Waters™

Nota applicativa

Multi-Residue Analysis of Pharmaceuticals, Personal Care Products (PPCPs) and Pesticides in Water by Direct Injection Using LC-MS/MS

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Abstract

In this application note, we investigate a list of over 190 pharmaceuticals, and personal care products (PPCPs) and pesticides (including their degradation products) in both drinking and surface water using a direct aqueous injection, multi-residue LC-MS/MS technique. This method addresses the continuously evolving European Union (EU) Water Framework and Drinking Water Directives and Watch Lists, which aim to establish regulatory standards and enhance the data used for identifying and monitoring an expanding list of substances of concern.

A method performance study was conducted using the ACQUITY™ Premier System paired with the Xevo™ TQ Absolute Tandem Quadrupole Mass Spectrometer and electrospray ionization (ESI) on three typical water matrices: tap water, surface water, and bottled mineral water. The performance of all analytes was evaluated at three spike levels (10, 25, and 125 ng/L), with six replicates for each level. For the most complex matrix, river water, the average method performance for trueness was 92%, with values ranging from 57% to 131% across all spike levels. The average trueness RSD was 5%, with 99% of all sample types and fortification levels showing an RSD below 20%.

Benefits

- Sensitivity of Xevo TQ Absolute allows for the trace level detection of PPCPs and pesticides in drinking and surface waters without the need for lengthy clean-up or concentration steps
- The direct injection approach increases productivity and provides faster turn-around time for reporting of results while being well aligned with green analytical chemistry principles
- More than 150 analytes reach limits of quantification of 10 ng/L, making this method suitable for screening for multi-class analytes in water matrices

Introduction

In recent years, there has been increasing concern about the presence of pesticides, pharmaceuticals and personal care products (PPCPs) in water bodies throughout the world.[1] The effect of these emerging contaminants on human health and their potential impact on the environment is not yet fully understood.

The updated Drinking Water Directive entered into force in January 2021 and is the EU's main law for drinking water. The Directive applies to all water, either in its original state or after treatment, intended for drinking, cooking, food preparation or other domestic purposes, regardless of its origin and whether it is supplied from a distribution network, supplied from a tanker or put into bottles or containers.[2] It further protects human health thanks to updated water quality standards, in accordance with World Health Organisation (WHO) recommendations, addressing emerging pollutants, such as endocrine disruptors, and promoting a preventive, risk-based approach to reduce pollution at its source.

Water bodies such as rivers, lakes and groundwaters have their status defined in the EU Water Framework Directive.[3] An amendment to Directive 2013/39/EU sets environmental quality standards for hazardous substances that require monitoring in these waters. A Commission Implementing Decision[4] document, 2022/1307, includes Watch List analytes with Maximum Acceptable Method Detection Limits for compounds of concern across multiple chemical classes.

Numerous studies have demonstrated that PPCPs are present at parts-per-trillion (PPT) levels in rivers and streams highlighting the need for methods that are able to detect compounds at these trace levels.[5-10] In addition to the low-level detection of these compounds, a major analytical challenge lies in the wide chemical diversity of chemicals of concern. Furthermore, to establish a more complete understanding of water pollution it is necessary to monitor a wide variety of types of water.

This application note demonstrates the direct injection, separation and detection of PPCPs and pesticides including acidic, basic, and neutral compounds from multiple regulated analyte lists in a variety of water types.

Experimental

Sample Description

Water samples were collected from sources of known soft and hard water areas and from surface water locations in the UK. Mineral water was purchased from a UK retail outlet and stored in its original container. All samples were stored in refrigerated conditions.

Prior to analysis, acetic acid was added to the samples to a final concentration of 0.01%. The samples were then aliquoted into glass autosampler vials and sealed with preslit PTFE/silicon septa caps (p/n: 186005666CV < https://www.waters.com/nextgen/global/shop/vials-containers--collection-plates/186005666cv-truview-lcms-certified-clear-glass-12-x-32-mm-screw-neck-vial-wi.html>) for direct injection by UPLC-MS/MS.

Method Condition

Matrix-matched calibration standards were prepared in bottled mineral water at nine concentrations: 5, 10, 20, 50, 75, 100, 200, 500, and 1000 ng/L and used across all assessments. Spiked samples were prepared in all three matrices with 6 replicates at each level fortified with all compounds at 10, 25 and 125 ng/L. These levels were

chosen based on the typical contaminant levels expected in the samples. Internal standards were not included in this method.

Quantification of spiked samples was by matrix bracketed calibration. Bottled mineral water was used to create matrix-matched calibration standards throughout as it contained the fewest incurred contaminant levels compared to other matrices screened. Optimum dwell time for target compounds were determined by the auto dwell function.

LC Conditions

LC system:	ACQUITY Premier FTN
Vials:	TruView pH control LCMS certified clear glass 12 x 32 mm screw neck vial, with cap and preslit PTFE/silicone septum (p/n: 186005666CV)
Column:	ACQUITY™ Premier HSS T3 Column 1.8 µm, 2.1 x 100 mm (p/n: 186009468)
Column temperature.:	45 ºC
Sample temperature.:	10 ºC
Injection volume:	20 µL
Flow rate:	0.500 mL/min
Mobile phase A:	0.01% acetic acid in water
Mobile phase B:	0.01% acetic acid in 50:50 v/v methanol:acetonitrile

Gradient Table

Time (min)	%A	%B	Curve
0.00	99	1	Initial
0.50	99	1	6
3.50	60	40	6
12.50	15	85	6
12.60	1	99	6
15.00	1	99	6
15.10	99	1	6
19.00	99	1	6

MS Conditions

MS system:	Xevo TQ Absolute
Ionization mode:	ESI+ and ESI-
Capillary voltage:	Positive ion +0.5 kV, negative ion -0.5 kV
Desolvation temperature:	550 ºC
Source temperature:	140 ºC
Desolvation gas flow:	1000 L/hr
Cone gas flow:	150 L/hr
MRM method:	See Appendix

Data Management

Software:	waters_connect™ for Quantitation Software

Results and Discussion

Despite the chemical diversity of the compounds analyzed, the method demonstrated retention complying with the requirements in the ISO 21253–2:2019 standard for water quality as applied to multi-compound class methods[11], exhibiting Gaussian chromatographic peak shapes and good retention time stability throughout the study, independent of water type, as demonstrated in Figure 1. Fast polarity switching maximized compound coverage and the speed of switching ensured that good peak definition was obtained with sufficient data points across peaks in both positive and negative mode.

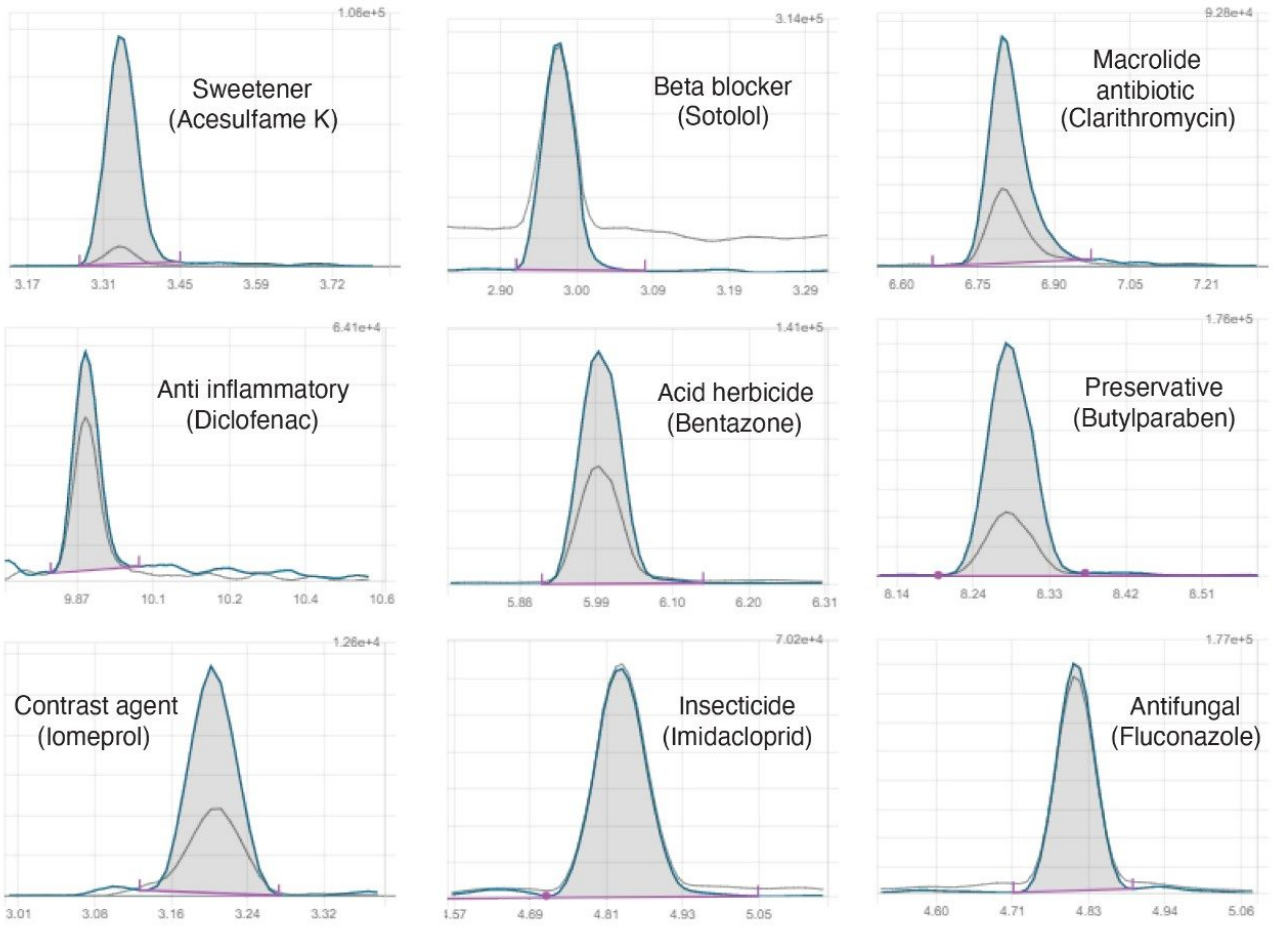

Figure 1. Representative chromatograms from different compound classes at 10 ng/L in mineral water.

Effect of sample composition on peak shape and sensitivity

To ensure optimal conditions for a diverse range of compounds with varying physiochemical properties, it is necessary to assess multiple parameters. During the study, the addition of various organic diluents to the aqueous sample was evaluated. It was observed that certain compounds, such as macrolide antibiotics, benefited from higher levels of organic content. However, it was found that a 100% aqueous composition was optimal for many compounds and proved to be the most practical choice, minimizing contamination risk and enhancing the method's efficiency. Furthermore, a small amount of acetic acid, similar to the content in the mobile phase, was added to each sample. This acidification improved the peak shape of certain compounds, such as Amoxicillin and Asulam. However, it was found to suppress the signal of some compounds, such as

Aldicarb. Optimization of these types of method conditions must be evaluated on a case-by-case basis taking into consideration the specific analyte list required for monitoring.

To improve the peak shape of the early eluting compounds, a 50 µL extension loop assembly (p/n: 430002012 < https://www.waters.com/nextgen/global/shop/service-parts--kits/430002012-assembly-extension-loop-50--l.html>) was installed between the injector valve and the analytical column. This provides extra system volume for thorough mixing of the sample aliquot in the mobile phase prior to loading onto the column.

Method Performance Study Results

Using matrix-matched calibration standards in bottled mineral water, 98% of 194 compounds could be described using a linear regression model with 1/X weighting, with residuals within ±20%. Either $1/X^2$ weighting or a second-order regression was used for the remaining analytes.

Most compounds (97%) displayed a coefficient of determination (R^2) value greater than 0.99 (>88% of compounds met criteria above 0.995). Example calibration curves and residuals across several compound classes are shown in Figure 2.

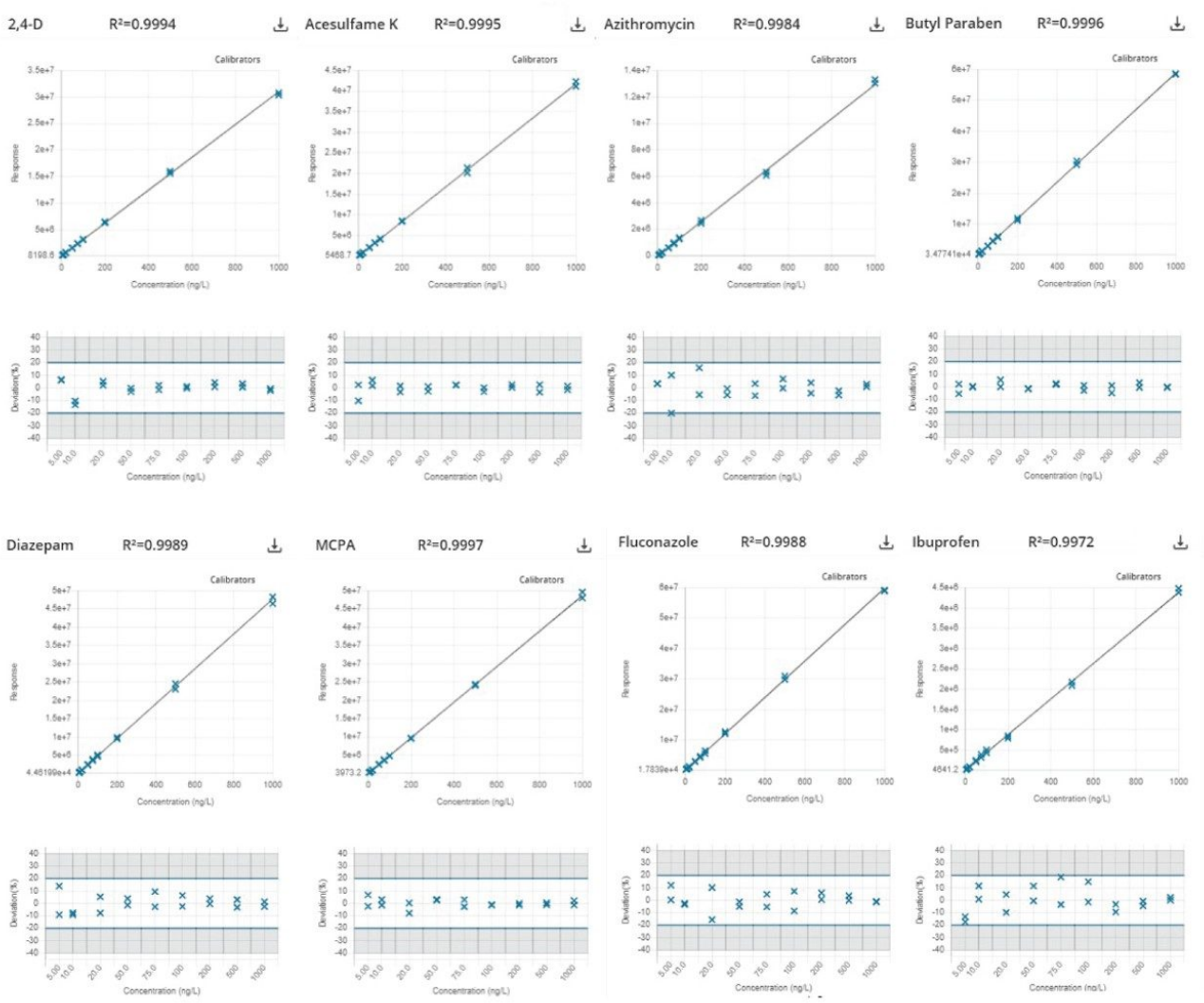

Figure 2. Calibration curves for representative compounds from different classes prepared in bottled mineral water over a concentration range of 5 to 1000 ng/L.

It was suspected that contributing factors to the compounds that fell below this coefficient of determination were solubility and stability. Daily preparation of standards was found to reduce these effects. Minimal matrix effects and losses throughout the run were observed, however, the use of internal standards would improve accuracy and account for these types of losses.

Figure 3 shows an example of Metconazole in different matrix samples. Peak shape and retention times were consistent while showing very little matrix effects.

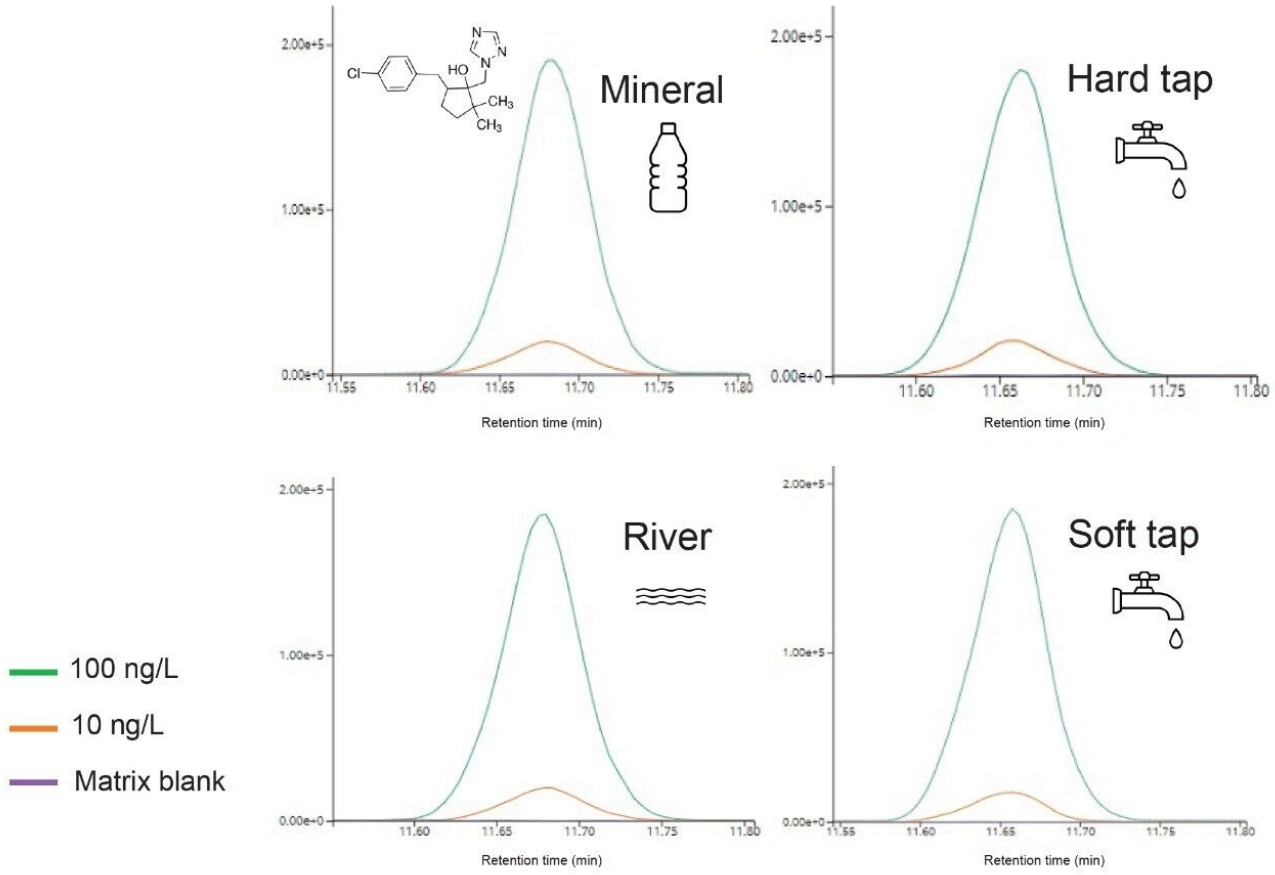

Figure 3. Triazole fungicide Metconazole, an analyte in the surface water watch list with a maximum acceptable method detection limit of 29 ng/L. At 10 ng/L S/N ratio (PtP) is >100 for all matrices.

The method's performance was evaluated across three validation batches, covering typical water types - soft and hard drinking water, and surface water. Each of the batches contained six spiked samples at three levels - 10, 25, and 125 ng/L. Among independent compounds and levels, 97% of spiked samples fell within the acceptable tolerance range of 70% to 120% (ISO 21253–2:2019). The data from the most complex matrix tested, surface water at three spike levels, is displayed in Figure 4.

Trueness of the method was assessed from the recovery samples. For bottled and tap water matrices 154 analytes achieved acceptable recoveries while for surface water 74 analytes succeeded. The percentage RSD values for the recovery data in surface water batch referenced above are summarized by error bars in Figure 4.

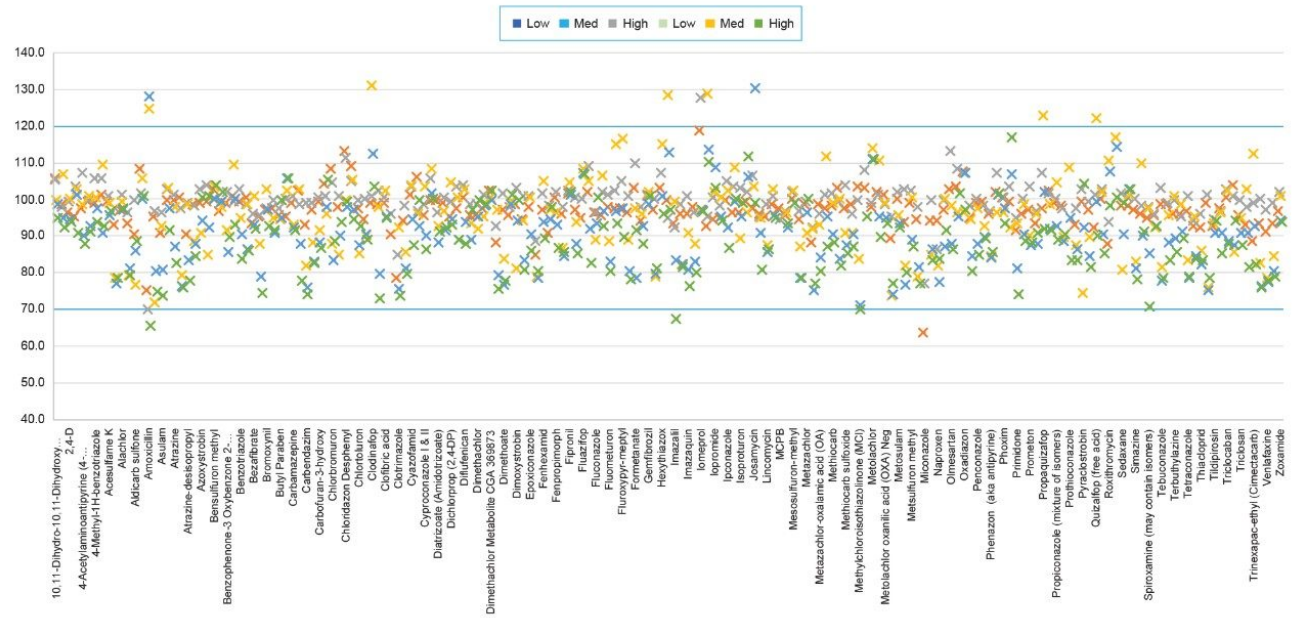

Figure 4. Trueness for surface water fortified at 10, 25 and 125 ng/L. Blue bars represent the acceptable recovery range of 70–120% (n=6).

Retention time for all analytes across the 3 method validation batches was stable, regardless of water type, with no significant change to peak shape (overall retention time within 3.2% RSD).

Conclusion

The updated EU Drinking Water and Water Framework Directives provide the regulatory framework for effective monitoring and management of water quality and include provisions for emerging contaminants. Ensuring compliance with these regulations and comprehensive coverage for an ever increasing analyte lists requires versatile, robust analytical methods and high performance LC/MS/MS systems. The direct-injection method investigated in this work is effective at detection of a wide range of PPCPs and pesticides at trace levels suitable for monitoring multiple water types for the presence of compound classes known or suspected to pose risks to human and environmental health. It further provides more rapid turn around time and greener operation than methods that rely upon high volumes of solvent and extensive sample preparation. Method performance was

assessed using criteria described in ISO 21253–2:2019. The calibration characteristics, linearity, and residuals were excellent over the concentration range studied. Accuracy and precision were evaluated at three matrix QC levels with six replicate spikes and found to provide excellent performance for 154 analytes in tap and bottled water and 74 analytes in surface water matrix.

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APPENDIX

MRM transitions for the analytes included in this app note. Optimum dwell time for target compounds was set automatically using the auto-dwell function so values may vary depending on acquisition windows. Quantitative transitions are in bold font. Analytes in ***blue italics*** are included in the EU WFD Annexes of October 26, 2022 (Document 52022PC0540).

Analyte	Ionization	Precursor (m/z)	Product (m/z)	Cone voltage (V)	Collision energy (eV)	Soft transmission enabled
10,11-Dihydro-10,11-Dihydroxy Carbamazepine	ESI+	271.0	180.1	15	30	
10,11-Dihydro-10,11-Dihydroxy Carbamazepine	**ESI+**	**271.0**	**236.0**	**15**	**10**	
2,4,5-T	ESI-	252.8	158.9	18	27	X
2,4,5-T	**ESI-**	**252.8**	**194.9**	**18**	**13**	**X**
2,4-D	ESI-	219.0	125.0	26	26	X
2,4-D	**ESI-**	**219.0**	**161.0**	**26**	**13**	**X**
2,4-DB	**ESI-**	**161.0**	**125.0**	**30**	**10**	
2,4-DB	ESI-	247.0	161.0	30	15	
4-Acetylaminoantipyrine (4-Acetamidoantipyrine)	ESI+	246.1	104.0	23	22	
4-Acetylaminoantipyrine (4-Acetamidoantipyrine)	**ESI+**	**246.1**	**228.1**	**23**	**13**	
4-Formylaminoantipyrine	**ESI+**	**232.1**	**104.0**	**28**	**21**	
4-Formylaminoantipyrine	ESI+	232.1	214.1	28	13	
4-Methyl-1H-benzotriazole	**ESI+**	**134.0**	**77.0**	**40**	**18**	
4-Methyl-1H-benzotriazole	ESI+	134.0	79.0	40	22	
Acephate	**ESI+**	**184.1**	**49.0**	**20**	**20**	**X**
Acephate	ESI+	184.1	143.0	20	10	X
Acesulfame K	ESI-	162.0	77.8	10	24	
Acesulfame K	**ESI-**	**162.0**	**81.8**	**10**	**14**	
Acetamiprid	*ESI+*	*223.0*	*56.1*	*30*	*15*	
Acetamiprid	***ESI+***	***223.0***	***126.0***	***30***	***20***	
Alachlor	**ESI+**	**270.2**	**162.1**	**2**	**20**	
Alachlor	ESI+	270.2	238.1	2	10	
Aldicarb	**ESI+**	**213.1**	**89.1**	**35**	**20**	
Aldicarb	ESI+	213.1	116.1	35	11	
Aldicarb sulfone	**ESI+**	**223.0**	**86.0**	**35**	**14**	X
Aldicarb sulfone	ESI+	223.0	148.0	35	10	X
Aldicarb sulfoxide	ESI+	207.0	89.0	20	15	
Aldicarb sulfoxide	**ESI+**	**207.0**	**132.0**	**20**	**5**	
Amoxicillin	ESI+	366.2	114.0	30	20	
Amoxicillin	**ESI+**	**366.2**	**349.1**	**30**	**8**	
Ampyrone (4-aminoantipyrine)	**ESI+**	**204.0**	**56.0**	**33**	**20**	
Ampyrone (4-aminoantipyrine)	ESI+	204.0	94.0	33	20	
Asulam	ESI+	230.9	92.0	22	22	X
Asulam	**ESI+**	**230.9**	**155.9**	**22**	**12**	X
Atenolol	ESI+	267.2	145.1	40	25	
Atenolol	**ESI+**	**267.2**	**190.1**	**40**	**20**	
Atrazine	*ESI+*	*216.1*	*96.1*	*39*	*23*	
Atrazine	***ESI+***	***216.1***	***174.1***	***39***	***18***	
Atrazine-desethyl	ESI+	188.0	78.9	34	26	
Atrazine-desethyl	**ESI+**	**188.0**	**146.0**	**34**	**16**	
Atrazine-desisopropyl	ESI+	174.0	78.9	40	18	
Atrazine-desisopropyl	**ESI+**	**174.0**	**96.0**	**40**	**18**	
Azithromycin	***ESI+***	***749.5***	***158.2***	***30***	***40***	
Azithromycin	*ESI+*	*749.5*	*591.5*	*30*	*30*	
Azoxystrobin	ESI+	404.1	328.9	15	30	
Azoxystrobin	**ESI+**	**404.1**	**372.0**	**15**	**16**	
Benalaxyl (Benalaxyl-M)	ESI+	326.1	91.0	25	30	
Benalaxyl (Benalaxyl-M)	**ESI+**	**326.1**	**148.0**	**25**	**20**	
Bensulfuron methyl	**ESI+**	**411.1**	**149.0**	**27**	**22**	
Bensulfuron methyl	ESI+	411.1	182.0	27	20	
Bentazone	**ESI-**	**238.9**	**132.1**	**30**	**24**	
Bentazone	ESI-	238.9	175.0	30	20	
Benzophenone-3	ESI+	229.1	105.0	40	20	
Benzophenone-3	**ESI+**	**229.1**	**151.0**	**40**	**20**	
Benzophenone-4 (Sulisobenzone)	ESI-	307.0	211.0	40	20	
Benzophenone-4 (Sulisobenzone)	**ESI-**	**307.0**	**227.0**	**40**	**20**	
Benzotriazole	**ESI+**	**120.1**	**65.0**	**40**	**20**	
Benzotriazole	ESI+	120.1	92.0	28	14	
Benzyl Paraben	ESI+	229.0	65.0	28	40	
Benzyl Paraben	**ESI+**	**229.0**	**151.0**	**28**	**22**	

Analyte	Ionization	Precursor (m/z)	Product (m/z)	Cone voltage (V)	Collision energy (eV)	Soft transmission enabled
Bezafibrate	ESI-	360.1	154.0	33	30	
Bezafibrate	**ESI-**	**360.1**	**274.0**	**33**	**15**	
Bisoprolol	ESI+	326.0	74.0	25	22	
Bisoprolol	**ESI+**	**326.0**	**116.0**	**25**	**16**	
Bromoxynil	ESI-	275.8	78.8	48	30	
Bromoxynil	**ESI-**	**275.8**	**80.8**	**48**	**30**	
Buturon	**ESI+**	**237.1**	**84.1**	**32**	**16**	
Buturon	ESI+	237.1	126.0	32	30	
Butyl Paraben	**ESI-**	**193.0**	**92.0**	**30**	**20**	
Butyl Paraben	ESI-	193.1	135.9	20	16	
Candesartan	**ESI+**	**441.0**	**263.0**	**24**	**12**	
Candesartan	ESI+	441.0	423.0	24	12	
Carbamazepine	*ESI+*	*237.0*	*179.0*	*38*	*34*	
Carbamazepine	***ESI+***	***237.1***	***194.1***	***34***	***20***	
Carbaryl	ESI+	202.0	117.0	20	25	X
Carbaryl	**ESI+**	**202.0**	**145.0**	**20**	**10**	**X**
Carbendazim	ESI+	192.1	132.1	10	30	
Carbendazim	**ESI+**	**192.1**	**160.1**	**10**	**15**	
Carbofuran	ESI+	222.1	123.0	5	20	
Carbofuran	**ESI+**	**222.1**	**165.1**	**5**	**10**	
Carbofuran-3-hydroxy	ESI+	238.1	163.0	30	15	
Carbofuran-3-hydroxy	**ESI+**	**238.1**	**181.0**	**30**	**10**	
Chlorantraniliprole	**ESI+**	**481.9**	**283.9**	**25**	**15**	
Chlorantraniliprole	ESI+	481.9	450.9	25	15	
Chlorbromuron	ESI+	292.9	182.0	30	16	
Chlorbromuron	**ESI+**	**292.9**	**203.9**	**30**	**18**	
Chloridazon	ESI+	222.0	77.0	56	30	
Chloridazon	**ESI+**	**222.0**	**92.0**	**56**	**30**	
Chloridazon Desphenyl	ESI+	145.8	54.1	23	20	
Chloridazon Desphenyl	**ESI+**	**145.8**	**116.9**	**23**	**20**	
Chloridazon-methyl-desphenyl	**ESI+**	**159.9**	**87.9**	**25**	**26**	
Chloridazon-methyl-desphenyl	ESI+	159.9	116.4	25	22	
Chlortoluron	ESI+	213.0	46.0	25	15	
Chlortoluron	**ESI+**	**213.0**	**72.0**	**25**	**15**	
Ciprofloxacin	**ESI+**	**332.1**	**288.1**	**35**	**18**	
Ciprofloxacin	ESI+	332.1	314.1	35	22	
Clarithromycin	*ESI+*	*748.5*	*590.5*	*30*	*18*	
Clarithromycin	***ESI+***	***748.5***	***158.1***	***30***	***25***	
Clodinafop	ESI+	312.0	238.2	42	24	
Clodinafop	**ESI+**	**312.0**	**265.8**	**42**	**16**	
Clodinafop-propargyl	ESI+	350.0	91.0	36	32	
Clodinafop-propargyl	**ESI+**	**350.0**	**266.0**	**36**	**16**	
Clofibric acid	ESI-	212.9	84.9	18	10	X
Clofibric acid	**ESI-**	**212.9**	**127.0**	**18**	**15**	X
Clopyralid	ESI+	191.9	110.0	30	30	
Clopyralid	**ESI+**	**191.9**	**145.9**	**30**	**20**	
Clotrimazole	**ESI+**	**277.1**	**165.2**	**40**	**27**	
Clotrimazole	ESI+	277.1	241.0	40	28	
Cyanazine	ESI+	241.0	96.0	41	25	
Cyanazine	**ESI+**	**241.0**	**214.0**	**41**	**17**	
Cyazofamid	**ESI+**	**325.0**	**107.9**	**25**	**15**	
Cyazofamid	ESI+	325.0	261.0	25	10	
Cyclamate (Sodium cyclamate)	**ESI-**	**178.1**	**79.9**	**56**	**24**	
Cyclamate (Sodium cyclamate)	ESI-	178.1	95.0	56	14	
Cyproconazole I & II	**ESI+**	**292.2**	**70.2**	**5**	**20**	
Cyproconazole I & II	ESI+	292.2	125.1	5	30	
Cyromazine	**ESI+**	**167.0**	**60.2**	**40**	**20**	
Cyromazine	ESI+	167.0	68.1	40	25	
Cyromazine	ESI+	167.0	108.1	35	20	
Diatrizoate (Amidotrizoate)	**ESI+**	**614.5**	**360.9**	**53**	**18**	
Diatrizoate (Amidotrizoate)	ESI+	614.5	487.8	53	10	
Diazepam	**ESI+**	**285.0**	**154.0**	**25**	**26**	
Diazepam	ESI+	285.0	193.1	25	30	
Dichlorprop (2,4-DP)	ESI-	233.0	125.0	28	25	X

Analyte	Ionization	Precursor (m/z)	Product (m/z)	Cone voltage (V)	Collision energy (eV)	Soft transmission enabled
Dichlorprop (2,4-DP)	**ESI-**	**233.0**	**161.0**	**28**	**13**	**X**
Diclofenac	***ESI+***	***296.0***	***214.0***	***23***	***30***	
Diclofenac	*ESI+*	*296.0*	*250.0*	*23*	*12*	
Diflufenican	ESI+	395.0	246.0	28	36	
Diflufenican	**ESI+**	**395.0**	**266.0**	**28**	**24**	
Dimefuron	**ESI+**	**339.0**	**72.0**	**42**	**26**	
Dimefuron	ESI+	339.0	166.9	42	20	
Dimethachlor	ESI+	256.2	148.2	29	25	
Dimethachlor	**ESI+**	**256.2**	**224.2**	**29**	**15**	
Dimethachlor ESA Metabolite (CGA 354742)	**ESI-**	**299.9**	**79.8**	**38**	**28**	
Dimethachlor ESA Metabolite (CGA 354742)	**ESI-**	**299.9**	**120.9**	**38**	**22**	
Dimethachlor Metabolite CGA 369873	ESI-	242.0	79.9	33	28	
Dimethachlor Metabolite CGA 369873	ESI-	242.0	121.0	33	18	
Dimethachlor OA	ESI+	252.0	132.1	18	24	
Dimethachlor OA	**ESI+**	**252.0**	**220.1**	**18**	**12**	
Dimethoate	ESI+	230.0	124.8	20	22	X
Dimethoate	**ESI+**	**230.0**	**198.8**	**20**	**10**	**X**
Dimethomorph I & II	ESI+	388.1	165.0	30	30	
Dimethomorph I & II	**ESI+**	**388.1**	**301.0**	**30**	**20**	
Dimoxystrobin	ESI+	327.1	116.1	20	21	
Dimoxystrobin	**ESI+**	**327.1**	**205.2**	**20**	**10**	
Diuron	*ESI+*	*233.0*	*46.3*	*35*	*15*	
Diuron	***ESI+***	***233.0***	***72.1***	***25***	***18***	
Epoxiconazole	ESI+	330.0	101.0	15	50	
Epoxiconazole	**ESI+**	**330.0**	**121.0**	**15**	**22**	
Erythromycin (mix of A, B and C isomers)	***ESI+***	***734.2***	***158.1***	***33***	***30***	
Erythromycin (mix of A, B and C isomers)	*ESI+*	*734.2*	*576.2*	*33*	*19*	
Ethofumesate	**ESI+**	**287.1**	**121.1**	**25**	**15**	
Ethofumesate	ESI+	287.1	259.1	25	10	
Famoxadone	**ESI+**	**392.2**	**238.0**	**20**	**15**	
Famoxadone	ESI+	392.2	331.1	20	10	
Fenhexamid	ESI+	302.0	55.2	35	35	
Fenhexamid	**ESI+**	**302.0**	**97.1**	**35**	**25**	
Fenoprop (2,4,5-TP)	**ESI-**	**267.0**	**195.0**	**28**	**15**	**X**
Fenoprop (2,4,5-TP)	ESI-	268.9	196.9	28	15	X
Fenpropimorph	ESI+	304.2	57.2	25	30	
Fenpropimorph	**ESI+**	**304.2**	**147.1**	**25**	**30**	
Fenuron	ESI+	165.0	45.9	15	15	
Fenuron	**ESI+**	**165.0**	**71.9**	**15**	**15**	
Fipronil	ESI-	434.7	249.9	33	28	
Fipronil	**ESI-**	**434.7**	**329.8**	**33**	**17**	
Florasulam	ESI+	360.0	108.9	40	50	
Florasulam	**ESI+**	**360.0**	**129.0**	**40**	**22**	
Fluazifop	**ESI+**	**328.1**	**254.1**	**30**	**26**	
Fluazifop	ESI+	328.1	282.1	30	16	
Fluazifop-butyl and Fluazifop-P-butyl	**ESI+**	**384.1**	**282.1**	**38**	**22**	
Fluazifop-butyl and Fluazifop-P-butyl	ESI+	384.1	328.1	38	16	
Fluconazole	**ESI+**	**307.1**	**220.1**	**28**	**20**	
Fluconazole	ESI+	307.1	238.0	28	14	
Flufenacet	ESI+	364.0	152.1	25	20	
Flufenacet	**ESI+**	**364.0**	**194.1**	**25**	**10**	
Fluometuron	ESI+	233.0	46.1	28	15	
Fluometuron	**ESI+**	**233.0**	**72.0**	**28**	**17**	
Fluroxypyr	ESI-	252.7	158.9	18	28	X
Fluroxypyr	**ESI-**	**252.7**	**194.9**	**18**	**15**	**X**
Fluroxypyr-meptyl	ESI+	367.0	181.0	21	32	
Fluroxypyr-meptyl	**ESI+**	**367.0**	**254.9**	**21**	**11**	
Flurtamone	ESI+	334.0	178.0	44	45	
Flurtamone	**ESI+**	**334.0**	**247.0**	**44**	**27**	

Analyte	Ionization	Precursor (m/z)	Product (m/z)	Cone voltage (V)	Collision energy (eV)	Soft transmission enabled
Flutriafol	**ESI+**	**302.1**	**70.1**	**25**	**16**	
Flutriafol	ESI+	302.1	122.9	25	30	
Formetanate	ESI+	222.0	46.0	30	26	
Formetanate	**ESI+**	**222.0**	**165.0**	**30**	**15**	
Gabapentin	**ESI+**	**172.1**	**137.1**	**25**	**15**	
Gabapentin	ESI+	172.1	154.1	24	14	
Gemfibrozil	**ESI-**	**249.0**	**121.1**	**18**	**15**	**X**
Gemfibrozil	ESI-	249.0	127.1	18	10	X
Hexazinone	ESI+	253.1	71.0	25	30	
Hexazinone	**ESI+**	**253.1**	**171.1**	**25**	**16**	
Hexythiazox	ESI+	353.0	168.1	10	25	
Hexythiazox	**ESI+**	**353.0**	**228.1**	**10**	**15**	
Ibuprofen	*ESI-*	*205.1*	*161.1*	*10*	*5*	*X*
Ibuprofen	***ESI-***	***273.0***	***161.1***	***40***	***13***	***X***
Imazalil	ESI+	297.0	69.0	25	20	
Imazalil	**ESI+**	**297.0**	**159.0**	**25**	**20**	
Imazamox	ESI+	306.0	193.0	38	24	
Imazamox	**ESI+**	**306.0**	**261.0**	**38**	**20**	
Imazaquin	ESI+	312.2	86.2	40	28	
Imazaquin	**ESI+**	**312.2**	**267.2**	**40**	**20**	
Imidacloprid	***ESI+***	***256.1***	***174.9***	***25***	***20***	
Imidacloprid	*ESI+*	*256.1*	*209.0*	*25*	*12*	
Iomeprol	**ESI+**	**777.6**	**404.9**	**70**	**40**	
Iomeprol	ESI+	777.6	531.8	70	30	
Iopamidol	ESI+	777.6	386.9	70	38	
Iopamidol	**ESI+**	**777.6**	**558.8**	**70**	**24**	
Iopromide	**ESI+**	**791.6**	**299.8**	**75**	**60**	
Iopromide	ESI+	791.6	572.7	75	24	
Ioxynil	**ESI-**	**369.7**	**126.8**	**40**	**30**	
Ioxynil	ESI-	369.7	215.0	40	30	
Ipconazole	**ESI+**	**334.2**	**70.0**	**50**	**25**	
Ipconazole	ESI+	334.2	125.0	50	25	
Iprodione	**ESI+**	**329.9**	**244.9**	**31**	**15**	
Iprodione	ESI+	329.9	287.9	31	12	
Isoproturon	*ESI+*	*207.1*	*46.2*	*28*	*15*	
Isoproturon	***ESI+***	***207.1***	***72.0***	***28***	***15***	
Isoxaben	ESI+	333.1	107.1	31	58	
Isoxaben	**ESI+**	**333.1**	**165.1**	**31**	**18**	
Josamycin	**ESI+**	**828.5**	**109.1**	**28**	**46**	
Josamycin	ESI+	828.5	174.2	28	30	
Lamotrigine	ESI+	256.0	145.1	50	38	
Lamotrigine	**ESI+**	**256.0**	**211.1**	**50**	**24**	
Lincomycin	**ESI+**	**407.2**	**126.1**	**30**	**25**	
Lincomycin	ESI+	407.2	359.2	30	15	
MCPA	**ESI-**	**199.0**	**141.0**	**30**	**13**	**X**
MCPA	ESI-	201.0	143.0	30	13	X
MCPB	**ESI-**	**227.0**	**141.0**	**20**	**15**	
MCPB	ESI-	229.0	143.0	20	15	
MCPP (Mecoprop)	ESI-	213.0	71.0	25	15	X
MCPP (Mecoprop)	**ESI-**	**213.0**	**141.0**	**25**	**20**	**X**
Mesosulfuron-methyl	ESI+	504.0	82.9	38	60	
Mesosulfuron-methyl	**ESI+**	**504.0**	**182.0**	**38**	**24**	
Metamitron	ESI+	203.1	104.0	34	22	
Metamitron	**ESI+**	**203.1**	**175.1**	**34**	**16**	
Metazachlor	**ESI+**	**278.0**	**134.0**	**16**	**24**	**X**
Metazachlor	ESI+	278.0	210.0	16	10	X
Metazachlor-oxalamic acid (OA)	**ESI+**	**274.0**	**134.0**	**20**	**18**	**X**
Metazachlor-oxalamic acid (OA)	ESI+	274.0	162.0	20	7	X
Metconazole	**ESI+**	**320.1**	**70.0**	**5**	**25**	
Metconazole	ESI+	320.1	125.0	5	30	
Methiocarb	ESI+	226.1	121.0	20	15	X
Methiocarb	**ESI+**	**226.1**	**169.0**	**20**	**10**	**X**
Methiocarb Sulfone	ESI+	258.1	107.1	40	35	X
Methiocarb Sulfone	**ESI+**	**258.1**	**122.1**	**31**	**19**	**X**
Methiocarb sulfoxide	ESI+	242.0	122.0	26	28	

Analyte	Ionization	Precursor (m/z)	Product (m/z)	Cone voltage (V)	Collision energy (eV)	Soft transmission enabled
Methiocarb sulfoxide	**ESI+**	**242.0**	**185.0**	**26**	**14**	
Methyl Paraben	**ESI-**	**151.1**	**91.8**	**20**	**20**	
Methyl Paraben	ESI-	151.1	135.9	20	14	
Methylchloroisothiazolinone (MCI)	**ESI+**	**150.0**	**115.0**	**30**	**16**	
Methylchloroisothiazolinone (MCI)	ESI+	150.0	118.9	30	18	
Methylisothiazolinone (MIT)	**ESI+**	**115.9**	**70.8**	**30**	**16**	
Methylisothiazolinone (MIT)	ESI+	115.9	100.8	30	18	
Metolachlor	ESI+	284.1	176.1	17	25	
Metolachlor	**ESI+**	**284.1**	**252.1**	**17**	**15**	
Metolachlor ethane sulfonic acid (ESA)	ESI+	330.1	202.1	23	28	X
Metolachlor ethane sulfonic acid (ESA)	**ESI+**	**330.1**	**298.0**	**23**	**15**	**X**
Metolachlor oxanilic acid (OXA)	ESI-	278.0	174.0	18	17	
Metolachlor oxanilic acid (OXA)	**ESI-**	**278.0**	**206.1**	**18**	**12**	
Metoprolol	**ESI+**	**268.2**	**116.1**	**40**	**15**	
Metoprolol	ESI+	268.2	176.1	17	25	
Metosulam	ESI+	418.0	140.0	41	52	
Metosulam	**ESI+**	**418.0**	**175.0**	**41**	**28**	
Metoxuron	**ESI+**	**229.0**	**72.0**	**26**	**18**	
Metoxuron	ESI+	229.0	155.9	26	25	
Metsulfuron methyl	**ESI+**	**382.0**	**167.0**	**28**	**16**	
Metsulfuron methyl	ESI+	382.0	198.9	28	22	
Mevinphos	**ESI+**	**225.1**	**127.1**	**15**	**15**	**X**
Mevinphos	ESI+	225.1	193.1	15	10	X
Miconazole	ESI+	417.1	69.0	40	25	
Miconazole	**ESI+**	**417.1**	**161.1**	**40**	**30**	
N4-Acetylsulfamethoxazole (Acetylsulfamethoxazole)	**ESI+**	**295.9**	**134.1**	**28**	**24**	
N4-Acetylsulfamethoxazole (Acetylsulfamethoxazole)	ESI+	295.9	198.0	28	18	
Naproxen	**ESI-**	**229.1**	**170.1**	**15**	**15**	
Nicosulfuron	*ESI+*	*411.0*	*106.0*	*26*	*32*	
Nicosulfuron	***ESI+***	***411.0***	***182.0***	***26***	***22***	
Olmesartan	**ESI+**	**447.0**	**207.0**	**18**	**22**	
Olmesartan	ESI+	447.0	429.1	18	13	
Omethoate	ESI+	214.0	124.8	25	22	
Omethoate	**ESI+**	**214.0**	**182.8**	**25**	**10**	
Oxadiazon	ESI+	344.9	219.9	50	20	
Oxadiazon	**ESI+**	**344.9**	**302.9**	**50**	**13**	
Oxazepam	ESI+	287.1	104.0	35	36	
Oxazepam	**ESI+**	**287.1**	**241.1**	**30**	**20**	
Penconazole	**ESI+**	**284.0**	**70.1**	**15**	**15**	
Penconazole	ESI+	284.0	159.0	15	25	
Phenazon (aka antipyrine)	**ESI+**	**189.1**	**56.1**	**60**	**26**	
Phenazon (aka antipyrine)	ESI+	189.1	77.0	60	32	
Phenmedipham	**ESI+**	**301.0**	**136.0**	**45**	**20**	**X**
Phenmedipham	ESI+	301.0	168.0	45	10	X
Phoxim	**ESI+**	**299.0**	**129.0**	**12**	**13**	
Phoxim	ESI+	299.0	153.0	12	7	
Picoxystrobin	**ESI+**	**368.0**	**145.1**	**10**	**25**	
Picoxystrobin	ESI+	368.0	205.1	10	10	
Primidone	ESI+	219.2	91.2	29	25	
Primidone	**ESI+**	**219.2**	**162.2**	**29**	**12**	
Prochloraz	ESI+	376.0	70.1	20	25	
Prochloraz	**ESI+**	**376.0**	**307.9**	**20**	**12**	
Prometon	ESI+	226.0	86.3	15	30	
Prometon	**ESI+**	**226.0**	**184.3**	**15**	**20**	
Propamocarb	**ESI+**	**189.1**	**102.0**	**15**	**15**	
Propamocarb	ESI+	189.1	144.0	15	10	
Propaquizafop	**ESI+**	**444.2**	**100.0**	**25**	**20**	
Propaquizafop	ESI+	444.2	163.1	25	60	
Propazine	ESI+	230.2	146.1	40	24	
Propazine	**ESI+**	**230.2**	**188.1**	**40**	**18**	
Propiconazole	ESI+	342.1	69.1	35	30	
Propiconazole	**ESI+**	**342.1**	**158.9**	**35**	**20**	
Propyphenazone (4-Isopropylantipyrine)	**ESI+**	**231.1**	**189.1**	**43**	**20**	
Propyphenazone (4-Isopropylantipyrine)	ESI+	231.1	201.0	43	23	

Analyte	Ionization	Precursor (m/z)	Product (m/z)	Cone voltage (V)	Collision energy (eV)	Soft transmission enabled
Prothioconazole	ESI+	344.0	189.0	20	20	
Prothioconazole	**ESI+**	**344.0**	**326.0**	**20**	**10**	
Pymetrozine	ESI+	218.0	79.0	15	30	
Pymetrozine	**ESI+**	**218.0**	**105.0**	**15**	**20**	
Pyraclostrobin	ESI+	388.1	163.0	25	25	
Pyraclostrobin	**ESI+**	**388.1**	**193.9**	**25**	**12**	
Quinmerac	ESI+	222.2	141.1	17	30	
Quinmerac	**ESI+**	**222.2**	**204.2**	**17**	**15**	
Quizalfop	ESI+	345.0	272.0	34	20	
Quizalfop	**ESI+**	**345.0**	**299.0**	**34**	**28**	
Quizalofop-ethyl	ESI+	373.0	91.1	30	32	
Quizalofop-ethyl	ESI+	373.0	299.1	30	18	
Roxithromycin	**ESI+**	**837.6**	**158.1**	**40**	**35**	
Roxithromycin	ESI+	837.6	679.5	40	20	
Sedaxane	**ESI+**	**332.0**	**159.0**	**13**	**18**	
Sedaxane	ESI+	332.0	292.1	13	15	
Siduron	**ESI+**	**233.0**	**93.8**	**35**	**20**	
Siduron	ESI+	233.0	137.0	35	15	
Simazine	ESI+	202.0	96.0	40	22	
Simazine	**ESI+**	**202.0**	**124.0**	**40**	**16**	
Sotalol (Bentapace)	ESI+	273.1	213.1	25	20	
Sotalol (Bentapace)	**ESI+**	**273.2**	**133.2**	**2**	**24**	
Spiroxamine	ESI+	298.0	100.0	10	32	
Spiroxamine	**ESI+**	**298.0**	**144.0**	**10**	**20**	
Sucralose	**ESI-**	**395.1**	**358.9**	**42**	**12**	
Sucralose	ESI-	397.0	361.0	42	12	
Sulfamethoxazole	ESI+	254.1	92.0	30	25	
Sulfamethoxazole	**ESI+**	**254.1**	**156.0**	**30**	**15**	
Tebuconazole	**ESI+**	**308.2**	**70.1**	**30**	**24**	
Tebuconazole	ESI+	308.2	124.9	30	40	
Temazepam	**ESI+**	**301.1**	**255.1**	**35**	**22**	
Temazepam	ESI+	301.1	283.1	35	15	
Terbuthylazine	ESI+	230.0	96.0	28	28	
Terbuthylazine	**ESI+**	**230.0**	**174.0**	**28**	**16**	
Terbuthylazine-desethyl	ESI+	202.1	79.1	30	26	
Terbuthylazine-desethyl	**ESI+**	**202.1**	**146.1**	**30**	**16**	
Tetraconazole	**ESI+**	**372.0**	**70.1**	**15**	**20**	
Tetraconazole	ESI+	372.0	159.0	15	25	
Thiabendazole	ESI+	202.0	130.9	45	30	
Thiabendazole	**ESI+**	**202.0**	**174.9**	**45**	**25**	
Thiacloprid	ESI+	253.0	90.1	35	35	
Thiacloprid	***ESI+***	***253.0***	***125.8***	***35***	***20***	
Thiacloprid	*ESI+*	*253.0*	*130.9*	*45*	*30*	
Thiamethoxam (isomers)	*ESI+*	*292.0*	*132.0*	*25*	*20*	
Thiamethoxam (isomers)	***ESI+***	***292.0***	***211.1***	***25***	***10***	
Tildipirosin	**ESI+**	**734.3**	**98.1**	**30**	**40**	
Tildipirosin	ESI+	734.3	561.5	30	26	
Tribenuron methyl	**ESI+**	**396.1**	**154.9**	**24**	**14**	
Tribenuron methyl	ESI+	396.1	180.9	24	22	
Triclocaban	ESI-	313.0	126.0	40	24	
Triclocaban	**ESI-**	**313.0**	**160.0**	**40**	**12**	
Triclopyr	ESI-	253.8	195.8	20	10	X
Triclopyr	**ESI-**	**255.9**	**197.8**	**20**	**10**	**X**
Triclosan	***ESI-***	***286.9***	***34.9***	***13***	***8***	
Triclosan	*ESI-*	*286.9*	*142.0*	*13*	*34*	
Trimethoprim	**ESI+**	**291.3**	**123.0**	**40**	**30**	
Trimethoprim	ESI+	291.3	230.2	40	30	
Trinexapac-ethyl (Cimectacarb)	**ESI+**	**252.9**	**69.0**	**33**	**12**	
Trinexapac-ethyl (Cimectacarb)	ESI+	252.9	207.0	33	12	
Tylosin	**ESI+**	**916.2**	**174.1**	**59**	**38**	
Tylosin	ESI+	916.2	772.3	59	30	
Valsartan	ESI+	436.2	207.1	30	20	
Valsartan	**ESI+**	**436.2**	**235.1**	**30**	**15**	
Valsartanic acid	ESI+	267.1	178.1	40	28	
Valsartanic acid	**ESI+**	**267.1**	**206.0**	**40**	**17**	
Venlafaxine	**ESI+**	**278.2**	**58.1**	**30**	**15**	
Venlafaxine	ESI+	278.2	121.0	20	46	
Venlafaxine-O-desmethyl (O-desmethylvenlafaxine)	ESI+	264.2	58.1	30	15	
Venlafaxine-O-desmethyl (O-desmethylvenlafaxine)	ESI+	264.2	107.0	30	30	
Zoxamide	**ESI+**	**336.0**	**158.9**	**30**	**40**	
Zoxamide	ESI+	336.0	186.9	30	25	

Featured Products

ACQUITY Premier System <https://www.waters.com/nextgen/global/products/chromatography/chromatography-systems/acquity-premier-system.html>

Xevo TQ Absolute Triple Quadrupole Mass Spectrometer <https://www.waters.com/nextgen/global/products/mass-spectrometry/mass-spectrometry-systems/xevo-tq-absolute.html>

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