



**Accelerate your Quantitative LC/MS
Workflows with a Fully Integrated
UHPLC-QQQ Platform**

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Pittcon

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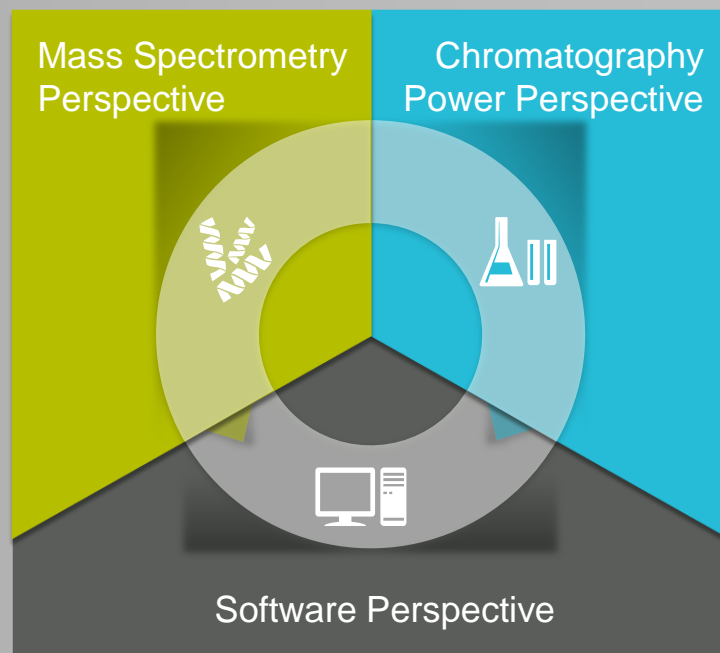
Outline

- Thermo Scientific™ Vanquish™ UHPLC System
- Thermo Scientific™ TSQ Endura™ Triple Quadrupole Mass Spectrometer (MS) and Thermo Scientific™ Quantiva™ Triple Quadrupole Mass Spectrometer
- Thermo Scientific™ Dionex™ Chromeleon™ Chromatography Data System (CDS) Software 7.2 for LCMS

Why a New UHPLC?

Customers told us they need:

- More resolution
- More sensitivity
- Easier and less method development
- More productivity
- Easier interaction and operation
- More robust and more reliable
- More sample capacity
- More access to experts
- More and fast service
- New, fresh & exciting instruments
- Better results in shorter time



The New Thermo Scientific Vanquish UHPLC System



We heard you! And we:

- Started with a complete new design in line with MS portfolio
- Put in 30 years of experience and know-how
- Developed a new and unique technology
- Closed gaps and pushed beyond previous limitations
- Boosted robustness
- Developed a new column technology
- Built the best UPHLC around the column/user
- Further leveraged our gold standard CDS software
- Boosted serviceability beyond established concepts

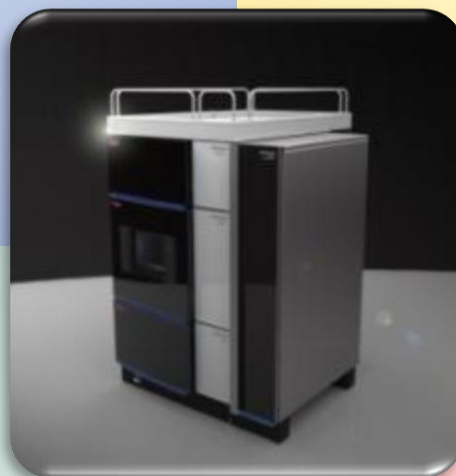
Vanquish System...Provides More Solutions!

- Vanquish UHPLC is not only a system – it is a problem-solving solution philosophy



Better integration with the world's best mass spectrometers

Maximum speed and resolution with new Thermo Scientific™ Accucore™ Vanquish™ columns



Revolutionary ease-of-use experience by new Chromeleon CDS features and workflows

More throughput capacity with the new Thermo Scientific Vanquish Charger module



Vanquish System is...

Confidence



Controlling the separation with more confidence

- 2 thermostating modes
- 5 °C to 120 °C temperature range
- Active preheating

Power



Driving the separation with more power

- 1500 bar (22,000 psi) of pump pressure
- Flow rate up to 5 mL/min
- 2 × 3 solvent channels

Sensitivity



Detecting the analyte with more sensitivity

- Linear up to 3000 mAU
- Noise levels down to $\pm 3 \mu\text{AU}$
- Lowest dispersion with Thermo Scientific™ LightPipe™ technology

Accuracy



Handling the sample with more accuracy

- Up to 23 well plates for up to 8832 samples
- Unsurpassed sample dosage
- Automation of workflows with barcode reading



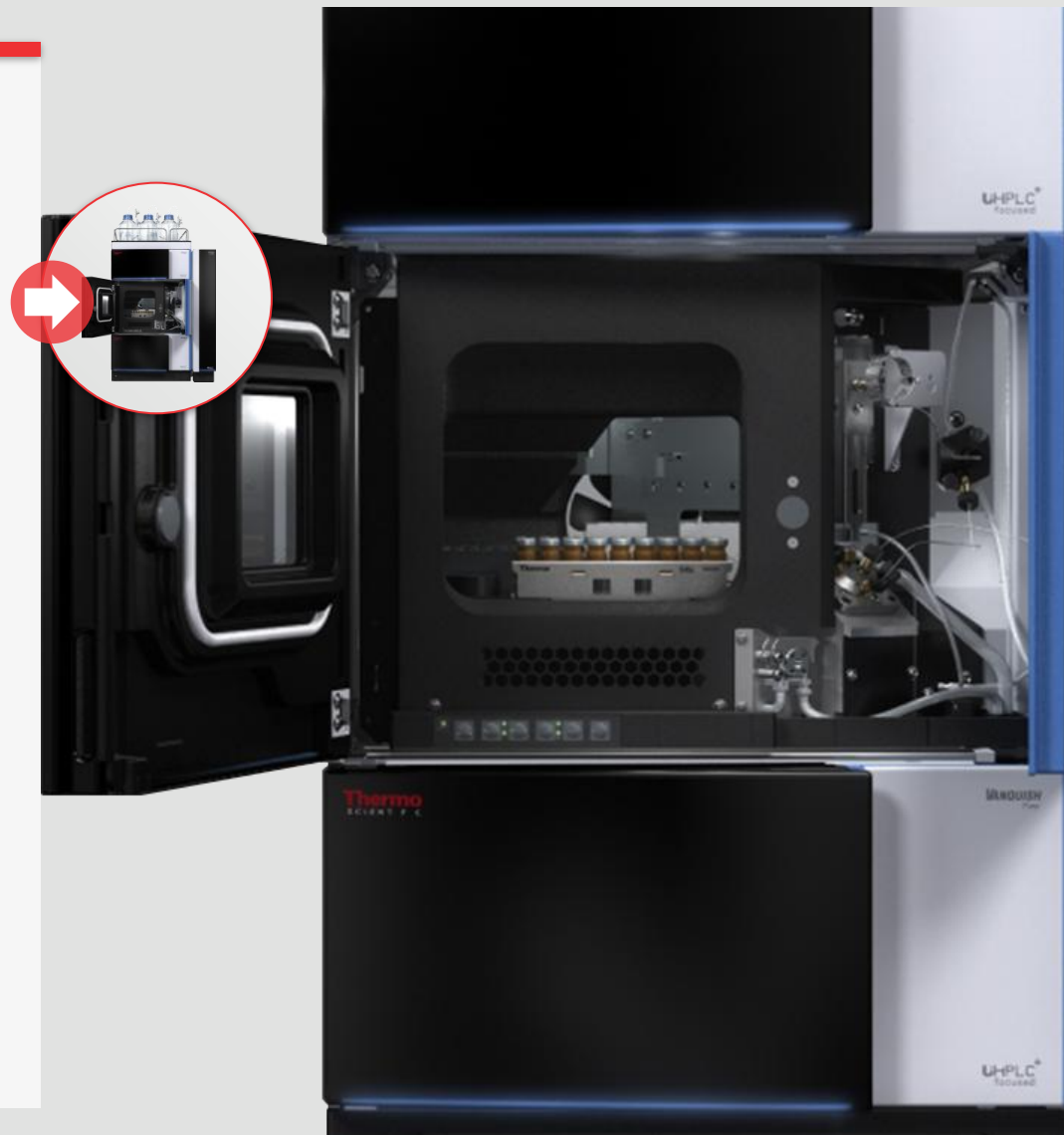
Vanquish Binary Pump

Feature	Benefit
1500 bar / 22 000 psi Up to 5000 $\mu\text{L}/\text{min}$	Flexibility for all working conditions
New parallel dual piston principle	very small pressure ripple => column and sensitivity
Adaptive Thermal Effect Compensation (ATEC™)	best flow and gradient performance => RT stable
2 × 3 solvent channels	9 different solvent combinations
Fingertight check valve design	Easy to service



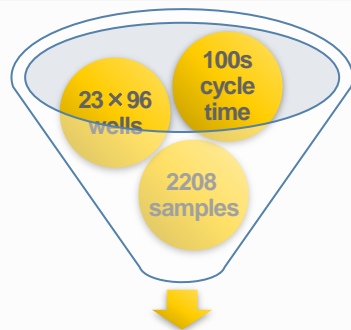
Vanquish Split Sampler

Feature	Benefit
New switching valve	no maintenance
Adjustable GDV	easy method transfer
Automatic sample pre-compression	<ul style="list-style-type: none">• reduced physical stress on column = longer lifetime• better retention time reproducibility
New air-to-air cooling concept	no condensation
Increased sample capacity	4 racks or well plates
Automated barcode reader	Rack tracking (esp. with Charger)



Vanquish Charger Module

- Fully integrated robotic unit with less than 1 min cycle time
- Hosts up to 9 additional racks/ deep well plates or 20 shallow well plates
- Up to 9000 samples – temperature controlled
- Precise temperature control using new designed air stream cooling concept
 - 4 – 40 °C
- Integrated barcode reader



One weekend full of results



The Vanquish Column Compartment

Feature	Benefit
Active Pre-Heater	Perfect temperature control (QC)
Two thermostating modes	Easy method transfer
Three independent column compartments	Method scouting, different temperature zones



Vanquish Column Compartment for MS integration

Feature	Benefit
Column compartment is vertical	The column outlet is closer to the MS ion source
Position of the column compartment can be to the left or to the right	Better integration with all Thermo Scientific Mass Spectrometers



Vanquish Diode Array Detector

- LightPipe technology for an unmatched detection experience
 - 10 mm standard flow cell
 - 60 mm high sensitivity flow cell
- Best signal-to-noise performance
- Lowest baseline noise
- Ultra-wide dynamic range
 - Up to 3000 mAU
 - For simultaneous detection of highly concentrated compounds and trace impurities
- Variable slit width for optimum resolution
1 – 8 nm
- Low peak dispersion
- Reduced RI and thermal effects

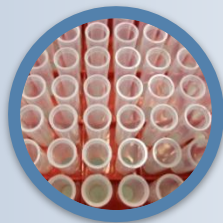


Vanquish System Features & Benefits for LC-MS Users

- Improved separation performance

FEATURE	BENEFIT
<ul style="list-style-type: none">• Better resolution• Minimal peak dispersion	<ul style="list-style-type: none">• Less matrix effects• More consistent quantification• More consistent sensitivity
<ul style="list-style-type: none">• Faster analysis	<ul style="list-style-type: none">• Improved LCMS productivity
<ul style="list-style-type: none">• Rock solid retention time stability	<ul style="list-style-type: none">• More reliable identification• More reliable quantification
<ul style="list-style-type: none">• New core enhanced 1.5 μm columns	<ul style="list-style-type: none">• Less method development• Less peaks of interest in the void volume

Challenges in Quantitative Mass Spectrometry

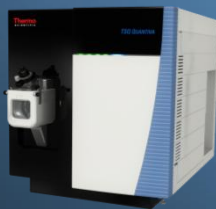


Large Sample Numbers



Low Concentration

Triple Quads



TSQ Endura MS and TSQ Quantiva MS



TSQ Endura MS

Extreme Quantitative Value

- Best-in-class sensitivity
- Unprecedented usability
- Ultimate robustness



TSQ Quantiva MS

Extreme Quantitative Performance

- Attogram sensitivity
- Unprecedented usability
- Exceptional robustness

Sensitivity, Speed & Robustness for High-Throughput Laboratories



TSQ Quantiva MS

Extreme quantitative performance

- Designed for the most challenging assays.
- For scientists needing to stay at the forefront of analytical technology

	TSQ Quantiva MS	TSQ Endura MS
Mass Range	10-1850	10-3400
Max SRM Number	30,000 SRMs	30,000 SRMs
SRM/Sec	500 SRMs/sec	500 SRMs/sec
Ion Optics	Active Ion Management (AIM)	S- LENS with Beam Blocker Technology
Quadrupole Design	<ul style="list-style-type: none">• Ion Max NG source• Electrodynamic ion funnel• ion beam guide with neutral blocker• 6 mm HyperQuad quadrupoles with asymmetric RF drive	4mm Quadrupoles with Asymmetric RF
Reserpine Specification	100,000 :1 S/N for 1 pg Reserpine	10,000 :1 S/N for 1 pg Reserpine

TSQ Endura MS

Extreme quantitative value

- Designed for non-stop operation.
- For scientist who need to run routine samples day in and day out.

Low Sample Concentration



Challenge

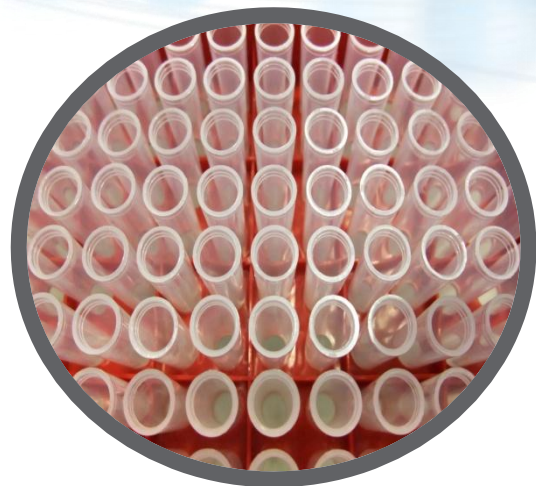
Demanding assays which require the absolute lowest limit of detection



TSQ Quantiva MS

Powered by AIM (Active Ion Management) technology, the TSQ Quantiva MS is the world's most sensitive triple quadrupole MS, detecting compounds at the ppt level.

Large Sample Numbers



Challenge

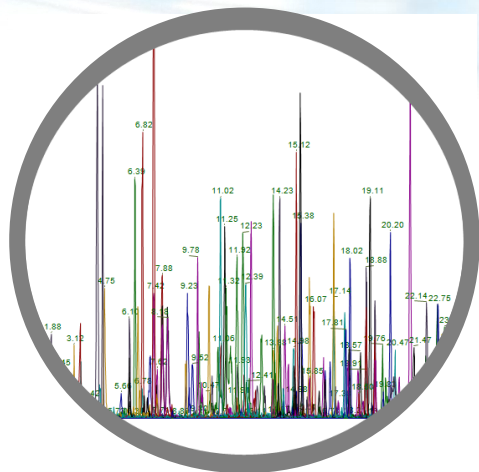
Need to analyze multi-residue analytes in very short run times, using UHPLC with robust performance 24/7



Vanquish System with Charger and TSO Quantiva MS

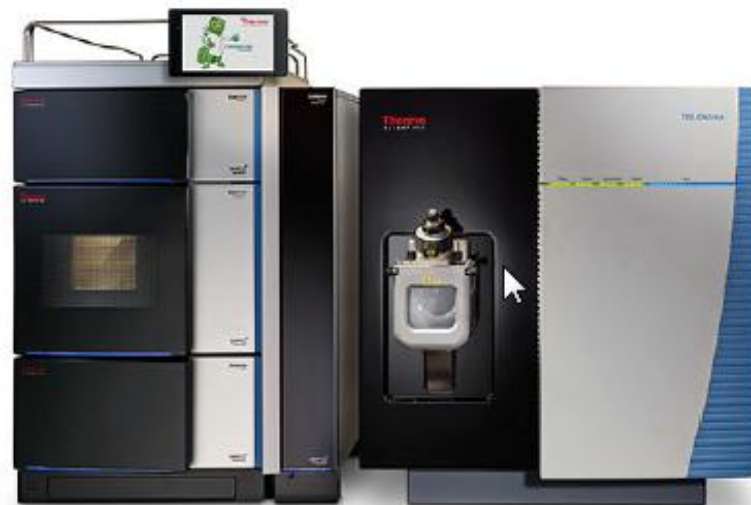
The AIM technology includes an ultra fast collision cell designed for fast SRMS with no loss in sensitivity. Neutral clusters eliminated for robustness.

Routine Quantitation



Challenge

Robust and reliable quantitation



TSQ Endura MS

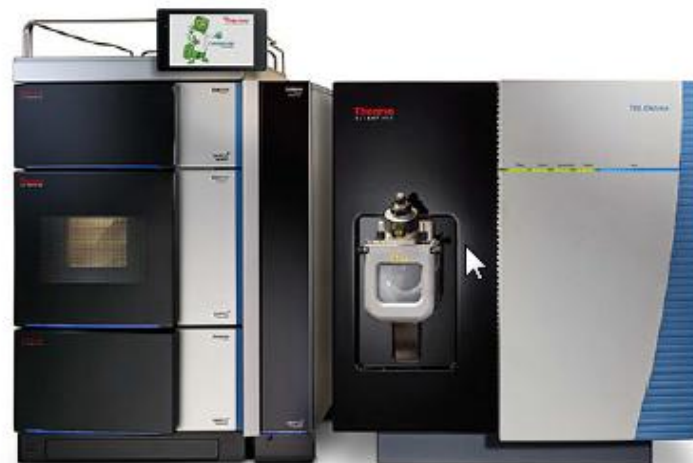
LODs and LOQs unrivaled in its class. It delivers this best-in-class quantitation run-after-run and day-after-day regardless of sample type or matrix.

TSQ Quantiva MS: Ease-of-Use



Challenge

Analysts don't have time to waste learning new software or optimizing methods.

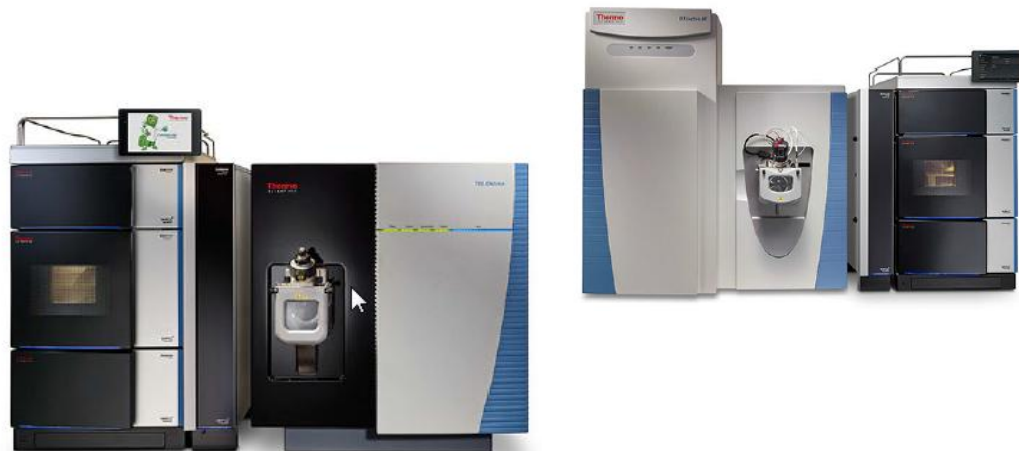


Vanquish System and TSQ MS with Chromeleon CDS Control

The entire software workflow has been redesigned to remove un-needed parameters.

Introduction

- How can you include MS in your laboratory CDS?
 - Currently it's on a workstation and there is no way to work remotely
- Chromeleon™ 7.2 Chromatography Data System is the first CDS to support MS instrument control and data processing with all main front-end separation techniques (GC, LC, IC) in an enterprise environment

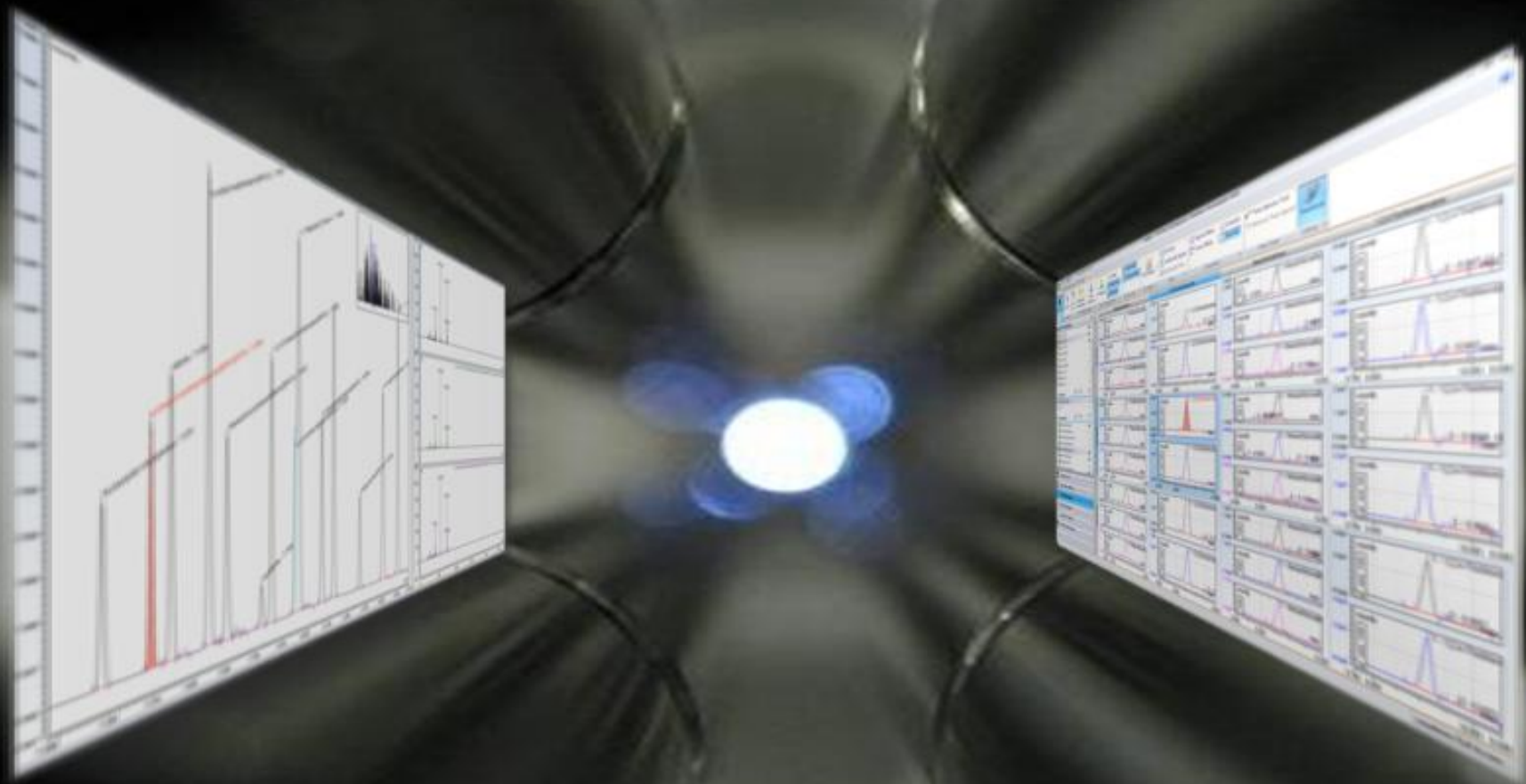


Quantiva & Endura - Fully Integrated within Chromeleon CDS

- Chromeleon 7.2 CDS supported workflows
 - Compliance, scalability, suite of quantification features
 - MS-specific data organization at component level
 - Context menu to open data in MS applications (e.g. Thermo Scientific™ Xcalibur™ Software)
- Key benefits
 - Only need to install, validate and learn one software package
 - Can use all compliance and processing features of Chromeleon CDS
 - Enhanced data security
 - Easily start analyses with eWorkflows™
 - Additional MS-specific detection algorithms (Genesis, ICIS)



MS Data Visualization



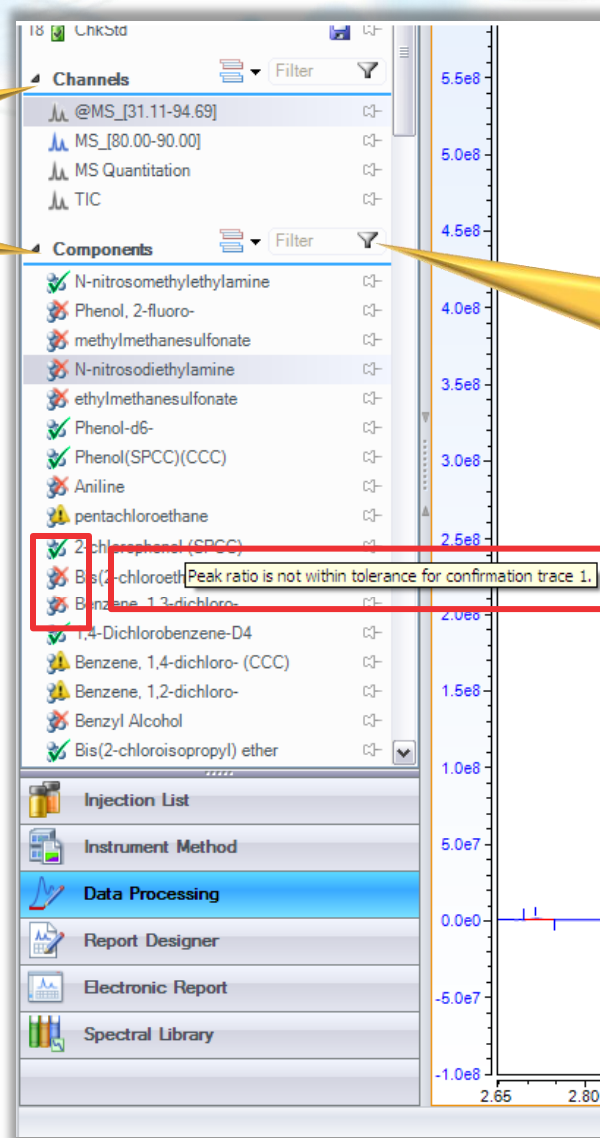
Seeing is believing...

Component and Channel Centric Data Viewing

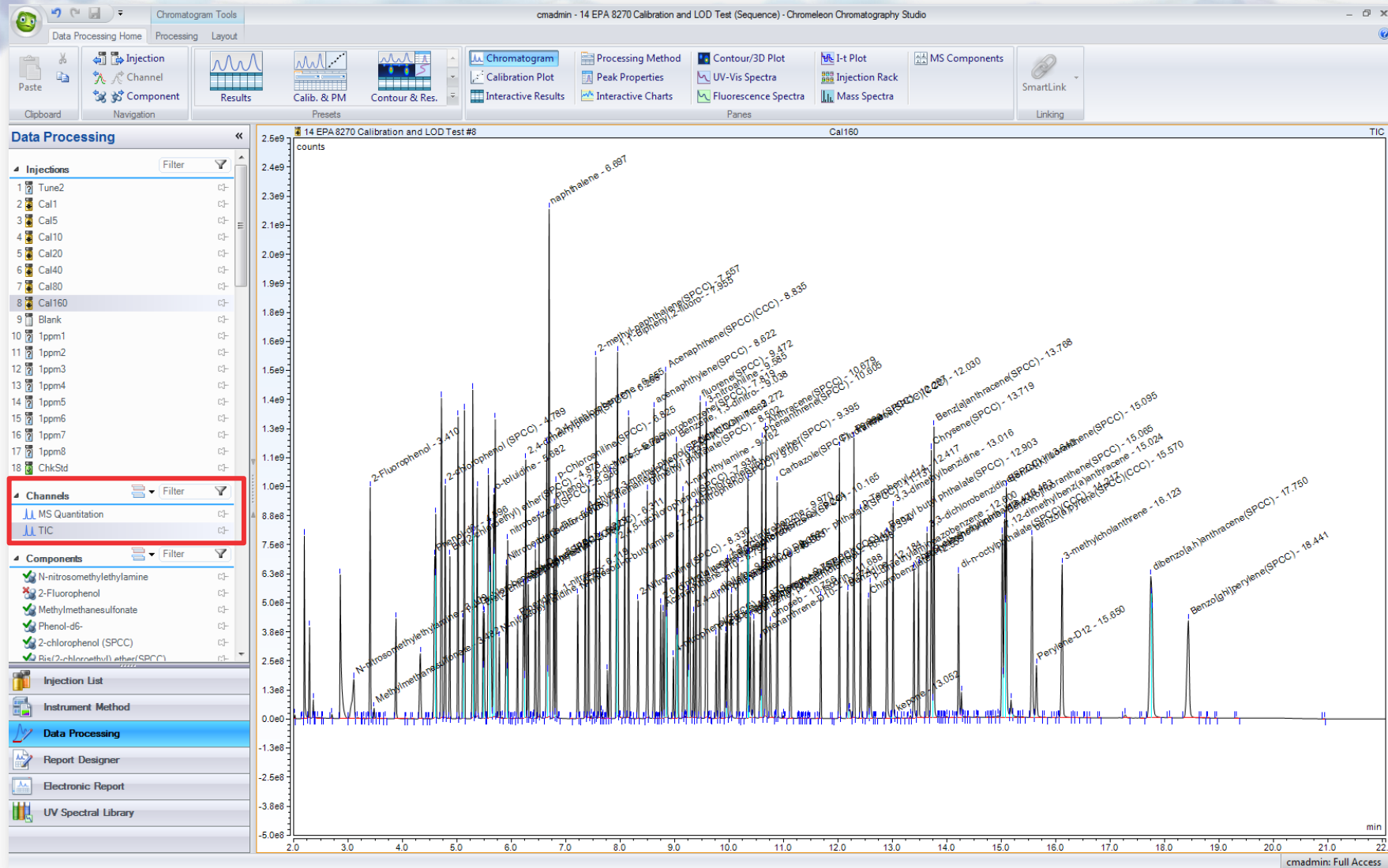
All channels and components listed and multi-selectable

Filter box to quickly narrow list of components or channels

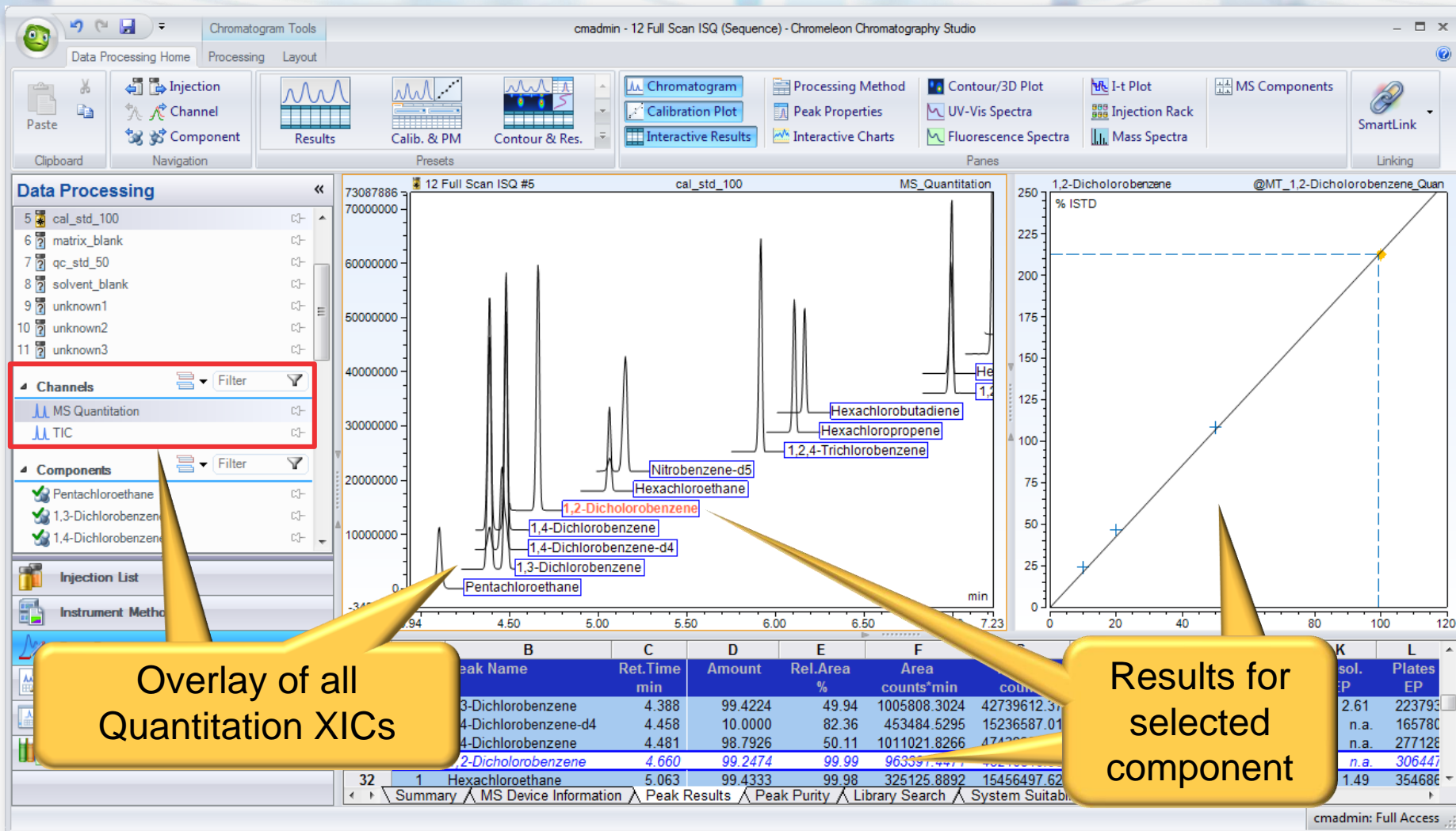
Components are tagged with tool tips, indicating analysis results



MS Data Views – Total Ion Chromatogram (TIC)



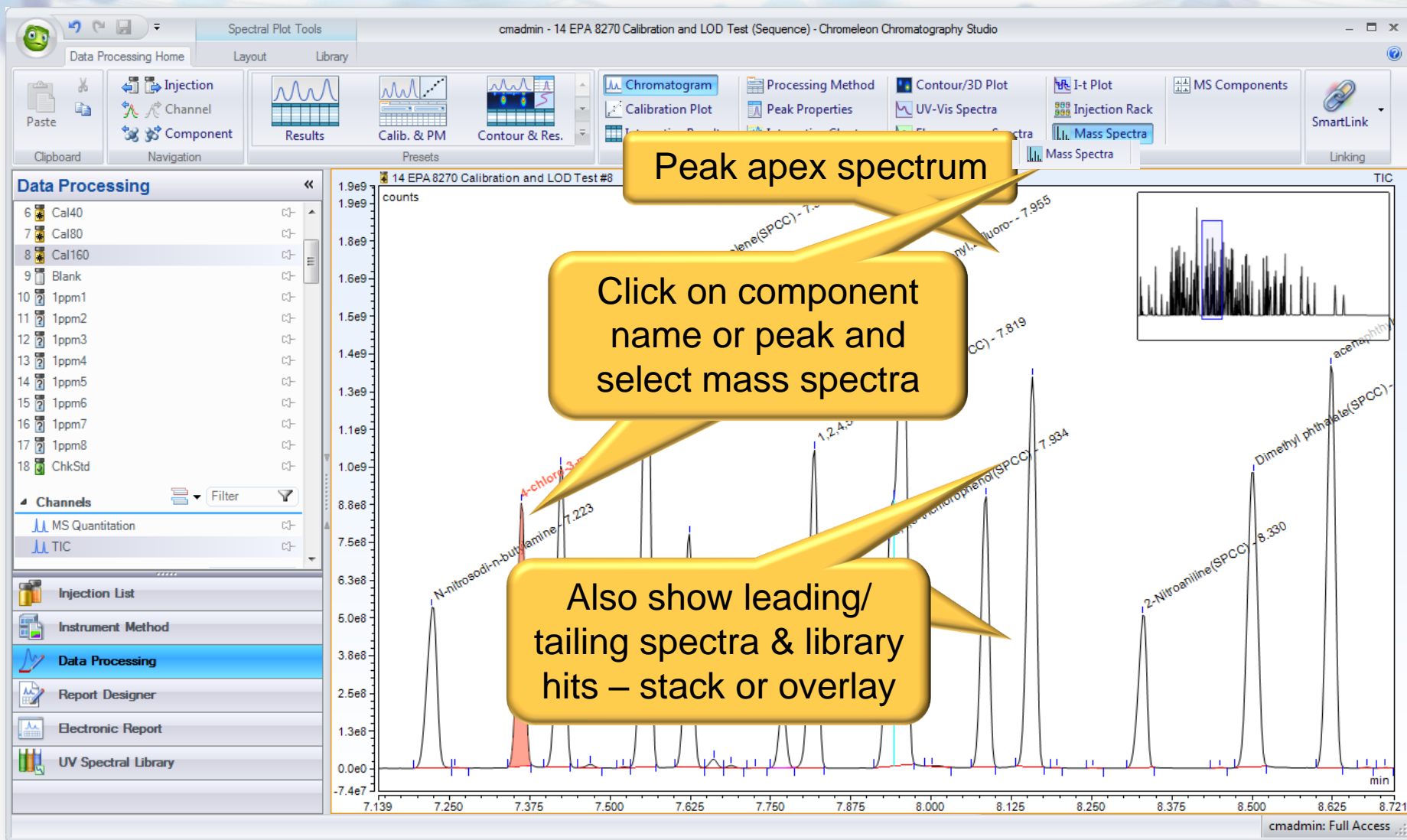
MS Data Views – MS Quantitation Channel



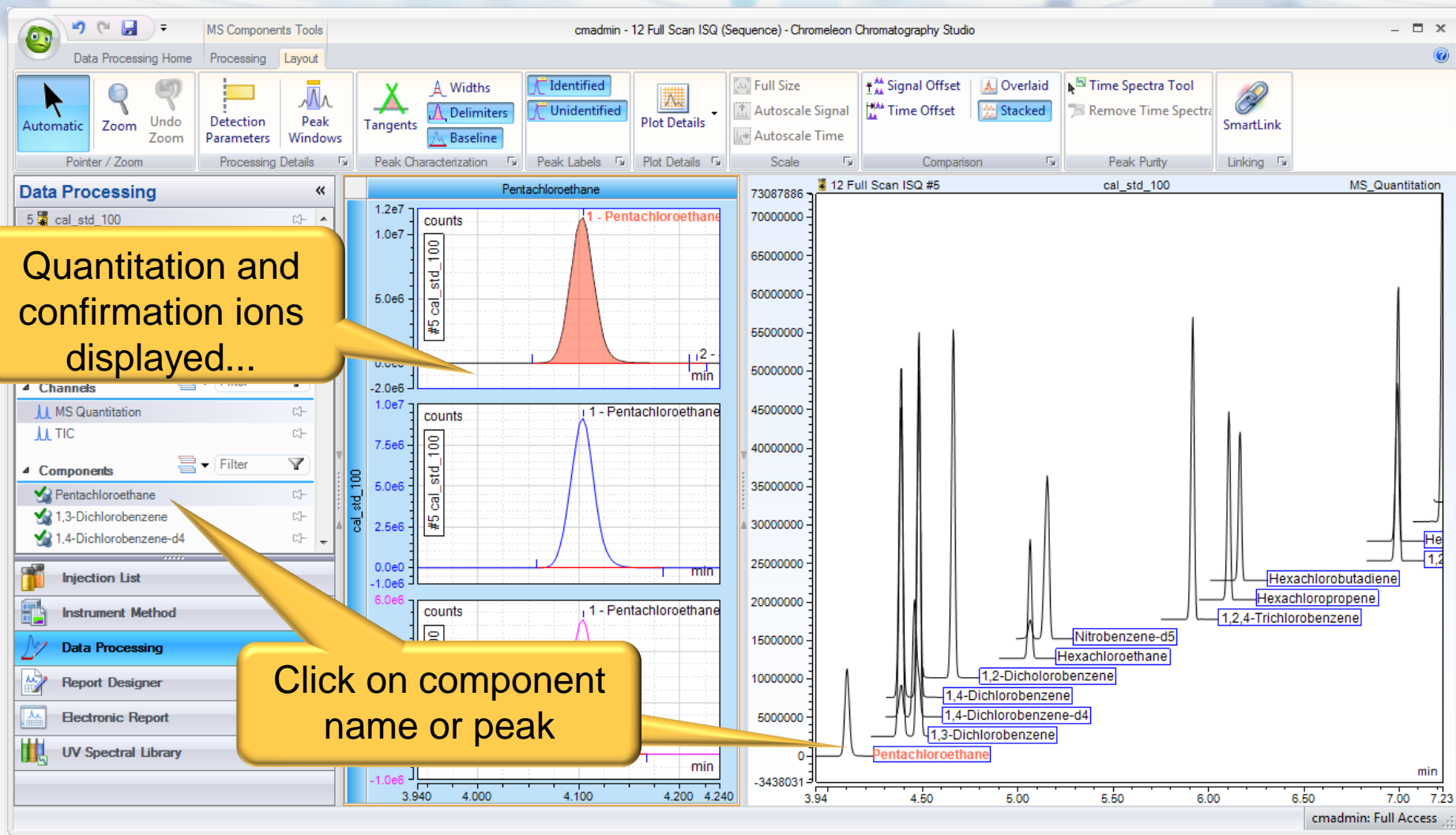
Overlay of all Quantitation XICs

Results for selected component

MS Data Views – Mass Spectrum Plot

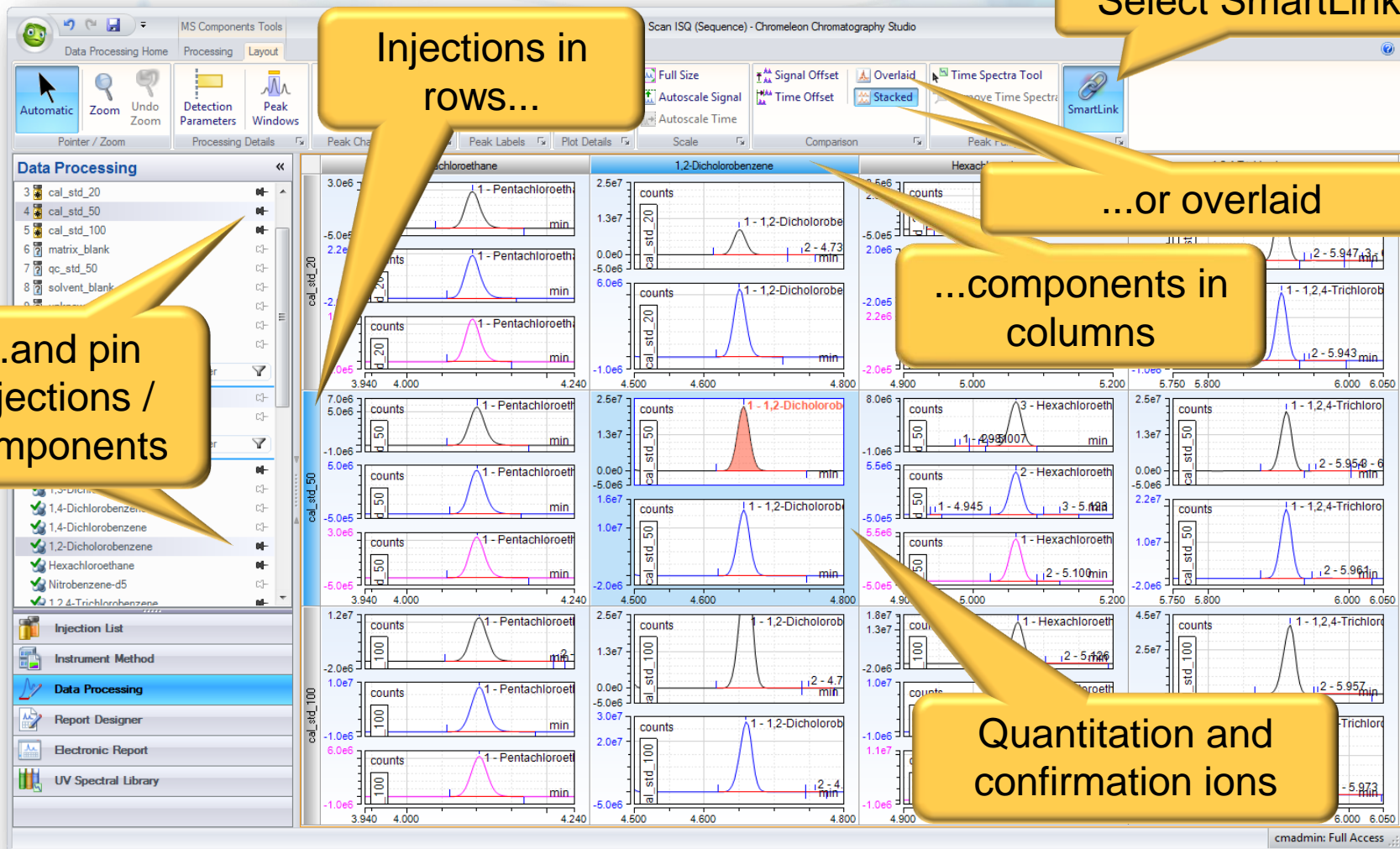


MS Data Views – Component Traces



Data Visualization – Multiple Components / Injections

- Using SmartLink and Component Traces...



MS Data Processing

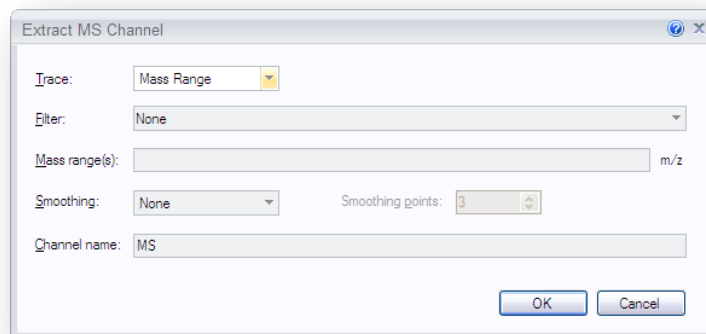


MS Data Processing

- With multiple traces and possibly hundreds of components, how can you quickly and easily process your MS data?
- How can you rapidly and accurately setup your component table?
- Existing data processing tools in Chromeleon CDS are now complimented by a suite of MS-specific tools for fast and efficient MS data processing, including:
 - Easy extracted ion chromatogram (XIC) creation
 - Additional MS-specific detection algorithms
 - Full processing control on a component-by-component basis
 - MS Library searching

MS Data Processing

- Apply all existing calibration modes and options to MS
- Easy extracted ion chromatogram creation
- Additional MS-specific detection algorithms
 - Genesis, ICIS
- Full processing control on a component-by-component basis
 - Additional MS-specific parameters in component table – quantitation and confirming ions, CAS numbers, molecular formulas, etc.



MS Data Processing – Extracted Ion Chromatograms

- Manual extraction of XIC

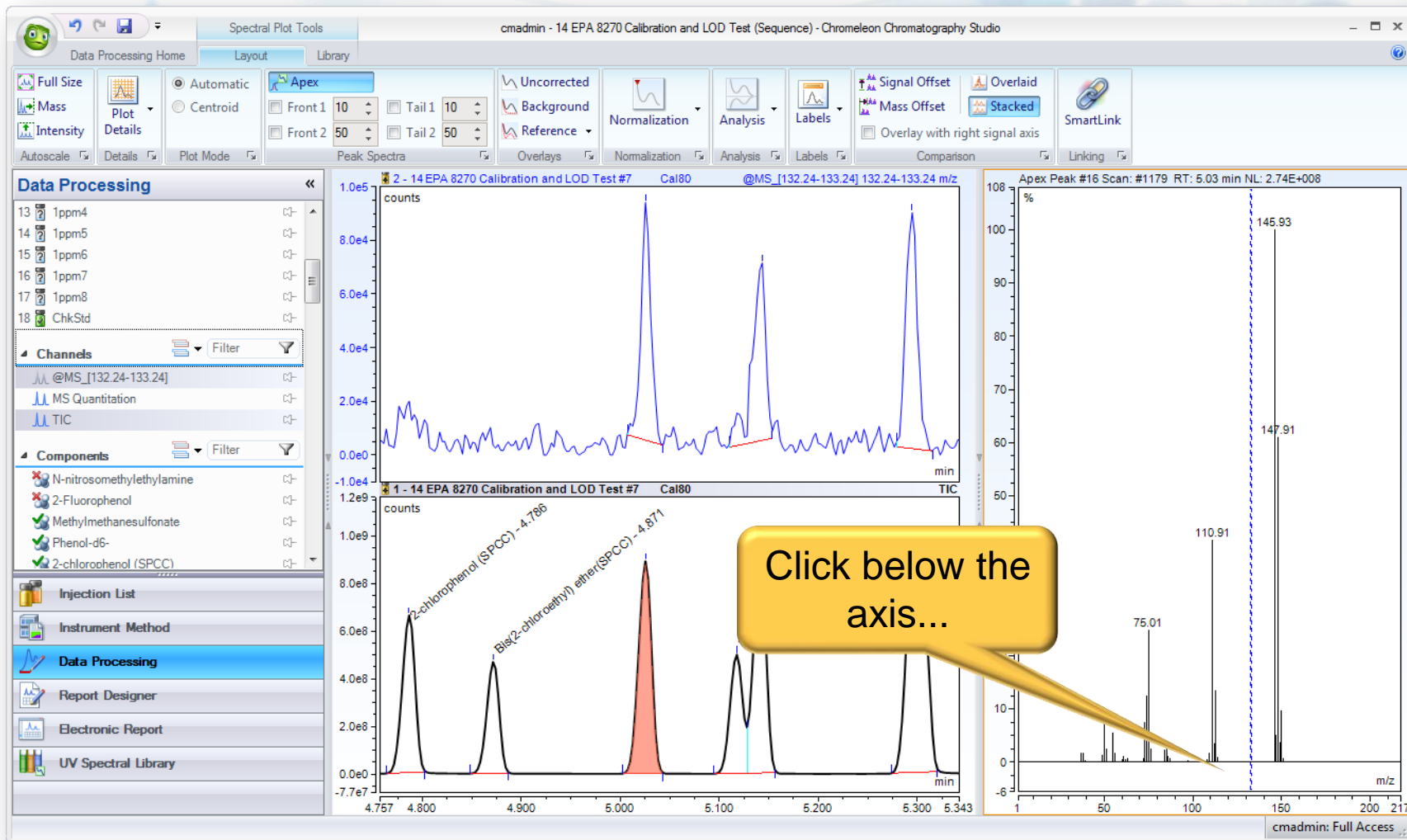
The screenshot displays the Chromeleon Chromatography Studio interface. The main window shows a chromatogram plot with a peak labeled '2-chlorophenol (SP)'. A context menu is open over the plot, with 'Extract MS Channel...' selected. The 'Extract MS Channel' dialog box is overlaid on the plot, showing the following settings:

- Trace: Mass Range
- Filter: {0,0} + c EI Full ms [35.00-500.00]
- Mass range(s): (empty field) m/z
- Smoothing: None Smoothing points: 3
- Channel name: MS_F1

Buttons for 'OK' and 'Cancel' are visible at the bottom right of the dialog box. A yellow callout box points to the 'Extract MS Channel...' option in the context menu with the text: 'Right-click on Channel or MS Plot'.

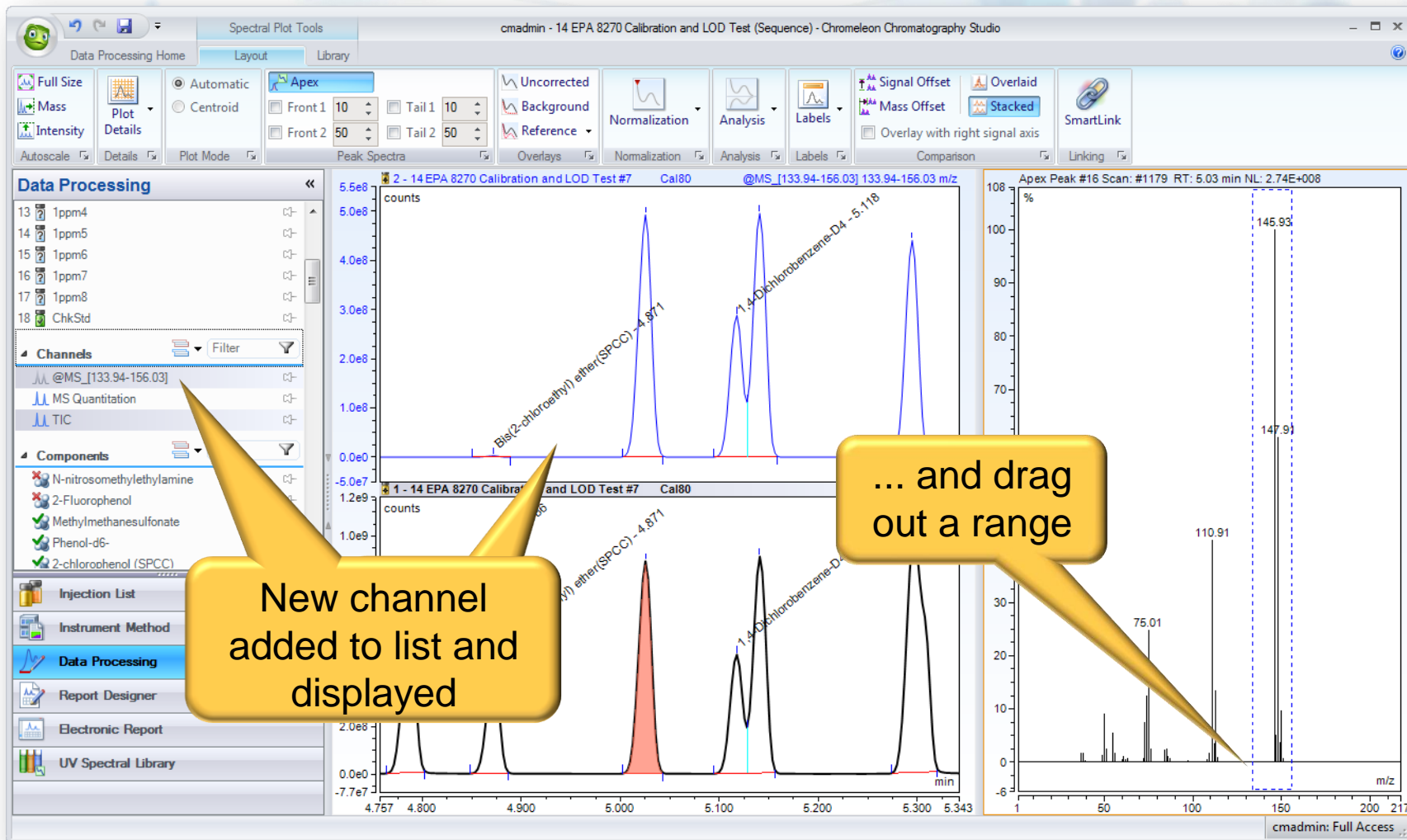
MS Data Processing – Extracted Ion Chromatograms

- Graphical extraction



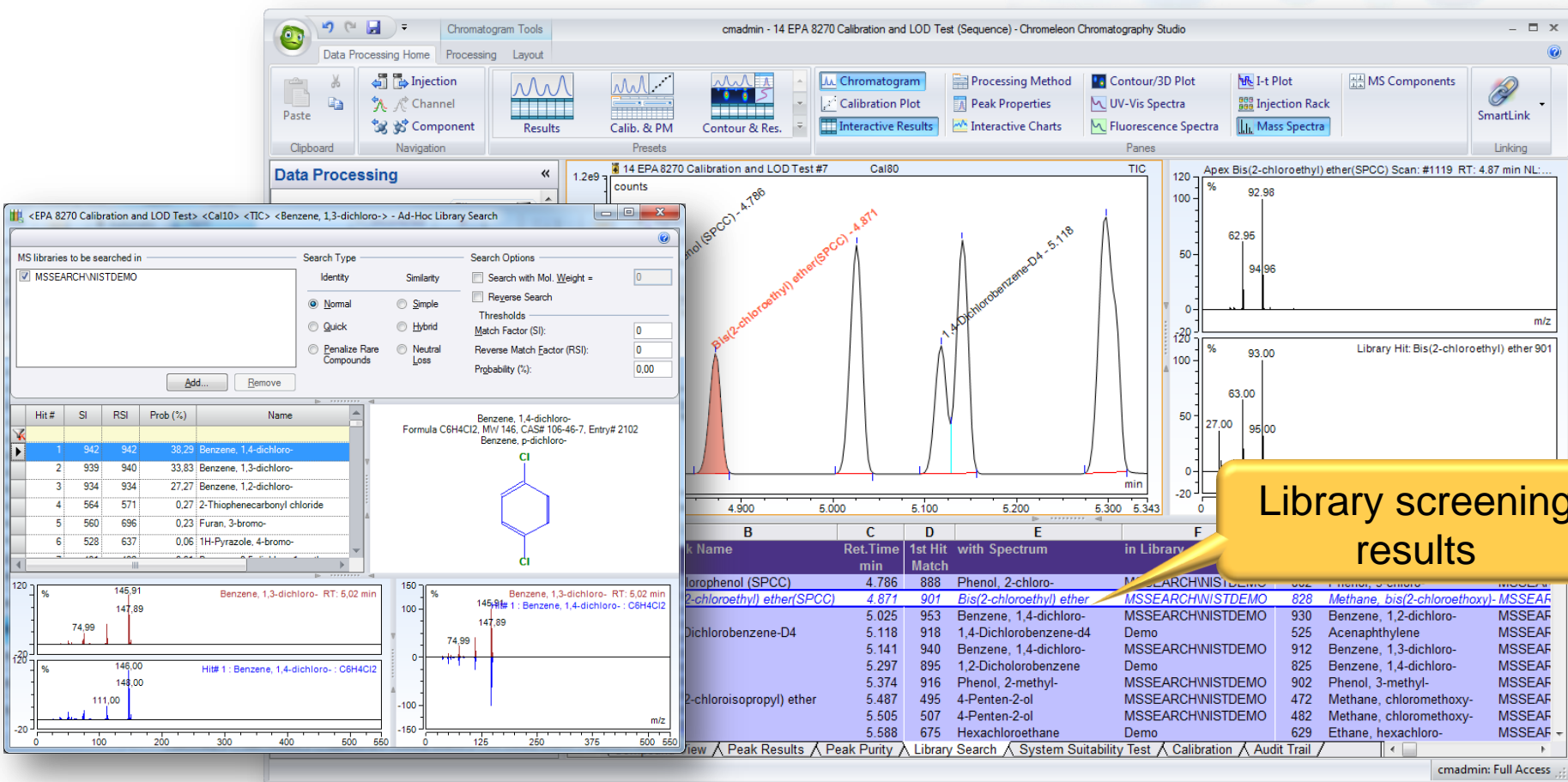
MS Data Processing – Extracted Ion Chromatograms

- Graphical extraction



Integrated NIST Library Search

- Use NIST libraries for spectral library screening and ad-hoc library search



Import from Compound Databases and NIST Libraries

- Quickly populate processing method component tables
- Use library searches
 - NIST
 - User libraries
- Use predefined compound data bases
 - Thermo Scientific™ TraceFinder™ software
- Use Xcalibur software raw files with component info

Compound Data Import

Data Source

NIST Libraries Path: C:\Program Files\NISTMS\MSSEARCH\NISTDEMO

Drag a column header here to group by that column.

	Name	Hit Probability (%)	Experiment Type	Category
1	Digitoxin	26,91	SIM	EI
2	Phenol, pentachloro-	98,79	SIM	EI
3	Benzenamine, 4-nitroso-N-phenyl-	5,35	SIM	EI
4	Pregn-4-ene-3,20-dione, 11-hydroxy-, (11 α)-	29,21	SIM	EI
5	Hydrocortisone Acetate	24,62	SIM	EI
6	4a,7-Methano-4aH-naphth[1,8a-b]oxirene, octahydro-4,4,8,8-tetramethyl-	29,96	SIM	EI
7	4a,7-Methano-4aH-naphth[1,8a-b]oxirene, octahydro-4,4,8,8-tetramethyl-	29,50	SIM	EI
8	Benzidine	91,34	SIM	EI

1 Quan Peak

	Mass	RT	Window (sec)	Polarity
1	184,02	6,25	6,78	+

2 Confirming Ions

	Mass
1	92,02
2	185,11

9 p,p'-DDT 43,90 SIM EI

Select All Unselect All Expand All Collapse All Import Cancel

MS Data Reporting

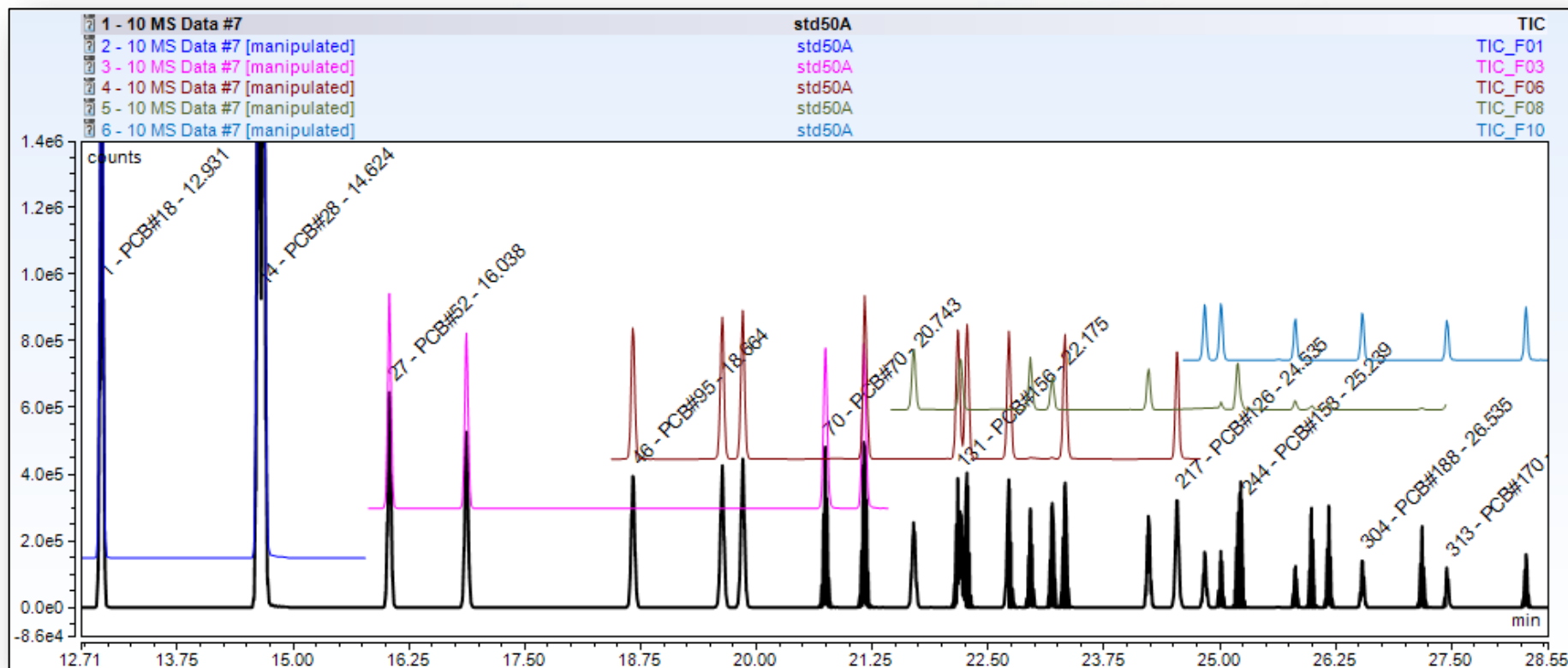


MS Data Reporting

- Can be a very time-consuming activity!
- Multiple components and traces make generic reporting tricky, if not impossible
- How do you effectively report such large quantities of data?
- Several new additions to Chromeleon CDS reporting tools
 - New MS based reporting objects
 - Mass Spectral Plot
 - Component Traces Plot
 - MS related report variables and tables
 - New tools for reporting of large amounts of multi-channel data
 - Consolidated Report Tables
 - Autorepeat Area Enhancements

MS Data Reporting

MS peaks often only appear in certain detection channels (filters) – how do you create a report for your peaks of interest?



MS Data Reporting – Consolidated Report Tables

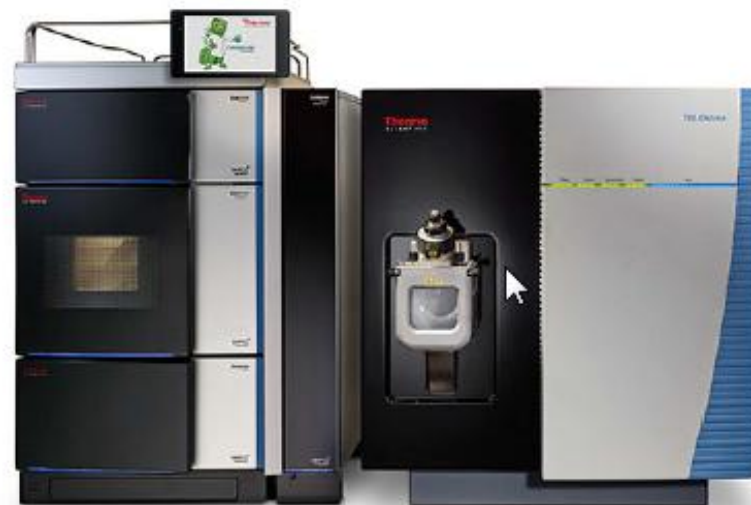
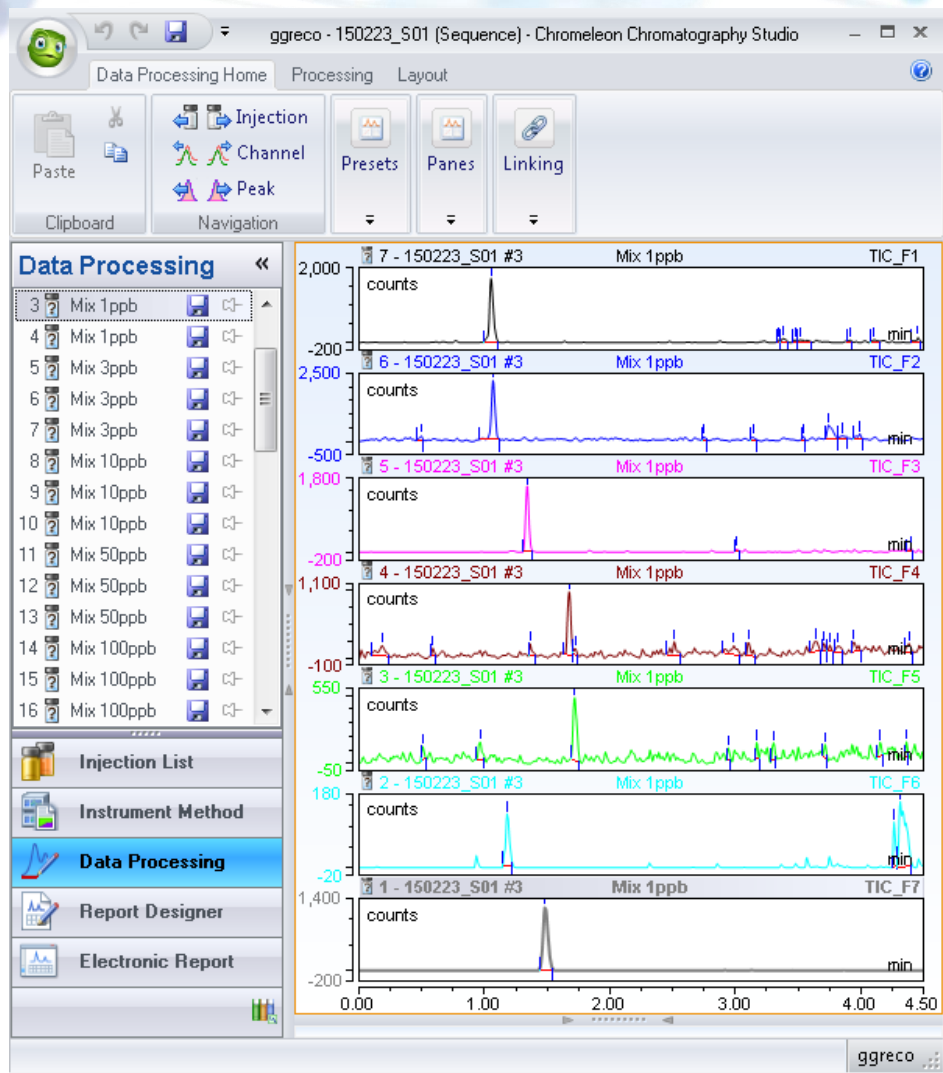
Chromeleon CDS Consolidated Report Tables

- Automatically report for the Channel with the highest response

No.	Peak Name	Area counts*min	Channel
TIC	TIC	Highest Response	Highest Response
3	PCB#18	15392	TIC_F01
10	PCB#28	19480	TIC_F01
11	PCB#33	17945	TIC_F01
25	PCB#52	5455	TIC_F03
34	PCB#95	3640	TIC_F06
50	PCB#70	2364	TIC
79	PCB#156	3650	TIC_F06
145	PCB#126	2757	TIC_F06
179	PCB#153	4781	TIC_F07
219	PCB#188	1100	TIC_F10
225	PCB#170	889	TIC_F10

- Useful for reporting large quantities of MS data in a generic, compact table

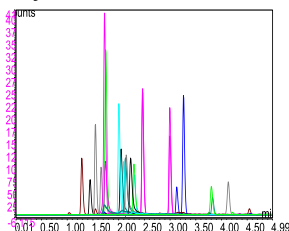
Antibiotics 1 ppb



36 Antibiotics Targeted Screening

Accucore Vanquish C18 column, 1.5 μ m x 2.1mm x 100mm

Overlaid selected reaction monitoring chromatograms showing detection of 36 antibiotics within a 5 minute detection window, binary Vanquish system and TSQ Vantage MS



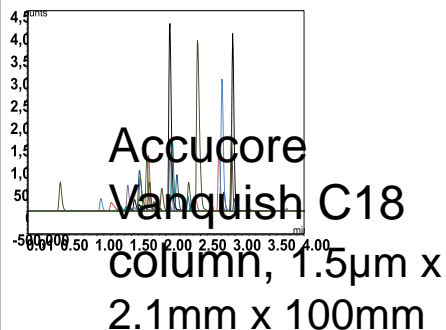
Mobile phase A: 0.1% formic acid / Water
Mobile phase B: 0.1% formic acid / MeOH
Flow rate: 400 μ L/min
Column temperature: 40 ° C, active preheating
Injection volume 2 μ L

Table 1. LC gradient conditions

Time (min)	%B
0.000	10
4.375	90
5.000	90
5.125	10
8.750	10

47 Drugs in 4 Minutes

Overlaid selected reaction monitoring chromatograms showing detection of 47 drugs within a 4 minute detection window, binary Vanquish system and TSQ Vantage MS

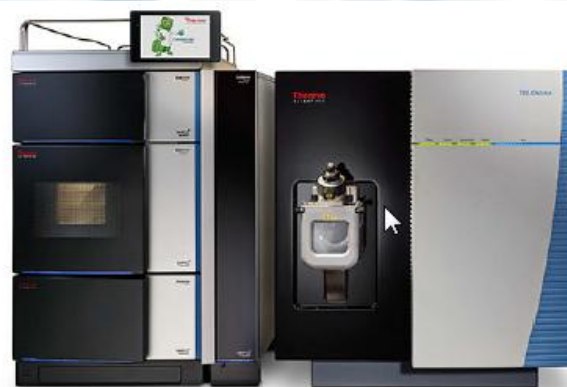


Mobile phase A:	10 mM ammonium acetate in water
Mobile phase B:	0.1% formic acid in methanol
Flow rate:	500 µL/min
Column temperature:	50 ° C, with active preheating
Injection volume:	2 µL

Table 1. LC gradient conditions

Time (min)	%B
0.00	10
0.16	10
2.88	90
3.20	90
3.28	10
5.60	10

Summary – Bringing It All Together



Chromeleon CDS has all the tools to help you process and report your MS data in the shortest time!



Thank You!

Any Questions?