



Answers for Science.
Knowledge for Life.™

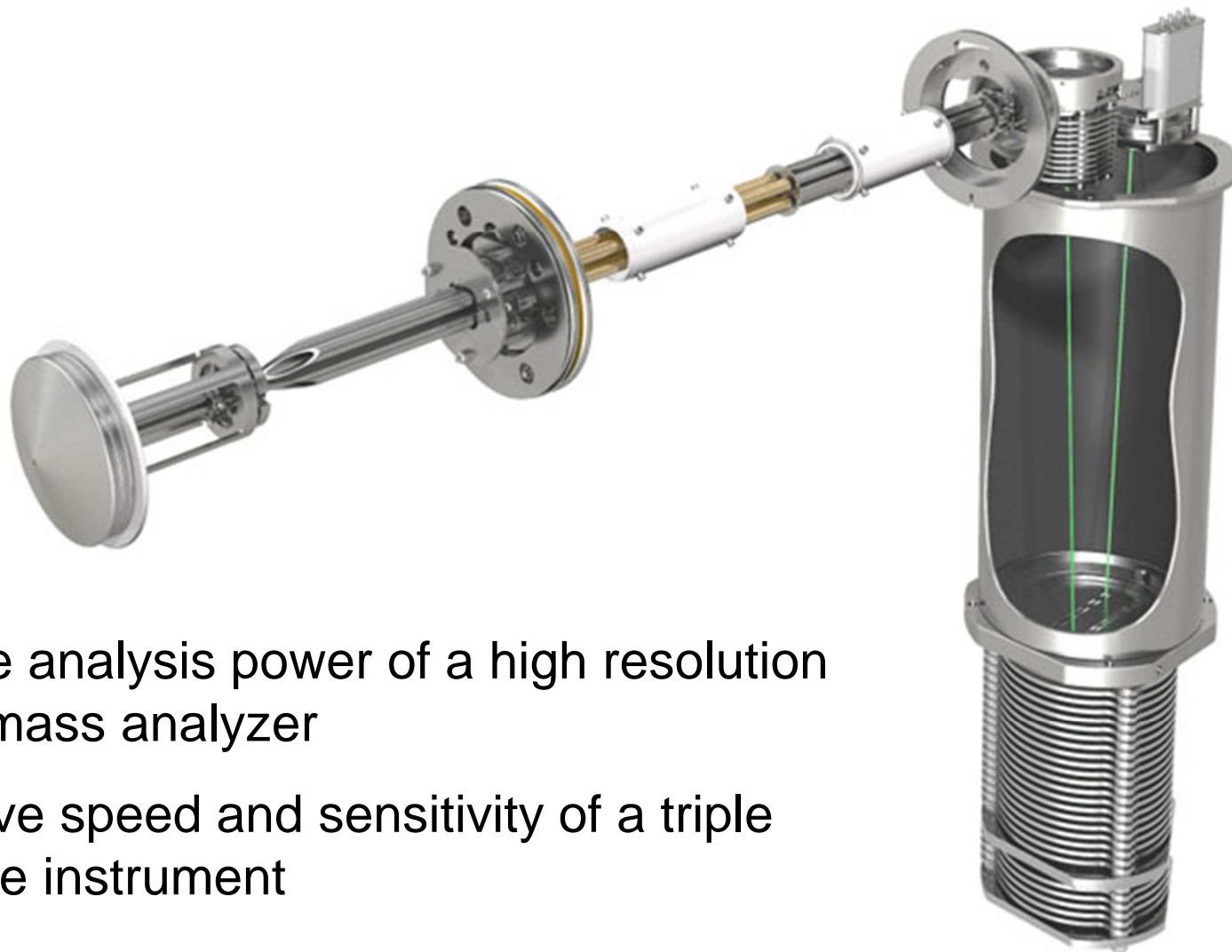


Ignite your Routine Testing Methods

Daniel McMillan, SCIEX
Budapest, 27th April 2016

AB SCIEX TripleTOF™ 4600 System

Ion Path Innovations – The Best of Both Worlds



- Qualitative analysis power of a high resolution accurate mass analyzer
- Quantitative speed and sensitivity of a triple quadrupole instrument

What's New?

SCIEX X500R QTOF System powered by SCIEX OS Software



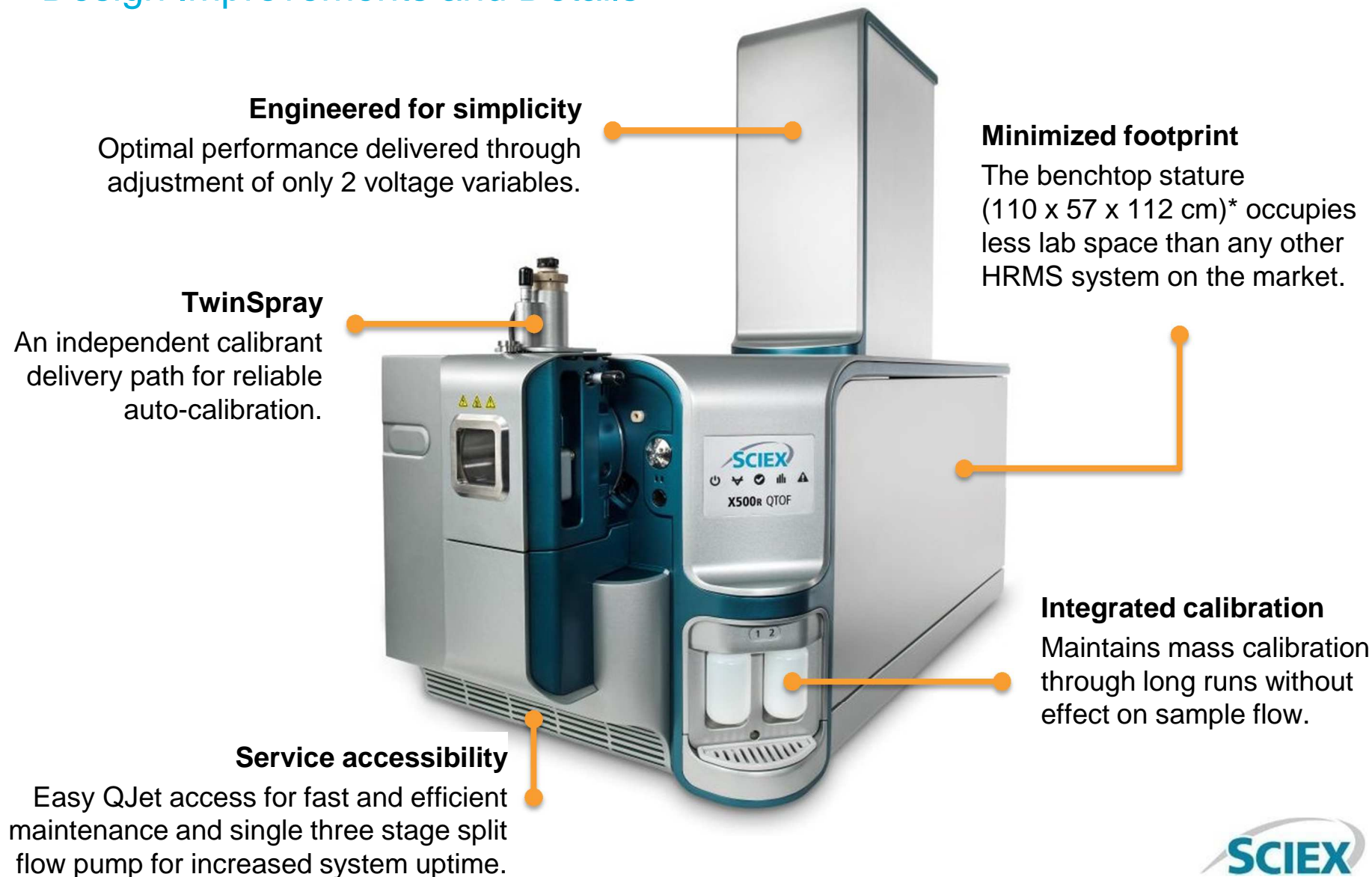
SCIEX X500R QTOF system

SCIEX ExionLC™ AC system

SCIEX OS software

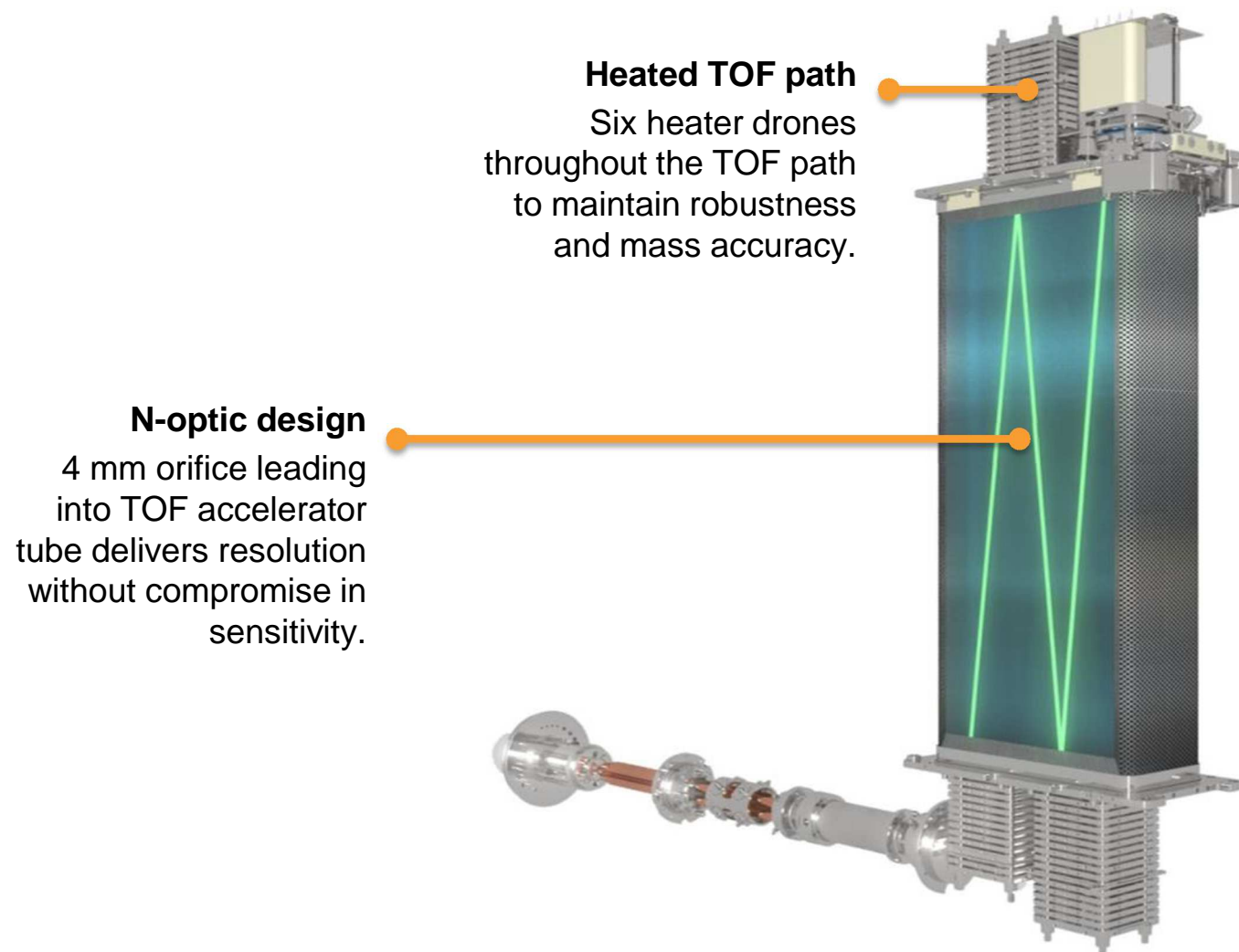
Introducing the SCIEX X500R QTOF System

Design Improvements and Details



Introducing the SCIEX X500R QTOF System

Design Improvements and Details

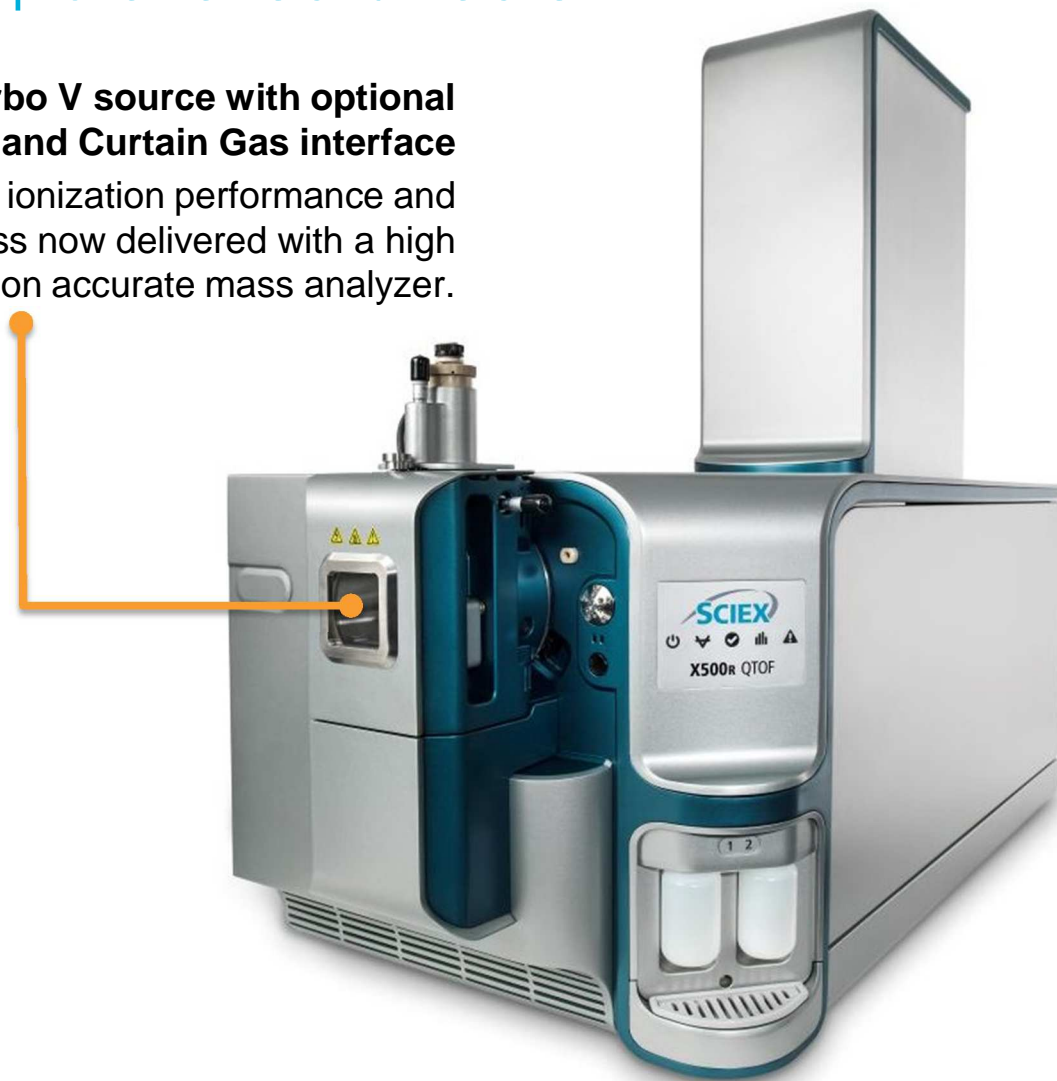


Introducing the SCIEX X500R QTOF System

Design Improvements and Details

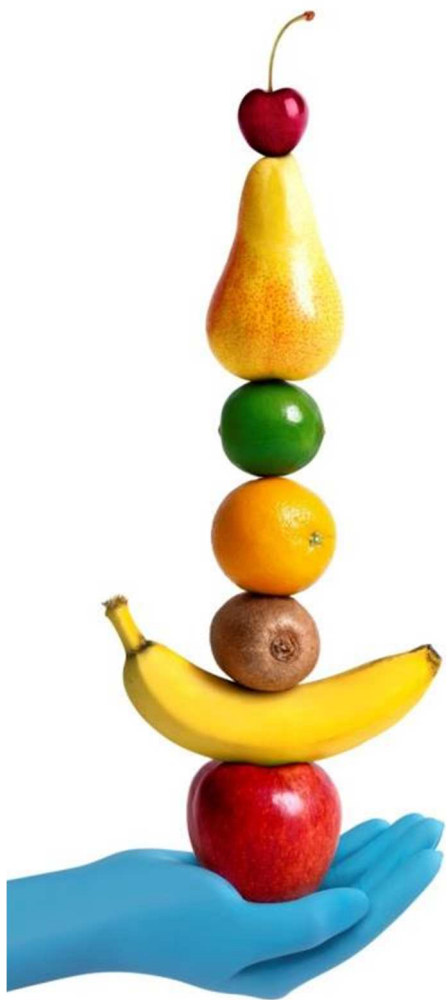
Legendary Turbo V source with optional IonDrive and Curtain Gas interface

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



Perfect Balance to Elevate Your Lab's Performance

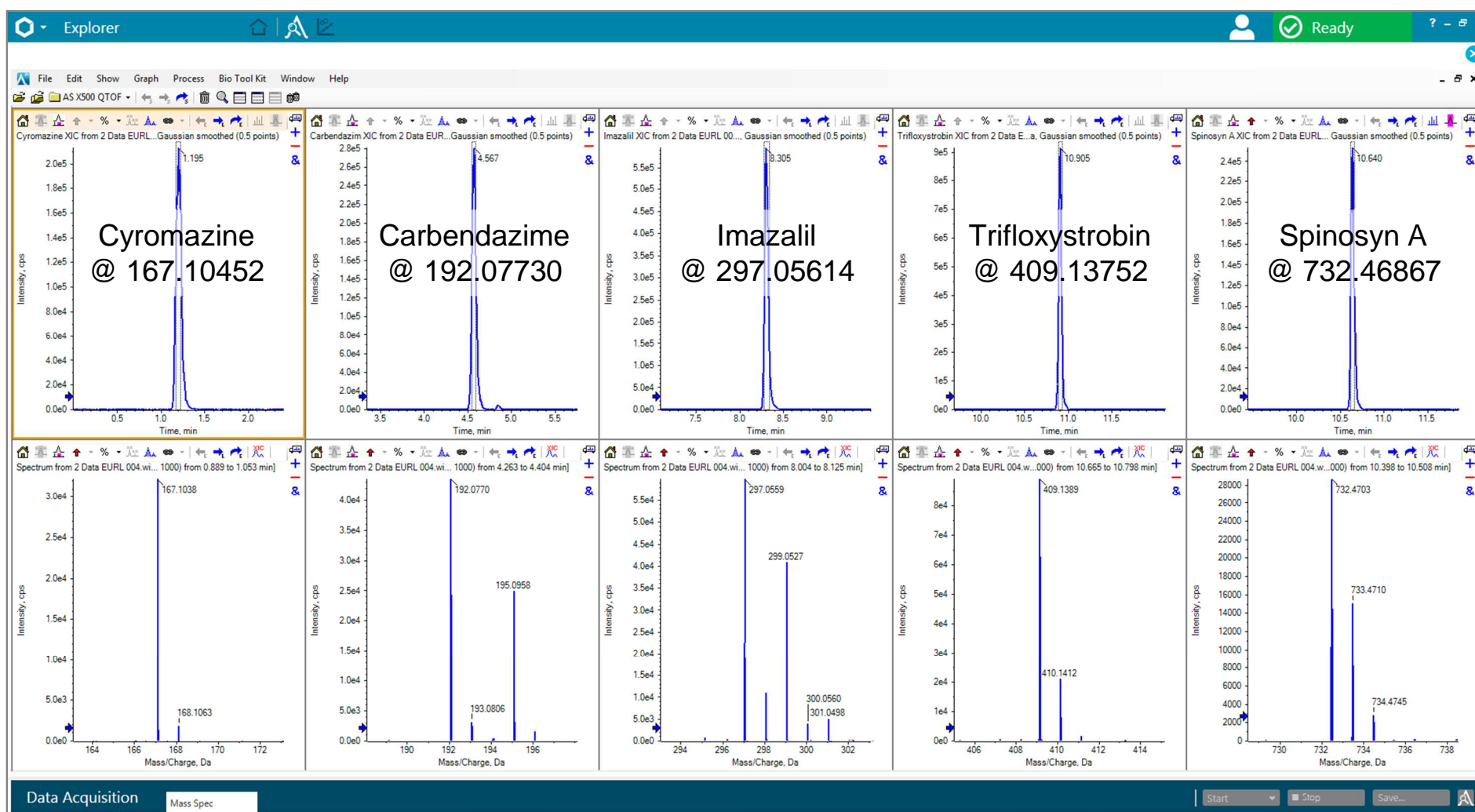
SCIEX X500R QTOF System



- 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

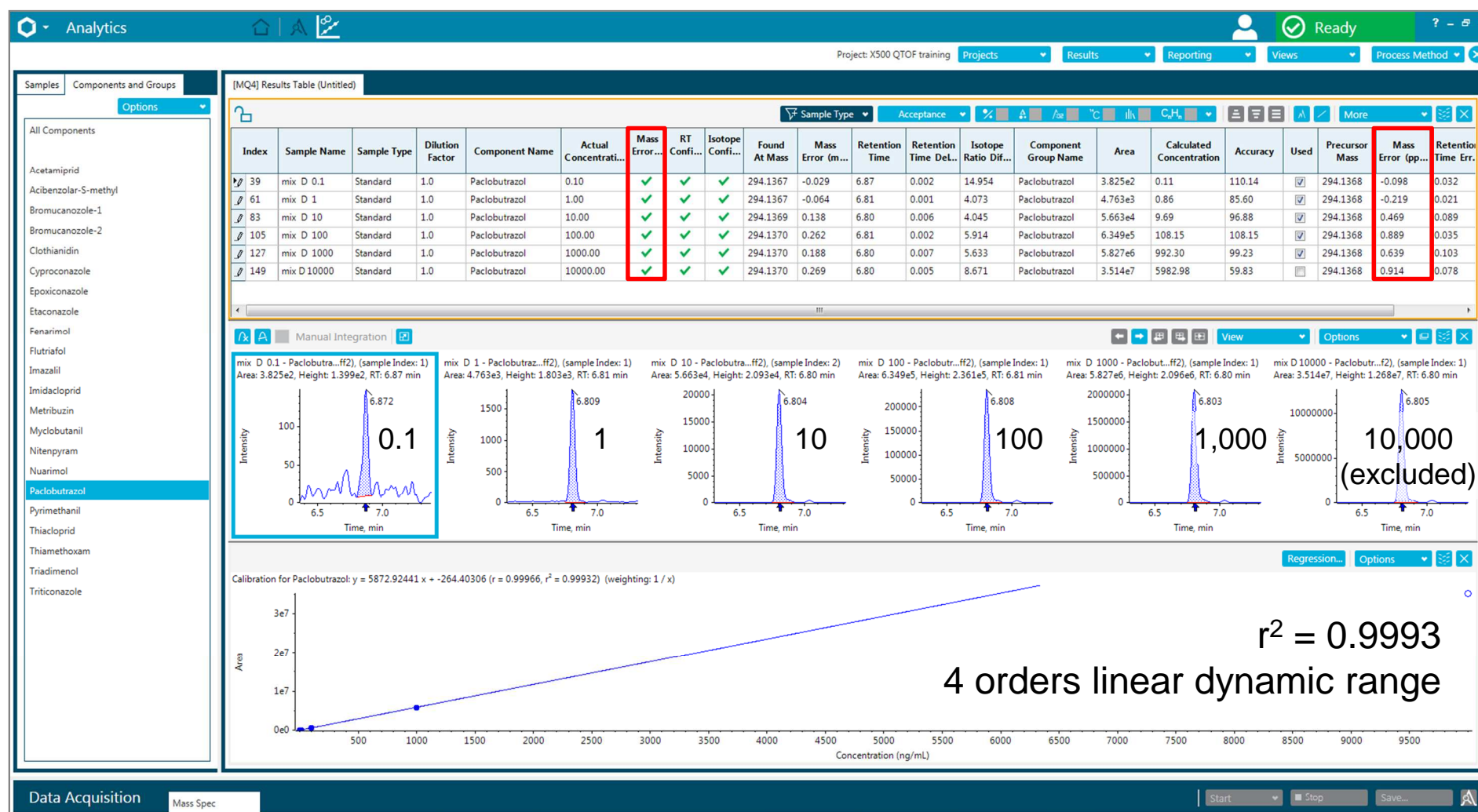
The SCIEX X500R QTOF System – Performance

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



The SCIEX X500R QTOF System – Performance

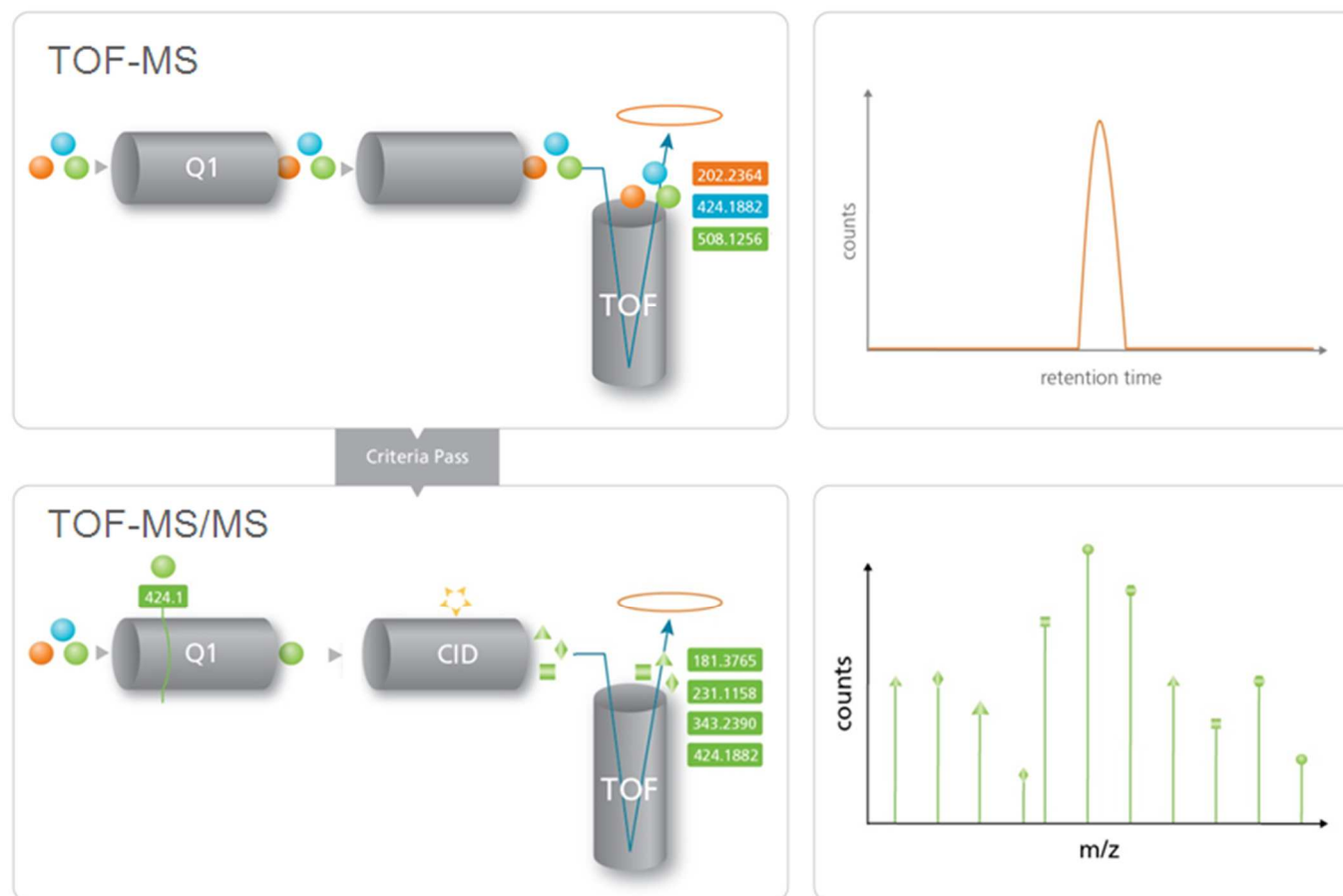
Linearity and Mass Accuracy (Paclobutrazol 0.1 to 10,000 ng/mL)



Mass error = -0.2 to 0.91 ppm

Information Dependent Acquisition of MS/MS (IDA)

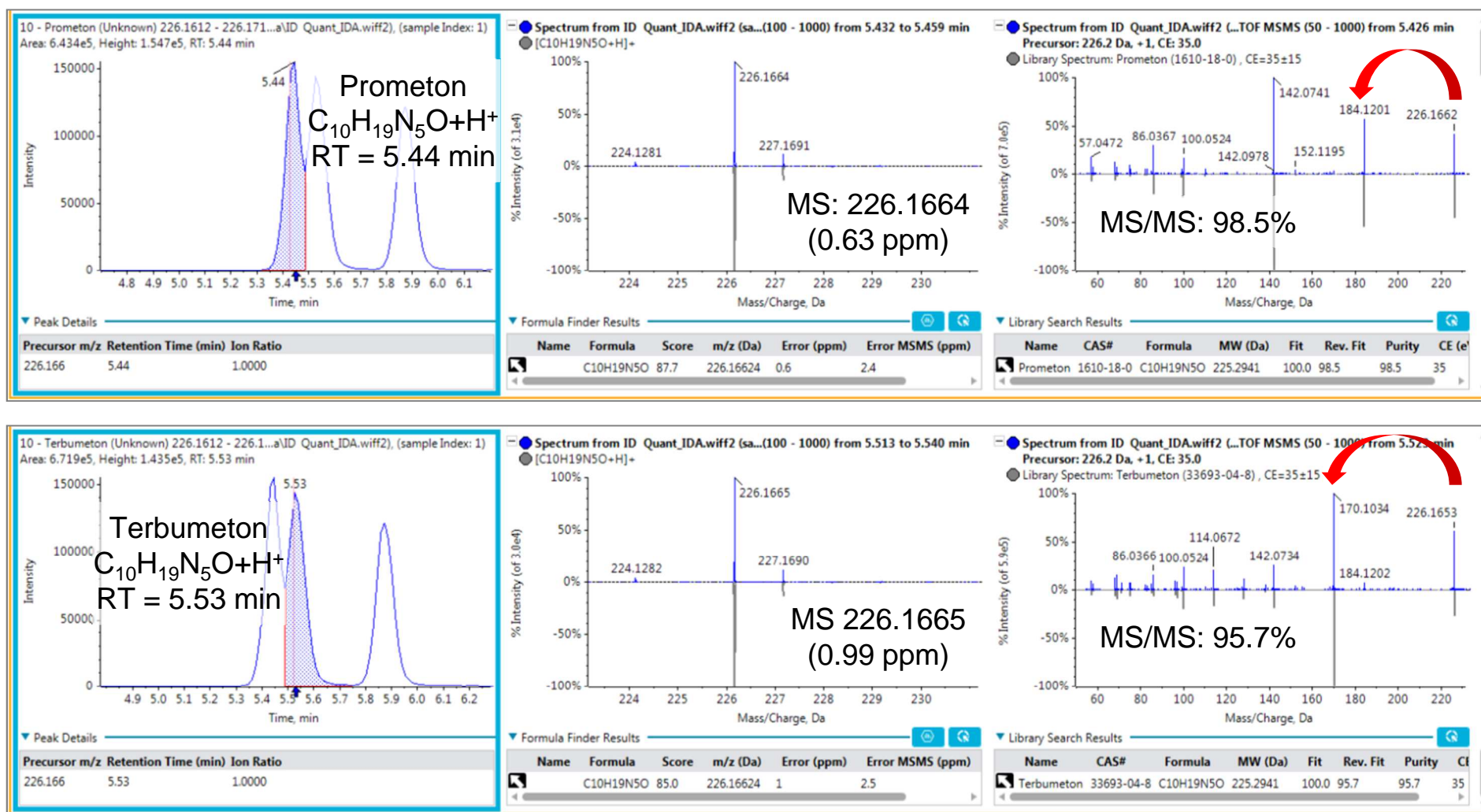
Provides MS/MS Spectra with High Selectivity (Q1 Resolution unit)



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

The SCIEX X500R QTOF System – IDA

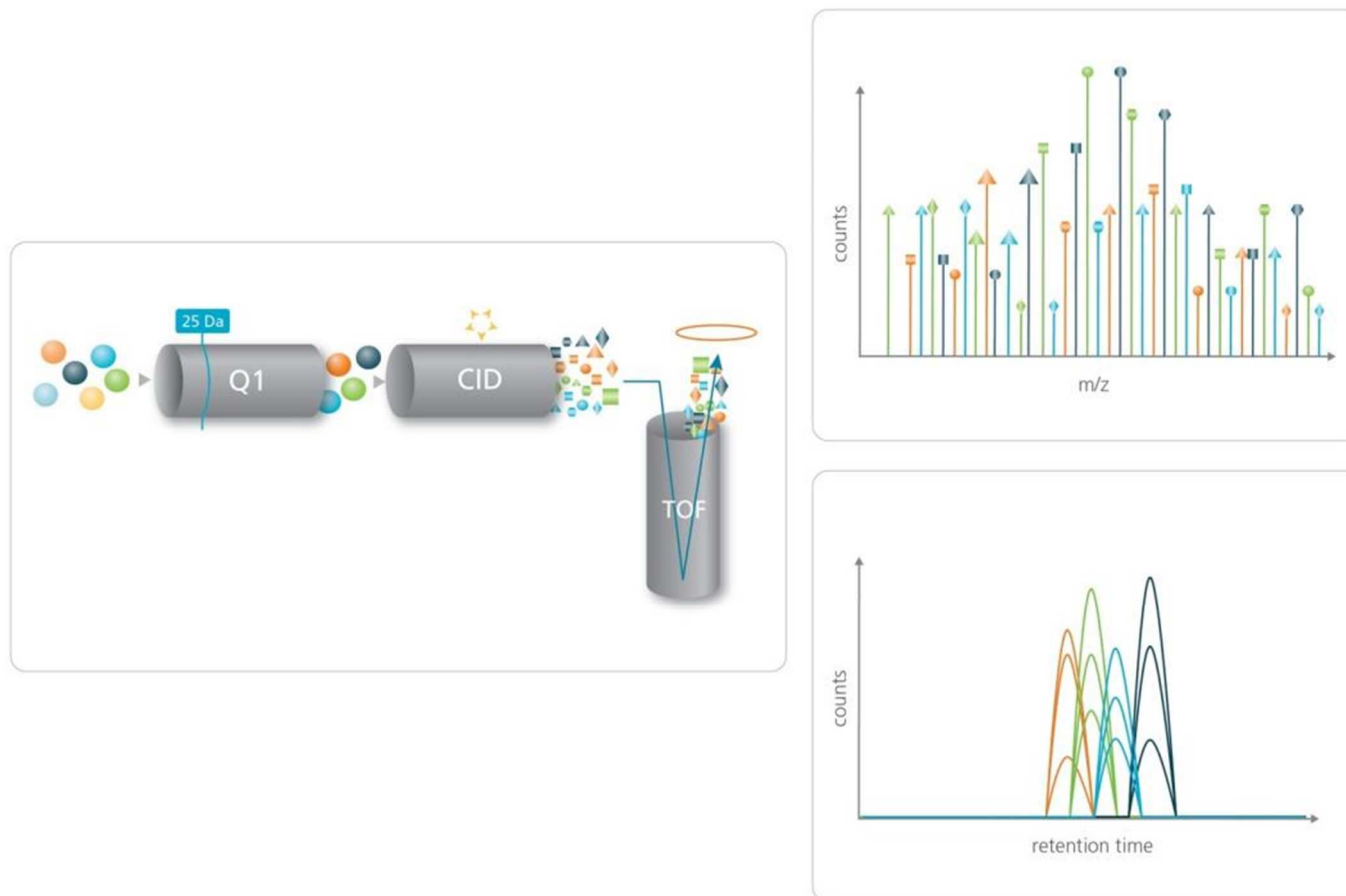
Confident Identification of Isomers using MS/MS (Prometon vs. Terbumeton)



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

MS/MS^{ALL} using SWATH™ Acquisition

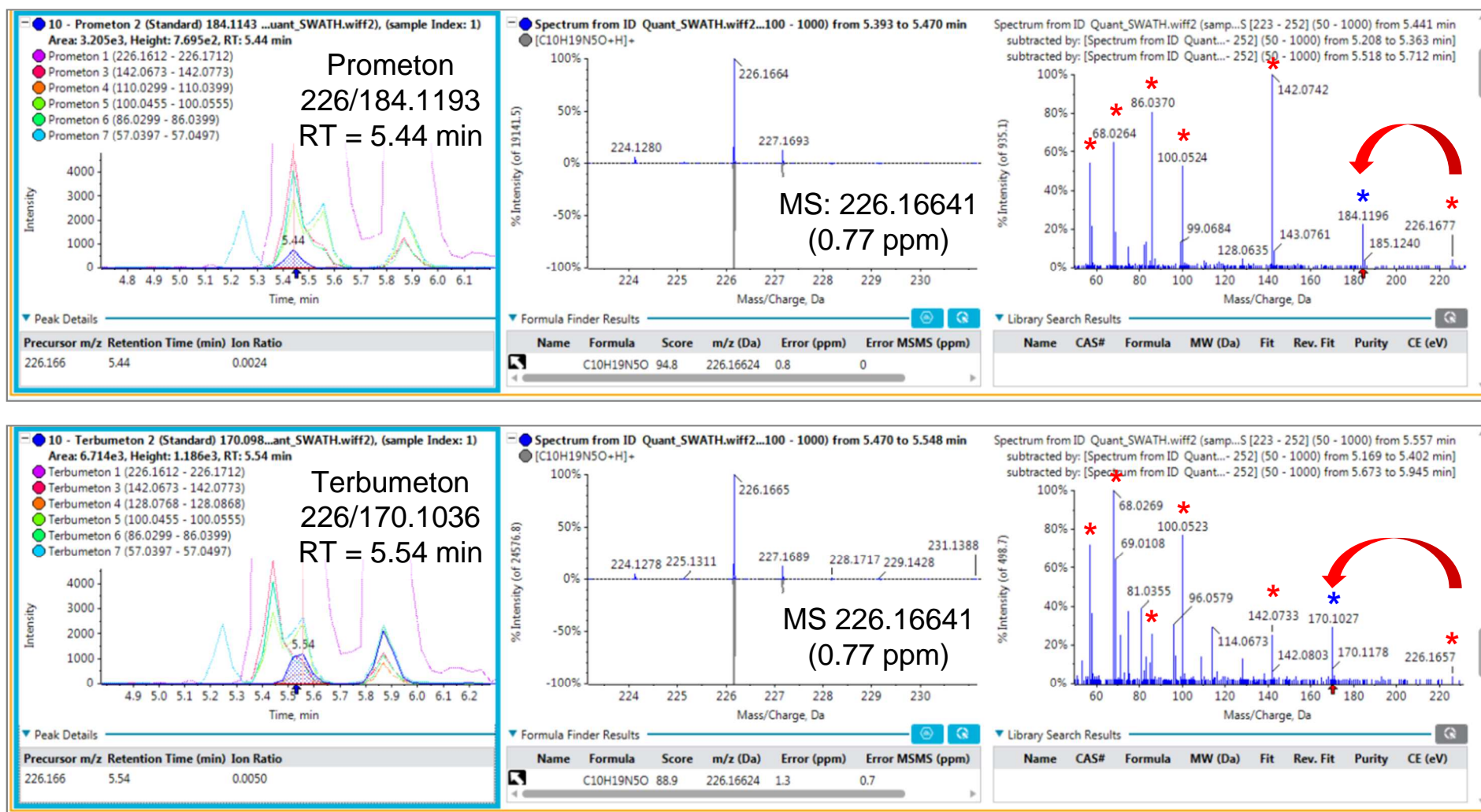
A Mode of Data Independent Acquisition Providing MS/MS^{ALL}



SWATH™: Wide Q1 Isolation Window is Stepped Across the Mass Range

The SCIEX X500R QTOF System – SWATH™ MS/MS^{ALL}

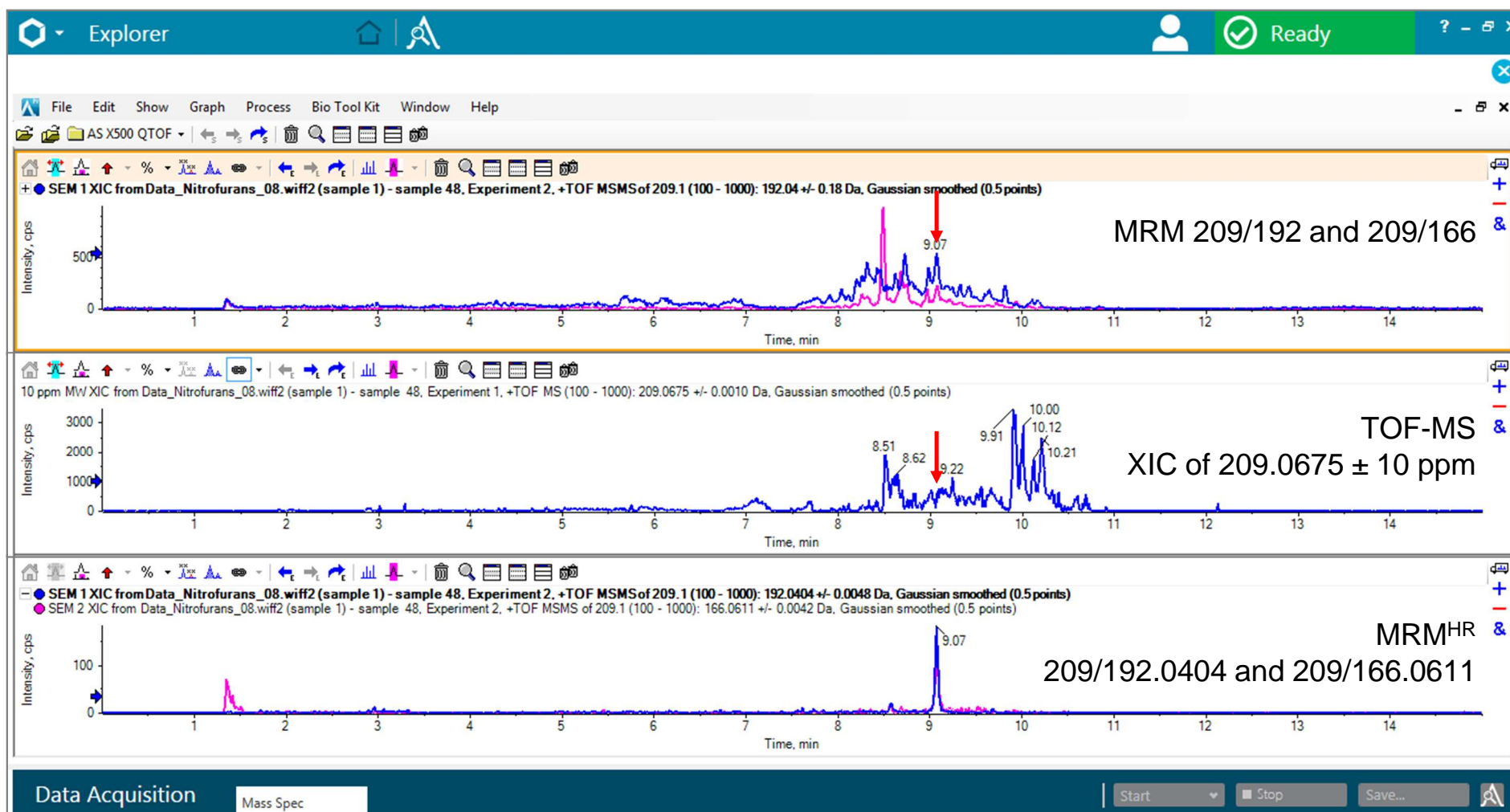
Confident Identification of Isomers using SWATH (Prometon vs. Terbumeton)



Identification based on unique fragment ions and their ratios

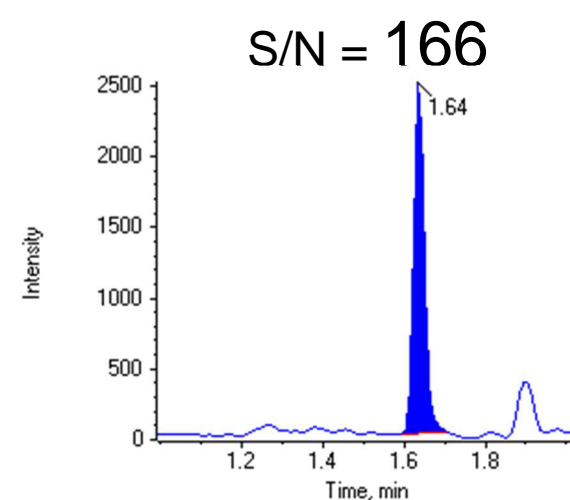
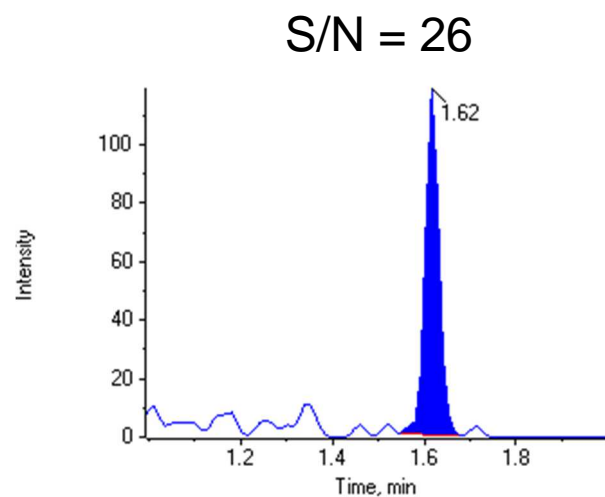
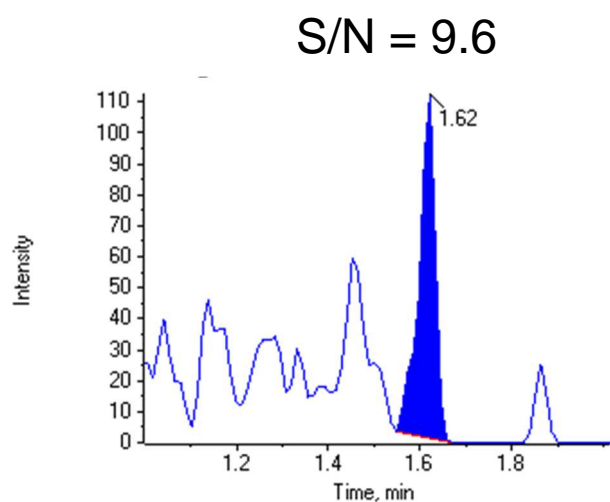
Increased Selectivity using MRM^{HR}

Feed Sample Tested Positive for NP-Semicarbazide



Comparison of TOF MS vs. SWATH vs. MRM^{HR} Quant

Loratidine



TOF MS



SWATH



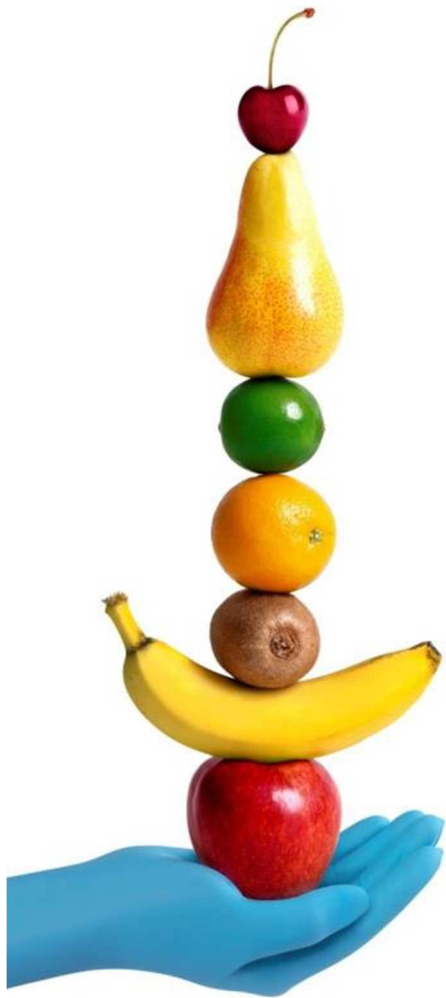
MRM^{HR}

Selectivity

Sensitivity

Perfect Balance to Elevate Your Lab's Performance

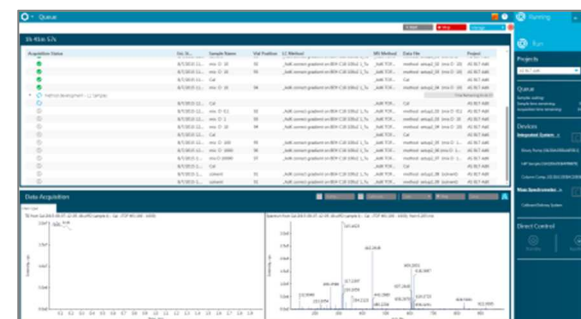
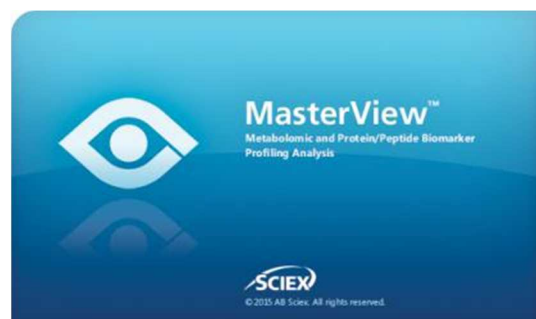
SCIEX X500R QTOF System Powered by SCIEX OS Software



- 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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 - 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



SCIEX OS Software – Home



Everything in a Single Software Platform

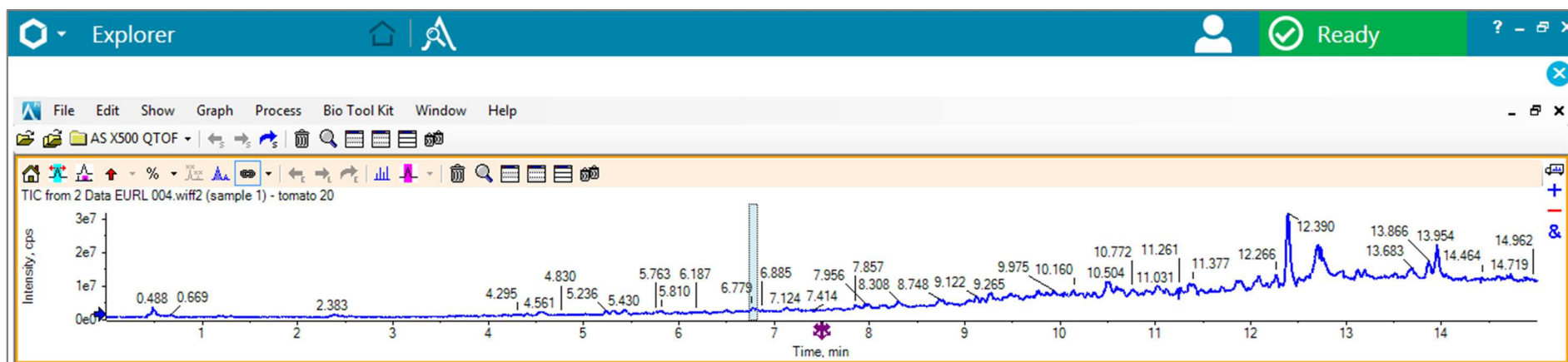
The screenshot shows the SCIEX OS software interface. At the top is a blue header bar with the SCIEX OS logo on the left and a status bar on the right containing a user icon, a green 'Ready' indicator, and window control buttons. Below the header, the main workspace displays the SCIEX OS logo on the left and a central menu titled 'Processing: Simultaneous Identification and quantitation'. This menu is divided into three columns: 'Acquisition', 'Processing', and 'Management'. The 'Acquisition' column contains icons for 'Batch', 'Queue', 'MS Method', 'LC Method', and 'MS Tune'. The 'Processing' column contains icons for 'Explorer' and 'Analytics'. The 'Management' column contains icons for 'Configuration', 'Library', 'Event Log', and 'Users'. Below the 'Acquisition' column, there is a section titled 'Acquisition' with the text 'Build MS and LC methods', 'Create batches', and 'Run samples'. Below the 'Management' column, there is a section titled 'Management' with the text 'Adjust hardware, software, and user settings'.

Processing
Simultaneous Identification
and quantitation

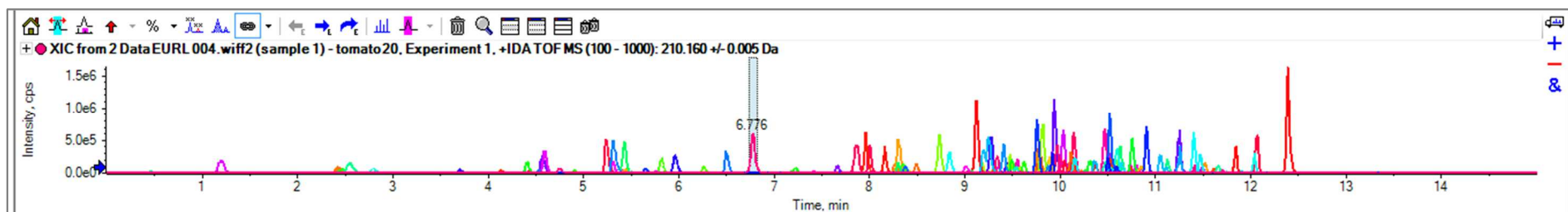
Acquisition
Build MS and LC methods
Create batches
Run samples

Management
Adjust hardware, software,
and user settings

Targeted Data Processing Workflow

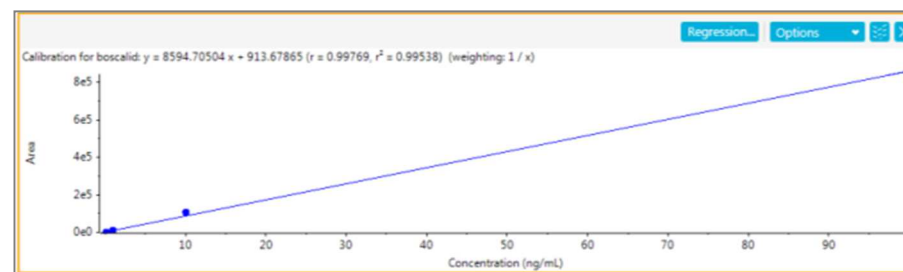
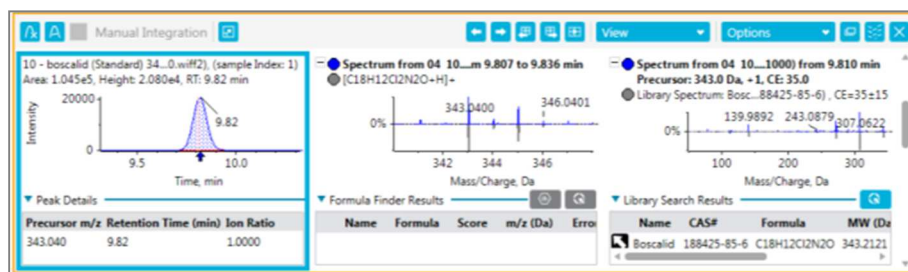


XIC generation for each target



Identification

Quantitation



RT ✓

Mass
Isotopes ✓

MS/MS search ✓

Above reporting level

SCIEX

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

Integration

Library Search

Acceptance Criteria

Confidence Limits

Qualitative Rules

Ion Ratio

Advanced

Formula Finder

Non-targeted Peaks

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...	acetamidiprid	C10H11CIN4	[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"/>	alldoxyc...	alldoxycarb	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"/>	chloryp...	chlorypyrifos	C9H11Cl3NO3PS	[M+H] ⁺	349.93356		0.02	11.49	
20	<input type="checkbox"/>	chloryp...	chlorypyrifos-me...	C7H7Cl3NO3PS	[M+H] ⁺	321.90226		0.02	10.79	
21	<input type="checkbox"/>	clofent...	clofentazine	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 checked="" type="checkbox"/>	% Difference Isotope Ratio	< 20	< 40	>= 40	20
<input checked="" type="checkbox"/>	Library Hit Score	> 70	> 50	<= 50	20
<input type="checkbox"/>	Formula Finder Score	> 50	> 20	<= 20	20

☐ Error %

☒ Absolute

Identification and Quantitation in SCIEX OS Software

3. Review Qualitative and Quantitative Results

Analytics

Project: X500 QTOF training

Ready

[IMQ4] 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

Integration

Minimum Peak Width: 3 points
Minimum Peak Height: 100.00
Gaussian Smooth Width: 1.0 points
Noise Percentage: 80.0 %
Baseline Subtract Window: 2.00 min
Peak Splitting: 2 points

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
[C14H14Cl2N2O+H]⁺

Spectrum from NVWA 10 - IDA.w...MS (50 - 1000) from 6.069 min
Precursor: 297.1 Da, +1, CE: 35.0
Library Spectrum: Imazalil (35554-44-0), CE=35±15

Formula Finder Results

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

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: $y = 3.42166e4 x + 26821.06121$ ($r = 0.99903$, $r^2 = 0.99806$) (weighting: 1 / x)

Review of peak integration, spectra and calibration line

Area

Concentration (ng/mL)

Data Acquisition

Mass Spec

Start Stop Save...

SCIEX OS Software – Unknown Identification



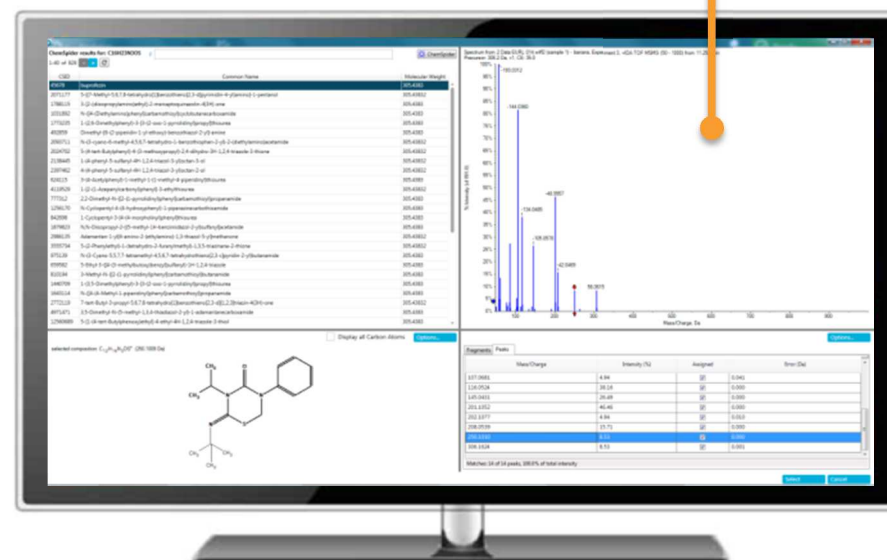
Software Improvements and Details

Automatic sample-control comparison

Non-Target peak finding

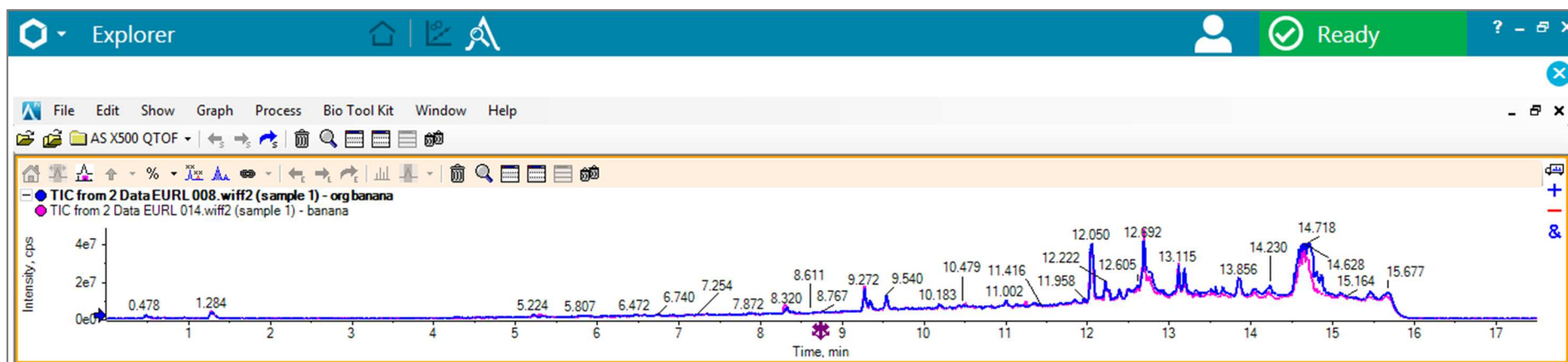
ChemSpider searching

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

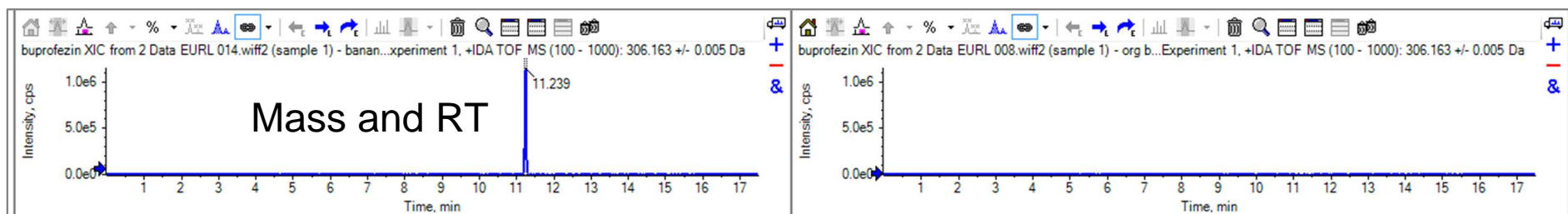


Automatic MS/MS library searching and formula finding

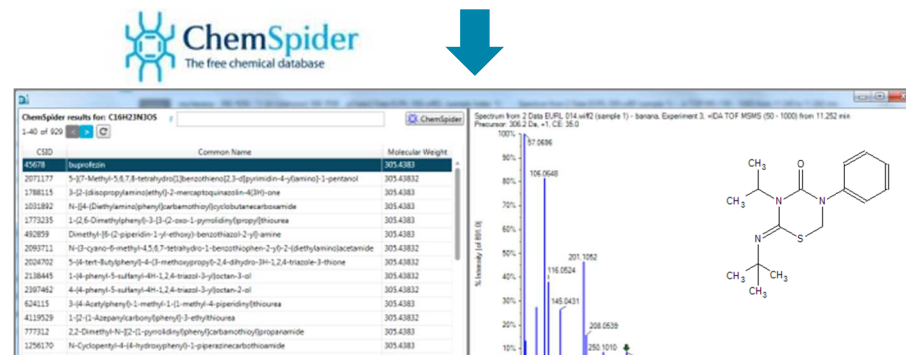
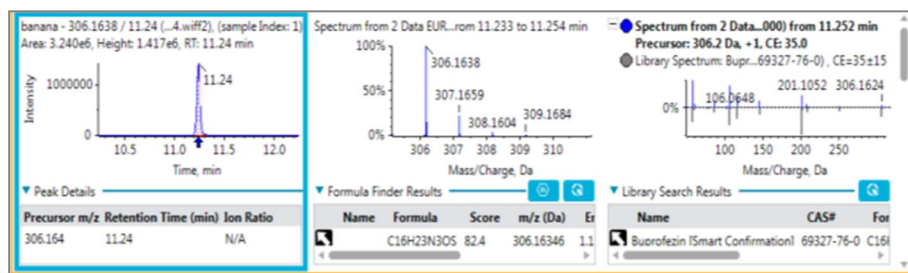
Non-Targeted Data Processing Workflow



Sample-control comparison



Identification



Formula finding ✓

MS/MS search ✓

Unknown Identification in SCIEX OS Software

1. Define Non-Target Peak Finding and Identification Parameters

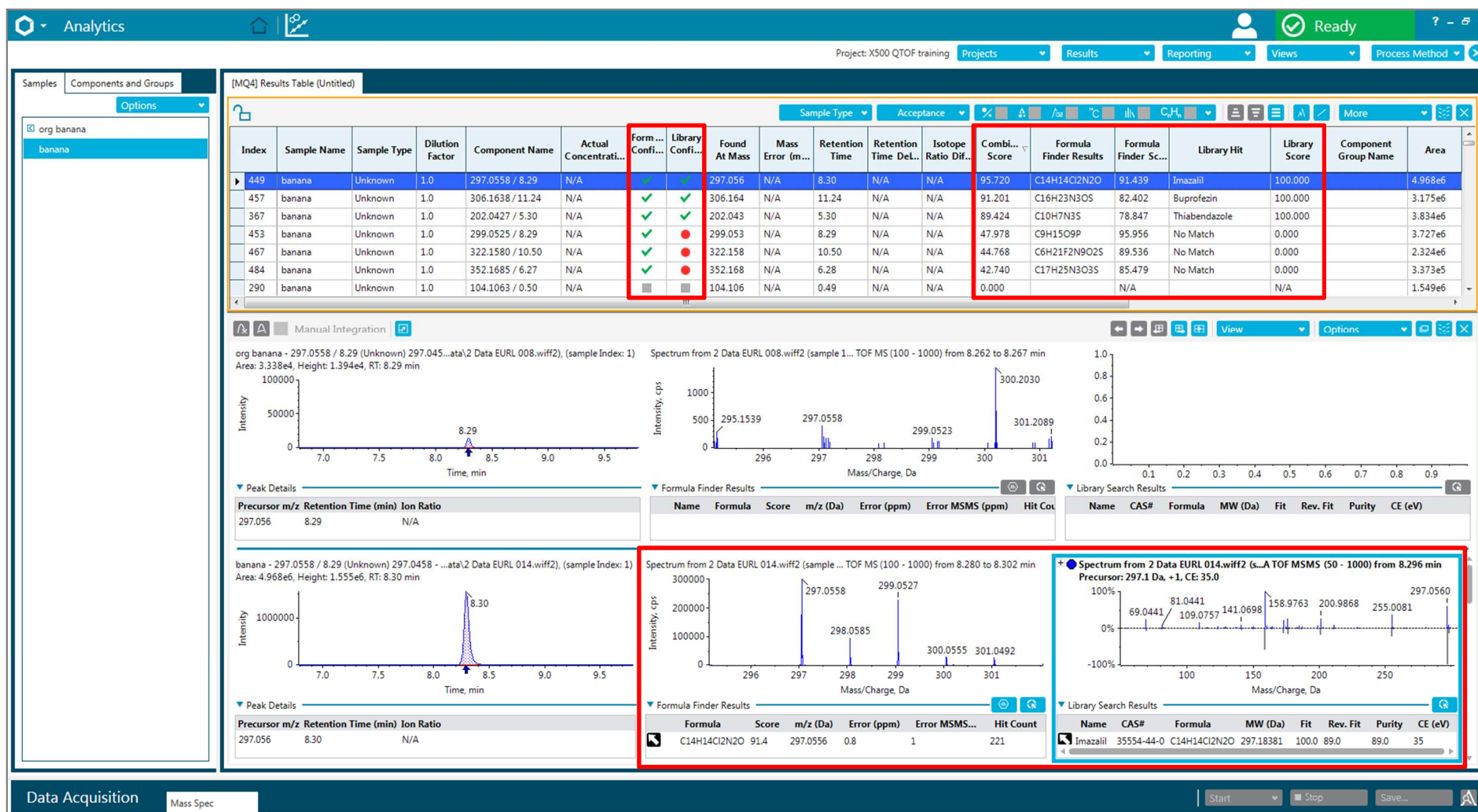
The first screenshot shows the 'Workflow' tab selected in the '[MQ4] Untitled Method' window. The 'Non-targeted screening' option is checked under the 'Select the workflow and then select a reference sample, if applicable' section. Below this, a message states: 'The recommended Reference Sample has been automatically selected. Change the selection only if required.' A table lists the selected reference samples:

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

The second screenshot shows the 'Formula Finder' tab selected in the same window. The 'Use Formula Finder' checkbox is checked. Under 'Type of Compound', 'Man-Made Compounds' is selected. Under 'Limits', the 'Max. Element' is set to 'C50 H100 Br3 Cl5 F3 I3 N10 O20 P1 S3', 'Mass Tolerance' is 5 ppm, and 'Area Ratio Threshold (Unknown/Comparison)' is 10.

Unknown Identification in SCIEX OS Software

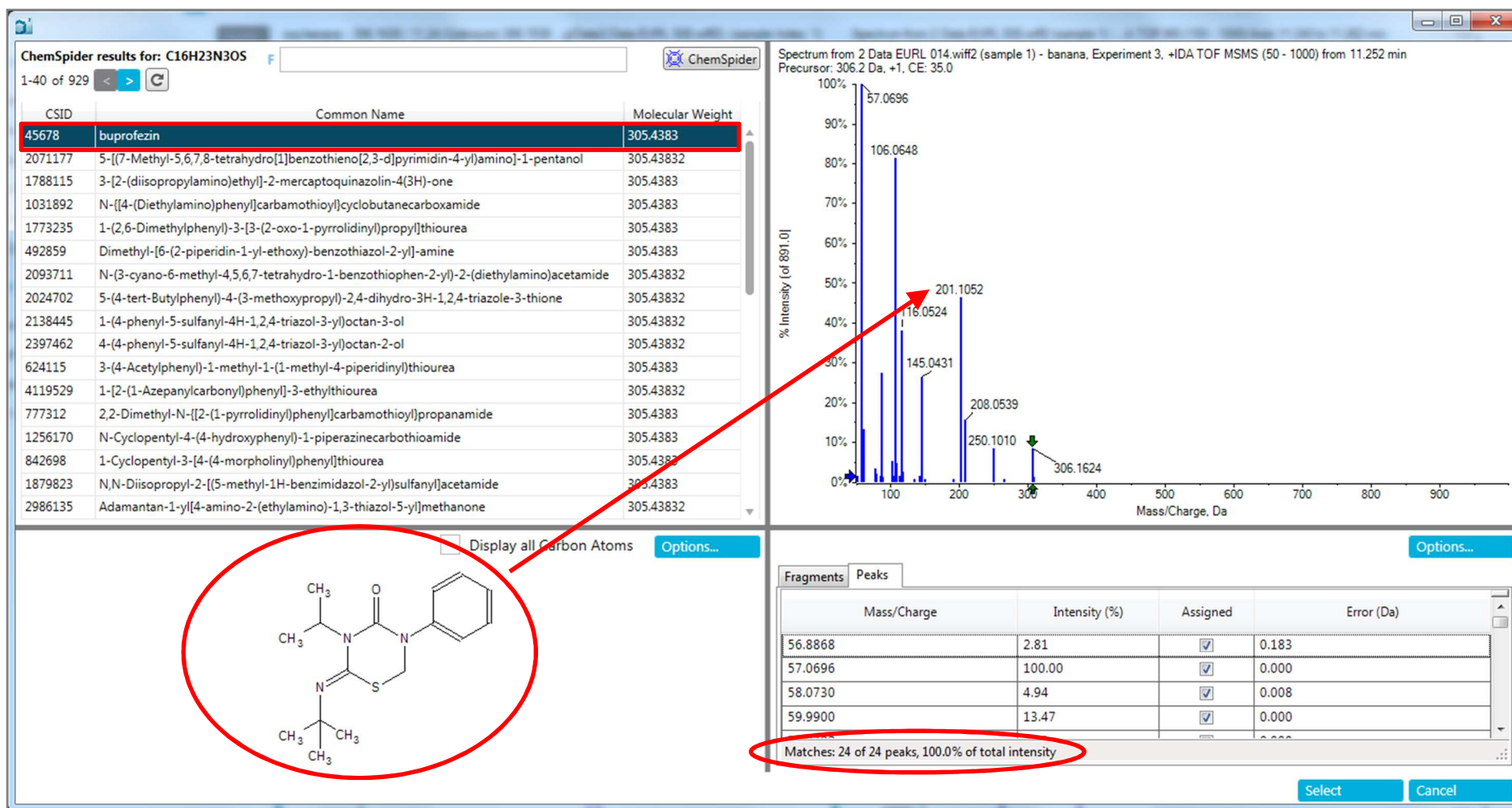
2. Automatic Sample-Control Comparison and Compound Identification



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

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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