

# 2022 AOCS Annual Meeting & Expo

## Analytical Program

*As of March 23, 2022. Subject to change.*

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### Dutton Award Symposium

#### FEATURED SESSION

*Organizers: Giorgia Purcaro, University of Liège, Belgium; and Michal Holčapek, University of Pardubice, Czech Republic*

Monday, May 2, 2022 | 7:25–9:30 a.m. EDT (Atlanta, USA; UTC-4)

*Each year, the AOCS Analytical Division assigns the Herbert J. Dutton Award to professionals who have made significant contributions in the analysis of oils, fats and lipids. This year's speakers will share career insights on lipids as biomolecules; chromatography and mass spectrometry; metabolome and lipidome atlas; foodomics; and lipodomic analysis in food.*

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**Comprehensive analysis of lipids: From plant oil analysis towards lipidomic cancer screening.** Michal Holčapek\* (**Herbert J. Dutton Award Winner**)  
, Department of Analytical Chemistry, University of Pardubice, Czech Republic

**Adventures in multiple dimensions of chromatography and mass spectrometry for lipidomic Analysis.** William C. Byrdwell\*<sup>1</sup>, Hari Karin Kotapati<sup>2</sup>, <sup>1</sup>*Methods and Application of Food Composition Lab, USDA ARS BHNRC MAFCL, United States;* <sup>2</sup>*University of Maryland, Nutrition and Food Science, United States*

**MetaboAtlas21: A comprehensive metabolome and lipidome atlas of mouse tissues and biofluids.** Tomas Cajka\*, Lucie Rudl Kulhava, Michaela Novakova, Jiri Hricko, Ondrej Kuda, Michaela Paucova, *Institute of Physiology of the Czech Academy of Sciences, Czech Republic*

**Lipidomic analysis in food: The role of a detailed elucidation of intact lipids in functional foods for investigating on nutritional aspects.** Paola Dugo\*, Francesca Rigano, Luigi Mondello, *Universita Di Messina, Italy*

**Foodomics study of the neuroprotective potential of natural products.** Alberto Valdés\*, Rocío Gallego, Zully J. Suárez-Montenegro, José David Sánchez-Martínez, Elena Ibañez, Miguel Herrero, Alejandro Cifuentes, *Institute of Food Science Research (CIAL-CSIC), Spain*

## AOCS Official Methods

ANALYTICAL

*Chairs: Susan Seegers, Bunge North America, USA; and Mark Collison, Retired ADM, USA*  
Monday, May 2, 2022 | 9:55 a.m.–Noon EDT (Atlanta, USA; UTC-4)

*The AOCS Official Methods session includes updates and changes to AOCS Official Methods and Procedures: Antioxidants, Liquid Chromatographic Method; Writing and Approval of Methods and Certified Laboratories (Criteria); Standardized Method to Quantify MCPDE and GE in edible oils.*

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**Changes to AOCS evaluation and design of test methods.** Scott Bloomer\*, *Technical Services, American Oil Chemists' Society, United States*

**Ce 6a-2021 HPLC analysis of phenolic antioxidants: A successful collaborative trial during the Covid pandemic.** Mark Collison\*, *Retired, United States*

**Development of ISO18363-4/AOCS Cd29f-2021: A new standardized method to quantify MCPDE and GE in edible oils.** Ralph Zwagerman\*, *Analytical Development, Lodders Croklaan BV, Netherlands*

**New AOCS Methods and Methods under development.** Xin Wu\*, Fiona Liu, Scott Bloomer, *Technical Services, American Oil Chemists' Society, United States*

## Authentication of Olive Oil

ANALYTICAL

*Chairs: Selina Wang, University of California, Davis, USA; and Enrico Valli, Università di Bologna, Italy*  
Monday, May 2, 2022 | 1:25–3:30 p.m. EDT (Atlanta, USA; UTC-4)

*The Authentication of Olive Oil session highlights an easier and greener way to accurately measure peroxide content; an overview of the results of the EU H2020 OLEUM project for the authenticity of olive oils; a new method for detecting lower-grade soft-deodorized olive oil contamination; and the use of AI olfactometry instruments to quantify sensory defects and more.*

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**The results of the EU H2020 OLEUM project for the authenticity of olive oils.** Tullia Gallina Toschi\*, *Department of Food and Agriculture Sciences, University of Bologna, Italy*

**Metabolic fingerprinting strategies for authentication challenge: EVOO adulterated by soft deodorized olive oil.** Jana Hajslova\*<sup>1</sup>, Klara Navratilova<sup>1</sup>, Enrico Valli<sup>2</sup>, Tullia Gallina Toschi<sup>3</sup>, <sup>1</sup>*Department of Food Analysis and Nutrition, University of Chemistry and Technology, Prague, Czech Republic;* <sup>2</sup>*Department of Agricultural and Food Sciences and Interdepartmental Centre of Agri-Food Industrial Research, Alma*

*Mater Studiorum—Università di Bologna, Italy; <sup>3</sup>Department of Food and Agriculture Sciences, Università di Bologna, Italy*

**Artificial Intelligence smelling machines based on multidimensional gas chromatography: Capturing extra-virgin olive oil aroma blueprint and unique identity.** Chiara Emilia Cordero\*<sup>1</sup>, Simone Squara<sup>1</sup>, Federico Stilo<sup>1</sup>, Erica Liberto<sup>1</sup>, Carlo Bicchi<sup>1</sup>, Stephen Reichenbach<sup>2</sup>, Luis Cuadros Rodriguez<sup>3</sup>, Humberto Bizzo<sup>4</sup>, <sup>1</sup>*Dipartimento di Scienza e Tecnologia del Farmaco, Università Degli Studi di Torino, Italy;* <sup>2</sup>*University of Nebraska Lincoln, United States;* <sup>3</sup>*Univesity of Granada, Spain;* <sup>4</sup>*Embrapa Agroindústria de Alimentos, Brazil*

**Easy and green method for the peroxide value determination in olive oil.** Francesco Longobardi\*<sup>1</sup>, Vito Michele Paradiso<sup>2</sup>, <sup>1</sup>*Chemistry, University of Bari A. Moro, Italy;* <sup>2</sup>*Università del Salento, Italy*

## Panel discussion

## General Analytical Methods

### ANALYTICAL

*Chairs: Pierluigi Delmonte, US Food and Drug Administration, USA; and Lisa Clement, Cargill Inc., USA*  
Monday, May 2, 2022 | 3:55–6 p.m. EDT (Atlanta, USA; UTC-4)

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**Detection of partially hydrogenated vegetable oils in food products based on fatty acid composition.** Pierluigi Delmonte\*<sup>1</sup>, Sarah Prebihalo<sup>1</sup>, Andrea Milani<sup>2</sup>, <sup>1</sup>*Office of Regulatory Science, Bioanalytical Methods Branch, U.S. Food & Drug Administration, United States;* <sup>2</sup>*U.S. Food & Drug Administration, United States*

**Analysis of hopanes by LC-GCxGC-ToF MS/FID, and their use for the confirmation of mineral oil contamination.** Carlos Martin Alberca\*<sup>1</sup>, Marian Steverink<sup>1</sup>, Torsten Tonak<sup>2</sup>, Thomas Gude<sup>2</sup>, <sup>1</sup>*Cargill, Global Edible Oils Solutions, Europe; R&D, Cargill, Netherlands;* <sup>2</sup>*Swiss Quality Testing Services (SQTS), Switzerland*

**Development of a method for the identification and quantification of terpenes and cannabinoids in hemp using multidimensional gas chromatography and quadrupole-orbitrap mass spectrometry.** Sarah Prebihalo\*, Rahul S. Pawar, Geoffrey Dubrow, Pierluigi Delmonte, *Office of Regulatory Science, Bioanalytical Methods Branch, U.S. Food & Drug Administration, United States*

**Isolation and purification phenolic compounds in California olive pomace by pilot-scale C18 gel chromatography.** Hefei Zhao\*, Selina Wang, *Department of Food Science and Technology, University of California, Davis, United States*

**Enhancing techno-functional and bioactive properties of whey proteins by conjugation with quercetin using combined treatment of redox pair and ultrasonication.** Waqas N. Baba\*, Sajid Maqsood, *Food Science, UAE University, United Arab Emirates*

## Authentication of Avocado and other High-Value Oils

### ANALYTICAL

*Chairs: Selina Wang, University of California, Davis, USA; and Jill Winkler-Moser, USDA ARS NCAUR, USA*  
Tuesday, May 3, 2022 | 7:25–9:30 a.m. EDT (Atlanta, USA; UTC-4)

*The Authentication of Avocado and Other High-Value Oils session discusses how avocado and other high-value oils are gaining in popularity but lack standards for purity and quality; new methods of testing for*

*adulteration in avocado and argon oils using LF-NMR and NMR; how region, fruit quality and other factors influence the chemical composition of avocados and affect standards; progress of the Codex Committee on Fats and Oils on the creation of world-wide standards for avocado oil.*

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**Update on the progress of the Codex Alimentarius standard for avocado oil.** Jill Winkler-Moser\*, USDA ARS NCAUR, United States

**Avocado oil chemical composition varies with harvest time, growing region, and fruit quality, demonstrating important considerations for standard development.** Hilary Green\*, Selina Wang, Department of Food Science and Technology, University of California, Davis, United States (**Analytical Division Student Award Winner**)

**Differentiating avocado oil from other vegetable oils using low-field NMR spectroscopy and chemometrics.** Fenfen Tang\*<sup>1</sup>, Hilary Green<sup>2</sup>, Selina Wang<sup>2</sup>, Emmanuel Hatzakis<sup>1</sup>, <sup>1</sup>Department of Food Science and Technology, The Ohio State University, United States; <sup>2</sup>Department of Food Science and Technology, University of California, Davis, United States

**High throughput authenticity screening of high value edible oils with benchtop NMR.** James Sagar<sup>1</sup>, Marcel Lachenmann\*<sup>2</sup>, Rachel Brignall<sup>1</sup>, Yvonne Gunning<sup>3</sup>, Kate Kemsley<sup>3</sup>, <sup>1</sup>Oxford Instruments, United Kingdom; <sup>2</sup>Oxford Instruments Inc., United States; <sup>3</sup>Quadram Institute Bioscience, United Kingdom

## Panel discussion

## Standard/Novel Analytical Methods for Protein Analysis in Food

### ANALYTICAL

Joint session with the Protein and Co-Products Division

Chairs: Sneh Bhandari, Independent Consultant, USA; Janitha Wanasundara, Agriculture and Agri-Food Canada, Canada; and Frederic Baudouin, Improve SAS, France

Tuesday, May 3, 2022 | 7:25–9:30 a.m. EDT (Atlanta, USA; UTC-4)

*This session features measuring chymotrypsin inhibitor activity; the need for standardization of protein functionality methodologies; nitrogen to protein conversion factors; prediction of protein and amino acid contents in lentils; and cross-reactivity risks of canary seed to related grains.*

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**Nitrogen to protein conversion factors—an update and practical guidance for their use and for determining specific factors for novel protein sources.** Elaine S. Krul\*, EKSci, LLC, United States

**Allergenicity risk assessment of glabrous canaryseed as a novel food protein source.** Lamia L'Hocine\*<sup>1</sup>, Mélanie Pitre<sup>2</sup>, Emily Mason<sup>2</sup>, Allaoua Achouri<sup>2</sup>, <sup>1</sup>Saint-Hyacinthe Research and Development Centre, Agriculture & Agri-Food Canada, Canada; <sup>2</sup>Agriculture and Agri-Food Canada, Canada

**Methodological inconsistencies in novel plant protein functional properties, and improvements for water absorption capacity determinations.** Analiese Goins\*, Sara Griffin, Department of Food Science and Nutrition, California State University, Fresno, United States

**Developing an optimized method for measuring chymotrypsin inhibitor activity in protein products.** Keshun Liu\*, Mike Woolman, Agricultural Research Service, US Dept. of Agriculture, United States

**Prediction of protein and amino acid contents in whole and ground lentils using near-infrared reflectance spectroscopy.** Jiayi Hang\*<sup>1</sup>, Da Shi<sup>1</sup>, James House<sup>1</sup>, Jason Neufeld<sup>1</sup>, Kirstin Bett<sup>2</sup>, <sup>1</sup>University of Manitoba, Canada; <sup>2</sup>University of Saskatchewan, Canada

## Analysis of Less-Abundant Lipids

ANALYTICAL

*Chairs: Kim Ekroos, Lipidomics Consulting Ltd, Finland; and Federico Torta, National University of Singapore, Singapore*

Tuesday, May 3, 2022 | 1:25–3:30 p.m. EDT (Atlanta, USA; UTC-4)

*This Analysis of Less Abundant Lipids session discusses cheminformatics toolbox for visualization of lipidomic data; the role of essential fatty-acid derived mediators in inflammation resolution; the role of isoprostanooids; analytical challenges of LC-MS/MS methods; and oxidation of lipids in aged emulsified foods.*

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**Quantification of minor lipid species in mammalian samples—strategies and pitfalls.** Gerhard Liebisch\*, Sabrina Krautbauer, Marcus Höring, *University Hospital Regensburg, Germany*

**The wonders of isoprostanooids in biological systems.** Jetty Chung-Yung Lee\*<sup>1</sup>, Jean-Marie Glanao<sup>2</sup>, Thierry Durand<sup>2</sup>, <sup>1</sup>*The University of Hong Kong, Hong Kong*; <sup>2</sup>*Institut des Biomolécules Max Mousseron, (IBMM), UMR 5247, CNRS, Université de Montpellier, ENSCM, France*

**Structure elucidation and biological evaluations of sulfido-conjugated specialized pro-resolving mediators.** Jesmond Dalli\*<sup>1</sup>, Kimberly Pistorius<sup>1</sup>, Ana Rodriguez<sup>2</sup>, Bernd Spur<sup>2</sup>, Charles Serhan<sup>3</sup>, <sup>1</sup>*Queen Mary University of London, United Kingdom*; <sup>2</sup>*Rowan University, United States*; <sup>3</sup>*Brigham and Women's Hospital, United States*

**An online structural-based connectivity and omic phenotype evaluations (SCOPE) cheminformatics toolbox for lipidomic data visualization.** Melanie Odenkirk\*<sup>1</sup>, Erin Baker<sup>1</sup>, David Reif<sup>2</sup>, <sup>1</sup>*Department of Chemistry, North Carolina State University, United States*; <sup>2</sup>*Department of Biological Sciences, North Carolina State University, United States*

**Selective ionization of oxidized versus non-oxidized lipid species using different solvent additives in direct infusion MS.** Eleni Lazaridi\*<sup>1</sup>, Marie Hennebelle<sup>1</sup>, Boudewijn Hollebrands<sup>2</sup>, Jean-Paul Vincken<sup>1</sup>, Hans-Gerd Janssen<sup>3</sup>, <sup>1</sup>*Wageningen University and Research, Netherlands*; <sup>2</sup>*Unilever, Netherlands*; <sup>4</sup>*Unilever, United States*

## Surface Methods and Analysis

ANALYTICAL

Joint session with the Surfactants and Detergents Division

*Chair: Rick Theiner, Evonik Industries, USA and Jeff Botts, Corbion, USA*

Tuesday, May 3, 2022 | 1:25–3:30 p.m. EDT (Atlanta, USA; UTC-4)

*The Surface Methods and Analysis session includes research on methods to quantify surfactant performance in laundry detergents; a technique to study interfaces at low interfacial tensions; contact angle measurements; a 1H NMR method to distinguish between emulsifier and surfactant classes; rheological-based approach to gel curve analysis; and properties and applications of docosanol and higher alcohol ethoxylates.*

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**Use of 1H NMR as a rapid analytical technique to distinguish between emulsifier and surfactant classes coupled with cosine similarity computations as part of a raw material surveillance program.** Margaret Walsh\*<sup>1</sup>, Jeff Botts<sup>2</sup>, <sup>1</sup>*Emulsifiers, Corbion, United States*; <sup>2</sup>*Sustainable Food Solutions, Corbion, United States*

**Understanding interfaces: Using contact angle measurements to determine surface tension, interfacial tension, and kinetic properties from contact angle hysteresis.** Daniel Scholz\*<sup>1</sup>, Paul Simutis<sup>2</sup>,  
<sup>1</sup>DataPhysics Instruments GmbH, Germany; <sup>2</sup>DataPhysics Instruments USA Corp., United States

**The spinning drop method: An accurate technique to study interfaces at low interfacial tensions.** Ronald Marquez\*<sup>1</sup>, Jose Maria Zamora<sup>2</sup>, <sup>1</sup>Laboratoire Physico-Chimie des Interfaces Complexes, TotalEnergies, Lille Univ., ESPCI, France; <sup>2</sup>CITEC ULA, Venezuela

**Fundamental interfacial properties and industrial applications of a new class of surface active docosanols and higher alcohol ethoxylates.** Ramesh Varadaraj\*, Ollie Normand, Dustin Landry, R&D, Sasol North America, United States

**Rheological-based approach to gel curve analysis of alcohol ethoxylates.** Timothy King\*<sup>1</sup>, Franklin Caputo<sup>1</sup>, Auriana Hughes<sup>1</sup>, Julian Barnes<sup>2</sup>, <sup>1</sup>Shell Global Solutions US Inc., United States, <sup>2</sup>Shell Global Solutions International B.V., United States

**Good, better, best: 3 Methods to quantify surfactant performance in laundry detergent tests.** Caspar van Leeuwen, Remco Langedijk\*, Patrick Zwamborn, Center for Testmaterials BV, Netherlands

## Edible Oil Contaminants—Analysis and Industrial Perspective

ANALYTICAL

Joint session with the Processing Division

Sponsored by Clariant

Chairs: Jan Kuhlmann, SGS Germany GmbH, Germany; and Wim de Greyt, Desmet Ballestra Group, Belgium

Tuesday, May 3, 2022 | 1:25–3:30 p.m. EDT (Atlanta, USA; UTC-4)

*The Edible Oil Contaminants session includes: the regulatory status of MOSH/MOAH; recent methods for determining MOSH/MOAH; method for detecting MCPD and GE applied to fats and oils; the introduction of an AOCS Official method adaptation for food emulsifiers; reducing GE using silica-based materials; and mitigation of MCPD.*

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**Mitigation of MCPD in physically refined palm oil.** Kornél Nagy\*, Marine Nicolas, Karine Redeuil, Xanthippe Theurillat, Nestlé Research—Société Des Produits Nestlé SA, Switzerland

**MCPD and glycidyl esters—presentation of a modular analysis method for oils and fats as well as compound foods.** Martin Kaminski\*, Department 5, BVL, Germany

**Determination of 3-MCPD and glycidol in food emulsifiers: Analytical solution and multi-laboratory validation.** Jan Kuhlmann\*, SGS Germany GmbH, Germany

**Recent analytical methodologies for the determination of MOSH/MOAH in edible oils & fats.** Susanne Kühn\*, Michael Koch, Institut Kirchhoff Berlin GmbH part of Mérieux NutriSciences, Germany

**MOSH/MOAH in edible oils and fats: Current status and mitigation solutions.** Antonios Papastergiadis\*, Wim De Greyt, R&D Centre, Desmet Ballestra Group, Belgium

## Advanced Methods of Analysis, Including Lipidomics

ANALYTICAL

Chairs: William C. Byrdwell, USDA ARS BHNRC MAFCL, USA; and Hari Kiran Kotapati, USDA ARS MAFCL, USA

Tuesday, May 3, 2022 | 3:55–6 p.m. EDT (Atlanta, USA; UTC-4)

*This session includes talks on the Lipidomics Standards Initiative; fast method for analyzing pulse oils; methodology for the characterization and quantification of lipid mediators; de novo identification and quantification of fatty acids in lipid extracts; and travelling wave cyclic ion mobility.*

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**Combining near-complete characterization with quantitation for lipid analysis in matrix using electron activated dissociation.** Mackenzie J. Pearson\*, Paul Norris, Ryan Anderson, *SCIEX, United States*

**Lipid separation and structural characterization using travelling wave cyclic ion mobility.** Giorgis Isaac\*, Hernando Olivos, Robert Plumb, *Biomedical Research, Waters Corporation, United States*

**Unknown unknowns in lipidomics: A *de novo* method for fatty acid discovery.** Stephen Blanksby\*, Philipp Menzel, Reuben Young, David Marshall, Berwyck Poad, *Queensland University of Technology, Australia*

**Potential of lipid class separation—mass spectrometry approaches for high-throughput lipidomic quantitation.** Michal Holčápek\*, *Department of Analytical Chemistry, University of Pardubice, Czech Republic*

**Fast chromatography with dual parallel mass spectrometry for lipidomic analysis and regioisomer quantification of pulse lipids.** William C. Byrdwell\*<sup>1</sup>, Hari Karin Kotapati<sup>2</sup>, <sup>1</sup>*Methods and Application of Food Composition Lab, USDA ARS BHNRC MAFCL, United States*; <sup>2</sup>*Nutrition and Food Science, University of Maryland, United States*

**Update on guidelines for lipidomics analysis and reporting.** Kim Ekroos\*<sup>1</sup>, Robert Ahrends<sup>2</sup>, Christer Ejsing<sup>3</sup>, Nils Hoffmann<sup>4</sup>, Michal Holčápek<sup>5</sup>, Harald Köfeler<sup>6</sup>, Jeffrey McDonald<sup>7</sup>, Gerhard Liebisch<sup>8</sup>, <sup>1</sup>*Lipidomics Consulting Ltd, Finland*; <sup>2</sup>*University of Vienna, Austria*; <sup>3</sup>*European Molecular Biology Laboratory, Germany*; <sup>4</sup>*Universität Bielefeld, Germany*; <sup>5</sup>*Department of Analytical Chemistry, University of Pardubice, Czech Republic*; <sup>6</sup>*Lipidomics Research Center Graz, Austria*; <sup>7</sup>*UT Southwestern, United States*; <sup>8</sup>*University of Regensburg, Germany*

## Trace Contaminants

ANALYTICAL

Chairs: Jessica Beekman, *US Food & Drug Admin, USA*; and Jan Kuhlmann, *SGS Germany GmbH, Germany*  
Wednesday, May 4, 2022 | 7:25–9:30 a.m. EDT (Atlanta, USA; UTC-4)

*The Trace Contaminants session features talks on measuring and identifying the major trace contaminants in fats and oils methods for quantifying mineral oil hydrocarbons, mycotoxins, chlorinated paraffins and MCPD and glycidyl; and recent developments in EU policy on contaminants in vegetable oils.*

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**Analysis of MCPD and glycidyl esters: Recent occurrence data in U.S. infant formulas and effects of cooking on contaminant concentrations in frozen fried foods.** Jessica Beekman\*, Samanta Popol, Steven Peyton, Shaun MacMahon, *Center for Food Safety and Applied Nutrition, U.S. FDA, United States*

**LC-GC×GC-TOFMS/FID: Extra dimensionality to untangle mineral oil contamination: A particular look into the MOAH fraction.** Gregory Bauwens, Giorgia Purcaro\*, *Gembloux Agro-Bio Tech, University of Liege, Belgium*

**Determination of MOSH and MOAH—German standard method with improved precision data.** Ludger Ruehl\*, *Institut für Sicherheit und Qualität bei Getreide, Max Rubner-Institut, Germany*

**Solutions for modern routine analysis of mycotoxins in edible oils.** Jan Kuhlmann, Nicolaus von Mouillard\*, *SGS Germany GmbH, Germany*

**Gas chromatography-mass spectrometry (GC-MS) and liquid chromatography-high resolution mass spectrometry (LC-HRMS) approaches for analysis of chlorinated paraffins in edible fats and oils.**

Thomas J McGrath\*<sup>1</sup>, Franck Limonier<sup>2</sup>, Giulia Poma<sup>1</sup>, Jasper Bombeke<sup>1</sup>, Raf Winand<sup>3</sup>, Kevin Vanneste<sup>3</sup>, Mirjana Andjelkovic<sup>2</sup>, Els Van Hoeck<sup>2</sup>, Laure Joly<sup>2</sup>, Adrian Covaci<sup>1</sup>, <sup>1</sup>*Toxicological Centre, University of Antwerp, Belgium*; <sup>2</sup>*Chemical and Physical Health Risks Department, Sciensano, Belgium*; <sup>3</sup>*Transversal activities in Applied Genomics, Sciensano, Belgium*

**EU policy on certain processing contaminants in vegetable oils and foods containing vegetable oils: recent developments and outlook.** Frans Verstraete\*, *Directorate General for Health and Food Safety, European Commission, Belgium*

## Phospholipid Analysis in Food and Nutrition Research

ANALYTICAL

Joint session with the Phospholipid Division

*Chairs: Michael Bukowski, USDA ARS, USA; and Francesca Giuffrida, Nestle Research Center, Switzerland*

Wednesday, May 4, 2022 | 7:25–9:30 a.m. EDT (Atlanta, USA; UTC-4)

*The Phospholipid Analysis session includes an open-source application to facilitate high-throughput lipidomics; using supercritical fluid chromatography and high resolution mass spectrometry to identify minor lipid classes; challenges in phospholipid analysis in bovine milk; and differentiating animal sources of milk.*

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**Current challenges in phospholipid analysis in bovine milk.** Zhiqian Liu\*, Simone Rochfort, *Agriculture Victoria Research, Australia*

**Differentiation of the animal source of milk and milk products by means of <sup>1</sup>H NMR and <sup>31</sup>P NMR spectroscopy.** Bernd Diehl\*, *Spectre Service AG, Germany*

**Identification of glycerophospholipid species in food and biological matrices by supercritical fluid chromatography coupled with high resolution mass spectrometry.** Francesca Giuffrida\*, *Societe des produits Nestlé, Switzerland*

**Shotgun lipidomics assistant: An open-source application to facilitate high-throughput, comprehensive lipidomics.** Baolong Su<sup>1</sup>, Mackenzie J. Pearson<sup>2</sup>, Steven J. Bensinger<sup>3</sup>, Kevin J. Williams\*<sup>1</sup>, <sup>1</sup>*Biological Chemistry, UCLA, United States*; <sup>2</sup>*SCIEX, United States*; <sup>3</sup>*Microbiology, Immunology, & Molecular Genetics, UCLA, United States*

**Panel discussion**

## Rapid and High-throughput Screening Methods

ANALYTICAL

*Chairs: David Barr, Bruker BioSpin Corp., USA; and Torben Kuechler, Eurofins Analytik GmbH, Germany*

Wednesday, May 4, 2022 | 9:55 a.m.–Noon EDT (Atlanta, USA; UTC-4)



*The Rapid and High-throughput Screening Methods session features a low-cost, portable system to determine solid fat content; using 1H-NMR spectroscopy to analyze deviations from the origin lot in olive oil; and calibrating NMR for fat analysis in chocolate.*

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**1H-NMR spectral fingerprints of extra virgin olive oils: Confirmation of the identity and homogeneity within commercial lots.** Torben Kuechler\*, Ole Winkelmann, Eurofins Analytik GmbH, Germany

**Single-wavelength near-infrared analysis as a rapid and field-deployable tool to determine the solid fat content in fats and oils.** Marco Grossi<sup>1</sup>, Enrico Valli\*<sup>2</sup>, Virginia Teresa Glicerina<sup>2</sup>, Pietro Rocculi<sup>2</sup>, Tullia Gallina Toschi<sup>3</sup>, Bruno Riccò<sup>1</sup>, <sup>1</sup>Department of Electrical Energy and Information Engineering Guglielmo Marconi, Alma Mater Studiorum—Università di Bologna, Italy; <sup>2</sup>Department of Agricultural and Food Sciences and Interdepartmental Centre of Agri-Food Industrial Research, Alma Mater Studiorum—Università di Bologna, Italy; <sup>3</sup>Department of Food and Agriculture Sciences, University of Bologna, Italy

**Demystifying chemometrics: How multivariate analysis allows spectroscopy to be used to solve most analytical problems.** Jonathon Speed\*, Keit Spectrometers, United Kingdom

**Calibration of NMR for total fat analysis in chocolate manufacturing.** Dika Lau\*<sup>1</sup>, Rebecca Kuehn<sup>1</sup>, Linsen Liu<sup>2</sup>, <sup>1</sup>R&D, Guittard Chocolates Company, United States, <sup>2</sup>Sciences, Guittard Chocolates Company, United States

**Palm oil extraction process control using TD-NMR—study of losses reduction case.** Daniel M. Consalter\*<sup>1</sup>, Silvia P. De Azevedo, Lucas Topp, Cristina Consalter, Bruno Caravieri, Gabriel Torresam Fine Instrument Technology, Brazil

**A nondestructive method for oil distribution evaluation in healthy fried food developing by Raman imaging.** Peijin Tong\*<sup>1</sup>, Lingling Wei<sup>2</sup>, Junmei Liang<sup>2</sup>, Wenming Cao<sup>1</sup>, <sup>1</sup>Wilmar (Shanghai) Biotechnology Research & Development Center Co., Ltd, China (People's Republic); <sup>2</sup>Wilmar Global R&D Center, China (People's Republic)

## Novel Analytical Tools to Assess Oil Quality and Oxidation

ANALYTICAL

Joint session with the Lipid Oxidation and Quality Division

Sponsored by Kalsec

Chairs: Matthew Phaner, University of Michigan-Flint, USA; Richard Della Porta, PepsiCo/Frito-Lay, USA; and Fernanda Furlan Goncalves Dias, University of California, Davis, USA

Wednesday, May 4, 2022 | 9:55 a.m.–Noon EDT (Atlanta, USA; UTC-4)

*This session includes a novel method for quantitative assessment of epoxides; new tool for evaluating oxidation stability of specialty oils; green solvents for antioxidant analysis in frying oils; a rapid and efficient analytical method of oil oxidation steps; and irradiation-specific changes in irradiated meat matrices.*

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**Novel and Versatile Tool for Investigating the Oxidation Stability of Specialty Oils.** Carolin Edinger\* Anton Paar PROVEVEK GMBH, Germany

**Time Domain (TD) NMR Proton (<sup>1</sup>H) Mobility Sensor to Assess Oil Quality and Oxidation.** Zeev Wiesman\*, Tatiana Osheter, Charles Linder, Biotechnology Engineering, Ben Gurion University of the Negev, Israel

**Analysis of lipid radiolysis in irradiated dried meat products.** Umut Yucel\*, Food Science Institute, Animal Sciences and Industry Department, Kansas State University, United States

**Implementation of Green Solvents to Monitor Thermal Oxidation of Common Frying Oils.** Matthew Phaner\*, *Department of Natural Sciences, University of Michigan–Flint, United States*

**Quantitative assessment of epoxide formation in bulk oil and mayonnaise by <sup>1</sup>H-<sup>13</sup>C HSQC NMR spectroscopy.** Vincent Boerkamp<sup>1</sup>, Donny Merckx<sup>2</sup>, Jianli Wang<sup>1</sup>, Jean-Paul Vincken<sup>1</sup>, John Van Duynhoven<sup>3</sup>, Marie Hennebelle\*<sup>1</sup>, *<sup>1</sup>Wageningen University, Netherlands; <sup>2</sup>Unilever, Netherlands; <sup>3</sup>Unilever R&D Vlaardingen, Netherlands*

## Analytical Poster Session

*Chairs: Lisa Clement, Cargill Inc., USA; and Ali Reza Fardin Kia, U.S. Food and Drug Administration, USA*

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**ANA-01 Development of a near-infrared spectroscopy calibration model to predict methionine content in whole soybeans.** Maria Erazo\*, William M. Singer, Nick Lord, Maria L. Rosso, Bo Zhang *School of Plant and Environmental Sciences, Virginia Tech, United States*

**ANA-02 Identification of soybean germplasm with higher concentrations of long chain fatty acids** Patrick Bewick\*<sup>1</sup>, Eva Collakova<sup>1</sup>, Bo Zhang<sup>2</sup>, *<sup>1</sup>Virginia Tech, United States; <sup>2</sup>School of Plant and Environmental Sciences, Virginia Tech, United States*

**ANA-03 Simultaneous determination of free and esterified fatty acids of food fats using a rapid gas chromatographic method.** Aubreyona Migliori\*<sup>1</sup>, Robert E. Ward<sup>2</sup>, Silvana Martini<sup>1</sup>, Melissa Marsh<sup>3</sup> *<sup>1</sup>Utah State University, United States; <sup>2</sup>Nutrition, Dietetics and Food Sciences, Utah State University, United States; <sup>3</sup>Food Science, Utah State University, United States*

**ANA-04 Consistent units are required when using the activated complex theory in oil evaluation process.** Liyou Zheng\*<sup>1</sup>, Hongyan Guo<sup>1</sup>, Jun Jin<sup>2</sup>, Qingzhe Jin<sup>2</sup>, *<sup>1</sup>Anhui Polytechnic University, China (People's Republic); <sup>2</sup>Jiangnan University, China (People's Republic)*

**ANA-05 Enhance HS-SPME extraction kinetics by vacuum-assisted headspace and multi-cumulative trapping SPME and the combination of them for olive oil volatile profiling.** Steven Mascrez\*, Giorgia Purcaro, *Gembloux Agro-Bio Tech, University of Liege, Belgium*

**ANA-06 Increase the throughput and reliability of fatty acid characterization in food by using a rapid single step microwave-assisted extraction and derivatization method followed by GC×GC-FID.** Steven Mascrez\*, Angelica Fina, Giorgia Purcaro, *Gembloux Agro-Bio Tech, University of Liege, Belgium*

**ANA-07 Nutrient content and carotenoid bioaccessibility of underutilized taro varieties from Hawaii.** Kento Senga\*<sup>1</sup>, Kacie Ho<sup>1</sup>, Jon-Paul Bingham<sup>1</sup>, Marisa Wall<sup>2</sup>, *<sup>1</sup>University of Hawaii at Manoa, United States; <sup>2</sup>United States Department of Agriculture, United States*

**ANA-08 Thoughtful optimization of microwave-assisted saponification and extraction of MOSH&MOAH in edible oil.** Grégory Bauwens\*<sup>1</sup>, Giorgia Purcaro<sup>2</sup>, *<sup>1</sup>Analytical Chemistry, University of Liege, Belgium; <sup>2</sup>Gembloux Agro-Bio Tech, University of Liege, Belgium*