

Owlstone Medical boosts efficiency—in and out of the lab—with upgrade to Chromeleon 7.3.2 CDS

"We have been using Chromeleon CDS for several years. It's robust and intuitive, with all the features needed to run our workflows. Since the upgrade to version 7.3.2, we can now perform all our analyses and reporting in one streamlined step to both process and export our results for all 250 components, taking us from days of processing time to less than four hours, which is a game changer."

—Dr. Kayleigh Arthur, Owlstone Medical Ltd.

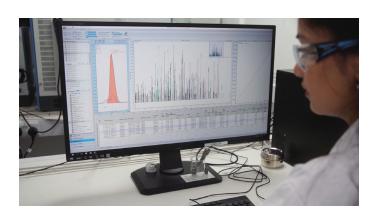
Introduction

Owlstone Medical is the global leader in Breath Biopsy®, a non-invasive way to capture and analyze volatile metabolites in breath to rapidly gain insight into the metabolic changes associated with cancer at its earliest stages. By focusing on areas such as lung cancer, liver disease, and more, the company aims to save 100,000 lives and \$1.5B in healthcare costs. Owlstone's ground-breaking approach relies on the ultra-sensitive, information-rich high-resolution accuratemass (HRAM) data produced by Thermo Scientific™ Orbitrap™ mass spectrometers combined with the Thermo Scientific™

Chromeleon™ Chromatography Data System (CDS) in a cloud-based enterprise installation for high-throughput data acquisition, processing and management in a secure, centralized environment. To enhance laboratory efficiency, Owlstone upgraded their Chromeleon CDS enterprise installation to version 7.3.2 long-term support (LTS). The upgrade provided a massive 15-fold increase in data-processing and reporting speeds compared to the previous version. It also enabled Owlstone to perform analyses and reporting for all target components in one method, substantially reducing processing time from days to a few hours.

"With Chromeleon CDS version 7.3.2, Thermo Fisher has produced an upgrade that really addressed our pain points and helps us work much more efficiently in and outside the lab. We are very happy to work with Chromeleon 7.3.2 CDS as a cloud-based solution for our MS analysis."

-Dr. Kayleigh Arthur, Owlstone Medical Ltd.



Non-invasive approach for disease detection

Exhaled breath contains hundreds of informative volatile organic compounds (VOCs) that provide a rich source of biological information. Unlike blood and tissue sampling, breath sampling offers a non-invasive, pain-free way to monitor human biology for early disease detection and treatment optimization for precision medicine. One of the benefits of using breath for early detection is that, unlike genetic tests, the results represent an individual's current metabolomic state, not just the life-long predisposition towards specific health issues. Using Orbitrap mass spectrometers and Chromeleon CDS, Owlstone Medical provides a reliable sample-to-results breath-testing workflow—Breath Biopsy—that represents a new way to measure the chemical composition of breath.

Chromeleon 7.3.2 CDS delivers efficient MS data processing and reporting for breath testing

Reliable breath testing depends on sensitive detection, which is why Orbitrap mass analyzer technology is a key part of the Breath Biopsy platform. Due to the volume of HRAM data produced during analysis of the complex set of compounds in breath, the CDS must be able to process and generate reports from large mass spectrometry (MS) data files rapidly and in the background, so analysts can continue to use the software to perform other tasks.

Dr. Kayleigh Arthur, Lead Validity and Compliance Scientist at Owlstone Medical, described the challenge presented by MS methods: "The size of the targeted panel for our application created issues due to the generation of huge amounts of data. We were processing around 250 components with each analysis and previously had to process in batches and simplify reports to reduce reporting time."

The Chromeleon 7.3.2 CDS enterprise installation addresses MS data processing and reporting challenges with fast, serverbased processing of large data files, reducing the time from injection to final results. Processing and report generation occur in the background, keeping the user interface available so analysts can continue to work. Dr. Arthur explained, "Chromeleon 7.3.2 software addressed our concerns about software speeds, for example, we have seen an increase of processing time over 15 times compared to the previous version. Since the upgrade, we can now perform all our analyses and reporting in one process and export for all 250 components, taking us from days of processing time to less than a few hours, which is a game changer for us. Even simple things have been improved dramatically, like the speed of moving between injections and the ability to work with the software while processing is running to help avoid delays. Everything is so much faster."

Easy upgrade

The upgrade to Chromeleon CDS version 7.3.2 was included free of charge as part of Owlstone's software enterprise support contract, which also provides support from Thermo Fisher Scientific enterprise specialists. The upgrade process was straightforward and required little to no downtime, allowing Owlstone to perform the upgrade themselves. Dr. Arthur noted "as it is deployed in an enterprise environment connected to a Cloud server, having an enterprise support contract is critical as it gives us access to Thermo Fisher enterprise support specialists who help us resolve any issues quickly, keeping any downtime to a minimum. The upgrade process itself was very straightforward—we actually did it ourselves—but we did have direct support from Thermo Fisher available in case we needed help."

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Robust, intuitive, and capable

Owlstone's Chromeleon software enterprise installation controls, acquires, processes, and reports data from several instruments including five Thermo Scientific™ Q Exactive™ GC Orbitrap™ GC-MS/MS systems, two Thermo Scientific™ Orbitrap™ Exploris™ GC mass spectrometers, and a Thermo Scientific™ TRACE™ 1600 gas chromatograph with a flame ionization detector (FID), all with thermal desorption and/or liquid injection. The software acquires, processes and reports results in a seamless workflow with a robust audit trial for data integrity.

From the beginning, Owlstone has been very satisfied with the software. Dr. Arthur explained, "We have used Chromeleon CDS for several years to control our thermal desorbers and Orbitrap GC-MS instruments and we are very impressed with its robustness and capabilities. The lab users and I find the software extremely intuitive, making it very easy to learn and use day-to-day. It has all the features needed to run our workflows. In just a few steps you can acquire, integrate, and identify compounds of interest and create detailed reports, which significantly reduces our data processing time."

Secure, cloud-based centralized installation for efficient, compliant operations

Companies like Owlstone need to control instruments and manage data in a secure centralized environment to enable remote access and compliance. For this reason, a few years prior to upgrading to Chromeleon 7.3.2 CDS, Owlstone had migrated to a centrally managed enterprise installation of Chromeleon software that resides on cloud-based servers. In this configuration, Owlstone can easily manage backups, set user roles and privileges, and query any data from the entire CDS installation. This saves time and money, ensures the best possible software performance, and makes IT's job easier.



"We wanted to have a centrally managed system with cloud servers, and Chromeleon CDS was able to support this easily," said Dr. Arthur. "With Chromeleon software we can manage all our instruments and work with data remotely via a centralized server, which means we don't need to be in the laboratory to access our data. This was particularly important during the COVID-19 pandemic, when we were still able to continue working from our homes. Our IT team can make sure everything is backed up properly, set user roles and privileges accordingly, and query any data from the entire installation with a simple mouse click. This saves Owlstone a lot of time and money with data management while providing users with the best performance for the software, which definitely makes everyone's work much easier."

"One of the key benefits of using breath is that it's based on current metabolic activities which is the most appropriate way to detect diseases in their earliest stages. This depends heavily on sensitivity of detection, which is why we use high-resolution accurate-mass Orbitrap mass spectrometers coupled with Chromeleon CDS. The software provides enhanced data acquisition, management, and processing, giving us an end-to-end solution for our high-throughput Breath Biopsy laboratory."

—Dr. Kayleigh Arthur, Owlstone Medical Ltd.

Conclusion

In a cloud-based enterprise installation, Chromeleon 7.3.2 CDS fully addresses Owlstone's MS data acquisition, processing, reporting, and management challenges, substantially increasing productivity. Owlstone now carries out MS analyses and meets reporting requirements in one streamlined process, saving substantial amounts of time from injection to final reporting of results. To meet future sample-analysis needs, the enterprise installation can be scaled up with additional instruments, offering further cost and efficiency gains. In combination with GC Orbitrap systems, Chromeleon CDS version 7.3.2 provides the end-to-end enterprise solution required to manage the logistics of ever-increasing demands for Owlstone's Breath Biopsy analyses.





About Kayleigh Arthur

Dr. Kayleigh Arthur is a Lead Validity and Compliance Scientist at Owlstone Medical Ltd. in Cambridge, UK. She is an analytical chemist and mass spectrometrist with over nine years of experience with LC-MS, GC-MS, and ion mobility spectrometry. Her work is focused on the incorporation of GC Orbitrap technology to investigate a variety of volatile organic compounds in Breath Biopsy research. Dr. Arthur was a PhD student at Loughborough University's Centre for Analytical Science and has a Master of Chemistry (MChem) First-class Hons, Chemistry with Analytical Science, also from Loughborough University's Centre for Analytical Science.

About Owlstone Medical

Headquartered in Cambridge, UK, with offices in London, Owlstone Medical's vision is to save 100,000 lives by realizing the promise of breath-based diagnostics through the development and application of Breath Biopsy®, a unique platform capable of both biomarker discovery and use in routine clinical testing. The platform includes ReCIVA® Breath Sampler, a proprietary sample collection device, the world's only commercial Breath Biopsy Laboratory, and the Breath Biopsy VOC Atlas, the most extensive catalogue of identified volatile organic compounds (VOCs) commonly found on breath.

Owlstone Medical's Research Products and Services are deployed at over 100 sites around the world with large pharmaceutical companies including AstraZeneca, Actelion, GlaxoSmithKline, and leading academic institutions. These are supported by Breath Biopsy OMNI®, a solution for end-to-end global breath VOC analysis, which is helping researchers advance biomarker discovery and disease research to find clinically relevant breath biomarkers.







