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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Preface

The purpose of this guide is to assist chromatographers with the selection of the best HPLC/UHPLC column and conditions for their LC methods, by providing good examples of successful separations.

However, the information in this guide is provided for reference purposes only and Advanced Chromatography Technologies assumes no risk or liabilities that may result from its use by others. Furthermore, Advanced Chromatography Technologies makes no representations or warranties that the information provided in this guide will address any particular need or purpose of any user of the Application Guide.

Send us your application and receive a free ACE column

Send us your application on an ACE column and help extend our applications database. Your proven method will enable your chromatography colleagues to benefit and if we select your application for publication we'll send you a **FREE** ACE analytical column of your choice.

To submit your application e-mail us at: info@ace-hplc.com

ACE® Food and Beverage Applications: Application Index

New ACE® Food and Beverage Applications

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ACE® Food and Beverage Applications: Analyte Index

ACE® Food and Beverage Applications: Analyte Index

Additives and Intense Sweeteners

ACE®
Ultra-inert
UHPLC & HPLC Columns

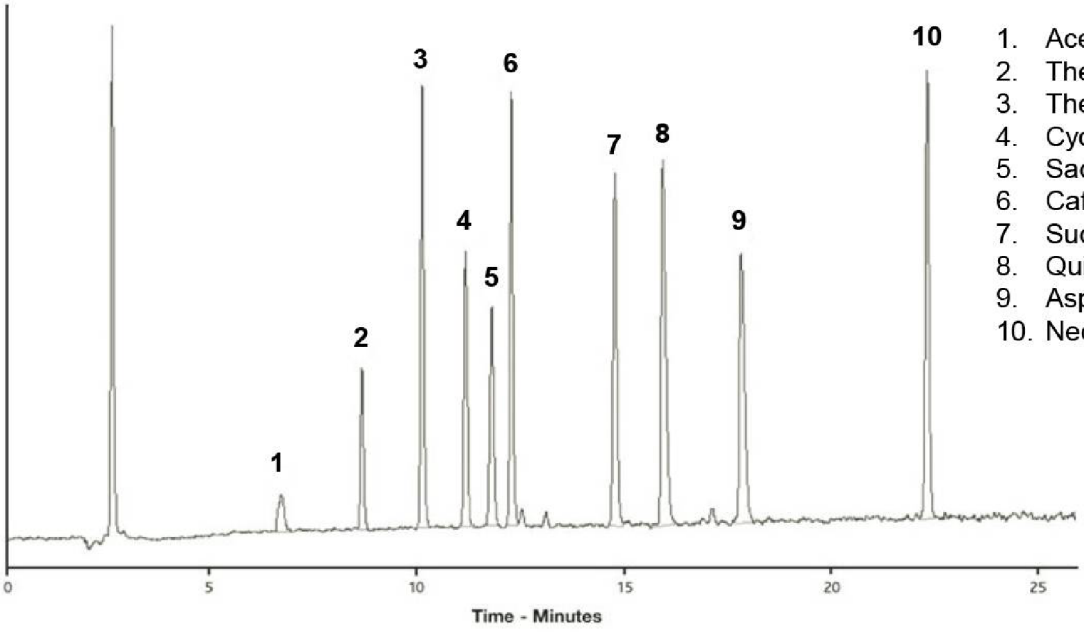
Application #**AN2950**

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

Agricultural Pesticides by LC-MS/MS

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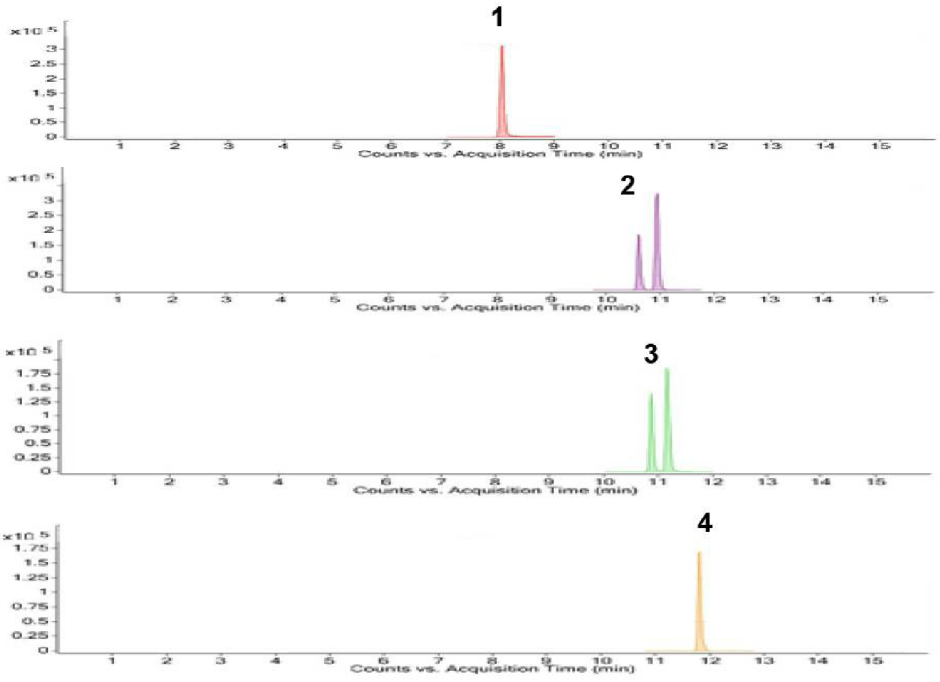
Application #**AN1290**

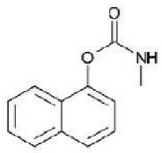
Conditions

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)

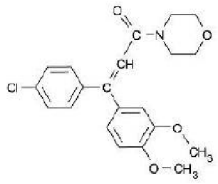
Time (mins)	%B
0.00	0
1.00	0
15.00	100
18.00	100
18.05	0
20.00	0

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

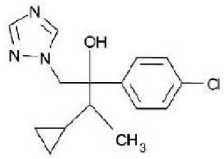




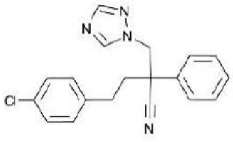
1. Carbaryl
(*m/z* 202.10 → 145.10)



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

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

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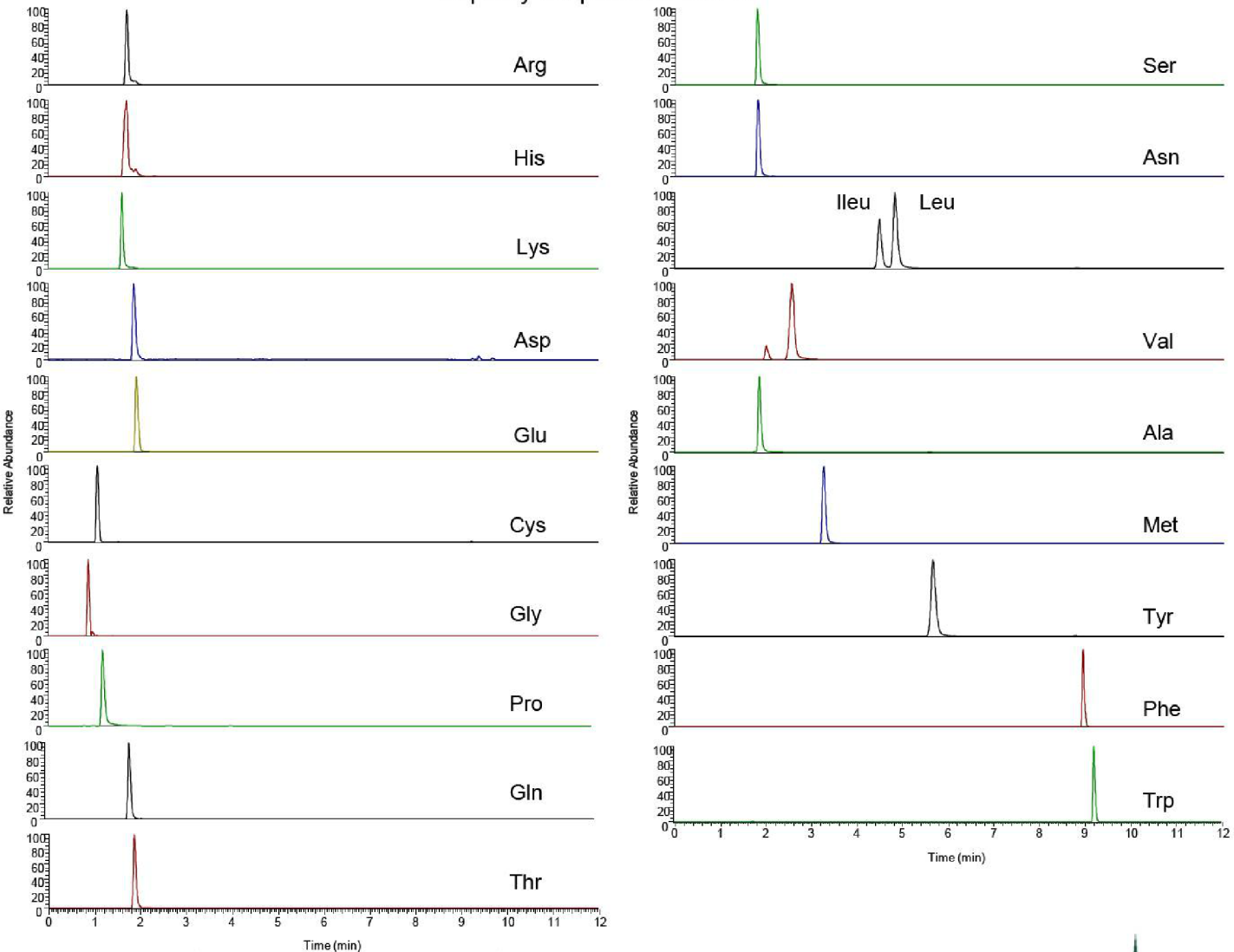
Application #AN2660

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



Amino Acids and Biogenic Amines in Wine and Beer

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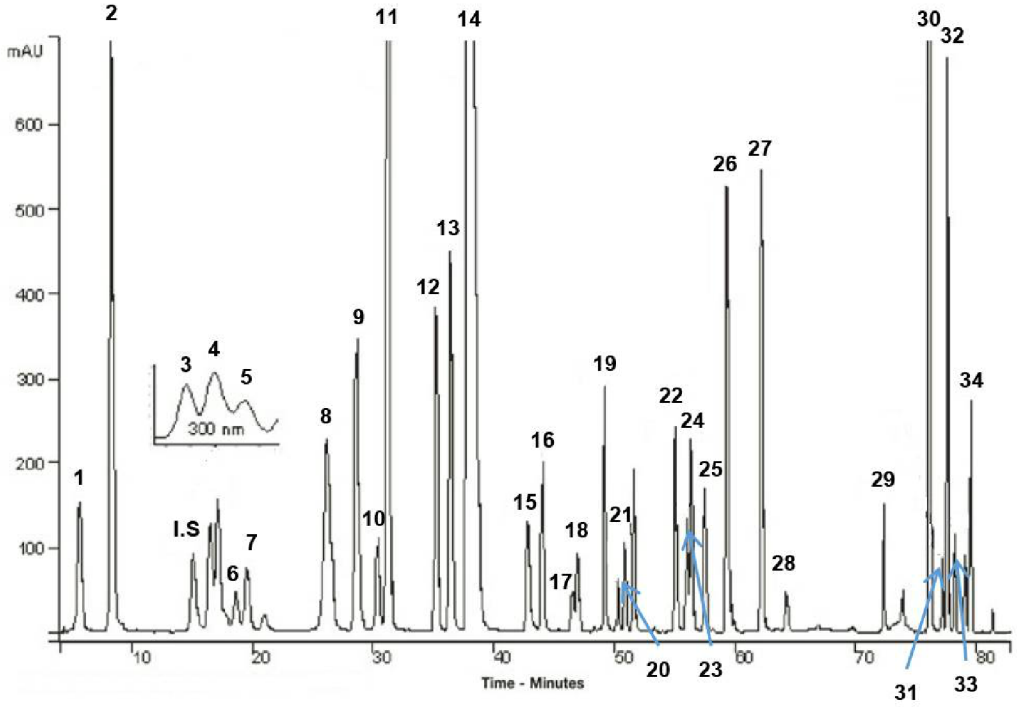
Application #**AN2800**

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
Sample:	Derivatised with diethyl ethoxymethylmalonate



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

Aminoglycosides in Eggs

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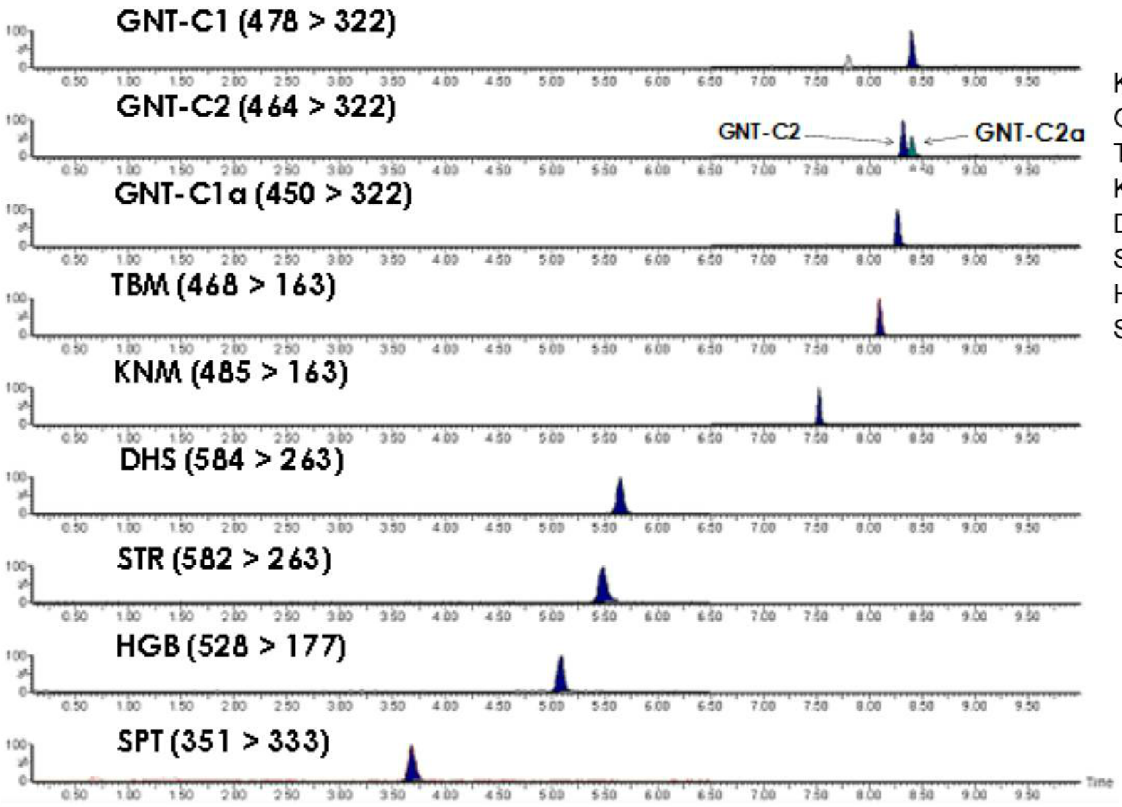
Application #**AN1920**

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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Annatto

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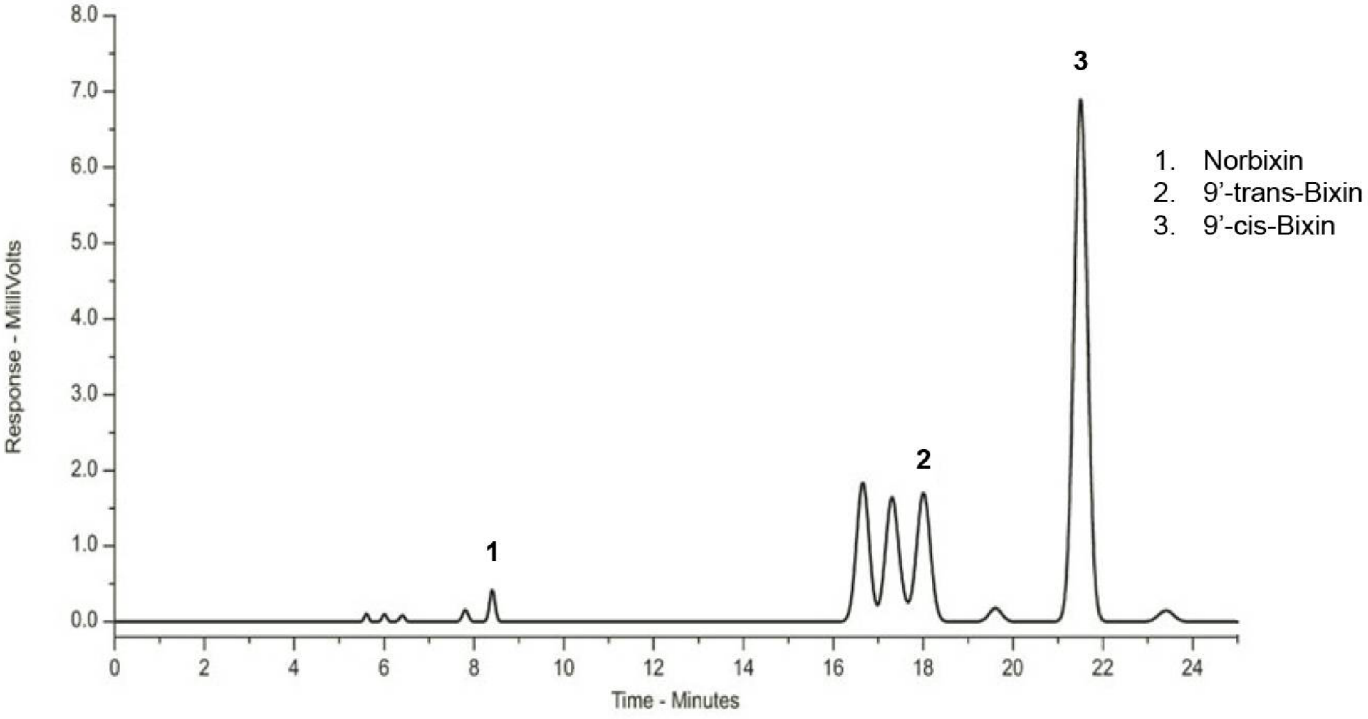
Application #**AN2840**

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



Anthocyanins from *Sambucus Nigra* (Elderberry)

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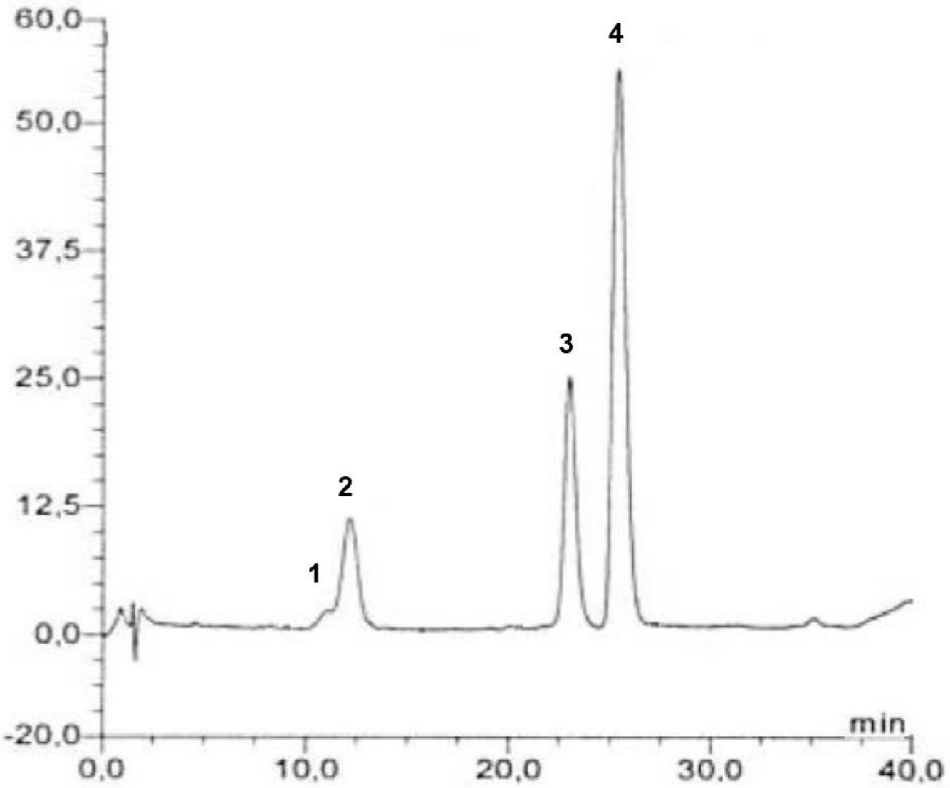
Application #AN2750

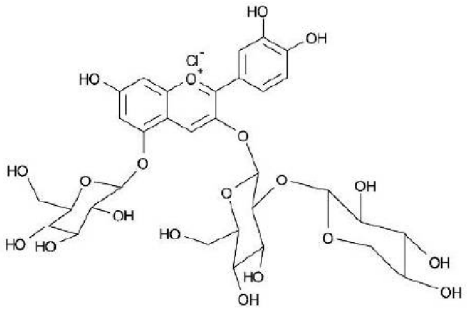
Conditions

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

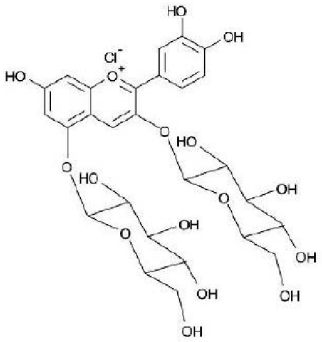
Time (mins)	%B
0	5
35	10
55	65
65	65

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

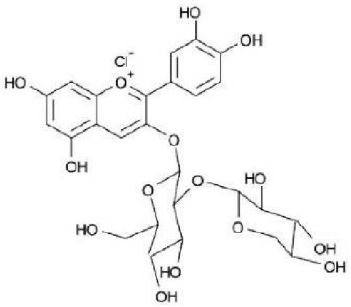




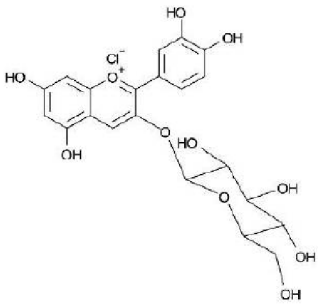
1. Cyanidin-3-sambubioside-5-glucoside



2. Cyanidin-3,5-diglucoside



3. Cyanidin-3-sambubioside



4. Cyanidin-3-glucoside

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Appetite Suppressants by LC-MS

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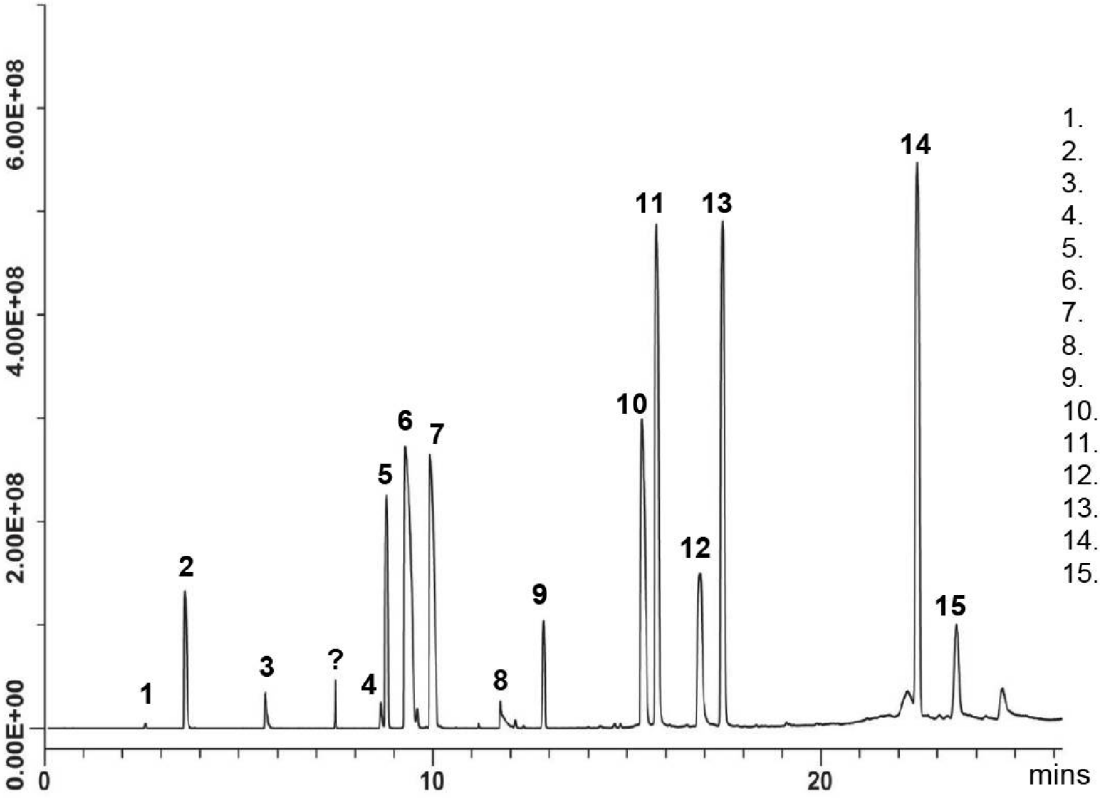
Application #**AN1960**

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	100.00
23.0	100.00

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

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

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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

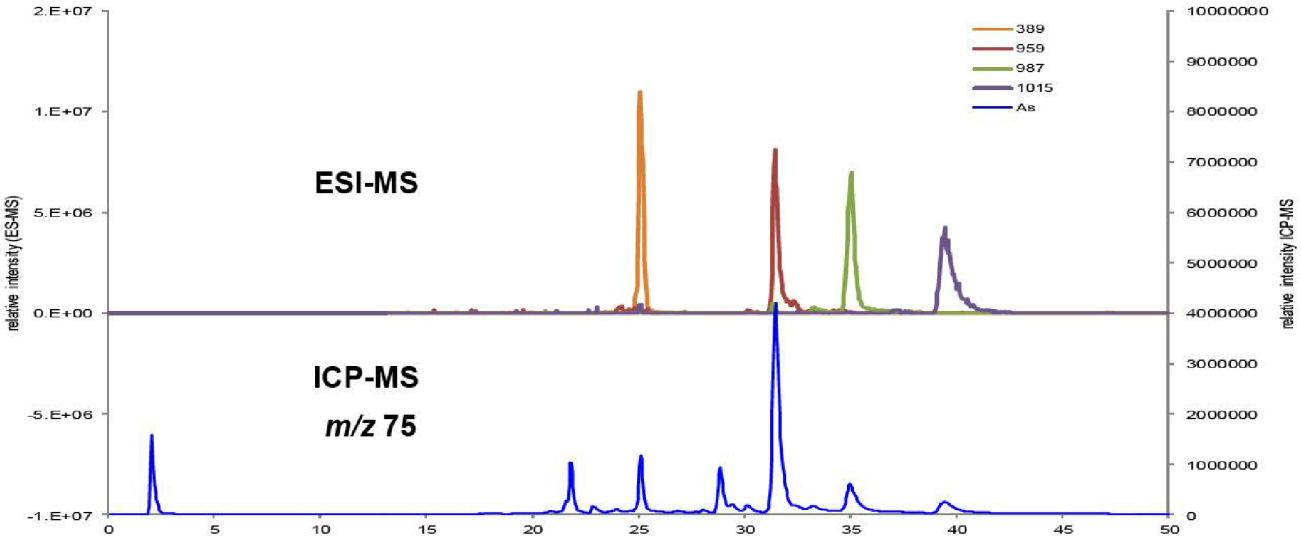
Flow Rate:	1 mL/min
Injection:	100 µL
Temperature:	45 °C
Detection:	Split ratio: 75% ESI-MS: 25% ICP-MS Thermo Scientific Element 2 ICP-MS Mode: Organic mode Medium resolution Thermo Scientific Orbitrap Discovery Positive ESI mode Spray voltage: 4.5 kV Capillary temperature: 320 °C Capillary voltage: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



Artificial Colours (Water Soluble)

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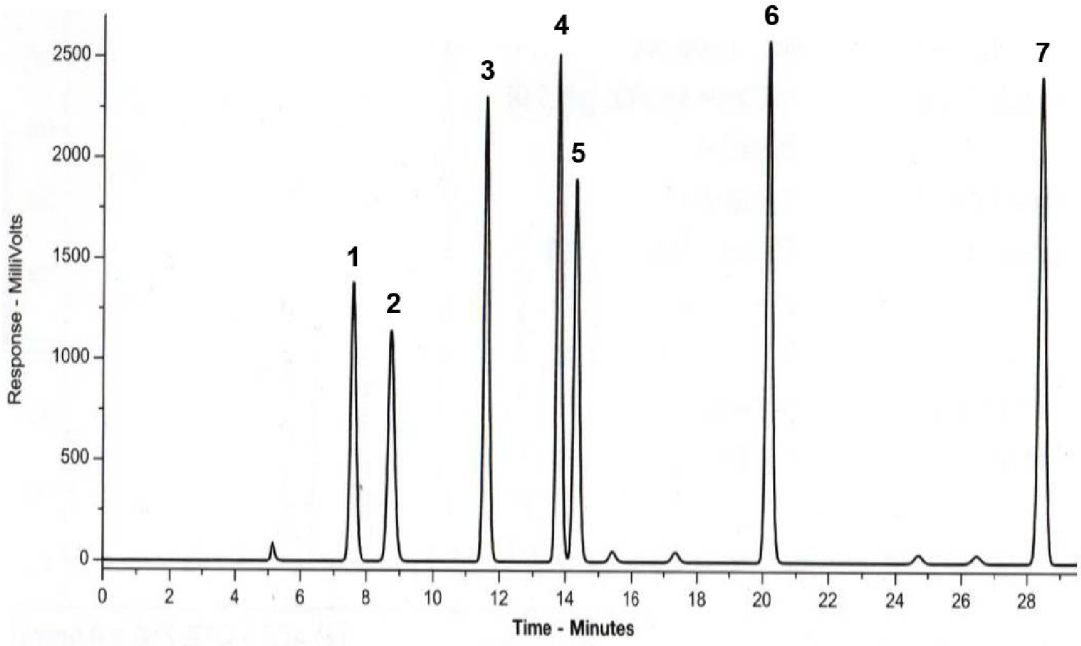
Application #**AN3010**

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

Artificial Food Colours

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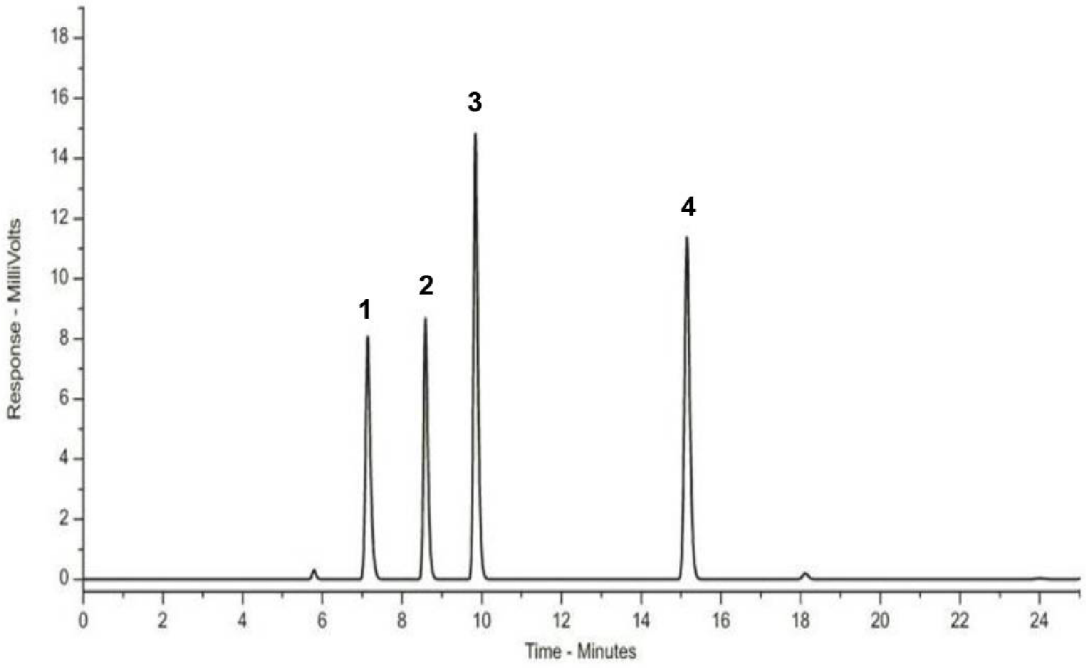
Application #**AN2960**

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

Artificial Sweeteners Global Method

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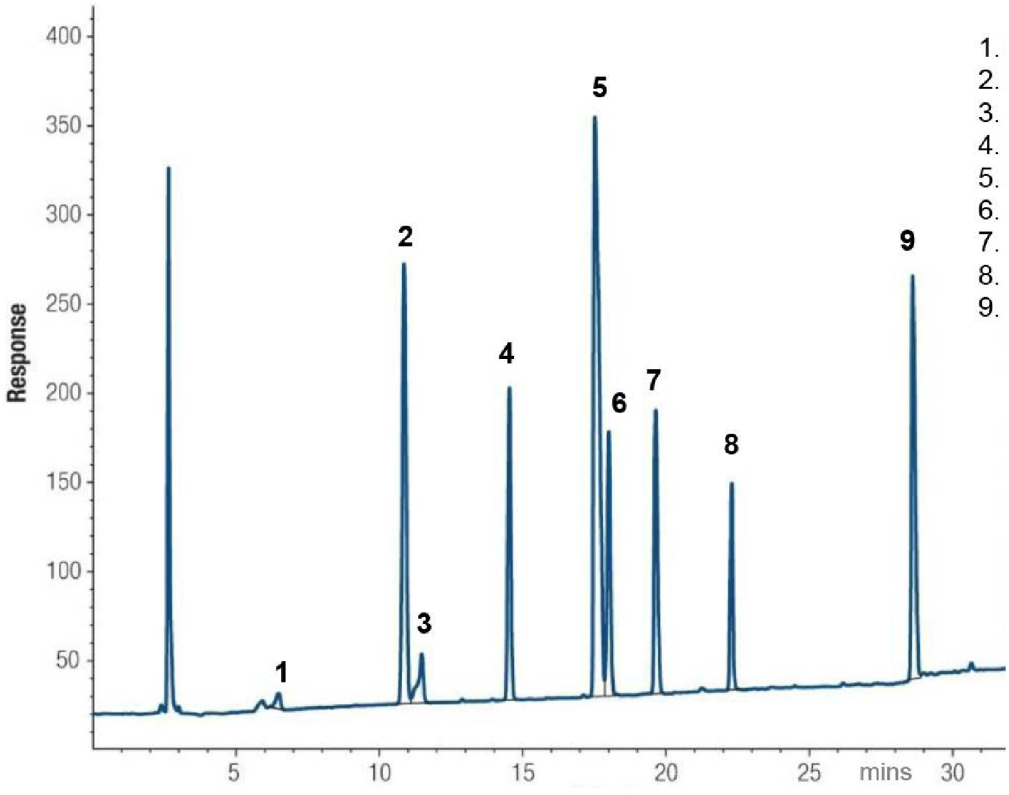
Application #AN1980

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

Artificial Sweeteners (Stevia Glycosides)

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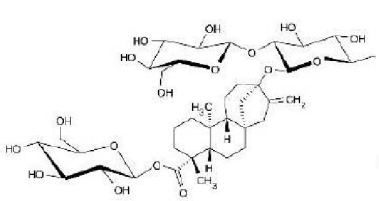
Application #**AN1020**

Conditions

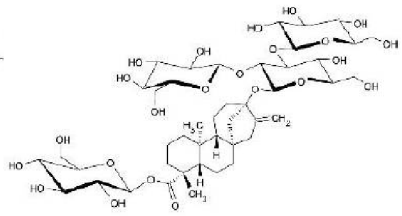
Column:	ACE Excel 2 SuperC18
Dimensions:	150 x 2.1 mm
Part Number:	EXL-1011-1502U
Mobile Phase:	A: 10 mM sodium dihydrogen phosphate pH 2.8 in H_2O
	B: 10 mM sodium dihydrogen phosphate pH 2.8 in H_2O/MeCN (80:20 v/v)

Time (mins)	%B
0	39.5
4	48.0

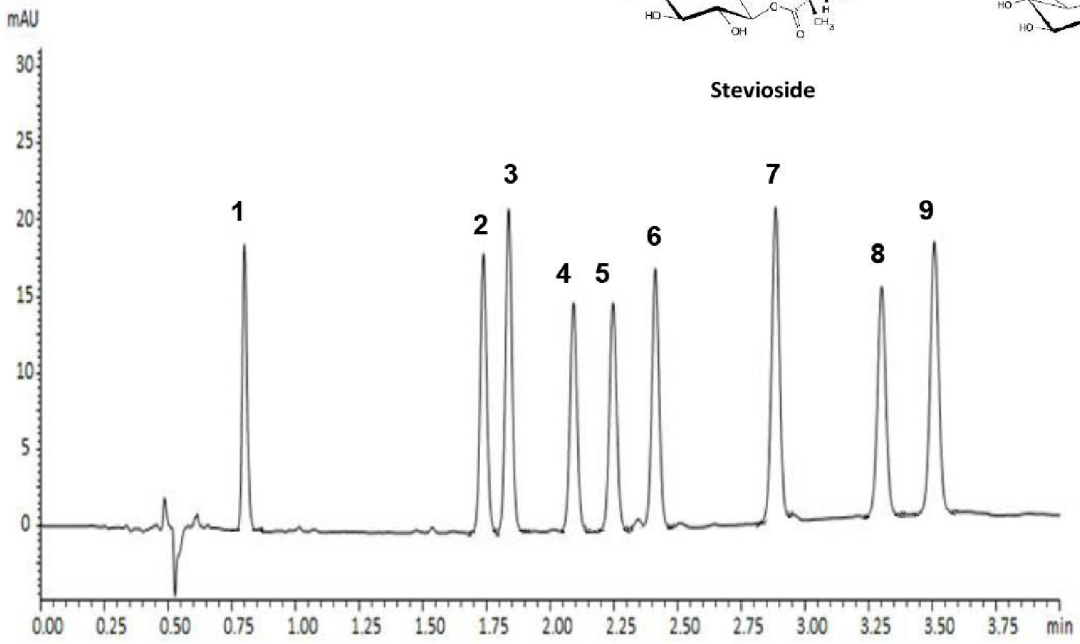
Flow Rate:	0.6 mL/min
Injection:	1 µL
Temperature:	50 °C
Detection:	UV, 200 nm



Stevioside



Rebaudioside A



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

Avenacins

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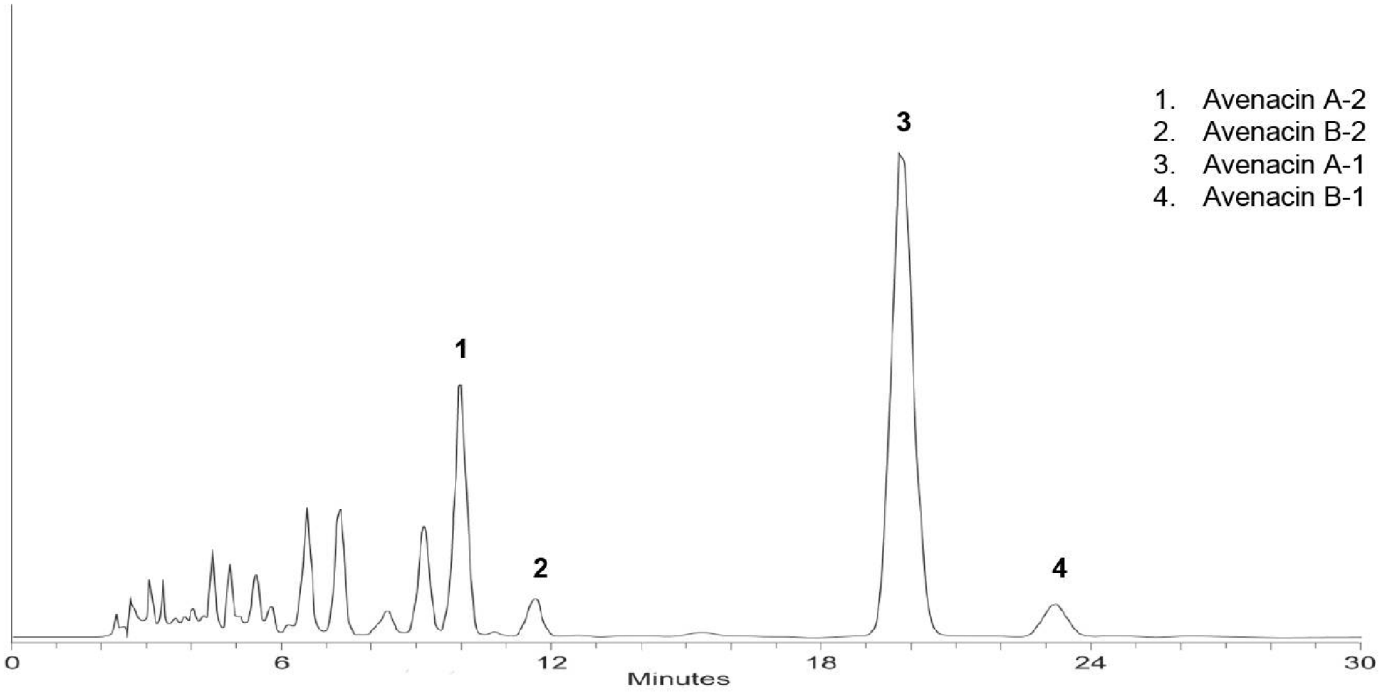
Application #**AN2740**

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

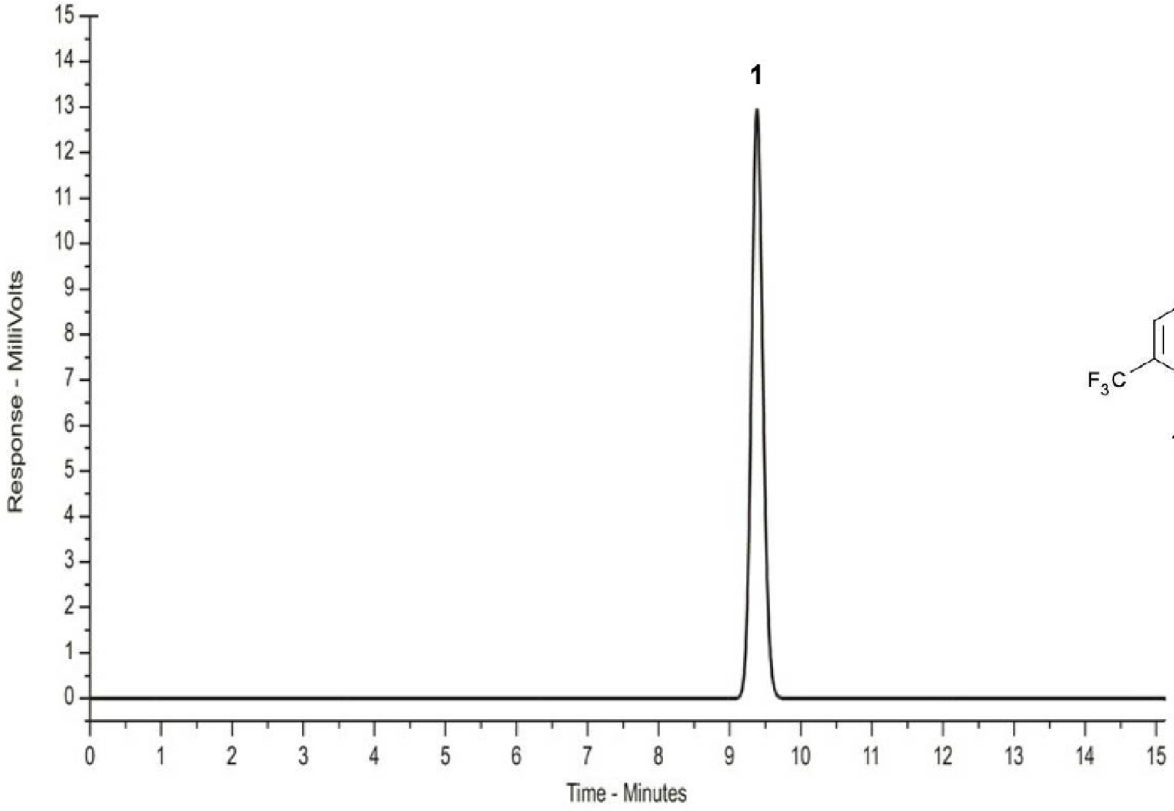


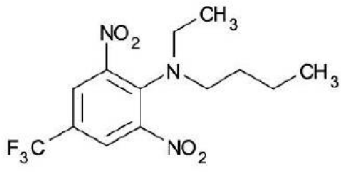
Benfluralin (Herbicide)

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

Caffeine and Metabolites

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Application #AN2010

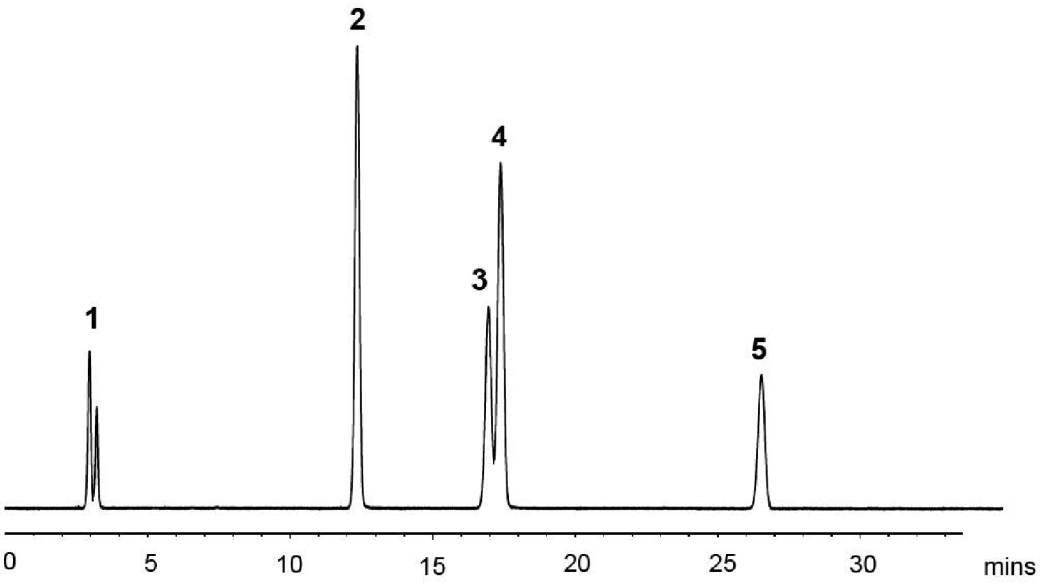
Conditions

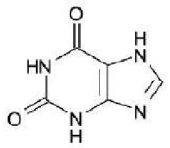
Column:	ACE 5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1211-1546U
Mobile Phase:	A: 20 mM ammonium acetate pH 7.0 in H_2O
	B: 20 mM ammonium acetate pH 7.0 in MeCN/H_2O (90:10 v/v)

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

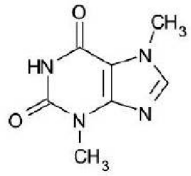
Post time 10 minutes

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

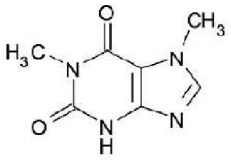




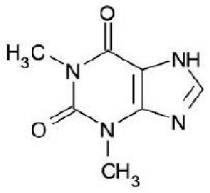
1. Xanthine



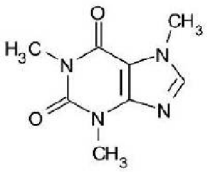
2. Theobromine



3. Paraxanthine



4. Theophylline



5. Caffeine

Chloramphenicol in Milk by LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN2030

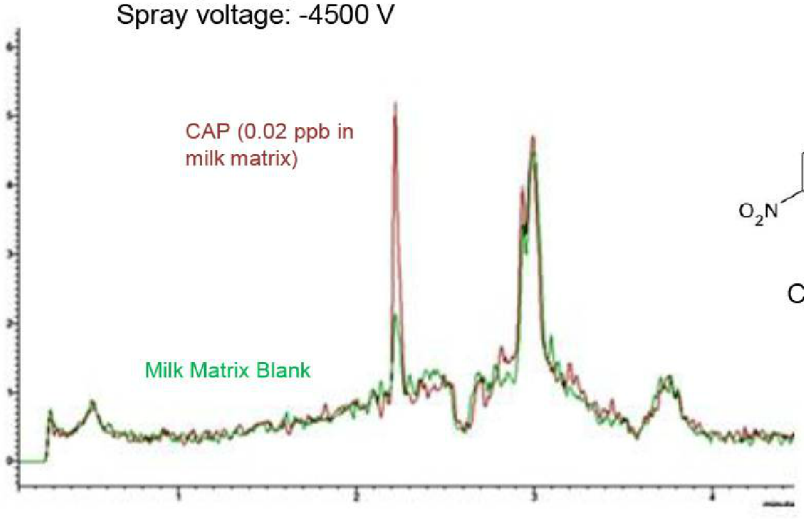
Conditions

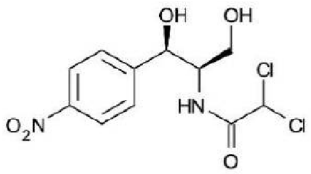
Column:	ACE 3 C18
Dimensions:	50 x 2.1 mm
Part Number:	ACE-111-0502
Mobile Phase:	A: H_2O
	B: MeOH

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

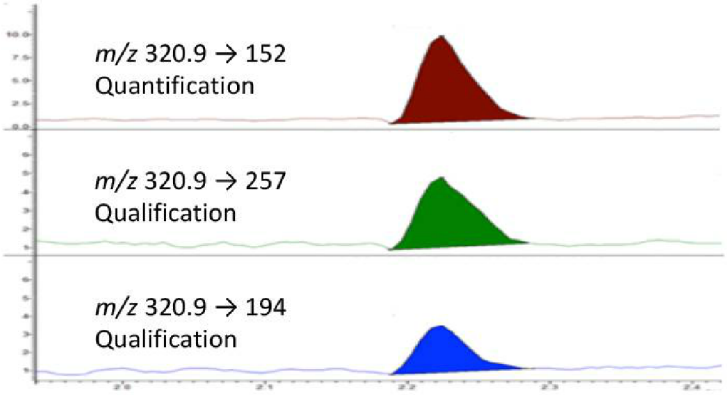
TIC of 3 MRMs of 0.02 ppb chloramphenicol spiked in milk matrix





Chloramphenicol

MRM chromatograms of 0.05 ppb chloramphenicol in milk



Chocolate Analysis

ACE®
Ultra-inert
UHPLC & HPLC Columns

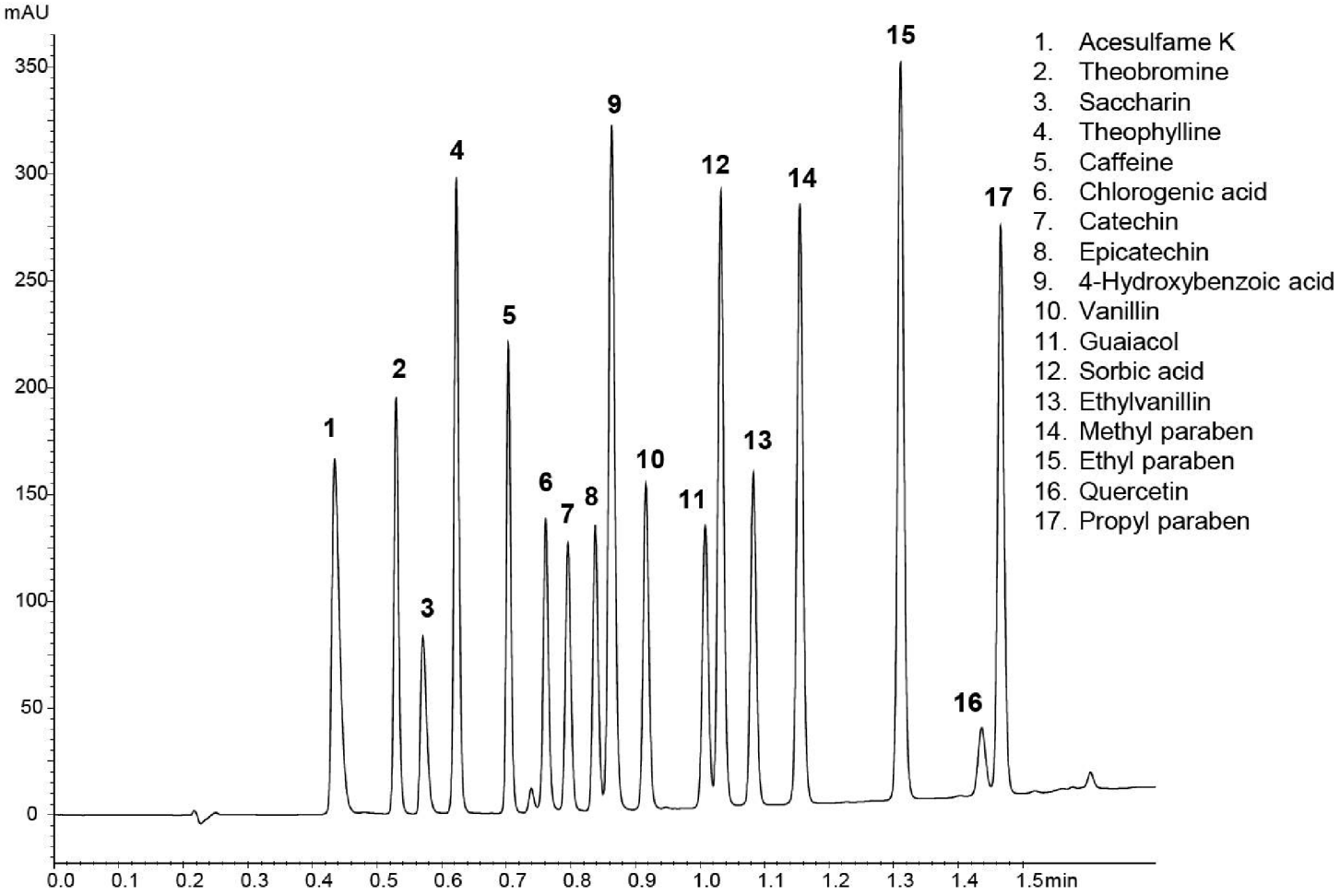
Application #AN2040

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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Coffee Metabolite Profiling by LC-MS

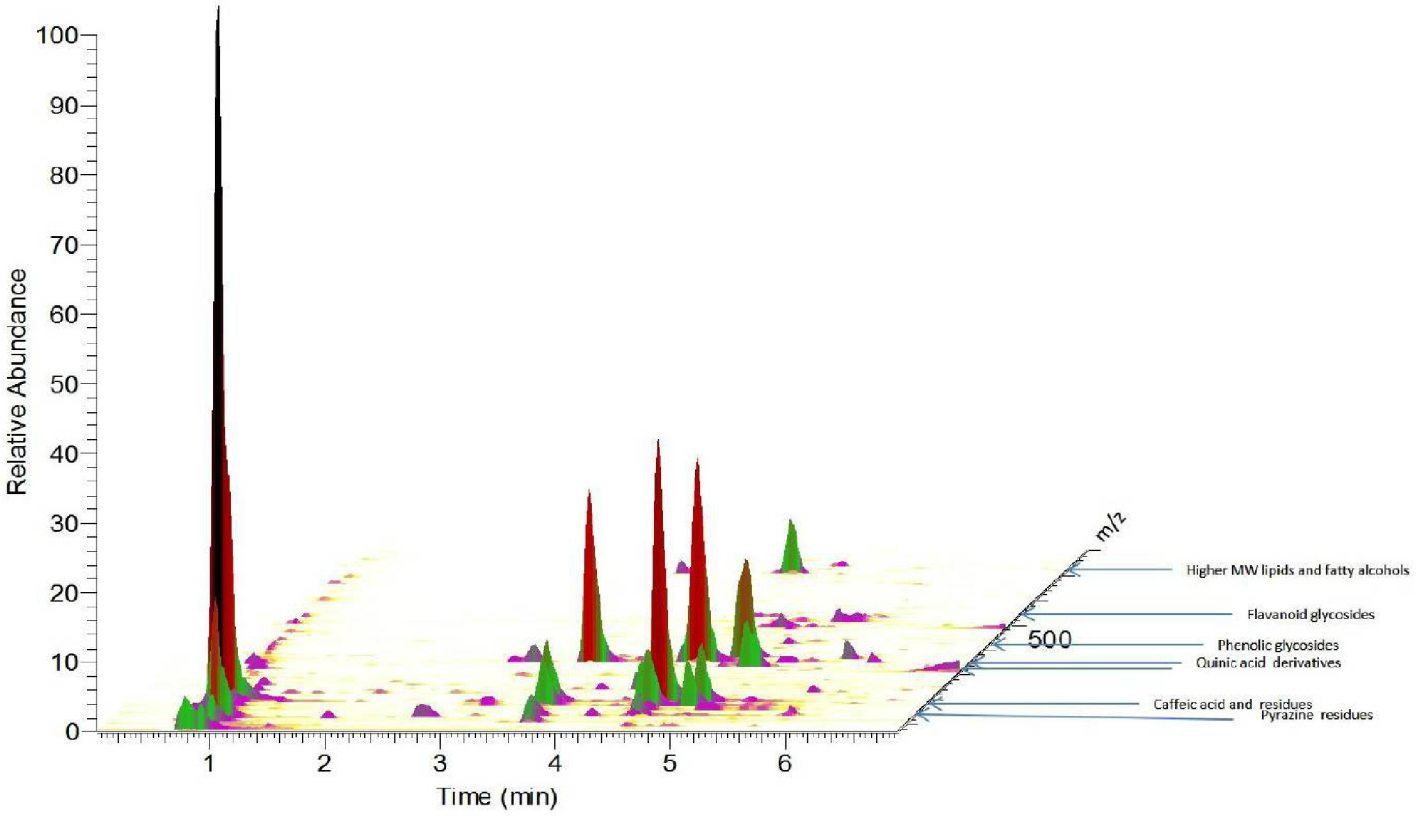
Application #**AN2590**

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



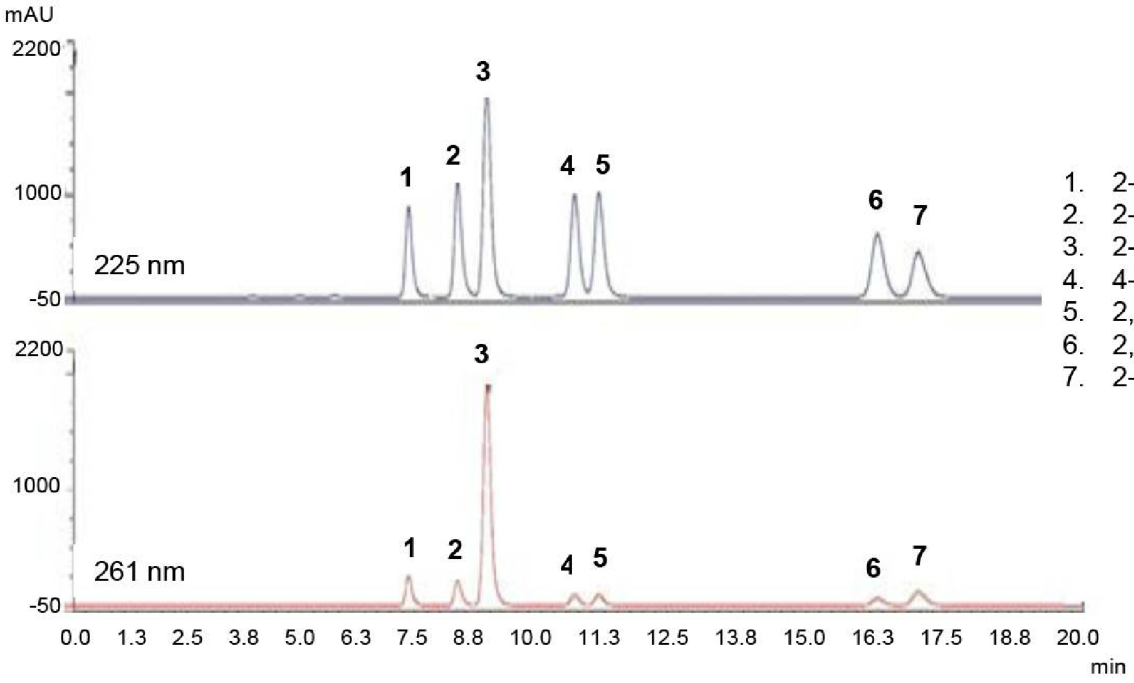
Cyclodextrin-Encapsulated Flavour Compounds in Beer

ACE®
Ultra-inert
UHPLC & HPLC Columns

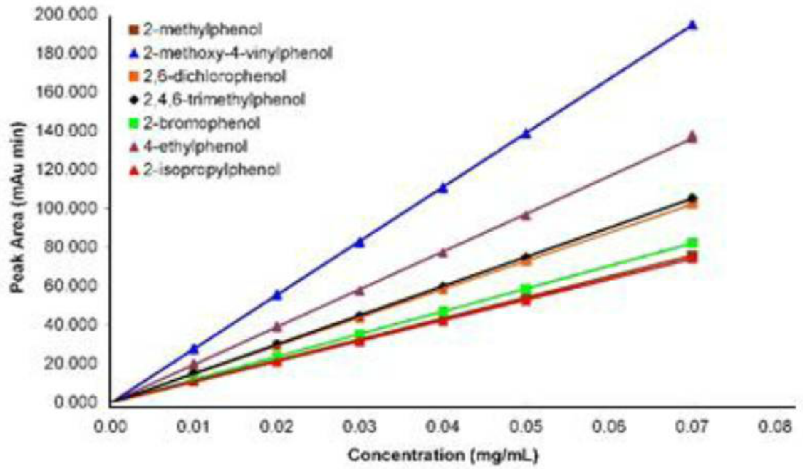
Application #**AN2300**

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



Defensins (Human) in Saliva Matrix

ACE®
Ultra-inert
UHPLC & HPLC Columns

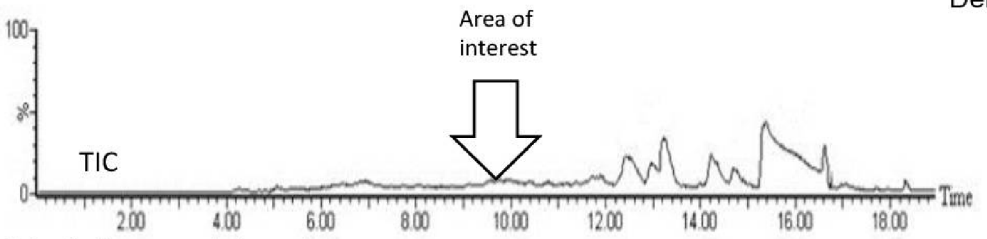
Application #AN1270

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

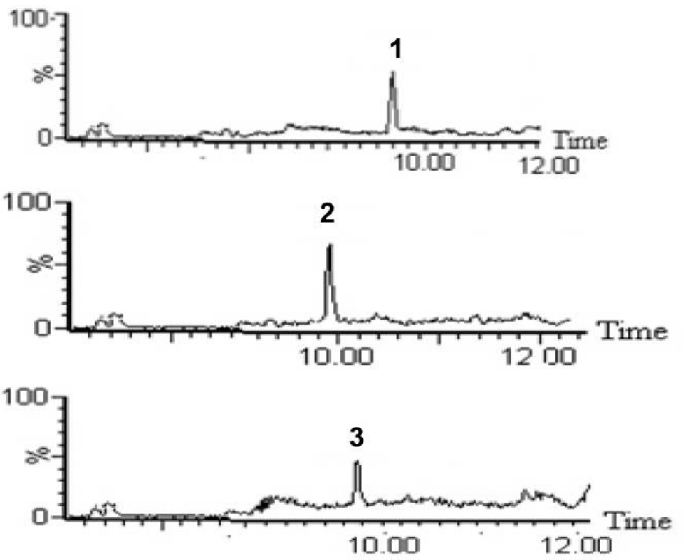
Time (mins)	%B
0	2
2	2
17	50
19	95
20	95

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

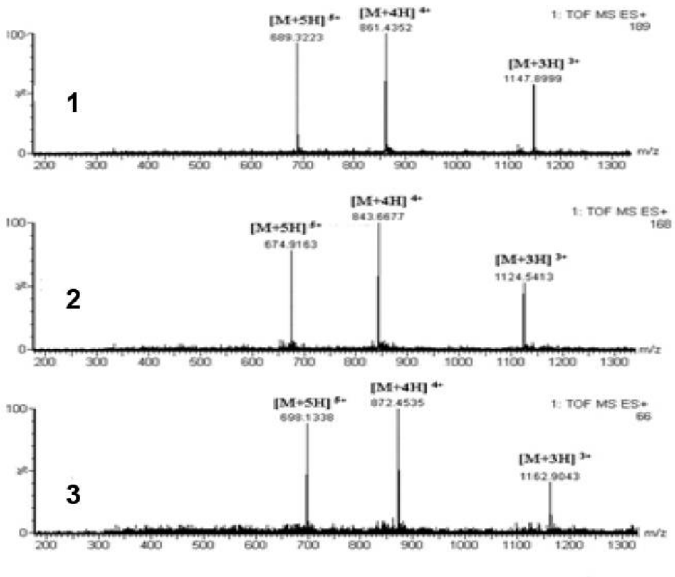


Defensin Human Neutrophil Peptides
1. HNP-1
(30 amino acid residues)
2. HNP-2
(29 amino acid residues)
3. HNP-3
(30 amino acid residues)

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



Mass spectra



Ethanol Extract from Seed Cover (*Acacia Farnesiana)*

ACE®
Ultra-inert
UHPLC & HPLC Columns

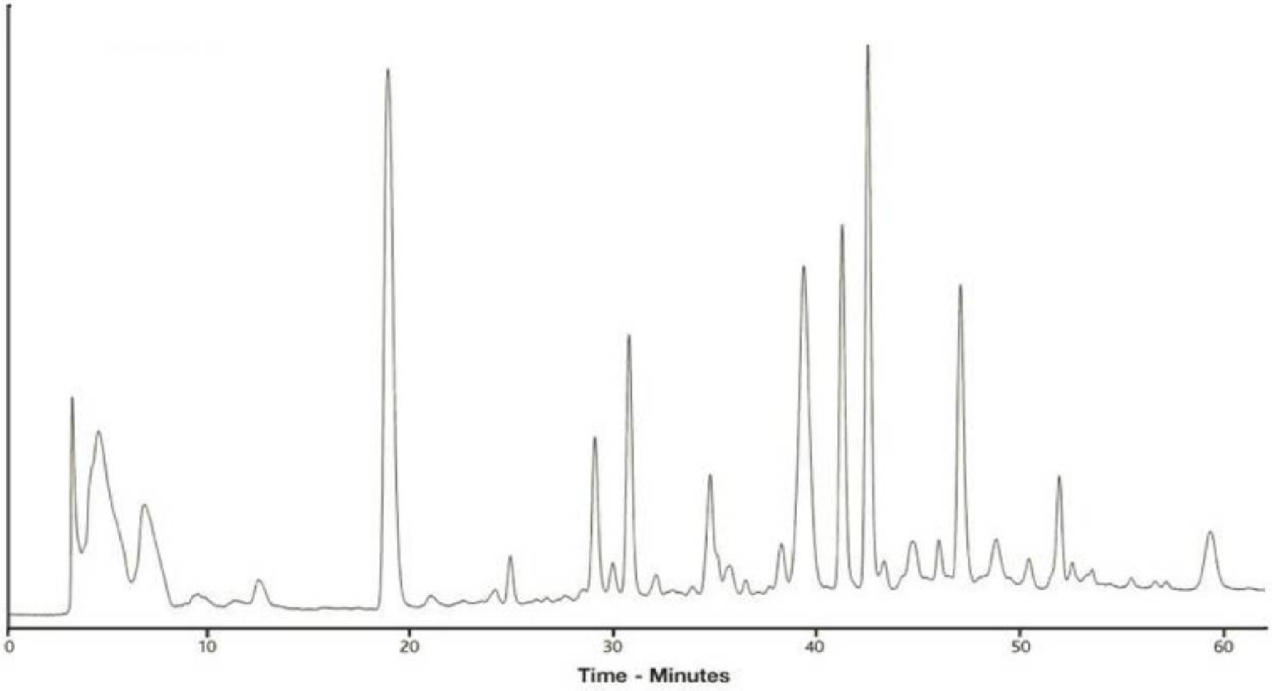
Application #**AN2900**

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



Flavone and Dibucaine

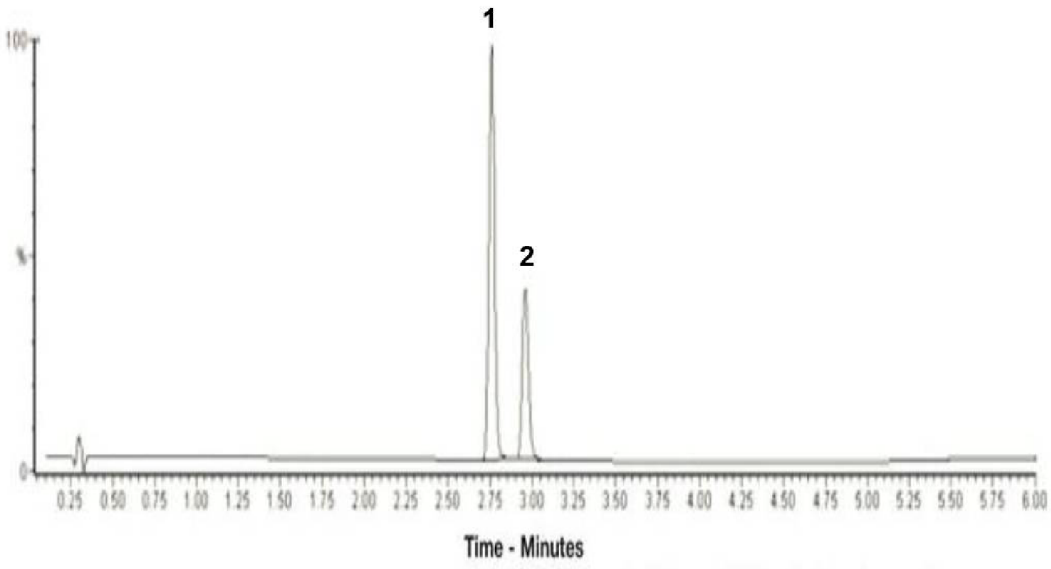
Application #**AN2850**

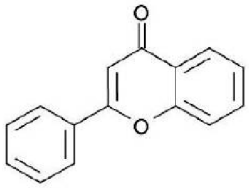
Conditions

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

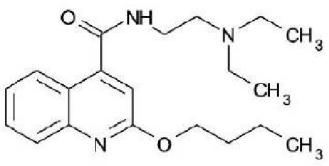
Time (mins)	%A	%B	%C
0.0	80	10	10
5.2	0	50	50
5.6	0	0	100

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





1. Flavone

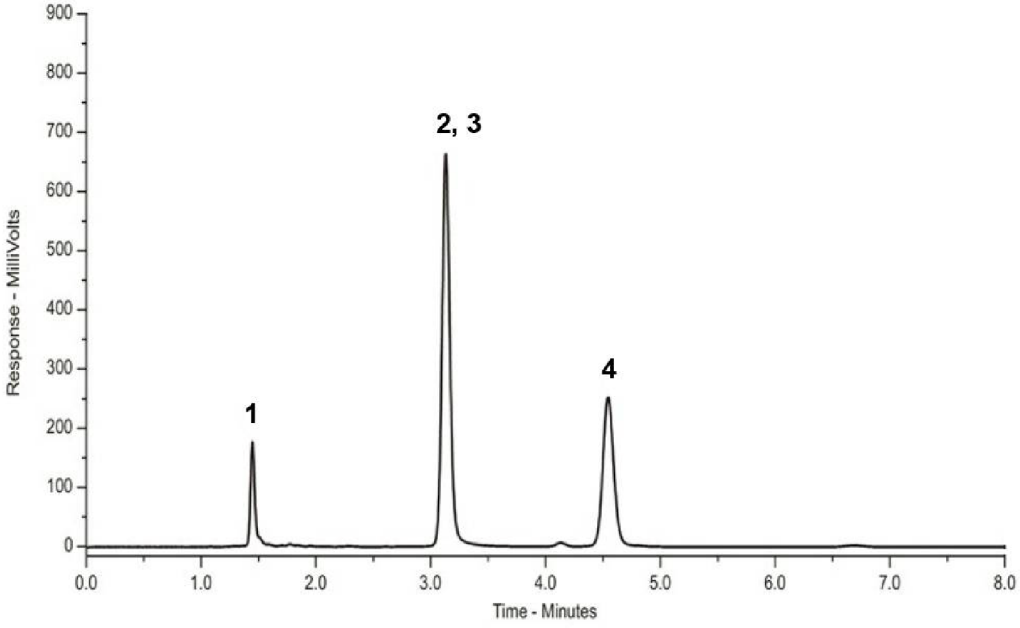


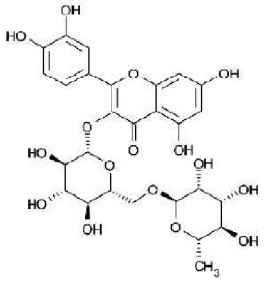
2. Dibucaine

Application #AN2810

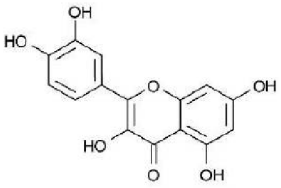
Conditions

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

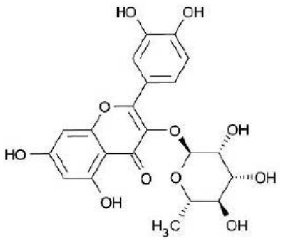




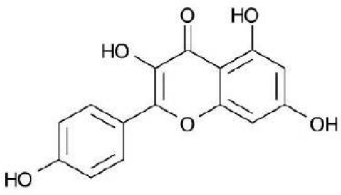
1. Rutin



2. Quercetin



3. Quercitrin



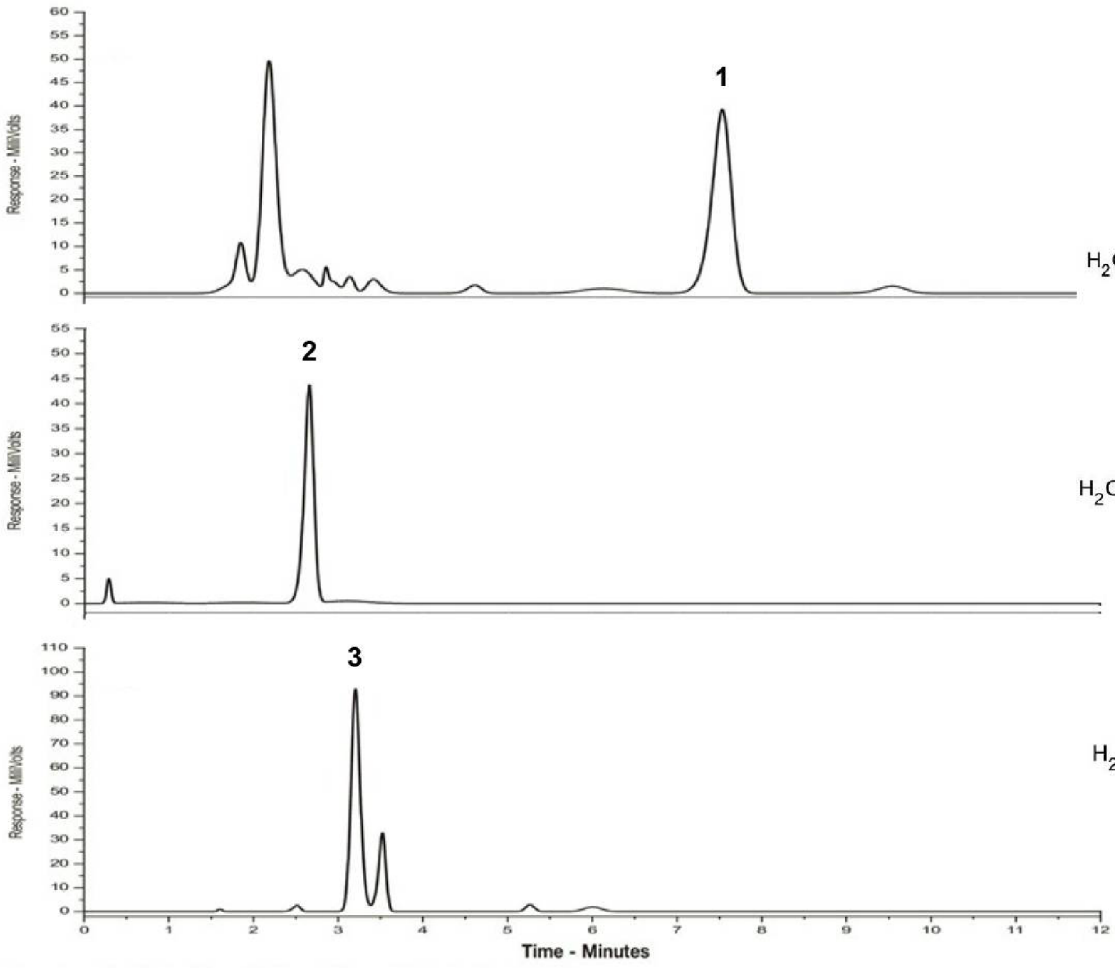
4. Kaempferol

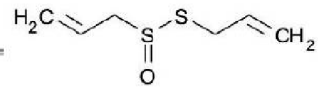
Garlic Analysis (I)

Application #**AN2820**

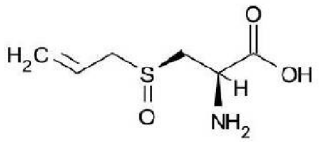
Conditions

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

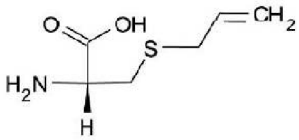




1. Allicin



2. Alliin



3. Deoxyalliin

Garlic Analysis (II)

ACE®
Ultra-inert
UHPLC & HPLC Columns

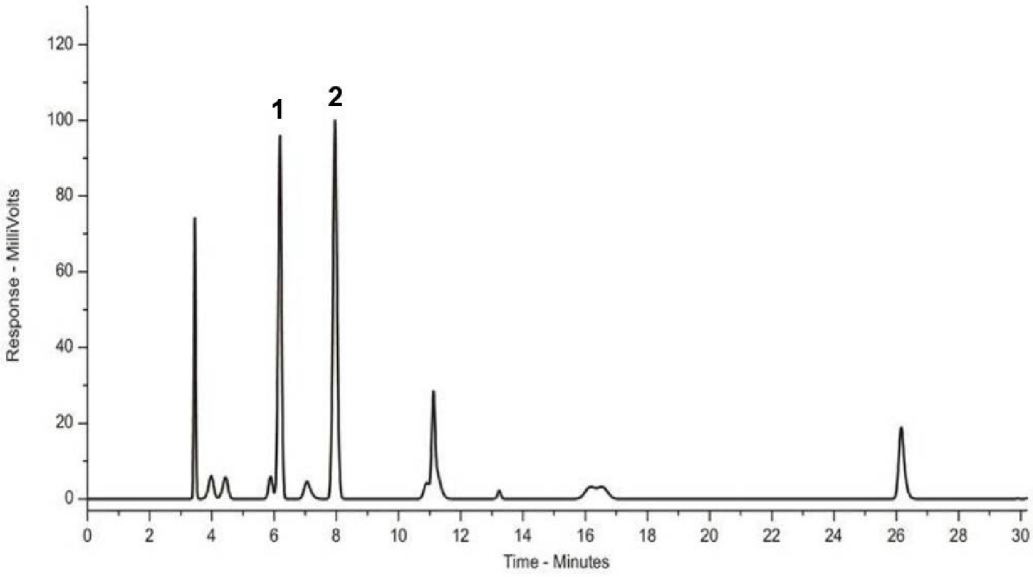
Application #**AN2830**

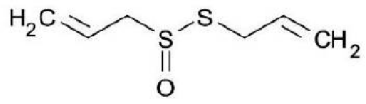
Conditions

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

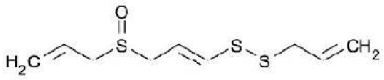
Time (mins)	%B
0	40
20	100
25	100

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





1. Allicin



2. Ajoene

Green Tea Metabolite Profiling by LC-MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

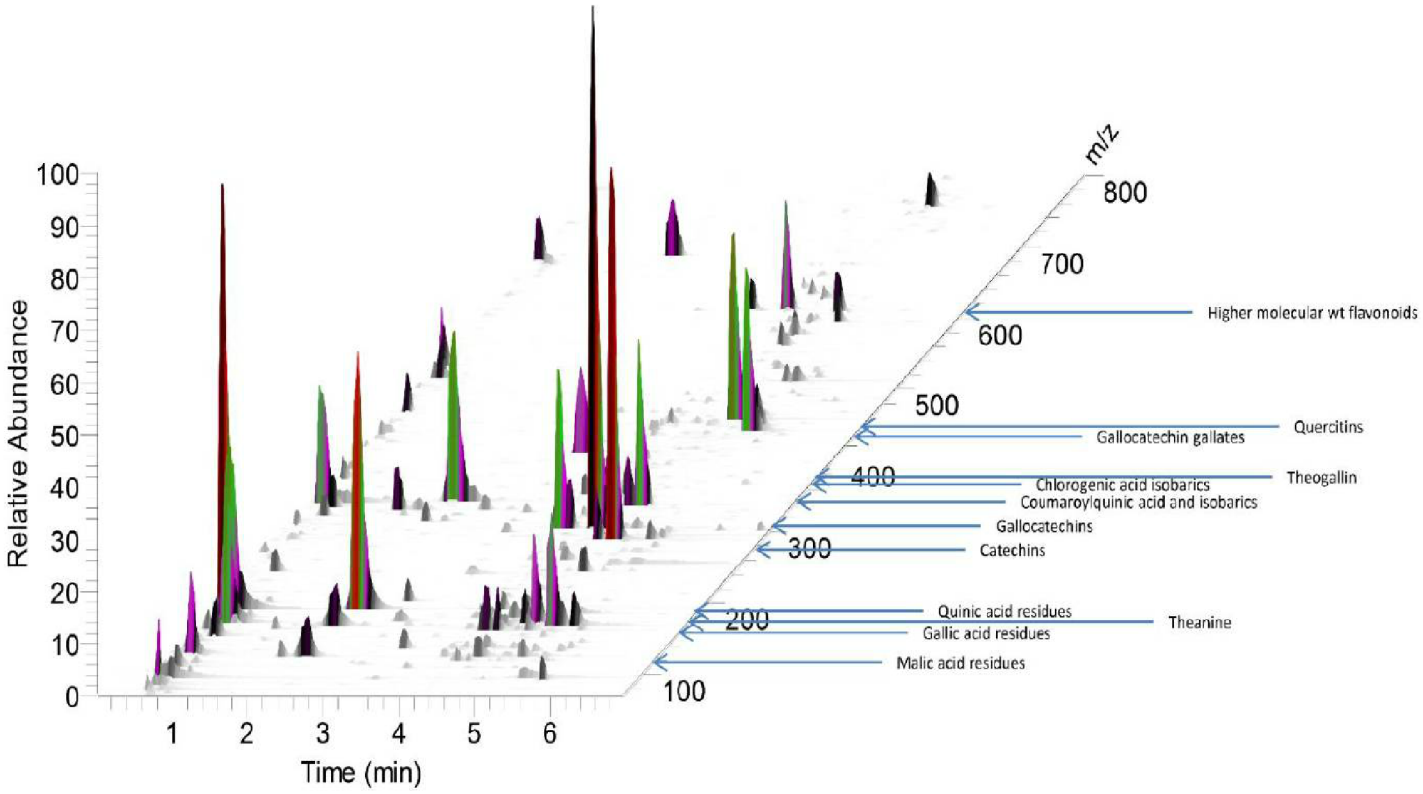
Application #AN2580

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



Herbicide Impurity Profile

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2130**

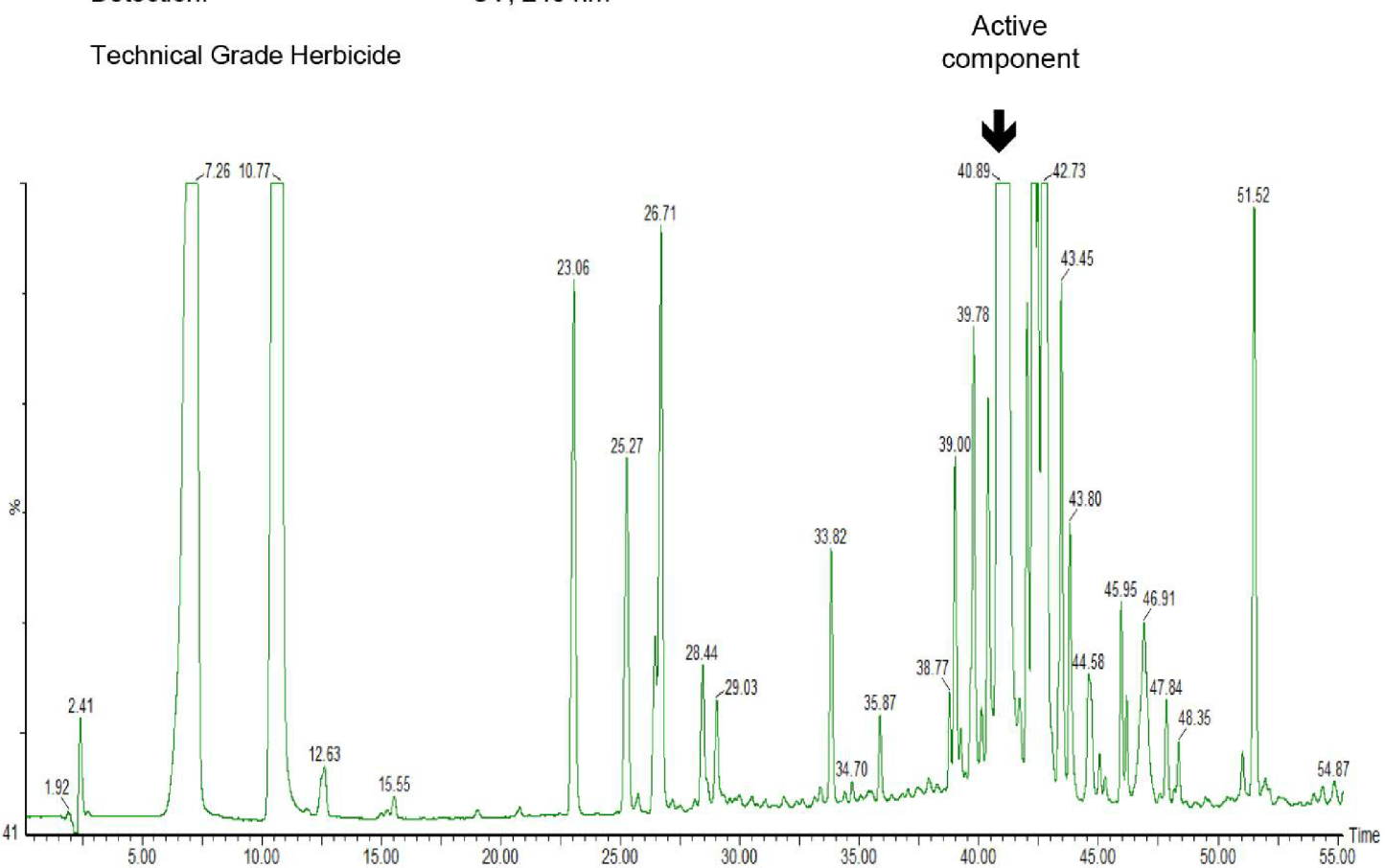
Conditions

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



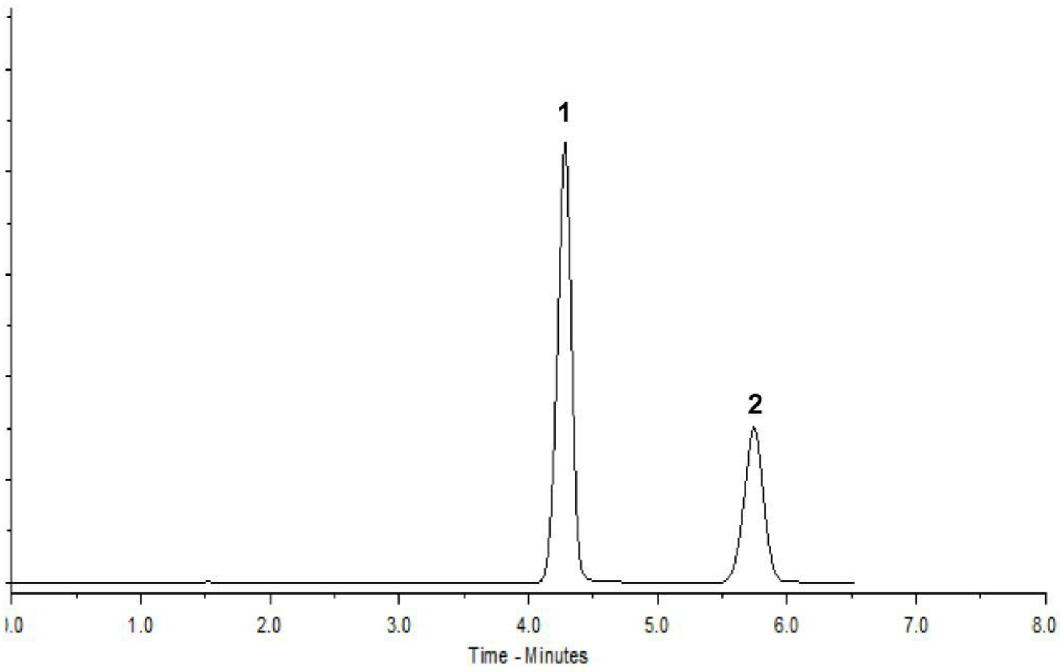
Hippuric Acid

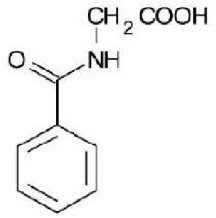
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN2760

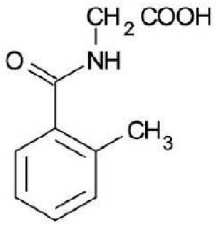
Conditions

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

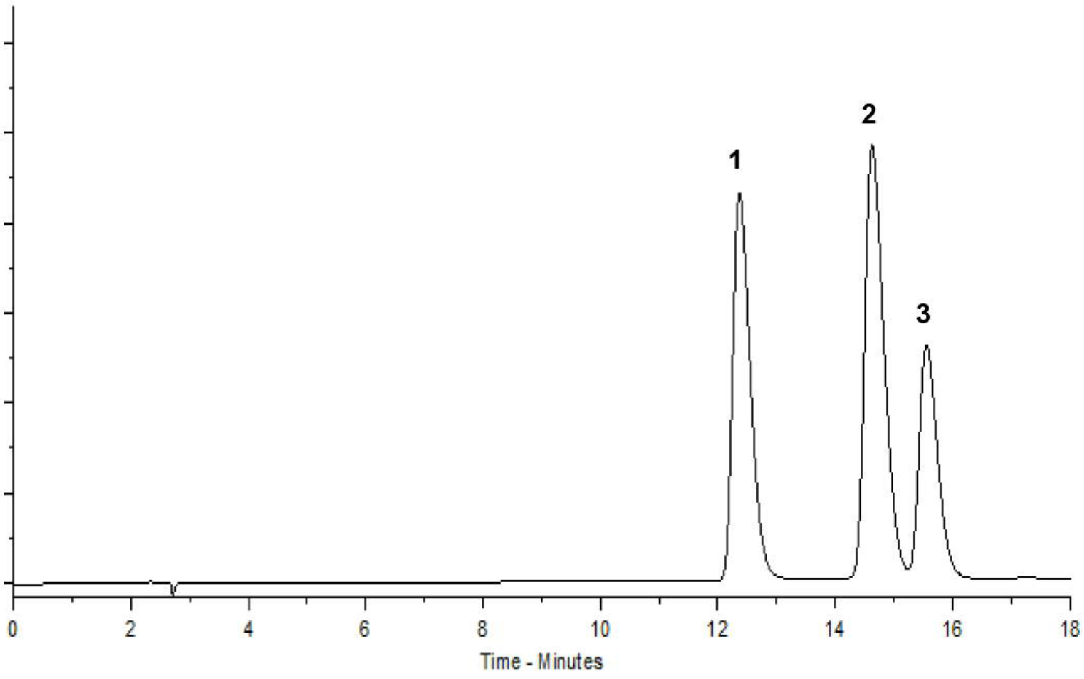
Application #AN2770

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



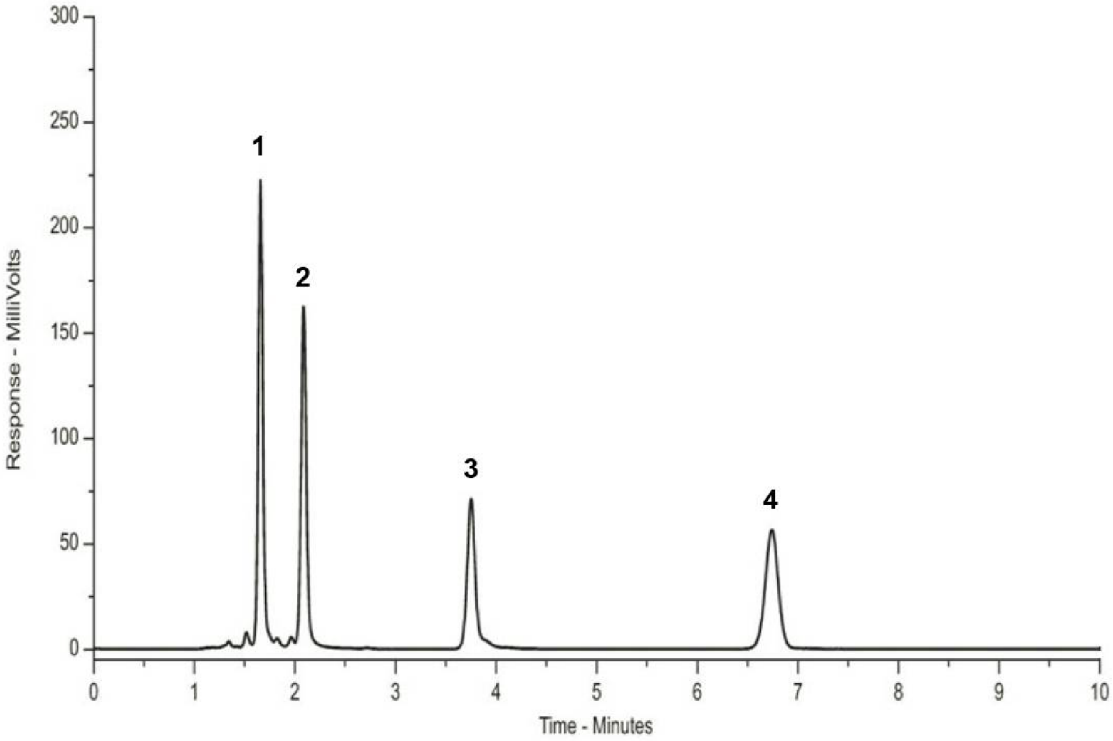
1. Bovine insulin
2. Human insulin
3. Porcine insulin

Isoflavones

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

Isoflavones in Red Clover and Soy Extract

ACE®
Ultra-inert
UHPLC & HPLC Columns

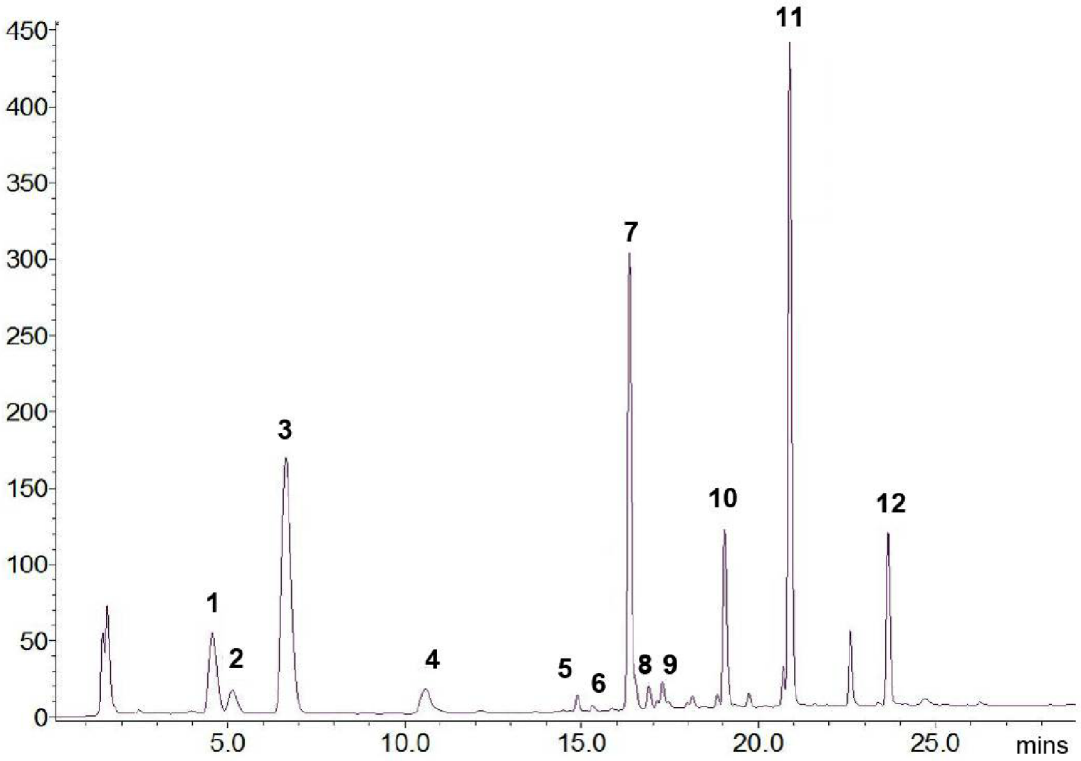
Application #AN1130

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. Acetyldaidzin
6. Acetylglycitin
7. Daidzein
8. Glycitein
9. Acetylgenistin
10. Genistein
11. Formononetin
12. Biochanin A

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

Liquorice Extracts Fingerprint

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2090**

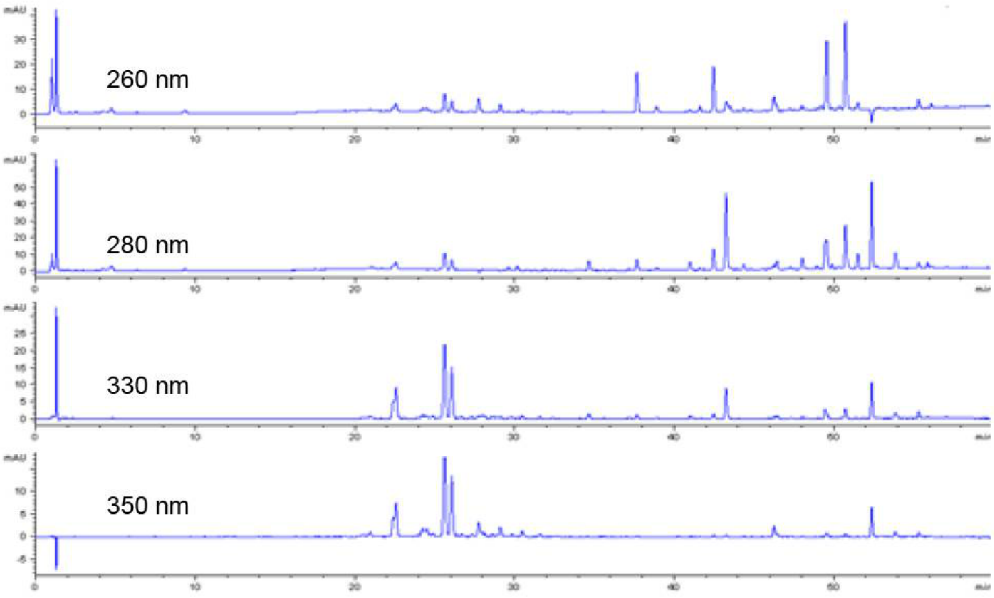
Conditions

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

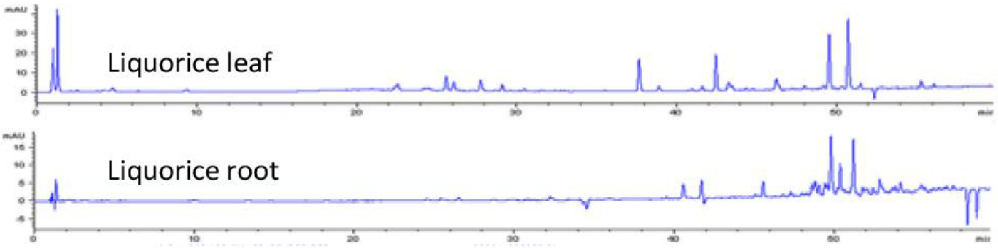
Time (mins)	%B
0	10
1	10
11	15
55	90
60	100

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



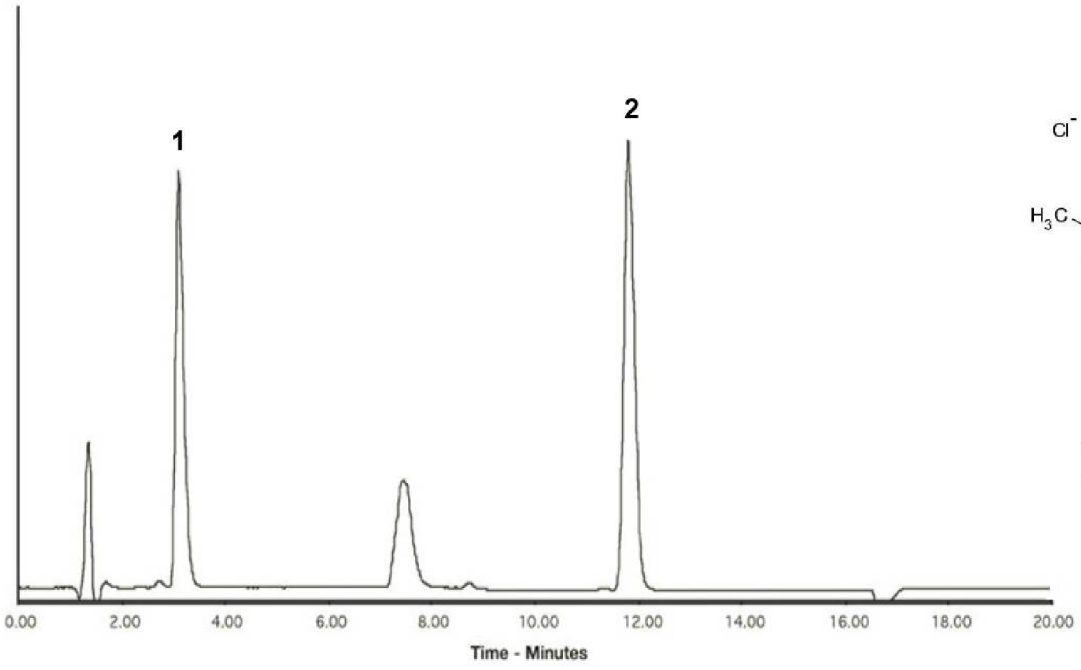
Malachite Green

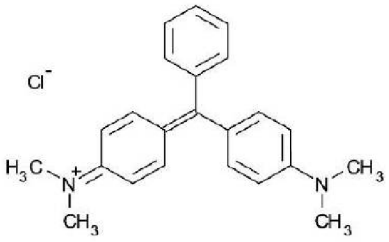
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2860**

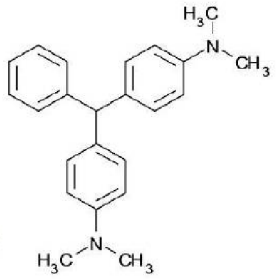
Conditions

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

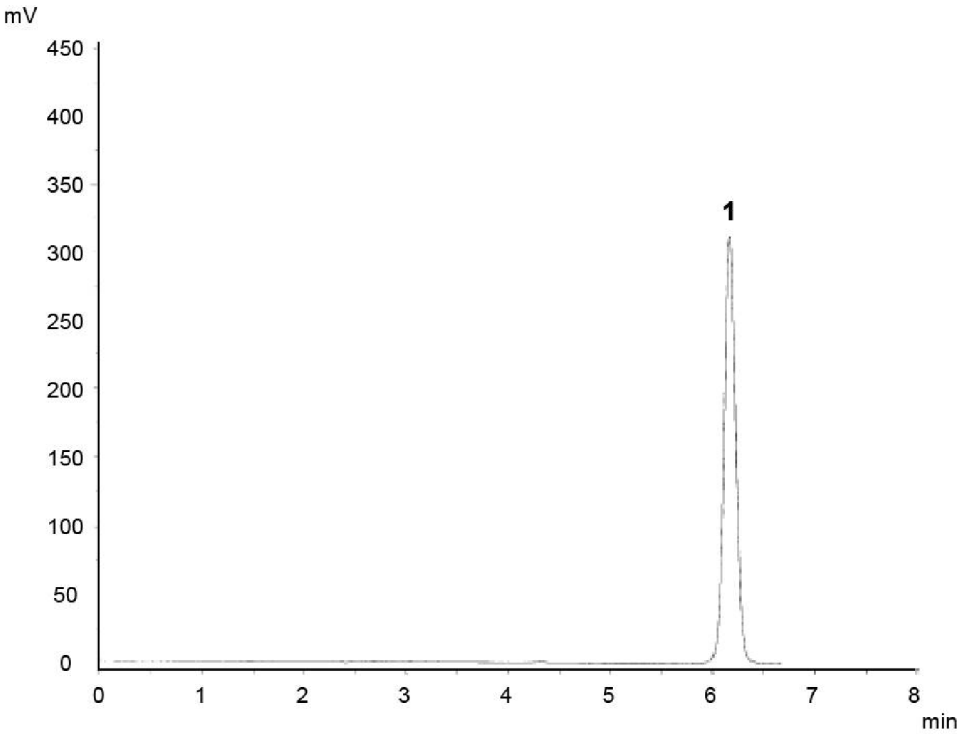
Melamine using Ion-Pairing Reagent

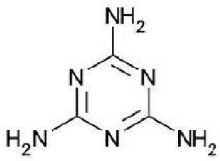
ACE®
Ultra-inert
UHPLC & HPLC Columns

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

Microcystins from Blue/Green Algae in Drinking Water

ACE®
Ultra-inert
UHPLC & HPLC Columns

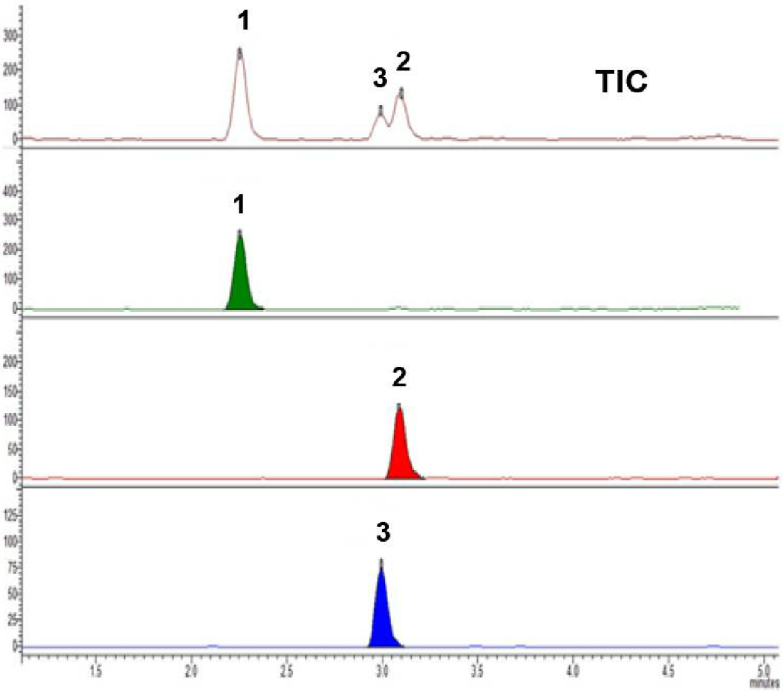
Application #**AN1190**

Conditions

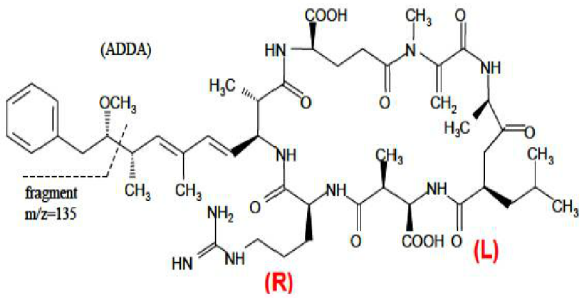
Column:	ACE Excel 2 C18
Dimensions:	100 x 2.1 mm
Part Number:	EXL-101-1002U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: MeCN

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

Milk Proteins

ACE®
Ultra-inert
UHPLC & HPLC Columns

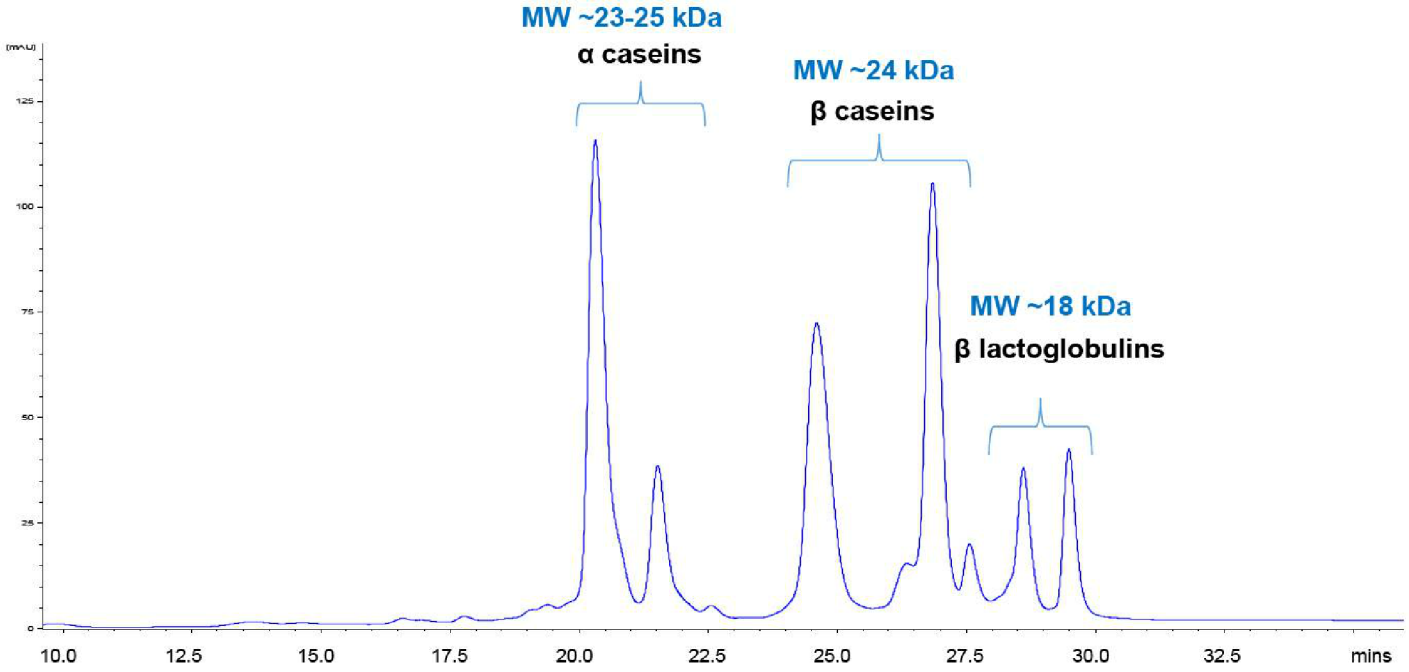
Application #**AN1540**

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



Mycotoxins by LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

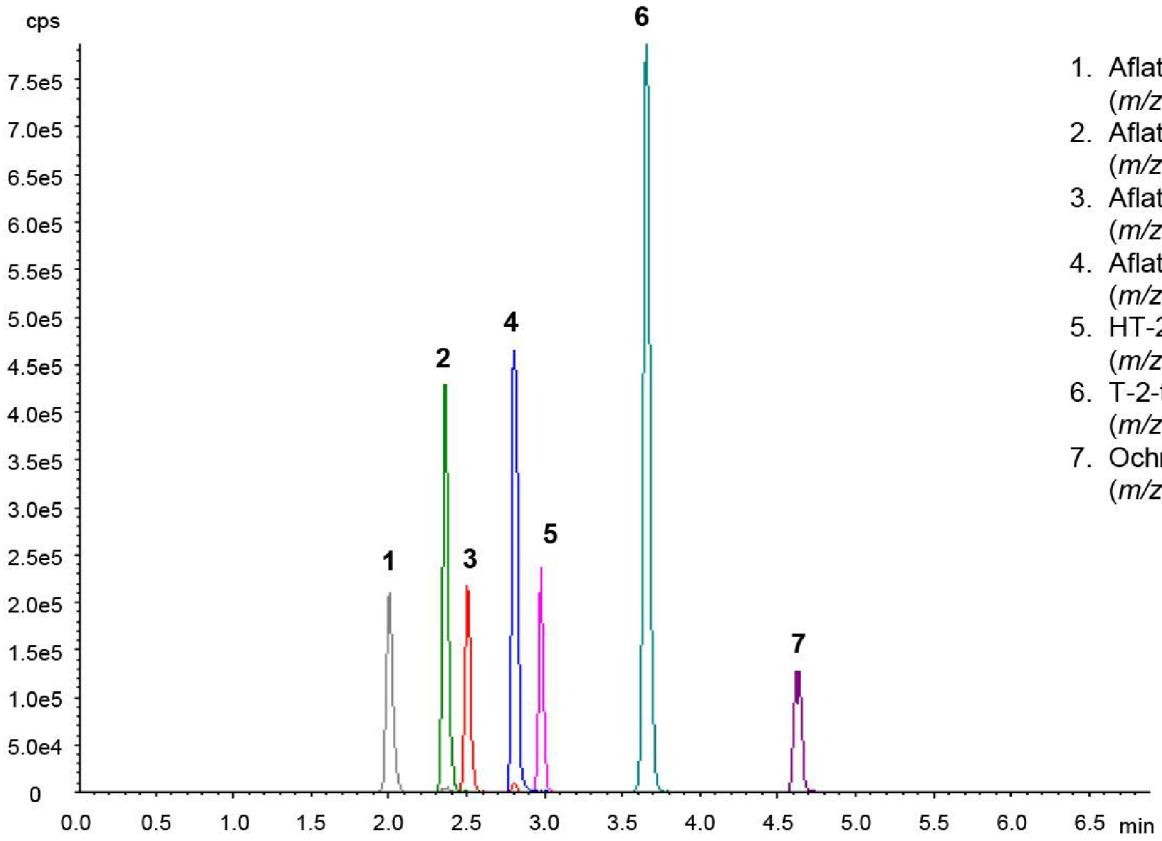
Application #**AN2330**

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)

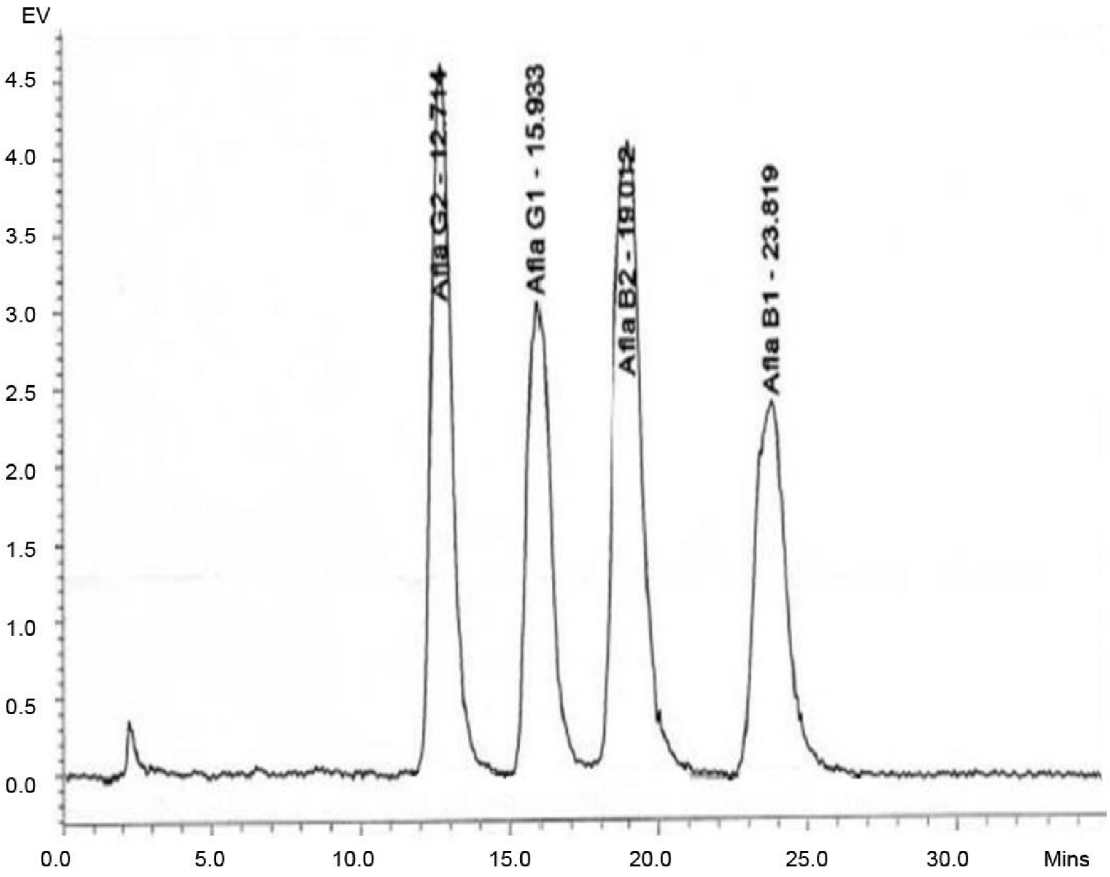
Mycotoxins / Aflatoxins from Peppers

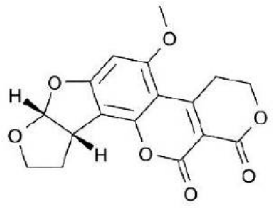
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1200**

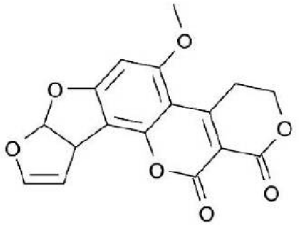
Conditions

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

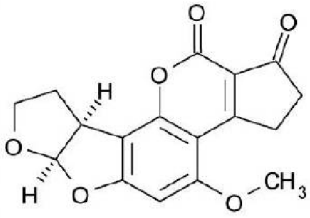




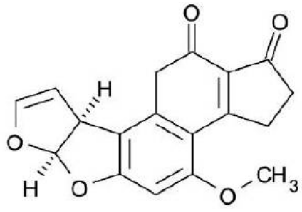
1. Aflatoxin G2



2. Aflatoxin G1



3. Aflatoxin B2



4. Aflatoxin B1

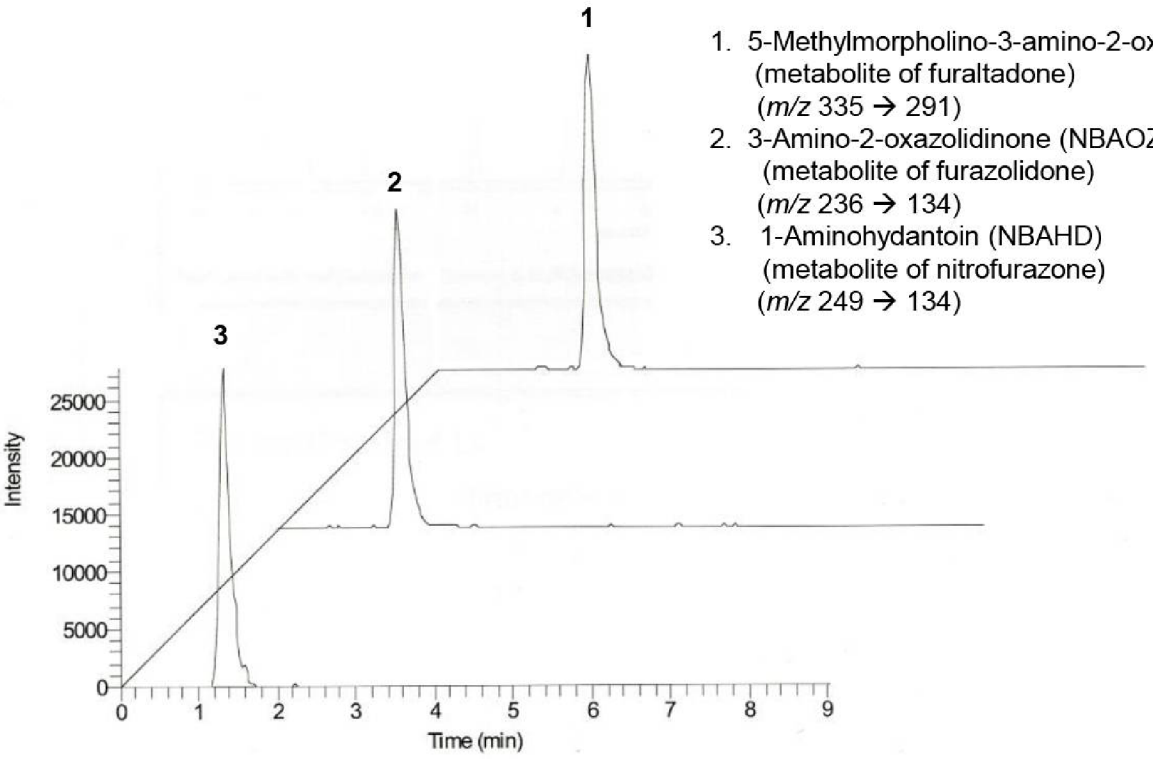
Nitrofuran Metabolites by LC-MS/MS

ACE®
Ultra-inert
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



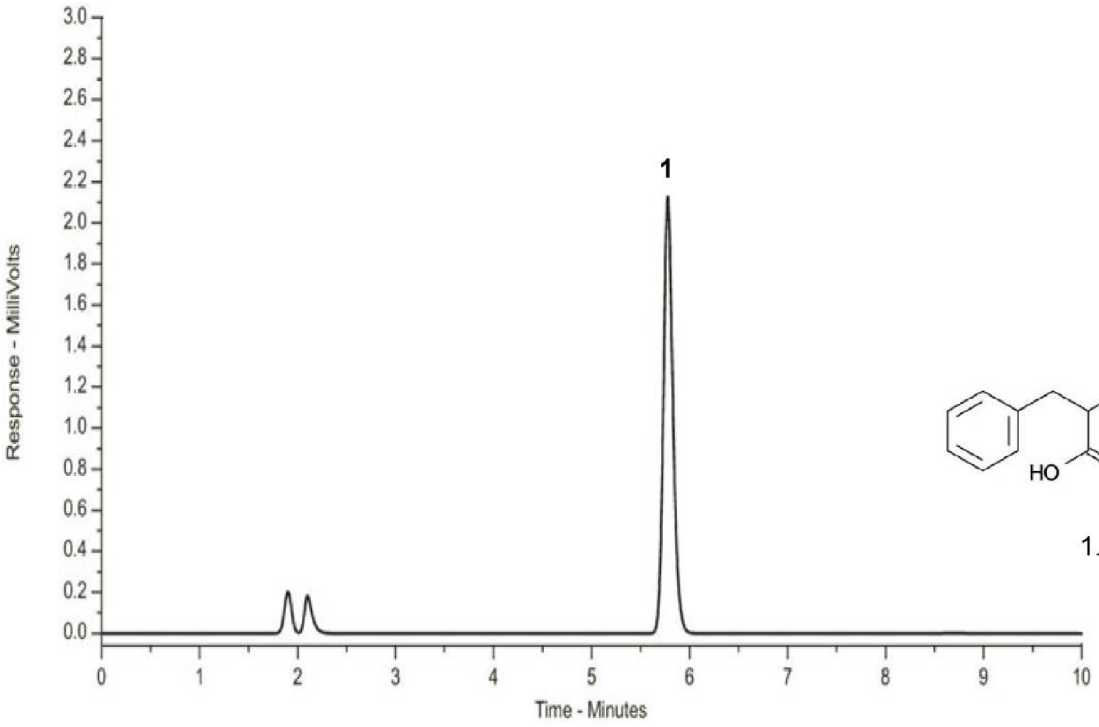
1. 5-Methylmorpholino-3-amino-2-oxazolidinone (NBAMOZ)
   (metabolite of furaltadone)
   (*m/z* 335 → 291)
2. 3-Amino-2-oxazolidinone (NBAOZ)
   (metabolite of furazolidone)
   (*m/z* 236 → 134)
3. 1-Aminohydantoin (NBAHD)
   (metabolite of nitrofurazone)
   (*m/z* 249 → 134)

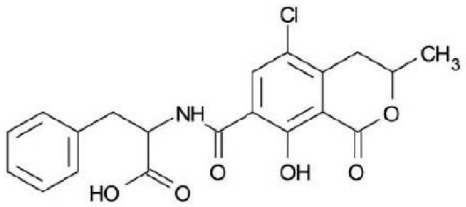
Ochratoxin A

Application #**AN2870**

Conditions

Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	MeCN/H_2O/Acetic acid (51:47:2 v/v)
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	Fluorescence – λ_{ex} 333 nm, λ_{em} 443 nm





1. Ochratoxin A

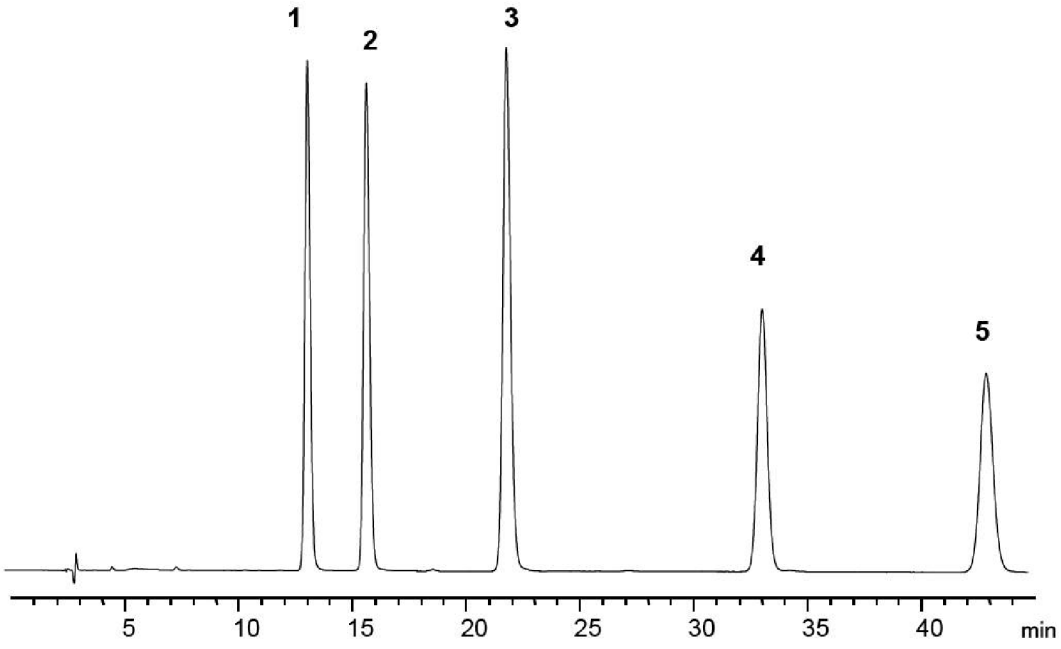
Organic Acids (I)

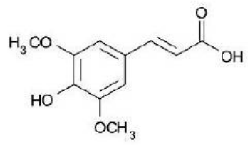
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1570**

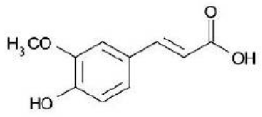
Conditions

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

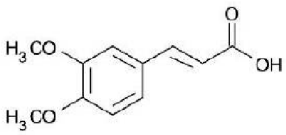




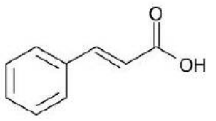
1. Sinapic acid



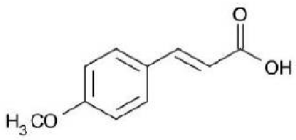
2. Ferulic acid



3. 3,4-Dimethoxycinnamic acid



4. Cinnamic acid



5. 4-Methoxycinnamic acid

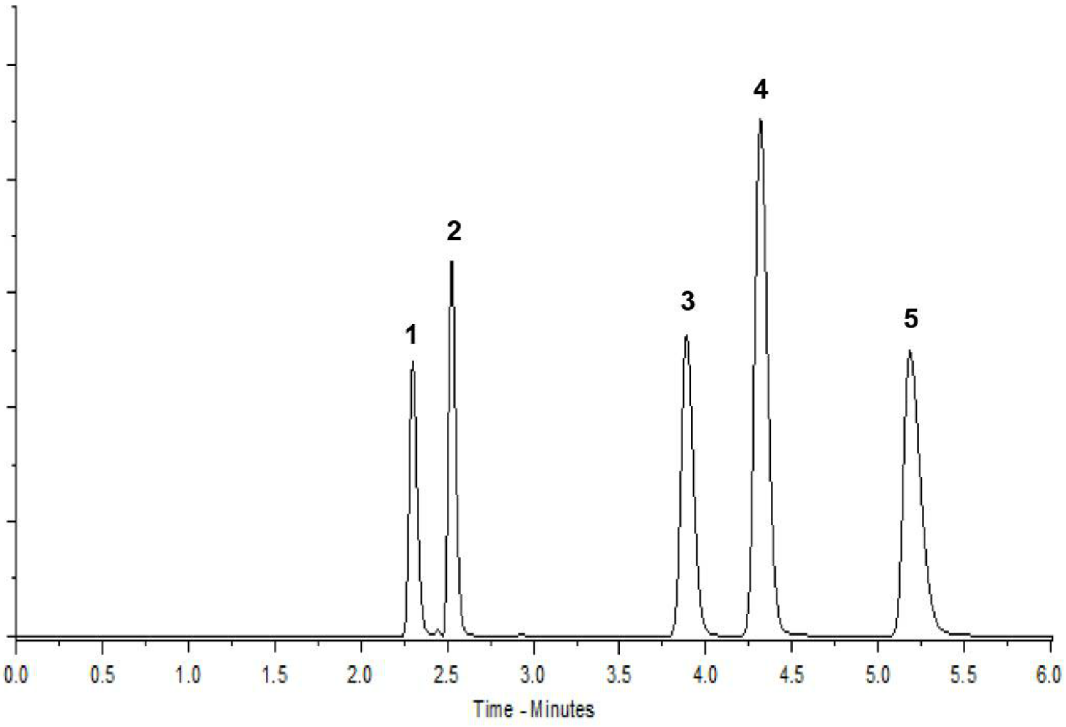
Organic Acids (II)

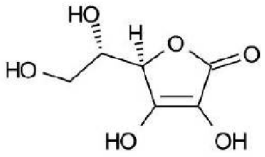
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2780**

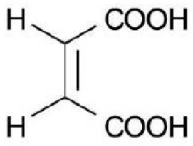
Conditions

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

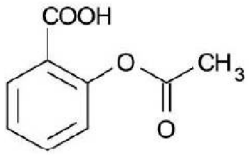




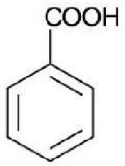
1. L-Ascorbic acid



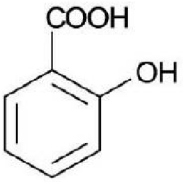
2. Maleic acid



3. Acetylsalicylic acid



4. Benzoic acid



5. Salicylic acid

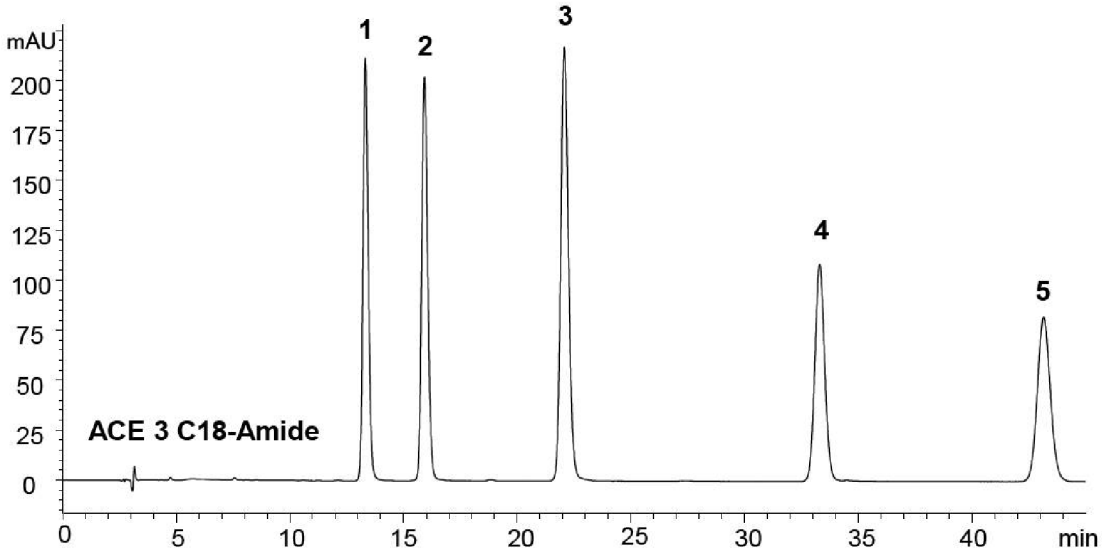
Organic Acids (III)

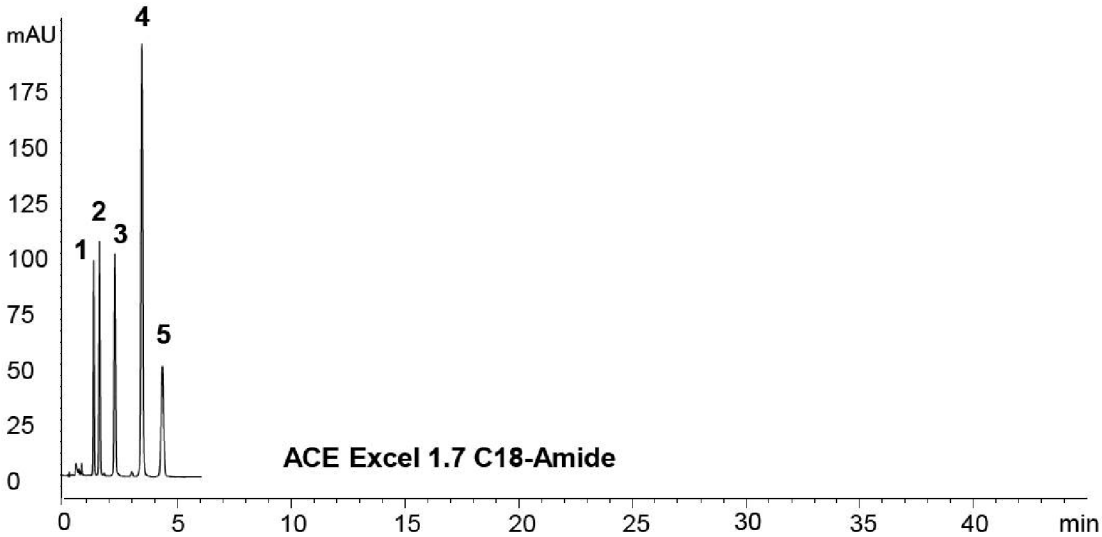
ACE®
Ultra-inert
UHPLC & HPLC Columns

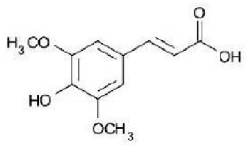
Application #AN2200

Conditions

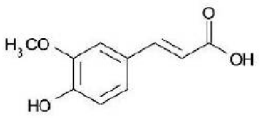
Column:	ACE 3 C18-Amide ACE Excel 1.7 C18-Amide
Dimensions:	250 x 2.1 mm 50 x 3.0 mm
Part Number:	250 x 2.1 mm (EXL-1112-2502U), 50 x 3 mm (EXL-1712-0503U)
Mobile Phase:	20 mM H_3PO_4 in MeOH/H_2O (40:60 v/v)
Flow Rate:	0.21 mL/min (250 x 2.1 mm) 0.8 mL/min (50 x 3.0 mm)
Injection:	5 µL (250 x 2.1 mm)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



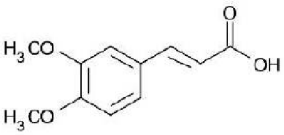




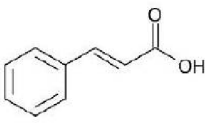
1. Sinapic acid



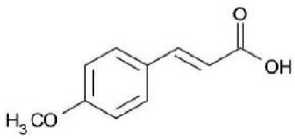
2. Ferulic acid



3. 3,4-Dimethoxycinnamic acid



4. Cinnamic acid



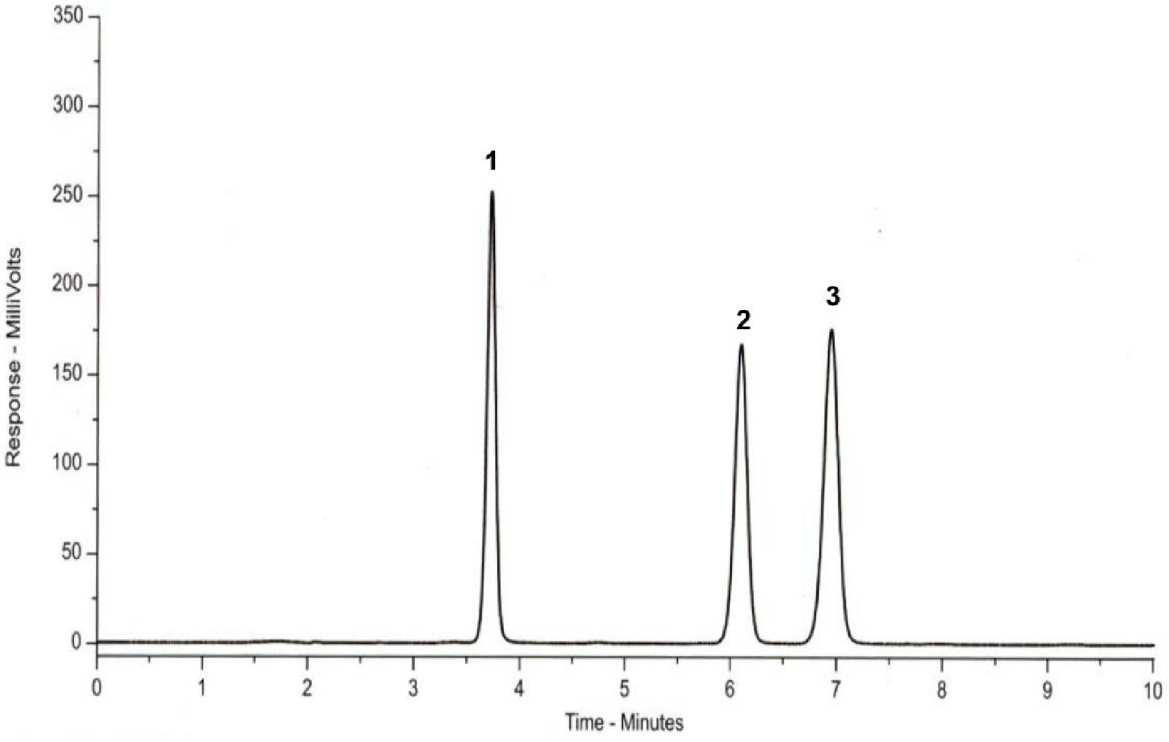
5. 4-Methoxycinnamic acid

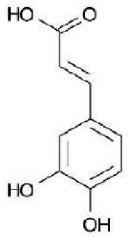
Organic Acids (IV)

Application #**AN3030**

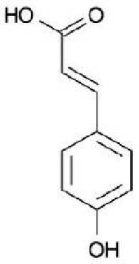
Conditions

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

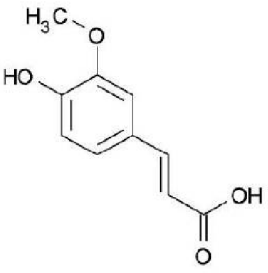




1. Caffeic acid



2. p-Coumaric acid



3. Ferulic acid

Organophosphorus Flame Retardants in Water by LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN1240

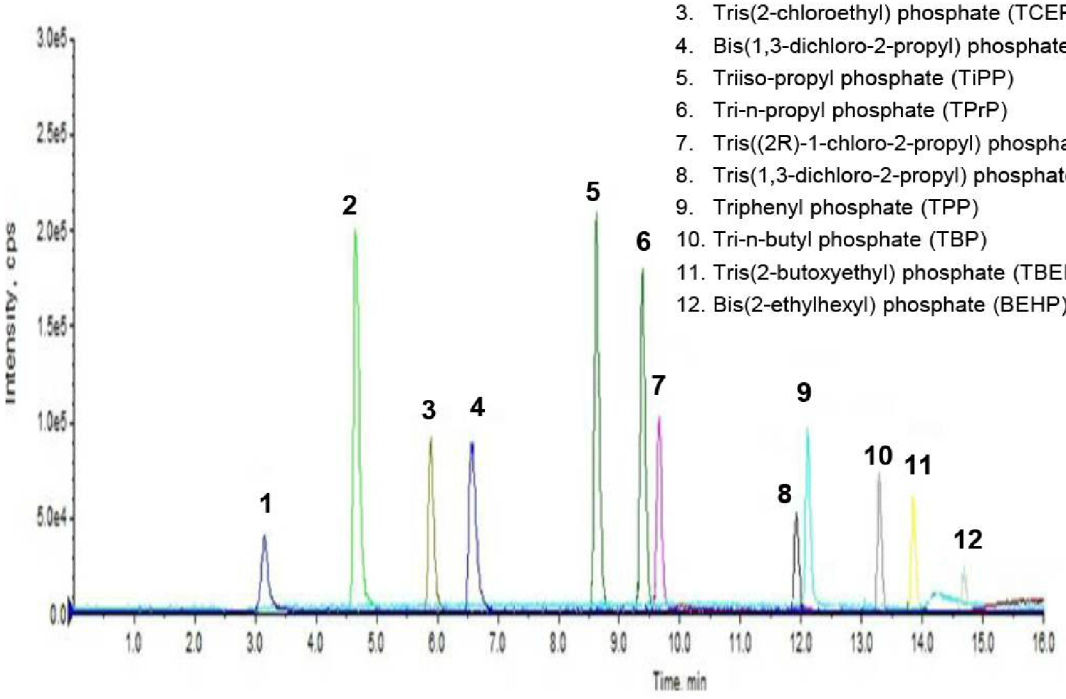
Conditions

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



Organophosphorus Isomer Flame Retardants in Water

ACE®
Ultra-inert
UHPLC & HPLC Columns

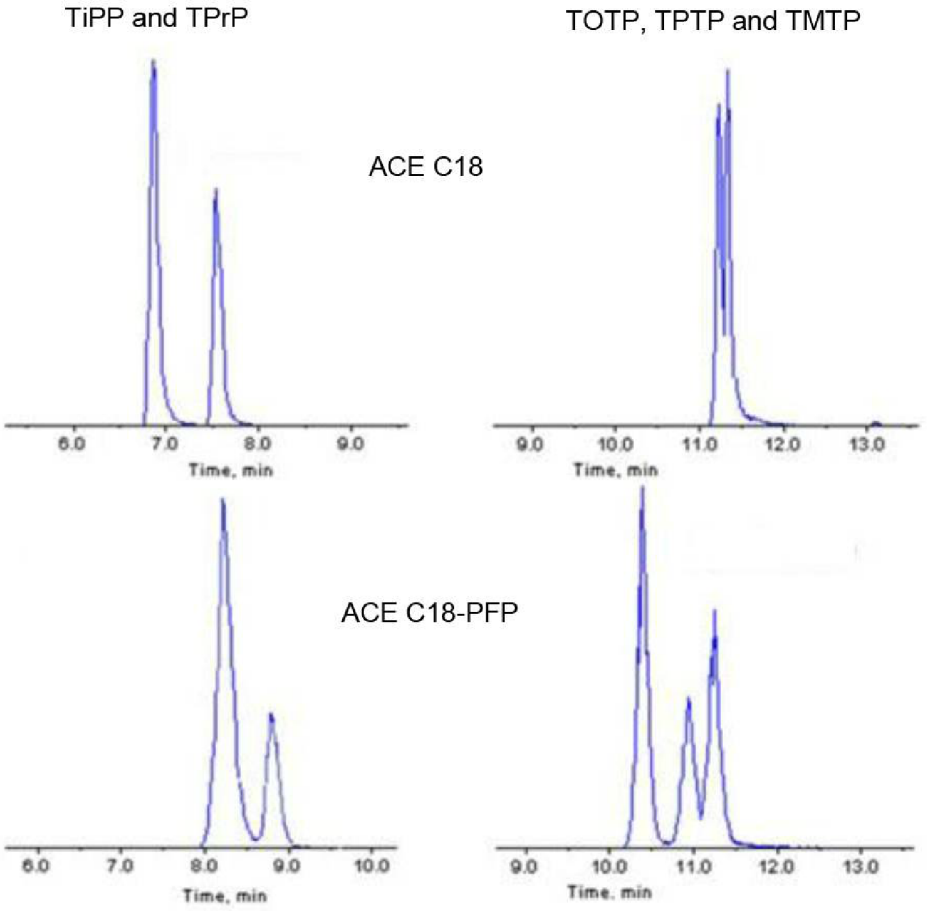
Application #AN1140

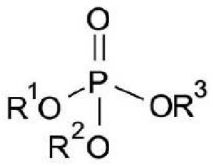
Conditions

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





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

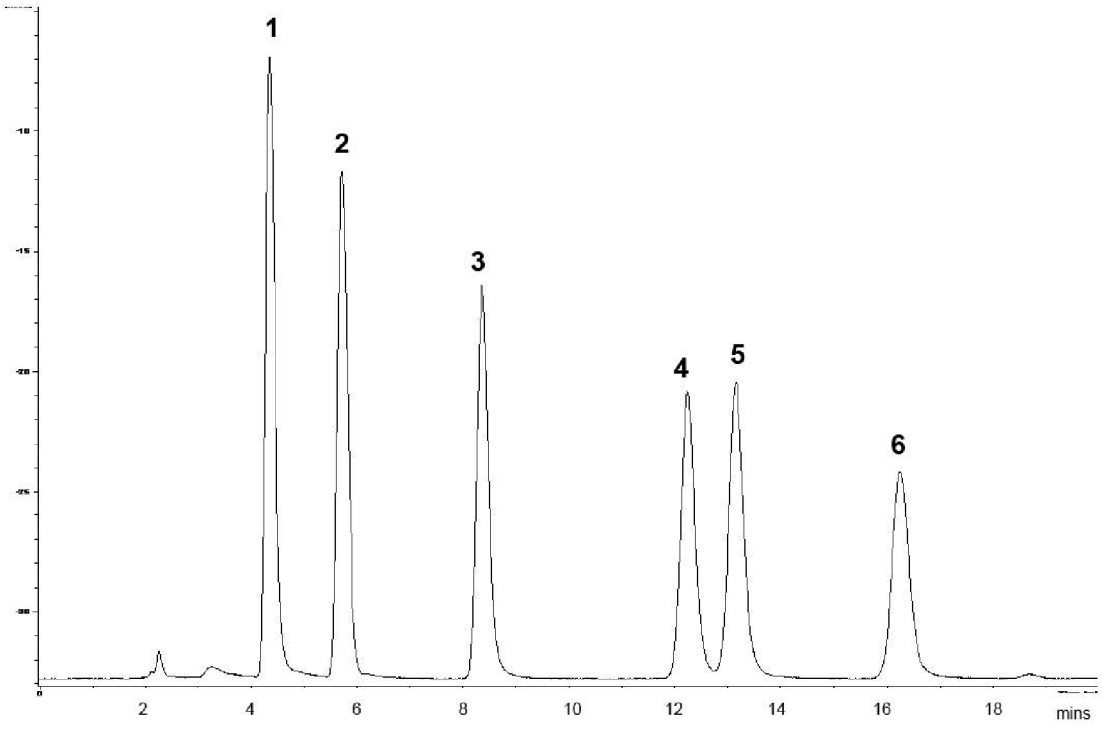
Paraben Preservatives

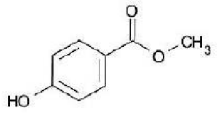
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN1250

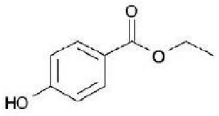
Conditions

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

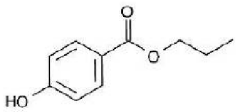




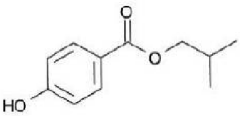
1. Methyl paraben



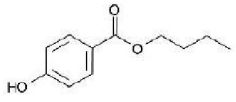
2. Ethyl paraben



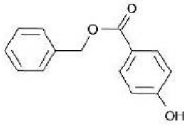
3. n-Propyl paraben



4. i-Butyl paraben



5. n-Butyl paraben



6. Benzyl paraben

Perfluoro Acids by LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

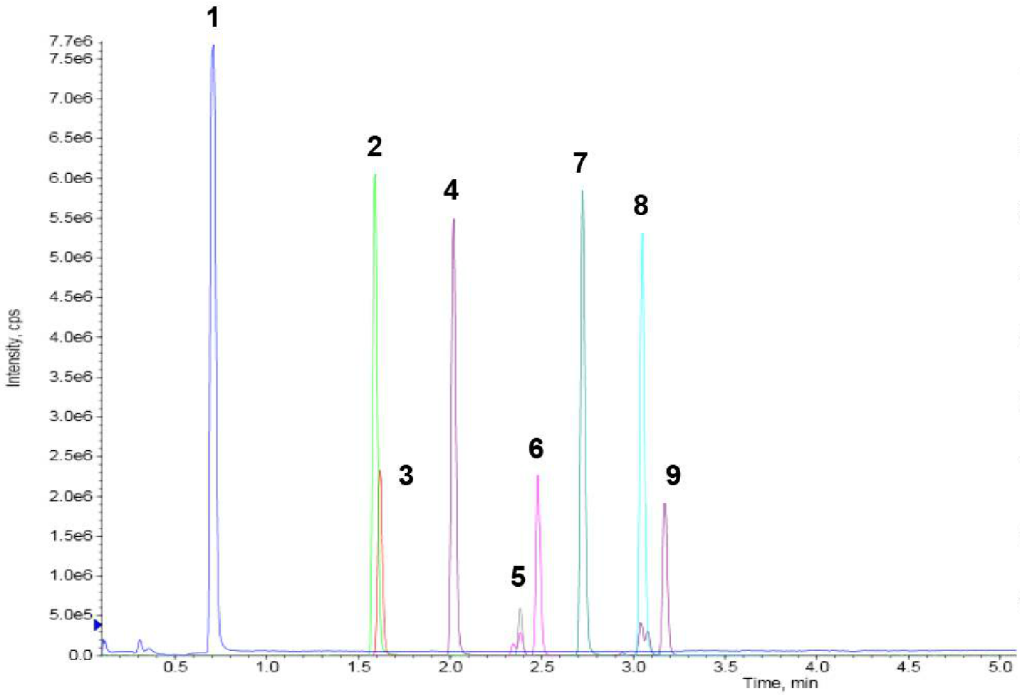
Application #AN1280

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. Perfluorobutanesulfonic acid (*m/z* 299 → 79.9)
4. Perfluoroheptanoic acid (*m/z* 363 → 319)
5. Perfluorooctanoic acid (*m/z* 413 → 368.9)
6. Perfluorohexanesulfonic 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)

Perfluoroalkyl Substances by Ion-Pairing LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

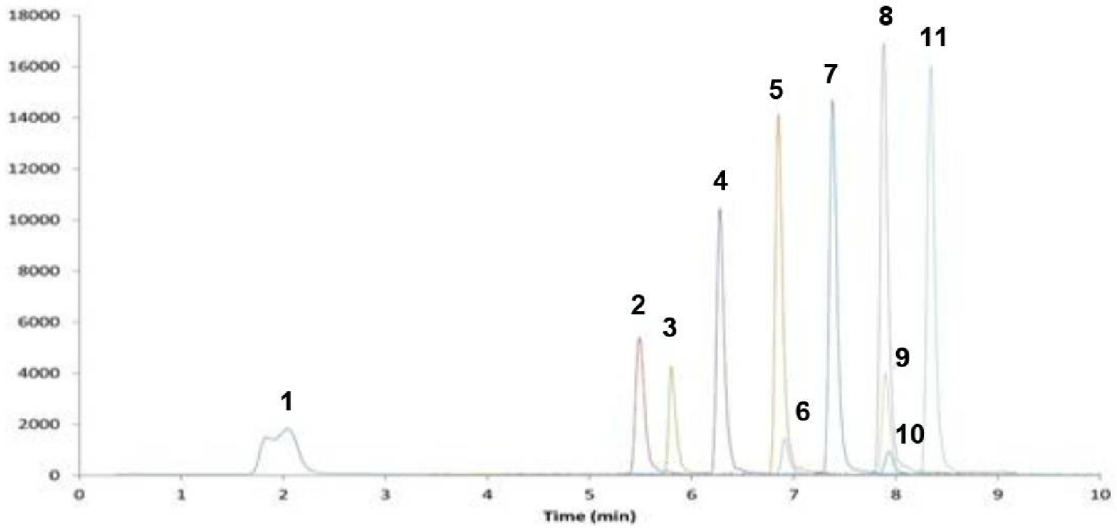
Application #**AN2560**

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)

Perfluorinated Compounds in Water by LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

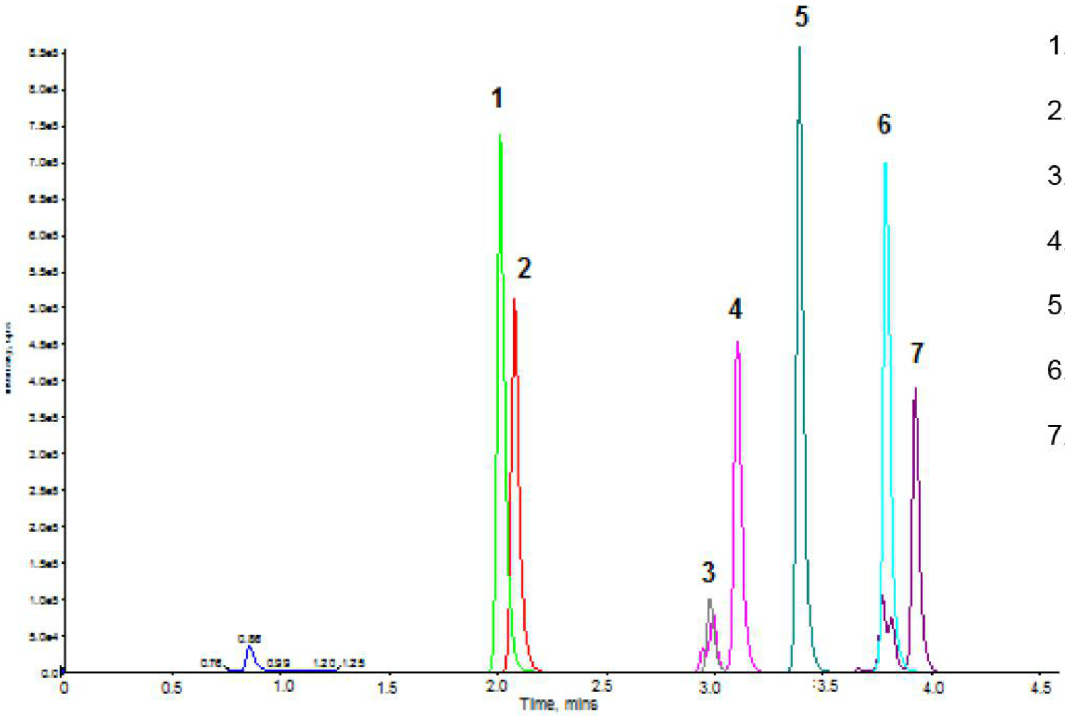
Application #AN2260

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

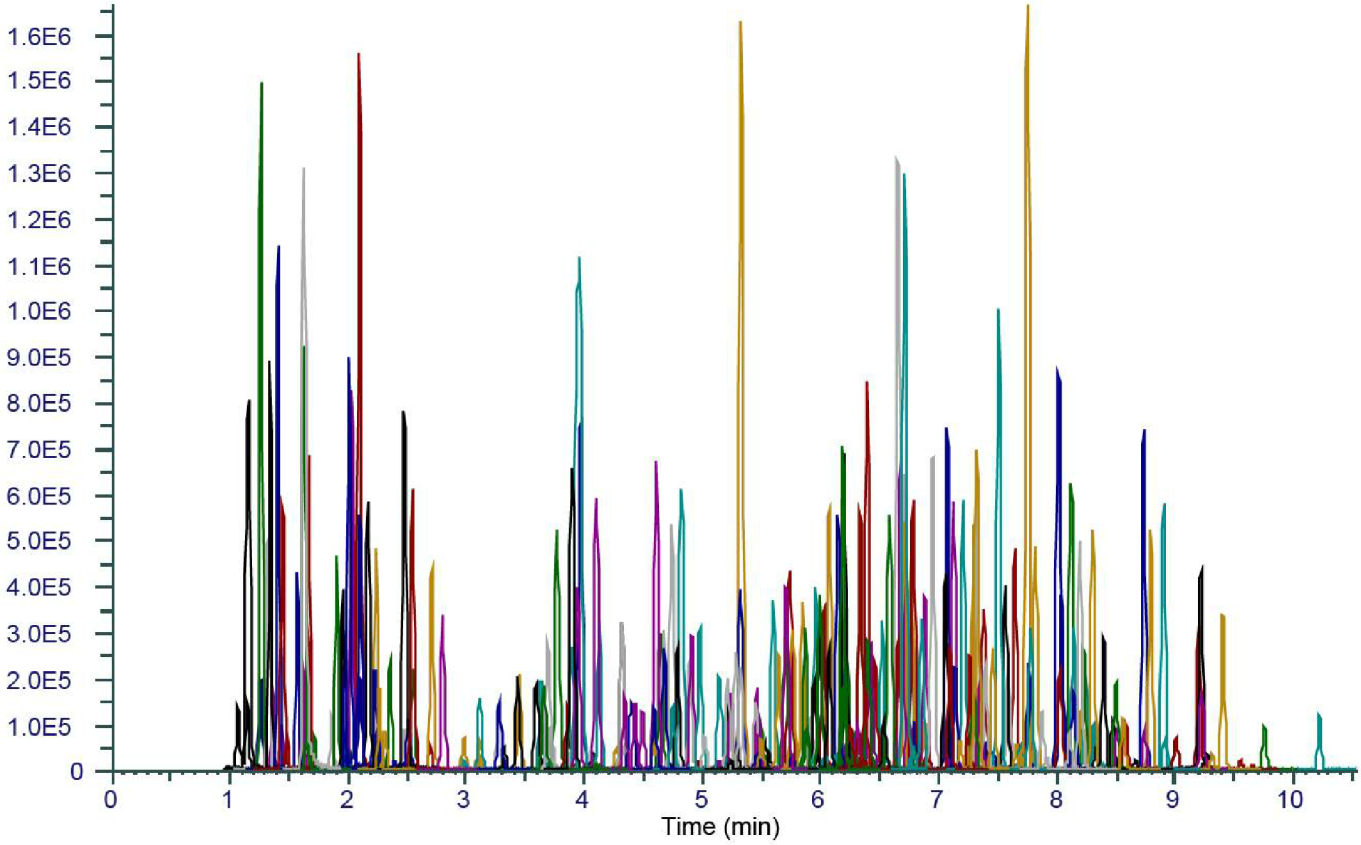
ACE®
Ultra-inert
UHPLC & HPLC Columns

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



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

250 Pesticide Screen using LC-MS/MS

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
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

250 Pesticide Screen using LC-MS/MS

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						

Pesticides by LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

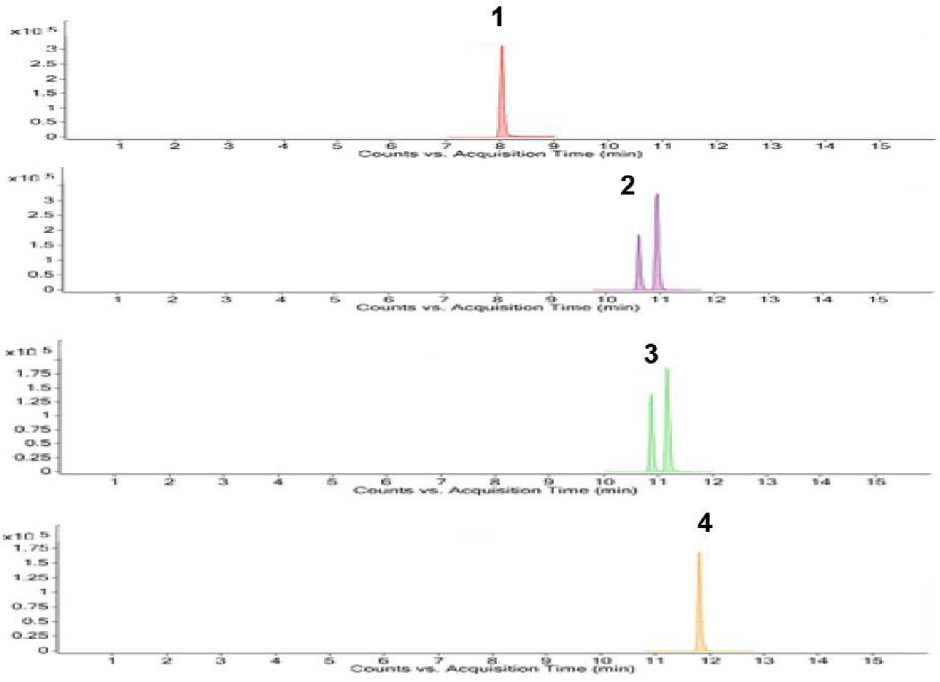
Application #AN1290

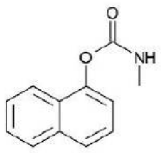
Conditions

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)

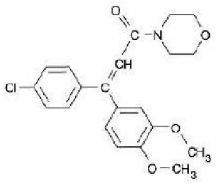
Time (mins)	%B
0.00	0
1.00	0
15.00	100
18.00	100
18.05	0
20.00	0

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

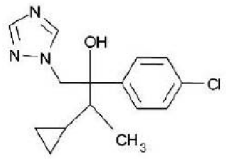




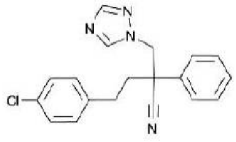
1. Carbaryl
(*m/z* 202.10 → 145.10)



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

Pesticides in Water

ACE®
Ultra-inert
UHPLC & HPLC Columns

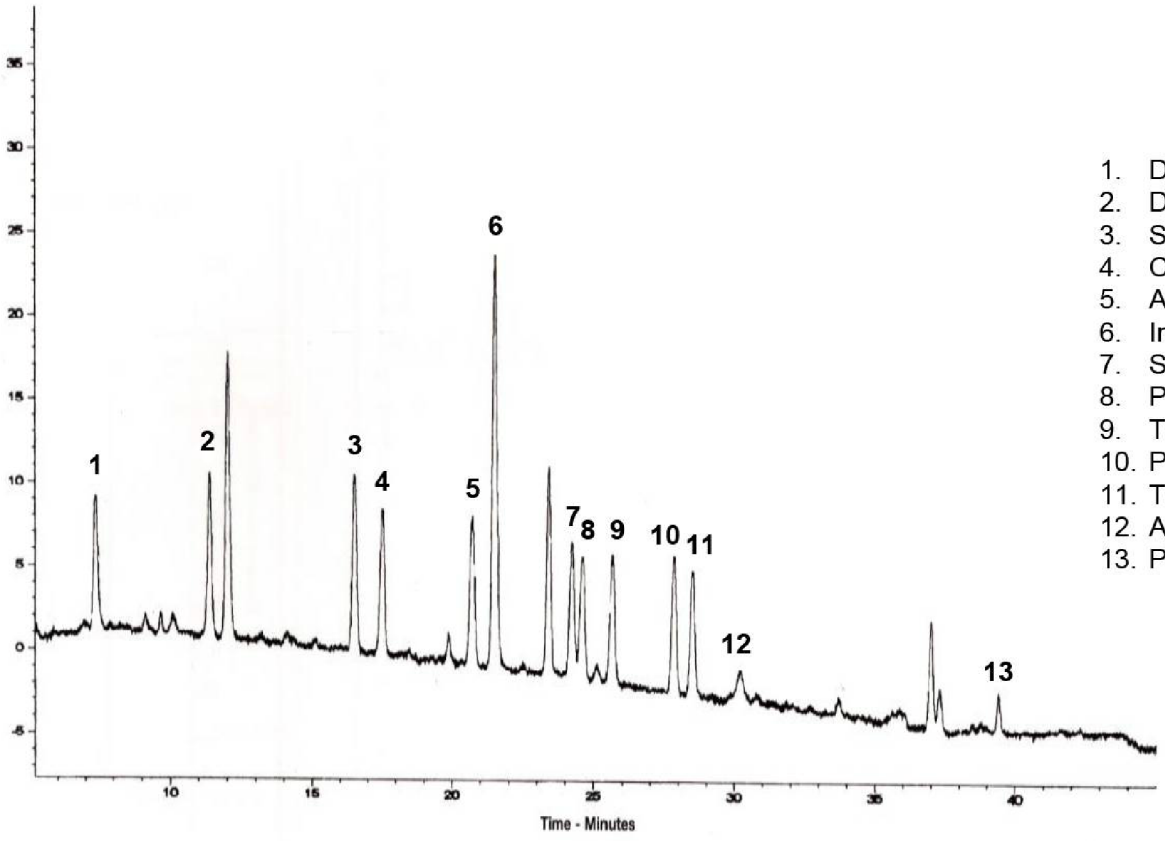
Application #AN3020

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

Phenolic Compounds in Ground Water & Landfill Leachates

ACE®
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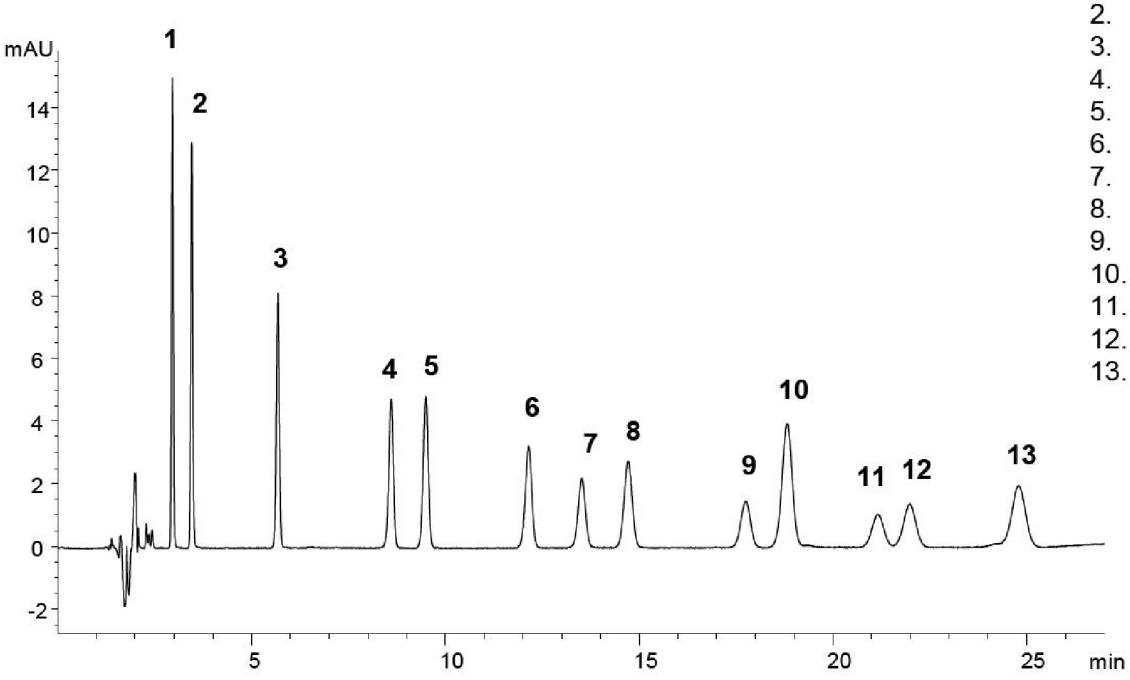
UHPLC & HPLC Columns

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

Phenol and Phenoxy Acid Herbicides

ACE®
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UHPLC & HPLC Columns

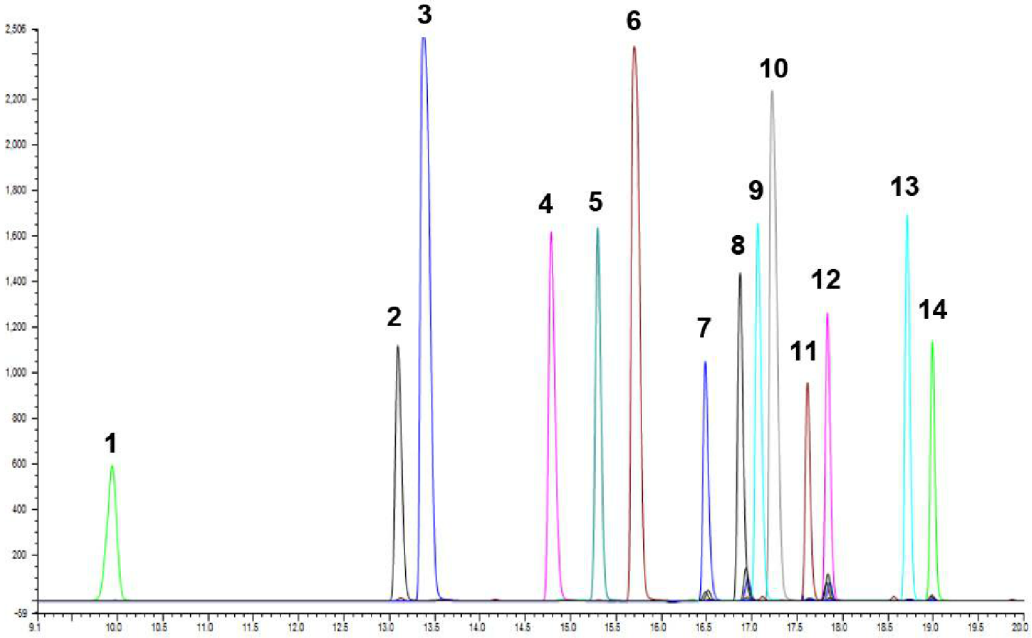
Application #AN2290

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

Phenols in Purple Coneflower (*Echinacea Purpurea)*

ACE®
Ultra-inert
UHPLC & HPLC Columns

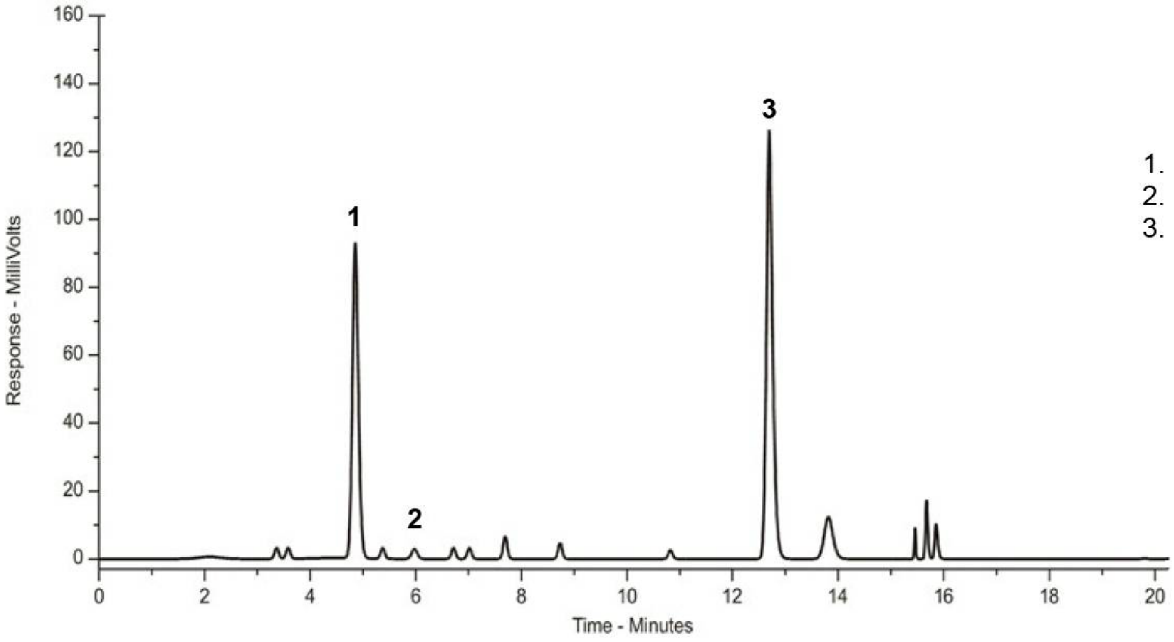
Application #**AN2920**

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

Phytoestrogens from Hop Extract by LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

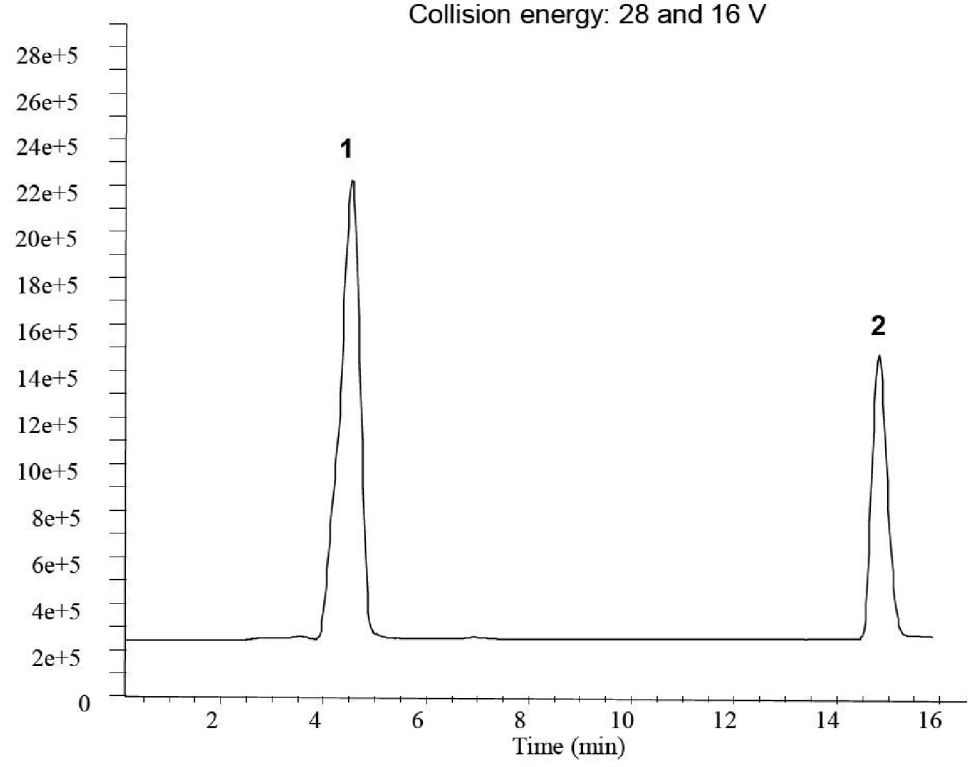
Application #AN1160

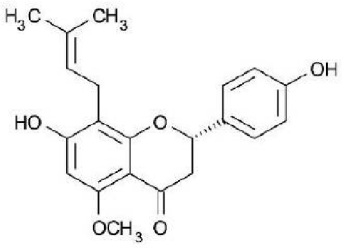
Conditions

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

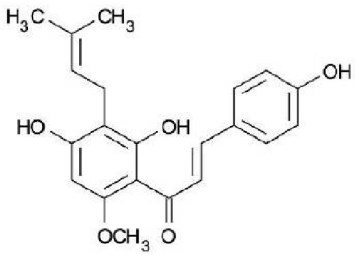
Time (mins)	%A	%B	%C	%D
0	56	0	44	0
8	51	5	44	0
10	51	5	44	0
17	95	5	0	0
22	95	0	0	5

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

Preservatives (I)

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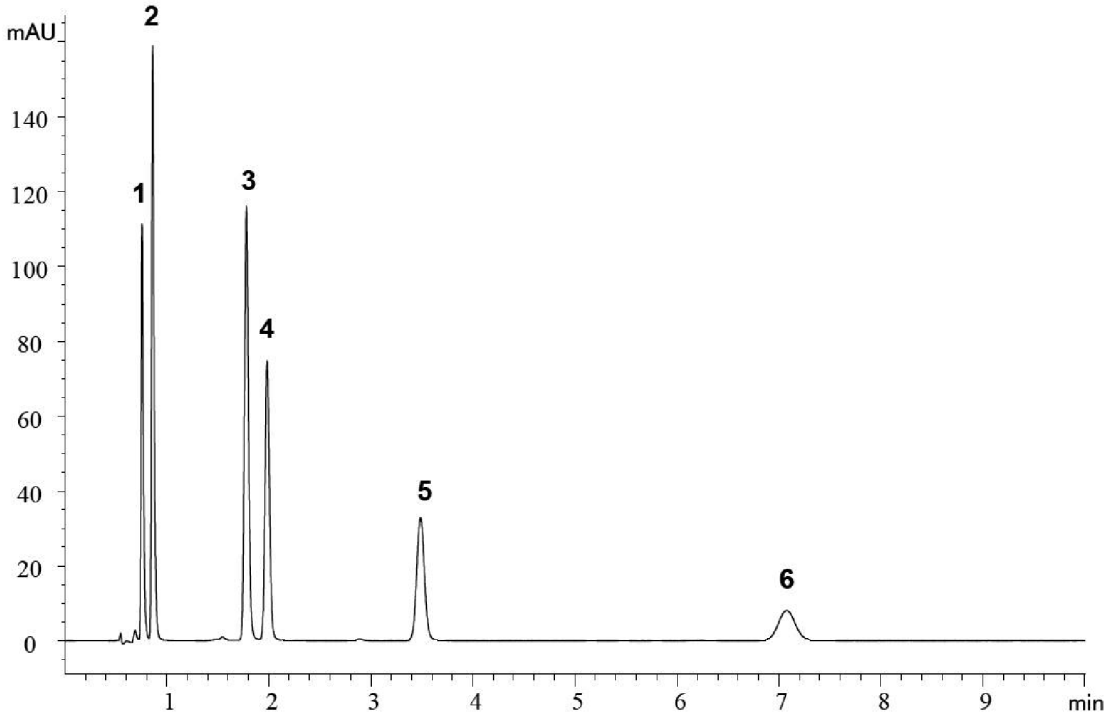
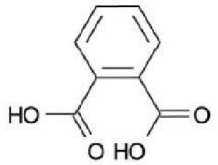
UHPLC & HPLC Columns

Application #AN2230

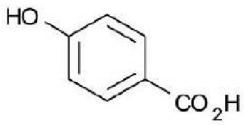
Conditions

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

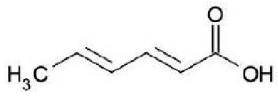




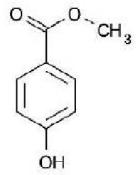
1. Phthalic acid



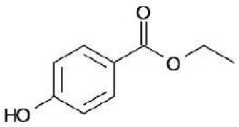
2. 4-Hydroxybenzoic acid



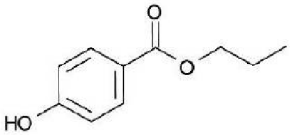
3. Sorbic acid



4. Methyl paraben



5. Ethyl paraben



6. Propyl paraben

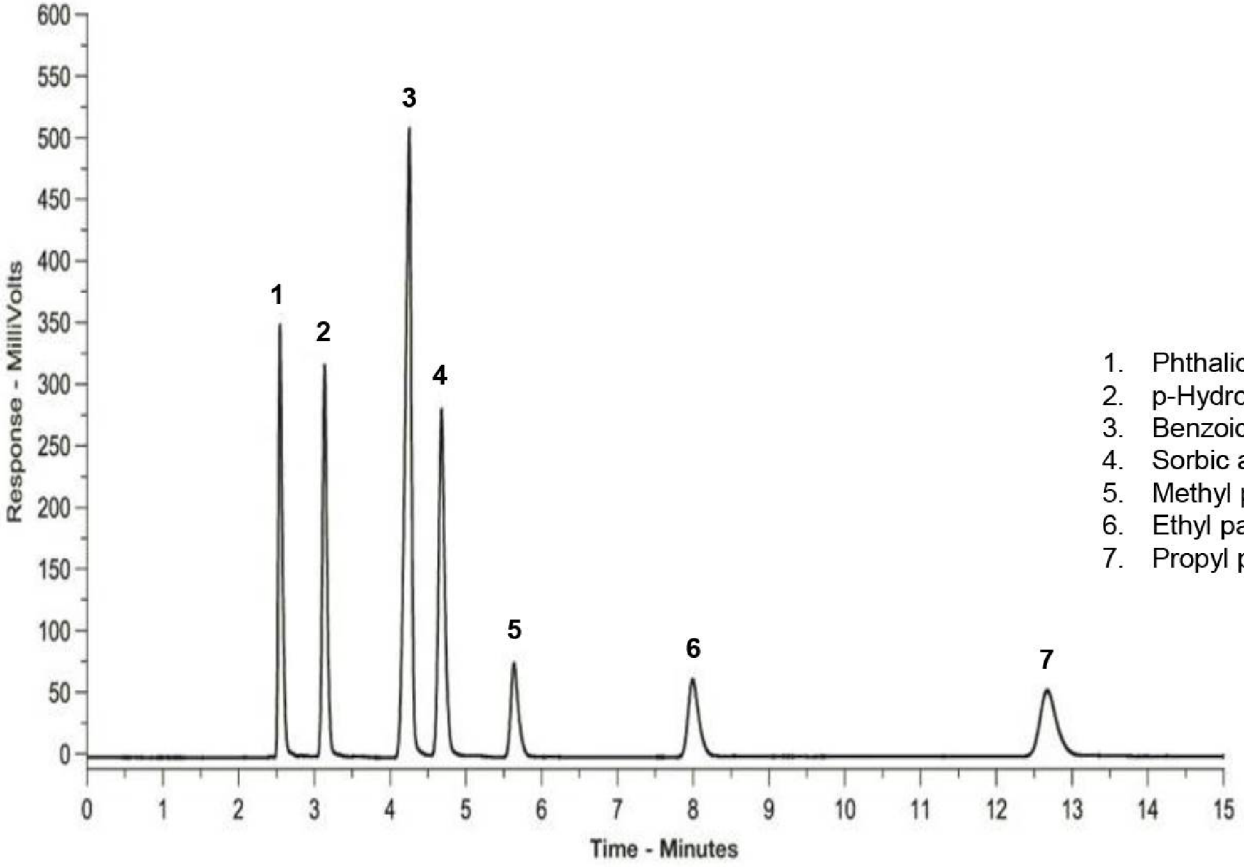
Preservatives (II)

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

Sennosides in Traditional Chinese Medicine

ACE®
Ultra-inert
UHPLC & HPLC Columns

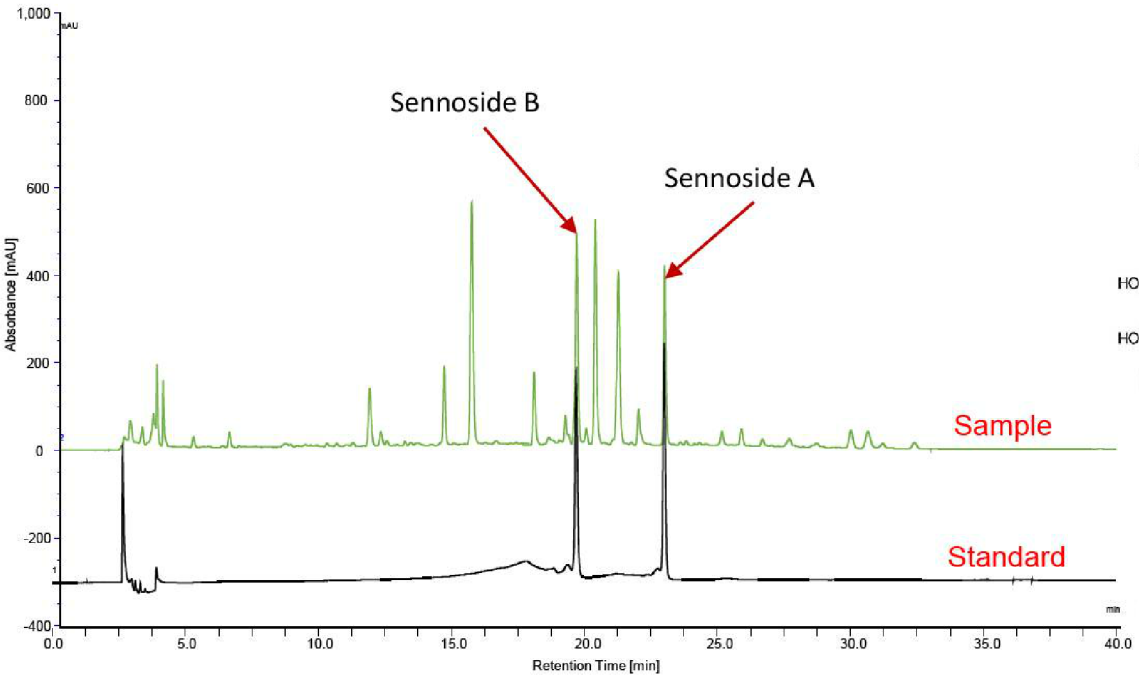
Application #AN1390

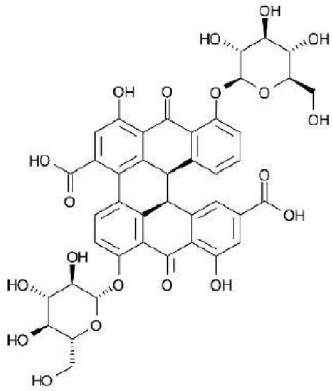
Conditions

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)

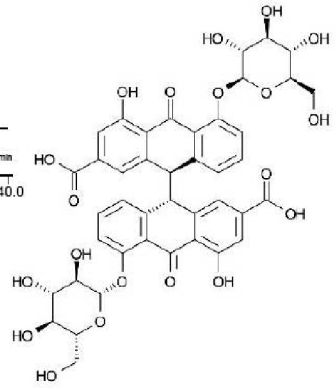
Time (mins)	%B
0	9
23	28
40	28

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

Spice Analysis for Illegal Dyes

ACE®
Ultra-inert
UHPLC & HPLC Columns

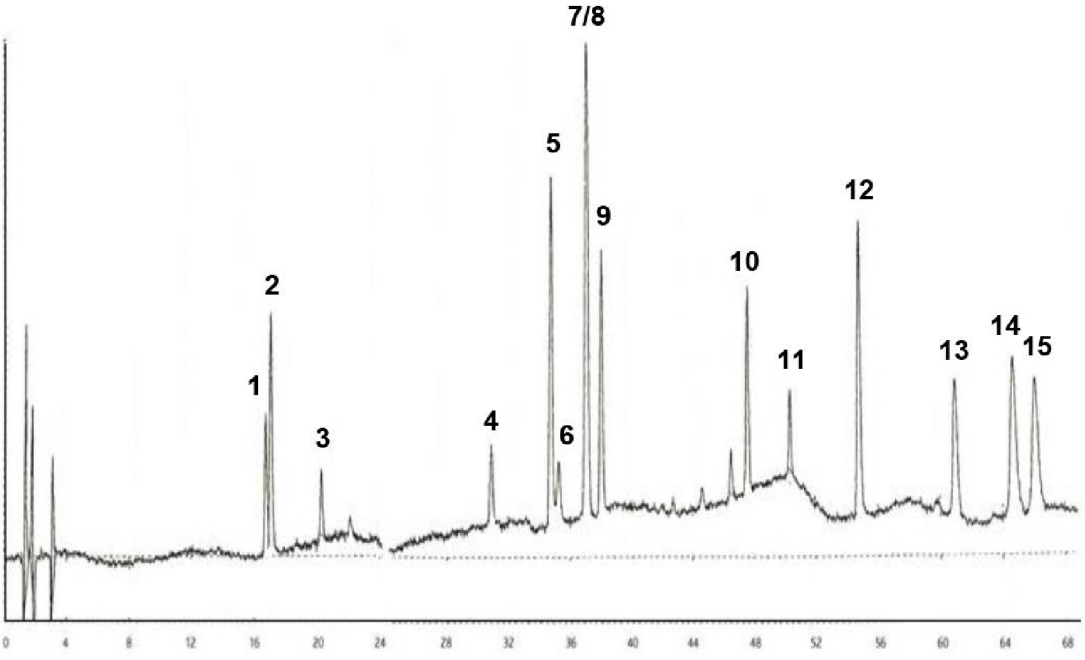
Application #**AN2910**

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

Sulfonamides

ACE®
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UHPLC & HPLC Columns

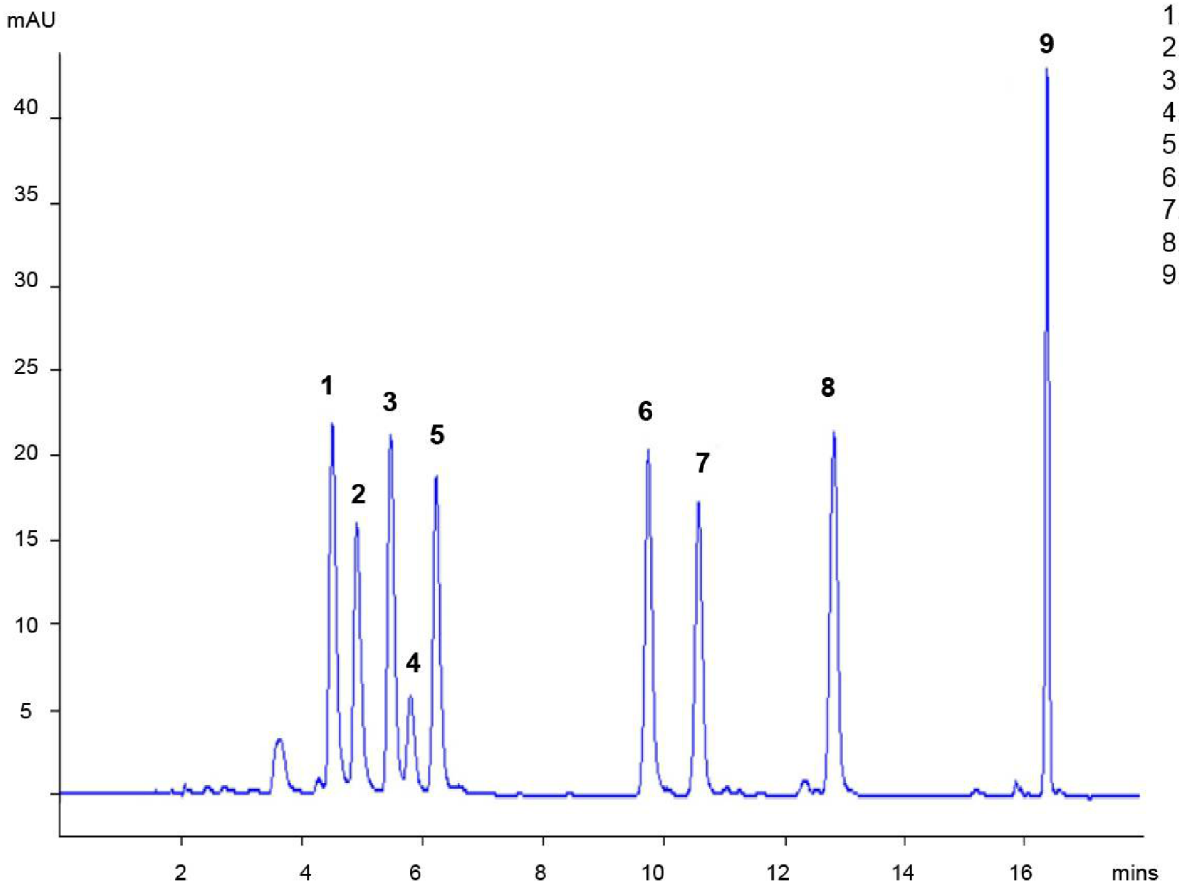
Application #**AN1610**

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

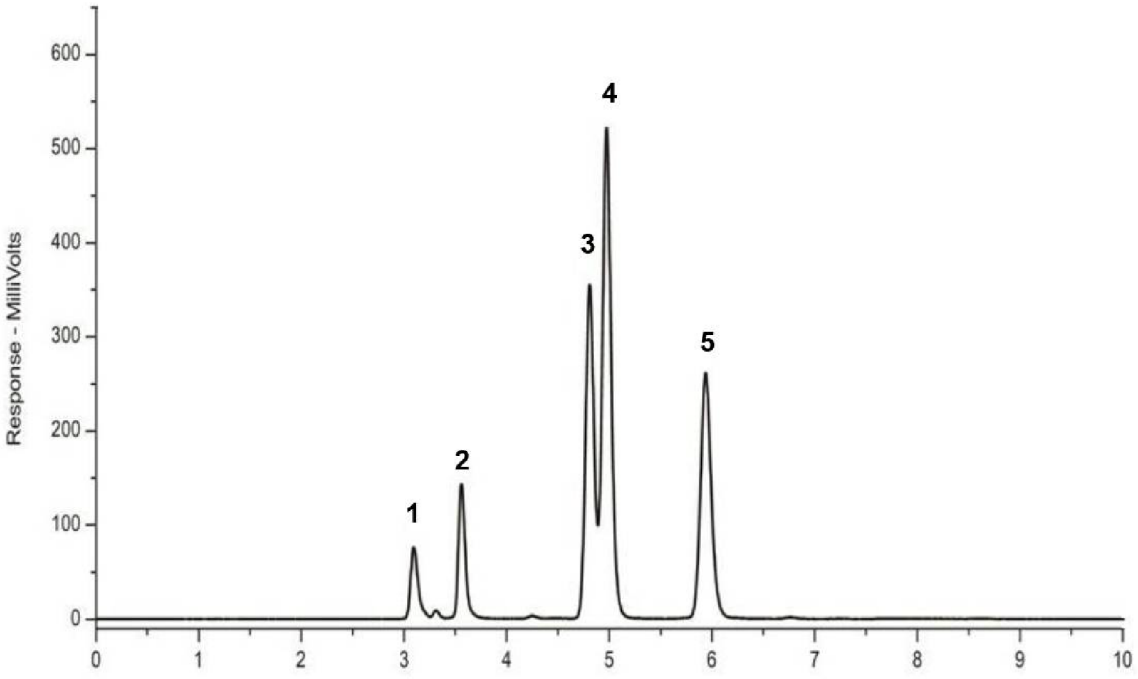
Tocopherols

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

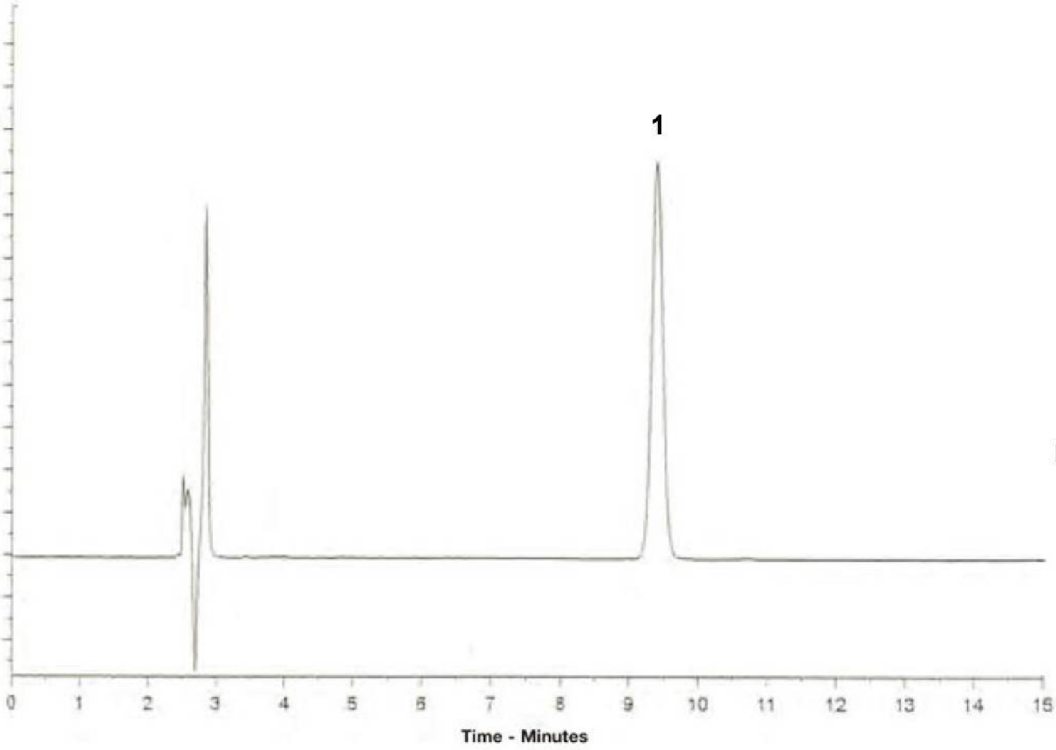
Trifluralin (Herbicide)

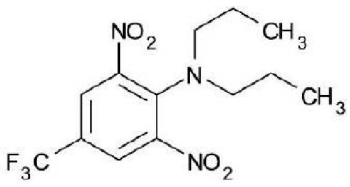
ACE®
Ultra-inert
UHPLC & HPLC Columns

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

BSA Tryptic Digest Profiling

ACE®
Ultra-inert
UHPLC & HPLC Columns

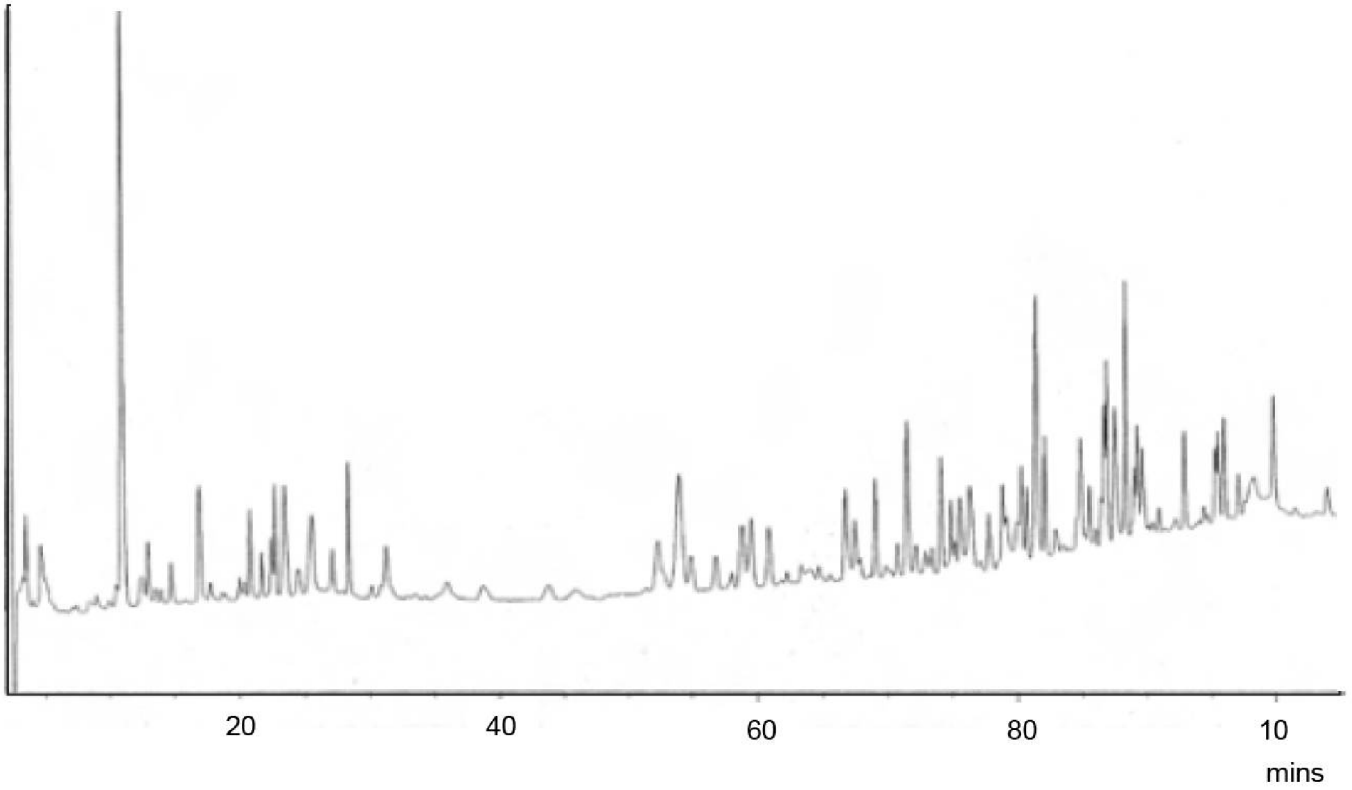
Application #**AN2000**

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



Vanillins

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN1620

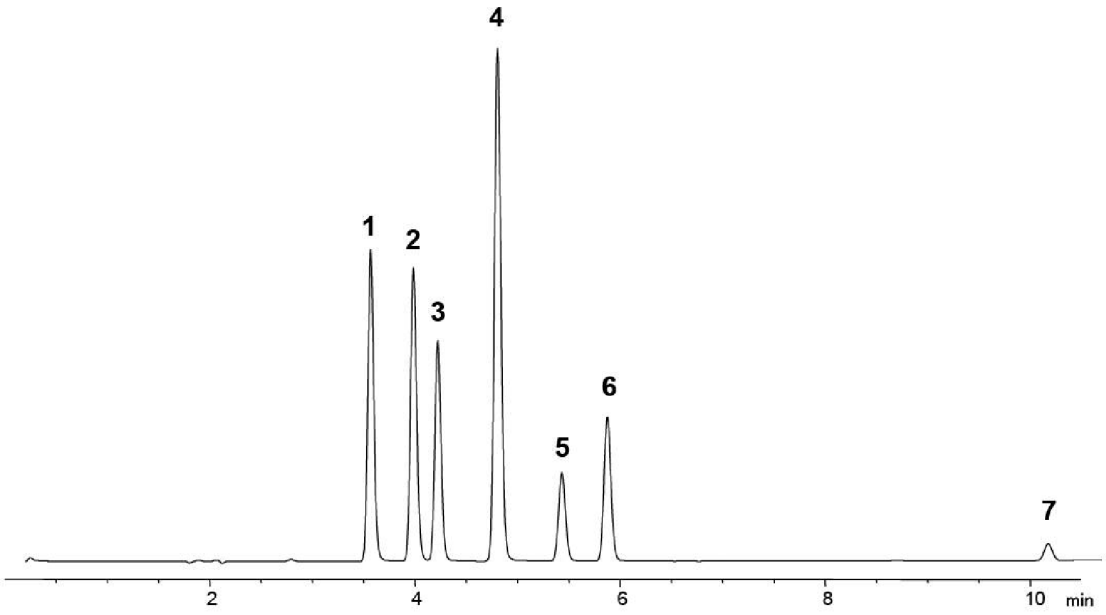
Conditions

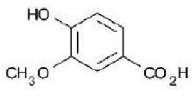
Column:	ACE 3 C18-Amide
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1112-1546U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

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

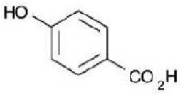
Post time 5 minutes

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

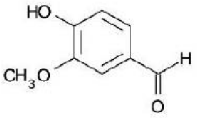




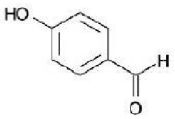
1. Vanillic acid



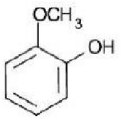
2. 4-Hydroxybenzoic acid



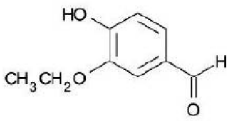
3. Vanillin



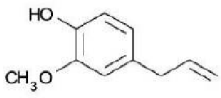
4. 4-Hydroxybenzaldehyde



5. Guaiacol



6. Ethyl Vanillin



7.Eugenol

Vanillins – Fast Analysis

ACE®
Ultra-inert
UHPLC & HPLC Columns

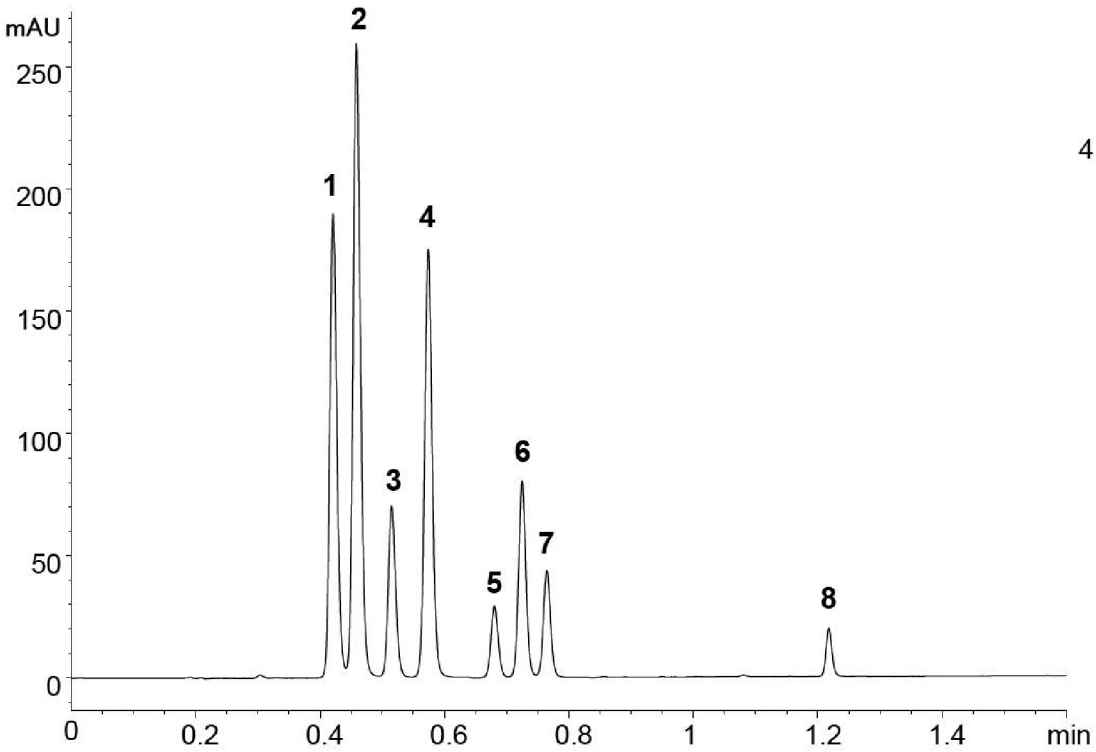
Application #AN2240

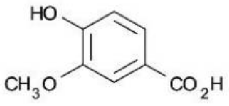
Conditions

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

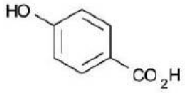
Time (mins)	%B
0.00	25
1.32	75
1.49	75
1.60	25

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

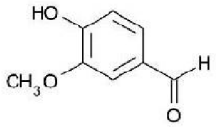




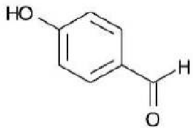
1. Vanillic acid



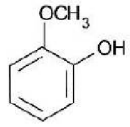
2. 4-Hydroxybenzoic acid



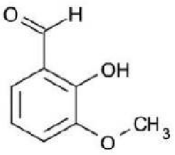
3. Vanillin



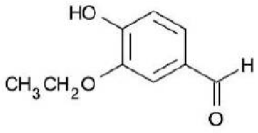
4. 4-Hydroxybenzaldehyde



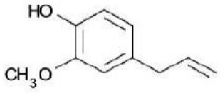
5. Guaiacol



6. o-Vanillin



7. Ethyl vanillin



8. Eugenol

Veterinary Steroids by LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

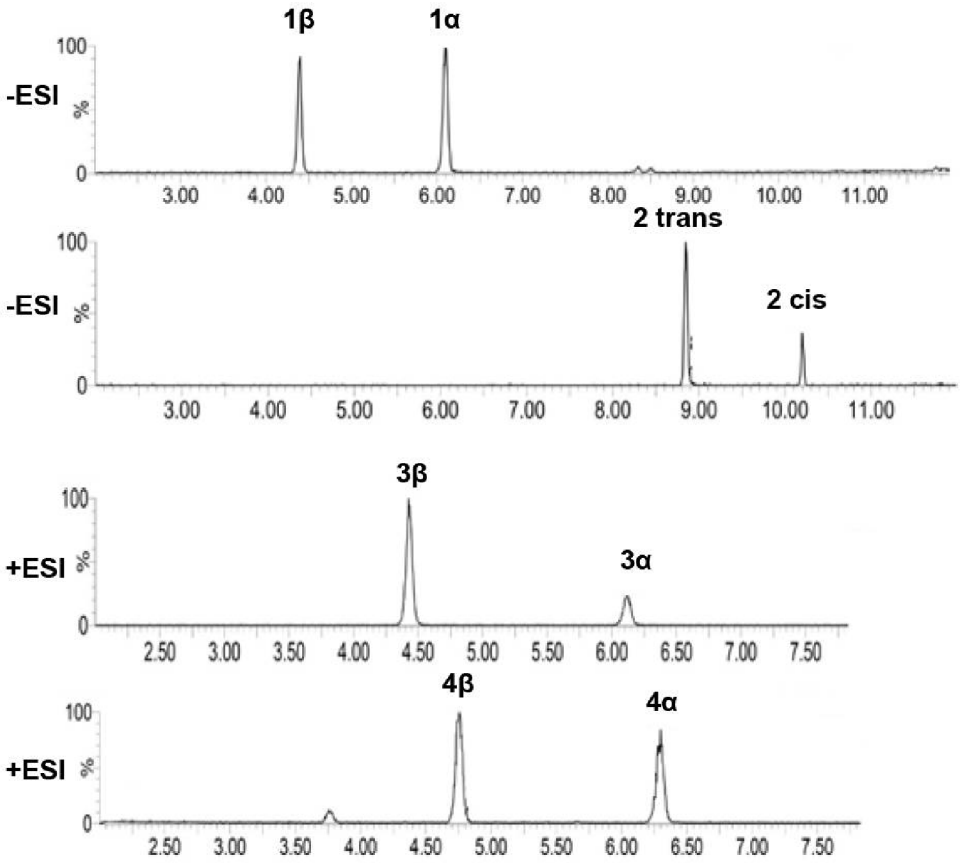
Application #**AN1830**

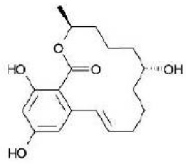
Conditions

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

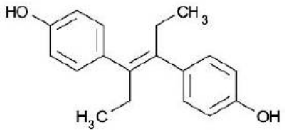
Time (mins)	%B
0.0	25
0.5	25
7.0	35
7.5	35
10.5	60
12.5	90

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



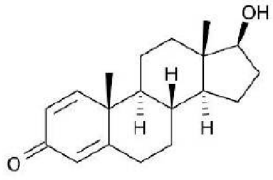


1. α- and β-Zearalenol
(*m/z* 319.17 → 275.12)

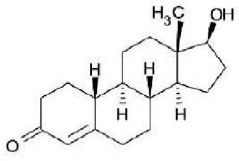


2. Diethylstilbestrol-d8
(*m/z* 275.23 → 245.09)

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

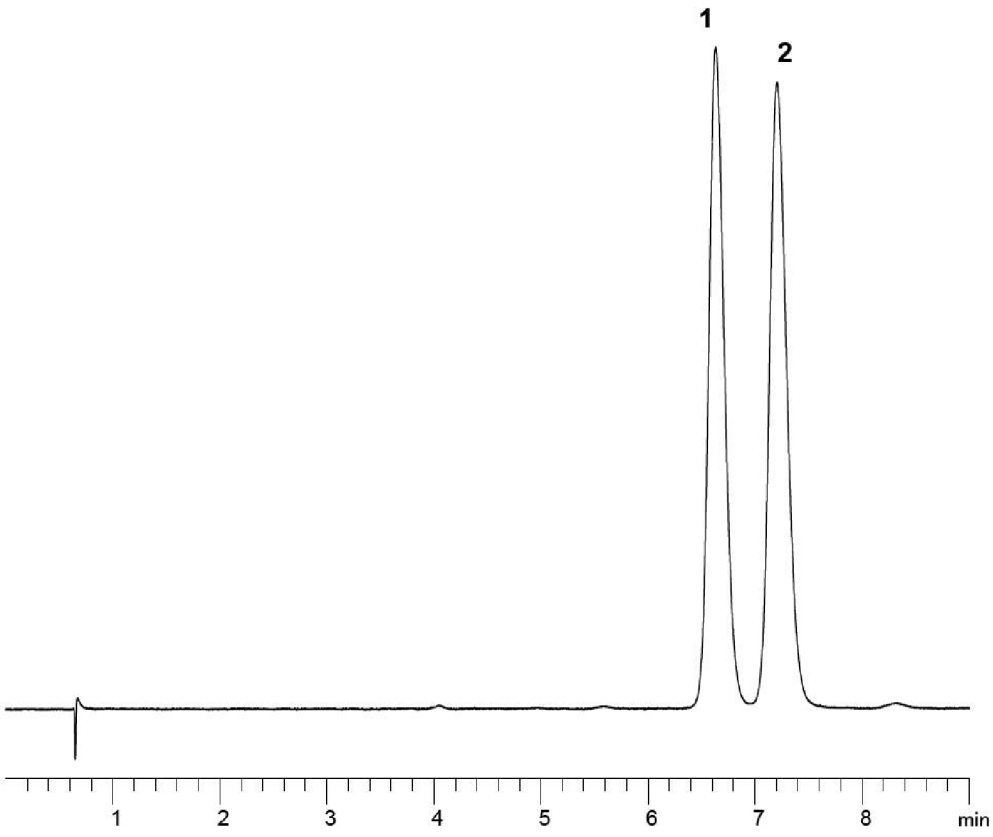
Vitamin D2/D3

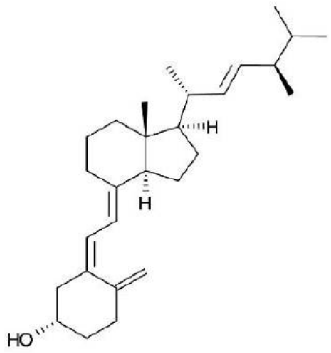
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1840**

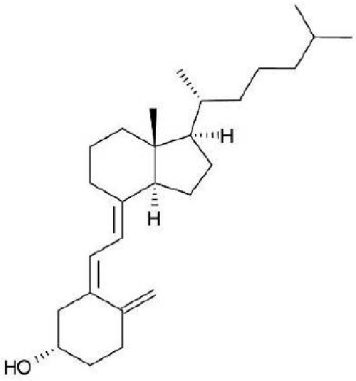
Conditions

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)

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

ACE®
Ultra-inert
UHPLC & HPLC Columns

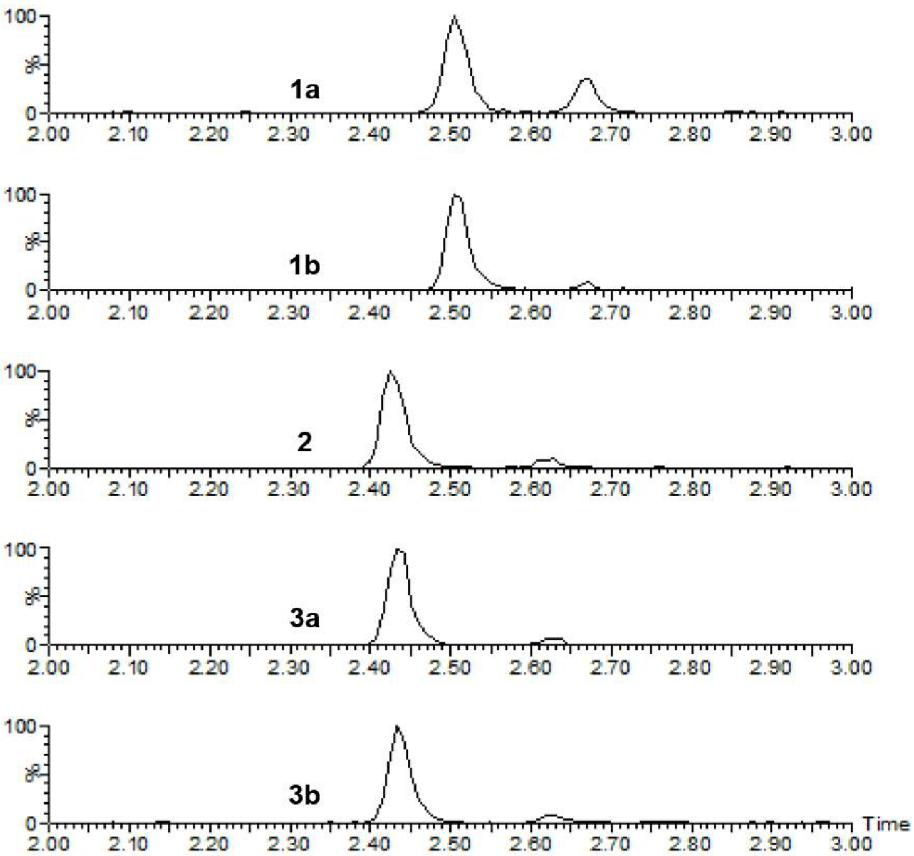
Application #AN2390

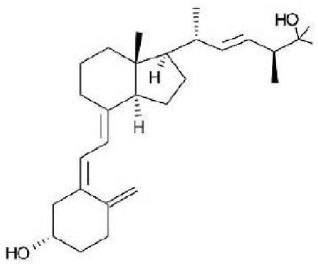
Conditions

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

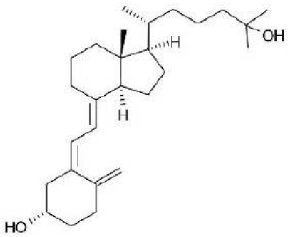
Time (mins)	%B
0.0	75
3.0	100
4.0	100

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)

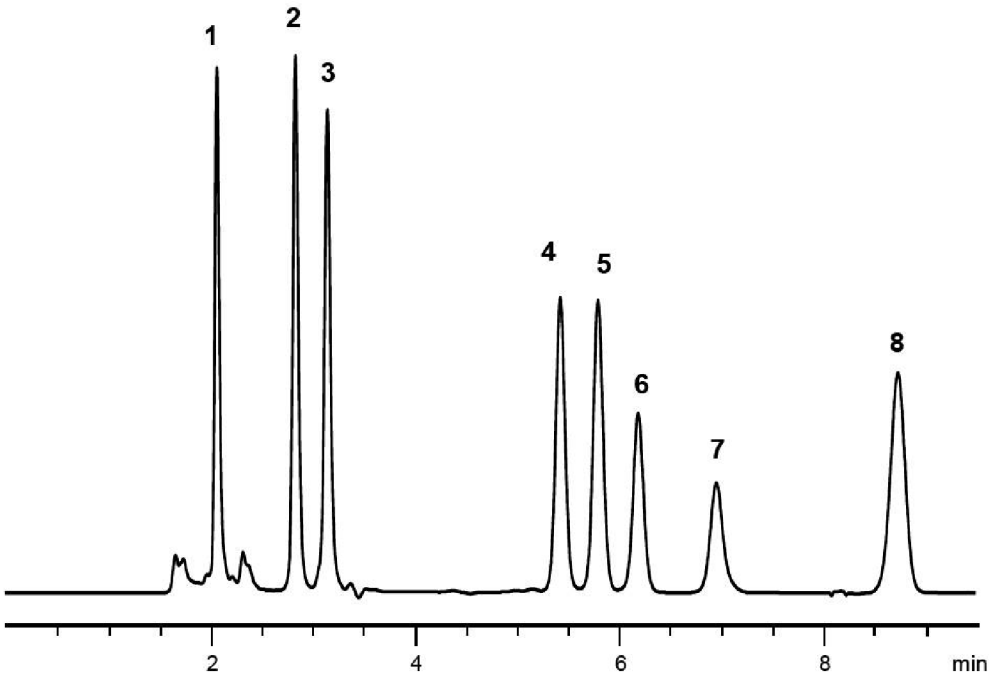
Vitamins – Fat Soluble

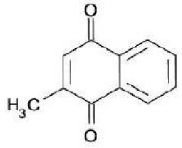
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN2420

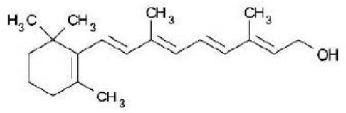
Conditions

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

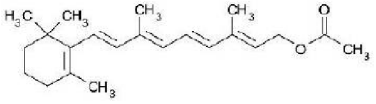




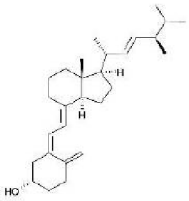
1. Menadione (Vitamin K3)



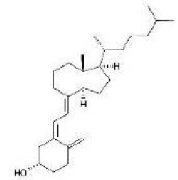
2. Retinol (Vitamin A)



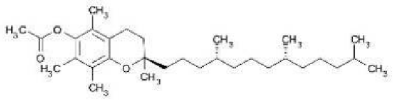
3. Vitamin A acetate



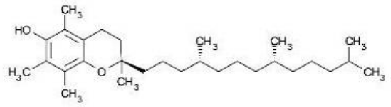
4. Ergocalciferol (Vitamin D2)



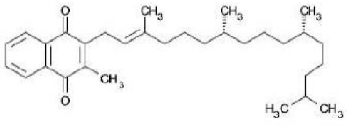
5. Cholecalciferol (Vitamin D3)



6. Vitamin E acetate



7. α-Tocopherol (Vitamin E)



8. Vitamin K1

Vitamins in Fruit Juice by Fast LC-MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

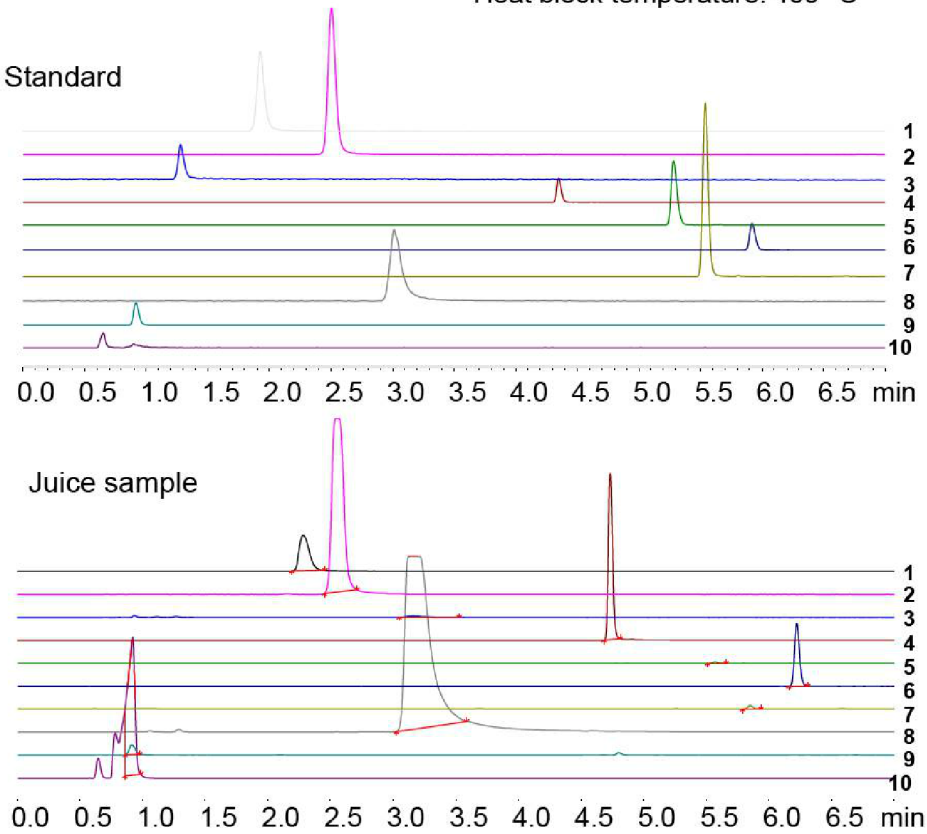
Application #AN2610

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 Heat 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)

Vitamins – Water Soluble (Gradient 1)

ACE®
Ultra-inert
UHPLC & HPLC Columns

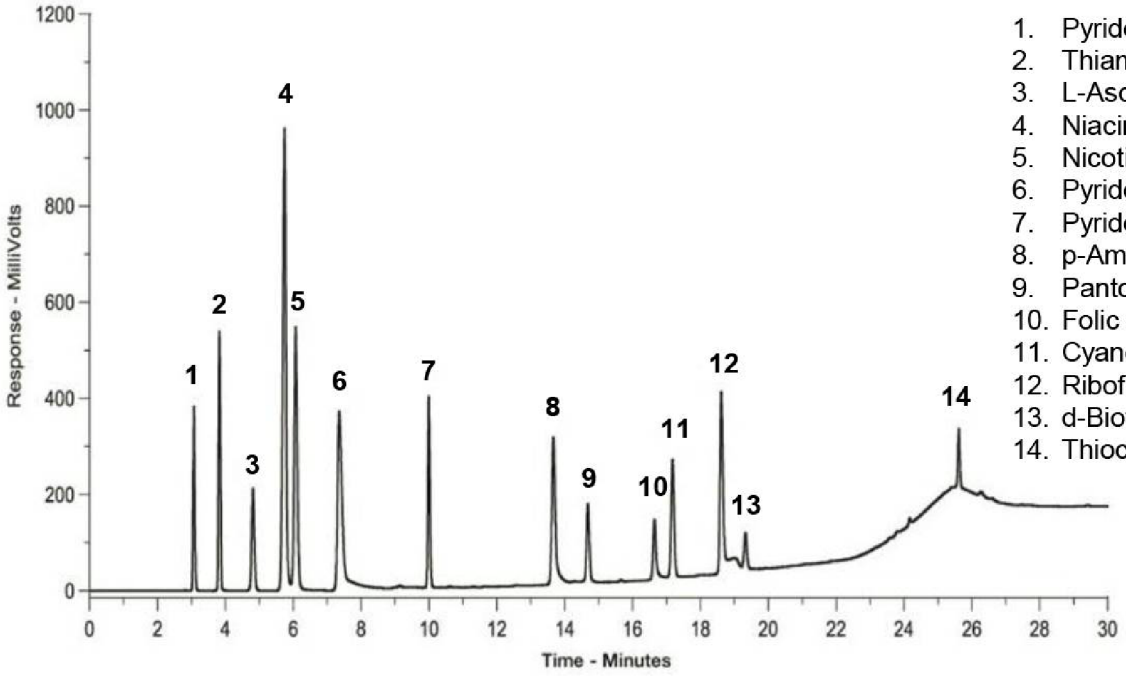
Application #**AN2940**

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

Vitamins – Water Soluble (Gradient 2)

ACE®
Ultra-inert
UHPLC & HPLC Columns

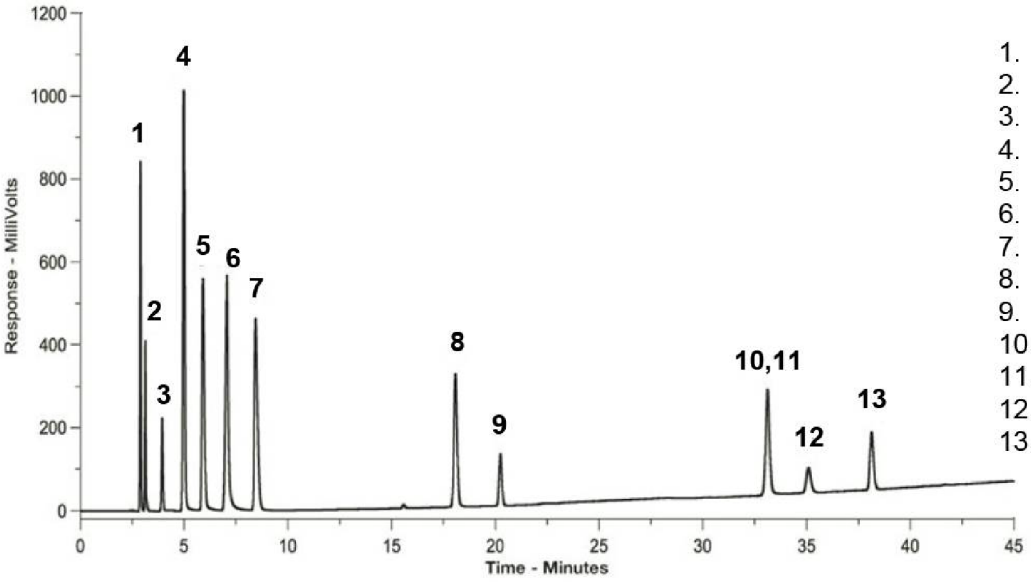
Application #**AN2930**

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)

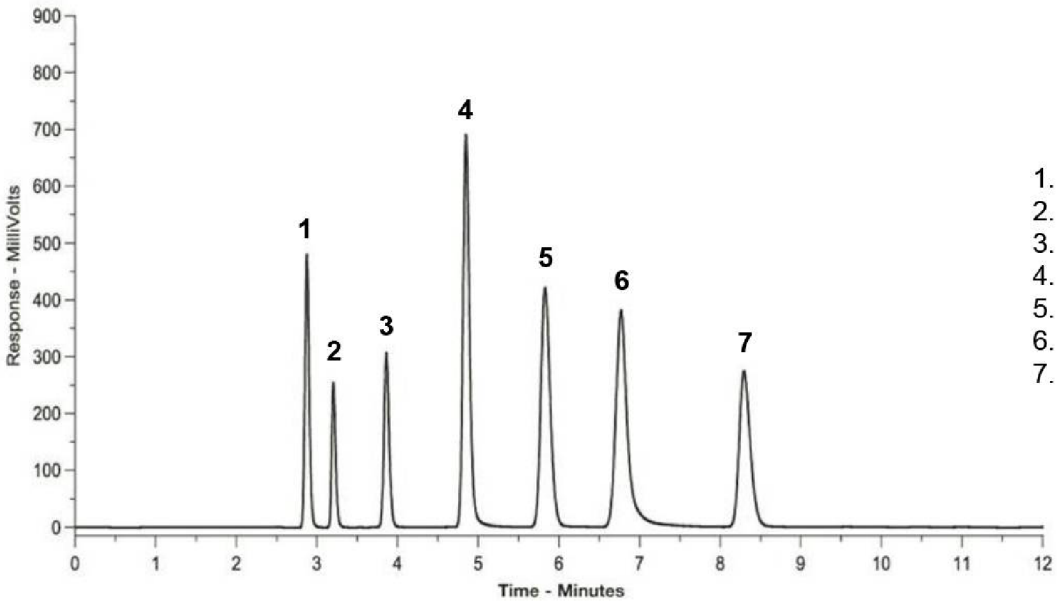
Vitamins – Water Soluble (Isocratic 1)

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

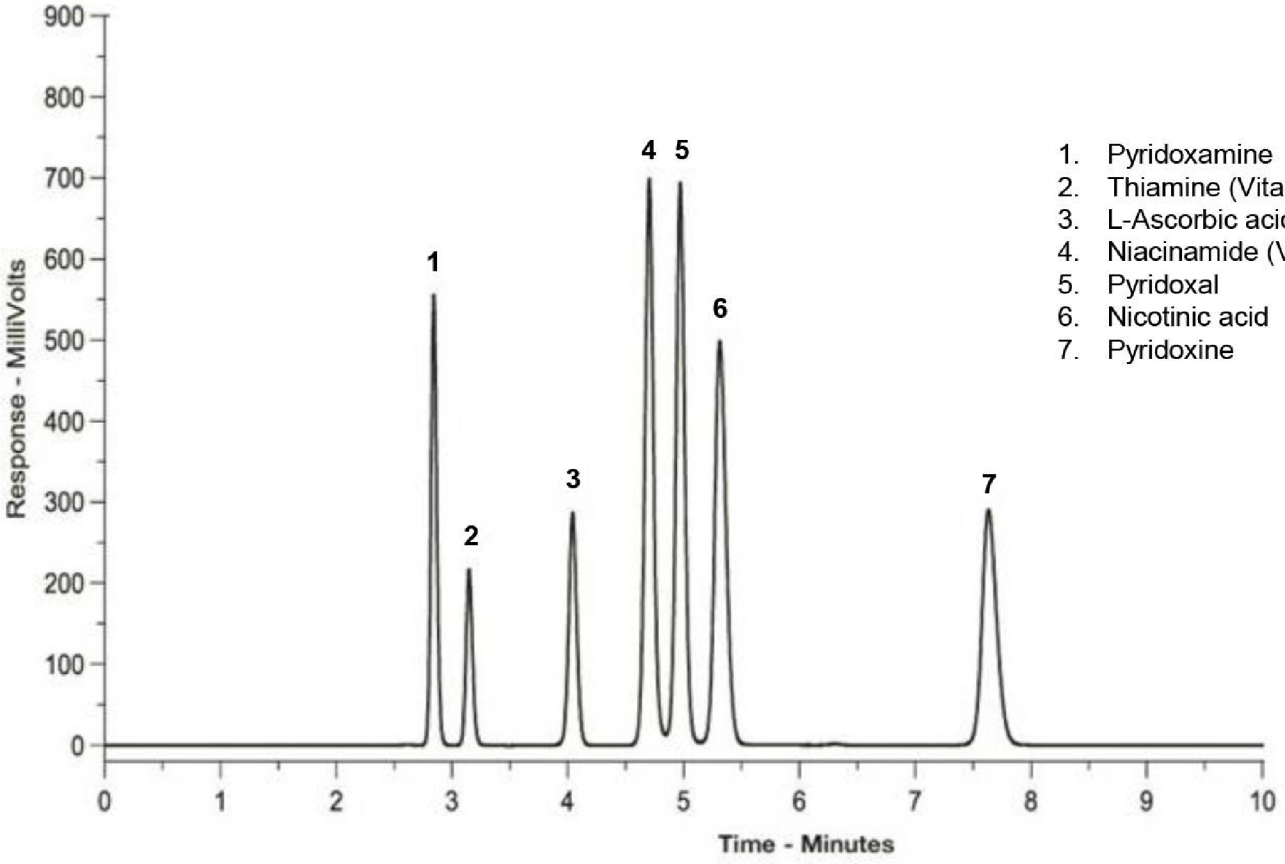
Vitamins – Water Soluble (Isocratic 2)

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

Water Soluble Vitamins (I)

ACE®
Ultra-inert
UHPLC & HPLC Columns

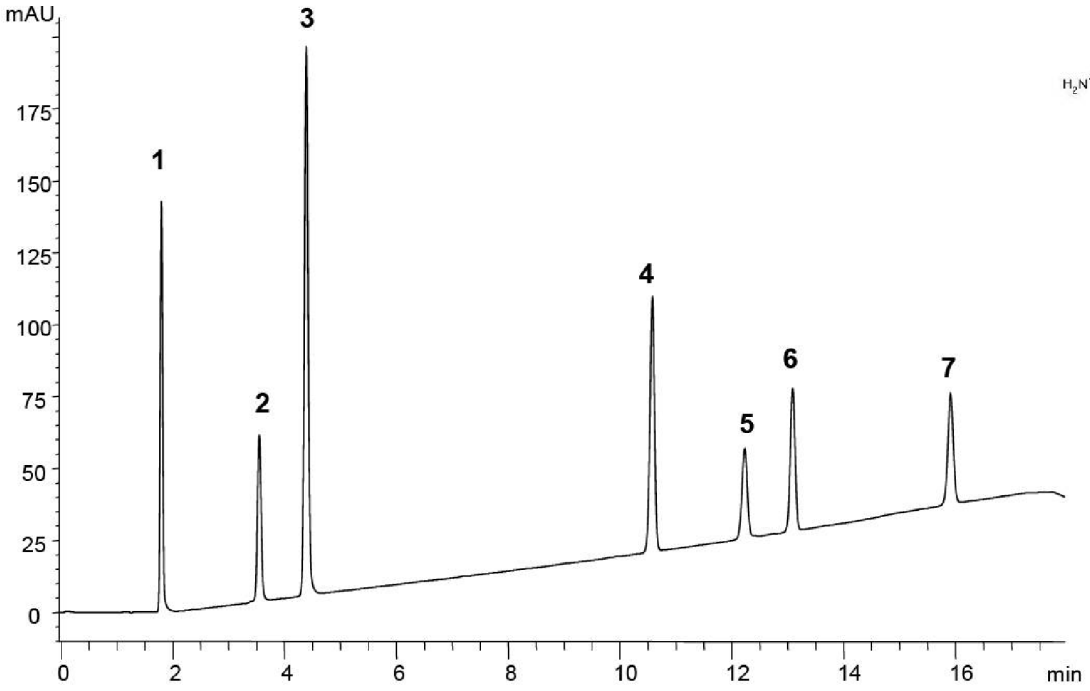
Application #AN1870

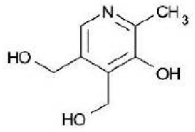
Conditions

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)

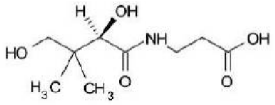
Time (mins)	%B
0	20
15	70

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

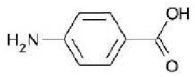




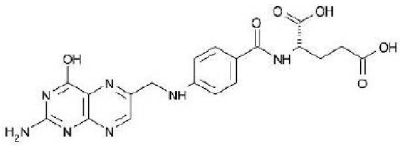
1. Pyridoxine (Vitamin B6)



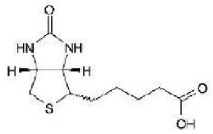
2. Pantothenic acid (Vitamin B5)



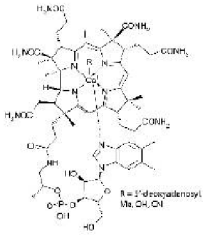
3. p-Aminobenzoic acid



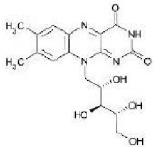
4. Folic acid (Vitamin B9/ Vitamin M)



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



6. Cyanocobalamin (Vitamin B12)



7. Riboflavin (Vitamin B2)

Water Soluble Vitamins (II)

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN1880

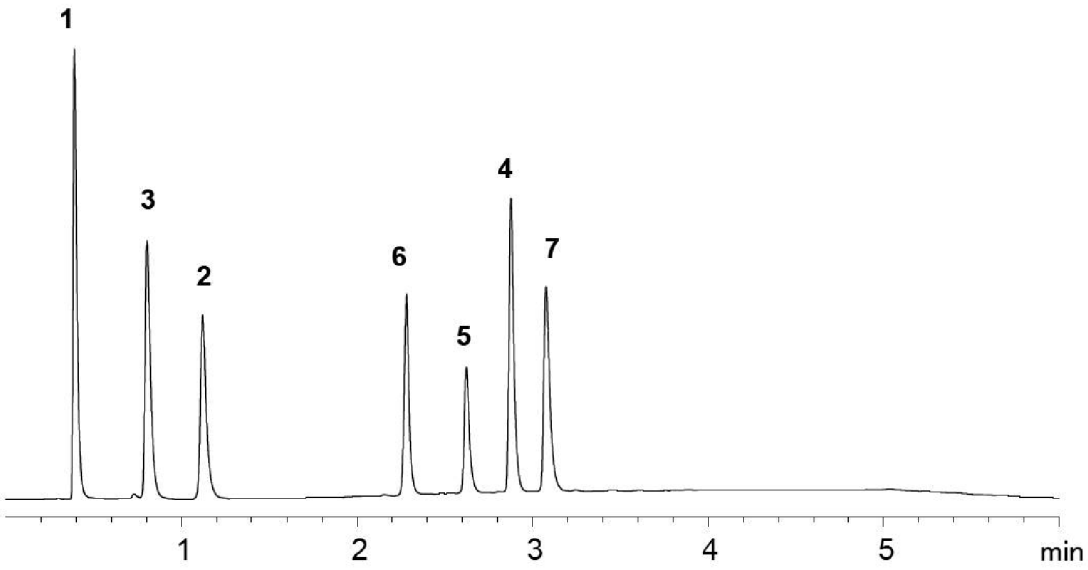
Conditions

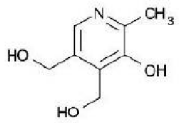
Column:	ACE Ultracore 2.5 SuperPhenylHexyl
Dimensions:	50 x 2.1 mm
Part Number:	CORE-25B-0502U
Mobile Phase:	A: 20 mM KH_2PO_4, pH 2.7 B: 20 mM KH_2PO_4, pH 2.7 in MeOH/H_2O (50:50 v/v)

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

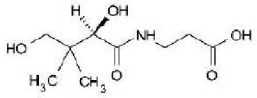
Post time 4.5 minutes

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

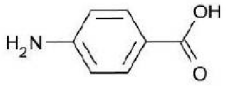




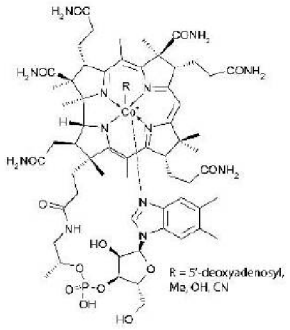
1. Pyridoxine



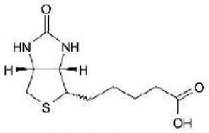
2. Pantothenic acid



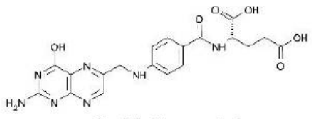
3. p-Aminobenzoic acid



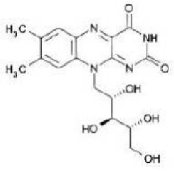
4. Cyanocobalamin



5. d-Biotin



6. Folic acid



7. Riboflavin

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

ACE®
Ultra-inert
UHPLC & HPLC Columns

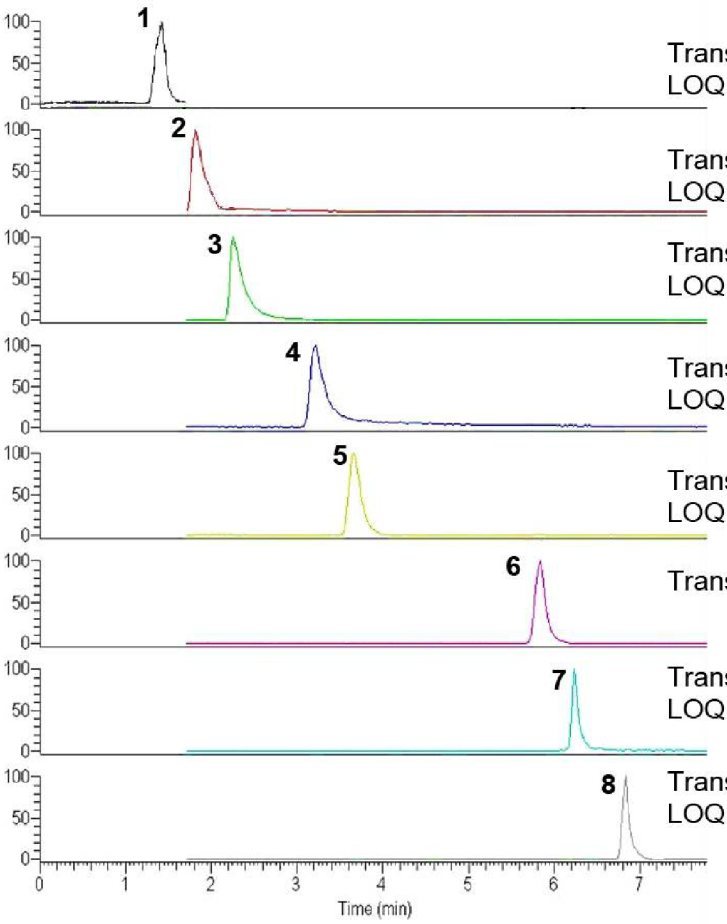
Application #AN1860

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

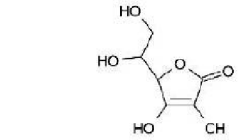
Transition *m/z* 123.0 → 80.3
LOQ 13.2 ng/mL

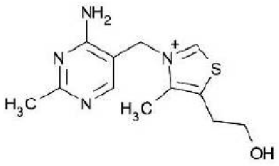
Transition *m/z* 220.0 → 202.1
LOQ 23.3 ng/mL

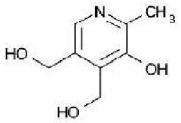
Transition *m/z* 180.1 → 105.2

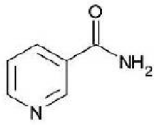
Transition *m/z* 442.0 → 294.9
LOQ 1.9 ng/mL

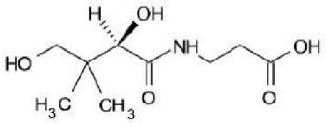
Transition *m/z* 377.1 → 243.0
LOQ 0.2 ng/mL

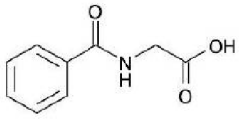

1. Ascorbic acid

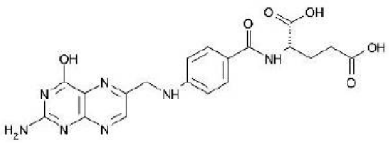

2. Thiamine

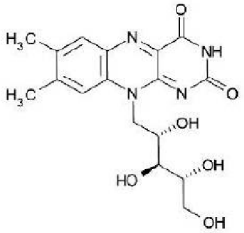

3. Pyridoxine


4. Nicotinamide


5. Pantothenic acid


6. Hippuric acid (IS)


7. Folic acid


8. Riboflavin

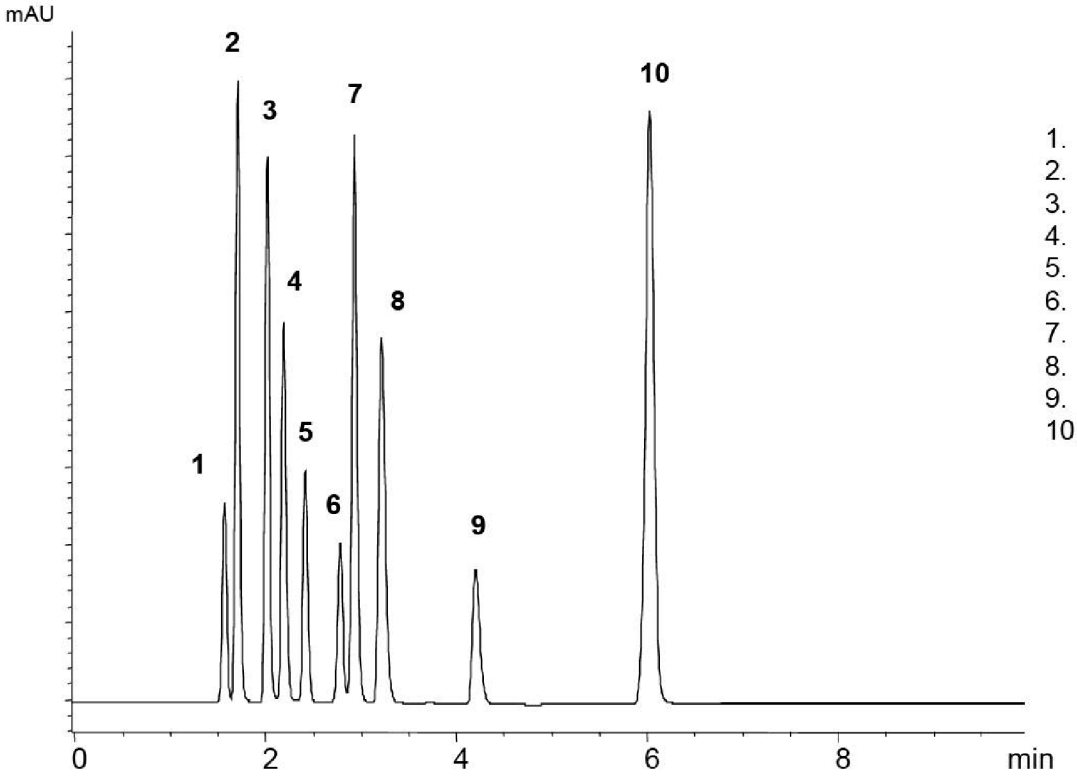
Water Soluble Vitamins and Polar Molecules

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

Whey Proteins from Whole Milk

ACE®
Ultra-inert
UHPLC & HPLC Columns

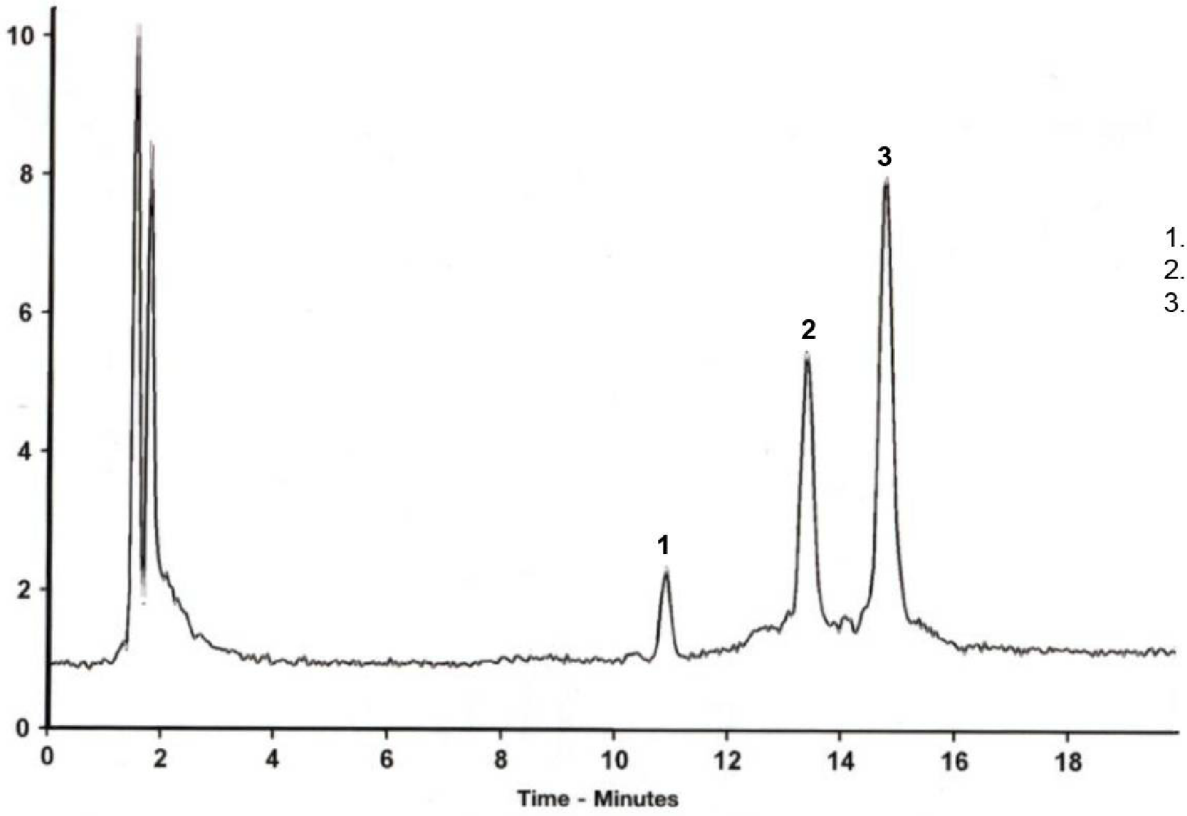
Application #**AN3000**

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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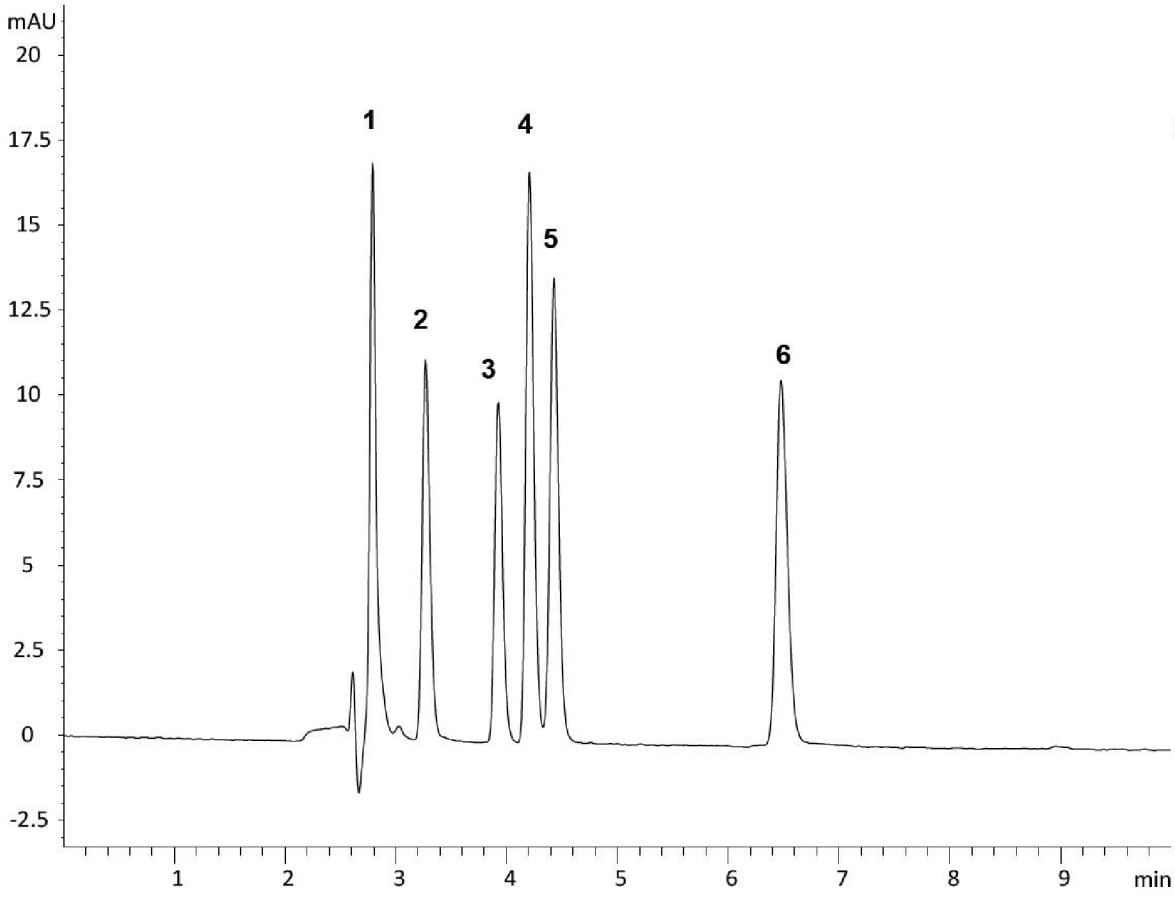
Wine Acid Analysis

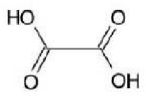
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1890**

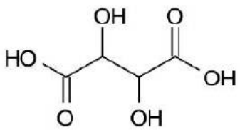
Conditions

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

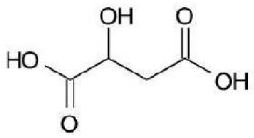




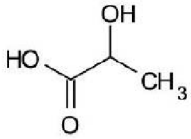
1. Oxalic acid



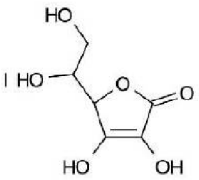
2. Tartaric acid



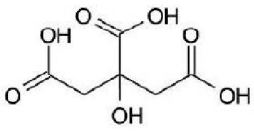
3. Malic acid



4. Lactic acid



5. Ascorbic acid



6. Citric acid

Amino Acid Enantiomer Separation of Seawater Samples

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN3880**

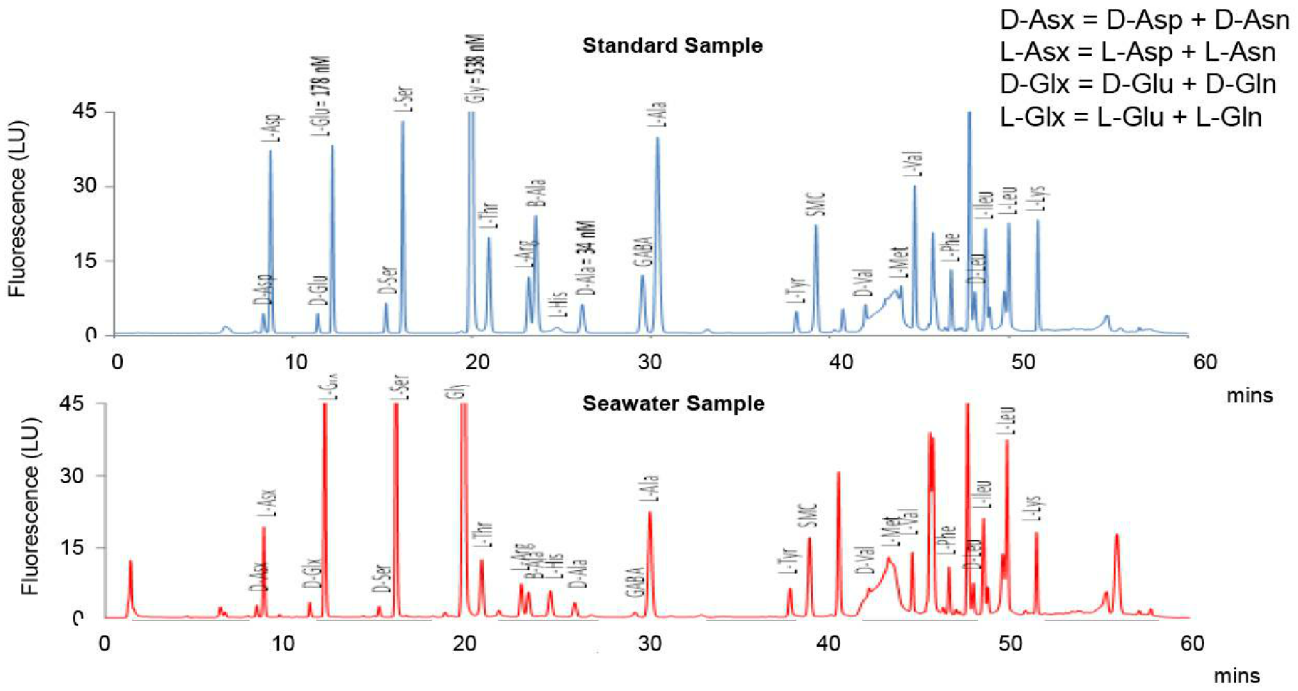
Conditions

Column:	ACE UltraCore 5 SuperC18
Dimensions:	250 x 3.0 mm
Part Number:	CORE-5A-2503U
Mobile Phase:	A: 95% 40 mM KH_2PO_4 pH 6.15 in H_2O + MeOH/MeCN (93:7 v/v) B: 62% MeOH/MeCN (93:7 v/v) + 38% A

Time (mins)	%B
0.0	0
13.0	27
33.0	36
38.0	58
54.0	92
55.0	100
57.5	0
60.0	0

Flow Rate:	0.7 mL/min
Temperature:	45 °C
Detection:	Fluorescence, λ_{ex} 330 nm λ_{em} 450 nm

This method enables the quantification of free, dissolved combined, particulate and total amino acid enantiomers from seawater. After hydrolysis, hydrolysates are evaporated, dissolved in borate buffer (pH 10) and centrifuged to remove flocculate. Samples are derivatised with OPA/IBDC (N-isobutyryl-D-cysteine) and SMC (S-methyl-L-cysteine) added as internal standard. Enantiomer elution order can be reversed by using IBLC (N-isobutyryl-L-cysteine)



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Amino Acid Profile of Edible Stink Bugs by LC-MS

ACE®
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UHPLC & HPLC Columns

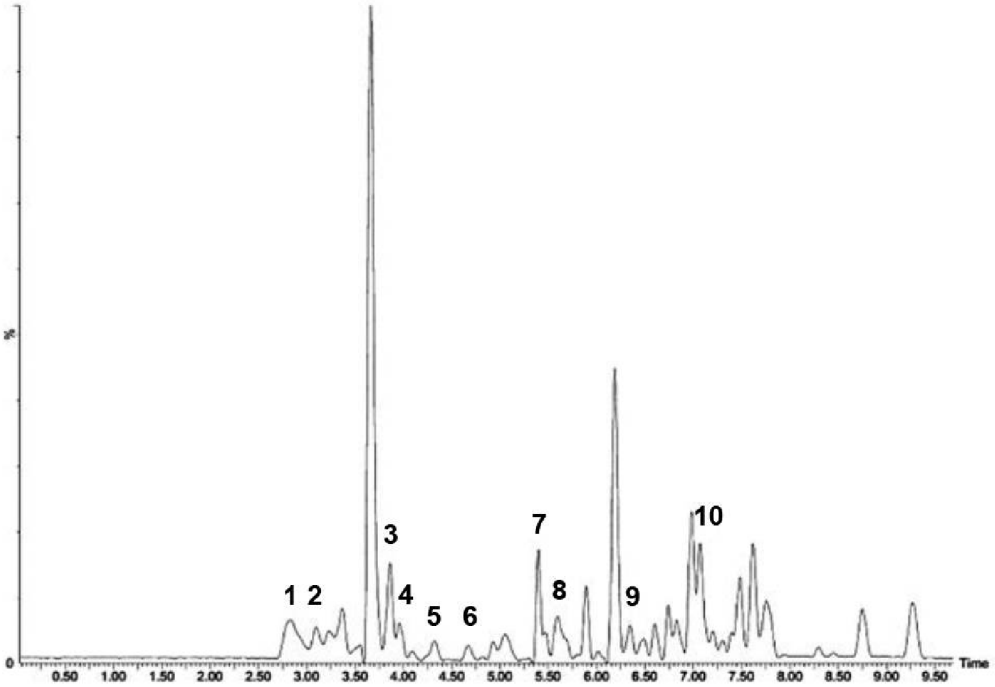
Application #AN3530

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	A: 0.01% formic acid in H_2O
	B: 0.01% formic acid in MeCN

Time (mins)	%B
0.0	5
3.0	30
6.0	30
7.5	80
10.5	80
13.0	100
18.0	100
20.0	5
22.0	5

Flow Rate:	0.7 mL/min
Injection:	1 µL
Detection:	Waters QToF-MS ESI in positive ion mode Scan range: *m/z* 100-700
Sample:	Profile of edible stink bugs (*Encosternum delegorguei* Spinola) after acid hydrolysis of extracted proteins



1. Arginine
2. Isoleucine
3. Leucine
4. Proline
5. Valine
6. Methionine
7. Hydroxyproline
8. Tyrosine
9. Lysine
10. Phenylalanine

Musundire R, Osuga IM, Cheseto X, Irungu J, Torto B (2016) Aflatoxin Contamination Detected in Nutrient and Anti-Oxidant Rich Edible Stink Bug Stored in Recycled Grain Containers. PLoS ONE 11(1): e0145914. doi:10.1371/journal.pone.0145914

Brazilian Red Propolis Biomarkers by LC-FTMS

ACE®
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UHPLC & HPLC Columns

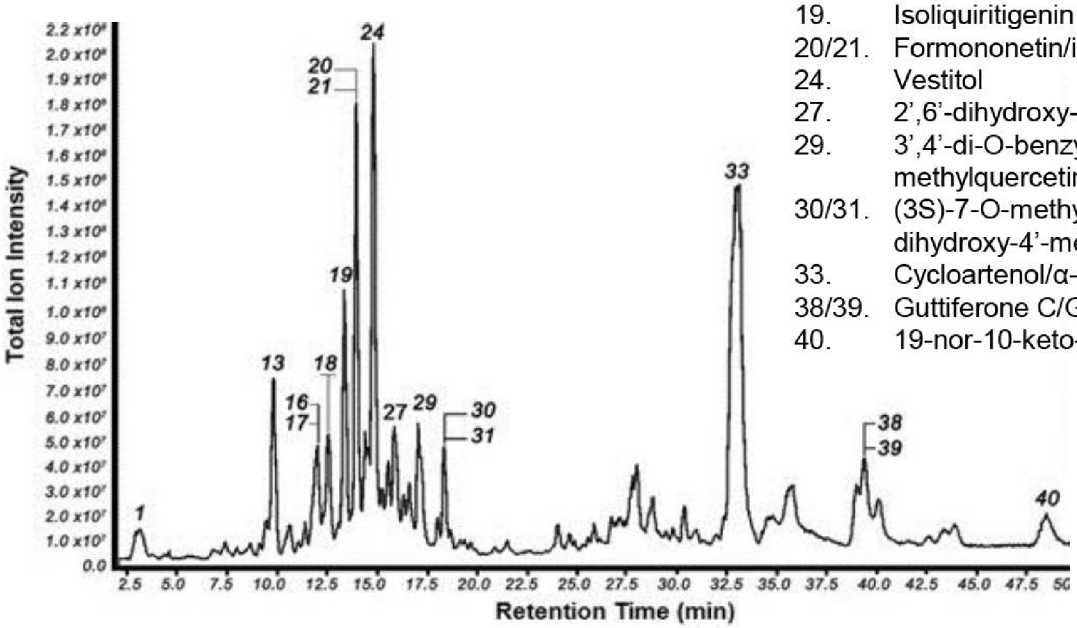
Application #AN3370

Conditions

Column:	ACE 5 C18
Dimensions:	100 x 4.6 mm
Part Number:	ACE-121-1046
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

Time (mins)	%B
0	30
6	45
10	60
14	75
18	90
22	100
47	100
52	30
58	30

Flow Rate:	0.3 mL/min
Injection:	10 µL
Detection:	Thermo Scientific LC-Orbitrap FTMS
	Negative ion mode
	Scan range 50-1200 amu
Sample:	Ethanolic extract of red propolis



1. Caffeic acid
13. Liquiritigenin
16/17. Naringenin/Pinobanksin
19. Isoliquiritigenin
20/21. Formononetin/isoformonetin
24. Vestitol
27. 2',6'-dihydroxy-4'-methoxydihydrochalcone
29. 3',4'-di-O-benzyl-7O-(2-hydroxyethyl)-3-O-methylquercetin
30/31. (3S)-7-O-methylvestitol/Calycosin/7,3'-dihydroxy-4'-methoxy-8-methylflavane
33. Cycloartenol/α-amyrin/β-amyrin
38/39. Guttiferone C/Guttiferone D
40. 19-nor-10-keto-25-hydroxyvitamin D3

Reference: de Mendonca et al, BMC Complement Altern Med. 2015; 15: 357. Published online 2015 Oct 14, doi:10.1186/s12906-015-0888-9

Caffeoylquinic and Dicaffeoylquinic Acids

ACE®
Ultra-inert
UHPLC & HPLC Columns

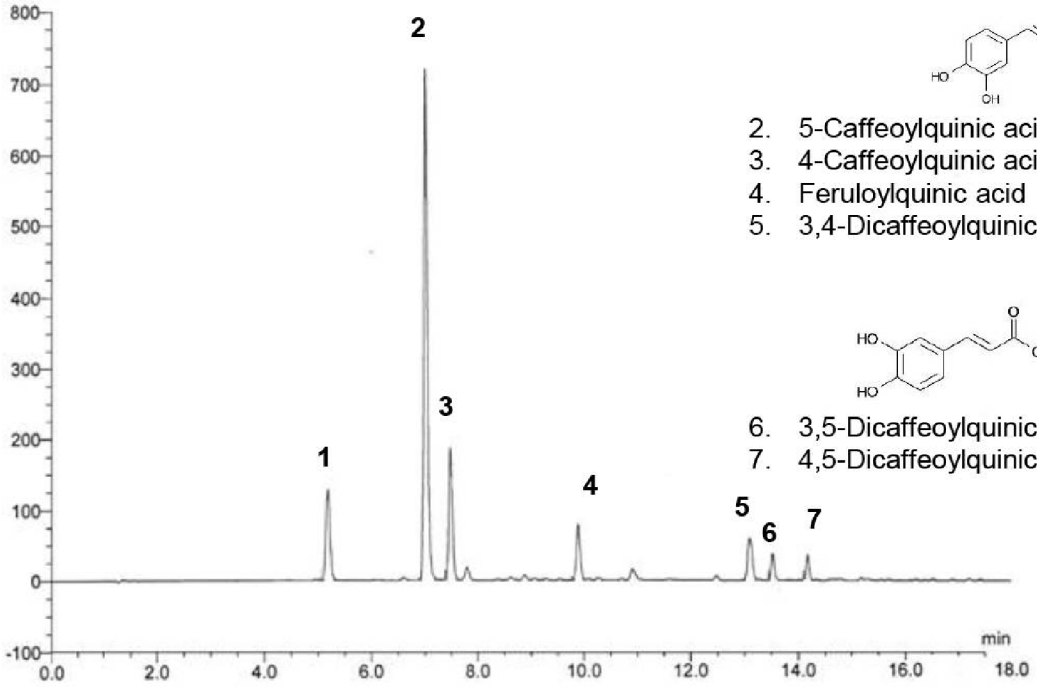
Application #AN3520

Conditions

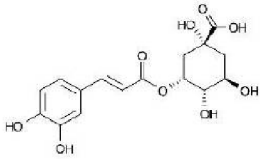
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	100 x 4.6 mm
Part Number:	CORE-25A-1046U
Mobile Phase:	A: 0.2% phosphoric acid in H_2O
	B: MeCN

Time (mins)	%B
0	5
1	5
9	18
14	28
15	70

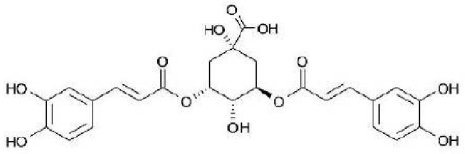
Flow Rate:	0.8 mL/min
Temperature:	35 °C
Detection:	UV-Vis, 327 nm



1. 3-Caffeoylquinic acid (chlorogenic acid)



2. 5-Caffeoylquinic acid (neochlorogenic acid)
3. 4-Caffeoylquinic acid (cryptochlorogenic acid)
4. Feruloylquinic acid
5. 3,4-Dicaffeoylquinic acid (isochlorogenic acid B)



6. 3,5-Dicaffeoylquinic acid (isochlorogenic acid A)
7. 4,5-Dicaffeoylquinic acid (isochlorogenic acid C)

Ginsenosides from Chinese Medicine by UHPLC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

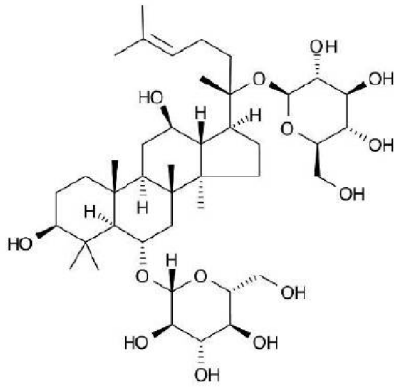
Application #AN3540

Conditions

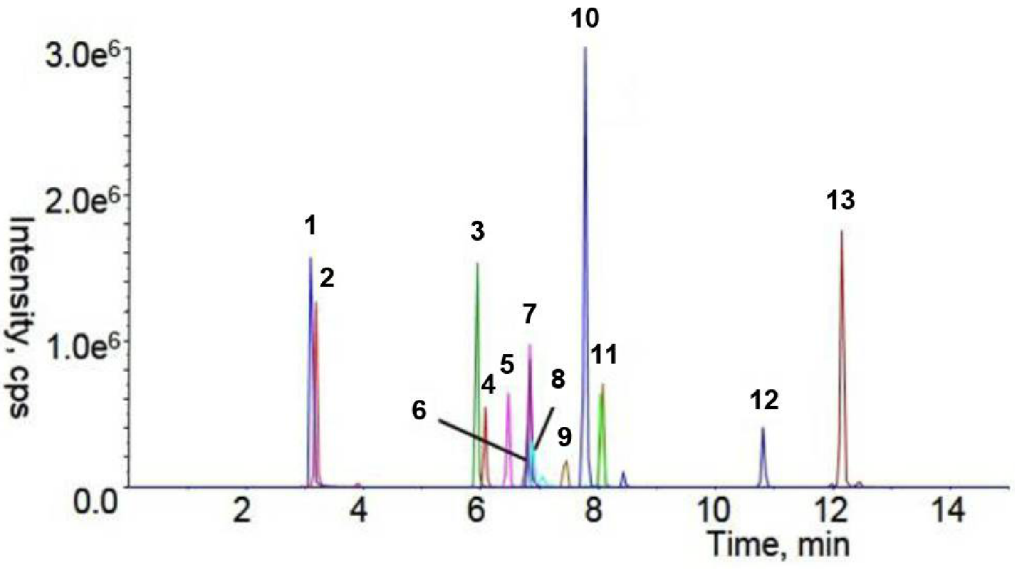
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	150 x 3.0 mm
Part Number:	CORE-25A-1503U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

Time (mins)	%B
0	25
13	60
15	95
17	95

Flow Rate:	0.4 mL/min
Injection:	2 µL
Temperature:	45 °C
Detection:	AB SCIEX 5500 Qtrap MS
	ESI in negative ion mode
	Source temperature: 450 °C
	Sprayer voltage: -4500 V
	Stepwise MRM mode for $[M + HCOO]^-$ > $[M - H]^-$ ion transitions
	Mass range 501 – 1250 u (step size 2 u)



Ginsenoside Rg1



1. Ginsenoside Re (*m/z* 991 → 945)
2. Ginsenoside Rg1 (*m/z* 845 → 799)
3. Ginsenoside Rf (*m/z* 845 → 799)
4. Ginsenoside Rb1 (*m/z* 1153 → 1107)
5. Ginsenoside Rc (*m/z* 1123 → 1077)
6. Ginsenoside Ro (*m/z* 1001 → 955)
7. Ginsenoside Rb2 (*m/z* 1123 → 1077)
8. Ginsenoside Rg2 (*m/z* 829 → 783)
9. Ginsenoside Rh1 (*m/z* 683 → 637)
10. Ginsenoside Rd (*m/z* 991 → 945)
11. Ginsenoside F1 (*m/z* 683 → 637)
12. Ginsenoside F2 (*m/z* 829 → 783)
13. Ginsenoside Rg3 (*m/z* 829 → 783)

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Paralytic Shellfish Poisoning (PSP) Toxins

ACE®
Ultra-inert
UHPLC & HPLC Columns

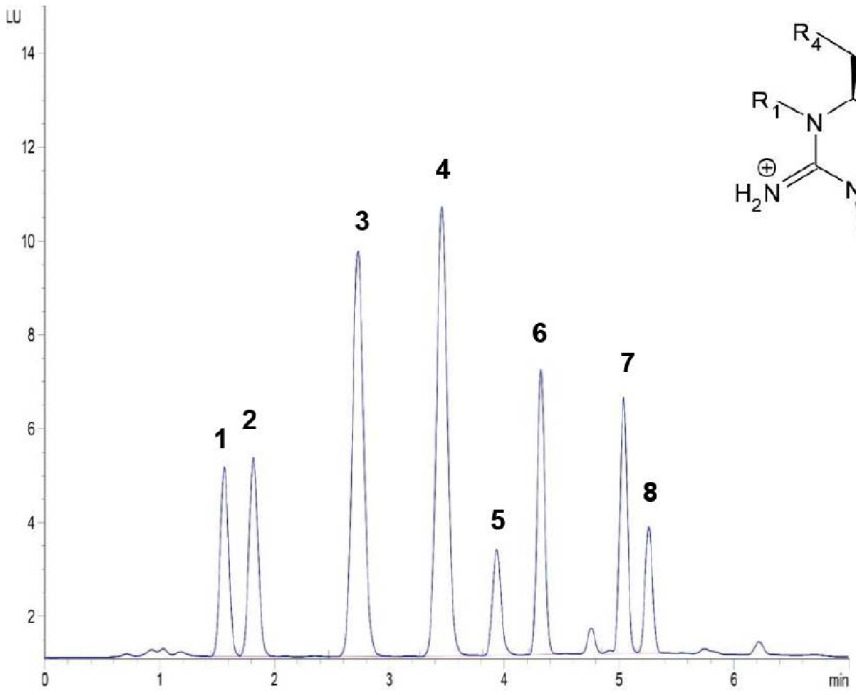
Application #**AN3180**

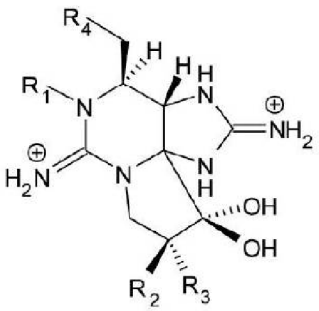
Conditions

Column:	ACE UltraCore 5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	CORE-5A-1546U
Mobile Phase:	A: 0.1 M ammonium formate in H_2O
	B: 0.1 M ammonium formate in H_2O/MeOH (95:5 v/v)

Time (mins)	%B
0.00	0
2.00	0
4.00	80
5.50	80
5.51	0
7.00	0

Flow Rate:	2 mL/min
Injection:	30 µL
Temperature:	20 °C
Detection:	Fluorescence λ_{Ex} 340 nm, λ_{Em} 395 nm
Sample:	Prechromatographic oxidation with hydrogen peroxide and periodate





1. dcGTX2,3
2. GTX1/4 + dcGTX2,3
3. C1,2
4. dcSTX + dcNEO
5. dcSTX + NEO
6. GTX2/3 + GTX1/4
7. GTX5
8. STX + NEO

PST Variant	R1	R2	R3	R4
STX	H	H	H	H_2N-COO
NEO	OH	H	H	H_2N-COO
GTX1	OH	H	OSO_3^-	H_2N-COO
GTX2	H	H	OSO_3^-	H_2N-COO
GTX3	H	OSO_3^-	H	H_2N-COO
GTX4	OH	OSO_3^-	H	H_2N-COO
GTX5 (B1)	H	H	H	O_3S-NH-COO
C1	H	H	OSO_3^-	O_3S-NH-COO
C2	H	OSO_3^-	H	O_3S-NH-COO
dcSTX	H	H	H	OH
dcNEO	OH	H	H	OH
dcGTX1	OH	H	OSO_3^-	OH
dcGTX2	H	H	OSO_3^-	OH
dcGTX3	H	OSO_3^-	H	OH

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300 Pesticide Screen by LC-MS/MS

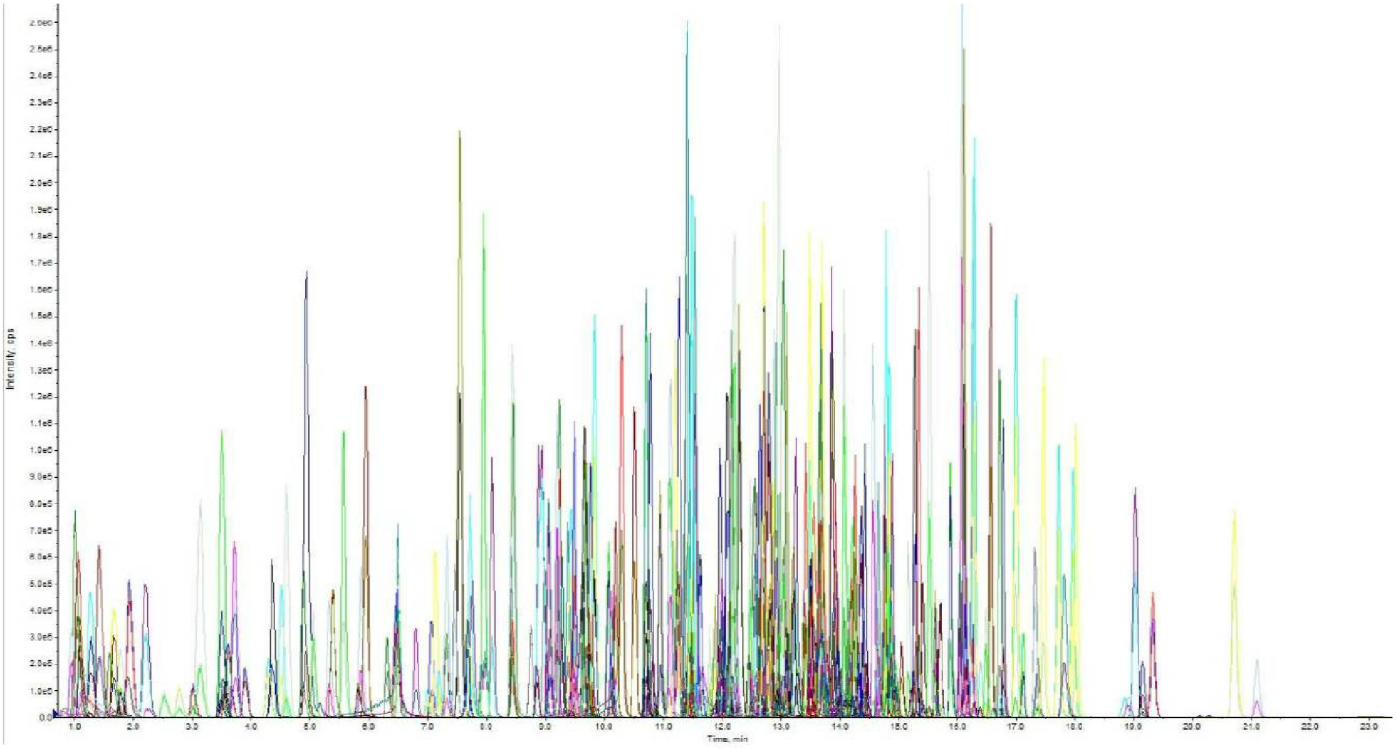
ACE®
Ultra-inert
UHPLC & HPLC Columns

Conditions

Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	100 x 2.1 mm
Part Number:	CORE-25A-1002U
Mobile Phase:	A: 5 mM ammonium formate in H_2O/MeOH (9:1 v/v) B: 5 mM ammonium formate in H_2O/MeOH (1:9 v/v)

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

Flow Rate:	0.3 mL/min
Injection:	6 µL
Temperature:	24 °C
Detection:	AB SCIEX 4000 QTRAP TurbolonSpray ESI positive mode Capillary voltage: 5000 V Heater gas temperature: 450 °C
Sample:	Sample prepared using QuEChERs methodology. Method validated using cucumber matrix spiked at 0.01 mg/kg. 265 analytes successfully validated (Analytes in black)



300 Pesticide Screen by LC-MS/MS

Analyte	Retention time (mins)	MRM transitions
3-Hydroxycarbofuran	3.5	238.1 → 163.1, 238.1 → 181.1
Acephate	1.0	184.1 → 142.9, 184.1 → 124.8
Acetamiprid	3.6	223.2 → 126.1, 225.2 → 128.1
Aclonifen	13.9	265.0 → 248.0, 267.0 → 250.0
Alachlor	12.9	270.2 → 238.2, 270.2 → 162.1
Aldicarb	5.4	208.0 → 89.0, 208.0 → 116.0
Aldicarb sulfone	1.2	240.0 → 86.0, 223.0 → 148.0
Aldicarb sulfoxide	1.1	207.0 → 132.0, 207.2 → 88.9
Ametryn	11.1	228.2 → 186.1, 228.2 → 68.0
Aminopyralid	0.8	207.0 → 160.9, 207.0 → 133.9
Amitrole	0.8	85.1 → 58.1, 85.1 → 57.1
Atrazine	9.3	216.2 → 174.0, 218.1 → 176.1
Atrazine-desethyl	4.4	188.2 → 146.0, 190.1 → 148.0
Atrazine-desisopropyl	2.4	174.1 → 104.1, 174.1 → 132.1
Avermectin B1a	18.2	876.5 → 553.0, 876.5 → 291.0
Avermectin B1b	19.1	890.5 → 305.0, 890.5 → 567.0
Azamethiphos	6.9	325.0 → 183.0, 325.0 → 138.9
Azinphos-ethyl	13.0	346.0 → 132.1, 346.0 → 160.1
Azinphos-methyl	10.9	318.1 → 132.1, 318.1 → 260.8
Aziprotryne	11.8	226.0 → 156.0, 226.0 → 125.0
Azoxystrobin	11.4	404.2 → 372.3, 404.2 → 344.1
Benalaxyl	14.0	326.2 → 148.1, 326.2 → 294.1
Benfuracarb	15.7	411.2 → 252.1, 411.2 → 195.1
Benthiavalicarb-isopropyl	12.0	382.3 → 116.0, 382.3 → 197.0
Bifenazate	12.5	301.2 → 198.1, 301.2 → 170.2
Bifenox	14.9	359.0 → 342.0, 359.0 → 310.0
Bifenthrin	21.0	440.0 → 181.1, 440.0 → 166.1
Bitertanol	14.6	338.2 → 269.0, 338.2 → 99.1
Bixafen	13.6	414.0 → 393.9, 416.1 → 395.9
Boscalid	11.7	343.1 → 306.8, 343.1 → 139.9
Bromfenvinfos-ethyl	14.3	405.0 → 155.0, 403.0 → 155.0
Bromuconazole A	12.2	378.0 → 159.1, 378.0 → 161.0
Bromuconazole B	13.5	378.1 → 159.1, 378.1 → 161.0
Bupirimate	13.5	317.2 → 166.2, 317.2 → 107.9
Buprofezin	16.1	306.3 → 201.1, 306.3 → 116.1
Cadusafos	14.8	271.1 → 158.9, 271.1 → 214.9
Carbaryl	8.3	202.2 → 145.1, 202.2 → 127.1
Carbendazim	4.7	192.2 → 160.1, 192.0 → 132.0
Carbofuran	7.4	222.2 → 165.1, 222.2 → 122.9
Carbosulfan	19.3	381.2 → 160.1, 381.2 → 118.1
Carboxin	8.3	236.1 → 143.1, 236.1 → 87.0
Carfentrazone-ethyl	13.8	412.2 → 345.9, 412.2 → 383.9
Chlorantraniliprole	10.7	484.0 → 452.9, 484.0 → 285.9
Chlorbromuron	11.7	295.1 → 205.9, 293.1 → 182.0
Chlorfenvinfos A	14.3	359.0 → 155.0, 358.9 → 99.0
Chloridazon	3.7	222.1 → 104.0, 222.1 → 77.1
Chlorpyrifos	16.8	349.9 → 198.1, 349.9 → 115.0
Chlorpyrifos-methyl	15.2	322.0 → 124.9, 324.0 → 125.1
Chlortoluron	9.1	213.2 → 72.0, 215.1 → 72.1
Cinidon-ethyl	16.3	394.0 → 348.0, 394.0 → 366.0
Clethodim A	12.8	360.1 → 164.1, 360.1 → 268.1
Clethodim B	10.2	360.1 → 164.1, 360.1 → 268.1
Clofentezine	15.1	303.1 → 137.9, 305.1 → 102.0
Clomazone	10.7	240.1 → 124.9, 242.2 → 127.1
Cloquintocet-mexyl	16.1	336.2 → 238.0, 336.2 → 192.1
Clothianidin	2.9	250.1 → 169.0, 250.1 → 132.0

Analyte	Retention time (mins)	MRM transitions
Coumaphos	14.3	363.0 → 227.0, 363.0 → 211.1
Cyanazine	6.7	241.1 → 214.1, 243.1 → 216.1
Cyazofamid	13.2	325.2 → 107.9, 327.2 → 107.9
Cycloate	14.9	216.2 → 83.1, 216.2 → 154.1
Cycloxydim A	13.1	326.3 → 280.0, 326.3 → 180
Cycloxydim B	8.4	326.3 → 280.0, 326.3 → 180
Cymoxanil	4.2	199.2 → 128.0, 199.2 → 111.1
Cyproconazole A	12.5	292.0 → 70.0, 292.0 → 125.0
Cyproconazole B	12.0	292.0 → 70.0, 292.0 → 125.0
Cyprodinil A	14.1	226.2 → 93.0, 226.2 → 77.0
Demeton-S-methyl	7.7	231.1 → 88.8, 231.1 → 61.0
Demeton-S-methyl sulfone	1.6	263.0 → 168.9, 263.0 → 120.8
Desmedipham	10.6	318.1 → 182.1, 318.1 → 136.0
Desmethyl-pirimicarb	5.8	225.2 → 72.0, 225.2 → 168.1
Diafenthiuron	17.4	385.2 → 329.2, 385.2 → 278.2
Diazinon	14.2	305.1 → 169.1, 305.1 → 97.0
Dichlofluanid	12.8	333.0 → 223.9, 333.0 → 122.9
Diclobutrazol A	13.7	328.0 → 70.0, 330.0 → 70.0
Dicrotofos	2.1	238.1 → 112.1, 238.1 → 193.1
Diethofencarb	11.1	268.1 → 226.1, 268.1 → 124.0
Difenoconazole	14.8	406.1 → 251.1, 408.2 → 253.1
Diflubenzuron	13.5	311.0 → 158.2, 311.0 → 141.1
Diflufenican	15.4	395.0 → 266.0, 395.0 → 246.0
Dimethachlor	10.2	256.2 → 224.0, 256.2 → 148.1
Dimethenamid	11.3	276.1 → 244.0, 278.1 → 246.0
Dimethoate	3.6	230.1 → 198.8, 230.1 → 124.9
Dimethomorph	11.7	388.1 → 301.0, 388.1 → 165.1
Dimoxystrobin	13.7	327.1 → 205.0, 327.1 → 116.0
Diniconazole	14.8	326.0 → 70.0, 328.0 → 70.0
Disulfoton	15.0	275.1 → 89.0, 275.1 → 61.0
Disulfoton sulfone	9.6	307.1 → 153.0, 307.1 → 171.0
Disulfoton sulfoxide	9.2	291.1 → 212.9, 291.1 → 185.0
Ditalimfos	13.1	300.1 → 148.0, 300.1 → 130.0
Diuron	10.0	233.1 → 71.9, 235.1 → 72.0
DMST	8.0	215.2 → 106.0, 215.2 → 78.9
Dodine	13.6	228.3 → 57.0, 228.3 → 60.1
Epoxiconazole	12.9	330.1 → 120.9, 330.1 → 75.2
Ethion	16.5	385.0 → 199.0, 385.0 → 143.0
Ethirimol	9.7	210.3 → 140.1, 210.3 → 98.0
Ethofumesate	11.3	287.1 → 121.0, 287.1 → 259.0
Ethoprofos	12.7	243.0 → 131.0, 243.0 → 97.0
Ethoxyquin A	12.9	218.2 → 148.0, 218.2 → 174.1
Ethoxyquin B	10.7	218.2 → 148.0, 218.2 → 174.1
Etofenprox	20.6	394.0 → 177.0, 394.0 → 359.0
Etrimfos	14.2	293.1 → 125.0, 293.1 → 265.1
Famoxadone NH4+	14.4	392.0 → 331.0, 392.0 → 238.0
Fenamidone	11.5	312.1 → 92.1, 312.1 → 236.1
Fenamifos	13.4	304.0 → 217.0, 304.0 → 202.0
Fenamifos sulfone	8.4	336.0 → 308.0, 336.0 → 266.0
Fenamifos sulfoxide	7.9	320.0 → 171.0, 320.0 → 233.0
Fenarimol	12.7	331.2 → 268.0, 331.2 → 139.0
Fenazaquin	18.0	307.1 → 161.1, 307.1 → 147.0
Fenbuconazole	13.2	337.0 → 124.9, 337.0 → 70.0
Fenbutatin oxide	22.9	519.3 → 463.3, 519.3 → 197.0
Fenhexamid	12.6	302.2 → 96.9, 304.2 → 97.0
Fenoxycarb	13.6	302.2 → 87.9, 302.2 → 116.0

300 Pesticide Screen by LC-MS/MS

Analyte	Retention time (mins)	MRM transitions
Fenpropathrin	17.3	367.0 → 125.0, 350.0 → 125.0
Fenpropidin	10.8	274.0 → 147.0, 274.0 → 117.0
Fenpropimorph	18.7	304.0 → 147.0, 304.0 → 117.0
Fenpyroximate	17.4	422.2 → 366.1, 422.2 → 135.1
Fensulfothion	10.0	309.1 → 280.8, 309.1 → 252.9
Fensulfothion sulfone	10.4	325.1 → 268.9, 325.1 → 297.0
Fenthion sulfone	9.0	311.1 → 125.0, 311.1 → 278.8
Fenthion sulfoxide	8.4	295.1 → 279.7, 295.1 → 108.9
Flonicamid	1.7	230.0 → 203.0, 230.0 → 148.0
Flubendiamide NH4+	13.8	700.0 → 407.9, 682.9 → 407.9
Fludioxonil NH4+	11.8	266.0 → 229.0, 266.0 → 227.1
Flufenacet	12.8	364.1 → 194.1, 364.1 → 152.2
Flufenoxuron	17.1	489.0 → 158.0, 489.0 → 141.1
Flumethrin NH4+	20.2	527.2 → 510.0, 527.2 → 267.0
Flumetsulam	2.0	326.2 → 128.8, 326.2 → 128.3
Flumioxazin	10.7	355.0 → 327.0, 355.0 → 299.0
Fluometuron	8.9	233.0 → 72.0, 233.0 → 160.0
Fluopicolide	11.9	383.0 → 173.0, 385.1 → 174.9
Fluopiram	12.5	397.0 → 173.0, 397.0 → 208.0
Fluoxastrobin	12.8	459.1 → 427.1, 459.1 → 188.1
Fluquinconazole	12.6	376.1 → 307.1, 376.1 → 349.1
Flusilazole	13.3	316.2 → 247.0, 316.2 → 165.1
Flutolanil	12.0	324.0 → 262.0, 324.0 → 242.0
Flutriafol	9.7	302.1 → 70.1, 302.1 → 123.0
Fomesafen (NH4-Adduct)	11.3	456.1 → 344.0, 458.1 → 346.0
Fonofos	14.3	247.0 → 109.0, 247.0 → 127.0
Fosthiazate	8.9	284.1 → 227.9, 284.1 → 104.0
Fuberidazole	6.9	185.0 → 157.0, 185.0 → 65.0
Furathiocarb	15.9	383.1 → 195.0, 383.1 → 252.1
Heptenofos	10.1	251.0 → 127.0, 251.0 → 124.8
Hexaconazole	14.3	314.0 → 70.0, 316.0 → 70.0
Hexaflumuron	15.5	461.1 → 158.2, 461.1 → 141.1
Hexazinone	7.3	253.2 → 71.0, 253.2 → 85.0
Hexythiazox	16.6	353.0 → 168.0, 353.0 → 228.0
Imazalil	13.6	297.2 → 159.1, 299.1 → 160.9
Imidacloprid	2.7	256.1 → 209.0, 256.1 → 175.0
Indoxacarb	15.2	528.1 → 248.9, 528.1 → 292.9
Ipconazole	15.3	334.2 → 70.0, 334.2 → 125.0
Iprodione	13.3	332.1 → 246.9, 330.0 → 245.0
Iprovalicarb	12.6	321.3 → 119.0, 321.3 → 203.1
Isofenfos	14.7	346.1 → 245.1, 346.1 → 217.1
Isofenfos-methyl	13.8	332.1 → 231.0, 332.1 → 273.0
Isoprocarb	9.4	194.1 → 95.0, 194.1 → 137.0
Isoprothiolane	12.1	291.1 → 231.0, 291.1 → 189.0
Isoproturon	9.7	207.2 → 72.0, 207.2 → 165.2
Isoxadifen-ethyl	13.9	313.2 → 296.1, 313.2 → 263.0
Isoxaflutole	10.0	360.1 → 251.1, 377.0 → 251.0
Kresoxim-methyl	13.9	314.0 → 116.0, 314.0 → 131.1
Lenacil	9.5	235.3 → 153.2, 235.3 → 136.2
Linuron	11.3	249.0 → 159.9, 249.0 → 182.0
Lufenuron	16.4	511.0 → 158.0, 511.0 → 141.0
Malaoxon	7.9	315.1 → 99.1, 315.1 → 127.1
Mandipropamid	11.9	412.1 → 328.1, 412.2 → 125.0
Mecarbam	13.0	330.1 → 227.0, 330.1 → 198.9
Mepanipyrim	12.9	224.2 → 106.0, 224.2 → 77.1
Mepronil	12.1	270.1 → 119.0, 270.1 → 228.1

Analyte	Retention time (mins)	MRM transitions
Mesotrione	1.2	340.0 → 228.0, 357.1 → 227.9
Metaflumizone	16.1	507.1 → 178.1, 507.1 → 287.1
Metalaxyl	9.8	280.1 → 220.2, 280.1 → 192.2
Metamitron	3.4	203.1 → 175.0, 203.1 → 104.2
Metazachlor	9.6	278.1 → 209.9, 278.1 → 134.2
Metconazole	14.4	320.1 → 70.0, 320.1 → 125.0
Methacrifos	10.7	241.0 → 208.9, 241.0 → 124.9
Methamidofos	0.9	142.0 → 93.9, 142.0 → 112.1
Methiocarb	11.4	226.2 → 169.1, 226.2 → 121.2
Methiocarb sulfone	4.1	258.1 → 122.0, 258.1 → 200.9
Methiocarb sulfoxide	3.0	242.1 → 185.0, 242.1 → 122.1
Methomyl	1.6	163.0 → 106.0, 163.0 → 88.0
Methoxyfenozide	12.2	369.1 → 149.1, 369.1 → 313.2
Metobromuron	9.4	259.0 → 170.0, 259.0 → 148.1
Metolachlor	13.0	284.1 → 252.0, 286.1 → 254.0
Metoxuron	5.7	229.1 → 72.0, 231.1 → 71.9
Metrafenone	14.8	409.2 → 209.1, 411.2 → 209.1
Metribuzin	7.1	215.2 → 187.1, 215.2 → 84.1
Mevinfos A	4.9	225.0 → 193.0, 225.0 → 127.0
Mevinfos B	3.4	225.0 → 193.0, 225.0 → 127.0
Molinate	12.0	188.2 → 126.2, 188.2 → 55.1
Monocrotofos	1.8	224.2 → 192.9, 224.2 → 126.9
Monolinuron	8.7	215.1 → 126.1, 215.1 → 148.1
Myclobutanil	12.2	289.2 → 70.0, 289.2 → 125.0
Napropamide	12.9	272.2 → 129.1, 272.2 → 171.1
Nitenpyram	1.3	271.1 → 189.2, 271.1 → 126.0
Novaluron	15.6	493.0 → 158.1, 493.0 → 141.1
Nuarimol	11.2	315.0 → 252.0, 315.0 → 81.0
Ofurace	7.6	282.0 → 160.1, 282.0 → 236.3
Omethoate	1.0	214.0 → 183.0, 214.0 → 125.0
Oxadiazon	16.2	345.0 → 220.0, 345.0 → 303.0
Oxadixyl	6.4	279.0 → 219.0, 279.0 → 133.0
Oxamyl NH4+	1.2	237.1 → 72.0, 220.2 → 72.0
Oxycarboxin	4.5	268.1 → 174.9, 268.1 → 147.0
Oxydemeton-methyl	1.4	247.0 → 108.9, 247.0 → 168.9
Paclobutrazol	11.8	294.0 → 70.0, 294.0 → 125.0
Paraoxon	9.4	275.9 → 219.9, 275.9 → 248.0
Paraoxon-methyl	6.1	248.1 → 202.1, 248.1 → 90.0
Parathion	13.8	292.0 → 236.0, 292.0 → 264.1
Penconazole	13.7	248.1 → 70.0, 284.1 → 159.0
Pencycuron	14.8	329.3 → 125.1, 331.3 → 127.0
Pendimethalin	16.9	282.2 → 212.1, 282.2 → 194.1
Pethoxamid	12.7	296.2 → 131.0, 296.2 → 250.0
Phenmedipham	10.8	301.2 → 168.0, 301.2 → 136.0
Phenthoate	13.9	321.0 → 247.0, 321.0 → 275.1
Phorate sulfone	9.6	293.0 → 170.8, 293.0 → 96.7
Phorate sulfoxide	9.2	277.0 → 199.0, 277.0 → 171.0
Phosalone	14.6	368.0 → 182.0, 369.9 → 183.9
Phosphamidon	6.4	300.2 → 127.1, 300.2 → 226.8
Phoxim	14.7	299.2 → 129.2, 299.2 → 77.1
Picloram	1.2	243.0 → 224.9, 241.0 → 222.9
Picolinafen	16.2	377.1 → 238.0, 377.1 → 359.0
Picoxystrobin	13.6	368.0 → 205.0, 368.0 → 145.0
Piperonyl butoxide	16.2	356.2 → 177.2, 356.2 → 119.0
Pirimicarb	9.0	239.2 → 72.0, 239.2 → 182.3
Pirimiphos-ethyl	16.3	334.1 → 198.0, 334.1 → 182.3

300 Pesticide Screen by LC-MS/MS

Analyte	Retention time (mins)	MRM transitions
Pirimiphos-methyl	14.8	306.2 → 108.0, 306.2 → 164.3
Prochloraz	14.4	376.0 → 308.0, 376.0 → 70.0
Profenofos	15.6	375.0 → 304.9, 373.0 → 302.9
Prometryn	12.6	242.2 → 158.1, 242.2 → 200.0
Propachlor	9.6	212.0 → 170.0, 212.0 → 94.1
Propamocarb	1.1	189.0 → 102.0, 189.0 → 144.0
Propaquizafop	16.0	444.2 → 100.0, 444.2 → 371.0
Propargite NH4+	17.0	368.2 → 231.1, 368.2 → 175.0
Propazine	11.0	230.2 → 188.1, 230.2 → 146.1
Propetamfos	12.4	282.1 → 138.0, 282.1 → 156.1
Propham	9.4	180.1 → 138.1, 180.1 → 120.1
Propiconazole	14.0	342.1 → 159.0, 342.1 → 69.0
Propisochlor	14.0	284.2 → 224.0, 284.2 → 148.0
Propoxur	7.2	210.1 → 111.1, 210.1 → 168.0
Propyzamide	11.9	256.1 → 190.0, 256.1 → 173.0
Proquinazid	17.7	373.2 → 330.9, 373.2 → 289.0
Prosulfocarb	15.5	252.2 → 91.0, 252.2 → 128.1
Prosulfuron	9.0	420.1 → 141.0, 420.1 → 167.1
Prothioconazole	14.1	344.1 → 326.0, 346.1 → 328.1
Prothioconazole-desthio	13.0	312.0 → 70.0, 312.0 → 125.0
Pymetrozine	1.5	218.0 → 105.0, 218.0 → 78.0
Pyraclostrobin	14.5	388.1 → 194.0, 388.1 → 163.0
Pyrazophos	14.8	374.0 → 222.0, 374.0 → 194.0
Pyridaben	18.0	365.0 → 309.0, 365.0 → 147.0
Pyridapenthion	12.4	341.0 → 189.0, 341.0 → 205.0
Pyridate	19.1	379.1 → 206.9, 379.1 → 350.9
Pyrifenox	13.0	295.1 → 93.0, 297.1 → 93.0
Pyrimethanil	11.3	200.0 → 82.0, 200.0 → 107.0
Pyriproxyfen	16.7	322.0 → 96.0, 322.0 → 185.0
Pyroxsulam	5.6	435.0 → 195.1, 435.0 → 194.0
Quinalfos	13.9	299.0 → 271.0, 299.0 → 243.0
Quinoclamine	6.8	208.0 → 105.0, 208.0 → 77.0
Quinoxyfen	16.4	308.0 → 197.0, 308.0 → 162.0
Rotenone	13.4	395.1 → 213.1, 395.1 → 192.0
Secbumeton	10.6	226.2 → 170.1, 226.2 → 100.0
Silthiofam	13.5	268.0 → 252.0, 268.0 → 73.0
Simazine	7.2	202.02 → 132.1, 202.2 → 104.0
Simetryn	9.4	214.1 → 124.1, 214.1 → 144.0
Spinosyn A	17.3	732.5 → 142.0, 732.5 → 98.0
Spinosyn D	18.3	746.5 → 142.0, 746.5 → 98.0
Spirodiclofen	17.4	313.1 → 295.0, 313.1 → 213.0

Analyte	Retention time (mins)	MRM transitions
Spiromesifen	16.8	371.2 → 273.1, 371.2 → 255.2
Spirotetramat	12.8	374.2 → 302.2, 374.2 → 330.2
Spiroxamine	13.3	298.3 → 100.1, 298.3 → 144.1
Sulfotep	14.0	323.0 → 97.0, 323.0 → 115.0
Tau-fluvalinate	18.9	503.0 → 208.0, 503.0 → 181.0
Tebuconazole	13.9	308.1 → 70.0, 308.1 → 125.0
Tebufenozide	13.5	353.2 → 297.2, 353.2 → 133.0
Tebufenpyrad	15.9	334.0 → 145.0, 334.0 → 117.0
Teflubenzuron	16.3	381.1 → 158.2, 381.1 → 141.2
Tembotrione (NH4 adduct)	5.9	458.0 → 340.9, 458.0 → 441.0
Terbufos	16.1	289.1 → 103.1, 289.1 → 232.9
Terbufos sulfone	11.1	321.1 → 171.0, 321.1 → 115.0
Terbufos sulfoxide	11.0	305.1 → 187.2, 305.1 → 131.1
Terbumeton	11.3	226.2 → 170.1, 226.2 → 142.0
Terbuthylazine	11.4	230.2 → 174.0, 232.2 → 176.0
Terbutryn	12.9	242.1 → 186.1, 242.1 → 96.0
Tetrachlorvinfos	13.5	367.0 → 127.0, 365.0 → 127.0
Tetraconazole	12.9	372.0 → 159.0, 374.0 → 161.2
Thiabendazole	6.2	202.1 → 174.9, 202.1 → 131.0
Thiacloprid	4.7	253.1 → 126.1, 253.1 → 99.1
Thiencarbazone-methyl	2.3	391.0 → 130.0, 391.0 → 230.0
Thiodicarb	9.2	355.0 → 88.0, 355.0 → 108.0
Thiophanate-methyl	7.6	343.0 → 151.1, 343.0 → 311.0
Tiamethoxam	1.7	292.0 → 211.0, 292.0 → 181.0
Tolclophos-methyl	14.9	301.2 → 268.9, 303.1 → 270.9
Tolylfluanid	13.9	347.0 → 237.8, 347.0 → 137.1
Topramezone	1.6	364.1 → 334.1, 364.1 → 125.0
Triadimefon	12.1	294.2 → 197.2, 294.2 → 225.0
Triadimenol	12.4	296.2 → 70.0, 298.2 → 70.0
Triallate	16.7	304.1 → 142.9, 304.1 → 86.2
Triazofos	12.6	314.0 → 162.0, 314.2 → 119.0
Trichlorfon	3.4	257.0 → 108.9, 257.0 → 220.8
Tricyclazole	5.2	190.1 → 136.1, 190.1 → 163.0
Trifloxystrobin	15.3	409.0 → 186.0, 409.0 → 206.0
Triflumizole	15.3	346.0 → 278.0, 346.0 → 73.0
Triflumuron	14.6	359.1 → 156.2, 359.1 → 139.0
Triforin	10.6	435.0 → 390.0, 437.0 → 392.0
Triticonazole A	12.7	318.0 → 70.0, 318.0 → 125.0
Triticonazole B	10.9	318.0 → 70.0, 318.0 → 125.0
Vamidothion	3.4	288.1 → 146.0, 288.1 → 118.0
Zoxamide	14.2	336.0 → 187.0, 338.0 → 189.0

Phenolic Compounds from Red Grape Seed Extract

ACE®
Ultra-inert
UHPLC & HPLC Columns

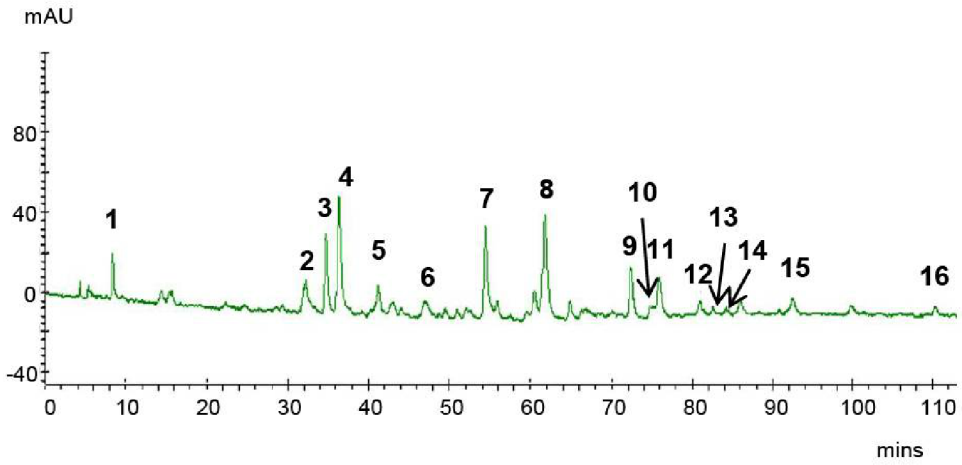
Application #AN3790

Conditions

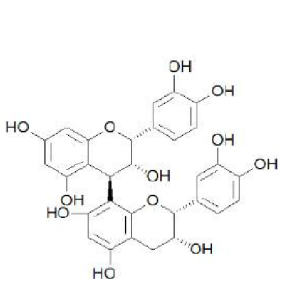
Column:	ACE 3 C18-AR
Dimensions:	200 x 4.6 mm
Part Number:	ACE-119-2046
Mobile Phase:	A: 2% acetic acid in H_2O
	B: 2% acetic acid in MeCN

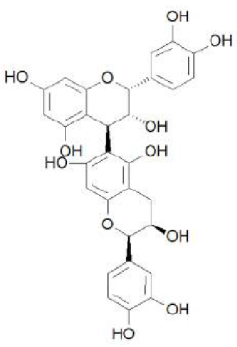
Time (mins)	%B
0	0
80	20
115	28
120	100
130	100

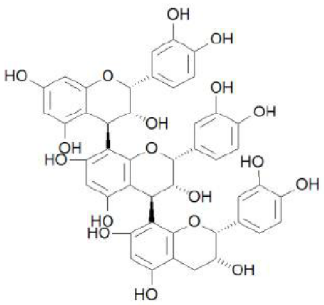
Flow Rate:	0.6 mL/min
Detection:	UV, 280 nm
	Peak identities established by combination of retention times, UV, fluorescence, NMR and ESI-MS (negative ion mode)

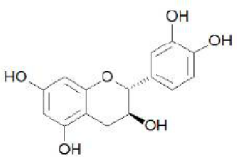


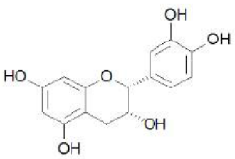
1. Gallic acid
2. Procyanidin B3 (dimer) + procyanidin C2 (trimer)
3. Procyanidin B1 (dimer)
4. (+)-Catechin
5. Procyanidin C3 (trimer)
6. Procyanidin B4 (dimer)
7. Procyanidin B2 (dimer)
8. (-)-Epicatechin
9. Procyanidin B3 gallate (dimer)
10. Procyanidin B7 (dimer)
11. Procyanidin C1 (trimer)
12. Procyanidin tetramer
13. Procyanidin pentamer
14. Procyanidin hexamer
15. (-)-Epigallocatechin
16. Procyanidin B5 (dimer)


Procyanidin B2


Procyanidin B5


Procyanidin C1


(+)-Catechin


(-)-Epicatechin

Grases F, Prieto R, Fernandez-Cabot R, Costa-Bauza A, Sanchez A, Prodanov M (2015) Effect of consuming a grape seed supplement with abundant phenolic compounds on the oxidative status of healthy human volunteers. Nutrition Journal 14:94 (2015) doi: 10.1186/s12937-015-0083-3

Tocopherols Mixture Separation

ACE®
Ultra-inert
UHPLC & HPLC Columns

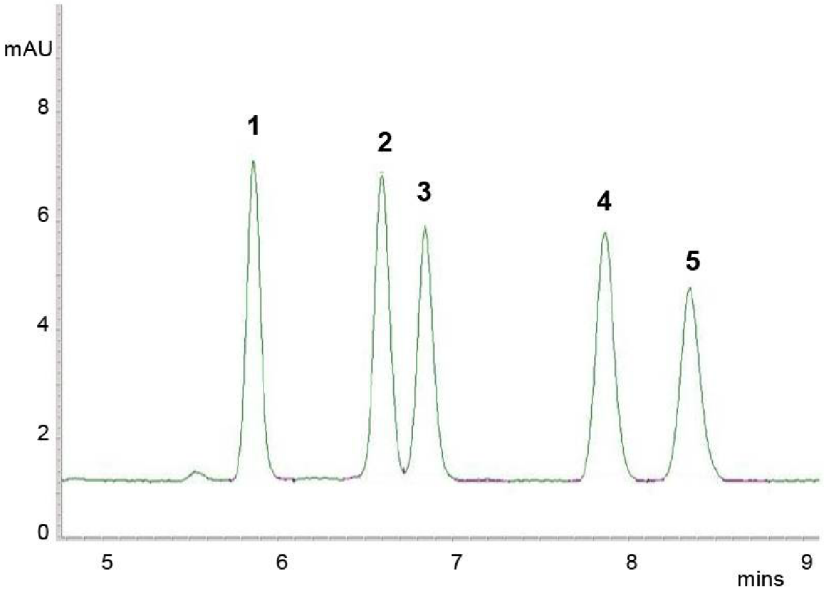
Application #**AN3390**

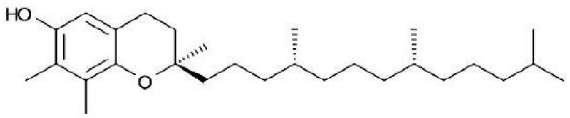
Conditions

Column:	ACE Excel 3 C18-PFP
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1110-1546U
Mobile Phase:	A: 0.1% H_3PO_4/MeCN (1:3 v/v)
	B: MeCN

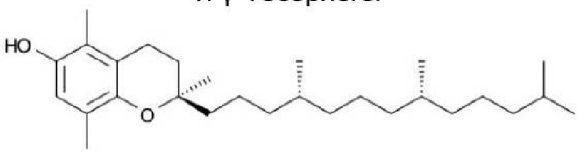
Time (mins)	%B
0.00	0
0.10	0
0.11	80
8.00	80
8.01	100
12.00	100
12.01	0
14.00	0

Flow Rate:	1.2 mL/min
Injection:	10 µL
Temperature:	40 °C
Detection:	UV, 285 nm

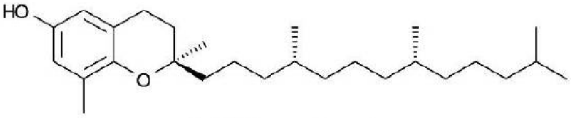




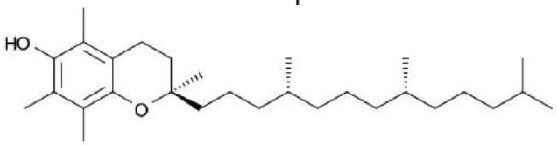
1. γ-Tocopherol



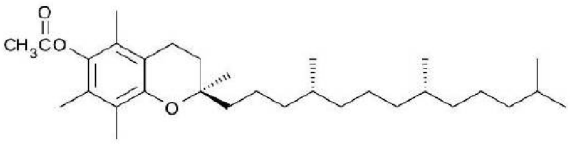
2. β-Tocopherol



3. δ-Tocopherol



4. α-Tocopherol



5. α-Tocopherol acetate

Sugars - Lactulose

ACE®
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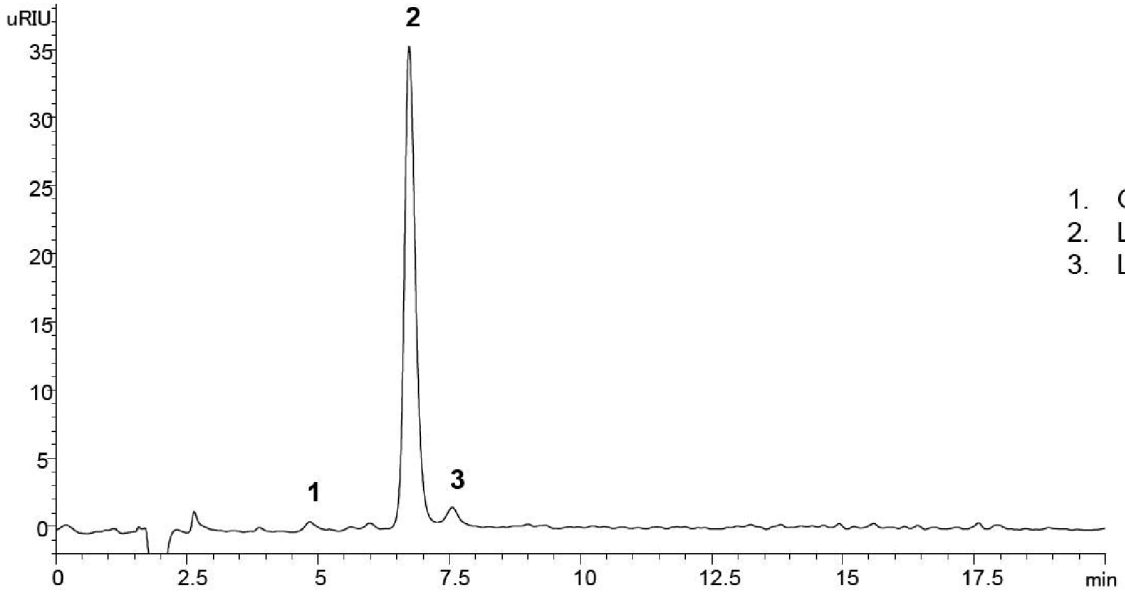
UHPLC & HPLC Columns

Application #**AN4020**

Conditions

Column:	ACE Excel 5 NH_2
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1214-1546U
Mobile Phase:	MeCN/H_2O (70:30 v/v)
Flow Rate:	1 mL/min
Injection:	10 µL
Temperature:	35 °C
Detection:	RI, 35 °C



1. Galactose
2. Lactulose
3. Lactose

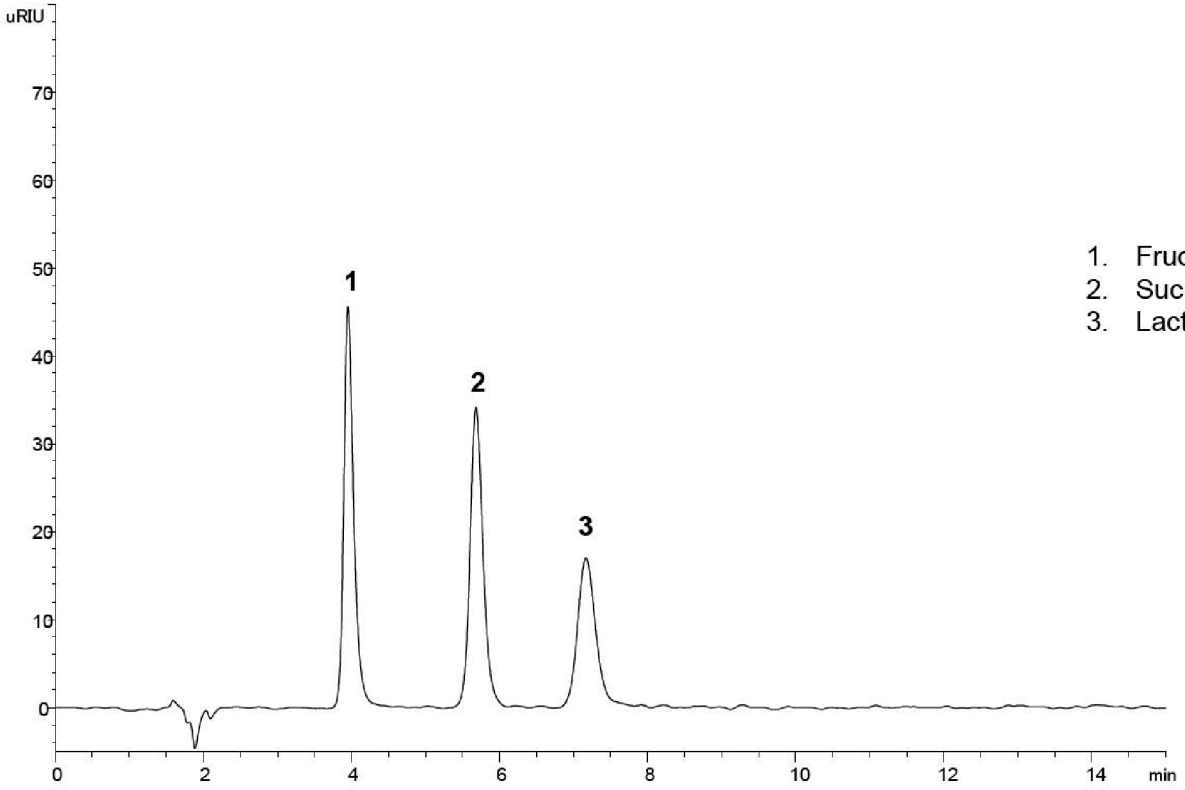
Sugars Separation

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN4030**

Conditions

Column:	ACE Excel 5 NH_2
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1214-1546U
Mobile Phase:	MeCN/H_2O (70:30 v/v)
Flow Rate:	1 mL/min
Injection:	10 µL
Temperature:	35 °C
Detection:	RI, 35 °C



1. Fructose
2. Sucrose
3. Lactose

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