

ACE[®]

UHPLC and HPLC Columns

Clinical, Forensic and Bioanalysis Applications Guide





Ultra-Inert Base Deactivated UHPLC/HPLC Columns

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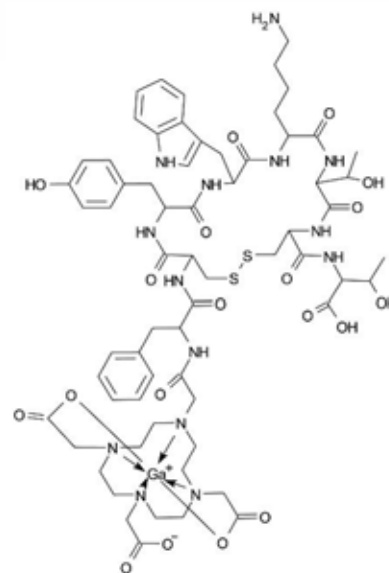
ACE®
Ultra-inert
UHPLC & HPLC Columns

Column:	ACE 3 C18
Dimensions:	50 x 4.6 mm
Part Number:	ACE-111-0546
Mobile Phase:	A: 0.1% formic acid in H ₂ O B: 0.1% formic acid in MeCN

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

Chemical structures shown:

- 4-Hydroxyphenyl group: Oc1ccc(cc1)
- DOTA-like structure (part of DOTATATE): O=C1OCCN(CC1)C2=CC=CC=C2



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Acylcarnitines by LC-MS/MS

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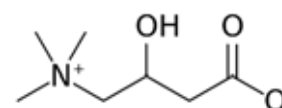
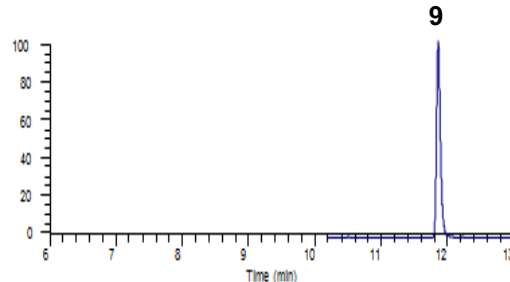
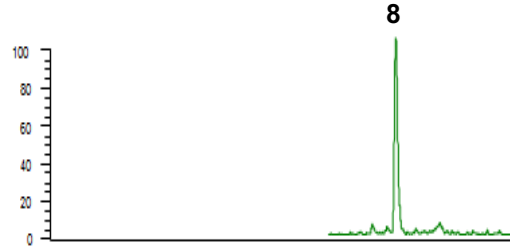
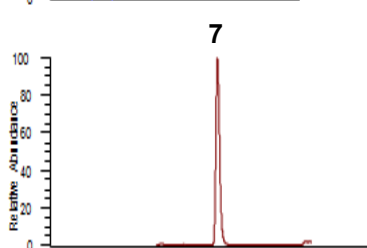
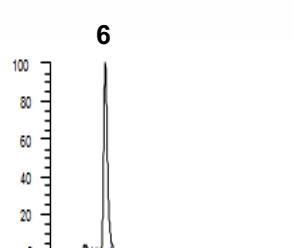
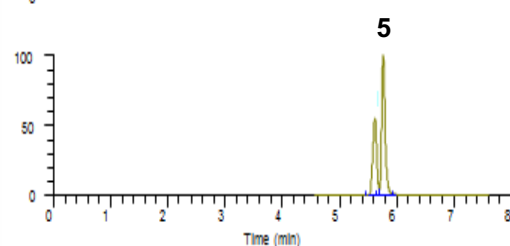
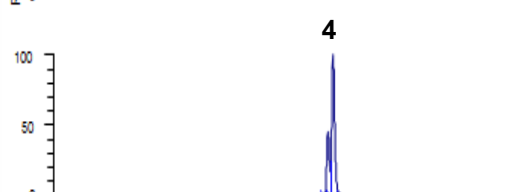
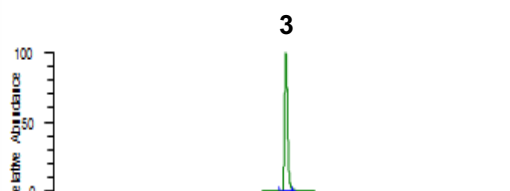
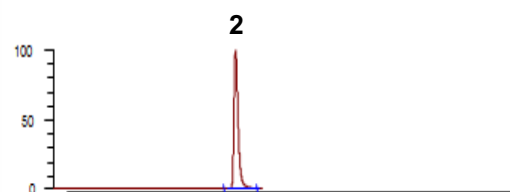
Application #AN1150

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 H₂O
B: 0.1% formic acid in MeOH

Time (mins)	%B
0.0	0.5
0.5	0.5
9.0	90.0
13.0	90.0

Flow Rate: 0.3 mL/min
Sample: Dried serum extract
Detection: Positive mode ESI



1. Carnitine
(*m/z* 162.16 → 85.25-85.35)
2. Acetylcarnitine
(*m/z* 204.13 → 85.25-85.35)
3. Propionylcarnitine
(*m/z* 218.13 → 85.25-85.35)
4. Butyrylcarnitine & Isobutyrylcarnitine
(*m/z* 232.15 → 85.25-85.35)
5. Isovaleryl-, 2-Methylbutyryl-, and Hexanoylcarnitine
(*m/z* 246.20 → 85.25-85.35)
6. Octanoylcarnitine
(*m/z* 260.20 → 85.25-85.35)
7. Myristoylcarnitine
(*m/z* 288.20 → 85.25-85.35)
8. Palmitoylcarnitine
(*m/z* 372.30 → 85.25-85.35)
9. Peak at 12.30 min
(*m/z* 400.30 → 85.25-85.35)

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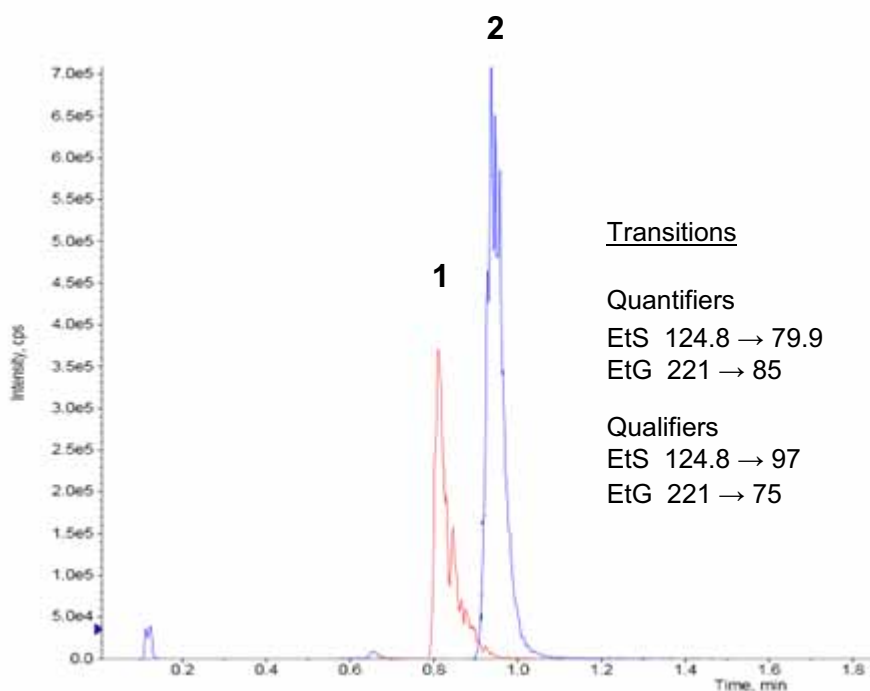
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Conditions

Column: ACE Excel 1.7 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-171-1002U
Mobile Phase: A: 1 mM ammonium fluoride
B: MeCN

Time (mins)	%B
0.0	0
0.5	20
1.5	20
2.0	100
4.0	100
4.5	0

Flow Rate: 0.4 mL/min
Injection: 1 µL
Temperature: 40 °C
Detection: AB SCIEX triple quad 5500
Negative ESI MRM
Source temperature: 750 °C
IonSpray voltage: -4500 V



Transitions

Quantifiers

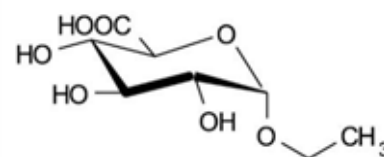
EtS 124.8 → 79.9

EtG 221 → 85

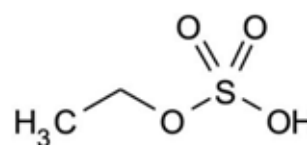
Qualifiers

EtS 124.8 → 97

EtG 221 → 75



1. Ethyl glucuronide (EtG)



2. Ethyl sulphate (EtS)

Fluoride counter-ion thought to enhance negative ESI response

Detection limit ~ 1 ng/mL in oral fluid



Amino Acids Derivatised with Dabsyl Chloride

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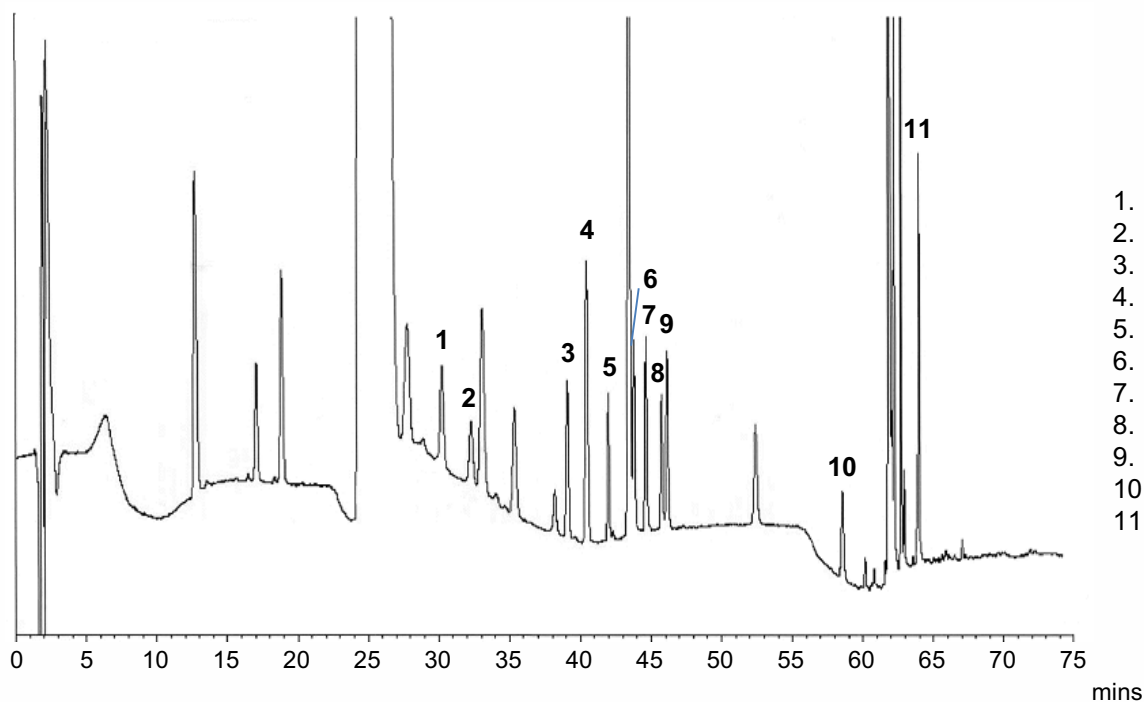
Application #AN3420

Conditions

Column: ACE 3 C18
Dimensions: 150 x 3.0 mm
Part Number: ACE-111-1503
Mobile Phase: A: 10 mM potassium dihydrogen phosphate pH 6.55 in H₂O
B: MeCN/IPA (70:30 v/v)

Time (mins)	%B
0.0	10
3.0	18
17.0	18
27.0	22
35.0	22
50.0	35
57.0	35
70.0	65
70.1	65
89.0	10
90.0	10

Flow Rate: 0.5 mL/min
Injection: 20 µL
Temperature: 50 °C
Detection: UV, 436 nm



1. L-Arginine
2. L-Threonine
3. L-Proline
4. L-Valine
5. L-Methionine
6. L-Isoleucine
7. L-Tryptophan
8. L-Norleucine
9. L-Leucine
10. Ammonium ion
11. L-Lysine

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Amino Acids by HPLC-HRAM-MS

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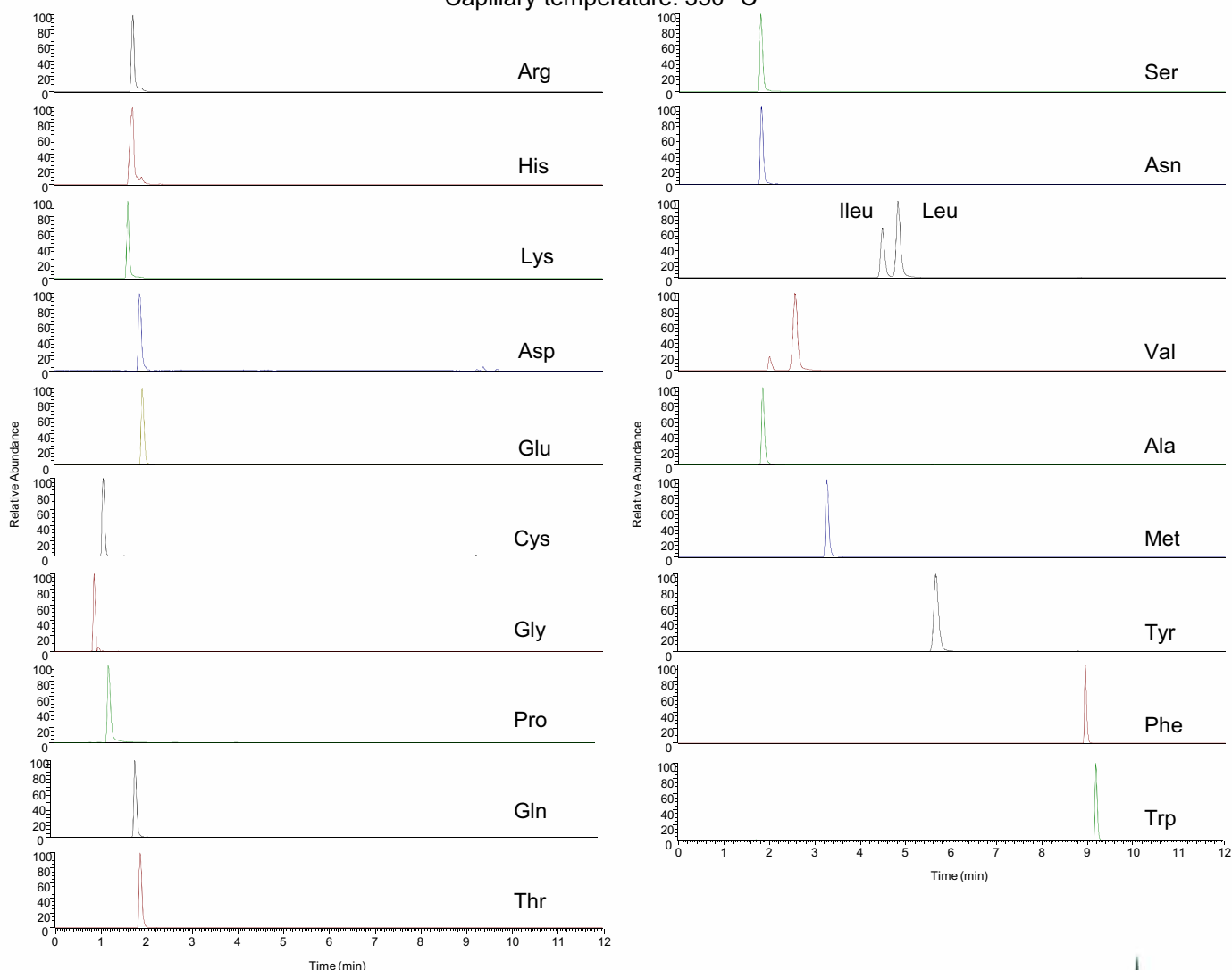
Application #AN2660

Conditions

Column: ACE 3 AQ
Dimensions: 150 x 3.0 mm
Part Number: ACE-116-1503
Mobile Phase: A: 0.1% formic acid in H₂O
B: 0.1% formic acid in MeCN

Time (mins)	%B
0	0
10	100

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



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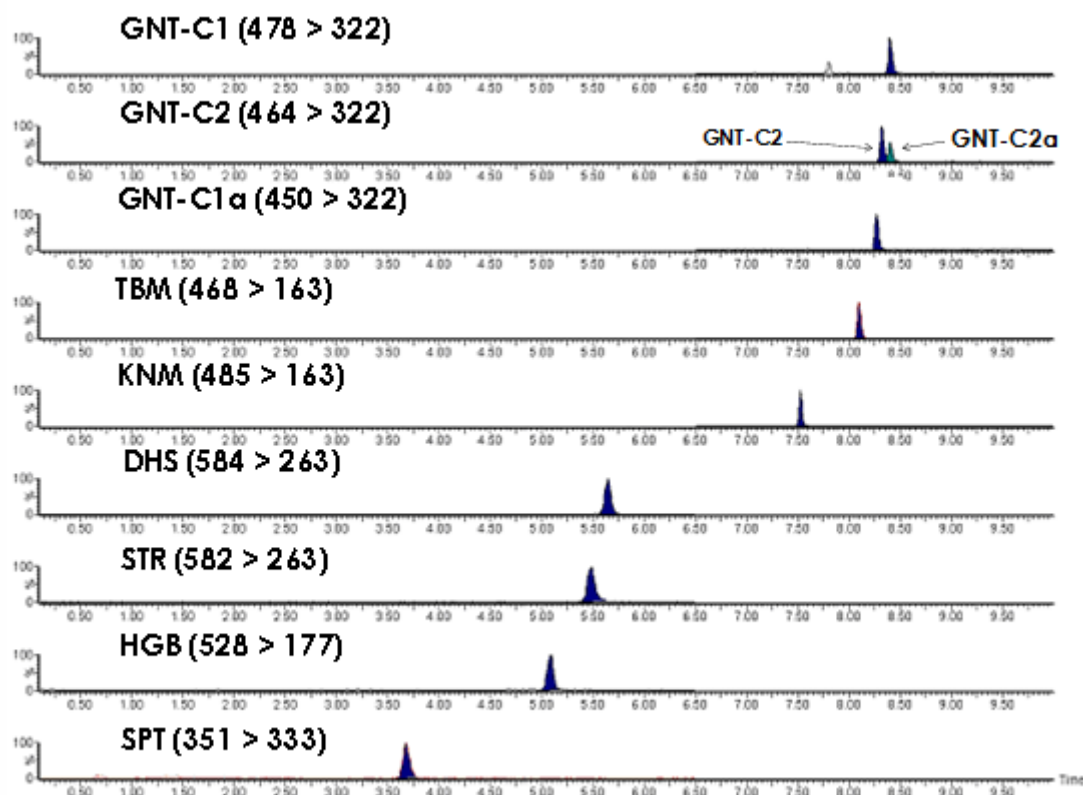

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Conditions

Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: A: 20 mM HFBA in H₂O/MeCN (98:2 v/v)
B: 20 mM HFBA in MeCN/H₂O (98:2 v/v)

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

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



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

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Amphetamines In Urine by LC-MS/MS

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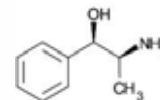
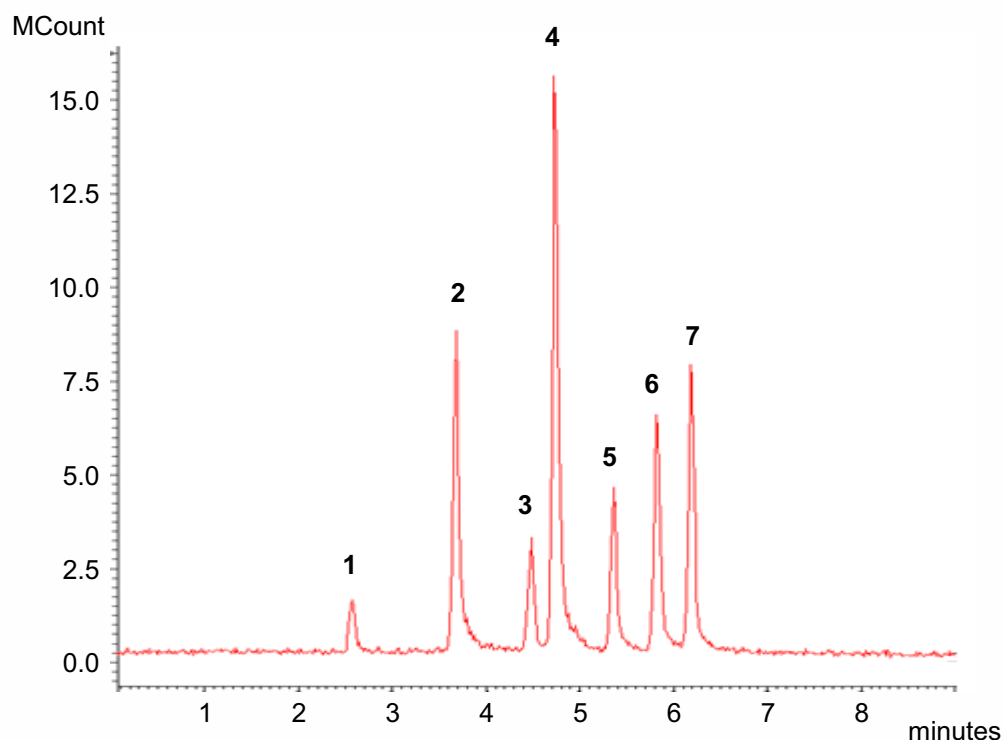
Application #AN1010

Conditions

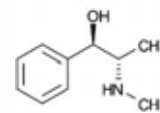
Column: ACE Excel 3 SuperC18
Dimensions: 75 x 2.1 mm
Part Number: EXL-1111-7502U
Mobile Phase: A: 5 mM ammonium hydroxide pH 10.8 in H₂O
B: 5 mM ammonium hydroxide pH 10.8 in MeOH/H₂O (90:10 v/v)

Time (mins)	%B
0	30
8	95

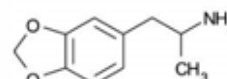
Flow Rate: 0.6 mL/min
Injection: 2 µL
Temperature: 60 °C
Detection: Varian 320 Triple Quadrupole MS
Electrospray voltage: +5 kV
Inlet capillary voltage: 30 V
CID with argon at 1.5 mTorr
Collision cell potential ranges from 5 to 17 V
Drying gas (nitrogen) temperature: 325 °C
Nebulizing gas (nitrogen)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



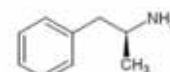
1. Phenylpropanolamine
LOD (est) 4 ppb
(*m/z* 151.6 → 134.0)



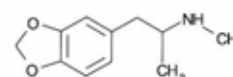
2. (l)-Ephedrine
LOD (est) 2 ppb
(*m/z* 166.2 → 148.0)



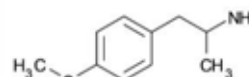
3. (dl)-3,4-MDA
LOD (est) 30 ppb
(*m/z* 179.7 → 163.0)



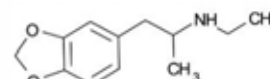
4. (d)-Amphetamine
LOD (est) 4 ppb
(*m/z* 135.8 → 90.9)



5. (dl)-3,4-MDMA
LOD (est) 2 ppb
(*m/z* 193.7 → 163.0)



6. 4-Methylthioamphetamine
LOD (est) 10 ppb
(*m/z* 182.2 → 165.0)



7. (±)-MDEA
LOD (est) 1 ppb
(*m/z* 207.7 → 165.0)

Anabolic Steroids from Horse Urine by LC-MS/MS

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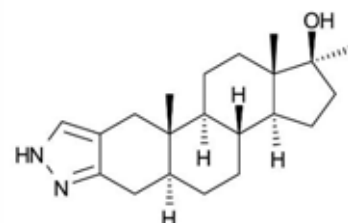
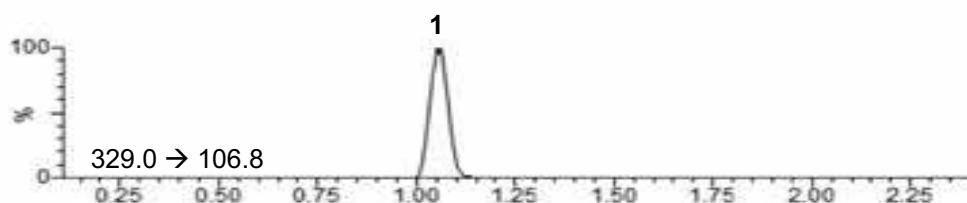
Application #AN2360

Conditions

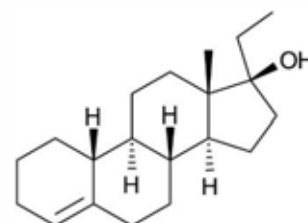
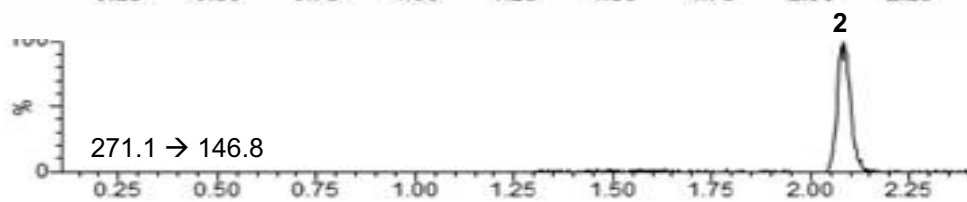
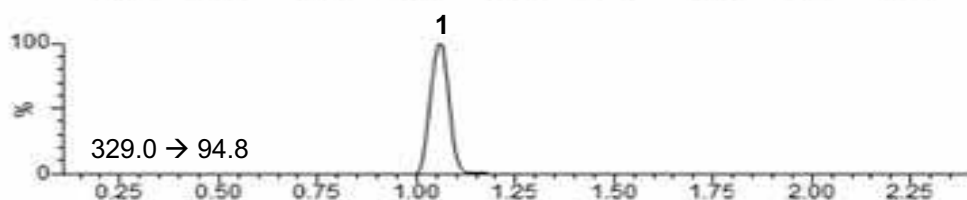
Column: ACE Excel 2 C18
Dimensions: 50 x 2.1 mm
Part Number: EXL-101-0502U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% formic acid in H₂O
B: 2 mM ammonium acetate, 0.1% formic acid in MeOH

Time (mins)	%B
0.00	75
0.25	75
1.50	90
1.51	100
3.50	100
3.51	75
4.00	75

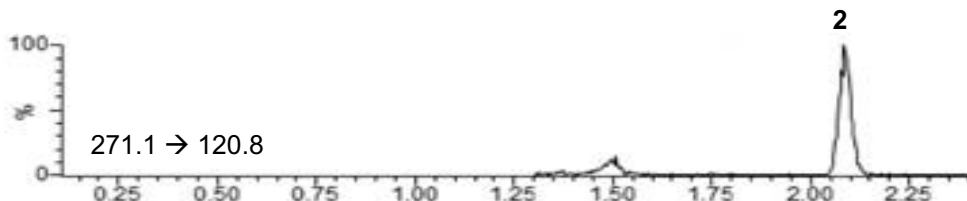
Flow Rate: 0.4 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: Premier XE triple quad MS
MRM positive ion mode
Desolvation temperature: 450 °C
Ion Source temperature: 120 °C



1. Stanozolol
(m/z 329.0 → 94.8)
(m/z 329.0 → 106.8)



2. Ethylestrenol
(m/z 271.1 → 120.8)
(m/z 271.1 → 146.8)



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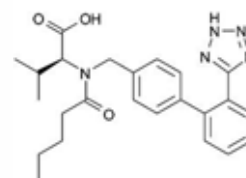
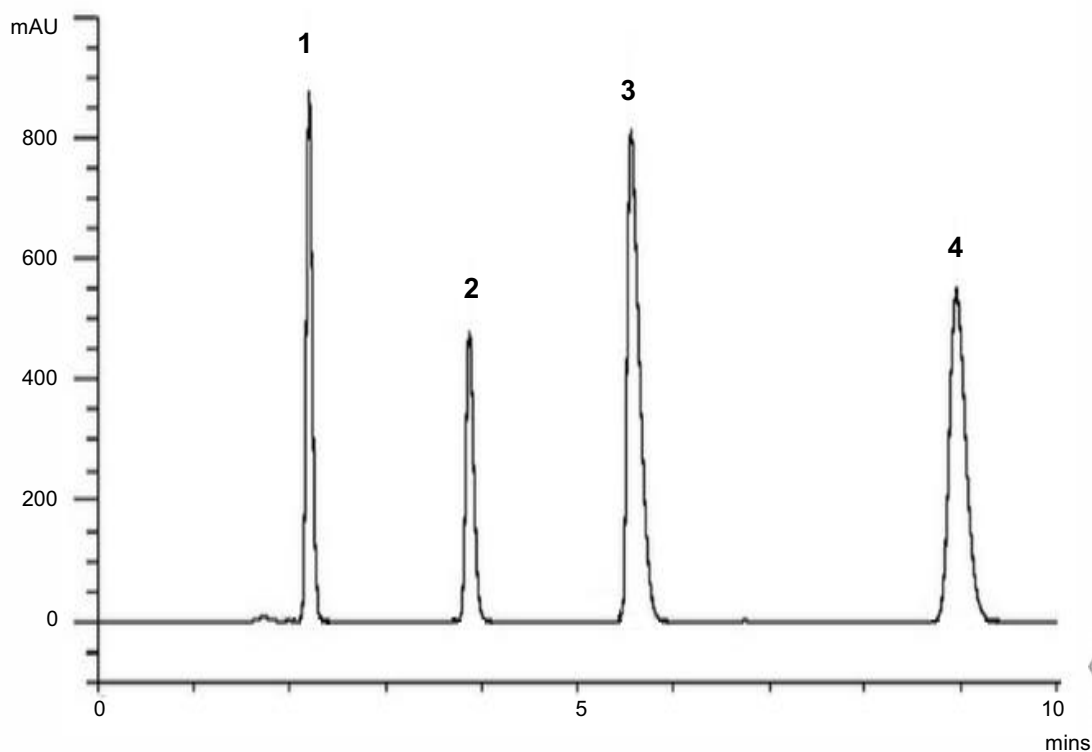
Angiotensin II Receptor Antagonists by LC-UV

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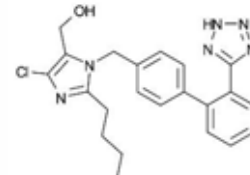
Application #AN3460

Conditions

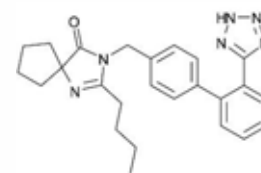
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 0.025 M KH₂PO₄ pH 6.0/MeCN (65:35 v/v)
Flow Rate: 1.5 mL/min
Temperature: 40 °C
Detection: UV, 220 nm



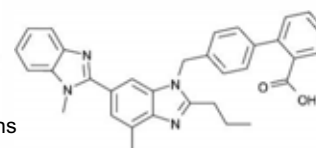
1. Valsartan



2. Losartan



3. Irbesartan



4. Telmisartan

Elshanawane AA, Abdelaziz LM, Hafez HM (2012) Stability Indicating HPLC Method for Simultaneous Determination of Several Angiotensin-II Receptor Antagonists in Their Dosage Forms. Pharmaceut Anal Acta 3:175. doi:10.4172/2153-2435.1000175

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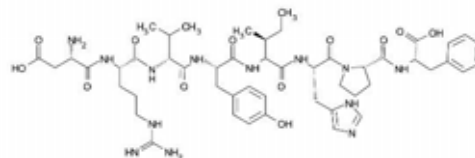
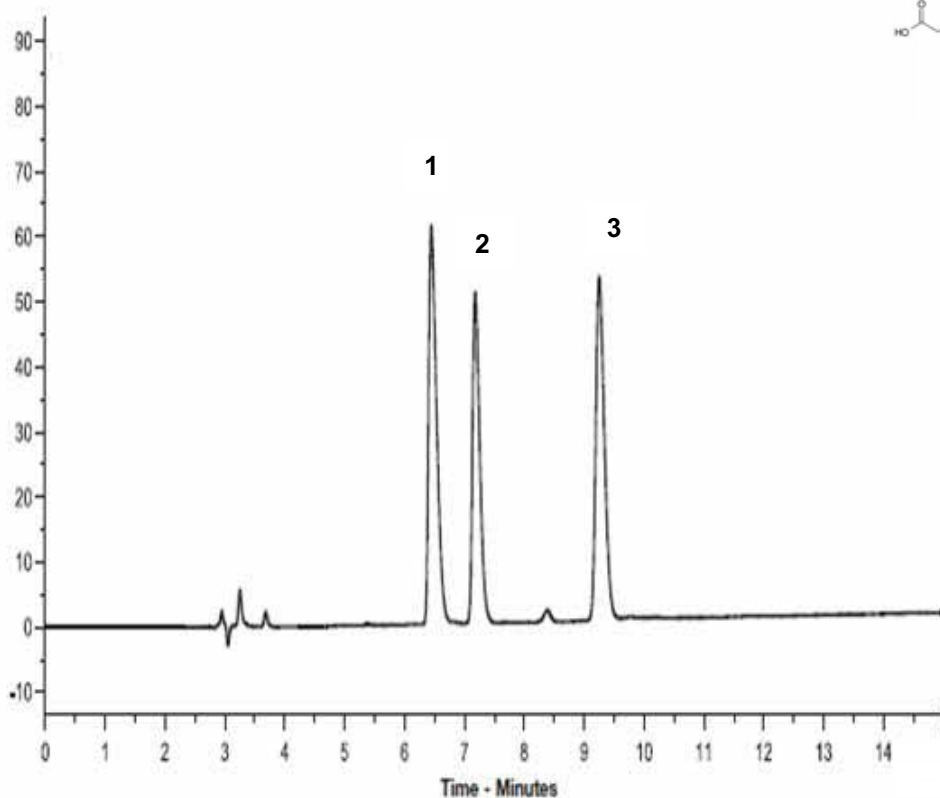
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Conditions

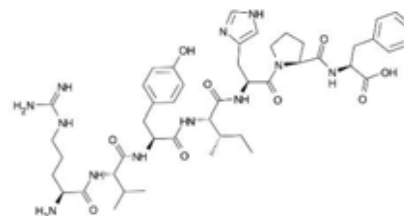
Column: ACE 5 C18-300
Dimensions: 250 x 4.6 mm
Part Number: ACE-221-2546
Mobile Phase: A: 0.1 % TFA in H₂O
B: 0.1% TFA in H₂O/MeCN (80:20 v/v)

Time (mins)	%B
0	25
15	40

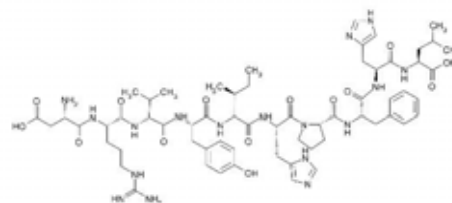
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 215 nm



1. Angiotensin II
(*m/z* 1046.2)



2. Angiotensin III
(*m/z* 931.1)



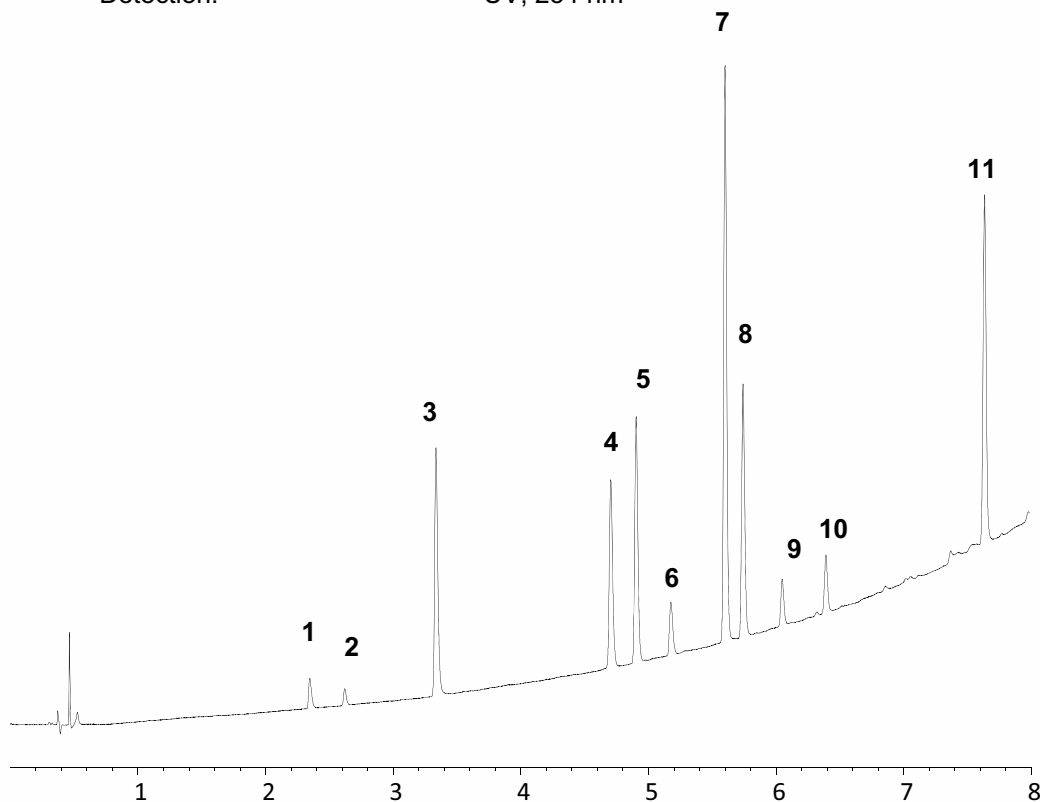
3. Angiotensin I
(*m/z* 1296.5)

Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 3.0 mm
Part Number: CORE-25A-1003U
Mobile Phase: A: 20 mM ammonium formate pH 3.0 in H₂O
B: 20 mM ammonium formate pH 3.0 in MeOH/H₂O (9:1 v/v)

Flow Rate: 1.2 mL/min
Injection: 2 µL
Temperature: 25 °C
Detection: UV, 254 nm

Time (mins)	%B
0.0	0
7.5	100
8.5	100
9.0	0



1. Pseudoephedrine
2. Scopolamine
3. Doxylamine
4. Chlorpheniramine
5. Triprolidine
6. Diphenhydramine
7. Acrivastine
8. Promethazine
9. Fexofenadine
10. Cetirizine
11. Loratadine



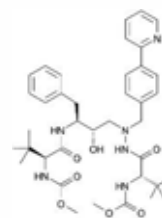
Antiretrovirals in Human Mononuclear Cell Extracts by LC-MS/MS

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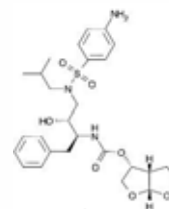
Application #AN3470

Conditions

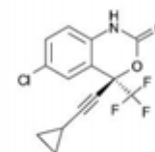
Column: ACE 3 C18
Dimensions: 100 x 3.0 mm
Part Number: ACE-111-1003
Mobile Phase: MeCN/H₂O/formic acid (60:40:0.1 v/v/v)
Flow Rate: 0.5 mL/min
Injection: 40 µL
Temperature: 40 °C
Detection: SCIEX API 6500 triple quad MS
Positive ion mode ESI (negative mode for efavirenz)
Ion spray voltage: +5500 V (-4500 V for efavirenz)
Temperature: 450 °C (650 °C for efavirenz)



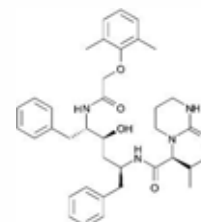
1. Atazanavir
(*m/z* 705.4 → 168.2)
LLOQ: 0.04 fmol/sample



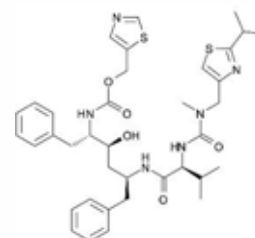
2. Darunavir
(*m/z* 548.3 → 392.3)
LLOQ: 1.0 fmol/sample



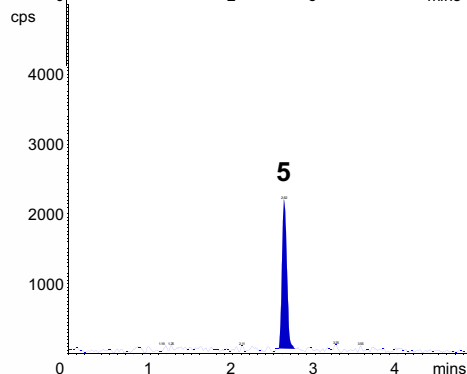
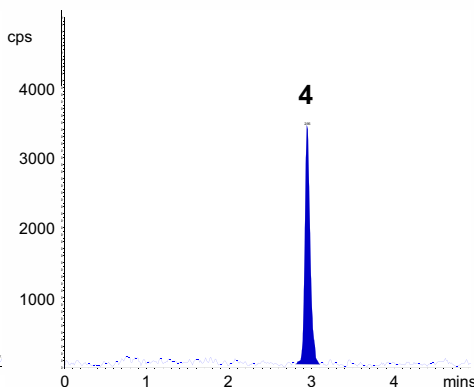
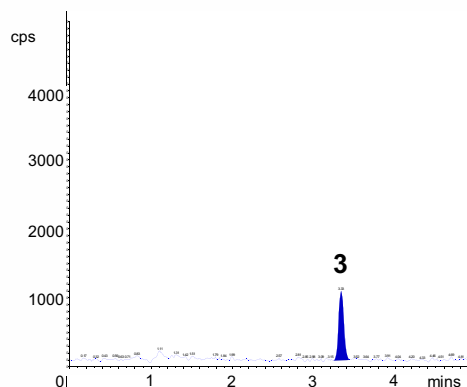
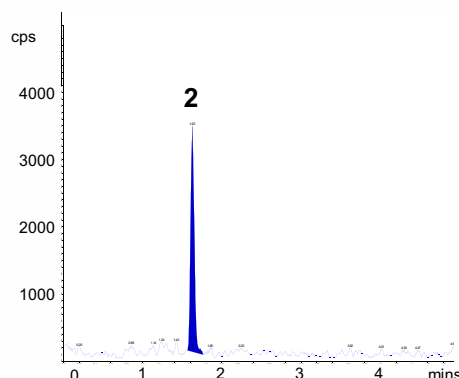
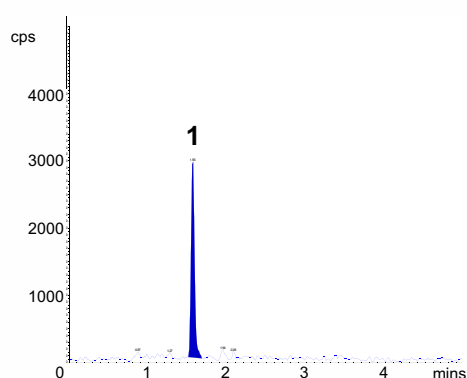
3. Efavirenz
(*m/z* 313.9 → 244.0)
LLOQ: 4.0 fmol/sample



4. Lopinavir
(*m/z* 629.4 → 447.3)
LLOQ: 1.0 fmol/sample



5. Ritonavir
(*m/z* 721.4 → 268.2)
LLOQ: 1.0 fmol/sample



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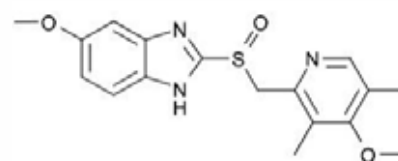
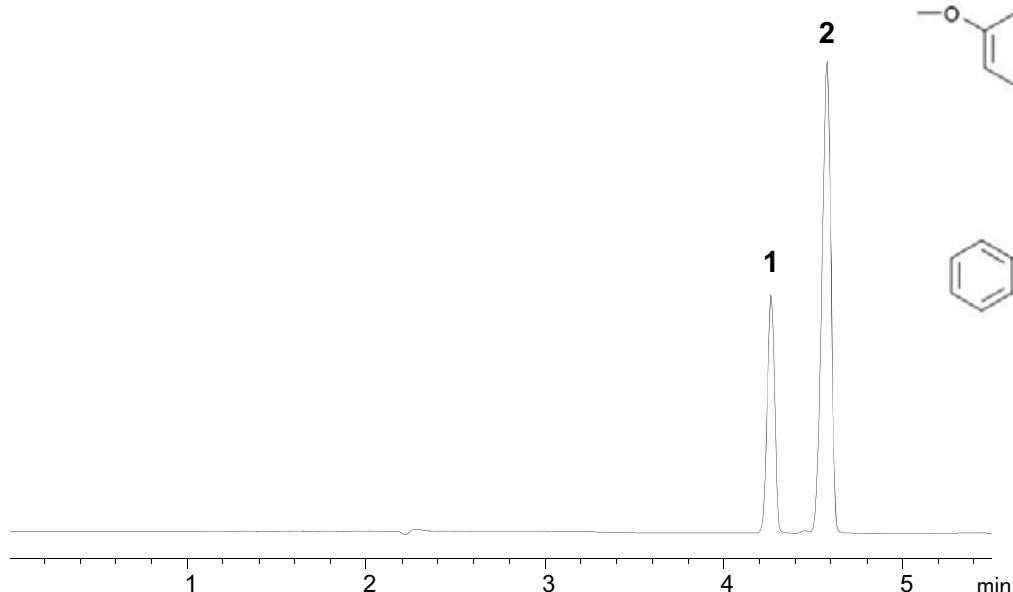
Anti-Ulcer Drugs in Basic Mobile Phase Conditions

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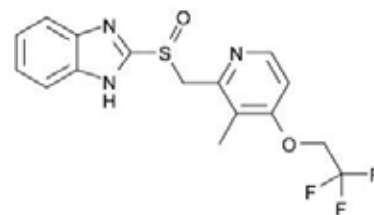
Application #AN1950

Conditions

Column: ACE 5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: EXL-1211-1546U
Mobile Phase: A: 0.1% ammonia in H₂O
B: 0.1% ammonia in MeCN/H₂O (90:10 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 30 °C
Detection: UV, 280 nm



1. Omeprazole



2. Lansoprazole



Appetite Suppressants by LC-MS

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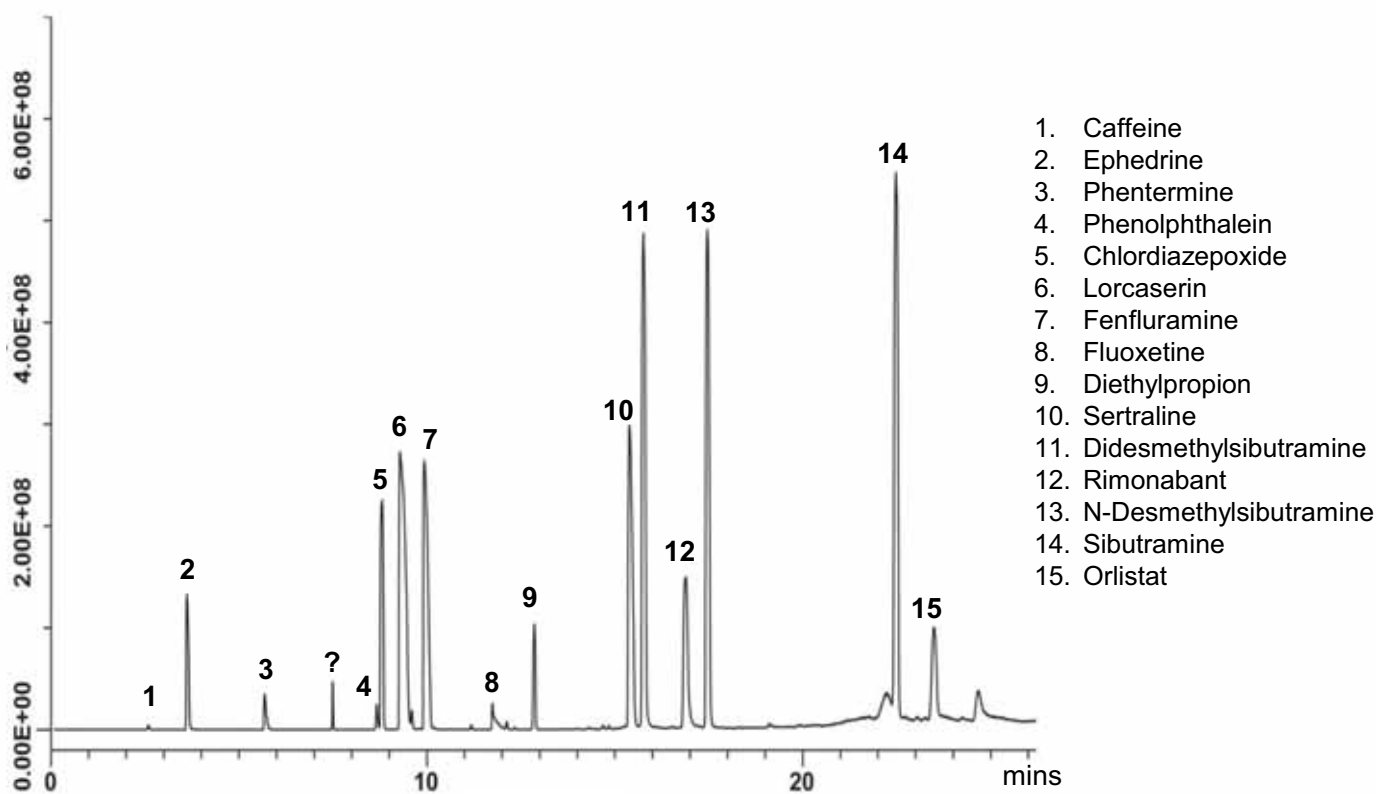
Application #AN1960

Conditions

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

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

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



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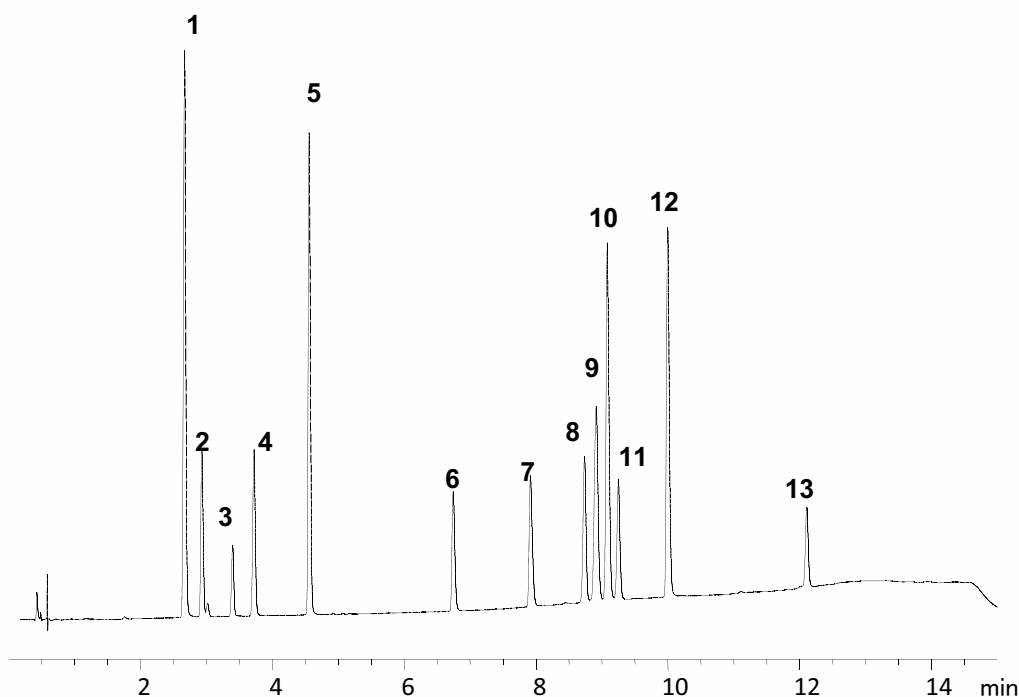
Conditions

Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-111-1002
Mobile Phase: A: 20 mM KH₂PO₄, pH 2.7
B: 20 mM KH₂PO₄, pH 2.7 in MeCN/H₂O (65:35 v/v)

Time (mins)	%B
0	5
1	5
12	95
13	95
14	5

Post time 3 minutes

Flow Rate: 0.6 mL/min
Injection: 2 µL
Temperature: 36 °C
Detection: UV, 214 nm

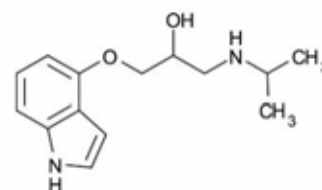
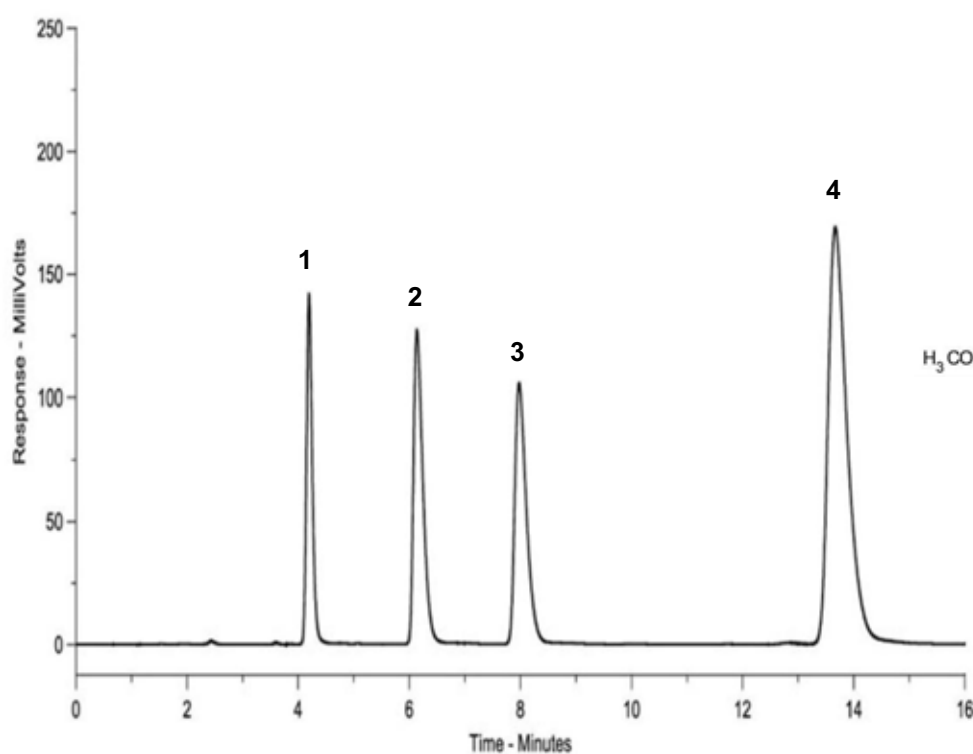


1. Hydrochlorothiazide
2. Sotalol
3. Amiloride
4. Atenolol
5. Pindolol
6. Metoprolol
7. Oxprenolol
8. Furosemide
9. Indapamide
10. Propranolol
11. Bendroflumethiazide
12. Carvedilol
13. Spironolactone

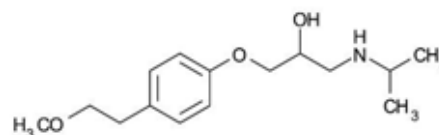


Conditions

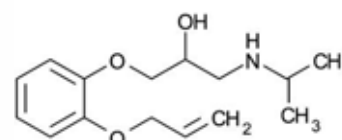
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 50 mM 1-methylpiperidine pH 11/MeOH (35:65 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 215 nm



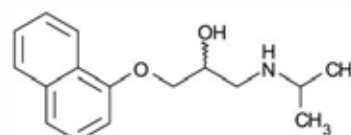
1. Pindolol



2. Metoprolol



3. Oxprenolol



4. Propranolol

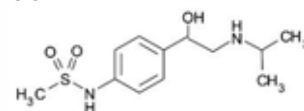
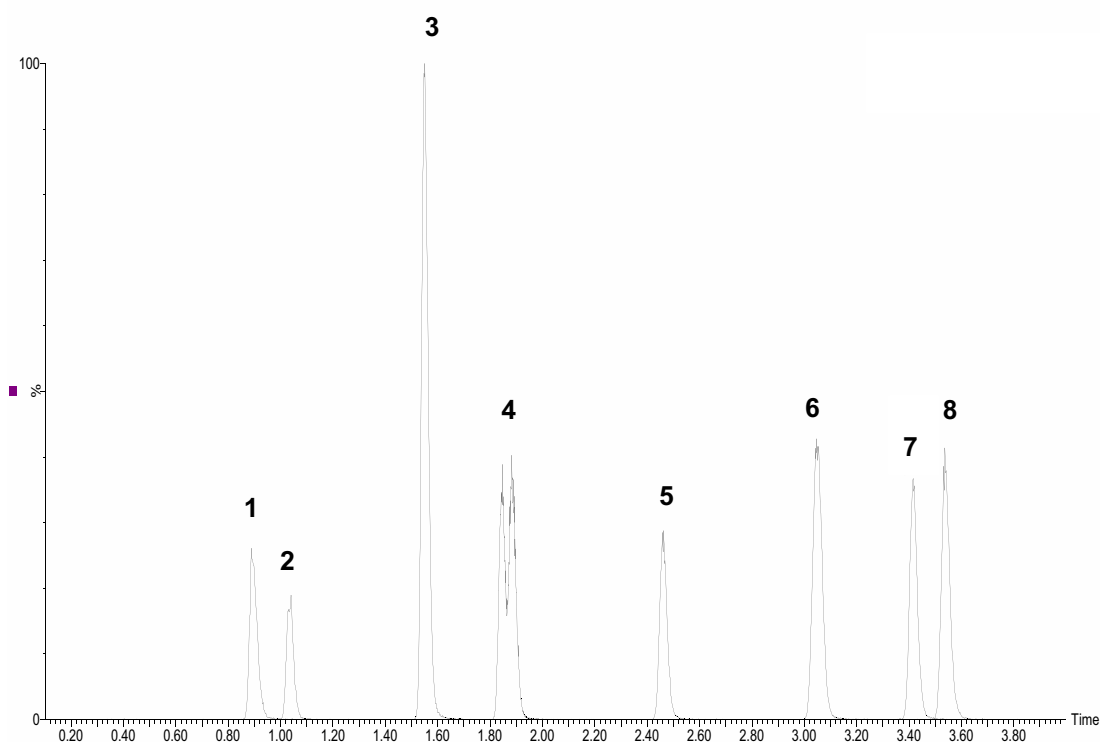


Conditions

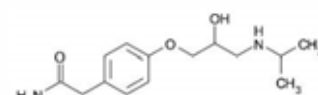
Column: ACE Excel 2 C18
Dimensions: 50 x 2.1 mm
Part Number: EXL-101-0502U
Mobile Phase: A: 2 mM ammonium acetate + 0.1% formic acid in H₂O
B: 2 mM ammonium acetate + 0.1% formic acid in MeOH

Time (mins)	%B
0.0	10
3.0	50
3.1	10

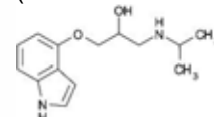
Flow Rate: 0.4 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: MS/MS
Sample: ESI in positive ion mode
2.5 pg/µL



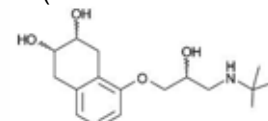
1. Sotalol
(*m/z* 272.9 → 212.8)



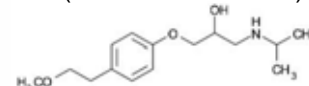
2. Atenolol
(*m/z* 267.0 → 189.8)



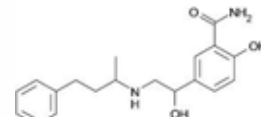
3. Pindolol
(*m/z* 248.9 → 115.8)



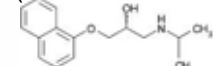
4. Nadolol diastereomers
(*m/z* 310.0 → 253.9)



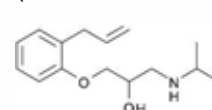
5. Metoprolol
(*m/z* 268.0 → 115.8)



6. Labetalol
(*m/z* 329.1 → 161.8)



7. Propranolol
(*m/z* 260.0 → 115.7)



8. Alprenolol
(*m/z* 250.0 → 115.8)

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Benzo(a)pyrene-7,8-quinone Derived Deoxynucleotide DNA Adducts

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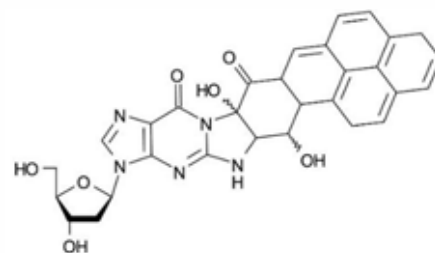
Application #AN3170

Conditions

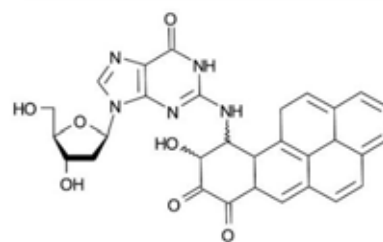
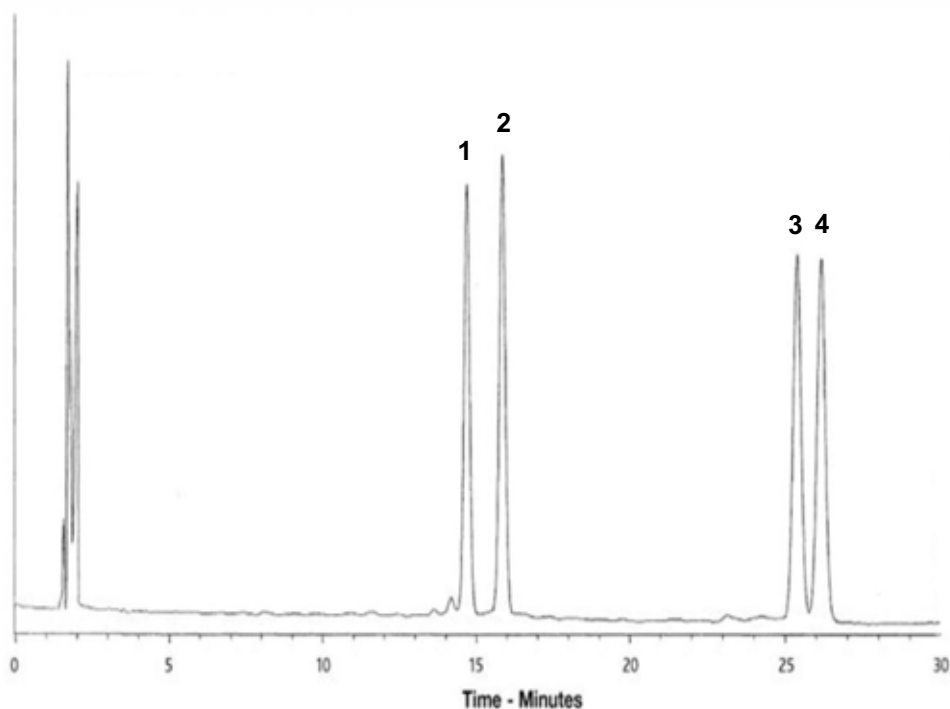
Column: ACE 3 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-111-1546
Mobile Phase: A: 0.1% formic acid in H₂O
B: MeCN

Time (mins)	%B
0	25
8	55

Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 35 °C
Detection: UV, 285 nm



1. BPQ-dG#1
2. BPQ-dG#2



3. BPQ-dG#3
4. BPQ-dG#4

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Biomarker Analysis for Gaucher Disease by LC-MS/MS

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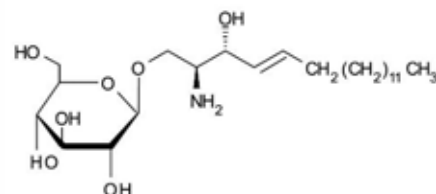
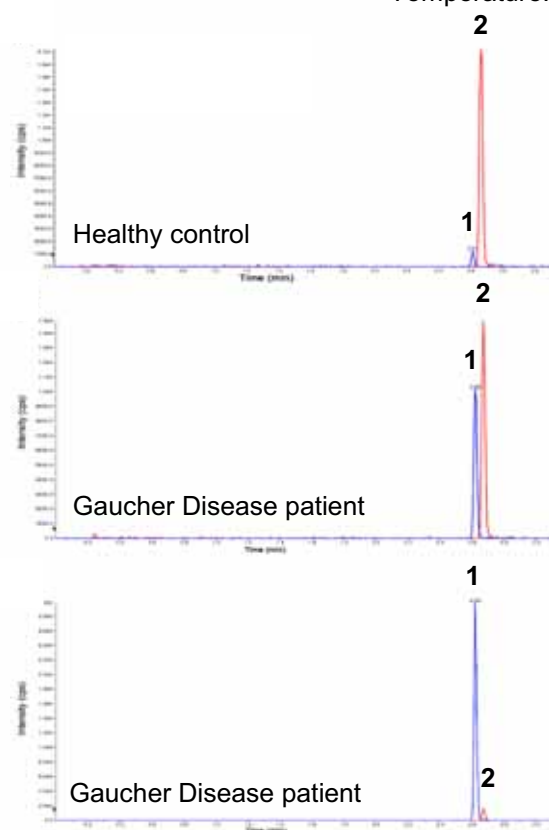
Application #AN3490

Conditions

Column: ACE 3 C8
Dimensions: 50 x 2.1 mm
Part Number: ACE-112-0502
Mobile Phase: A: 50 mM formic acid in H₂O
B: 50 mM formic acid in MeCN/acetone (1:1 v/v)

Time (mins)	%B
0.0	5
4.0	66
4.1	100
5.1	100
5.9	5

Flow Rate: 0.9 mL/min
Injection: 5 µL
Temperature: 60 °C
Detection: API 4000 triple quad MS
ESI in positive ion mode
Temperature: 500 °C



1. Glucosylsphingosine
(*m/z* 462 → 282)

2. Lyso-Gb2 (IS)
(*m/z* 624 → 282)

Rolfs A, Giese AK, Grittner U, Mascher D, Elstein D, et al. (2013) Glucosylsphingosine Is a Highly Sensitive and Specific Biomarker for Primary Diagnostic and Follow-Up Monitoring in Gaucher Disease in a Non-Jewish, Caucasian Cohort of Gaucher Disease Patients. PLoS ONE 8(11): e79732. doi:10.1371/journal.pone.0079732

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Biomarker for Niemann-Pick Type C1 Disease by LC-MS/MS

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Application #AN3480

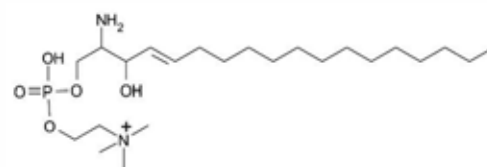
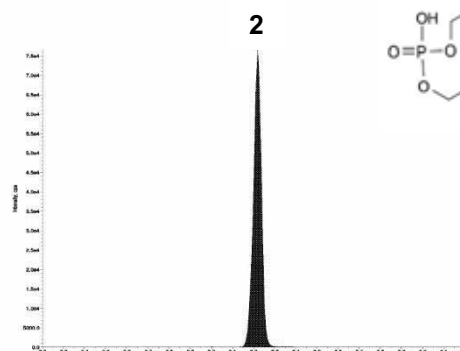
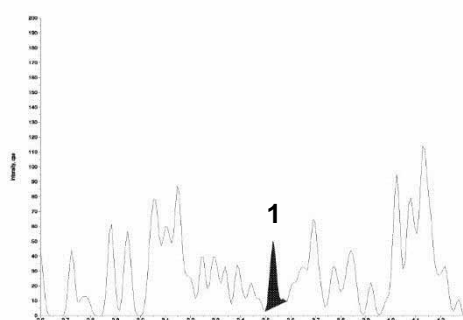
Conditions

Column: ACE 3 C8
Dimensions: 50 x 2.1 mm
Part Number: ACE-112-0502
Mobile Phase: A: 50 mM formic acid in H₂O
B: 50 mM formic acid in MeCN/acetone (1:1 v/v)

Time (mins)	%B
0.0	5
4.0	66
4.1	100
5.1	100
5.9	5

Flow Rate: 0.9 mL/min
Injection: 5 µL
Temperature: 60 °C
Detection: API 4000 triple quad MS
ESI in positive ion mode
Temperature: 500 °C

Human Control Plasma

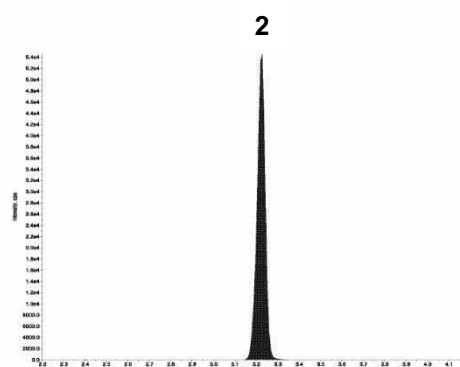
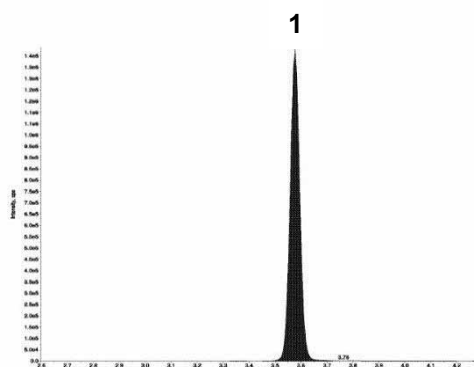


Lyso-SM (lyso-sphingomyelin)

1. Lyso-SM-509
(*m/z* 509 → 184)

2. Lyso-Gb2 (IS)
(*m/z* 624 → 282)

Niemann-Pick Patient Sample



Giese A, Mascher H, Grittner U, Eichler S, Kramp G, Lukas J, te Vrugte D, Eisa N, Cortina-Borja M, Porter F, Platt F, Rolfs A. Orphanet Journal of Rare Diseases (2015) 10:78 A novel, highly sensitive and specific biomarker for Niemann-Pick type C1 disease. DOI 10.1186/s13023-015-0274-1

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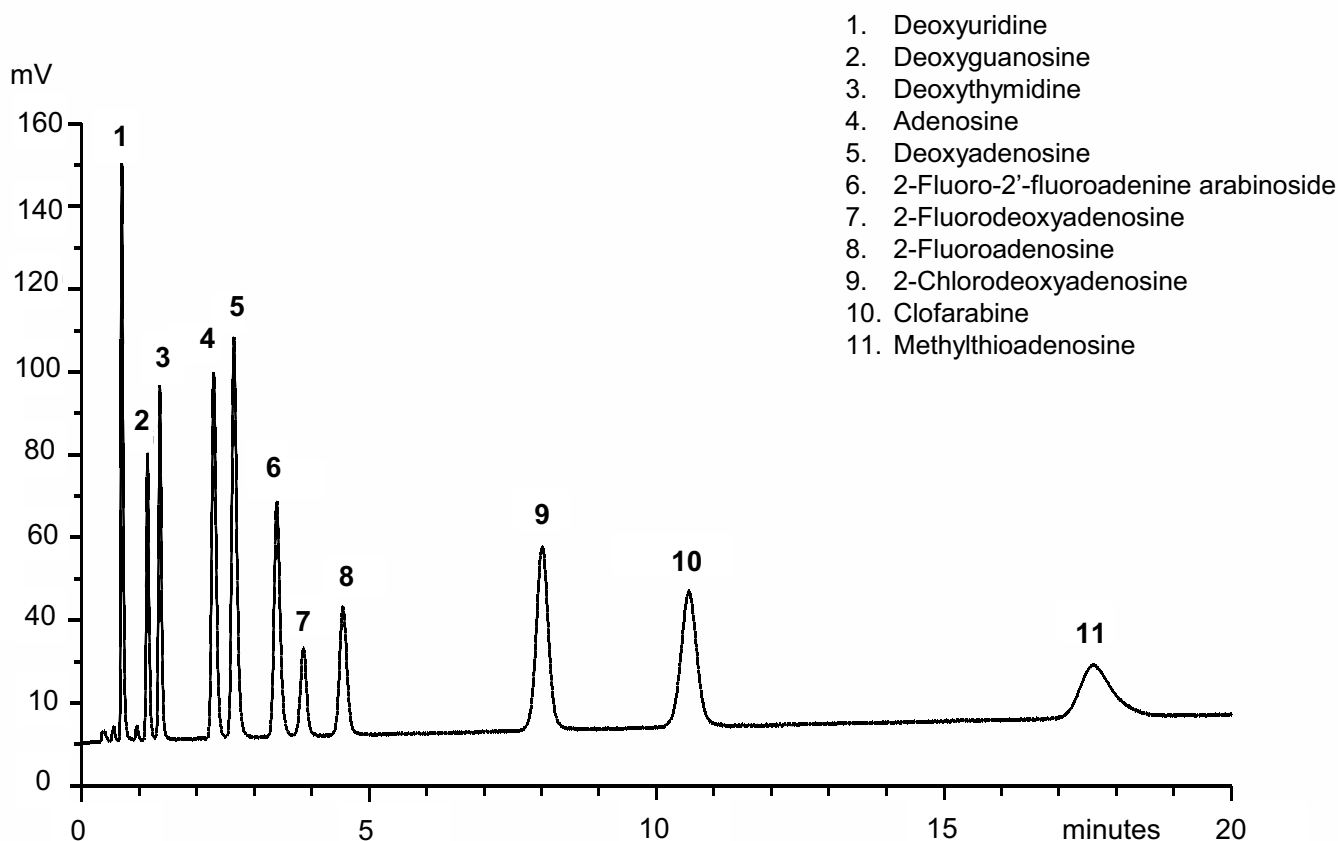


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Conditions

Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 2.1 mm
Part Number: CORE-25A-1502U
Mobile Phase: A: 7% methanol, 2.1 mM tetrabutylammonium bisulphate + 84 mM KH₂PO₄, pH 6 with KOH
B: 7% methanol, 2.1 mM tetrabutylammonium bisulphate + 8.4 mM KH₂PO₄, pH 6 with KOH
A/B (90:10 v/v)
Flow Rate: 0.4 mL/min
Injection: 2 µL
Temperature: Ambient
Detection: UV, 260 nm



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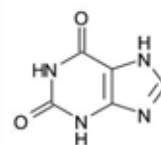
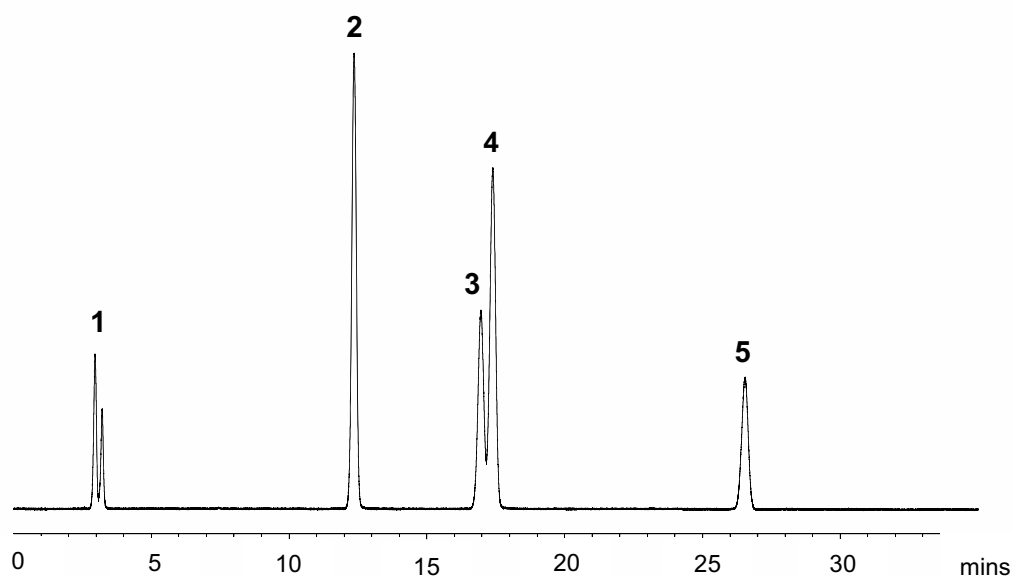


Conditions

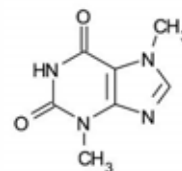
Column: ACE 5 SuperC18
Dimensions: 150 x 4.6 mm
Part Number: EXL-1211-1546U
Mobile Phase: A: 20 mM ammonium acetate pH 7.0 in H₂O
B: 20 mM ammonium acetate pH 7.0 in MeCN/H₂O (90:10 v/v)

Time (mins)	%B
0	2
45	15
48	15
49	2
Post time 10 minutes	

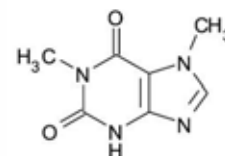
Flow Rate: 1 mL/min
Injection: 1 µL
Temperature: 60 °C
Detection: UV, 273 nm



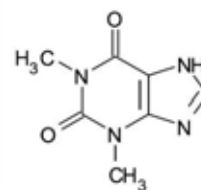
1. Xanthine



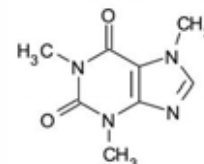
2. Theobromine



3. Paraxanthine



4. Theophylline



5. Caffeine



Cannabinoids in Rat Plasma

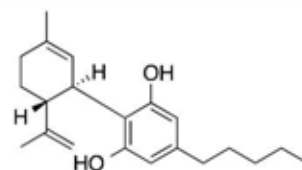
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Application #AN2310

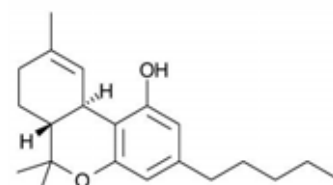
Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1110-1546
Mobile Phase: H₂O/MeCN (38:62 v/v)
Flow Rate: 1 mL/min
Injection: 30 µL
Temperature: 55 °C
Detection: UV, 220 nm

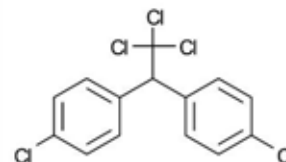
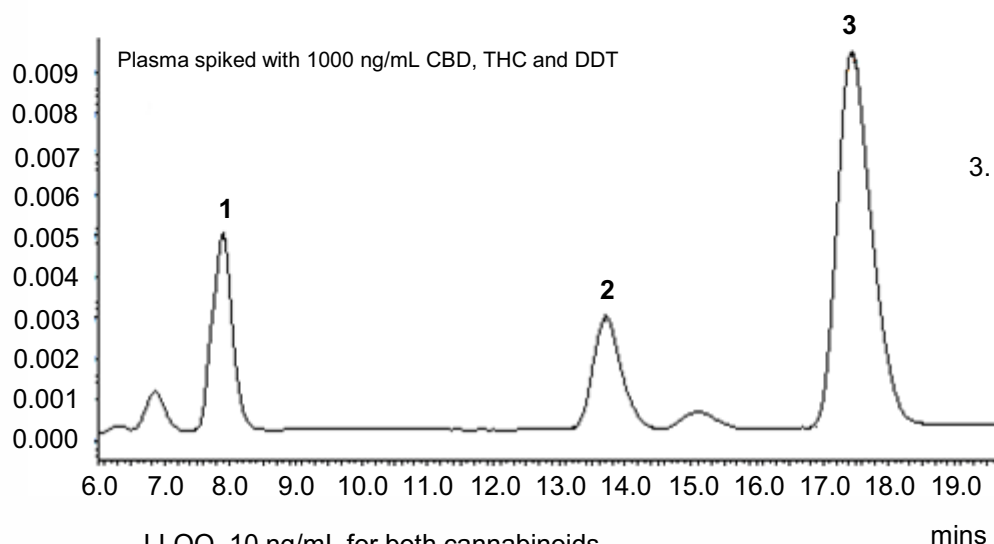
AU



1. Cannabidiol(CBD)



2. Δ⁹-Tetrahydrocannabinol (THC)



3. 4,4-Dichlorodiphenyltrichloroethane (DDT) (IS)

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

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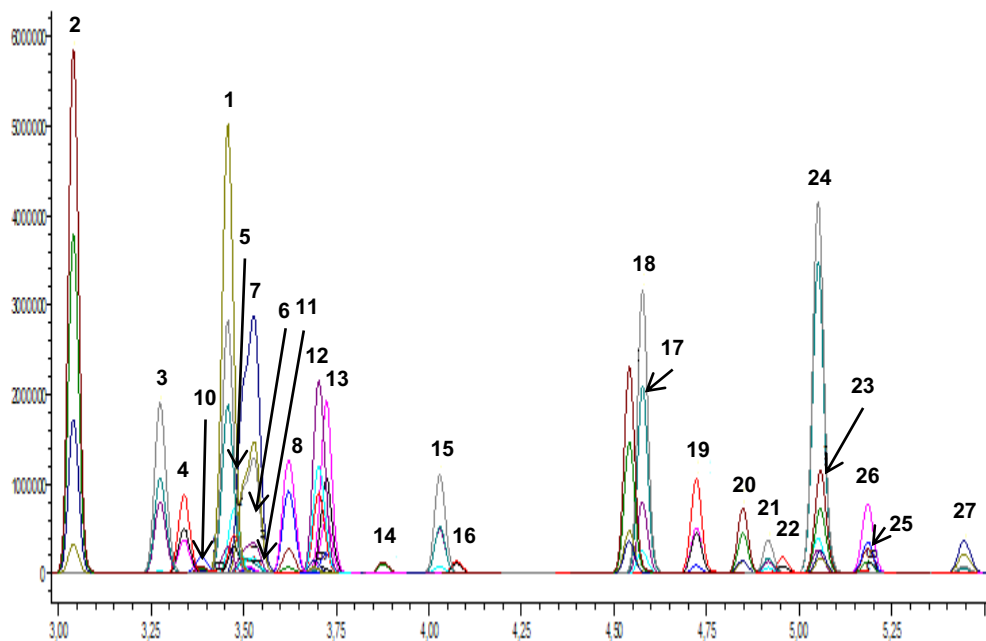
Conditions

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 H₂O
B: 0.1% formic acid in MeCN

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

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

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)



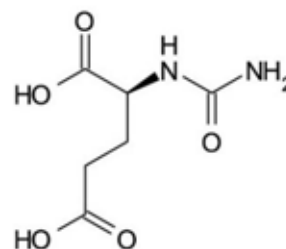
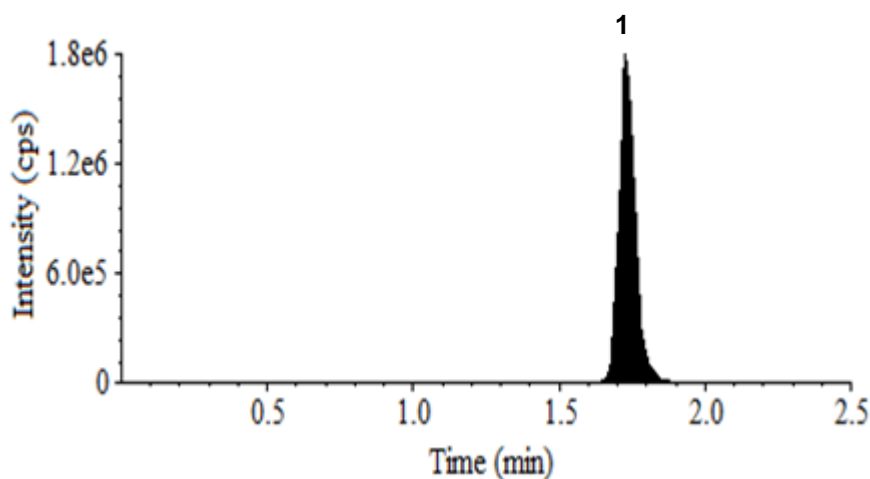
Carglumic Acid in Human Plasma by LC-MS/MS

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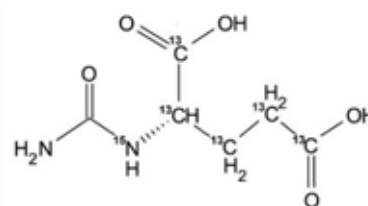
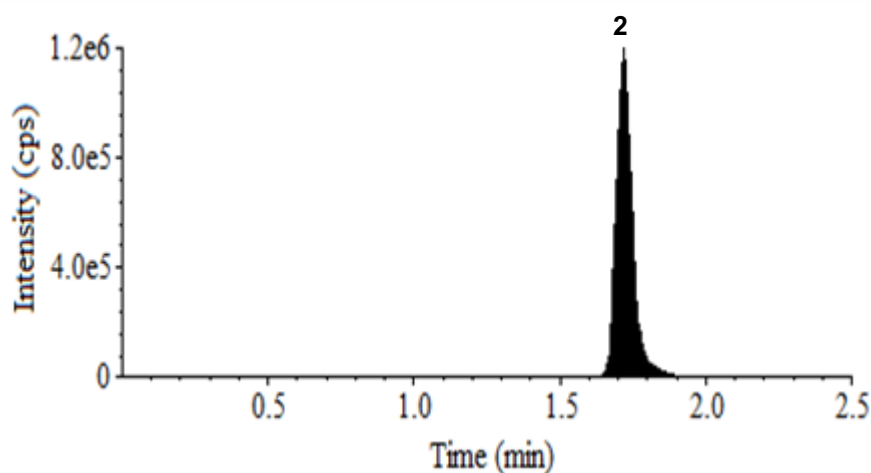
Application #AN3750

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



1. Carglumic acid
(m/z 189 $\rightarrow$ 146)
(LLOQ 6.0 ng/mL)



2. Carglumic acid-13C 15N (I.S.)
(m/z 195 $\rightarrow$ 152)

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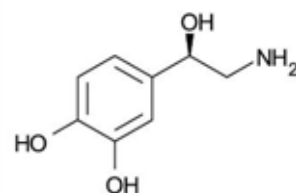
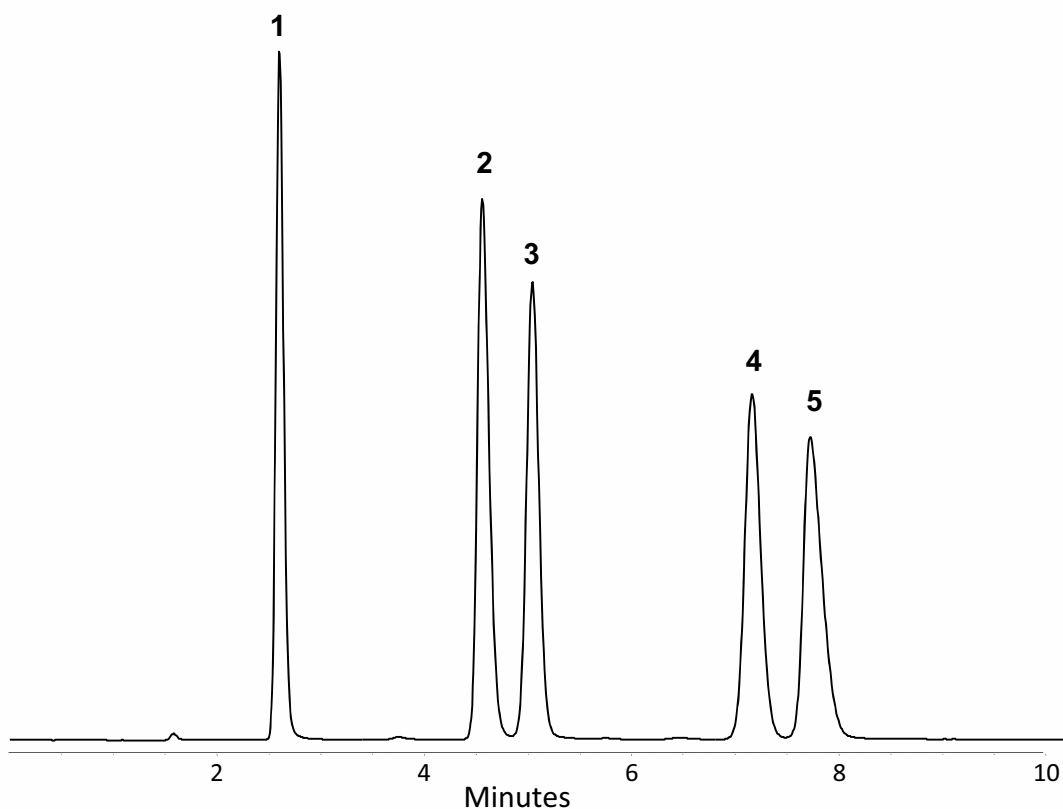
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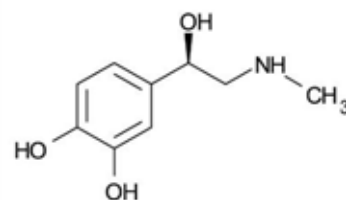
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Columns

Conditions

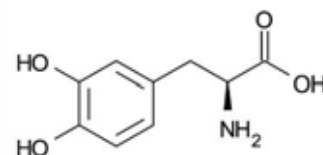
Column: ACE 5 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1210-1546
Mobile Phase: 12.5 mM ammonium formate pH 3.0 in H₂O
Flow Rate: 1 mL/min
Temperature: 22 °C
Detection: UV, 266 nm



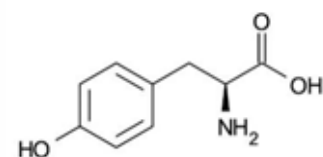
1. Norepinephrine



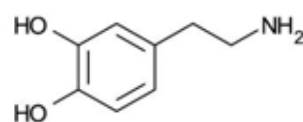
2. Epinephrine



3. Levodopa



4. Tyrosine



5. Dopamine



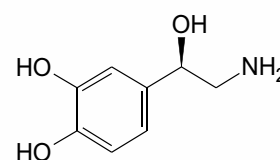
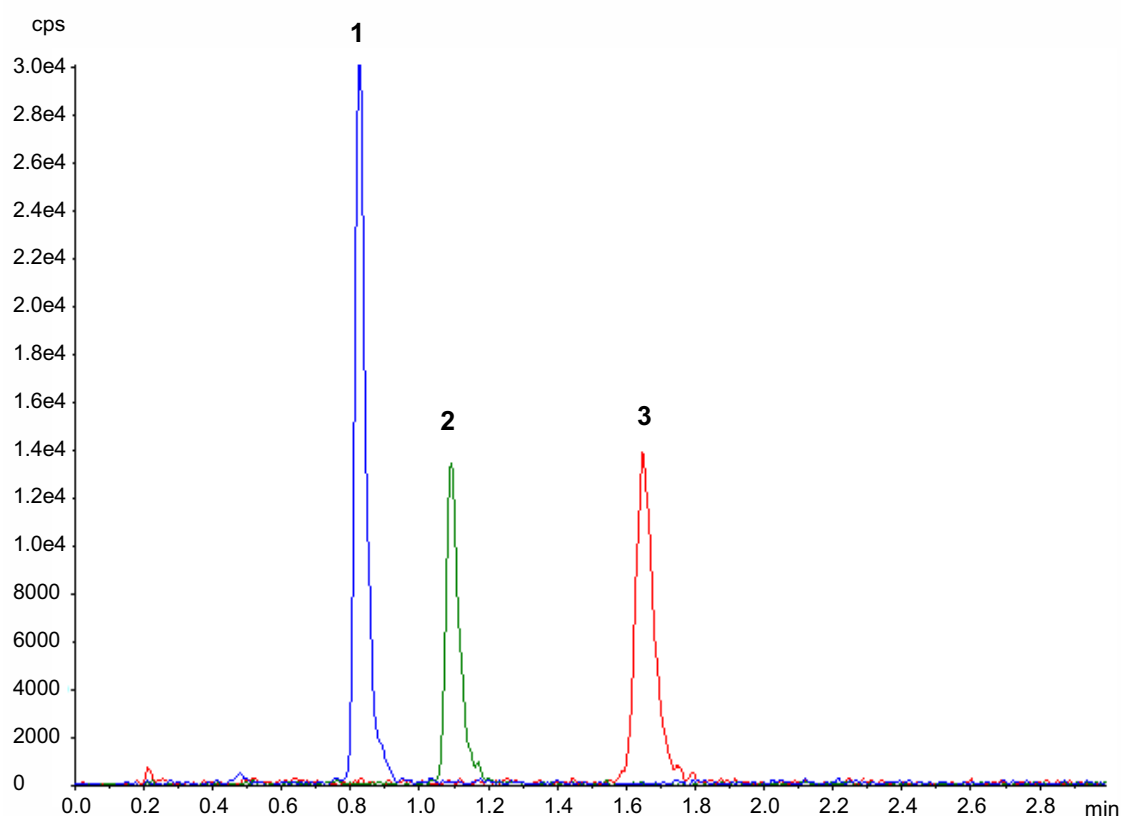
Catecholamines by LC-MS/MS

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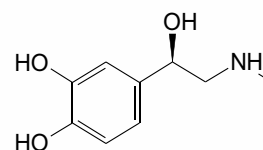
Application #AN2320

Conditions

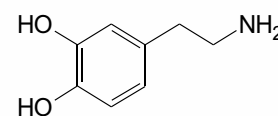
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: 2 mM ammonium formate pH 3.2/MeOH (98:2 v/v)
Flow Rate: 0.4 mL/min
Injection: 20 µL
Temperature: 40 °C
Detection: AB SCIEX triple quad 5500
Positive ESI mode
Source temperature: 700 °C
IonSpray voltage: 5500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



1. Norepinephrine
(m/z 152.1 $\rightarrow$ 107.1)



2. Epinephrine
(m/z 166.1 $\rightarrow$ 107.1)



3. Dopamine
(m/z 154.1 $\rightarrow$ 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 Metanephrines Separation (Gradient)

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Application #AN1480

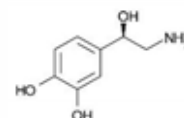
Conditions

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 H₂O
B: 20 mM ammonium formate pH 3.0 in MeOH/H₂O (90:10 v/v)

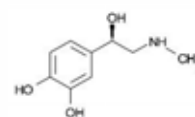
Time (mins)	%B
0	0
5	40
6	40
7	0

Post time 10 minutes

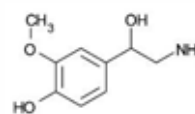
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: UV, 260 nm



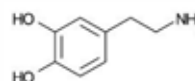
1. Norepinephrine



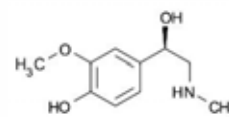
2. Epinephrine



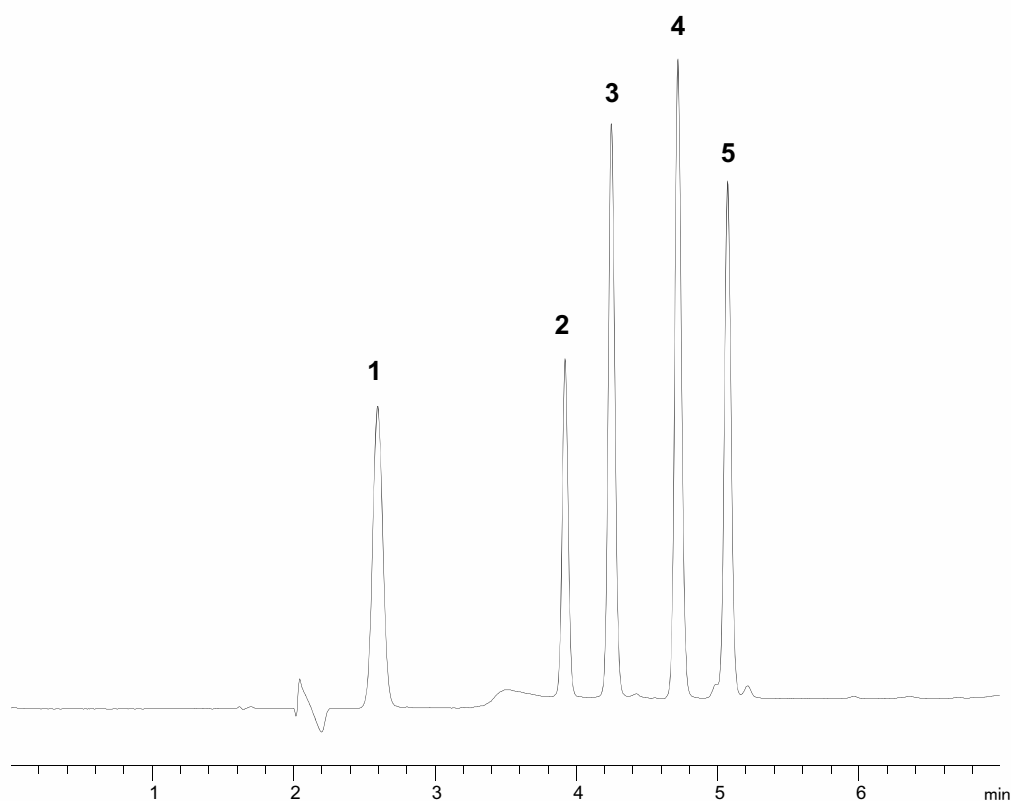
3. Normetanephrine



4. Dopamine



5. Metanephrine



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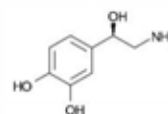
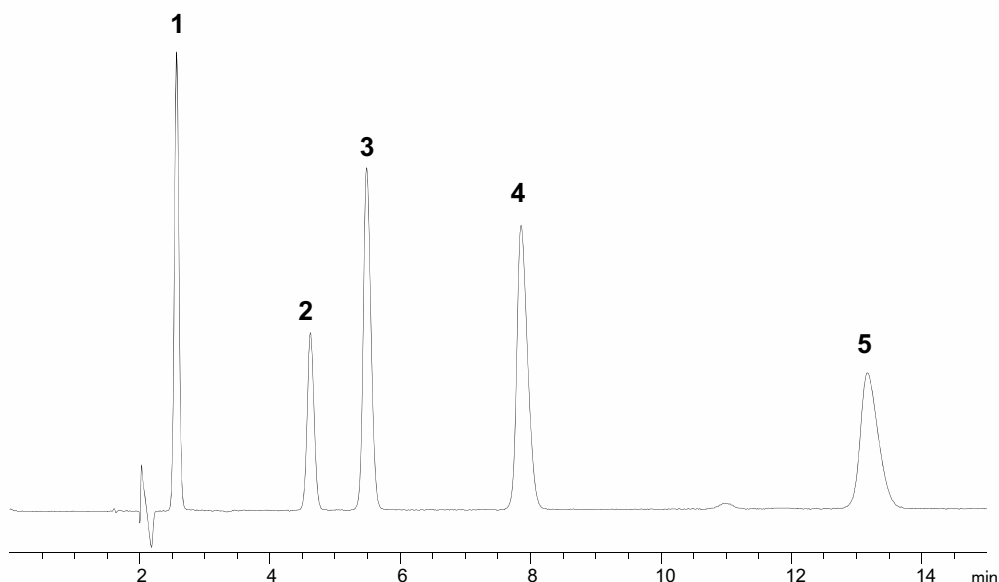
Catecholamines and Metanephrines Separation (Isocratic)

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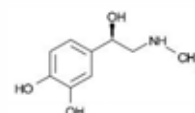
Application #AN1490

Conditions

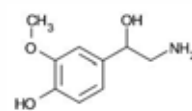
Column: ACE 5 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: ACE-1210-1546
Mobile Phase: 20 mM ammonium formate pH 3.0 in H₂O
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 25 °C
Detection: UV, 260 nm



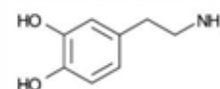
1. Norepinephrine



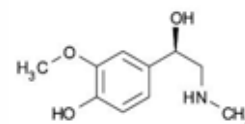
2. Epinephrine



3. Normetanephrine



4. Dopamine



5. Metanephrine



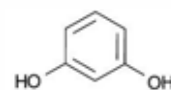
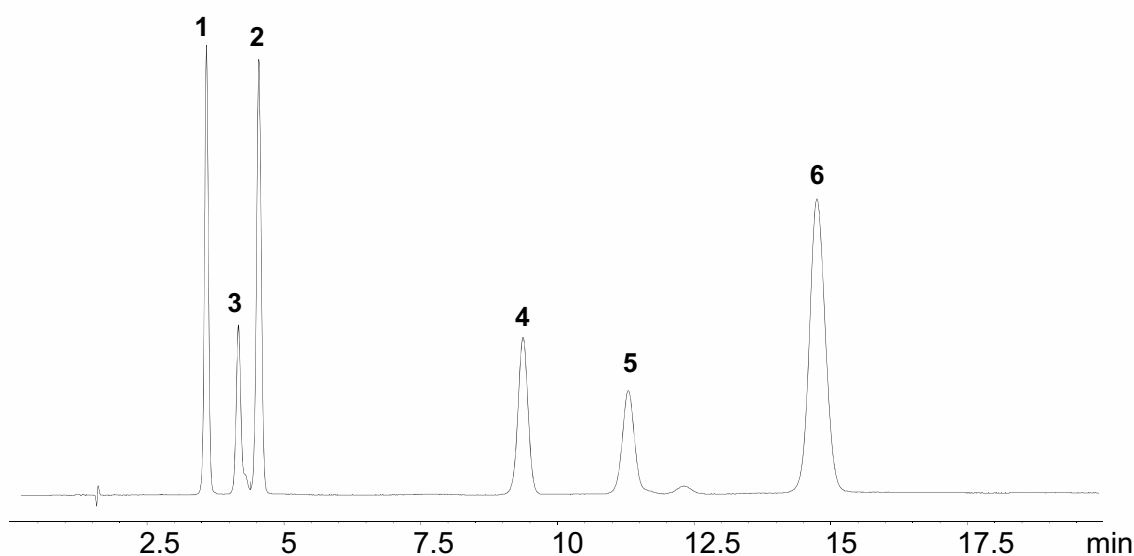
Catechols Mixture Separation (I)

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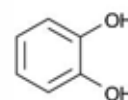
Application #AN1430

Conditions

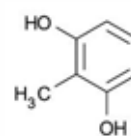
Column: ACE 3 CN-ES
Dimensions: 150 x 4.6 mm
Part Number: EXL-1113-1546U
Mobile Phase: 20 mM H₃PO₄ in MeCN/H₂O (25:75 v/v)
Flow Rate: 1.5 mL/min
Injection: 5 µL
Temperature: 30 °C
Detection: UV, 270 nm



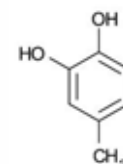
1. Resorcinol



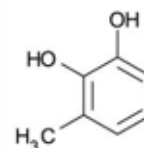
2. Catechol



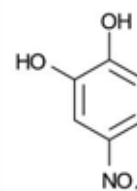
3. 2-Methylresorcinol



4. 4-Methylcatechol



5. 3-Methylcatechol



6. 4-Nitrocatechol



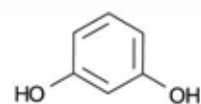
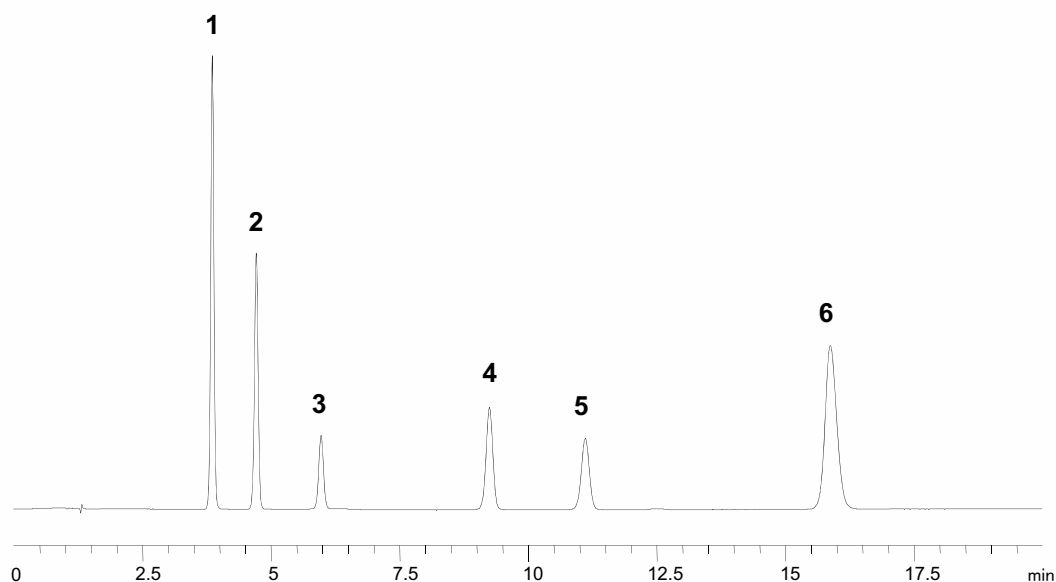
Catechols Mixture Separation (II)

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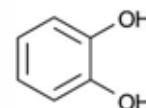
Application #AN1440

Conditions

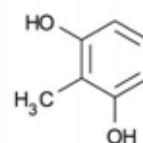
Column: ACE 3 C18-Amide
Dimensions: 150 x 4.6 mm
Part Number: EXL-1112-1546U
Mobile Phase: 20 mM H₃PO₄ in MeCN/H₂O (10:90 v/v)
Flow Rate: 1.5 mL/min
Injection: 5 µL
Temperature: 30 °C
Detection: UV, 270 nm



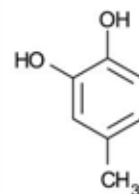
1. Resorcinol



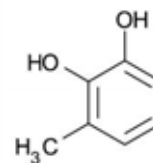
2. Catechol



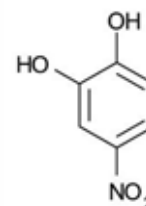
3. 2-Methylresorcinol



4. 4-Methylcatechol



5. 3-Methylcatechol



6. 4-Nitrocatechol

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Cathinone Psychoactive Substances by LC-UV and LC-Amperometry

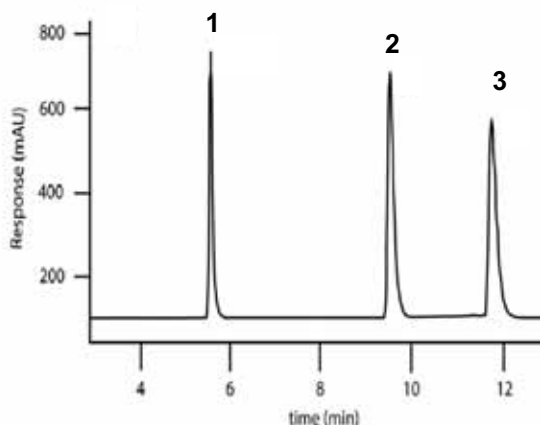
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Application #AN3500

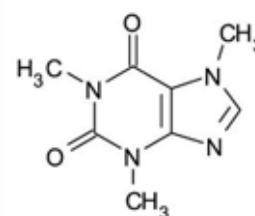
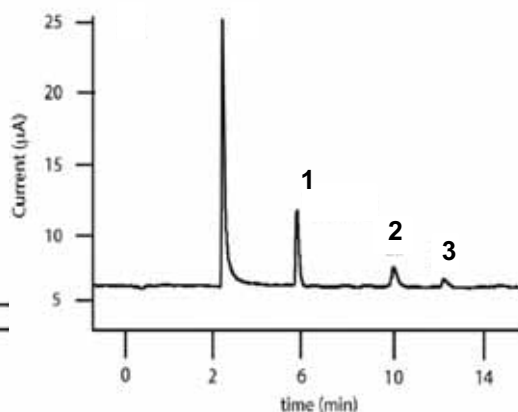
Conditions

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

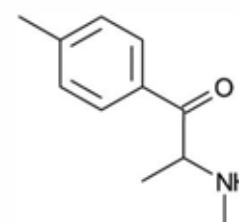
UV Detection



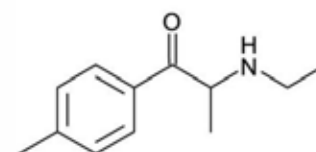
Amperometric Detection



1. Caffeine



2. 4-Methylmethcathinone
(4-MMC, mephedrone)



3. 4-Methylethcathinone
(4-MEC)

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

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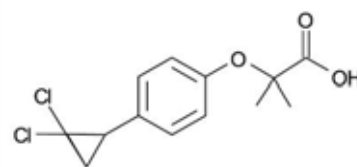
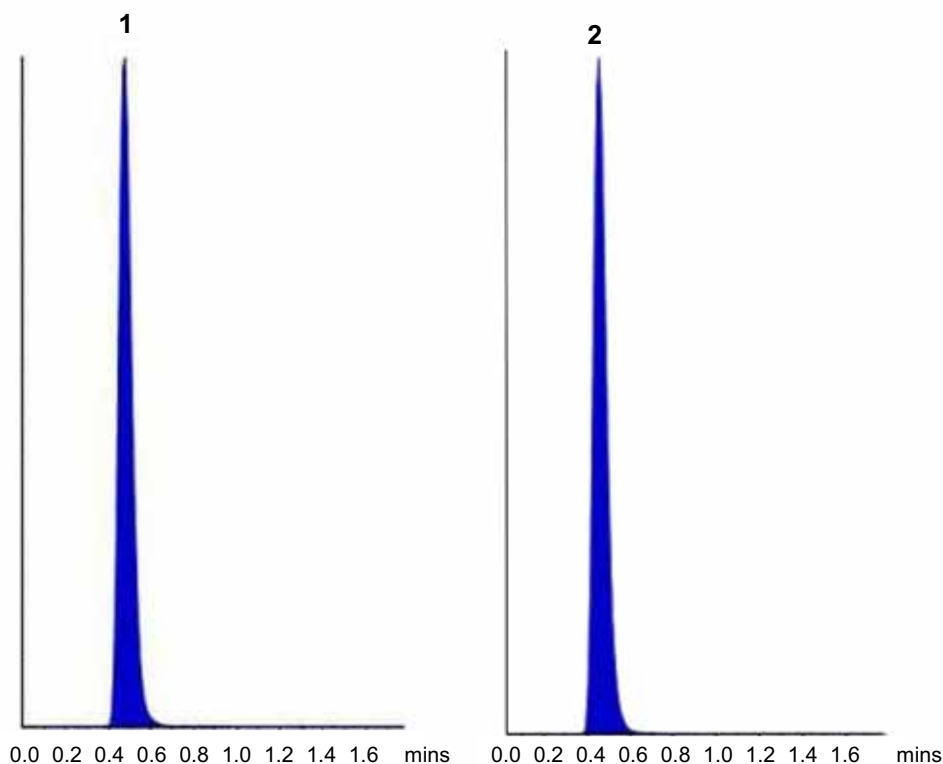
Ciprofibrate from Human Plasma by LC-MS/MS

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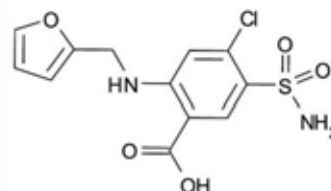
Application #AN2670

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 ₂ O (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



1. Ciprofibrate
(*m/z* 287.0 → 85.0)



2. Furosemide (IS)
(*m/z* 328.9 → 204.9)

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Clenbuterol in Equine Plasma by LC-MS/MS

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Application #AN2050

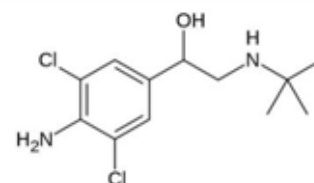
Conditions

Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002
Mobile Phase: A: 0.2% formic acid in H₂O
B: 0.2% formic acid in MeCN

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

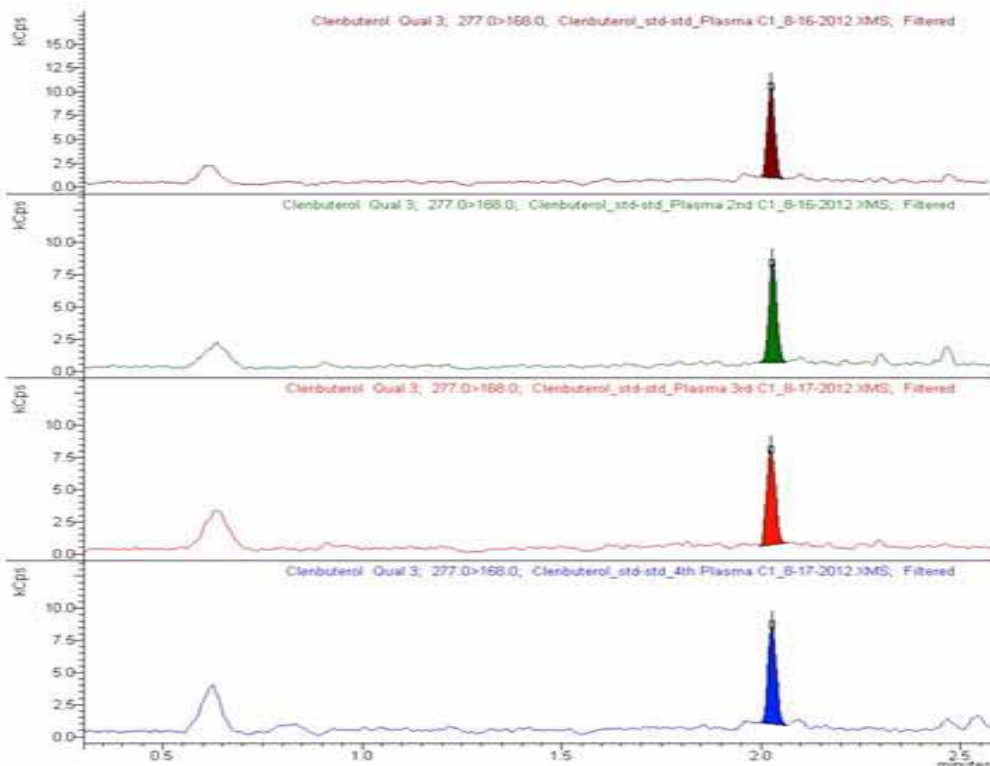
Flow Rate: 0.45 mL/min
Injection: 30 µL
Detection: Bruker EVOQ Elite triple quad MS
VIP heated-ESI temperature: 300 °C
Cone gas temperature: 300 °C
Spray voltage: +3500 V

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



1. Clenbuterol
(*m/z* 227.1 → 168)

2. d9-Clenbuterol (IS)
(*m/z* 286.1 → 204)



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Clonidine Hydrochloride Oral Solution Containing Preservatives

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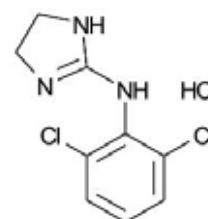
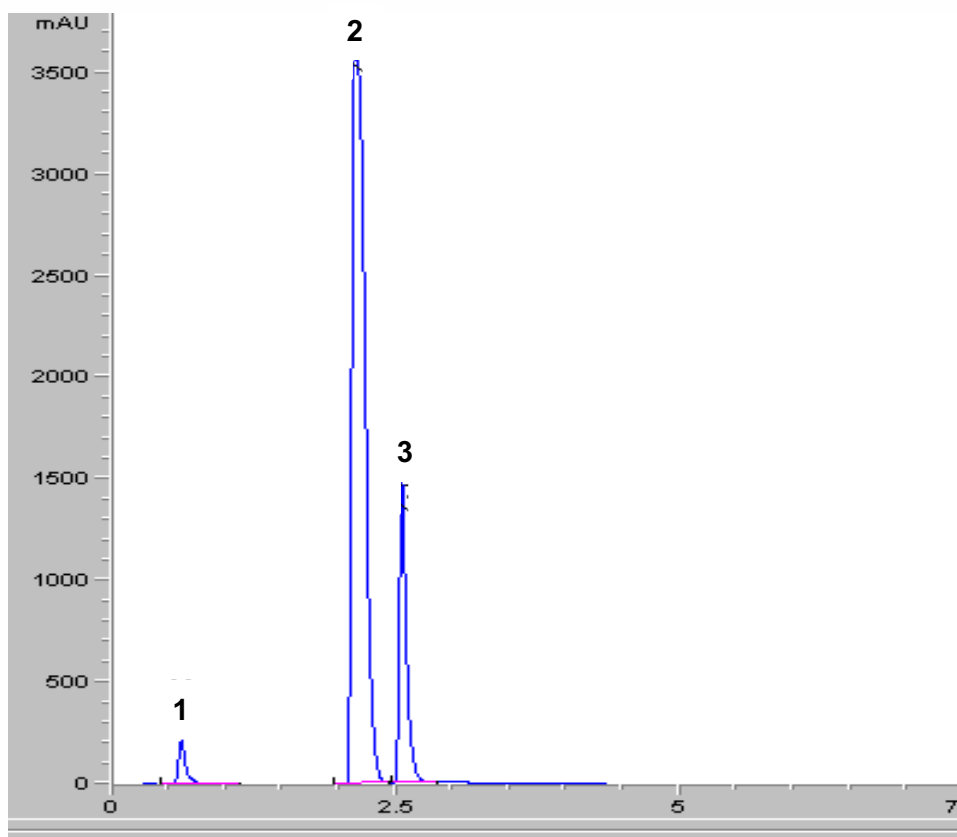
Application #AN2060

Conditions

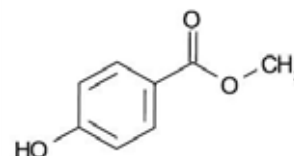
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 4.6 mm
Part Number: CORE-25A-0546U
Mobile Phase: A: 0.2% w/v phosphate buffer/MeOH/MeCN (80:10:10 v/v)
B: MeCN

Time (mins)	%B
0	0
0.8	0
2.1	70
3.4	70
3.5	0

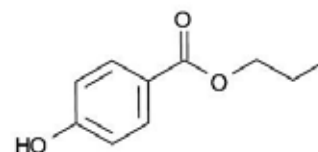
Flow Rate: 2 mL/min
Injection: 100 µL
Temperature: 20 °C
Detection: UV, 220 nm



1. Clonidine HCl
(10 µg/mL)



2. Methyl paraben
(1.5 g/mL)



3. Propyl paraben
(1.5 g/mL)

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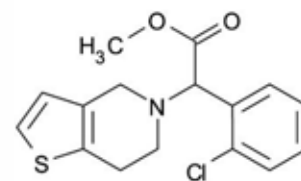
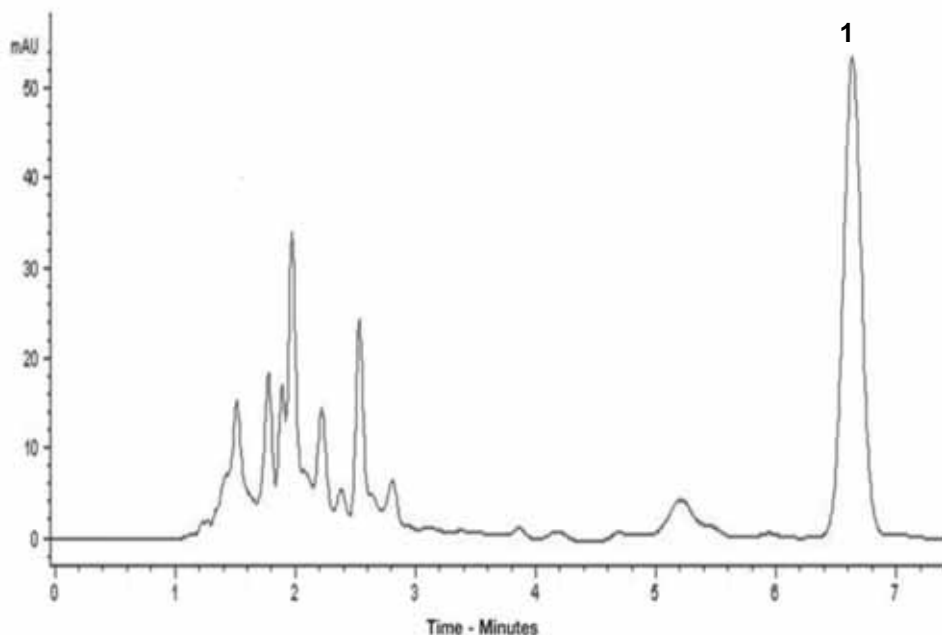
Clopidogrel and Photodegradation Products

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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 ₃ PO 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



1. Clopidogrel

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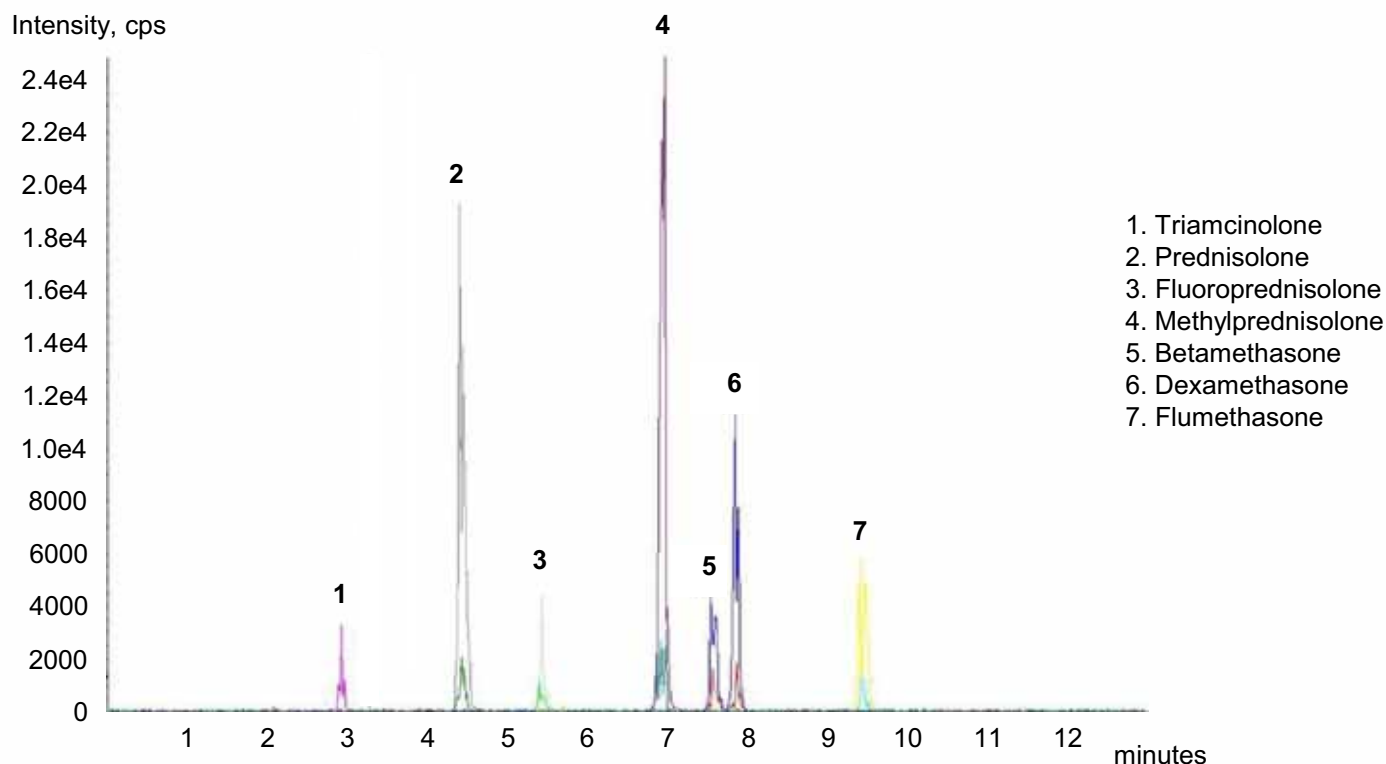

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Conditions

Column: ACE 3 C18-PFP
Dimensions: 150 x 2.1 mm
Part Number: ACE-1110-1502
Mobile Phase: A: 0.1% formic acid in H₂O
B: MeCN/0.1% formic acid in H₂O (90:10 v/v)

Time (mins)	%B
0.0	30
14.0	50
17.0	95
20.0	30

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



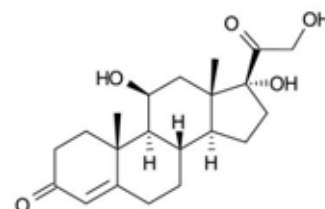
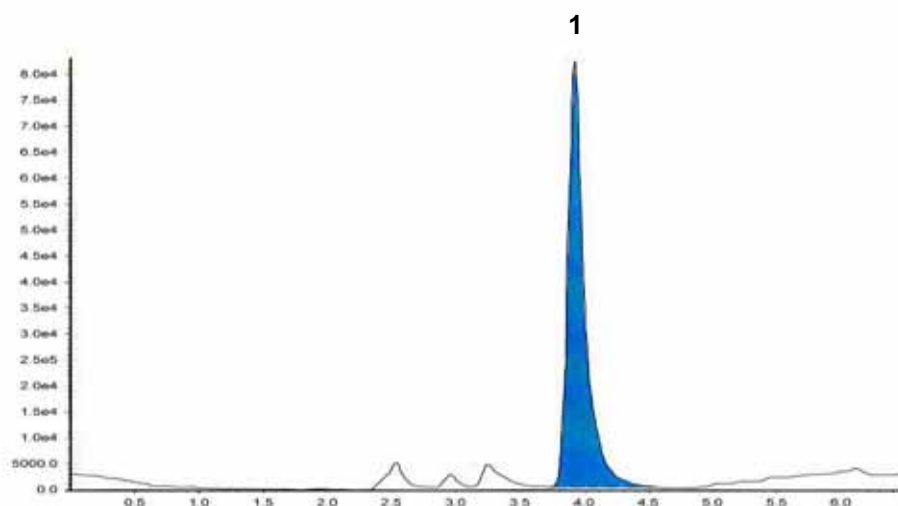
Cortisol in Urine by LC-MS/MS

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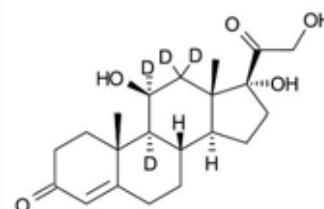
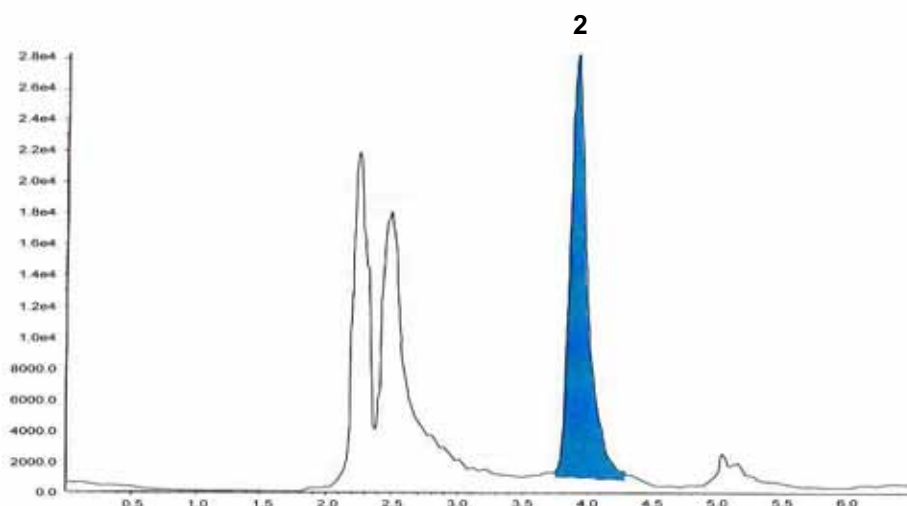
Application #AN2680

Conditions

Column: ACE Excel 2 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-101-1002U
Mobile Phase: 4 mM ammonium acetate in H₂O/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)



1. Cortisol
(*m/z* 363.5 → 121.3)



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

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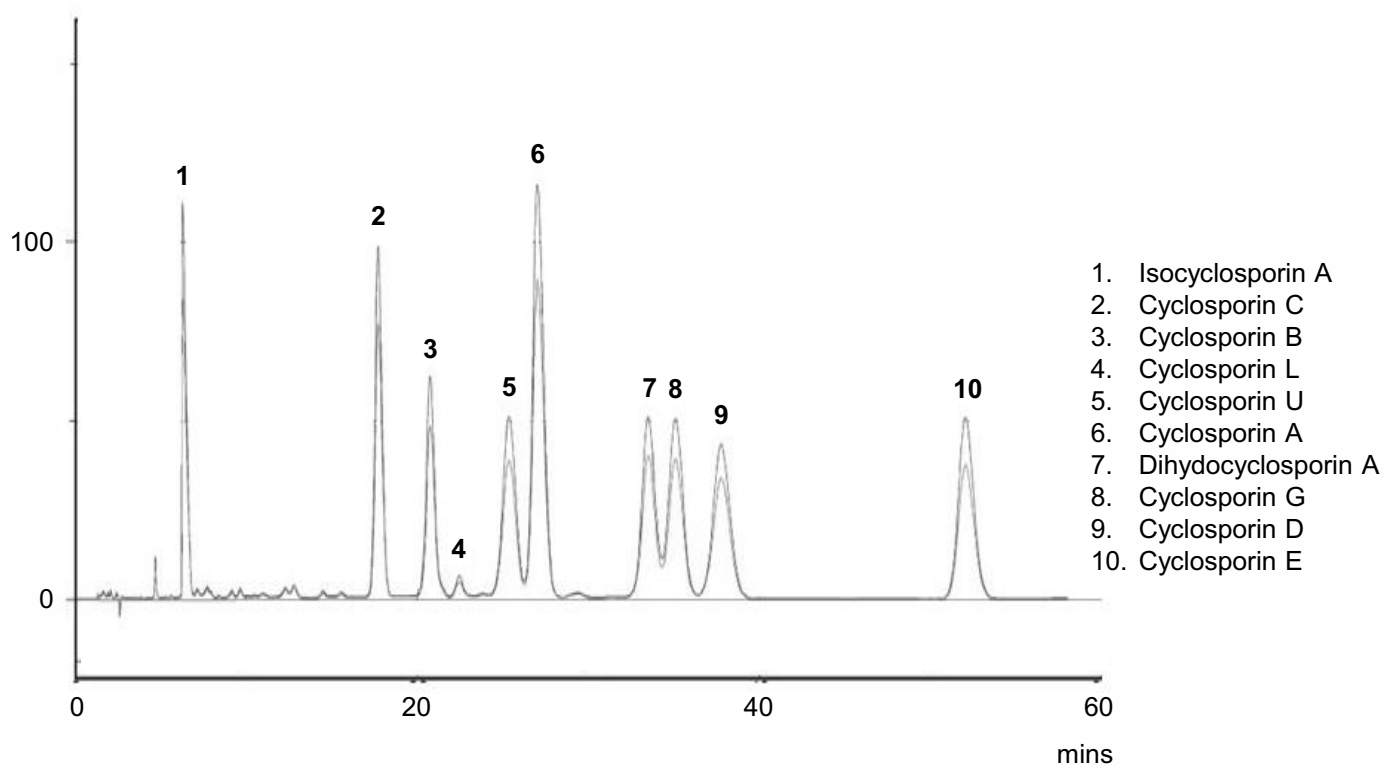
Cyclosporin Mixture

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UHPLC & HPLC Columns

Application #AN3270

Conditions

Column: ACE 5 C18
Dimensions: 250 x 3.0 mm
Part Number: ACE-121-2503
Mobile Phase: H₂O/MeCN/MTBE/H₃PO₄ (46:51:3:0.1 v/v/v/v)
Flow Rate: 0.8 mL/min
Temperature: 80 °C
Detection: UV, 210 nm



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Cytarabine Analogues by Ion-Pairing LC-MS/MS

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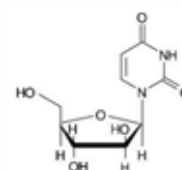
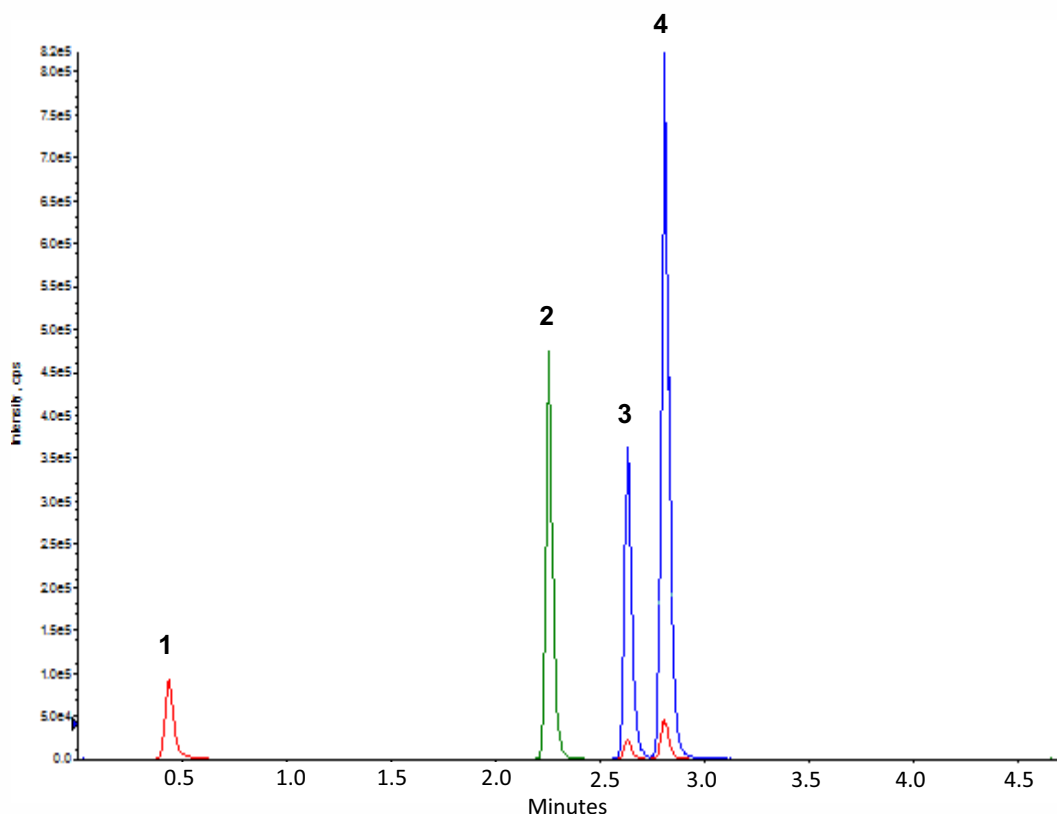
Application #AN2070

Conditions

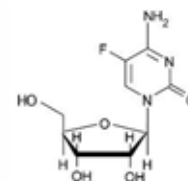
Column: ACE 3 C18
Dimensions: 50 x 2.1 mm
Part Number: ACE-111-0502
Mobile Phase: A: 0.1% perfluoropentanoic acid + 0.1% formic acid in H₂O
B: 0.1% perfluoropentanoic acid + 0.1% formic acid in MeCN

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

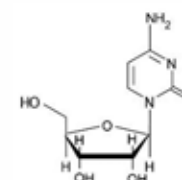
Flow Rate: 0.7 mL/min
Detection: API 4000 MS
TurbolonSpray, positive mode
Source Temperature 550 °C



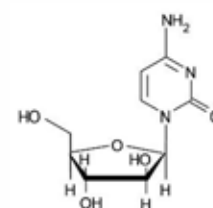
1. Uracil arabinofuranoside
(*m/z* 245 → 113)



2. 5-Fluorocytidine (IS)
(*m/z* 262 → 130)



3. Cytidine
(*m/z* 244 → 112)



4. Cytarabine
(*m/z* 244 → 112)

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Dermorphin in Equine Urine by LC-MS/MS

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Application #AN1040

Conditions

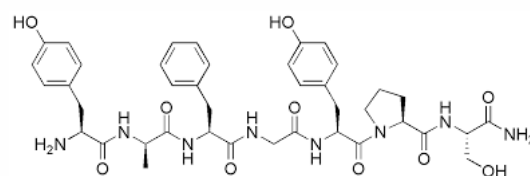
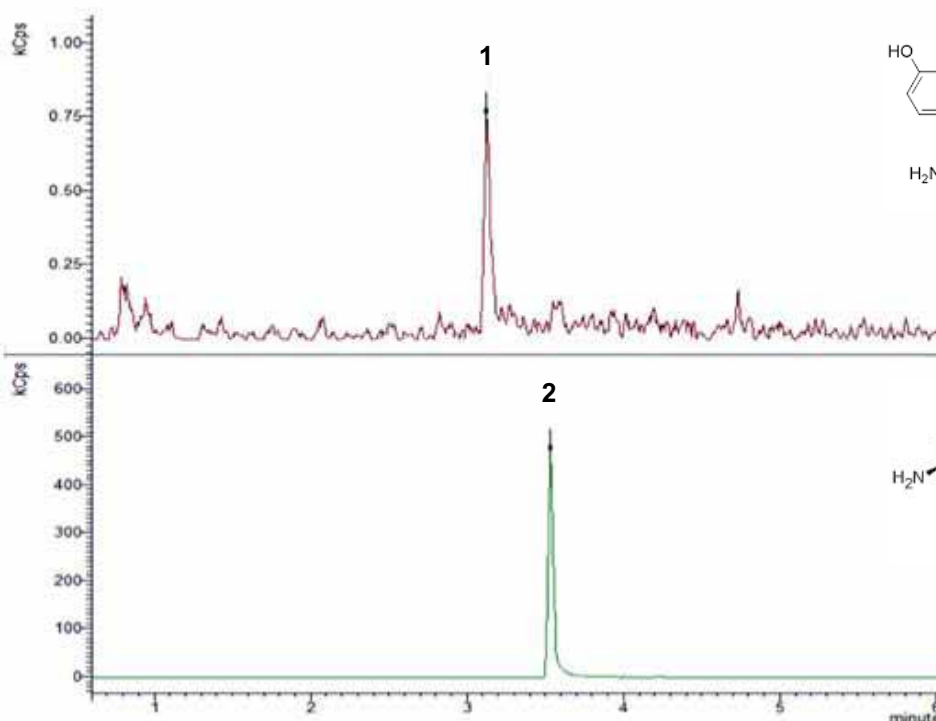
Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002
Mobile Phase: A: 0.2% formic acid in H₂O
B: 0.2% formic acid in MeCN

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

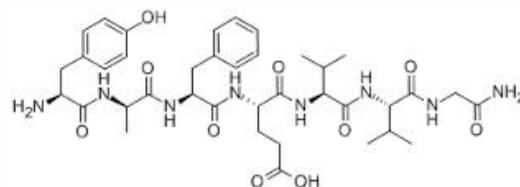
Flow Rate: 0.4 mL/min
Injection: 40 µL
Detection: Bruker EVOQ Elite triple quad MS
VIP heated-ESI temperature: 350 °C
Cone gas temperature: 250 °C
Spray voltage: +4000 V

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

LLOQ = 0.05 ng/mL



1. Dermorphin
(m/z 803.4 → 602 (Quantifier ion))
(m/z 803.4 → 202 (Qualifier ion))



2. Deltorhin-II (IS)
(m/z 783 → 277)

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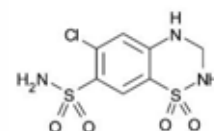
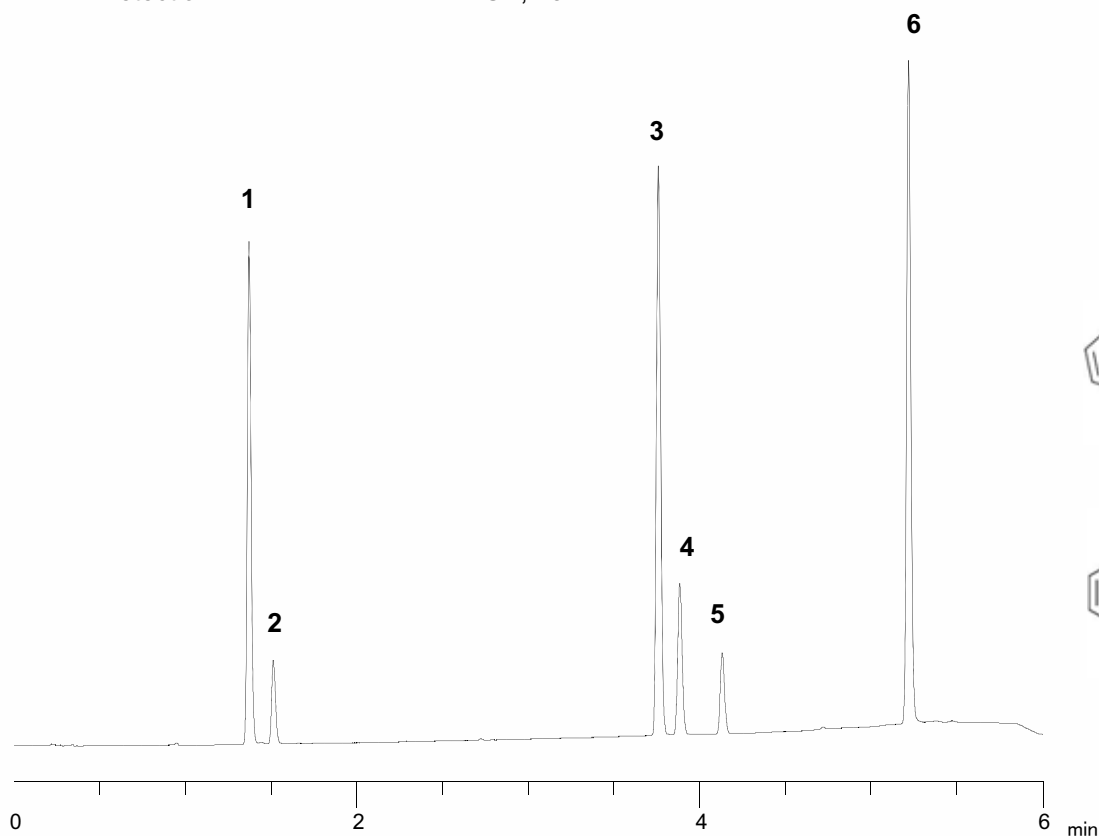
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Conditions

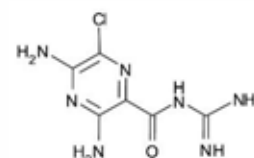
Column: ACE Excel 2 C18-PFP
Dimensions: 50 x 3.0 mm
Part Number: EXL-1010-0503U
Mobile Phase: A: 10 mM ammonium formate pH 3.0 in H₂O
B: 10 mM ammonium formate pH 3.0 in MeOH/H₂O (9:1 v/v)

Flow Rate: 1 mL/min
Injection: 2 µL
Temperature: 60 °C
Detection: UV, 254 nm

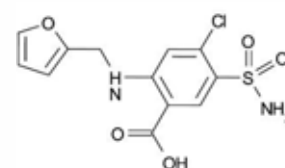
Time (mins)	%B
0.0	5
0.5	5
5.0	0
5.5	70
6.0	5



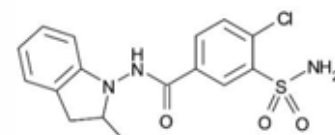
1. Hydrochlorothiazide



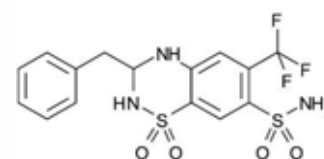
2. Amiloride



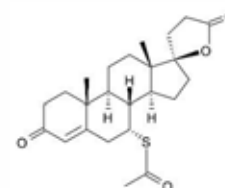
3. Furosemide



4. Indapamide



5. Bendroflumethiazide

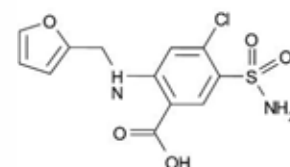
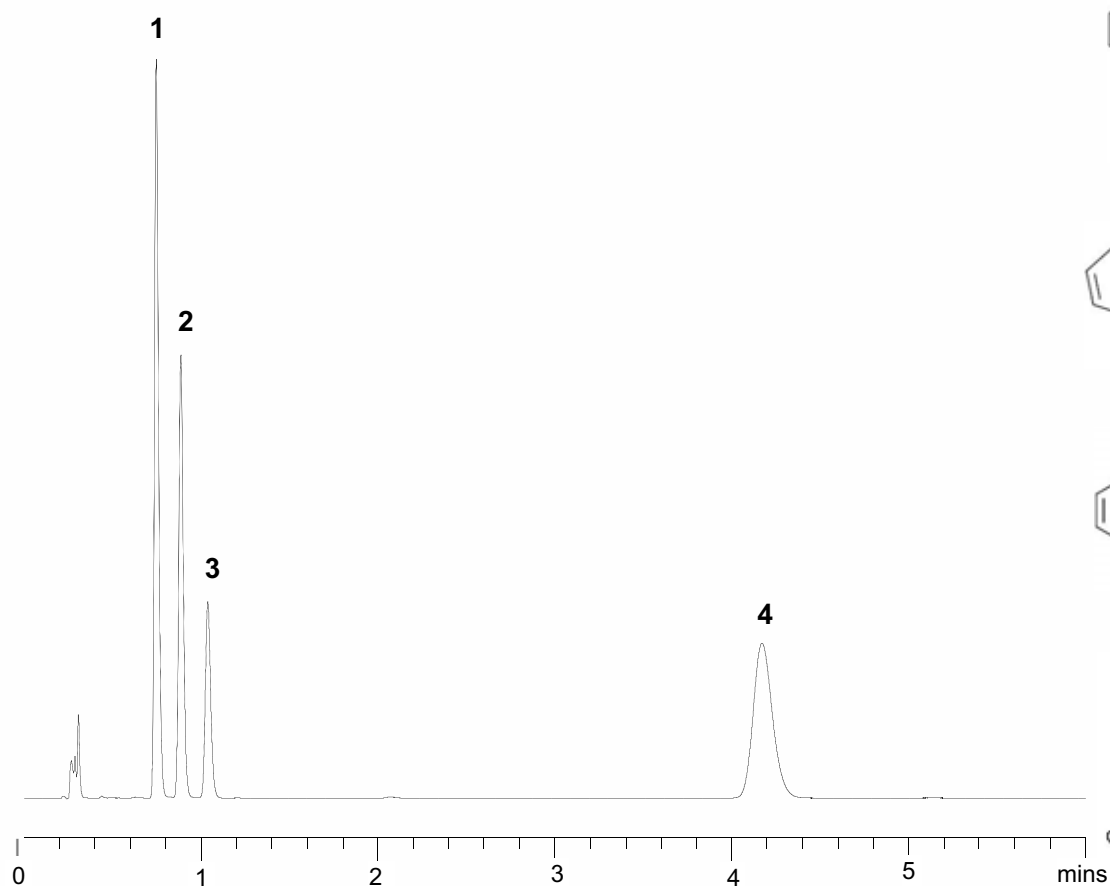


6. Spironolactone

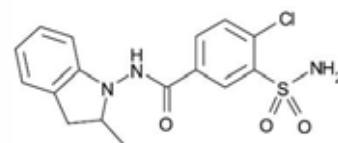


Conditions

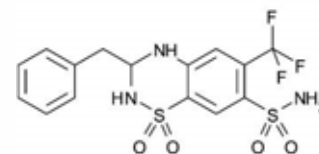
Column:	ACE Excel 2 C18-PFP
Dimensions:	50 x 3.0 mm
Part Number:	EXL-1010-0503U
Mobile Phase:	10 mM ammonium formate pH 3.0 in MeOH/H ₂ O (45:55 v/v)
Flow Rate:	1 mL/min
Injection:	2 µL
Temperature:	60 °C
Detection:	UV, 254 nm



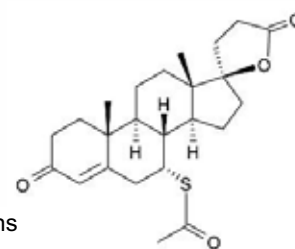
1. Furosemide



2. Indapamide



3. Bendroflumethiazide



4. Spironolactone

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Drugs of Abuse Screen by UHPLC-MS/MS

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Application #AN2190

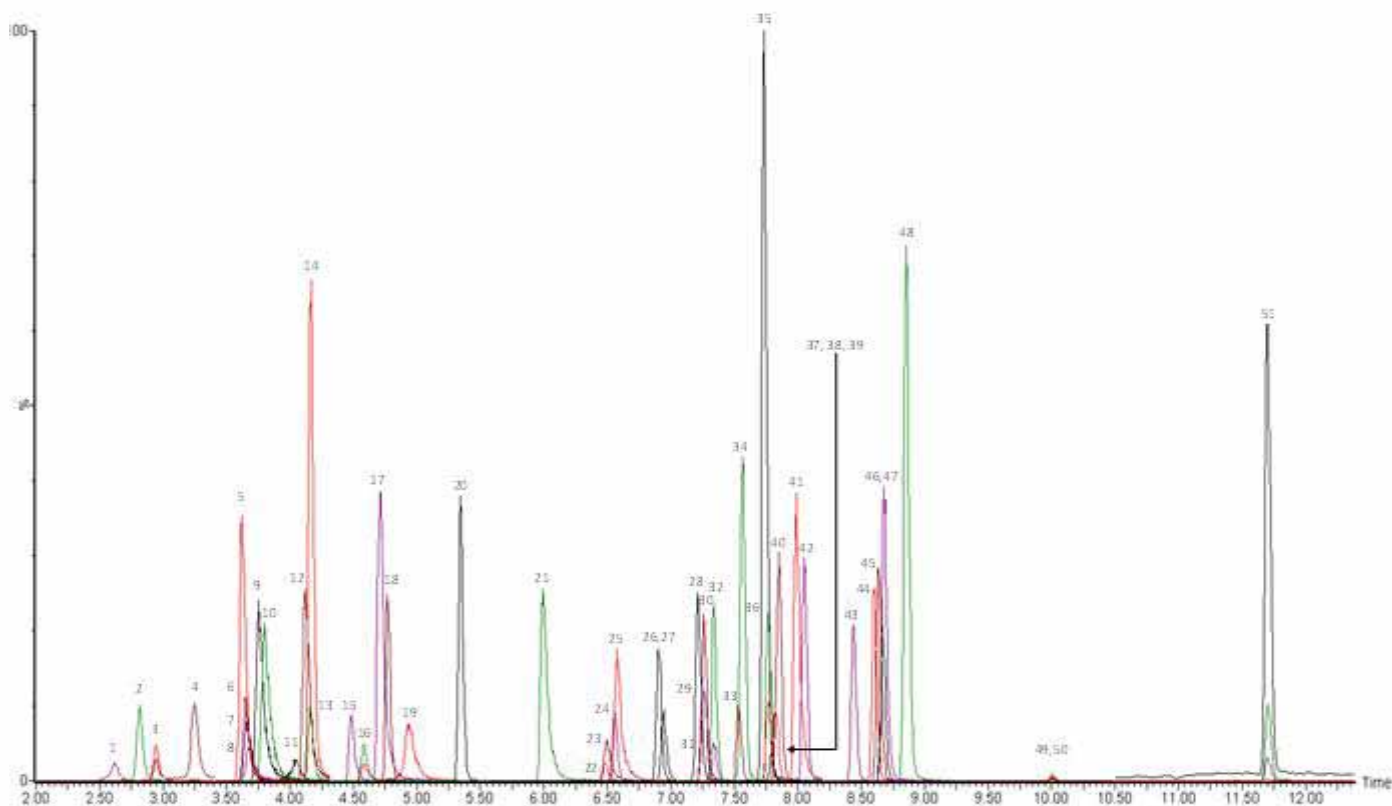
Page 1 of 2

Conditions

Column: ACE Excel 1.7 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-171-1002U
Mobile Phase: A: 5 mM ammonium acetate in H₂O
B: 5 mM ammonium acetate in MeOH

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 10⁻⁴ mbar



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Drugs Of Abuse Screen By UHPLC-MS/MS

Peak	Analyte	Rt	Q1 (Da)	Q3 (Da)	Peak	Analyte	Rt	Q1 (Da)	Q3 (Da)
1	Oxymorphone	2.62	302.2	198.1	27	Bromazepam	6.95	316.1	182.1
2	Morphine-D3	2.82	289.2	201.0	28	Ketamine	7.21	238.1	124.9
3	Morphine	2.95	286.2	201.0	29	Clonazepam	7.26	316.1	270.1
4	Hydromorphone	3.25	286.2	185.1	30	Nitrazepam	7.26	282.2	236.1
5	Amphetamine-D5	3.62	141.0	123.9	31	α -hydroxytriazolam	7.34	359.1	331.1
6	Amphetamine	3.65	136.0	118.9	32	Flunitrazepam	7.34	314.2	268.2
7	Dihydrocodeine	3.66	302.2	199.1	33	α -hydroxyalprazolam	7.54	325.2	297.1
8	MDA	3.67	180.1	105.0	34	Estazolam	7.56	295.2	267.2
9	MDMA	3.75	194.1	163.0	35	Zolpidem	7.73	308.2	235.1
10	Methamphetamine	3.80	150.0	90.9	36	Triazolam	7.77	343.0	308.1
11	Oxycodone	4.03	316.2	241.2	37	2-Hydroxyethylflurazepam	7.77	333.2	109.0
12	MDEA	4.12	208.2	163.0	38	Lorazepam	7.80	321.1	275.1
13	BZE-D3	4.15	293.1	171.0	39	Oxazepam	7.82	287.2	241.0
14	BZE	4.17	290.1	168.0	40	Alprazolam	7.85	309.2	281.2
15	6-MAM	4.48	328.2	165.1	41	Methadone	7.99	310.2	265.2
16	Codeine	4.59	300.3	215.1	42	Temazepam	8.05	301.1	255.1
17	Norfentanyl	4.71	233.1	84.0	43	Nordiazepam	8.44	271.1	139.9
18	7-Amino-clonazepam	4.77	286.2	121.0	44	Midazolam	8.61	326.2	291.2
19	Hydrocodone	4.94	300.2	199.1	45	Diazepam-D5	8.63	290.2	154.0
20	7-Amino-flunitrazepam	5.34	284.2	135.0	46	Diazepam	8.67	285.2	154.0
21	Cocaine	5.99	304.2	182.0	47	Flurazepam	8.68	388.2	315.1
22	Norbuprenorphine	6.47	414.3	101.0	48	Fentanyl	8.85	337.3	105.0
23	PCP	6.49	244.2	159.9	49	THC-COOH-D3	9.98	348.2	302.2
24	Zaleplon	6.55	306.2	264.2	50	THC-COOH	10.01	345.2	299.2
25	EDDP	6.58	278.2	234.2	51	Buprenorphine	11.70	468.3	101.0
26	Norketamine	6.90	224.1	124.9					



Ethyl Glucuronide in Water by LC-MS/MS

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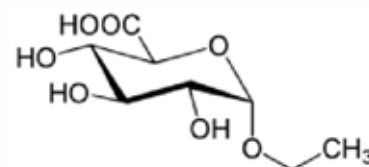
Application #AN1100

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 H₂O
B: MeOH

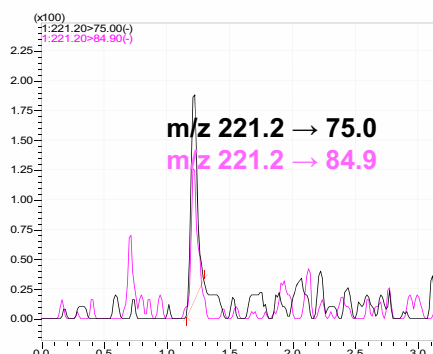
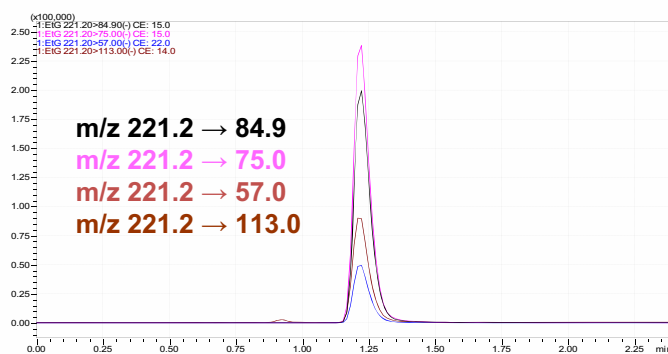
Time (mins)	%B
0.00	5
4.00	70
6.00	95
7.00	95
7.01	5

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

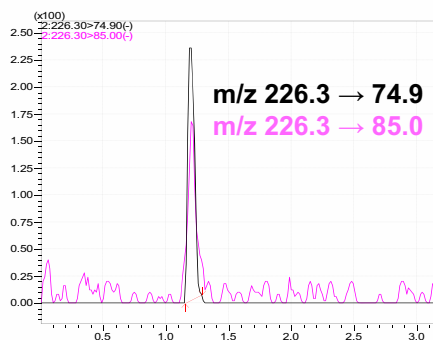
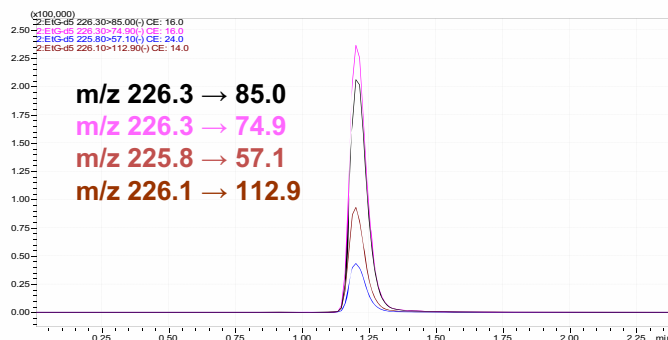


Ethyl glucuronide

Ethyl glucuronide (EtG)
LOQ in H₂O 300 fg on-column



Ethyl glucuronide-d5 (EtG-d5)



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Formoterol in Human Plasma by LC-MS/MS

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Application #AN3100

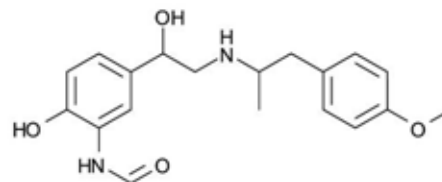
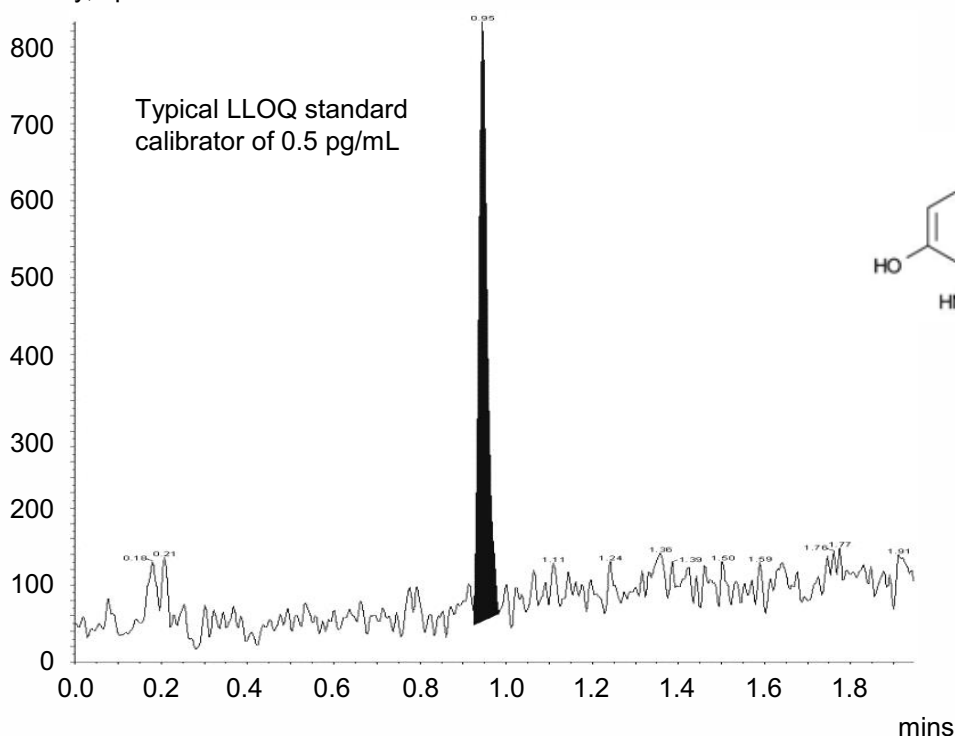
Conditions

Column: ACE Excel 2 C18-AR
Dimensions: 50 x 2.1 mm
Part Number: EXL-1012-0502U
Mobile Phase: A: 0.02% formic acid in H₂O
B: 0.02% formic acid in H₂O/MeOH (2:98 v/v)

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

Intensity, cps



1. Formoterol
(*m/z* 345 → 149)

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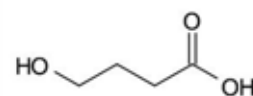
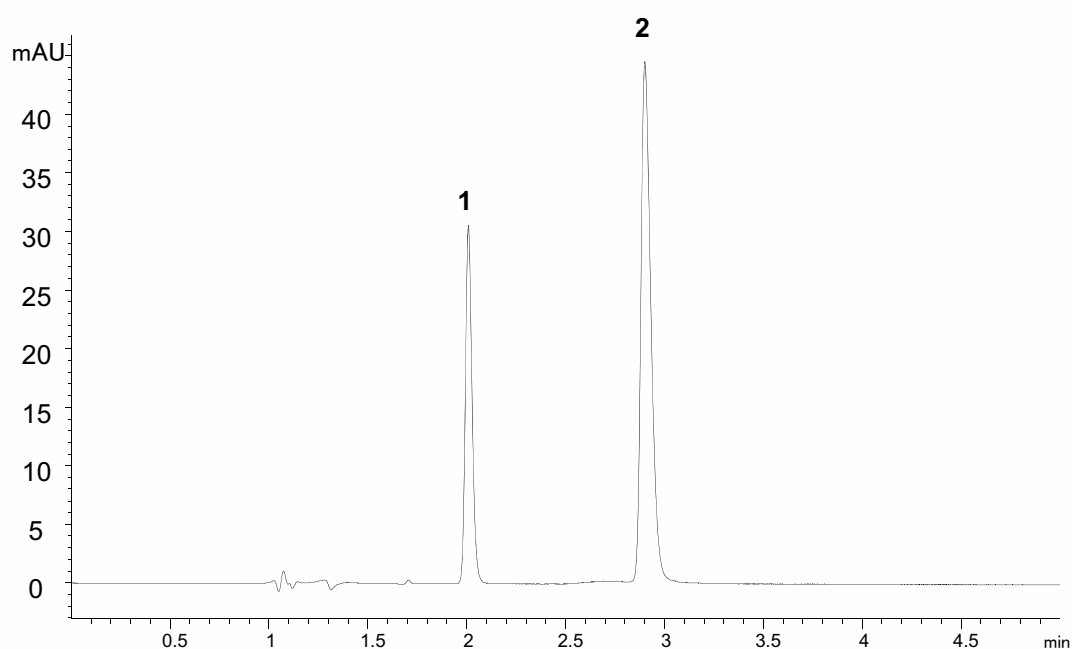
Gamma Hydroxybutyric Acid (GHB) and Gamma Butyrolactone (GBL)

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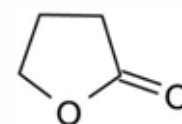
Application #AN1500

Conditions

Column: ACE Excel 2 C18-AR
Dimensions: 100 x 3.0 mm
Part Number: EXL-109-1003
Mobile Phase: 20 mM KH₂PO₄ pH 2.5 H₂O/MeCN (98:2 v/v)
Flow Rate: 0.43 mL/min
Injection: 2 µL
Temperature: 30 °C
Detection: UV, 215 nm



1. GHB



2. GBL



Hepcidin-25 and Truncated Isoforms by LC-HR-MS

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Application #AN3090

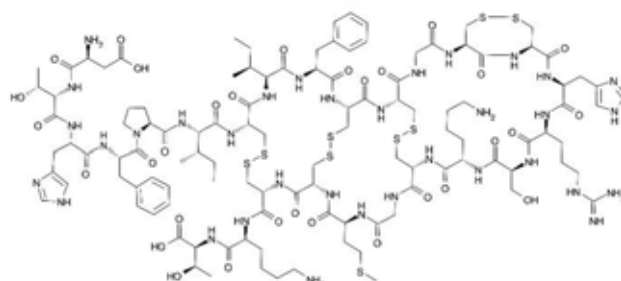
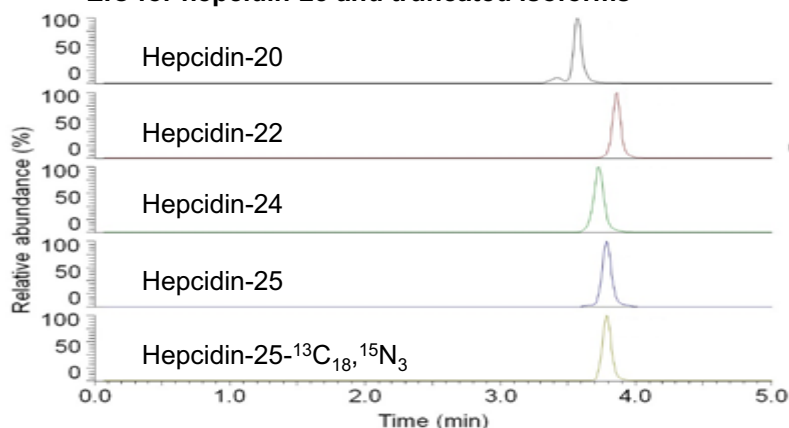
Conditions

Column: ACE 3 C18
Dimensions: 100 x 2.1 mm
Part Number: ACE-111-1002
Mobile Phase: A: 0.1% formic acid in H₂O
B: 0.1% formic acid in MeCN

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

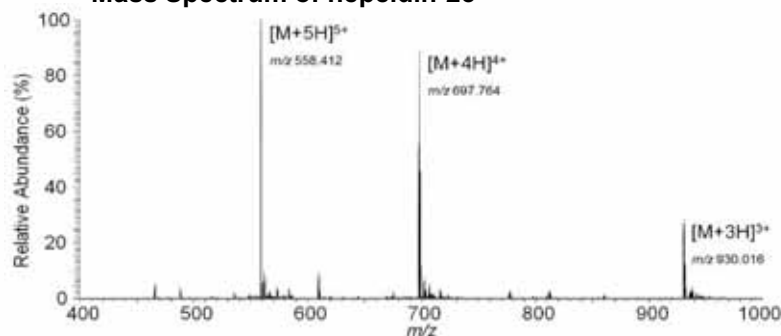
Flow Rate: 0.25 mL/min
Injection: 100 µL
Temperature: 60 °C
Detection: ThermoFisher Scientific Q-Exactive[™] high resolution MS
Heated electrospray ionisation (positive mode)
Spray voltage: 4.5 kV
Vaporiser temperature: 200 °C
Capillary temperature: 320 °C
Detection: Full scan m/z 400 – 1000
Extracted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

EIC for hepcidin-25 and truncated isoforms



Hepcidin-25
(MW 2789)

Mass Spectrum of hepcidin-25



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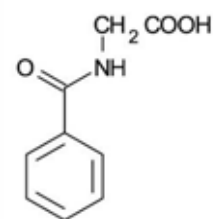
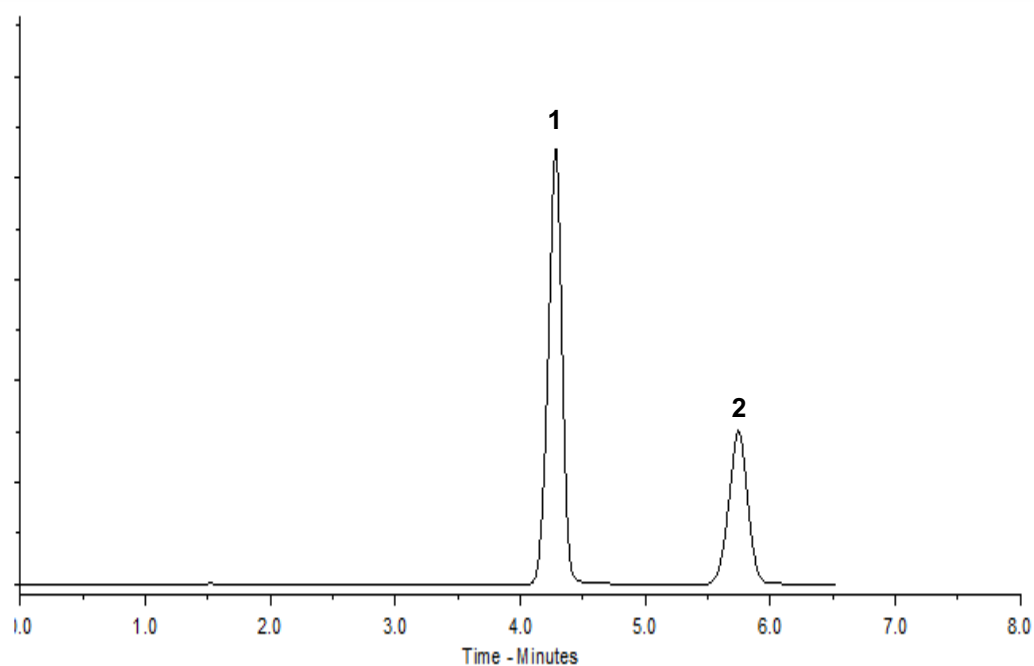
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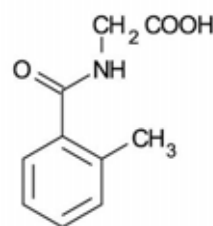
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Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 10 mM KH₂PO₄ pH 3.5 in H₂O/MeCN (15:85 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 254 nm



1. Hippuric acid



2. 2-Methylhippuric acid

Human Defensins in a Saliva Matrix

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Application #AN1270

Conditions

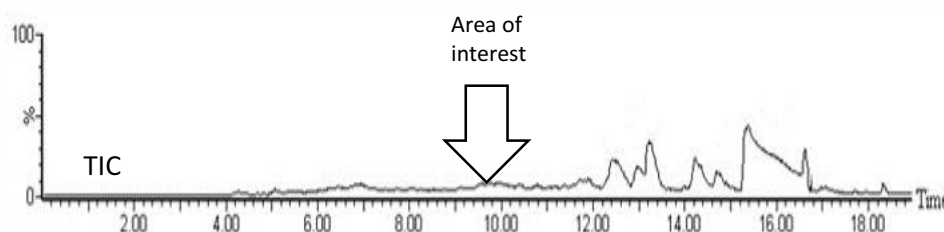
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 50 x 3.0 mm
Part Number: CORE-25A-1503U
Mobile Phase: A: 0.1% formic acid in H₂O
B: 0.1% formic acid in MeCN

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

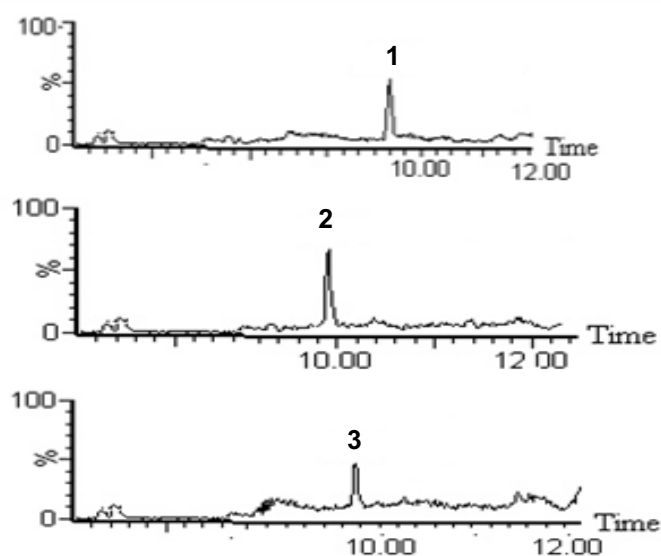
Flow Rate: 0.6 mL/min
Sample Preparation: SPE on C18
Detection: Synapt G1 QToF +ESI MS
Sampling cone voltage: 40 V
Source temperature: 150 °C
Capillary voltages: 4.8 kV
Extraction cone voltages: 41 kV
Desolvation temperature: 500 °C
Acquisition: 100-2000 m/z

Defensin Human Neutrophil Peptides

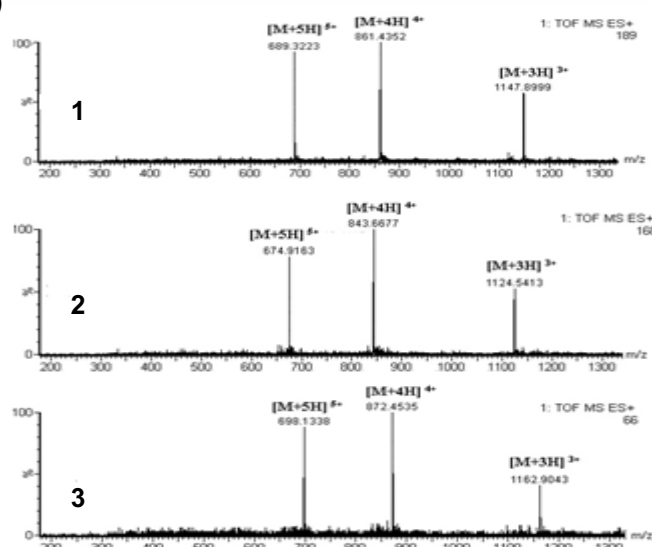
1. HNP-1
(30 amino acid residues)
2. HNP-2
(29 amino acid residues)
3. HNP-3
(30 amino acid residues)



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



Mass spectra



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Human Urine Metabolite Profiling by LC-MS

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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 H₂O
B: 0.01% formic acid in MeCN

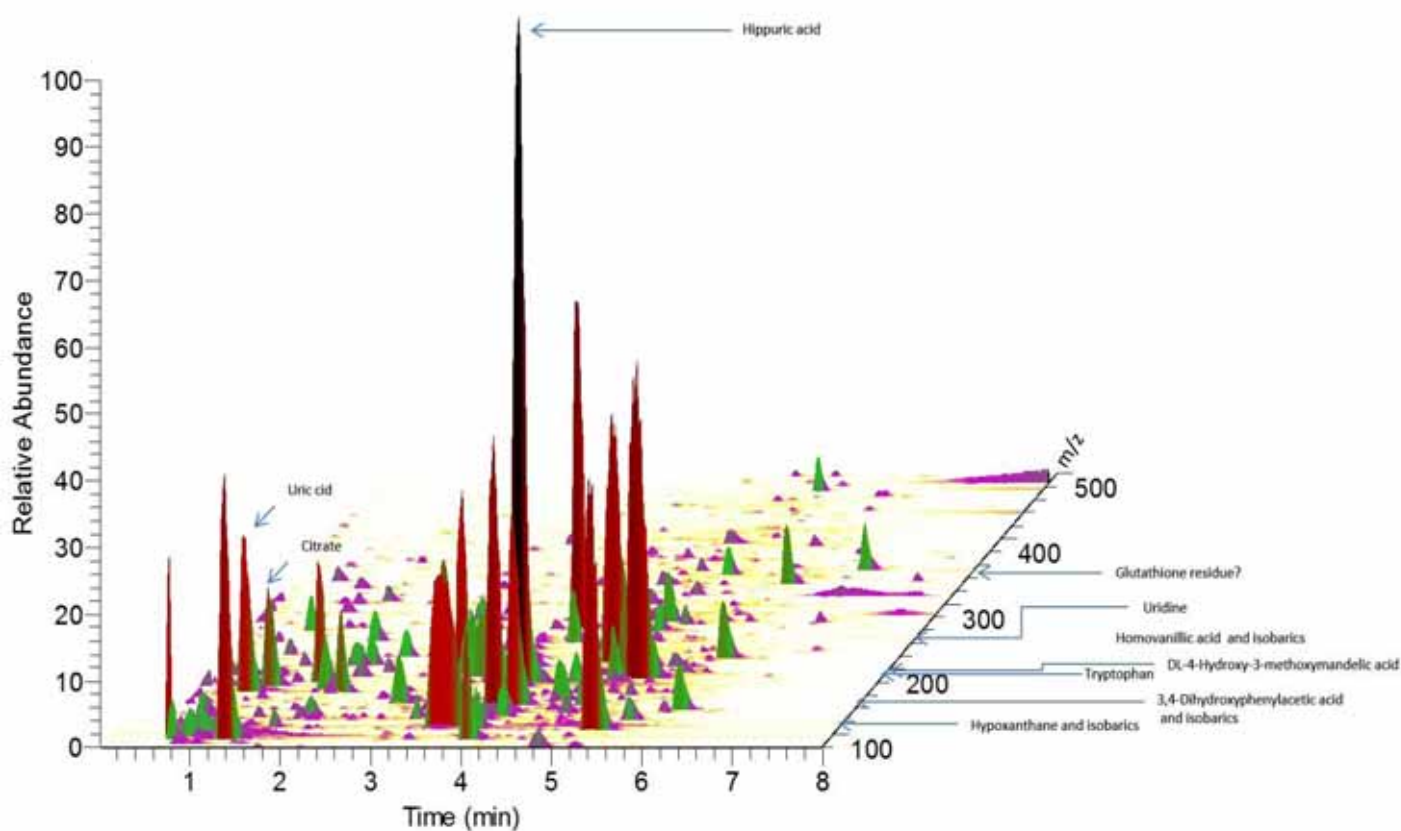
Time (mins)	%B
0.0	3
2.5	10
8.0	100
8.5	3
10.0	3

Flow Rate: 0.5 mL/min

Detection: Exactive accurate mass MS system
ESI in negative ion mode

Analytes between *m/z* 70-800 monitored

Sample: 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

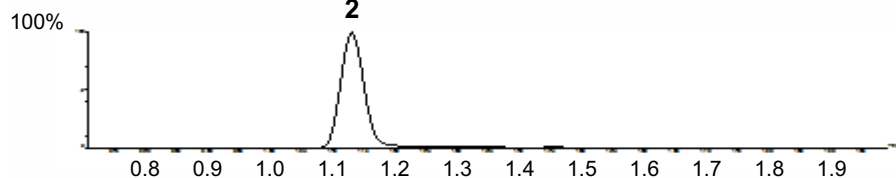
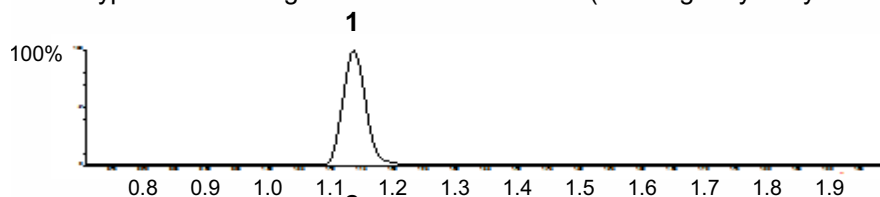
Conditions

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 H₂O
B: 0.5% Ammonium hydroxide in MeCN

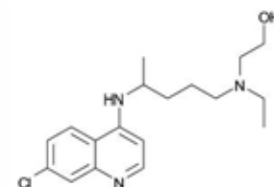
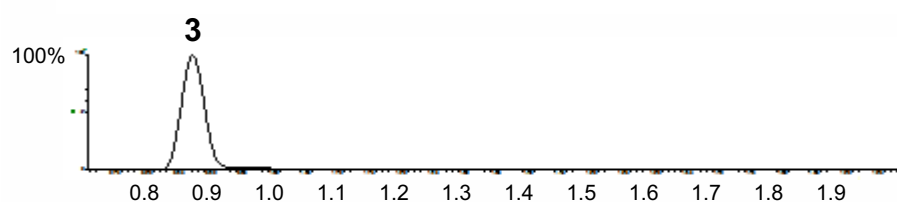
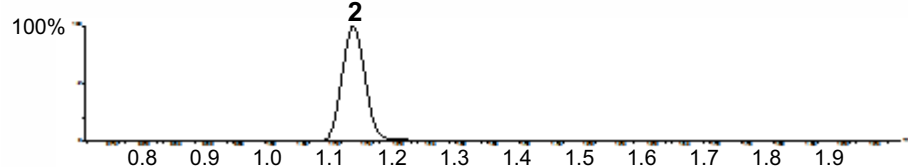
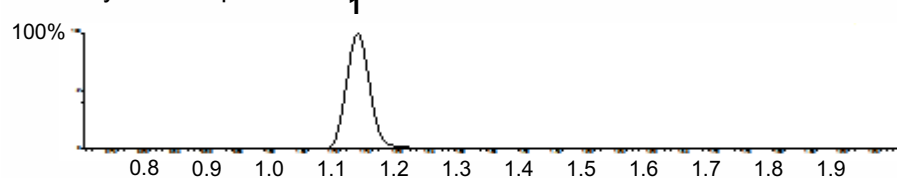
Time (mins)	%B
0.00	30
1.50	100
2.50	100
2.51	30

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

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



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



1. Hydroxychloroquine
(*m/z* 336 → 247)

2. D4-Hydroxychloroquine (IS)
(*m/z* 340 → 251)

3. Desethylhydroxychloroquine
(*m/z* 308 → 247)

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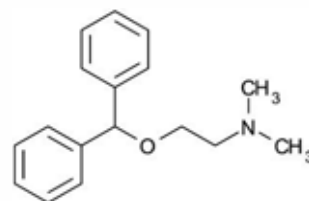
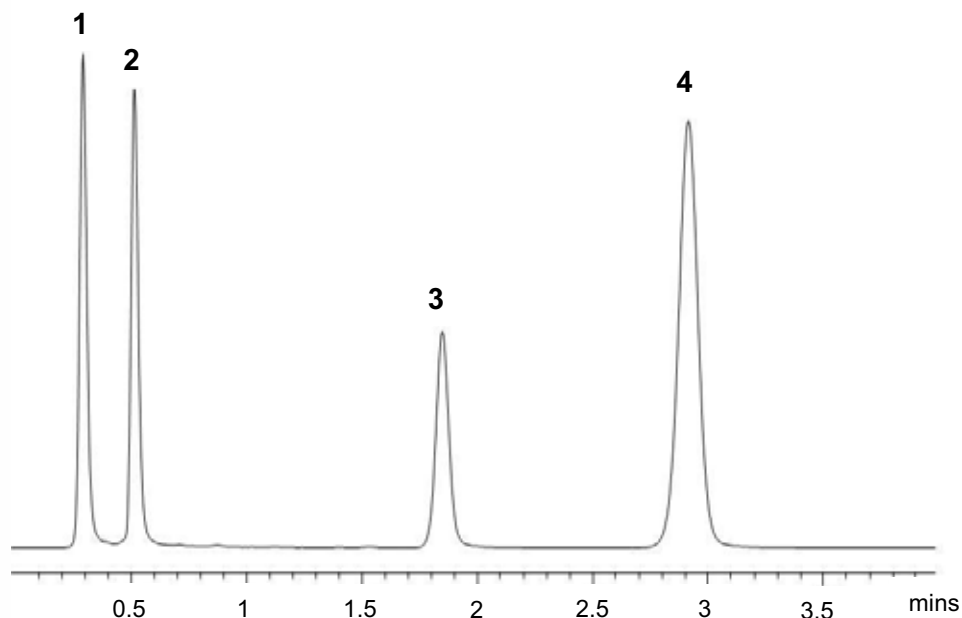
Ibuprofen in Combination with Antihistamine and Decongestant

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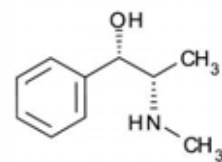
Application #AN2120

Conditions

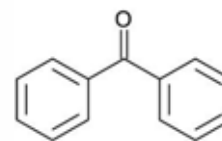
Column:	ACE Excel 3 C18-Amide
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1112-1546U
Mobile Phase:	0.01% potassium dihydrogen phosphate/MeCN (60:40 v/v)
Flow Rate:	0.6 mL/min
Injection:	0.5 µL
Temperature:	45 °C
Detection:	UV, 214 nm



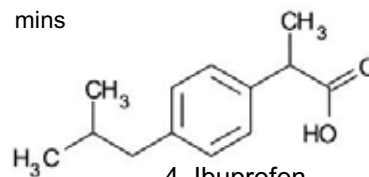
1. Diphenhydramine



2. Pseudoephedrine



3. Benzophenone



4. Ibuprofen

Insulin Analogues in Clinical and Post-Mortem Analyses

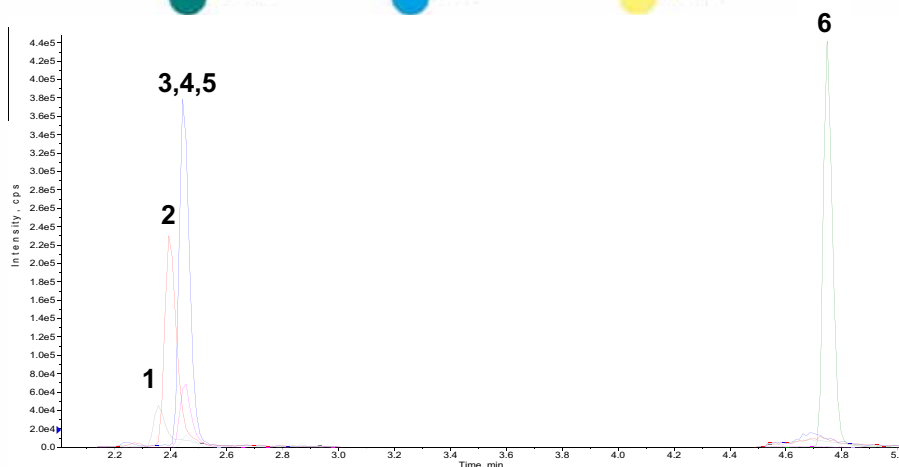
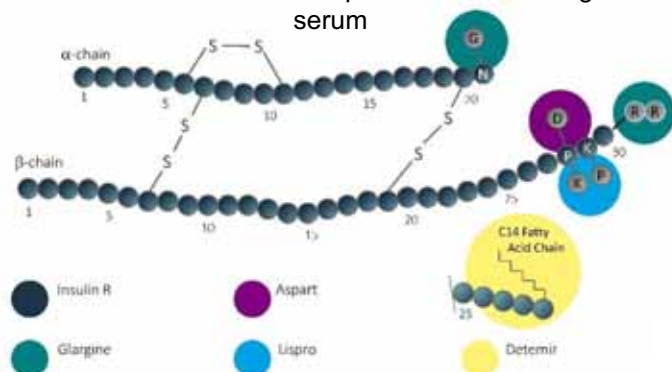
Application #AN3350

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 H₂O
B: 0.1% acetic acid in IPA/MeCN (25:75 v/v)

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



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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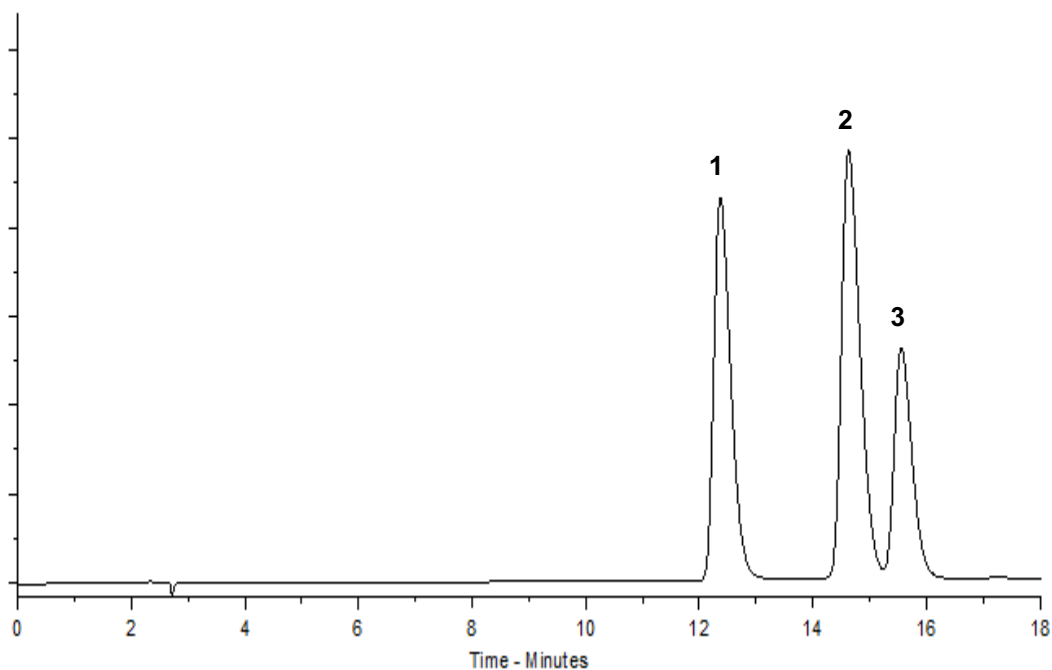


Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: A: 0.1% TFA in H₂O/MeCN (71:29 v/v)
B: 0.1% TFA in H₂O/MeCN (68:32 v/v)

Time (mins)	%B
0	10
16	90

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



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

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

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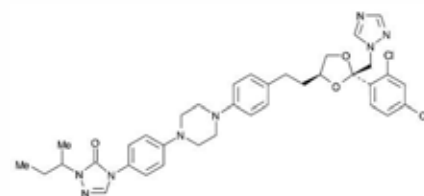
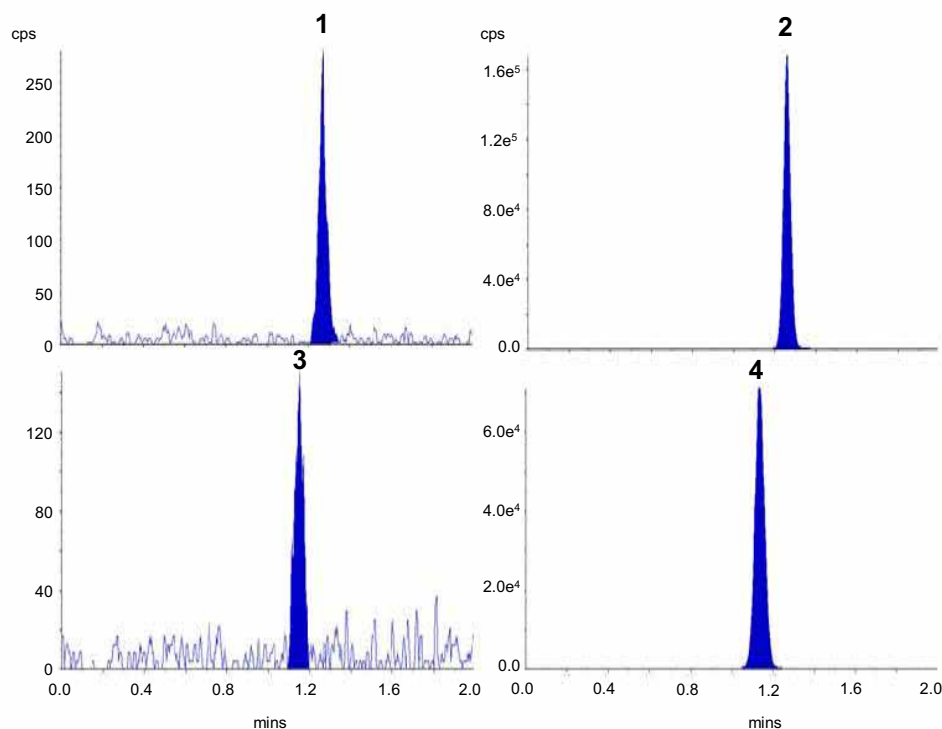
Application #AN3380

Conditions

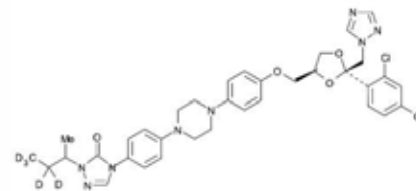
Column: ACE 3 C18-AR
Dimensions: 50 x 2.1 mm
Part Number: ACE-119-0502
Mobile Phase: A: 10 mM ammonium acetate in H₂O
B: 10 mM ammonium acetate in MeOH

Time (mins)	%B
0	75
2	98
3	98

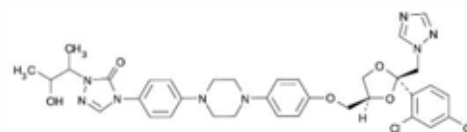
Flow Rate: 0.7 mL/min
Temperature: 45 °C
Detection: AB Sciex 4000
ESI positive ion mode
Sample: 1.0 ng/mL human whole blood (LLOQ)



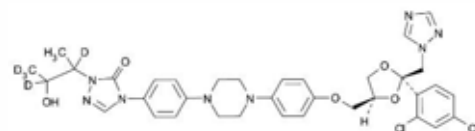
1. Itraconazole
(*m/z* 705.3 → 392.3)



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)

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

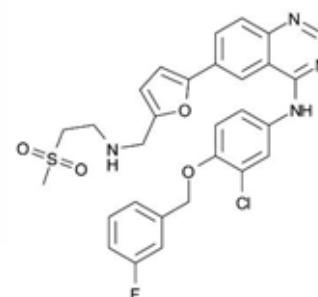
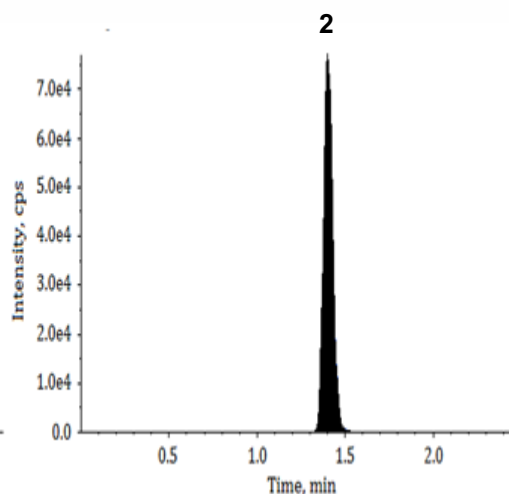
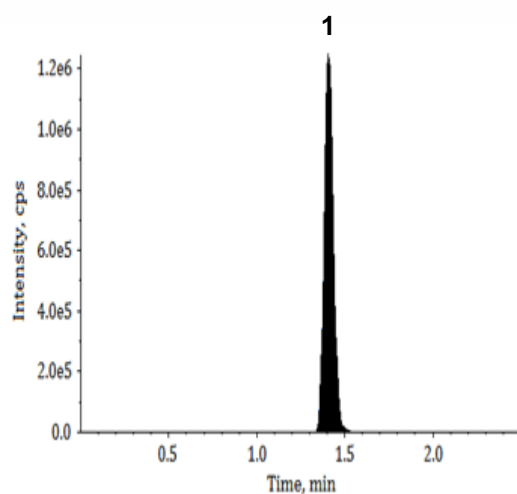
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Application #AN3360

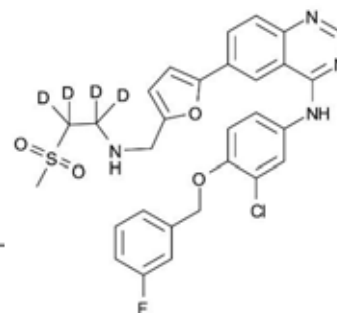
Conditions

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

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



1. Lapatinib
(m/z 581.1 $\rightarrow$ 365.2)
Concentration 1000 ng/mL



2. Lapatinib-d4 (IS)
(m/z 585.1 $\rightarrow$ 365.0)
Concentration 100 ng/mL

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Lidocaine in Saliva by LC-MS/MS

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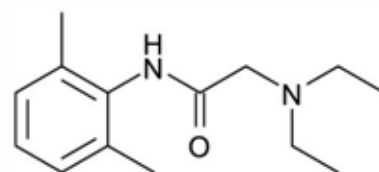
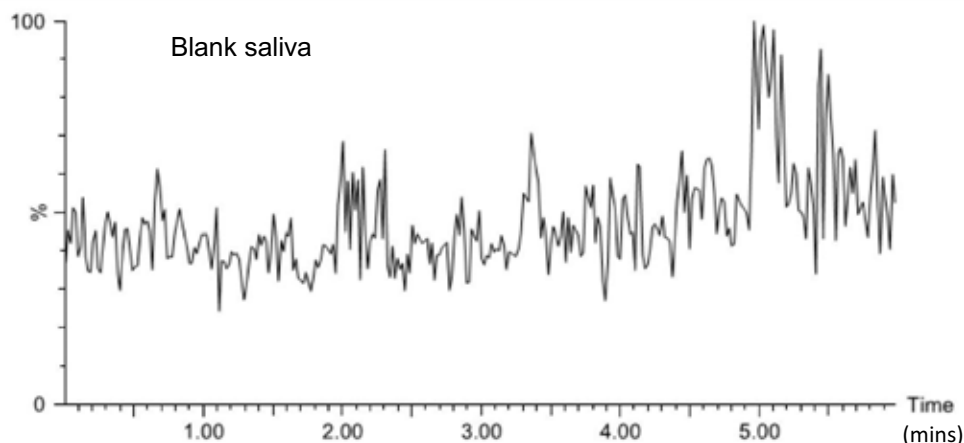
Application #AN2570

Conditions

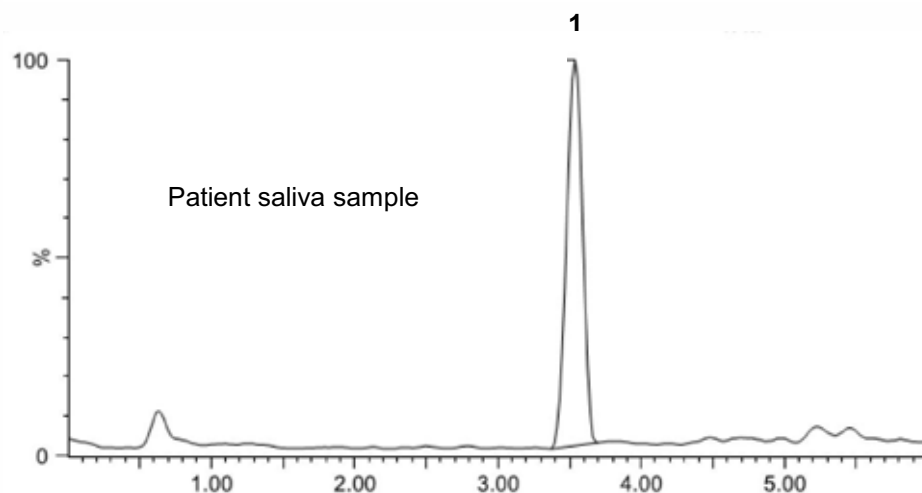
Column: ACE 3 C18
Dimensions: 100 x 3.0 mm
Part Number: ACE-111-1003
Mobile Phase: A: 0.1% formic acid in MeCN/H₂O (20:80 v/v)
B: 0.1% formic acid in MeCN/H₂O (80:20 v/v)

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: Quatro-Micro triple quad MS
Positive ion mode ESI



1. Lidocaine
(*m/z* 235 → 86)



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

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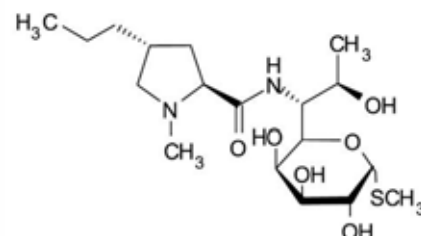
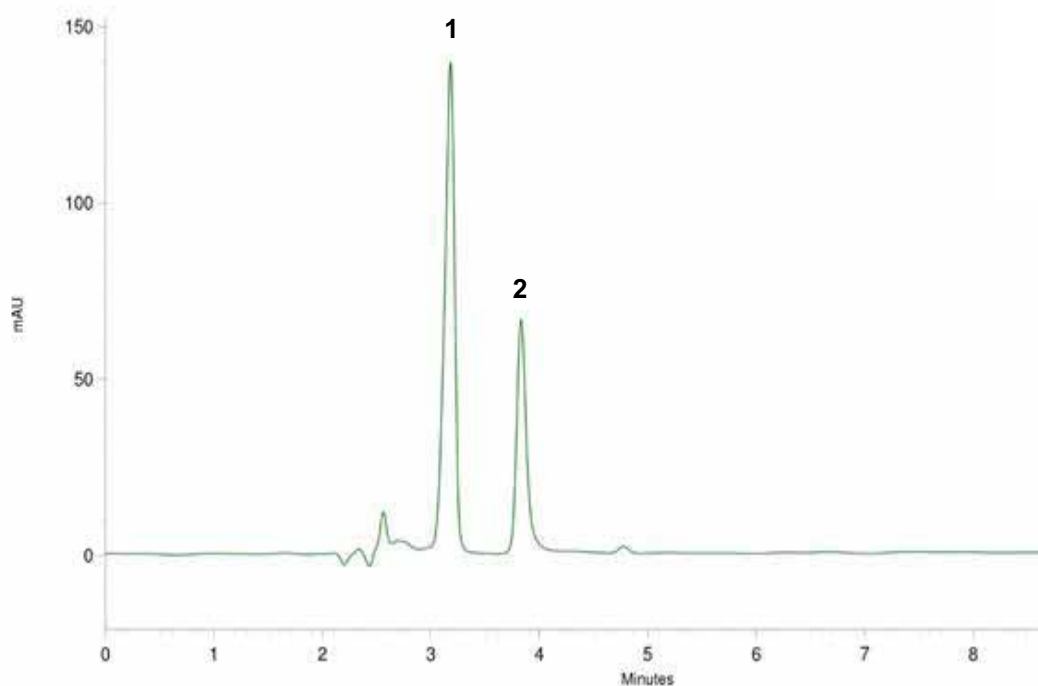
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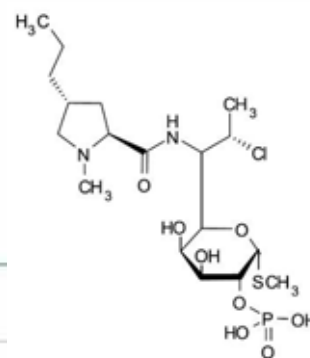
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Conditions

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



1. Lincomycin HCl



2. Clindamycin phosphate

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Lipid Classes Separation from *Drosophila Melanogaster*

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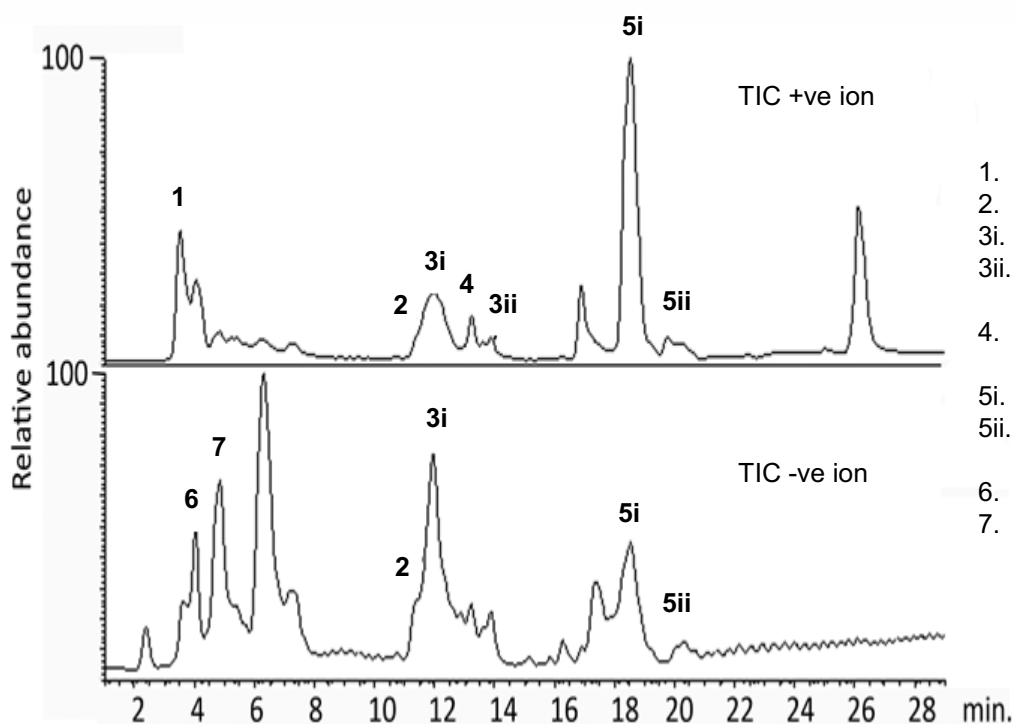
Application #AN1530

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)

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



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

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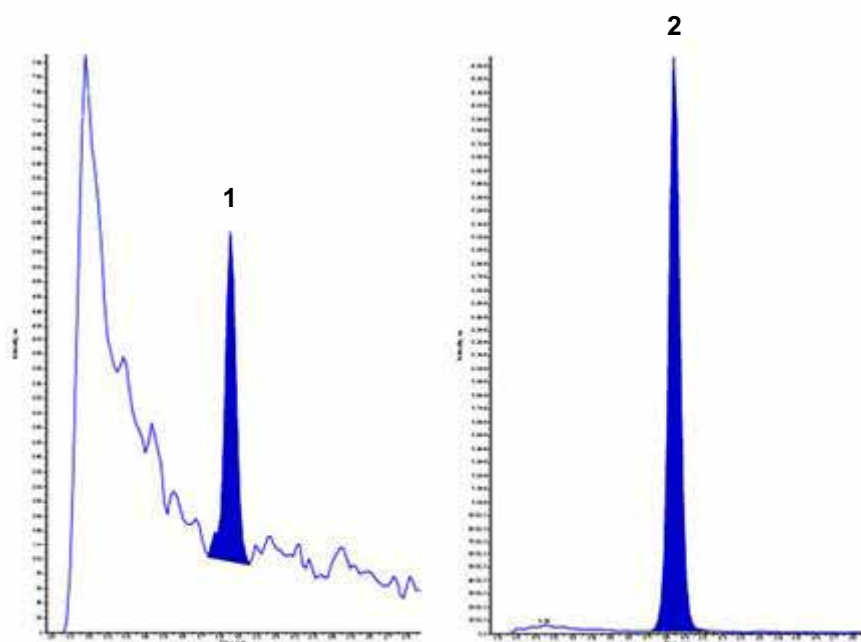
15-Hydroxy Lubiprostone in Human Plasma

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Application #AN1900

Conditions

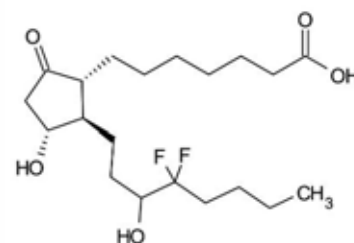
Column: ACE Excel 2 C18
Dimensions: 50 x 3.0 mm
Part Number: EXL-101-0503U
Mobile Phase: A: 0.1% formic acid in H₂O
B: MeCN
Flow Rate: 0.65 mL/min
Injection: 15 µL
Temperature: 35 °C
Detection: MDS Sciex API 5000
Turbolonspray negative mode
IonSpray voltage -4500 V
Source Temperature 450 °C



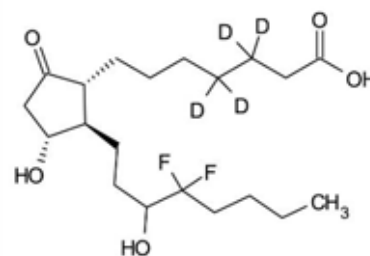
Lowest calibration standard sample containing 2.0 pg/mL in human EDTA K3 plasma.

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.



1. 15-Hydroxy lubiprostone
m/z 392.5
Transition: 391.2 → 373.2



2. 15-Hydroxy lubiprostone-d4 (IS)
m/z 396.5
Transition: 395.2 → 377.2

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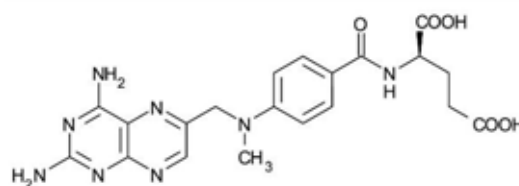
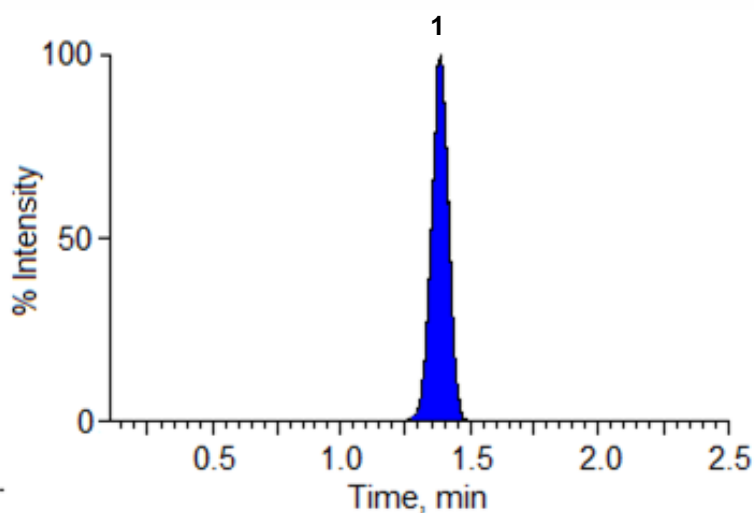
Methotrexate in K₃EDTA Human Plasma by LC-MS/MS

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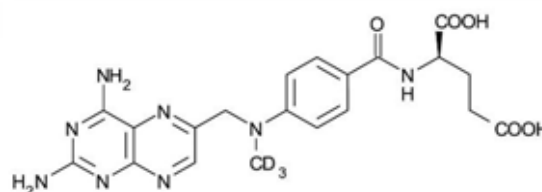
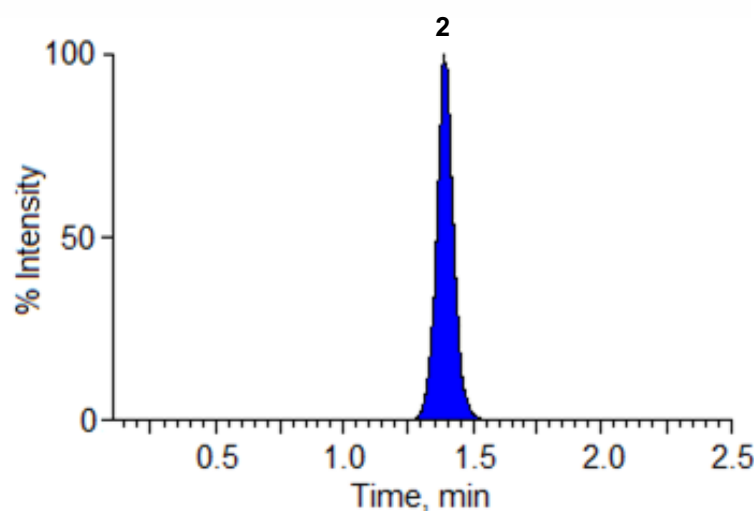
Application #AN3760

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



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)

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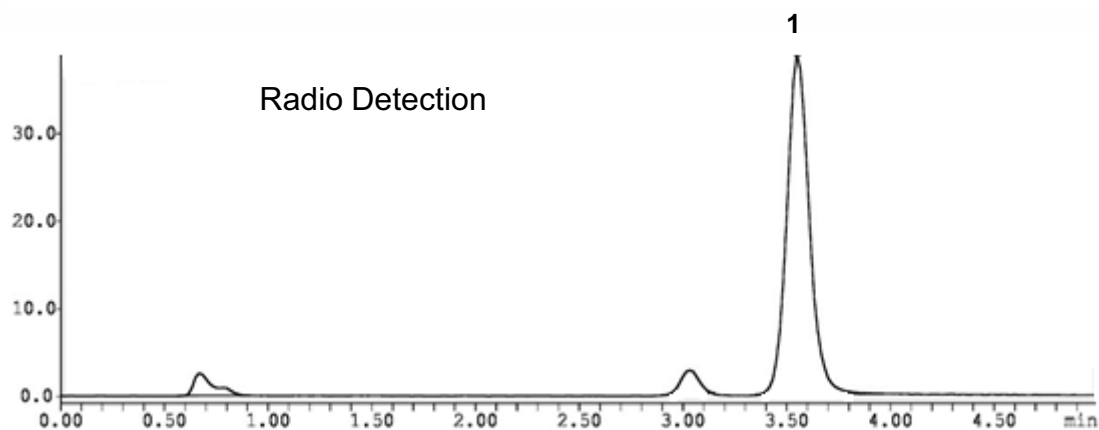
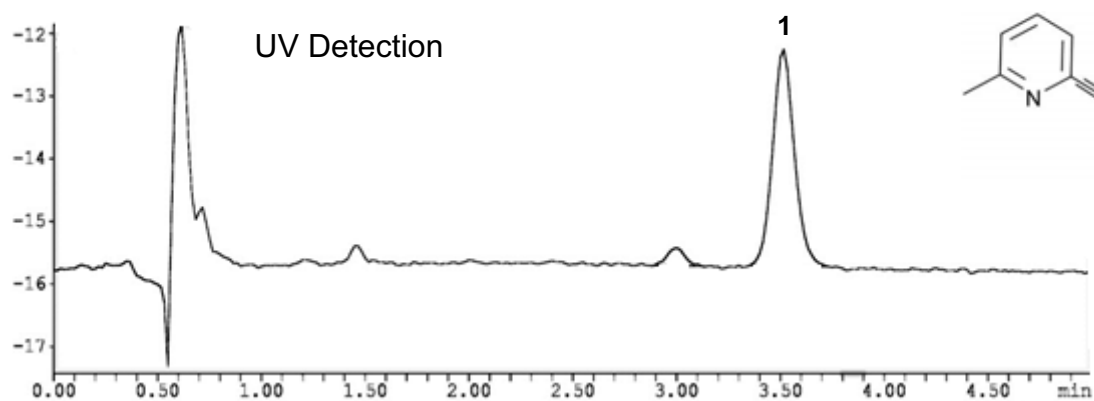
mGluR5 PET Tracer by Radio HPLC Analysis

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Application #AN2700

Conditions

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



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Non-Steroidal Anti-Inflammatory Drugs (I)

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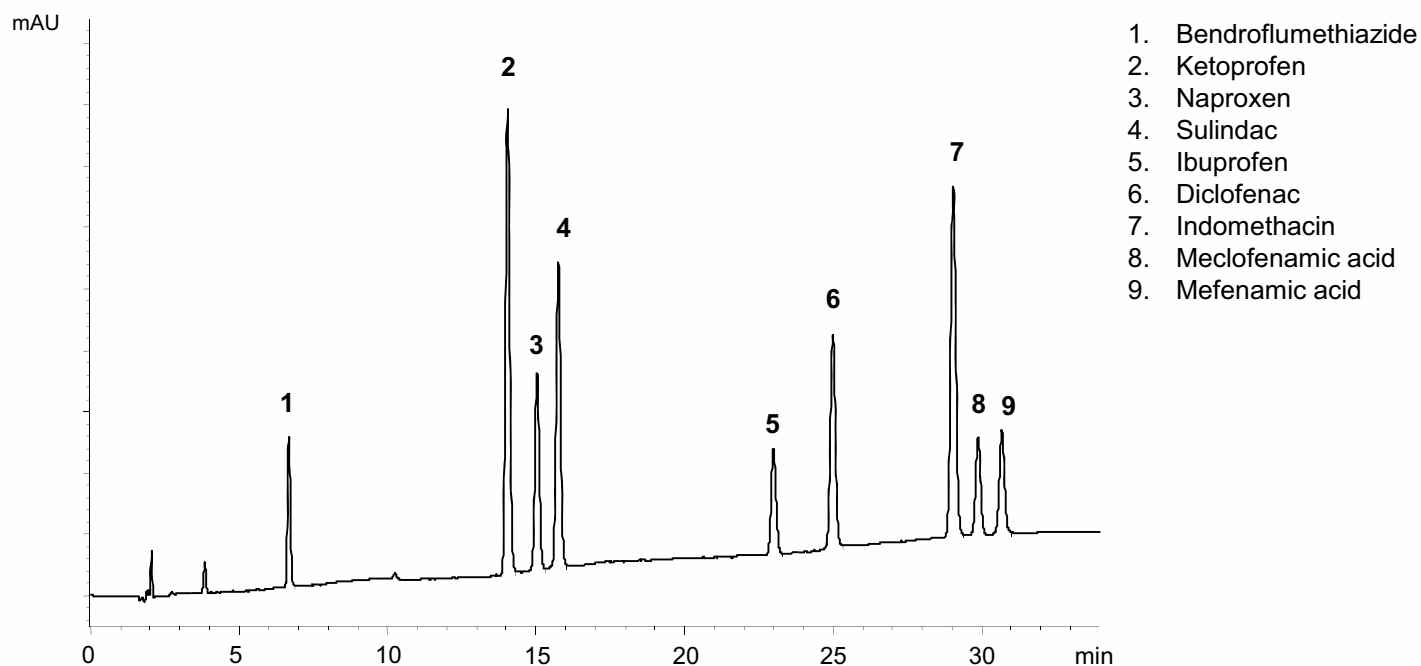
Application #AN1210

Conditions

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

Time (mins)	%B
0	52
28	74
33	74
38	52
Post time 10 minutes	

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



Non-Steroidal Anti-Inflammatory Drugs (II)

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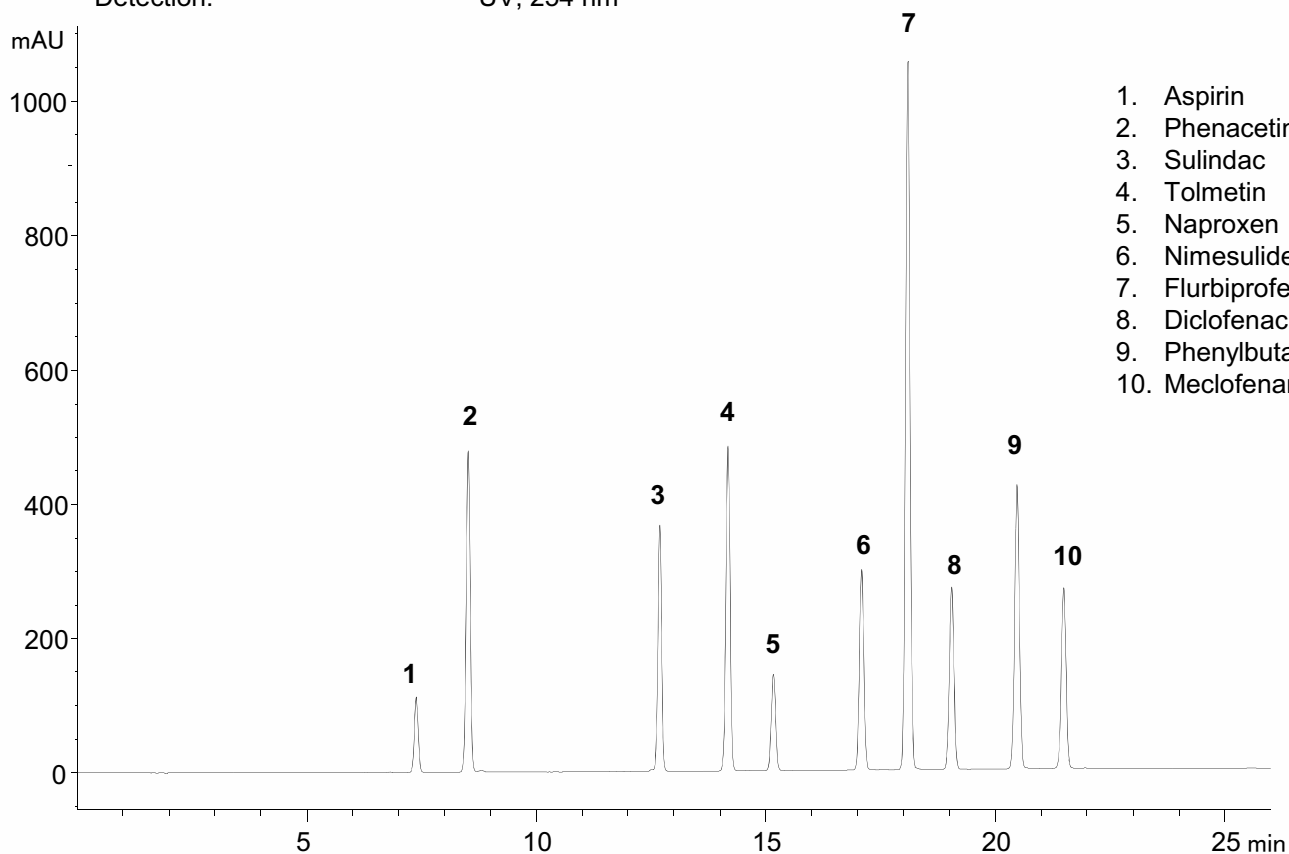
Application #AN1220

Conditions

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

Time (mins)	%B
0	20
20	70
25	70
36	20

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



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

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

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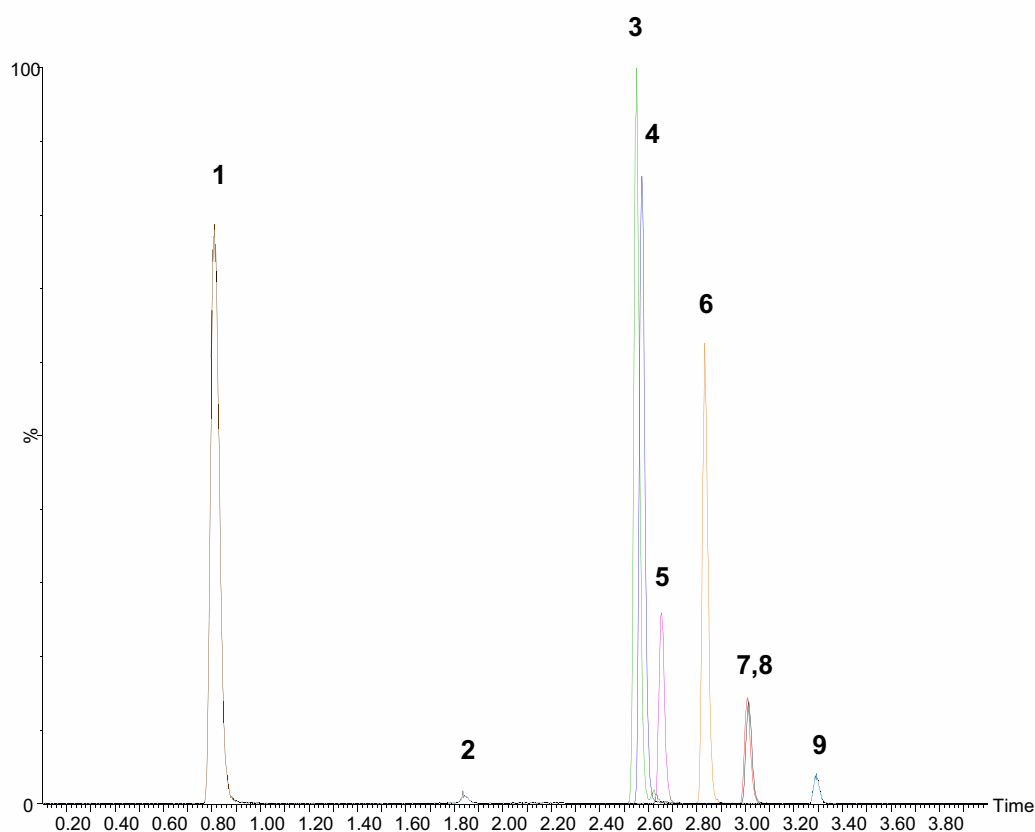
Application #AN2630

Conditions

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

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

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



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

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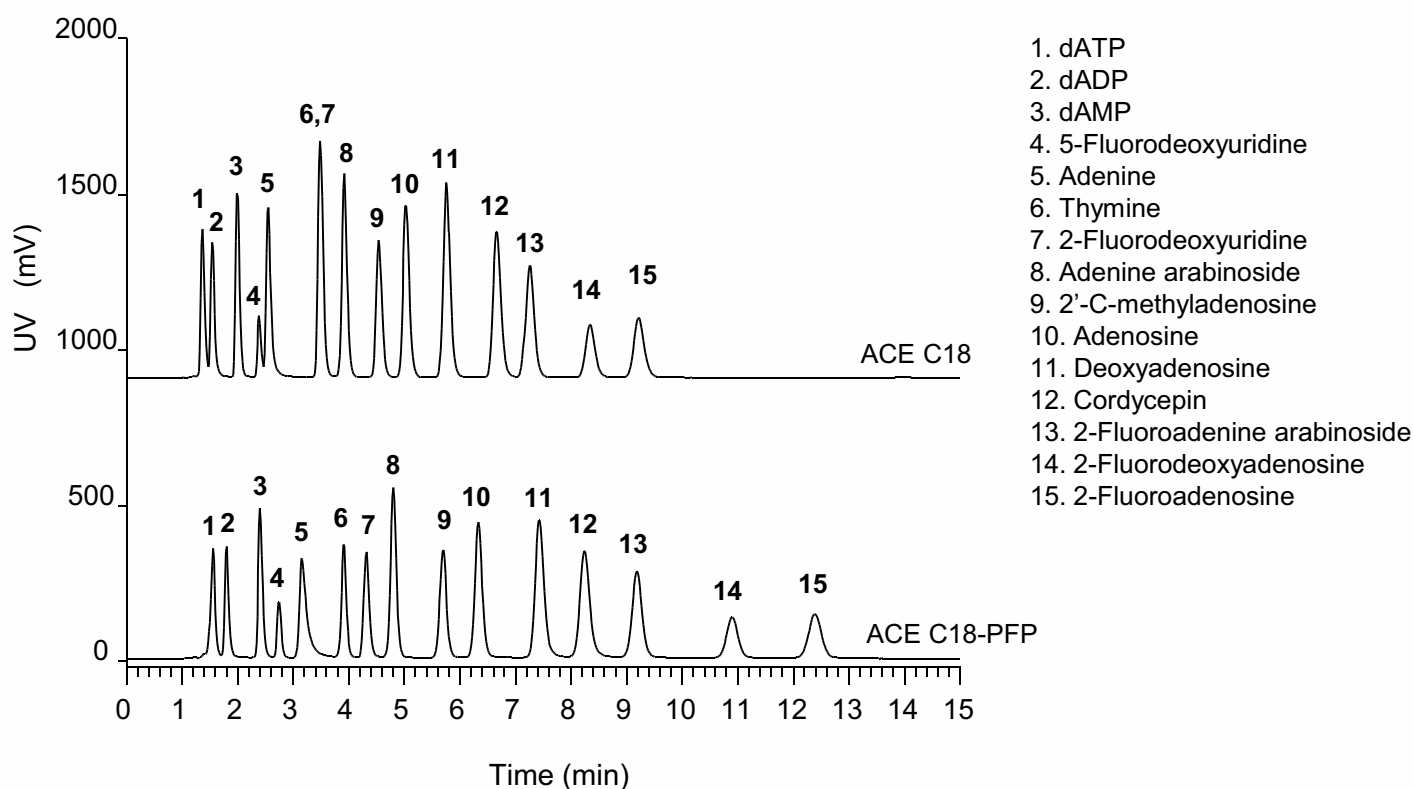
Nucleic Acids / Disease Biomarker Profiling (I)

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Application #AN1080

Conditions

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



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Nucleic Acids/ Disease Biomarker Profiling (II)

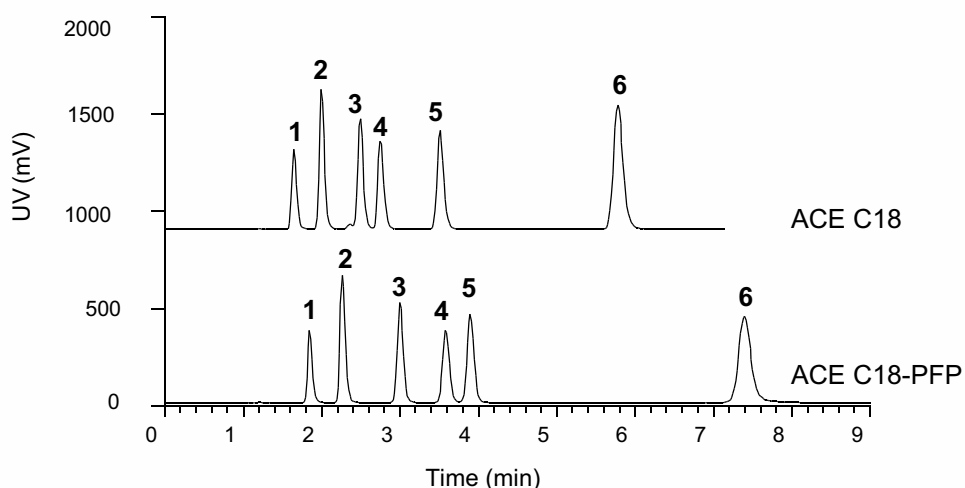
ACE[®]
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Application #AN1090

Conditions

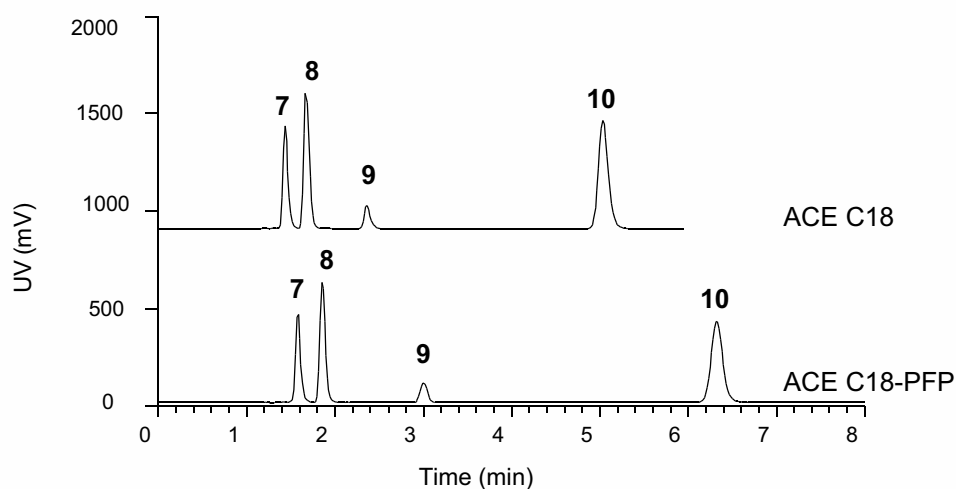
Column: ACE 3 C18-PFP
ACE 3 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-1110-1046, ACE-111-1046
Mobile Phase: 33 mM potassium phosphate pH 6.2 with KOH/MeOH (88:12 v/v)
Flow Rate: 1 mL/min
Temperature: Ambient
Detection: UV, 260 nm

Deoxyribonucleosides



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

Ribonucleosides



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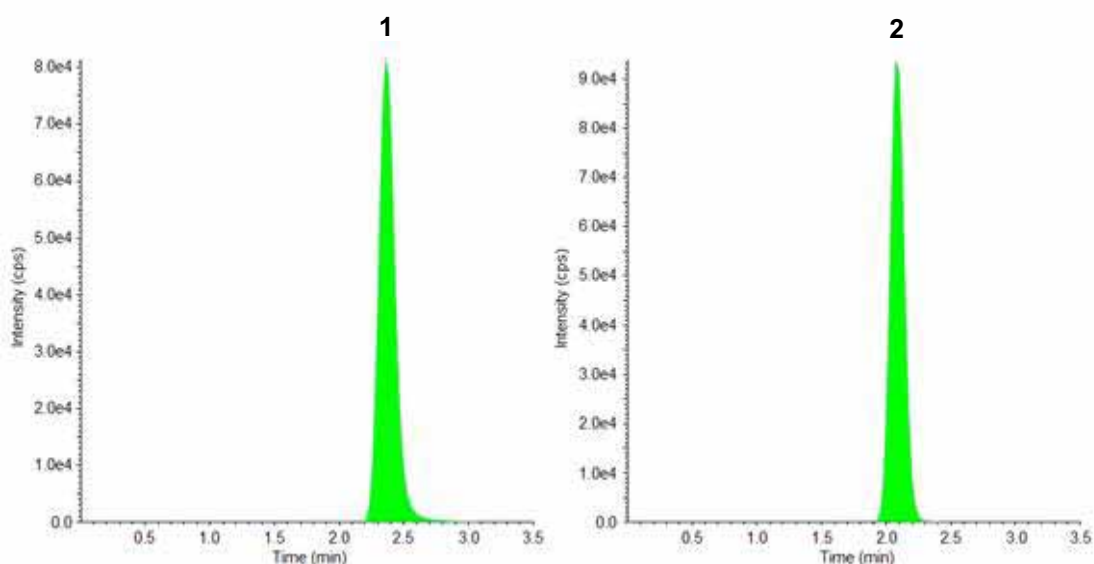
Olanzapine in Human Plasma by LC-MS/MS

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UHPLC & HPLC Columns

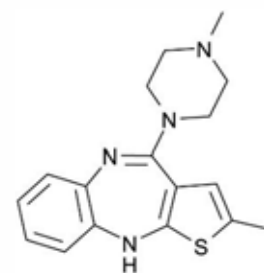
Application #AN2520

Conditions

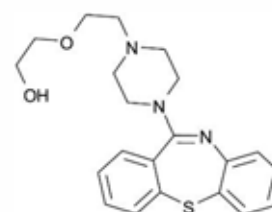
Column: ACE 5 C18-300
Dimensions: 100 x 4.6 mm
Part Number: ACE-221-1046
Mobile Phase: MeCN/0.01% ammonia in 2 mM ammonium formate pH 6.6 (85:15 v/v)
Flow Rate: 0.9 mL/min
Injection: 5 µL
Detection: API 4000 triple quad MS
Turbo Ion Spray in positive mode
Ion Spray voltage: 5500 V
Temperature: 550 °C



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



1. Olanzapine
(m/z 313.2 $\rightarrow$ 256.2)



2. Quetiapine (IS)
(m/z 384.2 $\rightarrow$ 253.2)

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Opiates In Urine by LC-MS/MS

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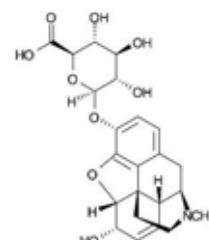
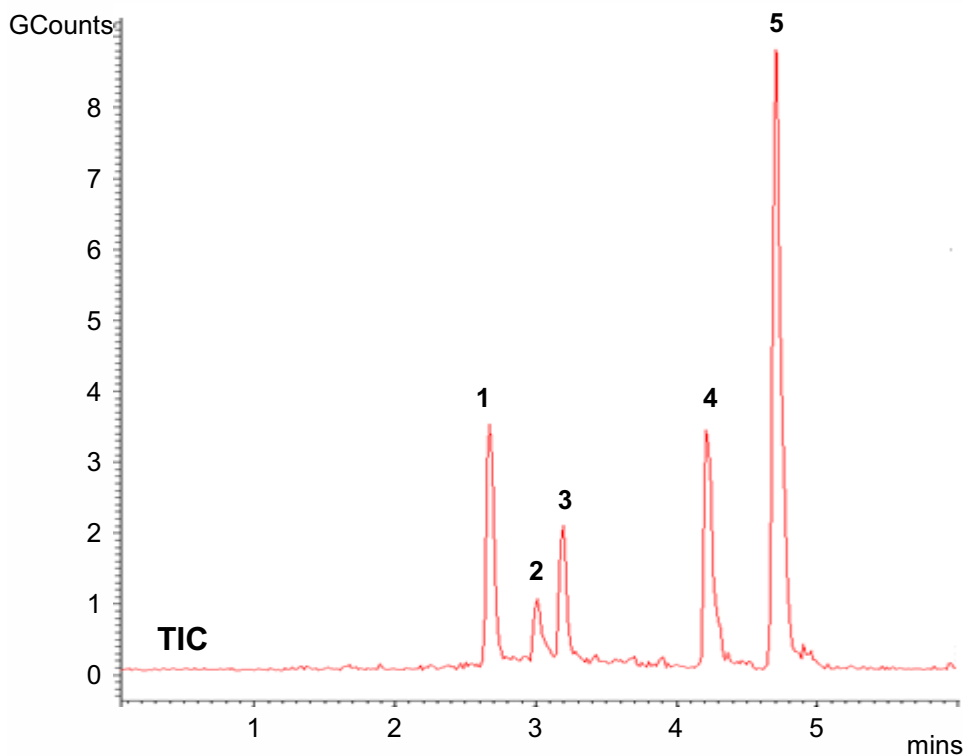
Application #AN1230

Conditions

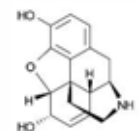
Column: ACE Excel 3 SuperC18
Dimensions: 75 x 2.1 mm
Part Number: EXL-1111-7502U
Mobile Phase: A: 5 mM ammonium hydroxide pH 10.8 in H₂O
B: 5 mM ammonium hydroxide pH 10.8 in MeOH/H₂O (90:10 v/v)

Time (mins)	%B
0	30
5	95

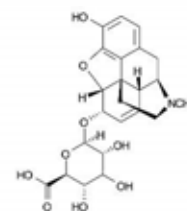
Flow Rate: 0.6 mL/min
Injection: 2 µL
Temperature: 60 °C
Detection: Varian 320 Triple Quadrupole MS
Electrospray voltage: +5 kV
Inlet capillary voltage: 30 V
CID with argon at 1.5 mTorr
Collision cell potential ranges from 5 to 17 V
Drying gas (nitrogen) temperature: 325 °C
Nebulizing gas (nitrogen)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



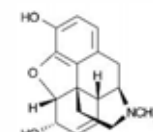
1. Morphine 3-β-D-glucuronide
LOD (est) 100 ppb
(*m/z* 462.0 → 285.9)



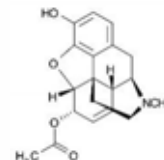
2. Normorphine
LOD (est) 100 ppb
(*m/z* 272.0 → 165.0)



3. Morphine 6-β-D-glucuronide
LOD (est) 100 ppb
(*m/z* 462.0 → 285.9)



4. Morphine
LOD (est) 20 ppb
(*m/z* 286.0 → 200.9)



5. 6-Acetylmorphine
LOD (est) 10 ppb
(*m/z* 328.0 → 164.9)

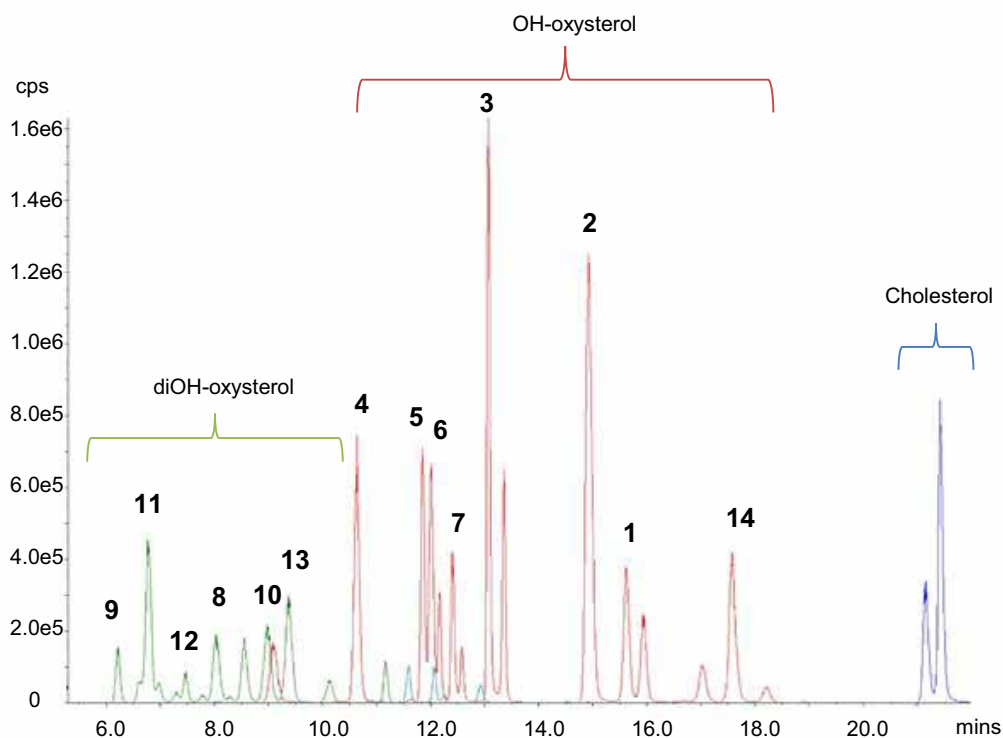


Conditions

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

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

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



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

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

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Paralytic Shellfish Poisoning (PSP) Toxins

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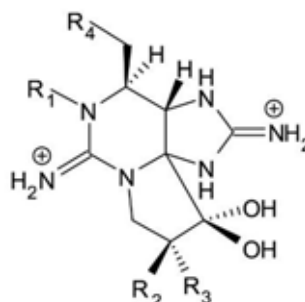
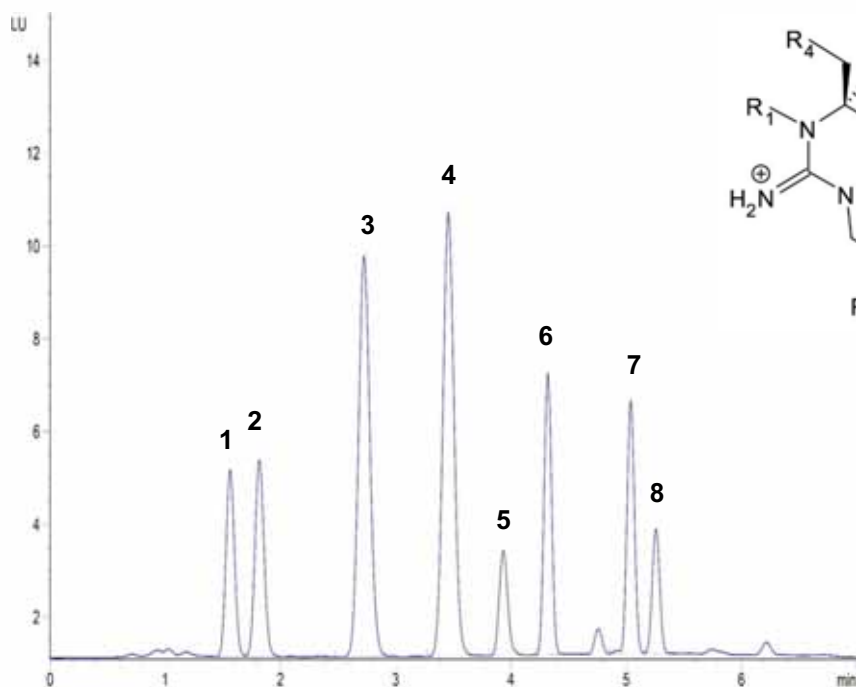
Application #AN3180

Conditions

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

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

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



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

PST Variant	R1	R2	R3	R4
STX	H	H	H	H ₂ N-COO
NEO	OH	H	H	H ₂ N-COO
GTX1	OH	H	OSO ₃ ⁻	H ₂ N-COO
GTX2	H	H	OSO ₃ ⁻	H ₂ N-COO
GTX3	H	OSO ₃ ⁻	H	H ₂ N-COO
GTX4	OH	OSO ₃ ⁻	H	H ₂ N-COO
GTX5 (B1)	H	H	H	O ₃ S-NH-COO
C1	H	H	OSO ₃ ⁻	O ₃ S-NH-COO
C2	H	OSO ₃ ⁻	H	O ₃ S-NH-COO
dcSTX	H	H	H	OH
dcNEO	OH	H	H	OH
dcGTX1	OH	H	OSO ₃ ⁻	OH
dcGTX2	H	H	OSO ₃ ⁻	OH
dcGTX3	H	OSO ₃ ⁻	H	OH

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Peptides – Selectivity Changes with Bonded Phase and Mobile Phase

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Application #AN3430

Conditions

Column: ACE 5 C18-300; ACE 5 C8-300; ACE 5 C4-300; ACE 5 Phenyl-300; ACE 5 CN-300

Dimensions: 250 x 4.6 mm

Part Number: ACE-221-2546, ACE-222-2546, ACE-223-2546, ACE-225-2546, ACE-224-2546

Mobile Phase: A: 0.1% TFA or 0.1% formic acid in H₂O

B: MeCN

Time (mins) %B

0 10

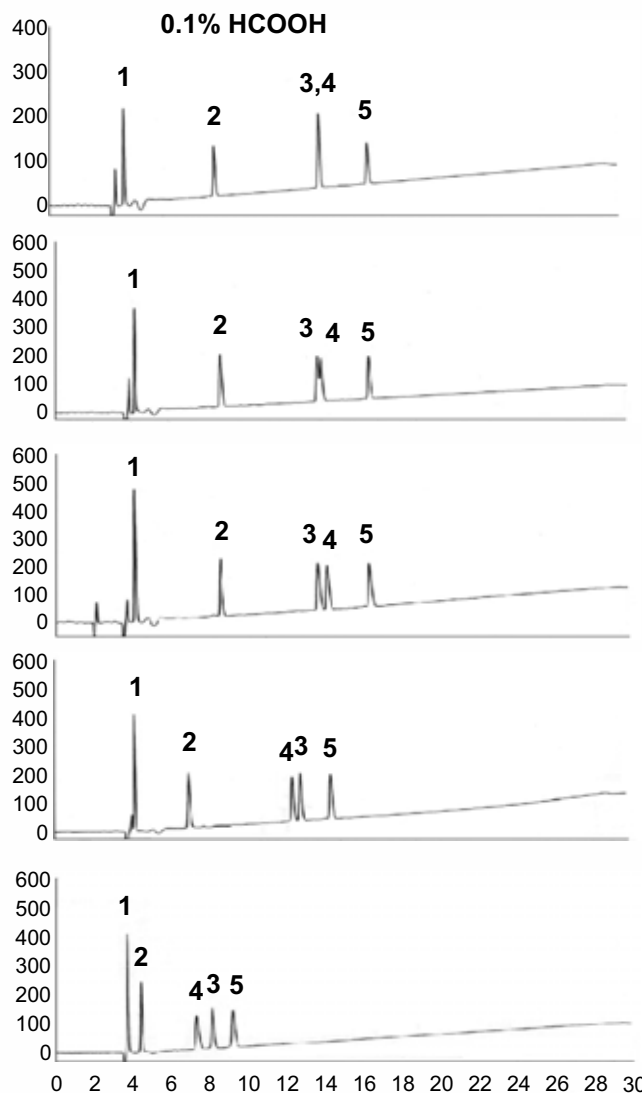
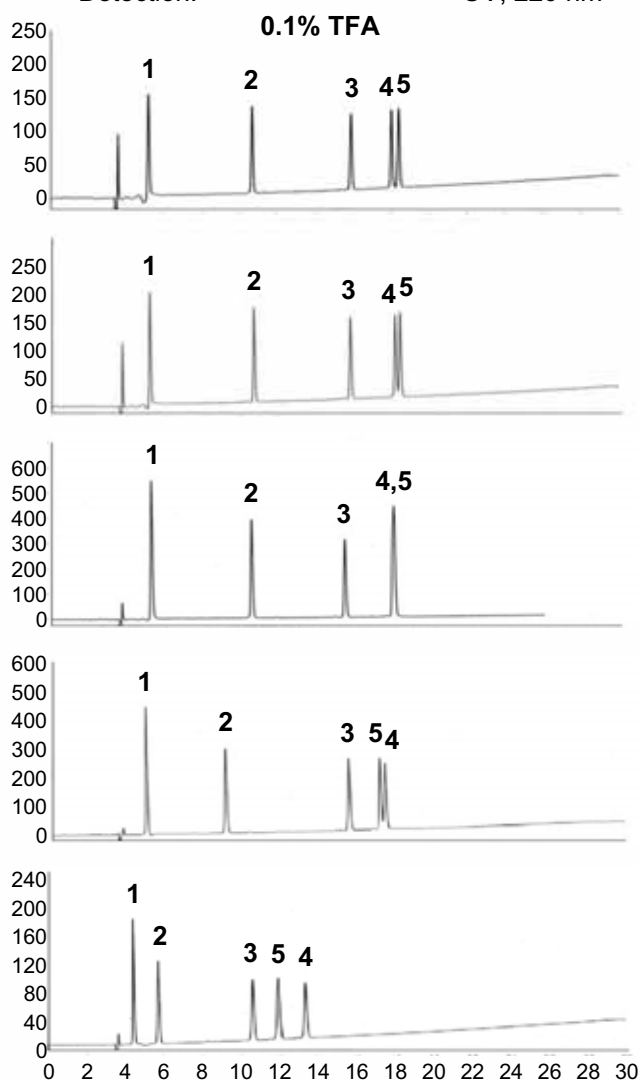
25 40

Flow Rate: 1 mL/min

Temperature: Ambient

Detection: UV, 220 nm

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



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Phosphatidylethanol Biomarker Analysis by UHPLC-MS/MS

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Application #AN3400

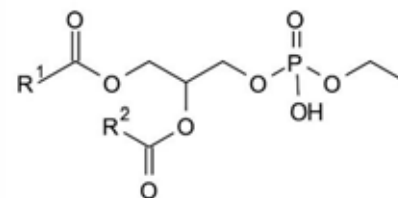
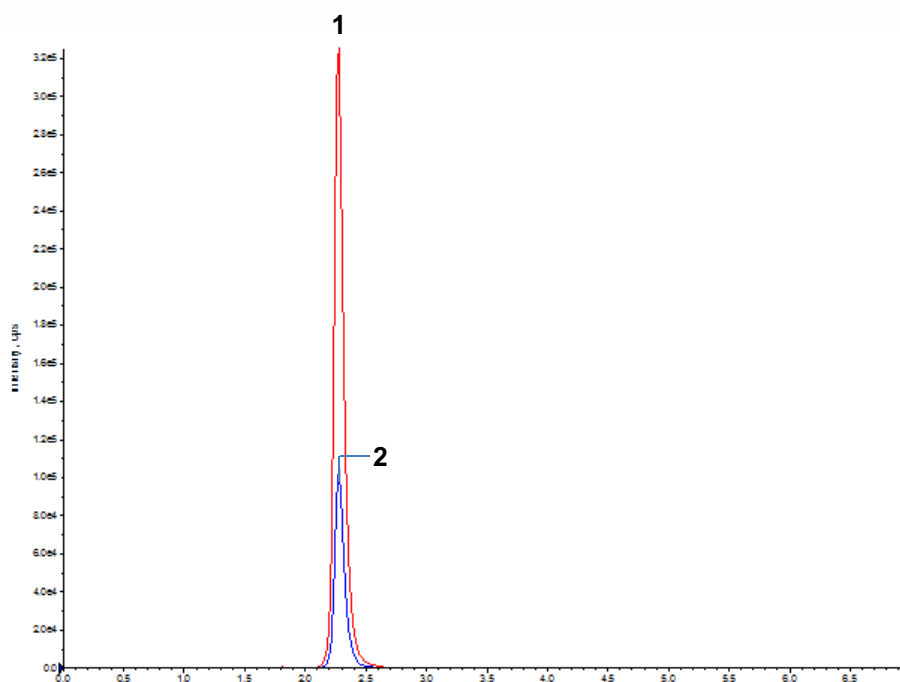
Conditions

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

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

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

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



Phosphatidylethanol

1. R1/R2 = 18:1/18:1
(m/z 701.4 → 281.2)

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

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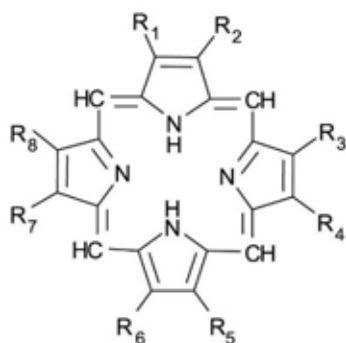
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Conditions

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

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

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



Where:

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

1. Uroporphyrin I
(R₁:A, R₂:P, R₃:A, R₄:P, R₅:A, R₆:P, R₇:A, R₈:P)
(m/z 831 → 727, 623, 655)

2. 7-Carboxyporphyrin I
(R₁:A, R₂:P, R₃:A, R₄:P, R₅:A, R₆:P, R₇:M, R₈:P)
(m/z 787 → 683, 670, 623)

3. 6-Carboxyporphyrin I
(R₁:M, R₂:P, R₃:A, R₄:P, R₅:A, R₆:P, R₇:M, R₈:P)
(m/z 743 → 639, 507, 521)

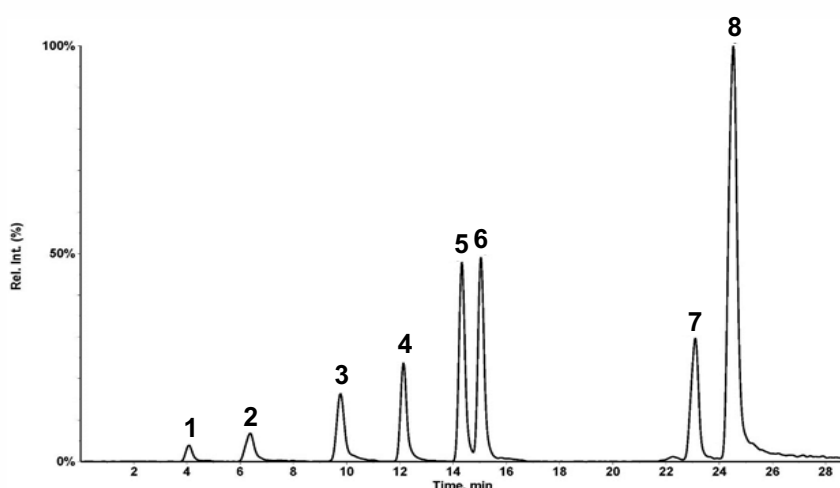
4. 5-Carboxyporphyrin I
(R₁:M, R₂:P, R₃:M, R₄:P, R₅:A, R₆:P, R₇:M, R₈:P)
(m/z 699 → 463, 595, 640)

5. Coproporphyrin I
(R₁:M, R₂:P, R₃:M, R₄:P, R₅:M, R₆:P, R₇:M, R₈:P)
(m/z 655 → 537, 596, 523)

6. Coproporphyrin III
(R₁:M, R₂:P, R₃:M, R₄:P, R₅:M, R₆:P, R₇:P, R₈:M)
(m/z 655 → 537, 596, 523)

7. Mesoporphyrin IX
(R₁:M, R₂:E, R₃:M, R₄:E, R₅:M, R₆:P, R₇:M, R₈:P)
(m/z 567 → 449, 479, 508)

8. Protoporphyrin IX
(R₁:M, R₂:V, R₃:M, R₄:V, R₅:M, R₆:P, R₇:P, R₈:M)
(m/z 563 → 445, 504, 489)



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

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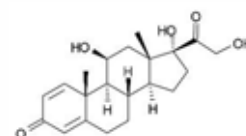
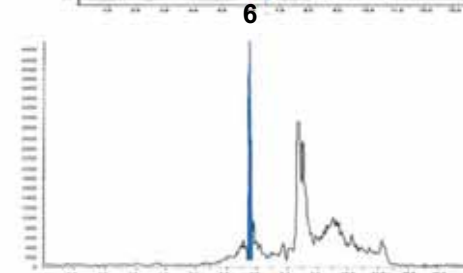
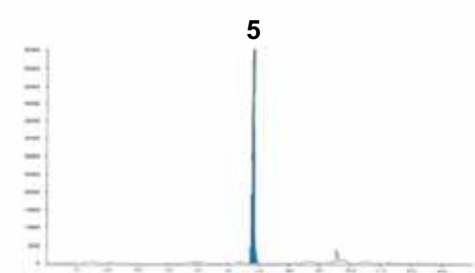
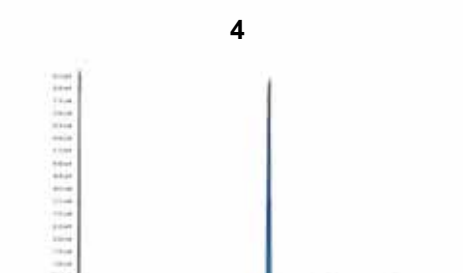
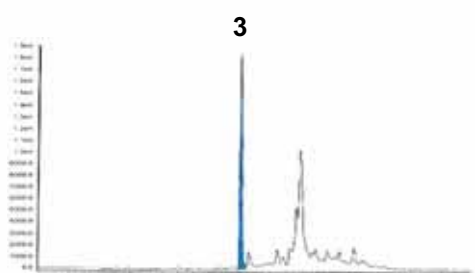
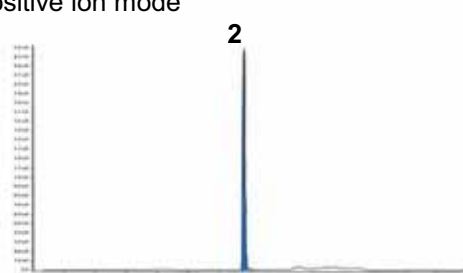
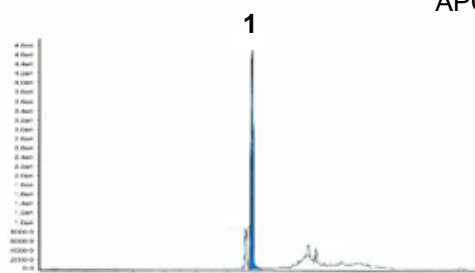
Application #AN2690

Conditions

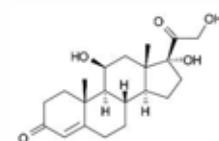
Column: ACE Excel 2 C18
Dimensions: 100 x 2.1 mm
Part Number: EXL-101-1002U
Mobile Phase: A: 4 mM ammonium acetate in H₂O
B: 0.2% (v/v) formic acid in MeOH

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

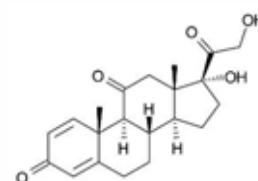
Flow Rate: 0.2 mL/min
Injection: 50 µL
Temperature: 50 °C
Detection: Applied Biosystems 5000 MS/MS
APCI in positive ion mode



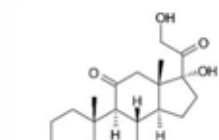
1. Prednisolone
(*m/z* 361.5 → 147.1)



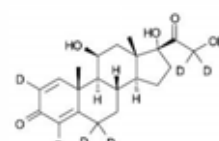
2. Cortisol
(*m/z* 363.5 → 121.3)



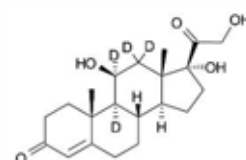
3. Prednisone
(*m/z* 359.4 → 147.1)



4. Cortisone
(*m/z* 361.5 → 163.3)



5. Prednisolone-d6 (IS)
(*m/z* 367.4 → 150.3)



6. Cortisol-d4 (IS)
(*m/z* 367.3 → 331.3)

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Pristinamycin Components in Plasma by LC-MS/MS

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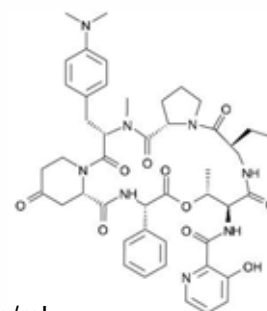
Application #AN1360

Conditions

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

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

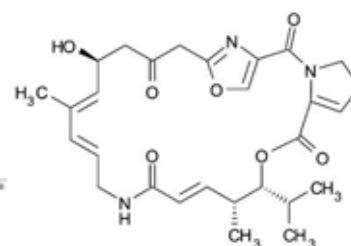
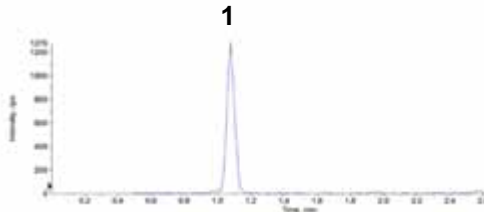
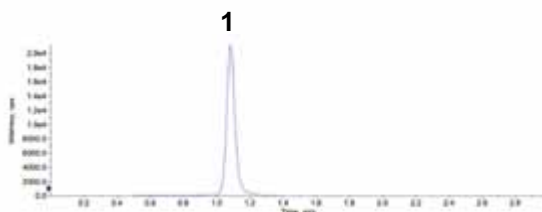
Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: 25 °C
Detection: MDS Sciex API 4000
Turbolonspray positive mode



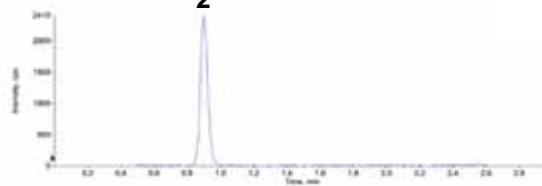
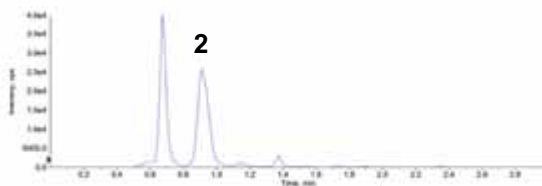
Processed study sample containing pristinamycin IA and IIA

Low calibration standard containing 2.5 ng/mL each of pristinamycin IA and IIA in human NaF/K₂C₂O₄ plasma

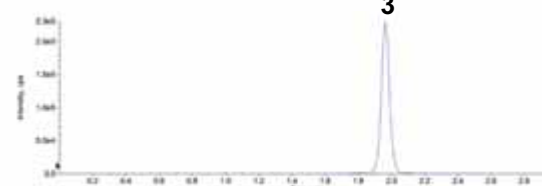
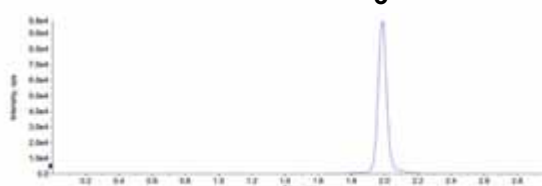
1. Pristinamycin IA
(*m/z* 867.5 → 134.2)



2. Pristinamycin IIA
(*m/z* 526.3 → 355.1)



3. Virginiamycin (IS)
(*m/z* 824.6 → 134.0)



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Prostaglandins using LC-MS/MS

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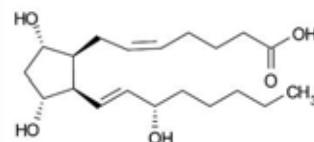
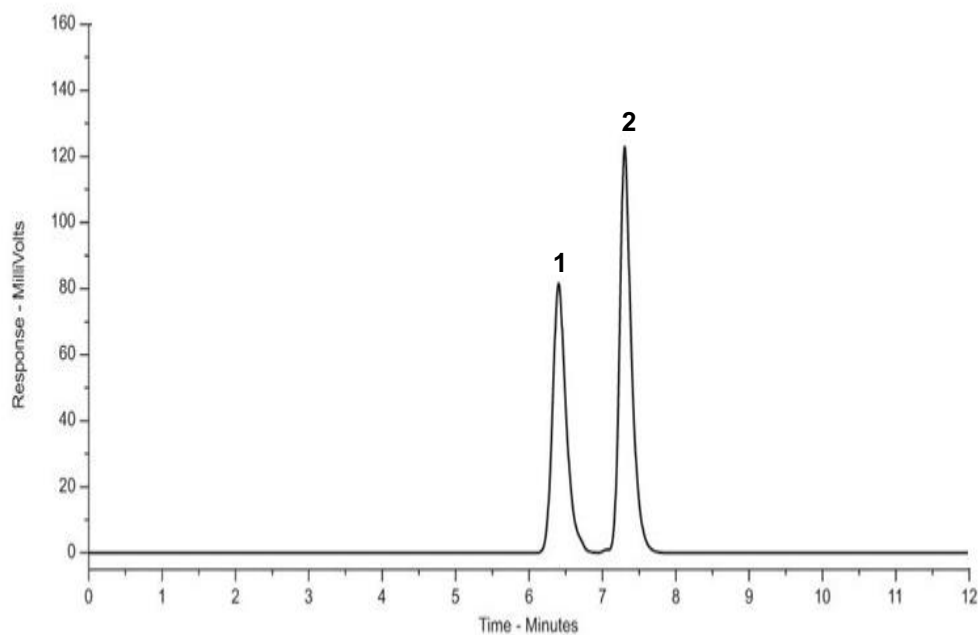
Application #AN3260

Conditions

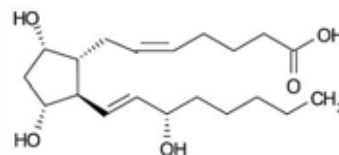
Column: ACE 3 C18
Dimensions: 50 x 2.1 mm
Part Number: ACE-111-0502
Mobile Phase:
A: H₂O
B: MeOH
C: MeCN

Time (mins)	%A	%B	%C
0	70	20	10
9	10	60	30
10	0.1	66.6	33.3

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



1. 8-iso-Prostaglandin F_{2α}



2. Prostaglandin F_{2α}

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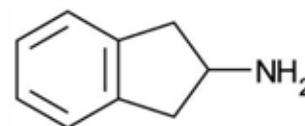
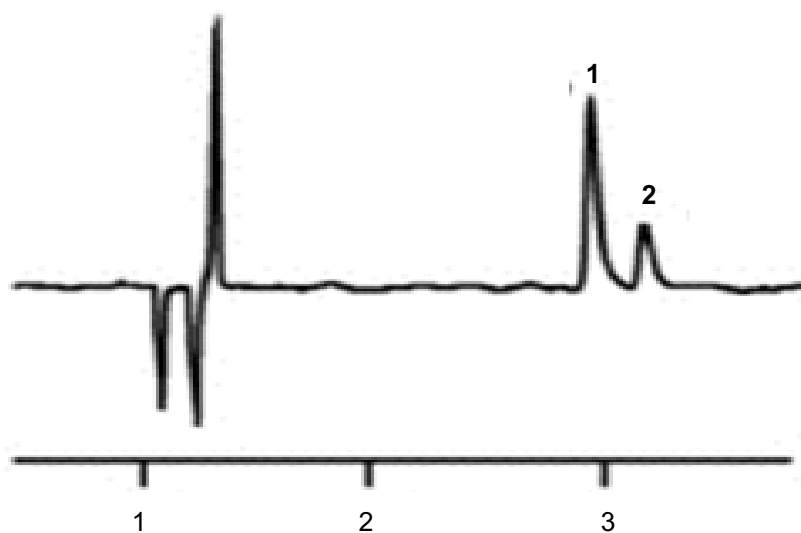
Psychoactive Substances in 'Synthacaine' by LC-UV

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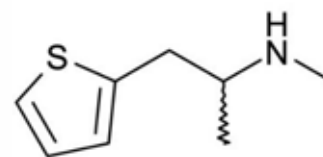
Application #AN3440

Conditions

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



1. 2-Aminoindane
LOD 0.83 µg/mL



2. Methiopropamine
LOD 0.31 µg/mL

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

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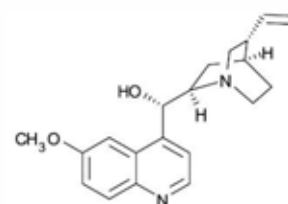
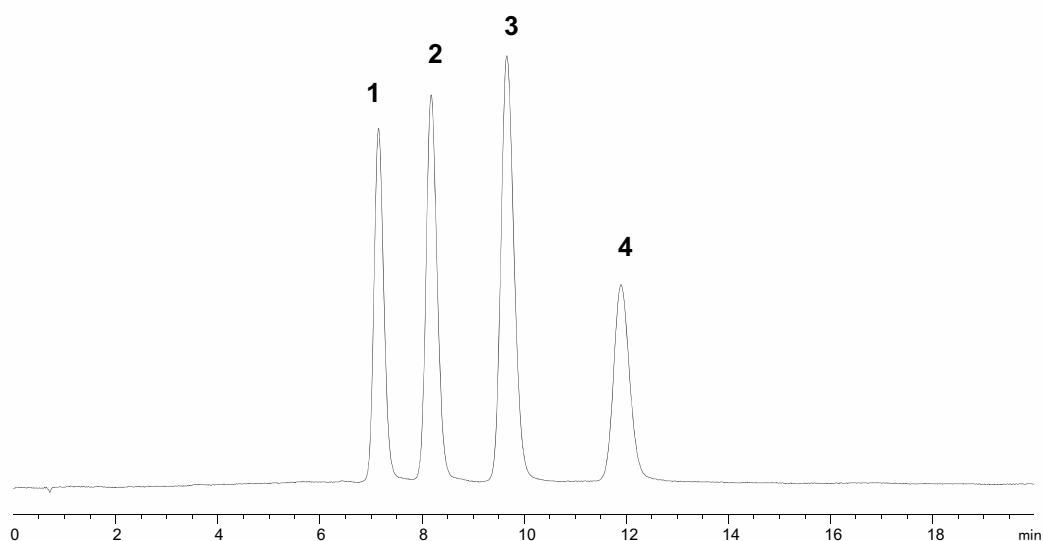
Quinidine, Quinine and their Hydroderivatives Separation

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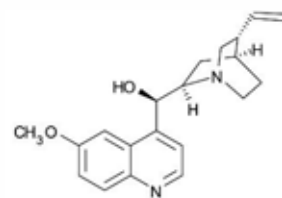
Application #AN1600

Conditions

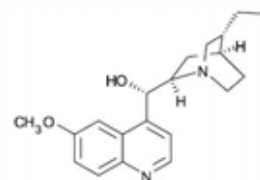
Column: ACE 3 C18-AR
Dimensions: 50 x 4.6 mm
Part Number: ACE-119-0546
Mobile Phase: 20 mM ammonium formate pH 3.0 in MeOH/H₂O (30:70 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: 30 °C
Detection: UV, 254 nm



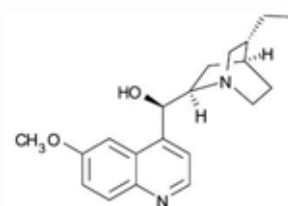
1. Quinidine



2. Quinine



3. Hydroquinidine



4. Hydroquinine

Ranitidine Hydrochloride and Related Impurities

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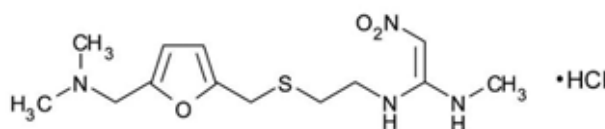
Application #AN3450

Conditions

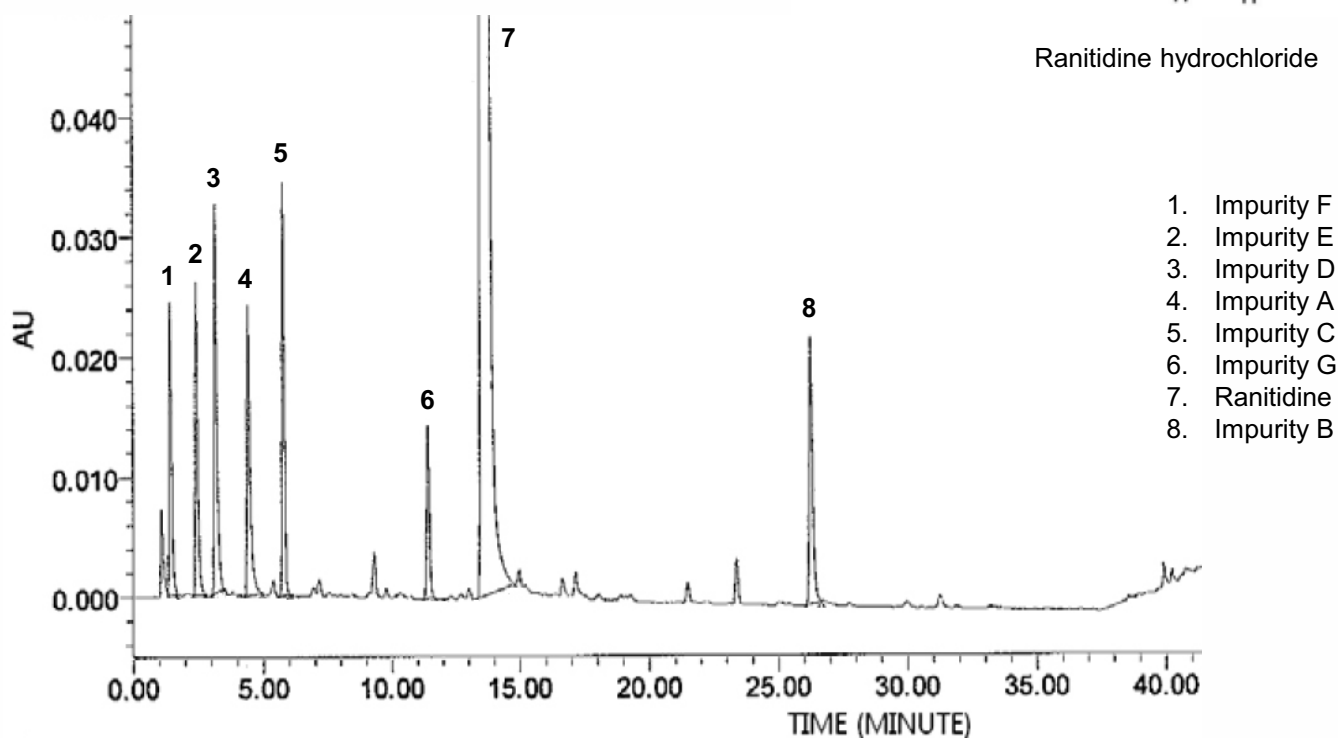
Column: ACE 3 C18
Dimensions: 100 x 4.6 mm
Part Number: ACE-111-1046
Mobile Phase: A: 0.05 M KH₂PO₄ pH 6.5 in H₂O/MeCN (98:2 v/v)
B: H₂O/MeCN (5:95 v/v)

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

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



Ranitidine hydrochloride



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

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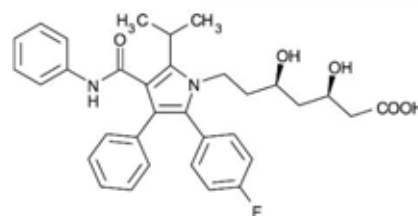
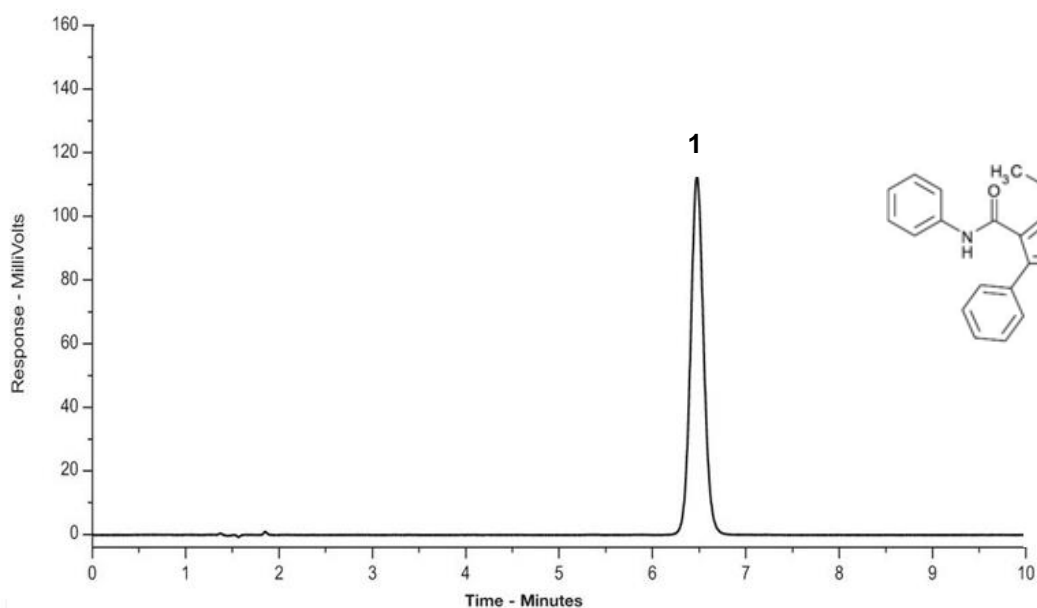
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Conditions

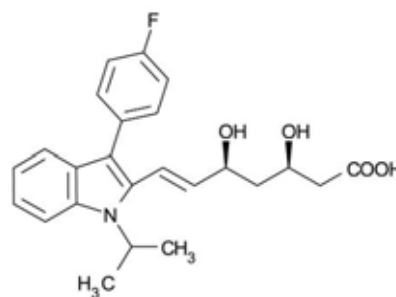
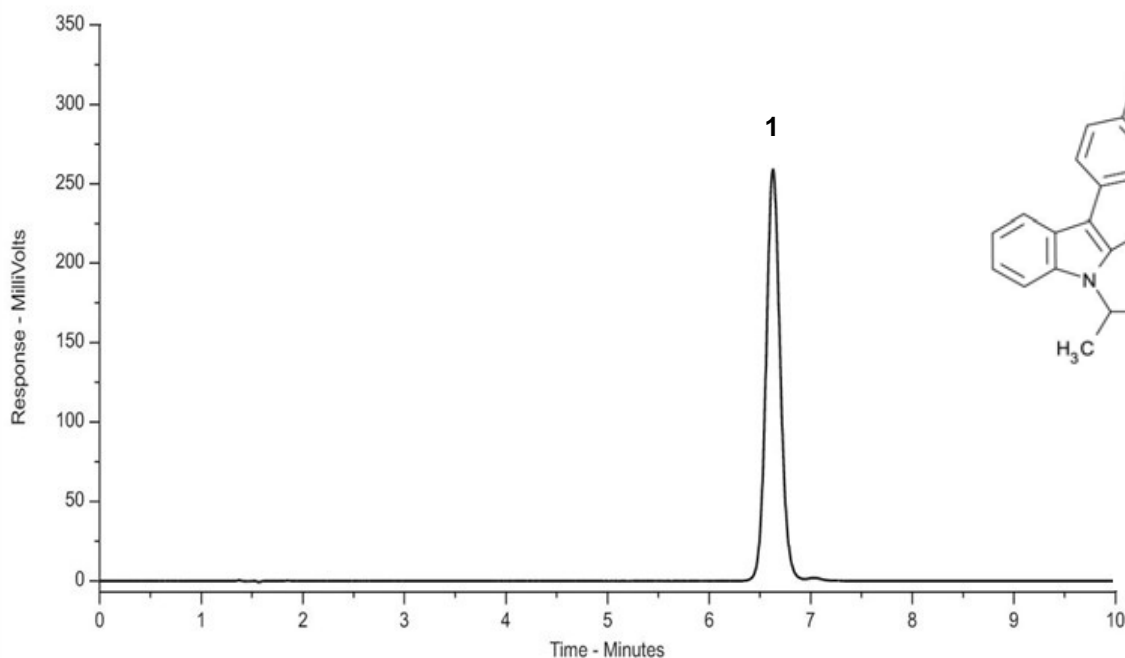
Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	10 mM ammonium formate pH 3.0/MeCN (47:53 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	Ambient
Detection:	UV, 254 nm



1. Atorvastatin

Conditions

Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	10 mM ammonium formate pH 3.0/MeCN (47:53 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	Ambient
Detection:	UV, 254 nm

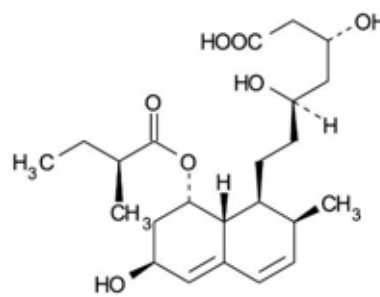
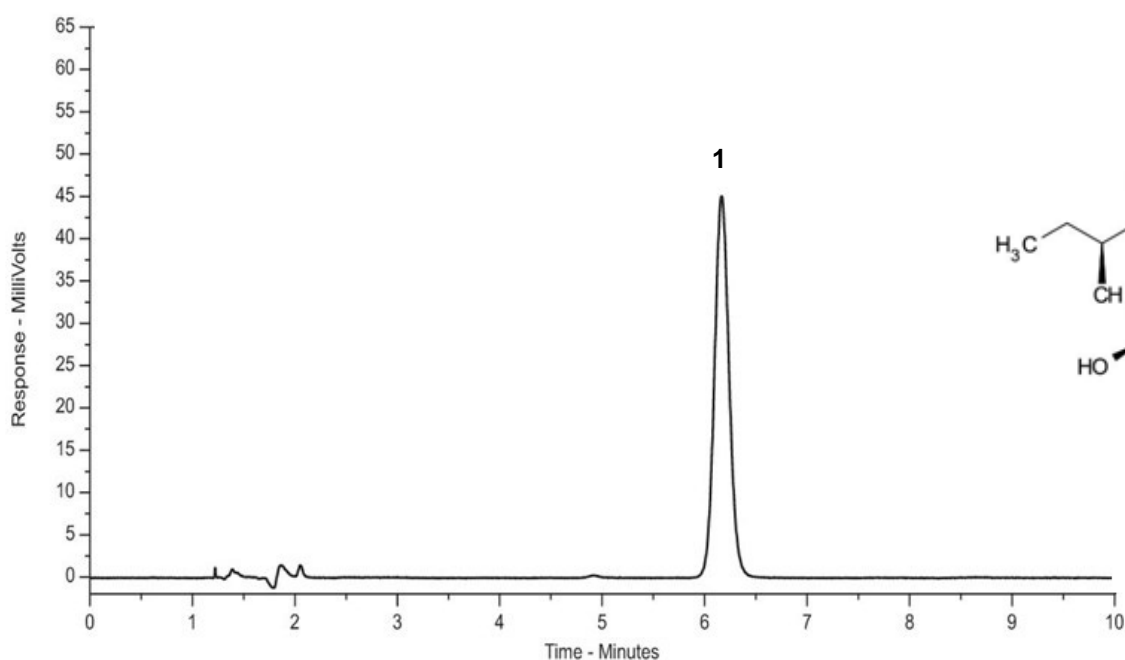


1. Fluvastatin



Conditions

Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	10 mM ammonium formate pH 3.0/MeCN (68:32 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	Ambient
Detection:	UV, 254 nm

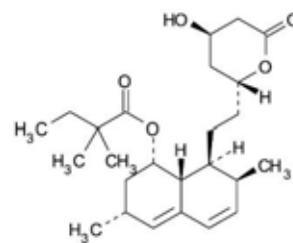
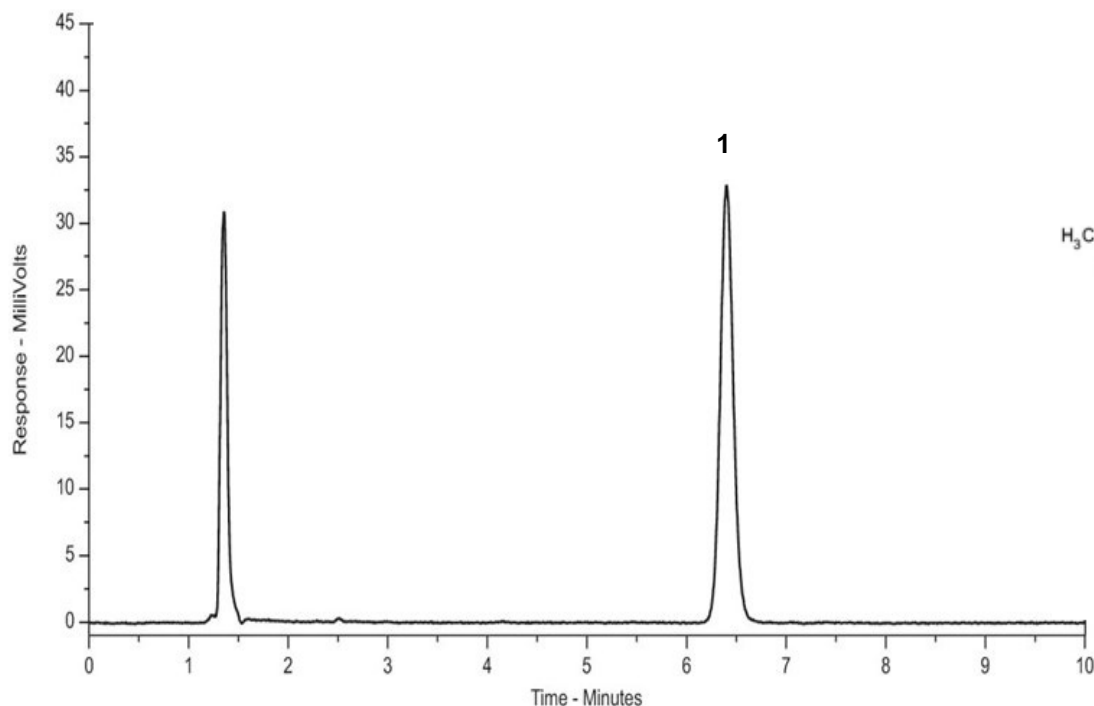


1. Pravastatin



Conditions

Column: ACE 5 C18
Dimensions: 150 x 4.6 mm
Part Number: ACE-121-1546
Mobile Phase: 10 mM ammonium formate pH 3.0/MeCN (25:75 v/v)
Flow Rate: 1 mL/min
Injection: 5 µL
Temperature: Ambient
Detection: UV, 254 nm

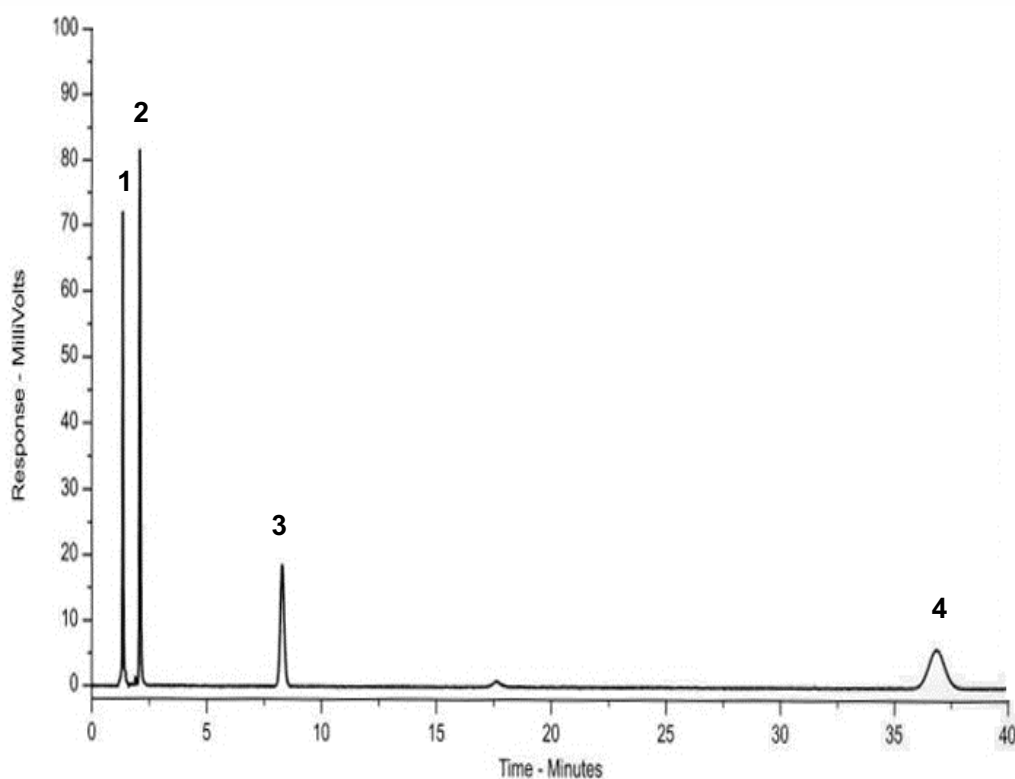


1. Simvastatin



Conditions

Column:	ACE 5 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-121-1546
Mobile Phase:	10 mM ammonium formate pH 3.0/MeCN (50:50 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	Ambient
Detection:	UV, 254 nm



1. Impurity
2. Pravastatin
3. Atorvastatin
4. Simvastatin



Steroid Hormones (Endogenous) by LC-MS/MS

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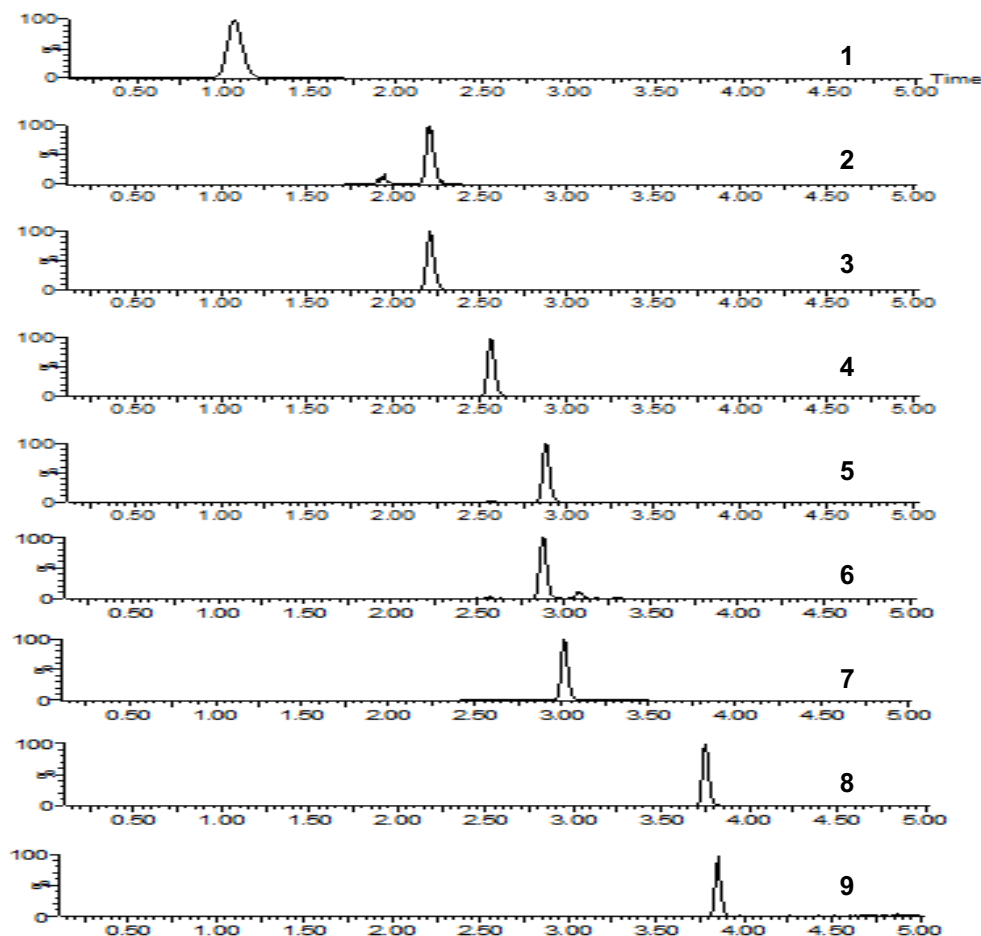
Application #AN2640

Conditions

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

Time (mins)	%B
0.0	50
0.8	50
4.2	81
4.3	100
5.3	100
5.8	50
6.8	50

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



1. Aldosterone
(*m/z* 361.4 → 315.4)
2. 21-Deoxycortisol
(*m/z* 347.4 → 311.4)
3. 11-Deoxycortisol
(*m/z* 347.4 → 97.0)
4. Androstendione
(*m/z* 287.3 → 97.0)
5. Testosterone
(*m/z* 289.4 → 97.0)
6. DHEA
(*m/z* 289.4 → 253.2)
7. 17 α -Hydroxyprogesterone
(*m/z* 331.4 → 97.0)
8. Progesterone
(*m/z* 315.4 → 97.0)
9. Androsterone
(*m/z* 291.3 → 255.4)

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Steroid Mixture Separation (I)

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Application #AN1060

Conditions

Column:

ACE 3 C18

ACE 3 Phenyl

ACE 3 C18-AR

Dimensions:

150 x 4.6 mm

Part Number:

ACE-111-1546, ACE-115-1546, ACE-119-1546

Mobile Phase:

A: H₂O

B: MeCN

Time (mins)

%B

0

25

24

46

26

6

27

25

Flow Rate:

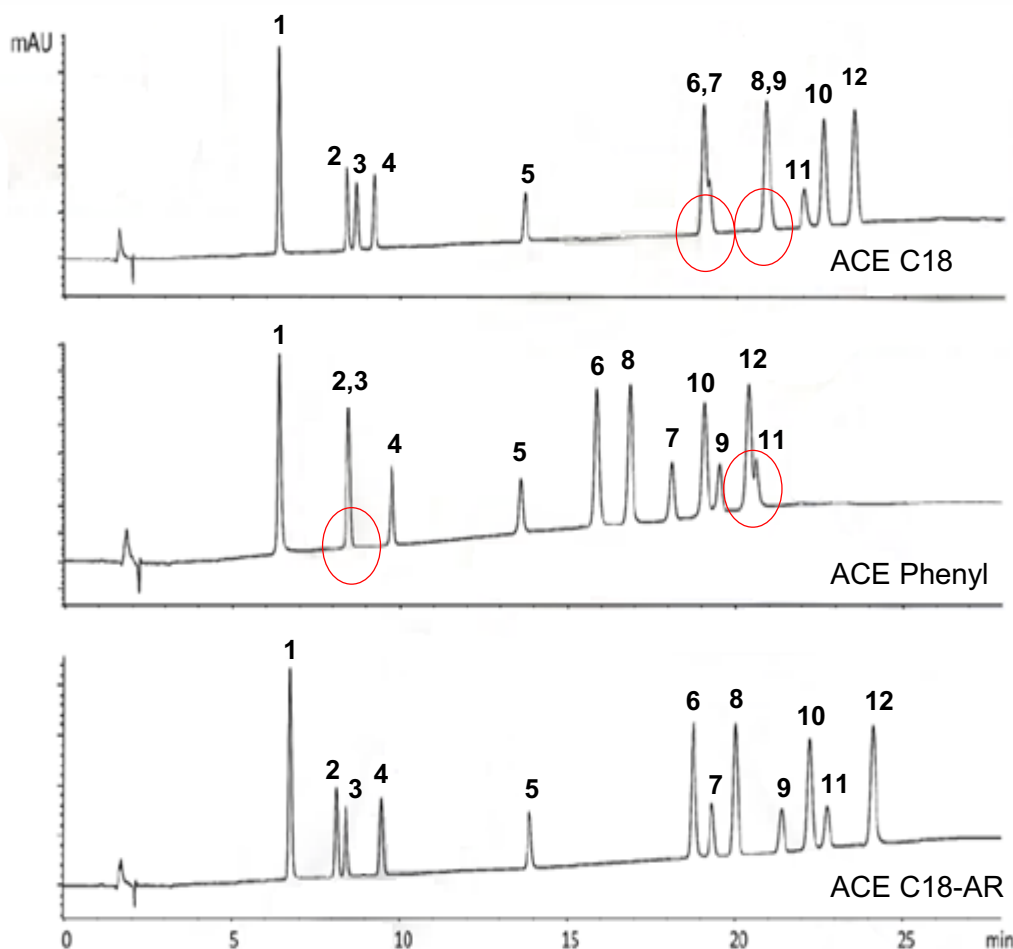
1 mL/min

Temperature:

20 °C

Detection:

UV, 214 nm



1. Estriol
2. Prednisolone
3. Hydrocortisone
4. Cortisone
5. Corticosterone
6. 17β-Estradiol
7. Cortisone-21-acetate
8. 17α-Estradiol
9. 19-Norethindrone
10. 17α-Ethinylestradiol
11. 21-Hydroxyprogesterone
12. Estrone

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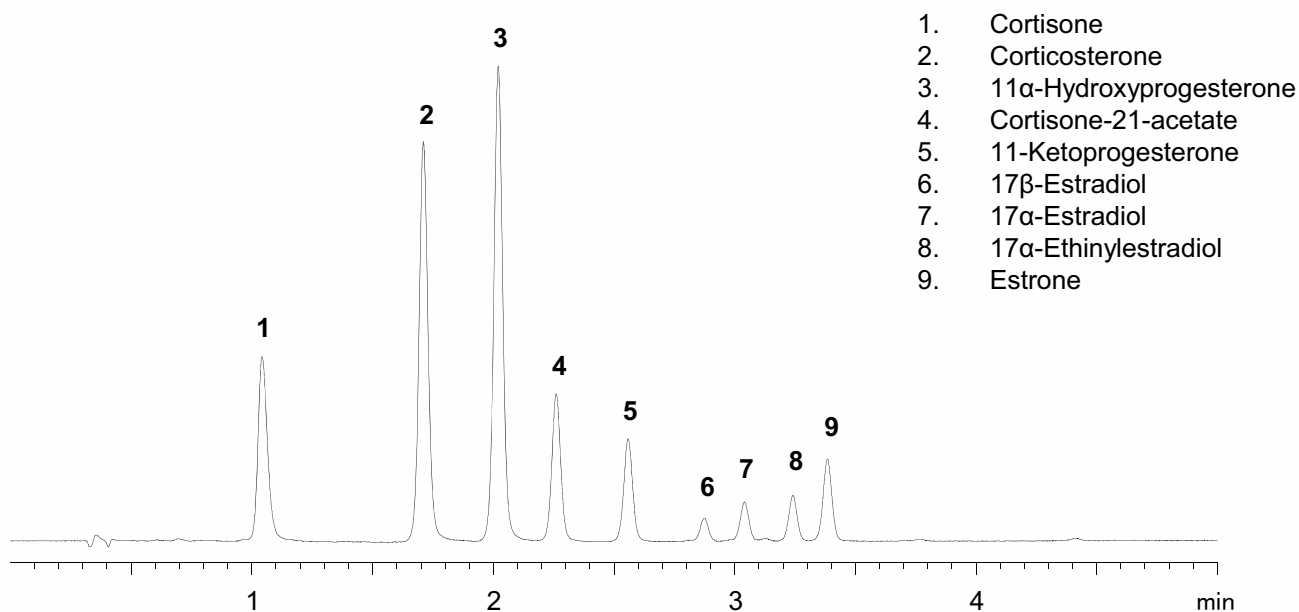
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Steroid Mixture Separation (II)

Application #AN1550

Conditions

Column: ACE Excel 2 CN-ES
Dimensions: 50 x 2.1 mm
Part Number: EXL-1013-0502U
Mobile Phase: A: 0.1% formic acid in H₂O
B: 0.1% formic acid in MeOH
Flow Rate: 0.4 mL/min
Injection: 1 µL
Temperature: 40 °C
Detection: UV, 214 and 260 nm

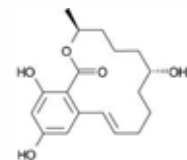
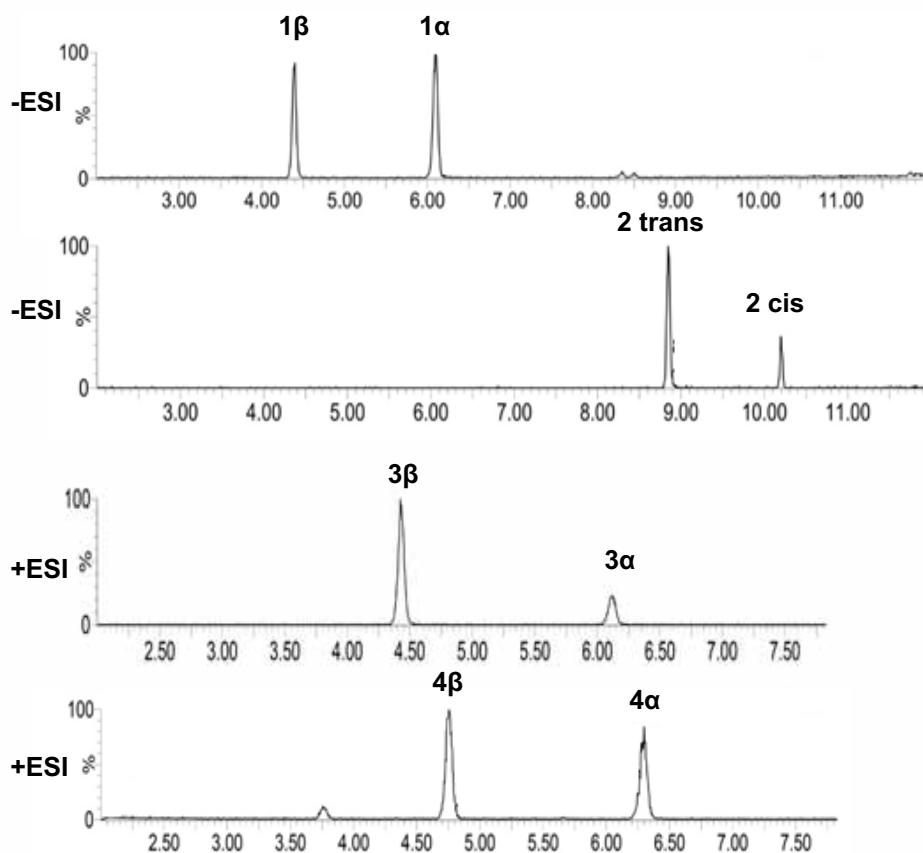


Conditions

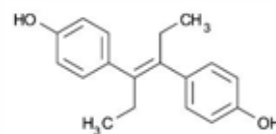
Column: ACE UltraCore 2.5 SuperC18
Dimensions: 100 x 2.1 mm
Part Number: CORE-25A-1002U
Mobile Phase: A: 0.01 mM ammonium fluoride + 0.001% formic acid
B: MeCN

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

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

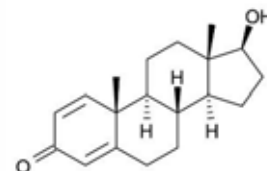


1. α - and β -Zearalenol
(m/z 319.17 $\rightarrow$ 275.12)

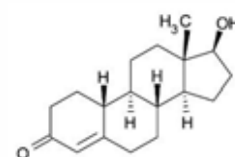


2. Diethylstilbestrol-d8
(m/z 275.23 $\rightarrow$ 245.09)

Also analysed in -ESI:
Talaranol and zearanol-d4
Talaranol and zearanol
Zearalenone
Hexestrol
Diethylstilbestrol
Dienesterol



3. α - and β -Boldenone
(m/z 287.17 $\rightarrow$ 121.12)



4. α - and β -Nortestosterone
(m/z 275.23 $\rightarrow$ 109.09)

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



Steroids Separation using Enhanced Polar Selectivity

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Application #AN2470

Conditions

Column: ACE Excel 3 C18-Amide
Dimensions: 50 x 2.1 mm
Part Number: EXL-1112-0502U
Mobile Phase:

A: 0.1% formic acid in H₂O

B: 0.1% formic acid in MeCN

Time (mins) %B

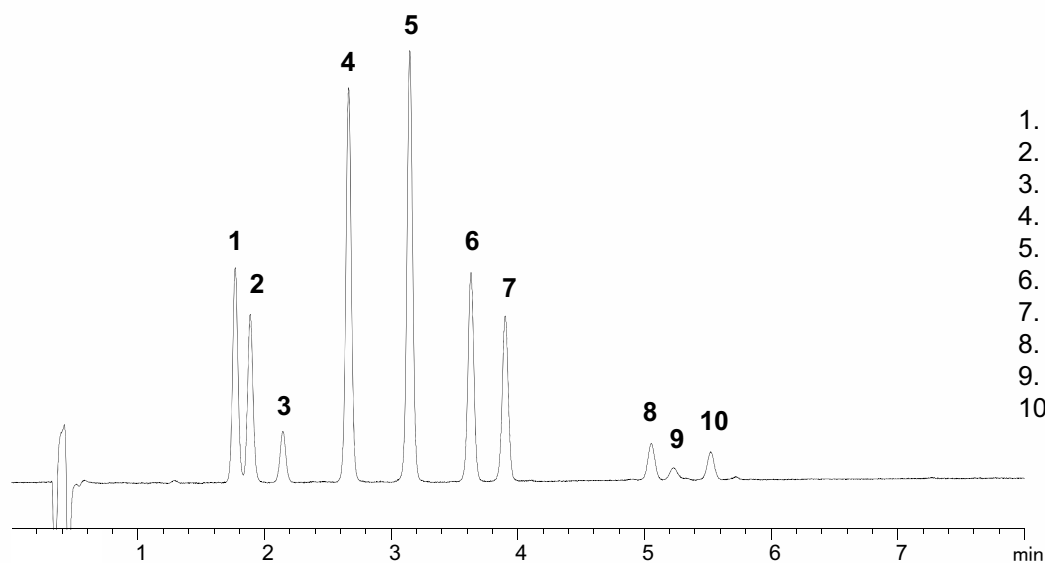
0 25

10 80

Flow Rate: 0.4 mL/min

Temperature: 20 °C

Detection: UV, 260 nm



1. Prednisone
2. Prednisolone
3. Estriol
4. Corticosterone
5. 11 α -Hydroxyprogesterone
6. 11-Ketoprogesterone
7. 21-Hydroxyprogesterone
8. 17 β -Estradiol
9. 17 α -Estradiol
10. 17 α -Ethinylestradiol



Steroids UHPLC-UV Analysis and Comparison

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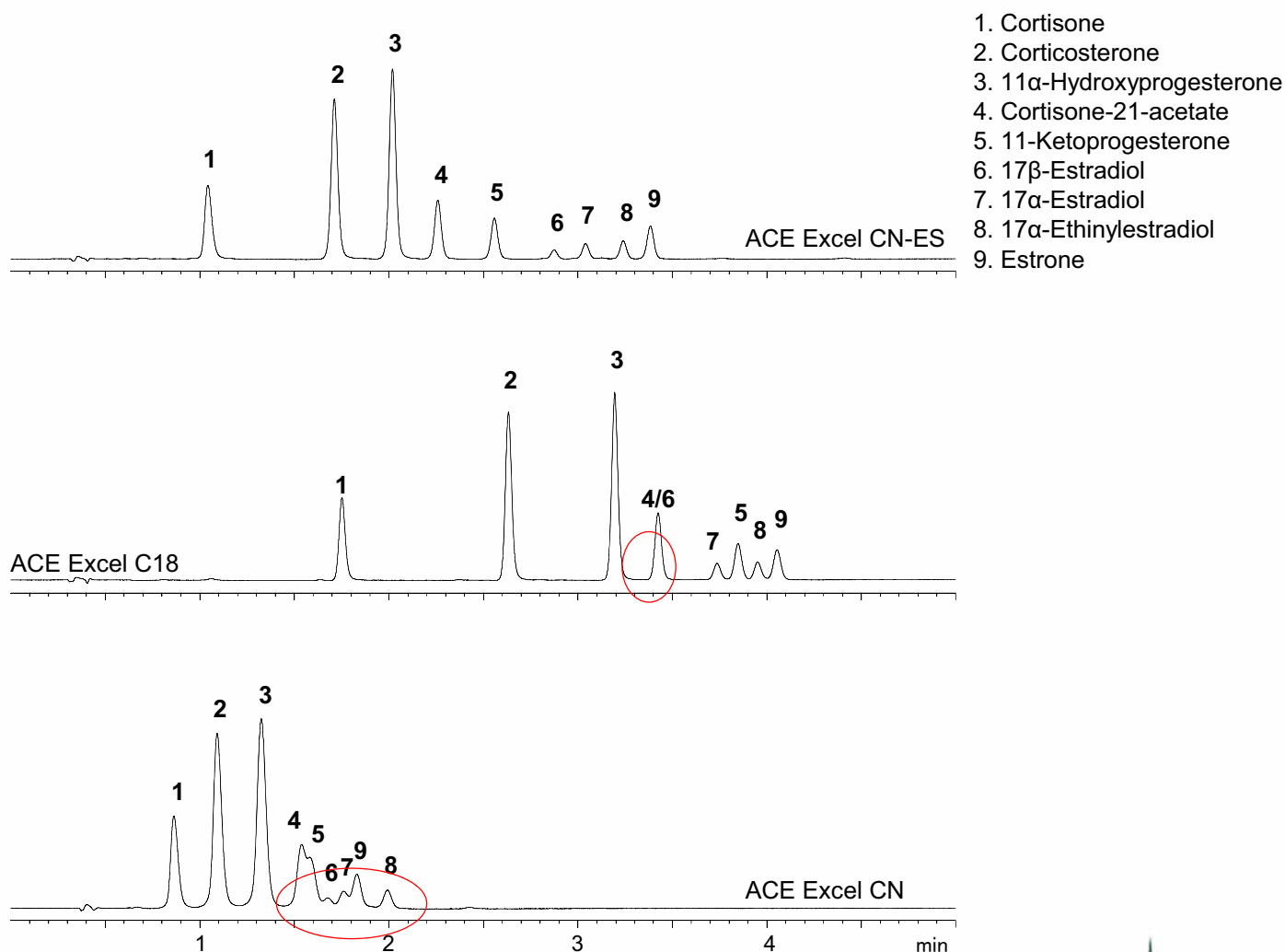
Application #AN1640

Conditions

Column: ACE Excel 2 CN-ES
ACE Excel 2 C18
ACE Excel 2 CN
Dimensions: 50 x 2.1 mm
Part Number: EXL-1013-0502U, EXL-101-0502U, EXL-104-0502U
Mobile Phase: A: 0.1% formic acid in H₂O
B: 0.1% formic acid in MeCN

Time (mins)	%B
0.0	25
10.0	80
10.5	80
11.0	25

Flow Rate: 0.4 mL/min
Temperature: 40 °C
Detection: UV, 260 nm



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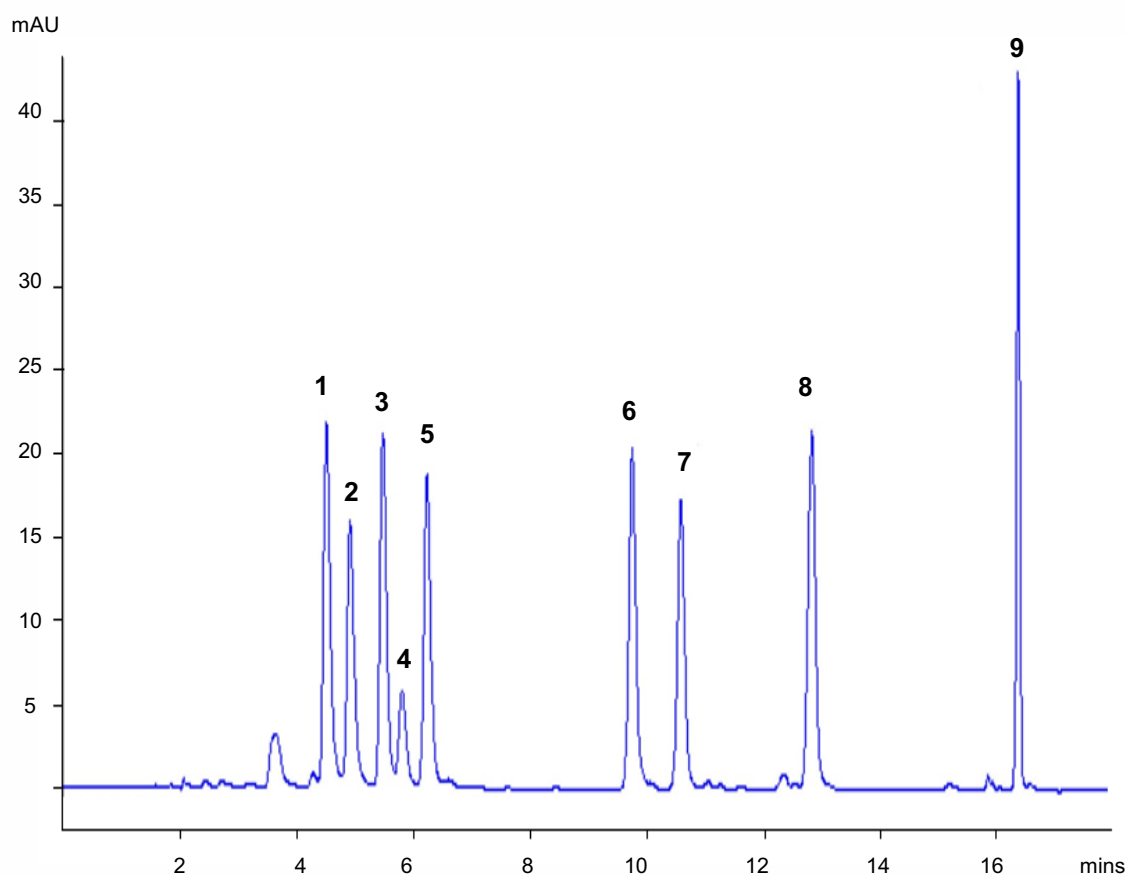
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Conditions

Column: ACE Excel 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: EXL-1110-1546U
Mobile Phase: A: H₂O
B: MeCN
C: 10% formic acid

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

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



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

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Sumatriptan and Promethazine by LC-MS/MS

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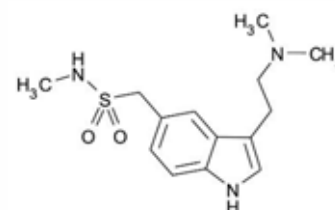
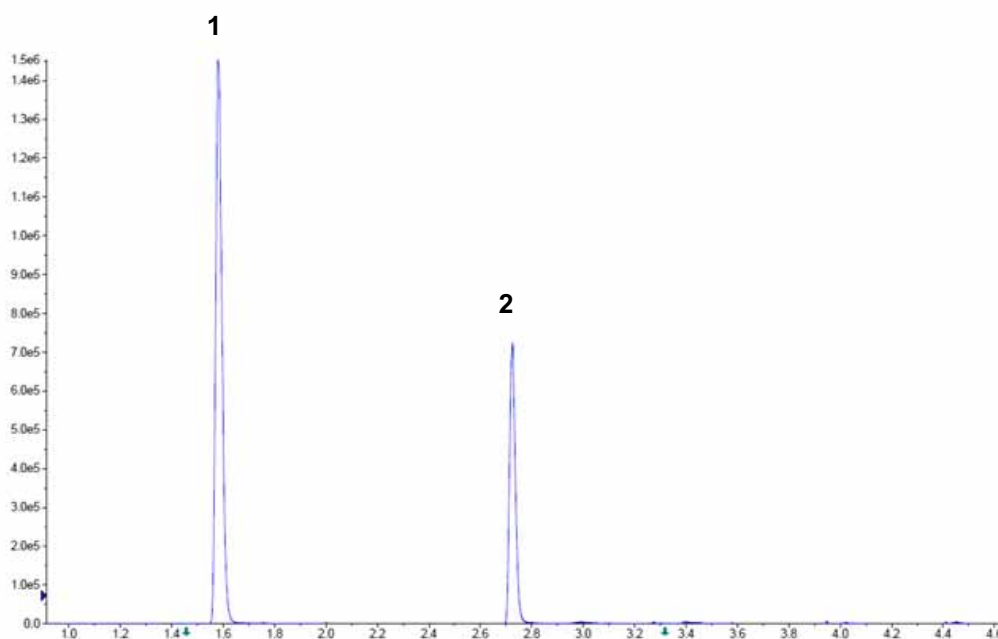
Application #AN2530

Conditions

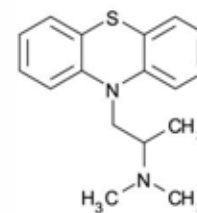
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: A: 0.1% formic acid in H₂O
B: 0.1% formic acid in MeOH

Time (min)	%B
0.0	15
0.5	15
2.5	90
3.5	90
5.5	15

Flow Rate: 0.7 mL/min
Temperature: 50 °C
Detection: AB Sciex QTRAP 6500
DuoSpray Ion source (ESI/APCI)
Positive ion MRM mode



1. Sumatriptan
(*m/z* 296 → 58)



2. Promethazine
(*m/z* 286 → 86)

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ACE[®]
UHPLC & HPLC
Columns

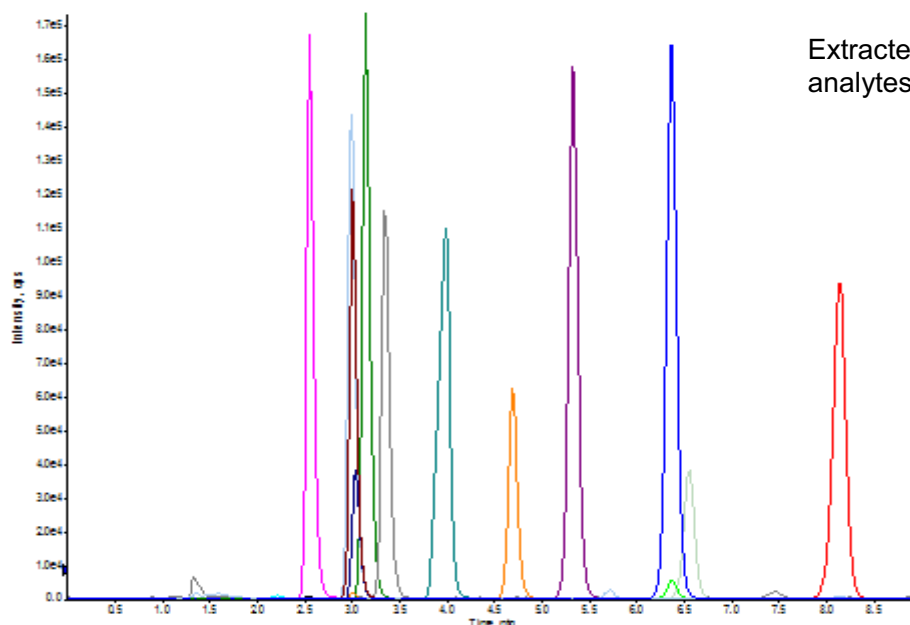
Synthetic Cannabinoids (SPICE) from Oral Fluid

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UHPLC & HPLC Columns

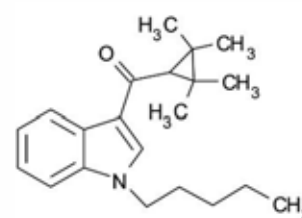
Application #AN1650

Conditions

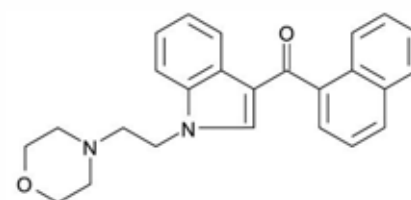
Column: ACE Excel 2 C18-AR
Dimensions: 100 x 2.1 mm
Part Number: EXL-109-1002U
Mobile Phase: 0.1% formic acid in MeOH/H₂O (85:15 v/v)
Flow Rate: 0.3 mL/min
Temperature: Ambient
Detection: Applied Biosystems/MDS Sciex 4000 Q-Trap
Positive mode Turbo Ionspray



Extracted ion chromatogram for SPICE analytes fortified in neat oral fluid at 20 ng/mL



UR-144



JWH-200

Retention Time (minutes)	Analyte	MRM Transition	Decustering Potential (DP)	Collision Energy (CE)	Cell Exit Potential (CXP)
2.55	JWH-250 N-(5-hydroxypentyl)	352>120.9	40	30	16
2.99	JWH-073 N-(3-hydroxybutyl)	344>155	40	30	16
3.00	UR-144 5-Hydroxy-pentyl	328.5>125	30	35	16
3.03	UR-144 Pentanoic Acid	342.5>125	30	35	16
3.14	d5-JWH-018 N-(4-hydroxypentyl)	363.5>155	40	35	16
3.14	JWH-018 N-(4-hydroxypentyl)	358>155	40	30	16
3.34	JWH-018 5-pentanoic acid	372>155	40	30	16
3.98	JWH-200	385>155	40	30	16
4.69	XLR-11	330>125	30	35	16
5.32	JWH-250	336>121	40	30	16
6.36	JWH-073	328>155	40	30	16
6.37	UR-144 5-Chloro-pentyl	346.9>125	30	35	16
6.55	UR-144	312.5>125	30	35	16
8.14	JWH-018	342>155	40	30	16

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Columns

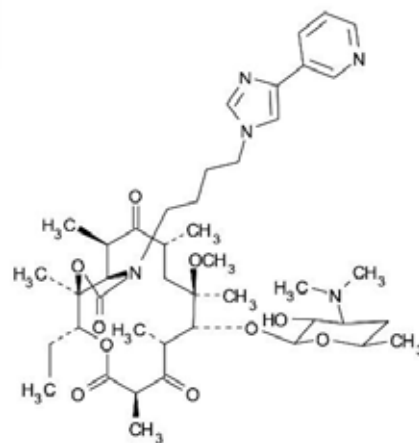
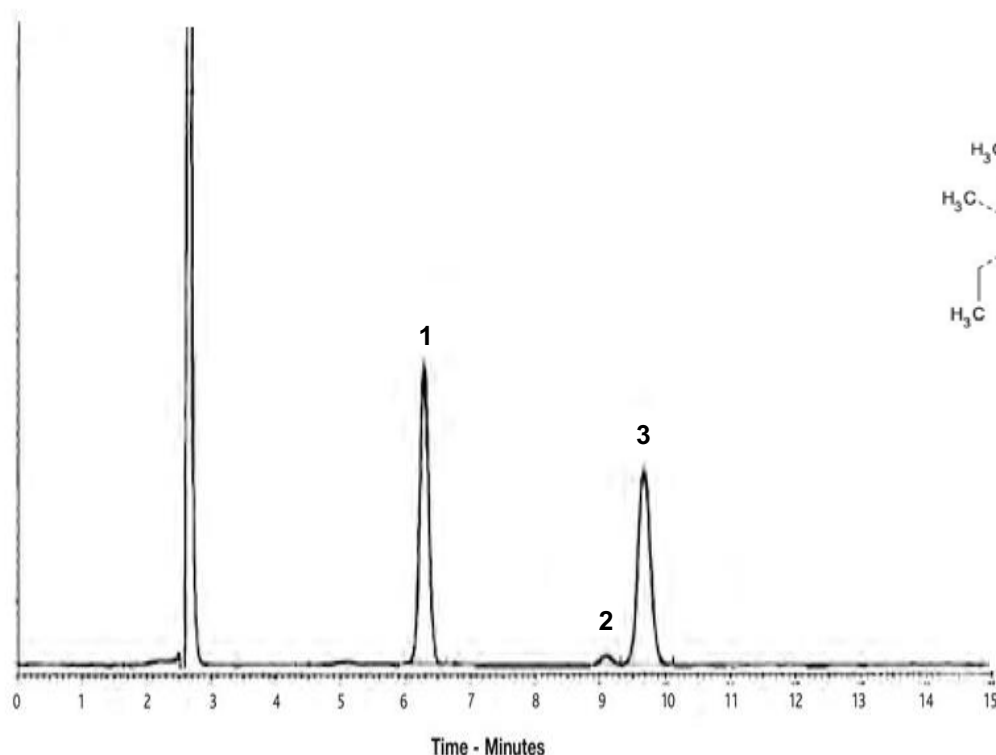
Telithromycin Analysis

ACE[®]
Ultra-inert
UHPLC & HPLC Columns

Application #AN3280

Conditions

Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 0.05 M phosphate buffer pH 4.0/MeOH (45:55 v/v)
Flow Rate: 1 mL/min
Injection: 20 µL
Temperature: 50 °C
Detection: UV, 265 nm
Sample: Exposed to 3% H₂O₂ for 1 hour



1. Telithromycin
2. Degradant 1
3. Degradant 2

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Terfenadine and Fexofenadine in Rat Plasma

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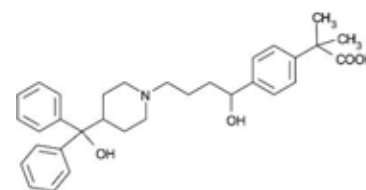
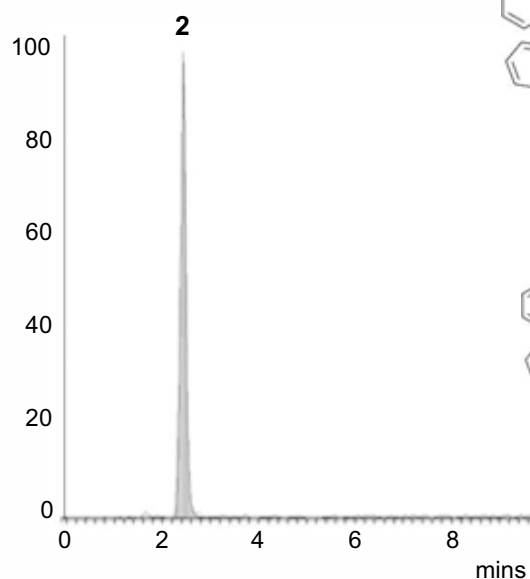
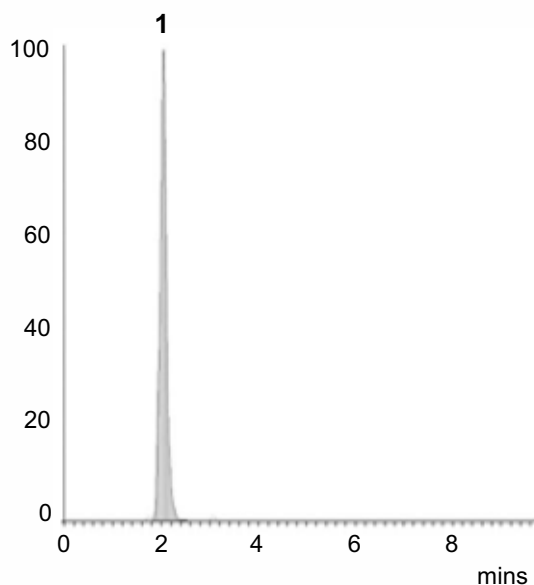
Application #AN3290

Conditions

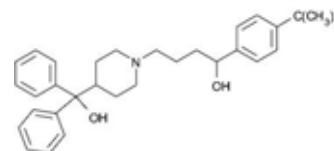
Column: ACE 5 AQ
Dimensions: 50 x 3.0 mm
Part Number: ACE-126-0503
Mobile Phase: A: 0.1% formic acid in H₂O
B: MeOH

Time (mins)	%B
0.0	10
1.5	90
2.0	90
3.0	10

Flow Rate: 1 mL/min
Injection: 10 µL
Temperature: Ambient
Detection: Turbo IonSpray MS/MS
Positive ion mode



1. Fexofenadine
(m/z 502.3 → 466.3)



2. Terfenadine
(m/z 472.3 → 436.3)

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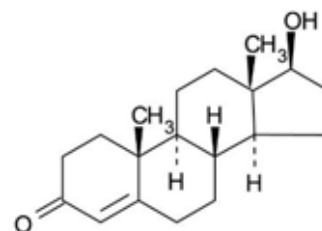
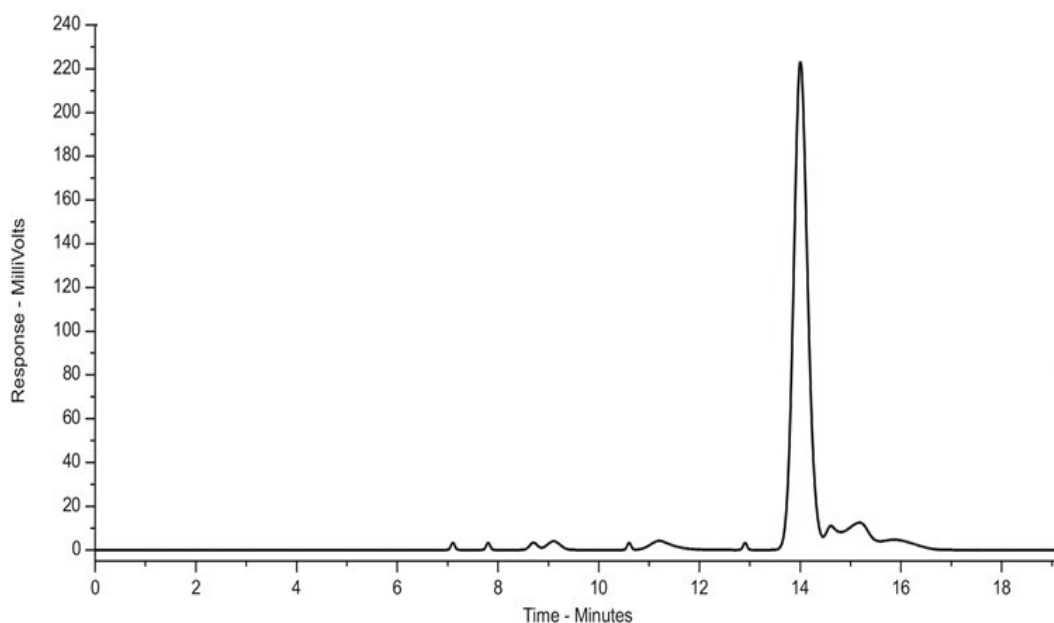
ACE[®]
UHPLC & HPLC
Columns

Conditions

Column: ACE 5 C18
Dimensions: 150 x 0.075 mm
Part Number: ACE-121-1500075
Mobile Phase: A: 0.1% formic acid in MeCN/0.1% formic acid in H₂O (10:90 v/v)
B: 0.1% formic acid in MeCN/0.1% formic acid in H₂O (90:10 v/v)

Time (mins)	%B
0	40
5	40
30	95

Flow Rate: 1 µL/min
Temperature: Ambient
Detection: ESI MS/MS
Positive ion mode



1. Testosterone

Thyroid Hormones by LC-MS/MS (I)

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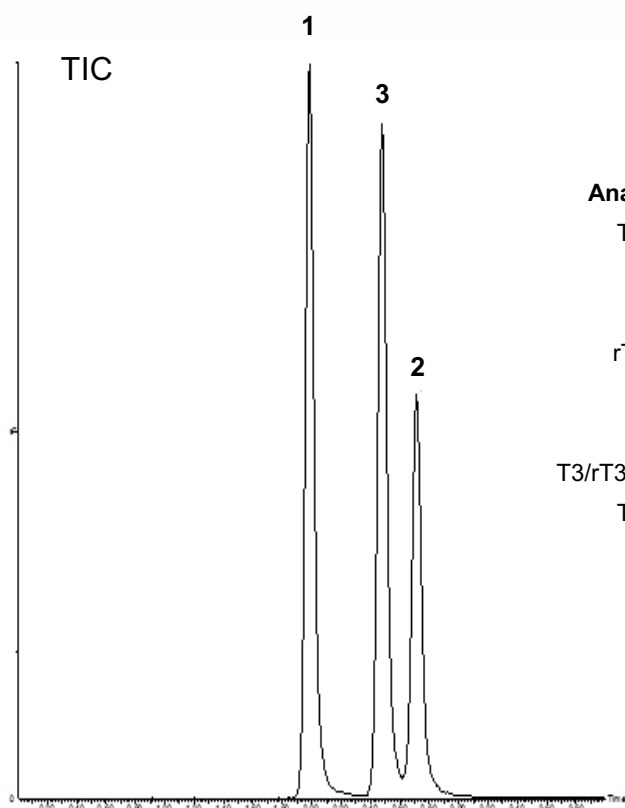
Application #AN2170

Conditions

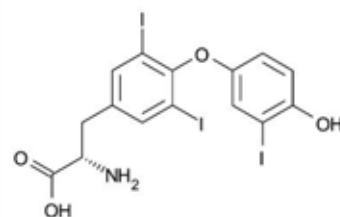
Column: ACE Excel 2 C18-AR
Dimensions: 100 x 2.1 mm
Part Number: EXL-109-1002U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% formic acid in H₂O
B: 2 mM ammonium acetate, 0.1% formic acid in MeOH

Time (mins)	%B
0.0	60
3.0	77
3.1	60

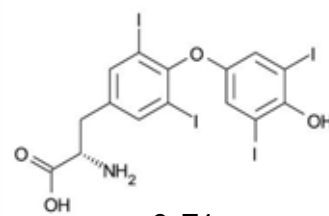
Flow Rate: 0.4 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: XEVO TQS triple quad MS
Desolvation temperature: 500 °C
Ion source temperature: 150 °C
Positive mode ESI, MRM



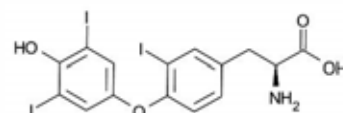
Analyte	Q1 (Da)	Q3 (Da)
T3	651.8 (651.8)	605.8 (507.8)
rT3	651.8 (651.8)	605.8 (478.9)
T3/rT3-d6 I.S.	657.8	611.8
T4	777.7 (777.7)	731.7 (351)
		(777.7) (633.8)



1. T3
(Tri-iodothyronine)



2. T4
(Thyroxine)



3. rT3
(Reversed tri-iodothyronine)

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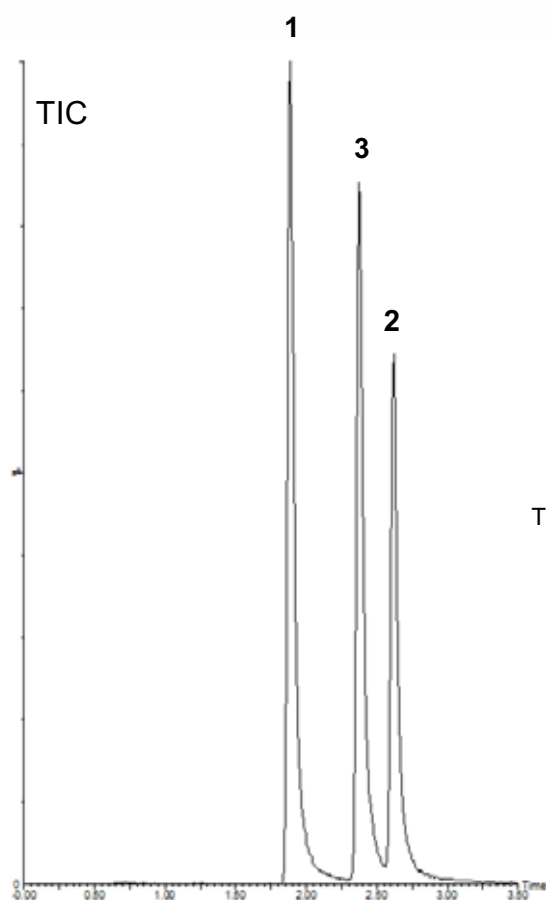
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Columns

Conditions

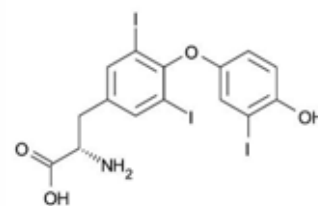
Column: ACE Excel 1.7 C18-AR
Dimensions: 100 x 2.1 mm
Part Number: EXL-179-1002U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% formic acid in H₂O
B: 2 mM ammonium acetate, 0.1% formic acid in MeOH

Time (mins)	%B
0.0	60
3.0	77
3.1	60

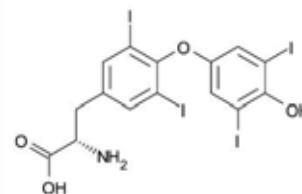
Flow Rate: 0.4 mL/min
Injection: 10 µL
Temperature: 40 °C
Detection: XEVO TQS triple quad MS
Desolvation temperature: 500 °C
Ion source temperature: 150 °C
Positive mode ESI, MRM



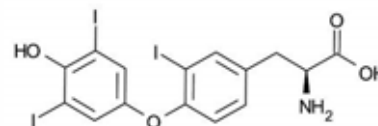
Analyte	Q1 (Da)	Q3 (Da)
T3	651.8	605.8
	(651.8)	(507.8)
	(651.8)	(478.9)
rT3	651.8	605.8
	(651.8)	(507.8)
	(651.8)	(478.9)
T3/rT3-d6 I.S.	657.8	611.8
T4	777.7	731.7
	(777.7)	(351)
	(777.7)	(633.8)



1. T3
(Tri-iodothyronine)



2. T4
(Thyroxine)



3. rT3
(Reversed tri-iodothyronine)

Tocopherol Mixture Separation

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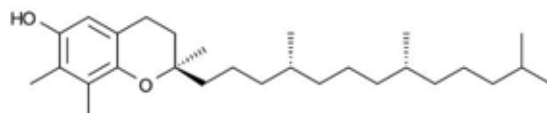
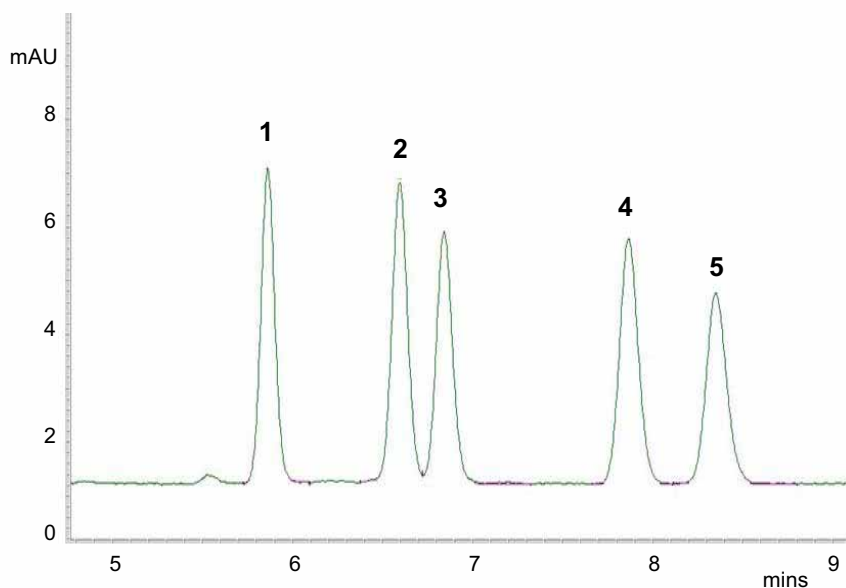
Application #AN3390

Conditions

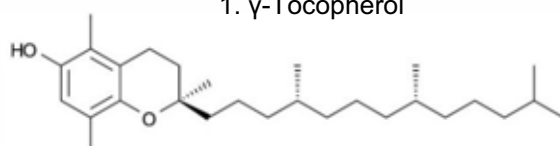
Column: ACE Excel 3 C18-PFP
Dimensions: 150 x 4.6 mm
Part Number: EXL-1110-1546U
Mobile Phase: A: 0.1% H₃PO₄/MeCN (1:3 v/v)
B: MeCN

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

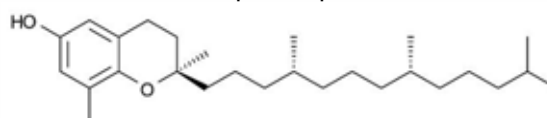
Time (mins)	%B
0.00	0
0.10	0
0.11	80
8.00	80
8.01	100
12.00	100
12.01	0
14.00	0



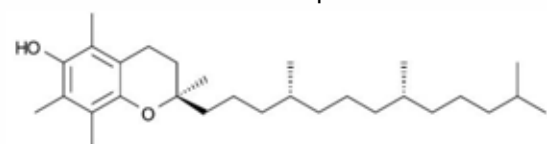
1. γ-Tocopherol



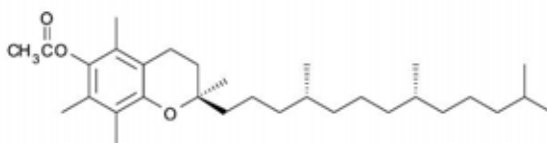
2. β-Tocopherol



3. δ-Tocopherol



4. α-Tocopherol



5. α-Tocopherol acetate

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Tricyclic Antidepressants (Gradient)

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Application #AN1690

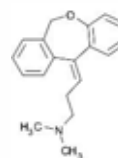
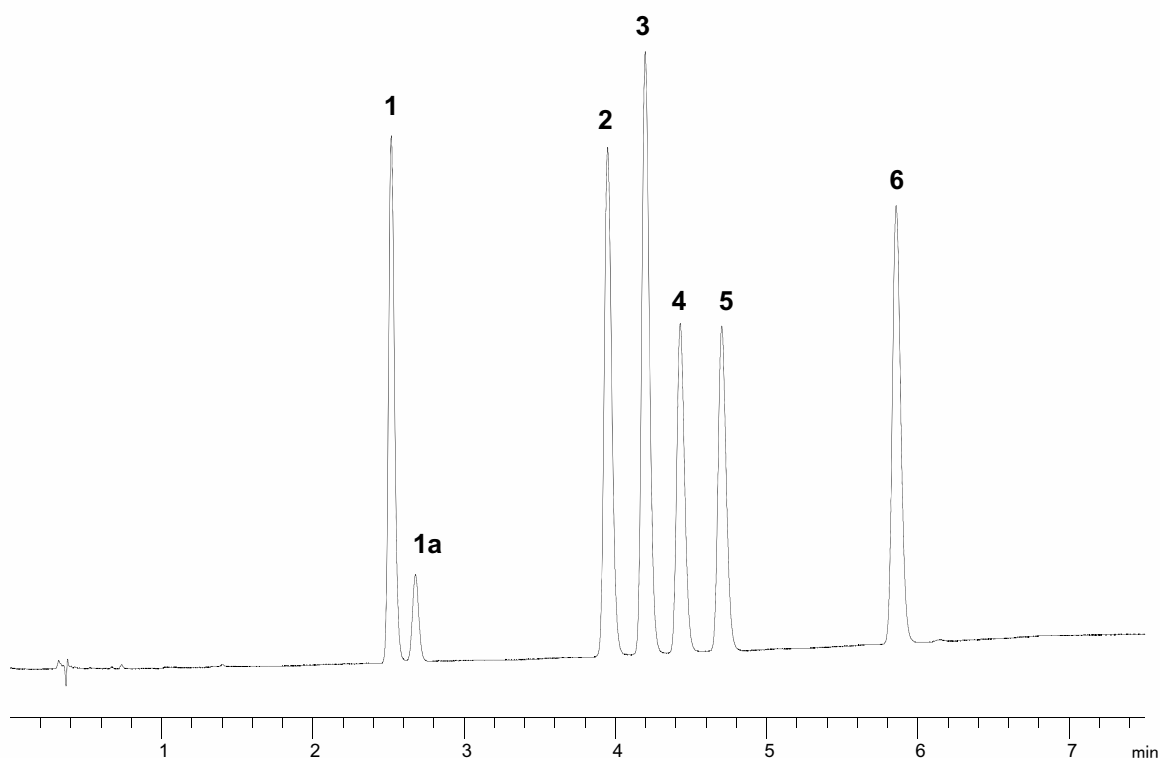
Conditions

Column: ACE Excel 2 SuperC18
Dimensions: 100 x 3.0 mm
Part Number: EXL-1011-1003U
Mobile Phase: A 20 mM ammonium formate pH 3.0 in H₂O
B 20 mM ammonium formate pH 3.0 in MeOH/H₂O (9:1 v/v)

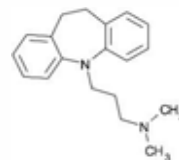
Time (mins)	%B
0.0	50
6.0	70
7.5	2

Post time 10 minutes

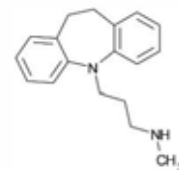
Flow Rate: 1.2 mL/min
Injection: 2 µL
Temperature: 40 °C
Detection: UV, 260 nm



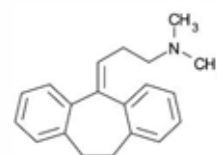
1. Doxepin + isomer



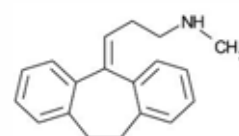
2. Imipramine



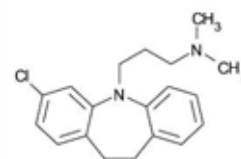
3. Desipramine



4. Amitriptyline



5. Nortriptyline



6. Clomipramine

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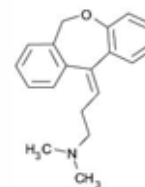
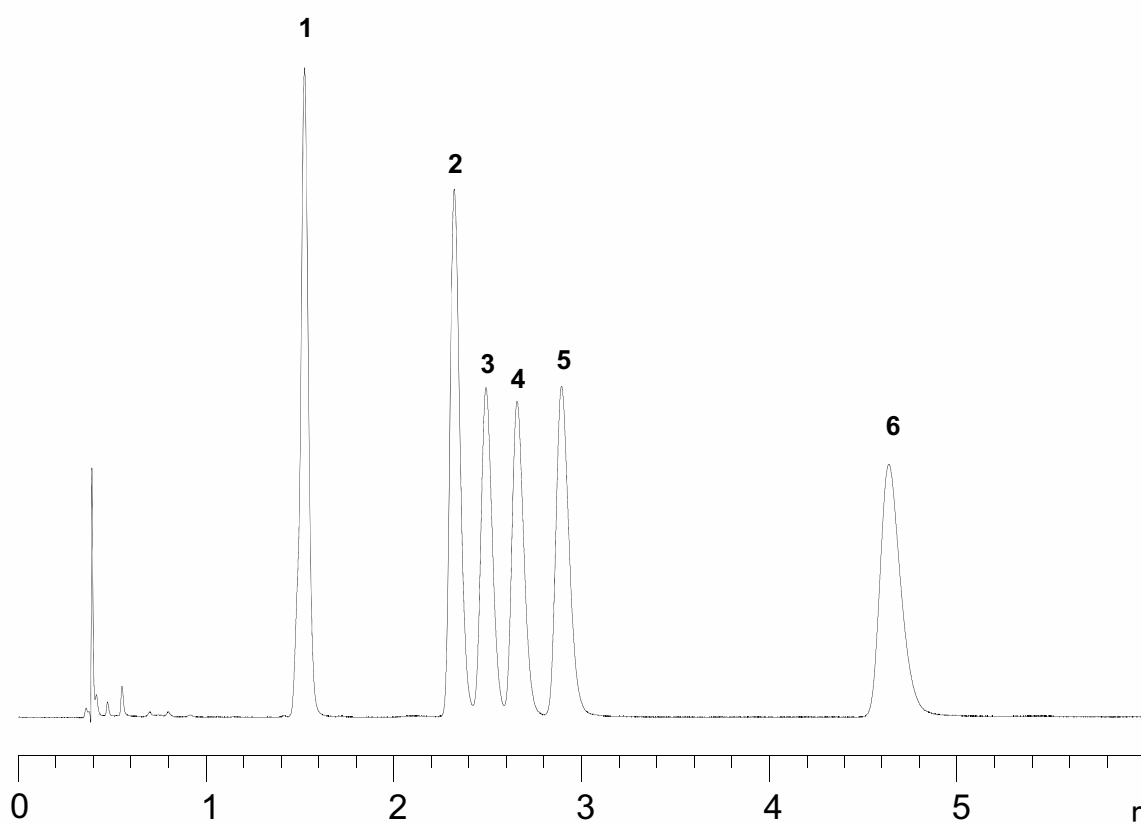
Tricyclic Antidepressants (Isocratic)

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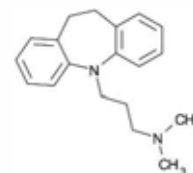
Application #AN1680

Conditions

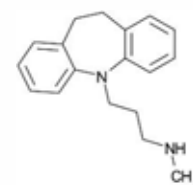
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 3.0 mm
Part Number: EXL-1010-1003U
Mobile Phase: 20 mM ammonium formate pH 3.0 in MeOH/H₂O (54:46 v/v)
Flow Rate: 1.2 mL/min
Injection: 2 µL
Temperature: 40 °C
Detection: UV, 260 nm



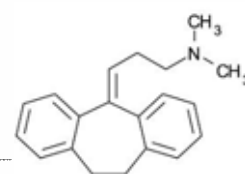
1. Doxepin



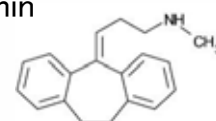
2. Imipramine



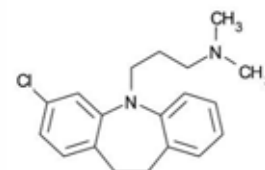
3. Desipramine



4. Amitriptyline



5. Nortriptyline



6. Clomipramine



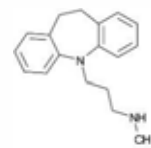
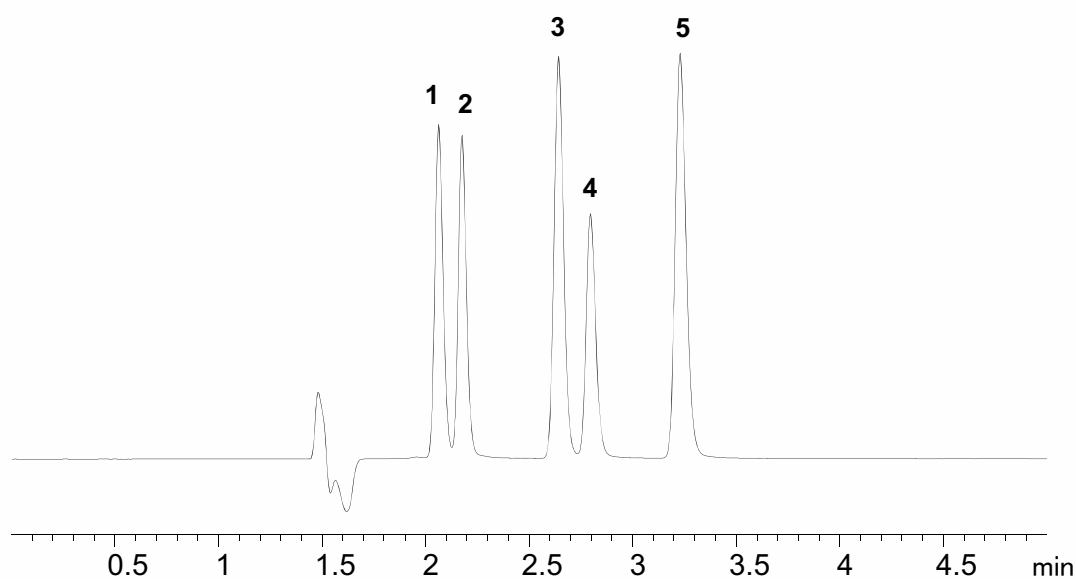
Tricyclic Antidepressants (Isocratic Rapid Analysis)

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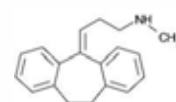
Application #AN1700

Conditions

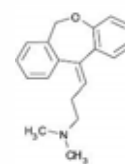
Column: ACE 5 C18
Dimensions: 250 x 4.6 mm
Part Number: ACE-121-2546
Mobile Phase: 20 mM ammonium acetate pH 6.3 MeCN/H₂O (65:35 v/v)
Flow Rate: 1.5 mL/min
Injection: 10 µL
Temperature: 60 °C
Detection: UV, 215 nm



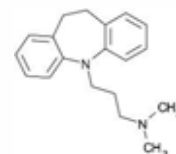
1. Desipramine



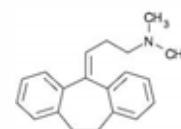
2. Nortriptyline



3. Doxepin



4. Imipramine



5. Amitriptyline



25-Hydroxy Vitamin D2/D3 in Serum by LC-MS/MS

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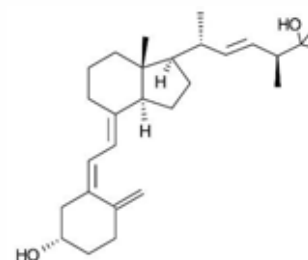
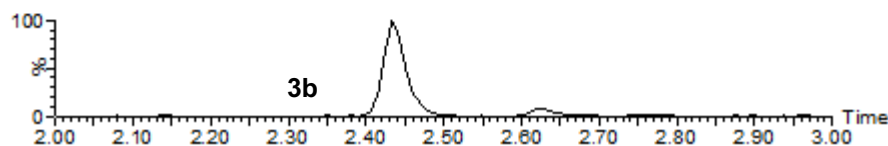
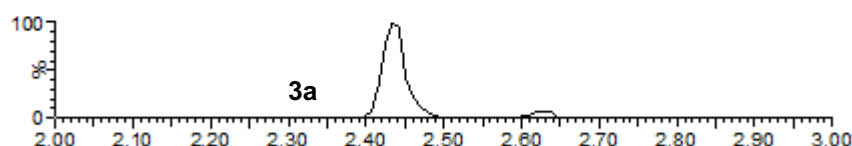
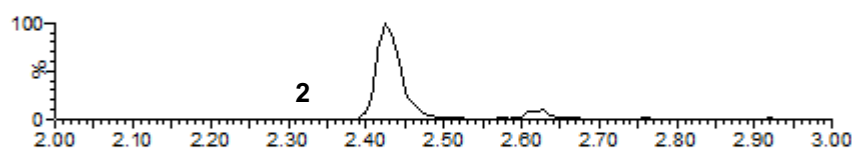
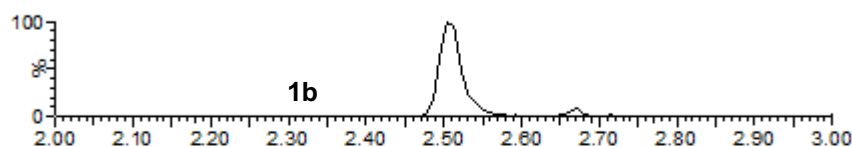
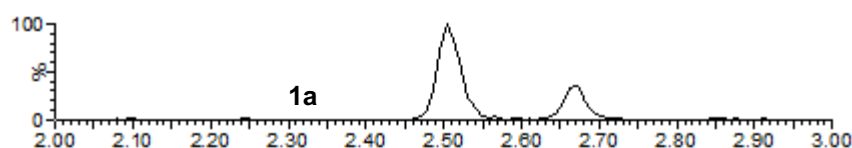
Application #AN2390

Conditions

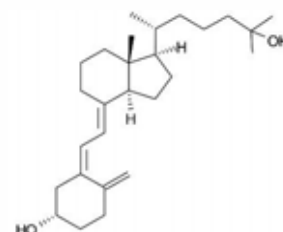
Column: ACE Excel 2 C18-PFP
Dimensions: 100 x 2.1 mm
Part Number: EXL-1010-1002U
Mobile Phase: A: 2 mM ammonium acetate, 0.1% formic acid in H₂O
B: 0.1% formic acid in MeOH

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

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



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



- 3a. 25-OH Vitamin D3
(m/z 383.5 $\rightarrow$ 257.5)
- 3b. 25-OH Vitamin D3
(m/z 383.5 $\rightarrow$ 107.2)

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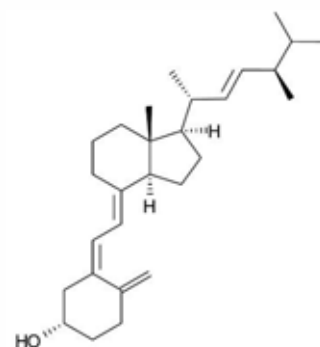
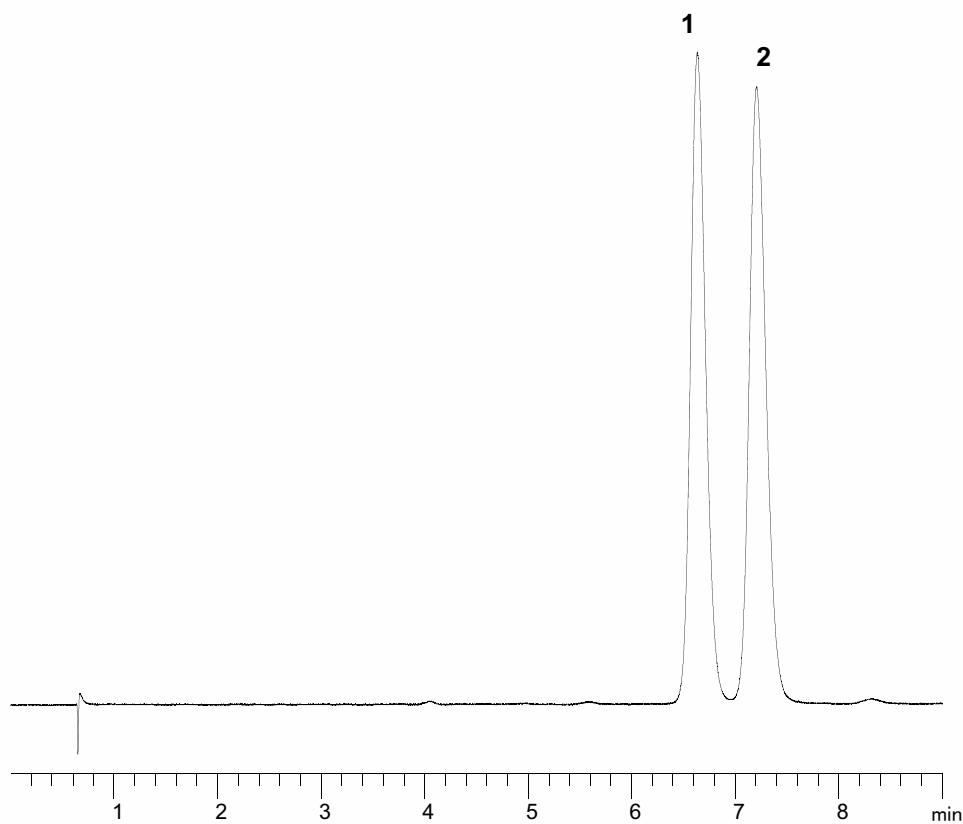
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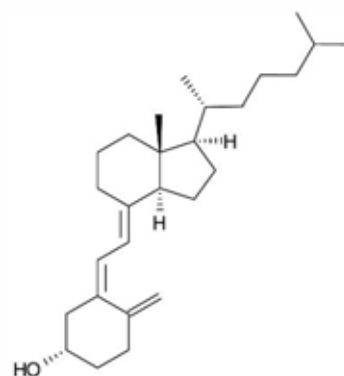
ACE[®]
UHPLC & HPLC
Columns

Conditions

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



1. Ergocalciferol (D2)

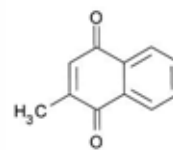
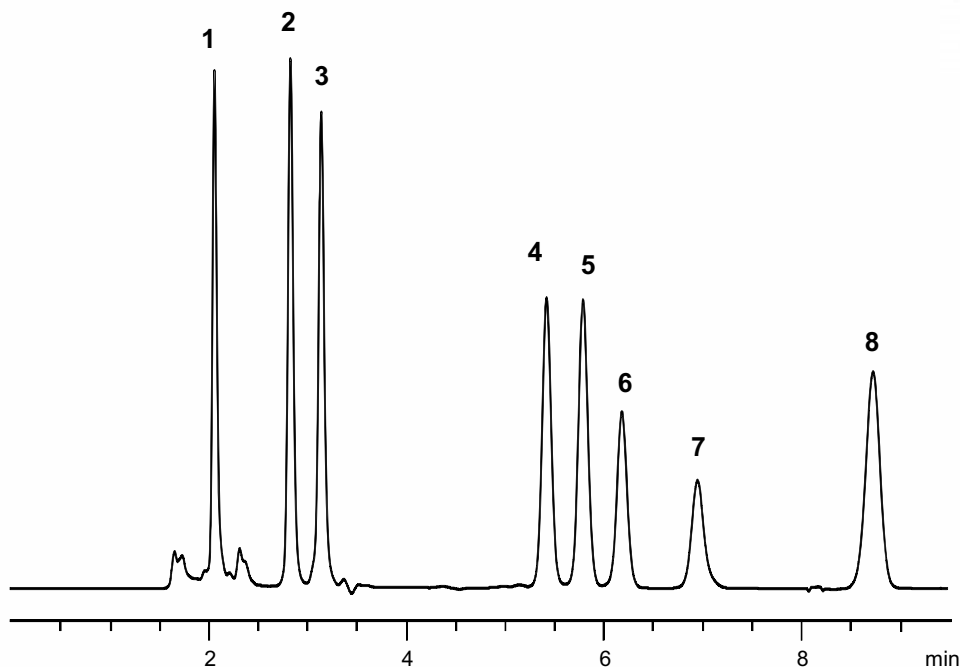


2. Cholecalciferol (D3)

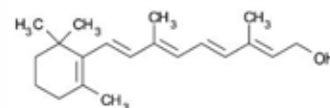
Application #AN2420

Conditions

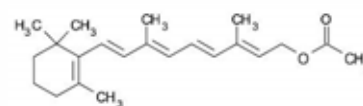
Column: ACE 3 C18-Amide
Dimensions: 150 x 4.6 mm
Part Number: EXL-1112-1546U
Mobile Phase: MeOH/MeCN (90:10 v/v)
Flow Rate: 1 mL/min
Temperature: 20 °C
Detection: UV, 280 nm



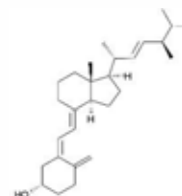
1. Menadione (Vitamin K3)



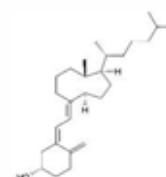
2. Retinol (Vitamin A)



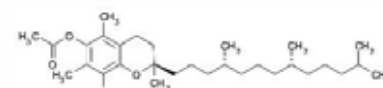
3. Vitamin A acetate



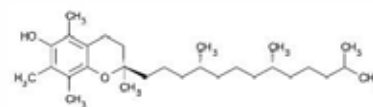
4. Ergocalciferol (Vitamin D2)



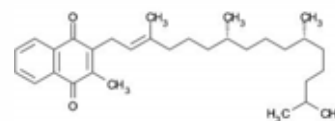
5. Cholecalciferol (Vitamin D3)



6. Vitamin E acetate



7. α-Tocopherol (Vitamin E)



8. Vitamin K1



Water Soluble Vitamins (I)

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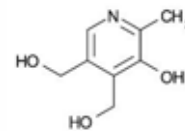
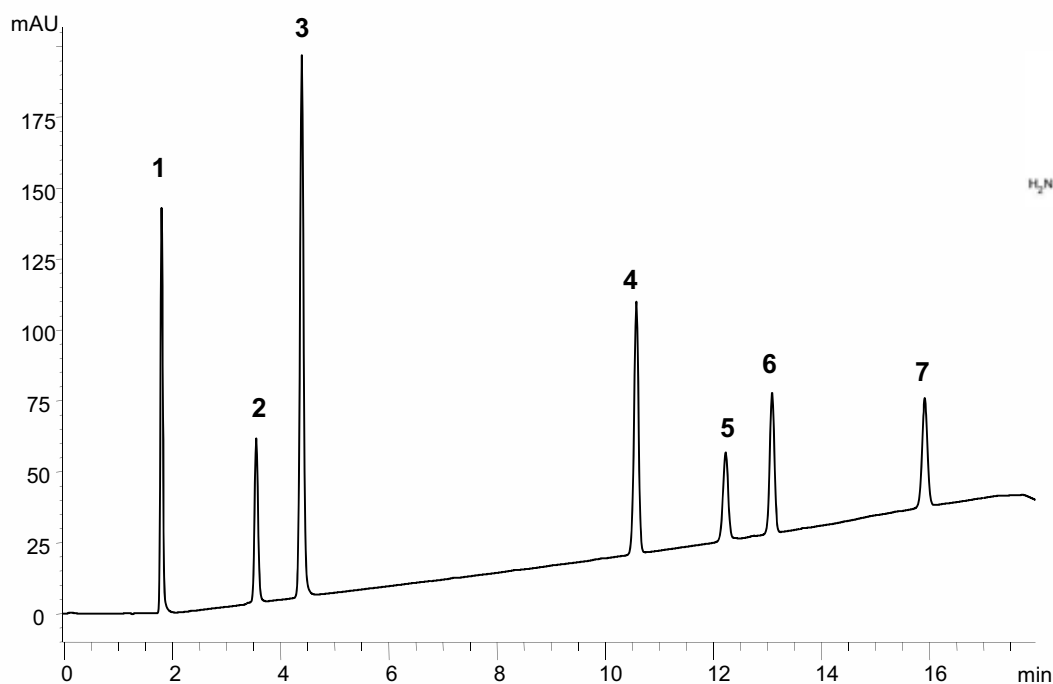
Application #AN1870

Conditions

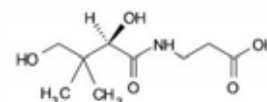
Column: ACE 3 C18-AR
Dimensions: 150 x 4.6 mm
Part Number: ACE-119-1546
Mobile Phase: A: 20 mM potassium phosphate pH 2.83 in H₂O
B: 20 mM potassium phosphate pH 2.83 in MeOH/H₂O (50:50 v/v)

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

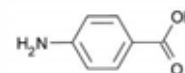
Time (mins)	%B
0	20
15	70



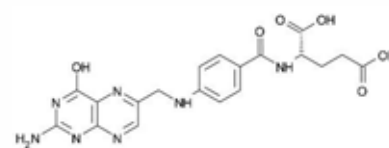
1. Pyridoxine
(Vitamin B6)



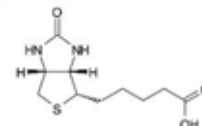
2. Pantothenic acid
(Vitamin B5)



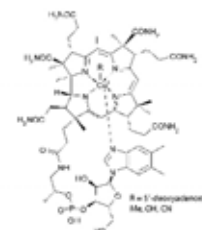
3. p-Aminobenzoic acid



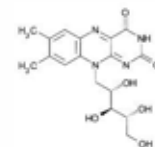
4. Folic acid
(Vitamin B9/ Vitamin M)



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



6. Cyanocobalamin
(Vitamin B12)



7. Riboflavin
(Vitamin B2)

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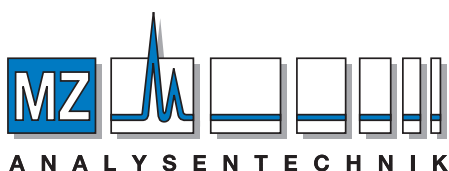


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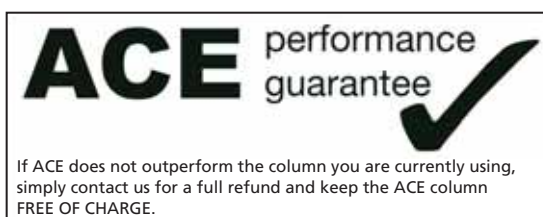


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MZ-Analysentechnik GmbH, Barcelona-Allee 17 • D-55129 Mainz

Tel +49 6131 880 96-0, Fax +49 6131 880 96-20

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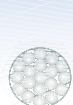


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