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Chromatography Solutions

Avantor® ACE® HPLC and UHPLC columns Cannabis applications guide

Avantor® ACE®

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.

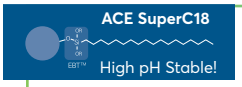
Table of contents

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

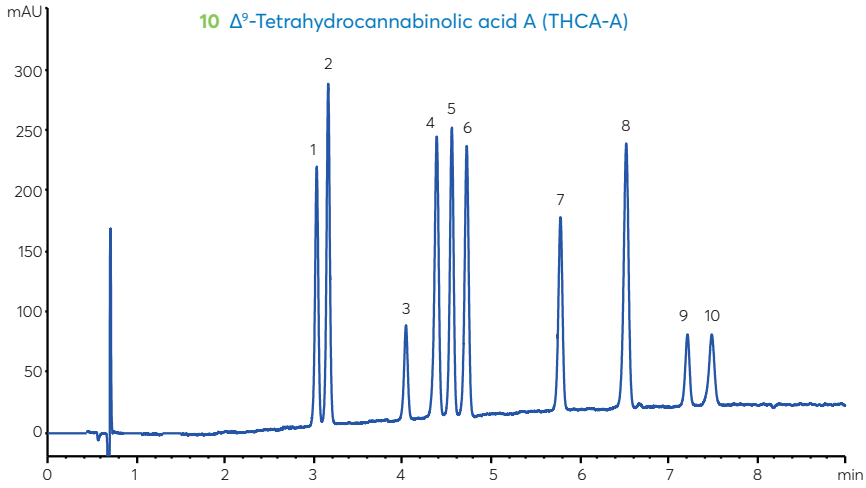


CONDITIONS

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_2O 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 µL
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

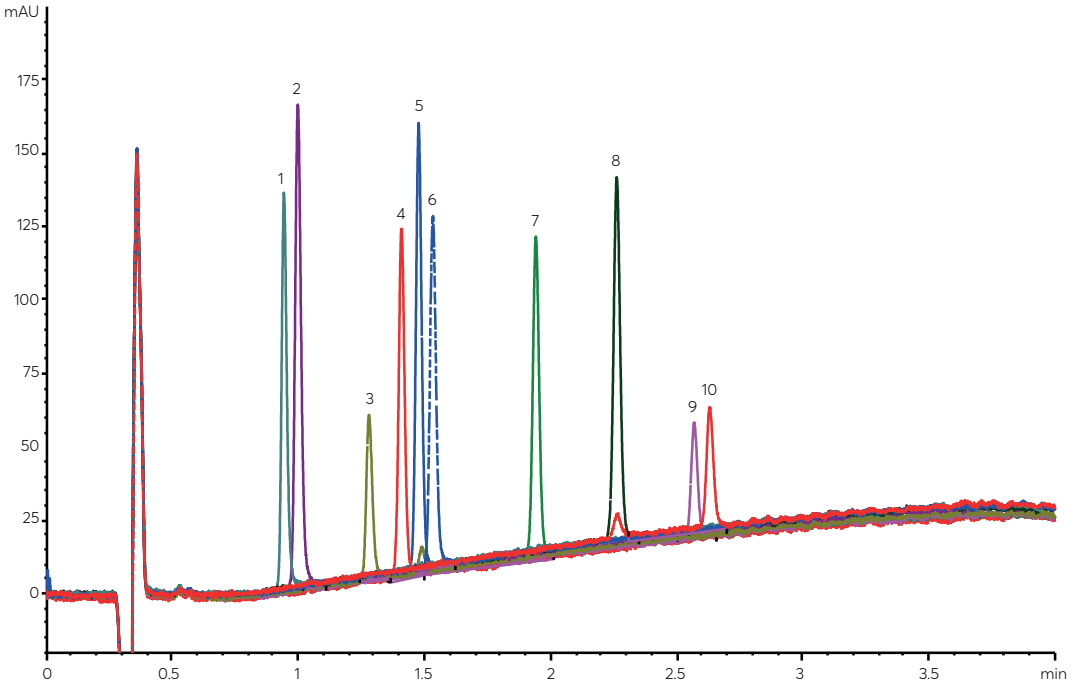
UltraCore SuperC18
High pH Stable!

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 H_2O 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

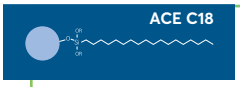
ANALYTES

1. (-)-11-Nor-9-carboxy-Δ⁹-tetrahydrocannabinol (THC-COOH)
2. Cannabidivarin (CBDV)
3. Cannabidiolic acid (CBDA)
4. Cannabigerol (CBG)
5. Cannabidiol (CBD)
6. Tetrahydrocannabivarin (THCV)
7. Cannabinol (CBN)
8. (-)-trans-Δ⁹-Tetrahydrocannabinol (THC)
9. Cannabichromene (CBC)
10. Δ⁹-Tetrahydrocannabinolic acid A (THCA-A)



LOW LEVEL DETERMINATION OF CANNABIS USE FROM HAIR SAMPLES

APPLICATION AN7070

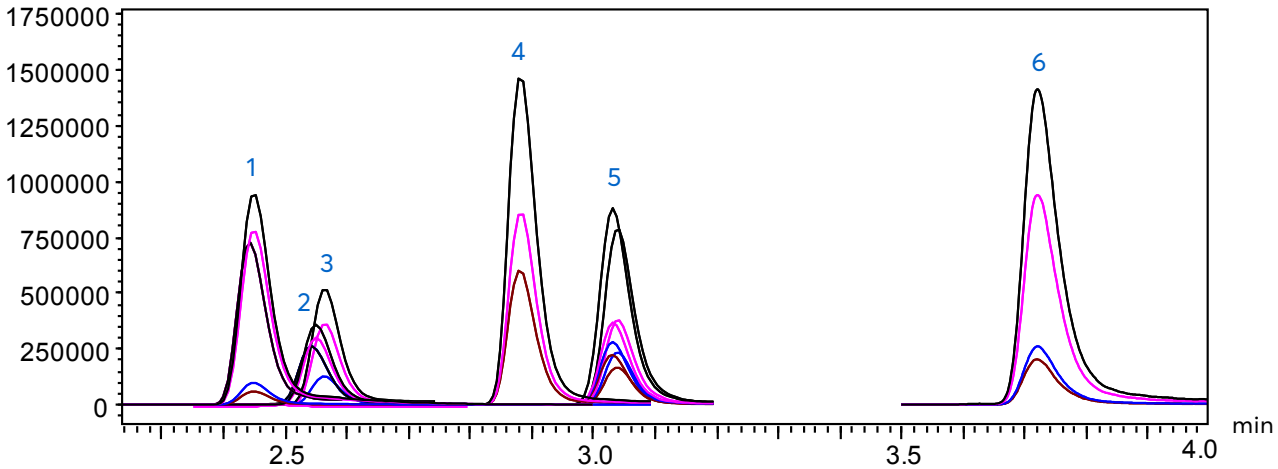


CONDITIONS

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 H_2O 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 mode
Sample:	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

1. 11-Hydroxy-Δ^9-tetrahydrocannabinol (THC-OH)
2. 11-Nor-9-carboxy-Δ^9-Tetrahydrocannabinol (THC-COOH)
3. Cannabidiol (CBD)
4. Cannabinol (CBN)
5. Tetrahydrocannabinol (THC)
6. Δ^9-Tetrahydrocannabinolic acid-A (THCA-A)



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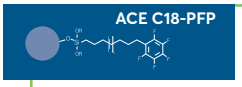
SEPARATION OF TERPENES USING LC/MS FRIENDLY CONDITIONS

APPLICATION AN7040



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 H_2O B: 0.1% formic acid in MeCN

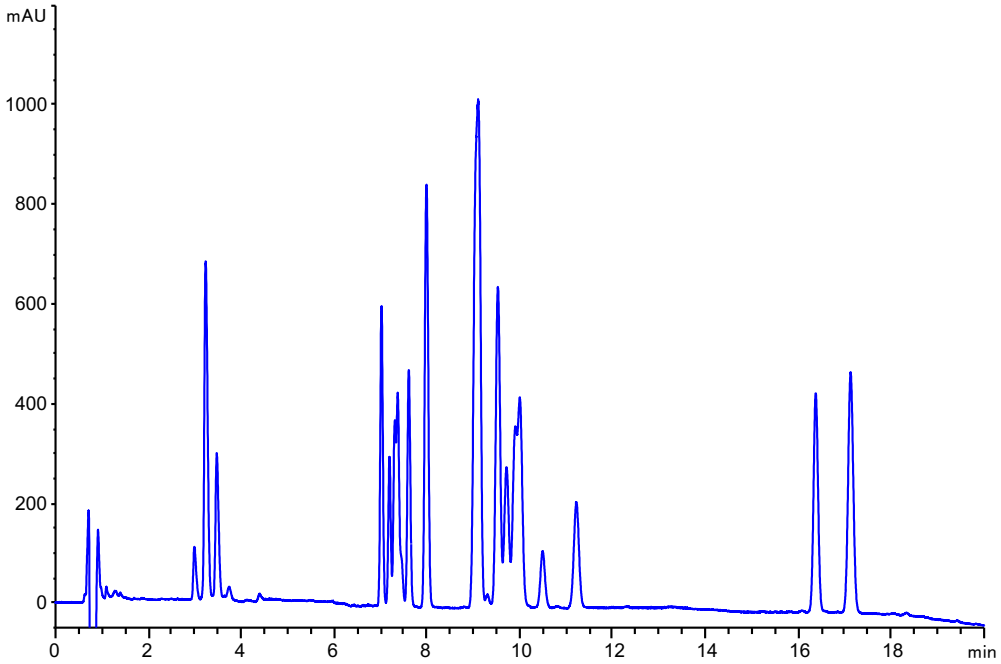
Gradient:

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 µL
Temperature:	30 °C
Detection:	UV, 210 nm

ANALYTES

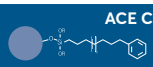
a-Pinene	Camphene
(-)-β-Pinene	β-Mycene
δ-3-Carene	a-Terpinene
D-Limonene	Ocimene
γ-Terpinene	Terpinolene
Linalool	(-)-Isopulegol
Geraniol	β-Caryophyllene
a-Humulene	Nerolidol
(-)-Guaiol	(-)-a-Bisabolol
1,8-Cineole (Eucalyptol)	p-Cymene
(-)-Caryophyllene oxide	



SYNTHETIC CANNABINOIDS BY LC-MS/MS

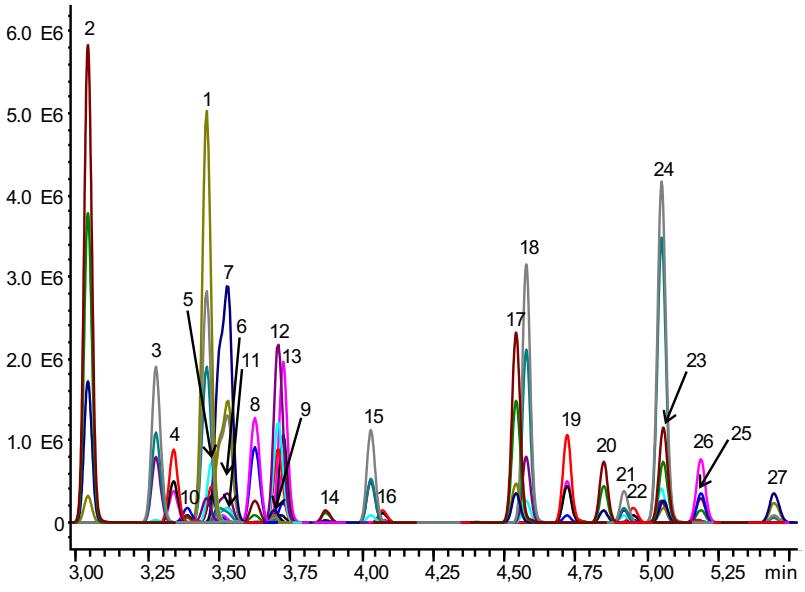
APPLICATION AN2540

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 H_2O 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

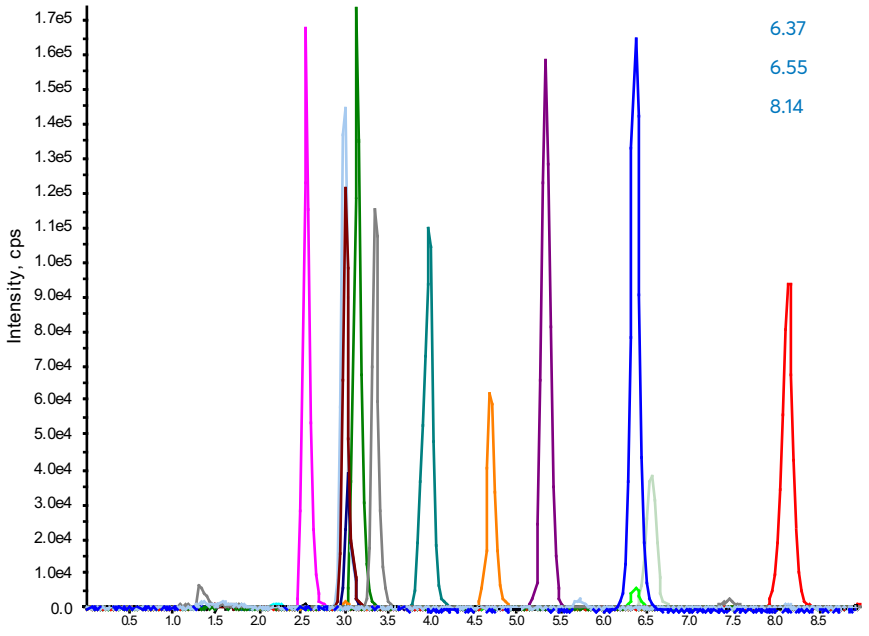
APPLICATION AN1650

ACE C18-AR

CONDITIONS

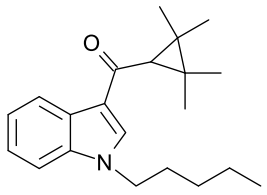
Column:	**ACE Excel 2 C18-AR**
Dimensions:	100 x 2.1 mm
Part Number:	EXL-109-1002U
Mobile Phase:	0.1% formic acid in MeOH/H_2O (85:15 v/v)
Flow Rate:	0.3 mL/min
Temperature:	Ambient
Detection:	Applied Biosystems/MDS Sciex 4000 Q-Trap Positive mode Turbo Ionspray

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

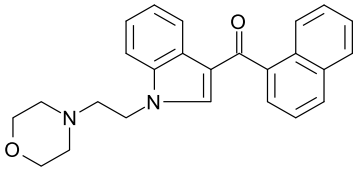


ANALYTES

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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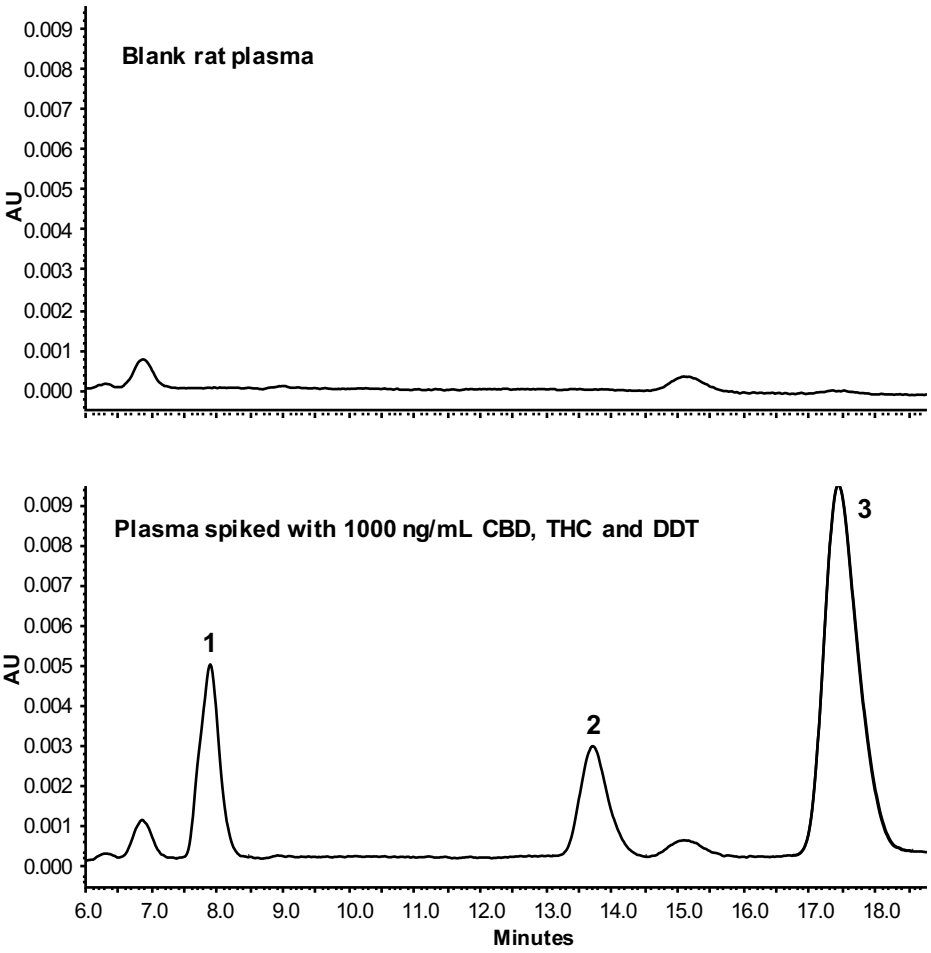
CANNABINOIDS IN RAT PLASMA

APPLICATION AN2310

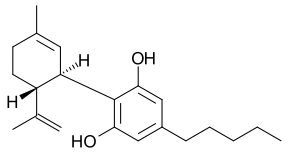
ACE C18-PFP



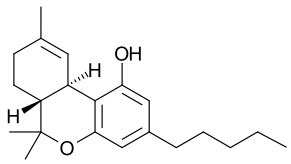
LLOQ 10 ng/mL for both cannabinoids
Method linearity 10 – 10,000 ng/mL

CONDITIONS

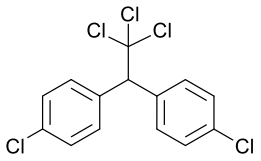
Column:	**ACE 3 C18-PFP**
Dimensions:	150 x 4.6 mm
Part Number:	ACE-1110-1546
Mobile Phase:	MeCN/H_2O (62:38 v/v)
Flow Rate:	1 mL/min
Injection:	30 µL
Temperature:	55 °C
Detection:	UV, 220 nm



1. Cannabidiol(CBD)



2. Δ^9-Tetrahydrocannabinol (THC)



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

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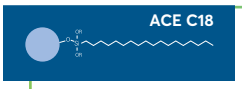
Mycotoxins

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

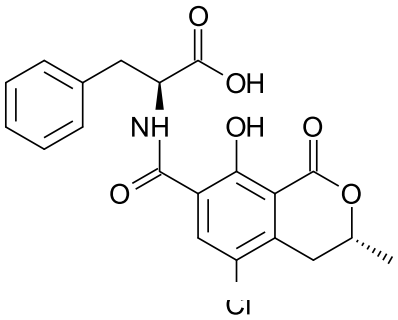


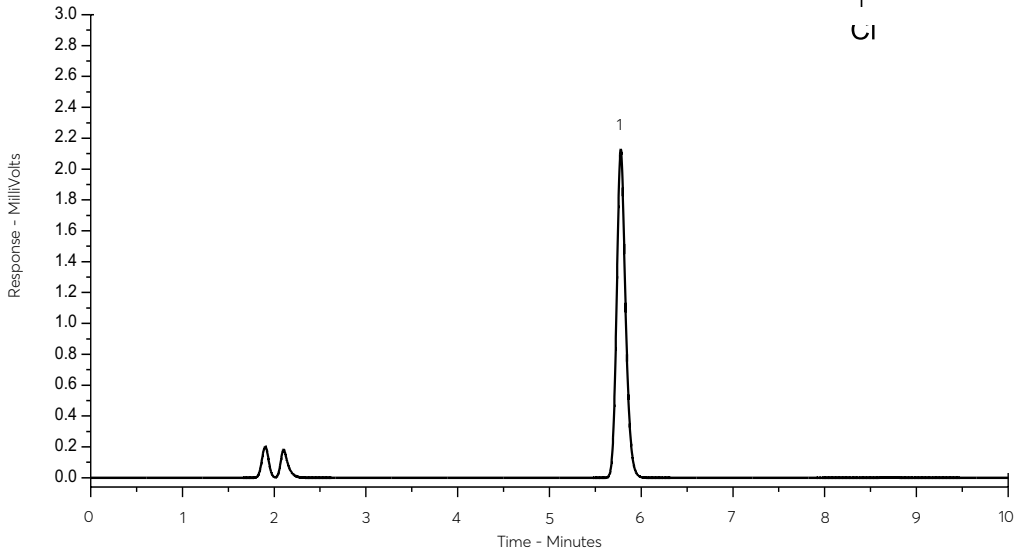
CONDITIONS

Column:	**ACE 5 C18**
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	MeCN/H_2O/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

ANALYTES

1 Ochratoxin A





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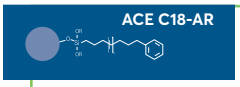
MYCOTOXINS BY LC-MS/MS

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 H_2O B: 1 mM ammonium acetate, 0.5% acetic acid in 95% MeOH

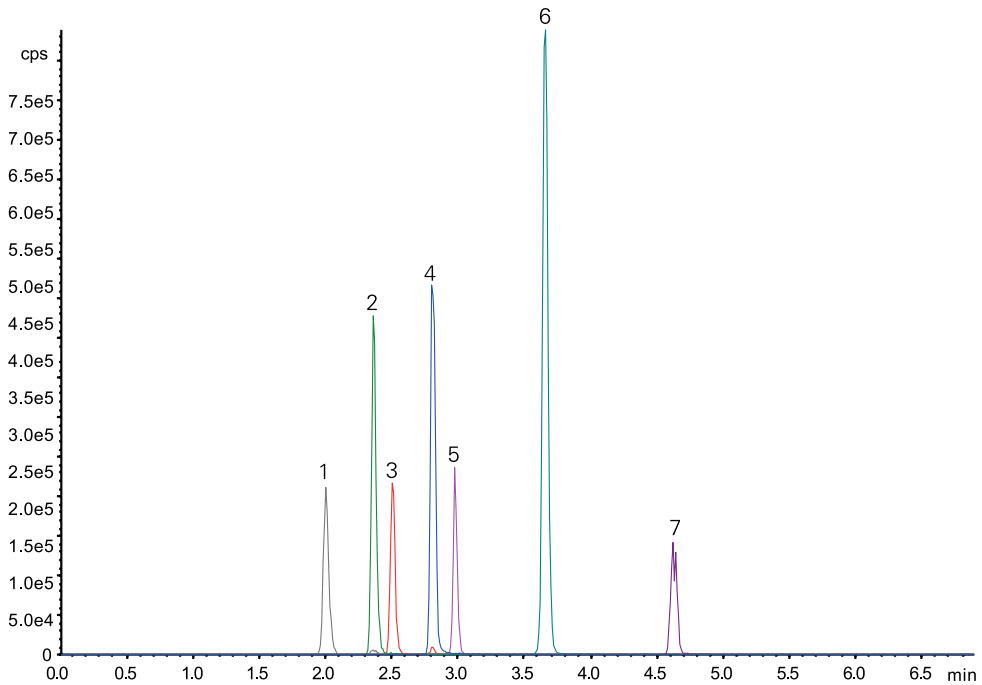
Gradient:

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

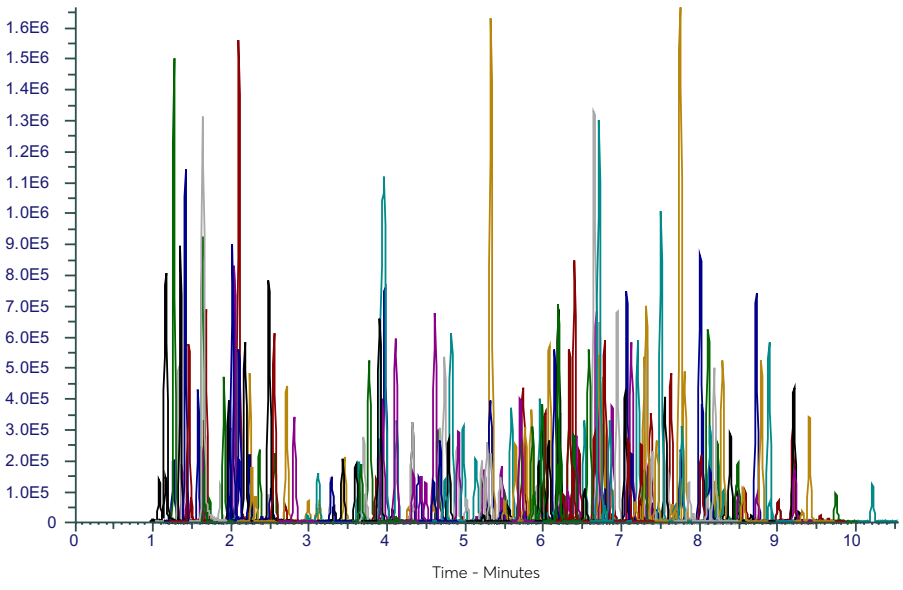
CONDITIONS

Column:	**ACE Excel 2 C18**
Dimensions:	100 x 2.1 mm
Part Number:	EXL-101-1002U
Mobile Phase:	A: 10 mM ammonium formate + 0.05% formic acid in H_2O B: 10 mM ammonium formate + 0.05% formic acid in MeOH

Gradient:

Time (mins)	% B
0.00	2
0.25	30
10.00	100
12.00	100
12.50	2
14.50	2

Flow Rate:	0.5 mL/min
Temperature:	50 °C
Detection:	TSQ Quantiva triple quad MS Positive mode HESI Spray voltage: 3500 V Ion transfer tube temperature: 350 °C Vaporizer temperature: 300 °C



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APPLICATION AN3060 - Page 2 of 4

ANALYTE	t_R/mins	Adduct	Precusor Ion m/z	Quant Ion m/z	Conf Ion m/z
3-OH Carbofuran	2.25	$[M+H]^+$	238.1	181.2	163.1
5-OH Thiabendazole	1.66	$[M+H]^+$	218.0	147.2	191.1
Abamectin	9.45	$[M+NH_4]^+$	890.5	305.3	567.5
Acephate	1.26	$[M+H]^+$	184.0	143.1	125.1
Acetamiprid	2.24	$[M+H]^+$	223.1	126.1	90.1
Aldicarb	2.95	$[M+NH_4]^+$	208.1	116.1	89.0
Aldicarb sulfone	1.44	$[M+NH_4]^+$	240.1	148.0	86.0
Aldicarb sulfoxide	1.37	$[M+NH_4]^+$	224.1	132.0	89.1
Allethrin	8.33	$[M+H]^+$	303.2	135.1	123.1
Ametoctradin	7.64	$[M+H]^+$	276.2	149.1	176.2
Atrazine	4.64	$[M+H]^+$	2.16.1	174.0	104.0
Azinphos ethyl	6.30	$[M+H]^+$	346.0	132.1	223.0
Azinphos methyl	5.14	$[M+H]^+$	318.0	132.0	124.9
Azinphos methyl OA	2.98	$[M+H]^+$	302.0	132.2	160.0
Azoxystrobin	5.59	$[M+H]^+$	404.1	372.1	344.1
Bendiocarb	3.72	$[M+H]^+$	224.1	174.0	109.1
Benoxacor	5.23	$[M+H]^+$	260.1	134.1	120.1
Bifenazate	6.27	$[M+H]^+$	301.1	198.0	170.1
Bitertanol	7.41	$[M+H]^+$	338.2	269.3	99.1
Boscalid	5.85	$[M+H]^+$	343.0	307.0	140.0
Bupirimate	6.68	$[M+H]^+$	317.2	210.2	237.3
Buprofezin	8.24	$[M+H]^+$	306.1	201.1	106.1
Cadusafos	7.58	$[M+H]^+$	271.1	159.0	131.0
Carbaryl	4.07	$[M+NH_4]^+$	219.1	145.1	127.0
Carbendazim	2.10	$[M+H]^+$	192.1	160.1	132.1
Carbofuran	3.77	$[M+H]^+$	222.1	165.2	123.2
Carboxin	3.97	$[M+H]^+$	236.1	143.0	93.0
Carfentrazone ethyl	6.88	$[M+H]^+$	412.0	346.1	366.0
Chlorantraniliprole	5.24	$[M+H]^+$	484.0	286.0	194.0
Chlorfenvinphos	7.21	$[M+H]^+$	359.0	170.0	99.1
Chlorimuron ethyl	5.73	$[M+H]^+$	415.1	186.0	83.0
Chlorpyrifos	8.47	$[M+H]^+$	349.9	198.0	97.0
Chlorpyrifos OA	6.65	$[M+H]^+$	334.0	278.0	197.9
Clethodim	7.71	$[M+H]^+$	360.3	164.1	136.1
Clofentezine	7.38	$[M+H]^+$	303.0	138.1	102.0
Cloransulam methyl	4.13	$[M+H]^+$	430.0	398.1	370.0
Clothianidin	1.99	$[M+H]^+$	250.0	169.1	132.0
Coumaphos	7.07	$[M+H]^+$	363.0	227.1	307.1
Crotoxyphos	5.86	$[M+NH_4]^+$	332.1	127.1	193.1
Crufomate	6.77	$[M+H]^+$	292.1	236.1	108.1
Cyantraniliprole	4.33	$[M+2+H]^+$	475.0	286.0	444.1
Cyazofamid	6.52	$[M+H]^+$	325.1	108.1	261.2
Cyflufenamid	7.42	$[M+H]^+$	413.1	295.1	203.0
Cymoxanil	2.48	$[M+H]^+$	199.1	128.1	111.1
Cyphenothrin	9.27	$[M+NH_4]^+$	393.2	151.2	123.2
Cyprosulfamide	3.30	$[M+H]^+$	375.1	135.1	254.1
Cyromazine	1.15	$[M+H]^+$	167.1	125.2	68.2
DEF	9.20	$[M+H]^+$	315.1	169.0	113.0
Demeton-S sulfone	2.55	$[M+H]^+$	291.1	235.1	263.1
Dialifos	7.46	$[M+H]^+$	394.0	208.1	181.0
Diazinon	7.12	$[M+H]^+$	305.1	169.1	153.2
Diazinon OA	5.32	$[M+H]^+$	289.1	153.2	233.1
Dichlormid	3.85	$[M+H]^+$	208.0	140.0	81.2
Dichlorvos	3.63	$[M+H]^+$	221.0	109.1	127.0
Dicrotophos	1.87	$[M+H]^+$	238.1	112.2	193.1
Diethofencarb	5.53	$[M+H]^+$	268.2	124.1	180.2
Diflubenzuron	6.66	$[M+H]^+$	311.0	158.0	141.0
Dimethenamid	5.70	$[M+H]^+$	276.1	244.1	168.2
Dimethoate	2.23	$[M+H]^+$	230.1	199.0	125.0
Dimethomorph	5.76, 6.07	$[M+H]^+$	388.1	301.0	165.1
Dinotefuran	1.36	$[M+H]^+$	203.1	129.1	114.2
Dioxacarb	2.26	$[M+H]^+$	224.1	123.1	167.1
Dioxathion	8.10	$[M-C_4H_{10}O_2PS_2]^+$	271.1	97.0	125.0
Disulfoton sulfone	4.59	$[M+H]^+$	307.0	261.1	125.0
Disulfoton sulfoxide	4.49	$[M+H]^+$	291.0	185.1	213.1
Diuron	4.82	$[M+H]^+$	233.0	72.1	160.0
DMST	3.90	$[M+H]^+$	215.1	106.1	151.0
Dodine	7.56	$[M+H]^+$	228.3	186.3	60.1
Emamectin	8.57	$[M+H]^+$	886.5	158.1	126.1
Ethiofencarb	4.27	$[M+H]^+$	226.1	107.1	169.1
Ethiofencarb sulfone	1.90	$[M+NH_4]^+$	275.1	107.1	201.1
Ethiofencarb sulfoxide	1.98	$[M+H]^+$	242.1	107.1	185.0
Ethion	8.31	$[M+H]^+$	385.0	199.1	143.0
Ethion monoxon	6.73	$[M+H]^+$	369.0	199.0	143.0
Ethiprole	5.77	$[M+NH_4]^+$	413.9	351.0	255.0
Ethofumesate	5.55	$[M+H]^+$	287.1	121.1	241.1
Ethoprop	6.46	$[M+H]^+$	243.1	173.0	131.0
Etofenprox	9.75	$[M+NH_4]^+$	394.2	177.2	107.1
Etoxazole	8.73	$[M+H]^+$	360.2	141.0	304.2
Famoxadone	7.24	$[M+H]^+$	392.2	331.1	238.0
Fenamidone	5.76	$[M+H]^+$	312.1	236.1	92.2
Fenamiphos	6.71	$[M+H]^+$	304.1	217.1	202.0
Fenamiphos sulfone	4.10	$[M+H]^+$	336.1	266.1	188.1
Fenamiphos sulfoxide	3.96	$[M+H]^+$	320.1	233.1	171.1
Fenazaquin	9.21	$[M+H]^+$	307.2	161.2	57.2
Fenhexamid	6.39	$[M+H]^+$	302.1	178.0	97.2
Fenobucarb	5.49	$[M+H]^+$	208.1	95.0	152.0
Fenoxaprop ethyl	8.04	$[M+H]^+$	362.1	288.1	91.1
Fenoxycarb	6.80	$[M+H]^+$	302.1	88.1	116.1
Fenpropimorph	6.42	$[M+H]^+$	304.3	147.2	119.1

APPLICATION AN3060 - Page 3 of 4

ANALYTE	t_R/mins	Adduct	Precusor Ion m/z	Quant Ion m/z	Conf Ion m/z
Fenpyroximate	8.90	$[M+H]^+$	422.2	366.1	214.2
Fensulfothion	4.89	$[M+H]^+$	309.0	235.0	281.1
Fenuron	2.17	$[M+H]^+$	165.1	72.1	77.1
Flonicamid	1.66	$[M+H]^+$	230.1	203.0	98.0
Fluazifop P butyl	8.12	$[M+NH_4]^+$	384.1	282.2	328.2
Fludioxonil	5.76	$[M+H]^+$	266.1	158.1	131.0
Flufenoxuron	8.79	$[M+H]^+$	489.0	158.1	141.1
Flufenpyr ethyl	6.72	$[M+H]^+$	409.1	335.0	307.0
Flumetsulam	2.03	$[M+H]^+$	326.1	129.1	109.0
Flumiclorac pentyl	8.13	$[M+NH_4]^+$	441.1	308.1	354.1
Fluometuron	4.31	$[M+H]^+$	233.1	72.2	46.3
Fluopicolide	6.00	$[M+H]^+$	383.0	173.0	145.0
Fluopyram	6.33	$[M+H]^+$	397.1	173.0	208.0
Fluoxastrobin	6.40	$[M+H]^+$	459.1	427.2	188.1
Fluridone	5.32	$[M+H]^+$	330.1	309.1	290.0
Flusilazole	6.77	$[M+H]^+$	316.1	247.2	165.1
Fluthiacet methyl	6.88	$[M+H]^+$	404.0	344.0	273.9
Flutolanil	5.95	$[M+H]^+$	324.1	262.0	282.0
Flutriafol	4.74	$[M+H]^+$	302.1	70.1	123.1
Fluxapyroxad	6.02	$[M+H]^+$	382.1	342.1	314.1
Forchlorfenuron	4.78	$[M+H]^+$	248.1	129.1	93.1
Formetanate HCl	1.26	$[M+H]^+$	222.0	165.1	120.0
Fosthiazate	4.40	$[M+H]^+$	284.1	104.1	228.1
Hexaconazole	7.29	$[M+H]^+$	314.1	158.9	70.0
Hexythiazox	8.51	$[M+H]^+$	353.1	228.0	168.0
Imazalil	5.14	$[M+H]^+$	297.1	159.1	255.1
Imazosulfuron	5.28	$[M+H]^+$	413.0	153.0	156.1
Imidacloprid	1.96	$[M+H]^+$	256.1	209.1	175.0
Imiprothrin	6.34	$[M+H]^+$	319.2	151.1 209.1	123.1
Indaziflam	6.58	$[M+H]^+$	302.2	158.1	145.1
Indoxacarb	7.75	$[M+H]^+$	528.1	249.0	150.1
Ipconazole	7.81	$[M+H]^+$	334.2	70.1	125.0
Iprovalicarb	6.31	$[M+H]^+$	321.2	119.1	186.2
Isofenphos	7.39	$[M+H]^+$	346.1	217.0	245.1
Isoprocarb	4.67	$[M+H]^+$	194.1	95.1	152.2
Isoproturon	4.79	$[M+H]^+$	207.2	72.2	165.2
Kresoxim methyl	6.90	$[M+H]^+$	314.1	267.2	222.1
Lactofen	8.22	$[M+NH_4]^+$	479.1	344.1	223.0
Lenacil	4.67	$[M+H]^+$	235.1	153.1	136.1
Leptophos OA	7.75	$[M+2+H]^+$	396.9	155.1	364.9
Linuron	5.46	$[M+H]^+$	249.0	182.1	160.1
Malathion	5.92	$[M+H]^+$	331.0	127.1	285.1
Malathion OA	3.89	$[M+H]^+$	315.1	127.1	99.0
Mandipropamid	5.94	$[M+H]^+$	412.1	328.2	356.2
Mefenpyr diethyl	7.26	$[M+H]^+$	373.1	327.1	160.0
Mepanipyrim	6.21	$[M+H]^+$	224.1	106.2	77.1
Mesotrione	2.01	$[M+H]^+$	340.1	228.1	104.1
Metaflumizone	8.30	$[M+H]^+$	507.1	178.0	287.1
Metalaxyl	4.91	$[M+H]^+$	280.1	220.1	192.1
Metaldehyde	2.02	$[M+NH_4]^+$	194.1	62.2	45.3
Metconazole	7.32	$[M+H]^+$	320.2	70.1	125.0
Methamidophos	1.16	$[M+H]^+$	142.0	94.2	125.1
Methidathion	4.97	$[M+NH_4]^+$	320.0	145.1	85.1
Methiocarb	5.64	$[M+H]^+$	226.1	169.2	121.1
Methiocarb sulfone	2.35	$[M+H]^+$	275.0	122.1	201.1
Methiocarb sulfoxide	2.10	$[M+H]^+$	242.1	185.1	122.1
Methomyl	1.61	$[M+H]^+$	163.1	106.1	88.1
Methoxyfenozide	6.04	$[M+H]^+$	369.2	149.1	313.1
Metolcarb	3.28	$[M+H]^+$	166.1	109.1	94.1
Metribuzin	3.59	$[M+H]^+$	215.1	187.1	131.1
Mevinphos	2.70	$[M+NH_4]^+$	242.1	193.1	127.1
Monocrotophos	1.71	$[M+H]^+$	224.1	193.0	127.0
Monolinuron	4.16	$[M+H]^+$	215.1	126.1	148.1
Myclobutanil	6.15	$[M+H]^+$	289.1	125.0	70.1
Nicosulfuron	3.45	$[M+H]^+$	411.1	182.0	213.0
Norflurazon	4.98	$[M+H]^+$	304.0	160.0	140.0
Norflurazon desmethyl	4.43	$[M+H]^+$	290.0	179.0	140.0
Omethoate	1.33	$[M+H]^+$	214.0	183.0	125.0
Oxamyl	1.48	$[M+NH_4]^+$	237.1	72.0	90.0
Oxamyl oxime	1.34	$[M+H]^+$	163.1	72.1	90.1
Oxydemeton methyl	1.57	$[M+H]^+$	247.0	169.1	109.1
Oxydemeton methyl sulfone	1.62	$[M+H]^+$	263.0	169.0	109.0
Parathion methyl OA	3.10	$[M+H]^+$	248.0	202.0	109.1
Parathion OA	4.61	$[M+H]^+$	276.1	220.1	248.1
Pencycuron	7.50	$[M+H]^+$	329.1	125.1	89.1
Penflufen	6.95	$[M+H]^+$	318.2	234.1	141.0
Penthiopyrad	7.05	$[M+H]^+$	360.1	177.1	276.1
Phenothrin	9.56	$[M+H]^+$	351.2	183.1	168.0
Phenthoate	6.81	$[M+H]^+$	321.0	247.1	79.1
Phorate OA	5.10	$[M+H]^+$	245.0	75.2	47.2
Phorate OA Sulfone	2.51	$[M+H]^+$	277.0	155.0	127.0
Phorate OA Sulfoxide	2.31	$[M+H]^+$	261.0	153.0	81.0
Phorate Sulfone	4.61	$[M+H]^+$	293.0	114.9	171.0
Phorate Sulfoxide	4.49	$[M+H]^+$	277.0	170.9	199.0
Phosalone	7.35	$[M+H]^+$	368.0	182.0	111.1
Phosmet	5.21	$[M+H]^+$	318.0	160.1	133.1
Phosmet OA	3.12	$[M+H]^+$	302.0	160.0	133.0
Phosphamidon	3.43	$[M+H]^+$	300.1	127.1	174.1
Phoxim	7.25	$[M+H]^+$	299.1	77.2	129.1
Picoxystrobin	6.79	$[M+H]^+$	368.1	145.0	115.0

APPLICATION AN3060 - Page 4 of 4

ANALYTE	t_R/mins	Adduct	Precusor Ion m/z	Quant Ion m/z	Conf Ion m/z
Pirimicarb	4.24	$[M+H]^+$	239.2	182.1	72.0
Pirimicarb Desmethyl	2.71	$[M+H]^+$	225.1	168.2	72.1
Pirimiphos Methyl	7.34	$[M+H]^+$	306.1	164.2	108.1
Prallethrin	7.69	$[M+H]^+$	301.2	133.0	151.2
Prochloraz	7.39	$[M+H]^+$	376.0	308.1	70.1
Profoxydim	7.71, 9.00	$[M+H]^+$	466.2	280.0	180.0
Promecarb	5.88	$[M+H]^+$	208.1	109.0	151.1
Propamocarb	1.41	$[M+H]^+$	189.1	102.0	144.0
Propaquizafop	8.21	$[M+H]^+$	444.1	299.2	371.2
Propargite	8.74	$[M+NH_4]^+$	368.2	231.2	175.1
Propetamphos	6.13	$[M+H]^+$	282.1	138.1	156.1
Propoxur(S)	3.69	$[M+H]^+$	210.1	168.2	111.1
Prosulfuron	5.29	$[M+H]^+$	420.1	167.1	141.1
Pymetrozine	1.44	$[M+H]^+$	218.1	105.1	78.1
Pyraclostrobin	7.30	$[M+H]^+$	388.1	163.1	194.1
Pyraflufen Ethyl	7.13	$[M+H]^+$	413.0	339.0	253.1
Pyrazophos	7.31	$[M+H]^+$	374.1	222.2	194.1
Pyridaben	9.22	$[M+H]^+$	365.1	309.0	147.1
Pyridalyl	10.21	$[M+2+H]^+$	492.0	110.9	164.0
Pyrimethanil	5.45	$[M+H]^+$	200.1	107.1	168.1
Pyriproxyfen	8.39	$[M+H]^+$	322.1	96.0	227.1
Quinalphos	6.78	$[M+H]^+$	299.1	163.1	147.1
Quinoxyfen	8.50	$[M+H]^+$	308.0	197.1	214.1
Quizalofop Ethyl	8.01	$[M+H]^+$	373.1	299.2	255.1
Resmethrin	9.40	$[M+H]^+$	339.2	128.1	171.1
Rimsulfuron	3.94	$[M+H]^+$	432.1	182.1	139.0
Rotenone	6.71	$[M+H]^+$	395.2	213.2	192.1
Saflufenacil	5.32	$[M+H]^+$	501.1	349.1	198.0
Sedaxane	6.20, 6.54	$[M+H]^+$	332.2	159.0	139.0
Sethoxydim	8.03	$[M+H]^+$	328.2	178.0	220.1
Simazine	3.66	$[M+H]^+$	202.1	104.1	132.1
Spinetoram	8.14	$[M+H]^+$	748.5	142.1	203.1
Spinosad A	7.69	$[M+H]^+$	732.5	142.1	98.0
Spinosad D	8.10	$[M+H]^+$	746.5	142.1	98.0
Spirodiclofen	8.91	$[M+H]^+$	411.1	313.1	71.1
Spiromesifen	8.66	$[M+NH_4]^+$	388.1	273.1	187.0
Spiromesifen Alcohol	5.01	$[M+H]^+$	273.2	187.1	179.1
Spirotetramat	6.38	$[M+H]^+$	374.2	302.3	216.2
Spiroxamine	5.95	$[M+H]^+$	298.3	144.2	100.2
Sulfoxaflor	2.39	$[M+NH_4]^+$	295.2	174.1	154.1
Sulprofos	8.56	$[M+H]^+$	323.0	219.1	139.1
TCMTB	5.48	$[M+H]^+$	239.0	180.0	136.0
Tebufenozide	6.78	$[M+H]^+$	353.2	133.0	104.8
Tebufenpyrad	8.19	$[M+H]^+$	334.2	117.1	145.1
Tebuthiuron	3.89	$[M+H]^+$	229.1	172.0	116.0
Tepraloxydim	4.10, 6.19	$[M+H]^+$	342.2	250.1	166.1
Terbufos Sulfone	5.46	$[M+H]^+$	321.0	115.0	143.0
Terbufos Sulfoxide	5.49	$[M+H]^+$	305.1	97.0	187.0
Terbuthylazine	5.71	$[M+H]^+$	230.1	174.1	104.1
Tetrachlorvinphos	6.86	$[M+2+H]^+$	366.9	127.1	206.0
Tetramethrin	7.91, 8.10	$[M+H]^+$	332.2	164.1	135.1
Thiabendazole	2.48	$[M+H]^+$	202.0	175.0	131.1
Thiacloprid	2.55	$[M+H]^+$	253.0	126.1	99.1
Thiamethoxam	1.65	$[M+H]^+$	292.0	211.1	181.1
Thifensulfuron Methyl	3.28	$[M+H]^+$	388.0	167.1	205.0
Thiobencarb	7.46	$[M+H]^+$	258.1	125.0	89.0
Thiodicarb	4.34	$[M+H]^+$	355.1	163.2	88.1
Thionazin	4.74	$[M+H]^+$	249.1	193.1	97.0
Topramezone	1.63	$[M+H]^+$	364.1	334.1	125.1
Triadimefon	6.07	$[M+H]^+$	294.1	197.0	225.0
Triadimenol	6.25	$[M+H]^+$	296.1	70.2	99.0
Triazophos	6.19	$[M+H]^+$	314.1	162.1	119.1
Tribenuron Methyl	4.59	$[M+H]^+$	396.1	155.1	181.1
Trichlorfon	2.26	$[M+H]^+$	256.9	109.0	221.0
Tricyclazole	2.80	$[M+H]^+$	190.0	163.1	136.1
Trifloxystrobin	7.78	$[M+H]^+$	409.1	186.2	206.2
Triflumizole	7.87	$[M+H]^+$	346.1	278.0	73.0
Triforine	5.23	$[M+2+H]^+$	434.9	213.0	98.2
Zoxamide	7.09	$[M+H]^+$	336.0	187.0	159.0

300 PESTICIDE SCREEN USING LC-MS/MS

APPLICATION AN3120 - Page 1 of 5

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/H_2O (1:9 v/v)
	B: 5 mM ammonium formate in MeOH/H_2O (9:1 v/v)

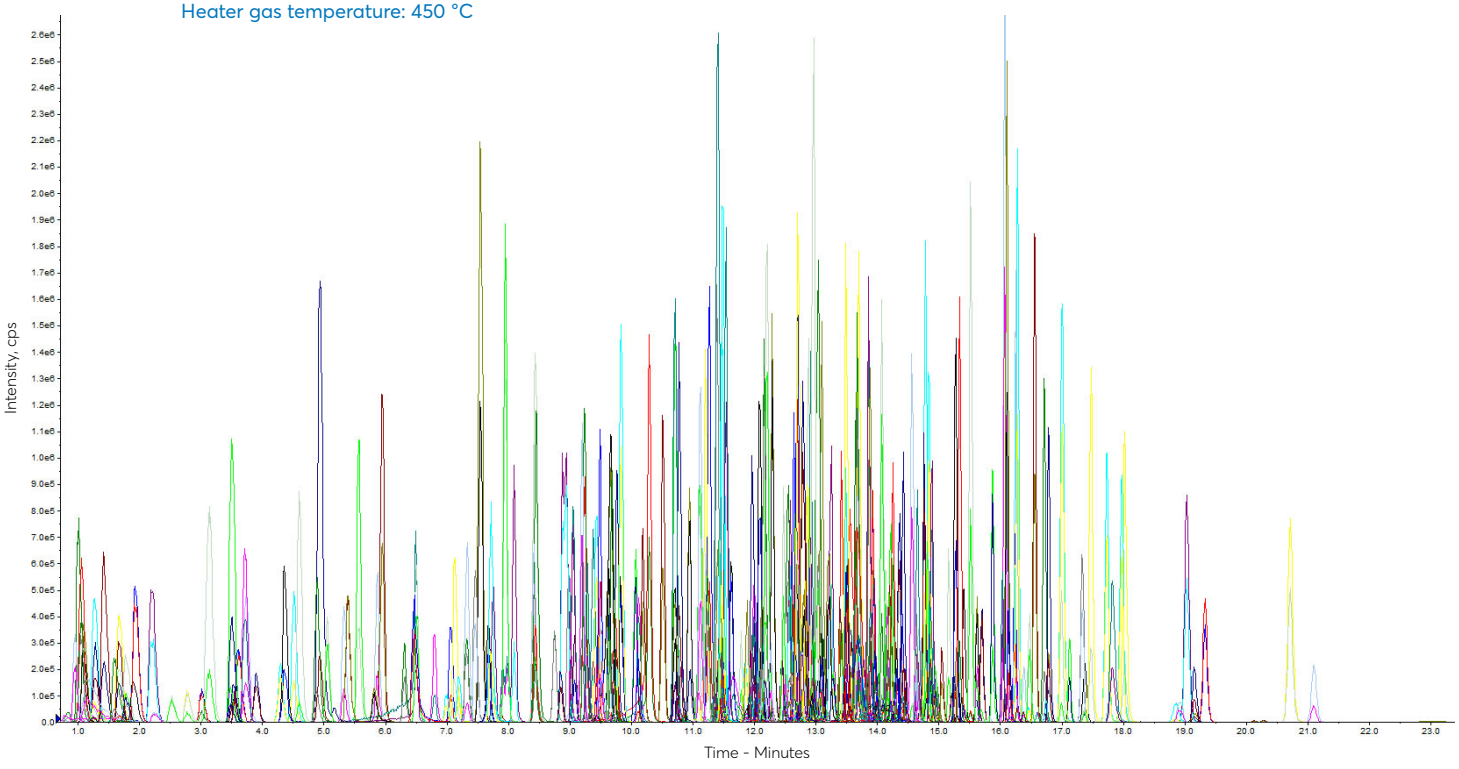
Gradient:

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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APPLICATION AN3120 - Page 2 of 5

ANALYTE	t_R/mins	MRM transitions (m/z)
3-Hydroxycarbofuran	3.5	238.1 → 163.1, 238.1 → 181.1
Acephate	1.0	184.1 → 142.9, 184.1 → 124.8
Acetamiprid	3.6	223.2 → 126.1, 225.2 → 128.1
Aclonifen	13.9	265.0 → 248.0, 267.0 → 250.0
Alachlor	12.9	270.2 → 238.2, 270.2 → 62.1
Aldicarb	5.4	208.0 → 89.0, 208.0 → 116.0
Aldicarb sulfone	1.2	240.0 → 86.0, 223.0 → 148.0
Aldicarb sulfoxide	1.1	207.0 → 132.0, 207.2 → 88.9
Ametryn	11.1	228.2 → 186.1, 228.2 → 68.0
Aminopyralid	0.8	207.0 → 160.9, 207.0 → 133.9
Amitrole	0.8	85.1 → 58.1, 85.1 → 57.1
Atrazine	9.3	216.2 → 174.0, 218.1 → 176.1
Atrazine-desethyl	4.4	188.2 → 146.0, 190.1 → 148.0
Atrazine-desisopropyl	2.4	174.1 → 104.1, 174.1 → 132.1
Avermectin B1a	18.2	876.5 → 553.0, 876.5 → 291.0
Avermectin B1b	19.1	890.5 → 305.0, 890.5 → 567.0
Azamethiphos	6.9	325.0 → 183.0, 325.0 → 138.9
Azinphos-ethyl	13.0	346.0 → 132.1, 346.0 → 160.1
Azinphos-methyl	10.9	318.1 → 132.1, 318.1 → 260.8
Aziprotryne	11.8	226.0 → 156.0, 226.0 → 125.0
Azoxystrobin	11.4	404.2 → 372.3, 404.2 → 344.1
Benalaxyl	14.0	326.2 → 148.1, 326.2 → 294.1
Benfuracarb	15.7	411.2 → 252.1, 411.2 → 195.1
Benthiavalicarb-isopropyl	12.0	382.3 → 116.0, 382.3 → 197.0
Bifenazate	12.5	301.2 → 198.1, 301.2 → 170.2
Bifenox	14.9	359.0 → 342.0, 359.0 → 310.0
Bifenthrin	21.0	440.0 → 181.1, 440.0 → 166.1
Bitertanol	14.6	338.2 → 269.0, 338.2 → 99.1
Bixafen	13.6	414.0 → 393.9, 416.1 → 395.9
Boscalid	11.7	343.1 → 306.8, 343.1 → 139.9
Bromfenvinfos-ethyl	14.3	405.0 → 155.0, 403.0 → 155.0
Bromuconazole A	12.2	378.0 → 159.1, 378.0 → 161.0
Bromuconazole B	13.5	378.1 → 159.1, 378.1 → 161.0
Bupirimate	13.5	317.2 → 166.2, 317.2 → 107.9
Buprofezin	16.1	306.3 → 201.1, 306.3 → 116.1
Cadusafos	14.8	271.1 → 158.9, 271.1 → 214.9
Carbaryl	8.3	202.2 → 145.1, 202.2 → 127.1
Carbendazim	4.7	192.2 → 160.1, 192.0 → 132.0
Carbofuran	7.4	222.2 → 165.1, 222.2 → 122.9
Carbosulfan	19.3	381.2 → 160.1, 381.2 → 118.1
Carboxin	8.3	236.1 → 143.1, 236.1 → 87.0
Carfentrazone-ethyl	13.8	412.2 → 345.9, 412.2 → 383.9
Chlorantraniliprole	10.7	484.0 → 452.9, 484.0 → 285.9
Chlorbromuron	11.7	295.1 → 205.9, 293.1 → 182.0
Chlorfenvinfos A	14.3	359.0 → 155.0, 358.9 → 99.0
Chloridazon	3.7	222.1 → 104.0, 222.1 → 77.1
Chlorpyrifos	16.8	349.9 → 198.1, 349.9 → 115.0

ANALYTE	t_R/mins	MRM transitions (m/z)
Chlorpyrifos-methyl	15.2	322.0 → 124.9, 324.0 → 125.1
Chlortoluron	9.1	213.2 → 72.0, 215.1 → 72.1
Cinidon-ethyl	16.3	394.0 → 348.0, 394.0 → 366.0
Clethodim A	12.8	360.1 → 164.1, 360.1 → 268.1
Clethodim B	10.2	360.1 → 164.1, 360.1 → 268.1
Clofentezine	15.1	303.1 → 137.9, 305.1 → 102.0
Clomazone	10.7	240.1 → 124.9, 242.2 → 127.1
Cloquintocet-mexyl	16.1	336.2 → 238.0, 336.2 → 192.1
Clothianidin	2.9	250.1 → 169.0, 250.1 → 132.0
Coumaphos	14.3	363.0 → 227.0, 363.0 → 211.1
Cyanazine	6.7	241.1 → 214.1, 243.1 → 216.1
Cyazofamid	13.2	325.2 → 107.9, 327.2 → 107.9
Cycloate	14.9	216.2 → 83.1, 216.2 → 154.1
Cycloxydim A	13.1	326.3 → 280.0, 326.3 → 180
Cycloxydim B	8.4	326.3 → 280.0, 326.3 → 180
Cymoxanil	4.2	199.2 → 128.0, 199.2 → 111.1
Cyproconazole A	12.5	292.0 → 70.0, 292.0 → 125.0
Cyproconazole B	12.0	292.0 → 70.0, 292.0 → 125.0
Cyprodinil A	14.1	226.2 → 93.0, 226.2 → 77.0
Demeton-S-methyl	7.7	231.1 → 88.8, 231.1 → 61.0
Demeton-S-methyl sulfone	1.6	263.0 → 168.9, 263.0 → 120.8
Desmedipham	10.6	318.1 → 182.1, 318.1 → 136.0
Desmethyl-pirimicarb	5.8	225.2 → 72.0, 225.2 → 168.1
Diafenthiuron	17.4	385.2 → 329.2, 385.2 → 278.2
Diazinon	14.2	305.1 → 169.1, 305.1 → 97.0
Dichlofluanid	12.8	333.0 → 223.9, 333.0 → 122.9
Diclobutrazol A	13.7	328.0 → 70.0, 330.0 → 70.0
Dicrotofos	2.1	238.1 → 112.1, 238.1 → 193.1
Diethofencarb	11.1	268.1 → 226.1, 268.1 → 124.0
Difenoconazole	14.8	406.1 → 251.1, 408.2 → 253.1
Diflubenzuron	13.5	311.0 → 158.2, 311.0 → 141.1
Diflufenican	15.4	395.0 → 266.0, 395.0 → 246.0
Dimethachlor	10.2	256.2 → 224.0, 256.2 → 148.1
Dimethenamid	11.3	276.1 → 244.0, 278.1 → 246.0
Dimethoate	3.6	230.1 → 198.8, 230.1 124.9
Dimethomorph	11.7	388.1 → 301.0, 388.1 → 165.1
Dimoxystrobin	13.7	327.1 → 205.0, 327.1 → 116.0
Diniconazole	14.8	326.0 → 70.0, 328.0 → 70.0
Disulfoton	15.0	275.1 → 89.0, 275.1 → 61.0
Disulfoton sulfone	9.6	307.1 → 153.0, 307.1 → 171.0
Disulfoton sulfoxide	9.2	291.1 → 212.9, 291.1 → 185.0
Ditalimfos	13.1	300.1 → 148.0, 300.1 → 130.0
Diuron	10.0	233.1 → 71.9, 235.1 → 72.0
DMST	8.0	215.2 → 106.0, 215.2 → 78.9
Dodine	13.6	228.3 → 57.0, 228.3 → 60.1
Epoxiconazole	12.9	330.1 → 120.9, 330.1 → 75.2
Ethion	16.5	385.0 → 199.0, 385.0 → 143.0

APPLICATION AN3120 - Page 3 of 5

ANALYTE	t_R/mins	MRM transitions (m/z)
Ethirimol	9.7	210.3 → 140.1, 210.3 → 98.0
Ethofumesate	11.3	287.1 → 121.0, 287.1 → 259.0
Ethoprofos	12.7	243.0 → 131.0, 243.0 → 97.0
Ethoxyquin A	12.9	218.2 → 148.0, 218.2 → 174.1
Ethoxyquin B	10.7	218.2 → 148.0, 218.2 → 174.1
Etofenprox	20.6	394.0 → 177.0, 394.0 → 359.0
Etrimfos	14.2	293.1 → 125.0, 293.1 → 265.1
Famoxadone NH_4+	14.4	392.0 → 331.0, 392.0 → 238.0
Fenamidone	11.5	312.1 → 92.1, 312.1 → 236.1
Fenamifos	13.4	304.0 → 217.0, 304.0 → 202.0
Fenamifos sulfone	8.4	336.0 → 308.0, 336.0 → 266.0
Fenamifos sulfoxide	7.9	320.0 → 171.0, 320.0 → 233.0
Fenarimol	12.7	331.2 → 268.0, 331.2 → 139.0
Fenazaquin	18.0	307.1 → 161.1, 307.1 → 147.0
Fenbuconazole	13.2	337.0 → 124.9, 337.0 → 70.0
Fenbutatin oxide	22.9	519.3 → 463.3, 519.3 → 197.0
Fenhexamid	12.6	302.2 → 96.9, 304.2 → 97.0
Fenoxycarb	13.6	302.2 → 87.9, 302.2 → 116.0
Fenpropathrin	17.3	367.0 → 125.0, 350.0 → 125.0
Fenpropidin	10.8	274.0 → 147.0, 274.0 → 117.0
Fenpropimorph	18.7	304.0 → 147.0, 304.0 → 117.0
Fenpyroximate	17.4	422.2 → 366.1, 422.2 → 135.1
Fensulfothion	10.0	309.1 → 280.8, 309.1 → 252.9
Fensulfothion sulfone	10.4	325.1 → 268.9, 325.1 → 297.0
Fenthion sulfone	9.0	311.1 → 125.0, 311.1 → 278.8
Fenthion sulfoxide	8.4	295.1 → 279.7, 295.1 → 108.9
Flonicamid	1.7	230.0 → 203.0, 230.0 → 148.0
Flubendiamide NH_4+	13.8	700.0 → 407.9, 682.9 → 407.9
Fludioxonil NH_4+	11.8	266.0 → 229.0, 266.0 → 227.1
Flufenacet	12.8	364.1 → 194.1, 364.1 → 152.2
Flufenoxuron	17.1	489.0 → 158.0, 489.0 → 141.1
Flumethrin NH_4+	20.2	527.2 → 510.0, 527.2 → 267.0
Flumetsulam	2.0	326.2 → 128.8, 326.2 → 128.3
Flumioxazin	10.7	355.0 → 327.0, 355.0 → 299.0
Fluometuron	8.9	233.0 → 72.0, 233.0 → 160.0
Fluopicolide	11.9	383.0 → 173.0, 385.1 → 174.9
Fluopiram	12.5	397.0 → 173.0, 397.0 → 208.0
Fluoxastrobin	12.8	459.1 → 427.1, 459.1 → 188.1
Fluquinconazole	12.6	376.1 → 307.1, 376.1 → 349.1
Flusilazole	13.3	316.2 → 247.0, 316.2 → 165.1
Flutolanil	12.0	324.0 → 262.0, 324.0 → 242.0
Flutriafol	9.7	302.1 → 70.1, 302.1 → 123.0
Fomesafen (NH_4-Adduct)	11.3	456.1 → 344.0, 458.1 → 346.0
Fonofos	14.3	247.0 → 109.0, 247.0 → 127.0
Fosthiazate	8.9	284.1 → 227.9, 284.1 → 104.0
Fuberidazole	6.9	185.0 → 157.0, 185.0 → 65.0
Furathiocarb	15.9	383.1 → 195.0, 383.1 → 252.1

ANALYTE	t_R/mins	MRM transitions (m/z)
Heptenofos	10.1	251.0 → 127.0, 251.0 → 124.8
Hexaconazole	14.3	314.0 → 70.0, 316.0 → 70.0
Hexaflumuron	15.5	461.1 → 158.2, 461.1 → 141.1
Hexazinone	7.3	253.2 → 71.0, 253.2 → 85.0
Hexythiazox	16.6	353.0 → 168.0, 353.0 → 228.0
Imazalil	13.6	297.2 → 159.1, 299.1 → 160.9
Imidacloprid	2.7	256.1 → 209.0, 256.1 → 175.0
Indoxacarb	15.2	528.1 → 248.9, 528.1 → 292.9
Ipconazole	15.3	334.2 → 70.0, 334.2 → 125.0
Iprodione	13.3	332.1 → 246.9, 330.0 → 245.0
Iprovalicarb	12.6	321.3 → 119.0, 321.3 → 203.1
Isofenfos	14.7	346.1 → 245.1, 346.1 → 217.1
Isofenfos-methyl	13.8	332.1 → 231.0, 332.1 → 273.0
Isoprocarb	9.4	194.1 → 95.0, 194.1 → 137.0
Isoprothiolane	12.1	291.1 → 231.0, 291.1 → 189.0
Isoproturon	9.7	207.2 → 72.0, 207.2 → 165.2
Isoxadifen-ethyl	13.9	313.2 → 296.1, 313.2 → 263.0
Isoxaflutole	10.0	360.1 → 251.1, 377.0 → 251.0
Kresoxim-methyl	13.9	314.0 → 116.0, 314.0 → 131.1
Lenacil	9.5	235.3 → 153.2, 235.3 → 136.2
Linuron	11.3	249.0 → 159.9, 249.0 → 182.0
Lufenuron	16.4	511.0 → 158.0, 511.0 → 141.0
Malaoxon	7.9	315.1 → 99.1, 315.1 → 127.1
Mandipropamid	11.9	412.1 → 328.1, 412.2 → 125.0
Mecarbam	13.0	330.1 → 227.0, 330.1 → 198.9
Mepanipyrim	12.9	224.2 → 106.0, 224.2 → 77.1
Mepronil	12.1	270.1 → 119.0, 270.1 → 228.1
Mesotrione	1.2	340.0 → 228.0, 357.1 → 227.9
Metaflumizone	16.1	507.1 → 178.1, 507.1 → 287.1
Metalaxyl	9.8	280.1 → 220.2, 280.1 → 192.2
Metamitron	3.4	203.1 → 175.0, 203.1 → 104.2
Metazachlor	9.6	278.1 → 209.9, 278.1 → 134.2
Metconazole	14.4	320.1 → 70.0, 320.1 → 125.0
Methacrifos	10.7	241.0 → 208.9, 241.0 → 124.9
Methamidofos	0.9	142.0 → 93.9, 142.0 → 112.1
Methiocarb	11.4	226.2 → 169.1, 226.2 → 121.2
Methiocarb sulfone	4.1	258.1 → 122.0, 258.1 → 200.9
Methiocarb sulfoxide	3.0	242.1 → 185.0, 242.1 → 122.1
Methomyl	1.6	163.0 → 106.0, 163.0 → 88.0
Methoxyfenozide	12.2	369.1 → 149.1, 369.1 → 313.2
Metobromuron	9.4	259.0 → 170.0, 259.0 → 148.1
Metolachlor	13.0	284.1 → 252.0, 286.1 → 254.0
Metoxuron	5.7	229.1 → 72.0, 231.1 → 71.9
Metrafenone	14.8	409.2 → 209.1, 411.2 → 209.1
Metribuzin	7.1	215.2 → 187.1, 215.2 → 84.1
Mevinfos A	4.9	225.0 → 193.0, 225.0 → 127.0
Mevinfos B	3.4	225.0 → 193.0, 225.0 → 127.0

APPLICATION AN3120 - Page 4 of 5

ANALYTE	t_R/mins	MRM transitions (m/z)
Molinate	12.0	188.2 → 126.2, 188.2 → 55.1
Monocrotofos	1.8	224.2 → 192.9, 224.2 → 126.9
Monolinuron	8.7	215.1 → 126.1, 215.1 → 148.1
Myclobutanil	12.2	289.2 → 70.0, 289.2 → 125.0
Napropamide	12.9	272.2 → 129.1, 272.2 → 171.1
Nitenpyram	1.3	271.1 → 189.2, 271.1 → 126.0
Novaluron	15.6	493.0 → 158.1, 493.0 → 141.1
Nuarimol	11.2	315.0 → 252.0, 315.0 → 81.0
Ofurace	7.6	282.0 → 160.1, 282.0 → 236.3
Omethoate	1.0	214.0 → 183.0, 214.0 → 125.0
Oxadiazon	16.2	345.0 → 220.0, 345.0 → 303.0
Oxadixyl	6.4	279.0 → 219.0, 279.0 → 133.0
Oxamyl NH_4+	1.2	237.1 → 72.0, 220.2 → 72.0
Oxycarboxin	4.5	268.1 → 174.9, 268.1 → 147.0
Oxydemeton-methyl	1.4	247.0 → 108.9, 247.0 → 168.9
Paclobutrazol	11.8	294.0 → 70.0, 294.0 → 125.0
Paraoxon	9.4	275.9 → 219.9, 275.9 → 248.0
Paraoxon-methyl	6.1	248.1 → 202.1, 248.1 → 90.0
Parathion	13.8	292.0 → 236.0, 292.0 → 264.1
Penconazole	13.7	248.1 → 70.0, 284.1 → 159.0
Pencycuron	14.8	329.3 → 125.1, 331.3 → 127.0
Pendimethalin	16.9	282.2 → 212.1, 282.2 → 194.1
Pethoxamid	12.7	296.2 → 131.0, 296.2 → 250.0
Phenmedipham	10.8	301.2 → 168.0, 301.2 → 136.0
Phenthoate	13.9	321.0 → 247.0, 321.0 → 275.1
Phorate sulfone	9.6	293.0 → 170.8, 293.0 → 96.7
Phorate sulfoxide	9.2	277.0 → 199.0, 277.0 → 171.0
Phosalone	14.6	368.0 → 182.0, 369.9 → 183.9
Phosphamidon	6.4	300.2 → 127.1, 300.2 → 226.8
Phoxim	14.7	299.2 → 129.2, 299.2 → 77.1
Picloram	1.2	243.0 → 224.9, 241.0 → 222.9
Picolinafen	16.2	377.1 → 238.0, 377.1 → 359.0
Picoxystrobin	13.6	368.0 → 205.0, 368.0 → 145.0
Piperonyl butoxide	16.2	356.2 → 177.2, 356.2 → 119.0
Pirimicarb	9.0	239.2 → 72.0, 239.2 → 182.3
Pirimiphos-ethyl	16.3	334.1 → 198.0, 334.1 → 182.3
Pirimiphos-methyl	14.8	306.2 → 108.0, 306.2 → 164.3
Prochloraz	14.4	376.0 → 308.0, 376.0 → 70.0
Profenofos	15.6	375.0 → 304.9, 373.0 → 302.9
Prometryn	12.6	242.2 → 158.1, 242.2 → 200.0
Propachlor	9.6	212.0 → 170.0, 212.0 → 94.1
Propamocarb	1.1	189.0 → 102.0, 189.0 → 144.0
Propaquizafop	16.0	444.2 → 100.0, 444.2 → 371.0
Propargite NH_4+	17.0	368.2 → 231.1, 368.2 → 175.0
Propazine	11.0	230.2 → 188.1, 230.2 146.1
Propetamfos	12.4	282.1 → 138.0, 282.1 156.1
Propham	9.4	180.1 → 138.1, 180.1 → 120.1

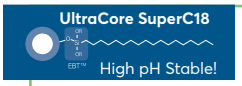
ANALYTE	t_R/mins	MRM transitions (m/z)
Propiconazole	14.0	342.1 → 159.0, 342.1 → 69.0
Propisochlor	14.0	284.2 → 224.0, 284.2 → 148.0
Propoxur	7.2	210.1 → 111.1, 210.1 → 168.0
Propyzamide	11.9	256.1 → 190.0, 256.1 → 173.0
Proquinazid	17.7	373.2 → 330.9, 373.2 → 289.0
Prosulfocarb	15.5	252.2 → 91.0, 252.2 → 128.1
Prosulfuron	9.0	420.1 → 141.0, 420.1 → 167.1
Prothioconazole	14.1	344.1 → 326.0, 346.1 → 328.1
Prothioconazole-desthio	13.0	312.0 → 70.0, 312.0 → 125.0
Pymetrozine	1.5	218.0 → 105.0, 218.0 → 78.0
Pyraclostrobin	14.5	388.1 → 194.0, 388.1 → 163.0
Pyrazophos	14.8	374.0 → 222.0, 374.0 → 194.0
Pyridaben	18.0	365.0 → 309.0, 365.0 → 147.0
Pyridapenthion	12.4	341.0 → 189.0, 341.0 → 205.0
Pyridate	19.1	379.1 → 206.9, 379.1 → 350.9
Pyrifenox	13.0	295.1 → 93.0, 297.1 → 93.0
Pyrimethanil	11.3	200.0 → 82.0, 200.0 → 107.0
Pyriproxyfen	16.7	322.0 → 96.0, 322.0 → 185.0
Pyroxsulam	5.6	435.0 → 195.1, 435.0 → 194.0
Quinalfos	13.9	299.0 → 271.0, 299.0 → 243.0
Quinoclamine	6.8	208.0 → 105.0, 208.0 → 77.0
Quinoxyfen	16.4	308.0 → 197.0, 308.0 → 162.0
Rotenone	13.4	395.1 → 213.1, 395.1 → 192.0
Secbumeton	10.6	226.2 → 170.1, 226.2 → 100.0
Silthiofam	13.5	268.0 → 252.0, 268.0 → 73.0
Simazine	7.2	202.02 → 132.1,202.2 104.0
Simetryn	9.4	214.1 → 124.1, 214.1 → 144.0
Spinosyn A	17.3	732.5 → 142.0, 732.5 → 98.0
Spinosyn D	18.3	746.5 → 142.0, 746.5 → 98.0
Spirodiclofen	17.4	313.1 → 295.0, 313.1 → 213.0
Spiromesifen	16.8	371.2 → 273.1, 371.2 → 255.2
Spirotetramat	12.8	374.2 → 302.2, 374.2 → 330.2
Spiroxamine	13.3	298.3 → 100.1, 298.3 → 144.1
Sulfotep	14.0	323.0 → 97.0, 323.0 → 115.0
Tau-fluvalinate	18.9	503.0 → 208.0, 503.0 → 181.0
Tebuconazole	13.9	308.1 → 70.0, 308.1 → 125.0
Tebufenozide	13.5	353.2 → 297.2, 353.2 → 133.0
Tebufenpyrad	15.9	334.0 → 145.0, 334.0 → 117.0
Teflubenzuron	16.3	381.1 → 158.2, 381.1 → 141.2
Tembotrione (NH_4 adduct)	5.9	458.0 → 340.9, 458.0 → 441.0
Terbufos	16.1	289.1 → 103.1, 289.1 → 232.9
Terbufos sulfone	11.1	321.1 → 171.0, 321.1 → 115.0
Terbufos sulfoxide	11.0	305.1 → 187.2, 305.1 → 131.1
Terbumeton	11.3	226.2 → 170.1, 226.2 → 142.0
Terbuthylazine	11.4	230.2 → 174.0, 232.2 → 176.0
Terbutryn	12.9	242.1 → 186.1, 242.1 → 96.0
Tetrachlorvinfos	13.5	367.0 → 127.0, 365.0 → 127.0

APPLICATION AN3120 - Page 5 of 5

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
Tolylfluanid	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

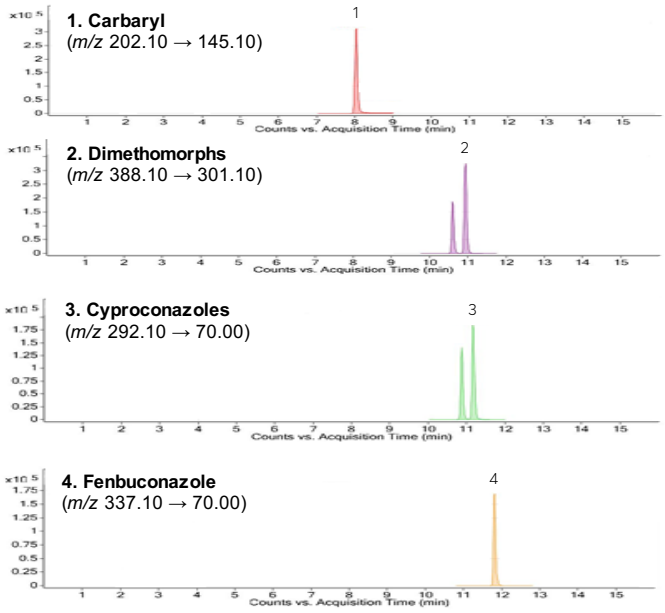
PESTICIDES BY LC-MS/MS

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_2O (1:9 v/v) B: 0.1% formic acid + 5 mM ammonium formate in MeOH/H_2O (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



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ANALYTES

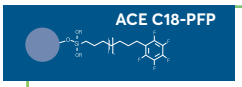
Also analysed under same conditions: Acephate, Acetamiprid, Aldicarb, Aldicarb sulfone, Aldicarb sulfoxide, Benomyl, Carbendazim, Carbofuran, Clofentezine, Clothianidin, Cyfluthrin, Demeton S-methylsulfone, Demeton S-methylsulfoxide, Dicrotophos, Dimethoate, Dinotefuran, DMA, DMPF, Flubendiamide, Folpet,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

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

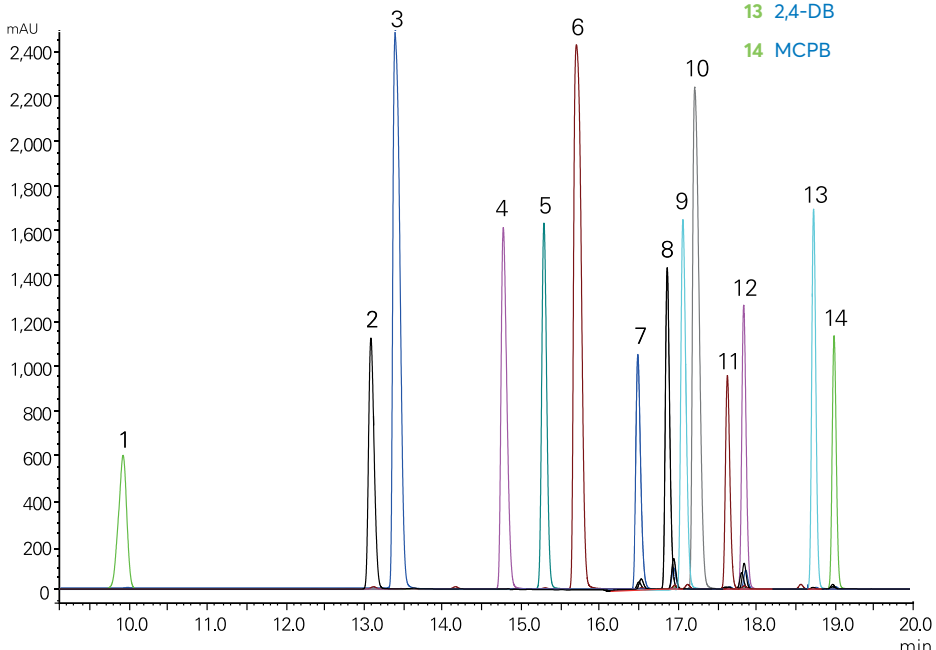


CONDITIONS

Column:	**ACE 3 C18-PFP**
Dimensions:	150 x 4.6 mm
Part Number:	ACE-1110-1546
Mobile Phase:	A: 0.1% formic acid in H_2O B: MeOH
Gradient:	Time (mins) % B 0.0 10 20.0 100
Flow Rate:	1 mL/min
Injection:	10 µL
Temperature:	35 °C
Detection:	UV, 280 nm

ANALYTES

1 1-Phenol
2 o-Cresol
3 2-Chlorophenol
4 4-Chlorophenol
5 2,6-Dichlorophenol
6 6-CP
7 2,4-D
8 MCPA
9 PCOC
10 2,4-DCP
11 2,4-DP
12 CMPP
13 2,4-DB
14 MCPB



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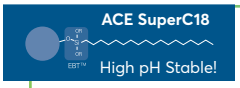
GLYPHOSATE AND RELATED COMPOUNDS AS FMOC DERIVATIVES (GRADIENT)

APPLICATION AN3850



CONDITIONS

Column: **ACE Excel 3 SuperC18**

Dimensions: 150 x 2.1 mm

Part Number: EXL-1111-1502U

Mobile Phase: A: H_2O
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

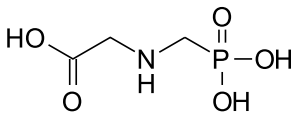
Temperature: 60 °C

Detection: UV, 254 nm

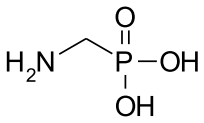
Sample: Standards derivatised with FMOC-Cl

ANALYTES

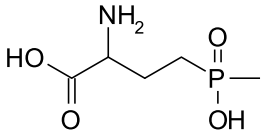
1 Glyphosate

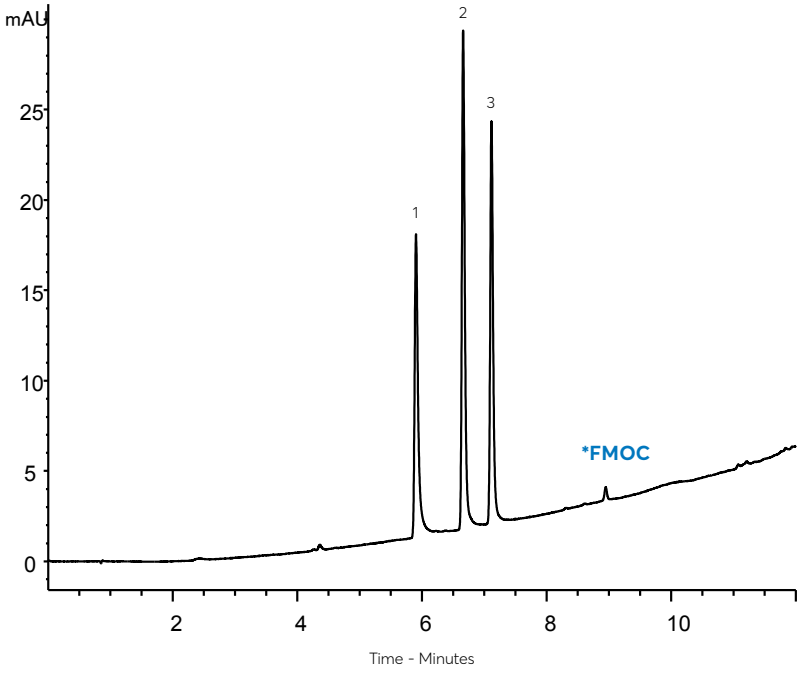


2 Aminomethylphosphonic acid (AMPA)



3 Glufosinate





GLYPHOSATE AND RELATED COMPOUNDS AS FMOC DERIVATIVES (ISOCRATIC)

APPLICATION AN3860

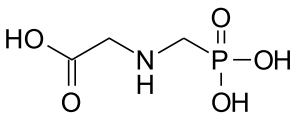
ACE SuperC18
High pH Stable!

CONDITIONS

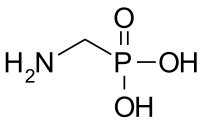
Column:	**ACE Excel 3 SuperC18**
Dimensions:	150 x 2.1 mm
Part Number:	EXL-1111-1502U
Mobile Phase:	5 mM ammonium formate pH 3.0 in MeOH/H_2O (45:55 v/v)
Flow Rate:	0.4 mL/min
Injection:	0.1 µL
Temperature:	25 °C
Detection:	UV, 254 nm
Sample:	Standards derivatised with FMOC-Cl

ANALYTES

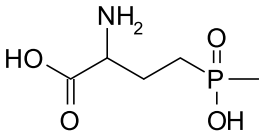
1 Glyphosate

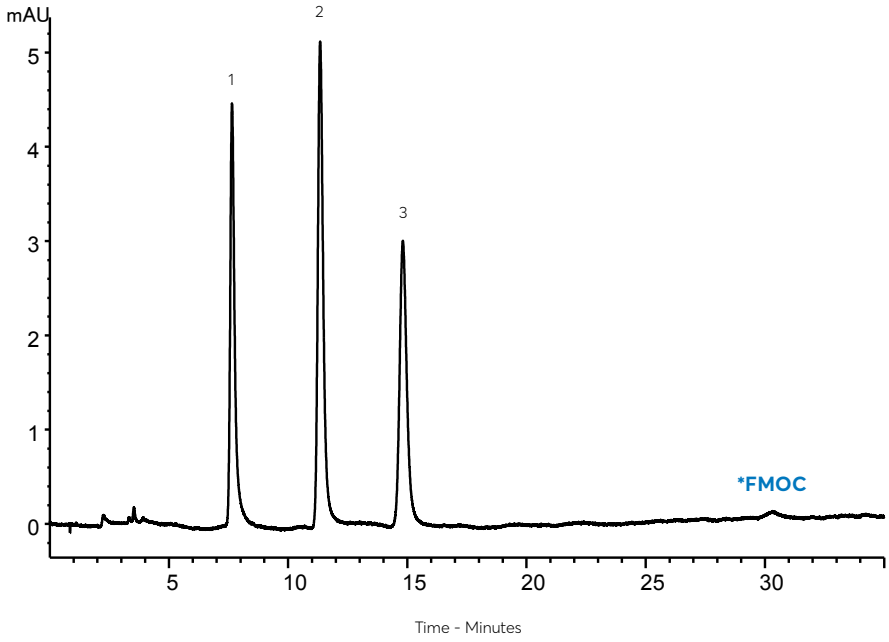


2 Aminomethylphosphonic acid (AMPA)



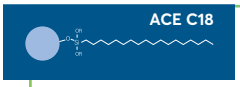
3 Glufosinate





HERBICIDE – BENFLURALIN

APPLICATION AN2880

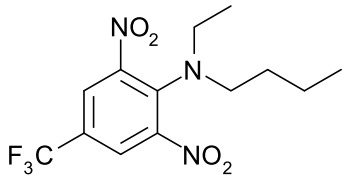


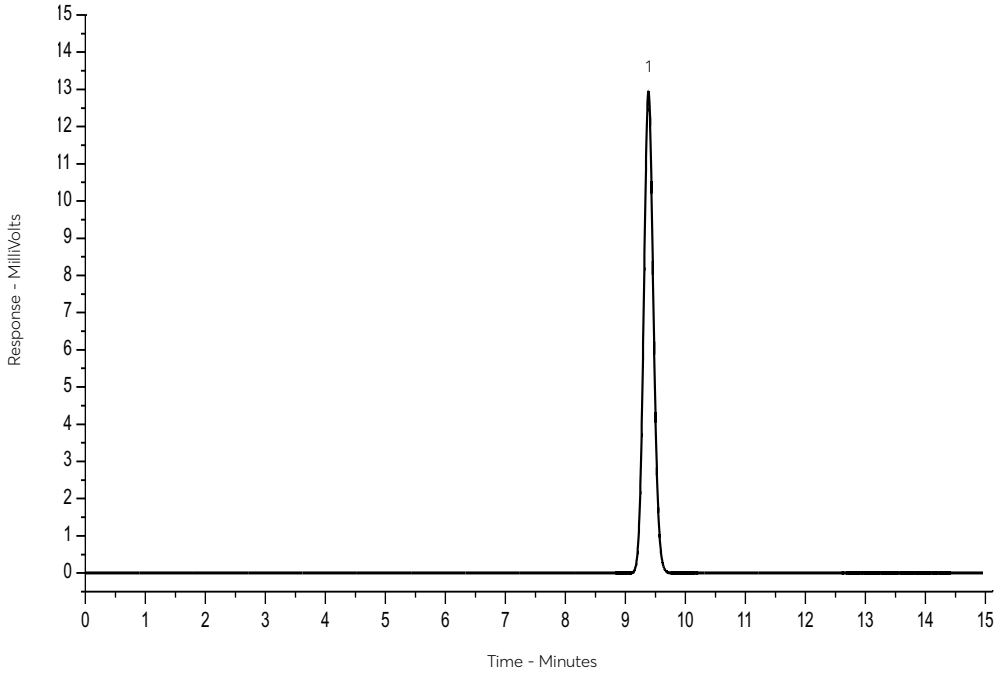
CONDITIONS

Column:	**ACE 5 C18**
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	MeOH/H_2O (85:15 v/v)
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 254 nm

ANALYTES

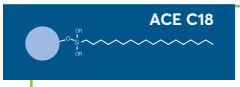
1 Benfluralin





HERBICIDE – TRIFLURALIN

APPLICATION AN2890

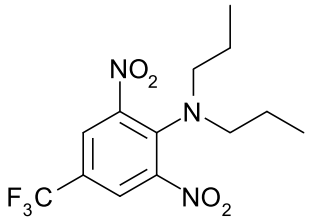


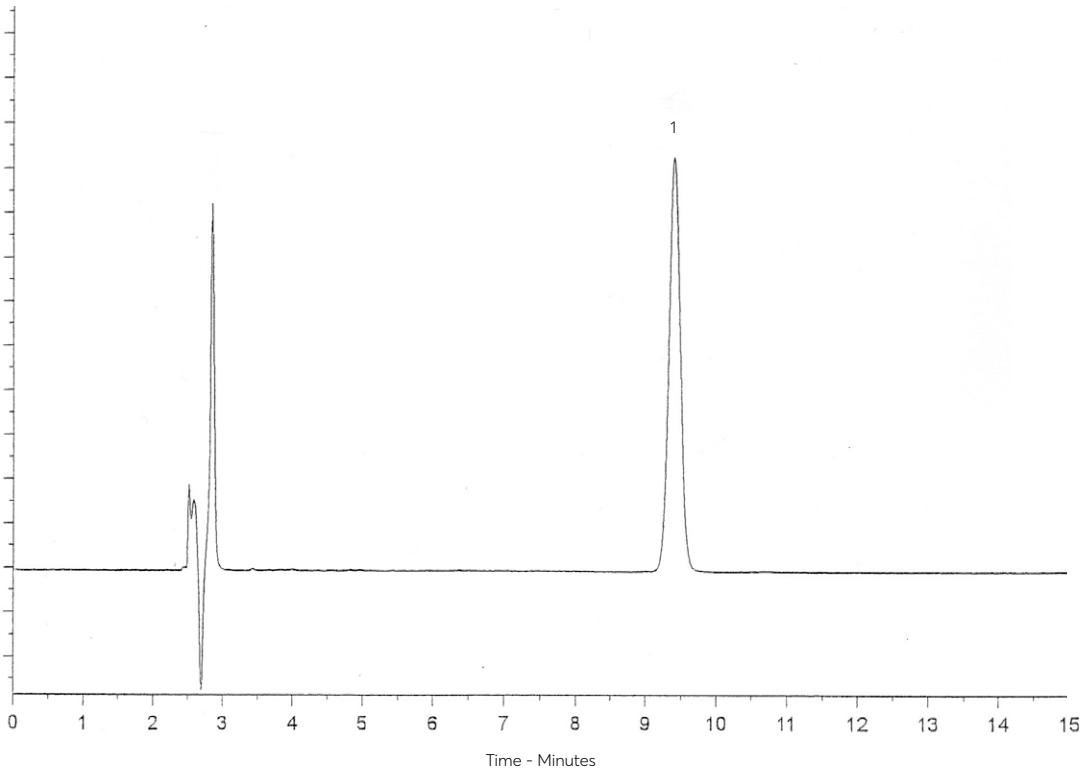
CONDITIONS

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	MeOH/H_2O (85:15 v/v)
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 254 nm

ANALYTES

1 Trifluralin





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	ACE C18-PFP	****	*** (acceptor)	****	***	****
ACE Extended Method Development Kit	ACE SuperC18	****	-	-	-	**
	ACE C18-Amide	****	-	**	****	**/***
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	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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