

Environmental Method

Illicit drugs analysis in water

Elevate your environmental testing with the X500R QTOF System

Method details and access to HR-MS/MS libraries to detect, quantify, and confirm illicit drugs in water samples using HPLC coupled with the X500R QTOF system, powered by SCIEX OS Software.

Sample Prep

Step 1

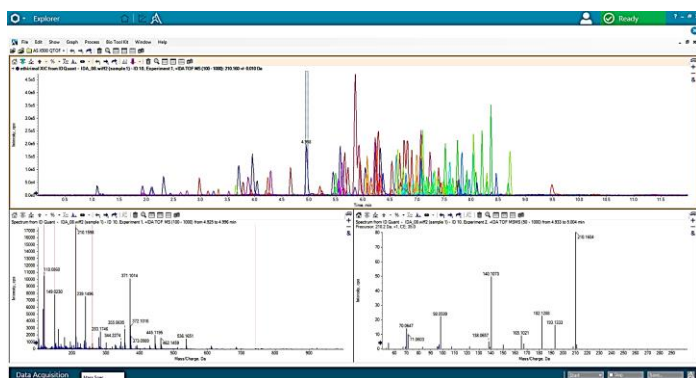
• Samples acidified to pH 2 using HCL and stored in the dark at 4°C until required

Step 2

• Transfer 1mL of sample into an analytical vial



SCIEX OS can deliver faster method set-up



SCIEX OS delivers enhanced data exploration of your acquired TOF MS and TOF MS/MS data

LC Method

Column	Phenomenex Kinetex C18, 100 x 4.6 mm, 5 um column	
Mobile Phase A	0.1% formic acid in water + 2mM ammonium formate	
Mobile Phase B	Acetonitrile	
Flow rate	0.9 mL/min	
Column temperature	30 °C	
Injection volume	100 uL	
Gradient profile	Time (min)	% B
	0	2
	1	2
	7	65
	7.1	100
	9	100
	9.1	2
	12	2

 MS Method

MS Method

Running

IDA 10MSM50msec

Method Overview

Device: X500 QTOF
Ion Source: TurboSpray

IDA

0 min → 20 min

Method duration: 20 min
Estimated cycles: 1577

Total scan time: 0.760605 sec

Add Experiment

Source and Gas Parameters

Ion source gas 1: 50 psi
Ion source gas 2: 70 psi

Curtain gas: 30
CAD gas: 7

Temperature: 450 °C

Experiment IDA

Polarity: Positive V
Spray voltage: 3500 V

TOF MS
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
CE spread: 0 V

IDA Criteria Small molecule

Maximum candidate ions: 10
Intensity threshold exceeds: 100 cps

☒ Dynamic background subtraction
☐ Exclude former candidate ions
For 6 sec
After 1 occurrences

Advanced Criteria

TOF MSMS

Presursor ion: 810 Da
TOF start mass: 50 Da
TOF stop mass: 1000 Da

Declustering potential: 80 V
DP spread: 0 V
Accumulation time: 0.05 sec

Collision energy: 35 V
CE spread: 15 V

Data Acquisition

Mass Scan

Start

Stop

Save

Suggested IDA (Information Dependent Acquisition) conditions for routine environmental testing as displayed in SCIEX OS.

Data Processing



Review your results with utmost efficiency using SCIEX OS for simultaneous quantitation and MS/MS library confirmation.

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X500R High Resolution Libraries

Genbank Accession	CDS Number	Protein	Transcript Length
U12008.1	2088-0.4	C18H20N2	19-1008
U12008.1	9888-0.4	C18H20N2	207-2494
U12008.1	9890-0.4	C18H20N2	207-2494
U12008.1	9892-0.4	C18H20N2	207-2494
U12008.1	9894-0.4	C18H20N2	207-2494
U12008.1	9896-0.4	C18H20N2	207-2494
U12008.1	9898-0.4	C18H20N2	207-2494
U12008.1	9900-0.4	C18H20N2	207-2494
U12008.1	9902-0.4	C18H20N2	207-2494
U12008.1	9904-0.4	C18H20N2	207-2494
U12008.1	9906-0.4	C18H20N2	207-2494
U12008.1	9908-0.4	C18H20N2	207-2494
U12008.1	9910-0.4	C18H20N2	207-2494
U12008.1	9912-0.4	C18H20N2	207-2494
U12008.1	9914-0.4	C18H20N2	207-2494
U12008.1	9916-0.4	C18H20N2	207-2494
U12008.1	9918-0.4	C18H20N2	207-2494
U12008.1	9920-0.4	C18H20N2	207-2494
U12008.1	9922-0.4	C18H20N2	207-2494
U12008.1	9924-0.4	C18H20N2	207-2494
U12008.1	9926-0.4	C18H20N2	207-2494
U12008.1	9928-0.4	C18H20N2	207-2494
U12008.1	9930-0.4	C18H20N2	207-2494
U12008.1	9932-0.4	C18H20N2	207-2494
U12008.1	9934-0.4	C18H20N2	207-2494
U12008.1	9936-0.4	C18H20N2	207-2494
U12008.1	9938-0.4	C18H20N2	207-2494
U12008.1	9940-0.4	C18H20N2	207-2494
U12008.1	9942-0.4	C18H20N2	207-2494
U12008.1	9944-0.4	C18H20N2	207-2494
U12008.1	9946-0.4	C18H20N2	207-2494
U12008.1	9948-0.4	C18H20N2	207-2494
U12008.1	9950-0.4	C18H20N2	207-2494
U12008.1	9952-0.4	C18H20N2	207-2494
U12008.1	9954-0.4	C18H20N2	207-2494
U12008.1	9956-0.4	C18H20N2	207-2494
U12008.1	9958-0.4	C18H20N2	207-2494
U12008.1	9960-0.4	C18H20N2	207-2494
U12008.1	9962-0.4	C18H20N2	207-2494
U12008.1	9964-0.4	C18H20N2	207-2494
U12008.1	9966-0.4	C18H20N2	207-2494
U12008.1	9968-0.4	C18H20N2	207-2494
U12008.1	9970-0.4	C18H20N2	207-2494
U12008.1	9972-0.4	C18H20N2	207-2494
U12008.1	9974-0.4	C18H20N2	207-2494
U12008.1	9976-0.4	C18H20N2	207-2494
U12008.1	9978-0.4	C18H20N2	207-2494
U12008.1	9980-0.4	C18H20N2	207-2494
U12008.1	9982-0.4	C18H20N2	207-2494
U12008.1	9984-0.4	C18H20N2	207-2494
U12008.1	9986-0.4	C18H20N2	207-2494
U12008.1	9988-0.4	C18H20N2	207-2494
U12008.1	9990-0.4	C18H20N2	207-2494
U12008.1	9992-0.4	C18H20N2	207-2494
U12008.1	9994-0.4	C18H20N2	207-2494
U12008.1	9996-0.4	C18H20N2	207-2494
U12008.1	9998-0.4	C18H20N2	207-2494
U12008.1	10000-0.4	C18H20N2	207-2494
U12008.1	10002-0.4	C18H20N2	207-2494
U12008.1	10004-0.4	C18H20N2	207-2494
U12008.1	10006-0.4	C18H20N2	207-2494
U12008.1	10008-0.4	C18H20N2	207-2494
U12008.1	10010-0.4	C18H20N2	207-2494
U12008.1	10012-0.4	C18H20N2	207-2494
U12008.1	10014-0.4	C18H20N2	207-2494

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XIC List**

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