mGluR5 PET Tracer by Radio HPLC Analysis

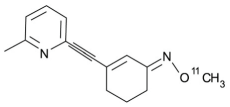
Application #AN2700

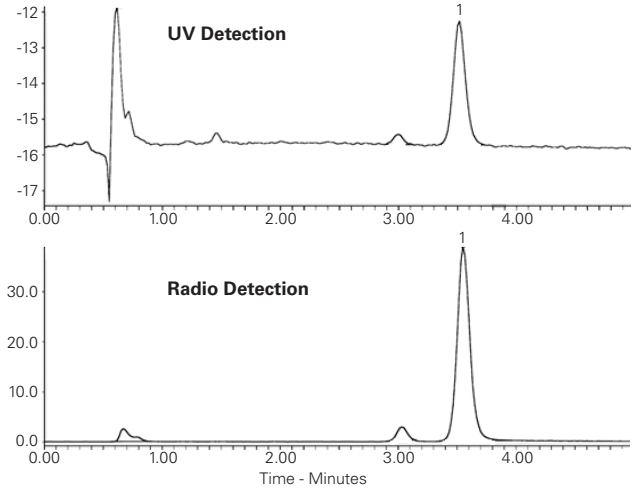
Conditions

Column: ACE 3 C18
Dimensions: 50 x 4.6 mm
Part Number: ACE-111-0546
Mobile Phase: 0.1% TFA in H_2O/MeCN (55:45 v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Detection: UV, 254 nm
Radio detection

Analyte

1. ^{11}C-ABP688





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Barcelona-Allee 17 • D-55129 Mainz
Tel +49 6131 880 96-0
Fax +49 6131 880 96-20
e-mail: info@mz-at.de
www.mz-at.de
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For additional column dimensions

Please enquire
email: info@ace-hplc.com

Microbial Extract by LC-MS

Application #AN1180

Conditions

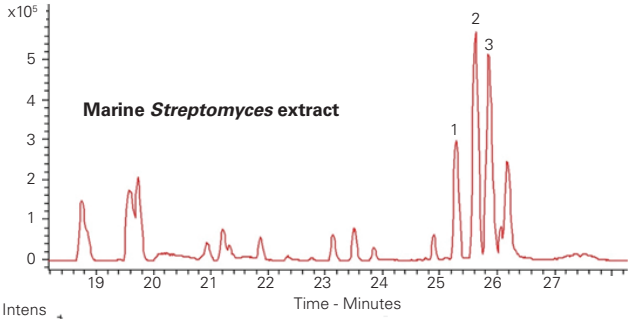
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 150 x 2.1 mm
Part Number: CORE-25A-1502U
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN
Gradient:

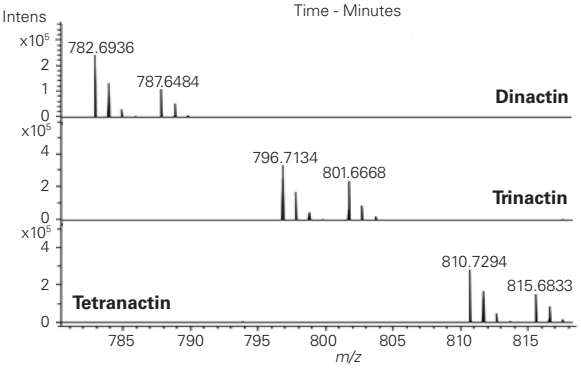
Time (mins)	%B
0.0	5
5.0	5
20.0	100
25.0	100

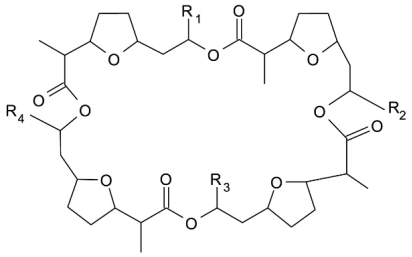
Flow Rate: 0.2 mL/min
Detection: Dionex 3000RS UHPLC system
coupled with Bruker MaXis Q-TOF MS
Electrospray MS positive mode
Source end plate offset -500 V
Nebuliser gas (N_2) 1.6 bar
Drying gas (N_2) temp 180 °C
Collision energy 5.0 eV
Collision RF 600 Vpp

Analytes

Macrotetralides
1. Dinactin $R_1 = R_3 = CH_2CH_3$, $R_2 = R_4 = CH_3$
2. Trinactin $R_1 = R_2 = R_3 = CH_2CH_3$, $R_4 = CH_3$
3. Tetranactin $R_1 = R_2 = R_3 = R_4 = CH_2CH_3$







Macrotetralides

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Microcystins from Blue/Green Algae in Drinking Water

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

Gradient:

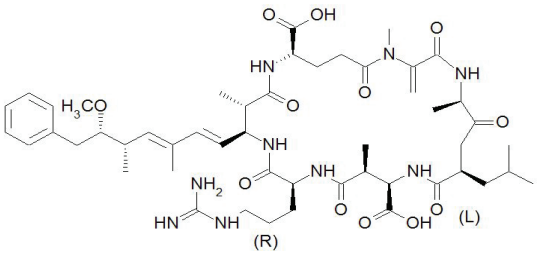
Time (mins)	%B
0.0	30
1.0	30
7.0	95
7.1	30
10.0	30

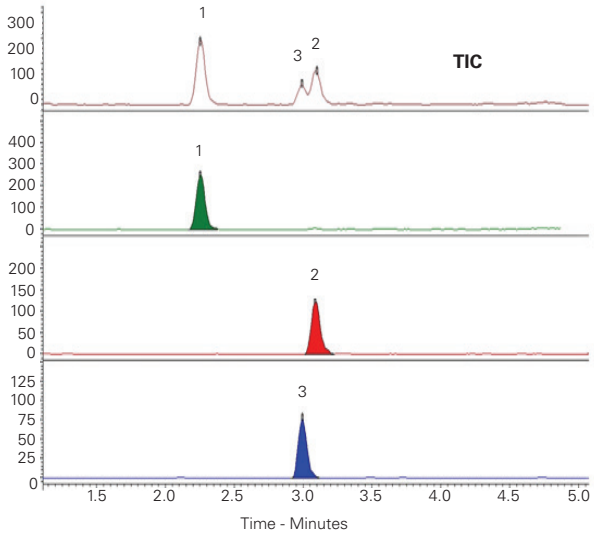
Flow Rate: 0.4 mL/min
Injection: 50 µL
Temperature: 40 °C
Sample: 0.05 ppb
Detection: Bruker EVOQ Elite triple quad MS
VIP heated-ESI temperature: 350 °C
Cone gas temperature: 200 °C
Spray voltage: 4500 V (+)
Collision gas: argon 1.5 mTorr

Analytes

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

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





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Milk Proteins

Application #AN1540

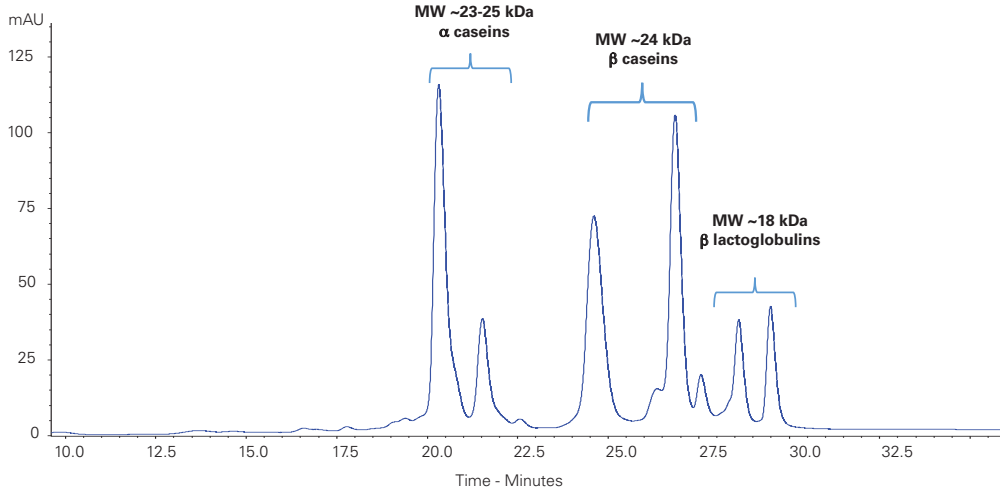
Conditions

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

Gradient:

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

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



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Mycotoxins by LC-MS/MS

Application #AN2330

Conditions

Column: ACE Excel 2 C18-AR
Dimensions: 50 x 2.1 mm
Part Number: EXL-109-0502U
Mobile Phase: A: 1 mM ammonium acetate, 0.5% acetic acid in H_2O
B: 1 mM ammonium acetate, 0.5% acetic acid in 95% MeOH

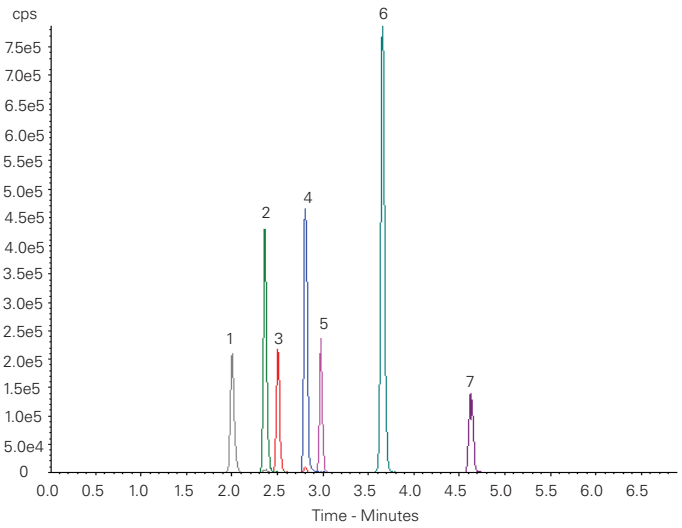
Gradient:

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

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

Analytes

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



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Mycotoxins/Aflatoxins from Peppers

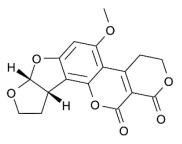
Application #AN1200

Conditions

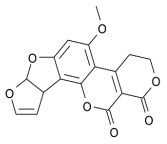
Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: H_2O/MeOH (60:40 v/v)
Flow Rate: 1 mL/min
Injection: 100 µL
Temperature: 45 °C
Detection: Fluorescence, λ_{Ex} 362 nm, λ_{Em} 425 nm

Analytes

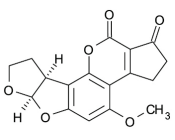
1. Aflatoxin G2
2. Aflatoxin G1
3. Aflatoxin B2
4. Aflatoxin B1



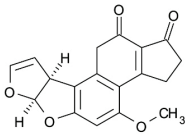
Aflatoxin G2



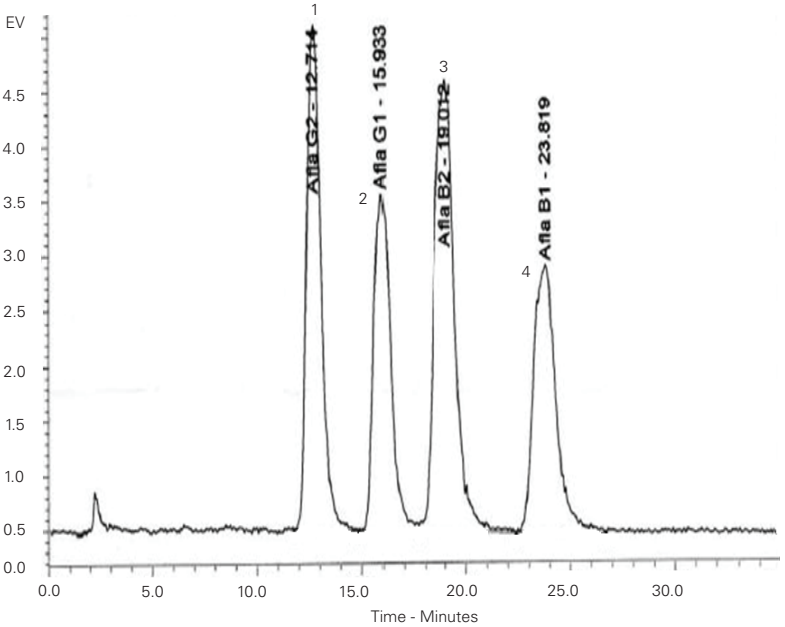
Aflatoxin G1



Aflatoxin B2



Aflatoxin B1



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Naphthalenes (Substituted)

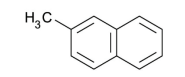
Application #AN3690

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	MeCN/H_2O (51:49 v/v)
Flow Rate:	1.5 mL/min
Temperature:	18 °C
Detection:	UV, 225 nm

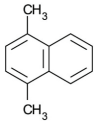
Analytes

1. 2-Methylnaphthalene
2. 1-Ethylnaphthalene
3. 1,4-Dimethylnaphthalene
4. 2-Ethylnaphthalene
5. n-Butylbenzene

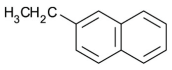


2-Methylnaphthalene

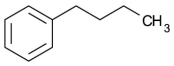
1-Ethylnaphthalene



1,4-Dimethylnaphthalene



2-Ethylnaphthalene



n-Butylbenzene

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Neonicotinoids in Honey by LC-MS/MS

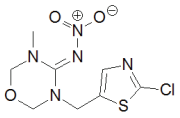
Application #AN4050

Conditions

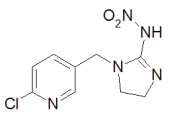
Column:	ACE UltraCore 2.5 SuperC18	
Dimensions:	100 x 2.1 mm	
Part Number:	CORE-25A-1002U	
Mobile Phase:	A: 0.05% ammonia in H_2O	
	B: 0.05% ammonia in MeOH	
Gradient:	**Time (mins)**	**%B**
	0	5
	3	100
Flow Rate:	0.6 mL/min	
Injection:	1 µL (POISe mode)	
Temperature:	30 °C	
Detection:	Shimadzu LCMS-8060	
	Positive ion mode HESI	
Sample:	Honey spiked at 0.1 ppb	
	(QuEChERS extract)	

Analytes

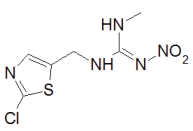
1. Thiamethoxam
   (*m/z* 292 → 211)
2. Imidacloprid
   (*m/z* 256 → 175)
3. Clothianidin
   (*m/z* 250 → 169)
4. Acetamiprid
   (*m/z* 223 → 126)
5. Thiacloprid
   (*m/z* 253 → 126)



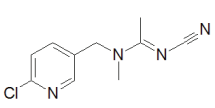
Thiamethoxam



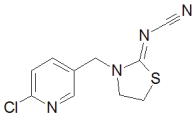
Imidacloprid



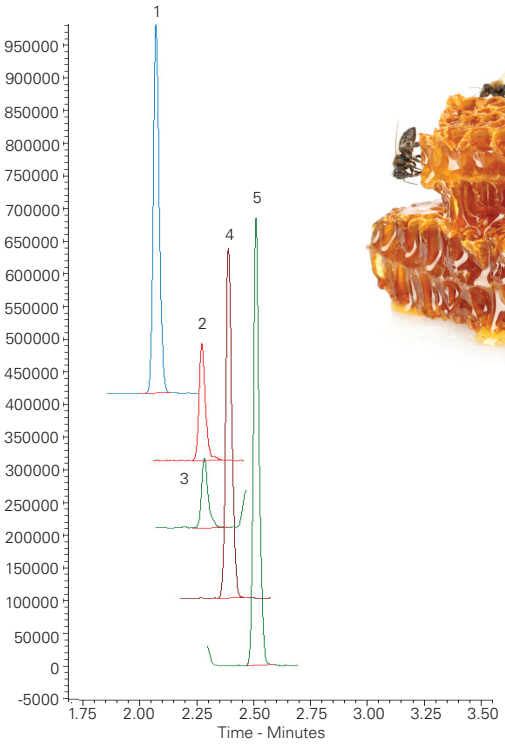
Clothianidin



Acetamiprid



Thiacloprid



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Neurotransmitters and Metabolites from Rat Brain by LC-MS/MS

Application #AN3870

Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: A: 0.2% formic acid in H_2O
B: MeCN

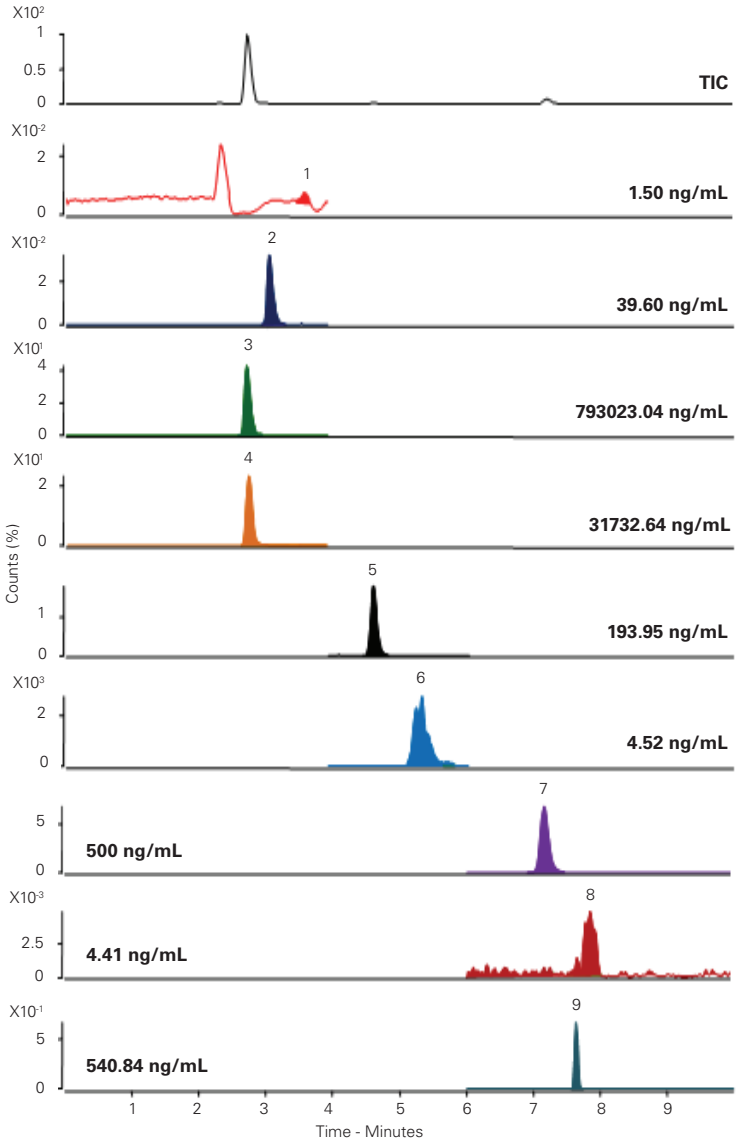
Gradient:

Time (mins)	%B
0	5
2	5
5	90
8	90
10	5
14	5

Flow Rate: 0.6 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: Agilent 6410 triple quad
ESI in positive ion mode (negative ion mode for MHPG)
Capillary Voltage: 1950 kV
Sample: Rat brain samples homogenised in aqueous formic acid, centrifuged and proteins removed by precipitation with acetonitrile

Analytes

	Quantifier	Qualifier	LLOQ (ng/mL)
1. Adrenaline	*m/z* 184.2 → 166.2	*m/z* 184.2 → 57.1	0.25
2. Noradrenaline	*m/z* 170.2 → 107.1	*m/z* 170.2 → 152.1	0.5
3. Glutamic acid	*m/z* 148.1 → 84.1	*m/z* 148.1 → 130.1	250
4. GABA	*m/z* 104 → 45	*m/z* 104 → 87	250
5. Dopamine	*m/z* 154.1 → 137.1	*m/z* 154.1 → 91.1	0.25
6. MHPG (3-Methoxy-4-hydroxyphenylglycol)	*m/z* 263 → 165.1	*m/z* 263 → 165.1	1
7. Isoprenaline (IS)	*m/z* 212.2 → 194.1		
8. 5-Hydroxyindoleacetic acid	*m/z* 192 → 145.9	*m/z* 192 → 90.9	1
9. Serotonin	*m/z* 177.2 → 160.2	*m/z* 177.2 → 132.1	10



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Nitroanilines (I)

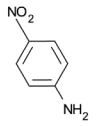
Application #AN3240

Conditions

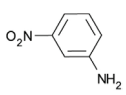
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 50 mM KH_2PO_4 pH 3.15/ MeCN (50:50 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analytes

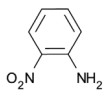
1. p-Nitroaniline
2. m-Nitroaniline
3. o-Nitroaniline



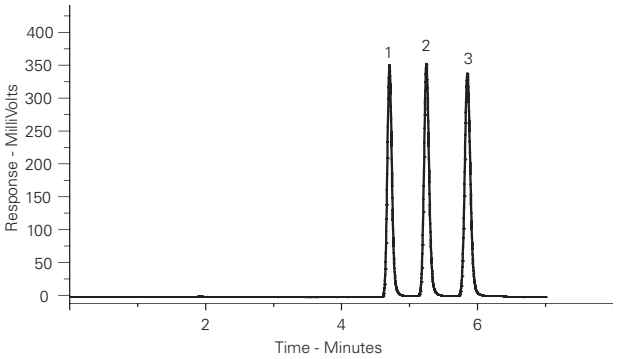
p-Nitroaniline



m-Nitroaniline



o-Nitroaniline



Nitroanilines (II)

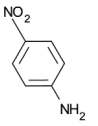
Application #AN3250

Conditions

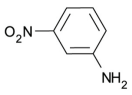
Column: ACE 5 CN
Dimensions: 250 x 4.6 mm
Part Number: ACE-124-2546
Mobile Phase: Heptane/Ethyl acetate (90:10 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analytes

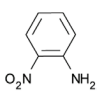
1. p-Nitroaniline
2. m-Nitroaniline
3. o-Nitroaniline



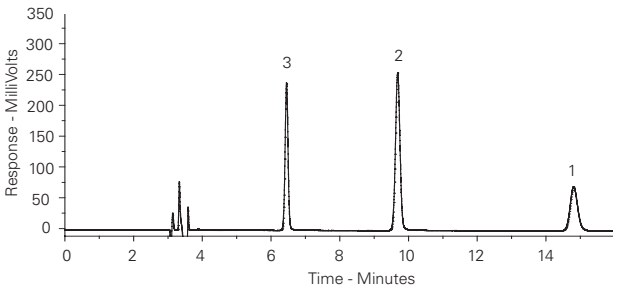
p-Nitroaniline



m-Nitroaniline



o-Nitroaniline



Nitrofuran Metabolites by LC-MS/MS

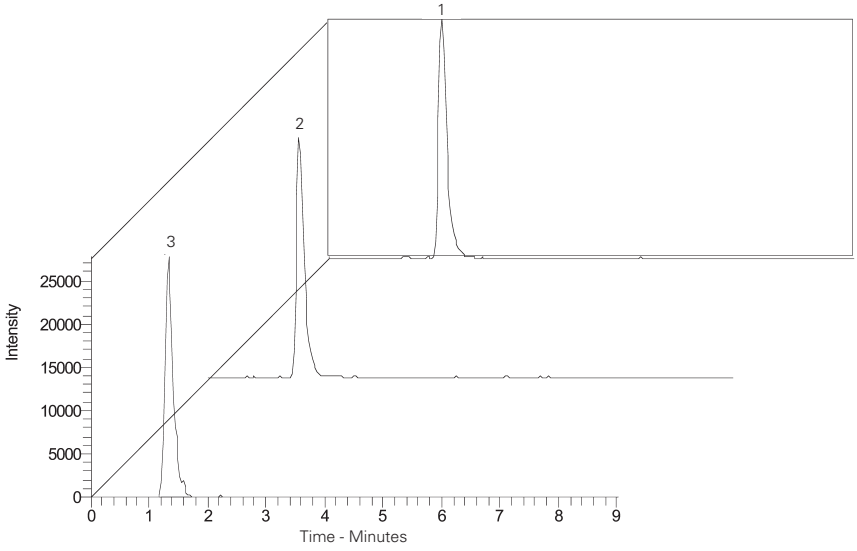
Application #AN3050

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

Analytes

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



Nitrosamines European Toy Standard Method by LC-MS/MS

Application #AN1110

Conditions

Column:	ACE Excel 2 C18-PFP
Dimensions:	150 x 3.0 mm
Part Number:	EXL-1010-1503U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeOH

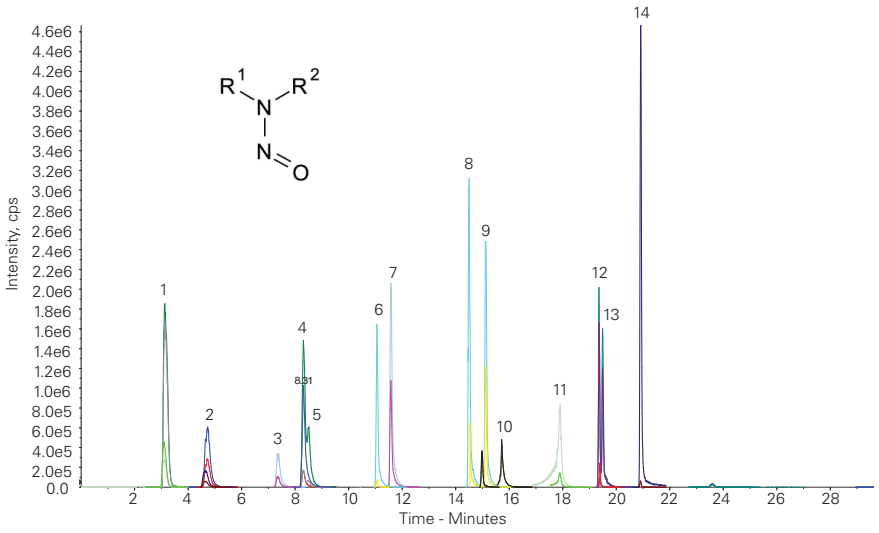
Gradient:	**Time (mins)**	**%B**
	0.0	5
	1.0	5
	10.0	65
	14.0	65
	15.0	90
	20.0	90
	21.0	5
	30.0	5

Flow Rate:	0.35 mL/min
Injection:	20 µL
Temperature:	40 °C
Sample Temperature:	4 °C
Detection:	Applied Biosystems 4000 Q-Trap MS
	Source: APCI (positive mode)
	Collision energy: 10-30 V
	Source temperature: 300 °C

European Union EN 71-12 Safety of Toys:
N-Nitrosamines and N-nitrosatable substances e.g.
Analysis of nitrosamines in balloon extracts

Analytes

1. NDELA (*m/z* 135.2 ⟶ 74.2, 135.2 ⟶ 104.2)
2. NDMA (*m/z* 74.9 ⟶ 43.2, 74.9 ⟶ 58.2)
3. Nmorph (*m/z* 117.1 ⟶ 86.3, 117.1 ⟶ 73.3)
4. Npyrr (*m/z* 101.2 ⟶ 55.3, 101.2 ⟶ 59.2)
5. NMEA (*m/z* 89.2 ⟶ 61.1, 89.2 ⟶ 43.3)
6. NDEA (*m/z* 103.1 ⟶ 75.2, 103.1 ⟶ 47.2)
7. NPIP (*m/z* 115.1 ⟶ 69.1, 115.1 ⟶ 41.2)
8. NDnPA (*m/z* 131.2 ⟶ 89.2, 131.2 ⟶ 43.3)
9. NdiPA (*m/z* 131.2 ⟶ 89.2, 131.2 ⟶ 43.3)
10. NMPhA (*m/z* 137.2 ⟶ 107.2, 137.2 ⟶ 66.1)
11. NEPhA (*m/z* 151.1 ⟶ 77.1, 151.1 ⟶ 95.3)
12. NDiBA (*m/z* 159.3 ⟶ 57.2, 159.3 ⟶ 103.2)
13. NDnBA (*m/z* 159.3 ⟶ 103.2, 159.3 ⟶ 57.2)
14. NDBzA (*m/z* 227.2 ⟶ 91.1, 227.2 ⟶ 181.2)



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Non-Steroidal Anti-Inflammatory Drugs (I)

Application #AN1210

Conditions

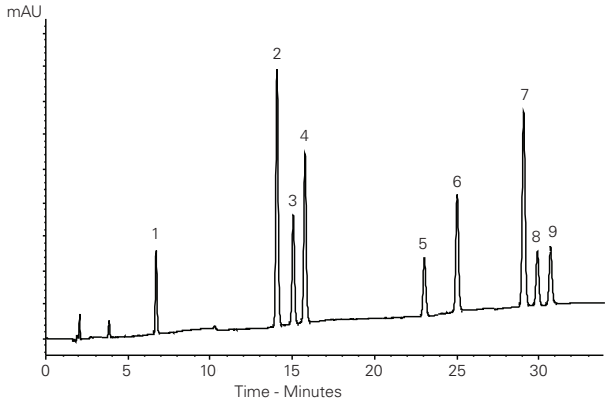
Column:	ACE 3 C18-AR
Dimensions:	150 x 4.6 mm
Part Number:	ACE-119-1546
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeOH

Gradient:	**Time (mins)**	**%B**
	0	52
	28	74
	33	74
	38	52
	48	52

Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	40 °C
Detection:	UV, 254 nm

Analytes

1. Bendroflumethiazide
2. Ketoprofen
3. Naproxen
4. Sulindac
5. Ibuprofen
6. Diclofenac
7. Indomethacin
8. Meclofenamic acid
9. Mefenamic acid



Non-Steroidal Anti-Inflammatory Drugs (II)

Application #AN1220

Conditions

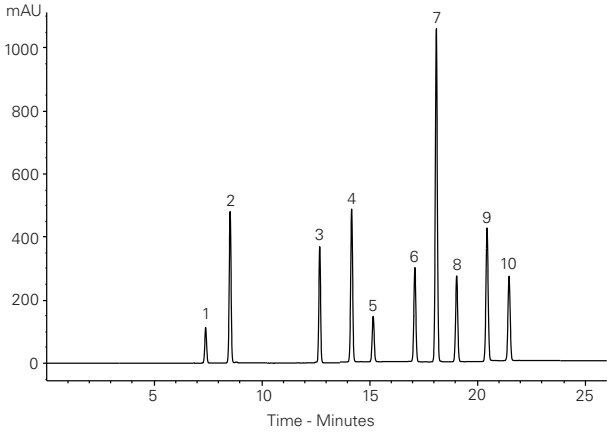
Column:	ACE Excel 5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1211-1546U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

Gradient:	**Time (mins)**	**%B**
	0	20
	20	70
	25	70
	36	20

Flow Rate:	1 mL/min
Injection:	10 µL
Temperature:	40 °C
Detection:	UV, 254 nm

Analytes

1. Aspirin
2. Phenacetin
3. Sulindac
4. Tolmetin
5. Naproxen
6. Nimesulide
7. Flurbiprofen
8. Diclofenac
9. Phenylbutazone
10. Meclofenamic acid



Non-Steroidal Anti-Inflammatory Drugs (III)

Application #AN3570

Conditions

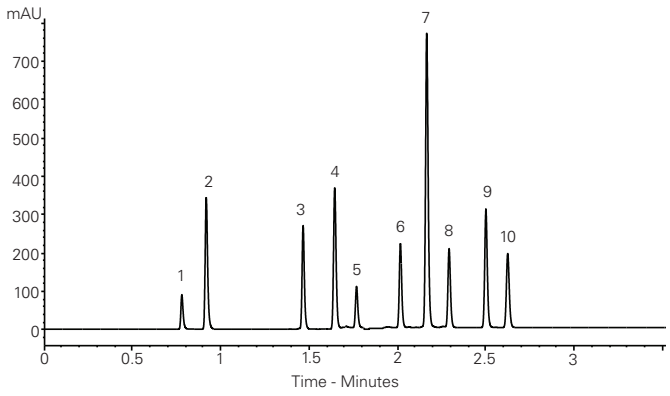
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	50 x 3.0 mm
Part Number:	CORE-25A-0503U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

Gradient:	**Time (mins)**	**%B**
	0.02	20
	2.71	70
	3.39	70
	3.52	20

Flow Rate:	0.85 mL/min
Injection:	1.04 µL
Temperature:	40 °C
Detection:	UV, 254 nm

Analytes

1. Aspirin
2. Phenacetin
3. Sulindac
4. Tolmetin
5. Naproxen
6. Nimesulide
7. Flurbiprofen
8. Diclofenac
9. Phenylbutazone
10. Meclofenamic acid



Non-Steroidal Anti-Inflammatory Drugs – Fast Analysis

Application #AN2080

Conditions

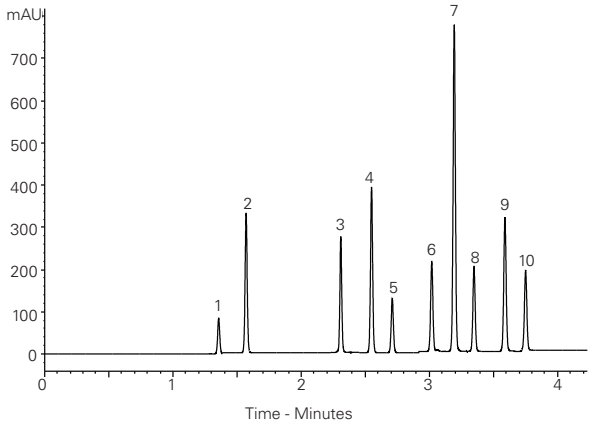
Column:	ACE Excel 2 SuperC18
Dimensions:	50 x 3.0 mm
Part Number:	EXL-1011-0503U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

Gradient:	**Time (mins)**	**%B**
	0.00	20
	0.25	20
	3.50	70
	4.00	20
	4.25	20

Flow Rate:	0.86 mL/m
Injection:	1.4 µL
Temperature:	40 °C
Detection:	UV, 254 nm

Analytes

1. Aspirin
2. Phenacetin
3. Sulindac
4. Tolmetin
5. Naproxen
6. Nimesulide
7. Flurbiprofen
8. Diclofenac
9. Phenylbutazone
10. Meclofenamic acid



Non-Steroidal Anti-Inflammatory Drugs by LC-MS/MS

Application #AN2630

Conditions

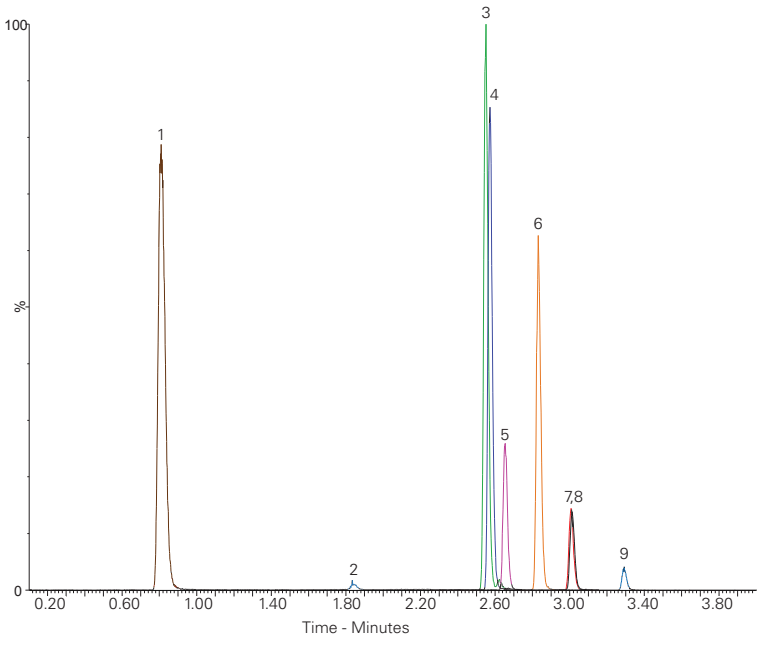
Column:	ACE Excel 2 C18
Dimensions:	50 x 2.1 mm
Part Number:	EXL-101-0502U
Mobile Phase:	A: 2 mM ammonium acetate, 0.1% formic acid in H_2O
	B: 2 mM ammonium acetate, 0.1% formic acid in MeOH

Gradient:	**Time (mins)**	**%B**
	0.0	15
	2.0	70
	3.0	90
	3.3	15

Flow Rate:	0.4 mL/min
Injection:	10 µL
Temperature:	40 °C
Detection:	MS/MS
	ESI in positive ion mode
Sample:	10 pg/µL

Analytes

1. Acetaminophen (*m/z* 151.7 → 109.7)
2. Salicylic acid (*m/z* 136.7 → 92.7)
3. Sulindac (*m/z* 357.0 → 233.1)
4. Ketoprofen (*m/z* 255.0 → 209.0)
5. Naproxen (*m/z* 231.0 → 184.9)
6. Phenylbutazone (*m/z* 309.1 → 119.8)
7. Indomethacin (*m/z* 357.9 → 138.7)
8. Diclofenac (*m/z* 295.8 → 213.9)
9. Mefenamic acid (*m/z* 242.0 → 208.8)



Nucleic Acids / Disease Biomarker Profiling (I)

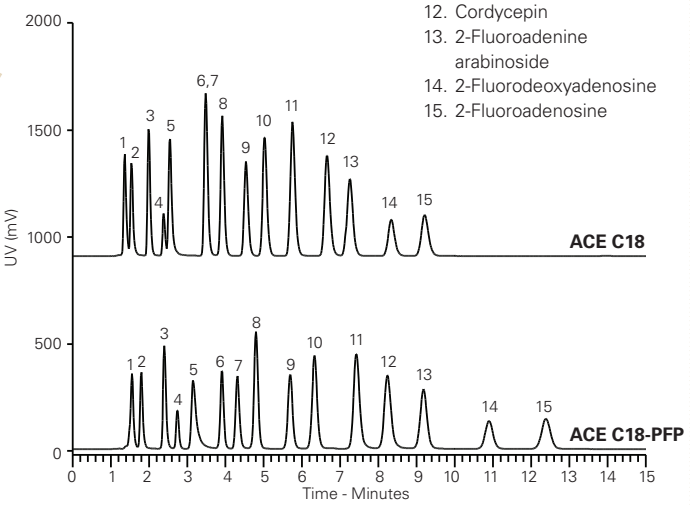
Application #AN1080

Conditions

Column: ACE 3 C18-PFP
ACE 3 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-1110-1046, ACE-111-1046
Mobile Phase: 33 mM potassium phosphate pH 6.2 with KOH/MeOH (88:12 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 260 nm

Analytes

1. dATP
2. dADP
3. dAMP
4. 5-Fluorodeoxyuridine
5. Adenine
6. Thymine
7. 2-Fluorodeoxyuridine
8. Adenine arabinoside
9. 2'-C-methyladenosine
10. Adenosine
11. Deoxyadenosine
12. Cordycepin
13. 2-Fluoroadenine arabinoside
14. 2-Fluorodeoxyadenosine
15. 2-Fluoroadenosine



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Nucleosides and Vitamins

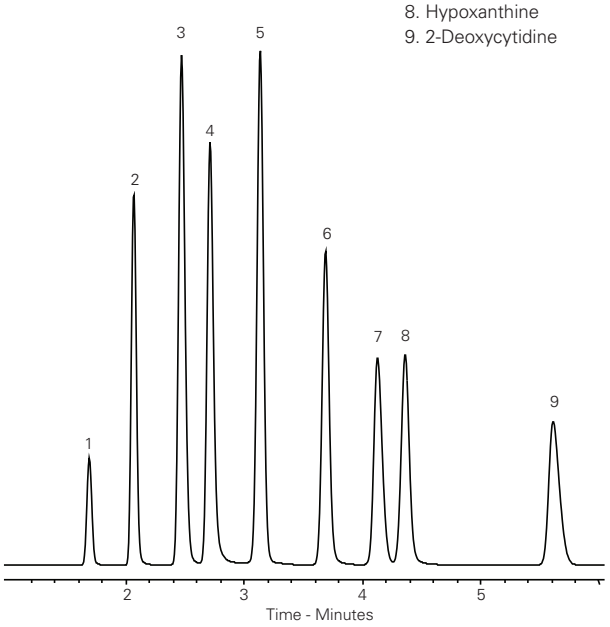
Application #AN1330

Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: 20 mM H_3PO_4 in H_2O
Flow Rate: 1 mL/min
Temperature: 22 °C
Detection: UV, 254 nm

Analytes

1. Pyridoxamine (Vitamin B6)
2. Cytosine
3. Thiamine (Vitamin B1)
4. Nicotinamide
5. L-Ascorbic acid (Vitamin C)
6. Uracil
7. Cytidine
8. Hypoxanthine
9. 2-Deoxycytidine



Nucleic Acids / Disease Biomarker Profiling (II)

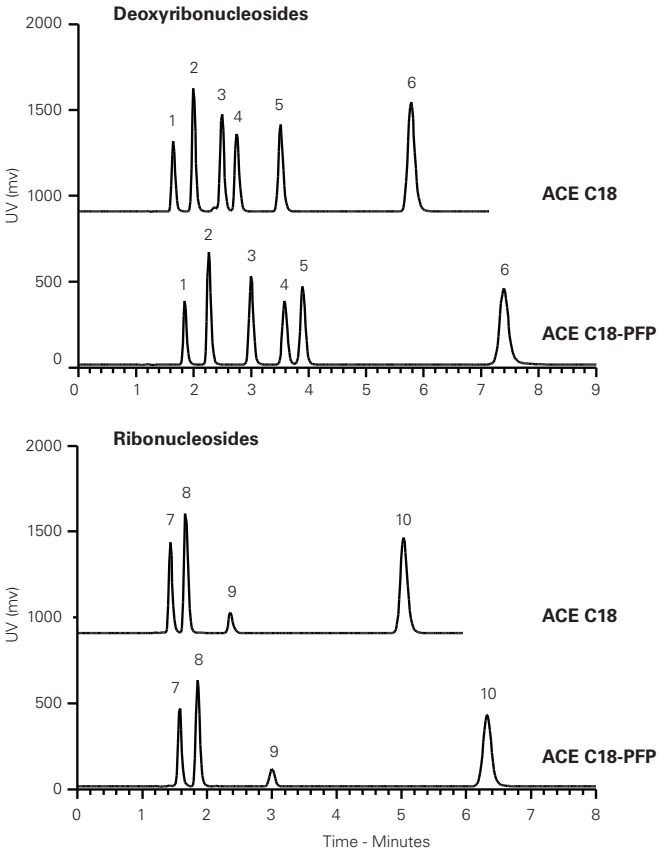
Application #AN1090

Conditions

Column: ACE 3 C18-PFP
ACE 3 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-1110-1046, ACE-111-1046
Mobile Phase: 33 mM potassium phosphate pH 6.2 with KOH/MeOH (88:12 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 260 nm

Analytes

1. Deoxycytidine
2. Deoxyuridine
3. Deoxyinosine
4. Deoxyguanosine
5. Thymidine
6. Deoxyadenosine
7. Cytidine
8. Uridine
9. Guanosine
10. Adenosine



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Ochratoxin A

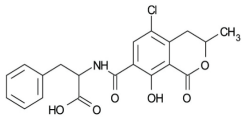
Application #AN2870

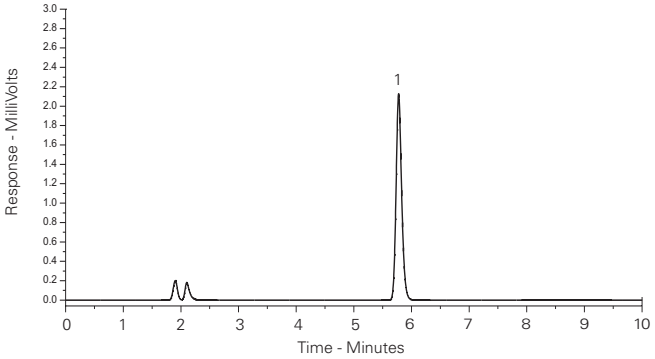
Conditions

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

Analyte

1. Ochratoxin A





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Olanzapine in Human Plasma by LC-MS/MS

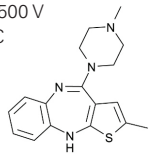
Application #AN2520

Conditions

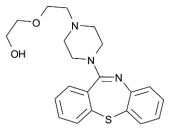
Column: ACE 5 C18-300
Dimensions: 100 x 4.6 mm
Part Number: ACE-221-1046
Mobile Phase: MeCN/0.01% ammonia in 2 mM ammonium formate pH 6.6 (85:15 v/v)
Flow Rate: 0.9 mL/min
Injection: 5 µL
Detection: API 4000 triple quad MS
Turbo Ion Spray in positive mode
Ion Spray voltage: 5500 V
Temperature: 550 °C

Analytes

1. Olanzapine (*m/z* 313.2 → 256.2)
2. Quetiapine (IS) (*m/z* 384.2 → 253.2)

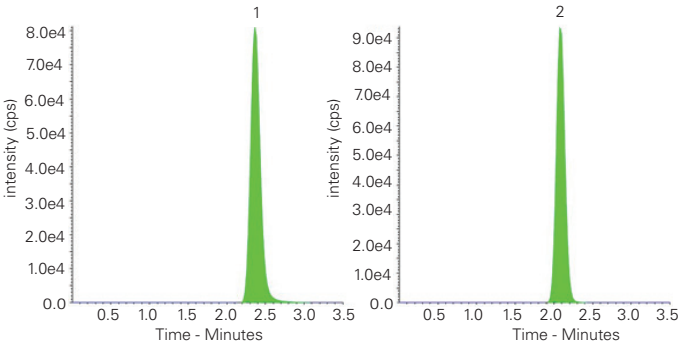


Olanzapine



Quetiapine (IS)

MRM chromatograms of plasma sample after administration of 5 mg dose of olanzapine



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Omeprazole and Degradation Products after Acidic Hydrolysis in 0.1 M HCl

Application #AN1560

Conditions

Column: ACE Excel 5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: EXL-1211-1546U
Mobile Phase: A: 0.1% ammonia in H_2O
B: 0.1% ammonia in MeCN/H_2O (90:10 v/v)

Gradient:

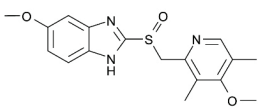
Time 1 (mins)	Time 2 (mins)	Time 3 (mins)	%B
0.0	0.0	0.0	10
15.0	30.0	45.0	90
15.5	30.5	45.5	90
18.0	33.0	48.0	10

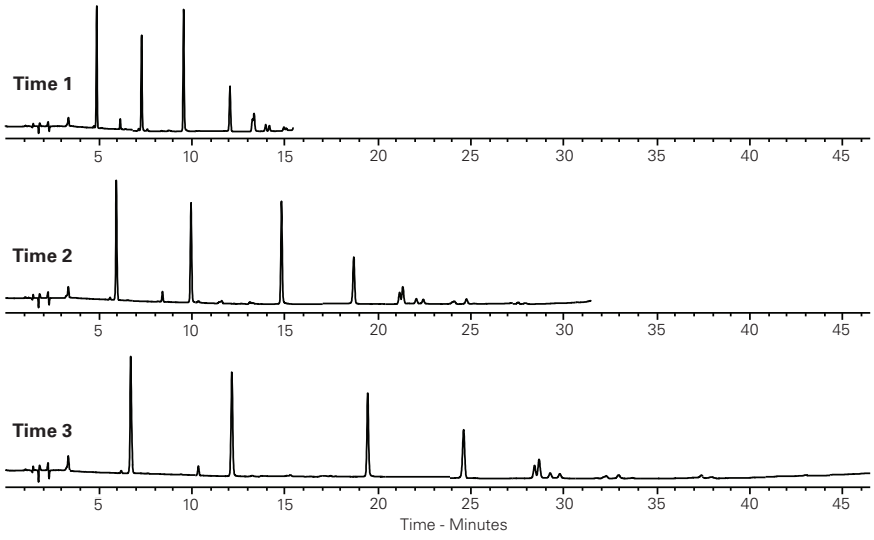
Post time 10 minutes

Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 30 °C
Detection: UV, 280 nm

Analyte

Omeprazole





Opiates from Drugs of Abuse Screen (#AN2190)

Application #AN2340

Conditions

Column: ACE Excel 1.7 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-171-1002U
Mobile Phase: A: 5 mM ammonium acetate in H_2O
B: 5 mM ammonium acetate in MeOH

Gradient:

Time (mins)	%B
0.0	10
10.0	90
11.9	90
13.4	10
15.5	10

Flow Rate: 0.3 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: MS Quattro Premier XE triple quad
MRM, positive and negative ESI mode
Desolvation temperature: 450 °C
IonSource temperature: 150 °C
Collision gas pressure: 3.5 x 10^{-3} mbar

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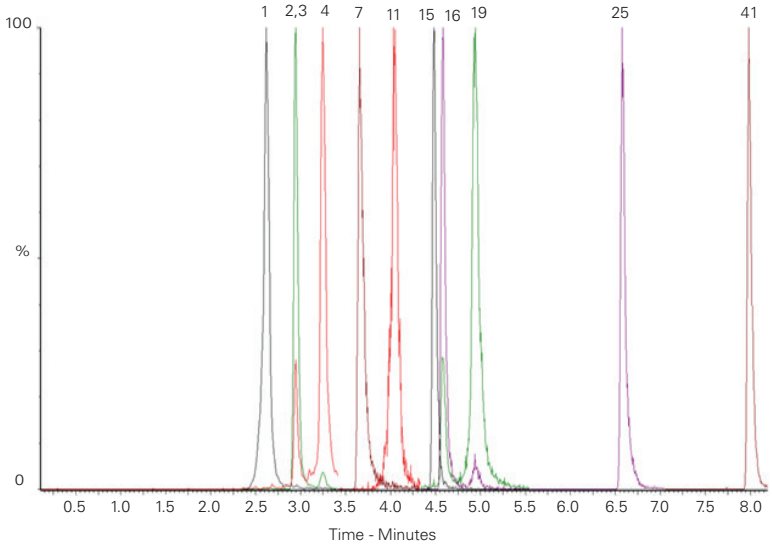
Analytes

1. Oxymorphone (*m/z* 302.2 → 198.1)
2. Morphine-d3 (*m/z* 289.2 → 201.0)
3. Morphine (*m/z* 286.2 → 201.0)
4. Hydromorphone (*m/z* 286.2 → 185.1)
7. Dihydrocodeine (*m/z* 302.2 → 199.1)
11. Oxycodone (*m/z* 316.2 → 241.2)
15. 6-MAM (*m/z* 328.2 → 165.1)
16. Codeine (*m/z* 300.3 → 215.1)
19. Hydrocodone (*m/z* 300.2 → 199.1)
25. EDDP (*m/z* 278.2 → 234.2)
41. Methadone (*m/z* 310.2 → 265.2)



Opiates in Urine by LC-MS/MS

Application #AN1230

Conditions

Column: ACE Excel 3 SuperC18
Dimensions: 75 x 2.1 mm
Part Number: EXL-1111-7502U
Mobile Phase: A: 5 mM ammonium hydroxide pH 10.8 in H_2O
B: 5 mM ammonium hydroxide pH 10.8 in MeOH/H_2O (90:10 v/v)

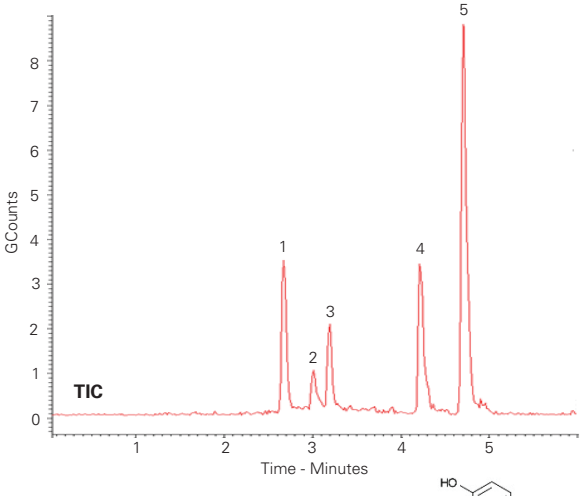
Gradient:

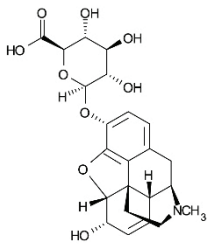
Time (mins)	%B
0	30
5	95

Flow Rate: 0.6 mL/min
Injection: 2 µL
Temperature: 60 °C
Detection: Varian 320 Triple Quadrupole MS
Electrospray voltage: +5 kV
Inlet capillary voltage: 30 V
CID with argon at 1.5 mTorr
Collision cell potential ranges from 5 to 17 V
Drying gas (nitrogen) temperature: 325 °C
Nebulizing gas (nitrogen) pressure: 35 psi
Extended Dynamic Range

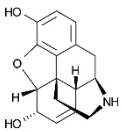
Analytes

1. Morphine 3-β-D-glucuronide
LOD (est) 100 ppb
(*m/z* 462.0 → 285.9)
2. Normorphine
LOD (est) 100 ppb
(*m/z* 272.0 → 165.0)
3. Morphine 6-β-D-glucuronide
LOD (est) 100 ppb
(*m/z* 462.0 → 285.9)
4. Morphine
LOD (est) 20 ppb
(*m/z* 286.0 → 200.9)
5. 6-Acetylmorphine
LOD (est) 10 ppb
(*m/z* 328.0 → 164.9)

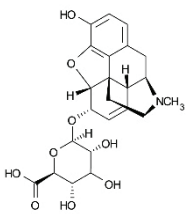




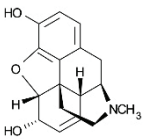
Morphine 3-β-D-glucuronide



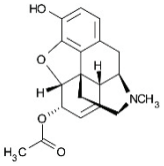
Normorphine



Morphine 6-β-D-glucuronide



Morphine



6-Acetylmorphine

Organic Acids

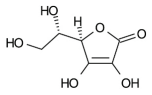
Application #AN2780

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

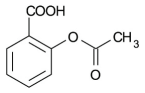
Analytes

1. L-Ascorbic acid
2. Maleic acid
3. Acetylsalicylic acid
4. Benzoic acid
5. Salicylic acid



L-Ascorbic acid

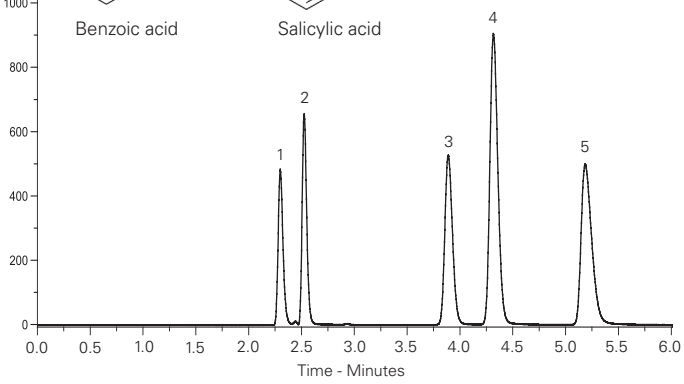
Maleic acid



Acetylsalicylic acid

Benzoic acid

Salicylic acid



For further applications

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

Organic Acids – Fast Separation

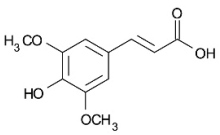
Application #AN2200

Conditions

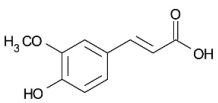
Column:	ACE Excel 3 C18-Amide ACE Excel 1.7 C18-Amide
Dimensions:	250 x 2.1 mm, 50 x 3.0 mm
Part Number:	250 x 2.1 mm (EXL-1112-2502U), 50 x 3 mm (EXL-1712-0503U)
Mobile Phase:	20 mM H_3PO_4 in MeOH/H_2O (40:60 v/v)
Flow Rate:	0.21 mL/min (250 x 2.1 mm) 0.8 mL/min (50 x 3.0 mm)
Injection:	5 µL (250 x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

Analytes

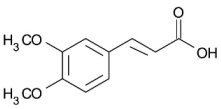
1. Sinapic acid
2. Ferulic acid
3. 3,4-Dimethoxycinnamic acid
4. Cinnamic acid
5. 4-Methoxycinnamic acid



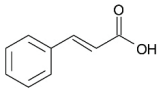
Sinapic acid



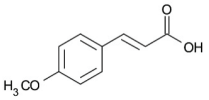
Ferulic acid



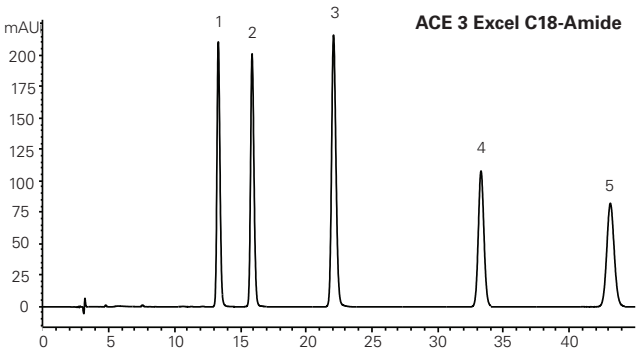
3,4-Dimethoxycinnamic acid

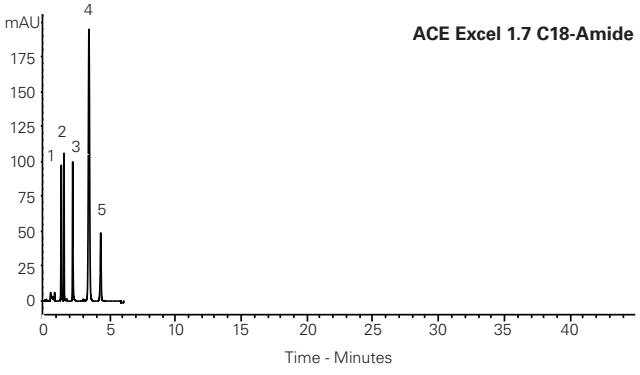


Cinnamic acid



4-Methoxycinnamic acid





Organophosphorus Flame Retardants in Water by LC-MS/MS

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)

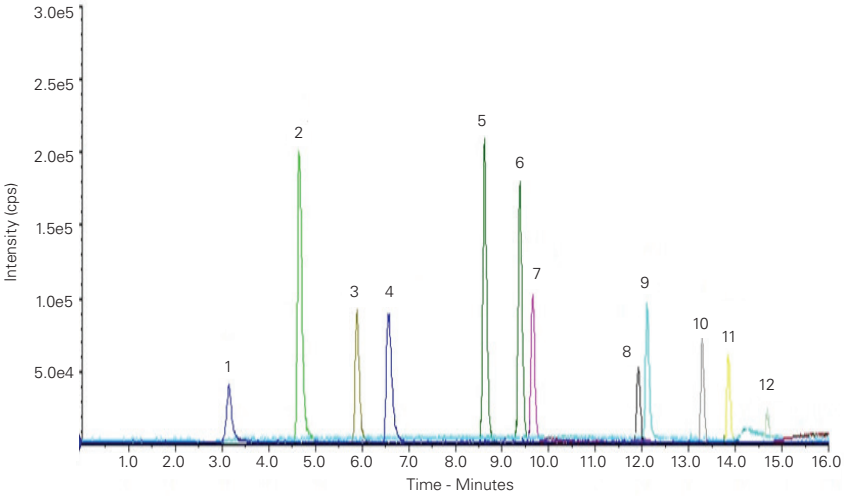
Gradient:

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

Analytes

		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



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Organophosphorus (Isomeric) Flame Retardants in Water

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)

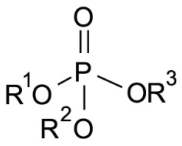
Gradient:

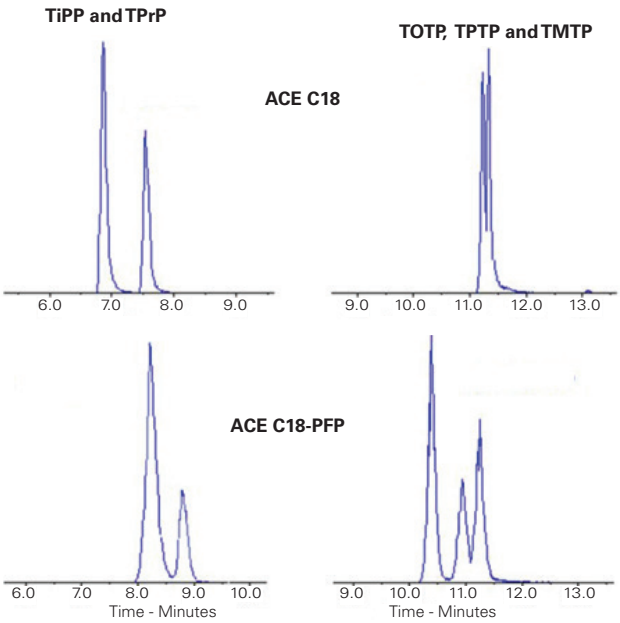
Time (mins)	%B
0.1	50
12.0	90
13.0	100
15.0	100
15.1	50
20.0	50

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

Analytes

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)





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Organotin Compounds

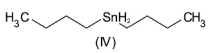
Application #AN3650

Conditions

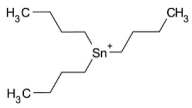
Column: ACE 3 C18
Dimensions: 150 x 2.1 mm
Part Number: ACE-111-1502
Mobile Phase: H_2O/MeCN/acetic acid/TEA (23:65:12:0.05 v/v/v/v)
Flow Rate: 0.2 mL/min
Detection: ICP-MS

Analytes

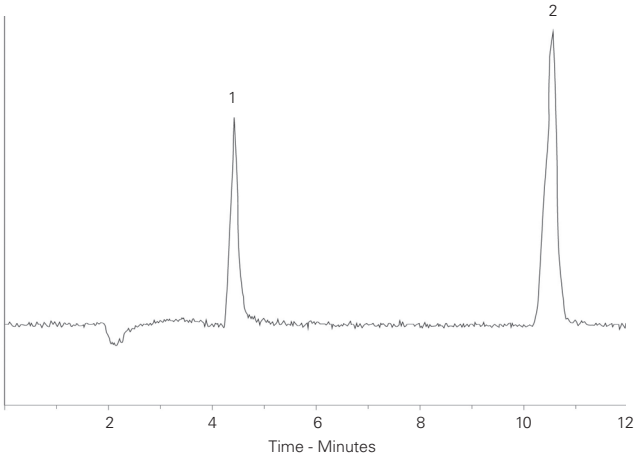
1. Dibutyltin
2. Tributyltin



Dibutyltin



Tributyltin



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OTC Gastric Drugs

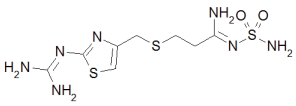
Application #AN3940

Conditions

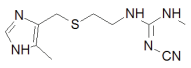
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeCN/10 mM ammonium bicarbonate pH 8.0 in H_2O (18:82)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analytes

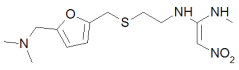
1. Famotidine
2. Cimetidine
3. Ranitidine



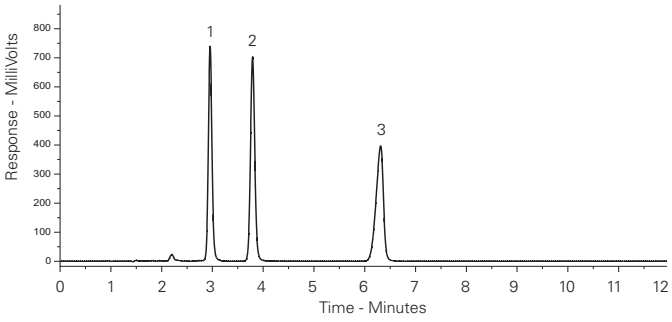
Famotidine



Cimetidine



Ranitidine



Oxysterols by LC-MS/MS

Application #AN2380

Conditions

Column: ACE 3 C18-AR
Dimensions: 150 x 2.1 mm
Part Number: ACE-119-1502
Mobile Phase: A: 0.1% formic acid in H_2O/MeOH (70:30 v/v)
B: 0.1% formic acid in MeOH

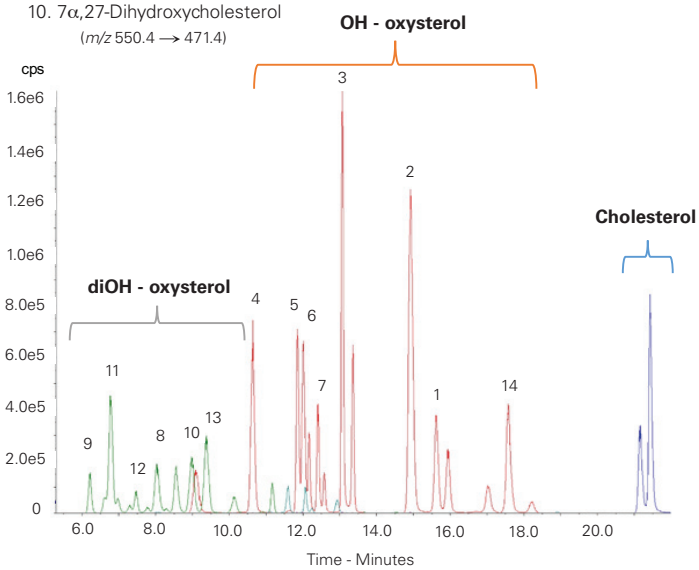
Gradient:

Time (mins)	%B
0.0	20
1.0	20
3.5	60
8.5	60
11.5	80
16.5	80
20.0	90
22.5	90
25.0	20

Flow Rate: 0.3 mL/min
Temperature: 40 °C
Detection: AB SCIEX API 4000 MS Turbo IonSpray, positive mode MRM
Sample: Derivatised with Girard P reagent

Analytes

1. 7α-Hydroxycholesterol (*m/z* 534.4 → 455.4)
2. 7β-Hydroxycholesterol (*m/z* 534.4 → 455.4)
3. 22(S)-Hydroxycholesterol (*m/z* 534.4 → 455.4)
4. 22(R)-Hydroxycholesterol (*m/z* 534.4 → 455.3)
5. 24(S)-Hydroxycholesterol (*m/z* 534.5 → 455.4)
6. 25-Hydroxycholesterol (*m/z* 534.4 → 455.4)
7. 27-Hydroxycholesterol (*m/z* 534.4 → 455.4)
8. 7α,25-Dihydroxycholesterol (*m/z* 550.4 → 471.4)
9. 7β,25-Dihydroxycholesterol (*m/z* 550.4 → 471.4)
10. 7α,27-Dihydroxycholesterol (*m/z* 550.4 → 471.4)
11. 7β,27-Dihydroxycholesterol (*m/z* 550.4 → 471.4)
12. 3β,25-Dihydroxy-5-cholesten-7-one (*m/z* 550.4 → 471.4)
13. 3β,27-Dihydroxy-5-cholesten-7-one (*m/z* 550.4 → 471.4)
14. 5α,6α-Epoxycholestanol (*m/z* 534.4 → 455.4)



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Oxymetazoline in Nasal Spray Formulation

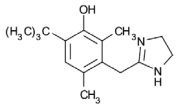
Application #AN3660

Conditions

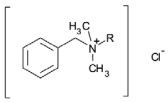
Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: aq. Na_2HPO_4 pH 7.0/MeCN (50:50 v/v)
Flow Rate: 1.5 mL/min
Temperature: 30 °C
Detection: UV, 214 nm

Analytes

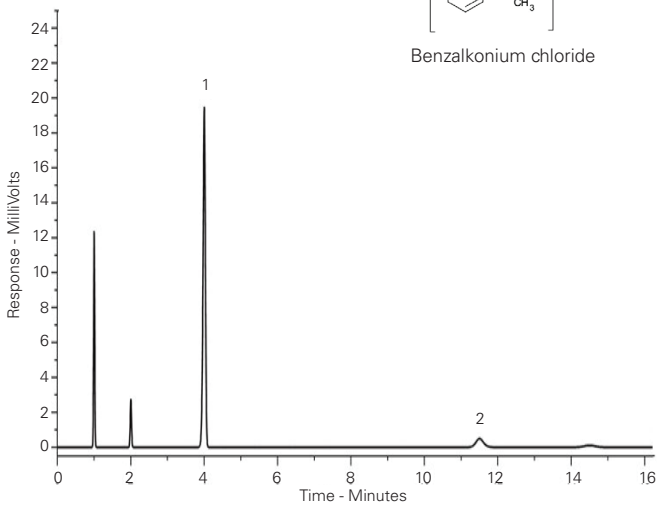
1. Oxymetazoline
2. Benzalkonium chloride



Oxymetazoline



Benzalkonium chloride



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Paclitaxel

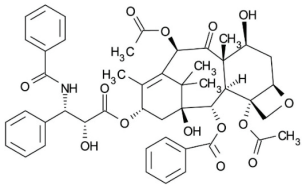
Application #AN3670

Conditions

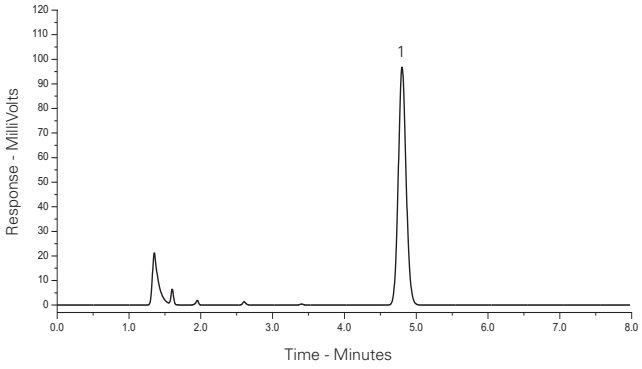
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: H_2O/MeCN (45:55 v/v)
Flow Rate: 1 mL/min
Temperature: 40 °C
Detection: UV, 227 nm

Analyte

1. Paclitaxel



Paclitaxel



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Paeonia Lactiflora Extract HPLC Fingerprint

Application #AN3820

Conditions

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

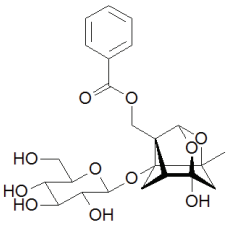
Gradient:

Time (mins)	%B
0	10
5	15
25	22
45	70
46	80
50	80

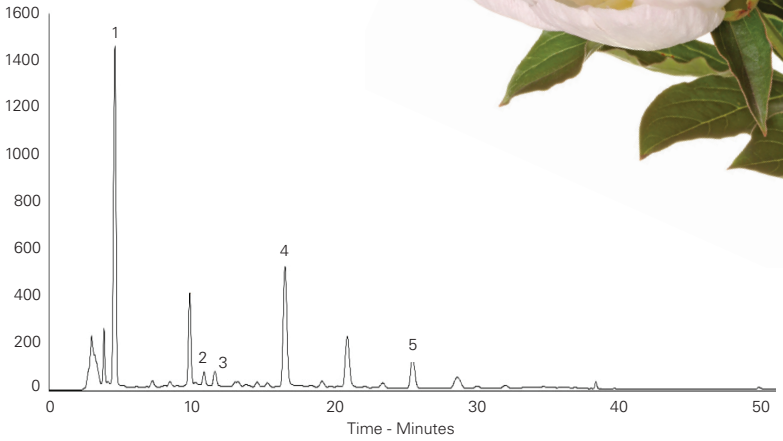
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 25 °C
Detection: UV, 254 nm
Sample: *P. lactiflora* root extracted with boiling water and polysaccharides removed by precipitation

Analytes

1. Gallic acid
2. Catechin hydrate
3. Methyl gallate
4. Paeoniflorin
5. Benzoic acid



Paeoniflorin



Choi H-J, Chung T-W, Park M-J, Lee KS, Yoon Y, Kim HS, Lee JH, Kwon S-M, Lee S-O, Kim K-J, Baek J-H, Ha K-T. (2016) *Paeonia lactiflora* Enhances the Adhesion of Trophoblast to the Endometrium via Induction of Leukemia Inhibitory Factor Expression. PloS ONE 11(2): e0148232. doi:10.137/journal.pone.0148232

Paraben Preservatives

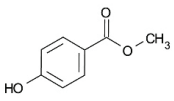
Application #AN1250

Conditions

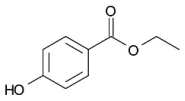
Column:	ACE 3 Phenyl
Dimensions:	150 x 2.1 mm
Part Number:	ACE-115-1502
Mobile Phase:	25 mM ammonium acetate pH 6.8 in H_2O/MeOH (50:50 v/v)
Flow Rate:	0.2 mL/min
Injection:	2 µL
Temperature:	40 °C
Detection:	UV, 240 nm

Analytes

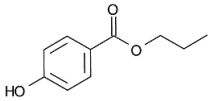
1. Methyl paraben
2. Ethyl paraben
3. n-Propyl paraben
4. i-Butyl paraben
5. n-Butyl paraben
6. Benzyl paraben



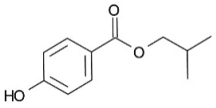
Methyl paraben



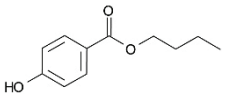
Ethyl paraben



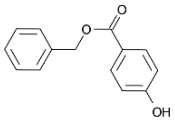
n-Propyl paraben



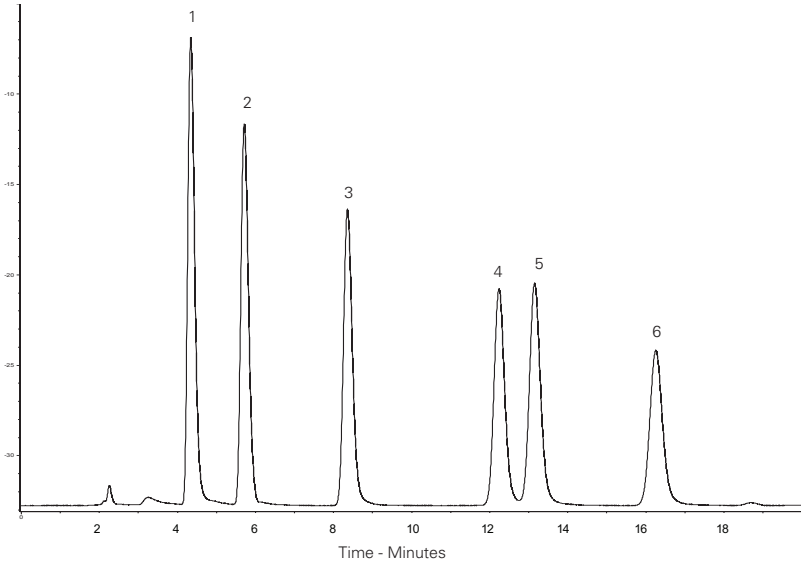
i-Butyl paraben



n-Butyl paraben



Benzyl paraben



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Paracetamol and Related Compounds

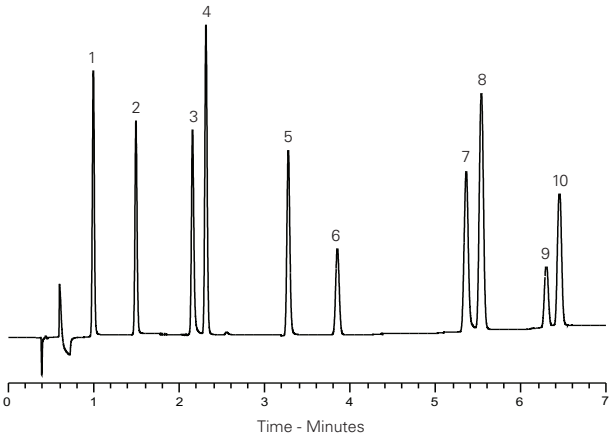
Application #AN1260

Conditions

Column:	ACE Excel 2 C18-PFP	
Dimensions:	100 x 3.0 mm	
Part Number:	EXL-1010-1003U	
Mobile Phase:	A: 20 mM ammonium acetate pH 6.0 in H_2O	
	B: 20 mM ammonium acetate pH 6.0 in MeOH/H_2O (90:10 v/v)	
Gradient:	**Time (mins)**	**%B**
	0.0	6
	5.5	63
Flow Rate:	1.2 mL/min	
Injection:	2 µL	
Temperature:	27 °C	
Detection:	UV, 220 nm	

Analytes

1. 4-Aminophenol
2. Hydroquinone
3. 2-Aminophenol
4. Paracetamol
5. 2-Acetamidophenol
6. Phenol
7. 4-Nitrophenol
8. 2-Nitrophenol
9. 4-Chloroacetanilide
10. 4-Chlorophenol



Paracetamol and Related Substances – Fast Analysis (I)

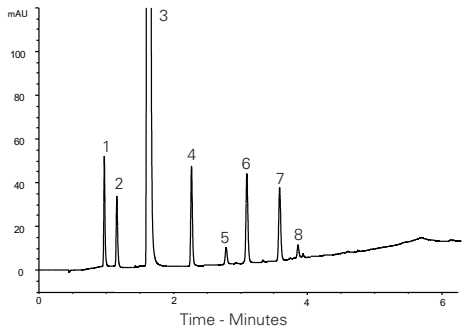
Application #AN2210

Conditions

Column:	ACE Excel 1.7 C18	
Dimensions:	50 x 3.0 mm	
Part Number:	EXL-171-0503U	
Mobile Phase:	A: 10 mM ammonium acetate pH 6.0 in H_2O	
	B: 10 mM ammonium acetate pH 6.0 in MeOH/H_2O (90:10 v/v)	
Gradient:	**Time (mins)**	**%B**
	0.00	5
	0.08	5
	5.08	95
	6.76	95
	7.09	5
	10.00	5
Flow Rate:	0.51 mL/min	
Injection:	0.7 µL	
Temperature:	40 °C	
Detection:	UV, 230 nm	

Analytes

1. 4-Aminophenol
2. Hydroquinone
3. Paracetamol
4. 2-Acetamidophenol
5. Phenol
6. 4-Nitrophenol
7. 2-Nitrophenol
8. 4-Chloroacetanilide



For enhanced resolution of paracetamol and related compounds, see AN2220.

Paracetamol and Related Substances – Enhanced Resolution

Application #AN2220

Conditions

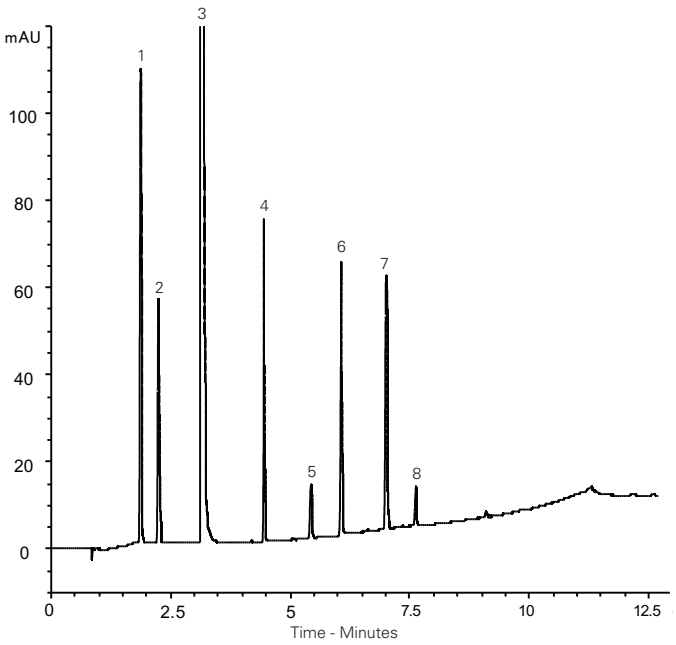
Column:	ACE Excel 1.7 C18
Dimensions:	100 x 3.0 mm
Part Number:	EXL-171-1003U
Mobile Phase:	A: 10 mM ammonium acetate pH 6.0 in H_2O
	B: 10 mM ammonium acetate pH 6.0 in MeOH/H_2O (90:10 v/v)

Gradient:	**Time (mins)**	**%B**
	0.00	5
	0.21	5
	10.23	95
	13.56	95
	14.16	5
	20.24	5

Flow Rate:	0.51 mL/min
Injection:	1.4 µL
Temperature:	40 °C
Detection:	UV, 230 nm

Analytes

1. 4-Aminophenol
2. Hydroquinone
3. Paracetamol
4. 2-Acetamidophenol
5. Phenol
6. 4-Nitrophenol
7. 2-Nitrophenol
8. 4-Chloroacetanilide



For enhanced speed of paracetamol and related compounds, see AN2210.

Paracetamol and Related Substances – Phase Selectivity

Application #AN3580

Conditions

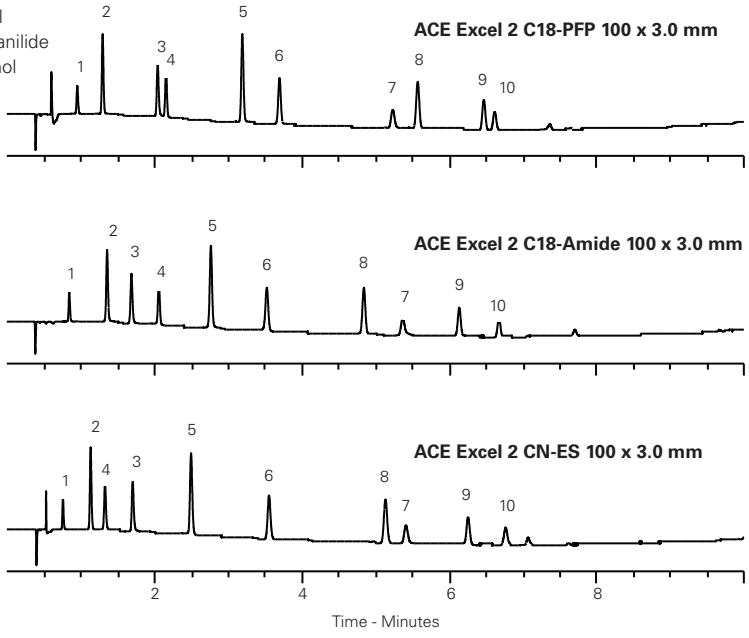
Column:	ACE Excel 2 C18-PFP, ACE Excel 2 C18-Amide, ACE Excel 2 CN-ES
Dimensions:	100 x 3.0 mm
Part Number:	EXL-1010-1003U, EXL-1012-1003U, EXL-1013-1003U
Mobile Phase:	A: 20 mM ammonium acetate pH 6.0 in H_2O
	B: 20 mM ammonium acetate pH 6.0 in MeOH/H_2O (90:10 v/v)

Gradient:	**Time (mins)**	**%B**
	0.0	5
	10.0	95
	12.5	95
	13.0	5

Flow Rate:	1.2 mL/min
Injection:	2 µL
Temperature:	40 °C
Detection:	UV, 210 nm

Analytes

1. 4-Aminophenol
2. Hydroquinone
3. 2-Aminophenol
4. Paracetamol
5. 2-Acetamidophenol
6. Phenol
7. 4-Nitrophenol
8. 2-Nitrophenol
9. 4-Chloroacetanilide
10. 4-Chlorophenol



Paralytic Shellfish Poisoning (PSP) Toxins

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)

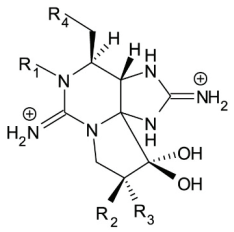
Gradient:

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

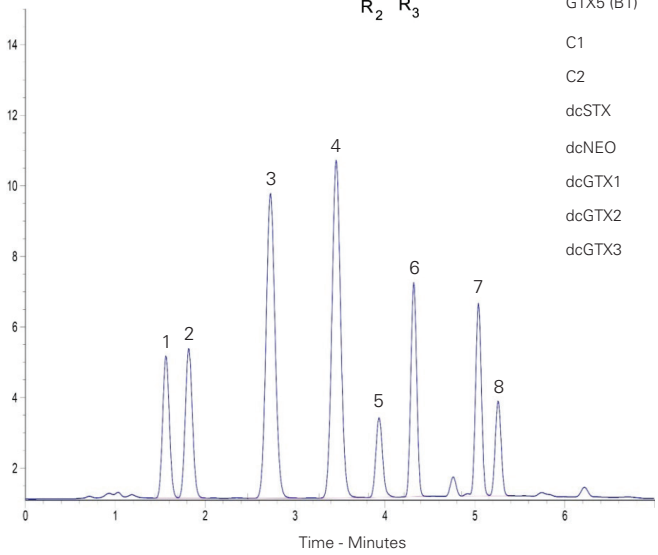
Flow Rate: 2 mL/min
Injection: 30 µL
Temperature: 20 °C
Detection: Fluorescence λ_{Ex} 340 nm, λ_{Em} 395 nm
Sample: Prechromatographic oxidation with hydrogen peroxide and periodate

Analytes

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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Parotoid Macrogland Secretions from South American Toads

Application #AN3970

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
B: 0.1% TFA in MeCN/H_2O (90:10 v/v)

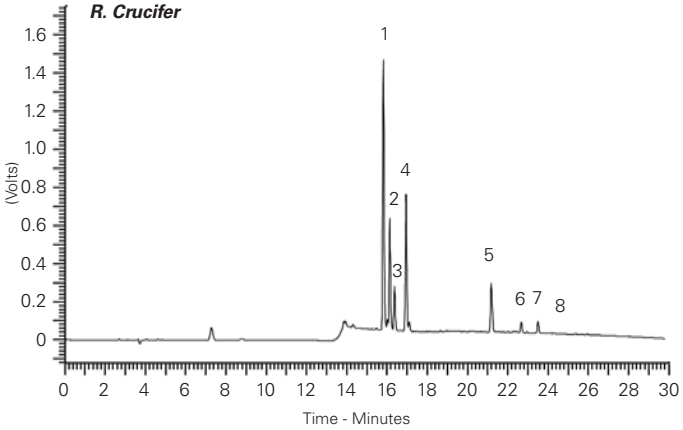
Gradient:

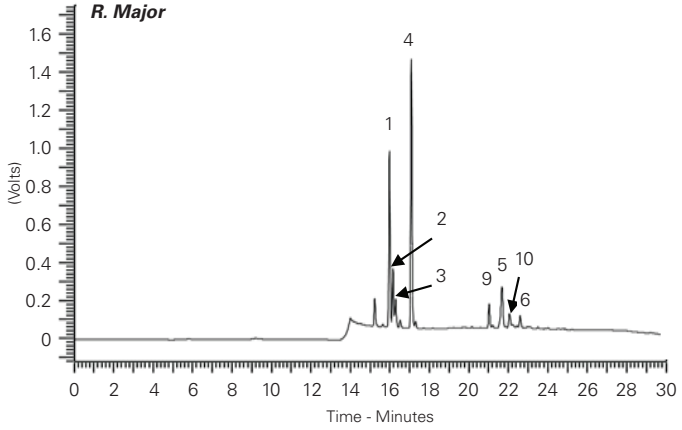
Time (mins)	%B
0	0
5	0
25	100

Flow Rate: 1 mL/min
Detection: PDA, 214 nm (Scanning 200-500 nm)

Analytes

1. Serotonin
2. N-Methylserotonin
3. N,N-Dimethylserotonin (bufotenine)
4. Dehydrobufotenine
5. Hellebrigenin
6. Marinobufagin
7. Telocinobufagin
8. Bufalin
9. Hellebrigenol-3-O-sulphate
10. Desacetylcinobufagin





Sciani JM, Angeli CB, Antoniazzi MM, Jared C, Pimenta DC. Differences and Similarities among Parotoid Macrogland Secretions in South American Toads: A Preliminary Biochemical Delineation.The Scientific World Journal 2013, http://dx.doi.org/10.1155/2013/937407

Paroxetine and Desfluoro Analogue

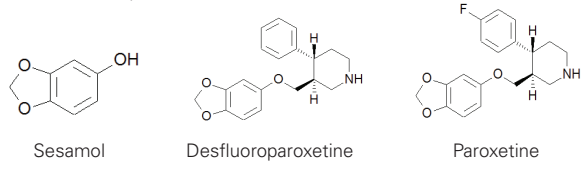
Application #AN3890

Conditions

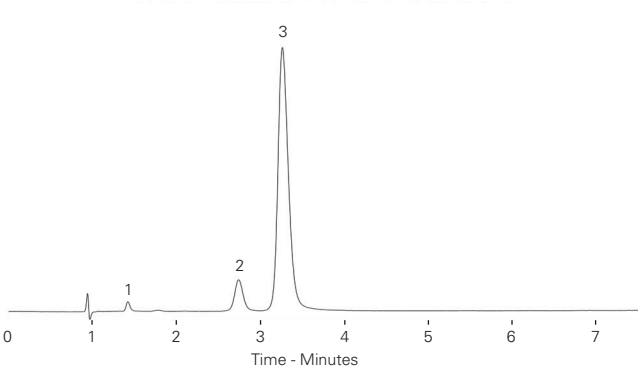
Column:	ACE 5 CN
Dimensions:	150 x 4.6 mm
Part Number:	ACE-124-1546
Mobile Phase:	20 mM ammonium formate pH 3.0/MeOH (60:40 v/v)
Flow Rate:	2 mL/min
Injection:	20 µL
Temperature:	Ambient
Detection:	UV, 295 nm

Analytes

1. Sesamol
2. Desfluoroparoxetine
3. Paroxetine



Sesamol | Desfluoroparoxetine | Paroxetine



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Peptide Test Mix

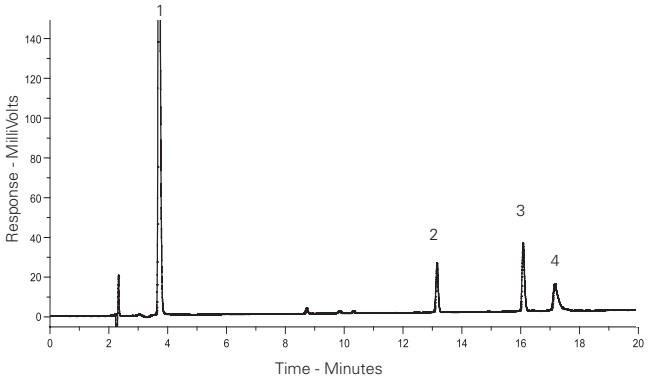
Application #AN3930

Conditions

Column:	ACE 5 C18-300	
Dimensions:	250 x 4.6 mm	
Part Number:	ACE-221-2546	
Mobile Phase:	A: 0.1% TFA in H_2O	
	B: 0.1% TFA in MeCN	
Gradient:	**Time (mins)**	**%B**
	0	10
	25	40
Flow Rate:	2 mL/min	
Injection:	5 µL	
Temperature:	Ambient	
Detection:	UV, 220 nm	

Analytes

1. Gly-Tyr (MW: 238.34)
2. Oxytocin (MW: 1007)
3. Angiotensin II (MW: 1046.18)
4. Neurotensin (MW: 1672.92)



Peptides – Varying pH

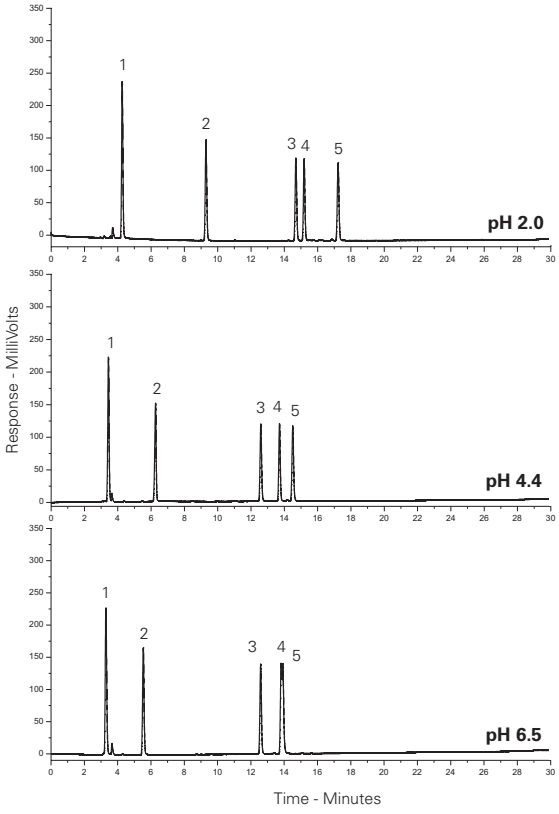
Application #AN3990

Conditions

Column:	ACE 5 C18-300	
Dimensions:	250 x 4.6 mm	
Part Number:	ACE-221-2546	
Mobile Phase:	A: 20 mM KH_2PO_4 in H_2O (pH as indicated)	
	B: MeCN	
Gradient:	**Time (mins)**	**%B**
	0	10
	25	40
Flow Rate:	1 mL/min	
Temperature:	Ambient	
Detection:	UV, 220 nm	

Analytes

1. Gly-Tyr (MW: 238.34)
2. Val-Tyr-Val (MW: 379.45)
3. Methionine enkephalin (MW: 573.67)
4. Angiotensin II (MW: 1046.18)
5. Leucine enkephalin (MW: 555.62)



Peptides – Selectivity Changes with Bonded Phase and Mobile Phase

Application #AN3430

Conditions

Column: ACE 5 C18-300; ACE 5 C8-300; ACE 5 C4-300; ACE 5 Phenyl-300; ACE 5 CN-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546, ACE-222-2546, ACE-223-2546, ACE-225-2546, ACE-224-2546
Mobile Phase: A: 0.1% TFA or 0.1% formic acid in H_2O
B: MeCN

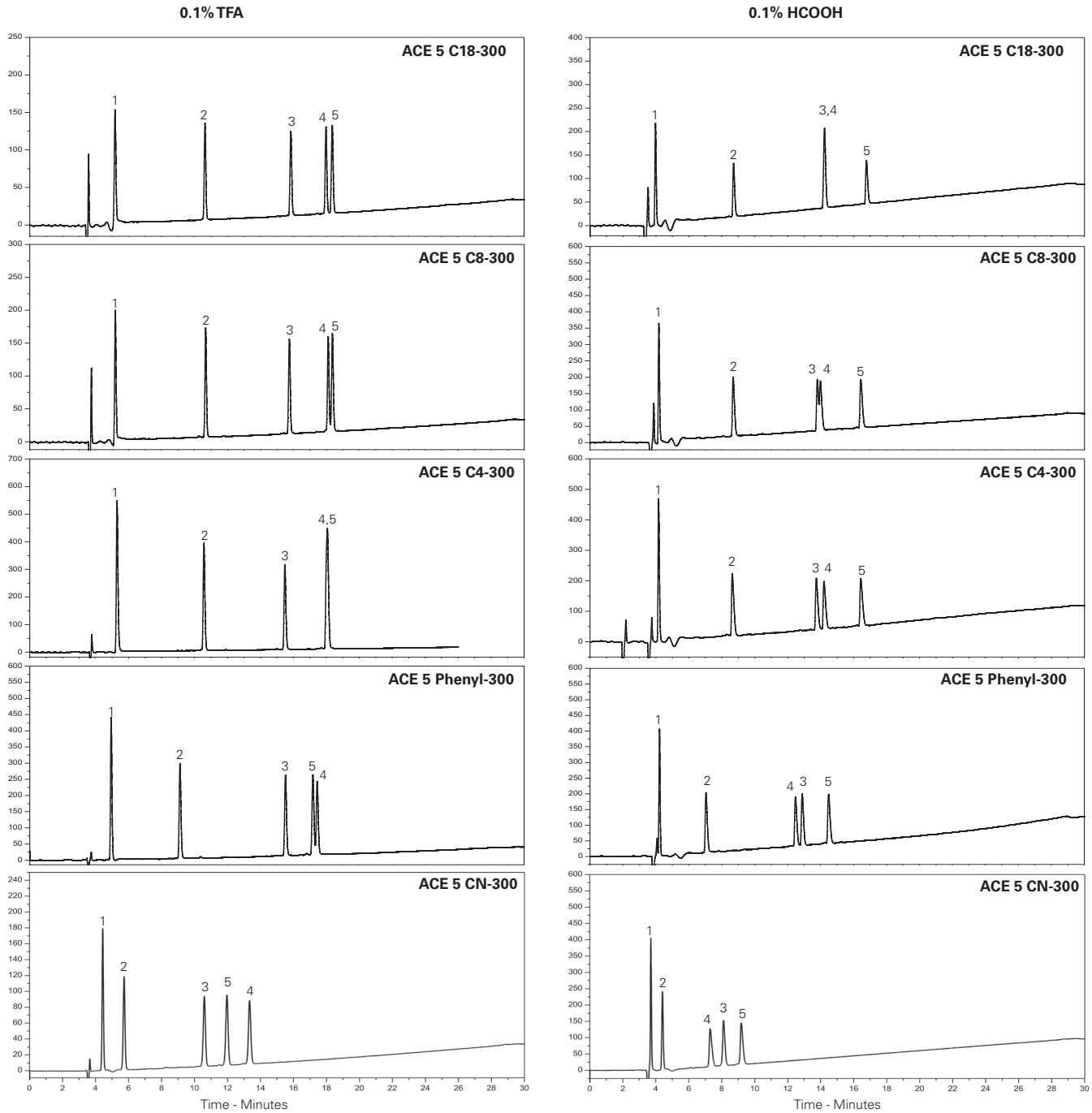
Gradient:

Time (mins)	%B
0.0	10
25.0	40

Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 220 nm

Analytes

1. Gly-Tyr (MW: 238.34)
2. Val-Tyr-Val (MW: 379.45)
3. Methionine enkephalin (MW: 573.67)
4. Angiotensin II (MW: 1046.18)
5. Leucine enkephalin (MW: 555.62)



Perfluoro Acids by LC-MS/MS

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)

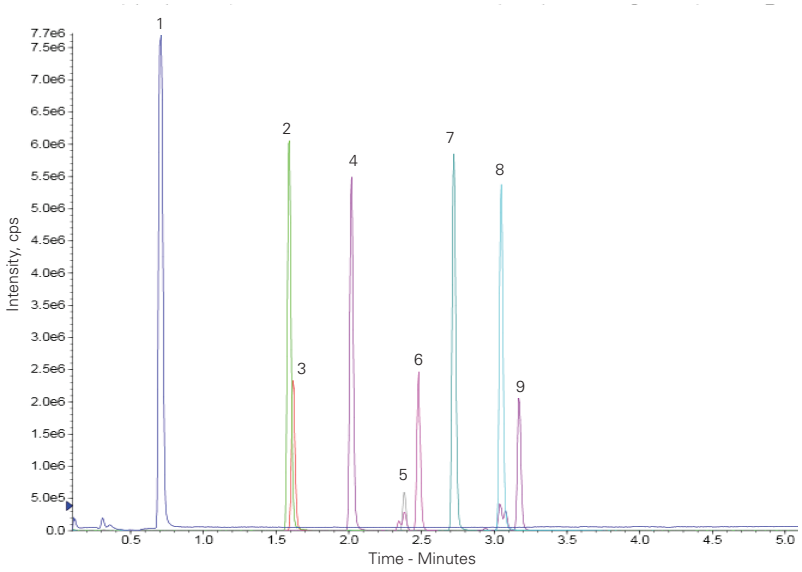
Gradient:

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

Analytes

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)



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Perfluoroalkyl Substances by Ion-Pairing LC-MS/MS

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)

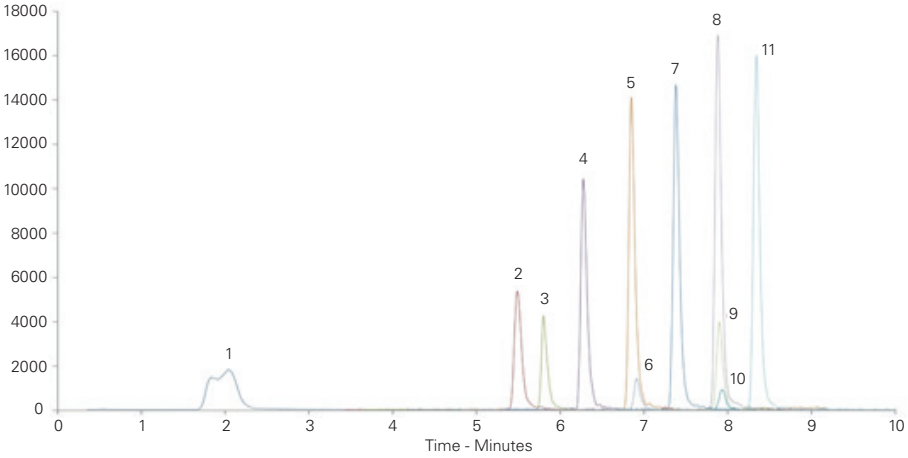
Gradient:

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

Analytes

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



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Perfluorinated Compounds in Water by LC-MS/MS

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)

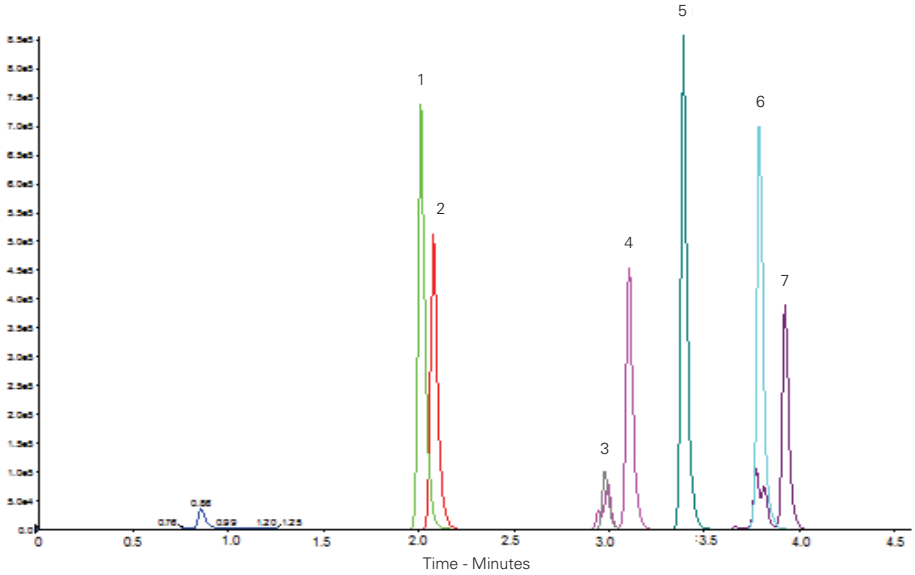
Gradient:

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

Analytes

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 by LC-MS/MS

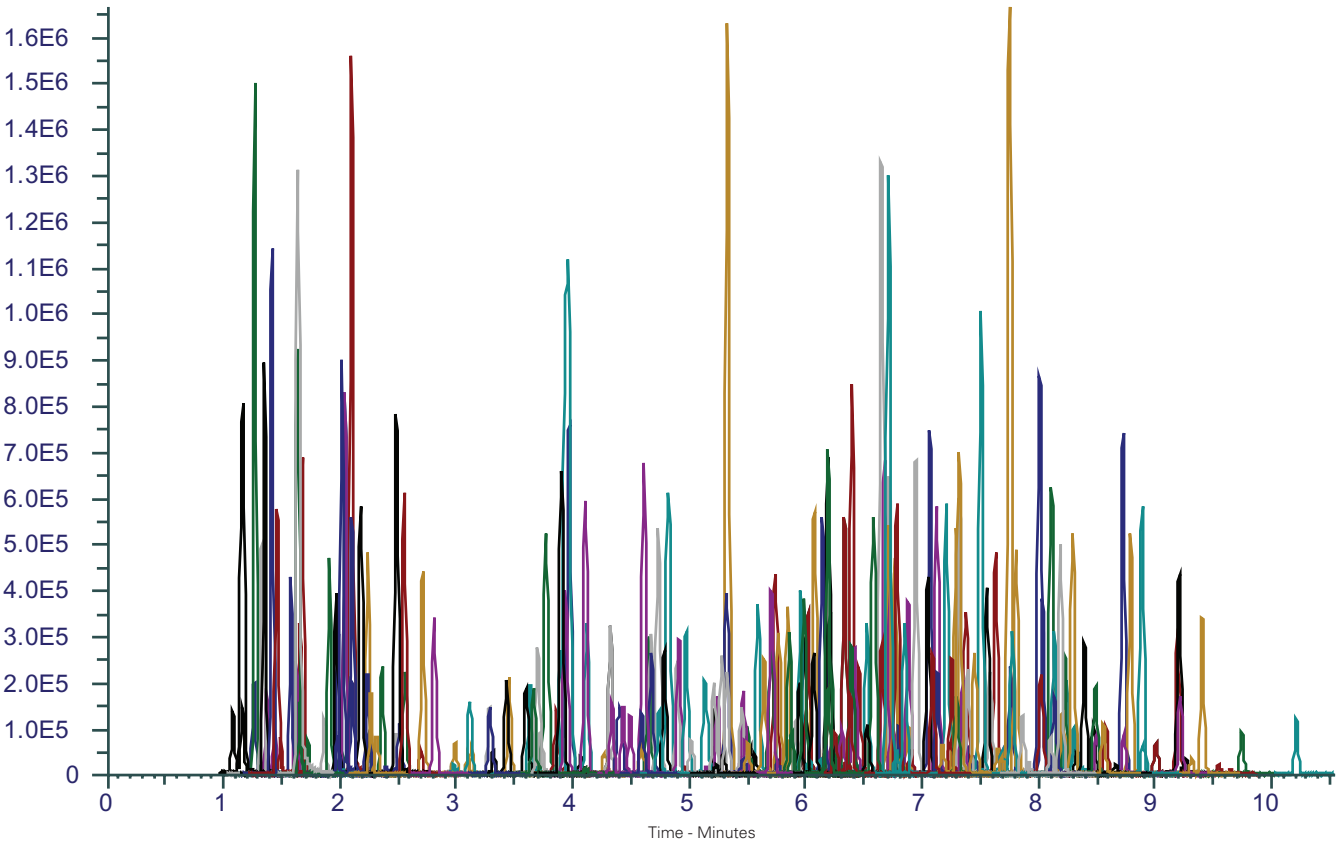
Conditions

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

Gradient:

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

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



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250 Pesticide Screen by LC-MS/MS

Analyte	R_t (mins)	Adduct	Precusor Ion *m/z*	Quant Ion *m/z*	Conf Ion *m/z*
3-OH Carbofuran	2.25	$[M+H]^+$	238.1	181.2	163.1
5-OH Thiabendazole	1.66	$[M+H]^+$	218.0	147.2	191.1
Abamectin	9.45	$[M+NH_4]^+$	890.5	305.3	567.5
Acephate	1.26	$[M+H]^+$	184.0	143.1	125.1
Acetamiprid	2.24	$[M+H]^+$	223.1	126.1	90.1
Aldicarb	2.95	$[M+NH_4]^+$	208.1	116.1	89.0
Aldicarb sulfone	1.44	$[M+NH_4]^+$	240.1	148.0	86.0
Aldicarb sulfoxide	1.37	$[M+NH_4]^+$	224.1	132.0	89.1
Allethrin	8.33	$[M+H]^+$	303.2	135.1	123.1
Ametoctradin	7.64	$[M+H]^+$	276.2	149.1	176.2
Atrazine	4.64	$[M+H]^+$	216.1	174.0	104.0
Azinphos ethyl	6.30	$[M+H]^+$	346.0	132.1	223.0
Azinphos methyl	5.14	$[M+H]^+$	318.0	132.0	124.9
Azinphos methyl OA	2.98	$[M+H]^+$	302.0	132.2	160.0
Azoxystrobin	5.59	$[M+H]^+$	404.1	372.1	344.1
Bendiocarb	3.72	$[M+H]^+$	224.1	167.1	109.1
Benoxacor	5.23	$[M+H]^+$	260.1	134.1	120.1
Bifenazate	6.27	$[M+H]^+$	301.1	198.0	170.1
Bitertanol	7.41	$[M+H]^+$	338.2	269.3	99.1
Boscalid	5.85	$[M+H]^+$	343.0	307.0	140.0
Bupirimate	6.68	$[M+H]^+$	317.2	210.2	237.3
Buprofezin	8.24	$[M+H]^+$	306.1	201.1	106.1
Cadusafos	7.58	$[M+H]^+$	271.1	159.0	131.0
Carbaryl	4.07	$[M+NH_4]^+$	219.1	145.1	127.0
Carbendazim	2.10	$[M+H]^+$	192.1	160.1	132.1
Carbofuran	3.77	$[M+H]^+$	222.1	165.2	123.2
Carboxin	3.97	$[M+H]^+$	236.1	143.0	93.0
Carfentrazone ethyl	6.88	$[M+H]^+$	412.0	346.1	366.0
Chlorantraniliprole	5.24	$[M+H]^+$	484.0	286.0	194.0
Chlorfenvinphos	7.21	$[M+H]^+$	359.0	170.0	99.1
Chlorimuron ethyl	5.73	$[M+H]^+$	415.1	186.0	83.0
Chlorpyrifos	8.47	$[M+H]^+$	349.9	198.0	97.0
Chlorpyrifos OA	6.65	$[M+H]^+$	334.0	278.0	197.9
Clethodim	7.71	$[M+H]^+$	360.3	164.1	136.1
Clofentezine	7.38	$[M+H]^+$	303.0	138.1	102.0
Cloransulam methyl	4.13	$[M+H]^+$	430.0	398.1	370.0
Clothianidin	1.99	$[M+H]^+$	250.0	169.1	132.0
Coumaphos	7.07	$[M+H]^+$	363.0	227.1	307.1
Crotoxyphos	5.86	$[M+NH_4]^+$	332.1	127.1	193.1
Crufomate	6.77	$[M+H]^+$	292.1	236.1	108.1
Cyantraniliprole	4.33	$[M+2+H]^+$	475.0	286.0	444.1
Cyazofamid	6.52	$[M+H]^+$	325.1	108.1	261.2
Cyflufenamid	7.42	$[M+H]^+$	413.1	295.1	203.0
Cymoxanil	2.48	$[M+H]^+$	199.1	128.1	111.1
Cyphenothrin	9.27	$[M+NH_4]^+$	393.2	151.2	123.2
Cyprosulfamide	3.30	$[M+H]^+$	375.1	135.1	254.1
Cyromazine	1.15	$[M+H]^+$	167.1	125.2	68.2
DEF	9.20	$[M+H]^+$	315.1	169.0	113.0
Demeton-S sulfone	2.55	$[M+H]^+$	291.1	235.1	263.1
Dialifos	7.46	$[M+H]^+$	394.0	208.1	181.0
Diazinon	7.12	$[M+H]^+$	305.1	169.1	153.2
Diazinon OA	5.32	$[M+H]^+$	289.1	153.2	233.1
Dichlormid	3.85	$[M+H]^+$	208.0	140.0	81.2
Dichlorvos	3.63	$[M+H]^+$	221.0	109.1	127.0
Dicrotophos	1.87	$[M+H]^+$	238.1	112.2	193.1
Diethofencarb	5.53	$[M+H]^+$	268.2	124.1	180.2
Diflubenzuron	6.66	$[M+H]^+$	311.0	158.0	141.0
Dimethenamid	5.70	$[M+H]^+$	276.1	244.1	168.2
Dimethoate	2.23	$[M+H]^+$	230.1	199.0	125.0
Dimethomorph	5.76, 6.07	$[M+H]^+$	388.1	301.0	165.1
Dinotefuran	1.36	$[M+H]^+$	203.1	129.1	114.2
Dioxacarb	2.26	$[M+H]^+$	224.1	123.1	167.1
Dioxathion	8.10	$[M-C_4H_{10}O_2PS_2]^+$	271.1	97.0	125.0
Disulfoton sulfone	4.59	$[M+H]^+$	307.0	261.1	125.0
Disulfoton sulfoxide	4.49	$[M+H]^+$	291.0	185.1	213.1
Diuron	4.82	$[M+H]^+$	233.0	72.1	160.0
DMST	3.90	$[M+H]^+$	215.1	106.1	151.0
Dodine	7.56	$[M+H]^+$	228.3	186.3	60.1
Emamectin	8.57	$[M+H]^+$	886.5	158.1	126.1
Ethiofencarb	4.27	$[M+H]^+$	226.1	107.1	169.1
Ethiofencarb sulfone	1.90	$[M+NH_4]^+$	275.1	107.1	201.1
Ethiofencarb sulfoxide	1.98	$[M+H]^+$	242.1	107.1	185.0
Ethion	8.31	$[M+H]^+$	385.0	199.1	143.0
Ethion monoxon	6.73	$[M+H]^+$	369.0	199.0	143.0
Ethiprole	5.77	$[M+NH_4]^+$	413.9	351.0	255.0
Ethofumesate	5.55	$[M+H]^+$	287.1	121.1	241.1
Ethoprop	6.46	$[M+H]^+$	243.1	173.0	131.0
Etofenprox	9.75	$[M+NH_4]^+$	394.2	177.2	107.1
Etoxazole	8.73	$[M+H]^+$	360.2	141.0	304.2
Famoxadone	7.24	$[M+NH_4]^+$	392.2	331.1	238.0
Fenamidone	5.76	$[M+H]^+$	312.1	236.1	92.2
Fenamiphos	6.71	$[M+H]^+$	304.1	217.1	202.0
Fenamiphos sulfone	4.10	$[M+H]^+$	336.1	266.1	188.1
Fenamiphos sulfoxide	3.96	$[M+H]^+$	320.1	233.1	171.1
Fenazaquin	9.21	$[M+H]^+$	307.2	161.2	57.2
Fenhexamid	6.39	$[M+H]^+$	302.1	178.0	97.2
Fenobucarb	5.49	$[M+H]^+$	208.1	95.0	152.0
Fenoxaprop ethyl	8.04	$[M+H]^+$	362.1	288.1	91.1
Fenoxycarb	6.80	$[M+H]^+$	302.1	88.1	116.1
Fenpropimorph	6.42	$[M+H]^+$	304.3	147.2	119.1

250 Pesticide Screen by LC-MS/MS

Analyte	R_t (mins)	Adduct	Precusor Ion *m/z*	Quant Ion *m/z*	Conf Ion *m/z*
Fenpyroximate	8.90	$[M+H]^+$	422.2	366.1	214.2
Fensulfothion	4.89	$[M+H]^+$	309.0	235.0	281.1
Fenuron	2.17	$[M+H]^+$	165.1	72.1	77.1
Flonicamid	1.66	$[M+H]^+$	230.1	203.0	98.0
Fluazifop-p-butyl	8.12	$[M+H]^+$	384.1	282.2	328.2
Fludioxonil	5.76	$[M+NH_4]^+$	266.1	158.1	131.0
Flufenoxuron	8.79	$[M+H]^+$	489.0	158.1	141.1
Flufenpyr ethyl	6.72	$[M+H]^+$	409.1	335.0	307.0
Flumetsulam	2.03	$[M+H]^+$	326.1	129.1	109.0
Flumiclorac pentyl	8.13	$[M+NH_4]^+$	441.1	308.1	354.1
Fluometuron	4.31	$[M+H]^+$	233.1	72.2	46.3
Fluopicolide	6.00	$[M+H]^+$	383.0	173.0	145.0
Fluopyram	6.33	$[M+H]^+$	397.1	173.0	208.0
Fluoxastrobin	6.40	$[M+H]^+$	459.1	427.2	188.1
Fluridone	5.32	$[M+H]^+$	330.1	309.1	290.0
Flusilazole	6.77	$[M+H]^+$	316.1	247.2	165.1
Fluthiacet methyl	6.88	$[M+H]^+$	404.0	344.0	273.9
Flutolanil	5.95	$[M+H]^+$	324.1	262.0	282.0
Flutriafol	4.74	$[M+H]^+$	302.1	70.1	123.1
Fluxapyroxad	6.02	$[M+H]^+$	382.1	342.1	314.1
Forchlorfenuron	4.78	$[M+H]^+$	248.1	129.1	93.1
Formetanate HCl	1.26	$[M+H]^+$	222.0	165.1	120.0
Fosthiazate	4.40	$[M+H]^+$	284.1	104.1	228.1
Hexaconazole	7.29	$[M+H]^+$	314.1	158.9	70.0
Hexythiazox	8.51	$[M+H]^+$	353.1	228.0	168.0
Imazalil	5.14	$[M+H]^+$	297.1	159.1	255.1
Imazosulfuron	5.28	$[M+H]^+$	413.0	153.0	156.1
Imidacloprid	1.96	$[M+H]^+$	256.1	209.1	175.0
Imiprothrin	6.34	$[M+H]^+$	319.2	151.1	123.1
Indaziflam	6.58	$[M+H]^+$	302.2	158.1	145.1
Indoxacarb	7.75	$[M+H]^+$	528.1	249.0	150.1
Ipconazole	7.81	$[M+H]^+$	334.2	70.1	125.0
Iprovalicarb	6.31	$[M+H]^+$	321.2	119.1	186.2
Isofenphos	7.39	$[M+H]^+$	346.1	217.0	245.1
Isoprocarb	4.67	$[M+H]^+$	194.1	95.1	152.2
Isoproturon	4.79	$[M+H]^+$	207.2	72.2	165.2
Kresoxim methyl	6.90	$[M+H]^+$	314.1	267.2	222.1
Lactofen	8.22	$[M+NH_4]^+$	479.1	344.1	223.0
Lenacil	4.67	$[M+H]^+$	235.1	153.1	136.1
Leptophos OA	7.75	$[M+2+H]^+$	396.9	155.1	364.9
Linuron	5.46	$[M+H]^+$	249.0	182.1	160.1
Malathion	5.92	$[M+H]^+$	331.0	127.1	285.1
Malathion OA	3.89	$[M+H]^+$	315.1	127.1	99.0
Mandipropamid	5.94	$[M+H]^+$	412.1	328.2	356.2
Mefenpyr diethyl	7.26	$[M+H]^+$	373.1	327.1	160.0

Analyte	R_t (mins)	Adduct	Precusor Ion *m/z*	Quant Ion *m/z*	Conf Ion *m/z*
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 by LC-MS/MS

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

300 Pesticide Screen by LC-MS/MS

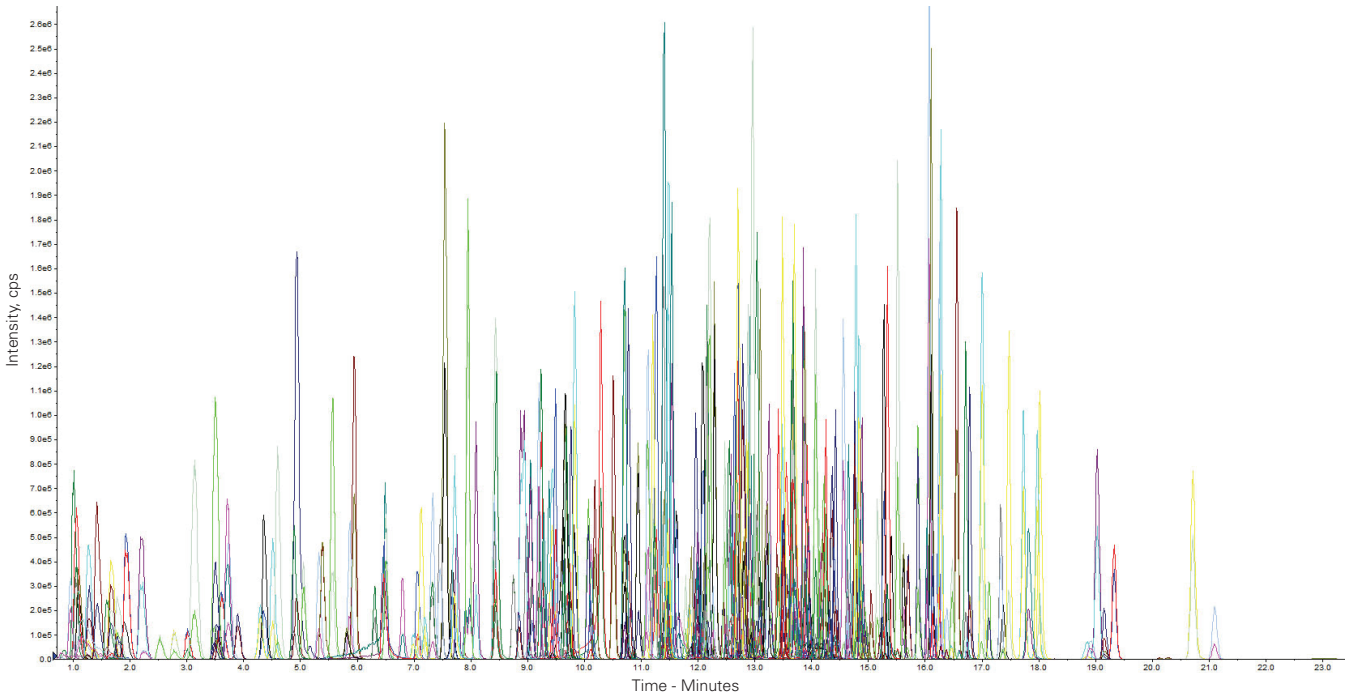
Conditions

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)

Gradient:

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

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



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300 Pesticide Screen by LC-MS/MS

Analyte	Retention Time (mins)	MRM transitions (*m/z*)
3-Hydroxycarbofuran	3.5	238.1 → 163.1, 238.1 → 181.1
Acephate	1.0	184.1 → 142.9, 184.1 → 124.8
Acetamiprid	3.6	223.2 → 126.1, 225.2 → 128.1
Aclonifen	13.9	265.0 → 248.0, 267.0 → 250.0
Alachlor	12.9	270.2 → 238.2, 270.2 → 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

Analyte	Retention Time (mins)	MRM transitions (*m/z*)
Chlorpyrifos-methyl	15.2	322.0 → 124.9, 324.0 → 125.1
Chlortoluron	9.1	213.2 → 72.0, 215.1 → 72.1
Cinidon-ethyl	16.3	394.0 → 348.0, 394.0 → 366.0
Clethodim A	12.8	360.1 → 164.1, 360.1 → 268.1
Clethodim B	10.2	360.1 → 164.1, 360.1 → 268.1
Clofentezine	15.1	303.1 → 137.9, 305.1 → 102.0
Clomazone	10.7	240.1 → 124.9, 242.2 → 127.1
Cloquintocet-mexyl	16.1	336.2 → 238.0, 336.2 → 192.1
Clothianidin	2.9	250.1 → 169.0, 250.1 → 132.0
Coumaphos	14.3	363.0 → 227.0, 363.0 → 211.1
Cyanazine	6.7	241.1 → 214.1, 243.1 → 216.1
Cyazofamid	13.2	325.2 → 107.9, 327.2 → 107.9
Cycloate	14.9	216.2 → 83.1, 216.2 → 154.1
Cycloxydim A	13.1	326.3 → 280.0, 326.3 → 180.0
Cycloxydim B	8.4	326.3 → 280.0, 326.3 → 180.0
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

300 Pesticide Screen by LC-MS/MS

Analyte	Retention Time (mins)	MRM transitions (*m/z*)
Ethirimol	9.7	210.3 → 140.1, 210.3 → 98.0
Ethofumesate	11.3	287.1 → 121.0, 287.1 → 259.0
Ethoprofos	12.7	243.0 → 131.0, 243.0 → 97.0
Ethoxyquin A	12.9	218.2 → 148.0, 218.2 → 174.1
Ethoxyquin B	10.7	218.2 → 148.0, 218.2 → 174.1
Etofenprox	20.6	394.0 → 177.0, 394.0 → 359.0
Etrimfos	14.2	293.1 → 125.0, 293.1 → 265.1
Famoxadone 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
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

Analyte	Retention Time (mins)	MRM transitions (*m/z*)
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
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

300 Pesticide Screen by LC-MS/MS

Analyte	Retention Time (mins)	MRM transitions (*m/z*)
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
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	202.2 → 132.1,202.2→ 104.0
Simetryn	9.4	214.1 → 124.1, 214.1 → 144.0
Spinosyn A	17.3	732.5 → 142.0, 732.5 → 98.0
Spinosyn D	18.3	746.5 → 142.0, 746.5 → 98.0
Spirodiclofen	17.4	313.1 → 295.0, 313.1 → 213.0
Spiromesifen	16.8	371.2 → 273.1, 371.2 → 255.2
Spirotetramat	12.8	374.2 → 302.2, 374.2 → 330.2
Spiroxamine	13.3	298.3 → 100.1, 298.3 → 144.1
Sulfotep	14.0	323.0 → 97.0, 323.0 → 115.0
Tau-fluvalinate	18.9	503.0 → 208.0, 503.0 → 181.0
Tebuconazole	13.9	308.1 → 70.0, 308.1 → 125.0
Tebufenozide	13.5	353.2 → 297.2, 353.2 → 133.0
Tebufenpyrad	15.9	334.0 → 145.0, 334.0 → 117.0
Teflubenzuron	16.3	381.1 → 158.2, 381.1 → 141.2
Tembotrione (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

300 Pesticide Screen by LC-MS/MS

Analyte	Retention Time (mins)	MRM transitions (*m/z*)
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
Thiamethoxam	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

Analyte	Retention Time (mins)	MRM transitions (*m/z*)
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

Pesticides by LC-MS/MS

Application #AN1290

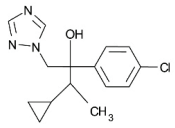
Conditions

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

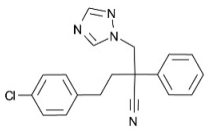
Gradient:

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

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



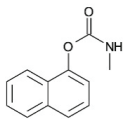
Cyproconazoles



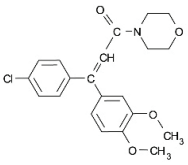
Fenbuconazole

Analytes

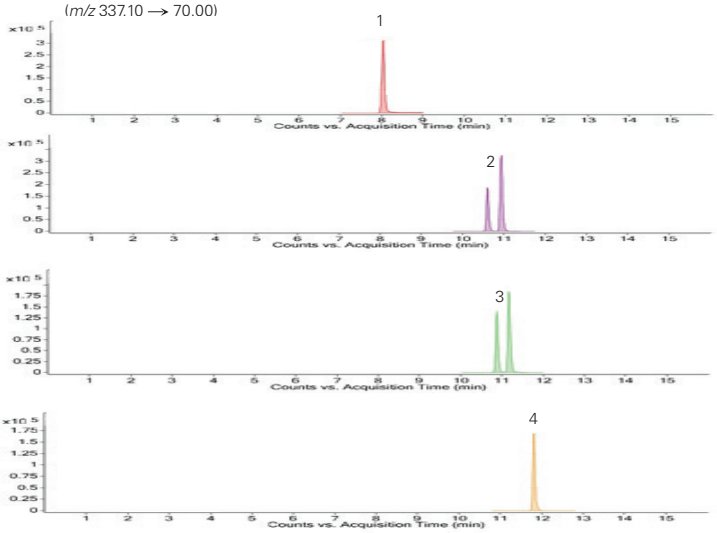
1. Carbaryl
   (*m/z* 202.10 → 145.10)
2. Dimethomorphs
   (*m/z* 388.10 → 301.10)
3. Cyproconazoles
   (*m/z* 292.10 → 70.00)
4. Fenbuconazole
   (*m/z* 337.10 → 70.00)



Carbaryl



Dimethomorphs



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

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Pesticides in Water

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

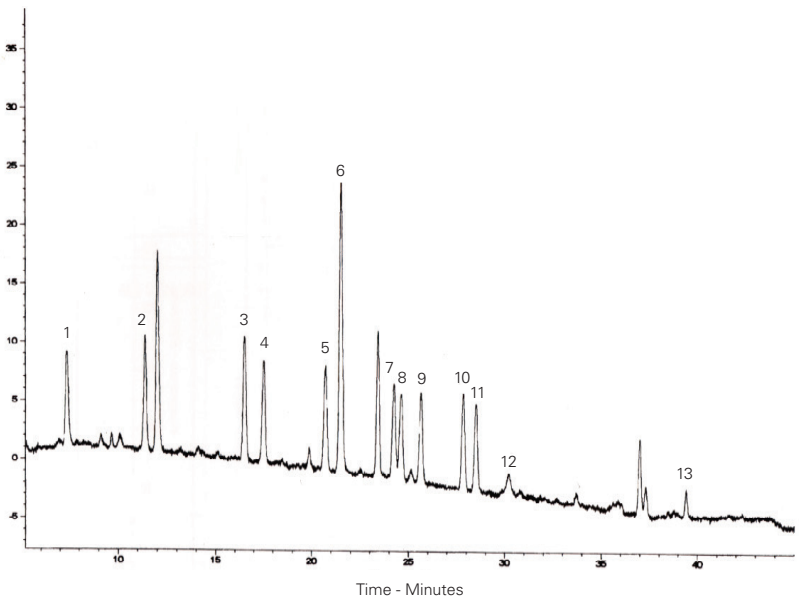
Gradient:

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)

Analytes

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



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Pharmaceutically Relevant Compounds (II)

Application #AN1630

Conditions

Column: ACE Excel 3 CN-ES
ACE Excel 3 C18-Amide
ACE Excel 3 C18-PFP
Dimensions: 100 x 3.0 mm
Part Numbers: EXL-1113-1003U, EXL-1112-1003U, EXL-1110-1003U
Mobile Phase: A: 20 mM ammonium formate in H_2O
B: 20 mM ammonium formate in MeOH

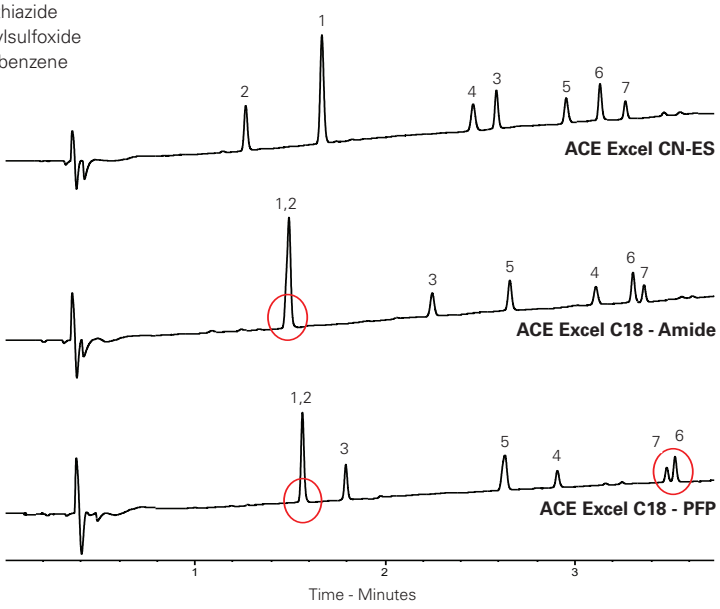
Gradient:

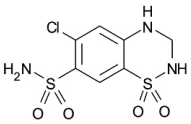
Time (mins)	%B
0.0	3
5.0	100
6.0	100
6.5	3

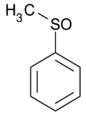
Flow Rate: 0.6 mL/min
Temperature: 40 °C
Detection: UV

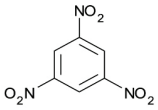
Analytes

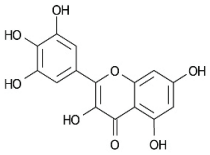
1. Hydrochlorothiazide
2. Methylphenylsulfoxide
3. 1,3,5-Trinitrobenzene
4. Myricetin
5. p-Cresol
6. Sulindac
7. Toluene

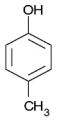


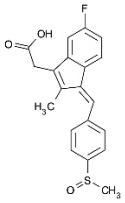

Hydrochlorothiazide


Methylphenylsulfoxide


1,3,5-Trinitrobenzene


Myricetin


p-Cresol


Sulindac


Toluene

Pharmaceutically Relevant Compounds (III)

Application #AN2400

Conditions

Column: ACE 5 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1210-1546
Mobile Phase: A: 5 mM formic acid in H_2O
B: 5 mM formic acid in MeOH

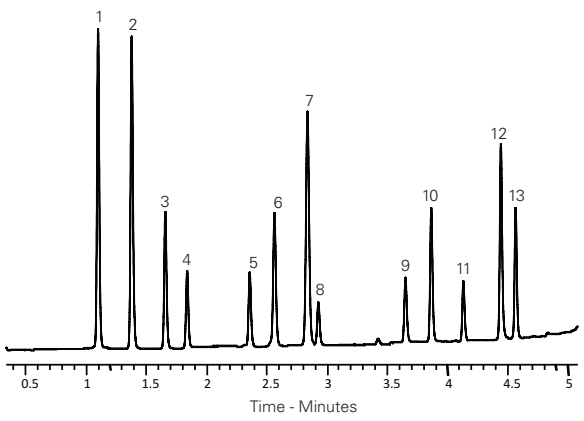
Gradient:

Time (mins)	%B
0.0	3
5.0	100
5.5	100
6.0	3
8.5	3

Flow Rate: 1.5 mL/min
Injection: 5 µL
Temperature: 40 °C
Detection: UV, 254 nm

Analytes

1. Paracetamol
2. Hydrochlorothiazide
3. Methylphenylsulfoxide
4. Methylphenylsulfone
5. Aspirin
6. Phenacetin
7. 1,3-Dinitrobenzene
8. 1,2,4-Trimethoxybenzene
9. Ethylbenzoate
10. Nimesulide
11. Ibuprofen
12. Indomethacin
13. Mefenamic acid



Pharmaceutically Relevant Compounds (IV)

Application #AN2460

Conditions

Column: ACE Excel 3 CN-ES
Dimensions: 100 x 2.1 mm
Part Number: EXL-1113-1002U
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN

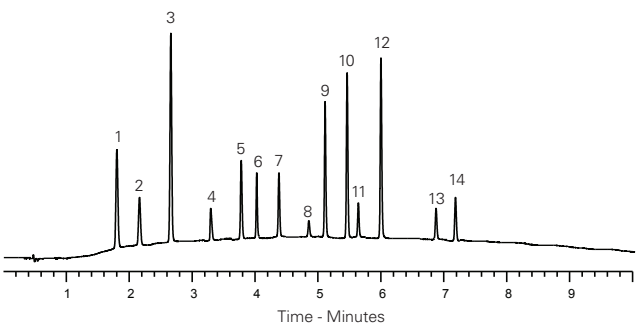
Gradient:

Time (mins)	%B
0	3
10	100

Flow Rate: 0.6 mL/min
Temperature: 40 °C
Detection: UV, 210 nm

Analytes

1. 1,3-Dihydroxybenzene
2. Catechol
3. Hydrochlorothiazide
4. Oxprenolol
5. Salicylic acid
6. Myricetin
7. Piroxicam
8. 1,2-Dinitrobenzene
9. Tolmetin
10. 1-Naphthol
11. Piperine
12. Diflunisal
13. Propylbenzene
14. 1,2,3-Trichlorobenzene



Pharmaceutically Relevant Compounds (V)

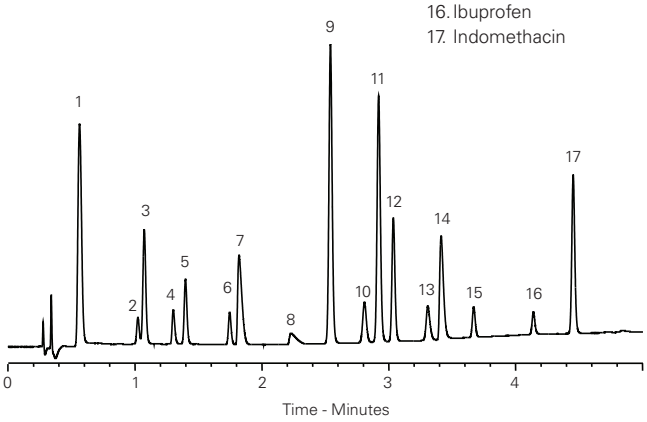
Application #AN2500

Conditions

Column:	ACE 3 C18-PFP
Dimensions:	50 x 2.1 mm
Part Number:	ACE-1110-0502
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeOH
Gradient:	**Time (mins) %B**
	0 3
	5 100
Flow Rate:	0.6 mL/min
Temperature:	40 °C
Detection:	UV, 254 nm

Analytes

1. Sulphanilamide
2. Nizatidine
3. Metronidazole
4. Amiloride
5. Hydrochlorothiazide
6. Caffeine
7. Pindolol
8. Metoprolol
9. Phenacetin
10. 1,3-Dinitrobenzene
11. Hexobarbital
12. Furosemide
13. Piroxicam
14. Carvedilol
15. Ketoprofen
16. Ibuprofen
17. Indomethacin



Please contact us for further information and advice on specific applications or for method development support

Pharmaceutically Relevant Mixture (I) – Different Selectivity Using pH

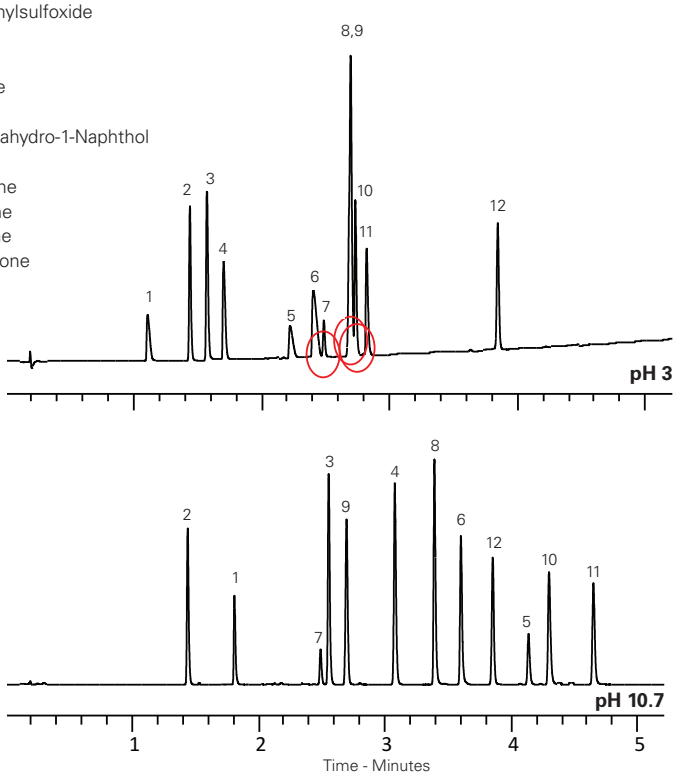
Application #AN1310

Conditions

Column:	ACE Ultracore 2.5 SuperC18
Dimensions:	50 x 2.1 mm
Part Number:	CORE-25A-0502U
Mobile Phase:	A1: 10 mM ammonium formate pH 3 in H_2O
	A2: 0.1% ammonia pH 10.7 in H_2O
	B1: 10 mM ammonium formate pH 3 in MeCN/H_2O (90:10 v/v)
	B2: 0.1% ammonia pH 10.7 in MeCN/H_2O (90:10 v/v)
Gradient:	**Time (mins) %B**
	0 3
	5 100
	6 100
Flow Rate:	0.6 mL/min
Temperature:	40 °C
Detection:	UV, 254 nm

Analytes

1. Atenolol
2. Methylphenylsulfoxide
3. Eserine
4. Prilocaine
5. Bupivacaine
6. Tetracaine
7. 1,2,3,4-Tetrahydro-1-Naphthol
8. Carvedilol
9. Nitrobenzene
10. Methdilazine
11. Amitriptyline
12. Valerophenone



Pharmaceutically Relevant Mixture (II) – Different Selectivity Using pH

Application #AN1300

Conditions

Column: ACE Ultracore 2.5 SuperPhenylHexyl
Dimensions: 50 x 2.1 mm
Part Number: CORE-25B-0502U
Mobile Phase: A1: 10 mM ammonium formate pH 3 in H_2O
A2: 0.1% ammonia pH 10.7 in H_2O
B1: 10 mM ammonium formate pH 3 in MeCN/H_2O (90:10 v/v)
B2: 0.1% ammonia pH 10.7 in MeCN/H_2O (90:10 v/v)

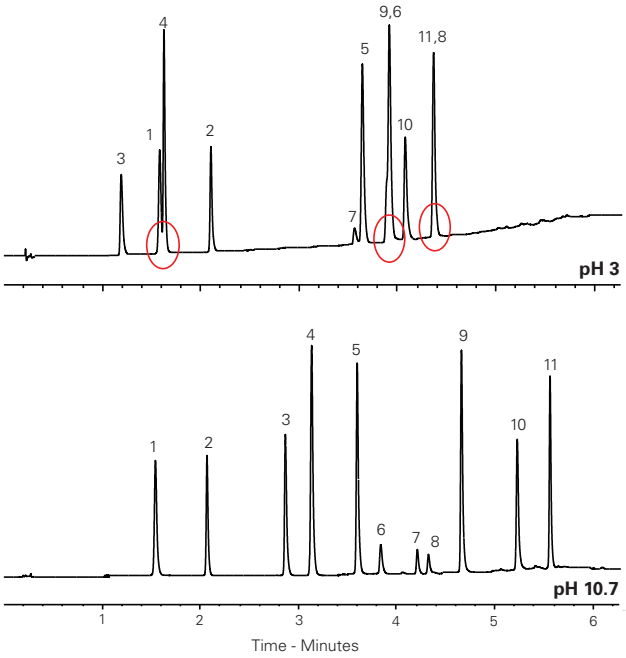
Gradient:

Time (mins)	%B
0	3
5	100
6	100

Flow Rate: 0.6 mL/min
Temperature: 40 °C
Detection: UV, 254 nm

Analytes

1. Benzamide
2. Caffeine
3. Procainamide
4. N-Acetylprocainamide
5. Propiophenone
6. Toluene
7. Remacemide
8. Ethylbenzene
9. Carvedilol
10. Nortriptyline
11. Clomipramine



Phenelzine in Human Plasma by LC-MS/MS

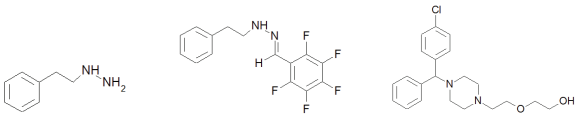
Application #AN4200

Conditions

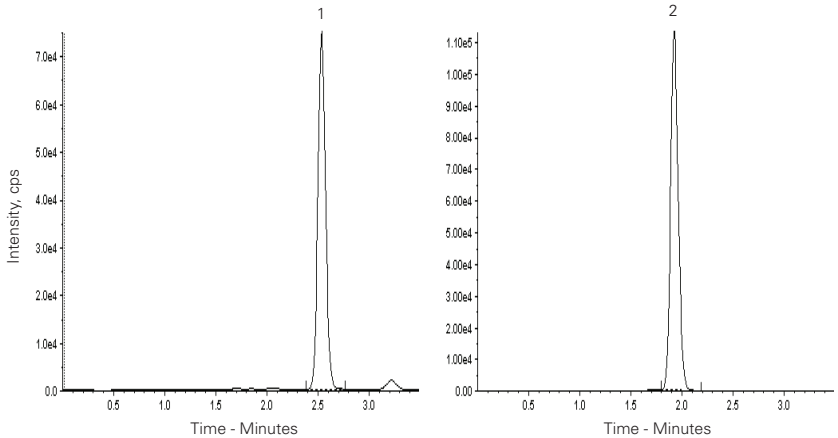
Column: ACE 5 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-121-1046
Mobile Phase: 10 mM ammonium acetate in H_2O, pH 4.0/MeOH (20:80 v/v)
Flow Rate: 1 mL/min with 70% split flow into MS
Injection: 10 µL
Temperature: 45 °C
Detection: AB Sciex API-4000 MS
MRM using ESI in positive ion mode
TurboIonSpray Interface Temperature: 600 °C
IonSpray Voltage: 5500 V
Sample: Phenelzine derivatised with pentafluorobenzaldehyde, followed by SPE extraction of derivative and hydroxyzine (I.S.) from 200 µL human plasma.

Analytes

1. Phenelzine derivative
(*m/z* 305.1 ⟶ 105.1)
20.2 ng/mL
2. Hydroxyzine
(*m/z* 375.3 ⟶ 201.1)
25 ng/mL



Spiked human plasma



Phenol and Phenoxy Acid Herbicides

Application #AN2290

Conditions

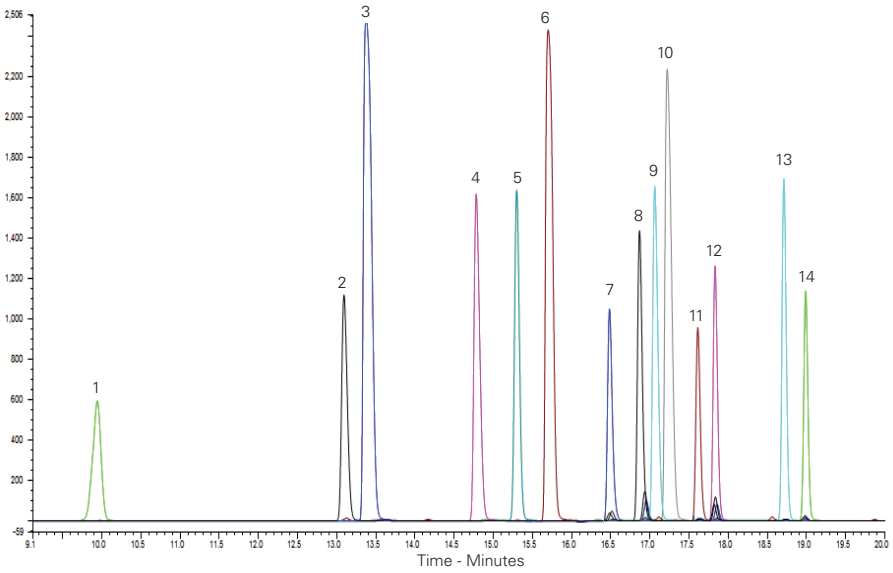
Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: A: 0.1% formic acid in H_2O
B: MeOH
Gradient:

Time (mins)	%B
0.0	10
20.0	100

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

Analytes

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



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Phenolic Acids

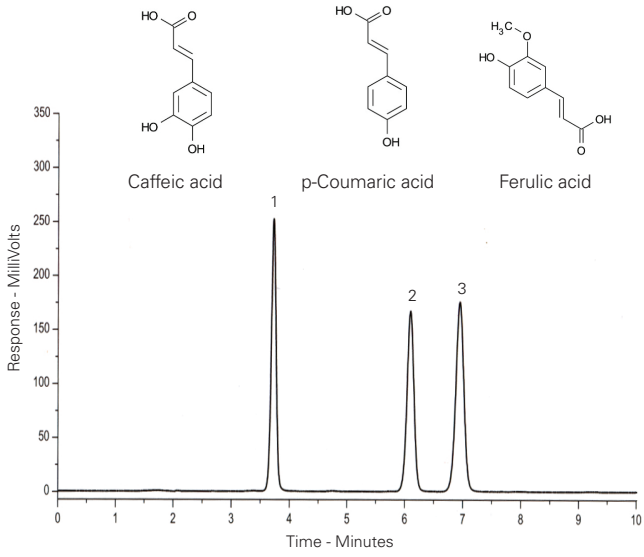
Application #AN3030

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

Analytes

1. Caffeic acid
2. p-Coumaric acid
3. Ferulic acid



Phenolic Compounds in Ground Water & Landfill Leachates

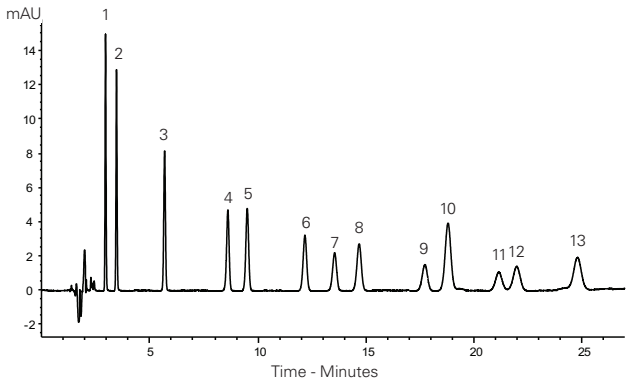
Application #AN3070

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: 1 mL/min
Injection: 10 µL
Temperature: 30 °C
Detection: UV, 274 nm

Analytes

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



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Phenolic Compounds from Red Grape Seed Extract

Application #AN3790

Conditions

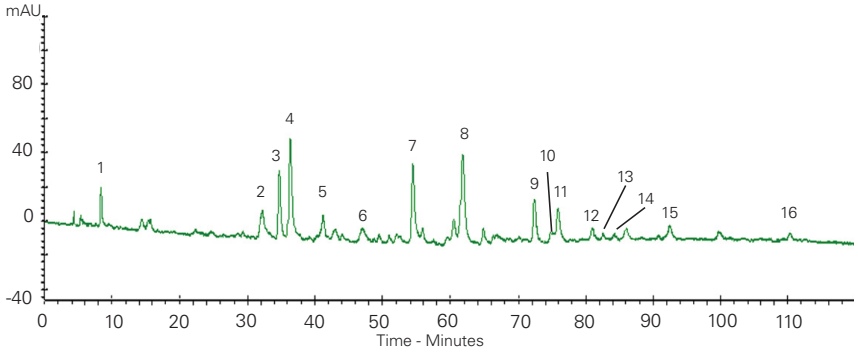
Column: ACE 3 C18-AR
Dimensions: 200 x 4.6 mm
Part Number: ACE-119-2046
Mobile Phase: A: 2% acetic acid in H_2O
B: 2% acetic acid in MeCN
Gradient:

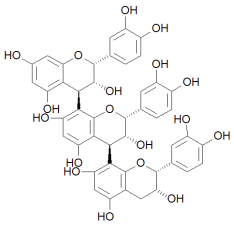
Times (mins)	%B
0	0
80	20
115	28
120	100
130	100

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)

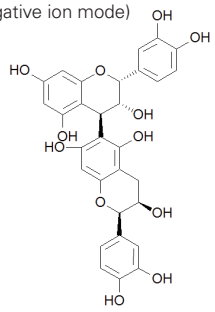
Analytes

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)

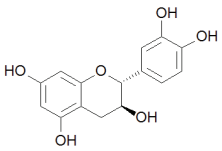




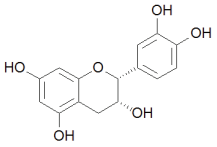
Procyanidin C1



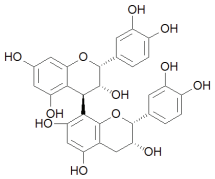
Procyanidin B5



(+)-Catechin



(-)-Epicatechin



Procyanidin B2

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

Phenols in Purple Coneflower *(Echinacea Purpurea)*

Application #AN2920

Conditions

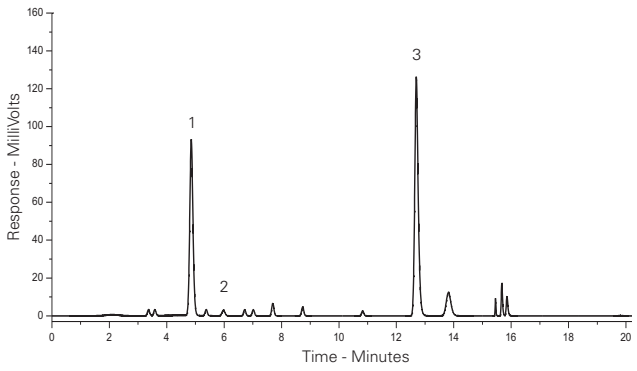
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.1% H_3PO_4 in H_2O
B: MeCN
Gradient:

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

Analytes

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



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Echinacea Purpurea

Phosphatidylethanol Biomarker Analysis by UHPLC-MS/MS

Application #AN3400

Conditions

Column: ACE 2 C4
Dimensions: 100 x 2.1 mm
Part Number: EXL-103-1002U
Mobile Phase: A: 2 mM ammonium acetate/MeCN (20:80 v/v)
B: IPA

Gradient:

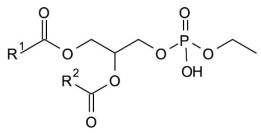
Time (mins)	%B
0.00	10
1.00	10
3.00	60
3.01	100
5.00	100
5.10	10

Flow Rate: 0.4 mL/min
Injection: 5 µL
Temperature: 40 °C
Detection: AB SCIEX triple quad 5500
Turbo IonSpray negative mode ESI
IonSpray Voltage: -4500 V
Temperature: 650 °C

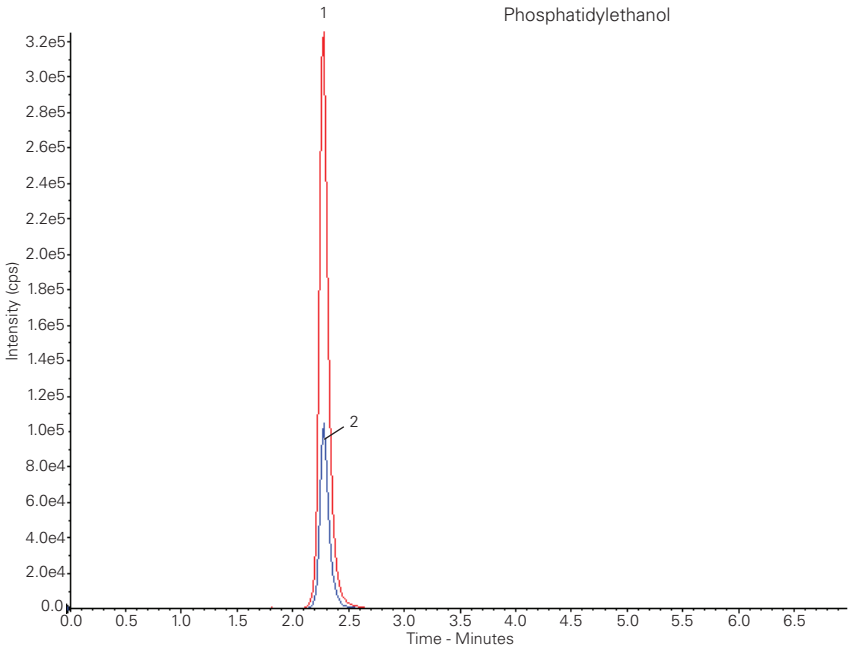
Phosphatidylethanol (PEth) measurement in blood is used as a biomarker of chronic alcohol use/abuse.

Analytes

1. R1/R2 = 18:1/18:1
(*m/z* 701.4 → 281.2)
2. R1/R2 = 16:1/16:1
(*m/z* 701.4 → 255.1)



Phosphatidylethanol



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Phytoestrogens from Hop Extract by LC-MS/MS

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

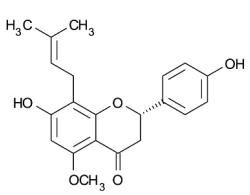
Gradient:

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

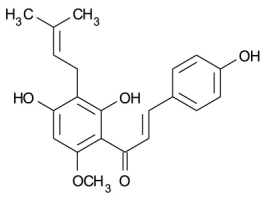
Flow Rate: 0.6 mL/min
Detection: TSQ-Quantum triple quad ESI
Spray voltage: -4500 V
Precursor ion: 355.4 $[M+H]^+$
MRM transition ions: 179 and 299
Collision energy: 28 and 16 V

Analytes

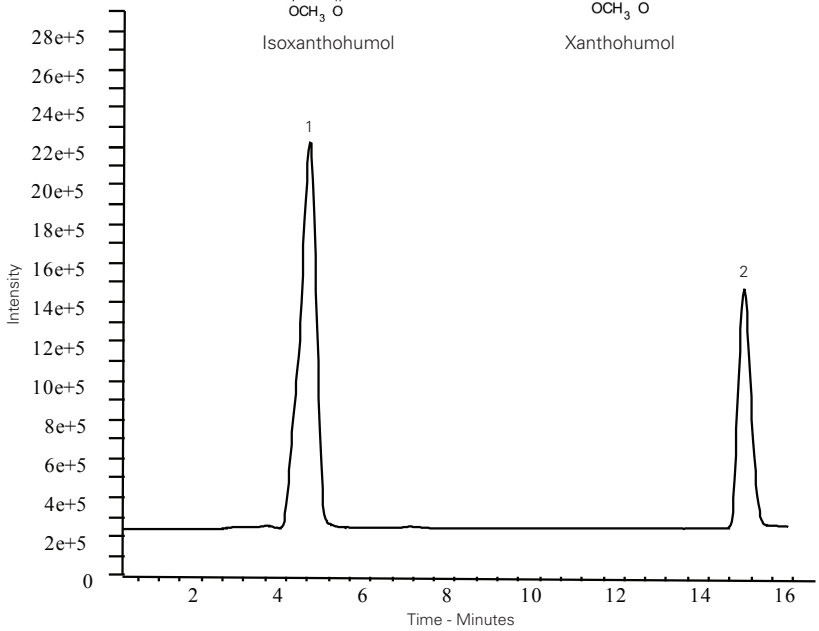
1. Isoxanthohumol
LOQ 0.07 µg/mL
2. Xanthohumol
LOQ 0.01 µg/mL



Isoxanthohumol



Xanthohumol



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Pilocarpine

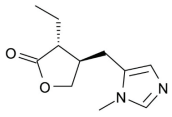
Application #AN3720

Conditions

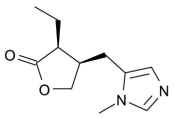
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 2 mM tetrabutylammonium dihydrogen phosphate/MeCN (85:15 v/v)
Flow Rate: 1 mL/min
Detection: UV, 254 nm

Analytes

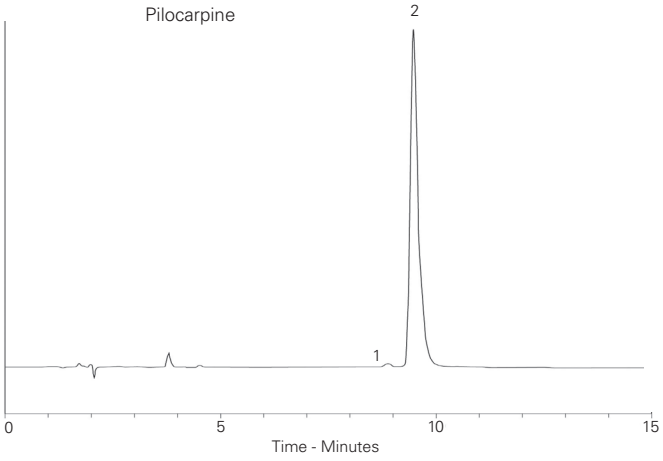
1. Isopilocarpine
2. Pilocarpine



Isopilocarpine



Pilocarpine



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Plant Hormones Involved in Abiotic Stresses

Application #AN4010

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: CORE-25A-1546U
Mobile Phase: A: 0.1% formic acid in H_2O
B: MeCN
Gradient:

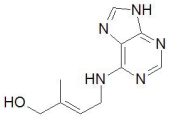
Time (mins)	%B
0	0
2	40
5	60
13	100
15	20

Flow Rate: 0.5 mL/min
Temperature: 40 °C
Detection: Shimadzu LCMS-8040 triple quad MS ESI positive and negative mode
Sample: Crude extract of *Arabidopsis thaliana* rosette leaves

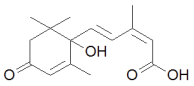
Plant hormones are involved in the regulation of response to exposure of abiotic stresses such as drought or salt

Analytes

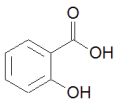
1. Zeatin (+ ESI)
   (*m/z* 220 → 119)
2. (±)-Abscisic acid (+ ESI)
   (*m/z* 247 → 91)
3. Salicylic acid (- ESI)
   (*m/z* 137 → 93)
4. (±)-Jasmonic acid (- ESI)
   (*m/z* 209 → 59)
5. Brassinolide (+ ESI)
   (*m/z* 481 → 95)



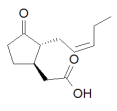
Zeatin



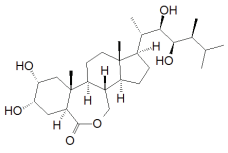
(±)-Abscisic acid



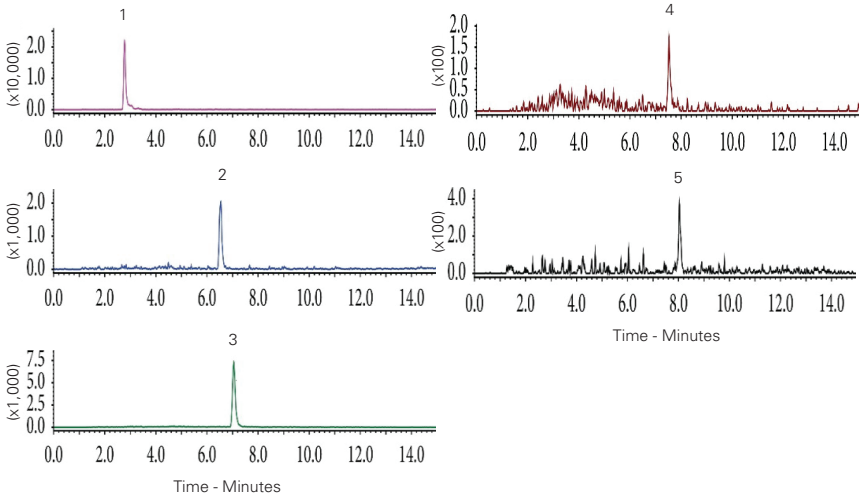
Salicylic acid



(±)-Jasmonic acid



Brassinolide



Kasote DM, Ghosh R, Chung JY, Kim J, Bae I, Bae H. Multiple Reaction Monitoring Mode Based Liquid Chromatography-Mass Spectrometry Method for Simultaneous Quantification of Brassinolide and other Plant Hormones Involved in Abiotic Stresses. International Journal of Analytical Chemistry (2016). http://dx.doi.org/10.1155/2016/7214087

Polar Compounds Separation

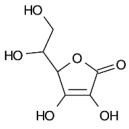
Application #AN1590

Conditions

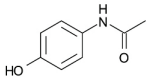
Column: ACE Excel 5 CN-ES
Dimensions: 150 x 4.6 mm
Part Number: EXL-1213-1546U
Mobile Phase: MeOH/H_2O (50:50 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 20 °C
Detection: UV, 254 nm

Analytes

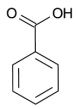
1. Ascorbic acid
2. Paracetamol
3. Benzoic acid
4. Salicylic acid



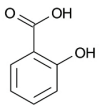
Ascorbic acid



Paracetamol



Benzoic acid



Salicylic acid

Polyamines

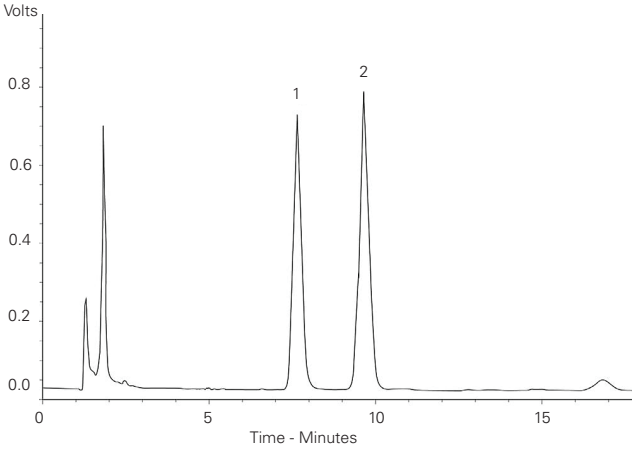
Application #AN3740

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: TRIS buffer pH 7.0/MeOH (10:90 v/v)
Flow Rate: 1.2 mL/min
Detection: Fluorescence – λ_{ex} 340 nm, λ_{em} 450 nm

Analytes

1. Putrescine
2. Cadaverine
(as OPA derivatives)



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Polycyclic Tetracarboxylic Acids

Application #AN1340

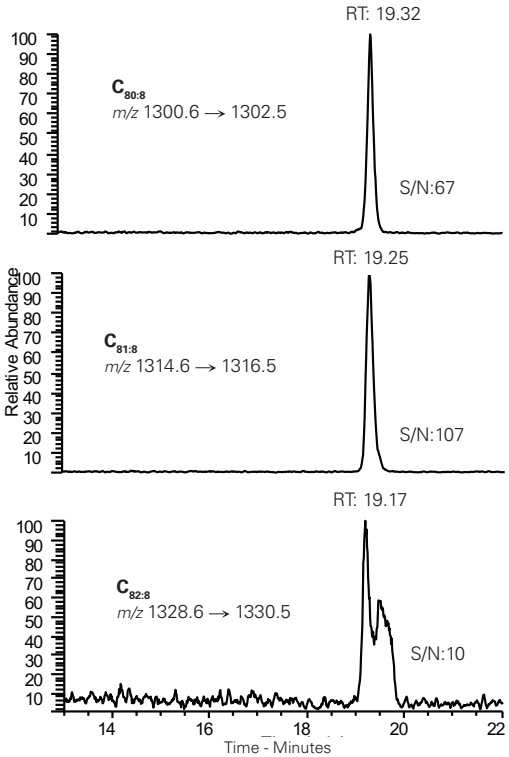
Conditions

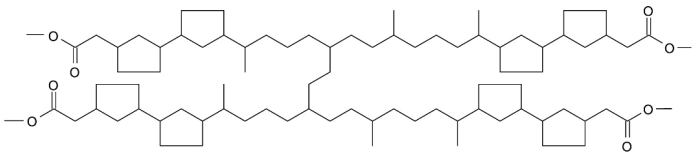
Column: ACE UltraCore 2.5 SuperPhenylHexyl
Dimensions: 100 x 2.1 mm
Part Number: CORE-25B-1002U
Mobile Phase: A: 10 mM ammonium acetate in MeOH/H_2O (98:2 v/v)
B: 10 mM ammonium acetate in IPA/H_2O (98:2 v/v)
Gradient:

Time (mins)	%B
0.0	0
1.0	0
15.0	100
25.0	100

Flow Rate: 0.15 mL/min
Injection: 5 µL
Temperature: Ambient
Detection: LCQ Ion trap MS
LC-ESI-MS extracted ion chromatograms
Compounds detected as ammoniated quasimolecular ions $[M+NH_4]^+$
Detection limit ~ 0.1 ppm

C_{80-82} polycyclic tetracarboxylic acids isolated from oilfield deposits





Tetramethyl ester of $C_{80:8}$ ring acid

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Polyethylene Glycol 1000

Application #AN3900

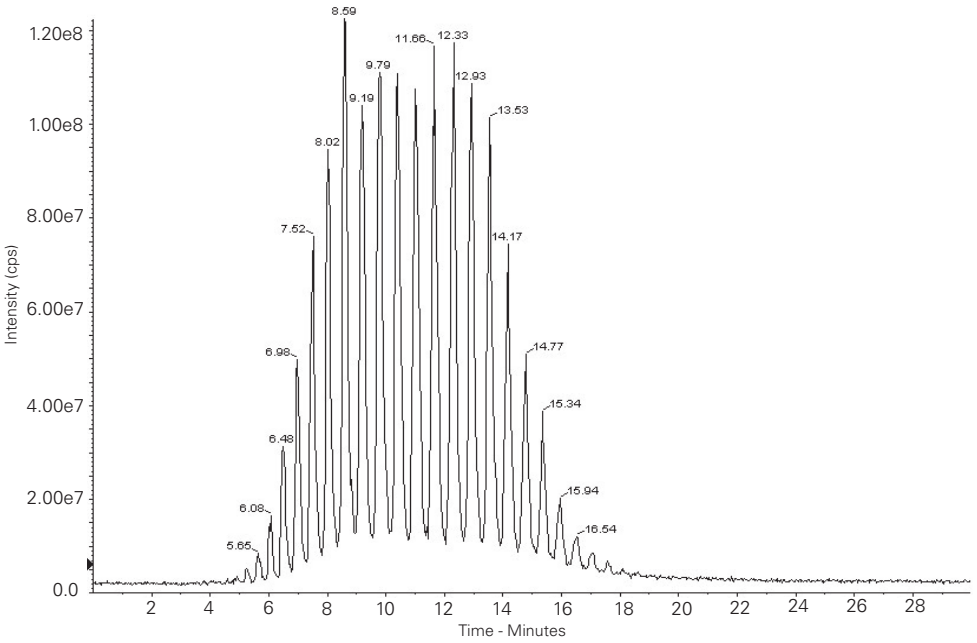
Conditions

Column: ACE 3 C8
Dimensions: 150 x 4.6 mm
Part Number: ACE-112-1546
Mobile Phase: A: 0.1% formic acid in H_2O
B: MeOH

Gradient:

Time (mins)	%B
0	50
45	85
50	50
60	50

Flow Rate: 1 mL/min
Detection: APCI (negative ion)



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[^{14}C]Pomalidomide and Metabolites in Human Plasma and Urine

Application #AN4240

Conditions

Column: ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-111-1546
Mobile Phase: A: 25 mM ammonium acetate pH 5.5 in H_2O
B: MeOH

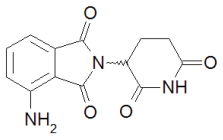
Gradient:

Time (mins)	%B
0	0
2	0
38	36
44	100
48	100
50	0

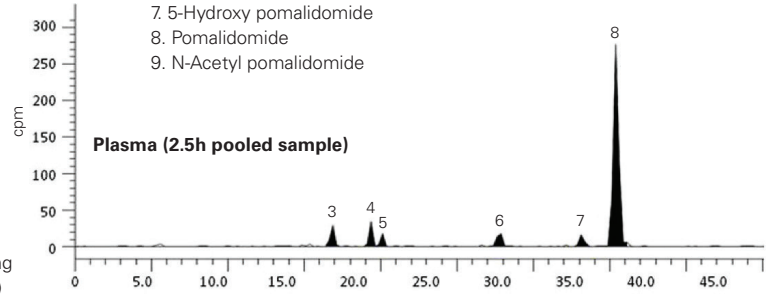
Flow Rate: 0.7 mL/min
Temperature: 30 °C
Detection: Radiometric
Metabolites characterised using LC-MS/MS (positive ion mode)

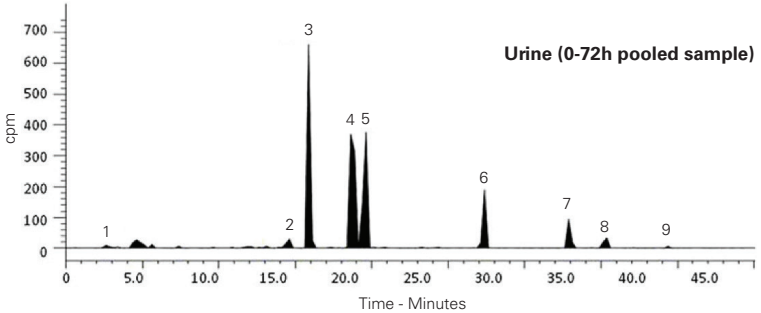
Analytes

1. 3-Aminophthalic acid
2. Hydrolysis product of pomalidomide
3. Hydrolysis product of pomalidomide
4. Glucuronide conjugate of 5-hydroxy pomalidomide
5. Glucuronide conjugate of 5-hydroxy pomalidomide
6. 7-Hydroxy pomalidomide
7. 5-Hydroxy pomalidomide
8. Pomalidomide
9. N-Acetyl pomalidomide



Pomalidomide





Hoffmann M, Kasserra C, Reyes J, Schafer P, Kosek J, Capone L, Parton A, Kim-Kang H, Surapaneni S, Kumar G. Absorption, Metabolism and Excretion of [^{14}C] Pomalidomide in Humans following Oral Administration. Cancer Chemotherapy and Pharmacology 71, 489-501 (2013) doi 10.1007/s00280-012-2040-6

Porphyrins in Oral Bacteria by LC-MS/MS

Application #AN3080

Conditions

Column: ACE 3 C18-PFP
Dimensions: 75 x 2.1 mm
Part Number: ACE-1110-7502
Mobile Phase: A: 0.1% formic acid in H_2O/MeCN (95:5 v/v)
B: 0.1% formic acid in H_2O/MeCN (5:95 v/v)

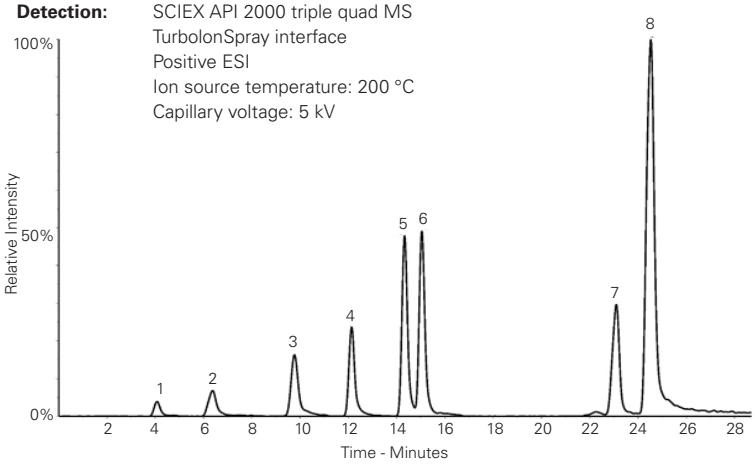
Gradient:

Time (mins)	%B
0.0	30
10.0	50
10.2	100
35.0	100

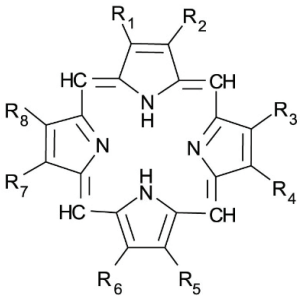
Flow Rate: 0.1 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: SCIEX API 2000 triple quad MS
TurbolonSpray interface
Positive ESI
Ion source temperature: 200 °C
Capillary voltage: 5 kV

Analytes

1. Uroporphyrin I
(R_1:A, R_2:P, R_3:A, R_4:P, R_5:A, R_6:P, R_7:A, R_8:P)
(*m/z* 831 → 727, 623, 655)
2. 7-Carboxyporphyrin I
(R_1:A, R_2:P, R_3:A, R_4:P, R_5:A, R_6:P, R_7:M, R_8:P)
(*m/z* 787 → 683, 670, 623)
3. 6-Carboxyporphyrin I
(R_1:M, R_2:P, R_3:A, R_4:P, R_5:A, R_6:P, R_7:M, R_8:P)
(*m/z* 743 → 639, 507, 521)
4. 5-Carboxyporphyrin I
(R_1:M, R_2:P, R_3:M, R_4:P, R_5:A, R_6:P, R_7:M, R_8:P)
(*m/z* 699 → 463, 595, 640)
5. Coproporphyrin I
(R_1:M, R_2:P, R_3:M, R_4:P, R_5:M, R_6:P, R_7:M, R_8:P)
(*m/z* 655 → 537, 596, 523)
6. Coproporphyrin III
(R_1:M, R_2:P, R_3:M, R_4:P, R_5:M, R_6:P, R_7:P, R_8:M)
(*m/z* 655 → 537, 596, 523)
7. Mesoporphyrin IX
(R_1:M, R_2:E, R_3:M, R_4:E, R_5:M, R_6:P, R_7:M, R_8:P)
(*m/z* 567 → 449, 479, 508)
8. Protoporphyrin IX
(R_1:M, R_2:V, R_3:M, R_4:V, R_5:M, R_6:P, R_7:P, R_8:M)
(*m/z* 563 → 445, 504, 489)



Where:
A: $-CH_2COOH$
E: $-CH_2CH_3$
M: $-CH_3$
P: $-CH_2CH_2COOH$
V: $-CH=CH_2$



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Pravastatin and Isomers by LC-MS/MS

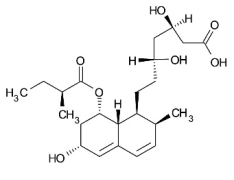
Application #AN1350

Conditions

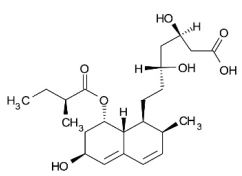
Column: ACE 3 C18
Dimensions: 50 x 3.0 mm
Part Number: ACE-111-0503
Mobile Phase: MeCN/MeOH/THF/H_2O/Acetic Acid
(15:20:5:60:0.1 v/v/v/v/v)
Flow Rate: 0.6 mL/min
Injection: 2 µL
Temperature: Ambient
Detection: API 3000 triple quad MS
TurbolonSpray – negative mode
Extracted ion chromatogram
of MRM *m/z* 423.3 → 321.1

Analytes

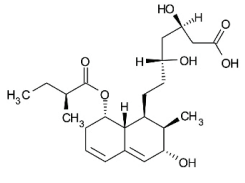
1. 6-epi-Pravastatin
(MW 424)
2. Pravastatin
(MW 424)
3. 3α-iso-Pravastatin
(MW 424)



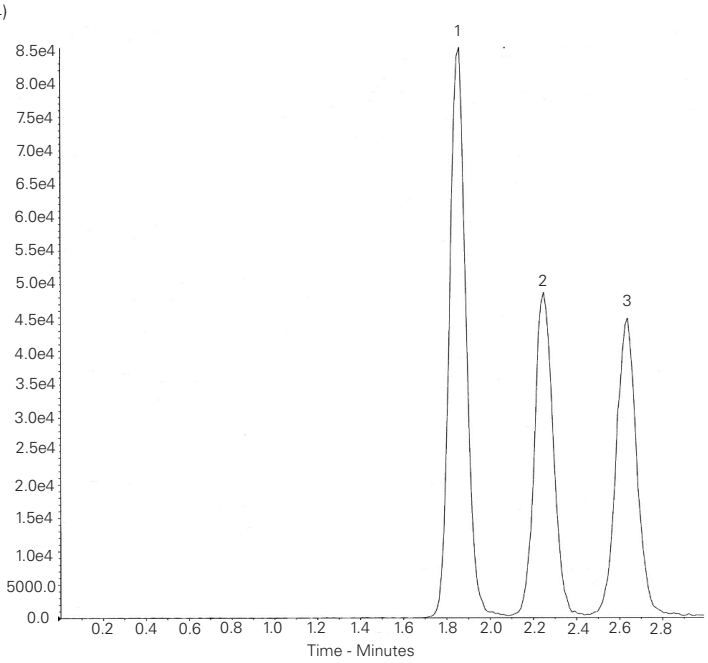
6-epi-Pravastatin



Pravastatin



3α-iso-Pravastatin



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Pravastatin in Cell Lysate Samples by LC-MS/MS

Application #AN4350

Conditions

Column: ACE Excel 3 SuperC18
Dimensions: 100 x 3.0 mm
Part Number: EXL-1111-1003U
Mobile Phase: A: 5 mM ammonium acetate pH 4.5 in H_2O
B: MeCN

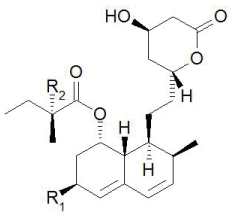
Gradient:

Time (mins)	%B
0	65
4	65
5	75
7	75
8	65

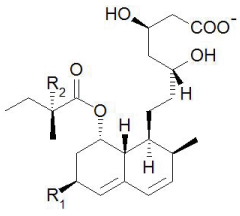
Flow Rate: 0.3 mL/min
Temperature: 40 °C
Detection: Quattro Ultima triple quad MS
ESI MRM mode: +ve (lactones)
–ve (hydroxy acids)
Source temperature: 125 °C
Desolvation temperature: 350 °C

Analytes

1. Lactone form (pharmacologically inactive)
2. Hydroxy acid form (pharmacologically active)



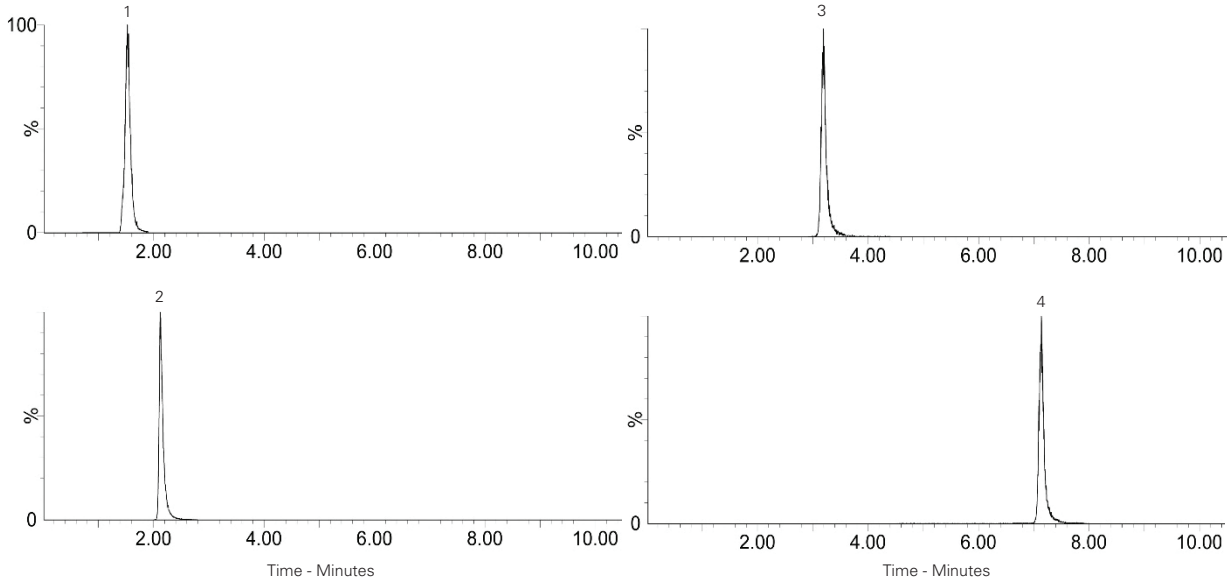
Lactone form
(pharmacologically inactive)



Hydroxy acid form
(pharmacologically active)

Peak	Analyte	Precursor ion	MRM transition *(m/z)*	LLOQ (ng/mL)
1	Pravastatin hydroxy acid	$[M-H]^-$	423.23 → 321.37	2.23
2	Pravastatin lactone	$[M+H]^+$	407.46 → 183.22	2.03
3	Lovastatin hydroxy acid (IS)	$[M-H]^-$	421.08 → 319.54	n/a
4	Lovastatin lactone (IS)	$[M+Na]^+$	427.15 → 325.36	n/a

Pravastatin: R_1 = OH, R_2 = H
Lovastatin (IS): R_1 = CH_3, R_2 = H



Taha DA, de Moor CH, Barrett DA, Lee JB, Gandhi RD, Hoo CW, Gershkovich P, (2016) The role of acid-base imbalance in statin-induced myotoxicity. Translational Research, The Journal of Laboratory and Clinical Medicine. http://dx.doi.org/10.1016/j.trsl.2016.03.015

Prednisolone, Prednisone, Cortisol and Cortisone in Serum by LC-MS/MS

Application #AN2690

Conditions

Column: ACE Excel 2 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-101-1002U
Mobile Phase: A: 4 mM ammonium acetate in H_2O
B: 0.2% (v/v) formic acid in MeOH

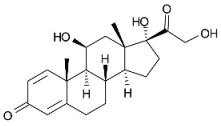
Gradient:

Time (mins)	%B
0.00	30
0.25	30
3.90	70
6.00	70
6.01	95
7.00	95
7.01	100

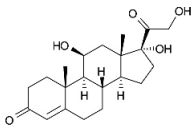
Flow Rate: 0.2 mL/min
Injection: 50 µL
Temperature: 50 °C
Detection: Applied Biosystems 5000 MS/MS
APCI in positive ion mode

Analytes

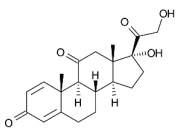
1. Prednisolone
(*m/z* 361.5 ⟶ 147.1)
2. Cortisol
(*m/z* 363.5 ⟶ 121.3)
3. Prednisone
(*m/z* 359.4 ⟶ 147.1)
4. Cortisone
(*m/z* 361.5 ⟶ 163.3)
5. Prednisolone-d6 (IS)
(*m/z* 367.4 ⟶ 150.3)
6. Cortisol-d4 (IS)
(*m/z* 367.3 ⟶ 331.3)



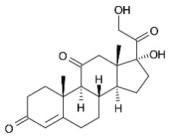
Prednisolone



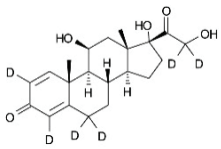
Cortisol



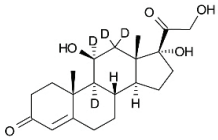
Prednisone



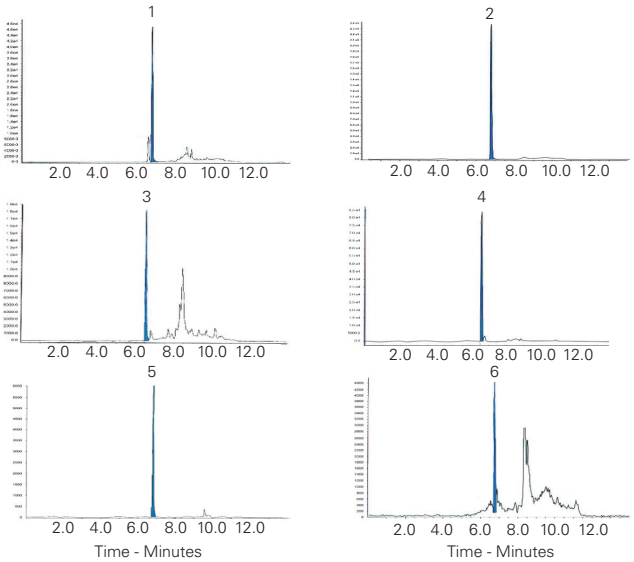
Cortisone



Prednisolone-d6 (IS)



Cortisol-d4 (IS)



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Preservatives (I)

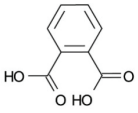
Application #AN2230

Conditions

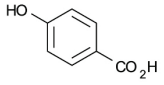
Column: ACE Excel 1.7 C18
Dimensions: 50 x 3.0 mm
Part Number: EXL-171-0503U
Mobile Phase: 20 mM potassium phosphate
pH 2.5 in MeCN/H_2O (30:70 v/v)
Flow Rate: 0.43 mL/min
Injection: 0.7 µL
Temperature: 20 °C
Detection: UV, 230 nm

Analytes

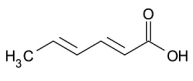
1. Phthalic acid
2. 4-Hydroxybenzoic acid
3. Sorbic acid
4. Methyl paraben
5. Ethyl paraben
6. Propyl paraben



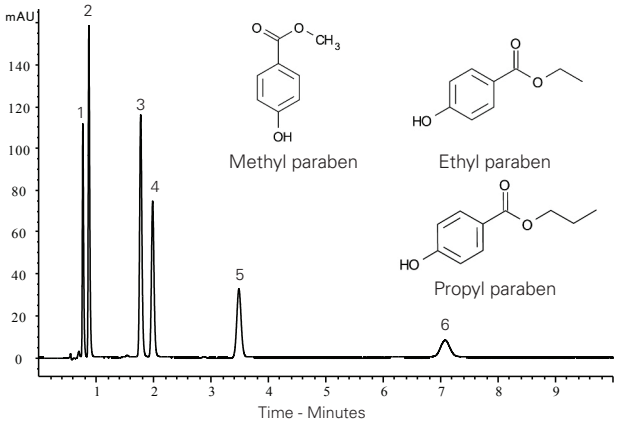
Phthalic acid



4-Hydroxybenzoic acid



Sorbic acid



Methyl paraben

Ethyl paraben

Propyl paraben

Preservatives (II)

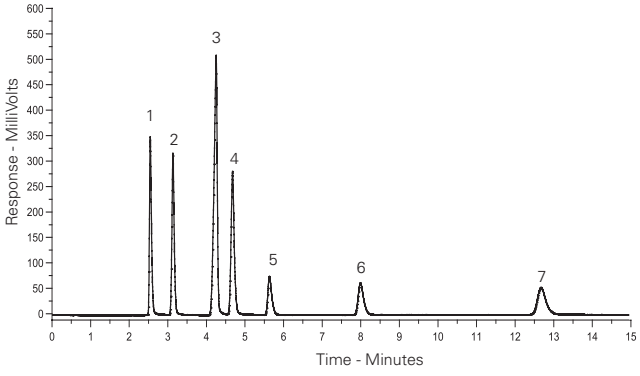
Application #AN3040

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

Analytes

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



Pristinamycin Components in Plasma by LC-MS/MS

Application #AN1360

Conditions

Column: ACE 3 C18
Dimensions: 30 x 3.0 mm
Part Number: ACE-111-0303
Mobile Phase: A: 1 mM ammonium formate + 0.1% formic acid in MeCN/H_2O (35:65 v/v)
B: MeCN

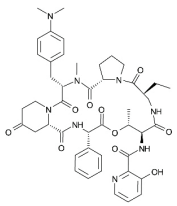
Gradient:

Time (mins)	%B
0.00	0
0.30	0
0.31	10
1.60	10
1.61	100
2.60	100
2.61	0
4.00	0

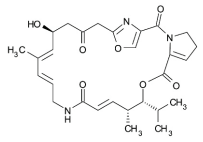
Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: 25 °C
Detection: MDS Sciex API 4000 TurbolonSpray positive mode

Analytes

1. Pristinamycin IA
   (*m/z* 867.5 → 134.2)
2. Pristinamycin IIA
   (*m/z* 526.3 → 355.1)
3. Virginiamycin (IS)
   (*m/z* 824.6 → 134.0)



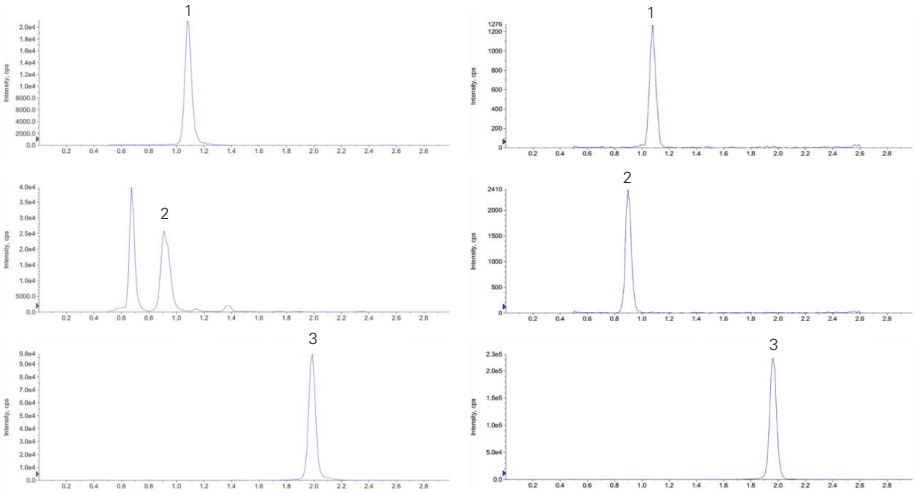
Pristinamycin IA



Pristinamycin IIA

Processed study sample containing pristinamycin IA and IIA

Low calibration standard containing 2.5 ng/mL each of pristinamycin IA and IIA in human $NaF/K_2C_2O_4$ plasma



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Proanthocyanidins from Cinnamon Bark Extract

Application #AN3510

Conditions

Column: ACE 3 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-111-2546
Mobile Phase: A: 1% acetic acid in H_2O
B: MeCN

Gradient:

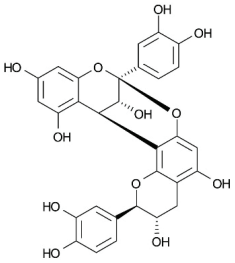
Time (mins)	%B
0	36
35	36
40	50
45	100
55	0
60	0

Flow Rate: 0.75 mL/min
Temperature: Ambient
Detection: UV, 280 nm
Sample: Cinnamon bark extract thiolysed with benzyl mercaptan

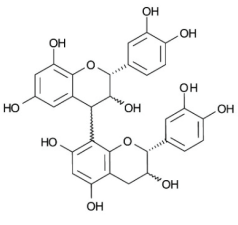
Analytes

1. Catechin
2. A-type PC dimer
3. A-type PC trimer
4. Epicatechin
5. A-type PC trimer
6. IS
7. cis-Cinnamic acid
8. A-type PC-BM trimer
9. trans-Cinnamic acid
10. cis-Catechin-BM
11. Epicatechin-BM
12. A-type PC-BM dimer

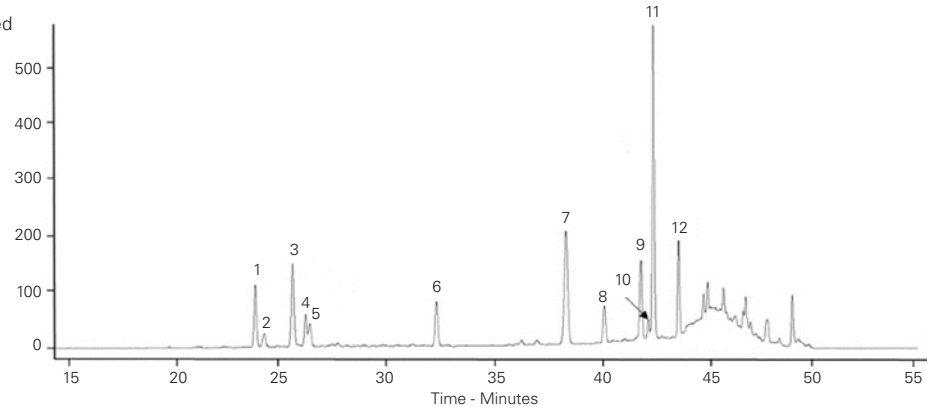
PC = Procyanidin
BM = Benzyl mercaptan adduct



Example of A type procyanidin dimer



Example of B type procyanidin dimer



Williams, A. R. et al. Anthelmintic activity of trans-cinnamaldehyde and A and B-type proanthocyanidins derived from cinnamon (*Cinnamomum verum*). Sci. Rep. 5, 14791; doi:10.1038/srep14791 (2015).

Procaine and p-Aminobenzoic Acid Separation

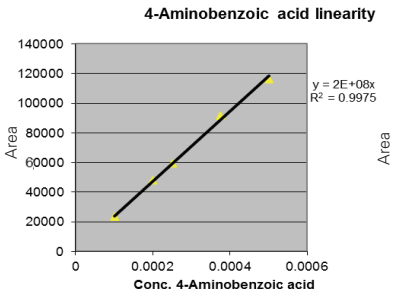
Application #AN1660

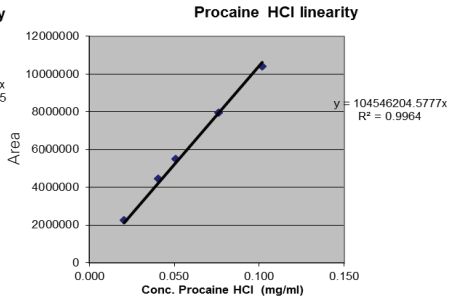
Conditions

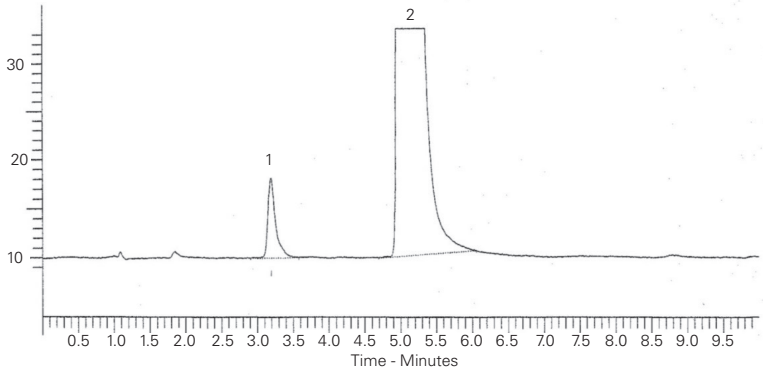
Column: ACE 3 C18-PFP
Dimensions: 100 x 4.6 mm
Part Number: ACE-1110-1046
Mobile Phase: 0.6% acetic acid in H_2O/MeOH (81:19 v/v), adjusted to pH 4.7 with 20% NaOH
Flow Rate: 1 mL/min
Detection: UV, 279 nm
S/N limit: 10
Sample: Procaine 0.0002 mg/mL, p-Aminobenzoic acid 0.00005 mg/mL

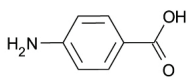
Analytes

1. p-Aminobenzoic acid (4-Aminobenzoic acid)
2. Procaine

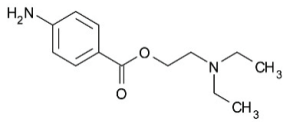








p-Aminobenzoic Acid



Procaine

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Propolis Phenolic Acids Applied to Human Skin

Application #AN4230

Conditions

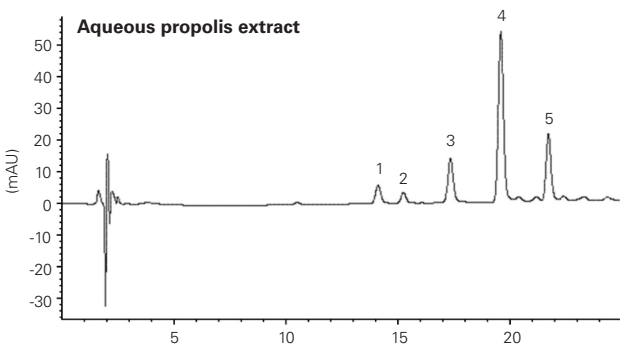
Column: ACE 5 C18
Dimensions: 150 x 0.5 mm
Part Number: ACE-121-15005
Mobile Phase: A: 0.5% acetic acid in H_2O
B: MeCN

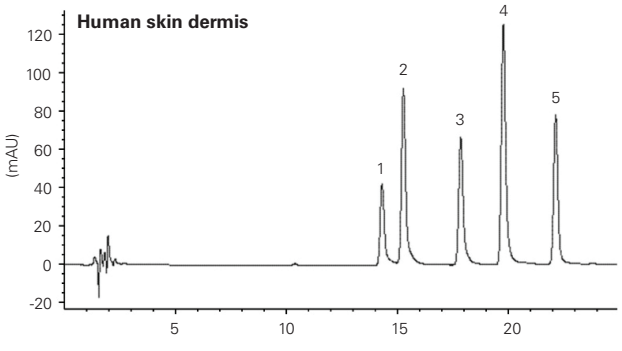
Gradient:	**Time (mins)**	**%B**
	0	1
	25	21

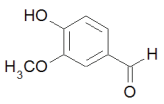
Flow Rate: 20 µL/min
Injection: 0.2 µL
Temperature: 25 °C
Detection: UV, 290 nm

Analytes

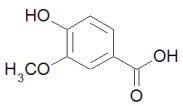
1. Vanillic acid
2. Caffeic acid
3. Vanillin
4. Coumaric acid
5. Ferulic acid



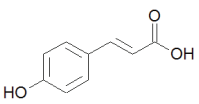




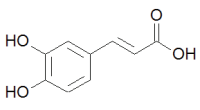
Vanillin



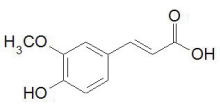
Vanillic acid



Coumaric acid



Caffeic acid



Ferulic acid

Zilius M, Ramanauskiene K, Briedis V. Release of Propolis Phenolic Acids from Semisolid Formulations and their Penetration into the Human Skin in vitro. Evidence-based Complementary and Alternative Medicine (2013) http://dx.doi.org/10.1155/2013/958717

Prostaglandins using LC-MS/MS

Application #AN3260

Conditions

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

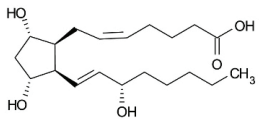
Gradient:

Time (mins)	%A	%B	%C
0	70.0	20.0	10.0
9	10.0	60.0	30.0
10	0.1	66.6	33.3

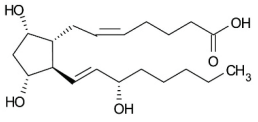
Flow Rate: 0.2 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: ESI (-) MS/MS
MRM *m/z* 353.3 → 193

Analytes

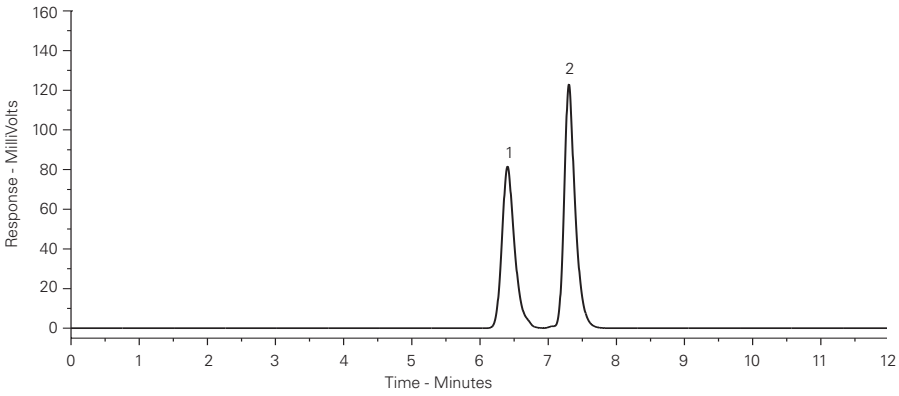
1. 8-iso-Prostaglandin $F2_\alpha$
2. Prostaglandin $F2_\alpha$



8-iso-Prostaglandin $F2_\alpha$



Prostaglandin $F2_\alpha$



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Protein Test Mix

Application #AN3730

Conditions

Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 0.1% TFA in H_2O
B: 0.1% TFA in MeCN

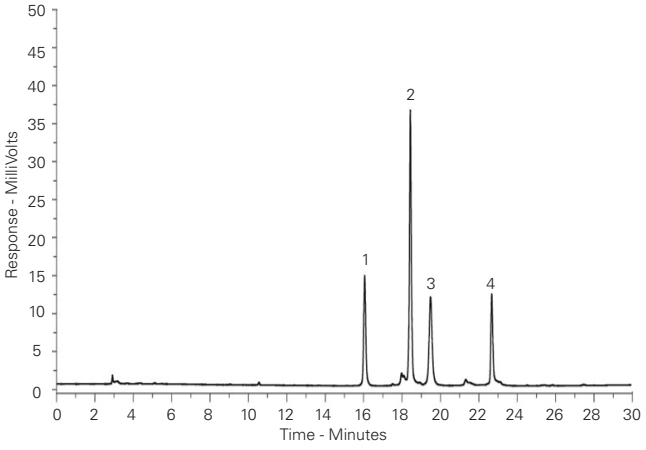
Gradient:

Time (mins)	%B
0	5
30	70

Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 280 nm

Analytes

1. Ribonuclease A (MW ~14 kDa)
2. Cytochrome C (MW ~12 kDa)
3. Holo-transferrin (MW ~77 kDa)
4. Apomyoglobin (MW ~17 kDa)



Proton Pump Inhibitors (PPIs)

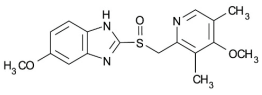
Application #AN3710

Conditions

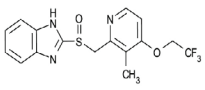
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 10 mM ammonium formate pH 3.0/MeCN (65:35 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analytes

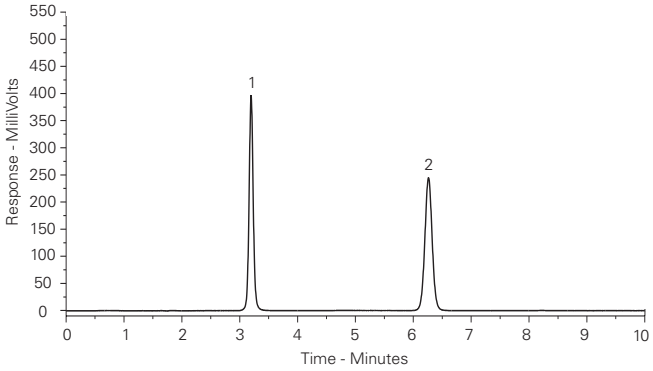
1. Omeprazole
2. Lansoprazole



Omeprazole



Lansoprazole



Psychoactive Substances in 'Synthacaine' by LC-UV

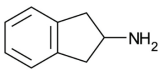
Application #AN3440

Conditions

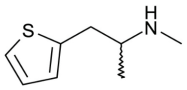
Column:	ACE 3 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-111-1546
Mobile Phase:	10 mM ammonium formate pH 3.5/MeCN (90:10 v/v)
Flow Rate:	1.2 mL/min
Temperature:	22 °C
Detection:	UV, 207 nm (2-Aminoindane) and 233 nm (Methiopropamine)
Sample:	Synthacaine 40 µg/mL

Analytes

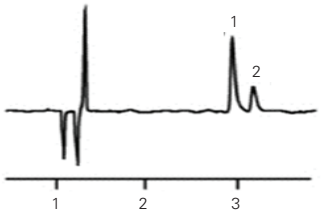
1. 2-Aminoindane
   LOD 0.83 µg/mL
2. Methiopropamine
   LOD 0.31 µg/mL



2-Aminoindane



Methiopropamine



Time - Minutes

Cumba L, Kolliopoulos A, Smith J, Thompson P, Evans P, Sutcliffe O, do Carmo D, Banks C (2015) Forensic electrochemistry: indirect electrochemical sensing of the components of the new psychoactive substance 'Synthacaine'. Analyst 140, 5536. doi:10.1039/c5an00858a

Quinidine, Quinine and their Hydroderivatives Separation

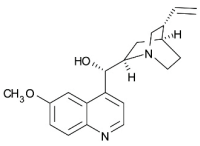
Application #AN1600

Conditions

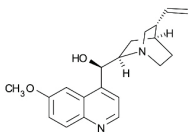
Column:	ACE 3 C18-AR
Dimensions:	50 x 4.6 mm
Part Number:	ACE-119-0546
Mobile Phase:	20 mM ammonium formate pH 3.0 in MeOH/H_2O (30:70 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	30 °C
Detection:	UV, 254 nm

Analytes

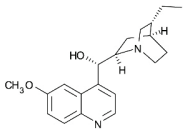
1. Quinidine
2. Quinine
3. Hydroquinidine
4. Hydroquinine



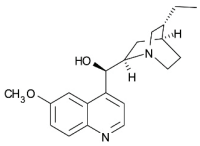
Quinidine



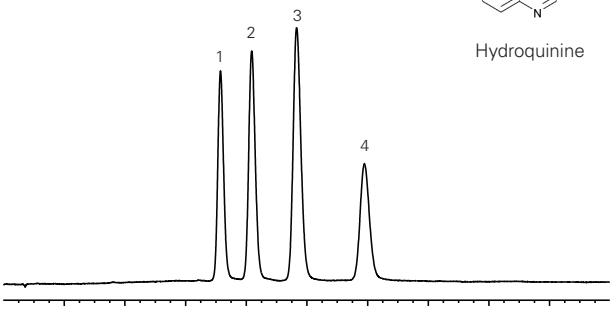
Quinine



Hydroquinidine



Hydroquinine



Time (minutes)

Need a custom column for your application?

Please enquire
email: info@ace-hplc.com

Ranitidine Hydrochloride and Related Impurities

Application #AN3450

Conditions

Column: ACE 3 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-111-1046
Mobile Phase: A: 0.05 M KH_2PO_4 pH 6.5 in H_2O/MeCN (98:2 v/v)
B: H_2O/MeCN (5:95 v/v)

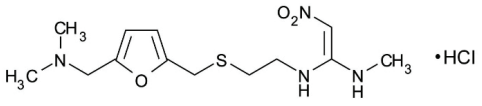
Gradient:

Time (mins)	%B
0	0
10	5
25	15
35	20
40	55
55	0

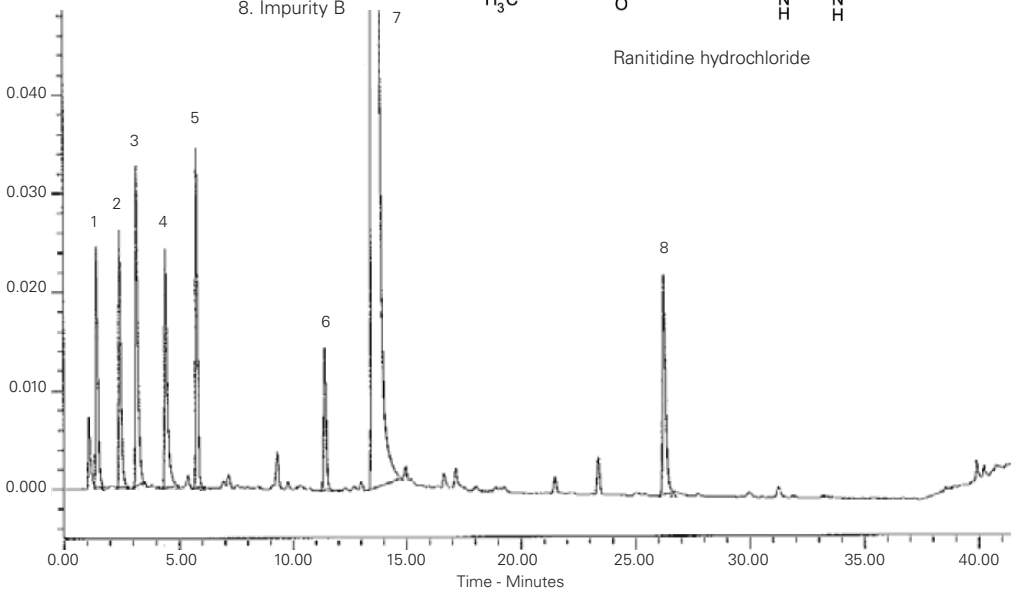
Flow Rate: 1 mL/min
Injection: 40 µL
Temperature: 40 °C
Detection: UV, 230 nm

Analytes

1. Impurity F
2. Impurity E
3. Impurity D
4. Impurity A
5. Impurity C
6. Impurity G
7. Ranitidine
8. Impurity B



Ranitidine hydrochloride



Sharma N, Rao S, Kumar N, Reddy P, Reddy A (2011) A Validated Stability-Indicating Liquid-Chromatographic Method for Ranitidine Hydrochloride in Liquid Oral Dosage Form. Sci Pharm. 79, 309. doi:10.3797/scipharm.1101-06

Recombinant hGMCSF Purified from *Escherichia Coli*

Application #AN3840

Conditions

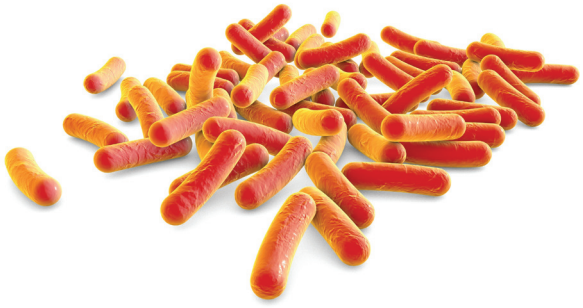
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: A: 0.1% TFA in H_2O/MeCN (90:10 v/v)
B: 0.1% TFA in H_2O/MeCN (10:90 v/v)

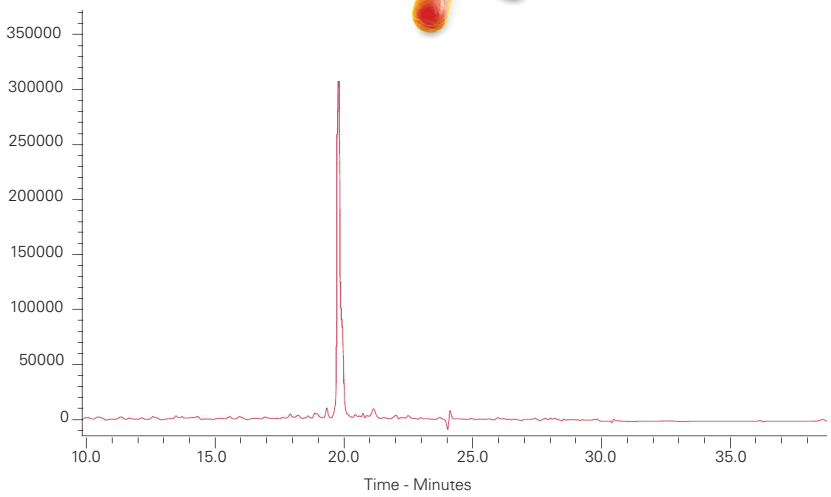
Gradient:

Time (mins)	%B
0	10
20	65
23	100

Flow Rate: 1 mL/min
Temperature: 30 °C
Detection: UV, 215 nm

hGMCSF = human Granulocyte Macrophage Colony Stimulating Factor, a 127 amino acid residue cytokine with a molecular weight of 14,477 Da





Das KMP, Banerjee S, Shekhar N, Damodaran K, Nair R, Somani S, Raiker VP, Jain S, Padmanabhan S. Cloning, Soluble Expression and Purification of High Yield Recombinant hGMCSF in *Escherichia coli*. Int. J. Mol. Sci. 2011, 12, 2064-2076; doi:10.3390/ijms12032064

Rifamycin Anti-tubercular Antibiotics in Human Plasma

Application #AN4090

Conditions

Column: ACE 3 C18
Dimensions: 100 x 3.0 mm
Part Number: ACE-111-1003
Mobile Phase: A: 15 mM ammonium formate pH 5.0 with formic acid in H_2O
B: 0.1% formic acid in MeOH

Gradient:

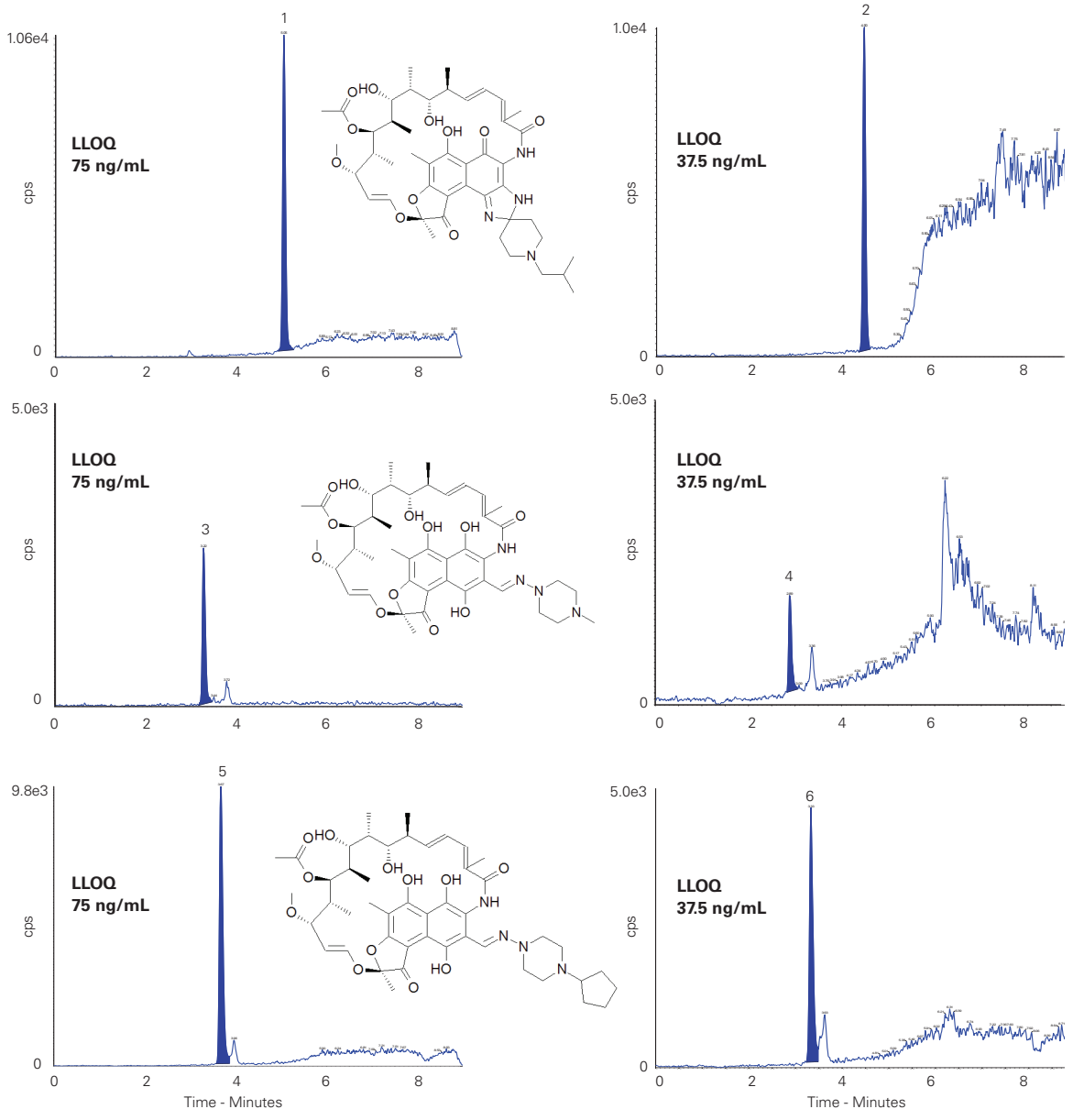
Time (mins)	%B
0.0	60
4.0	95
7.0	95
7.2	60
9.0	60

Flow Rate: 0.35 mL/min
Injection: 2 µL
Temperature: 30 °C
Detection: API 5000 triple quad MS
ESI in positive ion mode

Assay for simultaneous quantification of rifamycin antibiotics and their corresponding active desacetyl metabolites

Analytes

1. Rifabutin
   (*m/z* 847.5 → 815.5)
2. Desacetyl rifabutin
   (*m/z* 805.5 → 773.4)
3. Rifampicin
   (*m/z* 823.5 → 791.4)
4. Desacetyl rifampicin
   (*m/z* 781.5 → 749.4)
5. Rifapentine
   (*m/z* 877.5 → 845.4)
6. Desacetyl rifapentine
   (*m/z* 835.5 → 803.5)



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