Answers for Science.
Knowledge for Life.™

Sciex X500R a new Screening Platform for Food, Environmental & Forensic Analysis

Alexandre Paccou
Sr Manager, Support, EMEA

What's New?

SCIEX X500R QTOF System powered by SCIEX OS Software

SCIEX X500R QTOF system

SCIEX ExionLC™ AC system

SCIEX OS software

Outline

- 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® and Turbo pump access for fast and efficient maintenance, increasing system uptime.

Minimized footprint

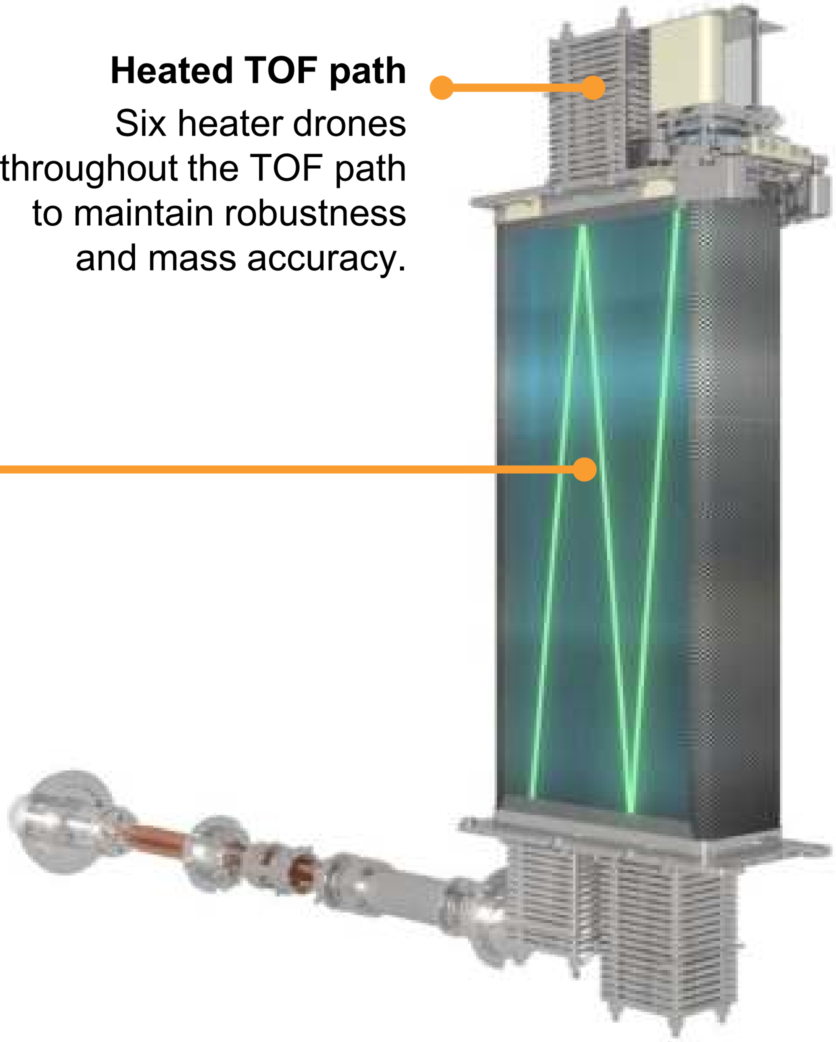
The benchtop stature (110 x 57 x 112 cm)* occupies less lab space than any other HRMS system on the market.

Integrated calibration

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

Introducing the SCIEX X500R QTOF System

Design Improvements and Details



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

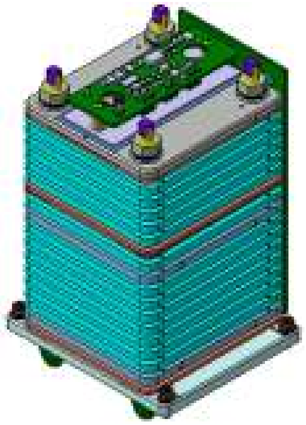
Design Improvements and Details

Dynamic Background Calibration
Use of background ions to maintain stable mass axis without calibrant.

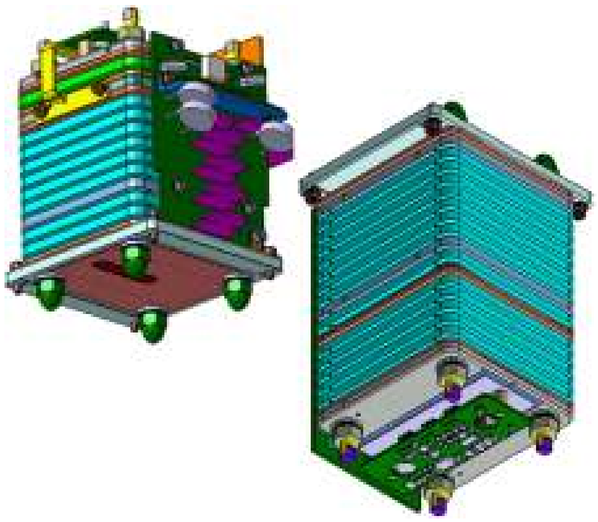
TwinSprayer

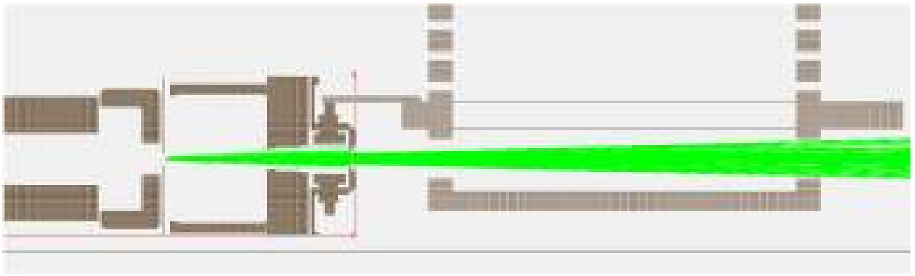
History 5

TOF Details



- Simplified ion transfer optics
- No slits… all ions go in (increased sensitivity)
- Focusing… high resolution without compromise in sensitivity
- Single pulse acceleration (6kV)
- 2 mirrors and direct thermal stabilization





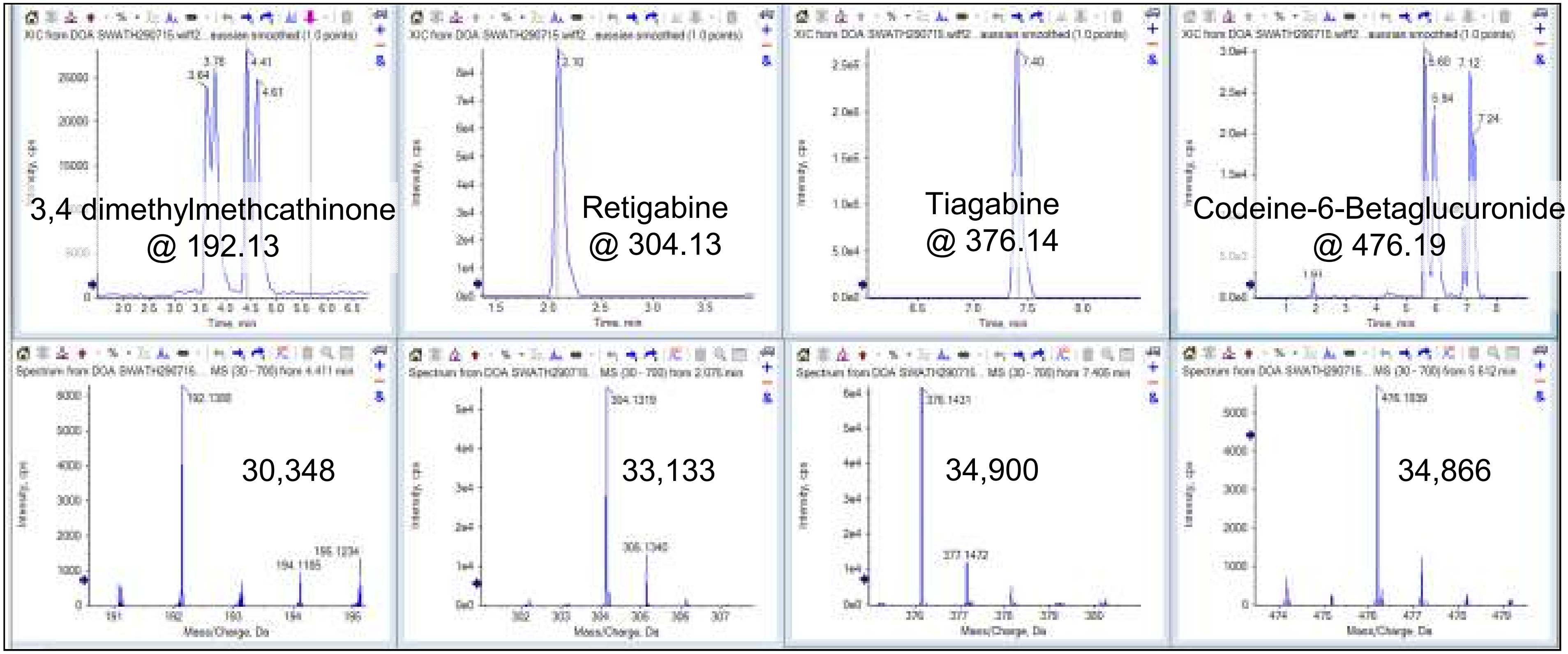
Perfect Balance to Elevate Your Lab's Performance

SCIEX X500R QTOF System

- The first robust, high performance high resolution MS/MS system designed for routine use.
  - Sensitivity to easily detect required drug cutoff concentration levels
  - Resolving power to remove interference from complex forensic matrices
  - Linearity to quantify up to 4 orders of magnitude
  - Identify compounds based on mass accuracy
  - Confident identification based MS/MS (IDA, MS/MS^{ALL} with SWATH™ Acquisition and ion ratios)
  - Industry leading robustness of Turbo V™ source and Curtain Gas™ interface

The SCIEX X500R QTOF System

Sensitivity and Resolution (20 ng/mL forensic drugs in urine, 10 μL injected)



3,4 dimethylmethcathinone
@ 192.13

Retigabine
@ 304.13

Tiagabine
@ 376.14

Codeine-6-Betaglucuronide
@ 476.19

30,348

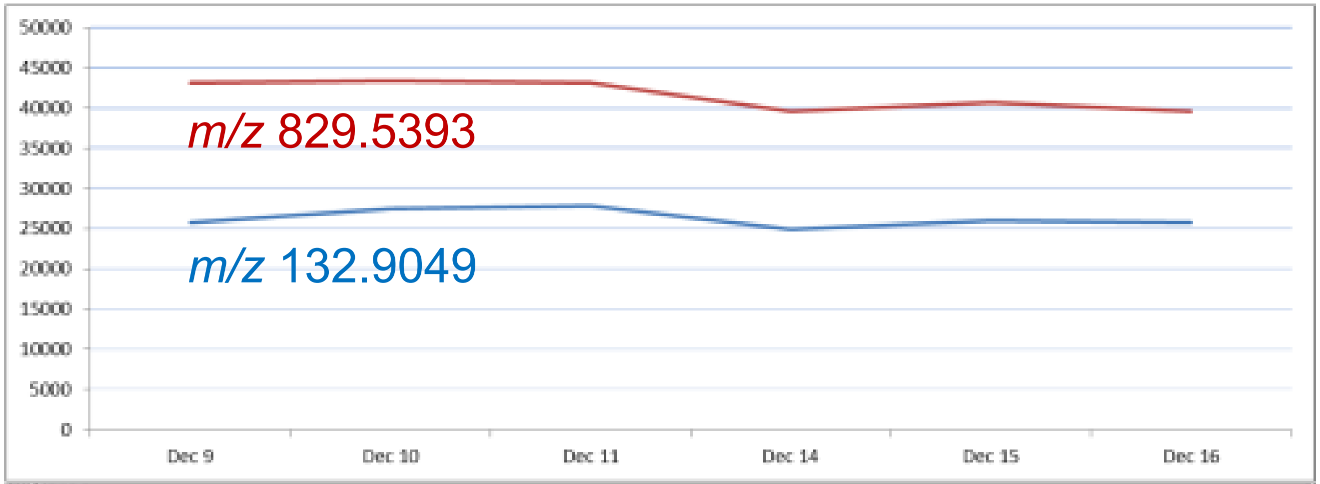
33,133

34,900

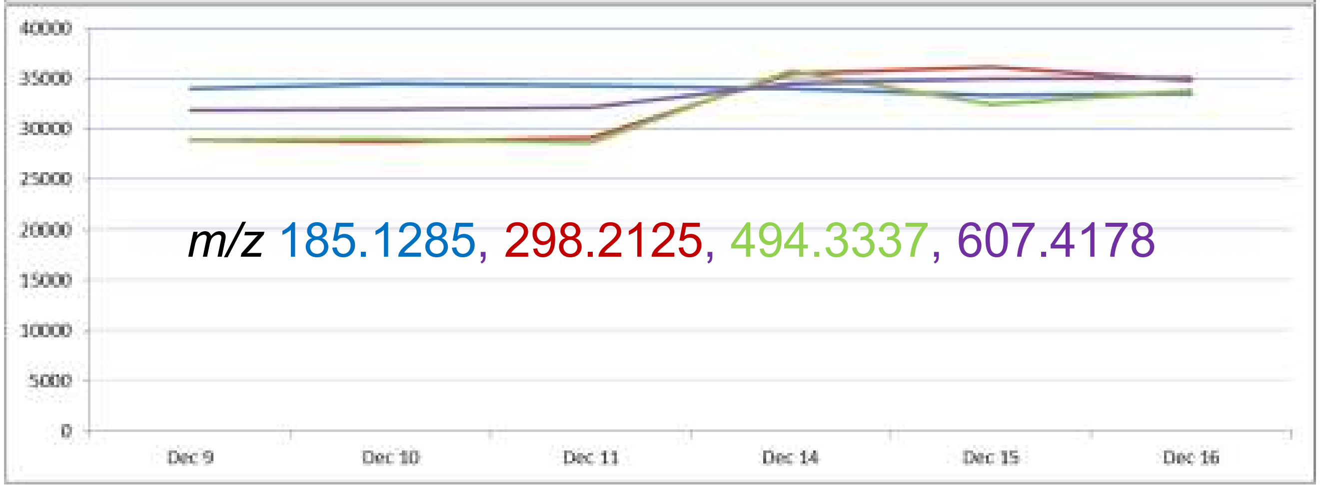
34,866

Resolution

Resolution from Dec 9 to Dec 16

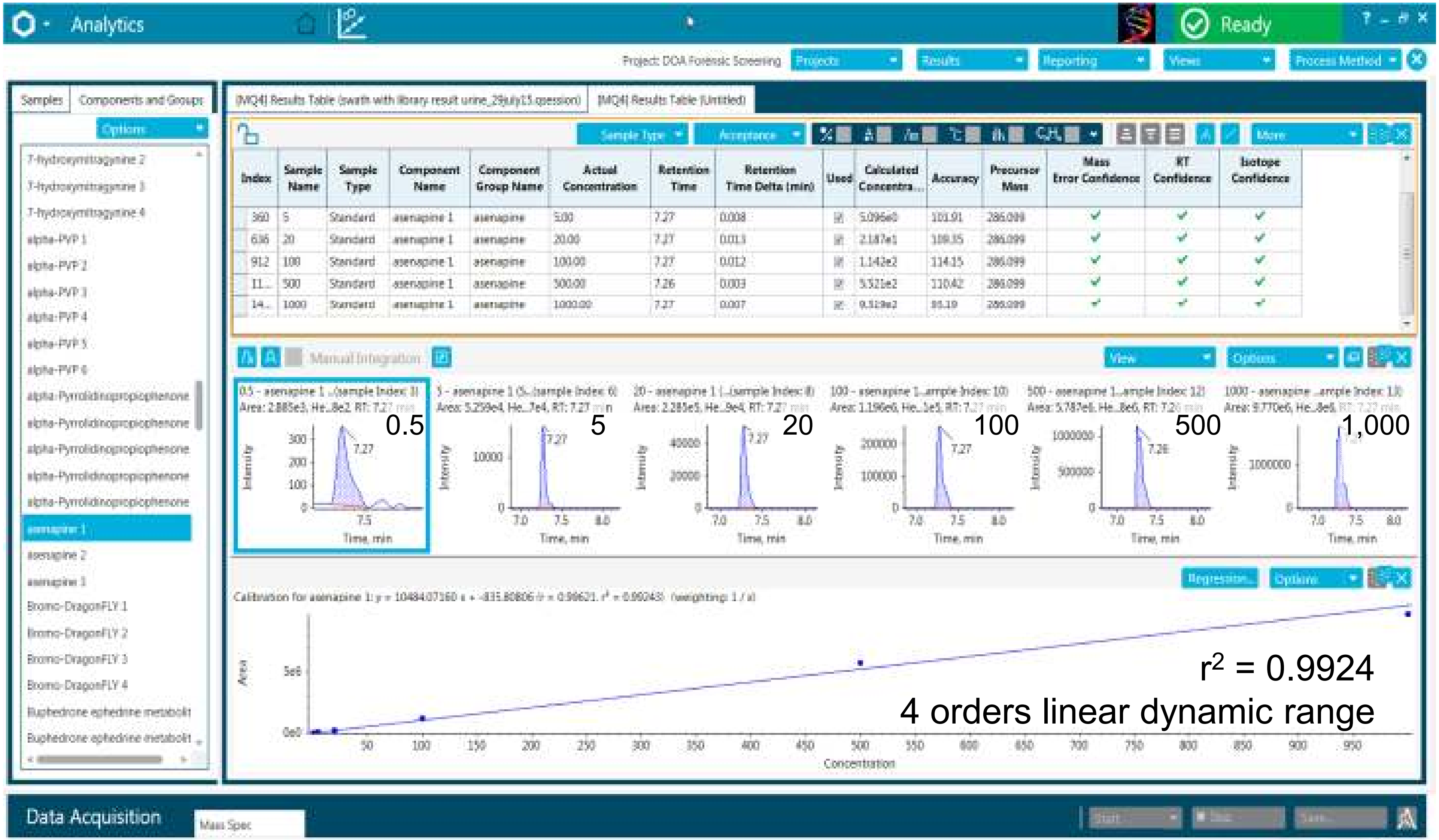


TOF-MS



TOF-MS/MS

The SCIEX X500R QTOF System – Linearity



Index	Sample Name	Sample Type	Component Name	Component Group Name	Actual Concentration	Retention Time	Retention Time Delta (min)	Used	Calculated Concentra...	Accuracy	Precursor Mass	Mass Error Confidence	RT Confidence	Isotope Confidence
360	5	Standard	asenapine 1	asenapine	5.00	7.27	0.008	☑	5.096e0	101.91	286.099	✓	✓	✓
636	20	Standard	asenapine 1	asenapine	20.00	7.27	0.013	☑	2.187e1	109.35	286.099	✓	✓	✓
912	100	Standard	asenapine 1	asenapine	100.00	7.27	0.012	☑	1.142e2	114.15	286.099	✓	✓	✓
11...	500	Standard	asenapine 1	asenapine	500.00	7.26	0.003	☑	5.521e2	110.42	286.099	✓	✓	✓
14...	1000	Standard	asenapine 1	asenapine	1000.00	7.27	0.007	☑	9.519e2	95.19	286.099	✓	✓	✓

0.5

5

20

100

500

1,000

Calibration for asenapine 1: y = 10484.07160 x + -835.80806 (r = 0.99621, r^2 = 0.99243) (weighting: 1 / x)

$r^2 = 0.9924$

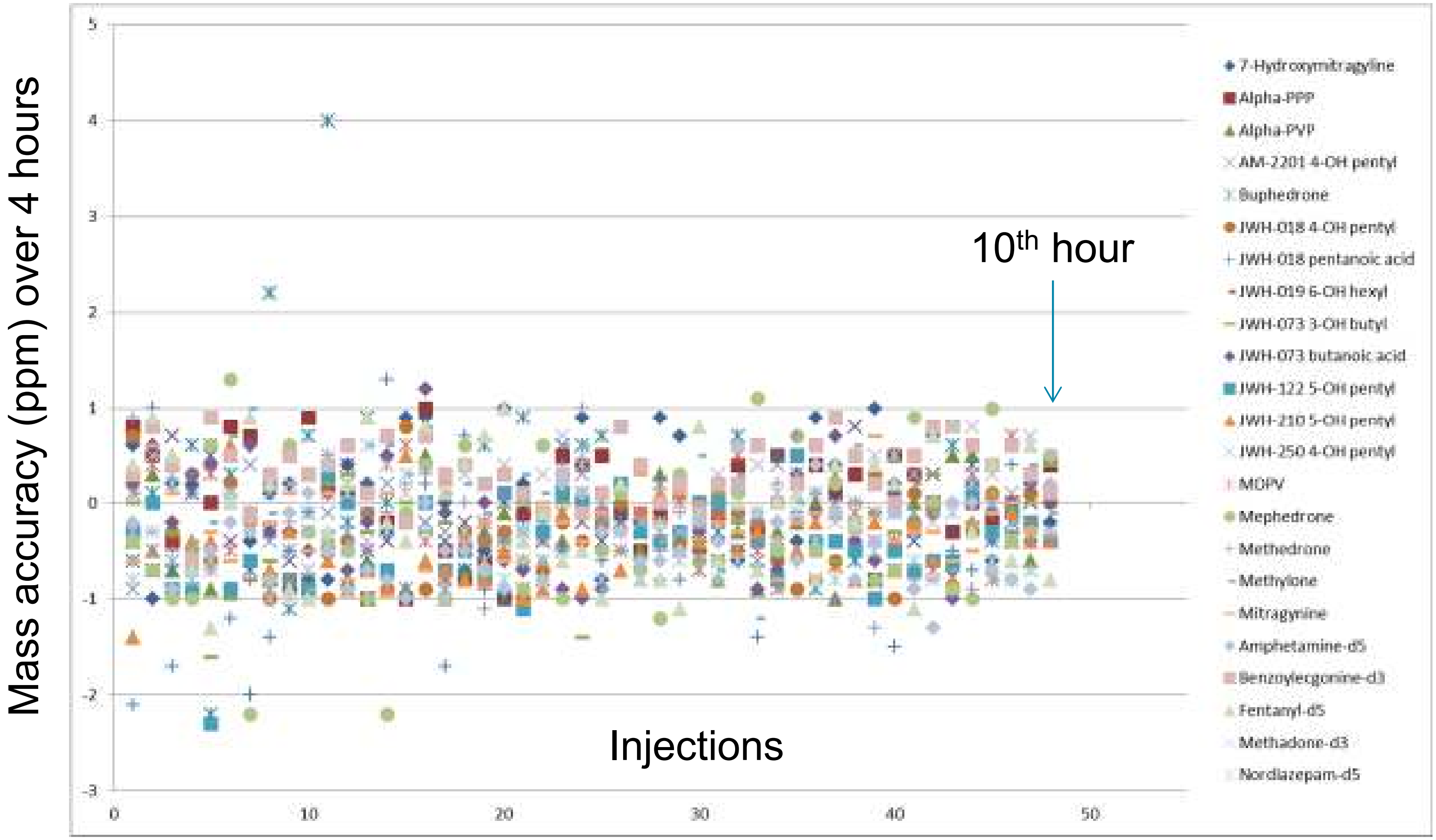
4 orders linear dynamic range

Linearity (Asenapine 0.5 to 1000 ng/mL)

RUO-MKT-11-3046-A

Mass Accuracy in urine samples without autocalibration

ppm in all injections over a 10-hour period (no calibration in between)

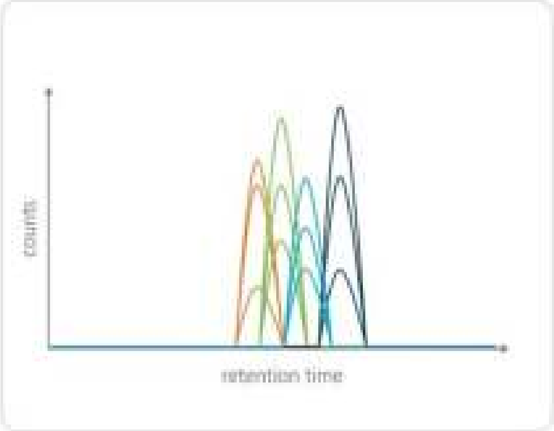


This is a plot for 6 urine samples with same analytes in different concentrations over a 10-hour period without any calibration.

MS/MS^{ALL} using SWATH® Acquisition

A Mode of Data Independent Acquisition Providing all MS/MS Spectra

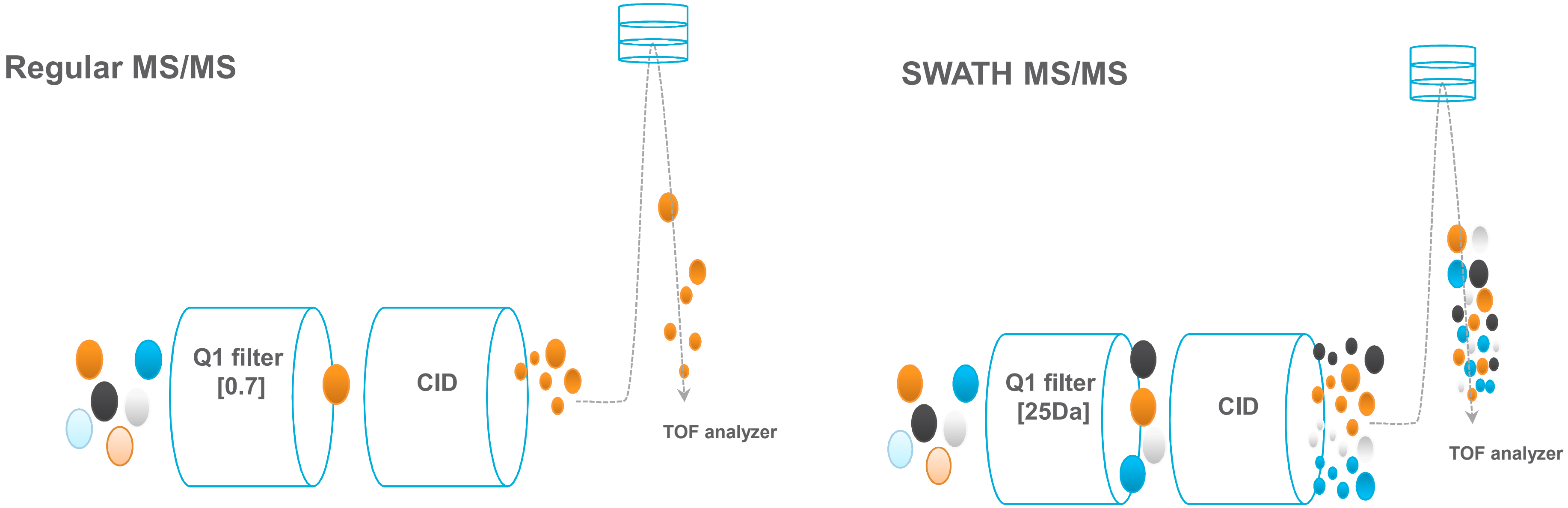
Wide Q1 Isolation Window is Stepped Across the Mass Range



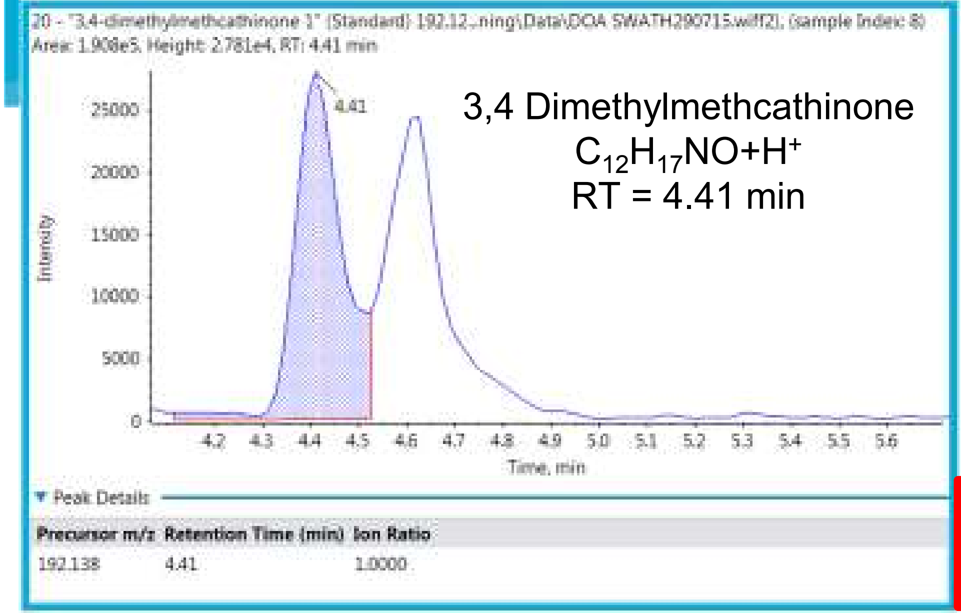
SWATH® acquisition can be used with variable Q1 isolation windows across the mass range

SWATH® Acquisition

- A mode of Data Independent Acquisition
- Provides MS/MS^{ALL}

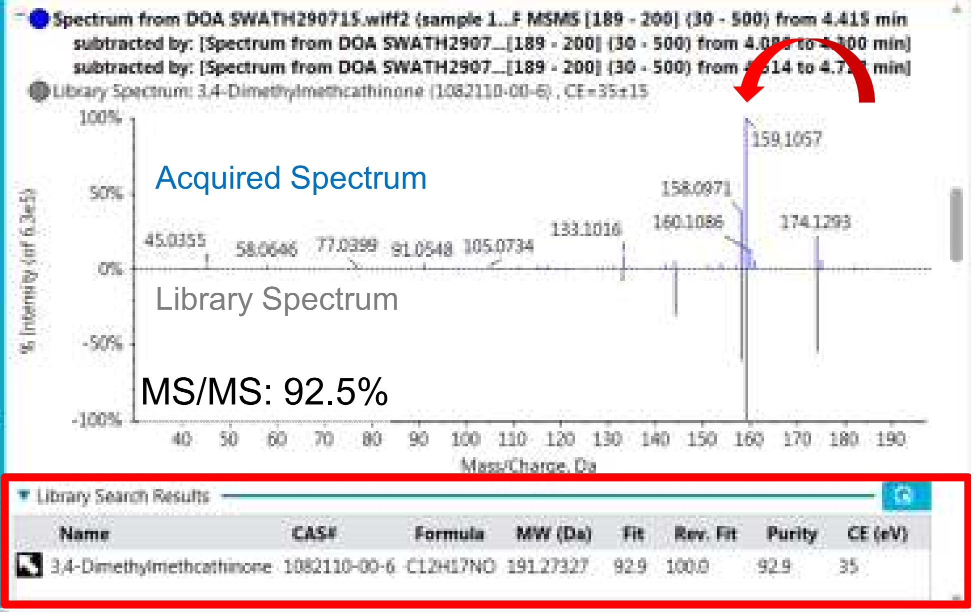


The SCIEX X500R QTOF System – SWATH® Acquisition


20 - "3,4-dimethylmethcathinone 1" (Standard) 192.12...ning\Data\DOA SWATH290715.wiff2), (sample Index: 8)
Area: 1.908e5, Height: 2.781e4, RT: 4.41 min

3,4 Dimethylmethcathinone
$C_{12}H_{17}NO+H^+$
RT = 4.41 min

Precursor m/z	Retention Time (min)	Ion Ratio
192.138	4.41	1.0000

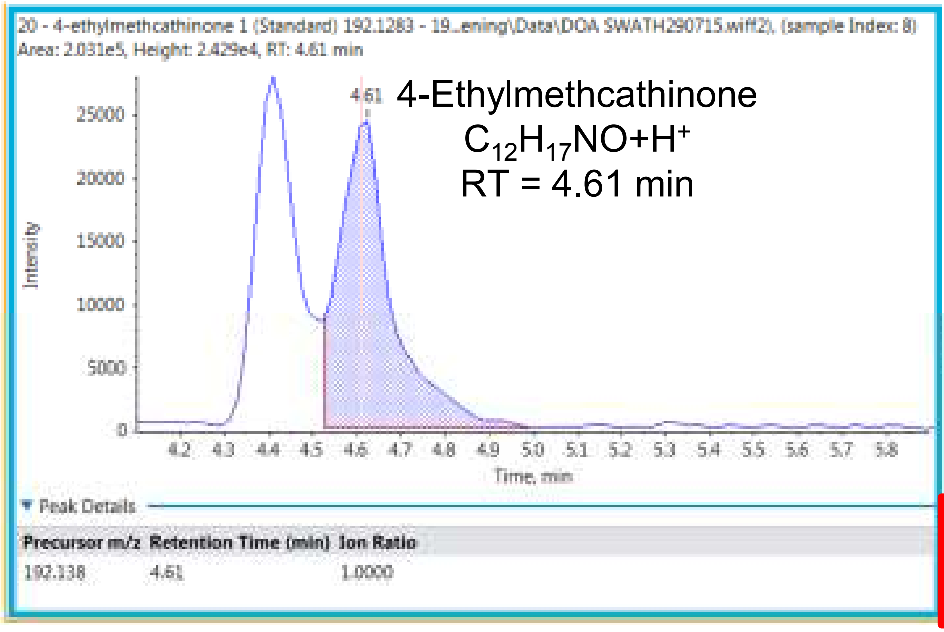

Spectrum from DOA SWATH290715.wiff2 (sample 1...F MSMS [189 - 200] (30 - 500) from 4.415 min
subtracted by: [Spectrum from DOA SWATH2907...[189 - 200] (30 - 500) from 4.0[illegible] to [illegible]00 min]
subtracted by: [Spectrum from DOA SWATH2907...[189 - 200] (30 - 500) from [illegible]14 to 4.7[illegible] min]
Library Spectrum: 3,4-Dimethylmethcathinone (1082110-00-6) , CE=35±15

Acquired Spectrum

Library Spectrum

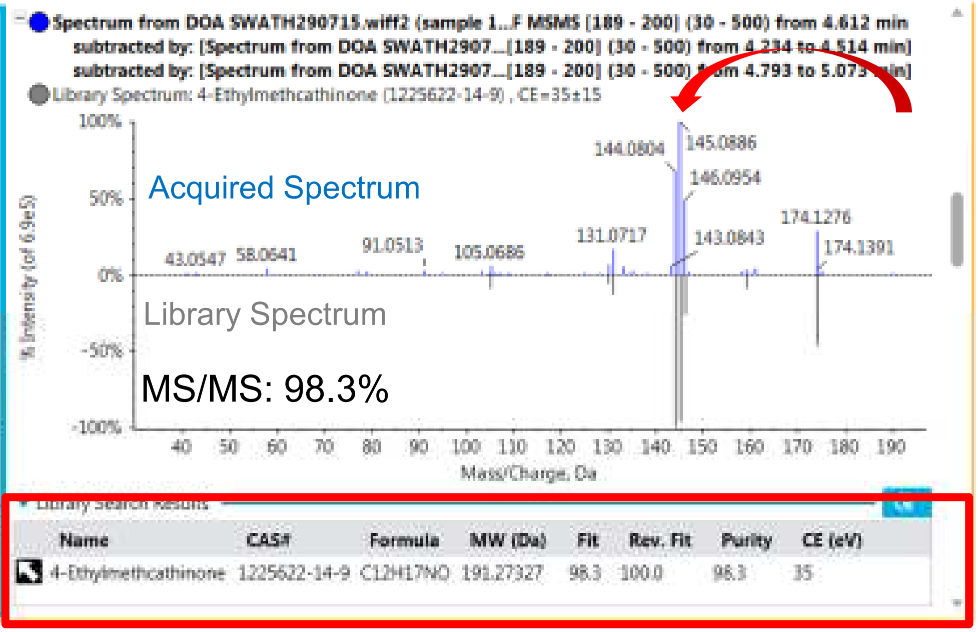
MS/MS: 92.5%

Name	CAS#	Formula	MW (Da)	Fit	Rev. Fit	Purity	CE (eV)
3,4-Dimethylmethcathinone	1082110-00-6	C12H17NO	191.27327	92.9	100.0	92.9	35


20 - 4-ethylmethcathinone 1 (Standard) 192.1283 - 19...ening\Data\DOA SWATH290715.wiff2), (sample Index: 8)
Area: 2.031e5, Height: 2.429e4, RT: 4.61 min

4-Ethylmethcathinone
$C_{12}H_{17}NO+H^+$
RT = 4.61 min

Precursor m/z	Retention Time (min)	Ion Ratio
192.138	4.61	1.0000


Spectrum from DOA SWATH290715.wiff2 (sample 1...F MSMS [189 - 200] (30 - 500) from 4.612 min
subtracted by: [Spectrum from DOA SWATH2907...[189 - 200] (30 - 500) from 4.234 to 4.514 min]
subtracted by: [Spectrum from DOA SWATH2907...[189 - 200] (30 - 500) from 4.793 to 5.073 min]
Library Spectrum: 4-Ethylmethcathinone (1225622-14-9) , CE=35±15

Acquired Spectrum

Library Spectrum

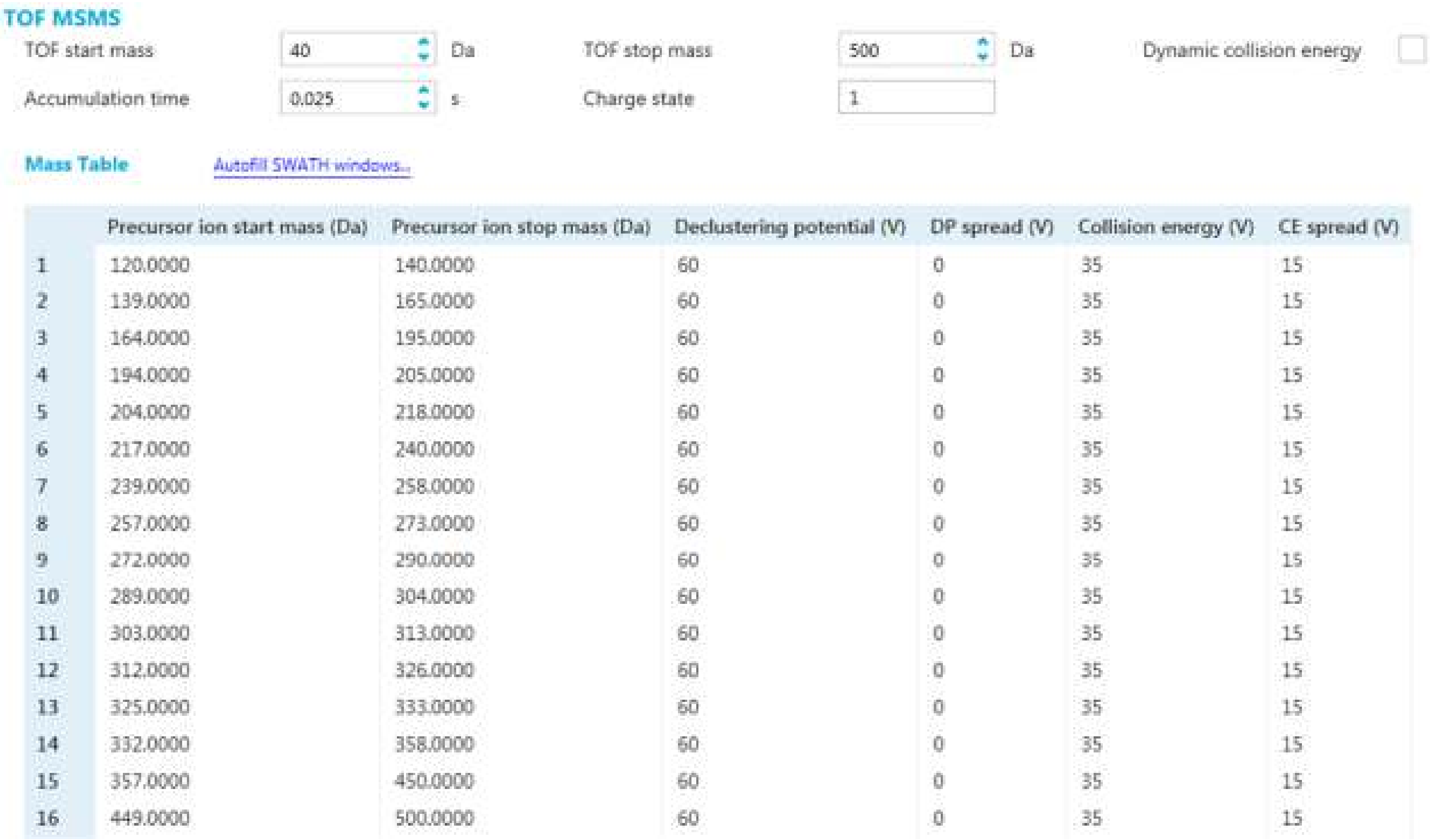
MS/MS: 98.3%

Name	CAS#	Formula	MW (Da)	Fit	Rev. Fit	Purity	CE (eV)
4-Ethylmethcathinone	1225622-14-9	C12H17NO	191.27327	98.3	100.0	98.3	35

Confident Identification of Isomers using MS/MS

Acquisition method

SWATH with variable windows, 8 min



TOF MSMS

TOF start mass: 40 Da

TOF stop mass: 500 Da

Dynamic collision energy ☐

Accumulation time: 0.025 s

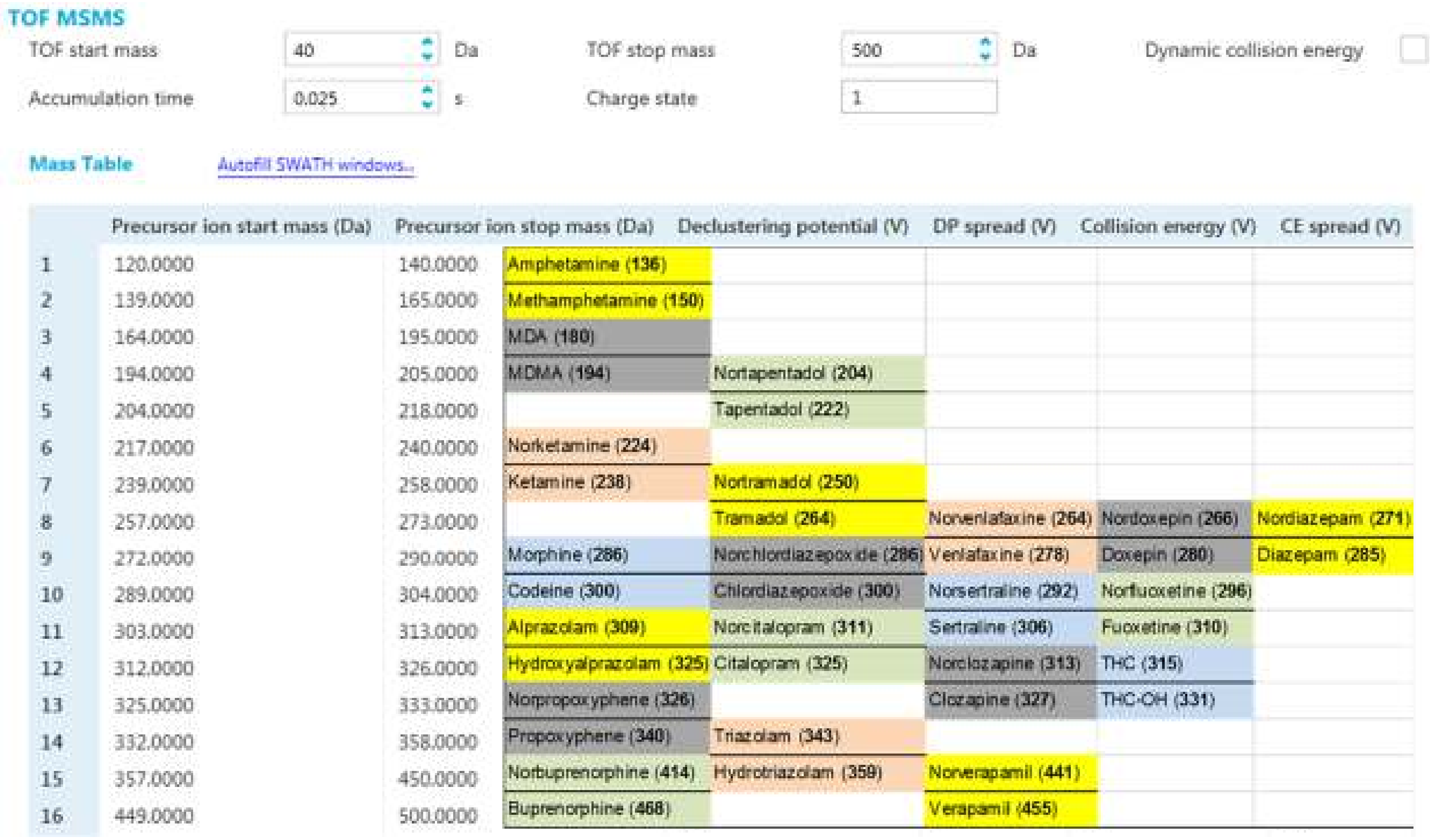
Charge state: 1

Mass Table

	Precursor ion start mass (Da)	Precursor ion stop mass (Da)	Declustering potential (V)	DP spread (V)	Collision energy (V)	CE spread (V)
1	120.0000	140.0000	60	0	35	15
2	139.0000	165.0000	60	0	35	15
3	164.0000	195.0000	60	0	35	15
4	194.0000	205.0000	60	0	35	15
5	204.0000	218.0000	60	0	35	15
6	217.0000	240.0000	60	0	35	15
7	239.0000	258.0000	60	0	35	15
8	257.0000	273.0000	60	0	35	15
9	272.0000	290.0000	60	0	35	15
10	289.0000	304.0000	60	0	35	15
11	303.0000	313.0000	60	0	35	15
12	312.0000	326.0000	60	0	35	15
13	325.0000	333.0000	60	0	35	15
14	332.0000	358.0000	60	0	35	15
15	357.0000	450.0000	60	0	35	15
16	449.0000	500.0000	60	0	35	15

Acquisition method

SWATH with variable windows, 8 min



TOF MSMS

TOF start mass: 40 Da
TOF stop mass: 500 Da
Dynamic collision energy ☐
Accumulation time: 0.025 s
Charge state: 1

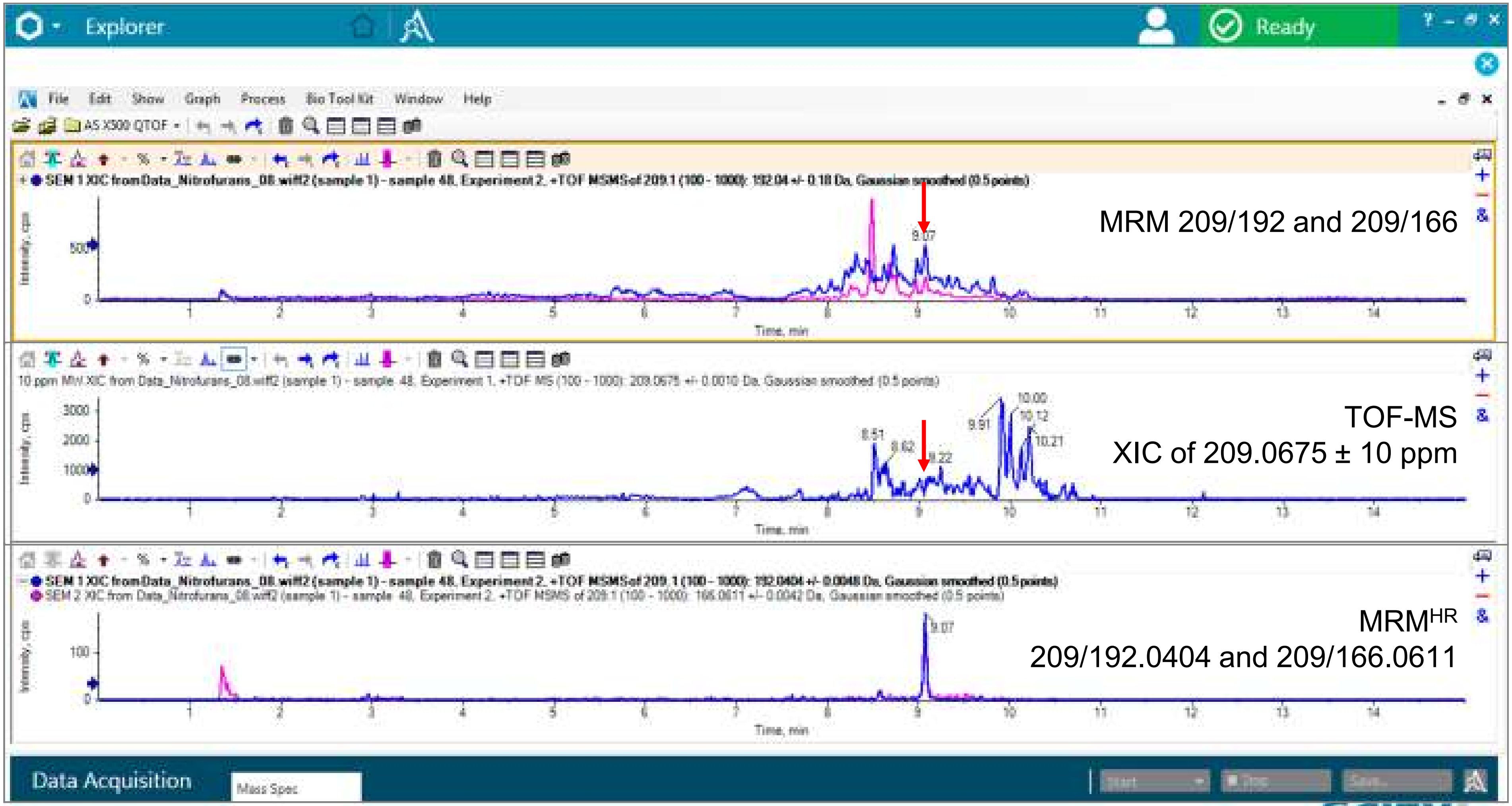
Mass Table

	Precursor ion start mass (Da)	Precursor ion stop mass (Da)		Declustering potential (V)	DP spread (V)	Collision energy (V)	CE spread (V)
1	120.0000	140.0000	Amphetamine (136)				
2	139.0000	165.0000	Methamphetamine (150)				
3	164.0000	195.0000	MDA (180)				
4	194.0000	205.0000	MDMA (194)	Nortapentadol (204)			
5	204.0000	218.0000		Tapentadol (222)			
6	217.0000	240.0000	Norketamine (224)				
7	239.0000	258.0000	Ketamine (238)	Nortramadol (250)			
8	257.0000	273.0000		Tramadol (264)	Norvenlafaxine (264)	Nordoxepin (266)	Nordiazepam (271)
9	272.0000	290.0000	Morphine (286)	Norchlordiazepoxide (286)	Venlafaxine (278)	Doxepin (280)	Diazepam (285)
10	289.0000	304.0000	Codeine (300)	Chlordiazepoxide (300)	Norsertraline (292)	Norfluoxetine (296)	
11	303.0000	313.0000	Alprazolam (309)	Norcitalopram (311)	Sertraline (306)	Fluoxetine (310)	
12	312.0000	326.0000	Hydroxyalprazolam (325)	Citalopram (325)	Norclozapine (313)	THC (315)	
13	325.0000	333.0000	Norpropoxyphene (326)		Clozapine (327)	THC-OH (331)	
14	332.0000	358.0000	Propoxyphene (340)	Triazolam (343)			
15	357.0000	450.0000	Norbuprenorphine (414)	Hydrotriazolam (359)	Norverapamil (441)		
16	449.0000	500.0000	Buprenorphine (468)		Verapamil (455)		

The SCIEX X500R QTOF System – MRM^{HR}

Increased selectivity with MRM^{HR}: Avoiding false negatives

Feed Sample Tested Positive for NP-Semicarbazide



SEM 1 XIC from Data_Nitrofurans_08.wiff2 (sample 1) - sample 48, Experiment 2, +TOF MSMS of 209.1 (100 - 1000): 192.04 +/- 0.10 Da, Gaussian smoothed (0.5 points)

MRM 209/192 and 209/166

10 ppm MW XIC from Data_Nitrofurans_08.wiff2 (sample 1) - sample 48, Experiment 1, +TOF MS (100 - 1000): 209.0675 +/- 0.0010 Da, Gaussian smoothed (0.5 points)

TOF-MS

XIC of 209.0675 ± 10 ppm

SEM 1 XIC from Data_Nitrofurans_08.wiff2 (sample 1) - sample 48, Experiment 2, +TOF MSMS of 209.1 (100 - 1000): 192.0404 +/- 0.0048 Da, Gaussian smoothed (0.5 points)

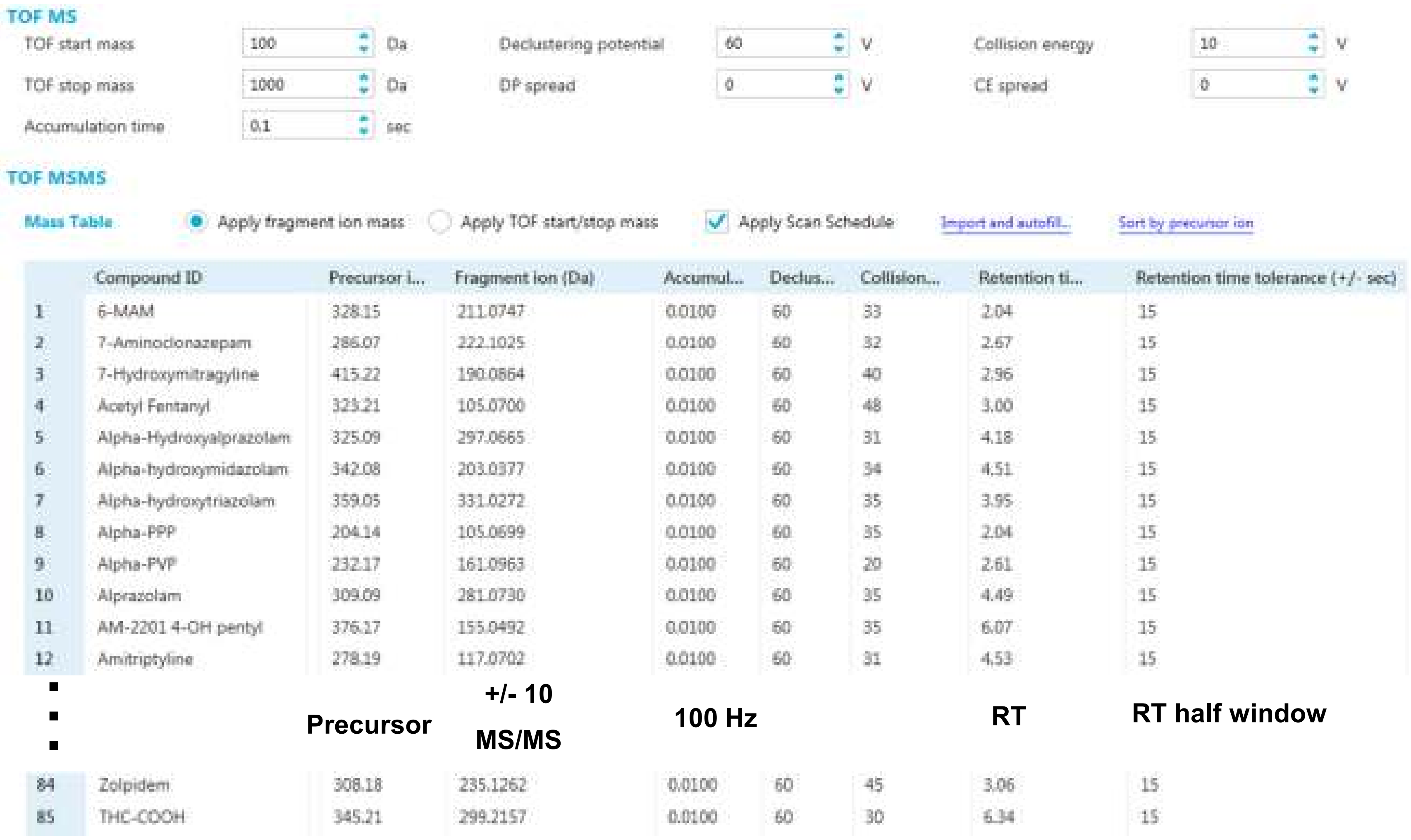
SEM 2 XIC from Data_Nitrofurans_08.wiff2 (sample 1) - sample 48, Experiment 2, +TOF MSMS of 209.1 (100 - 1000): 166.0611 +/- 0.0042 Da, Gaussian smoothed (0.5 points)

MRM^{HR}

209/192.0404 and 209/166.0611

Acquisition method

Scheduled MRM^{HR}, 8 min, Fragment±10 *m/z*



TOF MS

TOF start mass	100 Da	Declustering potential	60 V	Collision energy	10 V
TOF stop mass	1000 Da	DP spread	0 V	CE spread	0 V
Accumulation time	0.1 sec				

TOF MSMS

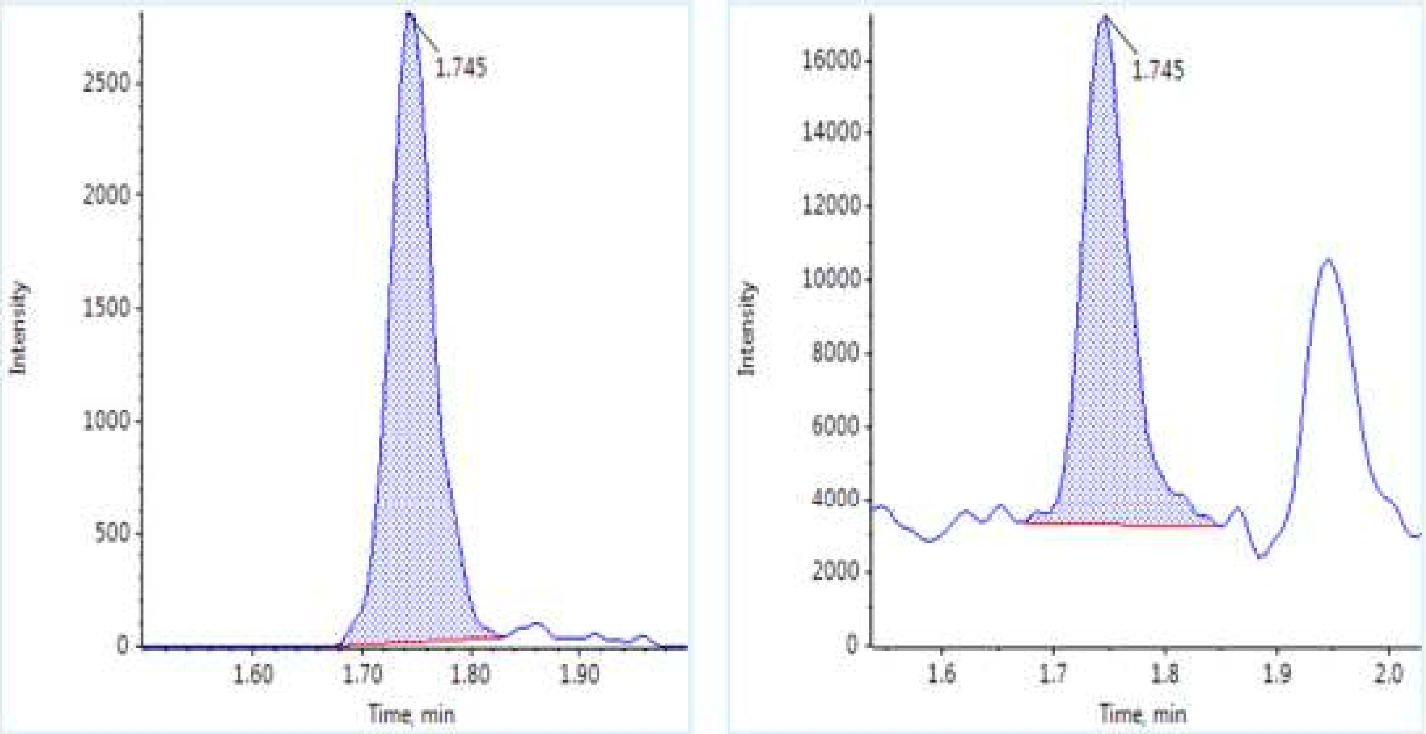
Mass Table ● Apply fragment ion mass ○ Apply TOF start/stop mass ☑ Apply Scan Schedule

	Compound ID	Precursor i...	Fragment ion (Da)	Accumul...	Declus...	Collision...	Retention ti...	Retention time tolerance (+/- sec)
1	6-MAM	328.15	211.0747	0.0100	60	33	2.04	15
2	7-Aminoclonazepam	286.07	222.1025	0.0100	60	32	2.67	15
3	7-Hydroxymitragyline	415.22	190.0864	0.0100	60	40	2.96	15
4	Acetyl Fentanyl	323.21	105.0700	0.0100	60	48	3.00	15
5	Alpha-Hydroxyalprazolam	325.09	297.0665	0.0100	60	31	4.18	15
6	Alpha-hydroxymidazolam	342.08	203.0377	0.0100	60	34	4.51	15
7	Alpha-hydroxytriazolam	359.05	331.0272	0.0100	60	35	3.95	15
8	Alpha-PPP	204.14	105.0699	0.0100	60	35	2.04	15
9	Alpha-PVP	232.17	161.0963	0.0100	60	20	2.61	15
10	Alprazolam	309.09	281.0730	0.0100	60	35	4.49	15
11	AM-2201 4-OH pentyl	376.17	155.0492	0.0100	60	35	6.07	15
12	Amitriptyline	278.19	117.0702	0.0100	60	31	4.53	15
⋮		**Precursor**	**+/- 10 MS/MS**	**100 Hz**			**RT**	**RT half window**
84	Zolpidem	308.18	235.1262	0.0100	60	45	3.06	15
85	THC-COOH	345.21	299.2157	0.0100	60	30	6.34	15

The SCIEX X500R QTOF System – MRM^{HR}

Scheduled MRM^{HR} (vs TOF scan)

Buphedrone (5 ng/mL in urine, 10-fold dilution, 10 μL injection)

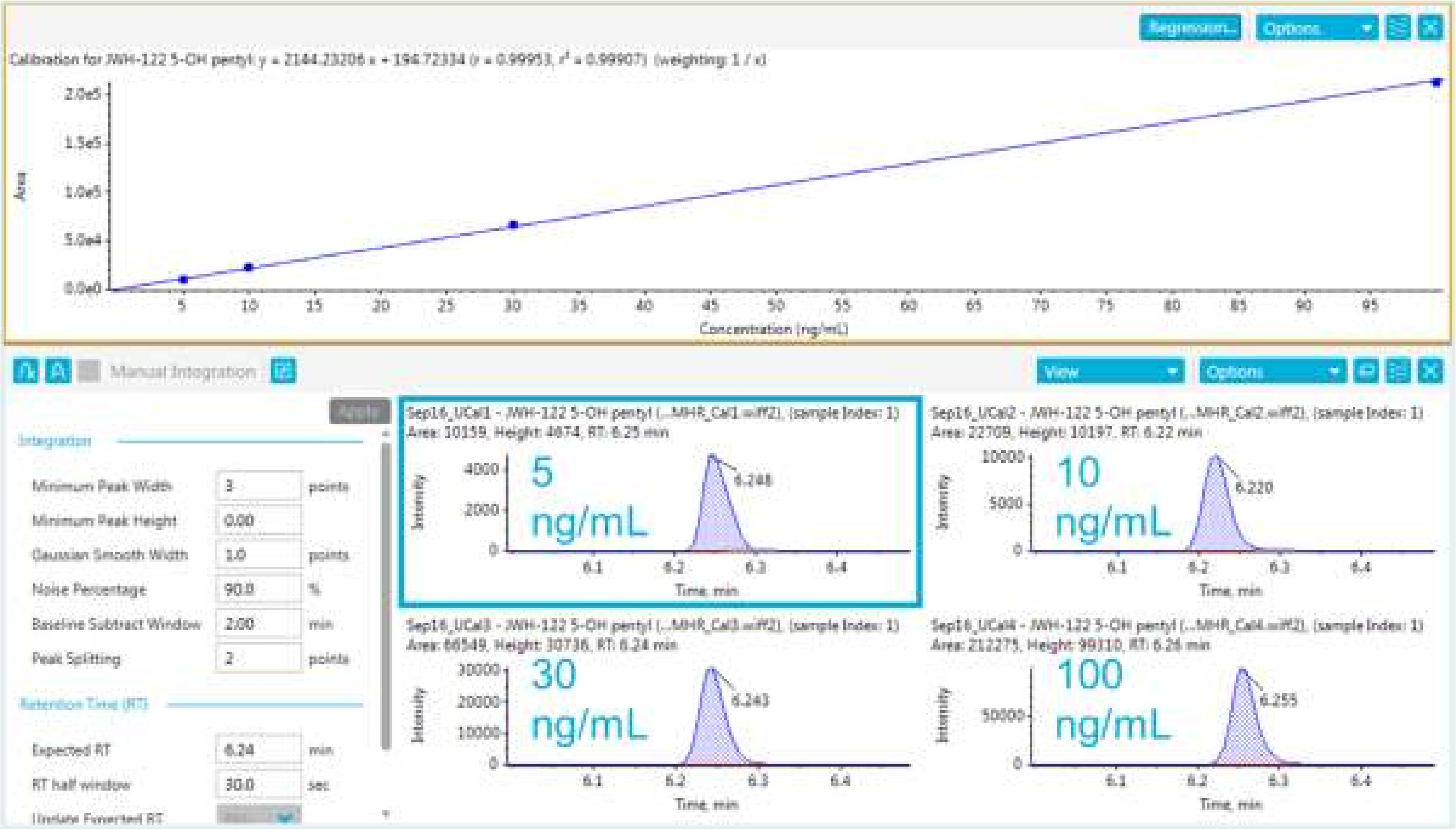


MRM^{HR}: 178.1→131.070±0.01 *m/z*

TOF-MS: 178.1226±0.005 *m/z*

The SCIEX X500R QTOF System – MRM^{HR}

Scheduled MRM^{HR}, 372.2→169.0644±0.0100 *m/z*



Calibration for JWH-122 5-OH pentyl: y = 2144.23206 x + 194.72334 (r = 0.99953, r^2 = 0.99907) (weighting: 1 / x)

Integration

Minimum Peak Width	3	points
Minimum Peak Height	0.00	
Gaussian Smooth Width	1.0	points
Noise Percentage	90.0	%
Baseline Subtract Window	2.00	min
Peak Splitting	2	points

Retention Time (RT)

Expected RT	6.24	min
RT half window	30.0	sec
Update Expected RT		

Sep16_UCal1 - JWH-122 5-OH pentyl (...MHR_Cal1.wiff2), (sample Index: 1)
Area: 10159, Height: 4674, RT: 6.25 min

Sep16_UCal2 - JWH-122 5-OH pentyl (...MHR_Cal2.wiff2), (sample Index: 1)
Area: 22709, Height: 10197, RT: 6.22 min

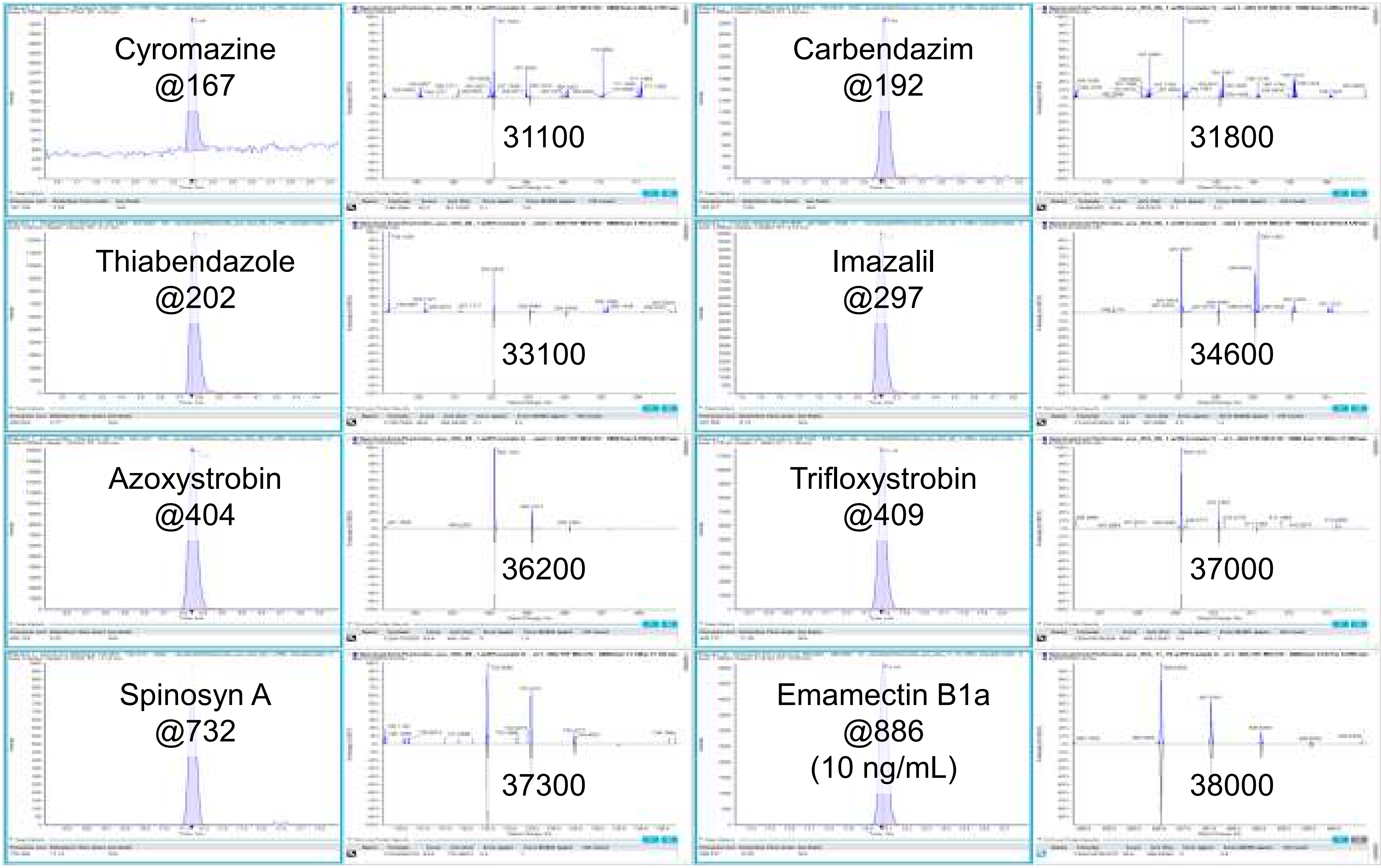
Sep16_UCal3 - JWH-122 5-OH pentyl (...MHR_Cal3.wiff2), (sample Index: 1)
Area: 66549, Height: 30736, RT: 6.24 min

Sep16_UCal4 - JWH-122 5-OH pentyl (...MHR_Cal4.wiff2), (sample Index: 1)
Area: 212275, Height: 99310, RT: 6.26 min

JWH-122 5-OH pentyl in urine (Urine was diluted 10-fold, 10 µL injection)

The SCIEX X500R QTOF System – Performance

Sensitivity and Resolution (1 ng/mL Pesticides , 5 µL injected, XIC ± 5 mDa)



Cyromazine
@167

31100

Carbendazim
@192

31800

Thiabendazole
@202

33100

Imazalil
@297

34600

Azoxystrobin
@404

36200

Trifloxystrobin
@409

37000

Spinosyn A
@732

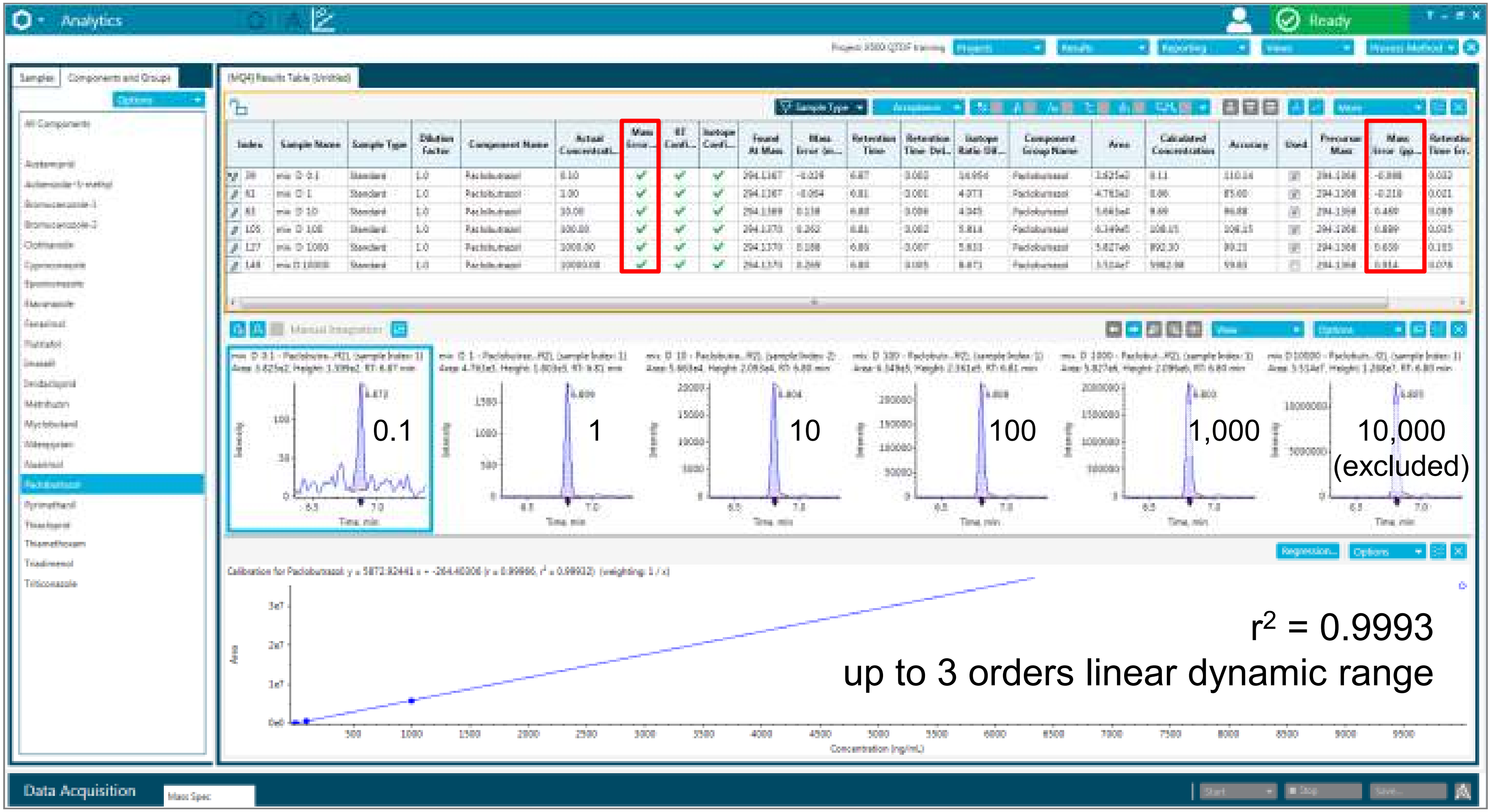
37300

Emamectin B1a
@886
(10 ng/mL)

38000

The SCIEX X500R QTOF System – Performance

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



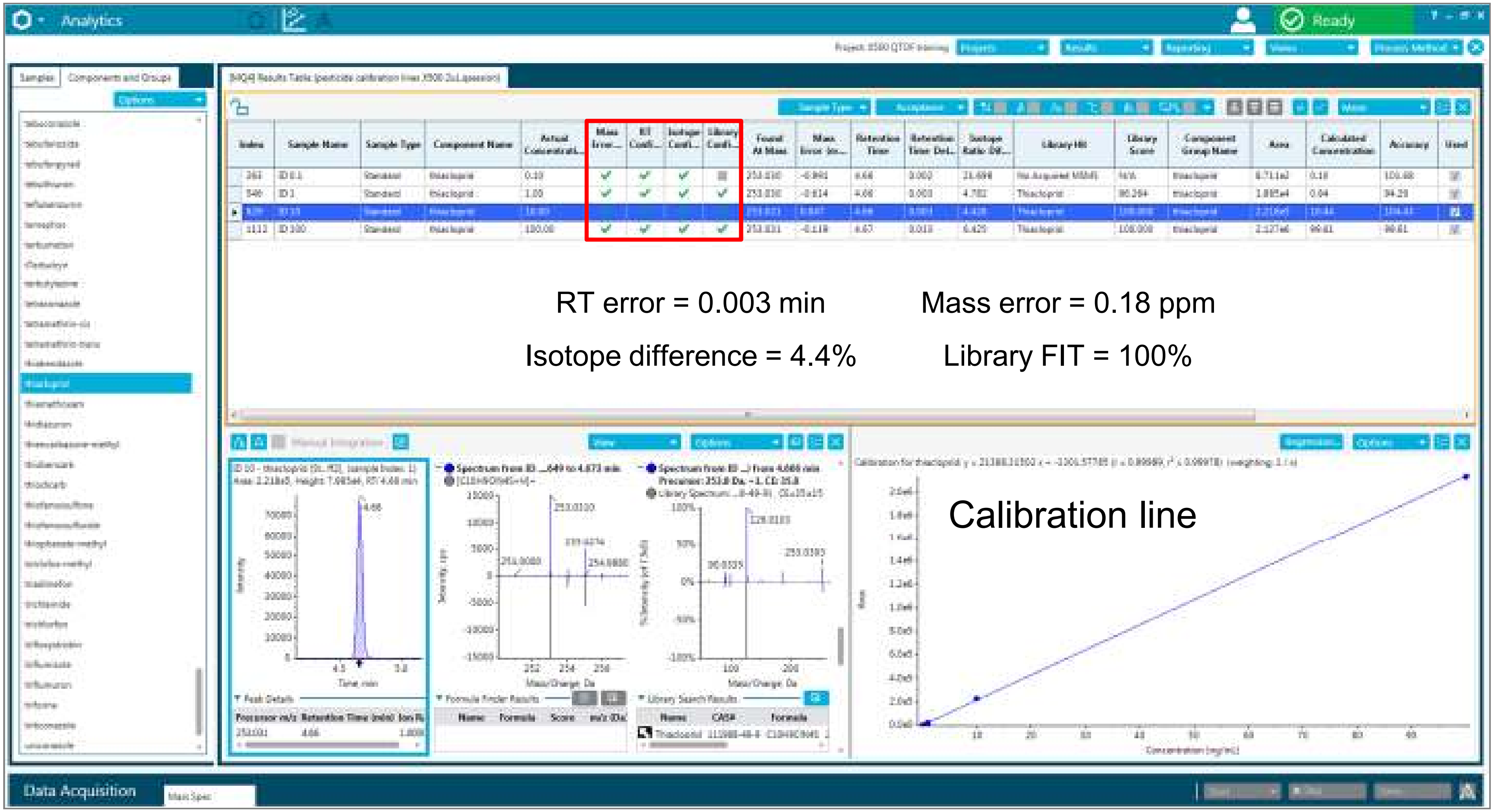
$r^2 = 0.9993$

up to 3 orders linear dynamic range

Mass error = -0.2 to 0.91 ppm, resolution of 30500 @ 294

The SCIEX X500R QTOF System – Performance

MS/MS Identification of Thiacloprid (10 ng/mL)



RT error = 0.003 min

Mass error = 0.18 ppm

Isotope difference = 4.4%

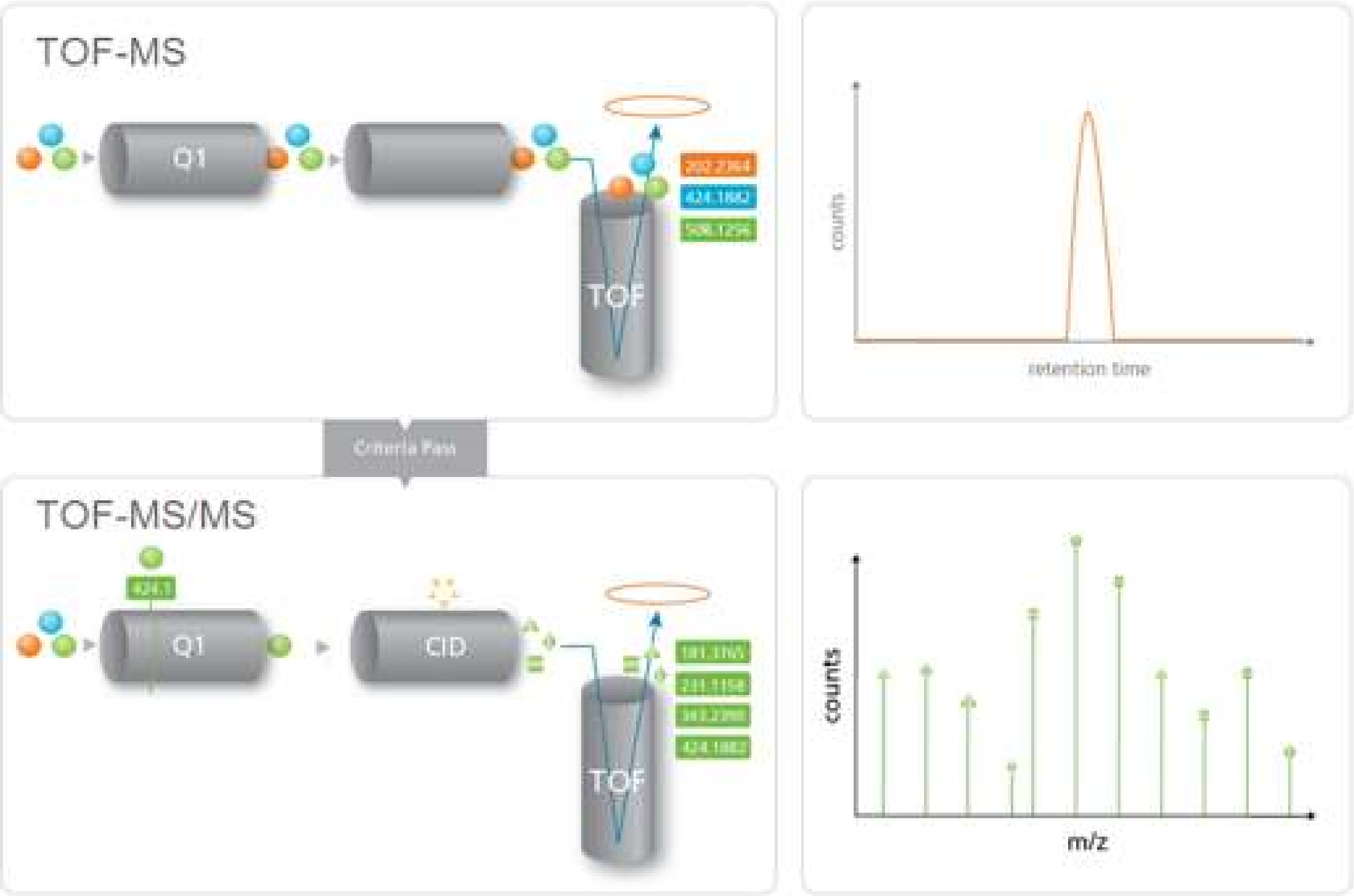
Library FIT = 100%

Calibration line

Review of XIC, MS and MS/MS

Information Dependent Acquisition of MS/MS (IDA)

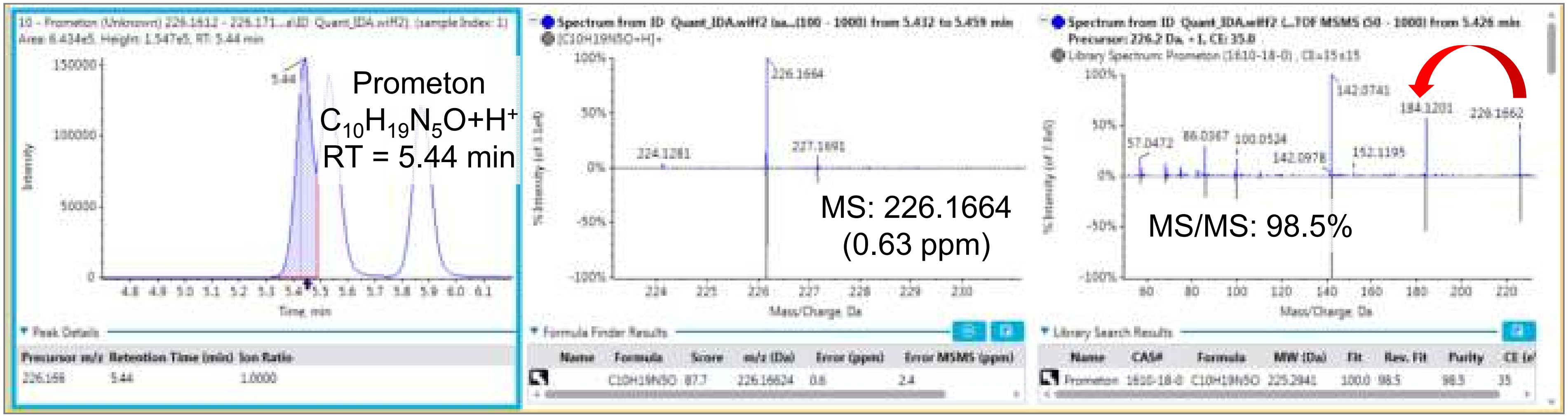
Provides MS/MS Spectra with High Selectivity (Q1 Resolution unit)



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)



10 - Prometon (Unknown) 226.1612 - 226.171...a)ID Quant_IDA.wiff2), (sample Index: 1)
Area: 6.434e5, Height: 1.547e5, RT: 5.44 min

Spectrum from ID Quant_IDA.wiff2 (sa...(100 - 1000) from 5.432 to 5.459 min
[C10H19N5O+H]+

Spectrum from ID Quant_IDA.wiff2 (...TOF MSMS (50 - 1000) from 5.426 min
Precursor: 226.2 Da, +1, CE: 35.0
Library Spectrum: Prometon (1610-18-0) , CE=35±15

Prometon
$C_{10}H_{19}N_5O+H^+$
RT = 5.44 min

MS: 226.1664
(0.63 ppm)

MS/MS: 98.5%

Peak Details

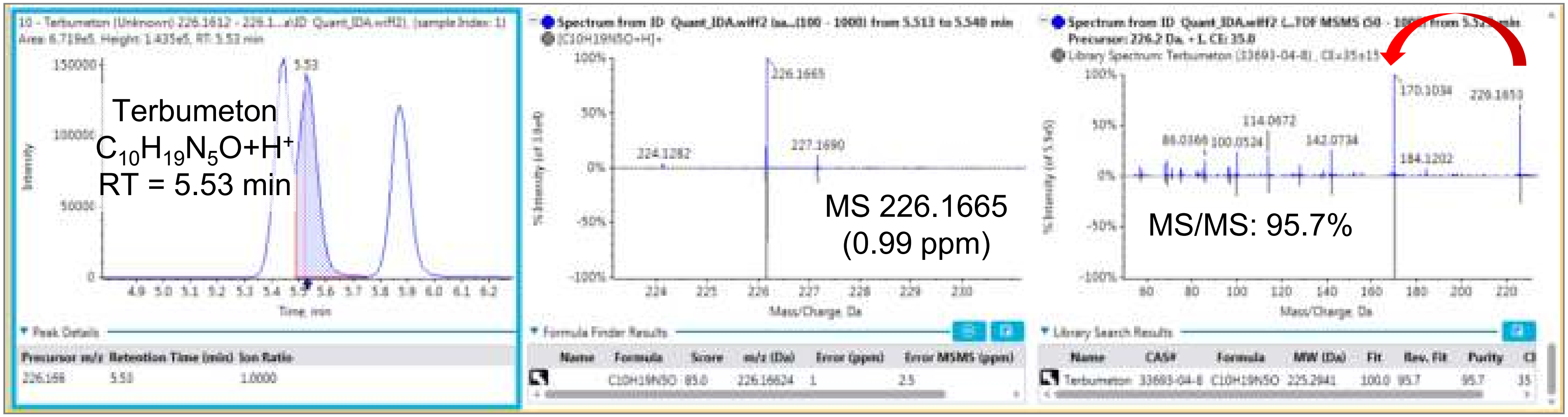
Precursor m/z	Retention Time (min)	Ion Ratio
226.168	5.44	1.0000

Formula Finder Results

Name	Formula	Score	m/z (Da)	Error (ppm)	Error MSMS (ppm)
	C10H19N5O	87.7	226.16624	0.6	2.4

Library Search Results

Name	CAS#	Formula	MW (Da)	Fit	Rev. Fit	Purity	CE (e
Prometon	1610-18-0	C10H19N5O	225.2941	100.0	98.5	98.5	35



10 - Terbumeton (Unknown) 226.1612 - 226.1...a)ID Quant_IDA.wiff2), (sample Index: 1)
Area: 6.719e5, Height: 1.435e5, RT: 5.53 min

Spectrum from ID Quant_IDA.wiff2 (sa...(100 - 1000) from 5.513 to 5.540 min
[C10H19N5O+H]+

Spectrum from ID Quant_IDA.wiff2 (...TOF MSMS (50 - 1000) from 5.52 min
Precursor: 226.2 Da, +1, CE: 35.0
Library Spectrum: Terbumeton (33693-04-8) , CE=35±15

Terbumeton
$C_{10}H_{19}N_5O+H^+$
RT = 5.53 min

MS 226.1665
(0.99 ppm)

MS/MS: 95.7%

Peak Details

Precursor m/z	Retention Time (min)	Ion Ratio
226.168	5.53	1.0000

Formula Finder Results

Name	Formula	Score	m/z (Da)	Error (ppm)	Error MSMS (ppm)
	C10H19N5O	85.0	226.16624	1	2.5

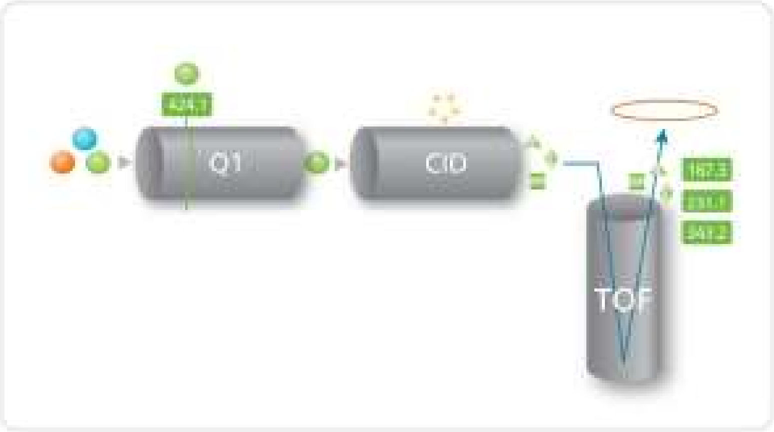
Library Search Results

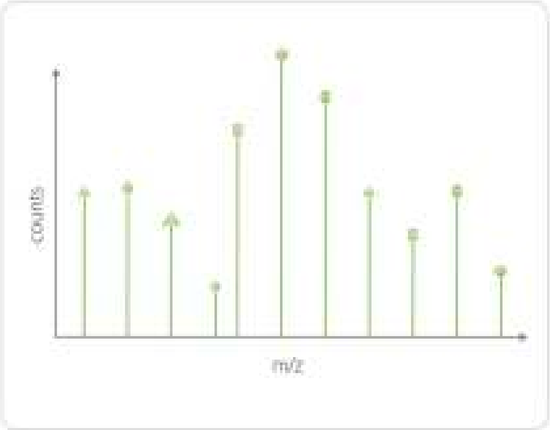
Name	CAS#	Formula	MW (Da)	Fit	Rev. Fit	Purity	CE
Terbumeton	33693-04-8	C10H19N5O	225.2941	100.0	95.7	95.7	35

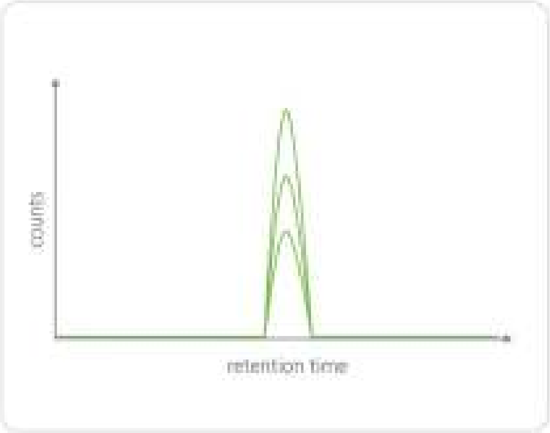
Identification based on MS/MS library searching (Q1 at unit resolution)

MRM^{HR}

Combining Selectivity of MRM and High Resolution



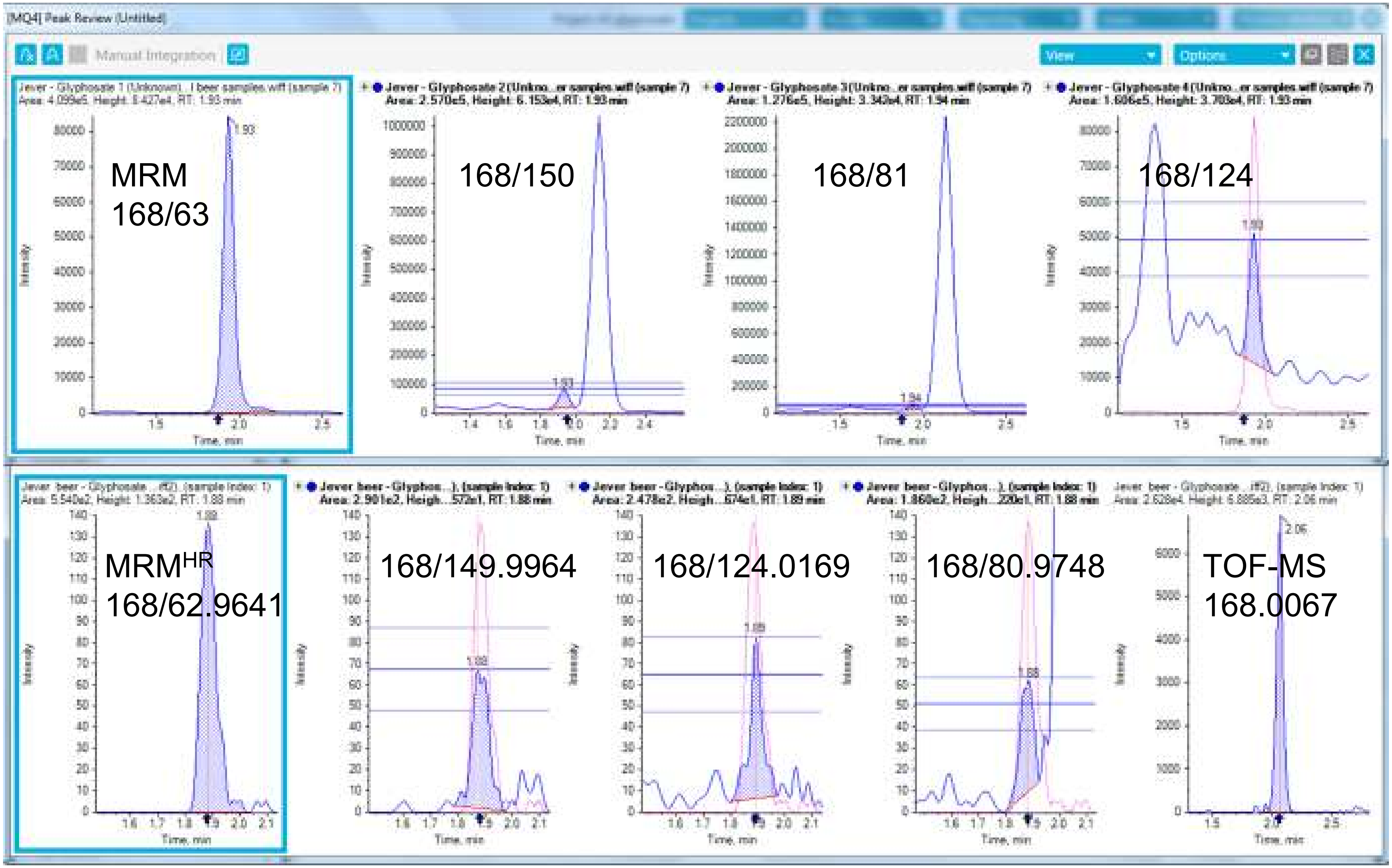




Unit Q1 isolation, fragmentation using optimized CE and narrow XIC of product ion

The SCIEX X500R QTOF System – MRM^{HR}

24 µg/L Glyphosate in a Beer Sample



MRM
168/63

168/150

168/81

168/124

MRM^{HR}
168/62.9641

168/149.9964

168/124.0169

168/80.9748

TOF-MS
168.0067

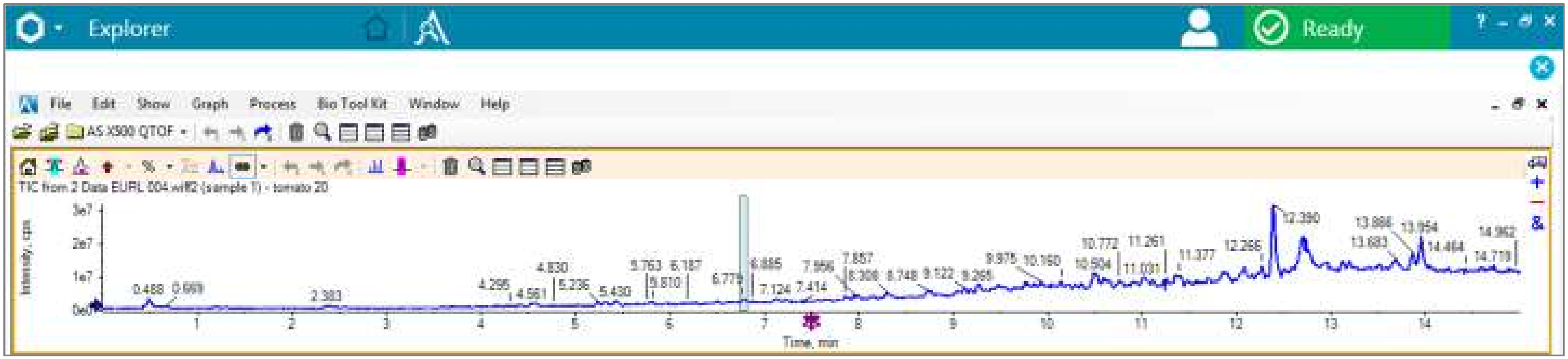
Perfect Balance to Elevate Your Lab's Performance

SCIEX X500R QTOF System Powered by SCIEX OS Software

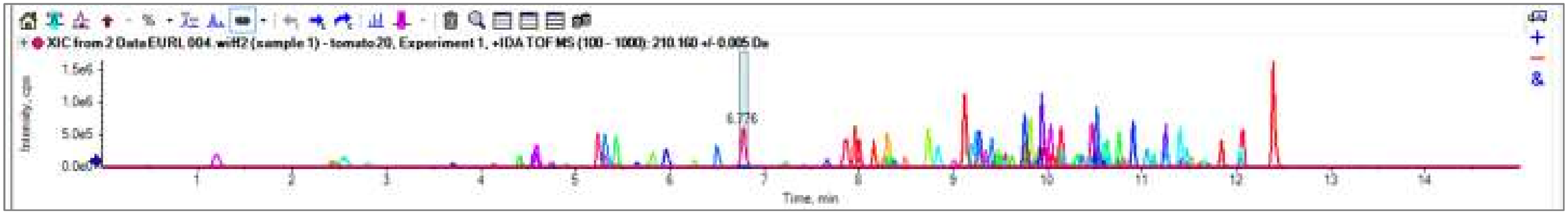
- The first robust, high performance high resolution MS/MS system designed for routine use.
  - Sensitivity to easily detect required drug cutoff concentration levels
  - Resolving power to remove interference from complex forensic matrices
  - Linearity to quantify up to 4 orders of magnitude
  - Identify compounds based on mass accuracy
  - Confident identification based MS/MS (IDA, MS/MS^{ALL} with SWATH™ Acquisition and ion ratios
  - 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.

SCIEX

Targeted Data Processing Workflow

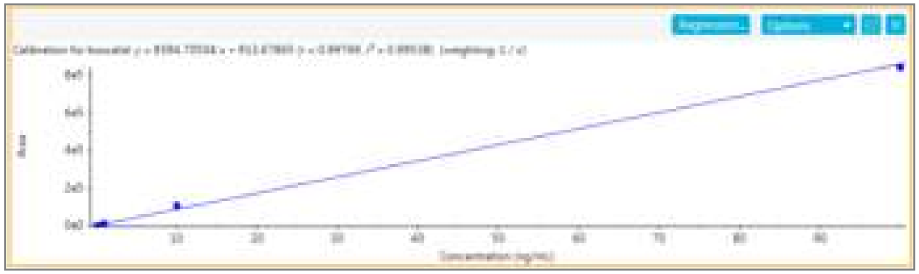


XIC generation for each target



Identification

Quantitation



RT ✓

Mass ✓

Isotopes ✓

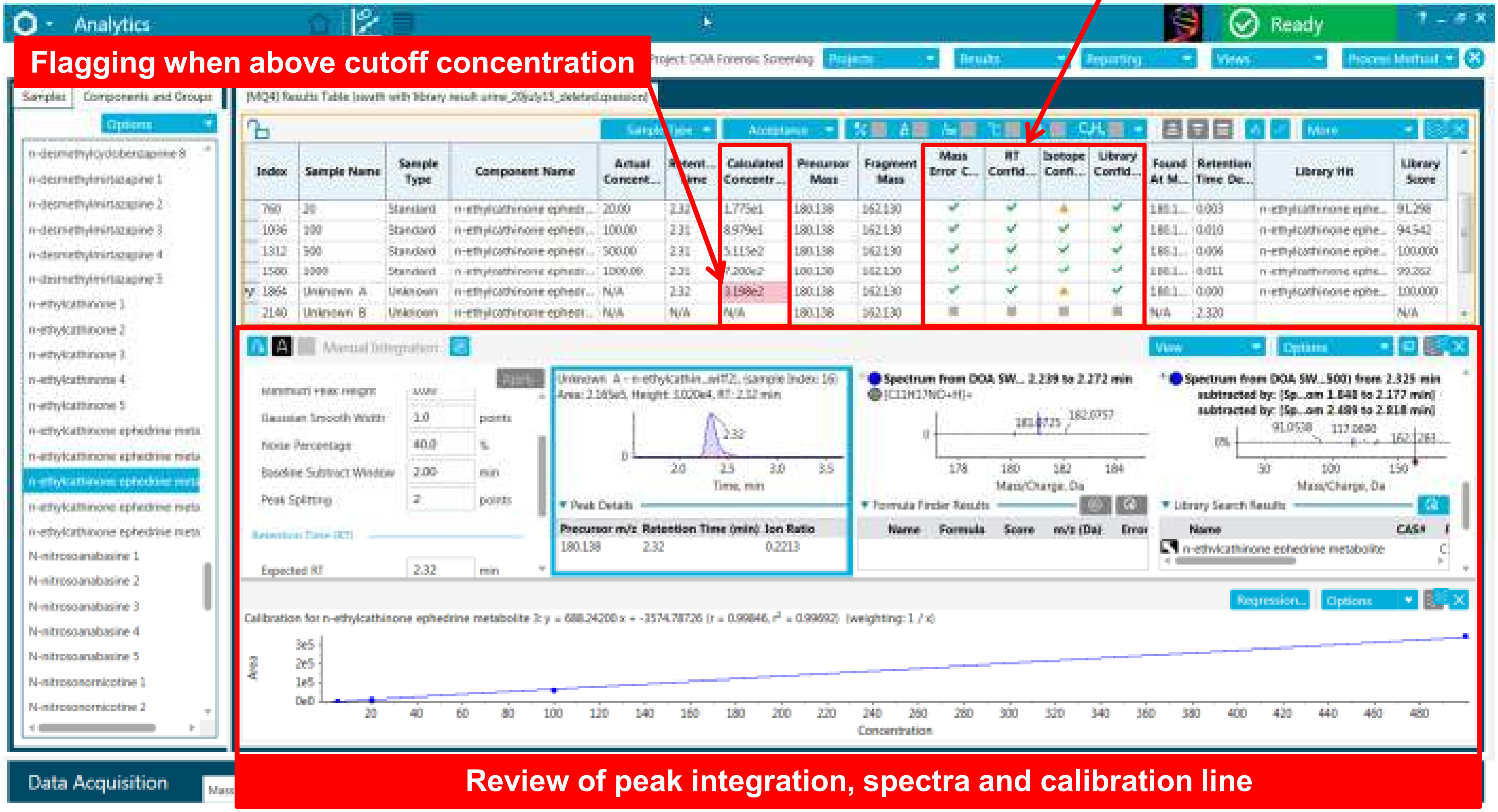
MS/MS search ✓

Above reporting level

Identification and Quantification in SCIEX OS Software

3. Review Quantitative and Qualitative Results

Traffic Lights to indicate confidence



Flagging when above cutoff concentration

Review of peak integration, spectra and calibration line

Index	Sample Name	Sample Type	Component Name	Actual Concent...	Retent... Time	Calculated Concentr...	Precursor Mass	Fragment Mass	Mass Error C...	RT Confid...	Isotope Confi...	Library Confid...	Found At M...	Retention Time De...	Library Hit	Library Score
760	20	Standard	n-ethylcathinone ephedr...	20.00	2.32	1.775e1	180.138	162.130	✓	✓	▲	✓	180.1...	0.003	n-ethylcathinone ephe...	91.298
1036	100	Standard	n-ethylcathinone ephedr...	100.00	2.31	8.979e1	180.138	162.130	✓	✓	✓	✓	180.1...	0.010	n-ethylcathinone ephe...	94.542
1312	500	Standard	n-ethylcathinone ephedr...	500.00	2.31	5.115e2	180.138	162.130	✓	✓	✓	✓	180.1...	0.006	n-ethylcathinone ephe...	100.000
1588	1000	Standard	n-ethylcathinone ephedr...	1000.00	2.31	7.200e2	180.138	162.130	✓	✓	✓	✓	180.1...	0.011	n-ethylcathinone ephe...	99.262
1864	Unknown A	Unknown	n-ethylcathinone ephedr...	N/A	2.32	3.198e2	180.138	162.130	✓	✓	▲	✓	180.1...	0.000	n-ethylcathinone ephe...	100.000
2140	Unknown B	Unknown	n-ethylcathinone ephedr...	N/A	N/A	N/A	180.138	162.130	■	■	■	■	N/A	2.320		N/A

Minimum Peak Height

Gaussian Smooth Width: 1.0 points

Noise Percentage: 40.0 %

Baseline Subtract Window: 2.00 min

Peak Splitting: 2 points

Retention Time (RT)

Expected RT: 2.32 min

Unknown A - n-ethylcathin...wiff2, (sample Index: 16)
Area: 2.165e5, Height: 3.020e4, RT: 2.32 min

Peak Details

Precursor m/z	Retention Time (min)	Ion Ratio
180.138	2.32	0.2213

Spectrum from DOA SW... 2.239 to 2.272 min
[C11H17NO+H]+

Formula Finder Results

Name	Formula	Score	m/z (Da)	Error

Spectrum from DOA SW...500) from 2.325 min
subtracted by: (Sp...om 1.848 to 2.177 min)
subtracted by: (Sp...om 2.489 to 2.818 min)

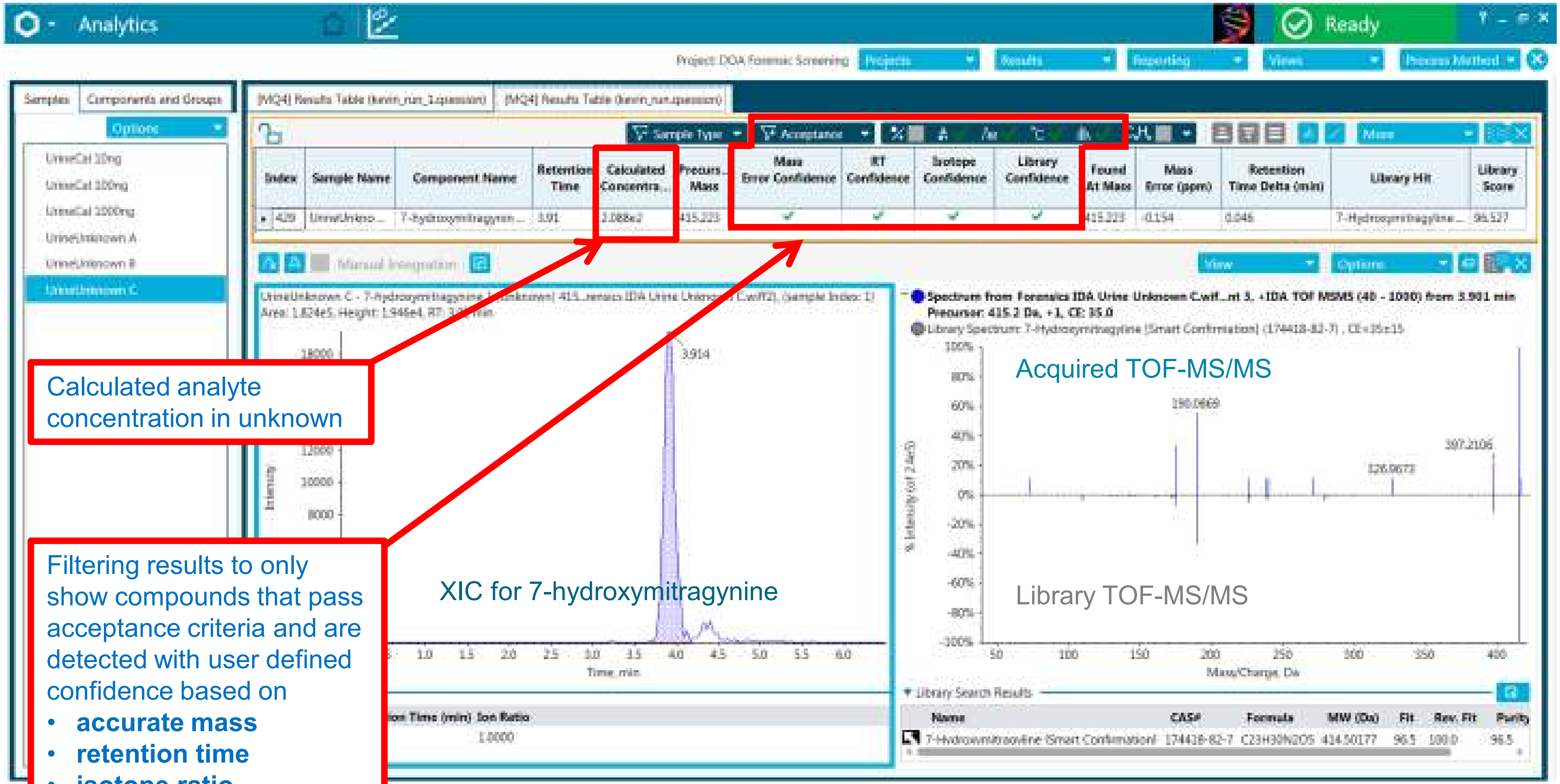
Library Search Results

Name	CAS#
n-ethylcathinone ephedrine metabolite	C

Calibration for n-ethylcathinone ephedrine metabolite 3: y = 688.24200 x + -3574.78726 (r = 0.99846, r^2 = 0.99692) (weighting: 1 / x)

Identification and Quantification in SCIEX OS Software

3. Review Quantitative and Qualitative Results



Index	Sample Name	Component Name	Retention Time	Calculated Concentra...	Precurs... Mass	Mass Error Confidence	RT Confidence	Isotope Confidence	Library Confidence	Found At Mass	Mass Error (ppm)	Retention Time Delta (min)	Library Hit	Library Score
429	UrineUnkno...	7-hydroxymitragynin...	3.91	2.088e2	415.223	✓	✓	✓	✓	415.223	-0.154	0.046	7-Hydroxymitragyline...	96.527

UrineUnknown C - 7-hydroxymitragynine (Unknown) 415...remaics IDA Urine Unknown C.wiff2), (sample Index: 1)
Area: 1.824e5, Height: 1.946e4, RT: 3.91 min

Spectrum from Forensics IDA Urine Unknown C.wif...nt 3, +IDA TOF MSMS (40 - 1000) from 3.901 min
Precursor: 415.2 Da, +1, CE: 35.0
Library Spectrum: 7-Hydroxymitragynine (Smart Confirmation) (174418-82-7) , CE=35±15

Library Search Results

Name	CAS#	Formula	MW (Da)	Fit	Rev. Fit	Purity
7-Hydroxymitragynine (Smart Confirmation)	174418-82-7	C23H30N2O5	414.50177	96.5	100.0	96.5

Calculated analyte concentration in unknown

Filtering results to only show compounds that pass acceptance criteria and are detected with user defined confidence based on

- **accurate mass**
- **retention time**
- **isotope ratio**
- **library matching**

XIC for 7-hydroxymitragynine

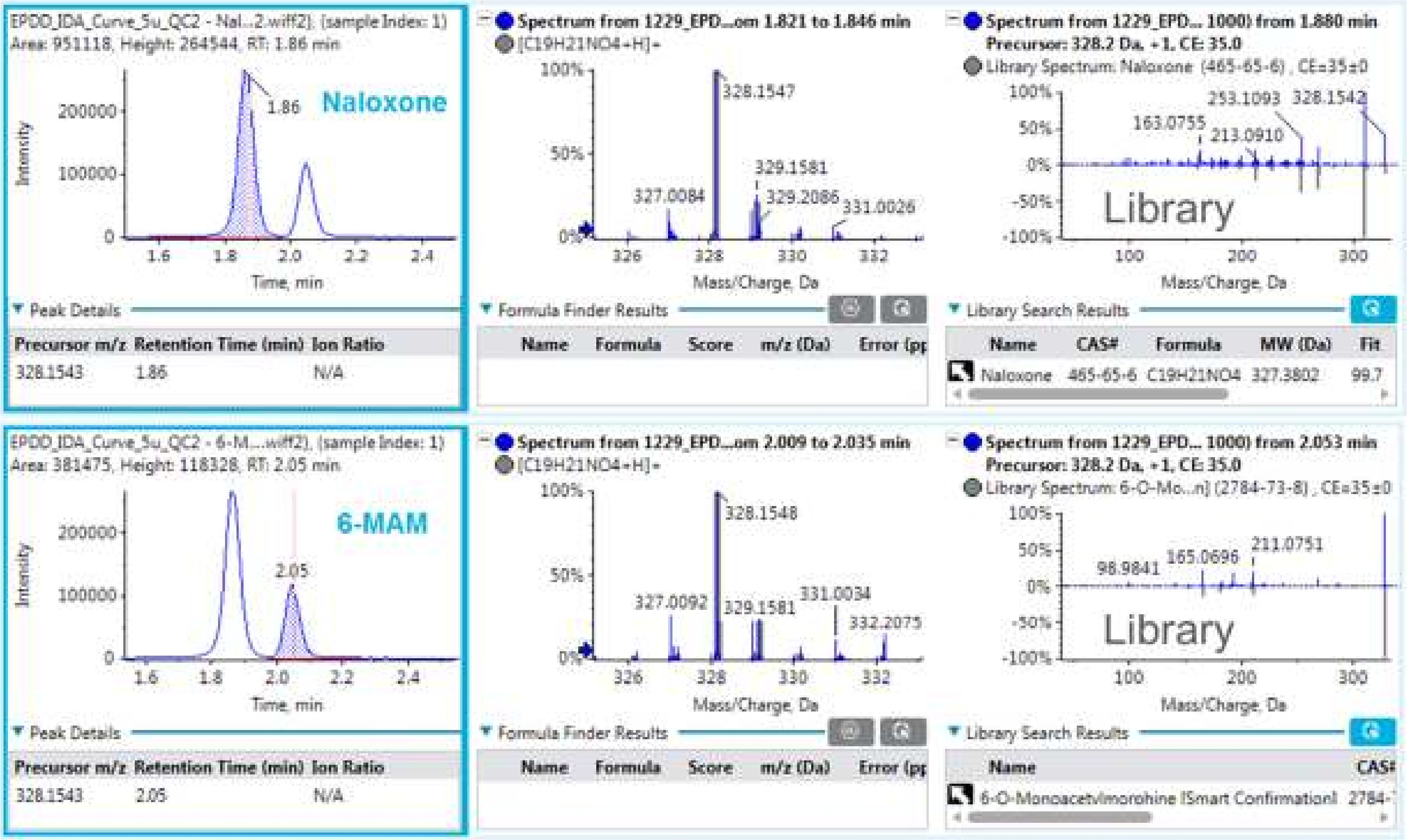
Acquired TOF-MS/MS

Library TOF-MS/MS

Targeted Data Processing of TOF-MS -Information Dependent Acquisition- TOF-MS/MS acquired data

Identification and Quantification in SCIEX OS Software

Highest confidence gained through library MS/MS comparison



EPDD_IDA_Curve_5u_QC2 - Nal...2.wiff2), (sample Index: 1)
Area: 951118, Height: 264544, RT: 1.86 min

Peak Details

Precursor m/z	Retention Time (min)	Ion Ratio
328.1543	1.86	N/A

Spectrum from 1229_EPD...om 1.821 to 1.846 min
[C19H21NO4+H]+

Formula Finder Results

Name	Formula	Score	m/z (Da)	Error (pp

Spectrum from 1229_EPD... 1000) from 1.880 min
Precursor: 328.2 Da, +1, CE: 35.0
Library Spectrum: Naloxone (465-65-6), CE=35±0

Library Search Results

Name	CAS#	Formula	MW (Da)	Fit
Naloxone	465-65-6	C19H21NO4	327.3802	99.7

EPDD_IDA_Curve_5u_QC2 - 6-M....wiff2), (sample Index: 1)
Area: 381475, Height: 118328, RT: 2.05 min

Peak Details

Precursor m/z	Retention Time (min)	Ion Ratio
328.1543	2.05	N/A

Spectrum from 1229_EPD...om 2.009 to 2.035 min
[C19H21NO4+H]+

Formula Finder Results

Name	Formula	Score	m/z (Da)	Error (pp

Spectrum from 1229_EPD... 1000) from 2.053 min
Precursor: 328.2 Da, +1, CE: 35.0
Library Spectrum: 6-O-Mo...n] (2784-73-8), CE=35±0

Library Search Results

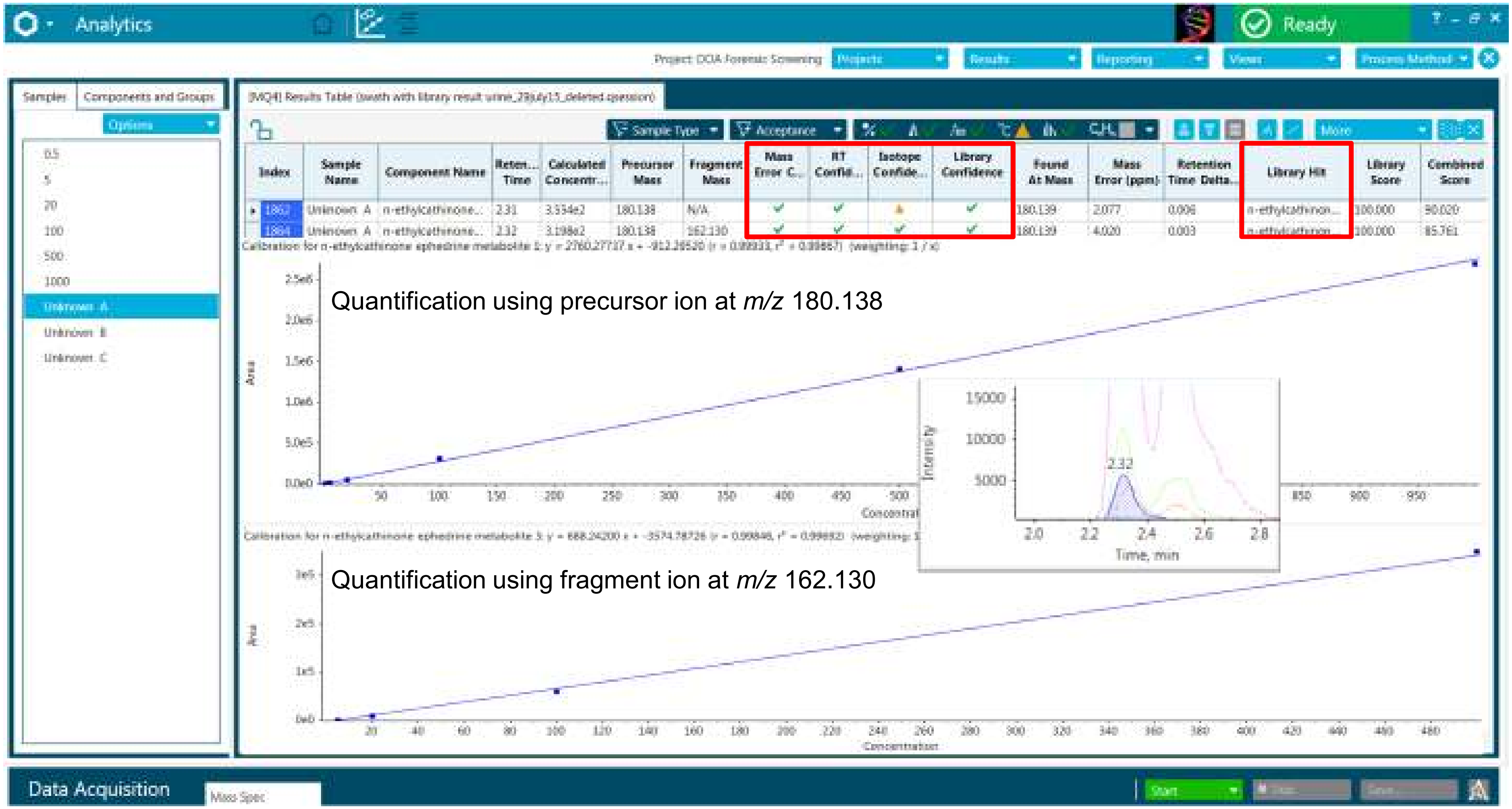
Name	CAS#
6-O-Monoacetylmorphine [Smart Confirmation]	2784-

XIC chromatograms

MS spectra

MS/MS spectra

Confirmation and quantitation using SWATH® acquisition for forensic drug screening



[MQ4] Results Table (swath with library result urine_28july15_deleted.qsession)

Index	Sample Name	Component Name	Reten... Time	Calculated Concentr...	Precursor Mass	Fragment Mass	Mass Error C...	RT Confid...	Isotope Confide...	Library Confidence	Found At Mass	Mass Error (ppm)	Retention Time Delta...	Library Hit	Library Score	Combined Score
1862	Unknown A	n-ethylcathinone...	2.31	3.534e2	180.138	N/A	✓	✓	⚠	✓	180.139	2.077	0.006	n-ethylcathinon...	100.000	90.020
1864	Unknown A	n-ethylcathinone...	2.32	3.198e2	180.138	162.130	✓	✓	✓	✓	180.139	4.020	0.003	n-ethylcathinon...	100.000	85.761

Calibration for n-ethylcathinone ephedrine metabolite 1: y = 2760.27737 x + -912.26520 (r = 0.99933, r² = 0.99867) (weighting: 1 / x)

Quantification using precursor ion at *m/z* 180.138

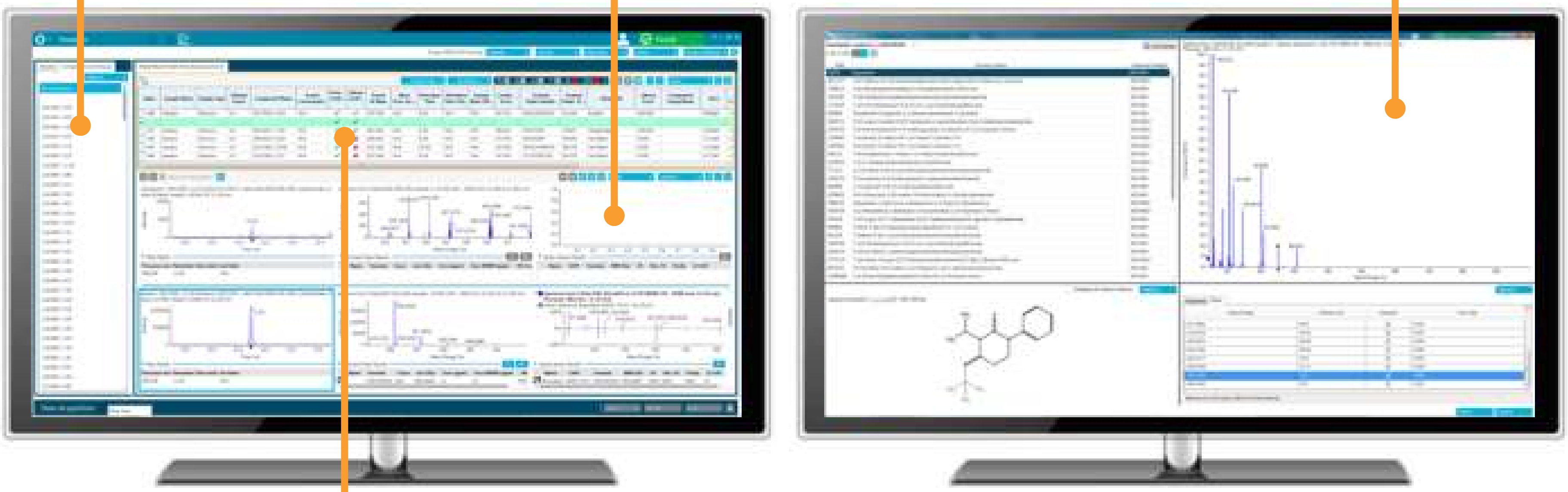
Calibration for n-ethylcathinone ephedrine metabolite 3: y = 688.24200 x + -3574.78726 (r = 0.99846, r² = 0.99692) (weighting: 1

Quantification using fragment ion at *m/z* 162.130

1. **Identification based on unique fragment ions and their ratios as well as MS/MS library searching**
2. **Quantitation on both precursor ion and fragment ions**

SCIEX OS Software – Unknown Identification

Software Improvements and Details



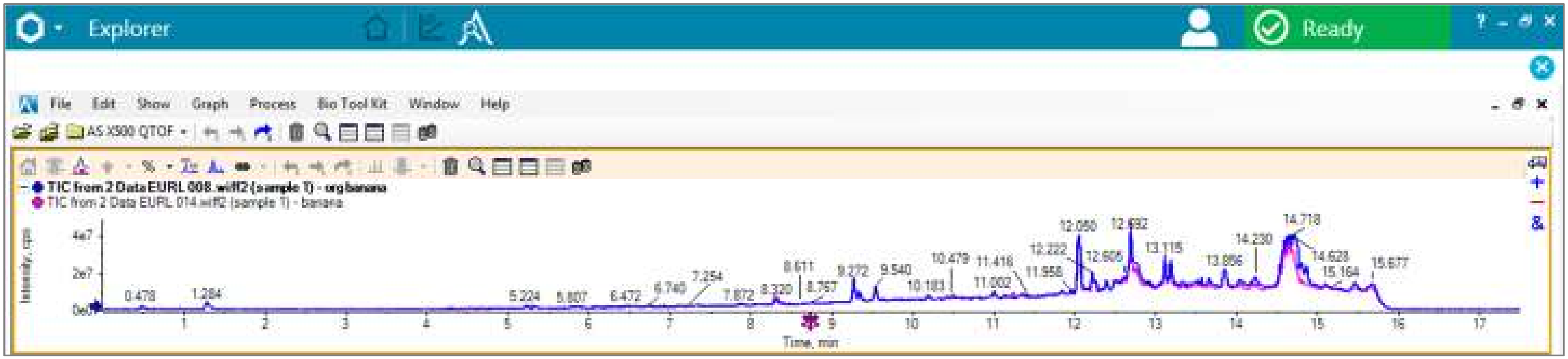
Automatic sample-control comparison

Non-Target peak finding

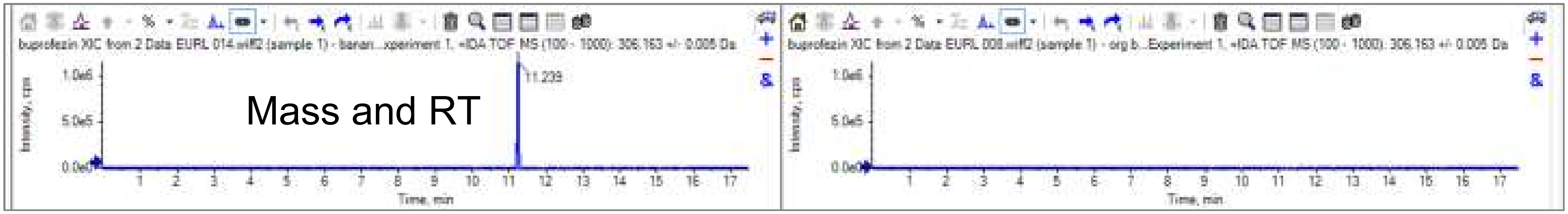
ChemSpider searching
Sorting by number of references and automatic structure elucidation to identify unknowns

Automatic MS/MS library searching and formula finding

Non-Targeted Data Processing Workflow



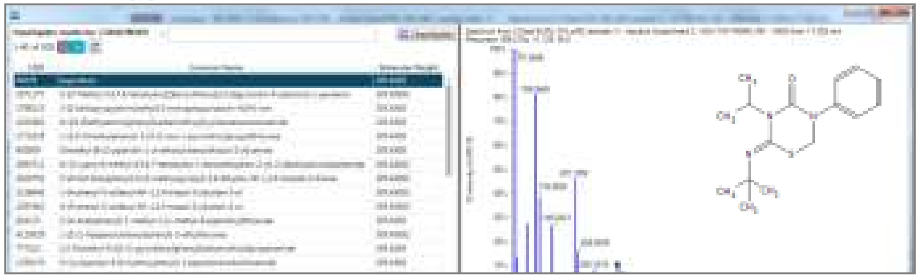
Sample-control comparison



Mass and RT

Identification

ChemSpider

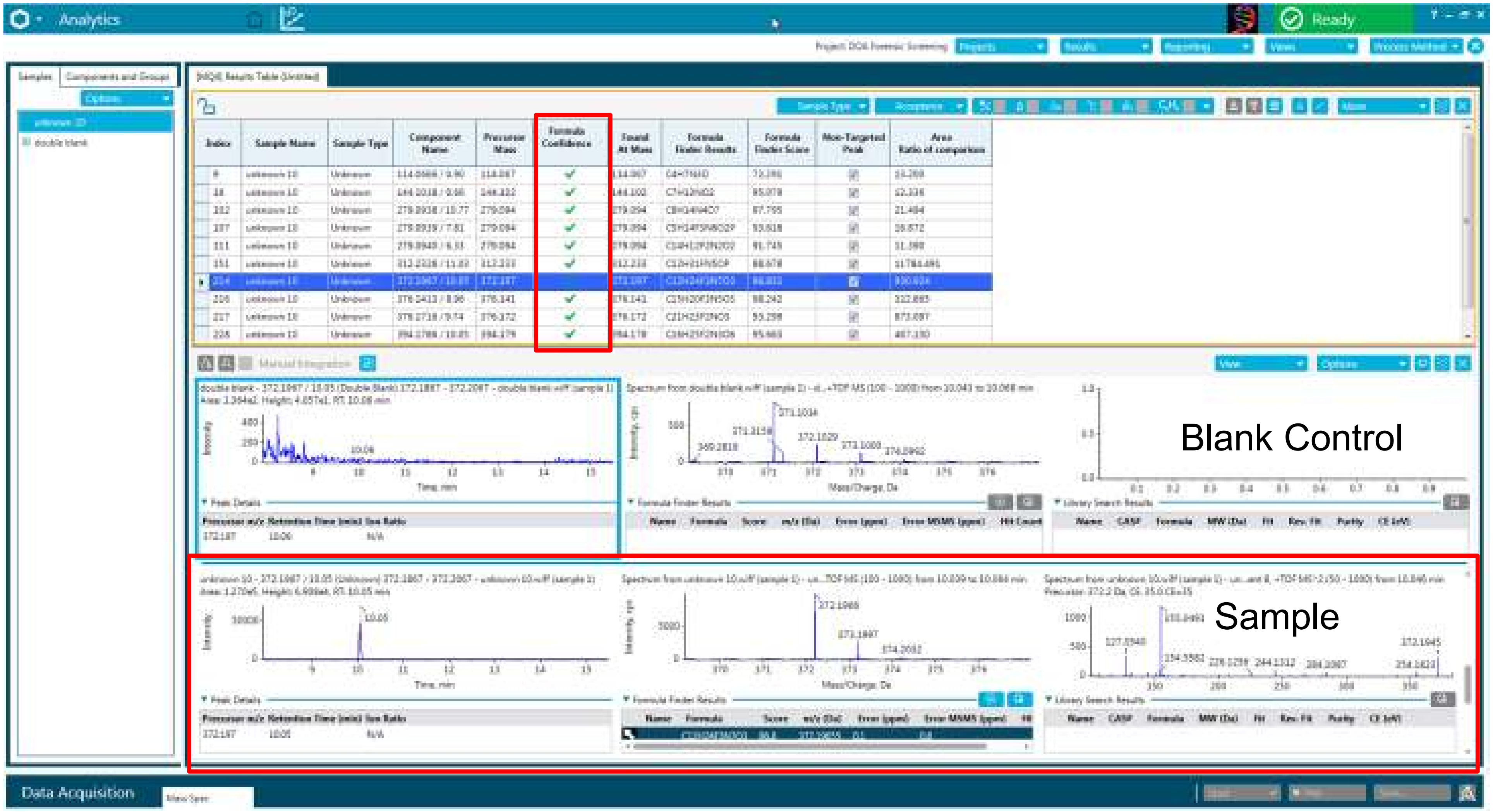


Formula finding ✓

MS/MS search ✓

Unknown Identification in SCIEX OS Software

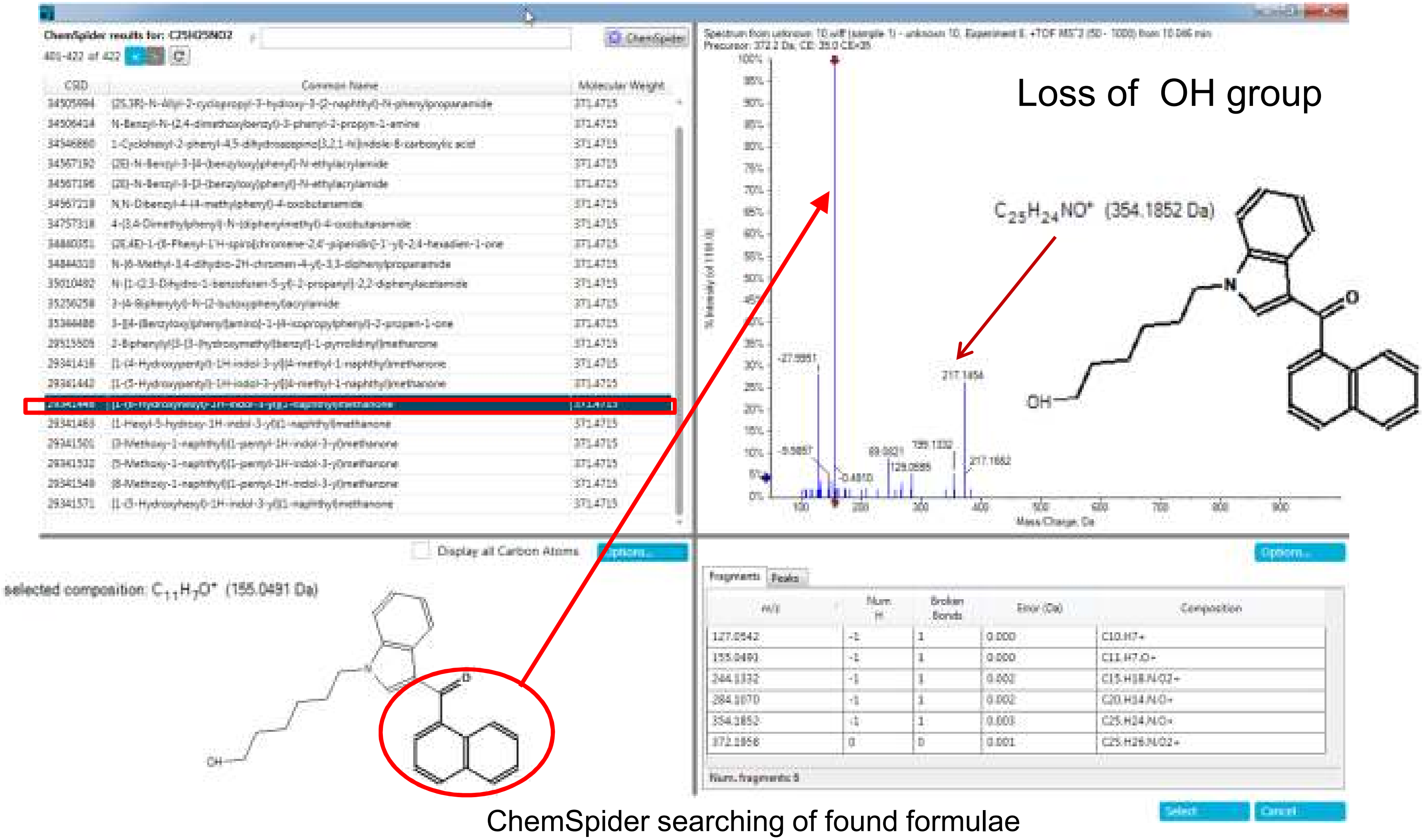
1. Automatic Sample-Control Comparison and Compound Identification



Automatic formula finding

Unknown Identification in SCIEX OS Software

1. Automatic Sample-Control Comparison and Compound Identification



ChemSpider results for: C25H25NO2

401-422 of 422

CSID	Common Name	Molecular Weight
34505994	(2S,3R)-N-Allyl-2-cyclopropyl-3-hydroxy-3-(2-naphthyl)-N-phenylpropanamide	371.4715
34506414	N-Benzyl-N-(2,4-dimethoxybenzyl)-3-phenyl-2-propyn-1-amine	371.4715
34546880	1-Cyclohexyl-2-phenyl-4,5-dihydroazepino[3,2,1-hi]indole-8-carboxylic acid	371.4715
34567192	(2E)-N-Benzyl-3-[4-(benzyloxy)phenyl]-N-ethylacrylamide	371.4715
34567198	(2E)-N-Benzyl-3-[3-(benzyloxy)phenyl]-N-ethylacrylamide	371.4715
34567218	N,N-Dibenzyl-4-(4-methylphenyl)-4-oxobutanamide	371.4715
34757318	4-(3,4-Dimethylphenyl)-N-(diphenylmethyl)-4-oxobutanamide	371.4715
34880351	(2E,4E)-1-(6-Phenyl-1'H-spiro[chromene-2,4'-piperidin]-1'-yl)-2,4-hexadien-1-one	371.4715
34884310	N-(6-Methyl-3,4-dihydro-2H-chromen-4-yl)-3,3-diphenylpropanamide	371.4715
35010482	N-[1-(2,3-Dihydro-1-benzofuran-5-yl)-2-propanyl]-2,2-diphenylacetamide	371.4715
35256258	3-(4-Biphenylyl)-N-(2-butoxyphenyl)acrylamide	371.4715
35344488	3-{[4-(Benzyloxy)phenyl]amino}-1-(4-isopropylphenyl)-2-propen-1-one	371.4715
29515505	2-Biphenylyl{3-[3-(hydroxymethyl)benzyl]-1-pyrrolidinyl}methanone	371.4715
29341418	[1-(4-Hydroxypentyl)-1H-indol-3-yl](4-methyl-1-naphthyl)methanone	371.4715
29341442	[1-(5-Hydroxypentyl)-1H-indol-3-yl](4-methyl-1-naphthyl)methanone	371.4715
29341448	[1-(6-Hydroxyhexyl)-1H-indol-3-yl](1-naphthyl)methanone	371.4715
29341463	(1-Hexyl-5-hydroxy-1H-indol-3-yl)(1-naphthyl)methanone	371.4715
29341501	(3-Methoxy-1-naphthyl)(1-pentyl-1H-indol-3-yl)methanone	371.4715
29341532	(5-Methoxy-1-naphthyl)(1-pentyl-1H-indol-3-yl)methanone	371.4715
29341548	(8-Methoxy-1-naphthyl)(1-pentyl-1H-indol-3-yl)methanone	371.4715
29341571	[1-(3-Hydroxyhexyl)-1H-indol-3-yl](1-naphthyl)methanone	371.4715

m/z	Num. H	Broken Bonds	Error (Da)	Composition
127.0542	-1	1	0.000	C10.H7+
155.0491	-1	1	0.000	C11.H7.O+
244.1332	-1	1	0.002	C15.H18.N.O2+
284.1070	-1	1	0.002	C20.H14.N.O+
354.1852	-1	1	0.003	C25.H24.N.O+
372.1856	0	0	0.001	C25.H26.N.O2+

Num. fragments: 6

ChemSpider searching of found formulae

Automatic structure elucidation using HR-MS/MS spectra

Summary

- 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

Thank you for your attention!

You ready to get behind the wheel?

Trademarks/Licensing