

[ VION IMS QTOF ]



BEYOND RESOLUTION



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.®

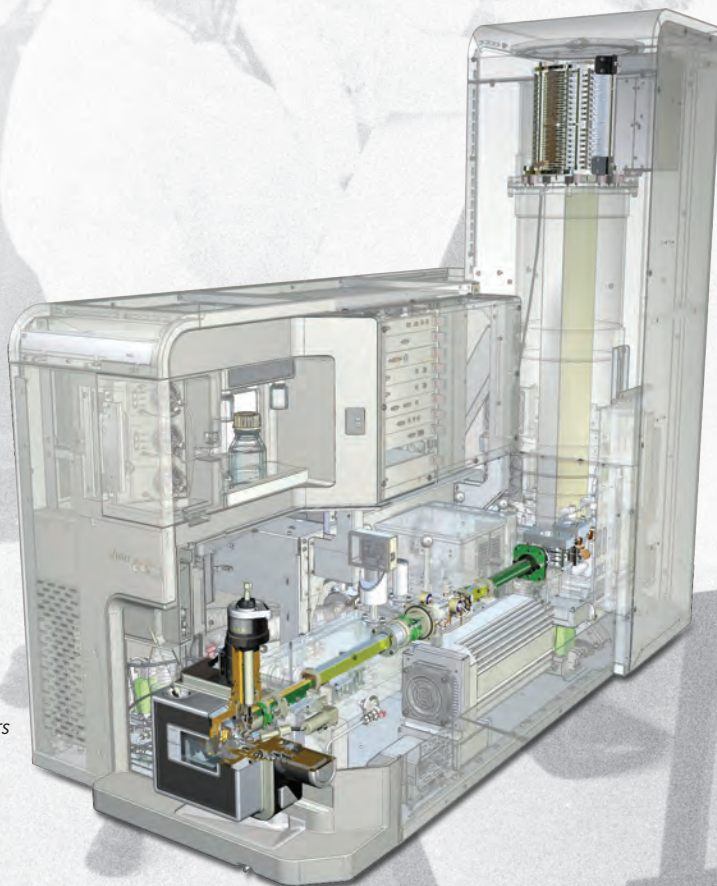
# Vion

**THE BENEFITS ARE CLEAR** and routinely available,

Complex samples give complex data with overlapping spectra and background interferences, making compound identification difficult and method development costly and time consuming. Sometimes resolution and accurate mass are not enough to identify analytes, so additional experiments are needed, making even routine analysis slow and inefficient.

Vion™ IMS QTof moves ion mobility mass spectrometry from research to routine. Rely on ion mobility to clean up and simplify every spectrum, so interpreting your data is easier than ever before. Find, identify and quantify your analytes confidently, enabling faster method development and higher sample throughput.

Waters' innovation and commitment to ion mobility brings you our most exciting benchtop platform: Vion IMS QTof, a high resolution benchtop QTof mass spectrometer that delivers the selectivity of ion mobility to every scientist, for every analysis.



..... The ion mobility capability of Vion IMS QTof is powered by T-Wave™ technology, which means it has higher transmission than any other form of ion mobility. QuanTof2™ technology delivers the dynamic range to make ion mobility quantitative and routinely usable.

# seamlessly from samples to answers.

## Just press start

You'll have more time to focus on the things that matter to you. It couldn't be simpler; just press start and Vion IMS QToF is calibrated and ready for you to acquire data.

## Simply acquire

Vion IMS QToF delivers high resolution, high sensitivity, sub 1 ppm mass accuracy, and enhanced quantitative performance without any compromises. Data acquisition methods use ion mobility as standard and are simple and straightforward to set up. Vion IMS QToF does the work you need it to do – freeing up more of your time.

## Get to the answers

UNIFI® Scientific Information System automates processing, enables data visualisation, and produces reports, presenting the data so that you can quickly and easily get to the answers you need.



# Vion

## BEYOND RESOLUTION

How much resolution do you need when sample variation and complexity cause common analytical challenges? Retention time shifts, isobaric analytes, and spectral interferences: only when ion mobility is a routine part of your analyses can you confidently overcome these challenges.

### Detect more compounds

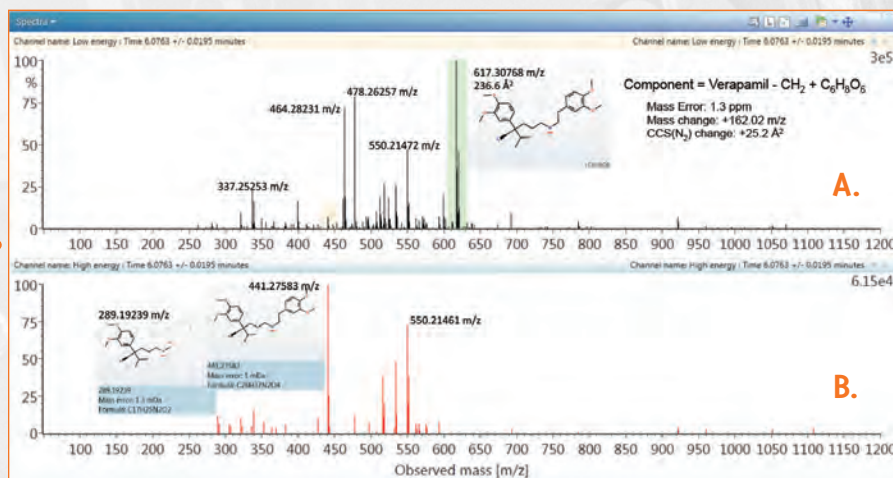
Ion mobility cleans up and simplifies your spectra, enabling identification of all the compounds in your sample. Discover analytes you didn't even know were there. Fully characterize your sample with confidence and make informed decisions.

### Confidently identify your compounds

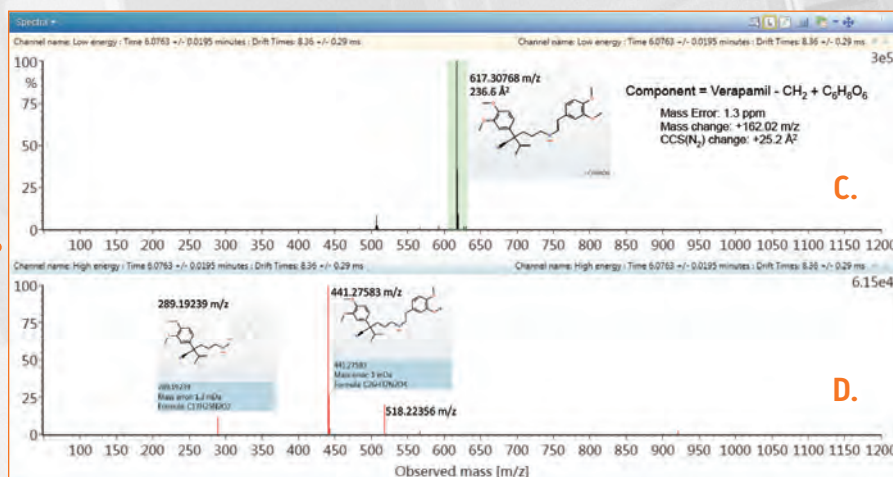
With CCS values available for every ion in every analysis, you have new levels of confidence in your identifications. Retention time is prone to vary with different chromatographic conditions and changing matrices. However, identifications based on CCS and  $m/z$  are precise and independent of retention time. Analyte identifications are right first time, every time.

LC Run (min)	Matrix	Observed ( $m/z$ )	Mass error (mDa)	Mass error (ppm)	Observed RT (min)	Observed CCS ( $\text{\AA}^2$ )
3	Solvent	609.2808	0.2	0.32	1.17	248.38
10	Plasma	609.2807	0.1	0.15	3.18	248.15
30	Urine	609.2803	-0.3	-0.56	7.64	247.69
RMS ppm error = 0.38			%RSD Observed CCS = 0.14			

The data presented above demonstrates that CCS values obtained for reserpine are precise and are matrix and retention time independent.



Retention time aligned LC-MS<sup>2</sup> data obtained for a protonated desmethyl glucuronide metabolite detected in rat bile after the administration of verapamil. (A) shows the precursor ion spectrum and (B) shows the associated higher energy fragment ion spectrum.



HDMS<sup>2</sup> adds clarity to your data. The addition of drift time alignment enables detection of (C) a single component precursor ion spectrum for the protonated desmethyl glucuronide metabolite detected in rat bile after the administration of verapamil and (D) the associated product ion spectrum. This level of clarity aids data interpretation and cannot be achieved with mass resolution alone.

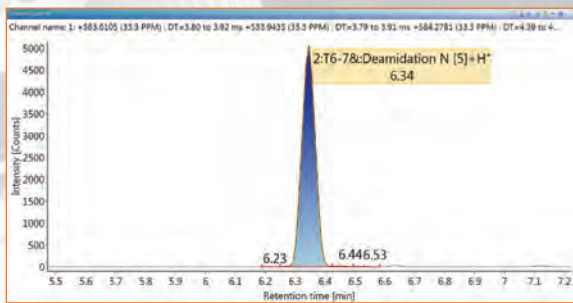
# HDMS<sup>E</sup>: UNLIMITED PRODUCT ION ACQUISITION

Have confidence in your data. HDMS<sup>E</sup> Unlimited Product Ion data independent acquisition combines the information content of high resolution MS/MS with the selectivity of ion mobility separation.

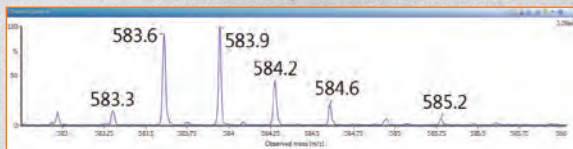
Ion mobility separation not only allows chromatographically coeluting compounds, but also structural isomers, to be resolved. This enables single component precursor/product ion spectra to be generated as ion mobility allows drift and retention time alignment of product ions and their respective

precursors. This provides unparalleled specificity for a data independent acquisition.

Two analytes at the same retention time, but at different drift times, result in product ion spectra that are fully separated from one another, enabling easier, automated data interpretation. The data collected are comprehensive with retention time and drift time aligned precursor and product ion spectra for all ions. If you need to know more, simply re-interrogate your data.

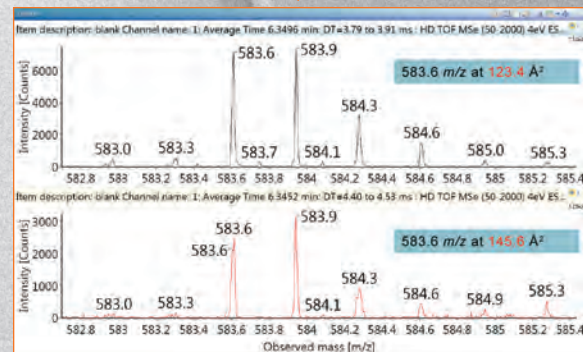
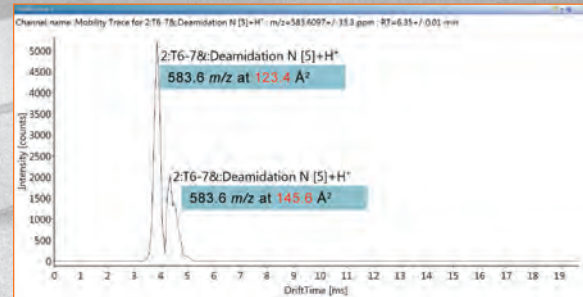


High resolution LC-MS spectrum yields one peptide ID



More resolution does not always give you more information. The data here illustrates that only with ion mobility can you see all the components in your sample.

High resolution IMS enabled LC-HDMS spectrum yields two peptide ID's that differ only by observed CCS

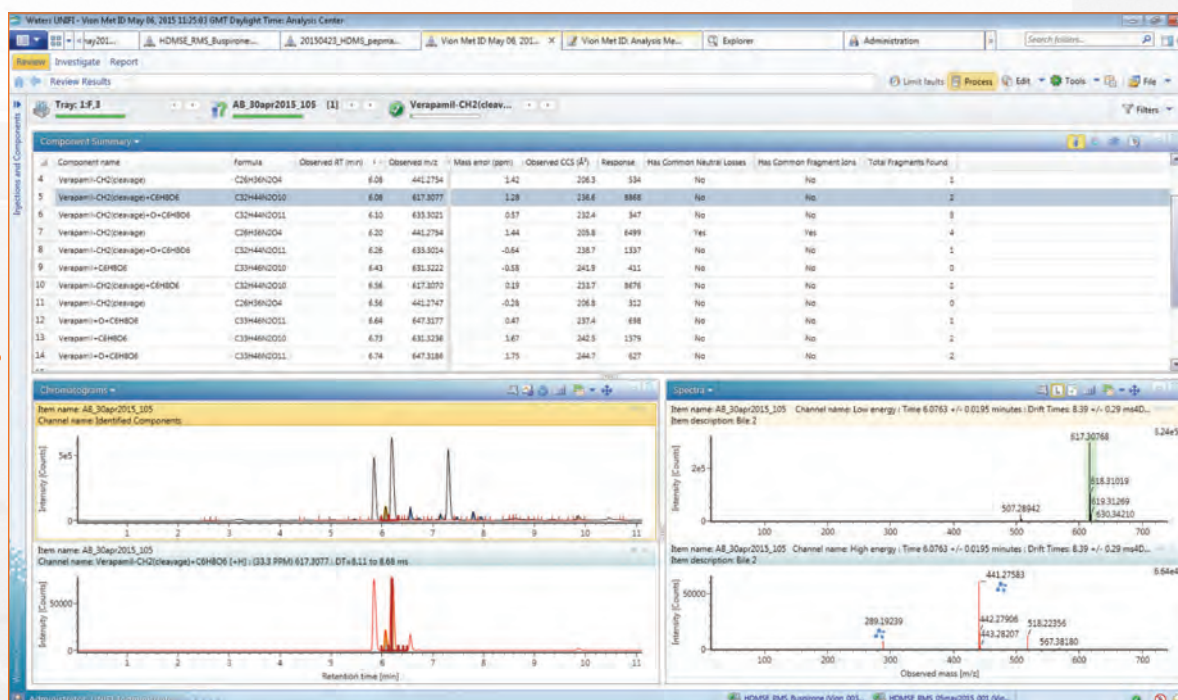


# Vion

## UNIFI TAKING DATA TO KNOWLEDGE

UNIFI Scientific Information System drives Vion IMS QToF to deliver the most comprehensive analytical workflows.

Target, identify, quantify, review, and report using streamlined analytical workflows that enable more confident results across a wide range of applications. Make better decisions faster when CCS values are incorporated into your workflow, to reduce both false positives and false negatives, increase throughput, and boost laboratory productivity.



Simplify your workflow. The latest version of UNIFI incorporates all the tools you need to confidently identify all drug metabolites. CCS values are available for every metabolite since IMS /CCS data reduction is embedded in UNIFI processing. Take advantage of the IMS dimension when HDMS<sup>E</sup> is your routine acquisition method.

### BE ASSURED. CHOOSE WATERS GLOBAL SERVICES.

Waters Global Services focuses on optimizing Waters products with superior service, support, upgrades, training, and Waters Quality Parts.<sup>®</sup>

### PROVEN SATISFACTION

For 14 consecutive years, an independent quality auditing firm has ranked Waters Global Services as "Best-in-Class" in providing expert technical knowledge, quick resolution of system issues, and process support.<sup>1</sup>



1. Achievement in Customer Excellence Award, Comfirm/Customersat, Inc., 2007-2014; NorthFace ScoreBoard Awards;<sup>™</sup> Omega Management Group Corporation, 2001-2003.

## VION WORKING FOR YOU

### Screening

Screening and quantification are daily activities for many scientists across a wide range of scientific disciplines. Meeting legislative and regulatory demands requires the utmost confidence in your data. UNIFI informatics workflows integrate the value of CCS, reducing false positives and false negatives driving laboratory efficiency.

### Pharma

The pharmaceutical industry is driven by the need to improve health and quality of life. The combination of UNIFI and Vion IMS QToF brings ion mobility to your drug discovery experiments while maintaining the ease and efficiency you need for your routine Met ID processes. Use CCS for confidence in component identification and structural characterization from cleaner product ion spectra.

### Omics

Increasing requirements to improve understanding of biological processes are driving the rapidly evolving analytical approaches applied in life and health sciences omics research. A recurring challenge for these omics studies is the identification and structural elucidation of metabolites, lipids, and peptides of interest. Incorporating Vion IMS QToF into your workflow gives you not only CCS data for every component, but also increased analytical space and resolution. Using this additional information increases the identification confidence compared to traditional analytical approaches.

Component name	m/z	Collision cross section error (%)	Observed collision cross section (Å²)	Expected collision cross section (Å²)	Mass error (ppm)	Expected RT (min)
1 Carbendazim	192.0774	-0.48	78.33	78.71	3.58	2.17
2 EPN	324.0445	-0.58	104.26	104.66	-2.72	8.70
3 Imazali	297.0560	-0.28	101.82	102.11	1.34	5.08
4 Indoxacarb	528.0790	-0.06	136.49	136.57	1.66	8.74
5 isofenphos-methyl	332.1082	3.49	108.50	104.84	0.50	8.26
6 Prochloraz	307.9996	-0.14	99.03	99.17	-3.24	6.67
7 Pyriproxyfen	322.1438	-0.22	115.87	116.13	0.18	9.21
8 Spirosad	732.4704	0.00	201.00	201.01	3.13	7.07
9 Thiabendazole	202.0449	-0.23	78.42	78.65	7.68	2.34

False positive

False negative

Screening for known Pesticides with CCS in a small scale proficiency test. Using CCS values as an additional filter for molecular identification enables false positive and false negative identifications to be minimized, improving confidence and efficiency of the analysis. The additional specificity afforded by CCS measurements minimizes false negatives by allowing m/z and/or rt tolerances to be relaxed.

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