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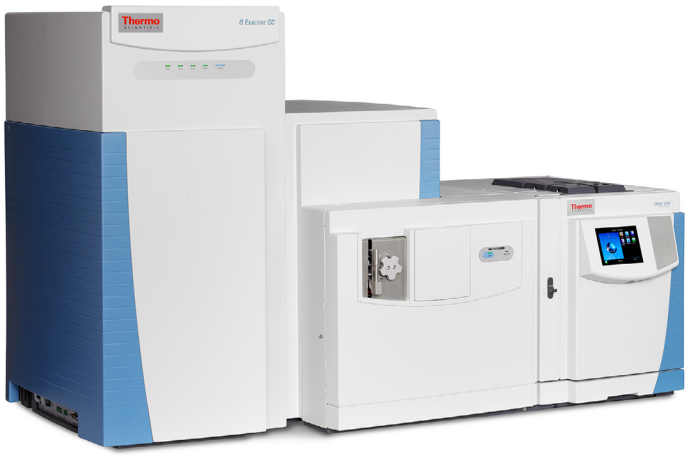
CASE STUDY
UCLA Pasarow Mass Spectrometry Laboratory

Orbitrap GC-MS Technology Advances Full Spectrum of Research



The Q Exactive GC Orbitrap GC-MS/MS system is used to identify and quantify small molecules with high chromatographic and mass resolution, and with high sensitivity.

Answering important research questions

Mass spectrometry (MS) is answering important questions in an increasingly broad spectrum of research around the world. However, available resources and MS expertise mean that it is not always feasible for labs to effectively deploy MS instruments on their own. This is where facilities that provide MS expertise and services can help.

The UCLA Pasarow Mass Spectrometry Laboratory is a center of MS expertise devoted to performing collaborative research, emphasizing the development and application of MS methods. The laboratory conducts a remarkably broad spectrum of collaborative research with UCLA and other research groups. For Kym Francis Faull, Ph.D., Professor and Laboratory Director, focus areas range from basic biochemistry to archaeology. Of the nine MS systems used in the laboratory, the Thermo Scientific™ Q Exactive™ GC Orbitrap™ GC-MS/MS system is applied to research that requires exceptional mass accuracy and sensitivity.

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Photo courtesy of UCLA Pasarow Mass Spectrometry Laboratory

"The Q Exactive is doing all the work we were able to do before, but better—due to greater sensitivity and more accuracy. It is a huge leap forward for us."

—Kym Francis Faull, Ph.D.,
Professor and Laboratory Director,
UCLA Pasarow Mass Spectrometry Laboratory

Q Exactive GC Orbitrap GC-MS/MS addresses broad scope of research

The availability of a sensitive and accurate Q Exactive GC Orbitrap GC-MS/MS system is essential to advancing the broad scope of research problems Pasarow addresses. This research includes:

- More sensitive, less costly assays to detect components of ruptured breast implants in blood. Though MRI is currently used, it lacks sufficient sensitivity and is expensive.
- More sensitive assays to detect early-stage kidney transplant rejection in urine where current tests likewise provide insufficient sensitivity
- Improved assays to detect early-stage Alzheimer's disease
- Organic residue analysis for archaeological research to provide valuable information about archaeological sites and artifact use
- Pharmacokinetics of potential new drugs; measuring drug concentrations in biological matrices

Unequivocal mass assignment and unprecedented sensitivity

With the Q Exactive GC Orbitrap GC-MS/MS system, mass (*m/z*) assignments are virtually unequivocal, enabling the laboratory to identify compounds with greater certainty than before. Accuracy of *m/z* assignment is particularly important for their biomarker profiling experiments to accurately and reproducibly "bin" MS data into the correct biological groups without overlap.

Often the most important sample components are present in the lowest concentrations. Extraordinary sensitivity provides the laboratory with two notable advantages. Clearly, enhanced sensitivity enables Pasarow's scientists to detect trace components in complex sample matrices such as blood with much greater certainty. It also means the laboratory can inject smaller sample volumes and still obtain very high-quality data. With smaller sample volumes, contamination of the GC injector port, GC column, and mass spectrometer ion source are reduced.

According to Dr. Faull, the Q Exactive GC Orbitrap GC-MS/MS system is user-friendly and easy to learn to use, with robust automated tuning and calibration that works very well to prepare the instrument for reproducible data acquisition day after day.

"The accuracy of *m/z* assignment is a defining feature of the Q Exactive GC-MS. The sensitivity is extraordinary and it is easy to use."

—Kym Francis Faull, Ph.D.

Dr. Faull explains GC-MS to students in Yaounde, Cameroon, West Africa.

Photo courtesy of UCLA Pasarow Mass Spectrometry Laboratory

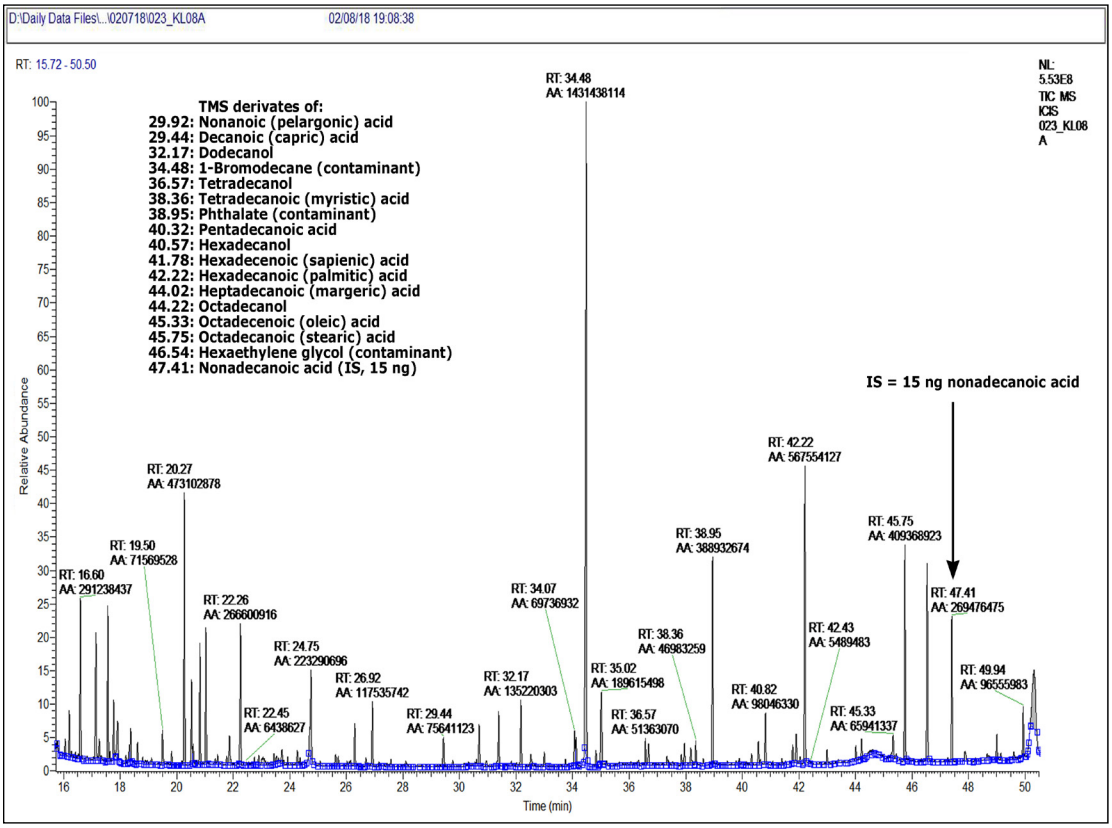
> "We are much more than a core lab because we do collaborative research with many different groups. When we're intellectually involved in the work, its more interesting, fun, and productive."
>
> —Kym Francis Faull, Ph.D.

Q Exactive GC Orbitrap GC-MS/MS in archaeological research: How was an ancient vessel used?

As described by Nigra, Faull, and Barnard,[1] archaeological unglazed pottery provides excellent loci for the preservation of organic molecules because their ceramic matrix retains and, to some extent, protects from destructive forces. GC-MS analysis to identify retained small organic molecules such as fatty acids, lipids, sterols, terpenoids, alkaloids, and carbohydrates present in a vessel can help archaeologists to determine if it was used for utilitarian or decorative purposes.

Conclusion

The Q Exactive GC Orbitrap GC-MS/MS system has brought the power of the high-resolution GC and high-resolution accurate-mass (HRAM) Orbitrap MS to the Pasarow Mass Spectrometry Laboratory. With the Q Exactive GC Orbitrap GC-MS/MS system, the laboratory accesses the exact masses of more compounds, at significantly lower levels, with singular confidence. The result is a broader and deeper understanding of the components in samples derived from a wide range of research collaborations.



Q Exactive GC Orbitrap GC-MS/MS analysis of extracted organic residues in a Neolithic potsherd (ca. 5400–5200 BC) from Albania. The samples were treated with BSTFA to convert the components to the TMS derivatives. The suite of fatty acids and their relative ratios suggest a vegetable source, possibly seeds. The chromatographic peak at 47.41 results from 15 ng of nonadecanoic acid added as internal standard. The chromatogram shows the abundance of other compounds, which were identified using the NIST database. The sample was prepared and analyzed by Gazmend Elezi and Jacob Damm, Cotsen Institute of Archaeology, under the supervision of Hans Barnard and Kym Faull. Courtesy of Dr. Hans Barnard, Cotsen Institute of Archaeology, University of California, Los Angeles.

About Dr. Kym F. Faull

Department of Psychiatry & Biobehavioral Sciences, and Laboratory Director, UCLA Pasarow Mass Spectrometry Laboratory. He earned his Bachelor of Agricultural Science with honors in Agricultural Biochemistry, and his Ph.D. in Plant Physiology from University of Adelaide, South Australia. After a post-doctoral fellowship at the University of Wollongong, New South Wales in GC/MS and human metabolic diseases, he joined the research staff at Stanford University School of Medicine, Department of Psychiatry and Behavioral Sciences in 1976. In 1990, Faull joined the faculty at UCLA. His publications reflect a deep background in biochemistry, and experience in the characterization and quantitation of biomolecules by MS. In addition to a wide range of research from biochemistry to archaeology, his work includes metabolic screening using GC-MS for organic acidurias and other inherited diseases, and work on biogenic amines and related compounds in major neuropsychiatric illnesses.

About UCLA Pasarow Mass Spectrometry Laboratory

The UCLA Pasarow Mass Spectrometry Laboratory is an intellectually vibrant group of individuals who share a commitment to the advancement of science and training of students through innovative research and educational endeavors. The Laboratory, located in the Semel Institute for Neuroscience and Human Behavior building at UCLA, conducts collaborative research and services for the entire UCLA campus and beyond, with emphasis on developing and applying MS methods to global and targeted identification and quantification of small molecules and proteins. The availability of gas and liquid chromatography and electron impact (EI), chemical (CI), electrospray (ESI), and laser desorption (LD) ionization methods together in one facility is vital to the wide variety of chemical and biochemical research its scientists help to advance. Its scientists are also involved in the development of computational analysis tools for mass spectrometric data, which include algorithms for feature identification and selection, deconvolution, and multivariate modeling.

> "Because the *m/z* assignment of ions is virtually unequivocal, we can identify compounds with greater certainty than before."
>
> —Kym Francis Faull, Ph.D.

Photo courtesy of UCLA Pasarow Mass Spectrometry Laboratory

Reference

1. Nigra, B. T.; Faull, K. F.; and Barnard, H. Analytical Chemistry in Archaeological Research. *Anal Chem.* **2015,** *87* (1), 3–18.

Find out more at **thermofisher.com/OrbitrapGCMS**

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