

# Case Study

## Implementing LC/MS to Ensure the Safety of Food, through Accurate, Rapid, and Cost Efficient Analysis

Food and Environmental  
Research Agency Case Study



The Food and Environment  
Research Agency

*The Food and Environment Research Agency (Fera) is an executive agency of the UK government's Department for Environment, Food and Rural Affairs (Defra). The agency was founded in April 2009 to encompass a number of Defra departments, including the Central Science Laboratory (CSL), the UK Government Decontamination Service (GDS), the Plant Health and Seeds Inspectorate (PHSI), Plant Variety Rights Office and Seeds Division (PVS) and Plant Health Division (PHD).*

*In 2009, Fera sought a liquid chromatography-mass spectrometry (LC-MS) system to enable the non-targeted detection of chemicals in food. The company implemented the Thermo Scientific Exactive benchtop LC-MS system to provide a high resolution, accurate and time efficient method of analyzing dirty samples and make routine analyses of food samples commercially viable.*

### Background

Fera's main purpose is to support and develop a sustainable food chain and to protect the global community from biological and chemical risks, particularly within food. To fulfill this role, the agency must provide robust evidence, rigorous analysis and professional advice to government, international organizations and the private sector. Fera has expertise in rapidly diagnosing threats, evaluating risks and informing on policy in food and environmental areas, as well as responding to and recovering from unforeseen or emergency situations. Fera also provides advice on policy issues, particularly relating to seed and plant health, and offers inspection services necessary to ensure protection for seeds, crops and horticulture. As issues such as food security, climate change and environmental sustainability present countries with significant, complex and often interrelated challenges, Fera plays a vital role, increasingly on a world stage, in anticipating the issues, assessing the risks and gathering the evidence to guide policy response.

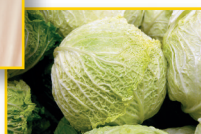
**“The Exactive system is a forerunner in mass spectrometry due to its high resolution capabilities.”**

Adrian Charlton,  
Head of Chemical and  
Biochemical Profiling, Fera

Fera manages more than 600 research projects, analyzing over 50,000 plant and food samples a year and is the National Reference Laboratory for chemicals in food, pesticides, veterinary drugs, dioxins and polychlorinated biphenyls (PCBs) in feed. Fera's main laboratory facility is located on a 32 hectare site at Sand Hutton near York in the United Kingdom and is occupied by almost 1000 employees, of whom approximately 600 are scientists. The company has more than 40,000 customers and 1,000 collaboration partners spread throughout 102 countries.

Fera's Biochemical and Chemical Profiling team currently uses non-targeted LC/MS and nuclear magnetic resonance (NMR) spectroscopy to analyze food samples for potential contamination. Fera selected the Exactive™ LC-MS system to enable the routine, accurate time and cost-efficient analysis of these samples.





### Business Challenge

The food testing industry has a high demand for analytical methodologies for the holistic monitoring of food, an approach often referred to as profiling or screening. Currently, chemical analysis of food is largely limited to the direct determination of compounds that are specified prior to analysis, which is known as the “target list” approach. While this approach is highly relevant to the enforcement of regulatory parameters relating to known food contamination issues, such as

the detection of pesticides and veterinary drug metabolites in foods, it does little to address those components in food that are not anticipated.

A number of high-profile issues, such as the deliberate adulteration of milk with melamine in China, have highlighted the need for Fera to perform

broad range analysis of the composition of foodstuffs. By obtaining a detailed understanding of what is naturally and normally present in foods, it becomes possible to monitor the food chain for abnormalities.

In order to look for a wide range of potential contaminants in the areas of food fraud and food safety, Fera needed a high-resolution and high mass accuracy

instrument that would enable non-targeted screening of food samples. New technology was required to enable the agency’s Biochemical and Chemical Profiling team to use generic and holistic approaches to look at the composition of foods and the potential for food contamination. They also hoped for time and cost savings if the instrument was capable of analyzing dirty samples – as this would preclude the need for lengthy sample clean up. Once equipped with the tools to screen all ingredients that go into a food product, Fera would be able to better support the food industry and Government in relation to food safety issues.

Adrian Charlton, Head of Chemical and Biochemical Profiling at Fera explains, “As we are continually being faced with new food safety challenges, it is important that our laboratory is equipped with the industry’s most advanced instrumentation. While holistic monitoring of food has been the desired method for a number of years, it is only in recent times that instrumentation technology has advanced to the point where this has become feasible. We needed a high resolution mass spectrometer that would enable us to perform non-targeted LC/MS screening of food samples, including dirty samples, saving time and cost in our laboratory and ensuring accurate results.”

### Vendor Selection

As a research and development team, Fera’s Biochemical and Chemical Profiling team required an instrument that would enable them to look at individual samples in great detail, extracting as much information as possible. The company also needed an instrument that would be compatible with and add value to its NMR spectroscopy instruments as this is a key technique in Fera’s laboratory. Adrian Charlton comments, “The Exactive system is a forerunner in mass spectrometry due to its high resolution capabilities. We felt that it would be ideal to have an LC/MS instrument that would complement the NMR approach and we found that the Exactive system is that instrument.”

Adrian explains that Fera had always wanted to perform non-targeted screening of food samples using LC/MS but until recently, the required technology had not been available. He continues, “While in the past LC/MS analyses have been largely targeted, instruments such as the Exactive LC-MS system have become available, making non-targeted LC/MS screening possible. Science has driven the development of high resolution mass spectrometers to ensure food safety through accurate and time-efficient analyses and this need has been met by Thermo Fisher.”

**“Since introducing the Exactive benchtop LC-MS system into our processes it has been extremely reliable and easy to use...”**



## Implementation

Fera implemented the Exactive LC-MS system in September 2009. The agency is currently using the Exactive system to analyze a range of samples, including testing plant materials for issues

such as genetic modification to discover how this impacts the nutritional quality of final food products.

The Exactive system is also used at Fera to analyze food materials such as honey for bioactive

properties and botanical markers to verify labeling claims and ensure authenticity. Fera is using the instrument to look at animals and plants in terms of biomarkers of disease, biomarkers of environmental exposure to pesticides and biomarkers of manipulation of the genome.

The main reason Exactive system was selected was that the instrument's high resolution would make non-targeted screening using LC/MS possible. Since implementation, Fera has also found that the Exactive system enables dirty samples to be analyzed, resulting in significant time and cost savings.

## Benefits

Since the installation of the Exactive system in 2009, the instrument has performed extremely accurate and cost-effective analyses of a wide range of samples. The high mass

resolution and accurate mass measurement of the Exactive system has made it possible for Fera to analyze dirty matrices, removing the need for lengthy sample clean-up and leaving more time to focus on results. The mass resolution has also enabled Fera to be much more specific when

determining molecular weights.

Since its implementation, the Exactive system has also enabled Fera to perform certain food analyses more routinely by offering a commercially viable option. The Exactive system has been used for proteomics and metabolomics research, particularly to investigate food authenticity issues. The EU has recently been faced with such issues. For example non-chicken products, such as beef, pork and water, have been added to chicken to make it heavier which increases its price. The Exactive system is currently being used to investigate this issue,

addressing economic, ethical and religious concerns raised by the substitution of chicken with other meat. Adrian Charlton comments, "Proteomics in particular has much potential for the future and we have found that the Exactive system is a good instrument for performing this type of research routinely and cost-effectively in our laboratory."

The Exactive system is a reasonably priced, benchtop instrument with the power of a much bigger instrument, yet it requires minimal space in the laboratory. Fera has successfully used the Exactive system for quantitative measurements and targeted analyses. Adrian continues, "Since introducing the Exactive benchtop LC-MS system into our processes it has been extremely reliable and easy to use by non-specialist instrument users, making routine operation very straightforward. As the method set-up does not require our most advanced instrument users, this also increases instrument usability and leaves our scientists with more time to focus on results."

In addition, data acquired using the Exactive system can be processed and de-convoluted using advanced Thermo Scientific SIEVE software, simplifying results analysis. Furthermore, The Exactive system's software can be easily integrated with external databases, allowing easy collaboration between Fera and its research partners.

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## Conclusion

Fera is using the Exactive benchtop LC-MS system to support governments and food producers worldwide by accurately analyzing food samples for contaminants and potential food safety risks. Using the instrument, the laboratory has benefited from substantial time and cost savings, while the high resolution of the Exactive system has ensured accurate and reliable results.

Adrian Charlton concludes: "Thermo Fisher is one of the biggest providers of scientific instruments in the world and has been responsible for the invention of well-regarded mass spectrometry technology, with the Exactive system a forerunner in the field. The resolution of the Exactive system is exceptional; we have been able to get down to a much higher mass resolution than we expected, removing large matrix interference completely. The instrument has become an integral part of our laboratory and has enabled Fera to make significant progress towards ensuring a sustainable food chain and protecting consumers from biological and chemical risks within food."

For more information on the work of Fera visit <http://www.fera.defra.gov.uk>.

*The Exactive system recently enabled Fera to analyze wine samples for natamycin, a naturally occurring fungicide in white and red wine, by injecting the wine directly onto the system without the need for sample clean-up.*



*The LC/MS method was applied to the analysis of 190 wine samples, originating mainly from South Africa and South America, during the period from December 2009 to March 2010. Fifty samples (26%) gave positive results for natamycin ( $> 5 \mu\text{g/L}^{-1}$ ) all of which originated from South America. The resolution of the Exactive system enabled the analysis of natamycin in wines at low  $\mu\text{g/L}^{-1}$  (ppb) levels in commercial samples of white and red wine, meaning the instrument can be used as a regulatory enforcement tool. The combination of LC and high-resolution MS proved to be a rapid, sensitive and highly selective method for the determination of natamycin in wine, enabling Fera to help Argentinean wine producers ensure the authenticity of their produce. The Exactive system also enables Fera to comply with EU regulations list compounds that can be included in wine sold in the EU.*



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