFERENCE OPENING PLENARY,** Hall A **Julia Laskin,** *Purdue University* ASMS Vice President for Programs **7:00 - 7:45 pm**  Of Stem Cells, Niches and Networks **Judith Kimble** *University of Wisconsin-Madison*
7:45 - 9:00 PM	**WELCOME RECEPTION,** Halls BC All are invited to join us for a festive opening to the conference featuring Corporate Member exhibits. Reception includes display and judging for the Undergraduate Student Poster Competition.

Consult online planner or mobile app for detailed program.

MONDAY

7:00 AM	**CORPORATE BREAKFAST SEMINARS,** Convention Center and Hilton Minneapolis
8:30 - 10:30 AM	**ORAL SESSIONS** MOA am: Post-translational Modifications: Qualitative & Quantitative Analysis, *Hall A* MOB am: Instrumentation: High-Resolution Mass Spectrometry, *Room L100* MOC am: Clinical Analysis: Applications, *Ballroom A* MOD am: Informatics: Multiomics Integration and Applications, *Ballroom B* MOE am: Fundamentals: Formation and Structures of Big Ions, *Auditorium* MOF am: Ion Mobility: Structure Determination & Applications, *Room 101* MOG am: H/D Exchange: Innovations and Applications, *Room 102* MOH am: Plants and Natural Products, *Room 103*
10:30 AM - 2:30 PM	**POSTER SESSION AND EXHIBITS,** Monday Posters, *Hall BC* **Odd-number posters present:** 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm **Even-number posters present:** 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm 11:30 am - 1:00 pm: **Undergraduate students** look for reserved tables and free lunch vouchers to ***Meet the Experts***
2:30 - 4:30 PM	**ORAL SESSIONS** MOA pm: Biomarkers: Quantitative Analysis, *Hall A* MOB pm: Instrumentation: New Developments in Ionization and Sampling, *Room L100* MOC pm: Drug Metabolism and Pharmacokinetics, *Ballroom A* MOD pm: Informatics: Peptide and Protein Identification, Proteomics, *Ballroom B* MOE pm: Fundamentals of Ionization, *Auditorium* MOF pm: Brain and Neurodegenerative Disease Research (in Memory of Sanford 'Sandy' P. Markey), *Room 101* MOG pm: Exposomics, Toxicology, and Health Outcomes, *Room 102* MOH pm: Environmental: Non-Target Analysis and Emerging Contaminants, *Room 103*
4:45 - 5:30 PM	**AWARD LECTURE,** Hall A  **John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry** preceded by Al Yergey MS Scientist Awards Presentations **Evan R. Williams** *University of California, Berkeley*
5:45 - 7:00 PM	**WORKSHOPS** There are light refreshments in foyers, 5:30 - 5:45 pm. 01 Machine Learning: How is it Enhancing Mass Spectrometry? (Independent), *Room L100* 02 Trans-Proteomic Pipeline: Recent Advances and Future Directions (Independent), *Room M100 BC* 03 Incorporating Hands-on Tutorials into Undergraduate Curriculum (Interest Group: Undergraduate Research in MS), *Room M100 DE* 04 Botanical Dietary Supplements: How mass spectrometry is impacting the assessment of the quality (Interest Group: Pharmaceuticals), *Room M100 FG* 05 Molecular Coverage in Ambient Ionization (Interest Group: Ambient Sampling & Ionization), *Ballroom A* 06 Recent development and ongoing challenges with HDX/CL/XL (Interest Group: HDX Covalent Labeling & Cross Linking), *Auditorium Main* 07 Ensuring QA/QC through the Harmonization of Microsampling Techniques in Clinical Chemistry Applications (Interest Group: Clinical Chemistry), *Auditorium Room 1* 08 The NIH and NSF Review and Funding Process (Independent), *Auditorium Room 2* 09 Mass Spectral Libraries: Current and Future Applications (Independent), *Auditorium Room 3* 10 Networking for Scientists: Celebrating Women Mass Spectrometrists (Independent), *Room 101* 11 Career Opportunities for Chinese Students and Scholars (Independent), *Room 102* 12 Real-time Mass Spectrometry in Proteomics and Beyond (Independent), *Room 103* 13 Developing World Outreach (Interest Group: Developing World Outreach), *Room 200 BC* 14 FTMS: FAIR Data for the Masses (Interest Group: FTMS), *Room 200 DE* 15 Polymeric Materials: Coupling of Thermal Polymer Analysis Techniques to MS (Interest Group: Polymeric Materials), *Room 200 FG* 16 The Exposome, Success Stories and the Way Forward (Interest Group: Exposomics), *Room 200 HI*
7:00 - 8:00 PM	**SPECIAL GAP HOUR RECEPTION SPONSORED BY AGILENT,** Room 101 Reception immediately following the Celebrating Women Mass Spectrometrists evening workshop (see 10 above). All are welcome to attend. The goal is to foster networking among the FeMS community and their supporters.
AFTER 8:00 PM	**CORPORATE HOSPITALITY SUITES AT HILTON MINNEAPOLIS**

TUESDAY

7:00 AM	**CORPORATE BREAKFAST SEMINARS,** Convention Center and Hilton Minneapolis
8:30 - 10:30 AM	**ORAL SESSIONS** TOA am: Biomarkers: Qualitative Analysis, *Hall A* TOB am: Instrumentation: Ionization and Detection of High-Mass Analytes, *Room L100* TOC am: Metabolomics: New Technologies and Applications, *Ballroom A* TOD am: Challenges in MS Analysis of Complex Mixtures, *Ballroom B* TOE am: Fundamentals: Reactions of Gaseous and Solvated Ions, *Auditorium* TOF am: Quantitative Proteomics in Systems Biology, *Room 101* TOG am: GC/MS: Instrumentation and Applications, *Room 102* TOH am: Imaging: Spatially-Resolved Omics, *Room 103*
10:30 AM - 2:30 PM	**POSTER SESSION AND EXHIBITS,** Tuesday Posters, Halls BC **Odd-number posters present:** 10:30 - 11:30 am PLUS 12:30 – 2:30 pm **Even-number posters present:** 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm
2:30 - 4:30 PM	**ORAL SESSIONS** TOA pm: Glycopeptides and Glycoproteins, *Hall A* TOB pm: Instrumentation: New Hybrid and Multimodal Approaches, *Room L100* TOC pm: Drug Discovery and Development: Qualitative and Quantitative Analysis, *Ballroom A* TOD pm: Artificial Intelligence in MS Instrumentation and Applications, *Ballroom B* TOE pm: Fundamentals: Ion Activation and Dissociation, *Auditorium* TOF pm: Lipidomics: New MS Technologies and Applications, *Room 101* TOG pm: Stable Isotope Labeling: Applications, *Room 102* TOH pm: Industry: Trace Analysis, Quality Control, and Automation, *Room 103*
4:45 - 5:30 PM	**AWARD LECTURE,** Ballroom B  **Biemann Medal Lecture** preceded by **Research Award Presentations** **Erin Baker** *North Carolina State University*
5:45 - 7:00 PM	**WORKSHOPS** There are light refreshments in foyers, 5:30 - 5:45 pm. 01 Big Data Analytics for Energy, Petroleum and Biofuels. (Interest Group: Energy Petroleum & Biofuels), *Room L100* 02 Best Practices for Maintaining Research Continuity in the Shared Resource Laboratory (Interest Group: Analytical Lab Managers), *Room M100 BC* 03 Ion traps and other Technologies that Brought Miniature Mass Spectrometers Mainstream (Interest Group: Ion Trap MS), *Room M100 DE* 04 From Academia to Industry: How Native MS works with complementary technologies to elucidate protein structure. (Interest Group: Native Mass Spectrometry), *Room M100 FG* 05 Reward Those Who Step Up: Helping to Prevent the Burnout of Underrepresented Groups in the Rollout of DEI Activities (ASMS Diversity & Inclusion Committee), *Ballroom A* 06 Isotopes - the Curse and Blessing of Mass Spectrometry (Interest Group: Fundamentals), *Ballroom B* 07 Utilizing GC/MS and Peripheral Technologies for Problem Solving in the Development of FFF Products (Interest Group: Flavor Frangrance & Foodstuff), *Auditorium Main* 08 Extractable and Leachable Testing in Pharmaceutical Industry (Independent), *Auditorium Room 1* 09 Top-Down Mass Spectrometry: Panel Discussion to Address the Community's Challenges (Interest Group: Top-Down Proteomics), *Auditorium Room 2* 10 Kahoot LC-MS Trivia! Stress free fun about LC-MS, ASMS, and Minneapolis! (Interest Group: LCMS & Related Topics), *Auditorium Room 3* 11 How to Kick Start Your Career in Academic or National/Federal Labs (part 1) (Interest Group: Young Mass Spectrometrists), *Room 101* 12 Imaging MS: Opportunities for Artificial Intelligence and Machine Learning (Interest Group: Imaging MS), *Room 102* 13 Towards probability-based metabolite identification confidence (Independent), *Room 103* 14 HUPO Proteomics Standards Initiative and ProteomeXchange for FAIR Biological MS (Independent), *Room 200 BC* 15 Photoionization MS: How to Identify the Best Technique for an Analytical Problem? (Interest Group: Photoionization MS), *Room 200 DE* 16 Recent Advances in ADME Biomarkers (Interest Group: DMPK), *Room 200 FG* 17 Visualization of Mass Spectrometry related data (Interest Group: Bioinformatics MS), *Room 200 HI*
7:00 - 8:00 PM	**SPECIAL GAP HOUR RECEPTION SPONSORED BY MOBILON,** Ballrom A Reception immediately following the ASMS Diversity & Inclusion Committee's evening workshop (see 05 above). All are welcome to attend. The goal is to foster networking among those interested in issues of diversity and inclusion.
AFTER 8:00 PM	**CORPORATE HOSPITALITY SUITES AT HILTON MINNEAPOLIS**

WEDNESDAY

7:00 AM	**CORPORATE BREAKFAST SEMINARS,** Convention Center and Hilton Minneapolis
8:30 - 10:30 AM	**ORAL SESSIONS** WOA am: Biotherapeutics: Proteins, Antibodies, and Antibody/Drug Conjugates, *Hall A* WOB am: Instrumentation: Innovative Separations Approaches Coupled to MS, *Room L100* WOC am: Imaging: Pharmaceuticals, Metabolites, Lipids, and Glycans, *Ballroom A* WOD am: Informatics: Metabolomics, *Ballroom B* WOE am: Fundamentals: Ion Structures and Energetics (In Memory of Fred W. McLafferty), *Auditorium* WOF am: Lipidomics: Targeted and Untargeted, *Room 101* WOG am: Forensics: Innovations and Applications, *Room 102* WOH am: Environmental: Innovative Approaches and Instrumentation, *Room 103*
10:30 AM - 2:30 PM	**POSTER SESSION AND EXHIBITS,** Wednesday Posters, Hall AB **Odd-number posters present:** 10:30 - 11:30 am PLUS 12:30 – 2:30 pm **Even-number posters present:** 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm
2:30 - 4:30 PM	**ORAL SESSIONS** WOA pm: Biotherapeutics: Characterization and Quantitation, *Hall A* WOB pm: Instrumentation: Ambient Ionization and Applications, *Room L100* WOC pm: Metabolomics: Untargeted Profiling, *Ballroom A* WOD pm: Nucleic Acids and Oligonucleotides, *Ballroom B* WOE pm: Fundamentals Beyond Mass Analysis: Structural Characterization of Isomers, *Auditorium* WOF pm: Protein-Ligand and Protein-Protein Interactions, *Room 101* WOG pm: Microbiome and Interactome, *Room 102* WOH pm: Viruses and Virus-Like Particles, *Room 103*
4:45 - 5:30 PM	**ASMS MEETING,** Hall A. Awards, board reports, wine, beer, soft drinks - and more!
5:45 - 7:00 PM	**WORKSHOPS** There are light refreshments in the foyers, 5:30 - 5:45 pm. 01 Current Landscape of High Throughput Sample Preparation in Quantitative MS (Independent), *Room L100* 02 Multi-Attribute Method (MAM): New Aspects in Development (Interest Group: Biotherapeutics), *Room M100 BC* 03 Periodic Table of Food Initiative: Engaging the Mass Spectrometry Community in the Development of a Democratized Foodomics Technology Platform (Independent), *Room M100 DE* 04 Recent Advances in Oligonucleotides & Peptides Bioanalysis by Triple Quad and HRMS (Interest Group: Regulated Bioanalysis), *Auditorium Main* 05 Efficient Analysis of Wastewater by Advanced Mass Spectrometry Techniques (Interest Group: Environmental Applications), *Auditorium Room 1* 06 Forensic Mass Spectral Technology: The Transition from Research to Practical Application (Interest Group: Forensics & Homeland Security), *Auditorium Room 2* 07 Data Independent Acquisition Goes Mainstream? (Interest Group: Data Independent Acquisition), *Ballroom A* 08 Single-cell proteomics: From Sample Preparation to Data Analysis (Independent), *Ballroom B* 09 How to Kick Start Your Career in Industry (part 2) (Interest Group: Young Mass Spectrometrists), *Room 101* 10 Cannabis & Hemp Science: The Importance of Mass Spectrometry (Independent), *Room 102* 11 Characterizing Greatness: Celebrating Fred McLafferty (Independent), *Room 103* 12 Democratizing Metabolomics: Lessons learned and future directions from US regional core facilities (Interest Group: Metabolomics), *Room 200 BC* 13 Allyship: Embracing Diversity and Inclusion in Your Workplace (Interest Group: Career Development), *Room 200 DE* 14 Cloud Resources for Proteomics Analysis (Independent), *Room 200 FG* 15 Ion Mobility Spectrometry: What's next? (Interest Group: Ion Mobility MS), *Room 200 HI*
AFTER 8:00 PM	**CORPORATE HOSPITALITY SUITES AT HILTON MINNEAPOLIS**

Consult online planner or mobile app for detailed program.

THURSDAY

7:00 AM	**CORPORATE BREAKFAST SEMINARS,** Convention Center and Hilton Minneapolis
8:30 - 10:30 AM	**ORAL SESSIONS** ThOA am: Structural Biology, *Hall A* ThOB am: Ion Mobility: Instrumentation & Method Development, *Room L100* ThOC am: Single Cell Omics, *Ballroom A* ThOD am: Informatics: Data-Independent Acquisition and Multiplexing, *Ballroom B* ThOE am: Fundamentals: Unconventional Approaches in MS (Honoring R. Graham Cooks), *Auditorium* ThOF am: Cancer Research, *Room 101* ThOG am: Food Safety & Chemistry: Innovations, *Room 102* ThOH am: High Throughput MS, *Room 103*
10:30 AM - 2:30 PM	**POSTER SESSION AND EXHIBITS,** Thursday Posters, Hall AB **Odd-number posters present:** 10:30 - 11:30 am PLUS 12:30 – 2:30 pm **Even-number posters present:** 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm
2:30 - 4:30 PM	**ORAL SESSIONS** ThOA pm: Top Down Protein Analysis, *Hall A* ThOB pm: Imaging: Instrumentation & Method Development, *Room L100* ThOC pm: Clinical Analysis: Innovations, *Ballroom A* ThOD pm: Informatics: Innovations, *Ballroom B* ThOE pm: Covalent Labeling and Chemical Crosslinking, *Auditorium* ThOF pm: Glycomics, *Room 101* ThOG pm: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements, *Room 102* ThOH pm: Small Molecules: Structural Characterization and Quantitation, *Room 103*
4:45 - 5:30 PM	**PLENARY LECTURE,** Hall A  *Homo naledi* and the Chamber of Secrets **Jeremy DeSilva** *Dartmouth College*
6:30 – 10:30 PM	**CLOSING EVENT: DINNER & PURPLEXPERIENCE CONCERT,** Hall D Advance Purchase Ticket Required, Sales close at 12pm noon MONDAY (June 6). Purchase your ticket online via Registration portal.

附錄二：壁報發表主題

POSTER OVERVIEW

Poster Presentation Schedule
Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm
Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm

MONDAY POSTERS

Set up all Monday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Monday posters
7:00 - 8:00 pm

TUESDAY POSTERS

Set up all Tuesday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Tuesday posters
7:00 - 8:00 pm

Consult online planner or mobile app for detailed program.

Poster Presentation Schedule
Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm
Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm

WEDNESDAY POSTERS

Set up all Wednesday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Wednesday posters
7:00 - 8:00 pm

THURSDAY POSTERS

Set up all Thursday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Thursday posters
7:00 - 8:00 pm