

# Freedom to Focus on What Matters

## Agilent MassHunter WalkUp Software Brings Welcome Changes to University of Bath Analytical Lab

For Dr. Shaun Reeksting at the University of Bath, versatility is the name of the game. In his role as mass spectrometry instrument specialist at the **University's Material and Chemical Characterisation Facility (MC<sup>2</sup>)**, Dr. Reeksting is tasked with recommending routes of sample characterization to a user base that varies as widely in their analytical needs as they do in their skill and experience in MS analysis.

Faced with a daily array of samples from such fields as synthetic organic chemistry, chemical engineering, architecture, food science, materials science, proteomics, and more, Reeksting and his fellow MC<sup>2</sup> experts have often found themselves treating many samples on what amounts to a case-by-case basis – a challenging, labor-intensive approach.

"Up until a couple of years ago, it wasn't unusual for us to start out by trying five or six different methods, swapping out mobile phases and columns, in an effort to try and understand how to recommend the best way forward for a particular analysis," Reeksting says. "In the middle of this, we began to take a careful look at the services we offered, especially the time and effort required, and value provided. It was becoming clear that the system we had in place wasn't ticking all the boxes in terms of the stated remit of the facility and the needs and expectations of our user community."



Dr. Shaun Reeksting, PhD

Mass Spectrometry Instrument Specialist  
University of Bath

## Enter the Agilent 6545 LC/Q-TOF and WalkUp software

In an effort to bridge this gap, Reeksting and colleagues began auditioning solutions. "We evaluated hardware and software packages from different vendors and found the Agilent WalkUp software combined with Agilent 6545 LC/Q-TOF to be versatile, robust, and well-rounded platform for handling automated sample submissions from a multidisciplinary userbase" he says. "The submission software allowed us to accommodate various levels of user expertise, manage a large user database easily, and automate emailing of results to individual users. The combined versatility of the instrument and the comprehensive submission and processing software surpassed our expectations and ticked all the boxes for the range of applications we had".

From the start, MC<sup>2</sup> staff were quick to take advantage of the power and flexibility of WalkUp software. Methods were easily integrated and adapted by key technical staff, allowing multiple columns to be used (four column and mobile phase selection options) in combination with various mass spec analysis methods and appropriate postacquisition data processing routines (Qual, BioConfirm, or Quant) depending on the workflow chosen by the user.

Importantly, the user base has also embraced this new solution. "Since the user interface can be tailored to suit different user skill levels as well as different sample types, including adding sequence information for intact protein samples, our users have found the interface intuitive and easy to operate," Reeksting says. "For many of them, it seems to be a much less intimidating process now, less of a question mark. They have a clearer picture of what to expect; there's a renewed sense of being connected to the analysis and in control of the data."

## A solution that continues to grow

As the MC<sup>2</sup> has brought additional features of WalkUp software online, the value of the solution has continued to grow. "Additional features that we've found useful include the automated vial disposal facility and level of error reporting for when solvents levels were low," Reeksting explains. "The software platform also allows further future expansion of our services to include multiple acquisition instruments through the OpenLab Server."

"After 2 1/2 years and around 20k samples, we are still impressed with the features of WalkUp," says Reeksting. "Also, we continue to be surprised at the versatility of the hardware/software combination."

"We are also very satisfied with the level of support we received from Agilent," he continues. "The app support team is responsive and helpful, service engineers are knowledgeable, and the instrument hardware has proven to be resilient. The whole solution has surpassed our expectations."

## A fresh approach, a fresh outlook

From the beginning, Reeksting and his colleagues were confident WalkUp software would make their lives – and those of their users – easier. What they didn't expect was the extent to which the Agilent solution would free them up to expand their roles.

"Compared to before, my day has changed a lot more toward results and interpretation," he says. "I feel more involved, and overall, it's a lot more rewarding. Now, we're having in-depth result discussions with users and clients, really helping them look into what the data is telling them, rather than spending hours changing columns and trying to get samples to work. There's a strong sense that we're helping our users solve research questions in depth, where before there really was only time to skim the surface."

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