

Chromatography Solutions

Avantor® ACE® HPLC and UHPLC columns Cannabis applications guide



Introduction

As the market for medicinal and recreational cannabis derived products expands globally, there is an ever increasing demand for the detailed analysis of key cannabis components, such as cannabinoids and terpenes, to provide accurate strain identification, potency testing and quality control. In addition, the detection and determination of potential contaminants, such as pesticides, mycotoxins and herbicides, is essential for product safety. The scope of testing and the range of target analytes requiring determination vary from region to region, making cannabis analysis a rapidly evolving and complex challenge. This guide brings together newly-developed key applications, utilising Avantor ACE HPLC and UHPLC column technology, for important analyte classes that require testing in the cannabis industry.

Avantor ACE HPLC and UHPLC columns are manufactured using ultra-inert, base-deactivated silica which delivers exceptional performance and column lifetime. In addition, the extended range of Avantor ACE novel-selectivity stationary phase chemistries provide chromatographers with powerful tools to explore separation selectivity. Avantor ACE columns are therefore ideally suited for application to the varied and complex challenges faced in the analysis of cannabis products.



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Cannabinoids & Terpenes

Cannabis samples are complex and contain several target compound classes that are of interest from analytical and regulatory perspectives. Cannabinoids and terpenes are major components and are therefore of primary importance for potency testing, profiling and strain identification. To date, over 100 cannabinoids and over 140 terpenes have been isolated from cannabis. Regulatory requirements for testing are highly varied and may require determination of several key cannabinoids, for example: Δ^9 -Tetrahydrocannabinol (Δ^9 -THC), Cannabidiol

(CBD), Δ^9 -Tetrahydrocannabinolic acid (THCA), Cannabidiolic acid (CBDA), Cannabigerol (CBG) and Cannabinol (CBN). In this section, analytical methods are presented that may be utilised for the routine determination of key cannabinoid and terpene components required for regulatory compliance and quality control purposes, using LC-MS compatible conditions. Additionally, applications are included for the determination of synthetic cannabinoid components that could potentially be utilised for the adulteration of cannabis products.

10 DIFFERENT CANNABINOIDS AND COMPOUNDS OF INTEREST

APPLICATION AN6850

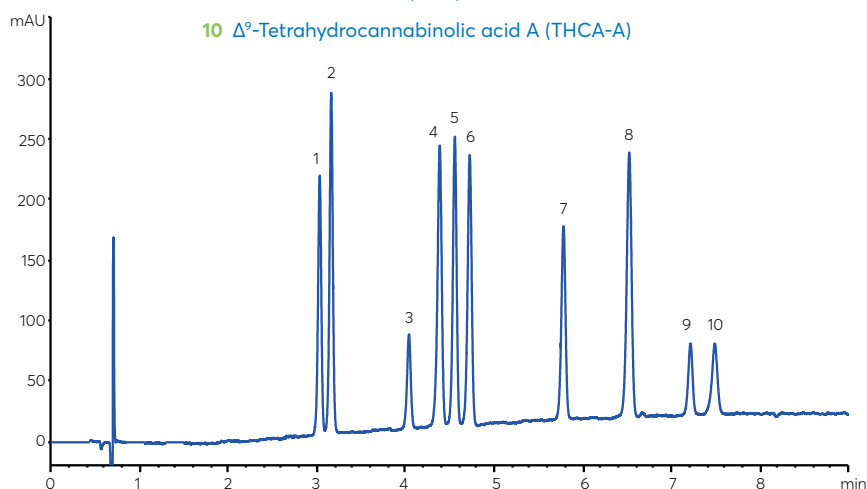


CONDITIONS

Column:	ACE Excel 2 SuperC18	
Dimensions:	100 x 3.0 mm	
Part Number:	EXL-1011-1003U	
Mobile Phase:	A: 0.075% formic acid in H ₂ O B: 0.1% formic acid in MeCN	
Gradient:	Time (mins)	% B
	0.0	70
	1.0	70
	10.0	100
	12.0	100
Flow Rate:	0.6 mL/min	
Injection:	5 μ L	
Temperature:	40 °C	
Detection:	UV, 210 nm	

ANALYTES

- 1 (-)-11-Nor-9-carboxy- Δ^9 -tetrahydrocannabinol (THC-COOH)
- 2 Cannabidivarin (CBDV)
- 3 Cannabidiolic acid (CBDA)
- 4 Cannabigerol (CBG)
- 5 Cannabidiol (CBD)
- 6 Tetrahydrocannabivarin (THCV)
- 7 Cannabinol (CBN)
- 8 (-)-trans- Δ^9 -Tetrahydrocannabinol (THC)
- 9 Cannabichromene (CBC)
- 10 Δ^9 -Tetrahydrocannabinolic acid A (THCA-A)



RAPID CANNABINOIDS ANALYSIS – OVERLAID INJECTIONS

APPLICATION AN6900

UltraCore SuperC18

High pH Stable!

CONDITIONS

Column: **ACE UltraCore 2.5 SuperC18**

Dimensions: 50 x 3.0 mm

Part Number: CORE-25A-0503U

Mobile Phase: A: 0.075% formic acid in H₂O
B: 0.1% formic acid in MeCN

Gradient:	Time (mins)	% B
	0.0	70
	0.25	70
	4.18	100
	5.05	100

Flow Rate: 0.6 mL/min

Injection: 2 µL

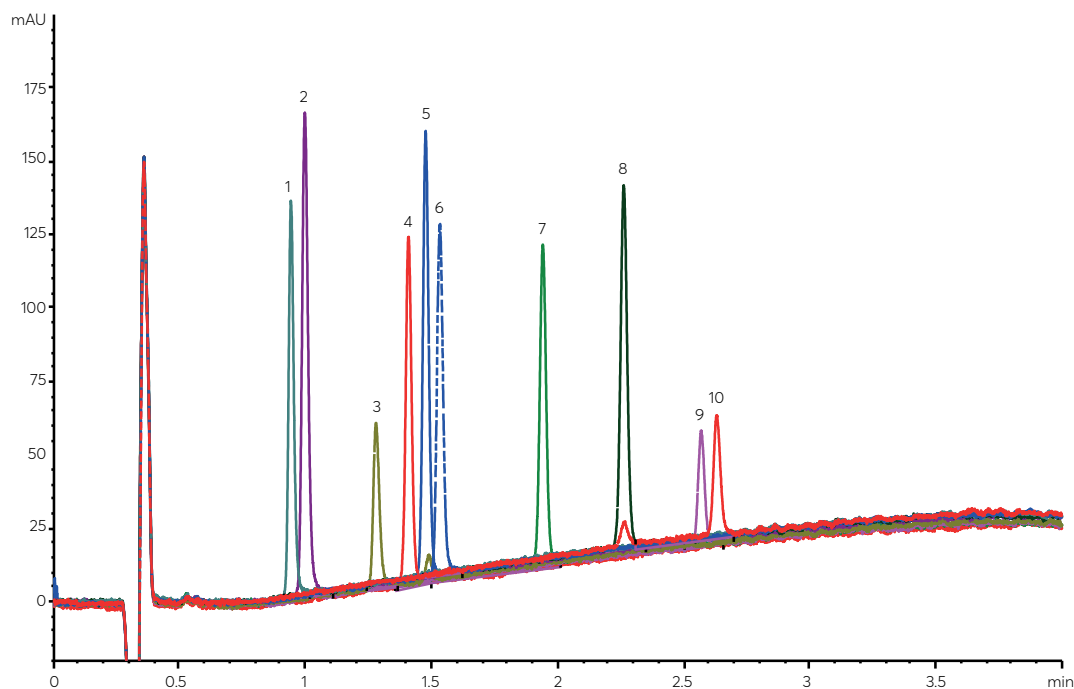
Temperature: 40 °C

Detection: UV, 210 nm

Mass on Column: 20 ng per analyte

ANALYTES

- 1 (-)-11-Nor-9-carboxy- Δ^9 -tetrahydrocannabinol (THC-COOH)
- 2 Cannabidiol (CBD)
- 3 Cannabidiolic acid (CBDA)
- 4 Cannabigerol (CBG)
- 5 Cannabidiol (CBD)
- 6 Tetrahydrocannabivarin (THCV)
- 7 Cannabinol (CBN)
- 8 (-)-trans- Δ^9 -Tetrahydrocannabinol (THC)
- 9 Cannabichromene (CBC)
- 10 Δ^9 -Tetrahydrocannabinolic acid A (THCA-A)



LOW LEVEL DETERMINATION OF CANNABIS USE FROM HAIR SAMPLES

APPLICATION AN7070

ACE C18



CONDITIONS

Column: **ACE Excel 1.7 C18**

Dimensions: 50 x 2.1 mm

Part Number: EXL-171-0502U

Mobile Phase: A: 0.01 % Acetic acid in H₂O
B: 0.01 % Acetic acid in MeOH

Gradient:	Time (mins)	% B
	0.0	50
	0.50	80
	2.00	90
	4.00	90
	4.01	50

Flow Rate: 0.3 mL/min

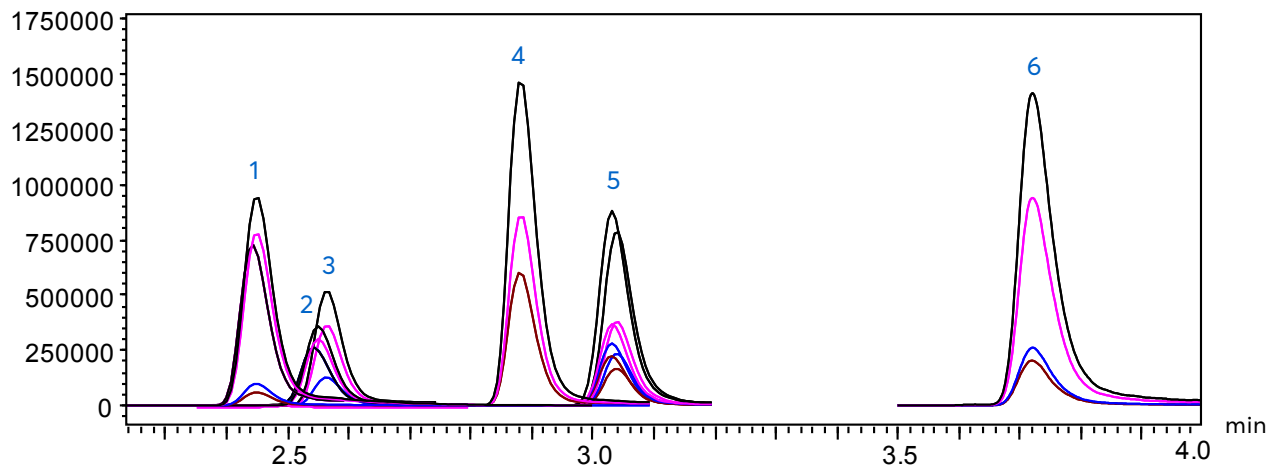
Injection: 5 µL

Temperature: 50 °C

Detection: Shimadzu 8060 Triple Quad MS
MRM, positive and negative ESI modeSample: THC and metabolites extracted from human hair using
matrix micro pulverization and clean up with supported
liquid extraction prior to LC/MS-MS analysis

ANALYTES

- 11-Hydroxy- Δ^9 -tetrahydrocannabinol (THC-OH)
- 11-Nor-9-carboxy- Δ^9 -Tetrahydrocannabinol (THC-COOH)
- Cannabidiol (CBD)
- Cannabinol (CBN)
- Tetrahydrocannabinol (THC)
- Δ^9 -Tetrahydrocannabinolic acid-A (THCA-A)



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SEPARATION OF TERPENES USING LC/MS FRIENDLY CONDITIONS

APPLICATION AN7040

ACE C18-PFP

CONDITIONS

Column: **ACE Excel 2 C18-PFP**

Dimensions: 100 x 3.0 mm

Part Number: EXL-1010-1003U

Mobile Phase: A: 0.1% formic acid in H₂O
B: 0.1% formic acid in MeCN

Gradient:

Time (mins)	% B
0.0	43
3.4	50
5.3	63
9.3	65
12.1	66
13.8	75
16.7	77
19.4	94
28.2	94

Flow Rate: 0.6 mL/min

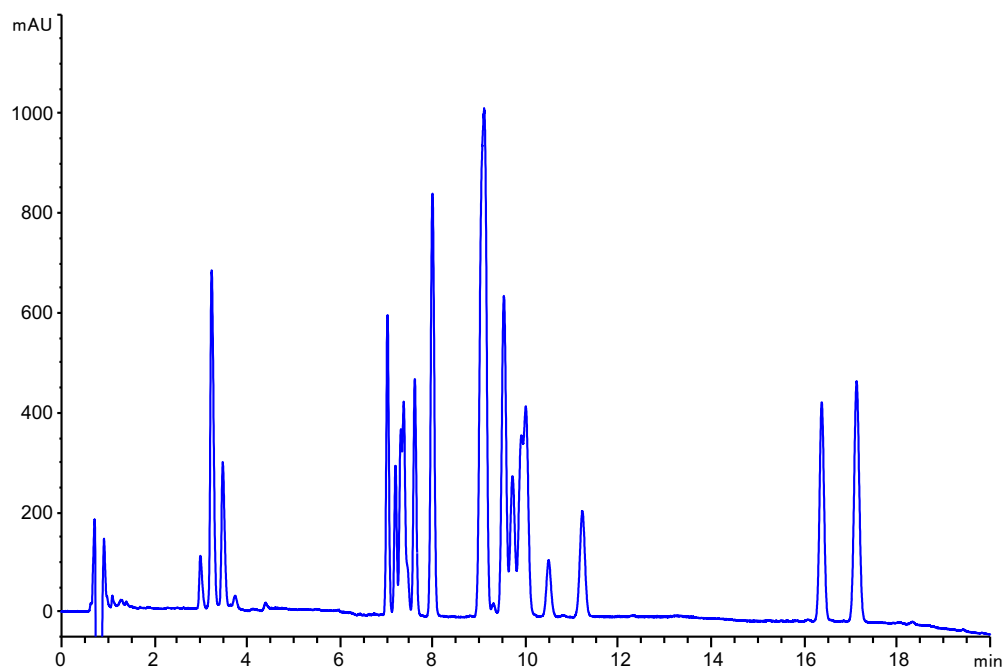
Injection: 2 μ L

Temperature: 30 °C

Detection: UV, 210 nm

ANALYTES

α -Pinene	Camphene
(-)- β -Pinene	β -Mycene
δ -3-Carene	α -Terpinene
D-Limonene	Ocimene
γ -Terpinene	Terpinolene
Linalool	(-)-Isopulegol
Geraniol	β -Caryophyllene
α -Humulene	Nerolidol
(-)-Guaïol	(-)- α -Bisabolol
1,8-Cineole (Eucalyptol)	p-Cymene
(-)-Caryophyllene oxide	



SYNTHETIC CANNABINOIDS BY LC-MS/MS

APPLICATION AN2540

ACE C18-AR

CONDITIONS

Column: **ACE Excel 3 C18-AR**

Dimensions: 100 x 3.0 mm

Part Number: EXL-119-1003U

Mobile Phase: A: 15 mM ammonium formate pH 4.0 in H₂O
B: 0.1% formic acid in MeCN

Gradient:

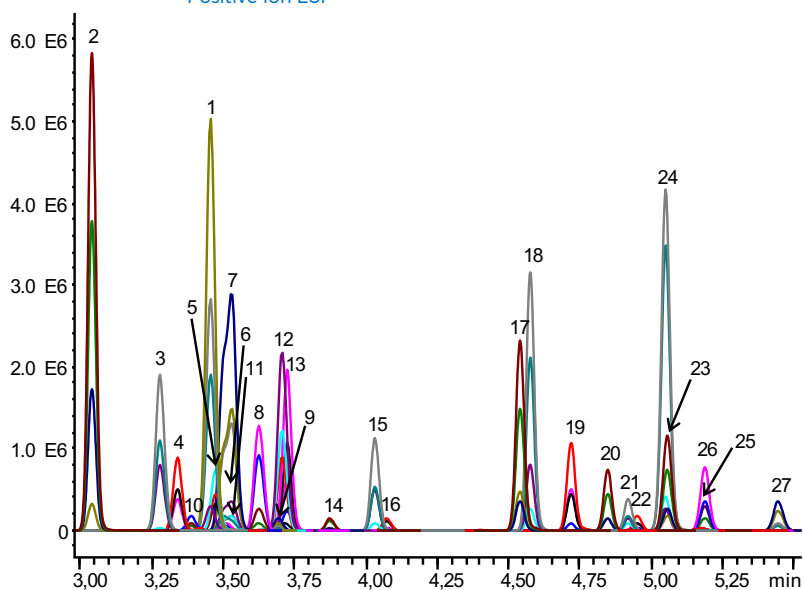
Time (mins)	% B
0.0	40
3.74	90
8.00	90
8.50	40

Flow Rate: 0.5 mL/min

Injection: 10 µL

Temperature: 40 °C

Detection: Shimadzu LCMS 8040 MS
Positive ion ESI



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ANALYTES

- 1 JWH-018 N-5-OH-pentyl-d5 (m/z 362.90 → 155.05; 127.00; 128.05)
- 2 JWH-250 N-5-OH-pentyl (m/z 352.20 → 121.15; 91.10; 186.05)
- 3 JWH-073 N-4-OH-butyl (m/z 344.20 → 155.00; 127.10; 54.95)
- 4 JWH-018 N-pentanoic (m/z 372.20 → 155.05; 127.10)
- 5 JWH-018 N-5-OH-pentyl (m/z 357.80 → 155.05; 127.05)
- 6 AM2201 N-4-OH-pentyl (m/z 376.40 → 155.00; 127.00; 144.00)
- 7 AM2201 5/6-OH-indole (m/z 375.90 → 155.05; 127.05; 248.10)
- 8 JWH-081 N-5-OH-pentyl (m/z 388.20 → 185.05; 157.05; 114.15)
- 9 MAM2201 N-4-OH-pentyl (m/z 389.60 → 169.00; 141.05; 115.15)
- 10 AB-CHMINACA (m/z 356.70 → 241.05; 312.20; 340.15)
- 11 UR-144 N-pentanoic (m/z 341.60 → 125.10; 55.05; 57.10)
- 12 JWH-019 N-6-OH-hexyl (m/z 371.80 → 155.05; 127.00; 144.00)
- 13 JWH-122 N-5-OH-pentyl (m/z 372.20 → 169.05; 141.05; 115.15)
- 14 AKB48 N-pentanoic (m/z 395.60 → 135.00; 93.10; 79.05)
- 15 JWH-018 5-OH-indole (m/z 358.20 → 155.00; 127.05; 230.05)
- 16 AKB48 N-5-OH-pentyl (m/z 381.60 → 135.10; 93.10; 79.05)
- 17 JWH-210 5-OH-indole (m/z 386.10 → 183.05; 153.10; 155.05)
- 18 PB-22 (m/z 358.80 → 214.05; 144.05; 116.00)
- 19 JWH-073 (m/z 328.20 → 127.10; 155.05; 200.10)
- 20 EAM2201 (m/z 387.70 → 183.10; 232.10; 155.10)
- 21 JWH-122 N-4-pentenyl (m/z 353.70 → 169.05; 141.10; 115.10)
- 22 JWH-018 (m/z 341.70 → 155.00; 127.05; 214.10)
- 23 JWH-081 (m/z 372.10 → 185.05; 157.15; 127.10)
- 24 AKB48F (m/z 384.30 → 135.15; 107.10; 93.10)
- 25 THJ-018 (m/z 342.60 → 215.10; 145.05; 90.00)
- 26 JWH-122 (m/z 356.30 → 169.05; 141.10; 115.15)
- 27 JWH-210 (m/z 370.10 → 183.10; 155.10; 153.10)

SYNTHETIC CANNABINOIDS (SPICE) FROM ORAL FLUID

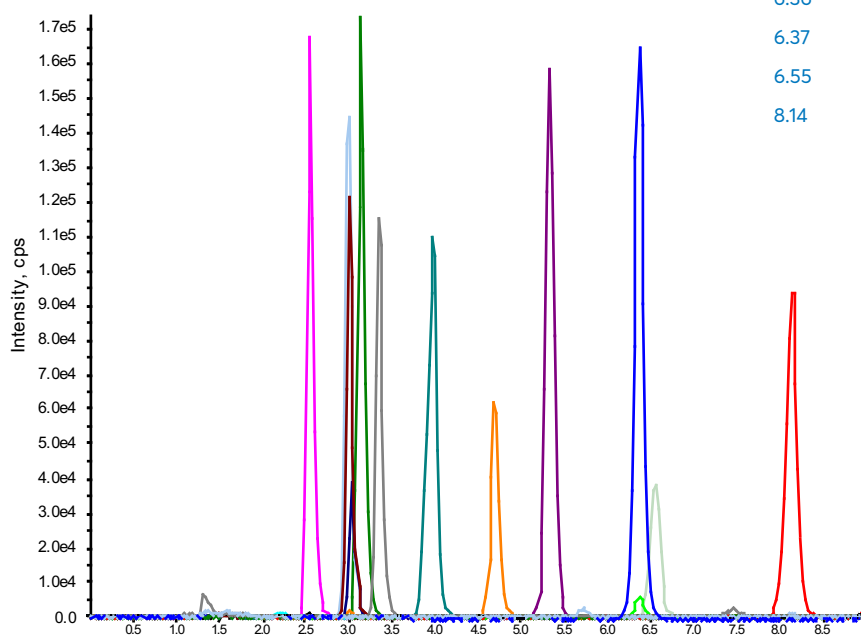
APPLICATION AN1650

ACE C18-AR

CONDITIONS

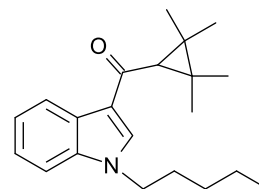
Column: **ACE Excel 2 C18-AR**
 Dimensions: 100 x 2.1 mm
 Part Number: EXL-109-1002U
 Mobile Phase: 0.1% formic acid in MeOH/H₂O (85:15 v/v)
 Flow Rate: 0.3 mL/min
 Temperature: Ambient
 Detection: Applied Biosystems/MDS Sciex 4000 Q-Trap
 Positive mode Turbo Ionspray

Extracted ion chromatogram for SPICE analytes fortified
in neat oral fluid at 20 ng/mL

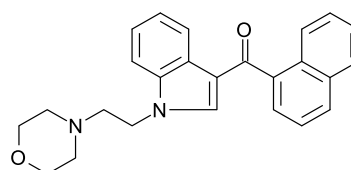


ANALYTES

t_R (min)	Analyte	MRM Transition
2.55	JWH-250 N-(5-hydroxypentyl)	352>120.9
2.99	JWH-073 N-(3-hydroxybutyl)	344>155
3.00	UR-144 5-hydroxypentyl	328.5>125
3.03	UR-144 pentanoic Acid	342.5>125
3.14	d5-JWH-018 N- (4-hydroxypentyl)	363.5>155
3.14	JWH-018 N- (4-hydroxypentyl)	358>155
3.34	JWH-018 5-pentanoic acid	372>155
3.98	JWH-200	385>155
4.69	XLR-11	330>125
5.32	JWH-250	336>121
6.36	JWH-073	328>155
6.37	UR-144 5-chloropentyl	346.9>125
6.55	UR-144	312.5>125
8.14	JWH-018	342>155



UR-144

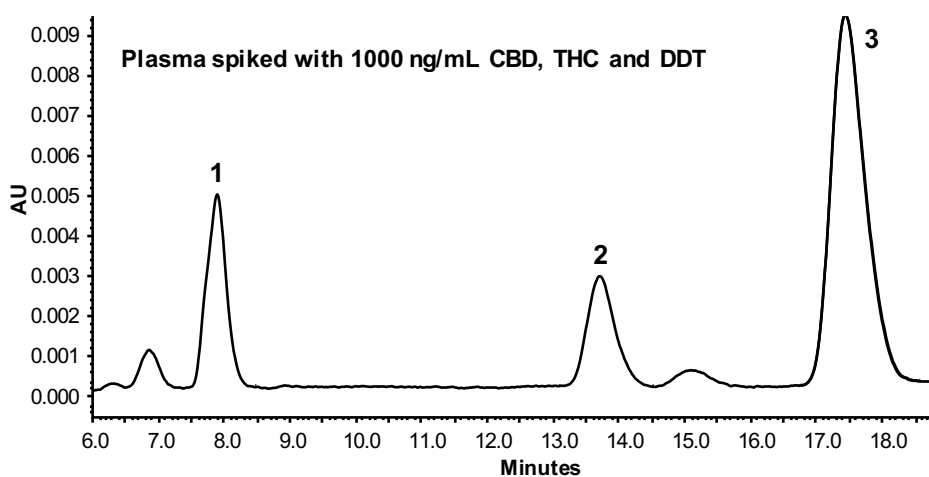
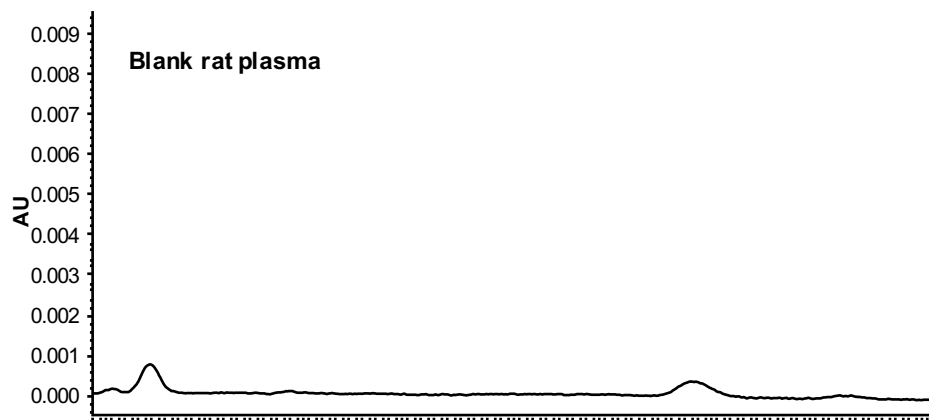
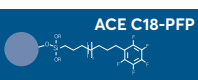


JWH-200

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CANNABINOIDS IN RAT PLASMA

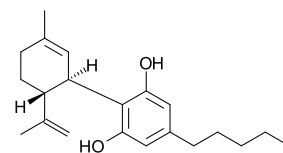
APPLICATION AN2310



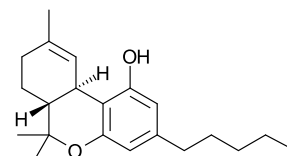
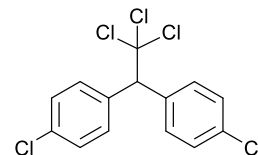
LLOQ 10 ng/mL for both cannabinoids
Method linearity 10 – 10,000 ng/mL

CONDITIONS

Column: **ACE 3 C18-PFP**
 Dimensions: 150 x 4.6 mm
 Part Number: ACE-1110-1546
 Mobile Phase: MeCN/H₂O (62:38 v/v)
 Flow Rate: 1 mL/min
 Injection: 30 µL
 Temperature: 55 °C
 Detection: UV, 220 nm



1. Cannabidiol(CBD)

2. Δ⁹-Tetrahydrocannabinol (THC)

3. 4,4'-Dichlorodiphenyltrichloroethane (DDT) (IS)

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Mycotoxins

Mycotoxins are secondary metabolites produced by several species of fungi and are considered one of the most important contaminants of agricultural commodities, including cannabis products. Although hundreds of mycotoxins are known, relatively few are considered to pose a significant health risk. Aflatoxins, in particular aflatoxin B₁, are genotoxic and carcinogenic and may cause liver cancer in humans, whilst ochratoxin A and the

trichothecenes HT-2 and T-2 can cause various toxic effects. Due to their potential toxicity at low levels to both humans and animals, monitoring and control of certain mycotoxins is important. The applications included in this guide detail the separation and identification of some of the most concerning mycotoxins from a food safety perspective.

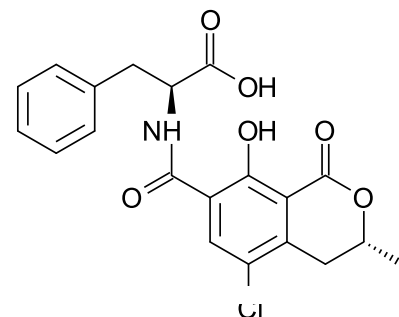
OCHRATOXIN A

APPLICATION AN2870



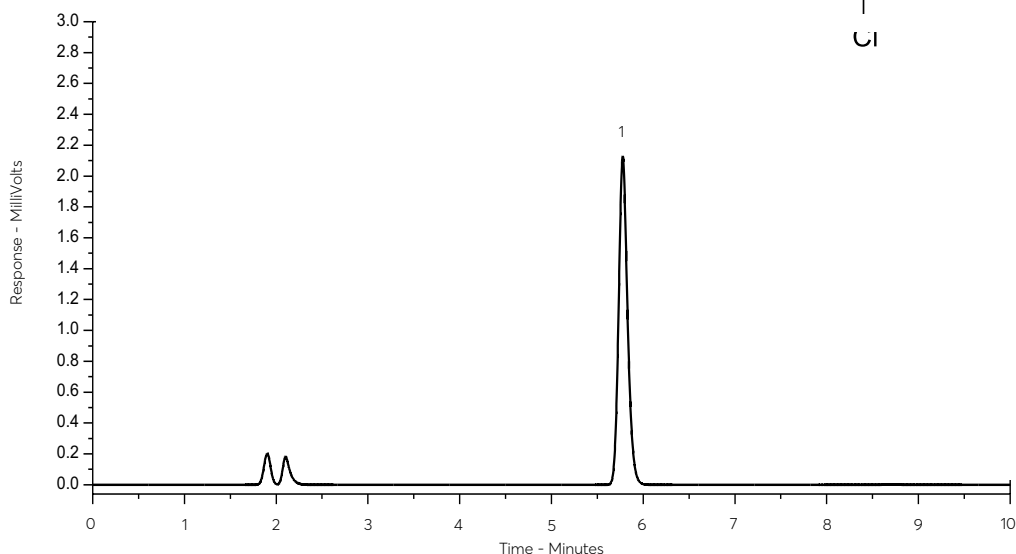
ANALYTES

1 Ochratoxin A



CONDITIONS

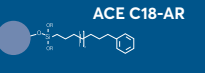
Column: **ACE 5 C18**
 Dimensions: 150 x 4.6 mm
 Part Number: ACE-121-1546
 Mobile Phase: MeCN/H₂O/Acetic acid (51:47:2 v/v/v)
 Flow Rate: 1 mL/min
 Temperature: Ambient
 Detection: Fluorescence –
 λ_{ex} 333 nm, λ_{em} 443 nm



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MYCOTOXINS BY LC-MS/MS

APPLICATION AN2330



CONDITIONS

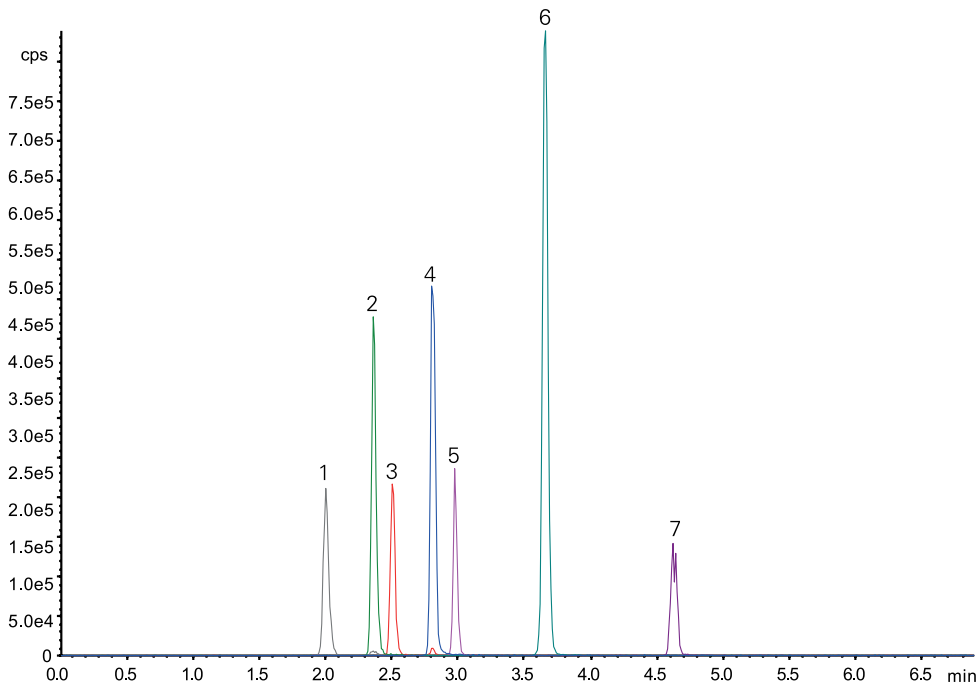
Column: **ACE Excel 2 C18-AR**
Dimensions: 50 x 2.1 mm
Part Number: EXL-109-0502U
Mobile Phase: A: 1 mM ammonium acetate, 0.5% acetic acid in H₂O
B: 1 mM ammonium acetate, 0.5% acetic acid in 95% MeOH
Gradient:

Time (mins)	% B
0.0	40
1.0	40
2.4	60
6.8	87

Flow Rate: 0.6 mL/min
Injection: 2 µL
Temperature: 40 °C
Detection: AB SCIEX triple quad 5500
Positive ESI mode
Source temperature: 500 °C
IonSpray voltage: 5500 V

ANALYTES

- 1 Aflatoxin G2 (m/z 331.1 → 313.1)
- 2 Aflatoxin G1 (m/z 329.0 → 243.1)
- 3 Aflatoxin B2 (m/z 315.1 → 287.0)
- 4 Aflatoxin B1 (m/z 313.1 → 285.0)
- 5 HT-2-toxin (m/z 442.2 → 263.1)
- 6 T-2-toxin (m/z 484.2 → 305.1)
- 7 Ochratoxin A (m/z 404.1 → 239.0)



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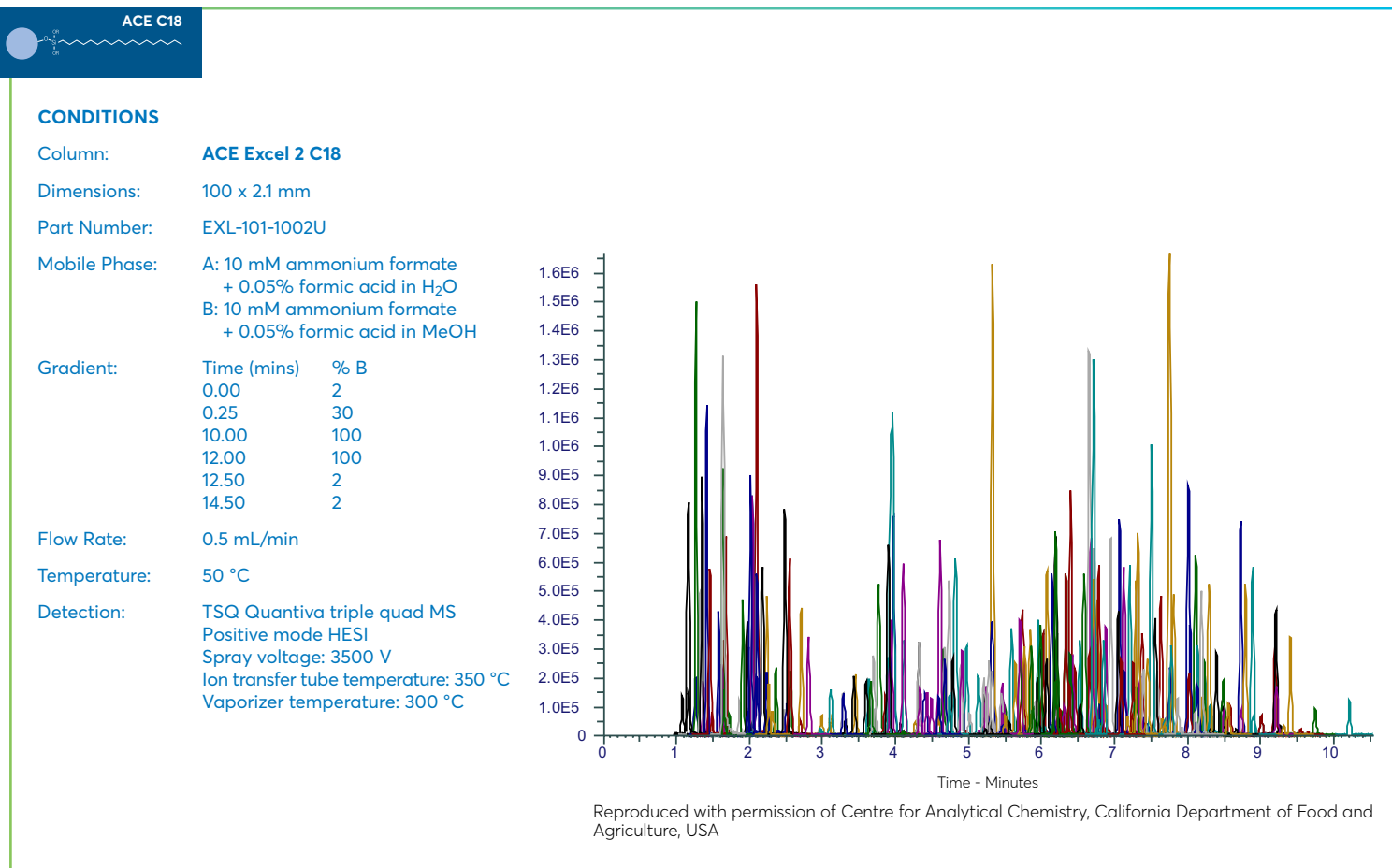
Pesticides

Testing for pesticide residues in cannabis products is important from health and environmental perspectives. Specific target compound lists and their required testing levels are often dynamic and may vary significantly on a regional level, but typically require testing for the presence of a range of authorised and restricted pesticides. High quality and comprehensive methods that enable the accurate detection of a wide range of pesticides

are therefore essential. LC-MS/MS is widely applied to achieve sensitive, low-level determination of residues in a variety of sample matrices. This section demonstrates the application of Avantor ACE solid-core and fully porous column technology to achieve rapid, high-sensitivity detection of a broad range of pesticide components, suitable for application to cannabis plant materials and final product.

250 PESTICIDE SCREEN USING LC-MS/MS

APPLICATION AN3060 - Page 1 of 4



APPLICATION AN3060 - Page 2 of 4

ANALYTE	t _R /mins	Adduct	Precursor Ion m/z	Quant Ion m/z	Conf Ion m/z	ANALYTE	t _R /mins	Adduct	Precursor Ion m/z	Quant Ion m/z	Conf Ion m/z
3-OH Carbofuran	2.25	[M+H] ⁺	238.1	181.2	163.1	Cyprosulfamide	3.30	[M+H] ⁺	375.1	135.1	254.1
5-OH Thiabendazole	1.66	[M+H] ⁺	218.0	147.2	191.1	Cyromazine	1.15	[M+H] ⁺	167.1	125.2	68.2
Abamectin	9.45	[M+NH ₄] ⁺	890.5	305.3	567.5	DEF	9.20	[M+H] ⁺	315.1	169.0	113.0
Acephate	1.26	[M+H] ⁺	184.0	143.1	125.1	Demeton-S sulfone	2.55	[M+H] ⁺	291.1	235.1	263.1
Acetamiprid	2.24	[M+H] ⁺	223.1	126.1	90.1	Dialifos	7.46	[M+H] ⁺	394.0	208.1	181.0
Aldicarb	2.95	[M+NH ₄] ⁺	208.1	116.1	89.0	Diazinon	7.12	[M+H] ⁺	305.1	169.1	153.2
Aldicarb sulfone	1.44	[M+NH ₄] ⁺	240.1	148.0	86.0	Diazinon OA	5.32	[M+H] ⁺	289.1	153.2	233.1
Aldicarb sulfoxide	1.37	[M+NH ₄] ⁺	224.1	132.0	89.1	Dichlorimid	3.85	[M+H] ⁺	208.0	140.0	81.2
Allethrin	8.33	[M+H] ⁺	303.2	135.1	123.1	Dichlorvos	3.63	[M+H] ⁺	221.0	109.1	127.0
Ametoctradin	7.64	[M+H] ⁺	276.2	149.1	176.2	Dicrotophos	1.87	[M+H] ⁺	238.1	112.2	193.1
Atrazine	4.64	[M+H] ⁺	216.1	174.0	104.0	Diethofencarb	5.53	[M+H] ⁺	268.2	124.1	180.2
Azinphos ethyl	6.30	[M+H] ⁺	346.0	132.1	223.0	Diflubenzuron	6.66	[M+H] ⁺	311.0	158.0	141.0
Azinphos methyl	5.14	[M+H] ⁺	318.0	132.0	124.9	Dimethenamid	5.70	[M+H] ⁺	276.1	244.1	168.2
Azinphos methyl OA	2.98	[M+H] ⁺	302.0	132.2	160.0	Dimethoate	2.23	[M+H] ⁺	230.1	199.0	125.0
Azoxystrobin	5.59	[M+H] ⁺	404.1	372.1	344.1	Dimethomorph	5.76, 6.07	[M+H] ⁺	388.1	301.0	165.1
Bendiocarb	3.72	[M+H] ⁺	224.1	174.0	109.1	Dinotefuran	1.36	[M+H] ⁺	203.1	129.1	114.2
Benoxacor	5.23	[M+H] ⁺	260.1	134.1	120.1	Dioxacarb	2.26	[M+H] ⁺	224.1	123.1	167.1
Bifenazate	6.27	[M+H] ⁺	301.1	198.0	170.1	Dioxathion	8.10	[M-C ₄ H ₁₀ O ₂ PS ₂] ⁺	271.1	97.0	125.0
Bitertanol	7.41	[M+H] ⁺	338.2	269.3	99.1	Disulfoton sulfone	4.59	[M+H] ⁺	307.0	261.1	125.0
Boscalid	5.85	[M+H] ⁺	343.0	307.0	140.0	Disulfoton sulfoxide	4.49	[M+H] ⁺	291.0	185.1	213.1
Bupirimate	6.68	[M+H] ⁺	317.2	210.2	237.3	Diuron	4.82	[M+H] ⁺	233.0	72.1	160.0
Buprofezin	8.24	[M+H] ⁺	306.1	201.1	106.1	DMST	3.90	[M+H] ⁺	215.1	106.1	151.0
Cadusafos	7.58	[M+H] ⁺	271.1	159.0	131.0	Dodine	7.56	[M+H] ⁺	228.3	186.3	60.1
Carbaryl	4.07	[M+NH ₄] ⁺	219.1	145.1	127.0	Emamectin	8.57	[M+H] ⁺	886.5	158.1	126.1
Carbendazim	2.10	[M+H] ⁺	192.1	160.1	132.1	Ethiofencarb	4.27	[M+H] ⁺	226.1	107.1	169.1
Carbofuran	3.77	[M+H] ⁺	222.1	165.2	123.2	Ethiofencarb sulfone	1.90	[M+NH ₄] ⁺	275.1	107.1	201.1
Carboxin	3.97	[M+H] ⁺	236.1	143.0	93.0	Ethiofencarb sulfoxide	1.98	[M+H] ⁺	242.1	107.1	185.0
Carfentrazone ethyl	6.88	[M+H] ⁺	412.0	346.1	366.0	Ethion	8.31	[M+H] ⁺	385.0	199.1	143.0
Chlorantraniliprole	5.24	[M+H] ⁺	484.0	286.0	194.0	Ethion monoxon	6.73	[M+H] ⁺	369.0	199.0	143.0
Chlorfenvinphos	7.21	[M+H] ⁺	359.0	170.0	99.1	Ethiprole	5.77	[M+NH ₄] ⁺	413.9	351.0	255.0
Chlorimuron ethyl	5.73	[M+H] ⁺	415.1	186.0	83.0	Ethofumesate	5.55	[M+H] ⁺	287.1	121.1	241.1
Chlorpyrifos	8.47	[M+H] ⁺	349.9	198.0	97.0	Ethoprop	6.46	[M+H] ⁺	243.1	173.0	131.0
Chlorpyrifos OA	6.65	[M+H] ⁺	334.0	278.0	197.9	Etofenprox	9.75	[M+NH ₄] ⁺	394.2	177.2	107.1
Clethodim	7.71	[M+H] ⁺	360.3	164.1	136.1	Etoazole	8.73	[M+H] ⁺	360.2	141.0	304.2
Clofentezine	7.38	[M+H] ⁺	303.0	138.1	102.0	Famoxadone	7.24	[M+H] ⁺	392.2	331.1	238.0
Cloransulam methyl	4.13	[M+H] ⁺	430.0	398.1	370.0	Fenamidone	5.76	[M+H] ⁺	312.1	236.1	92.2
Clothianidin	1.99	[M+H] ⁺	250.0	169.1	132.0	Fenamiphos	6.71	[M+H] ⁺	304.1	217.1	202.0
Coumaphos	7.07	[M+H] ⁺	363.0	227.1	307.1	Fenamiphos sulfone	4.10	[M+H] ⁺	336.1	266.1	188.1
Crotoxyphos	5.86	[M+NH ₄] ⁺	332.1	127.1	193.1	Fenamiphos sulfoxide	3.96	[M+H] ⁺	320.1	233.1	171.1
Crufomate	6.77	[M+H] ⁺	292.1	236.1	108.1	Fenazaquin	9.21	[M+H] ⁺	307.2	161.2	57.2
Cyantraniliprole	4.33	[M+2+H] ⁺	475.0	286.0	444.1	Fenhexamid	6.39	[M+H] ⁺	302.1	178.0	97.2
Cyazofamid	6.52	[M+H] ⁺	325.1	108.1	261.2	Fenobucarb	5.49	[M+H] ⁺	208.1	95.0	152.0
Cyflufenamid	7.42	[M+H] ⁺	413.1	295.1	203.0	Fenoxaprop ethyl	8.04	[M+H] ⁺	362.1	288.1	91.1
Cymoxanil	2.48	[M+H] ⁺	199.1	128.1	111.1	Fenoxycarb	6.80	[M+H] ⁺	302.1	88.1	116.1
Cyphenothrin	9.27	[M+NH ₄] ⁺	393.2	151.2	123.2	Fenpropimorph	6.42	[M+H] ⁺	304.3	147.2	119.1

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ANALYTE	t _R /mins	Adduct	Precursor Ion m/z	Quant Ion m/z	Conf Ion m/z	ANALYTE	t _R /mins	Adduct	Precursor Ion m/z	Quant Ion m/z	Conf Ion m/z
Fenpyroximate	8.90	[M+H] ⁺	422.2	366.1	214.2	Mepanipyrim	6.21	[M+H] ⁺	224.1	106.2	77.1
Fensulfothion	4.89	[M+H] ⁺	309.0	235.0	281.1	Mesotrione	2.01	[M+H] ⁺	340.1	228.1	104.1
Fenuron	2.17	[M+H] ⁺	165.1	72.1	77.1	Metaflumizone	8.30	[M+H] ⁺	507.1	178.0	287.1
Flonicamid	1.66	[M+H] ⁺	230.1	203.0	98.0	Metalaxyl	4.91	[M+H] ⁺	280.1	220.1	192.1
Fluazifop P butyl	8.12	[M+NH ₄] ⁺	384.1	282.2	328.2	Metalddehyde	2.02	[M+NH ₄] ⁺	194.1	62.2	45.3
Fludioxonil	5.76	[M+H] ⁺	266.1	158.1	131.0	Metconazole	7.32	[M+H] ⁺	320.2	70.1	125.0
Flufenoxuron	8.79	[M+H] ⁺	489.0	158.1	141.1	Methamidophos	1.16	[M+H] ⁺	142.0	94.2	125.1
Flufenpyr ethyl	6.72	[M+H] ⁺	409.1	335.0	307.0	Methidathion	4.97	[M+NH ₄] ⁺	320.0	145.1	85.1
Flumetsulam	2.03	[M+H] ⁺	326.1	129.1	109.0	Methiocarb	5.64	[M+H] ⁺	226.1	169.2	121.1
Flumiclorac pentyl	8.13	[M+NH ₄] ⁺	441.1	308.1	354.1	Methiocarb sulfone	2.35	[M+H] ⁺	275.0	122.1	201.1
Fluometuron	4.31	[M+H] ⁺	233.1	72.2	46.3	Methiocarb sulfoxide	2.10	[M+H] ⁺	242.1	185.1	122.1
Fluopicolide	6.00	[M+H] ⁺	383.0	173.0	145.0	Methomyl	1.61	[M+H] ⁺	163.1	106.1	88.1
Fluopyram	6.33	[M+H] ⁺	397.1	173.0	208.0	Methoxyfenozide	6.04	[M+H] ⁺	369.2	149.1	313.1
Fluoxastrobin	6.40	[M+H] ⁺	459.1	427.2	188.1	Metolcarb	3.28	[M+H] ⁺	166.1	109.1	94.1
Fluridone	5.32	[M+H] ⁺	330.1	309.1	290.0	Metribuzin	3.59	[M+H] ⁺	215.1	187.1	131.1
Flusilazole	6.77	[M+H] ⁺	316.1	247.2	165.1	Mevinphos	2.70	[M+NH ₄] ⁺	242.1	193.1	127.1
Fluthiacet methyl	6.88	[M+H] ⁺	404.0	344.0	273.9	Monocrotophos	1.71	[M+H] ⁺	224.1	193.0	127.0
Flutolanil	5.95	[M+H] ⁺	324.1	262.0	282.0	Monolinuron	4.16	[M+H] ⁺	215.1	126.1	148.1
Flutriafol	4.74	[M+H] ⁺	302.1	70.1	123.1	Myclobutanil	6.15	[M+H] ⁺	289.1	125.0	70.1
Fluxapyroxad	6.02	[M+H] ⁺	382.1	342.1	314.1	Nicosulfuron	3.45	[M+H] ⁺	411.1	182.0	213.0
Forchlorfenuron	4.78	[M+H] ⁺	248.1	129.1	93.1	Norflurazon	4.98	[M+H] ⁺	304.0	160.0	140.0
Formetanate HCl	1.26	[M+H] ⁺	222.0	165.1	120.0	Norflurazon desmethyl	4.43	[M+H] ⁺	290.0	179.0	140.0
Fosfiazate	4.40	[M+H] ⁺	284.1	104.1	228.1	Omethoate	1.33	[M+H] ⁺	214.0	183.0	125.0
Hexaconazole	7.29	[M+H] ⁺	314.1	158.9	70.0	Oxamyl	1.48	[M+NH ₄] ⁺	237.1	72.0	90.0
Hexythiazox	8.51	[M+H] ⁺	353.1	228.0	168.0	Oxamyl oxime	1.34	[M+H] ⁺	163.1	72.1	90.1
Imazalil	5.14	[M+H] ⁺	297.1	159.1	255.1	Oxydemeton methyl	1.57	[M+H] ⁺	247.0	169.1	109.1
Imazosulfuron	5.28	[M+H] ⁺	413.0	153.0	156.1	Oxydemeton methyl sulfone	1.62	[M+H] ⁺	263.0	169.0	109.0
Imidacloprid	1.96	[M+H] ⁺	256.1	209.1	175.0	Parathion methyl OA	3.10	[M+H] ⁺	248.0	202.0	109.1
Imiprothrin	6.34	[M+H] ⁺	319.2	151.1 209.1	123.1	Parathion OA	4.61	[M+H] ⁺	276.1	220.1	248.1
Indaziflam	6.58	[M+H] ⁺	302.2	158.1	145.1	Pencycuron	7.50	[M+H] ⁺	329.1	125.1	89.1
Indoxacarb	7.75	[M+H] ⁺	528.1	249.0	150.1	Penflufen	6.95	[M+H] ⁺	318.2	234.1	141.0
Ipconazole	7.81	[M+H] ⁺	334.2	70.1	125.0	Penthiopyrad	7.05	[M+H] ⁺	360.1	177.1	276.1
Iprovalicarb	6.31	[M+H] ⁺	321.2	119.1	186.2	Phenothrin	9.56	[M+H] ⁺	351.2	183.1	168.0
Isofenphos	7.39	[M+H] ⁺	346.1	217.0	245.1	Phenthoate	6.81	[M+H] ⁺	321.0	247.1	79.1
Isoprocab	4.67	[M+H] ⁺	194.1	95.1	152.2	Phorate OA	5.10	[M+H] ⁺	245.0	75.2	47.2
Isoproturon	4.79	[M+H] ⁺	207.2	72.2	165.2	Phorate OA Sulfone	2.51	[M+H] ⁺	277.0	155.0	127.0
Kresoxim methyl	6.90	[M+H] ⁺	314.1	267.2	222.1	Phorate OA Sulfoxide	2.31	[M+H] ⁺	261.0	153.0	81.0
Lactofen	8.22	[M+NH ₄] ⁺	479.1	344.1	223.0	Phorate Sulfone	4.61	[M+H] ⁺	293.0	114.9	171.0
Lenacil	4.67	[M+H] ⁺	235.1	153.1	136.1	Phorate Sulfoxide	4.49	[M+H] ⁺	277.0	170.9	199.0
Leptophos OA	7.75	[M+2+H] ⁺	396.9	155.1	364.9	Phosalone	7.35	[M+H] ⁺	368.0	182.0	111.1
Linuron	5.46	[M+H] ⁺	249.0	182.1	160.1	Phosmet	5.21	[M+H] ⁺	318.0	160.1	133.1
Malathion	5.92	[M+H] ⁺	331.0	127.1	285.1	Phosmet OA	3.12	[M+H] ⁺	302.0	160.0	133.0
Malathion OA	3.89	[M+H] ⁺	315.1	127.1	99.0	Phosphamidon	3.43	[M+H] ⁺	300.1	127.1	174.1
Mandipropamid	5.94	[M+H] ⁺	412.1	328.2	356.2	Phoxim	7.25	[M+H] ⁺	299.1	77.2	129.1
Mefenpyr diethyl	7.26	[M+H] ⁺	373.1	327.1	160.0	Picoxystrobin	6.79	[M+H] ⁺	368.1	145.0	115.0

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ANALYTE	t _R /mins	Adduct	Precursor Ion m/z	Quant Ion m/z	Conf Ion m/z	ANALYTE	t _R /mins	Adduct	Precursor Ion m/z	Quant Ion m/z	Conf Ion m/z
Pirimicarb	4.24	[M+H] ⁺	239.2	182.1	72.0	Spiromesifen	8.66	[M+NH ₄] ⁺	388.1	273.1	187.0
Pirimicarb Desmethyl	2.71	[M+H] ⁺	225.1	168.2	72.1	Spiromesifen Alcohol	5.01	[M+H] ⁺	273.2	187.1	179.1
Pirimiphos Methyl	7.34	[M+H] ⁺	306.1	164.2	108.1	Spirotetramat	6.38	[M+H] ⁺	374.2	302.3	216.2
Prallethrin	7.69	[M+H] ⁺	301.2	133.0	151.2	Spiroxamine	5.95	[M+H] ⁺	298.3	144.2	100.2
Prochloraz	7.39	[M+H] ⁺	376.0	308.1	70.1	Sulfoxaflor	2.39	[M+NH ₄] ⁺	295.2	174.1	154.1
Profoxydim	7.71, 9.00	[M+H] ⁺	466.2	280.0	180.0	Sulprofos	8.56	[M+H] ⁺	323.0	219.1	139.1
Promecarb	5.88	[M+H] ⁺	208.1	109.0	151.1	TCMTB	5.48	[M+H] ⁺	239.0	180.0	136.0
Propamocarb	1.41	[M+H] ⁺	189.1	102.0	144.0	Tebufenozide	6.78	[M+H] ⁺	353.2	133.0	104.8
Propaquizafop	8.21	[M+H] ⁺	444.1	299.2	371.2	Tebufenpyrad	8.19	[M+H] ⁺	334.2	117.1	145.1
Propargite	8.74	[M+NH ₄] ⁺	368.2	231.2	175.1	Tebuthiuron	3.89	[M+H] ⁺	229.1	172.0	116.0
Propetamphos	6.13	[M+H] ⁺	282.1	138.1	156.1	Tepraloxymdim	4.10, 6.19	[M+H] ⁺	342.2	250.1	166.1
Propoxur(S)	3.69	[M+H] ⁺	210.1	168.2	111.1	Terbufos Sulfone	5.46	[M+H] ⁺	321.0	115.0	143.0
Prosulfuron	5.29	[M+H] ⁺	420.1	167.1	141.1	Terbufos Sulfoxide	5.49	[M+H] ⁺	305.1	97.0	187.0
Pymetrozine	1.44	[M+H] ⁺	218.1	105.1	78.1	Terbuthylazine	5.71	[M+H] ⁺	230.1	174.1	104.1
Pyraclostrobin	7.30	[M+H] ⁺	388.1	163.1	194.1	Tetrachlorvinphos	6.86	[M+2+H] ⁺	366.9	127.1	206.0
Pyraflufen Ethyl	7.13	[M+H] ⁺	413.0	339.0	253.1	Tetramethrin	7.91, 8.10	[M+H] ⁺	332.2	164.1	135.1
Pyrazophos	7.31	[M+H] ⁺	374.1	222.2	194.1	Thiabendazole	2.48	[M+H] ⁺	202.0	175.0	131.1
Pyridaben	9.22	[M+H] ⁺	365.1	309.0	147.1	Thiacloprid	2.55	[M+H] ⁺	253.0	126.1	99.1
Pyridalyl	10.21	[M+2+H] ⁺	492.0	110.9	164.0	Thiamethoxam	1.65	[M+H] ⁺	292.0	211.1	181.1
Pyrimethanil	5.45	[M+H] ⁺	200.1	107.1	168.1	Thifensulfuron Methyl	3.28	[M+H] ⁺	388.0	167.1	205.0
Pyriproxyfen	8.39	[M+H] ⁺	322.1	96.0	227.1	Thiobencarb	7.46	[M+H] ⁺	258.1	125.0	89.0
Quinalphos	6.78	[M+H] ⁺	299.1	163.1	147.1	Thiodicarb	4.34	[M+H] ⁺	355.1	163.2	88.1
Quinoxifen	8.50	[M+H] ⁺	308.0	197.1	214.1	Thionazin	4.74	[M+H] ⁺	249.1	193.1	97.0
Quizalofop Ethyl	8.01	[M+H] ⁺	373.1	299.2	255.1	Topramezone	1.63	[M+H] ⁺	364.1	334.1	125.1
Resmethrin	9.40	[M+H] ⁺	339.2	128.1	171.1	Triadimefon	6.07	[M+H] ⁺	294.1	197.0	225.0
Rimsulfuron	3.94	[M+H] ⁺	432.1	182.1	139.0	Triadimenol	6.25	[M+H] ⁺	296.1	70.2	99.0
Rotenone	6.71	[M+H] ⁺	395.2	213.2	192.1	Triazophos	6.19	[M+H] ⁺	314.1	162.1	119.1
Saflufenacil	5.32	[M+H] ⁺	501.1	349.1	198.0	Tribenuron Methyl	4.59	[M+H] ⁺	396.1	155.1	181.1
Sedaxane	6.20, 6.54	[M+H] ⁺	332.2	159.0	139.0	Trichlorfon	2.26	[M+H] ⁺	256.9	109.0	221.0
Sethoxydim	8.03	[M+H] ⁺	328.2	178.0	220.1	Tricyclazole	2.80	[M+H] ⁺	190.0	163.1	136.1
Simazine	3.66	[M+H] ⁺	202.1	104.1	132.1	Trifloxystrobin	7.78	[M+H] ⁺	409.1	186.2	206.2
Spinetoram	8.14	[M+H] ⁺	748.5	142.1	203.1	Triflumizole	7.87	[M+H] ⁺	346.1	278.0	73.0
Spinosad A	7.69	[M+H] ⁺	732.5	142.1	98.0	Triforine	5.23	[M+2+H] ⁺	434.9	213.0	98.2
Spinosad D	8.10	[M+H] ⁺	746.5	142.1	98.0	Zoxamide	7.09	[M+H] ⁺	336.0	187.0	159.0
Spirodiclofen	8.91	[M+H] ⁺	411.1	313.1	71.1						

300 PESTICIDE SCREEN USING LC-MS/MS

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UltraCore SuperC18

High pH Stable!

CONDITIONS

Column: **ACE UltraCore 2.5 SuperC18**

Dimensions: 100 x 2.1 mm

Part Number: CORE-25A-1002U

Mobile Phase: A: 5 mM ammonium formate in MeOH/H₂O (1:9 v/v)B: 5 mM ammonium formate in MeOH/H₂O (9:1 v/v)

Gradient:	Time (mins)	% B
	0.0	30
	0.5	30
	15.0	100
	22.0	100
	22.1	30
	27.0	30

Flow Rate: 0.3 mL/min

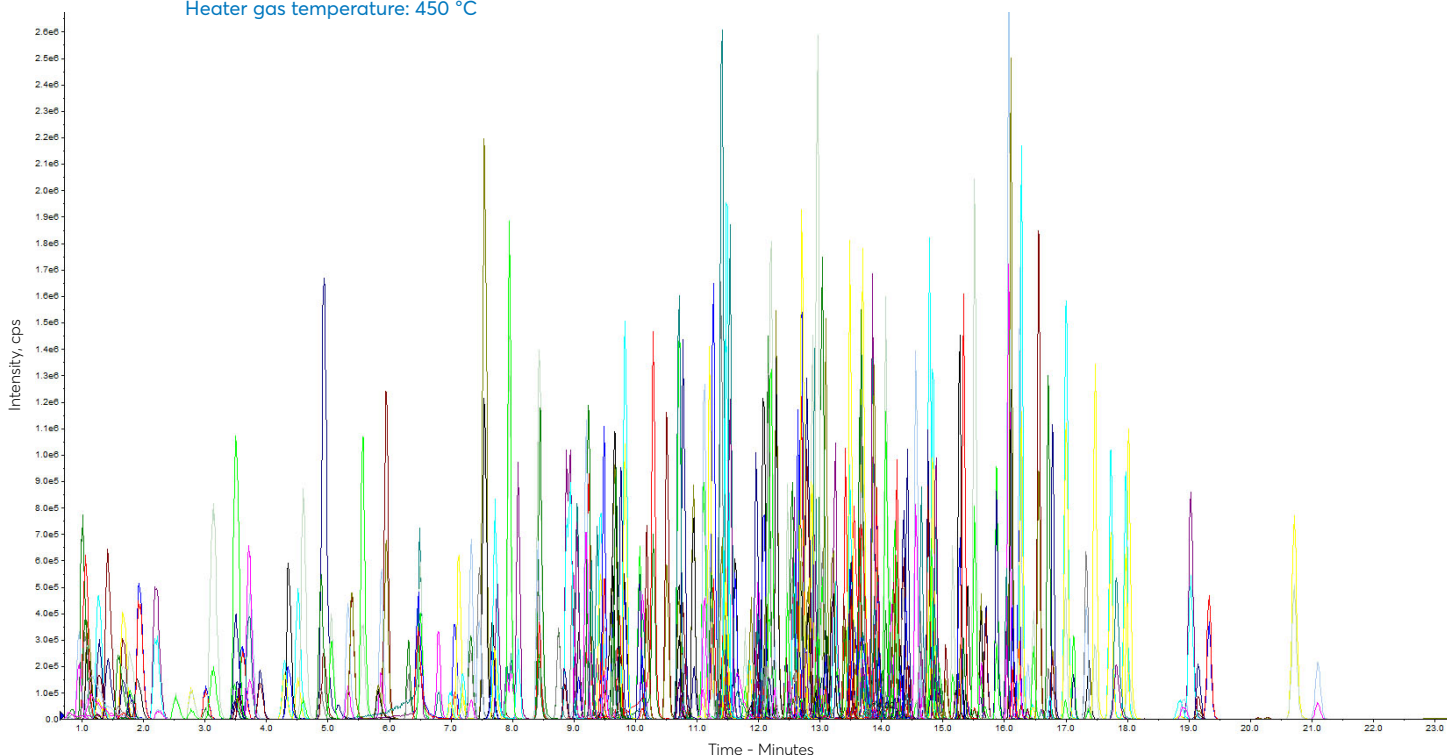
Injection: 6 µL

Temperature: 24 °C

Detection: AB SCIEX 4000 QTRAP
 TurbolonSpray ESI positive mode
 Capillary voltage: 5000 V
 Heater gas temperature: 450 °C

Sample: Sample prepared using QuEChERS methodology

Method validated using cucumber matrix spiked at 0.01 mg/kg.
 265 analytes successfully validated (analytes in black)



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ANALYTE	t _R /mins	MRM transitions (m/z)	ANALYTE	t _R /mins	MRM transitions (m/z)
3-Hydroxycarbofuran	3.5	238.1 → 163.1, 238.1 → 181.1	Chlorpyrifos-methyl	15.2	322.0 → 124.9, 324.0 → 125.1
Acephate	1.0	184.1 → 142.9, 184.1 → 124.8	Chlortoluron	9.1	213.2 → 72.0, 215.1 → 72.1
Acetamiprid	3.6	223.2 → 126.1, 225.2 → 128.1	Cinidon-ethyl	16.3	394.0 → 348.0, 394.0 → 366.0
Aclonifen	13.9	265.0 → 248.0, 267.0 → 250.0	Clethodim A	12.8	360.1 → 164.1, 360.1 → 268.1
Alachlor	12.9	270.2 → 238.2, 270.2 → 62.1	Clethodim B	10.2	360.1 → 164.1, 360.1 → 268.1
Aldicarb	5.4	208.0 → 89.0, 208.0 → 116.0	Clofentezine	15.1	303.1 → 137.9, 305.1 → 102.0
Aldicarb sulfone	1.2	240.0 → 86.0, 223.0 → 148.0	Clomazone	10.7	240.1 → 124.9, 242.2 → 127.1
Aldicarb sulfoxide	1.1	207.0 → 132.0, 207.2 → 88.9	Cloquintocet-mexyl	16.1	336.2 → 238.0, 336.2 → 192.1
Ametryn	11.1	228.2 → 186.1, 228.2 → 68.0	Clothianidin	2.9	250.1 → 169.0, 250.1 → 132.0
Aminopyralid	0.8	207.0 → 160.9, 207.0 → 133.9	Coumaphos	14.3	363.0 → 227.0, 363.0 → 211.1
Amitrole	0.8	85.1 → 58.1, 85.1 → 57.1	Cyanazine	6.7	241.1 → 214.1, 243.1 → 216.1
Atrazine	9.3	216.2 → 174.0, 218.1 → 176.1	Cyazofamid	13.2	325.2 → 107.9, 327.2 → 107.9
Atrazine-desethyl	4.4	188.2 → 146.0, 190.1 → 148.0	Cycloate	14.9	216.2 → 83.1, 216.2 → 154.1
Atrazine-desisopropyl	2.4	174.1 → 104.1, 174.1 → 132.1	Cycloxydim A	13.1	326.3 → 280.0, 326.3 → 180
Avermectin B1a	18.2	876.5 → 553.0, 876.5 → 291.0	Cycloxydim B	8.4	326.3 → 280.0, 326.3 → 180
Avermectin B1b	19.1	890.5 → 305.0, 890.5 → 567.0	Cymoxanil	4.2	199.2 → 128.0, 199.2 → 111.1
Azamethiphos	6.9	325.0 → 183.0, 325.0 → 138.9	Cyproconazole A	12.5	292.0 → 70.0, 292.0 → 125.0
Azinphos-ethyl	13.0	346.0 → 132.1, 346.0 → 160.1	Cyproconazole B	12.0	292.0 → 70.0, 292.0 → 125.0
Azinphos-methyl	10.9	318.1 → 132.1, 318.1 → 260.8	Cyprodinil A	14.1	226.2 → 93.0, 226.2 → 77.0
Aziprotryne	11.8	226.0 → 156.0, 226.0 → 125.0	Demeton-S-methyl	7.7	231.1 → 88.8, 231.1 → 61.0
Azoxystrobin	11.4	404.2 → 372.3, 404.2 → 344.1	Demeton-S-methyl sulfone	1.6	263.0 → 168.9, 263.0 → 120.8
Benalaxyl	14.0	326.2 → 148.1, 326.2 → 294.1	Desmedipham	10.6	318.1 → 182.1, 318.1 → 136.0
Benfuracarb	15.7	411.2 → 252.1, 411.2 → 195.1	Desmethyl-pirimicarb	5.8	225.2 → 72.0, 225.2 → 168.1
Benthiavalicarb-isopropyl	12.0	382.3 → 116.0, 382.3 → 197.0	Diafenthiuron	17.4	385.2 → 329.2, 385.2 → 278.2
Bifenazate	12.5	301.2 → 198.1, 301.2 → 170.2	Diazinon	14.2	305.1 → 169.1, 305.1 → 97.0
Bifenox	14.9	359.0 → 342.0, 359.0 → 310.0	Dichlofluanid	12.8	333.0 → 223.9, 333.0 → 122.9
Bifenthrin	21.0	440.0 → 181.1, 440.0 → 166.1	Diclobutrazol A	13.7	328.0 → 70.0, 330.0 → 70.0
Bitertanol	14.6	338.2 → 269.0, 338.2 → 99.1	Dicrotofos	2.1	238.1 → 112.1, 238.1 → 193.1
Bixafen	13.6	414.0 → 393.9, 416.1 → 395.9	Diethofencarb	11.1	268.1 → 226.1, 268.1 → 124.0
Boscalid	11.7	343.1 → 306.8, 343.1 → 139.9	Difenoconazole	14.8	406.1 → 251.1, 408.2 → 253.1
Bromfeninfos-ethyl	14.3	405.0 → 155.0, 403.0 → 155.0	Diflubenzuron	13.5	311.0 → 158.2, 311.0 → 141.1
Bromuconazole A	12.2	378.0 → 159.1, 378.0 → 161.0	Diflufenican	15.4	395.0 → 266.0, 395.0 → 246.0
Bromuconazole B	13.5	378.1 → 159.1, 378.1 → 161.0	Dimethachlor	10.2	256.2 → 224.0, 256.2 → 148.1
Bupirimate	13.5	317.2 → 166.2, 317.2 → 107.9	Dimethenamid	11.3	276.1 → 244.0, 278.1 → 246.0
Buprofezin	16.1	306.3 → 201.1, 306.3 → 116.1	Dimethoate	3.6	230.1 → 198.8, 230.1 → 124.9
Cadusafos	14.8	271.1 → 158.9, 271.1 → 214.9	Dimethomorph	11.7	388.1 → 301.0, 388.1 → 165.1
Carbaryl	8.3	202.2 → 145.1, 202.2 → 127.1	Dimoxystrobin	13.7	327.1 → 205.0, 327.1 → 116.0
Carbendazim	4.7	192.2 → 160.1, 192.0 → 132.0	Diniconazole	14.8	326.0 → 70.0, 328.0 → 70.0
Carbofuran	7.4	222.2 → 165.1, 222.2 → 122.9	Disulfoton	15.0	275.1 → 89.0, 275.1 → 61.0
Carbosulfan	19.3	381.2 → 160.1, 381.2 → 118.1	Disulfoton sulfone	9.6	307.1 → 153.0, 307.1 → 171.0
Carboxin	8.3	236.1 → 143.1, 236.1 → 87.0	Disulfoton sulfoxide	9.2	291.1 → 212.9, 291.1 → 185.0
Carfentrazone-ethyl	13.8	412.2 → 345.9, 412.2 → 383.9	Ditalimfos	13.1	300.1 → 148.0, 300.1 → 130.0
Chlorantraniliprole	10.7	484.0 → 452.9, 484.0 → 285.9	Diuron	10.0	233.1 → 71.9, 235.1 → 72.0
Chlorbromuron	11.7	295.1 → 205.9, 293.1 → 182.0	DMST	8.0	215.2 → 106.0, 215.2 → 78.9
Chlorfeninfos A	14.3	359.0 → 155.0, 358.9 → 99.0	Dodine	13.6	228.3 → 57.0, 228.3 → 60.1
Chloridazon	3.7	222.1 → 104.0, 222.1 → 77.1	Epoxiconazole	12.9	330.1 → 120.9, 330.1 → 75.2
Chlorpyrifos	16.8	349.9 → 198.1, 349.9 → 115.0	Ethion	16.5	385.0 → 199.0, 385.0 → 143.0

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ANALYTE	t _R /mins	MRM transitions (m/z)	ANALYTE	t _R /mins	MRM transitions (m/z)
Ethirimol	9.7	210.3 → 140.1, 210.3 → 98.0	Heptenofos	10.1	251.0 → 127.0, 251.0 → 124.8
Ethofumesate	11.3	287.1 → 121.0, 287.1 → 259.0	Hexaconazole	14.3	314.0 → 70.0, 316.0 → 70.0
Ethoprofos	12.7	243.0 → 131.0, 243.0 → 97.0	Hexaflumuron	15.5	461.1 → 158.2, 461.1 → 141.1
Ethoxyquin A	12.9	218.2 → 148.0, 218.2 → 174.1	Hexazinone	7.3	253.2 → 71.0, 253.2 → 85.0
Ethoxyquin B	10.7	218.2 → 148.0, 218.2 → 174.1	Hexythiazox	16.6	353.0 → 168.0, 353.0 → 228.0
Etofenprox	20.6	394.0 → 177.0, 394.0 → 359.0	Imazalil	13.6	297.2 → 159.1, 299.1 → 160.9
Etrimfos	14.2	293.1 → 125.0, 293.1 → 265.1	Imidacloprid	2.7	256.1 → 209.0, 256.1 → 175.0
Famoxadone NH ₄ ⁺	14.4	392.0 → 331.0, 392.0 → 238.0	Indoxacarb	15.2	528.1 → 248.9, 528.1 → 292.9
Fenamidone	11.5	312.1 → 92.1, 312.1 → 236.1	Ipconazole	15.3	334.2 → 70.0, 334.2 → 125.0
Fenamifos	13.4	304.0 → 217.0, 304.0 → 202.0	Iprodione	13.3	332.1 → 246.9, 330.0 → 245.0
Fenamifos sulfone	8.4	336.0 → 308.0, 336.0 → 266.0	Iprovalicarb	12.6	321.3 → 119.0, 321.3 → 203.1
Fenamifos sulfoxide	7.9	320.0 → 171.0, 320.0 → 233.0	Isofenfos	14.7	346.1 → 245.1, 346.1 → 217.1
Fenarimol	12.7	331.2 → 268.0, 331.2 → 139.0	Isofenfos-methyl	13.8	332.1 → 231.0, 332.1 → 273.0
Fenazaquin	18.0	307.1 → 161.1, 307.1 → 147.0	Isoproc carb	9.4	194.1 → 95.0, 194.1 → 137.0
Fenbuconazole	13.2	337.0 → 124.9, 337.0 → 70.0	Isoprothiolane	12.1	291.1 → 231.0, 291.1 → 189.0
Fenbutatin oxide	22.9	519.3 → 463.3, 519.3 → 197.0	Isoproturon	9.7	207.2 → 72.0, 207.2 → 165.2
Fenhexamid	12.6	302.2 → 96.9, 304.2 → 97.0	Isoxadifen-ethyl	13.9	313.2 → 296.1, 313.2 → 263.0
Fenoxycarb	13.6	302.2 → 87.9, 302.2 → 116.0	Isoxaflutole	10.0	360.1 → 251.1, 377.0 → 251.0
Fenpropathrin	17.3	367.0 → 125.0, 350.0 → 125.0	Kresoxim-methyl	13.9	314.0 → 116.0, 314.0 → 131.1
Fenpropidin	10.8	274.0 → 147.0, 274.0 → 117.0	Lenacil	9.5	235.3 → 153.2, 235.3 → 136.2
Fenpropimorph	18.7	304.0 → 147.0, 304.0 → 117.0	Linuron	11.3	249.0 → 159.9, 249.0 → 182.0
Fenpyroximate	17.4	422.2 → 366.1, 422.2 → 135.1	Lufenuron	16.4	511.0 → 158.0, 511.0 → 141.0
Fensulfothion	10.0	309.1 → 280.8, 309.1 → 252.9	Malaoxon	7.9	315.1 → 99.1, 315.1 → 127.1
Fensulfothion sulfone	10.4	325.1 → 268.9, 325.1 → 297.0	Mandipropamid	11.9	412.1 → 328.1, 412.2 → 125.0
Fenthion sulfone	9.0	311.1 → 125.0, 311.1 → 278.8	Mecarbam	13.0	330.1 → 227.0, 330.1 → 198.9
Fenthion sulfoxide	8.4	295.1 → 279.7, 295.1 → 108.9	Mepanipyrim	12.9	224.2 → 106.0, 224.2 → 77.1
Flonicamid	1.7	230.0 → 203.0, 230.0 → 148.0	Mepronil	12.1	270.1 → 119.0, 270.1 → 228.1
Flubendiamide NH ₄ ⁺	13.8	700.0 → 407.9, 682.9 → 407.9	Mesotrione	1.2	340.0 → 228.0, 357.1 → 227.9
Fludioxonil NH ₄ ⁺	11.8	266.0 → 229.0, 266.0 → 227.1	Metaflumizone	16.1	507.1 → 178.1, 507.1 → 287.1
Flufenacet	12.8	364.1 → 194.1, 364.1 → 152.2	Metalaxyl	9.8	280.1 → 220.2, 280.1 → 192.2
Flufenoxuron	17.1	489.0 → 158.0, 489.0 → 141.1	Metamitron	3.4	203.1 → 175.0, 203.1 → 104.2
Flumethrin NH ₄ ⁺	20.2	527.2 → 510.0, 527.2 → 267.0	Metazachlor	9.6	278.1 → 209.9, 278.1 → 134.2
Flumetsulam	2.0	326.2 → 128.8, 326.2 → 128.3	Metconazole	14.4	320.1 → 70.0, 320.1 → 125.0
Flumioxazin	10.7	355.0 → 327.0, 355.0 → 299.0	Methacrifos	10.7	241.0 → 208.9, 241.0 → 124.9
Fluometuron	8.9	233.0 → 72.0, 233.0 → 160.0	Methamidofos	0.9	142.0 → 93.9, 142.0 → 112.1
Fluopicolide	11.9	383.0 → 173.0, 385.1 → 174.9	Methiocarb	11.4	226.2 → 169.1, 226.2 → 121.2
Fluopiram	12.5	397.0 → 173.0, 397.0 → 208.0	Methiocarb sulfone	4.1	258.1 → 122.0, 258.1 → 200.9
Fluoxastrobin	12.8	459.1 → 427.1, 459.1 → 188.1	Methiocarb sulfoxide	3.0	242.1 → 185.0, 242.1 → 122.1
Fluquinconazole	12.6	376.1 → 307.1, 376.1 → 349.1	Methomyl	1.6	163.0 → 106.0, 163.0 → 88.0
Flusilazole	13.3	316.2 → 247.0, 316.2 → 165.1	Methoxyfenozide	12.2	369.1 → 149.1, 369.1 → 313.2
Flutolanil	12.0	324.0 → 262.0, 324.0 → 242.0	Metobromuron	9.4	259.0 → 170.0, 259.0 → 148.1
Flutriafol	9.7	302.1 → 70.1, 302.1 → 123.0	Metolachlor	13.0	284.1 → 252.0, 286.1 → 254.0
Fomesafen (NH ₄ -Adduct)	11.3	456.1 → 344.0, 458.1 → 346.0	Metoxuron	5.7	229.1 → 72.0, 231.1 → 71.9
Fonofos	14.3	247.0 → 109.0, 247.0 → 127.0	Metrafenone	14.8	409.2 → 209.1, 411.2 → 209.1
Fosthiazate	8.9	284.1 → 227.9, 284.1 → 104.0	Metribuzin	7.1	215.2 → 187.1, 215.2 → 84.1
Fuberidazole	6.9	185.0 → 157.0, 185.0 → 65.0	Mevinfos A	4.9	225.0 → 193.0, 225.0 → 127.0
Furathiocarb	15.9	383.1 → 195.0, 383.1 → 252.1	Mevinfos B	3.4	225.0 → 193.0, 225.0 → 127.0

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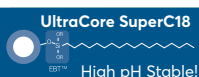
ANALYTE	t _R /mins	MRM transitions (m/z)	ANALYTE	t _R /mins	MRM transitions (m/z)
Molinate	12.0	188.2 → 126.2, 188.2 → 55.1	Propiconazole	14.0	342.1 → 159.0, 342.1 → 69.0
Monocrotopos	1.8	224.2 → 192.9, 224.2 → 126.9	Propisochlor	14.0	284.2 → 224.0, 284.2 → 148.0
Monolinuron	8.7	215.1 → 126.1, 215.1 → 148.1	Propoxur	7.2	210.1 → 111.1, 210.1 → 168.0
Myclobutanil	12.2	289.2 → 70.0, 289.2 → 125.0	Propyzamide	11.9	256.1 → 190.0, 256.1 → 173.0
Napropamide	12.9	272.2 → 129.1, 272.2 → 171.1	Proquinazid	17.7	373.2 → 330.9, 373.2 → 289.0
Nitenpyram	1.3	271.1 → 189.2, 271.1 → 126.0	Prosulfocarb	15.5	252.2 → 91.0, 252.2 → 128.1
Novaluron	15.6	493.0 → 158.1, 493.0 → 141.1	Prosulfuron	9.0	420.1 → 141.0, 420.1 → 167.1
Nuarimol	11.2	315.0 → 252.0, 315.0 → 81.0	Prothioconazole	14.1	344.1 → 326.0, 346.1 → 328.1
Ofurace	7.6	282.0 → 160.1, 282.0 → 236.3	Prothioconazole-desthio	13.0	312.0 → 70.0, 312.0 → 125.0
Omethoate	1.0	214.0 → 183.0, 214.0 → 125.0	Pymetrozine	1.5	218.0 → 105.0, 218.0 → 78.0
Oxadiazon	16.2	345.0 → 220.0, 345.0 → 303.0	Pyraclostrobin	14.5	388.1 → 194.0, 388.1 → 163.0
Oxadixyl	6.4	279.0 → 219.0, 279.0 → 133.0	Pyrazophos	14.8	374.0 → 222.0, 374.0 → 194.0
Oxamyl NH ₄ ⁺	1.2	237.1 → 72.0, 220.2 → 72.0	Pyridaben	18.0	365.0 → 309.0, 365.0 → 147.0
Oxycarboxin	4.5	268.1 → 174.9, 268.1 → 147.0	Pyridapenthion	12.4	341.0 → 189.0, 341.0 → 205.0
Oxydemeton-methyl	1.4	247.0 → 108.9, 247.0 → 168.9	Pyridate	19.1	379.1 → 206.9, 379.1 → 350.9
Paclobutrazol	11.8	294.0 → 70.0, 294.0 → 125.0	Pyrifeno	13.0	295.1 → 93.0, 297.1 → 93.0
Paraoxon	9.4	275.9 → 219.9, 275.9 → 248.0	Pyrimethanil	11.3	200.0 → 82.0, 200.0 → 107.0
Paraoxon-methyl	6.1	248.1 → 202.1, 248.1 → 90.0	Pyriproxyfen	16.7	322.0 → 96.0, 322.0 → 185.0
Parathion	13.8	292.0 → 236.0, 292.0 → 264.1	Pyroxsulam	5.6	435.0 → 195.1, 435.0 → 194.0
Penconazole	13.7	248.1 → 70.0, 284.1 → 159.0	Quinalfos	13.9	299.0 → 271.0, 299.0 → 243.0
Pencycuron	14.8	329.3 → 125.1, 331.3 → 127.0	Quinoclamine	6.8	208.0 → 105.0, 208.0 → 77.0
Pendimethalin	16.9	282.2 → 212.1, 282.2 → 194.1	Quinoxifen	16.4	308.0 → 197.0, 308.0 → 162.0
Pethoxamid	12.7	296.2 → 131.0, 296.2 → 250.0	Rotenone	13.4	395.1 → 213.1, 395.1 → 192.0
Phenmedipham	10.8	301.2 → 168.0, 301.2 → 136.0	Secbumeton	10.6	226.2 → 170.1, 226.2 → 100.0
Phenthoate	13.9	321.0 → 247.0, 321.0 → 275.1	Silthiofam	13.5	268.0 → 252.0, 268.0 → 73.0
Phorate sulfone	9.6	293.0 → 170.8, 293.0 → 96.7	Simazine	7.2	202.02 → 132.1, 202.2 104.0
Phorate sulfoxide	9.2	277.0 → 199.0, 277.0 → 171.0	Simetryn	9.4	214.1 → 124.1, 214.1 → 144.0
Phosalone	14.6	368.0 → 182.0, 369.9 → 183.9	Spinosyn A	17.3	732.5 → 142.0, 732.5 → 98.0
Phosphamidon	6.4	300.2 → 127.1, 300.2 → 226.8	Spinosyn D	18.3	746.5 → 142.0, 746.5 → 98.0
Phoxim	14.7	299.2 → 129.2, 299.2 → 77.1	Spirodiclofen	17.4	313.1 → 295.0, 313.1 → 213.0
Picloram	1.2	243.0 → 224.9, 241.0 → 222.9	Spiromesifen	16.8	371.2 → 273.1, 371.2 → 255.2
Picolinafen	16.2	377.1 → 238.0, 377.1 → 359.0	Spirotetramat	12.8	374.2 → 302.2, 374.2 → 330.2
Picoxystrobin	13.6	368.0 → 205.0, 368.0 → 145.0	Spiroxamine	13.3	298.3 → 100.1, 298.3 → 144.1
Piperonyl butoxide	16.2	356.2 → 177.2, 356.2 → 119.0	Sulfotep	14.0	323.0 → 97.0, 323.0 → 115.0
Pirimicarb	9.0	239.2 → 72.0, 239.2 → 182.3	Tau-fluvalinate	18.9	503.0 → 208.0, 503.0 → 181.0
Pirimiphos-ethyl	16.3	334.1 → 198.0, 334.1 → 182.3	Tebuconazole	13.9	308.1 → 70.0, 308.1 → 125.0
Pirimiphos-methyl	14.8	306.2 → 108.0, 306.2 → 164.3	Tebufenozide	13.5	353.2 → 297.2, 353.2 → 133.0
Prochloraz	14.4	376.0 → 308.0, 376.0 → 70.0	Tebufenpyrad	15.9	334.0 → 145.0, 334.0 → 117.0
Profenofos	15.6	375.0 → 304.9, 373.0 → 302.9	Teflubenzuron	16.3	381.1 → 158.2, 381.1 → 141.2
Prometryn	12.6	242.2 → 158.1, 242.2 → 200.0	Tembotrione (NH ₄ adduct)	5.9	458.0 → 340.9, 458.0 → 441.0
Propachlor	9.6	212.0 → 170.0, 212.0 → 94.1	Terbufos	16.1	289.1 → 103.1, 289.1 → 232.9
Propamocarb	1.1	189.0 → 102.0, 189.0 → 144.0	Terbufos sulfone	11.1	321.1 → 171.0, 321.1 → 115.0
Propaquizafop	16.0	444.2 → 100.0, 444.2 → 371.0	Terbufos sulfoxide	11.0	305.1 → 187.2, 305.1 → 131.1
Propargite NH ₄ ⁺	17.0	368.2 → 231.1, 368.2 → 175.0	Terbumeton	11.3	226.2 → 170.1, 226.2 → 142.0
Propazine	11.0	230.2 → 188.1, 230.2 146.1	Terbuthylazine	11.4	230.2 → 174.0, 232.2 → 176.0
Propetamfos	12.4	282.1 → 138.0, 282.1 156.1	Terbutryn	12.9	242.1 → 186.1, 242.1 → 96.0
Propham	9.4	180.1 → 138.1, 180.1 → 120.1	Tetrachlorvinfos	13.5	367.0 → 127.0, 365.0 → 127.0

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ANALYTE	t _R /mins	MRM transitions (m/z)	ANALYTE	t _R /mins	MRM transitions (m/z)
Tetraconazole	12.9	372.0 → 159.0, 374.0 → 161.2	Triallate	16.7	304.1 → 142.9, 304.1 → 86.2
Thiabendazole	6.2	202.1 → 174.9, 202.1 → 131.0	Triazofos	12.6	314.0 → 162.0, 314.2 → 119.0
Thiacloprid	4.7	253.1 → 126.1, 253.1 → 99.1	Trichlorfon	3.4	257.0 → 108.9, 257.0 → 220.8
Thiencarbazone-methyl	2.3	391.0 → 130.0, 391.0 → 230.0	Tricyclazole	5.2	190.1 → 136.1, 190.1 → 163.0
Thiodicarb	9.2	355.0 → 88.0, 355.0 → 108.0	Trifloxystrobin	15.3	409.0 → 186.0, 409.0 → 206.0
Thiophanate-methyl	7.6	343.0 → 151.1, 343.0 → 311.0	Triflumizole	15.3	346.0 → 278.0, 346.0 → 73.0
Tiamethoxam	1.7	292.0 → 211.0, 292.0 → 181.0	Triflumuron	14.6	359.1 → 156.2, 359.1 → 139.0
Tolclophos-methyl	14.9	301.2 → 268.9, 303.1 → 270.9	Triforin	10.6	435.0 → 390.0, 437.0 → 392.0
Tolyfluanid	13.9	347.0 → 237.8, 347.0 → 137.1	Triticonazole A	12.7	318.0 → 70.0, 318.0 → 125.0
Topramezone	1.6	364.1 → 334.1, 364.1 → 125.0	Triticonazole B	10.9	318.0 → 70.0, 318.0 → 125.0
Triadimefon	12.1	294.2 → 197.2, 294.2 → 225.0	Vamidothion	3.4	288.1 → 146.0, 288.1 → 118.0
Triadimenol	12.4	296.2 → 70.0, 298.2 → 70.0	Zoxamide	14.2	336.0 → 187.0, 338.0 → 189.0

PESTICIDES BY LC-MS/MS

APPLICATION AN1290

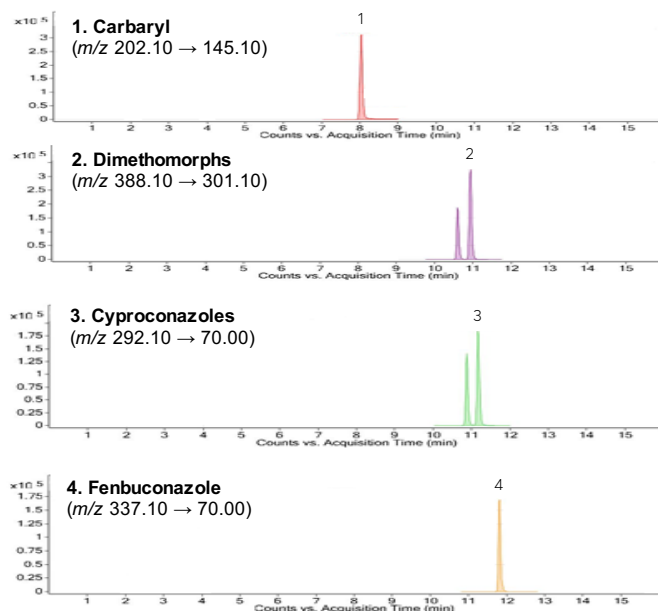


CONDITIONS

Column:	ACE UltraCore 2.5 SuperC18	
Dimensions:	50 x 2.1 mm	
Part Number:	CORE-25A-0502U	
Mobile Phase:	A: 0.1% formic acid + 5 mM ammonium formate in MeOH/H ₂ O (1:9 v/v) B: 0.1% formic acid + 5 mM ammonium formate in MeOH/H ₂ O (9:1 v/v)	
Gradient:	Time (mins)	% B
	0.00	0
	1.00	0
	15.00	100
	18.00	100
	18.05	0
	20.00	0
Flow Rate:	0.4 mL/min	
Injection:	20 µL	
Temperature:	40 °C	
Detection:	Agilent 6420 Triple Quadrupole MS, +ve mode ESI, Dynamic MRM	

ANALYTES

Also analysed under same conditions: Acephate, Acetamiprid, Aldicarb, Aldicarb sulfone, Aldicarb sulfoxide, Benomyl, Car bendazim, Carbofuran, Clofentezine, Clothianidin, Cyfluthrin, Demeton S-methylsulfone, Demeton S-methylsulfoxide, Dicrotophos, Dimethoate, Dinotefuran, DMA, DMPF, Flubendiamide, Folpet, Formetanate, Hexaconazole, Hexaflumuron, Imidacloprid, Indoxacarb, Mandipropamid, Methamidophos, Methomyl, Monocrotophos, Nicotine, Omethoate, Oxamyl, Pencycuron, Prochloraz, Propargite, Thiabendazole, Thiacloprid, Thiamethoxam, Thiodicarb, Thiophanate methyl and Triforine



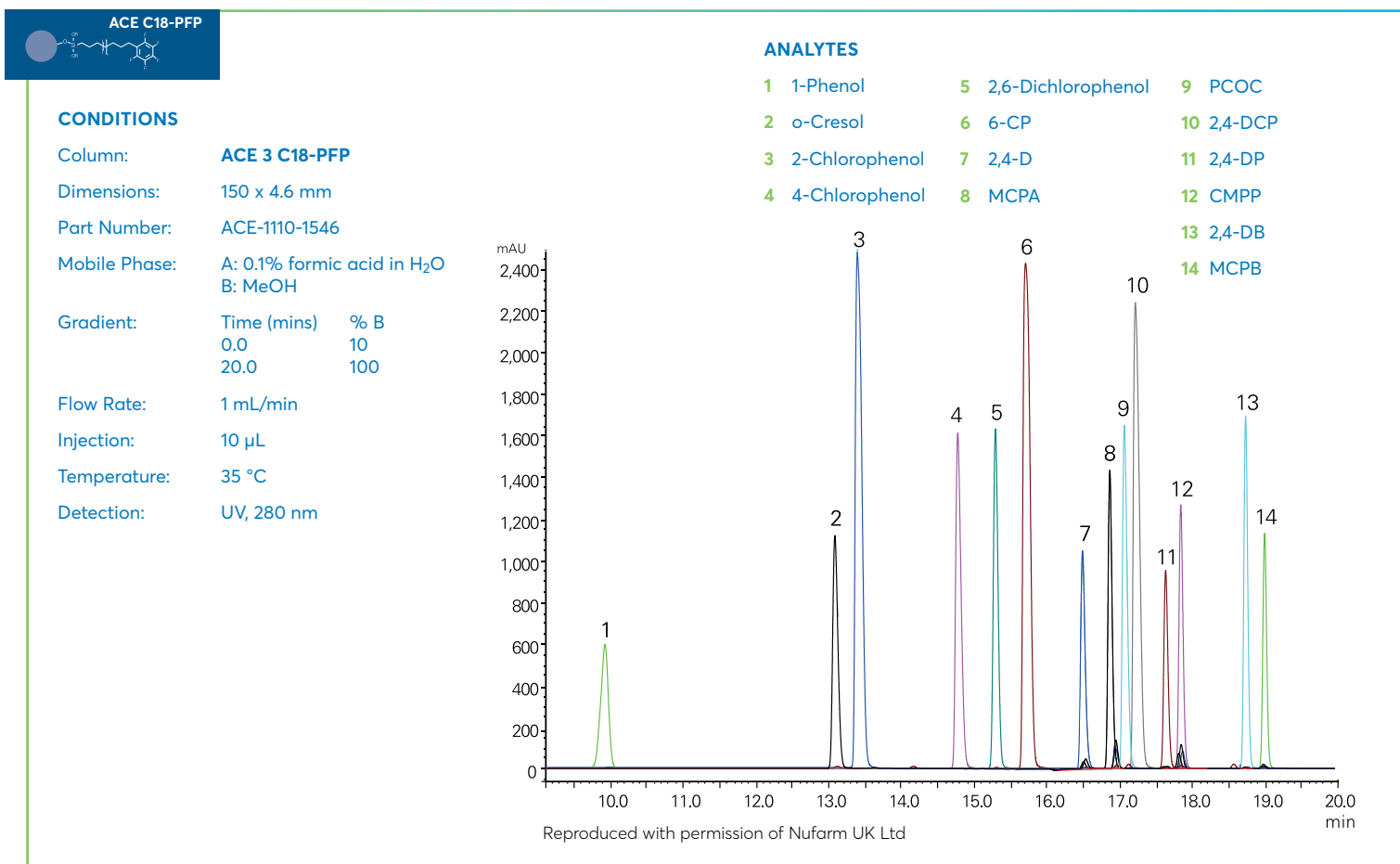
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Herbicides

Herbicides are a vital part of crop production and are widely utilised to improve crop quantity and quality. However, there is concern that once introduced, some herbicides and their degradation products may have negative environmental impacts and may impact human health. Powerful methods for the determination of a variety of herbicide components in different matrices are therefore highly valuable. The following section highlights the use of liquid chromatography for the detection of herbicides, and includes examples of the use of the novel Avantor ACE SuperC18 and Avantor ACE C18-PFP stationary phases.

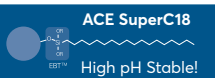
PHENOL AND PHENOXY ACID HERBICIDES

APPLICATION AN2290



GLYPHOSATE AND RELATED COMPOUNDS AS Fmoc DERIVATIVES (GRADIENT)

APPLICATION AN3850

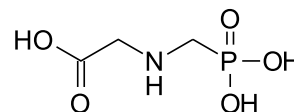


CONDITIONS

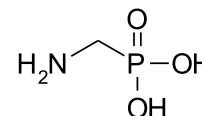
Column:	ACE Excel 3 SuperC18			
Dimensions:	150 x 2.1 mm			
Part Number:	EXL-1111-1502U			
Mobile Phase:	A: H ₂ O B: MeOH C: 200 mM ammonium formate pH 3.0			
Gradient:	Time (mins)	A %	B %	C %
	0	62.5	35.0	2.5
	10	2.5	95.0	2.5
	11	2.5	95.0	2.5
	12	62.5	35.0	2.5
	22	62.5	35.0	2.5
Flow Rate:	0.4 mL/min			
Injection:	0.1 µL			
Temperature:	60 °C			
Detection:	UV, 254 nm			
Sample:	Standards derivatised with Fmoc-Cl			

ANALYTES

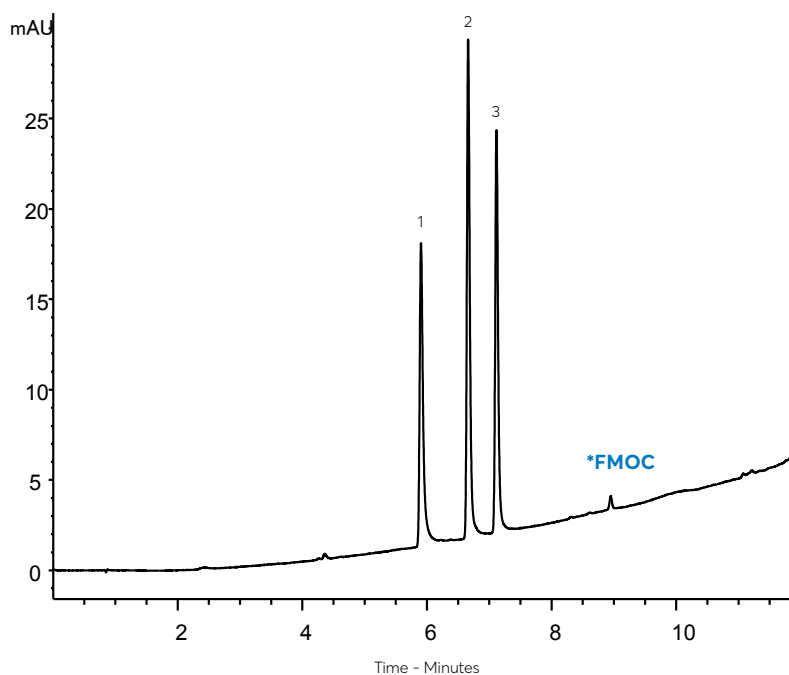
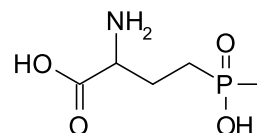
1 Glyphosate



2 Aminomethylphosphonic acid (AMPA)



3 Glufosinate



GLYPHOSATE AND RELATED COMPOUNDS
AS FMOC DERIVATIVES (ISOCRATIC)

APPLICATION AN3860

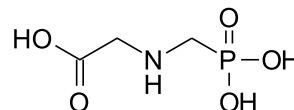


CONDITIONS

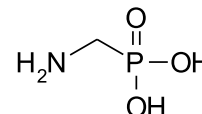
Column:	ACE Excel 3 SuperC18
Dimensions:	150 x 2.1 mm
Part Number:	EXL-1111-1502U
Mobile Phase:	5 mM ammonium formate pH 3.0 in MeOH/H ₂ O (45:55 v/v)
Flow Rate:	0.4 mL/min
Injection:	0.1 µL
Temperature:	25 °C
Detection:	UV, 254 nm
Sample:	Standards derivatised with FMOC-Cl

ANALYTES

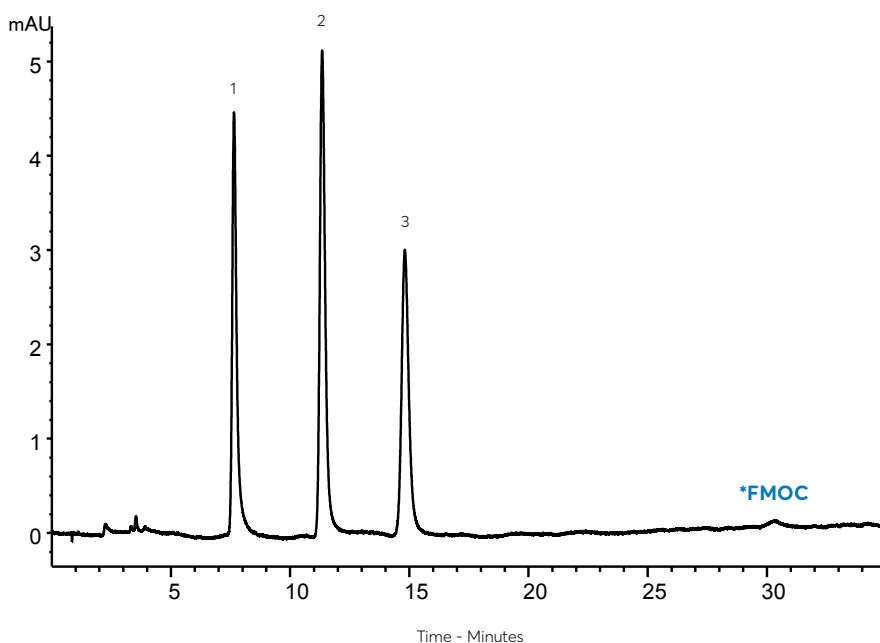
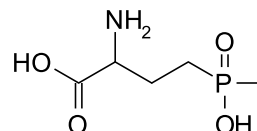
1 Glyphosate



2 Aminomethylphosphonic acid (AMPA)



3 Glufosinate



HERBICIDE – BENFLURALIN

APPLICATION AN2880

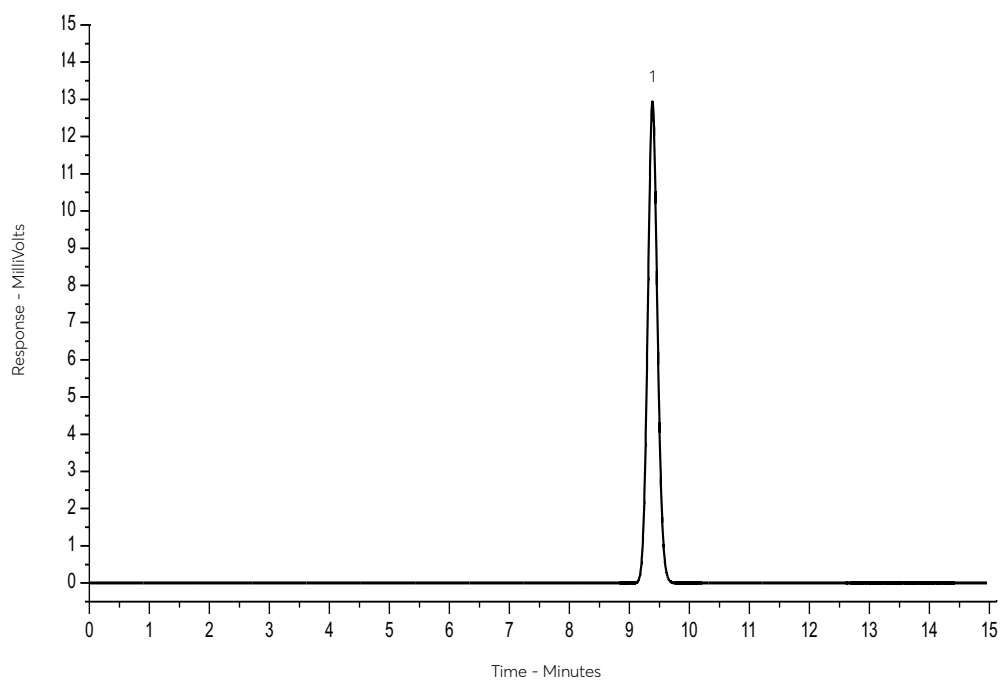
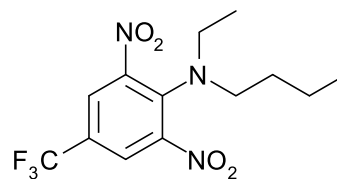
ACE C18

CONDITIONS

Column: **ACE 5 C18**
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: MeOH/H₂O (85:15 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

ANALYTES

1 Benfluralin



HERBICIDE – TRIFLURALIN

APPLICATION AN2890



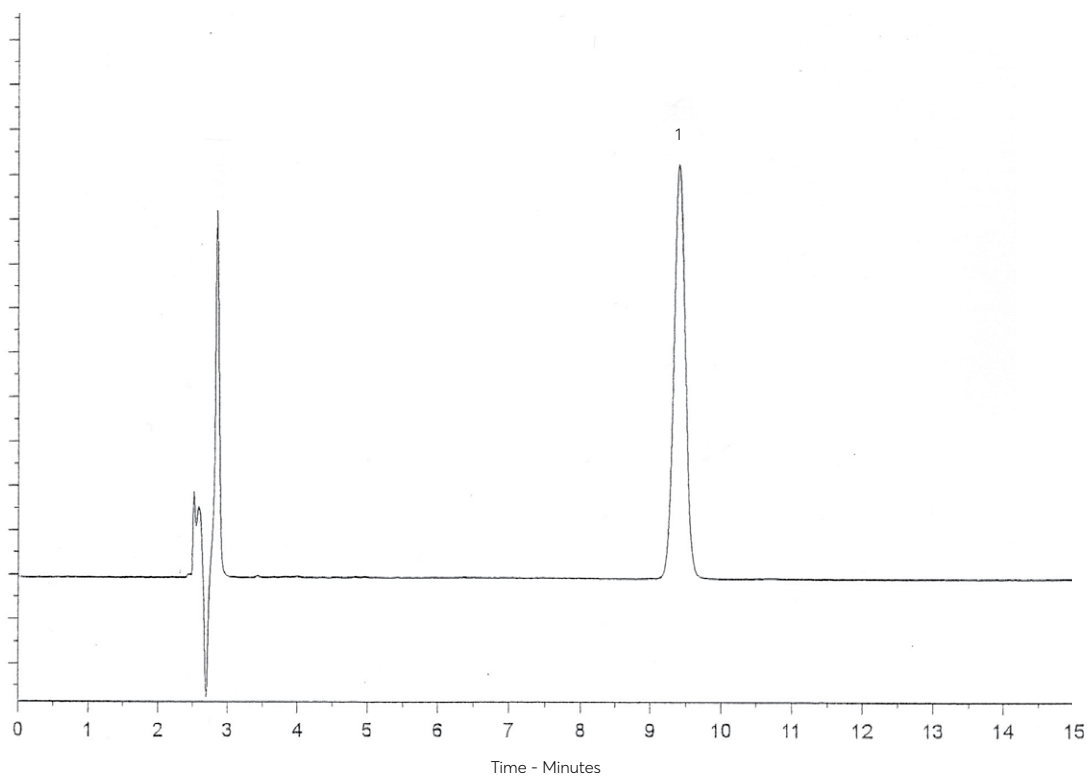
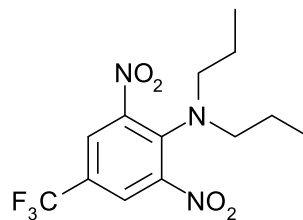
ACE C18

CONDITIONS

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: MeOH/H₂O (85:15 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

ANALYTES

1 Trifluralin



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- Each ACE phase provides different selectivity due to differing interactions

	Bonded Phase	SEPARATION MECHANISM AND RELATIVE STRENGTH ¹				
		Hydrophobic Binding	π-π Interaction	Dipole-Dipole	Hydrogen Bonding	Shape Selectivity
ACE Advanced Method Development Kit	ACE C18	****	–	–	*	**
	ACE C18-AR	****	*** (donor)	*	**	***
	ACE C18-PFP	****	*** (acceptor)	****	***	****
ACE Extended Method Development Kit	ACE SuperC18	****	–	–	–	**
	ACE C18-Amide	****	–	**	****	**/**
	ACE CN-ES	***	*	***	**	*
ACE UltraCore Method Development Kit	ACE UltraCore SuperC18	***	–	–	–	**
	ACE UltraCore SuperPhenylHexyl	**	*** (donor)	*	**	***

¹ Approximate value – determined by semi-quantitative mechanism weightings and/or by reference to other ACE phases using >100 characterising analytes.

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