SCIEX

Answers for Science.
Knowledge for Life.™

Ignite your Routine Testing Methods

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SCIEX, Concord, Ontario (Canada)

Overview

- Update to the SCIEX LC-MS/MS product portfolio
  - New SCIEX ExionLC™ systems
  - New SCIEX Triple Quad™ and QTRAP® 6500+ systems
  - New

- Application in Food Testing
  - Monofluoroacetate (1080) in milk in infant formula
  - Pesticide screening using ultra-fast polarity switching
  - Triazole derivative metabolites in fruits and vegetables
  - Target identification and quantitation using HR-MS/MS
  - Unknown screening using HR-MS/MS

New SCIEX ExionLC™ Systems

- ExionLC™ 100
  - Simple, non-intimidating, all-in-one box
  - Standard quaternary pump at HPLC pressures for more robustness, less downtime

- ExionLC™ AC
  - Consistent UHPLC performance
  - Minimal downtime

- ExionLC™ AD
  - Full UHPLC, high pressure ratings
  - Lowest carryover system

✓ Fully controlled by Analyst® software 1.6.3

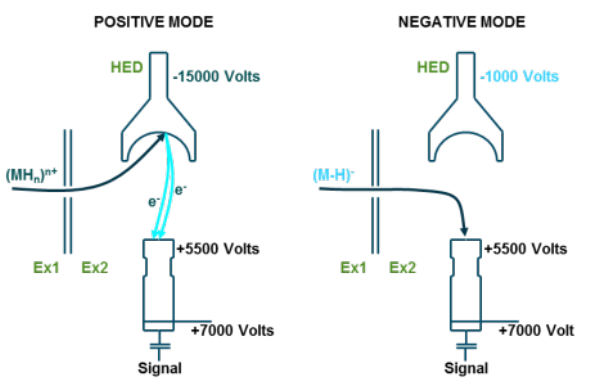
✓ Improved software integration for better stability

New SCIEX Triple Quad™ and QTRAP® 6500+ Systems

- Improved *Ion*Drive™ detection system
  - Quantify with lowest limits of quantitation and up to six orders of linear dynamic range
  - Ultra fast polarity switching with *Scheduled* MRM™ Pro algorithm for multi-target quantitation
- Elevated SelexION® technology
  - Differential Mobility Spectrometry with improved transmission and no effect on resolution
- Audible noise reduction (active exhaust)

- ✓ Industry proven performance of IonDrive™ Turbo V ion source and QJet® ion guide
- ✓ Results in less time – fast, high-throughput, simplified data processing tools
- ✓ Service and support resources for success

Improved *Ion*Drive™ Detection System



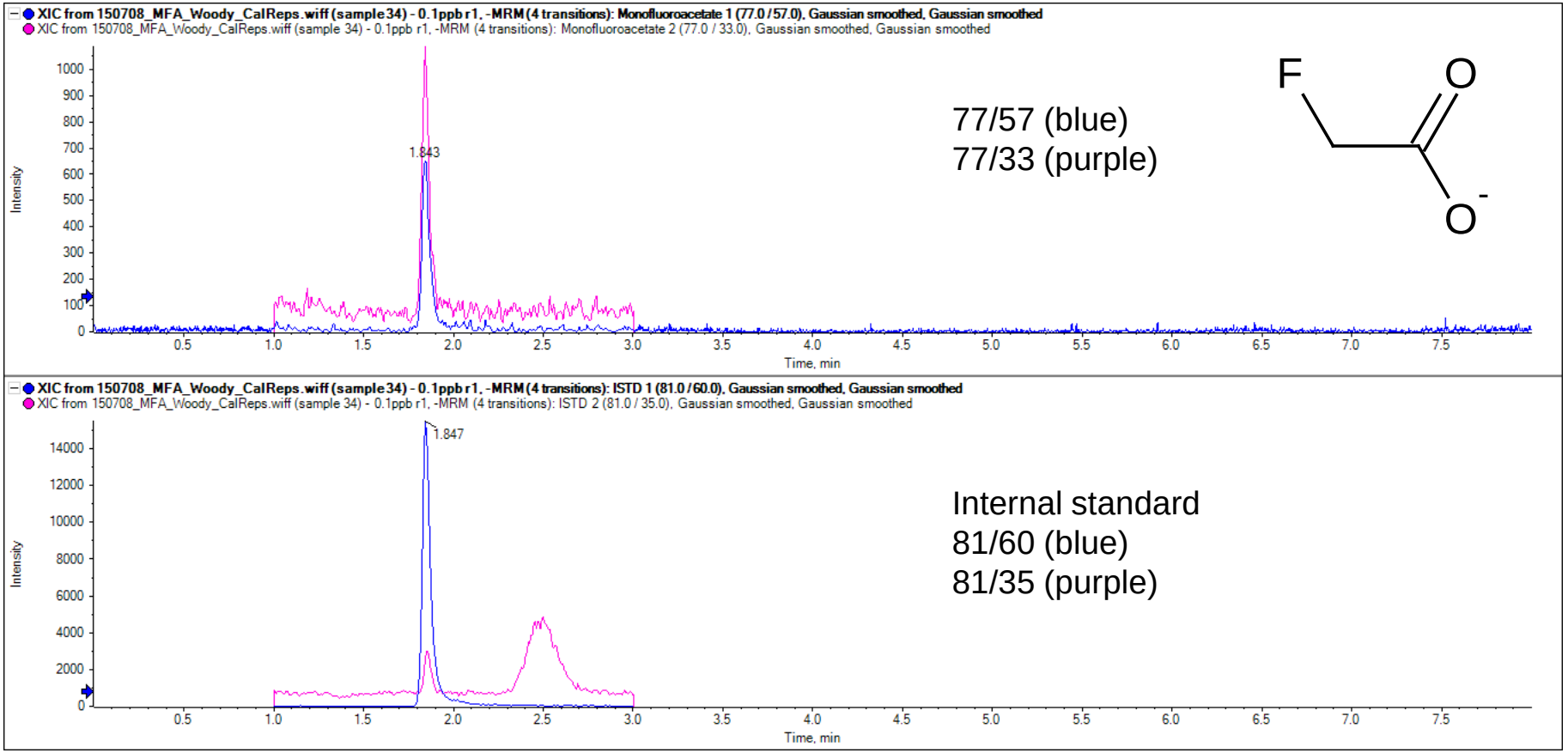
- New detector
  - Larger detection area
- New power supply
  - High energy dynode at 15 kV improves sensitivity
  - Enables faster ***5 msec*** polarity switching
- "Floated" design
  - Ions in negative polarity directed straight into the detector

✓ Contributes to significant signal gains in negative mode Q3 fragment ion <100 Da

✓ Improved data quality in screening applications with ultra-fast polarity switching

Detection of 0.1 ng/mL Monofluoroacetate

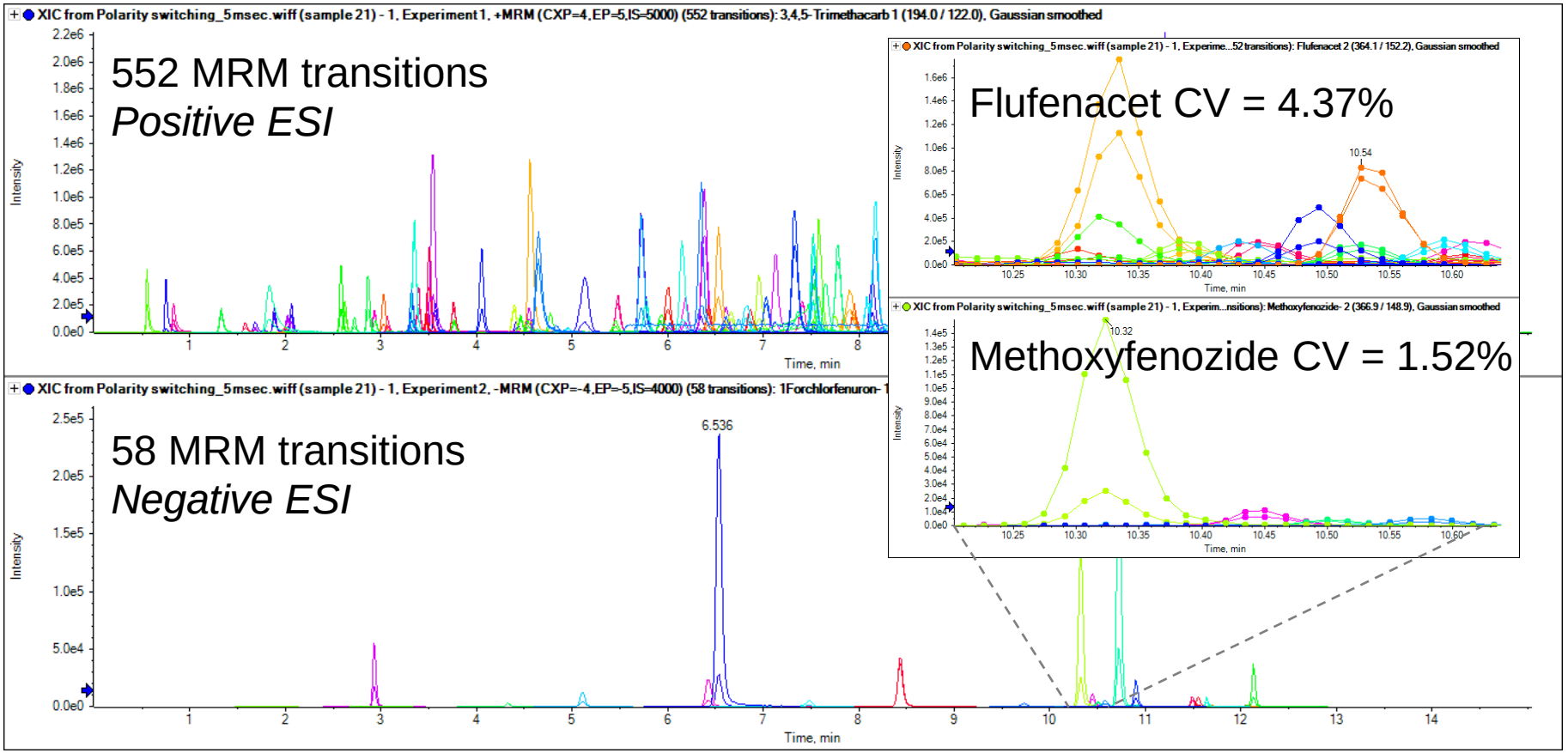
High Sensitivity in Negative Polarity using the QTRAP® 6500+ system



Sample preparation protocol and LC conditions adopted from the **AOAC First Action Official Method 2015.03**, MS/MS using QTRAP® 6500+ system

Pesticide Screening with Ultra-Fast Polarity Switching

Switching between positive and negative polarity in 5 msec



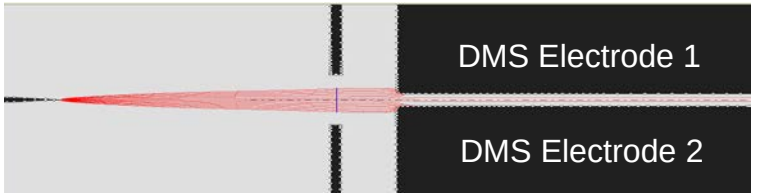
Phenomenex Kinetex™ Biphenyl 2.6u (50 x 2.1mm) column
Gradient of water/methanol + 5 mM ammonium formate
~300 pesticides at 1 ng/mL, MS/MS using QTRAP® 6500+ system

SelexION®+ DMS with Jet Injector Technology

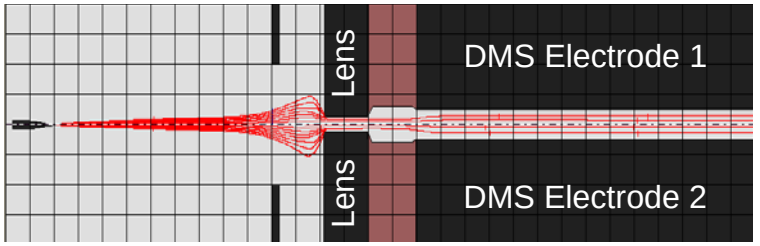
- New DMS cell designed to improve ion transmission by ~2x without loss in selectivity or resolution
  - Addition of lens increases ion velocities into DMS cell
  - Reduces transit times through detrimental fringing fields

✓ Continually driving selectivity improvements

SelexION cell



SelexION+ cell

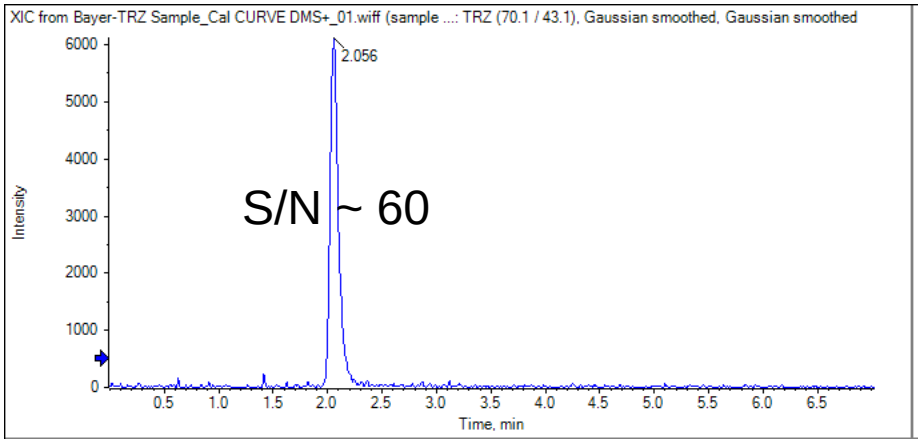


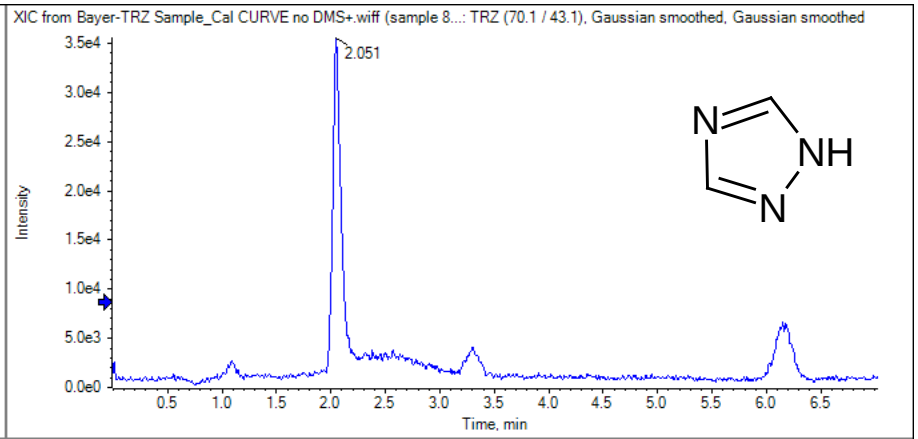
Reduced Noise and Interferences when Using DMS

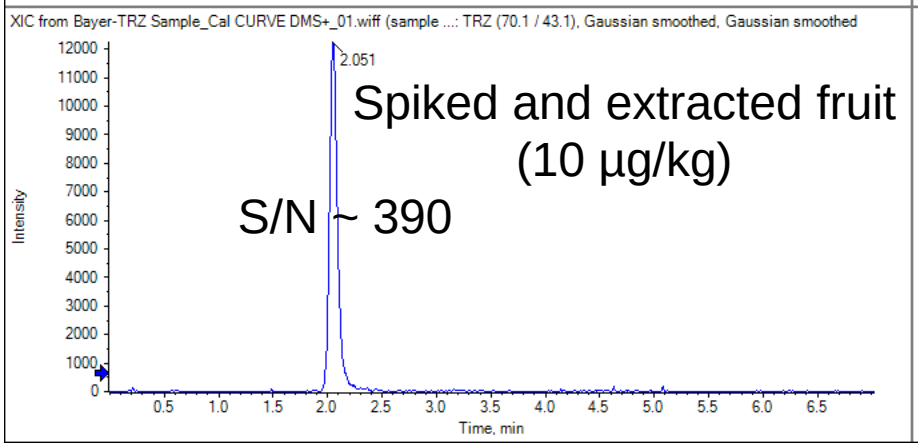
Example: Triazole in Fruit and Vegetable Extracts

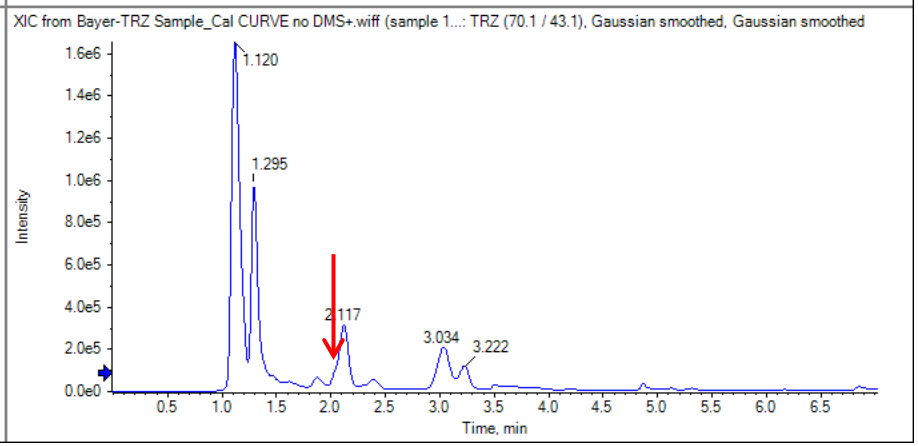
6500+ with DMS

6500+ DMS removed



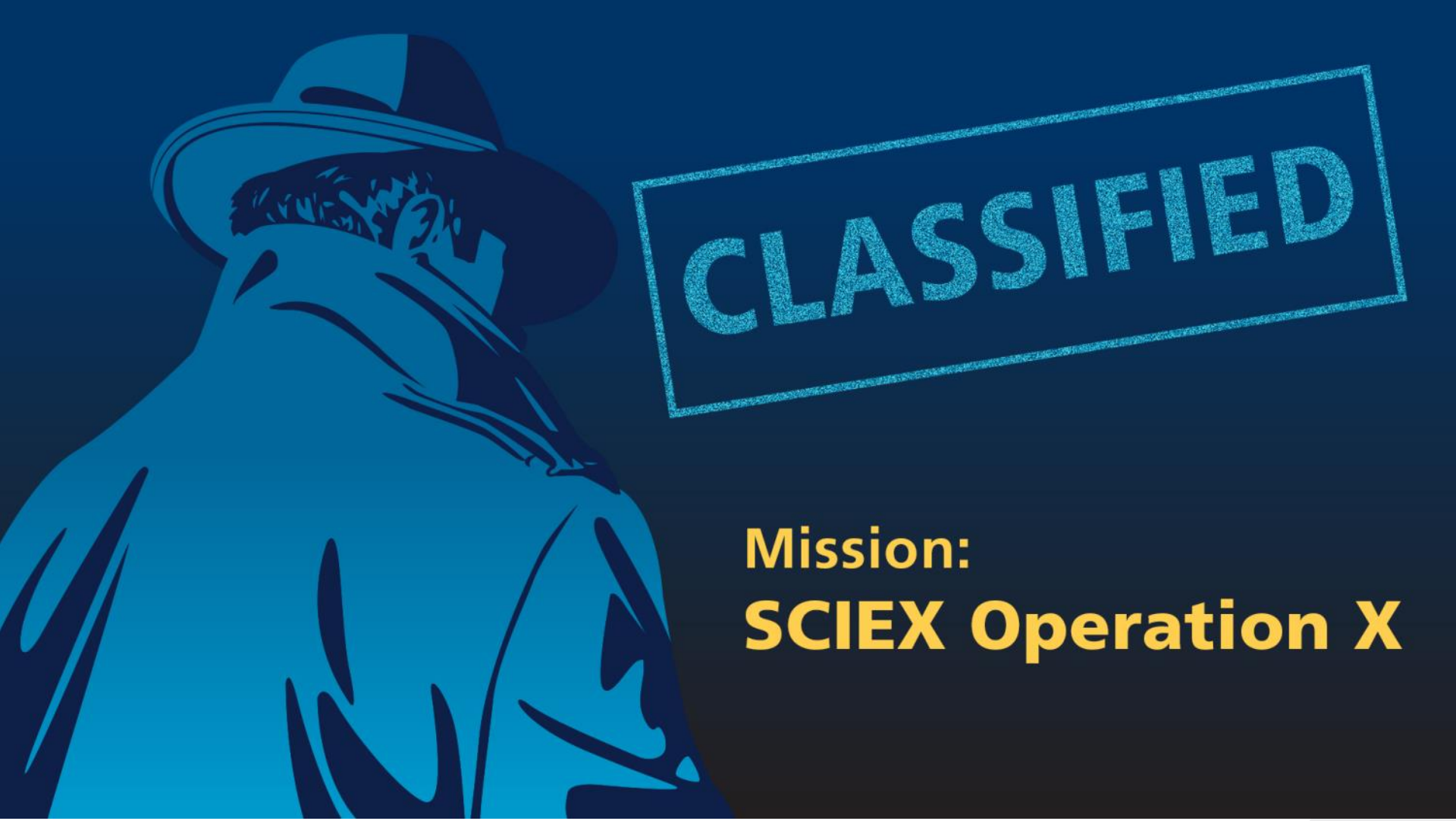






Original method developed by J. Jasak and R. Schöning,
also published as “EURL-SRM QuPPe-Method 8” by M. Anastassiades et al.

MS/MS using QTRAP® 6500+ system



A new high resolution mass spec system is on the horizon

Mission Complete >

What's New?

SCIEX X500R QTOF System powered by SCIEX OS Software

SCIEX X500R QTOF system

SCIEX ExionLC™ AC system

SCIEX OS software

Introducing the SCIEX X500R QTOF System

- Hardware
  - SCIEX ExionLC™ Systems
    - Fully controlled by SCIEX OS software
    - Improved software integration for better stability
  - SCIEX X500R QTOF System
    - N-optic design
    - Heated TOF path
    - Minimized footprint, engineered for simplicity and service accessibility
- Software
  - SCIEX OS Software
    - New user interface
    - Simultaneous identification and quantitation
    - Automatic unknown identification
- Application data
    - Target identification and quantitation
    - Unknown screening

Introducing the SCIEX X500R QTOF System

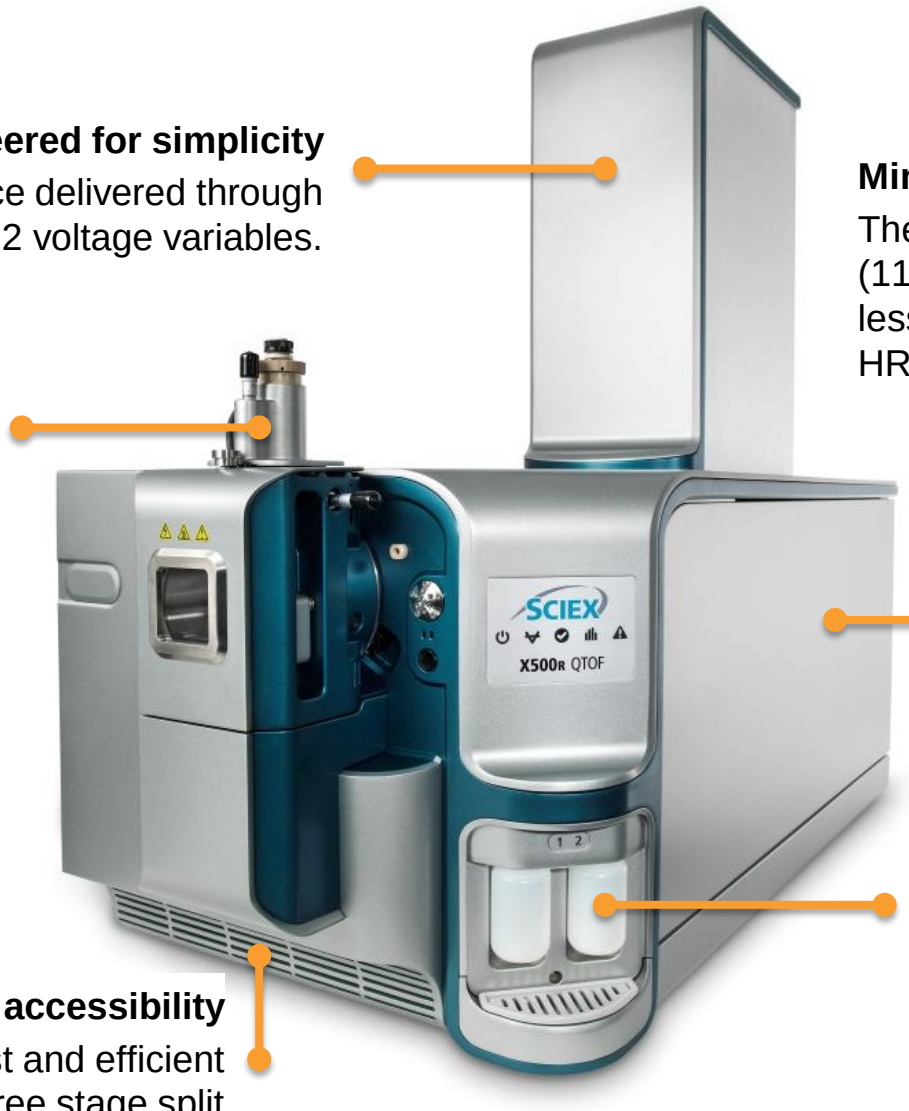
Design Improvements and Details

Engineered for simplicity

Optimal performance delivered through adjustment of only 2 voltage variables.

TwinSpray

An independent calibrant delivery path for reliable auto-calibration.



Minimized footprint

The benchtop stature (110 x 57 x 112 cm)* occupies less lab space than any other HRMS system on the market.

Integrated calibration

Maintains mass calibration through long runs without effect on sample flow.

Service accessibility

Easy QJet access for fast and efficient maintenance and single three stage split flow pump for increased system uptime.

Introducing the SCIEX X500R QTOF System

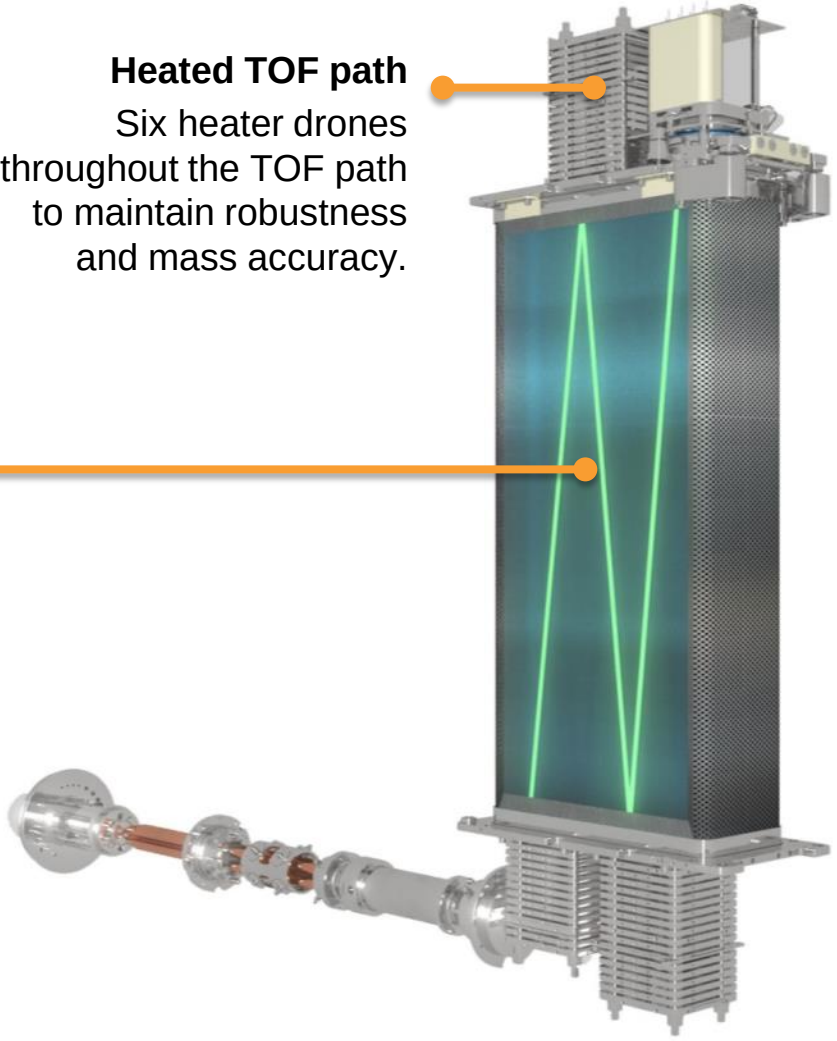
Design Improvements and Details

Heated TOF path

Six heater drones throughout the TOF path to maintain robustness and mass accuracy.

N-optic design

4 mm orifice leading into TOF accelerator tube delivers resolution without compromise in sensitivity.



Introducing the SCIEX X500R QTOF System

Design Improvements and Details

Legendary Turbo V source with optional IonDrive and Curtain Gas interface

Renowned ionization performance and ruggedness now delivered with a high resolution accurate mass analyzer.

Perfect Balance to Elevate Your Lab's Performance

SCIEX X500R QTOF System

- The first robust, high performance high resolution MS/MS system designed for routine use.
  - Sensitivity to easily detect maximum residue levels
  - Resolving power to remove interference from complex food matrices
  - Linearity to quantify over up to 4 orders of magnitude
  - Mass accuracy to identify compounds following regulatory guidelines
  - Confident identification based MS/MS (IDA and SWATH™ MS/MS^{ALL}, ion ratios and MS/MS spectra)
  - Industry leading robustness of Turbo V™ source and Curtain Gas™ interface

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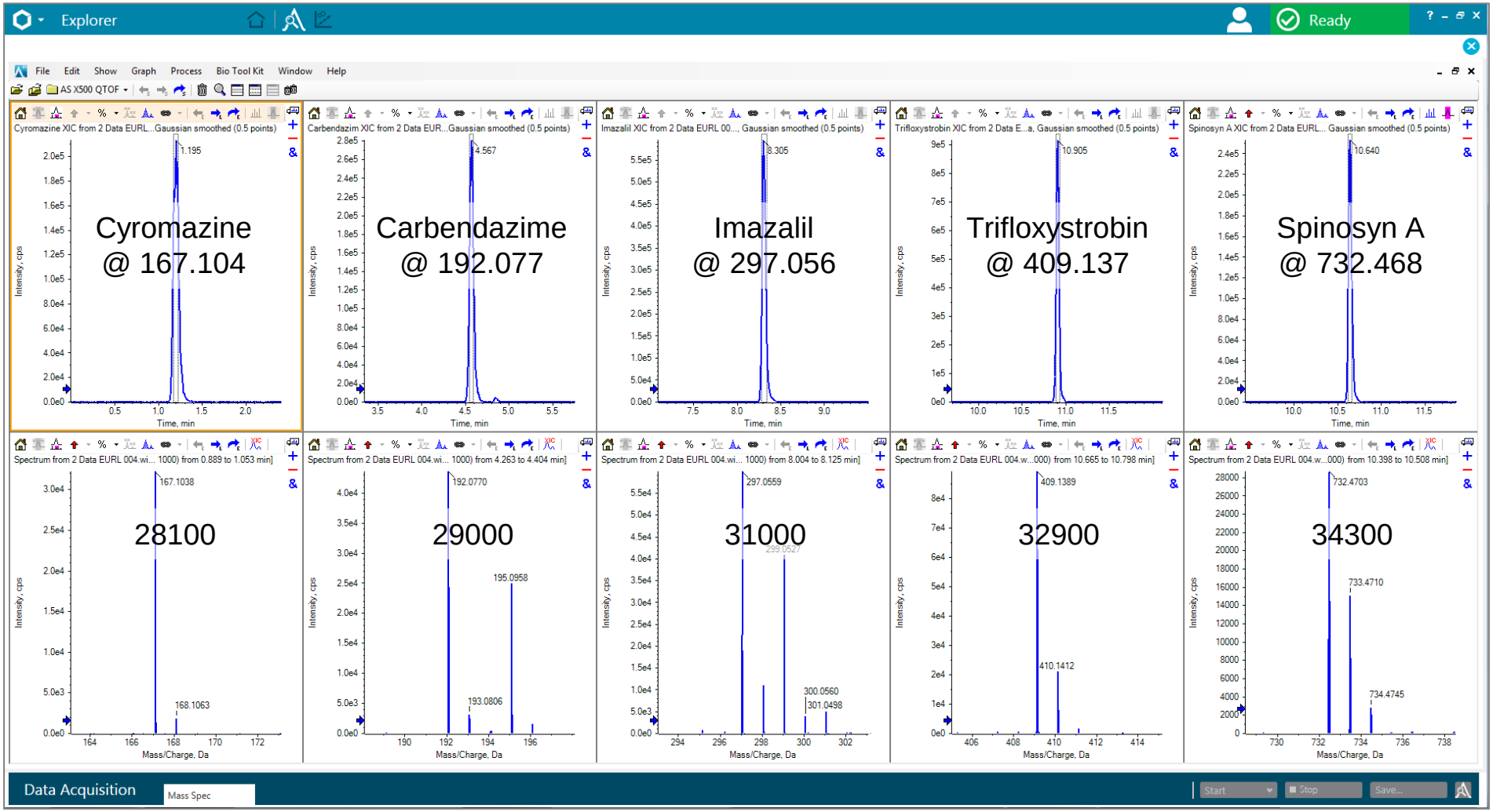
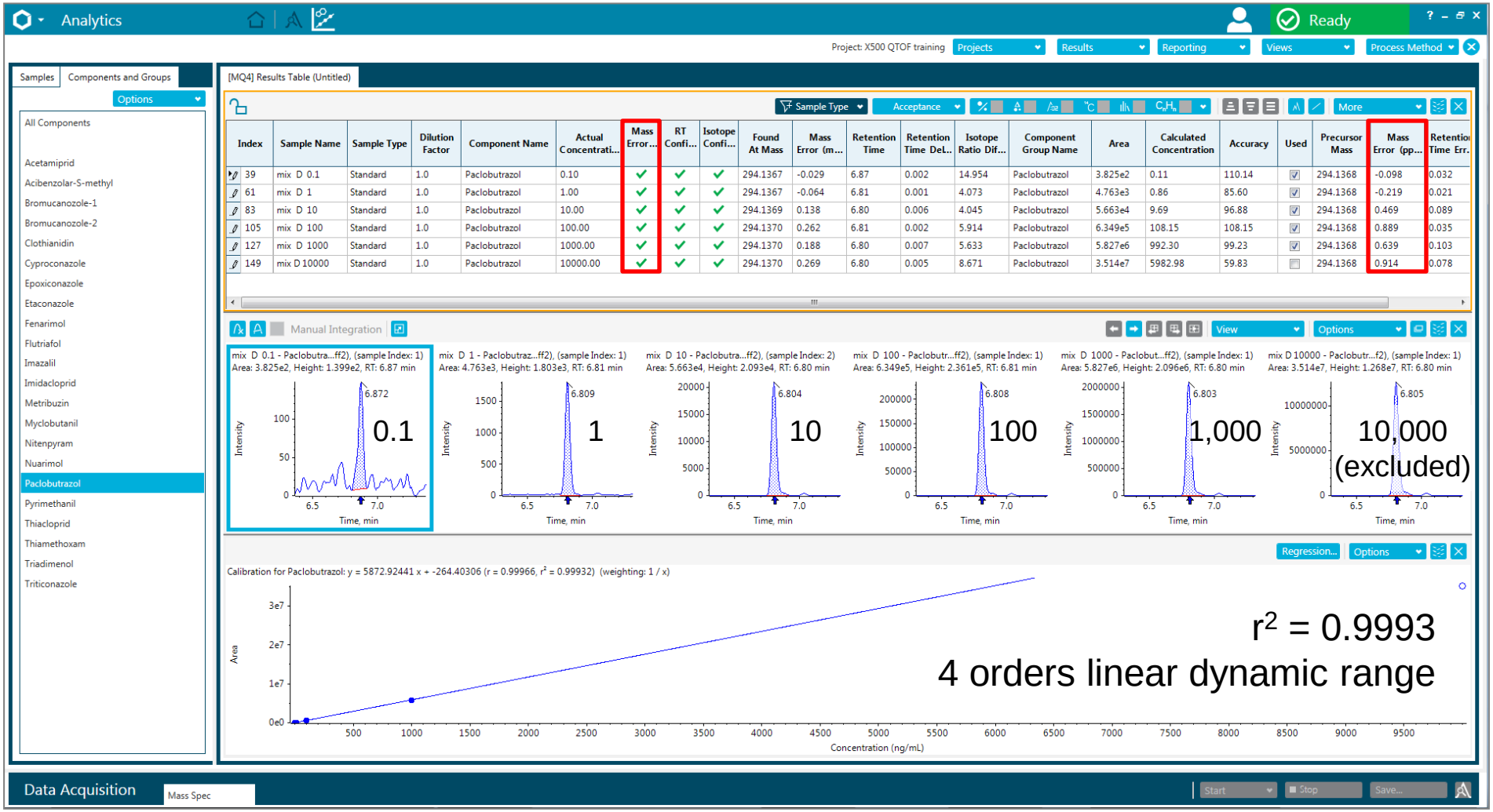
The SCIEX X500R QTOF System – Performance

Sensitivity and Resolution (20 µg/kg Pesticides in Fruit, 5 µL injected)



The SCIEX X500R QTOF System – Performance

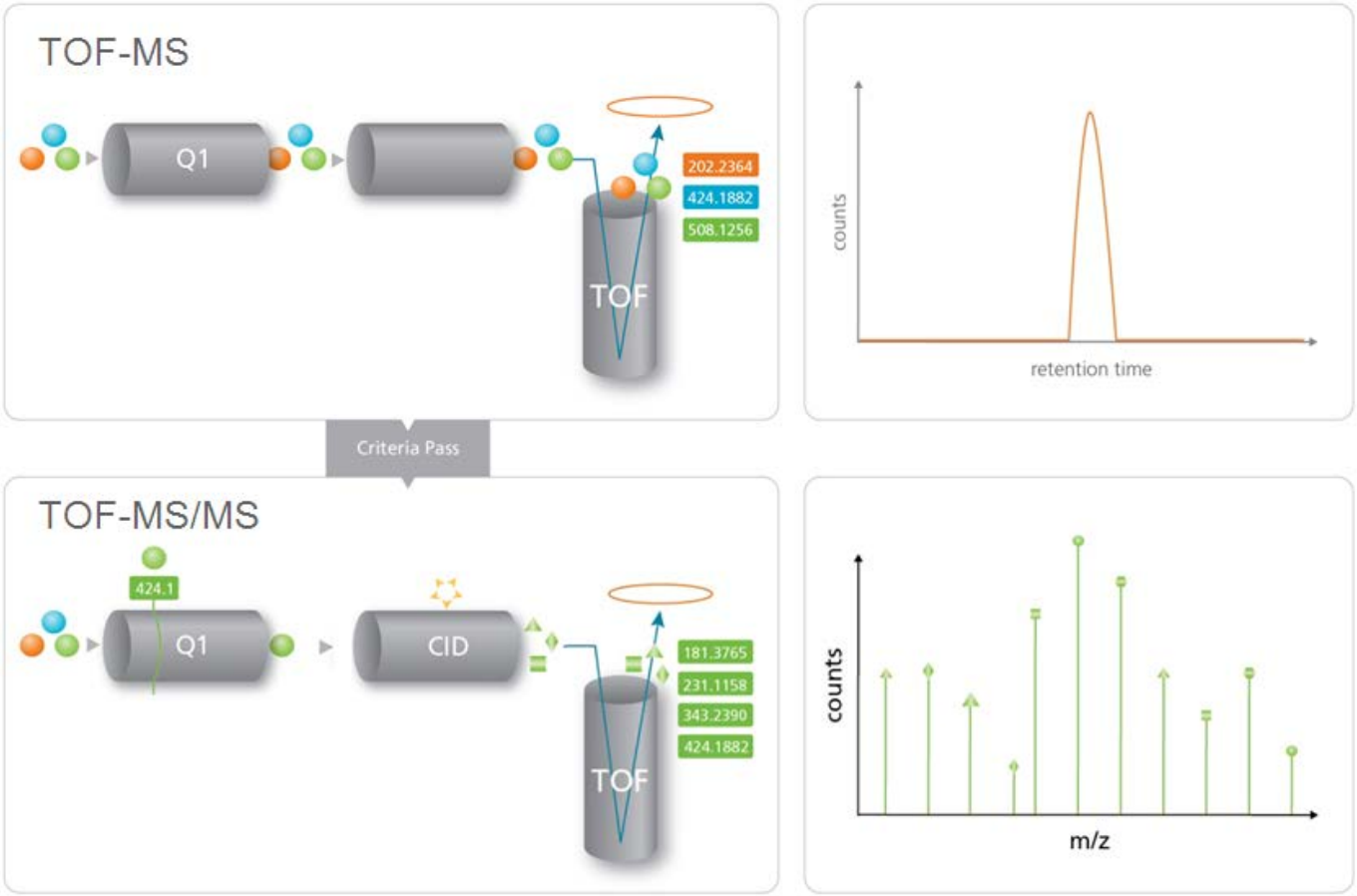
Linearity and Mass Accuracy (Paclobutrazol 0.1 to 10,000 ng/mL)



Mass error = -0.2 to 0.91 ppm

Information Dependent Acquisition of MS/MS (IDA)

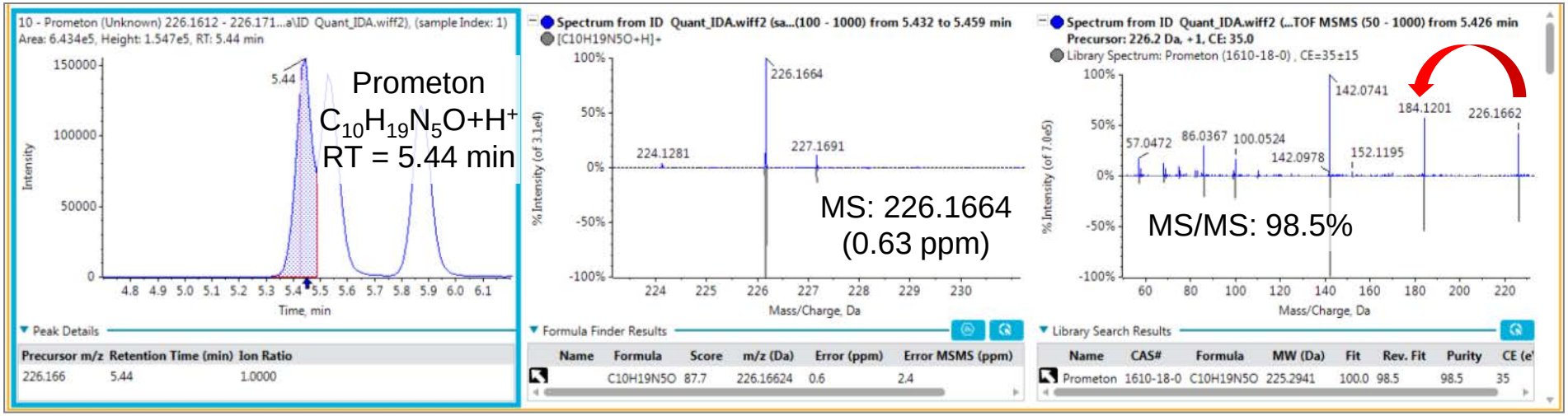
Provides MS/MS Spectra with High Selectivity (Q1 Resolution unit)

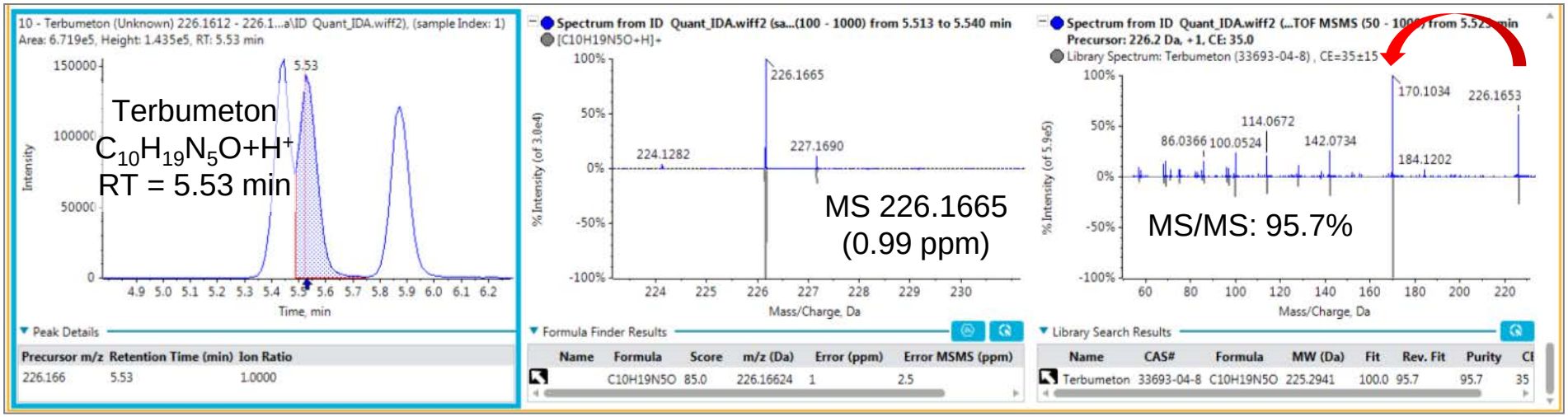


IDA can be used with and without inclusion list for target or non-target screening

The SCIEX X500R QTOF System – IDA

Confident Identification of Isomers using MS/MS (Prometon vs. Terbumeton)

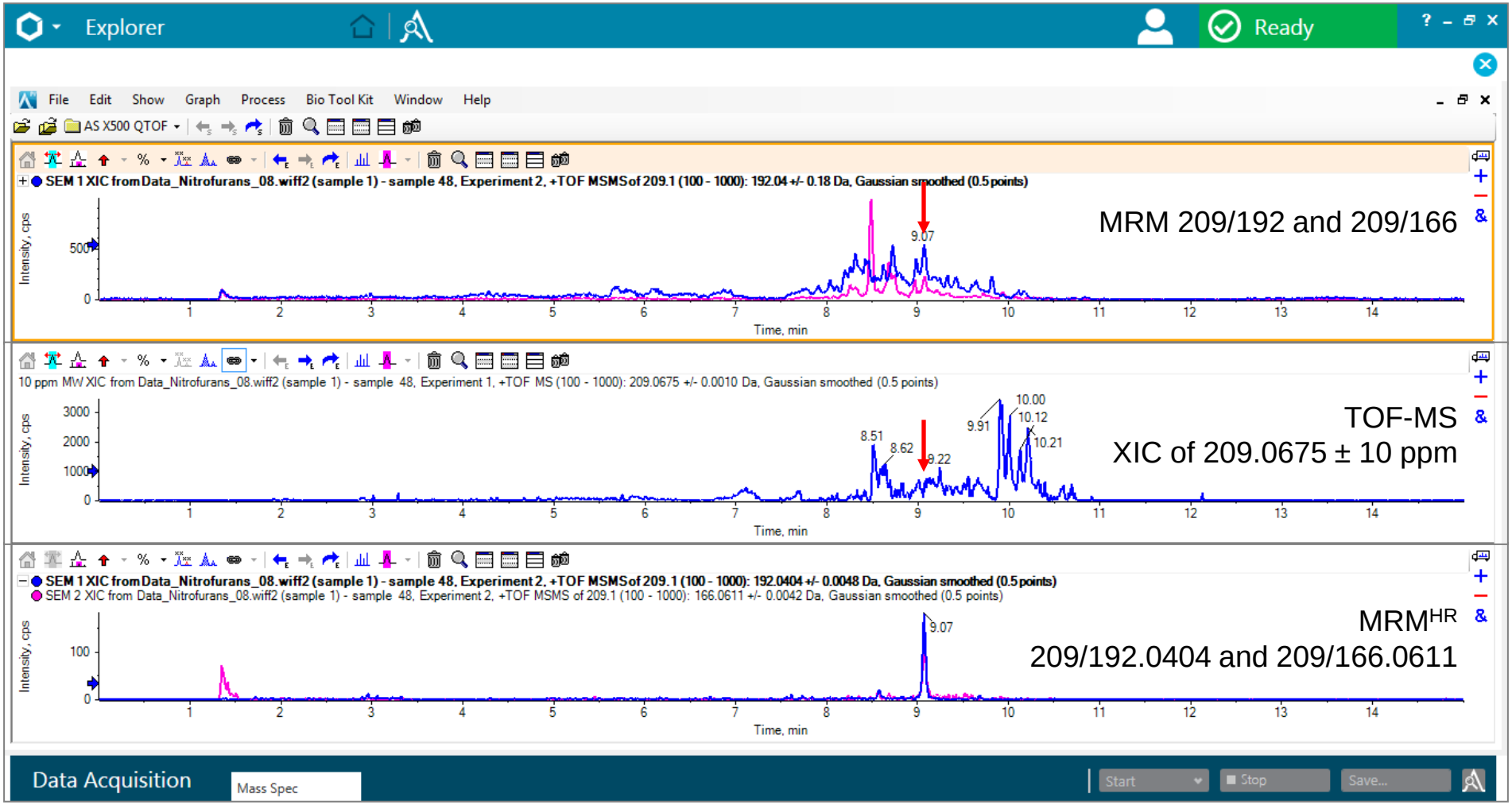




Identification based on MS/MS library searching (Q1 at unit resolution)

Increased Selectivity using MRM^{HR}

Feed Sample Tested Positive for NP-Semicarbazide



Perfect Balance to Elevate Your Lab's Performance

SCIEX X500R QTOF System Powered by SCIEX OS Software

- The first robust, high performance high resolution MS/MS system designed for routine use.
  - Sensitivity to easily detect maximum residue levels
  - Resolving power to remove interference from complex food matrices
  - Linearity to quantify over up to 4 orders of magnitude
  - Mass accuracy to identify compounds following regulatory guidelines
  - Confident identification based MS/MS (IDA and SWATH™ MS/MS^{ALL}, ion ratios and MS/MS spectra)
  - Industry leading robustness of Turbo V™ source and Curtain Gas™ interface
- Simple software workflows that deliver reliable results, it's the solution that's ready to meet your challenges today and for the future, from the trusted LC-MS/MS industry leader.

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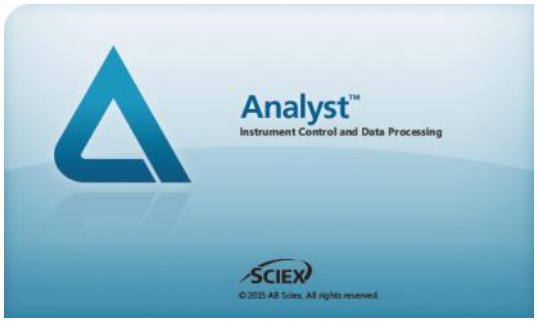
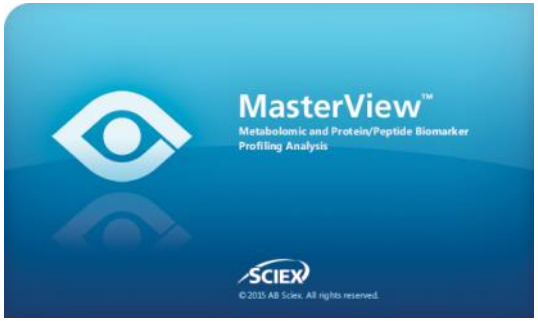
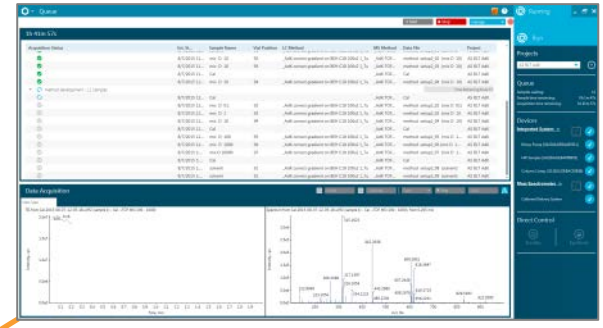
Introducing the SCIEX OS Software

Single Software Platform for MS Control, Data Processing and Reporting







SCIEX OS Software

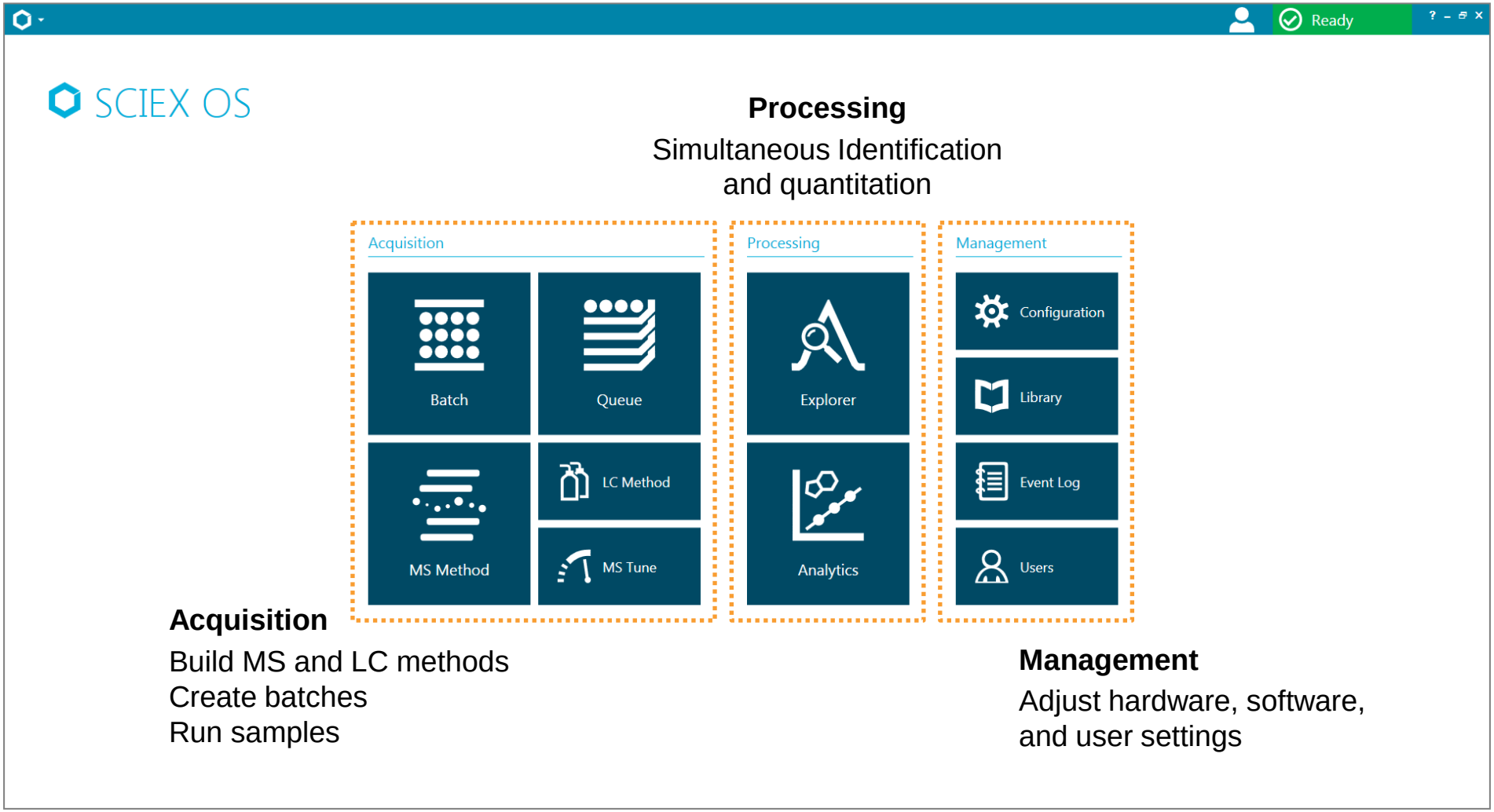
Software Improvements and Details

New user interface
Thoughtfully designed for faster learning and improved productivity

Acquire, analyze, report
Run the mass spectrometer and perform data processing, review and reporting in the same software

SCIEX OS Software – Home

Everything in a Single Software Platform



Processing

Simultaneous Identification
and quantitation

Acquisition

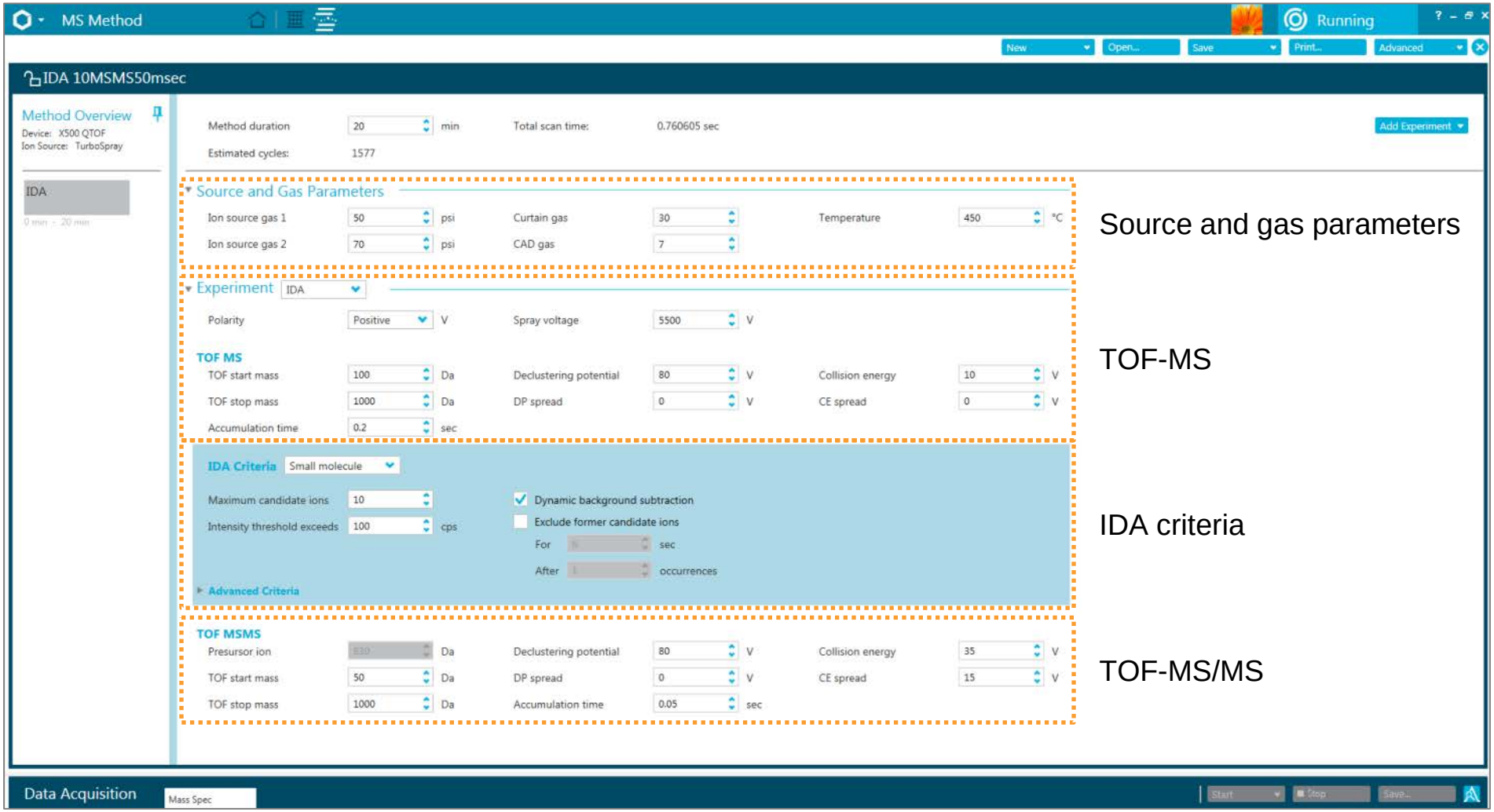
Build MS and LC methods
Create batches
Run samples

Management

Adjust hardware, software,
and user settings

SCIEX OS Software – Data Acquisition

1. Separate Method Editor for LC and MS Methods



Source and gas parameters

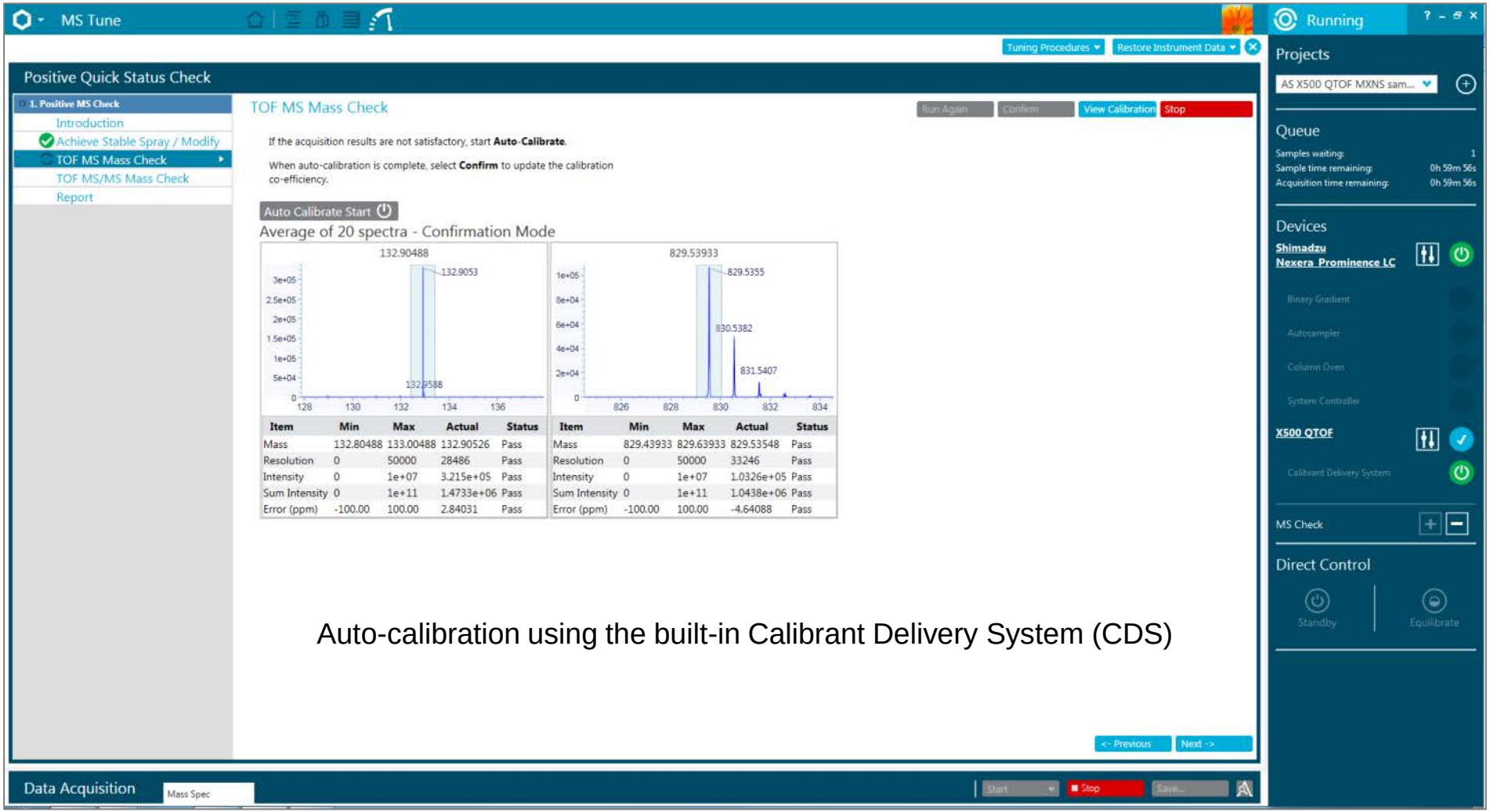
TOF-MS

IDA criteria

TOF-MS/MS

SCIEX OS Software – Auto-Calibration

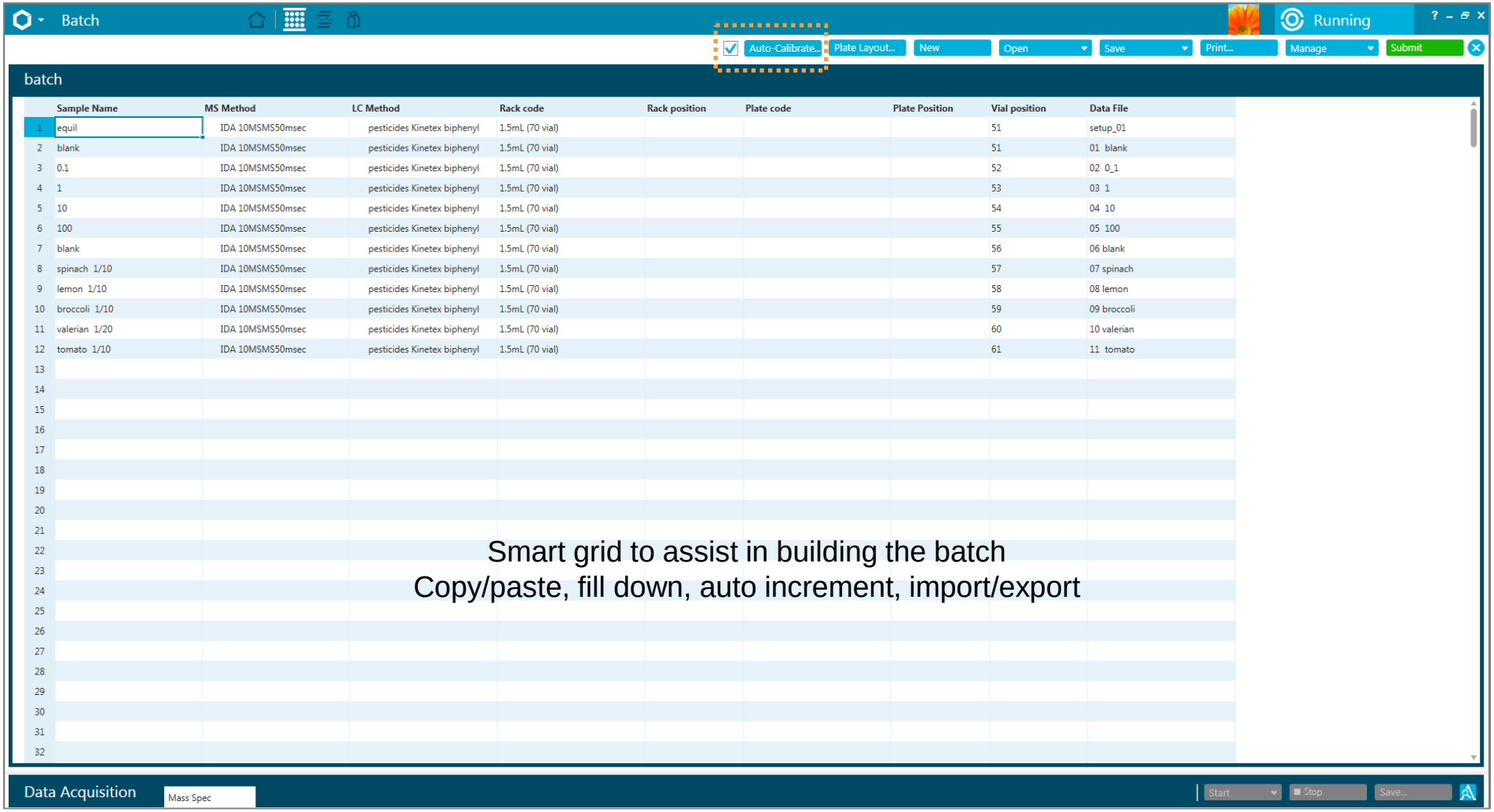
2. Auto-Calibration of TOF-MS and MS/MS and Reporting



Auto-calibration using the built-in Calibrant Delivery System (CDS)

SCIEX OS Software – Building a Batch

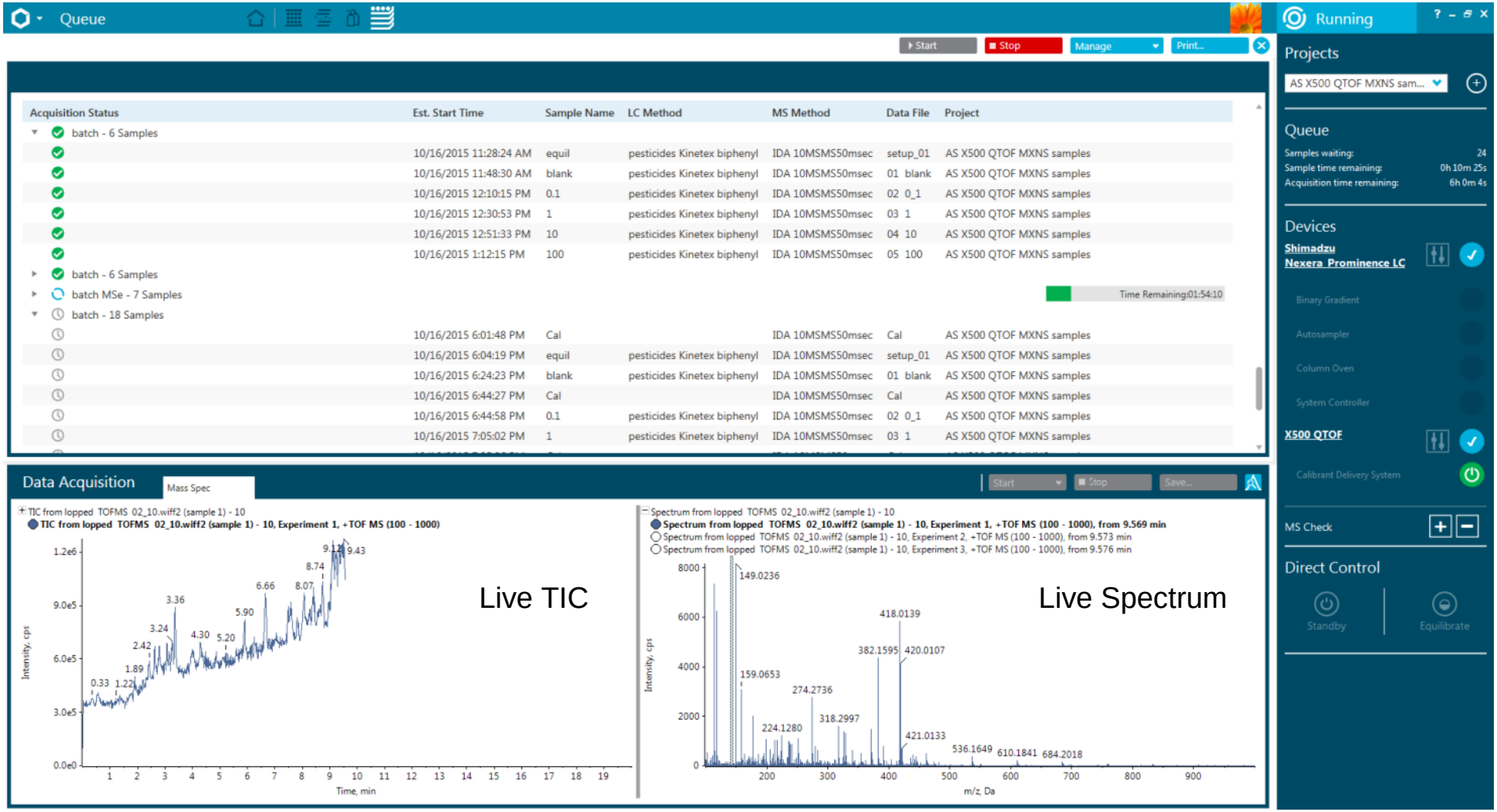
3. Batch Editor and Setup for Auto-Calibration



SCIEX OS Software – Queue, Live View and Status

4. Queue Manager with Inserted Auto-Cal Samples

Detailed instrument status



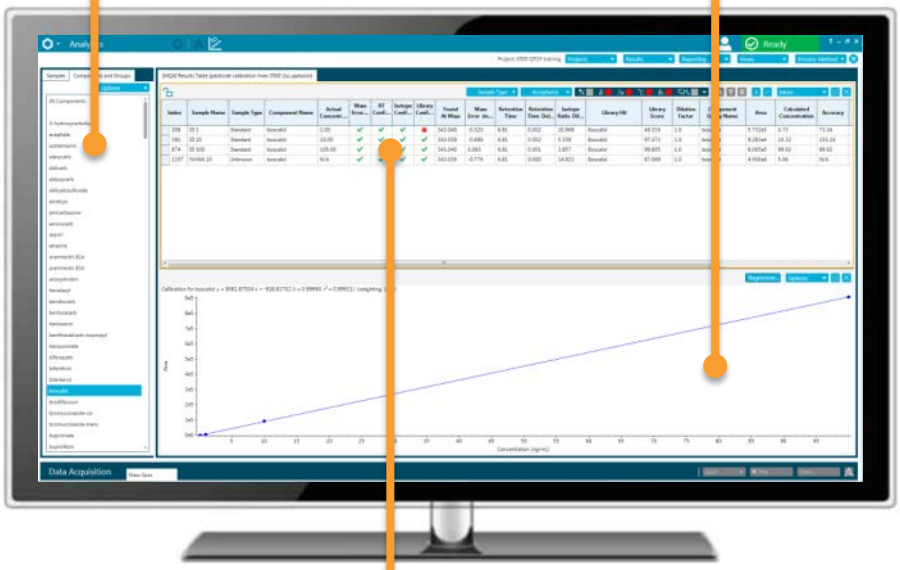
SCIEX OS Software – Identification and Quantitation

Software Improvements and Details

Triple quadrupole like quantitation

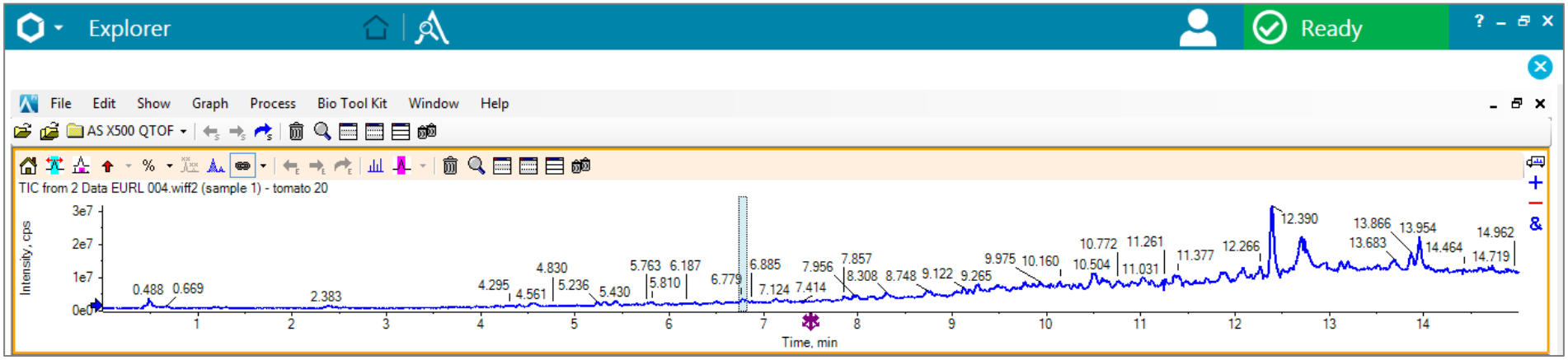
Processing of large compound lists

Simultaneous identification and quantitation
Powerful new tools to deliver quantitative and qualitative results from high resolution MS and MS/MS data.

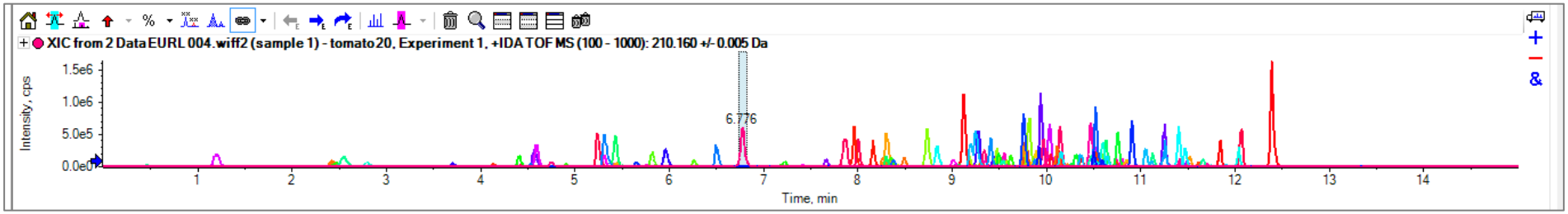


Intuitive Filtering for easy data review

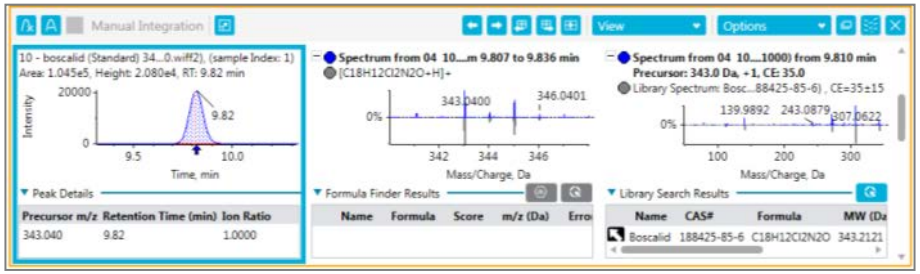
Targeted Data Processing Workflow



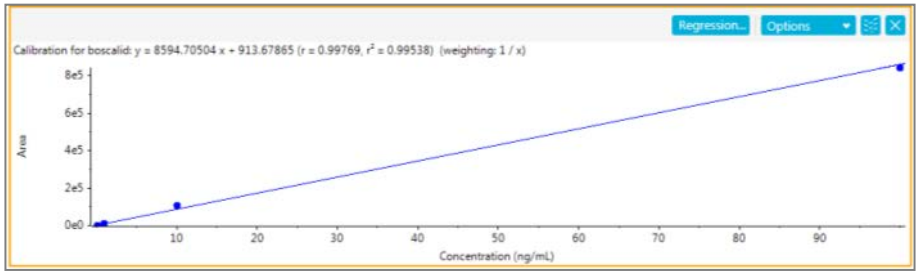
XIC generation for each target



Identification



Quantitation



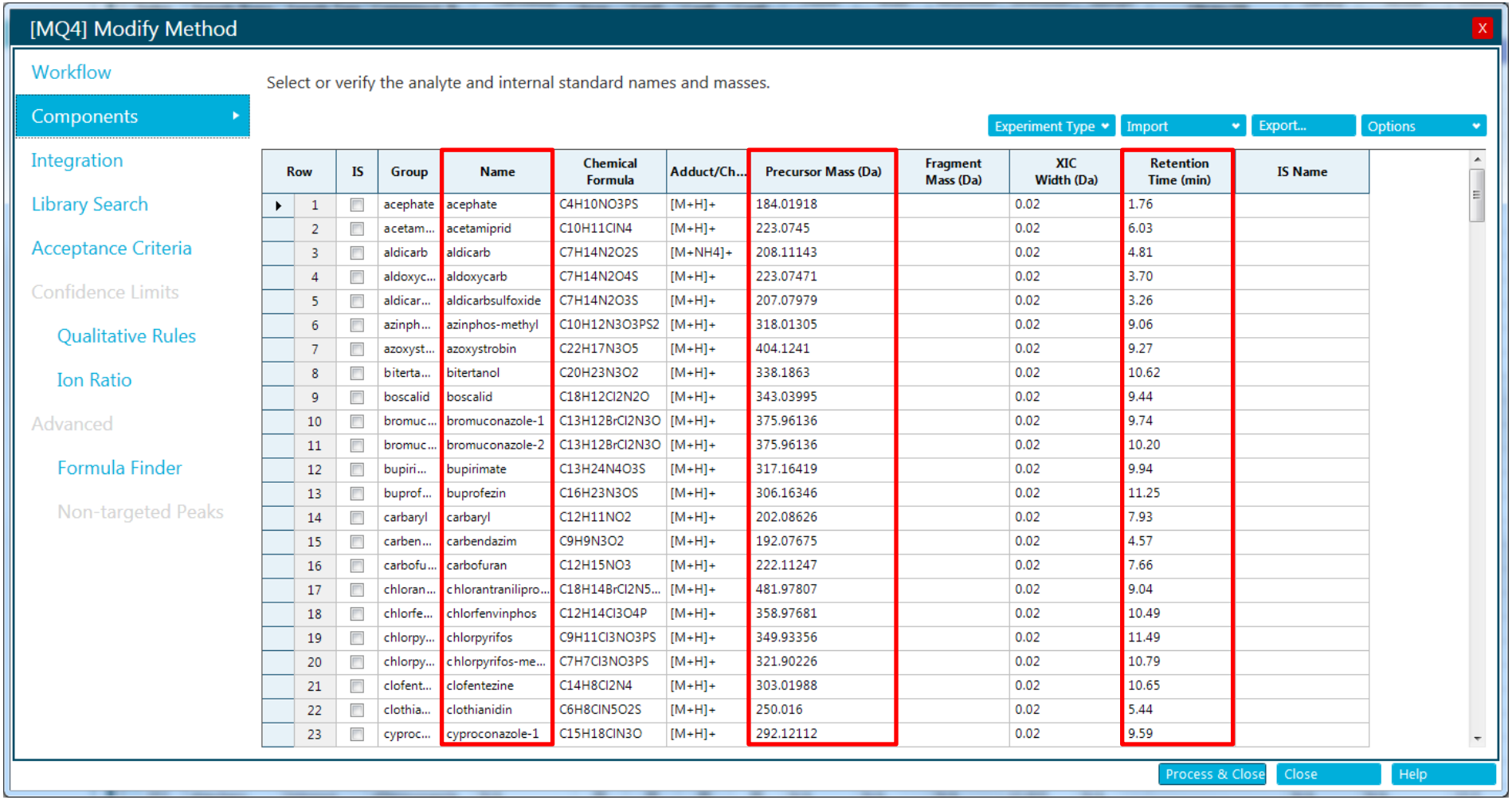
RT ✓ Mass ✓ MS/MS search ✓

Isotopes ✓

Above reporting level

Identification and Quantitation in SCIEX OS Software

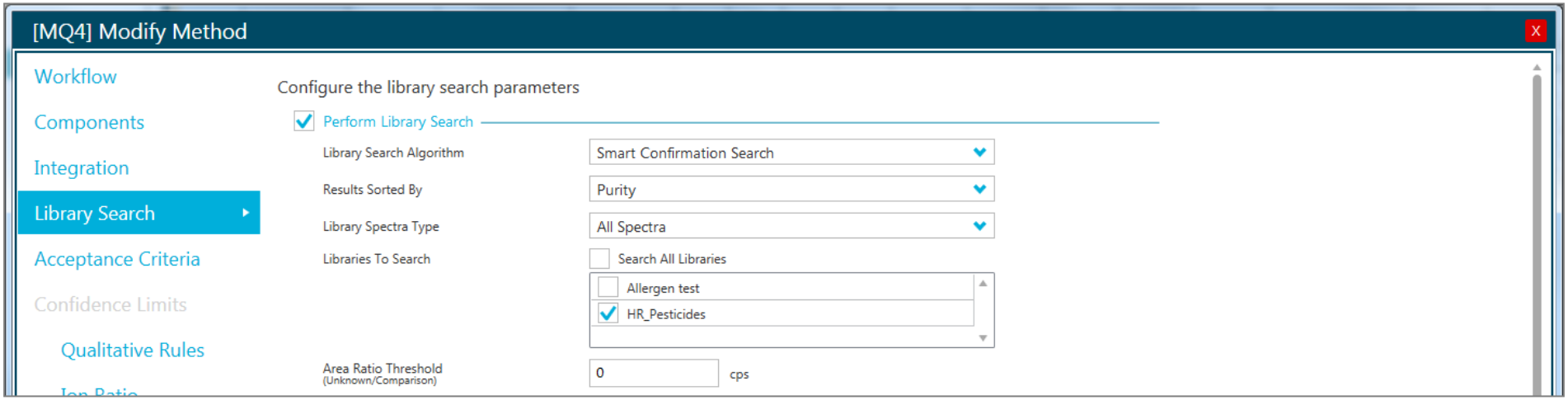
1. Define Retention Time and Accurate Mass for Each Target Analyte

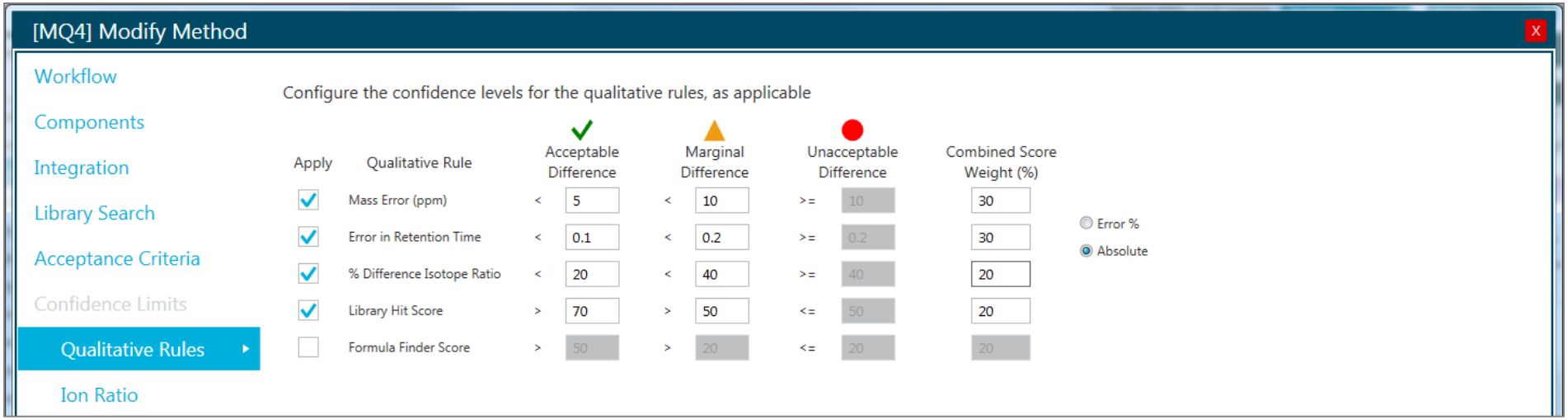


Row	IS	Group	Name	Chemical Formula	Adduct/Ch...	Precursor Mass (Da)	Fragment Mass (Da)	XIC Width (Da)	Retention Time (min)	IS Name
1		acephate	acephate	C4H10NO3PS	[M+H]+	184.01918		0.02	1.76	
2		acetam...	acetamiprid	C10H11ClN4	[M+H]+	223.0745		0.02	6.03	
3		aldicarb	aldicarb	C7H14N2O2S	[M+NH4]+	208.11143		0.02	4.81	
4		aldoxyc...	aldoxycarb	C7H14N2O4S	[M+H]+	223.07471		0.02	3.70	
5		aldicar...	aldicarbsulfoxide	C7H14N2O3S	[M+H]+	207.07979		0.02	3.26	
6		azinph...	azinphos-methyl	C10H12N3O3PS2	[M+H]+	318.01305		0.02	9.06	
7		azoxyst...	azoxystrobin	C22H17N3O5	[M+H]+	404.1241		0.02	9.27	
8		biterta...	bitertanol	C20H23N3O2	[M+H]+	338.1863		0.02	10.62	
9		boscalid	boscalid	C18H12Cl2N2O	[M+H]+	343.03995		0.02	9.44	
10		bromuc...	bromuconazole-1	C13H12BrCl2N3O	[M+H]+	375.96136		0.02	9.74	
11		bromuc...	bromuconazole-2	C13H12BrCl2N3O	[M+H]+	375.96136		0.02	10.20	
12		bupiri...	bupirimate	C13H24N4O3S	[M+H]+	317.16419		0.02	9.94	
13		buprof...	buprofezin	C16H23N3OS	[M+H]+	306.16346		0.02	11.25	
14		carbaryl	carbaryl	C12H11NO2	[M+H]+	202.08626		0.02	7.93	
15		carben...	carbendazim	C9H9N3O2	[M+H]+	192.07675		0.02	4.57	
16		carbofu...	carbofuran	C12H15NO3	[M+H]+	222.11247		0.02	7.66	
17		chloran...	chlorantranilipro...	C18H14BrCl2N5...	[M+H]+	481.97807		0.02	9.04	
18		chlorfe...	chlorfenvinphos	C12H14Cl3O4P	[M+H]+	358.97681		0.02	10.49	
19		chlorpy...	chlorpyrifos	C9H11Cl3NO3PS	[M+H]+	349.93356		0.02	11.49	
20		chlorpy...	chlorpyrifos-me...	C7H7Cl3NO3PS	[M+H]+	321.90226		0.02	10.79	
21		clofent...	clofentezine	C14H8Cl2N4	[M+H]+	303.01988		0.02	10.65	
22		clothia...	clothianidin	C6H8ClN5O2S	[M+H]+	250.016		0.02	5.44	
23		cyproc...	cyproconazole-1	C15H18ClN3O	[M+H]+	292.12112		0.02	9.59	

Identification and Quantitation in SCIEX OS Software

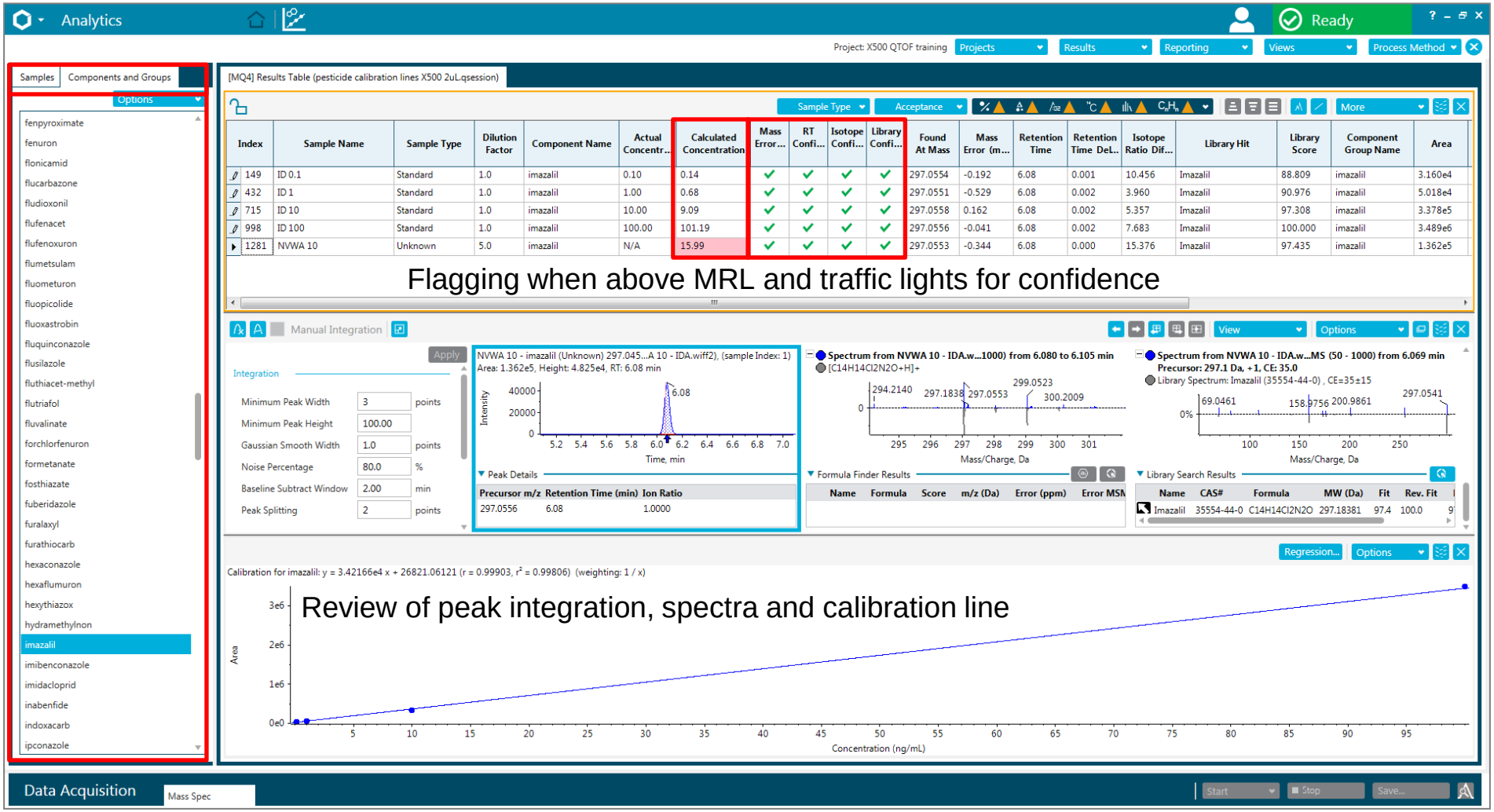
2. Define Identification Criteria and Confidence Settings





Identification and Quantitation in SCIEX OS Software

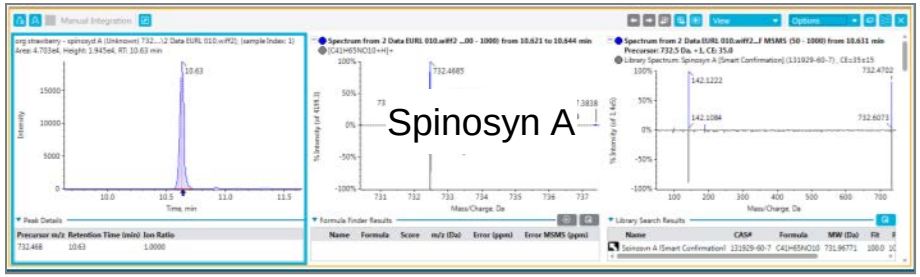
3. Review Quantitative and Quantitative Results



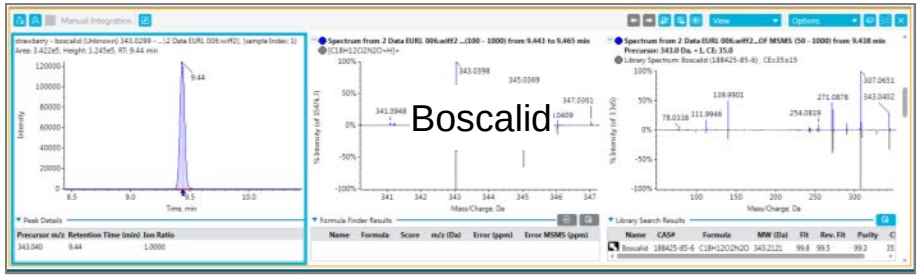
Pesticides in Store-bought Fruits and Vegetables

QuEChERS Extracts with 10x Dilution (5 µL Injection)

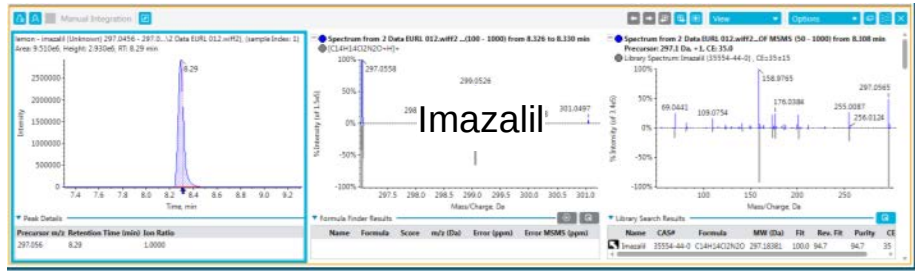
Organic strawberry



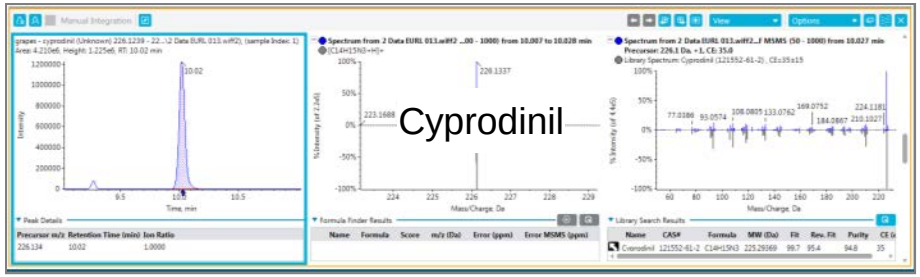
Strawberry



Lemon



Grapes



Pesticides (> 5 µg/kg) in Store-bought Fruits and Vegetables

Sample	Pesticide	Concentration (µg/kg)	RT error (%)	Mass error (ppm)	Isotope ratio error (%)	MS/MS PUR (%)
Organic strawberry	Spinosyn A	13.9	0.01	0.55	9.1	100.0
	Spinosyn D	33.3	0.01	1.63	6.0	99.4
Strawberry	Acetamiprid	19.2	0.08	-0.35	6.5	98.7
	Boscalid	161	0.00	-0.49	4.9	99.3
	Myclobutanil	85.0	0.00	-0.31	13.9	100.0
	Pyraclostrobin	40.5	0.00	1.33	16.3	99.0
	Pyrimethanil	391	0.00	0.32	4.7	97.3
Blueberry	n.d.	-	-	-	-	-
Organic Banana	Spinosyn D	12.6	0.00	2.33	19.8	100.0
Banana	Buprofezin	341	0.01	0.32	3.5	100.0
	Imazalil	565	0.02	0.79	15.1	91.5
	Thiabendazole	444	0.01	-1.51	13.9	97.6
Lemon	Imazalil	1080	0.02	0.74	7.3	94.7
	Pyrimethanil	164	0.01	-0.77	1.0	99.2
	Pyriproxyfen	31.6	0.01	0.43	11.4	95.3
Spinach	n.d.	-	-	-	-	-
Grapes	Boscalid	115	0.01	-0.80	8.8	97.2
	Buprofezin	17.3	0.01	0.22	7.3	99.6
	Cyprodinil	412	0.01	-0.87	3.3	94.8
	Imadacloprid	82.5	0.01	-0.58	14.6	96.1
	Pyraclostrobin	46.7	0.00	-1.31	4.8	100.0

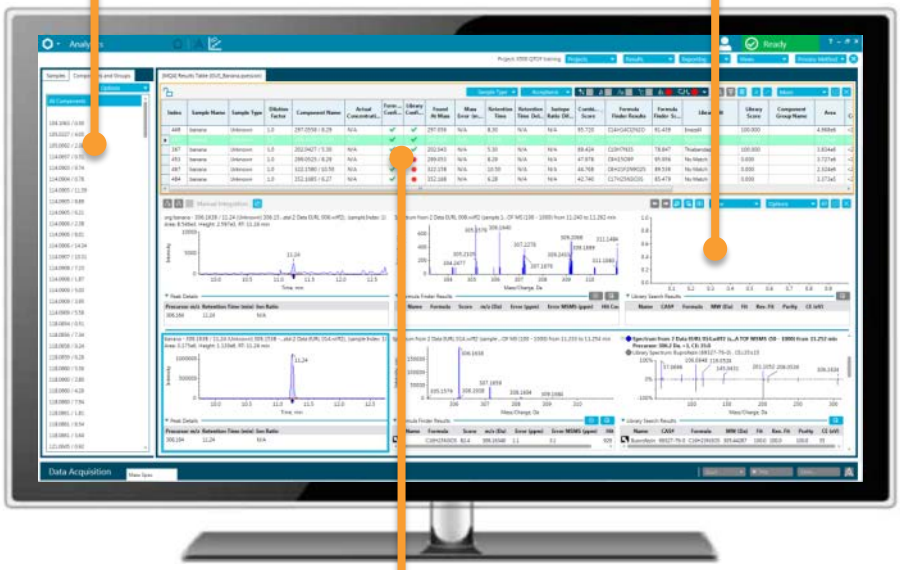
SCIEX OS Software – Unknown Identification

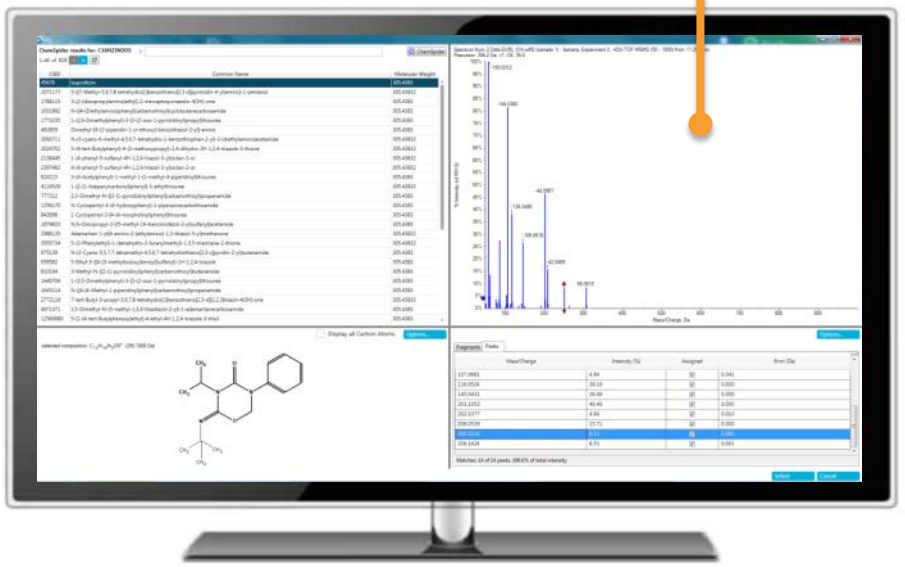
Software Improvements and Details

Automatic sample-control comparison

Non-Target peak finding

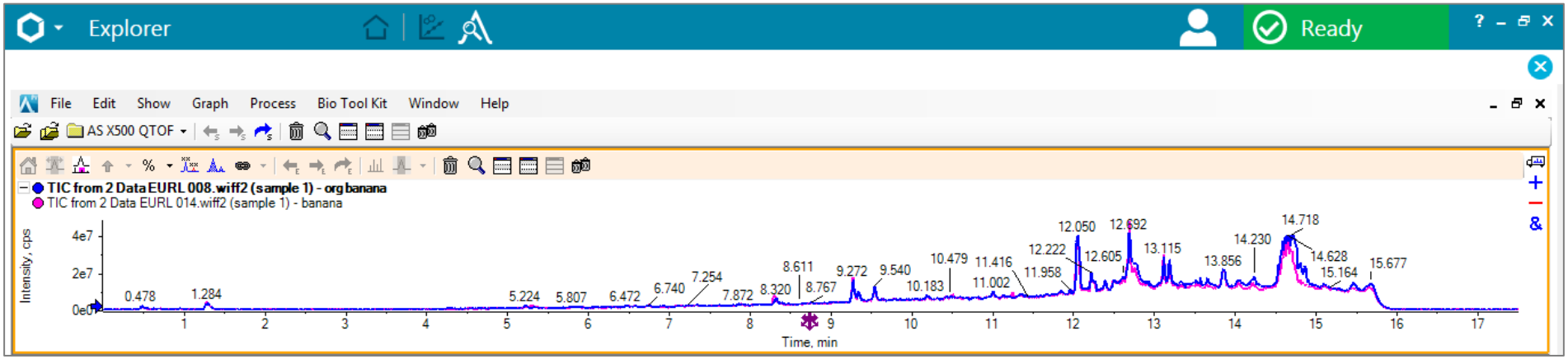
ChemSpider searching
Sorting by number of references and automatic structure elucidation to identify unknowns



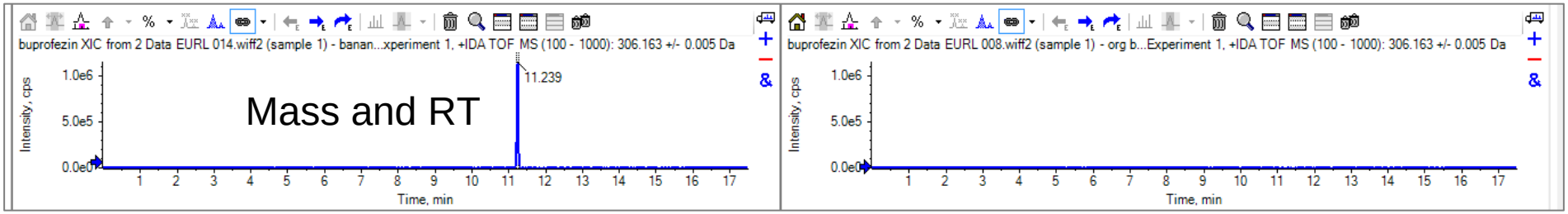


Automatic MS/MS library searching and formula finding

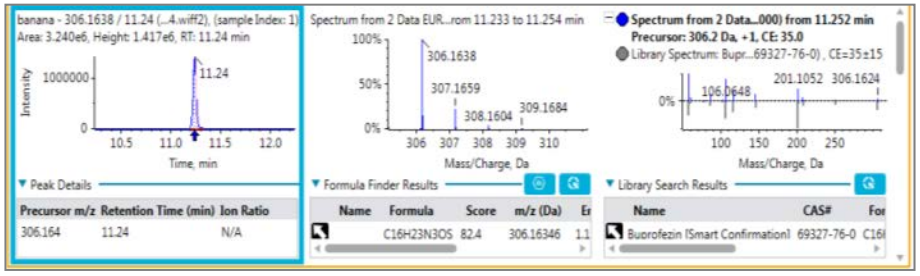
Non-Targeted Data Processing Workflow



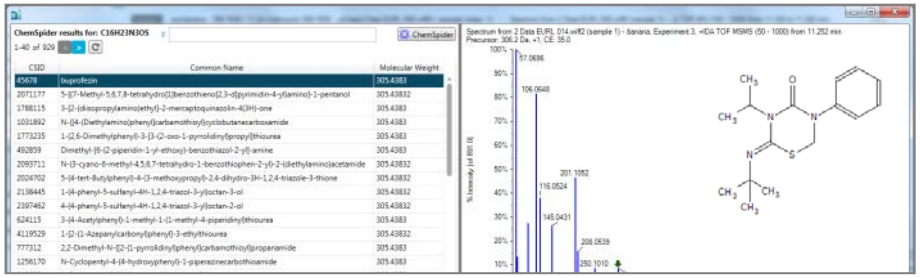
Sample-control comparison



Identification



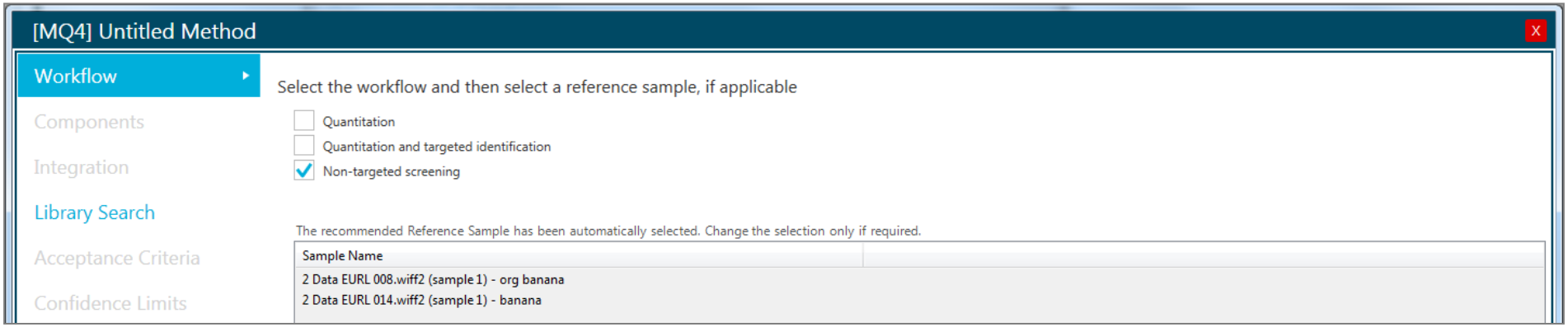
ChemSpider
The free chemical database

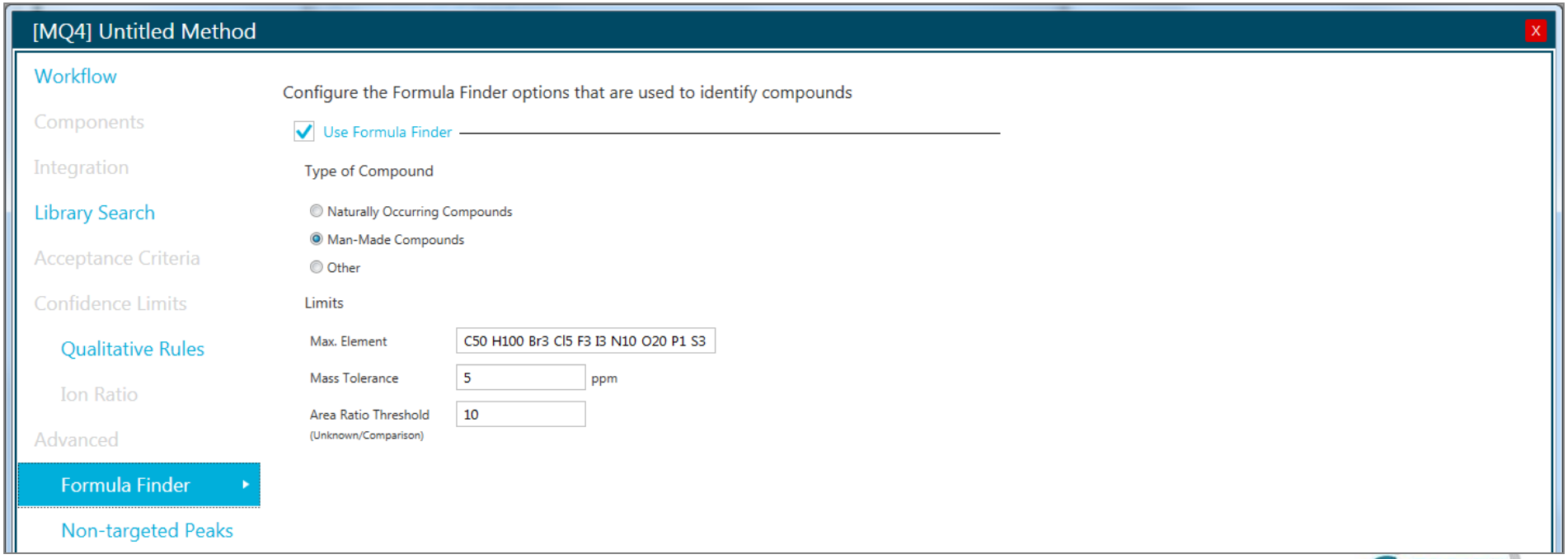


Formula finding ✓ MS/MS search ✓

Unknown Identification in SCIEX OS Software

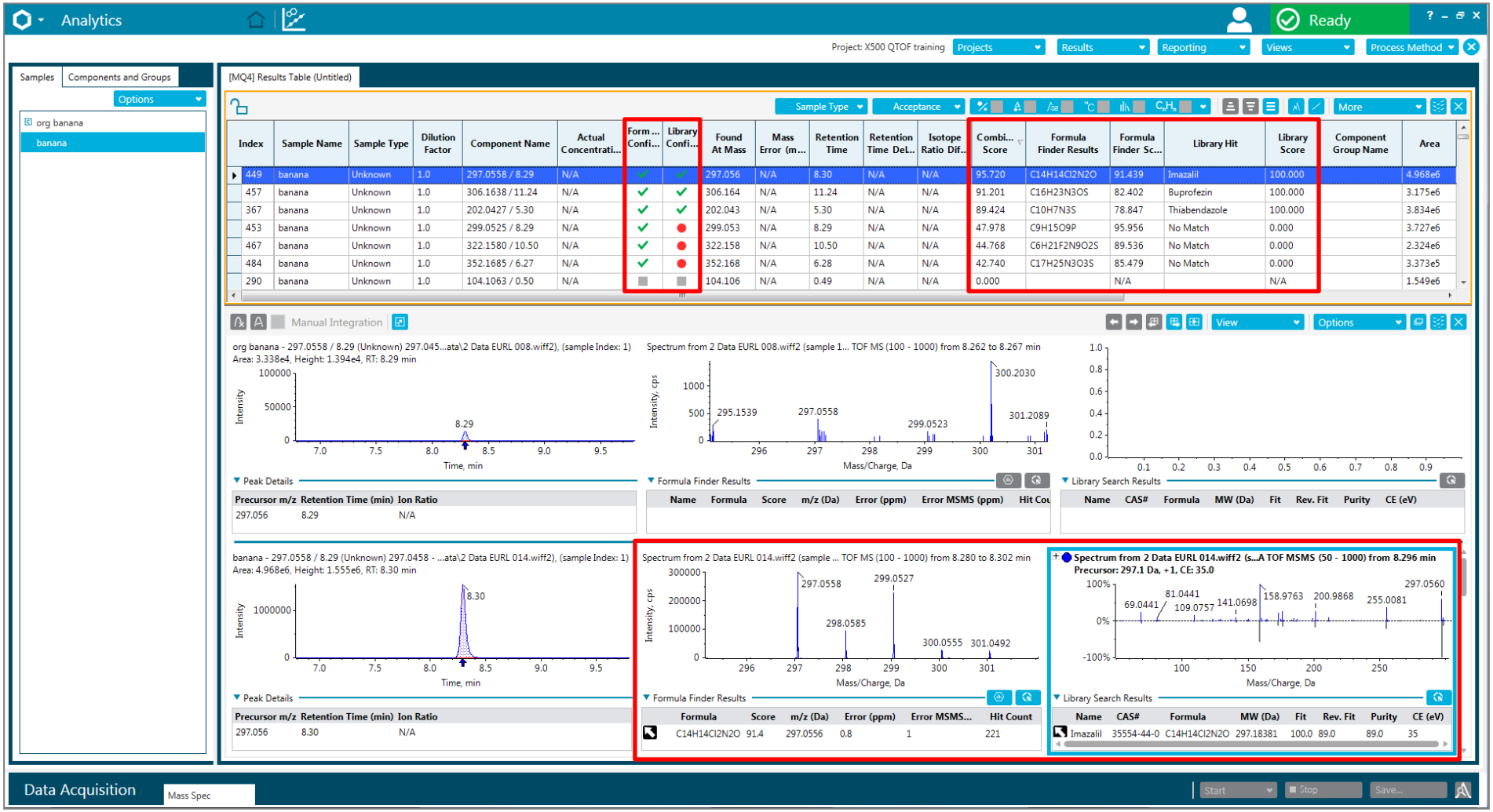
1. Define Non-Target Peak Finding and Identification Parameters





Unknown Identification in SCIEX OS Software

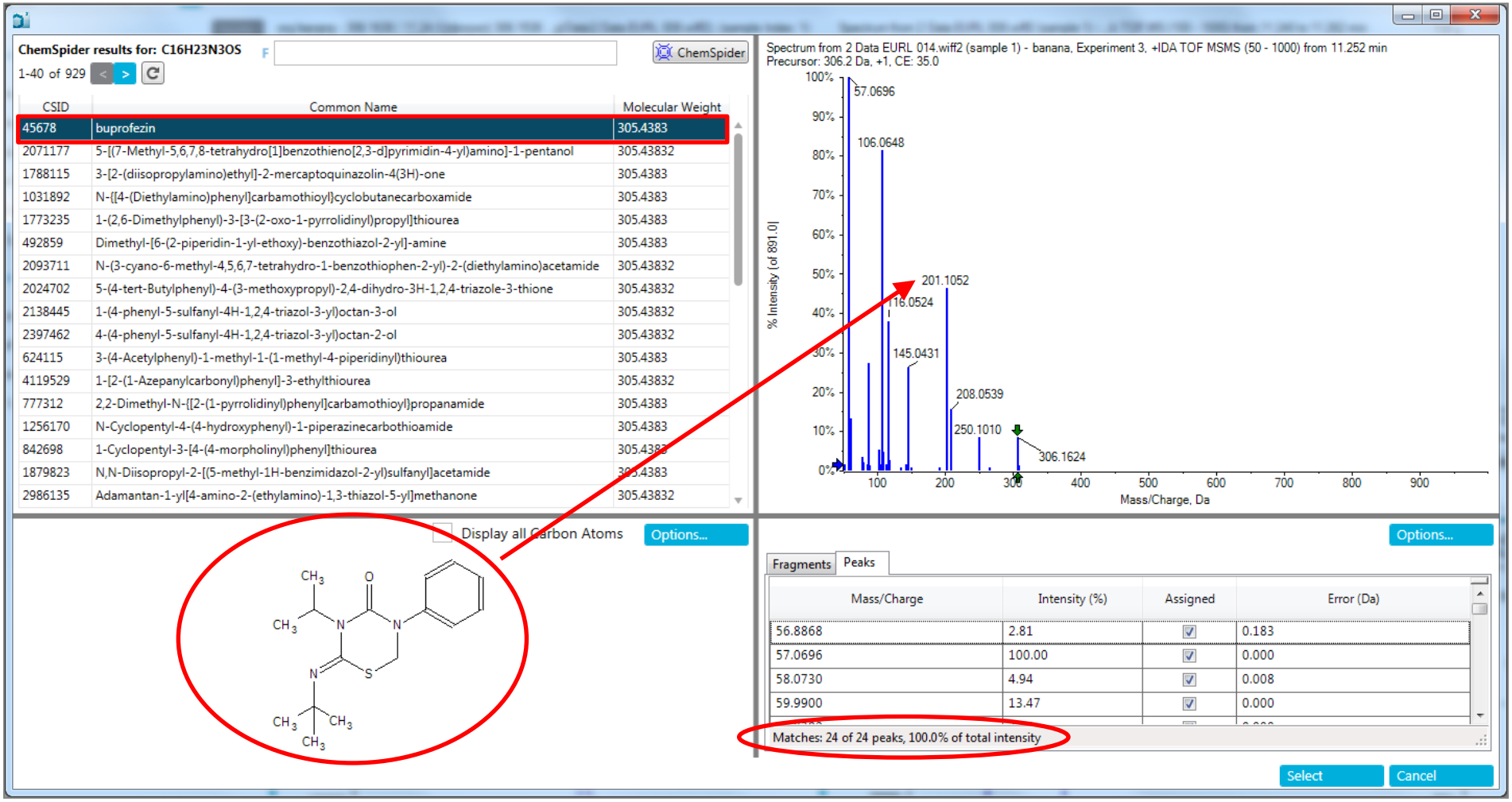
2. Automatic Sample-Control Comparison and Compound Identification



Automatic formula finding and MS/MS library searching

Unknown Identification in SCIEX OS Software

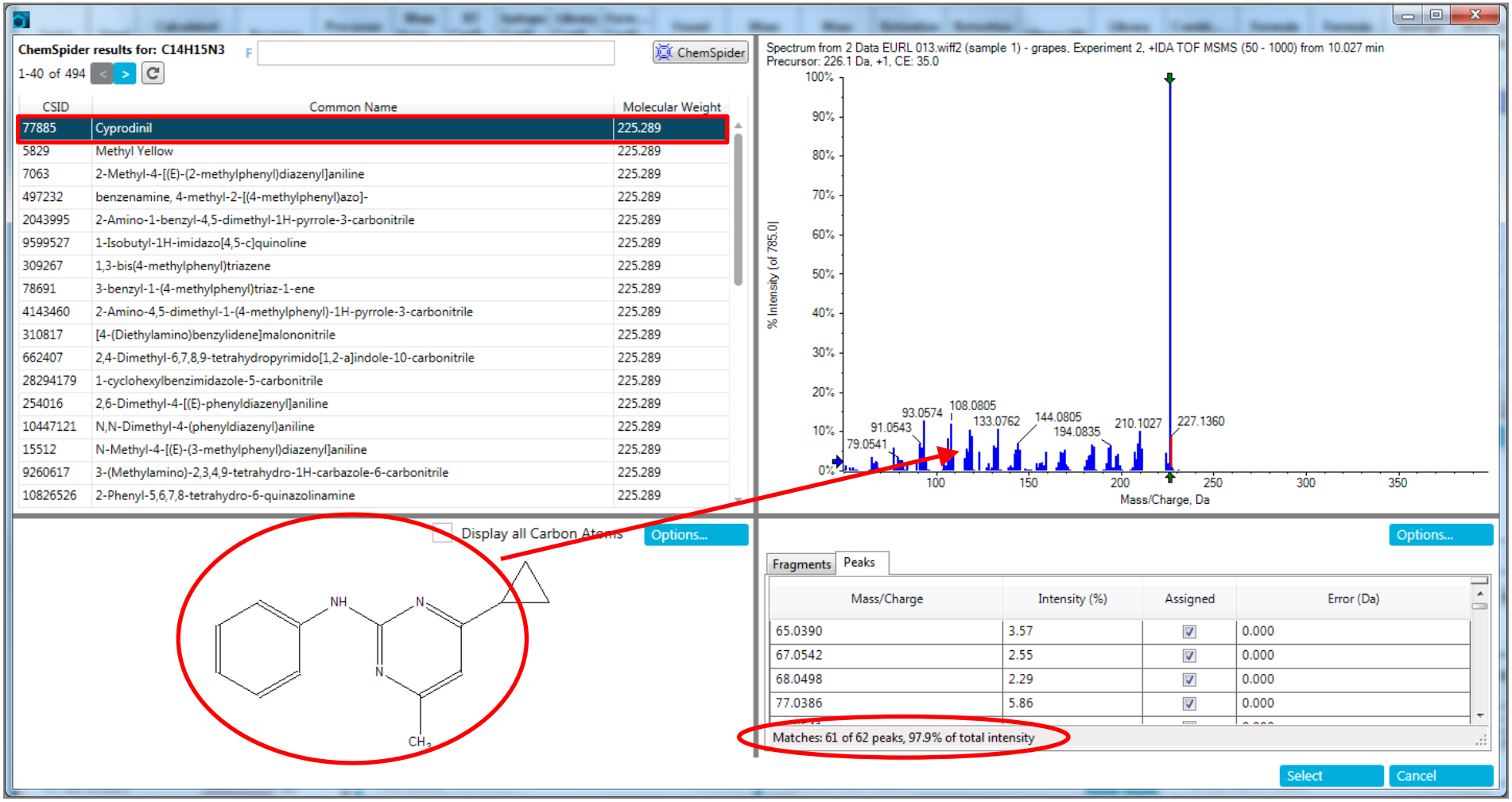
3. ChemSpider Searching and Structure Elucidation



ChemSpider searching of found formulae
Automatic structure elucidation using HR-MS/MS spectra

Unknown Identification in SCIEX OS Software

3. ChemSpider Searching and Structure Elucidation



ChemSpider searching of found formulae
Automatic structure elucidation using HR-MS/MS spectra

Summary

- Hardware and Software
  - New SCIEX ExionLC™ systems
    - Fully controlled by SCIEX OS software
  - New SCIEX Triple Quad™ and QTRAP® 6500+ systems
    - Improved IonDrive™ detection system
    - Elevated SelexION® technology
  - New SCIEX X500R QTOF System
    - N-optic design
    - Heated TOF path
    - Minimized footprint, engineered for simplicity and service accessibility
  - New SCIEX OS Software
    - New user interface
    - Simultaneous identification and quantitation
    - Automatic unknown identification
- Application data

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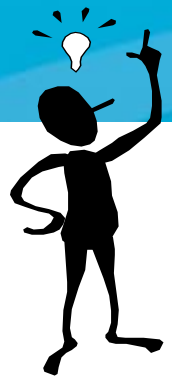

Thank you for your attention!