



Answers for Science.
Knowledge for Life.™



Ignite your Routine Testing Methods

André Schreiber
SCIEX, Concord, Ontario (Canada)

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

Mission:
SCIEX Operation X



CLASSIFIED

- 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

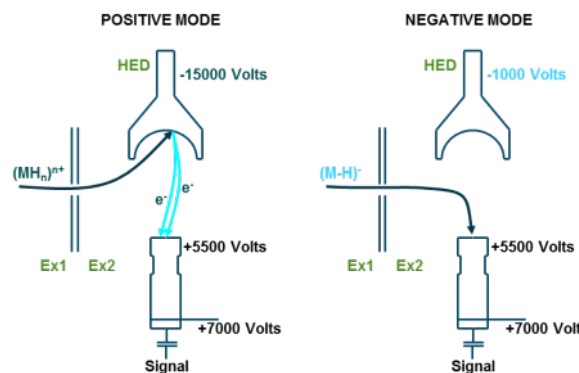


- Improved *IonDrive*™ detection system
 - Quantify with lowest limits of quantitation and up to six orders of linear dynamic range
 - Ultra fast polarity switching with *Scheduled MRM*™ Pro algorithm for multi-target quantitation
- Elevated *SelexION*® technology
 - Differential Mobility Spectrometry 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

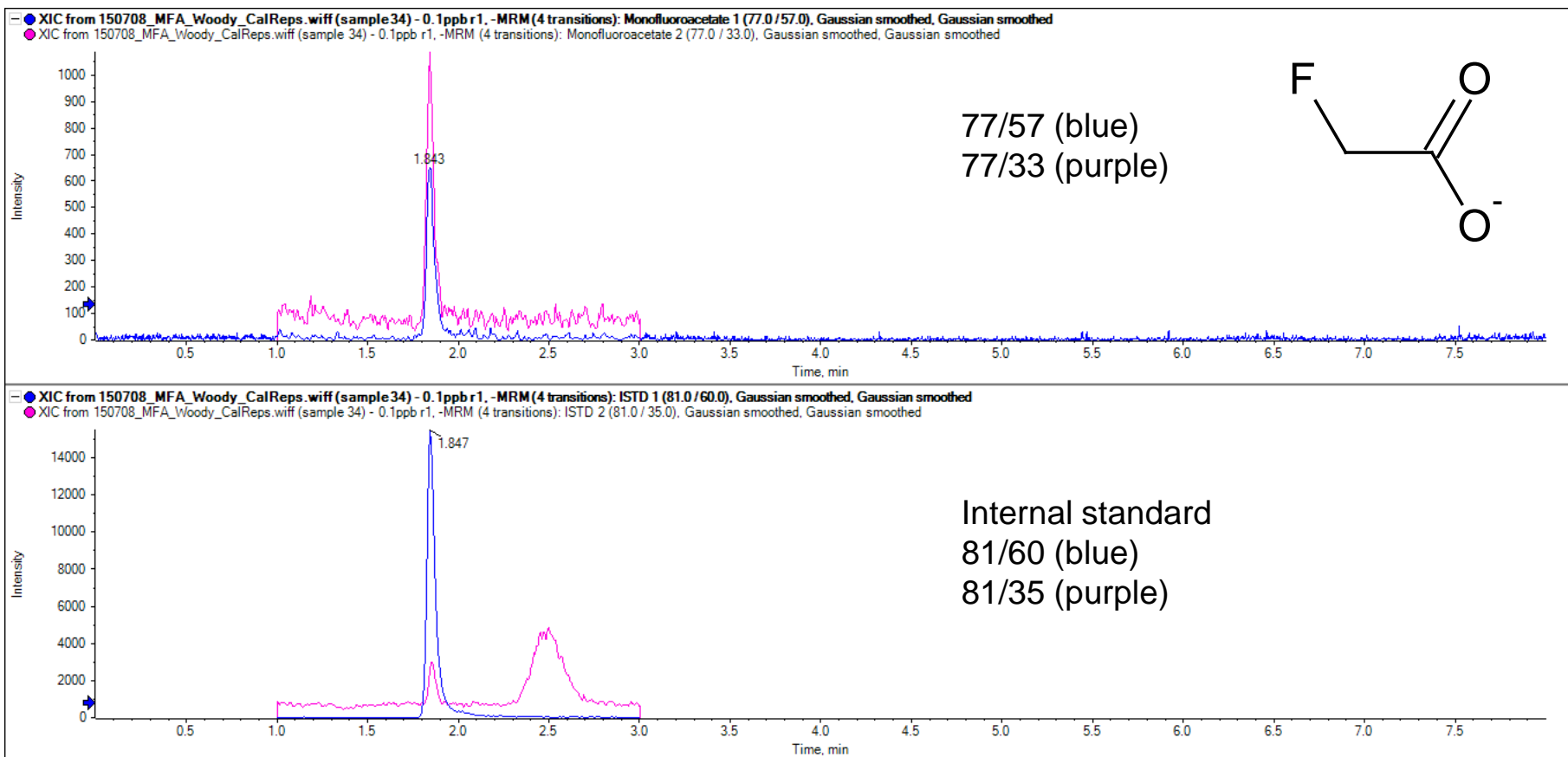
Improved *IonDrive*[™] Detection System

- 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

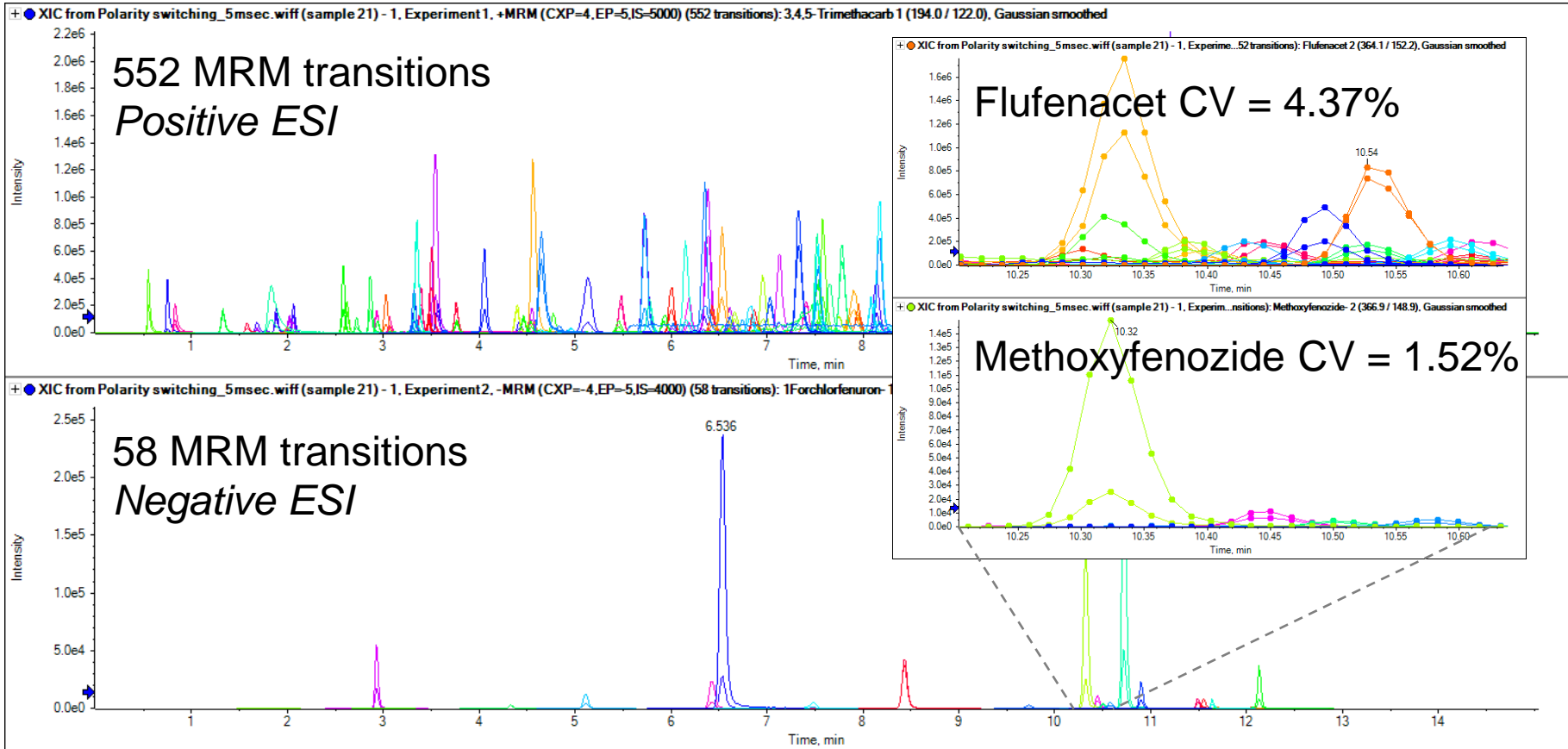
High Sensitivity in Negative Polarity using the QTRAP[®] 6500+ system



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



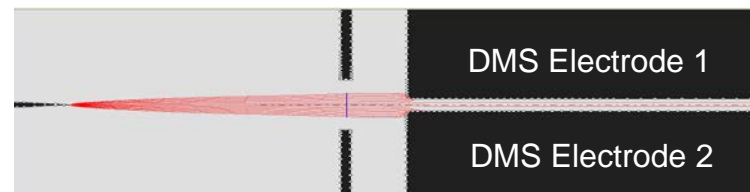
Phenomenex Kinetex™ Biphenyl 2.6u (50 x 2.1mm) column
Gradient of water/methanol + 5 mM ammonium formate
~300 pesticides at 1 ng/mL, MS/MS using QTRAP® 6500+ system

SelexION[®]+ DMS with Jet Injector Technology

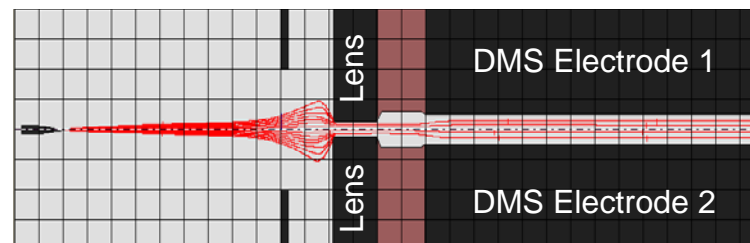
- New DMS cell designed to improve ion transmission by ~2x without loss in selectivity or resolution
 - Addition of lens increases ion velocities into DMS cell
 - Reduces transit times through detrimental fringing fields
- ✓ Continually driving selectivity improvements



SelexION cell



SelexION+ cell

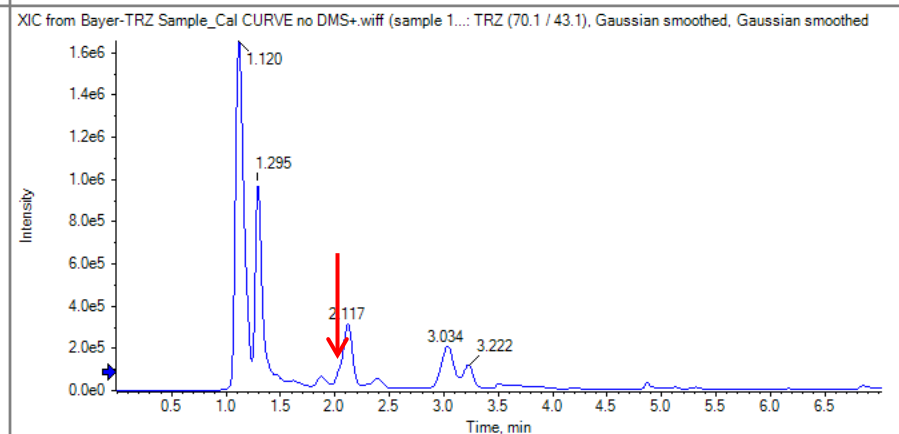
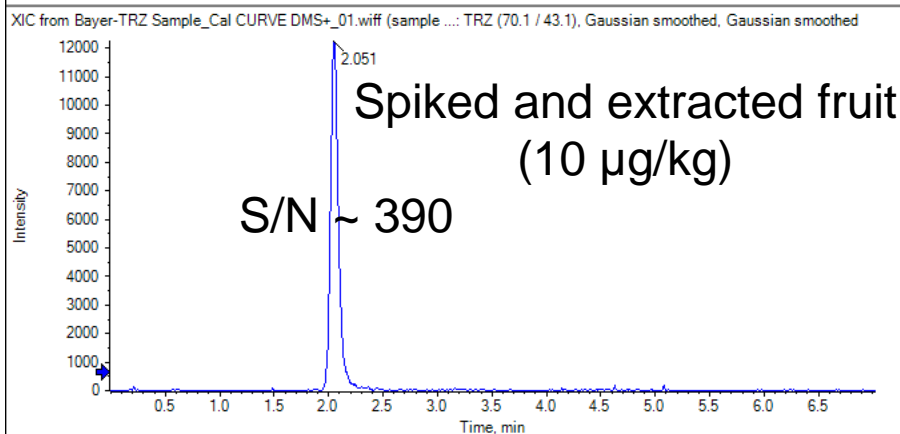
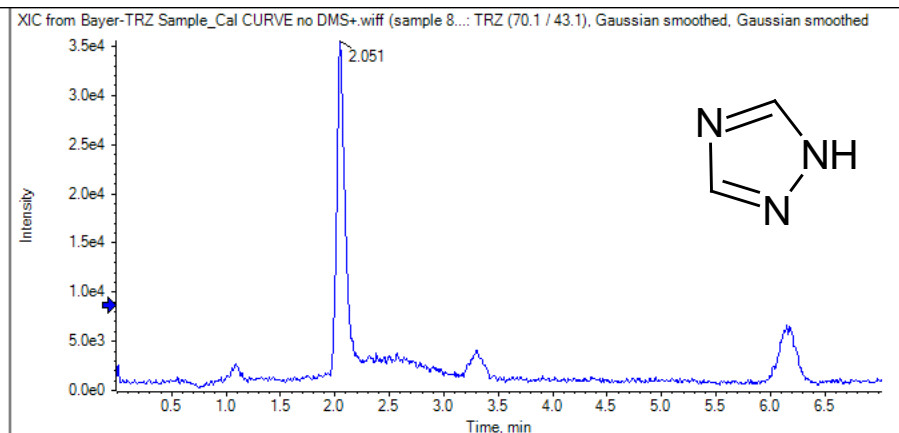
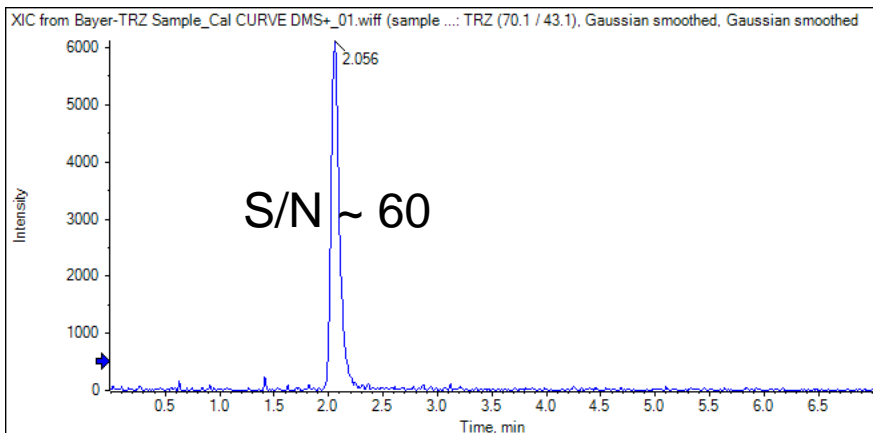


Reduced Noise and Interferences when Using DMS

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



CLASSIFIED

**Mission:
SCIEX Operation X**

**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

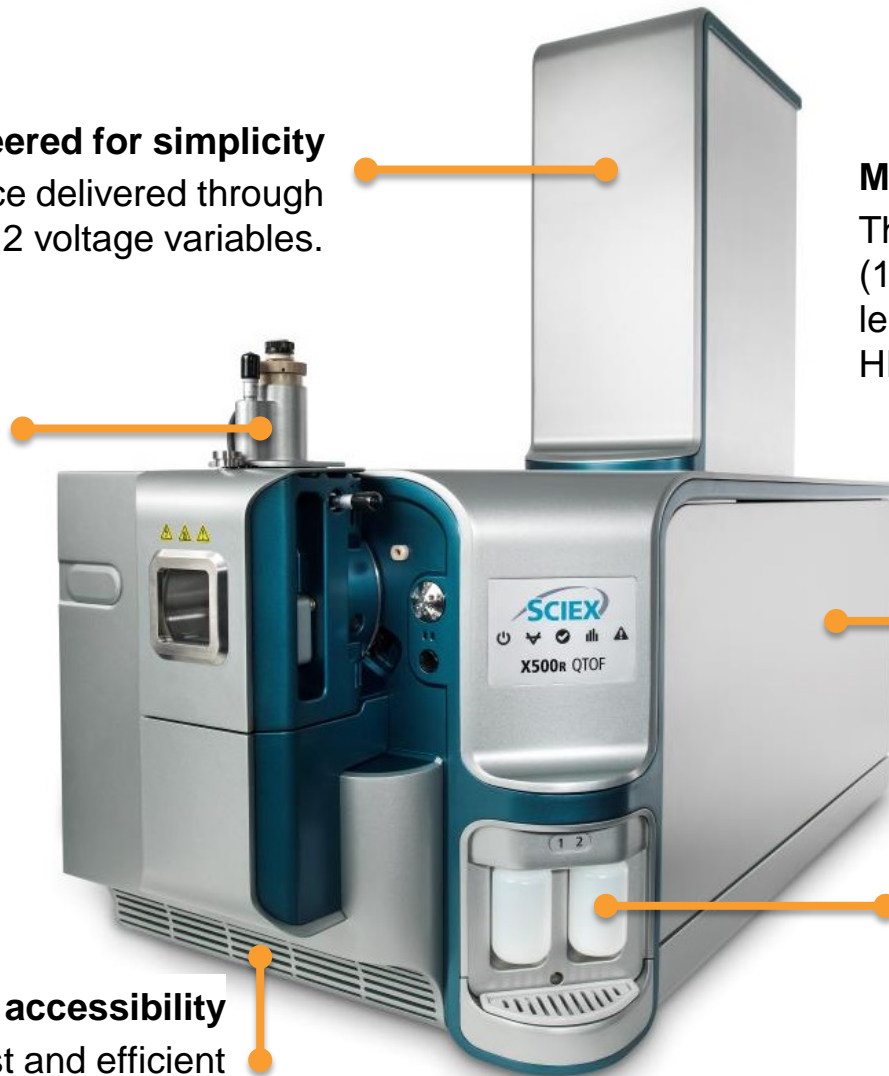
Optimal performance delivered through adjustment of only 2 voltage variables.

TwinSpray

An independent calibrant delivery path for reliable auto-calibration.

Service accessibility

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



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

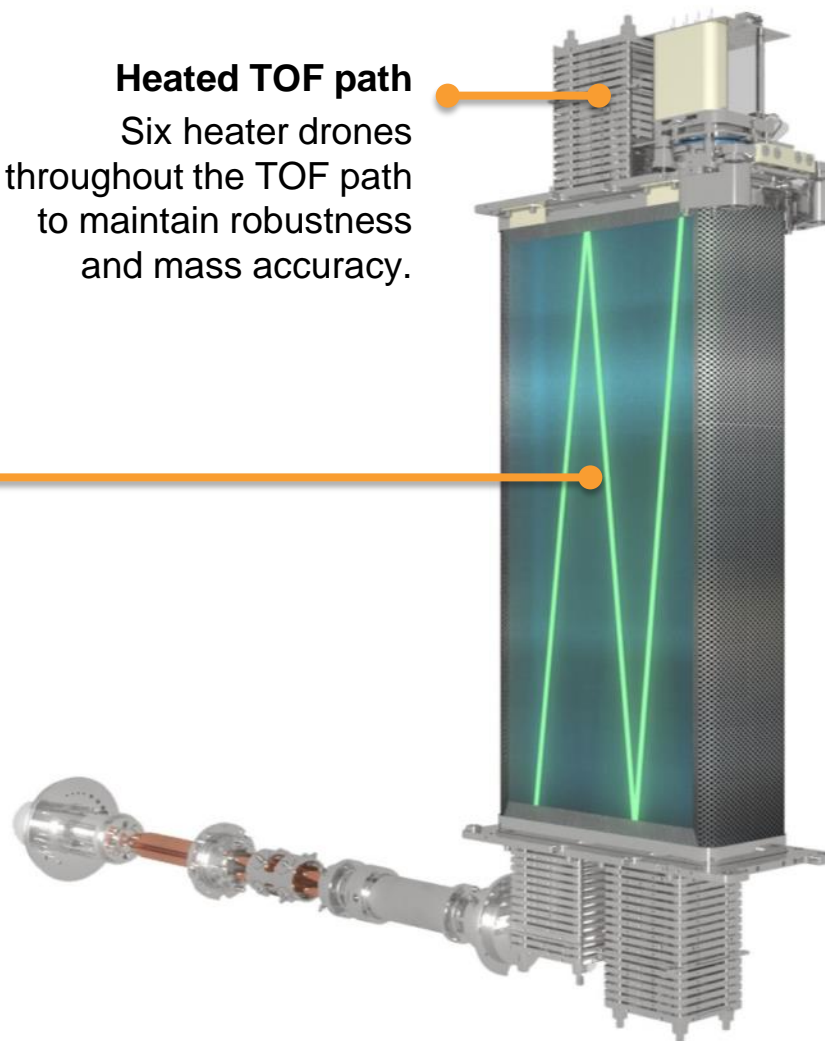
Maintains mass calibration through long runs without effect on sample flow.

Introducing the SCIEX X500R QTOF System

Design Improvements and Details

N-optic design
4 mm orifice leading into TOF accelerator tube delivers resolution without compromise in sensitivity.

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



Introducing the SCIEX X500R QTOF System

Design Improvements and Details

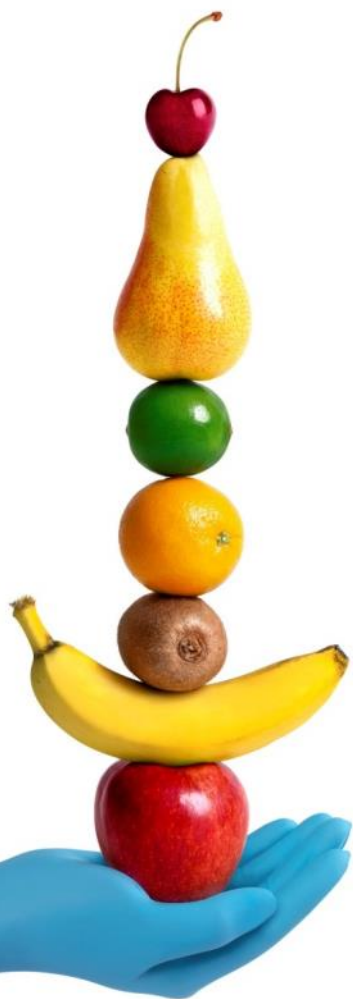
Legendary Turbo V source with optional IonDrive and Curtain Gas interface

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



Perfect Balance to Elevate Your Lab's Performance

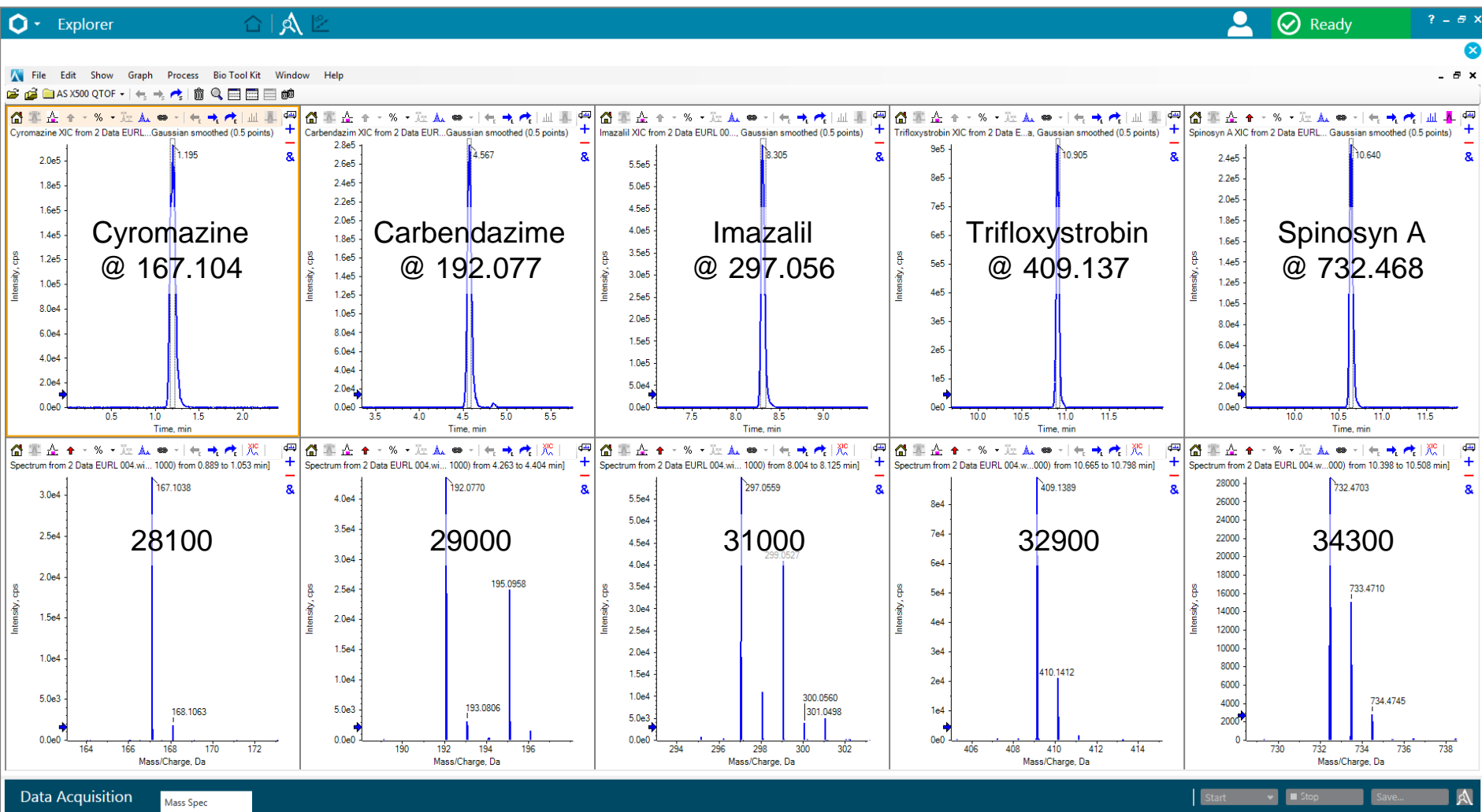
SCIEX X500R QTOF System



- 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

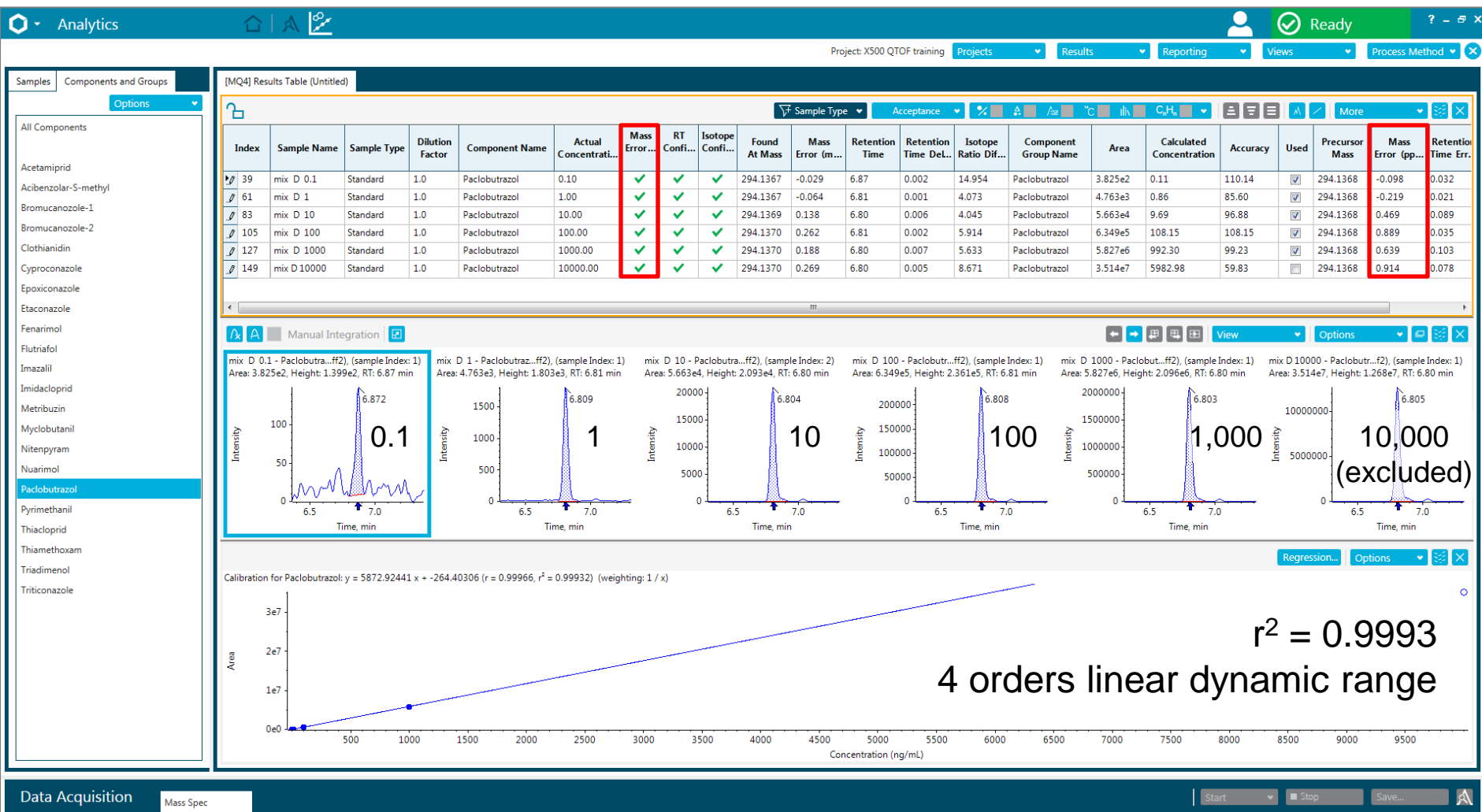
The SCIEX X500R QTOF System – Performance

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



The SCIEX X500R QTOF System – Performance

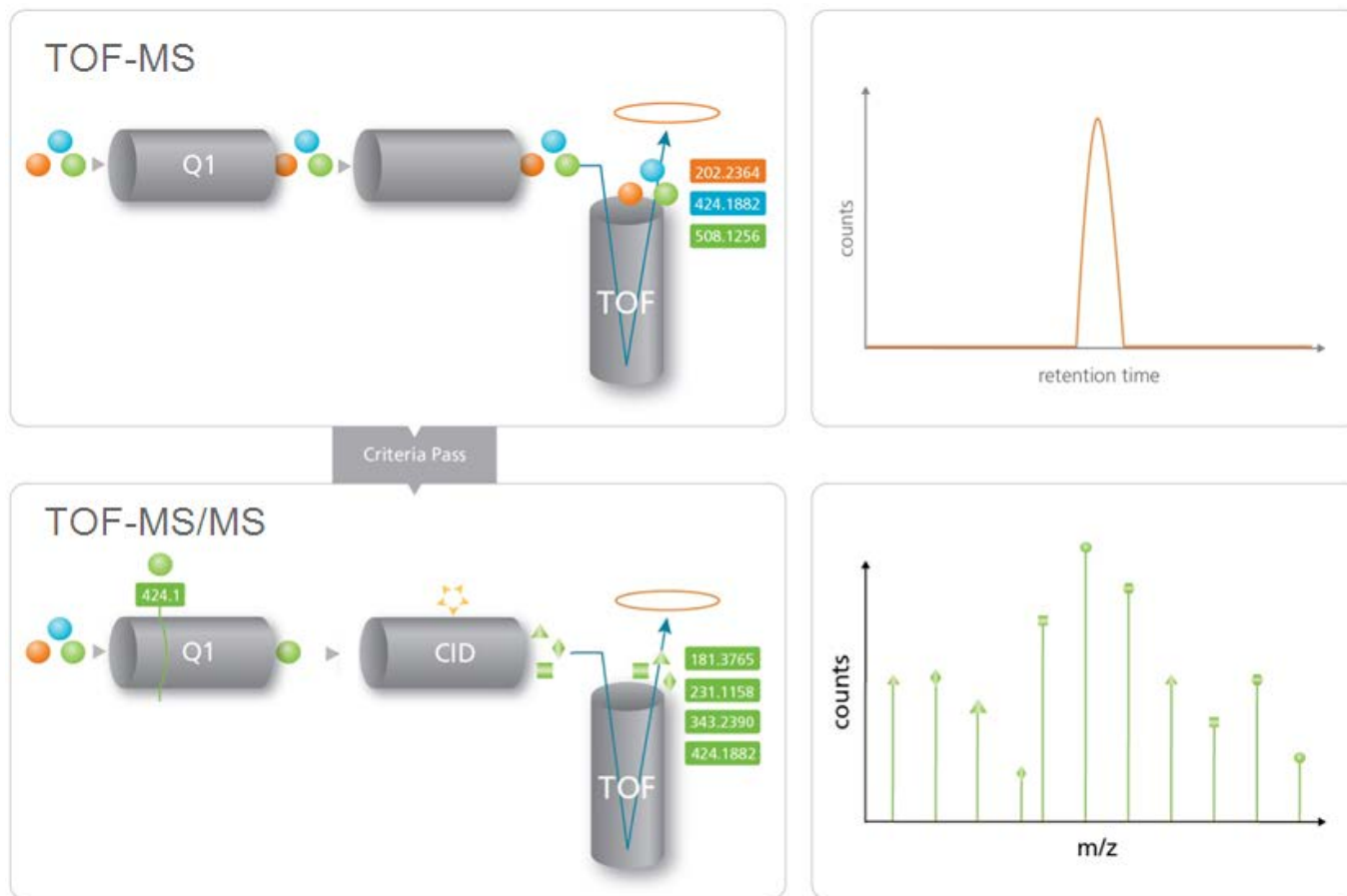
Linearity and Mass Accuracy (Paclobutrazol 0.1 to 10,000 ng/mL)



Mass error = -0.2 to 0.91 ppm

Information Dependent Acquisition of MS/MS (IDA)

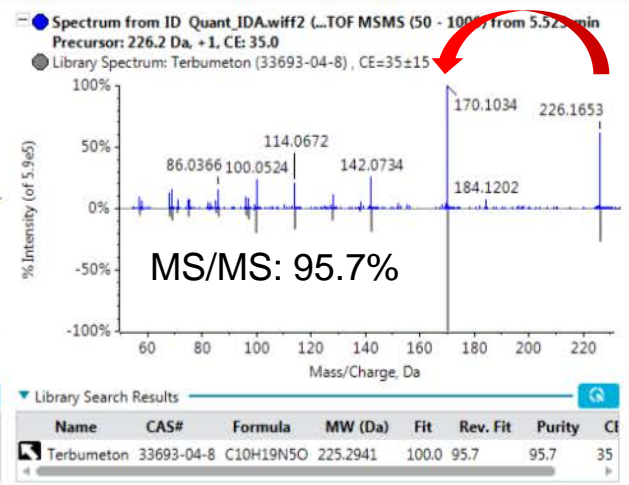
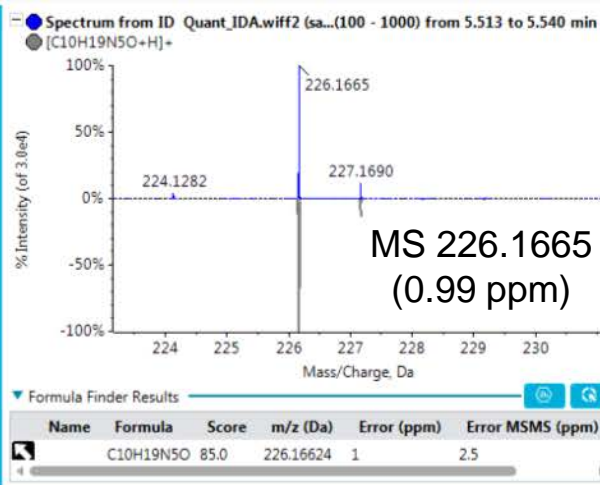
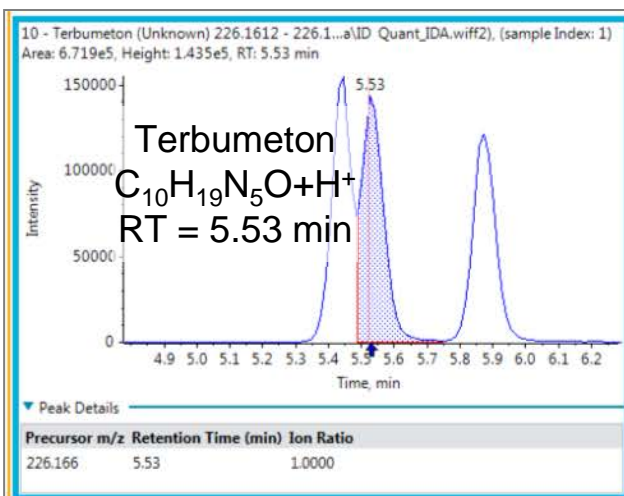
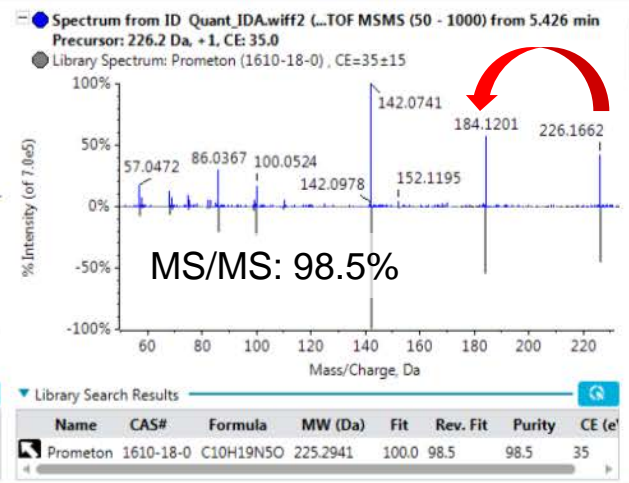
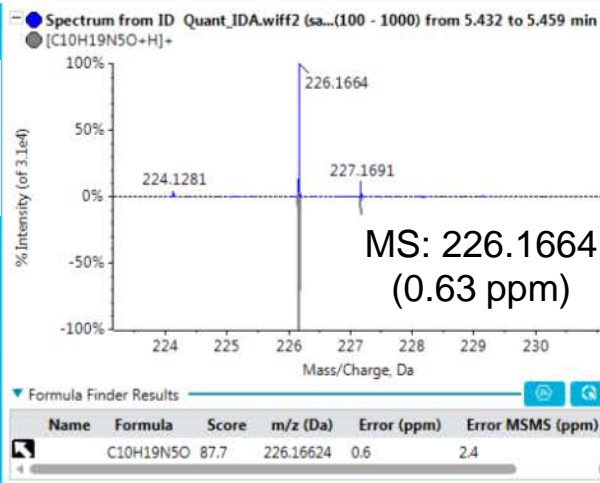
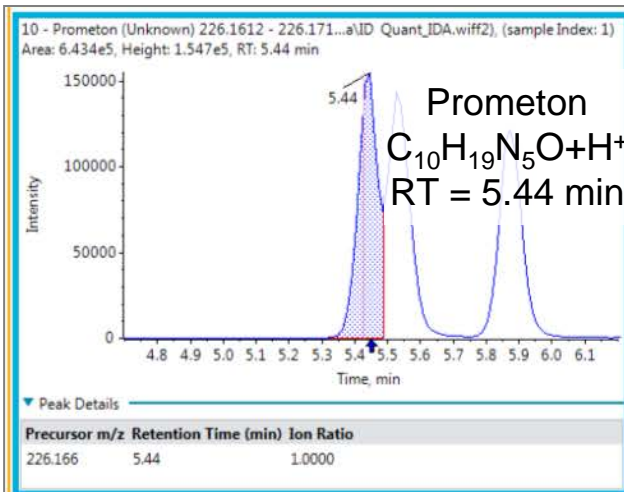
Provides MS/MS Spectra with High Selectivity (Q1 Resolution unit)



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

The SCIEX X500R QTOF System – IDA

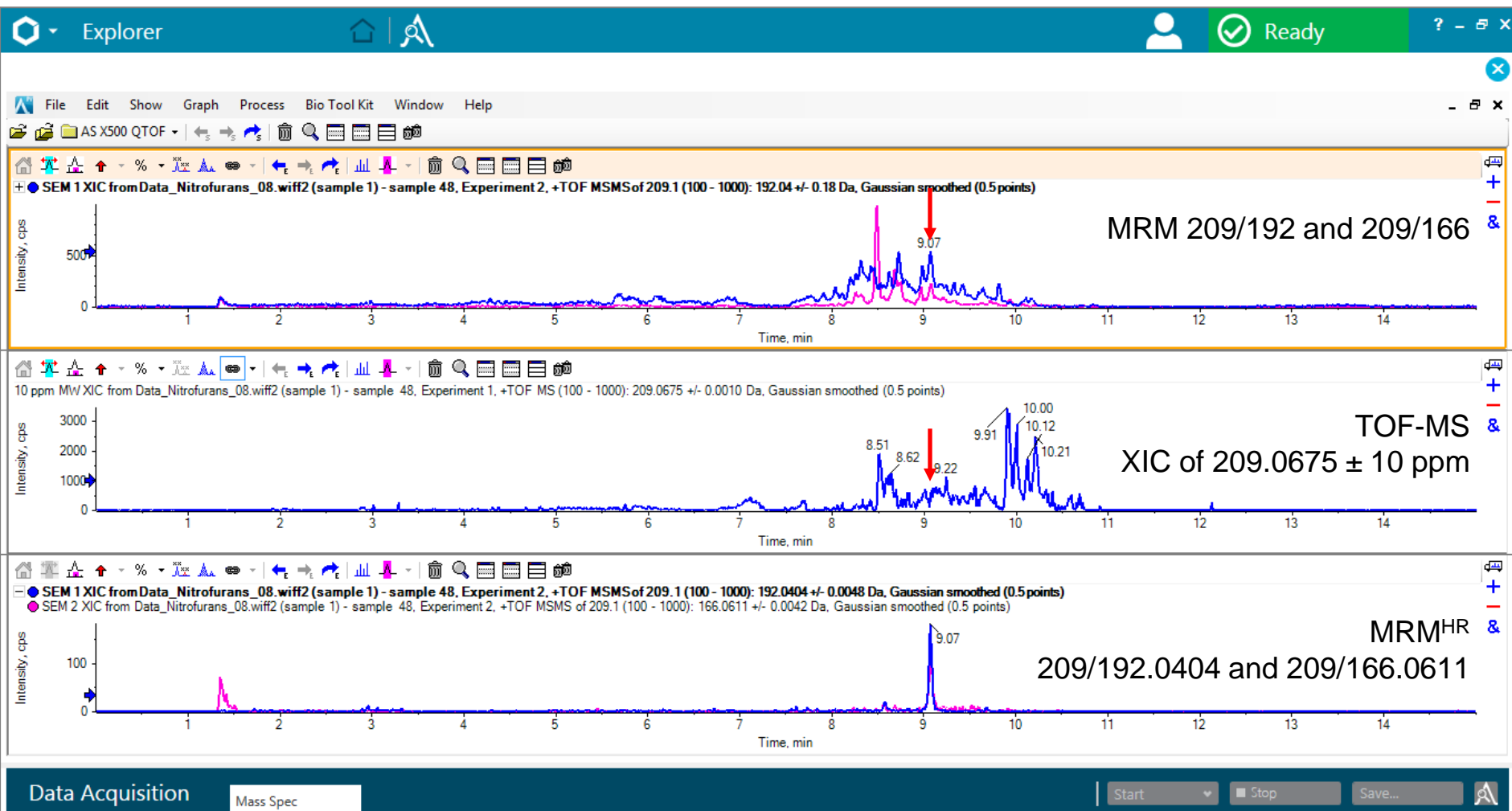
Confident Identification of Isomers using MS/MS (Prometon vs. Terbumeton)



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

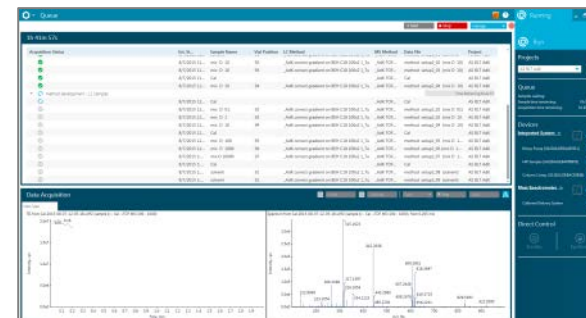
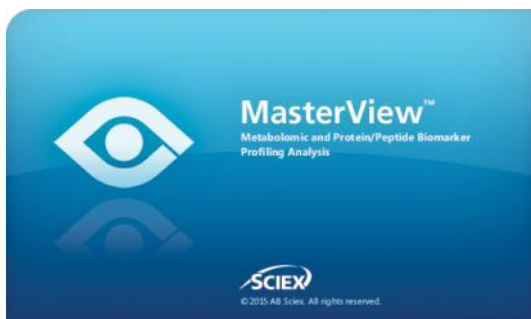
SCIEX X500R QTOF System Powered by SCIEX OS Software



- The first robust, high performance high resolution MS/MS system designed for routine use.
 - Sensitivity to easily detect maximum residue levels
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 - 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.

Introducing the SCIEX OS Software

Single Software Platform for MS Control, Data Processing and Reporting





Software Improvements and Details

New user interface

Thoughtfully designed for faster learning and improved productivity

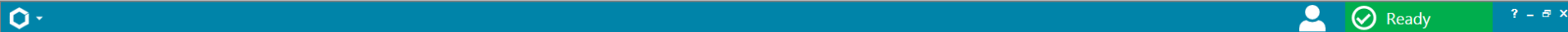
Acquire, analyze, report

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





Everything in a Single Software Platform



SCIEX OS

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

The screenshot displays the SCIEX OS software interface for editing a method named "IDA 10MSMS50msec". The interface is organized into several sections, each with its own set of parameters:

- Method Overview:** Shows "Method duration" set to 20 min and "Total scan time" as 0.760605 sec. "Estimated cycles" are 1577.
- Source and Gas Parameters:** Includes "Ion source gas 1" (50 psi), "Ion source gas 2" (70 psi), "Curtain gas" (30 psi), "CAD gas" (7 psi), and "Temperature" (450 °C).
- Experiment:** Shows "Polarity" as Positive V and "Spray voltage" as 5500 V.
- TOF MS:** Includes "TOF start mass" (100 Da), "TOF stop mass" (1000 Da), "Accumulation time" (0.2 sec), "Declustering potential" (80 V), "DP spread" (0 V), "Collision energy" (10 V), and "CE spread" (0 V).
- IDA Criteria:** Set to "Small molecule". Parameters include "Maximum candidate ions" (10), "Intensity threshold exceeds" (100 cps), and checkboxes for "Dynamic background subtraction" (checked) and "Exclude former candidate ions" (unchecked). It also has "For" and "After" time/occurrence settings.
- TOF MSMS:** Includes "Presursor ion" (E30 Da), "Declustering potential" (80 V), "Collision energy" (35 V), "TOF start mass" (50 Da), "DP spread" (0 V), "CE spread" (15 V), "TOF stop mass" (1000 Da), and "Accumulation time" (0.05 sec).

Labels on the right side of the image identify these sections: "Source and gas parameters", "TOF-MS", "IDA criteria", and "TOF-MS/MS".

SCIEX OS Software – Auto-Calibration

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

Positive Quick Status Check

- 1. Positive MS Check
 - Introduction
 - Achieve Stable Spray / Modify
 - TOF MS Mass Check**
 - TOF MS/MS Mass Check
 - Report

TOF MS Mass Check

If the acquisition results are not satisfactory, start **Auto-Calibrate**.

When auto-calibration is complete, select **Confirm** to update the calibration co-efficiency.

Auto Calibrate Start

Average of 20 spectra - Confirmation Mode

Mass Spectrum 1: 132.90488, 132.9053, 132.9588

Mass Spectrum 2: 829.53933, 829.5355, 830.5382, 831.5407

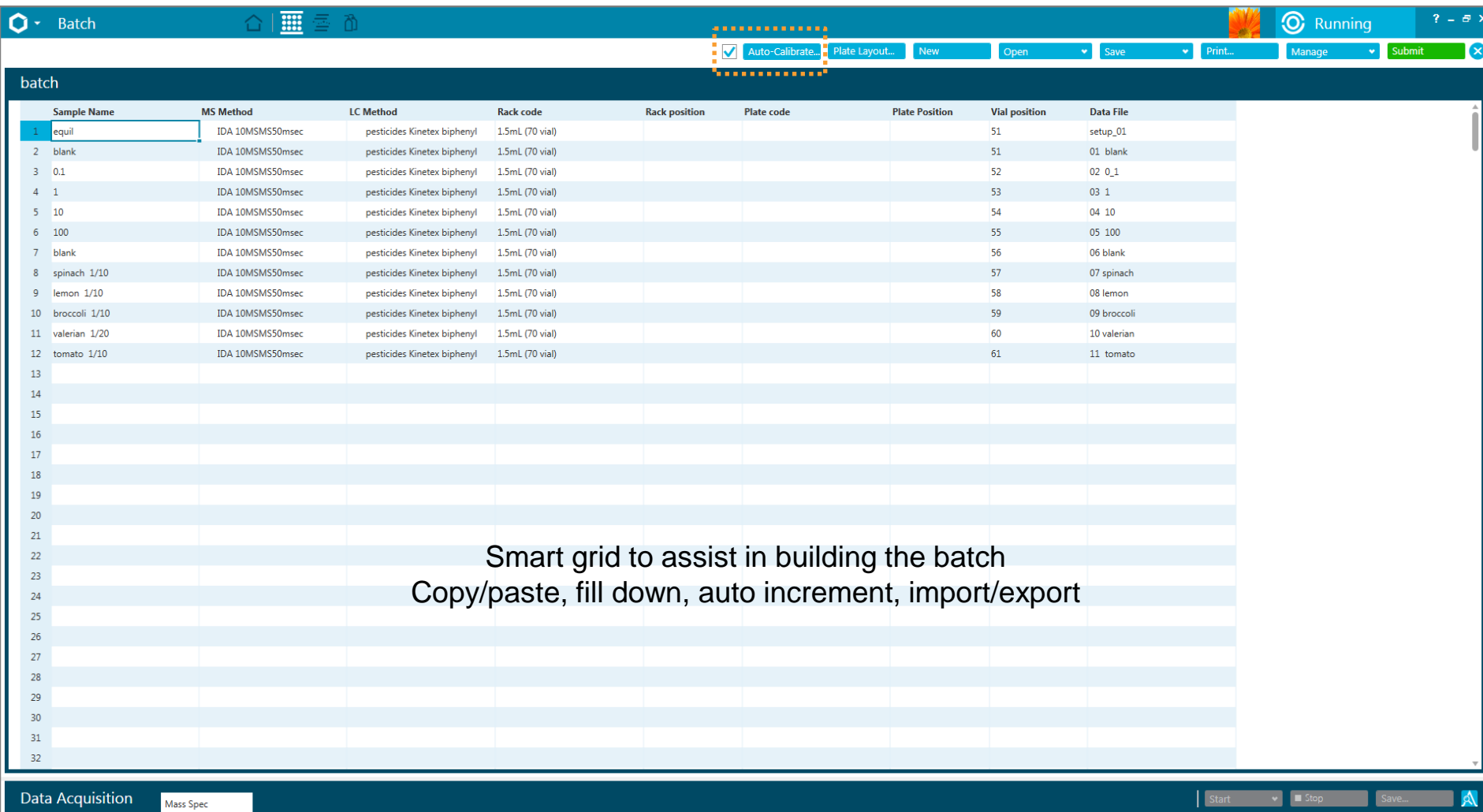
Item	Min	Max	Actual	Status
Mass	132.80488	133.00488	132.90526	Pass
Resolution	0	50000	28486	Pass
Intensity	0	1e+07	3.215e+05	Pass
Sum Intensity	0	1e+11	1.4733e+06	Pass
Error (ppm)	-100.00	100.00	2.84031	Pass

Item	Min	Max	Actual	Status
Mass	829.43933	829.63933	829.53548	Pass
Resolution	0	50000	33246	Pass
Intensity	0	1e+07	1.0326e+05	Pass
Sum Intensity	0	1e+11	1.0438e+06	Pass
Error (ppm)	-100.00	100.00	-4.64088	Pass

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

SCIEX OS Software – Building a Batch

3. Batch Editor and Setup for Auto-Calibration



The screenshot displays the SCIEX OS Batch Editor interface. At the top, a toolbar contains several buttons: 'Auto-Calibrate...' (highlighted with a dashed orange box), 'Plate Layout...', 'New', 'Open', 'Save', 'Print...', 'Manage', and 'Submit'. The main area is a table titled 'batch' with the following columns: Sample Name, MS Method, LC Method, Rack code, Rack position, Plate code, Plate Position, Vial position, and Data File. The table contains 12 rows of data, with the first row highlighted. Below the table, a text overlay reads: 'Smart grid to assist in building the batch Copy/paste, fill down, auto increment, import/export'. At the bottom of the interface, there is a 'Data Acquisition' section with 'Mass Spec' selected, and buttons for 'Start', 'Stop', and 'Save...'. The status bar at the top right shows 'Running'.

Sample Name	MS Method	LC Method	Rack code	Rack position	Plate code	Plate Position	Vial position	Data File
1 equil	IDA 10MSMS50msec	pesticides Kinetex biphenyl	1.5mL (70 vial)				51	setup_01
2 blank	IDA 10MSMS50msec	pesticides Kinetex biphenyl	1.5mL (70 vial)				51	01 blank
3 0.1	IDA 10MSMS50msec	pesticides Kinetex biphenyl	1.5mL (70 vial)				52	02 0_1
4 1	IDA 10MSMS50msec	pesticides Kinetex biphenyl	1.5mL (70 vial)				53	03 1
5 10	IDA 10MSMS50msec	pesticides Kinetex biphenyl	1.5mL (70 vial)				54	04 10
6 100	IDA 10MSMS50msec	pesticides Kinetex biphenyl	1.5mL (70 vial)				55	05 100
7 blank	IDA 10MSMS50msec	pesticides Kinetex biphenyl	1.5mL (70 vial)				56	06 blank
8 spinach 1/10	IDA 10MSMS50msec	pesticides Kinetex biphenyl	1.5mL (70 vial)				57	07 spinach
9 lemon 1/10	IDA 10MSMS50msec	pesticides Kinetex biphenyl	1.5mL (70 vial)				58	08 lemon
10 broccoli 1/10	IDA 10MSMS50msec	pesticides Kinetex biphenyl	1.5mL (70 vial)				59	09 broccoli
11 valerian 1/20	IDA 10MSMS50msec	pesticides Kinetex biphenyl	1.5mL (70 vial)				60	10 valerian
12 tomato 1/10	IDA 10MSMS50msec	pesticides Kinetex biphenyl	1.5mL (70 vial)				61	11 tomato
13								
14								
15								
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SCIEX OS Software – Queue, Live View and Status

4. Queue Manager with Inserted Auto-Cal Samples

Detailed instrument status

The screenshot displays the SCIEX OS software interface, divided into several key sections:

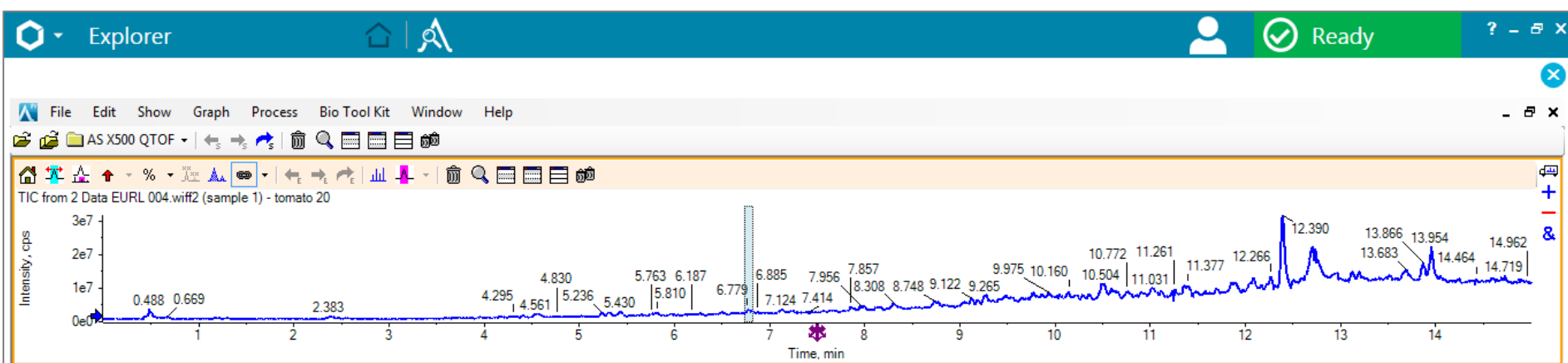
- Queue Manager:** A table listing acquisition status, start times, sample names, LC methods, MS methods, data files, and projects. It shows a sequence of samples including 'equil', 'blank', and 'Cal' (auto-calibration) samples interspersed with regular samples.
- Data Acquisition:** A section for monitoring the current acquisition, including a 'Mass Spec' tab and a 'Live TIC' (Total Ion Chromatogram) plot showing intensity versus time.
- Live View:** A section for monitoring the current spectrum, including a 'Live Spectrum' plot showing intensity versus m/z.
- Right Panel:** A detailed instrument status panel showing the instrument is 'Running', the project name, and the status of various components like the Shimadzu Nexera Prominence LC, Binary Gradient, Autosampler, Column Oven, System Controller, X500 QTOF, and Calibrant Delivery System.

Acquisition Status	Est. Start Time	Sample Name	LC Method	MS Method	Data File	Project
batch - 6 Samples						
✓	10/16/2015 11:28:24 AM	equil	pesticides Kinetex biphenyl	IDA 10MSMS50msec	setup_01	AS X500 QTOF MXNS samples
✓	10/16/2015 11:48:30 AM	blank	pesticides Kinetex biphenyl	IDA 10MSMS50msec	01 blank	AS X500 QTOF MXNS samples
✓	10/16/2015 12:10:15 PM	0.1	pesticides Kinetex biphenyl	IDA 10MSMS50msec	02 0_1	AS X500 QTOF MXNS samples
✓	10/16/2015 12:30:53 PM	1	pesticides Kinetex biphenyl	IDA 10MSMS50msec	03 1	AS X500 QTOF MXNS samples
✓	10/16/2015 12:51:33 PM	10	pesticides Kinetex biphenyl	IDA 10MSMS50msec	04 10	AS X500 QTOF MXNS samples
✓	10/16/2015 1:12:15 PM	100	pesticides Kinetex biphenyl	IDA 10MSMS50msec	05 100	AS X500 QTOF MXNS samples
batch - 6 Samples						
batch MSe - 7 Samples						
batch - 18 Samples						
⌚	10/16/2015 6:01:48 PM	Cal		IDA 10MSMS50msec	Cal	AS X500 QTOF MXNS samples
⌚	10/16/2015 6:04:19 PM	equil	pesticides Kinetex biphenyl	IDA 10MSMS50msec	setup_01	AS X500 QTOF MXNS samples
⌚	10/16/2015 6:24:23 PM	blank	pesticides Kinetex biphenyl	IDA 10MSMS50msec	01 blank	AS X500 QTOF MXNS samples
⌚	10/16/2015 6:44:27 PM	Cal		IDA 10MSMS50msec	Cal	AS X500 QTOF MXNS samples
⌚	10/16/2015 6:44:58 PM	0.1	pesticides Kinetex biphenyl	IDA 10MSMS50msec	02 0_1	AS X500 QTOF MXNS samples
⌚	10/16/2015 7:05:02 PM	1	pesticides Kinetex biphenyl	IDA 10MSMS50msec	03 1	AS X500 QTOF MXNS samples

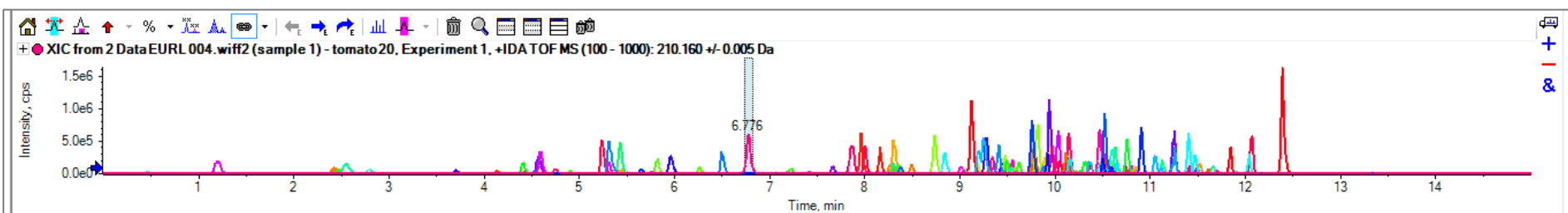
Live TIC

Live Spectrum

Targeted Data Processing Workflow



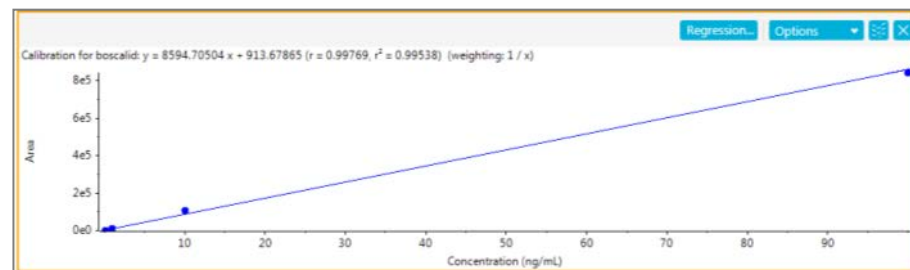
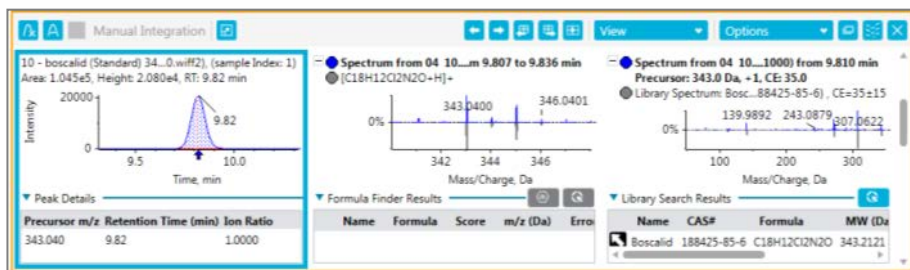
XIC generation for each target



Identification



Quantitation



RT ✓

Mass
Isotopes ✓

MS/MS search ✓

Above reporting level

Identification and Quantitation in SCIEX OS Software

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

[MQ4] Modify Method

Workflow Select or verify the analyte and internal standard names and masses.

Components Experiment Type Import Export... Options

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

Process & Close Close Help

Identification and Quantitation in SCIEX OS Software

2. Define Identification Criteria and Confidence Settings

[MQ4] Modify Method

Workflow

Components

Integration

Library Search

Acceptance Criteria

Confidence Limits

Qualitative Rules

Ion Ratio

Configure the library search parameters

Perform Library Search

Library Search Algorithm: Smart Confirmation Search

Results Sorted By: Purity

Library Spectra Type: All Spectra

Libraries To Search

Search All Libraries

Allergen test

HR_Pesticides

Area Ratio Threshold (Unknown/Comparison): 0 cps

[MQ4] Modify Method

Workflow

Components

Integration

Library Search

Acceptance Criteria

Confidence Limits

Qualitative Rules

Ion Ratio

Configure the confidence levels for the qualitative rules, as applicable

Apply	Qualitative Rule	Acceptable Difference	Marginal Difference	Unacceptable Difference	Combined Score Weight (%)	
<input checked="" type="checkbox"/>	Mass Error (ppm)	< 5	< 10	>= 10	30	
<input checked="" type="checkbox"/>	Error in Retention Time	< 0.1	< 0.2	>= 0.2	30	<input type="radio"/> Error %
<input checked="" type="checkbox"/>	% Difference Isotope Ratio	< 20	< 40	>= 40	20	<input checked="" type="radio"/> Absolute
<input checked="" type="checkbox"/>	Library Hit Score	> 70	> 50	<= 50	20	
<input type="checkbox"/>	Formula Finder Score	> 50	> 20	<= 20	20	

Identification and Quantitation in SCIEX OS Software

3. Review Quantitative and Quantitative Results

Analytics Ready

Project: X500 QTOF training Projects Results Reporting Views Process Method

Samples Components and Groups

Options

- fenpyroximate
- fenuron
- flonicamid
- flucarbazone
- fludioxonil
- flufenacet
- flufenoxuron
- flumetsulam
- fluometuron
- fluopicolide
- fluoxastrobin
- fluquinconazole
- flusilazole
- fluthiacet-methyl
- flutriafol
- fluvinate
- forchlorfenuron
- formetanate
- fosthiazate
- fuferidazole
- furalaxyl
- furathiocarb
- hexaconazole
- hexaflumuron
- hexythiazox
- hydramethylnon
- imazalil**
- imibenconazole
- imidacloprid
- inabenfide
- indoxcarb
- ipconazole

[MQ4] Results Table (pesticide calibration lines X500 2uL.qsession)

Index	Sample Name	Sample Type	Dilution Factor	Component Name	Actual Concentr...	Calculated Concentration	Mass Error...	RT Confi...	Isotope Confi...	Library Confi...	Found At Mass	Mass Error (m...	Retention Time	Retention Time Del...	Isotope Ratio Dif...	Library Hit	Library Score	Component Group Name	Area
149	ID 0.1	Standard	1.0	imazalil	0.10	0.14	✓	✓	✓	✓	297.0554	-0.192	6.08	0.001	10.456	Imazalil	88.809	imazalil	3.160e4
432	ID 1	Standard	1.0	imazalil	1.00	0.68	✓	✓	✓	✓	297.0551	-0.529	6.08	0.002	3.960	Imazalil	90.976	imazalil	5.018e4
715	ID 10	Standard	1.0	imazalil	10.00	9.09	✓	✓	✓	✓	297.0558	0.162	6.08	0.002	5.357	Imazalil	97.308	imazalil	3.378e5
998	ID 100	Standard	1.0	imazalil	100.00	101.19	✓	✓	✓	✓	297.0556	-0.041	6.08	0.002	7.683	Imazalil	100.000	imazalil	3.489e6
1281	NVWA 10	Unknown	5.0	imazalil	N/A	15.99	✓	✓	✓	✓	297.0553	-0.344	6.08	0.000	15.376	Imazalil	97.435	imazalil	1.362e5

Flagging when above MRL and traffic lights for confidence

Manual Integration

NVWA 10 - imazalil (Unknown) 297.045...A 10 - IDA.wiff2), (sample Index: 1)
Area: 1.362e5, Height: 4.825e4, RT: 6.08 min

Peak Details

Precursor m/z	Retention Time (min)	Ion Ratio
297.0556	6.08	1.0000

Spectrum from NVWA 10 - IDA.w...10000) from 6.080 to 6.105 min
Precursor: [C14H14Cl2N2O+H]+

Formula Finder Results

Name	Formula	Score	m/z (Da)	Error (ppm)	Error MSN
Imazalil	C14H14Cl2N2O	97.4	297.18381	100.0	9

Spectrum from NVWA 10 - IDA.w...MS (50 - 1000) from 6.069 min
Precursor: 297.1 Da, +1. CE: 35.0

Library Search Results

Name	CAS#	Formula	MW (Da)	Fit	Rev. Fit
Imazalil	35554-44-0	C14H14Cl2N2O	297.18381	97.4	100.0

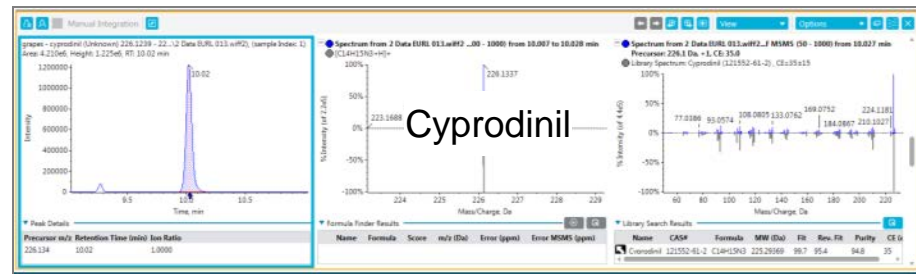
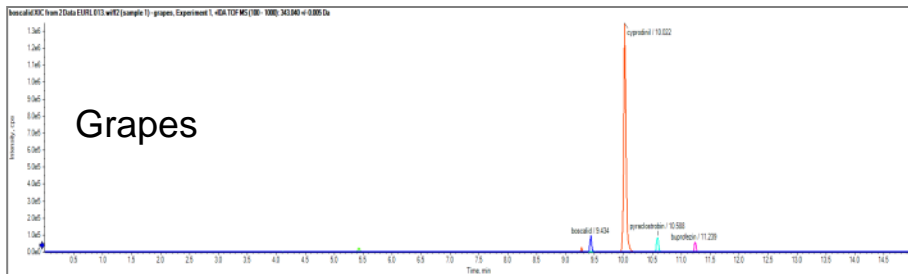
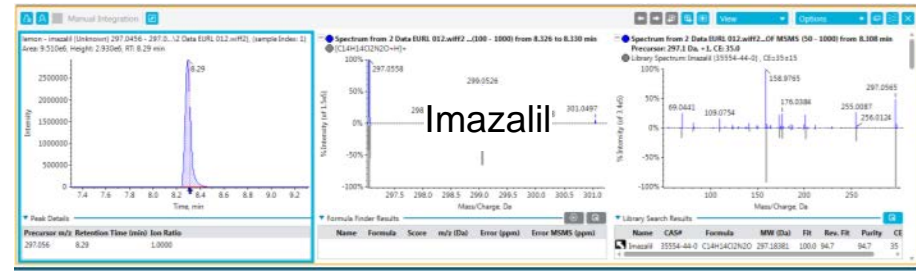
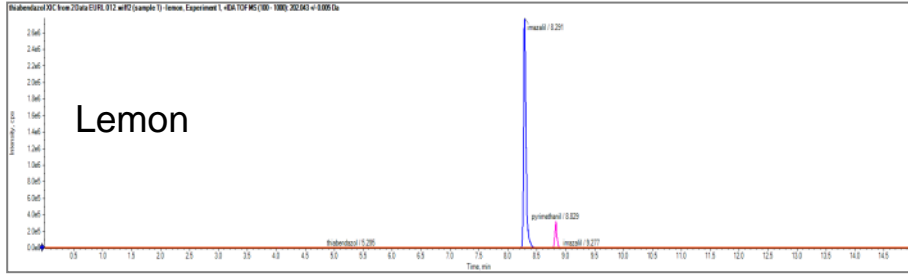
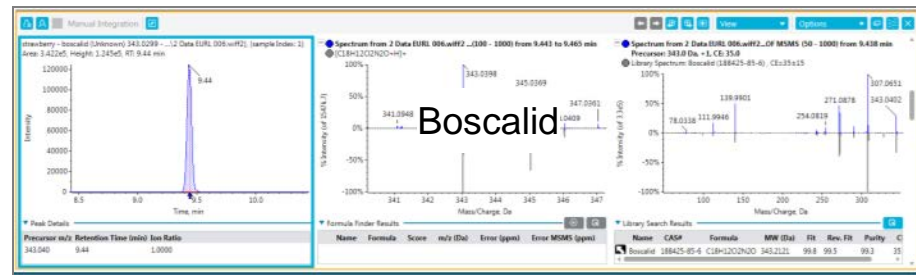
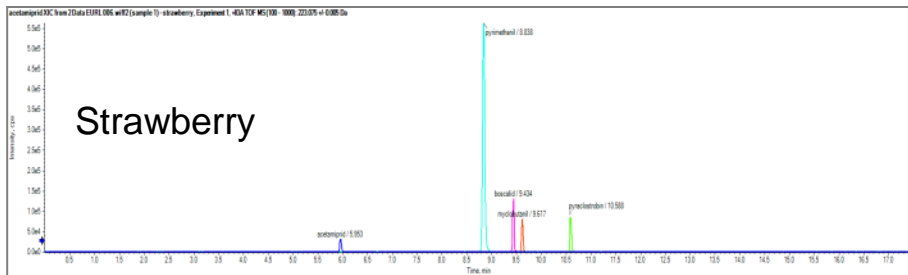
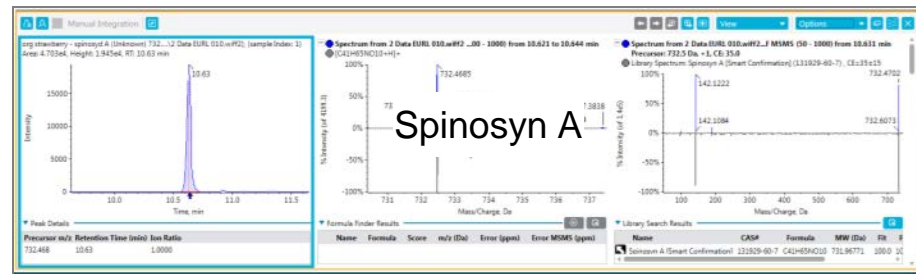
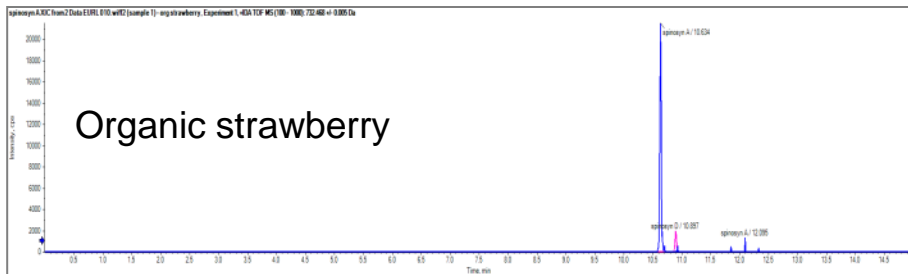
Calibration for imazalil: $y = 3.421664x + 26821.06121$ ($r = 0.99993$, $r^2 = 0.99806$) (weighting: 1 / x)

Review of peak integration, spectra and calibration line

Data Acquisition Mass Spec Start Stop Save...

Pesticides in Store-bought Fruits and Vegetables

QuEChERS Extracts with 10x Dilution (5 µL Injection)



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 (%)
<i>Organic strawberry</i>	Spinosyn A	13.9	0.01	0.55	9.1	100.0
	Spinosyn D	33.3	0.01	1.63	6.0	99.4
<i>Strawberry</i>	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
<i>Blueberry</i>	n.d.	-	-	-	-	-
<i>Organic Banana</i>	Spinosyn D	12.6	0.00	2.33	19.8	100.0
<i>Banana</i>	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
<i>Lemon</i>	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
<i>Spinach</i>	n.d.	-	-	-	-	-
<i>Grapes</i>	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





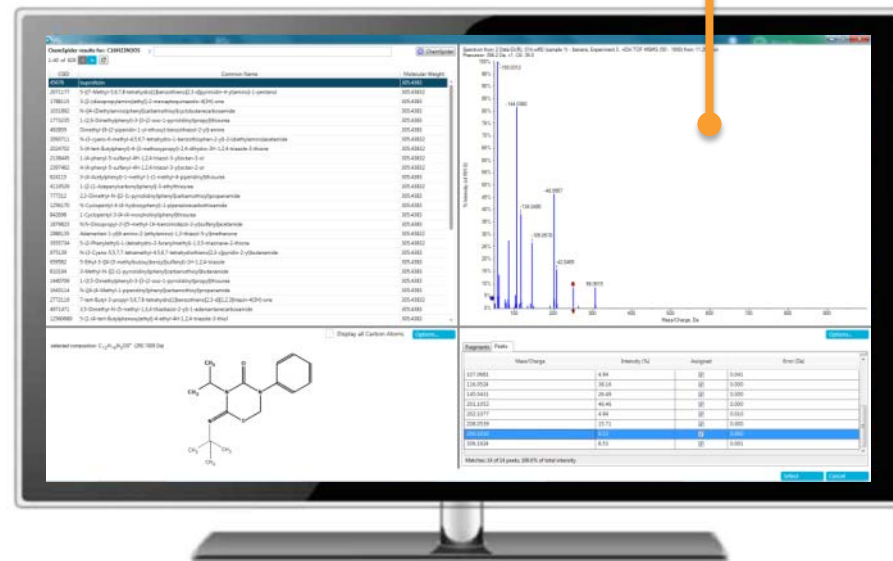
Software Improvements and Details

Automatic sample-control comparison

ChemSpider searching

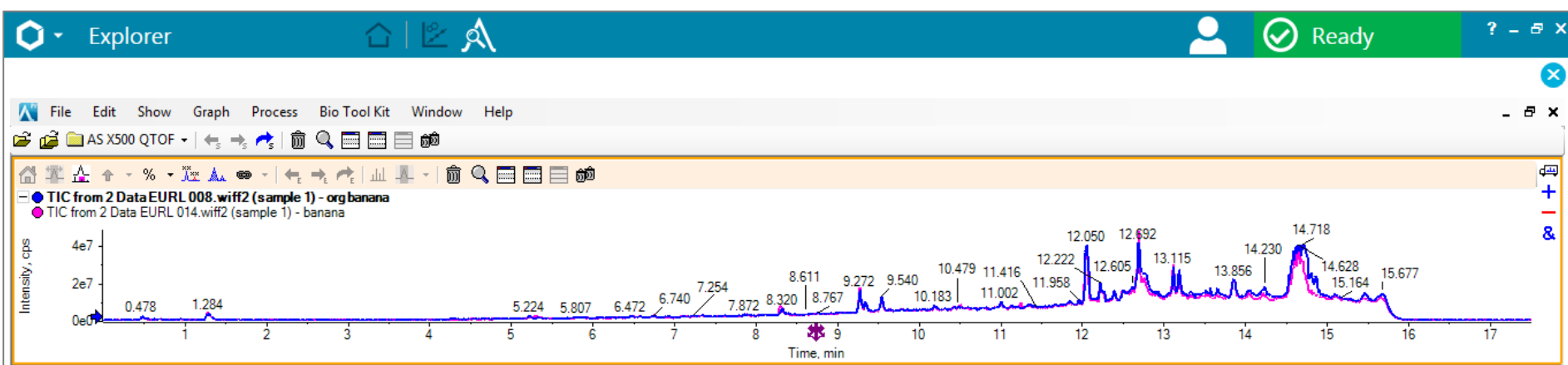
Sorting by number of references and automatic structure elucidation to identify unknowns

Non-Target peak finding

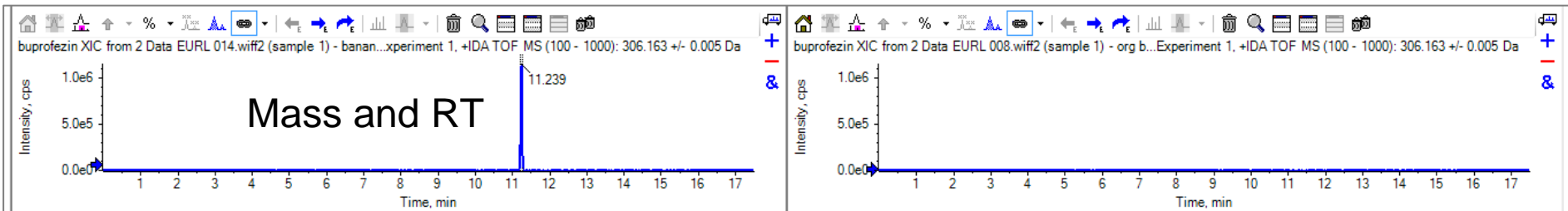


Automatic MS/MS library searching and formula finding

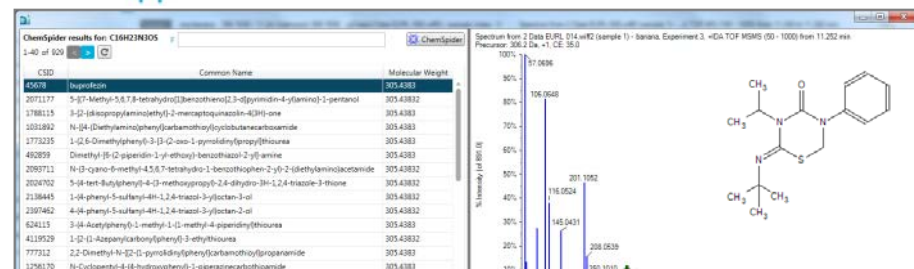
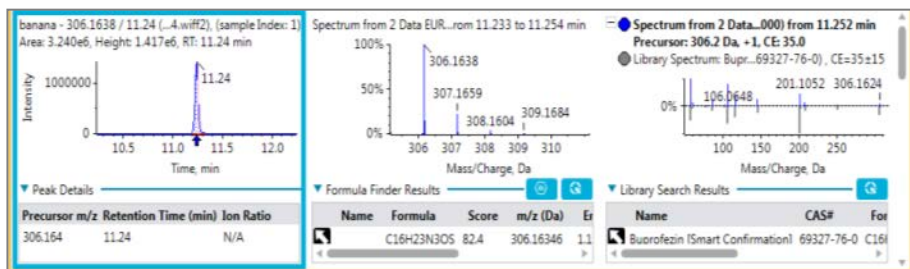
Non-Targeted Data Processing Workflow



Sample-control comparison



Identification



Formula finding ✓

MS/MS search ✓

Unknown Identification in SCIEX OS Software

1. Define Non-Target Peak Finding and Identification Parameters

[MQ4] Untitled Method

Workflow Select the workflow and then select a reference sample, if applicable

Components Quantitation

Integration Quantitation and targeted identification

Library Search Non-targeted screening

Acceptance Criteria The recommended Reference Sample has been automatically selected. Change the selection only if required.

Confidence Limits

Sample Name
2 Data EURL 008.wiff2 (sample 1) - org banana
2 Data EURL 014.wiff2 (sample 1) - banana

[MQ4] Untitled Method

Workflow Configure the Formula Finder options that are used to identify compounds

Components Use Formula Finder

Integration Type of Compound

Library Search Naturally Occurring Compounds

Acceptance Criteria Man-Made Compounds

Confidence Limits Other

Qualitative Rules Limits

Ion Ratio Max. Element C50 H100 Br3 Cl5 F3 I3 N10 O20 P1 S3

Advanced Mass Tolerance 5 ppm

Area Ratio Threshold 10 (Unknown/Comparison)

Formula Finder

Non-targeted Peaks

Unknown Identification in SCIEX OS Software

2. Automatic Sample-Control Comparison and Compound Identification

The screenshot displays the SCIEX OS software interface. At the top, the 'Analytics' menu is visible. The main window shows a 'Results Table (Untitled)' for project 'X500 QTOF training'. The table lists sample data with columns for Index, Sample Name, Sample Type, Dilution Factor, Component Name, Actual Concentration, Form Conf., Library Conf., Found At Mass, Mass Error, Retention Time, Retention Time Del., Isotope Ratio Dif., Combi Score, Formula Finder Results, Formula Finder Sc..., Library Hit, Library Score, Component Group Name, and Area. A red box highlights the 'Form Conf.', 'Library Conf.', 'Combi Score', and 'Library Score' columns.

Index	Sample Name	Sample Type	Dilution Factor	Component Name	Actual Concentrati...	Form ... Conf...	Library Conf...	Found At Mass	Mass Error (m...	Retention Time	Retention Time Del...	Isotope Ratio Dif...	Combi... Score	Formula Finder Results	Formula Finder Sc...	Library Hit	Library Score	Component Group Name	Area
449	banana	Unknown	1.0	297.0558 / 8.29	N/A	✓	✓	297.056	N/A	8.30	N/A	N/A	95.720	C14H14Cl2N2O	91.439	Imazali	100.000		4.968e6
457	banana	Unknown	1.0	306.1638 / 11.24	N/A	✓	✓	306.164	N/A	11.24	N/A	N/A	91.201	C16H23N3O5	82.402	Buprofezin	100.000		3.175e6
367	banana	Unknown	1.0	202.0427 / 5.30	N/A	✓	✓	202.043	N/A	5.30	N/A	N/A	89.424	C10H7N3S	78.847	Thiabenzazole	100.000		3.834e6
453	banana	Unknown	1.0	299.0525 / 8.29	N/A	✓	●	299.053	N/A	8.29	N/A	N/A	47.978	C9H15O9P	95.956	No Match	0.000		3.727e6
467	banana	Unknown	1.0	322.1580 / 10.50	N/A	✓	●	322.158	N/A	10.50	N/A	N/A	44.768	C6H21F2N9O2S	89.536	No Match	0.000		2.324e6
484	banana	Unknown	1.0	352.1685 / 6.27	N/A	✓	●	352.168	N/A	6.28	N/A	N/A	42.740	C17H25N3O3S	85.479	No Match	0.000		3.373e5
290	banana	Unknown	1.0	104.1063 / 0.50	N/A	■	■	104.106	N/A	0.49	N/A	N/A	0.000		N/A		N/A		1.549e6

Below the table, two mass spectra are shown. The first spectrum is for peak 449 (8.29 min) and the second is for peak 467 (8.30 min). Each spectrum includes a 'Peak Details' table and a 'Library Search Results' table. A red box highlights the 'Library Search Results' table for the 8.30 min peak, which identifies the compound as Imazali.

Peak Details for 8.30 min:

Precursor m/z	Retention Time (min)	Ion Ratio
297.056	8.30	N/A

Library Search Results for 8.30 min:

Name	CAS#	Formula	MW (Da)	Fit	Rev. Fit	Purity	CE (eV)
Imazali	35554-44-0	C14H14Cl2N2O	297.18381	100.0	89.0	89.0	35

Automatic formula finding and MS/MS library searching

Unknown Identification in SCIEX OS Software

3. ChemSpider Searching and Structure Elucidation

The screenshot displays the SCIEX OS interface for unknown identification. The top-left panel shows ChemSpider search results for the molecular formula C₁₆H₂₃N₃O₃. The first result, buprofezin (CSID 45678), is highlighted with a red box. The top-right panel shows a mass spectrum with the base peak at m/z 57.0696. A red arrow points from this peak to the chemical structure of buprofezin in the bottom-left panel. The bottom-right panel shows a table of identified peaks with a 100% match rate.

CSID	Common Name	Molecular Weight
45678	buprofezin	305.4383
2071177	5-[(7-Methyl-5,6,7,8-tetrahydro[1]benzothieno[2,3-d]pyrimidin-4-yl)amino]-1-pentanol	305.43832
1788115	3-[2-(diisopropylamino)ethyl]-2-mercaptoquinazolin-4(3H)-one	305.4383
1031892	N-[[4-(Diethylamino)phenyl]carbamothioyl]cyclobutanecarboxamide	305.4383
1773235	1-(2,6-Dimethylphenyl)-3-[3-(2-oxo-1-pyrrolidinyl)propyl]thiourea	305.4383
492859	Dimethyl-[6-(2-piperidin-1-yl-ethoxy)-benzothiazol-2-yl]-amine	305.4383
2093711	N-(3-cyano-6-methyl-4,5,6,7-tetrahydro-1-benzothiophen-2-yl)-2-(diethylamino)acetamide	305.43832
2024702	5-(4-tert-Butylphenyl)-4-(3-methoxypropyl)-2,4-dihydro-3H-1,2,4-triazole-3-thione	305.43832
2138445	1-(4-phenyl-5-sulfanyl-4H-1,2,4-triazol-3-yl)octan-3-ol	305.43832
2397462	4-(4-phenyl-5-sulfanyl-4H-1,2,4-triazol-3-yl)octan-2-ol	305.43832
624115	3-(4-Acetylphenyl)-1-methyl-1-(1-methyl-4-piperidinyl)thiourea	305.4383
4119529	1-[2-(1-Azepanylcarbonyl)phenyl]-3-ethylthiourea	305.43832
777312	2,2-Dimethyl-N-[(2-(1-pyrrolidinyl)phenyl]carbamothioyl]propanamide	305.4383
1256170	N-Cyclopentyl-4-(4-hydroxyphenyl)-1-piperazinecarbothioamide	305.4383
842698	1-Cyclopentyl-3-[4-(4-morpholinyl)phenyl]thiourea	305.4383
1879823	N,N-Diisopropyl-2-[(5-methyl-1H-benzimidazol-2-yl)sulfanyl]acetamide	305.4383
2986135	Adamantan-1-yl[4-amino-2-(ethylamino)-1,3-thiazol-5-yl]methanone	305.43832

Mass/Charge	Intensity (%)	Assigned	Error (Da)
56.8868	2.81	<input checked="" type="checkbox"/>	0.183
57.0696	100.00	<input checked="" type="checkbox"/>	0.000
58.0730	4.94	<input checked="" type="checkbox"/>	0.008
59.9900	13.47	<input checked="" type="checkbox"/>	0.000

Matches: 24 of 24 peaks, 100.0% of total intensity

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 results for: C₁₄H₁₅N₃

CSID	Common Name	Molecular Weight
77885	Cyprodinil	225.289
5829	Methyl Yellow	225.289
7063	2-Methyl-4-[(E)-(2-methylphenyl)diazenyl]aniline	225.289
497232	benzenamine, 4-methyl-2-[(4-methylphenyl)azo]-	225.289
2043995	2-Amino-1-benzyl-4,5-dimethyl-1H-pyrrole-3-carbonitrile	225.289
9599527	1-Isobutyl-1H-imidazo[4,5-c]quinoline	225.289
309267	1,3-bis(4-methylphenyl)triazene	225.289
78691	3-benzyl-1-(4-methylphenyl)triaz-1-ene	225.289
4143460	2-Amino-4,5-dimethyl-1-(4-methylphenyl)-1H-pyrrole-3-carbonitrile	225.289
310817	[4-(Diethylamino)benzylidene]malononitrile	225.289
662407	2,4-Dimethyl-6,7,8,9-tetrahydropyrimido[1,2-a]indole-10-carbonitrile	225.289
28294179	1-cyclohexylbenzimidazole-5-carbonitrile	225.289
254016	2,6-Dimethyl-4-[(E)-phenyldiazenyl]aniline	225.289
10447121	N,N-Dimethyl-4-(phenyldiazenyl)aniline	225.289
15512	N-Methyl-4-[(E)-(3-methylphenyl)diazenyl]aniline	225.289
9260617	3-(Methylamino)-2,3,4,9-tetrahydro-1H-carbazole-6-carbonitrile	225.289
10826526	2-Phenyl-5,6,7,8-tetrahydro-6-quinazolinamine	225.289

Spectrum from 2 Data EURL 013.wiff2 (sample 1) - grapes, Experiment 2, +IDA TOF MSMS (50 - 1000) from 10.027 min
Precursor: 226.1 Da, +1, CE: 35.0

Options...
Display all Carbon Atoms

Options...

Mass/Charge	Intensity (%)	Assigned	Error (Da)
65.0390	3.57	<input checked="" type="checkbox"/>	0.000
67.0542	2.55	<input checked="" type="checkbox"/>	0.000
68.0498	2.29	<input checked="" type="checkbox"/>	0.000
77.0386	5.86	<input checked="" type="checkbox"/>	0.000

Matches: 61 of 62 peaks, 97.9% of total intensity

Select Cancel

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!

