

Environmental Method

PPCP 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 pharmaceuticals and personal care products in water samples using HPLC coupled with the X500R QTOF system, powered by SCIEX OS Software.

Sample Prep

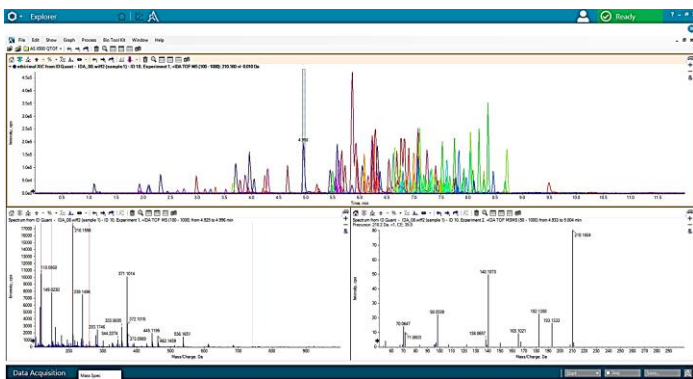
- Step 1 • Direct aqueous injection



SCIEX OS can deliver faster method set-up

LC Method

Column	Phenomenex Kinetex Biphenyl, 100 x 2.1 mm, 2.6 µm column	
Mobile Phase A	0.1% formic acid in water	
Mobile Phase B	0.1% formic acid in methanol	
Flow rate	0.6 mL/min	
Column temperature	30°C	
Injection volume	100 µL	
Gradient profile	Time (min)	% B
	0	2
	1	2
	7	65
	7.1	100
	9	100
	9.1	2
	12	2



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

MS Method

Method Overview
 Device: X500 QTOF
 Ion Source: TurboSpray

Method duration: 20 min | Total scan time: 0.76065 sec
 Estimated cycles: 1577

Source and Gas Parameters
 Ion source gas 1: 50 psi | Curtain gas: 30 | Temperature: 450 °C
 Ion source gas 2: 70 psi | CAD gas: 7

Experiment IDA
 Polarity: Positive V | Spray voltage: 5500 V

TOF MS
 TOF start mass: 100 Da | Declustering potential: 80 V | Collision energy: 10 V
 TOF stop mass: 1000 Da | DP spread: 0 V | CE spread: 0 V
 Accumulation time: 0.2 sec

IDA Criteria Small molecule
 Maximum candidate ions: 10 | Dynamic background subtraction:
 Intensity threshold exceeds: 100 cps | Exclude former candidate ions:
 For: 5 sec | After: 1 occurrences

Advanced Criteria

TOF MSMS
 Precursor ion: 5-20 Da | Declustering potential: 80 V | Collision energy: 35 V
 TOF start mass: 50 Da | DP spread: 0 V | CE spread: 15 V
 TOF stop mass: 1000 Da | Accumulation time: 0.05 sec

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

Data Processing

Index	Sample Name	Sample Type	Method	Component Name	Actual Concentration	Mean (Std. Dev.)	Min (Max)	Retention Time	Retention Time (Std. Dev.)	Component Description	Area	Calculated Concentration	Accuracy	Precursor Mass	Retention Time (Std. Dev.)
17	01	Standard	1.0	Permethrin	0.25	264.1287	0.028	8.87	0.028	Permethrin	7.12062	0.13	200.24	86	264.1288
18	01	Standard	1.0	Permethrin	0.50	264.1287	0.028	8.87	0.028	Permethrin	14.24124	0.26	400.48	86	264.1288
19	01	Standard	1.0	Permethrin	1.00	264.1288	0.028	8.88	0.028	Permethrin	28.48248	0.52	800.96	86	264.1288
20	01	Standard	1.0	Permethrin	2.00	264.1288	0.028	8.88	0.028	Permethrin	56.96496	1.04	1601.92	86	264.1288
21	01	Standard	1.0	Permethrin	4.00	264.1289	0.028	8.89	0.028	Permethrin	113.92992	2.08	3203.84	86	264.1288
22	01	Standard	1.0	Permethrin	8.00	264.1290	0.028	8.89	0.028	Permethrin	227.85984	4.16	6407.68	86	264.1288

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

Compound	CAS Number	Formula	Elemental Weight
2,2-Dimethylbutane	2880-64-4	C7H16	100.206
2,2-Dimethylpropane	68-127-6	C5H12	72.1506
2,2,4-Trimethylpentane	100-91-0	C8H18	114.231
2,2,4,4-Tetramethylpentane	68-139-0	C9H20	128.264
2,2,4,4-Tetramethylhexane	68-141-1	C10H22	142.298
2,2,4,4,4-Pentamethylhexane	68-143-3	C11H24	156.332
2,2,4,4,4-Pentamethylheptane	68-145-5	C12H26	170.366
2,2,4,4,4-Pentamethyloctane	68-147-7	C13H28	184.400
2,2,4,4,4-Pentamethylnonane	68-149-9	C14H30	198.434
2,2,4,4,4-Pentamethyldecane	68-151-1	C15H32	212.468
2,2,4,4,4-Pentamethylundecane	68-153-3	C16H34	226.502
2,2,4,4,4-Pentamethyltridecane	68-155-5	C17H36	240.536
2,2,4,4,4-Pentamethylpentadecane	68-157-7	C18H38	254.570
2,2,4,4,4-Pentamethylheptadecane	68-159-9	C19H40	268.604
2,2,4,4,4-Pentamethylnonadecane	68-161-1	C20H42	282.638
2,2,4,4,4-Pentamethylheneicosane	68-163-3	C21H44	296.672
2,2,4,4,4-Pentamethyltricosane	68-165-5	C22H46	310.706
2,2,4,4,4-Pentamethyltetracosane	68-167-7	C23H48	324.740
2,2,4,4,4-Pentamethylpentacosane	68-169-9	C24H50	338.774
2,2,4,4,4-Pentamethylhexacosane	68-171-1	C25H52	352.808
2,2,4,4,4-Pentamethylheptacosane	68-173-3	C26H54	366.842
2,2,4,4,4-Pentamethyleicosane	68-175-5	C27H56	380.876
2,2,4,4,4-Pentamethyltriacontane	68-177-7	C28H58	394.910
2,2,4,4,4-Pentamethyltriacontane	68-179-9	C29H60	408.944
2,2,4,4,4-Pentamethyltriacontane	68-181-1	C30H62	422.978
2,2,4,4,4-Pentamethyltriacontane	68-183-3	C31H64	437.012
2,2,4,4,4-Pentamethyltriacontane	68-185-5	C32H66	451.046
2,2,4,4,4-Pentamethyltriacontane	68-187-7	C33H68	465.080
2,2,4,4,4-Pentamethyltriacontane	68-189-9	C34H70	479.114
2,2,4,4,4-Pentamethyltriacontane	68-191-1	C35H72	493.148
2,2,4,4,4-Pentamethyltriacontane	68-193-3	C36H74	507.182
2,2,4,4,4-Pentamethyltriacontane	68-195-5	C37H76	521.216
2,2,4,4,4-Pentamethyltriacontane	68-197-7	C38H78	535.250
2,2,4,4,4-Pentamethyltriacontane	68-199-9	C39H80	549.284
2,2,4,4,4-Pentamethyltriacontane	68-201-1	C40H82	563.318

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