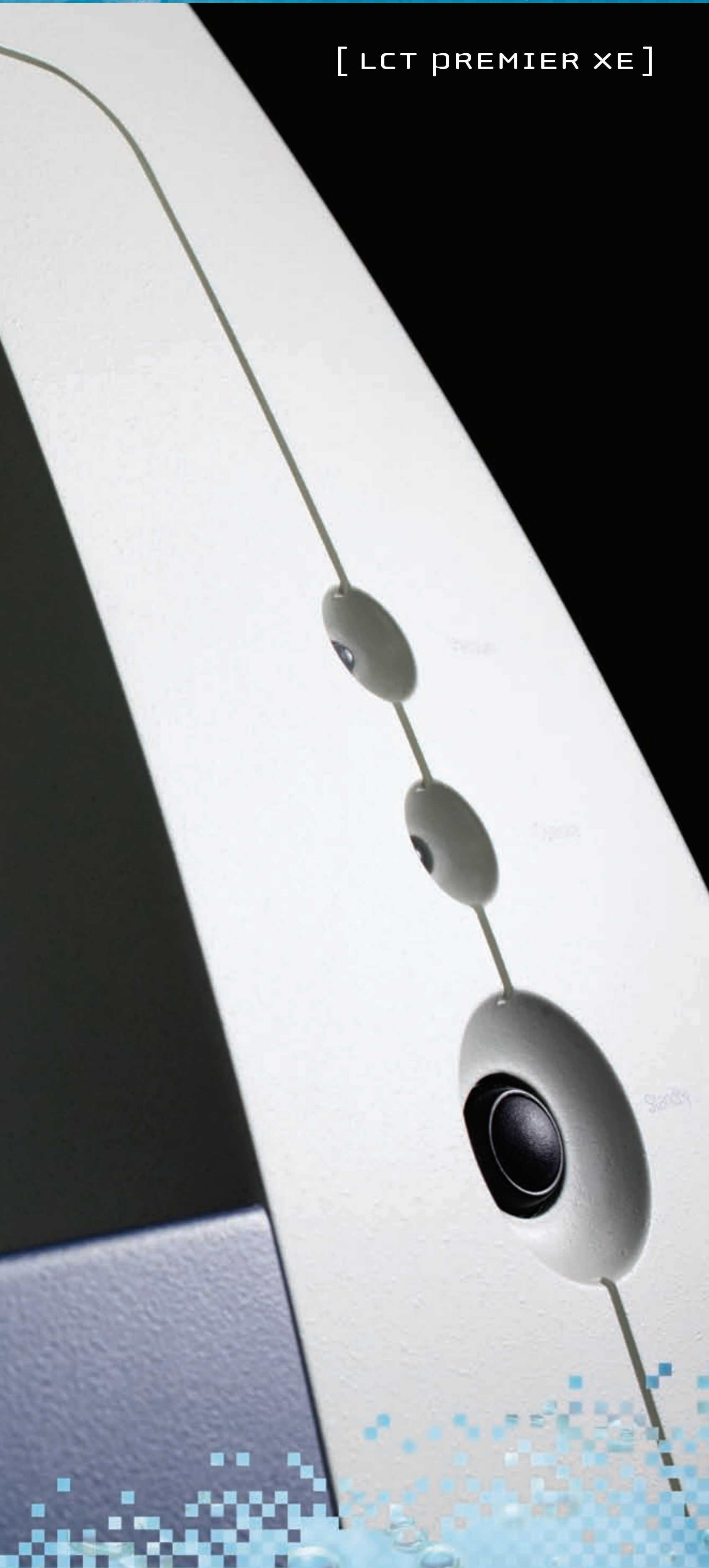
[LCT PREMIER XE]

EXACT MASS IN AN EASY-TO-USE PLATFORM



Waters

THE SCIENCE OF WHAT'S POSSIBLE.™

FAST, ACCURATE QUALITATIVE RESULTS.

Delivered just the way you want them.

You need to meet rigorous day-to-day requirements to confirm the identity of known compounds, rapidly identify unknowns, and characterize complex sample components. ■ For your specific needs, Waters offers a solution that pairs the exact mass, high resolution, and wide linear dynamic range of the LCT Premier™ XE Mass Spectrometer with the resolution, speed, and sensitivity of the ACQUITY UPLC® System. ■ Add powerful software Application Managers options to capture, store, and process data – and get your customized qualitative results – for everything from intact proteins to drug metabolites, process impurities, and pesticide residues.

A unique exact mass UPLC®/MS solution for high-resolution, high-sensitivity analyses: Waters® ACQUITY UPLC System with the LCT Premier XE Mass Spectrometer.

> "...we conclude that a mass spectrometer capable of 3 ppm mass accuracy and 2% error for isotopic abundance patterns outperforms mass spectrometers with less than 1 ppm mass accuracy...that do not include isotope information in the calculation of molecular formulae."

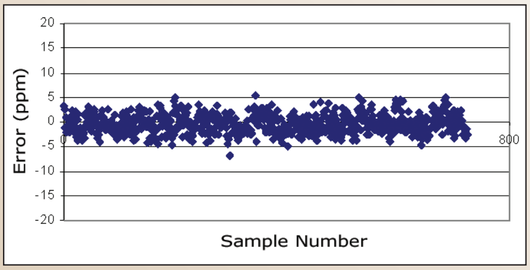
KIND T, FIEHN O.
Metabolomic database annotations via query of elemental compositions: Mass accuracy is insufficient even at less than 1 ppm.
BMC Bioinformatics. 2006 Apr 28;7:234.

THE BENEFIT OF EXACT MASS

You've measured the mass of your compound. How confident are you that you've identified it correctly?

The more accurate your measurement, the more confident you can be in your results. The LCT Premier XE, with its orthogonal acceleration time-of-flight (oa-TOF) analyzer, provides the capability of routine exact mass measurement (sub-3 ppm) when compared to instruments such as scanning quadrupole or ion trap style, which only provide nominal mass at best (0.1 Da).

Exact mass measurement enables you to identify the elemental composition of compounds with greater confidence. Even if you currently use a more expensive MS/MS system, nominal mass data can still make spectra difficult to interpret. Get more significant information using the increased accuracy of exact mass measurement with the easy-to-use LCT Premier XE Mass Spectrometer. Exact mass can also be obtained with in-source CID (collision induced dissociation) on the LCT Premier XE, providing fragmentation to aid in structural identification.



Exact mass measurement over long time periods. Compound X was analyzed via repeat injections over a time course of 10 days. The mean RMS mass measurement error for these data = 1.9 ppm.

Compound	Actual Mass	Measured Mass	mDa Error	ppm Error
4-acetamidophenol	152.0711	152.0807	-0.3	-2.0
sulfaguanidine	215.0602	215.0597	-0.5	-2.3
Sulfadimethoxine	311.0814	311.081	-0.4	-1.3
Val-Tyr-Val	380.2185	380.219	0.5	1.3
Terfenadine	472.3215	472.321	-0.5	-1.1
Leucine enkephalin	556.2771	556.2775	0.4	0.7
Reserpine	609.2812	609.2828	1.6	2.6
Erythromycin	734.469	734.4695	0.5	0.7
			RMS ppm error	1.6

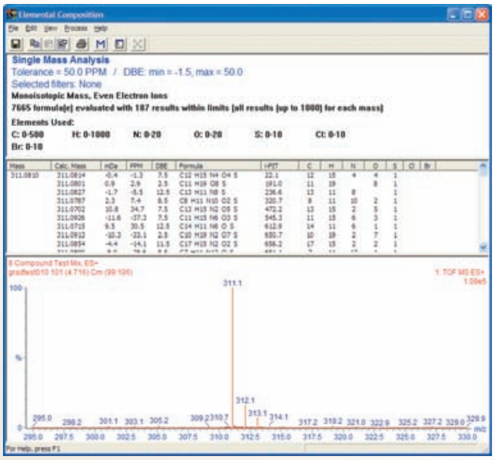
Exact mass measurement for a range of compounds from LC/MS analysis. Exact mass measurement is obtained for each compound with the mean RMS error = 1.6 ppm.

CONFIDENCE IN COMPOSITION, STRUCTURE, AND SPECIFICITY

Nominal mass measurement does not give you the complete picture – even with MS/MS.

With spectral resolution in excess of 12,000 FWHM provided by the high efficiency, high sensitivity and fast acquisition oa-TOF analyzer, automated exact mass measurement, in combination with the LockSpray™ ionization interface, is easy on the LCT Premier XE.

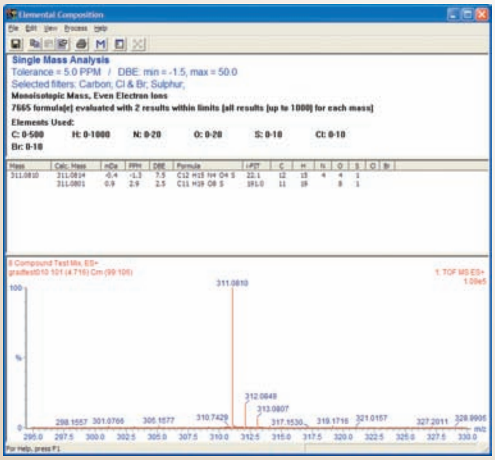
The accurate isotope patterns produced by the LCT Premier XE have allowed the provision of highly sophisticated pattern matching and elemental prediction algorithms to be incorporated into MassLynx™ Software. With MassLynx i-FIT,™ elemental composition calculations can be carried out utilizing a wide range of elements, and with the confidence of a simplified results list.



Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None
Monoisotopic Mass, Even Electron Ions
7665 formula(e) evaluated with 187 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-20 O: 0-20 S: 0-10 Cl: 0-10
Br: 0-10

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	C	H	N	O	S	Cl	Br
311.0810	311.0814	-0.4	-1.3	7.5	C12 H15 N4 O4 S	22.1	12	15	4	4	1		
	311.0801	0.9	2.9	2.5	C11 H19 O8 S	191.0	11	19		8	1		
	311.0827	-1.7	-5.5	12.5	C13 H11 N8 S	236.6	13	11	8		1		
	311.0787	2.3	7.4	8.5	C8 H11 N10 O2 S	320.7	8	11	10	2	1		
	311.0702	10.8	34.7	7.5	C13 H15 N2 O5 S	472.2	13	15	2	5	1		
	311.0926	-11.6	-37.3	7.5	C11 H15 N6 O3 S	545.3	11	15	6	3	1		
	311.0715	9.5	30.5	12.5	C14 H11 N6 O S	612.9	14	11	6	1	1		
	311.0912	-10.2	-33.1	2.5	C10 H19 N2 O7 S	650.7	10	19	2	7	1		
	311.0854	-4.4	-14.1	11.5	C17 H15 N2 O2 S	656.2	17	15	2	2	1		

At m/z 311, with nominal mass measurement accuracy, there are 620 possible elemental combinations. (Using element: $C_{500}H_{10000}N_{20}O_{20}S_{10}Cl_{10}Br_{10}$).



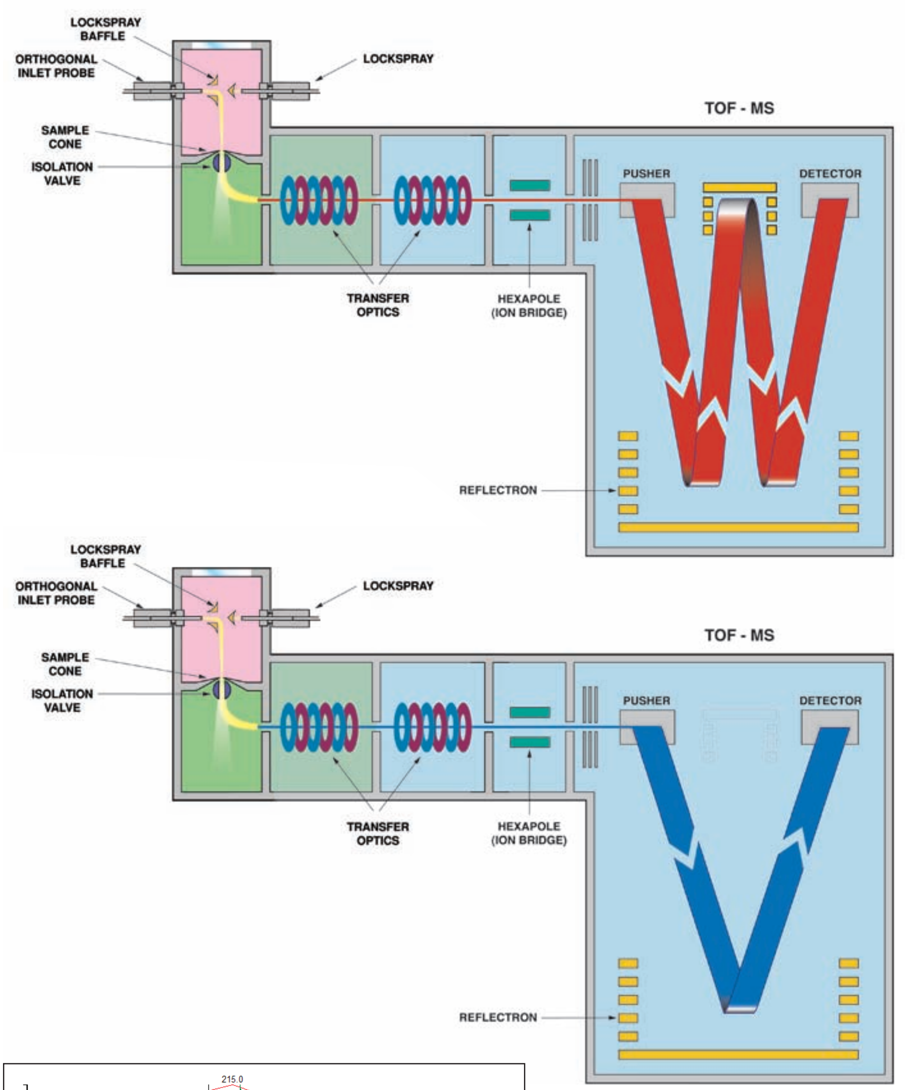
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: Carbon; Cl & Br; Sulphur;
Monoisotopic Mass, Even Electron Ions
7665 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-20 O: 0-20 S: 0-10 Cl: 0-10
Br: 0-10

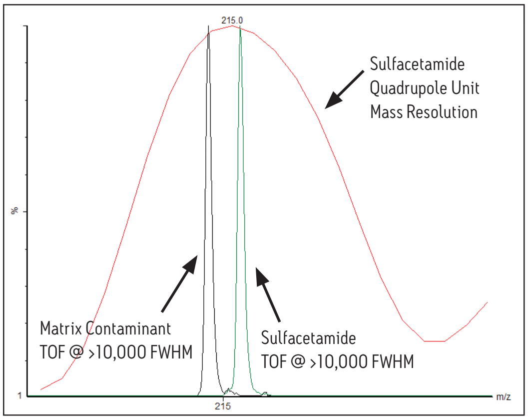
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	C	H	N	O	S	Cl	Br
311.0810	311.0814	-0.4	-1.3	7.5	C12 H15 N4 O4 S	22.1	12	15	4	4	1		
	311.0801	0.9	2.9	2.5	C11 H19 O8 S	191.0	11	19		8	1		

With exact mass measurement (sub 5 ppm) and isotope interpretation with MassLynx Software (i-FIT), there are only two possible elemental compositions with the top results being the correct formula.

W-OPTICS AND V-OPTICS

W-Optics™ is a novel method for enhancing resolution without increasing instrument footprint. By activating an additional ion mirror in the TOF analyzer, the unique flight path of the ions is effectively doubled, producing two-times improvement in resolution with negligible loss in signal-to-noise (S/N) detection. With the LCT Premier XE, W-Optics provides up to 15,000 FWHM, with greater than 10,000 FWHM at low m/z values, to provide you with greater confidence in your answer.





Improved specificity with exact mass measurement makes it possible to differentiate between analyte and matrix, increasing confidence in your answer.

HIGH RESOLUTION

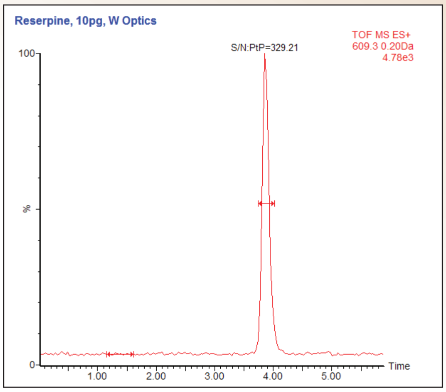
Enhanced resolution is vital for identifying components in complex mixtures, and is also essential for enabling automated exact mass measurements. High resolution minimizes potential interferences to the peak shape of your analyte of interest. By removing matrix effects, a more accurate measurement of m/z can be made.

The inherent high resolution of an oa-TOF, in conjunction with exact mass MS, enables compounds to be more easily identified and aids determination of elemental composition. Data processing tools also rely heavily on the specificity of exact mass measurements, such as database searching.

LOWER DETECTION LIMITS ACROSS FULL MASS RANGE

LCT Premier XE delivers unsurpassed sensitivity for full spectrum LC/MS

The dual-stage ion guide transfer region has lowered detection limits by an order of magnitude over the previous generation of oa-TOF systems. As a result, the LCT Premier XE not only provides you with the sensitivity you need to confirm analytes of interest in your sample, but it also enables you to identify low levels of unexpected components that scanning systems or selected ion recording may miss.

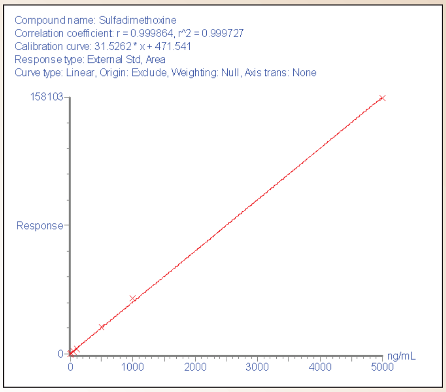


This example shows 10 pg of reserpine injected on-column. S/N is typically in excess of 100:1.

DYNAMIC RANGE ENHANCEMENT (DRE)

LCT Premier XE has the widest proven detection dynamic range of any oa-TOF available

The advantage of the full mass range spectra produced by the LCT Premier XE enables a wide range of components, both known and unknown, to be detected with high sensitivity. Full mass range spectra are beneficial when trying to fully characterize samples in terms of component identity and quantity. The extended dynamic range of the LCT Premier XE delivers up to four orders of magnitude for exact mass measurement and quantitative studies, allowing you to maximize the information produced from a single analysis.



This example of sulfadimethoxine (0.5-5000 ng/mL) demonstrates up to 4 orders linear dynamic range with DRE enabled.

POWERFUL TECHNOLOGY PLATFORM

LCT Premier XE Mass Spectrometer provides a powerful platform for your application analysis needs

- **Compact Size** – Powerful oa-TOF technology that uses minimal linear bench space
- **High Resolution** – Greater than 12,000 FWHM and 10,000 FWHM below 200 m/z
- **High Mass Measurement Accuracy** – Routine exact mass measurement (3 ppm RMS) with LockSpray
- **High Sensitivity Analyzer** – Low femtomole/picogram full spectrum detection
- **Wide Dynamic Range** – Over 4 orders of magnitude for exact mass measurement and quantitation
- **High m/z TOF Analyzer** – Up to 30,000 m/z ideal for protein applications
- **ZSpray™ Enabled** – Premium API interface for unsurpassed ruggedness and sensitivity
- **LockSpray with ESI as Standard** – Dual ESI ion source for simple exact mass measurement
- **ESCi® Multi Mode Ionization Source with LockSpray** – Dual ESI and APCI ionization during a single analysis for diverse compound coverage and exact mass
- **Fast Acquisition** – 20 spectra/sec providing compatibility for UPLC separations
- **Positive/Negative Ionization** – Alternating ionization modes with exact mass measurement
- **Wizard-Driven Software Technology** – Simplified instrument setup and calibration at the click of a button

Options

- **IonSABRE™ APCI with LockSpray** – For polar/non-polar analytes
- **NanoLockSpray™** – Exact mass ion source for low flow rate and nanoLC applications
- **Dual APPI/APCI Ion Source** – Dual ionization capability for the comprehensive analysis of non-polar compounds
- **Oil-free Scroll Pumps** – Alternative to standard oil-filled rotary backing pumps
- **Non-Covalent Enhancement Option** – Capability of analyzing non-covalent protein complexes

LCT PREMIER XE OPTIONS

The LCT Premier XE provides sensitive, full spectrum MS with exact mass measurement for the detection of components in each of these key applications

Open Access (Walk-up) Exact Mass

- Exact mass MS for elemental composition calculations with i-FIT
- Integrated LC and autosampler with environmental control for samples
- Automated exact mass data processing using OpenLynx™ Application Manager

Pesticide Residue Screening

- High sensitivity full spectrum detection for multiple analyte detection over a wide dynamic range
- Low ppb detection
- Exact mass with LockSpray for enhanced data confidence
- ChromaLynx with library searching for compound identification

Natural Product Identification

- High-sensitivity, full-spectrum detection for multiple analyte detection
- Exact Mass and in-source CID for accurate identification
- Automated exact mass data processing

Metabonomics

- Exact mass MS for elemental composition calculation with i-FIT to facilitate biomarker identification
- Integrated LC control for superior solvent delivery and sample management
- High sensitivity MS for low level detection
- Dynamic statistical processing and visualization of complex data sets using MarkerLynx™ Application Manager

Metabolite Identification

- Exact mass MS for elemental composition determination
- Wide detection dynamic range for combined rate and route studies
- Automated ID of metabolites using MetaboLynx™ Application Manager

Biological/Protein Characterization

- Enhanced sensitivity for low abundance proteins
- High m/z TOF analyzer for non-covalent protein detection
- Wide dynamic range detection
- High mass accuracy for Peptide Analysis or Protein Identification and Characterization
- Analyze and assign results to define the sequence of known proteins using BiopharmaLynx™ Application Manager

MASSLYNX APPLICATION MANAGERS

MassLynx Software can be further enhanced with a range of Application Managers to supplement the capabilities of your system

OpenLynx Application Manager

Provides walk-up LC/MS capabilities and automated batch processing of single or large batches of compounds, exact mass data with i-FIT elemental composition calculations

MetaboLynx Application Manager

Automates metabolite identification with an advanced control comparison

MarkerLynx Application Manager

Offers seamless multivariate statistical processing for large, complex metabonomics LC/MS data sets

BiopharmaLynx Application Manager

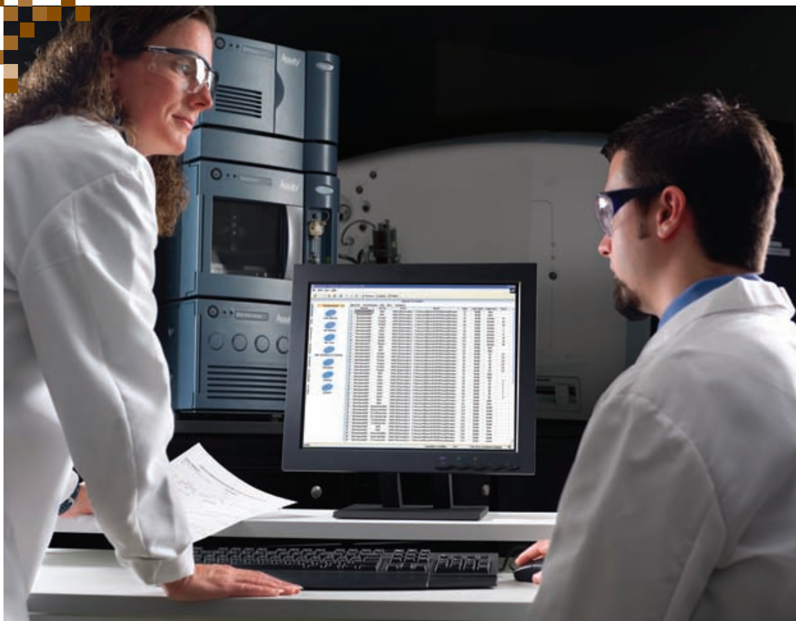
Designed to efficiently process, analyze, and report peptide and intact protein mass data for streamlining the characterization of biopharmaceutical products

TargetLynx™ Application Manager

Enables advanced quantification of target compounds with a full range of automatic quality control checks. Uses confirmatory ions for confident quantification of regulated compounds

ChromaLynx™ Application Manager

Facilitates the rapid detection, identification and semi-quantitative determination of components in complex mixtures. Provides library searching with exact mass scoring and elemental composition calculation with i-FIT



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