



# SCIEX QTRAP

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*All you need is ...*

**AMEDIS** 30let  
*s Vámi...*

**SCIEX** 50  
The Power of Precision

# SCIEX mass spectrometry portfolio: 2023

## SCIEX Triple Quad and QTRAP systems



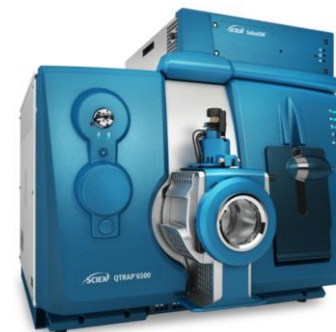
Triple Quad 3500 system



QTRAP/TQ 4500 system



SCIEX 5500+ system



QTRAP/TQ 6500+ system



SCIEX 7500 system

## Pushing the limits

X500R QTOF system



X500B QTOF system



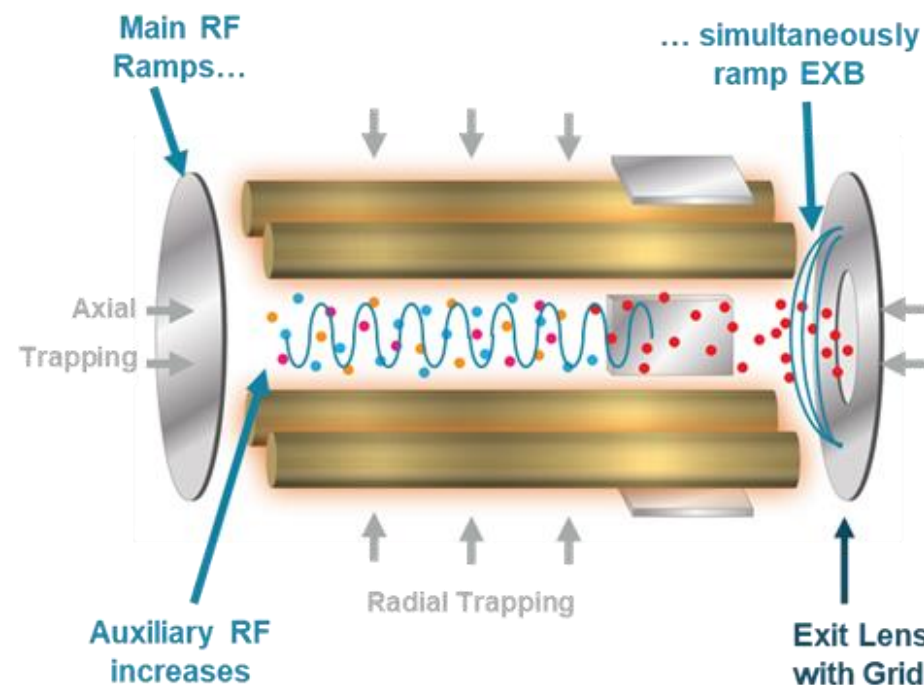
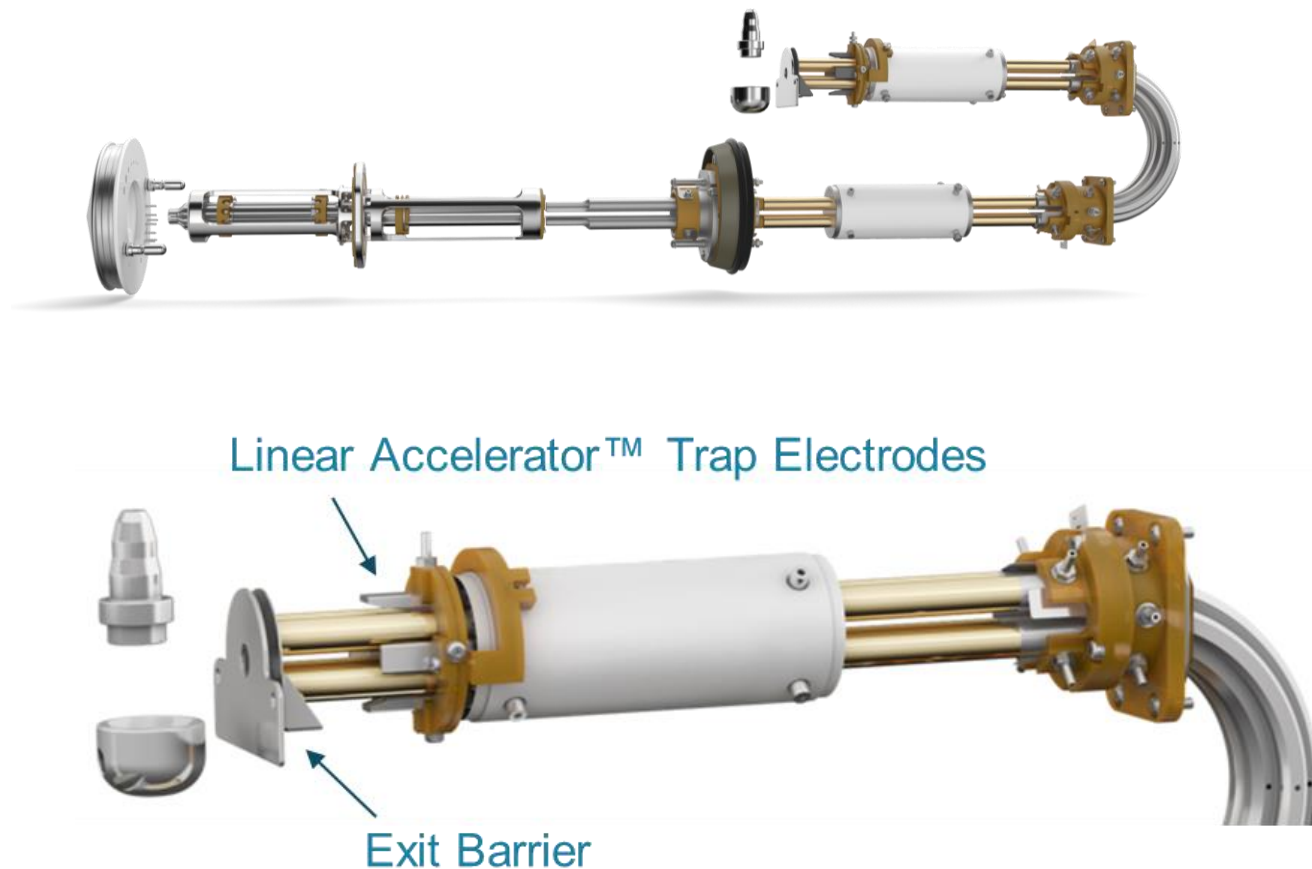
ZenoTOF 7600 system



## SCIEX HRMS products

# QTRAP - Built on a legacy of performance

## SCIEX QTRAP SYSTEM



# QTRAP - Triple Quadrupole / Linear Ion Trap MS

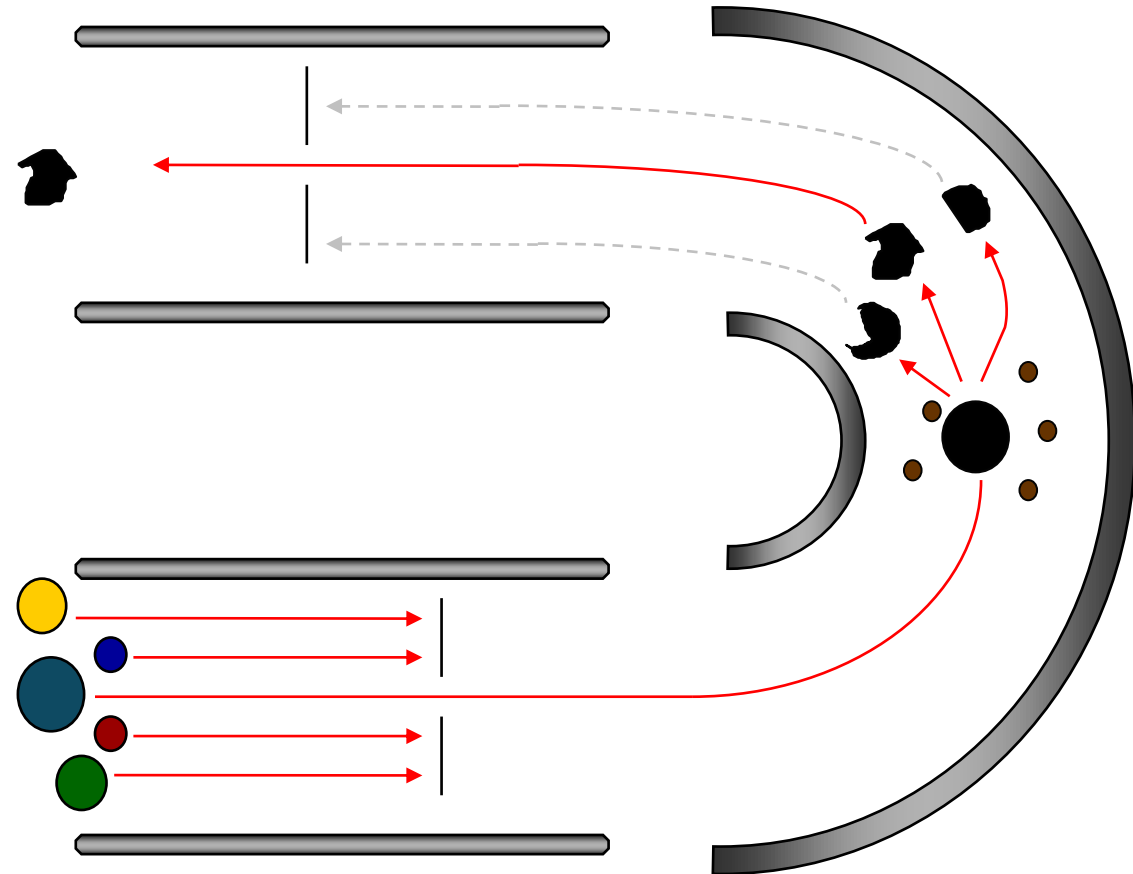
- All QqQ modes of operation
  - Identical sensitivity in MRM
  - Wide dynamic range for quantitation
  - Neutral Loss (NL)
  - Precursor Ion Scan (PI)
  - MRM
- Additional simultaneous functions of linear ion trap
  - **Enhanced MS (EMS)**
  - Enhanced Resolution (ER)
  - **Enhanced Product Ion Scan (EPI)**
  - **MS<sup>3</sup>**
  - Enhanced Multiply Charged Scan (EMC)

# Multiple Reaction Monitoring (MRM) - Quantitation

**Q1: SIM**

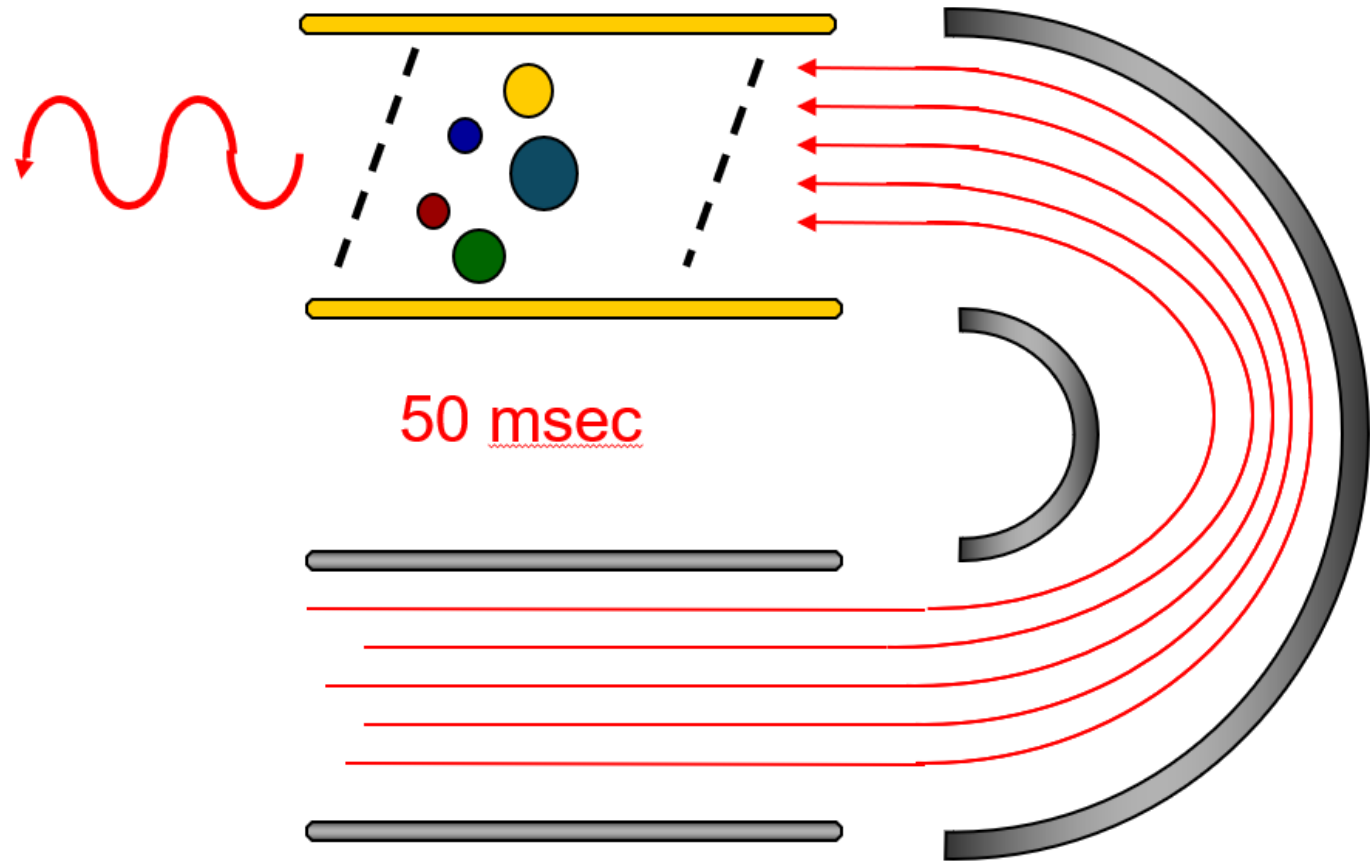
**Q2: Fragmentation**

**Q3: SIM**



# Enhanced MS Scan (EMS) - Search for Present Ions

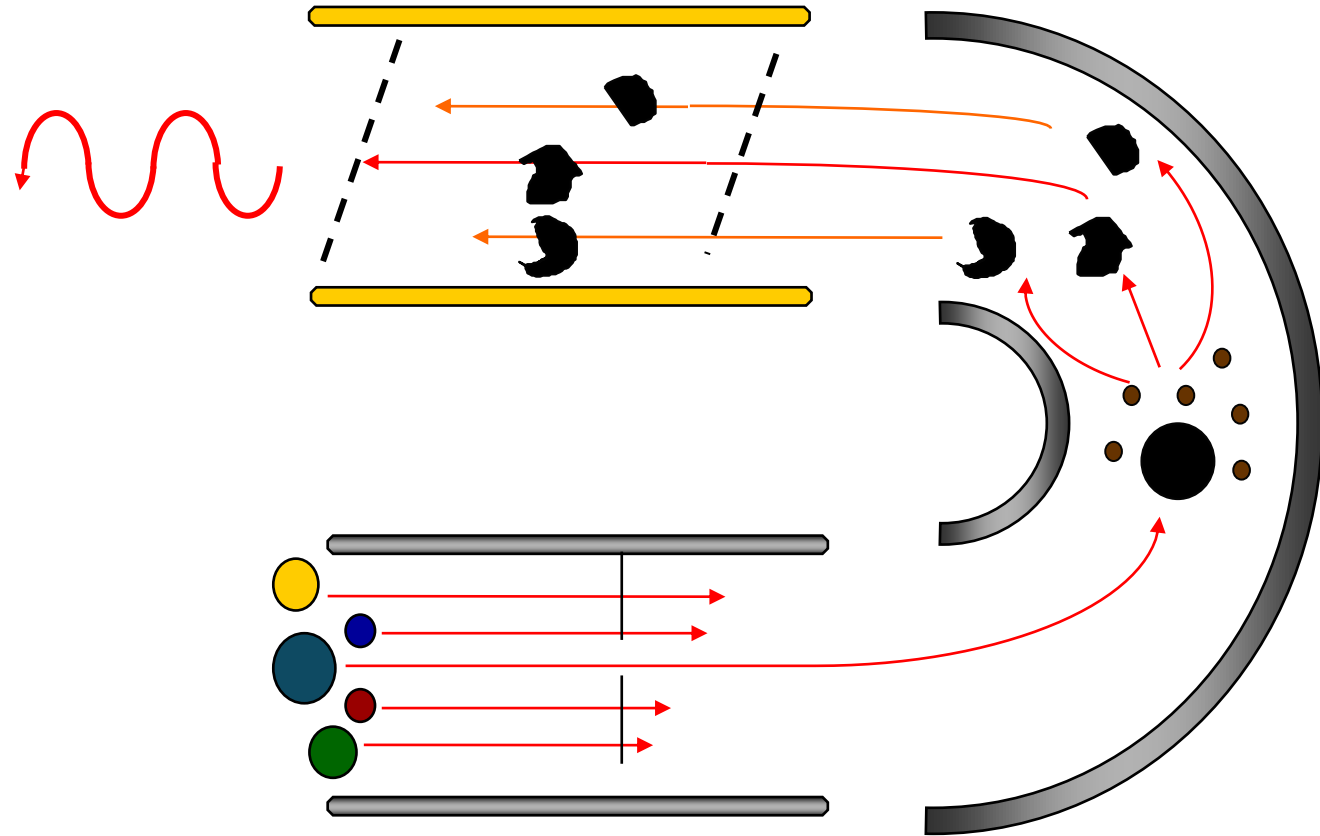
- Q1: RF only
- Q2: RF only
- LIT (Q3): Trap scan



# Enhanced Product Ion Scan (EPI)

Fragmentation pattern with good sensitivity

- Q1: SIM
- Q2: Fragmentation
- LIT (Q3): Trap scan





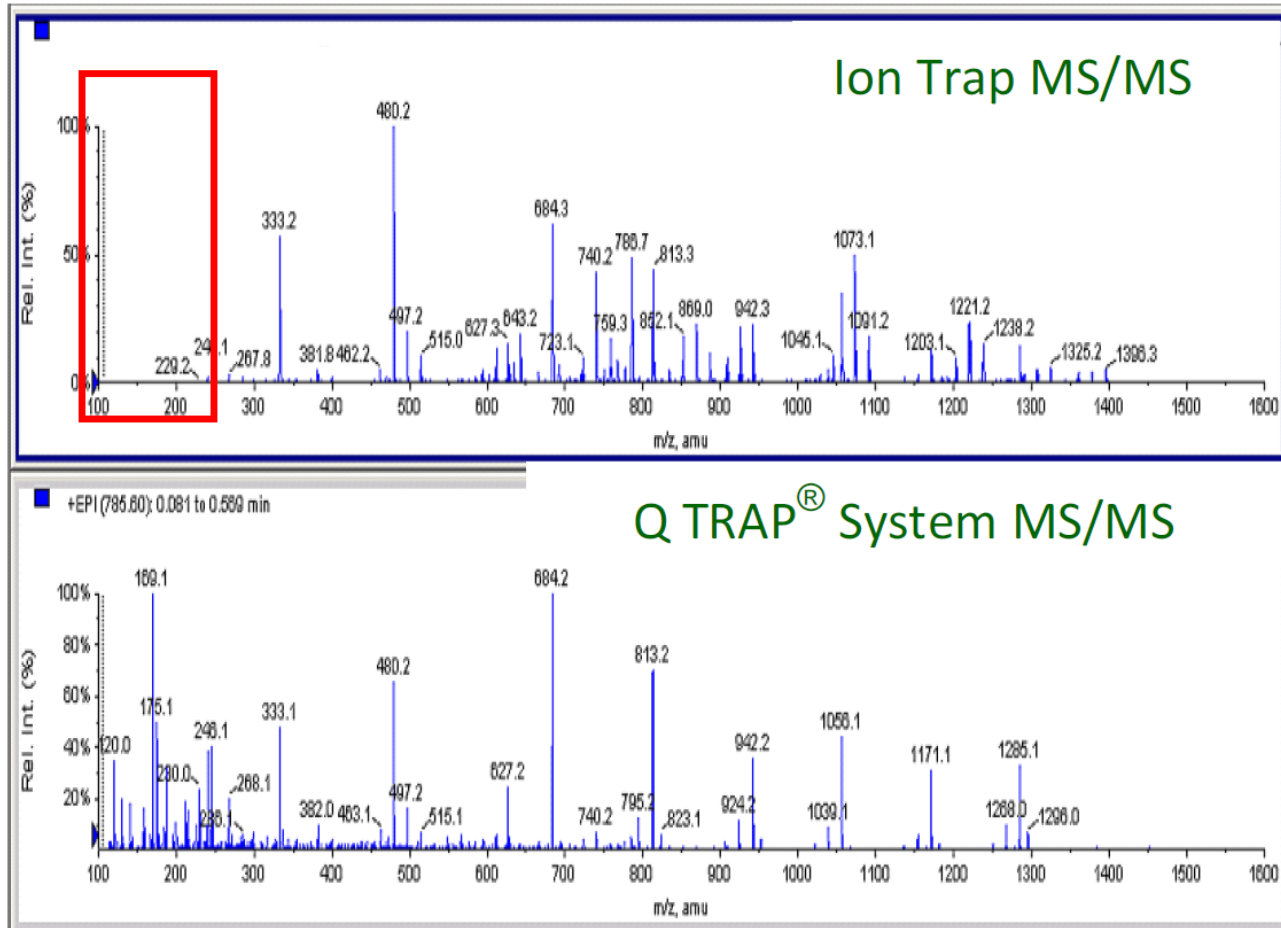
# QTRAP MS/MS

## QTRAP Enables Qualitative Workflows on a Quantitative Platform.

QTRAP systems in linear ion trap mode is typically >50-100x more sensitive than the equivalent scan in quadrupole mode.

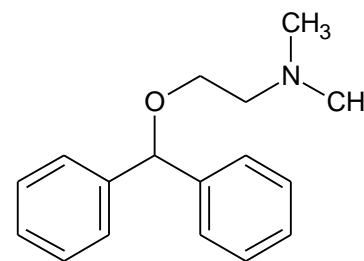
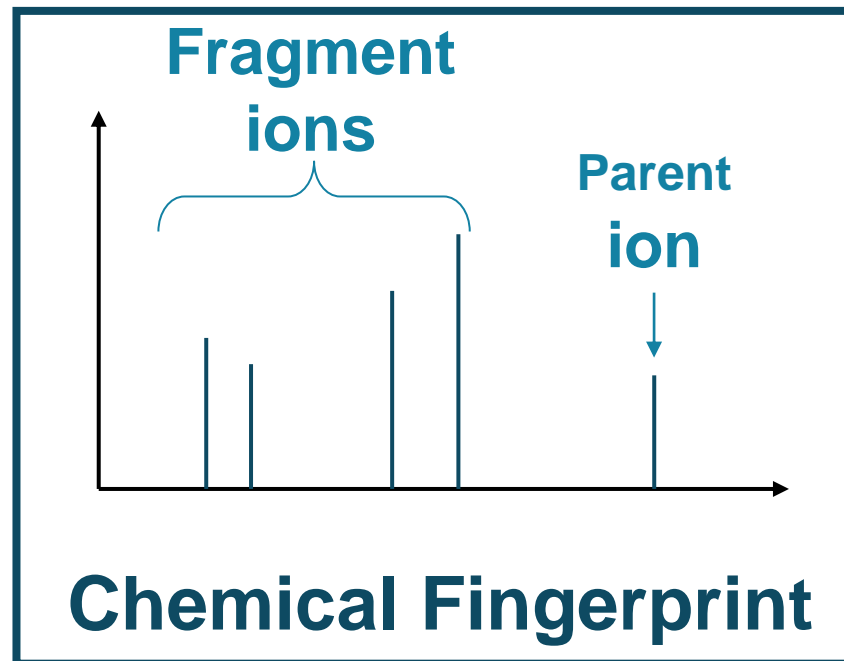
Without the low mass cut-off typically observed with conventional trap-based instruments.

This hybrid functionality makes the QTRAP system the only triple quadrupole based instrument that can do full quantitative and qualitative workflows *and* hybrid quantitative / qualitative workflows.





# MS/MS Library Searching



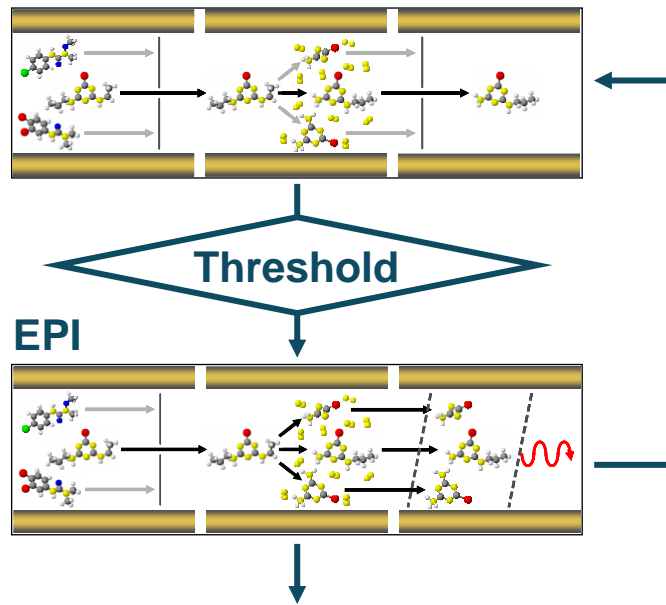
Multi-target Screening  
General Unknown Screening

MRM-EPI  
EMS – EPI

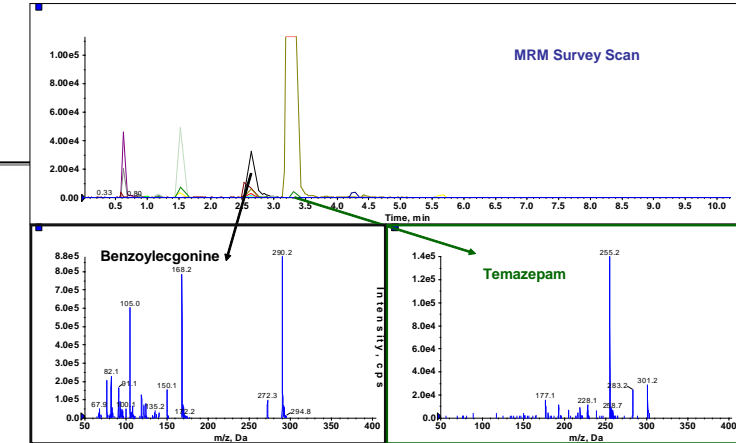
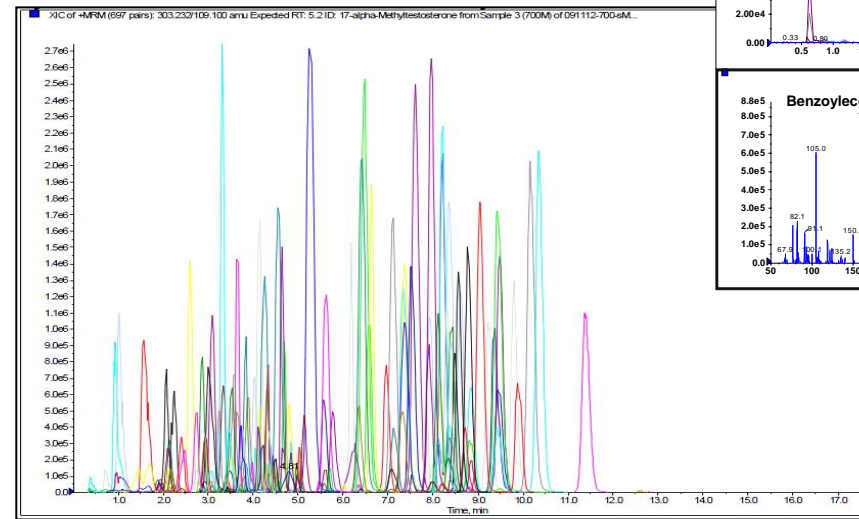
# Multi-Target Screening Approach with MRM

- MRM detection provides ultimate sensitivity and selectivity
- MS/MS library searching provides unambiguous confirmation
- Screening for hundreds of compounds is possible
- Only compounds on the “target list” are detected

## Scheduled MRM™ Algorithm



Library Search

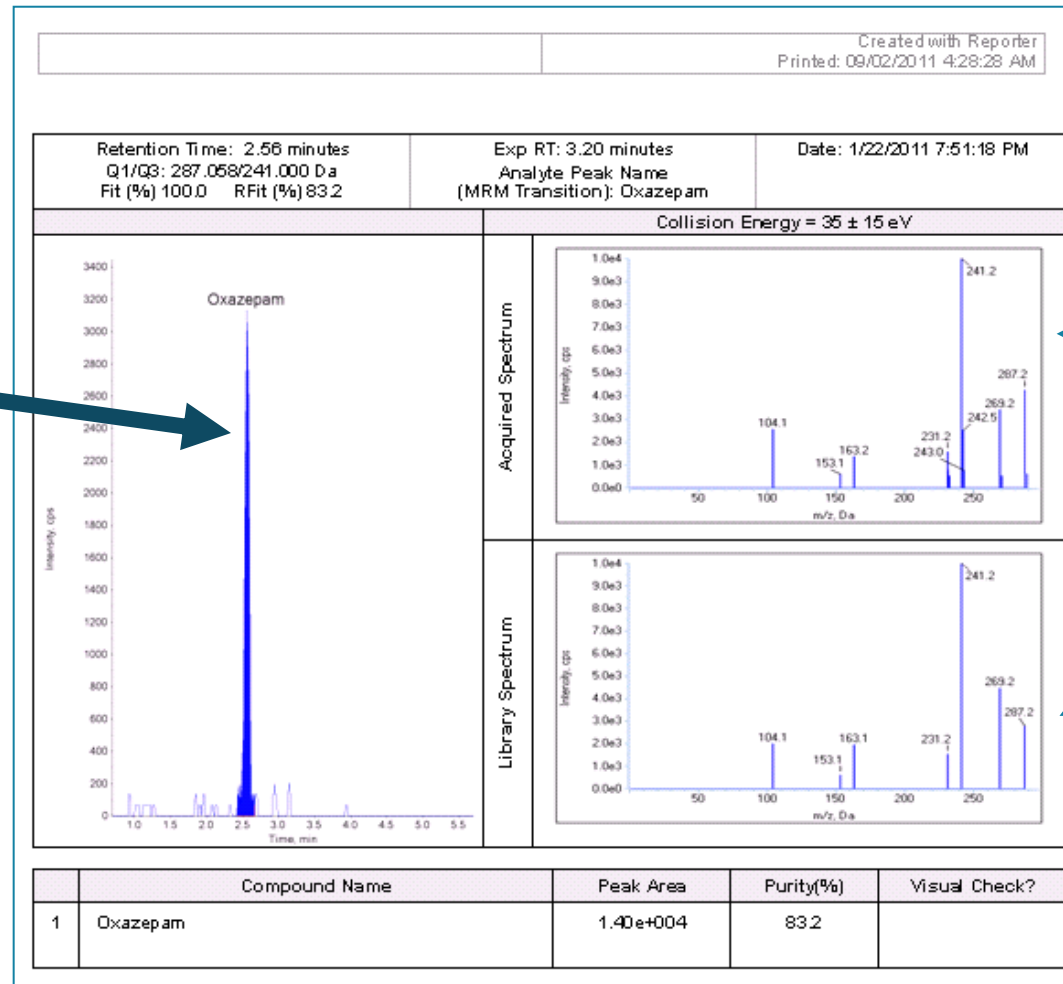


Example: Urine screen for 700 target drugs using AB SCIEX 3200 QTRAP® system

# Multi-Target Screening + Confirmation

- Survey Scan: MRM, Dependent Scan: EPI

**Detection**  
MRM of  
Oxazepam  
287.1/241.  
0



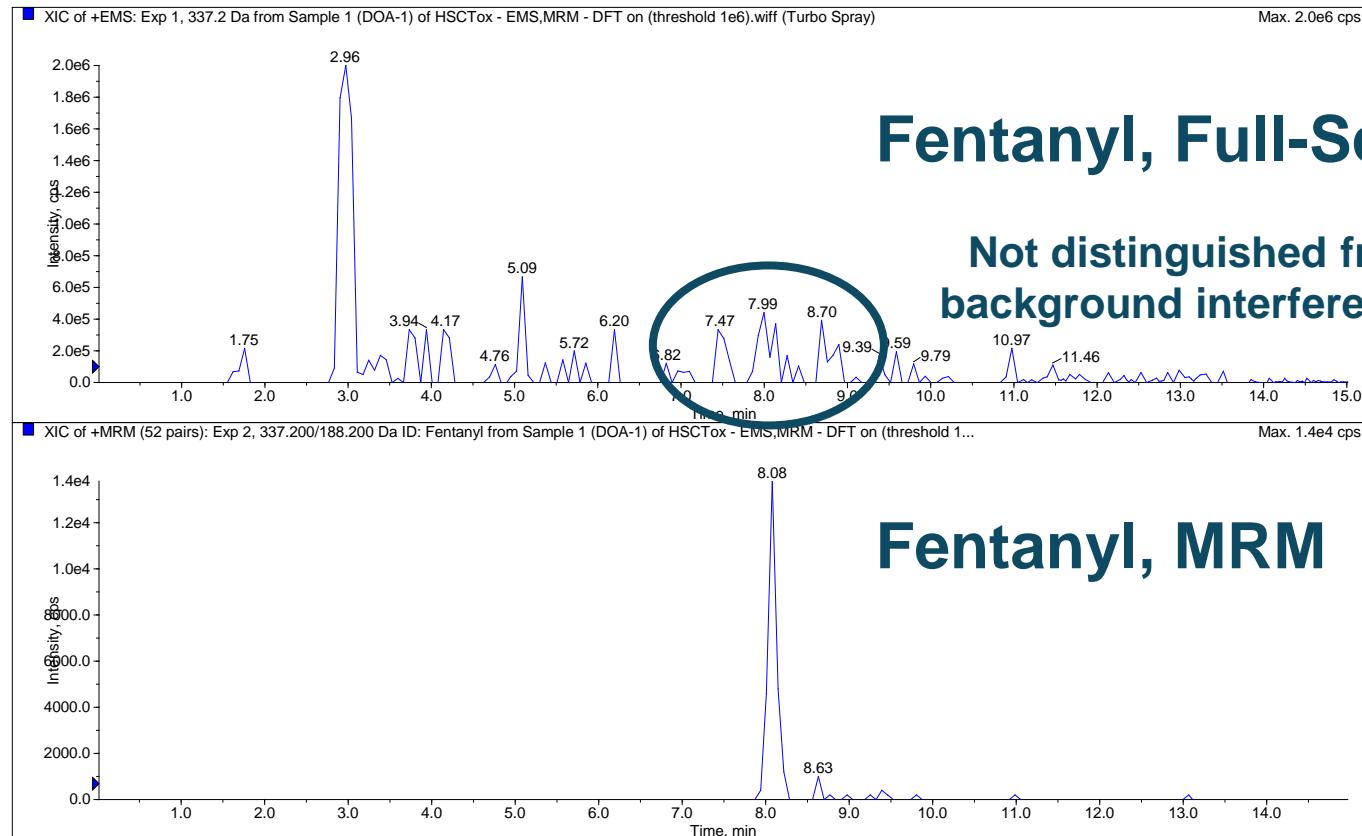
**Confirmation**

← Acquired spectrum

← Library spectrum of Oxazepam

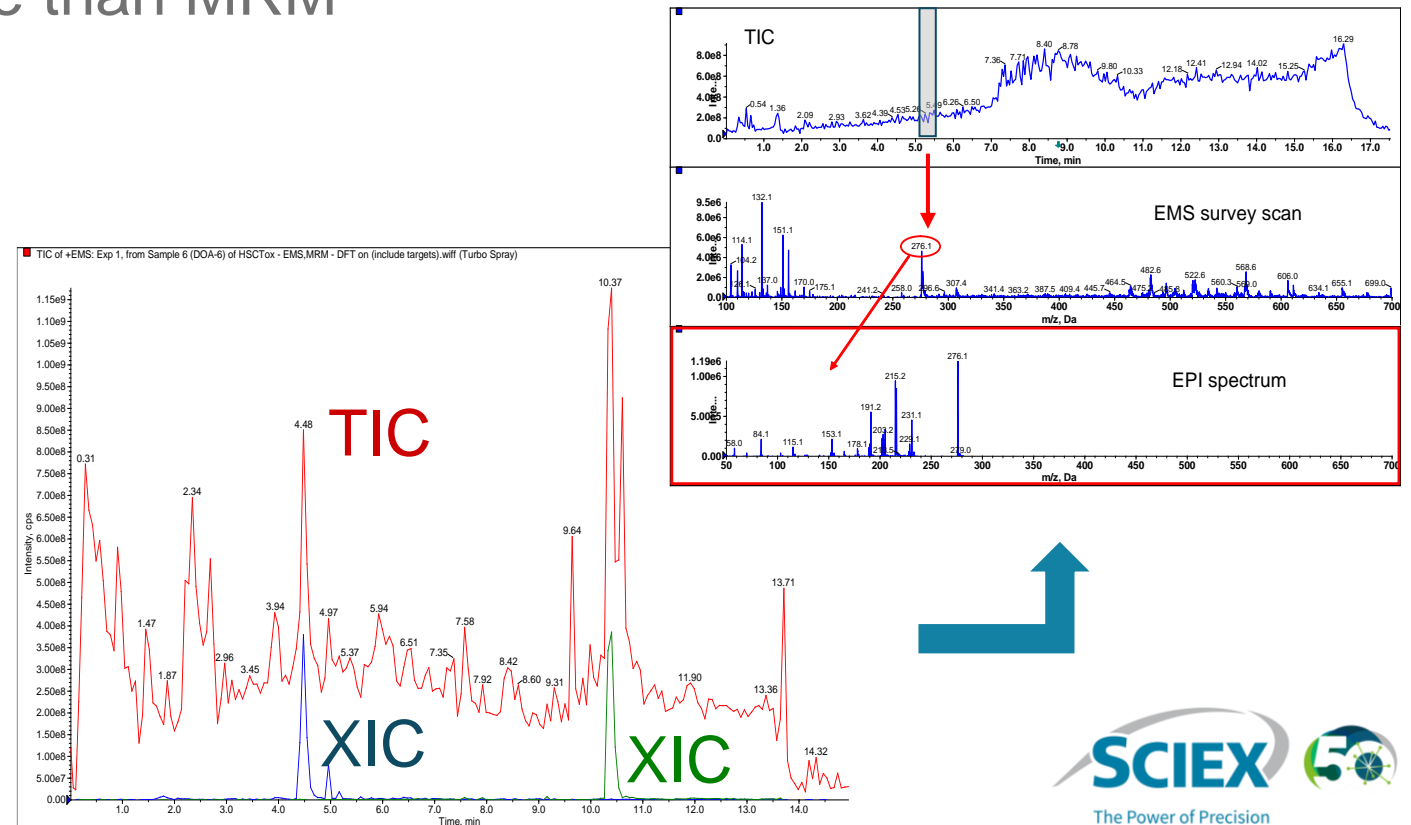
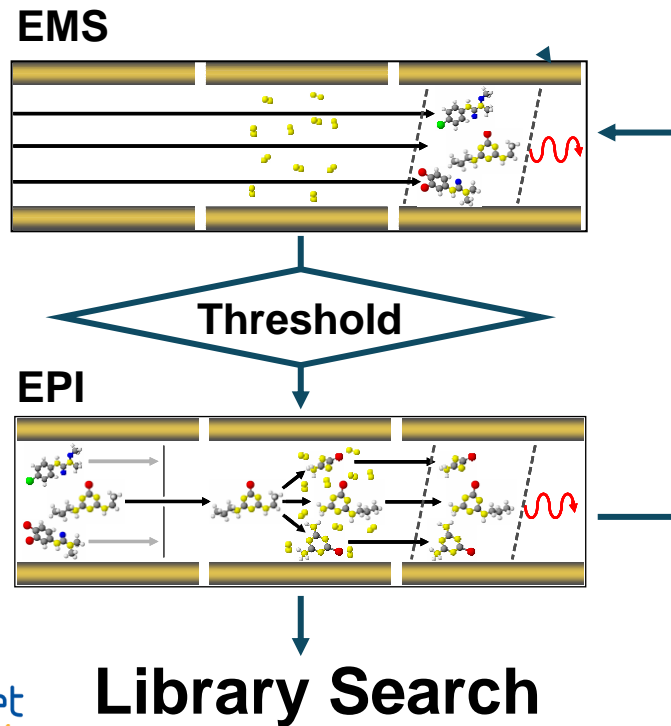
# Reminder: Tandem MS Provides Greater Selectivity

- Single-stage mass spectrometry cannot provide the *selectivity* and *specificity* required to distinguish analytes at low levels



# General Unknown Screening with EMS

- Full-scan EMS detection identifies all compounds and metabolites
- MS/MS library searching provides confirmation
- Data “mining” is laborious; automated software is very helpful
- Sensitivity and selectivity is worse than MRM



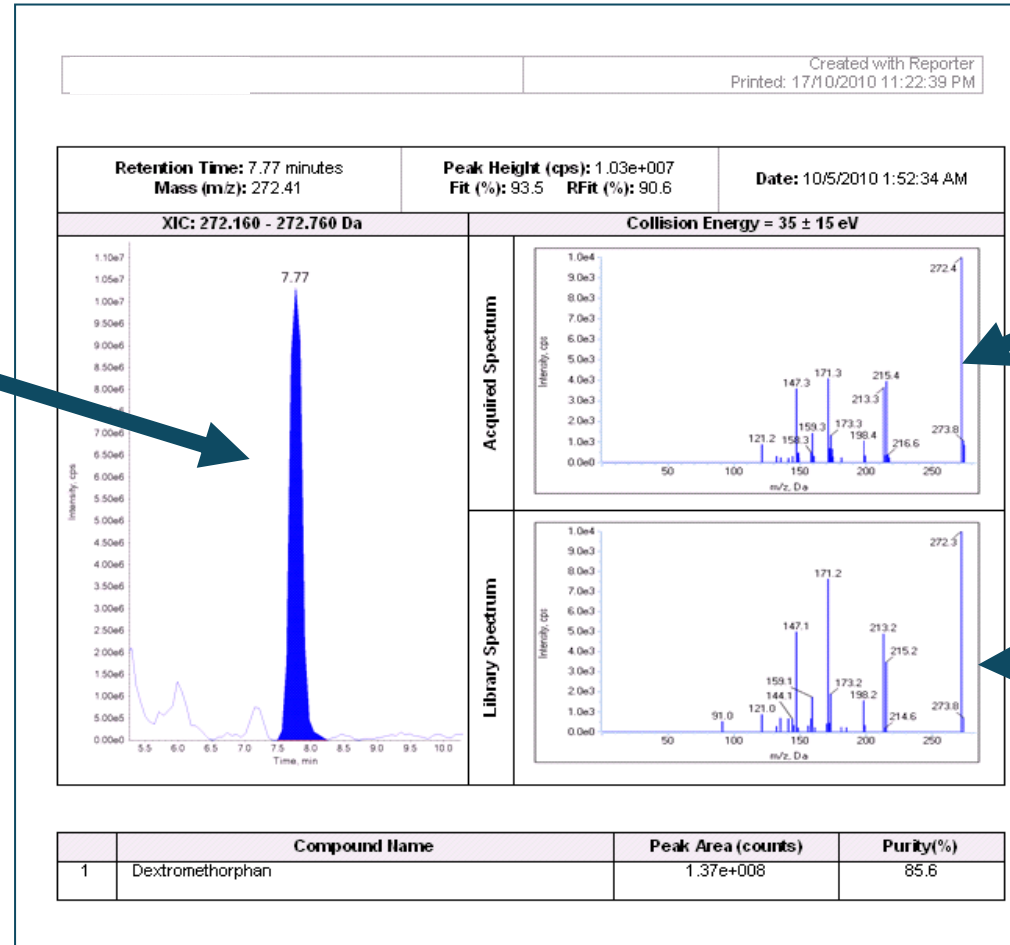


# General Unknown Screening + Confirmation on QTRAP®

- Survey Scan: EMS, Dependent Scan: EPI

## Detection

XIC of EMS peak  
(272.2-272.8)



## Confirmation

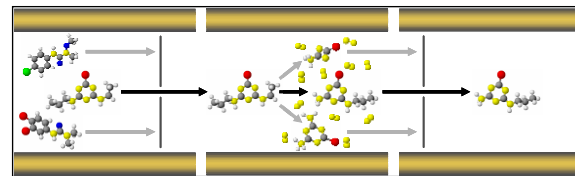
Acquired spectrum

Library spectrum:  
Dextromethorphan

# A New Approach: Combining Methodology

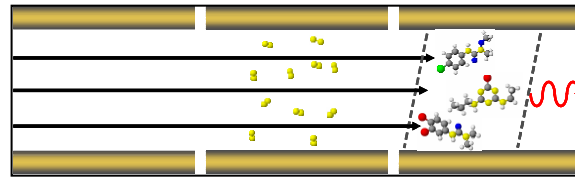
Why not combine “targeted” and “unknown” screening in a single method?

## Scheduled MRM™ Algorithm



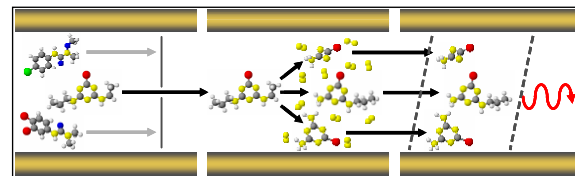
EMS

+



Threshold

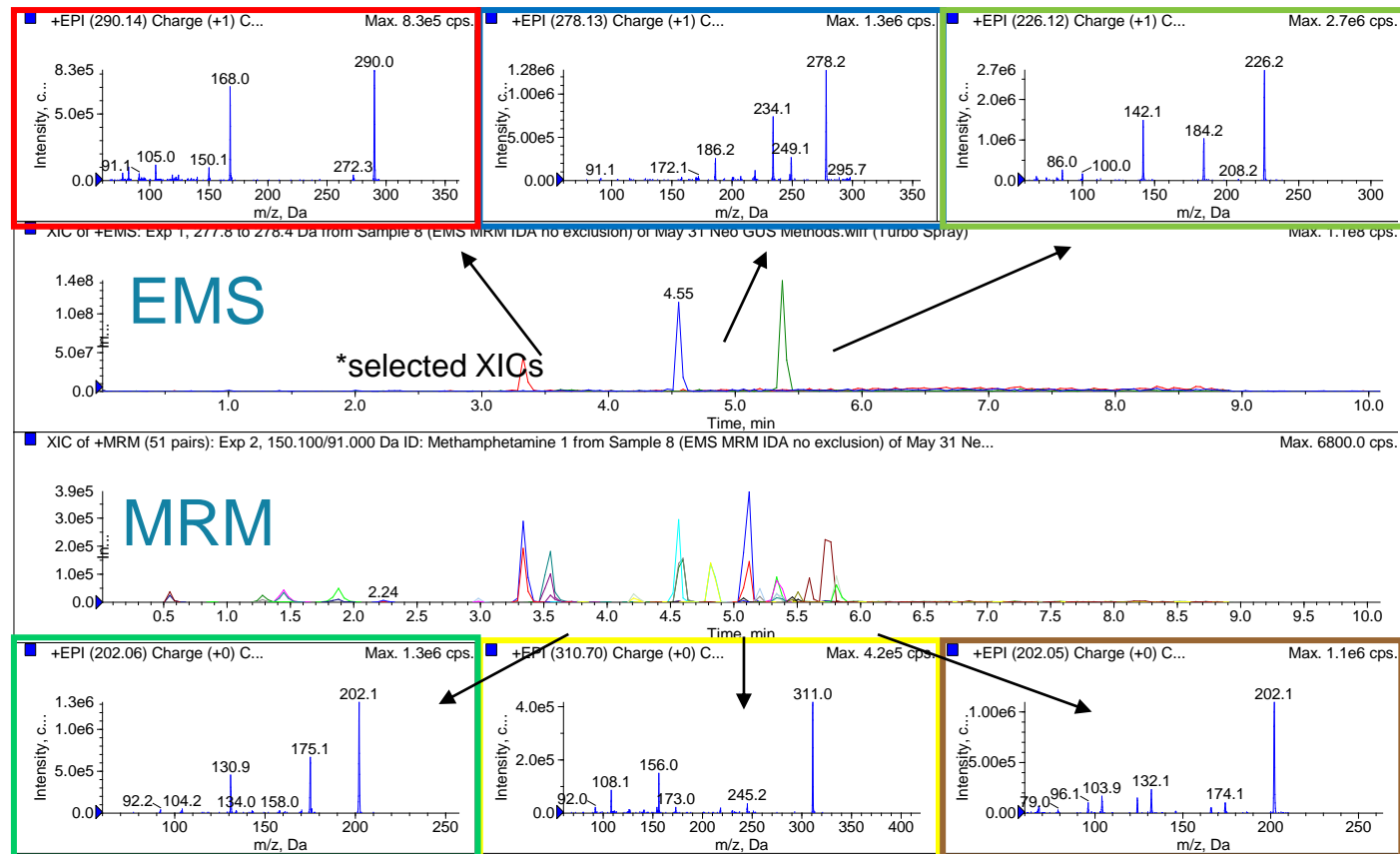
EPI



Library Search

# Targeted + Unknown Screening on a QTRAP<sup>®</sup> System

- EPI spectra are triggered from EMS and MRM survey scans
- EPI spectra are library-searched for confirmation of compound IDs



# Multi-target Screening vs. General Unknown Screening

- Multi-target screening (with MRM) cannot detect unknowns
- Multi-target screening (with MRM) offers the best sensitivity, and will detect low-abundance target compounds
- General Unknown Screening (with EMS) can detect all compounds and metabolites
- General Unknown Screening (with EMS) will not detect all of the low-abundance compounds

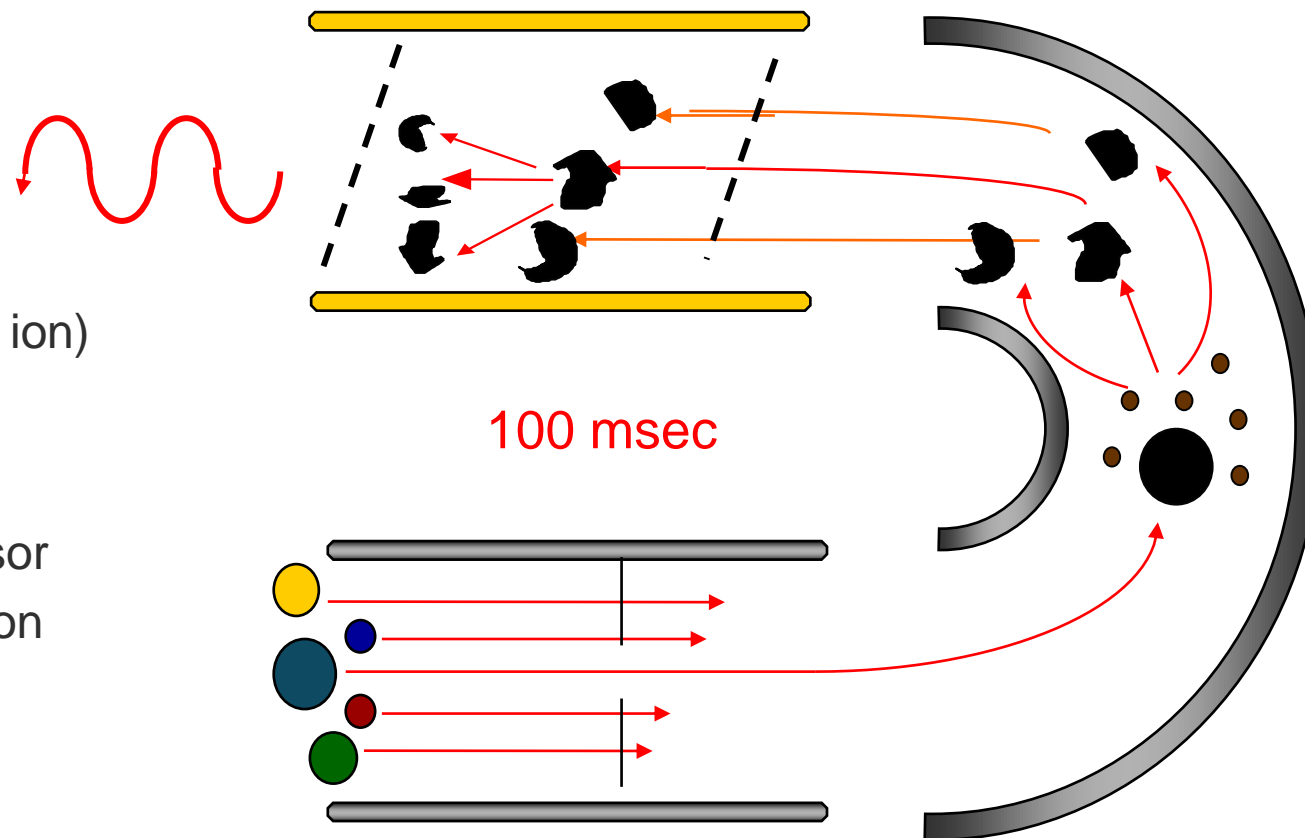
*MTS and GUS are truly complementary screening techniques.*

# MS/MS/MS with QTRAP MRM<sup>3</sup>



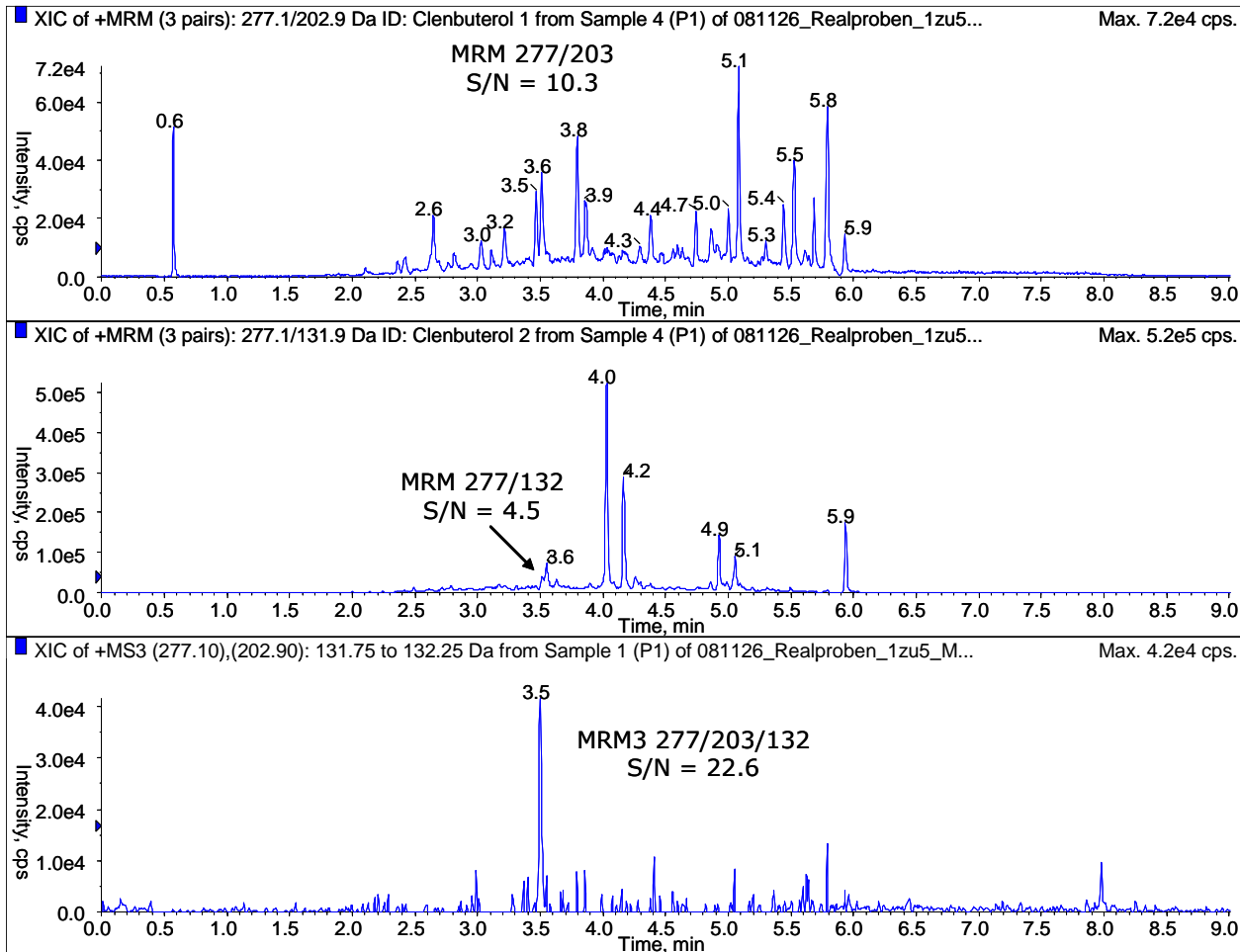
# MS/MS/MS - MRM3 added level of selectivity

- Q1:** **SIM** (selection of 1<sup>st</sup> precursor ion)
- Q2:** **Fragmentation**
- LIT (Q3):** **Trapping, isolation and fragmentation** of 2<sup>nd</sup> precursor ion by single frequency excitation





# MRM3 gives an added level of selectivity – increase sensitivity



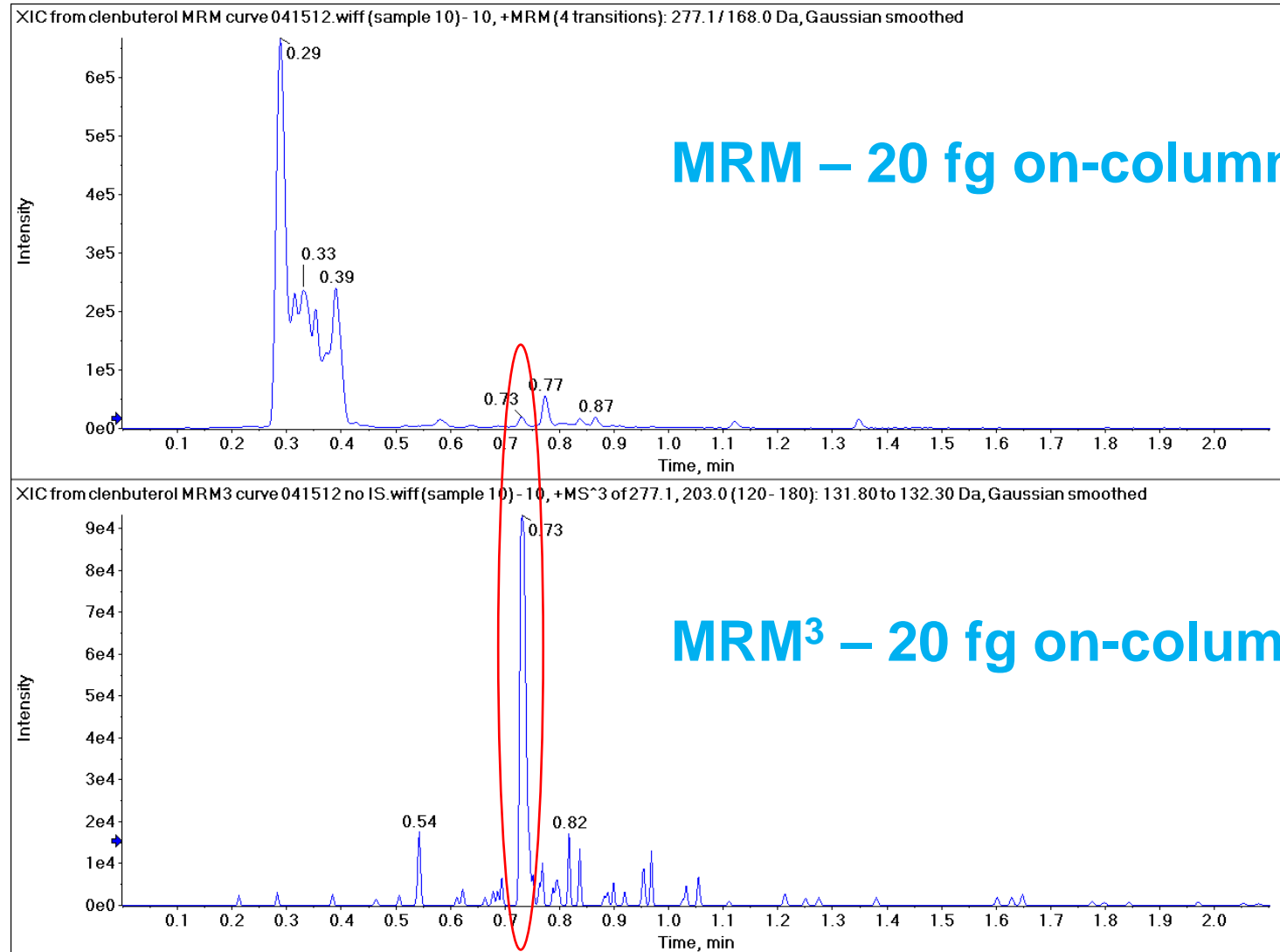
## Clenbuterol in urine:

← MRM transition 1:  
*Lots of peaks!*

← MRM transition 2:  
*Not very sensitive!*

← MRM<sup>3</sup>:  
*Well-resolved peak, matrix effects eliminated!*

# Clenbuterol in Urine – MRM<sup>3</sup>



# Conclusions

- Multi-target Screening (MRM-based) and General Unknown Screening (EMS-based) are truly complementary techniques:
  - MTS provides the ultimate sensitivity for detection of low-abundance compounds
  - GUS provides detection of unknowns
- The **QTRAP**<sup>®</sup> system allows rapid acquisition of **full-scan MS/MS** during MRM and EMS analysis, for additional confidence in IDs.
- The speed and versatility of the **QTRAP**<sup>®</sup> system allows users to **simultaneously detect** “target” and “unknown” compounds, by combining two survey scan-types in a single experiment.
- The collection of EMS “full-scan” spectra throughout acquisition allows the user to **re-interrogate the data** for additional “unknowns” at a later date.