ACE®

UHPLC and HPLC Columns

Food and Beverage Applications Guide

ACE®

UHPLC and HPLC Columns

Ultra-Inert Base Deactivated UHPLC / HPLC Columns

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Separation of Additives and Intense Sweeteners

ACE® Ultra-inert UHPLC & HPLC Columns

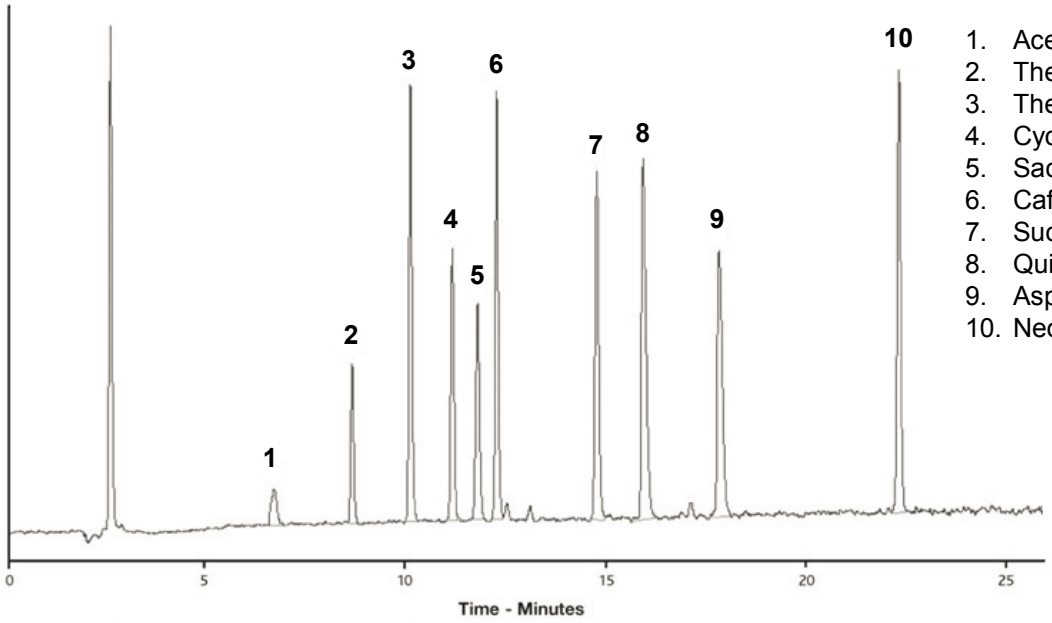
Application #AN2950

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.0 mm
Part Number: ACE-121-2504
Mobile Phase: A: H_2O
B: MeCN
C: 1% TFA in H_2O

Time (mins)	%A	%B	%C
0	88	2	10
25	50	40	10
30	30	60	10
35	88	2	10

Flow Rate: 1 mL/min
Temperature: 30 °C
Detection: ELSD



1. Acesulfame K
2. Theobromine
3. Theophylline
4. Cyclamate
5. Saccharin
6. Caffeine
7. Sucralose
8. Quinine sulphate
9. Aspartame
10. Neohesperidin dihydrochalcone

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Pesticides by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

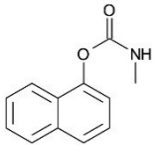
Application #AN1290

Conditions

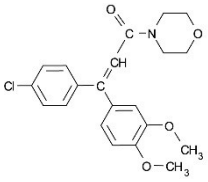
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
Mobile Phase: A: 0.1% formic acid + 5 mM ammonium formate in H_2O/MeOH (90:10 v/v)
B: 0.1% formic acid + 5 mM ammonium formate in H_2O/MeOH (10:90 v/v)

Time (mins)	%B
0.00	0
1.00	0
15.00	100
18.00	100
18.05	0
20.00	0

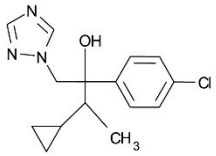
Flow Rate: 0.4 mL/min
Injection: 20 µL
Temperature: 40 °C
Detection: Agilent 6420 Triple Quadrupole MS, +ve mode ESI Dynamic MRM



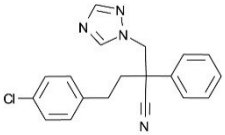
1. Carbaryl
(*m/z* 202.10 → 145.10)



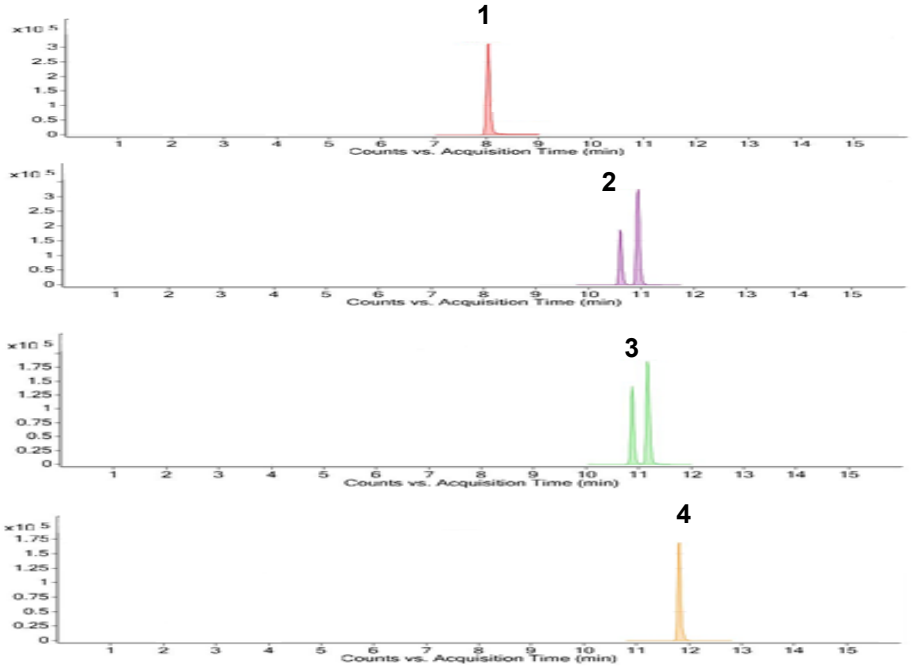
2. Dimethomorphs
(*m/z* 388.10 → 301.10)



3. Cyproconazoles
(*m/z* 292.10 → 70.00)



4. Fenbuconazole
(*m/z* 337.10 → 70.00)



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

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Free Amino Acids in Peas (*Pisum sativum*) by HPLC-HRAM-MS

ACE® Ultra-inert UHPLC & HPLC Columns

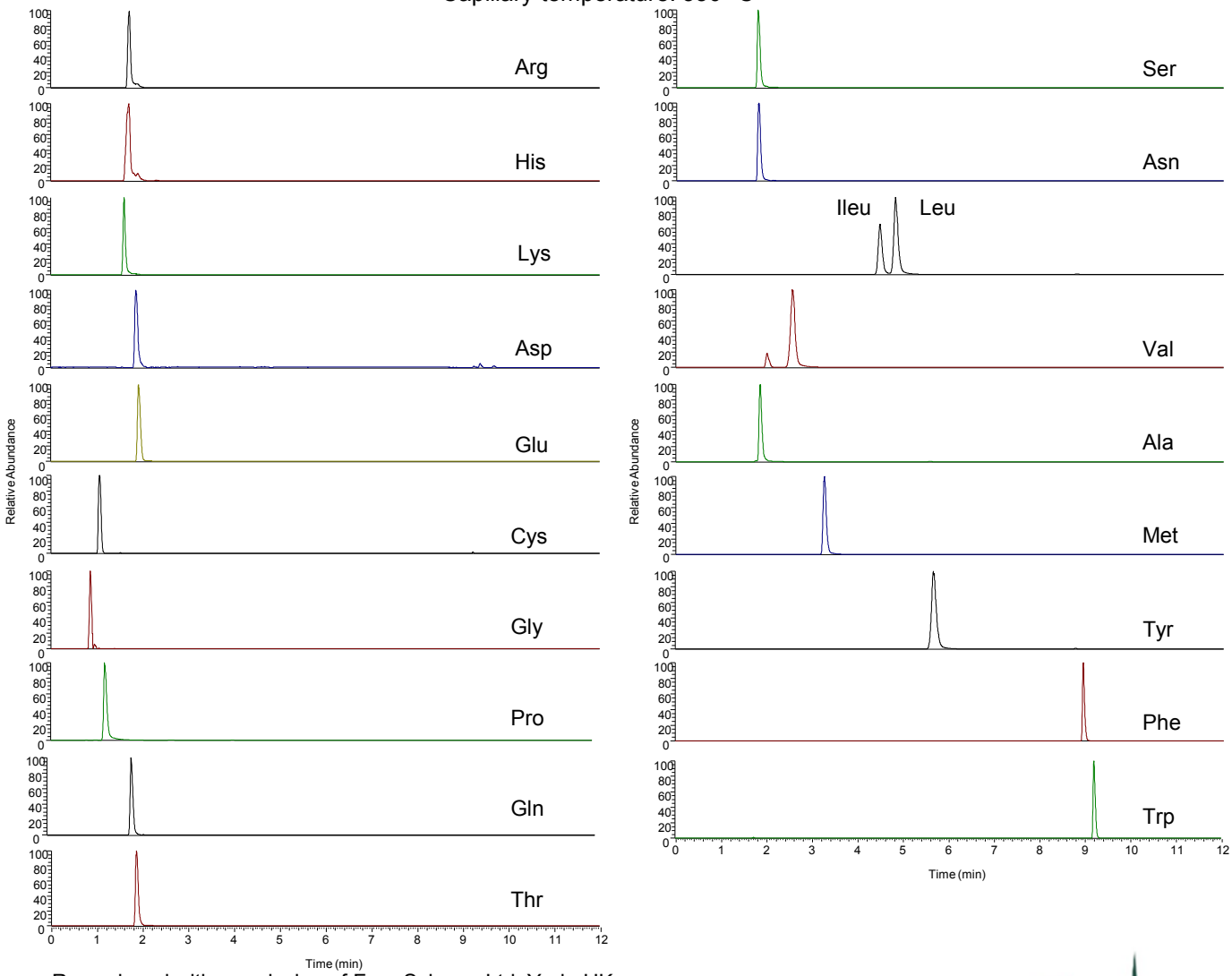
Application #**AN2660**

Conditions

Column:	ACE 3 AQ
Dimensions:	150 x 3.0 mm
Part Number:	ACE-116-1503
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

Time (mins)	**%B**
0	0
10	100

Flow Rate:	0.4 mL/min
Injection:	5 µL
Temperature:	30 °C
Detection:	Exactive Orbitrap high resolution MS
	ESI positive ion mode
	Capillary temperature: 350 °C



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Amino Acids and Biogenic Amines in Wine and Beer

ACE® Ultra-inert UHPLC & HPLC Columns

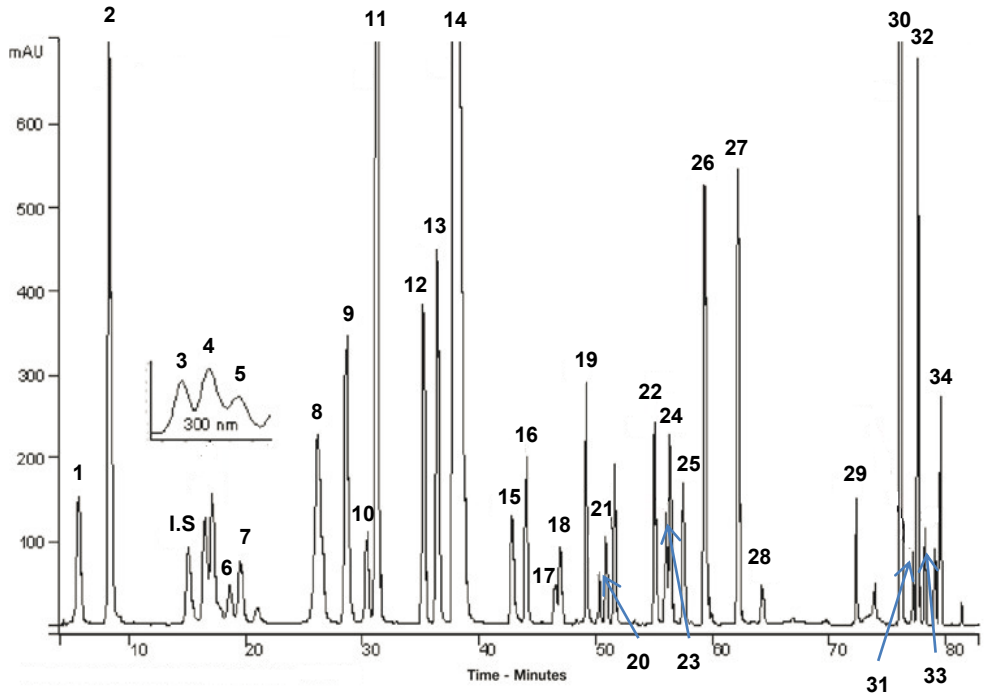
Application #**AN2800**

Conditions

Column: ACE 5 C18-HL
Dimensions: 250 x 4.6 mm
Part Number: ACE-321-2546
Mobile Phase: A: 25 mM acetate buffer pH 5.8 in H_2O
B: MeCN/MeOH (80:20 v/v)

Time (mins)	%B
0.0	45
20.0	60
30.5	17
33.5	17
65.0	40
73.0	72
78.0	82
82.0	100
85.0	100

Flow Rate: 0.8 mL/min
Injection: 20 µL
Temperature: 16 °C
Detection: UV, 269 nm, 280,nm and 300 nm



1. Aspartic acid
2. Glutamic acid
3. Asparagine
4. Serine
5. Hydroxyproline
6. Glutamine
7. Histidine
8. Glycine
9. Threonine
10. β-Alanine
11. Arginine
12. α-Alanine
13. GABA
14. Proline
15. Histamine
16. Tyrosine
17. Ammonium ion
18. Agmatine
19. Valine
20. Methionine
21. Cysteine
22. Isoleucine
23. Tryptophan
24. Leucine
25. Phenylalanine
26. Ornithine
27. Lysine
28. Spermidine
29. Tyramine
30. Putrescine
31. Tryptamine
32. Cadaverine
33. Phenylethylamine
34. Isoamylamine

I.S. L-2-Aminoadipic acid

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Aminoglycosides in Eggs

ACE® Ultra-inert UHPLC & HPLC Columns

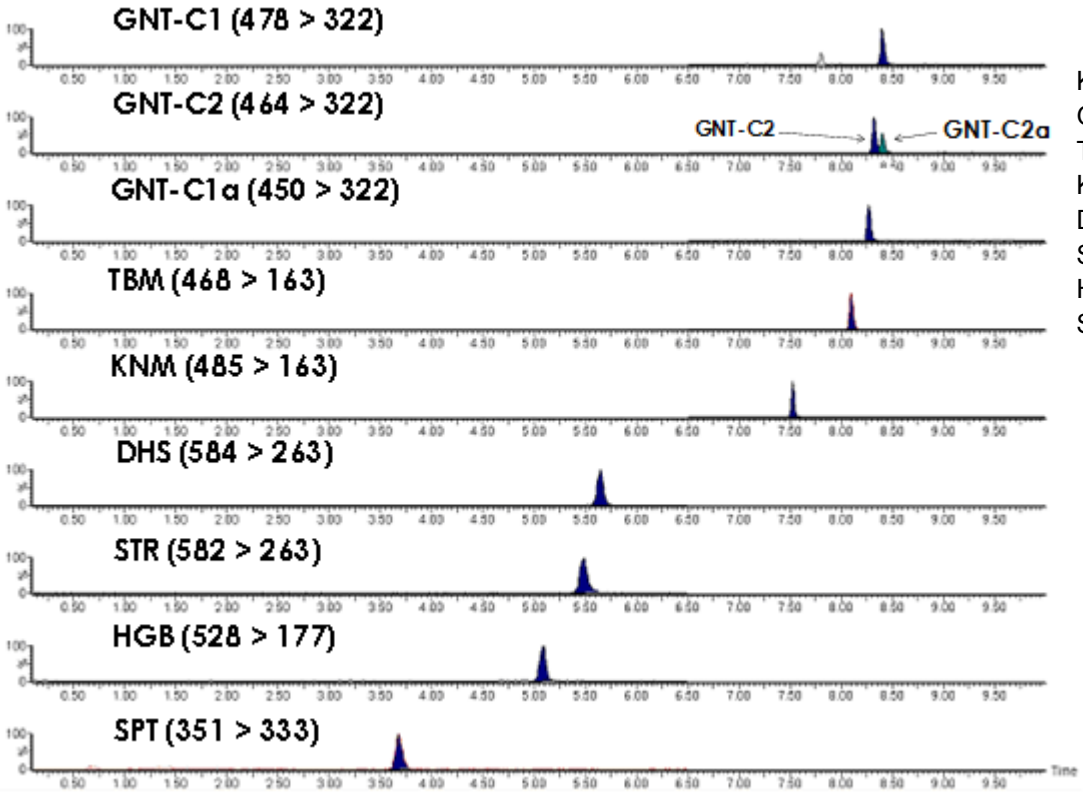
Application #**AN1920**

Conditions

Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: A: 20 mM HFBA in H_2O/MeCN (98:2 v/v)
B: 20 mM HFBA in MeCN/H_2O (98:2 v/v)

Time (mins)	%B	Curve
0.0	5.0	-
2.0	15.0	6
4.5	19.0	6
5.5	19.5	8
6.0	22.0	6
7.0	35.0	6
9.0	48.0	8
9.5	5.0	6

Flow Rate: 0.4 mL/min
Temperature: 40 °C
Detection: Positive ESI MRM (transitions as shown)
Sample: Extraction at low pH, clean up with WCX SPE cartridge
Egg sample spiked at 100 µg/kg (CCα)



Key
GNT Gentamicin
TBM Tobramycin
KNM Kanamycin
DHS Dihydrostreptomycin
STR Streptomycin
HGB Higromycin-B
SPT Spectinomycin

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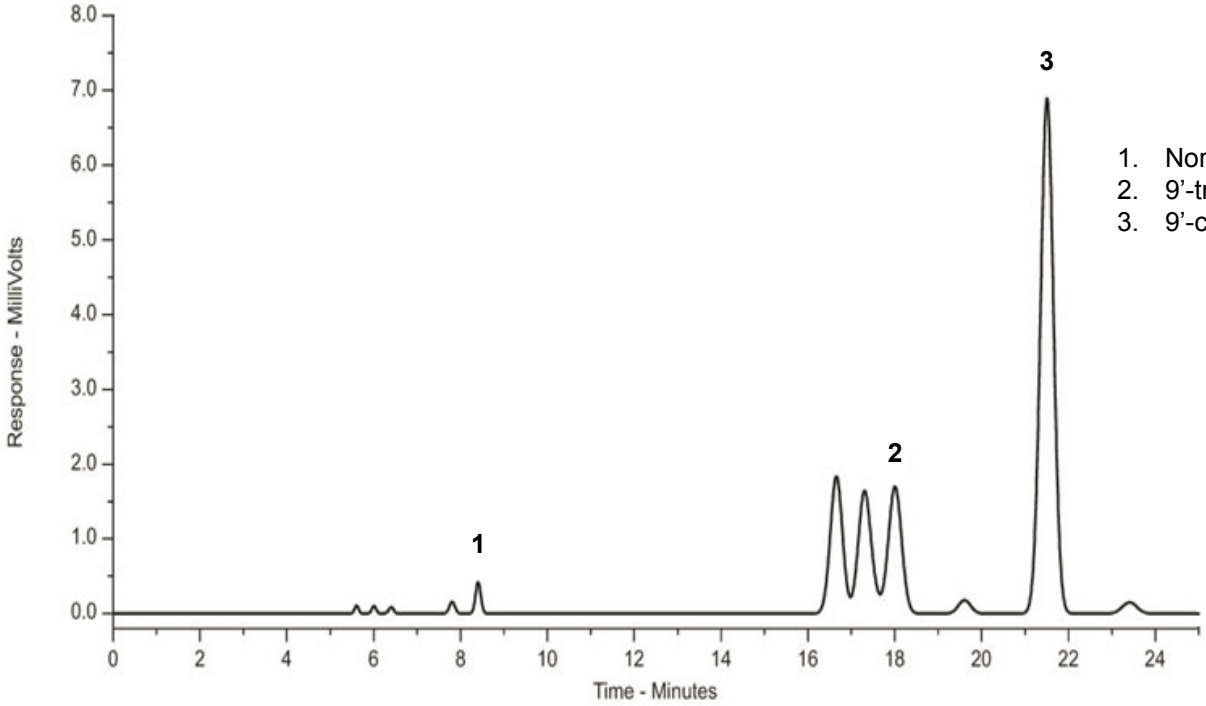
Detection of Annatto

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2840**

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	MeCN/0.16% acetic acid in H_2O (70:30 v/v)
Flow Rate:	1.2 mL/min
Temperature:	Ambient
Detection:	UV-Vis, 478 nm



1. Norbixin
2. 9'-trans-Bixin
3. 9'-cis-Bixin

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Anthocyanins from *Sambucus Nigra* (Elderberry)

ACE®
Ultra-inert
UHPLC & HPLC Columns

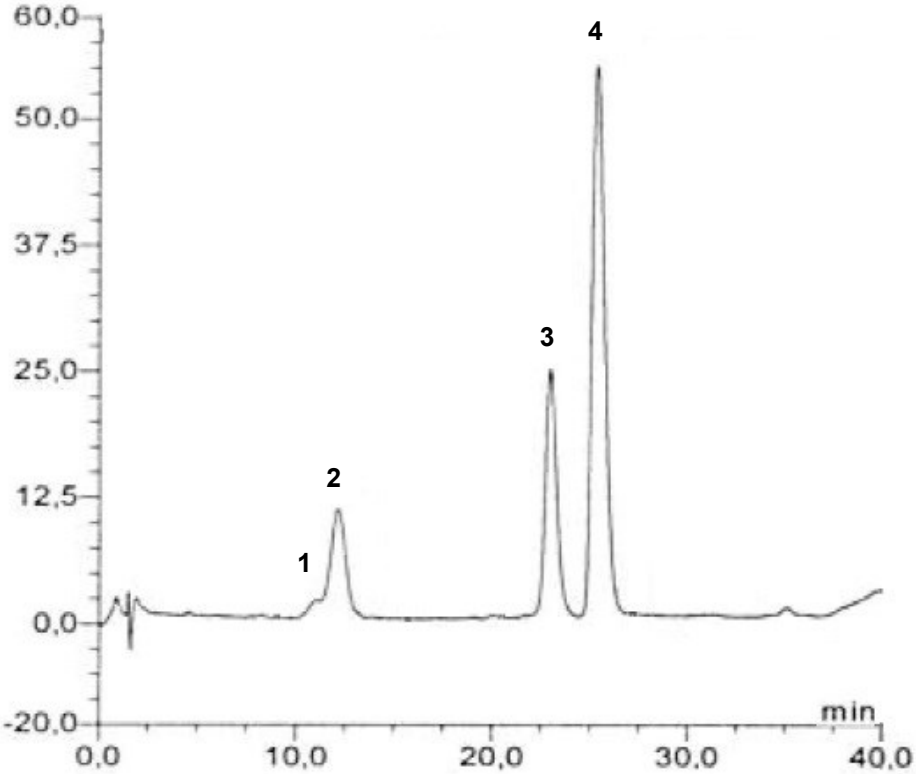
Application #AN2750

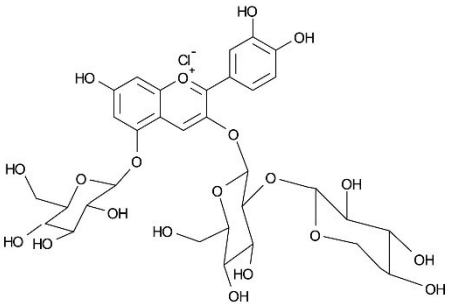
Conditions

Column:	ACE UltraCore 5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	CORE-5A-1546U
Mobile Phase:	A: 5% formic acid in H_2O
	B: MeOH

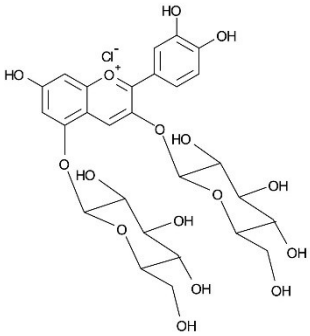
Time (mins)	%B
0	5
35	10
55	65
65	65

Flow Rate:	1 mL/min
Temperature:	40 °C
Detection:	UV-Vis, 525 nm

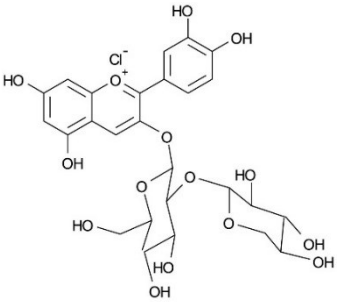




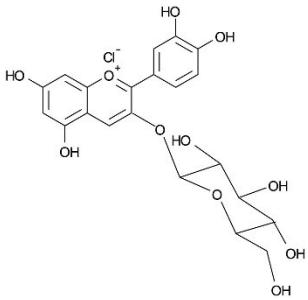
1. Cyanidin-3-sambubioside-5-glucoside



2. Cyanidin-3,5-diglucoside



3. Cyanidin-3-sambubioside



4. Cyanidin-3-glucoside

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Appetite Suppressants by LC-MS

ACE® Ultra-inert UHPLC & HPLC Columns

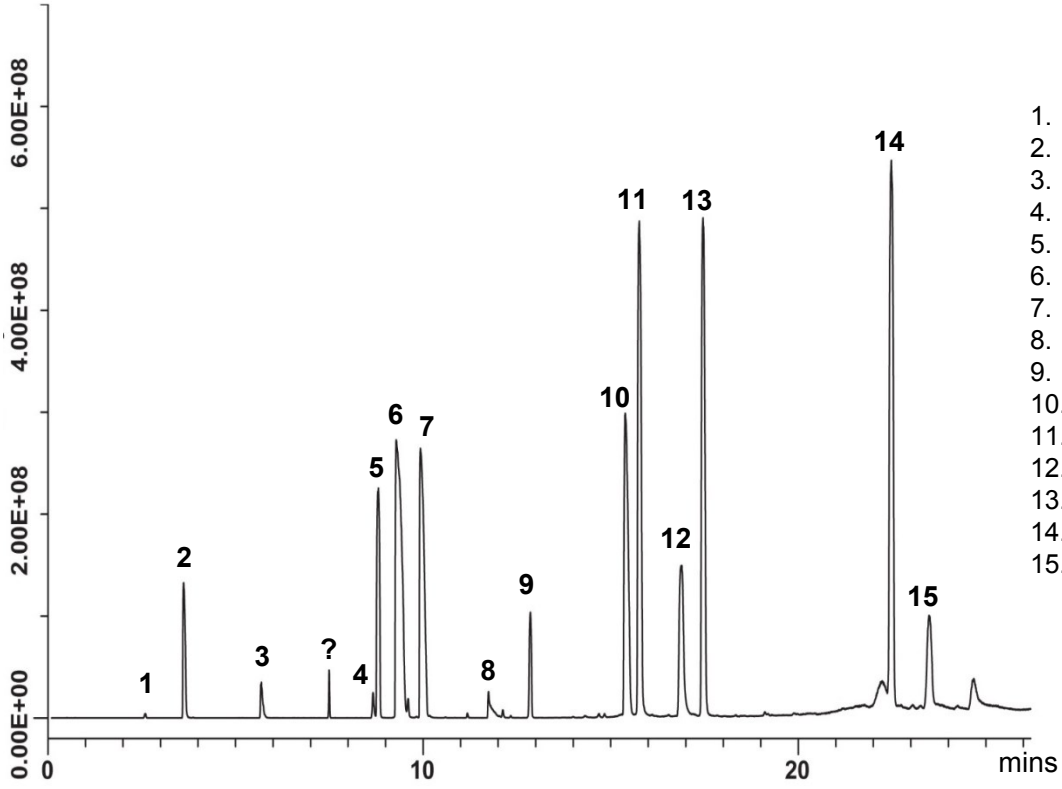
Application #AN1960

Conditions

Column:	ACE Excel 2 SuperC18
Dimensions:	100 x 2.1 mm
Part Number:	EXL-1011-1002U
Mobile Phase:	A: 10 mM ammonium acetate pH 9.35 with ammonium hydroxide B: 10 mM ammonium acetate pH 9.35/MeCN (10:90 v/v)

Time (mins)	%B
0.0	11.11
1.0	11.11
21.0	100
23.0	100

Flow Rate:	0.5 mL/min
Injection:	2 µL
Temperature:	25 °C
Detection:	MS



1. Caffeine
2. Ephedrine
3. Phentermine
4. Phenolphthalein
5. Chlordiazepoxide
6. Lorcaserin
7. Fenfluramine
8. Fluoxetine
9. Diethylpropion
10. Sertraline
11. Didesmethylsibutramine
12. Rimonabant
13. N-Desmethylsibutramine
14. Sibutramine
15. Orlistat

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Arsenolipids from Edible Seaweed by LC-ICP-MS and LC-ESI-MS

ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN1970

Conditions

Column:	ACE 3 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-111-1546
Mobile Phase:	A: 0.1% formic acid in H_2O B: 0.1% formic acid in MeOH

Time (mins)	%B
0	0
20	100
45	100

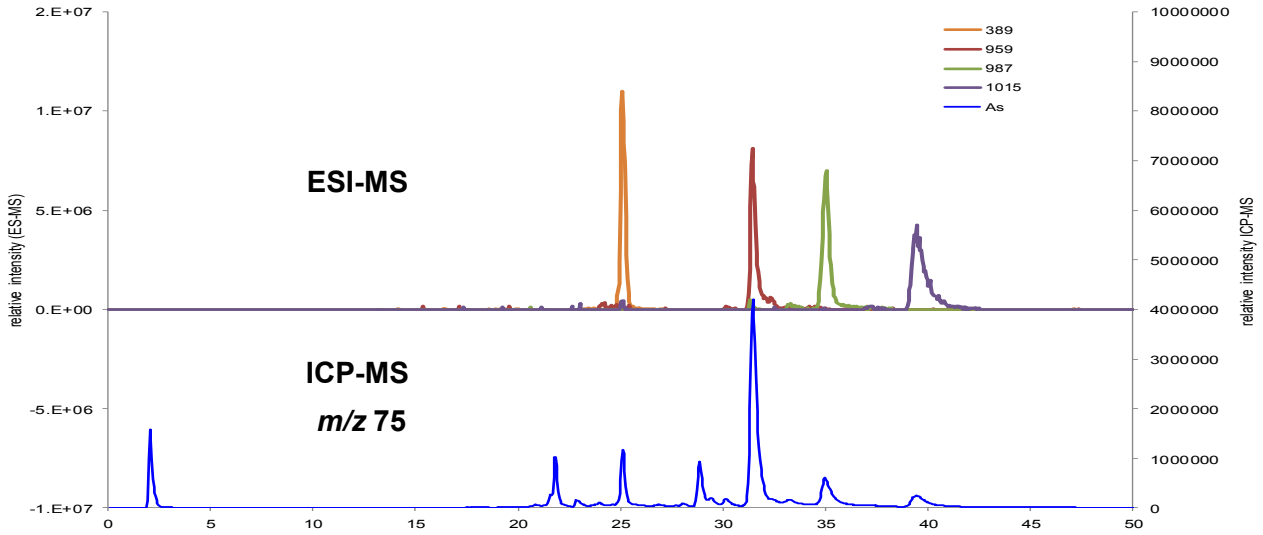
Flow Rate:	1 mL/min
Injection:	100 µL
Temperature:	45 °C
Detection:	Split ratio: 75% ESI-MS: 25% ICP-MS Thermo Scientific Element 2 ICP-MS Mode: Organic mode Medium resolution Thermo Scientific Orbitrap Discovery Positive ESI mode Spray voltage: 4.5 kV Capillary temperature: 320 °C Capillary voltage: 42 V

Arsenic-containing hydrocarbon:

m/z 389 [M + H]+ for $C_{21}H_{46}AsO$

Arsenic-containing phospholipids:

m/z 959 [M + H]+ for $C_{45}H_{89}AsO_{14}P$ (C16:0/C16:0)
m/z 987 [M + H]+ for $C_{47}H_{93}AsO_{14}P$ (C18:0/C16:0)
m/z 1015 [M + H]+ for $C_{49}H_{97}AsO_{14}P$ (C20:0/C16:0)



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Water Soluble Artificial Colours

ACE®
Ultra-inert
UHPLC & HPLC Columns

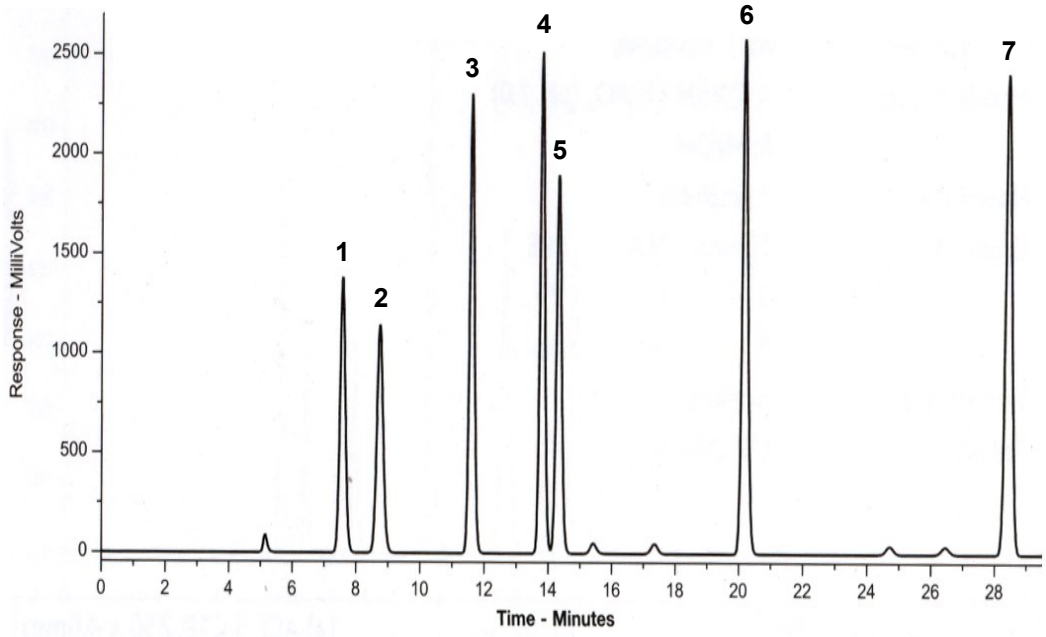
Application #**AN3010**

Conditions

Column:	ACE 3 C18
Dimensions:	100 x 4.6 mm
Part Number:	ACE-111-1046
Mobile Phase:	A: 3 mM tetrabutylammonium bromide and 5 mM KH_2PO_4 in H_2O B: 5 mM tetrabutylammonium bromide in MeOH

Time (mins)	%B
0	45
20	70
30	45
40	45

Flow Rate:	0.8 mL/min
Injection:	10 µL
Temperature:	Ambient
Detection:	UV-Vis, 420 nm, 520 nm and 600 nm



1. Amaranth
2. Sunset Yellow
3. Allura Red
4. Red 2G
5. Ponceau 4R
6. Carmoisine
7. Erythrosine

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Separation of Artificial Food Colours

ACE®
Ultra-inert
UHPLC & HPLC Columns

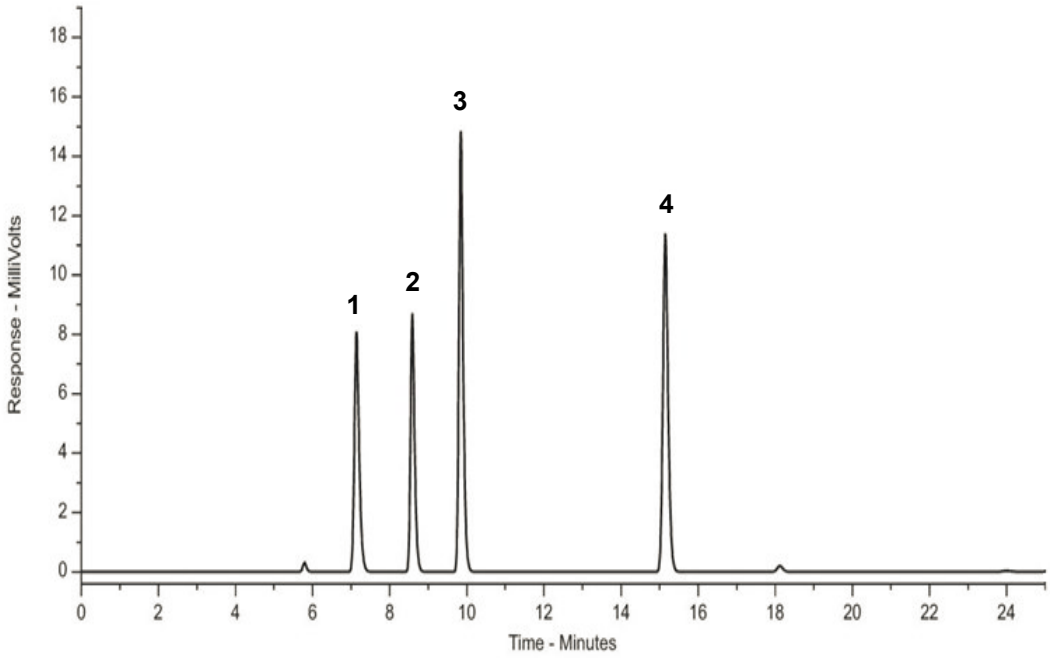
Application #**AN2960**

Conditions

Column:	ACE 3 C18
Dimensions:	100 x 4.6 mm
Part Number:	ACE-111-1046
Mobile Phase:	A: 3.1 mM tetrabutylammonium bromide and 5 mM KH_2PO_4 in H_2O B: 5 mM KH_2PO_4 in MeOH

Time (mins)	%B
0	45
12	60
25	45

Flow Rate:	0.8 mL/min
Injection:	10 µL
Temperature:	Ambient
Detection:	UV-Vis, 480 nm



1. Tartrazine
2. Amaranth
3. Sunset Yellow
4. Ponceau 4R

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Artificial Sweeteners Global Method

ACE® Ultra-inert UHPLC & HPLC Columns

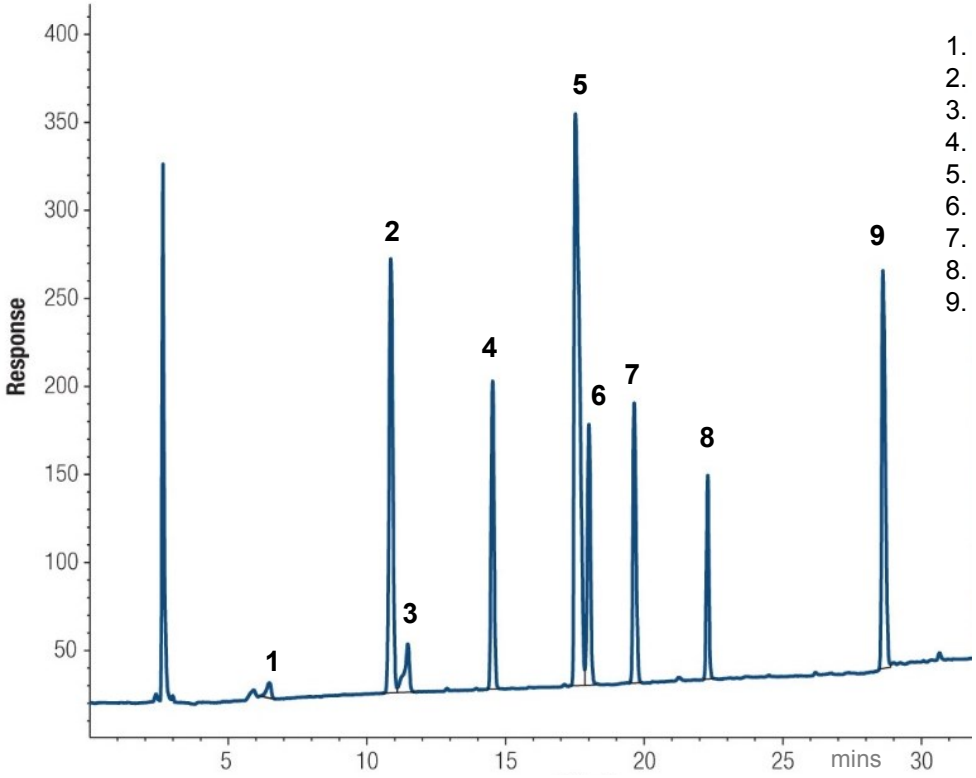
Application #AN1980

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: H_2O
B: MeCN
C: 0.1% TFA

Time (mins)	%A	%B	%C
0	88	2	10
25	50	40	10
30	30	60	10
35	88	2	10

Flow Rate: 1 mL/min
Injection: 50 µL
Temperature: 30 °C
Detection: Corona CAD



1. Acesulfame K
2. Cyclamate
3. Saccharin
4. Sucralose
5. Aspartame
6. Neotame
7. Alitame
8. Neohesperidin dihydrochalcone
9. Dulcin

Data courtesy of Durham County Council Scientific Services, UK

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Artificial Sweeteners (Stevia Glycosides)

ACE®
Ultra-inert
UHPLC & HPLC Columns

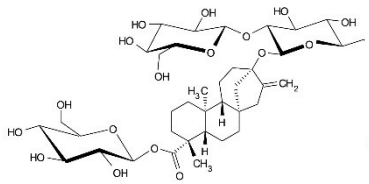
Application #**AN1020**

Conditions

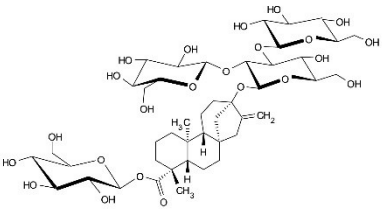
Column:	ACE Excel 2 SuperC18
Dimensions:	150 x 2.1 mm
Part Number:	EXL-1011-1202U
Mobile Phase:	A: 10 mM sodium dihydrogen phosphate pH 2.8 in H_2O
	B: 10 mM sodium dihydrogen phosphate pH 2.8 in H_2O/MeCN (80:20 v/v)

Time (mins)	%B
0	39.5
4	48.0

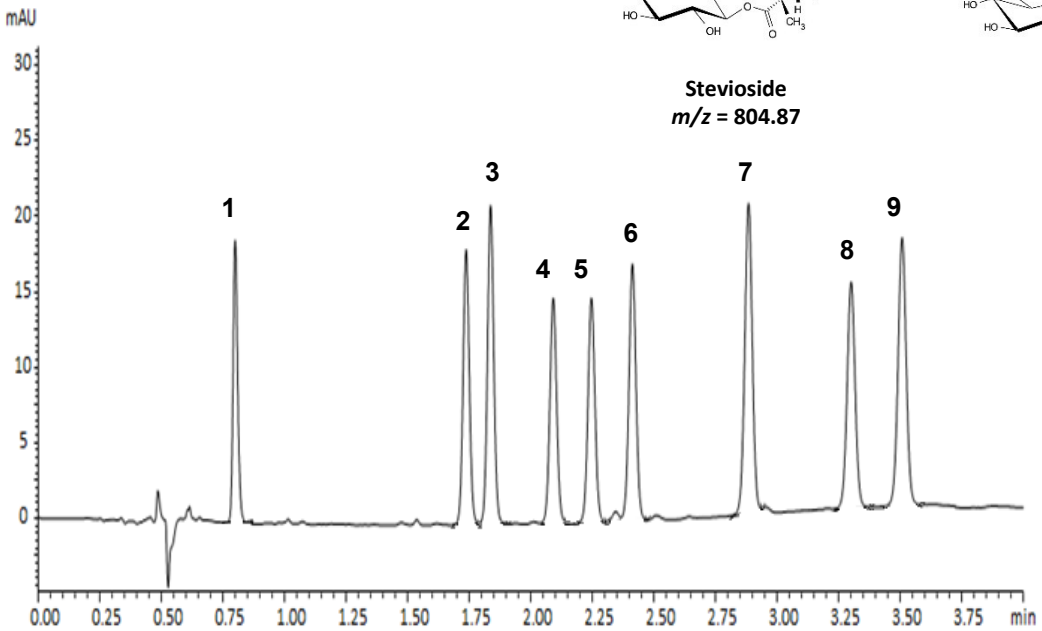
Flow Rate:	0.6 mL/min
Injection:	1 µL
Temperature:	50 °C
Detection:	UV, 200 nm



Stevioside
***m/z* = 804.87**



Rebaudioside
***m/z* = 967.01**



1. Rebaudioside D
2. Rebaudioside A
3. Stevioside
4. Rebaudioside F
5. Rebaudioside C
6. Dulcoside A
7. Rubusoside
8. Rebaudioside B
9. Steviolbioside

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http://images2.advanstar.com/PixelMags/lcgc-eu/pdf/2013-10-sp.pdf

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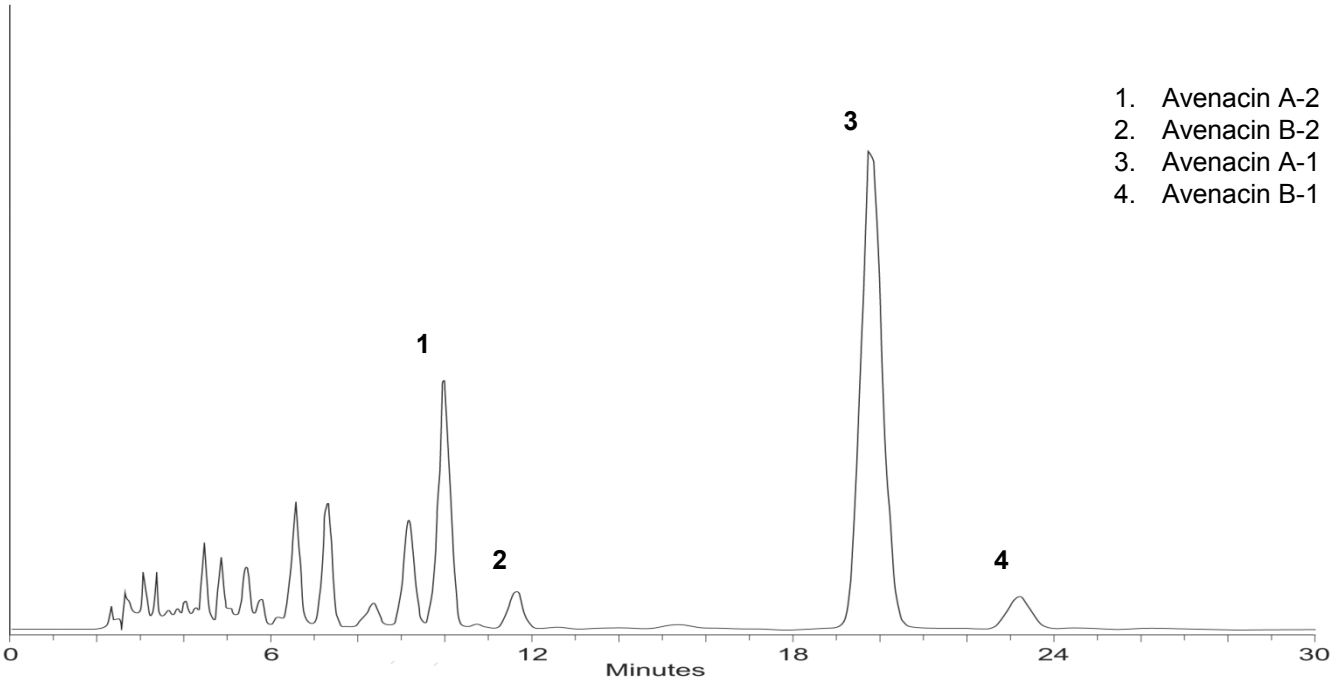
Detection of Avenacins

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2740**

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	H_2O/MeOH (30:70 v/v)
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 225 nm
Sample:	Partially purified extract from oat root



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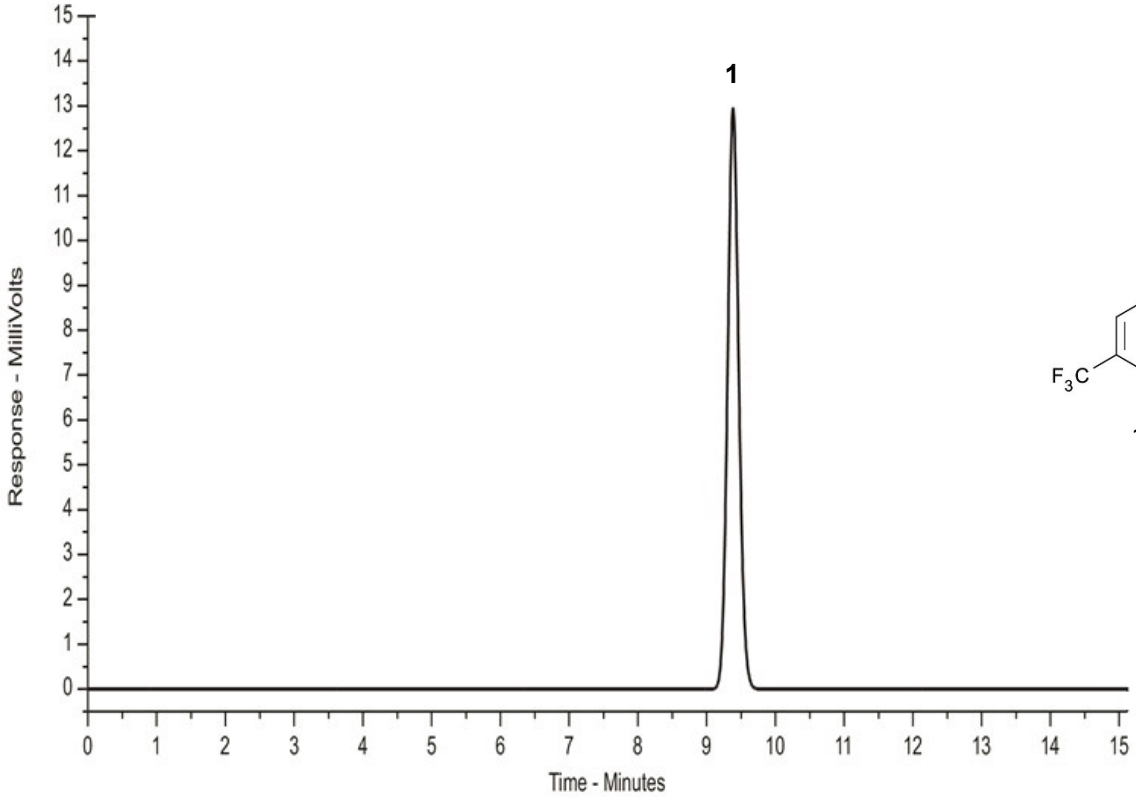
Detection of the Herbicide Benfluralin

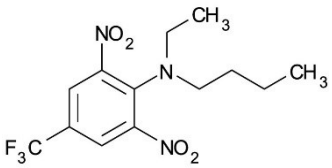
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2880**

Conditions

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





1. Benfluralin

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ACE®
UHPLC & HPLC
Columns

Caffeine and Metabolites

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2010**

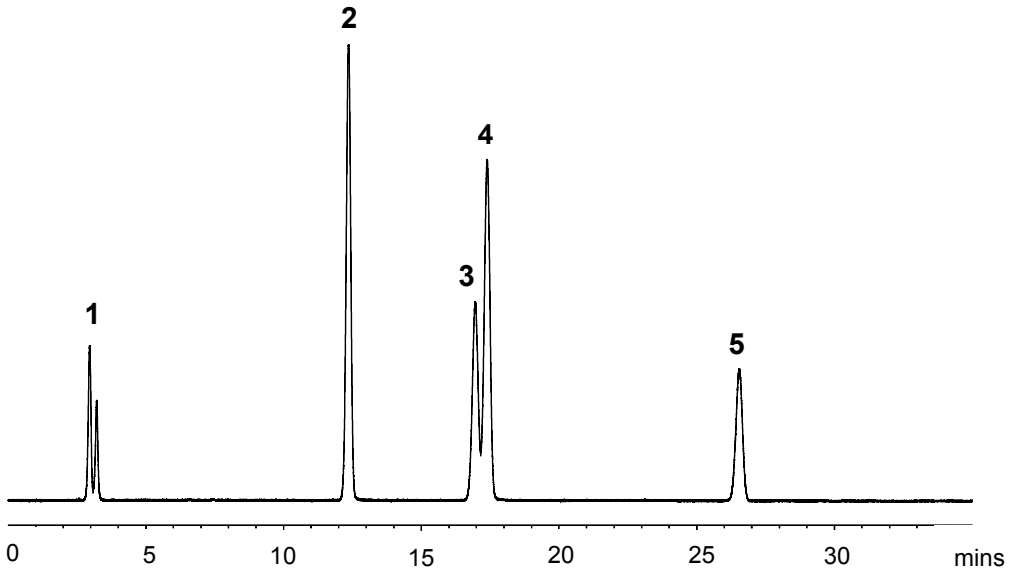
Conditions

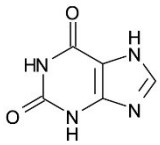
Column:	ACE 5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1211-1546U
Mobile Phase:	A: 20 mM ammonium acetate pH 7.0 in H_2O
	B: 20 mM ammonium acetate pH 7.0 in MeCN/H_2O (90:10 v/v)

Time (mins)	%B
0	2
45	15
48	15
49	2

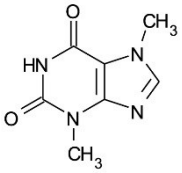
Post time 10 minutes

Flow Rate:	1 mL/min
Injection:	1 µL
Temperature:	60 °C
Detection:	UV, 273 nm

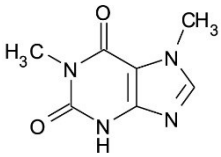




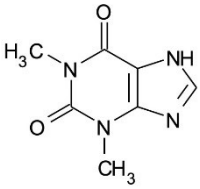
1. Xanthine



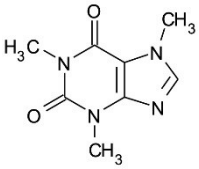
2. Theobromine



3. Paraxanthine



4. Theophylline



5. Caffeine

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Chloramphenicol in Milk by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN2030

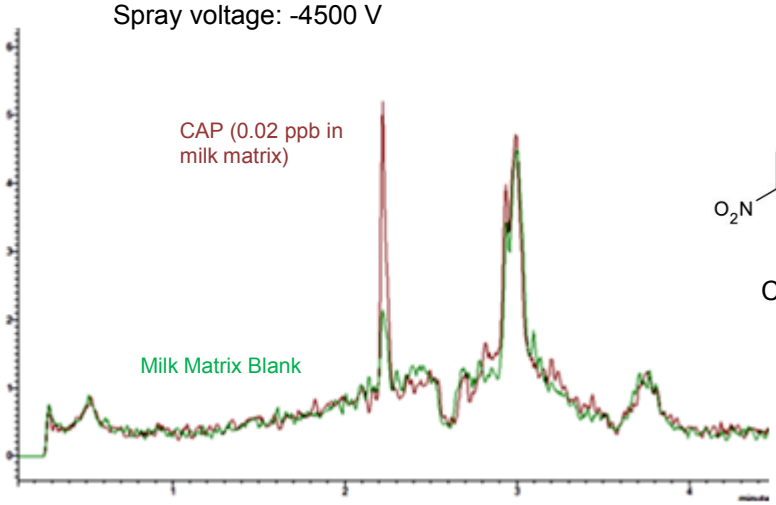
Conditions

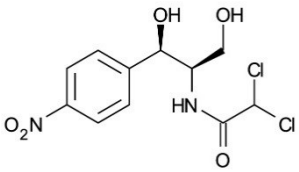
Column: ACE 3 C18
Dimensions: 50 x 2.1 mm
Part Number: ACE-111-0502
Mobile Phase: A: H_2O
B: MeOH

Time (mins)	%B
0.00	10
0.05	10
2.50	95
3.00	95
3.10	10
4.50	10

Flow Rate: 0.5 mL/min
Injection: 10 µL
Detection: Bruker EVOQ Elite triple quad MS
VIP heated-ESI temperature: 400 °C
Cone gas temperature: 350 °C
Spray voltage: -4500 V

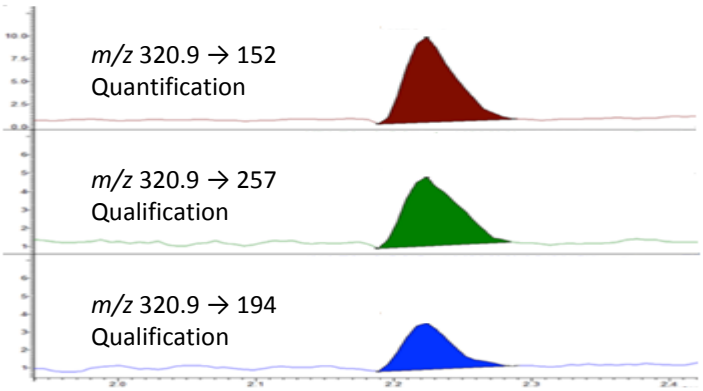
TIC of 3 MRMs of 0.02 ppb chloramphenicol spiked in milk matrix





Chloramphenicol

MRM chromatograms of 0.05 ppb chloramphenicol in milk



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Chocolate Analysis

ACE® Ultra-inert UHPLC & HPLC Columns

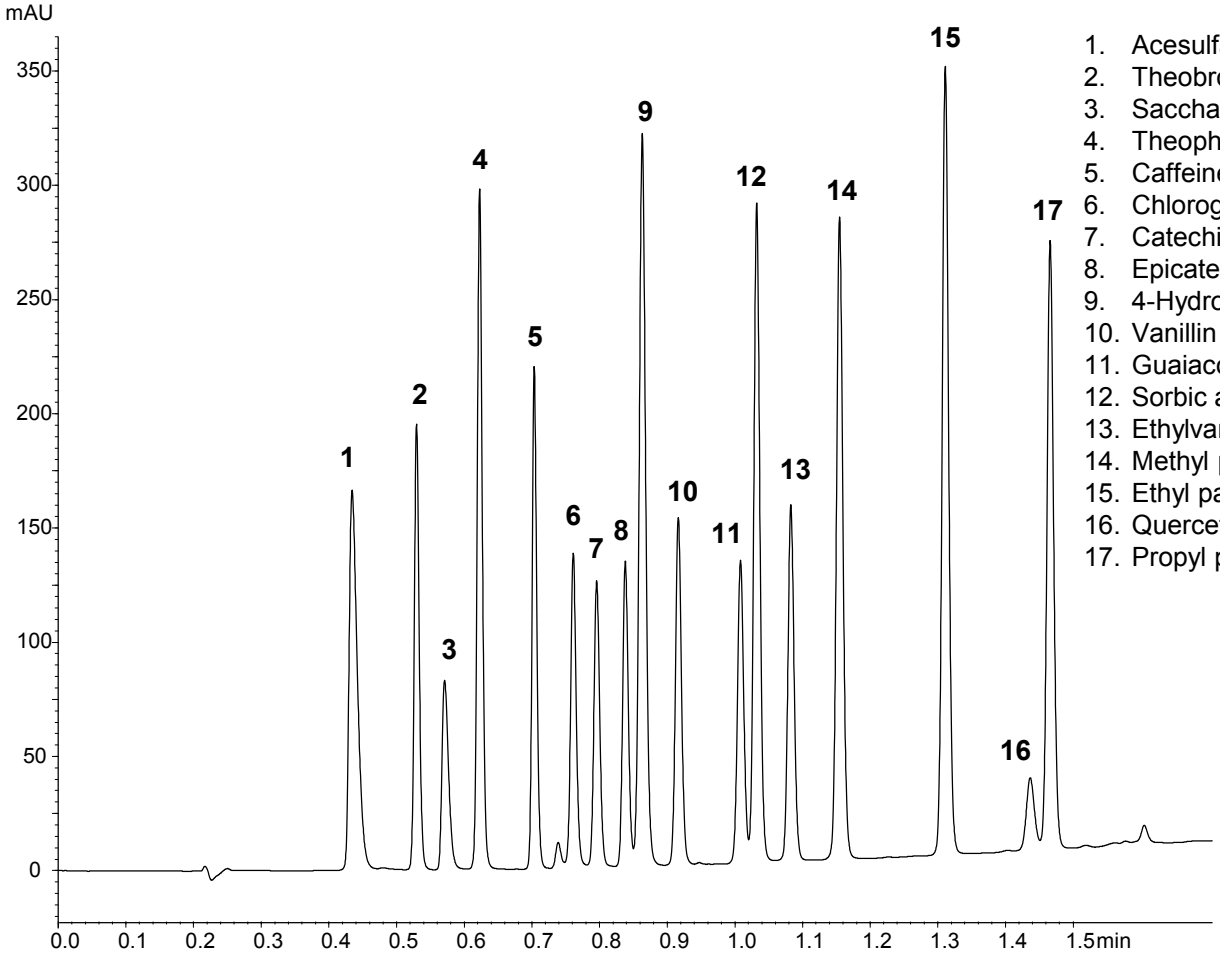
Application #**AN2040**

Conditions

Column:	ACE Excel 2 C18-Amide
Dimensions:	100 x 2.1 mm
Part Number:	EXL-1012-1002U
Mobile Phase:	A: 10 mM ammonium formate pH 2.8 in H_2O
	B: 10 mM ammonium formate pH 2.8 in MeCN/H_2O (90:10 v/v)

Time (mins)	%B
0.0	5
1.5	85

Flow Rate:	1.2 mL/min
Temperature:	42 °C
Detection:	UV, 254 nm



1. Acesulfame K
2. Theobromine
3. Saccharin
4. Theophylline
5. Caffeine
6. Chlorogenic acid
7. Catechin
8. Epicatechin
9. 4-Hydroxybenzoic acid
10. Vanillin
11. Guaiacol
12. Sorbic acid
13. Ethylvanillin
14. Methyl paraben
15. Ethyl paraben
16. Quercetin
17. Propyl paraben

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Metabolite Profiling of Coffee by LC-MS

ACE® Ultra-inert UHPLC & HPLC Columns

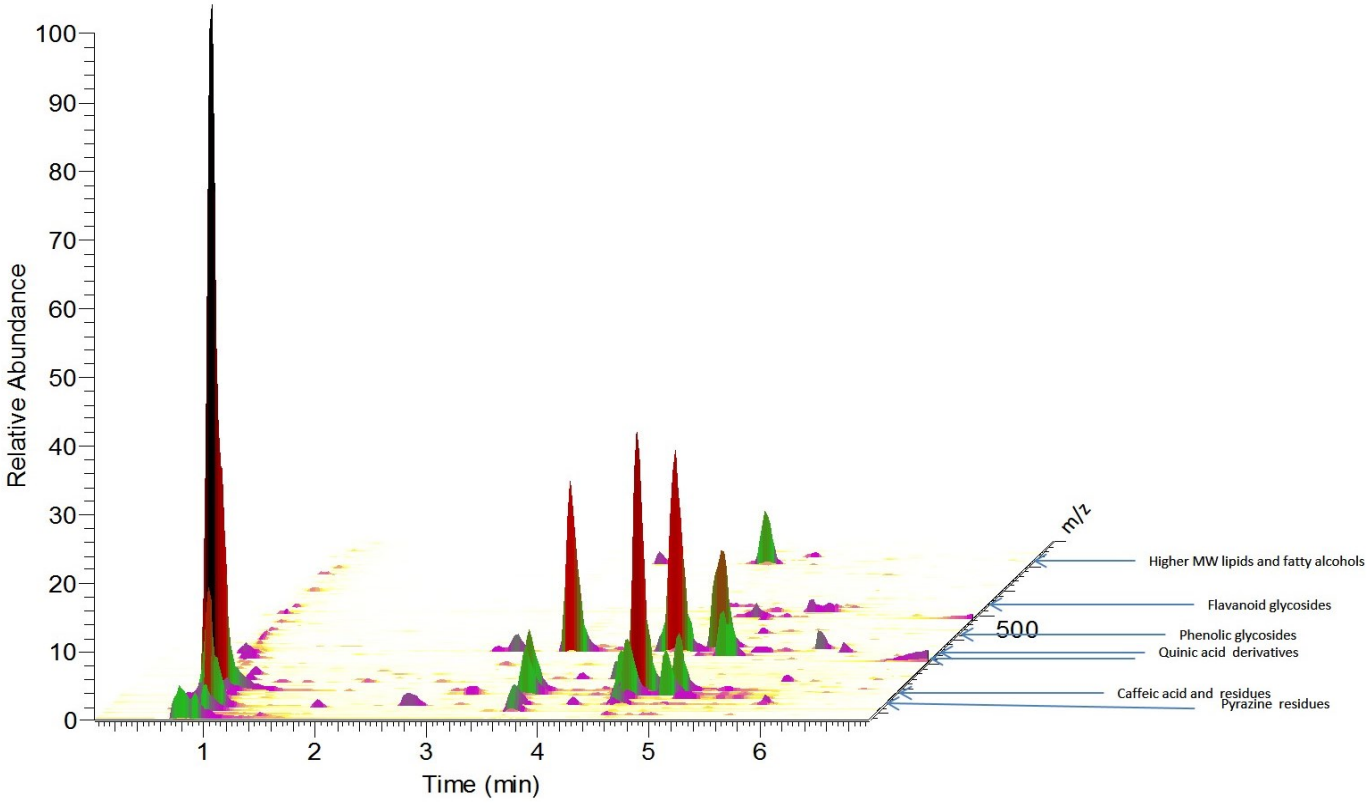
Application #**AN2590**

Conditions

Column: ACE Excel 1.7 C18-Amide
Dimensions: 100 x 2.1 mm
Part Number: EXL-1712-1002U
Mobile Phase: A: 0.01% formic acid in H_2O
B: 0.01% formic acid in MeCN

Time (mins)	%B
0.0	3
2.5	10
8.0	100
8.5	3
10.0	3

Flow Rate: 0.5 mL/min
Detection: Exactive accurate mass MS system
ESI in negative ion mode
Analytes between *m/z* 70-800 monitored
Sample: Metabolites from coffee extracted into cold water by vortexing for 20 mins. Samples filtered prior to injection onto column and modular Accela LC system



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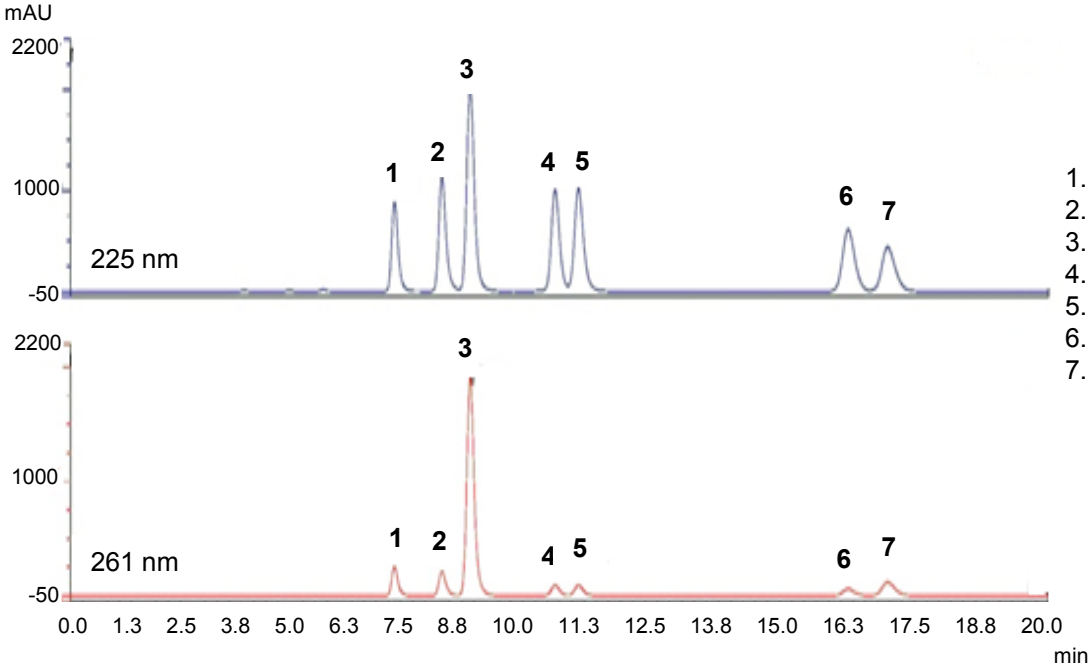
Cyclodextrin-Encapsulated Flavour Compounds in Beer

ACE® Ultra-inert UHPLC & HPLC Columns

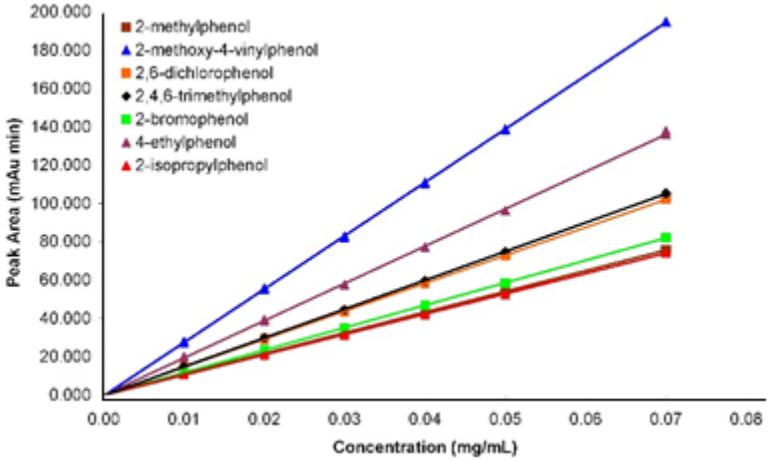
Application #**AN2300**

Conditions

Column:	ACE 3 C18
Dimensions:	150 x 4.0 mm
Part Number:	ACE-111-1504
Mobile Phase:	0.1% phosphoric acid in MeOH/H_2O (53:47 v/v)
Flow Rate:	0.5 mL/min
Injection:	20 µL
Temperature:	35 °C
Detection:	UV, 225 nm



1. 2-Methylphenol
2. 2-Bromophenol
3. 2-Methoxy-4-vinylphenol
4. 4-Ethylphenol
5. 2,4-Dichlorophenol
6. 2,4,6-Trimethylphenol
7. 2-Isopropylphenol



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Human Defensins in a Saliva Matrix

ACE®
Ultra-inert
UHPLC & HPLC Columns

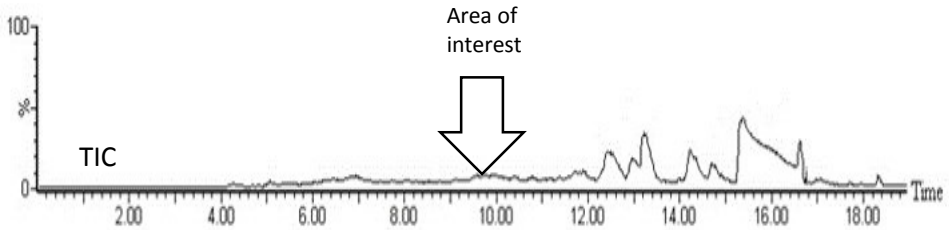
Application #**AN1270**

Conditions

Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	50 x 3.0 mm
Part Number:	CORE-25A-1503U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

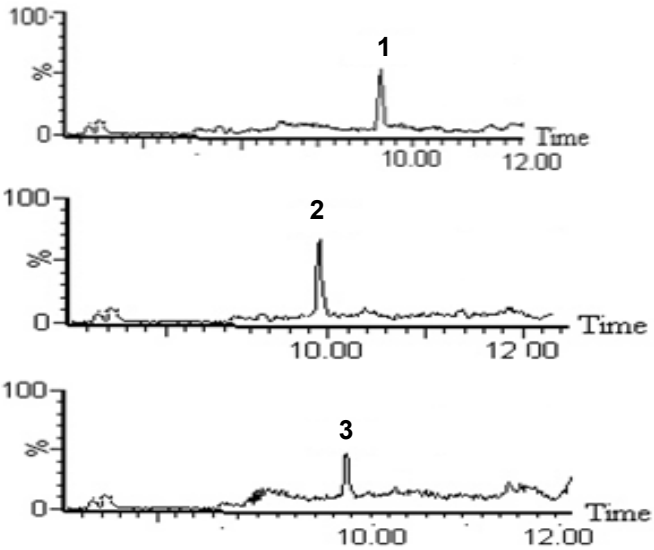
Time (mins)	**%B**
0	2
2	2
17	50
19	95
20	95

Flow Rate:	0.6 mL/min
Sample Preparation:	SPE on C18
Detection:	Synapt G1 QToF +ESI MS
	Sampling cone voltage: 40 V
	Source temperature: 150 °C
	Capillary voltages: 4.8 kV
	Extraction cone voltages: 41 kV
	Desolvation temperature: 500 °C
	Acquisition: 100-2000 m/z

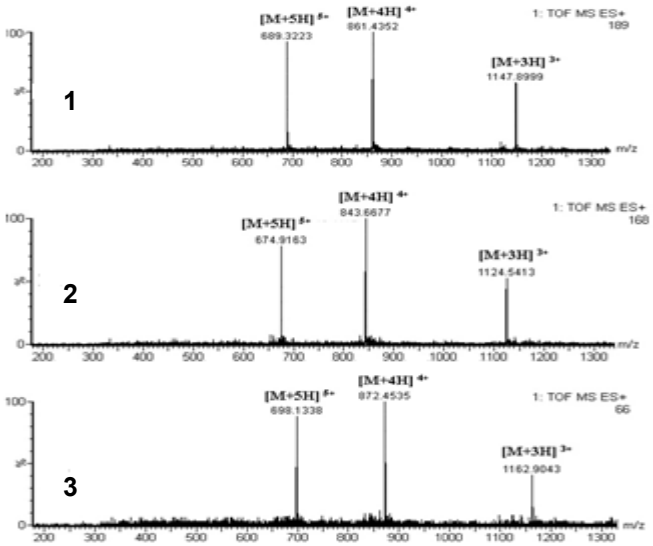


Defensin Human Neutrophil Peptides
1. HNP-1
(30 amino acid residues)
2. HNP-2
(29 amino acid residues)
3. HNP-3
(30 amino acid residues)

Extracted ion current chromatograms
(sum of multiply protonated ions $[M+3H]^{3+}$, $[M+4H]^{4+}$ and $[M+5H]^{5+}$)



Mass spectra



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Ethanol Extract from Seed Cover (*Acacia Farnesiana)*

ACE® Ultra-inert UHPLC & HPLC Columns

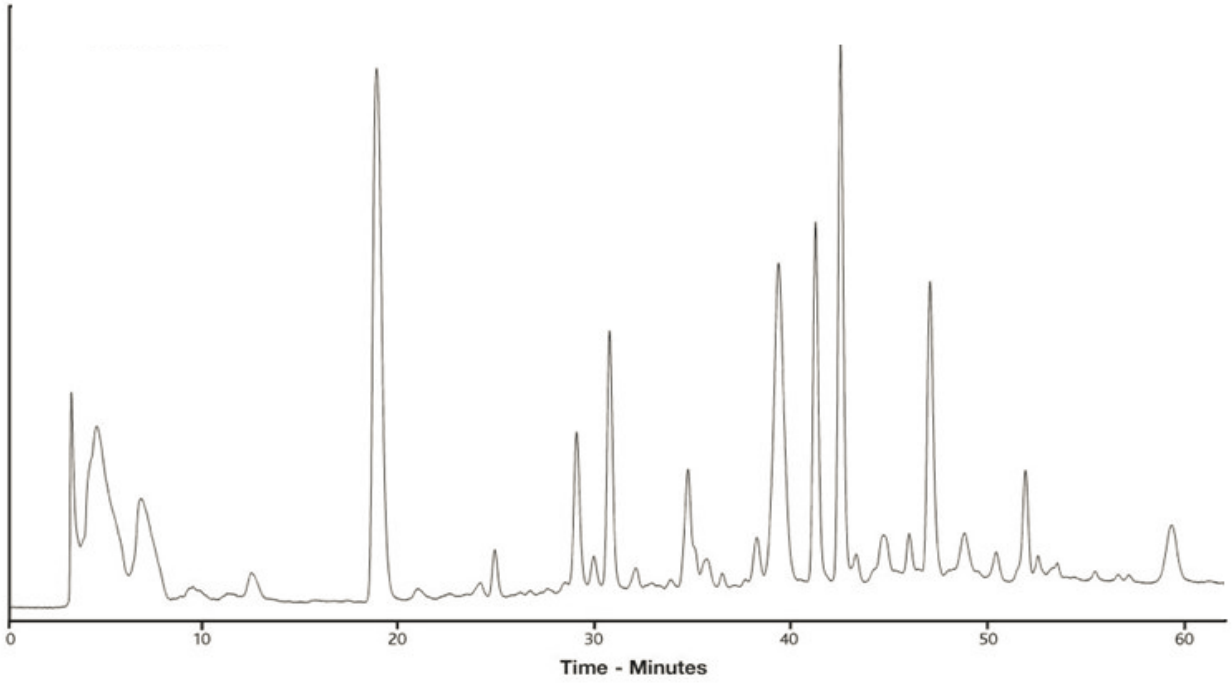
Application #**AN2900**

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	A: MeOH
	B: H_2O

Time (mins)	%B
0.0	85
2.5	85
60.0	50
62.5	50
70.0	85

Flow Rate:	2 mL/min
Temperature:	Ambient
Detection:	UV, 230 nm



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Detection of Flavone and Dibucaine

ACE®
Ultra-inert
UHPLC & HPLC Columns

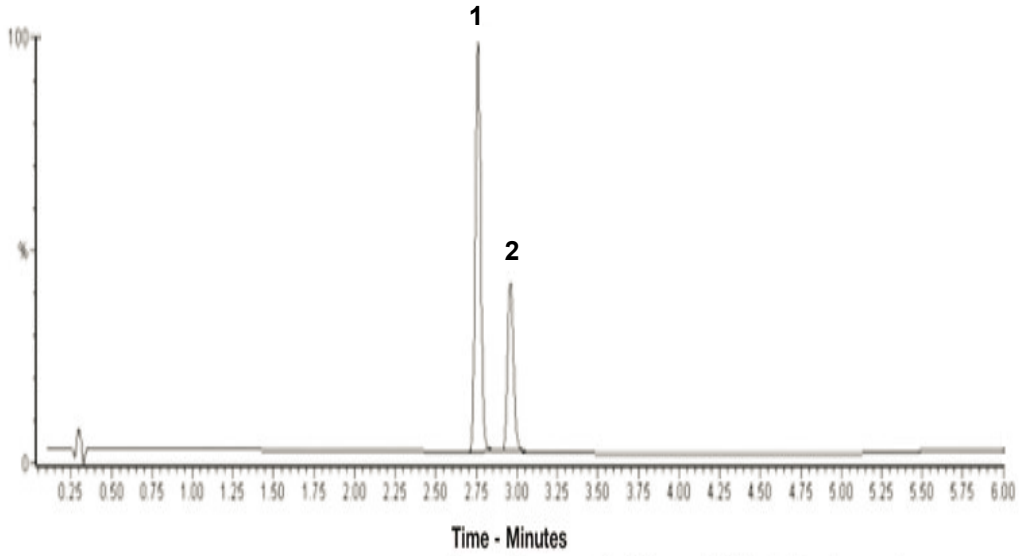
Application #**AN2850**

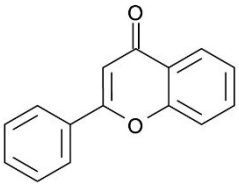
Conditions

Column: ACE 3 C18
Dimensions: 30 x 4.6 mm
Part Number: ACE-111-0346
Mobile Phase: A: 6.5 mM ammonium acetate in H_2O
B: MeCN
C: MeOH

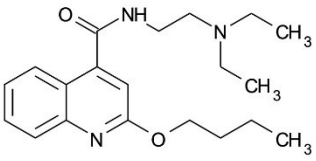
Time (mins)	%A	%B	%C
0.0	80	10	10
5.2	0	50	50
5.6	0	0	100

Flow Rate: 2 mL/min
Temperature: 60 °C
Detection: UV, 200-450 nm





1. Flavone



2. Dibucaine

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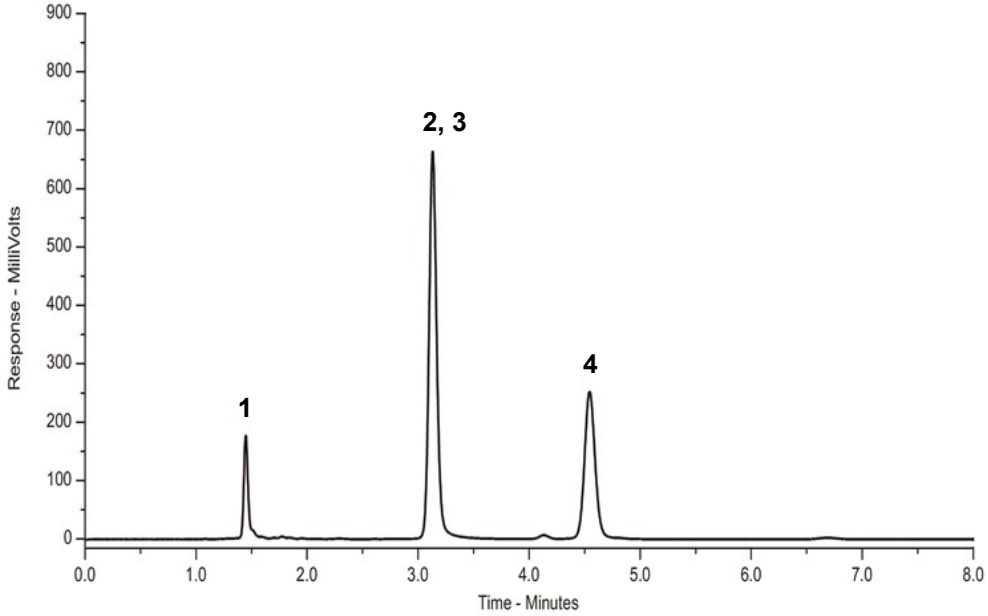
Analysis of Flavonoids

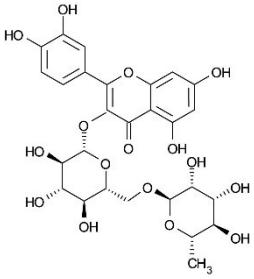
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN2810

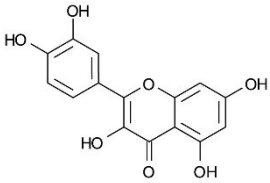
Conditions

Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	MeCN/0.1% formic acid in H_2O (40:60 v/v)
Flow Rate:	1 mL/min
Injection:	1 µL
Temperature:	Ambient
Detection:	UV, 254 nm

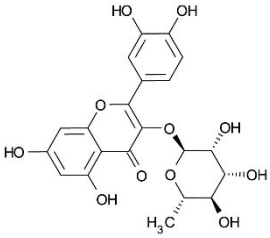




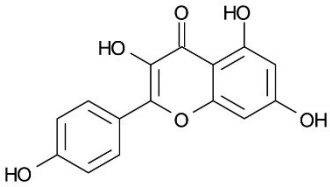
1. Rutin



2. Quercetin



3. Quercitrin



4. Kaempferol

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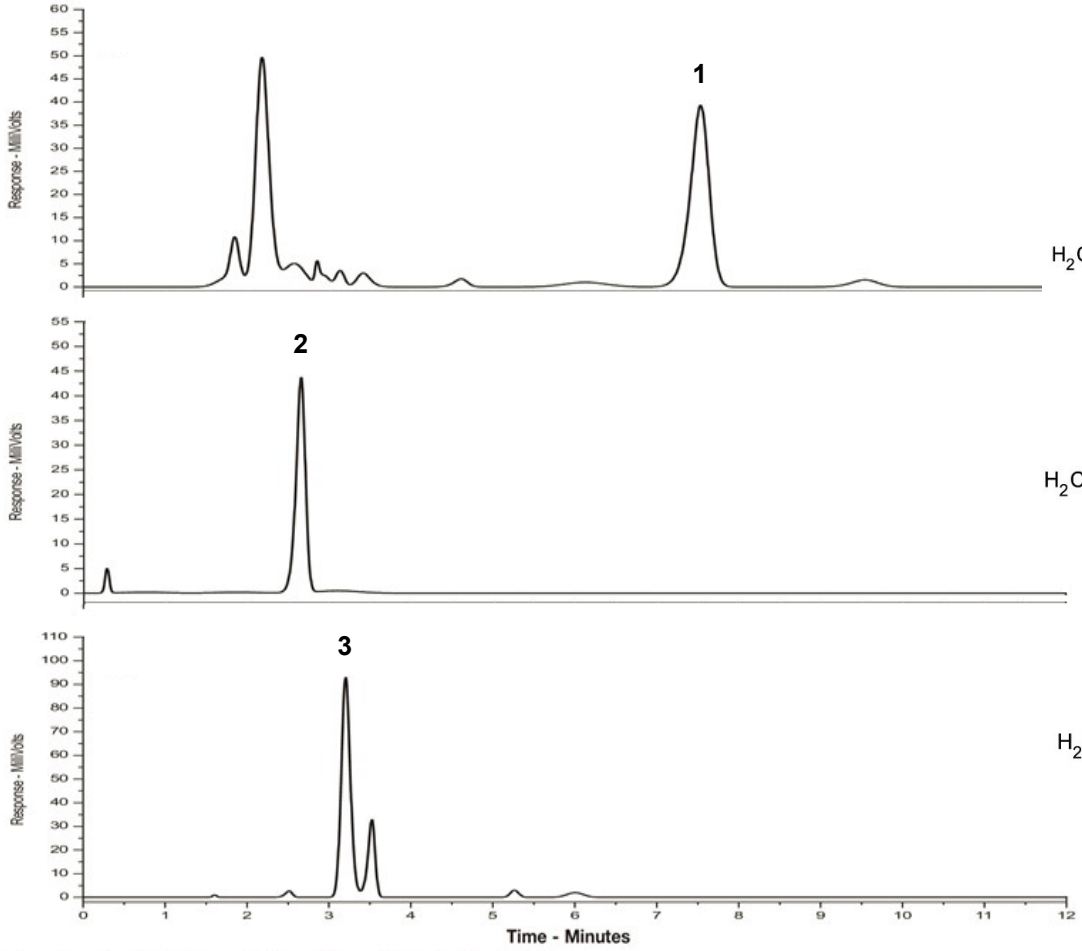
Analysis of Garlic (I)

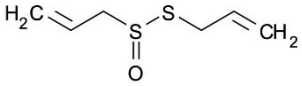
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2820**

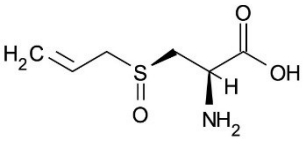
Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	H_2O/MeOH (50:50 v/v)
Flow Rate:	1 mL/min
Injection:	20 µL
Temperature:	30 °C
Detection:	UV, 210 nm

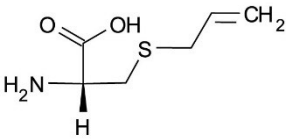




1. Allicin



2. Alliin



3. Deoxyalliin

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Analysis of Garlic (II)

ACE®
Ultra-inert
UHPLC & HPLC Columns

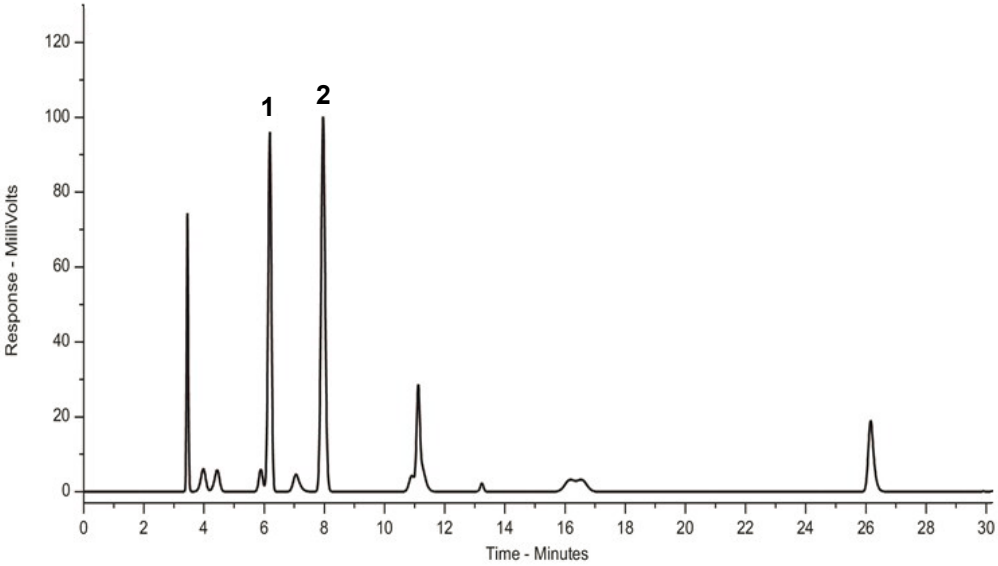
Application #**AN2830**

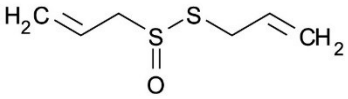
Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	A: H_2O
	B: MeCN

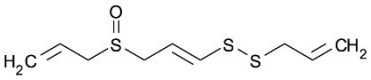
Time (mins)	%B
0	40
20	100
25	100

Flow Rate:	1 mL/min
Injection:	20 µL
Temperature:	30 °C
Detection:	UV, 254 nm





1. Allicin



2. Ajoene

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Metabolite Profiling of Green Tea by LC-MS

ACE® Ultra-inert UHPLC & HPLC Columns

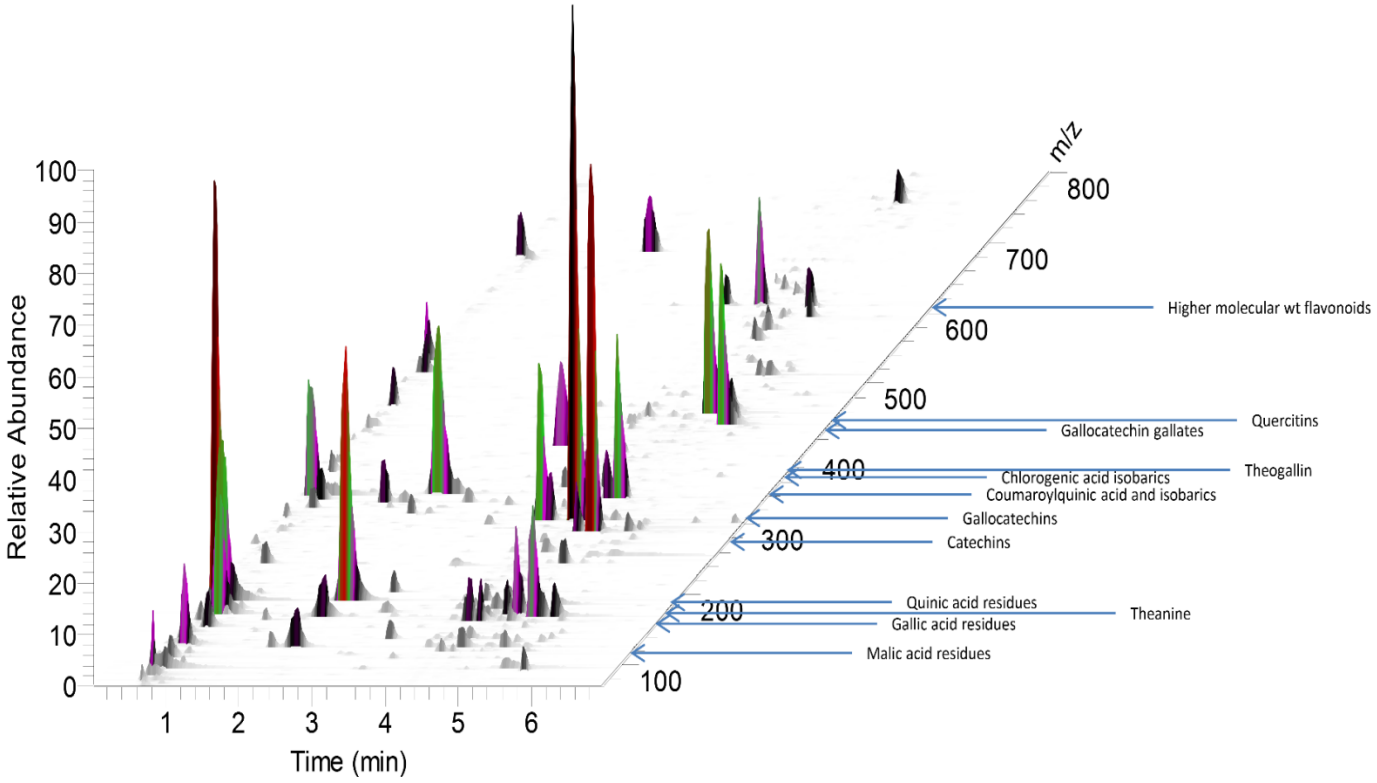
Application #AN2580

Conditions

Column: ACE Excel 1.7 C18-Amide
Dimensions: 100 x 2.1 mm
Part Number: EXL-1712-1002U
Mobile Phase: A: 0.01% formic acid in H_2O
B: 0.01% formic acid in MeCN

Time (mins)	%B
0.0	3
2.5	10
8.0	100
8.5	3
10.0	3

Flow Rate: 0.5 mL/min
Detection: Exactive accurate mass MS system
ESI in negative ion mode
Analytes between *m/z* 70-800 monitored
Sample: Metabolites from green tea extracted into cold water by vortexing for 20 mins. Samples filtered prior to injection onto column and modular Accela LC system



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Impurity Profile of a Herbicide

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2130**

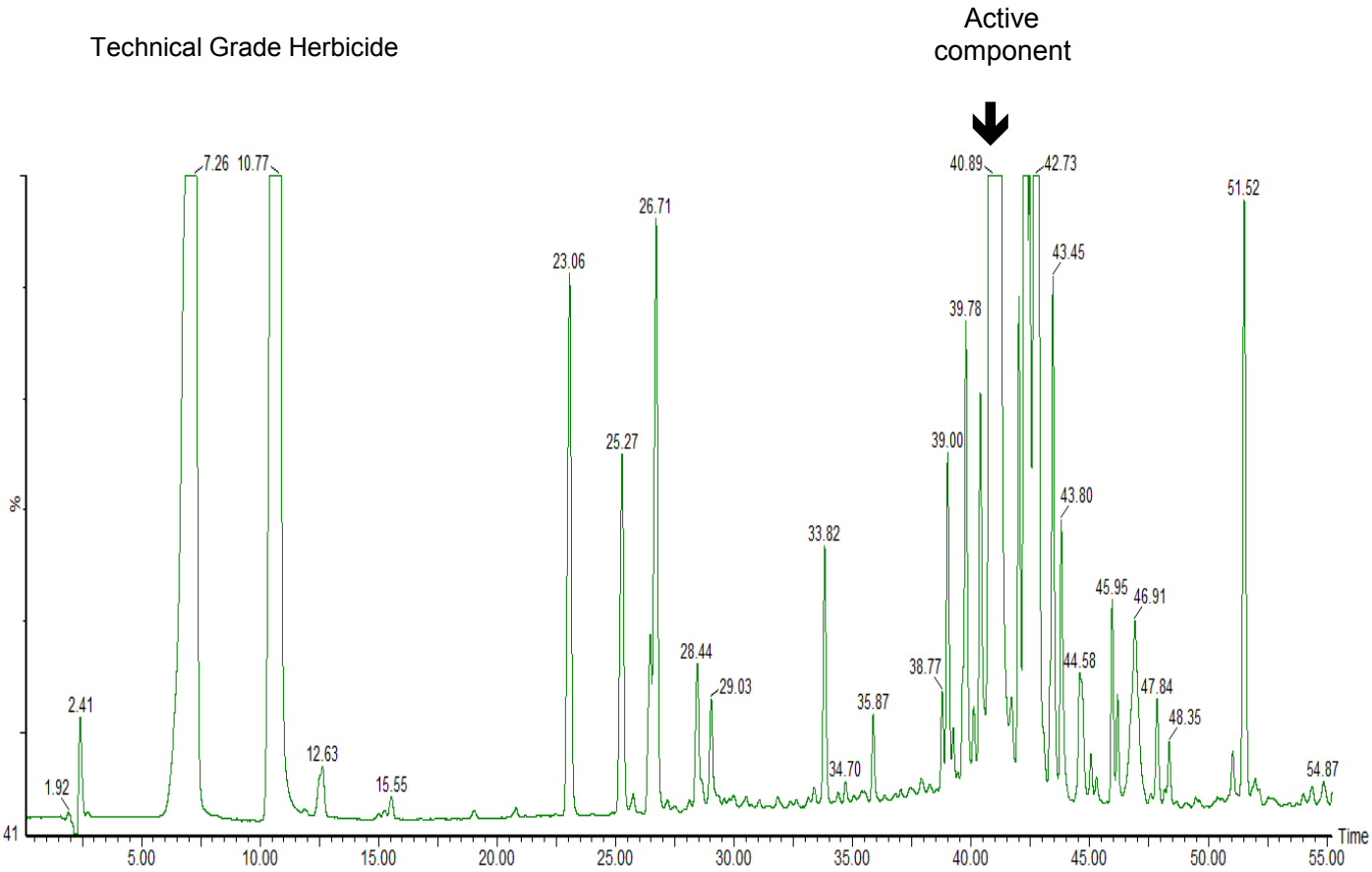
Conditions

Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	CORE-25A-1546U
Mobile Phase:	A: MeCN/H_2O/TFA (5:95:0.05 v/v/v)
	B: MeCN/TFA (99.9:0.05 v/v)

Time (mins)	%B
0	10
3	10
35	100
55	100
56	10
60	10

Flow Rate:	0.6 mL/min
Injection:	10 µL
Temperature:	25 °C
Detection:	UV, 240 nm

Technical Grade Herbicide



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www.ace-hplc.com or email: info@ace-hplc.com

ACE®
UHPLC & HPLC
Columns

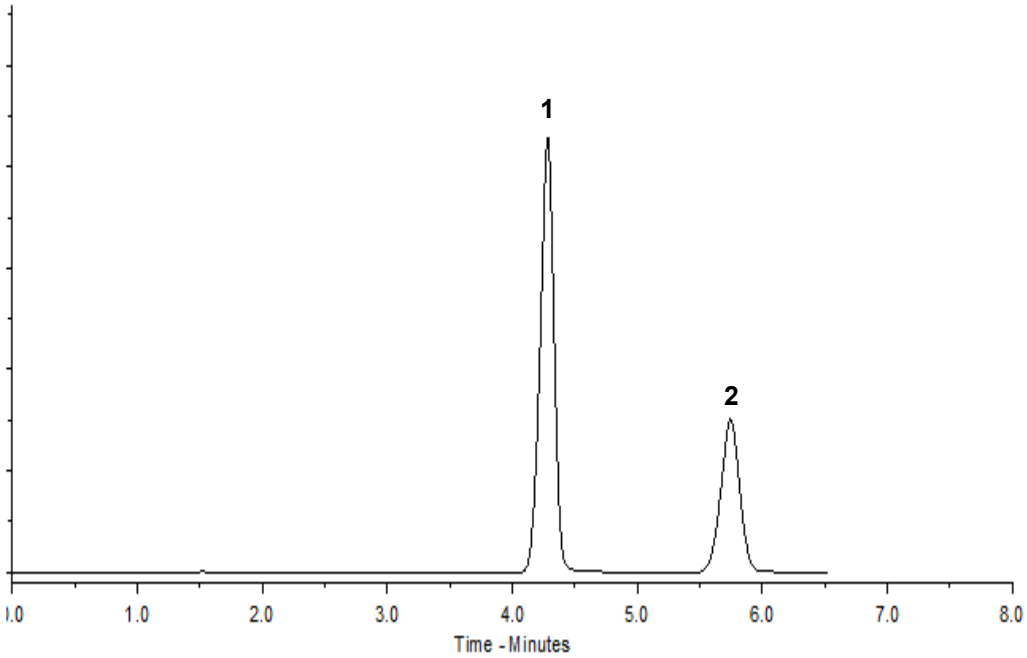
Separation of Hippuric Acid

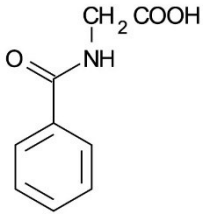
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2760**

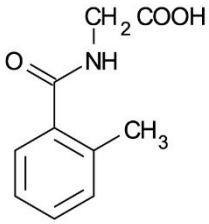
Conditions

Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	10 mM KH_2PO_4 pH 3.5 in H_2O/MeCN (15:85 v/v)
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 254 nm





1. Hippuric acid



2. 2-Methylhippuric acid

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Insulins

ACE®
Ultra-inert
UHPLC & HPLC Columns

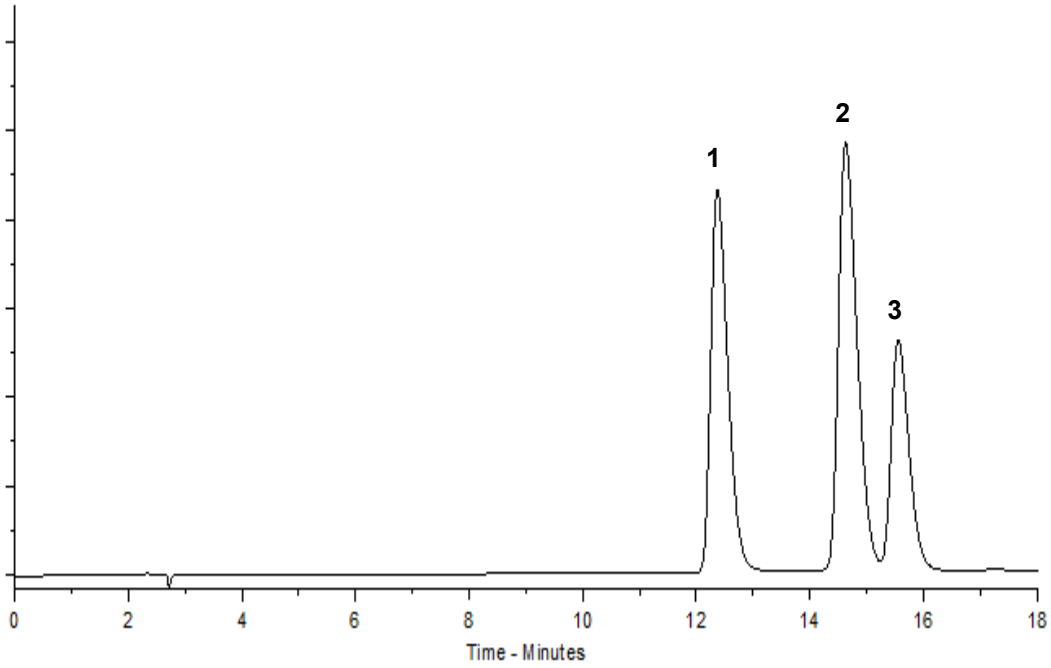
Application #**AN2770**

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	A: 0.1% TFA in H_2O/MeCN (71:29 v/v) B: 0.1% TFA in H_2O/MeCN (68:32 v/v)

Time (mins)	%B
0	10
16	90

Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 215 nm



1. Bovine insulin
2. Human insulin
3. Porcine insulin

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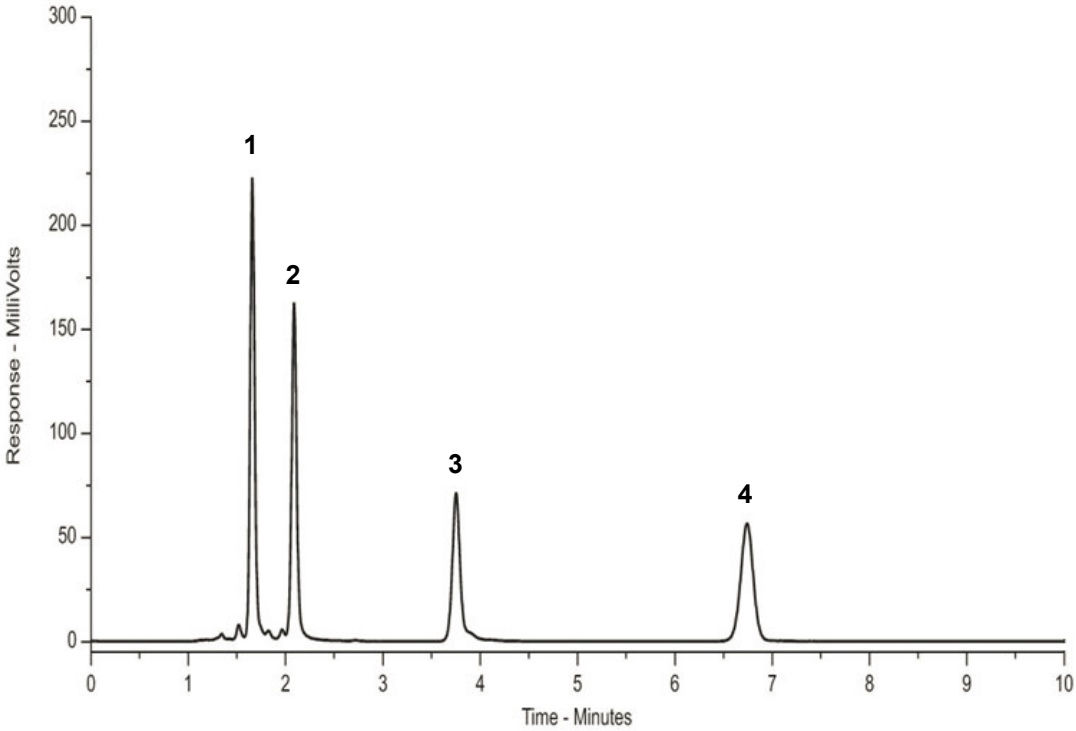
Separation of Isoflavones

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2970**

Conditions

Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	MeCN/0.1% formic acid in H_2O (35:65 v/v)
Flow Rate:	1 mL/min
Injection:	1 µL
Temperature:	Ambient
Detection:	UV, 254 nm



1. Daidzin
2. Genistin
3. Daidzein
4. Genistein

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Isoflavones in Red Clover and Soy Extract

ACE® Ultra-inert UHPLC & HPLC Columns

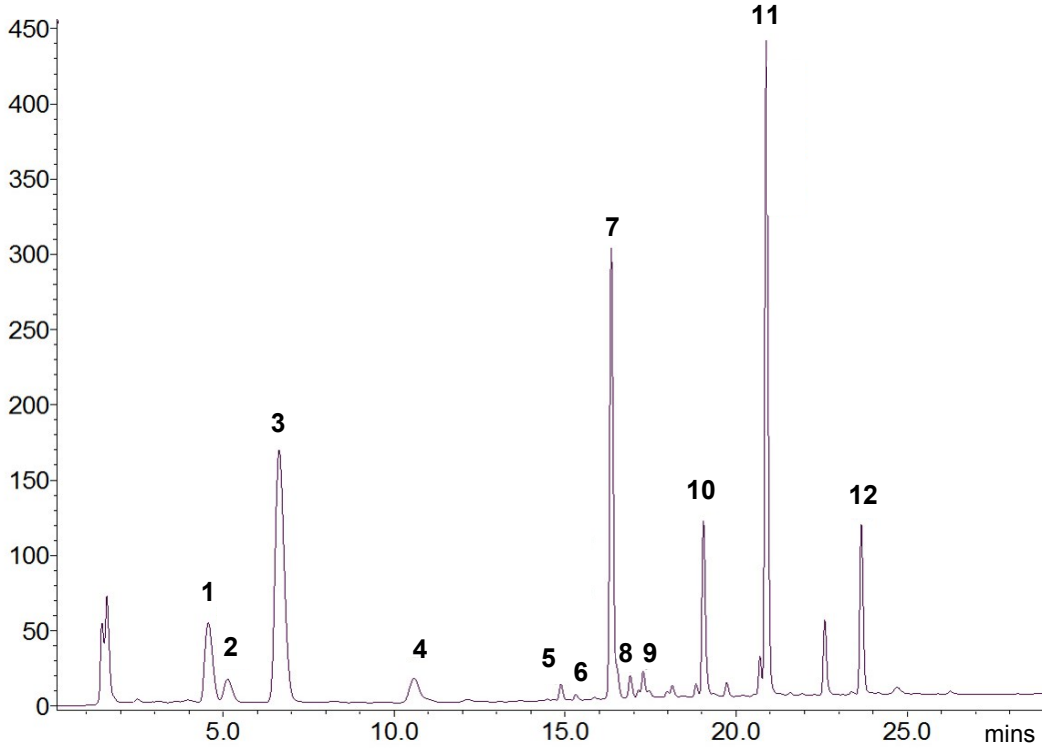
Application #**AN1130**

Conditions

Column:	ACE 3 C18-AR
Dimensions:	150 x 2.1 mm
Part Number:	ACE-119-1502
Mobile Phase:	A: Acetic acid in H_2O pH 2.8 B: 0.6% Acetic acid in MeCN

Time (min)	%B
0	15
7	15
27	75

Flow Rate:	0.35 mL/min
Injection:	3 µL
Temperature:	25 °C
Detection:	UV, 254 nm



1. Daidzin
2. Glycitin
3. Rutin (Int. Standard)
4. Genistin
5. Acetyl-Daidzin
6. Acetyl-Glycitin
7. Daidzein
8. Glycitein
9. Acetyl-Genistin
10. Genistein
11. Formononetin
12. Biochanin A

K. Weinfurter et al. Forsch. Komplementmed. 21 (Suppl.1): 45 (2014)

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Fingerprinting of Liquorice Extracts

ACE® Ultra-inert UHPLC & HPLC Columns

Application #**AN2090**

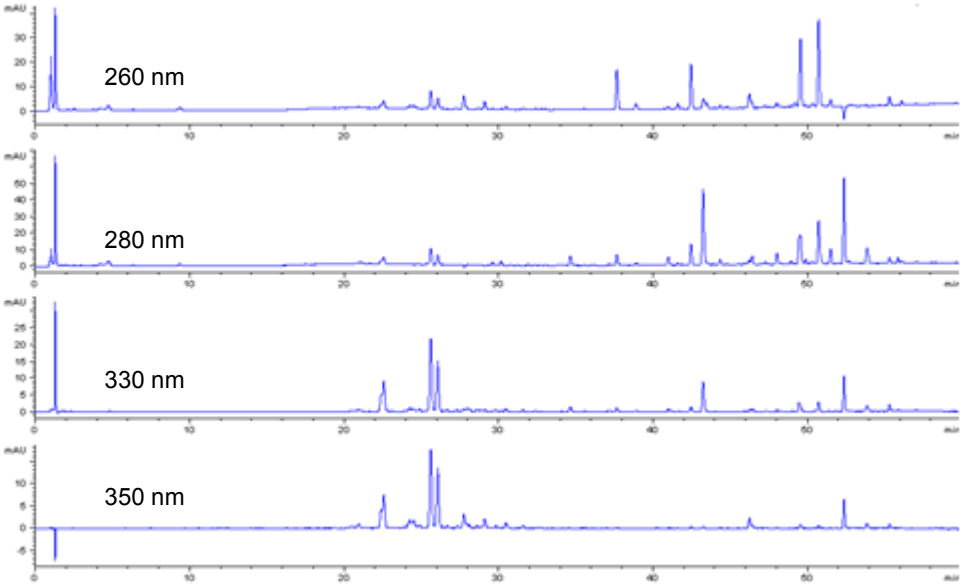
Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: Ammonium acetate in H_2O pH 4
B: MeOH

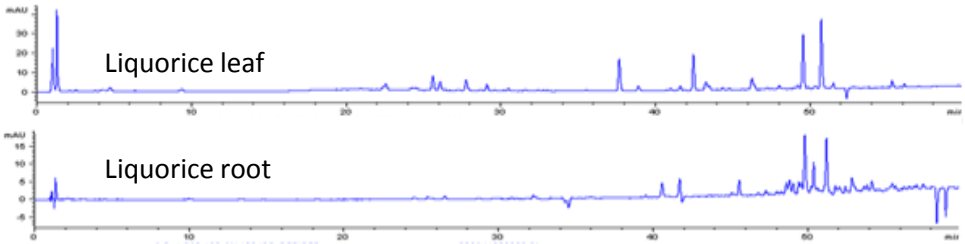
Time (mins)	%B
0	10
1	10
11	15
55	90
60	100

Flow Rate: 0.4 mL/min
Injection: 2 µL
Temperature: 40 °C
Detection: UV, 260, 280, 330 and 350 nm
Sample: Plant material ground to a fine powder in pestle and mortar. Powdered material extracted into methanol by ultrasonification for 30 minutes, followed by centrifugal filtration.

Methanolic liquorice leaf extract at different wavelengths



Comparison of methanolic extracts at 260 nm



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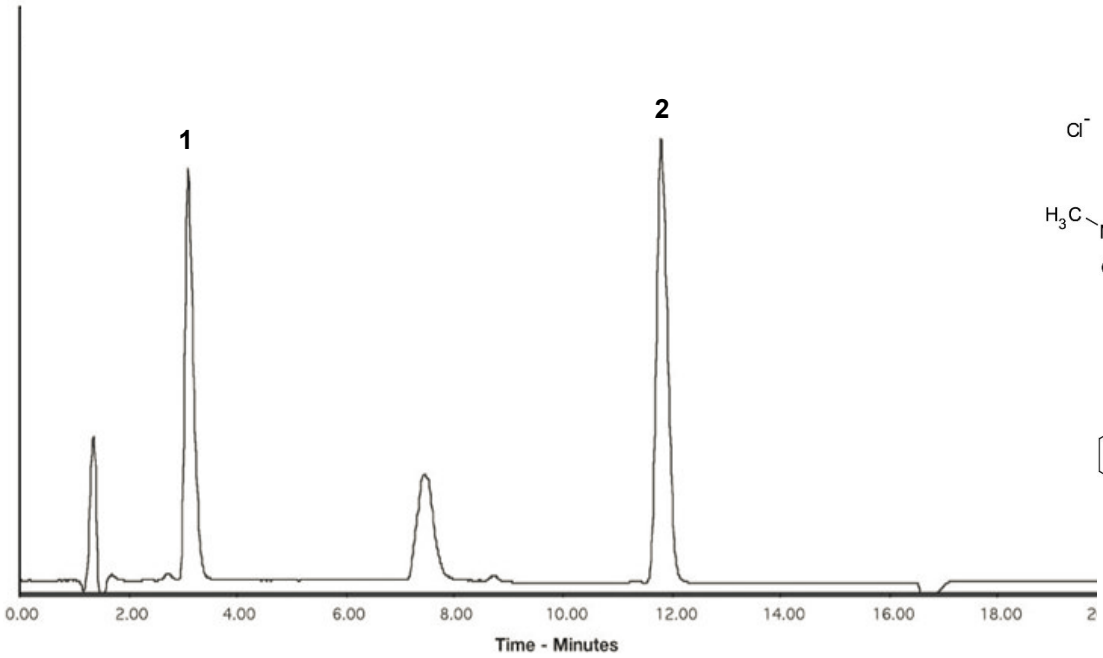
Detection of Malachite Green

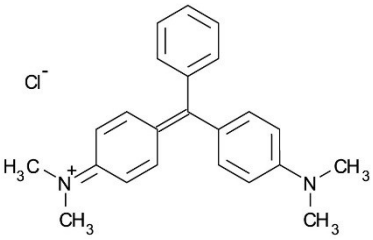
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2860**

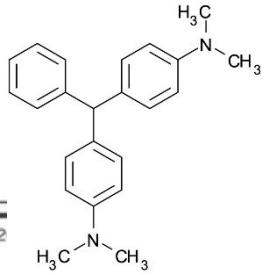
Conditions

Column:	ACE 5 C18
Dimensions:	150 x 3.0 mm
Part Number:	ACE-121-1503
Mobile Phase:	10 mM oxalic acid pH 2.9 in H_2O/MeCN (80:20 v/v)
Flow Rate:	0.4 mL/min
Temperature:	Ambient
Detection:	UV-Vis, 618 nm





1. Malachite green



2. Leucomalachite green

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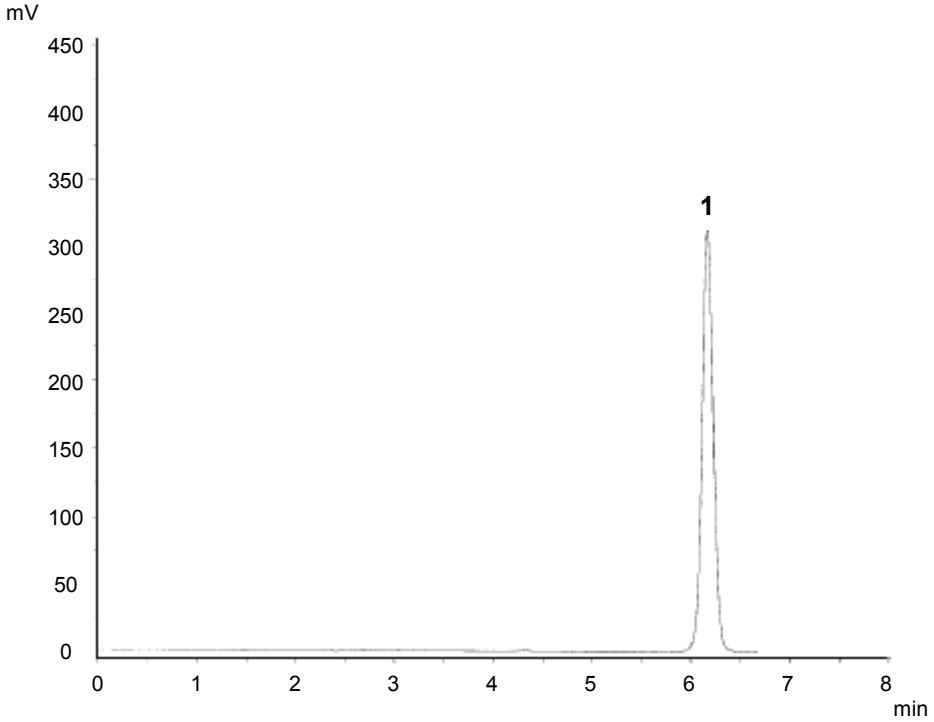
Detection of Melamine using Ion-Pairing Reagent

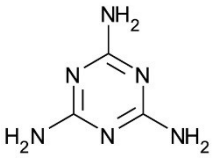
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2510**

Conditions

Column:	ACE 5 C8
Dimensions:	150 x 4.6 mm
Part Number:	ACE-122-1546
Mobile Phase:	5 mM heptafluorobutyric acid:MeCN (95:5 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	Ambient
Detection:	UV, 240 nm





1. Melamine

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Microcystins from Blue/Green Algae in Drinking Water

ACE® Ultra-inert UHPLC & HPLC Columns

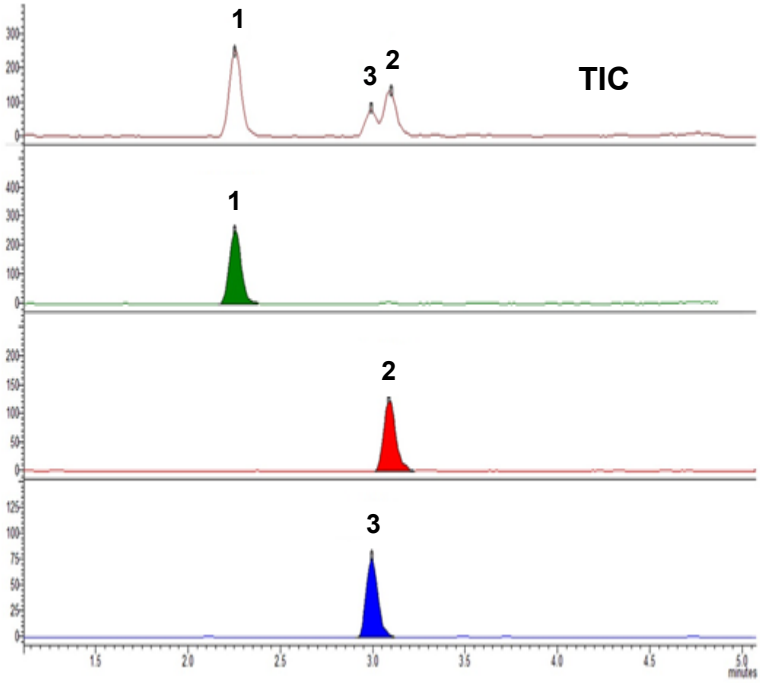
Application #**AN1190**

Conditions

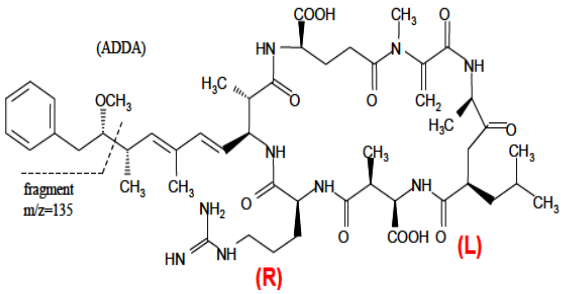
Column:	ACE Excel 2 C18
Dimensions:	100 x 2.1 mm
Part Number:	EXL-101-1002U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: MeCN

Time (mins)	%B
0.0	30
1.0	30
7.0	95
7.1	30
10.0	30

Flow Rate:	0.4 mL/min
Injection:	50 µL
Temperature:	40 °C
Sample:	0.05 ppb
Detection:	Bruker EVOQ Elite triple quad MS
	VIP heated-ESI temperature: 350 °C
	Cone gas temperature: 200 °C
	Spray voltage: 4500 V (+)
	Collision gas: argon 1.5 mTorr



1. Microcystin RR (MW 1038) (*m/z* 520 → 135)
2. Microcystin LR (MW 995) (*m/z* 498 → 135)
3. Microcystin YR (MW 1045) *m/z* 523 → 135)



Variants	R	L
Microcystin-LR	Leucine	Arginine
Microcystin-RR	Arginine	Arginine
Microcystin-YR	Tyrosine	Arginine

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Separation of Milk Proteins

ACE®
Ultra-inert
UHPLC & HPLC Columns

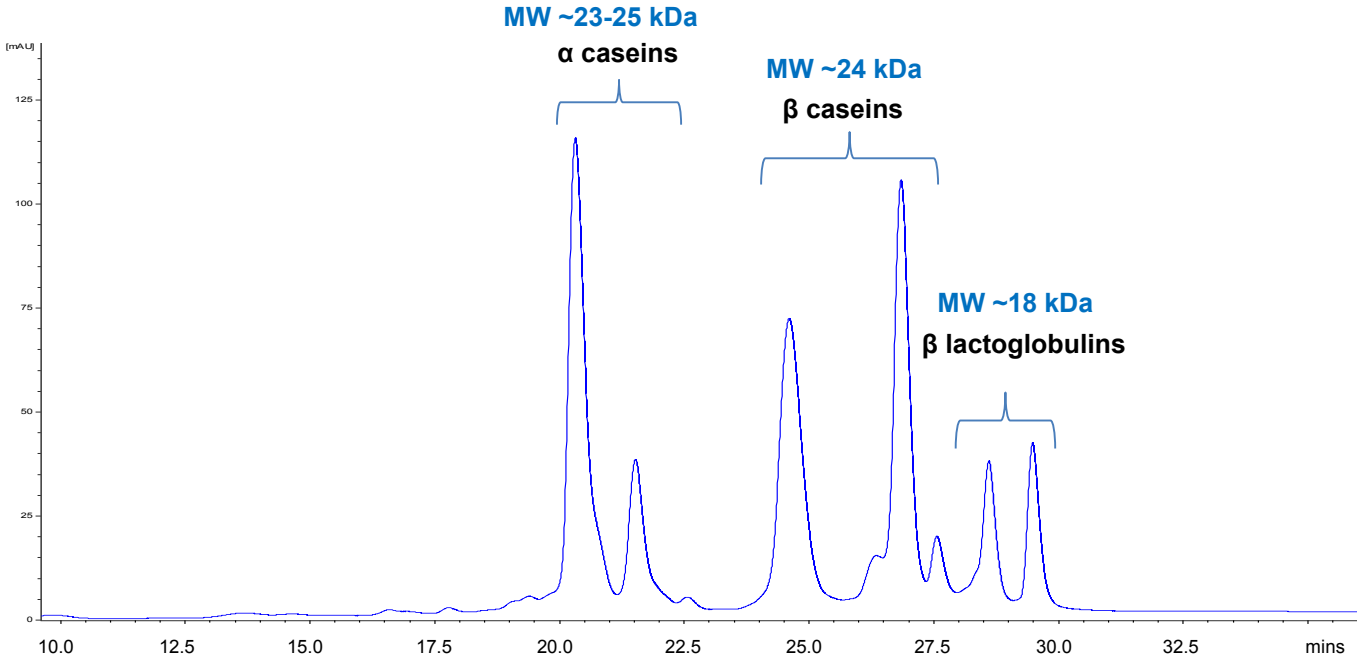
Application #**AN1540**

Conditions

Column:	ACE 5 C18-300
Dimensions:	150 x 2.1 mm
Part Number:	ACE-221-1502
Mobile Phase:	A: 0.01% TFA in H_2O
	B: 0.01% TFA in MeCN

Time (mins)	%B
0.0	33
5.0	33
9.0	35
18.0	37
22.0	40
27.5	41
28.0	41
43.0	43

Flow Rate:	0.2 mL/min
Temperature:	45 °C
Detection:	UV, 214 nm



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Mycotoxins by LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

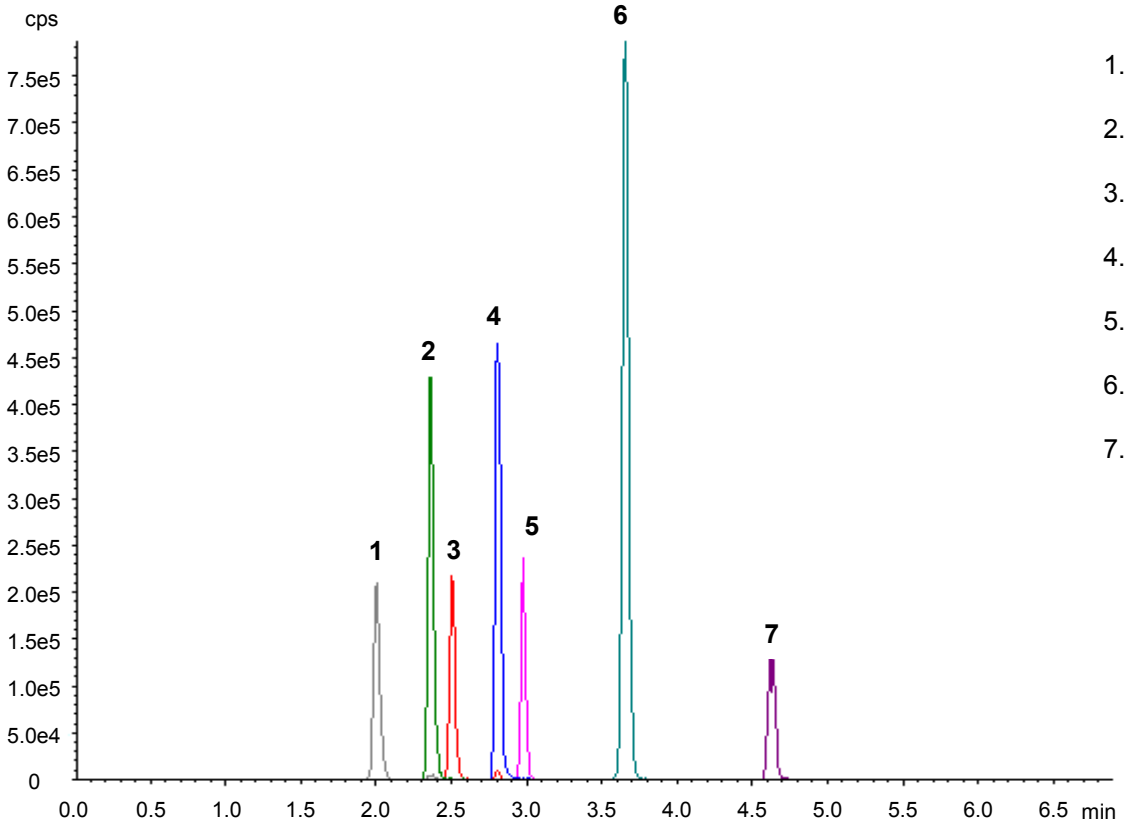
Application #**AN2330**

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

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



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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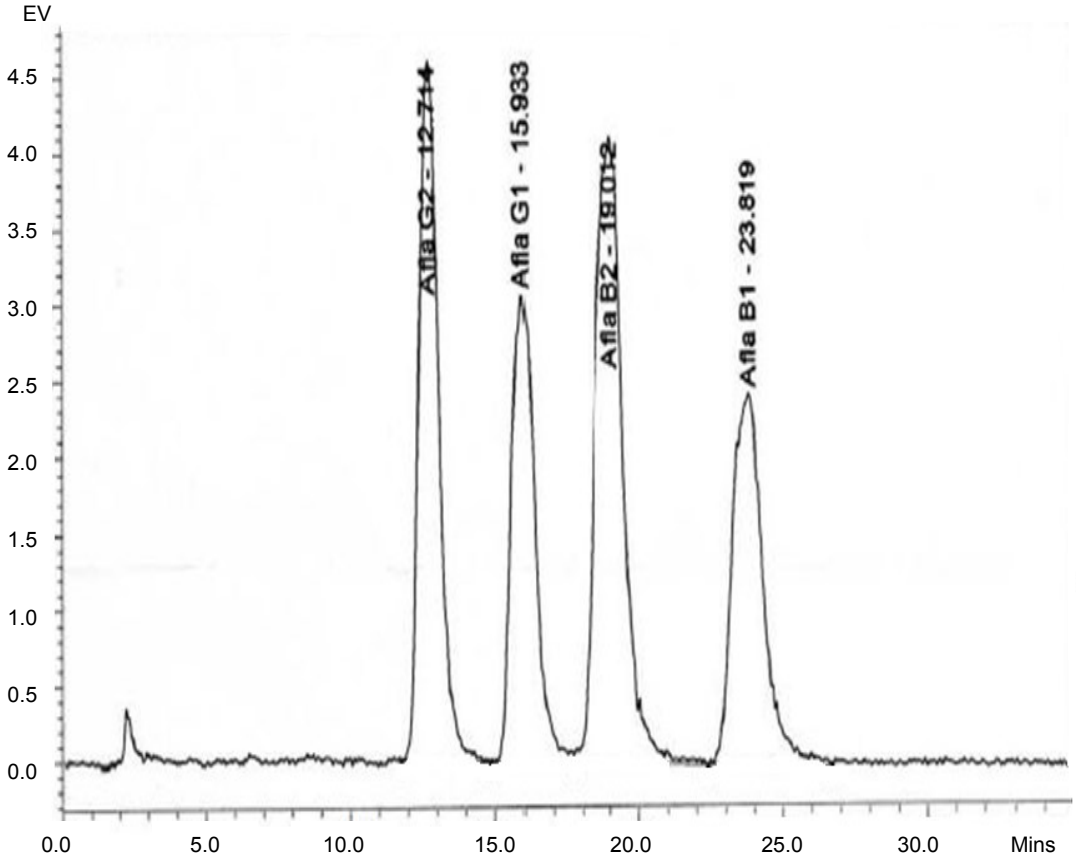
Mycotoxins / Aflatoxins from Peppers

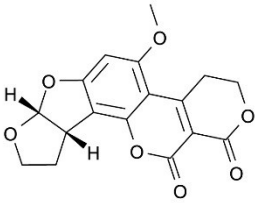
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1200**

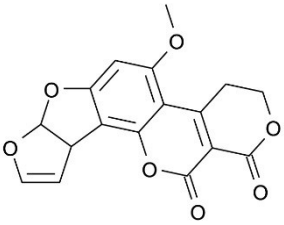
Conditions

Column:	ACE 3 C18-PFP
Dimensions:	150 x 4.6 mm
Part Number:	ACE-1110-1546
Mobile Phase:	H_2O/MeOH (60:40 v/v)
Flow Rate:	1 mL/min
Injection:	100 µL
Temperature:	45 °C
Detection:	Fluorescence, Ex λ 362 nm, Em λ 425 nm

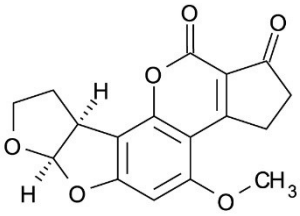




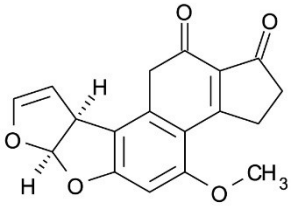
1. Aflatoxin G2



2. Aflatoxin G1



3. Aflatoxin B2



4. Aflatoxin B1

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Nitrofuran Metabolites by LC-MS/MS

ACE®
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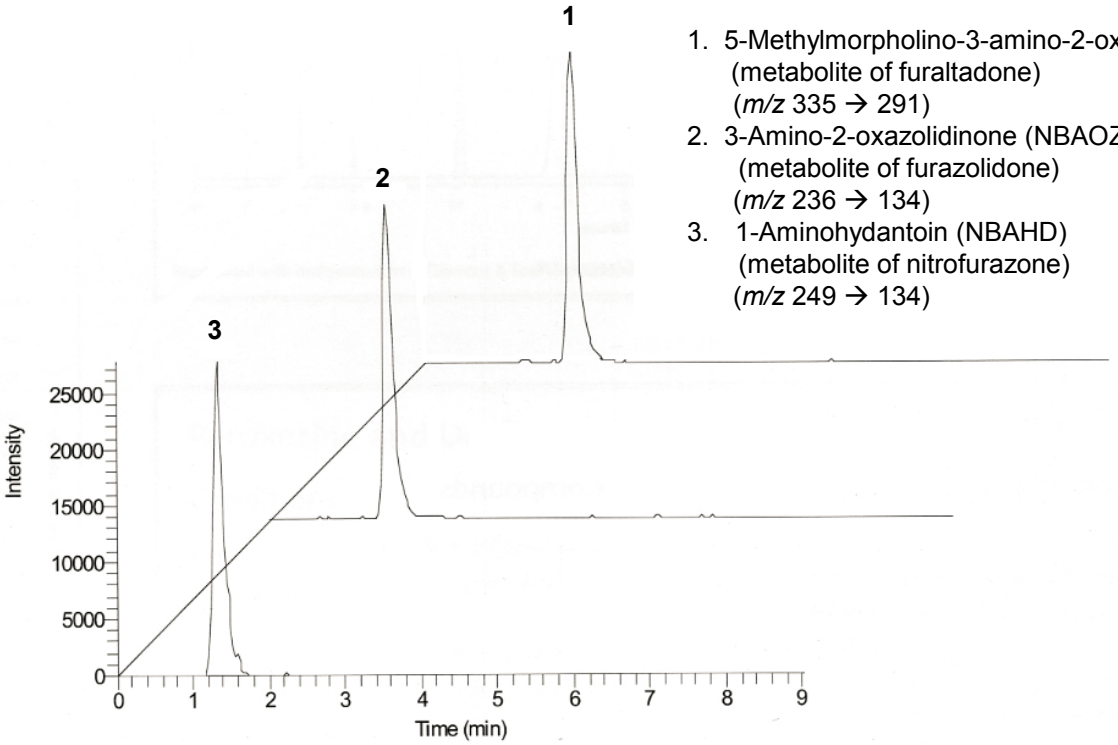
UHPLC & HPLC Columns

Application #**AN3050**

Conditions

Column:	ACE 3 C18
Dimensions:	50 x 2.1 mm
Part Number:	ACE-111-0502
Mobile Phase:	MeOH/0.5 mM ammonium acetate in H_2O (50:50 v/v)
Flow Rate:	0.2 mL/min
Injection:	20 µL
Temperature:	Ambient
Detection:	ESI MS/MS (+ve mode)
Sample:	Metabolites derivatised with 2-nitrobenzaldehyde to form nitrophenyl derivatives, prior to LC-MS analysis



1. 5-Methylmorpholino-3-amino-2-oxazolidinone (NBAMOZ)
   (metabolite of furaltadone)
   (*m/z* 335 → 291)
2. 3-Amino-2-oxazolidinone (NBAOZ)
   (metabolite of furazolidone)
   (*m/z* 236 → 134)
3. 1-Aminohydantoin (NBAHD)
   (metabolite of nitrofurazone)
   (*m/z* 249 → 134)

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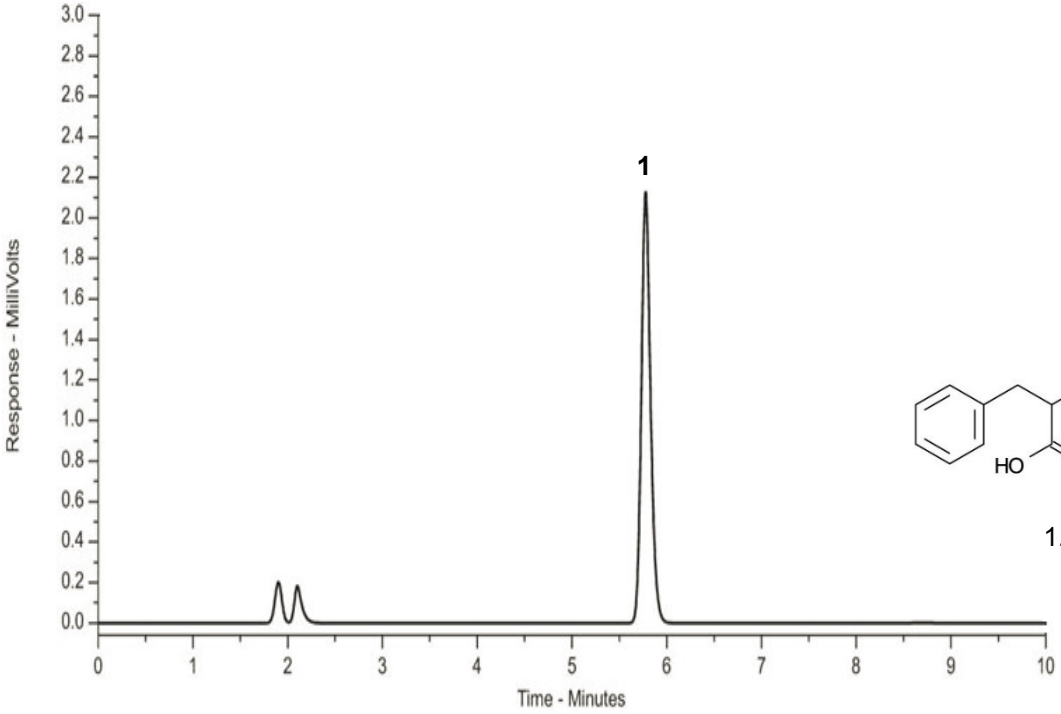
Detection of Ochratoxin A

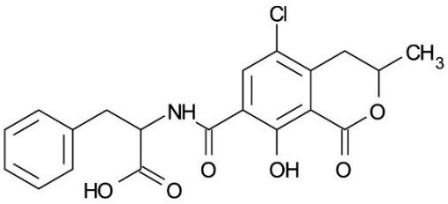
ACE®
Ultra-inert
UHPLC & HPLC Columns

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)
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	Fluorescence – λ_{ex} 333 nm, λ_{em} 443 nm





1. Ochratoxin A

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Separation of Organic acids

ACE®
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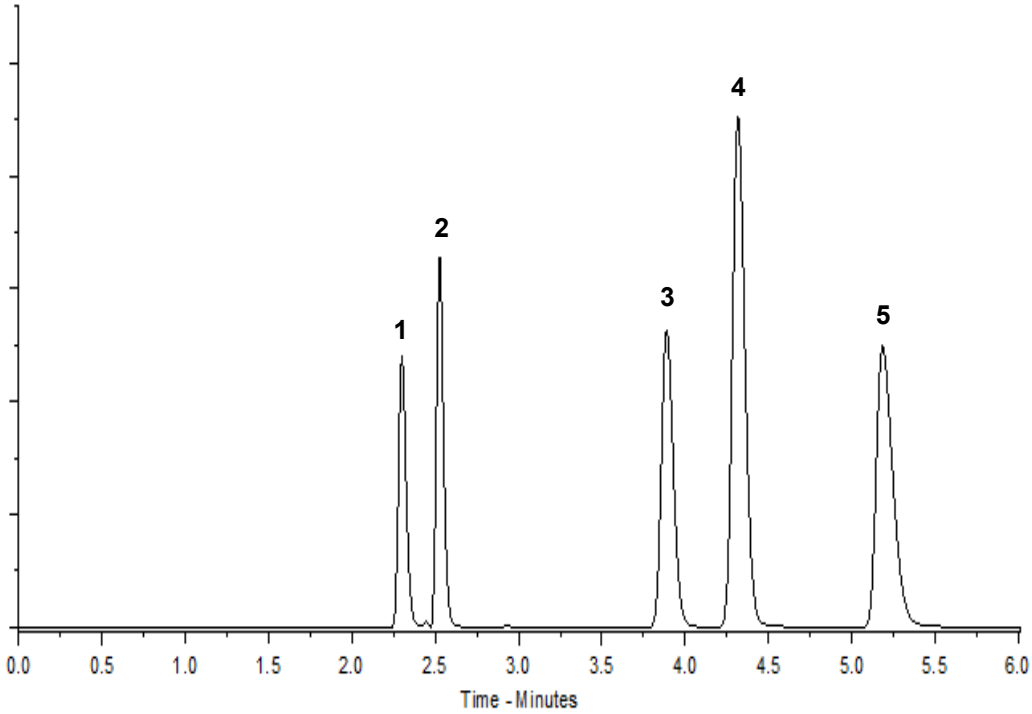
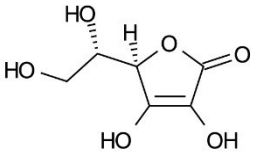
Application #**AN2780**

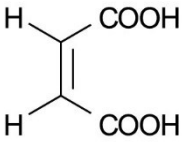
Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	50 mM KH_2PO_4 pH 5.7 in H_2O/MeOH (70:30 v/v)
Flow Rate:	1 mL/min
Temperature:	22 °C
Detection:	UV, 220 nm

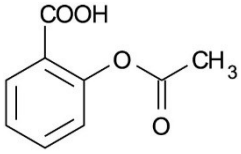




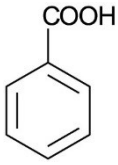
1. L-Ascorbic acid



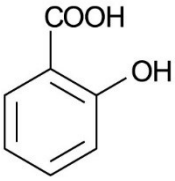
2. Maleic acid



3. Acetylsalicylic acid



4. Benzoic acid



5. Salicylic acid

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Separation of Organic Acids

ACE®
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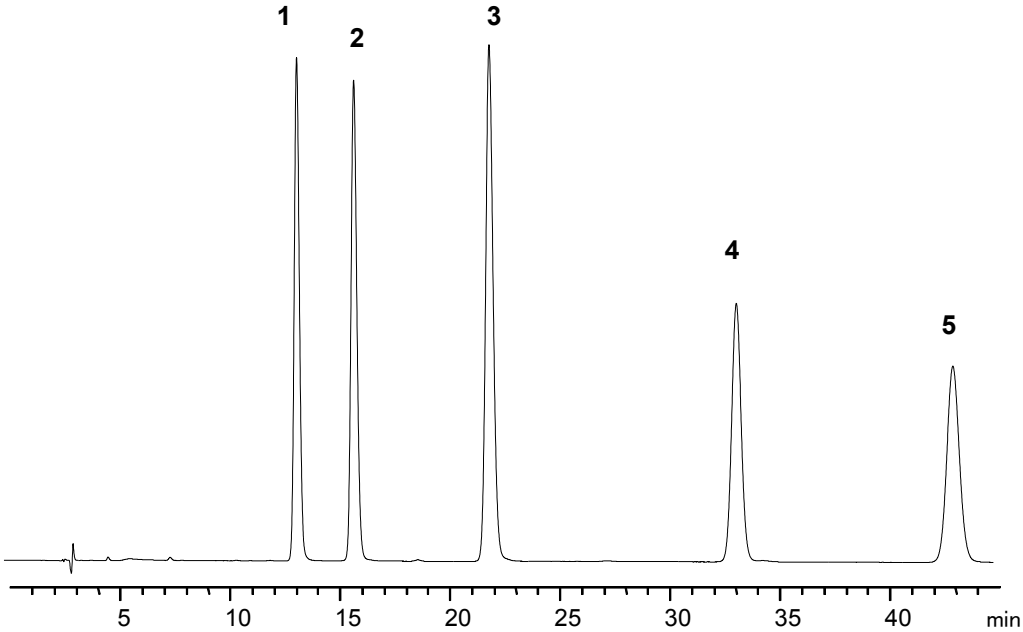
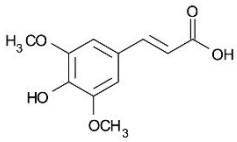
Application #**AN1570**

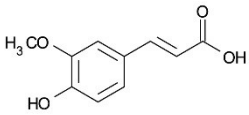
Conditions

Column:	ACE 3 C18-Amide
Dimensions:	250 x 2.1 mm
Part Number:	EXL-1112-2502U
Mobile Phase:	20 mM H_3PO_4 in MeOH/H_2O (40:60 v/v)
Flow Rate:	0.21 mL/min
Injection:	5 µL
Temperature:	20 °C
Detection:	UV, 210 nm

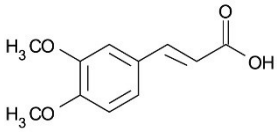




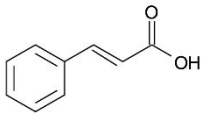
1. Sinapic acid



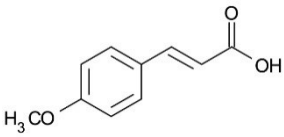
2. Ferulic acid



3. 3,4-Dimethoxycinnamic acid



4. Cinnamic acid



5. 4-Methoxycinnamic acid

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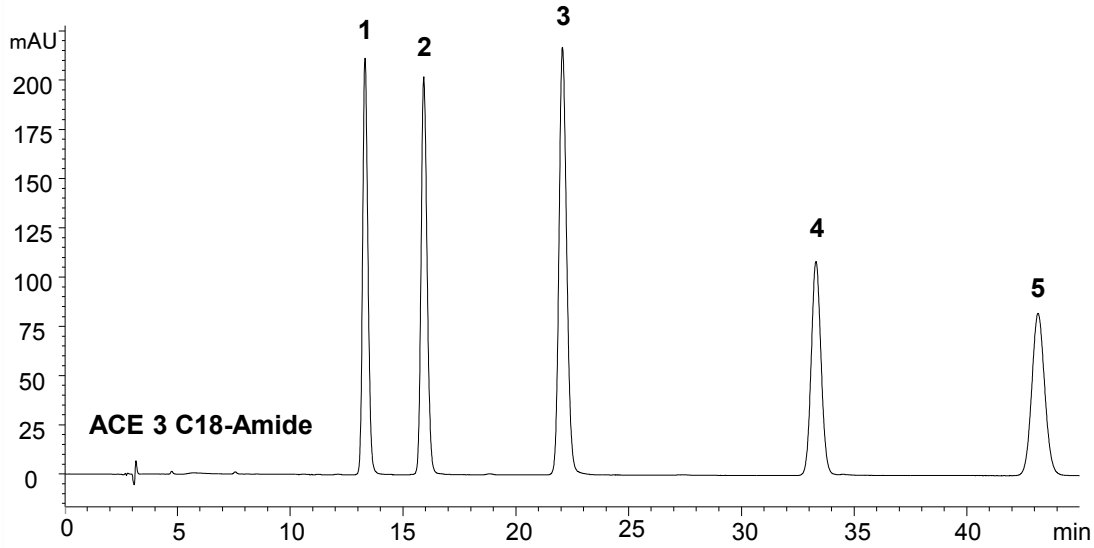
Fast Separation of Organic Acids

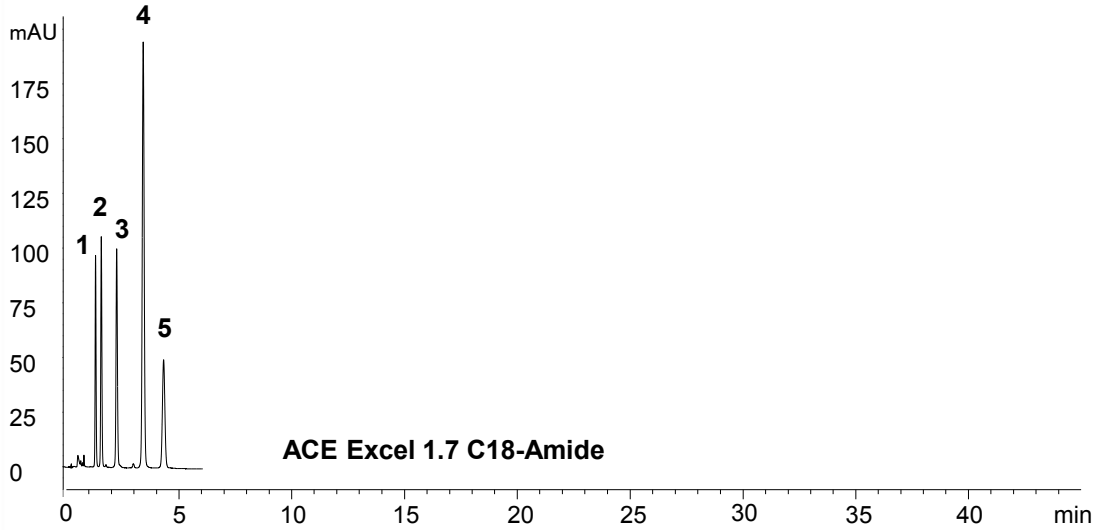
ACE®
Ultra-inert
UHPLC & HPLC Columns

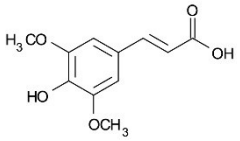
Application #**AN2200**

Conditions

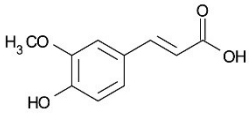
Column:	ACE 3 C18-Amide
	ACE Excel 1.7 C18-Amide
Dimensions:	250 x 2.1 mm
	50 x 3.0 mm
Part Number:	250 x 2.1 mm (EXL-1112-2502U), 50 x 3 mm (EXL-1712-0503U)
Mobile Phase:	20 mM H_3PO_4 in MeOH/H_2O (40:60 v/v)
Flow Rate:	0.21 mL/min (250 x 2.1 mm)
	0.8 mL/min (50 x 3.0 mm)
Injection:	5 µL (250 x 2.1 mm)
	2 µL (50 x 3.0 mm)
Temperature:	20 °C
Detection:	UV, 210 nm



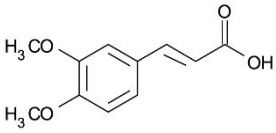




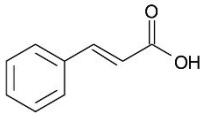
1. Sinapic acid



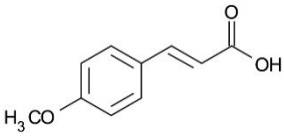
2. Ferulic acid



3. 3,4-Dimethoxycinnamic acid



4. Cinnamic acid



5. 4-Methoxycinnamic acid

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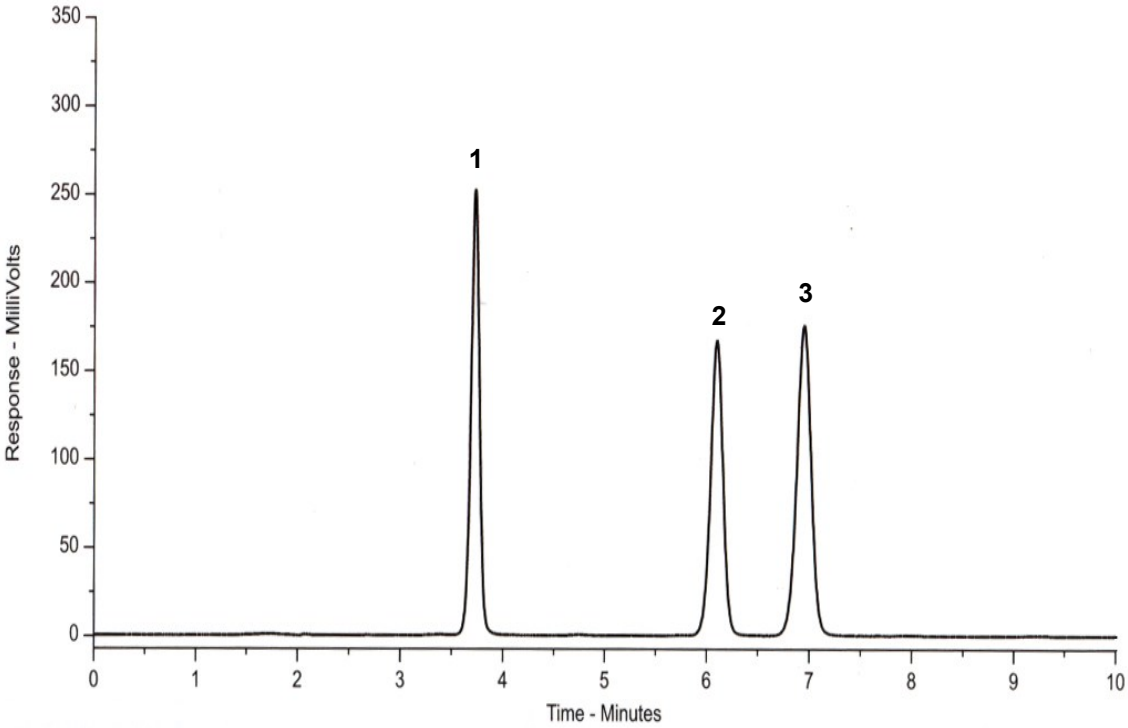
Separation of Phenolic Acids

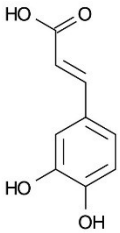
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN3030**

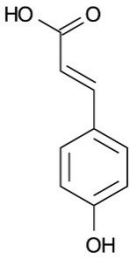
Conditions

Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	MeCN/0.1% formic acid in H_2O (20:80 v/v)
Flow Rate:	1 mL/min
Injection:	1 µL
Temperature:	Ambient
Detection:	UV, 254 nm

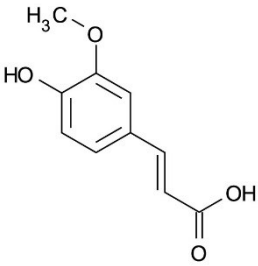




1. Caffeic acid



2. p-Coumaric acid



3. Ferulic acid

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Organophosphorus Flame Retardants in Water by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN1240

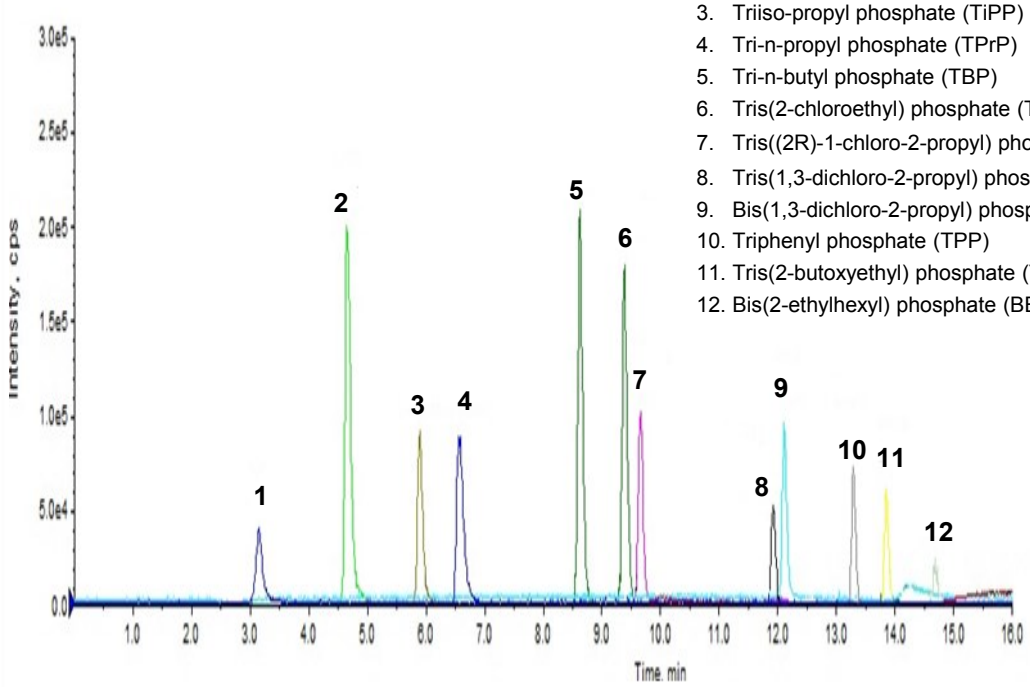
Conditions

Column:	ACE 3 C18
Dimensions:	100 x 2.1 mm
Part Number:	ACE-111-1002
Mobile Phase:	A: 0.05 mM ammonium formate + 0.005% formic acid in H_2O B: MeOH/MeCN (95:5 v/v)

Time (mins)	%B
0.1	50
12.0	90
13.0	100
15.0	100
15.1	50
20.0	50

Flow Rate:	0.25 mL/min
Injection:	80 µL
Temperature:	25 °C
Detection:	MS/MS

	Q1 Mass	Q3 Mass
1. Trimethyl phosphate (TMP)	141	109
2. Triethyl phosphate (TEP)	183	127
3. Triiso-propyl phosphate (TiPP)	225	99
4. Tri-n-propyl phosphate (TPrP)	225	99
5. Tri-n-butyl phosphate (TBP)	267	211
6. Tris(2-chloroethyl) phosphate (TCEP)	285	223
7. Tris((2R)-1-chloro-2-propyl) phosphate (TCPP)	327	99
8. Tris(1,3-dichloro-2-propyl) phosphate (TDCPP)	431	99
9. Bis(1,3-dichloro-2-propyl) phosphate (BDCP)	321	99
10. Triphenyl phosphate (TPP)	327	215
11. Tris(2-butoxyethyl) phosphate (TBEP)	399	299
12. Bis(2-ethylhexyl) phosphate (BEHP)	323	99



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Isomeric Organophosphorus Flame Retardants in Water

ACE® Ultra-inert UHPLC & HPLC Columns

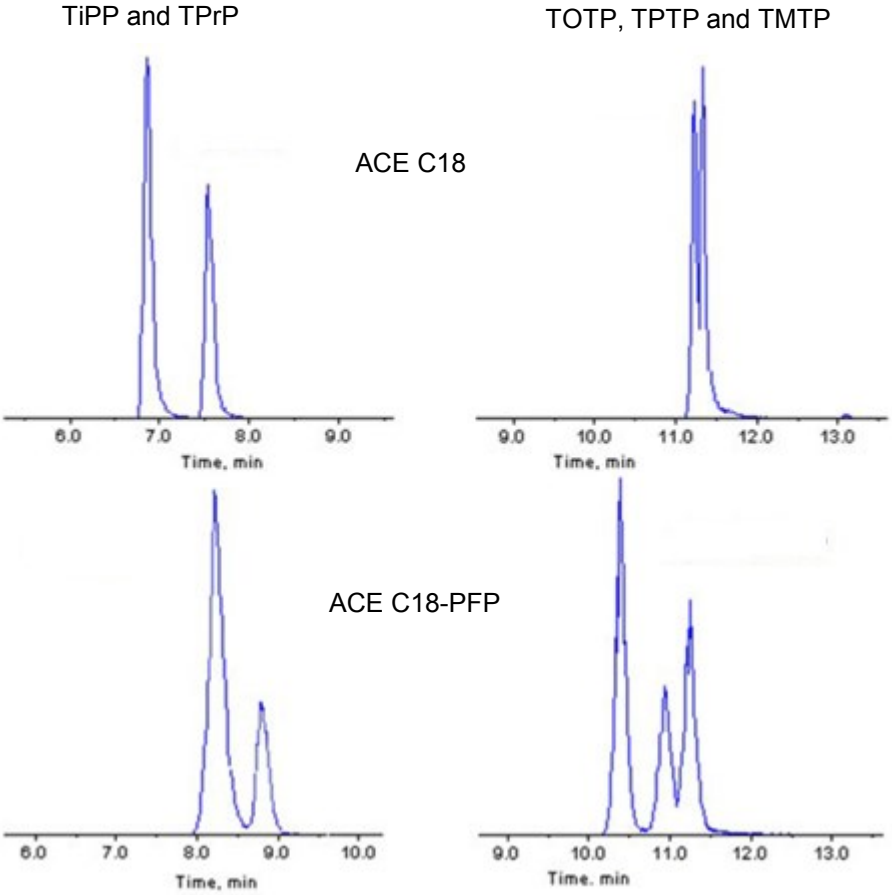
Application #**AN1140**

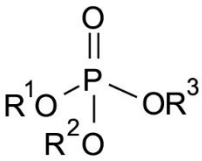
Conditions

Column:	ACE 3 C18 ACE 3 C18-PFP
Dimensions:	100 x 2.1 mm
Part Number:	ACE-111-1002, ACE-1110-1002
Mobile Phase:	A: 0.05 mM ammonium formate + 0.005% formic acid in H_2O B: MeOH/MeCN (95:5 v/v)

Time (mins)	**%B**
0.1	50
12.0	90
13.0	100
15.0	100
15.1	50
20.0	50

Flow Rate:	0.25 mL/min
Injection:	80 µL
Temperature:	25 °C
Detection:	MS/MS





1. Triiso-propyl phosphate (TiPP) (*m/z* 225 → 99)
2. Tri-n-propyl phosphate (TPrP) (*m/z* 225 → 99)
3. Tri-o-tolyl phosphate (TOTP) (*m/z* 369 → 91)
4. Tri-p-tolyl phosphate (TPTP) (*m/z* 369 → 91)
5. Tri-m-tolyl phosphate (TMTP) (*m/z* 369 → 91)

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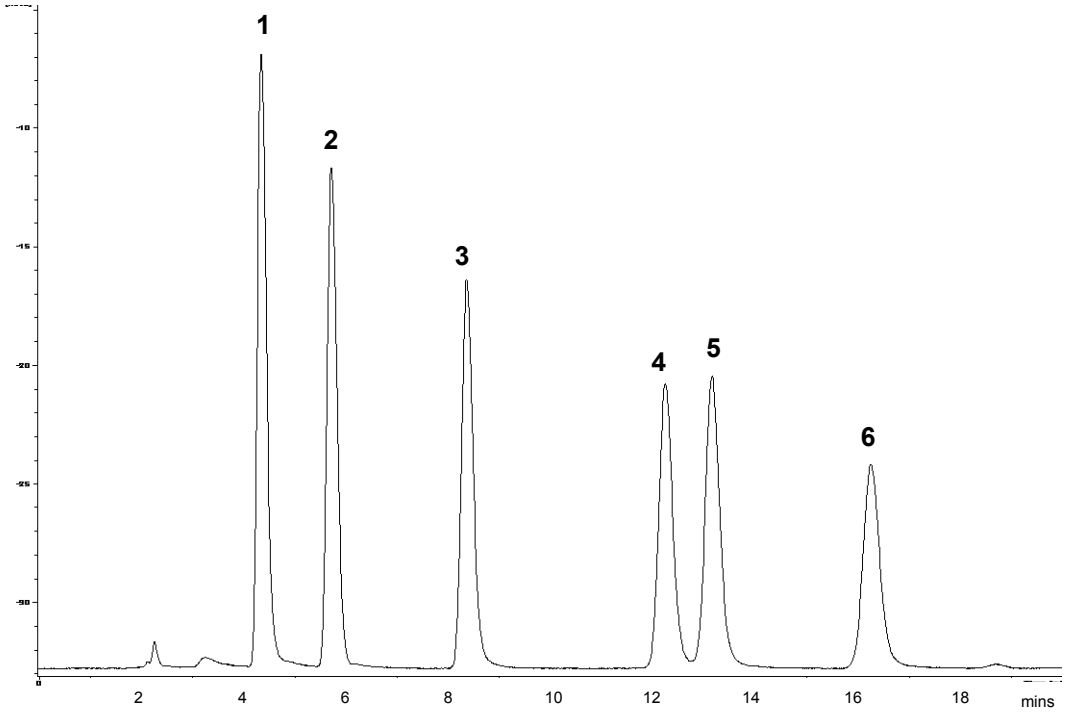
Paraben Preservatives

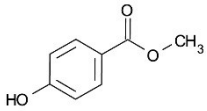
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1250**

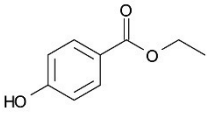
Conditions

Column:	ACE 3 Phenyl
Dimensions:	150 x 2.1 mm
Part Number:	ACE-115-1502
Mobile Phase:	25 mM ammonium acetate pH 6.8 in H_2O/MeOH (50:50 v/v)
Flow Rate:	0.2 mL/min
Injection:	2 µL
Temperature:	40 °C
Detection:	UV, 240 nm

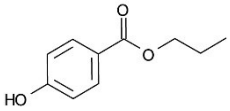




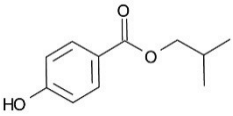
1. Methyl paraben



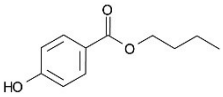
2. Ethyl paraben



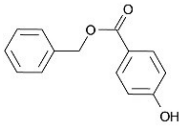
3. n-Propyl paraben



4. i-Butyl paraben



5. n-Butyl paraben



6. Benzyl paraben

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Perfluoro Acids by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

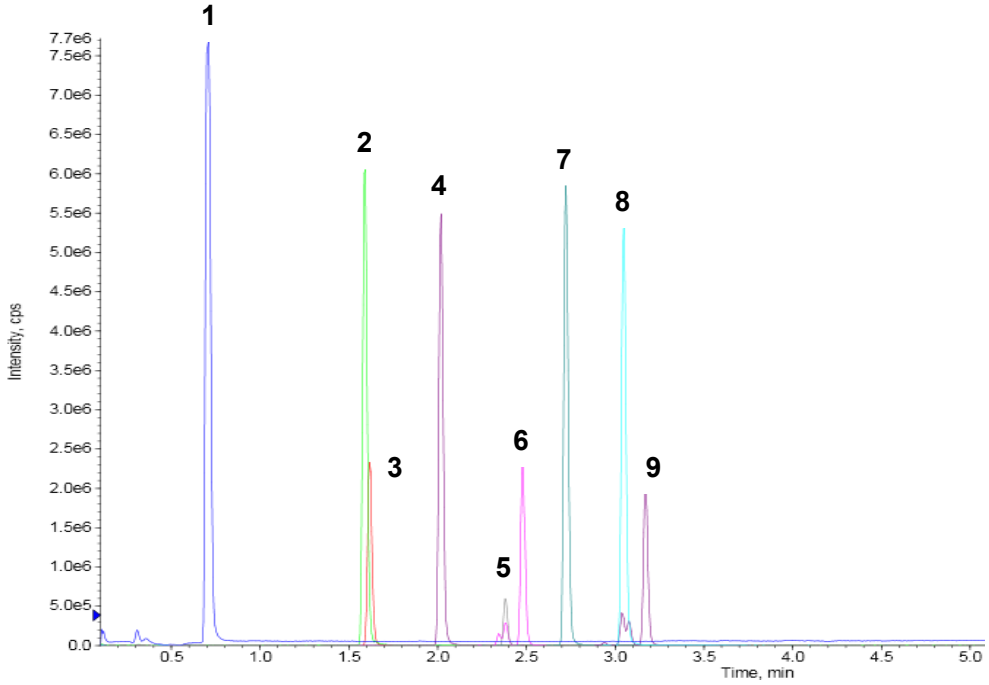
Application #**AN1280**

Conditions

Column:	ACE Excel 2 C18
Dimensions:	50 x 2.1 mm
Part Number:	EXL-101-0502U
Mobile Phase:	A: 2 mM ammonium acetate, 0.1% acetic acid/MeCN (95:5 v/v) B: 2 mM ammonium acetate, 0.1% acetic acid/MeCN (5:95 v/v)

Time (mins)	**%B**
0.0	25
0.5	25
5.5	95
7.5	95
8.0	25
10.0	25

Flow Rate:	0.5 mL/min
Injection:	20 µL
Temperature:	40 °C
Detection:	AB SCIEX triple quad 5500 Negative ESI MRM Source temperature: 450 °C IonSpray voltage: -2400 V



1. Heptafluorobutyric acid (*m/z* 212.9 → 168.9)
2. Perfluorohexanoic acid (*m/z* 313 → 268.9)
3. Perfluorobutylsulfonic acid (*m/z* 299 → 79.9)
4. Perfluoroheptanoic acid (*m/z* 363 → 319)
5. Perfluorooctanoic acid (*m/z* 413 → 368.9)
6. Perfluorohexylsulfonic acid (*m/z* 399 → 80)
7. Perfluorononanoic acid (*m/z* 463 → 419)
8. Perfluorodecanoic acid (*m/z* 513 → 469)
9. Perfluorooctanesulfonic acid (*m/z* 499 → 80)

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Perfluoroalkyl Substances by Ion-Pairing LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

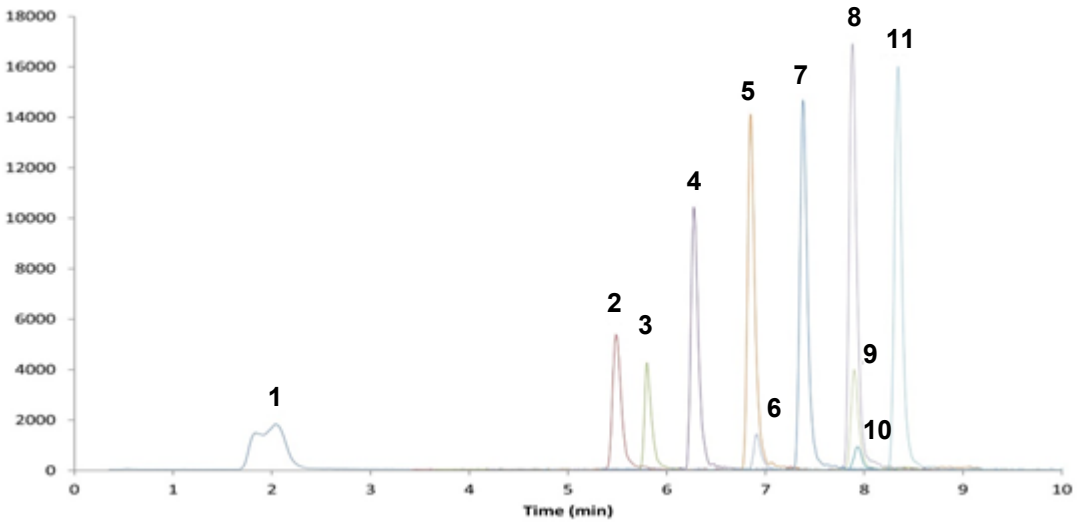
Application #**AN2560**

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
Mobile Phase: A: 2 mM ammonium acetate + 5 mM 1-methylpiperidine in MeOH/H_2O (5:95 v/v)
B: 2 mM ammonium acetate + 5 mM 1-methylpiperidine in MeOH/H_2O (95:5 v/v)

Time (mins)	%B
0.0	10
0.3	10
1.0	20
1.5	50
5.0	80
10.0	80
13.0	100
16.0	100

Flow Rate: 0.3 mL/min
Injection: 5 µL
Temperature: 35 °C
Detection: Agilent 6430 triple quad MS
ESI in negative ion mode
Capillary voltage: 3000 V
Nebulizer pressure: 50 psi



1. PFBA
   (*m/z* 213 → 169)
2. PFPeA
   (*m/z* 263 → 219)
   (*m/z* 263 → 175)
3. PFBS
   (*m/z* 299 → 99)
   (*m/z* 299 → 80)
4. PFHxA
   (*m/z* 313 → 269)
   (*m/z* 313 → 119)
5. PFHpA
   (*m/z* 363 → 319)
   (*m/z* 363 → 169)
6. PFHxS
   (*m/z* 399 → 99)
   (*m/z* 399 → 80)
7. PFOA
   (*m/z* 413 → 369)
   (*m/z* 413 → 169)
8. PFNA
   (*m/z* 463 → 419)
   (*m/z* 463 → 169)
9. PFOS
   (*m/z* 499 → 99)
   (*m/z* 499 → 80)
10. FOSA
    (*m/z* 498 → 498)
    (*m/z* 498 → 78)
11. PFDA
    (*m/z* 513 → 469)
    (*m/z* 513 → 269)

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Perfluorinated Compounds in Water by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

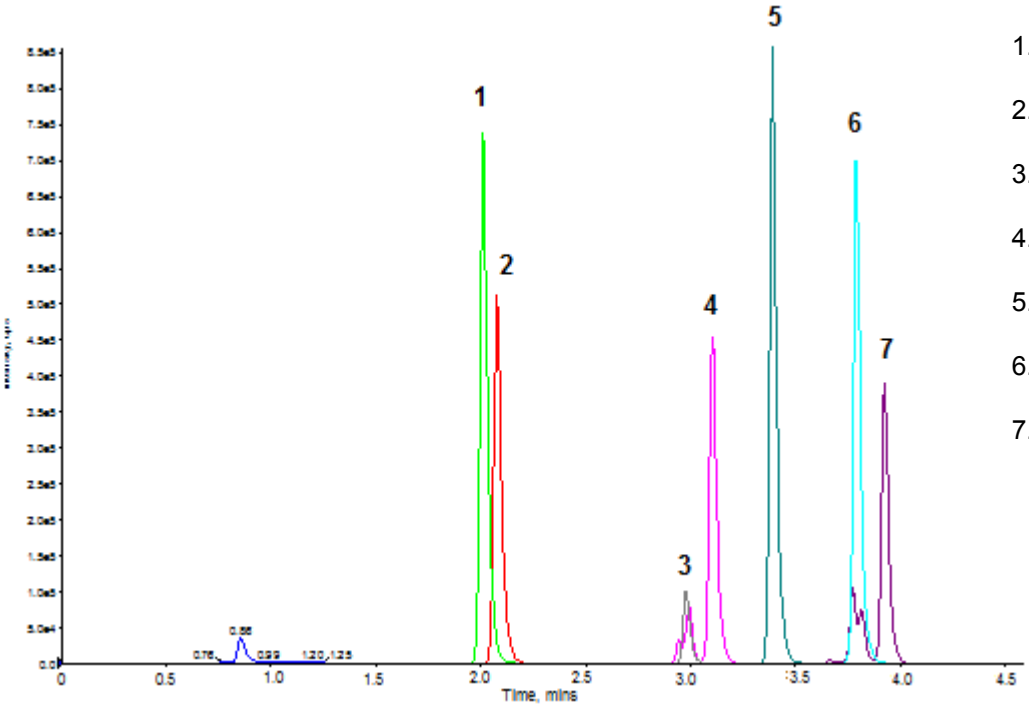
Application #AN2260

Conditions

Column:	ACE Excel 1.7 C18
Dimensions:	100 x 2.1 mm
Part Number:	EXL-171-1002U
Mobile Phase:	A: 2 mM ammonium acetate, 0.1% formic acid in H_2O/MeCN (90:10 v/v) B: 2 mM ammonium acetate, 0.1% formic acid in H_2O/MeCN (10:90 v/v)

Time (mins)	%B
0.0	25
0.5	25
3.5	70
4.0	100
5.5	100
6.0	25
9.0	25

Flow Rate:	0.5 mL/min
Injection:	10 µL
Temperature:	40 °C
Detection:	AB SCIEX triple quad 5500 Negative ESI MRM Source temperature: 450 °C IonSpray voltage: -2400 V



1. Perfluorohexanoic acid (*m/z* 313.0 → 268.9)
2. Perfluorobutanesulfonic acid (*m/z* 299.0 → 79.9)
3. Perfluorooctanoic acid (*m/z* 413.0 → 368.9)
4. Perfluorohexanesulfonic acid (*m/z* 399.0 → 80.0)
5. Perfluorononanoic acid (*m/z* 463.0 → 419.0)
6. Perfluorodecanoic acid (*m/z* 513.0 → 469.0)
7. Perfluorooctanesulfonic acid (*m/z* 499.0 → 80.0)

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250 Pesticide Screen using LC-MS/MS

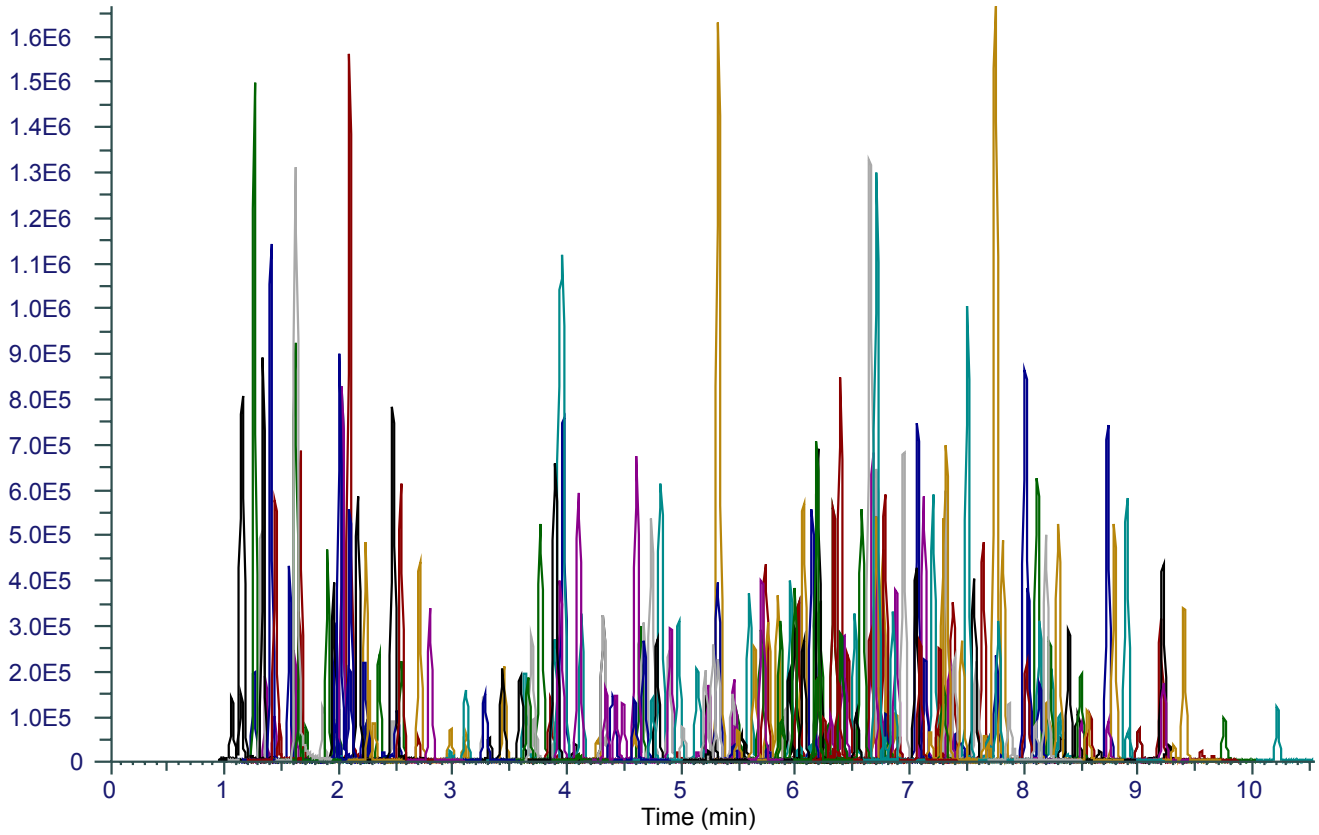
ACE®
Ultra-inert
UHPLC & HPLC Columns

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

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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250 Pesticide Screen using LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

Analyte	R_t	Adduct	Precursor Ion *m/z*	Quant Ion *m/z*	Conf Ion *mz*	Analyte	R_t	Adduct	Precursor Ion *m/z*	Quant Ion *m/z*	Conf Ion *mz*
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	Dichlormid	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	233.0	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	167.1	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	$[M-C_4H_{10}O_2PS_2]^+$	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	Etoxazole	8.73	$[M+H]^+$	360.2	141.0	304.2
Clofentezine	7.38	$[M+H]^+$	303.0	138.1	102.0	Famoxadone	7.24	$[M+NH_4]^+$	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	R_t	Adduct	Precursor Ion *m/z*	Quant Ion *m/z*	Conf Ion *mz*
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	$[M+H]^+$	384.1	282.2	328.2
Fludioxonil	5.76	$[M+NH_4]^+$	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	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

Analyte	R_t	Adduct	Precursor Ion *m/z*	Quant Ion *m/z*	Conf Ion *mz*
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	$[M+NH_4]^+$	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

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Analyte	R_t	Adduct	Precursor Ion *m/z*	Quant Ion *m/z*	Conf Ion *mz*	Analyte	R_t	Adduct	Precursor Ion *m/z*	Quant Ion *m/z*	Conf Ion *mz*
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	Tepraloxydim	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
Quinoxyfen	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						

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Pesticides by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

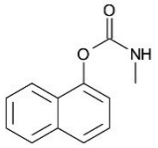
Application #AN1290

Conditions

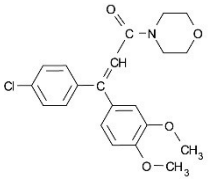
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
Mobile Phase: A: 0.1% formic acid + 5 mM ammonium formate in H_2O/MeOH (90:10 v/v)
B: 0.1% formic acid + 5 mM ammonium formate in H_2O/MeOH (10:90 v/v)

Time (mins)	%B
0.00	0
1.00	0
15.00	100
18.00	100
18.05	0
20.00	0

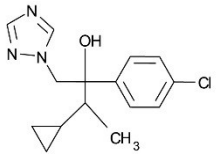
Flow Rate: 0.4 mL/min
Injection: 20 µL
Temperature: 40 °C
Detection: Agilent 6420 Triple Quadrupole MS, +ve mode ESI Dynamic MRM



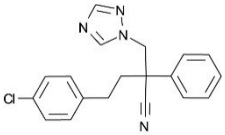
1. Carbaryl
(*m/z* 202.10 → 145.10)



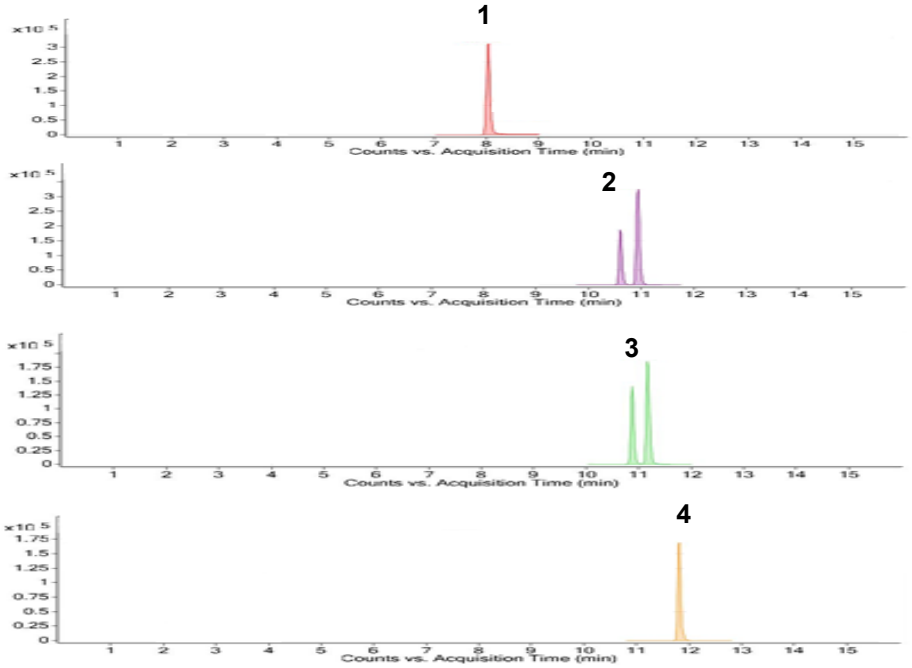
2. Dimethomorphs
(*m/z* 388.10 → 301.10)



3. Cyproconazoles
(*m/z* 292.10 → 70.00)



4. Fenbuconazole
(*m/z* 337.10 → 70.00)



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

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Pesticides in Water

ACE®
Ultra-inert
UHPLC & HPLC Columns

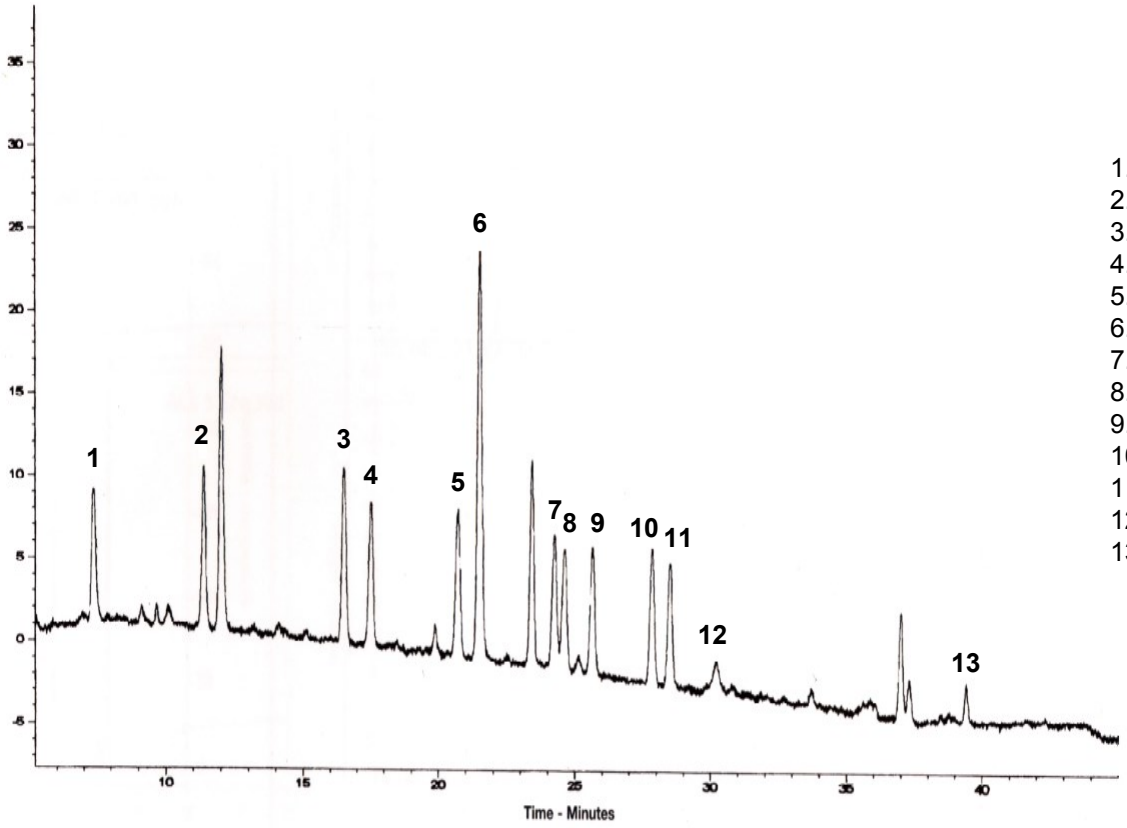
Application #**AN3020**

Conditions

Column:	ACE 3 C18
Dimensions:	150 x 2.1 mm
Part Number:	ACE-111-1502
Mobile Phase:	A: 0.1 M ammonium acetate in H_2O
	B: MeCN

Time (mins)	%B
0	10
40	80
47	90
49	10

Flow Rate:	0.3 mL/min
Injection:	25 µL
Temperature:	40 °C
Detection:	UV, 220 nm (Pendimethalin at 245 nm)
Sample:	0.05 µg/L standards in MeCN/H_2O 10:90 v/v)



1. Deisopropylatrazine
2. Desethylatrazine
3. Simazine
4. Cyanazine
5. Atrazine
6. Internal standard
7. Sebuthylazine
8. Propazine
9. Terbuthylazine
10. Prometryn
11. Terbutryn
12. Alachlor
13. Pendimethalin

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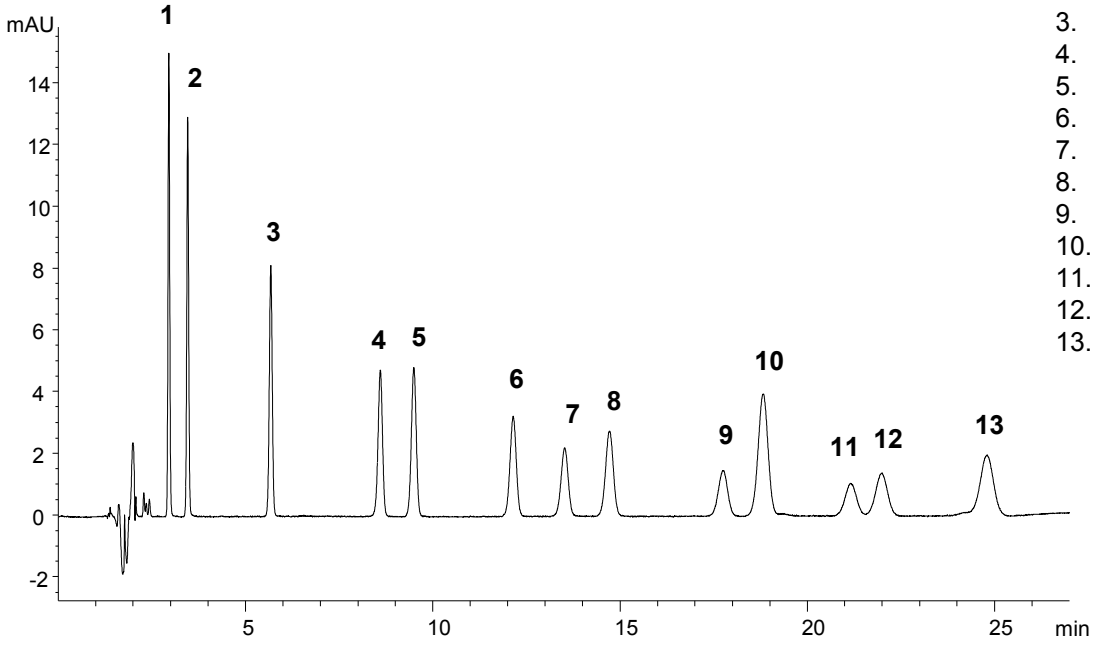
Detection of 13 Phenolic Compounds in Ground Water & Landfill Leachates

ACE® Ultra-inert UHPLC & HPLC Columns

Application #**AN3070**

Conditions

Column:	ACE Excel 3 C18-Amide
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1112-1546U
Mobile Phase:	0.1% formic acid v/v in H_2O/MeCN (65:35 v/v)
Flow Rate:	1mL/min
Injection:	10 µL
Temperature:	30 °C
Detection:	UV, 274 nm



1. Pyrocatechol
2. Resorcinol
3. Phenol
4. m-Cresol
5. o-Cresol
6. 2,4-Dimethylphenol
7. 3,4-Dimethylphenol
8. 3,5-Dimethylphenol
9. 1-Naphthol
10. 3,4,5-Trimethylphenol
11. 2,3,6-Trimethylphenol
12. 2,4,6-Trimethylphenol
13. 2-Naphthol

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Separation of Phenol and Phenoxy Acid Herbicides

ACE® Ultra-inert UHPLC & HPLC Columns

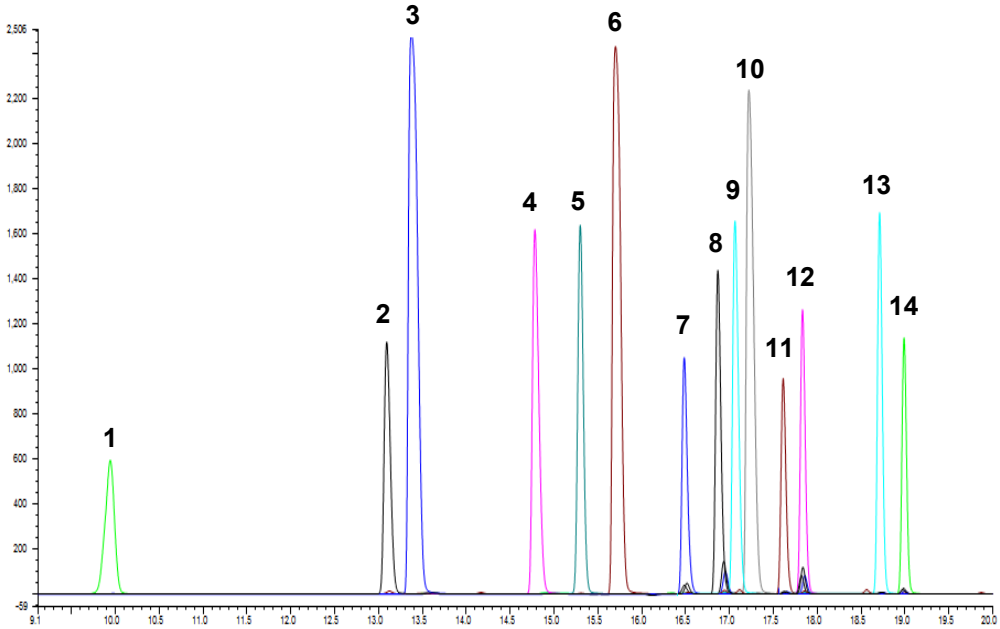
Application #AN2290

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

Time (mins)	%B
0.0	10
20.0	100

Flow Rate:	1 mL/min
Injection:	10 µL
Temperature:	35 °C
Detection:	UV, 280 nm



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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Phenols in Purple Coneflower (*Echinacea Purpurea)*

ACE® Ultra-inert UHPLC & HPLC Columns

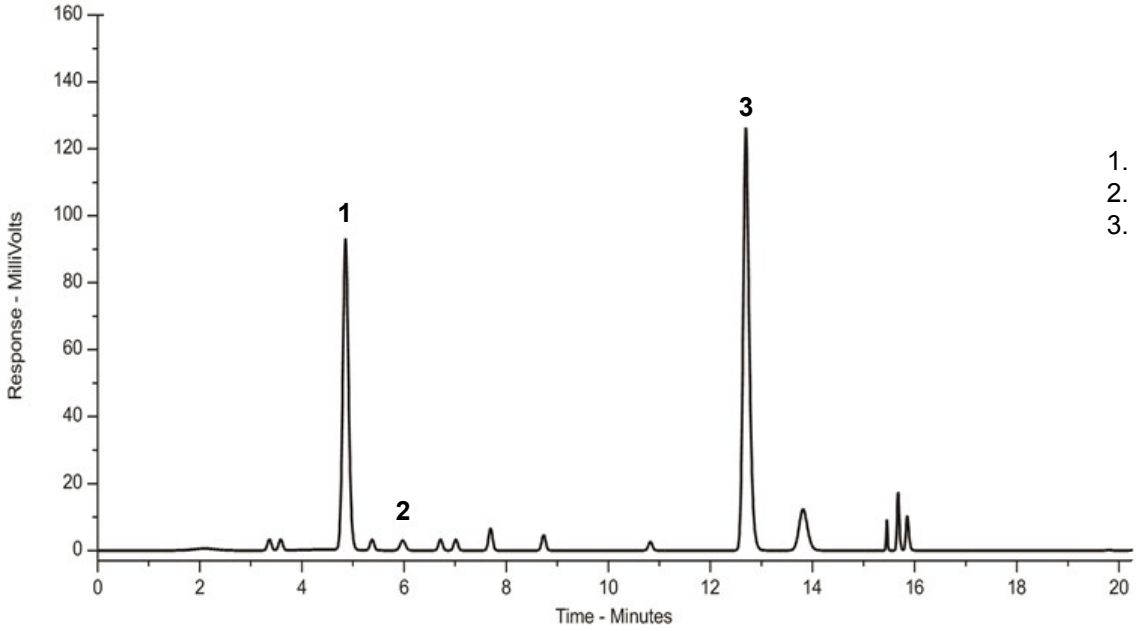
Application #**AN2920**

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	A: 0.1% H_3PO_4 in H_2O B: MeCN

Time (mins)	%B
0	10
13	22
14	40

Flow Rate:	1.5 mL/min
Injection:	10 µL
Temperature:	35 °C
Detection:	UV, 330 nm



1. Caftaric acid
2. Chlorogenic acid
3. Cichoric acid

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LC-MS/MS of Phytoestrogens from Hop Extract

ACE® Ultra-inert UHPLC & HPLC Columns

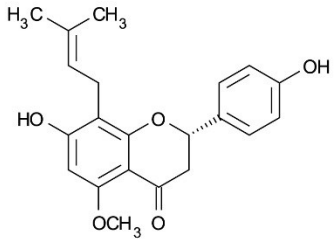
Application #**AN1160**

Conditions

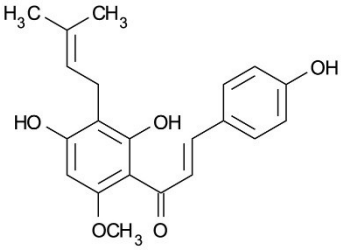
Column: ACE 3 C18-AR
Dimensions: 150 x 4.6 mm
Part Number: ACE-119-1546
Mobile Phase: A: 1% formic acid in MeCN
B: 1% formic acid in MeOH
C: 1% formic acid in H_2O
D: MeOH

Time (mins)	%A	%B	%C	%D
0	56	0	44	0
8	51	5	44	0
10	51	5	44	0
17	95	5	0	0
22	95	0	0	5

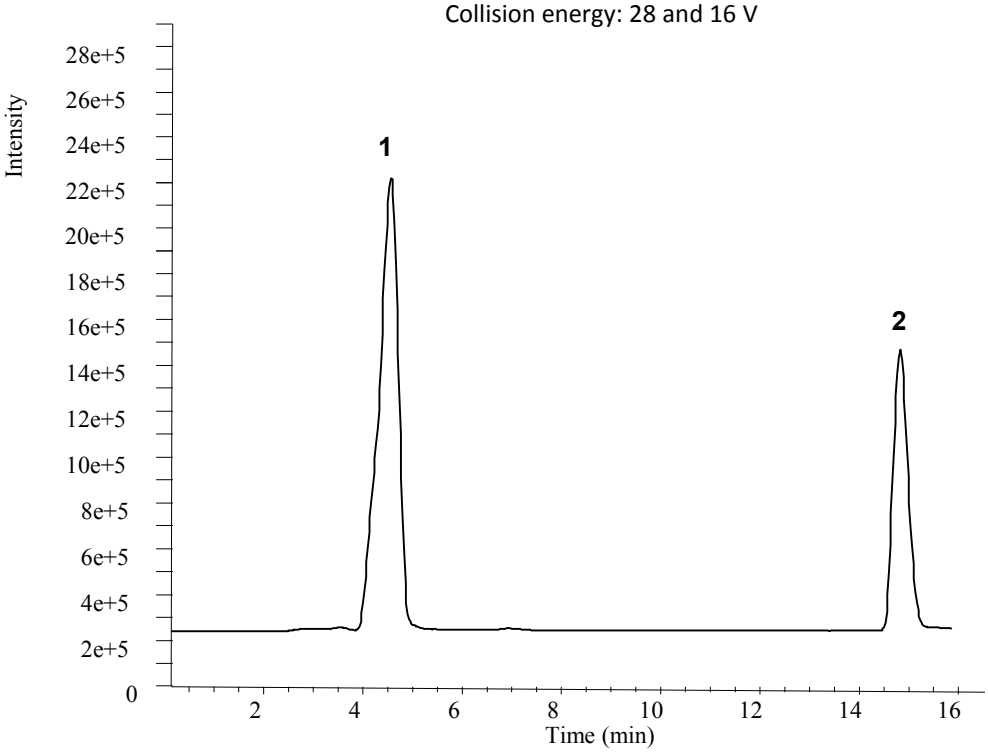
Flow Rate: 0.6 mL/min
Detection: TSQ-Quantum triple quad ESI
Spray voltage: -4500 V
Precursor ion: 355.4 $[M+H]^+$
MRM transition ions: 179 and 299
Collision energy: 28 and 16 V



1. Isoxanthohumol
LOQ 0.07 µg/mL



2. Xanthohumol
LOQ 0.01 µg/mL



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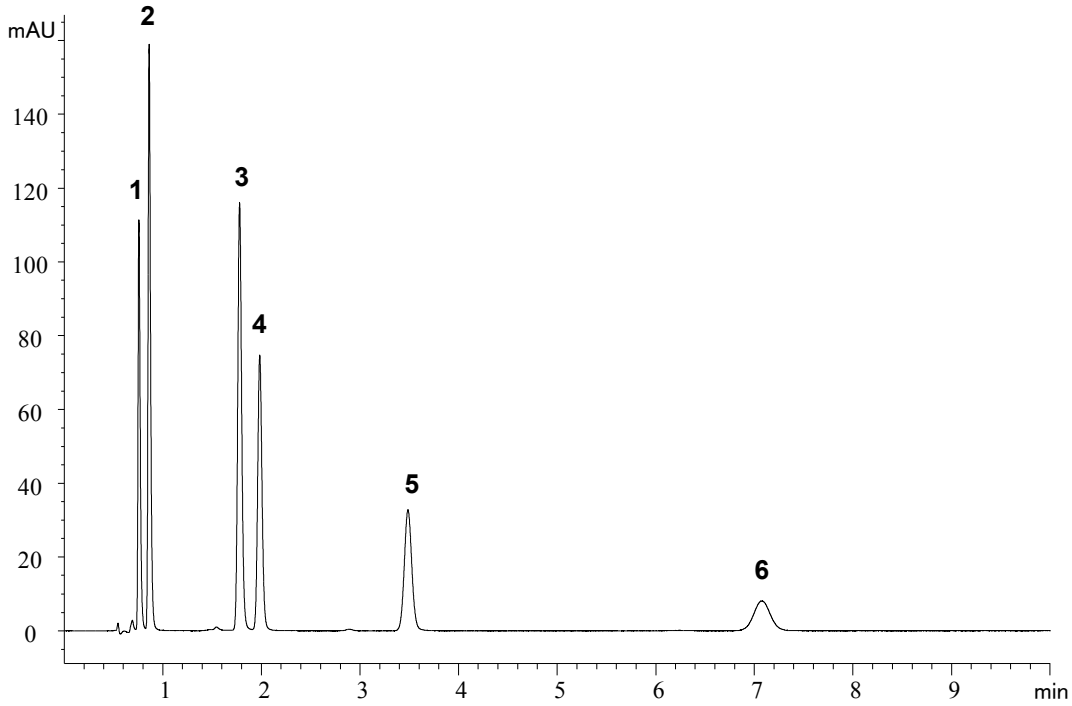
Separation of Preservatives

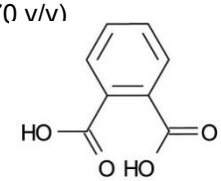
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2230**

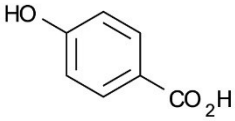
Conditions

Column:	ACE Excel 1.7 C18
Dimensions:	50 x 3.0 mm
Part Number:	EXL-171-0503U
Mobile Phase:	20 mM potassium phosphate pH 2.5 in MeCN/H_2O (30:70 v/v)
Flow Rate:	0.43 mL/min
Injection:	0.7 µL
Temperature:	20 °C
Detection:	UV, 230 nm

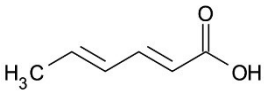




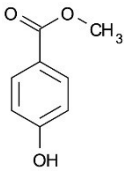
1. Phthalic acid



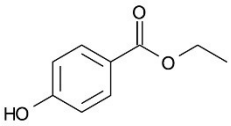
2. 4-Hydroxybenzoic acid



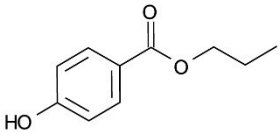
3. Sorbic acid



4. Methyl paraben



5. Ethyl paraben



6. Propyl paraben

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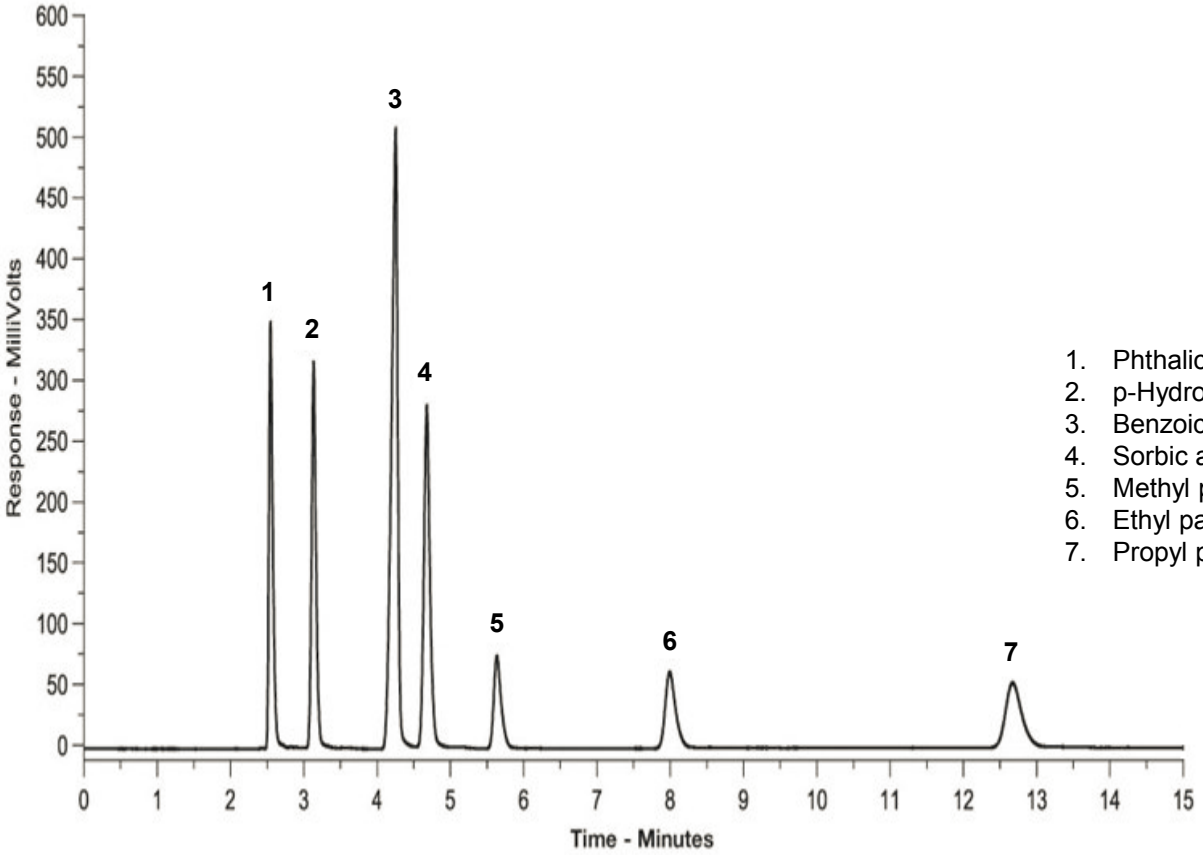
Separation of Seven Preservatives

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN3040**

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	MeCN/50 mM KH_2PO_4 pH 4.4 in H_2O (40:60 v/v)
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 230 nm



1. Phthalic acid
2. p-Hydroxybenzoic acid
3. Benzoic acid
4. Sorbic acid
5. Methyl paraben
6. Ethyl paraben
7. Propyl paraben

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Sennosides in Traditional Chinese Medicine

ACE®
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UHPLC & HPLC Columns

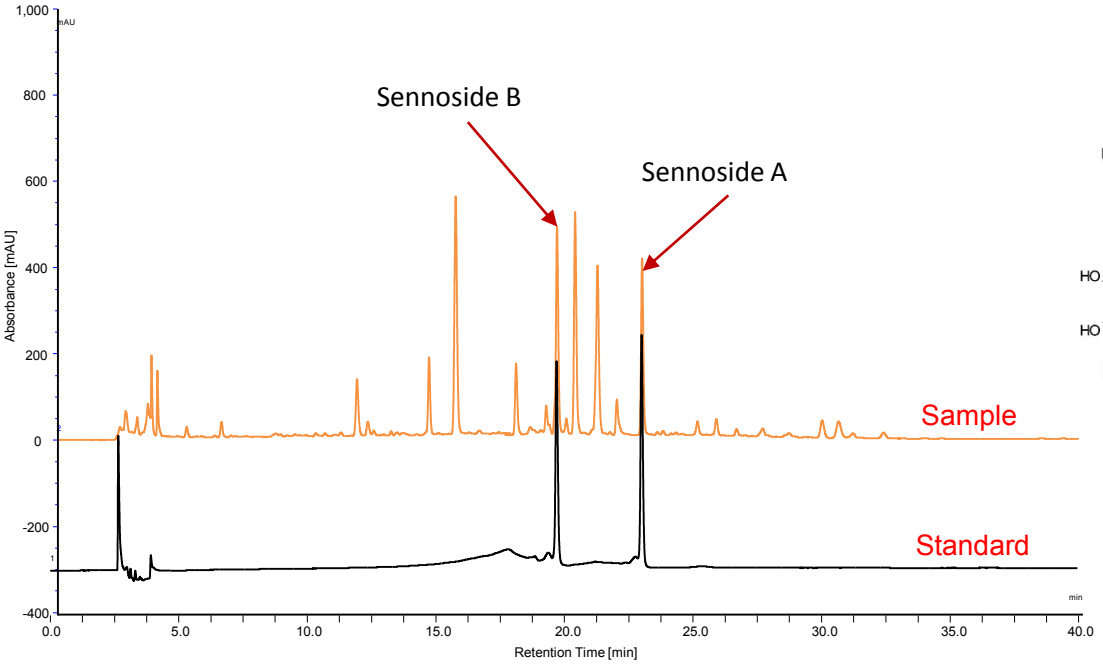
Application #AN1390

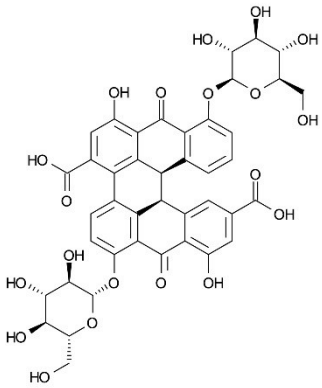
Conditions

Column:	ACE 3 C18-PFP
Dimensions:	150 x 4.6 mm
Part Number:	ACE-1110-1546
Mobile Phase:	A: 0.75% acetic acid in H_2O B: MeCN/MeOH (90:10 v/v)

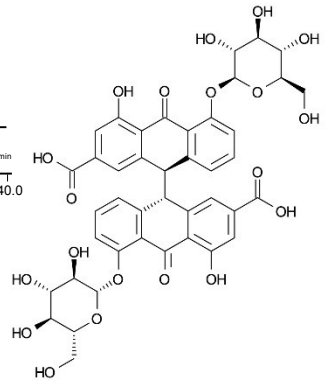
Time (mins)	%B
0	9
23	28
40	28

Flow Rate:	0.6 mL/min
Temperature:	35 °C
Detection:	UV, 271 nm
Sample:	Herbal tea bag containing Folium Sennae, Peppermint, Folium Mori, Folium Nelumbinis, Glycyrrhiza Uralensis and Lelang Grass Rhizome





Sennoside A



Sennoside B

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Illegal Dyes in Spices

ACE®
Ultra-inert
UHPLC & HPLC Columns

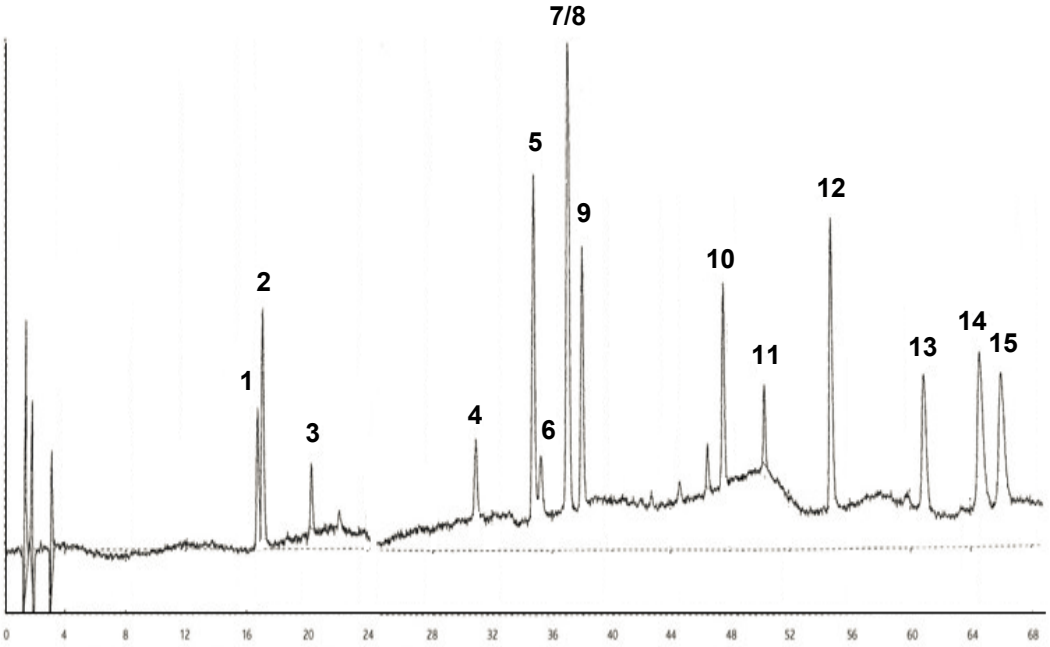
Application #**AN2910**

Conditions

Column: ACE 3 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-111-1046
Mobile Phase: A: H_2O
B: MeOH
C: 0.06 M Tetrabutylammonium bromide and 0.5 M KH_2PO_4 in H_2O pH 2.55

Time (mins)	%A	%B	%C
0	45	50	5
45	3	92	5
65	3	92	5
66	45	50	5
75	45	50	5

Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: Ambient
Detection: UV-Vis, 420 nm, 520 nm and 600 nm



1. Rhodamine B
2. Orange II
3. Metanil Yellow
4. Butter Yellow
5. Para Red
6. Sudan Orange G
7. Toluidine Red
8. Sudan I
9. Sudan Red G
10. Sudan II
11. Sudan Black
12. Sudan III
13. Sudan Red 7B
14. Sudan Red B
15. Sudan IV

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Separation of Sulfonamides

ACE® Ultra-inert UHPLC & HPLC Columns

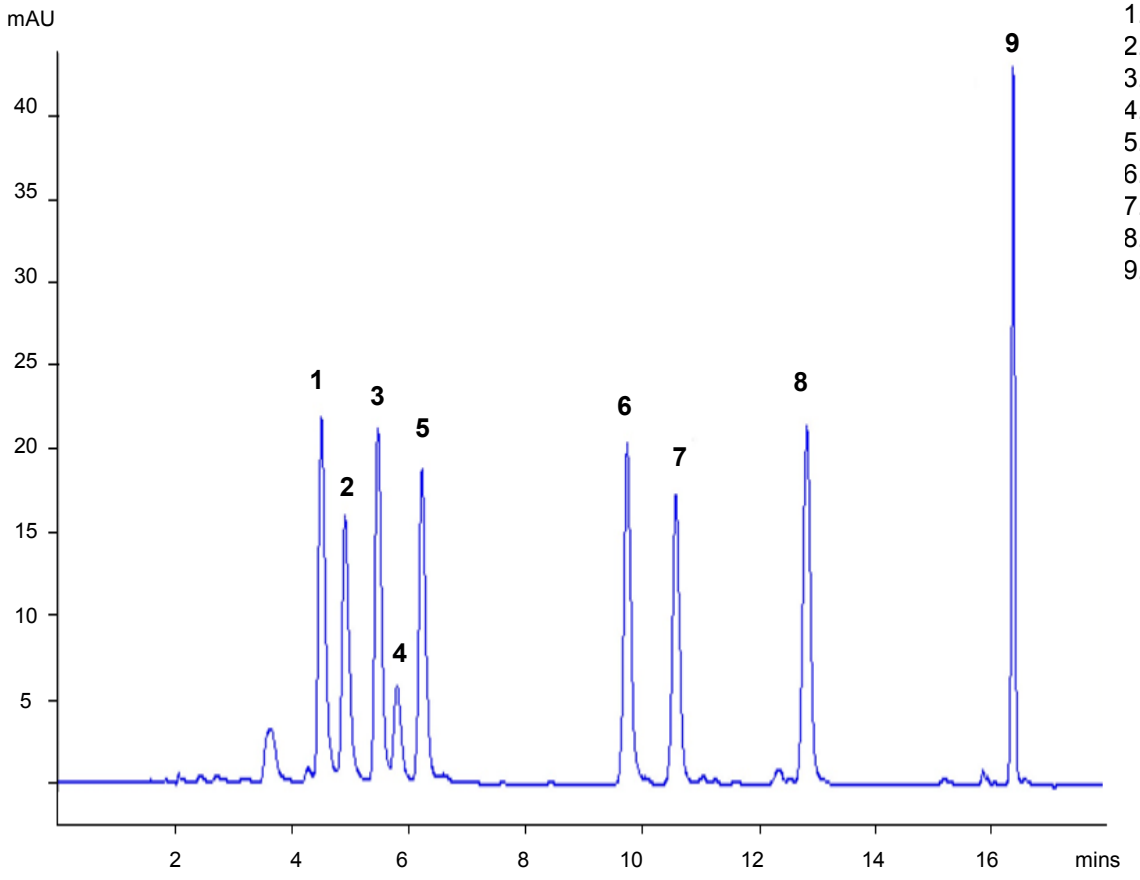
Application #**AN1610**

Conditions

Column: ACE Excel 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: EXL-1110-1546U
Mobile Phase: A: H_2O
B: MeCN
C: 10% formic acid

Time (mins)	%A	%B	%C
0	84	15	1
12	74	25	1
14	59	40	1
16	84	15	1
18	84	15	1

Flow Rate: 1 mL/min
Detection: UV, 268 nm



1. Sulfadiazine
2. Sulfapyridine
3. Sulfamerazine
4. Sulfamoxole
5. Sulfamethazine
6. Sulfamonomethoxine
7. Sulfachloropyridazine
8. Sulfamethoxazole
9. Sulfadimethoxine

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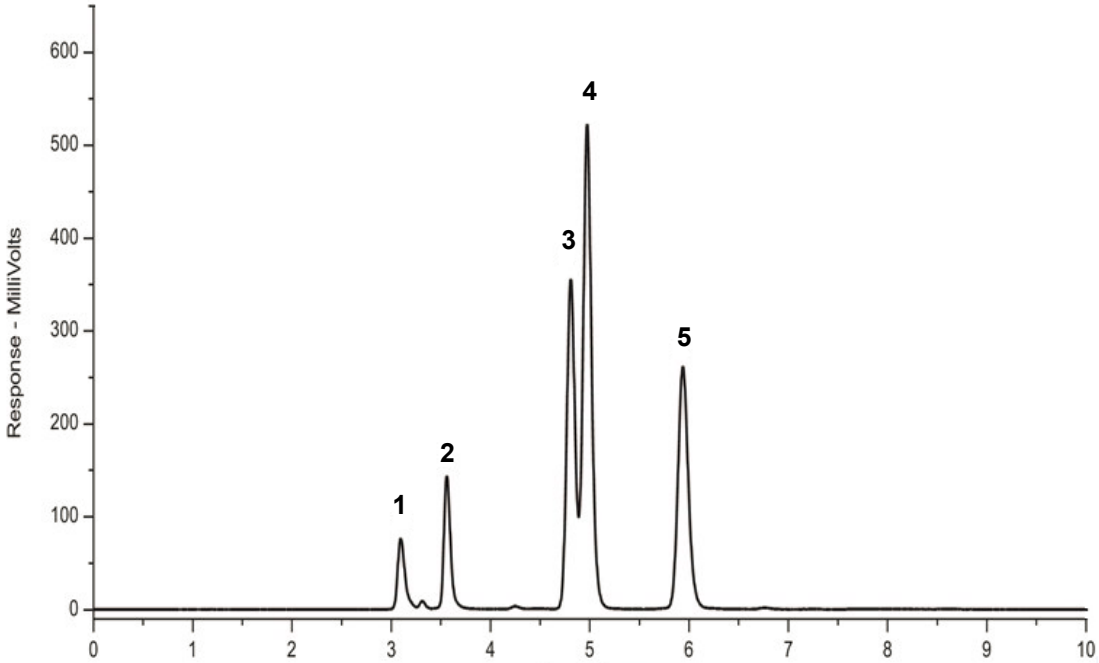
Separation of Tocopherols

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2790**

Conditions

Column:	ACE 5 SIL
Dimensions:	250 x 4.6 mm
Part Number:	ACE-127-2546
Mobile Phase:	Hexane/IPA (98:2 v/v)
Flow Rate:	1 mL/min
Injection:	1 µL
Temperature:	Ambient
Detection:	UV-Vis, 450 nm



1. γ-Tocopherol
2. α-Tocopherol
3. β-Tocopherol
4. β-Tocopherol
5. δ-Tocopherol

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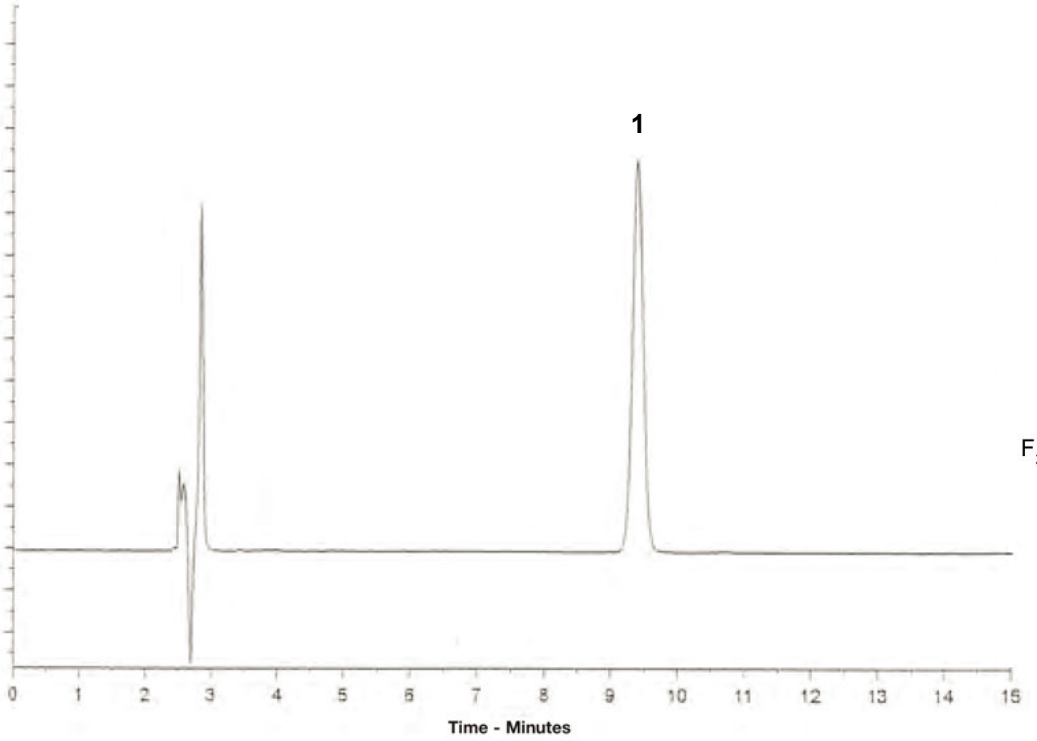
Detection of the Herbicide Trifluralin

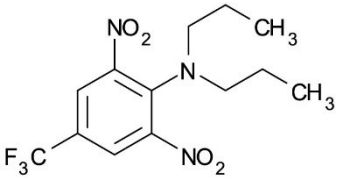
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2890**

Conditions

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





1. Trifluralin

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BSA Tryptic Digest Profiling

ACE®
Ultra-inert
UHPLC & HPLC Columns

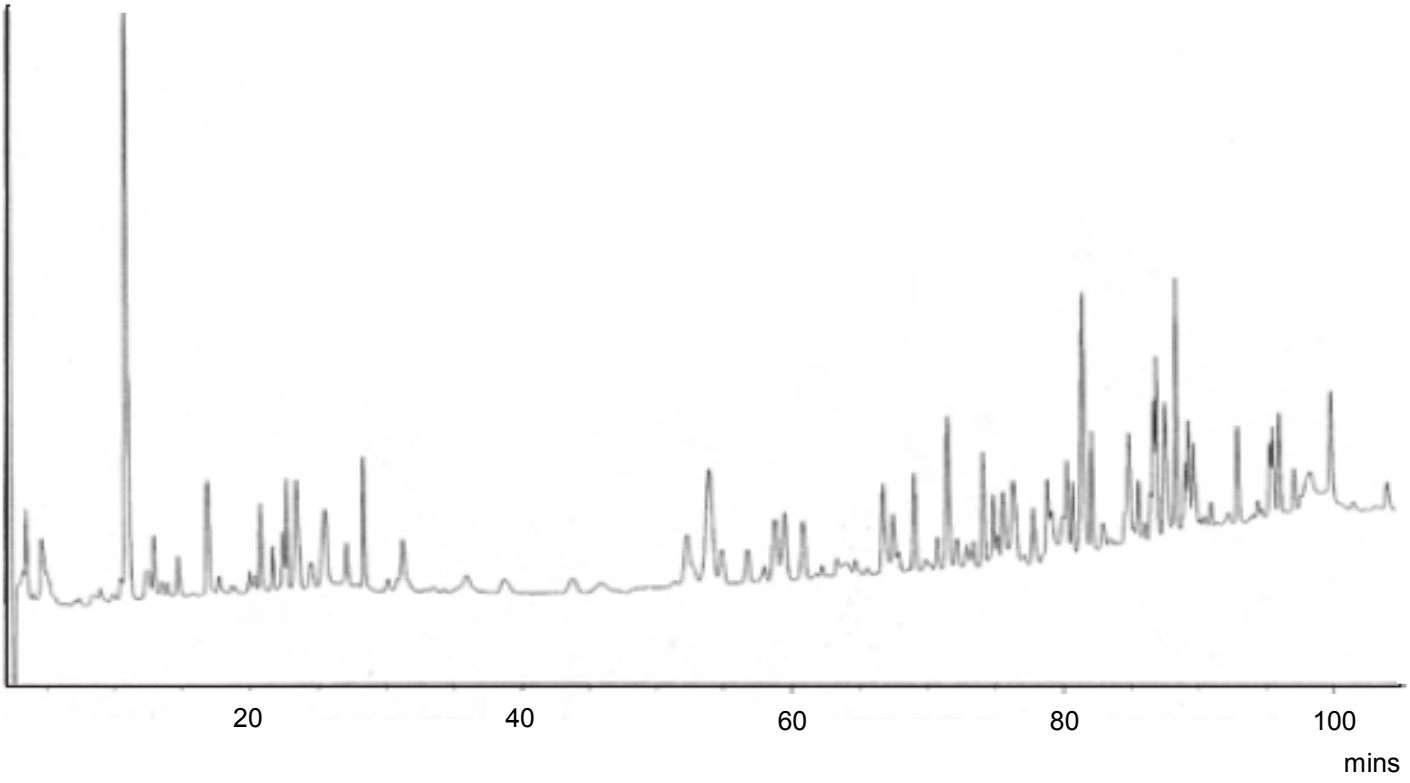
Application #**AN2000**

Conditions

Column: ACE 5 C18-300
Dimensions: 150 x 4.6 mm
Part Number: ACE-221-1546
Mobile Phase: A: 1% TFA in H_2O
B: 1% TFA in MeCN/H_2O (1:1 v/v)

Time (mins)	%B
0	4
5	4
25	20
45	20
75	40
95	65
115	70
120	4

Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 214 nm



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Separation of Vanillins

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1620**

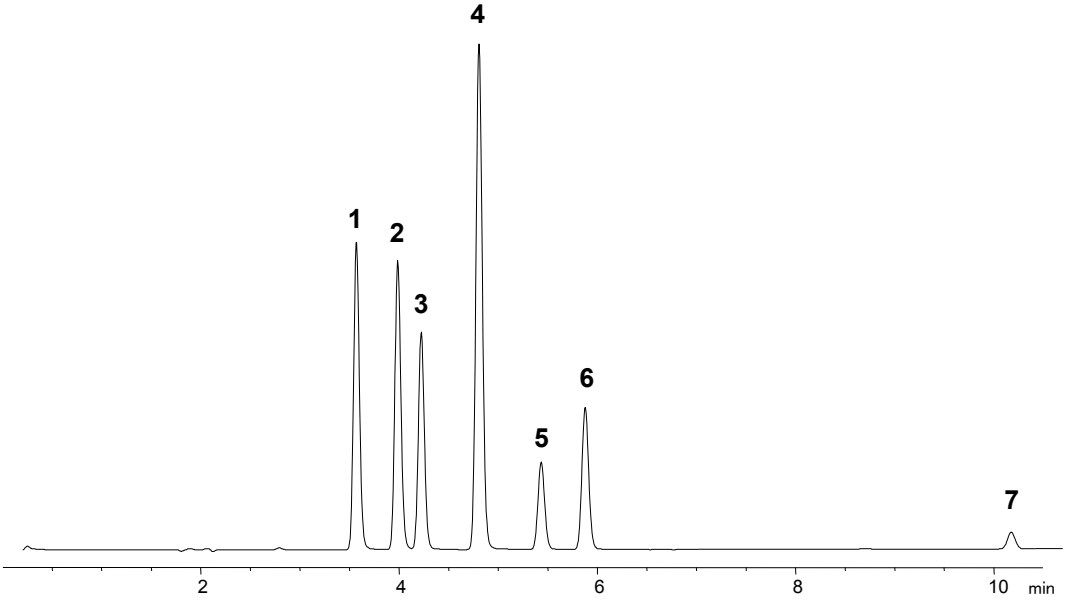
Conditions

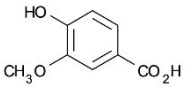
Column:	ACE 3 C18-Amide
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1112-1546U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

Time (mins)	%B
0.0	30
10.0	55
10.5	55
15.0	30

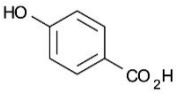
Post time 5 minutes

Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	40 °C
Detection:	UV, 260 nm

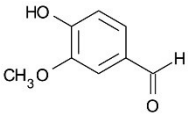




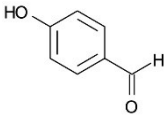
1. Vanillic acid



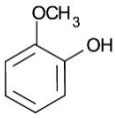
2. 4-Hydroxybenzoic acid



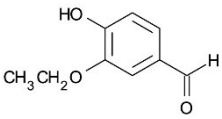
3. Vanillin



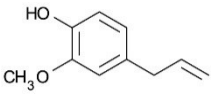
4. 4-Hydroxybenzaldehyde



5. Guaiacol



6. Ethyl Vanillin



7.Eugenol

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Fast Separation of Vanillin Compounds

ACE®
Ultra-inert
UHPLC & HPLC Columns

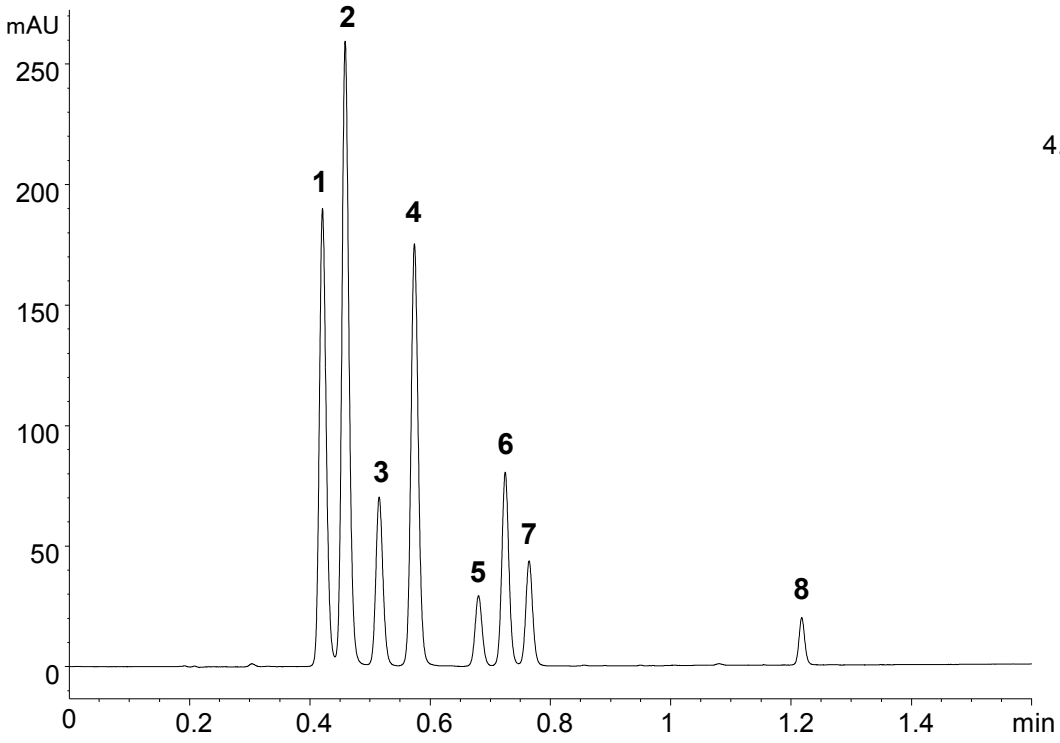
Application #**AN2240**

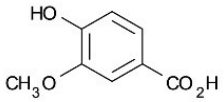
Conditions

Column:	ACE Excel 1.7 C18-Amide
Dimensions:	50 x 3.0 mm
Part Number:	EXL-1712-0503U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

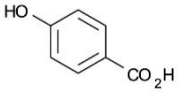
Time (mins)	%B
0.00	25
1.32	75
1.49	75
1.60	25

Flow Rate:	1.3 mL/min
Injection:	1 µL
Temperature:	45 °C
Detection:	UV, 260 nm

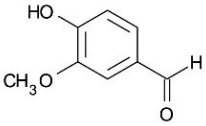




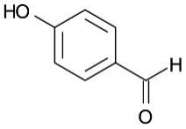
1. Vanillic acid



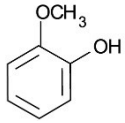
2. 4-Hydroxybenzoic acid



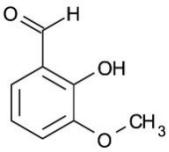
3. Vanillin



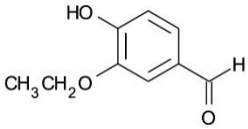
4. 4-Hydroxybenzaldehyde



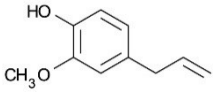
5. Guaiacol



6. o-Vanillin



7. Ethyl vanillin



8. Eugenol

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Veterinary Steroids by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

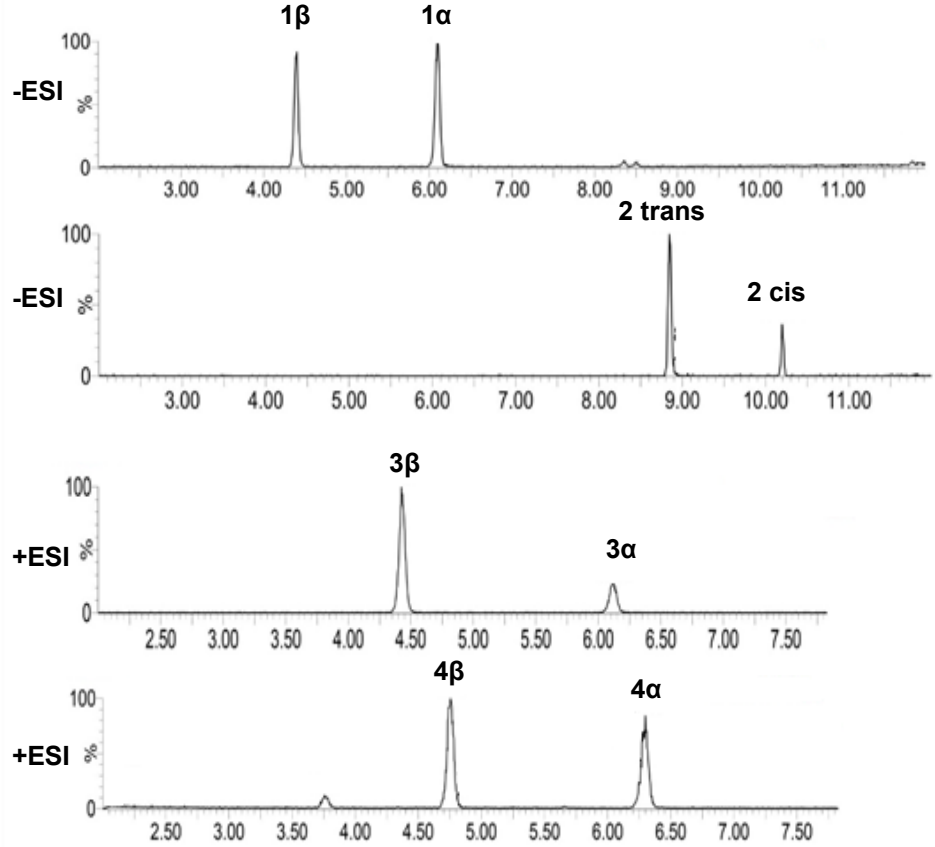
Application #**AN1830**

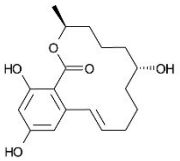
Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 2.1 mm
Part Number: CORE-25A-1002U
Mobile Phase: A: 0.01 mM ammonium fluoride + 0.001% formic acid
B: MeCN

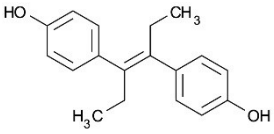
Time (mins)	%B
0.0	25
0.5	25
7.0	35
7.5	35
10.5	60
12.5	90

Flow Rate: 0.5 mL/min
Temperature: 45 °C
Detection: Positive or negative ESI
MRM data



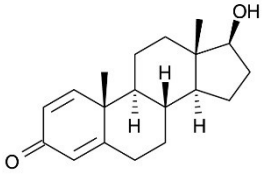


1. α- and β-Zearalenol (*m/z* 319.17 → 275.12)

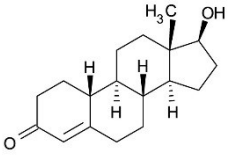


2. Diethylstilbestrol-d8 (*m/z* 275.23 → 245.09)

Also analysed in -ESI:
- Taleranol and zeranol-d4
- Taleranol and zeranol
- Zearalenone
- Hexestrol
- Diethylstilbestrol
- Dienesterol



3. α- and β-Boldenone (*m/z* 287.17 → 121.12)



4. α- and β-Nortestosterone (*m/z* 275.23 → 109.09)

Also analysed in +ESI:
- Hydroxystanozolol
- Hydroxystanozolol-d3
- Methyltestosterone
- Methyltestosterone-d3
- β-Nortestosterone-d3
- β-Trenbolone
- α-Trenbolone

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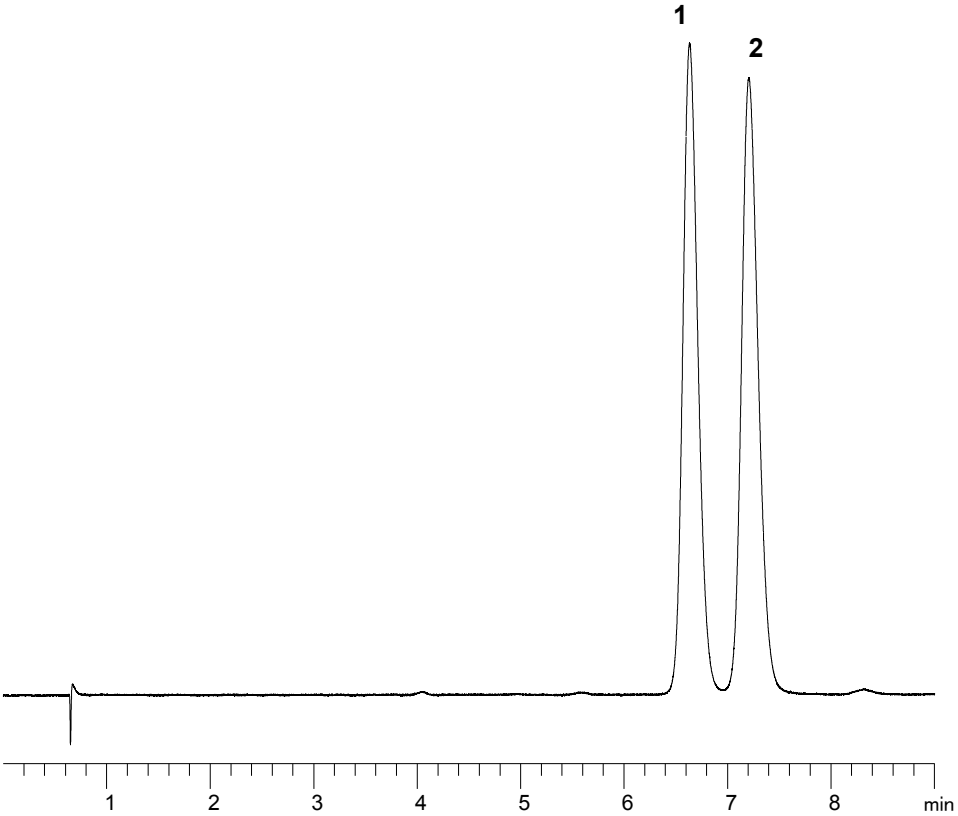
Vitamin D2/D3

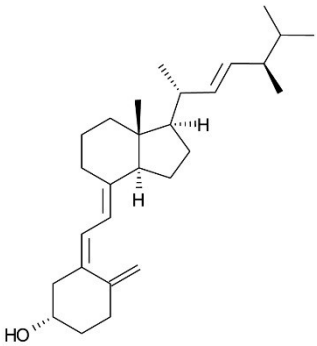
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1840**

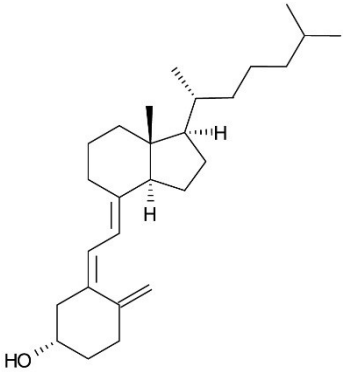
Conditions

Column:	ACE Excel 2 C18-Amide
Dimensions:	50 x 3.0 mm
Part Number:	EXL-1012-0503U
Mobile Phase:	100% MeCN
Flow Rate:	0.43 mL/min
Injection:	2 µL
Temperature:	20 °C
Detection:	UV, 265 nm





1. Ergocalciferol (D2)



2. Cholecalciferol (D3)

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25-Hydroxy Vitamin D in Serum by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

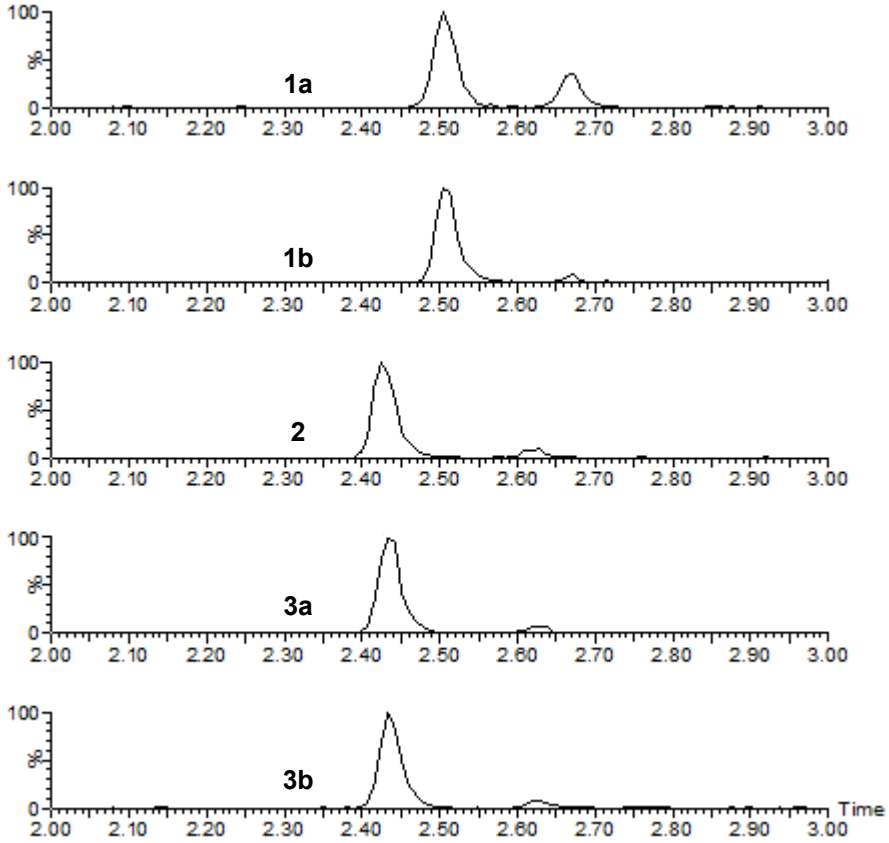
Application #**AN2390**

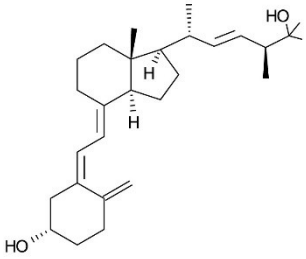
Conditions

Column:	ACE Excel 2 C18-PFP
Dimensions:	100 x 2.1 mm
Part Number:	EXL-1010-1002U
Mobile Phase:	A: 2 mM ammonium acetate, 0.1% formic acid in H_2O B: 0.1% formic acid in MeOH

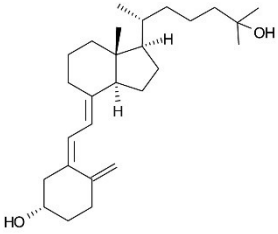
Time (mins)	%B
0.0	75
3.0	100
4.0	100

Flow Rate:	0.4 mL/min
Injection:	15 µL
Temperature:	40 °C
Detection:	Quattro Premier XE triple quad MS MRM positive ESI mode Desolvation temperature: 450 °C Ion source temperature: 150 °C





1a. 25-OH Vitamin D2 (*m/z* 395.5 → 269.5)
1b. 25-OH Vitamin D2 (*m/z* 395.5 → 119.2)
2. d6-25-OH Vitamin D3 (IS) (*m/z* 389.6 → 263.5)



3a. 25-OH Vitamin D3 (*m/z* 383.5 → 257.5)
3b. 25-OH Vitamin D3 (*m/z* 383.5 → 107.2)

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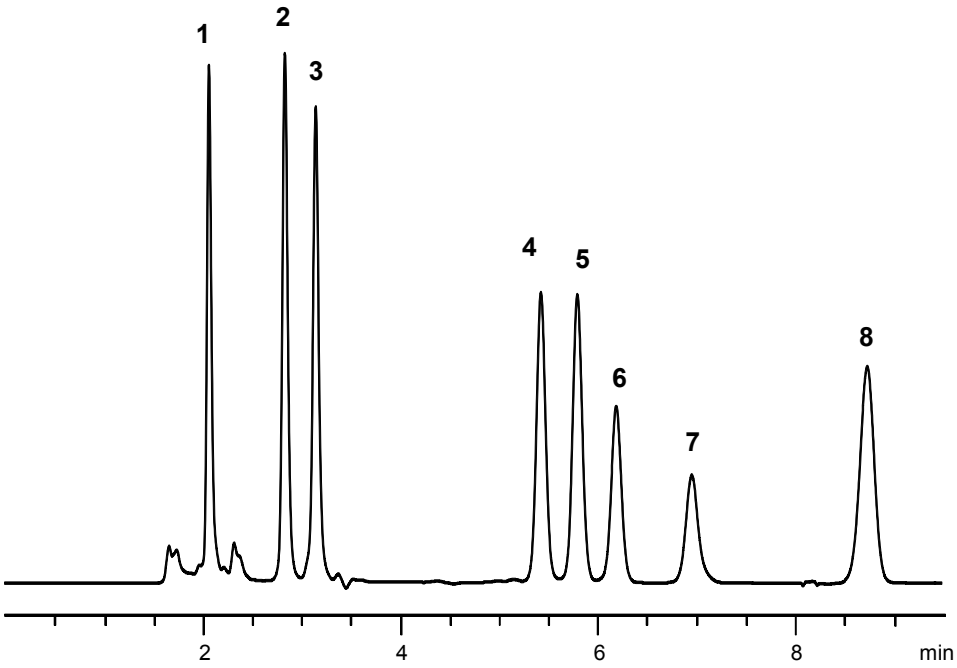
Separation of Fat Soluble Vitamins

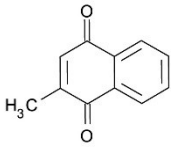
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN2420

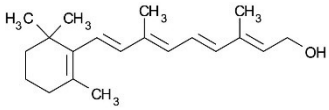
Conditions

Column:	ACE 3 C18-Amide
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1112-1546U
Mobile Phase:	MeOH/MeCN (90:10 v/v)
Flow Rate:	1 mL/min
Temperature:	20 °C
Detection:	UV, 280 nm

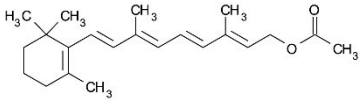




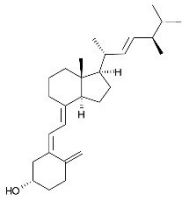
1. Menadione (Vitamin K3)



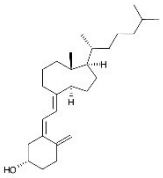
2. Retinol (Vitamin A)



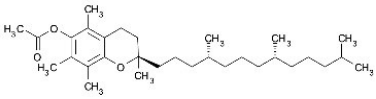
3. Vitamin A acetate



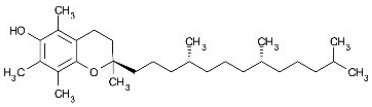
4. Ergocalciferol (Vitamin D2)



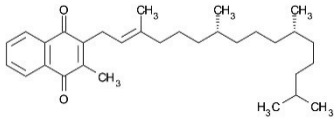
5. Cholecalciferol (Vitamin D3)



6. Vitamin E acetate



7. α-Tocopherol (Vitamin E)



8. Vitamin K1

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Fast LC-MS Analysis of Multivitamin Fruit Juice

ACE® Ultra-inert UHPLC & HPLC Columns

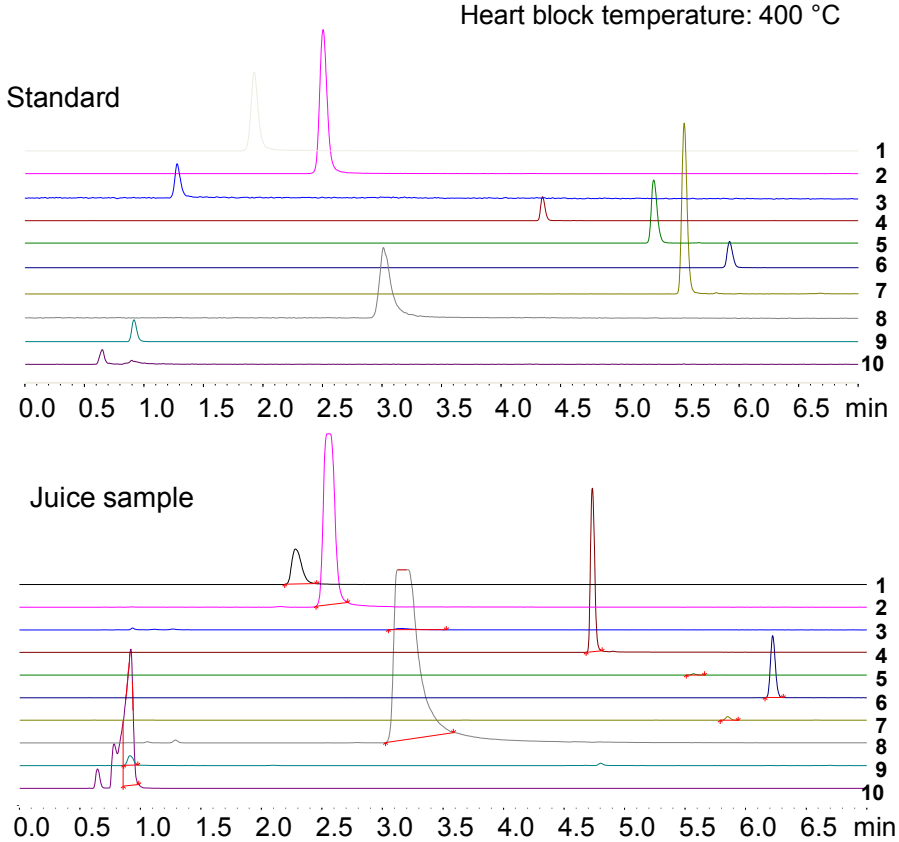
Application #AN2610

Conditions

Column: ACE Excel 3 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1110-1002U
Mobile Phase: A: 15 mM formic acid, adjusted to pH 3.8 with ammonia solution
B: MeOH

Time (mins)	%B
0.00	1
1.00	1
3.00	8
3.10	25
6.00	50
6.50	50
6.51	1
9.00	1

Flow Rate: 0.4 mL/min
Temperature: 30 °C
Detection: LCMS-8040 triple quad MS
ESI positive mode (ESI negative for ascorbic and citric acid)
DL temperature: 250 °C
Heart block temperature: 400 °C



1. Thiamine (Vitamin B1) (*m/z* 266.10 →122.15)
2. Pyridoxine (Vitamin B6) (*m/z* 170.20 →152.15)
3. Nicotinic acid (Vitamin B3) (*m/z* 124.00 →78.00)
4. Pantothenic acid (Vitamin B5) (*m/z* 220.30 →90.05)
5. Cyanocobalamin (Vitamin B12) (*m/z* 678.50→147.05)
6. Riboflavin (Vitamin B2) (*m/z* 377.20 →243.10)
7. Biotin (Vitamin B7) (*m/z* 245.10 →227.05)
8. Nicotinamide (Vitamin B3) (*m/z* 123.20 →80.05)
9. Ascorbic acid (Vitamin C) (*m/z* 175.10 →114.80)
10. Citric acid (*m/z* 191.10 →87.15)

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Separation of 14 Water Soluble Vitamins

ACE®
Ultra-inert
UHPLC & HPLC Columns

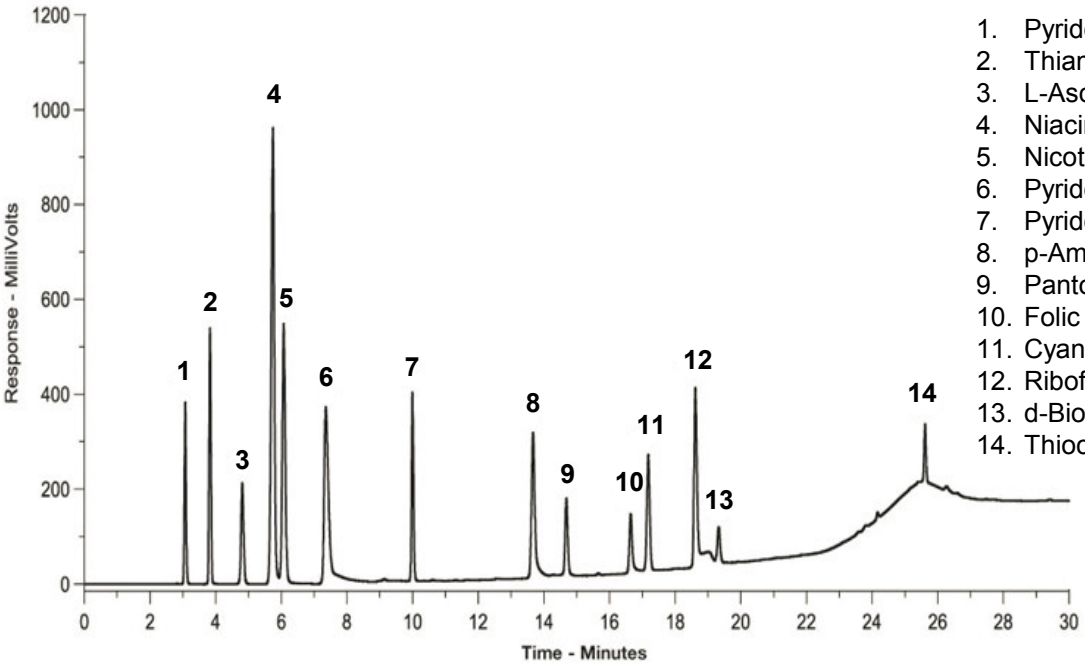
Application #**AN2940**

Conditions

Column:	ACE 5 C8
Dimensions:	250 x 4.6 mm
Part Number:	ACE-122-2546
Mobile Phase:	A: 50 mM KH_2PO_4 pH 2.5 in H_2O B: MeOH

Time (mins)	%B
0.0	0
3.0	0
16.5	45
19.5	80

Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 205 nm



1. Pyridoxamine
2. Thiamine (Vitamin B1)
3. L-Ascorbic acid (Vitamin C)
4. Niacinamide (Vitamin B3)
5. Nicotinic acid
6. Pyridoxal
7. Pyridoxine
8. p-Aminobenzoic acid
9. Pantothenic acid (Vitamin B5)
10. Folic acid (Vitamin B9)
11. Cyanocobalamin (Vitamin B12)
12. Riboflavin (Vitamin B2)
13. d-Biotin (Vitamin B7)
14. Thioctic acid

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Separation of 13 Water Soluble Vitamins using a Gradient

ACE® Ultra-inert UHPLC & HPLC Columns

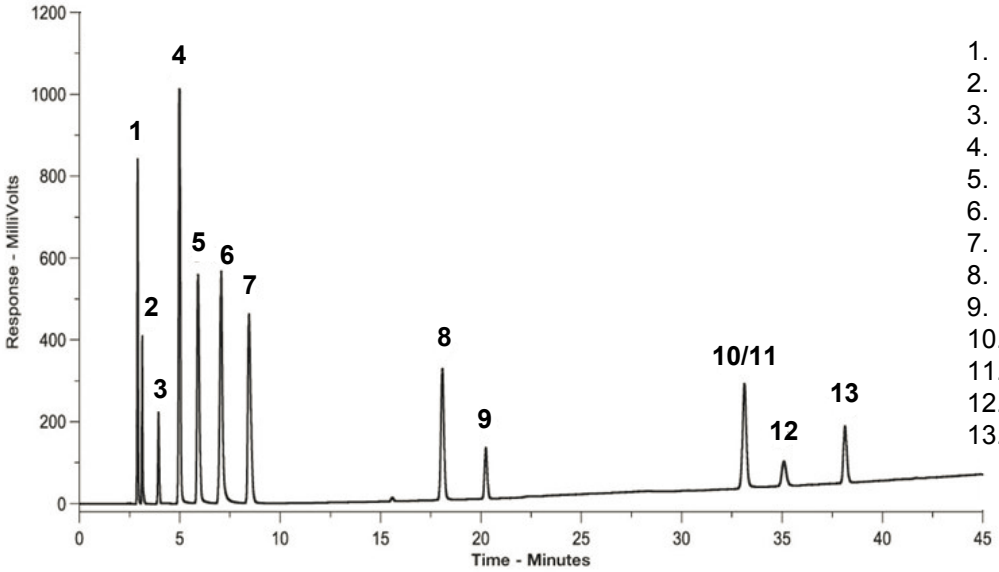
Application #AN2930

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 50 mM KH_2PO_4 pH 3.0 in H_2O
B: MeOH

Time (mins)	%B
0	3
5	3
45	45
50	80

Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 205 nm



1. Pyridoxamine
2. Thiamine (Vitamin B1)
3. L-Ascorbic acid (Vitamin C)
4. Nicotinic acid
5. Pyridoxal
6. Impurity
7. Pyridoxine
8. p-Aminobenzoic acid
9. Pantothenic acid (Vitamin B5)
10. Folic acid (Vitamin B9)
11. Cyanocobalamin (Vitamin B12)
12. d-Biotin (Vitamin B7)
13. Riboflavin (Vitamin B2)

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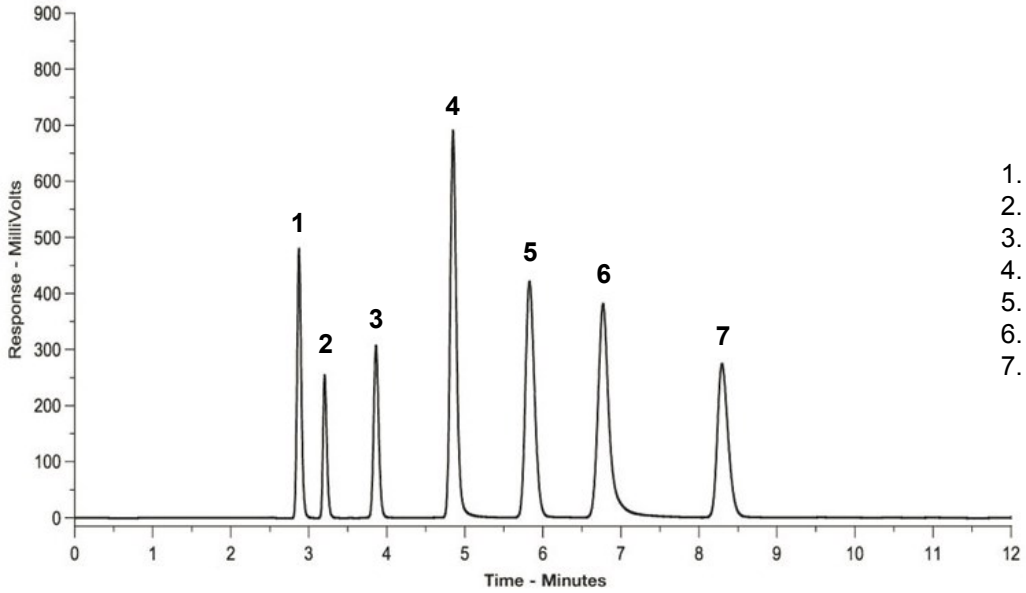
Separation of Seven Water Soluble Vitamins using Isocratic Conditions (I)

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2990**

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	50 mM KH_2PO_4 pH 3.0 in H_2O/MeOH (97:3 v/v)
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 205 nm



1. Pyridoxamine
2. Thiamine (Vitamin B1)
3. L-Ascorbic acid (Vitamin C)
4. Nicotinic acid
5. Pyridoxal
6. Impurity
7. Pyridoxine

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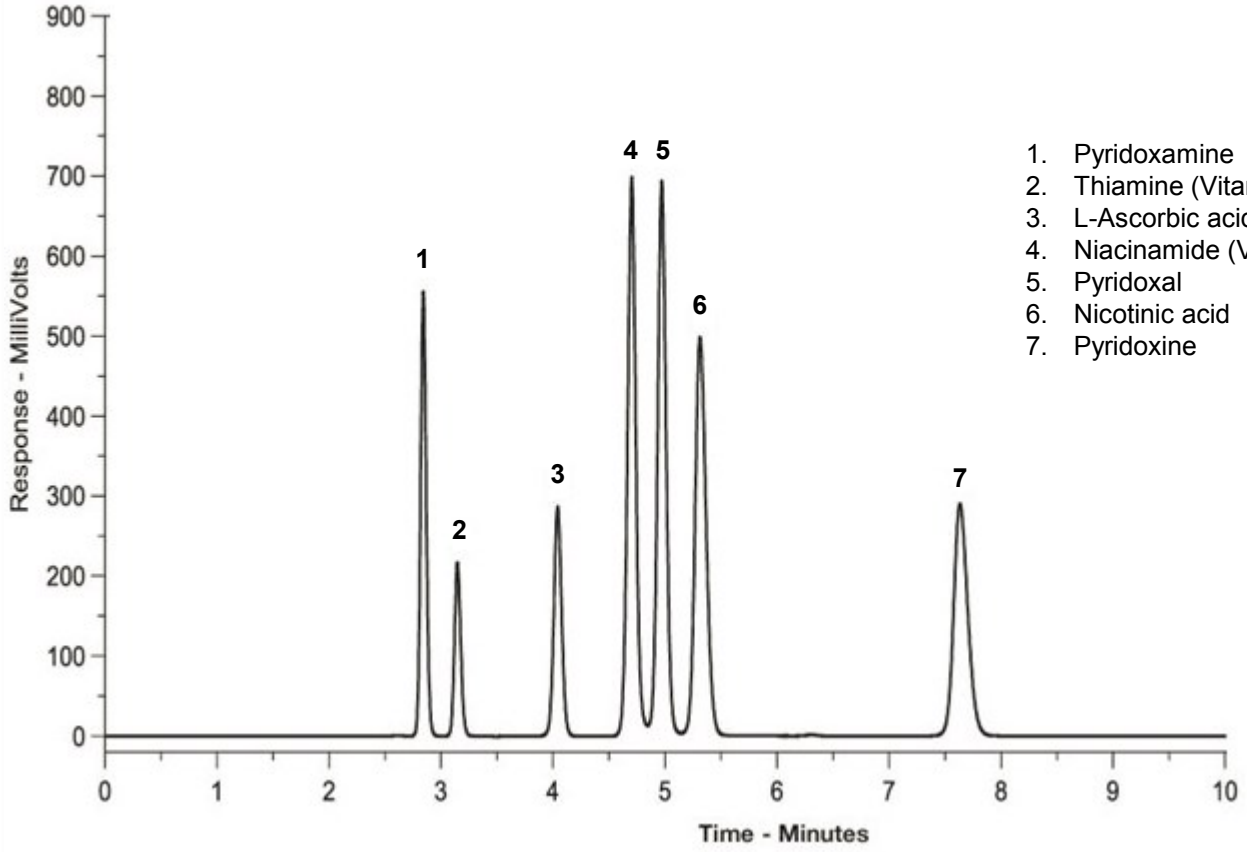
Separation of Seven Water Soluble Vitamins using Isocratic Conditions (II)

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2980**

Conditions

Column:	ACE 5 C8
Dimensions:	250 x 4.6 mm
Part Number:	ACE-122-2546
Mobile Phase:	50 mM KH_2PO_4 pH 2.5 in H_2O/MeOH (97:3 v/v)
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 205 nm



1. Pyridoxamine
2. Thiamine (Vitamin B1)
3. L-Ascorbic acid (Vitamin C)
4. Niacinamide (Vitamin B3)
5. Pyridoxal
6. Nicotinic acid
7. Pyridoxine

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Water Soluble Vitamins

ACE®
Ultra-inert
UHPLC & HPLC Columns

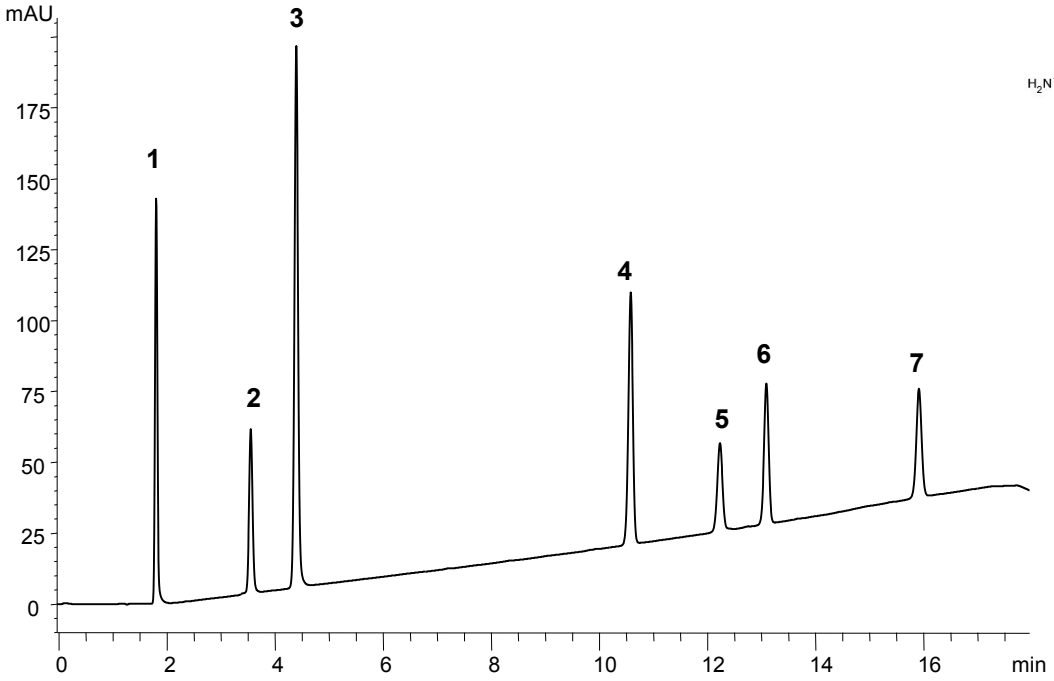
Application #AN1870

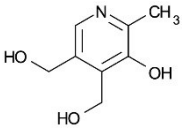
Conditions

Column:	ACE 3 C18-AR
Dimensions:	150 x 4.6 mm
Part Number:	ACE-119-1546
Mobile Phase:	A: 20 mM potassium phosphate pH 2.83 in H_2O B: 20 mM potassium phosphate pH 2.83 in MeOH/H_2O (50:50 v/v)

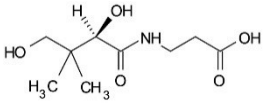
Time (mins)	%B
0	20
15	70

Flow Rate:	1.5 mL/min
Injection:	1 µL
Temperature:	40 °C
Detection:	UV, 205 nm

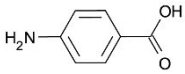




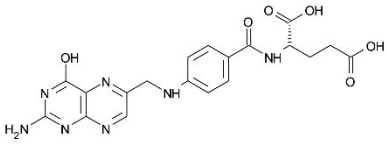
1. Pyridoxine (Vitamin B6)



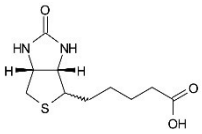
2. Pantothenic acid (Vitamin B5)



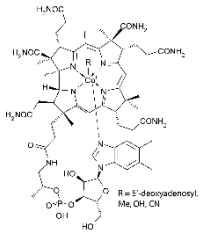
3. p-Aminobenzoic acid



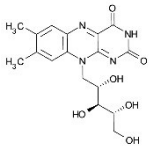
4. Folic acid (Vitamin B9/ Vitamin M)



5. D-Biotin (Vitamin B7/ Vitamin H)



6. Cyanocobalamin (Vitamin B12)



7. Riboflavin (Vitamin B2)

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Water Soluble Vitamins

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN1880

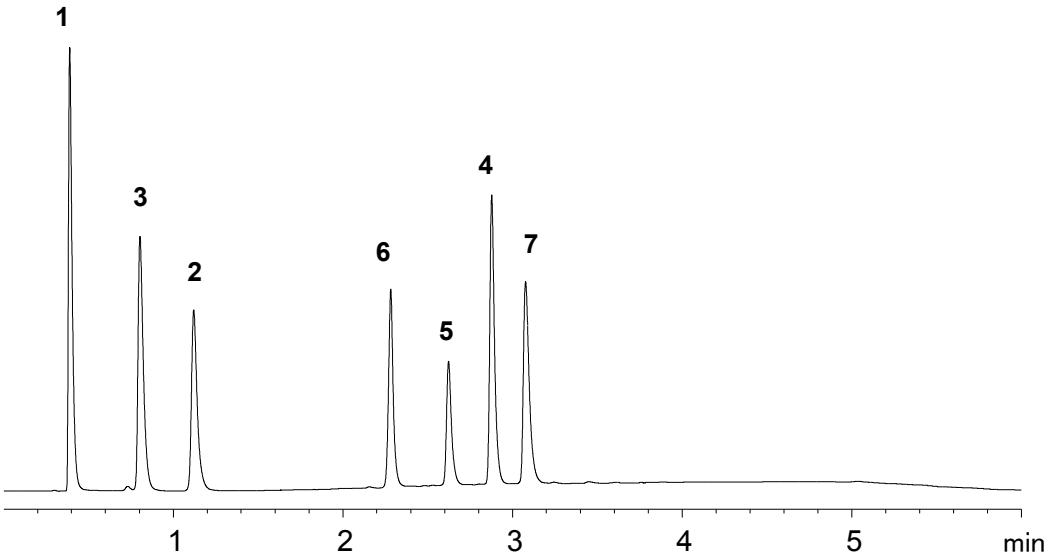
Conditions

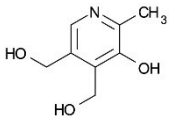
Column:	ACE Ultracore 2.5 SuperPhenylHexyl
Dimensions:	50 x 2.1 mm
Part Number:	CORE-25B-0502U
Mobile Phase:	A: 20 mM KH_2PO_4, pH 2.7
	B: 20 mM KH_2PO_4, pH 2.7 in MeOH/H_2O (50:50 v/v)

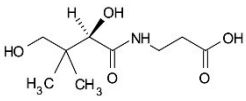
Time (mins)	%B
0.00	20
1.50	60
3.00	70
3.75	70
4.50	20

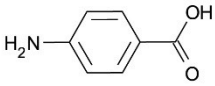
Post time 4.5 minutes

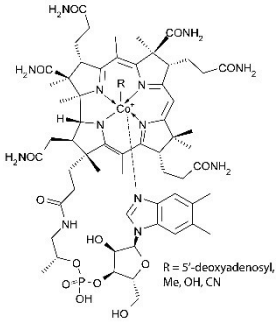
Flow Rate:	0.4 mL/min
Injection:	1 µL
Temperature:	40 °C
Detection:	UV, 205 and 254 nm



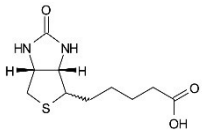

1. Pyridoxine

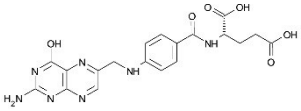

2. Pantothenic acid

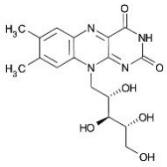

3. p-Aminobenzoic acid



4. Cyanocobalamin


5. d-Biotin


6. Folic acid


7. Riboflavin

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Water Soluble Vitamins in Green Vegetables by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

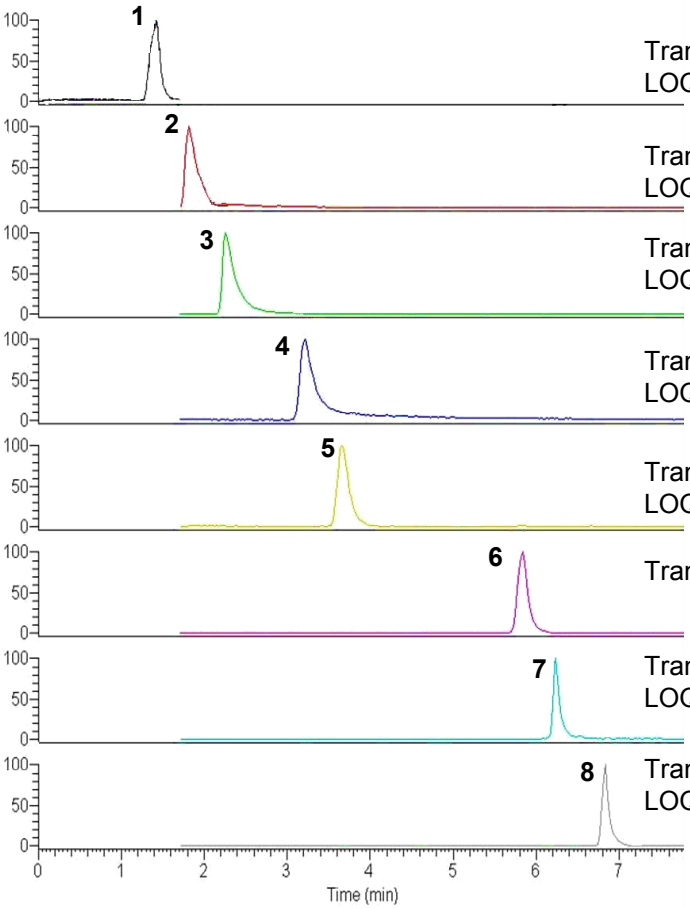
Application #AN1860

Conditions

Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002
Mobile Phase: A: 10 mM ammonium acetate in H_2O, pH 4.5
B: 0.1% acetic acid in MeOH
C: 0.3% acetic acid in MeOH

Time (mins)	%A	%B	%C
0	90	10	0
3	90	10	0
4	50	0	50
7	50	0	50
10	0	100	0

Flow Rate: 0.2 mL/min
Injection: 10 µL
Temperature: 20 °C
Detection: TSQ triple quad MS; SRM mode
-ESI for vitamin C
+ESI for B vitamins



Transition *m/z* 174.9 → 115.2
LOQ 128.1 ng/mL

Transition *m/z* 265.1 → 122.1
LOQ 2.4 ng/mL

Transition *m/z* 169.9 → 152.1
LOQ 0.6 ng/mL

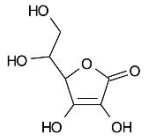
Transition *m/z* 123.0 → 80.3
LOQ 13.2 ng/mL

Transition *m/z* 220.0 → 202.1
LOQ 23.3 ng/mL

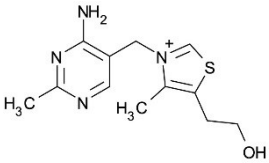
Transition *m/z* 180.1 → 105.2

Transition *m/z* 442.0 → 294.9
LOQ 1.9 ng/mL

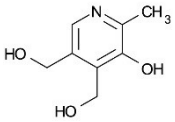
Transition *m/z* 377.1 → 243.0
LOQ 0.2 ng/mL



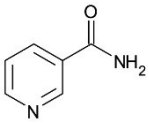
1. Ascorbic acid



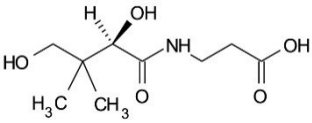
2. Thiamine



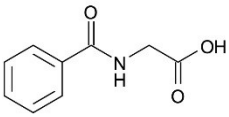
3. Pyridoxine



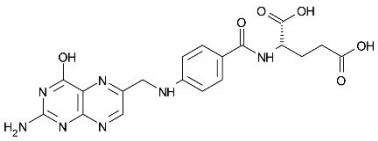
4. Nicotinamide



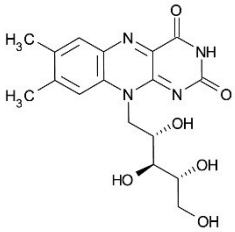
5. Pantothenic acid



6. Hippuric acid (IS)



7. Folic acid



8. Riboflavin

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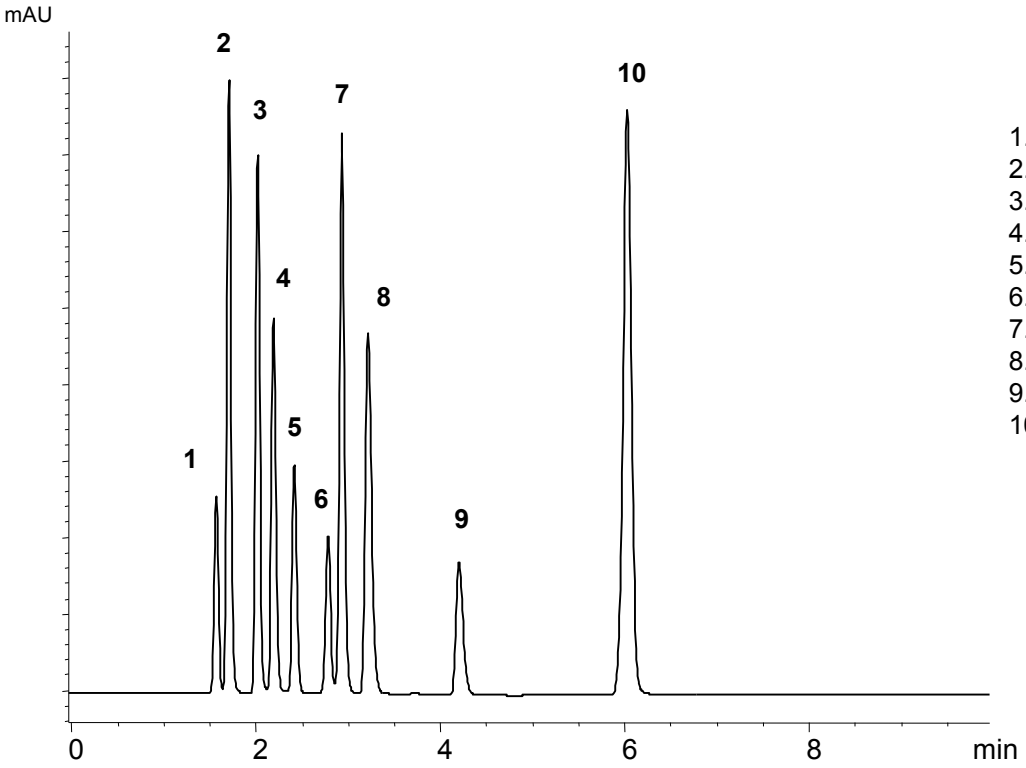
Water Soluble Vitamins and Polar Molecules

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1850**

Conditions

Column:	ACE 3 C18-AR
Dimensions:	150 x 4.6 mm
Part Number:	ACE-119-1546
Mobile Phase:	0.1 % phosphoric acid in H_2O/MeOH (96.5:3.5 v/v)
Flow Rate:	1 mL/min
Injection:	2 µL
Temperature:	22 °C
Detection:	UV, 260 nm



1. Pyridoxamine (Vitamin B6)
2. Thiamine (Vitamin B1)
3. Isonicotinamide
4. Nicotinamide
5. L-Ascorbic acid (Vitamin C)
6. Orotic Acid
7. Hypoxanthine
8. Pyridoxal (Vitamin B6)
9. Pyridoxine (Vitamin B6)
10. p-Aminobenzoic acid

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Whey Proteins from Whole Milk

ACE®
Ultra-inert
UHPLC & HPLC Columns

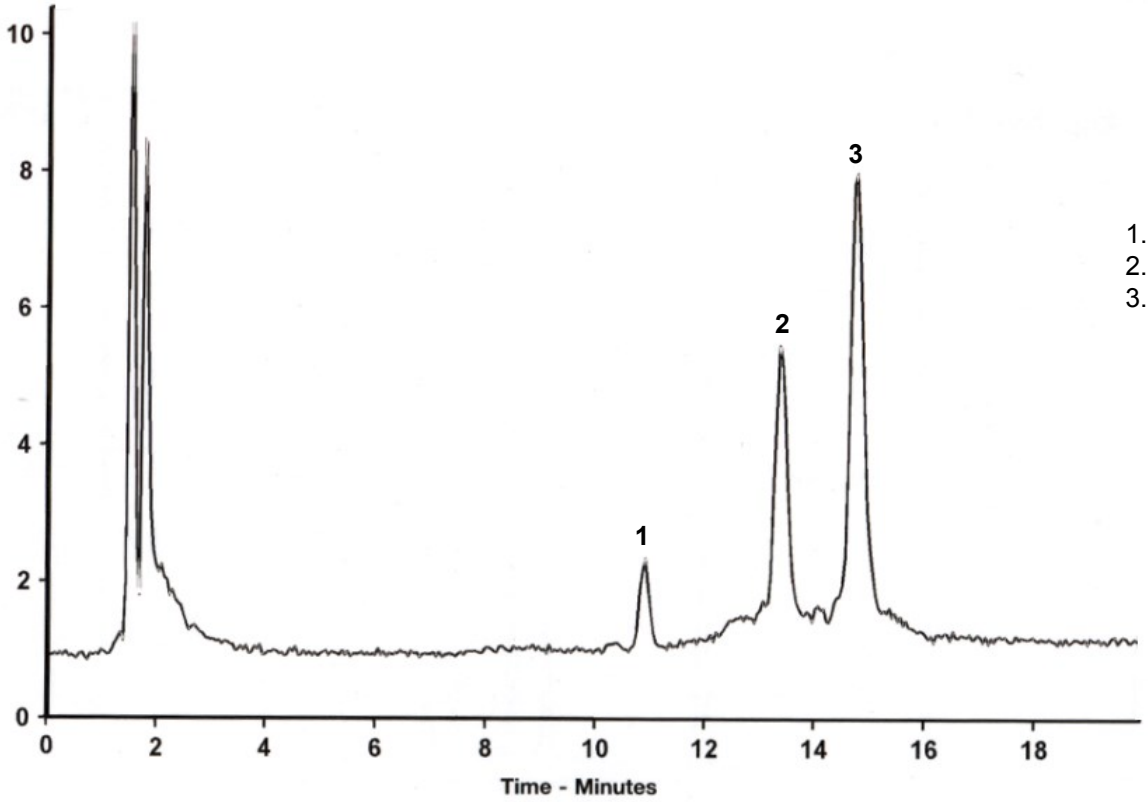
Application #**AN3000**

Conditions

Column: ACE 3 C4-300
Dimensions: 150 x 2.1 mm
Part Number: ACE-213-1502
Mobile Phase: A: 0.5% formic acid in H_2O
B: 0.5% formic acid in MeCN

Time (mins)	%B
0	35
16	43
17	80
20	80
21	35
31	35

Flow Rate: 0.4 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: ESI-MS (+ve)



1. α-Lactalbumin
2. β-Lactoglobulin B
3. β-Lactoglobulin A

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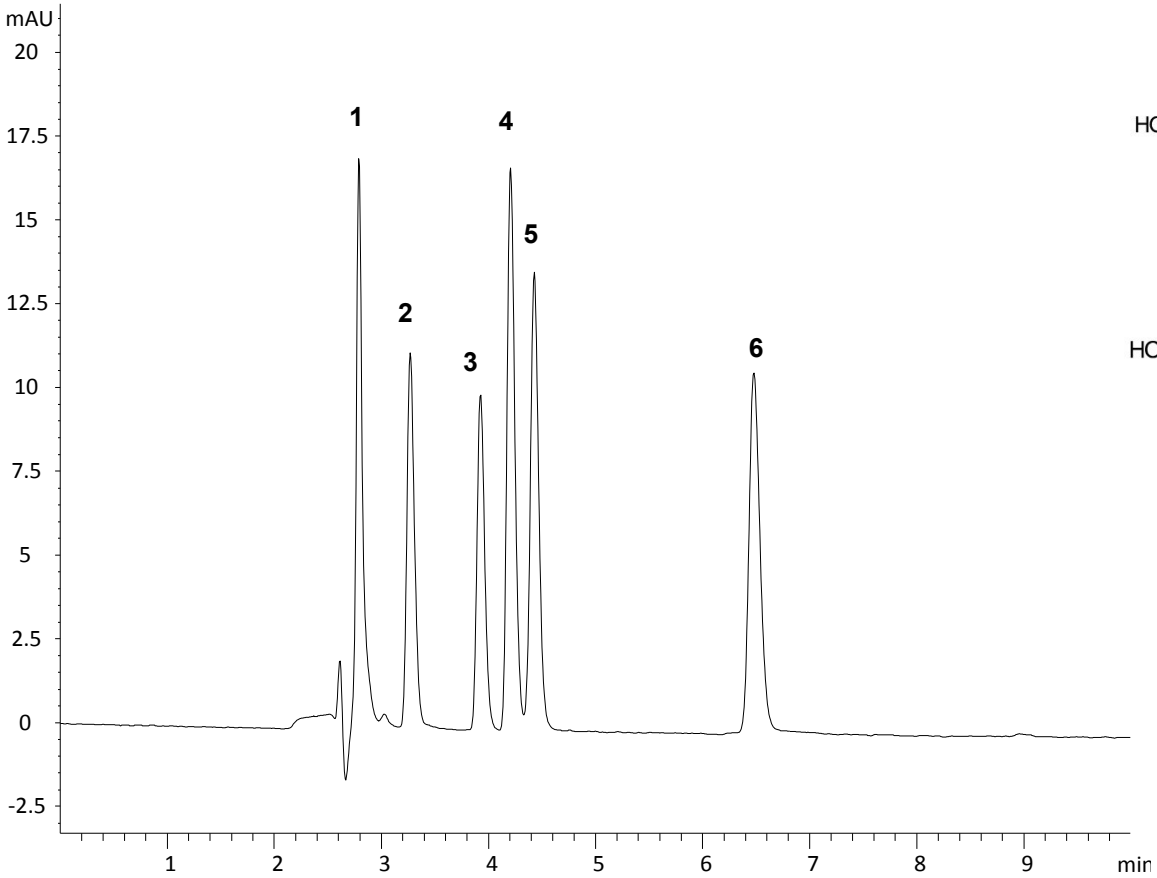
Wine Acid Analysis

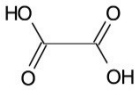
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1890**

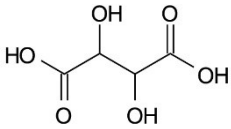
Conditions

Column:	ACE Excel 3 C18-Amide
Dimensions:	250 x 2.1 mm
Part Number:	EXL-1112-2502U
Mobile Phase:	40 mM ammonium phosphate pH 2.5 in H_2O
Flow Rate:	0.21 mL/min
Injection:	5 µL
Temperature:	25 °C
Detection:	UV, 214 nm

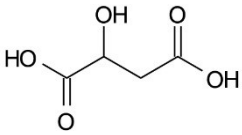




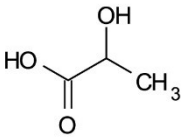
1. Oxalic acid



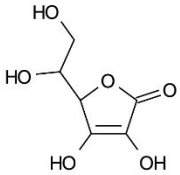
2. Tartaric acid



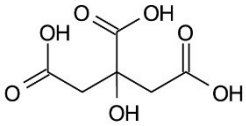
3. Malic acid



4. Lactic acid



5. Ascorbic acid



6. Citric acid

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For further details please contact:

Hichrom Limited
Tel: +44 (0)118 930 3660
Fax: +44 (0)118 932 3484
technical@hichrom.co.uk
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