ANALYTICAL SOLUTIONS FOR COSMETICS & PERSONAL CARE

A clear path to greater product innovation, safety, and compliance
A NEW FORMULA FOR SUCCESS
Driven by fast-moving trends and consumers’ unending search for novel beauty products, the personal care and cosmetics business is in constant motion. In an industry where fewer than 40% of new products succeed, the product pipeline can never be too full.

To meet your growth and profitability goals, you need to continuously pursue accelerated innovation and ever-shorter product development cycles. However, there are more than a few obstacles in your way, including:

• Growing regulatory requirements
• Increased pressure to validate product performance claims
• Consumer demand for more natural and organic products
• The constant threat of competitive pressure and counterfeiting.

The answer to many of these challenges can be found in the analytical laboratory – and Waters solutions can provide them, every step of the way.
According to a recent European Union study,\(^1\) counterfeiting costs the cosmetics and personal care industry $5.25 billion annually, tens of thousands of jobs, and deprives governments of $1.9 billion in tax revenues.

For consumers, it’s not just a matter of getting swindled. Counterfeit products may even cause physical harm, as many have been found to contain toxins and carcinogens. While luxury brands are the most frequent targets of counterfeiters, no personal care manufacturer is immune to the problem.

For all of these reasons, companies need to be able to test samples to identify counterfeits quickly and confidently, but catching them requires a high volume of painstaking analytical work.

**Identify Counterfeit Cosmetics with Multivariate Analysis**

What’s needed is a way to swiftly compare a suspect sample to the authentic product and determine if there are differences – and if necessary, provide a more detailed analysis in order to identify the individual components. Waters fulfills this need with an approach based on fast and simple multivariate analysis combining Liquid Chromatography (LC) or Atmospheric Pressure Gas Chromatography (APGC) with advanced time-of-flight Mass Spectrometry (MS).

**Counterfeit Testing Solutions:**

- ACQUITY UPLC® I-Class System
- UNIFI® Scientific Information System
- Xevo® G2-XS QTof Mass Spectrometer
- Atmospheric Pressure GC (APGC)
- ACQUITY UPLC Columns
- CORTECS® 1.6 µm Columns

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The key to any Waters counterfeit testing solution is the UNIFI Scientific Information System, which includes multivariate analysis tools. These tools enable you to reduce the multivariate dimensionality of large data sets by using statistical modeling and principle components analysis (PCA). An initial summary provides guidance for any further analysis that may be required, and the resulting marker sets can be labeled as authentic or counterfeit and saved. Subsequent samples of suspected counterfeit products can then be analyzed and compared to the authentic marker set and quickly identified.

With Waters, cosmetics and personal care product manufacturers now have the tools to protect their revenues, their consumers’ health, and their brand’s integrity.
RAW MATERIALS TESTING: ESTABLISHING ACTION AND SAFETY

While the marketing department often directs the path of new cosmetic and personal care product development, it is the responsibility of analytical laboratories to source the best raw materials and active ingredients and determine their efficacy and safety.

The challenge is to swiftly and thoroughly characterize each ingredient and ensure product safety. That’s particularly difficult when dealing with complex botanicals and other naturally-occurring compounds. From an analytical perspective, it means identifying all components in a sample, developing its chemical fingerprint, pinpointing toxins and allergens, and verifying the presence of the active ingredient in the final product.

Waters provides a wide range of technologies for screening, isolating and quantifying raw materials and active ingredients.

**Raw Material Testing Solutions:**
- Prep 100q SFC System
- ACQUITY UPLC I-Class and H-Class Systems
- Atmospheric Solids Analysis Probe (ASAP)
- Xevo TQD Mass Spectrometer
- Xevo G2-XS QTof Mass Spectrometer
- Viridis,® XBridge®, XSelect®, and ACQUITY UPLC Columns
- TruView™ Vials

Mass directed (m/z = 273, in source dimer) recovery of geraniol from orange oil with the Prep 100q SFC System. Sample recovery can be challenging by traditional preparative LC techniques due to the volatility of the compound. The use of supercritical fluid chromatography (SFC), which utilizes carbon dioxide as the primary mobile phase, enables up to 90% recovery for volatile compounds.
Case Study: Advancing the Characterization and Quality Control of Botanical Extracts with Mass Spectrometry

Bio-Botanica is a leading manufacturer of 500+ quality botanical extracts. To better identify extract constituents and meet the constant demands of a fast-paced laboratory environment, the company implemented the ACQUITY UPLC H-Class System with the Xevo TQD Mass Spectrometer. Scientific and business benefits included trace-level contaminant detection, method consolidation, reducing separation times by approximately 75%, and the ability to identify novel compounds that may have unique cosmetic applications.

Comprehensive characterization of botanicals with UPLC-MS/MS

Prep 100g SFC System
- Provides high-throughput, semi-preparative to preparative scale purification for higher productivity, greater flexibility, and lower costs per sample.
- Utilizes environmentally-friendly carbon dioxide (CO$_2$) as the primary mobile phase.
- Purification applications include chiral and achiral separations, impurity isolation, and natural products.
- Gas Liquid Separator (GLS) technology allows for more efficient fraction collection resulting in higher recovery of valuable compounds.
- Fully automated open-bed sample injection and fraction collection allows for the processing of hundreds of samples, or just a few.

Atmospheric Solids Analysis Probe (ASAP)
- Streamlines workflow by enabling rapid, direct analysis of volatile and semi-volatile solid and liquid samples in seconds.
- Simply dip a glass capillary into the sample, place the probe into the source, and the heated nitrogen desolvation gas will vaporize the sample, with corona discharge for sample ionization.
- Applications include the analysis of active components, such as UV absorbers in personal care products.
FORMULATION: ENSURING PERFORMANCE AND CHARACTERIZATION

New formulations are the lifeblood of the beauty industry. To keep the product pipeline full and moving steadily, laboratory chemists need to develop formulations that consistently deliver the desired efficacy, performance, safety, texture, fragrance, appearance, and stability — while also ensuring that the product packaging protects those attributes over time under a broad range of environmental conditions.

To a large extent, the success of your business depends on how swiftly and efficiently you can master this process. But there are many challenges that stand in your way, including high analytical throughput, the need to validate label claims, regulatory limits, and the complexity of product samples.

Waters addresses these challenges with unique liquid chromatography and mass detection technologies designed to enhance the effectiveness of your formulations laboratory.

Formulation Testing Solutions:
- ACQUITY® Arc™
- ACQUITY QDa® Detector
- Viridis, XBridge XP, XSelect XP, and ACQUITY UPLC Columns
- TruView Vials
Helping to Streamline Formulations Testing

With Waters® ACQUITY Arc System, significant productivity gains can be realized in formulation testing by deploying a single LC platform that allows the efficient transfer, adjustment, or improvement of methods from any LC platform - while the ACQUITY QDa Detector provides valuable mass spectral data within your existing workflows.

A mixture of six commercial biocides used in formulated shampoo and hand creams were analyzed using the ACQUITY Arc System to evaluate the impact of both conventional HPLC and UHPLC based chromatographic separations. ACQUITY Arc offers method compatibility for HPLC and UHPLC separations to aid organizations transitioning their methods from HPLC to UHPLC.

Whether you're testing for performance or characterization, Waters provides more ways to cut time and labor-intensive steps out of the process, without sacrificing scientific rigor.
Ensuring product safety is much more than a matter of fulfilling regulatory requirements. Your investments in product quality demonstrate a commitment to consumers’ health, environmental protection, and good corporate citizenship. Safety and regulatory testing also provide vital data to support label claims.

The continuing success of your business depends on your ability to protect your reputation as a quality brand. At the same time, as more stringent regulations require more testing, you’re under pressure to increase laboratory throughput. With the compliance burden only expected to grow you need a sure strategy to drive more efficient analyses.

Having served the demanding criteria of the pharmaceutical, food, and environmental industries for decades, Waters is constantly developing innovative technologies to detect a diverse range of compounds and address ever-changing regulatory environments.

Safety and Regulatory Testing Solutions:

- ACQUITY UPC2® System
- Xevo TQD
- ACQUITY UPLC I-Class System
- Xevo G2-XS QTof Mass Spectrometer
- UNIFI Scientific Information System
- ACQUITY UPC2 Trefoil™ Columns
- ACQUITY UPC2 Torus™ Columns
- UPC2 QC Reference Material

With Waters, regulatory compliance becomes a checklist item, not a resource-intensive obstacle.
Faster, More Cost Effective Allergen Detection
For the analysis of allergens, our solution is the UltraPerformance Convergence Chromatography™ (UPC²) System and Xevo TQD Mass Spectrometer. The world’s first Convergence Chromatography system, ACQUITY UPC² delivers a technology based on the principles of normal-phase LC that offers the ease-of-use of reversed-phase LC. The Xevo TQD was created to reduce the complexity of tandem (triple) quadrupole mass spectrometry – helping to ensure maximum productivity with minimal effort.

ACQUITY UPC² System
- Combines the performance of UPLC with SFC to deliver faster separations and superior resolution for chiral and achiral applications.
- Utilizes supercritical carbon dioxide (CO₂) as the primary mobile phase to provide a more cost-effective and greener technology by reducing the use of organic solvents.
- Streamlines sample preparation workflow by eliminating evaporation and reconstitution steps.
- Precisely varies mobile phase strength, pressure, and temperature to fine-tune resolving power and selectivity.
- Allows the use of gradients across the widest polarity range.

Xevo TQD Mass Spectrometer
- Enables simultaneous acquisition of high quality quantitative and qualitative data from the widest range of experiments.
- IntelliStart™ Technology simplifies MS setup and routine operation with automated quantification workflow tools.
- Observe MRM (multiple reaction monitoring) data and full scan background data simultaneously for faster, more robust method development.
- RADAR™ Technology provides the sensitivity and selectivity to monitor for sample matrix interferences, impurities, and degradants.

Rapidly Characterize Packaging Material Extracts
Likewise, the combination of the ACQUITY UPLC I-Class System, Xevo G2-XS QTof Mass Spectrometer, and UNIFI Scientific Information System is an effective solution for the non-targeted screening of packaging extracts. This LC-MS methodology streamlines the structural elucidation process by utilizing MS², an MS/MS technique that alternates between collecting accurate mass precursor and fragment ion information during a single analysis. This enables users to rapidly evaluate information for an unknown component (m/z) by ranking the possible elemental compositions and performing database searches for likely structures ranked based on fragmentation matching.
Product success can be made or broken in production. For example, delivering a product to market can be negatively affected by poor process control or an inability to confirm label claims.

With the US Food & Drug Administration and other regulatory bodies exerting greater influence on manufacturing best practices (e.g., cGMP), you need tools that enable you to continuously monitor production quality and back it up with the appropriate reports.

Waters supports Quality Control needs with systems and software that are robust enough to handle high-volume production at all your facilities, from in-process monitoring to final product QC.

**Quality Control Testing Solutions:**
- Empower® 3 Chromatography Software
- ACQUITY UPLC H-Class System
- ACQUITY UPLC PDA Detector
Process Monitoring – Make Faster Decisions

Process monitoring of cosmetic and personal care additives during manufacturing requires accurate and rapid decision-making information to ensure product quality and consistency. Waters ACQUITY H-Class System, along with the ACQUITY UPLC PDA Detector, and Empower 3 Software provides a solution. The system can separate multiple structurally similar biocides and UV filter agents simultaneously in a fraction of time required for traditional HPLC – and with PDA library matching and built-in advanced mathematical algorithms, each compound in the mixture can be identified and quantified. In addition, Empower 3’s Custom Calculation functionality allows the comparison of results to user/QC defined Pass/Fail criteria. The results can be automatically flagged in a standardized report helping to accelerate production workflow, as well as benefiting new product development and troubleshooting.

Empower 3 Custom Field Formula. The QC Pass/Fail criteria are based on biocide content.

Systems and software to support high volume production, from in-process monitoring to final product QC.
Many of the biggest challenges facing personal care and cosmetics laboratories revolve around data – capturing it, analyzing it, managing it, and reporting it accurately. Analytical data gathered from the product 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 and make sample management and the regulatory process as efficient and error-free as possible.

**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 development 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.
Given the diversity and complexity of cosmetic and personal care product samples, ensuring the most effective separations requires highly innovative column chemistries. Since the formation of the company in 1958, Waters has been developing leading-edge separation media designed for chromatography.

Our wide range of analytical columns can simplify method development, validation, and transfer throughout your organization.

**LC/UPC² Column Technologies:**

- ACQUITY UPLC BEH and XBridge BEH HPLC Columns are based on Waters patented organic/inorganic Hybrid Particle Technology (HPT). The second generation HPT, known as BEH Technology™, combines the high-pH dissolution resistance of a polymer with the efficiency and mechanical stability of silica. The extreme pH, temperature, and mechanical stability of BEH Technology allows you to harness the full power of pH in UPLC, UHPLC, and HPLC methods 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 UHPLC and 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 unequaled speed and unparalleled confidence.

**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.