Cannabinoids (Synthetic) by LC-MS/MS

Application #AN2540

Conditions

Column: ACE Excel 3 C18-AR
Dimensions: 100 x 3.0 mm
Part Number: EXL-119-1003U
Mobile Phase: A: 15 mM ammonium formate pH 4.0 in H_2O
B: 0.1% formic acid in MeCN

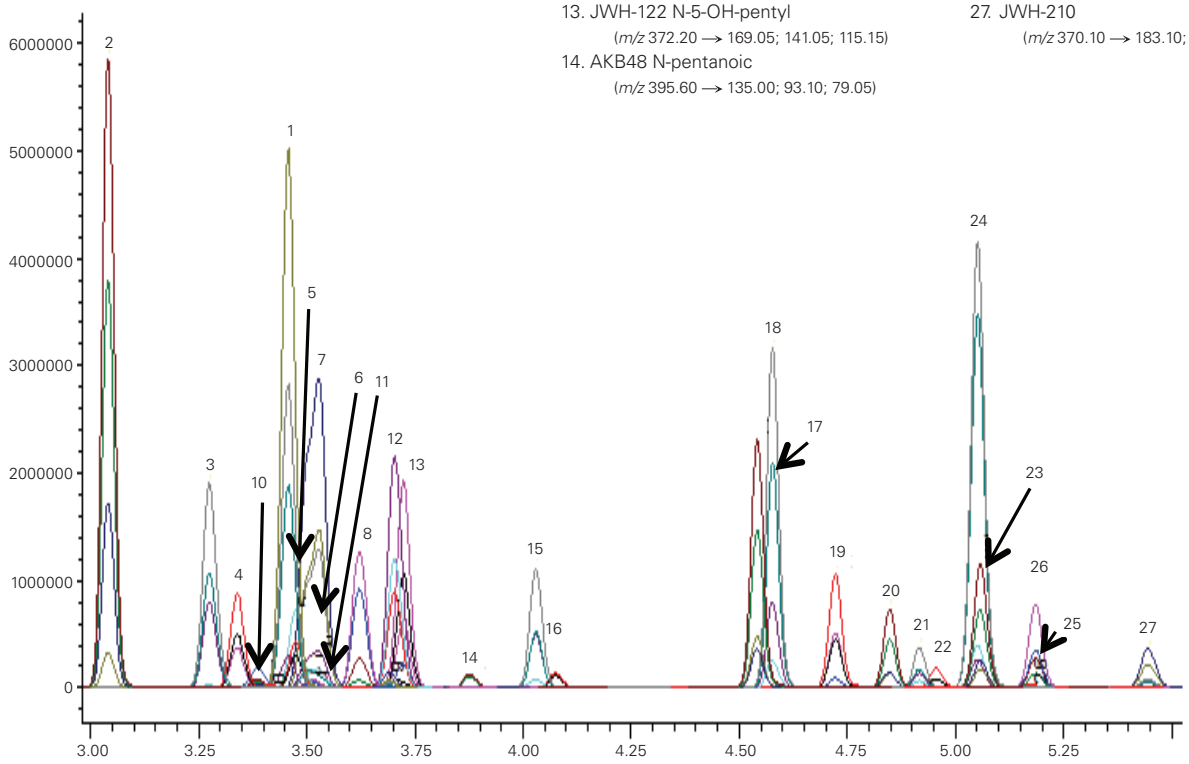
Gradient:

Time (mins)	%B
0.00	40
3.74	90
8.00	90
8.50	40

Flow Rate: 0.5 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: Shimadzu LCMS 8040 MS
Positive ion ESI

Analytes

1. JWH-018 N-5-OH-pentyl-d5
(*m/z* 362.90 → 155.05; 127.00; 128.05)
2. JWH-250 N-5-OH-pentyl
(*m/z* 352.20 → 121.15; 91.10; 186.05)
3. JWH-073 N-4-OH-butyl
(*m/z* 344.20 → 155.00; 127.10; 54.95)
4. JWH-018 N-pentanoic
(*m/z* 372.20 → 155.05; 127.10)
5. JWH-018 N-5-OH-pentyl
(*m/z* 357.80 → 155.05; 127.05)
6. AM2201 N-4-OH-pentyl
(*m/z* 376.40 → 155.00; 127.00; 144.00)
7. AM2201 5/6-OH-indole
(*m/z* 375.90 → 155.05; 127.05; 248.10)
8. JWH-081 N-5-OH-pentyl
(*m/z* 388.20 → 185.05; 157.05; 114.15)
9. MAM2201 N-4-OH-pentyl
(*m/z* 389.60 → 169.00; 141.05; 115.15)
10. AB-CHMINACA
(*m/z* 356.70 → 241.05; 312.20; 340.15)
11. UR-144 N-pentanoic
(*m/z* 341.60 → 125.10; 55.05; 57.10)
12. JWH-019 N-6-OH-hexyl
(*m/z* 371.80 → 155.05; 127.00; 144.00)
13. JWH-122 N-5-OH-pentyl
(*m/z* 372.20 → 169.05; 141.05; 115.15)
14. AKB48 N-pentanoic
(*m/z* 395.60 → 135.00; 93.10; 79.05)
15. JWH-018 5-OH-indole
(*m/z* 358.20 → 155.00; 127.05; 230.05)
16. AKB48 N-5-OH-pentyl
(*m/z* 381.60 → 135.10; 93.10; 79.05)
17. JWH-210 5-OH-indole
(*m/z* 386.10 → 183.05; 153.10; 155.05)
18. PB-22
(*m/z* 358.80 → 214.05; 144.05; 116.00)
19. JWH-073
(*m/z* 328.20 → 127.10; 155.05; 200.10)
20. EAM2201
(*m/z* 387.70 → 183.10; 232.10; 155.10)
21. JWH-122 N-4-pentenyl
(*m/z* 353.70 → 169.05; 141.10; 115.10)
22. JWH-018
(*m/z* 341.70 → 155.00; 127.05; 214.10)
23. JWH-081
(*m/z* 372.10 → 185.05; 157.15; 127.10)
24. AKB48F
(*m/z* 384.30 → 135.15; 107.10; 93.10)
25. THJ-018
(*m/z* 342.60 → 215.10; 145.05; 90.00)
26. JWH-122
(*m/z* 356.30 → 169.05; 141.10; 115.15)
27. JWH-210
(*m/z* 370.10 → 183.10; 155.10; 153.10)



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Cannabinoids in Rat Plasma

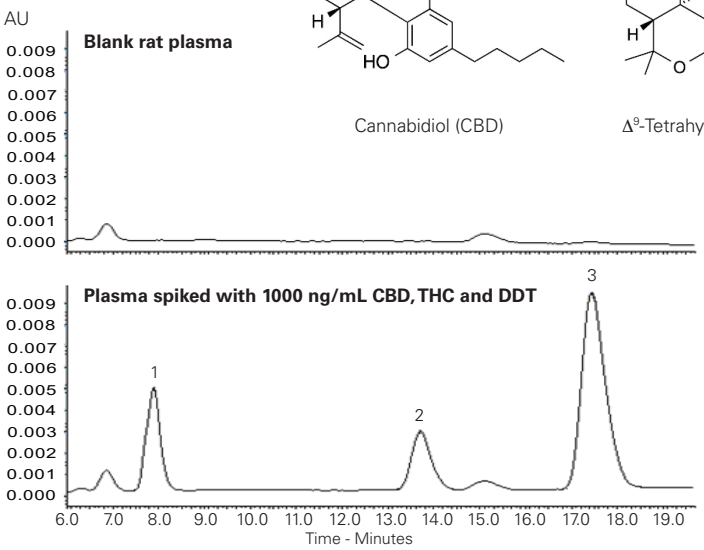
Application #AN2310

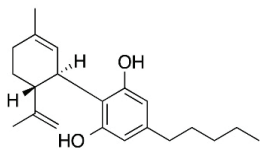
Conditions

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

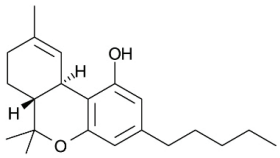
Analytes

1. Cannabidiol (CBD)
2. Δ^9-Tetrahydrocannabinol (THC)
3. 4,4-Dichlorodiphenyltrichloroethane (DDT) (IS)

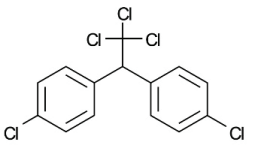




Cannabidiol (CBD)



Δ^9-Tetrahydrocannabinol (THC)



4,4-Dichlorodiphenyltrichloroethane (DDT) (IS)

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

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Carglumic Acid in Human Plasma by LC-MS/MS

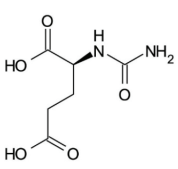
Application #AN3750

Conditions

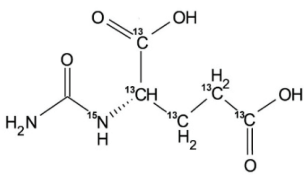
Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: MeCN/MeOH/0.1% acetic acid pH 3.2 (40:40:20 v/v/v)
Flow Rate: 1 mL/min
Temperature: 40 °C
Detection: MDS Sciex API-4000 triple quad MS
Negative ion mode ESI
Ion source temperature: 500 °C
Ion spray voltage: -4500 V
20% split flow to ion spray interface

Analytes

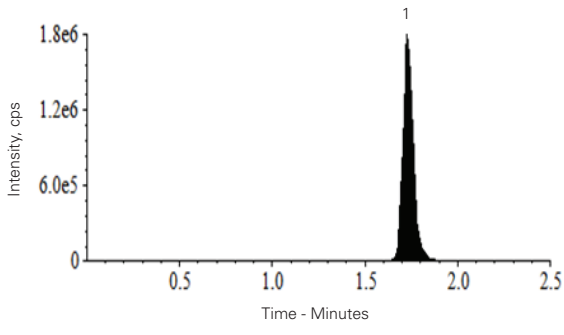
1. Carglumic acid
   (*m/z* 189 → 146)
   (LLOQ 6.0 ng/mL)
2. Carglumic acid-^{13}C ^{15}N (I.S)
   (*m/z* 195 → 152)

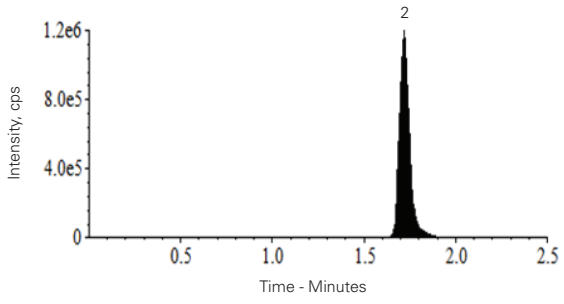


Carglumic acid



Carglumic acid-^{13}C ^{15}N (I.S.)





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Catechins

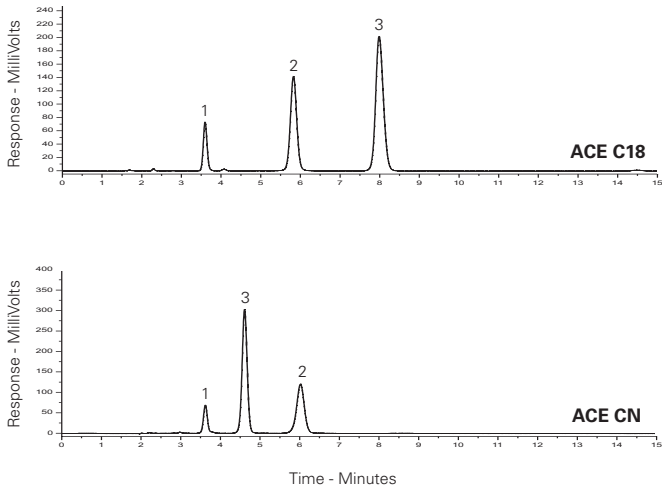
Application #AN3950

Conditions

Column: ACE 5 C18, ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546, ACE-124-1546
Mobile Phase: MeOH/0.1% formic acid in H_2O (25:75 v/v)
Flow Rate: 1 mL/min
Injection: 2 µL
Temperature: Ambient
Detection: UV, 280 nm

Analytes

1. Epigallocatechin
2. (+)-Epicatechin
3. Epigallocatechin gallate



Catecholamine Analysis (I)

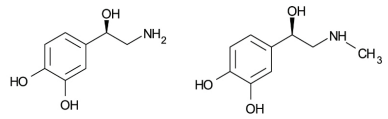
Application #AN2020

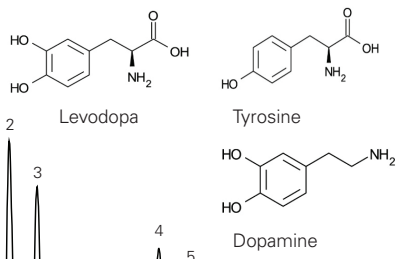
Conditions

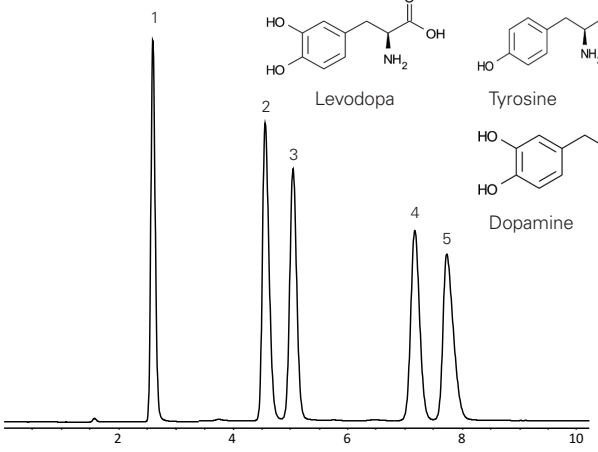
Column: ACE 5 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1210-1546
Mobile Phase: 12.5 mM ammonium formate pH 3.0 in H_2O
Flow Rate: 1 mL/min
Temperature: 22 °C
Detection: UV, 266 nm

Analytes

1. Norepinephrine
2. Epinephrine
3. Levodopa
4. Tyrosine
5. Dopamine







Catecholamine Analysis (II)

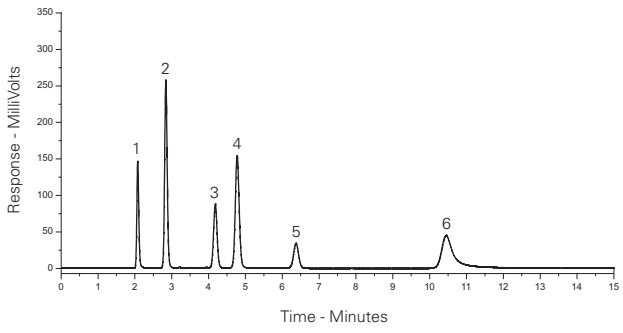
Application #AN3910

Conditions

Column: ACE 5 AQ
Dimensions: 150 x 4.6 mm
Part Number: ACE-126-1546
Mobile Phase: 50 mM KH_2PO_4 pH 3.0 in H_2O
Flow Rate: 1 mL/min
Injection: 2 µL
Temperature: Ambient
Detection: UV, 210 nm

Analytes

1. Noradrenaline (Norepinephrine)
2. Adrenaline (Epinephrine)
3. L-DOPA
4. Dopamine
5. L-Tyrosine
6. VMA (Vanillylmandelic acid)



Catecholamines by LC-MS/MS

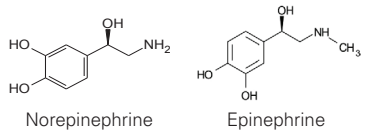
Application #AN2320

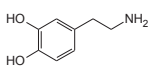
Conditions

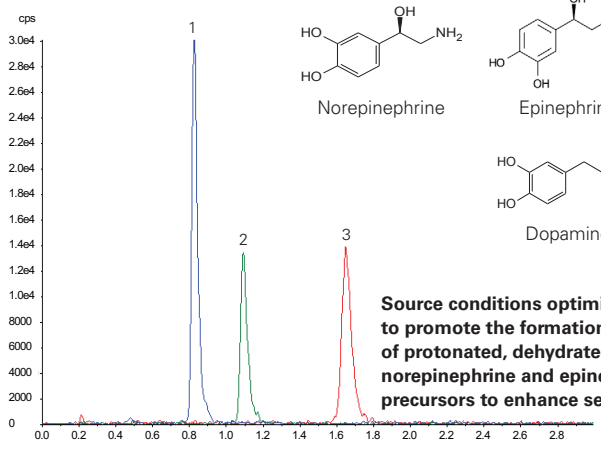
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: 2 mM ammonium formate pH 3.2/MeOH (98:2 v/v)
Flow Rate: 0.4 mL/min
Injection: 20 µL
Temperature: 40 °C
Detection: AB SCIEX triple quad 5500
Positive ESI mode
Source temperature: 700 °C
IonSpray voltage: 5500 V

Analytes

1. Norepinephrine
   (*m/z* 152.1 → 107.1)
2. Epinephrine
   (*m/z* 166.1 → 107.1)
3. Dopamine
   (*m/z* 154.1 → 91.1)







Source conditions optimised to promote the formation of protonated, dehydrated norepinephrine and epinephrine precursors to enhance sensitivity.

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Catecholamines and their Metabolites in Urine by LC-MS/MS

Application #AN4040

Conditions

Column: ACE UltraCore 2.5 SuperPhenylHexyl
Dimensions: 100 x 2.1 mm
Part Number: CORE-25B-1002U
Mobile Phase: A: 2 mM ammonium formate + 0.05% formic acid in H_2O
B: 2 mM ammonium formate + 0.05% formic acid in MeOH

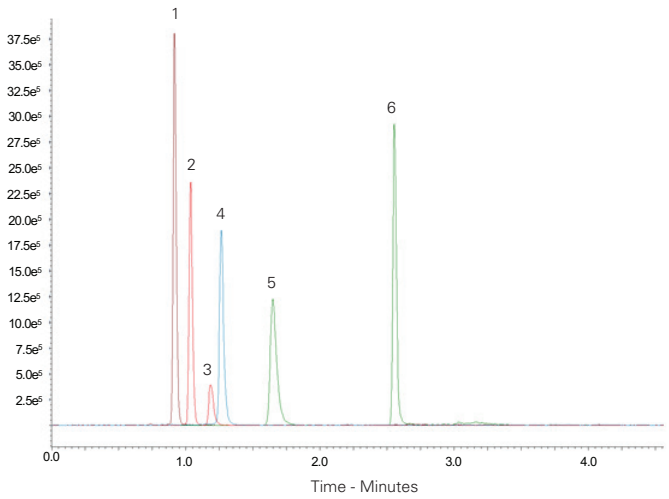
Gradient:

Time (mins)	%B
0.00	0
1.00	70
1.10	70
1.11	0
4.50	0

Flow Rate: 0.3 mL/min
Injection: 10 µL
Temperature: 30 °C
Detection: Shimadzu LCMS-8040
ESI in positive ion mode
Sample: Standard 100 ng/mL in urine (after SPE purification)

Analytes

1. Norepinephrine (*m/z* 170 → 107)
2. Epinephrine (*m/z* 184 → 166)
3. Normetanephrine (*m/z* 184 → 166)
4. Dopamine (*m/z* 154 → 91)
5. Metanephrine (*m/z* 198 → 180)
6. 3-Methoxytyramine (*m/z* 181 → 91)



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Catecholamines and Metanephrines Separation (Gradient)

Application #AN1480

Conditions

Column: ACE 5 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1210-1546
Mobile Phase: A: 20 mM ammonium formate pH 3.0 in H_2O
B: 20 mM ammonium formate pH 3.0 in MeOH/H_2O (90:10 v/v)

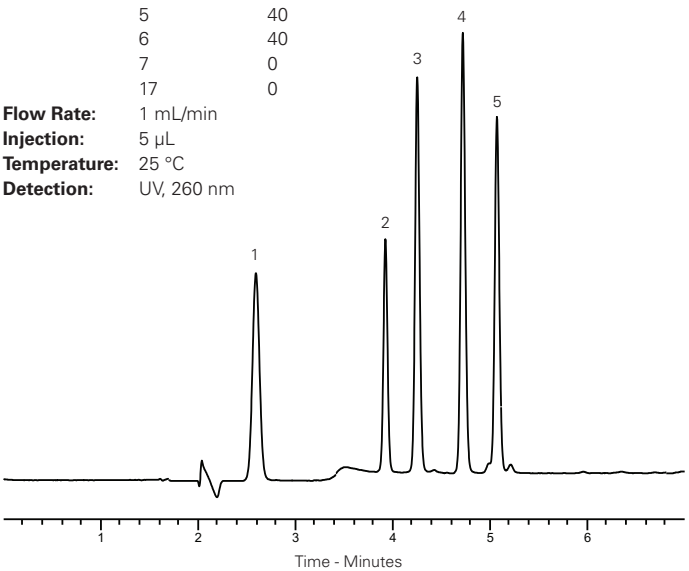
Gradient:

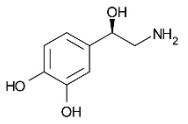
Time (mins)	%B
0	0
5	40
6	40
7	0
17	0

Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: UV, 260 nm

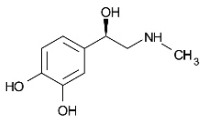
Analytes

1. Norepinephrine
2. Epinephrine
3. Normetanephrine
4. Dopamine
5. Metanephrine

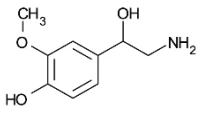




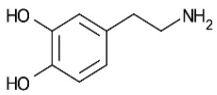
Norepinephrine



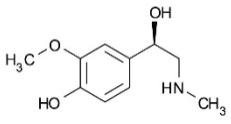
Epinephrine



Normetanephrine



Dopamine



Metanephrine

Catecholamines and Metanephrines Separation (Isocratic)

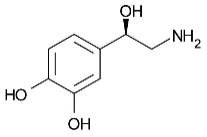
Application #AN1490

Conditions

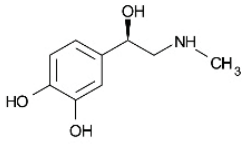
Column: ACE 5 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1210-1546
Mobile Phase: 20 mM ammonium formate pH 3.0 in H_2O
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: UV, 260 nm

Analytes

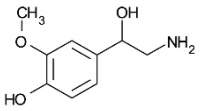
1. Norepinephrine
2. Epinephrine
3. Normetanephrine
4. Dopamine
5. Metanephrine



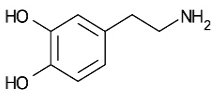
Norepinephrine



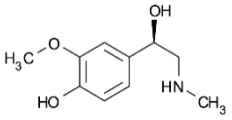
Epinephrine



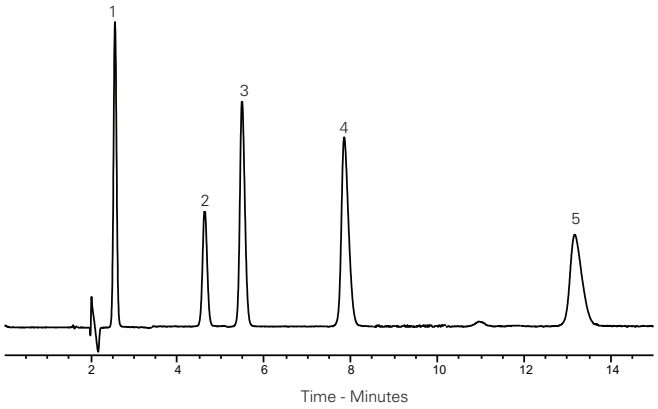
Normetanephrine



Dopamine



Metanephrine



Catecholamines from Plasma

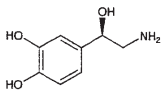
Application #AN3210

Conditions

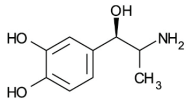
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 50 mM sodium acetate pH 7.0/MeCN/MeOH (50:35:15 v/v/v)
Flow Rate: 0.9 mL/min
Temperature: Ambient
Detection: Fluorescence – λ_{Ex} 350 nm, λ_{Em} 480 nm
Sample: Ion pair extraction using diphenyl-borate-ethanolamine. Derivatisation using diphenyl-ethylenediamine as fluorescent probe

Analytes

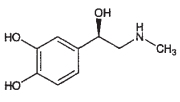
1. Noradrenaline (Norepinephrine)
2. 3,4-Dihydroxynorephedrine (I.S.)
3. Adrenaline (Epinephrine)



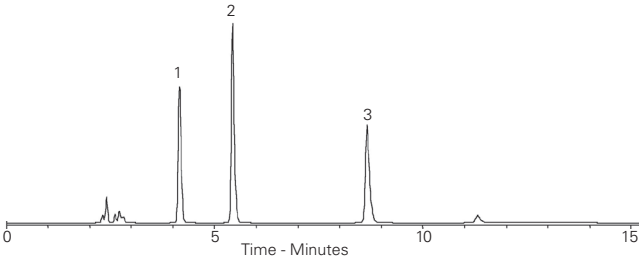
Noradrenaline



3,4-Dihydroxynorephedrine (I.S.)



Adrenaline



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Catecholamines from Urine

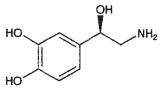
Application #AN3200

Conditions

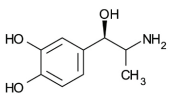
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 50 mM sodium acetate pH 7.0/MeCN/MeOH (50:35:15 v/v/v)
Flow Rate: 0.9 mL/min
Temperature: Ambient
Detection: Fluorescence – λ_{Ex} 350 nm, λ_{Em} 480 nm
Sample: Ion pair extraction using diphenyl-borate-ethanolamine. Derivatisation using diphenyl-ethylenediamine as fluorescent probe

Analytes

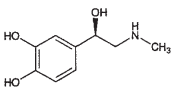
1. Noradrenaline (Norepinephrine)
2. 3,4-Dihydroxynorephedrine (I.S.)
3. Adrenaline (Epinephrine)
4. Dopamine



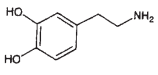
Noradrenaline



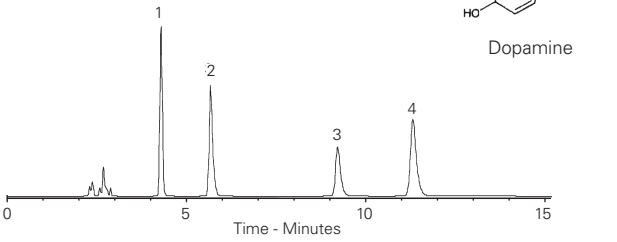
3,4-Dihydroxynorephedrine (I.S.)



Adrenaline



Dopamine



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Catechols Mixture Separations (I) and (II)

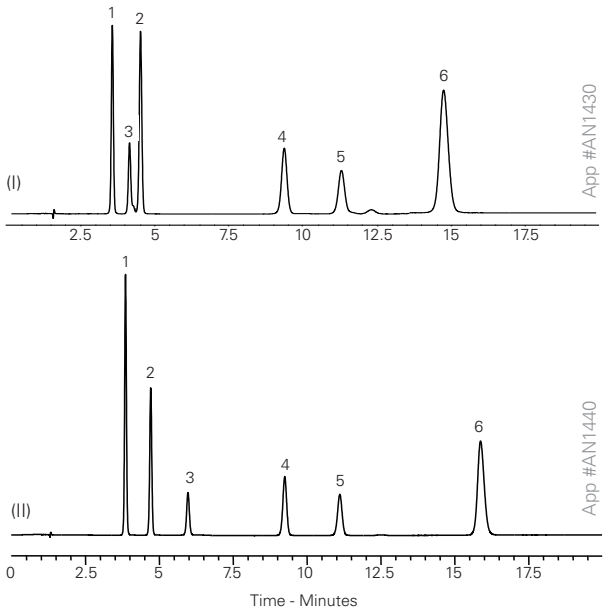
Application #AN1430 and #AN1440

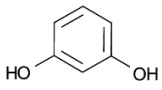
Conditions

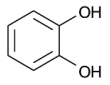
Column: (I) ACE Excel 3 CN-ES (II) ACE Excel 3 C18-Amide
Dimensions: 150 x 4.6 mm
Part Number: (I) EXL-1113-1546U (II) EXL-1112-1546U
Mobile Phase: (I) 20 mM H_3PO_4 in MeCN/H_2O (25:75 v/v)
(II) 20 mM H_3PO_4 in MeCN/H_2O (10:90 v/v)
Flow Rate: 1.5 mL/min
Injection: 5 µL
Temperature: 30 °C
Detection: UV, 270 nm

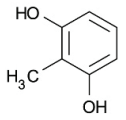
Analytes

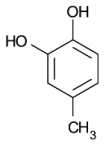
1. Resorcinol
2. Catechol
3. 2-Methylresorcinol
4. 4-Methylcatechol
5. 3-Methylcatechol
6. 4-Nitrocatechol

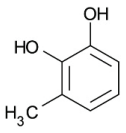


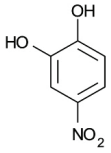

Resorcinol


Catechol


2-Methylresorcinol


4-Methylcatechol


3-Methylcatechol


4-Nitrocatechol

Cathinone Psychoactive Substances by LC-UV and LC-Amperometry

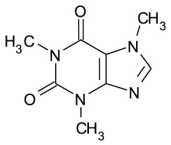
Application #AN3500

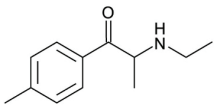
Conditions

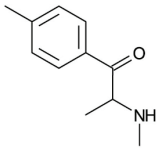
Column: ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-111-1546
Mobile Phase: 10 mM ammonium acetate-100 mM KCl pH 4.3/MeOH (70:30 v/v)
Flow Rate: 0.8 mL/min
Injection: 10 µL
Temperature: 22 °C
Detection: UV, 264 nm
Amperometric Potential +1.4 V

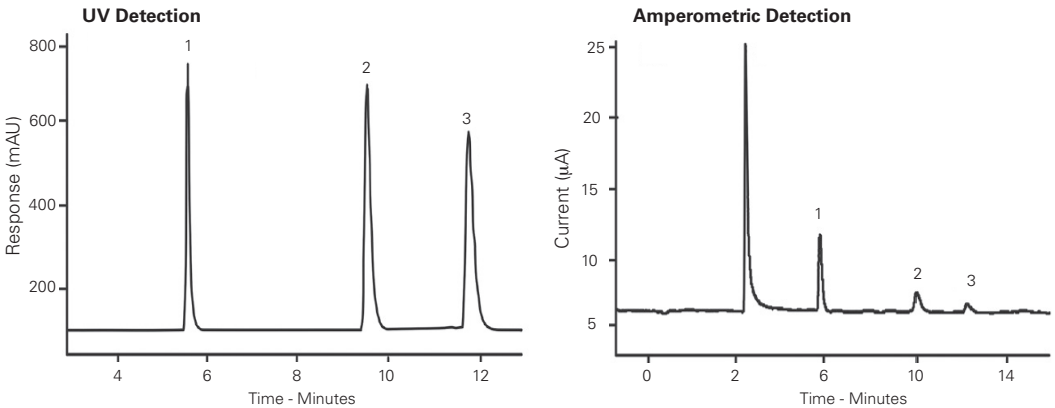
Analytes

1. Caffeine
2. 4-Methylmethcathinone (4-MMC, mephedrone)
3. 4-Methylethcathinone (4-MEC)


Caffeine


4-Methylethcathinone (4-MEC)


4-Methylmethcathinone (4-MMC, mephedrone)



Zuway K, Smith J, Foster C, Kapur N, Banks C, Sutcliffe O, (2015) Detection and quantification of new psychoactive substances (NPSs) within the evolved 'legal high' product, NRG-2, using high performance liquid chromatography-amperometric detection (HPLC-AD). Analyst 140, 6283. doi:10.1039/c5an01106j

Cefquinome by LC-MS

Application #AN3130

Conditions

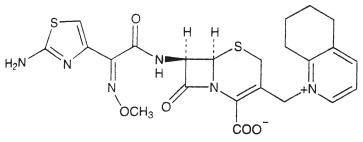
Column: ACE 5 C18
Dimensions: 150 x 2.1 mm
Part Number: ACE-121-1502
Mobile Phase: A: 2 mM formic acid in H_2O
B: 2 mM formic acid in MeCN
Gradient:

Time (mins)	%B
0	5
1	5
10	95
30	95

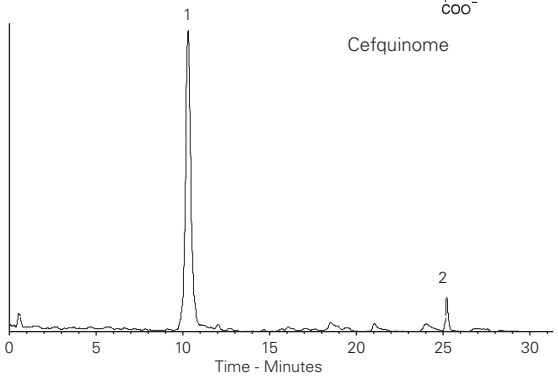
Flow Rate: 0.2 mL/min
Temperature: 25 °C
Detection: ESI-MS (+)

Analytes

1. Cefquinome (*m/z* 529.2)
2. Excipient



Cefquinome



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Ciprofibrate from Human Plasma by LC-MS/MS

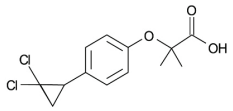
Application #AN2670

Conditions

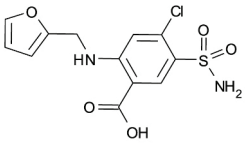
Column: ACE 5 C18
Dimensions: 50 x 4.6 mm
Part Number: ACE-121-0546
Mobile Phase: 0.001 % ammonia in MeOH/MeCN/H_2O (70:20:10 v/v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: API 3200 triple quad MS
ESI in negative ion mode
Ion source temperature: 550 °C
Ion spray voltage: 4500 V

Analytes

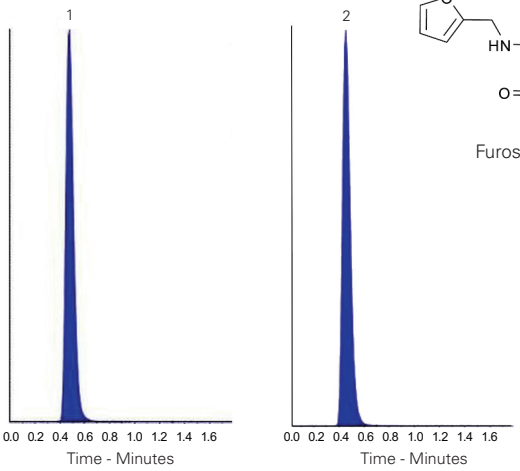
1. Ciprofibrate (*m/z* 287.0 → 85.0)
2. Furosemide (IS) (*m/z* 328.9 → 204.9)



Ciprofibrate



Furosemide (IS)



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Chloramphenicol in Milk by LC-MS/MS

Application #AN2030

Conditions

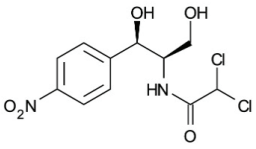
Column: ACE 3 C18
Dimensions: 50 x 2.1 mm
Part Number: ACE-111-0502
Mobile Phase: A: H_2O
B: MeOH
Gradient:

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

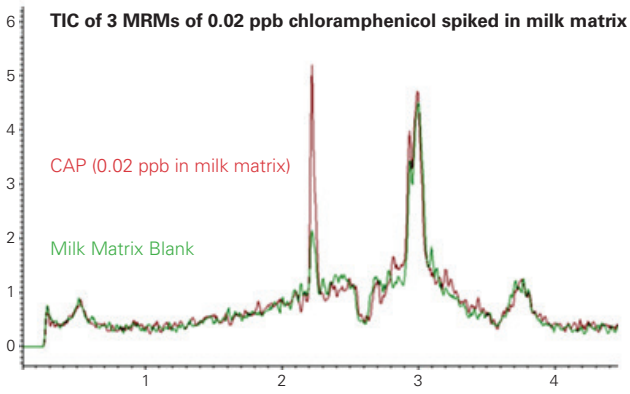
Flow Rate: 0.5 mL/min
Injection: 10 µL
Detection: Bruker EVOQ Elite triple quad MS
VIP heated-ESI temperature: 400 °C
Cone gas temperature: 350 °C
Spray voltage: -4500 V

Analyte

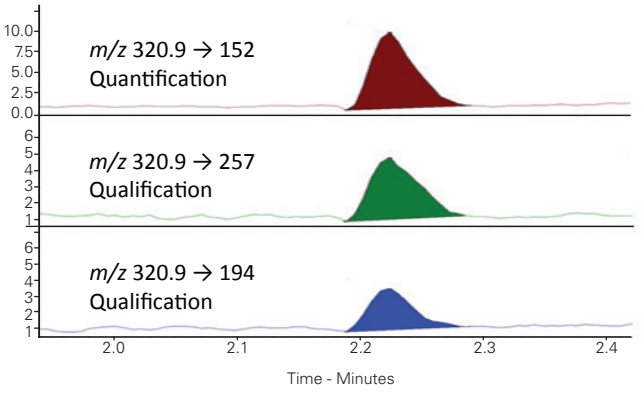
1. Chloramphenicol



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



MRM chromatograms of 0.05 ppb chloramphenicol in milk



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Chocolate Analysis

Application #AN2040

Conditions

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

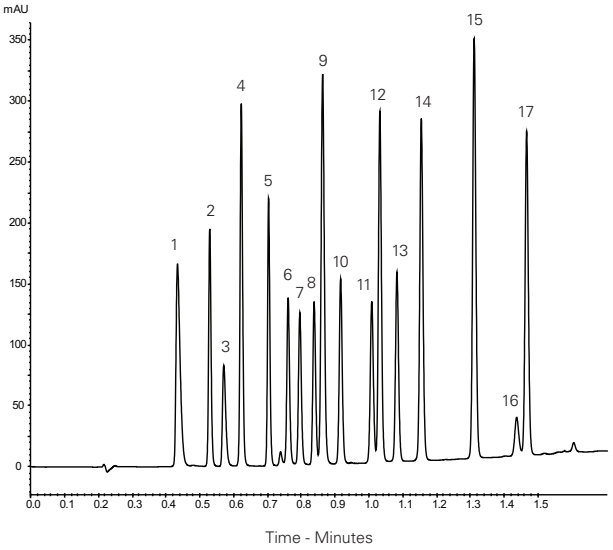
Gradient:

Time (mins)	%B
0.0	5
1.5	85

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

Analytes

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



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Clenbuterol in Equine Plasma by LC-MS/MS

Application #AN2050

Conditions

Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002
Mobile Phase: A: 0.2% formic acid in H_2O
B: 0.2% formic acid in MeCN

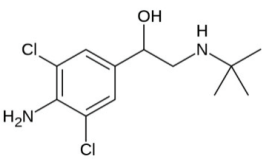
Gradient:

Time (mins)	%B
0.0	10
0.3	10
2.5	95
2.8	10
4.5	10

Flow Rate: 0.45 mL/min
Injection: 30 µL
Detection: Bruker EVOQ Elite triple quad MS
VIP heated-ESI temperature: 300 °C
Cone gas temperature: 300 °C
Spray voltage: +3500 V

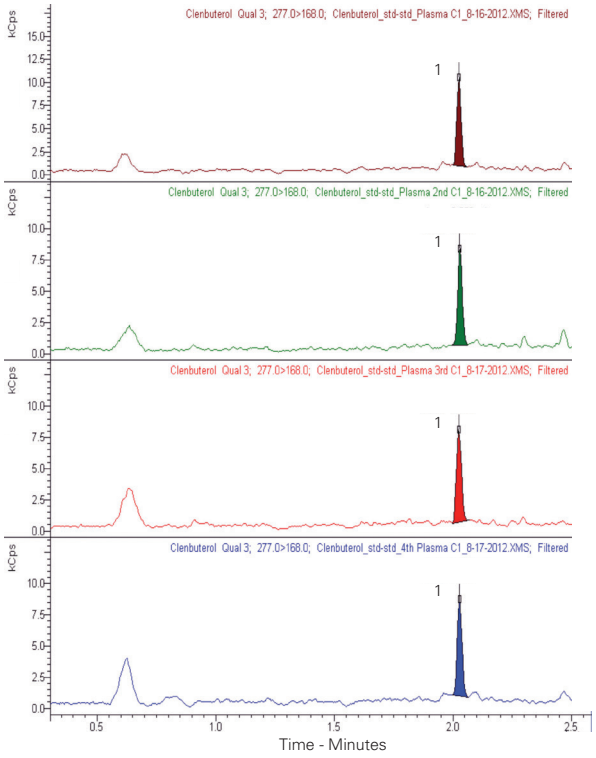
Analyte

1. Clenbuterol
(*m/z* 277.1 → 168)
d9-Clenbuterol (IS)
(*m/z* 286.1 → 204)



Clenbuterol

Representative MRM chromatograms of 5 ppt clenbuterol (150 fg on-column)



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Clonidine Hydrochloride Oral Solution Containing Preservatives

Application #AN2060

Conditions

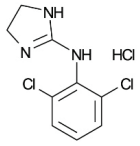
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	50 x 4.6 mm
Part Number:	CORE-25A-0546U
Mobile Phase:	A: 0.2% w/v phosphate buffer/ MeOH/MeCN (80:10:10 v/v/v) B: MeCN

Gradient:	**Time (mins)**	**%B**
	0.0	0
	0.8	0
	2.1	70
	3.4	70
	3.5	0

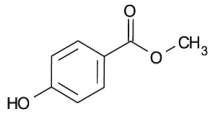
Flow Rate:	2 mL/min
Injection:	100 µL
Temperature:	20 °C
Detection:	UV, 220 nm

Analytes

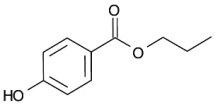
1. Clonidine HCl (10 µg/mL)
2. Methyl paraben (1.5 g/mL)
3. Propyl paraben (1.5 g/mL)



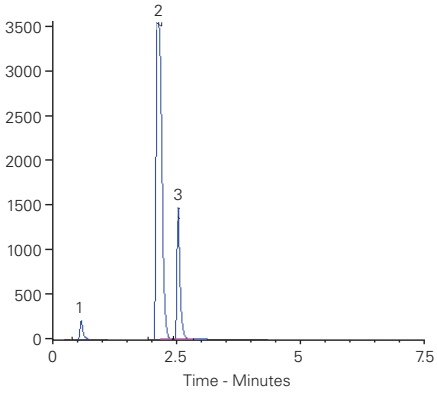
Clonidine HCl



Methyl paraben



Propyl paraben



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Clopidogrel and Photodegradation Products

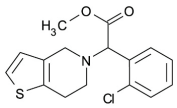
Application #AN3110

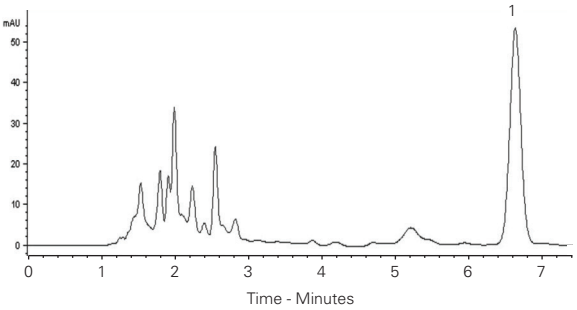
Conditions

Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	MeOH/aqueous TEA (pH 5.3 with H_3PO_4) (75:25 v/v)
Flow Rate:	1.2 mL/min
Injection:	20 µL
Temperature:	25 °C
Detection:	UV, 220 nm
Sample:	Exposed to UV light for 3.5 hours

Analyte

1. Clopidogrel





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

email: info@ace-hplc.com

Coffee Metabolite Profiling by LC-MS

Application #AN2590

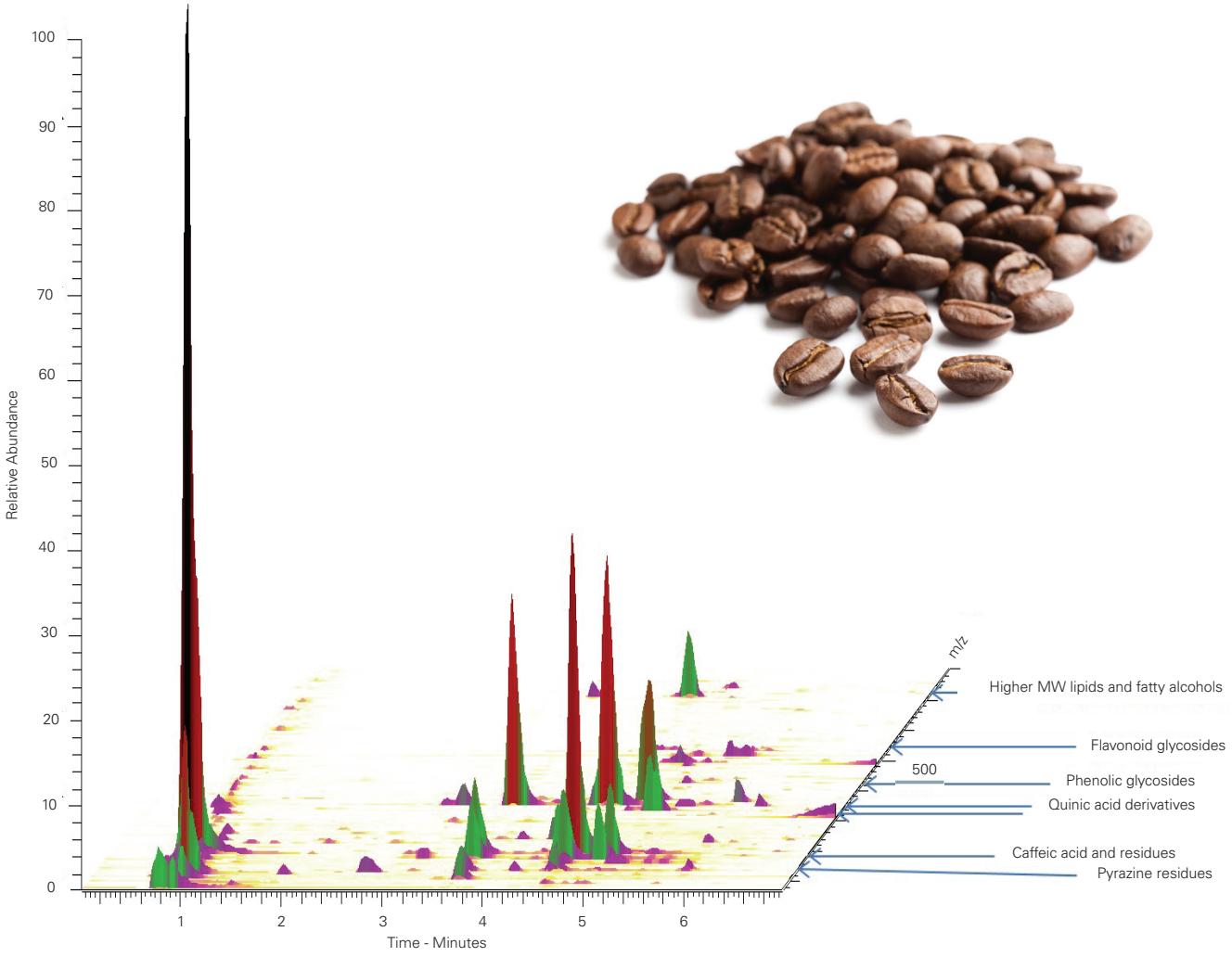
Conditions

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

Gradient:

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

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



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Cold Medicine Analytes (I) and (II)

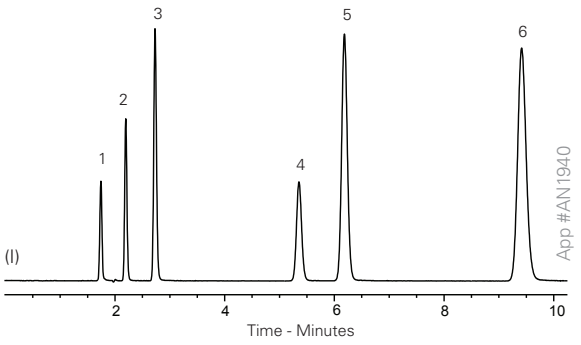
Application #AN1940 and #AN2410

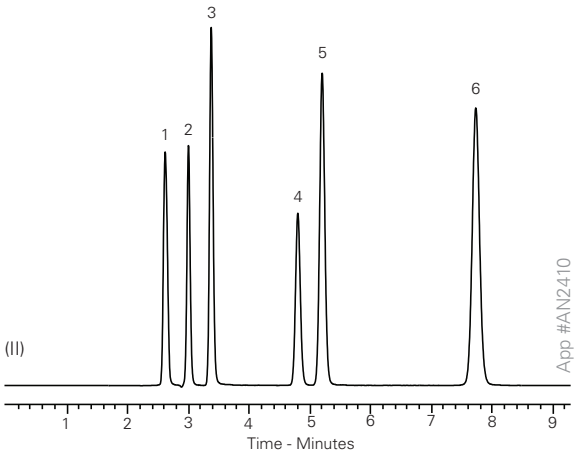
Conditions

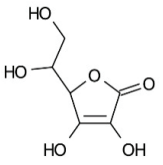
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: (I) 20 mM phosphoric acid in MeOH/H_2O (25:75 v/v)
(II) 0.1% formic acid in MeOH/H_2O (55:45 v/v)
Flow Rate: (I) 1.5 mL/min (II) 1.0 mL/min
Injection: 5 µL
Temperature: (I) 40 °C (II) 25 °C
Detection: (I) UV, 280 nm (II) UV, 275 nm

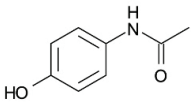
Analytes

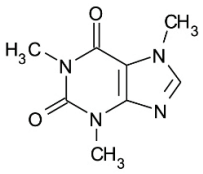
1. Ascorbic acid
2. Paracetamol
3. Caffeine
4. Aspirin
5. Ethenzamide
6. Salicylic acid

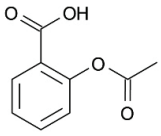


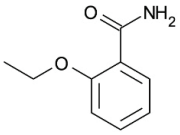


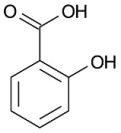

Ascorbic acid


Paracetamol


Caffeine


Aspirin


Ethenzamide


Salicylic acid

Corticosteroids by LC-MS/MS

Application #AN1030

Conditions

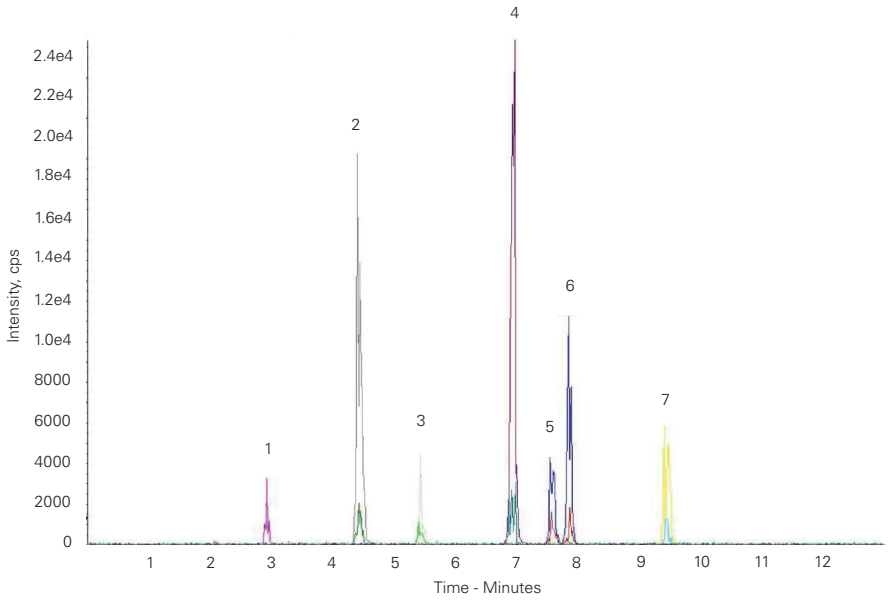
Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: 0.1% formic acid in H_2O
B: MeCN/0.1% formic acid in H_2O (90:10 v/v)
Gradient:

Time (mins)	%B
0	30
14	50
17	95
20	30

Flow Rate: 0.3 mL/min
Injection: 25 µL
Temperature: 15 °C
Detection: Turbospray, MRM

Analytes

1. Triamcinolone
2. Prednisolone
3. Fluoroprednisolone
4. Methylprednisolone
5. Betamethasone
6. Dexamethasone
7. Flumethasone



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Cortisol in Urine by LC-MS/MS

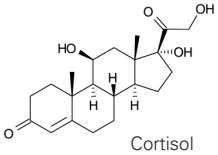
Application #AN2680

Conditions

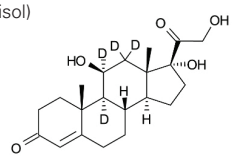
Column: ACE Excel 2 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-101-1002U
Mobile Phase: 4 mM ammonium acetate in H_2O/0.2% (v/v) formic acid in MeOH (71.5:28.5 v/v)
Flow Rate: 0.7 mL/min
Injection: 50 µL
Temperature: 50 °C
Detection: Applied Biosystems 5000 MS/MS APCI in positive ion mode
Sample: BioRad Liquichek Urine Quality Control standard (16 nmol/L cortisol)

Analytes

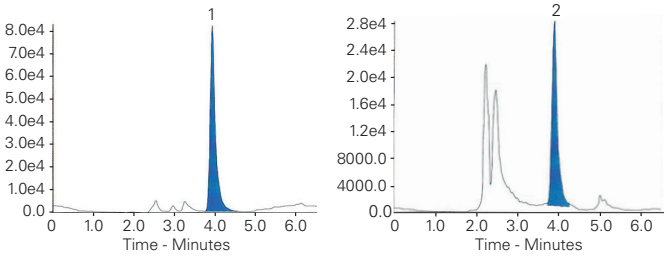
1. Cortisol
   (*m/z* 363.5 → 121.3)
2. Cortisol-d4 (IS)
   (*m/z* 367.3 → 331.3)



Cortisol



Cortisol-d4 (IS)



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Cyclosporin Mixture

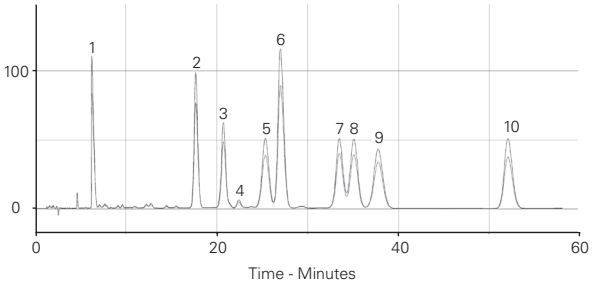
Application #AN3270

Conditions

Column: ACE 5 C18
Dimensions: 250 x 3.0 mm
Part Number: ACE-121-2503
Mobile Phase: H_2O/MeCN/MTBE/H_3PO_4 (46:51:3:0.1 v/v/v/v)
Flow Rate: 0.8 mL/min
Temperature: 80 °C
Detection: UV, 210 nm

Analytes

1. Isocyclosporin A
2. Cyclosporin C
3. Cyclosporin B
4. Cyclosporin L
5. Cyclosporin U
6. Cyclosporin A
7. Dihydrocyclosporin A
8. Cyclosporin G
9. Cyclosporin D
10. Cyclosporin E



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Cyclodextrin-Encapsulated Flavour Compounds in Beer

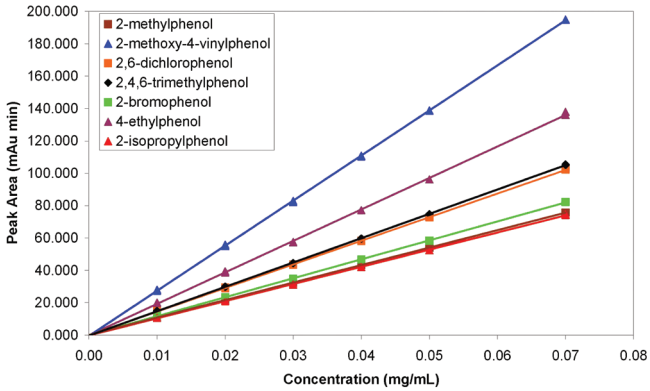
Application #AN2300

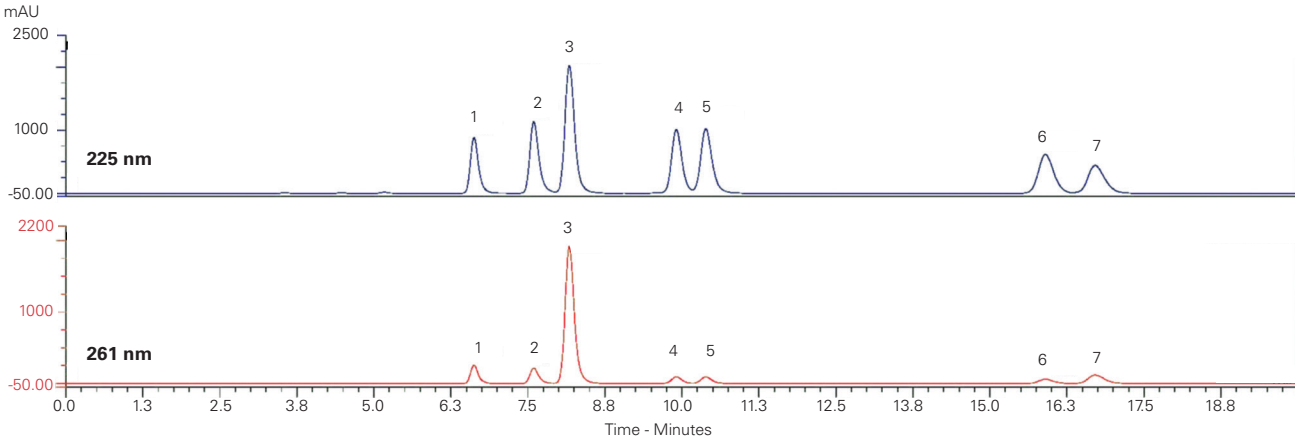
Conditions

Column: ACE 3 C18
Dimensions: 150 x 4.0 mm
Part Number: ACE-111-1504
Mobile Phase: 0.1% phosphoric acid in MeOH/H_2O (53:47 v/v)
Flow Rate: 0.5 mL/min
Injection: 20 µL
Temperature: 35 °C
Detection: UV, 225 nm and 261 nm

Analytes

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





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Cytarabine Analogues by Ion-Pairing LC-MS/MS

Application #AN2070

Conditions

Column: ACE 3 C18
Dimensions: 50 x 2.1 mm
Part Number: ACE-111-0502
Mobile Phase: A: 0.1% perfluoropentanoic acid + 0.1% formic acid in H_2O
B: 0.1% perfluoropentanoic acid + 0.1% formic acid in MeCN

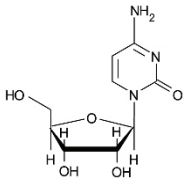
Gradient:

Time (mins)	%B
0.0	0
0.5	0
3.0	13
4.0	90
5.0	0

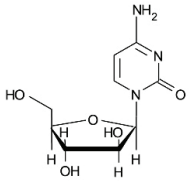
Flow Rate: 0.7 mL/min
Detection: API 4000 MS
TurbolonSpray, positive mode
Source Temperature 550 °C

Analytes

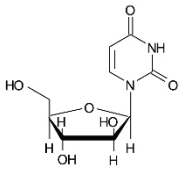
1. Uracil arabinofuranoside
   (*m/z* 245 → 113)
2. 5-Fluorocytidine (IS)
   (*m/z* 262 → 130)
3. Cytidine
   (*m/z* 244 → 112)
4. Cytarabine
   (*m/z* 244 → 112)



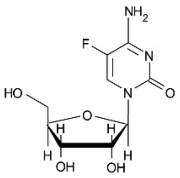
Cytidine



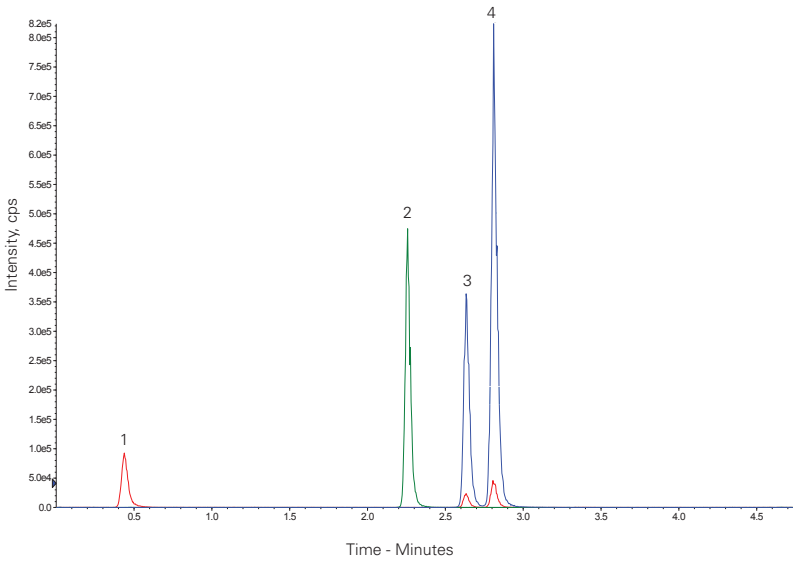
Cytarabine



Uracil arabinofuranoside



5-Fluorocytidine (IS)



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Cytotoxic Agents by UHPLC-MS/MS

Application #AN1070

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 2.1 mm
Part Number: CORE-25A-1002U
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN

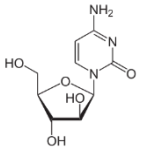
Gradient:

Time (mins)	%B
0.0	2
1.0	2
3.0	80
5.0	80
5.1	2
8.0	2

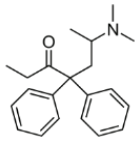
Flow Rate: 0.25 mL/min
Detection: Thermo Vantage triple quadrupole MS
MRM +ve ESI mode
Spray voltage: 3500 V
Nitrogen sheath and auxiliary gas
CID with argon: 1.5 mTorr

Analytes

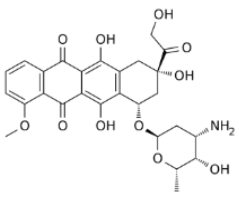
1. AraC
   (*m/z* 244.1 → 112.2)
2. Methadone
   (*m/z* 310.2 → 265.3)
3. Doxorubicin
   (*m/z* 544.2 → 361.2)
4. Etoposide
   (*m/z* 589.2 → 185.1)



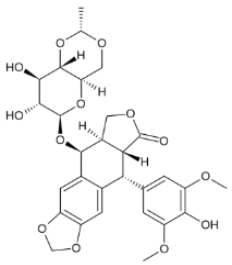
AraC



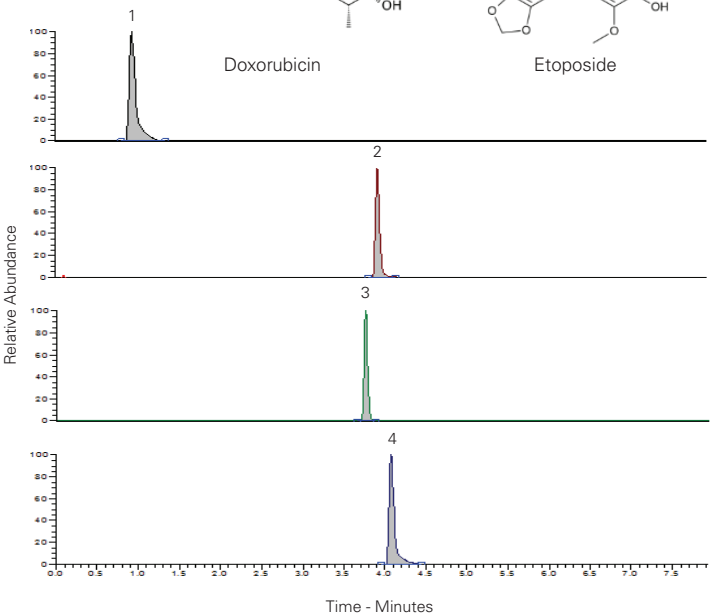
Methadone



Doxorubicin



Etoposide



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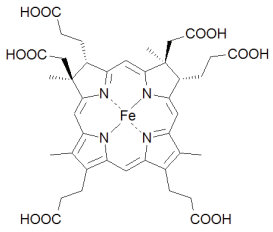
Decarboxylation of Sirohaem by Sirohaem Decarboxylase

Application #AN3830

Conditions

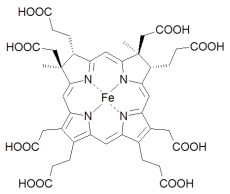
Column:	ACE 5 AQ	
Dimensions:	150 x 2.1 mm	
Part Number:	ACE-126-1502	
Mobile Phase:	A: 0.1% TFA in H_2O	
	B: MeCN	
Gradient:	**Time (mins)**	**%B**
	0	5
	6	20
	25	30
	35	100
	40	100
Flow Rate:	0.2 mL/min	
Detection:	DAD, 380 nm	



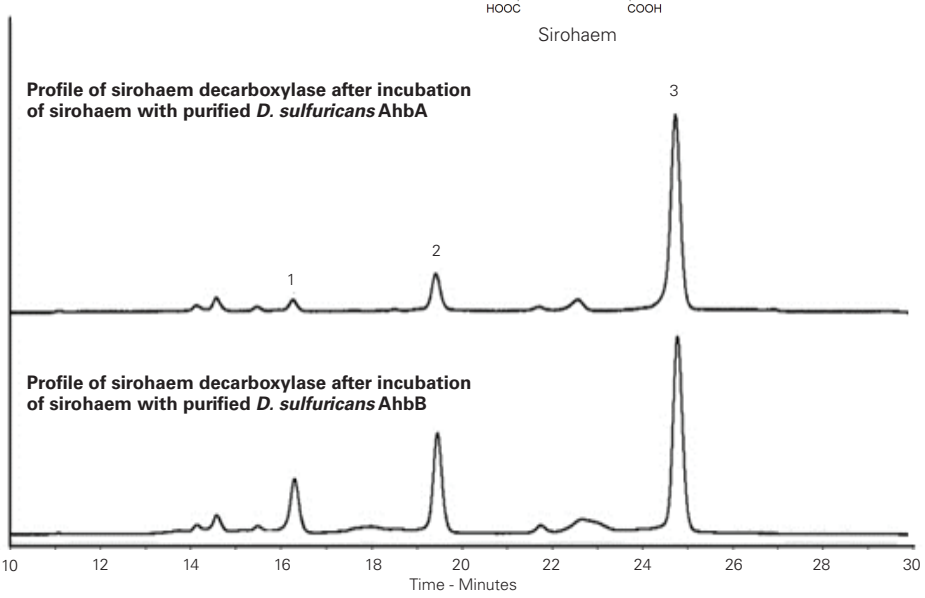
12,18-Didecarboxysirohaem

Analytes

1. Sirohaem
2. Monodecarboxysirohaem
3. 12,18-Didecarboxysirohaem



Sirohaem



Palmer DJ, Schroeder S, Lawrence AD, Deery E, Lobo SA, Saraiva LM, McLean KJ, Munro AW, Ferguson SJ, Pickersgill RW, Brown DG, Warren MJ. The structure, function and properties of sirohaem decarboxylase – an enzyme with structural homology to a transcription factor family that is part of an alternative haem biosynthesis pathway. Molecular Microbiology (2014) 93(2), 247-261. doi:10.1111/mmi.12656

Defensins (Human) in Saliva Matrix

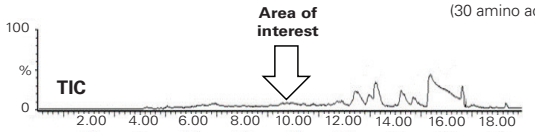
Application #AN1270

Conditions

Column:	ACE UltraCore 2.5 SuperC18	
Dimensions:	50 x 3.0 mm	
Part Number:	CORE-25A-0503U	
Mobile Phase:	A: 0.1% formic acid in H_2O	
	B: 0.1% formic acid in MeCN	
Gradient:	**Time (mins)**	**%B**
	0	2
	2	2
	17	50
	19	95
	20	95
Flow Rate:	0.6 mL/min	
Detection:	Synapt G1 QToF +ESI MS	
	Sampling cone voltage: 40 V	
	Source temperature: 150 °C	
	Capillary voltage: 4.8 kV	
	Extraction cone voltage: 41 kV	
	Desolvation temperature: 500 °C	
	Acquisition: 100-2000 *m/z*	
Sample:	SPE on C18	

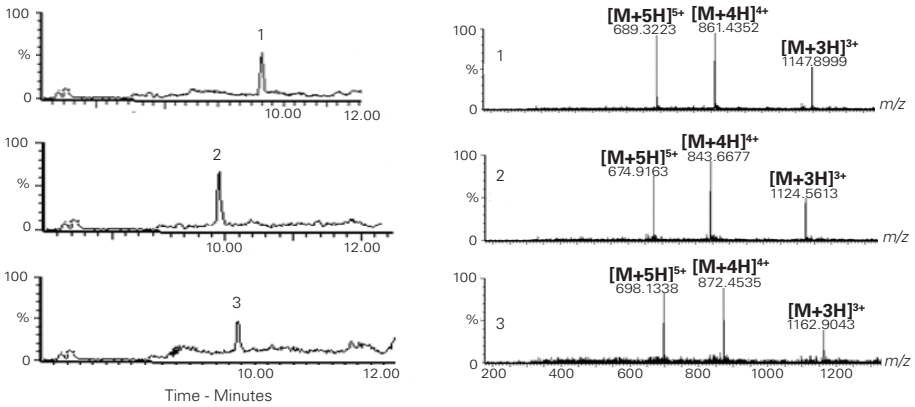
Defensin Human Neutrophil Peptides

1. HNP-1
   (30 amino acid residues)
2. HNP-2
   (29 amino acid residues)
3. HNP-3
   (30 amino acid residues)



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

Mass spectra



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Dermorphin in Equine Urine by LC-MS/MS

Application #AN1040

Conditions

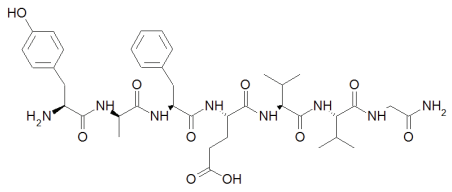
Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002
Mobile Phase: A: 0.2% formic acid in H_2O
B: 0.2% formic acid in MeCN

Gradient:

Time (mins)	%B
0.00	5
0.20	5
8.00	95
8.50	95
8.51	5
12.50	5

Flow Rate: 0.4 mL/min
Injection: 40 µL
Detection: Bruker EVOQ Elite triple quad MS
VIP heated-ESI temperature: 350 °C
Cone gas temperature: 250 °C
Spray voltage: +4000 V

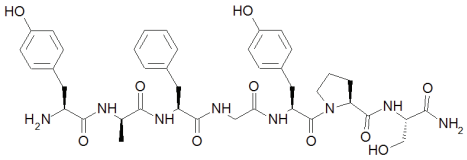
Accurate quantification of dermorphin in equine urine in range 0.05 – 100 ng/mL
LLOQ = 0.05 ng/mL



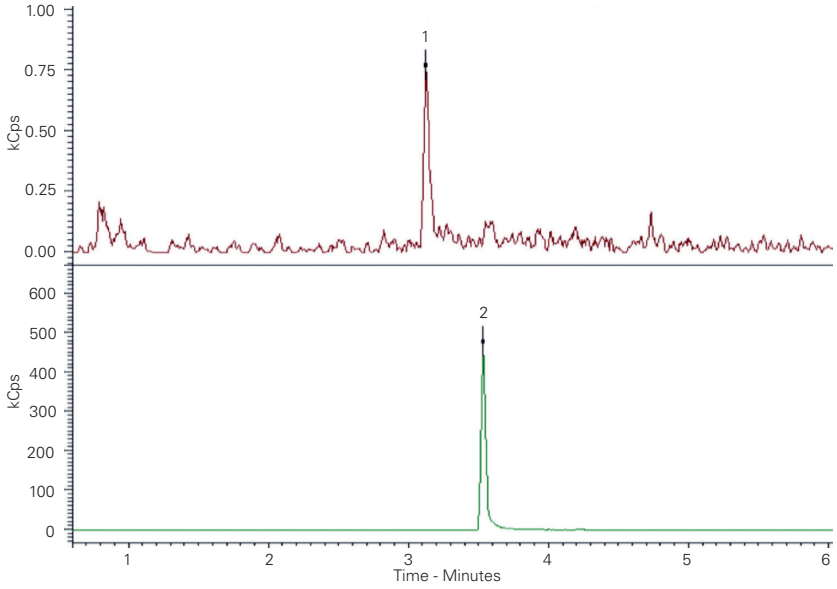
Deltorphin-II (IS)

Analytes

1. Dermorphin
(*m/z* 803.4 → 602 (Quantifier ion))
(*m/z* 803.4 → 202 (Qualifier ion))
2. Deltorphin-II (IS)
(*m/z* 783 → 277)



Dermorphin



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Didanosine

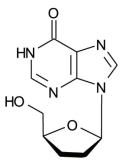
Application #AN3590

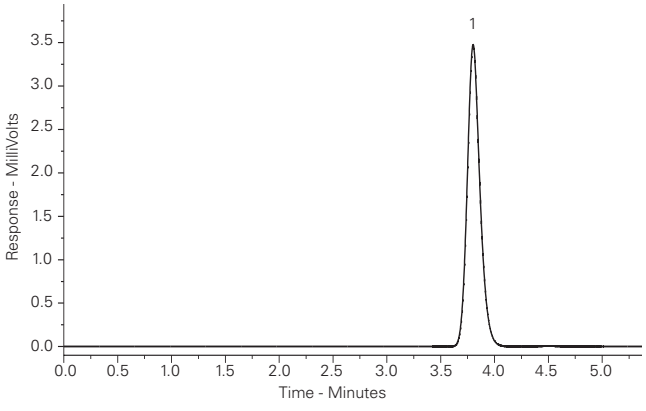
Conditions

Column: ACE 5 C18-HL
Dimensions: 250 x 4.6 mm
Part Number: ACE-321-2546
Mobile Phase: 50 mM ammonium acetate pH 8.0/MeOH (80:20 v/v)
Flow Rate: 1.5 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analyte

1. Didanosine





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Diuretics (Isocratic)

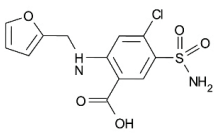
Application #AN2140

Conditions

Column: ACE Excel 2 C18-PFP
Dimensions: 50 x 3.0 mm
Part Number: EXL-1010-0503U
Mobile Phase: 10 mM ammonium formate pH 3.0 in MeOH/H_2O (45:55 v/v)
Flow Rate: 1 mL/min
Injection: 2 µL
Temperature: 60 °C
Detection: UV, 254 nm

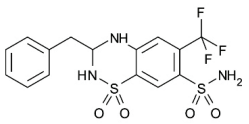
Analytes

1. Furosemide
2. Indapamide
3. Bendroflumethiazide
4. Spironolactone

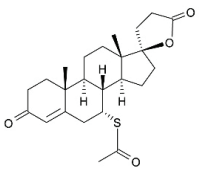


Furosemide

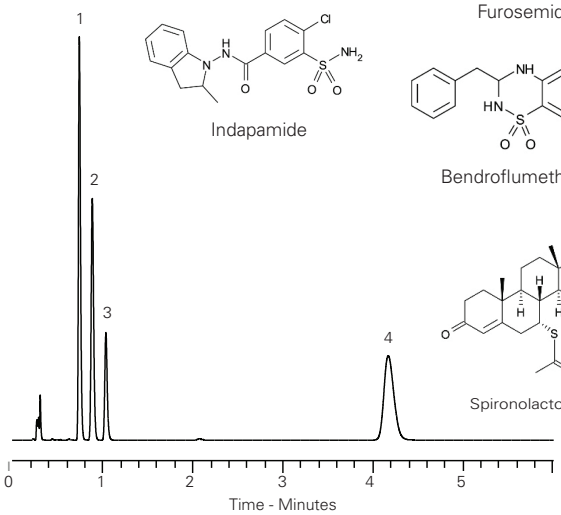
Indapamide



Bendroflumethiazide



Spironolactone



Diuretics

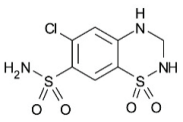
Application #AN1450

Conditions

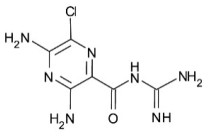
Column:	ACE Excel 2 C18-PFP
Dimensions:	50 x 3.0 mm
Part Number:	EXL-1010-0503U
Mobile Phase:	A: 10 mM ammonium formate pH 3.0 in H_2O B: 10 mM ammonium formate pH 3.0 in MeOH/H_2O (9:1 v/v)
Gradient:	**Time (mins) %B** 0.0 5 0.5 5 5.0 70 5.5 70 6.0 5
Flow Rate:	1 mL/min
Injection:	2 µL
Temperature:	60 °C
Detection:	UV, 254 nm

Analytes

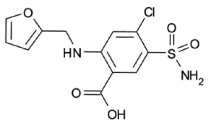
1. Hydrochlorothiazide
2. Amiloride
3. Furosemide
4. Indapamide
5. Bendroflumethiazide
6. Spironolactone



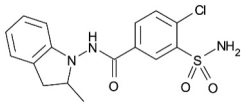
Hydrochlorothiazide



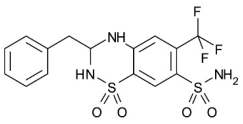
Amiloride



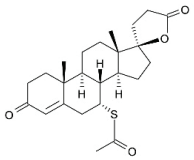
Furosemide



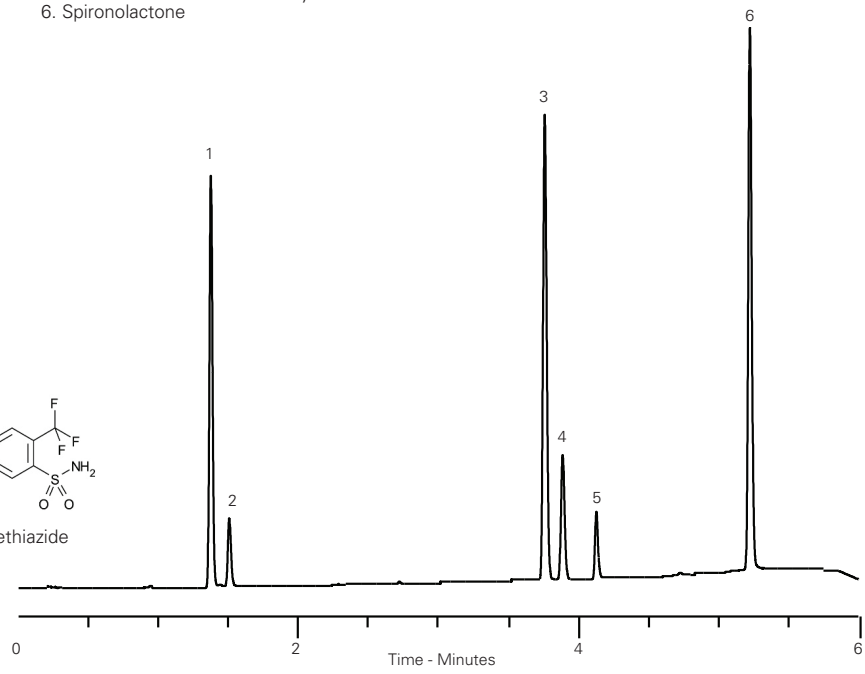
Indapamide



Bendroflumethiazide



Spironolactone



DOTATATE and Octreotide

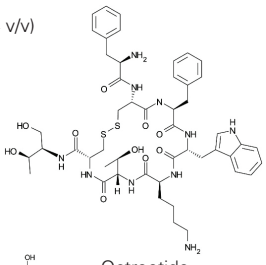
Application #AN2730

Conditions

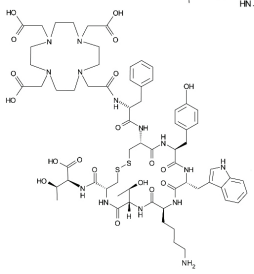
Column:	ACE 3 C18
Dimensions:	150 x 3.0 mm
Part Number:	ACE-111-1503
Mobile Phase:	0.1% TFA in H_2O/MeCN (76:24 v/v)
Flow Rate:	0.6 mL/min
Injection:	20 µL
Detection:	UV, 220 nm

Analytes

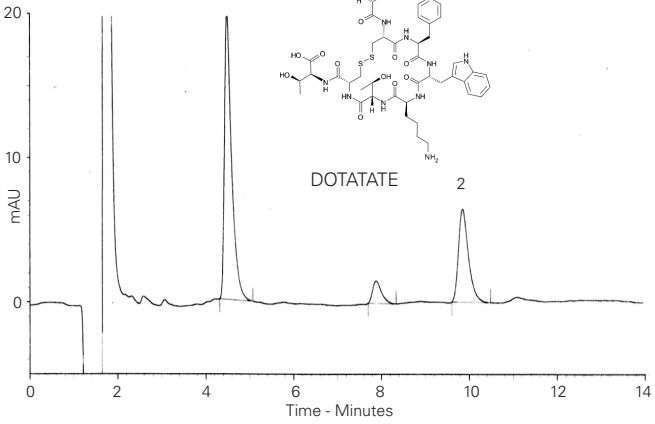
1. DOTATATE
2. Octreotide



Octreotide



DOTATATE



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^{68}Ga-DOTATATE QC Analysis by Radiometric Detection

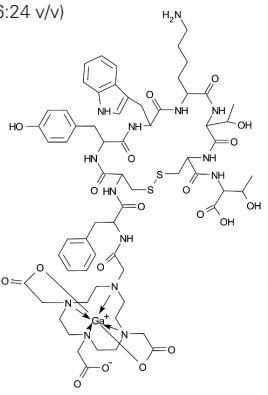
Application #AN2720

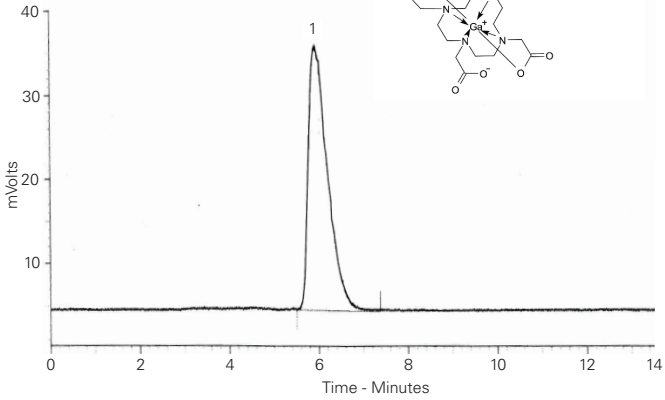
Conditions

Column:	ACE 3 C18
Dimensions:	150 x 3.0 mm
Part Number:	ACE-111-1503
Mobile Phase:	0.1% TFA in H_2O/MeCN (76:24 v/v)
Flow Rate:	0.6 mL/min
Injection:	20 µL
Detection:	Radiometric

Analyte

1. ^{68}Ga-DOTATATE





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^{68}Ga-DOTATATE PET Tracer by LC-MS/MS

Application #AN2710

Conditions

Column: ACE 3 C18
Dimensions: 50 x 4.6 mm
Part Number: ACE-111-0546
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN

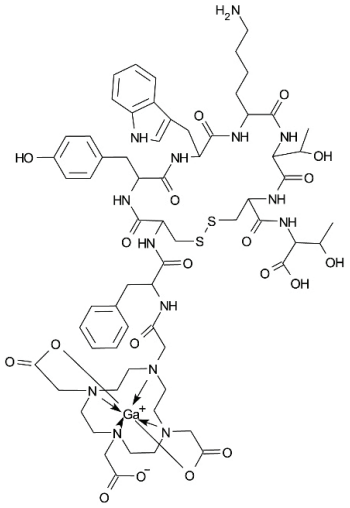
Gradient:

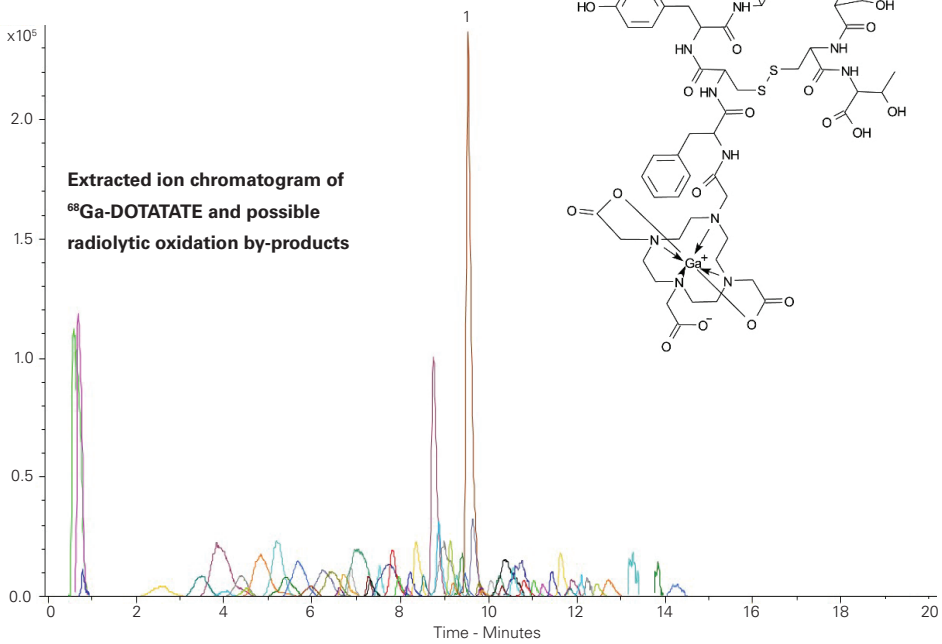
Time (mins)	%B
0	2
10	25
20	25

Flow Rate: 1 mL/min
Injection: 10 µL
Detection: Bruker ESI-Q-TOF
ESI positive ion mode

Analyte

1. ^{68}Ga-DOTATATE





Extracted ion chromatogram of ^{68}Ga-DOTATATE and possible radiolytic oxidation by-products

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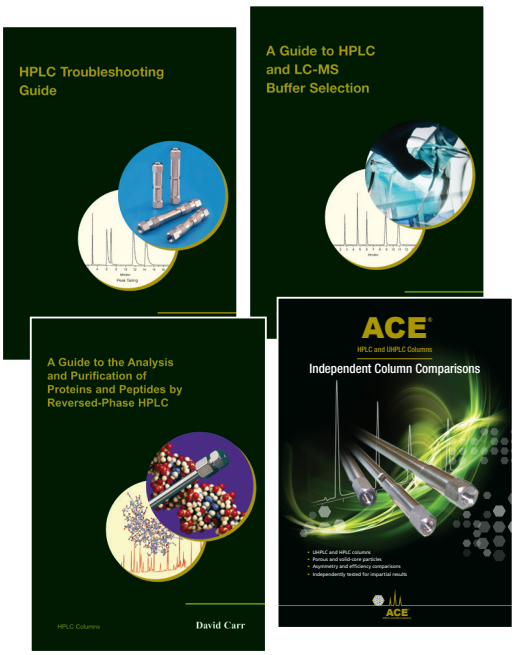

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Drugs of Abuse Screen by UHPLC-MS/MS

Application #AN2190

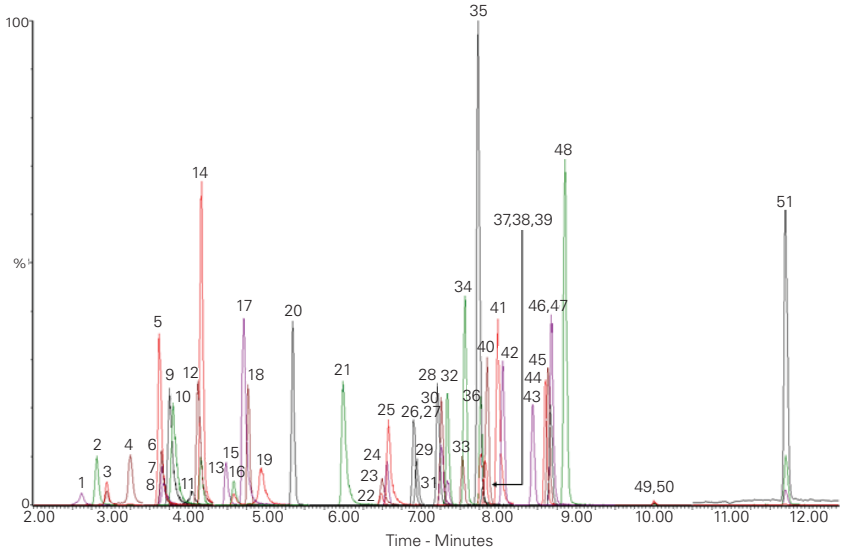
Conditions

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

Gradient:

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

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



Peak	Analyte	R_t (Mins)	Q1 (Da)	Q3 (Da)
1	**Oxymorphone**	2.62	302.2	198.1
2	**Morphine-d3**	2.82	289.2	201.0
3	**Morphine**	2.95	286.2	201.0
4	**Hydromorphone**	3.25	286.2	185.1
5	**Amphetamine-d5**	3.62	141.0	123.9
6	**Amphetamine**	3.65	136.0	118.9
7	**Dihydrocodeine**	3.66	302.2	199.1
8	**MDA**	3.67	180.1	105.0
9	**MDMA**	3.75	194.1	163.0
10	**Methamphetamine**	3.80	150.0	90.9
11	**Oxycodone**	4.03	316.2	241.2
12	**MDEA**	4.12	208.2	163.0
13	**BZE-d3**	4.15	293.1	171.0
14	**BZE**	4.17	290.1	168.0
15	**6-MAM**	4.48	328.2	165.1
16	**Codeine**	4.59	300.3	215.1
17	**Norfentanyl**	4.71	233.1	84.0
18	**7-Amino-clonazepam**	4.77	286.2	121.0
19	**Hydrocodone**	4.94	300.2	199.1
20	**7-Amino-flunitrazepam**	5.34	284.2	135.0
21	**Cocaine**	5.99	304.2	182.0
22	**Norbuprenorphine**	6.47	414.3	101.0
23	**PCP**	6.49	244.2	159.9
24	**Zaleplon**	6.55	306.2	264.2
25	**EDDP**	6.58	278.2	234.2
26	**Norketamine**	6.90	224.1	124.9

Peak	Analyte	R_t (Mins)	Q1 (Da)	Q3 (Da)
27	**Bromazepam**	6.95	316.1	182.1
28	**Ketamine**	7.21	238.1	124.9
29	**Clonazepam**	7.26	316.1	270.1
30	**Nitrazepam**	7.26	282.2	236.1
31	**α-Hydroxytriazolam**	7.34	359.1	331.1
32	**Flunitrazepam**	7.34	314.2	268.2
33	**α-Hydroxyalprazolam**	7.54	325.2	297.1
34	**Estazolam**	7.56	295.2	267.2
35	**Zolpidem**	7.73	308.2	235.1
36	**Triazolam**	7.77	343.0	308.1
37	**2-Hydroxyethylflurazepam**	7.77	333.2	109.0
38	**Lorazepam**	7.80	321.1	275.1
39	**Oxazepam**	7.82	287.2	241.0
40	**Alprazolam**	7.85	309.2	281.2
41	**Methadone**	7.99	310.2	265.2
42	**Temazepam**	8.05	301.1	255.1
43	**Nordiazepam**	8.44	271.1	139.9
44	**Midazolam**	8.61	326.2	291.2
45	**Diazepam-d5**	8.63	290.2	154.0
46	**Diazepam**	8.67	285.2	154.0
47	**Flurazepam**	8.68	388.2	315.1
48	**Fentanyl**	8.85	337.3	105.0
49	**THC-COOH-d3**	9.98	348.2	302.2
50	**THC-COOH**	10.01	345.2	299.2
51	**Buprenorphine**	11.70	468.3	101.0

Drugs of Abuse Screen (250 Analytes) in Urine by LC-MS/MS

Conditions

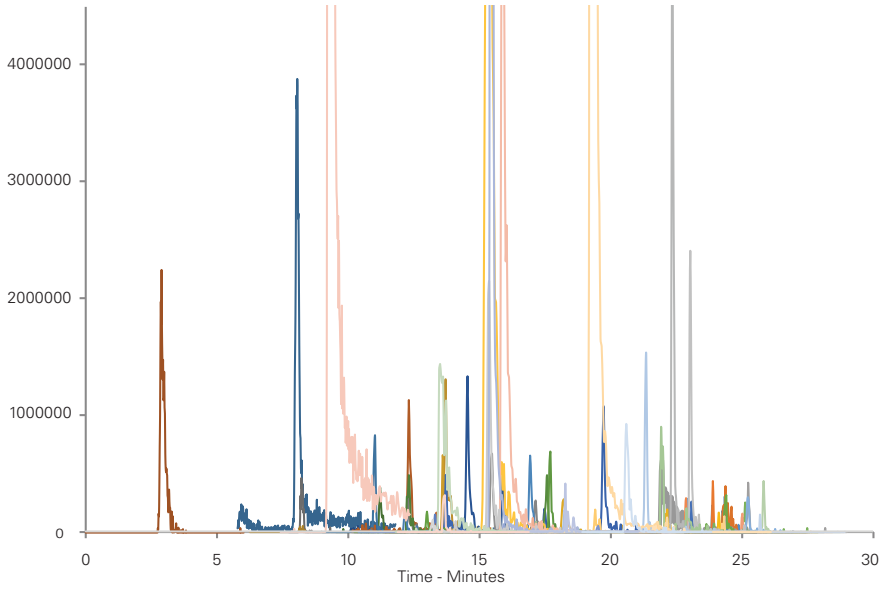
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: A: 2 mM ammonium acetate + 0.1% formic acid in H_2O
B: 2 mM ammonium acetate + 0.1% formic acid in MeOH

Gradient:

Time (mins)	%B
0	2
4	2
34	100
38	100
40	2

Flow Rate: 0.3 mL/min
Injection: 10 µL
Temperature: 37 °C
Detection: Thermo Quantum Ultra MS
ESI in positive ion mode

Analytes in blue are included in Extracted Ion Chromatogram



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Analyte	R_t (Mins)	MRM Transitions (*m/z*)
6-Acetylcodeine	16.9	342.2 > 165.1
Alfentanil	21.1	417.4 > 197.2
Alprazolam	23.3	309.11 > 205.1
Aminoclonazepam	13.9	286.2 > 222.3
Aminodesmethylflunitrazepam	20.0	270.1 > 121.1
Aminoflunitrazepam	16.2	284.1 > 135.1
Aminonitrazepam	10.9	252.1 > 94.1
Aminorex	12.2	163 > 120.1
Amiodarone	31.3	646.2 > 100
Amisulpride	16.2	370.1 > 242
Amitriptyline	24.4	278.2 > 91.1
Amlodipine	25.3	409.3 > 238.2
Amlodipine met	22.9	407 > 318
Amphetamine	11.6	136.1 > 65.2
Amphetamine-d6	11.6	142.2 > 67.2
Anhydroecgonine methyl ester	9.8	182.2 > 91.1
Aripiprazole	25.5	448.1 > 285.1
Atenolol	10.7	267.1 >145.1
Atomoxetine	23.1	256.2 > 44.1
Atomoxetine metabolite	22.5	242.2 > 44.1
Benzedrone	21.7	254 > 65.1
Benzoylecgonine	15.6	290.1 > 77.2
Benzoylecgonine-d3	15.6	293.2 > 77.2
Benzylpiperazine	5.1	177.2 > 65.1
Bisoprolol	19.9	326.3 > 116.1
Bromazepam	20.4	316 > 182.1

Analyte	R_t (Mins)	MRM Transitions (*m/z*)
Buphedrone	14.2	178.2 > 160.1
Buphedrone ephedrine	13.5	180.4 > 162.2
Bupivacaine	19.5	289.2 > 84.2
Buprenorphine glucuronide	18.1	644.4 > 468.4
Bupropion	19.5	240.1 > 131.1
Butylone	14.7	222.1 > 131.1
Caffeine	13.1	195.1 > 110.1
Camfetamine	18.7	202.2 > 67.1
Carbamazepine	21.5	237.1 > 192.2
Carbamazepine 10,11-Epoxide	18.6	253.2 > 180.1
Cathine	20.0	134.2 > 91.1
Cathinone	9.5	150.2 > 117.1
2C-B-FLY	20.1	286 > 269.1
Chlordiazepoxide	19.5	300.1 > 227.1
Chloroquine	18.5	320.1 > 142.1
Chlorpheniramine	20.4	275.1 > 167.2
Chlorpromazine	25.9	319.2 > 58.1
Citalopram	22.2	325.1 > 246.1
Clobazam	22.8	301.1 > 259.2
Clomethiazole	17.3	161.9 > 113
Clomipramine	27.0	315.1 > 86.1
Clonazepam	23.1	316.1 > 214.2
Clonidine	13.2	230 > 44.2
Clozapine	21.7	327.1 > 192.1
Cocaethylene	19.5	318.2 > 82.2
Cocaine	18.0	304.2 > 82.2

Drugs of Abuse Screen (250 Analytes) in Urine by LC-MS/MS

Analyte	R_t (Mins)	MRM Transitions (*m/z*)
Codeine	11.9	300.2 > 153.2
Cotinine	2.5	177.1 > 80.1
Creatinine	1.3	114 > 44
Cyclizine	22.5	267.1 > 167.1
D2PM (Diphenylprolinol)	7.3	254.1 > 130.1
Dehydroaripiprazole	25.3	446.1 > 285.1
Desipramine	24.3	267.1 > 72.2
N-Desmethylclozapine	21.0	313 > 192.1
Desmethylcitalopram	22.4	311.1 > 109.1
Desmethylflunitrazepam	22.5	300.1 > 254.2
Desmethylfluoxetine	25.4	296.2 > 134.1
N-Desmethylmirtazapine	16.1	252.1 > 195.1
Desmethylolanzapine	12.6	299.1 > 198.1
N-Desmethyltramadol	16.7	250.1 > 44.2
O-Desmethyltramadol	12.8	250.1 > 58.2
Desmethylvenlafaxine	15.5	264.3 > 58.1
N-Desmethylzopiclone	20.0	375.1 > 245.1
Desomorphine	13.1	272.1 > 152.1
Desoxypipradol	20.5	252.1 > 91.1
Dextromethorphan	20.0	272.2 > 171.1
Diamorphine	16.9	370.1 > 165.1
Diazepam	25.5	285.1 > 154.1
Didesmethylcitalopram	22.2	297 > 262.1
Digoxin	24.2	781.2 > 97
Dihydrocodeine	11.7	302.2 > 128.1
Diltiazem	22.7	415.1 > 178.1
Dimethocaine	16.3	279.3 > 92.1
Dinitrophenol	18.4	183 > 109
Diphenhydramine	21.2	256.1 > 167.1
Dipipanone	25.0	350.2 > 265.2
Donepezil	22.2	380.1 > 91
Dothiepin	23.7	296.2 > 202.2
Ecgonine ethyl ester	2.5	214.1 > 196.1
Ecgonine methyl ester	1.0	200.1 > 182.1
EDDP	21.4	278.2 > 219.2
Estazolam	22.5	295.1 > 267.1
Ethylamphetamine	14.5	164.1 > 91.2
Ethylmethcathinone	15.8	192.2 > 131.2
Ethylphenidate	19.2	248.1 > 56.2
Etizolam	23.5	343.1 > 314.2
Fenfluramine	20.3	232.1 > 159.1
Fentanyl	21.4	337.2 > 105.1
Flubromazolam	23.2	371.1 > 223.1
Flunitrazepam	23.5	314.1 > 269.3
2-Fluoroamphetamine	13.2	154.1 > 83.1
Fluoroamphetamine interferent	10.6	154 > 67.1
3-Fluoromethcathinone	20.0	182.1 > 149.1

Analyte	R_t (Mins)	MRM Transitions (*m/z*)
4-Fluoromethcathinone	20.0	182 > 148.1
Fluoxetine	25.3	310.1 > 44.2
Fluphenazine	28.1	438.3 > 143.1
Flurazepam	21.6	388 > 315
Fluvoxamine	26.0	319.1 > 71
Gabapentin	10.5	172.1 > 67.2
Glibenclamide	28.2	494.1 > 168.9
Gliclazide	24.6	324.1 > 110
Glimepiride	28.4	491.1 > 126
Glipizide	24.5	446.1 > 286
Haloperidol	23.1	376.1 > 95.1
Hippuric acid	10.9	180 > 77
Hydrocodone	13.1	300.1 > 199.1
Hydromorphone	10.4	286.2 > 185.1
Hydroxyalprazolam	22.4	325.1 > 216.1
4-Hydroxyamphetamine	5.4	152.1 > 107.1
Hydroxybupropion	18.5	253.1 > 130.1
4-Hydroxymethamphetamine	20.0	166.1 > 107.1
8-Hydroxymirtazapine	15.6	282.1 > 211
7-Hydroxymitragynine	18.2	415.3 > 175.1
3-Hydroxyphenazepam	23.3	366.9 > 320.8
7-Hydroxyquetiapine	15.3	400.3 > 208.1
9-Hydroxyrisperidone	19.5	427.2 > 69.1
Imipramine	24.2	281.1 > 86.2
5-Iodo-2-aminoindane	18.4	260.1 > 115.1
Ketamine	15.4	238.1 > 125.1
Lamotrigine	16.8	256.1 > 211.1
Levamisole	13.3	205.1 > 91.1
Levetiracetam	8.9	171.2 > 126.1
Lidocaine	14.8	235.1 > 86.2
Lorazepam	22.8	321 > 229.1
Lormetazepam	23.8	335 > 289.1
LSD	20.1	324.3 > 223.1
MCAT	5.4	164.2 > 130.1
mCPP	17.0	197.1 > 118.1
MDA	13.4	180.1 > 133.1
MDAI	12.3	178.19 > 161.1
MDEA	15.2	208.1 > 135.1
MDMA	14.1	194.1 > 135.2
MDPV	18.1	276.1 > 135.1
MEGX	13.4	207.1 > 58.1
MeOPP	13.3	193.2 > 133.1
Mephedrone	14.6	178.1 > 144.2
Mescaline	12.7	212.1 > 165.1
Metformin	2.5	130 > 60.1
Methadone	24.0	310.2 > 105.1
Methadone-d3	24.0	313.2 > 268.2

Drugs of Abuse Screen (250 Analytes) in Urine by LC-MS/MS

Analyte	R_t (Mins)	MRM Transitions (*m/z*)
Methamphetamine	12.8	150.1 > 91.2
Methaqualone	22.8	251.2 > 91.1
Methedrone	13.9	194.1 > 146.1
Methiopropamine	10.6	156.1 > 97
Methocarbamol	16.8	242.1 > 118.1
Methoxetamine	17.2	248.2 > 121.1
3-Methoxytyramine	6.6	168 > 91
Methylethcathinone	20.0	192.1 > 144.2
Methylhexanamine	13.4	116.1 > 57.3
Methylone	12.7	208.1 > 132.1
Methylphenidate	16.5	234.1 > 56.2
5-Methyltryptamine	16.9	175.1 > 143
Metoclopramide	17.2	300.1 > 227.1
Midazolam	20.9	326.1 > 249.1
Mirtazapine	16.6	266.1 > 72.2
Mitragynine	22.6	399.3 > 174.1
Modafinil	21.1	296.1 > 129
6-Monoacetylmorphine	12.9	328.1 > 165.1
Mono-N-desethylamiodarone	30.8	618.2 > 547.2
Morphine	7.7	286.1 > 152.2
Morphine glucuronide	2.7	462.2 > 201.1
Morphine-d3	7.7	289.2 > 152.2
Naloxone	20.0	328.3 > 212.1
Naphyrone	23.2	282.2 > 141.1
Nefopam	19.5	254.9 > 166.1
Nifoxipam	20.9	316.05 > 298.1
Nimetazepam	23.6	296.1 > 250.2
Nitrazepam	22.8	282.1 > 236.1
Noralfentanil/sufentanil	19.4	277.1 > 245.1
Norbuprenorphine glucuronide	15.5	590.3 > 414.3
Norcyclizine	21.9	253.2 > 167.1
Nordiazepam	24.4	271.1 > 140.1
Nordothiepin	24.4	282.1 > 202.1
Norfentanyl	15.6	233.2 > 56.2
Norketamine	14.8	224.1 > 125.1
Normorphine	3.8	272.1 > 165.2
Nornefopam	19.7	240.9 > 166.1
Noroxycodone	13.0	302.1 > 284.1
Norpropoxyphene	23.0	308 > 44.2
Norsertraline	20.0	275.3 > 159
Nortriptyline	24.6	264.1 > 91.1
Olanzapine	13.4	313.1 > 84.1
Orphenadrine	23.4	270.1 > 181.1
Oxazepam	23.5	287.1 > 104.1
Oxybutynin	24.6	358.1 > 141.9
Oxycodone	12.9	316.1 > 241.1
Oxymorphone	20.0	302 > 227

Analyte	R_t (Mins)	MRM Transitions (*m/z*)
Paracetamol	7.8	152.1 > 65.1
PCP	20.5	244.3 > 86.2
Pentazocine	19.5	286.3 > 175.2
Pentedrone	16.0	192.2 > 131.1
Phenazepam	24.5	350.9 > 206
Pheniramine	15.1	241.2 > 196.2
Phenytoin	20.0	253.1 > 77
Pholcodine	9.2	399.2 > 114.1
PMA	13.8	149.2 > 91.1
PMMA	14.6	180.2 > 121.1
Powder 20140730	18.7	248.3 > 84.2
Prazepam	27.0	325 > 140
Pregabalin	10.4	160.1 > 97.2
Procyclidine	22.4	288.3 > 42
Promethazine	20.0	285.1 > 86.2
Propofol	23.9	179 > 137
Propofol glucuronide	20.1	372.2 > 148.1
Propoxyphene	23.6	340.2 > 58.2
Propranolol	23.0	260.1 > 157.1
Quetiapine	21.7	384.1 > 221.1
Remifentanil	18.4	377.3 > 113.1
Risperidone	20.4	411.1 > 190.8
Ritalinic acid	14.4	220.2 > 56.1
Sertraline	25.6	306.1 > 159
Sildenafil	23.6	475.4 > 58.1
Sildenafil N-oxide	23.9	491.4 > 312.3
Sufentanil	22.9	387.3 > 140.2
Temazepam	24.2	301.1 > 177.1
Temazepam-d5	24.1	306.1 > 260.2
Tetrazepam	24.5	289.2 > 225.2
TFMPP	7.9	231.1 > 118.1
Theophylline	11.2	181.1 > 124.1
Tramadol	16.9	264.2 > 58.2
Trazodone	23.9	372.2 > 179.2
Trifluoperazine	28.8	408.2 > 113.2
Trihexyphenidyl	23.7	302.1 > 70.1
Varenicline	12.3	212.2 > 168.1
Venlafaxine	19.1	278.2 > 58.2
Verapamil	23.9	455.2 > 150.1
Vigabatrin	2.5	130.1 > 71.1
Warfarin	25.7	309.1 > 251.1
Zaleplon	21.5	306.1 > 236.2
Zolpidem	18.8	308.2 > 235.2
Zolpidem phenyl COOH	15.3	338 > 265.1
Zopiclone	16.5	389.1 > 217.1
Zopiclone N-oxide	17.6	405.2 > 217.1

Echinacea

Application #AN4270

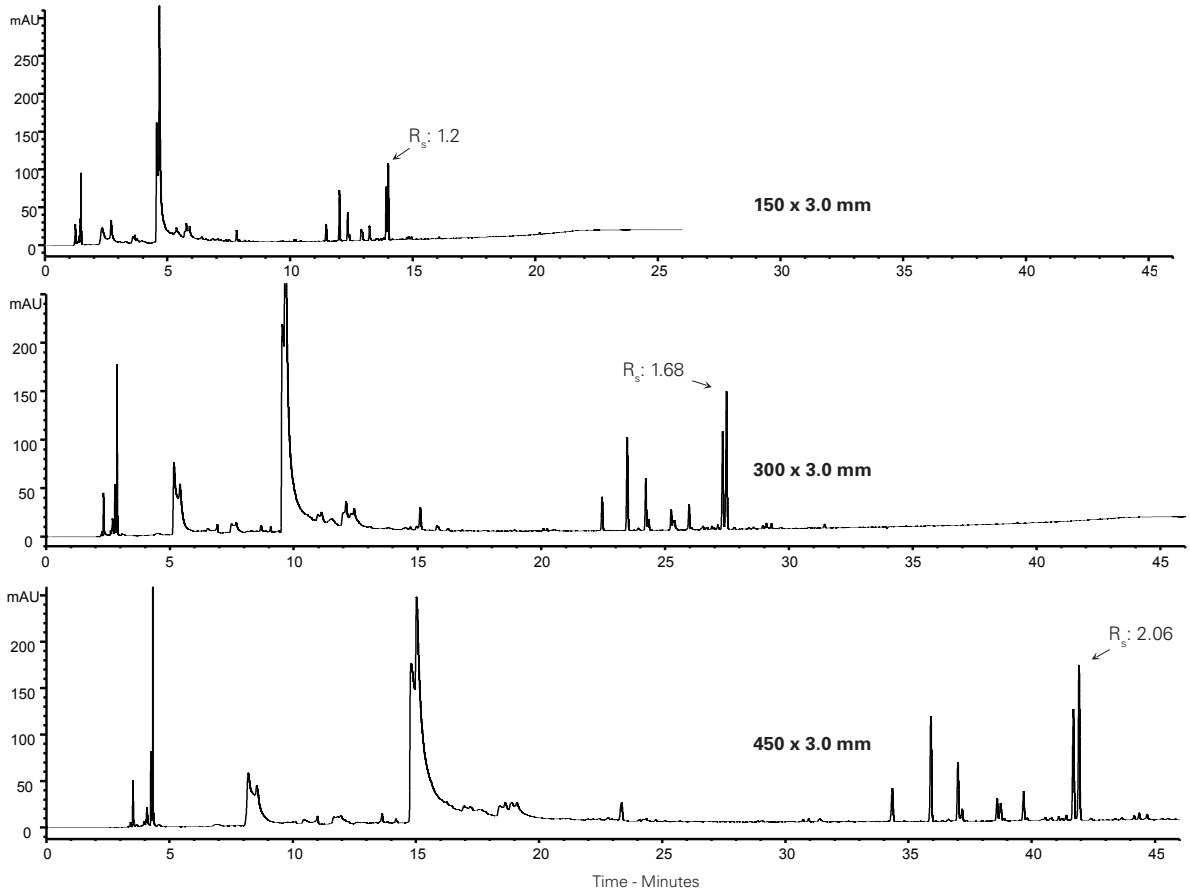
Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 150 x 3.0 mm; 2 x 150 x 3.0 mm (coupled); 3 x 150 x 3.0 mm (coupled)
Part Number: CORE-25A-1503U
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN

Gradient:

	Time (mins)			
	150 x 3.0 mm	**300 x 3.0 mm**	**450 x 3.0 mm**	**%B**
	-	0.00	0.00	5
	0.00	0.47	0.94	5
	20.00	40.47	60.94	100
	25.00	45.47	75.94	100
	26.00	46.47	76.94	5
	46.00	86.47	136.94	5

Flow Rate: 0.43 mL/min
Temperature: 80 °C
Detection: UV, 254 nm



Entacapone

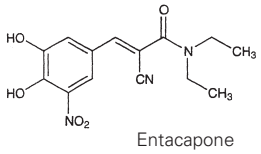
Application #AN3600

Conditions

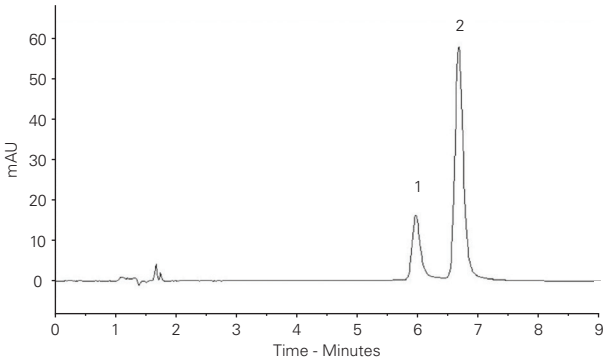
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: Phosphoric acid pH 3.0/MeCN (65:35 v/v)
Flow Rate: 2.0 mL/min
Injection: 20 µL
Temperature: 25 °C
Detection: UV, 305 nm
Sample: Entacapone standard in MeOH solution exposed to direct UV radiation (254 nm)

Analytes

1. Degradation Product
2. Entacapone



Entacapone



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Epanolol

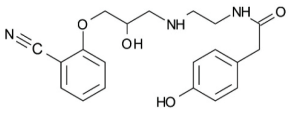
Application #AN3610

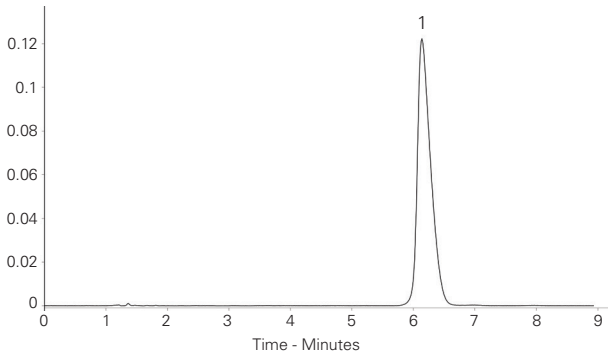
Conditions

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 (85:15 v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: Ambient
Detection: UV, 254 nm

Analyte

1. Epanolol





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Epinastine

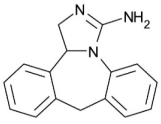
Application #AN3620

Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 0.3% TEA pH 4.0 with phosphoric acid/MeOH (60:40 v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 25 °C
Detection: UV, 254 nm

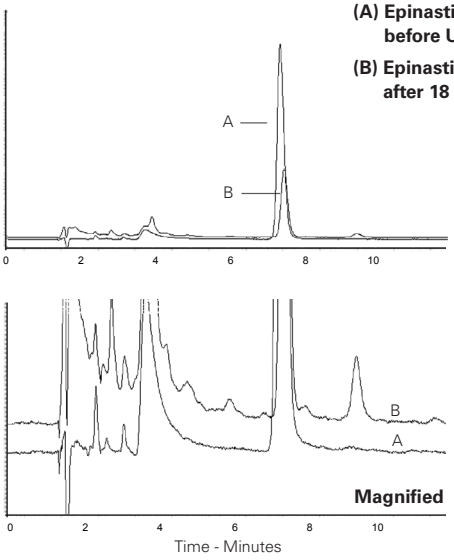
Analyte

1. Epinastine



(A) Epinastine Hydrochloride before UV radiation

(B) Epinastine Hydrochloride after 18 hours UV radiation



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Ethanol Extract from Seed Cover (*Acacia Farnesiana*)

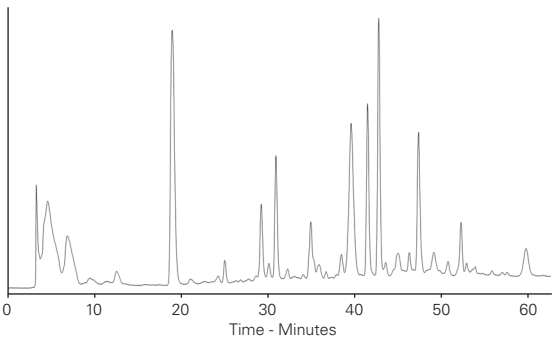
Application #AN2900

Conditions

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

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

Flow Rate: 2.0 mL/min
Temperature: Ambient
Detection: UV, 230 nm



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Ethyl Glucuronide in Water by LC-MS/MS

Application #AN1100

Conditions

Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: A: 0.05% formic acid in H_2O
B: MeOH

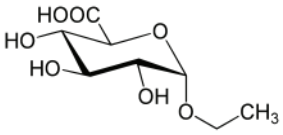
Gradient:

Time (mins)	%B
0.00	5
4.00	70
6.00	95
7.00	95
7.01	5

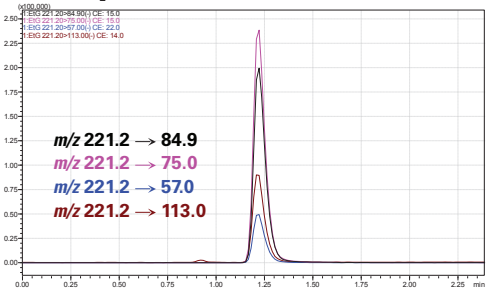
Flow Rate: 0.4 mL/min
Injection: 3 µL
Temperature: 40 °C
Detection: Shimadzu LCMS-8050
ESI voltage: -3 kV
Desolvation line: 250 °C
Interface heater: 380 °C
Nebulizing gas: 3 L/min
Heat block: 400 °C

Analyte

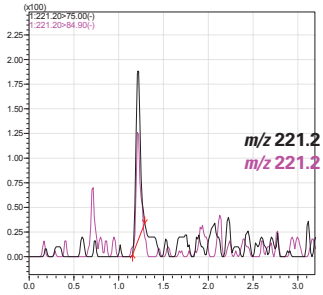
1. Ethyl glucuronide



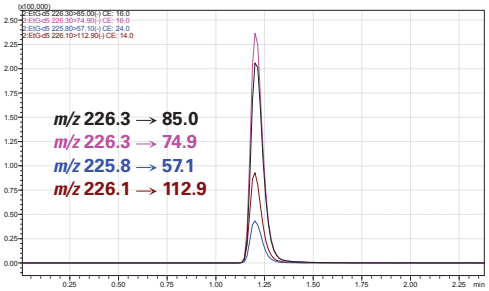
Ethyl glucuronide (EtG)
LOQ in H_2O 300 fg on-column



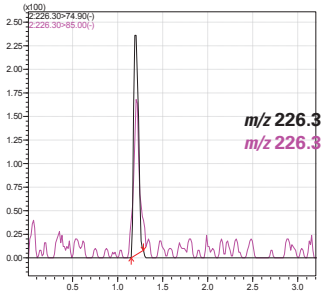
EtG 100 pg/mL



Ethyl glucuronide-d5 (EtG-d5)



EtG-d5 100 pg/mL



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Exploiting Selectivity by Adjusting pH

Application #AN2440

Conditions

Column: ACE Excel 2 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: EXL-1011-0502U
Mobile Phase: A1: 10 mM ammonium formate pH 3.0 in H_2O
A2: 0.1% ammonia pH 10.7 in H_2O
B1: 10 mM ammonium formate pH 3.0 in MeCN/H_2O (90:10 v/v)
B2: 0.1% ammonia pH 10.7 in MeCN/H_2O (90:10 v/v)

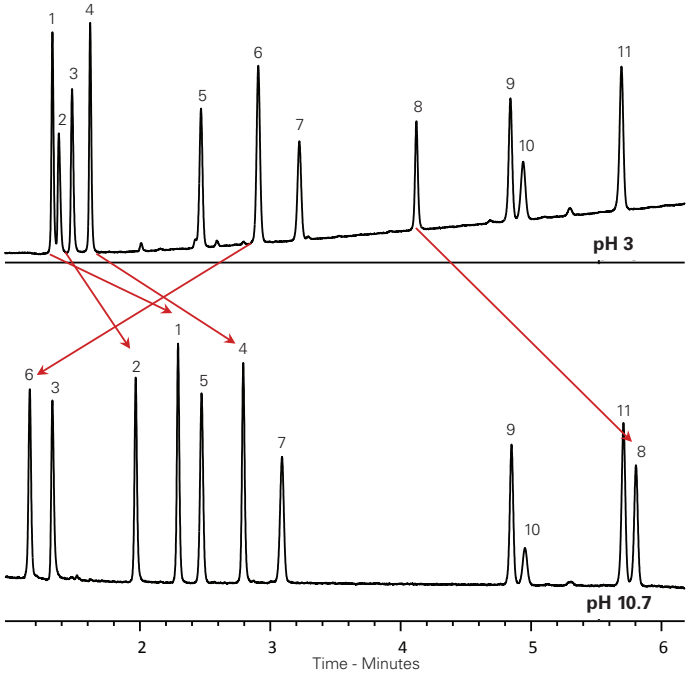
Gradient:

Time (mins)	%B
0.0	3
7.0	100
8.0	100
8.5	3
12.5	3

Flow Rate: 0.42 mL/min
Injection: 2 µL
Temperature: 40 °C
Detection: UV, 254 nm

Analytes

1. Nizatidine
2. Salbutamol
3. Amiloride
4. N-Acetylprocainamide
5. Quinoxaline
6. Methyl paraben
7. p-Cresol
8. Reserpine
9. Piperine
10. Toluene
11. Felodipine



Explosive Analytes (I)

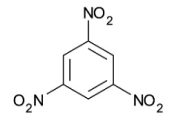
Application #AN1460

Conditions

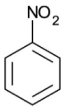
Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	MeOH/H_2O (50:50 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	20 °C
Detection:	UV, 254 nm

Analytes

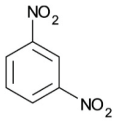
1. 1,3,5-Trinitrobenzene
2. Nitrobenzene
3. 1,3-Dinitrobenzene
4. 2,4-Dinitrotoluene



1,3,5-Trinitrobenzene

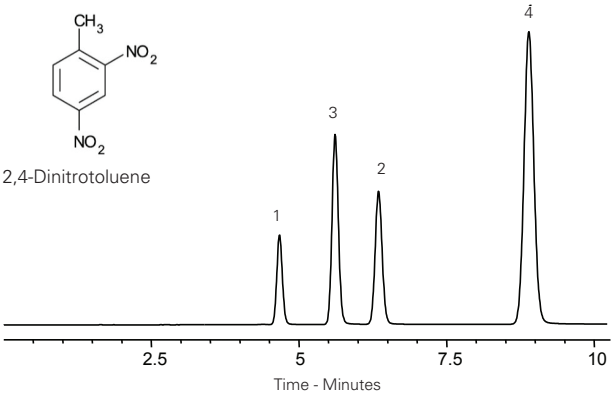


Nitrobenzene



1,3-Dinitrobenzene

2,4-Dinitrotoluene



Explosive Analytes (II)

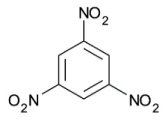
Application #AN1470

Conditions

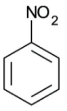
Column:	ACE 5 CN-ES
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1213-1546U
Mobile Phase:	MeOH/H_2O (50:50 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	20 °C
Detection:	UV, 254 nm

Analytes

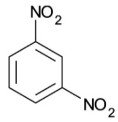
1. 1,3,5-Trinitrobenzene
2. Nitrobenzene
3. 1,3-Dinitrobenzene
4. 2,4-Dinitrotoluene



1,3,5-Trinitrobenzene

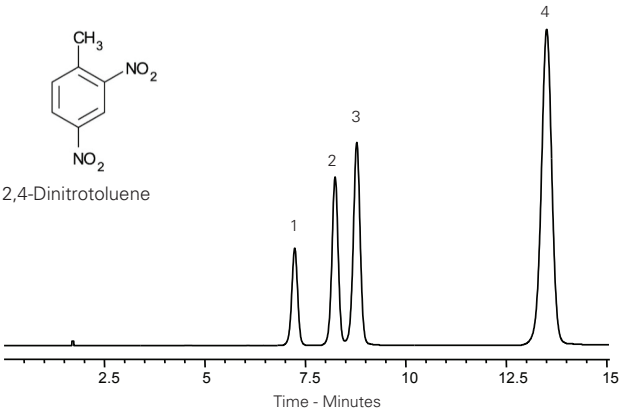


Nitrobenzene



1,3-Dinitrobenzene

2,4-Dinitrotoluene



Fingerprinting of *Cuscuta Chinensis* Flavonoids

Application #AN4250

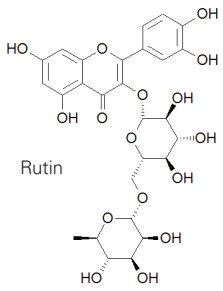
Conditions

Column:	ACE 5 C18	
Dimensions:	250 x 4.6 mm	
Part Number:	ACE-121-2546	
Mobile Phase:	A: 0.25% o-phosphoric acid in H_2O	
	B: MeCN	
Gradient:	**Time (mins)**	**%B**
	0	5
	2	5
	7	10
	10	15
	23	20
	28	30
	32	50
Flow Rate:	1 mL/min	
Injection:	10 µL	
Detection:	UV, 360 nm	

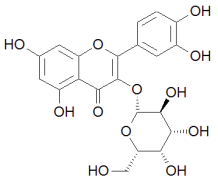
***Cuscuta chinensis* is used in traditional medicines in eastern and southern Asia**

Analytes

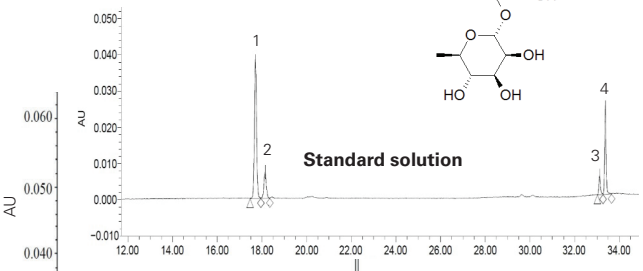
1. Rutin
2. Hyperoside
3. Isorhamnetin
4. Kaempferol

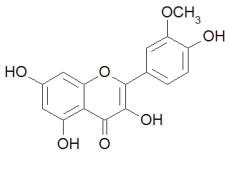


Rutin

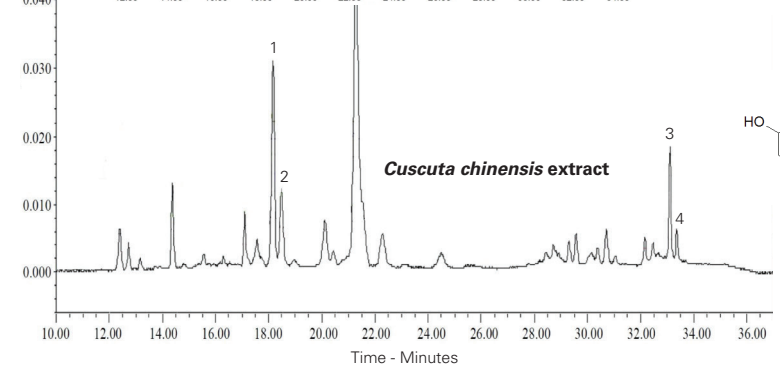


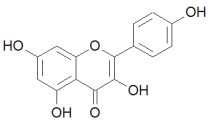
Hyperoside





Isorhamnetin





Kaempferol

Shekarchi M, Kondori BM, Hajimehdipoor H, Abdi L, Naseri M, Pourfarzib M, Amin G. (2014) Finger Printing and Quantitative Analysis of *Cuscuta chinensis* Flavonoid Contents from Different Hosts by RP-HPLC. Food and Nutrition Sciences, 5, 914-921. http://dx.doi.org/10.4236/fns.2014.510101

Flavone and Dibucaine

Application #AN2850

Conditions

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

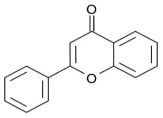
Gradient:

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

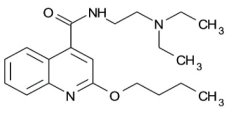
Flow Rate: 2 mL/min
Temperature: 60 °C
Detection: UV, 200-450 nm

Analytes

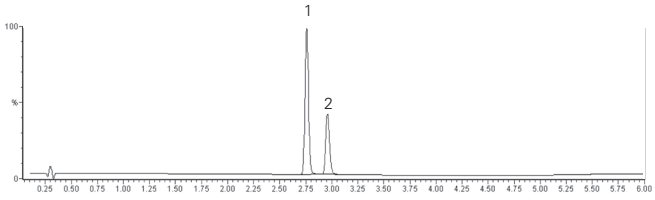
1. Flavone
2. Dibucaine



Flavone



Dibucaine



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Flavonoids

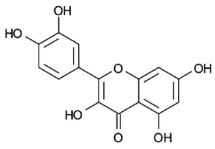
Application #AN2810

Conditions

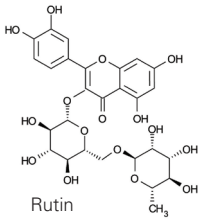
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: MeCN/0.1% formic acid in H_2O (40:60 v/v)
Flow Rate: 1 mL/min
Injection: 1 µL
Temperature: Ambient
Detection: UV, 254 nm

Analytes

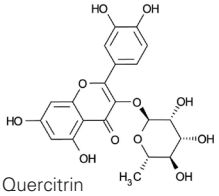
1. Rutin
2. Quercetin
3. Quercitrin
4. Kaempferol



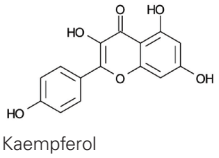
Quercetin



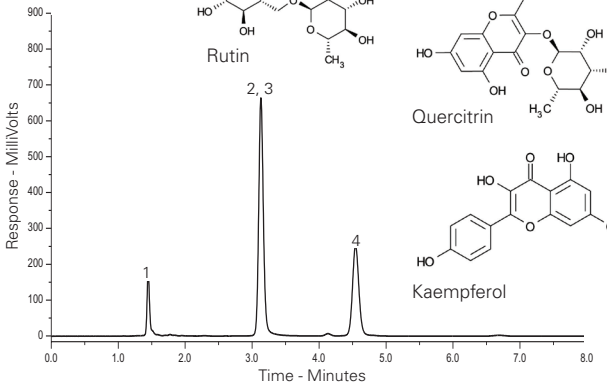
Rutin



Quercitrin



Kaempferol



Flurbiprofen and Related Substances

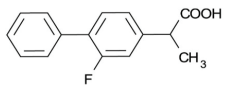
Application #AN3630

Conditions

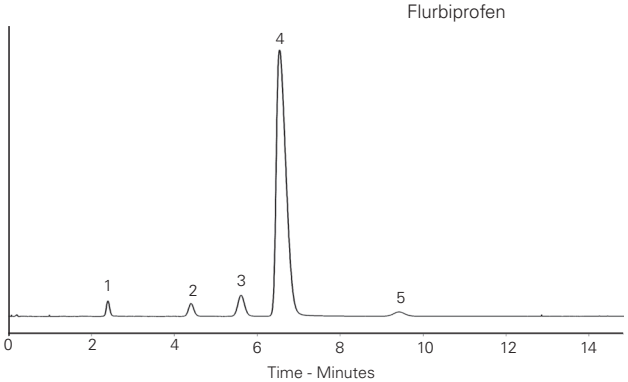
Column: ACE 3 C18
Dimensions: 50 x 4.6 mm
Part Number: ACE-111-0546
Mobile Phase: H_2O/MeCN/TFA (64:34:0.5 v/v/v)
Flow Rate: 2 mL/min
Injection: 20 µL
Temperature: 28 °C
Detection: UV, 254 nm

Analytes

1. 2-(2-Fluoro-4-biphenyl)-2-hydroxypropionic acid
2. cis-2-(2-Fluoro-4-biphenyl)-2-hydroxypropionic acid
3. 2-Fluoro-4-biphenyl-4-carboxylic acid
4. Flurbiprofen (2-(2-Fluorobiphenyl-4-yl)propionic acid)
5. 4-Acetyl-2-fluorobiphenyl



Flurbiprofen



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Formoterol from Human Plasma by LC-MS/MS

Application #AN3100

Conditions

Column: ACE Excel 2 C18-AR
Dimensions: 50 x 2.1 mm
Part Number: EXL-109-0502U
Mobile Phase: A: 0.02% formic acid in H_2O
B: 0.02% formic acid in H_2O/MeOH (2:98 v/v)

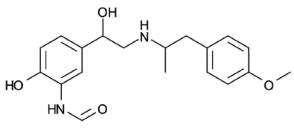
Gradient:

Time (mins)	%B
0.00	10
0.20	10
2.00	40
2.01	100
3.50	100
3.51	10
4.00	10

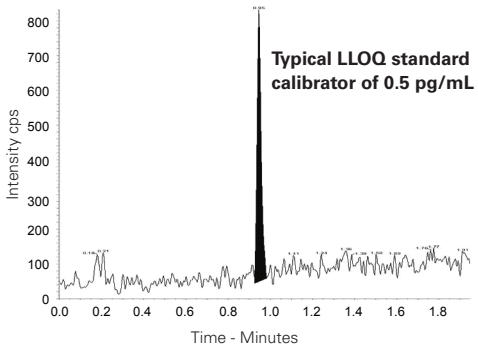
Flow Rate: 0.75 mL/min
Temperature: 60 °C
Detection: AB SCIEX QTRAP 5500 LC-MS/MS system
Sample: Extracted by mixed mode cation exchange SPE

Analyte

1. Formoterol (*m/z* 345 → 149)



Formoterol



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Galanthamine

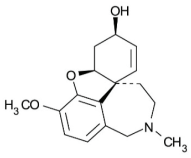
Application #AN3640

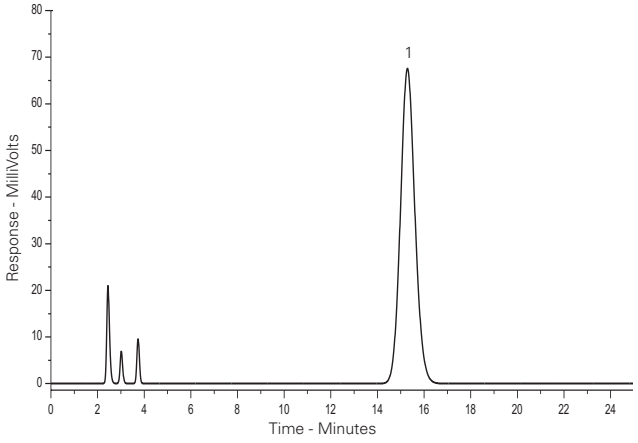
Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 0.1% TFA/MeCN (92:8 v/v)
Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: 20 °C
Detection: UV, 210 nm

Analyte

1. Galanthamine





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Gamma Hydroxybutyric Acid (GHB) and Gamma Butyrolactone (GBL) Separation

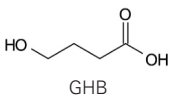
Application #AN1500

Conditions

Column: ACE Excel 2 C18-AR
Dimensions: 100 x 3.0 mm
Part Number: EXL-109-1003U
Mobile Phase: 20 mM KH_2PO_4 pH 2.5 in H_2O/MeCN (98:2 v/v)
Flow Rate: 0.43 mL/min
Injection: 2 µL
Temperature: 30 °C
Detection: UV, 215 nm

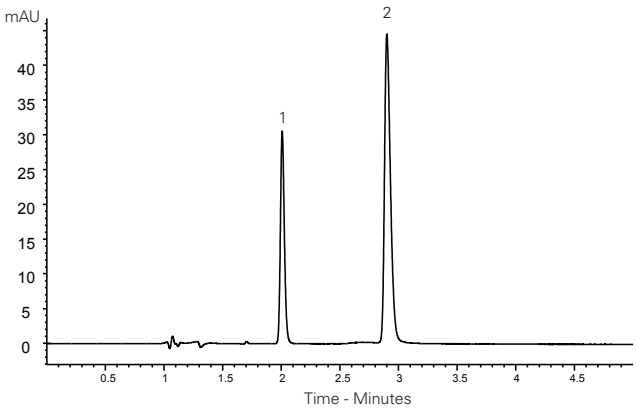
Analytes

1. GHB
2. GBL



GHB

GBL



Garlic Analysis (I)

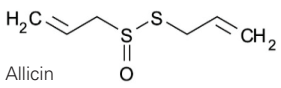
Application #AN2820

Conditions

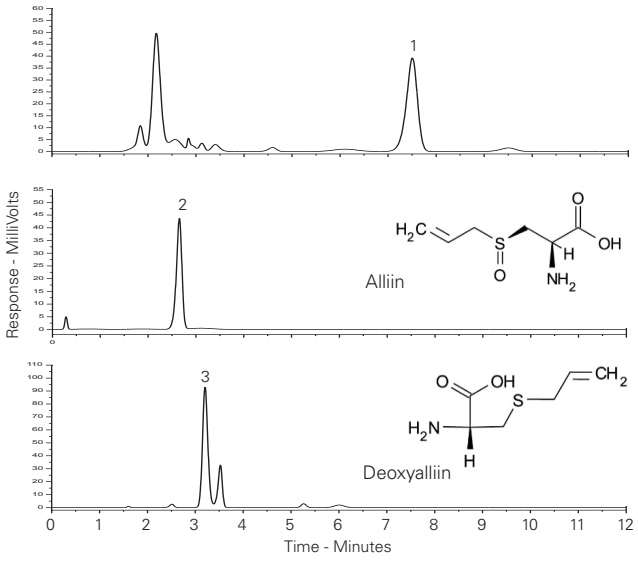
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: H_2O/MeOH (50:50 v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 30 °C
Detection: UV, 210 nm

Analytes

1. Allicin
2. Alliin
3. Deoxyalliin



Allicin



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Garlic Analysis (II)

Application #AN2830

Conditions

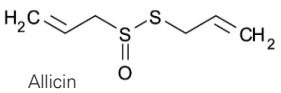
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: H_2O
B: MeCN

Gradient:	**Time (mins)**	**%B**
	0	40
	20	100
	25	100

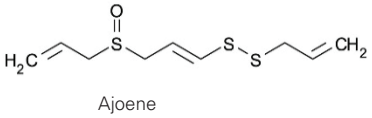
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 30 °C
Detection: UV, 254 nm

Analytes

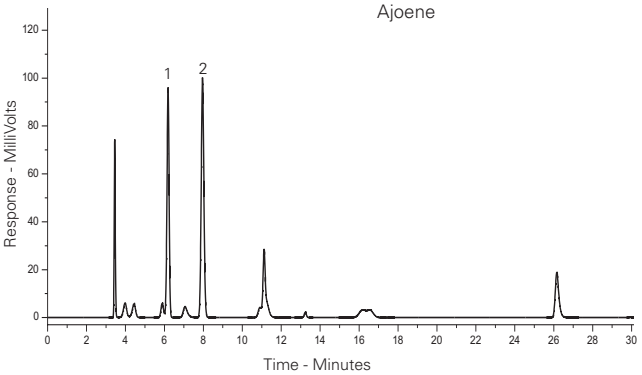
1. Allicin
2. Ajoene



Allicin



Ajoene



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Ginkgo Biloba – Ultra Resolution

Application #AN2270

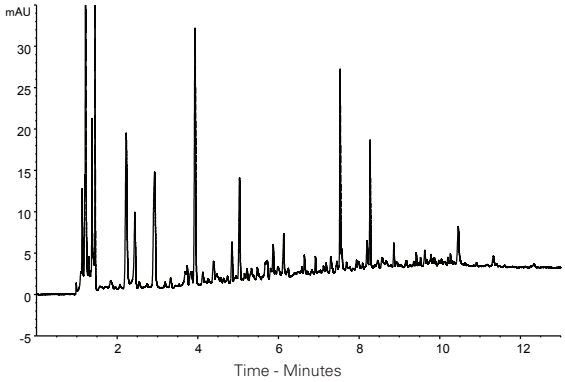
Conditions

Column: ACE Excel 1.7 C18-PFP
Dimensions: 2 x 100 x 3.0 mm (coupled)
Part Number: 2 x EXL-1710-1003U
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN

Gradient:

Time (mins)	%B
0.00	5
0.72	5
15.72	50
18.72	100
20.72	100
22.72	5

Flow Rate: 0.8 mL/min
Injection: 2 µL
Temperature: 80 °C
Detection: UV, 254 nm
Sample: Extract of *Ginkgo Biloba*



Need a custom column for your application?

Please enquire

email: info@ace-hplc.com

Ginkgo Biloba - Used in traditional medicine and as a source of food

Ginsenosides from Chinese Medicine by UHPLC-MS/MS

Application #AN3540

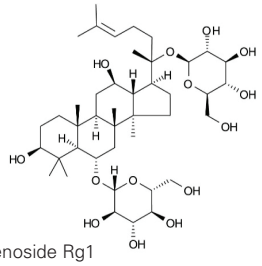
Conditions

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

Gradient:

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

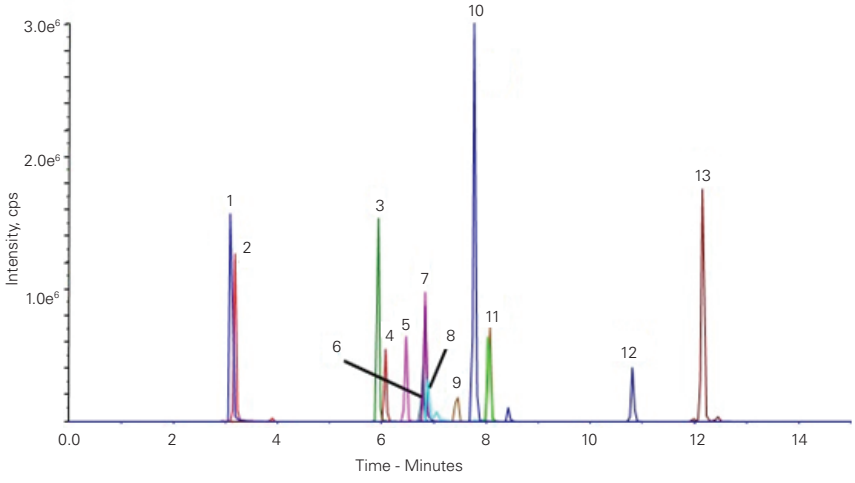
Flow Rate: 0.4 mL/min
Injection: 2 µL
Temperature: 45 °C
Detection: AB SCIEX 5500 Qtrap MS
ESI in negative ion mode
Source temperature: 450 °C
Sprayer voltage: -4500 V
Stepwise MRM mode for
$[M + HCOO]^-$ > $[M - H]^-$ ion transitions
Mass range 501 – 1250 u (step size 2 u)



Ginsenoside Rg1

Analytes

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



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Ginseng Extract

Application #AN4260

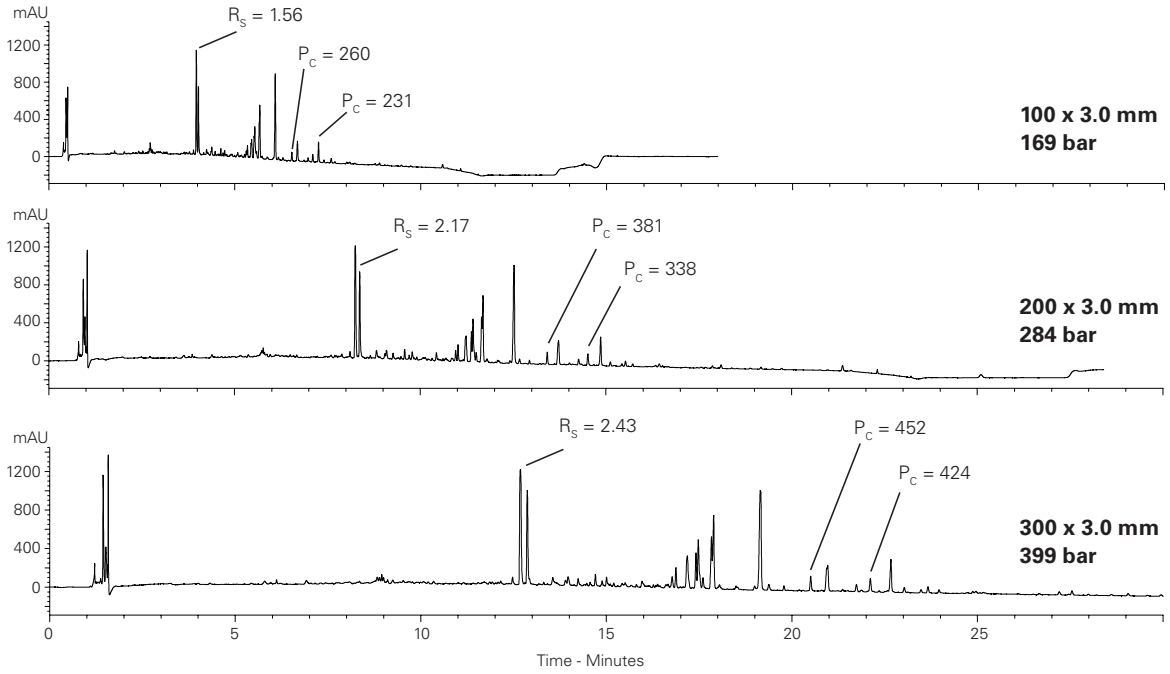
Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 3.0 mm; 2 x 100 x 3.0 mm (coupled); 3 x 100 x 3.0 mm (coupled)
Part Number: CORE-25A-1003U
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN

Gradient:

	Time (mins)			
	100 x 3.0 mm	**200 x 3.0 mm**	**300 x 3.0 mm**	**%B**
	-	0.00	0.00	5
	0.00	0.36	0.71	5
	10.00	20.36	30.71	70
	11.00	22.36	33.71	95
	13.00	26.36	39.71	95
	14.00	28.36	42.71	5
	22.00	44.36	66.71	5

Flow Rate: 0.8 mL/min
Injection: 2 µL (100 x 3.0 mm); 4 µL (200 x 3.0 mm); 6 µL (300 x 3.0 mm)
Temperature: 80 °C
Detection: UV, 203 nm
Sample: 5 x 75 mg tablets ground to fine powder and extracted with 10.0 mL MeCN/H_2O (1:1 v/v) for 15 minutes with ultrasonication. 100 µL supernatant diluted with 300 µL water and filtered using a Whatman Mini-Uniprep syringeless filter
System: Chromaster Ultra Rs



Gliotoxin from *Aspergillus Fumigatus* Liquid Culture

Application #AN3780

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.05% TFA in H_2O/MeCN (90:10 v/v)
B: 0.05% TFA in H_2O/MeCN (40:60 v/v)

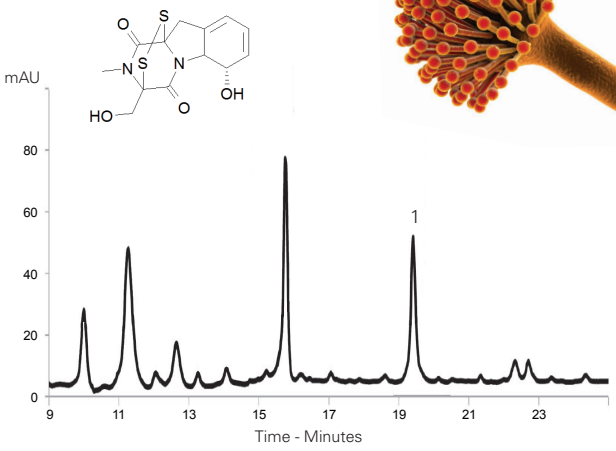
Gradient:

Time (mins)	%B
0	10
21	100

Flow Rate: 1 mL/min
Detection: UV, 254 nm

Analyte

1. Gliotoxin



Svahn KS, Goransson U, Chryssanthou E, Olsen B, Sjolin J, Stromstedt A. Induction of Gliotoxin Secretion in *Aspergillus fumigatus* by Bacteria-Associated Molecules. PloS ONE 9(4): e93685. doi:10.1371/journal.pone.0093685

Glyphosate and Related Compounds as FMOC Derivatives (Gradient)

Application #AN3850

Conditions

Column: ACE Excel 3 SuperC18
Dimensions: 150 x 2.1 mm
Part Number: EXL-1111-1502U
Mobile Phase: A: H_2O
B: MeOH
C: 200 mM ammonium formate pH 3.0

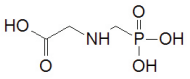
Gradient:

Time (mins)	%A	%B	%C
0	62.5	35.0	2.5
10	2.5	95.0	2.5
11	2.5	95.0	2.5
12	62.5	35.0	2.5
22	62.5	35.0	2.5

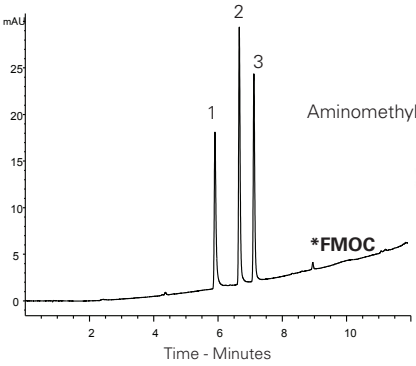
Flow Rate: 0.4 mL/min
Injection: 0.1 µL
Temperature: 60 °C
Detection: UV, 254 nm
Sample: Standards derivatised with FMOC-Cl

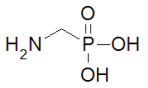
Analytes

1. Glyphosate
2. Aminomethylphosphonic acid (AMPA)
3. Glufosinate

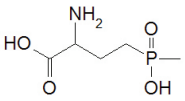


Glyphosate





Aminomethylphosphonic acid (AMPA)



Glufosinate

Glyphosate and Related Compounds as FMOC Derivatives (Isocratic)

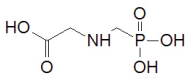
Application #AN3860

Conditions

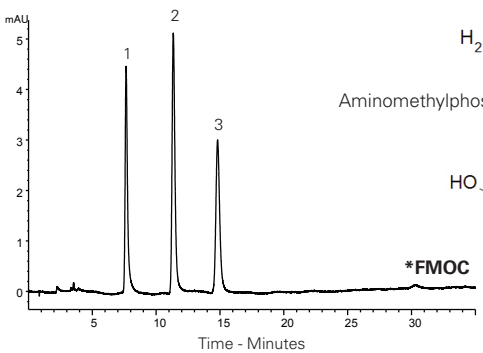
Column: ACE Excel 3 SuperC18
Dimensions: 150 x 2.1 mm
Part Number: EXL-1111-1502U
Mobile Phase: 5 mM ammonium formate pH 3.0 in H_2O/MeOH (55:45 v/v)
Flow Rate: 0.4 mL/min
Injection: 0.1 µL
Temperature: 25 °C
Detection: UV, 254 nm
Sample: Standards derivatised with FMOC-Cl

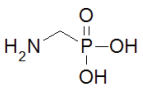
Analytes

1. Glyphosate
2. Aminomethylphosphonic acid (AMPA)
3. Glufosinate

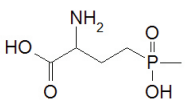


Glyphosate





Aminomethylphosphonic acid (AMPA)



Glufosinate

Green Tea Extract

Application #AN4280

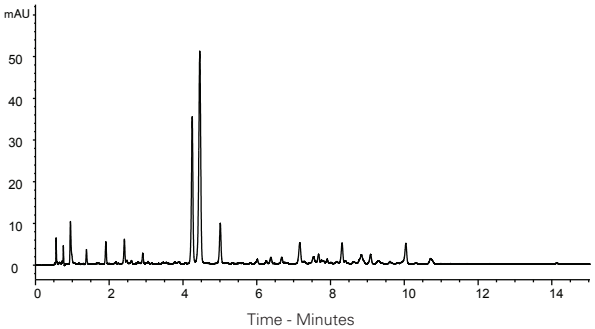
Conditions

Column: ACE Excel 1.7 SuperC18
Dimensions: 100 x 3.0 mm
Part Number: EXL-1711-1003U
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN

Gradient:

Time (mins)	%B
0	5
15	20
17	95
18	95
20	5
27	5

Flow Rate: 0.8 mL/min
Injection: 2 µL
Temperature: 80 °C
Detection: UV, 260 nm
Sample: Tablet ground to fine powder and extracted with MeCN/H_2O (1:1 v/v) with ultrasonication. Supernatant diluted with H_2O and filtered using Whatman Mini-Uniprep syringeless filter
System: Chromaster Ultra Rs



Green Tea Metabolite Profiling by LC-MS

Application #AN2580

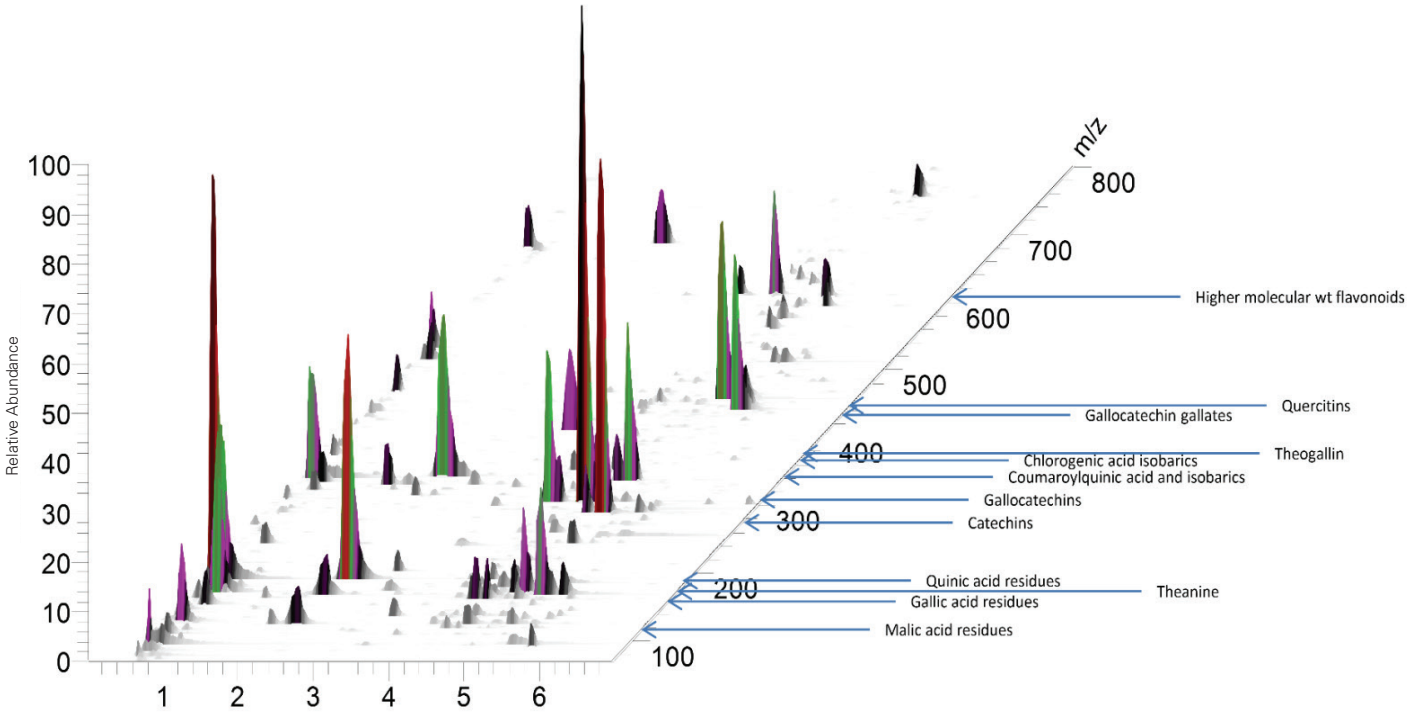
Conditions

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

Gradient:

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

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



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Hair Dye Restricted Components (I)

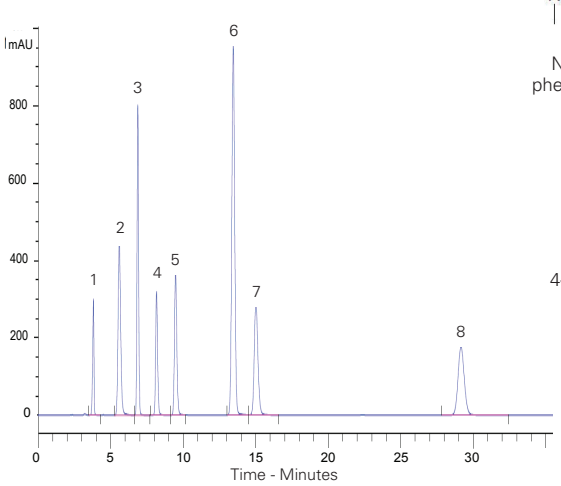
Application #AN2100

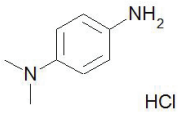
Conditions

Column: ACE Excel 5 C18-Amide
Dimensions: 250 x 4.6 mm
Part Number: EXL-1212-2546U
Mobile Phase: 1.8 g disodium phosphate dodecahydrate + 2.8 g potassium dihydrogen phosphate + 1.0 g sodium 1-heptanesulfonate (all diluted to 1.0 L with water)/MeCN (60:40 v/v)
Flow Rate: 1 mL/min
Temperature: 60 °C
Detection: UV, 280 nm

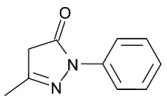
Analytes

1. N,N-Dimethyl-1,4-phenylenediamine HCl
2. 5-Methyl-2-phenyl-1,2-dihydropyrazole-3-one
3. 6-Hydroxyindole
4. 4-Chlororesorcinol
5. 2,7-Dihydroxynaphthalene
6. 4-Aminodiphenylamine
7. 1,5-Dihydroxynaphthalene
8. 1-Naphthol

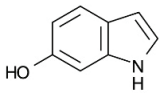




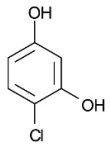
N,N-Dimethyl-1,4-phenylenediamine HCl



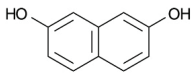
5-Methyl-2-phenyl-1,2-dihydropyrazol-3-one



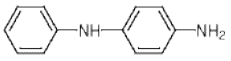
6-Hydroxyindole



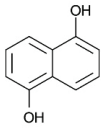
4-Chlororesorcinol



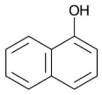
2,7-Dihydroxynaphthalene



4-Aminodiphenylamine



1,5-Dihydroxynaphthalene



1-Naphthol

Hair Dye Restricted Components (II)

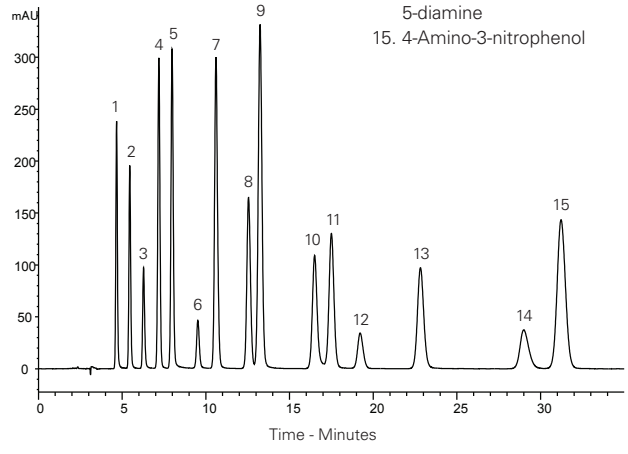
Application #AN2110

Conditions

Column: ACE Excel 5 C18-Amide
Dimensions: 250 x 4.6 mm
Part Number: EXL-1212-2546U
Mobile Phase: 1.8 g disodium phosphate dodecahydrate + 2.8 g potassium dihydrogen phosphate + 1.0 g sodium 1-heptanesulfonate (all diluted to 1.0 L with water)/MeCN (60:40 v/v)
Flow Rate: 1 mL/min
Temperature: 25 °C
Detection: UV, 280 nm

Analytes

1. p-Phenylenediamine
2. p-Aminophenol
3. Toluene-2,5-diamine
4. m-Aminophenol
5. o-Phenylenediamine
6. 2-Chloro-p-phenylenediamine
7. o-Aminophenol
8. Resorcinol
9. 2-Nitro-p-phenylenediamine
10. Toluene-3,4-diamine
11. 4-Amino-2-hydroxytoluene
12. 2-Methylresorcinol
13. 6-Amino-m-cresol
14. N,N-Diethyltoluene-2,5-diamine
15. 4-Amino-3-nitrophenol



Halogenated Positional Isomer Separations

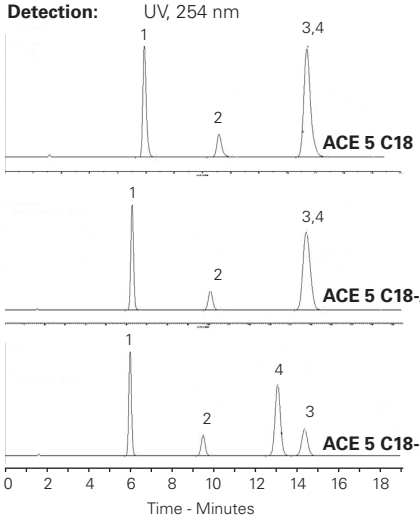
Application #AN1510

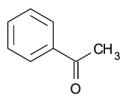
Conditions

Column: ACE 5 C18
ACE 5 C18-AR
ACE 5 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546,
ACE-129-1546,
ACE-1210-1546
Mobile Phase: H_2O/MeOH (50:50 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: Ambient
Detection: UV, 254 nm

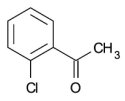
Analytes

1. Acetophenone
2. o-Chloroacetophenone
3. m-Chloroacetophenone
4. p-Chloroacetophenone

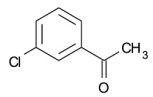




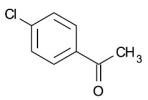
Acetophenone



o-Chloroacetophenone



m-Chloroacetophenone



p-Chloroacetophenone

Hepcidin-25 and Truncated Isoforms by LC-HRMS

Application #AN3090

Conditions

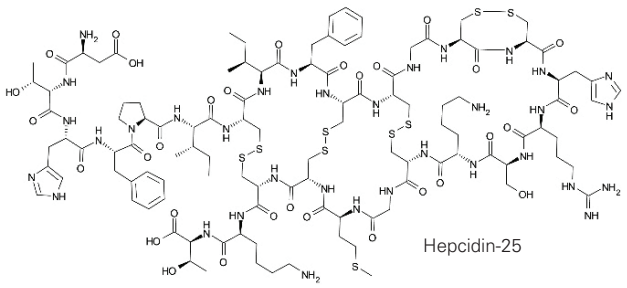
Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN
Gradient:

Time (mins)	%B
0	15
5	100
6	100

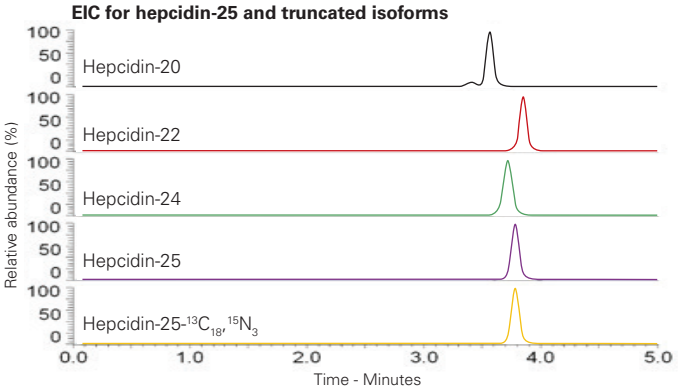
Flow Rate: 0.25 mL/min
Injection: 100 µL
Temperature: 60 °C
Detection: ThermoFisher Scientific Q-Exactive™ high resolution MS
Heated electrospray ionisation (positive mode)
Spray voltage: 4.5 kV
Vaporiser temperature: 200 °C
Capillary temperature: 320 °C
Detection: Full scan *m/z* 400 – 1000
Extracted ion chromatogram from sum of 6 most abundant isotopes of +3, +4 and +5 charge states

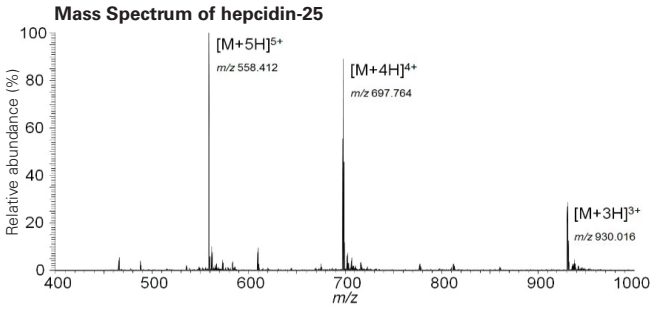
Analyte

1. Hepcidin-25
(MW 2789)



Hepcidin-25





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Herbicide – Benfluralin

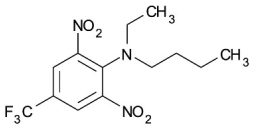
Application #AN2880

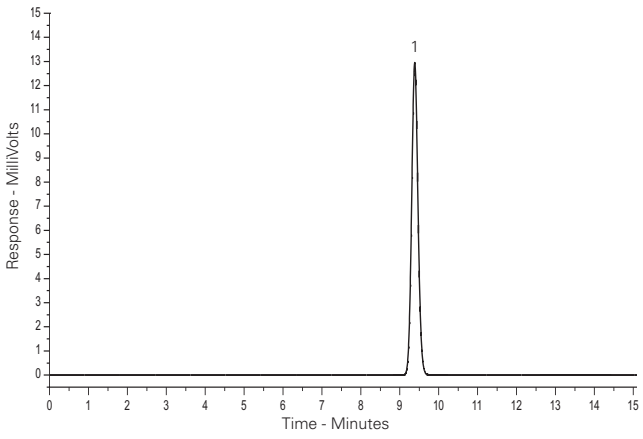
Conditions

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

Analyte

1. Benfluralin





Herbicide – Trifluralin

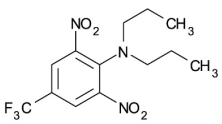
Application #AN2890

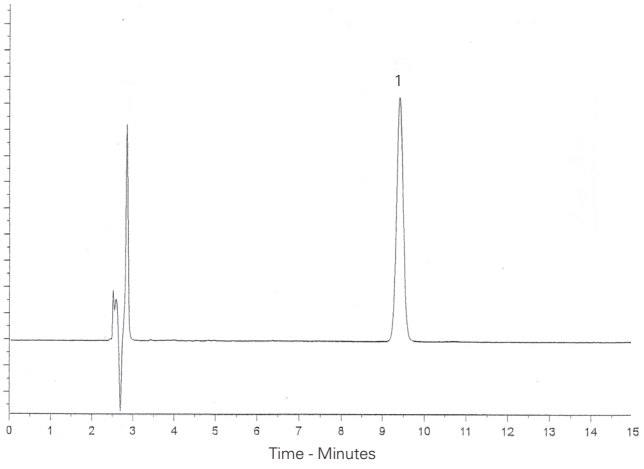
Conditions

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

Analyte

1. Trifluralin





Herbicide Impurity Profile

Application #AN2130

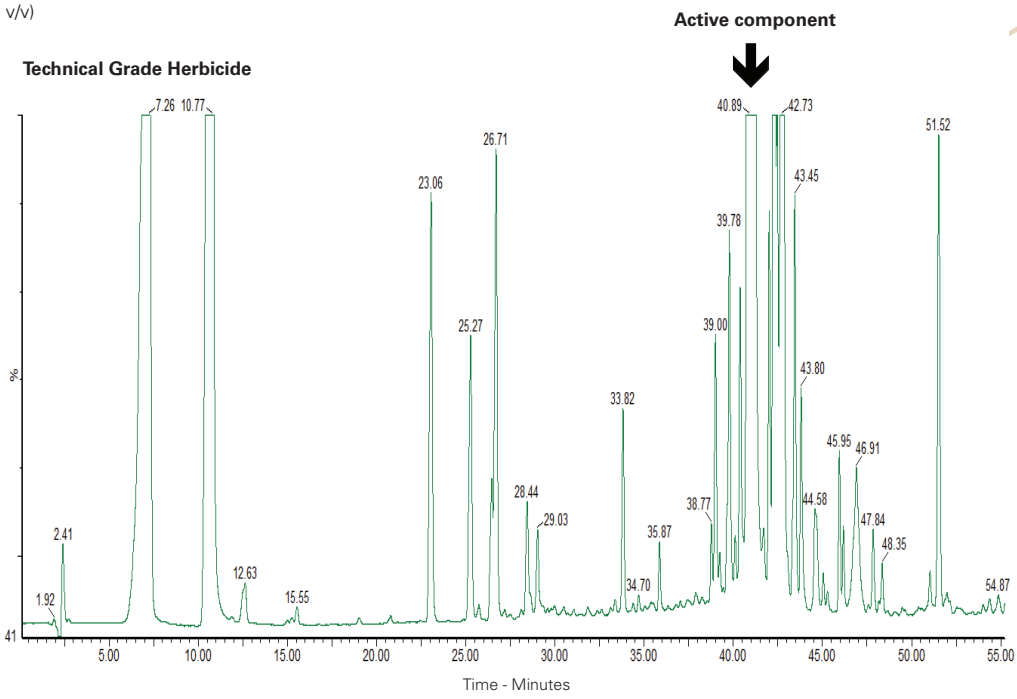
Conditions

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

Gradient:

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

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



Hippuric Acid

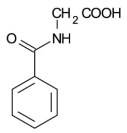
Application #AN2760

Conditions

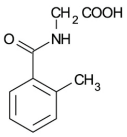
Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 10 mM KH_2PO_4 pH 3.5 in H_2O/MeCN (15:85 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm

Analytes

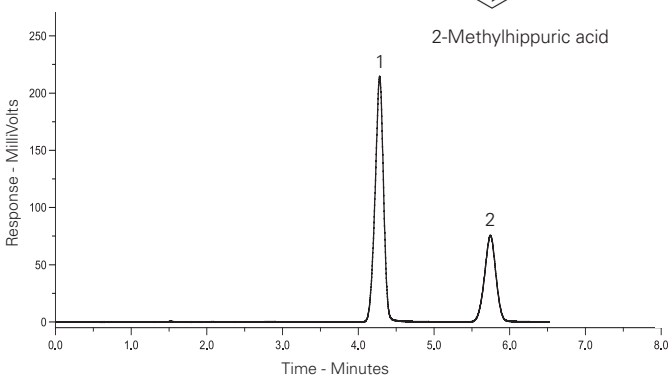
1. Hippuric acid
2. 2-Methylhippuric acid



Hippuric acid



2-Methylhippuric acid



Please enquire for details of our chromatography training, technical advice, applications support, batch reservation service and custom packing facility

email: info@ace-hplc.com

Human Urine Metabolite Profiling by LC-MS

Application #AN2600

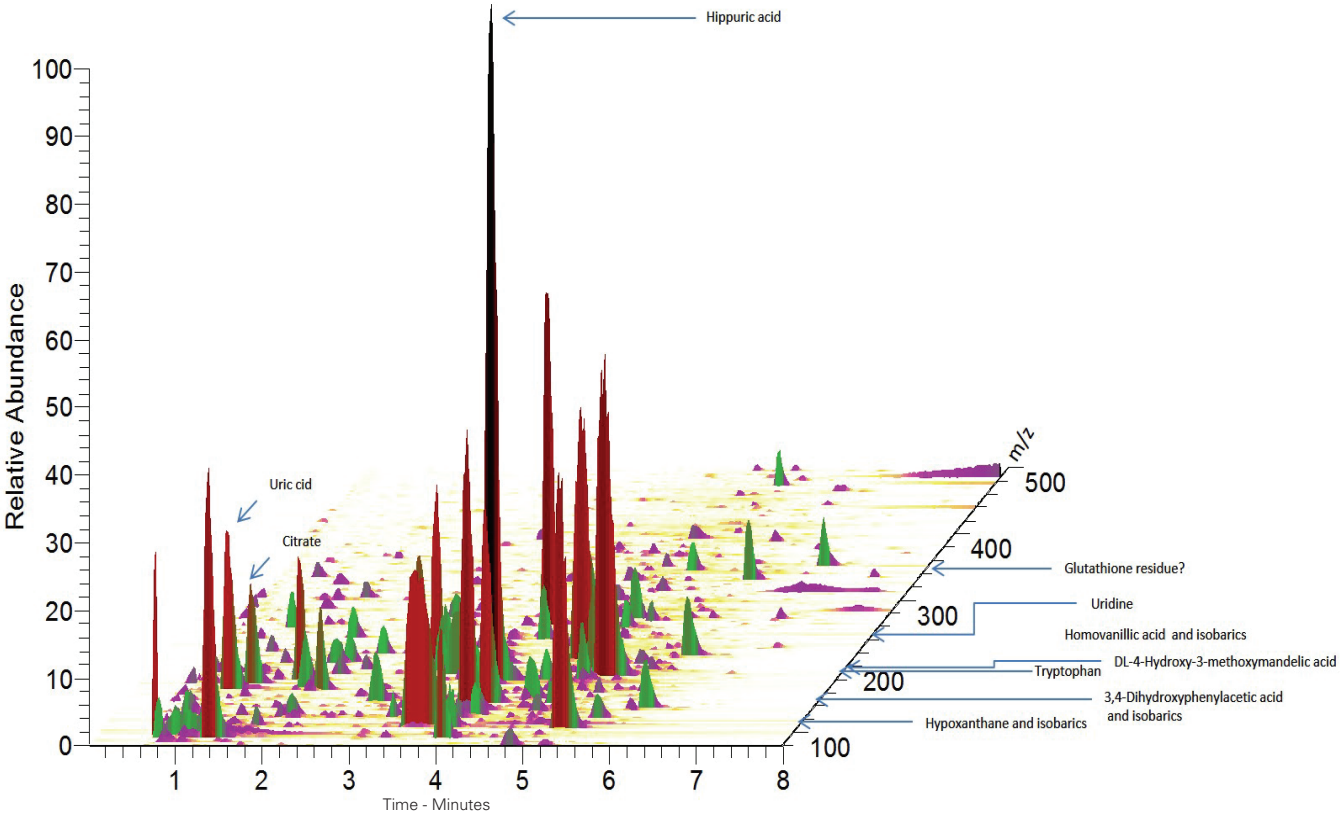
Conditions

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

Gradient:

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

Flow Rate: 0.5 mL/min
Detection: Exactive accurate mass MS system
ESI in negative ion mode
Analytes between *m/z* 70-800 monitored
Sample: Urine of healthy adult volunteer, filtered prior to injection onto column and modular Accela LC system.



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Hydroxychloroquine in Whole (EDTA) Blood by LC-MS/MS

Application #AN1120

Conditions

Column: ACE Excel 2 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: EXL-1011-0502U
Mobile Phase: A: 0.5% Ammonium hydroxide pH 10 in H_2O
B: 0.5% Ammonium hydroxide in MeCN

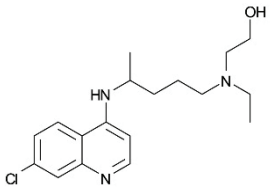
Gradient:

Time (mins)	%B
0.00	30
1.50	100
2.50	100
2.51	30

Flow Rate: 0.4 mL/min
Injection: 5 µL
Temperature: 40 °C
Detection: MS/MS detection with Waters TQD
ESI +ve ion mode

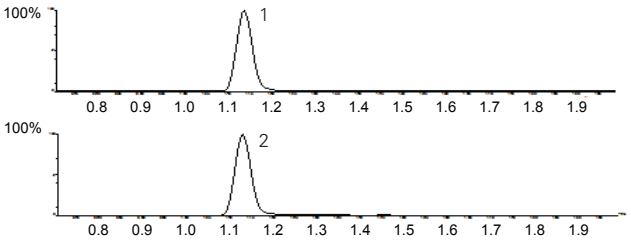
Analytes

1. Hydroxychloroquine (*m/z* 336 → 247)
2. d4-Hydroxychloroquine (IS) (*m/z* 340 → 251)
3. Desethylhydroxychloroquine (*m/z* 308 → 247)

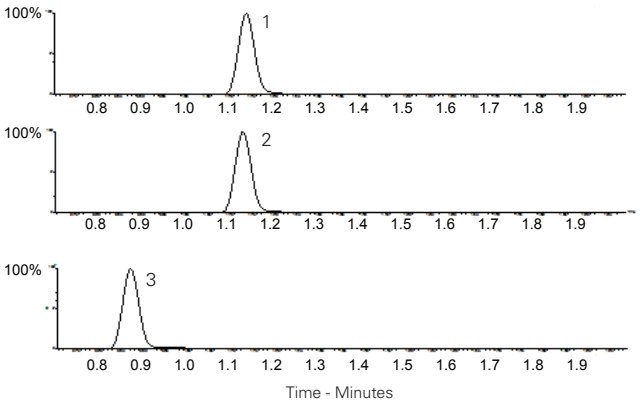


Hydroxychloroquine

Typical chromatogram for lowest calibrator (0.09 mg/L hydroxychloroquine)



Typical chromatogram for whole (EDTA) blood samples from patient with systemic lupus



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Combined Hypertension Therapy Drugs

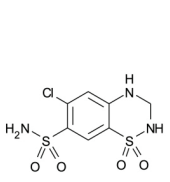
Application #AN4210

Conditions

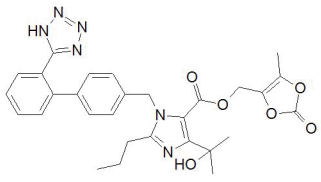
Column: ACE 5 CN
Dimensions: 200 x 4.6 mm
Part Number: ACE-124-2046
Mobile Phase: 10 mM phosphoric acid in H_2O, pH 2.5/MeCN/MeOH (80:7:13 v/v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 30 °C
Detection: UV, 235 nm
Sample: 1 µg/mL each analyte

Analytes

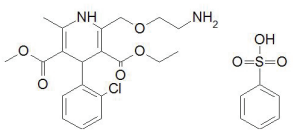
1. Hydrochlorothiazide
2. Olmesartan medoxomil
3. Amlodipine besylate
4. Valsartan



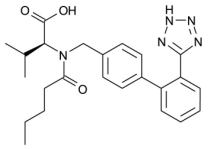
Hydrochlorothiazide



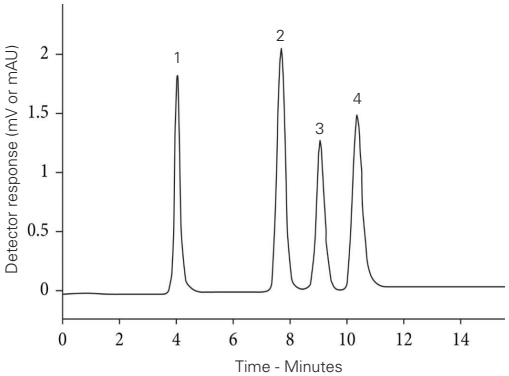
Olmesartan medoxomil



Amlodipine besylate



Valsartan



Tekkeli SEK. Development of an HPLC-UV Method for the Analysis of Drugs used for Combined Hypertension Therapy in Pharmaceutical Preparations and Human Plasma. Journal of Analytical Methods in Chemistry (2013) http://dx.doi.org/10.1155/2013/179627

Ibuprofen and Related Impurities

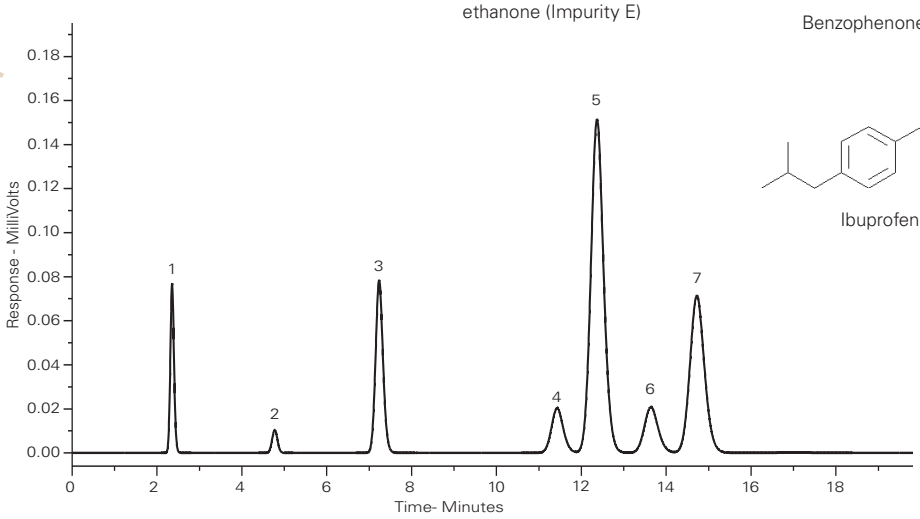
Application #AN4000

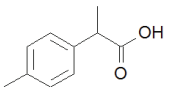
Conditions

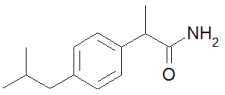
Column: ACE 5 C18
Dimensions: 150 x 3.0 mm
Part Number: ACE-121-1503
Mobile Phase: 0.1% TFA in H_2O/MeCN (64:36 v/v)
Flow Rate: 1.5 mL/min
Temperature: 40 °C
Detection: UV, 214 nm

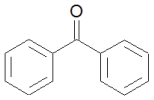
Analytes

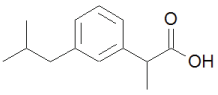
1. 2-(4-Methylphenyl) propanoic acid (Impurity D)
2. 2-(4-Isobutylphenyl) propanamide (Impurity C)
3. Benzophenone (IS)
4. 2-(3-Isobutylphenyl) propanoic acid (Impurity A)
5. Ibuprofen
6. 2-(4-Butylphenyl) propanoic acid (Impurity B)
7. 1-(4-Isobutylphenyl) ethanone (Impurity E)

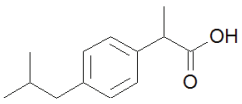


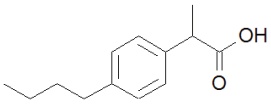

2-(4-Methylphenyl) propanoic acid (Impurity D)

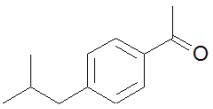

2-(4-Isobutylphenyl) propanamide (Impurity C)


Benzophenone (IS)


2-(3-Isobutylphenyl) propanoic acid (Impurity A)


Ibuprofen


2-(4-Butylphenyl) propanoic acid (Impurity B)


1-(4-Isobutylphenyl) ethanone (Impurity E)

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Ibuprofen in Combination with Antihistamine and Decongestant

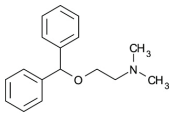
Application #AN2120

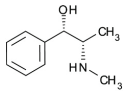
Conditions

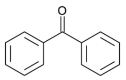
Column: ACE Excel 3 C18-Amide
Dimensions: 150 x 4.6 mm
Part Number: EXL-1112-1546U
Mobile Phase: 0.01% potassium dihydrogen phosphate/MeCN (60:40 v/v)
Flow Rate: 0.6 mL/min
Injection: 0.5 µL
Temperature: 45 °C
Detection: UV, 214 nm

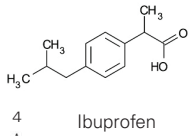
Analytes

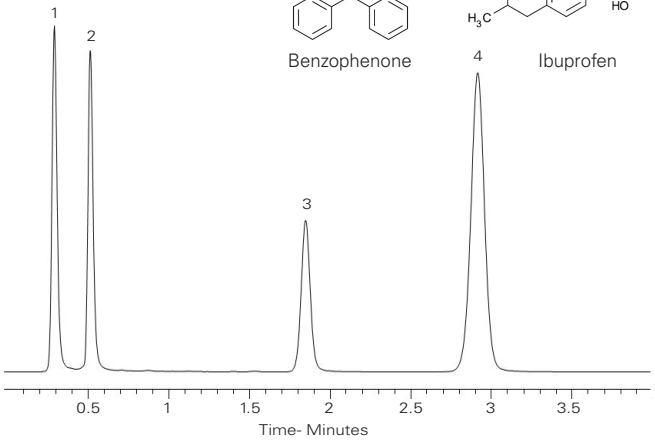
1. Diphenhydramine
2. Pseudoephedrine
3. Benzophenone
4. Ibuprofen


Diphenhydramine


Pseudoephedrine


Benzophenone


Ibuprofen



Alternative column dimensions available

Please enquire
email: info@ace-hplc.com

Illegal Dyes in Spices

Application #AN2910

Conditions

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

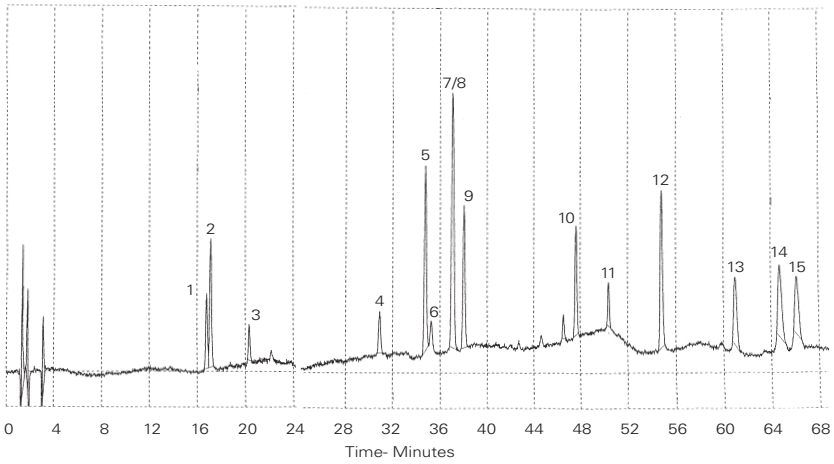
Gradient:

Time (mins)	%A	%B	%C	Curve
0	45	50	5	
45	3	92	5	6
65	3	92	5	11
66	45	50	5	1
75	45	50	5	1

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

Analytes

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



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Insulin Analogues in Clinical and Post-Mortem Analyses

Application #AN3350

Conditions

Column: ACE 5 C18-300
Dimensions: 50 x 2.1 mm
Part Number: ACE-221-0502
Mobile Phase: A: 0.1% acetic acid in H_2O
B: 0.1% acetic acid in IPA/MeCN (25:75 v/v)

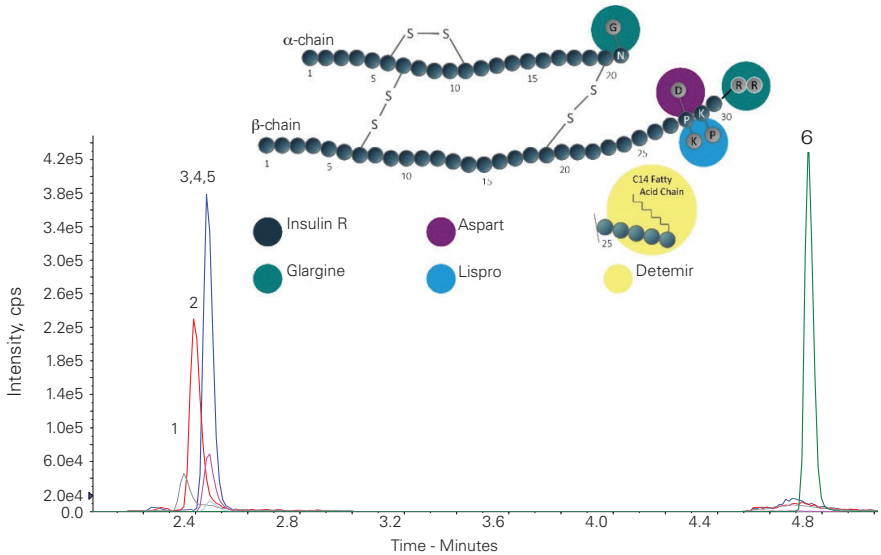
Gradient:

Time (mins)	%B
0.0	22
0.5	22
1.0	34
3.0	36
4.0	98
6.2	98
6.3	22

Flow Rate: 0.55 mL/min
Injection: 40 µL
Detection: AB Sciex QTRAP 5500
ESI positive ion mode
Ion spray voltage: 5500 V
Temperature: 600 °C
Sample: 100 µU/mL insulin analogues in steroid-free serum

Analytes

1. Glargine
   MW 6063
   Quantifier (*m/z* 867.2 → 136)
   Qualifier (*m/z* 1011.4 → 1164.2)
   Qualifier (*m/z* 1011.4 → 1179.4)
2. Bovine insulin (IS)
   MW~5800
   Quantifier (*m/z* 956.5 → 136.1)
   Qualifier (*m/z* N/A)
3. Aspart
   MW 5826
   Quantifier (*m/z* 971.7 → 136)
   Qualifier (*m/z* 1166 → 219)
   Qualifier (*m/z* 971.7 → 226.1)
4. Lispro
   MW 5808
   Quantifier (*m/z* 1162.4 → 217)
   Qualifier (*m/z* 968.6 → 217)
5. Insulin R
   MW 5808
   Quantifier (*m/z* 1162.4 → 345.2)
   Qualifier (*m/z* 1162.3 → 65.2)
   Qualifier (*m/z* 1162.4 → 226.1)
6. Detemir
   MW 5917
   Quantifier (*m/z* 1184 → 454.4)
   Qualifier (*m/z* 987 → 454.4)
   Qualifier (*m/z* 1184.0 → 357.4)



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Insulins

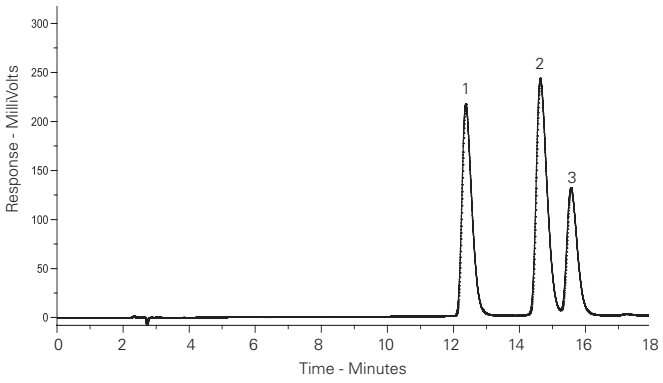
Application #AN2770

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	A: 0.1% TFA in H_2O/MeCN (71:29 v/v)
	B: 0.1% TFA in H_2O/MeCN (68:32 v/v)
Gradient:	**Time (mins) %B**
	0 10
	16 90
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 215 nm

Analytes

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



Isoflavones

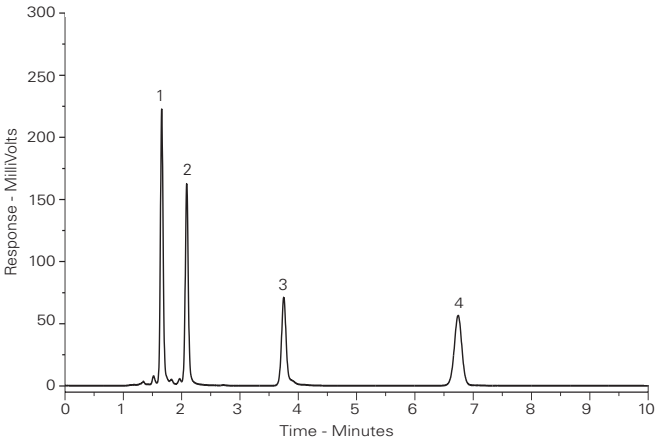
Application #AN2970

Conditions

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

Analytes

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



Isoflavones in Red Clover and Soy Extract

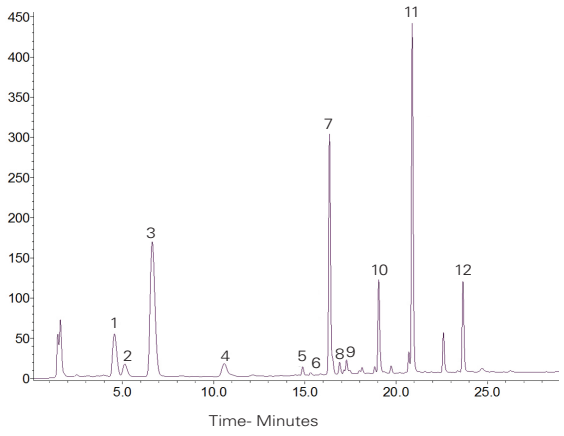
Application #AN1130

Conditions

Column:	ACE 3 C18-AR
Dimensions:	150 x 2.1 mm
Part Number:	ACE-119-1502
Mobile Phase:	A: Acetic acid in H_2O pH 2.8
	B: 0.6% Acetic acid in MeCN
Gradient:	**Time (mins) %B**
	0 15
	7 15
	27 75
Flow Rate:	0.35 mL/min
Injection:	3 µL
Temperature:	25 °C
Detection:	UV, 254 nm

Analytes

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



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

Red clover is a perennial herb that commonly grows wild in meadows throughout Europe and Asia.

Itraconazole and Hydroxyitraconazole in Human Whole Blood by LC-MS/MS

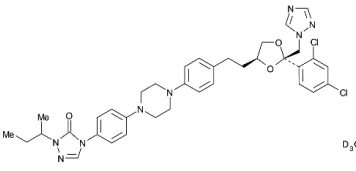
Application #AN3380

Conditions

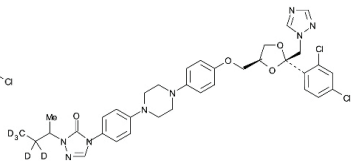
Column:	ACE 3 C18-AR
Dimensions:	50 x 2.1 mm
Part Number:	ACE-119-0502
Mobile Phase:	A: 10 mM ammonium acetate in H_2O
	B: 10 mM ammonium acetate in MeOH
Gradient:	**Time (mins) %B**
	0 75
	2 98
	3 98
Flow Rate:	0.7 mL/min
Temperature:	45 °C
Detection:	AB Sciex 4000
	ESI positive ion mode
Sample:	1.0 ng/mL human whole blood (LLOQ)

Analytes

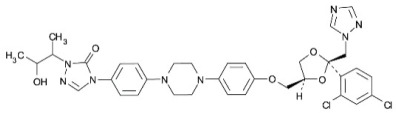
1. Itraconazole
   (*m/z* 705.3 → 392.3)
2. Itraconazole-d5
   (*m/z* 710.4 → 397.4)
3. Hydroxyitraconazole
   (*m/z* 721.3 → 408.2)
4. Hydroxyitraconazole-d5
   (*m/z* 726.4 → 413.3)



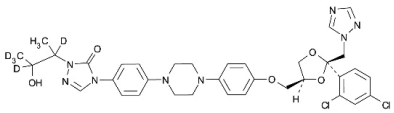
Itraconazole



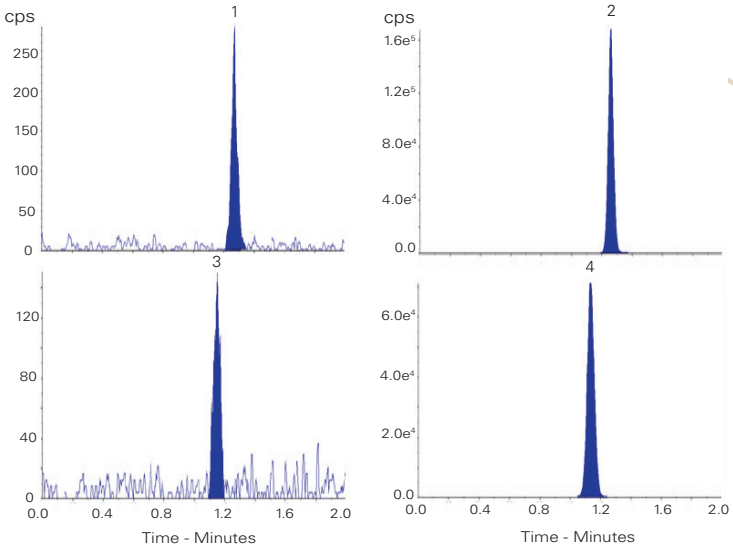
Itraconazole-d5



Hydroxyitraconazole



Hydroxyitraconazole-d5



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Lansoprazole and Degradation Products after Acidic Hydrolysis in 0.1 M HCl

Application #AN1520

Conditions

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

Gradient:

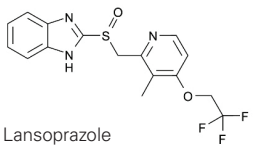
Time 1 (mins)	Time 2 (mins)	Time 3 (mins)	%B
0.0	0.0	0.0	10
15.0	30.0	45.0	90
15.5	30.5	45.5	90
18.0	33.0	48.0	10

Post time 10 minutes

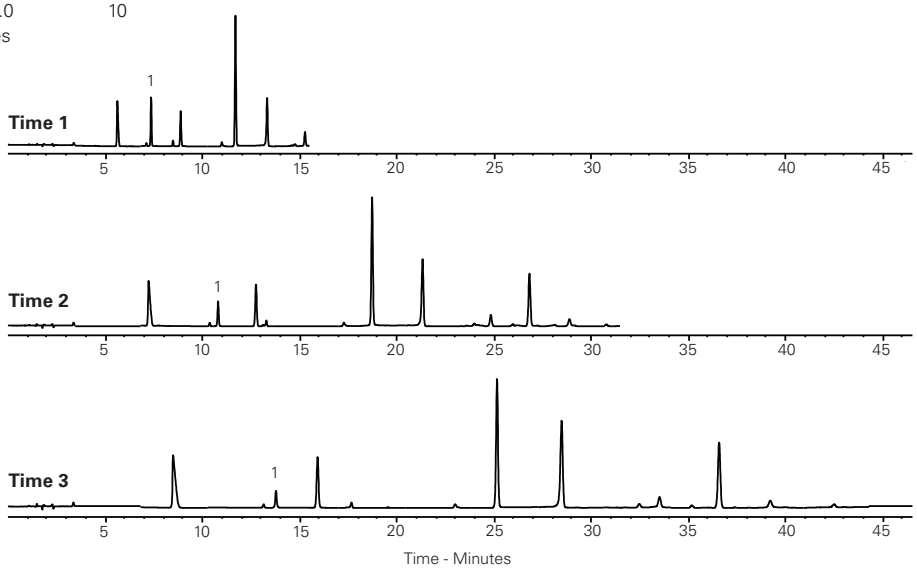
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 30 °C
Detection: UV, 280 nm

Analyte

1. Lansoprazole



Lansoprazole



Lapatinib Anticancer Drug in Human Plasma by LC-MS/MS

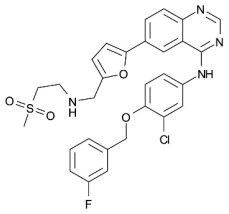
Application #AN3360

Conditions

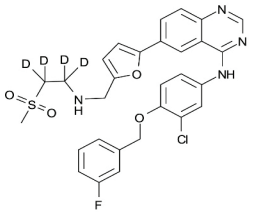
Column: ACE 5 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-121-1046
Mobile Phase: 10 mM ammonium formate pH 3.5/MeCN (10:90 v/v)
Flow Rate: 1 mL/min
Injection: 0.5 µL
Temperature: 40 °C
Detection: API 4000 triple quad MS
Positive ion mode ESI
Ion spray voltage: 5500 V
Temperature: 400 °C
Sample: Extracted from 100 µL plasma using liquid-liquid extraction

Analytes

1. Lapatinib
(*m/z* 581.1 ⟶ 365.2)
Concentration 1000 ng/mL
2. Lapatinib-d4 (IS)
(*m/z* 585.1 ⟶ 365.0)
Concentration 100 ng/mL

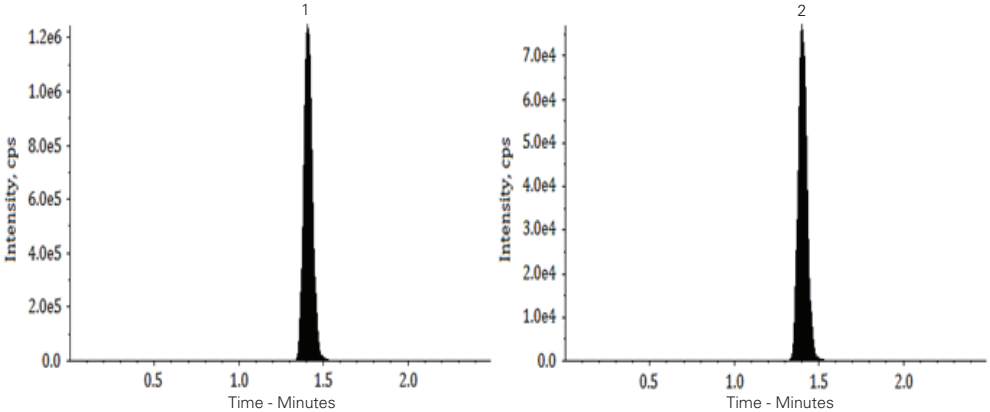


Lapatinib



Lapatinib-d4 (IS)

LLOQ	2.5 ng/mL
LOD	1.0 ng/mL
Method Linearity	2.5 – 2500 ng/mL



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Lidocaine in Saliva by LC-MS/MS

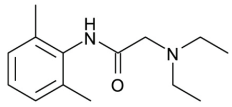
Application #AN2570

Conditions

Column:	ACE 3 C18
Dimensions:	100 x 3.0 mm
Part Number:	ACE-111-1003
Mobile Phase:	A: 0.1% formic acid in MeCN/H_2O (20:80 v/v)
	B: 0.1% formic acid in MeCN/H_2O (80:20 v/v)

Gradient:	**Time (mins)**	**%B**
	0.0	20
	1.0	20
	3.0	80
	4.5	80

Flow Rate:	0.3 mL/min
Injection:	10 µL
Detection:	Quattro-Micro triple quad MS Positive ion mode ESI

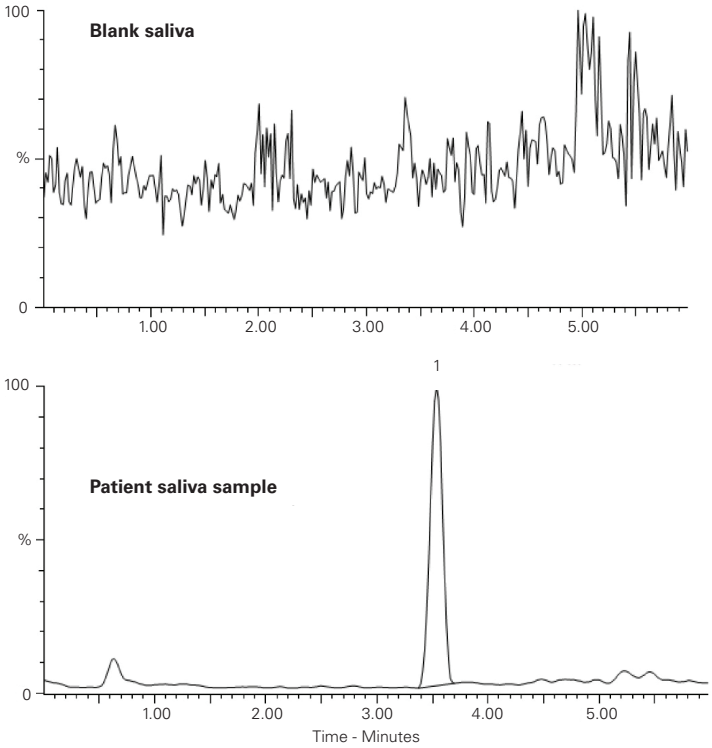


1. Lidocaine

Analyte

1. Lidocaine

(*m/z* 235 → 86)



Saliva samples taken after "Emla 5 %" application to skin

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Lincosamide Antibiotics

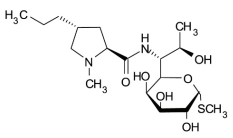
Application #AN2650

Conditions

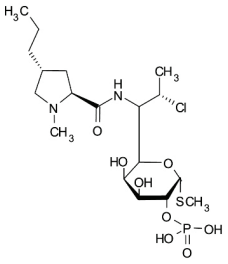
Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	0.02 M sodium phosphate dibasic pH 3.0/MeCN (70:30 v/v)
Flow Rate:	1 mL/min
Injection:	25 µL
Temperature:	25 °C
Detection:	UV, 205 nm

Analytes

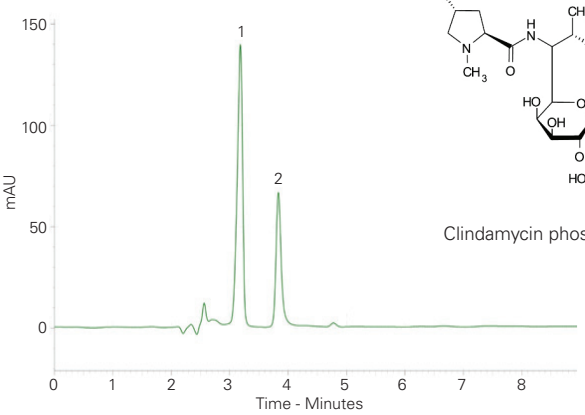
1. Lincomycin HCl
2. Clindamycin phosphate



Lincomycin HCl



Clindamycin phosphate



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Lipid Classes Separation from *Drosophila Melanogaster*

Application #AN1530

Conditions

Column: ACE 3 SIL
Dimensions: 150 x 3.0 mm
Part Number: ACE-117-1503
Mobile Phase: A: IPA/MeCN (20:80 v/v)
B: IPA/0.02 M ammonium formate (20:80 v/v)
Gradient:

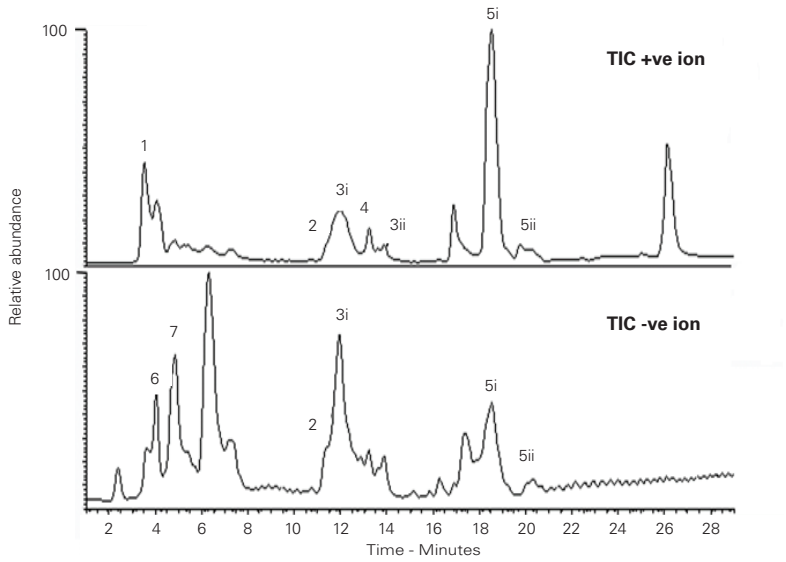
Time (mins)	%B
0.0	8
1.0	8
5.0	9
10.0	20
16.0	25
23.0	35
26.0	8

Flow Rate: 0.3 mL/min
Detection: LTQ Orbitrap MS
Positive and negative ion mode

Drosophila Melanogaster

Analytes

1. Triglyceride (TG)
2. Phosphoserine (PS)
3i. Phosphoethanolamine (PE)
3ii. Lyso phosphoethanolamine (Lyso PE)
4. Sphingomyelin phosphoethanolamine (SMPE)
5i. Phosphatidylcholine (PC)
5ii. Lyso phosphatidylcholine (Lyso PC)
6. Glycerophosphoglycerol (GPG)
7. Phosphoinositol (PI)



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Liquorice Extracts Fingerprint

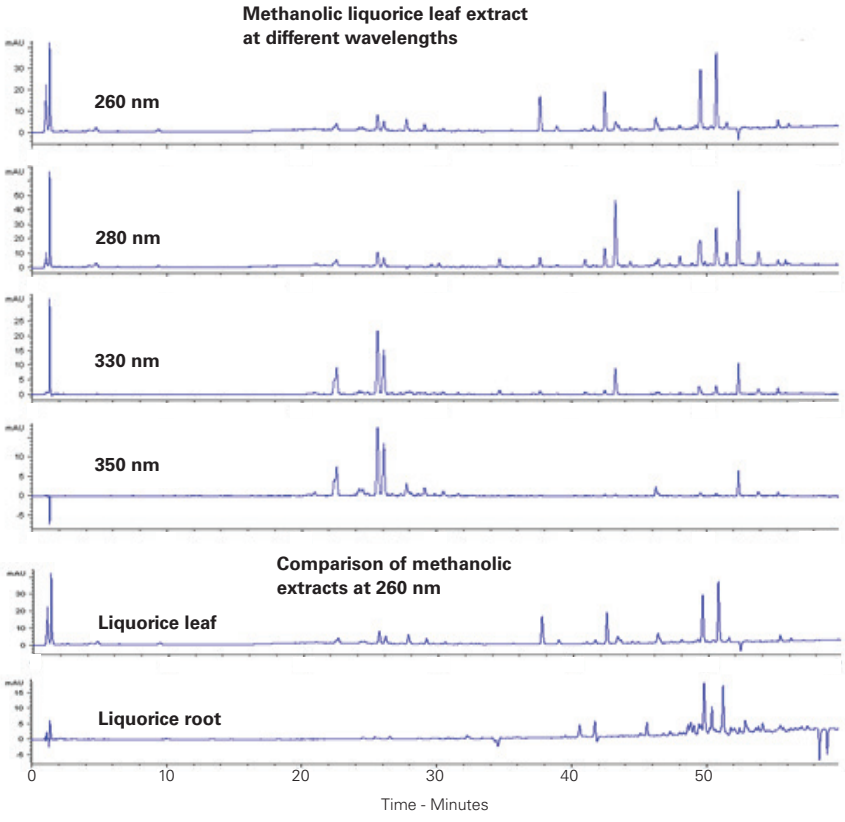
Application #AN2090

Conditions

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

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

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



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Local Anaesthetics

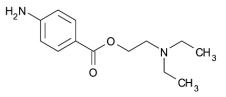
Application #AN3220

Conditions

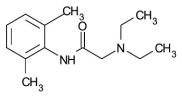
Column: ACE 5 AQ
Dimensions: 250 x 4.6 mm
Part Number: ACE-126-2546
Mobile Phase: MeCN/H_2O/2.5 M H_2SO_4 (21:79:0.1 v/v/v)
Flow Rate: 1.5 mL/min
Detection: UV

Analytes

1. Procaine
2. Lignocaine
3. Cocaine

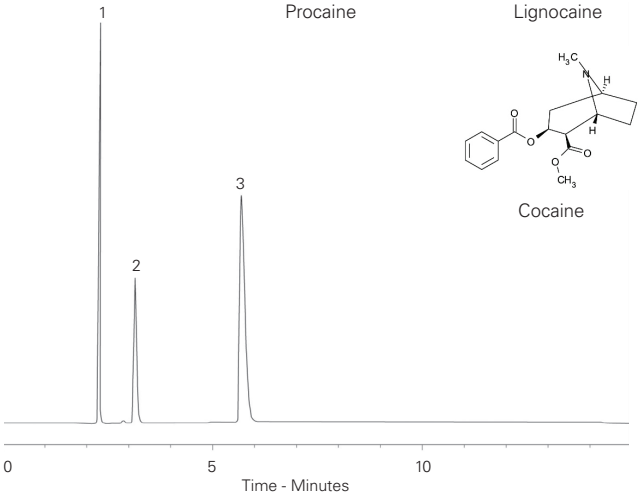


Procaine



Lignocaine

Cocaine



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15-Hydroxy Lubiprostone in Human Plasma

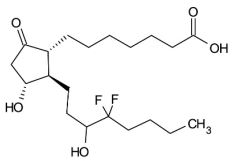
Application #AN1900

Conditions

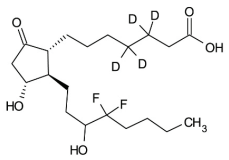
Column: ACE Excel 2 C18
Dimensions: 50 x 3.0 mm
Part Number: EXL-101-0503U
Mobile Phase: A: 0.1% formic acid in H_2O
B: MeCN
Flow Rate: 0.65 mL/min
Injection: 15 µL
Temperature: 35 °C
Detection: MDS Sciex API 5000
TurbolonSpray negative mode
IonSpray voltage -4500 V
Source Temperature 450 °C

Analytes

1. 15-Hydroxy lubiprostone
(m/z 391.2 ⟶ 373.2)
2. 15-Hydroxy lubiprostone-d4 (IS)
(m/z 395.2 ⟶ 377.2)

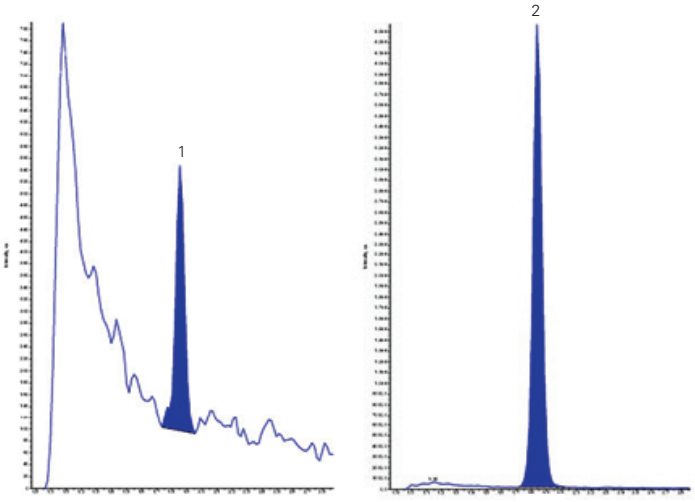


15-Hydroxy lubiprostone



15-Hydroxy lubiprostone-d4

Lowest calibration standard sample containing 2.0 pg/mL in human EDTA K3 plasma.
Lubiprostone, a fatty acid derived from prostaglandin E1, is rapidly metabolised to 15-hydroxy lubiprostone. Quantitation is based on 15-hydroxy lubiprostone, with the d4 analogue as internal standard.



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Lubricant Additives: ADPA/OPNA Antioxidants

Application #AN1170

Conditions

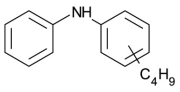
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	CORE-25A-1546U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN/IPA (1:2 v/v)

Gradient:	**Time (mins)**	**%B**
	0.0	65.0
	15.0	97.5
	25.0	97.5
	25.1	65.0

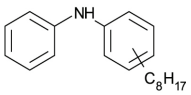
Flow Rate:	1 mL/min
Temperature:	60 °C
Detection:	UV, 220 nm

Analytes

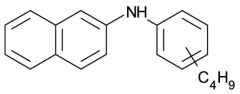
1. C4-ADPA
2. C8-ADPA
3. C4-OPNA
4. C12-ADPA
5. C16-ADPA



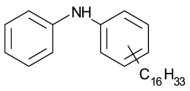
C4-ADPA



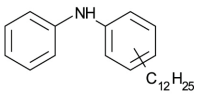
C8-ADPA



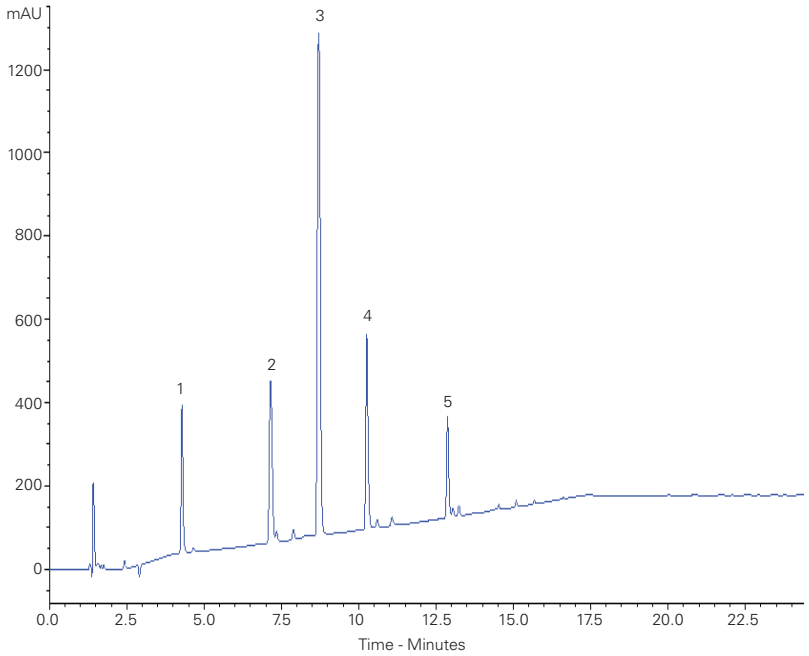
C4-OPNA



C16-ADPA



C12-ADPA



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Lurbinectedin in Plasma by LC-MS/MS

Application #AN3810

Conditions

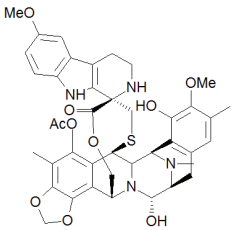
Column:	ACE 3 C18-PFP
Dimensions:	30 x 2.1 mm
Part Number:	ACE-1110-0302
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

Gradient:	**Time (mins)**	**%B**
	0.0	10
	2.5	90
	3.5	90
	3.6	10
	5.0	10

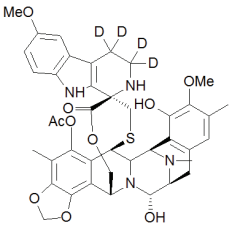
Flow Rate:	0.6 mL/min
Injection:	5 µL
Temperature:	50 °C
Detection:	API 4000 triple quad
	TurbolonSpray, ESI positive ion mode
	Turbo Temperature: 650 °C
	Ion Spray Potential: 5000 V

Analytes

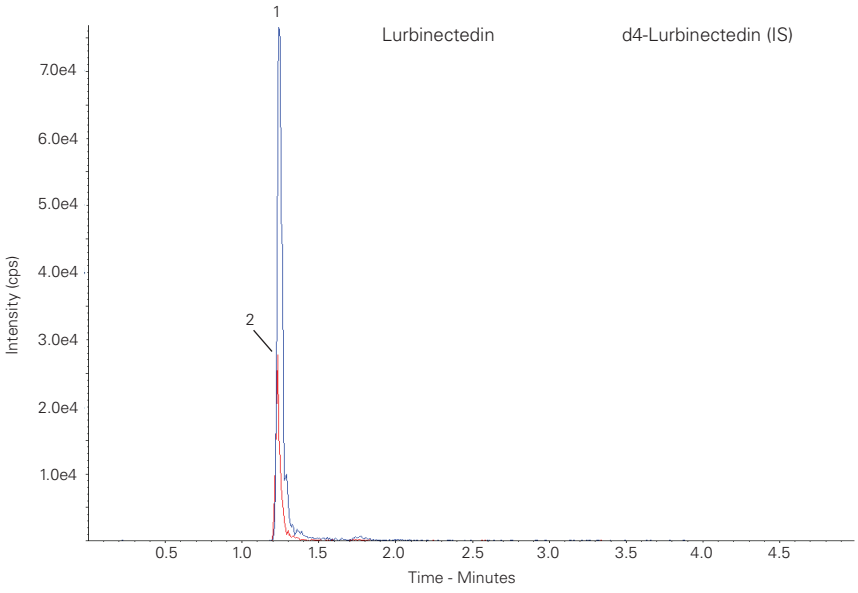
1. Lurbinectedin
   (*m/z* 767.3 → 273.0)
   (LLOQ 0.1 ng/mL)
2. d4-Lurbinectedin (IS)
   (*m/z* 771.4 → 277.0)



Lurbinectedin



d4-Lurbinectedin (IS)



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Malachite Green

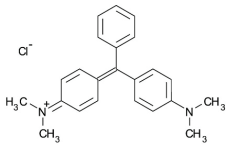
Application #AN2860

Conditions

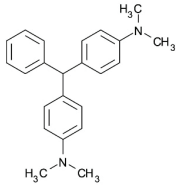
Column: ACE 5 C18
Dimensions: 150 x 3.0 mm
Part Number: ACE-121-1503
Mobile Phase: 10 mM oxalic acid pH 2.9 in H_2O/MeCN (80:20 v/v)
Flow Rate: 0.4 mL/min
Temperature: Ambient
Detection: UV-Vis, 618 nm

Analytes

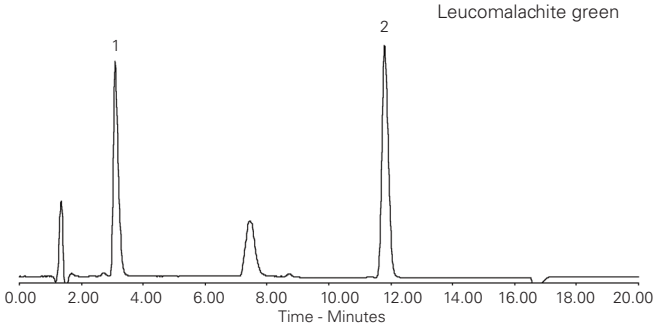
1. Malachite green
2. Leucomalachite green



Malachite green



Leucomalachite green



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Maleic and Fumaric Acids

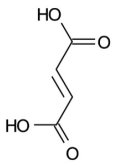
Application #AN3230

Conditions

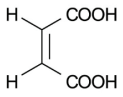
Column: ACE 5 AQ
Dimensions: 250 x 4.6 mm
Part Number: ACE-126-2546
Mobile Phase: 50 mM KH_2PO_4 pH 7.0 in H_2O
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 210 nm

Analytes

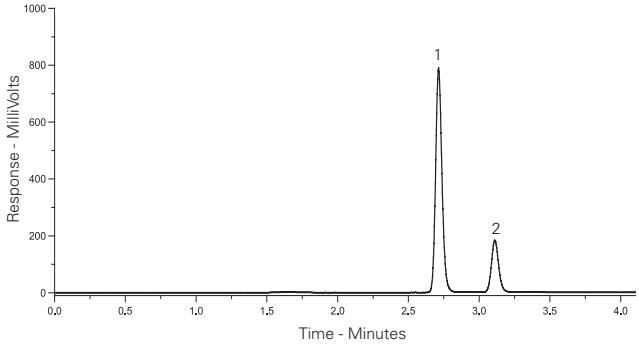
1. Fumaric acid
2. Maleic acid



Fumaric acid



Maleic acid



MDMA (Ecstasy) and PMA (Dr Death) Separation

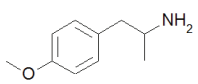
Application #AN4220

Conditions

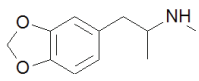
Column: ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-111-1546
Mobile Phase: 0.05 M KH_2PO_4 pH 3.2 in H_2O/MeCN (90:10 v/v)
Flow Rate: 1.2 mL/min
Injection: 10 µL
Temperature: 22 °C
Detection: UV, 210 nm

Analytes

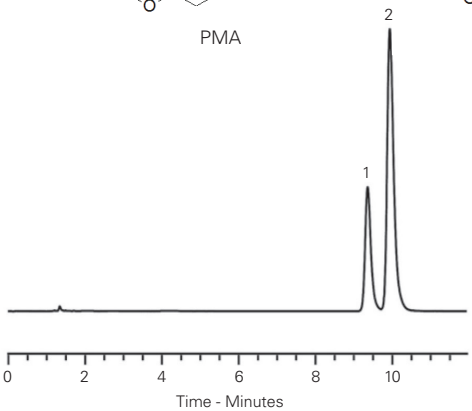
1. PMA
   (4-Methoxyamphetamine)
   LOD 0.08 µg/mL
   LOQ 0.26 µg/mL
2. MDMA
   (3,4-Methylenedioxy methamphetamine)
   LOD 0.04 µg/mL
   LOQ 0.12 µg/mL



PMA



MDMA



Cumba LR, Smith JP, Zuway KY, Sutcliffe OB, do Carmo DR, Banks CE. Forensic electrochemistry: simultaneous voltammetric detection of MDMA and its fatal counterpart 'Dr Death' (PMA). Anal. Methods, 8, 142-152 (2016) doi: 10.1039/c5ay02924d

Melamine using Ion-Pairing Reagent

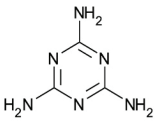
Application #AN2510

Conditions

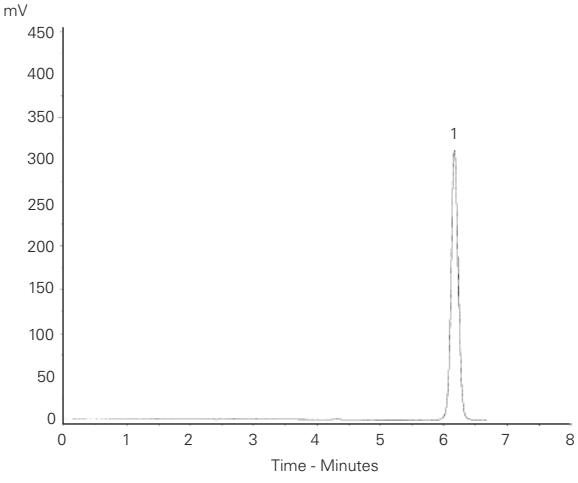
Column: ACE 5 C8
Dimensions: 150 x 4.6 mm
Part Number: ACE-122-1546
Mobile Phase: 5 mM heptafluorobutyric acid/MeCN (95:5 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: Ambient
Detection: UV, 240 nm

Analyte

1. Melamine



Melamine



Metabolomic Analysis of Extracted Jurkat T Cells by LC-HRMS

Application #AN3980

Conditions

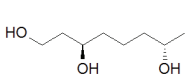
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN
Gradient:

Time (mins)	%B
0	0
1	0
11	65
13	65
18	95
20	95

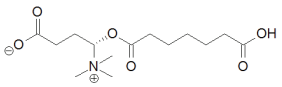
Flow Rate: 0.35 mL/min
Injection: 5 µL
Temperature: 35 °C
Detection: Thermo Scientific Q Exactive Orbitrap MS
Heated electrospray ionisation in positive mode
Spray Voltage: 3.3 kV
Capillary Temperature: 300 °C
Heater Temperature: 350 °C
Mass Scan Range: *m/z* 70-1000
Resolution: 70,000

Analytes

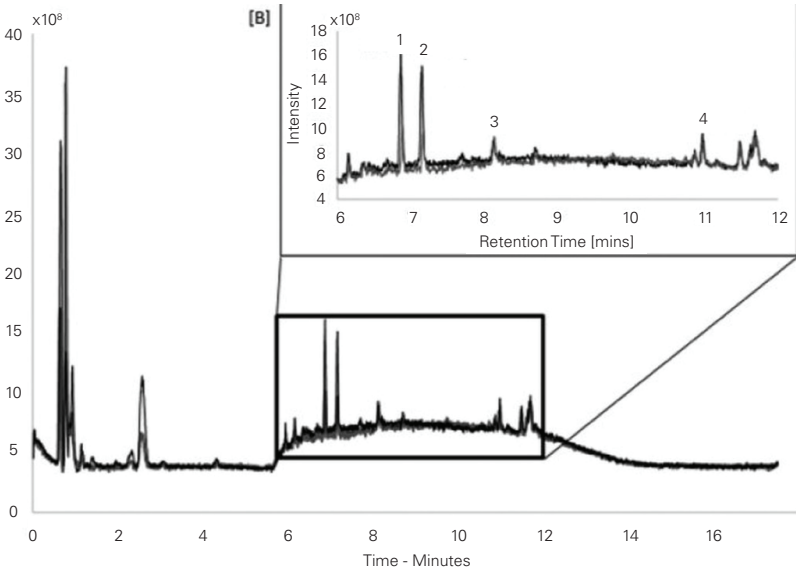
1. Caffeine-d3 (IS)
2. Tryptophan-d3 (IS)
3. 1,3,7-Octanetriol
4. Pimelylcarnitine



1,3,7-Octanetriol



Pimelylcarnitine



TIC overlay for Jurkat T-lymphocyte cells rinsed with either 0.3% ammonium formate (darker line) or 0.3% ammonium acetate.

Ulmer CZ, Yost RA, Chen J, Mathews CE, Garrett TJ. Liquid-Chromatography-Mass Spectrometry Metabolic and Lipidomic Sample Preparation Workflow for Suspension-Cultured Mammalian Cells using Jurkat T Lymphocyte Cells, J. Proteomics Bioinform, (2015), 8(6), 126-132. doi:10.4172/jpb.1000360

Metabolomic Biomarkers in Ethylmalonic Encephalopathy

Application #AN4130

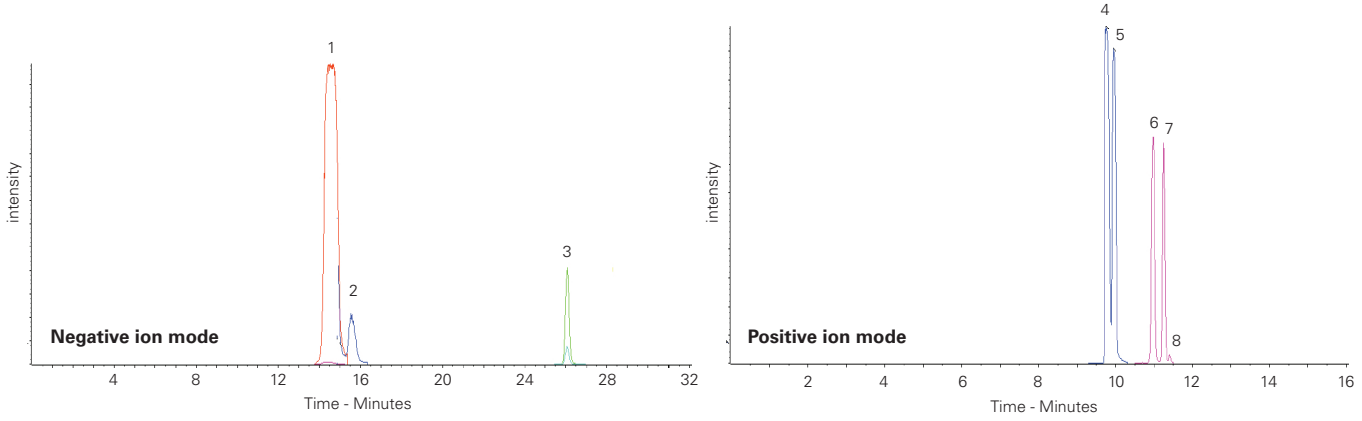
Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN
Detection: Sciex API 4000 triple quad MS
ESI in negative ion mode
Sample: Urine sample from patient with ethylmalonic encephalopathy is filtered and extracted with ice-cold methanol, evaporated to dryness and reconstituted in 0.1% formic acid in water

Please contact info@ace-hplc.com for additional information on the chromatographic conditions used for this analysis.

Analytes

1. Ethylmalonic acid (*m/z* 131 → 87)
2. Methylsuccinic acid (*m/z* 131 → 87)
3. Adipic acid (*m/z* 145 → 83)
4. Isobutyrylcarnitine (*m/z* 232 → 85)
5. Butyrylcarnitine (*m/z* 232 → 85)
6. 2-Methylbutyrylcarnitine (*m/z* 246 → 85)
7. Isovalerylcarnitine (*m/z* 246 → 85)
8. Valerylcarnitine (*m/z* 246 → 85)



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Metabolomics and Biochemical Genetics - Acylglycines

Application #AN4080

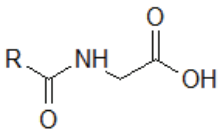
Conditions

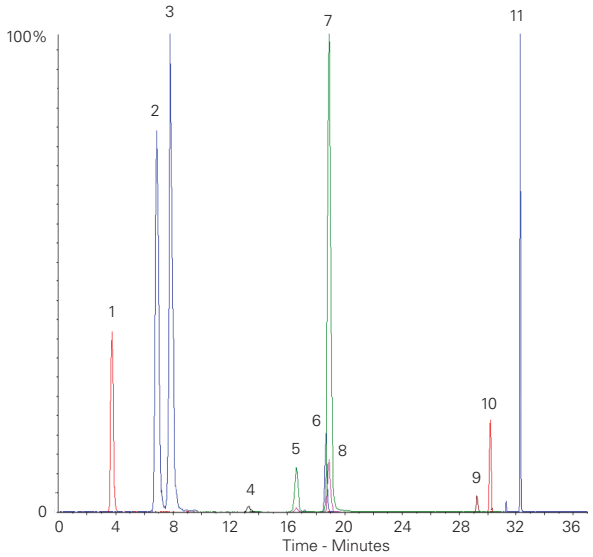
Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN
Detection: Sciex API 4000 triple quad MS
ESI in negative ion mode
Sample: Urine / plasma sample is filtered and extracted with ice-cold methanol, evaporated to dryness and reconstituted in 0.1% formic acid in water

Please contact info@ace-hplc.com for additional information on the chromatographic conditions used for this analysis.

Analytes

1. Propionylglycine (*m/z* 130 → 74)
2. Isobutyrylglycine (*m/z* 144 → 74)
3. Butyrylglycine (*m/z* 144 → 74)
4. 2-Methylbutyrylglycine (*m/z* 158 → 74)
5. Isovalerylglycine (*m/z* 158 → 74)
6. Tiglylglycine (*m/z* 156 → 112)
7. Valerylglycine (*m/z* 158 → 74)
8. 3-Methylcrotonylglycine (*m/z* 156 → 74)
9. Suberylglycine (*m/z* 230 → 74)
10. Hexanoylglycine (*m/z* 172 → 74)
11. Trans-Cinnamoylglycine (*m/z* 204 → 160)





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Metabolomics – C4 & C5 Hydroxy and Dicarboxylic Acids

Application #AN4110

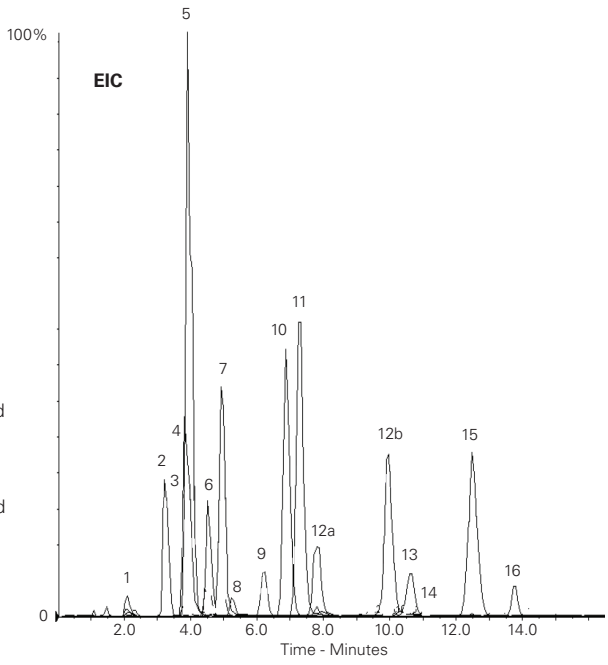
Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN
Detection: Sciex API 4000 triple quad MS
ESI in negative ion mode
Sample: Urine / plasma sample is filtered and extracted with ice-cold methanol, evaporated to dryness and reconstituted in 0.1% formic acid in water

Please contact info@ace-hplc.com for additional information on the chromatographic conditions used for this analysis.

Analytes

1. Isocitric acid (*m/z* 191 → 111)
2. 2-Hydroxyglutaric acid (*m/z* 147 → 129)
3. 3-Hydroxyglutaric acid (*m/z* 147 → 85)
4. Maleic acid (*m/z* 115 → 71)
5. Citric acid (*m/z* 191 → 111)
6. Fumaric acid (*m/z* 115 → 71)
7. Succinic acid (*m/z* 117 → 73)
8. Methylmalonic acid (*m/z* 117 → 55)
9. 3-Hydroxy-3-methylglutaric acid (*m/z* 161 → 99)
10. 2-Hydroxyadipic acid (*m/z* 161 → 143)
11. 3-Hydroxyisovaleric acid (*m/z* 117 → 59)
12. 3-Hydroxy-2-methylbutyric acid (*m/z* 117 → 73)
13. Glutaric acid (*m/z* 131 → 87)
14. 2-Ethyl-3-hydroxypropionic acid (*m/z* 117 → 87)
15. Ethylmalonic acid (*m/z* 131 → 87)
16. Methylsuccinic acid (*m/z* 131 → 87)



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Metabolomics – C4 Hydroxy Acids

Application #AN4120

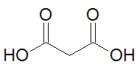
Conditions

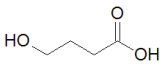
Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN
Detection: Sciex API 4000 triple quad MS
ESI in negative ion mode
Sample: Urine / plasma sample is filtered and extracted with ice-cold methanol, evaporated to dryness and reconstituted in 0.1% formic acid in water

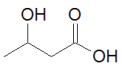
Please contact info@ace-hplc.com for additional information on the chromatographic conditions used for this analysis.

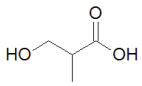
Analytes

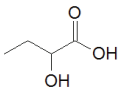
1. Malonic acid (*m/z* 103 → 59)
2. 4-Hydroxybutyric acid (*m/z* 103 → 57)
3. 3-Hydroxybutyric acid (*m/z* 103 → 59)
4. 3-Hydroxyisobutyric acid (*m/z* 103 → 73)
5. 2-Hydroxybutyric acid (*m/z* 103 → 57)

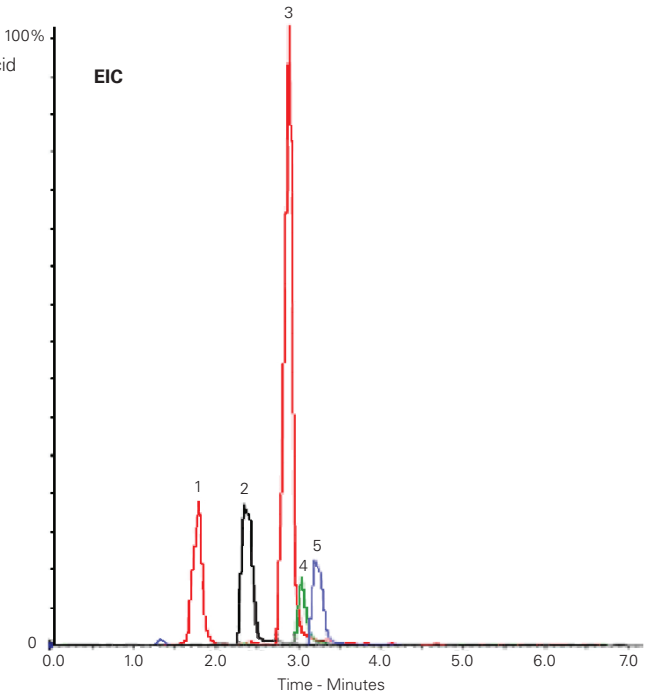

Malonic acid


4-Hydroxybutyric acid


3-Hydroxybutyric acid


3-Hydroxyisobutyric acid


2-Hydroxybutyric acid



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Metabolomics – C6 & C7 Hydroxy and Dicarboxylic Acids

Application #AN4100

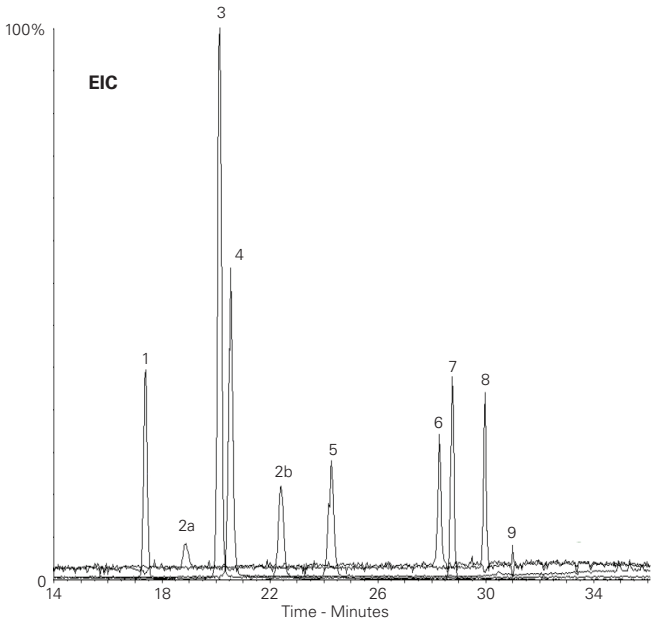
Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: 0.1% formic acid in H_2O
B: 0.1% formic acid in MeCN
Detection: Sciex API 4000 triple quad MS
ESI in negative ion mode
Sample: Urine / plasma samples filtered and extracted with ice-cold methanol, evaporated to dryness and reconstituted in 0.1% formic acid in water.

Please contact info@ace-hplc.com for additional information on the chromatographic conditions used for this analysis.

Analytes

1. 5-Hydroxyhexanoic acid (*m/z* 131 → 85)
2. 2-Hydroxy-3-methylvaleric acid (*m/z* 131 → 73)
3. 3-Methylglutaric acid (*m/z* 145 → 101)
4. Adipic acid (*m/z* 145 → 83)
5. 2-Hydroxyisocaproic acid (*m/z* 131 → 85)
6. 3-Methyladipic acid (*m/z* 159 → 115)
7. Pimelic acid (*m/z* 159 → 97)
8. 4-Hydroxyphenylacetic acid (*m/z* 151 → 107)
9. 2-Hydroxyphenylacetic acid (*m/z* 151 → 107)



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Methotrexate in K_3EDTA Human Plasma by LC-MS/MS

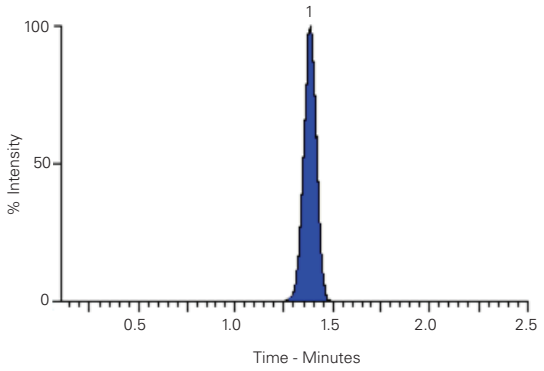
Application #AN3760

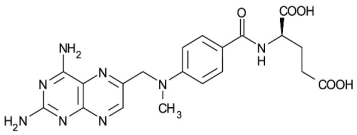
Conditions

Column: ACE 5 CN
Dimensions: 150 x 4.6 mm
Part Number: ACE-124-1546
Mobile Phase: 10 mM ammonium formate pH 7.0/MeOH (60:40 v/v)
Flow Rate: 1 mL/min
Temperature: 40 °C
Detection: Quattro Premier XE triple quad MS
Positive ion mode ESI
Ion source temperature: 120 °C
Desolvation temperature: 450 °C
Sample: Methotrexate and methotrexate-d3 extracted using solid phase extraction

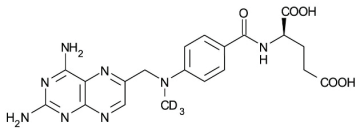
Analytes

1. Methotrexate
   (*m/z* 455 → 308)
   (LLOQ 1.0 ng/mL)
   (Concentration 100 ng/mL)
2. Methotrexate-d3 (I.S.)
   (*m/z* 458 → 311)
   (Concentration 50 ng/mL)

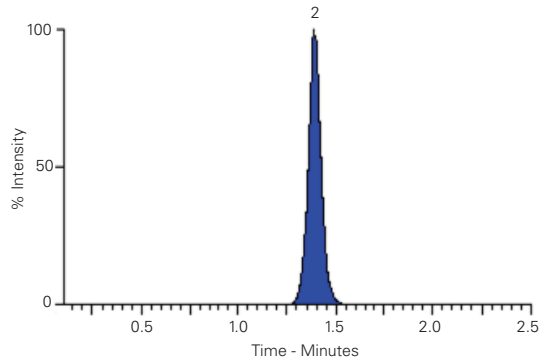




Methotrexate



Methotrexate-d3 (I.S.)



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17α-Methyltestosterone in Freshwater Tilapia Aquaculture

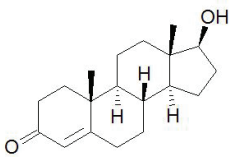
Application #AN4340

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: MeCN/H_2O (45:55 v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 25 °C
Detection: UV, 245 nm

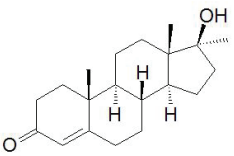
Analytes

1. Testosterone (IS)
2. 17α-Methyltestosterone

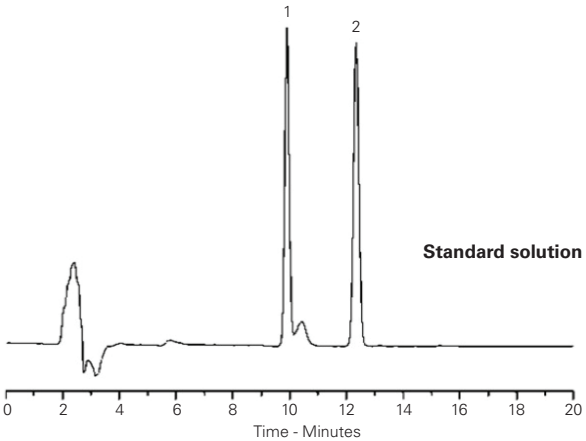


Testosterone (IS)

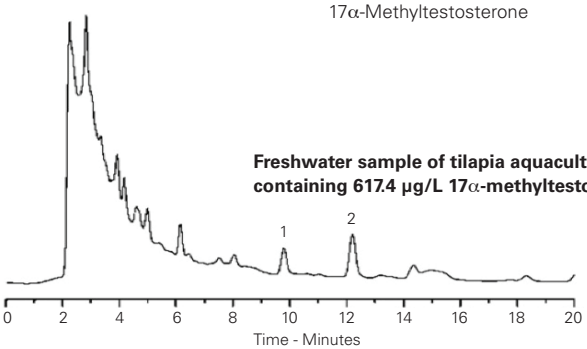
17α-Methyltestosterone is used for sex reversal of tilapia fish in order to avoid overpopulation in ponds. It therefore has to be monitored in aqueous matrices to prevent release into the environment.



17α-Methyltestosterone



Standard solution (600 µg/L)



Freshwater sample of tilapia aquaculture containing 617.4 µg/L 17α-methyltestosterone

Barbosa IR, Lopes S, Oliveira R, Domingues I, Soares AMVM, Nogueira AJA. Determination of 17α-Methyltestosterone in Freshwater Samples of Tilapia Farming by High Performance Liquid Chromatography, American Journal of Analytical Chemistry,(2013), 4, 207-211. http://dx.doi.org/10.4236/ajac.2013.44026