

APPLICATION SOLUTION

NATURAL PRODUCTS



Waters
THE SCIENCE OF WHAT'S POSSIBLE.®



THE FIRST OF ITS KIND, UNIFI COULD ONLY COME FROM WATERS

- Easy to use, with a workflow and templates that help you efficiently move from analysis to reports
- Reliably identifies, quantifies, and reports natural products compounds, minimizing false positives
- Characterizes chemical composition of herb-based products with speed and accuracy, and identifies plant of origin with integrated Traditional Medicine Library
- A next-generation solution built upon proven, category-leading Waters technology

The total solution for profiling the chemical ingredients of natural products.

The demand for knowledge of natural products has never been greater. Academic researchers are exploring new uses in the areas of botanicals, marine species, bacteria for drug discovery, and even toxicology. Commercial enterprises see tremendous opportunities in bringing breakthrough medicines, herbal remedies, and dietary supplements to market. Companies involved in flavor and fragrance look to add new and exotic appeal to their brands.

Even though the herbs, leaves, and roots of natural products have been around for centuries, there is still much that we do not know about them. How does a specific herb work? Why does it work? What impact can be expected from different combinations?

Researchers are looking to unlock these primeval secrets and confidently bring new products to market. In today's increasingly regulated environment, acceptance of natural products requires the most precise analysis and detailed, fit-for-purpose scientific reporting. To achieve this level of fully integrated workflow demands the combination of expertise, performance, and experience that only Waters can deliver.

Ideally suited for the analytical challenges to fully understanding and commercializing the vast possibilities of natural products, the Waters Natural Products Application Solution with UNIFI® gives scientists a tightly integrated set of tools to streamline the path from sample to knowledge... and from understanding to market.

LATEST TECHNOLOGIES REVEAL
NATURE'S SECRETS.

Integrating reporting into the workflow: The UNIFI advantage.

Laboratories today are being asked to work smarter and faster. Streamlining the workflow is an essential part of their success. The UNIFI Scientific Information System enables scientists to capture the complex data acquired by high-end mass spectrometry and chromatography with one platform.

Now, you are able to acquire, process, review, and communicate analyses then seamlessly generate reports that document findings – all within a single integrated workflow. Results are more accurate and reports can be tailored to a specific task.

You have the operational and scientific advantage of world-class analytical instruments, chemistries and consumables, standards and reagents, and software integrated through the entire workflow.

Acquisition

Together, the ACQUITY UPLC® I-Class System and Xevo® G2-S QTof MS provide a unified method for acquiring high-resolution data and deliver world-class analytical power. Acquired data travels to UNIFI, where the solution architecture intelligently captures and stores both data and methods. Scientists using UNIFI have exceptional flexibility to use and share data, encouraging the speed of new discoveries.

Process

UNIFI automatically brings together the LC and MS raw data, which can be processed in the background while acquisition continues. Single users or workgroups located across the lab and around the globe can access the information to use, re-use, and manage. Researchers can move more quickly from initial analysis to actionable results.

Review and confirm

Within UNIFI, you can display raw and processed data in a single interface. You can investigate peaks and spectra dynamically. The software's powerful Data Review Tools are fully customizable: create filters and dashboards and display only the information pertinent to your project. The entire review process is accelerated, yet more accurate and compliance-ready.

Report and communicate

You don't have to leave UNIFI to communicate results. Built-in reporting templates help you to quickly present precisely the information required. Information can be exchanged and transferred among teams, departments, facilities, and third-party partners anywhere in the world. Because all the data stays within UNIFI, you are building an expanding repository of scientific knowledge – improving the efficacy of future analyses while also compiling a historical record of analyses that can be applied to future explorations.



Natural Products Application Solution with UNIFI.

WORKFLOW THAT BREAKS WITH TRADITION.

Integrating world-class chromatography and mass spectrometry instrumentation with next-generation informatics.

Traditionally, data acquisition, processing, and report generation are distinct activities that often involve several analysts. The arrival of the Waters Natural Products Application Solution with UNIFI creates a holistic and streamlined workflow: from sample to instruments to informatics that includes an expansive Traditional Medicine Library. Projects move through analysis to reporting smoothly, quickly, and accurately – no matter how complex your sample is.

Example: Green Tea

Green Tea is found, savored, and valued nearly everywhere in the world. Variations among plants from different locations must be carefully determined and precisely measured.

Using green tea as an example, you can see that the Waters Natural Products Application Solution with UNIFI captures all of the complex LC/MS data on one platform, enabling you to explore and confirm within a single, integrated workflow.

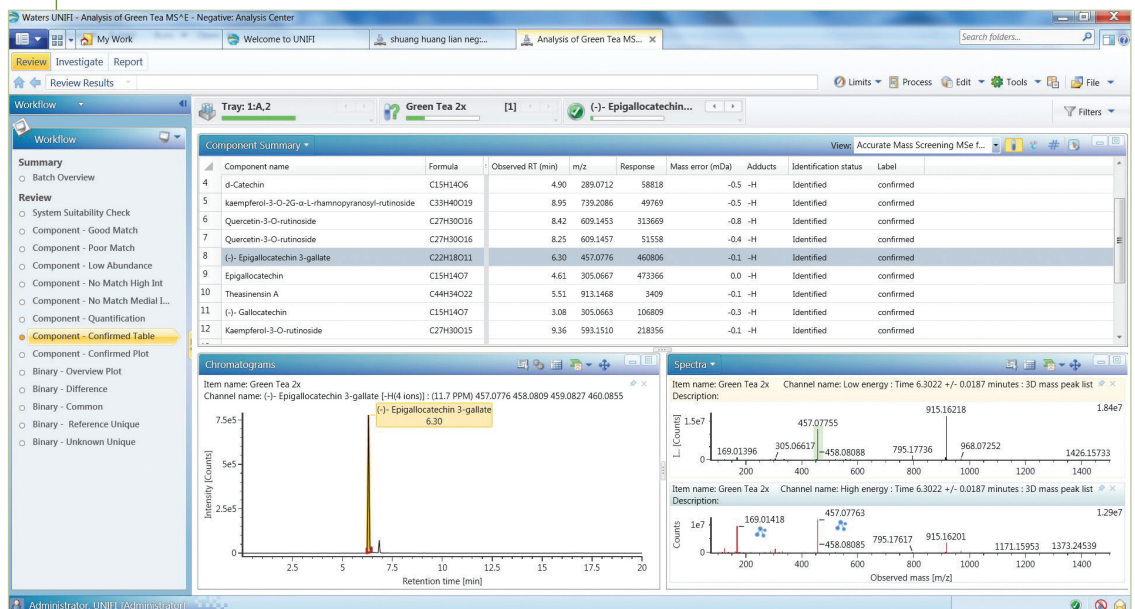
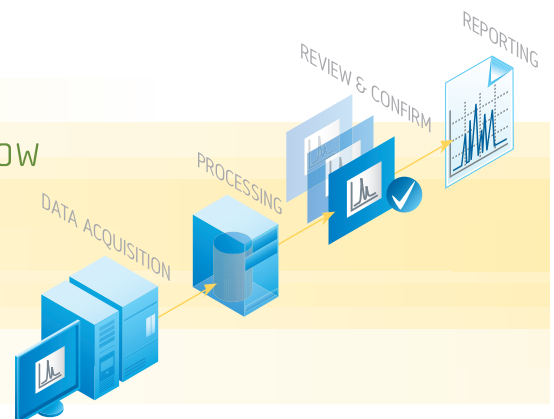


Figure 1. Reviewing processed results in UNIFI. The Review tab includes workflows, component summary, chromatogram, and spectrum (both low and high collision energy scans) correlating to each of the components listed in summary table above.

The fully streamlined workflow

Achieve highly precise analyses, then automatically and centrally store results in a relational database to greatly simplify data management.



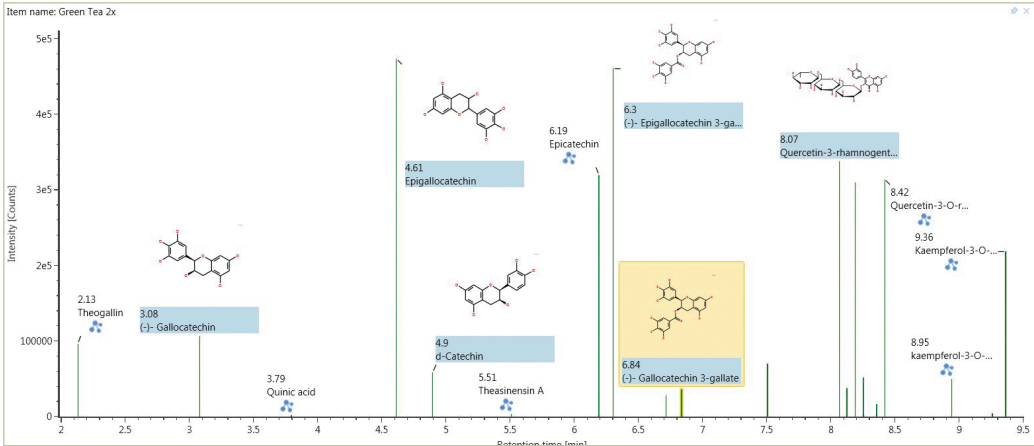


Figure 2. Confirmed chemical ingredients can be reviewed by a simple click of the Component-Confirmed Plot workflow. The chemical identity and structure of each confirmed component are clearly displayed, and many are directly matched with data in the Traditional Medicine Library.

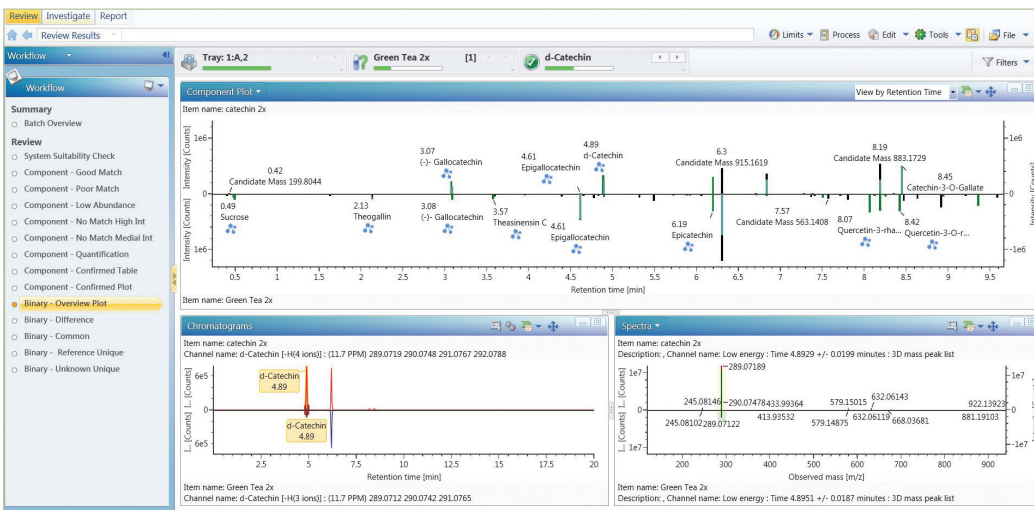


Figure 3. Another workflow enables scientists to perform binary comparisons to identify common and different components between two samples.

Top: Mirror plot of the two Component Plots for two samples to be compared.

Bottom: Mirror plot of the extracted ion chromatogram (left) and low collision energy MS spectrum of a component in two samples (right).

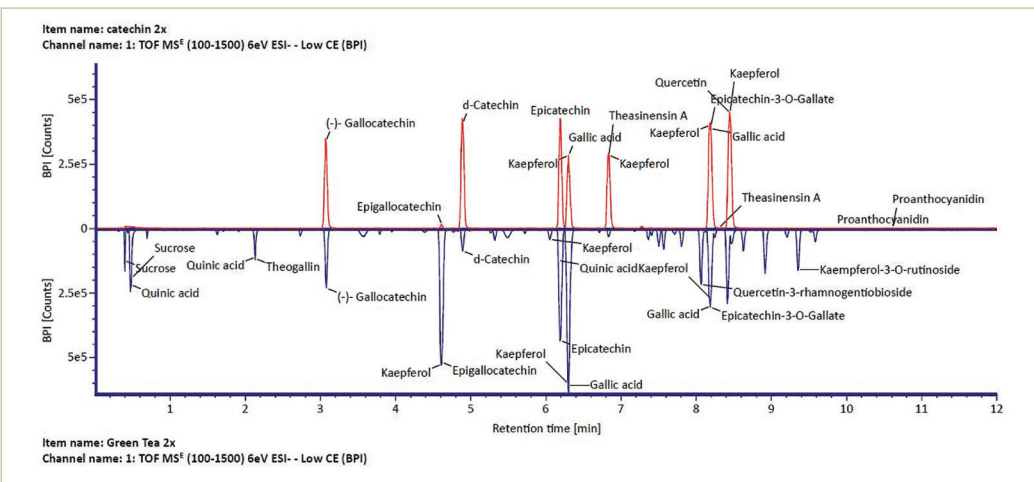
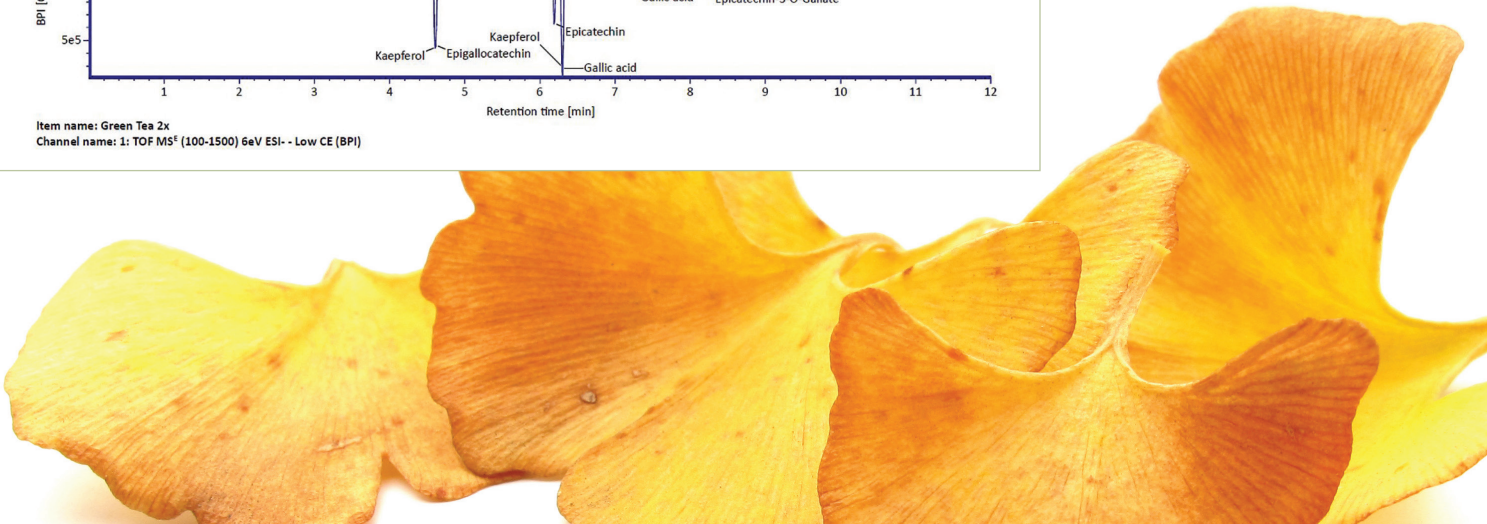


Figure 4. Mirror plot showing the comparison of the confirmed components in both samples.

Top: Catechin Standard Mix as the reference sample.

Bottom: Green Tea Extract as the unknown sample.



Specialized scientific reference library lets you to focus on exploration.

FULLY INTEGRATED TECHNOLOGY DELIVERS SUPERIOR RESULTS

The Natural Products Application Solution with UNIFI is a complete solution that provides high performance to your laboratory and enables you to collaborate with other colleagues around the world. By standardizing analytic laboratory processes across laboratories, it helps to expedite research progress and development decisions.

Natural products can be challenging to fully analyze. While there are many online databases available, investigations of Chinese herbal ingredients take researchers out of their workflow, slowing down analysis and data mining. The Waters Natural Products Application Solution with UNIFI fills this gap: its Traditional Medicine Library includes all of the herbs detailed in the 2010 edition of Chinese Pharmacopoeia and several thousand unique compound entries.

Every compound entry lists its:

- Chemical structure
- Molecular formula
- Molecular weight in exact mass
- Plant origin
- Name in English and Mandarin

Each herb is identified by:

- Chinese name
- Mandarin Pinyin
- Latin name

The screenshot displays the 'Scientific Library' application window. The main pane shows search results for 'Geniposide' from the 'Waters Traditional Medicine Library'. The 'Properties' section lists: TUPAC name (C17H24O11), Formula (C17H24O11), Hill formula (C17H24O11), Average molar mass (404.3659), and Monoisotopic mass (404.1319). The 'Item tag' field contains the chemical structure and its name in Chinese: 'Zhi, 栀子, Monoterpenoid Glycosides, STEMONARIN, FRUCTUS, Baibu, 百部'. The 'Synonyms' section lists 'Geniposide' as the English name and '栀子苷' as the Chinese name. A 'Select Item Tags' panel on the right shows a tree view of 'Traditional Chinese Medicines' with 'Geniposide' selected under 'Mandarin Pinyin'. A 'Search results (23 items found)' table at the bottom right lists various compounds with their library names and formulas.

Name	Library name	Formula
Oxymastemonine	Waters Traditional Medicine Library	C23H32NO7
Oxotuberostemonine	Waters Traditional Medicine Library	C23H31NO5
N-Oxy-tuberostemonine	Waters Traditional Medicine Library	C23H33NO5
Isomastemonine	Waters Traditional Medicine Library	C23H29NO6
Isodidehydro-tuberostemonine	Waters Traditional Medicine Library	C23H29NO4
Geniposide	Waters Traditional Medicine Library	C17H24O11
d-Sesamin	Waters Traditional Medicine Library	C20H38O6
Didehydro-tuberostemonine	Waters Traditional Medicine Library	C23H27NO4
Crocin A	Waters Traditional Medicine Library	C44H64O24
Chlorogenic acid	Waters Traditional Medicine Library	C16H18O9
Benzoic acid	Waters Traditional Medicine Library	C7H6O2
Asiic acid	Waters Traditional Medicine Library	C8H8O3

Figure 5. The Traditional Medicine Library's infrastructure links each compound to its plant(s) of origin and chemical classes. The library includes details such as plant names and compound information, such as chemical structure, molecular formula, average and monoisotopic molecular weight in exact mass.



When you consider that the UNIFI solution's Traditional Medicine Library features deeply detailed information, multiple languages, and the ability to cross-reference results, it's evident that you now have a powerful solution to merge modern and traditional knowledge.

INTEGRATED TRADITIONAL MEDICINE LIBRARY.

Drive your science forward.

The resolution, mass accuracy, specificity, and sensitivity that can be achieved with the ACQUITY UPLC I-Class System coupled to Xevo G2-S QToF MS provides more confidence in the building blocks of natural product research.

The UNIFI Scientific Information System is the first software platform to merge UPLC® and high performance MS data into a single solution that includes tools to meet your laboratory's needs today and tomorrow, from a scientific reference library to configurable compliance tools.

Together, this powerful application solution brings a new level of accuracy and optimized workflow to analyzing complex natural products.

ACQUITY UPLC I-CLASS SYSTEM

With superior chromatographic resolving power, develop the most accurate and reproducible separations to optimize MS performance. Get the most information possible to accelerate laboratory results.



XEVO G2-S QTOF

Uses proven quantitative ToF (QuanTof™) technology and StepWave™ ion optics to deliver superior UPLC-compatible mass resolution, dynamic range, quantitative performance, mass accuracy, and speed of analysis – simultaneously.



WATERS ANALYTICAL STANDARDS AND REAGENTS

Precisely formulated and ready-to-use to ensure your system is fit for purpose. Helps you derive optimal performance from your LC and MS instruments and ensure consistency from day to day, system to system, and lab to lab.



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