

Collaborative Software Development Accelerates Waters Newest App

A beta testing partnership between Waters and Primoris Belgium refined the capabilities of the new **waters_connect** for quantitative analysis app-based platform for method development, data processing, and data review

Technology: **waters_connect™** for Quantitative Analysis, **TargetLynx™** Application Manager, **MassLynx™** Mass Spectrometry Software, **Xevo™** TQ-S Micro Mass Spectrometer, **Xevo TQ-XS** Mass Spectrometer

FOOD AND FOOD ADDITIVES ANALYSIS AT PRIMORIS

As specialists in the routine analysis of food and feed stuffs, Primoris provides its international customers with analytical services for detecting pesticides, contaminants, genetically modified organisms (GMOs), and transmittable viruses in food and feed. The company also supports customers with risk analysis after a positive finding of the residue limits, which includes determining any potential risk for public health.

Primoris began as a spin-off of Ghent University in 2001. It has grown to become an international group comprising of Primoris Laboratories, CKCert Certification Company, and the Ciboris Knowledge Center.

Because of the multilateral and bilateral agreements within European co-operation for Accreditation (EA) and International Laboratory Accreditation Cooperation (ILAC), the company's nationally granted accreditations are recognized globally as equivalent by all participating accreditation organizations, and its certified laboratories include Primoris Belgium, Primoris Bulgaria, Primoris Colombia, Primoris Costa Rica, and Primoris Ecuador.



*The Primoris team believe the **waters_connect** for Quantitative Analysis Software offers business benefits to the company by removing tedious manual data reviews, as well as dramatically improving access to data.*

WORKING WITH WATERS

As a long-time customer, Primoris Belgium had extensive experience with Waters™ MassLynx and TargetLynx XS software, in addition to a wide variety of Waters analytical instrumentation.

Beta testing the new **waters_connect** for Quantitative Analysis Software offered a unique opportunity to collect feedback from experienced users in a routine laboratory environment.

Mr. Wendel D'Hondt, Primoris Belgium Team Leader, explains:

"There's a high level of trust between our two companies, and it was nice that we could influence the product before it was released. It's a win-win situation. Waters got a product that was designed to fit the needs of its customers. Primoris got a product that we can work with to improve our own efficiency."

“ We specialize in analysis of very difficult samples like food additives, food supplements, essential oils — anything that’s remotely related to food and will be used in food or feed applications. We cater to the needs of our customers by providing timely results and special requests. But our focus is always on quality. We want to provide our customers with good, reliable results.”

MR. WENDEL D’HONDT

Primoris Belgium Team Leader

That emphasis on quality means that Primoris continually invests in advanced analytical technology to provide small molecule quantitation data analysis services for its clients. That includes around 50 Waters instruments in the Belgium laboratory alone, comprising liquid chromatography (LC), gas chromatography (GC), and mass spectrometry (MS) systems. Mr. Tybo Mylle, Primoris Belgium Team Leader, describes the company’s strategy behind these investments:

“Our biggest service offerings are LC-MS and GC-MS methods, which we use for the wide screening of a general pesticide use. But the market is always changing, and we continually work to achieve lower reporting limits for all compounds. So, we need sensitive machines to keep ahead of our customers’ needs. We’re always trying to prepare for what is coming in the future.”



Primoris plans to continue working with Waters to provide training in the software’s technical controls and show users how these might be leveraged in the laboratory.

That business philosophy helped the Primoris Belgium team serve as excellent beta testers for the new waters_connect for Quantitative Analysis Software, helping Waters refine this new software platform to meet the needs of its customers.

TESTING FOOD AND FOOD STUFFS

Primoris began more than two decades ago by specializing in pesticide testing for food and feed, which includes fungicides, herbicides, insecticides, lures, rodenticides, and repellents. Over the years, the company has continually added to their analytical services, which now include the detection of mycotoxins, heavy metals, food contaminants and ingredients, and transmissible viruses.

As the food analysis industry relies on timeliness, quick turnarounds are a vital component of the laboratory’s services. Primoris adapts the speed of analysis to the customers’ needs, offering three different analysis times: standard is 3–5 working days, fast is 36 hours, and urgent is 8 hours. However, the company’s focus on quality means that Primoris can’t afford to lose any functionality at the same time. Mr. D’Hondt explains:

“We have to balance quality and speed. We do offer a special eight-hour service, which means the customer provides us with the sample before 11AM, and we promise results by that evening. But we also need to make sure the results are always reliable.”

Food testing labs face several challenges when running a targeted method for the quantitation of hundreds of analytes across many batches of different samples and matrices. The improvement in MS technologies and rapid advancements in new instrumentation have provided the field with powerful analytical capabilities in terms of sensitivity, selectivity, resolution, throughput, mass range, and mass accuracy.

“ Our biggest challenges are with our multi-residue methods. These methods detect a lot of compounds. For example, our main LC-MS method detects more than 300 compounds. In contrast, a pharmaceutical laboratory may only need to detect 10 compounds in their scope.”

MR. TYBO MYLLE

Primoris Belgium Team Leader

Other challenges include sample preparation and data processing. LC-MS systems generate enormous amounts of data in multi-residue analysis. One of the biggest bottlenecks for food analysis methods is associated with developing, managing, and curating error-free acquisition and data processing methods, which can be both time-consuming and cumbersome. Companies like Primoris often work with instrument manufacturers and analytical software developers to address these issues.

"We really love MassLynx and TargetLynx XS, but some things can be better. This was a great opportunity to get those things on the table, and Waters really listened to us. One of our biggest challenges is data size. Our clients always want more compounds to be in our multi-residue methods, and we continually add new ones. At some point, the software simply can't export everything at once, and we'll have to use workarounds to process all the data. But Waters really wants to help us with this issue, and the MS Quan app has the potential to make it better."

MS. JANNE DOMBRECHT

Primoris Belgium Lead of Analysis

Primoris explains that the data file sizes are now so large due to the many compounds in the multi-residue method, that it is impossible to export the file from TargetLynx XS. The workarounds take time, and include multiple stages (processing the list in TargetLynx XS, exporting in xml, importing into the LIMS) that result in at least a 30-minute delay in the lab's most common method. This data export used to take 5 minutes, but now an additional 30 minutes on every project causes workload bottlenecks.

BETA TESTING PROCESS

Waters developed the waters_connect for Quantitative Analysis Software to offer unique method development, data processing, and reviewing tools in a modern, app-based software platform. Collaboration efforts with Primoris Belgium as an early adopter helped to provide insight and guidance to small molecule quantitation data analysis needs in food.

As a result, Waters developers could design specific software functionality to enhance efficiency at every stage of the workflow, including faster time-to-result and increased efficiency in quantitative analysis. Mr. D'Hondt explains:

"We saw the future, and we were confident that we could help Waters make some adjustments that would reflect the needs of real users in the laboratory. Of course, analysts are very critical and very detail-focused. We knew we could provide a lot of good feedback to the Waters software development team."

That feedback took the form of numerous iterations of the MS Quan app, as well as frequent meetings between Primoris Belgium and Waters to refine the workflows and the user interface as changes were made. At one point, the Primoris Belgium team even sketched out suggestions for the app's screen layout. Mr. D'Hondt explains:

"The best way to communicate was to show Waters a drawing of how we wanted it to look. And they used a lot of our suggestions to build a new screen for unknowns. Everything we asked for is either addressed or already included in the newly launched app."

BENEFITS

The Primoris team's experience with the collaborative software development process has strengthened the company's confidence in the commitment of Waters to deliver new levels of usability, efficiency and confidence to its customers. The impact of this partnership can be seen in the recently launched waters_connect for Quantitative Analysis Software, which provides a single platform for LC and LC-MS applications that accelerate end-to-end scientific workflows.



Waters developed the waters_connect for Quantitative Analysis Software to offer unique method development, data processing, and reviewing tools in a modern, app-based software platform.

The partnership with Primoris helped Waters build an interface that enables users to focus on the data that needs attention most, including tailored rulesets and a unique summary dashboard. The waters_connect platform and its suite of applications also includes functionality that allows a regulated laboratory to simply configure and confidently demonstrate all the technical requirements for electronic records as prescribed by 21 CFR Part 11, Annex 11, and other regulatory agency guidance.

One of the key improvements was the MS Quan app's ability to reduce the time spent on quantitative data review by up to 50% with its unique Exception Focused Review (XFR) functionality. The app also enables companies like Primoris to process large sample batches faster with improved workflows that speed up and enhance method development. Laboratories can accelerate data processing and meet pressing project timelines by easily setting up methods through a user-friendly interface with simplified graphics. Libraries of methods, toolkits and other shared functions are accessible across users to facilitate transfer and reusability.

Speeding up access to results cannot come at a sacrifice to data integrity and laboratories like Primoris must always remain compliant with regulatory agencies. The waters_connect for quantitative analysis software was designed to help users confidently report results from accurate and reliable data using application-focused quantitative workflows with built-in traceability and data integrity. That helps Primoris and its customers meet regulatory requirements with a clear plan and a strategy for compliance.

" Whenever there's an issue, we must always show the data. That's why transparency is so important for us because we do a lot of quality checks. The new MS Quan app enables us to visualize the data better. As a result, we can answer questions from our internal quality review team, as well as from customers or regulatory agencies, like: can you show us the retention time? Can you show us the integration? Does that show what we need it to? Can you show us these specific results?"

MR. WENDEL D'HONDT
Primoris Belgium Team Leader

NEXT STEPS

With the waters_connect for Quantitative Analysis Software now available, Primoris Belgium plans to begin the process of integrating the software into its lab. With help from the Waters support team, the laboratory hopes to minimize the time needed to train team members. The leaders of the analysis team plan to take a methodical approach to the rollout process.

" Changing software is really a difficult thing to do when you need to keep up with your daily routine. We'll start small with maybe one or two instruments for small methods of 2-5 compounds. Then as our laboratory personnel become more comfortable using the waters_connect Software, we can roll it out to other machines. Our eventual goal is to replace all of the old software in the lab."

MS. JANNE DOMBRECHT
Primoris Belgium Lead of Analysis



The Primoris team's experience with the collaborative software development process has strengthened the company's confidence in the commitment of Waters to deliver.

The software's ability to generate high-quality data quickly and easily is one aspect that will make the platform easier to learn and to use. Primoris plans to continue working with Waters to provide training in the software's technical controls and show users how these might be leveraged in the laboratory.

Primoris sees the benefits already of working on a single vendor platform with single vendor software. Mr. D'Hondt describes how this enables training to be more seamless:

"Working with the software is easy, we only need to know one software to work on all the machines and it is easy for a new analyst to learn everything. It is also easy to switch between the machines, for example if one goes down, because the software is the same. This commonality will remain the same once the team learns the new software."

With regards to the large bottleneck on Primoris' main multi-residue LMS method, the team anticipates considerable time savings. They are impressed with Waters commitment to solving the delays in exporting data, and are confident this is addressed in the new MS Quan app. Mr. D'Hondt articulates the time savings that will be significant, removing the 30-minute bottlenecks from this method on a daily basis, as well as the impact on staff morale:

"The processing of data will go quicker: doing things faster, getting through more work as a result. If all our wasted time is expelled, we win so much time. With that time, we can do more work in one day, and we feel very productive."

The Primoris team believe the waters_connect for Quantitative Analysis Software offers business benefits to the company by removing tedious manual data reviews, as well as dramatically improving access to data.

These newfound efficiencies will help the company provide its customers with improved insights while also speeding up analysis time.

" We see a lot of improvements with waters_connect for Quantitative Analysis, things that we have needed before that are now possible with this new software. It could potentially improve our throughput. Our volume of work is one of the major challenges, so making things more efficient is very desirable. We can potentially eliminate some wasted time in our workflows, which will also free up time for our analysts to work on other projects. Plus, our team will be happier when they realize that waters_connect can help them become even more productive."

MR. WENDEL D'HONDT

Primoris Belgium Team Leader

Waters

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