

mGluR5 PET Tracer by Radio HPLC Analysis

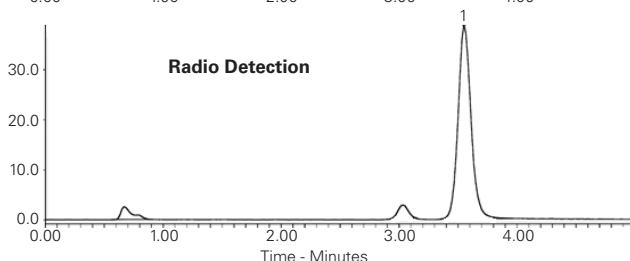
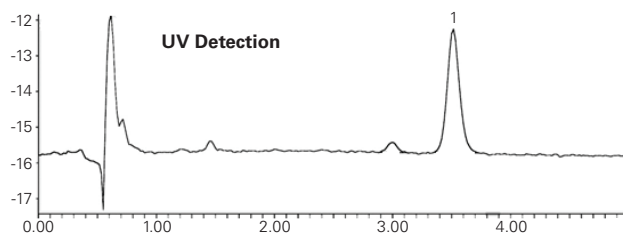
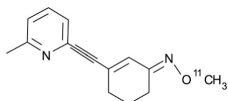
Application #AN2700

Conditions

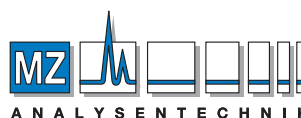
Column: ACE 3 C18
Dimensions: 50 x 4.6 mm
Part Number: ACE-111-0546
Mobile Phase: 0.1% TFA in H₂O/MeCN (55:45 v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Detection: UV, 254 nm
 Radio detection

Analyte

1. ¹¹C-ABP688



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 e-mail: info@mz-at.de
 www.mz-at.de

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 H₂O
 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:

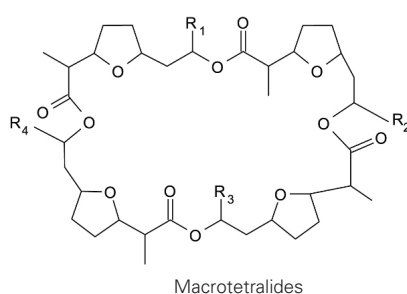
Detection:

0.2 mL/min
 Dionex 3000RS UHPLC system coupled with Bruker MaXis Q-TOF MS
 Electrospray MS positive mode
 Source end plate offset -500 V
 Nebuliser gas (N₂) 1.6 bar
 Drying gas (N₂) temp 180 °C
 Collision energy 5.0 eV
 Collision RF 600 Vpp

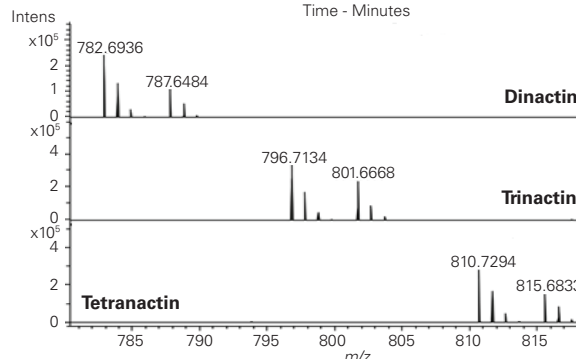
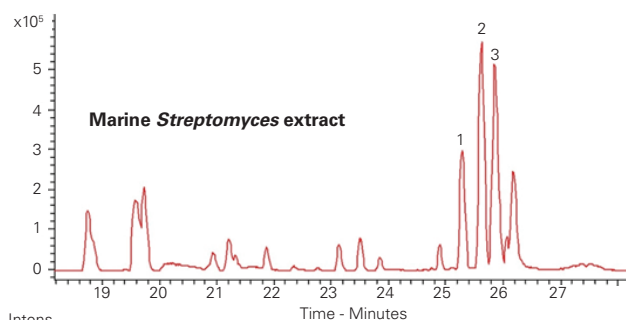
Analytes

Macrotetralides

1. Dinactin R₁ = R₃ = CH₂CH₃, R₂ = R₄ = CH₃
2. Trinactin R₁ = R₂ = R₃ = CH₂CH₃, R₄ = CH₃
3. Tetranactin R₁ = R₂ = R₃ = R₄ = CH₂CH₃



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 H₂O
 B: MeCN
Gradient:

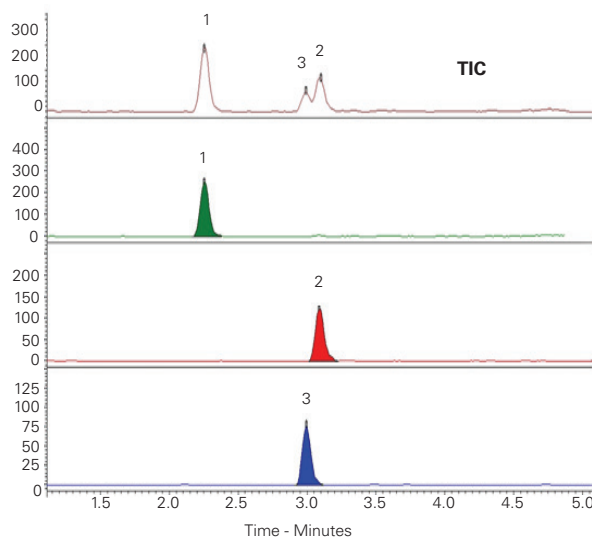
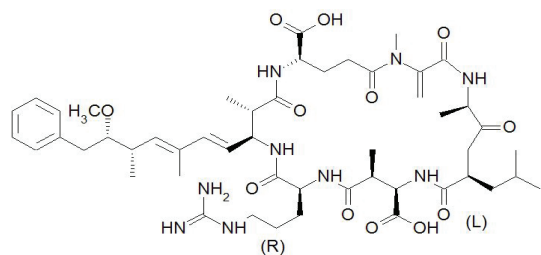
Time (mins)	%B
0.0	30
1.0	30
7.0	95
7.1	30
10.0	30

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

Analyses

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

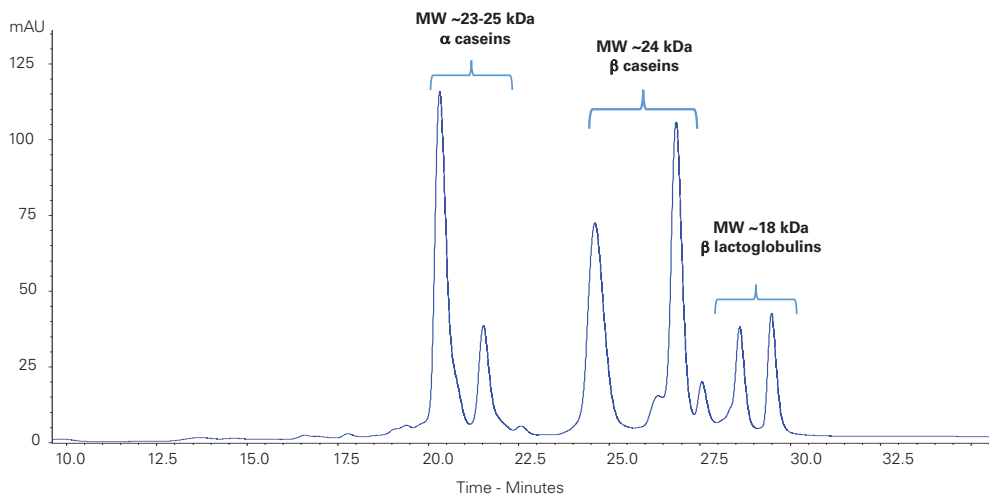
Application #AN1540

Conditions

Column: ACE 5 C18-300
Dimensions: 150 x 2.1 mm
Part Number: ACE-221-1502
Mobile Phase: A: 0.01 % TFA in H₂O
 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

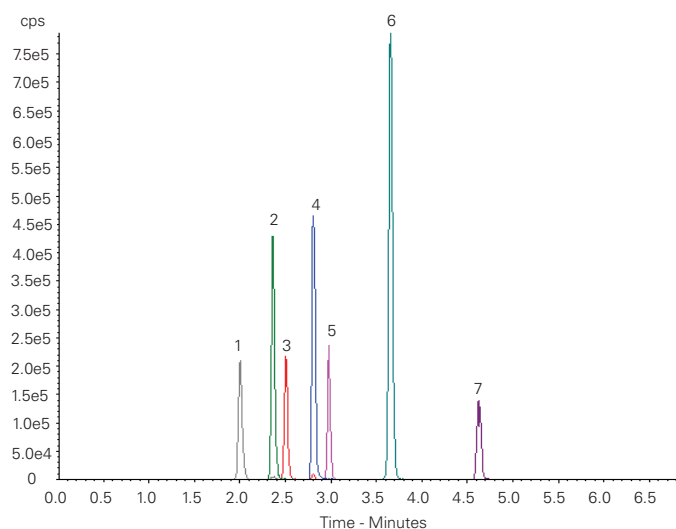
Column: ACE Excel 2 C18-AR
Dimensions: 50 x 2.1 mm
Part Number: EXL-109-0502U
Mobile Phase: A: 1 mM ammonium acetate, 0.5% acetic acid in H₂O
 B: 1 mM ammonium acetate, 0.5% acetic acid in 95% MeOH
Gradient:

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

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

Analytes

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



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Mycotoxins/Aflatoxins from Peppers

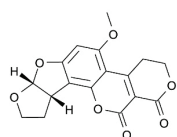
Application #AN1200

Conditions

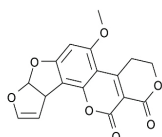
Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: H₂O/MeOH (60:40 v/v)
Flow Rate: 1 mL/min
Injection: 100 µL
Temperature: 45 °C
Detection: Fluorescence, λ_{Ex} 362 nm,
 λ_{Em} 425 nm

Analytes

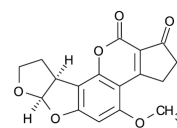
1. Aflatoxin G2
2. Aflatoxin G1
3. Aflatoxin B2
4. Aflatoxin B1



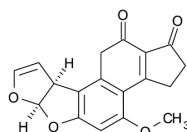
Aflatoxin G2



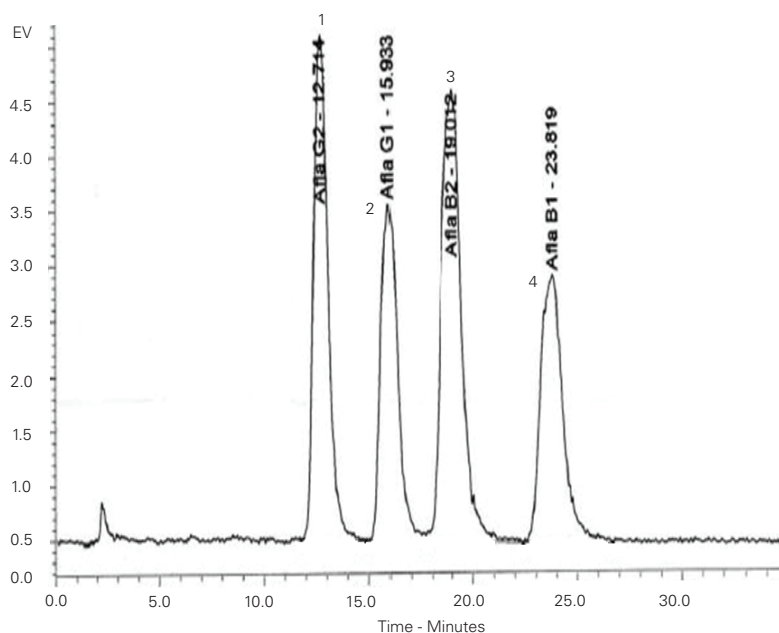
Aflatoxin G1



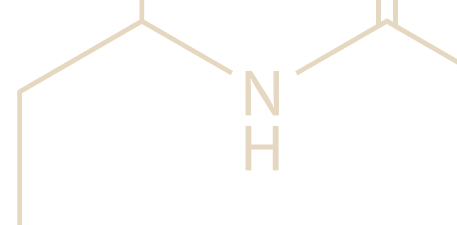
Aflatoxin B2



Aflatoxin B1



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Naphthalenes (Substituted)

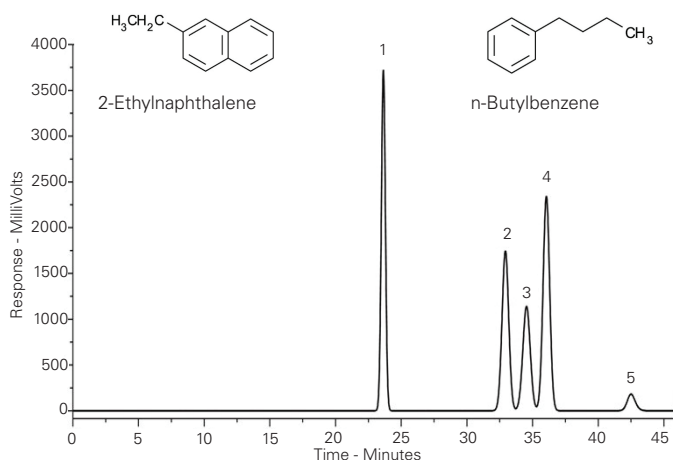
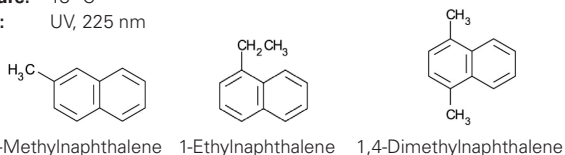
Application #AN3690

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: MeCN/H₂O (51:49 v/v)
Flow Rate: 1.5 mL/min
Temperature: 18 °C
Detection: UV, 225 nm

Analytes

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



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Neonicotinoids in Honey by LC-MS/MS

Application #AN4050

Conditions

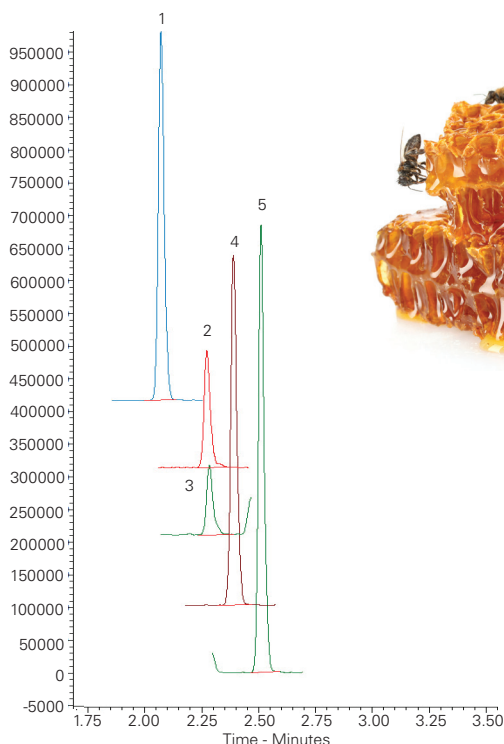
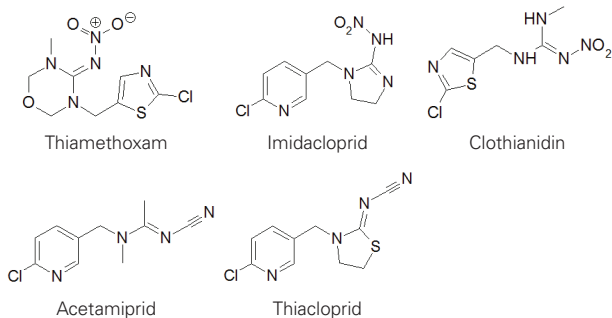
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 2.1 mm
Part Number: CORE-25A-1002U
Mobile Phase: A: 0.05% ammonia in H₂O
 B: 0.05% ammonia in MeOH
Gradient:

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. Thiocloprid (*m/z* 253 → 126)



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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 H₂O
 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

- Adrenaline
- Noradrenaline
- Glutamic acid
- GABA
- Dopamine
- MHPG
(3-Methoxy-4-hydroxyphenylglycol)
- Isoprenaline (IS)
- 5-Hydroxyindoleacetic acid
- Serotonin

Quantifier

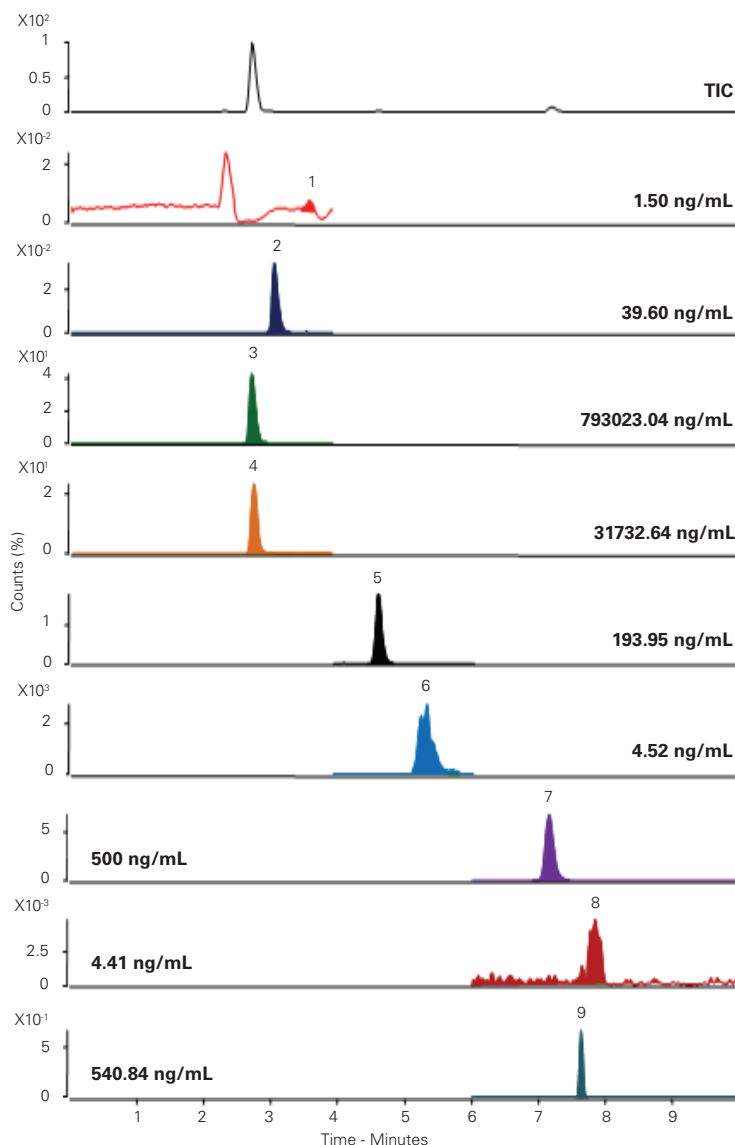
m/z 184.2 → 166.2
m/z 170.2 → 107.1
m/z 148.1 → 84.1
m/z 104 → 45
m/z 154.1 → 137.1
m/z 263 → 165.1
m/z 212.2 → 194.1
m/z 192 → 145.9
m/z 177.2 → 160.2

Qualifier

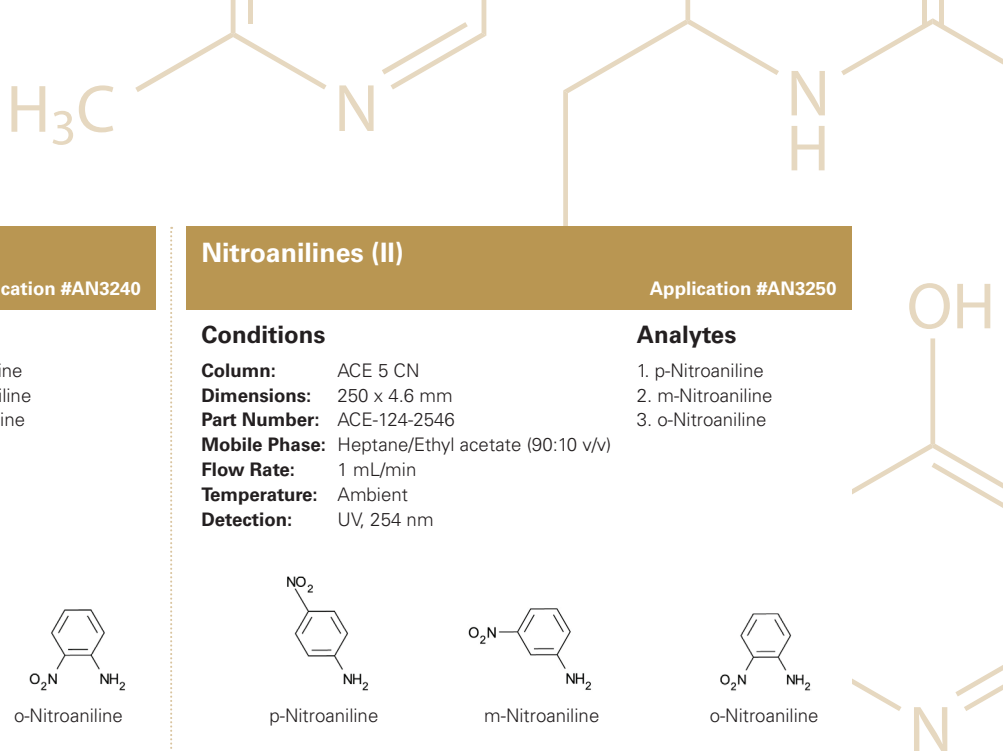
m/z 184.2 → 57.1
m/z 170.2 → 152.1
m/z 148.1 → 130.1
m/z 104 → 87
m/z 154.1 → 91.1
m/z 263 → 165.1
m/z 192 → 90.9
m/z 177.2 → 132.1

LLOQ (ng/mL)

0.25
 0.5
 250
 250
 0.25
 1
 1
 10



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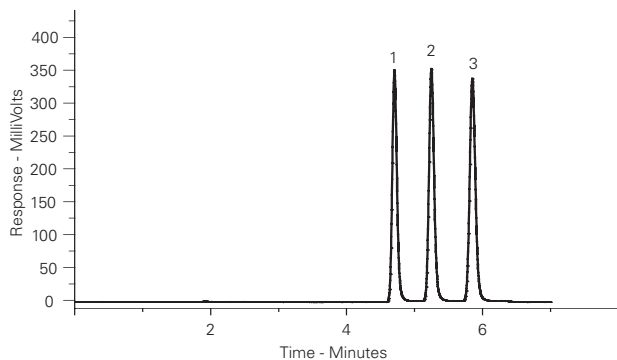
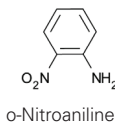
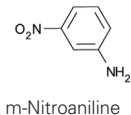
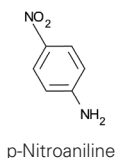
Nitroanilines (I) Application #AN3240

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 50 mM KH₂PO₄ 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



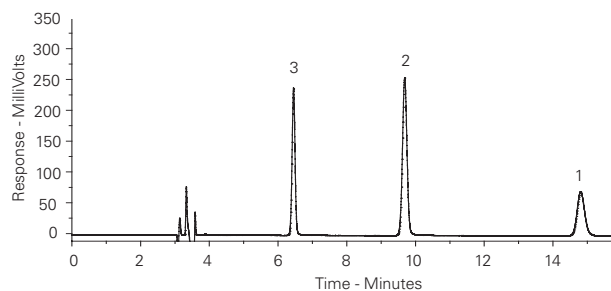
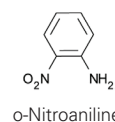
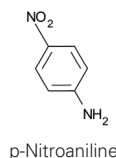
Nitroanilines (II) Application #AN3250

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



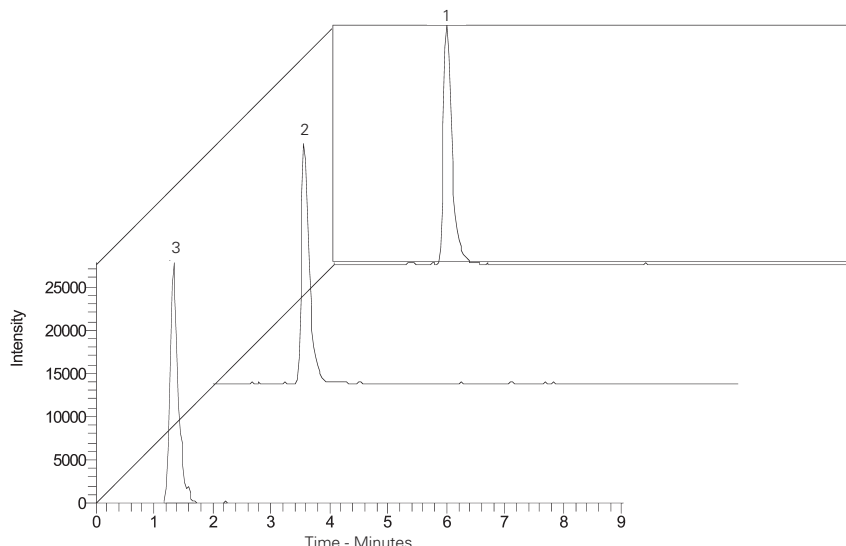
Nitrofurans Metabolites by LC-MS/MS Application #AN3050

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 H₂O (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 furalfadone) (*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

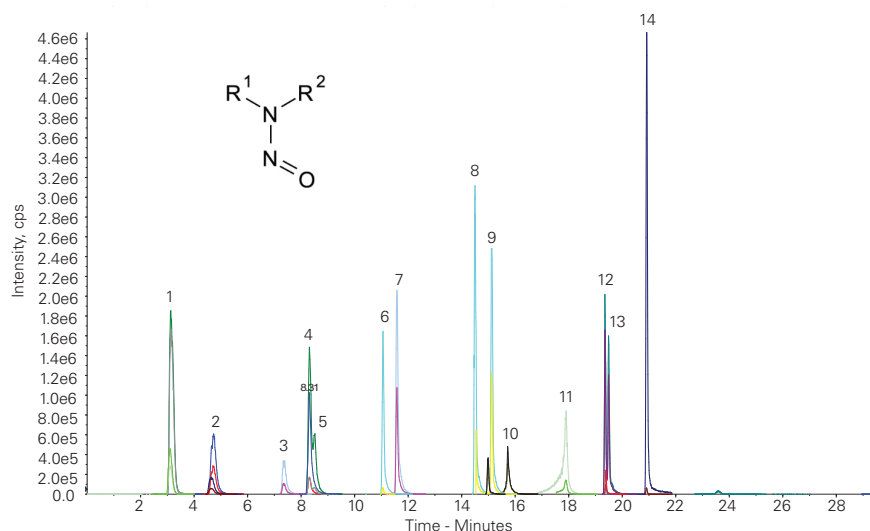
Column: ACE Excel 2 C18-PFP
Dimensions: 150 x 3.0 mm
Part Number: EXL-1010-1503U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeOH
Gradient:

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

Analytes

- | | | |
|---|--|--|
| 1. NDELA
(<i>m/z</i> 135.2 → 74.2, 135.2 → 104.2) | 6. NDEA
(<i>m/z</i> 103.1 → 75.2, 103.1 → 472) | 11. NEPhA
(<i>m/z</i> 151.1 → 77.1, 151.1 → 95.3) |
| 2. NDMA
(<i>m/z</i> 74.9 → 43.2, 74.9 → 58.2) | 7. NPIP
(<i>m/z</i> 115.1 → 69.1, 115.1 → 41.2) | 12. NDiBA
(<i>m/z</i> 159.3 → 57.2, 159.3 → 103.2) |
| 3. Nmorph
(<i>m/z</i> 117.1 → 86.3, 117.1 → 73.3) | 8. NDnPA
(<i>m/z</i> 131.2 → 89.2, 131.2 → 43.3) | 13. NDnBA
(<i>m/z</i> 159.3 → 103.2, 159.3 → 57.2) |
| 4. Npyrr
(<i>m/z</i> 101.2 → 55.3, 101.2 → 59.2) | 9. NdiPA
(<i>m/z</i> 131.2 → 89.2, 131.2 → 43.3) | 14. NDBzA
(<i>m/z</i> 227.2 → 91.1, 227.2 → 181.2) |
| 5. NMEA
(<i>m/z</i> 89.2 → 61.1, 89.2 → 43.3) | 10. NMPHA
(<i>m/z</i> 137.2 → 107.2, 137.2 → 66.1) | |



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

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Non-Steroidal Anti-Inflammatory Drugs (I)

Application #AN1210

Conditions

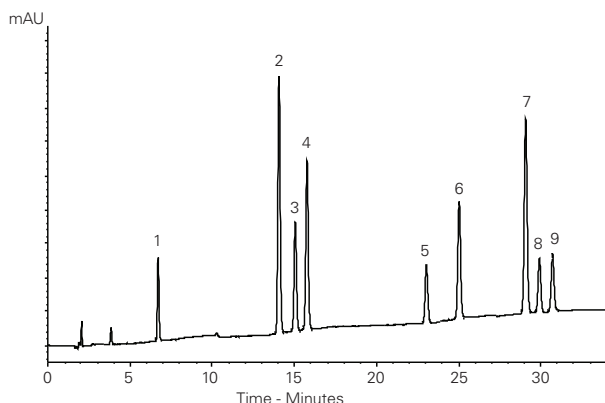
Column: ACE 3 C18-AR
Dimensions: 150 x 4.6 mm
Part Number: ACE-119-1546
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeOH
Gradient:

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

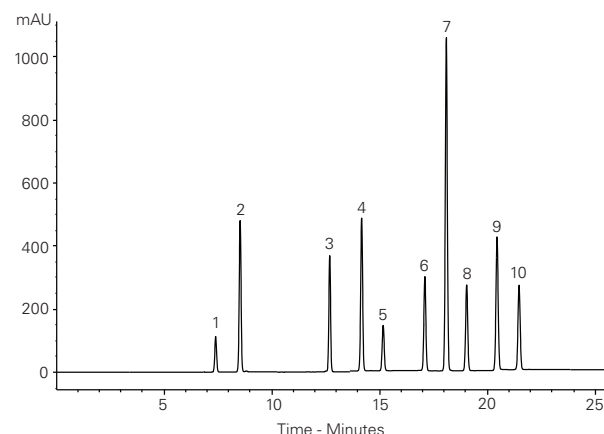
Column: ACE Excel 5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: EXL-1211-1546U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

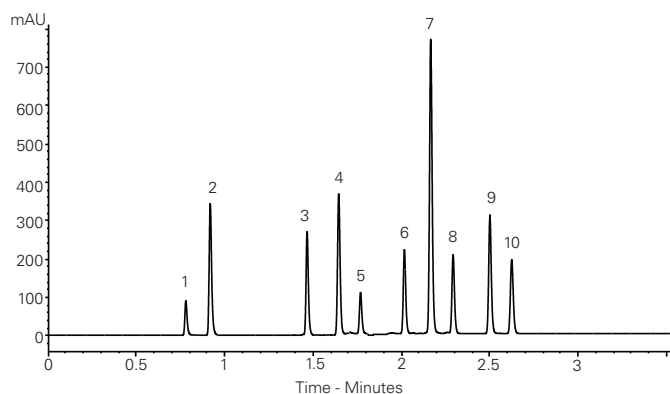
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 3.0 mm
Part Number: CORE-25A-0503U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

- Aspirin
- Phenacetin
- Sulindac
- Tolmetin
- Naproxen
- Nimesulide
- Flurbiprofen
- Diclofenac
- Phenylbutazone
- Meclofenamic acid



Non-Steroidal Anti-Inflammatory Drugs – Fast Analysis

Application #AN2080

Conditions

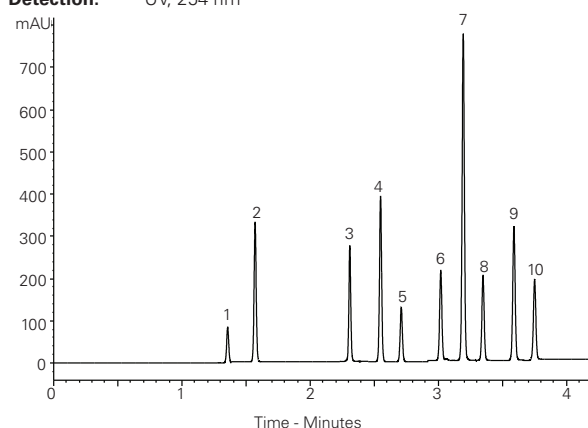
Column: ACE Excel 2 SuperC18
Dimensions: 50 x 3.0 mm
Part Number: EXL-1011-0503U
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeCN
Gradient:

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

- Aspirin
- Phenacetin
- Sulindac
- Tolmetin
- Naproxen
- Nimesulide
- Flurbiprofen
- Diclofenac
- Phenylbutazone
- Meclofenamic acid



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

Application #AN2630

Conditions

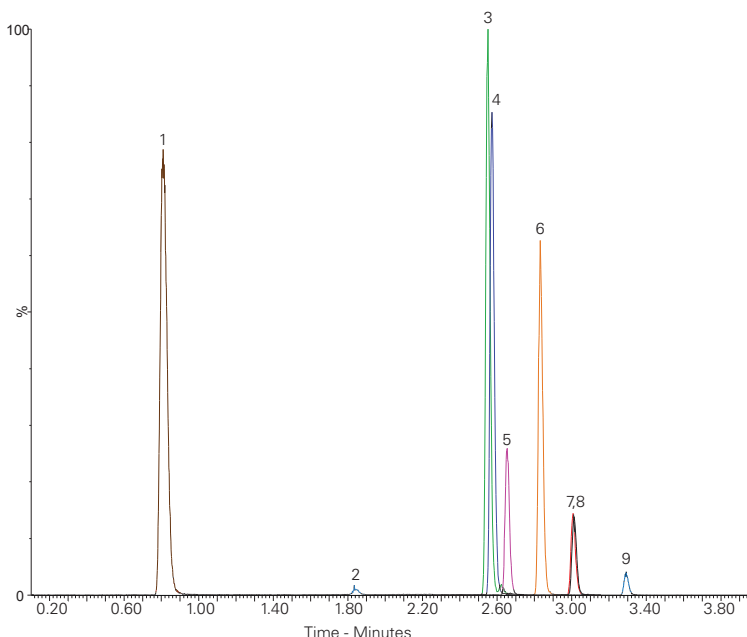
Column: ACE Excel 2 C18
Dimensions: 50 x 2.1 mm
Part Number: EXL-101-0502U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% formic acid in H₂O
 B: 2 mM ammonium acetate, 0.1% formic acid in MeOH
Gradient:

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
 Sample: ESI in positive ion mode
 10 pg/µL

Analytes

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



Nucleic Acids / Disease Biomarker Profiling (I)

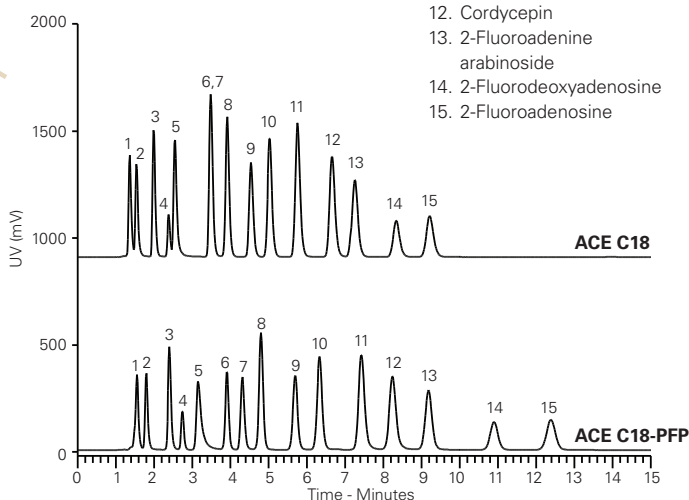
Application #AN1080

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

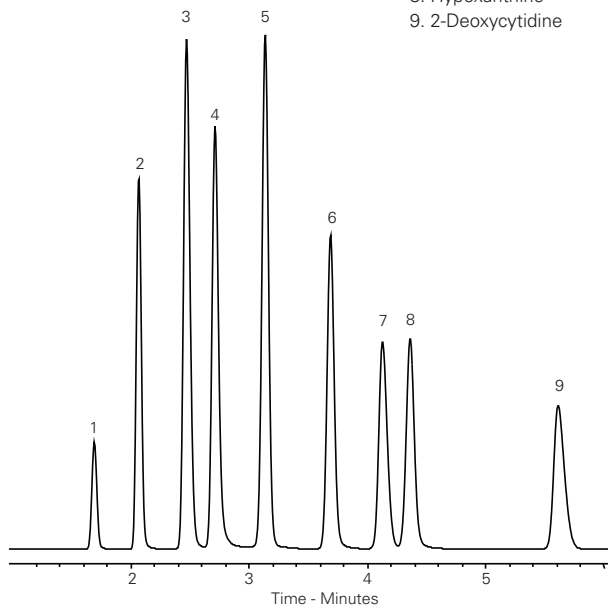
Application #AN1330

Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: 20 mM H₃PO₄ in H₂O
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)

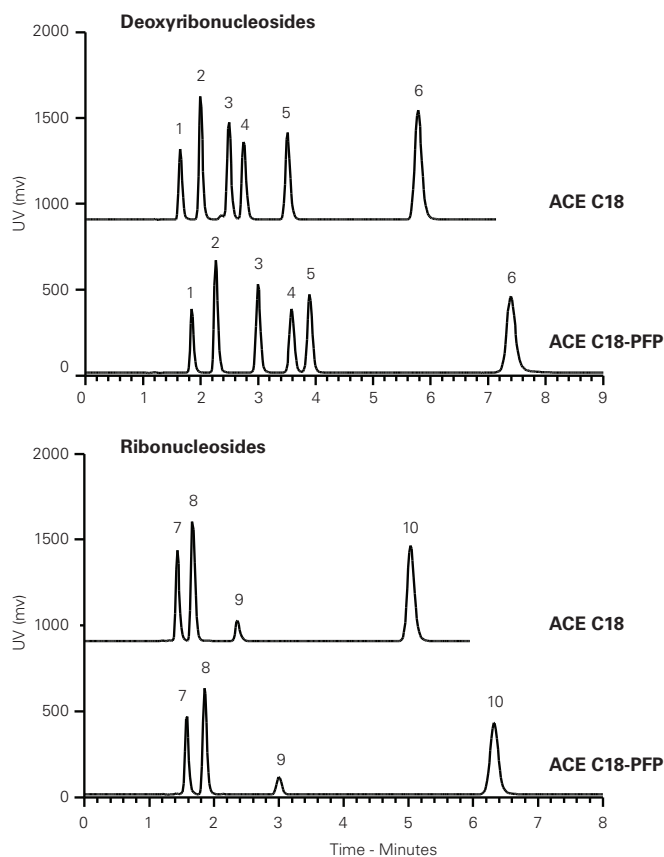
Application #AN1090

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

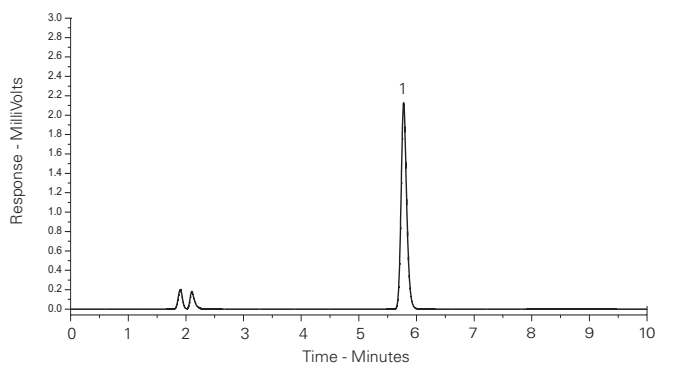
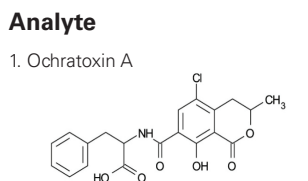


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Ochratoxin A Application #AN2870

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

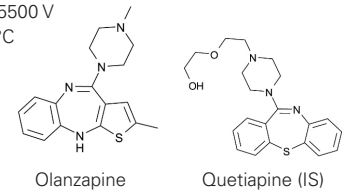


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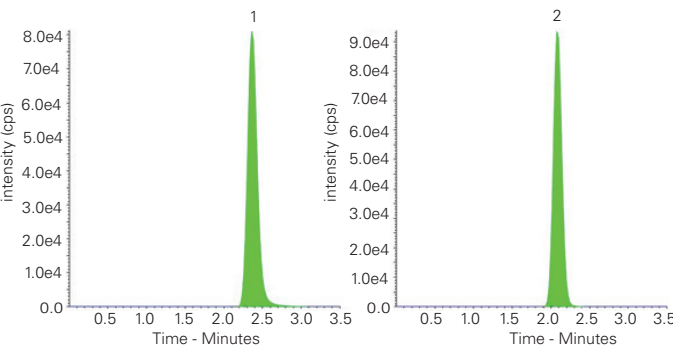
Olanzapine in Human Plasma by LC-MS/MS Application #AN2520

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)



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



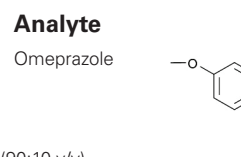
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Omeprazole and Degradation Products after Acidic Hydrolysis in 0.1 M HCl Application #AN1560

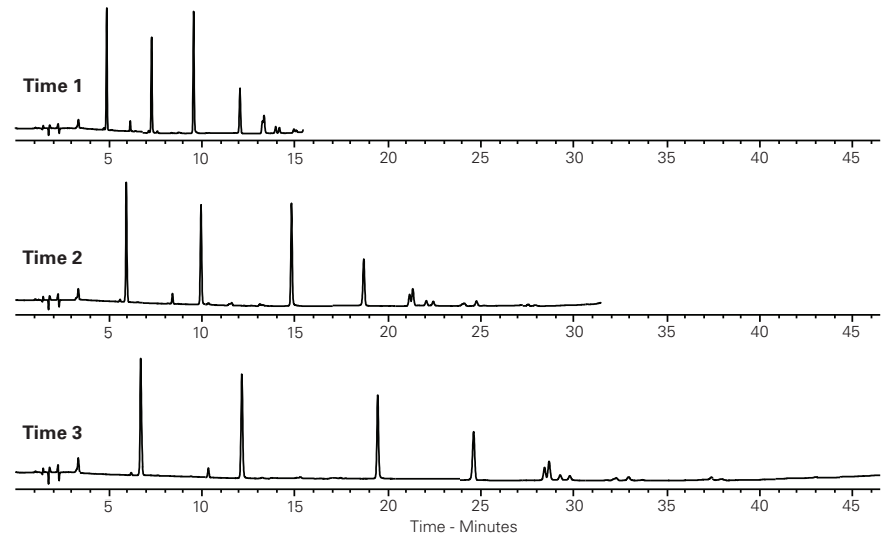
Conditions
Column: ACE Excel 5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: EXL-1211-1546U
Mobile Phase: A: 0.1% ammonia in H₂O
 B: 0.1% ammonia in MeCN/H₂O (90:10 v/v)
Gradient:

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



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 H₂O
 B: 5 mM ammonium acetate in MeOH
Gradient:

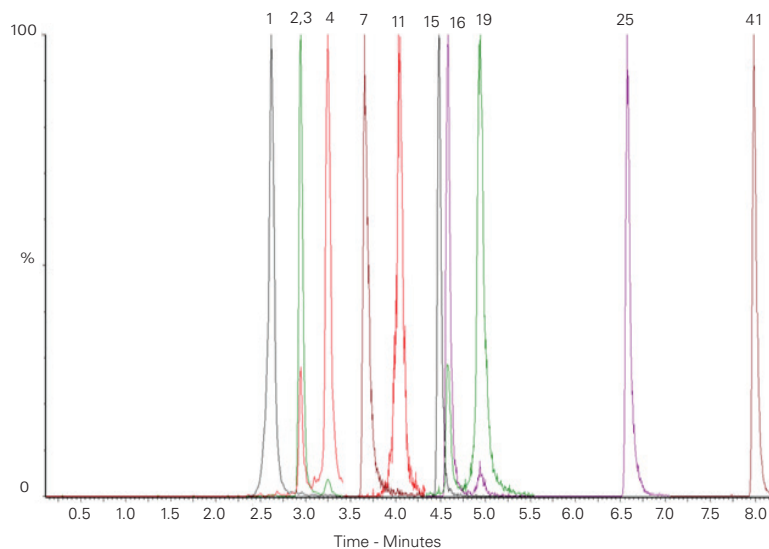
Time (mins)	%B
0.0	10
10.0	90
11.9	90
13.4	10
15.5	10

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



Analytes

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



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Opiates in Urine by LC-MS/MS

Application #AN1230

Conditions

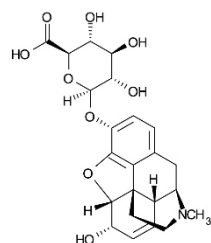
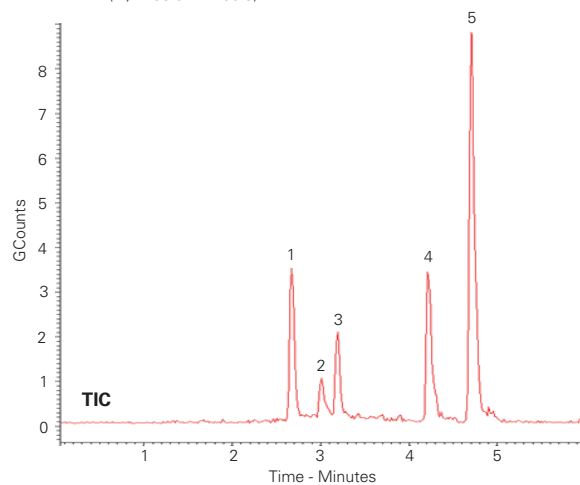
Column: ACE Excel 3 SuperC18
Dimensions: 75 x 2.1 mm
Part Number: EXL-1111-7502U
Mobile Phase: A: 5 mM ammonium hydroxide pH 10.8 in H₂O
 B: 5 mM ammonium hydroxide pH 10.8 in MeOH/H₂O (90:10 v/v)
Gradient:

Time (mins)	%B
0	30
5	95

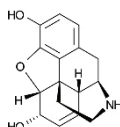
Flow Rate: 0.6 mL/min
Injection: 2 µL
Temperature: 60 °C
Detection: Varian 320 Triple Quadrupole MS
 Electrospray voltage: +5 kV
 Inlet capillary voltage: 30 V
 CID with argon at 1.5 mTorr
 Collision cell potential ranges from 5 to 17 V
 Drying gas (nitrogen) temperature: 325 °C
 Nebulizing gas (nitrogen)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

Analytes

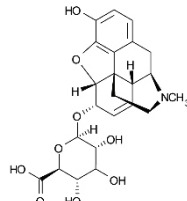
- | | | |
|---|---|--|
| 1. Morphine 3-β-D-glucuronide
LOD (est) 100 ppb
(<i>m/z</i> 462.0 → 285.9) | 3. Morphine 6-β-D-glucuronide
LOD (est) 100 ppb
(<i>m/z</i> 462.0 → 285.9) | 5. 6-Acetylmorphine
LOD (est) 10 ppb
(<i>m/z</i> 328.0 → 164.9) |
| 2. Normorphine
LOD (est) 100 ppb
(<i>m/z</i> 272.0 → 165.0)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



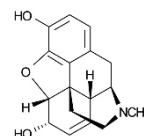
Morphine 3-β-D-glucuronide



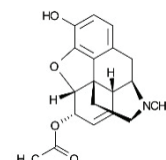
Normorphine



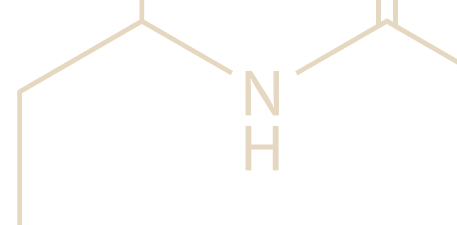
Morphine 6-β-D-glucuronide



Morphine



6-Acetylmorphine



Organic Acids

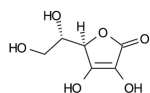
Application #AN2780

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 $\text{H}_2\text{O}/\text{MeOH}$ (70:30 v/v)
Flow Rate: 1 mL/min
Temperature: 22 °C
Detection: UV, 220 nm

Analytes

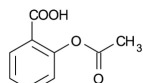
1. L-Ascorbic acid
2. Maleic acid
3. Acetylsalicylic acid
4. Benzoic acid
5. Salicylic acid



L-Ascorbic acid



Maleic acid



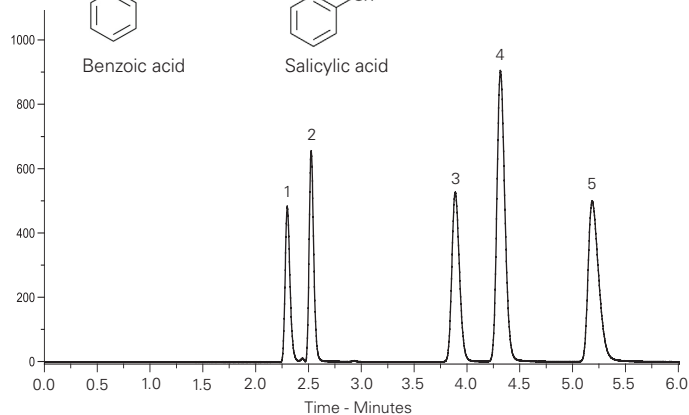
Acetylsalicylic acid



Benzoic acid



Salicylic acid



For further applications

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

Organic Acids – Fast Separation

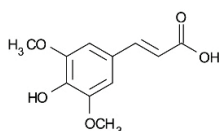
Application #AN2200

Conditions

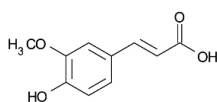
Column: ACE Excel 3 C18-Amide
 ACE Excel 1.7 C18-Amide
Dimensions: 250 x 2.1 mm, 50 x 3.0 mm
Part Number: 250 x 2.1 mm (EXL-1112-2502U),
 50 x 3 mm (EXL-1712-0503U)
Mobile Phase: 20 mM H_3PO_4 in
 $\text{MeOH}/\text{H}_2\text{O}$ (40:60 v/v)
Flow Rate: 0.21 mL/min (250 x 2.1 mm)
 0.8 mL/min (50 x 3.0 mm)
Injection: 5 μL (250 x 2.1 mm)
 2 μL (50 x 3.0 mm)
Temperature: 20 °C
Detection: UV, 210 nm

Analytes

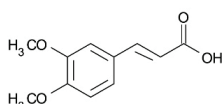
1. Sinapic acid
2. Ferulic acid
3. 3,4-Dimethoxycinnamic acid
4. Cinnamic acid
5. 4-Methoxycinnamic acid



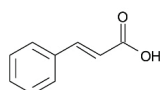
Sinapic acid



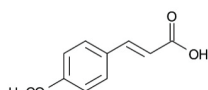
Ferulic acid



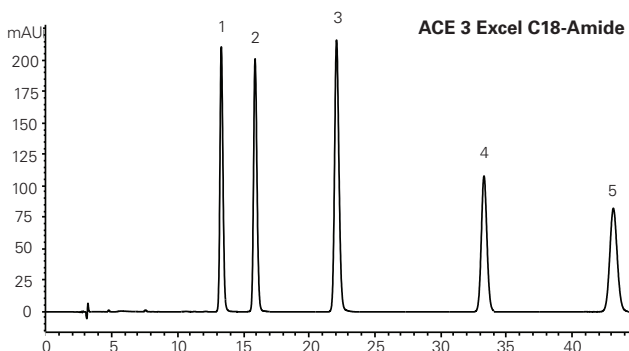
3,4-Dimethoxycinnamic acid



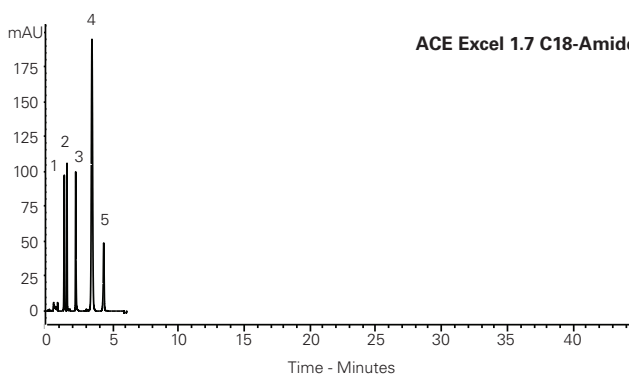
Cinnamic acid



4-Methoxycinnamic acid



ACE 3 Excel C18-Amide



ACE Excel 1.7 C18-Amide

Organophosphorus Flame Retardants in Water by LC-MS/MS

Application #AN1240

Conditions

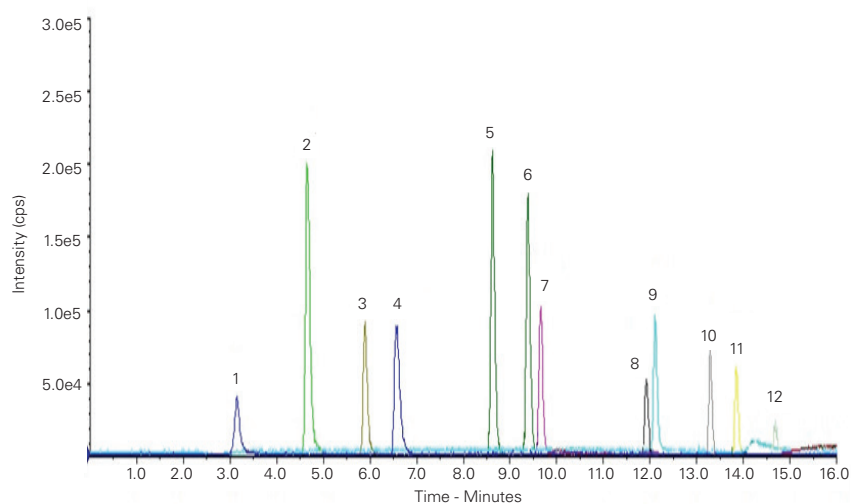
Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002
Mobile Phase: A: 0.05 mM ammonium formate + 0.005% formic acid in H₂O
 B: MeOH/MeCN (95:5 v/v)
Gradient:

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

Analyte	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 (BDPCP)	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

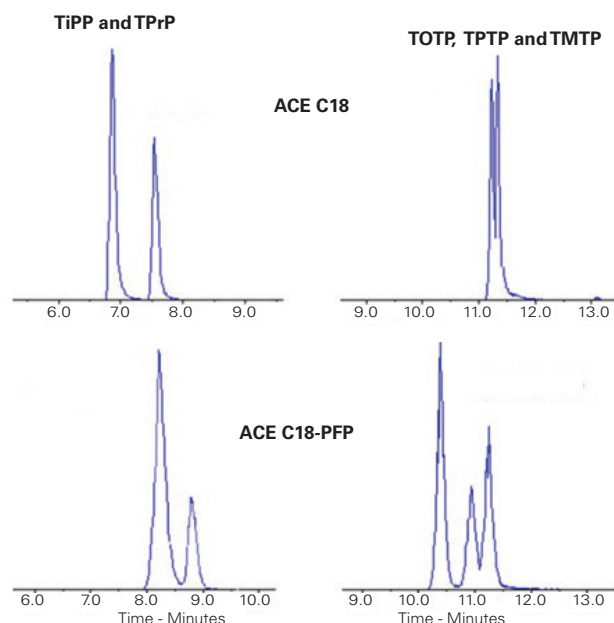
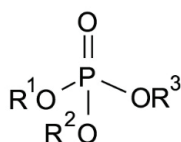
Column: ACE 3 C18
 ACE 3 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002, ACE-1110-1002
Mobile Phase: A: 0.05 mM ammonium formate + 0.005% formic acid in H₂O
 B: MeOH/MeCN (95:5 v/v)
Gradient:

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

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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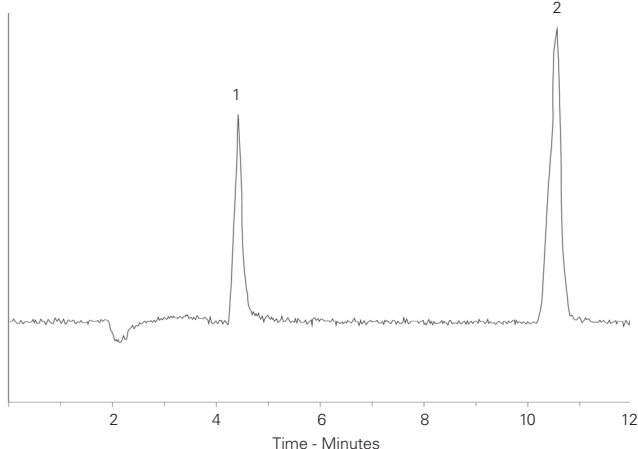
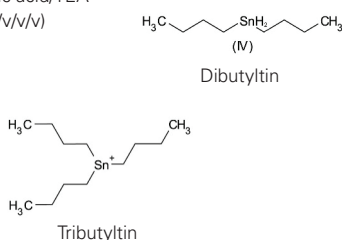
Organotin Compounds Application #AN3650

Conditions

Column: ACE 3 C18
Dimensions: 150 x 2.1 mm
Part Number: ACE-111-1502
Mobile Phase: H₂O/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



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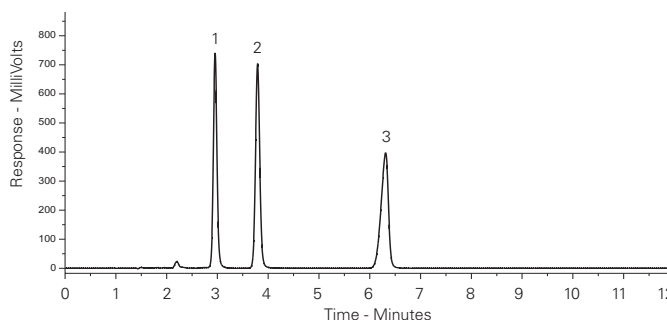
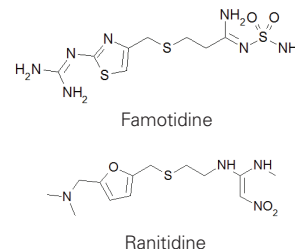
OTC Gastric Drugs Application #AN3940

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 H₂O (18:82)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analytes

1. Famotidine
2. Cimetidine
3. Ranitidine



Oxysterols by LC-MS/MS Application #AN2380

Conditions

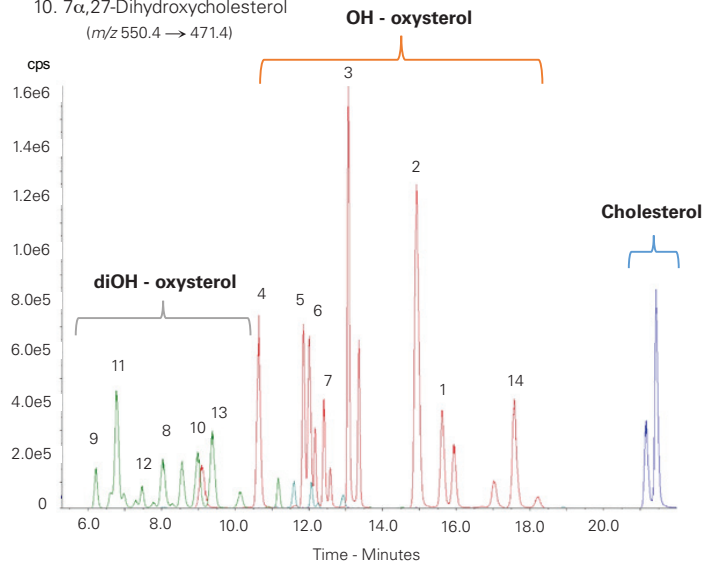
Column: ACE 3 C18-AR
Dimensions: 150 x 2.1 mm
Part Number: ACE-119-1502
Mobile Phase: A: 0.1% formic acid in H₂O/MeOH (70:30 v/v)
 B: 0.1% formic acid in MeOH
Gradient:

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: Derivatized with Girard P reagent

Analytes

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



Reproduced from supplement (pnas.org/content/suppl/2014/08/01/1322807111) to 'Oxysterols are agonist ligands of ROR γ t and drive Th17 cell differentiation', PNAS, 111 (33), 12163-12168 (2014)

Oxymetazoline in Nasal Spray Formulation

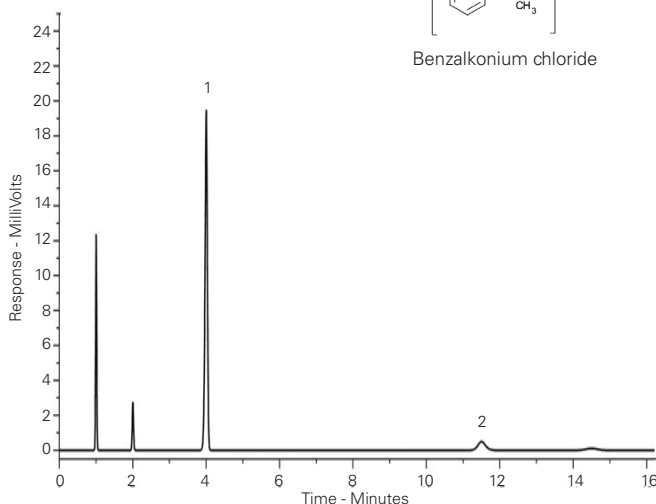
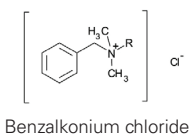
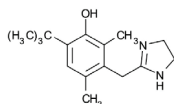
Application #AN3660

Conditions

Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: aq. Na₂HPO₄ 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



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Paclitaxel

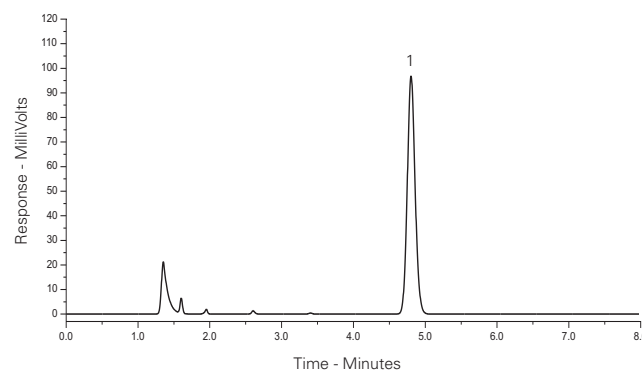
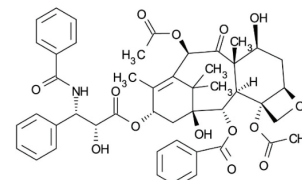
Application #AN3670

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: H₂O/MeCN (45:55 v/v)
Flow Rate: 1 mL/min
Temperature: 40 °C
Detection: UV, 227 nm

Analyte

1. Paclitaxel



Reproduced with permission of Biointeractions Ltd, Reading, UK

Paeonia Lactiflora Extract HPLC Fingerprint

Application #AN3820

Conditions

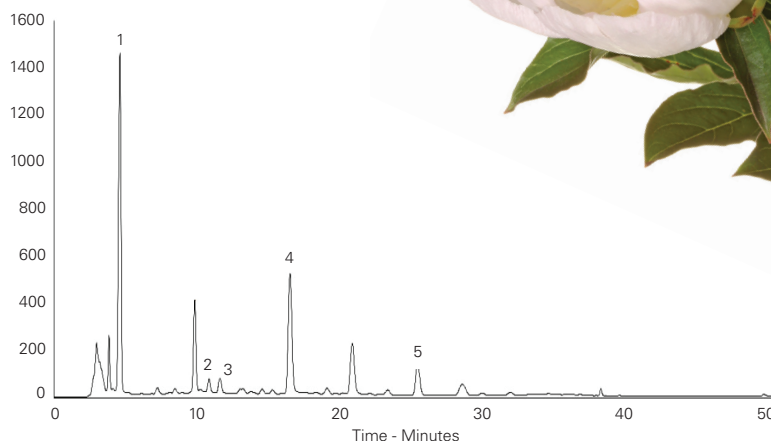
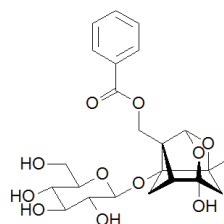
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.1% phosphoric acid in H₂O
 B: MeCN

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



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:10.1371/journal.pone.0148232



Paraben Preservatives

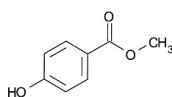
Application #AN1250

Conditions

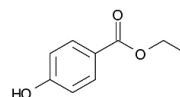
Column: ACE 3 Phenyl
Dimensions: 150 x 2.1 mm
Part Number: ACE-115-1502
Mobile Phase: 25 mM ammonium acetate pH 6.8 in H₂O/MeOH (50:50 v/v)
Flow Rate: 0.2 mL/min
Injection: 2 µL
Temperature: 40 °C
Detection: UV, 240 nm

Analytes

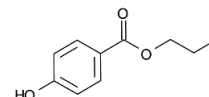
1. Methyl paraben
2. Ethyl paraben
3. n-Propyl paraben
4. i-Butyl paraben
5. n-Butyl paraben
6. Benzyl paraben



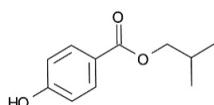
Methyl paraben



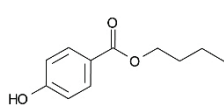
Ethyl paraben



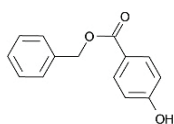
n-Propyl paraben



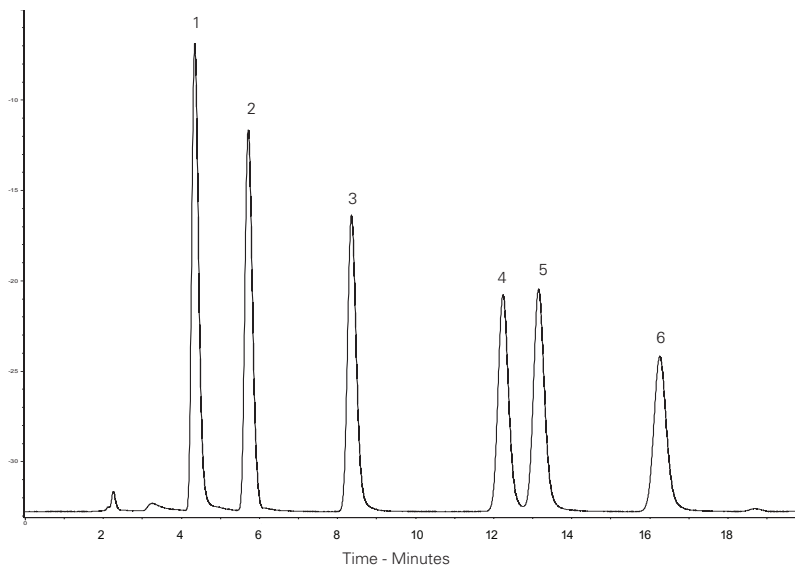
i-Butyl paraben



n-Butyl paraben



Benzyl paraben



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Paracetamol and Related Compounds

Application #AN1260

Conditions

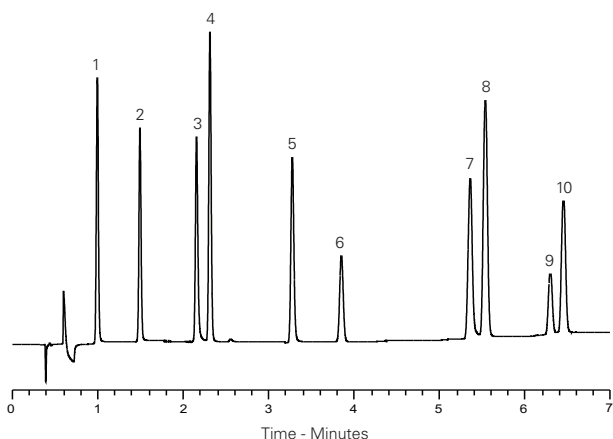
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 3.0 mm
Part Number: EXL-1010-1003U
Mobile Phase: A: 20 mM ammonium acetate pH 6.0 in H₂O
 B: 20 mM ammonium acetate pH 6.0 in MeOH/H₂O (90:10 v/v)
Gradient:

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

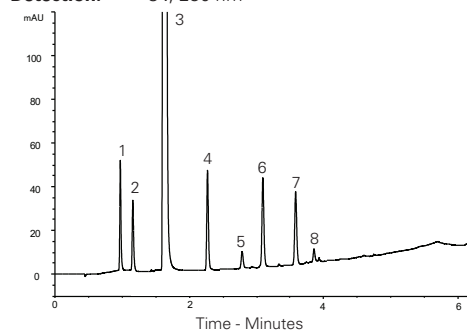
Column: ACE Excel 1.7 C18
Dimensions: 50 x 3.0 mm
Part Number: EXL-171-0503U
Mobile Phase: A: 10 mM ammonium acetate pH 6.0 in H₂O
 B: 10 mM ammonium acetate pH 6.0 in MeOH/H₂O (90:10 v/v)
Gradient:

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

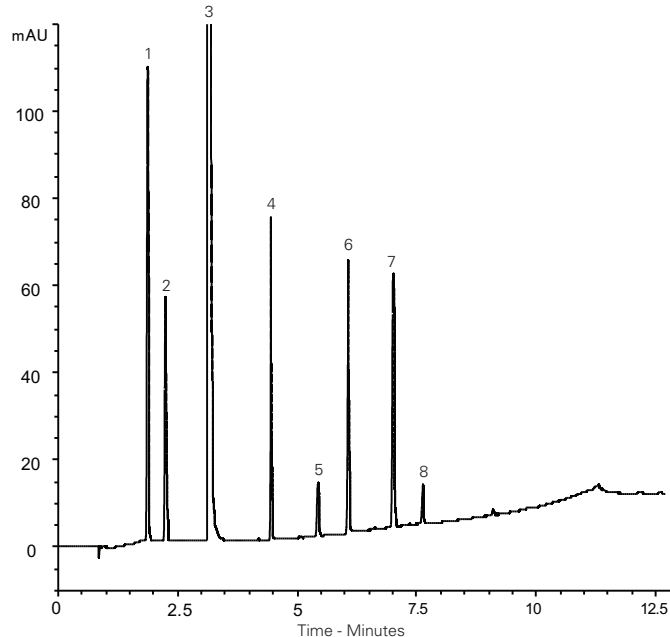
Column: ACE Excel 1.7 C18
Dimensions: 100 x 3.0 mm
Part Number: EXL-171-1003U
Mobile Phase: A: 10 mM ammonium acetate
 pH 6.0 in H₂O
 B: 10 mM ammonium acetate
 pH 6.0 in MeOH/H₂O (90:10 v/v)
Gradient:

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

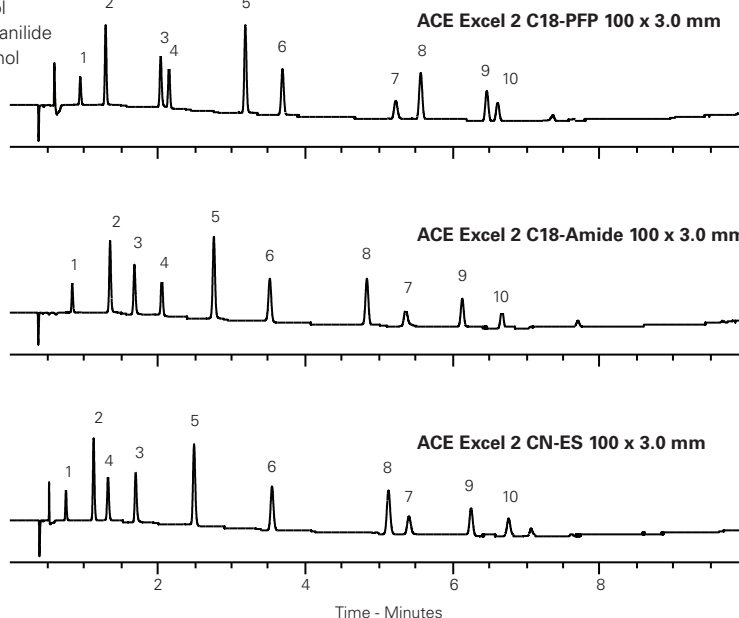
Column: ACE Excel 2 C18-PFP,
 ACE Excel 2 C18-Amide,
 ACE Excel 2 CN-ES
Dimensions: 100 x 3.0 mm
Part Number: EXL-1010-1003U,
 EXL-1012-1003U,
 EXL-1013-1003U
Mobile Phase: A: 20 mM ammonium acetate
 pH 6.0 in H₂O
 B: 20 mM ammonium acetate
 pH 6.0 in MeOH/H₂O (90:10 v/v)
Gradient:

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

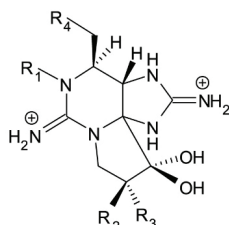
Column: ACE UltraCore 5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: CORE-5A-1546U
Mobile Phase: A: 0.1 M ammonium formate in H₂O
 B: 0.1 M ammonium formate in H₂O/MeOH (95:5 v/v)
Gradient:

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

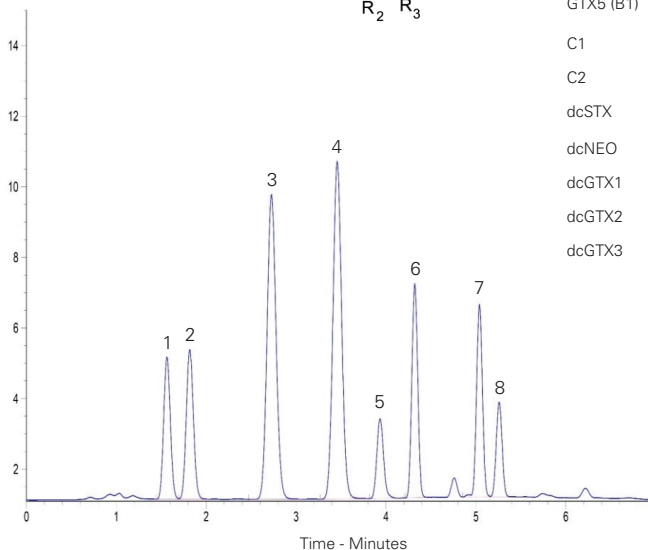
Flow Rate: 2 mL/min
Injection: 30 µL
Temperature: 20 °C
Detection: Fluorescence λ_{Ex} 340 nm, λ_{Em} 395 nm
Sample: Prechromatographic oxidation with hydrogen peroxide and periodate

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 ₂ N-COO
NEO	OH	H	H	H ₂ N-COO
GTX1	OH	H	OSO ₃ ⁻	H ₂ N-COO
GTX2	H	H	OSO ₃ ⁻	H ₂ N-COO
GTX3	H	OSO ₃ ⁻	H	H ₂ N-COO
GTX4	OH	OSO ₃ ⁻	H	H ₂ N-COO
GTX5 (B1)	H	H	H	O ₃ S-NH-COO
C1	H	H	OSO ₃ ⁻	O ₃ S-NH-COO
C2	H	OSO ₃ ⁻	H	O ₃ S-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

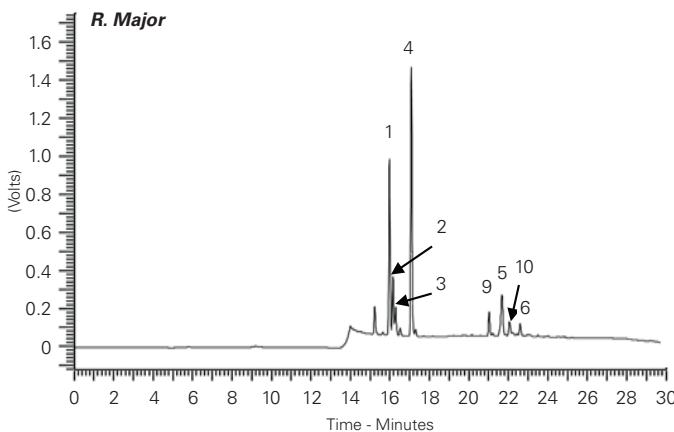
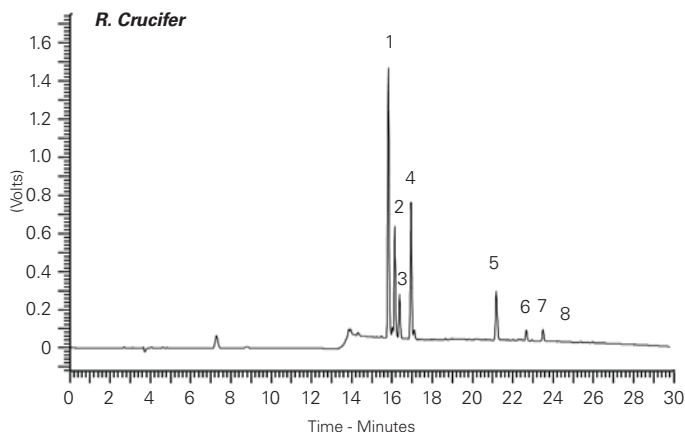
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.1% TFA in H₂O
 B: 0.1% TFA in MeCN/H₂O (90:10 v/v)
Gradient:

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

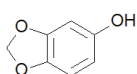
Application #AN3890

Conditions

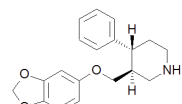
Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: 20 mM ammonium formate
 pH 3.0/MeOH (60:40 v/v)
Flow Rate: 2 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: UV, 295 nm

Analytes

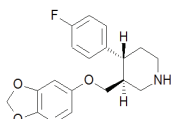
1. Sesamol
2. Desfluoroparoxetine
3. Paroxetine



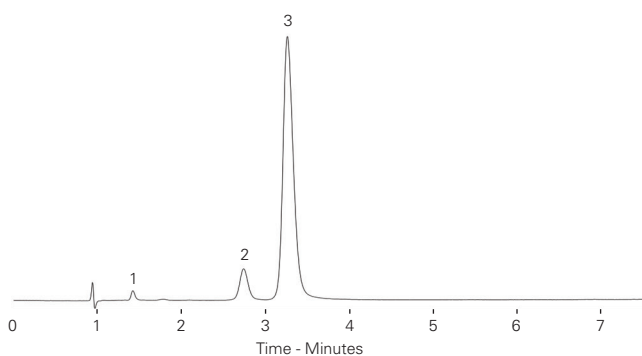
Sesamol



Desfluoroparoxetine



Paroxetine



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Peptide Test Mix

Application #AN3930

Conditions

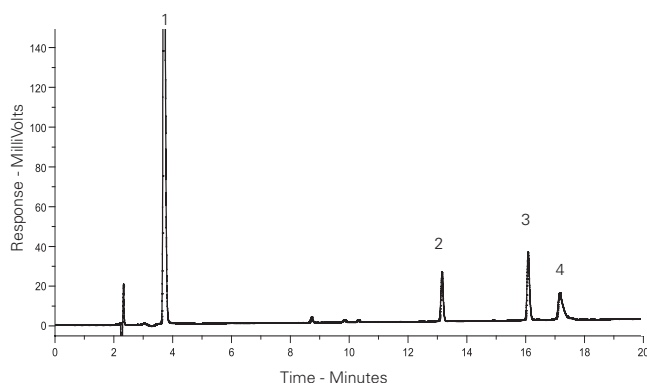
Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 0.1% TFA in H₂O
 B: 0.1% TFA in MeCN
Gradient:

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

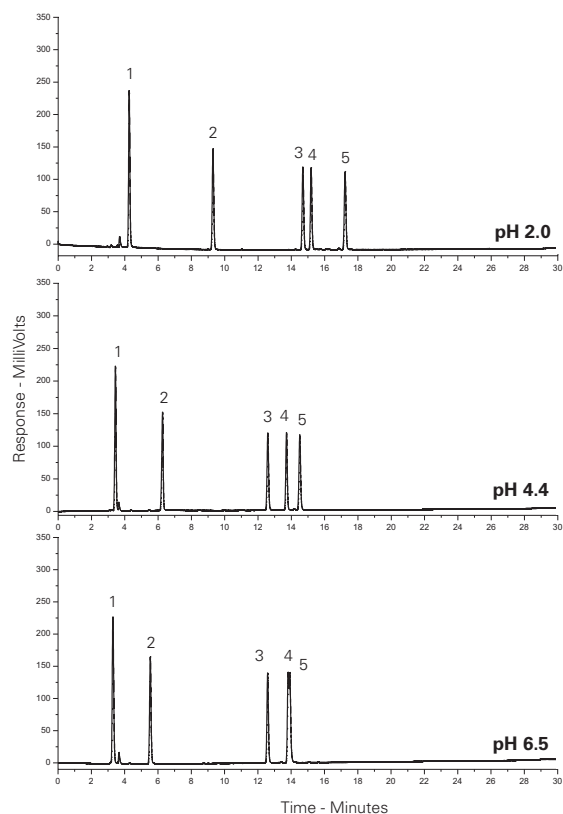
Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 20 mM KH₂PO₄ in
 H₂O (pH as indicated)
 B: MeCN
Gradient:

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 H₂O
B: MeCN

Gradient:

Time (mins)	%B
0.0	10
25.0	40

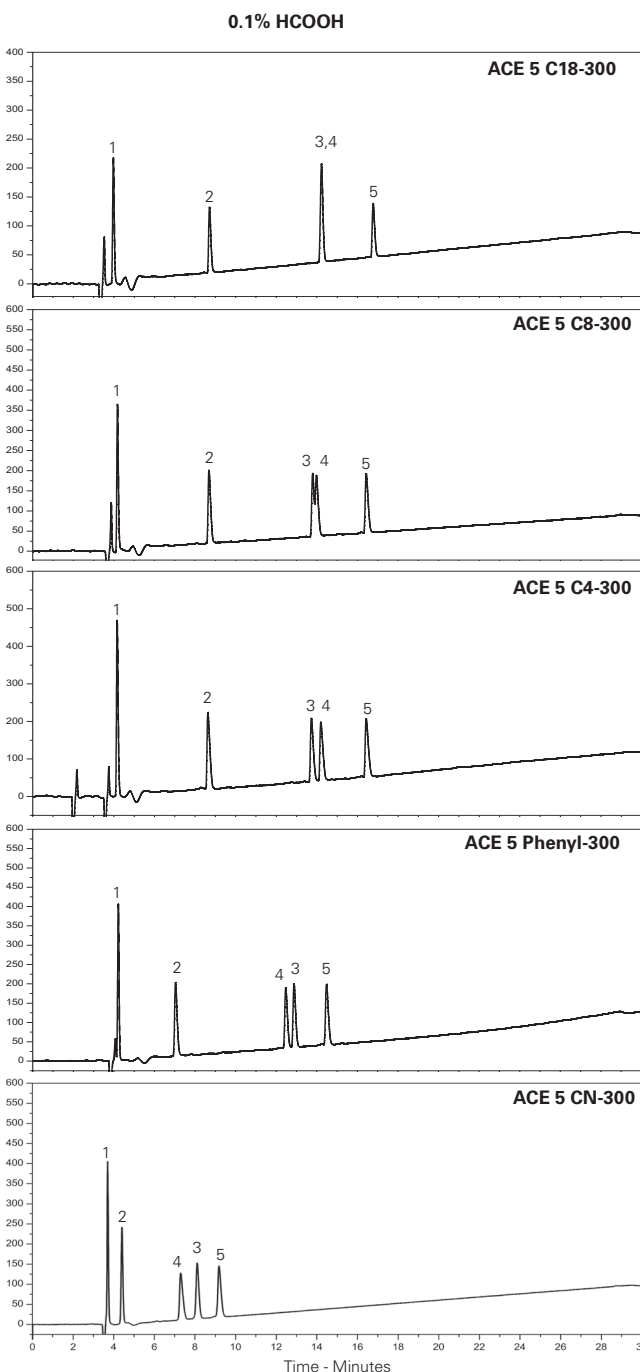
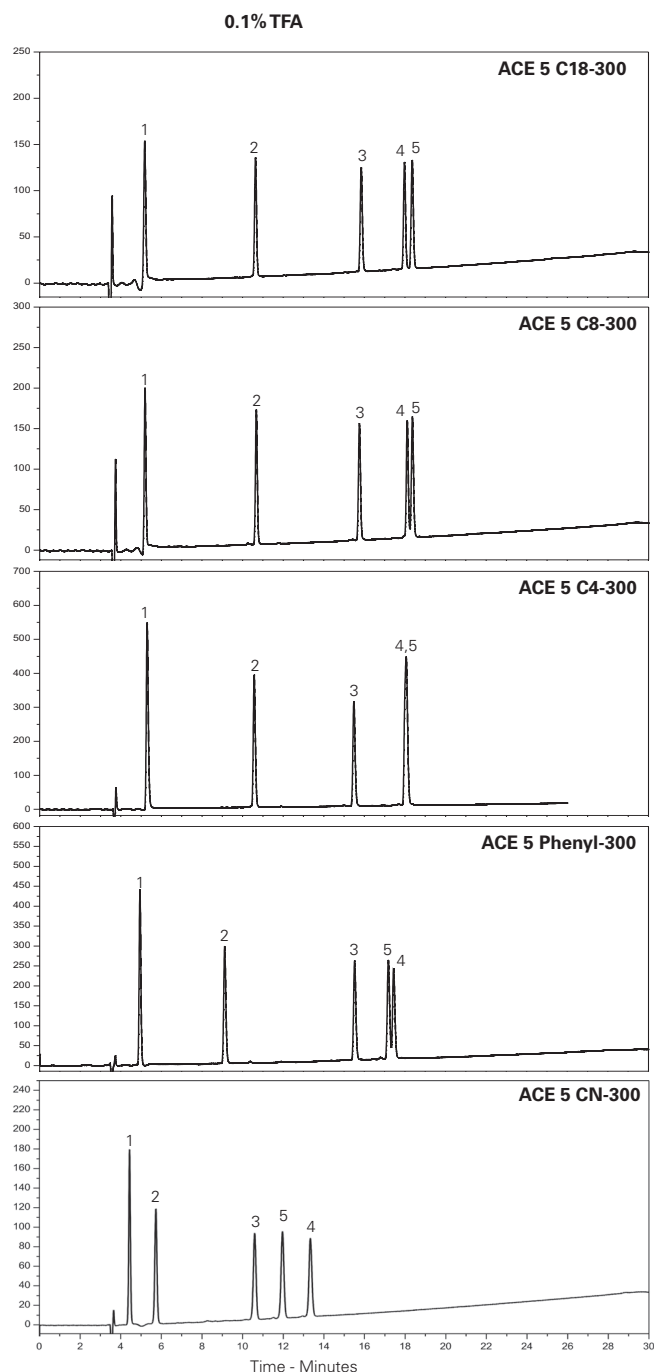
Flow Rate: 1 mL/min

Temperature: Ambient

Detection: UV, 220 nm

Analyses

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

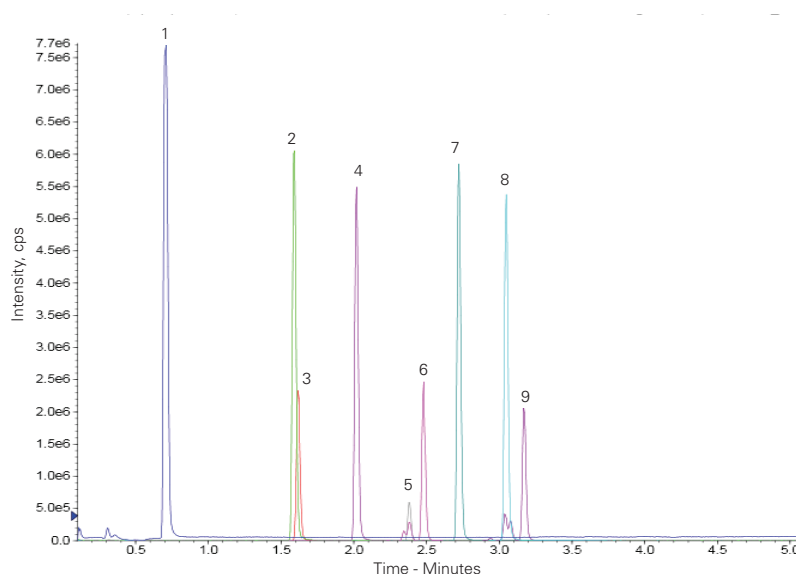
Column: ACE Excel 2 C18
Dimensions: 50 x 2.1 mm
Part Number: EXL-101-0502U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% acetic acid/MeCN (95:5 v/v)
 B: 2 mM ammonium acetate, 0.1% acetic acid/MeCN (5:95 v/v)
Gradient:

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
(<i>m/z</i> 212.9 → 168.9) | 4. Perfluoroheptanoic acid
(<i>m/z</i> 363 → 319) | 7. Perfluorononanoic acid
(<i>m/z</i> 463 → 419) |
| 2. Perfluorohexanoic acid
(<i>m/z</i> 313 → 268.9) | 5. Perfluorooctanoic acid
(<i>m/z</i> 413 → 368.9) | 8. Perfluorodecanoic acid
(<i>m/z</i> 513 → 469) |
| 3. Perfluorobutanesulfonic acid
(<i>m/z</i> 299 → 79.9) | 6. Perfluorohexanesulfonic acid
(<i>m/z</i> 399 → 80) | 9. Perfluorooctanesulfonic acid
(<i>m/z</i> 499 → 80) |



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Perfluoroalkyl Substances by Ion-Pairing LC-MS/MS

Application #AN2560

Conditions

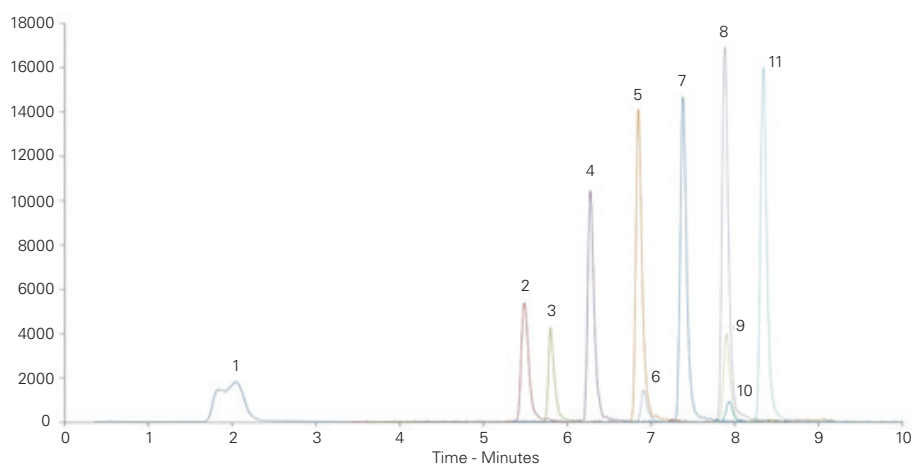
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
Mobile Phase: A: 2 mM ammonium acetate + 5 mM 1-methylpiperidine in MeOH/H₂O (5:95 v/v)
 B: 2 mM ammonium acetate + 5 mM 1-methylpiperidine in MeOH/H₂O (95:5 v/v)
Gradient:

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



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Perfluorinated Compounds in Water by LC-MS/MS

Application #AN2260

Conditions

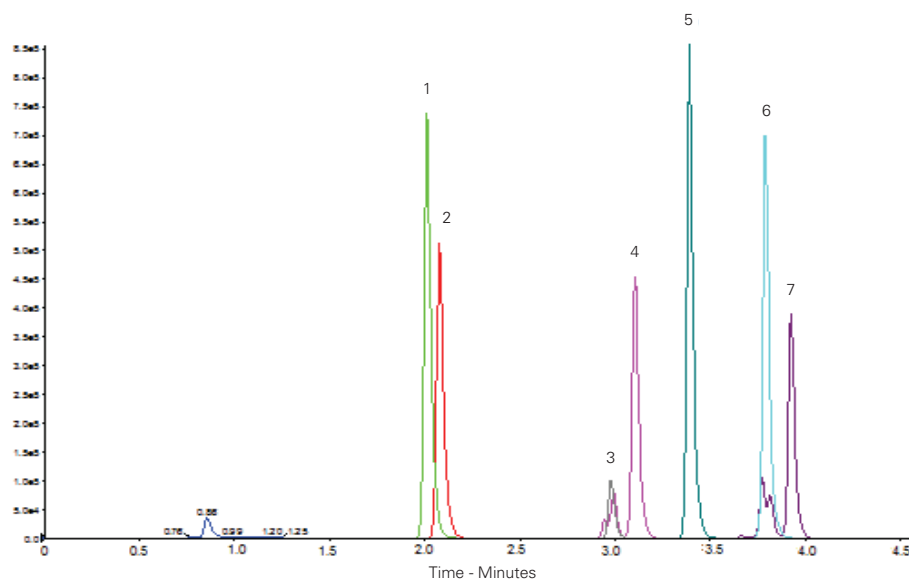
Column: ACE Excel 1.7 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-171-1002U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% formic acid in H₂O/MeCN (90:10 v/v)
 B: 2 mM ammonium acetate, 0.1% formic acid in H₂O/MeCN (10:90 v/v)
Gradient:

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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ACE Method Development Kits

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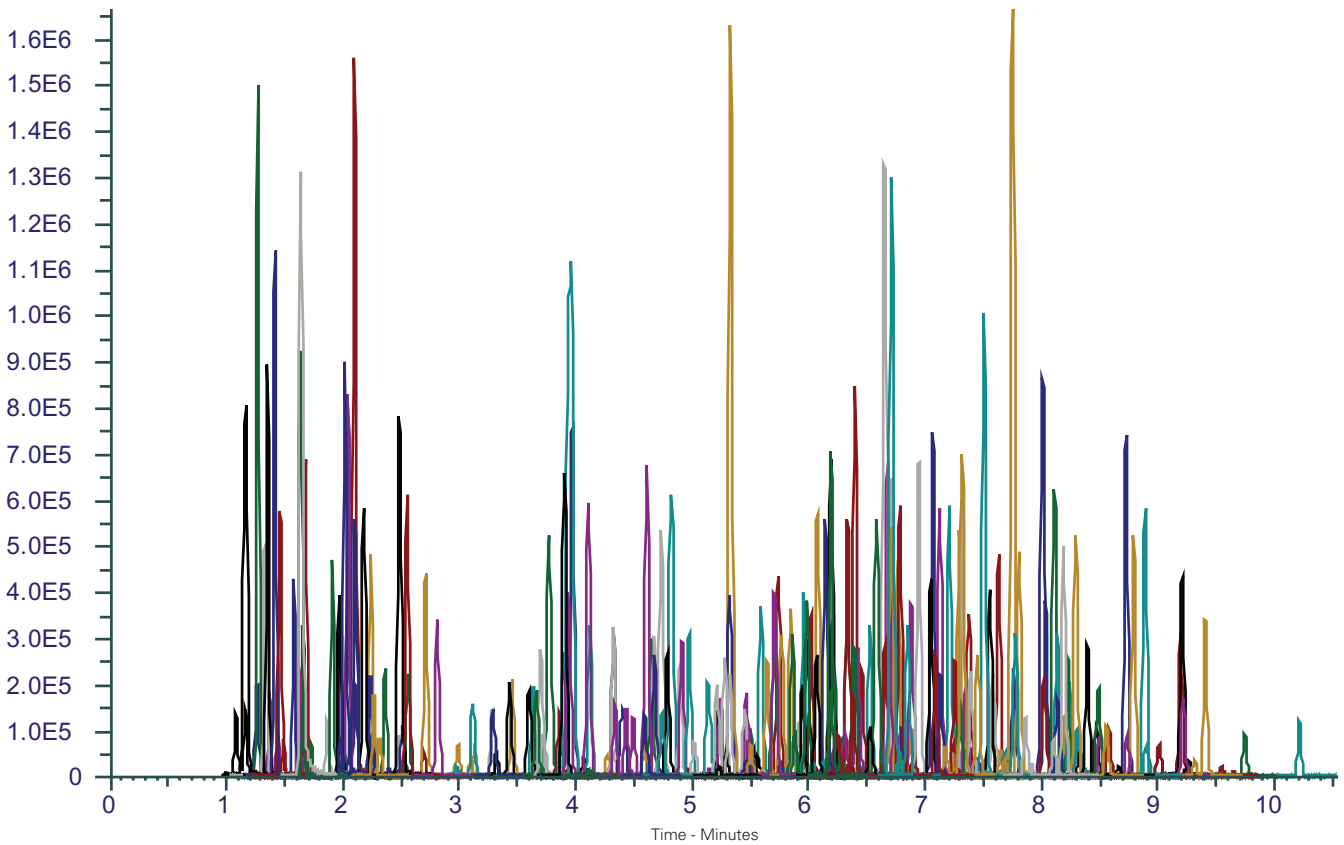
250 Pesticide Screen by LC-MS/MS

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 H₂O
 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

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Application #AN3060

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





250 Pesticide Screen by LC-MS/MS Page 3 of 4
Application #AN3060

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



250 Pesticide Screen by LC-MS/MS

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Application #AN3060

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

300 Pesticide Screen by LC-MS/MS

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Application #AN3120

Conditions

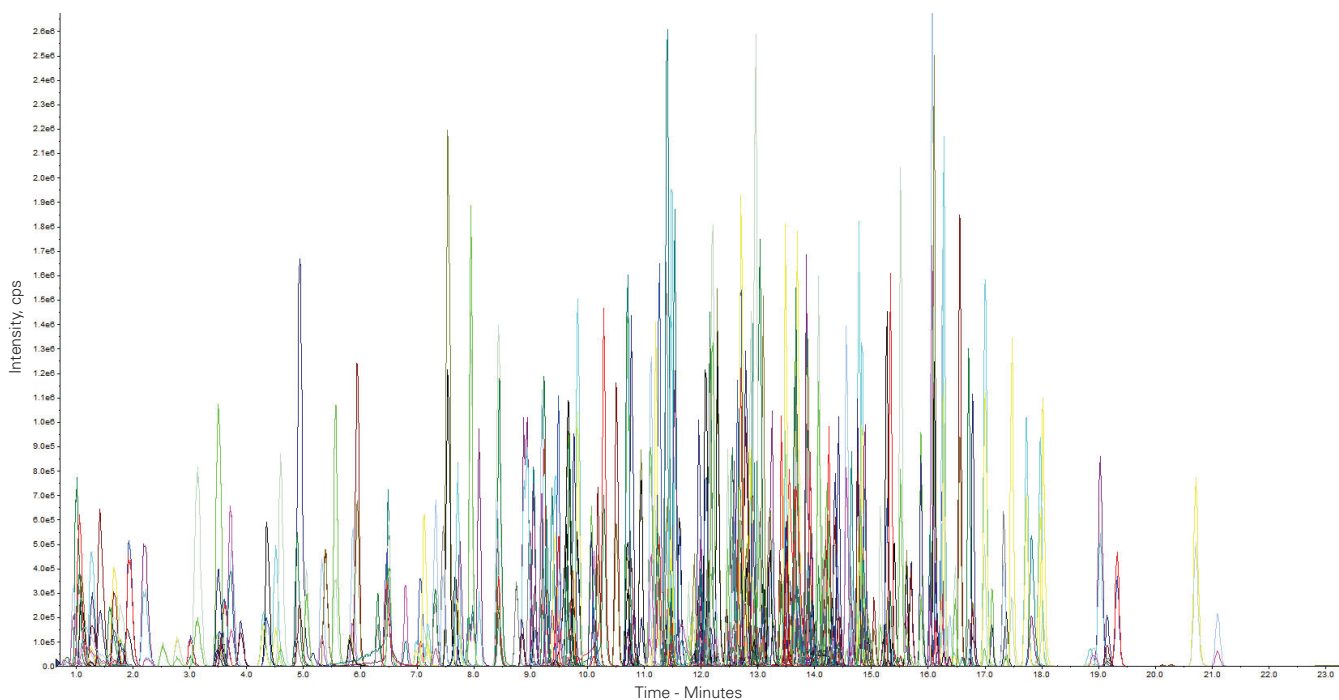
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 2.1 mm
Part Number: CORE-25A-1002U
Mobile Phase: A: 5 mM ammonium formate in H₂O/MeOH (9:1 v/v)
 B: 5 mM ammonium formate in H₂O/MeOH (1:9 v/v)

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

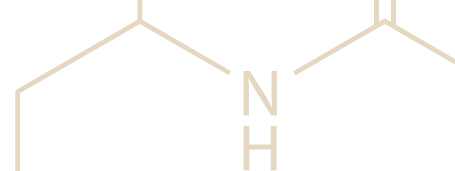
Flow Rate: 0.3 mL/min**Injection:** 6 µL**Temperature:** 24 °C

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

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Application #AN3120

Analyte	Retention Time (mins)	MRM transitions (m/z)	Analyte	Retention Time (mins)	MRM transitions (m/z)
3-Hydroxycarbofuran	3.5	238.1 → 163.1, 238.1 → 181.1	Chlorpyrifos-methyl	15.2	322.0 → 124.9, 324.0 → 125.1
Acephate	1.0	184.1 → 142.9, 184.1 → 124.8	Chlortoluron	9.1	213.2 → 72.0, 215.1 → 72.1
Acetamiprid	3.6	223.2 → 126.1, 225.2 → 128.1	Cinidon-ethyl	16.3	394.0 → 348.0, 394.0 → 366.0
Aclonifen	13.9	265.0 → 248.0, 267.0 → 250.0	Clethodim A	12.8	360.1 → 164.1, 360.1 → 268.1
Alachlor	12.9	270.2 → 238.2, 270.2 → 162.1	Clethodim B	10.2	360.1 → 164.1, 360.1 → 268.1
Aldicarb	5.4	208.0 → 89.0, 208.0 → 116.0	Clofentezine	15.1	303.1 → 137.9, 305.1 → 102.0
Aldicarb sulfone	1.2	240.0 → 86.0, 223.0 → 148.0	Clomazone	10.7	240.1 → 124.9, 242.2 → 127.1
Aldicarb sulfoxide	1.1	207.0 → 132.0, 207.2 → 88.9	Cloquintocet-mexyl	16.1	336.2 → 238.0, 336.2 → 192.1
Ametryn	11.1	228.2 → 186.1, 228.2 → 68.0	Clothianidin	2.9	250.1 → 169.0, 250.1 → 132.0
Aminopyralid	0.8	207.0 → 160.9, 207.0 → 133.9	Coumaphos	14.3	363.0 → 227.0, 363.0 → 211.1
Amitrole	0.8	85.1 → 58.1, 85.1 → 57.1	Cyanazine	6.7	241.1 → 214.1, 243.1 → 216.1
Atrazine	9.3	216.2 → 174.0, 218.1 → 176.1	Cyazofamid	13.2	325.2 → 107.9, 327.2 → 107.9
Atrazine-desethyl	4.4	188.2 → 146.0, 190.1 → 148.0	Cycloate	14.9	216.2 → 83.1, 216.2 → 154.1
Atrazine-desisopropyl	2.4	174.1 → 104.1, 174.1 → 132.1	Cycloxydim A	13.1	326.3 → 280.0, 326.3 → 180.0
Avermectin B1a	18.2	876.5 → 553.0, 876.5 → 291.0	Cycloxydim B	8.4	326.3 → 280.0, 326.3 → 180.0
Avermectin B1b	19.1	890.5 → 305.0, 890.5 → 567.0	Cymoxanil	4.2	199.2 → 128.0, 199.2 → 111.1
Azamethiphos	6.9	325.0 → 183.0, 325.0 → 138.9	Cyproconazole A	12.5	292.0 → 70.0, 292.0 → 125.0
Azinphos-ethyl	13.0	346.0 → 132.1, 346.0 → 160.1	Cyproconazole B	12.0	292.0 → 70.0, 292.0 → 125.0
Azinphos-methyl	10.9	318.1 → 132.1, 318.1 → 260.8	Cyprodinil A	14.1	226.2 → 93.0, 226.2 → 77.0
Aziprotryne	11.8	226.0 → 156.0, 226.0 → 125.0	Demeton-S-methyl	7.7	231.1 → 88.8, 231.1 → 61.0
Azoxystrobin	11.4	404.2 → 372.3, 404.2 → 344.1	Demeton-S-methyl sulfone	1.6	263.0 → 168.9, 263.0 → 120.8
Benalaxyl	14.0	326.2 → 148.1, 326.2 → 294.1	Desmedipham	10.6	318.1 → 182.1, 318.1 → 136.0
Benfuracarb	15.7	411.2 → 252.1, 411.2 → 195.1	Desmethyl-pirimicarb	5.8	225.2 → 72.0, 225.2 → 168.1
Benthiavalicarb-isopropyl	12.0	382.3 → 116.0, 382.3 → 197.0	Diafenthiuron	17.4	385.2 → 329.2, 385.2 → 278.2
Bifenazate	12.5	301.2 → 198.1, 301.2 → 170.2	Diazinon	14.2	305.1 → 169.1, 305.1 → 97.0
Bifenox	14.9	359.0 → 342.0, 359.0 → 310.0	Dichlofluanid	12.8	333.0 → 223.9, 333.0 → 122.9
Bifenthrin	21.0	440.0 → 181.1, 440.0 → 166.1	Diclobutrazol A	13.7	328.0 → 70.0, 330.0 → 70.0
Bitertanol	14.6	338.2 → 269.0, 338.2 → 99.1	Dicrotofos	2.1	238.1 → 112.1, 238.1 → 193.1
Bixafen	13.6	414.0 → 393.9, 416.1 → 395.9	Diethofencarb	11.1	268.1 → 226.1, 268.1 → 124.0
Boscalid	11.7	343.1 → 306.8, 343.1 → 139.9	Difenoconazole	14.8	406.1 → 251.1, 408.2 → 253.1
Bromfeninfos-ethyl	14.3	405.0 → 155.0, 403.0 → 155.0	Diflubenzuron	13.5	311.0 → 158.2, 311.0 → 141.1
Bromuconazole A	12.2	378.0 → 159.1, 378.0 → 161.0	Diflufenican	15.4	395.0 → 266.0, 395.0 → 246.0
Bromuconazole B	13.5	378.1 → 159.1, 378.1 → 161.0	Dimethachlor	10.2	256.2 → 224.0, 256.2 → 148.1
Bupirimate	13.5	317.2 → 166.2, 317.2 → 107.9	Dimethenamid	11.3	276.1 → 244.0, 278.1 → 246.0
Buprofezin	16.1	306.3 → 201.1, 306.3 → 116.1	Dimethoate	3.6	230.1 → 198.8, 230.1 → 124.9
Cadusafos	14.8	271.1 → 158.9, 271.1 → 214.9	Dimethomorph	11.7	388.1 → 301.0, 388.1 → 165.1
Carbaryl	8.3	202.2 → 145.1, 202.2 → 127.1	Dimoxystrobin	13.7	327.1 → 205.0, 327.1 → 116.0
Carbendazim	4.7	192.2 → 160.1, 192.0 → 132.0	Diniconazole	14.8	326.0 → 70.0, 328.0 → 70.0
Carbofuran	7.4	222.2 → 165.1, 222.2 → 122.9	Disulfoton	15.0	275.1 → 89.0, 275.1 → 61.0
Carbosulfan	19.3	381.2 → 160.1, 381.2 → 118.1	Disulfoton sulfone	9.6	307.1 → 153.0, 307.1 → 171.0
Carboxin	8.3	236.1 → 143.1, 236.1 → 87.0	Disulfoton sulfoxide	9.2	291.1 → 212.9, 291.1 → 185.0
Carfentrazone-ethyl	13.8	412.2 → 345.9, 412.2 → 383.9	Ditalimfos	13.1	300.1 → 148.0, 300.1 → 130.0
Chlorantraniliprole	10.7	484.0 → 452.9, 484.0 → 285.9	Diuron	10.0	233.1 → 71.9, 235.1 → 72.0
Chlorbromuron	11.7	295.1 → 205.9, 293.1 → 182.0	DMST	8.0	215.2 → 106.0, 215.2 → 78.9
Chlorfeninfos A	14.3	359.0 → 155.0, 358.9 → 99.0	Dodine	13.6	228.3 → 57.0, 228.3 → 60.1
Chloridazon	3.7	222.1 → 104.0, 222.1 → 77.1	Epoxiconazole	12.9	330.1 → 120.9, 330.1 → 75.2
Chlorpyrifos	16.8	349.9 → 198.1, 349.9 → 115.0	Ethion	16.5	385.0 → 199.0, 385.0 → 143.0





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Analyte	Retention Time (mins)	MRM transitions (m/z)	Analyte	Retention Time (mins)	MRM transitions (m/z)
Ethirimol	9.7	210.3 → 140.1, 210.3 → 98.0	Furathiocarb	15.9	383.1 → 195.0, 383.1 → 252.1
Ethofumesate	11.3	287.1 → 121.0, 287.1 → 259.0	Heptenofos	10.1	251.0 → 127.0, 251.0 → 124.8
Ethoprophos	12.7	243.0 → 131.0, 243.0 → 97.0	Hexaconazole	14.3	314.0 → 70.0, 316.0 → 70.0
Ethoxyquin A	12.9	218.2 → 148.0, 218.2 → 174.1	Hexaflumuron	15.5	461.1 → 158.2, 461.1 → 141.1
Ethoxyquin B	10.7	218.2 → 148.0, 218.2 → 174.1	Hexazinone	7.3	253.2 → 71.0, 253.2 → 85.0
Etofenprox	20.6	394.0 → 177.0, 394.0 → 359.0	Hexythiazox	16.6	353.0 → 168.0, 353.0 → 228.0
Etrimfos	14.2	293.1 → 125.0, 293.1 → 265.1	Imazalil	13.6	297.2 → 159.1, 299.1 → 160.9
Famoxadone NH4+	14.4	392.0 → 331.0, 392.0 → 238.0	Imidacloprid	2.7	256.1 → 209.0, 256.1 → 175.0
Fenamidone	11.5	312.1 → 92.1, 312.1 → 236.1	Indoxacarb	15.2	528.1 → 248.9, 528.1 → 292.9
Fenamifos	13.4	304.0 → 217.0, 304.0 → 202.0	Ipconazole	15.3	334.2 → 70.0, 334.2 → 125.0
Fenamifos sulfone	8.4	336.0 → 308.0, 336.0 → 266.0	Iprodione	13.3	332.1 → 246.9, 330.0 → 245.0
Fenamifos sulfoxide	7.9	320.0 → 171.0, 320.0 → 233.0	Iprovalicarb	12.6	321.3 → 119.0, 321.3 → 203.1
Fenarimol	12.7	331.2 → 268.0, 331.2 → 139.0	Isofenfos	14.7	346.1 → 245.1, 346.1 → 217.1
Fenazaquin	18.0	307.1 → 161.1, 307.1 → 147.0	Isofenfos-methyl	13.8	332.1 → 231.0, 332.1 → 273.0
Fenbuconazole	13.2	337.0 → 124.9, 337.0 → 70.0	Isoprocarb	9.4	194.1 → 95.0, 194.1 → 137.0
Fenbutatin oxide	22.9	519.3 → 463.3, 519.3 → 197.0	Isoprothiolane	12.1	291.1 → 231.0, 291.1 → 189.0
Fenhexamid	12.6	302.2 → 96.9, 304.2 → 97.0	Isoproturon	9.7	207.2 → 72.0, 207.2 → 165.2
Fenoxycarb	13.6	302.2 → 87.9, 302.2 → 116.0	Isoxadifen-ethyl	13.9	313.2 → 296.1, 313.2 → 263.0
Fenpropathrin	17.3	367.0 → 125.0, 350.0 → 125.0	Isoxaflutole	10.0	360.1 → 251.1, 377.0 → 251.0
Fenpropidin	10.8	274.0 → 147.0, 274.0 → 117.0	Kresoxim-methyl	13.9	314.0 → 116.0, 314.0 → 131.1
Fenpropimorph	18.7	304.0 → 147.0, 304.0 → 117.0	Lenacil	9.5	235.3 → 153.2, 235.3 → 136.2
Fenpyroximate	17.4	422.2 → 366.1, 422.2 → 135.1	Linuron 	11.3	249.0 → 159.9, 249.0 → 182.0
Fensulfothion	10.0	309.1 → 280.8, 309.1 → 252.9	Lufenuron	16.4	511.0 → 158.0, 511.0 → 141.0
Fensulfothion sulfone	10.4	325.1 → 268.9, 325.1 → 297.0	Malaoxon	7.9	315.1 → 99.1, 315.1 → 127.1
Fenthion sulfone	9.0	311.1 → 125.0, 311.1 → 278.8	Mandipropamid	11.9	412.1 → 328.1, 412.2 → 125.0
Fenthion sulfoxide	8.4	295.1 → 279.7, 295.1 → 108.9	Mecarbam	13.0	330.1 → 227.0, 330.1 → 198.9
Flonicamid	1.7	230.0 → 203.0, 230.0 → 148.0	Mepanipyrim	12.9	224.2 → 106.0, 224.2 → 77.1
Flubendiamide NH4+	13.8	700.0 → 407.9, 682.9 → 407.9	Mepronil	12.1	270.1 → 119.0, 270.1 → 228.1
Fludioxonil NH4+	11.8	266.0 → 229.0, 266.0 → 227.1	Mesotrione	1.2	340.0 → 228.0, 357.1 → 227.9
Flufenacet	12.8	364.1 → 194.1, 364.1 → 152.2	Metaflumizone	16.1	507.1 → 178.1, 507.1 → 287.1
Flufenoxuron	17.1	489.0 → 158.0, 489.0 → 141.1	Metalaxyl	9.8	280.1 → 220.2, 280.1 → 192.2
Flumethrin NH4+	20.2	527.2 → 510.0, 527.2 → 267.0	Metamitron	3.4	203.1 → 175.0, 203.1 → 104.2
Flumetsulam	2.0	326.2 → 128.8, 326.2 → 128.3	Metazachlor	9.6	278.1 → 209.9, 278.1 → 134.2
Flumioxazin	10.7	355.0 → 327.0, 355.0 → 299.0	Metconazole	14.4	320.1 → 70.0, 320.1 → 125.0
Fluometuron	8.9	233.0 → 72.0, 233.0 → 160.0	Methacrifos	10.7	241.0 → 208.9, 241.0 → 124.9
Fluopicolide	11.9	383.0 → 173.0, 385.1 → 174.9	Methamidofos	0.9	142.0 → 93.9, 142.0 → 112.1
Fluopiram	12.5	397.0 → 173.0, 397.0 → 208.0	Methiocarb	11.4	226.2 → 169.1, 226.2 → 121.2
Fluoxastrobin	12.8	459.1 → 427.1, 459.1 → 188.1	Methiocarb sulfone	4.1	258.1 → 122.0, 258.1 → 200.9
Fluquinconazole	12.6	376.1 → 307.1, 376.1 → 349.1	Methiocarb sulfoxide	3.0	242.1 → 185.0, 242.1 → 122.1
Flusilazole	13.3	316.2 → 247.0, 316.2 → 165.1	Methomyl	1.6	163.0 → 106.0, 163.0 → 88.0
Flutolanil	12.0	324.0 → 262.0, 324.0 → 242.0	Methoxyfenozide	12.2	369.1 → 149.1, 369.1 → 313.2
Flutriafol	9.7	302.1 → 70.1, 302.1 → 123.0	Metobromuron	9.4	259.0 → 170.0, 259.0 → 148.1
Fomesafen (NH4-Adduct)	11.3	456.1 → 344.0, 458.1 → 346.0	Metolachlor	13.0	284.1 → 252.0, 286.1 → 254.0
Fonofos	14.3	247.0 → 109.0, 247.0 → 127.0	Metoxuron	5.7	229.1 → 72.0, 231.1 → 71.9
Fosthiazate	8.9	284.1 → 227.9, 284.1 → 104.0	Metrafenone	14.8	409.2 → 209.1, 411.2 → 209.1
Fuberidazole	6.9	185.0 → 157.0, 185.0 → 65.0	Metribuzin	7.1	215.2 → 187.1, 215.2 → 84.1



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Application #AN3120

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 NH ₄ ⁺	1.2	237.1 → 72.0, 220.2 → 72.0
Oxycarboxin	4.5	268.1 → 174.9, 268.1 → 147.0
Oxydemeton-methyl	1.4	247.0 → 108.9, 247.0 → 168.9
Paclobutrazol	11.8	294.0 → 70.0, 294.0 → 125.0
Paraoxon	9.4	275.9 → 219.9, 275.9 → 248.0
Paraoxon-methyl	6.1	248.1 → 202.1, 248.1 → 90.0
Parathion	13.8	292.0 → 236.0, 292.0 → 264.1
Penconazole	13.7	248.1 → 70.0, 284.1 → 159.0
Pencycuron	14.8	329.3 → 125.1, 331.3 → 127.0
Pendimethalin	16.9	282.2 → 212.1, 282.2 → 194.1
Pethoxamid	12.7	296.2 → 131.0, 296.2 → 250.0
Phenmedipham	10.8	301.2 → 168.0, 301.2 → 136.0
Phenthoate	13.9	321.0 → 247.0, 321.0 → 275.1
Phorate sulfone	9.6	293.0 → 170.8, 293.0 → 96.7
Phorate sulfoxide	9.2	277.0 → 199.0, 277.0 → 171.0
Phosalone	14.6	368.0 → 182.0, 369.9 → 183.9
Phosphamidon	6.4	300.2 → 127.1, 300.2 → 226.8
Phoxim	14.7	299.2 → 129.2, 299.2 → 77.1
Picloram	1.2	243.0 → 224.9, 241.0 → 222.9
Picolinafen	16.2	377.1 → 238.0, 377.1 → 359.0
Picoxystrobin	13.6	368.0 → 205.0, 368.0 → 145.0
Piperonyl butoxide	16.2	356.2 → 177.2, 356.2 → 119.0
Pirimicarb	9.0	239.2 → 72.0, 239.2 → 182.3
Pirimiphos-ethyl	16.3	334.1 → 198.0, 334.1 → 182.3
Pirimiphos-methyl	14.8	306.2 → 108.0, 306.2 → 164.3
Prochloraz	14.4	376.0 → 308.0, 376.0 → 70.0
Profenofos	15.6	375.0 → 304.9, 373.0 → 302.9
Prometryn	12.6	242.2 → 158.1, 242.2 → 200.0
Propachlor	9.6	212.0 → 170.0, 212.0 → 94.1
Propamocarb	1.1	189.0 → 102.0, 189.0 → 144.0
Propaquizafop	16.0	444.2 → 100.0, 444.2 → 371.0
Propargite NH ₄ ⁺	17.0	368.2 → 231.1, 368.2 → 175.0

Analyte	Retention Time (mins)	MRM transitions (m/z)
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
Pyraclastrobin	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
Pyrifenoxy	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
Quinoxifen	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 (NH ₄ adduct)	5.9	458.0 → 340.9, 458.0 → 441.0
Terbufos	16.1	289.1 → 103.1, 289.1 → 232.9
Terbufos sulfone	11.1	321.1 → 171.0, 321.1 → 115.0
Terbufos sulfoxide	11.0	305.1 → 187.2, 305.1 → 131.1



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
Tolyfluanid	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

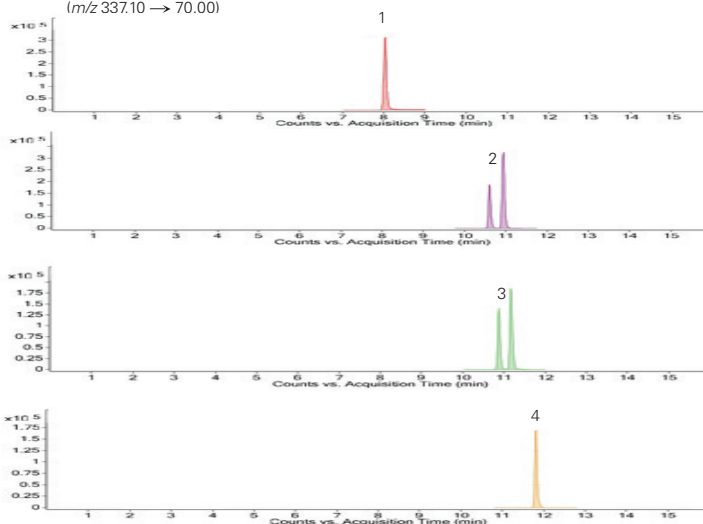
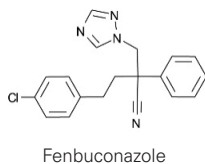
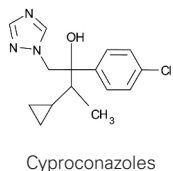
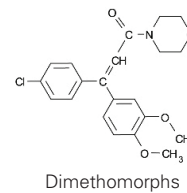
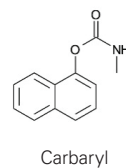
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
Mobile Phase: A: 0.1% formic acid + 5 mM ammonium formate in H₂O/MeOH (90:10 v/v)
 B: 0.1% formic acid + 5 mM ammonium formate in H₂O/MeOH (10:90 v/v)
Gradient:

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

Analytes

- Carbaryl (*m/z* 202.10 → 145.10)
- Dimethomorphs (*m/z* 388.10 → 301.10)
- Cyproconazoles (*m/z* 292.10 → 70.00)
- Fenbuconazole (*m/z* 337.10 → 70.00)



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

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Pesticides in Water Application #AN3020

Conditions

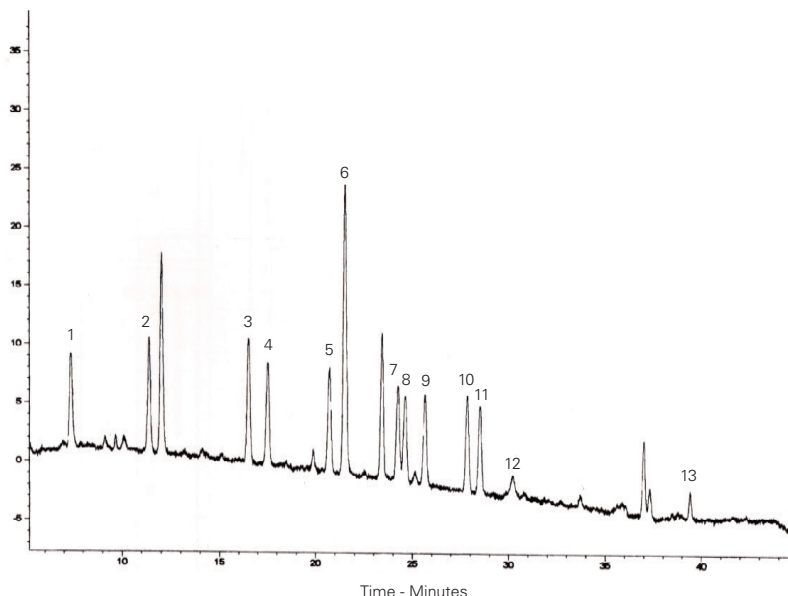
Column: ACE 3 C18
Dimensions: 150 x 2.1 mm
Part Number: ACE-111-1502
Mobile Phase: A: 0.1 M ammonium acetate in H₂O
 B: MeCN
Gradient:

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/H₂O (10:90 v/v)

Analytes

- Deisopropylatrazine
- Desethylatrazine
- Simazine
- Cyanazine
- Atrazine
- Internal standard
- Sebuthylazine
- Propazine
- Terbutylazine
- Terbutylazine
- Prometryn
- Terbutryn
- Alachlor
- 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

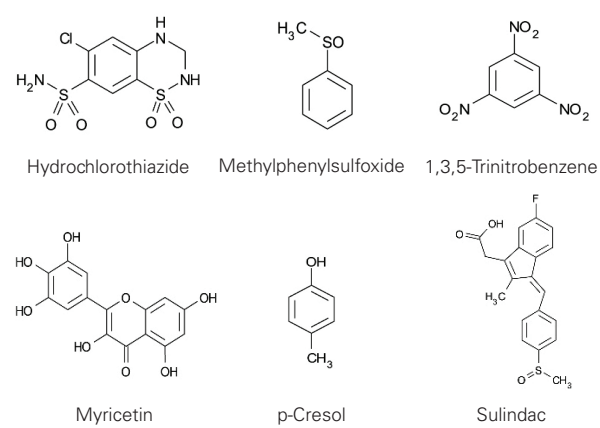
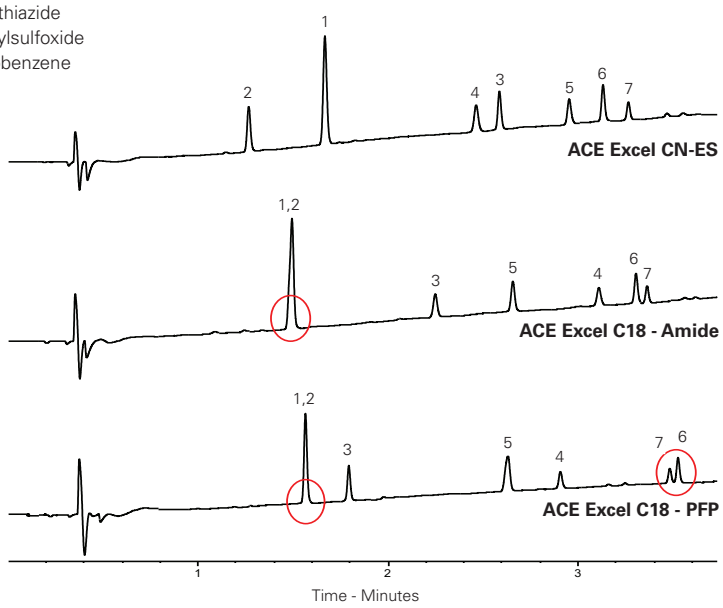
Mobile Phase: A: 20 mM ammonium formate in H₂O
B: 20 mM ammonium formate in MeOH

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**
- Hydrochlorothiazide
 - Methylphenylsulfonide
 - 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

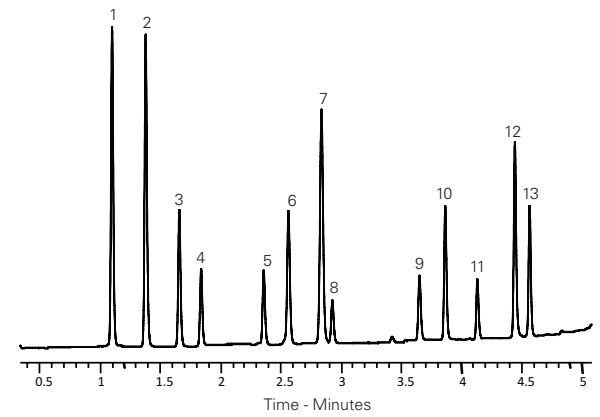
Mobile Phase: A: 5 mM formic acid in H₂O
B: 5 mM formic acid in MeOH

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**
- Paracetamol
 - Hydrochlorothiazide
 - Methylphenylsulfonide
 - Methylphenylsulfone
 - Aspirin
 - Phenacetin
 - 1,3-Dinitrobenzene
 - 1,2,4-Trimethoxybenzene
 - Ethylbenzoate
 - Nimesulide
 - Ibuprofen
 - Indomethacin
 - 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

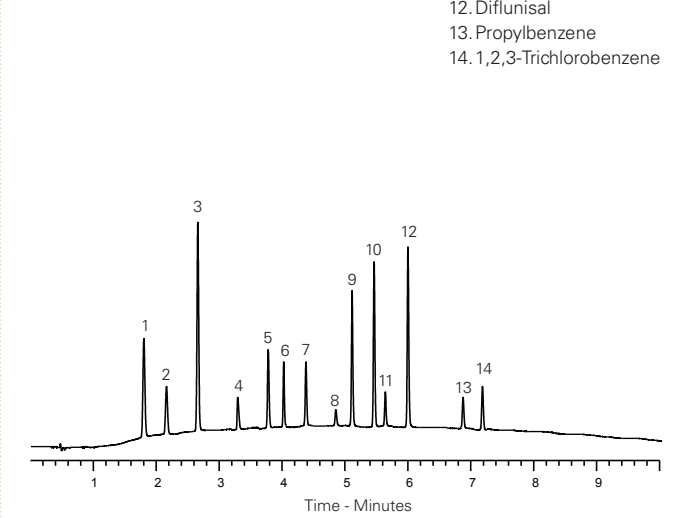
Mobile Phase: A: 0.1% formic acid in H₂O
B: 0.1% formic acid in MeCN

Gradient:

Time (mins)	%B
0	3
10	100

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

- Analytes**
- 1,3-Dihydroxybenzene
 - Catechol
 - Hydrochlorothiazide
 - Oxprenolol
 - Salicylic acid
 - Myricetin
 - Piroxicam
 - 1,2-Dinitrobenzene
 - Tolmetin
 - 1-Naphthol
 - Piperine
 - Diflunisal
 - Propylbenzene
 - 1,2,3-Trichlorobenzene





Pharmaceutically Relevant Compounds (V)
Application #AN2500

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

Conditions

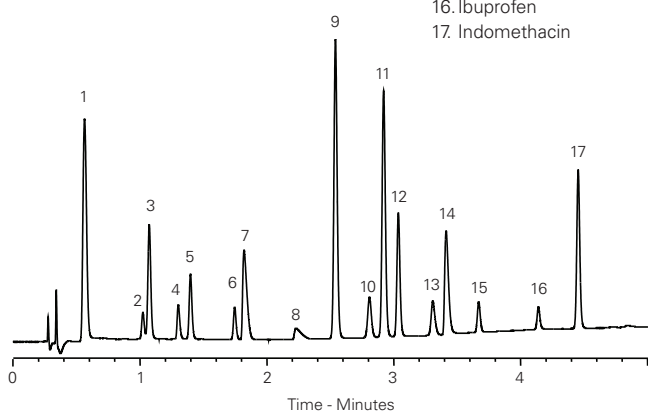
Column: ACE 3 C18-PFP
Dimensions: 50 x 2.1 mm
Part Number: ACE-1110-0502
Mobile Phase: A: 0.1% formic acid in H₂O
 B: 0.1% formic acid in MeOH
Gradient:

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



Pharmaceutically Relevant Mixture (I) – Different Selectivity Using pH
Application #AN1310

Conditions

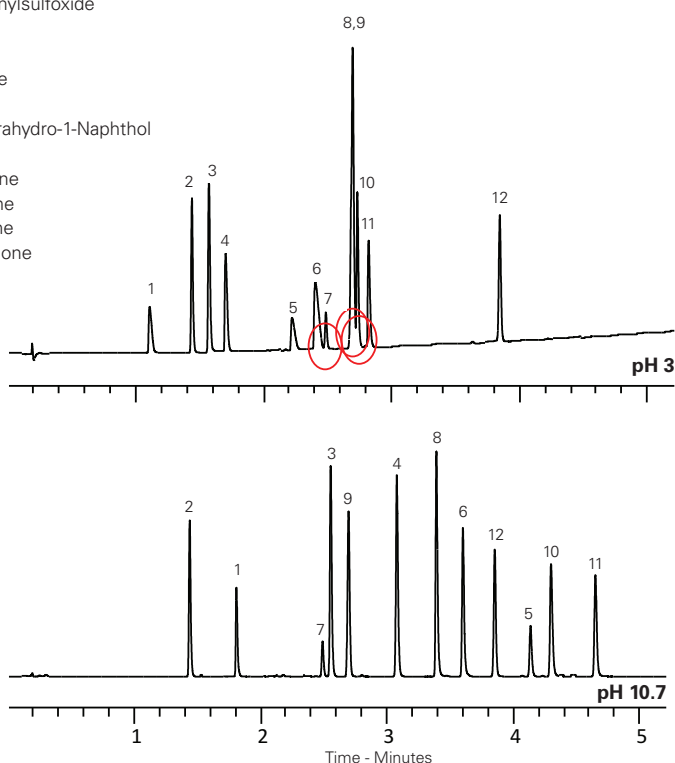
Column: ACE Ultracore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-0502U
Mobile Phase: A1: 10 mM ammonium formate pH 3 in H₂O
 A2: 0.1% ammonia pH 10.7 in H₂O
 B1: 10 mM ammonium formate pH 3 in MeCN/H₂O (90:10 v/v)
 B2: 0.1% ammonia pH 10.7 in MeCN/H₂O (90:10 v/v)
Gradient:

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

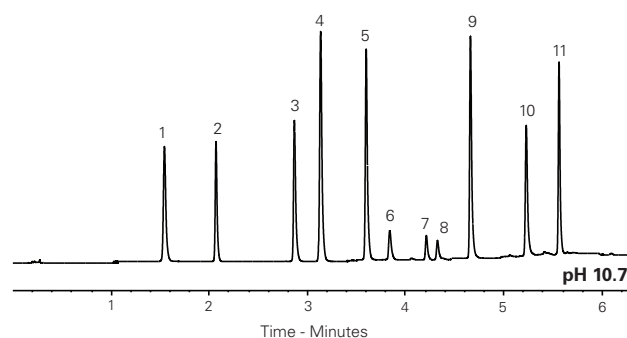
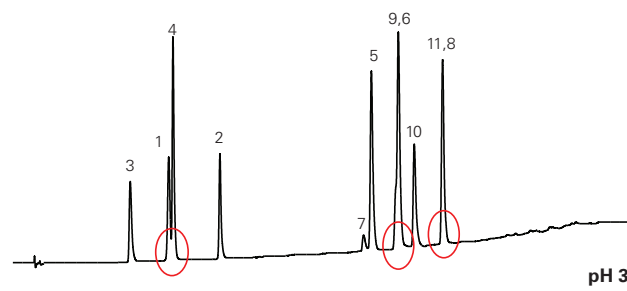
Column: ACE Ultracore 2.5 SuperPhenylHexyl
Dimensions: 50 x 2.1 mm
Part Number: CORE-25B-0502U
Mobile Phase: A1: 10 mM ammonium formate pH 3 in H₂O
 A2: 0.1% ammonia pH 10.7 in H₂O
 B1: 10 mM ammonium formate pH 3 in MeCN/H₂O (90:10 v/v)
 B2: 0.1% ammonia pH 10.7 in MeCN/H₂O (90:10 v/v)
Gradient:

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

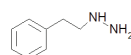
Application #AN4200

Conditions

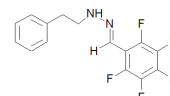
Column: ACE 5 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-121-1046
Mobile Phase: 10 mM ammonium acetate in H₂O, pH 4.0/MeOH (20:80 v/v)
Flow Rate: 1 mL/min with 70% split flow into MS
Injection: 10 µL
Temperature: 45 °C
Detection: AB Sciex API-4000 MS
 MRM using ESI in positive ion mode
 TurbolonSpray 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

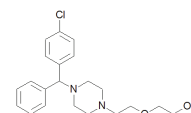
1. Phenelzine derivative
(*m/z* 305.1 → 105.1)
20.2 ng/mL
2. Hydroxyzine
(*m/z* 375.3 → 201.1)
25 ng/mL



Phenelzine

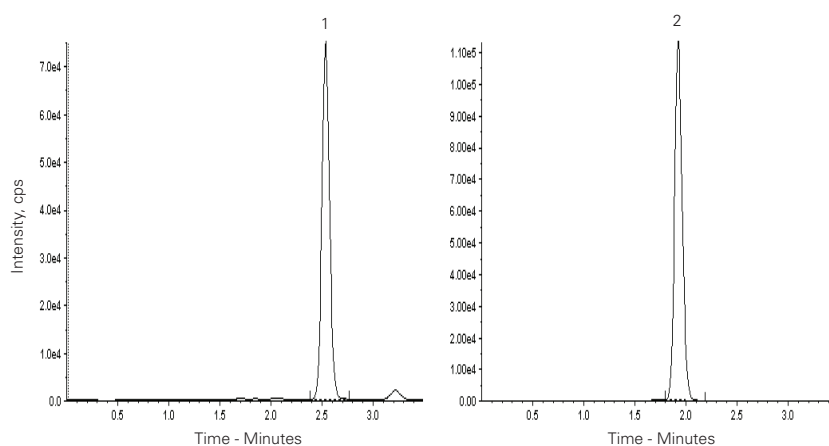


Phenelzine derivative



Hydroxyzine

Spiked human plasma





Phenol and Phenoxy Acid Herbicides

Application #AN2290

Conditions

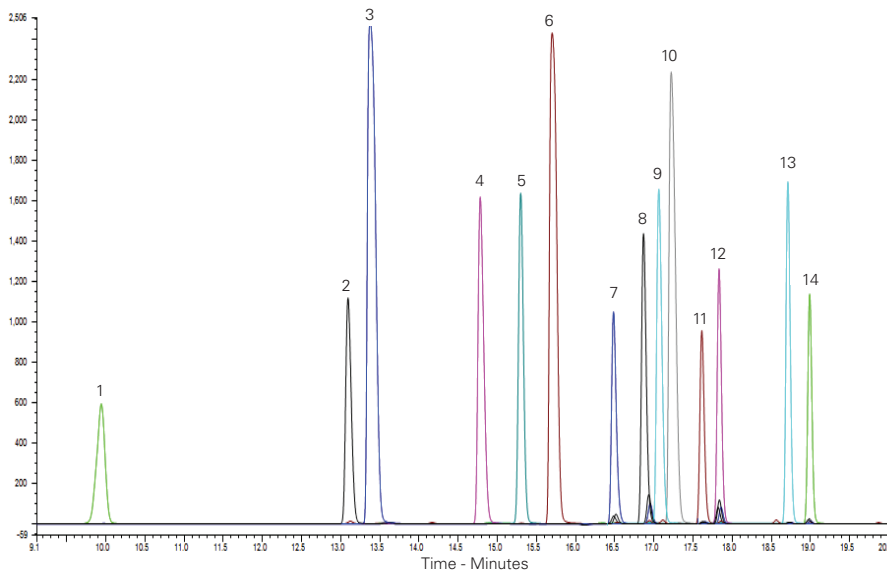
Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: A: 0.1% formic acid in H₂O
 B: MeOH
Gradient:

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



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Phenolic Acids

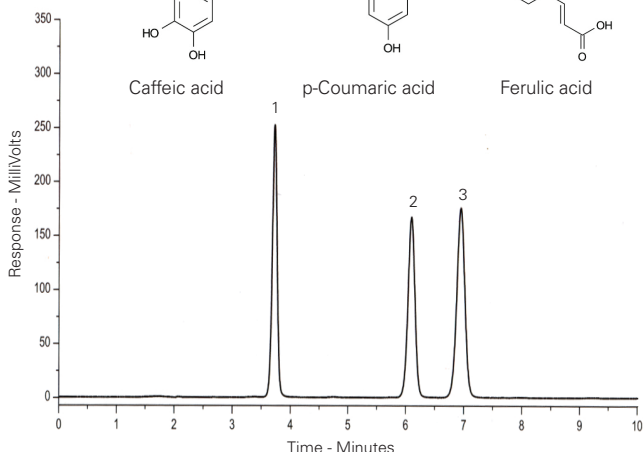
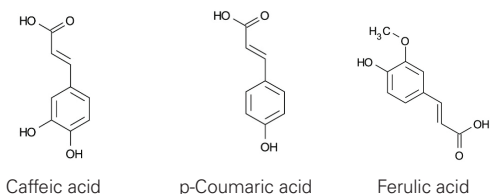
Application #AN3030

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeCN/0.1% formic acid in H₂O (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

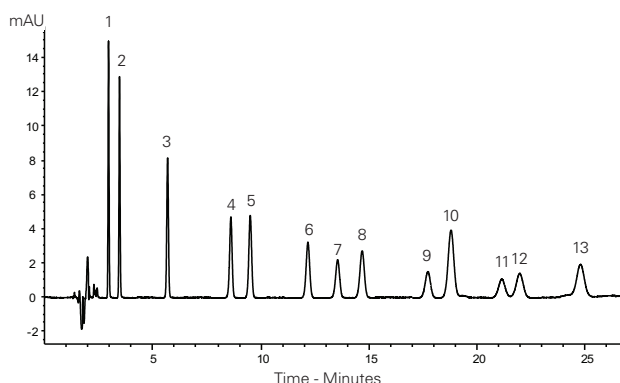
Application #AN3070

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 H₂O
 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

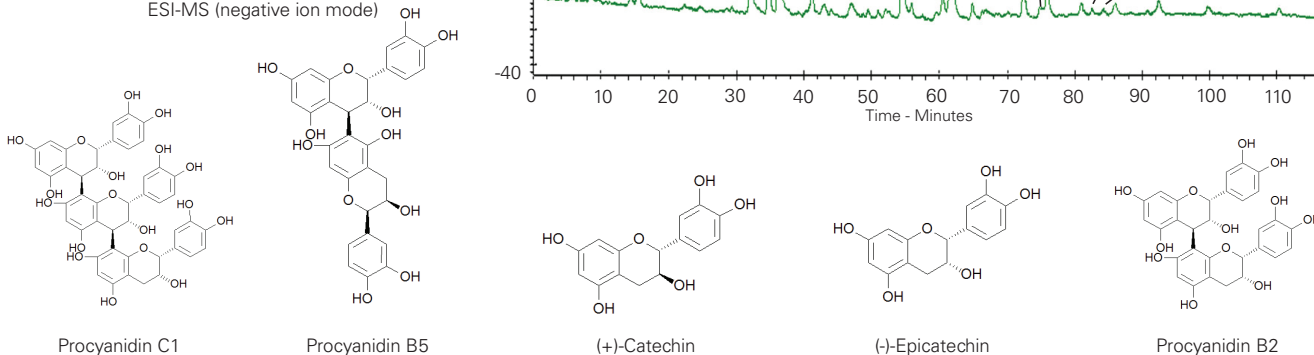
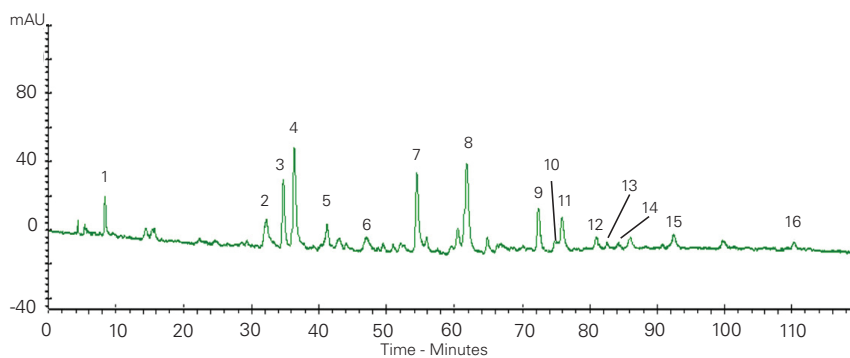
Column: ACE 3 C18-AR
Dimensions: 200 x 4.6 mm
Part Number: ACE-119-2046
Mobile Phase: A: 2% acetic acid in H₂O
 B: 2% acetic acid in MeCN
Gradient:

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



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

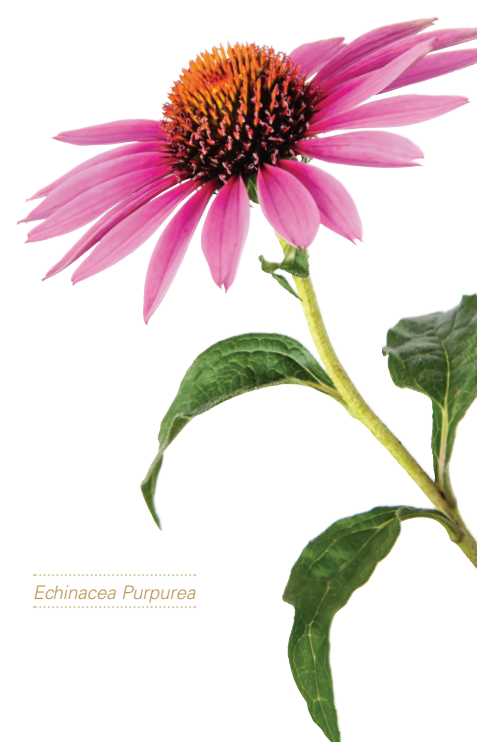
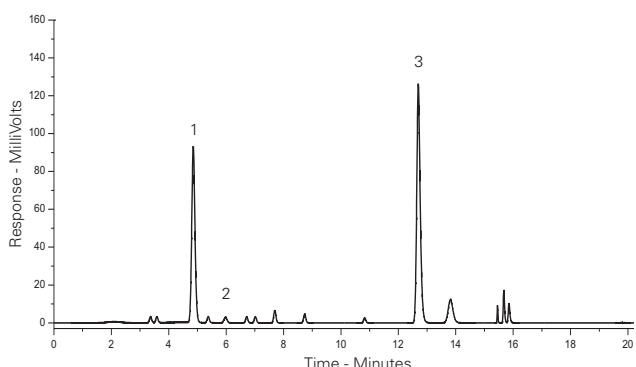
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.1% H₃PO₄ in H₂O
 B: MeCN
Gradient:

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



Echinacea Purpurea

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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

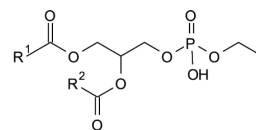
Gradient:	Time (mins)	%B
	0.00	10
	1.00	10
	3.00	60
	3.01	100
	5.00	100
	5.10	10

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

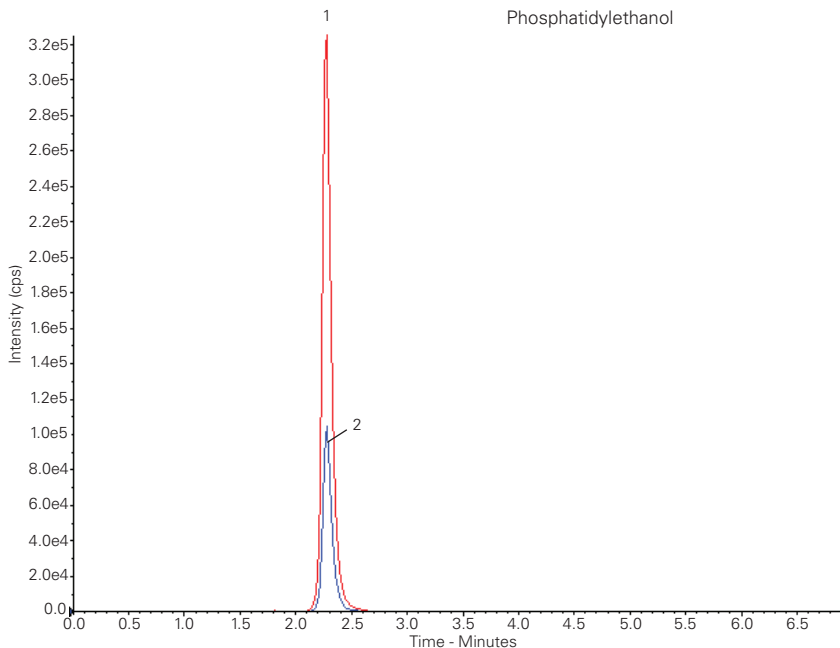
Phosphatidylethanol (PEth) measurement in blood is used as a biomarker of chronic alcohol use/abuse.

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 H₂O
 D: MeOH

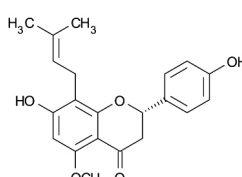
Gradient:	Time (mins)	%A	%B	%C	%D
	0	56	0	44	0
	8	51	5	44	0
	10	51	5	44	0
	17	95	5	0	0
	22	95	0	0	5

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

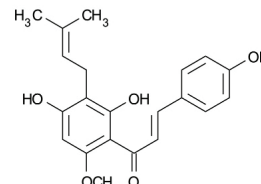


Analytes

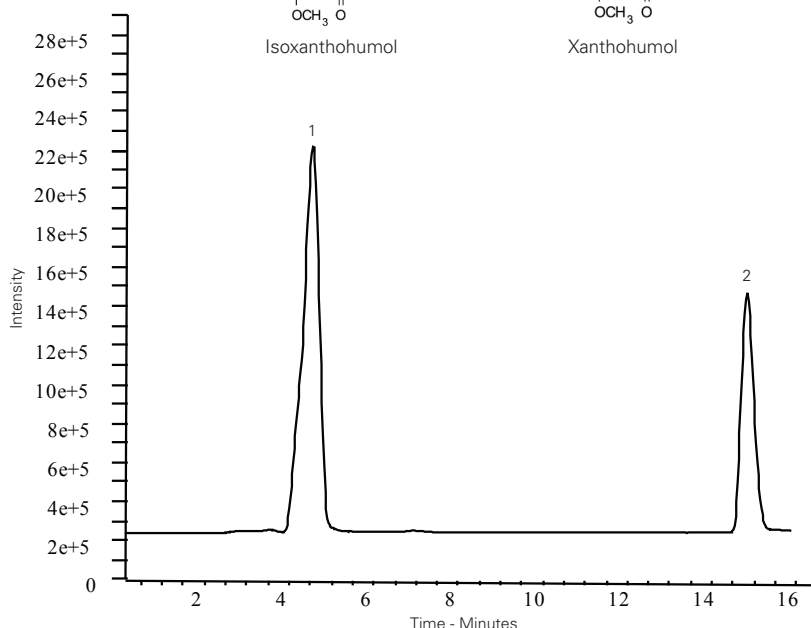
1. Isoxanthohumol
LOQ 0.07 µg/mL
2. Xanthohumol
LOQ 0.01 µg/mL



Isoxanthohumol



Xanthohumol



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Pilocarpine

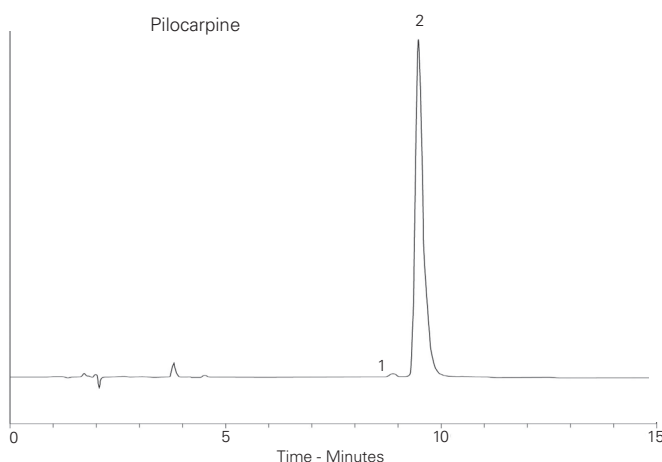
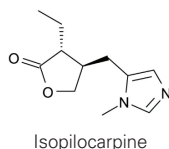
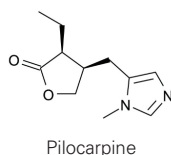
Application #AN3720

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



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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 H₂O
 B: MeCN
Gradient:

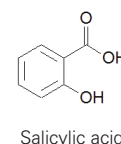
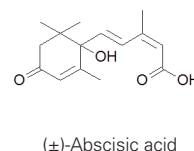
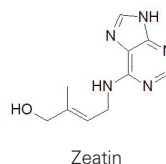
Time (mins)	%B
0	0
2	40
5	60
13	100
15	20

Flow Rate: 0.5 mL/min
Temperature: 40 °C
Detection: Shimadzu LCMS-8040 triple quad MS
 ESI positive and negative mode

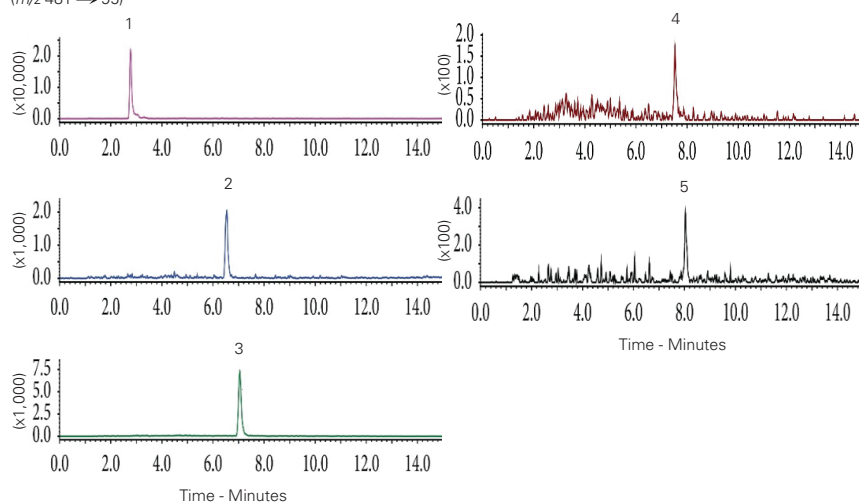
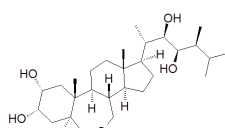
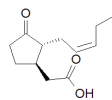
Sample: Crude extract of *Arabidopsis thaliana* rosette leaves

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)



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



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

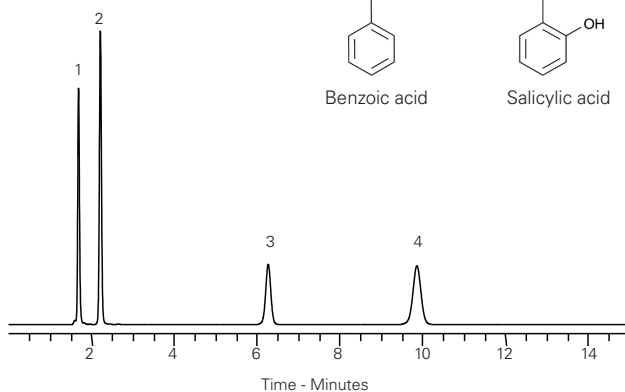
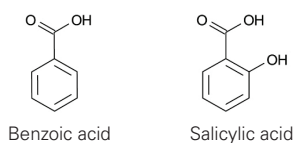
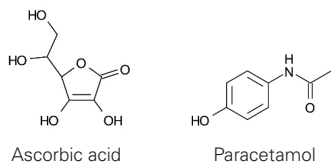
Application #AN1590

Conditions

Column: ACE Excel 5 CN-ES
Dimensions: 150 x 4.6 mm
Part Number: EXL-1213-1546U
Mobile Phase: MeOH/H₂O (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



Polyamines

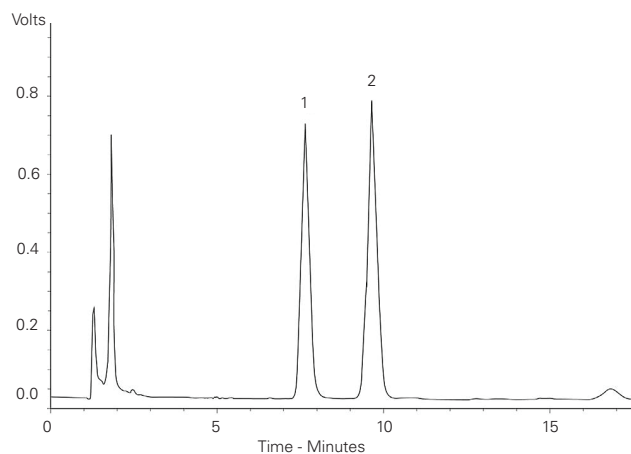
Application #AN3740

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

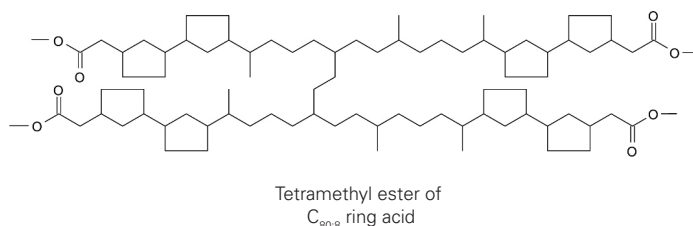
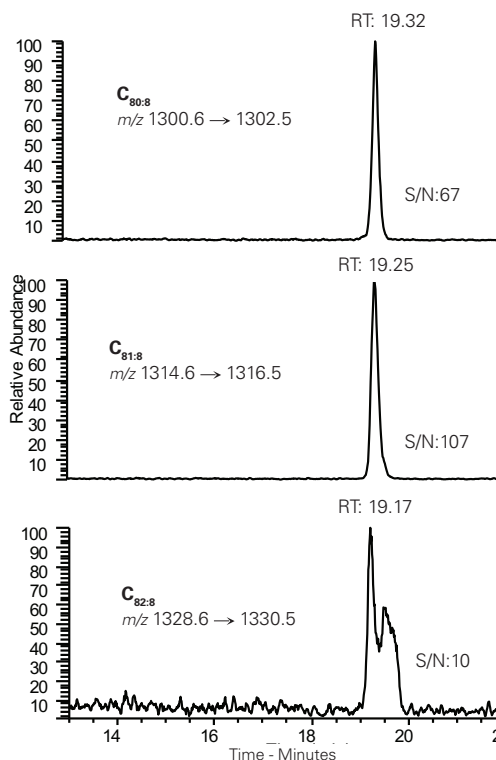
Conditions

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/H₂O (98:2 v/v)
 B: 10 mM ammonium acetate in IPA/H₂O (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+NH₄]⁺
 Detection limit ~ 0.1 ppm

C₈₀₋₈₂ polycyclic tetracarboxylic acids isolated from oilfield deposits



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Polyethylene Glycol 1000

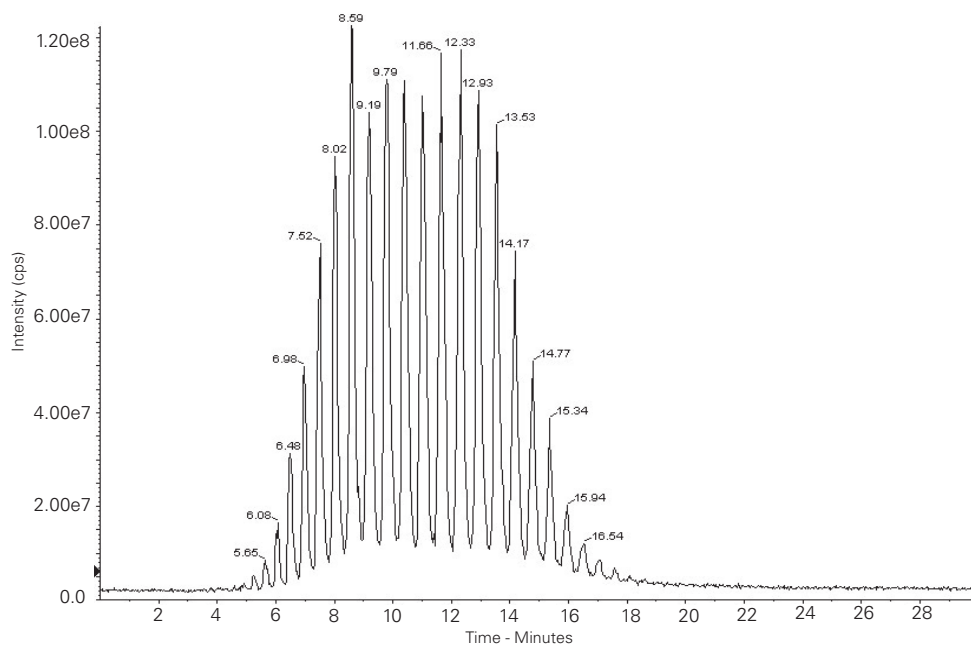
Application #AN3900

Conditions

Column: ACE 3 C8
Dimensions: 150 x 4.6 mm
Part Number: ACE-112-1546
Mobile Phase: A: 0.1% formic acid in H₂O
 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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[¹⁴C]Pomalidomide and Metabolites in Human Plasma and Urine

Application #AN4240

Conditions

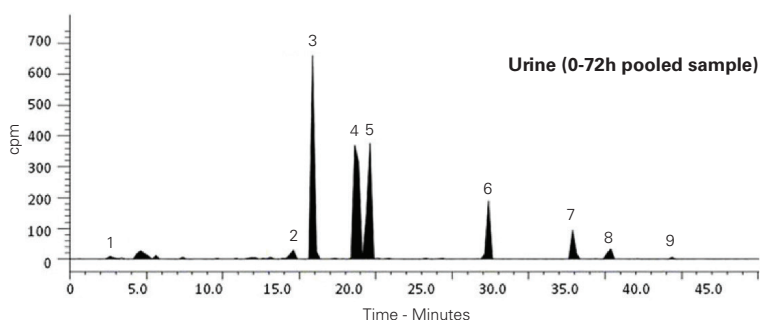
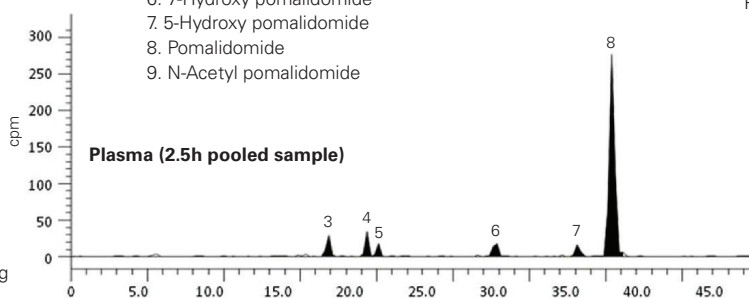
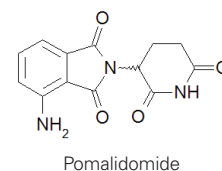
Column: ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-111-1546
Mobile Phase: A: 25 mM ammonium acetate pH 5.5 in H₂O
 B: MeOH
Gradient:

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

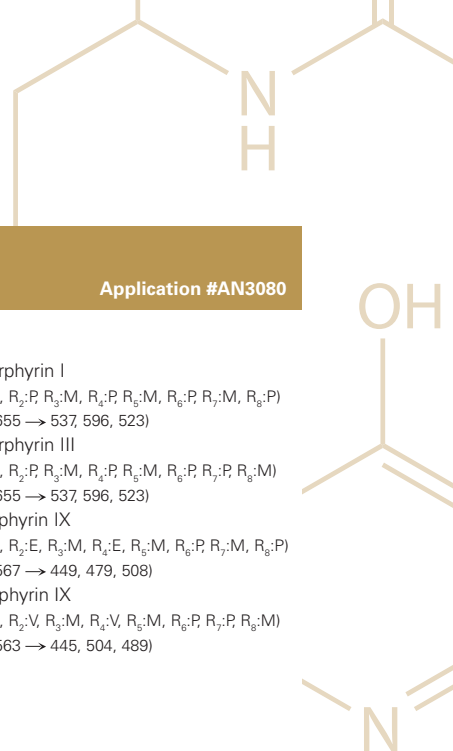
Flow Rate: 0.7 mL/min
Temperature: 30 °C
Detection: Radiometric
 Metabolites characterised using LC-MS/MS (positive ion mode)

Analytes

- 3-Aminophthalic acid
- Hydrolysis product of pomalidomide
- Hydrolysis product of pomalidomide
- Glucuronide conjugate of 5-hydroxy pomalidomide
- Glucuronide conjugate of 5-hydroxy pomalidomide
- 7-Hydroxy pomalidomide
- 5-Hydroxy pomalidomide
- Pomalidomide
- N-Acetyl 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 [¹⁴C] 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

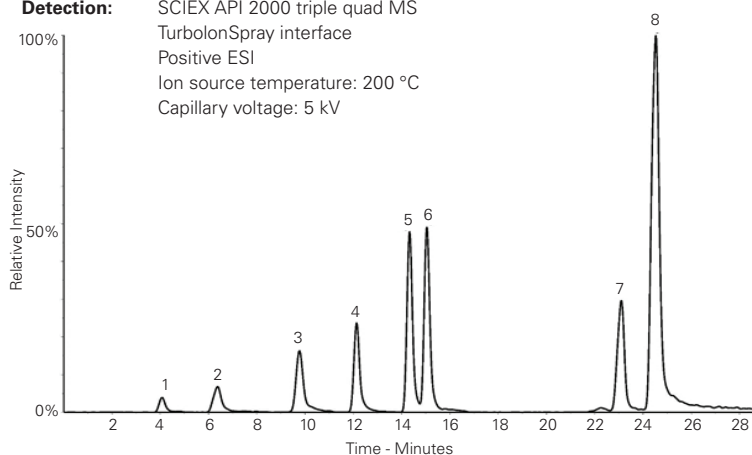
Column: ACE 3 C18-PFP
Dimensions: 75 x 2.1 mm
Part Number: ACE-1110-7502
Mobile Phase: A: 0.1% formic acid in H₂O/MeCN (95:5 v/v)
 B: 0.1% formic acid in H₂O/MeCN (5:95 v/v)
Gradient:

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

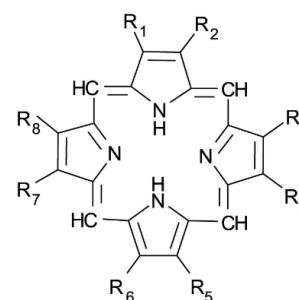
Flow Rate: 0.1 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: SCIEX API 2000 triple quad MS
 TurbolonSpray interface
 Positive ESI
 Ion source temperature: 200 °C
 Capillary voltage: 5 kV

Analytes

1. Uroporphyrin I
(R₁:A, R₂:P, R₃:A, R₄:P, R₅:A, R₆:P, R₇:A, R₈:P)
(*m/z* 831 → 727, 623, 655)
2. 7-Carboxyporphyrin I
(R₁:A, R₂:P, R₃:A, R₄:P, R₅:A, R₆:P, R₇:M, R₈:P)
(*m/z* 787 → 683, 670, 623)
3. 6-Carboxyporphyrin I
(R₁:M, R₂:P, R₃:A, R₄:P, R₅:A, R₆:P, R₇:M, R₈:P)
(*m/z* 743 → 639, 507, 521)
4. 5-Carboxyporphyrin I
(R₁:M, R₂:P, R₃:M, R₄:P, R₅:A, R₆:P, R₇:M, R₈:P)
(*m/z* 699 → 463, 595, 640)
5. Coproporphyrin I
(R₁:M, R₂:P, R₃:M, R₄:P, R₅:M, R₆:P, R₇:M, R₈:P)
(*m/z* 655 → 537, 596, 523)
6. Coproporphyrin III
(R₁:M, R₂:P, R₃:M, R₄:P, R₅:M, R₆:P, R₇:P, R₈:M)
(*m/z* 655 → 537, 596, 523)
7. Mesoporphyrin IX
(R₁:M, R₂:E, R₃:M, R₄:E, R₅:M, R₆:P, R₇:M, R₈:P)
(*m/z* 567 → 449, 479, 508)
8. Protoporphyrin IX
(R₁:M, R₂:V, R₃:M, R₄:V, R₅:M, R₆:P, R₇:P, R₈:M)
(*m/z* 563 → 445, 504, 489)



Where:
 A: -CH₂COOH
 E: -CH₂CH₃
 M: -CH₃
 P: -CH₂CH₂COOH
 V: -CH=CH₂



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Pravastatin and Isomers by LC-MS/MS

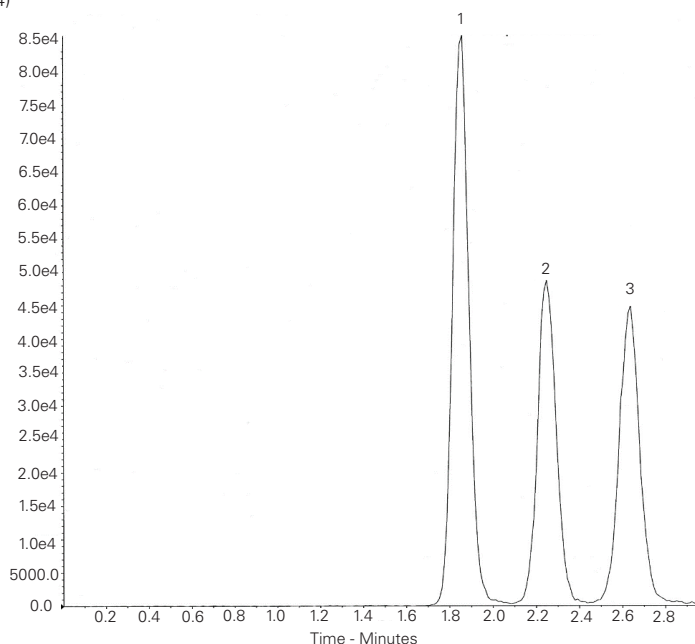
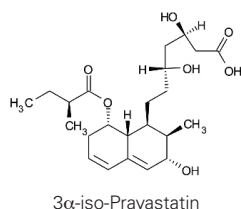
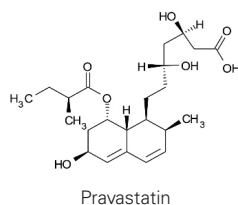
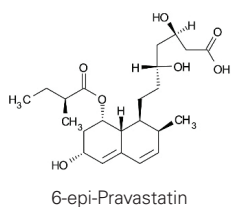
Application #AN1350

Conditions

Column: ACE 3 C18
Dimensions: 50 x 3.0 mm
Part Number: ACE-111-0503
Mobile Phase: MeCN/MeOH/THF/H₂O/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)



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Pravastatin in Cell Lysate Samples by LC-MS/MS

Application #AN4350

Conditions

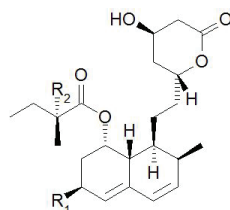
Column: ACE Excel 3 SuperC18
Dimensions: 100 x 3.0 mm
Part Number: EXL-1111-1003U
Mobile Phase: A: 5 mM ammonium acetate pH 4.5 in H₂O
 B: MeCN
Gradient:

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

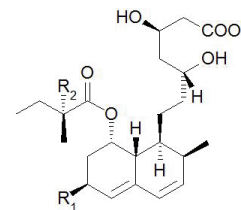
Flow Rate: 0.3 mL/min
Temperature: 40 °C
Detection: Quattro Ultima triple quad MS
 ESI MRM mode: +ve (lactones)
 -ve (hydroxy acids)
 Source temperature: 125 °C
 Desolvation temperature: 350 °C

Analytes

- Lactone form (pharmacologically inactive)
- Hydroxy acid form (pharmacologically active)



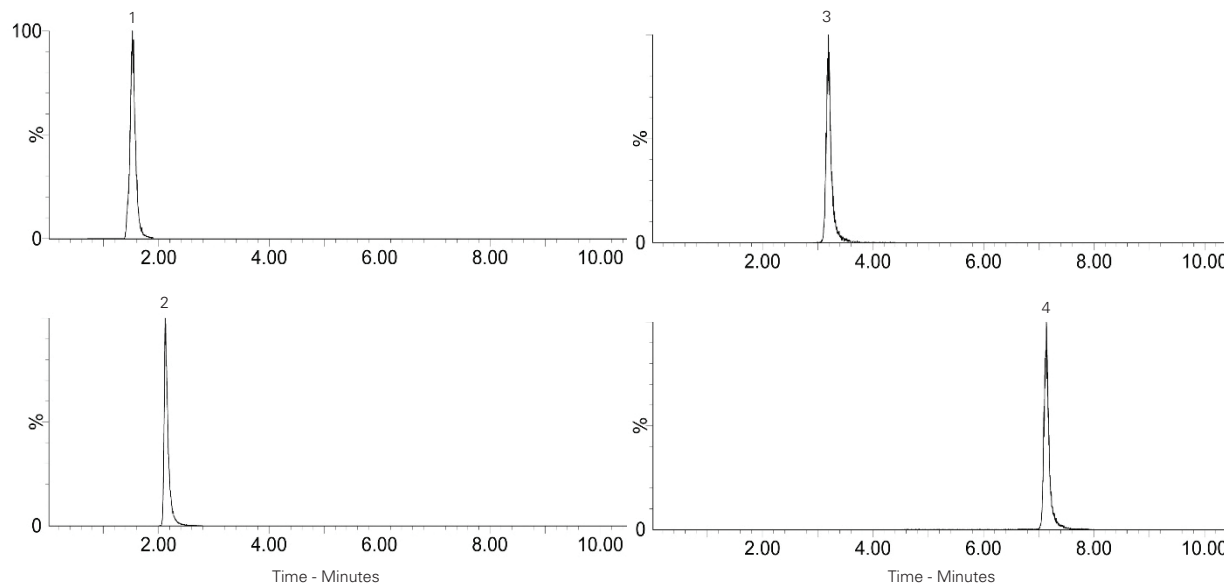
Lactone form
(pharmacologically inactive)



Hydroxy acid form
(pharmacologically active)

Peak	Analyte	Precursor ion	MRM transition (<i>m/z</i>)	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: R₁ = OH, R₂ = H
Lovastatin (IS): R₁ = CH₃, R₂ = 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

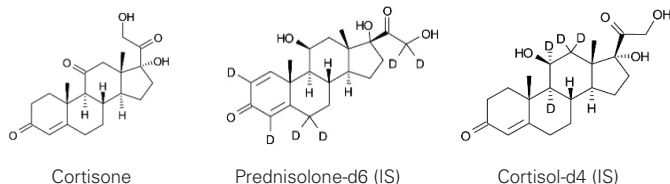
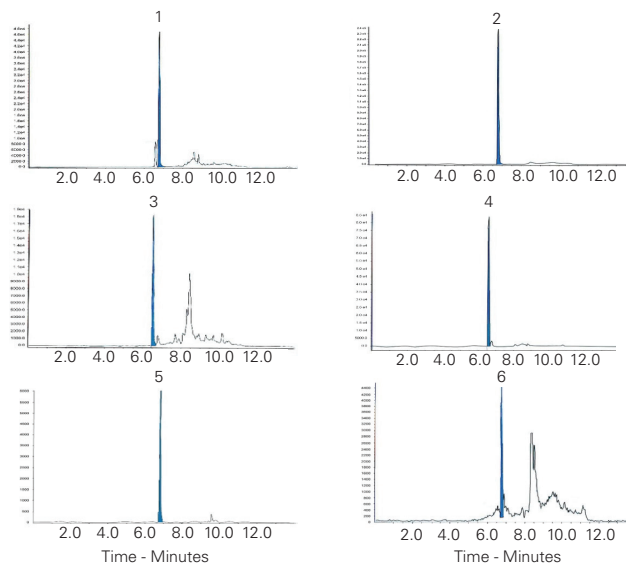
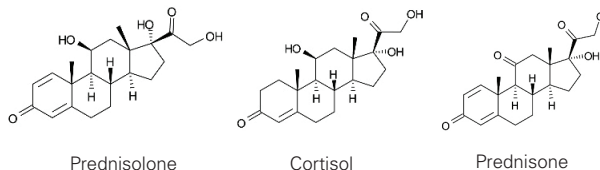
Column: ACE Excel 2 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-101-1002U
Mobile Phase: A: 4 mM ammonium acetate in H₂O
 B: 0.2% (v/v) formic acid in MeOH
Gradient:

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)



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Preservatives (I)

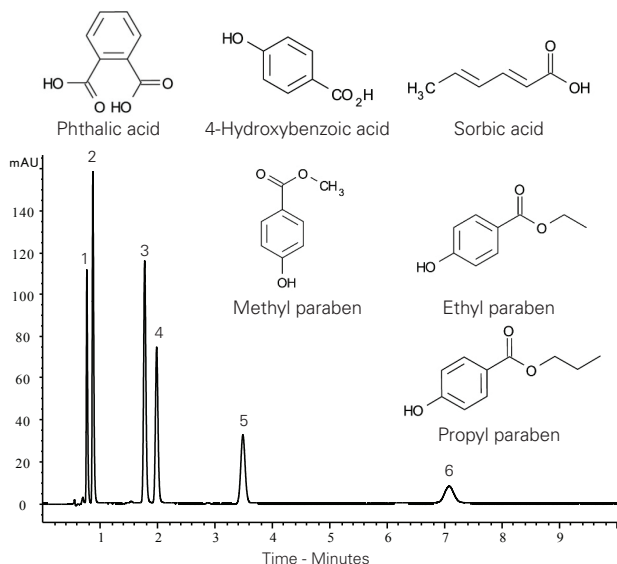
Application #AN2230

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/H₂O (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



Preservatives (II)

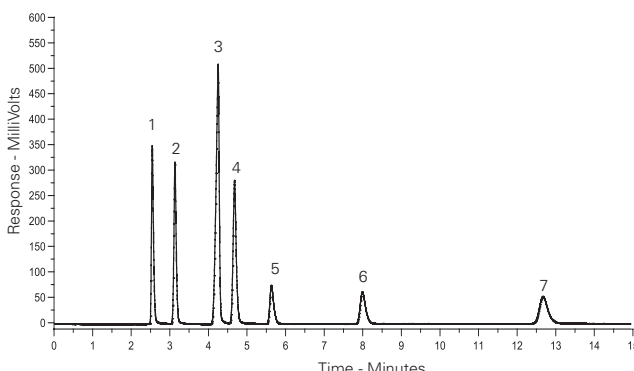
Application #AN3040

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: MeCN/50 mM KH₂PO₄
 pH 4.4 in H₂O (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

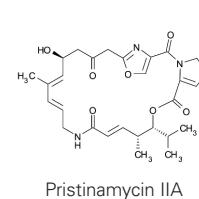
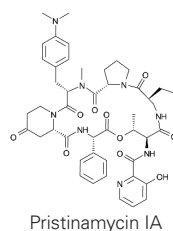
Column: ACE 3 C18
Dimensions: 30 x 3.0 mm
Part Number: ACE-111-0303
Mobile Phase: A: 1 mM ammonium formate + 0.1% formic acid in MeCN/H₂O (35:65 v/v)
 B: MeCN
Gradient:

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

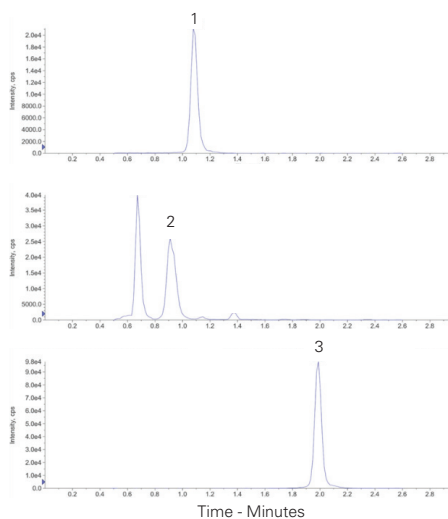
Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: 25 °C
Detection: MDS Sciex API 4000
 TurbolonSpray positive mode

Analytes

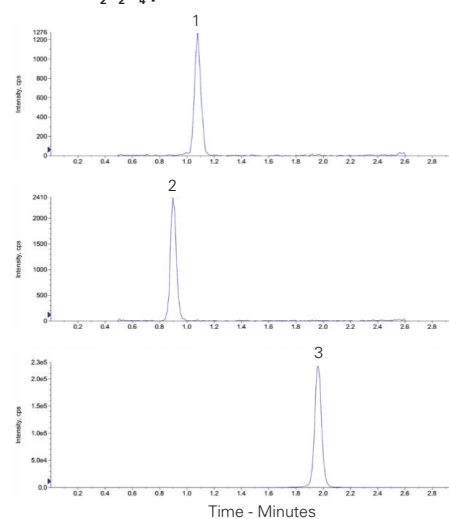
1. Pristinamycin IA
(m/z 8675 → 134.2)
2. Pristinamycin IIA
(m/z 526.3 → 355.1)
3. Virginiamycin (IS)
(m/z 824.6 → 134.0)



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/K₂C₂O₄ plasma



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Proanthocyanidins from Cinnamon Bark Extract Application #AN3510

Conditions

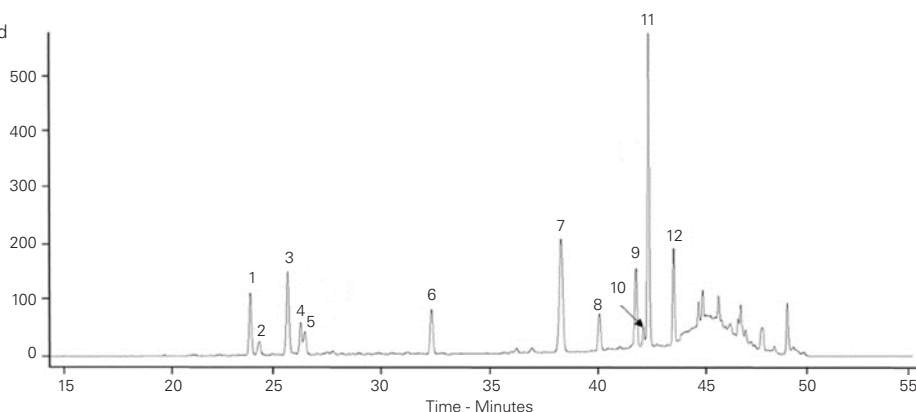
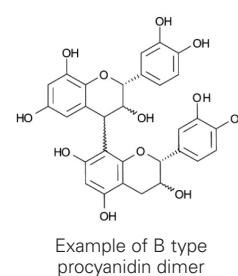
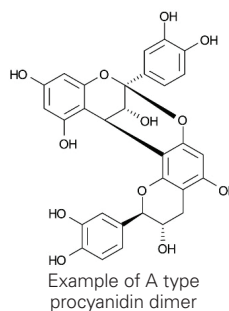
Column: ACE 3 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-111-2546
Mobile Phase: A: 1% acetic acid in H₂O
 B: MeCN
Gradient:

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



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

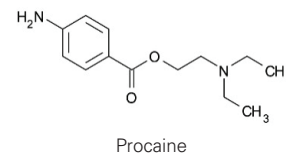
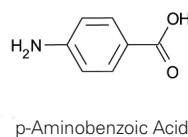
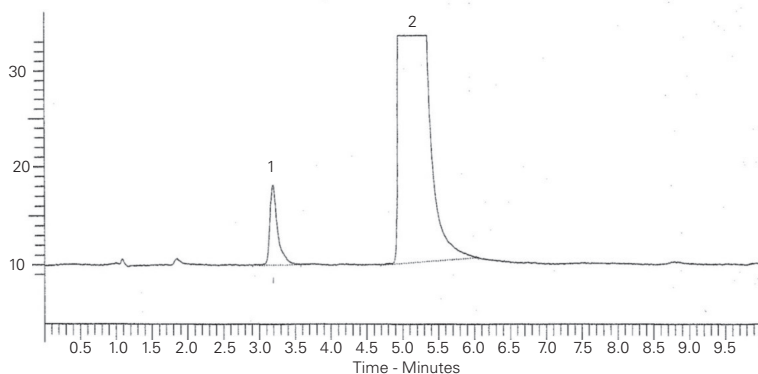
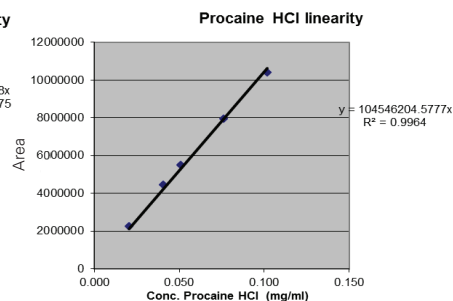
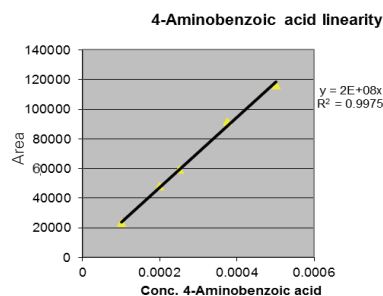
Application #AN1660

Conditions

Column: ACE 3 C18-PFP
Dimensions: 100 x 4.6 mm
Part Number: ACE-1110-1046
Mobile Phase: 0.6% acetic acid in H₂O/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



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Propolis Phenolic Acids Applied to Human Skin

Application #AN4230

Conditions

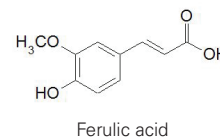
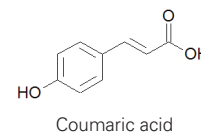
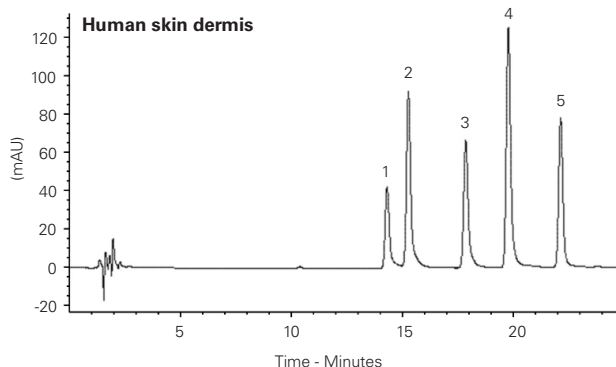
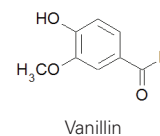
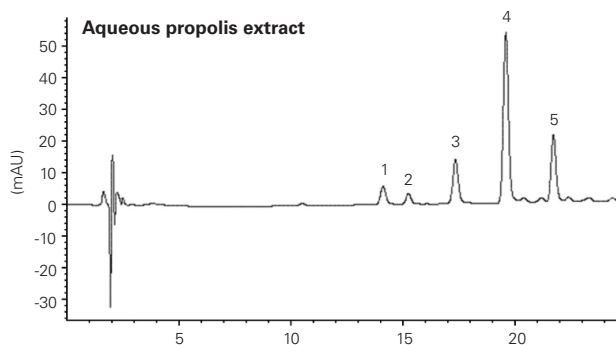
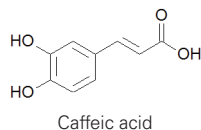
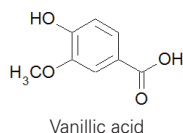
Column: ACE 5 C18
Dimensions: 150 x 0.5 mm
Part Number: ACE-121-15005
Mobile Phase: A: 0.5% acetic acid in H₂O
 B: MeCN
Gradient:

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



Zilius M, Ramanauskienė 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

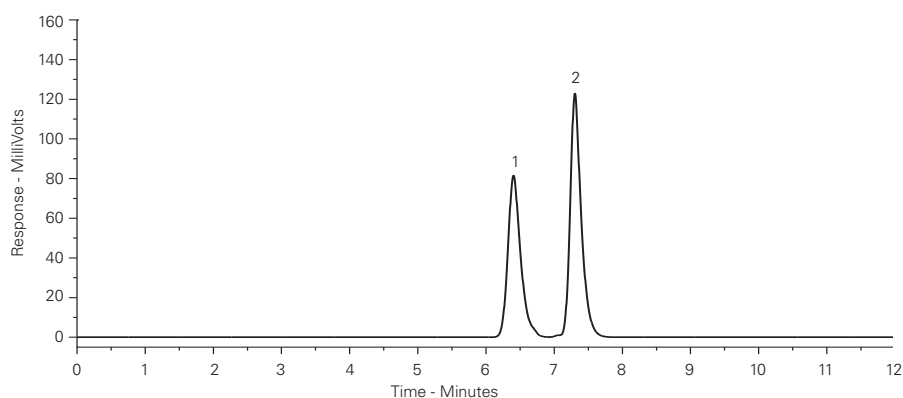
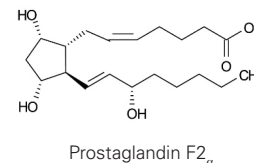
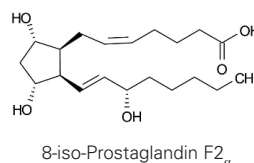
Column: ACE 3 C18
Dimensions: 50 x 2.1 mm
Part Number: ACE-111-0502
Mobile Phase: A: H₂O
 B: MeOH
 C: MeCN
Gradient:

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

- 8-iso-Prostaglandin F_{2α}
- Prostaglandin F_{2α}



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Protein Test Mix

Application #AN3730

Conditions

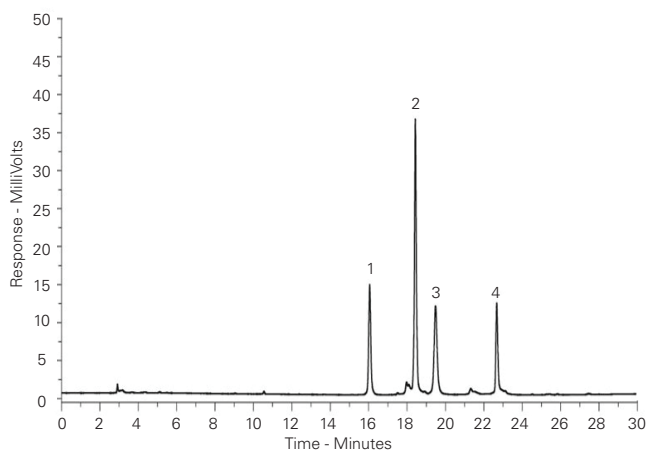
Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 0.1% TFA in H₂O
 B: 0.1% TFA in MeCN
Gradient:

Time (mins)	%B
0	5
30	70

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

Analytes

- Ribonuclease A (MW ~14 kDa)
- Cytochrome C (MW ~12 kDa)
- Holo-transferrin (MW ~77 kDa)
- Apomyoglobin (MW ~17 kDa)



Proton Pump Inhibitors (PPIs)

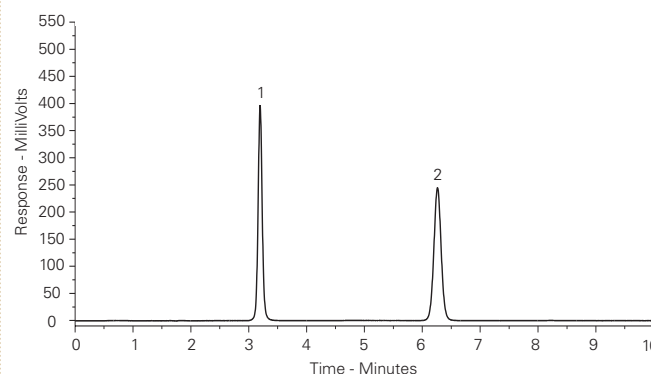
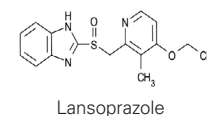
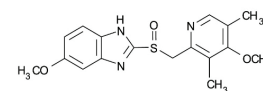
Application #AN3710

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

- Omeprazole
- Lansoprazole





Psychoactive Substances in 'Synthacaine' by LC-UV

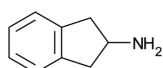
Application #AN3440

Conditions

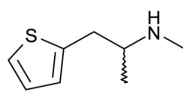
Column: ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-111-1546
Mobile Phase: 10 mM ammonium formate pH 3.5/MeCN (90:10 v/v)
Flow Rate: 1.2 mL/min
Temperature: 22 °C
Detection: UV, 207 nm (2-Aminoindane) and 233 nm (Methiopropamine)
Sample: Synthacaine 40 µg/mL

Analytes

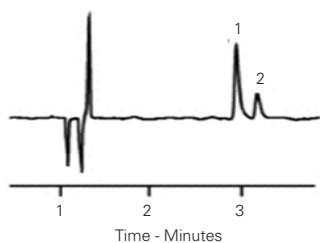
- 2-Aminoindane
LOD 0.83 µg/mL
- Methiopropamine
LOD 0.31 µg/mL



2-Aminoindane



Methiopropamine



Cumba L, Koliopoulos 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

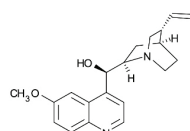
Application #AN1600

Conditions

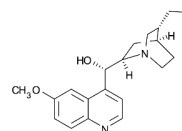
Column: ACE 3 C18-AR
Dimensions: 50 x 4.6 mm
Part Number: ACE-119-0546
Mobile Phase: 20 mM ammonium formate pH 3.0 in MeOH/H₂O (30:70 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 30 °C
Detection: UV, 254 nm

Analytes

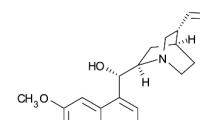
- Quinidine
- Quinine
- Hydroquinidine
- Hydroquinine



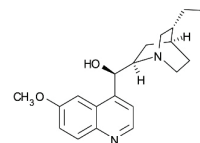
Quinine



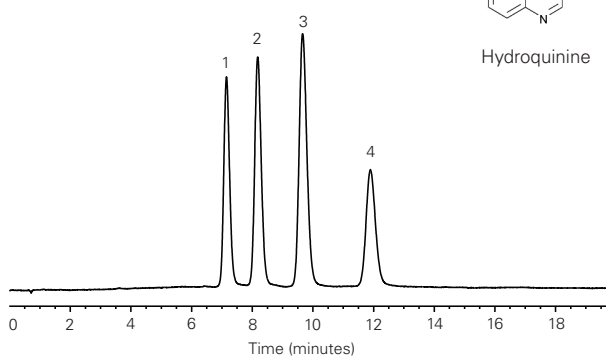
Hydroquinidine



Quinidine

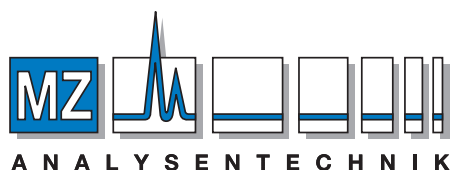


Hydroquinine



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e-mail: info@mz-at.de, www.mz-at.de

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 $\text{H}_2\text{O}/\text{MeCN}$ (98:2 v/v)
 B: $\text{H}_2\text{O}/\text{MeCN}$ (5:95 v/v)

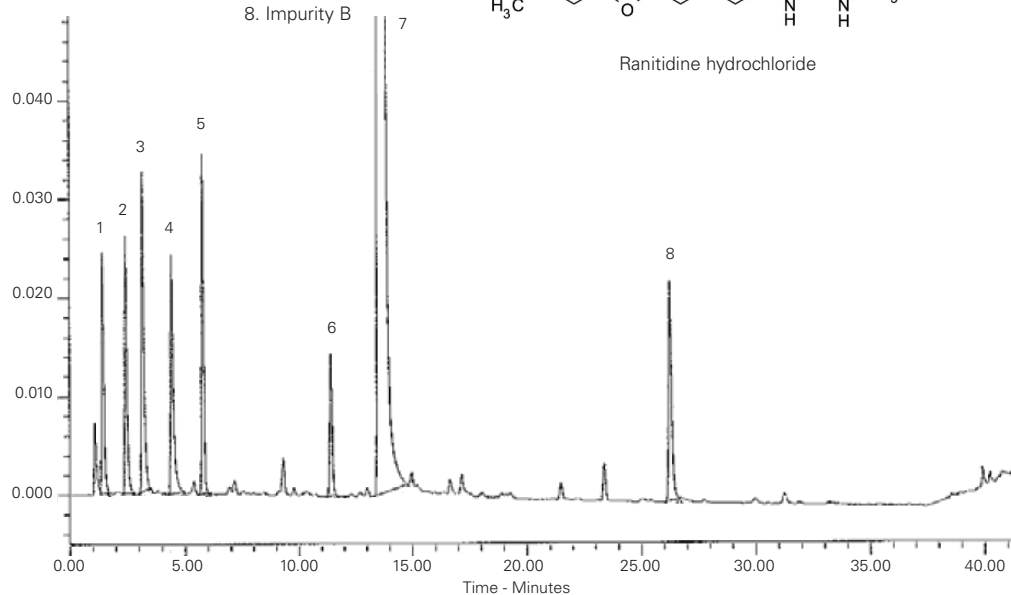
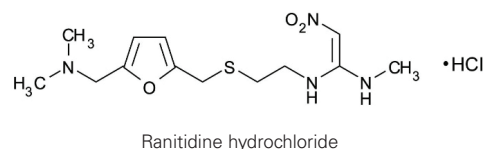
Gradient:

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 $^\circ\text{C}$
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



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

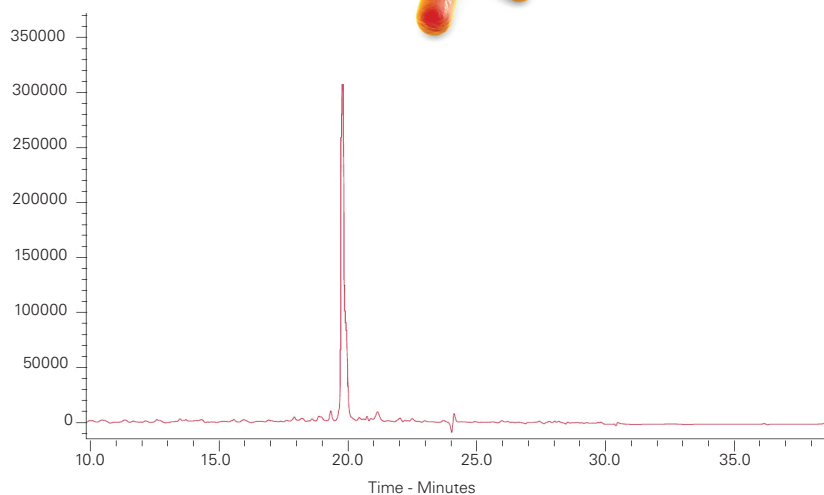
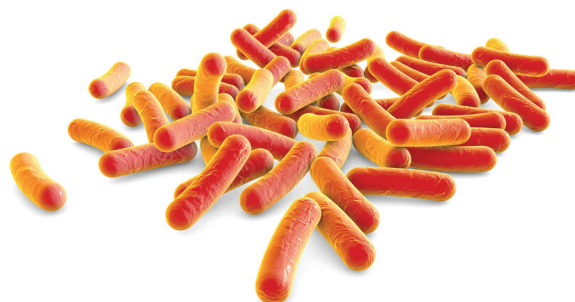
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: A: 0.1% TFA in $\text{H}_2\text{O}/\text{MeCN}$ (90:10 v/v)
 B: 0.1% TFA in $\text{H}_2\text{O}/\text{MeCN}$ (10:90 v/v)

Gradient:

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

Flow Rate: 1 mL/min
Temperature: 30 $^\circ\text{C}$
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 H₂O
 B: 0.1% formic acid in MeOH
Gradient:

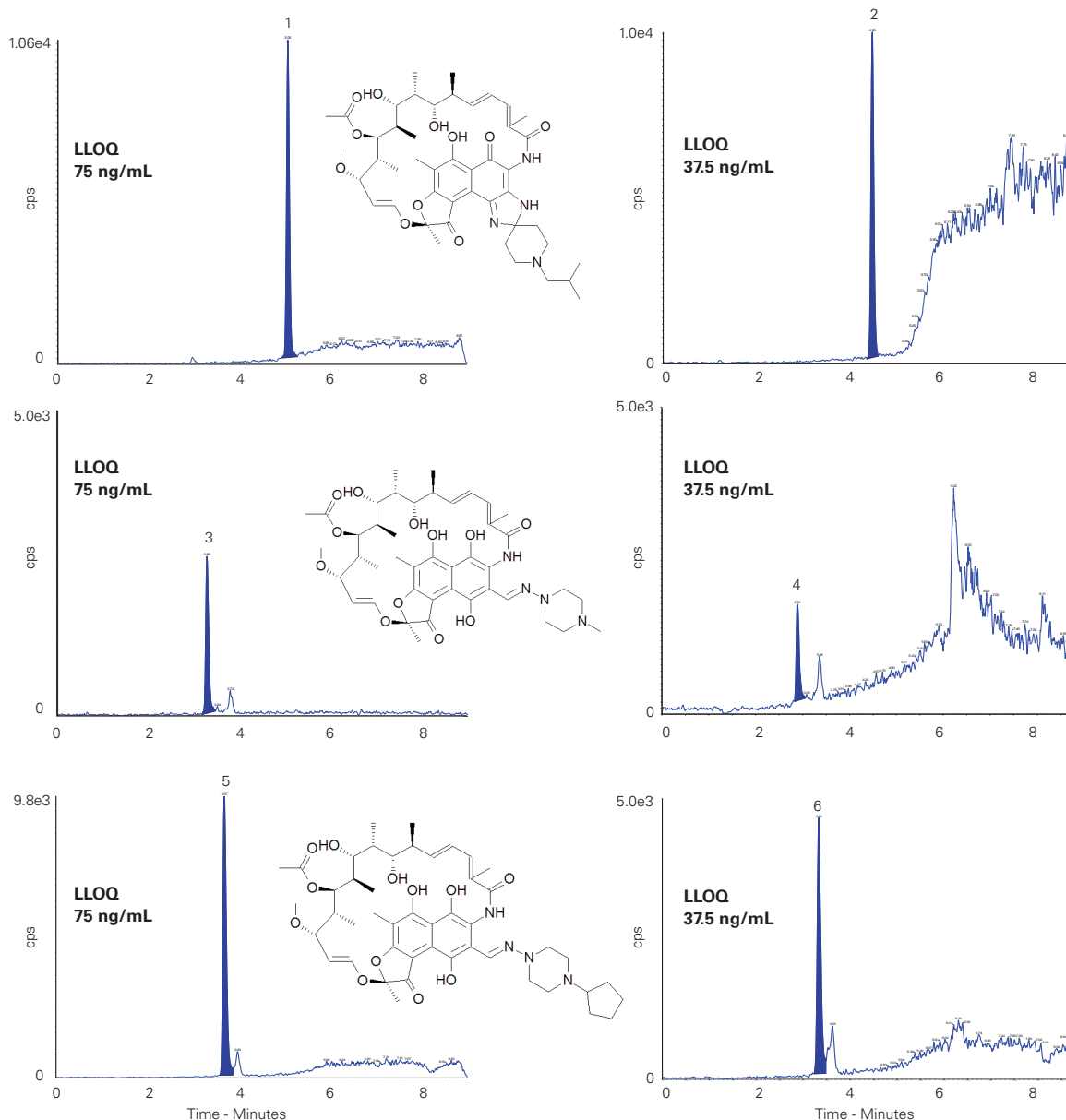
Time (mins)	%B
0.0	60
4.0	95
7.0	95
7.2	60
9.0	60

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

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)

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



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