

A close-up photograph of several golden wheat stalks, showing the intricate texture of the grain heads and the long, thin awns. The stalks are arranged diagonally across the frame, creating a sense of depth and movement. The lighting is warm, highlighting the natural colors of the wheat.

**ACCOMPLISH
MORE IN AN
INCREASINGLY
DEMANDING
INDUSTRY
LANDSCAPE**

Waters
THE SCIENCE OF WHAT'S POSSIBLE.®

Growing demand, growing pressure

Driven by the need to ensure a secure and sustainable global food supply, the agrochemicals industry is striving to improve productivity from arable lands and to increase efficient use of water resources.

As the global population grows, so does demand for new crop protection products that deliver greater effectiveness and lower environmental impact.





As an agrochemical producer, you face a mounting array of challenges in your efforts to meet growing demand:

- Regulatory testing and documentation requirements are increasing as governments exercise greater oversight of chemical use.
- Businesses and consumers alike are demanding more environmentally friendly chemicals.
- A growing generics market is putting downward pressure on pricing.
- You need to innovate and differentiate your products to better meet evolving market needs.

The costs incurred to address these challenges are considerable. The discovery and development process is long, costly, and resource-intensive. The data generation process necessary for product registration has created long backlogs at many laboratories. The drive for new, innovative products often results in more complex formulations that are more difficult to analyze and test, adding more time, effort, and costs to the process.

As you work to strengthen your position in this competitive marketplace, Waters provides analytical solutions that can make a direct, positive impact on your business, delivering value every step of the way:



Synthetic Chemistry

Purification

Formulation

Trace Detection

Metabolite ID

SYNTHETIC CHEMISTRY

Synthesis is at the heart of agrochemical discovery and development. In the search for new chemicals that have specific activity, an important goal is speed – achieving swift and efficient synthesis of candidate molecules for screening. Translated to analytical requirements, that means both high chromatographic resolution and high throughput for routine analysis – to reveal more in each sample with minimal effort and maximum consistency. Waters supports these needs with several key solutions.

Faster Sample Turnaround and Lower Costs For Liquid Chromatography Separations

ACQUITY UPLC H-Class System

Waters® ACQUITY UPLC® H-Class System offers the flexibility of a quaternary-based HPLC with the performance advantages of UPLC® – this means greater sample throughput, reduced cost per analysis, and better quality results for agrochemical laboratories that use traditional HPLC.

KEY FEATURES/BENEFITS

- Enable more rapid decision making with runtimes that are up to 10 times faster.
- Seamlessly transition existing HPLC methods to UPLC.
- Better resolve known components and discover unknown components with superior chromatographic resolution.
- Decrease solvent consumption by up to 95% for reduced costs and environmental impact.
- Increase laboratory productivity with significantly reduced method development times.
- Designed for UPLC systems, Waters Fraction Manager (WFM -A) minimizes fraction loss and carryover during purification.



ACQUITY UPLC H-Class System.



Waters Fraction Manager (WFM-A).

The Most Accessible, Affordable, and Usable Mass Detector

ACQUITY QDa Detector

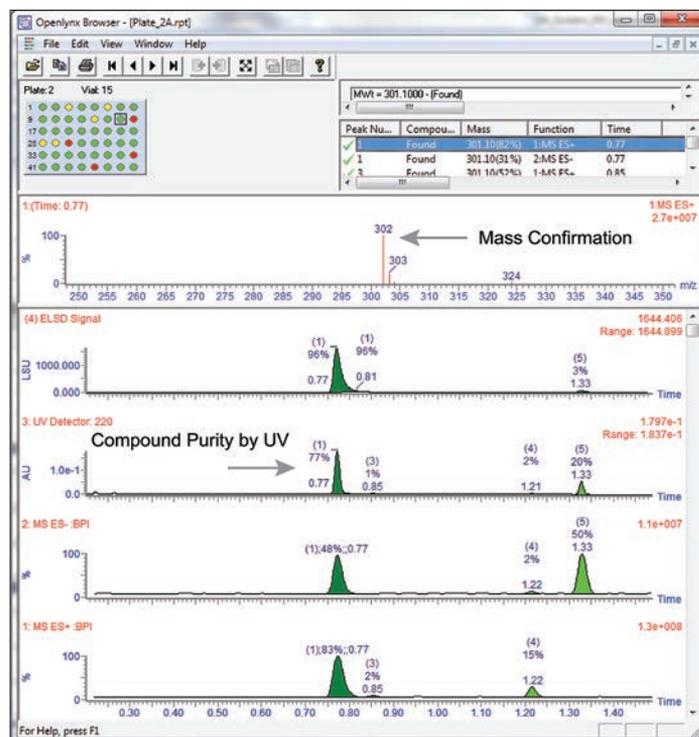
A mass detector for LC laboratories performing routine screening to confirm components, the ACQUITY® QDa® Detector offers a fast and easy solution that works within existing workflows. It is pre-optimized to work with your samples, without sample-specific or user adjustments typical of traditional mass spectrometers.

KEY FEATURES/BENEFITS

- Quantify compounds with no UV response at levels not amenable to or accessible by optical detection – broaden the scope of your sample analyses.
- As intuitive as an optical detector with the robustness to handle a wide range of analyses.
- Any scientist can generate the highest quality mass spectral data routinely and consistently – no special training or expertise required.
- Save space with the only mass detector that integrates with and fits on top of your instrument stack.
- Compatibility with Waters ACQUITY UPLC, ACQUITY UPC²®, Alliance® HPLC, and purification LC and SFC systems provides access to MS detection for all separation scientists.
- Full compatibility with Empower® Chromatography Software and MassLynx® Mass Spectrometry Software allows users to leverage the market leading platforms.
- Combines with OpenLynx™ Open Access Software to streamline workflow for the rapid separation and identification of reaction products from chemical synthesis.



ACQUITY QDa Detector.



OpenLynx Application Manager browser showing detection using evaporative light scattering detection (ELSD), UV for purity estimation, and electrospray positive and negative detection with ACQUITY QDa for mass confirmation.

PURIFICATION

Purification is an essential task in agrochemical R&D processes, including the isolation of high purity active ingredients from synthetic chemistry as well as significant impurities and reaction by-products that must be characterized for regulatory submissions or are needed in larger scale for further studies. Organizations must employ analytical separation technologies that can be predictively scaled up to yield the required quantity and purity of target compounds (actives and/or impurities) rapidly and cost effectively.

Mass Directed Purification

By applying mass spectrometry to purification, laboratories can streamline what is often a lengthy and cumbersome process. Mass-directed purification minimizes user intervention between isolation steps, lowering cost and saving time by collecting only specific target compounds, thereby reducing the number of fractions requiring analysis and handling.



*AutoPurification HPLC/MS System
with ACQUITY QDa Detector.*

Purification Without Complexity

AutoPurification System with ACQUITY QDa

The AutoPurification™ HPLC/MS System makes mass-directed purification more readily accessible to chromatographers. This solution provides flexible automated compound isolation options that simplify the purification workflow and increase process efficiency by empowering scientists to perform other tasks.

Supercritical Fluid Chromatography

Supercritical Fluid Chromatography (SFC) can lower the cost of purification further by reducing the use of expensive organic solvents and ensuring easier recovery of purified samples. When used for achiral compound purifications traditionally performed by reverse phase methods, orthogonal selectivity and significantly reduced dry down times are two key benefits. For larger scale chiral compound purification, SFC enables faster normal phase based separations for more challenging compounds, in addition to being the technique of choice for chiral purification.

Optimal Solutions to Meet Your Purification Needs

SFC 80/200/350 Preparative Systems

Waters' bulk-scale SFC purification systems build on the performance advantages of SFC by automating the preparative process. They feature co-solvent gradient, high-pressure separators for quantitative recovery of purified products, such as enantiomers, complex synthetic chemicals, and natural products.

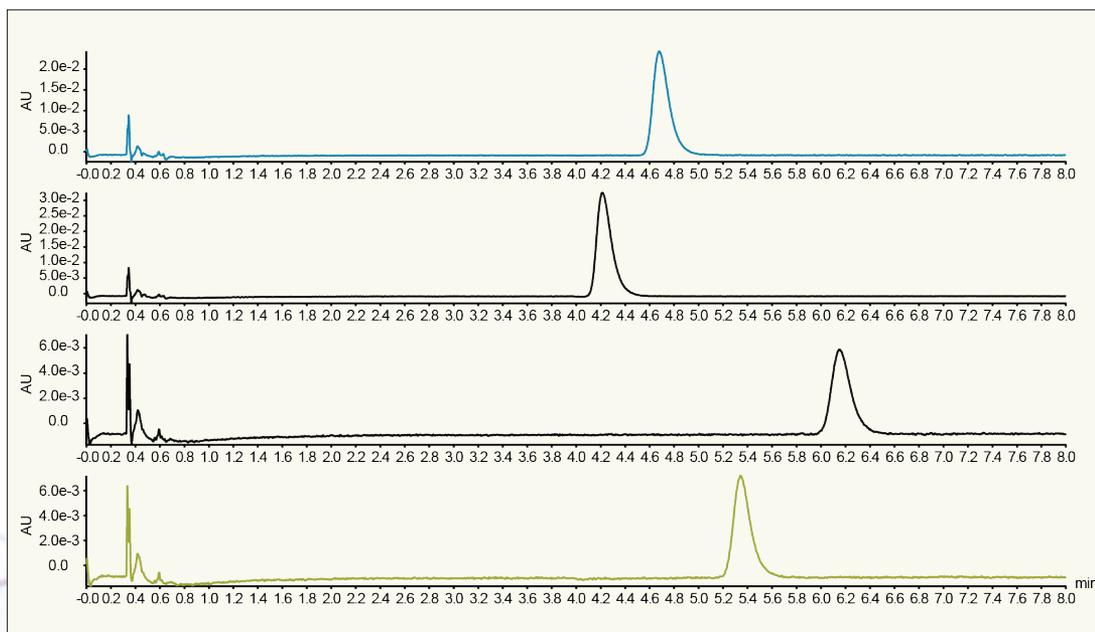


Prep 350
SFC System.

Increase Productivity, Reduce Costs

Prep 100q SFC System

The Waters Prep 100q SFC System provides high-throughput, preparative scale purification with PDA and/or MS directed purification, to meet the increased demand for higher productivity, greater flexibility, and lower costs per sample.



Preparative SFC was used to efficiently isolate trace impurities in a commercial formulation of the fungicide propiconazole (contains isomers and trace impurities at ~1% level) in sufficient amounts for structural elucidation and other studies. UPC² chiral analysis of four collected impurities from the Prep 100q SFC System with chiral prep columns demonstrated that each isomer had an enantiomeric excess (e.e.) >98%.

FORMULATION



Achieving the optimum formulation is essential to any crop protection product, and may provide a clear competitive advantage. The best pesticide formulations deliver a highly specific action with reduced application rates, are cost effective, and maintain stability during storage and transport. As a manufacturer, you must quickly determine which isomers are delivering the desired action by assessing the enantiomeric purity of chiral active ingredients, and for product registration purposes, specify and quantitate all other non-active components in the formulation.

Formulation imposes a demanding analytical workload, spanning everything from the characterization of raw materials, such as actives, additives, and surfactants, to the composition and stability of the formulated product. If you can shorten that process, you can ensure that your new product reaches the market – and makes a positive impact on your business performance – that much sooner.

Increased Confidence in Chiral Analysis

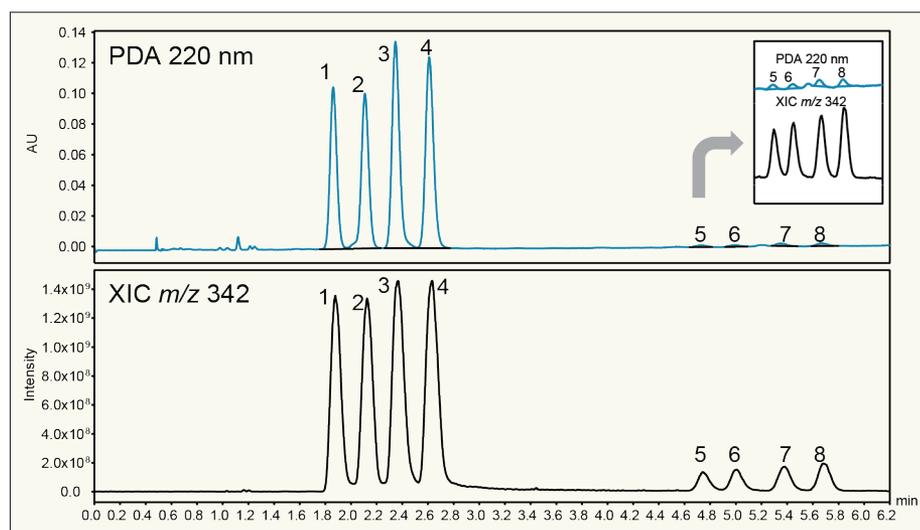
ACQUITY UPC² System

UltraPerformance Convergence Chromatography™ (UPC²) is a new category of separation science that combines the performance advantages of Waters' UPLC Technology with SFC – delivering faster separations and superior resolution for chiral and achiral applications.

KEY FEATURES/BENEFITS

- Utilizes supercritical carbon dioxide (CO₂) as the primary mobile phase to provide a more cost-effective and greener technology by lowering the use of organic solvents.
- Streamline sample preparation workflow dramatically by eliminating lengthy evaporation and reconstitution steps.

- Precisely vary mobile phase strength, pressure, and temperature to fine-tune resolving power and selectivity – exercise better control over the retention of analytes for analyzing structural analogs, isomers, and enantiomeric and diastereomeric mixtures.
- Enhance compound detection and identification by combining with the ACQUITY QDa Detector to generate fast and reliable mass spectral data within the existing chromatography workflow.
- An effective separations solution for a variety of agrochemical applications including formulation and synthetic chemistry.



ACQUITY UPC² UV chromatogram at 220 nm showing the chiral resolution of propiconazole stereoisomers and unknown chiral components in the formulation sample using the ACQUITY UPC² Trefoil AMY1 Column. Extracted ion chromatogram at m/z 342 is also shown.

TRACE DETECTION

Many of the registration requirements of new agrochemical products relate to understanding environmental fate, transport, and toxicity. Trace-level analysis in complex biological and environmental matrices is key to supporting both pre- and post-product registration activities.

High Performance MS/MS from a Compact Design

Xevo TQ-S micro

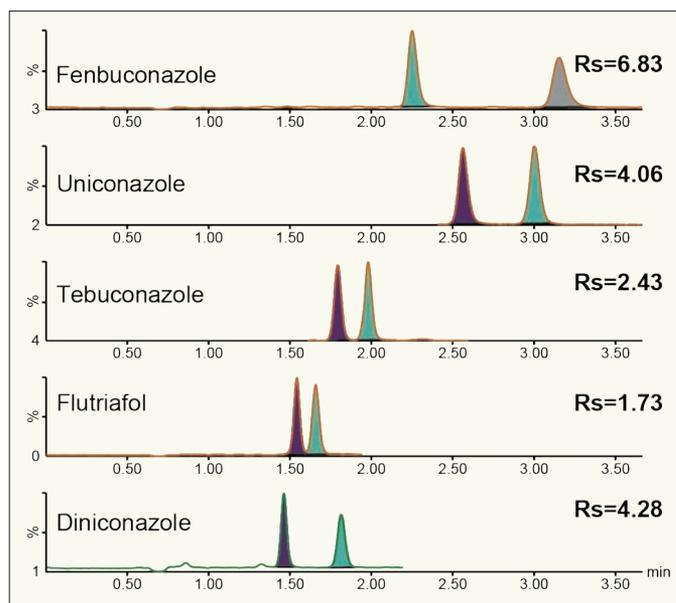
A tandem quadrupole instrument with a small footprint, this system delivers low levels of quantitation with a wide dynamic range. Designed to acquire sensitive, robust, and dependable data at accelerated rates of acquisition, the Xevo® TQ-S micro is able to reproduce high quality analytical performance injection after injection, even with the most complex sample matrices.

KEY FEATURES/BENEFITS

- Detect target compounds at very low concentrations, dilute samples to reduce matrix effects, and use smaller sample volumes with StepWave™ off-axis ion source technology.
- Minimize sample runtime and maximize the number of compounds assayed in a single method.
- Monitor matrix interferences and greatly improve the ease of quantitative MS/MS method development with RADAR™ Technology.
- Automated instrument optimization with IntelliStart™ Technology saves analysts' time and ensures high system performance.
- Search, manage, and automatically optimize quantitative methods with MassLynx workflow software tools including the Quanpedia™ Database.
- Universal ion source architecture ensures coverage of every application – use with ESI, ESCI, APCI, APPI, APGC, ASAP, nanoFlow™ ESI, and ionKey/MS.™
- Better reproducibility with more time spent monitoring specific MRMs and less time between MRMs using Xccelerated Ion Transfer (XIT).
- Useful for samples with a high concentration of active ingredient and low concentration impurity or metabolite, Xtended Dynamic Range (XDR) provides enhanced sensitivity and a wider dynamic range.



Xevo TQ-S micro with the ACQUITY UPC² System.



The ACQUITY UPC² System and Xevo TQ-S were used to analyze triazole fungicides in wheat grain and wheat straw. ACQUITY UPC²-MRM chromatograms show the enantioseparation of five triazole fungicides pre-spiked onto wheat grain at a level of 1 ng/g and extracted using QuEChERS with Oasis® MCX sample cleanup. Improved enantiomeric resolution and shorter analysis times were achieved compared with normal phase chiral separations resulting in higher sample throughput.

METABOLITE IDENTIFICATION

To properly determine the toxicological and environmental impact of an agrochemical, you need to detect, identify, and quantify all of the metabolites in your sample. For your laboratory productivity, that means a need for both process efficiency and scientific rigor.

Know More About Your Metabolites

Metabolite Identification Application Solution with UNIFI

The Waters Metabolite Identification Application Solution with UNIFI® is an all-inclusive system that provides agrochemical laboratories with the most comprehensive analytical tool for identifying and characterizing metabolites. Purpose-built for metabolite (Met) ID, this system brings unparalleled ease and efficiency to routine Met ID processes – scientists can rapidly derive results from complex data sets.

KEY FEATURES/BENEFITS

ACQUITY UPLC I-Class System

- Provides rapid, high-resolution separations to help resolve components of interest from complex matrix interference peaks faster than ever before.
- Maximizes peak capacity to enhance MS sensitivity.
- Provides the lowest carryover, complementing MS sensitivity and extending MS linear dynamic range.
- Purposefully engineered for the lowest dispersion.

Xevo G2-XS QTof

- Analyze the broadest range of compounds in the most complex samples.
- StepWave ion optics allow for unsurpassed levels of robust sensitivity.
- Delivers superior UPLC-compatible mass resolution, matrix-tolerant dynamic range, quantitative performance, mass accuracy, and speed of analysis – simultaneously.

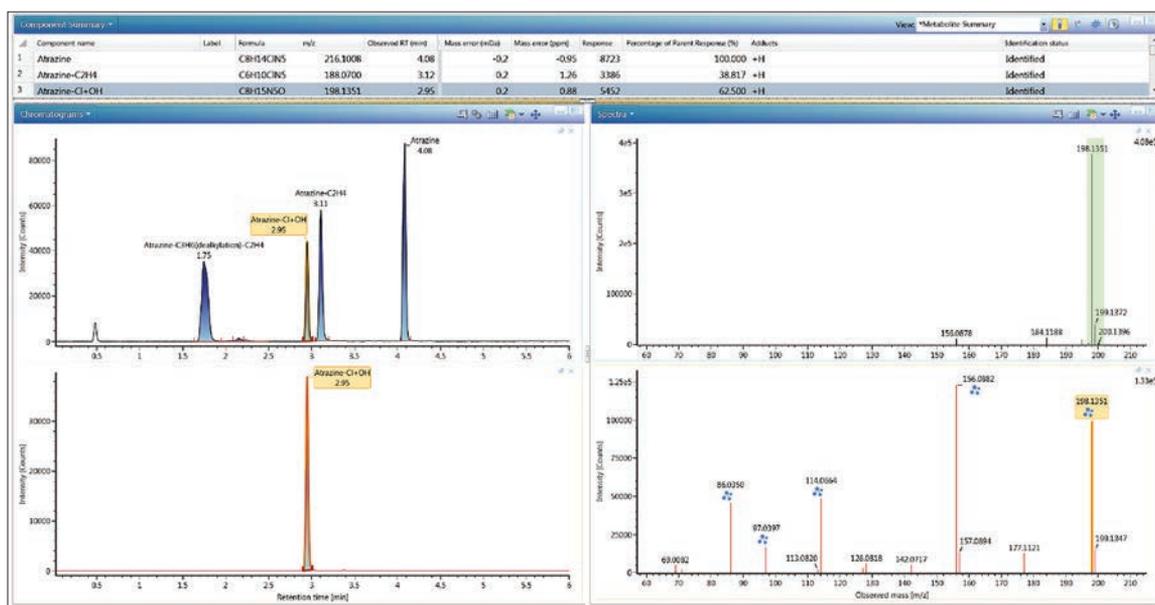


ACQUITY UPLC I-Class System with Xevo G2-XS QTof.



UNIFI Scientific Information System

- Enables workflow customization so you can generate information and integrate results into your current process.
- Predicts metabolic pathways based upon the structure of the molecule of interest.
- Should an unexpected metabolic event be discovered, UNIFI can record the occurrence and store it in its Scientific Library – the repository of information builds as each scientist contributes to it.
- Easily stores, makes use of, and allows sharing of data, methods, and reports.



Component Summary table presents details about the identified metabolites. Extracted ion chromatograms of all metabolites identified in the soil sample are displayed (top left) and the highlighted metabolite (bottom left). The MS^E high/low collision energy (CE) mass spectra showing precursor (low CE) and fragmentation (high CE) information for the selected metabolite are also visible. Note: Likely structure assignments are indicated by the blue molecule symbols to aid interpretation.

DATA MANAGEMENT

Many of the biggest challenges facing agrochemical laboratories revolve around data – capturing it, analyzing it, managing it, and reporting it accurately in registration documentation. Analytical data gathered from the discovery and development process can also provide insights to guide future product development. Waters fulfills these needs with an array of software solutions that allow organizations to:

- Manage increasingly large volumes of data from a broad range of analytical techniques.
- Make sample management and the regulatory submission process as efficient and error-free as possible.
- Employ software tools that will enhance the productivity of scientists.
- Share data openly and seamlessly across the enterprise.

LIMS Capabilities Without the Complexities

NuGenesis Lab Management System

Waters' NuGenesis® Lab Management System is a user-centric platform that uniquely combines synergistic data, workflow, and sample management capabilities to support the entire product lifecycle from discovery through manufacturing.

KEY FEATURES/BENEFITS

- NuGenesis SDMS automatically captures and catalogs data generated by instruments, scientists, and outside sources into a centralized data repository.
- NuGenesis ELN allows laboratories to document observations, control procedures, and exchange information with other software solutions.
- NuGenesis SampleShare is a web client that automates the submission of samples to NuGenesis-based laboratories for analysis.
- NuGenesis Stability is a stability protocol management and testing solution that delivers productivity improvements at every step of the process.
- NuGenesis Connectors provide a bi-directional link between the NuGenesis Lab Management System and business systems such as SAP supporting more accurate and rapid decision making.

Combining Power and Personalization

Empower 3 Chromatography Data Software

Empower 3 is Waters' compliance-ready chromatography data software (CDS) for advanced data acquisition, processing, and reporting that simplifies the management of chromatography test results.

KEY FEATURES/BENEFITS

- Empower's QuickStart interface makes it easy to conduct targeted tasks and workflows – users have the flexibility to customize interfaces to suit individual needs.
- Empower Laboratory Analytics assembles and displays chromatography performance data in easy-to-view, graphical dashboards – so you can determine which improvements are needed to increase efficiency.
- Empower Mobile provides wireless access to Empower Software from a tablet or smart phone – monitor system status, perform routine system administration tasks, and review reports no matter where you are.
- Empower 3's ApexTrack™ Technology provides automated and reliable peak integration, with effective detection of poorly-resolved or low-level peaks on noisy or sloping baselines.
- Comprehensive control of LC, GC, MS, SFC, IC, and CE systems from a wide variety of vendors – standardize on a single platform to reduce maintenance, training, and validation costs.



Paradigm Scientific Search

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User: CORP\JUSCTAM

Results Summary
Results Returned: 6
Total Artifacts: 7
Search Time: 0.310 sec
Total Time: 0.333 sec

Current Search
Sources: SDMS, ELN, ChemDev Reports, PharmSci DMS, PharmSci Reports, Syntex ELN 3, COV-2 Project, Image Collection, Waters Application Library, Applications, Risk Collection, Combinatorial Data, Chemogenomics, Run Handbook

Refine results using Facets
Score, Authors, File Extension, Source, Stars, Created Date, Modified Date, Document Creation Date, Document Modified Date, Document Page Count, Document Company, Document Slide Count

Search Again

Tebuconazole
n/a
1,000 Applications

Chiral guan
usuhehm
1,000 Applications

Tebuconazole
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1,000 Spectral Database

(R)-Tebuconazole
n/a
1,000 Applications

(S)-Tebuconazole
n/a
1,000 Applications

Enantioselective Degradation of...
n/a
1,000 Applications

Paradigm Scientific Search results for the fungicide Tebuconazole. Result indicates where the Tebuconazole structure (based on a structural jpeg image) was found in various documents.

Enterprise-Wide Scientific Information Access

Paradigm Scientific Search Software

Paradigm™ enables fast, easy, high-value searches of chemical and biological information across enterprise information repositories to drive product innovation, development, and manufacturing.

KEY FEATURES/BENEFITS

- Creates a searchable index of the data and content in instrument-based, science, business, and office applications.
- Search on text, documents, and science objects such as chemical structures and reactions, methods, chromatograms, spectra, and digital images.
- Retrieves only the most relevant results, filters them according to your area of interest, and ranks them by importance.
- Easy-to-use interface requires no specialized training.



YOUR CONSUMABLE PARTNER IN SEPARATION SCIENCE



CORTECS Columns.

Given the diversity and complexity of agrochemical samples, ensuring the most effective separations requires highly innovative sample preparation and column chemistries. Since the formation of the company in 1958, Waters has been developing leading edge separation media designed for chromatography. As the technique and supporting instrumentation evolve, Waters continues to deliver key products for routine and matrix specific or specialized applications.

Our wide range of analytical columns can simplify method development, validation, and transfer throughout your organization. In addition, Waters' sample preparation solutions for quantitative analysis make it easy to deliver samples that are reproducible, yield high recovery, and are free of interferences.

Innovation with a Purpose

With such a long history of product development, coupled with a commitment to continuous supply, the Waters consumable portfolio consists of thousands of products supporting new and legacy methods worldwide.

LC/UPC² Column Technologies

ACQUITY UPLC and XBridge[®] HPLC columns are built upon the revolutionary Hybrid Particle Technology. The wide pH range and extreme mechanical stability have established these products as the number one starting point for any routine LC method development.



XSelect® HPLC Columns have alternate selectivities to the conventional C₁₈ or C₈ phases. These chemistries are also available for UPLC under the ACQUITY CSH™ and ACQUITY HSS product names.

CORTECS® Columns were developed to fulfill the promise of core-shell based chromatography phases: CORTECS 1.6 µm for maximum efficiency of UPLC separations, and CORTECS 2.7 µm for improved speed of analysis and flexibility for HPLC.

ACQUITY UPC² Trefoil™ and Torus™ column chemistries, combined with the ACQUITY UPC² Platform, enable separation scientists to better access normal-phase chromatography with the ease and reliability of reversed-phase chromatography. They provide the ability to handle both chiral and achiral separations with unequalled speed and unparalleled confidence.



Waters Analytical Standards and Reagents.

Sample Preparation

Oasis Sample Preparation Products represent the first water wettable, generic, simple-to-use solid phase extraction media. It works extremely well for a wide range of applications by providing highly selective cleanup to increase sensitivity using mixed-mode reversed phase and ion-exchange functionalities.

Waters Analytical Standards and Reagents

A portfolio of differentiated and enabling standards, reference materials, and application solutions that provide simplified and faster workflows, along with a higher level of confidence, quality, and repeatability in your results.

Waters Global Services

Be Assured. Choose Waters Global Services.

Waters Global Services focuses on optimizing Waters products with superior service, support, upgrades, training, and Waters Quality Parts.® For 14 consecutive years, an independent quality auditing firm has ranked Waters Global Services Best-in-Class in providing expert technical knowledge, quick resolution of system issues, and process support.

¹ Achievement in Customer Excellence Award, CustomerSat, Inc., 2007-2014; NorthFace ScoreBoard Award,sm Omega Management Group Corporation, 2001-2006.

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