

## Single-vendor LC-MS and CDS system delivers benefits to Fondazione Edmund Mach Chemistry Lab

Since 2008, Fondazione Edmund Mach has continued the aims and activities of the Istituto Agrario di San Michele all'Adige, founded in 1874, and of the Alpine Ecology Centre established in 1992.

It is a highly prestigious institution, which over the years has achieved many important awards at the international level. They deliver a range of education, training and technology transfer programs in the fields of agriculture, food processing and sustainable development, with particular regard for the environment and the safeguarding of the territory of the Trentino region.





“Chromeleon 7.2 CDS is a very comprehensive and simple to use software. In a few steps, you can integrate, identify and quantify the interest compounds and create reports, charts and graphs reducing data processing time.”

Tiziana Nardin is a food technologist at the Fondazione Edmund Mach in Trento, Italy. She works in the chemistry laboratory in the Unità Chimica Enologica e Agroalimentare del Centro di Sperimentazione e Servizi Tecnologici where they provide analytical services to businesses and public bodies in the fields of agricultural and oenological chemistry and microbiology. Their applied research and experimentation activities involve studying advanced technical solutions for the environmental, social and economic sustainability of production and for the quality and healthiness of food and agricultural products.

“I have a degree in food technology and I’m currently getting my Ph.D. in agricultural science and biotechnology,” Tiziana said. “I have worked here for 14 years now and specialize in studying food and beverages. For many years, the chemistry laboratory has provided extensive support to the agroindustrial production world, and regional, national and international research institutions, through multiple analytical activities which range from official checks to technical support on site. This includes, defining conventions on the specific technological aspects of testing of wine and spirits in the field.”

The laboratory uses Thermo Scientific™ Chromeleon™ 7.2 Chromatography Data System (CDS) software to control several instruments including Thermo Scientific™ Dionex™ ICS-5000+ HPIC™ ion chromatography (IC) systems, Thermo Scientific™ UltiMate™ 3000 UHPLC systems and a Thermo Scientific™ Q Exactive™ Hybrid Quadrupole-Orbitrap™ Mass Spectrometer.

Here is a recent interview we had with Tiziana about how they use Chromeleon CDS software, what their experience has been using the LC-MS system and the benefits they see to having one software for control.

**Q: *What are the drivers, issues, and concerns of your lab?***

Tiziana: Our laboratory gives informative and analytical support to private companies and public institutions to help them solve technical issues related to food processing, traceability and quality assurance. So, as with many labs, we need to be able to foresee the possible needs of our customers, develop or adopt novel technical solutions, and support the transfer of new knowledge and practical solutions to our customers.

**Q: *How does Chromeleon CDS software help with compliance?***

Tiziana: Some of the analytical tests we perform are supervised by a national accreditation body and must comply with UNI CEI EN ISO/IEC 17025 (quality requirements for the competence of testing and calibration laboratories). Chromeleon CDS software allows us to manage the analytical activities, from sample sequences to personalized reports, meeting the prescribed requirements.



**Q: *What was your experience learning and using the software?***

Tiziana: We have used Chromeleon CDS software for several years to control our IC and LC systems and were very impressed with its features and capabilities. We found the software very easy to learn and to use day-to-day as it is extremely intuitive with a clean, user-friendly interface.

We have found Chromeleon CDS software to be a very comprehensive and simple to use software. In just a few steps you can integrate, identify, and quantify the compounds of interest and create reports, charts, and graphs which significantly reduces data processing time.

**Q: *What was your motivation for looking at adding MS to your lab?***

Tiziana: LC-MS is now a well-established technique in many leading labs and we also firmly believed that this was a necessary addition to our instrumentation in order to improve our advanced analytical proposal to our customers. LC-MS, and in particular UHPLC with a high resolution, accurate mass (HRAM) MS, would give us a series of advantages and benefits due to the high specificity and selectivity of these detectors especially for experimentation projects.



**Q: *You must have compared other mass spectrometers. Why did you consider the Q Exactive MS for your situation?***

Tiziana: We did consider several alternative MS systems but the Q Exactive mass spectrometer was shown to give us very good performance and versatility for our targeted and non-targeted screening and qualitative and quantitative analyses.

Also, from our good experiences with Chromeleon CDS software we decided it would be preferable and convenient if we were able to use it to control the high resolution MS. So naturally we were excited when we heard that Chromeleon CDS supported HRAM MS. Being able to use one software package to control both the LC and MS and the availability of features for targeted MS quantification were major factors in our decision.

**Q: *What is your experience with the LC-MS solution?***

Tiziana: Since the addition of the LC-MS system to the laboratory we have found that, when using it with Chromeleon CDS software for our targeted analyses, it is very flexible. Moreover, thanks to high-resolution technology and therefore the accurate mass analyses, we could broaden the field of our food analytical chemistry experimentation with untargeted screening research.

We immediately found the Q Exactive Mass Spectrometer to be a very robust instrument. The source does not require cleaning often, but if it is necessary the procedure is very fast and easy. Also we found the mass calibration to be stable for four or five days which allows us to analyze long sequences without stopping.

The LC-MS system has become an essential tool for our targeted and untargeted analyses. The heated electrospray source (HESI) increases the ionization of numerous compounds and the many different experiments that the instrument facilitates allow us to meet our customer's requirements.

With full scan analyses, we can obtain and record all sample data which can then be used for retrospective analysis if required and with the mass resolution up to 140,000 full width at half maximum (FWHM) eliminating isobaric interferences we have much greater confidence in our compound identification. Furthermore, the inclusion of the quadrupole allows us to select the precursor ion which, coupled with the higher-energy collisional dissociation (HCD) cell, enables us to identify and confirm compounds using fragmentation analyses.

**Q: *How many methods do you perform?***

Tiziana: We use the system for many different applications from targeted quality control analysis of, for example, simple phenols and alkaloids to untargeted research analysis of food and beverages including free and glycosylated phenols, alkaloids, pesticides, minor sugars, amines, vitamins, mycotoxins and many more. Coupled with Chromeleon CDS, the data analysis from the Q Exactive mass spectrometers becomes easy and fast to handle both for the acquisition and the processing of the data, and we have found that the available features for targeted quantification definitely make it faster and easier to use than any other software.

**Q: *Are there any benefits to having everything from one vendor?***

Tiziana: We have found several benefits to having one vendor for both software and instrumentation. The first was fast and easy connection to Thermo Fisher Scientific specialists who understand the full system and were therefore able to deliver better initial training and, later on, provide support for any issues and help us solve them very quickly. Chromeleon CDS software allows us to fully control the LC-MS instrument—managing full scan and data dependent experiments. It also supports the importing of databases with compound parameters, exporting and comparison of spectra, and processing and exporting of MS and MS/MS results.

**Q: *Did Chromeleon CDS change the way you do things in the lab?***

Tiziana: Yes. We have found Chromeleon CDS to be a very complete software package. It allows us to now manage our HPLCs, IC and all the detectors used with these instruments [including the MS] in one system. It is easy to control all the different instrument functions allowing us to streamline our methods and experiments which saves us time developing methods and therefore reduces our customer turnaround time.

We have also found some functions are now much easier and faster. The user interface is very intuitive and easy to use with minimal training. For example, in the audit trails you can easily filter to view any errors or warnings which facilitates instrument troubleshooting which in turn minimizes any downtime.

Overall I would definitely recommend it!

**Q Exactive Hybrid Quadrupole-Orbitrap Mass Spectrometer**

Identify, quantify and confirm more compounds rapidly and with confidence using the Q Exactive Mass Spectrometer. This benchtop LC-MS/MS system combines quadrupole precursor ion selection with high-resolution, accurate-mass Orbitrap detection to deliver exceptional performance and versatility. It is equally useful for untargeted or targeted screening and a broad range of qualitative and quantitative applications in drug discovery, proteomics, environmental and food safety, clinical research and forensic toxicology.

For more information, go to [Q Exactive Hybrid Quadrupole-Orbitrap MS System](#)

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**Chromeleon 7.2 CDS**

Chromeleon CDS software provides chromatography labs with compliance-ready data management, unified instrument control and simplified analysis and data reporting for chromatography and mass spectrometry. By extending Chromeleon CDS beyond chromatography into MS, labs can now streamline chromatography and MS workflows with a single software package.

For more information, go to the [Chromeleon CDS Resource Center](#)

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