West Virginia Purchasing Division

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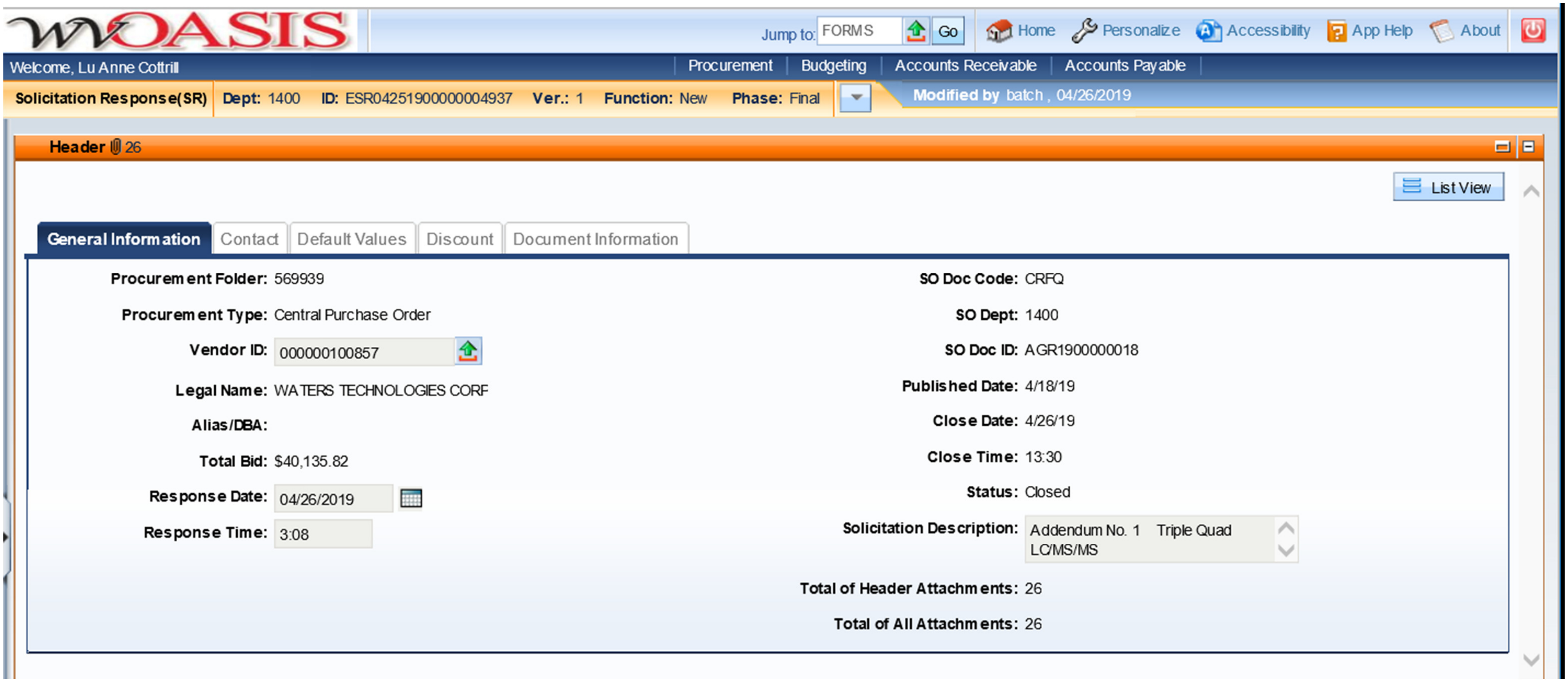
The following documentation is an electronically-submitted vendor response to an advertised solicitation from the *West Virginia Purchasing Bulletin* within the Vendor Self-Service portal at *wvOASIS.gov*. As part of the State of West Virginia's procurement process, and to maintain the transparency of the bid-opening process, this documentation submitted online is publicly posted by the West Virginia Purchasing Division at *WVPurchasing.gov* with any other vendor responses to this solicitation submitted to the Purchasing Division in hard copy format.



Welcome, Lu Anne Cottrill

Solicitation Response(SR) **Dept:** 1400 **ID:** ESR04251900000004937 **Ver.:** 1 **Function:** New **Phase:** Final

Modified by batch , 04/26/2019

Header 26

Procurement Folder: 569939

Procurement Type: Central Purchase Order

Vendor ID: 000000100857

Legal Name: WATERS TECHNOLOGIES CORP

Alias/DBA:

Total Bid: $40,135.82

Response Date: 04/26/2019

Response Time: 3:08

SO Doc Code: CRFQ

SO Dept: 1400

SO Doc ID: AGR1900000018

Published Date: 4/18/19

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Close Time: 13:30

Status: Closed

Solicitation Description: Addendum No. 1 Triple Quad LC/MS/MS

Total of Header Attachments: 26

Total of All Attachments: 26

Purchasing Division
2019 Washington Street East
Post Office Box 50130
Charleston, WV 25305-0130

State of West Virginia
Solicitation Response

Proc Folder : 569939
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Date issued	Solicitation Closes	Solicitation Response	Version
	2019-04-26 13:30:00	SR 1400 ESR04251900000004937	1

VENDOR

000000100857

WATERS TECHNOLOGIES CORP

Solicitation Number: CRFQ 1400 AGR1900000018

Total Bid : $40,135.82 **Response Date:** 2019-04-26 **Response Time:** 03:08:42

Comments:

FOR INFORMATION CONTACT THE BUYER
Melissa Pettrey
(304) 558-0094
melissa.k.pettrey@wv.gov

Signature on File **FEIN #** **DATE**

All offers subject to all terms and conditions contained in this solicitation

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Ln Total Or Contract Amount
1	LC/MS/MS, Workstation PC, Software, Printer, nitrogen	1.00000	EA	$10,200.000000	$10,200.00

Comm Code	Manufacturer	Specification	Model #
41100000			

Extended Description :	generator, uninterrupted power supply, specific test methods per section 3.1

Comments: Please see the price sheet, it appears online is missing some line items for the instrument.

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Ln Total Or Contract Amount
2	shipping charges & inside delivery	1.00000	EA	$2,649.190000	$2,649.19

Comm Code	Manufacturer	Specification	Model #
78121603			

Extended Description :	Shipping charges & inside delivery per section 3.1.6

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Ln Total Or Contract Amount
3	Installation/validation	1.00000	EA	$0.000000	$0.00

Comm Code	Manufacturer	Specification	Model #
73171605			

Extended Description :	Installation/Validation per section 3.1.6

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Ln Total Or Contract Amount
4	Training/warranty	1.00000	EA	$0.000000	$0.00

Comm Code	Manufacturer	Specification	Model #
73171605			

Extended Description :	Training/Warranty per section 3.1.6

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Ln Total Or Contract Amount
5	Service	1.00000	EA	$27,286.630000	$27,286.63

Comm Code	Manufacturer	Specification	Model #
73171605			

Extended Description : Service per section 3.1.6

Building Laboratory Capacity to Ensure Cannabis Safety, Quality, and Efficacy

Waters ACQUITY UPLC-MS/MS and Xevo TQ-S micro systems improve pesticide detection for ProVerde Laboratories, helping scientists ensure consumer safety for medical marijuana products

Technology: Waters ACQUITY UPLC, ACQUITY UPC^2, and Xevo TQ-S micro MS/MS systems

ESTABLISHING TESTING STANDARDS AT PROVERDE LABORATORIES

In 2013, Massachusetts legalized the use of medical marijuana (MMJ), creating a new marketplace in the state. ProVerde Laboratories, Inc. was launched the same year to meet the corresponding need for MMJ testing services, serving as one of the state's first ISO 17025 accredited, full-service analytical testing laboratories specializing in the cannabis and hemp industries.

From its onset, ProVerde was committed to using the latest scientific technologies to yield the most reliable analytical results, while maintaining an environmentally friendly, green approach. Headquartered in Milford, Massachusetts, the company's mission focuses on building lasting relationships with its customers and communities by providing services with reliability, quality, and integrity.

Cutting-edge analytical technology is the core of ProVerde's service offerings. These techniques include liquid chromatography (LC), gas chromatography (GC), and supercritical fluid chromatography (SFC) for method development, batch release testing, research, and consulting services.

These chromatography techniques are coupled with mass spectrometry (MS) detection to achieve the highest possible sensitivity for applications in pharmaceutical, food, materials science, petroleum, and clinical research. Other capabilities include analysis of elemental compositions using inductively coupled plasma mass spectrometry (ICP-MS) as well as screening for microbiological contaminants and pathogens.

ProVerde is the first ISO 17025 accredited lab in Massachusetts.

WORKING WITH WATERS

ProVerde's founders had a long working relationship with Waters, specifically in pharmaceutical and academic research. The opportunity to build a laboratory from the ground up enabled ProVerde to invest in the highest quality Waters instrumentation available – including ACQUITY™ UPLC™ with Xevo™ TQ-S micro tandem quad MS for pesticide analysis, UPLC, and UPC$^{2™}$ for cannabinoid analysis.

ProVerde Laboratories.

Dr. Hudalla credits his company's relationship with Waters as a key part of its business strategy: *"Part of our success is the vendors we choose for instrumentation. That's a major foundational component of what we're able to achieve from a quality perspective."*

The use of these advanced techniques for pesticide detection was relatively new for the cannabis industry. ProVerde positioned itself early on as a bridge between cutting-edge analytical techniques and the needs of the emerging MMJ marketplace, relying on its founders' expertise in the pharmaceutical industry.

> "We didn't set it up like a traditional cannabis lab. We knew what a pharmaceutical lab looked like, and we knew what a university research lab looked like. That's how we built out our laboratory from the start."
>
> DR. CHRISTOPHER HUDALLA
> *ProVerde Co-founder and CSO*

ProVerde currently serves clients in 36 different countries and 40 different states, providing a range of services that include:

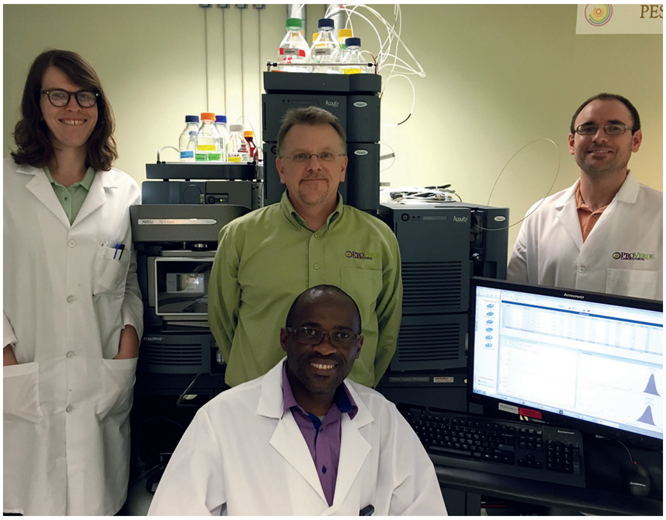
- Cannabinoid analysis
- Pesticide analysis
- Heavy metal and elemental analysis
- Terpene/residual solvent/VOC analysis
- Mycotoxin analysis
- Microbiological analysis
- Genetic sex determination

As MMJ legalization has grown, the company has several expansion projects underway, including a laboratory in Lesotho, Africa, in partnership with the country's government officials, and one in Portland, Maine. It is also looking to further expand its footprint in North America by adding labs in California, Colorado, South Carolina, and Oklahoma. There are further plans to add a lab in Canada.

ProVerde's relationship with Waters has proven to be a key element of the company's growth and success as it navigates the emerging MMJ industry.

EMERGING MARKETPLACE FOR MMJ PRODUCTS

When the state of Massachusetts legalized MMJ in 2013, ProVerde executives found themselves at the starting point of a new – and uncharted – marketplace. As public perception and legislation regarding MMJ evolved, ProVerde saw an opportunity to use its founders' expertise in laboratory research and cutting-edge analytical instrumentation to fill the growing need for certified MMJ testing laboratories.



Scientists in the laboratory at ProVerde.

MMJ is a nascent industry with constantly shifting regulations, which differ from state to state as well as from country to country. Governments are constantly writing and rewriting legislation regarding MMJ use, which challenges product testing laboratories to meet these changes as they occur.

The Massachusetts Department of Health was responsible for the state's laboratory guidelines, which mandated MMJ dispensaries develop a chemical profile of their products and test them for mold, mildew, and heavy metals as well as pesticides and residual solvents. ProVerde was active in the process from the beginning, even lobbying the agency to put many of these testing requirements in place.

The ProVerde founders knew credibility was key to establishing a successful product testing facility in any industry, and they focused on building trustworthiness from the beginning. The company established its reputation for high-quality MMJ testing services by investing heavily in skilled personnel with strong scientific backgrounds and the latest analytical instrumentation.

One major objective stood out above all others, however. As ProVerde navigated this new marketplace, the company's founders determined their top concern should be product safety and quality control above everything else.

The emphasis on consumer safety began in the company's very early days. As the state of Massachusetts hashed out the legislative details, Dr. Hudalla and the ProVerde team began conducting research to better understand the needs of the MMJ marketplace. One of those research projects was working with a mother who had a 13 month-old daughter with epilepsy.

Dr. Hudalla describes the experience: *"We worked closely with the mother to understand the production of the medicine. She had to produce it herself. We often have to source the product, and we were finding product that was heavily contaminated as we frequently do. These are cumulative toxins, and they are going to have a significant detrimental effect on a 13 month-old child. We were able to intercept it, so the contaminated product wasn't used for the creation of her daughter's medication."*

The experience put a face to the services the company was providing, something that differs significantly from most laboratories in that are conducting pharmaceutical-related research. The ProVerde team became very aware that they held a unique position to ensure consumer safety in the MMJ market.

Dr. Hudalla explains: *"I don't know who's consuming these products. So, I must assume the end user of this product is an infant or someone who has a compromised immune system – someone who may be on chemo who cannot tolerate the toxins that we might find in these products. That lends importance to what we do."*

As a result, today ProVerde executives see the company's role as more than simply a service provider. Dr. Hudalla views his company's services as a way to protect clients from liability by preventing contaminated products from getting into the marketplace. Additionally, the company offers its clients the ability to fix problems by identifying the source of contamination, determining how to remediate it, and ensuring the final product is safe.

Dr. Hudalla describes the company's viewpoint: *"We're on the frontline and see the impact of our work. It's about consumer safety. Our primary goal is making sure that consumers aren't put at risk."*

To do that, ProVerde turned to Waters to ensure it had the best instrumentation available to accomplish its goals.

Dr. Christopher Hudalla. ProVerde co-founder and CSO.

CUTTING-EDGE ANALYTICAL INSTRUMENTATION FOR CANNABINOIDS AND PESTICIDE TESTING

ProVerde scientists needed to detect and quantify pesticides down to the lowest possible levels, and in the presence of interferences from complex matrices. Large variations in the concentrations of different pesticides further added to this challenge.

Working closely with Waters, ProVerde scientists explored the use of multiple techniques to achieve the most reliable analytical results possible, while maintaining the company's goal for an environmentally friendly, green approach.

UltraPerformance Liquid Chromatography (UPLC)

From the beginning, ProVerde focused on UltraPerformance LC™ (UPLC) – one of the best techniques for cannabis analysis because of its ability to rapidly quantitate individual cannabinoids. Waters UPLC instrumentation offers the capability to analyze more samples, faster, and with better results.

UPLC is a Waters innovation with re-engineered LC particle technology, column design, injectors, pumps, and detectors. The increased performance of sub-2-μm hybrid columns, used in conjunction with Waters ACQUITY UPLC systems delivers mobile phase at high pressures with low dispersion, preserves the chromatographic benefits of such small-particle chemistries – producing sharper and more concentrated peaks.

> "UPLC is a higher-pressure method that is the same as HPLC, but faster and more efficient. It reduced our sample analysis time from 8–9 min to about 3.5 min per sample. That dramatically increased our throughput."
>
> DR. CHRISTOPHER HUDALLA
> *ProVerde Co-founder and CSO*

ProVerde scientists also found the ACQUITY UPLC System reduced solvent use without compromising analytical results. That benefit served ProVerde's goal to make as little impact to the environment as possible by minimizing the company's carbon footprint.

> "At ProVerde, we think green, and this applies to our technical methodology as well. Our goal is to ensure the most accurate results using the greenest technology – generating less hazardous waste and consuming less energy. When we use UPLC, we generate 60% less hazardous waste per test. Disposal of waste is a significant cost for us. By cutting the cost of disposal in half, it cuts the cost of analysis. It's a huge cost saving. Plus, UPLC gives us higher throughput, so we can also increase revenue that way."
>
> DR. CHRISTOPHER HUDALLA
> *ProVerde Co-founder and CSO*

Originally, ProVerde started with one Waters UPLC-MS/MS system in its Massachusetts lab for pesticide analysis and one UPLC-UV for cannabinoid analysis, but the company ended up purchasing three more UPLC-MS/MS systems to keep up with the demand. Today those instruments are churning out data 24/7.

The UPLC instrumentation also helps ProVerde maintain a strong quality control system in this fast-paced environment by enabling the company to perform continuous calibration examinations.

> "Waters has been very supportive in helping us optimize our processing methods. When we started, we would identify peaks by their retention time. Now we identify peaks by retention time and their UV spectral absorbance across that peak. We compare that to a library reference."
>
> DR. CHRISTOPHER HUDALLA
> *ProVerde Co-founder and CSO*

Pesticide detection for medical marijuana products.

Dr. Hudalla explains the value of that capability: *"Every 20th sample is a QC sample that is designed to determine if the system is performing as it should. I can document that the system is accurately quantitating my cannabinoids, and I'm able to do that in a high-throughput fashion. It's essential for my business."*

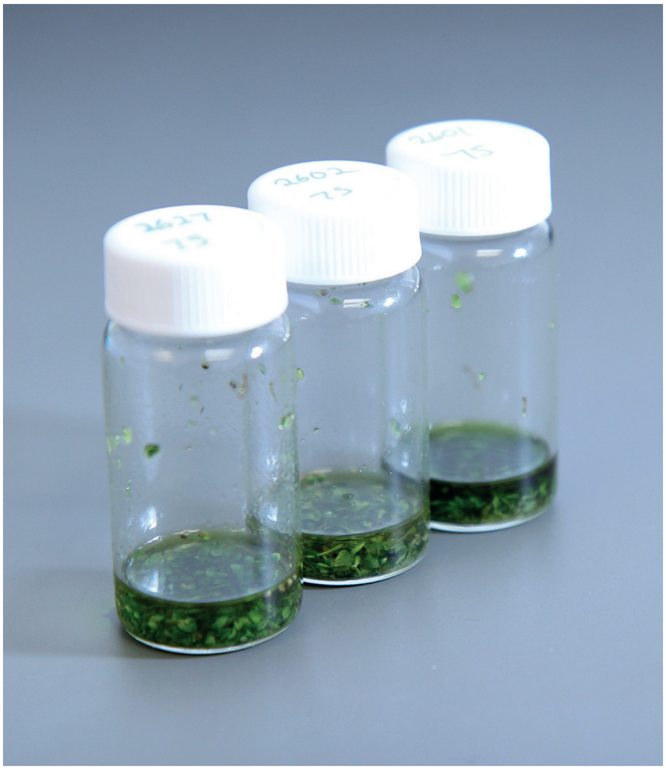
Dr. Hudalla continues to say: *"I'll frequently see products as being marketed as THC-free. Someone is making a cannabidiol (CBD)-based product, and they're advertising as no tetrahydrocannabinol (THC) in their product. Yet when I test it, I see a THC peak. Not just a peak, because that could just be matrix effect, but the UV absorbance spectrum for that peak matches THC. It has the exact match of weight and absorbance of THC, and it's enough information to give me confidence that I could defend it in a court of law, if necessary."*

UltraPerformance Convergence Chromatography

ProVerde also performs cannabinoid analysis and potency profiling using the UltraPerformance Convergence Chromatography™ System (UPC^2) from Waters, using CO_2 as the primary mobile phase component.

The ACQUITY UPC^2 System provides orthogonal selectivity to UPLC since polar metabolites elute later than the parent drug. Coupling UPC^2 with electrospray ionization and MS analysis can be a powerful and complementary technology in cannabis applications.

Waters' ACQUITY UPC^2 Technology represents one of the fastest, most reliable, and robust technologies available for chromatographic testing. At the same time, UPC^2 enables a dramatic reduction in the use of organic solvents, minimizing the amount of hazardous waste generated, making it one of the most environmentally friendly testing methodologies available and thus maintaining ProVerde's commitment to 'green'.



ProVerde specializes in medical marijuana testing.

While UPC^2 is a relatively new addition to MMJ testing methodology, it's a good match for cannabis analysis because of the large number of cannabinoids found in samples, which typically fall between 80–100. Waters UPC^2 Technology can separate and quantify all the major cannabinoid compounds, providing a more detailed, accurate profile of a marijuana extract.

This information allows dispensaries to issue proper doses and recommend the right cannabis strain for customers. For example, CBD is a component of marijuana that has been shown to help reduce seizures in children with epilepsy. But dispensaries want to ensure these products do not have THC, the psychoactive ingredient found in cannabis.

Dr. Hudalla explains: *"Children respond exceptionally well to high amounts of CBD, but you don't want to give them too much THC. You don't want to have your kid inebriated."*

Mass spectrometry

ProVerde uses UPLC with tandem mass spectrometry (UPLC-MS/MS) to screen for and quantitate pesticides – helping to ensure that compounds used during cultivation do not make their way into final consumer products. ProVerde develops matrix-specific pesticide preparation steps before analyzing products on Waters UPLC-MS/MS instrumentation.

The Xevo TQ-S micro Mass Spectrometer offered ProVerde a significant increase in sensitivity with no reduction in selectivity. Meaningful information was obtained for a greater number of components across a larger population of samples, giving a more complete picture for improved understanding and more confidence in results – two important benefits for the company.

That data also helps Dr. Hudalla and his team when accuracy is vital, such as verifying product marketing and packaging information.

Triple quad for pesticide testing

The variety of matrices for MMJ products is a significant challenge for ProVerde scientists. Again, the company's relationship with Waters proved fruitful when they discovered new analytical techniques could help address these issues – this time with UPLC coupled with the Xevo TQ-S mass spectrometry for pesticide testing, to ensure products are safe.

When analyzing MMJ samples, it can be difficult to separate pesticides in certain instances when they are eluting with cannabis resin components (such as THC) that are present in very high levels and cannot be separated by any reasonable cleanup.

> "Being able to use different approaches gives us increased confidence in the results. If we have a potential matrix effect, we can turn to complementary analytical technology to get the information we need."
>
> DR. CHRISTOPHER HUDALLA
> *ProVerde Co-founder and CSO*

ProVerde found UPLC worked well for detecting contaminants in MMJ samples when coupled with the Xevo TQ-S micro Mass Spectrometer. The company's scientists found the increased sensitivity of the Xevo TQ-S micro instrument enabled them to quantify and confirm trace components at lower levels in the most complex samples.

ADVANCING MMJ TESTING CAPABILITIES

MMJ is a new and emerging market in both the United States and throughout the world, and ProVerde sees a future that taps into the power of cutting-edge analytical technology and scientific expertise to ensure product quality and safety – just like in related industries such as pharmaceuticals, food, beverages, and dietary supplements.

As the MMJ market evolves, ProVerde and Waters plan to continue to work together to ensure consumer safety, in addition to meeting the growing need for regulatory compliance testing services. ProVerde's investment in the most advanced Waters analytical instrumentation is a key component of the company's long-term strategy to build trustworthiness and credibility in this emerging industry.

Dr. Hudalla summarizes the importance of the relationship between ProVerde and Waters to his company's approach:

> "Instrumentation is the most critical component of our business. Waters equipment is a foundational portion of our testing platform."
>
> DR. CHRISTOPHER HUDALLA
> *ProVerde Co-founder and CSO*

Waters
THE SCIENCE OF WHAT'S POSSIBLE.™

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

ACQUITY UPLC I-Class PLUS System (SM-FTN-I)

The Waters™ ACQUITY™ UPLC™ I-Class PLUS System's holistic design is targeted for investigative analysis where maximized peak capacity, throughput, and sensitivity are critical and is perfectly suited for running any MS-based applications. The system is comprised of a Binary Solvent Manager (BSM) and a Sample Manager with Flow-Through Needle (SM-FTN-I); this configuration offers excellent carryover performance.

ACQUITY UPLC I-CLASS PLUS SYSTEM FEATURES (WITH SM-FTN-I)

Total system bandspread,† 5σ	≤9 µL (default configuration)
Dwell volume (total system)†	≤100 µL (default configuration)
Gradient delay volume†	≤80 µL
Integrated leak management	Leak sensors, as standard, and safe leak handling
System synchronization	Injection synchronization between both pumps and the sample manager enhances retention time reproducibility
Operating flow rate range	0.001 to 2.000 mL/min, in 0.001 mL increments (firmware version 1.71 and later)
Maximum operating pressure	18,000 psi up to 1 mL/min, 12,000 psi up to 2 mL/min
pH range†	1 to 12.5
Unattended operation	Leak sensors, full 96-hour diagnostic data display through console software
Cycle time	≤15 s inject to inject, with load ahead enabled

BINARY SOLVENT MANAGER (BSM)

Number of solvents	Up to four, in combination of two, A1 or A2 and B1 or B2
Solvent conditioning	Integrated vacuum degassing, six lines with two allocated for the injector needlewash/purge solvents
Gradient formation	High pressure mixing, binary gradient
Gradient profiles	11 gradient curves (including linear, step [2], concave [4], and convex [4])
Primary check valves	Intelligent Intake Valves (i^2Valve)
Flow accuracy†	±1.0% of set flow rate at 0.500 mL/min, as per SystemsQT™
Flow precision†	≤0.075% RSD or 0.01 min SD, (0.2 to 2.0 mL/min), whichever is greater using premixed solvent
Composition ripple†	≤1.0 mAu
Composition precision†	≤0.15% RSD or ±0.01 min SD, whichever is greater
Composition accuracy†	±0.5% absolute from 5% to 95%, 0.2 to 2.0 mL/min

Pressure pulsation†	≤0.4% or 25 psi, whichever is greater
Compressibility compensation	Automatic, no user intervention required
Priming	Wet priming runs at a flow rate of 4 mL/min
Pump seal wash	Equipped with a programmable active wash system to flush the rear of the high pressure seals and the plungers
Flow ramping	Automatic
Primary wetted materials	316L stainless steel, UHMWPE blend, MP35N, titanium alloy, gold, sapphire, ruby, zirconia, Nitronic 60, DLC, fluoropolymer, PEEK, PEEK blend
Mixing options	Standard: 50 µL Optional: 100 µL and 380 µL

SAMPLE MANAGER-FTN (SM-FTN-I)

Injection volume range	0.1 to 10.0 µL as standard configuration Up to 1000.0 µL with optional extension loop
Accuracy	±0.2 µL, measured by fluid weight removed from vial with 10.0 µL injections averaged over 20 injections using standard 100-µL syringe
Precision†	≤0.25%, 5 to 50µl
Linearity†	≥0.999
Maximum sample capacity	Any two of the following: ▪ 96 and 384 microtiter plates ▪ 48 position 2.00-mL vial plates ▪ 48 position 0.65-mL micro-centrifuge tube plates ▪ 24 position 1.50-mL micro-centrifuge tube plates
Sample compartment temperature range	4.0 to 40.0 °C, settable in 0.1 °C increments; maintains 19 °C below ambient with a tolerance range between -2 and +4 °C
Temperature accuracy	±0.5 °C at sensor
Temperature stability	±1.0 °C at sensor
Sample manager heat time	≤30 min ambient-40 °C
Sample manager cool time	≤60 min ambient-4 °C
Injection needle wash	Integrated, active, programmable
Minimum sample required	3 µL residual, using Waters' Total Recovery 2-mL Vials (zero offset)
Sample carryover†	≤0.001% caffeine (UV) ≤0.001% sulphadimethoxine (MS)
Advanced sample manager capabilities	Auto-dilution and auto-addition
Primary wetted materials	316L stainless steel, polyimide, PEEK blend, DLC, PPS

COLUMN HEATERS (CH-A)

Column capacity	CH-A: Single column, up to 4.6 mm internal diameter (I.D.), up to 150 mm in length with filter or guard column. Mounting extends out for use with MS-based detector
Fittings	18,000 psi, low dispersion, with reusable column inlet fittings
Column compartment temperature range	Settable from 20.0 to 90.0 °C, settable in 0.1 °C increments
Column compartment temperature accuracy	±0.5 °C at sensor
Column compartment temperature stability	±0.3 °C at sensor
Column compartment heat time	≤15 min ambient-60 °C
Solvent conditioning	Active pre-heating as standard; passive pre-heating (for legacy method support)
Column tracking	eCord™ Technology column information management tracks and archives column usage history

COLUMN MANAGEMENT (CM-A)

Column capacity	CM-A: Two columns, as standard (maximum length of 150 mm with filter or guard column) up to 4.6 mm internal diameter (I.D.)
Switching valves	Two nine-port, eight-position valves (CM-A only); provides programmable access switching, waste and bypass positions for rapid solvent changeover
Column compartment(s) temperature range	4.0 to 90.0 °C, settable in 0.1 °C increments; two independent heat/cool zones
Column compartment(s) temperature accuracy	±0.5 °C at sensor
Column compartment(s) temperature stability	±0.3 °C at sensor
Column compartment heat time	≤15 min ambient-60 °C
Column compartment cool time	≤15 min 60–20 °C
Solvent conditioning	Active pre-heating as standard; passive pre-heating (for legacy method support)
Fittings	18,000 psi, low dispersion, with reusable column inlet fittings
Column tracking	eCord Technology column information management tracks and archives column usage history
2D support	Optional

SAMPLE ORGANIZER

Sample plate capacity	Sample plate capacity is configured based on the types and combinations of plates being used: ▪ Maximum of 19 standard microtiter plates, up to 15.5 mm high, or ▪ Maximum of 9 intermediate height plates (or 2-mL vial holders), up to 40.0 mm high, or ▪ Maximum of 6 deep well plates (or 4-mL vial holders), up to 47.0 mm high
Maximum sample capacity	Maximum of 7296 samples in nineteen 384-well plates
Sample compartment temperature range	4.0 to 40.0 °C, settable in 0.1 °C increments with a tolerance range between -2 and +4 °C
Temperature accuracy	±1 °C at the sensor
Temperature stability	±1 °C at the sensor

BASED INSTRUMENTAL CONTROL

External control	Empower™ Software, MassLynx™ Software, UNIFI™ Scientific Information System, or standalone through console software
External communications	Ethernet interfacing via RJ45 connection to host PC
Event inputs/outputs	Rear panel contact closure and/or TTL inputs/outputs
Connections INSIGHT™	Provides real-time monitoring and automatic notification of instrument performance and diagnostic information, allowing for quicker problem resolution

ENVIRONMENTAL SPECIFICATIONS

Acoustic noise	≤62 dBA, system
Humidity operating	20% to 80%, non-condensing
Operating temperature range	4 to 40 °C

ELECTRICAL SPECIFICATIONS

Power requirements	100 to 240 VAC
Line frequency	50 to 60 Hz
Power consumption	BSM: 360 VAC FTN: 400 VAC CM-A: 400 VAC

PHYSICAL SPECIFICATIONS

ACQUITY UPLC I-Class PLUS System: BSM, SM-FTN-I, and CH-A	Width: Height: Depth:	34.3 cm (13.5 in.) 71.1 cm (28.0 in.) 71.2 cm (28.0 in.)
ACQUITY UPLC I-Class PLUS System: BSM, SM-FTN-I, and CM-A	Width: Height: Depth:	34.3 cm (13.5 in.) 79.6 cm (31.4 in.) 71.2 cm (28.0 in.)
Sample Organizer	Width: Height: Depth:	25.4 cm (10.0 in.) 96.5 cm (38.0 in.) 71.1 cm (28.0 in.)

[†] For specific test conditions, contact your Waters sales representative.

Waters

THE SCIENCE OF WHAT'S POSSIBLE.™

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ACQUITY UPLC
I-Class PLUS

WHAT SEPARATES YOU FROM EVERYONE ELSE

Waters
THE SCIENCE OF WHAT'S POSSIBLE.™

COMPLEX CHALLENGES SOLVED

Looking for answers to the most complex scientific challenges is what you do. Your research could lead to ground-breaking medicines, cleaner drinking water, or safer food. The scientific tools you deploy, and the information it provides, can make all the difference.

With industry-leading separations performance, the ACQUITY™ UPLC™ I-Class PLUS System provides new possibilities of maximizing the resolution and sensitivity of your methods; enhancing the characterization of your samples, while improving productivity to advance the science of your laboratory.

AMPLIFY YOUR RESEARCH

- Highly efficient, rapid separations are facilitated by industry-leading ultra-low dispersion and delay volume.
- Ultra-efficient, narrow peaks enhance the sensitivity of any mass spectrometer to simplify the characterization of the most complex samples.

www.waters.com/iclassplus

Acquity UPLC® I-Class PLUS

LOW DISPERSION FOR ULTRA PERFORMANCE

Wide range of detection capabilities

UPLC-optimized detectors to match your application needs, including photodiode array, UV/Vis, fluorescence, refractive index, evaporative light scattering, and mass spectrometry.

Versatile column management

Support for analytical LC column dimensions up to 150 mm in length with automated selection between two columns with the optional column manager. Equipped with independently controlled temperature zones, active solvent pre-heating, and eCord™ Intelligent Chip Technology for each column.

Binary solvent manager

Delivers precise and accurate binary solvent blending at pressures up to 18,000 psi. Two integrated solvent select valves provides access to a total of four solvents. Automated solvent compressibility, integrated solvent degassing, and programmable seal wash maximize flow accuracy, precision, and reliability.

Ultra-low system dispersion

True UPLC performance with band spread as low as 4 μL.

Versatile autosampler options

Choose between two low dispersion flow-through-needle injectors (SM-FTN-H or SM-FTN-I) with a volume range of 0.1 to 1000 μL. Alternatively, a fixed loop injector (SM-FL-I) is available with a volume range of 0.1 to 250 μL.

Flexible sample support

Accepts either vials or ANSI well plate formats. Extend capacity for high throughput and open access environments with the optional Sample Organizer.

Gradient SmartStart

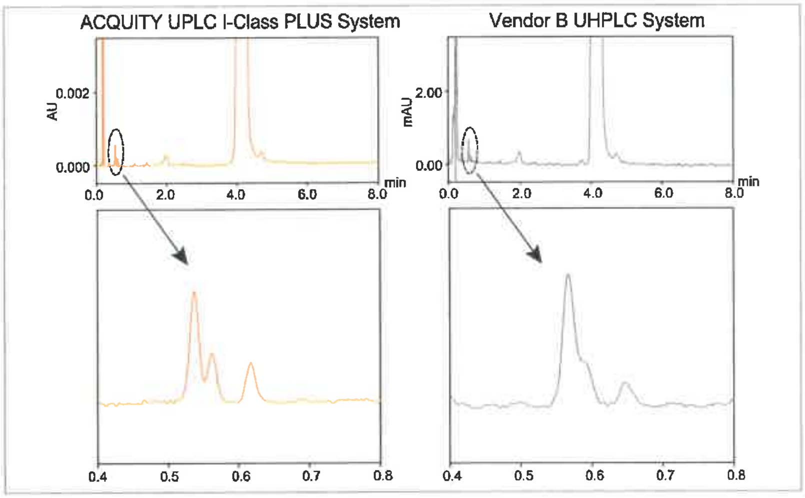
Easily adjust for system volume differences when transferring methods from an alternative LC system without alteration to the method table.

www.waters.com/iclassplus

DISPERSION MATTERS

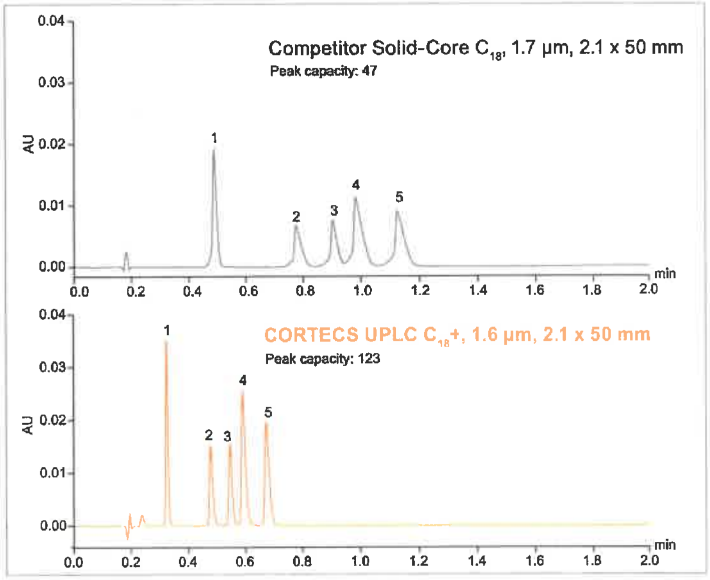
The pursuit of improved chromatographic performance has been made for decades, leading to the creation of novel particle technology, and the size of those particles, reduced. The potential of those particles, no matter how efficient they have become, are limited by the system in which they are run on. System band spread plays a key role, yet is often overlooked.

The ACQUITY UPLC I-Class PLUS System stands out, providing a clear view on what lies within the sample. When paired with CORTECS™ UPLC 1.6 µm solid-core Columns, scientists can achieve new levels of resolution and sensitivity that brings chromatographic performance to a new level.


ACQUITY UPLC I-Class PLUS System

Vendor B UHPLC System

In this example, the impurity analysis of tetracaine was run under the same conditions on the ACQUITY UPLC I-Class PLUS System (system band spread of 4 µL) and a UHPLC system (system band spread of 20 µL). Although the UHPLC system was optimized for lowest possible dispersion and system volume, the impact of system dispersion is clearly evident. Significantly better resolution was achieved with the ACQUITY UPLC I-Class PLUS System.


Competitor Solid-Core C_{18}, 1.7 µm, 2.1 x 50 mm
Peak capacity: 47

CORTECS UPLC C_{18}+, 1.6 µm, 2.1 x 50 mm
Peak capacity: 123

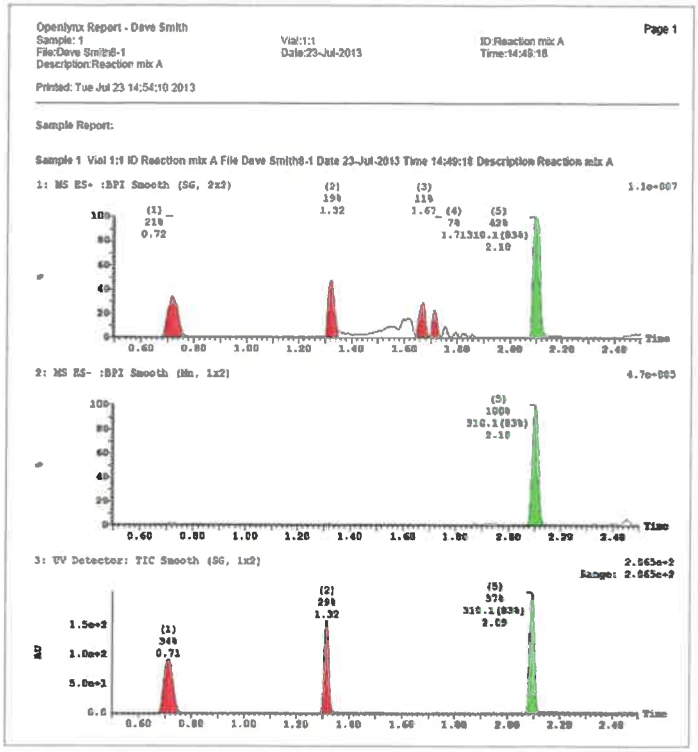
By pairing the ultra-low dispersion ACQUITY UPLC I-Class PLUS System with high-efficiency CORTECS Columns, you'll achieve new levels of UPLC performance. These 1.6 µm columns deliver exceptional levels of efficiency, performance, and throughput, resulting in narrower peaks and higher peak capacity.

THE IDEAL INLET TO MASS SPECTROMETRY

The ACQUITY UPLC I-Class PLUS System is designed specifically for the rapid pace of laboratories on the cutting edge of research where LC-MS plays a critical role:

- Narrow peak widths not only provide enhanced resolution, but also more efficient ionization, enhancing mass spectrometry sensitivity
- Ultra low delay volume results in exceptionally fast analysis times
- Sensitivity is enhanced through industry-leading carryover performance
- Multidimensional UPLC configurations lead to improved sample characterization through selective isolation

The ACQUITY UPLC I-Class PLUS System is designed to be the ideal inlet to mass spectrometry, maximizing the analytical value of each and every analysis. With the ability to achieve high resolution and high sensitivity methods rapidly, the answer you seek is not only obtained very quickly, but with new levels of clarity to enhance the characterization of even the most complex samples.



Openlynx Report - Dave Smith
Sample: 1
File:Dave Smith8-1
Description:Reaction mix A

Vial:1:1
Date:23-Jul-2013

ID:Reaction mix A
Time:14:49:18

Page 1

Printed: Tue Jul 23 14:54:10 2013

Sample Report:

Sample 1 Vial 1:1 ID Reaction mix A File Dave Smith8-1 Date 23-Jul-2013 Time 14:49:18 Description Reaction mix A

Typical MassLynx™-based Open Access report for a medicinal chemist using the ACQUITY UPLC I-Class PLUS System with ACQUITY QDa™ Mass Detector. The highlighted area shows how the ACQUITY QDa Mass Detector confirms that the required product (310 Da) has been successfully synthesized while the purity is determined from the ACQUITY UPLC PDA Detector.

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For your local sales office, please visit www.waters.com/contact

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Waters ACQUITY UPLC® I-Class System

Site Preparation Guide

Notice

Table of Contents

Introduction

This document serves as a guideline to help you prepare your laboratory facility for your Waters ACQUITY I-Class System. It describes the physical and environmental conditions, power, solvents, and sample preparation hardware required for the operation of the Waters ACQUITY I-Class System.

System description

The core Waters ACQUITY UPLC® I-Class System consists of a Binary Solvent Manager, Column Heater with Active Pre-heating (CH-A), (BSM), Sample Manager – Flow Through Needle (SM-FTN) or Sample Manager – Fixed Loop (SM-FL), and Solvent Tray Module.

Available as options are:

- Tunable UV detector (TUV)
- Photo-diode array (PDA) detector[1]
- Column Manager-A (CM-A)
- Common Platform Sample Organizer
- Evaporative Light Scattering (ELS) detector
- Fluorescence (FLR) detector
- Refractive Index (RI) detector
- Waters mass spectrometers* (several available)
- Flex Cart that includes casters for easy movement, adjustable table top, integrated power outlets, and storage space for the data system and waste container

***NOTE:** *If your system includes a mass spectrometer, refer to its site preparation guide for additional site requirements.*

Responsibilities

A certified Waters engineer will be responsible for installing and commissioning the system to ensure that the instrument is properly installed and fully operational. Your laboratory must meet the requirements specified in this guide and be prepared in advance to allow the engineer to perform the installation. Only after you prepare your laboratory and complete and return the checklist at the end of this document can the installation be scheduled.

A major part of the system installation is a series of tests designed to evaluate the instrument performance under specific operating conditions. At the end of each test, the result is entered in the Installation Checklist.

To help train the intended operator in basic system operation, it is important that you schedule the installation so that the operator is present to assist with the installation performance tests.

If you require specific training on the ACQUITY I-Class System or Empower™ or MassLynx™ software, arrange for this separately from the startup through your local Waters office.

If you have any questions regarding the information in this document or any particular site problems, contact your local Waters sales representative. If necessary, we will arrange to conduct a site survey.

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[1] *The term "ACQUITY PDA Detector" refers to two detectors: the ACQUITY UPLC Photodiode Array (PDA) Detector, and ACQUITY UPLC PDA Extended Wavelength (eλ or eLambda) Detector.*

Space and moving requirements

Carefully review the following sections.

- Example Waters ACQUITY UPLC® I-Class System configurations
- Space considerations
- Component dimensions
- Component weights
- Minimum door widths
- Lifting

NOTE: *Also, for more information about various I-CLass configurations, refer to the ACQUITY I-Class configuration document, P/N 715003144, available on the Waters Support Center at http://www.waters.com.*

Example Waters ACQUITY UPLC® I-Class System configurations

Figure 1 consists of the following components in a stacked position:

- Binary Solvent Manager (BSM)
- Sample Manager – Flow Through Needle (SM-FTN) or Sample Manager – Fixed Loop (SM – FL)
- Column Heater with Active Pre-heating (CH-A)
- Optional detector
- Solvent Tray Module

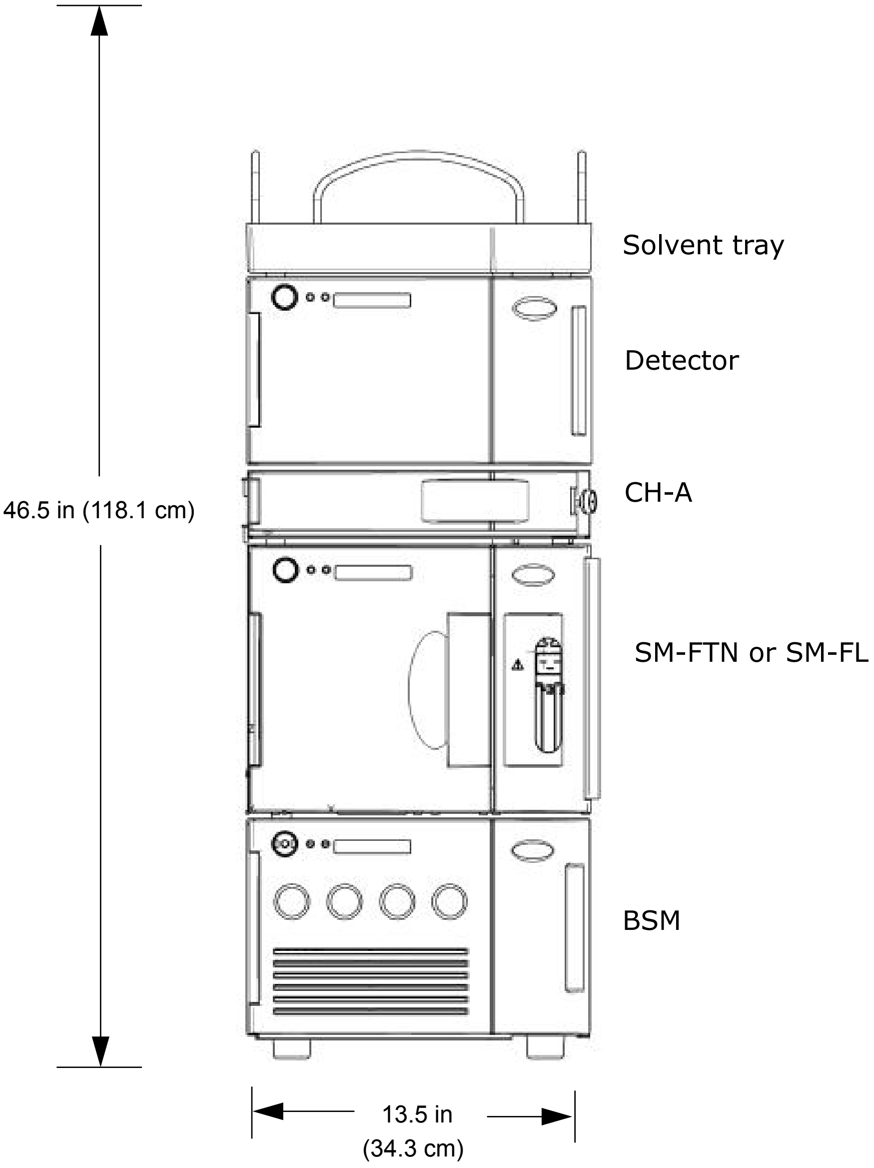


Figure 1 - ACQUITY I-Class System with Column Heater-A

NOTE: *The vertical dimension in Figure 1 includes extra 10-inch (25.4-cm) clearance for solvent tray access; see Table 1 for depth requirements.*

Figure 2 shows an ACQUITY I-Class System with an optional Column Manager (CM-A) positioned above the sample manager.

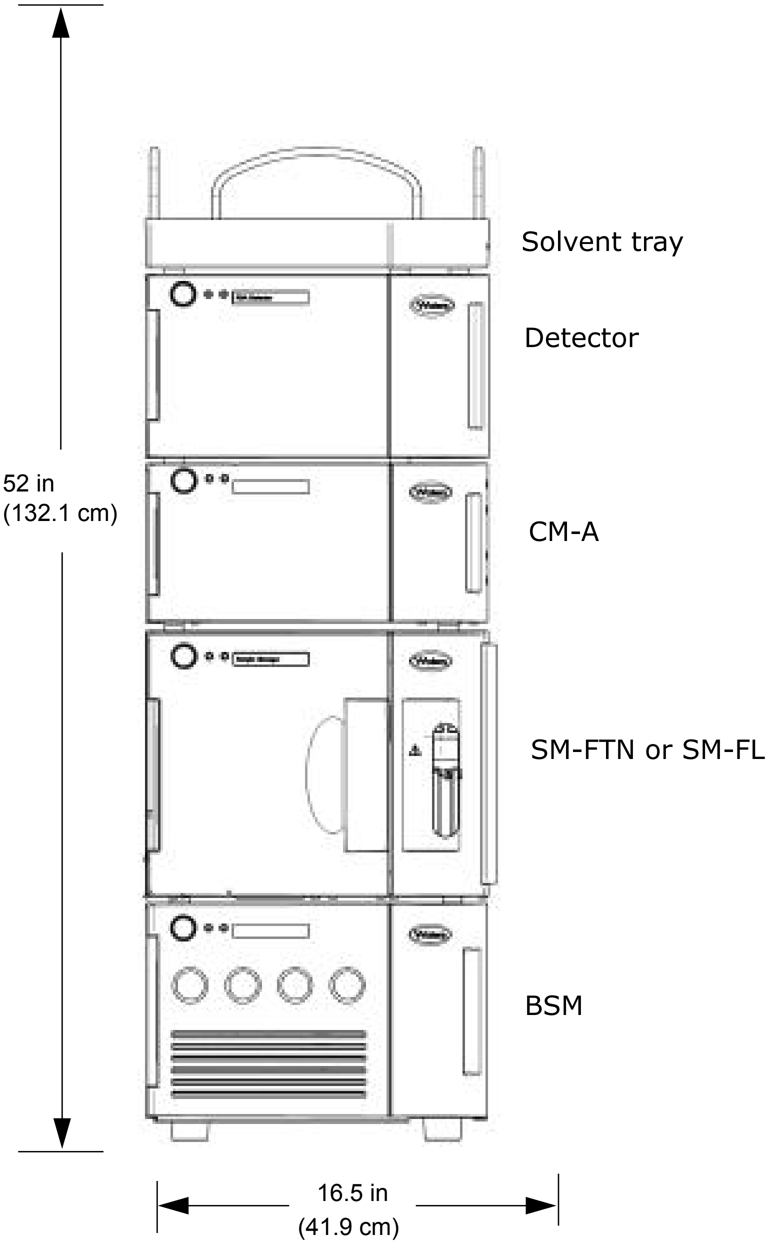


Figure 2 - ACQUITY I-Class System with Column Manager-A

NOTE: *The vertical dimension in Figure 2 includes an extra 10-inch (25.4-cm) clearance for solvent tray access; the horizontal dimension includes an extra 3-inch (7.6 cm) right-side clearance for SM-FTN and CM-A ventilation. See Table 1 for depth requirements.*

Figure 3 shows an ACQUITY I-Class System with an optional Common Platform Sample Organizer (CPSO) to the left of the stack.

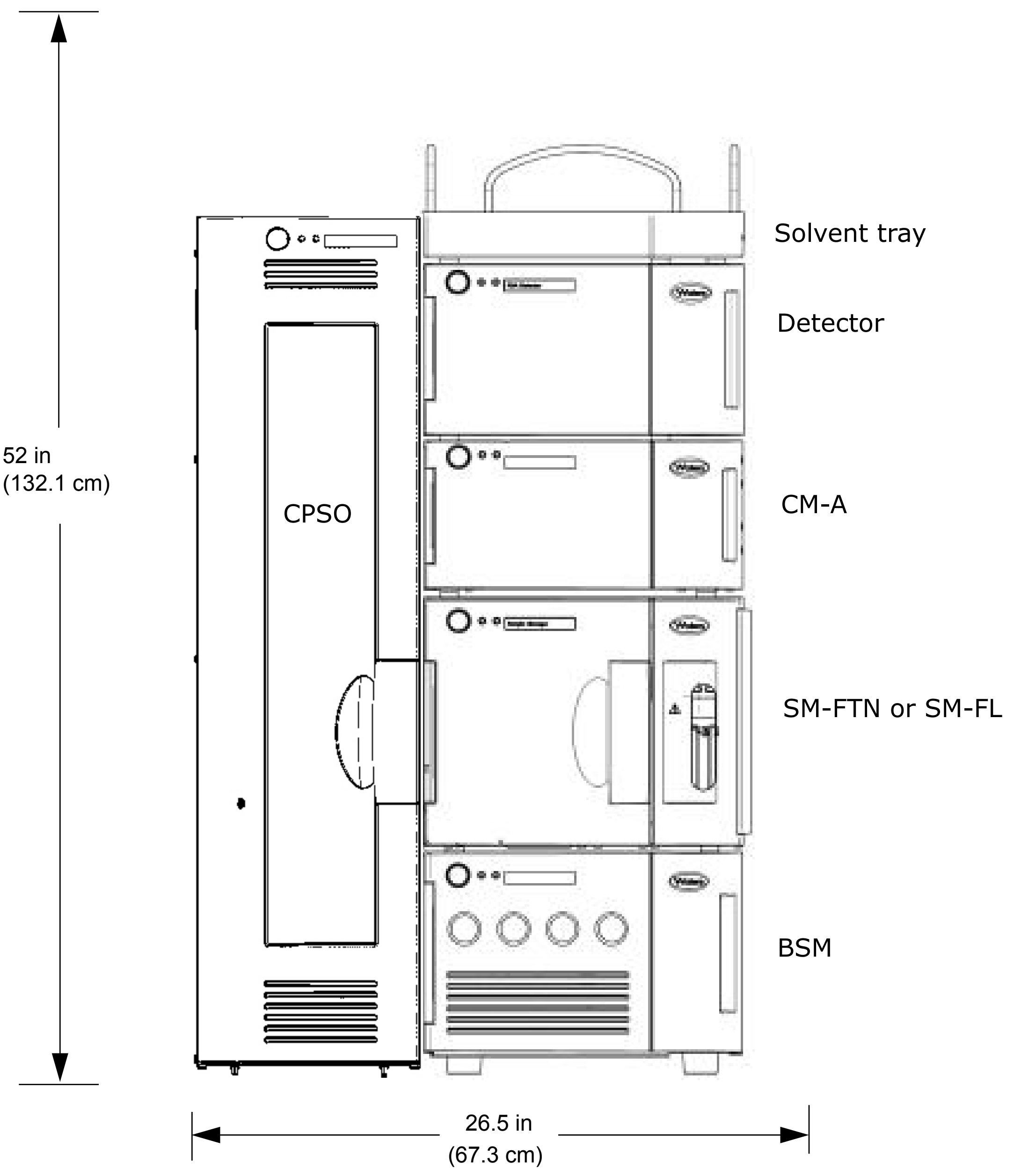


Figure 3 - ACQUITY I-Class System with Column Manager-A and CPSO

NOTE: *The vertical dimension in Figure 2 includes an extra 10-inch (25.4-cm) clearance for solvent tray access; the horizontal dimension includes an extra 3-inch (7.6 cm) right-side clearance for SM-FTN and CM-A ventilation. See Table 1 for depth requirements.*

Figure 4 provides an overhead view for systems with SQD or TQD mass spectrometers.

IMPORTANT: *If your system uses a different mass spectrometer, refer to its site preparation guide for dimensions and additional space requirements.*

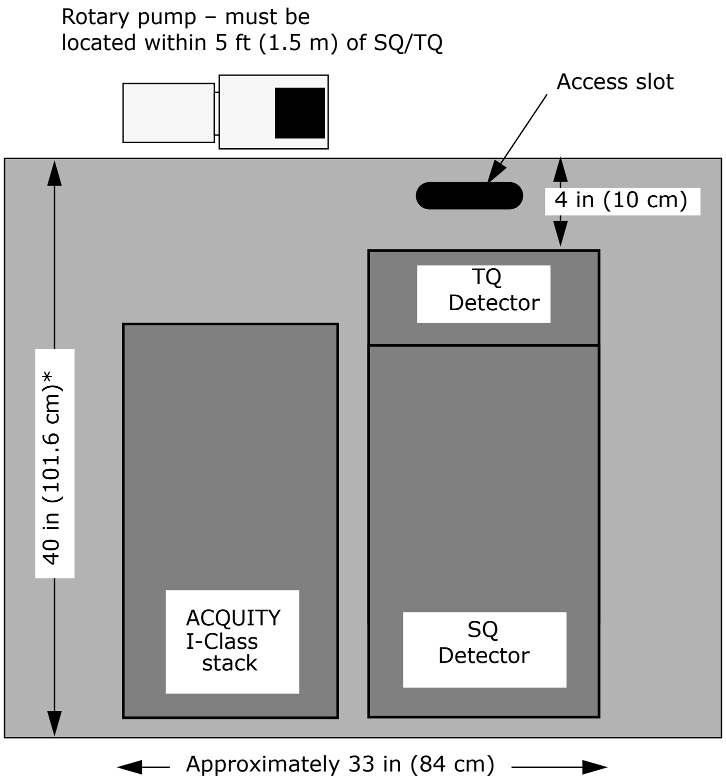


Figure 4 - Space requirements for systems with SQD or TQD mass spectrometers.

NOTE: *Also, for more information about various I-CLass configurations, refer to the ACQUITY I-Class configuration document, P/N 715003144, available on the Waters Support Center at http://www.waters.com.*

Space considerations

When determining the space requirements for your system, refer to the bulleted items listed below, Table 1 on page 12, and the *ACQUITY I-Class Configuration Guide.*

- For systems with a mass spectrometer, refer to its site preparation guide for specific site requirements.
- When choosing a location for the system, allow at least 6 inches (15.2 cm) behind the system for ventilation and rear panel connections. Also, allow enough space to remove the side panels for service access.
- The SM-FTN and CM-A require 3 inches (7.6 cm) of right-side ventilation clearance.
- When an optical detector is positioned above another detector in the stack, the multi-detector drip tray option must be installed on the upper detector. Two inches (5.1 cm) of right side clearance are required to accommodate its drain tubing.
- Some I-Class configurations that include a mass spectrometer and a CH-A, may require the use of an optional MS bracket kit to position the column heater to the right of the I-Class stack. Doing so reduces the length of the tubing that extends to the mass spectrometer inlet. Refer to the *ACQUITY I-Class Configuration Guide* to determine whether your system requires the MS bracket kit.
- All Waters instruments ship domestically with a 7.5-ft (2.3-m) power cord that must be plugged into the rear of the chassis. International power cords are 8.25 ft (2.5 m).
- The system may be placed either on a traditional laboratory bench or inside a fume hood. Ideally the system should be placed on a movable worktable (i.e. a laboratory bench on wheels).
- If installing the system inside a fume hood, you may need to carefully position the system on blocks to provide sufficient clearance for the Binary Solvent Manager door to open (above the entry shelf of the hood) and allow for proper drainage of the drip management system.
- All of the power on/off switches for the ACQUITY I-Class System are located on the upper-left front panels of each instrument.
- The data system (computer CPU, monitor, keyboard, Ethernet switch, and mouse) must be placed on a laboratory bench close to the system. These components require approximately 24 in (61.0 cm) of bench space. Standard length cables are provided with the system. If necessary, extension cables for any of these cables may be sourced locally from a PC vendor.

  NOTE: *An internet connection is required in order to enable the optional Connections INSIGHT® (Intelligent Services).*
- If using the ACQUITY I-Class System with a mass spectrometer, the data system must be located within 16 ft (5 m) of the mass spectrometer to allow connection of the communication cables. Also, an access slot may need to be cut in the bench top to allow the vacuum tubes and gas lines to be passed to and from the mass spectrometer. Refer to the appropriate mass spectrometer site preparation guide for details.
- Solvent supply reservoir(s) must be located on the top of the ACQUITY I-Class System in the Solvent Tray Module. For installation and removal of solvent bottles, plan for an additional 10 in. (25.4 cm) of space above the top of the bottles.
- If using the optional Waters ACQUITY Flex Cart (Figure 5) to support single-stack configurations, you must accommodate its footprint of 30 x 33 in (76.2 x 83.8 cm).You

can set the Flex Cart tabletop height from 30 to 44 in (76.2 to 111.8 cm). The Flex Cart can also house the system waste containers and data system.

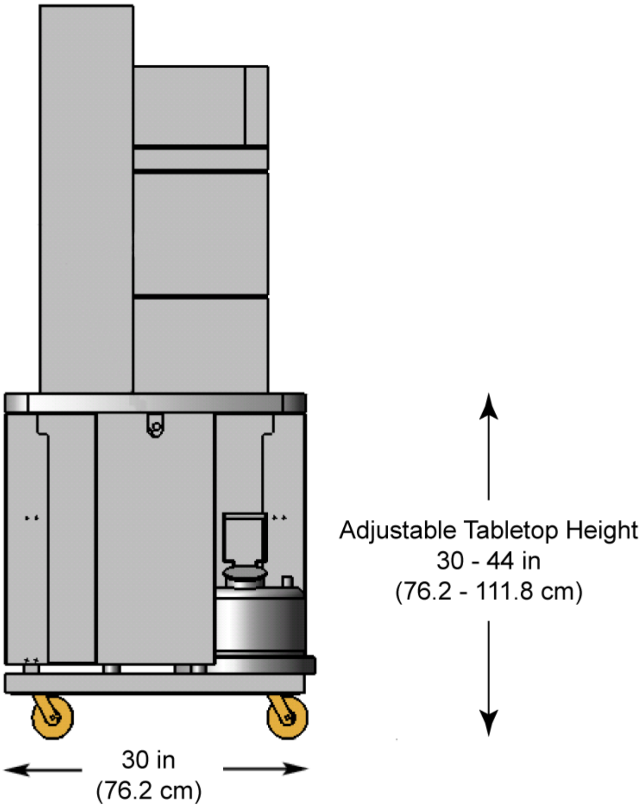


Figure 5 - ACQUITY System Flex Cart

Component dimensions

Table 1: Component dimensions [a]

System Component	Width	Depth	Height
Binary Solvent Manager	13.5 in (34.3 cm)	26.0 in (66.1 cm)	9.38 in (23.8 cm) with 0.875 in (2.2 cm) feet*
	Allow at least 6 in. (15.2 cm) clearance at the rear for ventilation and connections.		
Isocratic Solvent Manager	13.5 in (34.3 cm)	26.0 in (66.1 cm)	9.38 in (23.8 cm) with 0.875 in (2.2 cm) feet[a]
	Allow at least 6 in. (15.2 cm) clearance at the rear for ventilation and connections.		
Sample Manager (SM-FTN)	13.5 in (34.3 cm)	28.0 in (71.2 cm)	10.7 in (27.1 cm) with 0.25 in (0.64 cm) feet*
	Allow at least 6 in. (15.2 cm) clearance at the rear and 3 in. (7.6 cm) to the right for ventilation and connections. Additionally, the fluidics drawer of the sample manager slides outward 15.5 in (39.4 cm).		
Sample Manager (SM-FL)	13.5 in (34.3 cm)	28.0 in (71.2 cm)	10.7 in (27.1 cm) with 0.25 in (0.64 cm) feet*
	Allow at least 6 in. (15.2 cm) clearance at the rear and 3 in. (7.6 cm) to the right for ventilation and connections. Additionally, the fluidics drawer of the sample manager slides outward 15.5 in (39.4 cm).		
Column Heater-A	13.5 in (34.3 cm)	22.0 in (56.0 cm)	2.95 in (7.5 cm) with 0.25 in (0.64 cm) feet*
	If using with a mass spectrometer, allow 13.25 in (33.6 cm) of clearance for the Column Heater bracket in the extended position to right of the stack.		
Column Manager-A	13.5 in (34.3 cm)	24.0 in (61 cm)	7.8 in (20 cm)
	Allow at least 6 in. (15.2 cm) clearance at the rear and 3 in. (7.6 cm) to the right for ventilation and connections.		
TUV Detector	13.5 in (34.3 cm)	21.0 in (53.4 cm)	8.2 in (20.8 cm) with 0.25 in (0.64 cm) feet*
	Allow at least 6 in. (15.2 cm) clearance at the rear for ventilation and connections. When the multi-detector drip tray option is used, allow for an additional 2 in. (5.1 cm) drain tube clearance to the right of the detector.		
PDA Detector	13.5 in (34.3 cm)	24.0 in (61 cm)	8.5 in (21.6 cm) with 0.25 in (0.64 cm) feet*
	Allow at least 6 in. (15.2 cm) clearance at the rear for ventilation and connections. When the multi-detector drip tray option is used, allow for an additional 2 in. (5.1 cm) drain tube clearance to the right of the detector.		

Table 1: Component dimensions (Continued)[a]

ELS Detector	13.5 in (34.3 cm)	20.4 in (51.8 cm)	8.5 in (21.6 cm) with 0.25 in (0.64 cm) feet*
	Allow at least 6 in. (15.2 cm) clearance at the rear for ventilation and connections. When positioned in the left stack, allow for an additional 1 in. (2.54 cm) drain tube clearance between the left and right stacks.		
FLR Detector	13.5 in (34.3 cm)	20.4 in (51.8 cm)	8.5 in (21.6 cm) with 0.25 in (0.64 cm) feet*
	Allow at least 6 in. (15.2 cm) clearance at the rear for ventilation and connections.		
RI Detector	13.5 in (34.3 cm)	24.0 in (61 cm)	8.2 in (20.8 cm) with 0.25 in (0.64 cm) feet*
	Allow at least 6 in. (15.2 cm) clearance at the rear for ventilation and connections. When the multi-detector drip tray option is used, allow for an additional 2 in. (5.1 cm) drain tube clearance to the right of the detector.		
Solvent Tray Module	13.5 in (34.3 cm)	20.5 in (52.1 cm)	5.0 in (12.7 cm)
	* All instruments are equipped with 0.25 in (0.64 cm) high feet.		
QDa Detector	14 in (35.3 cm)	29.5 in (75 cm)	8 in (20 cm)
	Refer to the QDa Detector Site Preparation Guide, P/N 715002299, for space rotary pump requirements.		
SQ Detector 2	13.85 in. (35.2 cm)	29.0 in (74 cm)	23.25 in (59.3 cm)
SQ Detector	14.0 in. (35.6 cm)	25.0 in (63.5 cm)	21.0 in (53.4 cm)
TQ Detector	14.0 in. (35.6 cm)	33.5 in (85.1 cm)	21.0 in (53.4 cm)
Common Platform Sample Organizer	10 in (25.4 cm)	30.0 in (76.2 cm)	38.0 in (96.5 cm) including base
	Allow at least 6 in (15.2 cm) clearance at the rear for ventilation and connections.		

a. If a different mass spectrometer is included with the system, refer to its site preparation guide for dimensions.

Component weights

Ensure that your bench top is able to support the total weight of your system’s components (Table 2). Note that the Waters ACQUITY Flex Cart (Figure 5) is rated to safely handle the total weight of the components in a typical system.

Table 2: Component weights[a]

System Component	Weight
Binary Solvent Manager	57 lb (25.9 kg)
Isocratic Solvent Manager	57 lb (25.9 kg)
Sample Manager - FTN	57.5 lb (26.1 kg)

Table 2: Component weights[a] (Continued)

System Component	Weight
Sample Manager - FL	57 lb (25.9 kg)
Column Heater-A	12.5 lb (5.7 kg)
Column Manager-A	46 lb (21 kg)
TUV Detector	20.5 lb (9.3 kg)
Photodiode Array Detector	34.3 lb (15.6 kg)
ELS Detector	32.5 lb (14.7 kg)
FLR Detector	30 lb (13.6 kg)
RI Detector	34 lb (15.4 kg)
Solvent Tray Module	5 lb (2.3 kg)
QDa Detector (Standard) QDa Detector (Performance)	62 lb (28 kg) 55 lb (25 kg)
SQ Detector 2	176 lb (80 kg)
SQ Detector	127 lb (58 kg)
TQ Detector	189 lb (85.5 kg)
Common Platform Sample Organizer	125 lb (56.8 kg)

[a] If a different mass spectrometer is included with the system, refer to its site preparation guide for weight.

Minimum door widths

Doors through which the system will be moved must be a minimum of 25 in (63.5 cm) wide. If you are using the optional Waters ACQUITY Flex Cart, the minimum door width is 30 in (76.2 cm). Elevators and corridors must be wide enough to allow corners to be negotiated. Special arrangements may be required if you plan to move the system to the laboratory via a staircase. Mass spectrometers may require greater door widths.

Lifting

As a general guide before lifting, lowering, or moving the instruments:

- Assess the risk of injury
- Take action to eliminate risk
- Plan the operation in advance and in conjunction with our engineer when he/she arrives on site
- Comply with the appropriate country and/or company regulations

Solvent considerations

Depending on the solvent being used, suitable solvent containers may be placed on a magnetic stirrer/hotplate within the Solvent Tray Module on top of the system.

Due to the increased sensitivity that both the ACQUITY I-Class System and the new series of mass spectrometers offer, all solvents, including water and additives, must be of the highest chemical purity. Failure to use such solvents will result in high background contamination, low signal-to-noise, and loss of sensitivity. Waters recommends using clean, high-purity, submicron filtered solvents. Solvents that are submicron filtered by the manufacturer do not require any additional filtering.

Use ultrapure (i.e., particle-free, chemically clean, 18-megaohm cm resistivity) water. This will reduce the amount of impurities in the water that can collect on the column during equilibration with the weak solvent.

If your ACQUITY I-Class System includes a mass spectrometer, or is part of an application-based system, IPA will need to be supplied to perform a system flush. Refer to the mass spectrometer or application-based system site preparation guide for additional solvent requirements.

For further detail on controlling contamination, and information on solvent brands and mobile phase reservoirs, refer to the document *Controlling Contamination in UltraPerformance LC®/MS and HPLC/MS Systems*, part number 715001307, located in the Waters Support Center on the Web (www.waters.com).

Gas supply

WARNING: ***IF USING ZERO GRADE AIR, CONSIDER THE COMBUSTIBILITY OF THE SOLVENTS.***

Nitrogen gas for mass spectrometers

For systems with an optional mass spectrometer, you must provide a supply of dry, oil-free nitrogen with a purity of at least 95%. The nitrogen must be regulated at 7 bar (100 psi) outlet pressure. Refer to the mass spectrometer site preparation guide that ships with your system for additional nitrogen gas supply requirements.

Collision gas for mass spectrometers

Argon is required for the collision cell on systems that include some mass spectrometers. The argon must be dry, high purity (≥99.997%) and regulated at a pressure of 0.5 bar (7 psi). Refer to the mass spectrometer site preparation guide that ships with your system for additional collision gas supply requirements.

Nitrogen gas for an ELS detector

The ELS Detector requires a suitable supply of high purity nitrogen gas or zero grade air (e.g., oil- and particle-free gas). If using zero grade air, consider the combustibility of the solvents. Gas cylinders are not recommended due to their limited capacity. Waters recommends using a gas flow of approximately 3 - 4 L/min. A constant gas supply (65 - 90 psi at the regulator) is required to operate the detector.

Waste collection

The ACQUITY UPLC Drip Management System is a closed-architecture, gravity-driven drainage system that effectively collects and removes any solvent leaks and process waste from the needle and plunger seal washes. Each instrument uses a drip tray to collect and route the waste from one module tray to the one beneath it, eventually exiting the system through the elbow drain located below the Binary Solvent Manager compartment door.

Follow these waste collection requirements when preparing your laboratory:

- To maintain proper drainage and leak control, the ACQUITY I-Class System must be level.
- A waste container, such as a large-capacity carboy or safely enclosed glass container, must be positioned below the bench top to collect the waste.
- All waste tubing must be routed in a manner that prevents the formation of traps in the tubing.
- The Solvent Tray Module located on top of the system is capable of holding up to two liters of spilled solvent. You will need to supply a separate waste container of sufficient capacity to collect any spill from the waste line at the rear of the tray.
- When an optical detector is positioned above another detector in the stack, the Waters Multi-detector Drip Tray option (P/N 205000355) must be installed on the upper detector.

Power requirements

Refer to the following power requirements when preparing your laboratory:

- All ACQUITY I-Class System components require a dedicated, earthed (grounded) power source. The receptacles from this power source must be accessible to the ACQUITY I-Class System components, and must share a common ground.
- If your ACQUITY I-Class System has a mass spectrometer, refer to its site preparation guide for power requirements.
- The use of a line conditioner or an uninterruptible power supply (UPS) should also be considered for optimum long-term input voltage stability.
- The optional Flex Cart includes a 15A power strip with 10 receptacles to which the ACQUITY I-Class System components connect. The cart typically reduces the number of required VAC receptacles for the site to one or two.

Refer to Table 3 on page 17 for power requirements for each system component.

Table 3: Power requirements by component

System Component	Input Voltage/ Frequency	Fuse Rating	Max. Power Draw	Power Cord Supplied
Binary Solvent Manager	100 to 240 VAC 50/60 Hz	5.0 A	360 VA	7.5 ft (2.3 m) domestic 8.25 ft (2.5 m) international
Isocratic Solvent Manager	100 to 240 VAC 50/60 Hz	5.0 A	200 VA	7.5 ft (2.3 m) domestic 8.25 ft (2.5 m) international
Sample Manager - FTN (with a CH-A)	100 to 240 VAC 50/60 Hz	10.0 A	400 VA	7.5 ft (2.3 m) domestic 8.25 ft (2.5 m) international
TUV Detector	100 to 240 VAC 50/60 Hz	3.15 A	185 VA	7.5 ft (2.3 m) domestic 8.25 ft (2.5 m) international
PDA Detector	100 to 240 VAC 50/60 Hz	3.15 A	145 VA	7.5 ft (2.3 m) domestic 8.25 ft (2.5 m) international
ELS Detector	100 to 240 VAC 50/60 Hz	5.0 A	200 VA	7.5 ft (2.3 m) domestic 8.25 ft (2.5 m) international
FLR Detector	100 to 240 VAC 50/60 Hz	3.15 A	280 VA	7.5 ft (2.3 m) domestic 8.25 ft (2.5 m) international
RI Detector	100 to 240 VAC 50/60 Hz	3.15 A	145 VA	7.5 ft (2.3 m) domestic 8.25 ft (2.5 m) international
Column Manager-A	100 to 240 VAC 50/60 Hz	N/A	400 VA	7.5 ft (2.3 m) domestic 8.25 ft (2.5 m) international
QDa Detector	100 to 240 VAC 50/60 Hz	13 to 16 A	400 VA	7.5 ft (2.3 m) domestic 8.25 ft (2.5 m) international
- Diaphragm pump	24 VDC	N/A	64 VA	Connects to the QDa
- Rotary pump	100 to 240 VAC 50/60 Hz	13 to 16 A	300 VA	7.5 ft (2.3 m) domestic 8.25 ft (2.5 m) international
SQ Detector 2 (including rotary/scroll pump)	200 to 240 VAC 50/60 Hz	13 –16 A	See mass spec site prep guide	8.25 ft (2.5 m) – detector 6.5 ft (2 m) – pump
SQ Detector (including rotary pump)	200 to 240 VAC 50/60 Hz	13 –16 A	1430 VA	8.25 ft (2.5 m) – detector 6.5 ft (2 m) – pump
TQ Detector (including rotary pump)	200 to 240 VAC 50/60 Hz	13 –16 A	2000 VA	8.25 ft (2.5 m) – detector 6.5 ft (2 m) – pump
Common Platform Sample Organizer	100 to 240 VAC 50/60 Hz	10.0 A	540 VA	7.5 ft. (2.3 m) domestic 8.25 ft (2.5 m) international

Figure 6 shows the country- or region-specific plug types supplied with the Waters ACQUITY UPLC® I-Class System.

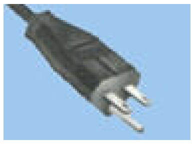
US/Canada (125 V)		5-15P (UL817 and CSA C.22.2)
US/Canada (250 V)		L6-15P (UL817 and CSA C.22.2)
US/Canada (250 V)		6-15P (UL817 and CSA C.22.2)
UK		3-pin (BS1363)
Europe		2-pin (CEE7)
Denmark		3-pin (Afsnit 107-2-D1)
Australia		3-pin (AS/NZS 3112)
China		3-pin (GB2099, 10A and 16A versions)

Figure 6 - Plug types supplied with the ACQUITY I-Class System

Environmental requirements

General

Follow these general environmental requirements when preparing your laboratory:

- Waters recommends that the ACQUITY I-Class System be installed in an environmentally controlled laboratory, in a draft-free position away from excessive amounts of dust.
- The air-conditioning or heating ventilation must not be positioned directly above the system.
- The relative humidity must not exceed 80%, non-condensing.
- The ACQUITY I-Class System must be installed in an environment that complies with Pollution Category 1 and Installation Category 2.

Temperature

Follow these temperature requirements and considerations when preparing your laboratory:

- The ambient temperature in the laboratory must be from 4 to 40 °C (39.2 to 104 °F). Failure to operate in this range will compromise the performance of the system and may result in instrument failure.

  CAUTION: *The CH-A is designed to accurately control the column temperature when the difference between the room and column temperatures is at least 5 °C (9 °F). Also, sample cooling in CM-A the will not reach 4 °C (39.2°F) if the ambient temperature is 25 °C (77 °F) or greater.*

- The optimum temperature range of the laboratory is 19 to 22 °C (66 to 72 °F). Short-term thermal variations should be no more than 2 °C (3.6 °F) per 1.5 hours.

Vibration

The Waters ACQUITY I-Class System must not be placed close to heavy machines such as compressors and generators which can create excessive floor vibration.

Magnetic fields

If using the Waters ACQUITY I-Class System as an inlet for a mass spectrometer, position the system with mass spectrometer away from strong magnetic fields such as those generated by NMR systems or magnetic sector mass spectrometers.

Radio emissions

The Waters ACQUITY I-Class System must be placed in an environment where Radio Frequency (RF) emission from surrounding sources is minimal.

Possible sources of RF emission include RF-linked alarm systems, mobile telephones, and hand-held transmitters.

Exhaust outlets

An in-line degasser, integral to the Binary Solvent Manager, exhausts dissolved gases from the eluents and condensate from the exhaust system through a vent line on the front of the Binary Solvent Manager. To avoid exposure to solvent vapors, it is recommended that you route the exhaust to a laboratory fume hood using the supplied tubing. A 3.5-foot (1.06 m) length of 1/8-inch (0.32-cm) I.D. tubing is supplied in the Binary Solvent Manager Startup Kit.

To properly vent the exhaust vapor to waste in an ELS Detector, a drying gas exhaust bottle is provided to trap any condensate that forms from vented vapor exiting the detector. A 3-foot (0.9-m) and 5-foot (1.5-m) length of black exhaust hose is also supplied to route exhaust from the detector to the bottle, and from the bottle to a laboratory exhaust system that applies gentle vacuum.

CAUTION: ***TO AVOID CONTACT WITH ELUENT GASES, CONNECT THE OUTLET VENT TO A SUITABLE EXHAUST, SUCH AS A PROPERLY FUNCTIONING HOOD.***

Test samples

CAUTION: ***HAZARDOUS SAMPLES MUST BE HANDLED IN A MANNER THAT CONFORMS TO THE MANUFACTURER'S GUIDELINES AS DEFINED IN THE RELEVANT HAZARD DATA SHEETS.***

The Waters service engineer will use the samples supplied with the ACQUITY I-Class System to test a system that includes a mass spectrometer or other ACQUITY I-Class System detector.

NOTE: *The Waters engineer will not carry test samples to the installation. If the test samples cannot be provided prior to the agreed installation date, the installation must be rescheduled. If the Waters engineer arrives on site and the necessary facilities are unavailable, the customer will be charged any costs incurred for the visit.*

If your laboratory practices require full sample certification documentation, Waters Analytical Standards and Reagents provide ready-to-use reference materials and reagents that are fully traceable and certified.

Supplies of high-purity water and acetonitrile are required to perform the tests. Refer to "Solvent considerations" for more information.

Items supplied by the customer

The following items must be supplied by the customer:

- Three 1-liter wash bottles
- Two solvent waste containers
- Two 2-liter or four 1-liter mobile phase bottles
- Appropriate glassware for sample and solvent preparation
- Solvents and solvent filtration apparatus

CAUTION: ***ENSURE THAT THESE ITEMS ARE NOT OR HAVE NOT BEEN WASHED WITH DETERGENT, WASHED WITH OTHER GLASSWARE, OR WASHED IN FACILITIES THAT MIGHT HAVE DETERGENT RESIDUE. WASHING GLASSWARE IN A COMMON DISHWASHING FACILITY CAN CONTAMINATE WITH DETERGENT RESIDUES WHICH MAY CONTAIN POLYETHYLENE GLYCOL AND OTHER "STICKY" SUBSTANCES. VINYL-COATED STEEL RACKS CAN BE ADDITIONAL SOURCES OF CONTAMINATION.***

For systems that include a mass spectrometer, refer to the mass spectrometer site preparation guide for specific requirements.

Computer Requirements

If you are planning to provide your own computer for an Empower- or MassLynx-controlled ACQUITY I-Class System, contact your sales person for details on the required computer hardware and operating system specifications.

Connections INSIGHT® installation requirements

Installation of the Waters Connections INSIGHT® software (Intelligent Services that provide real-time, remote system monitoring and notification) requires the following:

- An active Internet connection
- This Internet connection can either be direct or through a firewall or proxy server

NOTE: *The outgoing-initiated connection from the Connections INSIGHT Service Agent to the Waters Connections Enterprise Server uses SSL (Secure Sockets Layer) port 443. Information sent includes only instrument usage counters, error message text, and instrument configuration data. The Connections INSIGHT Service Agent does not have access to nor does it transmit business-sensitive information, and connects only to the Waters Connections Enterprise Server.*

ACQUITY I-Class System site preparation checklist

This checklist must be completed and returned to Waters when all the requirements are available.

> ***NOTE:*** *It is the customer's responsibility to ensure that ALL the laboratory supplies are correct. Please attach any additional information to this document where necessary.*

Space Requirements (without bench) - see page 5

The available bench space is adequate for the system. .... ☐

Floor Space Requirements (with bench) - see page 5

The available floor space is adequate for the system. .... ☐

Lifting and Carrying - see page 14

Suitable equipment or personnel will be available to lift the instrument onto the laboratory bench. .... ☐

Solvents and Samples - see page 14

Suitable solvent and solvent containers are available, and solvent and sample preparation facilities are in place. .... ☐

Gases and Regulators – see **page 15**

For systems with a mass spectrometer, a regulated (0.5 bar [7 psi]), dry, oil-free nitrogen source with a purity of at least 95% is available.................. ☐

For systems with a TQD or other mass spec, high purity (≥99.997%) argon gas regulated at 0.5 bar (7 psi) is available with a 3-mm (1/8-in.) adaptor .... ☐

For systems with an ELS detector, a supply of high purity nitrogen gas or zero grade air is available. .... ☐

Waste Collection - see page 15

Suitable waste containers are available. .... ☐

Power Requirements - see page 16

The specified power source requirements are met, and an appropriate number of power receptacles are available. .... ☐

Environmental Requirements - see page 19

The laboratory meets the temperature, humidity, vibration, magnetic fields, and radio emissions requirements. .... ☐

Exhaust Outlets - see page 19

A suitable fume hood is available. .... ☐

Ancillary Equipment

If you plan to use any other equipment with the system, provide details below.

Make/Type	Model	Already commissioned	To be commissioned

Test Samples - see page 20

The supplied test samples, required for installation, are available. .... ☐

Customer-supplied Items - see page 21

All customer-supplied items, including wash and mobile phases bottles, waste containers, glassware, solvents, and filtration apparatus are available... ☐

Minimum Computer Requirements - see page 21

If not purchasing the computer from Waters Corporation, a computer that meets the specified requirements is available. .... ☐

Waters Connections INSIGHT® Requirements - see page 21

If you are planning to install Waters Connections INSIGHT® software, an Internet connection is available. .... ☐

I confirm that all supplies are now available and that all specified environmental conditions have been met. During the installation, the operator intends to be available for demonstration and training by the Waters engineer:

At all times. .... ☐

Approximately ____% of the time. .... ☐

Not at all. .... ☐

During the likely period of installation, the following dates are NOT convenient:

____

Signed: ____

NOTE: *If an authorized Waters service engineer arrives on site to begin installation work and cannot complete the installation due to lack of facilities (i.e. power, laboratory readiness), costs incurred will be charged.*

Please complete the following sections in block letters:

Position: ____

Name: ____

Organization: ____

Street: ____

City/State: ____

Zip/Postal Code: ____

Country: ____

Telephone: ____

Fax: ____

Email: ____

NOTE: *The installation of your system cannot begin until pages 22 through 24 of this document have been fully completed and returned to the Sales Support Representative at your local Waters office.*

Purchasing Divison
2019 Washington Street East
Post Office Box 50130
Charleston, WV 25305-0130

State of West Virginia
Request for Quotation
13 — Equipment

Proc Folder: 569939

Doc Description: Addendum No. 1 Triple Quad LC/MS/MS

Proc Type: Central Purchase Order

Date Issued	Solicitation Closes	Solicitation No	Version
2019-04-18	2019-04-26 13:30:00	CRFQ 1400 AGR1900000018	2

BID RECEIVING LOCATION

BID CLERK
DEPARTMENT OF ADMINISTRATION
PURCHASING DIVISION
2019 WASHINGTON ST E
CHARLESTON WV 25305
US

VENDOR

Vendor Name, Address and Telephone Number:

Waters Technologies Corporation
34 Maple St
Milford, MA 01757
PH: 508-482-2000

FOR INFORMATION CONTACT THE BUYER

Melissa Pettrey
(304) 558-0094
melissa.k.pettrey@wv.gov

Signature X Kristen A. **FEIN #** 04-3234558 **DATE** 4/25/19

All offers subject to all terms and conditions contained in this solicitation

ADDITIONAL INFORMATION:

Addendum No. 1

Addendum No. 1 is issued to publish and distribute the attached information to the vendor community.
****

Central Request for Quotation

The West Virginia Purchasing Division is soliciting bids on behalf of the Agency, the West Virginia Department of Agriculture to establish a contract for the one time purchase of a Liquid Chromatography Triple Quadrupole Mass Spectrometer (LC/MS/MS), workstation PC, software, printer, nitrogen generator, uninterrupted power supply (UPS), specific test methods, shipping, installation, validation, warranty, training and service per the bid requirements, specifications, terms and conditions attached to this solicitation.

INVOICE TO	SHIP TO
PROCUREMENT OFFICER 304-558-2221 AGRICULTURE DEPARTMENT OF ADMINISTRATIVE SERVICES 1900 KANAWHA BLVD E CHARLESTON WV25305-0173 US	AUTHORIZED RECEIVER 304-558-2227 AGRICULTURE DEPARTMENT OF REGULATORY PROTECTION DIVISION 313 GUS R DOUGLAS LN, BLDG 11 CHARLESTON WV 25312 US

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Total Price
1	LC/MS/MS, Workstation PC, Software, Printer, nitrogen	1.00000	EA		

Comm Code	Manufacturer	Specification	Model #
41100000			

Extended Description :

generator, uninterrupted power supply, specific test methods per section 3.1

INVOICE TO	SHIP TO
PROCUREMENT OFFICER 304-558-2221 AGRICULTURE DEPARTMENT OF ADMINISTRATIVE SERVICES 1900 KANAWHA BLVD E CHARLESTON WV25305-0173 US	AUTHORIZED RECEIVER 304-558-2227 AGRICULTURE DEPARTMENT OF REGULATORY PROTECTION DIVISION 313 GUS R DOUGLAS LN, BLDG 11 CHARLESTON WV 25312 US

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Total Price
2	shipping charges & inside delivery	1.00000	EA		

Comm Code	Manufacturer	Specification	Model #
78121603			

Extended Description :

Shipping charges & inside delivery per section 3.1.6

INVOICE TO		SHIP TO	
PROCUREMENT OFFICER 304-558-2221		AUTHORIZED RECEIVER 304-558-2227	
AGRICULTURE DEPARTMENT OF		AGRICULTURE DEPARTMENT OF	
ADMINISTRATIVE SERVICES		REGULATORY PROTECTION DIVISION	
1900 KANAWHA BLVD E		313 GUS R DOUGLAS LN, BLDG 11	
CHARLESTON	WV25305-0173	CHARLESTON	WV 25312
US		US	

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Total Price
3	Installation/validation	1.00000	EA		

Comm Code	Manufacturer	Specification	Model #
73171605			

Extended Description :
Installation/Validation per section 3.1.6

INVOICE TO		SHIP TO	
PROCUREMENT OFFICER 304-558-2221		AUTHORIZED RECEIVER 304-558-2227	
AGRICULTURE DEPARTMENT OF		AGRICULTURE DEPARTMENT OF	
ADMINISTRATIVE SERVICES		REGULATORY PROTECTION DIVISION	
1900 KANAWHA BLVD E		313 GUS R DOUGLAS LN, BLDG 11	
CHARLESTON	WV25305-0173	CHARLESTON	WV 25312
US		US	

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Total Price
4	Training/warranty	1.00000	EA		

Comm Code	Manufacturer	Specification	Model #
73171605			

Extended Description :
Training/Warranty per section 3.1.6

INVOICE TO		SHIP TO	
PROCUREMENT OFFICER 304-558-2221		AUTHORIZED RECEIVER 304-558-2227	
AGRICULTURE DEPARTMENT OF		AGRICULTURE DEPARTMENT OF	
ADMINISTRATIVE SERVICES		REGULATORY PROTECTION DIVISION	
1900 KANAWHA BLVD E		313 GUS R DOUGLAS LN, BLDG 11	
CHARLESTON	WV25305-0173	CHARLESTON	WV 25312
US		US	

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Total Price
5	Service	1.00000	EA		

Comm Code	Manufacturer	Specification	Model #
73171605			

Extended Description :

Service per section 3.1.6

SOLICITATION NUMBER: AGR1900000018
Addendum Number: 1

The purpose of this addendum is to modify the solicitation identified as AGR1900000018 ("Solicitation") to reflect the change(s) identified and described below.

Applicable Addendum Category:

[ ] Modify bid opening date and time

[ ] Modify specifications of product or service being sought

[X] Attachment of vendor questions and responses

[ ] Attachment of pre-bid sign-in sheet

[ ] Correction of error

[ ] Other

Description of Modification to Solicitation:

1. **To publish Vendor questions and Agency responses.**
2. **Bid opening remains 04/26/2019 @ 1:30 P.M.**

Additional Documentation: Documentation related to this Addendum (if any) has been included herewith as Attachment A and is specifically incorporated herein by reference.

Terms and Conditions:

1. All provisions of the Solicitation and other addenda not modified herein shall remain in full force and effect.

2. Vendor should acknowledge receipt of all addenda issued for this Solicitation by completing an Addendum Acknowledgment, a copy of which is included herewith. Failure to acknowledge addenda may result in bid disqualification. The addendum acknowledgement should be submitted with the bid to expedite document processing.

CRFQ AGR1900000018
Vendor Q&A

Q1. Bid Instructions:

11. EXCEPTIONS AND CLARIFICATIONS states that a Vendor can submit exceptions and clarifications to the specifications of the contractual agreement and also states that submission of such may be grounds for disqualification.

> As part of a Vendor's Bid Package submission, we would like to request a few additions/ edits to the State's terms and conditions, without being disqualified. Would the State consider without disqualification, a request to include the vendors standard terms of service (if you need them), reference to the commercial EULA's included by clickwrap, the manufacturer's commercial warranty as the governing warranty and in addition to the State's, and a commercially reasonable limitation of liability for (i) consequential damages, (ii) indemnification for direct damages for personal injury and death or persons, and damage to property and (iii) IP infringement for the manufacture and state of subject products and reasonable remedies?
>
> We will provide the details of these requested changes in our submission but seek your approval in advance as to concept.

A1. Vendor must include any exceptions to terms and conditions in its bid. Should any exception be deemed to violate a mandatory requirement of the solicitation Vendor's proposal will be disqualified

Q2. Line item 3.1.1.19

For minimal tuning during method development and minimal maintenance of the ion path, the LC/MS/MS will require hot source induced desolvation interface to the mass analyzer by patented Larmnar Flow Ion Guide using gas flow. Submit evidence of instrument use with cannabis for at least 6 months without matrix induced cleaning and maintenance

> With evidence of 6 months operation without matrix induced cleaning and maintenance, will a reference lab name and contact information suffice to show evidence that they have been running for over six months without maintenance?
>
> Also, does the reference to no matrix induced cleaning and maintenance include routine source cleaning without breaking vacuum or the need to recalibrate? Please elaborate what can and cannot be included.

A2. Yes.
Yes, must submit evidence to support your instruments ruggedness and stability that satisfies the question.

ADDENDUM ACKNOWLEDGEMENT FORM
SOLICITATION NO.: AGR1900000018

Instructions: Please acknowledge receipt of all addenda issued with this solicitation by completing this addendum acknowledgment form. Check the box next to each addendum received and sign below. Failure to acknowledge addenda may result in bid disqualification.

Acknowledgment: I hereby acknowledge receipt of the following addenda and have made the necessary revisions to my proposal, plans and/or specification, etc.

Addendum Numbers Received:
(Check the box next to each addendum received)

[X] Addendum No. 1
[ ] Addendum No. 2
[ ] Addendum No. 3
[ ] Addendum No. 4
[ ] Addendum No. 5
[ ] Addendum No. 6
[ ] Addendum No. 7
[ ] Addendum No. 8
[ ] Addendum No. 9
[ ] Addendum No. 10

I understand that failure to confirm the receipt of addenda may be cause for rejection of this bid. I further understand that that any verbal representation made or assumed to be made during any oral discussion held between Vendor's representatives and any state personnel is not binding. Only the information issued in writing and added to the specifications by an official addendum is binding.

Waters Technologies Corporation
Company

Kristen A.
Authorized Signature

4/25/19
Date

NOTE: This addendum acknowledgement should be submitted with the bid to expedite document processing.

ADDENDUM ACKNOWLEDGEMENT FORM
SOLICITATION NO.:

Instructions: Please acknowledge receipt of all addenda issued with this solicitation by completing this addendum acknowledgment form. Check the box next to each addendum received and sign below. Failure to acknowledge addenda may result in bid disqualification.

Acknowledgment: I hereby acknowledge receipt of the following addenda and have made the necessary revisions to my proposal, plans and/or specification, etc.

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(Check the box next to each addendum received)

☑ Addendum No. 1
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☐ Addendum No. 7
☐ Addendum No. 8
☐ Addendum No. 9
☐ Addendum No. 10

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Waters Technologies Corporation
Company

Kristen A. Arakelian
Authorized Signature

4/25/19
Date

NOTE: This addendum acknowledgement should be submitted with the bid to expedite document processing.

[APPLICATION NOTE]

Waters
THE SCIENCE OF WHAT'S POSSIBLE.™

Analysis of Legacy and Emerging Perfluorinated Alkyl Substances (PFAS) in Environmental Water Samples Using Solid Phase Extraction (SPE) and LC-MS/MS

Kari Organtini,[1] Ken Rosnack,[1] Douglas Stevens,[1] and Euan Ross[2]
[1] Waters Corporation, Milford, MA, USA
[2] Waters Corporation, Wilmslow, UK

APPLICATION BENEFITS

Performing SPE sample preparation of water samples using the ISO 25101 method for PFAS analysis provides:

- Highly sensitive analysis using the Xevo™ TQ-S micro
- Detection limits in the low to sub- ng/L range to meet regulatory requirements
- A robust and reliable solution for monitoring PFAS compounds in environmental water matrices

WATERS SOLUTIONS

ACQUITY™ UPLC™ I-Class PLUS System

ACQUITY UPLC BEH C_{18} Column

Oasis™ WAX SPE Cartridges

PFC Analysis Kit

Xevo TQ-S micro

MassLynx™ MS Software

KEYWORDS

Perfluorinated, polyfluorinated, PFAS, PFC, AFFF, PFOS, PFOA, WAX SPE cartridge, TQ-S micro

INTRODUCTION

Perfluoroalkyl substances (PFAS) are a group of persistent and bioaccumulative anthropogenic pollutants that are common to consumer and industrial processes. They are introduced to the environment through a variety of sources ranging from industrial manufacturing of non-stick coatings to their use in firefighting foams. While this group of compounds encompasses thousands of unique compounds, most advisories currently focus on the two most commonly known, PFOS and PFOA. While there currently are no legal requirements for monitoring of PFASs globally, many countries worldwide do recommend they be monitored at some level. In the United States, the U.S. EPA has set an advisory limit of 70 ng/L (ppt) of total PFOS and PFOA;[1] while in Europe, the European Water Framework Directive has singled out PFOS and its derivatives. The Water Framework Directive is an environmental quality standard and advises an annual average value of 0.65 ng/L for inland surface waters.[2]

To reach detection limits low enough to satisfy advisories, either a highly sensitive mass spectrometer is required, or sample preparation that allows for sample enrichment must be employed. The first option was discussed in a previous application note utilizing the ASTM 7979 procedure with the Xevo TQ-XS.[3] This application note will detail the second approach using SPE extraction to enrich water samples with analysis performed on Waters™ Xevo TQ-S micro. Methodology was adapted from ISO 25101 which was written for analysis of PFOS and PFOA in environmental water samples.[4] Both approaches are valid options and it depends on a laboratory's resources and testing needs as to which method should be considered.

EXPERIMENTAL

The ISO 25101 method was utilized as a guideline for the sample preparation methodology used for this analysis. Currently, ISO 25101 covers the extraction and analysis of only PFOA and PFOS. For this method, an extended list of PFAS compounds were considered and added. Appendix A contains information on all of the PFAS compounds analyzed in this method, together with a subset of emerging compounds being used to replace the legacy PFAS compounds, including GenX. All standards were obtained from Wellington Laboratories (Guelph, Ontario).

A Certified QC Standard (cat no.: 731) from ERA (Golden, CO), for use with ground and surface waters, was utilized as an instrumental QC check throughout the analysis. The standard contained a mix of 12 PFAS compounds. Certified values and QC Performance Acceptance Limits for each compound in the mix are provided with the standard, making instrumental QC evaluation quick and straightforward.

Due to widespread use of PFAS substances there are many common sources of potential contamination to the analysis. Since required detection limits are in the low- to sub-ng/L, care must be taken during sample collection, preparation, and analysis. Considering there are many common sources of PFAS contamination in the field and laboratory, it is recommended that any laboratory supplies to be used for this analysis be checked for PFAS contamination before use, as is practical. Contamination is also unavoidable from the chromatographic system. Therefore steps should be taken to minimize any system contribution, and as such, the Waters PFC Analysis Kit (p/n: 176001744) for the UPLC system was utilized. The kit is comprised of PFAS-free components (such as PEEK tubing to replace the conventional Teflon coated solvent lines) and an isolator column that helps to delay any residual background interferences from co-eluting with the analytical peak. Installation of the PFC Analysis Kit is straightforward and quick.[5] In addition, special mobile phase solvents from Honeywell (Muskegon, MI) were used that were bottled in a manner to reduce residual background PFAS levels.

Sample preparation

Standards were prepared as a mix in methanol and calibration standards were appropriately diluted into 1:1 water:methanol to match the final solvent composition of the samples.

Environmental water samples were collected from various sources including surface water, ground water, influent waste water, and effluent waste water. The surface water and ground water samples were collected locally. Waste water samples were provided by Dr. David Reckhow (University of Massachusetts, Amherst). Samples were collected into pre-washed 250 mL HDPE bottles. A blank of each sample was retained for extraction and the remaining samples were spiked with various levels of PFAS compounds and corresponding isotopically labeled standards. The isotope labeled internal standards were utilized to correct for matrix effects as well as any recovery losses from sample preparation.

Sample extraction was performed using ISO 25101 as a guideline with minor method adjustments to accommodate the extended list of PFAS compounds. Oasis WAX 6 cc, 150 mg SPE Cartridges (p/n: 186002493) were used for the sample extraction of 250 mL water samples. The full method for sample preparation is outlined in Figure 1. This method provides a sample enrichment factor of 250×.

Figure 1. Full method details of SPE sample extraction for water samples.

LC conditions

LC system:	ACQUITY UPLC I-Class PLUS fitted with the PFC Analysis Kit (p/n: 176001744)
Column:	ACQUITY UPLC BEH C_{18} 2.1 × 100 mm, 1.7 µm (p/n: 186002352)
Column temp.:	35 °C
Sample temp.:	10 °C
Injection volume:	10 µL
Mobile phase A:	95:5 Water:methanol + 2 mM ammonium acetate
Mobile phase B:	Methanol + 2 mM ammonium acetate

Gradient:

Time (min)	Flow rate (mL/min)	%A	%B
0	0.3	100	0
1	0.3	80	20
6	0.3	55	45
13	0.3	20	80
14	0.4	5	95
17	0.4	5	95
18	0.3	100	0
22	0.3	100	0

MS conditions

MS system:	Xevo TQ-S micro
Ionization mode:	ESI-
Capillary voltage:	0.5 kV
Desolvation temp.:	350 °C
Desolvation gas flow:	900 L/hr
Cone gas flow:	100 L/hr
Source temp.:	100 °C
Method events:	Divert flow to waste from 16 to 21 minutes

MRM parameters for each compound were optimized using the QuanOptimize™ tool in MassLynx Software and are listed in Appendix A.

RESULTS AND DISCUSSION

INSTRUMENT PERFORMANCE AND DETECTION LIMITS

The LC-MS/MS method utilized was fit for purpose for the determination of a range of PFAS compounds of interest. An overlay chromatogram showing the chromatography of all the compounds is shown in Figure 2. Peak shape of the early eluting compounds suffer from slight broadening due to the significant difference in solvent composition between the starting LC gradient and sample.

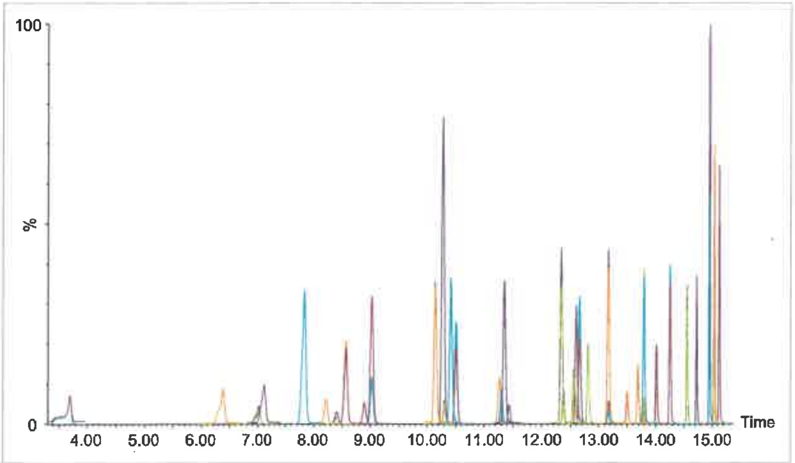

Figure 2. Overlay of all PFAS compounds analyzed in the method.

Detection limits can be seen for all compounds in Table 1. Due to the concentration enhancement provided from the sample preparation procedure, the detection limits are reported as both in-vial and in-sample (250-fold lower than vial concentration) limits. For the most part, in-sample detection limits were sub-ng/L (ppt), reaching to the pg/L (ppq) levels. A few of the less water soluble compounds had ng/L (ppt) detection limits. The detection limits detailed in Table 1 are suitable for current requirements for PFAS testing.

Calibration was very linear over several orders of magnitude for all compounds. An example of a typical solvent calibration curve can be seen in Figure 3, showing an example for PFOA, along with a chromatogram of PFOA at its detection limit.

During sample analysis, the ERA standard was used as a QC for instrument performance. The instrument performed within the designated Acceptance Limits for all compounds. The average error from the certified values was 15%, although many were below 10% error.

Table 1. Detection limits in vial and sample for all PFAS compounds.

Compound	LOD vial (ng/L)	LOD sample (ng/L)	R^2
PFBA	10	0.04	0.999
PFPeA	10	0.04	0.999
PFHxA	10	0.04	0.999
PFHpA	5	0.02	0.999
PFOA	<2	<0.01	0.999
PFNA	10	0.04	0.999
PFDA	10	0.04	0.999
PFUnDA	10	0.04	0.999
PFDoDA	10	0.04	0.999
PFTriDA	10	0.04	0.993
PFTreDA	10	0.04	0.999
PFHxDA	500	2.00	0.994
PFOcDA	2000	8.00	0.988
PFBS	4.4	0.02	0.999
PFPeS	4.7	0.02	0.999
PFHxS	3.7	0.01	0.999
PFHpS	9.5	0.04	0.999
PFOS	3.65	0.01	0.999
PFNS	4.8	0.02	0.999
PFDS	9.6	0.04	0.999
N-EtFOSAA	10	0.04	0.999
N-MeFOSAA	5	0.02	0.999
FHUEA	5	0.02	0.999
FOUEA	5	0.02	0.999
8:2 diPAP	500	2.00	0.997
4:2 FTS	23.4	0.09	0.999
6:2 FTS*	<95	<0.38	0.999
8:2 FTS	9.6	0.04	1.000
PFecHS	9.2	0.04	0.999
FHEA	20	0.08	0.999
FOEA	8	0.03	0.999
FDEA	20	0.08	0.999
FHpPA	5	0.02	0.999
GenX	20	0.08	0.999
ADONA	<2	<0.01	0.999
9Cl-PF3ONS	<1.9	<0.01	0.999
11Cl-PF3OUdS	9.42	0.04	0.996
NFHDA	5	0.02	0.999
PFEESA	<2	<0.01	0.999
PFMBA	<2	<0.01	0.999

**The true detection limit for 6:2 FTS cannot be determined due to contamination. The concentration listed here as the LOD signifies the approximate contamination level.*

SAMPLE PREPARATION PERFORMANCE

Overall performance of the sample preparation method can be summarized in the recovery values highlighted in Figure 4. A majority of the PFAS compounds fell within the recovery range of 75% to 130%. A few compounds had lower recoveries, including the C13 and C14 (PFTriDA and PFTreDA) carboxylates, as well as one of the emerging PFAS compounds, 11ClPF3OUdS. PFTriDA and PFTreDA are known to be less water soluble than the smaller chain PFCAs (perfluorinated carboxylic acids). Adjusting the final sample's solvent composition could be investigated to achieve better recoveries, but the impact to the remaining compounds must be evaluated. Also, a few compounds exhibited very high recovery rates, including PFBA, 6:2 FTS, and PFODA. PFBA and 6:2 FTS have been determined to be common contaminant compounds in the laboratory where the sample analysis was performed. Source(s) of the contamination was investigated but has not yet been able to be determined. PFODA appears to experience a matrix stabilization effect, and this was reported in a prior application note.[3] Use of the isotope labeled internal standards to correct for loss through sample prep improves the accuracy further, as demonstrated by the green bars in Figure 4.

Repeatability of the method was assessed from the analysis of six replicates of ground water spiked with the PFASs. The orange squares in Figure 4 represent the %RSD of the six replicates of ground water taken through the entire sample preparation method and analysis. All PFASs had a %RSD below 15%, with most being below 10%. This indicates the sample analysis method is reproducible.

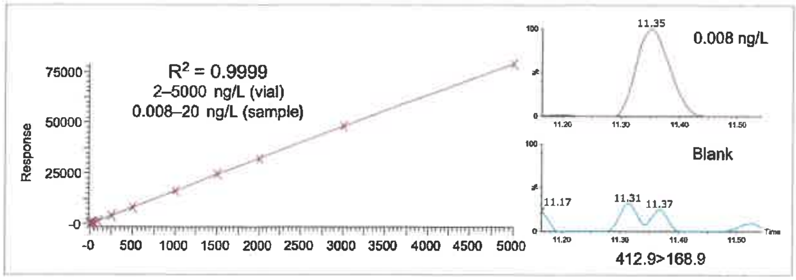

Figure 3. Demonstration of the linearity and sensitivity of PFOA showing calibration curve and peak at the detection limit of 0.008 ng/L compared to a blank.

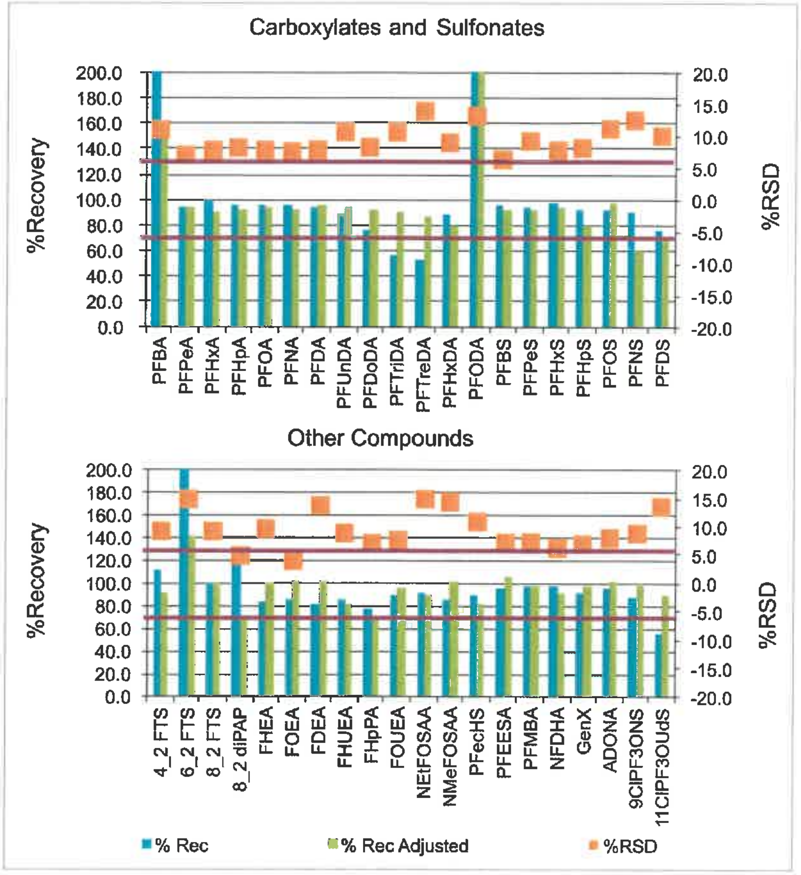

Figure 4. Method recovery (blue bars/left axis) and method reproducibility (orange squares/right axis) for all PFAS compounds covered in method. The adjusted recovery (green bars/left axis) represents the compound response corrected to its internal standard.

METHOD ROBUSTNESS

The robustness of the instrument over a series of matrix injections was evaluated using a spiked surface water extract. 20 replicate injections were performed to assess peak area, retention time, and ion ratio stability in a complex matrix. Stability of all three parameters over 20 injections are shown in Figure 5 for PFOA. Peak area is plotted in TrendPlot™ to determine the %RSD, a peak overlay is shown to represent the retention time is not shifting, and ion ratio data indicates the ion ratios are stable. In the example shown for PFOA, the %RSD of peak areas is approximately 3%. Overall, a %RSD of less than 10% was seen for all PFASs in the method.

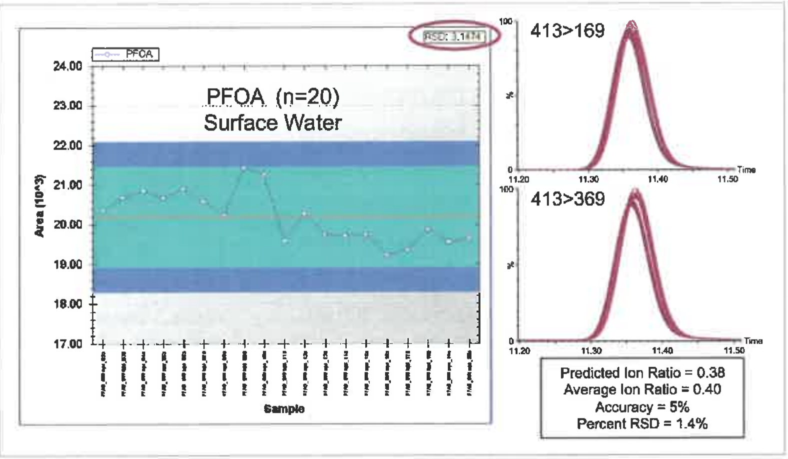

Figure 5. Repeatability assessed by 20 replicate injections of surface water. Peak area of PFOA for each injection is plotted in TrendPlot with an RSD of 3% (left) and the peak overlay of replicate injections with ion ratio information (right).

ANALYSIS OF ENVIRONMENTAL WATER SAMPLES

Four different types of environmental water samples were extracted and analyzed to test the described method including surface water, ground water, influent waste water, and final effluent waste water. A range of different PFASs were detected at varying concentrations in all samples. Figure 6 shows an example of a few PFASs identified in a surface water sample which include both legacy and emerging PFASs of interest. As shown in Figure 6, the identified PFASs were not present in the extraction blank and therefore can be confirmed as identified in the sample and not a from a source of background PFAS contamination.

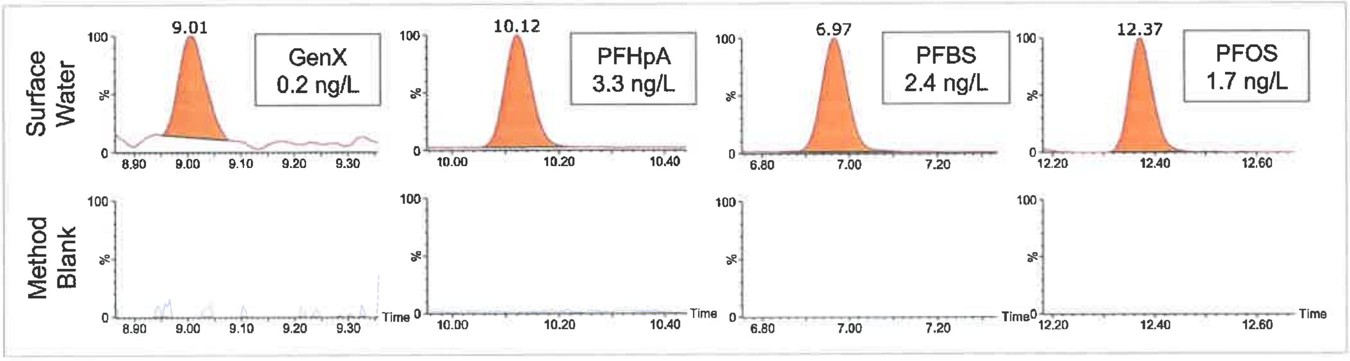

Figure 6. Identification of PFAS compounds in surface water sample extract (right) compared to the extraction blank (left). The blank is scaled to the surface water peak.

Figure 7 demonstrates the different patterns and concentrations of PFASs identified in the environmental water samples. From the list of 40 compounds screened, 27 were detected in the four samples. All samples contained both legacy and emerging PFAS compounds. Both waste water samples contained the highest levels and the largest numbers of different PFASs. Of the six PFASs detected in the ground water sample, half were emerging contaminants (PFEESA, PFMBA, and NFDHA).

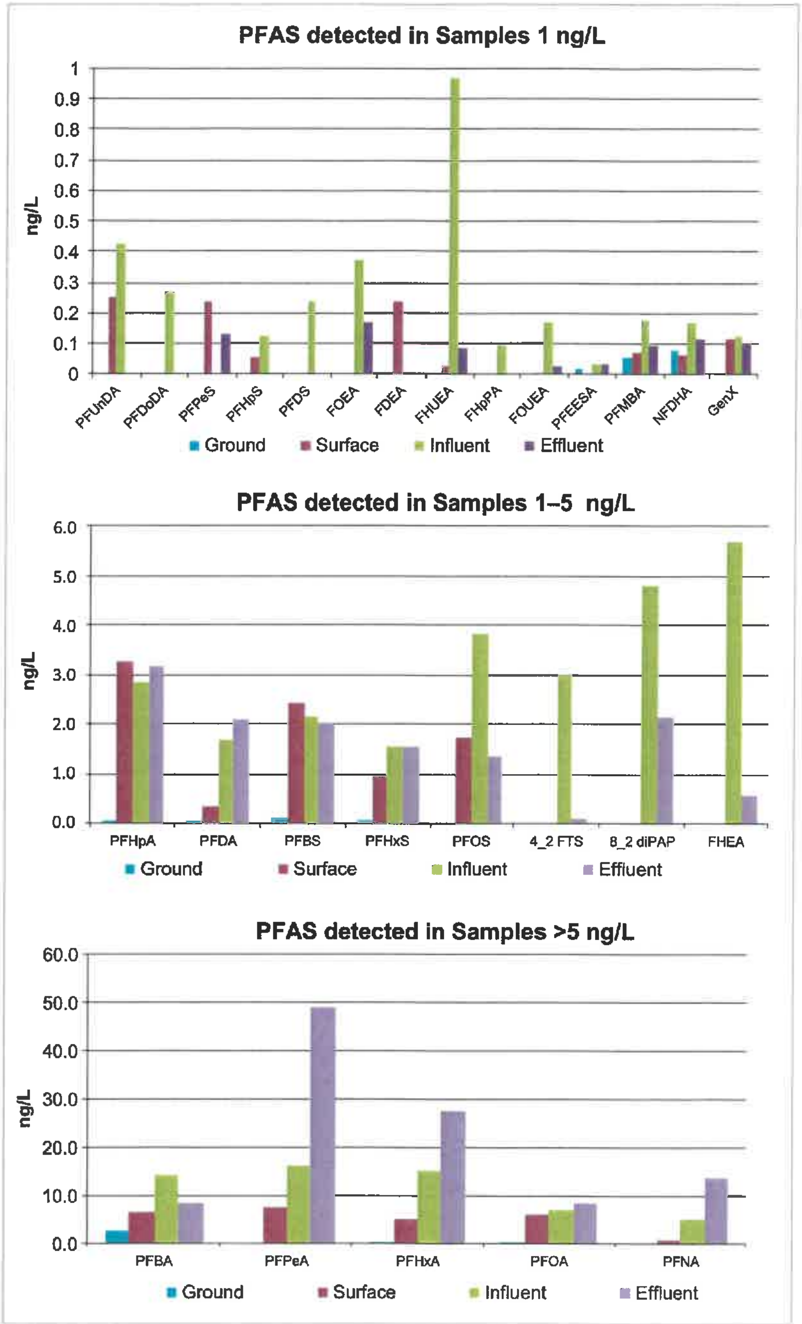

Figure 7. Patterns of PFASs detected in environmental water samples grouped by concentration level.

CONCLUSIONS

- Using SPE preparation of water samples provides a 250× enrichment of the sample allowing for analysis using the Xevo TQ-S micro.
- Achievable detection limits with this method on the Xevo TQ-S micro align with the necessary action levels set by the European Framework Directive and the U.S. EPA health advisory.
- Following the guidance of ISO 25101, analysis of environmental water samples can be accomplished for determination of both legacy and emerging PFASs.
- The method was verified by the use of the ERA certified QC standard, enhancing confidence in results.
- The method described is robust and has been applied to the analysis of a various range of environmental water samples including surface, ground, and waste waters.

Acknowledgements

The authors would like to acknowledge Honeywell for the productive conversations and considerations for providing the special mobile phase solvents for this work. The authors would also like to acknowledge Dr. David Reckhow and team at the University of Massachusetts, Amherst for providing waste water samples for this work.

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Appendix

Compound	CAS number	PFAS class	Type	Precursor	Product	CV	CE	RT
PFBA	375-22-4	carboxylate	legacy	212.9	169	10	10	3.6
PFPeA	2706-90-3	carboxylate	legacy	262.9	219	10	5	6.3
PFHxA	307-24-4	carboxylate	legacy	312.9	269 119	5	10 20	8.5
PFHpA	375-85-9	carboxylate	legacy	362.9	319 169	15	10 15	10.1
PFOA	335-67-1	carboxylate	legacy	412.9	369 169	10	10 15	11.3
PFNA	375-95-1	carboxylate	legacy	462.9	418.9 219	10	10 15	12.3
PFDA	335-76-2	carboxylate	legacy	512.9	468.9 219	15	10 15	13.1
PFUnDA	2058-94-8	carboxylate	legacy	562.9	518.9 269	25	10 20	13.8
PFDoDA	307-55-1	carboxylate	legacy	612.9	568.9 169	30	10 25	14.2
PFTriDA	72629-94-8	carboxylate	legacy	662.9	618.9 169	5	10 30	14.6
PFTreDA	376-06-7	carboxylate	legacy	712.9	668.9 169	10	15 25	14.7
PFHxDA	67905-19-5	carboxylate	legacy	812.9	768.8 169.2	40	10 40	15.0
PFODA	16517-11-6	carboxylate	legacy	912.9	868.9 169.2	35	15 35	15.1
PFBS	29420-49-3	sulfonate	legacy	298.9	80.1 99.1	15	30 30	7.0
PFPeS	2706-91-4	sulfonate	legacy	348.9	80.1 99.1	10	30 30	8.8
PFHxS	3871-99-6	sulfonate	legacy	398.9	80.1 99.1	10	35 30	10.3
PFHpS	375-92-8	sulfonate	legacy	448.9	80.2 99.1	15	35 35	11.4
PFOS	1763-23-1	sulfonate	legacy	498.9	80.2 99.1	15	40 40	12.3
PFNS	N/A	sulfonate	legacy	548.9	80.2 99.2	20	40 40	13.2
PFDS	335-77-3	sulfonate	legacy	598.9	80.2 99.1	25	40 40	13.8
N-MeFOSAA	2991-50-6	sulfonamidoacetic acid	legacy	569.9	418.9 219.1	35	20 25	13.5
N-EtFOSAA	2355-31-9	sulfonamidoacetic acid	legacy	584	418.8 525.9	15	20 20	13.8
FHUEA	70887-88-6	unsaturated telomer acid	legacy	356.9	292.9 243	10	10 35	10.4
FOUEA	70887-84-2	unsaturated telomer acid	legacy	456.9	393 343	10	10 40	12.6
8_2 diPAP	678-41-1	phosphate ester	legacy	989	97 542.5	10	40 20	15.0
4_2 FTS	757124-72-4	telomer sulfonate	legacy	326.9	307 81.1	15	15 35	8.4
6_2 FTS	29420-49-3	telomer sulfonate	legacy	426.9	407 344.9 81	15	20 10 35	11.3
8_2 FTS	39108-34-4	telomer sulfonate	legacy	526.9	506.8 444.6 81.2	15	25 10 40	13.1
PFecHS	67584-42-3	cyclic	legacy	460.9	380.9 99.1	40	30 30	11.2
FHEA	53826-12-3	telomer acid	legacy	376.9	292.9 313	5	15 5	10.5
FOEA	27854-31-5	telomer acid	legacy	476.9	393 413	5	10 5	12.6
FDEA	53826-13-4	telomer acid	legacy	576.9	492.9 512.9	15	15 5	14.0
FHpPA	812-70-4	other	legacy	440.9	336.9 317	15	10 20	12.5
ADONA	958445-44-8	other	emerging	376.9	251 85	10	10 25	10.2
9Cl-PF3ONS	73606-19-6	other	emerging	530.9	350.9 83	15	25 25	12.8

Compound	CAS number	PFAS class	Type	Precursor	Product	CV	CE	RT
11Cl-PF3OUdS	73606-19-6	other	emerging	630.9	450.8 83	30	30 30	14.0
GenX	13252-13-6	other	emerging	285	119 185	5	35 7	9.0
PFMBA	863090-89-5	other	emerging	278.9	85 235	10	10 5	7.0
NFDHA	151772-58-6	other	emerging	294.9	85 201	5	20 10	8.2
PFEESA	113507-82-7	other	emerging	314.9	83 135	15	20 20	7.8
13C-PFBA	–	–	–	216.9	172	10	10	3.6
13C5-PFPeA	–	–	–	267.9	223	10	5	6.3
13C5-PFHxA	–	–	–	317.9	272.9 119.9	10	5 20	8.5
13C4-PFHpA	–	–	–	366.9	321.9 169 172	15	10 15 15	10.1
13C8-PFOA	–	–	–	420.9	375.9 172	5	10 15	11.3
13C9-PFNA	–	–	–	471.9	426.9 223	10	10 15	12.3
13C6-PFDA	–	–	–	518.9	473.9 223	5	10 15	13.1
13C7-PFUnDA	–	–	–	569.9	524.9 274	5	10 15	13.8
13C-PFDoDA	–	–	–	614.9	569.9 169 269.1	10	10 25 20	14.2
13C2-PFTreDA	–	–	–	714.9	669.9 169	25	10 35	14.7
13C2-PFHxDA	–	–	–	815	769.9 169.3	30	15 35	15.0
13C3-PFBS	–	–	–	301.9	80 99	10	30 25	7.0
13C3-PFHxS	–	–	–	401.9	80.1 99.1	10	40 35	10.3
13C8-PFOS	–	–	–	506.9	80.1 99.1	15	40 40	12.3
D5-N-EtFOSAA	–	–	–	589	418.9 506.9	30	20 15	13.8
D3-N-MeFOSAA	–	–	–	572.9	418.9 482.7 514.7	35	20 15 20	13.5
13C-FOUEA	–	–	–	458.9	393.9 119.1	25	10 40	12.6
13C4-8:2 diPAP	–	–	–	993	97.3 544.8	30	40 25	15.0
13C2-4:2 FTS	–	–	–	328.9	308.9 81	40	15 25	8.4
13C2-6:2 FTS	–	–	–	428.9	367 408.8	10	10 20	11.3
13C2-8:2 FTS	–	–	–	528.9	508.9 81	10	20 35	13.1
13C-FHEA	–	–	–	378.9	293.9 64.1	5	10 5	10.5
13C-FOEA	–	–	–	478.9	393.9 64.1	10	15 10	12.6
13C-FDEA	–	–	–	578.9	493.9 64.2	25	5 5	14.0
13C3-GenX	–	–	–	287	169 119	5	12 12	9.0

[APPLICATION NOTE]

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Analysis of Residual Pesticides and Mycotoxins in Cannabis Using UPLC-MS/MS and GC-MS/MS to Meet California Regulatory Requirements

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Rebecca Stevens,[3] James Roush,[3] and Christopher Hudalla[3]
[1]Waters Corporation, Milford, MA, USA; [2]Waters Corporation, Beverly, MA, USA; [3]ProVerde Laboratories, Milford, MA, USA

APPLICATION BENEFITS

- Sensitive and reproducible workflow for screening the California list of pesticides and mycotoxins in cannabis
- Minimal sample preparation followed by rapid UPLC™ and GC separations
- Automated method generation using the Quanpedia™ Pesticide Database
- Ease of use with data analysis and reporting via MassLynx™ MS Software
- Meets or exceeds action levels for pesticides and mycotoxins testing for the State of California

WATERS SOLUTIONS

ACQUITY™ UPLC H-Class System

Xevo™ TQ-S micro Tandem Quadrupole Mass Spectrometer

XBridge™ BEH C_{18} XP Column 2.5 µm, 2.1 x 150 mm

MassLynx MS Software

Dispersive SPE (dSPE) cleanup tube

Xevo TQ-GC Tandem Quadrupole Mass Spectrometer

KEYWORDS

Cannabis, pesticides, mycotoxins, UPLC, TQ-GC, Quanpedia

INTRODUCTION

The increased use of both medical and recreational cannabis in combination with its expanding legal acceptance in several US states[1] has led to demanding cannabis safety and quality control testing. Analytical testing typically includes cannabinoids profiling/potency, mycotoxins, terpenes, residual solvents, metals, and pesticide residues analysis. Pesticides are of particular interest as they are widely used in the cultivation of cannabis plants to safeguard against harmful insects and to promote crop yields. The application of pesticides is strictly regulated,[2] and their residues in cannabis products are closely monitored by state regulatory agencies in order to protect consumers. The number of regulated pesticides that are required to be monitored varies by state as do the action limits which range from 0.01 µg/g (10 ppb) to above 1 µg/g (1 ppm).

In addition to pesticides, cannabis intended for inhalation, ingestion, or topical application must also be tested for mycotoxins. Mycotoxins, including aflatoxins and ochratoxins, are naturally occuring toxins produced by certain strains of mold. This mold, or mycotoxin contamination, can occur during either cultivation or storage and the toxins produced present a serious health risk to consumers. Routine testing for mycotoxins at low levels is critical to ensure the health of consumers, particularly those who may already have compromised health. As with pesticides, a robust and rapid test is critical and single simultaneous test for pesticides and mycotoxins is ideal.

Multi-residue compound detection is routinely performed using tandem quadrupole mass spectrometry (MS/MS) in combination with liquid chromatography (LC) and gas chromatography (GC). Both LC-MS/MS and GC-MS/MS are commonly used for multi-residue pesticide analysis as some residues are only amenable to either LC or GC. Tandem quadrupole MS is the detector of choice as it provides high sensitivity and selectivity for simultaneous analysis of hundreds of pesticides at low ng/g (ppb) levels in a single analysis.

In this application note, we present the use of a simple sample extraction and dSPE cleanup where the resulting extract is analyzed by UPLC-MS/MS and/or GC-MS/MS for rapidly monitoring pesticides and mycotoxins in cannabis matrix to meet California regulations. With the variety of residues to be monitored as well as the continued possibility of new ones being added, method generation can be a tedious task. In this study, full analytical methods full analytical methods including LC, GC and MS methods were utilized from Quanpedia eliminating the need for method development for the California pesticide and mycotoxin lists.

EXPERIMENTAL

Sample preparation

Standard compounds for 66 pesticides and 5 mycotoxins monitored on the California list were combined to produce a stock solution which was sequentially diluted to prepare the spiking solutions. The cannabis buds were first ground using a hand grinder. Aliquots of 0.5 g of ground material were weighed into 50-mL centrifuge tubes and spiked with 0.10 µg/g (100 ppb) and 0.50 µg/g (500 ppb) of the acetonitrile spiking solutions. A 5 mL volume of acetonitrile was added and the samples were processed using a Geno Grinder for 3 minutes (1500 rpm). The mycotoxins were spiked at 0.02 µg/g (20 ppb) and 0.10 µg/g (100 ppb). The samples were then centrifuged at 5000 rpm for 5 minutes.

A 1 mL aliquot of the supernatant was added to a dSPE tube (2 mL centrifuge tube containing 150 mg MgSO$_4$, 50 mg PSA, 50 mg C$_{18}$, 7.5 mg graphitized carbon black) [p/n 186009229], shaken for 1 minute, centrifuged, and the supernatant transferred to a sample vial for analysis by UPLC-MS/MS and/or GC-MS/MS. Extracted matrix that did not contain pesticide residues was used to generate matrix matched calibration curves. Prior to GC-MS/MS analysis, all samples were spiked with an internal standard mix (QuEChERS Internal Standard Mix for GC-MS Analysis from Restek).

Instrumentation and software

LC separations were performed on Waters™ ACQUITY UPLC H-Class System and the Xevo TQ-S micro Tandem Quadrupole Mass Spectrometer. MassLynx MS Software (v4.2) was used for data acquisition and processing. GC separations were performed on the Xevo TQ-GC Tandem Quadrupole Mass Spectrometer using MassLynx MS Software (v4.2) for data acquisition and processing The Quanpedia Database and method generation software was used to automatically generate MRM acquisition and TargetLynx™ processing methods for both LC-MS/MS and GC-MS/MS.

UPLC conditions

UPLC system:	ACQUITY UPLC H-Class
Separation mode:	Gradient
Column:	XBridge C$_{18}$ 2.5 µm, 2.1 × 150 mm
Solvent A:	5 mM ammonium formate with 0.020% formic acid in water
Solvent B:	Methanol
Flow rate:	0.400 mL/min
Column temp.:	50 °C
Injection volume:	5 µL

Gradient conditions:

Time (min)	%A	%B	Curve
0.00	98%	2%	–
0.20	98%	2%	6
4.00	30%	70%	6
10.00	30%	70%	6
12.00	1%	99%	6
15.00	1%	99%	6
15.01	98%	2%	1
17.00	98%	2%	1

MS conditions

MS system:	Xevo TQ-S micro
Ionization mode:	ESI+/ESI-
Capillary voltage:	3.0 kV (+); 2.5 kV (-)
Cone voltage:	Various V
Collision energy:	Various eV
Desolvation temp.:	550 °C
Source temp.:	150 °C
Desolvation gas:	800 (L/hr)
Cone gas:	50 (L/hr)

GC conditions

GC system:	Xevo TQ-GC
Column:	Rxi-5MS 20 m × 0.18 mm × 0.18 µm
Carrier gas:	Helium
Injection type:	Pulsed splitless
Injector temp.:	280 °C
Pulse time:	1.5 min
Pulse pressure:	45 psi
Inlet liner:	Single taper splitless with wool
Flow rate:	2 mL/min
Injection volume:	1 µL

GC oven program

Rate (°C/min)	Temp. (°C)	Hold (min)
—	60	0.45
18.70	330	2.25

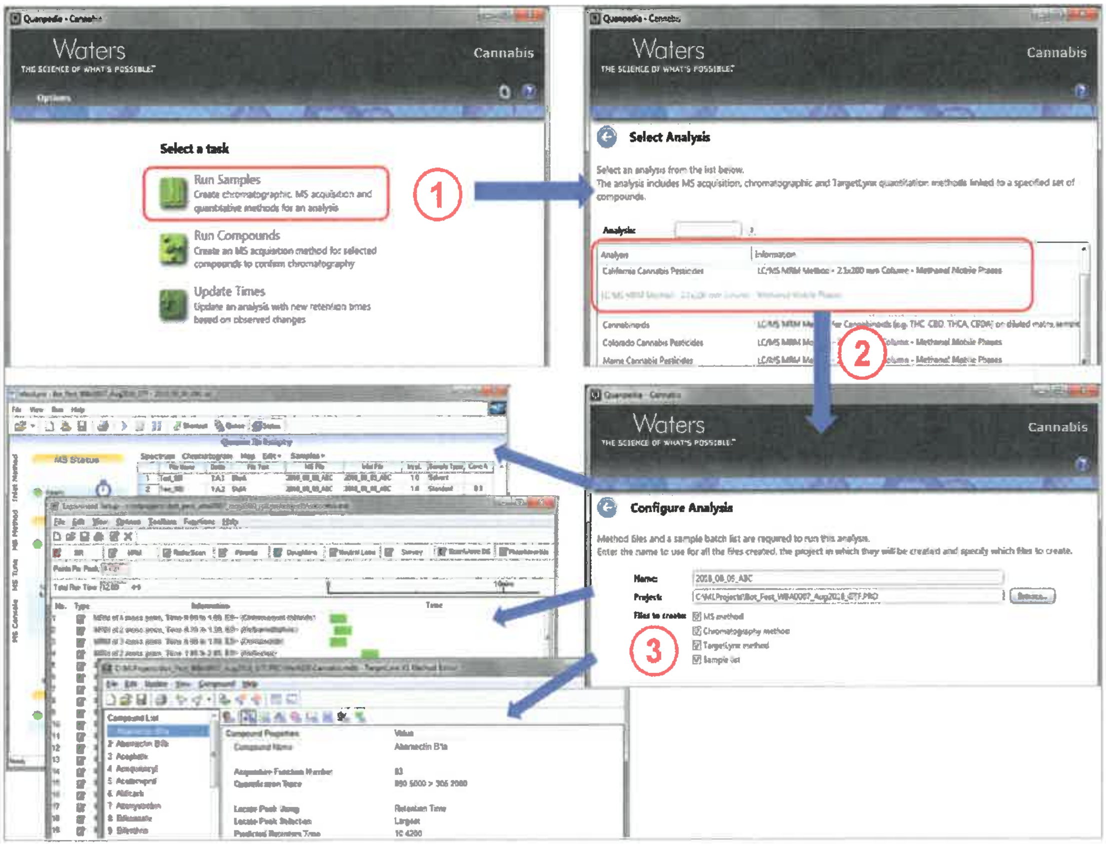
Total run time = 17.14 min

Ionization mode:	EI+, 70 eV
GC interface temp.:	300 °C
Source temp.:	250 °C
MS resolution:	IntelliStart™ Custom Resolution settings were used

RESULTS AND DISCUSSION

METHOD DEVELOPMENT AND OPTIMIZATION

Waters Quanpedia method database was used to automatically create the LC, GC, MS, and data processing methods (Figure 1) for the various target analytes to be monitored using the MRM transitions as listed in Appendix Tables 1 to 3. Users can quickly generate pre-defined LC-MS/MS, and GC-MS/MS methods in just three steps, which eliminates the level of potential error and the complexity involved in method development for large numbers of target analytes. Another advantage is that Quanpedia greatly decreases the amount of work, time, and resources required for laboratories to set up methods. Quanpedia also contains functionality to quickly adjust retention times associated with a method, eliminating the lengthy process of manually adjusting MRM time windows due to retention time shifts. This UPLC-MS/MS method contained 67 compounds (62 pesticides and 5 mycotoxins) and the GC-MS/MS method contained 54 compounds, fully covering the California requirements for pesticide and mycotoxin residue analysis.



Select a task

Run Samples
Create chromatographic, MS acquisition and quantitative methods for an analysis

Run Compounds
Create an MS acquisition method for selected compounds to confirm chromatography

Update Times
Update an analysis with new retention times based on observed changes

Select Analysis

Select an analysis from the list below.
The analysis includes MS acquisition, chromatographic and TargetLynx quantitation methods linked to a specified set of compounds.

Configure Analysis

Method files and a sample batch list are required to run this analysis.
Enter the name to use for all the files created, the project in which they will be created and specify which files to create.

Name: 2018_08_06_ABC
Project: C:\MLProjects\Bot_Fest_WBA0007_Aug2018_GTF.PRO
Files to create: ☑ MS method ☑ Chromatography method ☑ TargetLynx method ☑ Sample list

Figure 1. Rapid implementation of LC, GC, MS and data processing methods using Quanpedia method database.

PESTICIDES ANALYSIS BY LC-MS/MS

Currently, US states and Canada have defined different testing requirements for pesticide residue testing in cannabis. The list of pesticides varies with each state. Furthermore, the composition and complexity of the matrix varies widely across different cannabis strains (or cultivars). The combination of long lists of pesticides with variable and complex matrices presents a significant challenge in method development.

The State of California monitors 66 target pesticides in cannabis.[3] This list completely encompasses the Oregon pesticide[4] list minus MGK-264, and it has additional pesticides including spinetoram, captan, chlordane, pentachloronitrobenzene, chlorpyrifos, coumaphos, dimethomorph, fenhexamid and mevinphos. Representative MRM chromatograms for selected pesticides are displayed in Figure 2. Chromatogram 1 shows the cis and trans-isomers of mevinphos.

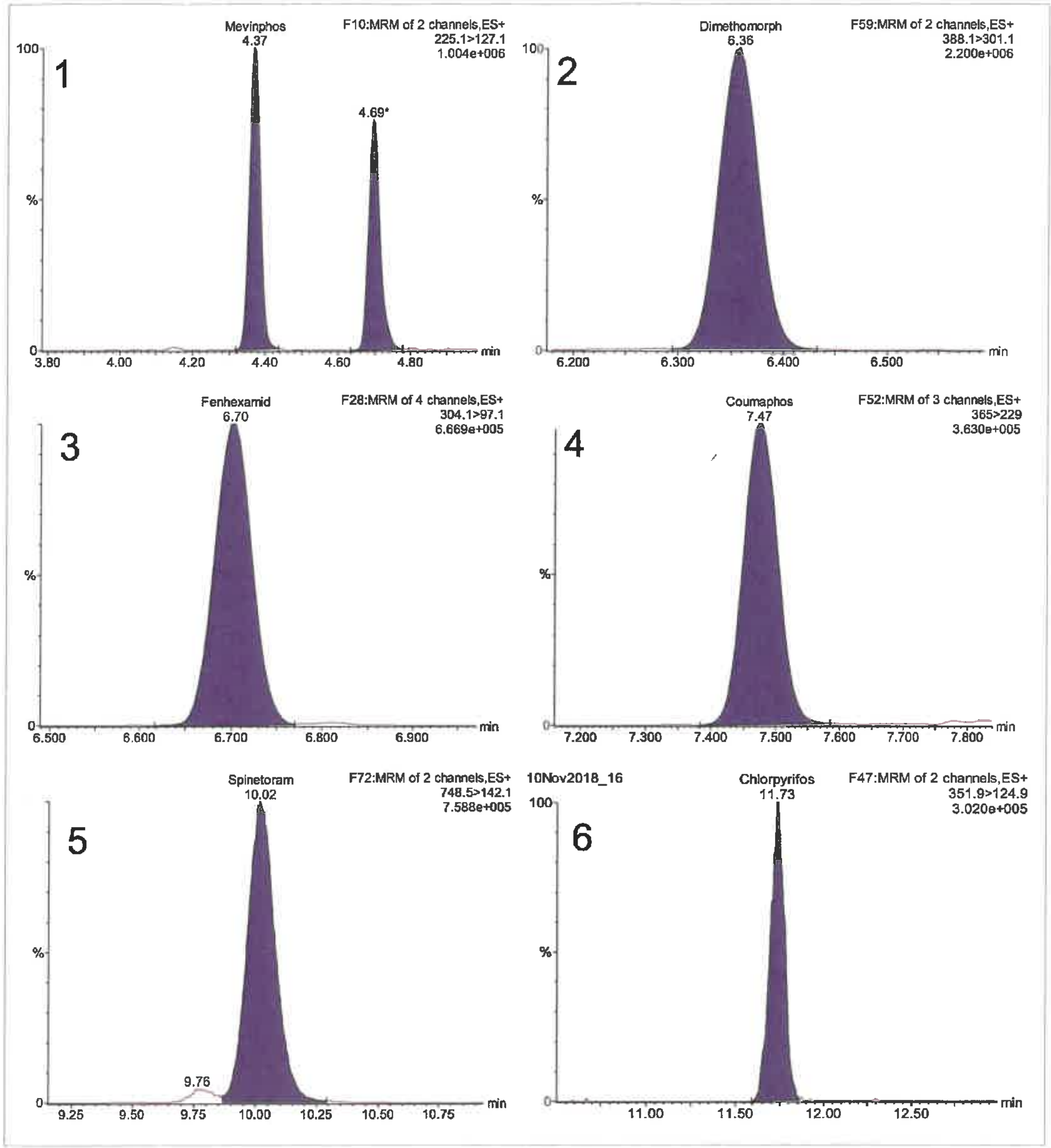
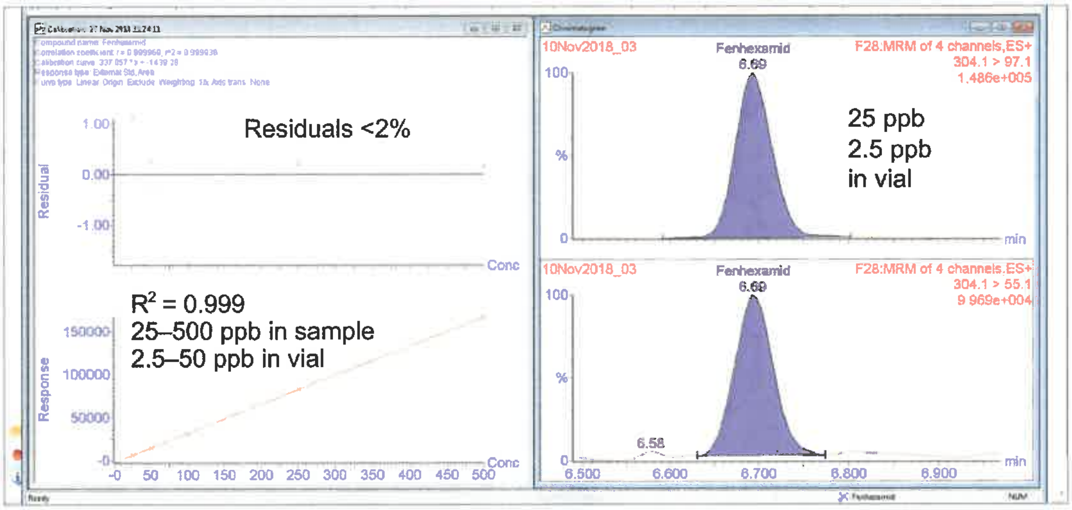


Figure 2. Representative MRM chromatograms for (1) mevinphos isomers, (2) dimethomorph, (3) fenhexamid, (4) coumaphos, (5) spinetoram, (6) chlorpyriphos spiked at a level of 0.10 µg/g in cannabis flower and extracted using the sample preparation protocol reported.

LINEARITY AND SENSITIVITY

Matrix matched calibration curves were generated using blank extracted cannabis. An example of the quantitation curve for the pesticide fenhexamid is shown in Figure 3. Linear calibration curves (R^2>0.990) for all pesticides were obtained over the range tested 0.025 to 0.50 µg/g (25 to 500 ppb in sample or 2.5 to 50 ppb in vial concentration).



Compound name: Fenhexamid
Correlation coefficient: r = 0.999969, r^2 = 0.999938
Calibration curve: 337.057 * x + -1439.28
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

Figure 3. Representative example of a quantitation curve for fenhexamid, demonstrating a linear range from 0.025 to 0.50 µg/g (25 to 500 ppb in sample or 2.5 to 50 ppb in vial concentration).

MULTI-RESIDUE METHOD CHALLENGES

Multi-pesticide residue analysis requires careful attention to the MRM transitions of co-eluting compounds since there can be signal interferences which can lead to inaccurate quantitation. The compounds spinetoram J and spinosad D share common structural features and produce the same primary and secondary ion fragments during collision induced dissociation (CID). The precursor *m/z* for spinosad D is 746.5 and that of spinetoram J is *m/z* 748.5. The isotopic form of spinosad D that contains two carbon-13 atoms gives rise to a signal in the same MRM channel used for analysis of spinetoram J (Figure 4). When both pesticides co-occur in a mixture, accurate quantitation of each individual pesticide requires chromatographic separation as shown in Figure 4.

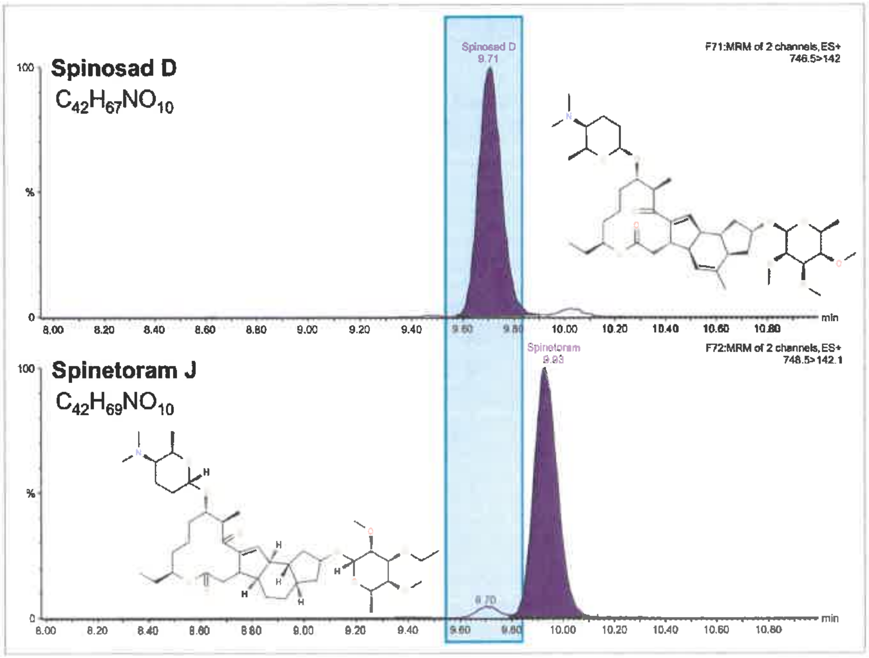


Figure 4. Representative MRM chromatograms for spinosad D and spinetoram J spiked at a level of 0.1 µg/g in cannabis flower and extracted using the sample preparation protocol reported.

MYCOTOXINS ANALYSIS BY LC-MS/MS

The LC-MS/MS analysis of mycotoxins can be combined with the analysis of pesticide residues in a single analytical injection, allowing trace level detection of aflatoxins G2, G1, B2, B1, and ochratoxin A. The calibration curves for all mycotoxins were linear (R^2>0.990) over the range tested 0.005 to 0.10 µg/g (5 to 100 ppb in sample or 0.5 to 10 ppb in vial concentration) in matrix matched calibration curves. Figure 5 shows the chromatograms of cannabis matrix spiked at 0.02 µg/g which is the action level set by the State of California for mycotoxins testing.

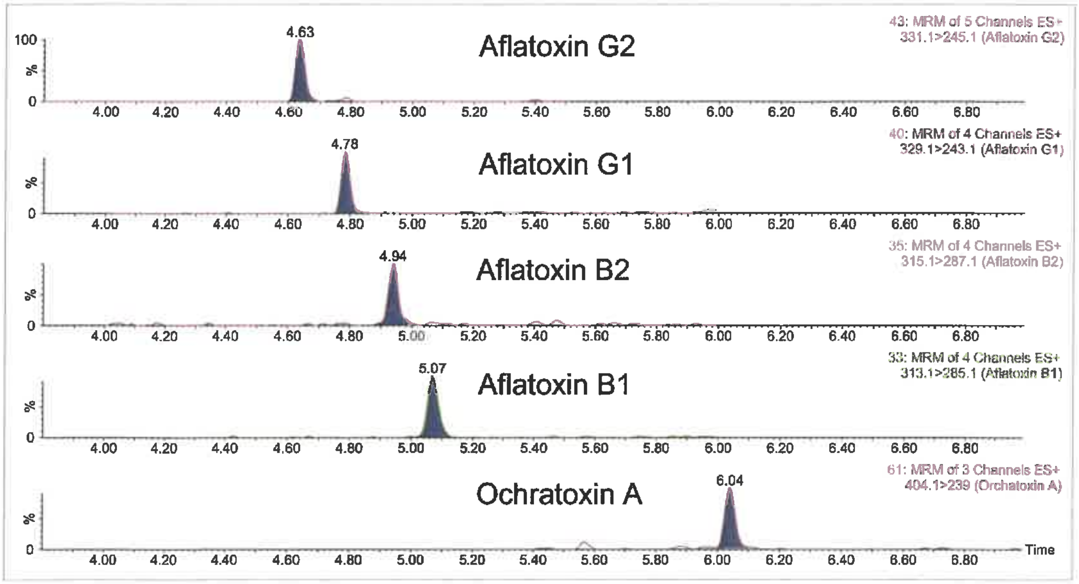


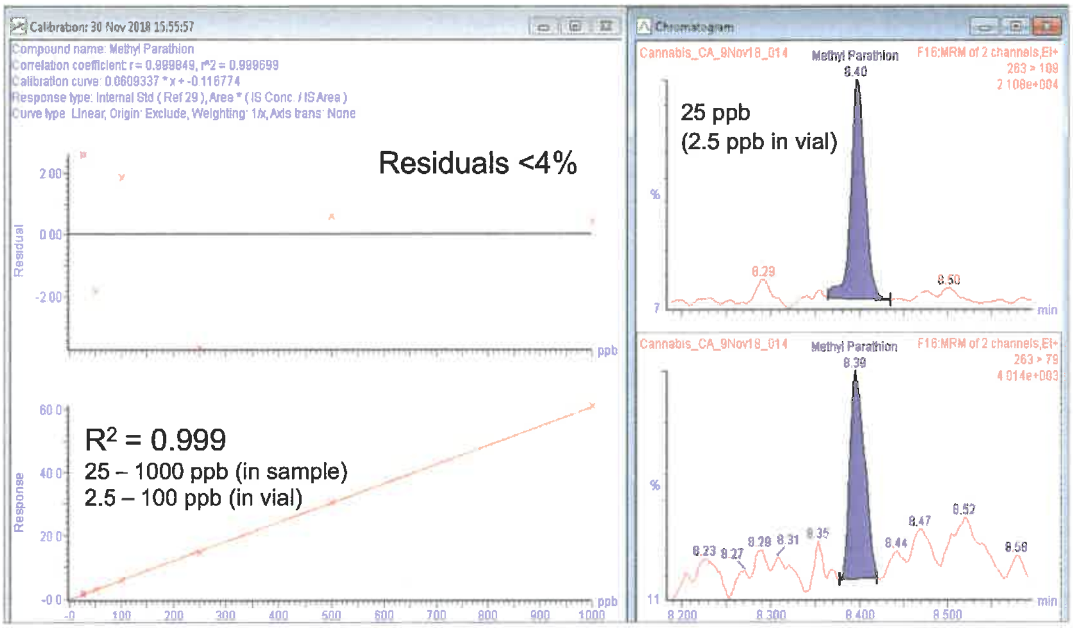
Figure 5. Representative MRM chromatograms for aflatoxins G2, G1, B2, B1, and ochratoxin A spiked at a level of 0.02 µg/g in cannabis matrix.

PESTICIDES ANALYSIS BY GC-MS/MS

Analysis for pesticide residues in the cannabis flower extracts also required GC-MS/MS to fully cover the California pesticide regulations. Compounds like chlordane, captan (analyzed as its degradant THPI), and pentachloronitrobenzene (PCNB) require GC-MS/MS due to poor ionization using electrospray ionization in LC-MS/MS. Conversely, compounds such as bifenthrin ionize well using both LC-MS/MS and GC-MS/MS, but experienced matrix interference to reach the required levels using LC-MS/MS. Additionally, there was a large subset of compounds that worked well using both techniques. Therefore, analysis on both systems allows for increased confidence in results and the GC-MS/MS data can be used as an added confirmatory technique.

LINEARITY AND SENSITIVITY

Matrix matched calibration curves were bracketed around injections of sample extracts. Continuing calibration checks were also run throughout the analysis sequence to ensure system performance was maintained through the runs. Linearity over the range of 0.025 to 1 µg/g (25 to 1000 ppb) was excellent with R^2 values >0.995 and residuals were within 20%. Figure 6 highlights an example of methyl parathion post spiked into the cannabis flower extract showing excellent linearity, residuals, and sensitivity. Figure 7 demonstrates an example of the pesticides that required GC-MS/MS analysis at the action limit extracted in cannabis flower samples. It is important to note that bifenthrin elutes close to the region where THC and other cannabinoids elute and therefore its peak shape is broadened due to the matrix.



Calibration: 30 Nov 2018 15:55:57

Compound name: Methyl Parathion
Correlation coefficient: r = 0.999849, r^2 = 0.999699
Calibration curve: 0.0609337 * x + -0.116774
Response type: Internal Std (Ref 29), Area * (IS Conc. / IS Area)
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

Figure 6. Representative example of a GC-MS/MS quantitation curve for methyl parathion demonstrating a linear range from 0.025 to 1 µg/g (25 to 1000 ppb in sample or 2.5 to 100 ppb in vial concentration).

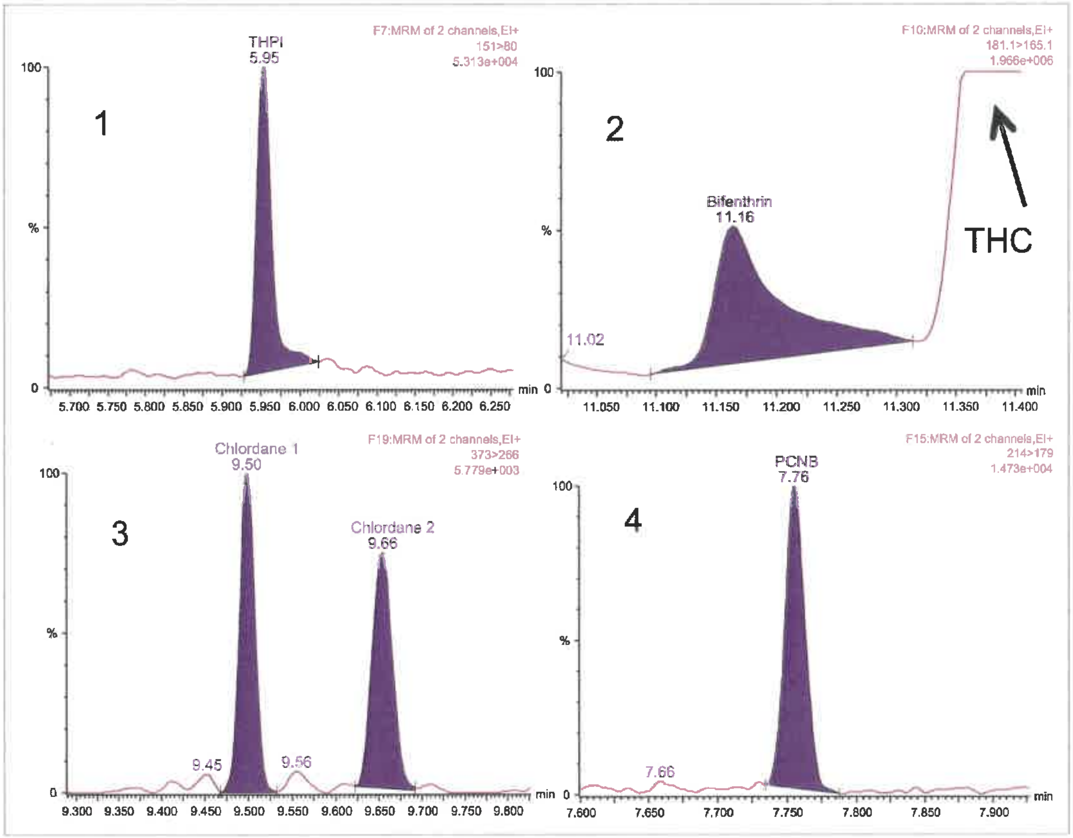


Figure 7. Representative MRM chromatograms for (1) THPI, captan degradation product; (2) bifenthrin; (3) trans and cis chlordane; (4) PCNB spiked at a level of 0.1 µg/g in cannabis flower 0.7 µg/g for THPI) and extracted using the sample preparation protocol reported.

REPRODUCIBILITY OF GC-MS/MS PESTICIDE DATA

Cannabis is a very challenging matrix that can quickly create a loss of response from the inlet liner and source components becoming dirty. It is essential to have a system that is robust enough to hold up to challenging matrices such as cannabis. Reproducibility of the GC-MS/MS response was assessed by injecting 50 replicates of cannabis matrix post spiked with the California pesticide suite at 0.1 µg/g. Figure 8 highlights three of the GC pesticides analyzed over the series of injections. The %RSD of the peak response were below 15% for the majority of the pesticides across the 50 replicate injections.

RECOVERY AND MATRIX EFFECTS

Method recovery was assessed by spiking pesticides at the 0.1 µg/g and 0.5 µg/g levels in cannabis flower and comparing the response to that observed from spiked matrix blanks (matrix matched standards). The mycotoxins were spiked at 0.02 µg/g and 0.10 µg/g. As shown in Figure 9, the recoveries observed for most pesticides were in the range of 80% to 120%. The dSPE cleanup provided significant reduction of matrix suppression for most compounds (data not shown). An example of the benefits of using dSPE to reduce suppression effects can be seen in a previous study using the Oregon list pesticides.[4] Compounds that eluted in the same range as the cannabis resin constituents such as THCA show greater ion suppression compared to compounds that eluted before the resin constituents.

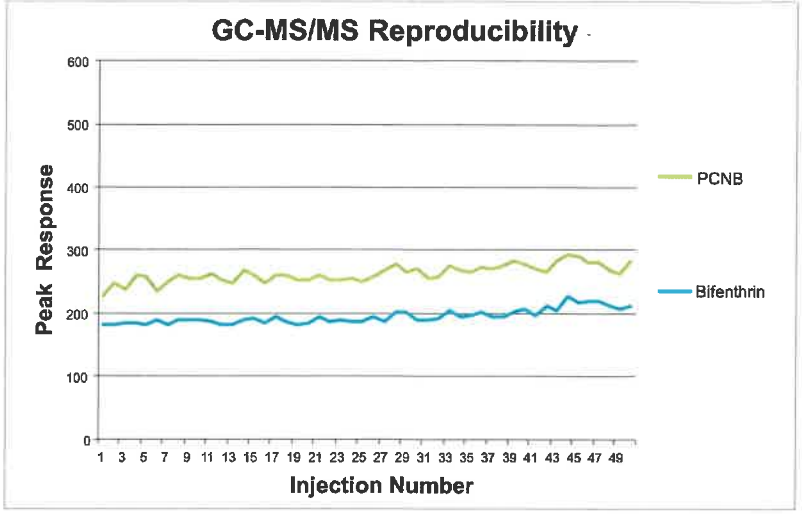


Figure 8. Peak area plotted over 50 replicate injections of cannabis matrix spiked with 0.1 µg/g pesticides highlighting the %RSD for the peak response.

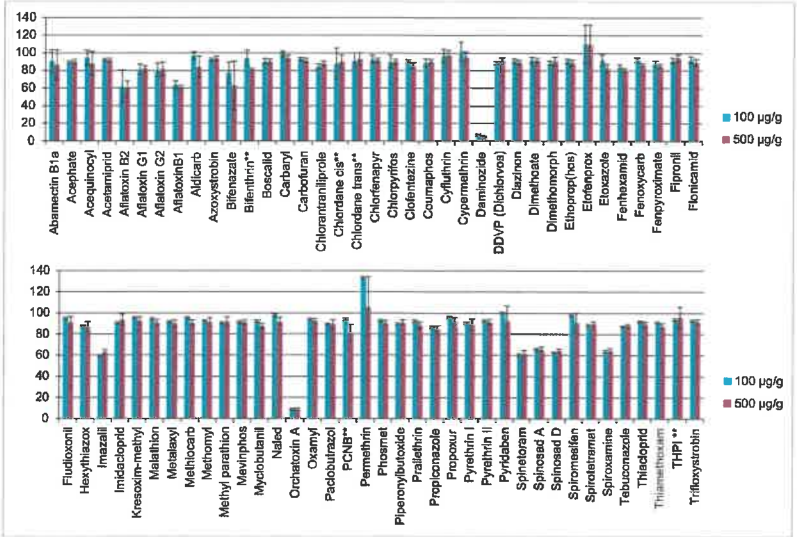


*Figure 9. % recovery of all pesticides and mycotoxins from the cannabis matrix (n = 6). Error bars indicate the standard deviation observed for each compound. Please note the reduced recoveries for ochratoxin A and daminozide are due to their interaction with the PSA sorbent during the dSPE cleanup step. ** Represents the recovery for GC pesticides.*

CONCLUSIONS

This simple sample extraction and dSPE cleanup method followed by UPLC-MS/MS and GC-MS/MS analysis provides a rapid, sensitive, and robust workflow for determination of the California pesticide list and mycotoxins in challenging cannabis matrix. Matrix suppression was significantly reduced using dSPE cleanup for many pesticides; thereby improving the data quality. This method is capable of meeting the action levels for the California pesticide list and mycotoxins in cannabis matrix.

References

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2. California Department of Pesticide Regulation Website, Retrieved on 17 December 2018 from https://www.cdpr.ca.gov/docs/cannabis/index.htm
3. Bureau of Medical Cannabis Regulation, Retrieved on 17 December 2018 from https://www.bcc.ca.gov/law_regs/cannabis_text.pdf
4. K Tran, M Twohig, M Young, A Aubin, N Meruva, G Fujimoto, R Stevens, J Roush, and C Hudalla. Determination of the Oregon Pesticide List in Cannabis Using a Simple Extraction Procedure With dSPE Cleanup and UPLC-MS/MS. Waters application note 720006373en. September 2018.

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Appendix

Appendix Table 1. LC-MS/MS retention times and MRM transitions for the LC amenable pesticides on the California list.

Analytes	Action level (0.1 µg/g)	RT	Quan trace Cone (V), Collision (eV)	Qual trace Cone (V), Collision (eV)
Abamectin	0.1	13.48	890.5>305.1(45,25)	890.5>145 (45,30)
Acephate	0.1	2.96	184>143 (15,6)	184>95 (15,19)
Acequinocyl	0.1	14.53	343.2>189.1 (35,20)	343.2>115 (35,40)
Acetamiprid	0.1	4.36	223>126 (30,20)	223>56.1 (30,15)
Aldicarb	0.1	4.91	208>116 (12,6)	208>89 (12,16)
Azoxystrobin	0.1	5.96	404.1>344.1 (25, 20)	404.1>372 (25,25)
Bifenazate	0.1	6.53	301.16>170.2 (28,22)	301.16>153 (28,28)
Boscalid	0.1	6.22	343>140 (25,20)	343>307 (25,12)
Carbaryl	0.5	5.41	202.1>145 (28,12)	202.1>127 (28,25)
Carbofuran	0.1	5.29	222.1>165 (5, 10)	222.1>123 (5,20)
Chlorantraniliprole	10	5.85	481.9>283.9 (15,23)	481.9>450.9 (15,25)
Chlorfenapyr	0.1	9.54	409.2>59 (58,16)	409.1>379.1 (58,10)
Chlorpyrifos	0.1	11.77	351.9>124.9 (40,19)	351.9>199.9 (40,19)
Cinerin I	0.5	12.8	317.2>149 (28,11)	317.2>107 (28,27)
Cinerin II	0.5	8.7	361.2>149 (28,7)	361.2>107 (28,20)
Clofentezine	0.1	8.05	303>138 (20,15)	303>102 (20,30)
Coumaphos	0.1	7.49	365>229 (40,23)	363>307 (40,15)
Cyfluthrin	2	13.07	451.1>191 (35,17)	453.1>193 (35,17)
Cypermethrin	1	13.25	433.1>191 (15,17)	435.1>193 (15,17)
Daminozide	1	1.2	161>143 (24,12)	161>61 (24,12)
DDVP (Dichlorvos)	0.1	5.25	221>109 (23,22)	221>79 (23,34)
Diazinon	0.1	7.73	305.1>169 (20,22)	305.1>153.1 (20,20)
Dimethoate	0.1	4.36	230>125 (5,10)	230>198.9 (5,20)
Dimethomorph	2	6.37	388.1>301.1 (45,19)	388.1>165.1 (45,30)
Ethoprop(hos)	0.1	6.88	243>130.9 (18,20)	243>97 (18,31)
Etofenprox	0.1	13.67	394.3>177 (26,15)	394.3>106.9 (26,43)
Etoxazole	0.1	12.7	360.2>141 (55,30)	360.2>113 (55,55)
Fenhexamid	0.1	6.71	302.1>97.1 (55,23)	302.1>55.1 (55,33)
Fenoxycarb	0.1	7.11	302.1>88(10,20)	302.1>116.1 (10,11)
Fenpyroximate	0.1	12.89	422.2>366.1 (35,20)	422.2>138.1 (35,30)
Fipronil	0.1	7.07	434.9>330 (42,13)	434.9>250 (42,25)
Flonicamid	0.1	3.74	230.1>203.1 (35,15)	230.1>148.1 (35,35)
Fludioxonil	0.1	6.16	247.2>126 (30,30)	247.2>180.2 (30,28)
Hexythiazox	0.1	12.07	353>228.1 (10,15)	353>168.1 (10,25)
Imazalil	0.1	5.94	297>69 (25,20)	297>159 (25,20)
Imidacloprid	5	4.11	256.1>175.1 (25,20)	256.1>209 (25,15)
Jasmolin I	0.5	13.27	331>121 (25,21)	331>107 (20,20)
Jasmolin II	0.5	10.47	375.2>163 (30,9)	375.2>107 (30,25)
Kresoxim-methyl	0.1	7.36	314.1>116 (5,15)	314.1>235 (5,20)
Malathion	0.5	6.3	331.1>127 (12,20)	331.1>285 (12,12)
Metalaxyl	2	5.77	280.2>220.1 (10,10)	280.2>192 (10,10)
Methiocarb	0.1	6.18	226>169 (25,10)	226>121 (25,20)
Methomyl	1	3.67	163.1>88 (10,10)	163.1>106 (10,10)
Methyl parathion	0.1	6.04	264.15>125.1 (38,18)	264.15>232.1 (38,14)
Mevinphos	0.1	4.37	225.1>127.1 (15,15)	225.1>193.1 (15,10)
Myclobutanil	0.1	6.45	289.122>69.97 (30,20)	289.122>125 (30,38)
Naled	0.1	5.85	381>127 (30,17)	381>109 (30,27)
Oxamyl	0.5	3.51	237.1>72.1 (5,10)	237.1>90.1 (5,10)
Paclobutrazol	0.1	6.32	294.1>70.2 (10,20)	294.1>125.1 (10,35)
Permethrin	0.5	13.49	408.1>183 (20,22)	410.1>185 (20,22)
Phosmet	0.1	5.88	318>160 (28,22)	318>133 (28,20)
Piperonylbutoxide	3	11.01	356.2>177.1 (20,10)	356.2>119 (20,35)
Prallethrin	0.1	8.92	301.2>133 (5,12)	301.2>169 (5,9)
Propiconazole	0.1	7.75	342.1>158.9 (15,25)	342.1>69 (15,20)
Propoxur	0.1	5.27	210.1>111 (15,15)	210.1>168 (15,5)
Pyrethrin I	0.5	12.91	329.1>161 (18,8)	329.1>133 (18,16)
Pyrethrin II	0.5	8.99	373.2>161 (37,8)	373.2>133 (37,19)
Pyridaben	0.1	13.25	365.2>147.1 (5,24)	365.2>309 (5,12)
Spinetoram	0.1	10.02	748.5>142.1 (75,30)	748.5>98.1 (75,60)
Spinosad A	0.1	8.38	732.6>142 (35,30)	732.6>98.1 (35,35)
Spinosad D	0.1	9.78	746.5>142 (40,31)	746.5>98.1 (40,35)
Spiromesifen	0.1	12.63	388.2>273.1 (28,14)	371.2>273.1 (43,10)
Spirotetramat	0.1	6.62	374>330 (20,15)	374>302 (20,30)
Spiroxamine	0.1	6.23	298>144 (40,20)	298>100 (40,32)
Tebuconazole	0.1	7.51	308.2>70.1 (10,20)	308.2>125 (10,35)
Thiacloprid	0.1	4.57	253>126 (40,20)	253>90.1 (40,35)
Thiamethoxam	5	3.74	292>211.2 (25,10)	292>132 (25,20)
Trifloxystrobin	0.1	9.18	409.1>186 (10,16)	409.1>145 (10,40)

Appendix Table 2. LC-MS/MS retention times and MRM transitions for mycotoxins on the California list.

Analytes	Action level (0.1 µg/g)	RT	Quan trace Cone (V), Collision (eV)	Qual trace Cone (V), Collision (eV)
AflatoxinB1	0.02	5.07	313.1>285.1 (35,21)	313.1>241.1 (35,35)
Aflatoxin B2	0.02	4.94	315.1>259.1 (35,28)	315.1>287.1(35,25)
Aflatoxin G1	0.02	4.79	329.1>243.1 (35,25)	329.1>311.1 (35,21)
Aflatoxin G2	0.02	4.64	331.1>245.1 (35,28)	331.1>189 (35,40)
Ochratoxin A	0.02	6.04	404.1>239 (45,23)	404.1>358.1 (45,13)

Appendix Table 3. GC-MS/MS retention times and MRM transitions for the GC amenable pesticides on the California list.

Pesticide	Action level (µg/g)	RT	Quan trace (CE)	Qual trace 1 (CE)
Acephate	0.1	5.7	136>94 (14)	136>42(10)
Acequinocyl	0.1	12.53	342>188(16)	189>115(26)
Azoxystrobin	0.1	13.39	344>172(44)	344>156(32)
Bifenazate	0.1	11.03	199>184(12)	300>258 (10)
Bifenthrin	3	11.03	181.1>165.1 (30)	181.1>166.1 (17)
Boscalid	0.1	12.44	140>112 (14)	140>76 (23)
Captan	0.7	9.2	114>79 (12)	79>77 (12)
Carbaryl	0.5	8.34	144>115 (26)	144>116 (16)
Carbofuran	0.1	7.44	164>103 (29)	164>149 (14)
Chlorantraniliprole	10	11.1	278>249 (25)	278>215 (24)
Chlordane, trans	0.1	9.35	375>266 (24)	373>266 (28)
Chlordane, cis	0.1	9.5	375>266 (24)	373>266 (28)
Chlorfenapyr	0.1	9.99	59>31 (6)	59>29 (8)
Chlorpyrifos	0.1	8.78	197>168.9 (14)	197>107 (38)
Coumaphos	0.1	12.03	362>109 (17)	210>182 (12)
Cyfluthrin 1	2	12.25	163>127(8)	226>206 (20)
Cyfluthrin 2	2	12.29	163>127 (8)	226>206 (20)
Cyfluthrin 3/4	2	12.34	163>127 (8)	226>206 (20)
Cypermethrin 1	1	12.39	163>127 (9)	163>91 (14)
Cypermethrin 2	1	12.39	163>127 (9)	163>91 (14)
Cypermethrin 3/4	1	12.39	163>127 (9)	163>91 (14)
Diazinon	0.1	7.77	137>84 (18)	199>93 (17)
Dichlorvos	0.1	4.25	185>93 (14)	109>79 (9)
Dimethoate	0.1	7.36	125>47 (12)	125>79 (10)
Dimethomorph	2	13.41	301>165 (14)	301>152 (48)
Ethoprophos	0.1	6.8	158>97 (15)	158>114 (7)
Etofenprox	0.1	12.55	163.1>107.1 (20)	163.1>135 (12)
Etoxazole	0.1	11.1	141>113 (17)	141>63.1 (28)
Fenhexamid	0.1	10.5	177>113 (16)	177>78 (24)
Fenoxycarb	0.1	11.01	116>88 (12)	255>186 (14)
Fenpyroximate	0.1	7.43	213>77 (25)	213>212 (15)
Fipronil	0.1	9.22	367>213 (38)	369>215 (38)
Flonicamid	0.1	6.66	174>69 (32)	146>126 (10)
Fludioxonil	0.1	9.72	248>154.1 (26)	248>182 (22)
Hexythiazox	0.1	9.4	155>111 (20)	155>120 (25)
Imazalil	0.1	9.53	215>173 (9)	217>175 (9)
Kresoxim-methyl	0.1	9.87	116>89 (15)	116>63 (24)
Malathion	0.5	8.67	173>99 (19)	173>127 (12)
Metalaxyl	2	8.41	160>130 (18)	160>145 (12)
Methiocarb	0.1	8.57	168>153 (14)	153>109 (10)
Methyl parathion	0.1	8.26	263>109 (16)	263>79 (30)
Mevinphos	0.1	5.52	127>109 (12)	192>127 (14)
Myclobutanil	0.1	9.81	179>125.1 (20)	179>152 (12)
Paclobutrazol	0.1	9.43	236>125 (18)	238>127 (16)
PCNB	0.1	7.61	214>179 (14)	295>237 (25)
Permethrin 1	0.5	11.97	163>127 (5)	165>129 (5)
Permethrin 2	0.5	12.03	163>127 (5)	165>129 (5)
Phosmet	0.1	10.97	160.1>77.1 (24)	160>133 (15)
Piperonyl butoxide	3	10.81	176>103 (26)	176>131 (12)
Prallethrin	0.1	9.35	123>81 (10)	123>79 (15)
Propiconazole 1	0.1	10.46	173>109 (26)	173>144.9 (19)
Propiconazole 2	0.1	10.52	173>109 (26)	173>144.9 (19)
Propoxur (Baygon)	0.1	6.67	110>64 (17)	110>63 (21)
Pyrethrin I	0.5	9.84	123>81 (10)	123>79 (15)
Pyrethrin II	0.5	10.35	133>105 (12)	133>91 (15)
Pyridaben	0.1	12.04	148>117 (24)	148>132 (16)
Spiromesifen	0.1	10.9	272>209 (17)	272>254 (8)
Spiroxamine 1	0.1	8.26	100>58 (15)	100>72 (13)
Spiroxamine 2	0.1	8.54	100>58 (15)	100>72 (13)
Tebuconazole	0.1	10.63	250.1>125 (30)	252.1>127 (28)
Thiamethoxam	5	9.05	212>139 (30)	212>125 (14)
THPI (captan)	0.7	5.83	151>80 (5)	151>77 (30)
Trifloxystrobin	0.1	10.51	116>89 (15)	116>63 (26)
Triphenylphosphate*	-	10.69	325>169 (24)	326>215 (20)
PCB 18*	-	7.67	256>186 (15)	258>186 (15)
PCB 28*	-	8.18	256>186 (15)	258>186 (15)
PCB 52*	-	8.54	290>220 (23)	292>220 (23)

** Indicates compound used as internal standard.*

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Melissa Pettrey
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melissa.k.pettrey@wv.gov

Signature X Kristen A **FEIN #** 04-3234558 **DATE** 4/25/19

All offers subject to all terms and conditions contained in this solicitation

ADDITIONAL INFORMATION:

Central Request for Quotation

The West Virginia Purchasing Division is soliciting bids on behalf of the Agency, the West Virginia Department of Agriculture to establish a contract for the one time purchase of a Liquid Chromatography Triple Quadrupole Mass Spectrometer (LC/MS/MS), workstation PC, software, printer, nitrogen generator, uninterrupted power supply (UPS), specific test methods, shipping, installation, validation, warranty, training and service per the bid requirements, specifications, terms and conditions attached to this solicitation.

INVOICE TO	SHIP TO
PROCUREMENT OFFICER 304-558-2221 AGRICULTURE DEPARTMENT OF ADMINISTRATIVE SERVICES 1900 KANAWHA BLVD E CHARLESTON WV25305-0173 US	AUTHORIZED RECEIVER 304-558-2227 AGRICULTURE DEPARTMENT OF REGULATORY PROTECTION DIVISION 313 GUS R DOUGLAS LN, BLDG 11 CHARLESTON WV 25312 US

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Total Price
1	LC/MS/MS, Workstation PC, Software, Printer, nitrogen	1.00000	EA		

Comm Code	Manufacturer	Specification	Model #
41100000			

Extended Description :

generator, uninterrupted power supply, specific test methods per section 3.1

INVOICE TO	SHIP TO
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Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Total Price
2	shipping charges & inside delivery	1.00000	EA		

Comm Code	Manufacturer	Specification	Model #
78121603			

Extended Description :

Shipping charges & inside delivery per section 3.1.6

INVOICE TO	SHIP TO
PROCUREMENT OFFICER 304-558-2221 AGRICULTURE DEPARTMENT OF ADMINISTRATIVE SERVICES 1900 KANAWHA BLVD E CHARLESTON WV25305-0173 US	AUTHORIZED RECEIVER 304-558-2227 AGRICULTURE DEPARTMENT OF REGULATORY PROTECTION DIVISION 313 GUS R DOUGLAS LN, BLDG 11 CHARLESTON WV 25312 US

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Total Price
3	Installation/validation	1.00000	EA		

Comm Code	Manufacturer	Specification	Model #
73171605			

Extended Description :

Installation/Validation per section 3.1.6

INVOICE TO	SHIP TO
PROCUREMENT OFFICER 304-558-2221 AGRICULTURE DEPARTMENT OF ADMINISTRATIVE SERVICES 1900 KANAWHA BLVD E CHARLESTON WV25305-0173 US	AUTHORIZED RECEIVER 304-558-2227 AGRICULTURE DEPARTMENT OF REGULATORY PROTECTION DIVISION 313 GUS R DOUGLAS LN, BLDG 11 CHARLESTON WV 25312 US

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Total Price
4	Training/warranty	1.00000	EA		

Comm Code	Manufacturer	Specification	Model #
73171605			

Extended Description :

Training/Warranty per section 3.1.6

INVOICE TO	SHIP TO
PROCUREMENT OFFICER 304-558-2221 AGRICULTURE DEPARTMENT OF ADMINISTRATIVE SERVICES 1900 KANAWHA BLVD E CHARLESTON WV25305-0173 US	AUTHORIZED RECEIVER 304-558-2227 AGRICULTURE DEPARTMENT OF REGULATORY PROTECTION DIVISION 313 GUS R DOUGLAS LN, BLDG 11 CHARLESTON WV 25312 US

Line	Comm Ln Desc	Qty	Unit Issue	Unit Price	Total Price
5	Service	1.00000	EA		

Comm Code	Manufacturer	Specification	Model #
73171605			

Extended Description :

Service per section 3.1.6

INSTRUCTIONS TO VENDORS SUBMITTING BIDS

1. REVIEW DOCUMENTS THOROUGHLY: The attached documents contain a solicitation for bids. Please read these instructions and all documents attached in their entirety. These instructions provide critical information about requirements that if overlooked could lead to disqualification of a Vendor's bid. All bids must be submitted in accordance with the provisions contained in these instructions and the Solicitation. Failure to do so may result in disqualification of Vendor's bid.

2. MANDATORY TERMS: The Solicitation may contain mandatory provisions identified by the use of the words "must," "will," and "shall." Failure to comply with a mandatory term in the Solicitation will result in bid disqualification.

3. PREBID MEETING: The item identified below shall apply to this Solicitation.

☑ A pre-bid meeting will not be held prior to bid opening

☐ A **NON-MANDATORY PRE-BID** meeting will be held at the following place and time:

☐ A **MANDATORY PRE-BID** meeting will be held at the following place and time:

All Vendors submitting a bid must attend the mandatory pre-bid meeting. Failure to attend the mandatory pre-bid meeting shall result in disqualification of the Vendor's bid. No one person attending the pre-bid meeting may represent more than one Vendor.

An attendance sheet provided at the pre-bid meeting shall serve as the official document verifying attendance. The State will not accept any other form of proof or documentation to verify attendance. Any person attending the pre-bid meeting on behalf of a Vendor must list on the attendance sheet his or her name and the name of the Vendor he or she is representing.

Additionally, the person attending the pre-bid meeting should include the Vendor's E-Mail address, phone number, and Fax number on the attendance sheet. It is the Vendor's responsibility to locate the attendance sheet and provide the required information. Failure to complete the attendance sheet as required may result in disqualification of Vendor's bid.

All Vendors should arrive prior to the starting time for the pre-bid. Vendors who arrive after the starting time but prior to the end of the pre-bid will be permitted to sign in, but are charged with knowing all matters discussed at the pre-bid.

Questions submitted at least five business days prior to a scheduled pre-bid will be discussed at the pre-bid meeting if possible. Any discussions or answers to questions at the pre-bid meeting are preliminary in nature and are non-binding. Official and binding answers to questions will be published in a written addendum to the Solicitation prior to bid opening.

4. VENDOR QUESTION DEADLINE: Vendors may submit questions relating to this Solicitation to the Purchasing Division. Questions must be submitted in writing. All questions must be submitted on or before the date listed below and to the address listed below in order to be considered. A written response will be published in a Solicitation addendum if a response is possible and appropriate. Non-written discussions, conversations, or questions and answers regarding this Solicitation are preliminary in nature and are nonbinding.

Submitted e-mails should have solicitation number in the subject line.

Question Submission Deadline: 04/17/2019 @ 3:00 P.M. EDT

Submit Questions to: Melissa Pettrey, Senior Buyer
2019 Washington Street, East
Charleston, WV 25305
Fax: (304) 558-4115 (Vendors should not use this fax number for bid submission)
Email: melissa.k.pettrey@wv.gov

5. VERBAL COMMUNICATION: Any verbal communication between the Vendor and any State personnel is not binding, including verbal communication at the mandatory pre-bid conference. Only information issued in writing and added to the Solicitation by an official written addendum by the Purchasing Division is binding.

6. BID SUBMISSION: All bids must be submitted electronically through wvOASIS or signed and delivered by the Vendor to the Purchasing Division at the address listed below on or before the date and time of the bid opening. Any bid received by the Purchasing Division staff is considered to be in the possession of the Purchasing Division and will not be returned for any reason. The Purchasing Division will not accept bids, modification of bids, or addendum acknowledgment forms via e-mail. Acceptable delivery methods include electronic submission via wvOASIS, hand delivery, delivery by courier, or facsimile.

The bid delivery address is:
Department of Administration, Purchasing Division
2019 Washington Street East
Charleston, WV 25305-0130

A bid that is not submitted electronically through wvOASIS should contain the information listed below on the face of the envelope or the bid may be rejected by the Purchasing Division.:

SEALED BID: CRFQ AGR1900000018
BUYER: Melissa Pettre, Senior Buyer
SOLICITATION NO.:
BID OPENING DATE: 04/26/2019
BID OPENING TIME: 1:30 P.M. EDT
FAX NUMBER: 304-558-3970

The Purchasing Division may prohibit the submission of bids electronically through wvOASIS at its sole discretion. Such a prohibition will be contained and communicated in the wvOASIS system resulting in the Vendor's inability to submit bids through wvOASIS. Submission of a response to an Expression or Interest or Request for Proposal is not permitted in wvOASIS.

For Request For Proposal ("RFP") Responses Only: In the event that Vendor is responding to a request for proposal, the Vendor shall submit one original technical and one original cost proposal plus ________________convenience copies of each to the Purchasing Division at the address shown above. Additionally, the Vendor should identify the bid type as either a technical or cost proposal on the face of each bid envelope submitted in response to a request for proposal as follows:

BID TYPE: (This only applies to CRFP)
☐ Technical
☐ Cost

7. **BID OPENING:** Bids submitted in response to this Solicitation will be opened at the location identified below on the date and time listed below. Delivery of a bid after the bid opening date and time will result in bid disqualification. For purposes of this Solicitation, a bid is considered delivered when confirmation of delivery is provided by wvOASIS (in the case of electronic submission) or when the bid is time stamped by the official Purchasing Division time clock (in the case of hand delivery).

Bid Opening Date and Time: 04/26/2019 @ 1:30 P.M. EDT

Bid Opening Location: Department of Administration, Purchasing Division
2019 Washington Street East
Charleston, WV 25305-0130

8. ADDENDUM ACKNOWLEDGEMENT: Changes or revisions to this Solicitation will be made by an official written addendum issued by the Purchasing Division. Vendor should acknowledge receipt of all addenda issued with this Solicitation by completing an Addendum Acknowledgment Form, a copy of which is included herewith. Failure to acknowledge addenda may result in bid disqualification. The addendum acknowledgement should be submitted with the bid to expedite document processing.

9. BID FORMATTING: Vendor should type or electronically enter the information onto its bid to prevent errors in the evaluation. Failure to type or electronically enter the information may result in bid disqualification.

10. ALTERNATE MODEL OR BRAND: Unless the box below is checked, any model, brand, or specification listed in this Solicitation establishes the acceptable level of quality only and is not intended to reflect a preference for, or in any way favor, a particular brand or vendor. Vendors may bid alternates to a listed model or brand provided that the alternate is at least equal to the model or brand and complies with the required specifications. The equality of any alternate being bid shall be determined by the State at its sole discretion. Any Vendor bidding an alternate model or brand should clearly identify the alternate items in its bid and should include manufacturer's specifications, industry literature, and/or any other relevant documentation demonstrating the equality of the alternate items. Failure to provide information for alternate items may be grounds for rejection of a Vendor's bid.

☐ This Solicitation is based upon a standardized commodity established under W. Va. Code § 5A-3-61. Vendors are expected to bid the standardized commodity identified. Failure to bid the standardized commodity will result in your firm's bid being rejected.

11. EXCEPTIONS AND CLARIFICATIONS: The Solicitation contains the specifications that shall form the basis of a contractual agreement. Vendor shall clearly mark any exceptions, clarifications, or other proposed modifications in its bid. Exceptions to, clarifications of, or modifications of a requirement or term and condition of the Solicitation may result in bid disqualification.

12. COMMUNICATION LIMITATIONS: In accordance with West Virginia Code of State Rules §148-1-6.6, communication with the State of West Virginia or any of its employees regarding this Solicitation during the solicitation, bid, evaluation or award periods, except through the Purchasing Division, is strictly prohibited without prior Purchasing Division approval. Purchasing Division approval for such communication is implied for all agency delegated and exempt purchases.

13. REGISTRATION: Prior to Contract award, the apparent successful Vendor must be properly registered with the West Virginia Purchasing Division and must have paid the $125 fee, if applicable.

14. UNIT PRICE: Unit prices shall prevail in cases of a discrepancy in the Vendor's bid.

15. PREFERENCE: Vendor Preference may be requested in purchases of motor vehicles or construction and maintenance equipment and machinery used in highway and other infrastructure projects. Any request for preference must be submitted in writing with the bid, must specifically identify the preference requested with reference to the applicable subsection of West Virginia Code § 5A-3-37, and should include with the bid any information necessary to evaluate and confirm the applicability of the requested preference. A request form to help facilitate the request can be found at: http://www.state.wv.us/admin/purchase/vrc/Venpref.pdf.

15A. RECIPROCAL PREFERENCE: The State of West Virginia applies a reciprocal preference to all solicitations for commodities and printing in accordance with W. Va. Code § 5A-3-37(b). In effect, non-resident vendors receiving a preference in their home states, will see that same preference granted to West Virginia resident vendors bidding against them in West Virginia. A request form to help facilitate the request can be found at: http://www.state.wv.us/admin/purchase/vrc/Venpref.pdf.

16. SMALL, WOMEN-OWNED, OR MINORITY-OWNED BUSINESSES: For any solicitations publicly advertised for bid, in accordance with West Virginia Code §5A-3-37(a)(7) and W. Va. CSR § 148-22-9, any non-resident vendor certified as a small, women-owned, or minority-owned business under W. Va. CSR § 148-22-9 shall be provided the same preference made available to any resident vendor. Any non-resident small, women-owned, or minority-owned business must identify itself as such in writing, must submit that writing to the Purchasing Division with its bid, and must be properly certified under W. Va. CSR § 148-22-9 prior to contract award to receive the preferences made available to resident vendors. Preference for a non-resident small, women-owned, or minority owned business shall be applied in accordance with W. Va. CSR § 148-22-9.

17. WAIVER OF MINOR IRREGULARITIES: The Director reserves the right to waive minor irregularities in bids or specifications in accordance with West Virginia Code of State Rules § 148-1-4.6.

18. ELECTRONIC FILE ACCESS RESTRICTIONS: Vendor must ensure that its submission in wvOASIS can be accessed and viewed by the Purchasing Division staff immediately upon bid opening. The Purchasing Division will consider any file that cannot be immediately accessed and viewed at the time of the bid opening (such as, encrypted files, password protected files, or incompatible files) to be blank or incomplete as context requires, and are therefore unacceptable. A vendor will not be permitted to unencrypt files, remove password protections, or resubmit documents after bid opening to make a file viewable if those documents are required with the bid. A Vendor may be required to provide document passwords or remove access restrictions to allow the Purchasing Division to print or electronically save documents provided that those documents are viewable by the Purchasing Division prior to obtaining the password or removing the access restriction.

19. NON-RESPONSIBLE: The Purchasing Division Director reserves the right to reject the bid of any vendor as Non-Responsible in accordance with W. Va. Code of State Rules § 148-1-5.3, when the Director determines that the vendor submitting the bid does not have the capability to fully perform, or lacks the integrity and reliability to assure good-faith performance."

20. ACCEPTANCE/REJECTION: The State may accept or reject any bid in whole, or in part in accordance with W. Va. Code of State Rules § 148-1-4.5. and § 148-1-6.4.b."

21. YOUR SUBMISSION IS A PUBLIC DOCUMENT: Vendor's entire response to the Solicitation and the resulting Contract are public documents. As public documents, they will be disclosed to the public following the bid/proposal opening or award of the contract, as required by the competitive bidding laws of West Virginia Code §§ 5A-3-1 et seq., 5-22-1 et seq., and 5G-1-1 et seq. and the Freedom of Information Act West Virginia Code §§ 29B-1-1 et seq.

DO NOT SUBMIT MATERIAL YOU CONSIDER TO BE CONFIDENTIAL, A TRADE SECRET, OR OTHERWISE NOT SUBJECT TO PUBLIC DISCLOSURE.

Submission of any bid, proposal, or other document to the Purchasing Division constitutes your explicit consent to the subsequent public disclosure of the bid, proposal, or document. The Purchasing Division will disclose any document labeled "confidential," "proprietary," "trade secret," "private," or labeled with any other claim against public disclosure of the documents, to include any "trade secrets" as defined by West Virginia Code § 47-22-1 et seq. All submissions are subject to public disclosure without notice.

22. INTERESTED PARTY DISCLOSURE: West Virginia Code § 6D-1-2 requires that the vendor submit to the Purchasing Division a disclosure of interested parties to the contract for all contracts with an actual or estimated value of at least $1 Million. That disclosure must occur on the form prescribed and approved by the WV Ethics Commission prior to contract award. A copy of that form is included with this solicitation or can be obtained from the WV Ethics Commission. This requirement does not apply to publicly traded companies listed on a national or international stock exchange. A more detailed definition of interested parties can be obtained from the form referenced above.

23. WITH THE BID REQUIREMENTS: In instances where these specifications require documentation or other information with the bid, and a vendor fails to provide it with the bid, the Director of the Purchasing Division reserves the right to request those items after bid opening and prior to contract award pursuant to the authority to waive minor irregularities in bids or specifications under W. Va. CSR § 148-1-4.6. This authority does not apply to instances where state law mandates receipt with the bid.

GENERAL TERMS AND CONDITIONS:

1. CONTRACTUAL AGREEMENT: Issuance of a Award Document signed by the Purchasing Division Director, or his designee, and approved as to form by the Attorney General's office constitutes acceptance of this Contract made by and between the State of West Virginia and the Vendor. Vendor's signature on its bid signifies Vendor's agreement to be bound by and accept the terms and conditions contained in this Contract.

2. DEFINITIONS: As used in this Solicitation/Contract, the following terms shall have the meanings attributed to them below. Additional definitions may be found in the specifications included with this Solicitation/Contract.

2.1. "Agency" or **"Agencies"** means the agency, board, commission, or other entity of the State of West Virginia that is identified on the first page of the Solicitation or any other public entity seeking to procure goods or services under this Contract.

2.2. "Bid" or **"Proposal"** means the vendors submitted response to this solicitation.

2.3. "Contract" means the binding agreement that is entered into between the State and the Vendor to provide the goods or services requested in the Solicitation.

2.4. "Director" means the Director of the West Virginia Department of Administration, Purchasing Division.

2.5. "Purchasing Division" means the West Virginia Department of Administration, Purchasing Division.

2.6. "Award Document" means the document signed by the Agency and the Purchasing Division, and approved as to form by the Attorney General, that identifies the Vendor as the contract holder.

2.7. "Solicitation" means the official notice of an opportunity to supply the State with goods or services that is published by the Purchasing Division.

2.8. "State" means the State of West Virginia and/or any of its agencies, commissions, boards, etc. as context requires.

2.9. "Vendor" or **"Vendors"** means any entity submitting a bid in response to the Solicitation, the entity that has been selected as the lowest responsible bidder, or the entity that has been awarded the Contract as context requires.

3. CONTRACT TERM; RENEWAL; EXTENSION: The term of this Contract shall be determined in accordance with the category that has been identified as applicable to this Contract below:

☐ **Term Contract**

Initial Contract Term: Initial Contract Term: This Contract becomes effective on ____________________ and extends for a period of ____________________ year(s).

Renewal Term: This Contract may be renewed upon the mutual written consent of the Agency, and the Vendor, with approval of the Purchasing Division and the Attorney General's office (Attorney General approval is as to form only). Any request for renewal should be delivered to the Agency and then submitted to the Purchasing Division thirty (30) days prior to the expiration date of the initial contract term or appropriate renewal term. A Contract renewal shall be in accordance with the terms and conditions of the original contract. Unless otherwise specified below, renewal of this Contract is limited to __________________ successive one (1) year periods or multiple renewal periods of less than one year, provided that the multiple renewal periods do not exceed the total number of months available in all renewal years combined. Automatic renewal of this Contract is prohibited. Renewals must be approved by the Vendor, Agency, Purchasing Division and Attorney General's office (Attorney General approval is as to form only)

> ☐ **Alternate Renewal Term** – This contract may be renewed for __________________ successive __________ year periods or shorter periods provided that they do not exceed the total number of months contained in all available renewals. Automatic renewal of this Contract is prohibited. Renewals must be approved by the Vendor, Agency, Purchasing Division and Attorney General's office (Attorney General approval is as to form only)

Delivery Order Limitations: In the event that this contract permits delivery orders, a delivery order may only be issued during the time this Contract is in effect. Any delivery order issued within one year of the expiration of this Contract shall be effective for one year from the date the delivery order is issued. No delivery order may be extended beyond one year after this Contract has expired.

☐ **Fixed Period Contract:** This Contract becomes effective upon Vendor's receipt of the notice to proceed and must be completed within ______________________ days.

☐ **Fixed Period Contract with Renewals:** This Contract becomes effective upon Vendor's receipt of the notice to proceed and part of the Contract more fully described in the attached specifications must be completed within ________________ days. Upon completion of the work covered by the preceding sentence, the vendor agrees that maintenance, monitoring, or warranty services will be provided for _______________ year(s) thereafter.

☑ **One Time Purchase:** The term of this Contract shall run from the issuance of the Award Document until all of the goods contracted for have been delivered, but in no event will this Contract extend for more than one fiscal year.

☐ **Other:** See attached.

4. NOTICE TO PROCEED: Vendor shall begin performance of this Contract immediately upon receiving notice to proceed unless otherwise instructed by the Agency. Unless otherwise specified, the fully executed Award Document will be considered notice to proceed.

5. QUANTITIES: The quantities required under this Contract shall be determined in accordance with the category that has been identified as applicable to this Contract below.

☐ **Open End Contract:** Quantities listed in this Solicitation are approximations only, based on estimates supplied by the Agency. It is understood and agreed that the Contract shall cover the quantities actually ordered for delivery during the term of the Contract, whether more or less than the quantities shown.

☐ **Service:** The scope of the service to be provided will be more clearly defined in the specifications included herewith.

☑ **Combined Service and Goods:** The scope of the service and deliverable goods to be provided will be more clearly defined in the specifications included herewith.

☐ **One Time Purchase:** This Contract is for the purchase of a set quantity of goods that are identified in the specifications included herewith. Once those items have been delivered, no additional goods may be procured under this Contract without an appropriate change order approved by the Vendor, Agency, Purchasing Division, and Attorney General's office.

6. EMERGENCY PURCHASES: The Purchasing Division Director may authorize the Agency to purchase goods or services in the open market that Vendor would otherwise provide under this Contract if those goods or services are for immediate or expedited delivery in an emergency. Emergencies shall include, but are not limited to, delays in transportation or an unanticipated increase in the volume of work. An emergency purchase in the open market, approved by the Purchasing Division Director, shall not constitute of breach of this Contract and shall not entitle the Vendor to any form of compensation or damages. This provision does not excuse the State from fulfilling its obligations under a One Time Purchase contract.

7. REQUIRED DOCUMENTS: All of the items checked below must be provided to the Purchasing Division by the Vendor as specified below.

☐ **BID BOND (Construction Only):** Pursuant to the requirements contained in W. Va. Code § 5-22-1(c), All Vendors submitting a bid on a construction project shall furnish a valid bid bond in the amount of five percent (5%) of the total amount of the bid protecting the State of West Virginia. The bid bond must be submitted with the bid.

☐ **PERFORMANCE BOND:** The apparent successful Vendor shall provide a performance bond in the amount of 100% of the contract. The performance bond must be received by the Purchasing Division prior to Contract award.

☐ **LABOR/MATERIAL PAYMENT BOND:** The apparent successful Vendor shall provide a labor/material payment bond in the amount of 100% of the Contract value. The labor/material payment bond must be delivered to the Purchasing Division prior to Contract award.

In lieu of the Bid Bond, Performance Bond, and Labor/Material Payment Bond, the Vendor may provide certified checks, cashier's checks, or irrevocable letters of credit. Any certified check, cashier's check, or irrevocable letter of credit provided in lieu of a bond must be of the same amount and delivered on the same schedule as the bond it replaces. A letter of credit submitted in lieu of a performance and labor/material payment bond will only be allowed for projects under $100,000. Personal or business checks are not acceptable. Notwithstanding the foregoing, West Virginia Code § 5-22-1 (d) mandates that a vendor provide a performance and labor/material payment bond for construction projects. Accordingly, substitutions for the performance and labor/material payment bonds for construction projects is not permitted.

☐ **MAINTENANCE BOND:** The apparent successful Vendor shall provide a two (2) year maintenance bond covering the roofing system. The maintenance bond must be issued and delivered to the Purchasing Division prior to Contract award.

☐ **LICENSE(S) / CERTIFICATIONS / PERMITS:** In addition to anything required under the Section of the General Terms and Conditions entitled Licensing, the apparent successful Vendor shall furnish proof of the following licenses, certifications, and/or permits prior to Contract award, in a form acceptable to the Purchasing Division.

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The apparent successful Vendor shall also furnish proof of any additional licenses or certifications contained in the specifications prior to Contract award regardless of whether or not that requirement is listed above.

8. INSURANCE: The apparent successful Vendor shall furnish proof of the insurance identified by a checkmark below and must include the State as an additional insured on each policy prior to Contract award. The insurance coverages identified below must be maintained throughout the life of this contract. Thirty (30) days prior to the expiration of the insurance policies, Vendor shall provide the Agency with proof that the insurance mandated herein has been continued. Vendor must also provide Agency with immediate notice of any changes in its insurance policies, including but not limited to, policy cancelation, policy reduction, or change in insurers. The apparent successful Vendor shall also furnish proof of any additional insurance requirements contained in the specifications prior to Contract award regardless of whether or not that insurance requirement is listed in this section.

Vendor must maintain:

☑ **Commercial General Liability Insurance** in at least an amount of: $1,000,000.00 per occurrence.

☑ **Automobile Liability Insurance** in at least an amount of: $100,000.00 per occurrence.

☐ **Professional/Malpractice/Errors and Omission Insurance** in at least an amount of: ____________________ per occurrence.

☐ **Commercial Crime and Third Party Fidelity Insurance** in an amount of: __________________ per occurrence.

☐ **Cyber Liability Insurance** in an amount of: ______________________________ per occurrence.

☐ **Builders Risk Insurance** in an amount equal to 100% of the amount of the Contract.

☐ **Pollution Insurance** in an amount of: ___________________ per occurrence.

☐ **Aircraft Liability** in an amount of: ___________________ per occurrence.

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Notwithstanding anything contained in this section to the contrary, the Director of the Purchasing Division reserves the right to waive the requirement that the State be named as an additional insured on one or more of the Vendor's insurance policies if the Director finds that doing so is in the State's best interest.

9. WORKERS' COMPENSATION INSURANCE: The apparent successful Vendor shall comply with laws relating to workers compensation, shall maintain workers' compensation insurance when required, and shall furnish proof of workers' compensation insurance upon request.

10. [Reserved]

11. LIQUIDATED DAMAGES: This clause shall in no way be considered exclusive and shall not limit the State or Agency's right to pursue any other available remedy. Vendor shall pay liquidated damages in the amount specified below or as described in the specifications:

☐ ________________________ for ________________________________

☐ Liquidated Damages Contained in the Specifications

12. ACCEPTANCE: Vendor's signature on its bid, or on the certification and signature page, constitutes an offer to the State that cannot be unilaterally withdrawn, signifies that the product or service proposed by vendor meets the mandatory requirements contained in the Solicitation for that product or service, unless otherwise indicated, and signifies acceptance of the terms and conditions contained in the Solicitation unless otherwise indicated.

13. PRICING: The pricing set forth herein is firm for the life of the Contract, unless specified elsewhere within this Solicitation/Contract by the State. A Vendor's inclusion of price adjustment provisions in its bid, without an express authorization from the State in the Solicitation to do so, may result in bid disqualification. Notwithstanding the foregoing, Vendor must extend any publicly advertised sale price to the State and invoice at the lower of the contract price or the publicly advertised sale price.

14. PAYMENT IN ARREARS: Payment in advance is prohibited under this Contract. Payment may only be made after the delivery and acceptance of goods or services. The Vendor shall submit invoices, in arrears.

15. PAYMENT METHODS: Vendor must accept payment by electronic funds transfer and P-Card. (The State of West Virginia's Purchasing Card program, administered under contract by a banking institution, processes payment for goods and services through state designated credit cards.)

16. TAXES: The Vendor shall pay any applicable sales, use, personal property or any other taxes arising out of this Contract and the transactions contemplated thereby. The State of West Virginia is exempt from federal and state taxes and will not pay or reimburse such taxes.

17. ADDITIONAL FEES: Vendor is not permitted to charge additional fees or assess additional charges that were not either expressly provided for in the solicitation published by the State of West Virginia or included in the unit price or lump sum bid amount that Vendor is required by the solicitation to provide. Including such fees or charges as notes to the solicitation may result in rejection of vendor's bid. Requesting such fees or charges be paid after the contract has been awarded may result in cancellation of the contract.

18. FUNDING: This Contract shall continue for the term stated herein, contingent upon funds being appropriated by the Legislature or otherwise being made available. In the event funds are not appropriated or otherwise made available, this Contract becomes void and of no effect beginning on July 1 of the fiscal year for which funding has not been appropriated or otherwise made available.

19. CANCELLATION: The Purchasing Division Director reserves the right to cancel this Contract immediately upon written notice to the vendor if the materials or workmanship supplied do not conform to the specifications contained in the Contract. The Purchasing Division Director may also cancel any purchase or Contract upon 30 days written notice to the Vendor in accordance with West Virginia Code of State Rules § 148-1-5.2.b.

20. TIME: Time is of the essence with regard to all matters of time and performance in this Contract.

21. APPLICABLE LAW: This Contract is governed by and interpreted under West Virginia law without giving effect to its choice of law principles. Any information provided in specification manuals, or any other source, verbal or written, which contradicts or violates the West Virginia Constitution, West Virginia Code or West Virginia Code of State Rules is void and of no effect.

22. COMPLIANCE WITH LAWS: Vendor shall comply with all applicable federal, state, and local laws, regulations and ordinances. By submitting a bid, Vendor acknowledges that it has reviewed, understands, and will comply with all applicable laws, regulations, and ordinances.

> **SUBCONTRACTOR COMPLIANCE:** Vendor shall notify all subcontractors providing commodities or services related to this Contract that as subcontractors, they too are required to comply with all applicable laws, regulations, and ordinances. Notification under this provision must occur prior to the performance of any work under the contract by the subcontractor.

23. ARBITRATION: Any references made to arbitration contained in this Contract, Vendor's bid, or in any American Institute of Architects documents pertaining to this Contract are hereby deleted, void, and of no effect.

24. MODIFICATIONS: This writing is the parties' final expression of intent. Notwithstanding anything contained in this Contract to the contrary no modification of this Contract shall be binding without mutual written consent of the Agency, and the Vendor, with approval of the Purchasing Division and the Attorney General's office (Attorney General approval is as to form only). Any change to existing contracts that adds work or changes contract cost, and were not included in the original contract, must be approved by the Purchasing Division and the Attorney General's Office (as to form) prior to the implementation of the change or commencement of work affected by the change.

25. WAIVER: The failure of either party to insist upon a strict performance of any of the terms or provision of this Contract, or to exercise any option, right, or remedy herein contained, shall not be construed as a waiver or a relinquishment for the future of such term, provision, option, right, or remedy, but the same shall continue in full force and effect. Any waiver must be expressly stated in writing and signed by the waiving party.

26. SUBSEQUENT FORMS: The terms and conditions contained in this Contract shall supersede any and all subsequent terms and conditions which may appear on any form documents submitted by Vendor to the Agency or Purchasing Division such as price lists, order forms, invoices, sales agreements, or maintenance agreements, and includes internet websites or other electronic documents. Acceptance or use of Vendor's forms does not constitute acceptance of the terms and conditions contained thereon.

27. ASSIGNMENT: Neither this Contract nor any monies due, or to become due hereunder, may be assigned by the Vendor without the express written consent of the Agency, the Purchasing Division, the Attorney General's office (as to form only), and any other government agency or office that may be required to approve such assignments.

28. WARRANTY: The Vendor expressly warrants that the goods and/or services covered by this Contract will: (a) conform to the specifications, drawings, samples, or other description furnished or specified by the Agency; (b) be merchantable and fit for the purpose intended; and (c) be free from defect in material and workmanship.

29. STATE EMPLOYEES: State employees are not permitted to utilize this Contract for personal use and the Vendor is prohibited from permitting or facilitating the same.

30. PRIVACY, SECURITY, AND CONFIDENTIALITY: The Vendor agrees that it will not disclose to anyone, directly or indirectly, any such personally identifiable information or other confidential information gained from the Agency, unless the individual who is the subject of the information consents to the disclosure in writing or the disclosure is made pursuant to the Agency's policies, procedures, and rules. Vendor further agrees to comply with the Confidentiality Policies and Information Security Accountability Requirements, set forth in http://www.state.wv.us/admin/purchase/privacy/default.html.

31. YOUR SUBMISSION IS A PUBLIC DOCUMENT: Vendor's entire response to the Solicitation and the resulting Contract are public documents. As public documents, they will be disclosed to the public following the bid/proposal opening or award of the contract, as required by the competitive bidding laws of West Virginia Code §§ 5A-3-1 et seq., 5-22-1 et seq., and 5G-1-1 et seq. and the Freedom of Information Act West Virginia Code §§ 29B-1-1 et seq.

DO NOT SUBMIT MATERIAL YOU CONSIDER TO BE CONFIDENTIAL, A TRADE SECRET, OR OTHERWISE NOT SUBJECT TO PUBLIC DISCLOSURE.

Submission of any bid, proposal, or other document to the Purchasing Division constitutes your explicit consent to the subsequent public disclosure of the bid, proposal, or document. The Purchasing Division will disclose any document labeled "confidential," "proprietary," "trade secret," "private," or labeled with any other claim against public disclosure of the documents, to include any "trade secrets" as defined by West Virginia Code § 47-22-1 et seq. All submissions are subject to public disclosure without notice.

32. LICENSING: In accordance with West Virginia Code of State Rules § 148-1-6.1.e, Vendor must be licensed and in good standing in accordance with any and all state and local laws and requirements by any state or local agency of West Virginia, including, but not limited to, the West Virginia Secretary of State's Office, the West Virginia Tax Department, West Virginia Insurance Commission, or any other state agency or political subdivision. Obligations related to political subdivisions may include, but are not limited to, business licensing, business and occupation taxes, inspection compliance, permitting, etc. Upon request, the Vendor must provide all necessary releases to obtain information to enable the Purchasing Division Director or the Agency to verify that the Vendor is licensed and in good standing with the above entities.

> **SUBCONTRACTOR COMPLIANCE:** Vendor shall notify all subcontractors providing commodities or services related to this Contract that as subcontractors, they too are required to be licensed, in good standing, and up-to-date on all state and local obligations as described in this section. Obligations related to political subdivisions may include, but are not limited to, business licensing, business and occupation taxes, inspection compliance, permitting, etc. Notification under this provision must occur prior to the performance of any work under the contract by the subcontractor.

33. ANTITRUST: In submitting a bid to, signing a contract with, or accepting a Award Document from any agency of the State of West Virginia, the Vendor agrees to convey, sell, assign, or transfer to the State of West Virginia all rights, title, and interest in and to all causes of action it may now or hereafter acquire under the antitrust laws of the United States and the State of West Virginia for price fixing and/or unreasonable restraints of trade relating to the particular commodities or services purchased or acquired by the State of West Virginia. Such assignment shall be made and become effective at the time the purchasing agency tenders the initial payment to Vendor.

34. VENDOR CERTIFICATIONS: By signing its bid or entering into this Contract, Vendor certifies (1) that its bid or offer was made without prior understanding, agreement, or connection with any corporation, firm, limited liability company, partnership, person or entity submitting a bid or offer for the same material, supplies, equipment or services; (2) that its bid or offer is in all respects fair and without collusion or fraud; (3) that this Contract is accepted or entered into without any prior understanding, agreement, or connection to any other entity that could be considered a violation of law; and (4) that it has reviewed this Solicitation in its entirety; understands the requirements, terms and conditions, and other information contained herein.

Vendor's signature on its bid or offer also affirms that neither it nor its representatives have any interest, nor shall acquire any interest, direct or indirect, which would compromise the performance of its services hereunder. Any such interests shall be promptly presented in detail to the Agency. The individual signing this bid or offer on behalf of Vendor certifies that he or she is authorized by the Vendor to execute this bid or offer or any documents related thereto on Vendor's behalf; that he or she is authorized to bind the Vendor in a contractual relationship; and that, to the best of his or her knowledge, the Vendor has properly registered with any State agency that may require registration.

35. VENDOR RELATIONSHIP: The relationship of the Vendor to the State shall be that of an independent contractor and no principal-agent relationship or employer-employee relationship is contemplated or created by this Contract. The Vendor as an independent contractor is solely liable for the acts and omissions of its employees and agents. Vendor shall be responsible for selecting, supervising, and compensating any and all individuals employed pursuant to the terms of this Solicitation and resulting contract. Neither the Vendor, nor any employees or subcontractors of the Vendor, shall be deemed to be employees of the State for any purpose whatsoever. Vendor shall be exclusively responsible for payment of employees and contractors for all wages and salaries, taxes, withholding payments, penalties, fees, fringe benefits, professional liability insurance premiums, contributions to insurance and pension, or other deferred compensation plans, including but not limited to, Workers' Compensation and Social Security obligations, licensing fees, etc. and the filing of all necessary documents, forms, and returns pertinent to all of the foregoing.

Vendor shall hold harmless the State, and shall provide the State and Agency with a defense against any and all claims including, but not limited to, the foregoing payments, withholdings, contributions, taxes, Social Security taxes, and employer income tax returns.

36. INDEMNIFICATION: The Vendor agrees to indemnify, defend, and hold harmless the State and the Agency, their officers, and employees from and against: (1) Any claims or losses for services rendered by any subcontractor, person, or firm performing or supplying services, materials, or supplies in connection with the performance of the Contract; (2) Any claims or losses resulting to any person or entity injured or damaged by the Vendor, its officers, employees, or subcontractors by the publication, translation, reproduction, delivery, performance, use, or disposition of any data used under the Contract in a manner not authorized by the Contract, or by Federal or State statutes or regulations; and (3) Any failure of the Vendor, its officers, employees, or subcontractors to observe State and Federal laws including, but not limited to, labor and wage and hour laws.

37. PURCHASING AFFIDAVIT: In accordance with West Virginia Code §§ 5A-3-10a and 5-22-1(i), the State is prohibited from awarding a contract to any bidder that owes a debt to the State or a political subdivision of the State, Vendors are required to sign, notarize, and submit the Purchasing Affidavit to the Purchasing Division affirming under oath that it is not in default on any monetary obligation owed to the state or a political subdivision of the state.

38. ADDITIONAL AGENCY AND LOCAL GOVERNMENT USE: This Contract may be utilized by other agencies, spending units, and political subdivisions of the State of West Virginia; county, municipal, and other local government bodies; and school districts ("Other Government Entities"), provided that both the Other Government Entity and the Vendor agree. Any extension of this Contract to the aforementioned Other Government Entities must be on the same prices, terms, and conditions as those offered and agreed to in this Contract, provided that such extension is in compliance with the applicable laws, rules, and ordinances of the Other Government Entity. A refusal to extend this Contract to the Other Government Entities shall not impact or influence the award of this Contract in any manner.

39. CONFLICT OF INTEREST: Vendor, its officers or members or employees, shall not presently have or acquire an interest, direct or indirect, which would conflict with or compromise the performance of its obligations hereunder. Vendor shall periodically inquire of its officers, members and employees to ensure that a conflict of interest does not arise. Any conflict of interest discovered shall be promptly presented in detail to the Agency.

40. REPORTS: Vendor shall provide the Agency and/or the Purchasing Division with the following reports identified by a checked box below:

☑ Such reports as the Agency and/or the Purchasing Division may request. Requested reports may include, but are not limited to, quantities purchased, agencies utilizing the contract, total contract expenditures by agency, etc.

☐ Quarterly reports detailing the total quantity of purchases in units and dollars, along with a listing of purchases by agency. Quarterly reports should be delivered to the Purchasing Division via email at purchasing.requisitions@wv.gov.

41. BACKGROUND CHECK: In accordance with W. Va. Code § 15-2D-3, the Director of the Division of Protective Services shall require any service provider whose employees are regularly employed on the grounds or in the buildings of the Capitol complex or who have access to sensitive or critical information to submit to a fingerprint-based state and federal background inquiry through the state repository. The service provider is responsible for any costs associated with the fingerprint-based state and federal background inquiry.

After the contract for such services has been approved, but before any such employees are permitted to be on the grounds or in the buildings of the Capitol complex or have access to sensitive or critical information, the service provider shall submit a list of all persons who will be physically present and working at the Capitol complex to the Director of the Division of Protective Services for purposes of verifying compliance with this provision. The State reserves the right to prohibit a service provider's employees from accessing sensitive or critical information or to be present at the Capitol complex based upon results addressed from a criminal background check.

Service providers should contact the West Virginia Division of Protective Services by phone at (304) 558-9911 for more information.

42. PREFERENCE FOR USE OF DOMESTIC STEEL PRODUCTS: Except when authorized by the Director of the Purchasing Division pursuant to W. Va. Code § 5A-3-56, no contractor may use or supply steel products for a State Contract Project other than those steel products made in the United States. A contractor who uses steel products in violation of this section may be subject to civil penalties pursuant to W. Va. Code § 5A-3-56. As used in this section:

a. "State Contract Project" means any erection or construction of, or any addition to, alteration of or other improvement to any building or structure, including, but not limited to, roads or highways, or the installation of any heating or cooling or ventilating plants or other equipment, or the supply of and materials for such projects, pursuant to a contract with the State of West Virginia for which bids were solicited on or after June 6, 2001.

b. "Steel Products" means products rolled, formed, shaped, drawn, extruded, forged, cast, fabricated or otherwise similarly processed, or processed by a combination of two or more or such operations, from steel made by the open heath, basic oxygen, electric furnace, Bessemer or other steel making process. The Purchasing Division Director may, in writing, authorize the use of foreign steel products if:

c. The cost for each contract item used does not exceed one tenth of one percent (.1%) of the total contract cost or two thousand five hundred dollars ($2,500.00), whichever is greater. For the purposes of this section, the cost is the value of the steel product as delivered to the project; or

d. The Director of the Purchasing Division determines that specified steel materials are not produced in the United States in sufficient quantity or otherwise are not reasonably available to meet contract requirements.

43. PREFERENCE FOR USE OF DOMESTIC ALUMINUM, GLASS, AND STEEL: In Accordance with W. Va. Code § 5-19-1 et seq., and W. Va. CSR § 148-10-1 et seq., for every contract or subcontract, subject to the limitations contained herein, for the construction, reconstruction, alteration, repair, improvement or maintenance of public works or for the purchase of any item of machinery or equipment to be used at sites of public works, only domestic aluminum, glass or steel products shall be supplied unless the spending officer determines, in writing, after the receipt of offers or bids, (1) that the cost of domestic aluminum, glass or steel products is unreasonable or inconsistent with the public interest of the State of West Virginia, (2) that domestic aluminum, glass or steel products are not produced in sufficient quantities to meet the contract requirements, or (3) the available domestic aluminum, glass, or steel do not meet the contract specifications. This provision only applies to public works contracts awarded in an amount more than fifty thousand dollars ($50,000) or public works contracts that require more than ten thousand pounds of steel products.

The cost of domestic aluminum, glass, or steel products may be unreasonable if the cost is more than twenty percent (20%) of the bid or offered price for foreign made aluminum, glass, or steel products. If the domestic aluminum, glass or steel products to be supplied or produced in a "substantial labor surplus area", as defined by the United States Department of Labor, the cost of domestic aluminum, glass, or steel products may be unreasonable if the cost is more than thirty percent (30%) of the bid or offered price for foreign made aluminum, glass, or steel products. This preference shall be applied to an item of machinery or equipment, as indicated above, when the item is a single unit of equipment or machinery manufactured primarily of aluminum, glass or steel, is part of a public works contract and has the sole purpose or of being a permanent part of a single public works project. This provision does not apply to equipment or machinery purchased by a spending unit for use by that spending unit and not as part of a single public works project.

All bids and offers including domestic aluminum, glass or steel products that exceed bid or offer prices including foreign aluminum, glass or steel products after application of the preferences provided in this provision may be reduced to a price equal to or lower than the lowest bid or offer price for foreign aluminum, glass or steel products plus the applicable preference. If the reduced bid or offer prices are made in writing and supersede the prior bid or offer prices, all bids or offers, including the reduced bid or offer prices, will be reevaluated in accordance with this rule.

44. INTERESTED PARTY SUPPLEMENTAL DISCLOSURE: W. Va. Code § 6D-1-2 requires that for contracts with an actual or estimated value of at least $1 million, the vendor must submit to the Agency a supplemental disclosure of interested parties reflecting any new or differing interested parties to the contract, which were not included in the original pre-award interested party disclosure, within 30 days following the completion or termination of the contract. A copy of that form is included with this solicitation or can be obtained from the WV Ethics Commission. This requirement does not apply to publicly traded companies listed on a national or international stock exchange. A more detailed definition of interested parties can be obtained from the form referenced above.

DESIGNATED CONTACT: Vendor appoints the individual identified in this Section as the Contract Administrator and the initial point of contact for matters relating to this Contract.

Alicia Shannon, Contract Specialist
(Name, Title)

(Printed Name and Title)
34 Maple St, Milford, MA 01757
(Address)
508-482-3699 / 508-482-8532
(Phone Number) / (Fax Number)
bid_desk@waters.com
(email address)

CERTIFICATION AND SIGNATURE: By signing below, or submitting documentation through wvOASIS, I certify that I have reviewed this Solicitation in its entirety; that I understand the requirements, terms and conditions, and other information contained herein; that this bid, offer or proposal constitutes an offer to the State that cannot be unilaterally withdrawn; that the product or service proposed meets the mandatory requirements contained in the Solicitation for that product or service, unless otherwise stated herein; that the Vendor accepts the terms and conditions contained in the Solicitation, unless otherwise stated herein; that I am submitting this bid, offer or proposal for review and consideration; that I am authorized by the vendor to execute and submit this bid, offer, or proposal, or any documents related thereto on vendor's behalf; that I am authorized to bind the vendor in a contractual relationship; and that to the best of my knowledge, the vendor has properly registered with any State agency that may require registration.

(Company)

(Authorized Signature) (Representative Name, Title)

(Printed Name and Title of Authorized Representative)

(Date)

(Phone Number) (Fax Number)

SPECIFICATIONS

1. **PURPOSE AND SCOPE:** The West Virginia Purchasing Division is soliciting bids on behalf of West Virginia Department of Agriculture to establish a contract for the one time purchase of a **Liquid Chromatography Triple Quadrupole Mass Spectrometer (LC/MS/MS), workstation PC, software, printer, nitrogen generator, uninterrupted power supply (UPS), specific test methods, shipping, installation, validation, warranty, training and service.**

2. **DEFINITIONS:** The terms listed below shall have the meanings assigned to them below. Additional definitions can be found in section 2 of the General Terms and Conditions.

   2.1 **"Contract Services"** means the LC/MS/MS with inside delivery, installation, validation, warranty, and training.

   2.2 **"Pricing Page"** means the pages, contained in wvOASIS or attached as Exhibit A, upon which Vendor should list its proposed price for the Contract Items.

   2.3 **"Solicitation"** means the official notice of an opportunity to supply the State with goods or services that is published by the Purchasing Division.

   2.4 **"Validation"** means is the process used to confirm that the analytical procedure employed for a specific test or matrices is suitable for its intended use.

   2.5 **"Installation"** means unpacking and setting instrumentation in place with all connections secured for the instrument(s) to be in working order including software installation on the computer connected to the instrument.

   2.6 **"Warranty"** means the written warranty of the manufacturer of a new instrument of its condition and fitness for use, including any terms or conditions precedent to the enforcement of obligations under that warranty.

   2.7 **"Training"** means teaching staff how to use and maintain the instrument and software.

   2.8 **"Service"** means performing routine maintenance work or repair to the instrument or software.

   2.9 **"APCI"** means atmospheric pressure chemical ionization.

   2.10 **"ESI"** means electrospray.

2.11 **"FG"** means femtogram.

2.12 **"LC/MS/MS"** means Liquid Chromatography Triple Quadrupole Mass Spectrometer.

2.13 **"MRM"** means multiple reactions monitoring.

2.14 **"MSMS"** means tandem mass spectrometry.

2.15 **"SIM"** means selected ion monitoring.

2.16 **"S/N"** means signal to noise.

2.17 **"M/Z"** means mass to charge ratio.

2.18 **"AMU"** means Atomic mass unit.

2.19 **"DA/S"** means Daltons per second.

2.20 **"UHPLC"** means Ultra High-performance liquid chromatography.

2.21 **"SLPM"** means standard liters per minute.

2.22 **"PSIG"** means pounds per square inch gauge.

2.23 **"UPS"** means uninterrupted power supply.

3. GENERAL REQUIREMENTS:

3.1 **Mandatory Contract Item Requirements:** Contract Item must meet or exceed the mandatory requirements listed below for the **Liquid Chromatography Triple Quadrupole Mass Spectrometer (LC/MS/MS), workstation PC, software, printer, nitrogen generator, uninterrupted power supply (UPS), specific test methods, shipping, installation, validation, warranty, training, and service.**

3.1.1 Liquid Chromatography Triple Quadrupole Mass Spectrometer (LC/MS/MS)

3.1.1.1 Must be capable of detecting a variety of analytes including pesticides, herbicides, toxins, drugs in matrices such as foods, soil, vegetation (including hemp), animal feed, and water.

3.1.1.2 The system provided must be capable of analyzing the list of pesticides from the Cannabis and hemp pesticide lists from Oregon and California. See 3.1.4.2

3.1.1.3 MSMS must have dual ion sources that operate independently which can be set to electrospray ionization (ESI) or atmospheric pressure chemical ionization (APCI). The instrument must enable combinations such as ESI/APCI, ESI/ESI, APCI/APCI with the same or opposite polarities without having to remove the sources to switch modes.

3.1.1.4 Minimum sensitivity requirement for positive ion mode: signal/noise (S/N) 2000:1 25 femtograms (fg) of reserpine on column. Minimum sensitivity requirement for negative ion mode: signal/noise (S/N)>2000:1, 25 femtograms (fg) of chloramphenicol on column.

3.1.1.5 The source probes must be easy to remove without the use of tools.

3.1.1.6 Ion source must have flat response across flow rate up to 3 milliliters per minute without loss of sensitivity.

3.1.1.7 Capable of switching between rapidly between positive and negative ion detection without high voltage switching.

3.1.1.8 Acquisition modes: Q1 scan, Q2 scan, multiple reactions monitoring (MRM), selected ion monitoring (SIM), Neutral Loss scans, Product Ion, Precursor Ion, Time managed MRM

3.1.1.9 Minimum mass range requirement: 5-1500 mass to charge ratio (m/z)

3.1.1.10 Mass stability required: 0.05 atomic mass unit (amu) in 24 hours

3.1.1.11 Mass accuracy needed: minimum 0.1 unit across mass range

3.1.1.12 Scan speed: ≤30,000 daltons per second (da/s)

3.1.1.13 Quad resolution: unit, low and high, minimal sensitivity loss at 0.1 Daltons resolutions

3.1.1.14 Polarity switching time: ≤15 milliseconds

3.1.1.15 Dynamic range: 6 orders

3.1.1.16 Minimum multiple reactions monitoring (MRM) Dwell Time: 1 millisecond

3.1.1.17 MRM transitions: 450 per time segment > 40,000 ion transactions per method

3.1.1.18 Must have high selectivity mass filter at 0.3 Daltons. Signal loss must not be more than 10%.

3.1.1.19 For minimal tuning during method development and minimal maintenance of the ion path, the LC/MS/MS will require hot source induced desolvation interface to the mass analyzer by patented Laminar Flow Ion Guide using gas flow. Submit evidence of instrument use with cannabis for at least 6 months without matrix induced cleaning and maintenance

3.1.1.20 High performance liquid chromatograph capable of solvent and column switching without user intervention

3.1.1.21 High performance liquid chromatograph capable of regulating column temperature of at least 2 different columns

3.1.1.22 The UHPLC pump must have 18,000 psi capability and a flow rate to 5mL/minute.

3.1.1.23 High performance liquid chromatograph with an autosampler

3.1.1.24 The LC/MS/MS instrument must be fully automated for analysis with a system controller that is loaded with the necessary software that can perform instrument diagnostics, monitor all operating and electrical parameters, and allow remote tuning capability in real time.

3.1.1.25 The LC/MS/MS must include a maintenance kit.

3.1.1.26 Vendor must provide documentation for recommended environmental conditions, electrical requirements, gas requirements, or any other factor that would affect instrument performance.

3.1.2 Nitrogen generator

3.1.2.1 The nitrogen generator must be capable of producing up to 18 standard liters per minute (slpm) of liquid chromatography mass spectrometer grade gases at 80 pounds per square inch (psig) or have the capacity for the needs stated in the gas requirements of the LCMSMS.

3.1.2.2 The vendor must include if there is another gas requirement or need for the specific instrument being quoted other than listed in 3.1.2.1.

3.1.3 Uninterrupted Power Supply (UPS)

3.1.3.1 The uninterrupted power supply (UPS) must provide protection and complete power conditioning where the output remains continuously regulated. Must be rated to a capacity at least 5200

VA or have the capacity for the needs stated in the electrical requirements of the LCMSMS.

3.1.3.2 The vendor must include if there is another UPS electrical requirement or need to maintain the integrity of the instrument for proper operation being quoted other than listed in 3.1.3.1.

3.1.4 Specific Test methods: Cannabis and hemp methods

3.1.4.1 The vendor must provide a standard operating procedure for Cannabis and hemp analysis that includes sample preparation and analysis of the complete Cannabis list from states such as Oregon or California which include the analytes in 3.1.4.2.

3.1.4.2 See Exhibit B.

3.1.5 Workstation and software

3.1.5.1 Data station with windows based operating system capable of multitasking allowing data processing and data acquisition simultaneously.

3.1.5.2 Operating system must be fully integrated to control LS/MS/MS.

3.1.6 Shipping, Installation, Validation, Warranty, Training (including Specific Test Methods Application), and Service

3.1.6.1 Vendor must be on-site for delivery and perform the installation (labor and supplies included) of the LCMSMS.

3.1.6.2 The vendor must provide a written validation of the instrument's performance after installation.

3.1.6.3 Vendor will provide a full one-year parts and labor warranty on all items, including 2 preventative maintenances.

3.1.6.4 Vendor must be able to perform resolutions to service requests within 72 hours which includes on-site resolutions.

3.1.6.5 Vendor will provide on-site training (labor and non-consumable supplies included) for all instruments and software.

3.1.6.6 Vendor will provide on-site applications assistance for implementation of standard operating procedures for Cannabis and hemp analysis related to 3.1.4 by an applications scientist familiar with the analysis.

3.1.6.7 Vendor will provide copies of all system manuals (operations, training, technical, service, maintenance).

4. CONTRACT AWARD:

4.1 Contract Award: The Contract is intended to provide Agencies with a purchase price for the Contract Items. The Contract shall be awarded to the Vendor that provides the Contract Items meeting the required specifications for the lowest overall total cost as shown on the Pricing Pages.

4.2 Pricing Page: Vendor should complete the Pricing Page Exhibit A by placing all inclusive information in each column for item number, model/brand name, unit price and extended amount. There should be a price for the LCMSMS, workstation, software, printer, shipping/inside delivery, installation, validation, warranty, training, specific methods, and service. If there is no charge for any deliverable, indicate in the cell with "no charge". The bidder/vendor information must be completed and include an authorize signature. Vendor should complete the Pricing Page in full as failure to complete the Pricing Page in its entirety may result in Vendor's bid being disqualified.

Vendor should type or electronically enter the information into the Pricing Page to prevent errors in the evaluation.

5. PAYMENT:

5.1 Payment: Vendor shall accept payment in accordance with the payment procedures of the State of West Virginia.

6. DELIVERY AND RETURN:

6.1 Shipment and Delivery: Vendor should ship the Contract Items immediately after being awarded this Contract and receiving a purchase order. Contract Items must be delivered to Agency at 313 Gus R. Douglass Lane, Charleston, WV 25312.

6.2 Late Delivery: The Agency placing the order under this Contract must be notified in writing if the shipment of the Contract Items will be delayed for any reason. Any delay in delivery that could cause harm to an Agency will be grounds for cancellation of the Contract, and/or obtaining the Contract Items from a third party.

Any Agency seeking to obtain the Contract Items from a third party under this provision must first obtain approval of the Purchasing Division.

6.3 **Delivery Payment/Risk of Loss:** Vendor shall deliver the Contract Items F.O.B. destination to the Agency's location.

6.4 **Return of Unacceptable Items:** If the Agency deems the Contract Items to be unacceptable, the Contract Items shall be returned to Vendor at Vendor's expense and with no restocking charge. Vendor shall either make arrangements for the return within five (5) days of being notified that items are unacceptable, or permit the Agency to arrange for the return and reimburse Agency for delivery expenses. If the original packaging cannot be utilized for the return, Vendor will supply the Agency with appropriate return packaging upon request. All returns of unacceptable items shall be F.O.B. the Agency's location. The returned product shall either be replaced, or the Agency shall receive a full credit or refund for the purchase price, at the Agency's discretion.

6.5 **Return Due to Agency Error**: Items ordered in error by the Agency will be returned for credit within 30 days of receipt, F.O.B. Vendor's location. Vendor shall not charge a restocking fee if returned products are in a resalable condition. Items shall be deemed to be in a resalable condition if they are unused and in the original packaging. Any restocking fee for items not in a resalable condition shall be the lower of the Vendor's customary restocking fee or 5% of the total invoiced value of the returned items.

7 VENDOR DEFAULT:

7.1 The following shall be considered a vendor default under this Contract.

7.1.1 Failure to provide Contract Items in accordance with the requirements contained herein.

7.1.2 Failure to comply with other specifications and requirements contained herein.

7.1.3 Failure to comply with any laws, rules, and ordinances applicable to the Contract Services provided under this Contract.

7.1.4 Failure to remedy deficient performance upon request.

7.2 The following remedies shall be available to Agency upon default.

7.2.1 Immediate cancellation of the Contract.

7.2.2 Immediate cancellation of one or more release orders issued under this Contract.

7.2.3 Any other remedies available in law or equity.

8 FACILITIES ACCESS: Performance of Services will require access to the facility.

8.1 Vendor must identify principal service personnel who will be asked for identification upon entrance to the facility.

8.2 Anyone performing under this Contract will be subject to Agency's security protocol and procedures.

8.3 Vendor shall inform all staff of Agency's security protocol and procedures.

Exhibit A CRFQ AGR1900000018

PRICING PAGE

Item No.	Description	Model No/Brand Name	Quanity	Unit Price	Extended Amount
1	LCMSMS, workstation PC, software, printer, nitrogen generator, UPS, specific test methods	Waters Xevo TQ-S micro System	1	$295,000	$295,000
	installation/validation	included in line 1	1		included in line 1
	training/warranty	included in line 1	1		included in line 1
	service	Waters	1	$27,286.63	$27,286.63
	Failure to use this form may result in disqualification			**GRAND TOTAL**	$322,286.63

	Bidder / Vendor Information
Name:	Waters Technologies Corporation
Address:	34 Maple St
	Milford, MA 01757
Phone:	800-252-4752
Email Address:	bid_desk@waters.com
Authorized Signature:	Kristen A Arakelian

Vendor should not alter pricing page and should fill out pricing page as it. The addition of alterations to the pricing page and/or addition of commodities other than those listed on the pricing page online or as an attachment will result in disqualification of bid submittal.

Please reference Waters' Quotation #21998299 for detailed information

Exhibit B

Analytes of interest for the LCMSMS for West Virginia Department of Agriculture

Tox2	T022
Colchicine	Aminopterin
Aflatoxin G1	Codeine
Aflatoxin B1	Oxycodone
T2 Toxin	Scopolamine
*Digoxin	Ouabain
*Strychnine	Hydrocodone
*Ricinine	Eserine
*Aconitine	Emetine
*alpha-amanitin	Apomorphine
*Brodifacoum	Brucine
Anti-Coagulants (ran in negative ion mode)	Atropine
Warfarin	Hyoscyamine
Coumachlor	Levorphenol
Diphacinone	Heroin
Dicoumarol	Hydrastine
Chlorophacinone	Yohimbine
Bromadiolone	Digoxigenin
Difethialone	Picrotin
*Brodifacoum	Solanine
	Pentazocine
Other Compounds	Lobeline
Fluoroacetic Acid	Digitoxigenin
Melamine	Digitoxin
	*Ricinine
	*alpha-amanitin
	*strychnine
	*digoxin
	*aconitine

Compounds with * are in multiple lists

T022 method additional compounds	
Aldicarb	Coumaphos
Aldicarb sulfone	Ethiofencarb
Aldicarb sulfoxide	Fenamiphos
Atropine	Fenamiphos sulfide
Berberine	Methamidiphos
*Brodifacoum	Methomyl
Carbanyl	Oxamyl
Carbofuran	Picrotin
*Colchicine	Propoxur

Pesticides	
2,4-D	Imazethapyr
2,4,5-T	Isoxaflutole
2,4-DB	Mesotrione
2,4-DP	MCPA (2-methyl-4-chlorophenoxyacetic acid)

Exhibit B

Aldicarb (+ degradates)
Aminocyclopyrachlor
Aminopyralid
Bentazon
Clopyralid
Dacthal (+ degradates)
Dicamba
Dinotefuran
Diuron
Glyphosate (+AMPA)
Imazapyr
Hexazinone (+ Metabolite B)
Metsulfuron-methyl
Metribuzin (+ DA, DADK, DK)
Napropamide
Picloram
Propiconazole
Rimsulfuron
Sulfometuron-methyl
Tebuthiuron
Thiamethoxam
Thifensulfuron-methy
Tralkoxydim
Triclopyr

STATE OF WEST VIRGINIA
Purchasing Division

PURCHASING AFFIDAVIT

CONSTRUCTION CONTRACTS: Under W. Va. Code § 5-22-1(i), the contracting public entity shall not award a construction contract to any bidder that is known to be in default on any monetary obligation owed to the state or a political subdivision of the state, including, but not limited to, obligations related to payroll taxes, property taxes, sales and use taxes, fire service fees, or other fines or fees.

ALL CONTRACTS: Under W. Va. Code §5A-3-10a, no contract or renewal of any contract may be awarded by the state or any of its political subdivisions to any vendor or prospective vendor when the vendor or prospective vendor or a related party to the vendor or prospective vendor is a debtor and: (1) the debt owed is an amount greater than one thousand dollars in the aggregate; or (2) the debtor is in employer default.

EXCEPTION: The prohibition listed above does not apply where a vendor has contested any tax administered pursuant to chapter eleven of the W. Va. Code, workers' compensation premium, permit fee or environmental fee or assessment and the matter has not become final or where the vendor has entered into a payment plan or agreement and the vendor is not in default of any of the provisions of such plan or agreement.

DEFINITIONS:

"Debt" means any assessment, premium, penalty, fine, tax or other amount of money owed to the state or any of its political subdivisions because of a judgment, fine, permit violation, license assessment, defaulted workers' compensation premium, penalty or other assessment presently delinquent or due and required to be paid to the state or any of its political subdivisions, including any interest or additional penalties accrued thereon.

"Employer default" means having an outstanding balance or liability to the old fund or to the uninsured employers' fund or being in policy default, as defined in W. Va. Code § 23-2c-2, failure to maintain mandatory workers' compensation coverage, or failure to fully meet its obligations as a workers' compensation self-insured employer. An employer is not in employer default if it has entered into a repayment agreement with the Insurance Commissioner and remains in compliance with the obligations under the repayment agreement.

"Related party" means a party, whether an individual, corporation, partnership, association, limited liability company or any other form or business association or other entity whatsoever, related to any vendor by blood, marriage, ownership or contract through which the party has a relationship of ownership or other interest with the vendor so that the party will actually or by effect receive or control a portion of the benefit, profit or other consideration from performance of a vendor contract with the party receiving an amount that meets or exceed five percent of the total contract amount.

AFFIRMATION: By signing this form, the vendor's authorized signer affirms and acknowledges under penalty of law for false swearing (*W. Va. Code* §61-5-3) that: (1) for construction contracts, the vendor is not in default on any monetary obligation owed to the state or a political subdivision of the state, and (2) for all other contracts, that neither vendor nor any related party owe a debt as defined above and that neither vendor nor any related party are in employer default as defined above, unless the debt or employer default is permitted under the exception above.

WITNESS THE FOLLOWING SIGNATURE:

Vendor's Name: Waters Technologies Corporation

Authorized Signature: Date: 4/25/19

State of Massachusetts

County of Worcester, to-wit:

Taken, subscribed, and sworn to before me this 25 day of April, 2019.

My Commission expires March 13, 2020.

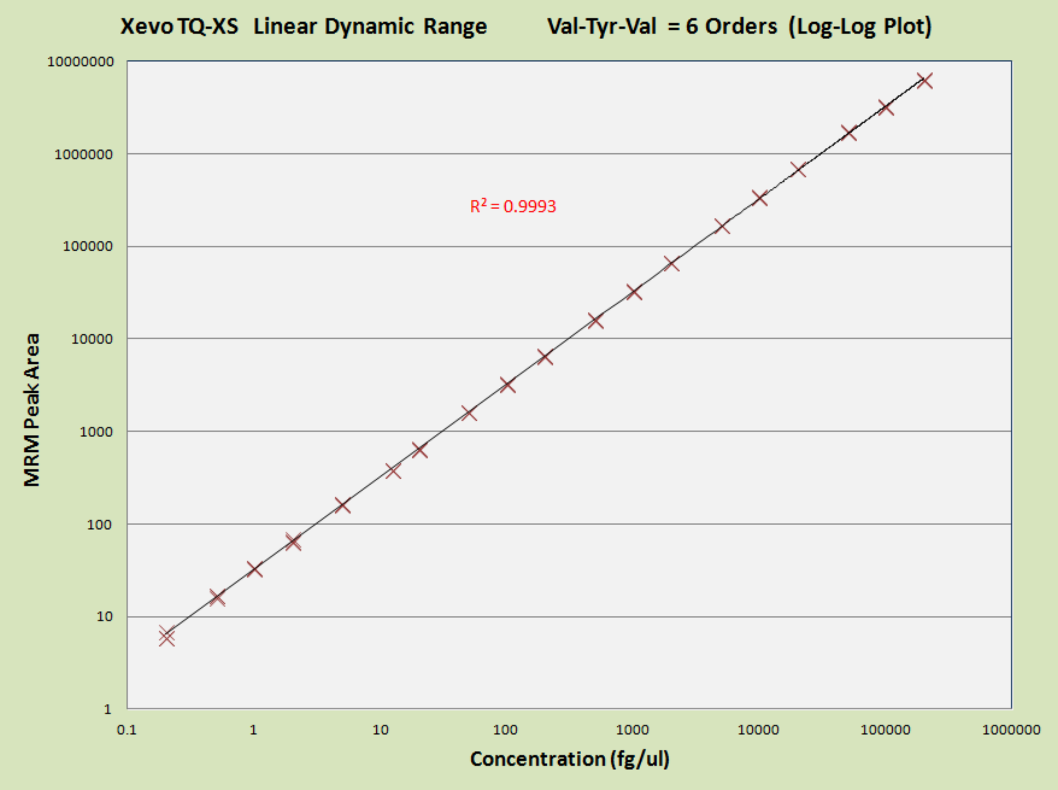
ROBIN M. FRIBERG
Notary Public
COMMONWEALTH OF MASSACHUSETTS
My Commission Expires
March 13 2020

AFFIX SEAL HERE . NOTARY PUBLIC

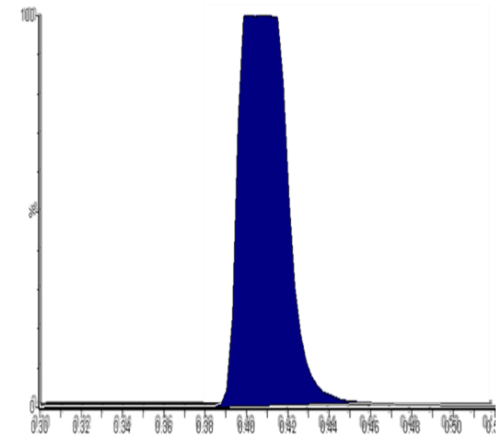
Improved Customer Experience
Xtended Dynamic Range detector

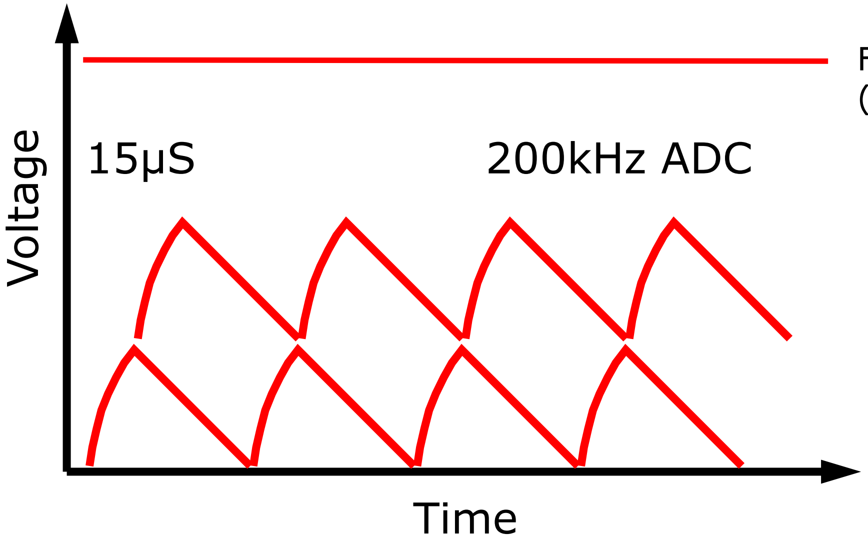
- Long-life photomultiplier technology
- Accessible sensitivity
  - data for peptide Val-Tyr-Val
  - UPLC/MRM ESI+, 6 orders linear dynamic range

Easy method transfer to a more sensitive instrument



XDR Detection System

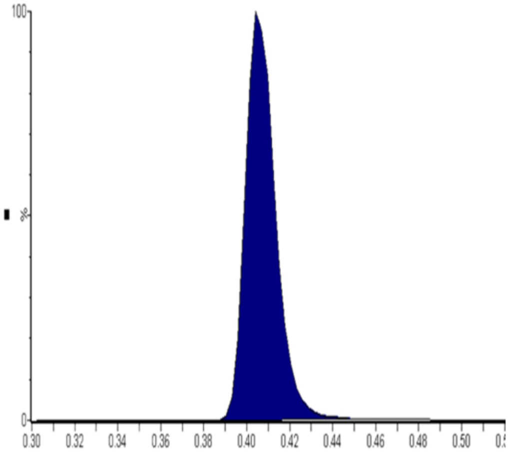


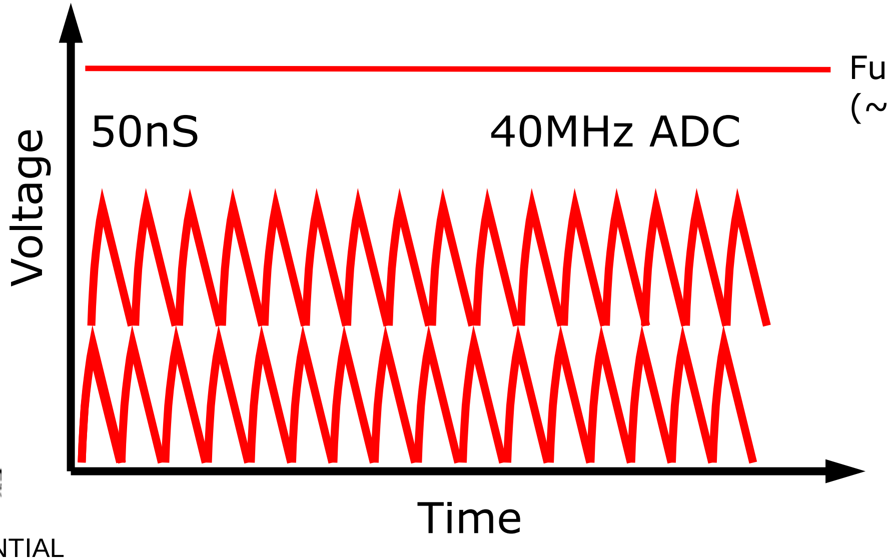


15μS

200kHz ADC

Full Scale
(~20 Million Ions/sec)





50nS

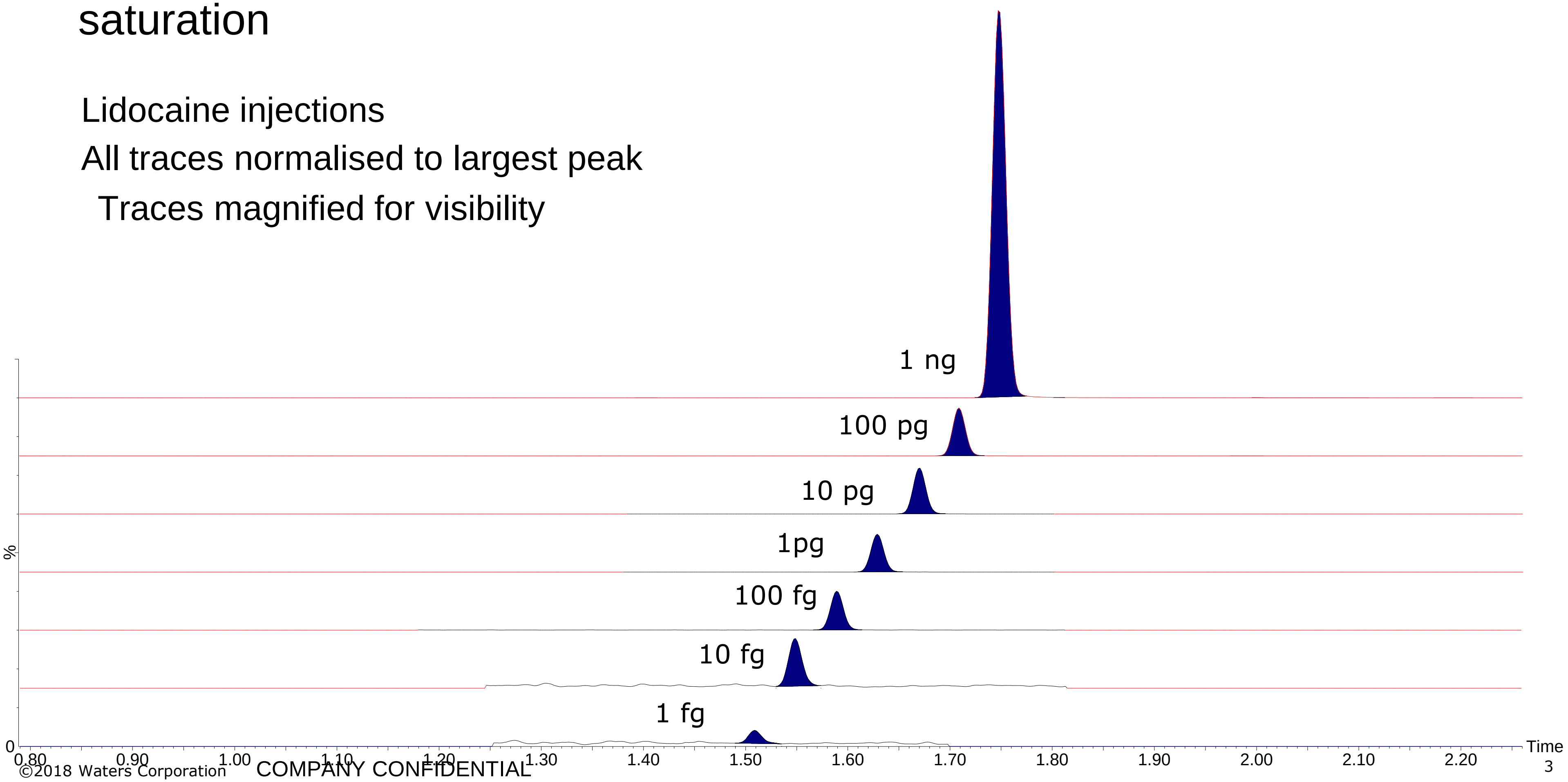
40MHz ADC

Full Scale
(~200 Million Ions/sec)

Detector Linear Dynamic Range

Xtended Dynamic Range™ (XDR)

- Easier to transfer methods from other instruments with higher or lower sensitivities
- Accessible sensitivity with up to 6 orders of linear dynamic range without saturation



Lidocaine injections

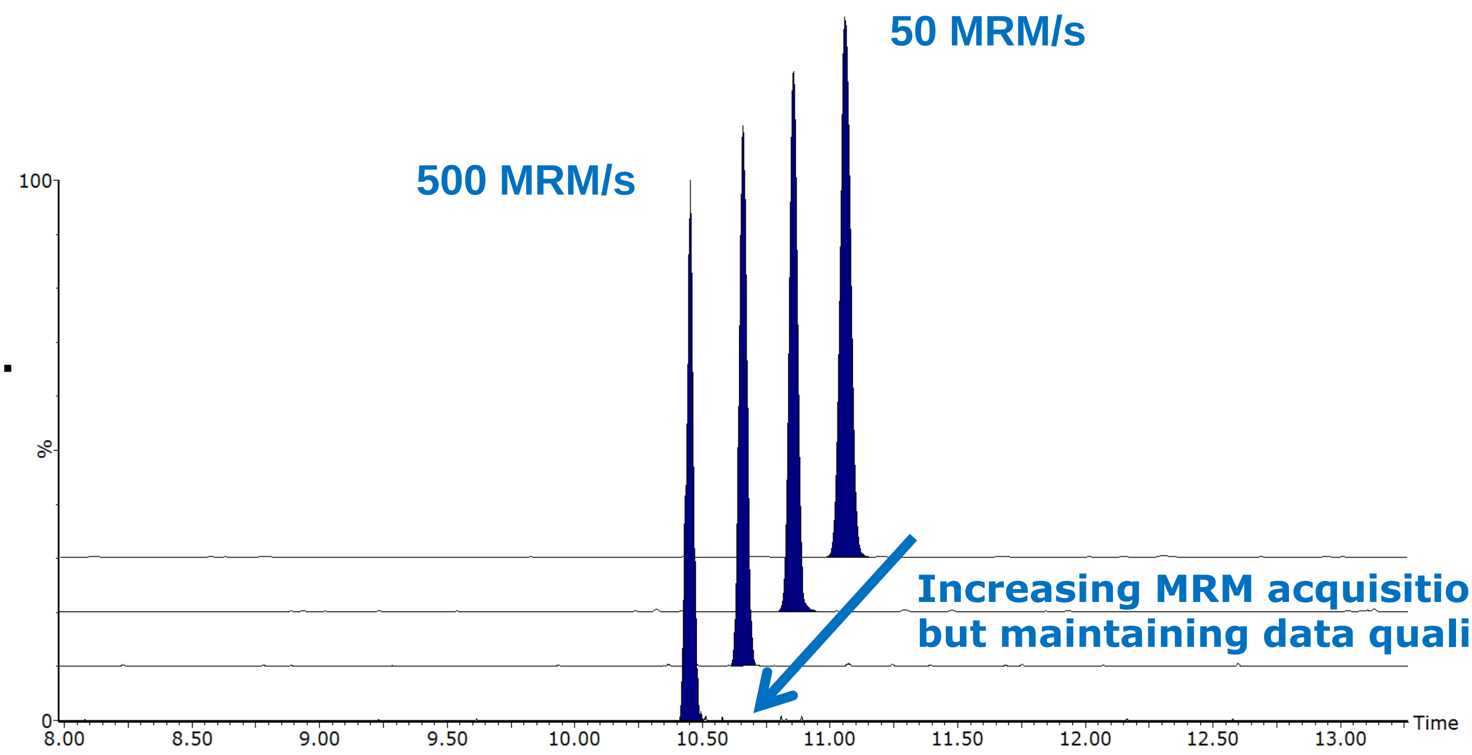
All traces normalised to largest peak

Traces magnified for visibility

Speed without Compromise

Xcelerated Ion Transfer™ (XIT)

- The new Xcelerated Ion Transfer (XIT) electronics, featuring SpaceWire technology, enable rapid data acquisition without performance loss

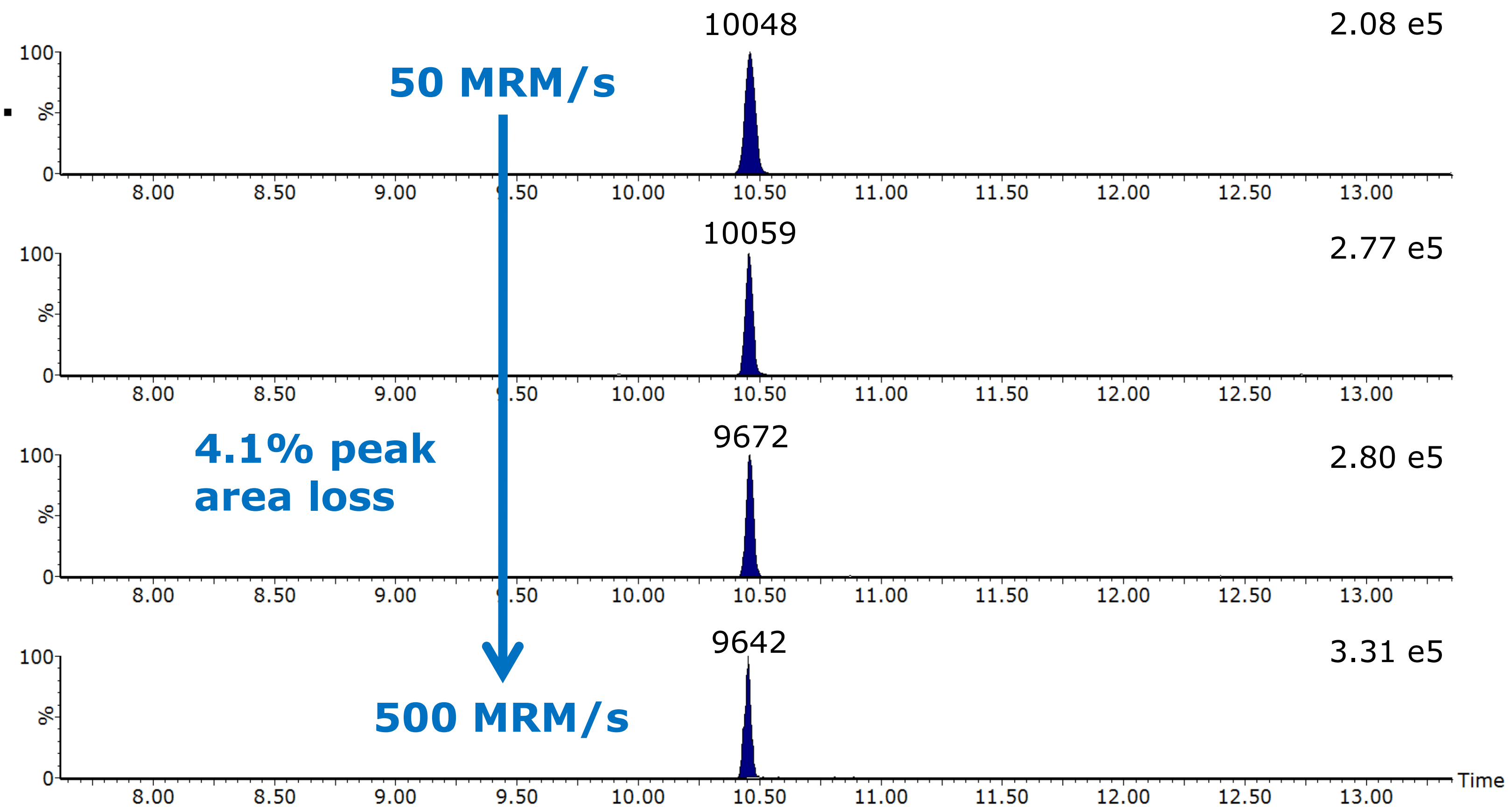


Increasing MRM acquisition speed but maintaining data quality

COMPANY CONFIDENTIAL

Data Quality and Speed

Data Quality at High Speed - Buprofezin



50 MRM/s

4.1% peak area loss

500 MRM/s

Dwell and Delay Time	%RSD (of 10 acquisitions)
10 ms	2.33
5 ms	5.08
3 ms	2.22
1 ms	5.49

[INSTRUMENT UPGRADE]

Waters
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ESCI MULTI-MODE IONIZATION SOURCE

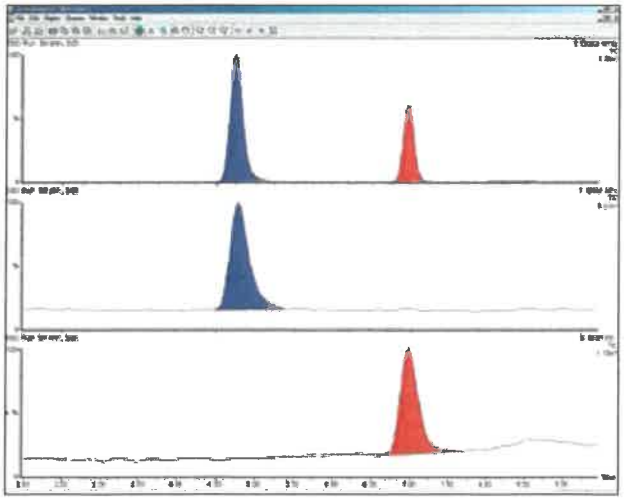
Enhance the capabilities of your Waters ZQ and Quattro micro mass spectrometers

NEED MULTIPLE IONIZATION TECHNIQUES TO ANALYZE YOUR LABORATORY'S DIVERSE SAMPLES?

- Save analysis time using ESI and APCI in a single run
- Minimize the number of failed samples
- Prevent inconvenience of changing ionization sources

Increased analysis success

Fast and accurate analytical methods are critical when trying to keep up with the speed with which samples are produced in your laboratory. Samples under analysis may have considerable differences in chemical structures and properties. Many laboratories use a combination of ionization techniques for the characterization of diverse samples including electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI). Typically, a change in ionization mode requires a change in instrument ion source and re-optimization of source parameters, resulting in lost analysis time.



By providing ESI and APCI in the same run, the ESCi Multi-Mode Ionization Source allows increased analysis success for diverse samples.

Improved productivity and ionization flexibility

For environments where ESI use predominates but occasional use of a complementary ionization mode is needed, the Waters ESCi® Multi-Mode Ionization Source minimizes the need for source changes and repeat injections by providing ESI and APCI in the same analysis. High-speed switching between ionization modes in the source enables ESI and APCI to occur throughout the analysis. The ESCi Multi-Mode Ionization Source uses ESI source hardware with the addition of an APCI corona needle and modified electronics. During ESCi operation, the electronics alternate between the electrospray capillary and the APCI corona needle within normal interscan delay times.

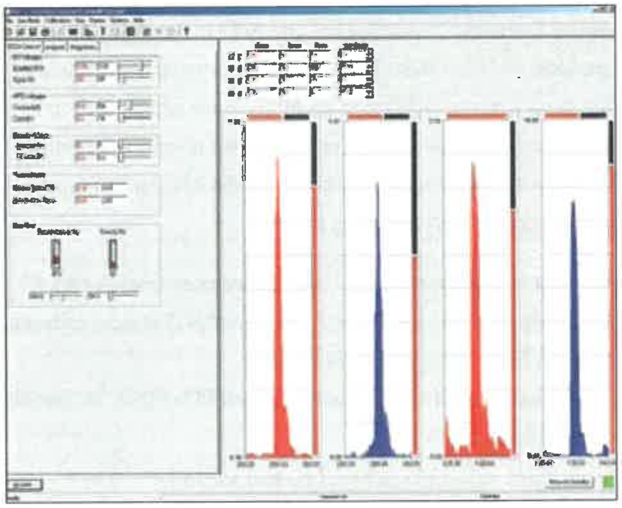
Together with the Waters ZQ™ Mass Detector or Quattro micro™ tandem quadrupole system and MassLynx™ 4.0 or later software, the ESCi Mulit-Mode Ionization Source:

- Allows for combinations of ESI-/ESI+/APCI+/APCI- for flexible sample ionization
- Enables 100 mS switching between ionization modes and polarities
- Operates from 50 µL/min to 1 mL/min and higher (using split flow)
- Enhances productivity by simplifying the workflow of samples in open access environments
- Frees up existing "dedicated ionization" systems to increase sample analysis capacity
- Minimizes the need to change ionization sources or transfer samples between LC/MS systems
- Permits multiple ionization mode data for a sample to be stored in one location—even one data file—rather than disparate LC/MS systems

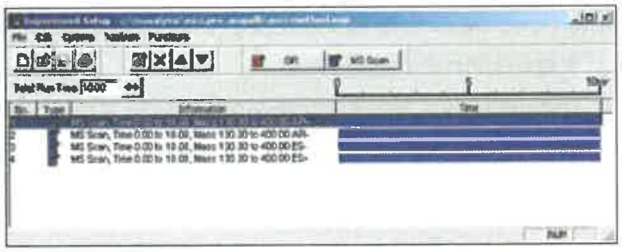
Simple operation in a MassLynx software environment

When the ESCi Multi-Mode Ionization Source is operating within a minimum of a MassLynx 4.0 software environment you can:

- Control short time constant settings, such as capillary and cone voltages, for each ionization mode
- Develop methods with ionization modes in various combinations and durations
- Review data easily using the standard MassLynx chromatogram and spectrum windows plus the intuitive OpenLynx™ Application Manager browser
- Use sample submission, data processing and results reporting capabilities via the OpenLynx Application Manager for open access and high throughput environments



Parameters for ESI and APCI can be optimized and signal can be monitored on the same MS tune page.



MS experiment setup is the same as with traditional ionization sources—only now, ionization modes can be chosen in various combinations and durations.

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Waters Global Services focuses on optimizing Waters products with superior service, support, upgrades, training, and Waters Quality Parts®

PROVEN SATISFACTION

For the sixth consecutive year, an independent quality auditing firm ranked Waters Global Services best-in-class in providing expert technical knowledge, quick resolution of system issues, and process support.[1]

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[1] *2006 Omega NorthFace ScoreBoard Award℠. Omega Management Group Corporation.*

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Korea 82 2 820 2700
Mexico 52 55 52 00 1860
The Netherlands 31 76 508 7200
Norway 47 6 384 6050
Poland 48 22 833 4400
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April 2008 720000104EN PC-PDF

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Waters Exceptions to State of West Virginia RFQ# 1400 AGR1900000018

General Terms and Conditions

1) Item 28. Warranty- Waters requests this language be deleted in its entirety and replaced with reference to our "Waters Licenses, Warranties, and Support Services" document attached herewith.

2) Item 35. Vendor Relationship- Waters requests removal of the 2nd paragraph

3) Item 36. Indemnification- Waters requests removal of this item in its entirety and replaced with "Intentionally Omitted"

4) Item 41. Background Check- Waters service employees are never regularly on a customer site and Waters employees do not have access to sensitive or critical information. What is required if this is the case?

   Additionally, Waters requests that certification of passed background checks conducted upon hire be provided in lieu of fingerprint-based background checks.

Specifications

5) Item 6.4 Return of Unacceptable Items- Waters requests this language be deleted in its entirety and replaced with "Waters may, in its sole discretion, authorize product returns in appropriate circumstances, subject to such conditions as Waters may specify. Any such return shall be subject to the express prior authorization of Waters and payment by Buyer of a restocking charge. No returns will be authorized after one hundred twenty (120) days following shipment to Buyer." In accordance with Waters standard commercial practice.

6) Item 6.5 Return Due to Agency Error- Waters requests removal of this item in its entirety and replaced with "Intentionally Omitted." All returns should be governed by Item 6.4, as amended, in accordance with Waters standard commercial practices.

Genius NM32LA-110V

Nitrogen Generator for LC-MS

Part Number : 10-6520 Service Kit : 08-4780

PEAK SCIENTIFIC

*Your local **gas generation** partner*

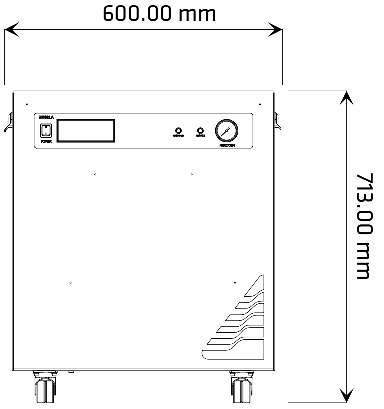
Description

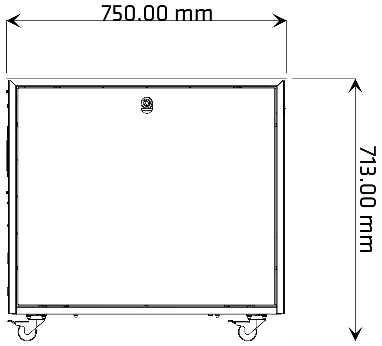
The Genius NM32LA-110V is a variant of our best-selling NM32LA nitrogen generator for LC-MS, engineered to operate at 110V rather than 230V as with the standard model. This tailored solution for laboratories operating at 110V (eg. USA), removes the requirement for a step-up transformer to boost supply to 230V in order to realize the benefits of the NM32LA.

The culmination of over a decade's work perfecting an on-site nitrogen gas generation for LC-MS, the Genius NM32LA is the pinnacle of our Genius series. NM32LA has become a proven and reliable on-demand nitrogen solution in countless laboratories worldwide. This system's popularity is underpinned by its compatibility with most mass specs available in the market.

Applications

- Perfect for labs with 110V electrical supply
- Ideal nitrogen gas source for MS instruments designed to operate in 110V facilities (eg. Waters Acquity QDa)





Genius Nm32la-110v Dimensions

Key Features

- Compressor based solution, generator can run on its own without the need for an external source of air
- Proven and reliable with 1000's in the field worldwide
- 110V electrical supply compatible, no step-up transformer required
- Duty and service indicators
- Latest generation, high specification compressor located in insulated chamber to minimize noise and vibration
- Once connected to the instrument and power is supplied, the system is fully operational
- The most cost effective method of gas supply
- Remove the hassle and safety concerns of ordering and changing out pressurized cylinders
- Gas is supplied on demand so generator works to your schedule

Technical Specifications	Genius NM32LA-110V
Max Flow Rate	32 L/min
Max Pressure	100 psi / 6.9 bar
Max Relative Humidity	80% Non-Condensing
Max Altitude	2000 Metres
Particles	< 0.01µm
Gas Outlets	1x 1/4" BSP Female
Phthalates	None
Suspended Liquids	None
Operating Temperature	5°C - 35°C / 41°F - 95°F
Electrical Requirements	100-115V 60Hz 11A
Power Consumption	1265 Watts
Noise Level	59 dB
Generator Dimensions (HxWxD)	713 x 600 x 750 mm/28.1 x 23.6 x 29.5 in
Generator Weight	95 Kg (209lbs)

Ordering Information	
Part Number	10-6520
Annual Service	08-4780
Standard Maintenance Plan	09-3110
Complete Maintenance Plan	09-3010

[PEAK Protected]™

Peak Scientific gas generators define the benchmark in reliability, convenience and performance in laboratories around the world, and come backed by a 12 month warranty. Beyond this period however you can ensure that you're investment continues to be **[Protected]** by our comprehensive generator care cover.

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Product Certifications

[APPLICATION NOTE]

Waters
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Multiresidue Analysis of Pesticides in Fruits and Vegetables Using UPLC-MS/MS

Dimple Shah, Naren Meruva, and Gareth Cleland
Waters Corporation, Milford, MA, USA

APPLICATION BENEFITS

- Multiresidue method for 190 pesticides in fruit and vegetable commodities showing excellent recoveries and precision at or below EU MRL.
- Detection of incurred residues confirmed in compliance with SANTE 11945/2015 guidelines.
- Method readily extendable for additional pesticides of interest, using DisQuE™ variations, MS/MS method database, and easily updated reporting criteria.

WATERS SOLUTIONS

ACQUITY® UPLC® H-Class System

Xevo® TQ-S micro

ACQUITY BEH C_{18} Column

MassLynx® MS Software

TargetLynx™ Application Manager

Quanpedia™ Database

DisQuE QuEChERS Dispersive Solid Phase Extraction

KEYWORDS

Pesticides, green beans, white grapes, QuEChERS, food safety, MRL

INTRODUCTION

Pesticides are widely used in agricultural farming across the world. Pesticide residue levels in food products are regulated and closely monitored. Most countries have established legislation imposing Maximum Residue Limits (MRLs) for pesticide residues in food commodities which require analytical techniques that are sensitive, selective, accurate, and robust. Multiresidue analysis is challenging due to the low limits of detection required to achieve MRL compliance for a diverse range of pesticides in a wide range of food commodities. There are currently in excess of 1000 pesticides commercially available, and laboratories are under increasing pressure to widen the scope of their analytical methods for routine pesticide monitoring.

In this application note, we describe the development of a multiresidue method for the routine determination of 190 pesticide residues in various fruit and vegetable matrices using UPLC-MS/MS. White grapes and green beans were selected for this application due to their relatively increased complexity, since they contain chlorophylls which are known to affect the extraction efficiency of pesticides from food matrices. A generic QuEChERS sample extraction procedure was used to extract the pesticides from the fruit and vegetable samples, followed by rapid and high resolution UPLC separation and trace level detection of pesticides using the Xevo TQ-S micro.

EXPERIMENTAL

UPLC conditions

LC system:	ACQUITY UPLC H-Class
Column:	ACQUITY BEH C_{18} 1.7 µm, 2.1 x 100 mm
Column temp.:	45 °C
Injection volume:	10 µL
Flow rate:	0.45 mL/min
Mobile phase A:	10 mM Ammonium acetate (pH 5) in water
Mobile phase B:	10 mM Ammonium acetate (pH 5) in methanol
Weak needle wash:	50/50 Water/methanol (v/v)
Strong needle wash:	10/90 Methanol/water (v/v)
Seal wash:	90/10 Water/methanol

Gradient:

Time (min)	Flow rate (mL/min)	%A	%B	Curve
Initial	0.450	98	2	6
0.25	0.450	98	2	6
12.25	0.450	1	99	6
13.00	0.450	1	99	6
13.01	0.450	98	2	6
17.00	0.450	98	2	6

MS conditions

MS system:	Xevo TQ-S micro
Ionization mode:	ESI+
Capillary voltage:	1.00 kV
Desolvation temp.:	500 °C
Desolvation gas flow:	1000 L/Hr
Source temp.:	150 °C

Two MRM transitions for each compound were obtained from the Quanpedia Database[1] which contains a compendium of methods, and monitored for all of the pesticides that were studied. The data were acquired and processed using MassLynx MS Software v.4.1 with TargetLynx XS Application Manager.

Standards

Waters® LC Multiresidue Pesticide Standards Kit (p/n 186007574) was used to make a mix of calibration standards. The stock solution of 10 µg/mL was prepared by combining 100 µL from each ampoule.

Sample description

The green beans and white grape samples investigated in this study were purchased from a local supermarket.

Sample preparation

15 g of homogenized samples were extracted with 15 mL of 1% glacial acetic acid in acetonitrile, followed by the addition of QuEChERS AOAC material (DisQuE Pouches, p/n 186006812). The tube was shaken for 1 minute and centrifuged at 3700 rpm for 5 minutes. Then 100 µL of the extract was taken and diluted to 1 mL with water before LC-MS/MS analysis.

To study linearity, solvent and matrix matched standards (MMS) calibration curves were created by spiking the pesticide mix from 0.001 to 0.50 mg/kg (1 ppb to 500 ppb) in solvent and the matrices, respectively.

RESULTS AND DISCUSSION

All pesticides were analyzed on an ACQUITY UPLC BEH C_{18} Column. For each pesticide, two MRM transitions were monitored, and AutoDwell was applied. Autodwell is a feature used in MassLynx Software to ensure that sufficient points across each chromatographic peak are achieved. A user simply enters the average peak width and number of points required, and the software automatically calculates the dwell time required to achieve the minimum number of points across the peak specified. With the rapid acquisition rate of the Xevo TQ-S micro, 380 MRMs were monitored with a 1 minute wide retention time window with at least 12 data points across the peak. False negatives are potentially avoided by extending the acquisition range.

Figure 1 shows an overlay of chromatograms (vertically linked) for all pesticides spiked at 10 ppb (0.01 mg/kg) in the green beans and white grapes.

LINEARITY

Linearity was studied with nine different levels of matrix-matched standards calibration. The concentrations of the calibration levels ranged from 1 to 500 ppb (sample equivalent to 0.001 to 0.5 mg/kg). A majority of the compounds (96%) showed a linear response with correlation coefficients >0.990 in both matrices. Example calibration curves of imidacloprid in white grapes and pyraclostrobin in green beans are shown in Figure 2.

RECOVERY

Method recovery was evaluated by spiking the reference standards in the samples and quantifying against the matrix-matched calibration curve. Green bean and white grape samples were pre-spiked with all of the pesticides at 10 ppb (0.01 mg/kg) in triplicate. The samples were extracted and quantified against the matrix matched calibration curve. Recoveries were calculated using TargetLynx XS Software. Recoveries for most of the pesticides (97% in white grapes and 96% in green beans) fell within the acceptable tolerance of 70% to 120% range (DG SANTE/11945/2015)[2] in both samples. The precision in terms of %RSD for most compounds (93%) in green beans and white grapes were less than 20%. The use of a suitable internal standard will significantly improve repeatability for those analytes. Recoveries for all the pesticides in green beans and white grapes are shown in Appendix A.

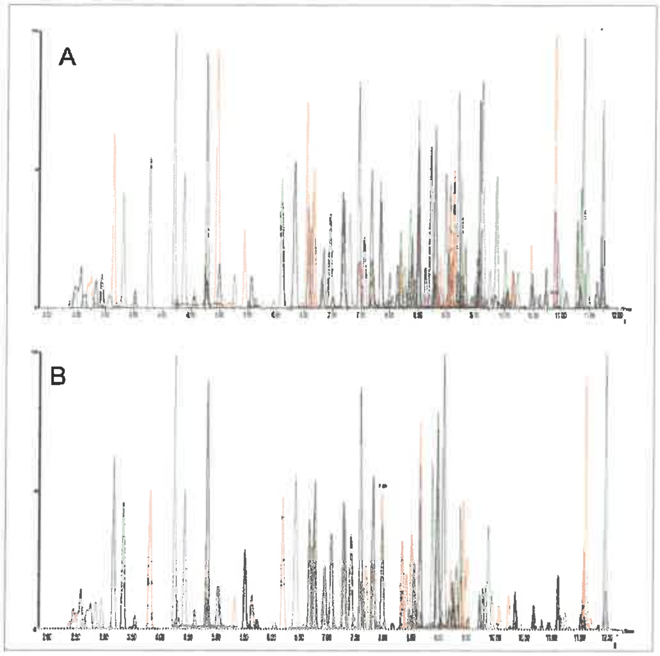


Figure 1. Total ion chromatogram of pesticides in A. green beans, and B. white grapes.

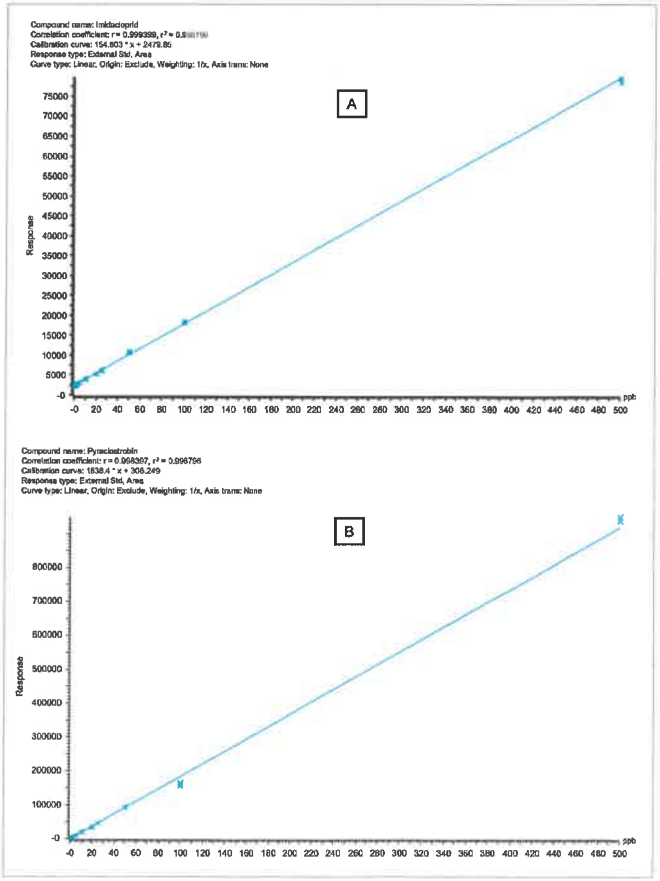
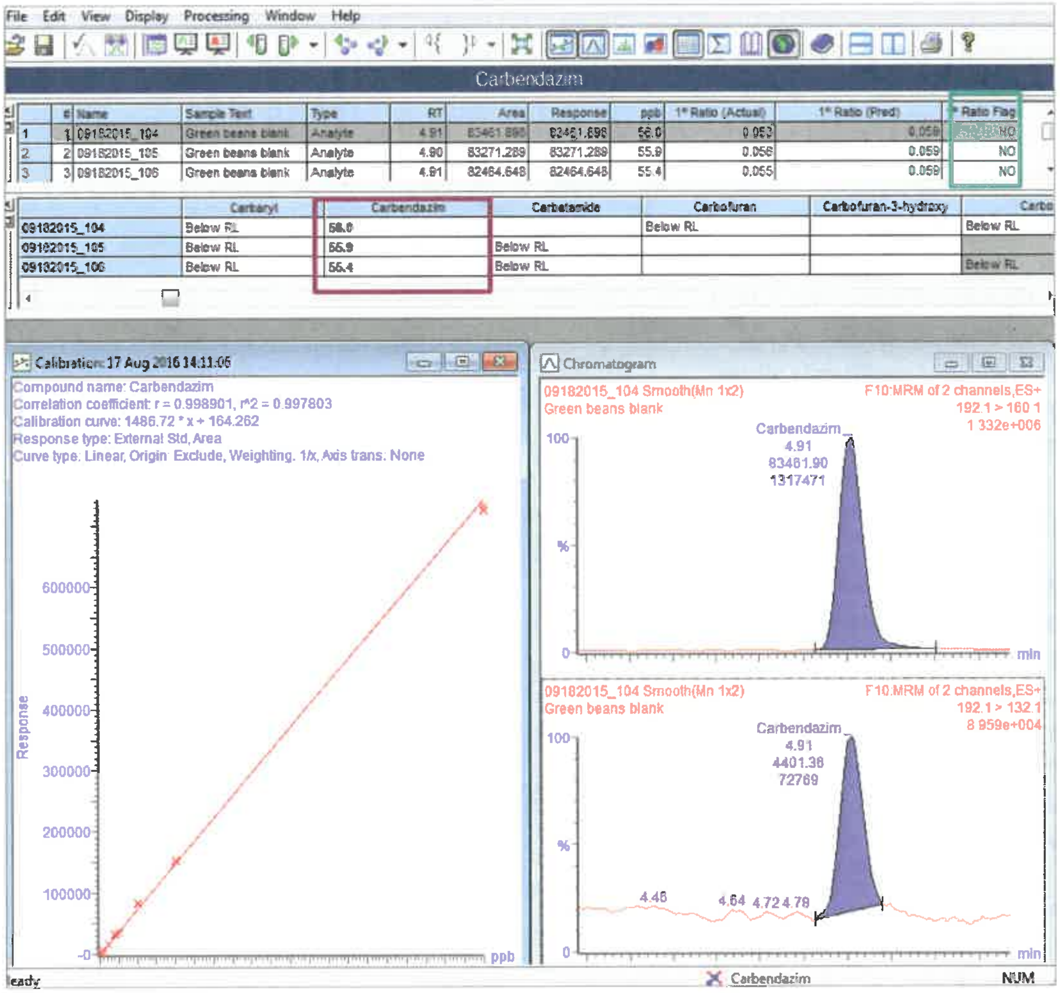


Figure 2. Matrix matched calibration curve of A. imidacloprid in white grapes, and B. pyraclostrobin in green beans.

SAMPLE ANALYSIS

To determine incurred residues, the white grape and green bean samples were prepared as described in the Sample preparation section and analyzed. From the obtained results, carbendazim, propamocarb, and pyrimethanil were observed in the green bean sample and quantified below 0.07 mg/kg. Boscalid, cyprodinil, fenhexaid, imidacloprid, methoxyfenozide, pyraclostrobin, and trifloxystrobin were observed in the grape sample and quantified at less than 0.25 mg/kg. For accurate quantification of incurred residues, a standard addition technique can be employed. Figure 3 shows an example of an incurred residue found in the green bean sample.

In order to avoid false identification, it is important to check the retention time tolerance and ion ratios of the incurred residues. TargetLynx automatically calculates ion ratios and provides accurate quantification for all incurred residues. All of the incurred pesticide residues detected in the green bean and white grape samples were identified in accordance with the criteria specified in the European Commission SANTE document 11945/2015,[2] [retention time (± 0.1 minute) and ion ratios (<30 %)] and compared against the reference.



	#	Name	Sample Text	Type	RT	Area	Response	ppb	1° Ratio (Actual)	1° Ratio (Pred)	* Ratio Flag
1	1	09182015_104	Green beans blank	Analyte	4.91	83461.898	83461.898	56.0	0.053	0.059	NO
2	2	09182015_105	Green beans blank	Analyte	4.90	83271.289	83271.289	55.9	0.056	0.059	NO
3	3	09182015_106	Green beans blank	Analyte	4.91	82464.648	82464.648	55.4	0.055	0.059	NO

	Carbaryl	Carbendazim	Carbetamide	Carbofuran	Carbofuran-3-hydroxy	Carbo
09182015_104	Below RL	56.0		Below RL		Below RL
09182015_105	Below RL	55.9	Below RL			
09182015_106	Below RL	55.4	Below RL			Below RL

Calibration: 17 Aug 2016 14:11:06

Compound name: Carbendazim
Correlation coefficient: r = 0.998901, r^2 = 0.997803
Calibration curve: 1486.72 * x + 164.262
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

Figure 3. Carbendazim identified in the green bean sample.

CONCLUSIONS

- A broad range of pesticides (190) of interest were successfully analyzed using an easy sample preparation procedure (QuEChERS) and UPLC-MS/MS determination in green bean and white grape samples.
- This method can easily detect all of the listed pesticides at 0.01 mg/kg which is at or below the maximum residue level limit (MRL).
- More than 95% of the pesticides were detected with recoveries within the range of 70% to 120% using a QuEChERS extraction procedure.
- TargetLynx Application Manager provides efficient and automated data processing tools for calculating recoveries and quantification of incurred residues.

References

1. Quanpedia Database: A Compendium of Compounds and Analyses for Rapid and Simple Multi-Residue LC-MS/MS Method Development. Waters Technology Brief No. 720004400en. 2012.
2. Guidance document on the analytical quality control and method validation procedures for pesticides residues analysis in food and feed.
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Appendix A

		White grapes		Green grapes	
Name	RT	Recovery 0.01 mg/kg (n=3)	% RSD	Recovery 0.01 mg/kg (n=3)	% RSD
Acephate	1.93	87.0	6.4	94.6	3.9
Acetamiprid	4.71	99.3	4.8	107.2	2.3
Acibenzolar-S-methyl	8.18	130.2	17.1	–	–
Aldicarb	5.6	98.9	6.8	109.3	4.5
Aldicarb sulfone	2.79	99.2	5.8	114.6	4.9
Aldicarb sulfoxide	2.65	64.8	7.8	107.5	3.5
Ametryn	8.36	100.8	5.3	101.6	7.2
Aminocarb	6.28	90.8	5.2	108.4	2.2
Azoxystrobin	8.46	101.0	6.0	103.8	5.0
Benalaxyl	9.82	103.9	4.8	102.6	5.0
Bendiocarb	6.57	103.3	5.8	106.4	2.5
Benzoximate	10.1	99.4	6.9	97.3	7.7
Bifenazate	9.07	171.8	16.1	62.0	6.6
Bitertanol	10.09	97.6	9.1	92.9	11.4
Boscalid	8.67	*		95.7	23.2
Bromuconazole I	8.96	98.9	23.2	97.4	19.8
Bromuconazole II	9.57	127.7	15.7	90.9	18.4
Bupirimate	9.51	107.7	9.6	105.7	12.9
Buprofezin	10.85	102.0	7.7	111.4	5.1
Butafenacil	9.16	107.8	8.1	96.2	6.3
Butocarboxim	5.51	98.0	6.5	105.4	2.6
Butoxycarboxim	2.79	98.2	6.0	107.2	3.5
Carbaryl	6.91	96.8	4.4	101.2	2.5
Carbendazim	4.91	97.8	6.0	*	
Carbetamide	6.05	97.7	5.6	106.4	2.8
Carbofuran	6.63	102.4	5.4	109.0	2.9
Carbofuran-3-hydroxy	4.75	103.7	6.4	118.2	3.8
Carboxin	6.8	99.5	5.3	103.4	4.1
Carfentrazone-ethyl	9.61	109.8	16.6	97.2	16.1
Chlorantraniliprole	8.14	89.2	14.0	106.3	15.4
Chlorfluazuron	11.57	139.9	32.2	102.6	30.7
Chloroxuron	9	109.0	7.0	108.6	7.2
Chlortoluron	7.25	103.8	5.0	108.1	3.0
Clethodim I	7.96	140.6	16.6	91.0	15.2
Clethodim II	9.39	97.4	16.7	96.5	18.5
Clofentezine	10	115.1	10.7	117.6	7.6
Clothianidin	4.17	102.2	11.1	105.6	5.1
Cyazofamid	9.3	108.2	6.4	102.8	6.6
Cycluron	7.81	104.2	6.1	109.5	3.2
Cymoxanil	4.94	101.0	6.9	104.9	2.5
Cyproconazole I	8.84	104.1	8.6	91.0	15.2

		White grapes		Green grapes	
Name	**RT**	**Recovery 0.01 mg/kg (n=3)**	**% RSD**	**Recovery 0.01 mg/kg (n=3)**	**% RSD**
Cyproconazole II	9.05	83.3	16.6	104.9	2.5
Cyprodinil	9.66	*		78.2	28.4
Cyromazine	2.09	96.2	19.9	93.5	5.6
Desmedipham	7.97	95.1	5.6	96.0	4.0
Diclobutrazol	9.5	97.9	9.5	100.5	7.2
Dicrotophos	4.16	94.3	5.3	100.0	1.5
Difenoconazole I	10.27	102.4	12.4	88.8	11.0
Difenoconazole II	10.31	97.5	5.5	82.5	9.7
Diflubenzuron	9.4	104.6	10.7	97.3	9.8
Dimethoate	4.52	92.1	10.0	97.6	17.4
Dimethomorph I	8.61	84.4	21.0	103.3	14.9
Dimethomorph II	8.61	98.6	16.9	92.5	17.0
Dimoxystrobin	9.59	106.0	4.5	103.2	6.5
Diniconazole	10.19	89.6	32.4	97.4	12.7
Dinotefuran	2.6	102.1	4.6	99.5	23.4
Diuron	7.66	114.4	7.4	90.1	4.7
Emamectin benzoate I	11.3	107.3	5.5	97.5	11.5
Emamectin benzoate II	11.3	109.4	8.8	97.4	14.2
Epoxiconazole	9.25	100.7	7.4	100.9	11.7
Eprinomectin	11.76	99.5	35.0	85.3	23.0
Etaconazole I	9.23	91.4	16.9	96.9	22.9
Etaconazole II	9.3	85.1	12.2	104.6	25.7
Ethiofencarb	7.12	100.1	6.4	99.4	2.6
Ethiprole	8.6	106.6	13.1	75.2	27.0
Ethofumesate	8.4	103.8	8.8	102.9	6.7
Famoxadone	9.94	103.1	7.0	99.0	5.0
Fenamidone	8.6	101.7	4.5	100.5	7.3
Fenarimol	9.21	122.2	14.0	–	–
Fenazaquin	11.6	102.9	15.4	82.6	6.8
Fenbuconazole	9.42	94.9	14.0	94.1	12.7
Fenhexamid	9.16	*		83.1	11.6
Fenobucarb	8.31	101.5	7.3	92.7	36.8
Fenoxycarb	9.53	123.3	7.2	119.9	2.6
Fenpropimorph	11.71	101.6	8.3	91.6	13.4
Fenpyroximat	11.39	100.1	3.3	98.6	4.2
Fenuron	4.33	102.0	4.4	110.4	1.5
Fipronil	9.53	–		72.6	32.1
Flonicamid	3.28	99.0	11.5	113.1	19.2
Flufenacet	9.22	108.0	5.7	102.3	5.4
Flufenoxuron	11.32	114.7	5.9	104.5	4.3
Fluomethuron	7.14	106.5	6.5	100.6	2.8
Fluoxastrobin	9.2	100.9	12.0	92.6	21.0
Fluquinconazole	9.06	74.0	31.9	79.0	23.3

		White grapes		Green grapes	
Name	**RT**	**Recovery 0.01 mg/kg (n=3)**	**% RSD**	**Recovery 0.01 mg/kg (n=3)**	**% RSD**
Flusilazole	9.51	100.8	8.8	107.7	18.0
Flutolanil	8.77	102.4	7.8	95.2	6.8
Flutriafol	7.63	96.9	11.2	87.9	7.5
Forchlorfenuron	7.65	99.9	8.9	96.7	11.1
Formetanate HCL	2.53	87.2	5.9	106.6	12.2
Fuberidazole	5.9	115.2	8.4	95.0	9.3
Furalaxyl	8.47	103.4	7.2	111.8	4.8
Furathiocarb	10.7	107.4	5.5	101.7	8.3
Halofenzoide	8.52	106.7	20.4	79.5	35.4
Hexaconazole	10	98.0	10.5	93.2	9.8
Hexythiazox	11.07	107.5	7.1	103.3	5.9
Hydramethylnon	10.67	76.4	17.3	103.3	7.4
Imazalil	9.52	113.9	11.8	88.8	21.0
Imidacloprid	4.21	*		102.3	7.7
Indoxacarb	10.42	124.6	13.1	107.5	6.5
Ipconazole I	10.31	98.4	14.8	94.1	4.1
Ipconazole II	10.45	97.2	6.1	95.2	3.5
Iprovalicarb I	9.03	101.5	6.1	98.1	2.2
Iprovalicarb II	9.1	106.4	6.0	98.7	4.7
Isocarbofos	7.84	95.2	21.8	–	–
Isoprocarb	7.52	102.0	6.0	101.5	3.3
Isoproturon	7.64	103.0	5.1	102.7	2.9
Ivermectine	12.47	123.9	31.0	87.7	28.0
Kresoxim-methyl	9.63	100.1	15.0	77.2	22.3
Linuron	8.28	103.6	7.6	93.2	6.1
Lufenuron	10.98	109.4	11.9	97.3	12.4
Mandipropamid	8.77	103.4	9.4	104.4	7.6
Mefenacet	8.95	105.4	5.2	102.5	6.8
Mepanipyrim	8.99	103.5	13.4	99.6	16.9
Mepronil	8.76	104.4	5.8	107.3	6.4
Mesotrione	2.87	85.6	17.2	84.1	12.3
Metalaxyl	7.8	102.9	6.2	108.9	3.4
Metconazole	10	98.2	7.9	93.4	3.5
Methabenzthiazuron	7.43	102.5	4.1	104.3	4.0
Methamidophos	1.61	75.3	8.3	94.8	11.0
Methiocarb	8.47	103.0	5.2	101.0	6.9
Methomyl	3.27	100.5	5.8	116.3	1.6
Methoprotryne	8.35	102.3	5.3	103.6	6.0
Methoxyfenozide	8.85	*		103.6	6.5
Metobromuron	7.3	103.6	10.4	106.8	4.4
Metribuzin	6.3	93.0	22.1	99.0	19.1
Mevinphos I	4.7	95.5	10.7	101.8	5.1
Mevinphos II	5.39	95.8	6.5	96.5	3.0

		White grapes		Green grapes	
Name	RT	Recovery 0.01 mg/kg (n=3)	% RSD	Recovery 0.01 mg/kg (n=3)	% RSD
Mexacarbate	8.77	96.2	8.0	96.4	4.8
Monocrotophos	3.73	95.2	5.4	98.8	1.6
Monolinuron	6.95	100.1	13.9	141.0	13.0
Myclobutanil	8.95	108.0	14.7	126.5	11.9
Neburon	9.51	114.7	10.4	121.3	16.6
Nitenpyram	3.19	98.0	8.8	102.2	7.6
Novaluron	10.57	118.6	19.3	108.6	11.3
Omethoate	2.44	87.6	10.2	98.9	4.0
Oxadixyl	6.12	105.3	4.6	107.0	13.1
Oxamyl	3.11	101.0	5.3	108.4	2.3
Paclobutrazol	8.73	94.7	11.8	88.8	7.9
Penconazole	9.17	99.1	15.6	88.9	8.9
Pencycuron	10.19	99.1	25.8	94.6	34.4
Phenmedipham	8.1	97.7	6.3	97.9	8.0
Picoxystrobin	9.55	108.1	5.4	110.9	5.7
Piperonyl butoxide	10.85	107.1	5.3	104.1	6.7
Pirimicarb	7.42	99.0	5.3	100.3	1.7
Procloraz	10.08	113.7	17.7	87.7	14.4
Promecarb	8.69	101.5	6.8	102.0	4.7
Prometon	8.22	101.4	5.9	93.9	15.2
Prometryn	9.11	100.4	9.0	100.7	8.1
Propamocarb	2.72	64.3	6.7	*	
Propargite	11.26	101.8	5.0	102.9	2.9
Propham	7.36	109.8	36.6	102.0	11.4
Propiconazole I	9.87	93.5	24.8	76.3	10.0
Propiconazole II	9.92	103.3	16.4	86.7	9.5
Propoxur	6.53	99.4	4.7	106.0	2.3
Pymetrozine	3.48	100.9	8.3	124.9	4.2
Pyracarbolid	6.61	100.2	6.7	105.0	2.0
Pyraclostrobin	9.97	*		110.5	5.4
Pyridaben	11.67	101.6	5.5	120.6	3.1
Pyrimethanil	8.33	90.2	28.3	*	*
Pyriproxifen	10.91	103.1	6.5	102.7	3.4
Secbumeton	8.16	100.5	7.1	99.2	3.2
Siduron	8.35	110.7	4.8	122.3	4.1
Simetryn	7.47	100.2	7.5	100.8	5.6
Spinosad A	11.34	105.7	4.5	85.8	5.1
Spirodiclofen	11.43	104.4	5.9	99.1	3.8
Spiromesifen	11.21	100.4	26.0	92.4	26.6
Spirotetramat	9.18	100.3	9.5	96.0	7.7
Spiroxamine I	9.29	102.5	6.2	110.9	4.1
Spiroxamine II	9.29	99.2	7.1	107.8	6.1
Sulfentrazone	6.93	102.3	11.2	101.5	8.4

		White grapes		Green grapes	
Name	RT	Recovery 0.01 mg/kg (n=3)	% RSD	Recovery 0.01 mg/kg (n=3)	% RSD
Tebuconazole	9.75	94.9	14.9	75.3	11.2
Tebufenozide	9.54	107.5	7.8	120.7	10.6
Tebuthiuron	6.76	99.7	6.1	103.2	2.9
Teflubenzuron	10.87	103.8	9.8	107.9	14.8
Terbumeton	8.47	104.5	6.3	103.7	3.6
Terbutryn	9.23	103.3	6.1	100.1	4.9
Tetraconazole	9.28	74.9	28.0	72.3	39.5
Thiabendazole	5.63	144.6	10.8	95.9	8.0
Thiacloprid	5.21	102.6	6.6	108.8	2.3
Thiamethoxam	3.48	105.3	6.4	104.9	4.5
Thidiazuron	6.42	94.4	7.0	92.7	6.3
Thiobencarb	10.11	105.2	6.3	98.8	6.3
Triadimefon	8.86	98.2	9.0	123.6	22.6
Triadimenol	9.04	95.9	3.9	90.7	8.4
Trichlorfon	4.51	92.7	6.4	84.5	8.7
Tricyclazole	5.47	98.6	9.1	104.6	5.5
Trifloxystrobin	10.42	*		102.1	4.6
Triflumizole	10.52	178.8	23.4	84.7	5.4
Triflumuron	10	108.8	6.3	103.0	5.5
Triticonazole	9.23	96.2	6.3	92.3	9.1
Vamidothion	4.73	95.9	4.9	102.4	1.2
Zoxamide	9.81	118.9	8.1	105.8	9.7

** Incurred residue*

- Not detected at spiked level

Determination of the Oregon Pesticide List in Cannabis Using a Simple Extraction Procedure With dSPE Cleanup and UPLC-MS/MS

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APPLICATION BENEFITS

- Sensitive and robust method for screening pesticides in cannabis per the Oregon Cannabis Pesticide Guide List
- Minimal sample preparation followed by rapid UPLC™ separation
- Automated UPLC-MS/MS method generation using the Quanpedia™ Database
- Ease of use with data analysis and reporting via MassLynx™ MS Software

WATERS SOLUTIONS

ACQUITY™ UPLC H-Class System

Xevo™ TQ-S micro Mass Spectrometer

XBridge™ BEH C_{18} *XP* Column

MassLynx MS Software

KEYWORDS

Cannabis testing, pesticides, multi-residue pesticide detection, LC-MS/MS

INTRODUCTION

The increased use of both medical and recreational cannabis in combination with its expanding legal acceptance in most US states[1] has led to rigorous cannabis safety and quality control testing. Pesticides are widely used in the cultivation of cannabis plants to safeguard against harmful insects and to promote better crop yields. The application of pesticides is regulated,[2] and their residues in cannabis products are closely monitored by state regulatory agencies. The number of pesticides and their action limits varies from state to state. In Oregon, 59 pesticides are monitored with action limits ranging from 100 to 2000 ppb. Therefore adopting a robust and rapid procedure for monitoring the Oregon pesticide list in cannabis products is critical.

Multi-residue pesticide detection is routinely performed using tandem quadrupole mass spectrometry (MS/MS) in combination with liquid chromatography (LC) and gas chromatography (GC). Both LC-MS/MS and GC-MS/MS are commonly used for multi-residue pesticide analysis as some pesticides are only amenable to either LC or GC. Tandem quadrupole MS is the detector of choice as it provides high sensitivity and selectivity for simultaneous analysis of hundreds of pesticides at low ppb (ng/g) levels in a single analysis.

In this application note we present the use of a simple sample extraction and dispersive solid phase extraction (dSPE) cleanup procedure followed by UPLC-MS/MS analysis for rapidly monitoring the Oregon Cannabis Pesticide Guide List[3] in cannabis matrix. With so many compounds to monitor, method generation can be a tedious task. In this study, the preexisting LC and MS methods from Waters™ Quanpedia Database were used to develop and implement a rapid solution for the Oregon pesticide list.

EXPERIMENTAL

Sample preparation

Standard compounds for the 59 pesticides monitored on the Oregon list were combined to produce a stock solution which was sequentially diluted to prepare the spiking solutions. Cannabis buds were first ground using a hand grinder. A 0.5 g portion of the ground material were weighed into 50 mL centrifuge tubes and spiked with 200 ppb of the acetonitrile spiking solutions. A 5-mL volume of acetonitrile was added and the samples were processed using a Geno Grinder (two stainless steel grinding balls, 11 mm) for 5 minutes (1500 rpm). The samples were then centrifuged at 5000 rpm for 5 minutes. For experiments where no further cleanup was performed, the supernatant was filtered using a 0.2 µm PTFE filter in preparation for analysis.

A 1 mL aliquot of the supernatant was added to a dSPE tube (2 mL centrifuge tube containing 150 mg $MgSO_4$, 50 mg PSA, 50 mg C_{18}, 7.5 mg graphitized carbon black), vortexed for 1 minute, centrifuged, and the supernatant transferred to a sample vial for analysis by UPLC-MS/MS.

Instrumentation and software

All separations were performed on the Waters™ ACQUITY UPLC H-Class System and the Xevo TQ-S micro Tandem Quadrupole Mass Spectrometer. MassLynx MS Software (v4.1) was used for data acquisition and processing. The Quanpedia Database can be used to automatically generate LC, MS acquisition, and TargetLynx™ data processing methods to reduce method setup times with minimal user interaction.

UPLC conditions

UPLC system: ACQUITY UPLC H-Class

Separation mode: Gradient

Column: XBridge BEH C_{18} *XP*, 130Å, 2.5 µm, 2.1 mm × 100 mm, P/N: 186006031

Solvent A: 5 mM Ammonium formate with 0.020% formic acid in water

Solvent B: Methanol

Flow rate: 0.50 mL/min

Column temp.: 30 °C

Injection volume: 5 µL

Gradient conditions:

Time (min)	%A	%B	Curve
0.00	98%	2%	–
0.20	98%	2%	6
11.50	1%	99%	6
13.00	1%	99%	6
13.25	98%	2%	1
15.00	98%	2%	1

MS conditions

MS system: Xevo TQ-S micro

Ionization mode: ESI+/ESI-

Capillary voltage: 2.5 kV (+); 2.4 kV (-)

Cone voltage: Various V

Collision energy: Various eV

Desolvation temp.: 450 °C

Source temp.: 150 °C

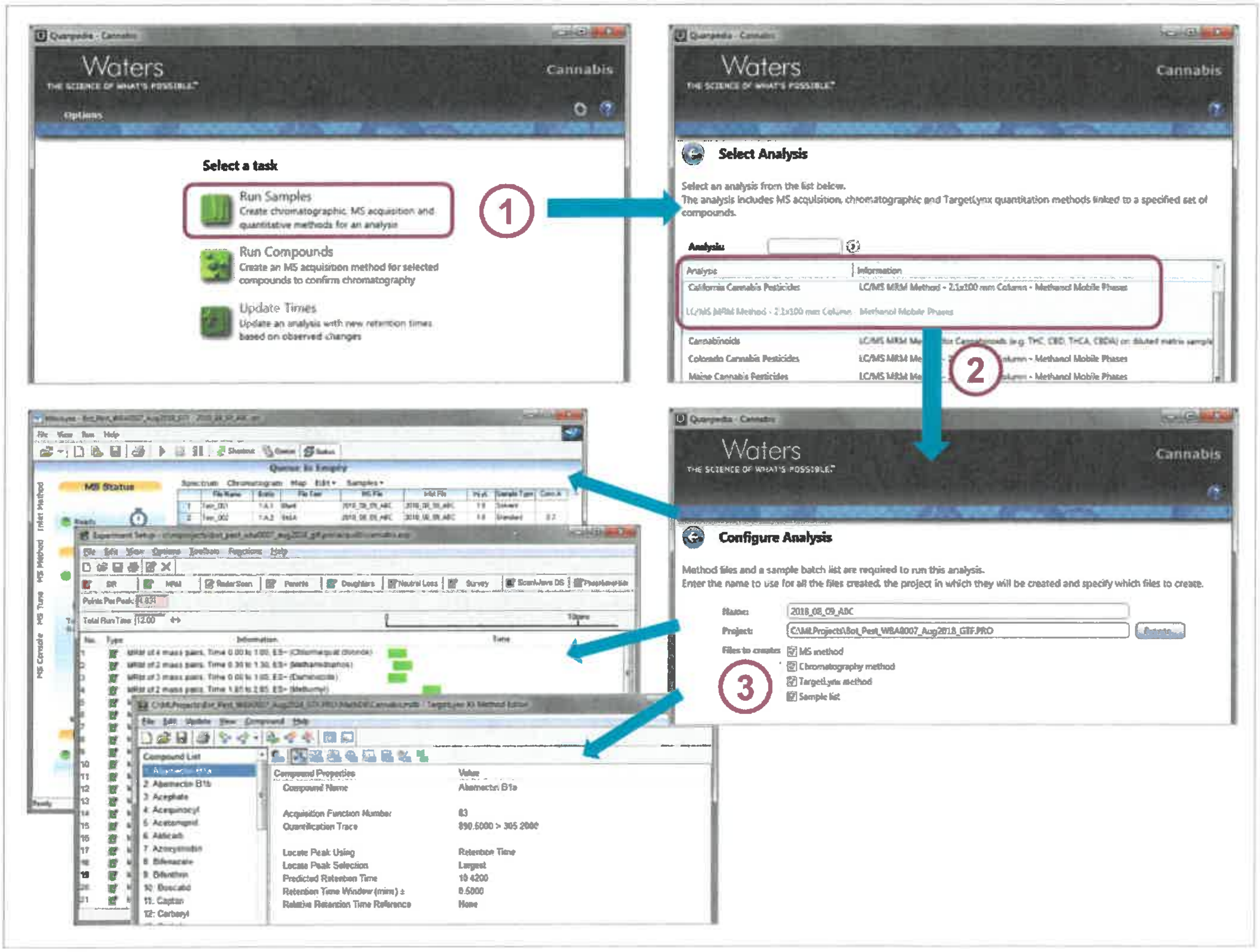
Desolvation gas flow: 1000 L/Hr

Cone gas: 50 L/Hr

RESULTS AND DISCUSSION

METHOD DEVELOPMENT AND OPTIMIZATION

Quanpedia Database was used to automatically create the LC, MS, and data processing methods (Figure 1) for the various target pesticides monitored using the transitions listed in Table 1. Users can quickly generate pre-defined LC-MS/MS methods in three easy steps, which greatly reduces the potential for error and level of complexity involved in method development for large numbers of target analytes. As a result, it decreases the amount of work, time, and resources required for laboratories to set up methods.



Select a task

Run Samples
Create chromatographic, MS acquisition and quantitative methods for an analysis

Run Compounds
Create an MS acquisition method for selected compounds to confirm chromatography

Update Times
Update an analysis with new retention times based on observed changes

Select Analysis

Select an analysis from the list below.
The analysis includes MS acquisition, chromatographic and TargetLynx quantitation methods linked to a specified set of compounds.

Analysis:

Analysis	Information
California Cannabis Pesticides	LC/MS MRM Method - 2.1x100 mm Column - Methanol Mobile Phases
LC/MS MRM Method - 2.1x100 mm Column	Methanol Mobile Phases
Cannabinoids	LC/MS MRM Me… for Cannabinoids (e.g. THC, CBD, THCA, CBDA) on diluted matrix sample
Colorado Cannabis Pesticides	LC/MS MRM Me… olumn - Methanol Mobile Phases
Maine Cannabis Pesticides	LC/MS MRM Me… olumn - Methanol Mobile Phases

Configure Analysis

Method files and a sample batch list are required to run this analysis.
Enter the name to use for all the files created, the project in which they will be created and specify which files to create.

Name: 2018_08_09_ABC
Project: C:\MLProjects\Bot_Pest_WBA0007_Aug2018_GTF.PRO
Files to create:
☑ MS method
☑ Chromatography method
☑ TargetLynx method
☑ Sample list

Compound List
2 Abamectin B1b
3 Acephate
4 Acequinocyl
5 Acetamiprid
6 Aldicarb
7 Azoxystrobin
8 Bifenazate
9 Bifenthrin
10 Boscalid
11 Captan
12 Carbaryl

Compound Properties	Value
Compound Name	Abamectin B1a
Acquisition Function Number	83
Quantification Trace	890.5000 > 305.2000
Locate Peak Using	Retention Time
Locate Peak Selection	Largest
Predicted Retention Time	10.4200
Retention Time Window (mins) ±	0.5000
Relative Retention Time Reference	None

Figure 1. Rapid implementation of LC, MS, and data processing methods using the Quanpedia Database.

Table 1. Retention times, MRM transitions, and %Recovery for the Oregon pesticide list in cannabis matrix. Data based on four replicate measurements.

Pesticides	RT (min)	%Recovery	Quan trace	Qual trace
Abamectin	11.72	71	890.7>305.3	890.7>145.1
Acephate	2.40	85	184.1>143.1	184.1>95.1
Acequinocyl	12.71	82	343.2>189.1	343.2>115.0
Acetamiprid	5.06	90	223.1>126.1	223.1>56.1
Aldicarb	5.76	108	208.1>89.1	208.1>116.1
Azoxystrobin	8.10	95	404.1>344.1	404.1>372.1
Bifenazate	8.70	94	301.1>170.2	301.1>153.1
Bifenthrin	12.01	96	440.1>166.2	440.2>181.2
Boscalid	8.32	94	343.1>307.1	343.1>140.1
Carbaryl	6.86	92	202.1>145.1	202.1>127.1
Carbofuran	6.54	92	222.1>165.1	222.1>123.1
Chlorantraniliprole	7.83	90	481.9>283.9	481.9>450.9
Chlorfenapyr	10.12	97	409.2>186.1	409.2>206.1
Chlorpyrifos	10.82	92	351.9>124.9	351.9>199.9
Clofentezine	9.73	90	303.1>138.1	303.1>102.1
Cyfluthrin	11.25	114	451.1>191.1	453.1>193.1
Cypermethrin	11.43	90	433.1>191.0	435.1>193.1
Daminozide	0.59	53	161.1>143.1	161.1>61.1
Diazinon	9.46	95	305.1>169.1	305.1>153.1
Dichlorvos	6.41	90	221.1>109.1	221.1>79.1
Dimethoate	4.92	92	230.1>125.1	230.1>198.9
Ethoprophos	8.82	87	243.1>130.9	243.1>97.1
Etofenprox	11.91	92	394.3>177.1	394.3>106.9
Etoxazole	11.05	87	360.2>141.1	360.2>113.1
Fenoxycarb	9.20	96	302.1>116.1	302.1>88.1
Fenpyroximate	11.20	90	422.2>366.1	422.2>138.1
Fipronil	9.21	101	434.9>330.1	434.9>250.1
Flonicamid	3.67	96	230.1>203.1	230.1>148.1
Fludioxinil	8.38	99	247.2>126.1	247.2>180.2
Hexythiazox	10.87	87	353.1>228.1	353.1>168.1
Imazalil	7.54	48	297.1>159.1	297.1>69.1
Imidacloprid	4.65	87	256.1>175.1	256.1>209.1
Kresoxim-methyl	9.26	98	314.1>116.1	314.1>235.1
Malathion	8.42	98	331.1>127.1	331.1>285.1
Metalaxyl	7.50	90	280.2>220.1	280.2>192.1
Methiocarb	8.22	92	226.1>121.1	226.1>169.1
Methomyl	3.67	93	163.1>88.1	163.1>106.1
MGK 264	9.96	90	276.1>210.1	276.1>71.1
Myclobutanil	8.63	88	289.1>69.9	289.1>125.1
Naled	7.68	96	381.1>127.1	381.1>109.1
Oxamyl	3.47	93	237.1>72.1	237.1>90.1
Paclobutrazol	8.39	88	294.1>70.2	294.1>125.1
Parathion methyl	8.07	94	264.2>125.1	264.2>232.1
Permethrin	11.86	90	408.1>183.1	410.1>185.1
Phosmet	7.89	92	318.1>160.1	318.1>133.1
Piperonyl butoxide	10.60	84	356.2>177.1	356.2>119.1
Prallethrin	10.04	102	301.2>133.1	301.2>169.1
Propiconazole	9.50	80	342.1>69.1	342.1>158.9
Propoxur	6.45	92	210.1>111.1	210.1>168.1
Pyrethrin I	11.19	91	329.1>161.1	329.1>133.1
Pyrethrin II	10.13	94	373.2>161.1	373.2>133.1
Pyridaben	11.46	85	365.2>147.1	365.2>309.1
Spinosad A	9.82	43	732.6>142.1	732.6>98.1
Spinosad D	10.25	40	746.5>142.1	746.5>98.1
Spiromesifen	8.11	94	372.3>344.2	372.3>329.2
Spirotetramat	8.77	87	374.1>330.1	374.1>302.1
Spiroxamine	8.31	42	298.1>144.1	298>100.1
Tebuconazole	9.43	85	308.2>70.1	308.2>125.1
Thiacloprid	5.50	90	253.1>126.1	253.1>90.1
Thiamethoxam	3.92	92	292.1>132.1	292.1>211.2
Trifloxystrobin	10.12	96	409.1>186.1	409.1>145.1

Figure 2 shows an overlay chromatogram of 59 pesticides analyzed by UPLC-MS/MS. MRM chromatograms of selected pesticides in cannabis matrix are shown in Figure 3.

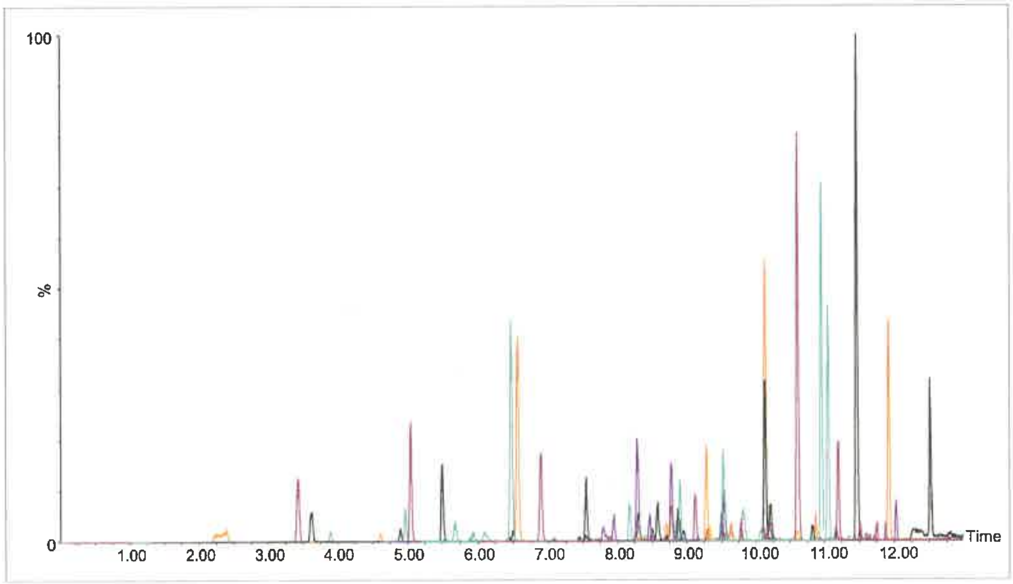


Figure 2. UPLC-MS/MS chromatogram overlay of 59 pesticides spiked at 200 ppb in the cannabis matrix.

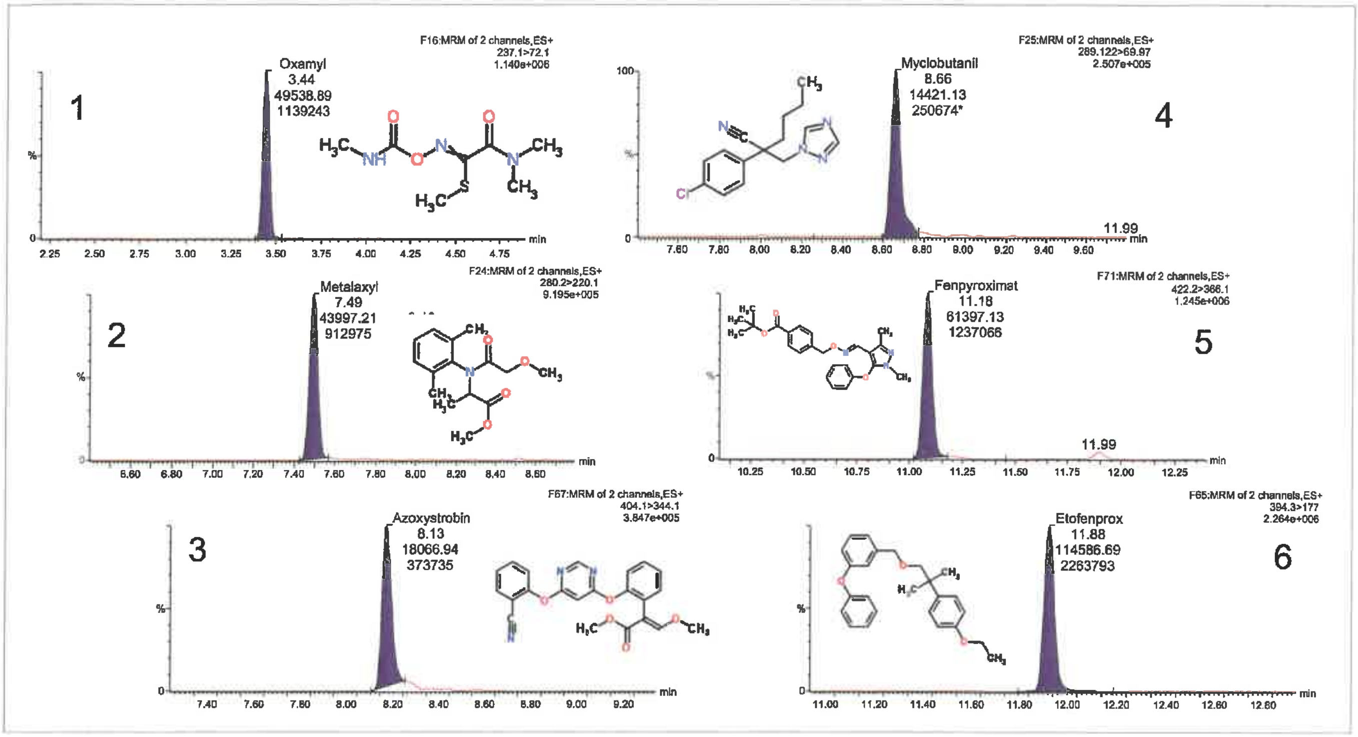
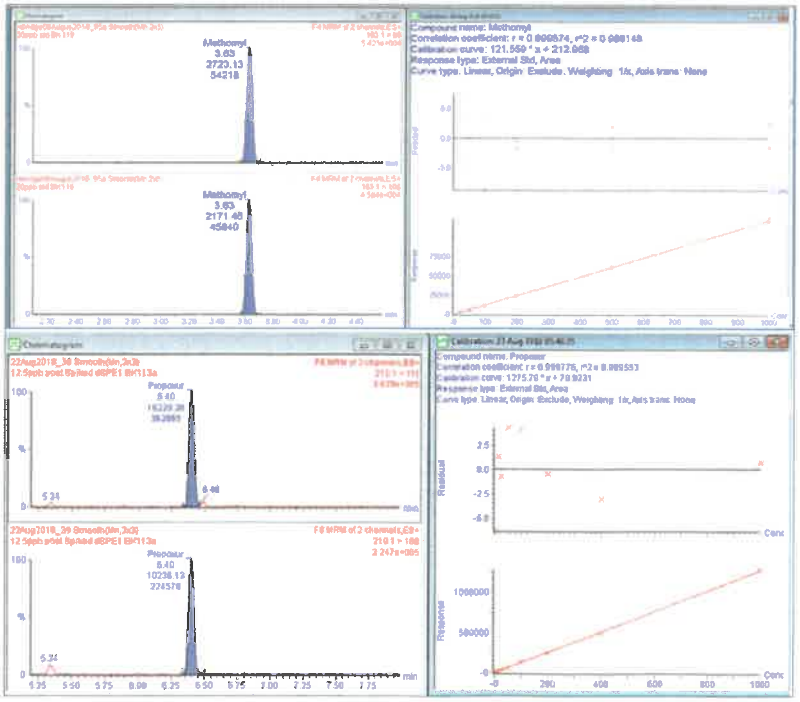


Figure 3. Representative MRM chromatograms for 1. oxamyl, 2. metalaxyl, 3. azoxystrobin, 4 myclobutanil, 5. fenpyroximat, and 6. etofenprox spiked at a level of 200 ppb and extracted using the sample preparation protocol reported.

LINEARITY

An example of the quantitation curve for methomyl and propoxur are shown in Figure 4. Linear calibration curves ($R^2>0.990$) for each pesticide were obtained over the range tested 6.25 to 1000 ppb in matrix. Table 2 highlights the limit of quantitation (LOQ) and action limits per the Oregon Cannabis Pesticide Guide List.[3]



Compound name: Methomyl
Correlation coefficient: r = 0.999574, r^2 = 0.999148
Calibration curve: 121.559 * x + 212.968
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

Compound name: Propoxur
Correlation coefficient: r = 0.999776, r^2 = 0.999553
Calibration curve: 1275.78 * x + 78.9231
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

Figure 4. Representative example of quantitation curves for methomyl and propoxur analyzed with a linearity range of 6.25 to 1000 ppb.

RECOVERY AND MATRIX EFFECTS

Method recovery was assessed by spiking pesticides at the 200 ppb and 1000 ppb levels in a cannabis flower matrix and comparing the response to that observed from spiked matrix blanks (matrix-matched standards). As shown in Figure 5, the recoveries observed for most of the pesticides were in the range of 80% to 120%. Matrix suppression was determined at the 200 ppb level by comparing the response observed in matrix-matched standards to the response observed in the solvent standards. Matrix suppression data is presented in Figure 6. Those compounds that co-eluted with the cannabis resin constituents (retention times from 9 to 12 minutes) showed the greatest suppression before dSPE cleanup. The dSPE cleanup provided a significant reduction of suppression for most of the compounds.

Table 2. Limit of quantitation (LOQ) for pesticide analytes and their action levels in the Oregon Cannabis Pesticide Guide List.

Pesticides	LOQ (ppb)	Action levels (ppb)	Pesticides	LOQ (ppb)	Action levels (ppb)
Abamectin	<200	500	Imazalil	<100	200
Acephate	<200	400	Imidacloprid	<100	400
Acequinocyl	<100	2000	Kresoxim-methyl	<100	400
Acetamiprid	<100	200	Malathion	<100	200
Aldicarb	<200	400	Metalaxyl	<100	200
Azoxystrobin	<100	200	Methiocarb	<100	200
Bifenazate	<100	200	Methomyl	<100	400
Bifenthrin	<100	200	MGK 264	<100	200
Boscalid	<100	400	Myclobutanil	<100	200
Carbaryl	<100	200	Naled	<100	500
Carbofuran	<100	200	Oxamyl	<100	1000
Chlorantraniliprole	<100	200	Paclobutrazol	<100	400
Chlorfenapyr	<100	1000	Parathion methyl	<100	200
Chlorpyrifos	<100	200	Permethrin	<100	200
Clofentezine	<100	200	Phosmet	<100	200
Cyfluthrin	<200	1000	Piperonyl butoxide	<100	2000
Cypermethrin	<200	1000	Prallethrin	<100	200
Daminozide	<1000	1000	Propiconazole	<100	400
Diazinon	<100	200	Propoxur	<100	200
Dichlorvos	<100	100	Pyrethrin	<200	1000
Dimethoate	<100	200	Pyridaben	<100	200
Ethoprophos	<100	200	Spinosad	<100	200
Etofenprox	<200	400	Spiromesifen	<200	200
Etoxazole	<100	200	Spirotetramat	<100	200
Fenoxycarb	<100	200	Spiroxamine	<100	400
Fenpyroximate	<100	400	Tebuconazole	<100	400
Fipronil	<100	400	Thiacloprid	<100	200
Flonicamid	<200	1000	Thiamethoxam	<100	200
Fludioxinil	<200	400	Trifloxystrobin	<100	200
Hexythiazox	<100	1000			

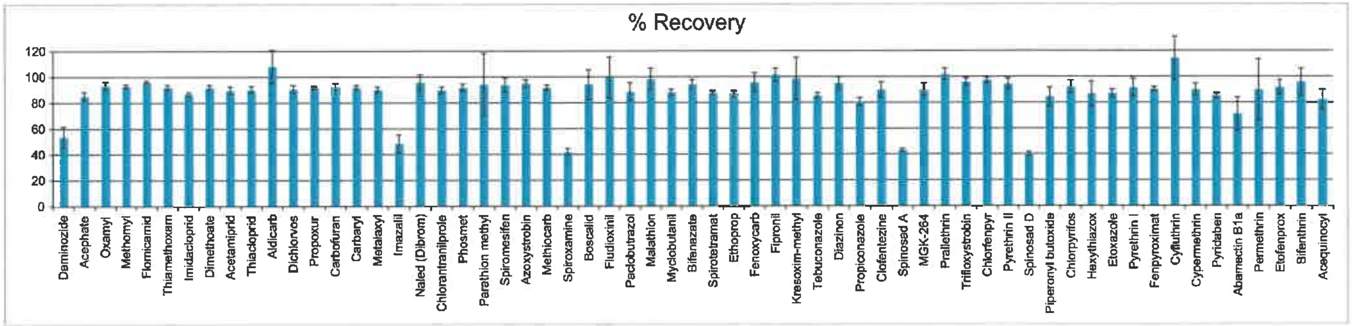


Figure 5. %Recovery of pesticides from the cannabis matrix (n = 4). Compounds are presented in order of retention (from 2.9 min for acephate to 12.8 min for acequinocyl). Error bars indicate the standard deviation observed for each compound. The combined recovery of spinosad A and D components is close to 85%.

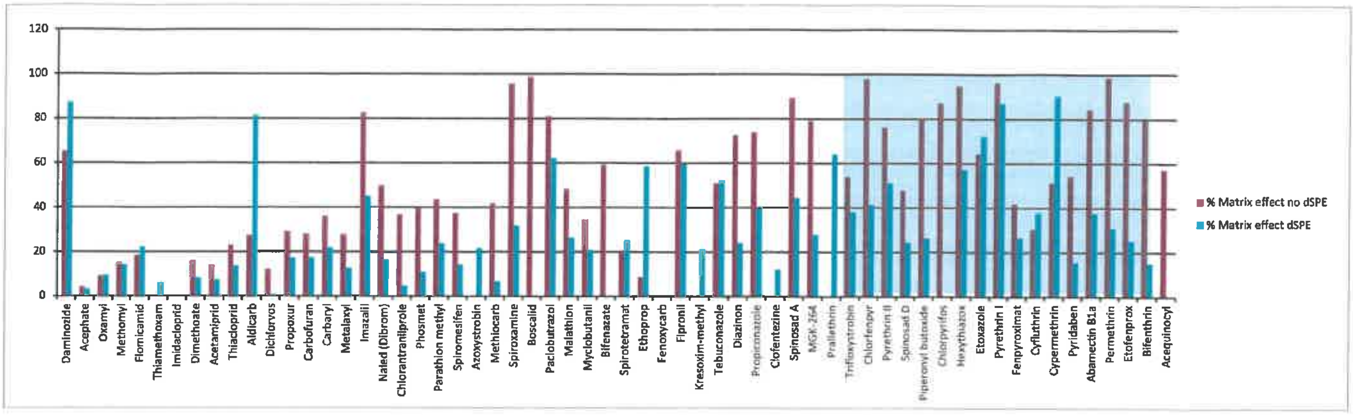


Figure 6. Matrix suppression at the 200 ppb level; the red bars indicate suppression observed without dSPE and the blue bars indicate suppression after dSPE cleanup. The shaded area indicates the compounds that co-eluted with the cannabis resin constituents.

CONCLUSIONS

This simple sample extraction and dSPE cleanup method followed by UPLC-MS/MS analysis using the ACQUITY UPLC H-Class System coupled to the Xevo TQ-S micro Tandem Quadrupole Mass Spectrometer provides a rapid, sensitive, and robust method for determination of the Oregon Cannabis Pesticide Guide List in a challenging cannabis matrix. Matrix suppression was significantly reduced by dSPE cleanup for many of the pesticides; thereby improving the data quality. This method is capable of meeting the MRLs for Oregon's pesticide list in cannabis matrix.

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1. Legality of cannabis by U.S. Jurisdiction, Retrieved on 22 August 2018 from Wikipedia https://en.wikipedia.org/wiki/Legality_of_cannabis_by_U.S._jurisdiction.
2. Oregon Guide List for Pesticides and Cannabis, Retrieved on 22 August 2018 from https://www.oregon.gov/ODA/shared/Documents/Publications/PesticidesPARC/GuidelistPesticideCannabis.pdf.
3. Oregon Health Authority Technical Report, Retrieved on 22 August 2018 from https://www.oregon.gov/oha/ph/PreventionWellness/marijuana/Documents/oha-8964-technical-report-marijuana-contaminant-testing.pdf.

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Waters Reference for Cannabis Analysis Using Proposed System

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ProVerde Laboratories
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Milford, MA 01757
(phone) 617-221-3356
(e-mail) Chris.Hudalla@ProVerdeLabs.com

Christopher has used Waters instrumentation for cannabis analysis. We have included a case study document in our bid response from ProVerde Laboratories. Christopher feels strongly that no major cleaning is needed on our instrument for a year, with a yearly preventative maintenance performed. The only regular cleaning needed does not break vacuum and involves changing the cone on the front of the source---this literally takes seconds and we include a spare part to readily change this out as needed. Christopher can attest to the robustness of the system running cannabis and hemp analysis.

Rapid Detection of 7 Illegal Veterinary Additives in Animal Feed Using Oasis PRiME HLB Clean-up and UPLC-MS/MS

DeFeng Huang , Xia Geng, and Xiaowei He
Waters Technologies (Shanghai) Co., Ltd.

APPLICATION BENEFITS

- Efficient, time-saving total solution for muti-residue analysis of veterinary drugs in animal feed formula
- Simple and rapid sample preparation with Oasis™ PRiME HLB
- Fast and sensitive UPLC™-MS/MS analysis

WATERS SOLUTIONS

ACQUITY™ UPLC I-Class System

Xevo™ TQ-S micro Mass Spectrometer

Oasis PRiME HLB Cartridge

KEYWORDS

Olaquindox, neomycin sulfate, sulfaquinoxaline, dihydropyridine, Oasis PRiME HLB Cartridge, formula feed, UPLC, MS, veterinary drug

INTRODUCTION

When discussing illegal additives in the feed, we immediately think of clenbuterol. Since the scandal of clenbuterol was exposed in 2011, the Chinese government has established a strict standard for the use of additives, and also tightened regulation for the illegal use of additives in feed. Nevertheless, some feed producers still have not stopped their illegal behavior. The "CCTV 3.15 party in 2017" exposed this situation and aroused great concern from the public. A reporter's survey found the abuse of veterinary drugs including olaquindox, neomycin sulfate, sulfaquinoxaline, and dihdropyridine in animal breeding.

Olaquindox is an alternative to clenbuterol, that can promote growth, reduce the feed and meat ratio, improve body size, and improve feed intake. It tends to be accumulated in animal tissue and leads to chromosomal abnormalities in cells if added to animal feed over a long period of time. However, the residues of these compounds also pose a health risk to the consumers.

Currently, the determination of olaquindox in the Chinese national standard (GB)[1] is mainly based on LC-UV and LC-MS/MS methods. Accurate quantification of Olaquindox is a challenge because of the complex matrices and potential to decompose during sample preparation and when exposed to light.

In this application note, a simple clean-up protocol using a novel SPE device was introduced for the analysis Olaquindox and six other illegal veterinary additives in animal feed. The extract was cleaned up by pass-through SPE using the Oasis PRiME HLB Cartridge prior to UPLC-MS/MS analysis. The spiked samples were quantified using an external standards method, and the recovery and reproducibility for each compound met the regulatory requirements of the quantitative method. This method is simple, rapid, accurate, suitable for the analysis of the highlighted veterinary drugs in animal feed.

EXPERIMENTAL

UPLC conditions

LC system:	ACQUITY UPLC I-Class
Column:	ACQUITY UPLC HSS T3, 1.8 µm, 2.1 x 100 mm
Temp.:	45 °C
Flow rate:	0.4 mL/min
Mobile phase A:	0.1% formic acid in water
Mobile phase B:	0.1% formic acid in methanol
Run time:	9 min
Injection vol.:	2 µL

Gradient:

Time	Flow rate (mL/min)	%A	%B
0.00	0.4	98	2
0.25	0.4	98	2
3.25	0.4	70	30
7.00	0.4	2	98
7.50	0.4	2	98
7.60	0.4	98	2
9.00	0.4	98	2

MS conditions

MS system:	Xevo TQ-S micro
Ionization mode:	ESI+
Capillary voltage:	3.0 kV
Desolvation temp.:	550 °C
Source temp.:	150 °C
Desolvation flow:	1000 L/h
Cone gas:	50 L/h

MRM conditions

Compound	Parent ion (*m/z*)	Product ion (*m/z*)	Cone voltage (V)	Collision energy (eV)
Olaquindox	264.1	143.0 212.1	32 32	30 23
Sulfaquinoxaline	301.0	92.0 155.9	32 32	30 13
Trimethoprim	291.1	123.0 230.1	40 40	27 28
Aminophylline	181.0	96.1 123.9	35 35	25 21
Diprophylline	255.1	123.9 181.0	35 35	35 22
Dexamethasone	393.2	355.2 373.2	20 20	10 10
Atropine	290.1	93.0 124.0	35 35	36 29

Sample preparation

Initial extraction

Step 1:	Weigh 1 g of feed sample into a 50 mL centrifuge tube;
Step 2:	Add 10 mL of extraction solvent (80% acetonitrile + 20% water) and shake well for 10 min;
Step 3:	Centrifuge at 6000 rpm for 5 min

Pass-through SPE clean-up

Step 1:	An Oasis PRiME HLB Cartridge (6 cc, 200 mg; p/n 186008057) was mounted on a pre-cleaned SPE vacuum manifold. Cartridge conditioning is not required and is not performed.
Step 2:	A 0.5 mL aliquot of the supernatant (sample extract) was passed through the Oasis PRiME HLB Cartridge and the eluant was discarded.
Step 3:	Install the collection tubes. Another 1 mL of supernatant was passed through the cartridge, and the eluant was collected. The eluant was diluted 1:3 with water and injected into Xevo TQ-S micro for analysis.

RESULTS AND DISCUSSION

METHOD RECOVERY AND STABILITY

The analyte recovery was determined by spiking standards into the blank matrix, a 1:1 mixture of rice and corn powders. The analytes were spiked at concentrations of low, medium (5 times low spike) and high levels (10 times low spike). The lowest spike for olaquindox was 10 ug/kg, sulfaquinoxaline was 0.5 ug/kg, trimethoprim and atropine was 2.5 ug/kg and the lowest spike for aminophylline, diprophylline and dexamethasone was 5.0 ug/kg). Each level of spiking was repeated in five replicates. All samples were processed according to the method described previously. The concentrations were calculated using a matrix-matched calibration curve. The recovery range of the high, medium, and low level samples ranged from 70.6% to 112%. The precision range of the high and medium level spike samples was 0.88% to 4.2% and the precision range was 4.3% to 8.8% for the low spike samples.

MATRIX EFFECTS AND MATRIX MATCHED CALIBRATION CURVE

The matrix effect was measured by comparing the peak area of solvent standards and post spiked samples in chicken feed and swine feed samples, where the spiked level was equal to 5 µg/kg for atropine and diprophylline, and 1 µg/kg for the other compounds.

Calibration curves ranged from 0.01 to 1.00 µg/L for sulfaquinoxaline, from 0.1 to 10 µg/L for olaquindox, aminophylline, diprophylline, and dexamethasone, and 0.05 to 5.0 µg/L for trimethoprim and atropine.

Table 1. Matrix effects of each compound and the correlation coefficients of their matrix matched calibration curves.

Veterinary drugs	Matrix effects (%)	Matrix matched calibration curve R^2
Olaquindox	(9.0)	0.9998
Sulfaquinoxaline	(14.9)	0.9997
Trimethoprim	7.2	0.9998
Atropine	16.1	0.9994
Aminophylline	(0.5)	0.9995
Diprophylline	9.6	0.9992
Dexamethasone	(14.7)	0.9991

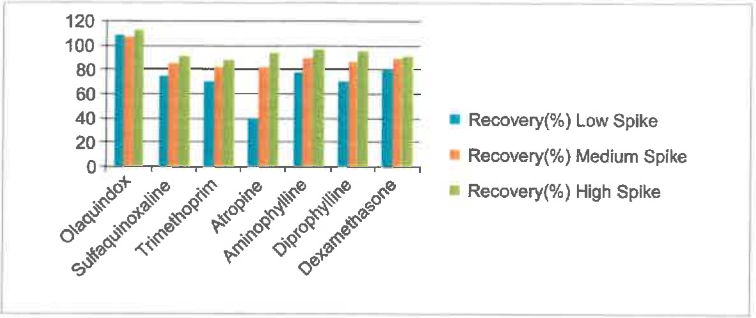

Figure 1. Summary of recoveries for spiked feed samples. The lowest spike for olaquindox was 10 ug/kg, sulfaquinoxaline was 0.5 ug/kg, trimethoprim and atropine was 2.5 ug/kg and the lowest spike for aminophylline, diprophylline and dexamethasone was 5.0 ug/kg).

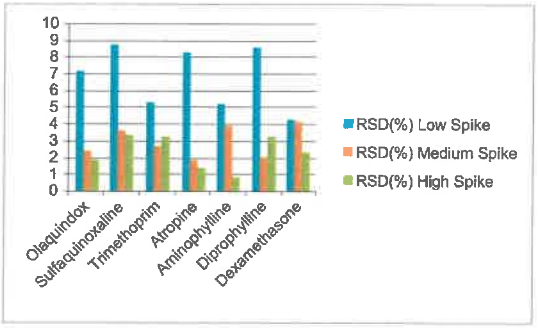

Figure 2. Precision of recoveries for spiked feed samples.

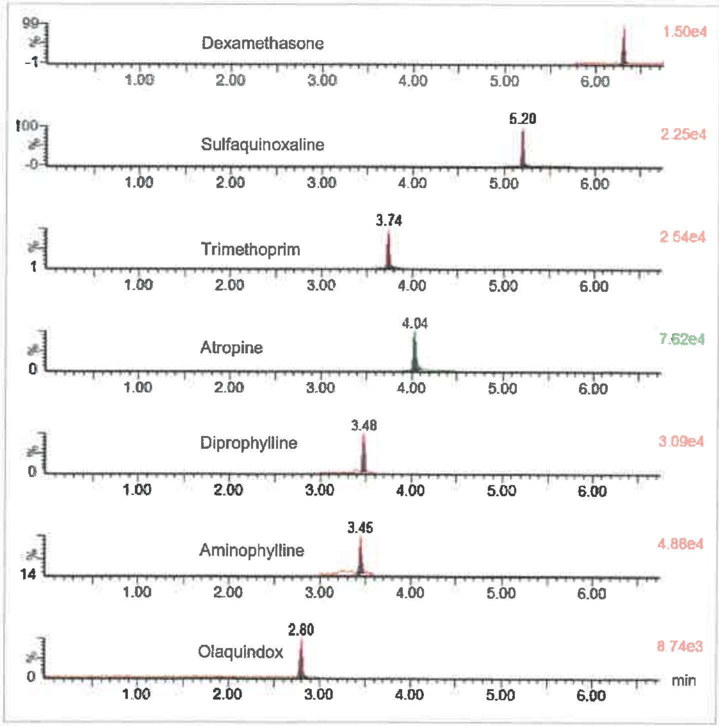

Figure 3. Typical chromatograms of spiked sample (sulfaquinoxaline spiked at 0.1 ppb; olaquindox, aminophylline, diprophylline, and dexamethasone spiked at 1.0 ppb; trimethoprim and atropine spiked at 0.5 ppb).

The established method was used for real sample analysis. Finally, an olaquindox content up to 1.9 to 18 mg/kg was detected in chicken feed and swine feed samples.

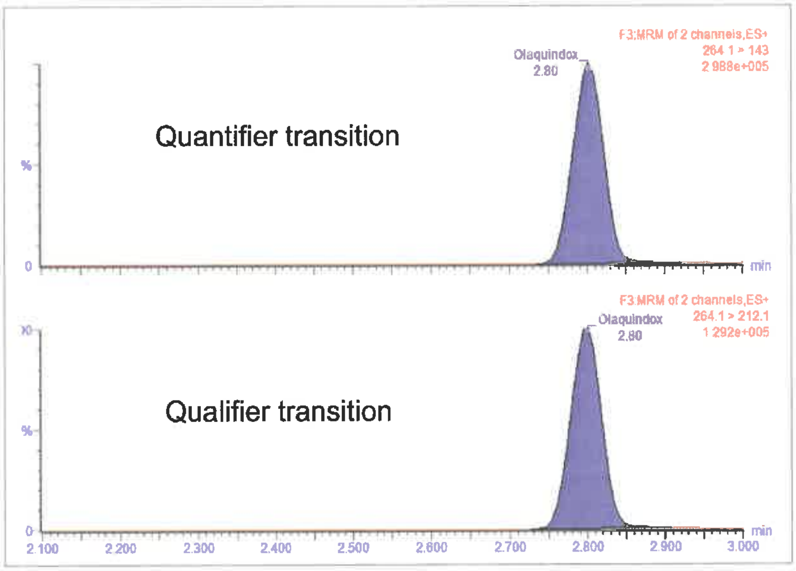

Figure 4. Chromatogram of olaquindox (1.9 mg/kg) in chicken feed.

CONCLUSIONS

- A simple and rapid analytical method was developed for the determination of seven illegal veterinary drug additives in animal feed. This method has been proven to achieve levels of detection that meet regulatory requirements.
- The Oasis PRiME HLB Cartridge provided effective clean-up and good recoveries for the target veterinary drugs in animal feeds.
- The ACQUITY UPLC I-Class System coupled with Xevo TQ-S micro offered good sensitivity and robust methodology.

Reference

1. Announcement No. 2086-5-2014 of the Ministry of Agriculture of the People's Republic of China: Determination of carbadox, mequindox, quinocetone and olaquindox in feeds – liquid chromatography – tandem mass spectrometry.

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Item	Product#	Qty	Description	Unit Price	Discount	Net Price
1	**176850043**	1	**Xevo TQ-S micro System**	452,495.00	- 198,754.66	253,740.34
			With the following configuration:			
	176003468	1	Xevo TQ-S micro			
	176003469	1	MS Ref Stds Xevo TQ-S micro			
	176002526	1	MassLynx Workstation with TL			
	668000273	1	MONITOR, Lenovo ThinkVision Flat Panel			
	176002685	1	Vac Rough Pump + Freq Conv			
	186007574	1	LC Multiresidue Pesticide Standards Kit			
	176003949	1	APcI Probe Option			
			ACQUITY UPLC I-Class PLUS System			
	176015111	1	ACQ. I-Class PLUS Sys. (CM-A) w/SM-FTN-I			
			Analytical Column Options			
	186006031	1	XBridge BEH C18 XP Column, 130Å, 2.5 µm, 2.1 mm X 100 mm, 1/pk			
	186006709	1	XBridge BEH C18 XP Column, 130Å, 2.5 µm, 2.1 mm X 150 mm, 1/pk			
			Installation, Training and Plans			
	741000321	1	TQD SYSTEM INSTALLATION CERT			
	750000487	1	NA - On-Site Field Apps Ed Cert (2 days)			
	176003950	1	Analytical LC-MS Solvent Install Kit			
2	668000275	1	Printer, HP Laser Jet, P3015dn, 110 Volt	1,135.00		1,135.00
3	186008060	1	NITROGEN GENERATOR NM32LA-110V	21,100.00		21,100.00
4	725000473	1	Power Supply, Uninterruptable 5.2KV	10,200.00		10,200.00
5	700004318	1	SOURCE SPARES KIT	1,070.00	- 476.15	593.85
6	**176003850**	1	**XEVO TQ-S Micro (Rotary) PM Kit W/CHEM**	3,322.00	- 1,478.30	1,843.70
	201000294	1	XEVO TQ-S MICRO (ROTARY) PERF MAINT KIT			
	186007976	1	Xevo TQ-S micro Set Up Solution			
	186006846	1	MS Cleaning Solution			
7	201000316	1	I-Class PLUS SM-FTN Perform Maint Kit	2,845.00	- 1,266.03	1,578.97
8	201000260	1	ACQUITY I-CLASS BSM PERFORM MAINT KIT	3,870.00	- 1,722.15	2,147.85
9	201000207	1	I-CLASS CM-A / CM-AUX & BIO PM KIT	20.00	- 8.90	11.10
			Items 5-9 must be purchased with item 1 on one purchase order for the discounts to be applicable			
10	720002242EN	1	Implementation Kit	1.00	- 1.00	0.00

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Product#	Qty	Description	Unit Price	Discount	Net Price
SERVICE PLANS					
		Preventative Maintenance Plans year 2.			
740005543	1	PMP Xevo TQ-S micro (1PM)	12,080.00	- 5,436.00	6,644.00
740005868	1	PMP ACQUITY PLUS BSM (1PM)	4,110.00	- 1,849.50	2,260.50
740005883	1	PMP ACQUITY I-Class PLUSSM-FTN-I (1PM)	3,340.00	- 1,503.00	1,837.00
740004221	1	PMP ACQUITY H-Class Col Mgr-Active (1PM)	345.00	- 155.26	189.74
740002549	1	Maint: MassLynx S/W 2nd Yr	2,230.00	- 992.35	1,237.65
TDS603152	1	SERVICE PLAN DISTANCE CHARGE ZONE 3	1,480.00		1,480.00
		Preventative Maintenance Plans year 3.			
740005543	1	PMP Xevo TQ-S micro (1PM)	12,080.00	- 5,436.00	6,644.00
740005868	1	PMP ACQUITY PLUS BSM (1PM)	4,110.00	- 1,849.50	2,260.50
740005883	1	PMP ACQUITY I-Class PLUSSM-FTN-I (1PM)	3,340.00	- 1,503.00	1,837.00
740004221	1	PMP ACQUITY H-Class Col Mgr-Active (1PM)	345.00	- 155.26	189.74
740002548	1	MassLynx Software 1 Year Plan	2,230.00	- 1,003.50	1,226.50
TDS603152	1	SERVICE PLAN DISTANCE CHARGE ZONE 3	1,480.00		1,480.00
SUBTOTAL				USD	**27,286.63**

Detail Product Description(s)

Product# Description

176003468 Xevo TQ-S micro

The Xevo® TQ-S micro is a sensitive but compact tandem quadrupole mass spectrometer featuring reliable performance with a wide dynamic range and high rates of data acquisition. Robust sensitivity is enabled by proven ZSpray" and StepWave" which facilitate the detection of analytes at low concentrations in complex matrices and enable low volume injections with consistent, precise and accurate results. Xtended dynamic range" (XDR) technology provides accessible sensitivity and method transfer. The Xevo® TQ-S micro makes it easier to confidently quantify more analytes using reproducible high acquisition rates with Xcellerated Ion Transfer" (XIT). Using RADAR, which enables rapid switching between MS full scan and MS/MS acquisition modes, analysts can understand sample complexity and improve method development.

The following items are included as part of the standard system:
Z SPRAY" API interface#Dual orthogonal interface for robust LC/MS
Electrospray (ESI) inlet probe#for efficient ionisation of a wide range of compounds
ESCi" ionisation capability#rapid switching source for both ESI and APCI in the same run
IntelliStart" fluidics#Automated tuning, calibration and method development
TargetLynx XS" #Application manager (requires license as provided with PC, below)
OpenLynx" #Application manager (requires license as provided with PC, below)

The standard system does not include the following items, which must be specified separately:
Additional inlet probes and ion source options (detailed below).
Acquisition PC data system and monitor
Additional Workstation data system terminals.
Printers.
Additional MassLynx" options (detailed below).
Vacuum backing pump options (rotary or oil-free combinations)
HPLC systems or other inlet options.

1. Z SPRAY" API INTERFACE
This instrument is equipped with an atmospheric pressure ionisation (API) LC interface. The source and spraying elements are visible through a transparent window in the enclosure and are easily accessible via a quick-release mechanism. The source elements may be wiped clean in situ or removed for cleaning without the need for tools and without breaking vacuum. The nebulized spray is orientated orthogonally and positioned off axis for maximum source longevity and analyser protection against 'dirty' samples. The source also includes facilities for de-clustering ions formed at atmospheric pressure. Positive and negative capability is included. Positive ion, negative ion and ESCi" capability is available as standard (allowing rapid switching between ESI and APCI, positive and negative in the same run). All source voltages and gases are under data system control.

2. INTELLISTART" FLUIDICS
The instrument is equipped with an on-board infusion system capable of delivering reference solutions from 3 built-in vial locations. The on-board fluidics system is controlled by the IntelliStart software to provide automated instrument setup, mass calibration and method development. The reference solutions are delivered via switching valves for either direct or combined (into an LC flow) infusion into the API source. The valves can in addition be programmed from the software to function as an LC flow divert. If required, the fluidics can be controlled manually via the system Console.

3. TANDEM QUADRUPOLE ANALYSER

Detail Product Description(s)

Product# Description

176003468 Xevo TQ-S micro - Continued

The instrument is equipped with two high performance quadrupole mass analysers with inter-element beam focusing and a mass range of 2-2000 amu. Pre-filters are fitted to the mass analysers to maximise resolution and transmission. The pre-filters also eliminate the need for cleaning of the quadrupole mass analysers. All lens and analyser voltages are digitally controlled. Analyser parameters may be programmed with respect to mass for optimal performance. Analyser parameters used for data acquisition are automatically recorded and appended to the relevant data file.

3. StepWave" ION TRANSFER OPTICS
This instrument is equipped with patented, off-axis StepWave " ion transfer optics. Uniquely the StepWave technology both dramatically increases the efficiency of ion transfer from the ion source to the quadrupole MS analyser at the same time as efficiently eliminating undesirable neutral contaminants. The technology employed allows Xevo TQ-S micro to deliver unprecedented levels of sensitivity, speed, and selectivity.

4. COLLISION CELL
The collision cell can be operated as a high efficiency travelling wave (T-Wave) device for collision induced dissociation. The travelling wave enables rapid cell clearance and refill for fast MRM transition switching while maintaining optimum signal to noise.

T-Wave" :
The cell can be operated as a high efficiency travelling wave (T-Wave) device for collision induced dissociation. The travelling wave enables rapid cell clearance and refill for fast MRM transition switching while maintaining optimum signal to noise.

RADAR" :
An information-rich acquisition approach that allows you to collect highly specific quantitative MRM data for target compounds while providing additional spectral data to help visualize all other components in the sample.

5. VACUUM SYSTEM
Clean, differentially pumped, automated vacuum system comprising:
Air-cooled Pfeiffer splitflow turbomolecular drag pump evacuating both the source & analyser.
Vacuum read backs and system vent/pump cycles are digitally monitored and controlled, to provide total software control and ensure fail-safe operation in the event of power failure.
The backing option must be ordered separately (See Backing Pump Options for part numbers and descriptions)

6. DETECTOR - Xtended Dynamic Range" (XDR)
The instrument is equipped with a low noise dynolite photomultiplier detector. The detector is positioned after the second analyzer. A High Voltage conversion dynode and phosphor are positioned at 90° off-axis to the analyser for the elimination of neutral noise. The detector features novel, integral focusing optics, which provides a detection efficiency approaching 100% for single ions. New XDR electronics incorporate 40 MS/s and 16 bit ADC to increase the dynamic range. The photomultiplier is enclosed in its own vacuum envelope for long life. The detector operates in both positive and negative ion mode, which can be switched rapidly under software digital control.

7. MASSLYNX" SOFTWARE / MS Workstation
The MS Workstation and MassLynx" 4.1 License for the application software for instrument control, data acquisition and processing must be ordered separately (See MS Workstation Variant Configurator section for part numbers and descriptions)

Detail Product Description(s)

Product# Description

176003468 Xevo TQ-S micro - Continued

Post acquisition processing and general data manipulation can be carried out by an additional computer workstation and software installation (See the MassLynx" Process-only Workstations section of the MassLynx Variant configurator 176706000).

176002526 MassLynx Workstation with TL

MassLynx" Workstation with License
MassLynx Application Software License includes key discs for TargetLynx" and OpenLynx"
Lenovo ThinkStation P520 Series with Windows 10 Enterprise LTSB
Processor: Intel® Xeon® W-2125 Processor (4.0 GHz 4c); Operating system: Windows 10 Enterprise LTSB (US English); Form factor: Tower 4x6 Mechanical; Motherboard: P520 - TPM Enabled; Total memory: 64 GB; Video adapter: NVIDIA Quadro P1000 4GB 4mDP HP; Audio adapter: Integrated Audio; RAID: Internal RAID - Not Enabled; Flash: 1x 512GB SSD M.2 PCIe OPAL; Hard drive: 1x 10TB SATA3 3.5" Hard Drive - 7200 rpm; First optical device bay: Lenovo 16x DVD +/- RW Dual Layer (Windows 10); Networking: Integrated Ethernet 10/100/1000, 1x Intel i210-t1 Ethernet 10/100/1000; Keyboard: Lenovo USB Preferred Pro Full Size Keyboard - US Euro; Pointing device: Lenovo Optical Wheel Mouse - USB Primax 400 DPI; Line Cord: US; Language Pack: English; System Warranty: Non-Return HDD - 4 Year Warranty US/EMEA/AP, Four year on-site warranty (parts and labour); Monitor: None; Printer: None

668000273 MONITOR, Lenovo ThinkVision Flat Panel

22" Flat Panel Monitor
Lenovo ThinkVision L2250p - LCD display - TFT - 22" - Widescreen - 1680 x 1050 / 75 Hz - 250 cd/m2 - 1000:1 - 5 ms -0.282 mm DVI-D, VGA - business black

176003949 APcI Probe Option

Dedicated tool-free probe option for Xevo TQ-XS atmospheric pressure chemical ionisation (APCI). The interface can be used at up to 2 ml/min without the need for flow splitting.

176015111 ACQ. I-Class PLUS Sys. (CM-A) w/SM-FTN-I

ACQUITY UPLC I-Class PLUS Column Manager System (CM-A) with SM-FTN-I
The ACQUITY UPLC I-Class PLUS Column Manager System has integrated solvent, sample and column heating configured for binary solvent delivery and sample introduction via a Flow-Through Needle sample manager (SM-FTN-I). The system may be configured with UV-based UPLC optical detectors and any currently supported Waters#mass detector, with a choice of instrument control and data management software.

The following items are included as part of the column manager system:
ACQUITY UPLC I-Class PLUSBinary Solvent Manager (BSM)
ACQUITY UPLC I-Class PLUSSample Manager # Flow-Through-Needle (SM-FTN-I)
Column Manager (CM-A)configured with two (2) 0.003#/0.076 mm I.D. ActivePre-Heaters, additional tubing and 18K PSI valve kit
ACQUITY UPLC I-Class PLUSColumn Manager System Start Up Kit
Total of 4 Leak Sensors
ACQUITY UPLC AbsorbanceStart-Up Solution

Detail Product Description(s)

Product# Description

176015111 ACQ. I-Class PLUS Sys. (CM-A) w/SM-FTN-I - Continued

Information Set
ACQUITY UPLC Solvent Tray Module
ACQUITY UPLC I-Class PLUS System Start Up Kit
ACQUITY UPLC BEH C18 Column, 2.1 x 50 mm, 1.7 µm
Vials
Replaces 176015074

741000321 TQD SYSTEM INSTALLATION CERT

Waters TQ Detector MS System Installation
Includes:
-System Set up and Specification Testing
-Product Familiarization Training
-1 Year Manufacturers Warranty
- Insight Remote Intelligent Services

176003950 Analytical LC-MS Solvent Install Kit

Analytical LC-MS Solvent Install Kit
The Analytical LC-MS Solvent Install Kit is intended to assist in effectively installing new LC-MS systems by minimizing sources of possible contamination. This kit includes the LC-MS Grade Solvent Kit (186008715) as well as the Waters Certified Container Kit (186007088). Additional kit components also include a formic acid additive, aqueous ammonia additive and nitrile gloves.
Note: Because this is a hazardous material and GHS requirements vary from country to country, Waters Corporation is only able to ship this item to specific countries worldwide. If the destination for this order (i.e. the ship to country) is changed to a non-permitted country at any point after this quote was generated, this item will be excluded from the final order.

668000275 Printer, HP Laser Jet, P3015dn, 110 Volt

HP LaserJet P3015DN Laser 42ppm, 110V, 1200x1200DPI LTR USB 128MB Duplex
/ Has Network Connection.

725000473 Power Supply, Uninterruptable 5.2KV

Power Supply, uninterruptible 5.2kVA
(This unit is modified from the standard to allow an overload capacity on Instrument Start-up)
Please Note that this requires an L6-30 wall socket

201000260 ACQUITY I-CLASS BSM PERFORM MAINT KIT

ACQUITY I-Class BSM 18K Performance Maintenance Kit

Waters General Sales Terms and Conditions

THIS TRANSACTION IS EXPRESSLY CONDITIONED UPON AND SUBJECT TO ALL OF THE FOLLOWING TERMS AND CONDITIONS:
1. Acceptance - Buyer's acceptance of the offer to purchase the products and/or services set forth on the front page made by Waters Technologies Corporation d/b/a Waters Corporation (Waters) of this quotation shall create a contract subject to and expressly limited by the terms and conditions contained on this form. Acceptance of this quotation may only be made on the exact terms and conditions set forth on this quotation; if additional or different terms are proposed by Buyer, such additional or different terms shall not become a part of the contract formed by Buyer's acceptance of the quotation. Receipt of the products sold hereunder or commencement of the services provided hereunder shall be deemed acceptance of the terms and conditions of this quotation.
2. Taxes and Payment - Any tax, duty, custom or other fee of any nature imposed upon this transaction by any federal, state or local governmental authority shall be paid by Buyer in addition to the price quoted. In the event Waters is required to prepay any such tax or fee, Buyer will reimburse Waters. Payment terms shall be net thirty (30) days after shipment and are subject to credit approval. An interest charge equal to 1 1/2% per month (18% per year) will be added to quotations outstanding beyond 30 days after shipment. In addition, Waters reserves the right, in its sole discretion, to require C.O.D. payment terms from any Buyer. Waters may also refuse to sell to any person until all prior overdue accounts are paid in full.
3. Delivery and Shipment - Delivery terms shall be F.O.B. Waters shipping point; identification of the products shall occur when they leave Waters shipping point at which time title and risk of loss shall pass to Buyer. All shipment costs shall be paid by Buyer and if prepaid by Waters the amount thereof shall be reimbursed to Waters. Waters will make reasonable commercial efforts to ship the products or provide the services hereunder in accordance with the delivery date set forth on the reverse side hereof provided, that Waters accepts no liability for any losses or for general, indirect special or consequential damages arising out of delays in delivery.
4. Warranty - The products and/or services shall be covered by the applicable Waters standard warranty, a copy of which is supplied with the products and/or services or upon request. NO OTHER WARRANTY, WHETHER EXPRESS OR IMPLIED, IS MADE WITH RESPECT TO THE PRODUCTS AND/OR SERVICES. WATERS EXPRESSLY EXCLUDES THE IMPLIED WARRANTIES OF MERCHANTABILITY AND OF FITNESS FOR A PARTICULAR PURPOSE. Any model or sample furnished to the Buyer is merely illustrative of the general types and quality of goods and does not represent that the products will conform to the model or sample. Buyer's remedies under Waters warranty shall be limited to repair or replacement of the product or component which failed to conform to Waters applicable standard warranty. WATERS SHALL NOT BE LIABLE FOR CONSEQUENTIAL, INCIDENTAL, SPECIAL OR ANY OTHER INDIRECT DAMAGES RESULTING FROM ECONOMIC LOSS OR PROPERTY DAMAGE SUSTAINED BY BUYER FROM THE USE OF ITS PRODUCTS OR SERVICES.
5. Returned Goods - Waters may, in its sole discretion, authorizeproduct returns in appropriate circumstances, subject to such conditions as Waters may specify. Any such return shall be subject to the express prior authorization of Waters and payment by Buyer of a restocking charge. No returns will be authorized after one hundred twenty (120) days following shipment to Buyer.
6. Technical Advice - Waters may, at Buyer's request furnish technical assistance, advice and information with respect to the products if and to the extent that such advice, assistance and information is conveniently available. It is expressly agreed that there is no obligation to provide such information, which is provided without charge at the Buyer's risk, and which is PROVIDED WITHOUT WARRANTY OF ANY KIND AND IS SUBJECT TO THE WARRANTY DISCLAIMERS AND LIMITATION OF LIABILITY SET FORTH IN PARAGRAPH 4.
7. Waters Right of Possession, etc. - Buyer hereby grants Waters a purchase money security interest in the goods offered by this quotation to secure the due and punctual payment of the purchase price specified in this quotation. In the event of default by Buyer in any payment due Waters, Waters shall have the right, in addition to any other remedies it may have at law or in equity, to withhold shipment, to recall goods in transit and retake the same, to repossess any goods which may be stored with Waters for Buyer's account without the necessity of Waters initiating any other proceedings. In addition, Waters shall have all of the rights and remedies of a secured party under the Massachusetts Uniform Commercial Code and may exercise all such rights and remedies in accordance therewith. Buyer shall execute such documents as Waters may request to effectuate the foregoing security interest.
8. Agents, etc. - No agent, employee or other representative has the right to modify or expand Waters standard warranty applicable to the products and/or services or to make any representations as to the products other than those set forth in the applicable user or operator's guide delivered with the products, and any such affirmation, representation or warranty, if made, should not be relied upon by Buyer and shall not form a part of contract between Waters and Buyer for the purchase of the products or services.
9. Fair Labor Standards - The products or services provided hereunder were produced and/or performed in compliance with the requirements of all sections of the Fair Labor Standards Act of 1938 as amended.
10. Equal Employment - Waters is an Equal Opportunity Employer. It does not discriminate in any phase of the employment process against any person because of race, color, creed, religion, national origin, sex, age, veteran or handicapped status.
11. Modifications, Waiver, Termination - The contract formed by Buyer's acceptance of this quotation may be modified and any breach thereunder may be waived only by a written and signed document by the party against whom enforcement thereof is sought.
12. Governing Law - The contract formed by Buyer's acceptance of this quotation shall be governed by and construed in accordance with the laws of the Commonwealth of Massachusetts, U.S.A.
13. Compliance with Laws - Buyer shall at all times comply with all applicable federal, state and local laws and regulations, including, without limitation, the provisions of the United States Export Control Laws as may be in effect for any of the products or services, and, if products or services hereunder are used in clinical applications, all applicable rules and regulations of the United States Food andDrug Administration and/or other domestic or international agencies with respect to the application of, as the case may be, Good Clinical Practices ("GCP"), Good Laboratory Practices ("GLP") or good Manufacturing Practices ("GMP").
14. Additional Terms and Conditions - This quotation is also subject to any Waters Special Terms and Conditions applicable to the products or services offered by this quotation, which appear on the front of this quotation. Any variance from the terms and conditions of this quotation in any order or other written notification from Buyer, will be of no effect. Should Buyer order products or services through a Waters office located outside of the United States, the terms and conditions of the quotation issued by the office outside of the United States shall govern such order.
15. Arbitration - Any and all disputes or controversies arising in connection with the contract formed by Buyer's acceptance of this quotation or the sale of products and/or performance of the services shall be resolved by final and binding arbitration in Boston, Massachusetts, under the rules of the American Arbitration Association then obtaining. The arbitrators shall have no power to add to, subtract from or modify any of these terms or conditions of this contract. Any award rendered in such arbitration may be enforced by either party in either the courts of the Commonwealth of Massachusetts or in the United States District Court for the District of Massachusetts, to whose jurisdiction for such purposes Waters and Buyer each hereby irrevocably consents and submits.
16. Software - To the extent there is any software included with the products, the software is being licensed, not sold and all rights, title and interest therein shall remain with Waters. Use of the software shall be in accordance with the applicable software license delivered with the products. U.S. Government Restricted Rights - RESTRICTED RIGHTS LEGEND. Use, duplication or disclosure by the Government is subject to restrictions as set forth in subparagraph (c)(1)(ii) of the Rights in Technical Data and Computer Software clause at DFARS 252.227-7013 or subparagraphs (c)(1) and (2) of the Commercial Computer Software - Restricted Rights clause at 48 CFR 52.227-19, as applicable.
17. Force Majeure - Waters shall have no liability for failure toperform, or delay in performance, in the delivery of any and all equipment manufactured or sold by Waters including instruments, supplies, components, systems, chemistry, accessories, replacement spare parts, or any and all services provided by Waters, caused by circumstances beyond its reasonable control including, but not limited to, acts of God, acts of nature, floods, fire, explosions, war or military mobilization, United States governmental action or inaction, request of governmental authority, delays of any kind in transportation or inability to obtain material or equipment, acts of other governments, strikes, or labor disturbances.
18. Diagnostic Products - Buyer acknowledges and agrees that only those products which are labeled and identified as in vitro diagnostic (#IVD#)

devices are intended to be used for IVD purposes. Buyer acknowledges and agrees that any products that are not labeled and identified as IVDs are general laboratory products intended for research and other general scientific uses and are not for use in IVD procedures.

[WHITE PAPER]

STEPWAVE

Enhancing MS Sensitivity and Robustness

Waters

THE SCIENCE OF WHAT'S POSSIBLE.™

INTRODUCTION

Of the key analytical requirements for any experiment, sensitivity is typically of primary concern. Having the selectivity to uncover an analyte within a complex matrix is inconsequential without the presence of sufficient ions of interest to detect.

Based on stacked-ring ion guide technology, Waters® StepWave™ is an elegant device designed to maximize ion transmission from the source to the mass analyzer. Through its unique design, StepWave also allows for the active removal of neutral contaminants, providing an enhancement to overall signal-to-noise, while importantly extending the robustness of the system.

Principles of operation

When sampling ions from an atmospheric pressure ion source, a significant quantity of gas enters the vacuum system. It is essential to remove the accompanying gas from the ions prior to the mass analyzer. The configuration of an off-axis ion guide featuring conjoined stacked rings enables the active separation of ions from the gas flow.

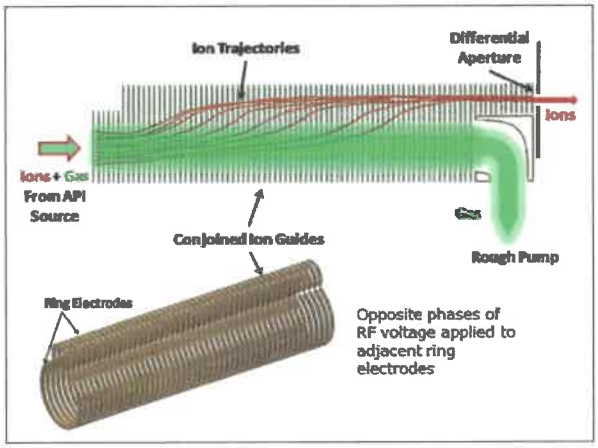


Figure 1. Diagrams of the conjoined stacked ring ion guides.

Figure 1 shows a schematic of a conjoined ion guide. The ions enter the larger diameter ion guide and are directed into the upper ion guide using a differential voltage; this focuses them into a narrow beam for transport into the mass analyzer. Gas, neutral species, and any non-desolvated material are directed to the rough pump inlet. The gap between the lower and upper guides allows the clear passage of ions without impact on the lenses, as shown in Figure 2. A reverse travelling wave on the lower guide ensures ions are not swept out with the high gas flow and have time to transfer into the upper guide. Once captured, they are propelled by T-Wave into the next stage.

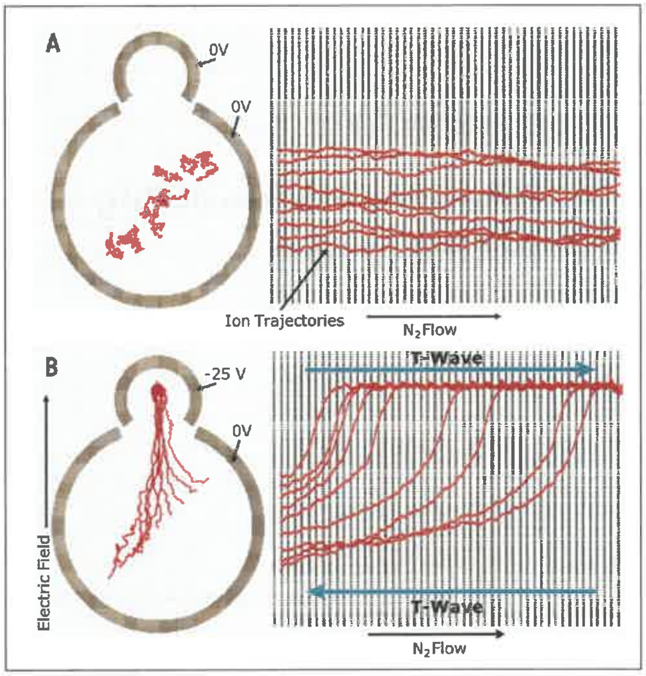


Figure 2. SIMION simulation of ion transit through the conjoined ion guide device: (a) with no potential difference between the sections (b) with 25 V.

Maximizing sensitivity

StepWave's design allows the handling of much larger gas loads into the instrument, permitting the use of a larger sampling orifice to capture significantly more ions from the source. Signal transmission is consequently increased more than 25X over the standard single ion guide designs, directly contributing to greater sensitivity across the mass range, as shown in Figure 3. Chemical noise is an undesirable consequence of the larger orifice; however StepWave can improve signal-to-noise compared to expected ratios, due to the active removal of the neutral or large cluster species.

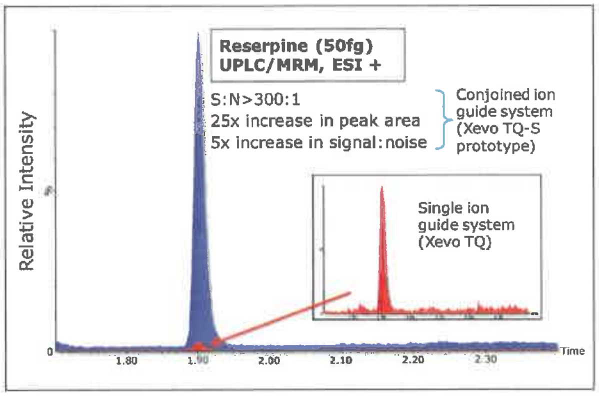


Figure 3. Reserpine, 50 fg on-column. 800 µL/min gradient elution on a 50 x 2.1 mm BEH C_{18} Column.

> "When compared to earlier generation mass spectrometer models, MicroConstants experienced a forty-fold increase in sensitivity with compounds tested internally in negative electrospray ionization mode. The significant increase in sensitivity can be attributed primarily to the system's new StepWave ion-transfer technology. This off-axis design dramatically increases the efficiency of ion transfer from the ion source to the quadrupole MS analyzer while at the same time actively eliminating undesirable neutral contaminants".
>
> **MICROCONSTANTS, INC., press release, 2 March 2011**

Extending robust use of the enhanced performance

Historically, one of the limiting factors of efforts to increase signal transmission was the impact on instrument robustness. The transfer of excessive solvent, matrix, and ion beam into the ion optics can quickly and dramatically reduce sensitivity over time. Any gains made in sensitivity are essentially made redundant if that performance cannot be repeated day after day.

Figure 4 illustrates the design robustness with no significant change in performance after 6000 repeat injections of verapamil in protein-precipitated plasma.

Other designs that offset the flight path of ions from the source to the analyzer can still lead to contamination of the surrounding optics, degrading sensitivity over time. However, the StepWave design protects the critical upper ion guide and the subsequent aperture from the direct line of sight of the high gas flow and contaminants. Key tuning parameters therefore remain unaffected, and sensitive methods are maintained over time.

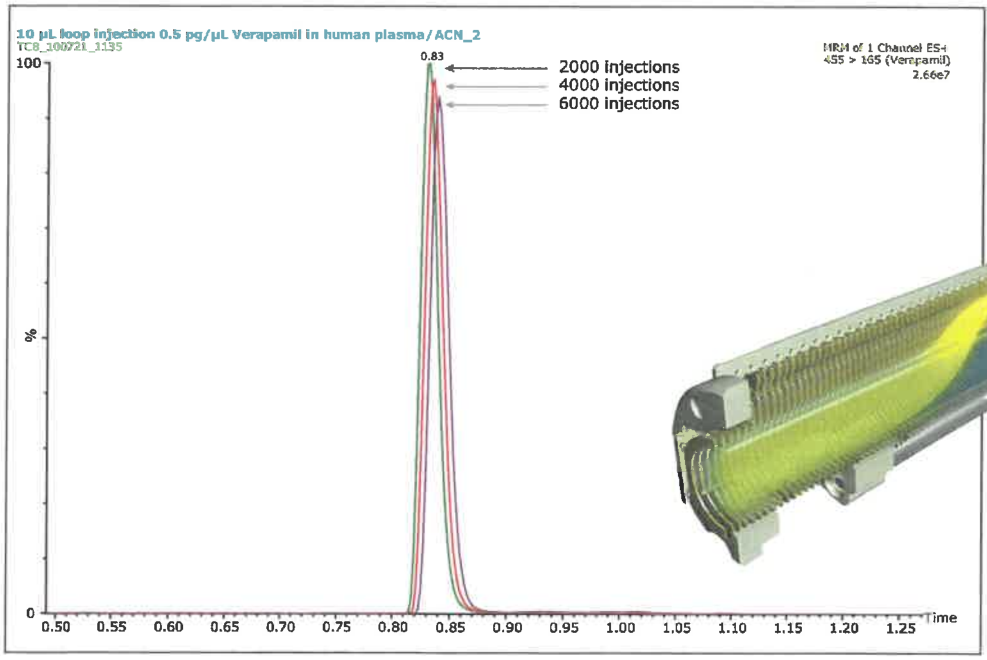
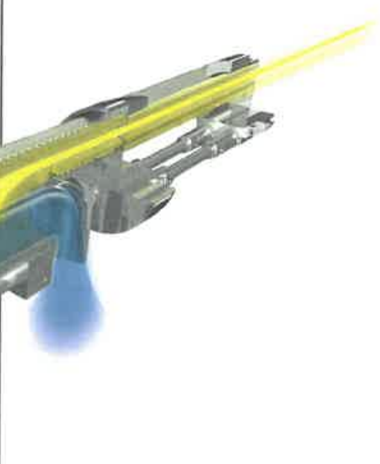


Figure 4. Robustness with no significant change in performance after 6000 repeat injections of verapamil in protein-precipitated plasma.



> "The Waters Xevo® TQ-S [featuring StepWave] has allowed us to greatly improve achievable sensitivity on a number of challenging assays, ranging from the analysis of very high potency small molecules to the quantification of therapeutic peptides."
>
> **MOHAMMED ABRAR, Method Development Manager, Unilabs York Bioanalytical Solutions, York, UK**

Remaining compatible with UPLC® speed and multi-function acquisitions

Manipulating ions in such a high flow environment introduces a significant challenge. The use of travelling waves in the conjoined guide allows the speed of ions to be finely controlled. By propelling ions through the device, the T-Wave™ aids the speed of transfer into the mass analyzer, thus maintaining the critical acquisition parameters required to carry out multimode tandem MS experiments over the narrow peak widths from UltraPerformance LC.®

SUMMARY

StepWave is a unique ion transfer device designed to maximize transmission from the ion source to the mass analyzer. Typical gains observed are 25 X increase in peak area and 10 X in signal-to-noise. Critically, the device also maintains instrument robustness and delivers significant improvements over alternative commercialized methods.

Further Reading

1. Applications of a travelling wave-based radio-frequency only stacked ring ion guide, *Rapid Commun. Mass Spectrom.*, 2004; 18: 2401-2414.
2. A new conjoined RF ion guide for enhanced ion transmission, K. Giles and D. Gordon, Application Note 720003606EN.
3. Dramatically Enhanced Analytical Sensitivity with the Use of Novel StepWave Ion Transfer Technology in the SYNAPT G2-S System. Waters Application Note, Literature No. 720003964EN.
4. Increasing Bioanalytical Assay Sensitivity For Low Exposure Compounds with Xevo TQ-S. Waters Application Note, Literature No. 720003419EN.
5. An Introduction to Waters T-Wave Devices, Unique Technology for Advanced MS Capabilities. Waters Literature No. 720004177EN.

Find further reading and animations online:
www.waters.com/wavedevices

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THE SCIENCE OF WHAT'S POSSIBLE.™

April 2012 720004175EN LB-PDF

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T: 1 508 478 2000
F: 1 508 872 1990
www.waters.com

REQUEST FOR QUOTATION
Liquid Chromatography/Mass Spectrometer (LC/MS) Instrument

Responses Bolded and Italicized after Each Requirement Below

SPECIFICATIONS

1. **PURPOSE SCOPE:** The West Virginia Purchasing Division is soliciting bids on behalf of West Virginia Department of Agriculture to establish a contract for the one time purchase of a **Liquid Chromatography Triple Quadrupole Mass Spectrometer (LC/MS/MS), workstation PC, software, printer, nitrogen generator, uninterrupted power supply (UPS), specific test methods, shipping, installation, validation, warranty, training and service.**

2. **DEFINITIONS:** The terms listed below shall have the meanings assigned to them below. Additional definitions can be found in section 2 of the General Terms and Conditions.

   2.1 **"Contract Services"** means the LC/MS/MS with inside delivery, installation, validation, warranty, and training.

   2.2 **"Pricing Page"** means the pages, contained in wvOASIS or attached as Exhibit A, upon which Vendor should list its proposed price for the Contract Items.

   2.3 **"Solicitation"** means the official notice of an opportunity to supply the State with goods or services that is published by the Purchasing Division.

   2.4 **"Validation"** means is the process used to confinn that the analytical procedure employed for a specific test or matrices is suitable for its intended use.

   2.5 **"Installation"** means unpacking and setting instrumentation in place with all connections secured for the instrument(s) to be in working order including software installation on the computer connected to the instrument.

   2.6 **"Warranty"** means the written warranty of the manufacturer of a new instrument of its condition and fitness for use, including any terms or conditions precedent to the enforcement of obligations under that warranty.

   2.7 **"Training"** means teaching staff how to use and maintain the instrument and software.

   2.8 **"Service"** means performing routine maintenance work or repair to the instrument or software.

   2.9 **"APCI"** means atmospheric pressure chemical ionization.

   2.10 **"ESI"** means electrospray.

2.11 **"FG"** means femtogram.

2.12 **"LC/MS/MS'"** means Liquid Chromatography Triple Quadrupole Mass Spectrometer.

2.13 **"MRM:"** means multiple reactions monitoring.

2.14 **"MSMS"** means tandem mass spectrometry.

2.15 **"SIM"** means selected ion monitoring.

2.16 ***"SIN"*** means signal to noise.

2.17 **"M/Z"** means mass to charge ratio.

2.18 **"AMU"** means Atomic mass unit.

2,19 **"DAIS"** means Daltons per second.

2.20 **"UHPLC"** means Ultra High-performance liquid chromatography.

2.21 **"SLPM"** means standard liters per minute.

2.22 **"PSIG"** means pounds per square inch gauge.

2.23 **"UPS"** means uninterrupted power supply.

3. GENERAL REQUIREMENTS:

3.1 **Mandatory Contract Item Requirements:** Contract Item must meet or exceed the mandatory requirements listed below for the **Liquid Chromatography Triple Quadrupole Mass Spectrometer (LC/MS/MS), workstation PC, software, printer, nitrogen generator, uninterrupted power supply (UPS), specific test methods, shipping, installation, validation, warranty, training, and service.**

The proposed system will meet all these requirements. The system contains an ACQUITY I-Class Plus UPLC, Xevo TQ-S Micro tandem quadrupole mass spectrometer (LC/MS/MS system). A MassLynx workstation PC with software for acquisition and processing is included along with a printer, nitrogen generator, UPS, application notes for test methods, and all costs associated with shipping, installation, validation, warranty, training, and service.

3.1.1 Liquid Chromatography Triple Quadrupole Mass Spectrometer (LC/MS/MS)

3.1.1.1 Must be capable of detecting a variety of analytes including pesticides, herbicides, toxins, drugs in matrices such as foods, soil, vegetation (including hemp), animal feed, and water.

The ACQUITY I-Class Plus UPLC and Xevo TQ-S Micro LC/MS/MS system are used across several application spaces and are more than capable of detecting the analytes included above. The system works to detect analytes from various matrices. Attached are application notes providing evidence of system use across a wide variety of analyte and application areas (Attached files are named: Analysis of Legacy and Emerging PFAS in Water Samples using SPE and LC-MSMS.pdf, Multiresidue Analysis of Pesticides in Fruits and Vegetables Using UPLC-MSMS.pdf and Rapid Detection of Illegal Veterinary Additives in Animal Feed using SPE and UPLC-MSMS.pdf showing a range of matrices and analytes.)

3.1.1.2 The system provided must be capable of analyzing the list of pesticides from the Cannabis and hemp pesticide lists from Oregon and California. See 3.1.4.2

Attached are two application notes (California Pesticides_List Cannabis.pdf and Oregon_Pesticides_List Cannabis.pdf) that show how our systems are capable of this analysis. (One note is that the California list contains some compounds that are only GC amenable. This would require the user to use a GC/MS/MS system for full pesticide analysis of the California list. This is independent of any LC-MS/MS based systems and is strictly based on chemical properties of those pesticides.)

3.1.1.3 MSMS must have dual ion sources that operate independently which can be set to electrospray ionization (ESI) or atmospheric pressure chemical ionization (APCI). The instrument must enable combinations such as ESI/APCI, ESI/ESI, APCI/APCI with the same or opposite polarities without having to remove the sources to switch modes.

The proposed system has a source design that can be readily switched between ESI and APCI modes in both positive and negative polarities. The modes supported for this source include ESI, APCI, and ESCI, a mode that uses both ESI and APCI to help with method development. A white paper regarding ESCI is included.

3.1.1.4 Minimum sensitivity requirement for positive ion mode: signal/noise **(SIN)** 2000:1 25 femtograms (fg) of reserpine on column. Minimum sensitivity requirement for negative ion mode: signal/noise (S/N)>2000:**1,** 25 femtograms (fg) of chloramphenicol on column.

The system has the following sensitivity specifications (also listed in attached specification sheet). MRM Sensitivity ESI+ : A 1 pg on-column injection of reserpine will give a chromatographic signal/noise greater than 200,000:1 using raw, unsmoothed data. MRM Sensitivity ESI- : A 1 pg on-column injection of chloramphenicol will give a chromatographic signal/noise greater than 100,000:1, using raw, unsmoothed data.

3.1.1.5 The source probes must be easy to remove without the use of tools.

Our source probes can be removed without the use of tools.

3.1.1.6 Ion source must have flat response across flow rate up to 3 milliliters per minute without loss of sensitivity.

Our system works in an operating range of 0.001 to 2.000 mL/min. For our applications, running at 3 mL/min is not necessary and this is a lockout specification not related to the ability to run pesticide, or other types of analysis.

Unlike UHPLC instruments UPLC based instruments are optimized to run at under 2 ml/min to reduce solvent consumption and to provide superior results.

3.1.1.7 Capable of switching between rapidly between positive and negative ion detection without high voltage switching.

Our system can switch between positive and negative ion modes in 15 ms without high voltage switching.

3.1.1.8 Acquisition modes: Ql scan, Q2 scan, multiple reactions monitoring (MRM), selected ion monitoring (SIM), Neutral Loss scans, Product Ion, Precursor Ion, Time managed MRM

Acquisition modes supported include: full scan MS, product ion scan, precursor ion scan, constant neutral loss, selected ion recording (SIR/SIM), multiple reaction monitoring (MRM), simultaneous full scan and MRM (RADAR), Survey scan modes: full scan MS triggered product ion scan, precursor ion scan triggered product ion scan, constant neutral loss triggered product ion scan.

Though not called "time-managed MRM (this is a lockout specification term specific to one vendor)," We have automated MRM scheduling where the dwell time, inter-channel delay time, and inter-scan delay time for individual channels in an MRM experiment can be automatically assigned to ensure the optimal number of MRM data points per chromatographic peak is acquired. This GREATLY simplifies MRM method creation, irrespective of number of compounds per assay, while ensuring the best quantitative performance for every experiment. MRM data acquisition rates will be optimal for the quantification of all analytes in a given assay.

3.1.1.9 Minimum mass range requirement: 5-1500 mass to charge ratio (m/z)

The mass range of the instrument is 2 – 2048 m/z.

3.1.1.10 Mass stability required: 0.05 atomic mass unit (amu) in 24 hours

The mass drift is < 0.1 Da over a 24 hour period. For nominal mass systems (single or tandem/triple quadrupole MS) this meets all requirements.

3.1.1.11 Mass accuracy needed: minimum 0.1 unit across mass range

Automatically adjusted to desired resolution 0.5 Da, 0.75 Da, or 1.00 Da FWHM. Mass accuracy is 0.1 Da or better across mass range.

3.1.1.12 Scan speed: 30,000 daltons per second (dais)

Scan speed is up to 20,000 Da/s. Examples of achievable acquisition rates: 20 scans/s (m/z 50-1000), 40 scans/s (m/z 50-500). A specification of 30,000 Da/s is a lockout specification that has no impact on the type of analysis being asked to perform as we have included application notes that demonstrate our instruments are more than capable for intended use.

3.1.1.13 Quad resolution: unit, low and high, minimal sensitivity loss at 0.1 Daltons resolutions

Automatically adjusted to desired resolution 0.5 Da, 0.75 Da, or 1.00 Da FWHM.

3.1.1.14 Polarity switching time: 15 milliseconds

The Xevo TQ-S micro has polarity switching time of 15 milliseconds to switch between positive and negative ion modes.

3.1.1.15 Dynamic range: 6 orders

The linearity of response relative to sample concentration, for a specified compound, is six orders of magnitude from the limit of detection. Attached is a pdf demonstrating the dynamic range (Dynamic_Range.pdf).

3.1.1.16 Minimum multiple reactions monitoring (MRM) Dwell Time: 1 millisecond

Minimum dwell time of 1 millisecond per MRM channel.

3.1.1.17 MRM transitions: 450 per time segment> 40,000 ion transactions per method

The system can perform a maximum acquisition rate of 500 MRM data points per second. There are up to 32,768 MRM channels (1024 functions, 32 channels per function) that can be monitored in a single acquisition. A fixed number of 40,000 ion transactions is a lockout specification for a single vendor and has no impact on the intended applications as we have attached application notes demonstrating the use of this instrument for the intended purposes.

3.1.1.18 Must have high selectivity mass filter at 0.3 Daltons. Signal loss must not be more than 10%.

In addition to the high resolution, high stability quadrupole analyzers, there are pre-filters that maximize resolution and ion transmission while preventing the contamination of the main analyzers. Additionally, the collision cell is made of a segmented quadrupole (T-Wave Collision cell, white paper attached) which enables optimal MS/MS performance by enhancement of ion transfer between the collision cell and quadrupole.

3.1.1.19 For minimal tuning during method development and minimal maintenance of the ion path, the LC/MS/MS will require hot source induced desolvation interface to the mass analyzer by patented Laminar Flow Ion Guide using gas flow. Submit evidence of instrument use with cannabis for at least 6 months without matrix induced cleaning and maintenance

To assist with minimal tuning during method development and to decrease instrument maintenance time, the proposed LC/MS/MS system is equipped with a StepWave source design. This off-axis ion guide increases instrument sensitivity by

removing neutrals and gas load as ions are actively moved upwards into the StepWave source on-axis to the mass analyzer. In addition, the instrument uses a Z-Spray ionization source design where after the ionization process, this orthogonal source design forces ions to make two 90 degree turns prior to entering the ion guide. Between Z-Spray and StepWave (StepWave white paper attached to bid documentation) the instrument is optimized for long-term uptime.

Additionally, we have submitted a reference and case study from ProVerde Laboratories who uses our equipment for use with cannabis and can attest to the robustness of the system. Our reference says it is very easy to continually use the system for 12 months (then get a preventative maintenance visit) with only needing to change the cone on the front end, which literally takes seconds and does not break vacuum.

Reference for instrument use with cannabis – Please contact with any questions.

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3.1.1.20 High performance liquid chromatograph capable of solvent and column switching without user intervention

Our system is capable of switching between columns with programmable access switching, waste and bypass positions for rapid solvent changeover.

3.1.1.21 High performance liquid chromatograph capable of regulating column temperature of at least 2 different columns

Our system can regulate column temperature of at least two different columns.

3.1.1.22 The UHPLC pump must have 18,000 psi capability and a flow rate to 5 mL/minute

The I-Class Plus UPLC has a maximum operating pressure of 18,000 psi. For the methods we have included for pesticide analysis, operating at a flow rate of 5 mL/min is not a requirement for performance of the system at high precision and accuracy. Our system has an operating flow rate range of 0.001 to 2.000 mL/min which is more than capable of our methods. UPLC instrumentation is optimized for flow rates under 2 mL/min to reduce solvent consumption and control peak shape.

The defined flow rate of 5 mL/min is a lockout specification which has no impact on the analysis. Additionally a specification of 5 ml/min does not match the previous specification for the Mass Spectrometer (3.1.1.6) which states it must be able to desolvate at 3 ml/min, both of these numbers are lockout specifications and have no relevance for the intended applications based on the request that our methods be included with the instrument which do not use flow rates above 2 mL/min.

3.1.1.23 High performance liquid chromatograph with an autosampler

The system is a UPLC system equipped with an autosampler.

3.1.1.24 The LC/MS/MS instrument must be fully automated for analysis with a system controller that is loaded with the necessary software that can perform instrument diagnostics, monitor all operating and electrical parameters, and allow remote tuning capability in real time.

The system has software capable of performing instrument diagnostics, monitoring operating and electrical parameters, and can be controlled externally as needed for remote tuning and access. The instrument also uses IntelliStart software for automated tuning of compounds and method development.

3.1.1.25 The LC/MS/MS must include a maintenance kit.

Preventative Maintenance Kits are included for all components of the LC/MS/MS instrument. Additionally we have included a source spares kit for commonly used parts.

3.1.1.26 Vendor must provide documentation for recommended environmental conditions, electrical requirements, gas requirements, or any other factor that would affect instrument performance.

Attached is the site preparation guide for both the ACQUITY I-Class Plus UPLC and Xevo TQ-S which can provide this information.

3.1.2 Nitrogen generator

3.1.2.1 The nitrogen generator must be capable of producing up to 18 standard liters per minute (slpm) of liquid chromatography mass spectrometer grade gases at 80 pounds per square inch (psig) or have the capacity for the needs stated in the gas requirements of the LC/MS/MS.

The nitrogen generator has a flow rate up to 32 L/min at a pressure of 100 psi. This generator by PEAK is paired to work optimally with the proposed system. The specifications are attached to this bid for the PEAK Genius NM32LA-110 V Nitrogen Generator.

3.1.2.2 The vendor must include if there is another gas requirement or need for the specific instrument being quoted other than listed in 3.1.2.1.

The instrument requires Argon gas as well. We recommend a lecture-size bottle of Argon for collision gas for doing MRM (fragmentation) work. This will last the life of the instrument. Both Ar and N_2 ***gas are commonly used for tandem MS experiments; the collision gas is dependent on vendor. (Argon is also a little better at energy transfer in the collision process.)***

3.1.3 Uninterrupted Power Supply (UPS)

3.1.3.1 The uninterrupted power supply (UPS) must provide protection and complete power conditioning where the output remains continuously regulated. Must be rated to a capacity at least 5200 VA or have the capacity for the needs stated in the electrical requirements of the LCMSMS.

The UPS quoted will provide protection for the system as discussed above. The UPS has a capacity of 5200 VA and meets the needs required for the LC/MS/MS system. The specifications for the UPS are included in this bid documentation.

3.1.3.2 The vendor must include if there is another UPS electrical requirement or need to maintain the integrity of the instrument for proper operation being quoted other than listed in 3.1.3.1.

There is no other UPS electrical requirement other than listed in 3.1.3.1. Specifications are attached for this UPS.

3.1.4 Specific Test methods: Cannabis and hemp methods

3.1.4.1 The vendor must provide a standard operating procedure for Cannabis and hemp analysis that includes sample preparation and analysis of the complete Cannabis list from states such as Oregon or California which include the analytes in 3.1.4.2.

Attached are two application notes (California Pesticides_List Cannabis.pdf and Oregon_Pesticides_List Cannabis.pdf) that show how our systems are capable of this analysis. (One note is that the California list contains some compounds that are only GC amenable. This would require the user to use a GC/MS/MS system for full pesticide analysis of the California list.)

3.1.4.2 See Exhibit B.

Other than the compounds on the California and Oregon state lists, we can work with the customer to provide LC/MS/MS methods for the compounds from the FERN list. Our demo lab recently has made a method for these compounds and we can provide such method on request (unpublished data this point but is available for our customers). Additionally, with use of IntelliStart software in MassLynx, adding more compounds to a method is very easy to do. Along with this, our QuanPedia library contains 100s of pesticide compounds with associated MRMs to continue to build the methods with new and emerging compounds of interest.

3.1.5 Workstation and software

3.1.5.1 Data station with windows based operating system capable of multitasking allowing data processing and data acquisition simultaneously.

Our workstation is a Windows 10 based and allows for processing and acquisition simultaneously in MassLynx.

3.1.5.2 Operating system must be fully integrated to control LC/MS/MS.

The operating system is fully integrated to control LC/MS/MS.

3.1.6 Shipping, Installation, Validation, Warranty, Training (including Specific Test Methods Application), and Service

3.1.6.1 Vendor must be on-site for delivery and perform the installation (labor and supplies included) of the LCMSMS.

We will be on-site for the delivery of the instrument. We will perform the installation of the LC/MS/MS system at a time agreed upon by the customer.

3.1.6.2 The vendor must provide a written validation of the instrument's performance after installation.

All of our instrument installations are required to meet system specifications. We will sign off on the instrument's performance meeting specifications after installation to provide this information.

3.1.6.3 Vendor will provide a full one-year parts and labor warranty on all items, including 2 preventative maintenances.

This is included in the "Service Plans" section of our quotation.

3.1.6.4 Vendor must be able to perform resolutions to service requests within 72 hours which includes on-site resolutions.

Technical support is part of our service plan included in our quotation. Waters Field Service Engineers make every effort to return calls promptly however no guarantee of a return time can be made. If you use our web based iRequest system you will receive an e-mail notification of receipt of request almost immediately. Onsite response time target for Waters is 48 hours or less 80% of the time, however, we cannot guarantee 72 hour on-site response.

3.1.6.5 Vendor will provide on-site training (labor and non-consumable supplies included) for all instruments and software.

Two days of on-site application training are included as part of the quote. We also have a regional applications laboratory at Northern Kentucky University. The chemist there will also provide training on the instrument and software. Additionally, we host regional free training classes for our software throughout the year and are available to provide additional training on site for new analysts as needed.

3.1.6.6 Vendor will provide on-site applications assistance for implementation of standard operating procedures for Cannabis and hemp analysis related to 3.1.4 by an applications scientist familiar with the analysis.

Two days of on-site application training are included as part of the quote. Our regional applications chemist is familiar with cannabis and hemp analysis and will assist with the training and method implementation.

3.1.6.7 Vendor will provide copies of all system manuals (operations, training, technical, service, maintenance).

We will provide all manuals for the instrumentation to the customer (these will have details on operations, technical, service, and maintenance and can be used for some training). Additionally, we will also provide any training materials used.

[WHITE PAPER]

T-WAVE DEVICES

Unique Technology for Advanced MS Capabilities

Waters

THE SCIENCE OF WHAT'S POSSIBLE.™

INTRODUCTION

Analytical chemists constantly search for better ways to meet their scientific challenges. To meet their needs, Waters is dedicated to engineering robust technology platforms that provide tangible improvements in the performance, versatility, and simplicity of its mass spectrometers.

A key technological component is the travelling wave (T-Wave™) ion guide that enables the precise manipulation of ions in a mass spectrometer in order to enhance sensitivity, selectivity, and analytical speed.

T-Wave devices enable ions to be contained, moved forwards or backwards at predefined speeds, focused, trapped, sequentially released according to *m/z*, and separated based on their mobility. Ions can be moved between two or more T-Wave devices if required. If necessary, a single T-Wave device can perform more than one function. T-Wave devices add capabilities that transcend the boundaries of conventional mass spectrometry. They can:

- Provide extremely high transmission of ions for unparalleled MS sensitivity
- Significantly improve the performance of scanning quadrupoles
- Allow extremely rapid acquisitions of tandem quadrupole MS/MS data
- Rapidly separate ions based on their mobilities

History

The universal need to get a comprehensive set of results in as short a time as possible is an important driver in the development of innovative analytical technologies. In recent years this need has required tandem quadrupole users to run analytical methods with ever increasing numbers of MS/MS data channels, reducing the acquisition time of each channel to acquire the data within the time constraints of an HPLC separation.

Unfortunately, in conventional mass spectrometers, rapid acquisition of MS/MS data can reduce sensitivity and increase cross-talk due to the slow transit times of ions through the gas-filled collision cell.

The problem was compounded by the introduction of the Waters® ACQUITY UPLC® System in 2004, the first UltraPerformance LC® System.[1] It was immediately adopted by an MS community already focused on faster and better analytical results. However, an ACQUITY UPLC System delivers sharp, concentrated peaks typically less than two seconds wide. This requires the mass spectrometer to generate data at even greater speeds, and conventional mass spectrometers simply cannot cope.

The problem was solved by the first commercially available T-Wave device, the Travelling Wave Ion Guide (TWIG) collision cell, first seen on the Waters Quattro Premier™ Mass Spectrometer in 2003.[2] Since then T-Wave Technology has found a diverse range of uses in every Waters mass spectrometer. From the TriWave®[3] device that allows ion mobility separations to take place inside a QTof instrument, to the ScanWave™[4] device that enhances the sensitivity of tandem quadrupole MS/MS scans and, most recently, the StepWave™[5] device that increases the overall sensitivity of a mass spectrometer twenty-five-fold. T-Wave devices are transforming the capabilities of the modern laboratory, helping scientists to better unravel the intricacies of complex chemical and biological systems.

Principles of Operation

The T-Wave device consists of a stacked ring ion guide in which a sequence of ring-shaped electrodes is arranged, as shown in Figure 1. Adjacent rings have opposite phases of Radio Frequency (RF) voltage applied to them, which radially confine the ions within the device while allowing them to pass unhindered along the axis.

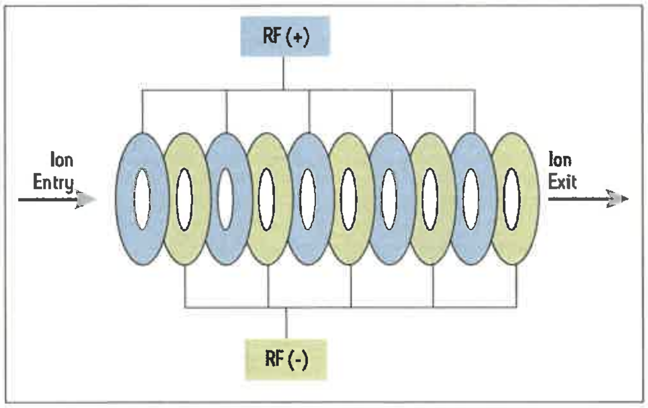

Figure 1. Stacked ring ion guide.

A Direct Current (DC) voltage can be applied to a pair of adjacent rings, which produces a potential barrier within the device that the ions cannot cross, as shown in Figure 2. If this DC potential is stepped to an adjacent set of rings then the ion barrier effectively moves forward a short distance, causing any ions in front of it to be propelled forwards. By stepping the ion barrier sequentially along the rings from one end of the device to the other it behaves as a travelling wave that drives the ions through the device. The process has been likened to surfers being propelled forward at the front of an ocean wave.

The electrode pairs are grouped in repeat patterns so that at any given time there are multiple waves passing through the device, as shown in Figure 3.

The speed of the travelling wave determines the residence time of ions in the device and can be accurately controlled. When filled with argon gas and used as a collision cell, the travelling waves are able to minimize ion transit times, allowing fast switching experiments with no loss in sensitivity. This allows the instruments to acquire high quality MS/MS data even when coupled to UPLC® Technology.

Potential barriers can also be generated in the device with radio frequency (RF) voltages as well as DC voltages. A particular feature of the RF barrier is that its amplitude is *m/z* dependent and can be scanned to provide *m/z* dependent ion transmission, extending system functionality as in the ScanWave device.[4]

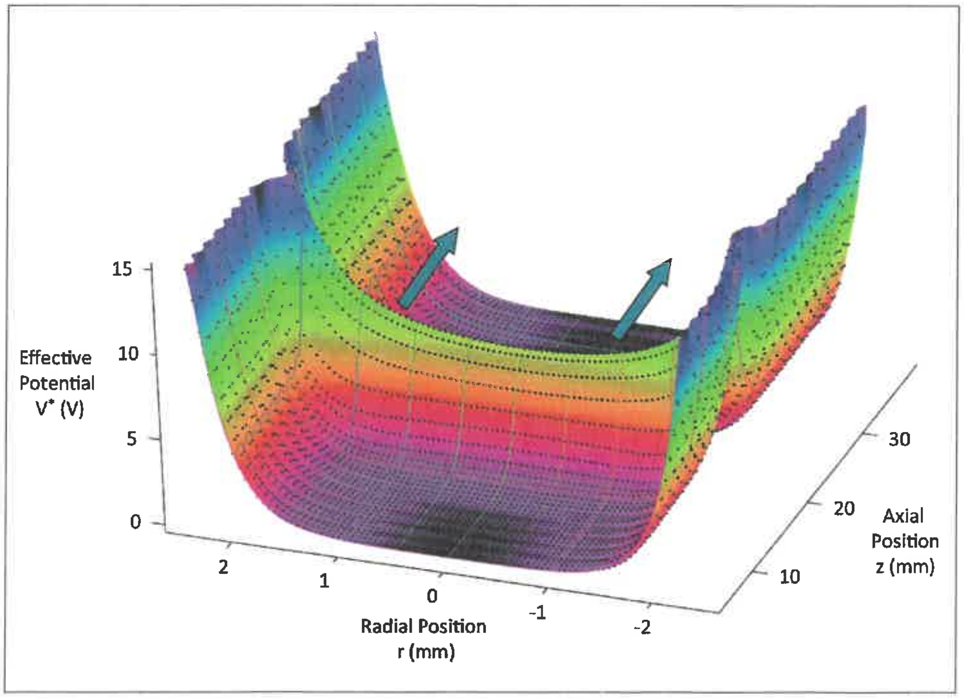

Figure 2. A three-dimensional representation of a potential barrier. Ions in front of the potential barrier are moved forward as the barrier is moved in the direction of the arrows.

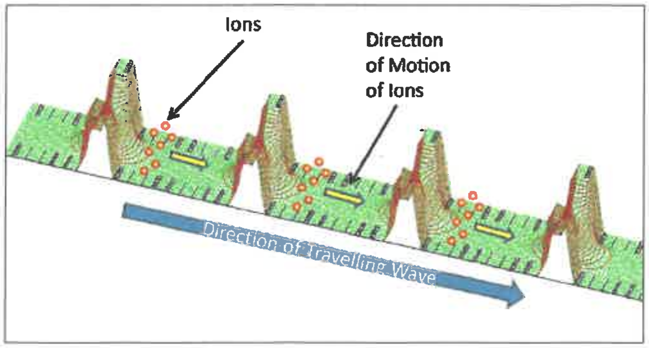

Figure 3. A sequential series of travelling waves moves from left to right through the device, maximizing the efficiency of ion transport.

In practice, the T-Wave device is constructed with the ring electrodes supported on printed circuit boards that deliver both the RF and DC voltages, as shown in Figure 4.

When using a conventional collision cell for MRM analyses, increasing the data acquisition rate leads to reduced sensitivity and increased cross-talk, shown in Figure 5A. Using a T-Wave collision cell, the sensitivity is maintained, even at high data acquisition rates, as shown in Figure 5B.

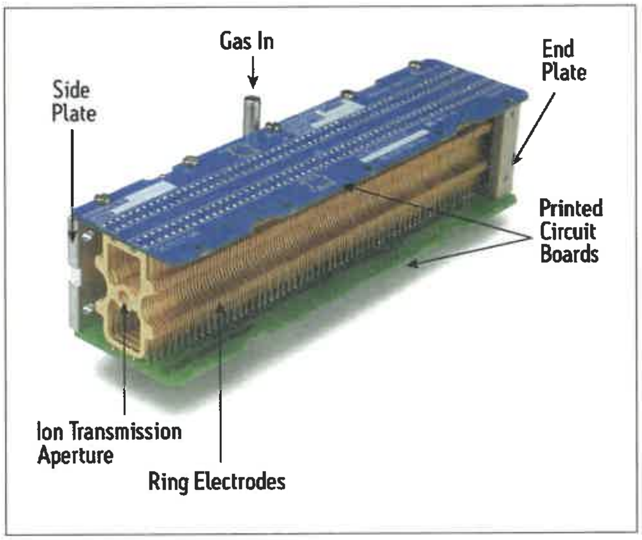

Figure 4. A T-Wave collision cell, showing the ring electrodes mounted on printed circuit boards for simplicity of construction.

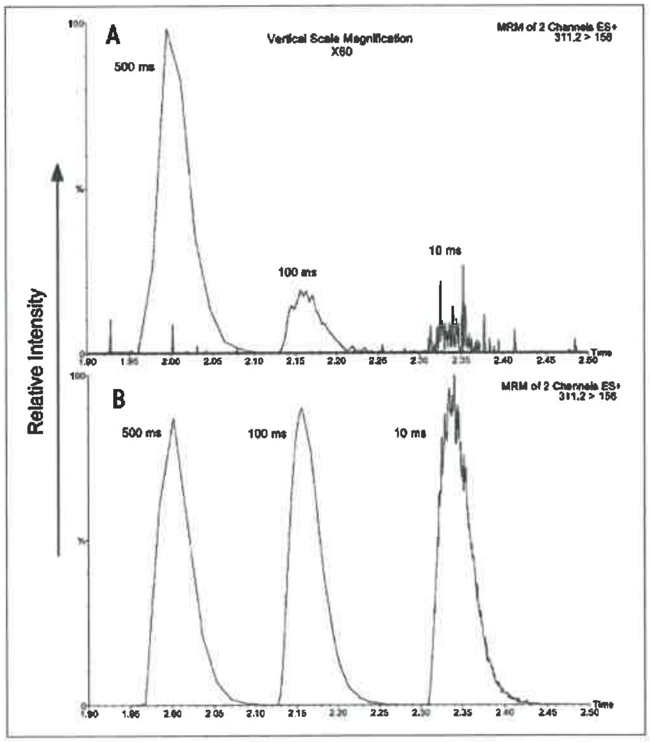

Figure 5. The upper trace (A) shows the reduction in signal seen on a conventional collision cell as dwell time is reduced from 500 to 10 ms. The lower trace (B) shows how the signal intensity is maintained when using a T-Wave collision cell.

Unique Capabilities

The ability to place ion barriers wherever they are needed, at any desired height, and the ability to remove them, or move them at any desired speed, provides total control of the ions within a Waters mass spectrometer. Since its inception as an advanced collision cell for tandem mass spectrometry, T-Wave Technology has been used in a number of creative and innovative ways to enhance the performance and functionality of Waters mass spectrometers, sometimes adding unique capabilities not possible by other means. Practical applications of this technology are discussed in the following documents:

1. ScanWave – Getting Better Full Scan Data from Tandem Quadrupole MS (720004174EN)
2. StepWave – Enhancing MS Sensitivity and Robustness (720004175EN)
3. TriWave – Complete Characterization of Mixtures and Molecules (720004176EN)

Further Reading

1. UPLC, An introduction and review, J. Liq. Chromatogr. Rel. Technol., 2005; 28: 1253-1263.
2. Applications of a traveling wave-based radio-frequency only stacked ring ion guide, Rapid Commun. Mass Spectrom., 2004; 18: 2401-2414.
3. An investigation of the mobility separation of some peptide and protein ions using a new hybrid quadrupole/traveling wave IMS/oa-ToF instrument, Int. J. Mass Spectrom., 2007; 261: 1-12.
4. ScanWave: A New Approach to Enhancing Spectral Data on a Tandem Quadrupole Mass Spectrometer, J. Am. Soc. Mass Spectrom., 2010; 21: 1061-1069.
5. A New Conjoined RF Ion Guide for Enhanced Ion Transmission, Poster presented at the 58th ASMS Conference on Mass Spectrometry and Allied Topics in Salt Lake City, Utah, 2010, Waters Literature No. 720003606en.

Find further reading and animations online:
www.waters.com/wavedevices

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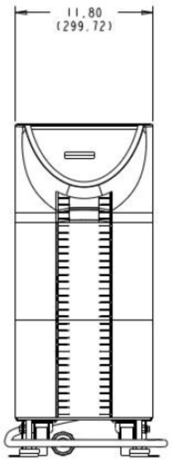
SPECIFICATIONS



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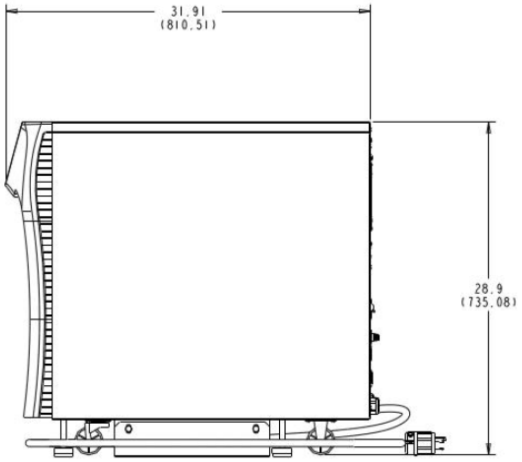
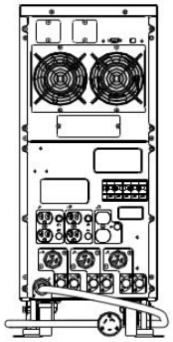


SIDE



REAR

	Model	**Waters Model ABCDEF5200-22 Part #22052-52R**				
	Topology	True On-Line, Double-Conversion, IGBT Design, Internal Isolation Transformer				
INPUT	Voltage (VAC)	200	208	220	230	240
	Voltage Range (VAC)	140-230	146-239	154-253	161-264	168-276
	Voltage Tolerance	+ 15% ~ -30% before switching to batteries				
	Frequency (Hz)	50/60				
	Frequency Tolerance	42 Hz to 69 Hz before switching to batteries				
	Input PF	> 0.95				
	Input Current THD	< 5.0%				
	Input Connection	Hardwired Standard: Line cord Optional (Consult factory)				
OUTPUT	Capacity	5200VA/ 4680W				
	Voltage (VAC)	200	120/208/240	220	230	120/208/240
	Voltage Regulation	± 3.0% Max, ± 1.0% Normal				
	Output Voltage THD	< 3.0%				
	Power Factor	0.9				
	Step Load Response	± 4.0% for 50% step load change ± 6.0% for 100% step load change Return to ±3.0% of nominal within 3 cycles				
	Crest Factor	3:1				
	Frequency (Hz)	50/60				
	Frequency Regulation	± 0.1Hz				
	Overload	125% for 2 minutes 150% for 30 seconds 300% for 500ms				
	Efficiency	AC-AC >85.0% DC-AC >81.0%				
	Common Mode Noise	< 0.5 VRMS				
	Output Connection	Hardwired Standard; Output Receptacles Optional (Consult factory)				
BYPASS	Input Voltage (VAC)	200	208	220	230	240
	Output Voltage (VAC)	200	120/208/240	220	230	120/208/240
	Transformer Voltage Regulation	± 3.0%				
	Overload	125% for 10 minutes 150% for 500ms 1000% for 1 cycle				
	Efficiency	> 95.0%				

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SPECIFICATIONS

BATTERY	Voltage (VDC)	96.0, nominal 109.2, float
	Battery	12V, 34W flame retardant High Rate, Sealed Lead-Acid
	Quantity	16
	Charge Current (ADC)	3.0
	Backup Time (min)	> 6.0
	Recharge Time	8 Hours to 90%
ENVIRONMENT	Temperature (°C)	0 to 40, operating -20 to 60, transit
	Altitude (m)	2,000, operating 12,000, transit
	Humidity	5.0% to 90.0%, non condensing
	Audible (dBA)	50-55 @ 1m from front of unit
	Heat Dissipation (BTU/hr)	2819.56
AGENCIES	EMC	FCC Part 15J Class A EN 55022 Class A/ CISPR 22 EN 50091-2 IEC 61000-3-2
	Safety Agencies	UL1778 cUL to CSA22.2 No.107.1 CE: IEC62040, w/CB report and certificate IEC61000-4-2, Electrostatic Discharge IEC61000-4-3, Radiated Electromagnetic Field Immunity IEC61000-4-4, Electrical Fast Transient/ Burst Immunity IEC61000-4-5, Surge Immunity IEC61000-4-6, Immunity to Conducted Radio Frequency Disturbances IEC61000-4-8, Power Frequency Magnetic Field Immunity IEC61000-4-11, Voltage Dips, Short Interruptions, and Voltage Variations
	RoHS	All units are RoHS compliant
OTHER	Communication	RS-232 USB DB-9 Dry Contacts Internal SNMP Adapter (option)
	Plug & Receptacle	L6-30P, (2) 5-20R Duplex, (3) L6-15R
	Unit Weight	299 lbs. / 136 kg.
	Shipping Weight	395 lbs. / 180 kg.

Warranty/Support: POWERVAR warrants the electronics and transformers used in its uninterruptible power managers to be free from defects in materials and workmanship for a period of three years from the date of shipment. Batteries are warranted for a period of two years from the date of shipment for standby use; 90 days for cyclic use. For North American service or support on any POWERVAR product, please contact POWERVAR Technical Support at (800) 369-7179 (in Illinois call (847-596-7000). For service and support in EMEA, contact POWERVAR, Ltd. in the United Kingdom at +44 (0) 1793 553980. Or visit the POWERVAR website at **www.powervar.com**.

Battery Life Disclaimer: Powervar's standard battery warranty applies only to UPS and UPM products which are continuously connected to AC mains power, except during utility power outages. Products which are regularly and intentionally disconnected from AC mains power will experience battery discharge/charge cycles potentially far more numerous than those for which the battery was designed. As a result, products used in such applications will experience substantially reduced battery life. For that reason, Powervar's standard battery warranty does not apply for applications in which the UPS or UPM product is regularly and intentionally disconnected from AC mains power. Powervar UPS and UPM products used in such applications shall receive a 90 day warranty on batteries.

POWERVAR, Inc. - 1450 Lakeside Drive, Waukegan, IL 60085
POWERVAR, Ltd. - Unit 5 Birch, Kembrey Park, Swindon, Wiltshire, UK SN2 8UU

Waters
THE SCIENCE OF
WHAT'S POSSIBLE.®

Waters Licenses, Warranties, and Support Services

71500029510
Revision G

Company information

The term "Waters" shall mean Waters Corporation and/or a Related Company of Waters Corporation. A Related Company of Waters Corporation means any corporation or other business entity that is directly controlled by Waters Corporation. Control means direct or indirect ownership of or other beneficial interest in fifty percent (50%) or more of the voting stock, other voting interest, or income of a corporation or other business entity.

Copyright notice

Trademarks

NuGenesis®, Waters®, Empower®, MassLynx®, THE SCIENCE OF WHAT'S POSSIBLE.®, and UNIFI®, are registered trademarks of Waters Corporation, and Breeze™, Waters NuGenesis SDMS™, Waters SDMS Vision Publisher™, Waters Analytical Workflow Manager™ are trademarks of Waters Corporation.

Other registered trademarks or trademarks are the sole property of their owners.

Contacting Waters

Contact Waters® with technical questions regarding the use, transportation, removal, or disposal of any Waters product. You can reach us via the Internet, telephone, or conventional mail.

Waters contact information:

Contacting medium	Information
Internet	The Waters Web site includes contact information for Waters locations worldwide. Visit www.waters.com.
Telephone and fax	For all worldwide location phone and fax numbers, please visit the Waters Web site.
Conventional mail	Waters Corporation 34 Maple Street Milford, MA 01757 USA
Online Service Request System - iRequest	Contact Waters online at www.waters.com/irequest

Table of Contents

License, Warranty, Support, Shipment, Damage, Claim, and Return Information

1.1 Software license and warranty

All use of the Waters Software shall be governed by the terms and conditions of the Waters Software License Agreement, attached hereto as Appendix A.

The term "Software" includes the object code version of the MassLynx software, Breeze software, Empower software, Waters NuGenesis Scientific Data Management System (SDMS) software, Waters SDMS Vision Publisher software, Waters Analytical Workflow Manager (AWM) software, Waters UNIFI software and/or such other software licensed to you by Waters.

1.2 Instrumentation and service warranty

1.2.1 Limited warranty: instrumentation

Waters warrants from the date of shipment for the applicable warranty period that its instrumentation identified and/or marketed as Waters products shall be free from defects in design, material, and workmanship and shall conform to and perform materially in accordance with the specifications set forth in the applicable operator or user manual when used in the proper operating environment under normal use and service. This warranty covers all new instrumentation products manufactured by Waters. Any warranty that may be applicable to third-party instrumentation products and accessories shall be provided by the respective manufacturers or suppliers of such third-party components.

Waters instruments are for use only by properly qualified personnel. Waters instruments labeled and identified as *in vitro* diagnostic ("IVD") devices may be used for IVD purposes. Such IVD uses must be in accordance with the instrument's intended use statement provided in the product literature. Any patient diagnosis or treatment determination made as a result of data generated using a Waters IVD instrument must be made by a qualified health care professional. Waters instruments that are not labeled and identified as IVDs are general laboratory instruments intended for research use only and are not for use in IVD procedures. Customer shall not use any such general laboratory instruments for IVD purposes.

This instrumentation limited warranty is subject to the conditions set forth below.

1.2.1.1 Exclusions

The foregoing limited warranty does not apply to any material deviation from the specifications by any instrumentation product that results from (a) use of the instrumentation for any purpose other than general purpose use unless specifically expressed otherwise in the product literature; (b) use of the instrumentation products for investigational use with or without confirmation of diagnosis by another, medically established diagnostic product or procedure; (c) errors or defects in any third-party component; (d) modification of the instrumentation products by anyone other than Waters; (e) failure by customer to install any standard enhancement or update in accordance with an update procedure or release of firmware or any operating system release; (f) any willful or negligent action or omission of customer; (g) any misuse, or incorrect use, of the instrumentation product; (h) any malfunction of any non-Waters information system or instrument with which the instrumentation product may be connected; or (i) failure to establish or maintain the operating environment for the instrumentation product in accordance with the applicable operator or user manual.

1.2.1.2 Exclusive remedy

In the event of any failure of a Waters' instrumentation product to perform in accordance with the foregoing limited warranty, Waters' sole liability and customer's sole and exclusive remedy, shall at Waters' sole discretion be the repair or replacement of the instrumentation product or refund of amounts paid by customer for the instrumentation product that does not meet the limited warranty.

1.2.1.3 Warranty service

Warranty service is performed at no charge and at Waters' option and in Waters' sole discretion in one of four ways:

- With your authorization, a service representative will access your system remotely.
- A service representative is dispatched to the customer facility.
- The instrumentation product is returned for repair at a Waters facility.
- Replacement parts with appropriate installation instructions are sent to the customer.

Warranty service is performed only if the customer notifies Waters during the applicable warranty period.

Unless otherwise agreed in writing at the time of sale, if the instrumentation product for which warranty service is sought has been removed from the initial installation geographic site, no warranty service will be provided.

Warranty service is provided during normal business hours (8:00 A.M. to 5:00 P.M., Monday through Friday). Service is not available when Waters offices are closed in observance of legal holidays.

1.2.1.3.1Warranty service exceptions for instrumentation

Warranty service is not performed on

- any instrumentation product or part that has been repaired by others, improperly installed, altered, or damaged in any way.
- any instrumentation product or parts not manufactured by Waters.
- any instrumentation product that malfunctions because the customer has failed to perform maintenance, calibration checks, or observe good operating procedures.
- any instrumentation product that malfunctions due to the use of unapproved maintenance, or repair parts, or operating supplies and computers not meeting minimum hardware requirements, or as a result of network-related problems.

Repair or replacement is not made

- for expendable items such as lamps, panel lights, fuses, batteries, filters, seals, and other items contained in a Performance Maintenance Kit, when such items were operable at the time of initial use.

- because of decomposition due to chemical action.
- because of poor facilities, operating conditions, or inadequate utilities.

1.2.1.3.2 Limited warranty: repair and maintenance service

Waters warrants repairs and maintenance services for a period of ninety (90) days from the date of delivery of such services. Waters also warrants the parts used shall be free from defects in design, material and workmanship and shall conform to and perform materially in accordance with the specifications set forth in the applicable operator or user manual when used in the proper operating environment under normal use and service.

Repair and maintenance warranty service is not provided for

- any instrument, maintenance or repair part that has been repaired by others, improperly installed, altered, or damaged in any way.
- any instrumentation product that malfunctions because the customer has failed to perform maintenance, calibration checks, or observe good operating procedures.
- any instrumentation product that malfunctions due to the use of unapproved maintenance or repair parts or operating supplies and computers not meeting minimum hardware requirements or as a result of network related problems.
- any system component or assembly that falls outside the scope of the repair or maintenance service that fails either during or within ninety (90) days of the service event.

Repair or replacement is not made

- because of decomposition due to chemical action.
- because of poor facilities, operating conditions, or inadequate utilities.

1.2.2 Warranty disclaimers

TO THE EXTENT PERMITTED BY APPLICABLE LAW, THE LIMITED WARRANTIES SET FORTH HEREIN ARE EXCLUSIVE AND IN LIEU OF ALL OTHER REPRESENTATIONS, WARRANTIES AND GUARANTEES, EXPRESS OR IMPLIED, INCLUDING WITHOUT LIMITATION ANY IMPLIED WARRANTIES OF MERCHANTABILITY, FITNESS OF THE PRODUCTS FOR A PARTICULAR PURPOSE, INCLUDING FITNESS FOR USE IN CLINICAL DIAGNOSTIC PROCEDURES OR FOR INVESTIGATIONAL USE WITH OR WITHOUT CONFIRMATION OF DIAGNOSIS BY ANOTHER MEDICALLY ESTABLISHED DIAGNOSTIC PRODUCT OR PROCEDURE, OR NONINFRINGEMENT, AND ANY WARRANTIES ARISING OUT OF COURSE OF DEALING OR COURSE OF PERFORMANCE. CUSTOMER EXPRESSLY ACKNOWLEDGES THAT BECAUSE OF THE COMPLEX NATURE OF THE PRODUCTS AND THEIR MANUFACTURE, WATERS CANNOT AND DOES NOT WARRANT THAT THE OPERATION OF THE PRODUCTS WILL BE WITHOUT INTERRUPTION OR ERROR-FREE OR WITHOUT DEFECT. CUSTOMER EXPRESSLY ACKNOWLEDGES THAT CUSTOMER IS SOLELY RESPONSIBLE FOR USE OF THE PRODUCTS IN CLINCIAL DIAGNOSTIC PROCEDURES OR FOR INVESTIGATIONAL USE WITH OR WITHOUT CONFIRMATION OF DIAGNOSIS BY ANOTHER MEDICALLY ESTABLISHED DIAGNOSTIC PRODUCT OR PROCEDURE.

TO THE EXTENT PERMITTED BY APPLICABLE LAW, IN NO EVENT SHALL WATERS OR ITS SUPPLIERS BE LIABLE FOR ANY INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, PUNITIVE OR CONSEQUENTIAL DAMAGES INCLUDING, WITHOUT LIMITATION, DAMAGES FOR LOSS OF BUSINESS INFORMATION OR PECUNIARY LOSS ARISING OUT OF THE USE OR

INABILITY TO USE THE PRODUCTS, EVEN IF WATERS HAS BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGES. WATERS' TOTAL LIABILITY IN ANY EVENT SHALL NOT EXCEED THE PURCHASE PRICE OF THE GOODS AND SERVICES TO WHICH THE DAMAGES RELATE AND, THE PARTIES AGREE THAT SUCH LIMITED LIABILITY IS A REASONABLE ALLOCATION OF THE RISKS INVOLVING THE PRODUCT.

1.2.3 Transfer of warranty

The warranty is not transferable from the original owner or original installation site to another geographic location without the written consent of Waters. In the event that the instrument(s) must be relocated within the same company and country during the warranty period, Waters offers relocation services to ensure proper care is taken when de-installing, packing and re-installing in order to maintain the warranty coverage.

1.2.4 Warranty periods

Note that warranty periods begin when products are shipped.

Instrumentation:

Warranted item	Component or components	Warranty period
Electronic and mechanical assemblies	Entire instrument, except for maintenance parts, operating supplies, and expendable components.	One year (12 months) from the date of shipment, unless otherwise stated in the instrument's accompanying user documentation.
Mechanical and electronic assemblies	Instruments that have served as demonstration models.	Ninety (90) days from date of shipment.
Normal wear and maintenance parts	As defined in the instrument Performance Maintenance Kit, if available.	Ninety (90) days from date of shipment.
Operating supplies and expendables	Autosampler vials, solvent and sample filters, and fuses.	Warranted to function properly when delivered.

Service:

Warranted item	Component or components	Warranty period
Parts installed during a demand service repair	Mechanical and electronic assemblies	Ninety (90) days from date of shipment.
Service labor	Service workmanship	Ninety (90) days from date of service delivery.

1.2.5 Warranty returns

No returns may be made without prior notification and authorization from Waters. If it is necessary to return products to Waters, contact Waters Customer Service, the Waters subsidiary nearest you, or your Waters representative for a return merchandise authorization (RMA) number and forwarding address.

1.2.6 Warranty: non-Waters hardware

Waters does not assemble, configure, or install software on any computer or computer peripheral that has not been purchased from Waters.

The warranty for hardware not manufactured by Waters follows the warranty, if any, of the original equipment manufacturer.

1.3 Support and extended coverage

Waters' USA and Canadian customers seeking service and support may contact Waters Technical Service (800 252-4752). Others may phone their local Waters subsidiary or Waters corporate headquarters in Milford, Massachusetts (USA), or they may visit the Waters Web site (http://www.waters.com) and click Support.

Total Assurance Warranty is available during the first 90 days of system ownership and receives the same discount as that of the system purchased. It provides full support coverage for two years and guarantees a scheduled Performance Maintenance (PM) visit in year two.

Total Assurance Plan is available at the end of the Warranty and is renewable annually, it also provides annual scheduled PM visit.

Both TAW, and TAP provide technical telephone support, priority service, repair visits and replacement parts as needed to ensure your system is running at peak performance.

1.4 Installation and extended training

1.4.1 Instrument startup

As part of the purchased installation charge, Waters offers familiarization training for a single, designated primary operator.

Instrument startup consists of these procedures:

- Assembling computer hardware and connecting a printer purchased from Waters.
- Connecting computer hardware to the system instruments.
- Configuring and testing a system for proper instrument function and data collection.

Optional installation services are available to purchasers of workstation add-on kit software products. The services consist of software installation, system configuration, and primary operator familiarization training. During this day of system installation service, a certified Waters field service technician will configure the customer's computer, load software, and interface the computer with the system.

1.4.2 Extended training

Waters Educational Services provides instrument and software training beyond that which is provided at startup. Courses are available at the customer site, our worldwide campus in Milford, Mass., U.S.A., in our Regional Training Centers in Europe and Asia, and at most Waters subsidiaries. Programs can be generic or customized to address specific challenges.

For details about the training and extended support programs, visit the Waters Web site (http://www.waters.com), and click Education, or Services & Support.

1.5 Shipments, damages, claims, and returns

All shipments are made free on board (FOB) shipping point. Waters suggests that you authorize insurance for all shipments. Instruments and major components are packed and shipped via ground transportation unless otherwise required. Supplies and/or replacement parts are packed and shipped via a ground courier, air parcel post, or parcel post, unless otherwise requested.

1.5.1 Damages

The U.S. Interstate Commerce Commission (ICC) has determined that carriers are as responsible for concealed damages that occur during transit as they are for obvious damages. Concealed damage is damage that occurs to the contents of a shipping package where the package exterior remains apparently undamaged. Therefore, unpack the instrument or component promptly after receiving it, aware that it may have sustained concealed damage while in transit.

1.5.2 Claims

If you discover the item shipped has sustained concealed damage, do not continue to unpack it. Instead, request the local agent or carrier to immediately inspect the unit, and secure a written (inspection) report of his or her findings to support the claim. You must make this request within 15 days of receiving the damaged unit, otherwise, the carrier will not honor the claim. Do not return damaged goods to Waters without first securing the inspection report and contacting Waters for a return merchandise authorization (RMA) number.

Ensure the shipment is protected and secure after you receive it. Components removed from the shipment, or damaged while awaiting installation, are the responsibility of the customer.

After a damage inspection report is secured, Waters cooperates fully in supplying replacements and handling a claim, which either party may initiate.

1.5.3 Returns

No returns may be made without prior notification and authorization, If for any reason it is necessary to return material to Waters, contact Waters Customer Service, the Waters subsidiary nearest you, or your local Waters representative for a return merchandise authorization (RMA) number and forwarding address.

A

Waters Software License Agreement

This is a legal agreement ("Agreement") between you (the "Customer") and Waters Corporation and/or a Related Company of Waters Corporation (collectively, "Waters"). A Related Company of Waters Corporation means any corporation or other business entity that is directly controlled by Waters Corporation. Control means direct or indirect ownership of or other beneficial interest in fifty percent (50%) or more of the voting stock, other voting interest, or income of a corporation or other business entity.

By using Waters' Software including any Upgrades (as defined below), you represent that you have the power and authority to enter into this Agreement on behalf of your company. In such event, "you" refers to your company. YOU MUST READ AND AGREE TO THE TERMS OF THIS AGREEMENT BEFORE ANY WATERS' SOFTWARE CAN BE INSTALLED OR USED. BY CLICKING ON THE "ACCEPT" BUTTON OF THIS AGREEMENT, OR BY INSTALLING OR USING WATERS' SOFTWARE, YOU ARE AGREEING TO BE BOUND BY THE TERMS AND CONDITIONS OF THIS AGREEMENT. IF YOU DO NOT AGREE WITH THE TERMS AND CONDITIONS OF THIS AGREEMENT, THEN YOU SHOULD EXIT THIS PAGE AND NOT INSTALL OR USE ANY WATERS' SOFTWARE. BY DOING SO YOU FOREGO ANY IMPLIED OR STATED RIGHTS TO INSTALL OR USE WATERS' SOFTWARE, AND YOU SHALL RETURN IT TO US FOR A FULL REFUND (IF APPLICABLE).

All use of Waters' Software shall be governed by the following terms and conditions.

1. **Definitions**.

a. The term “Software” includes the object code version of the MassLynx software, Breeze software, Empower software, Waters NuGenesis Scientific Data Management System (SDMS) software, Waters SDMS Vision Publisher software, Waters Analytical Workflow Manager (AWM) software, Waters UNIFI software and/or such other software indicated on the Waters' Quotation and accepted by you on your Purchase Order ("PO") and licensed to you by Waters. The Software is comprised of the computer programs, media containing the computer programs (including Oracle® Network Embedded Software, where applicable), user documentation, and any Upgrades that Waters may provide to you. You acknowledge and agree that the Software constitutes Waters' confidential information.

b. “Upgrades” shall mean and include any changes, additions, or corrections made by Waters to the Software.

c. “Quotation” shall mean a document provided by an authorized representative of Waters which describes the Software, Waters' products, and/or those certain Waters Partners' product(s), if any, that you, the Customer, may purchase, including pricing. All such Quotations shall include and be subject to the terms and conditions contained in this Agreement unless otherwise agreed in writing.

d. “Purchase Order” shall mean a written authorization from you, the Customer, to Waters for the purchase of Software and products. All such Purchase Orders shall reference a Quotation and be subject to the terms and conditions contained in this Agreement.

2. License and Usage of Software

Subject to the terms and conditions of this Agreement and upon payment of the applicable license fees, Waters hereby grants to you a non-exclusive, non-transferable, non-sublicenseable right and license during the Term (as defined below) to use the Software in connection with Waters' products and/or those certain Waters' Partner product(s) authorized by Waters, if any. In this regard, you may install, copy, operate and transmit the Software in whole or in part: (i) for single-seat licenses, only as necessary to use the Software either on a single personal computer or workstation, and (ii) for client/server licenses, in a reasonable manner to ensure that the number of users does not exceed the number of users for which you have paid license fees. The Software is protected by the copyright laws of the United States and international treaties. A "Waters' Partner" is an entity with which Waters has a business alliance.

3. Ownership of the Software.

The Software is licensed to you, not sold. Subject to the rights granted above, Waters and the manufacturers of any third-party software included within the Software retain all right, title and interest in and to the Software. You acknowledge that the Software is licensed in object code for use solely in conjunction with Waters' products. Use of the Software in conjunction with non-Waters products, other than those certain Waters' Partner product(s) authorized by Waters, if any, is not licensed hereunder and is prohibited.

4. General Usage Restrictions.

a. You may not use the Software for any purpose beyond the scope of the license granted in this Agreement.

b. Without limiting the generality of the foregoing, you will not: (i) authorize or permit use of the Software by persons not authorized to do so; (ii) market or distribute the Software; (iii) assign, sublicense, sell, lease or otherwise transfer, convey or pledge as security or otherwise encumber, your rights under the license granted in Section 2 above; (iv) use the Software in any time-sharing, subscription, rental or service bureau arrangement, including, without limitation, any use to provide services or process data for the benefit of, or on behalf of, any third party; (v) modify the Software; (vi) combine or integrate the Software with hardware, software or technology not provided to you by Waters; (vii) decompile, disassemble, reverse engineer (unless required by law for interoperability) or otherwise attempt to obtain or perceive the source code from which any component of the Software is compiled or interpreted, and you hereby acknowledge that nothing in this Agreement shall be construed to grant you any right to obtain or use such source code; (viii) disclose the results of any benchmark tests run on the Software (whether or not the results were obtained with assistance from Waters) to any party; or (ix) make copies of the Software other than a reasonable number of copies solely for archival purposes, provided that you reproduce and include Waters' and any third party manufacturer's copyright notices on any backup, disaster recovery or archival copies of the Software and on copies of any user documentation. It is understood and agreed that you may temporarily move, install and operate the Software at a different computer or workstation in the event of computer or workstation malfunction.

c. The Software is not for use by individuals other than properly qualified personnel. Generally, the Software is not intended for use in *in vitro* diagnostic ("IVD") procedures, but is general laboratory software intended for research use only. Customer shall not use any such general laboratory software for IVD purposes. Notwithstanding the foregoing, certain Software may be labeled and identified as an IVD device ("IVD Software") and as such may be used for IVD purposes. Customer shall not use such IVD Software except in accordance with the IVD Software's intended use statement provided in the product literature. Any patient diagnosis or treatment determination made as a result of data generated using the IVD Software must be made by a qualified health care professional.

5. Oracle Software.

a. Waters has provided, as part of the Software, access to certain Oracle embedded software as a convenience. To the extent that the Software contains Oracle software, you acknowledge that Oracle has no express or implied obligation to provide any technical or other support to you for such software. Please contact Waters directly for technical support and customer service related to the Oracle software.

b. Oracle may provide to its own customers, who may include you, as part of an Oracle software package source code identical to the Oracle source code embedded in the Software. Regardless of whether Oracle does do so, the Oracle source code embedded in the Software shall be governed solely by the terms of this Agreement. If you have obtained an Oracle software license, you must not attempt to use the Oracle software to access, use, reproduce, modify reverse, engineer or otherwise tamper with the Software.

c. Third party technology that is appropriate or necessary for use with some Oracle software, if any, is specified in the Software documentation or otherwise by Waters and such third party technology is licensed to you only for use with the Software under the terms of the third party license agreement specified in the Software documentation or otherwise by Waters and not under the terms of this Agreement.

d. Oracle is a third party beneficiary of the rights and obligations of this Agreement.

6. Exclusion of the Uniform Computer Information Transactions Act ("UCITA").

It is understood and agreed that the provisions of the UCITA do not apply to this Agreement and the license contained herein.

7. Warranties; Disclaimers.

a. **Representations and Warranties.** Each party to this Agreement hereby represents and warrants (i) that it is duly organized, validly existing and in good standing under the laws of its jurisdiction of incorporation; and (ii) that the first installation or use of the Software in the designated operating environment constitutes a valid and binding obligation between you and Waters and will be enforceable against you in accordance with the terms of this Agreement.

b. Waters Limited Warranty.

i.Waters warrants for a period of ninety (90) days from the date of shipment (the "Warranty Period") that the Software will, when used in the designated operating environment, perform substantially in accordance with the operating specifications set forth in the user manual as amended by any release notes issued during the Warranty Period and that the Software will be free of defects in materials and workmanship (the "Limited Warranty"). The Limited Warranty shall apply only to the most current version of the Software that was supplied to you by Waters.

ii. The Limited Warranty is subject to the conditions set forth below:

(a.) You must give written notice to Waters during the Warranty Period with an explanation of the circumstances of any claim that the Software fails to conform to this Limited Warranty.

(b.) Your sole and exclusive remedy in the event of any such failure is expressly limited to the correction or replacement of the defective Software or the refund of the fees paid for the defective Software.

(c.) The Limited Warranty shall not apply to any Software delivered to you that has been improperly installed or modified or that has been the subject of neglect, misuse, abuse, misapplication or alteration.

(d.) No representative of Waters is authorized to commit Waters to any warranty other than the Limited Warranty contained herein.

c. **Disclaimer.** SUBJECT TO THE LIMITED WARRANTY SET FORTH ABOVE, TO THE MAXIMUM EXTENT PERMITTED BY APPLICABLE LAW, WATERS AND ORACLE DISCLAIM ANY AND ALL PROMISES, REPRESENTATIONS AND WARRANTIES, WHETHER EXPRESS, IMPLIED OR STATUTORY, INCLUDING, BUT NOT LIMITED TO, ANY WARRANTIES OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE, DATA ACCURACY, SYSTEM INTEGRATION, TITLE, NON-INFRINGEMENT AND/OR QUIET ENJOYMENT, AND THE SOFTWARE, DOCUMENTATION AND ANY OTHER INFORMATION OR MATERIALS OTHERWISE PROVIDED ARE PROVIDED "AS IS" AND ARE SUBJECT TO NO OTHER WARRANTY. NO WARRANTY IS MADE BY

WATERS AND/OR ORACLE ON THE BASIS OF TRADE USAGE, COURSE OF DEALING OR COURSE OF TRADE. NEITHER WATERS NOR ORACLE WARRANTS THAT THE SOFTWARE WILL MEET YOUR REQUIREMENTS OR THAT THE OPERATION OF THE SOFTWARE WILL BE UNINTERRUPTED OR ERROR-FREE, OR THAT ALL ERRORS WILL BE CORRECTED. YOU ACKNOWLEDGE THAT WATERS' AND/OR ORACLE'S OBLIGATIONS UNDER THIS AGREEMENT ARE FOR YOUR BENEFIT ONLY.

d. **Exclusions of Remedies; Limitation of Liability.** OTHER THAN AS SET OUT IN SECTION 7.b ABOVE AND TO THE EXTENT PERMITTED BY APPLICABLE LAW, IN NO EVENT SHALL WATERS AND/OR ORACLE BE LIABLE TO YOU FOR ANY INCIDENTAL, INDIRECT, SPECIAL, CONSEQUENTIAL OR PUNITIVE DAMAGES, REGARDLESS OF THE NATURE OF THE CLAIM, INCLUDING, WITHOUT LIMITATION, LOST PROFITS, COSTS OF DELAY, ANY FAILURE OF DELIVERY, BUSINESS INTERRUPTION, COSTS OF LOST OR DAMAGED DATA OR DOCUMENTATION OR LIABILITIES TO THIRD PARTIES ARISING FROM ANY SOURCE, EVEN IF WATERS AND/OR ORACLE HAS BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGES. THIS LIMITATION UPON DAMAGES AND CLAIMS IS INTENDED TO APPLY WITHOUT REGARD TO WHETHER OTHER PROVISIONS OF THIS AGREEMENT HAVE BEEN BREACHED OR HAVE PROVEN INEFFECTIVE. TO THE EXTENT PERMITTED BY APPLICABLE LAW, ORACLE SHALL NOT BE LIABLE TO YOU FOR ANY OTHER DAMAGES, INCLUDING DIRECT DAMAGES. THE CUMULATIVE LIABILITY OF WATERS TO YOU FOR ALL CLAIMS ARISING FROM OR RELATING TO THIS AGREEMENT, INCLUDING,

WITHOUT LIMITATION, ANY CAUSE OF ACTION ARISING IN CONTRACT, TORT, OR STRICT LIABILITY, SHALL NOT EXCEED THE TOTAL AMOUNT OF ALL FEES, IF ANY, THEN PAID TO WATERS BY YOU DURING THE TWELVE (12) MONTH PERIOD IMMEDIATELY PRIOR TO THE EVENT, ACT OR OMISSION GIVING RISE TO SUCH LIABILITY. THIS LIMITATION OF LIABILITY IS INTENDED TO APPLY WITHOUT REGARD TO WHETHER OTHER PROVISIONS OF THIS AGREEMENT HAVE BEEN BREACHED OR HAVE PROVED INEFFECTIVE.

e. **Essential Basis.** The parties acknowledge and agree that the disclaimers, exclusions and limitations of liability set forth in this Section 7 form an essential basis of this Agreement, and that, absent any such disclaimers, exclusions or limitation of liability, the terms of this Agreement, including, without limitation, the economic terms, would be substantially different.

8. **Term and Termination.**

a. **Term.** This Agreement shall remain in effect for as long as you are not in violation of any material provision contained in this Agreement (the "Term"). A substantial deviation of Waters' hardware from the specifications in the corresponding documentation will not be considered a breach that allows you to terminate this Agreement.

b. **Rights to Terminate.**

i. Each party has the right to terminate this Agreement, by giving written notice of termination to the other party, if: (a) the other party breaches this Agreement and (b) either the breach cannot be cured or, if the breach can be cured, it is not cured by the breaching party within fifteen (15) days after receiving written notice of the breach from the non-breaching party; provided, however, in the event of a breach by you, at the discretion of Waters, this Agreement may be immediately revoked and terminated. In such event, Waters' shall have the following rights: (x) the right of termination as set forth above; (y) the right to obtain an injunction to enjoin your continued or repeated breaches; and (z) the right to all costs incurred by Waters as a result of the breach, including reasonable attorney's fees and costs.

ii. You may terminate this Agreement at any time by giving written notice of termination to Waters.

c. **Consequences of Termination**. When this Agreement expires or is terminated:

i.You must (a) immediately cease all use of the Software, (b) promptly return to Waters or destroy all copies of the Software in your possession or control and (c) certify in writing to Waters that you have complied with Sections (a) and (b).

ii. You will remain obligated to pay any amounts you owe to Waters at that time.

9. Export Control.

a. The Software is subject to export controls under the U.S. Export Administration Regulations. Therefore, the Software may not be exported or re-exported to entities within, or residents or citizens of, embargoed countries or countries subject to applicable trade sanctions, nor to prohibited or denied persons or entities without proper government licenses. Information about such restrictions can be found at the following websites: http://www.treas.gov/ofac/ and www.bis.doc.gov/complianceandenforcement/Liststocheck.htm. Countries embargoed by the U.S. include Cuba, Iran, North Korea, Sudan and Syria. You are responsible for any violation of the U.S. export control laws related to the Software. By accepting this Agreement, you confirm that you are not a resident or citizen of any country currently embargoed by the U.S. and that you are not otherwise prohibited from receiving the Software.

b. If you are a branch of the United States government, you shall have "restricted rights" to use, duplicate, or disclose the Software as set forth in subdivision (c)(1)(ii) of Rights in Technical Data and Computer Software Federal Acquisition Regulations in Technical Data and Computer Software Federal Acquisition Regulations Supplement (DFARS) 252.227-7013 or subparagraphs (c)(1) and (2) of the Commercial Computer Software-Restricted Rights at 48 CFR 52.227_19.

10. Audit Rights.

You shall maintain accurate records as to your use of the Software as authorized by this Agreement. During the Term hereof, Waters, or persons designated by Waters, will, at any time, be entitled to inspect such records and your computers, in order to verify that the Software is being used by you in accordance with the terms of this Agreement, provided that Waters may conduct no more than one (1) audit in any twelve (12) month period. Any such audit will be performed at Waters' expense during normal business hours, provided that you shall promptly reimburse Waters for the cost of such audit if such audit reveals that your use of the Software is not as authorized by this Agreement.

11. Transfer.

This Agreement shall be assignable by Waters. It shall not be assignable by you without the prior written consent of Waters.

12. Dispute Resolution.

a. All disputes arising in connection with this Agreement shall be finally settled under the Rules of Conciliation and Arbitration of the International Chamber of Commerce (the "Rules") by one or more arbitrators appointed in accordance with the Rules.

b. Notwithstanding the provisions of Section 12.a above, either party hereto shall be entitled to seek equitable relief against the other party in any competent court having jurisdiction over the parties without first submitting the matter to arbitration with respect to alleged breaches or threatened breaches of any material term or provision of this Agreement. The parties hereby irrevocably submit to the jurisdiction of any of said courts in any such claims and waive any claim or defense of inconvenient forum or lack of personal jurisdiction under any applicable law, decision, treaty or otherwise. In making the foregoing submission to jurisdiction, each party expressly waives the benefit of any contrary provision of the laws of the jurisdiction of its incorporation or where it is doing business. Both parties represent and warrant that they are not immune from judicial proceeding and will not claim immunity for themselves or their property in any claims that may arise hereunder. The parties further agree that service of process or notice in any such action, suit or proceeding shall be effective if delivered in the same manner as the Quotation and PO. You acknowledge that the breach of the terms or conditions of this Agreement by you, including any unauthorized use, reproduction or transfer of the Software, may substantially diminish the value of the Software and irrevocably harm Waters.

13. Entire Agreement.

This Agreement sets forth the entire understanding and agreement between you and Waters and may be amended only in writing signed by both parties. NO LICENSOR, DISTRIBUTOR, DEALER, RETAILER, RESELLER, SALES PERSON, OR EMPLOYEE IS AUTHORIZED TO MODIFY THIS AGREEMENT OR TO MAKE ANY REPRESENTATION OR PROMISE THAT IS DIFFERENT FROM, OR IN ADDITION TO, THE TERMS OF THIS AGREEMENT.

14. Waiver.

No waiver of any right under this Agreement will be effective unless in writing, signed by a duly authorized representative of the party to be bound. No waiver of any past or present right arising from any breach or failure to perform will be deemed to be a waiver of any future right arising under this Agreement.

15. Severability.

If any provision of this Agreement is invalid or unenforceable, that provision will be construed, limited, modified or, if necessary, severed, to the extent necessary, to eliminate its invalidity or unenforceability, and the other provisions of this Agreement will remain unaffected.

16. Relationship of the Parties; No Agency.

Nothing contained herein shall be construed to place Waters and you in a relationship of partners, joint ventures, principal agent or employer employee, and neither party shall have any authority to obligate or bind the other whatsoever, except as specifically provided by the terms of this

Agreement. In no event shall either party hold itself out to be an agent of the other with the authority to bind such other party to any agreement, contract or obligation.

17. Force Majeure.

Waters shall have no liability for failure to perform, or delay in performance, in the delivery of any and all Software caused by circumstances beyond Waters' reasonable control, including, but not limited to, acts of God, acts of nature, floods, fire, explosions, war or military mobilization, United States governmental action or inaction, request of governmental authority, delays of any kind in transportation or inability to obtain material or equipment, acts of other governments, strikes, or labor disturbances.

[XEVO TQ-S MICRO]

REDEFINING COMPACT PERFORMANCE

ROBUST SENSITIVITY BEYOND EXPECTATION

TQ-S micro

Waters

THE SCIENCE OF WHAT'S POSSIBLE.®

Xevo TQ-S micro

CLASS-LEADING PERFORMANCE THAT **CAN FIT INTO**

From the most powerful family of tandem quadrupole instruments, the Xevo® TQ-S micro from Waters® epitomizes our key elements of design. Reliable instrument operation is essential to maximize laboratory efficiency. The Xevo TQ-S micro is able to reproduce high quality analytical performance injection after injection, even with the most complex sample matrices.

Designed to acquire sensitive, robust and dependable data at accelerated rates of acquisition:

- Robust performance enabled by proven ZSpray™ and StepWave.™
  - Detect analytes at low concentrations in complex matrices.
  - Inject less sample with precision, accuracy and consistency.
- Xtended Dynamic Range™ (XDR) provides accessible sensitivity and method transfer.
- Confidently quantify more analytes using reproducible high acquisition rates with Xcelerated Ion Transfer™ (XIT) electronics.

ACQUITY UPLC I-Class with Xevo TQ-S micro

ANY LAB

UPLC/MRM comparison of Xevo TQ-S micro relative to Xevo TQD

Compound	Ionisation Mode	Relative S/N	Relative Peak Area
Bentazon	ESI-	3	4
Hexaflumuron	ESI-	3	7
Ioxynil	ESI-	12	10
Teflubenzuron	ESI-	5	10
Amphetamine	ESI+	2	10
Atrazine	ESI+	5	5
Buprofezin	ESI+	5	6
Chlortoluron	ESI+	4	6
Dicrotophos	ESI+	10	11
Hexazinone	ESI+	3	8
Methomyl	ESI+	5	5
Metolachlor	ESI+	4	6
Metoxuron	ESI+	3	6
Monolinuron	ESI+	3	5
Sebuthylazine	ESI+	5	5
Terbuthylazine	ESI+	5	4
Vitamin D	ESI+	4	16
Mean Value		**5**	**7**

GET AHEAD WITH FAST, **SENSITIVE DATA**

Reduced Laboratory Footprint

Innovative technological design has resulted in a mass spectrometer with a very small footprint (42% smaller than the Xevo TQ MS) that delivers unmatched performance in its class.

ENGINEERED SIMPLICITY

The design philosophy of Engineered Simplicity™ ensures maximum system performance with minimum effort.

- Uncomplicated IntelliStart™ software simplifies instrument set-up and operation.
- New features in TargetLynx XS™ provide quick and easy results review and reporting.
- Universal source architecture gives access to the widest range of ionization techniques in minutes.

T-Wave™

The next generation of collision cell technology further improving rapid, high quality, UPLC®-compatible MS/MS data acquisition.

Enabled by StepWave Technology

Revolutionary off-axis ion source technology that removes neutral molecules, reducing noise and providing robust performance.

XIT Electronics

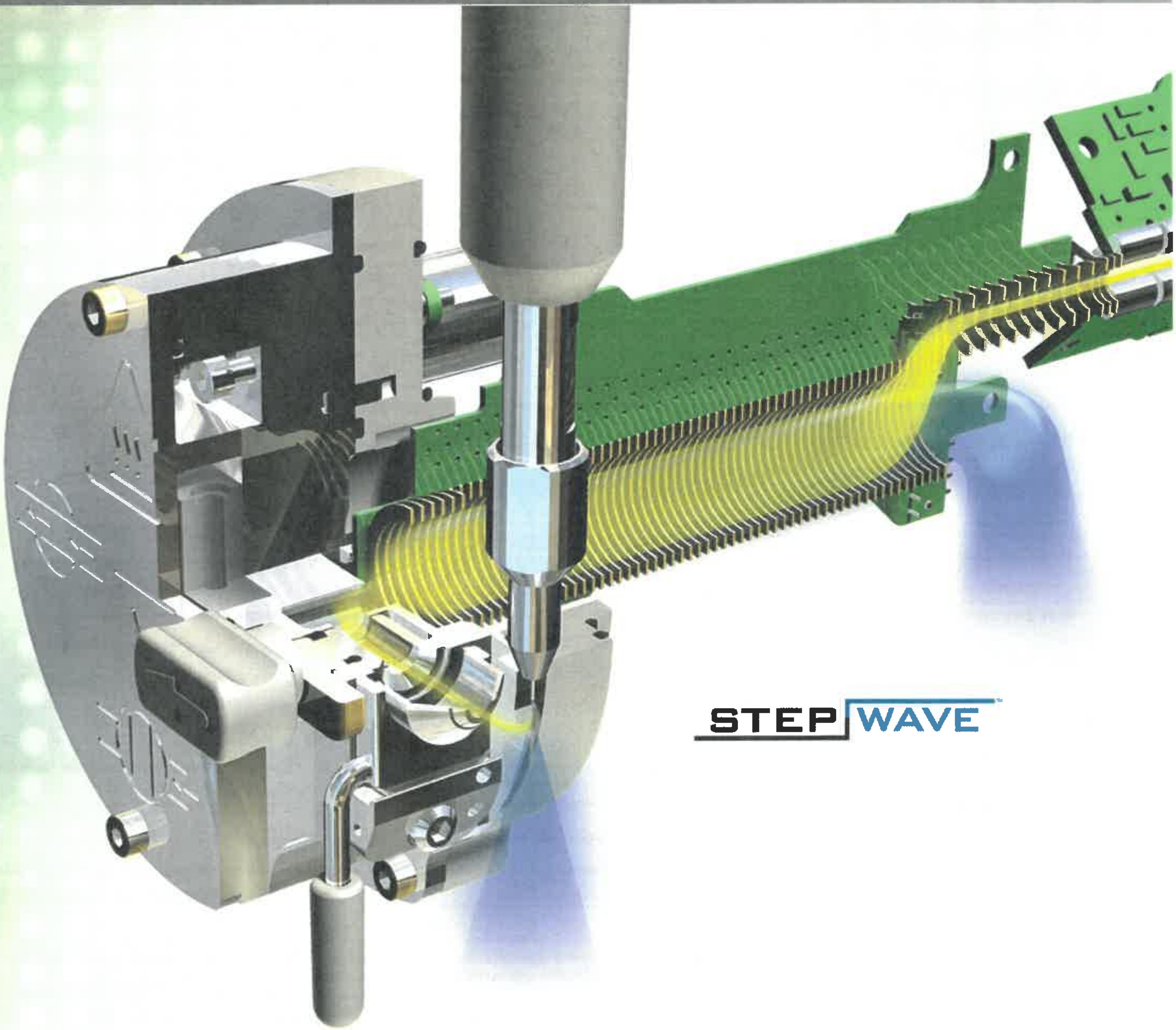
The new Xcelerated Ion Transfer electronics, featuring SpaceWire technology, enables rapid data acquisition so that narrow chromatographic peak widths are no barrier to reproducibility. Improved dynamic range is made possible by the XDR detector.

RADAR™

Using simultaneous quantitative and qualitative data acquisition it is possible to understand sample complexity, enabling intelligent method development while accurately quantifying target compounds with no compromise on performance.

PICs™

Product Ion Confirmation scanning is a data-directed product ion scanning acquisition capability, activated by a single check box, for additional confidence in analyte identification.

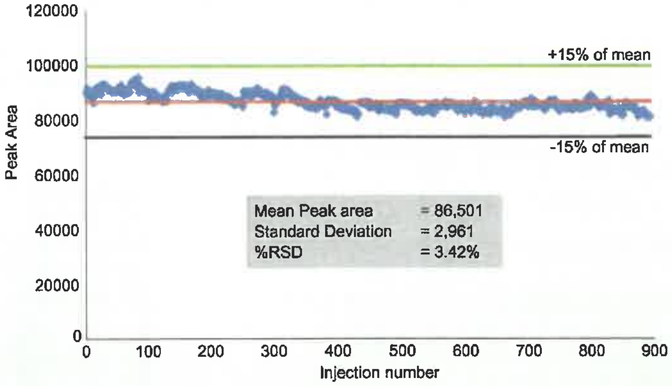


STEP WAVE

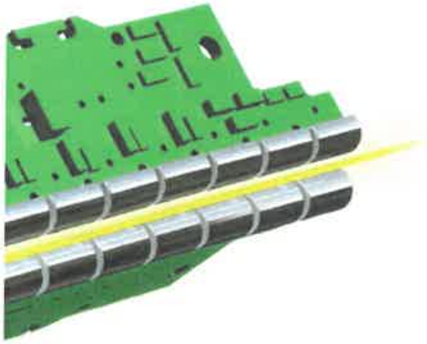
ROBUST **PERFORMANCE**

Robust performance begins in the source with proven ZSpray geometry, efficiently removing neutral molecules while drawing ions through the sample cone into the analyzer.

StepWave in the Xevo TQ-S micro is designed to cope with the challenges in the modern laboratory that are produced by high sample throughput and difficult matrices. Neutral molecules and gas load are passively removed for enhanced transmission, with the ion beam actively transferred into the mass analyzer, improving sensitivity and robustness.



Robust sensitivity for 900 injections of verapamil in protein-precipitated plasma (2.5 pg on column) with reproducibility of 3.4% RSD.



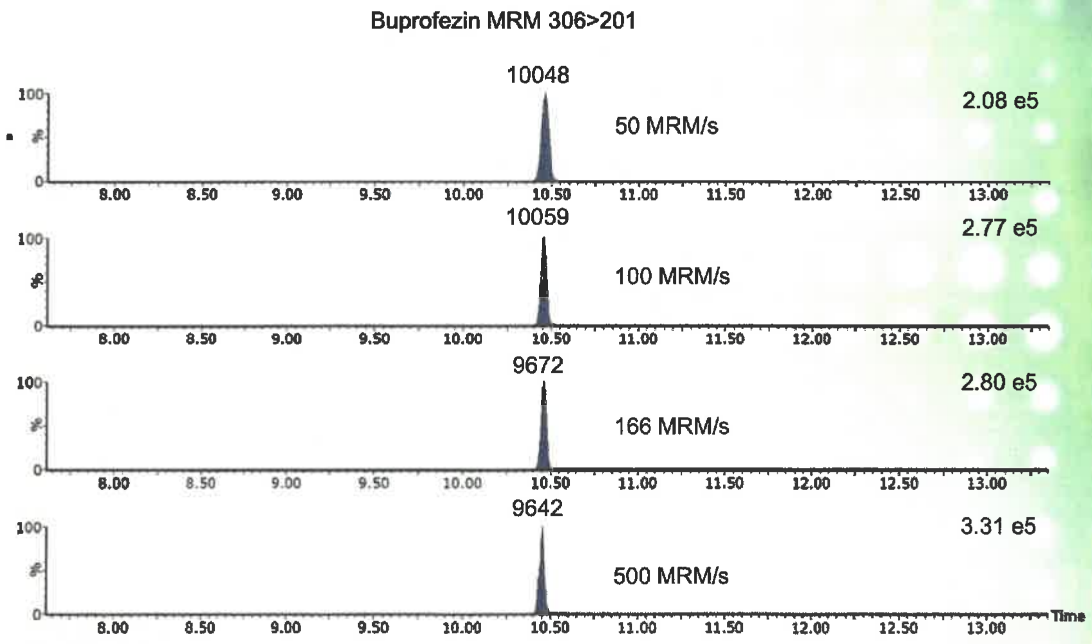
IMPROVED MRM ACQUISITION **PEAK CAPACITY**

Making Sensitivity Accessible with a Larger Dynamic Range

XIT electronics, using SpaceWire technology and the next generation of T-Wave collision cell, enable acquisition rates of 500 MRM/s with no compromise in data quality. The advanced XDR detector further increases the working range, allowing for easy method transfer.

As standard with the entire Xevo tandem quadrupole range, rapid polarity switching gives coverage of both positive and negative ionizing compounds in a single injection.

Repeatable Performance at High Speed



Injections of buprofezin pesticide showing only 4% loss in peak area (annotated above peaks) and no loss in peak height when increasing the rate of MRM transition acquisition from 50 MRM/s to 500 MRM/s. Ten injections were made at each rate of acquisition and reproducibility of peak area was excellent (<5.5% at each speed).

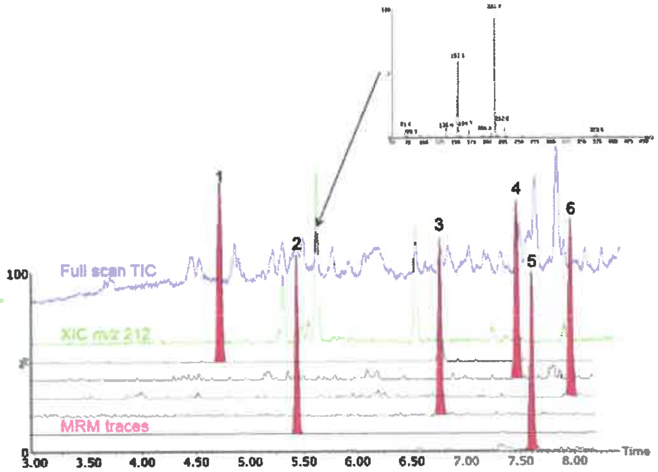
UNDERSTANDING **SAMPLE COMPLEXITY**

Use RADAR to Acquire Information – Rich Quantitative Data:

- Detect unexpected contaminants while performing routine quantitation.
- Characterize the background matrix for every sample, increasing data quality.
- Detect analytes that are not in a targeted MRM screening method.
- Improve method development by discovering more matrix components.
- Intelligent troubleshooting during routine analysis.

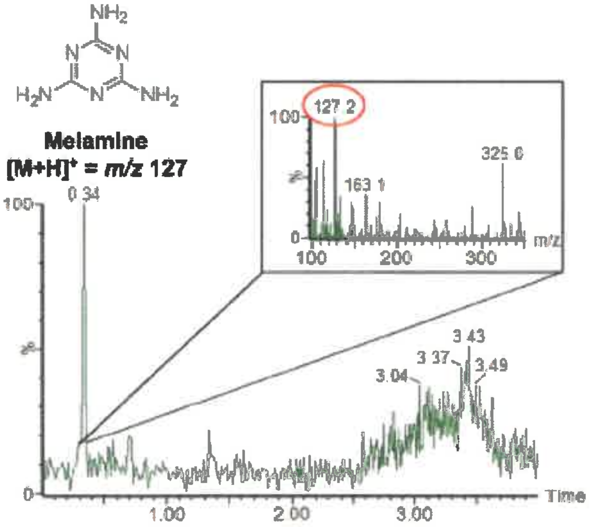
With RADAR it is possible to rapidly alternate between MS, MS/MS, positive and negative ion modes without compromising performance in any mode.

Characterization of the Background Matrix



Extracted MRM chromatograms for 6 pesticides (methomyl (1), dicrotophos (2), metoxuron (3), simazine (4), hexazinone (5) and monolinuron (6) in ginger matrix at 10 ppb) acquired using simultaneous MRM and full scan MS m/z 50-450. Inset is the full scan spectrum of a peak acquired at 5.63 min and the green trace shows the XIC for m/z 212.

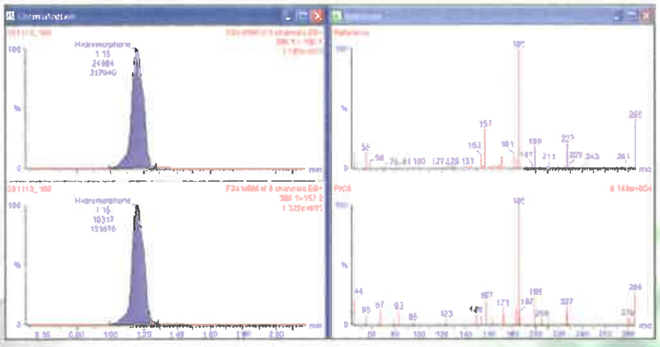
Unexpected Contaminant Detection



XIC for melamine from the full scan RADAR data Inset shows the background subtracted spectrum acquired at 0.34 minutes

Quantitate with Confidence

Product Ion Confirmation scanning (PICs) provides full confidence in results. Activated by a single check box in the method editor, PICs automatically triggers a product ion scan when a peak is detected by MRM.



Hydromorphone reference spectrum

Hydromorphone acquired PICs spectrum

INFORMATICS **EXPANDING CAPABILITIES**

Easy to Use, Even with Minimal Experience

Intellistart simplifies system setup with a user-friendly interface that automates routine tasks and reduces the burden of complicated operation.

Simple, Integrated Method Databases

The extensive and searchable QUANPEDIA™ database allows for efficient management and optimization of quantitative LC/MS/MS method information, including automatic scheduling of MRMs and automated generation of acquisition and processing methods.

Instant Critical QC Information Delivery

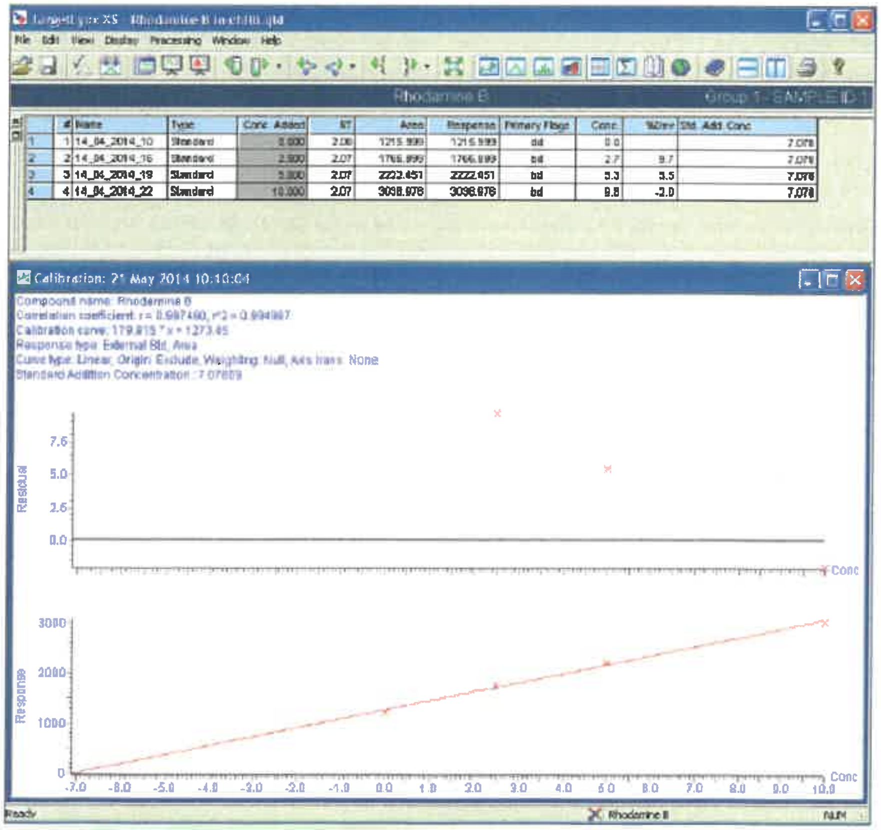
Automated real-time QC checking ensures that valuable samples are not wasted; if pre-defined tolerances are not met, QCMonitor will automatically send an email to notify the analyst.

Comprehensive Data Processing with Uncomplicated Results Review

TargetLynx XS now provides the ability to perform standard addition to accurately calculate analyte concentrations in complex samples despite extreme matrix variability. This software streamlines automated quantitative data review and reporting, minimizing the possibility of errors by providing a clear overview of QC checks and results.

Confidence in Your System Performance

Monitoring QC and sample results over time is easy with TrendPlot, which has simple graphical displays to enable quick decision making, allowing faster results delivery to the customer.



	#	Name	Type	Conc. Added	RT	Area	Response	Primary Flags	Conc.	%Dev	Std. Add Conc
1	1	14_04_2014_10	Standard	0.000	2.06	1215.999	1215.999	bd	0.0		7.078
2	2	14_04_2014_16	Standard	2.500	2.07	1766.999	1766.999	bd	2.7	9.7	7.078
3	3	14_04_2014_19	Standard	5.000	2.07	2222.451	2222.451	bd	5.3	5.5	7.078
4	4	14_04_2014_22	Standard	10.000	2.07	3098.978	3098.978	bd	9.8	-2.0	7.078

Calibration: 21 May 2014 10:10:04

Compound name: Rhodamine B
Correlation coefficient: r = 0.997400, r^2 = 0.994867
Calibration curve: 179.815 * x + 1273.45
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: Null, Axis trans: None
Standard Addition Concentration : 7.07869

The TargetLynx XS browser showing the use of standard addition to calculate the concentration of Rhodamine B.

FLEXIBLE SEPARATION TO **COVER EVERY APPLICATION**

High resolution chromatographic peaks require the increased rates of high quality data acquisition provided by the Xevo TQ-S micro. Waters market-leading separation technologies include the ACQUITY UPLC® family of LC systems, UPC^{2}® and APGC. Application flexibility is further enhanced by the range of quickly interchangeable ion source options made possible by universal ion source architecture.

ACQUITY UPC^{2}

ACQUITY UPLC H-Class

ACQUITY UPLC I-Class

ACQUITY UPLC M-Class

APGC – Atmospheric Pressure Gas Chromatography

APPI – Atmospheric Pressure Photo Ionization
APCI – Atmospheric Pressure Chemical Ionization

ionKey/MS™

nanoFlow™ ESI

ESI – Electrospray Ionization
APCI – Atmospheric Pressure Chemical Ionization
ESCi® – Dual ESI and APCi

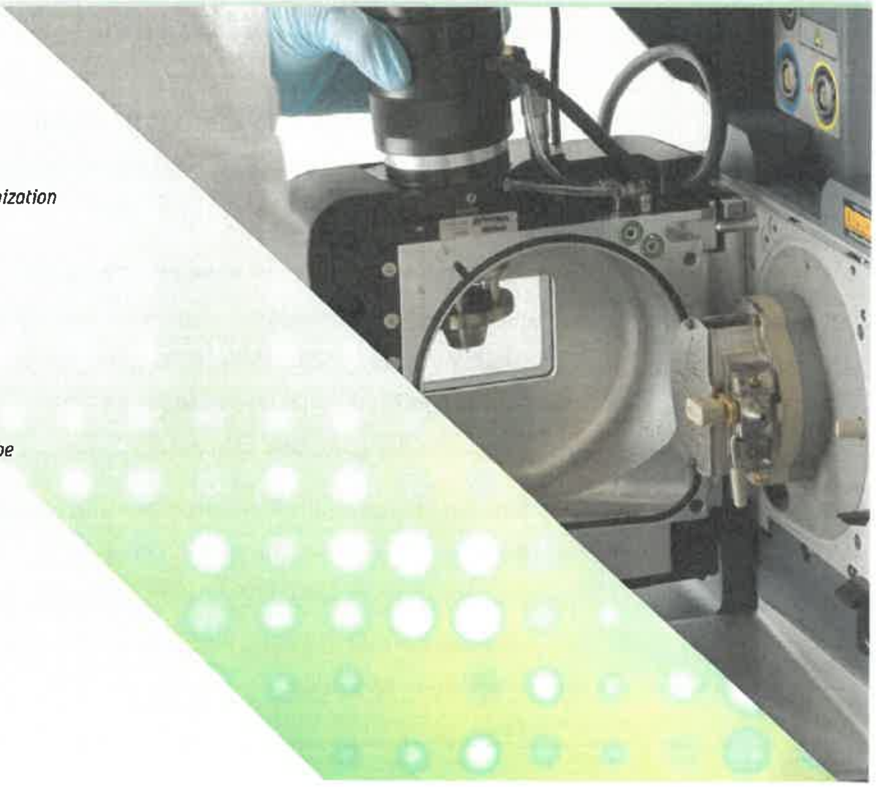
ASAP – Atmospheric Solids Analysis Probe

CHANGE YOUR ION SOURCES
NOT YOUR INSTRUMENTS

Universal Ion Source Architecture Covers Every Application, with Unlimited Potential.

The Xevo range of mass spectrometers all have multiple ion source options which are interchangeable in minutes and provide optimal ionization for each function required in the laboratory.

The Xevo TQ-S micro is compatible with ESI, ESCi,® APCI, APPI, APGC, ASAP and ionKey/MS™ and is also simply changed with DESI (Prosolia), DART (IonSense) and LDTD (Phytronix) ion sources.



The Power of Xevo

EXPAND YOUR CAPABILITIES

Xevo TQ-XS

ULTIMATE SENSITIVITY AND RELIABILITY

Xevo TQ-S micro

SENSITIVE, RELIABLE, AND COMPACT

Your world is changing and you need to be able to develop robust methods quickly, get the same result every time, and generate data you can trust.

Take your analyses to the next level by employing market-leading instrumentation, combined with the right chemistries and methodologies and unrivalled specialist support, allowing you to focus on what you do with the data, not how you get it.

Leap forward in your scientific challenges and benefit from the innovative and accomplished Xevo mass spectrometers, engineered to deliver reproducible and accurate quantitative data, with system versatility and simplicity of operation.

SENSITIVITY

Xevo G2-XS QTof

COMPREHENSIVE, QUANTITATIVE,
AND QUALITATIVE INFORMATION

Xevo TQD

ACCESSIBLE, RELIABLE, AND PROVEN

SENSITIVITY

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Malaysia 603 7841 1688
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Puerto Rico 1 787 747 8445
Singapore 65 6593 7100
Spain 34 93 600 9300
Sweden 46 8 555 115 00
Switzerland 41 56 676 7000
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UAE 971 4 214 62 38
UK 44 208 238 6100
US 1 800 252 4752

www.waters.com/TQSmicro

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November 2016 720005046EN TC-SIG

Waters® Xevo® TQ-S micro

Site Preparation Guide

Notice

Table of Contents

Introduction

This document describes the environmental conditions, power supplies and gas supplies that are required for the operation of the Xevo TQ-S micro. Operating the instrument in conformance with these conditions will enable the instrument to achieve its optimum performance.

Responsibilities

Warning: Observe Good Laboratory Practice (GLP) at all times, particularly when working with hazardous materials, and consult the safety representative for your organization regarding its protocols for handling such materials.

Warning: Safety glasses must be worn at all times when working with hazardous materials and pressured fluidics.

A Waters engineer will be responsible for installing and commissioning the system to ensure that the instrument is properly installed and operational. The laboratory must be prepared in advance to allow the engineer to carry out the installation efficiently. A site preparation checklist is included at the end of this document for you to fill in and return to Waters when the laboratory is ready.

Important: The installation of the system cannot begin until the checklist has been completed and returned to the mass spectrometer sales support representative at your local Waters office.

The installation time may vary, depending on the instrument options being installed. The site preparation checklist must be completed as accurately as possible to help minimize installation time.

A major aspect of the system installation is the implementation of tests designed to evaluate the instrument functionality under specific operating conditions. At the completion of each test, the actual test result obtained is entered in the Installation Checklist or Instrument Qualification Workbook, whichever is appropriate.

Important: A user who has been designated to be responsible for the normal use and upkeep of the instrument must be present during the installation.

The user must be present during the functionality tests at installation; this allows the user to be trained in the basic system operation. If there are foreseen periods when the intended user cannot be present, please notify us in advance; this will enable us to schedule the installation for a more convenient time.

If you have questions regarding the information in this document or any specific site problems, contact your local Waters sales representative. If necessary, we will arrange a site survey.

Storage

The following storage conditions are required prior to installation:

- Unopened shipping crates
- Crates stored away from heavy machinery such as compressors or generators, which generate excessive floor vibration
- Storage area temperature 0 to 40 °C (32 to 104 °F) and humidity <80%, non-condensing

Contact your local Waters representative if you need further advice regarding storage conditions.

Unpacking and moving

The instrument is delivered in several palletized cartons and crates. Their sizes may vary dependent on instrument specification and optional accessories, typical sizes for the instrument crate are:

Width	560 mm (22 inch)
Length	1100 mm (43.5 inch)
Height	1040 mm (41 inch)
Weight	130 kg (287 lbs)

It is a warranty condition that the shipping crates are unpacked only when the Waters engineer is present. At the end of the installation, it is the customer's responsibility to dispose of the crates and packaging.

It is essential that the instrument is not bumped or jolted during unpacking or any subsequent transport. If the instrument needs to be transported across an uneven surface, the instrument must be carried on a forklift truck or trolley.

Doorways must be at least 600 mm (24 inch) wide. Elevators and corridors (including corners) must be sufficiently wide for maneuvering of the instrument. Special handling arrangements may be necessary if access to the laboratory is via a staircase.

Lifting equipment

Once unpacked, the instrument weights are approximately as shown in Table 1:

Table 1: Instrument weights

Xevo TQ-S micro	100 kg (220 lbs)
Data system (computer, monitor, and optional printer)	<50 kg (110 lbs)
Rotary pump*	40 kg (88 lbs)
Scroll pump*	42 kg (93 lbs)

***System includes either a rotary or scroll pump option.

Warning: The instrument must only be lifted using lifting equipment capable of raising the instrument's weight safely. The instrument must not be lifted manually.

Important: It is essential that you provide suitable equipment for lifting the instrument. The installation cannot be implemented unless this equipment is made available. The engineer will require assistance lifting and positioning the instrument.

A forklift truck or A-frame hoist is recommended for lifting and transporting the instrument. The instrument is fitted with a lifting harness, which must be used to lift the instrument from the shipping crate onto the bench.

Bench loading

The bench must be able to support the combined weight of the mass spectrometer, data system and LC system. Nominal weights for the instrument and data system are shown in Table 1. Refer to the UPLC, HPLC, or GC system site preparation guide for specific weight information.

Space requirements

Instrument

The instrument has the following dimensions:

Width	352 mm (13.85 inch)
Length	913 mm (36.0 inch)
Height	593 mm (23.25 inch)

Note: A moveable workbench of suitable load rating is the preferred arrangement for the system setup, to provide ease of access for servicing.

For service access, a minimum clearance of 600 mm (23.6 inch) is required for the front, back, and right side of the instrument; a temporary clearance of 1000 mm (39.5 inch) is required for the left side of the instrument. If the instrument is placed on a bench that can be moved out during service visits, the minimum clearance at the back is 150 mm (6 inch) with the rotary/scroll pump positioned beneath the instrument. The mass spectrometer must be installed on a surface that is level to within ±1° in any direction.

The instrument is fitted with a 2.5-m (8-ft) power cable.

A possible layout for the Xevo TQ-S micro, rotary/scroll pump, data system, and ancillary equipment is shown in Figure 1 and Figure 2.

Note: An additional 150 mm (6 inch) is recommended behind the workbench to accommodate vacuum tubing.

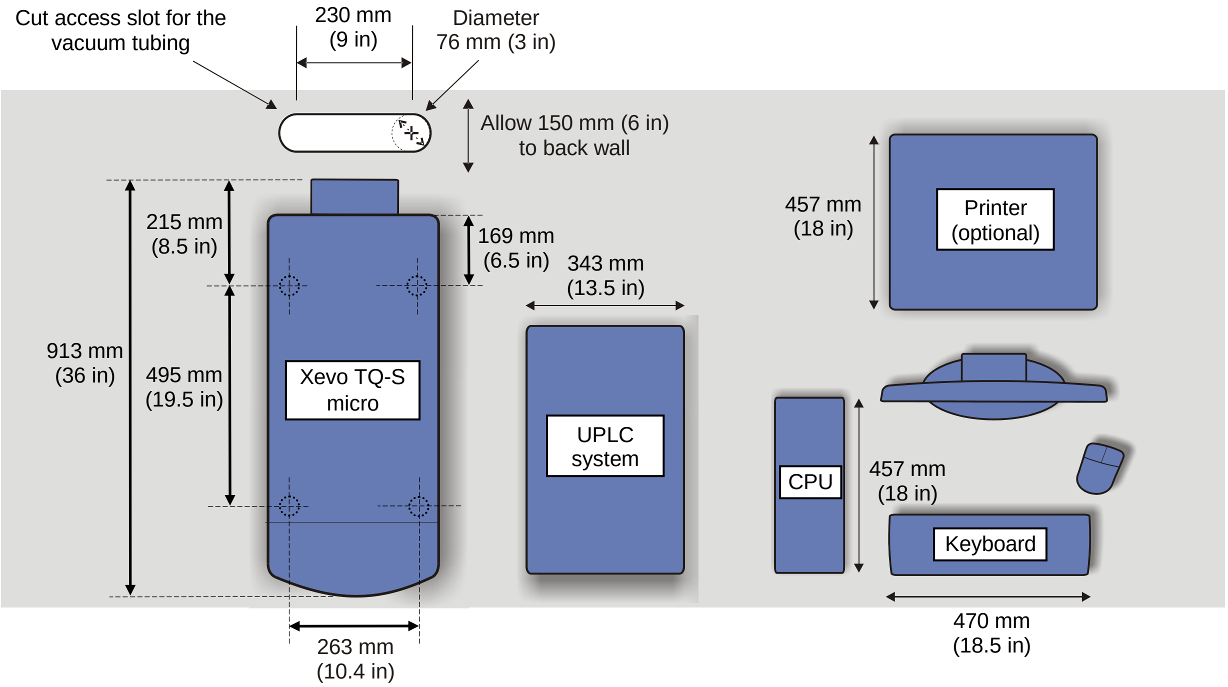

Figure 1 - Plan view, showing space requirements

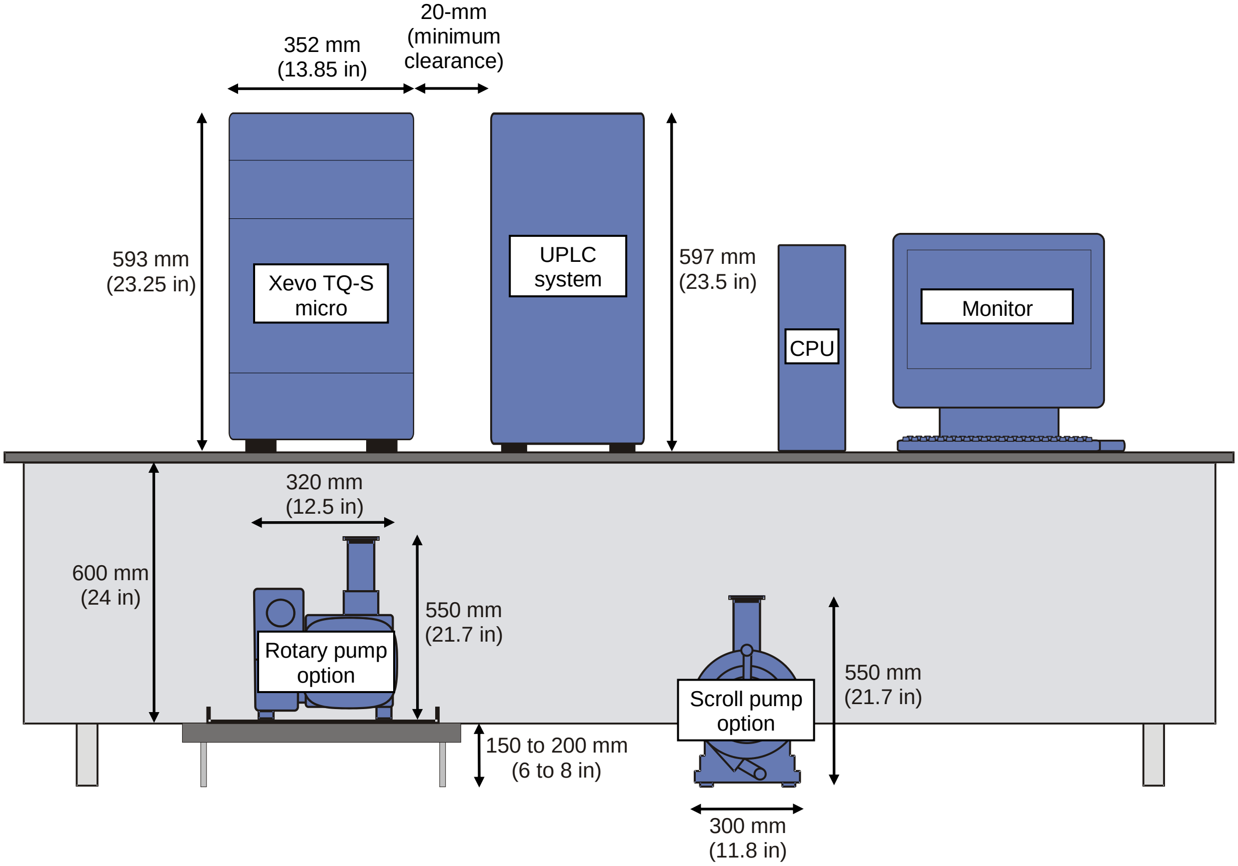

Figure 2 - Front view, showing space requirements

Rotary/scroll pump

The rotary pump or optional scroll pump must be positioned on the floor, either behind or underneath the instrument and within 1 m (3.3 ft) of the rear of the chassis. The pump is supplied with a 2-m (6.5-ft) power cable.

Make sure there is adequate ventilation around the rotary/scroll pump so that the ambient temperature around the pump does not exceed 40 °C.

Allow at least 150-mm clearance for the pump cooling fans.

LC system

Ensure that there is sufficient space to the left of the mass spectrometer for the LC system. Refer to the UPLC or HPLC system site preparation guide for the relevant space requirements.

Data system

The data system can be positioned on the same bench as the mass spectrometer or on a separate desk (available as an option). A 3-m (10-ft) X-wire network cable connects the computer to the mass spectrometer. The two data system power cables for the PC and monitor are approximately 2 m (6.5 ft) in length.

Warning: To avoid damage to and/or risk of electric shock and fire, the data system and any ancillary equipment must not be exposed to dripping or splashing liquids; nor should objects filled with liquid, such as solvent bottles, be placed on them.

Connections INSIGHT® Installation Requirements

Installation of the Waters Connections INSIGHT software (Intelligent Services that provide real-time system monitoring and notification), requires the following:

- An active Internet connection (direct, or through a firewall or proxy server)
- SSL (secure sockets layer) port 443 to be activated

Note: Connections INSIGHT software directly communicates with the Waters Enterprise Server using 128-bit data encryption. For further information see *Connections INSIGHT Frequently Asked Questions* (p/n 720001131EN).

Electrical safety

The Xevo TQ-S micro detector complies with the International Safety Standard IEC 61010-1:2001 and meets the European Low Voltage Directive 2006/95/EC by means of European Harmonized Standard EN 61010-1:2001.

For installations in Australia and New Zealand, the building installation must comply with AS3000: electrical installations for Australia and New Zealand.

The instrument is suitable for use in environments categorized as Pollution Degree 2 and Over-voltage Category II.

Power requirements

The Xevo TQ-S micro detector and rotary/scroll pump require one power socket each. The power supply sockets must be located within 2 m (6.5 ft.) of the instrument. Do not position the equipment so that it is difficult to disconnect the mains cable.

The data system typically requires two power sockets located adjacent to the Xevo TQ-S micro for the instrument PC and monitor. Further outlets may be required for optional equipment, such as a printer. Do not position the equipment so that it is difficult to disconnect the mains cable.

A typical LC system may require three or more additional sockets – refer to the relevant LC documentation for information.

Important: Mains voltage fluctuations must not exceed ±10%.

The power requirements for the equipment are summarized in Table 2.

Table 2: Summary of power requirements

	Nominal rated voltage	**Supply fuse / circuit breaker rating**	**Typical power consumption**	**Power connection**	**Power sockets**	**Power sockets** (with optional UPS)
Xevo TQ-S micro	200 to 240 V, 50/60 Hz	13 to 16 A	900 W	IEC 60320 C20 receptacle	1	1
Data system	100 to 127 V /200 to 240 V, 50/60 Hz	5 to 15 A 2.5 to 16 A	200 W	IEC 60320 C14 receptacles	2	
Scroll pump option						
XDS46i	200 to 230 V, 50/60 Hz	13 to 16 A	350 W	IEC 60320 C20 receptacles	1	
Rotary pump option						
SV40BI	200 to 240 V, 50 Hz	13 to 16 A	1.3 kW	CO16 3	1	
	200 to 240 V, 60 Hz	13 to 16 A	1.6 kW	CO16 3	1	
SV40BIFC	200 to 240 V, 50/60 Hz	13 to 16 A	1.5 kW	CO16 3	1	

Important: Voltage supply stability is critical for instrument operation. The nominal power supply voltage must fall within the ranges specified in Table 2 at all times to allow for the occasional 10% surge.

The supplies must be wired with a protective earth and fused or fitted with circuit-breakers of the specified ratings, in accordance with local regulations.

The mains supply must not have brown-outs/surges greater than ±10%, and must not exceed the specified maximum operating range for more than 0.3 sec. Transient voltage drops to half nominal voltage or less must have a duration of less than 20 ms. There must be less than 1.0 V RMS of ripple on the mains supply.

On pump start-up, currents of up to 36 A (200 to 240 V) or 50 A (115 to 120 V) may be drawn for several seconds, because of the initial pump loading. It is recommended that time delay fuses and circuit-breakers are used to prevent nuisance tripping.

The rotary/scroll pump is normally in continuous operation; it is recommended that the system is installed such that the supply cannot be inadvertently switched off.

It is also recommended that additional protection is provided for the instrument by means of:

- Residual Current Devices (RCD’s) for UK and Europe
- Ground Fault Circuit Interrupters (GFCI’s) for Rest of the World

In the case of instruments fitted with a transformer, the RCD/GFCI must be fitted on the primary (supply) side of the transformer.

Electrical transformers

If there is a possibility that the supply voltages will not meet the specified operating range under all conditions, a transformer must be used to change the primary supply voltage to the specified range. Mains conditioners/stabilizers are also available as an optional accessory. Contact Waters with advance notification if power supply problems are likely to be experienced and for additional advice.

In the case of instruments fitted with a transformer, the RCD/GFCI must be fitted on the primary (supply) side of the transformer.

If your order includes a nitrogen generator and the mains supply is known to run continuously at voltages less than 220 V, Waters and Peak Scientific recommend fitting one of the following transformers between the generator and mains supply.

Caution: Running nitrogen generators continuously at voltages less than 220 V is not recommended and extended periods at these extremes can affect the operation and life of the generator.

Table 3: Nitrogen generator transformer options

Model type	**06-3100**	**06-3110**
View		
Description	208 volt AC to 230 volt AC boost transformer	115 volt AC to 230 volt AC boost transformer

System plug options

The system plug options are shown in Table 4. The instrument is shipped with the plugs that were requested at the point of order. The user must provide appropriate sockets for the relevant type of plug used. If the available sockets are incompatible with the plugs supplied, the customer must supply appropriate cord sets for the instrument and pumps. The cord sets must comply with local regulations.

Computer equipment is typically rated at 100 to 120 V / 220 to 240 V, 50/60 Hz. In some cases, it may be necessary to set the appropriate voltage using a voltage selector switch before connecting the equipment to the power supply. For full details, refer to the instructions provided with the equipment.

Note: If ancillary equipment is to be installed (for example, compressors) additional power outlets, possibly requiring 3-phase supplies, may be needed. Such supplemental needs must be confirmed with the local Waters agent prior to the start of the installation.

Table 4: Power cords supplied by Waters

Plug option	Plug type	System components
US/Canada (125 V) 	5-15P (UL817 and CSA C.22.2)	Data System
US/Canada (250 V) 	L6-15P (UL817 and CSA C.22.2)	Mass Spectrometer Rotary/Scroll Pump Nitrogen Generator
UK 	3-pin (BS1363)	Data System Mass Spectrometer Rotary/Scroll Pump Nitrogen Generator
Europe 	2-pin (CEE7)	
Denmark 	3-pin (Afsnit 107-2-D1)	
Australia 	3-pin (AS/NZS 3112)	
China 	GB2099 (10 A version)	Data System
China 	GB2099 (16 A version)	Mass Spectrometer Rotary/Scroll Pump Nitrogen Generator

Uninterruptible power supply

To prevent instabilities in local mains power impacting system reliability and performance, Waters recommends the use of an uninterruptible power supply (UPS). In support of this recommendation, Waters supplies UPS units that have been specifically configured and evaluated for use with Waters MS systems. Your local Waters field sales representative can provide further details.

These UPS units step up single-phase line voltage to 230 V AC, provide power conditioning and protection for the MS system.

For North America, the UPS system requires one L6-30 (30 amp) wall socket. In other areas, the UPS system will typically connect to your laboratory mains power using the standard MS instrument power cord and wall socket required for your system. See Table 2 and Table 4.

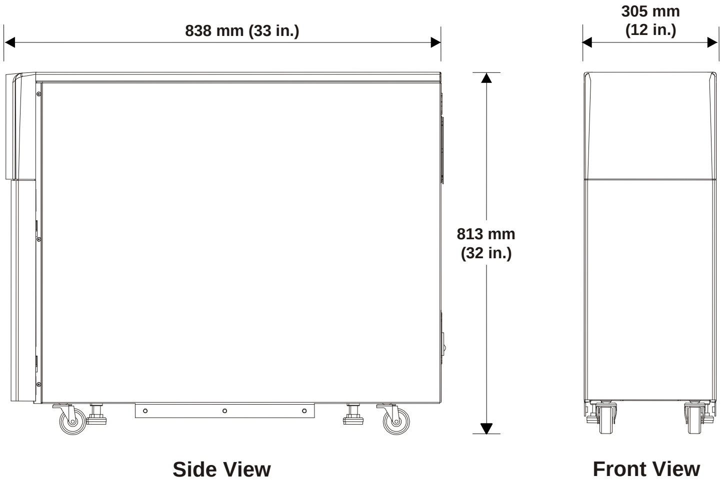

Figure 3 - Approximate maximum dimensions of the UPS

Environment requirements

Safety recommendations

Because of the operation of atmospheric pressure sources, the user must be aware of potential chemical hazards. In particular, the user must assess the risks associated with nitrogen gas (oxygen deficiency) and solvents vented into the laboratory. Note that because of the fluidic nature of the sample inlet, ionization and exhaust system, there is a potential for gas/liquid leaks to occur. The user must give due consideration to the laboratory environment (including volume and air changes) before installation and during operation of the system.

Warning: The active exhaust vent must provide a minimum vacuum of 2 millibar below atmospheric pressure (negative pressure). It must be capable of supporting a maximum instrument exhaust gas load of 2500 L/hour.

Warning: Exhaust venting must comply with all local safety and environmental regulations. The ANSI/AIHA Z9.2-2001 standard for “Fundamentals governing the design and operation of local exhaust ventilation systems” provides guidance on compliant exhaust systems.

Positioning

It is recommended that the instrument is installed in an air conditioned laboratory, in a draft-free position, away from excessive amounts of dust. Air conditioning units must not be positioned directly above the mass spectrometer. To avoid adverse operation, do not locate the instrument in direct sunlight.

Ventilation

The maximum overall heat dissipation into the room from the instrument and pumps is approximately 2.7 kW. This figure does not take into account the data system or other ancillary equipment such as LC systems. Air conditioning systems may have to be installed or upgraded to accommodate additional heat load into the room when these systems are installed.

Temperature

The ambient temperature range required for normal operation is 15 to 28 °C (59 to 82 °F).

Short-term (1.5 h) variations must be no more than 2 °C (3.5 °F).

Humidity

The relative humidity in which the instrument and pumps are to operate must be in the range of 20% to 80%, non-condensing.

Altitude

The instrument is designed and tested to operate below 2000 m (6500 ft).

Vibration

The instrument must not be placed close to heavy machinery such as compressors and generators, which may generate excessive floor vibration.

Magnetic fields

The instrument must be positioned away from magnetic fields of greater than 10 Gauss, such as those generated by NMR spectrometers and magnetic sector mass spectrometers.

Radio emissions

The instrument must not be placed within a Radio Frequency (RF) field of greater than 1.0 V/m.

Possible sources of RF emission include RF-linked alarm systems, Local Area Networks (LANs), mobile telephones, and hand-held transmitters.

Gases and regulators

Nitrogen gas

Caution: Where the APGC source is ordered, nitrogen purity must be >99.999%.

Refer to the *APGC Site Preparation Guide* (p/n 715002164) for specific external nitrogen gas supply and connection requirements.

The Xevo TQ-S micro requires a supply of dry, oil-free nitrogen with a purity of at least 95%. The nitrogen must be regulated at 6.75 ±0.25 bar (98 ±4 psi) outlet pressure, using a two-stage gas regulator with an appropriate outlet range, for example, 0 to 8 bar (0 to 116 psi).

Important: It is the customer's responsibility to provide a two-stage regulator fitted with an adapter to connect to a 6-mm push-in fitting, see Table 5.

Caution: The nitrogen must be connected using the 5-m (16 ft.) of 6-mm OD Teflon tubing supplied. Do not cut the tubing to size. The nitrogen line must be checked for leaks under pressure.

If copper tubing is used for the nitrogen line, the copper must be chemically cleaned; if stainless steel tubing is used, the stainless steel must be medical grade. Ensure that there are no soldered or brazed joints in the line, as these may result in contamination of the instrument with tin or lead oxide. Any joints in the nitrogen line must be compression fittings.

During API operation, typical nitrogen usage varies from 600 to 1200 L/h (at atmospheric pressure). This equates approximately to the consumption of a large cylinder of compressed nitrogen each day. You may prefer to use a liquid nitrogen Dewar, which will last for several weeks, consult your local gas supplier for an ideal gas supply configuration.

Note: The use of nitrogen cylinders is not recommended. Because of high consumption, a cylinder is likely to empty during long sample runs. The supply must be constant in case venting occurs.

Collision gas

Argon is required for the collision cell. The argon must be dry, high purity (99.997%), and regulated at a pressure of 0.5 ±0.1 bar (7 ±2 psi), using a two-stage high purity gas regulator with an appropriate outlet range, for example, 0 to 2 bar (0 to 29 psi).

Important: It is the customer's responsibility to provide a two-stage regulator fitted with an adapter to connect to a $^1/_8$-inch Swagelok type fitting, see Table 5.

Caution: Ensure that there are no soldered or brazed joints in the argon line, as these may result in contamination of the instrument with tin or lead oxide. Any joints in the collision gas line must be compression fittings.

The gas supply must be connected using the clean, $^1/_8$-inch OD, medical-grade stainless steel tubing supplied and checked for leaks under pressure.

Exhaust outlets

Rotary/scroll pump exhaust

The rotary/scroll pump exhaust gases must be vented to the atmosphere outside the laboratory via a user-supplied fume hood or industrial vent. The exhaust may be connected to an existing laboratory vent carrying gases from other sources.

Five meters (16 ft) of 12-mm ID PVC tubing is supplied. If this length is insufficient, the user must supply an adapter and tubing with an internal diameter of at least 51 mm (2 inch) for the extra distance to the vent point.

Note: The fume hood/industrial vent must be equipped with an extraction fan system to enable adequate displacement of the exhaust gases.

Source exhaust (nitrogen)

The source exhaust line must be connected to either a laboratory fume hood or to an active exhaust system.

Refer to the exhaust warnings in the Environment requirements section on page 15 for additional source exhaust information.

Caution: Severe contamination of the instrument may result if the source exhaust line is connected to the rotary pump exhaust line. The damage will occur when the nitrogen supply is turned off, or when the nitrogen runs out, as any rotary pump oil vapor will migrate via the source exhaust to the ion source and then through the sample cone into the analyzer.

Five meters (16 ft) of 12-mm OD Teflon tubing is supplied for the source exhaust. If this length is insufficient, the user must supply an adapter and tubing with an ID of at least 16 mm (⅝ inch) for the extra distance to the vent point.

The instrument software can be configured to switch the LC system off if it detects that the nitrogen gas supply has failed. In the event that the nitrogen gas is switched off (or runs out) and the LC system continues to operate, excess solvent is drained from the source via the source exhaust line.

Solvent delivery system

The instrument includes an ACQUITY ever-flow valve and syringe drive for infusion. A gas-tight, 250-µL syringe, with a flow rate range of 5 to 200 µL/min is included.

For ESI / ESCI / APCI, a UPLC / HPLC pump giving a stable, pulse-free flow of 50 to 2000 µL/min is required.

Before returning the checklist at the end of this document, please ensure that any locally supplied solvent delivery system has either already been commissioned or that a commissioning date has been scheduled.

Note: If a solvent delivery system suitable for running performance specifications will not be available at the time of installation (for example, in the case of instruments supplied with an ACQUITY M-Class) inform the local Waters service agent so that special arrangements can be made.

Test samples

Warning: Hazardous samples must be handled with care and in a manner that conforms to the manufacturers' guidelines.

Test samples are required for verifying the performance of instruments at the time of installation; they are also used for routine operations such as tuning and mass calibration.

Note: A Test Sample Kit is supplied with the instrument for the installation setup. It is the customer's responsibility, in conjunction with the local Waters sales representative, to ensure that any additional samples required for customer-specific tests and post-installation testing are available.

Note: The Waters engineer will not carry test samples to the installation. If the Waters engineer is unable to complete the installation because of a lack of facilities, costs incurred will be charged. The installation will be rescheduled when the chemicals are available.

Important: Storage instructions provided with the test samples must be adhered to; the use of inferior quality test chemicals caused by adverse storage conditions could impair the instrument installation.

Note: If your laboratory practices require full sample certification documentation, Waters Analytical Standards and Reagents provide ready-to-use reference materials and reagents that are fully traceable and certified (www.waters.com).

Solvents and reagents

Caution: Clean, high-purity solvents and reagents and clean glassware must be used to ensure the optimum performance of the LC-MS system. Significant delays to the installation may occur if clean solvents and glassware are not provided by the customer prior to commencing the installation.

High-purity solvents (i.e. LC-MS grade) are required, as shown in the following list; these are used for making up standard solutions for performance tests and for cleaning instrument components. For detail on controlling contamination, and information on solvent brands, refer to *Controlling Contamination in Ultra Performance LC™/MS and HPLC/MS Systems* (p/n 715001307), located in the Support area of the Waters website (www.waters.com).

- Water
- Acetonitrile
- Methanol
- Formic acid

Caution: If using a water purification system, maintain it regularly in accordance with the manufacturer's guidelines.

Sample preparation equipment

Facilities for making up test samples must be available at site. Typical equipment required for sample preparation includes (but is not limited to):

- Calibrated syringes - Eppendorf (or equivalent), spanning range 1 µL to 1 mL
- Measuring cylinders, spanning range 100 mL to 1 L
- Volumetric flasks - 10-mL flasks (up to 11 required); 50-mL flasks (up to 7 required)
- Calibrated analytical balance
- Nitrile gloves
- Lint-free tissue

Cleaning test sample glassware

For detailed information on properly cleaning glassware or other components, refer to *Controlling Contamination in Ultra Performance LC®/MS and HPLC/MS Systems* (p/n 715001307), located in the Support area of the Waters website (www.waters.com).

Cleaning equipment

An ultrasonic bath is required for the routine cleaning of instrument parts. The bath must be at least 300 mm x 150 mm x 100 mm deep (12 inch x 6 inch x 4 inch).

Caution: Surfactants must not be used for cleaning glassware or other components. Refer to the document *Controlling Contamination in Ultra Performance LC®/MS and HPLC/MS Systems* (p/n 715001307), located in the Support area of the Waters website (www.waters.com).

Surfactant-free glass vessels are required in which to place instrument components for cleaning. These vessels must be made available for use at the time of installation. The vessels must have a diameter of at least 120 mm (5 inch) and be approximately 120 mm (5 inch) high.

Summary of fittings

Table 5 shows a summary of the waste and gas connections for the installation of the Xevo TQ-S micro.

Table 5: Summary of instrument fittings required

	Fittings on the system	**Items supplied with the instrument**	**Items to be supplied by the customer**
Rotary/scroll pump exhaust	12-mm OD tail pipe	5-m (16-ft) PVC tube, 12-mm ID	Industrial vent or fume hood
Source exhaust (nitrogen)	12-mm push-in fitting	6-m (19.6-ft) Teflon tube, 12-mm OD	Industrial vent or fume hood
Liquid waste	0.375 x 0.25 ID one-touch fitting	2-m (6.5-ft), Tygon tubing	Waste bottle, 1 L (minimum)
Nitrogen supply (API)	6-mm push-in fitting	5-m (16-ft) Teflon tube, 6-mm OD	Nitrogen supply, regulated to 6.75 ±0.25 bar (98 ±4 psi) via a 6-mm adapter
Collision gas supply	$^{1}/_{8}$-inch fitting (Swagelok type)	3-m (10-ft) of $^{1}/_{8}$-inch OD stainless steel tubing	Argon supply, regulated to 0.5 ±0.1 bar (7 ±2 psi), via a $^{1}/_{8}$-inch adapter (Swagelok recommended)
ACQUITY Ever-Flow valve	Rheodyne nuts and ferrules	Tubing and Rheodyne nuts and ferrules	Tubing and Rheodyne nuts and ferrules

Xevo TQ-S micro site preparation checklist

This checklist must be completed and returned to Waters when all the amenities are available.

Note: If any items are on order, please indicate this on the checklist and include the anticipated arrival date.

Note: It is the customer's responsibility to ensure that all the correct laboratory supplies are present. If you need any additional information or have difficulties acquiring parts or samples, please contact your local Waters Sales representative.

Access (see page 5)
The instrument is located on the ground floor/basement/___ floor (delete as appropriate) .... ☐

All elevators, staircases, corridors and doorways through which the instrument must pass are adequate to allow easy access to the laboratory .... ☐

Lifting equipment (see page 6)
Suitable equipment is available to lift the instrument onto the laboratory bench .... ☐

Bench/floor space (see page 7)
Adequate bench or floor space is available for the system .... ☐

Connections INSIGHT® installation requirements (see page 9)
If you are planning to install Waters Connections INSIGHT software, an Internet connection is available .... ☐

Power supply (see page 10)
An appropriate number of sockets with earth connections are available and they meet the stipulated power requirements .... ☐

Positioning/ventilation (see page 15)
There is no direct air conditioning flow onto the instrument .... ☐

Temperature (see page 15)
The room temperature is as specified in this document .... ☐

Humidity (see page 15)
The humidity is as specified in this document .... ☐

Altitude (see page 15)
The instrument will be operated below 2000 m (6500 ft) .... ☐

Floor vibration (see page 16)
The site is free from known vibration .... ☐

Magnetic fields (see page 16)
The site is free from magnetic fields of greater than 10 Gauss .... ☐

Radio emissions (see page 16)
The RF field strength is less than 1 V/m .... ☐

Gases and regulators (see page 16)

Dry, oil-free, ≥95% purity nitrogen gas is available, regulated at 6.75 ±0.25 bar (98 ±4 psi) with a 6-mm adapter .... ☐

High purity ≥99.999% nitrogen gas is available when APGC source is supplied .... ☐

High purity ≥99.997% argon gas is available, regulated at 0.5 ±0.1 bar (7 ±2 psi) with a $^{1}/_{8}$-inch adapter .... ☐

Rotary/scroll pump exhaust (see page 17)

A suitable outlet is available for the rotary/scroll pump exhaust .... ☐

Source exhaust (see page 17)

A separate exhaust, 2 mbar below atmospheric pressure is available .... ☐

Solvent delivery system (see page 18)

Make and model of system to be used:

Make ______________________________

Model ______________________________

Flow rate capability of the system ______________________

Delivery system is already on site and commissioned .... ☐

or

Delivery system is scheduled to be commissioned on: ______________________________

A second (customer-supplied) syringe pump is available .... ☐

Ancillary equipment

If you plan to use any other equipment with the system (e.g. Gilson Autosampler; UV Detector), please give details below.

Make / type	**Model**	**Already commissioned**	**To be commissioned on**

Test samples (see page 18)
All samples required for the installation are available .... ☐

Solvents/reagents (see page 19)
Solvents are available .... ☐

Sample preparation equipment (see page 19)
Sample preparation equipment, as specified in this document, is available .... ☐

Cleaning (see page 20)
An ultrasonic bath is available .... ☐

Vessels for cleaning components are available .... ☐

I confirm all supplies are now available and all specified environmental conditions have been met*.

During the installation, the user intends to be available for demonstration and training by the Waters engineer:

At all times .... ☐

Approximately _______% of the time .... ☐

Not at all .... ☐

During the likely period of installation, the following dates are NOT convenient:

____

Signed: ____

***Important:** If an authorized Waters service engineer arrives on site to begin installation work and can not complete the installation because of lack of facilities (i.e. lifting equipment, power, water, test samples, laboratory readiness), costs incurred will be charged to the customer.

Please complete the following sections in block letters:

Name ____

Position ____

Organization ____

Street ____

City ____

ZIP/postcode ____

Country ____

Telephone ____

Fax ____

E Mail ____

Important: The installation of your system cannot begin until pages 21 through 26 of this document have been fully completed and returned to the Mass Spectrometer Sales Support Representative at your local Waters office.

Applications survey

As part of our commitment to provide greater customer service, we have found it necessary to obtain a little more information concerning our user base.

We would be grateful if you could take the time to complete the following questions to provide us with some information about how the instrument will be used.

This information will enable us to inform you of relevant current application notes and seminars and allows us to identify common interest groups so that we can promote cross transfer of information between customers.

What is your scientific field?
(e.g. pharmaceutical, environmental, general, etc.)

____

____

Which classes of compounds will be analyzed?
(e.g. carbohydrate, peptides, pesticides, etc.)

____

____

What is your application area?
(e.g. quantitation, purity analysis, structural determination, etc.)

____

____

Our sales team often requires reference sites for specific applications.
Would you be willing to be used as a contact reference site for prospective customers?

____

____

[INSTRUMENT SPECIFICATIONS]

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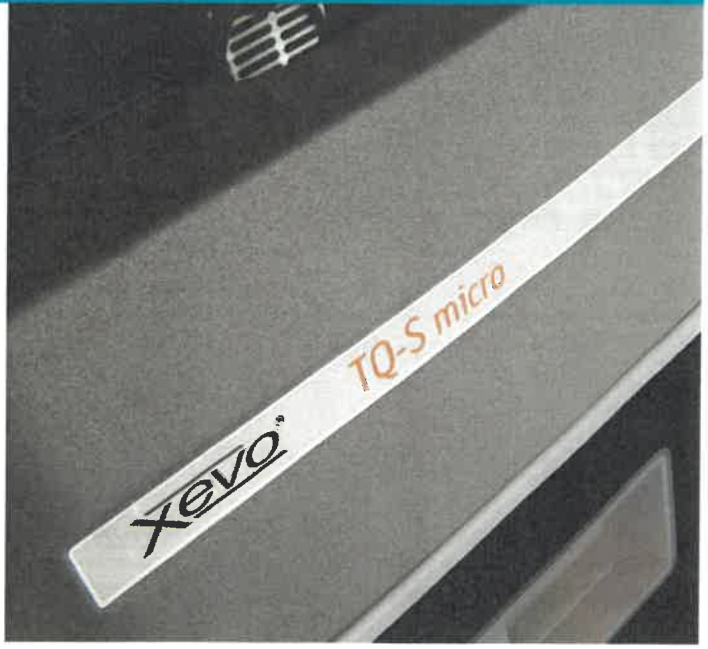

Xevo TQ-S micro

Xevo® TQ-S micro is a sensitive but compact tandem quadrupole mass spectrometer featuring reliable performance with a wide dynamic range and high rates of data acquisition. Robust sensitivity is enabled by proven ZSpray™ and StepWave™ which facilitate the detection of analytes at low concentrations in complex matrices and enable low volume injections with accurate, precise, and consistent results. Xtended Dynamic Range™ (XDR) technology provides accessible sensitivity and method transfer. The Xevo TQ-S micro makes it easier to confidently quantify more analytes using reproducible high acquisition rates with Xcelerated Ion Transfer™ (XIT). Using RADAR,™ which enables rapid switching between MS full scan and MS/MS acquisition modes, analysts can understand sample complexity and improve method development.

SYSTEM HARDWARE SPECIFICATIONS

API sources and ionization modes	High performance ZSpray dual-orthogonal API sources: 1) Multi mode source – ESI/APCI/ESCi® (standard) NB - Dedicated APCI requires an additional probe (optional) 2) APCI IonSABRE II probe (optional) 3) Dual mode APPI/APCI source (optional) 4) nanoFlow™ ESI source (optional) 5) ASAP (optional) 6) APGC ion source (optional) 7) ionKey/MS™ source (optional) Optimized gas flow dynamics for efficient ESI deslovation (supporting LC flow rates up to 2 mL/min) Tool-free source exchange Vacuum isolation valve Tool free access to customer serviceable elements Plug and play probes De-clustering cone gas Software control of gas flows and heating elements
Ion source transfer optics	StepWave ion transfer optics (Waters patent pending) delivering class leading UPLC®/MS/MS sensitivity. The unique off-axis design dramatically increases the efficiency of ion transfer from the ion source to the quadrupole MS analyzer at the same time as actively eliminating undesirable neutral contaminants.
Mass analyzer	Two high resolution, high stability quadrupole analyzers (MS1/MS2), plus pre-filters to maximize resolution and transmission while preventing contamination of the main analyzers

Collision cell	T-Wave™ enabled for optimal MS/MS performance at high data acquisition rates
Detector	Low noise, off axis, long life photomultiplier detector
Vacuum system	One split-flow air-cooled vacuum turbomolecular pump evacuating the source and analyzer; One vacuum backing pump
Dimensions	Width: 35.6 cm (14.0 in) Height: 60.0 cm (23.6 in) Depth: 93 cm (36.6 in)
Regulatory approvals/marks	CE, CB, NRTL (CAN/US), RCM

SYSTEM SOFTWARE SPECIFICATIONS

Software	Systems supported on MassLynx® version 4.1; OpenLynx™ and TargetLynx™ XS Application Managers are included as standard
IntelliStart™ Technology	System parameter checking and alerts Integrated sample/calibrant delivery system + programmable divert valve Automated mass calibration Automated sample tuning Automated SIR and MRM method development LC-MS System Check – automated on-column performance test
Quantification methods database	Quanpedia™ – a database for storing and sharing user defined LC/MRM acquisition methods and associated processing methods for the targeted quantification of named compounds is provided as standard; database entries for a number of applications are also provided as a standard
Automated MRM scheduling (acquisition rate assignment)	Dwell time, inter-channel delay time, and inter-scan delay time for individual channels in a multiple MRM experiment can be automatically assigned (using the Auto-Dwell feature) to ensure that the optimal number of MRM data points per chromatographic peak is acquired. The Auto-Dwell feature can dynamically optimize MRM cycle times to accommodate retention time windows that either partially or completely overlap. This greatly simplifies MRM method creation, irrespective of the number of compounds in a single assay, while at the same time ensuring the very best quantitative performance for every experiment
Automated MRM scheduling (acquisition rate assignment)	Multiple MRM experiments can be scheduled (manually or automatically using the database) using retention time windows to optimize the cycle time for each MRM channel monitored. If required, MRM retention time windows can overlap partially or completely. This ensures that MRM data acquisition rates will be optimal for the quantification of all analytes in a given assay

PERFORMANCE SPECIFICATIONS

Acquisition modes	Full scan MS Product ion scan Precursor ion scan Constant neutral loss Selected ion recording (SIR) Multiple reaction monitoring (MRM) Simultaneous full scan and MRM (RADAR)
Survey scan modes	Full scan MS triggered product ion scan Precursor ion scan triggered product ion scan Constant neutral loss triggered product ion scan
Product ion confirmation (PIC) mode	MRM acquisition acts as an automatic trigger for the acquisition of product ion spectra
RADAR	An information rich acquisition approach that allows you to collect highly specific quantitative data for target compounds while providing the ability to visualize all other components
Mass range	2 to 2048 *m/z*
Scan speed	Up to 20,000 Da/s Examples of achievable acquisition rates: 20 scans per second (*m/z* 50 to 1000) 40 scans per second (*m/z* 50 to 500)
Mass stability	Mass drift is <0.1 Da over a 24 hour period
Linearity of response	The linearity of response relative to sample concentration, for a specified compound, is six orders of magnitude from the limit of detection
Polarity switching time	15 ms to switch between positive and negative ion modes
MS to MS/MS switching time	3 ms
ESCi mode switching time	20 ms to switch between ESI and APCI
MRM acquisition rate	Maximum acquisition rate of 500 MRM data points per second; Minimum dwell time of 1 ms per MRM channel; Minimum inter-channel delay of 1 ms; At an MRM acquisition rate of 500 MRM data points per second there is no more than 20% loss in signal compared to 50 MRM data points per second
Inter-Channel cross talk	The inter-Channel cross talk between two MRM transitions will be less than 0.001% (less than 10 ppm)
Number of MRM channels	Up to 32,768 MRM channels (1024 functions, 32 channels per function) can be monitored in a single acquisition; up to 1,024 MRM channels when operating in GLP/secure mode (32 functions, 32 channels per function)
Mass resolution	Automatically adjusted (IntelliStart) to desired resolution; (0.50 Da, 0.75 Da or 1.00 Da FWHM)

MRM sensitivity (ESI+)	A 1 pg on-column injection of reserpine will give a chromatographic signal-to-noise greater than 200,000:1, using raw unsmoothed data (LC mobile phase flow rate of 0.4 mL/min, MRM transition 609 >195 *m/z*)
MRM sensitivity (ESI-)	A 1 pg on-column injection of Chloramphenicol will give a chromatographic signal-to-noise greater than 100,000:1, using raw unsmoothed data (LC mobile phase flow rate of 0.8 mL/min, MRM transition 321 >152 *m/z*)
MRM sensitivity (APCI+)	A 1 pg on-column injection of 17-α-hydroxyprogesterone will give a chromatographic signal-to-noise greater than 30:1, using raw unsmoothed data (LC mobile phase flow rate of 0.8 mL/min, MRM transition 331 >109 *m/z*)

It should be noted that the above are not standard installation specifications. All Xevo TQ-S micro instruments will be installed and tested in accordance with standard performance tests as detailed in Waters document (Xevo TQ-S micro Installation Checklist). Test criteria are routinely reviewed to ensure quality is maintained and are therefore subject to change without notice. See Site Preparation Guide and Product Release Notes for additional product and specification information.

Related patents:

1. ZSpray (US Patent 5,756,994).
2. StepWave (US Patent 8,581,181 and US Patent 8,581,182).

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