SCIEX

Answers for Science.
Knowledge for Life.™

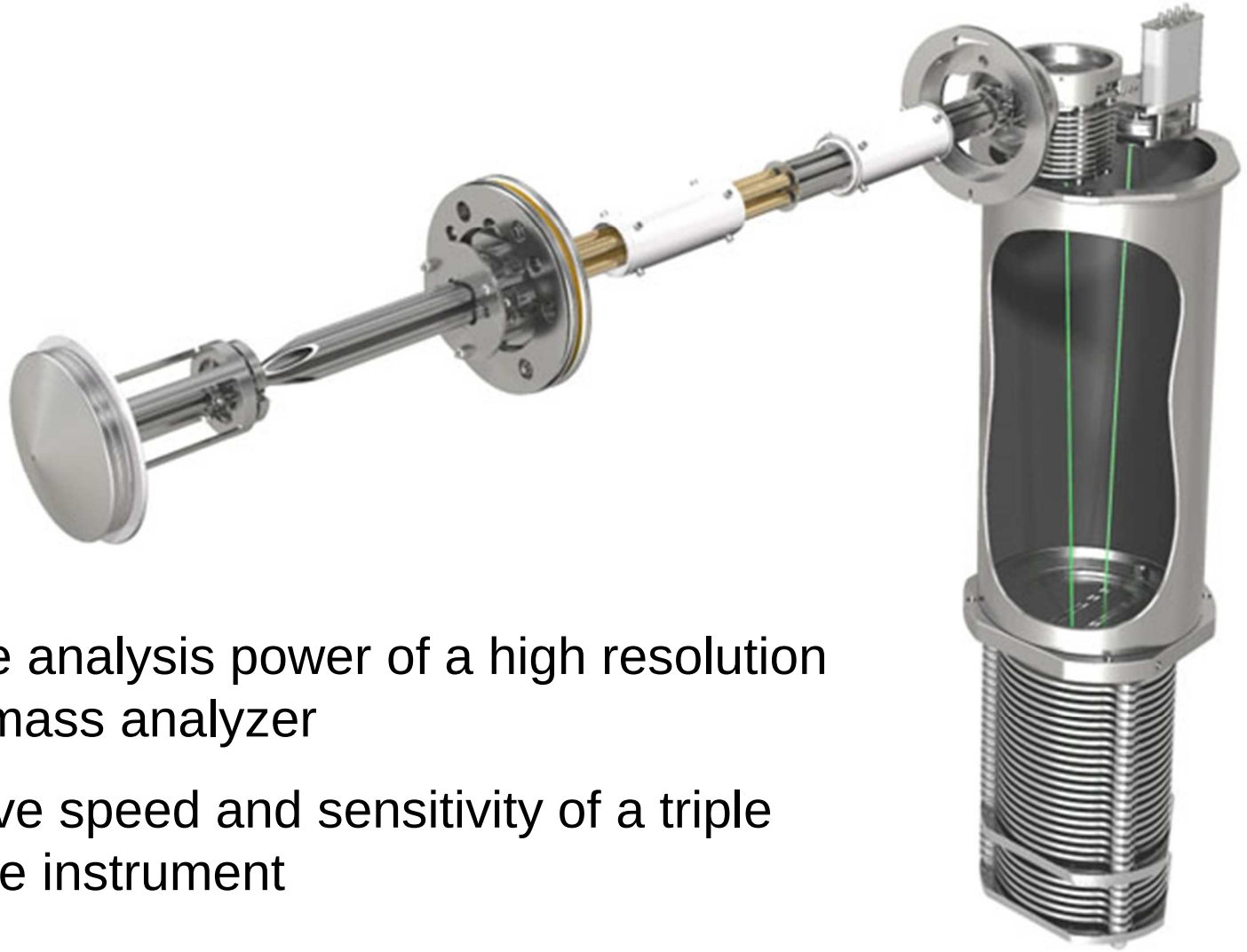
# Ignite your Routine Testing Methods

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

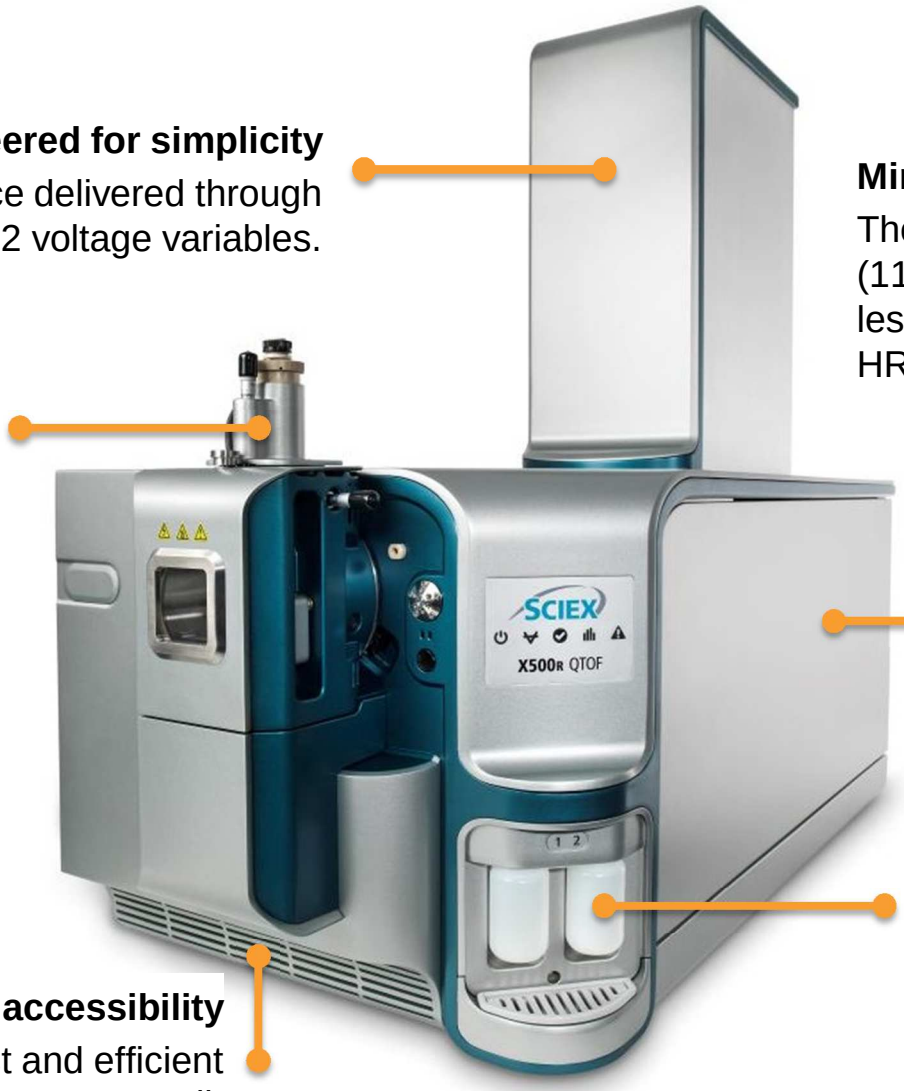
## Design Improvements and Details

**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

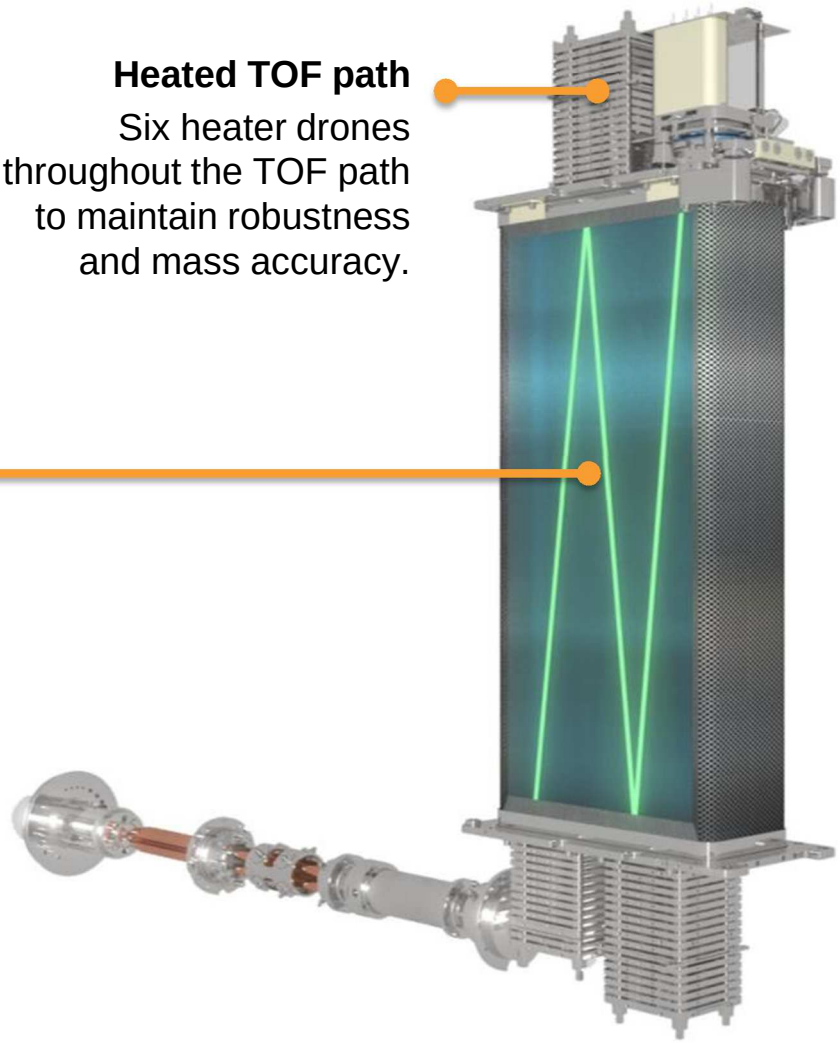
## Design Improvements and Details

**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

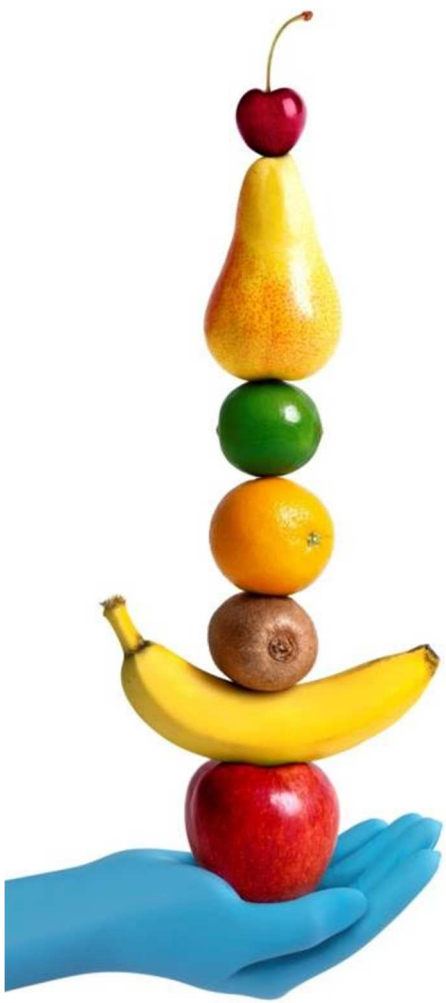
## Design Improvements and Details

**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

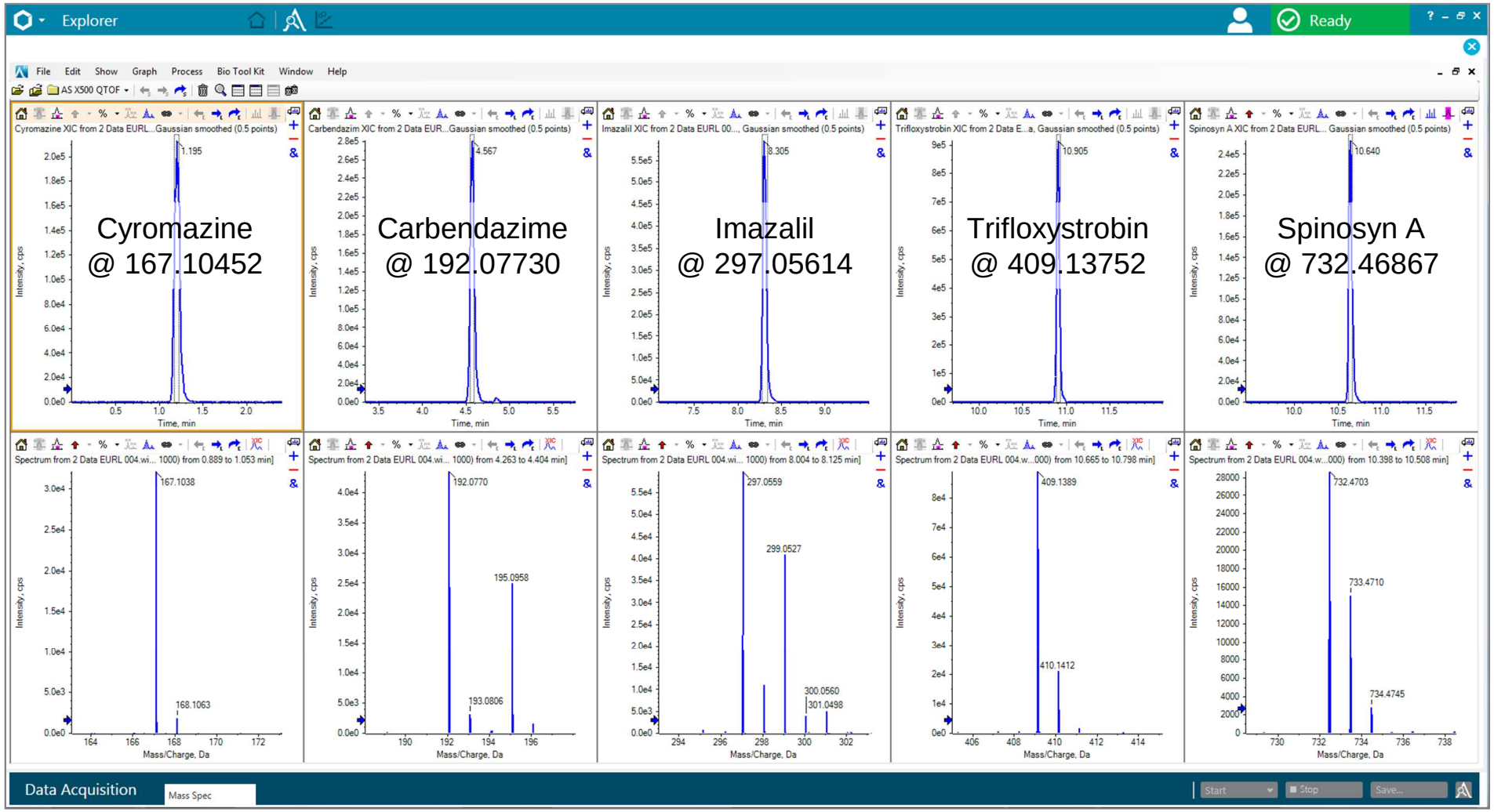
## SCIEX X500R QTOF System



- 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

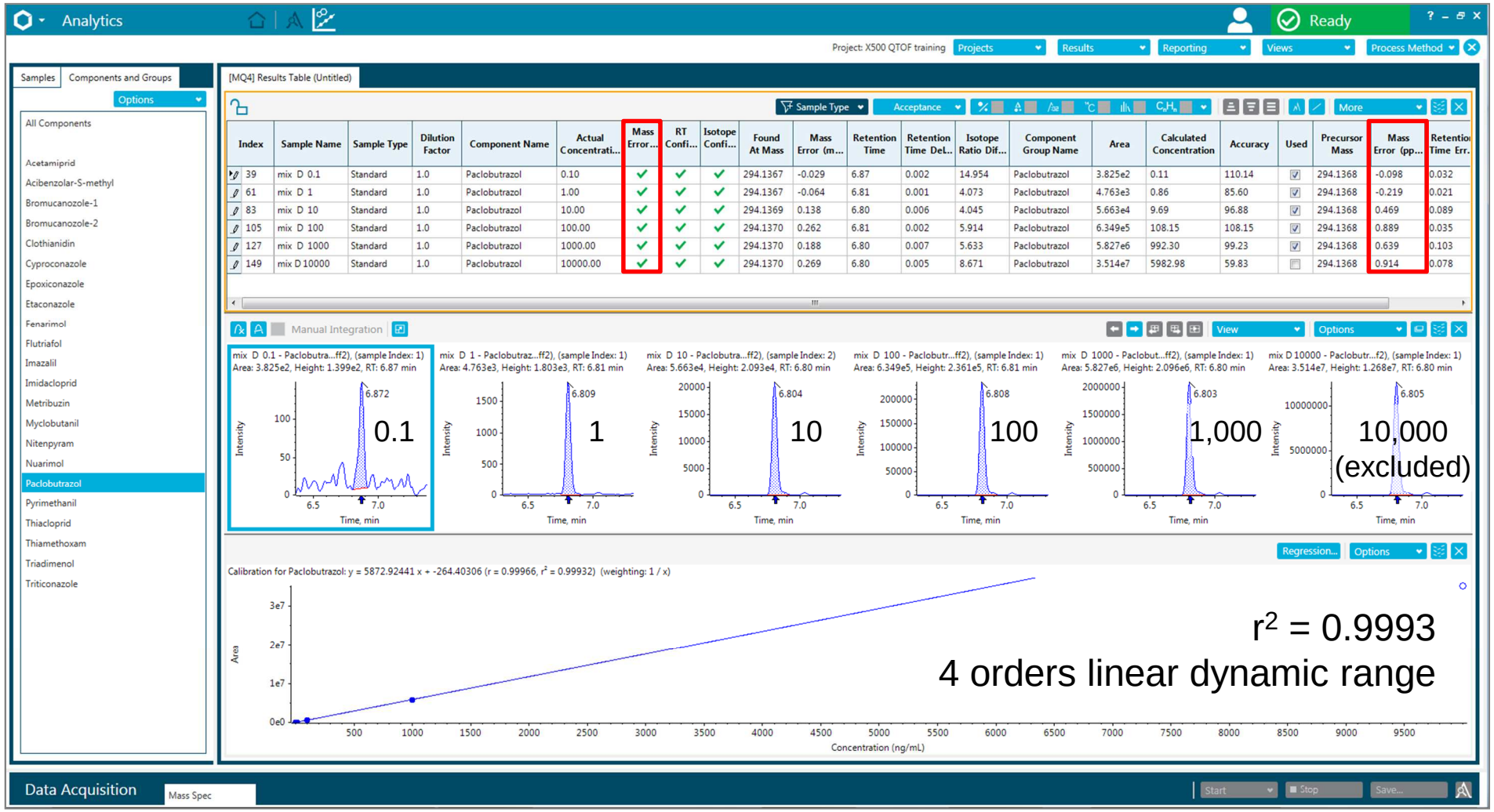
# The SCIEX X500R QTOF System – Performance

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



# The SCIEX X500R QTOF System – Performance

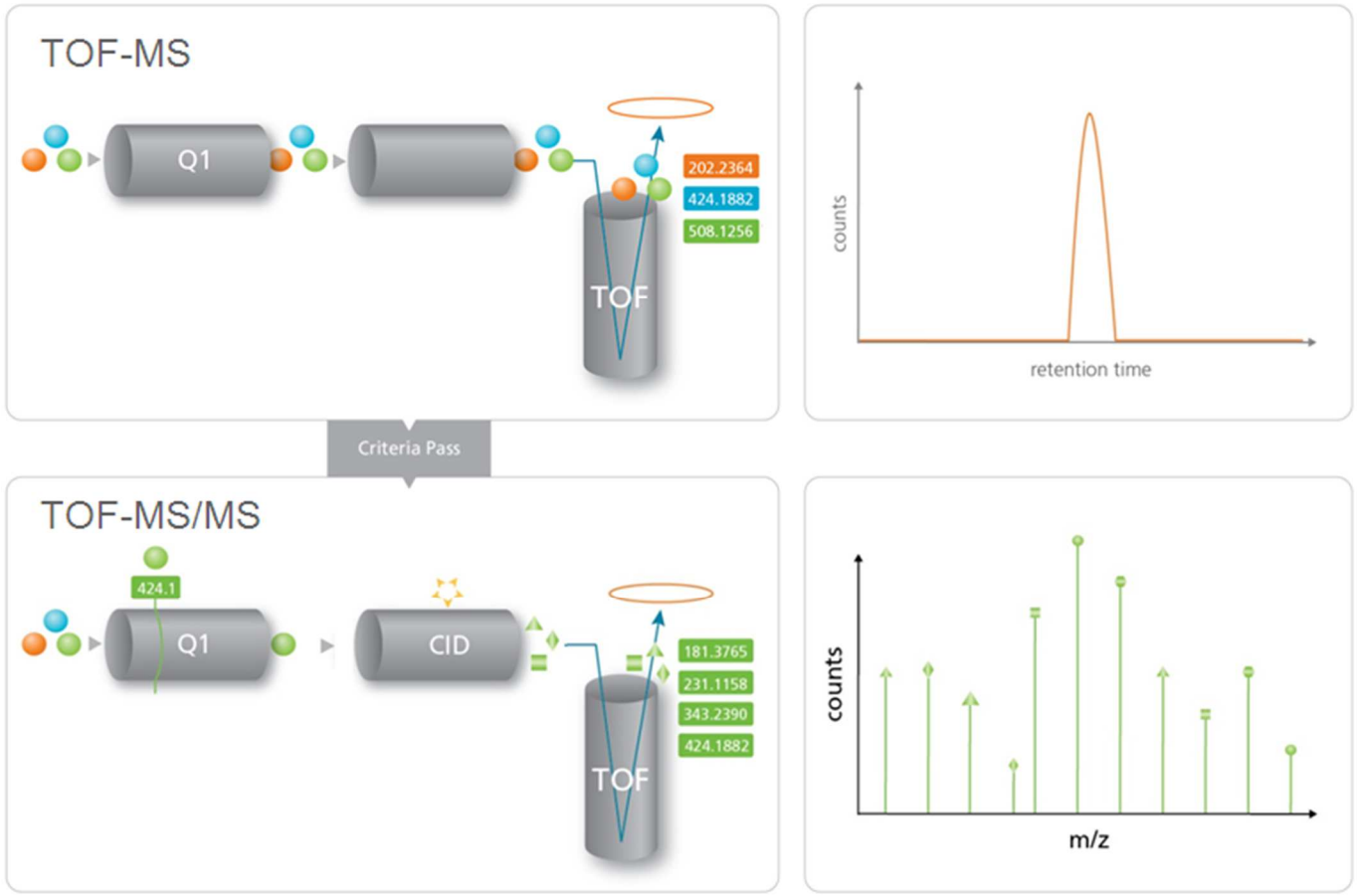
## Linearity and Mass Accuracy (Paclobutrazol 0.1 to 10,000 ng/mL)




Mass error = -0.2 to 0.91 ppm

# Information Dependent Acquisition of MS/MS (IDA)

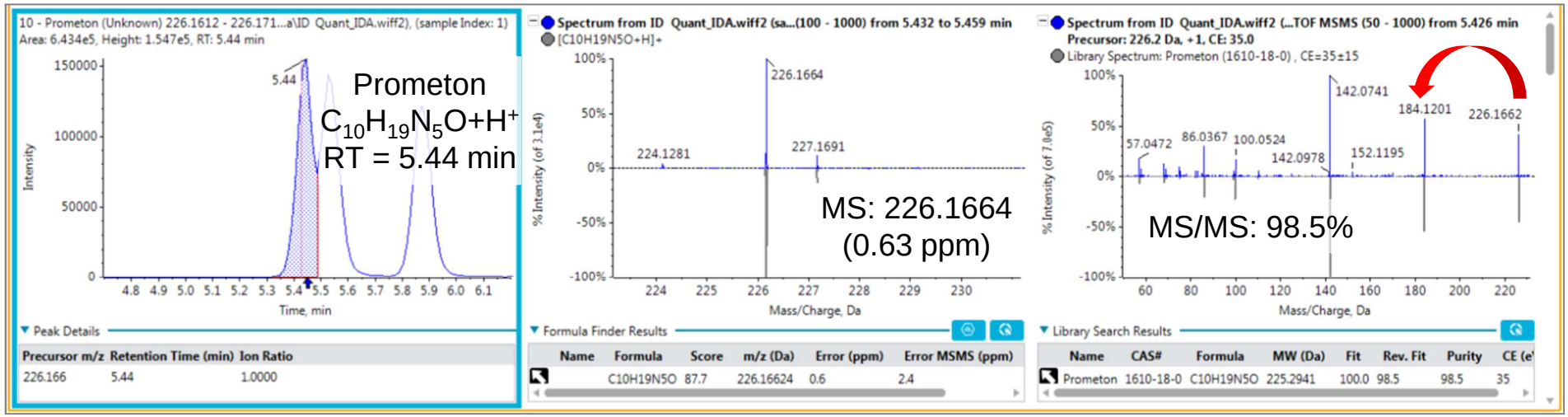
## Provides MS/MS Spectra with High Selectivity (Q1 Resolution unit)




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

# The SCIEX X500R QTOF System – IDA

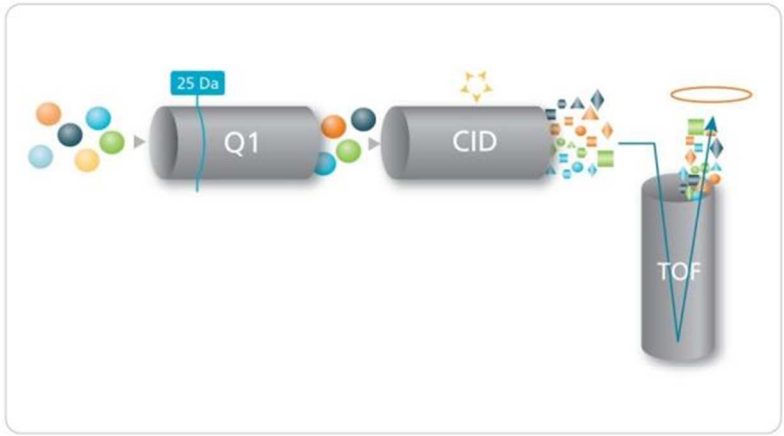
## Confident Identification of Isomers using MS/MS (Prometon vs. Terbumeton)

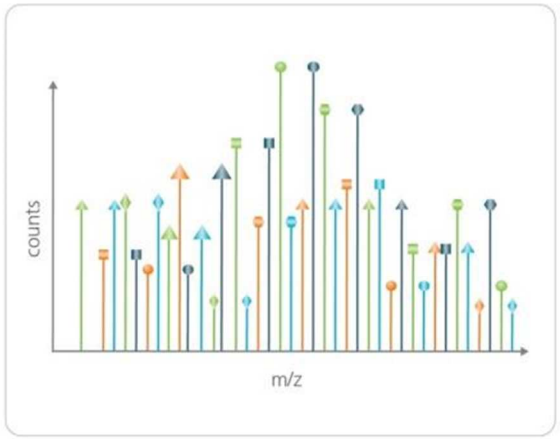



Identification based on MS/MS library searching (Q1 at unit resolution)

# MS/MS$^{ALL}$ using SWATH™ Acquisition

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



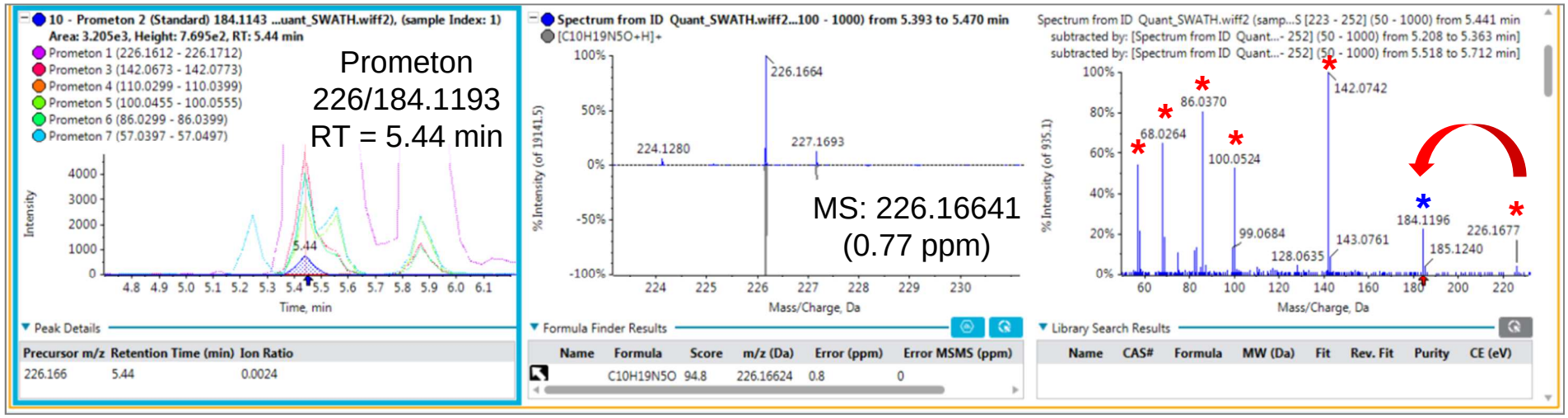





SWATH™: Wide Q1 Isolation Window is Stepped Across the Mass Range

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

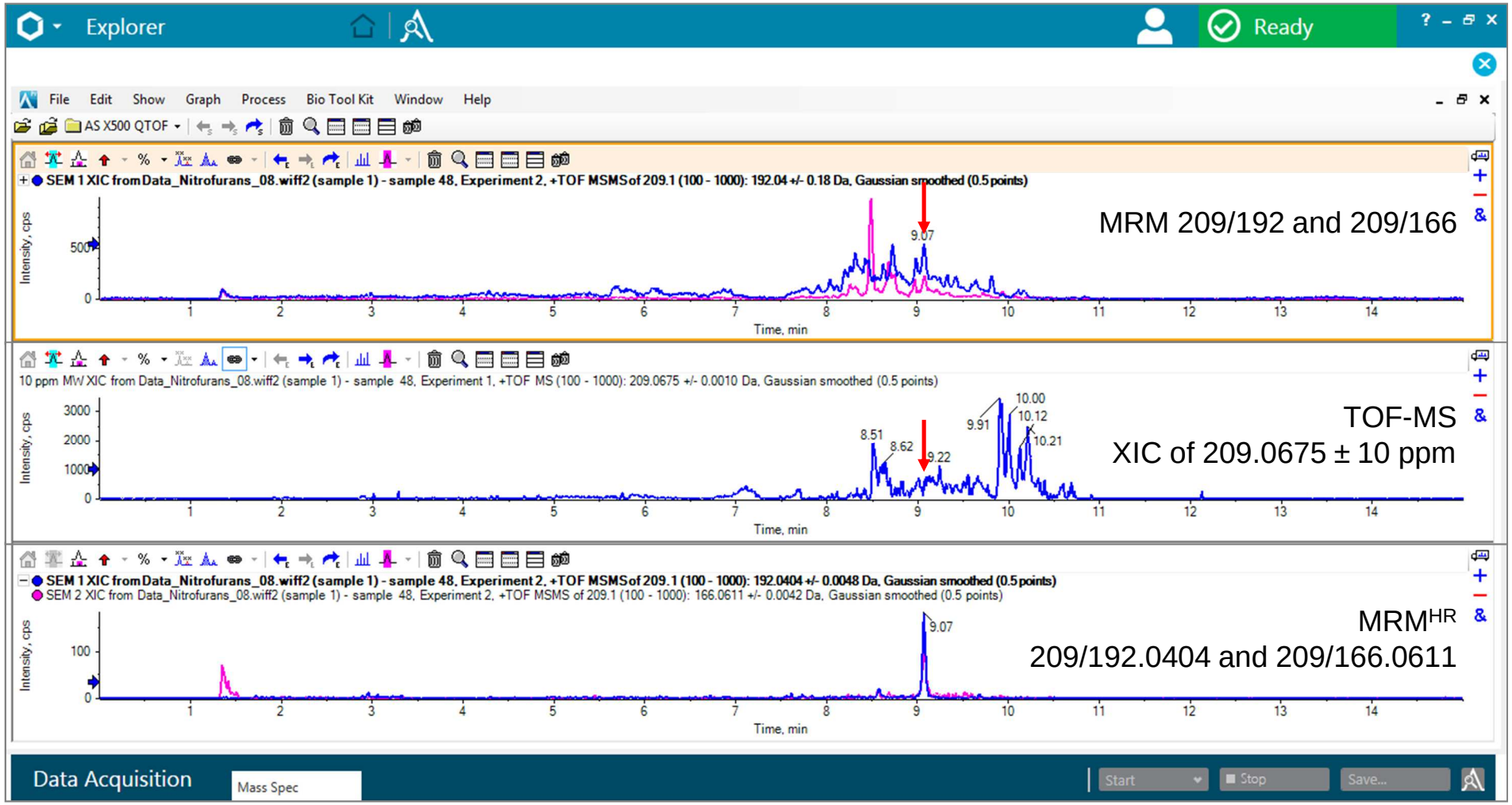
## Confident Identification of Isomers using SWATH (Prometon vs. Terbumeton)




Identification based on unique fragment ions and their ratios

# Increased Selectivity using MRM$^{HR}$

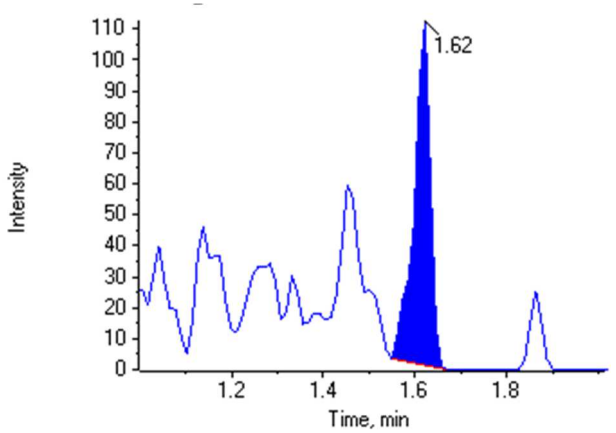
## Feed Sample Tested Positive for NP-Semicarbazide



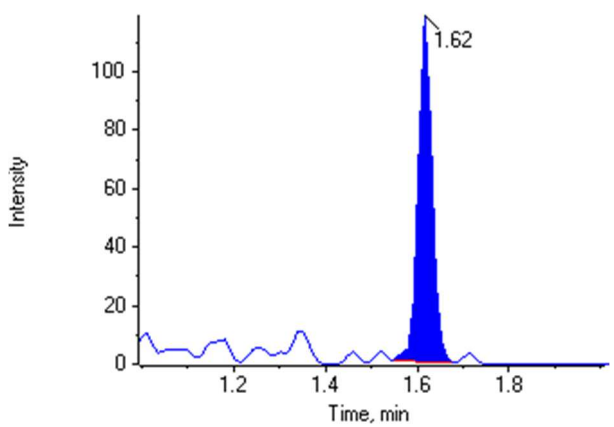
# Comparison of TOF MS vs. SWATH vs. MRM$^{HR}$ Quant

## Loratidine

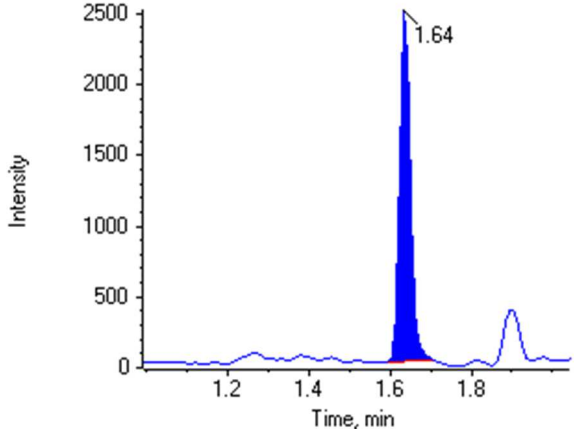
S/N = 9.6




S/N = 26




S/N = 166

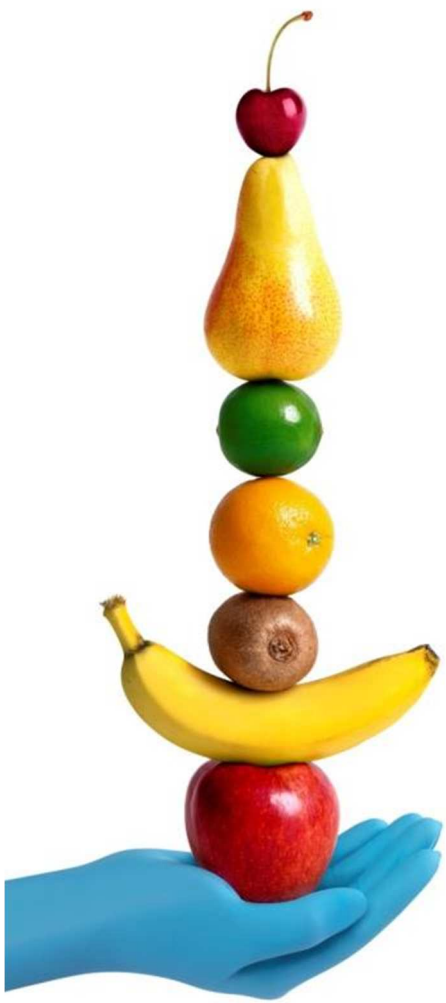



**TOF MS** → **SWATH** → **MRM$^{HR}$**

**Selectivity** **Sensitivity**

# Perfect Balance to Elevate Your Lab's Performance

## SCIEX X500R QTOF System Powered by SCIEX OS Software



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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.

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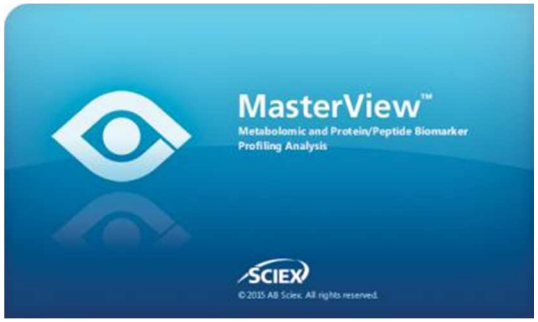
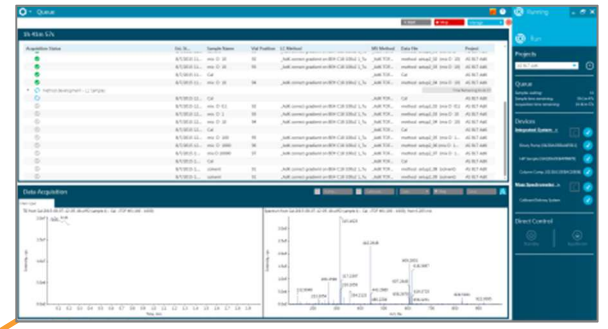
# Introducing the SCIEX OS Software

## Single Software Platform for MS Control, Data Processing and Reporting

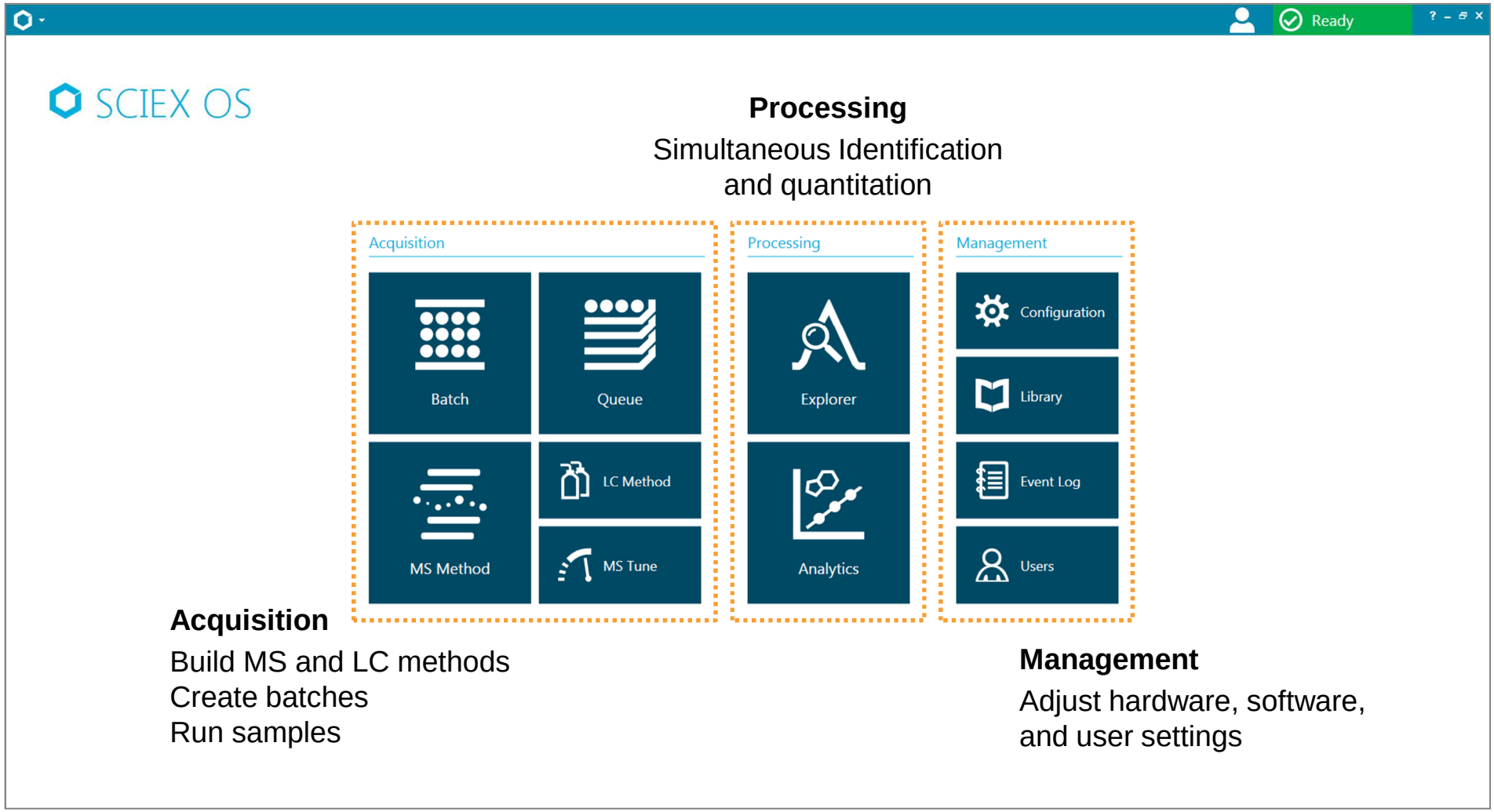





# SCIEX OS Software – Home

## Everything in a Single Software Platform




**Processing**

Simultaneous Identification
and quantitation

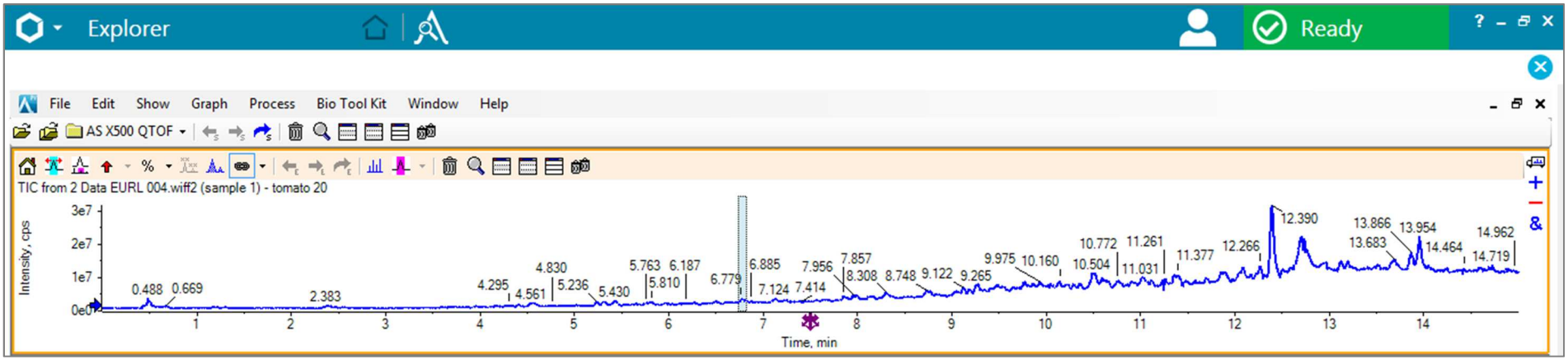
**Acquisition**

Build MS and LC methods
Create batches
Run samples

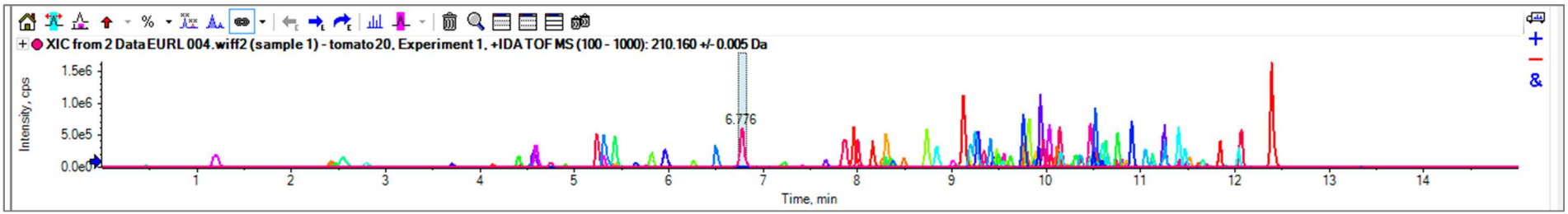
**Management**

Adjust hardware, software,
and user settings

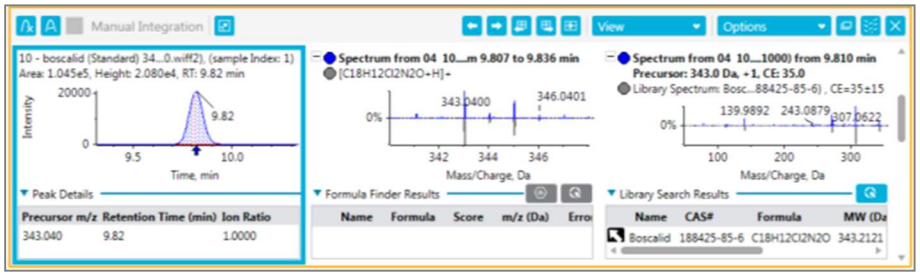
# Targeted Data Processing Workflow



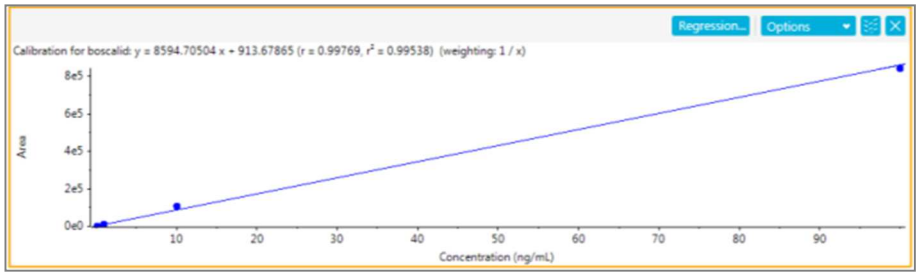

XIC generation for each target




Identification




Quantitation



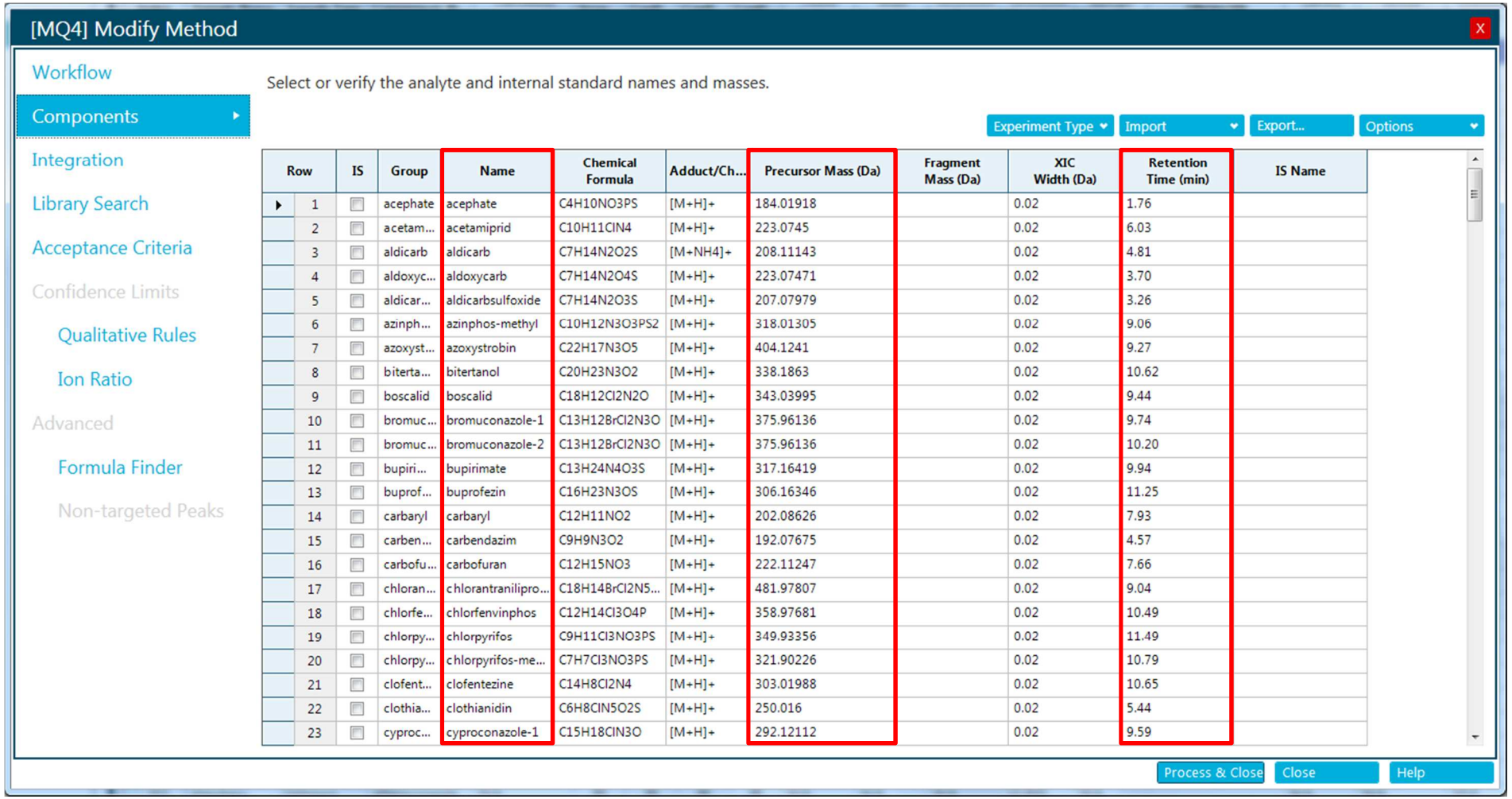

RT ✓ Mass ✓ MS/MS search ✓

Isotopes ✓

Above reporting level

# Identification and Quantitation in SCIEX OS Software

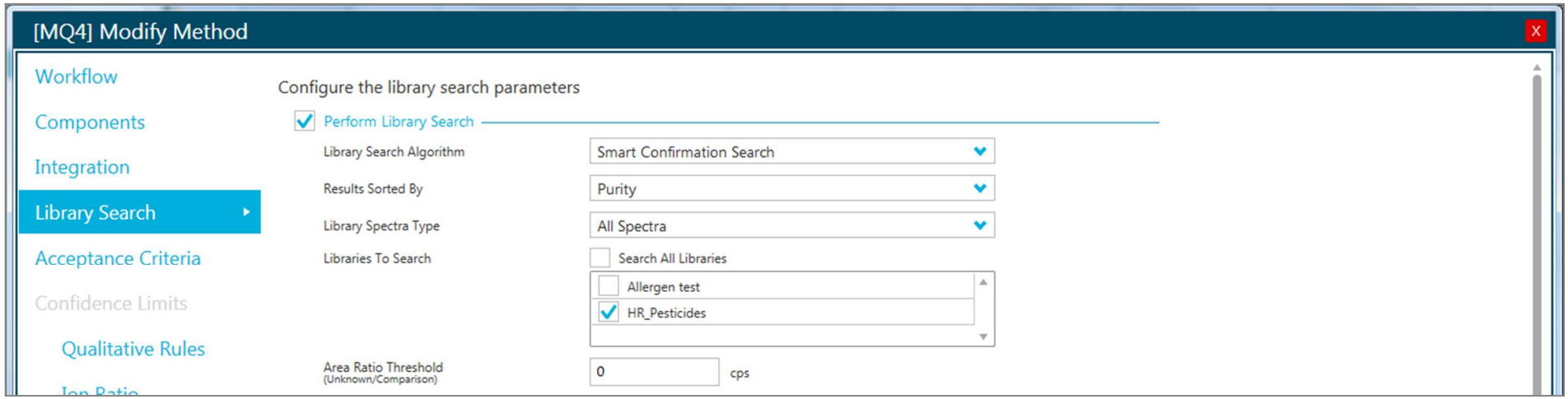
## 1. Define Retention Time and Accurate Mass for Each Target Analyte

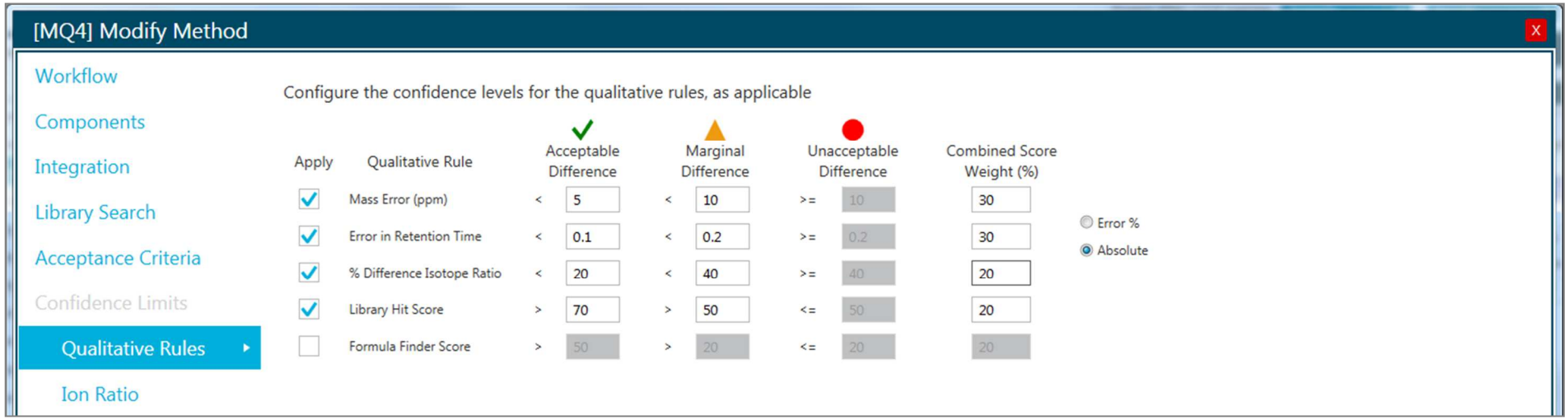



| Row | IS | Group | Name | Chemical Formula | Adduct/Ch... | Precursor Mass (Da) | Fragment Mass (Da) | XIC Width (Da) | Retention Time (min) | IS Name |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | | acephate | acephate | C4H10NO3PS | [M+H]+ | 184.01918 | | 0.02 | 1.76 | |
| 2 | | acetam... | 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

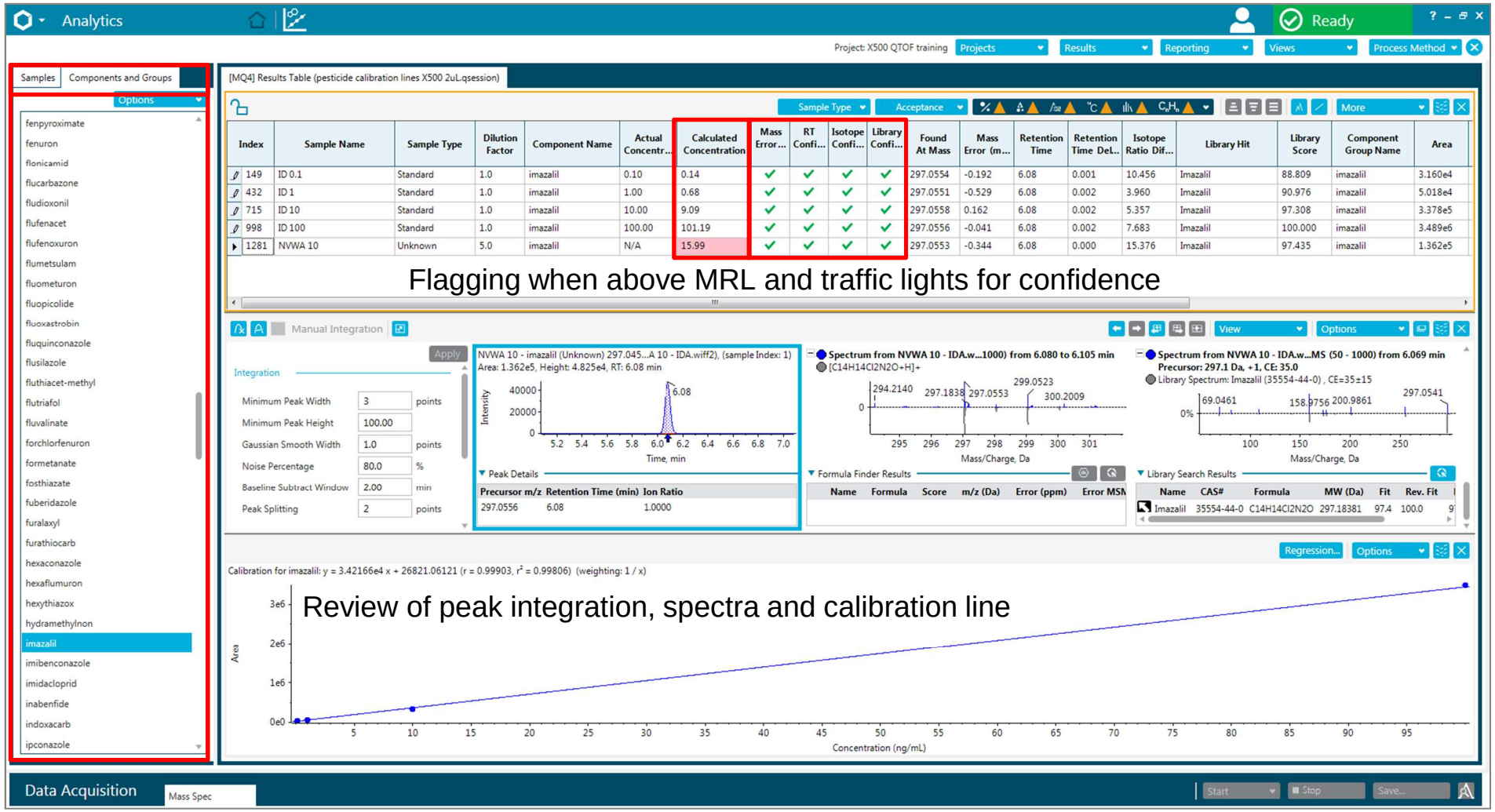
## 2. Define Identification Criteria and Confidence Settings



# Identification and Quantitation in SCIEX OS Software

## 3. Review Qualitative and Quantitative Results



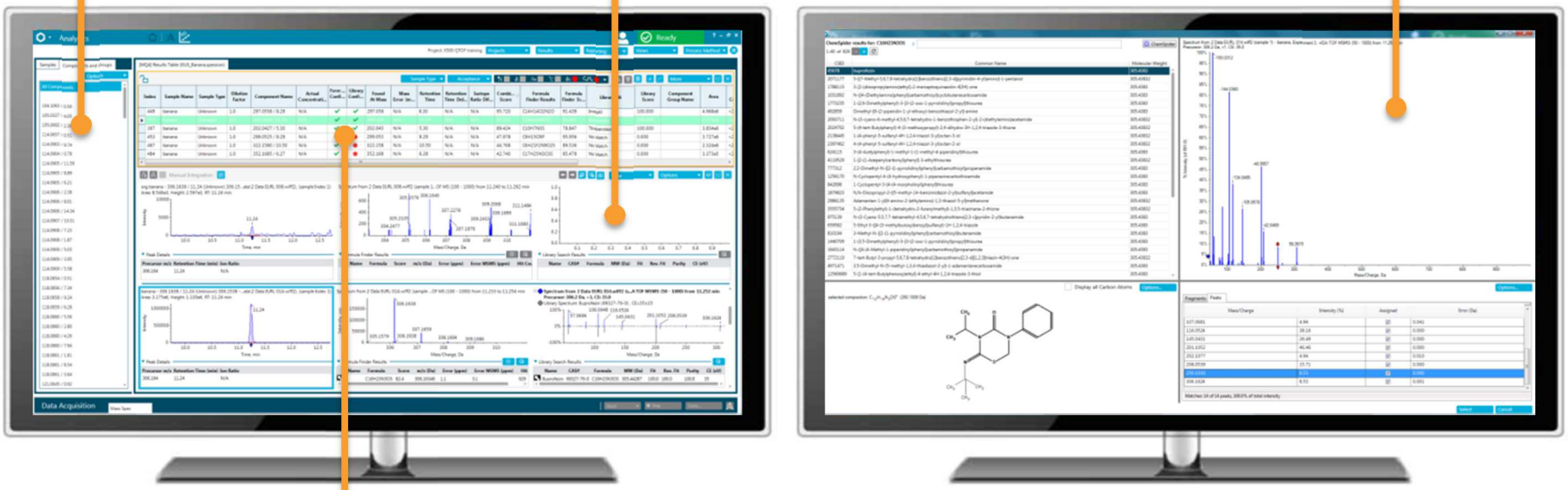
# SCIEX OS Software – Unknown Identification

## Software Improvements and Details

**Automatic sample-control comparison**

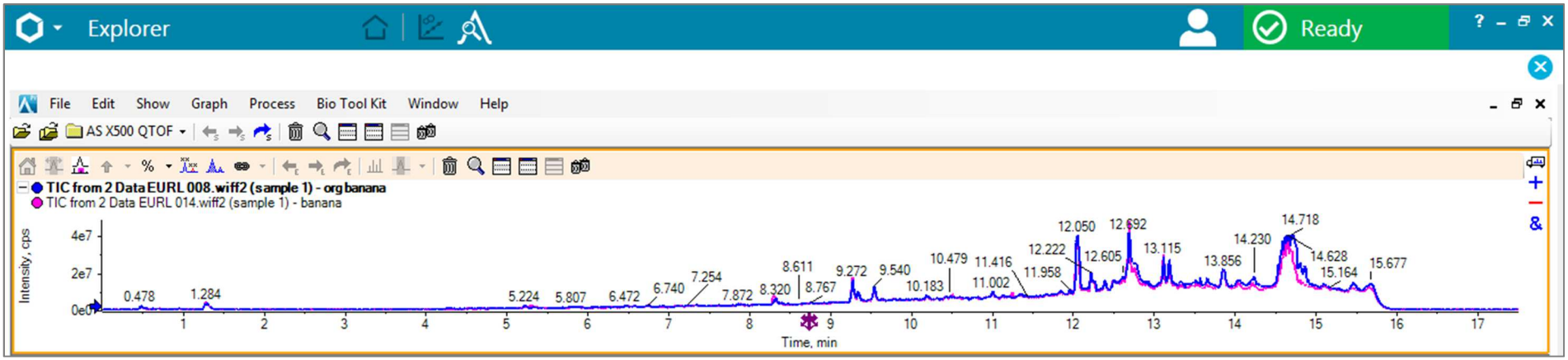
**Non-Target peak finding**

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

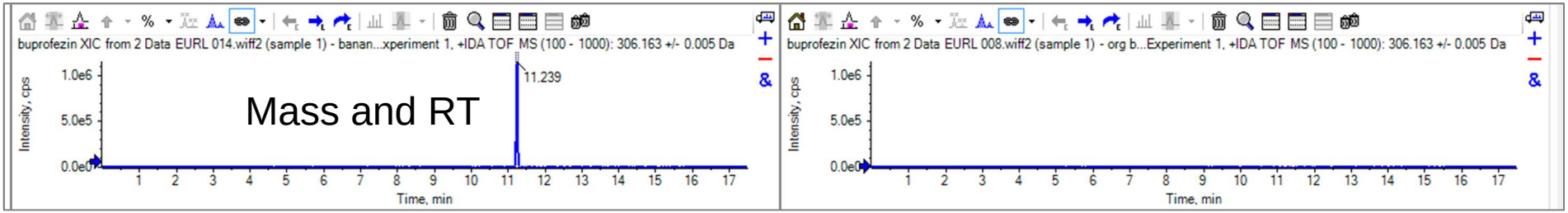


**Automatic MS/MS library searching and formula finding**

# Non-Targeted Data Processing Workflow

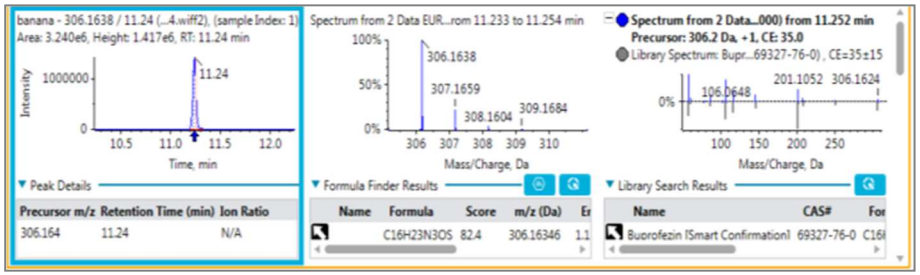



Sample-control comparison

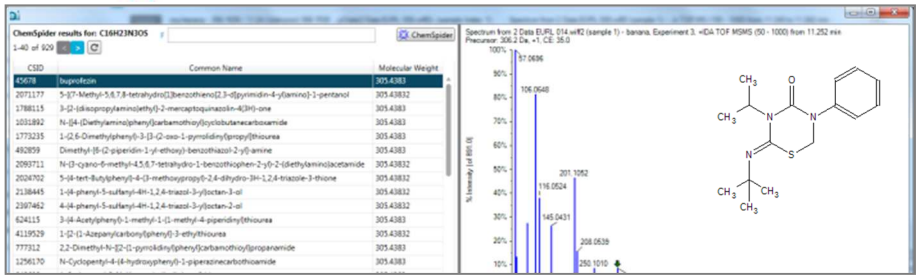



Mass and RT

Identification




ChemSpider
The free chemical database



Formula finding ✓ MS/MS search ✓

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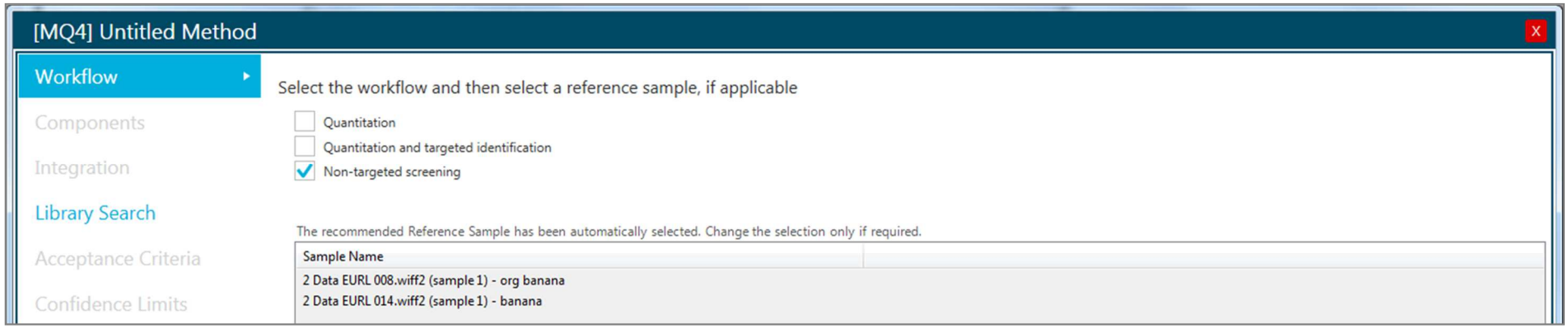
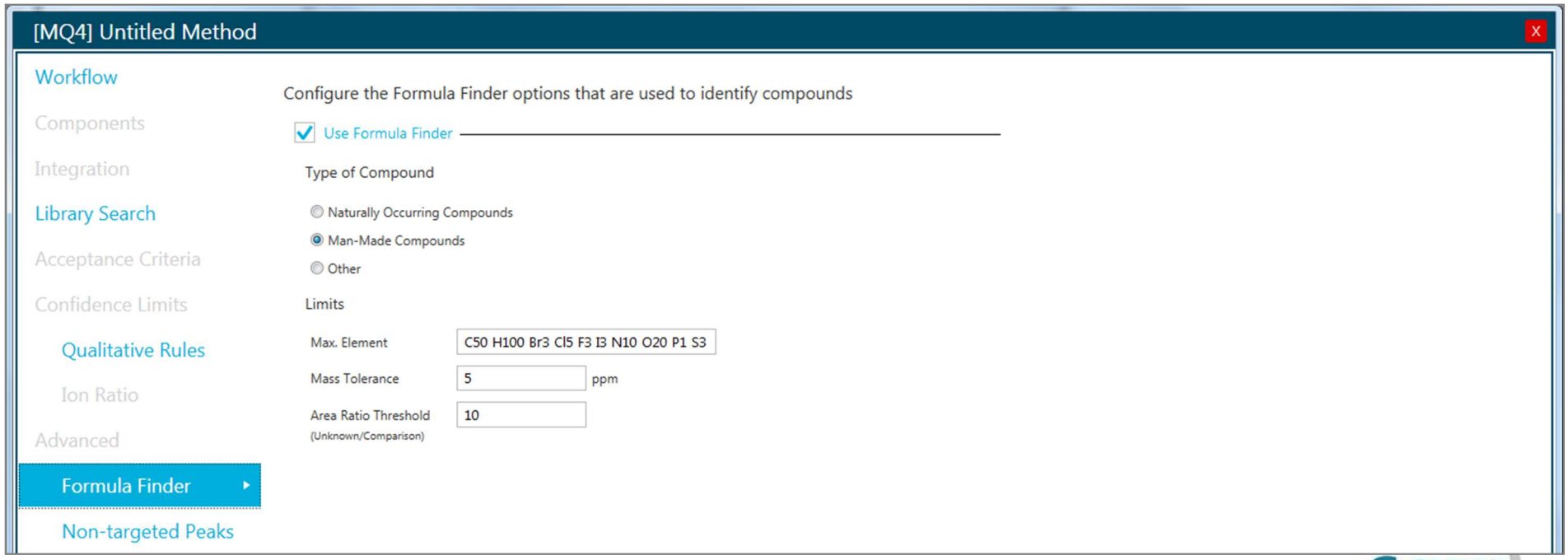
# Unknown Identification in SCIEX OS Software

## 1. Define Non-Target Peak Finding and Identification Parameters



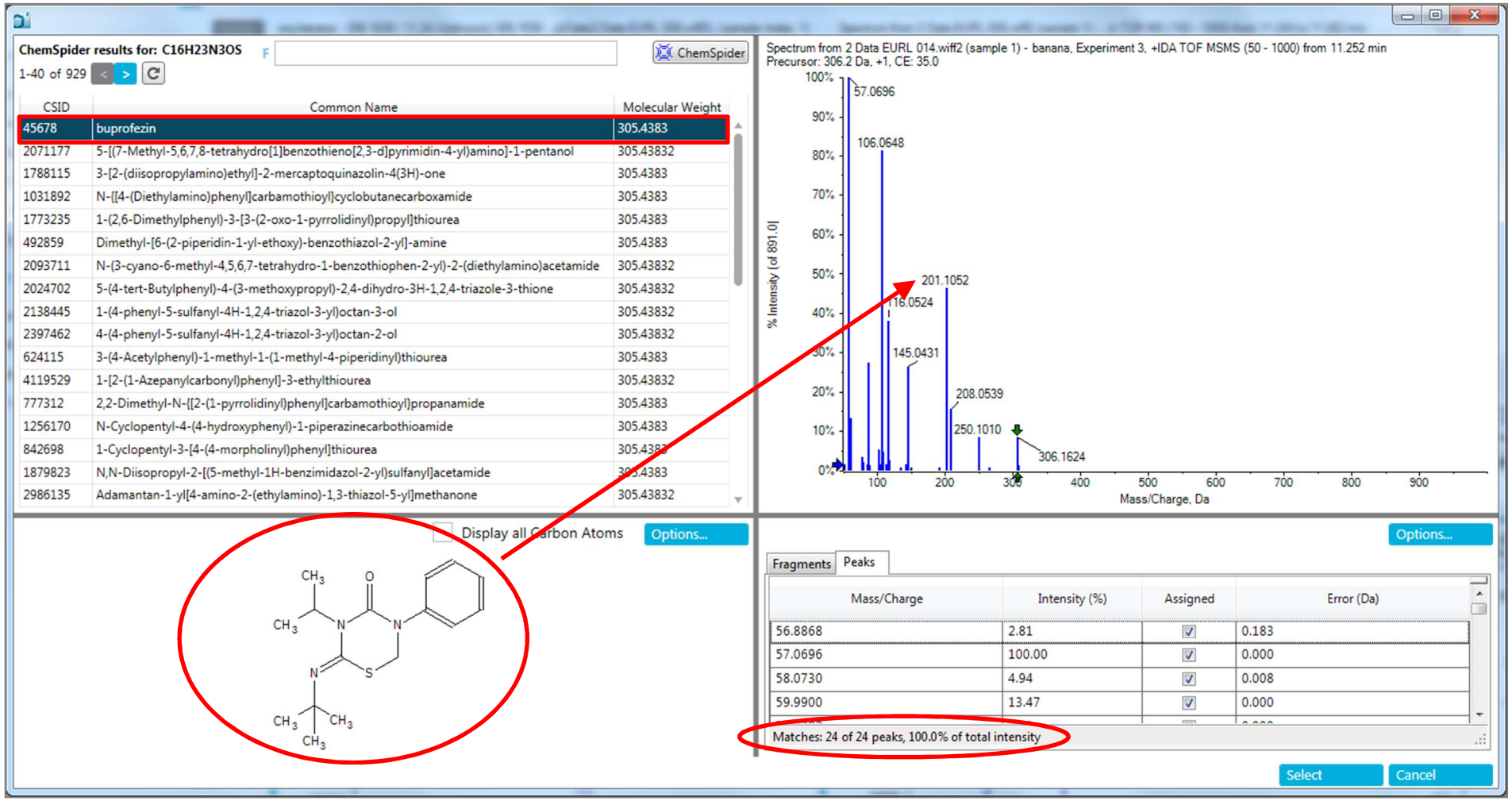
# Unknown Identification in SCIEX OS Software

## 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

# 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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