

Training the Next Generation of Mass Spectrometry Leaders

The Swansea University Medical School and Waters Corporation have partnered to strengthen student and professional training in mass spectrometry technology using the ACQUITY QDa Mass Detector

Technology: ACQUITY QDa Mass Detector

MASS SPECTROMETRY EDUCATION AT SWANSEA UNIVERSITY

Located in Wales, United Kingdom, the Swansea University Medical School is dedicated to educating and training the next generation of doctors, life scientists, health professionals, innovators, educators, researchers, and leaders. The school ranks first in the United Kingdom for its research environment and second for overall research quality, and it has established itself as a world-class place to learn, research, innovate, and collaborate.

Research is the cornerstone of the university's success, and faculty and staff members often collaborate with government and industry organizations in a joint effort to make a difference in the health and wellbeing of people around the world. Swansea University has long established itself as a center of excellence for mass spectrometry (MS), with the siting of the Royal Society Research Unit in 1975 followed by the Mass Spectrometry Research Unit and then the Engineering and Physical Sciences Research Council's (EPSRC) UK National Mass Spectrometry Service Center in 1987.

The National Mass Spectrometry Facility (NMSF, and the former EPSRC Service), which is located within Swansea University's Medical School, offers comprehensive MS facilities and services for leading university research groups throughout the UK, as well as commercial research opportunities. Across several laboratories, the University has more than 20 mass spectrometers, including 5 in R&D, 12 in the NMSF, and 3 in the Medical School and in the College of Engineering.



Inside the NMSF at Swansea University.

WORKING WITH WATERS

The relationship between Swansea University and Waters extends much further than this specific project with the ACQUITY™ QDa™ Mass Detector.

Waters is an affiliate of the Medical School, and has supported many of the university's research projects, both in monetary value and in-kind resources. The relationship has resulted in numerous joint projects, with the development and evaluation of technology that includes ionization sources and the ACQUITY QDa Mass Detector training module, in conjunction with Dr. Godfrey, being one of the more recent collaborations.

Dr. Godfrey explains: *"It's far more than just the instrument. Our relationship with Waters is an example of how to achieve all the right benefits from an industry collaboration. The university can access cutting-edge analytical technology, and Waters benefits from our findings and the potential impact on instrument development. There are a lot of synergies between our organizations."*

University students, faculty, and staff members work together with industry partners teaching method development; data analysis; databases and informatics; laboratory management such as quality assurance and quality control (QA-QC), Good Laboratory Practice (GLP), Good Manufacturing Practice (GMP) and safety; as well as applications in medical and life sciences (e.g. (nano)therapeutics); environmental analysis; chemistry; and forensic science.

In 2011 Swansea University established more formal MS training and education for its students – expanding research activity while at the same time nurturing new talent. This training included a greater emphasis on the background and fundamentals of MS, separation science, and sample handling and preparation skills.

“We realized that the graduate pool available for recruitment to our Ph.D. programs had a limited mass spec knowledge to really hit the ground running on research projects. We were also working with industry, including Waters, to determine MS training needs, both in terms of future graduates and current professionals. So, we identified the need to develop new training provision in MS.”

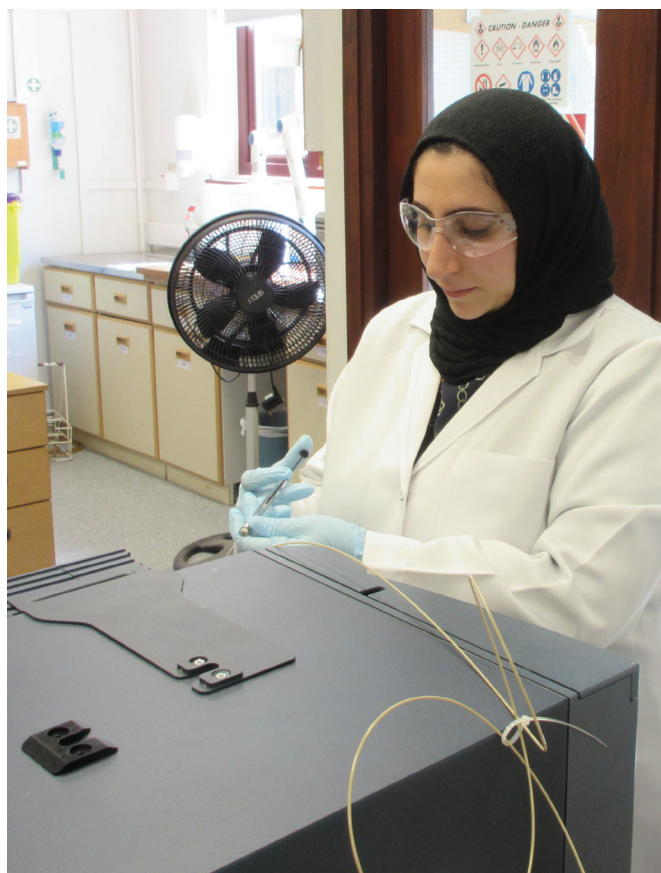
DR. RUTH GODFREY

Senior Lecturer at Swansea University
Medical School

As part of this process, Swansea University Medical School began collaborating with Waters to develop a practical training module for students to learn the fundamentals of MS using the ACQUITY QDa Mass Detector.

GROWING DEMAND FOR MASS SPECTROMETRY

MS is a technique that has become increasingly pervasive in both academic research and industry, providing qualitative and quantitative information across many different university departments. MS has historically required a great deal of scientific study and hands-on knowledge to perform correctly, so MS expertise was difficult to cultivate without lengthy and detailed training in the technique.



Waters technology being used in the NMSF at Swansea University.

At the same time, the demand for LC-MS analysis in industry has grown rapidly – about 10% annually.¹

Swansea University prides itself on its postgraduate and professional training courses in MS and separation sciences, which reflect the unique skills of the university as a center for mass spectrometry research, together with the NMSF. University leaders saw the need to expand its MS training for students to meet this growing demand as well as to ensure university coursework was based on the most recent developments in MS technology.

Dr. Godfrey explains: “MS is one of those subject areas where it’s expensive to purchase and maintain instrumentation, and to maintain the staff to look after and operate the instrumentation. We wanted to strengthen our masters and postgraduate training provision as a way of meeting that gap. The lack of trained graduates is essentially a problem for industry as well, and we wanted to take steps to make sure we had trained graduates to meet the need.”

Swansea University’s approach focused on educating its students about the science behind how MS instrumentation works, which they realized at the time wasn’t covered in sufficient depth.

"A student may run a sample, but they aren't seeing the target analyte. So, they may continue to increase the amount of sample into the mass spectrometer, inadvertently making it far dirtier and more insensitive. But perhaps the reason that they haven't seen the analyte in the first place is because they don't have the right sample preparation conditions, or perhaps they're running in positive mode when it needs to be running negative mode."

DR. RUTH GODFREY

*Senior Lecturer at Swansea University
Medical School*

To meet those challenges, Swansea University partnered with Waters to work with the ACQUITY QDa Mass Detector to develop learning and teaching resources to support students in gaining an understanding of theoretical and practical fundamentals of MS.

EDUCATIONAL USES OF THE ACQUITY QDa

The ACQUITY QDa Mass Detector was designed as a robust and reliable bench-top mass spectrometer that, amongst many other things, is ideal for teaching the fundamental principles of MS due to its ease of use.

Many academic laboratories still have perceived barriers associated with MS – including complexity, size, and affordability – that have prohibited researchers and students from realizing the benefits of mass data. This is not helped by those entering the world of mass spectrometry often coming from varied backgrounds without any experience of MS instrumentation. The ACQUITY QDa Mass Detector can reduce these barriers and meet the growing need to deliver mass data to new analysts and laboratories, who have limited (or no) MS experience but require the increased confidence in information and results that MS provides.

Dr. Godfrey explains: "In general in our laboratory we have the ethos, if you break it you fix it, if you dirty it you clean it. There is nothing more awkward than 'you have now used my instrument slot, and I cannot get back onto it for three days because someone has failed to return the instrument in working order'.

The high end, primarily research instrumentation, is only permitted to be used by the Masters students, who have to prove their lab competency and instrument training first. The ACQUITY QDa potentially bridges the gap to undergraduate study.

Generally, there is a lack of awareness of the instrumentation and what it takes to look after instrumentation. That is why we do not want to use the ACQUITY QDa to become totally a walk-up instrument for students. We do not want to make it too easy for them to lose the responsibility.

They only truly appreciate the costs once they have left us and become a project manager and start pricing up a project, realizing they could probably buy a house for the price of an instrument! Now, with the ACQUITY QDa educational package, they are more aware of the instrumentation and how to operate it."

The mobility of the ACQUITY QDa means it can easily be relocated as experimental requirements demand. This flexibility allowed it to be used for Outreach and STEM activities, including offerings at the British and Swansea Science Festivals and an event at the University of Birmingham. These activities have reached thousands of members of the public and are important in inspiring the next generation of analytical scientists.

Learning MS fundamentals

Swansea University partnered with Waters to use the ACQUITY QDa Mass Detector to introduce students to the principles of MS and mass spectral interpretation.



A researcher operating the ACQUITY QDa Mass Detector in the laboratory.



A student undertaking research in the NMSF at Swansea University.

The goal was to enable students to gain practical hands-on experience exploring MS fundamentals such as mass-to-charge ratio, monoisotopic versus average mass, isotopic patterns, formation of adducts, multiple-charging, fragmentation, and more.

Mr. Rhodri Owen, experimental officer in the Swansea University Medical School, describes the initial thought process: *“Waters already had some ideas about developing education classes, and they were doing initial investigations of the ACQUITY QDa’s ability to operate as a standalone mass spectrometer. They found that it was a possibility, and they were quite interested in developing the educational package to go with it.”*

Providing hands-on experience

Waters provided Swansea University with access to an ACQUITY QDa Mass Detector, enabling faculty and students to get hands-on experience with this cutting-edge mass detection technology. Initially, Mr. Owen and his team worked with the instrument by testing different compounds to see which ones were effective, generating good data, and showcasing the range of different ionization modes and different techniques for the ACQUITY QDa, as well as demonstrating the fundamentals of MS.

Dr. Godfrey explains: *“We evaluate technologies and develop methods for industry. We provide them with the opportunity to work with our graduate students on projects that can identify suitable applications for their instrumentation or maybe the instrument will form the basis of postgraduate project. If something comes out of that research, such as intellectual property or other in-kind benefits, we share that with the vendor. That’s part of what we do in terms of open innovation.”*

Developing a training module

At the same time, Swansea University researchers used the ACQUITY QDa Mass Detector to put together a training module to support students in gaining a practical understanding of MS fundamentals – including the instrumentation and its component parts, instrument operation, acquisition, spectral interpretation, and the generation of characteristic mass data as the basis of modern compound identification.

The training module included experiments designed to be either standalone or to incrementally build a student’s knowledge and experience about MS, such as the basic operation of the ACQUITY QDa, generation and interpretation of spectra using MassLynx™, and the interpretation of isotope patterns, polarity switching, analysis of simple mixtures, polymers, and fragmentation analysis.

“We put together a theoretical chapter just to give everybody a background of how MS works. Then we developed a series of individual experiments showcasing different aspects of how to generate the basic mass spectra through to interpretation of more complex mixtures and biomolecules. Each of the experiments were designed to be either standalone, or you could go through the full experiment and incrementally build your knowledge depending on your experience.”

MR. RHODRI OWEN

*Experimental Officer at Swansea University
Medical School*

Swansea University found several benefits of the ACQUITY QDa Mass Detector for teaching this series of practical experiments in MS.

BENEFITS OF THE ACQUITY QDA MASS DETECTOR

Perhaps the biggest benefit of the ACQUITY QDa Mass Detector in an educational setting is its ease of use, which makes it the ideal instrument for learning MS fundamentals. Swansea University researchers found the instrument enabled students with little MS experience to obtain useful mass information, which was helpful for the initial learning process.

Additionally, university students develop other transferable skills such as problem solving, laboratory skills, numerical and mathematical skills, data analysis, and effective communication – all of which are applicable in both educational and industry environments.

“Our goal was to enable the students to perform the tasks using the ACQUITY QDa without too much assistance. I was pleased that the students didn’t have many issues. The instrument was still in good working order afterwards, and it didn’t require cleaning. The students didn’t have problems in applying the protocols, and they had an opportunity for more hands-on experience. It was popular with the students, and they were very satisfied.”

DR. RUTH GODFREY

Senior Lecturer at Swansea University
Medical School

Student feedback: “Practical exercises such as this make it easier to visualize and understand mass spectrometry theory.”

Students were able to use the ACQUITY QDa Mass Detector training module to develop an understanding of theoretical and practical fundamentals of MS, including:

- Instrumentation: inlet, ion source, ionization techniques, mass analyzer, ion detection, and data acquisition.
- Instrument operation: sample introduction, data acquisition, polarity switching (positive and negative modes), full scan versus selected ion monitoring, and continuum versus centroid data.
- Interpretation of mass spectra: m/z , monoisotopic mass versus average mass, isotope patterns, adducts, fragmentation, multiple charges, and the nitrogen rule.

After a solid introduction to MS with the ACQUITY QDa Mass Detector, Dr. Godfrey believes students can continue to expand on this knowledge using other MS instruments with different capabilities.

Swansea University plans to continue to develop training to help students apply what they’ve learned to more complex MS instrumentation, such as tandem quadrupole (triple quadrupole), quadrupole time-of-flight and ion mobility mass spectrometers.

NEXT STEPS

Swansea University and Waters have successfully completed the first phase of their partnership with the development of the ACQUITY QDa Mass Detector training module. Additionally, Dr. Godfrey and her team have future plans for developing a continuing professional development (CPD) module as well as recognition by the Royal Society of Chemistry (RSC), the UK’s professional association for advancing the chemical sciences.

Dr. Godfrey explains: “We have quite a unique selection of training provisions here at Swansea. While our initial agreement with Waters was for education purposes, we see an opportunity to develop additional training packages. For example, this ACQUITY QDa training module would become a commercial module that would be part of the university’s CPD portfolio.”

As a result, the training module would be available to industry professionals who are new to MS technology or who require short training programs on specific types of instrumentation. Additionally, Swansea University researchers see an opportunity to develop training add-ons for Waters to use with other customers after instrument purchases.



The research team in the NMSF at Swansea University.



"The beauty of the Waters ACQUITY QDa Mass Detector is that it's very easy to use and is very low maintenance. It automatically calibrates itself once a year. The consumable parts are plugged in and plugged out, and if they get dirty or damaged, you can easily swap them out. It is ideal for somebody who's just learning about MS."

MR. RHODRI OWEN

*Experimental Officer at Swansea University
Medical School*

In the long term, Dr. Godfrey sees even more opportunities to use the ACQUITY QDa Mass Detector in future university research and development projects: *"Because of my focus on R&D, I'm very interested in evaluating the ACQUITY QDa Mass Detector for other applications within chemistry. I certainly see the scope to expand how we're using the instrument. Many academics could see a dedicated system for teaching as a luxury, but if they were able to combine the system for research and teaching, that is more appealing."*

References

1. *Scientific Digital Imaging report*, 2018
<https://scientificdigitalimaging.com/wp-content/uploads/2018/12/SDI-Interim-Report-2018.pdf>

Waters

THE SCIENCE OF WHAT'S POSSIBLE.™

Waters, The Science of What's Possible, ACQUITY, QDa, and MassLynx are trademarks of Waters Corporation. All other trademarks are the property of their respective owners.

Waters Corporation
34 Maple Street
Milford, MA 01757 U.S.A.
T: 1 508 478 2000
F: 1 508 872 1990
www.waters.com