ACE®

UHPLC and HPLC Columns

Clinical, Forensic and Bioanalysis Applications Guide

ACE®

UHPLC and HPLC Columns

Ultra-Inert Base Deactivated UHPLC/HPLC Columns

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

ACE® Ultra-inert UHPLC & HPLC Columns

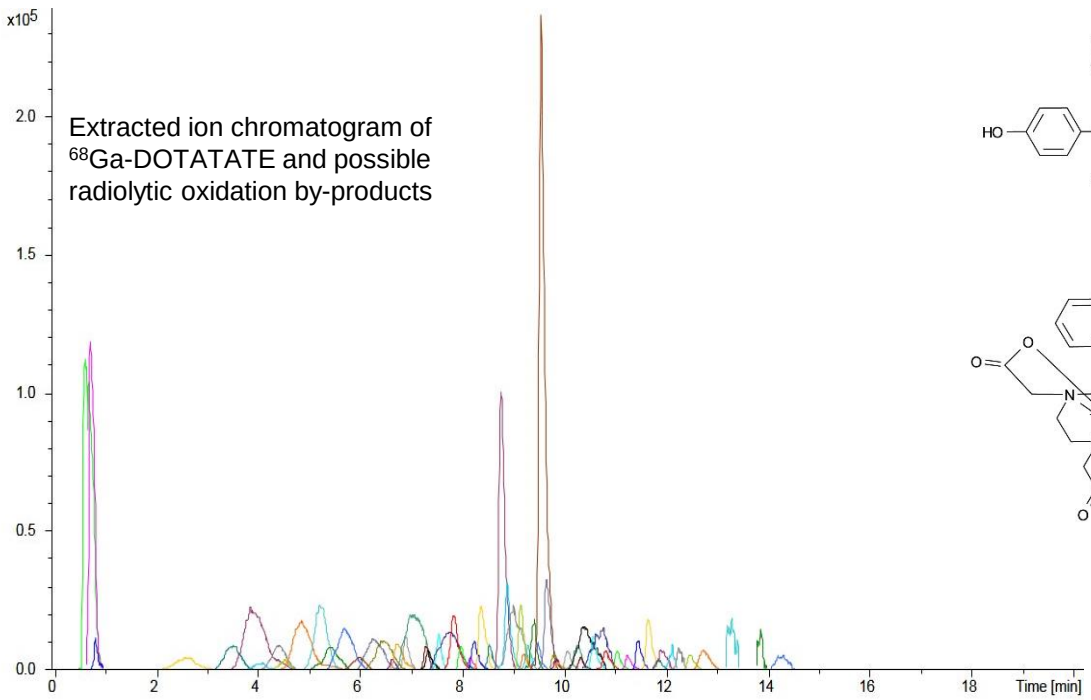
Application #AN2710

Conditions

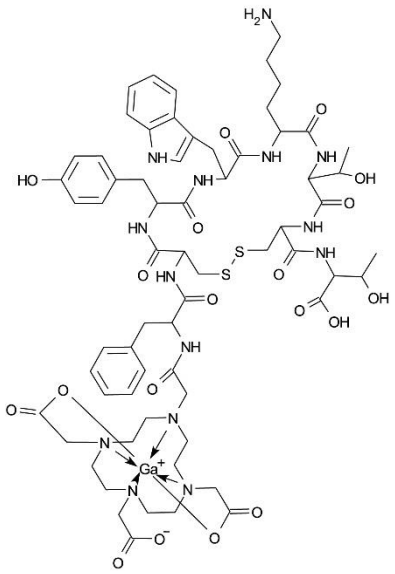
Column:	ACE 3 C18
Dimensions:	50 x 4.6 mm
Part Number:	ACE-111-0546
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

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

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



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



1. ^{68}Ga-DOTATATE

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Acylcarnitines by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

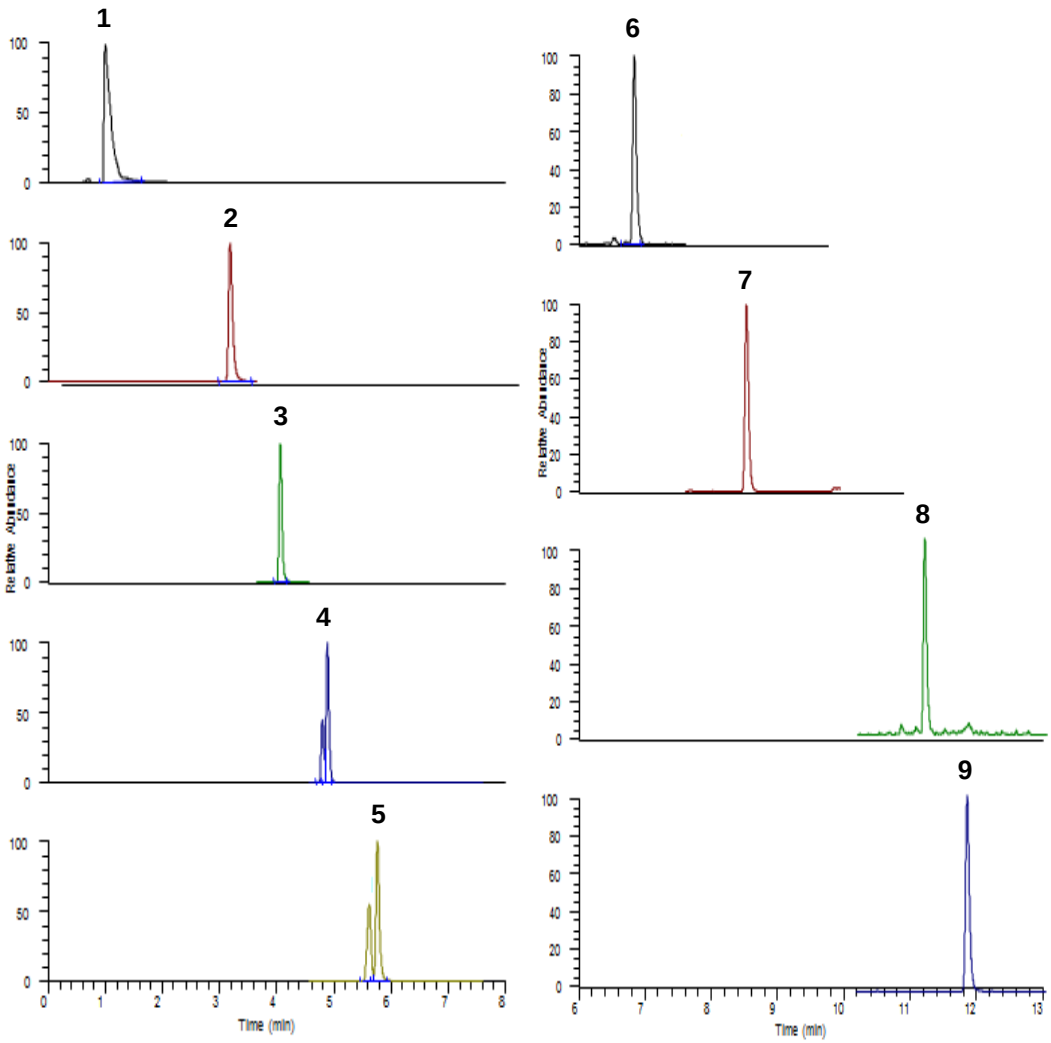
Application #**AN1150**

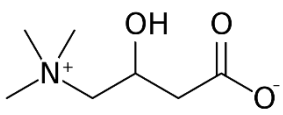
Conditions

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 H_2O
	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. Isovalerylcarnitine & 2-Methylbutyrylcarnitine
(*m/z* 246.20 → 85.25-85.35)
6. Hexanoylcarnitine
(*m/z* 260.20 → 85.25-85.35)
7. Octanoylcarnitine
(*m/z* 288.20 → 85.25-85.35)
8. Myristoylcarnitine
(*m/z* 372.30 → 85.25-85.35)
9. Palmitoylcarnitine
(*m/z* 400.30 → 85.25-85.35)

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Alcohol Biomarkers by UHPLC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

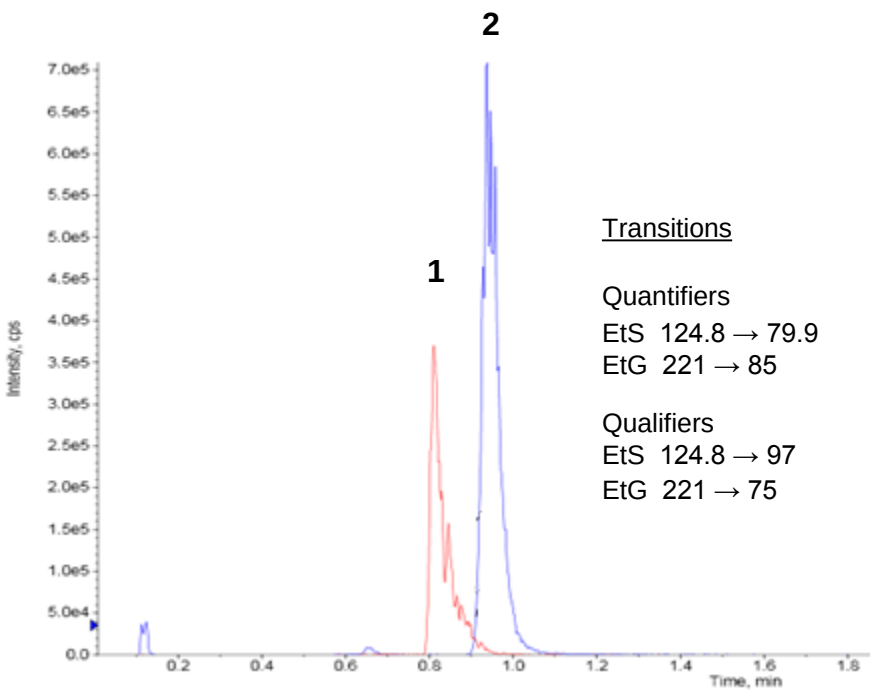
Application #**AN1910**

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

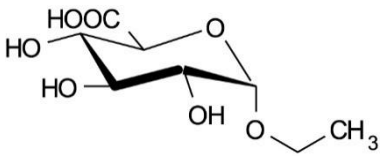
Flow Rate:	0.4 mL/min
Injection:	1 µL
Temperature:	40 °C
Detection:	AB SCIEX triple quad 5500 Negative ESI MRM Source temperature: 750 °C IonSpray voltage: -4500 V



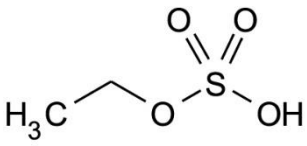
Transitions

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

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Amino Acids Derivatised with Dabsyl Chloride

ACE®
Ultra-inert
UHPLC & HPLC Columns

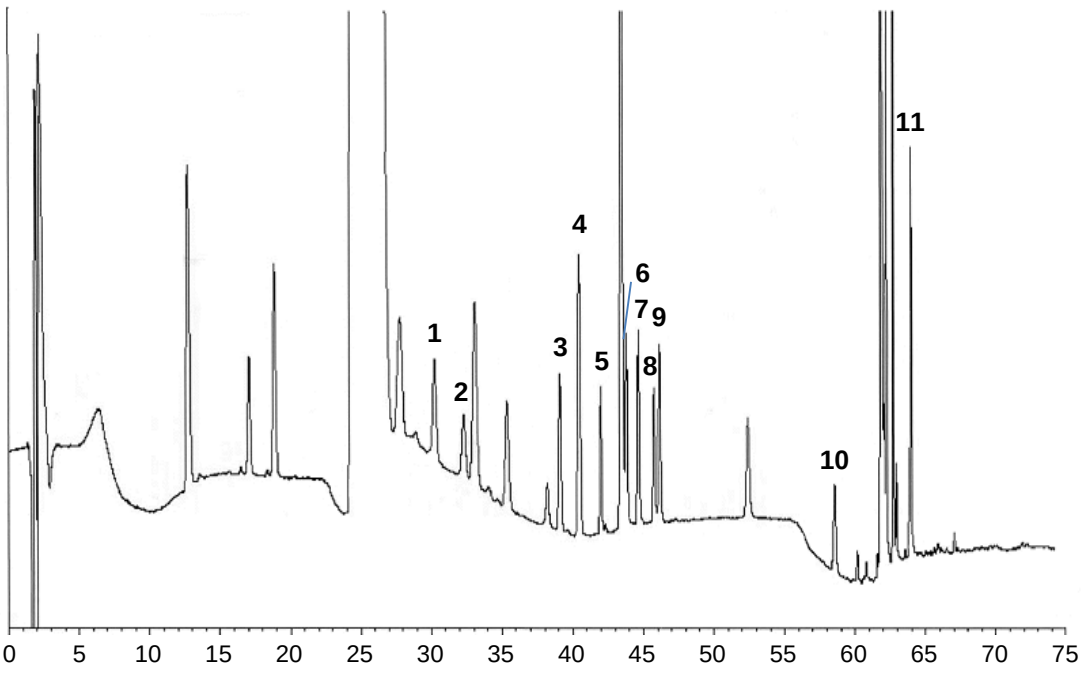
Application #AN3420

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 H_2O 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

ACE®
Ultra-inert
UHPLC & HPLC Columns

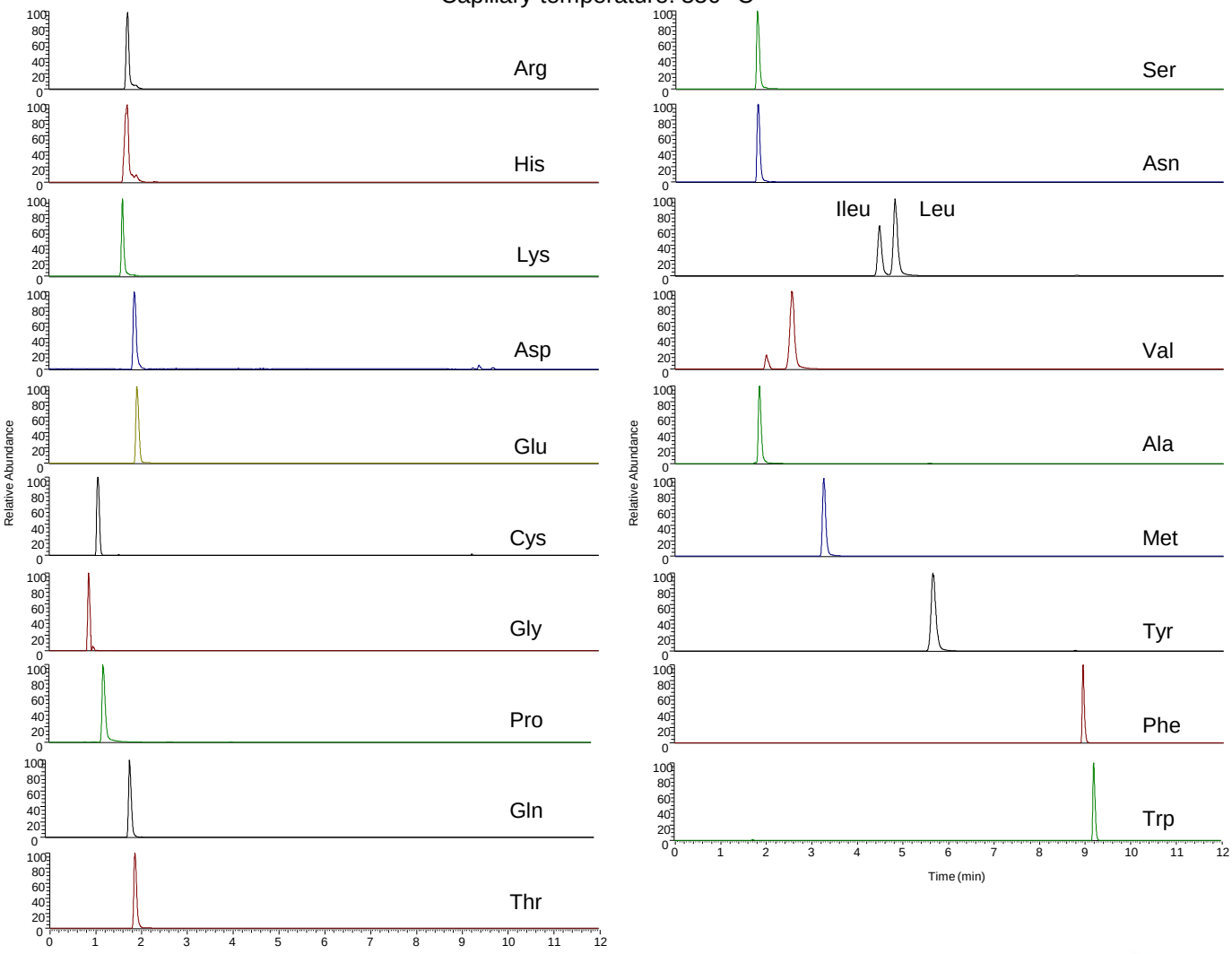
Application #AN2660

Conditions

Column:	ACE 3 AQ
Dimensions:	150 x 3.0 mm
Part Number:	ACE-116-1503
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: 0.1% formic acid in MeCN

Time (mins)	%B
0	0
10	100

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



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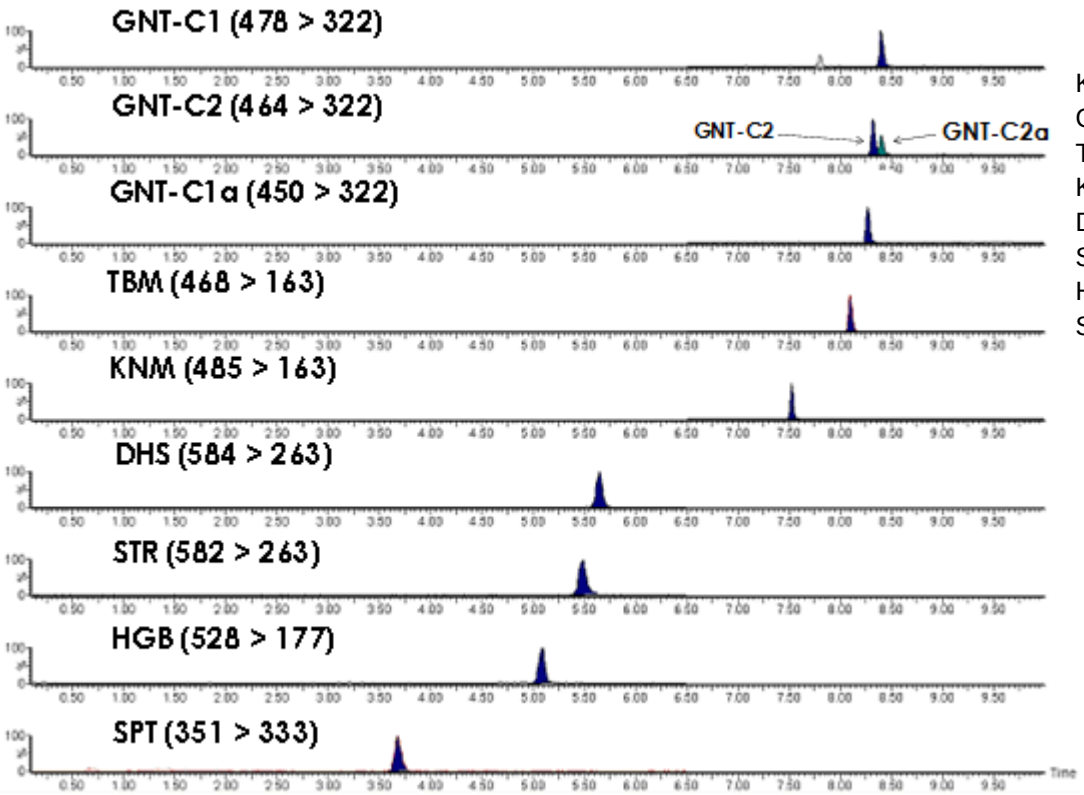
Application #AN1920

Conditions

Column:	ACE Excel 2 C18-PFP
Dimensions:	100 x 2.1 mm
Part Number:	EXL-1010-1002U
Mobile Phase:	A: 20 mM HFBA in H_2O/MeCN (98:2 v/v) B: 20 mM HFBA in MeCN/H_2O (98:2 v/v)

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

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



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

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Amphetamines In Urine by LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

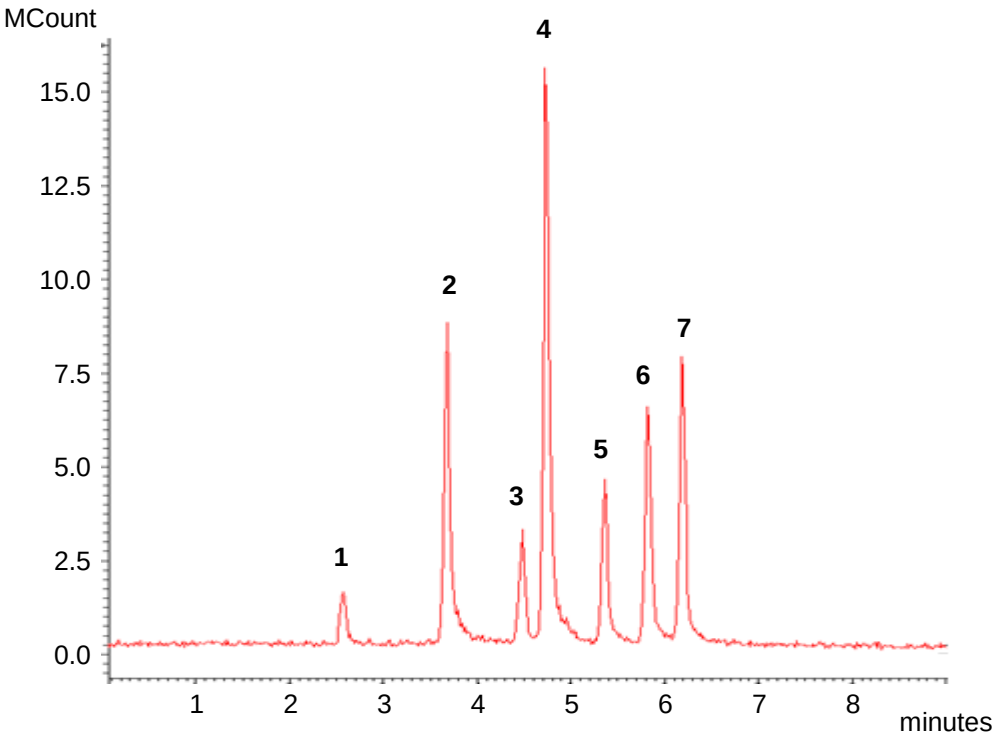
Application #AN1010

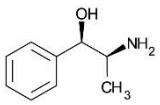
Conditions

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 H_2O
	B: 5 mM ammonium hydroxide pH 10.8 in MeOH/H_2O (90:10 v/v)

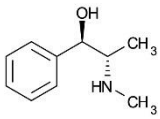
Time (mins)	%B
0	30
8	95

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

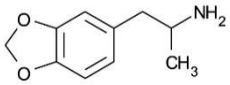




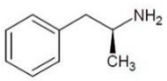
1. Phenylpropanolamine
LOD (est) 4 ppb
(*m/z* 151.6 → 134.0)



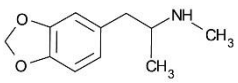
2. (l)-Ephedrine
LOD (est) 2 ppb
(*m/z* 166.2 → 148.0)



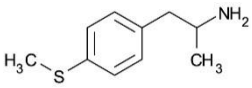
3. (dl)-3,4-MDA
LOD (est) 30 ppb
(*m/z* 179.7 → 163.0)



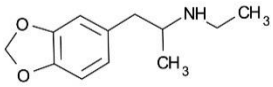
4. (d)-Amphetamine
LOD (est) 4 ppb
(*m/z* 135.8 → 90.9)



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)

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Anabolic Steroids from Horse Urine by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

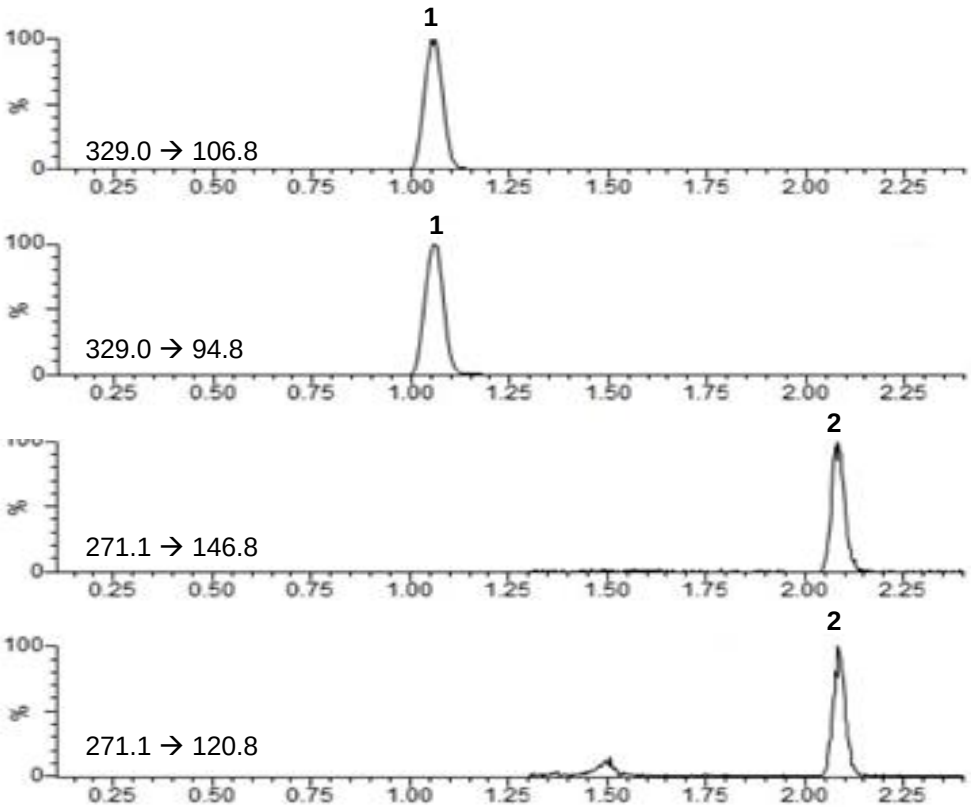
Application #AN2360

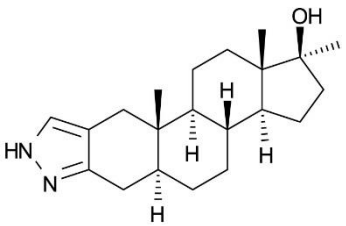
Conditions

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 H_2O
	B: 2 mM ammonium acetate, 0.1% formic acid in MeOH

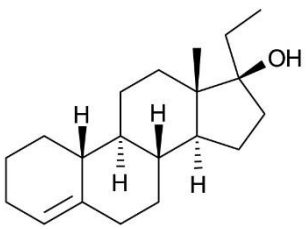
Time (mins)	%B
0.00	75
0.25	75
1.50	90
1.51	100
3.50	100
3.51	75
4.00	75

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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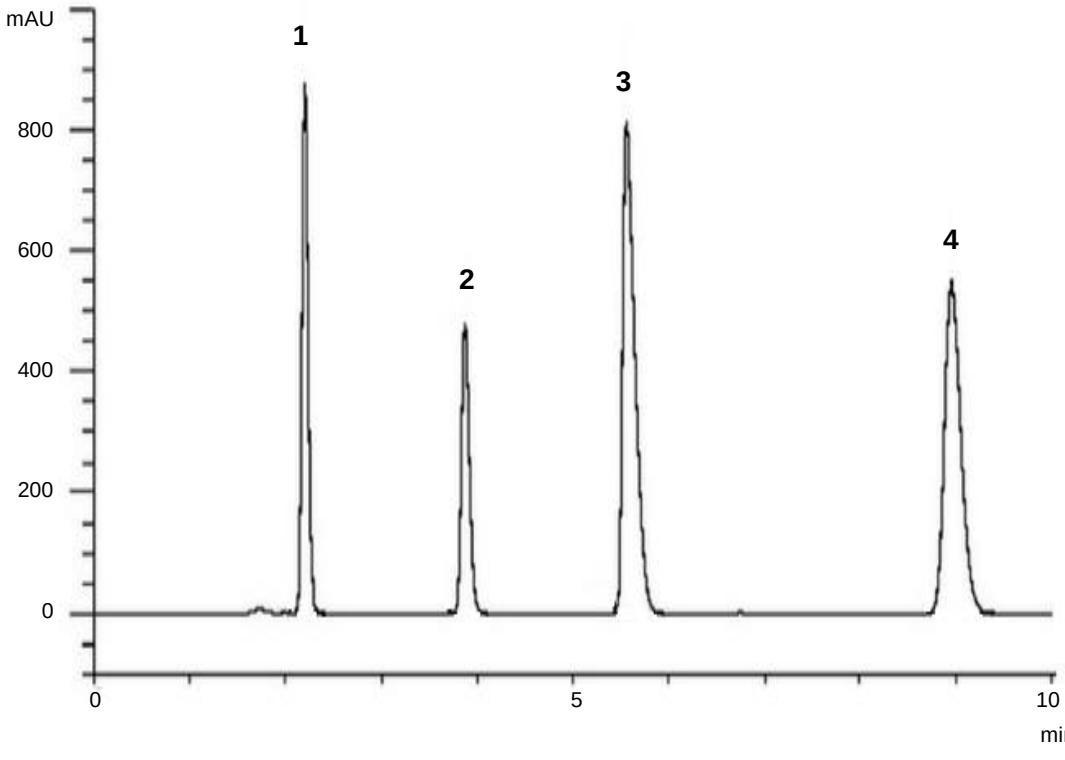
Angiotensin II Receptor Antagonists by LC-UV

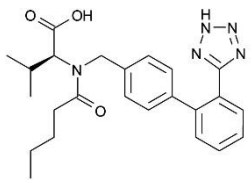
ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN3460

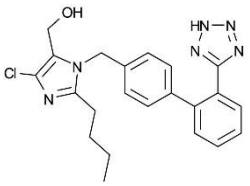
Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	0.025 M KH_2PO_4 pH 6.0/MeCN (65:35 v/v)
Flow Rate:	1.5 mL/min
Temperature:	40 °C
Detection:	UV, 220 nm

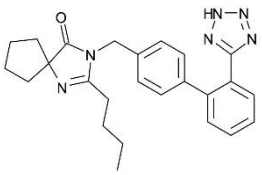




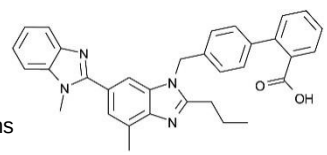
1. Valsartan



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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Angiotensin Peptides

ACE®
Ultra-inert
UHPLC & HPLC Columns

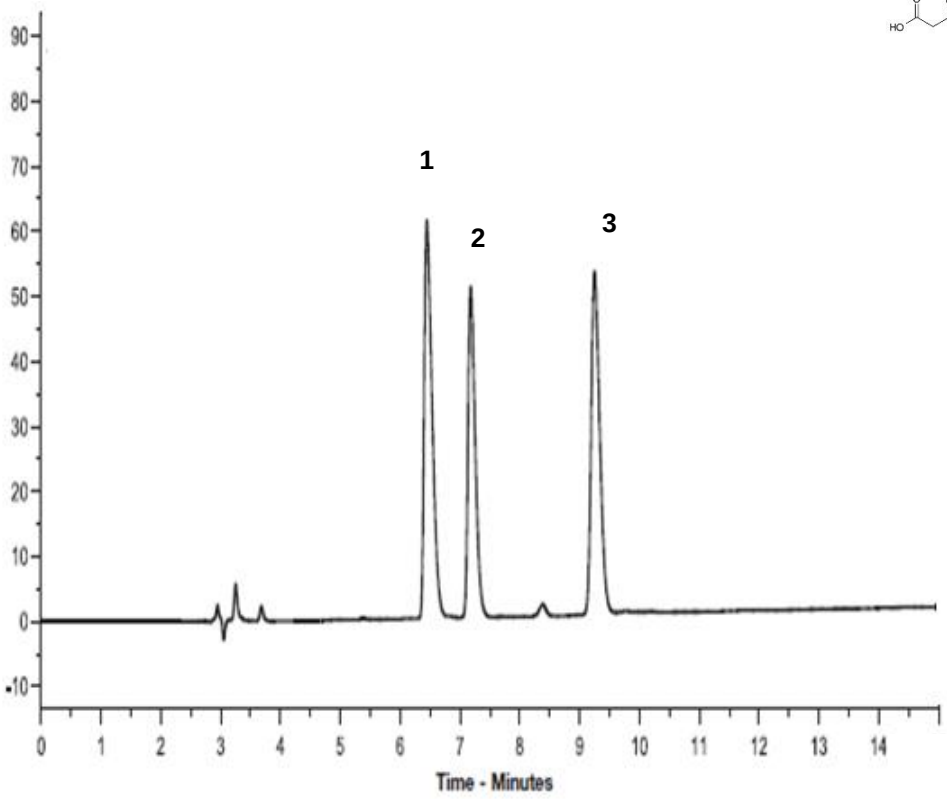
Application #AN2150

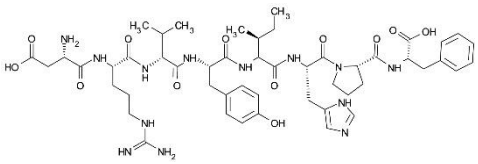
Conditions

Column:	ACE 5 C18-300
Dimensions:	250 x 4.6 mm
Part Number:	ACE-221-2546
Mobile Phase:	A: 0.1 % TFA in H_2O
	B: 0.1% TFA in H_2O/MeCN (80:20 v/v)

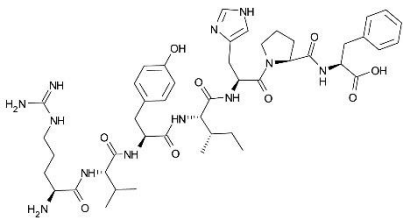
Time (mins)	%B
0	25
15	40

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

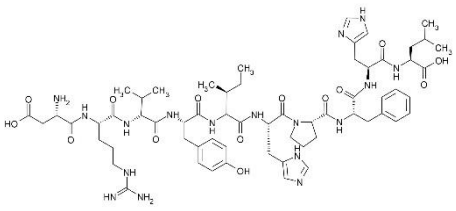




1. Angiotensin II
(*m/z* 1046.2)



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



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

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Antihistamines

ACE®
Ultra-inert
UHPLC & HPLC Columns

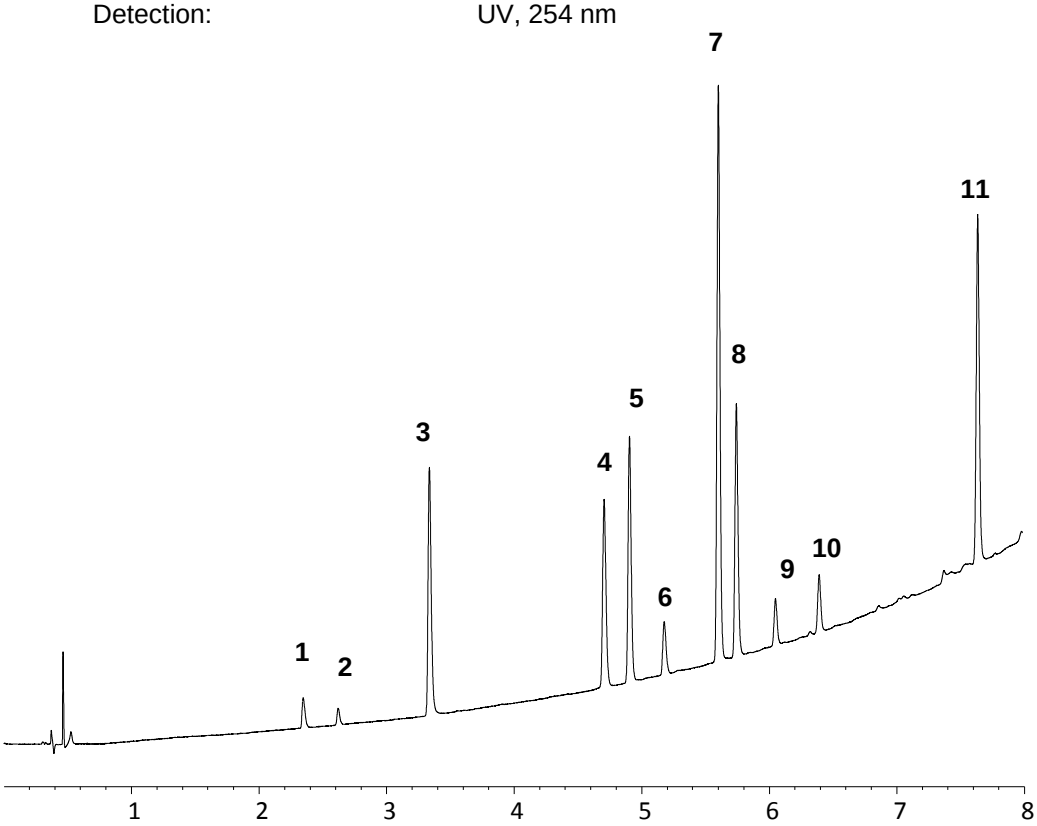
Application #AN1400

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 H_2O
	B: 20 mM ammonium formate pH 3.0 in MeOH/H_2O (9:1 v/v)

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

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



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

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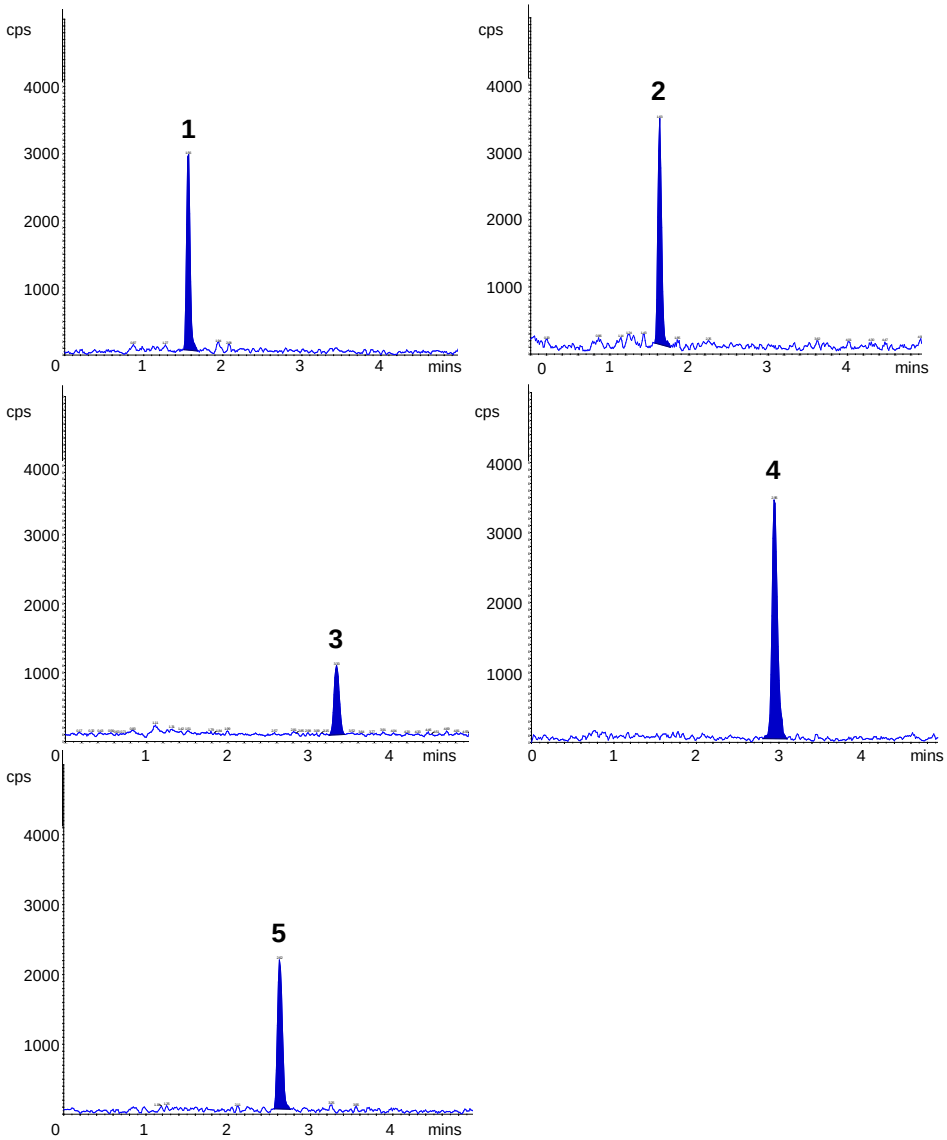
Antiretrovirals in Human Mononuclear Cell Extracts by LC-MS/MS

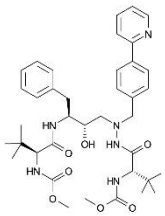
ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN3470

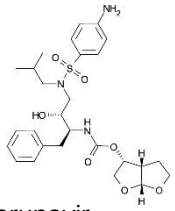
Conditions

Column:	ACE 3 C18
Dimensions:	100 x 3.0 mm
Part Number:	ACE-111-1003
Mobile Phase:	MeCN/H_2O/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)

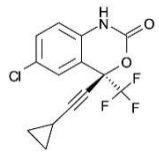




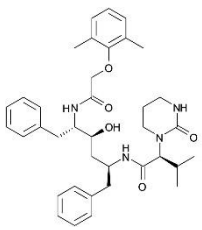
1. Atazanavir
(*m/z* 705.4 → 168.2)
LLOQ: 0.04 fmol/sample



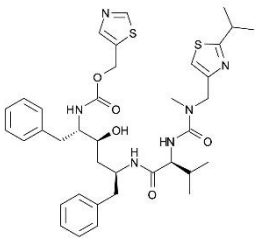
2. Darunavir
(*m/z* 548.3 → 392.3)
LLOQ: 1.0 fmol/sample



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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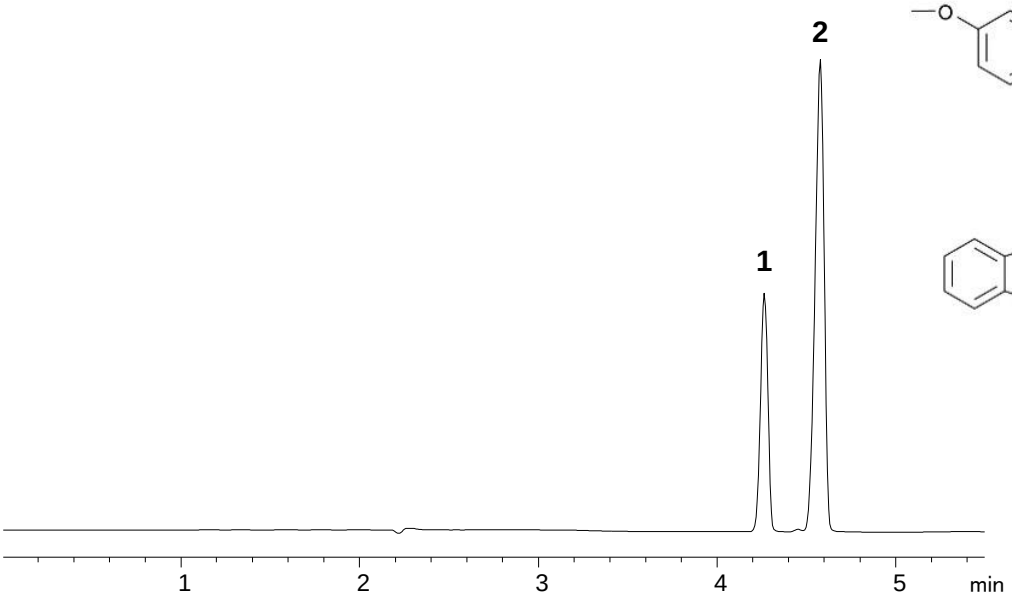
Anti-Ulcer Drugs in Basic Mobile Phase Conditions

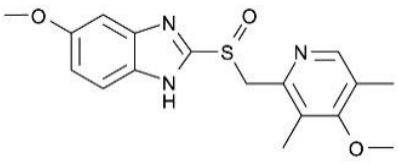
ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN1950

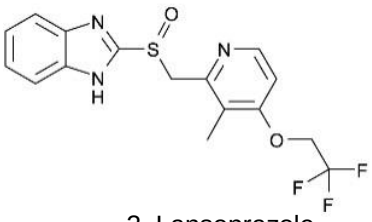
Conditions

Column:	ACE 5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1211-1546U
Mobile Phase:	A: 0.1% ammonia in H_2O
	B: 0.1% ammonia in MeCN/H_2O (90:10 v/v)
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	30 °C
Detection:	UV, 280 nm





1. Omeprazole



2. Lansoprazole

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Appetite Suppressants by LC-MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

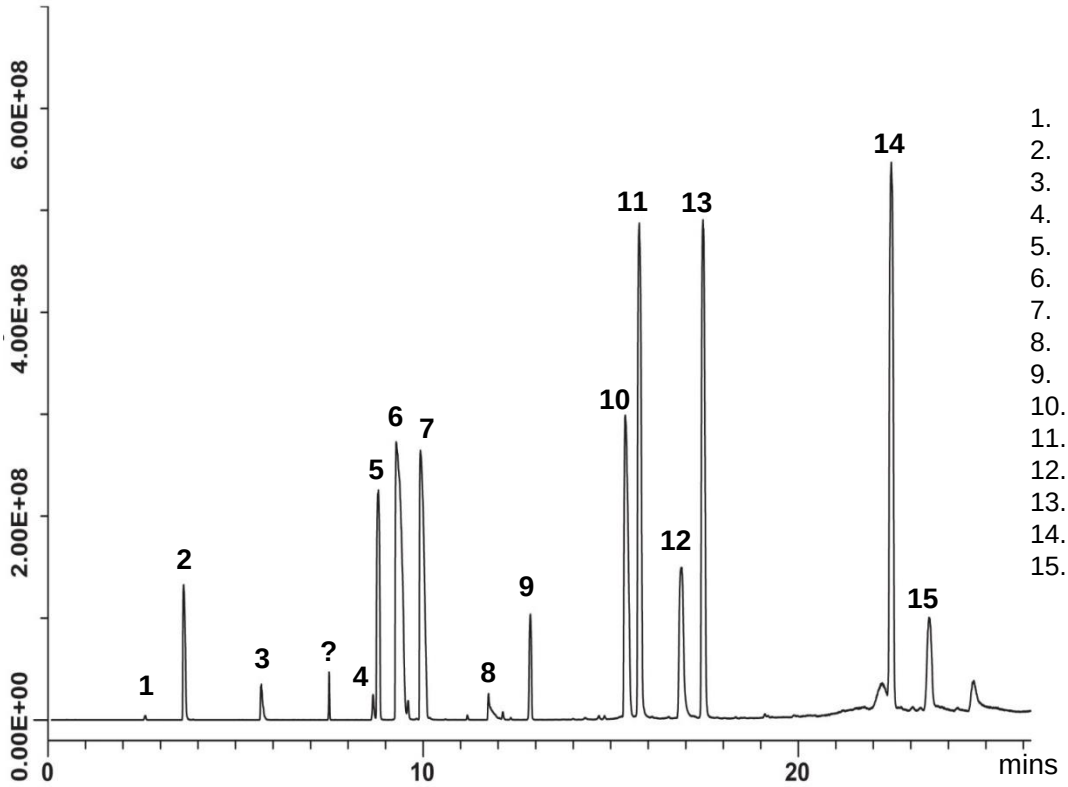
Application #AN1960

Conditions

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

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

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



1. Caffeine
2. Ephedrine
3. Phentermine
4. Phenolphthalein
5. Chlordiazepoxide
6. Lorcaserin
7. Fenfluramine
8. Fluoxetine
9. Diethylpropion
10. Sertraline
11. Didesmethylsibutramine
12. Rimonabant
13. N-Desmethylsibutramine
14. Sibutramine
15. Orlistat

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β-Antagonists and Diuretics

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN1410

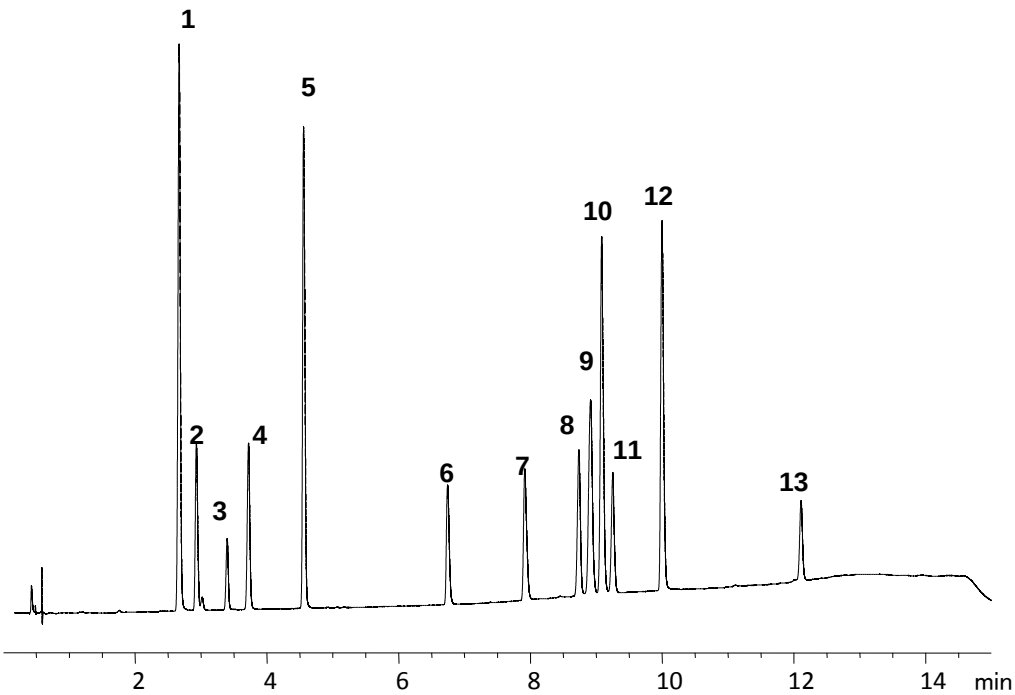
Conditions

Column:	ACE 3 C18
Dimensions:	100 x 2.1 mm
Part Number:	EXL-111-1002
Mobile Phase:	A: 20 mM KH_2PO_4, pH 2.7
	B: 20 mM KH_2PO_4, pH 2.7 in MeCN/H_2O (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

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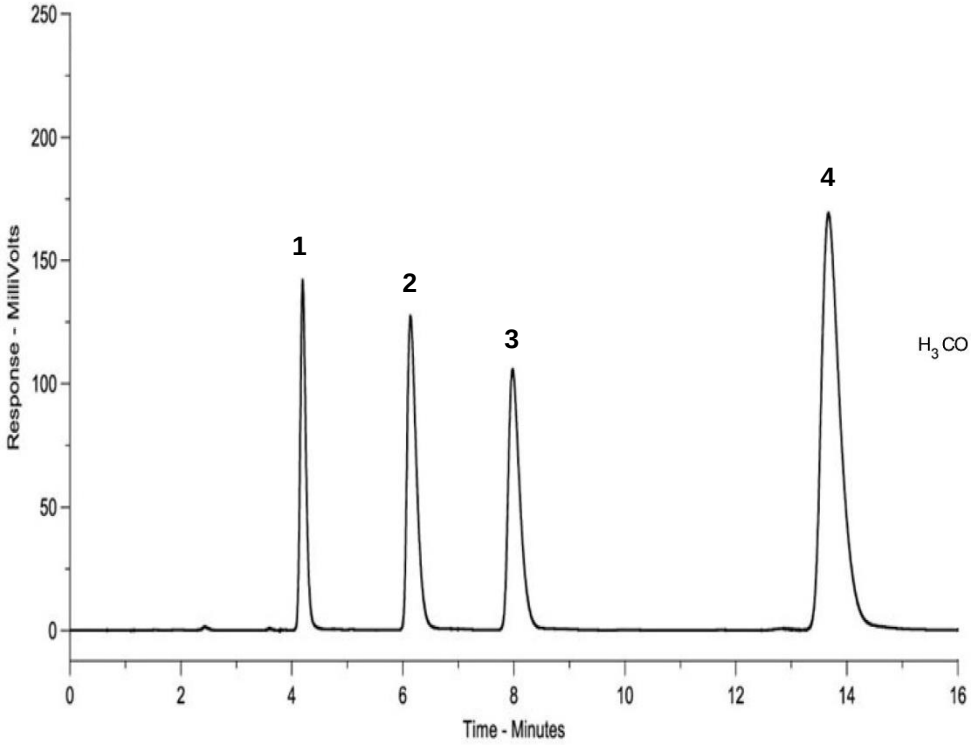
β-Blockers

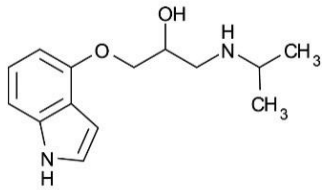
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN3160

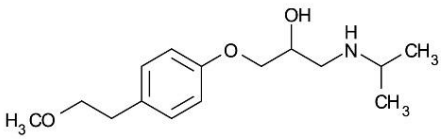
Conditions

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

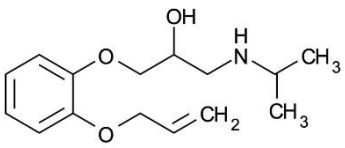




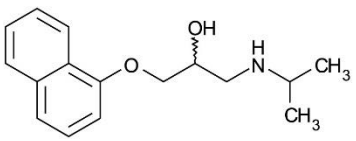
1. Pindolol



2. Metoprolol



3. Oxprenolol



4. Propranolol

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β-Blockers by LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

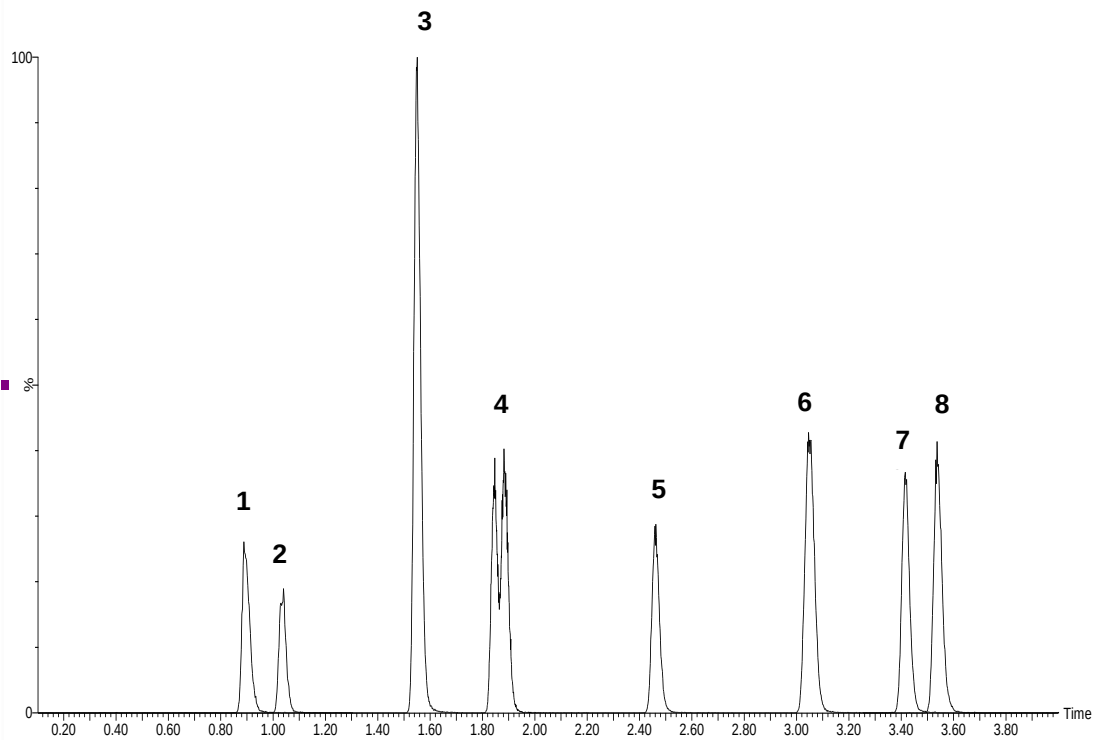
Application #AN2620

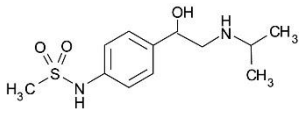
Conditions

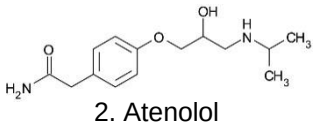
Column:	ACE Excel 2 C18
Dimensions:	50 x 2.1 mm
Part Number:	EXL-101-0502U
Mobile Phase:	A: 2 mM ammonium acetate + 0.1% formic acid in H_2O
	B: 2 mM ammonium acetate + 0.1% formic acid in MeOH

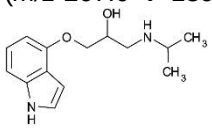
Time (mins)	%B
0.0	10
3.0	50
3.1	10

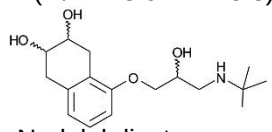
Flow Rate:	0.4 mL/min
Injection:	10 µL
Temperature:	40 °C
Detection:	MS/MS
	ESI in positive ion mode
Sample:	2.5 pg/µL

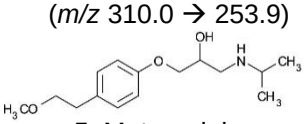


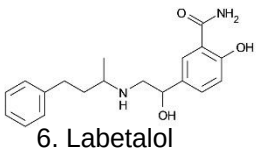

1. Sotalol
(*m/z* 272.9 → 212.8)

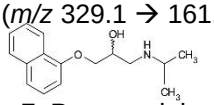

2. Atenolol
(*m/z* 267.0 → 189.8)

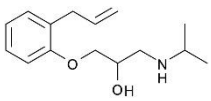

3. Pindolol
(*m/z* 248.9 → 115.8)


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

ACE® Ultra-inert UHPLC & HPLC Columns

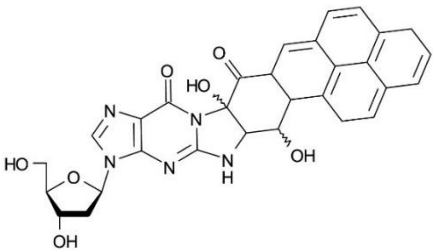
Application #AN3170

Conditions

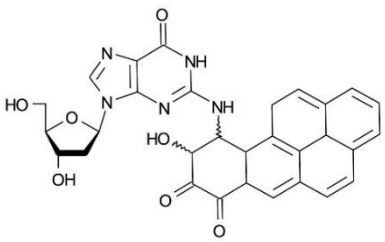
Column:	ACE 3 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-111-1546
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: MeCN

Time (mins)	%B
0	25
8	55

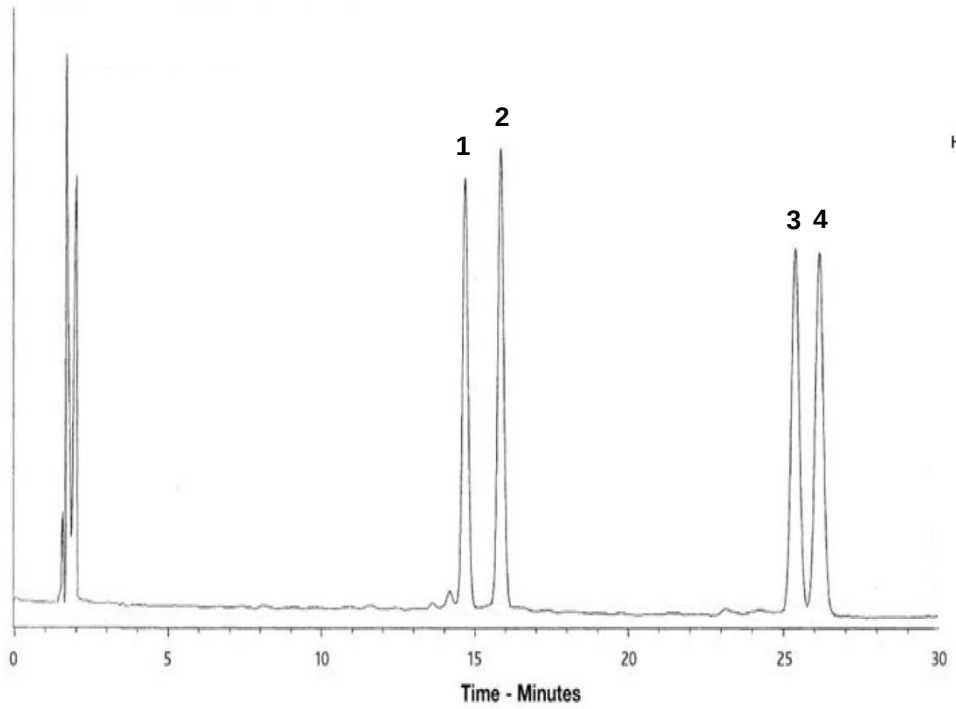
Flow Rate:	1 mL/min
Injection:	5 µL
Temperature:	35 °C
Detection:	UV, 285 nm



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

ACE® Ultra-inert UHPLC & HPLC Columns

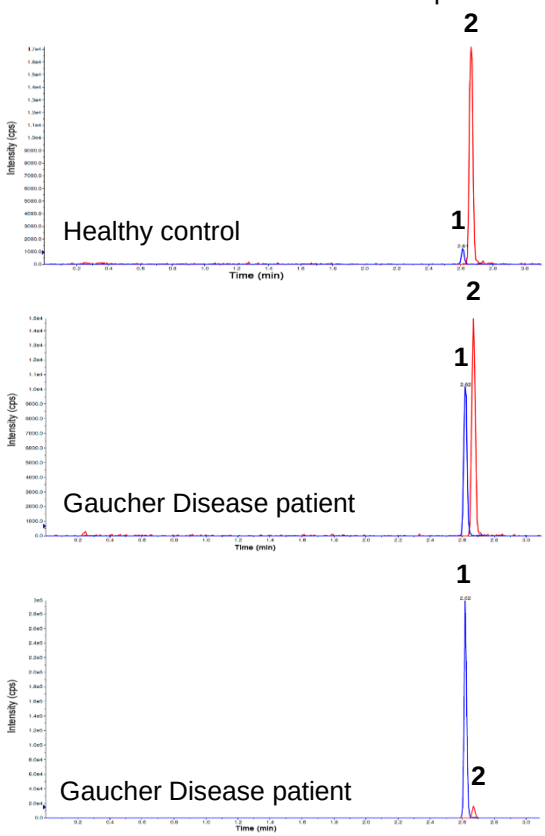
Application #AN3490

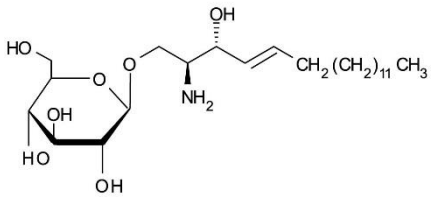
Conditions

Column:	ACE 3 C8
Dimensions:	50 x 2.1 mm
Part Number:	ACE-112-0502
Mobile Phase:	A: 50 mM formic acid in H_2O
	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

ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN3480

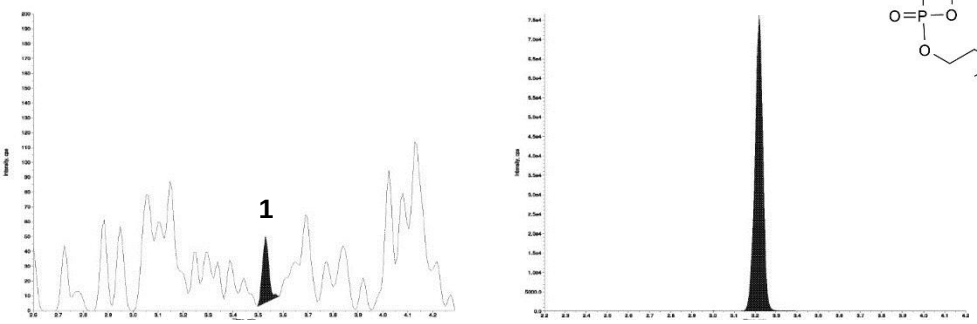
Conditions

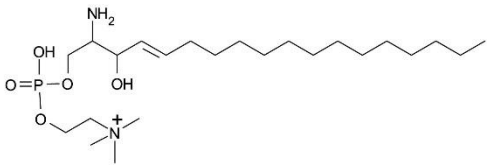
Column:	ACE 3 C8
Dimensions:	50 x 2.1 mm
Part Number:	ACE-112-0502
Mobile Phase:	A: 50 mM formic acid in H_2O
	B: 50 mM formic acid in MeCN/acetone (1:1 v/v)

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



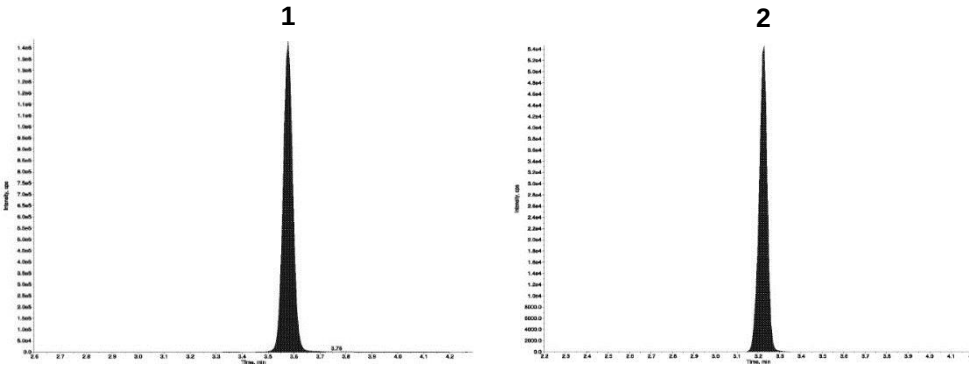


Lyso-SM (lyso-sphingomyelin)

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 Vruchte 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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Biomarker Profiling

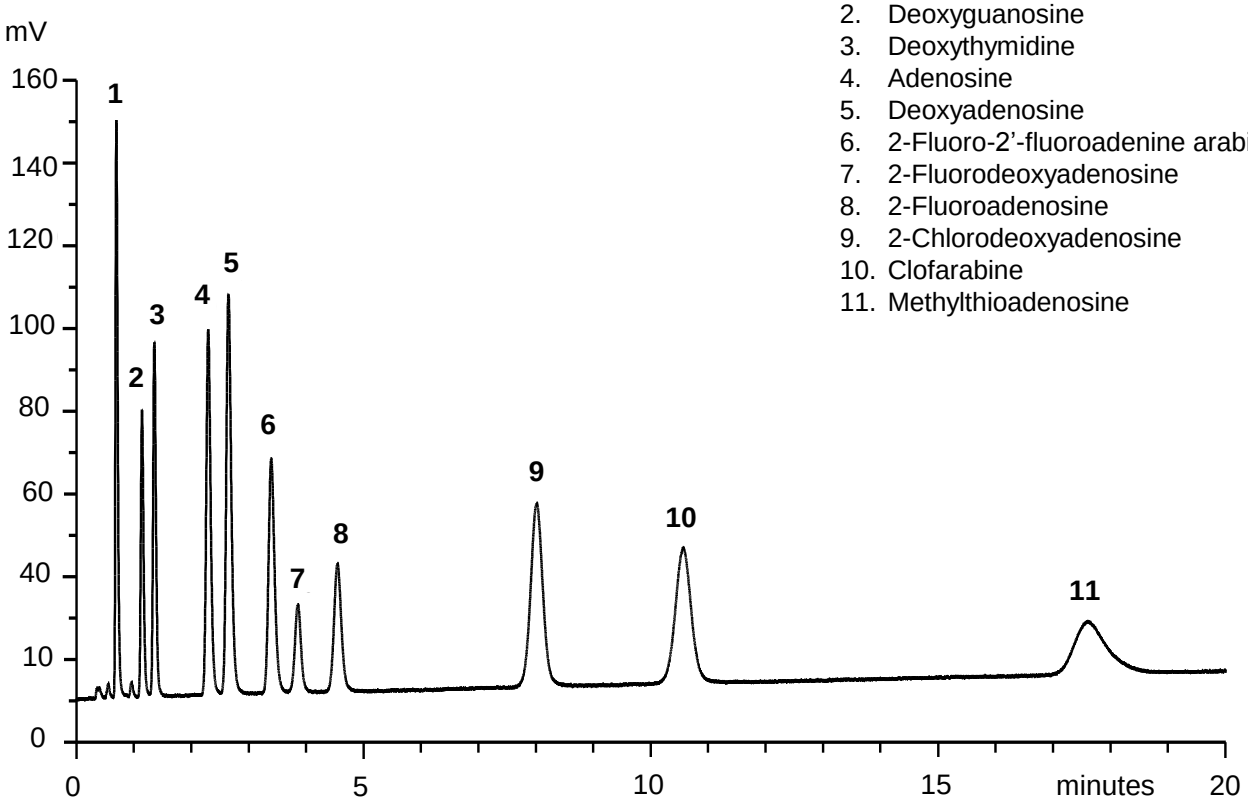
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN1990

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 KH_2PO_4, pH 6 with KOH B: 7% methanol, 2.1 mM tetrabutylammonium bisulphate + 8.4 mM KH_2PO_4, 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

1. Deoxyuridine
2. Deoxyguanosine
3. Deoxythymidine
4. Adenosine
5. Deoxyadenosine
6. 2-Fluoro-2'-fluoroadenine arabinoside
7. 2-Fluorodeoxyadenosine
8. 2-Fluoroadenosine
9. 2-Chlorodeoxyadenosine
10. Clofarabine
11. Methylthioadenosine



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Caffeine and Metabolites

ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN2010

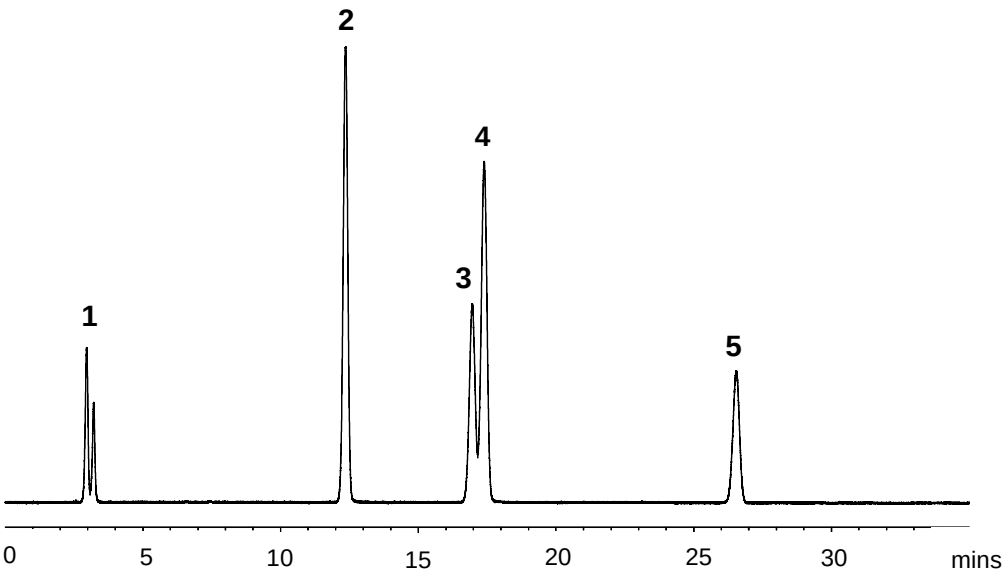
Conditions

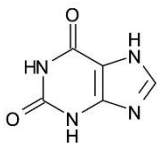
Column:	ACE 5 SuperC18
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1211-1546U
Mobile Phase:	A: 20 mM ammonium acetate pH 7.0 in H_2O
	B: 20 mM ammonium acetate pH 7.0 in MeCN/H_2O (90:10 v/v)

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

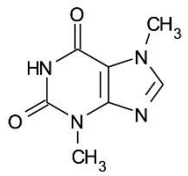
Post time 10 minutes

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

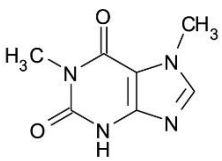




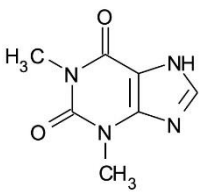
1. Xanthine



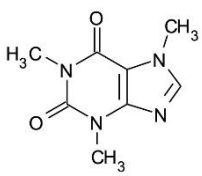
2. Theobromine



3. Paraxanthine



4. Theophylline



5. Caffeine

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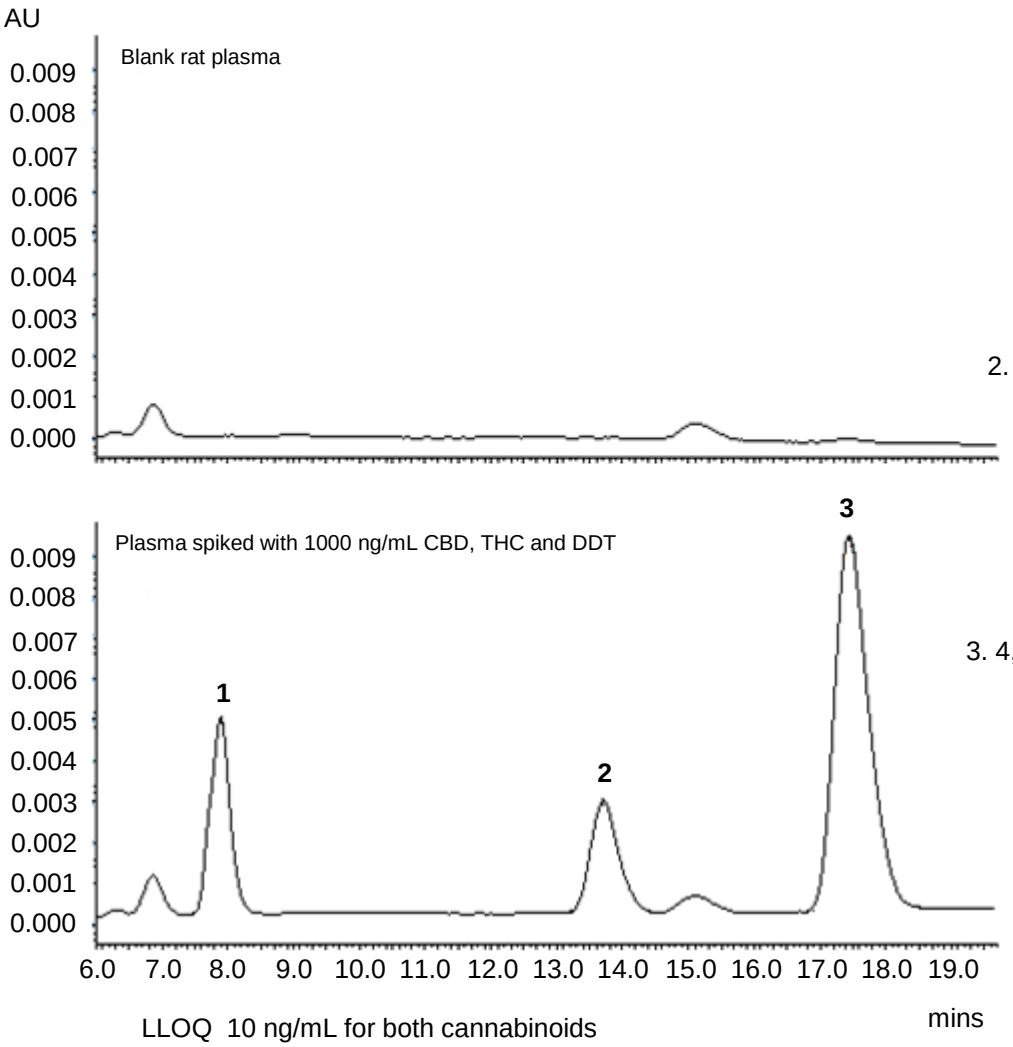
Cannabinoids in Rat Plasma

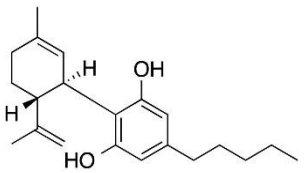
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN2310

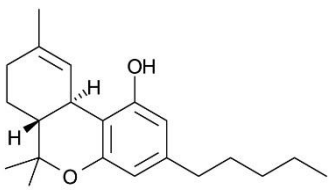
Conditions

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

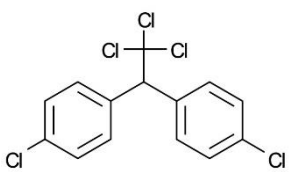




1. Cannabidiol(CBD)



2. Δ^9-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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Cannabinoids (Synthetic) by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

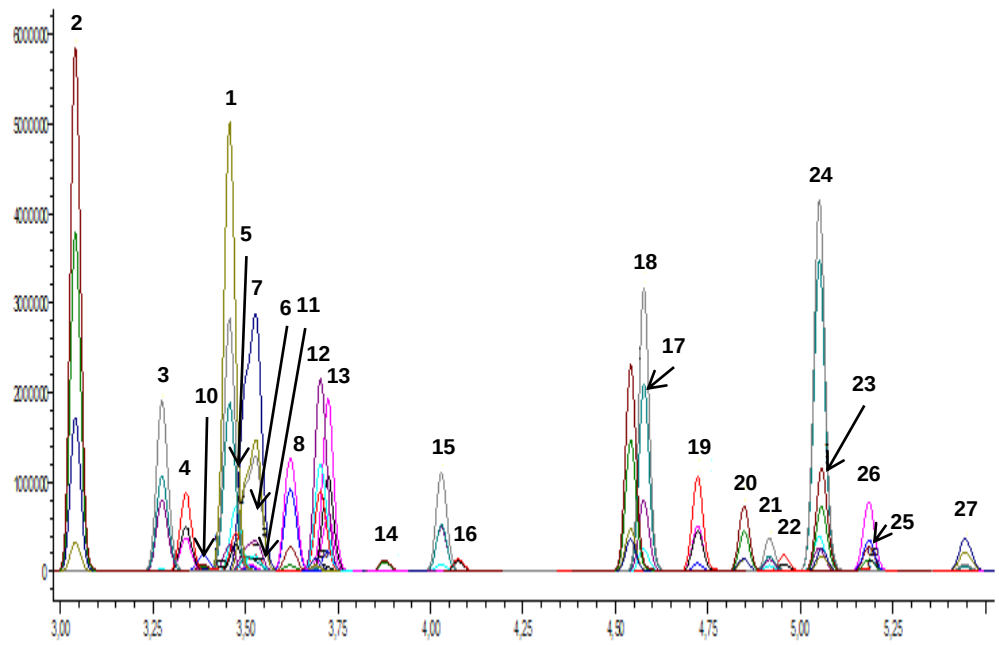
Application #AN2540

Conditions

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

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

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



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

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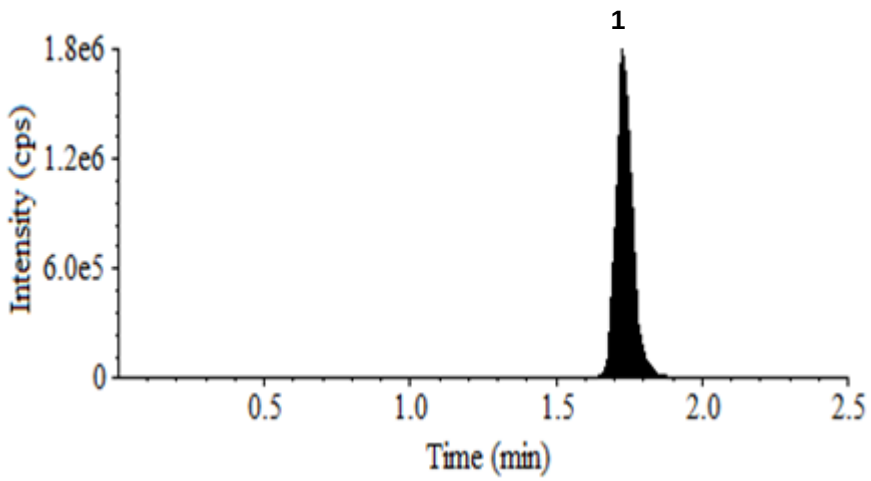
Carglumic Acid in Human Plasma by LC-MS/MS

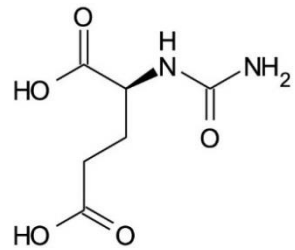
ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN3750

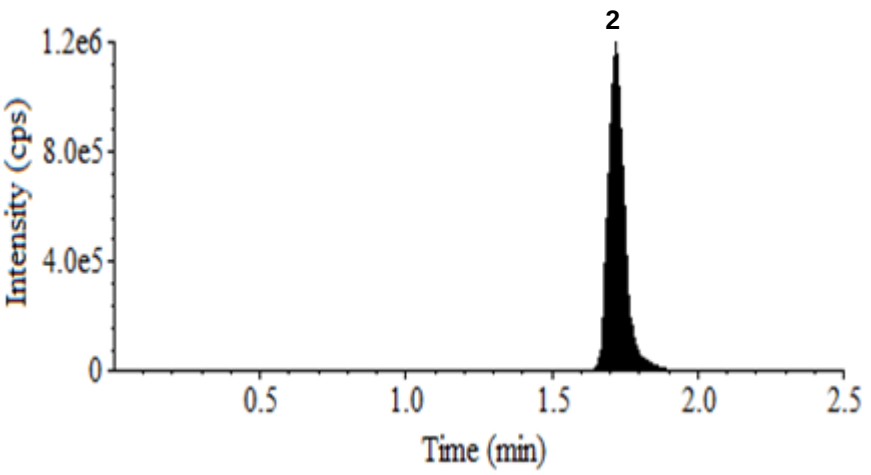
Conditions

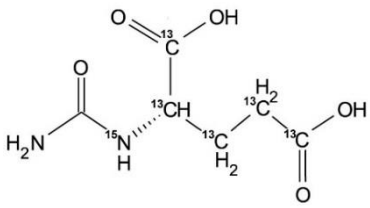
Column:	ACE 5 CN
Dimensions:	150 x 4.6 mm
Part Number:	ACE-124-1546
Mobile Phase:	MeCN/MeOH/0.1% acetic acid pH 3.2 (40:40:20 v/v/v)
Flow Rate:	1 mL/min
Temperature:	40 °C
Detection:	MDS Sciex API-4000 triple quad MS Negative ion mode ESI Ion source temperature: 500 °C Ion spray voltage: -4500 V 20%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





1. Carglumic acid
(*m/z* 189 → 146)
(LLOQ 6.0 ng/mL)





2. Carglumic acid-13C 15N (I.S.)
(*m/z* 195 → 152)

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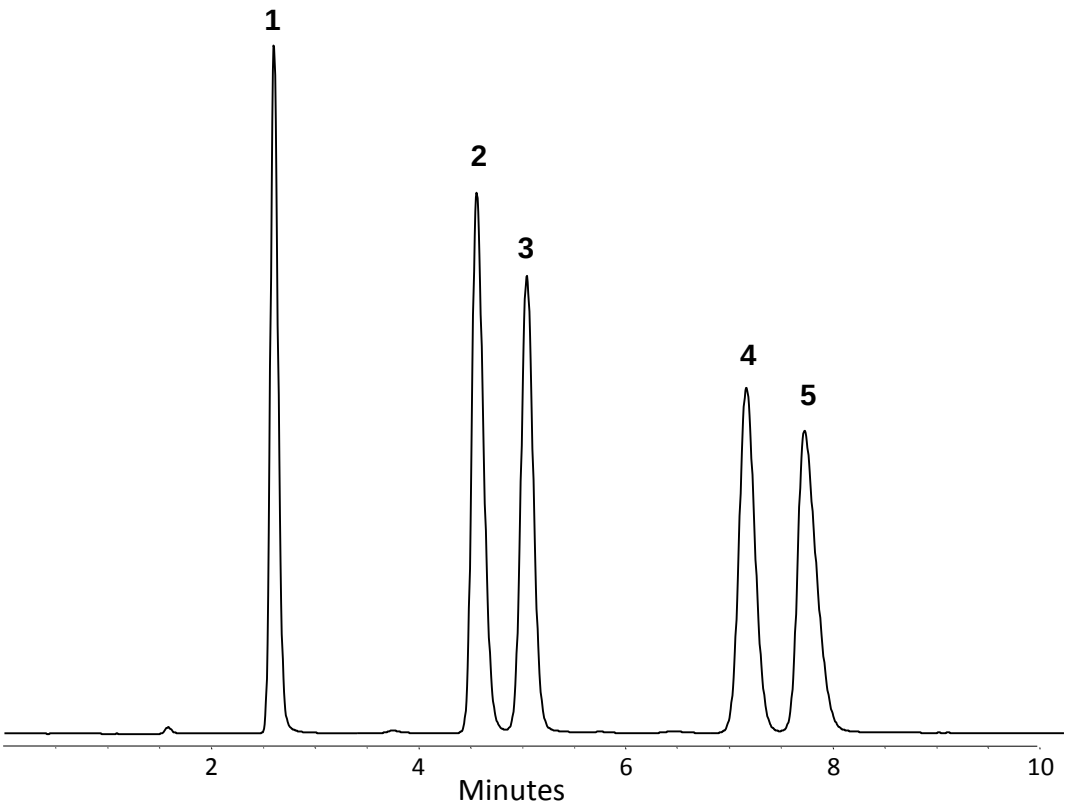
Catecholamine Analysis

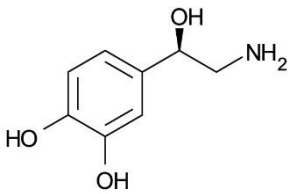
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN2020**

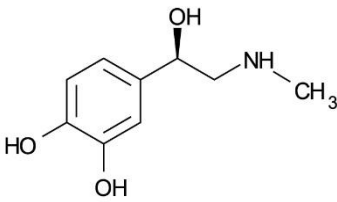
Conditions

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

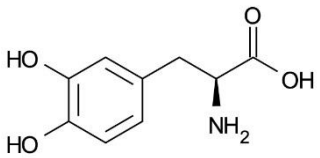




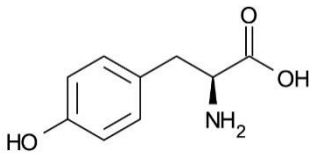
1. Norepinephrine



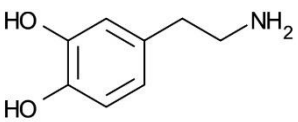
2. Epinephrine



3. Levodopa



4. Tyrosine



5. Dopamine

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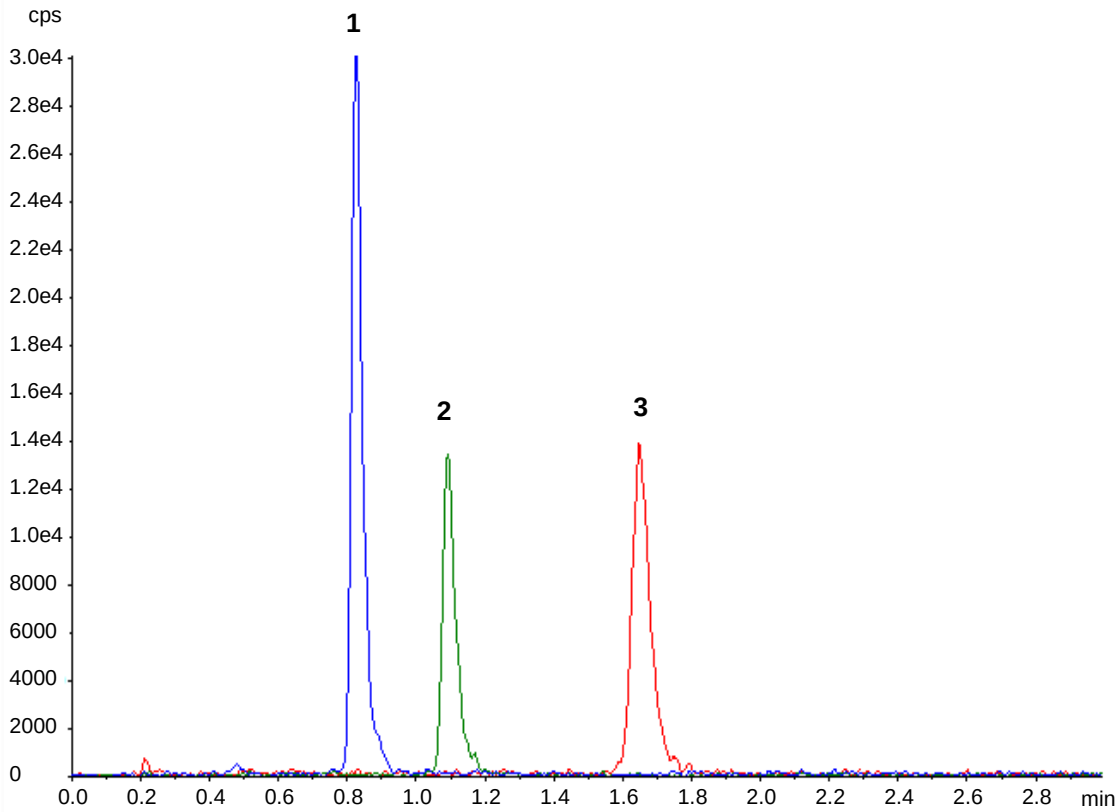
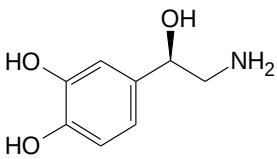
Catecholamines by LC-MS/MS

Application #**AN2320**

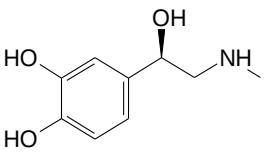
Conditions

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

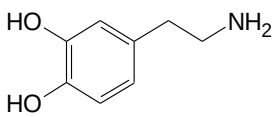




1. Norepinephrine
(*m/z* 152.1 → 107.1)



2. Epinephrine
(*m/z* 166.1 → 107.1)



3. Dopamine
(*m/z* 154.1 → 91.1)

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

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Catecholamines and Metanephrines Separation (Gradient)

ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN1480

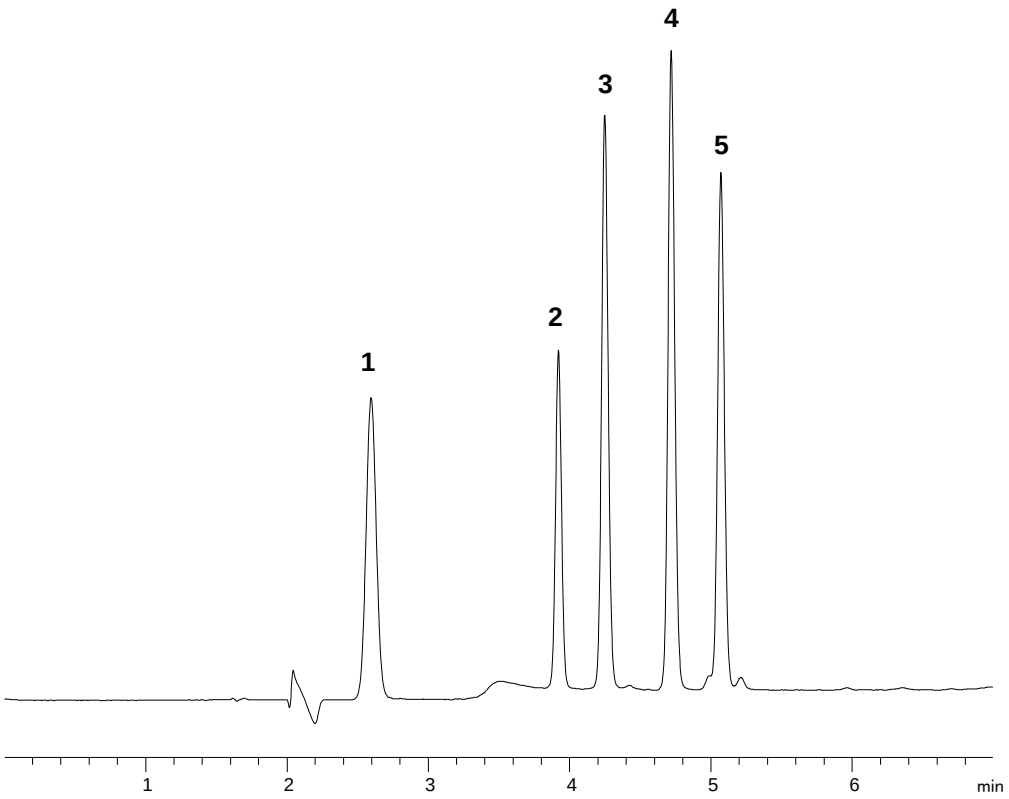
Conditions

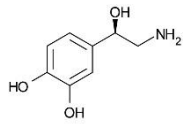
Column:	ACE 5 C18-PFP
Dimensions:	150 x 4.6 mm
Part Number:	ACE-1210-1546
Mobile Phase:	A: 20 mM ammonium formate pH 3.0 in H_2O
	B: 20 mM ammonium formate pH 3.0 in MeOH/H_2O (90:10 v/v)

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

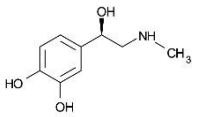
Post time 10 minutes

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

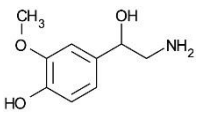




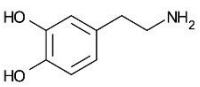
1. Norepinephrine



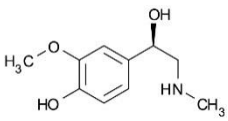
2. Epinephrine



3. Normetanephrine



4. Dopamine



5. Metanephrine

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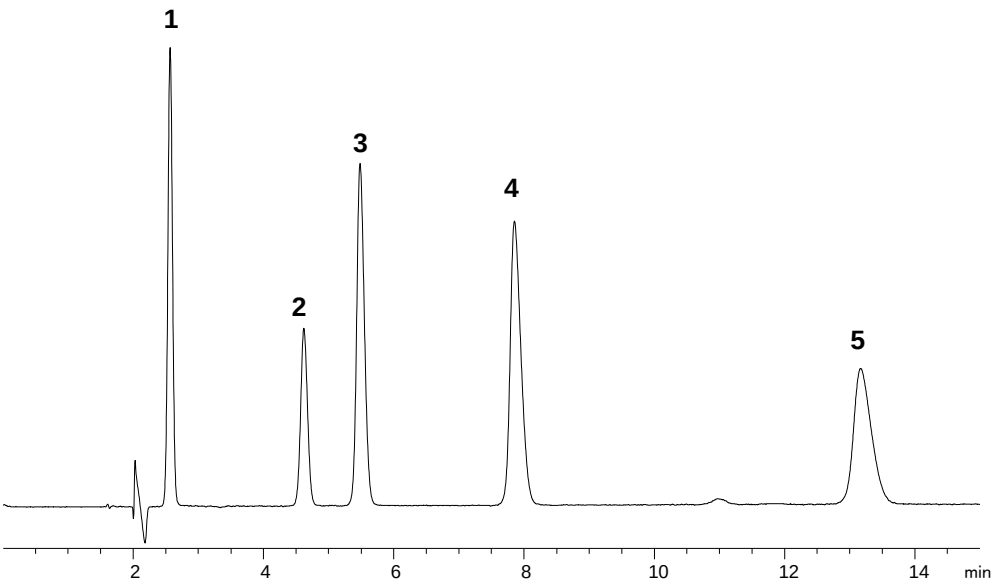
Catecholamines and Metanephrines Separation (Isocratic)

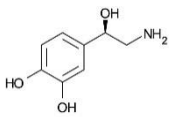
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN1490

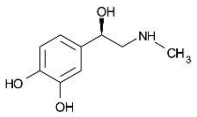
Conditions

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

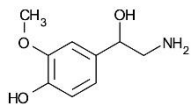




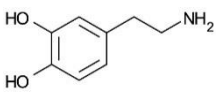
1. Norepinephrine



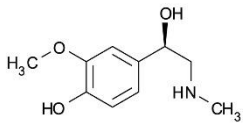
2. Epinephrine



3. Normetanephrine



4. Dopamine



5. Metanephrine

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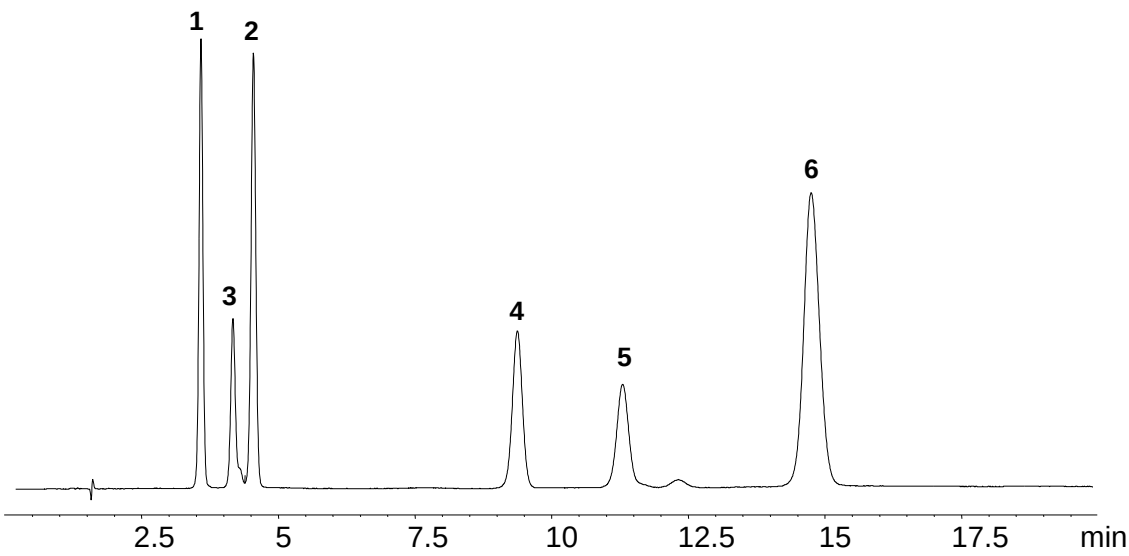
Catechols Mixture Separation (I)

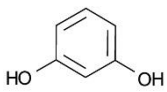
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN1430

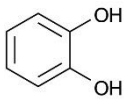
Conditions

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

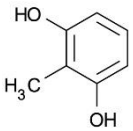




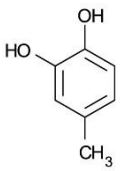
1. Resorcinol



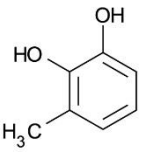
2. Catechol



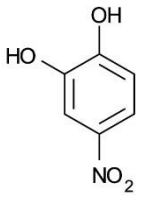
3. 2-Methylresorcinol



4. 4-Methylcatechol



5. 3-Methylcatechol



6. 4-Nitrocatechol

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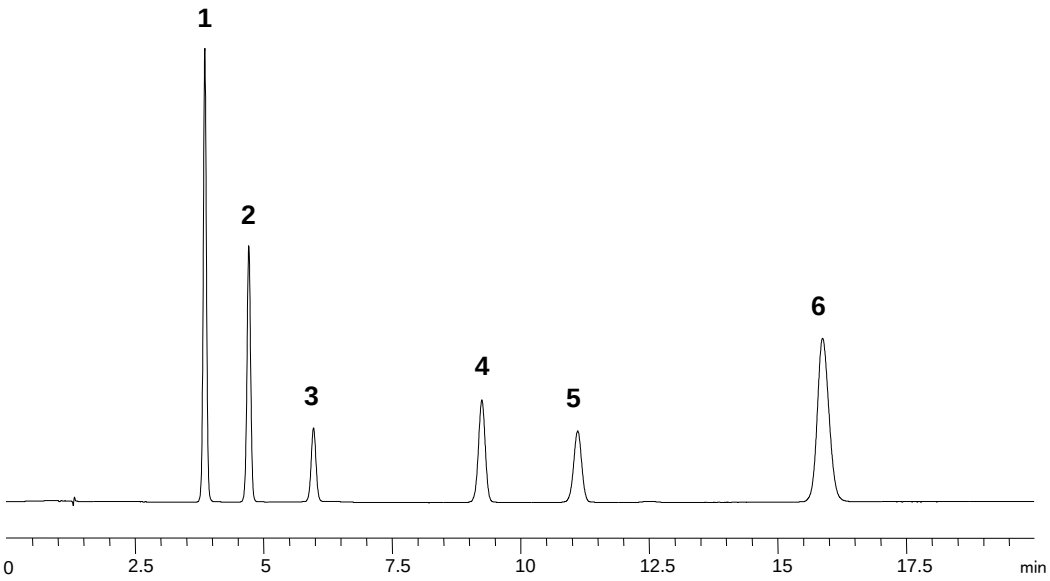
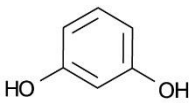
Catechols Mixture Separation (II)

Application #**AN1440**

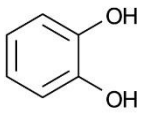
Conditions

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

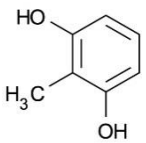




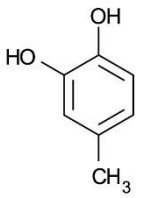
1. Resorcinol



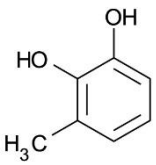
2. Catechol



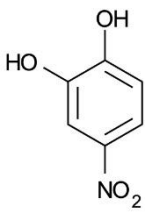
3. 2-Methylresorcinol



4. 4-Methylcatechol



5. 3-Methylcatechol



6. 4-Nitrocatechol

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Cathinone Psychoactive Substances by LC-UV and LC-Amperometry

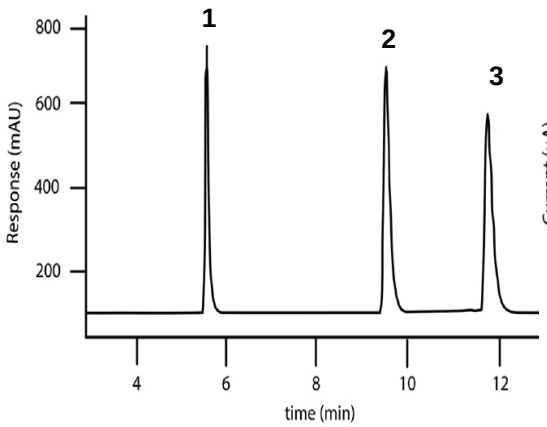
ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN3500

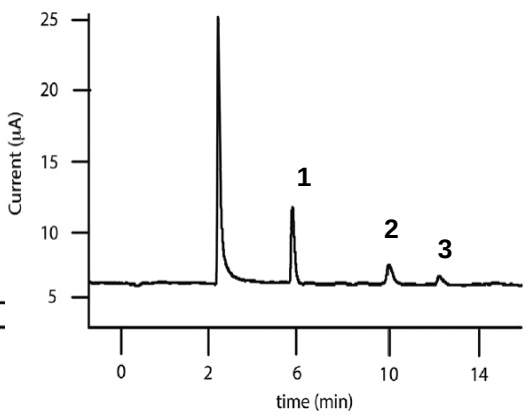
Conditions

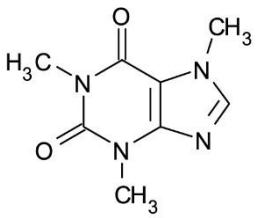
Column:	ACE 3 C18
Dimensions:	150 x 4.6 mm
Part Number:	ACE-111-1546
Mobile Phase:	10 mM ammonium acetate-100 mM KCl pH 4.3/MeOH (70:30 v/v)
Flow Rate:	0.8 mL/min
Injection:	10 µL
Temperature:	22 °C
Detection:	UV, 264 nm Amperometric Potential +1.4 V

UV Detection

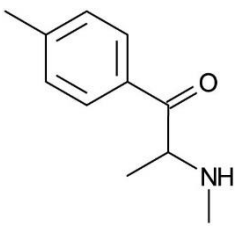


Amperometric Detection

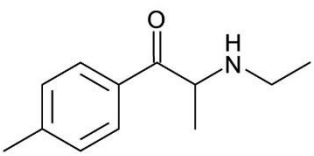




1. Caffeine



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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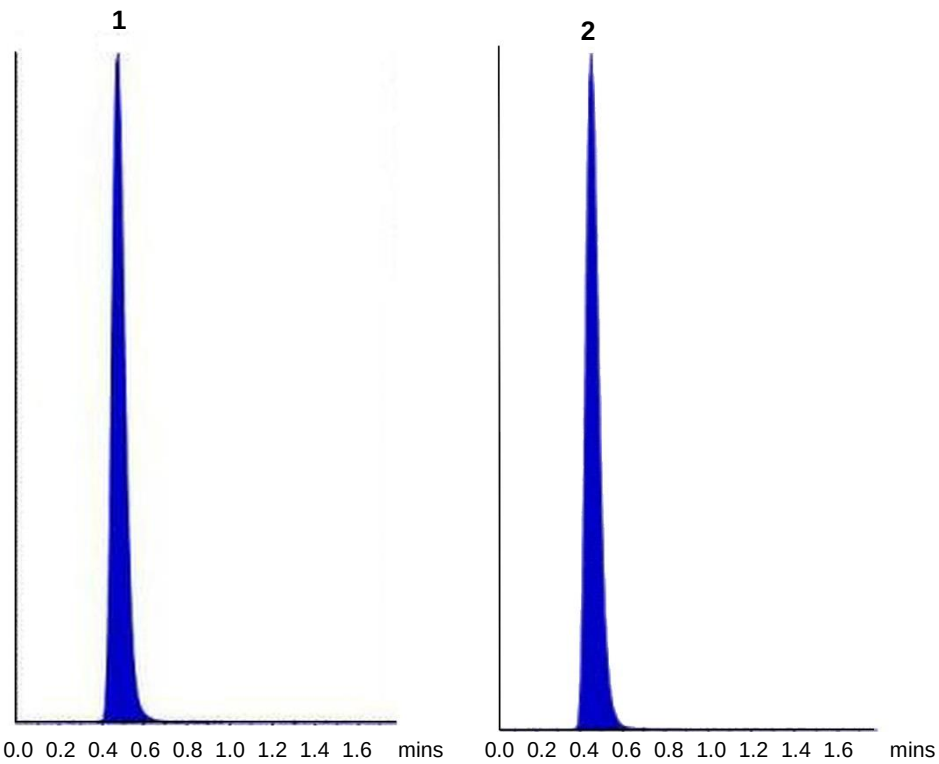
Ciprofibrate from Human Plasma by LC-MS/MS

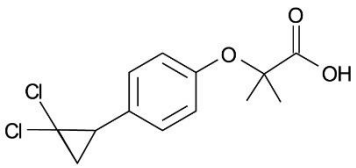
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN2670

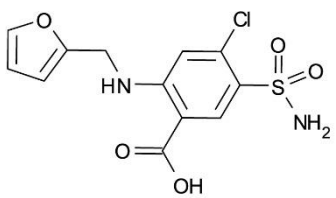
Conditions

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





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

ACE® Ultra-inert UHPLC & HPLC Columns

Application #**AN2050**

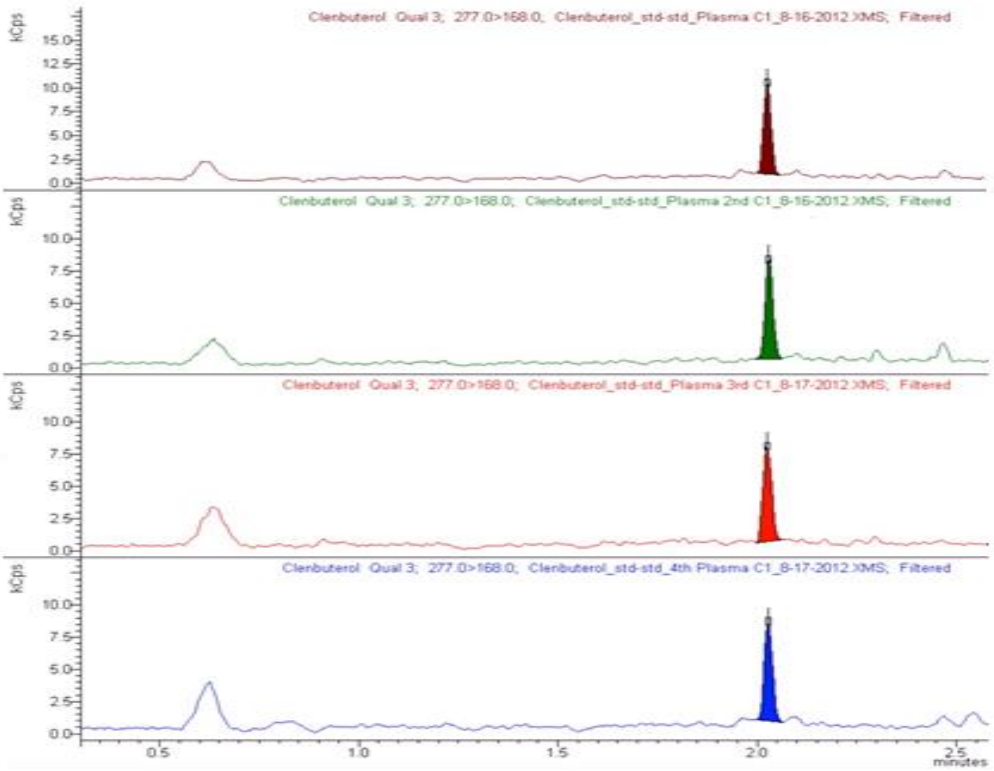
Conditions

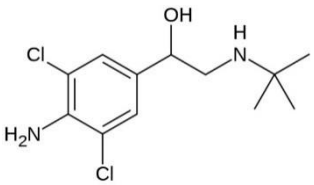
Column:	ACE 3 C18
Dimensions:	100 x 2.1 mm
Part Number:	ACE-111-1002
Mobile Phase:	A: 0.2% formic acid in H_2O
	B: 0.2% formic acid in MeCN

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

ACE® Ultra-inert UHPLC & HPLC Columns

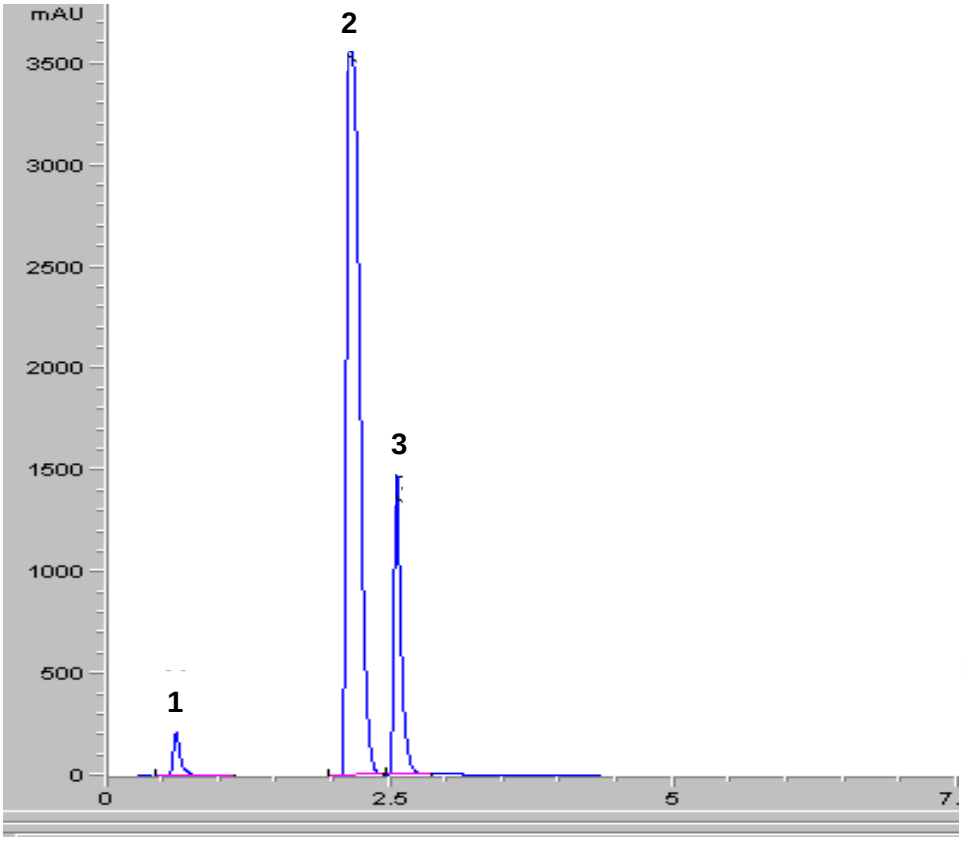
Application #AN2060

Conditions

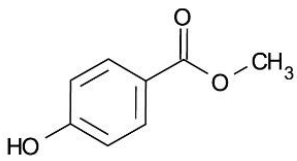
Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	50 x 4.6 mm
Part Number:	CORE-25A-0546U
Mobile Phase:	A: 0.2% w/v phosphate buffer/MeOH/MeCN (80:10:10 v/v) B: MeCN

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

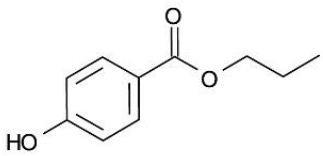
Flow Rate:	2 mL/min
Injection:	100 µL
Temperature:	20 °C
Detection:	UV, 220 nm



1. Clonidine HCl (10 µg/mL)



2. Methyl paraben (1.5 g/mL)



3. Propyl paraben (1.5 g/mL)

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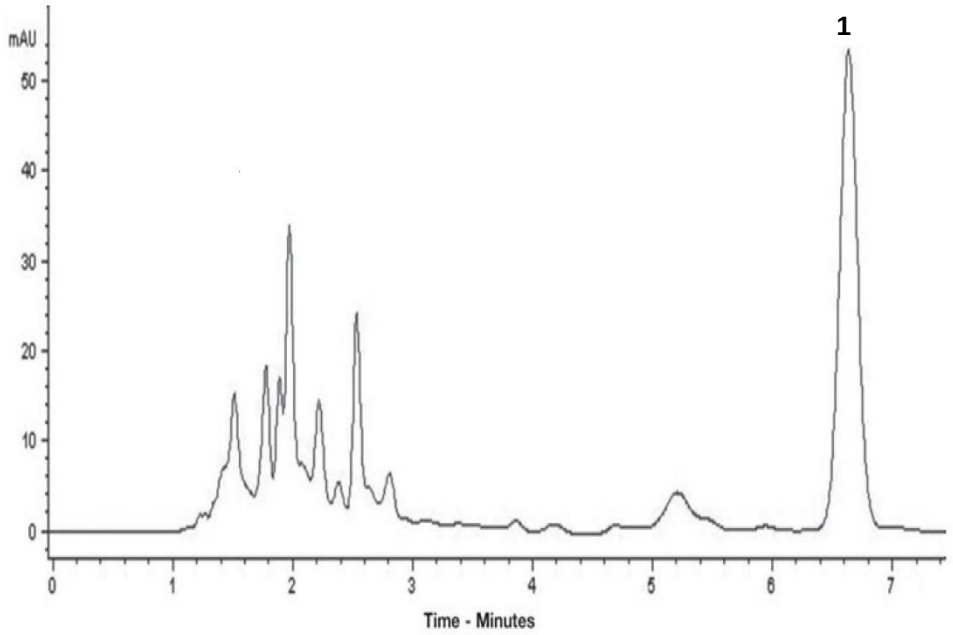
Clopidogrel and Photodegradation Products

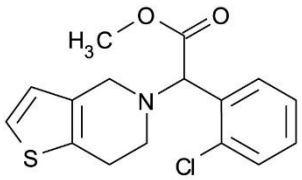
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN3110

Conditions

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





1. Clopidogrel

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Corticosteroids by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

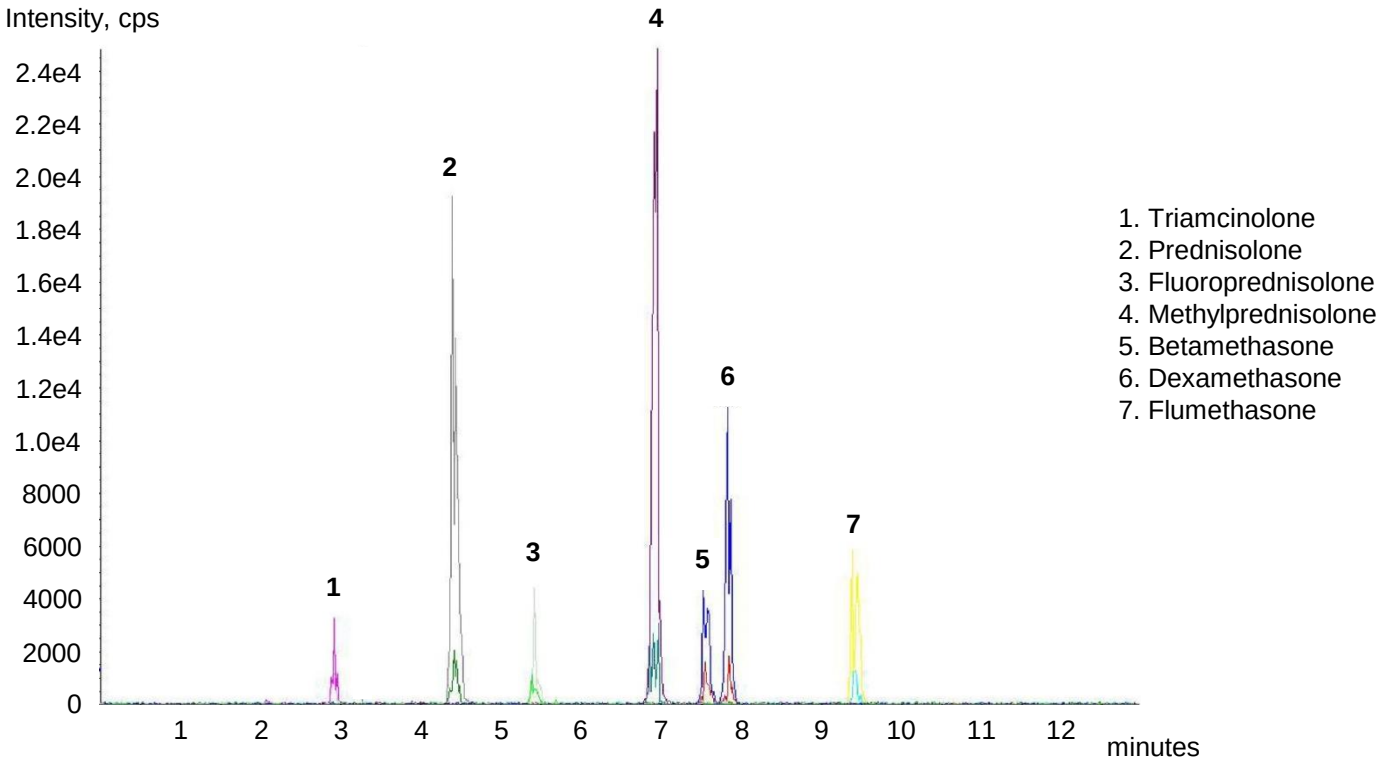
Application #**AN1030**

Conditions

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

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



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

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Cortisol in Urine by LC-MS/MS

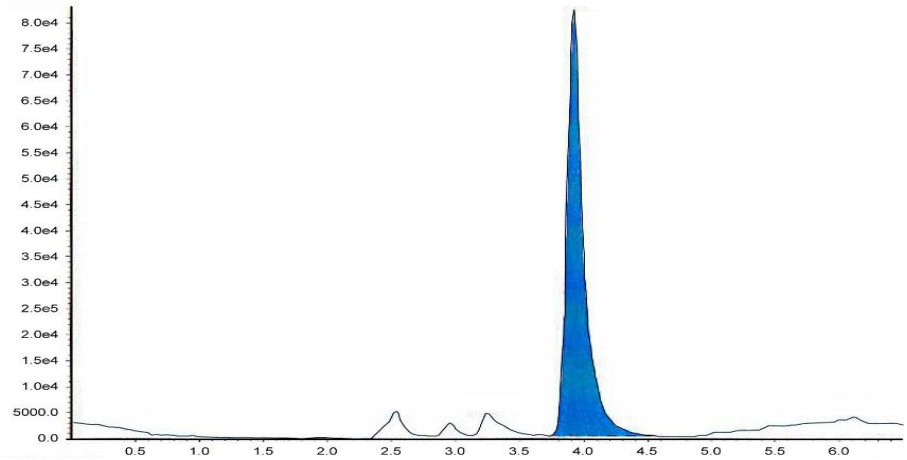
ACE® Ultra-inert UHPLC & HPLC Columns

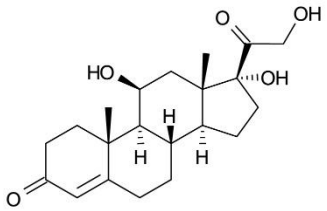
Application #AN2680

Conditions

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

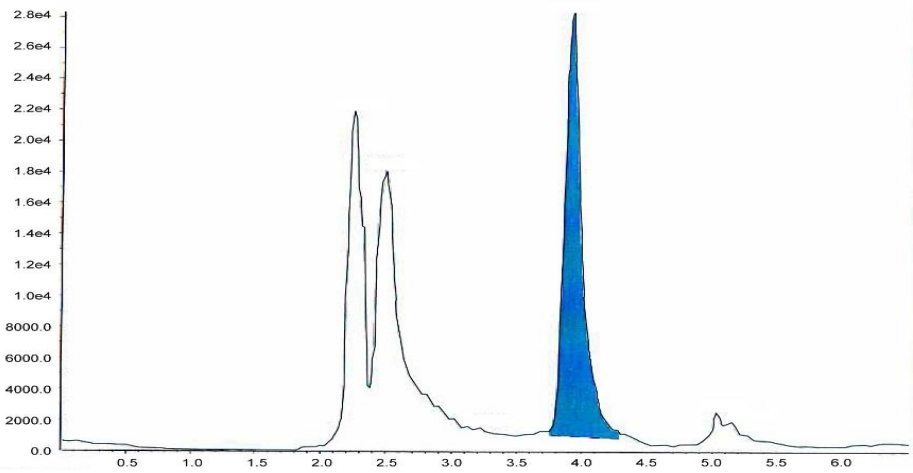
1

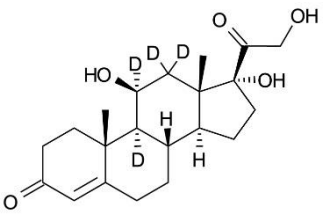




1. Cortisol
(*m/z* 363.5 → 121.3)

2





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

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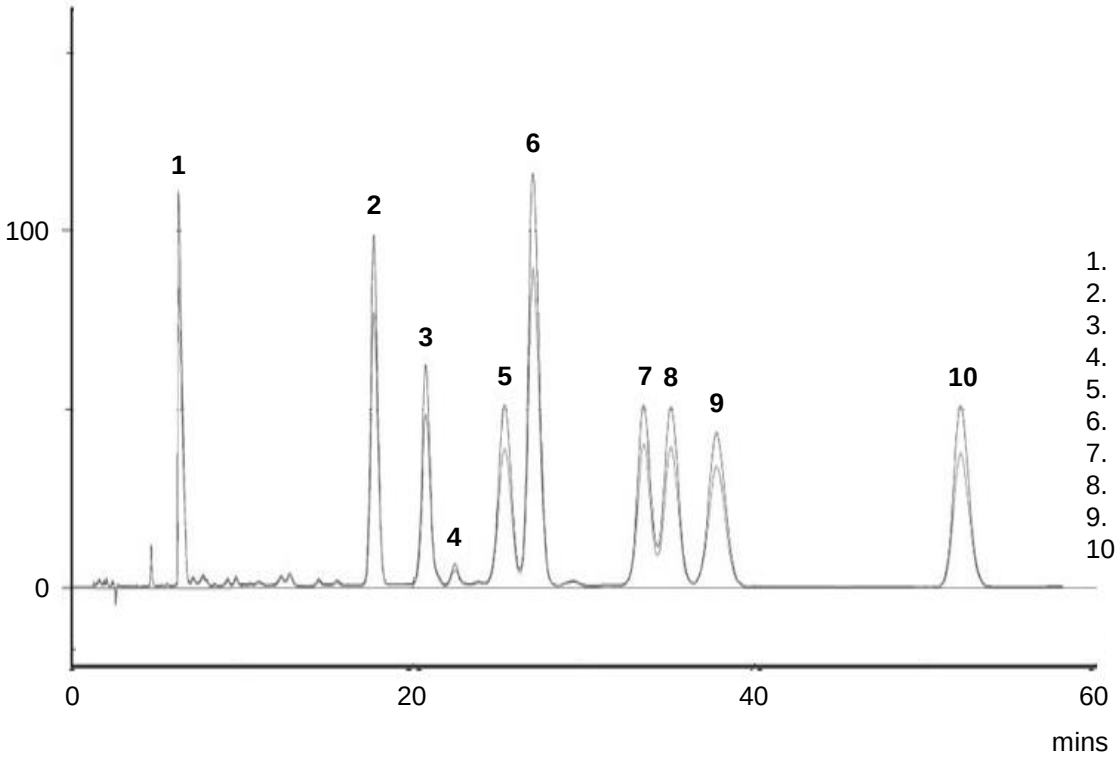
Cyclosporin Mixture

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN3270

Conditions

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



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

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Cytarabine Analogues by Ion-Pairing LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

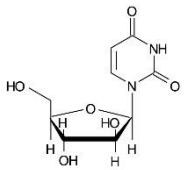
Application #**AN2070**

Conditions

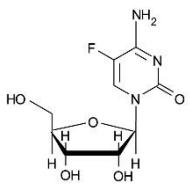
Column:	ACE 3 C18
Dimensions:	50 x 2.1 mm
Part Number:	ACE-111-0502
Mobile Phase:	A: 0.1% perfluoropentanoic acid + 0.1% formic acid in H_2O
	B: 0.1% perfluoropentanoic acid + 0.1% formic acid in MeCN

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

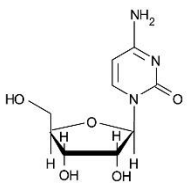
Flow Rate:	0.7 mL/min
Detection:	API 4000 MS
	TurbolonSpray, positive mode
	Source Temperature 550 °C



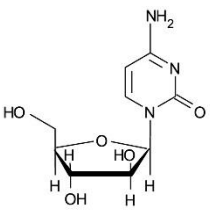
1. Uracil arabinofuranoside
(*m/z* 245 → 113)



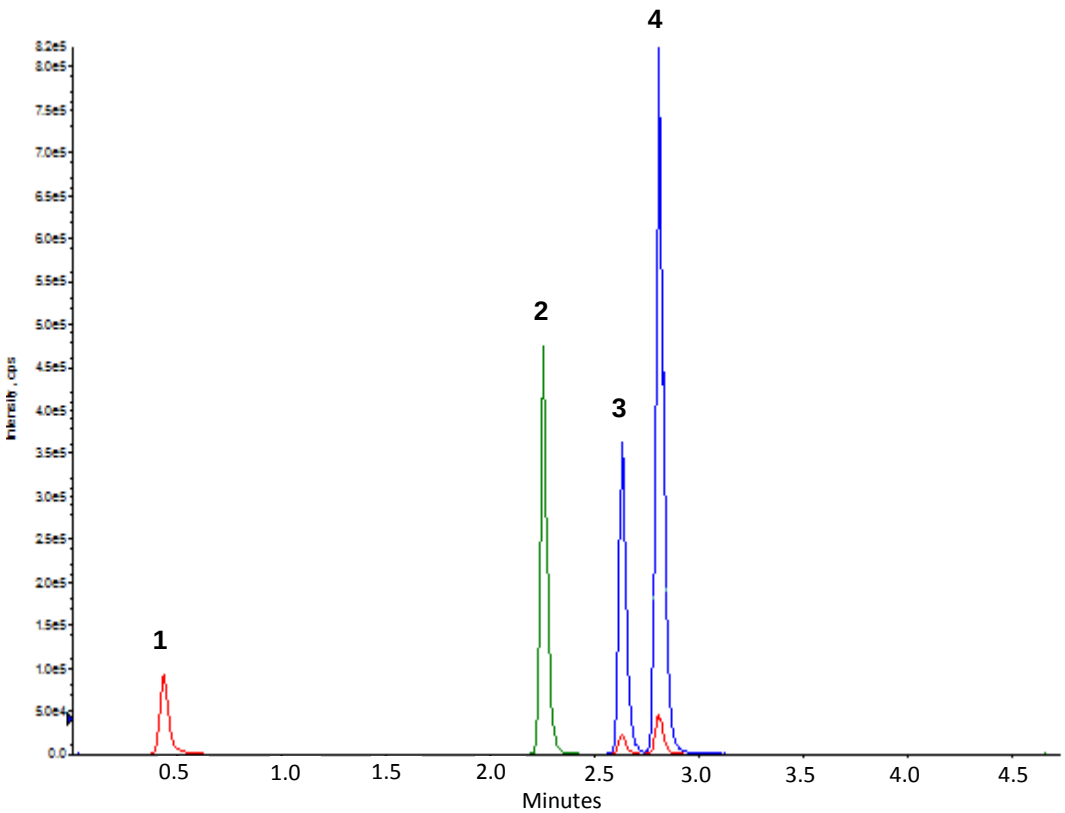
2. 5-Fluorocytidine (IS)
(*m/z* 262 → 130)



3. Cytidine
(*m/z* 244 → 112)



4. Cytarabine
(*m/z* 244 → 112)



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Cytotoxic Agents by UHPLC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

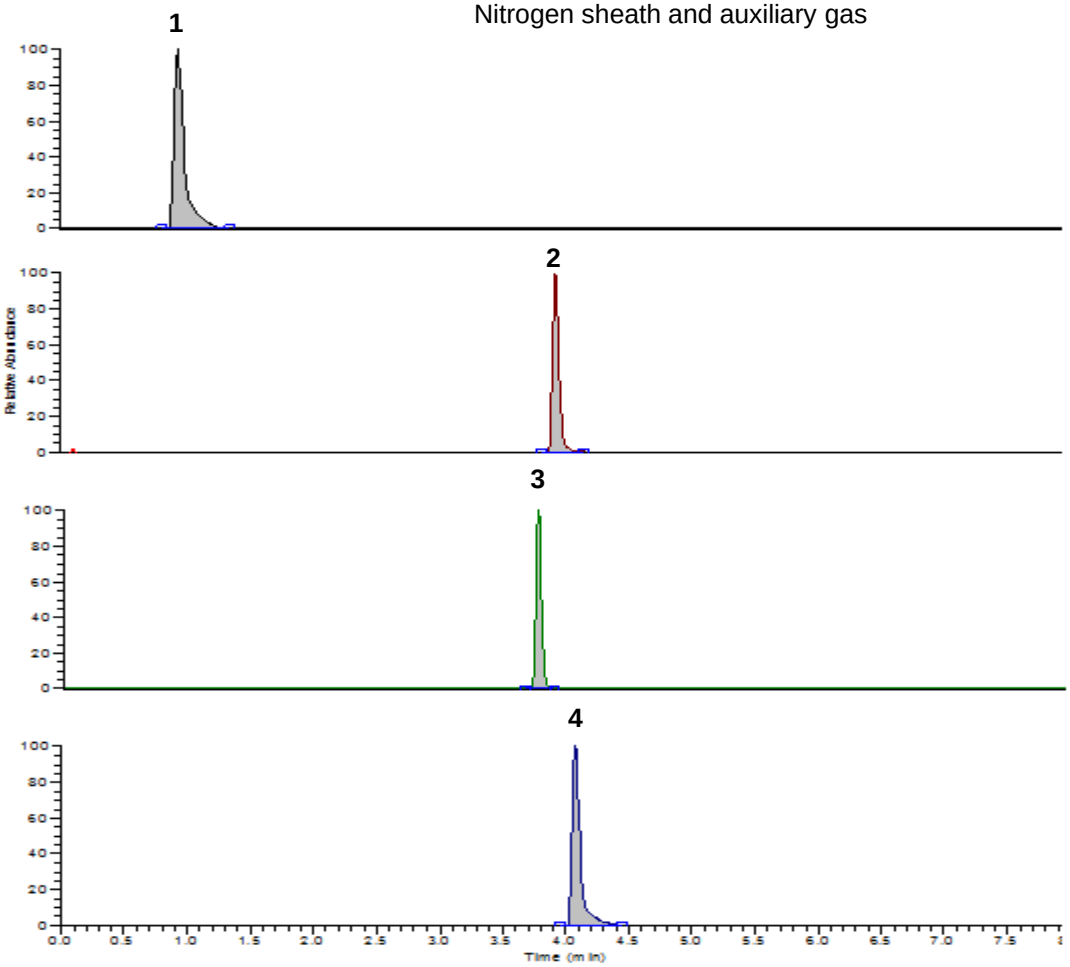
Application #**AN1070**

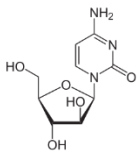
Conditions

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

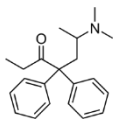
Time (mins)	%B
0.0	2
1.0	2
3.0	80
5.0	80
5.1	2
8.0	2

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

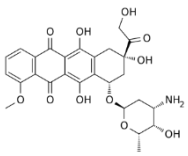




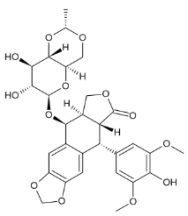
1. AraC
(*m/z* 244.1 → 112.2)



2. Methadone
(*m/z* 310.2 → 265.3)



3. Doxorubicin
(*m/z* 544.2 → 361.2)



4. Etoposide
(*m/z* 589.2 → 185.1)

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Dermorphin in Equine Urine by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

Application #**AN1040**

Conditions

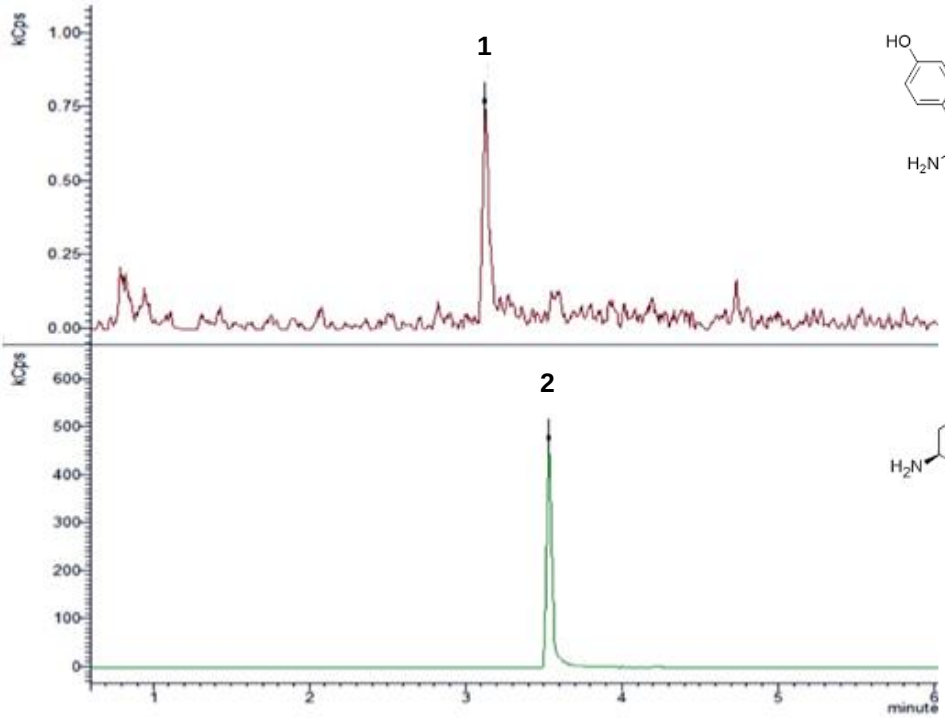
Column:	ACE 3 C18
Dimensions:	100 x 2.1 mm
Part Number:	ACE-111-1002
Mobile Phase:	A: 0.2% formic acid in H_2O
	B: 0.2% formic acid in MeCN

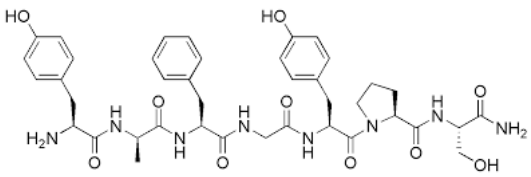
Time (mins)	%B
0.00	5
0.20	5
8.00	95
8.50	95
8.51	5
12.50	5

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

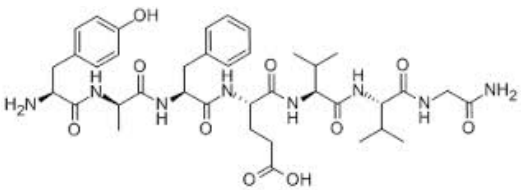
Accurate quantification of dermorphin in equine urine in range 0.05 – 100 ng/mL

LLOQ = 0.05 ng/mL





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



2. Deltorphin-II (IS)
(*m/z* 783 → 277)

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Diuretics (Gradient)

ACE®
Ultra-inert
UHPLC & HPLC Columns

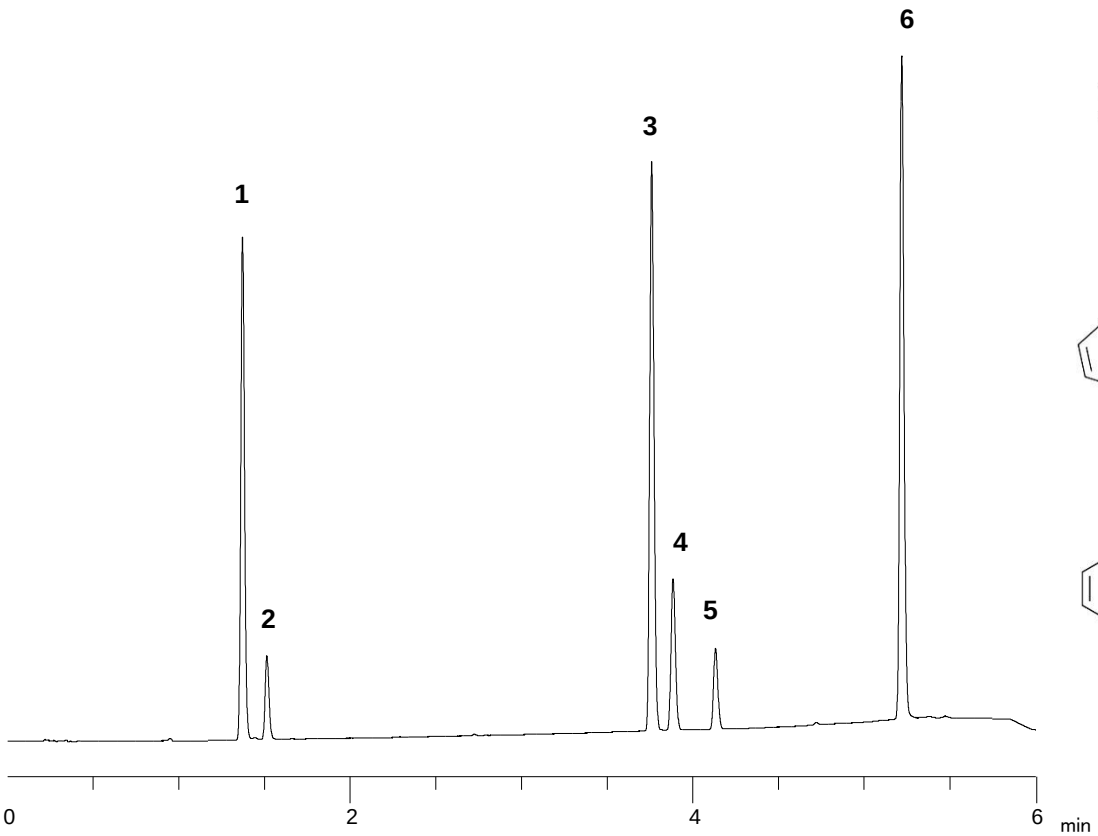
Application #AN1450

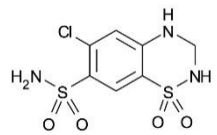
Conditions

Column:	ACE Excel 2 C18-PFP
Dimensions:	50 x 3.0 mm
Part Number:	EXL-1010-0503U
Mobile Phase:	A: 10 mM ammonium formate pH 3.0 in H_2O
	B: 10 mM ammonium formate pH 3.0 in MeOH/H_2O (9:1 v/v)

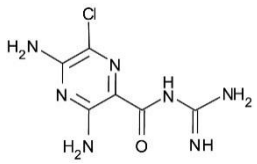
Time (mins)	%B
0.0	5
0.5	5
5.0	0
5.5	70
6.0	5

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

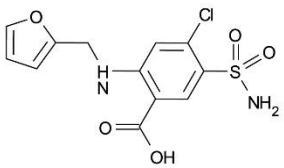




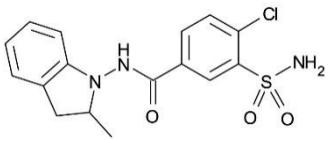
1. Hydrochlorothiazide



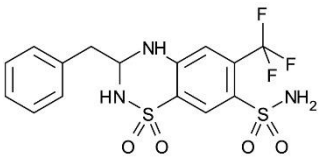
2. Amiloride



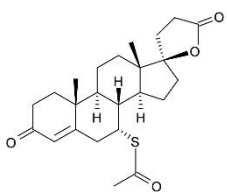
3. Furosemide



4. Indapamide



5. Bendroflumethiazide



6. Spironolactone

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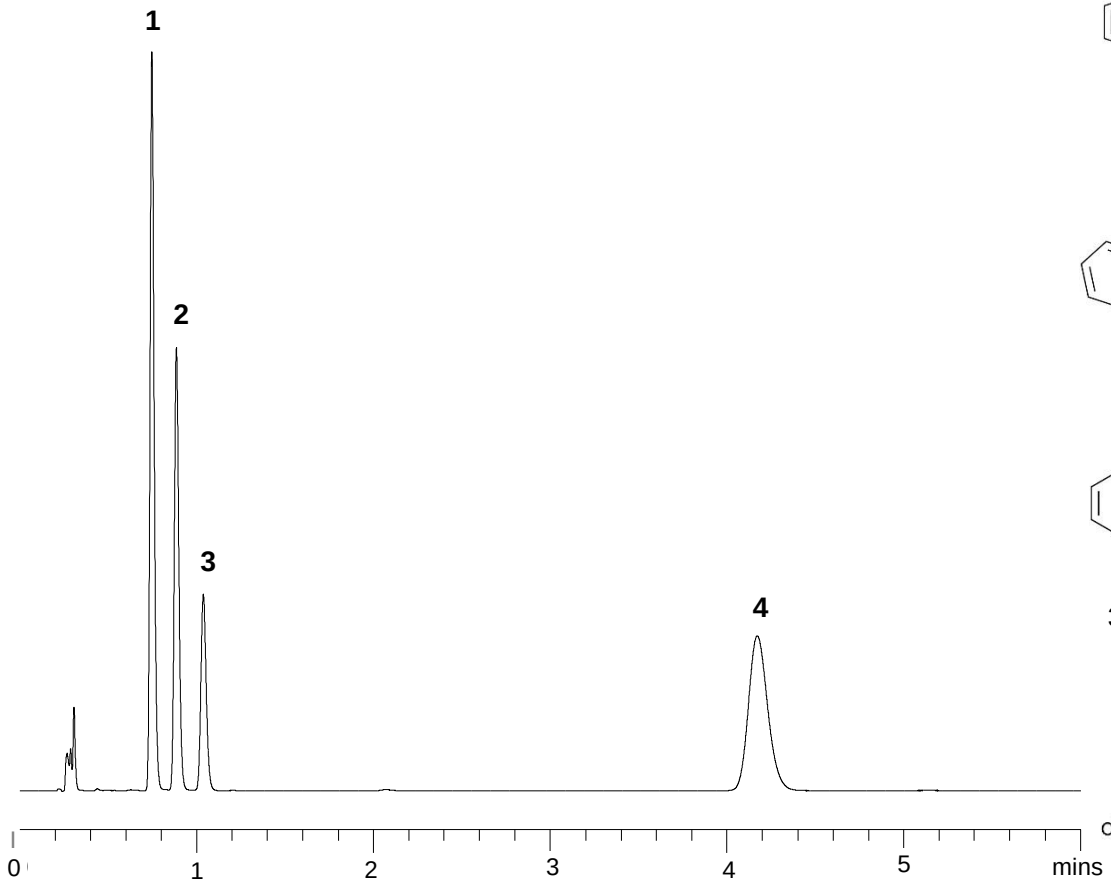
Diuretics (Isocratic)

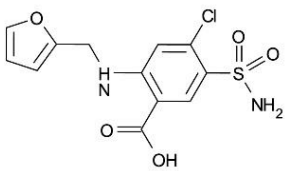
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN2140

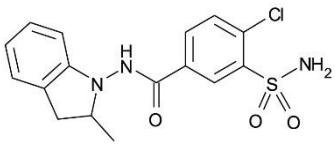
Conditions

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

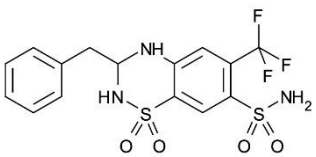




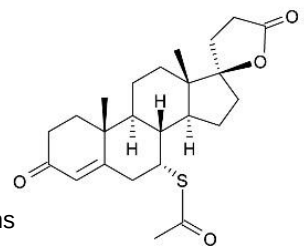
1. Furosemide



2. Indapamide



3. Bendroflumethiazide



4. Spironolactone

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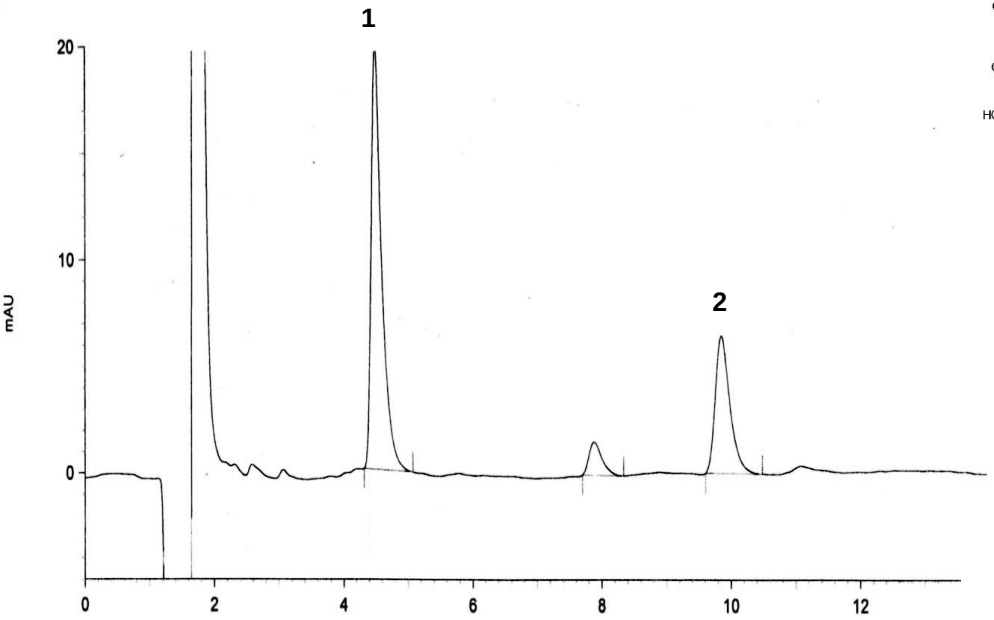
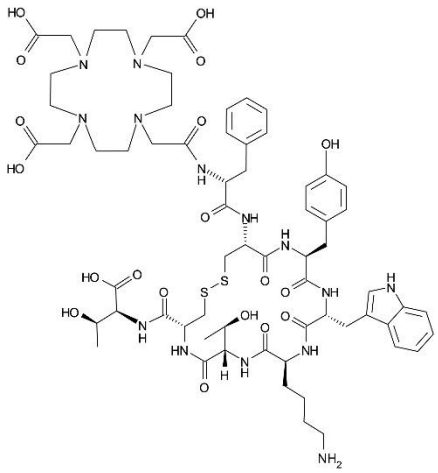
DOTATATE and Octreotide

Application #AN2730

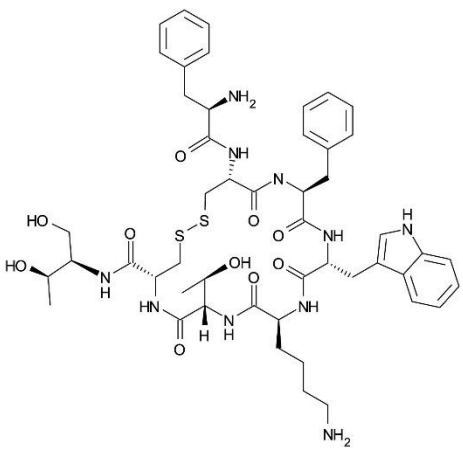
Conditions

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





1. DOTATATE



2. Octreotide

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Drugs of Abuse Screen by UHPLC-MS/MS

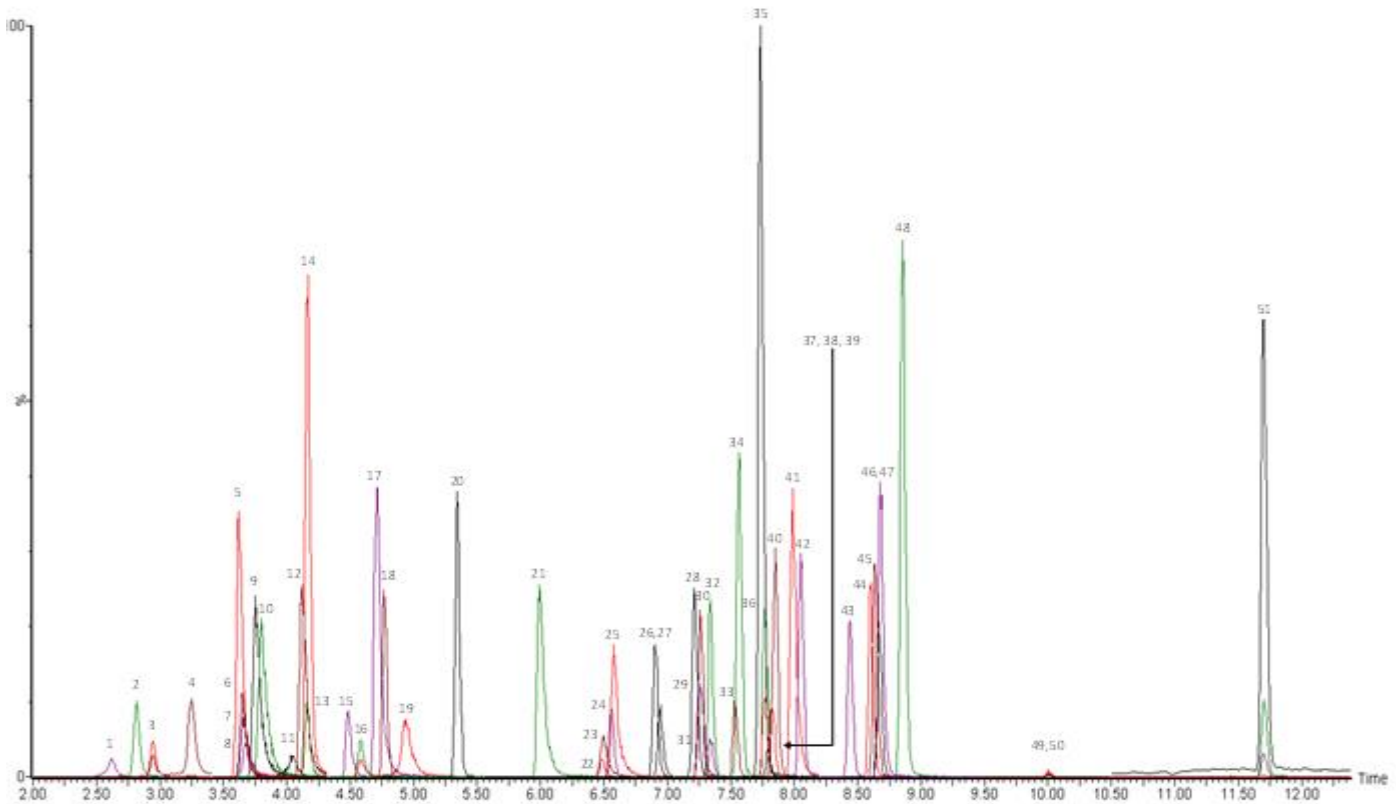
ACE® Ultra-inert UHPLC & HPLC Columns

Conditions

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

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 100^{-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					

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Ethyl Glucuronide in Water by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

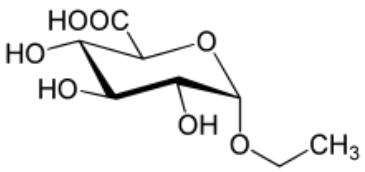
Application #**AN1100**

Conditions

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

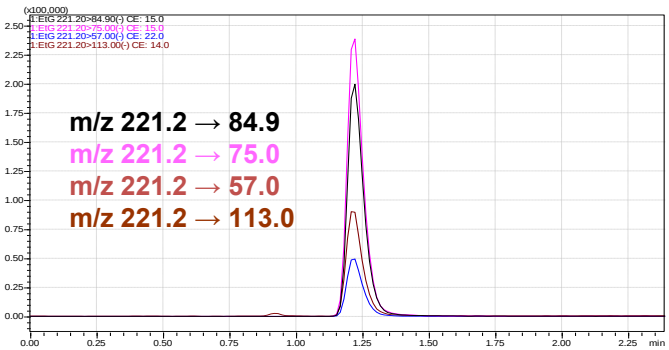
Time (mins)	%B
0.00	5
4.00	70
6.00	95
7.00	95
7.01	5

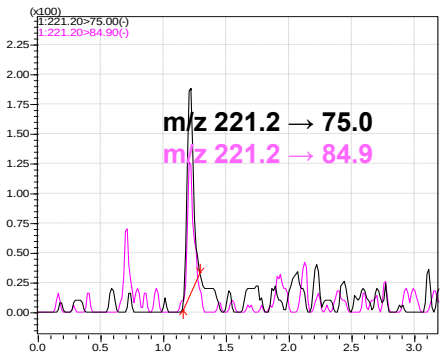
Flow Rate:	0.4 mL/min
Injection:	3 µL
Temperature:	40 °C
Detection:	Shimadzu LCMS-8050 ESI voltage: -3 kV Desolvation line: 250 °C Interface heater: 380 °C Nebulizing gas: 3 L/min Heat block: 400 °C



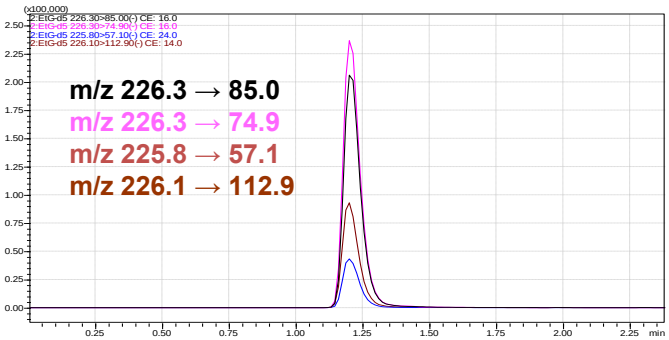
Ethyl glucuronide

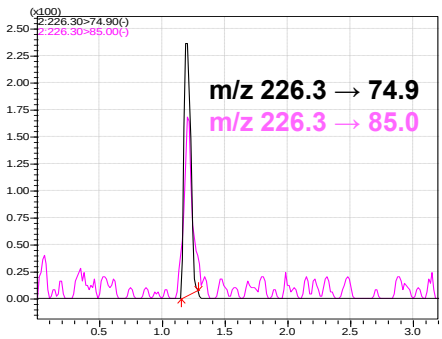
Ethyl glucuronide (EtG)
LOQ in H_2O 300 fg on-column





Ethyl glucuronide-d5 (EtG-d5)





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Formoterol in Human Plasma by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

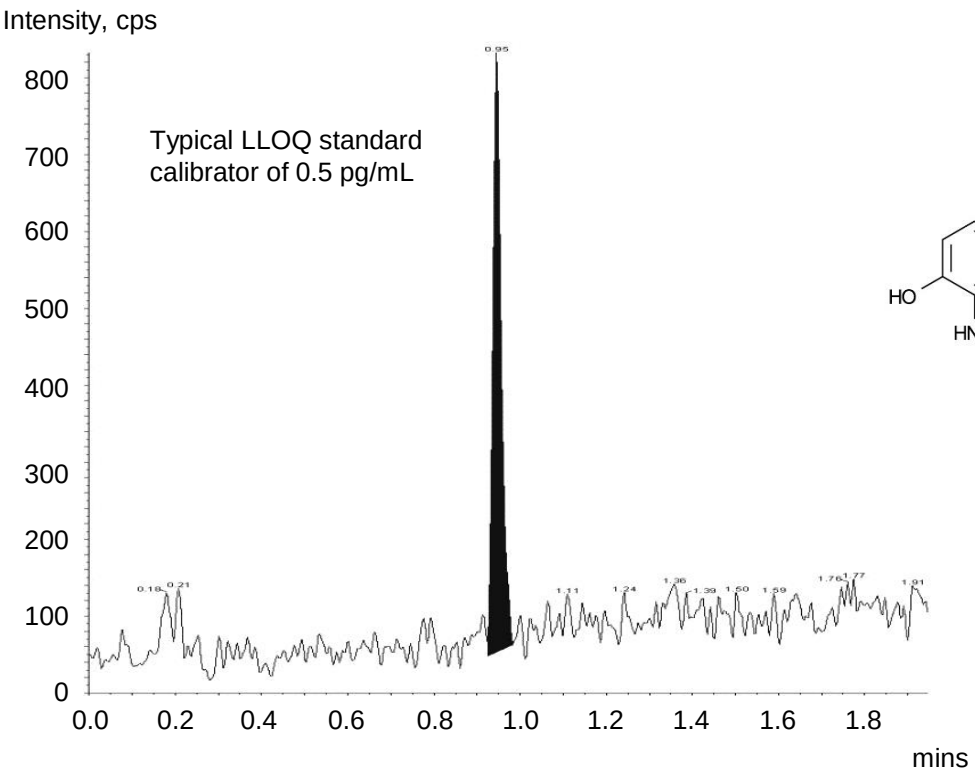
Application #AN3100

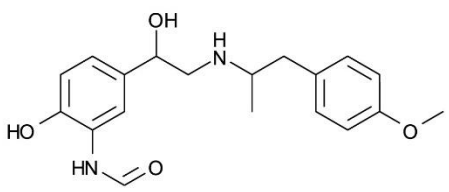
Conditions

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 H_2O
	B: 0.02% formic acid in H_2O/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





1. Formoterol
(*m/z* 345 → 149)

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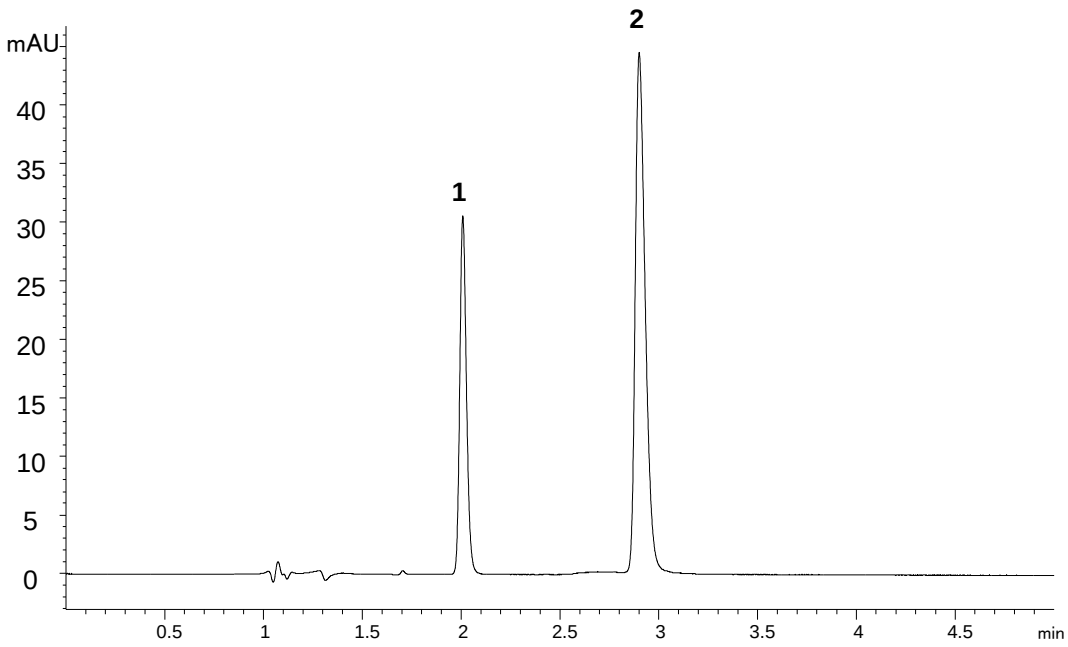
Gamma Hydroxybutyric Acid (GHB) and Gamma Butyrolactone (GBL)

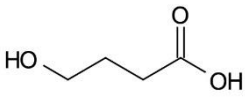
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN1500

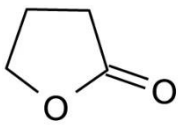
Conditions

Column:	ACE Excel 2 C18-AR
Dimensions:	100 x 3.0 mm
Part Number:	EXL-109-1003
Mobile Phase:	20 mM KH_2PO_4 pH 2.5 H_2O/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

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

ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN3090

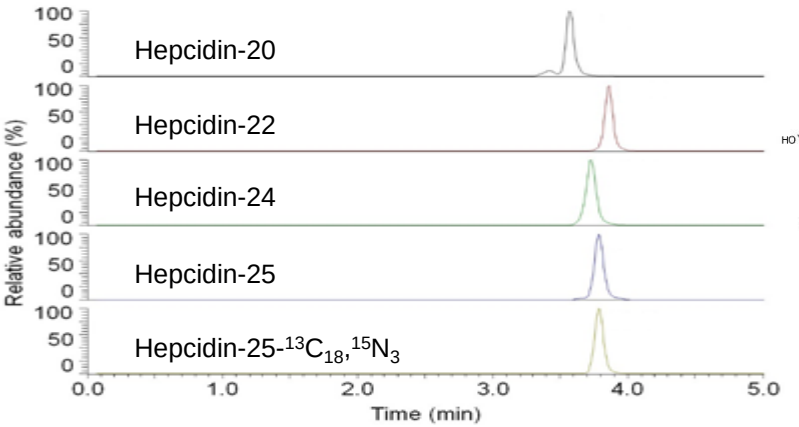
Conditions

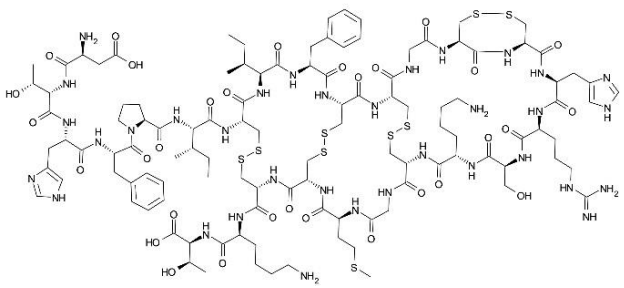
Column:	ACE 3 C18
Dimensions:	100 x 2.1 mm
Part Number:	ACE-111-1002
Mobile Phase:	A: 0.1% formic acid in H_2O B: 0.1% formic acid in MeCN

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

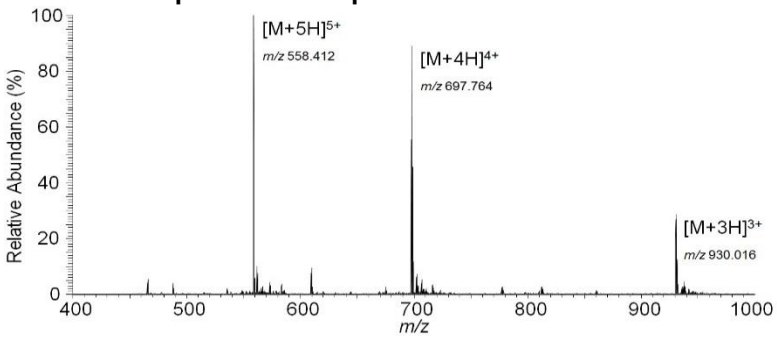
EIC for hepcidin-25 and truncated isoforms





Hepcidin-25
(MW 2789)

Mass Spectrum of hepcidin-25



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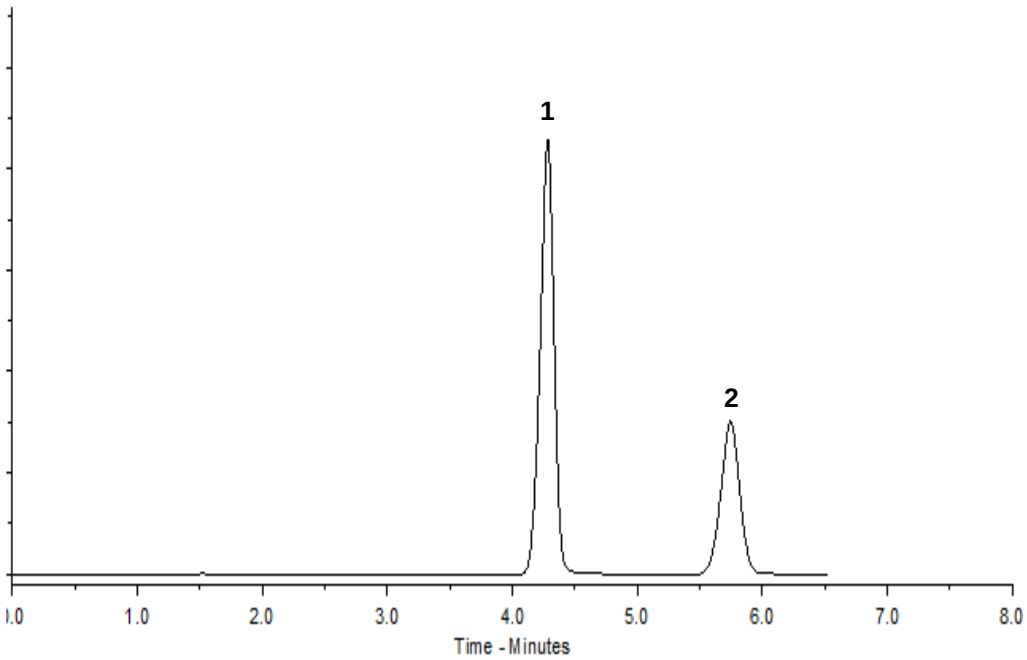
Hippuric Acid

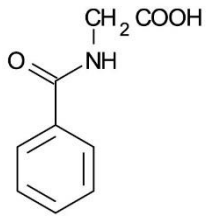
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN2760

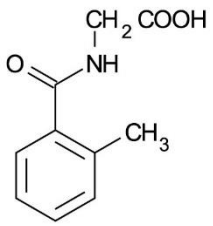
Conditions

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





1. Hippuric acid



2. 2-Methylhippuric acid

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Human Defensins in a Saliva Matrix

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1270**

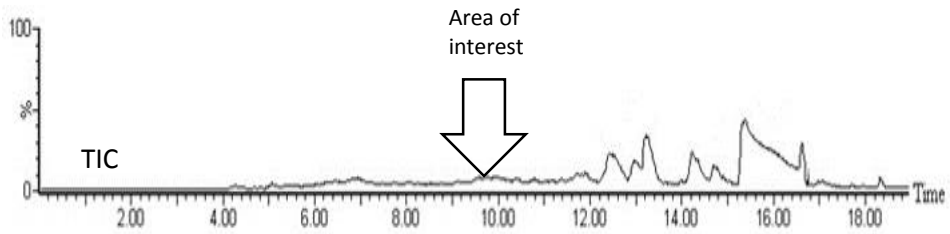
Conditions

Column:	ACE UltraCore 2.5 SuperC18
Dimensions:	50 x 3.0 mm
Part Number:	CORE-25A-1503U
Mobile Phase:	A: 0.1% formic acid in H_2O B: 0.1% formic acid in MeCN

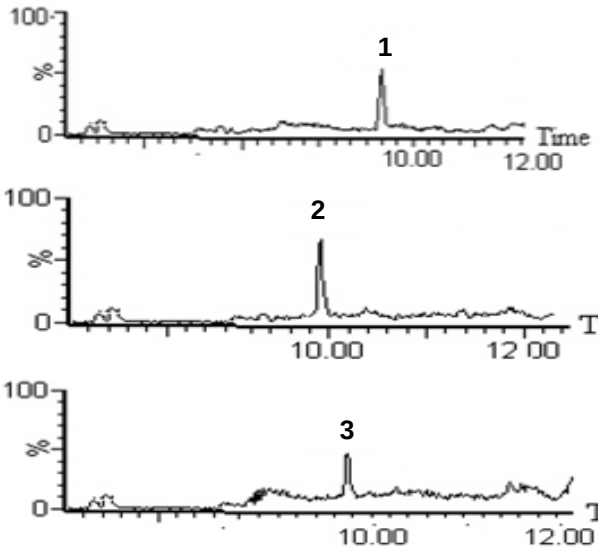
Time (mins)	%B
0	2
2	2
17	50
19	95
20	95

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

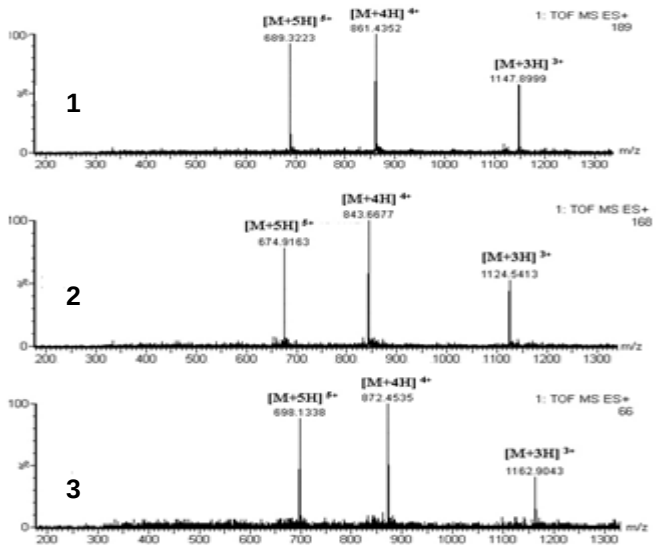
Defensin Human Neutrophil Peptides
1. HNP-1
(30 amino acid residues)
2. HNP-2
(29 amino acid residues)
3. HNP-3
(30 amino acid residues)



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



Mass spectra



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Human Urine Metabolite Profiling by LC-MS

ACE® Ultra-inert UHPLC & HPLC Columns

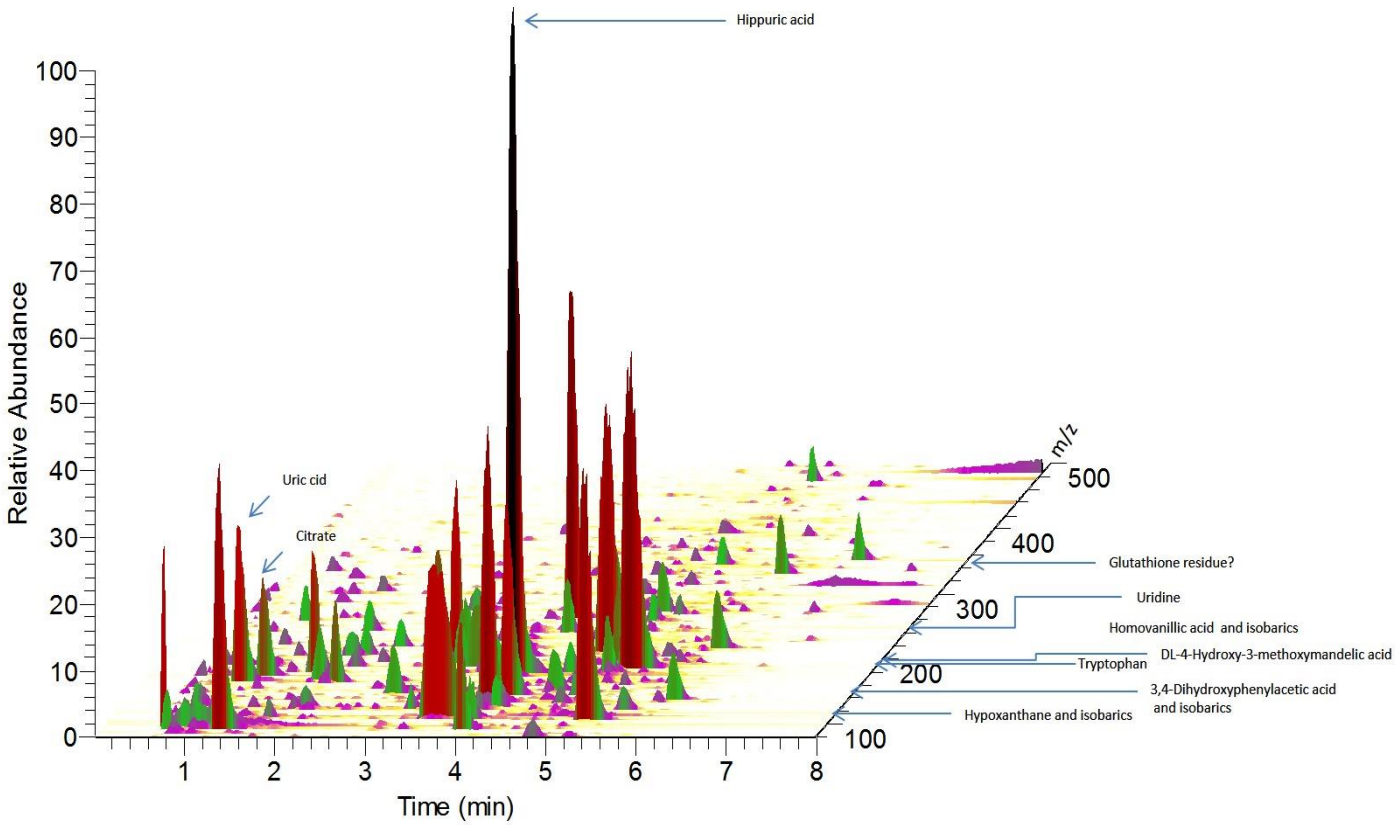
Application #**AN2600**

Conditions

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

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

ACE® Ultra-inert UHPLC & HPLC Columns

Application #**AN1120**

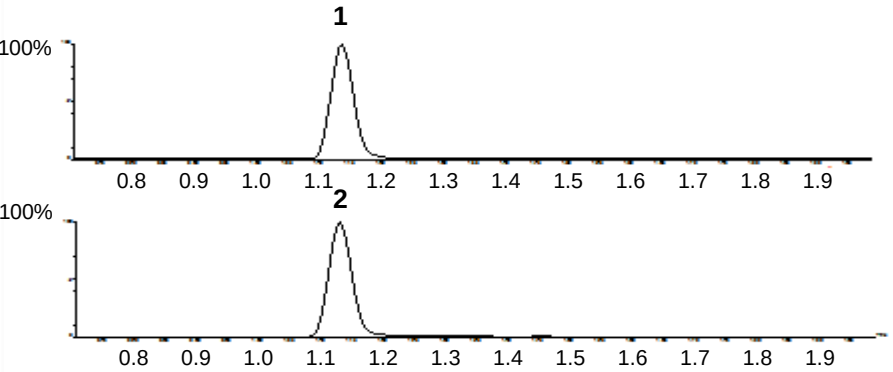
Conditions

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

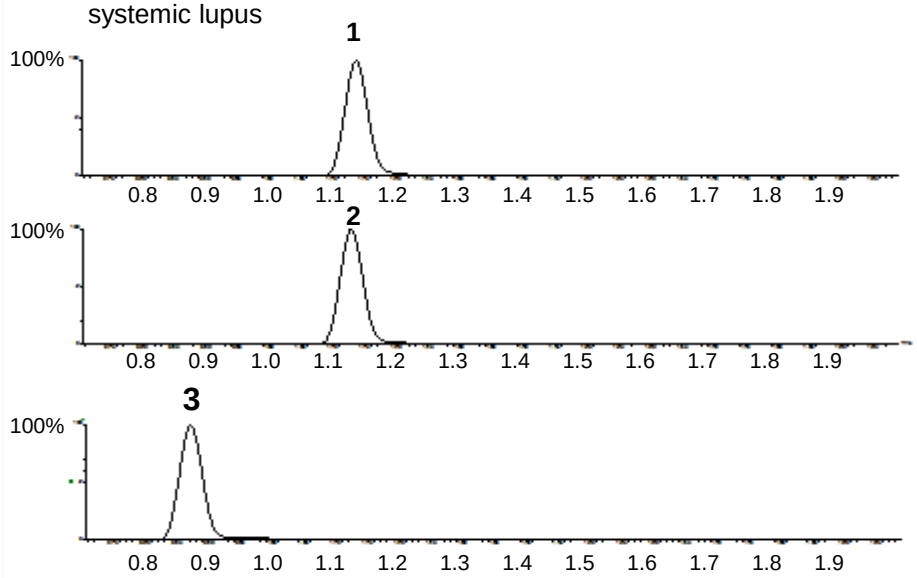
Time (mins)	%B
0.00	30
1.50	100
2.50	100
2.51	30

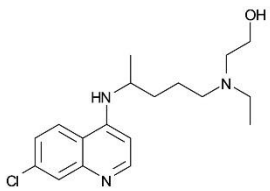
Flow Rate:	0.4 mL/min
Injection:	5 µL
Temperature:	40 °C
Detection:	MS/MS detection with Waters TQD
	ESI +ve ion mode

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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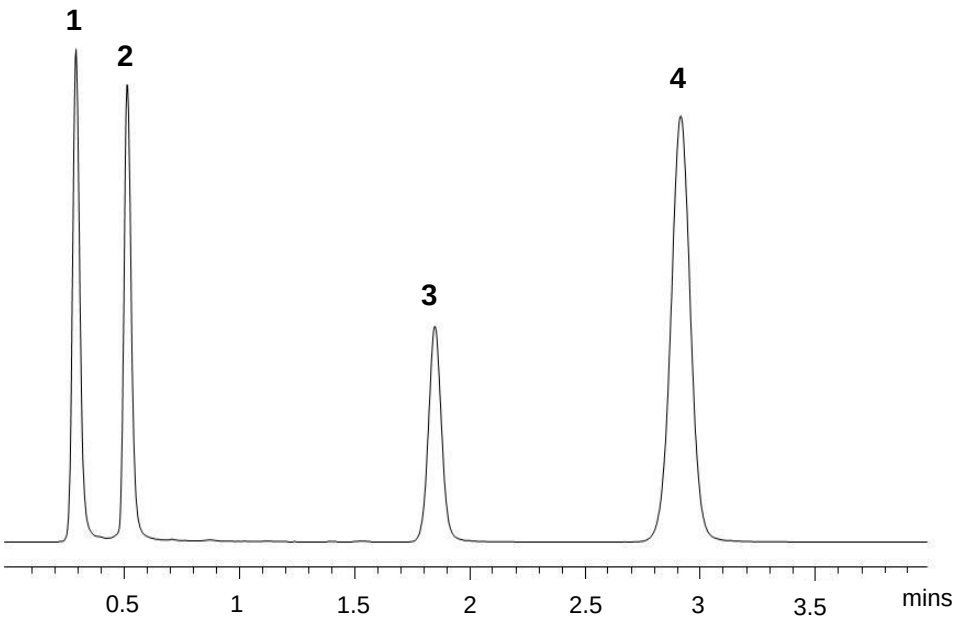
Ibuprofen in Combination with Antihistamine and Decongestant

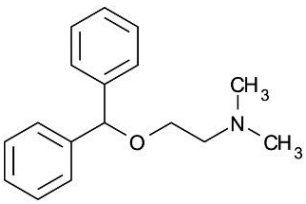
ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN2120

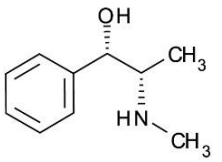
Conditions

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

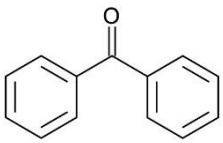




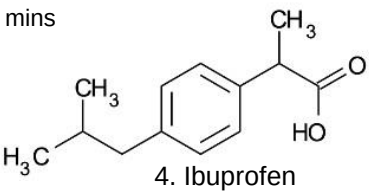
1. Diphenhydramine



2. Pseudoephedrine



3. Benzophenone



4. Ibuprofen

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Insulin Analogues in Clinical and Post-Mortem Analyses

ACE® Ultra-inert UHPLC & HPLC Columns

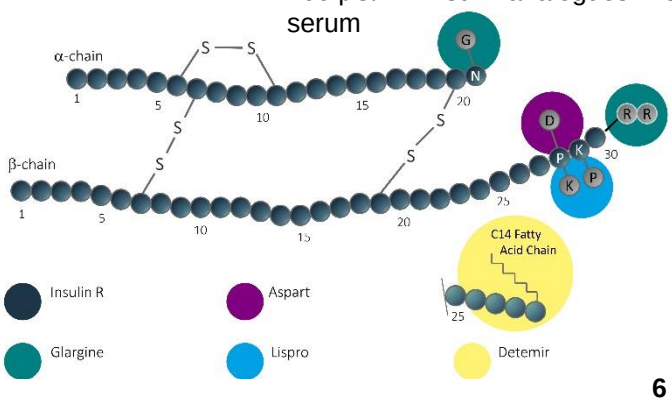
Application #AN3350

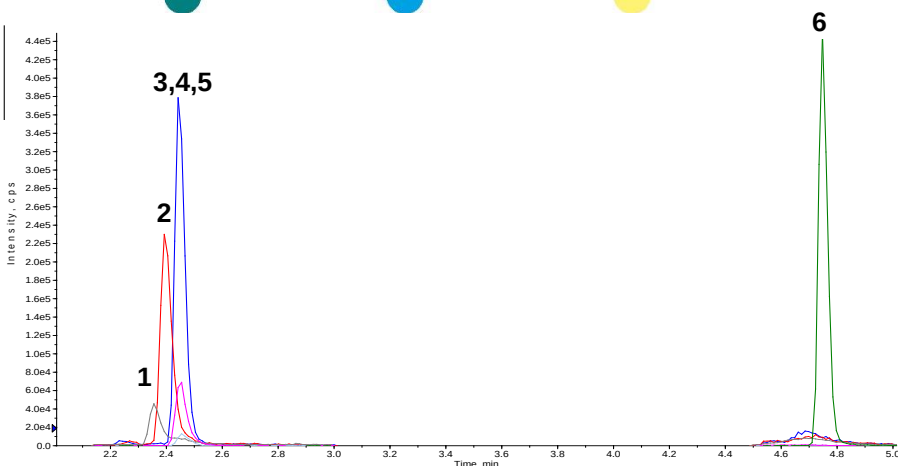
Conditions

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

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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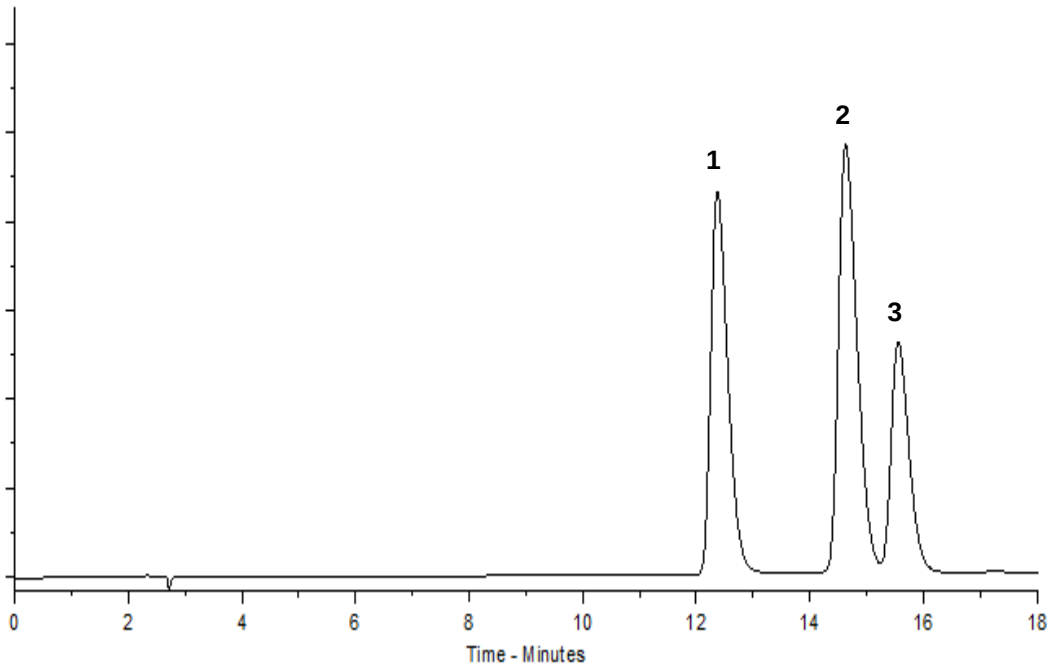
Application #**AN2770**

Conditions

Column:	ACE 5 C18
Dimensions:	250 x 4.6 mm
Part Number:	ACE-121-2546
Mobile Phase:	A: 0.1% TFA in H_2O/MeCN (71:29 v/v) B: 0.1% TFA in H_2O/MeCN (68:32 v/v)

Time (mins)	%B
0	10
16	90

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



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

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

ACE® Ultra-inert UHPLC & HPLC Columns

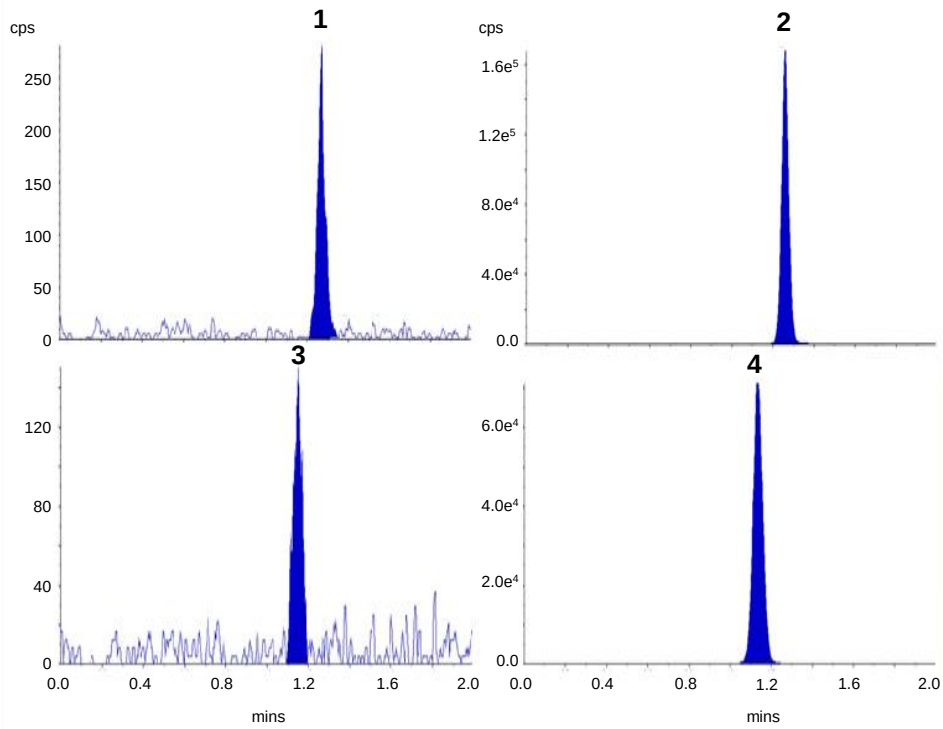
Application #AN3380

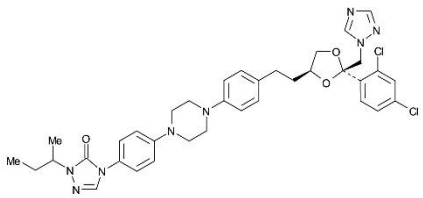
Conditions

Column:	ACE 3 C18-AR
Dimensions:	50 x 2.1 mm
Part Number:	ACE-119-0502
Mobile Phase:	A: 10 mM ammonium acetate in H_2O
	B: 10 mM ammonium acetate in MeOH

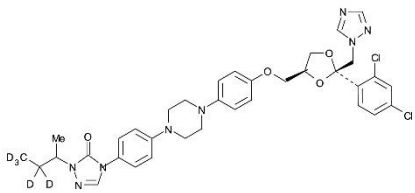
Time (mins)	%B
0	75
2	98
3	98

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)

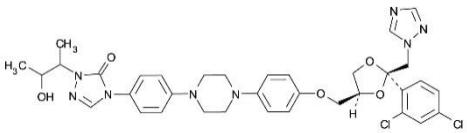




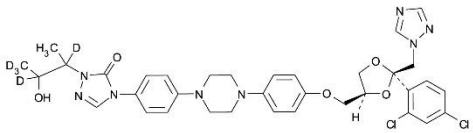
1. Itraconazole
(*m/z* 705.3 → 392.3)



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

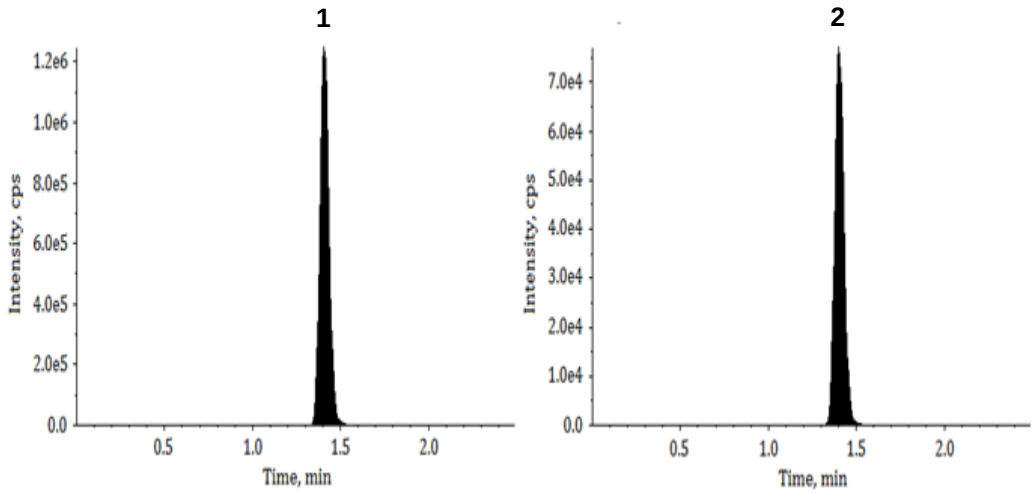
ACE®
Ultra-inert
UHPLC & HPLC Columns

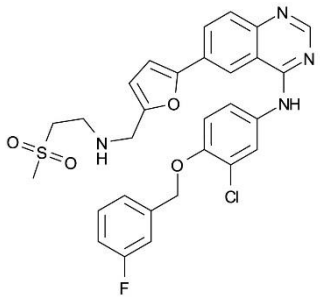
Application #AN3360

Conditions

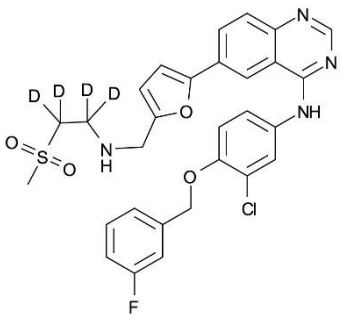
Column:	ACE 5 C18
Dimensions:	100 x 4.6 mm
Part Number:	ACE-121-1046
Mobile Phase:	10 mM ammonium formate pH 3.5/MeCN (10:90 v/v)
Flow Rate:	1 mL/min
Injection:	0.5 µL
Temperature:	40 °C
Detection:	API 4000 triple quad MS Positive ion mode ESI Ion spray voltage: 5500 V Temperature: 400 °C
Sample:	Extracted 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 → 365.2)
Concentration 1000 ng/mL



2. Lapatinib-d4 (IS)
(*m/z* 585.1 → 365.0)
Concentration 100 ng/mL

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Lidocaine in Saliva by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

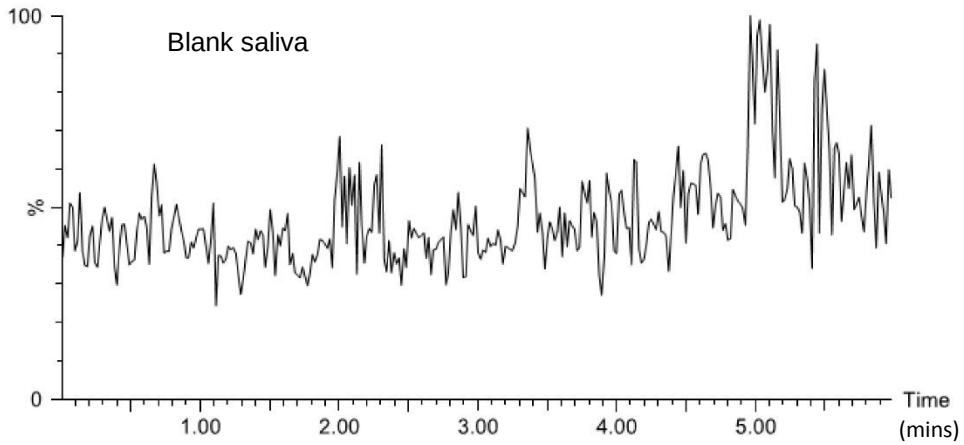
Application #AN2570

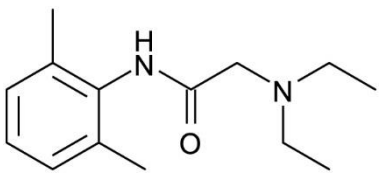
Conditions

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

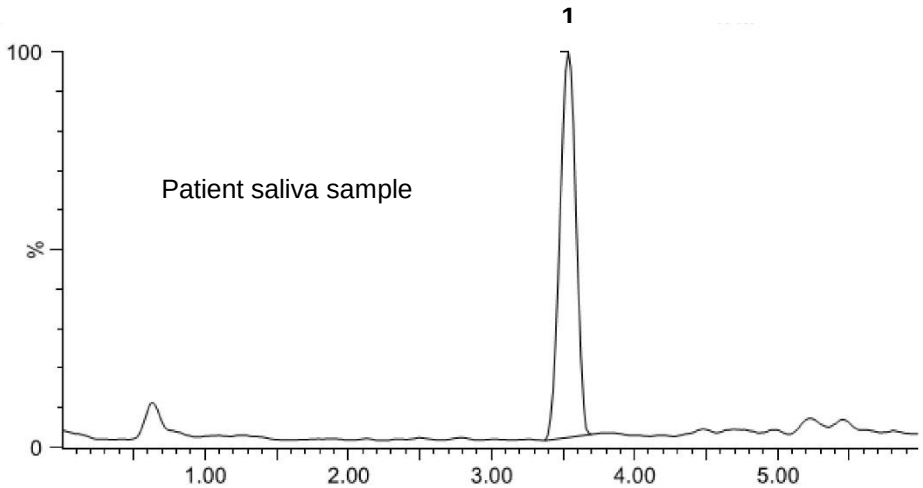
Time (mins)	%B
0.0	20
1.0	20
3.0	80
4.5	80

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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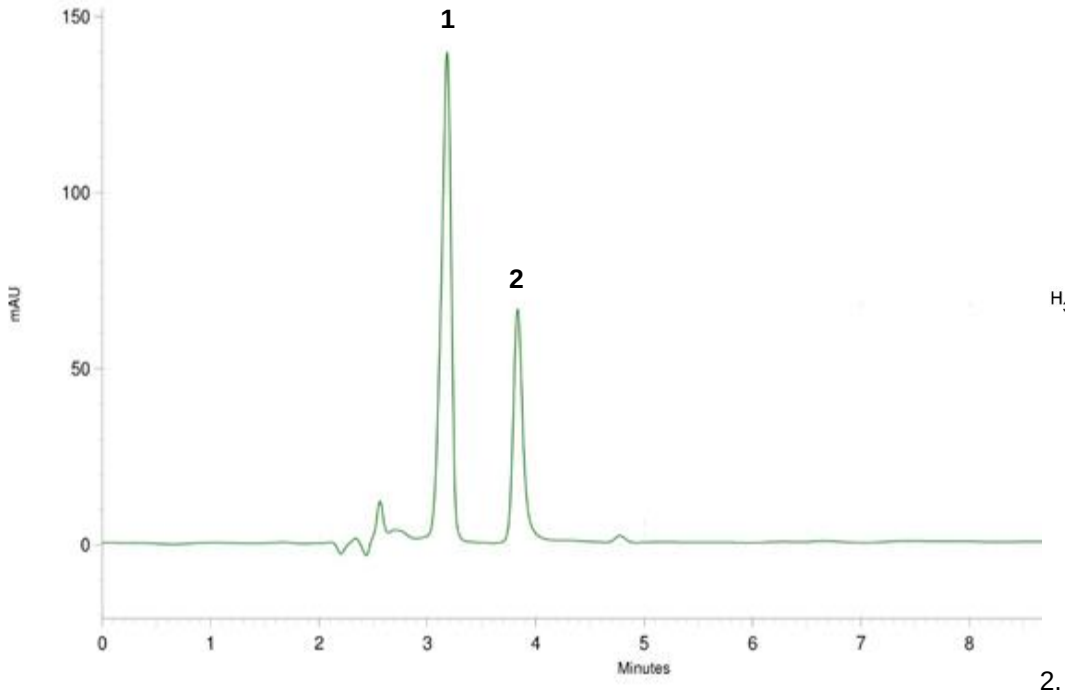
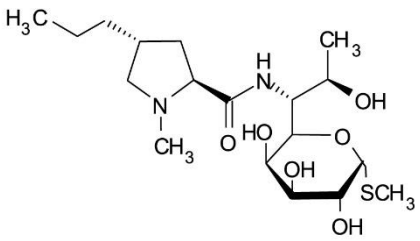
Lincosamide Antibiotics

Application #AN2650

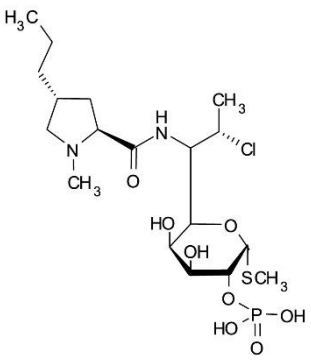
Conditions

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





1. Lincomycin HCl



2. Clindamycin phosphate

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Lipid Classes Separation from *Drosophila Melanogaster*

ACE® Ultra-inert UHPLC & HPLC Columns

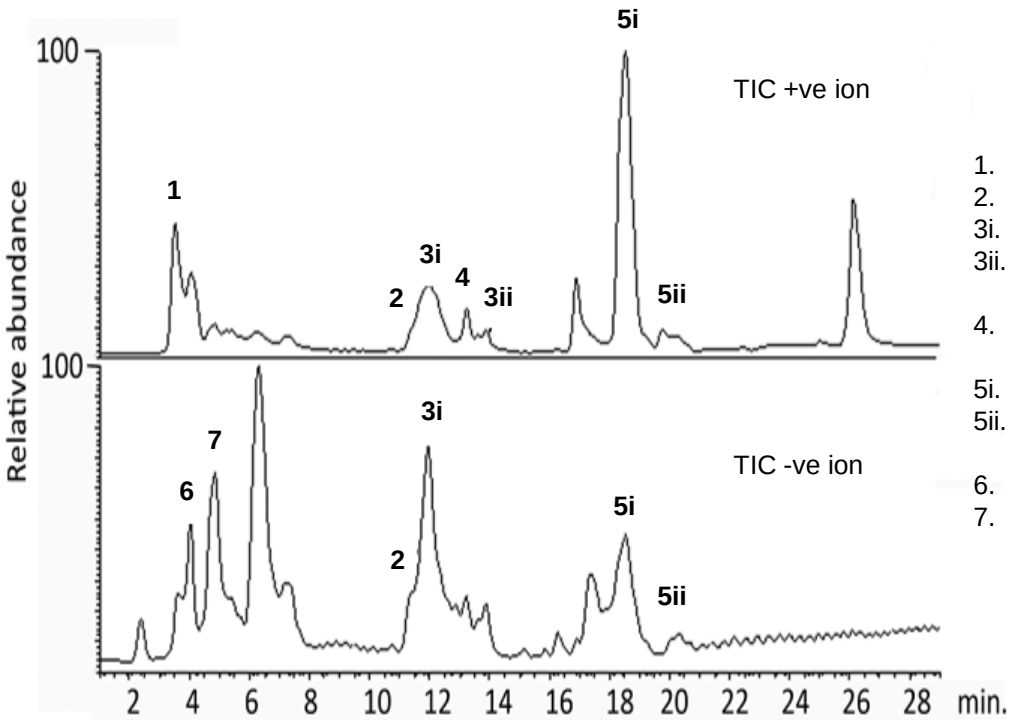
Application #AN1530

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 phosphotidylcholine (Lyso PC)
6. Glycerophosphoglycerol (GPG)
7. Phosphoinositol (PI)

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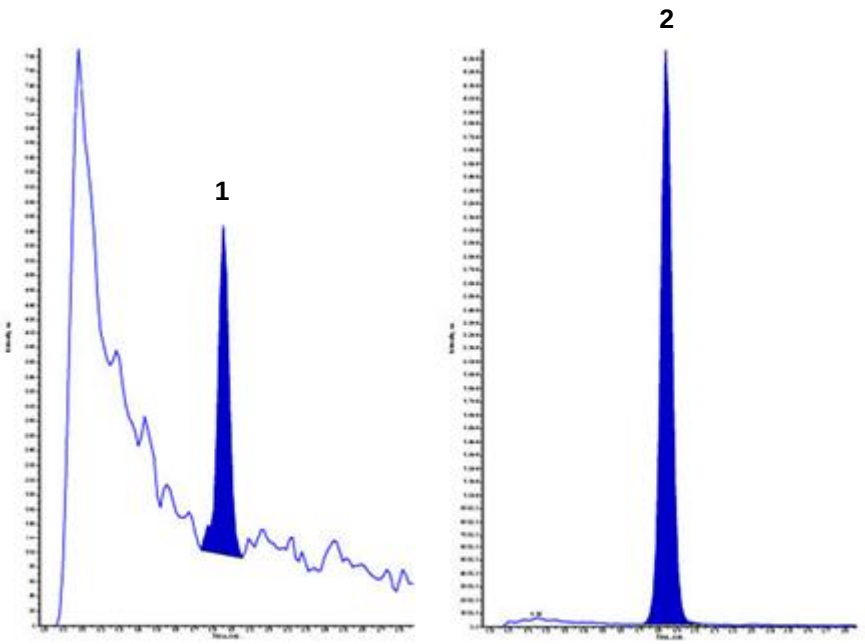
15-Hydroxy Lubiprostone in Human Plasma

ACE® Ultra-inert UHPLC & HPLC Columns

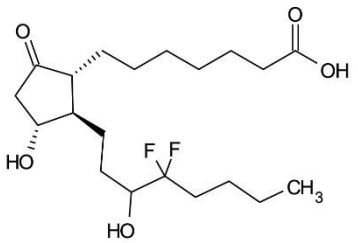
Application #AN1900

Conditions

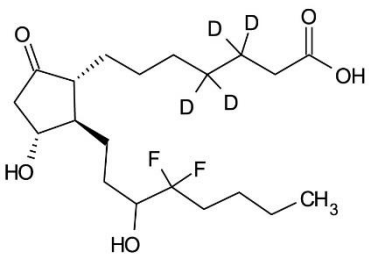
Column:	ACE Excel 2 C18
Dimensions:	50 x 3.0 mm
Part Number:	EXL-101-0503U
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: MeCN
Flow Rate:	0.65 mL/min
Injection:	15 µL
Temperature:	35 °C
Detection:	MDS Sciex API 5000
	TurbolonSpray negative mode
	IonSpray voltage -4500 V
	Source Temperature 450 °C



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



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

Lubiprostone, a fatty acid derived from prostaglandin E1, is rapidly metabolised to 15-hydroxy lubiprostone.

Quantitation is based on 15-hydroxy lubiprostone, with the d4 analogue as internal standard.

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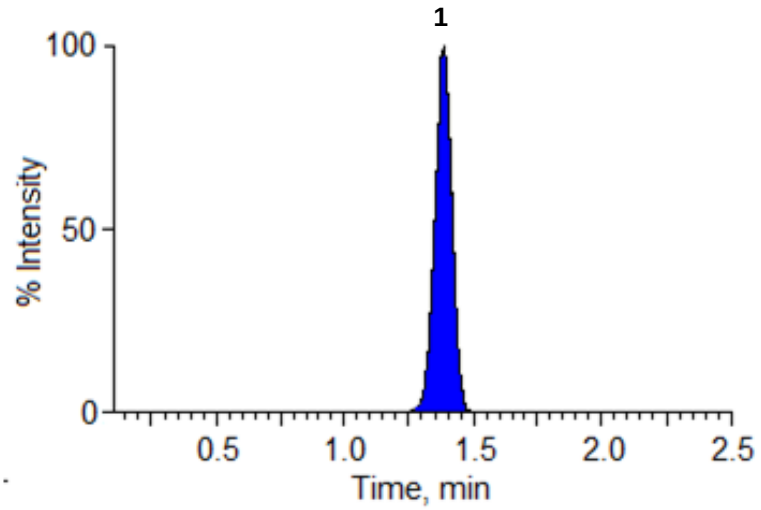
Methotrexate in K_3EDTA Human Plasma by LC-MS/MS

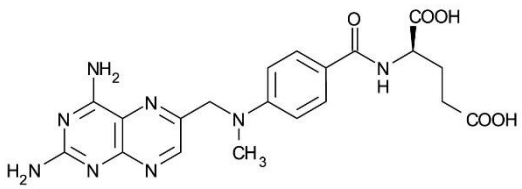
ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN3760

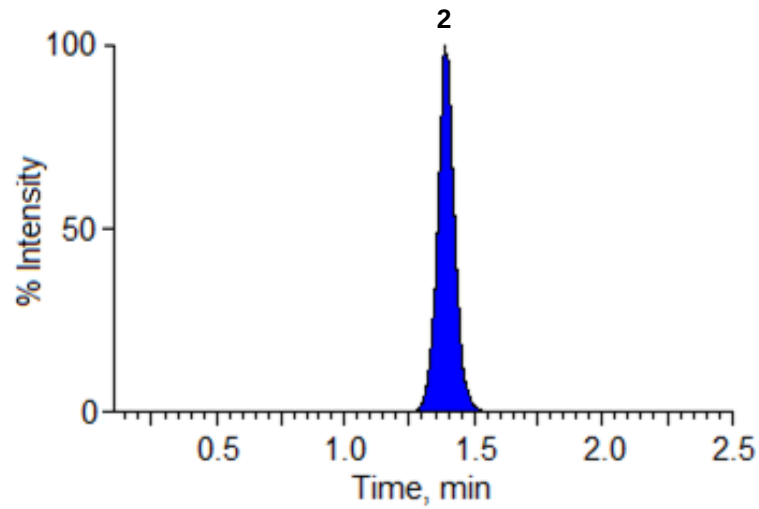
Conditions

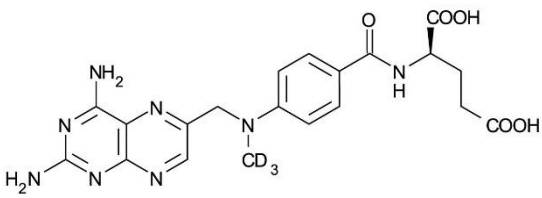
Column:	ACE 5 CN
Dimensions:	150 x 4.6 mm
Part Number:	ACE-124-1546
Mobile Phase:	10 mM ammonium formate pH 7.0/MeOH (60:40 v/v)
Flow Rate:	1 mL/min
Temperature:	40 °C
Detection:	Quattro Premier XE triple quad MS Positive ion mode ESI Ion source temperature: 120 °C Desolvation temperature: 450 °C
Sample:	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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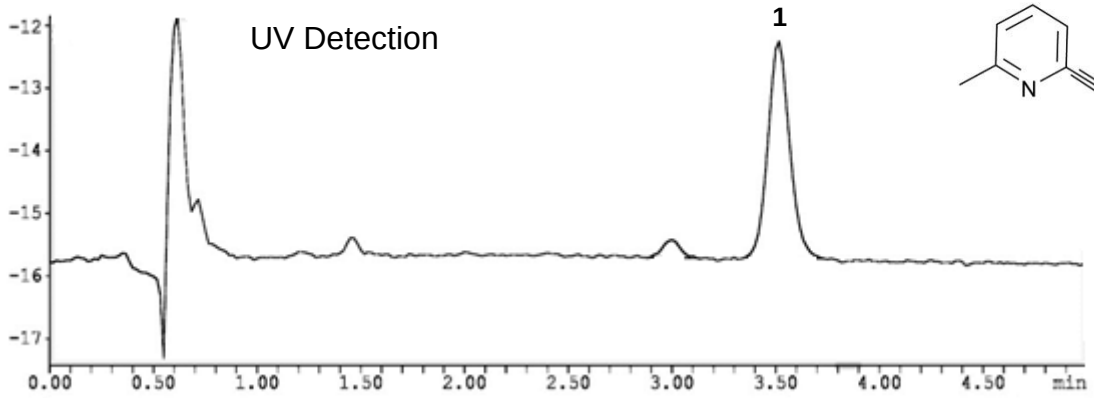
mGluR5 PET Tracer by Radio HPLC Analysis

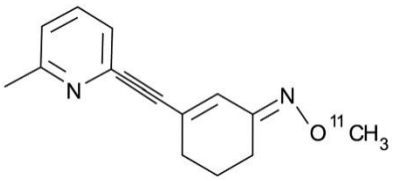
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN2700

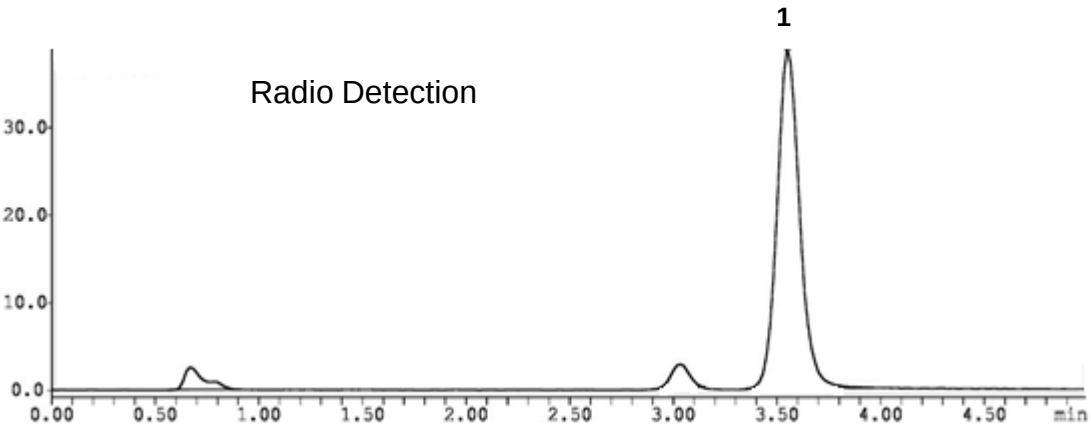
Conditions

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





l. ^{11}C-ABP688



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Non-Steroidal Anti-Inflammatory Drugs (I)

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN1210

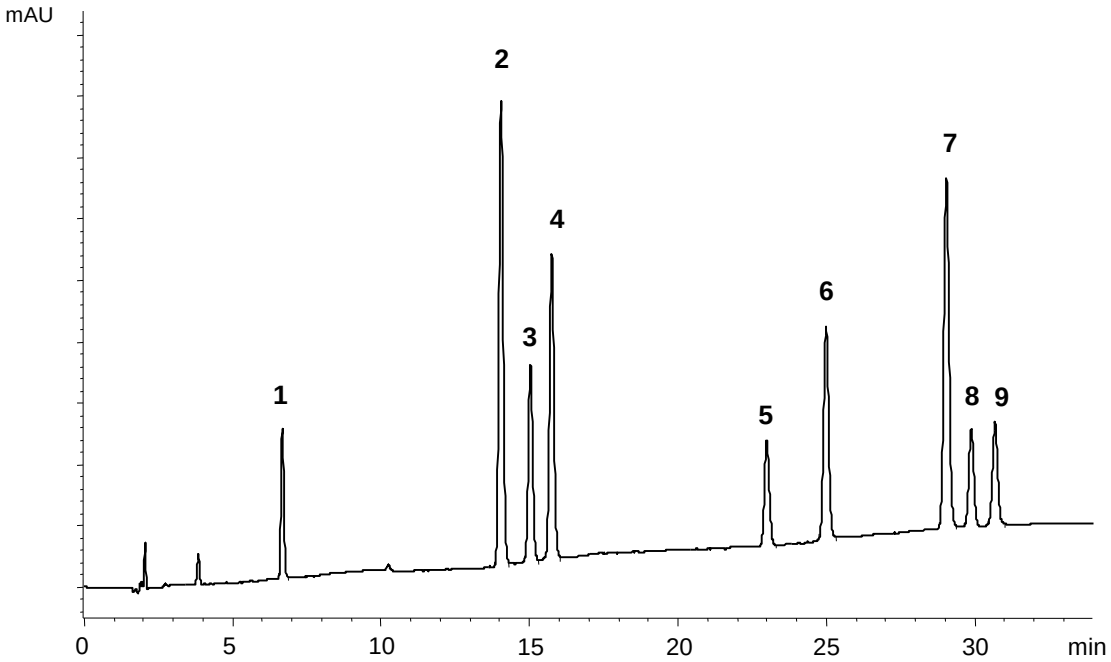
Conditions

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

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



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

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Non-Steroidal Anti-Inflammatory Drugs (II)

ACE® Ultra-inert UHPLC & HPLC Columns

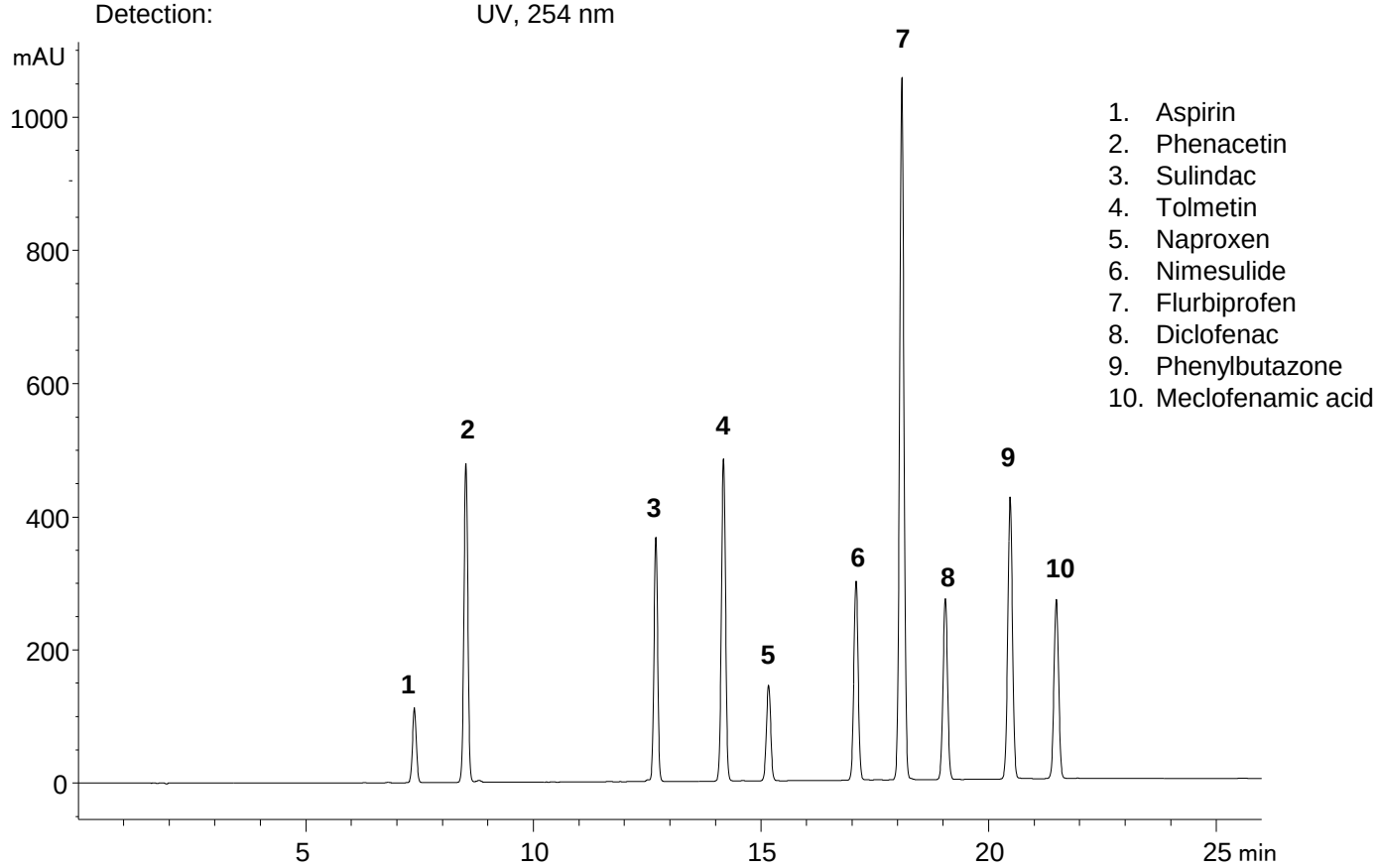
Application #AN1220

Conditions

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

ACE® Ultra-inert UHPLC & HPLC Columns

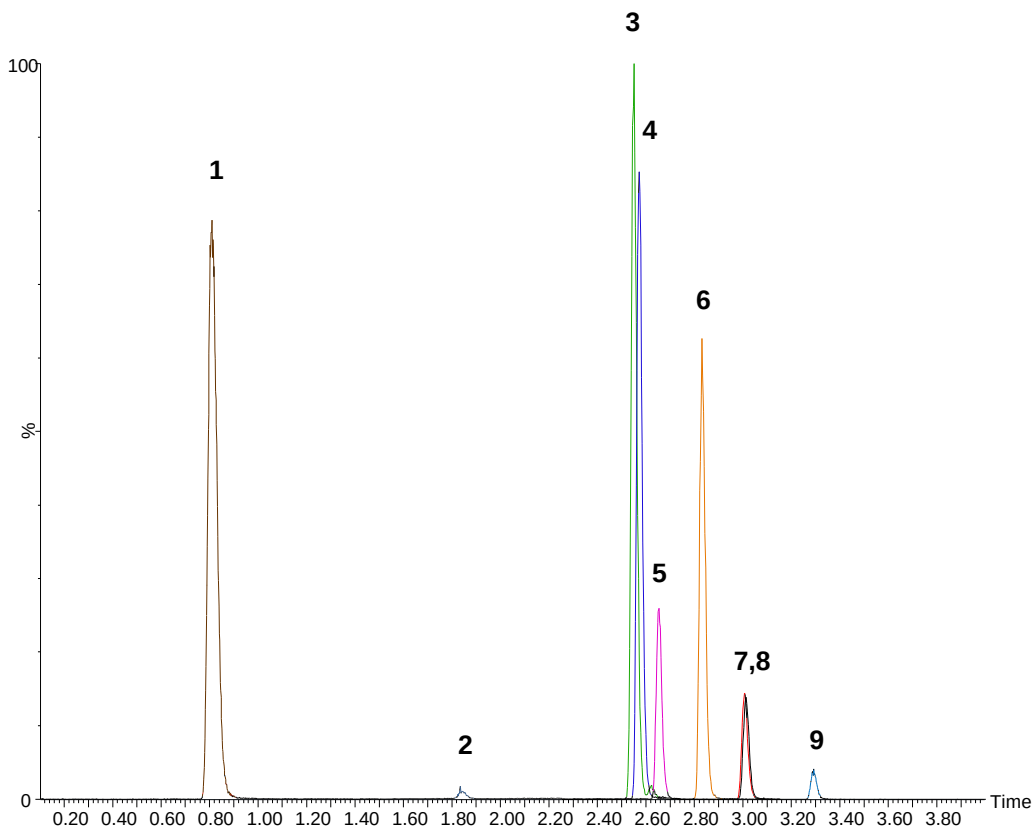
Application #**AN2630**

Conditions

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

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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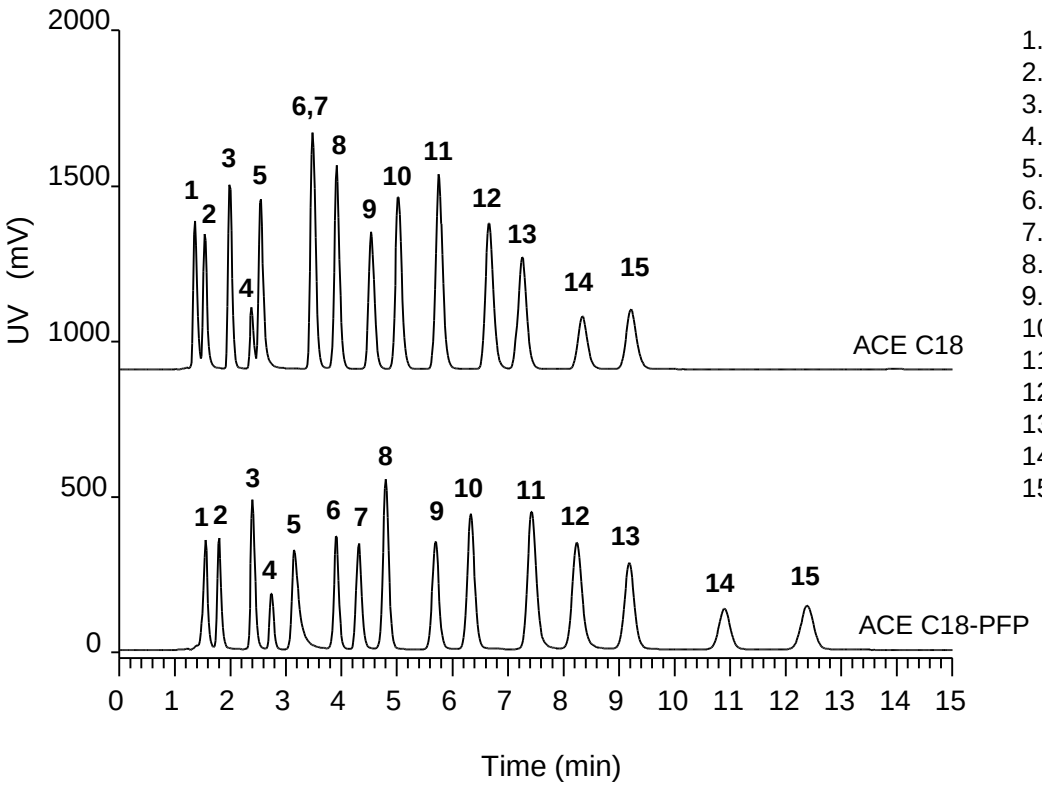
Nucleic Acids / Disease Biomarker Profiling (I)

ACE®
Ultra-inert
UHPLC & HPLC Columns

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



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

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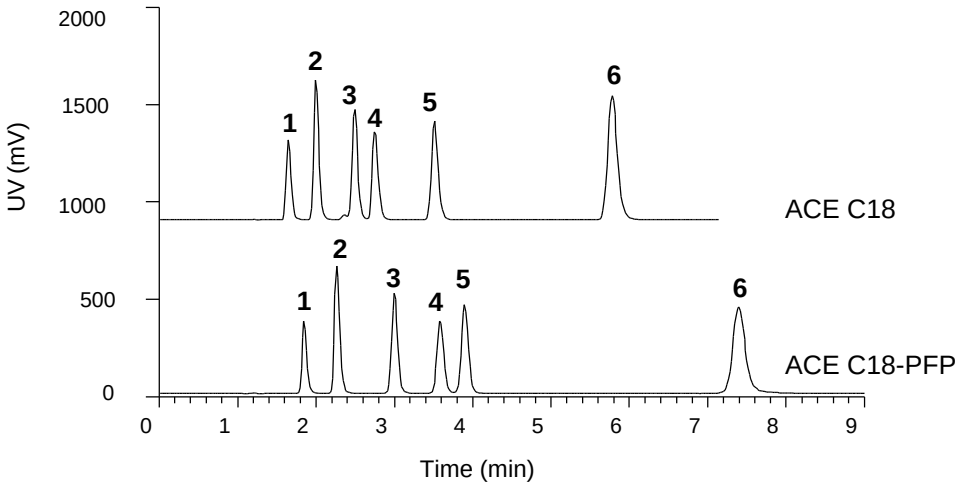
Nucleic Acids/ Disease Biomarker Profiling (II)

Application #**AN1090**

Conditions

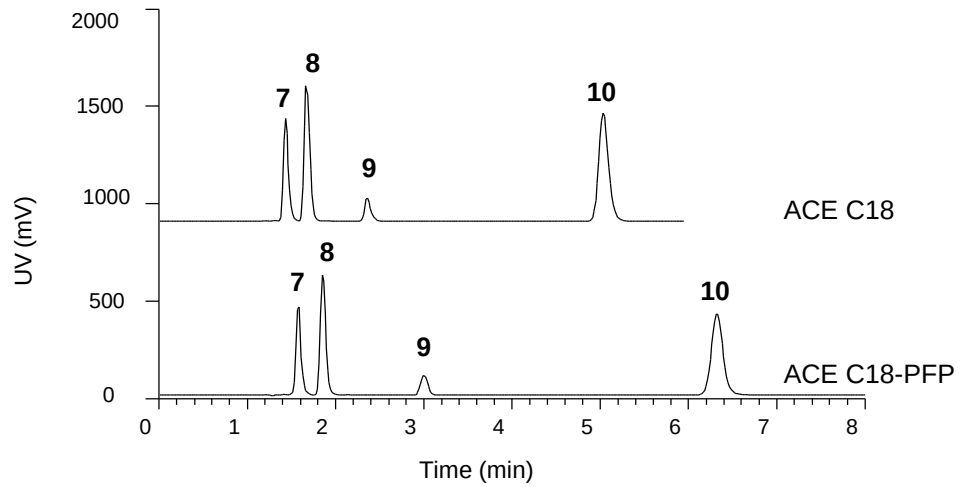
Column:	ACE 3 C18-PFP ACE 3 C18
Dimensions:	100 x 4.6 mm
Part Number:	ACE-1110-1046, ACE-111-1046
Mobile Phase:	33 mM potassium phosphate pH 6.2 with KOH/MeOH (88:12 v/v)
Flow Rate:	1 mL/min
Temperature:	Ambient
Detection:	UV, 260 nm

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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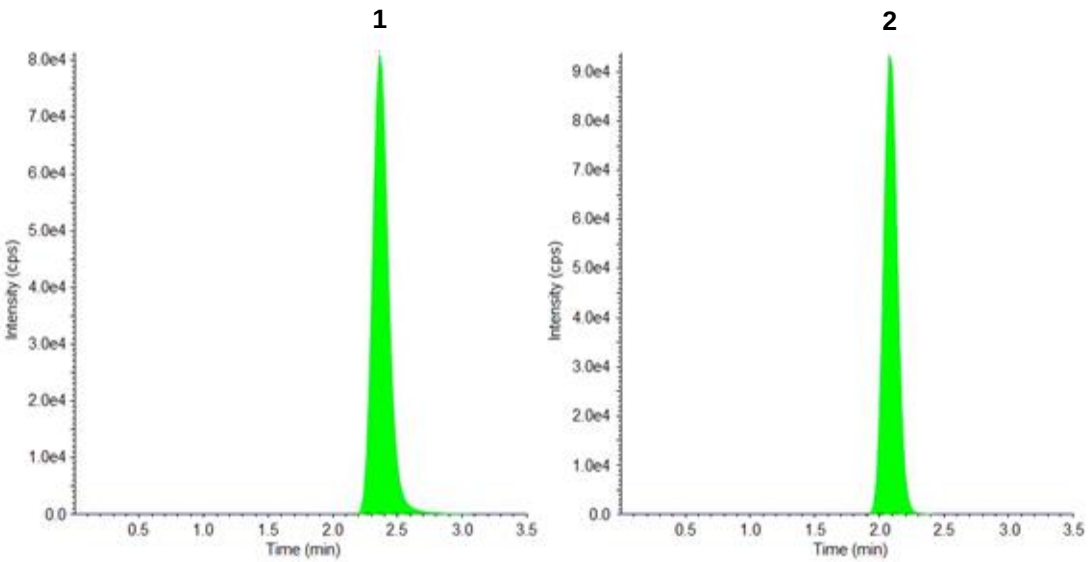
Olanzapine in Human Plasma by LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

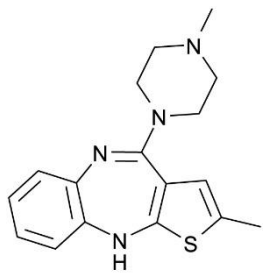
Application #AN2520

Conditions

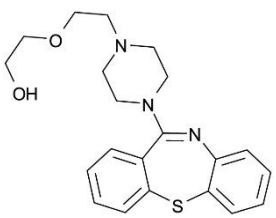
Column:	ACE 5 C18-300
Dimensions:	100 x 4.6 mm
Part Number:	ACE-221-1046
Mobile Phase:	MeCN/0.01% ammonia in 2 mM ammonium formate pH 6.6 (85:15 v/v)
Flow Rate:	0.9 mL/min
Injection:	5 µL
Detection:	API 4000 triple quad MS Turbo Ion Spray in positive mode Ion Spray voltage: 5500 V Temperature: 550 °C



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



1. Olanzapine
(*m/z* 313.2 → 256.2)



2. Quetiapine (IS)
(*m/z* 384.2 → 253.2)

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Opiates In Urine by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

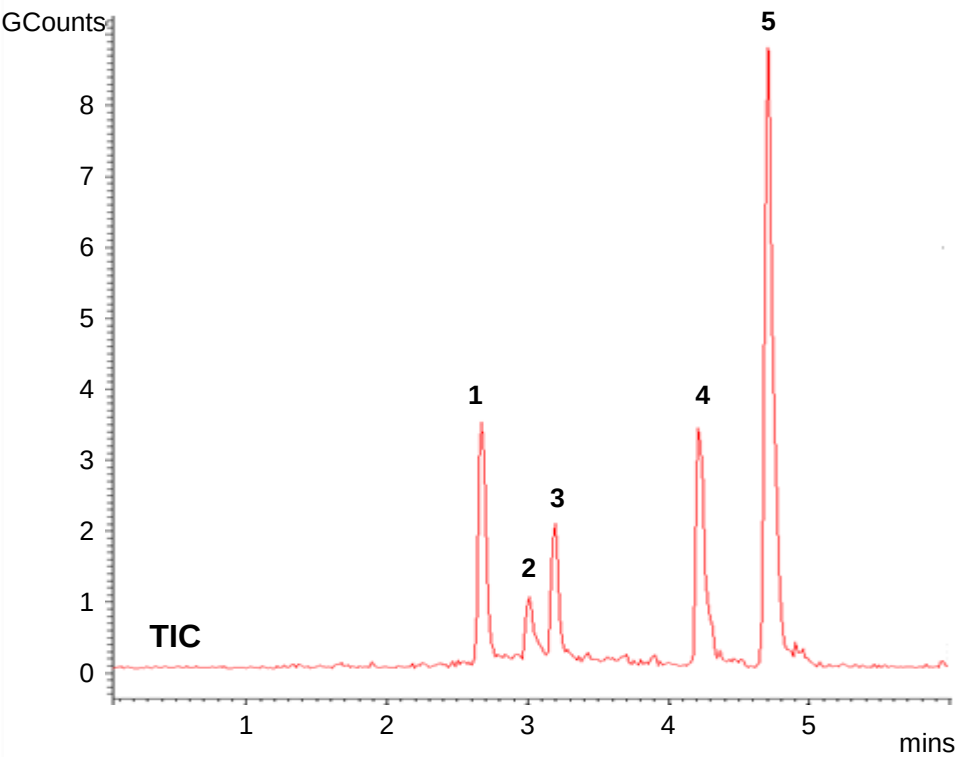
Application #**AN1230**

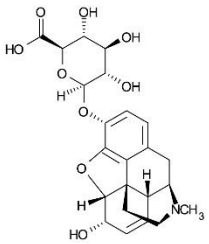
Conditions

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

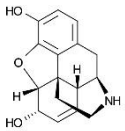
Time (mins)	%B
0	30
5	95

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

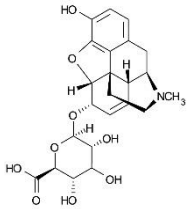




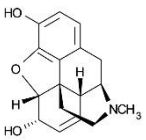
1. Morphine 3-β-D-glucuronide
LOD (est) 100 ppb
(*m/z* 462.0 → 285.9)



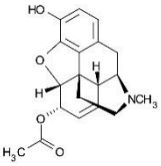
2. Normorphine
LOD (est) 100 ppb
(*m/z* 272.0 → 165.0)



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)

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Oxysterols by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

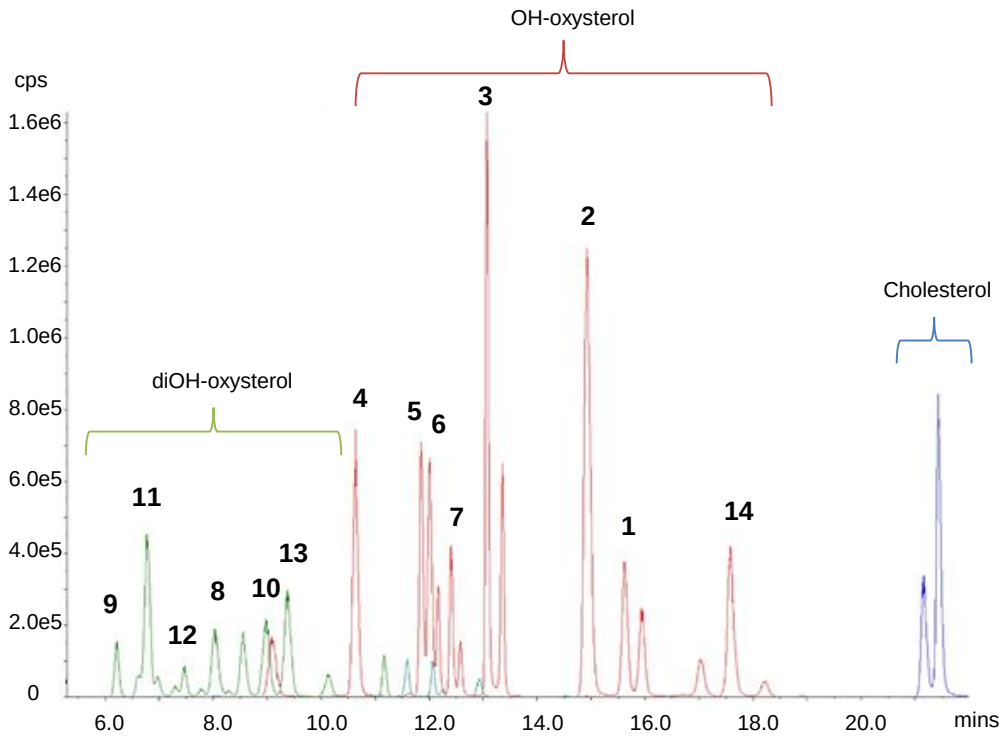
Application #**AN2380**

Conditions

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

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

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



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

Reproduced from supplement (pnas.org/content/suppl/2014/08/01/1322807111) to 'Oxysterols are agonist ligands of RORγt and drive Th17 cell differentiation', PNAS, 111 (33), 12163-12168 (2014)

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Paralytic Shellfish Poisoning (PSP) Toxins

ACE® Ultra-inert UHPLC & HPLC Columns

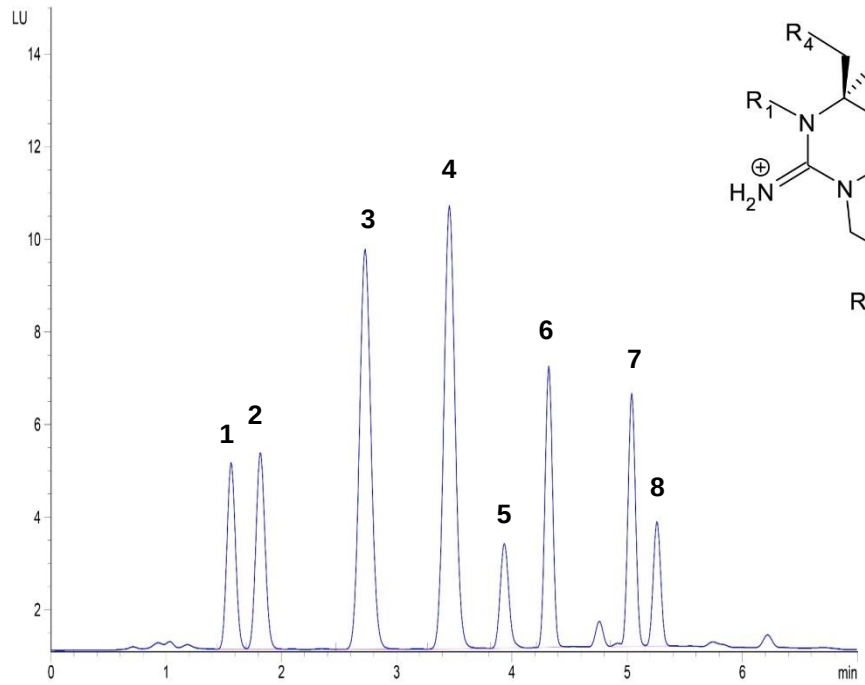
Application #AN3180

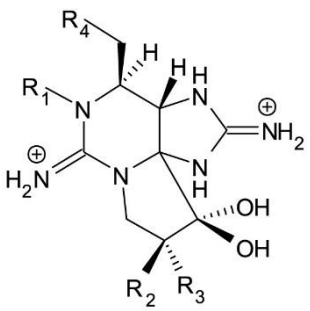
Conditions

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

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

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





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

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

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Peptides – Selectivity Changes with Bonded Phase and Mobile Phase

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN3430

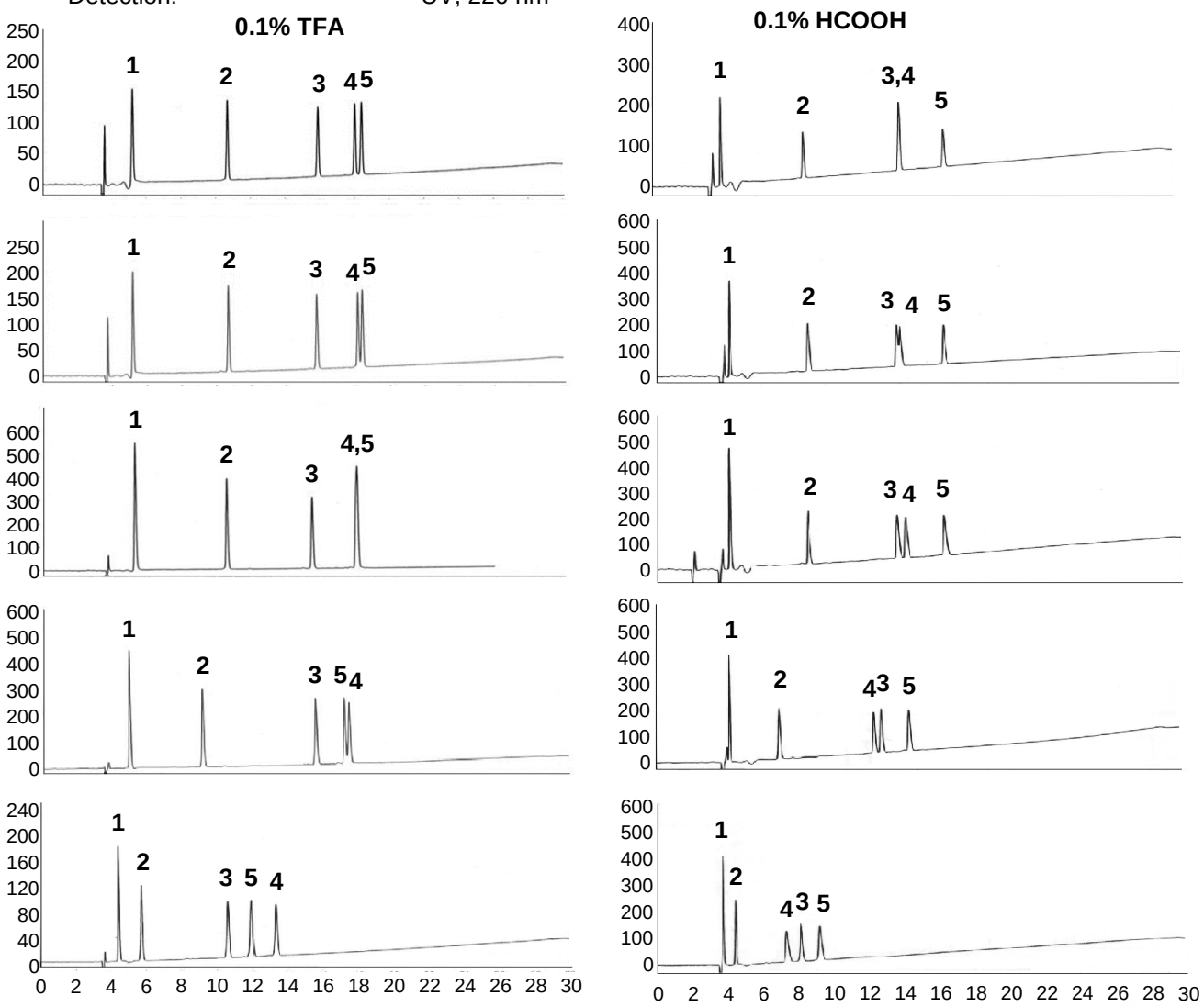
Conditions

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

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

ACE® Ultra-inert UHPLC & HPLC Columns

Application #**AN3400**

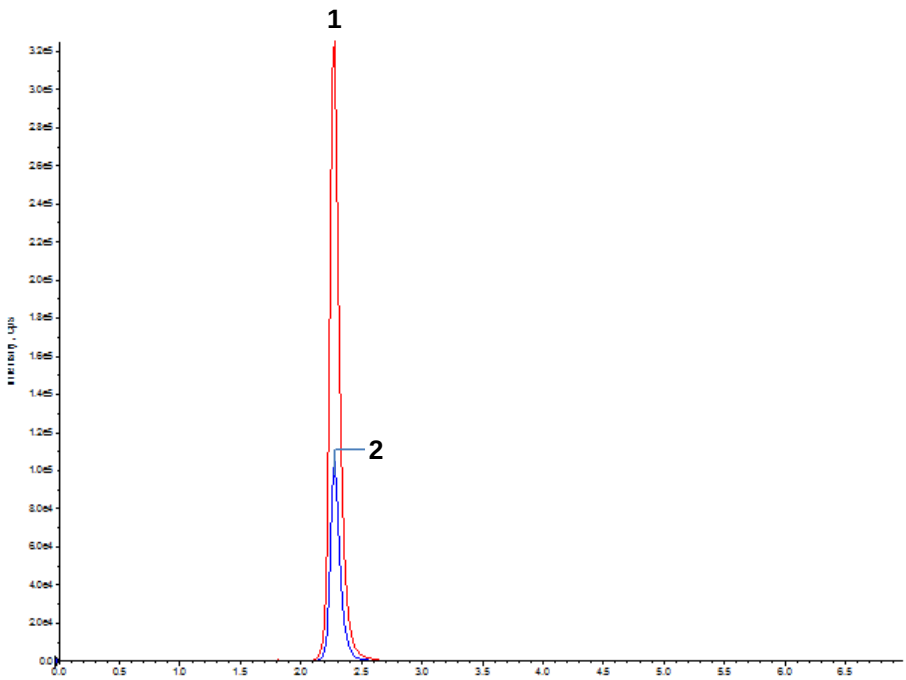
Conditions

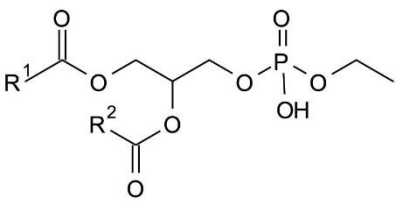
Column:	ACE 2 C4
Dimensions:	100 x 2.1 mm
Part Number:	EXL-103-1002U
Mobile Phase:	A: 2 mM ammonium acetate/MeCN (20:80 v/v)
	B: IPA

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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Porphyrins in Oral Bacteria by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

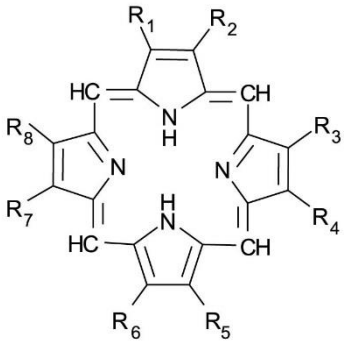
Application #AN3080

Conditions

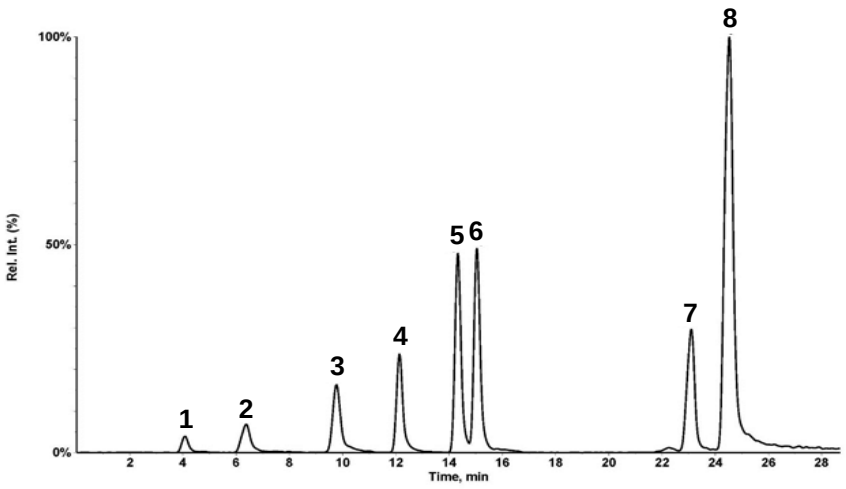
Column:	ACE 3 C18-PFP
Dimensions:	75 x 2.1 mm
Part Number:	ACE-1110-7502
Mobile Phase:	A: 0.1% formic acid in H_2O/MeCN (95:5 v/v)
	B: 0.1% formic acid in H_2O/MeCN (5:95 v/v)

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



1. Uroporphyrin I
(R_1:A, R_2:P, R_3:A, R_4:P, R_5:A, R_6:P, R_7:A, R_8:P)
(*m/z* 831 → 727, 623, 655)

2. 7-Carboxyporphyrin I
(R_1:A, R_2:P, R_3:A, R_4:P, R_5:A, R_6:P, R_7:M, R_8:P)
(*m/z* 787 → 683, 670, 623)

3. 6-Carboxyporphyrin I
(R_1:M, R_2:P, R_3:A, R_4:P, R_5:A, R_6:P, R_7:M, R_8:P)
(*m/z* 743 → 639, 507, 521)

4. 5-Carboxyporphyrin I
(R_1:M, R_2:P, R_3:M, R_4:P, R_5:A, R_6:P, R_7:M, R_8:P)
(*m/z* 699 → 463, 595, 640)

5. Coproporphyrin I
(R_1:M, R_2:P, R_3:M, R_4:P, R_5:M, R_6:P, R_7:M, R_8:P)
(*m/z* 655 → 537, 596, 523)

6. Coproporphyrin III
(R_1:M, R_2:P, R_3:M, R_4:P, R_5:M, R_6:P, R_7:P, R_8:M)
(*m/z* 655 → 537, 596, 523)

7. Mesoporphyrin IX
(R_1:M, R_2:E, R_3:M, R_4:E, R_5:M, R_6:P, R_7:M, R_8:P)
(*m/z* 567 → 449, 479, 508)

8. Protoporphyrin IX
(R_1:M, R_2:V, R_3:M, R_4:V, R_5:M, R_6:P, R_7:P, R_8:M)
(*m/z* 563 → 445, 504, 489)

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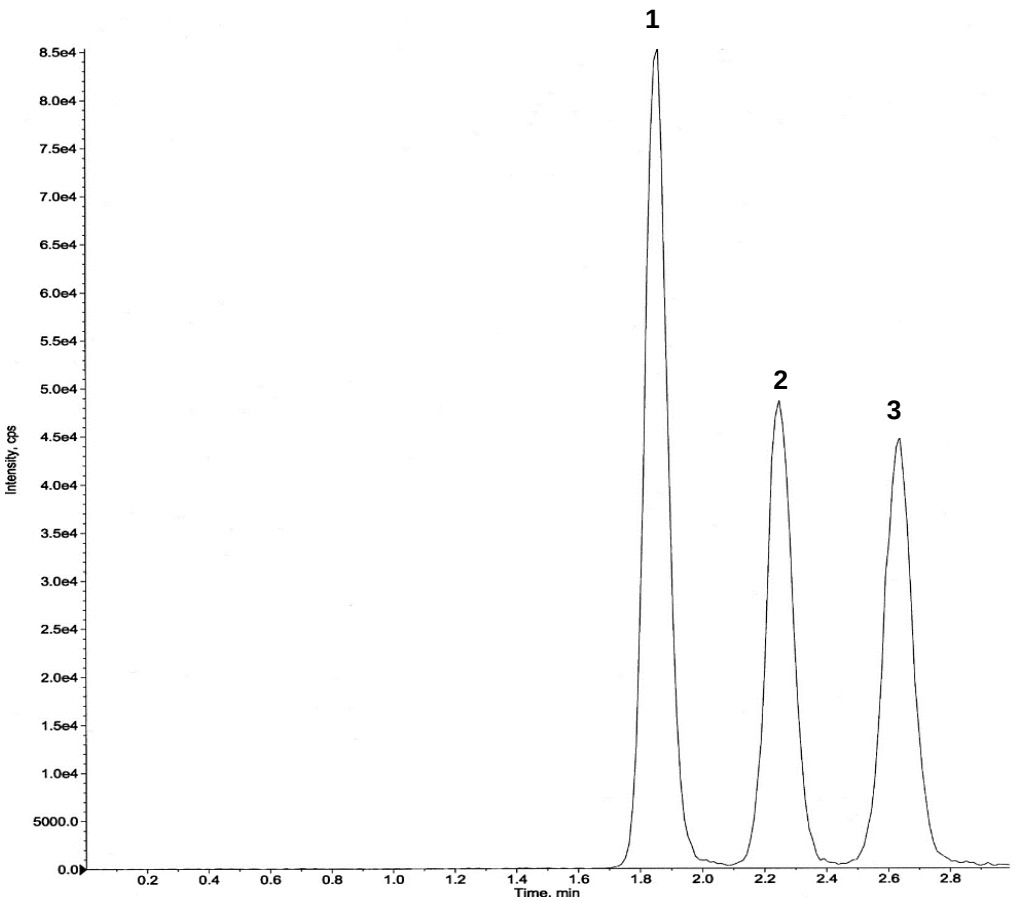
Pravastatin and Isomers by LC-MS/MS

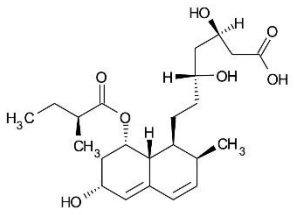
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN1350

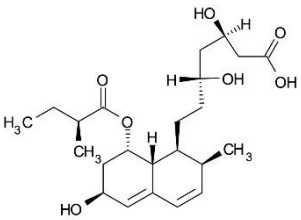
Conditions

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

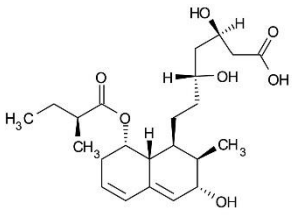




1. 6-epi-Pravastatin
(*m/z* 424)



2. Pravastatin
(*m/z* 424)



3. 3α-iso-Pravastatin
(*m/z* 424)

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

ACE® Ultra-inert UHPLC & HPLC Columns

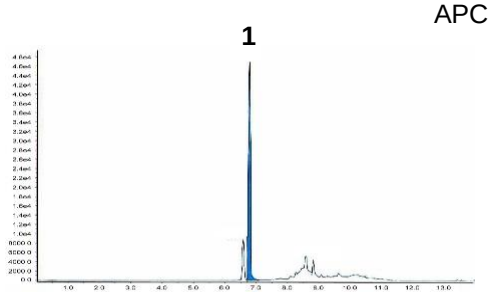
Application #AN2690

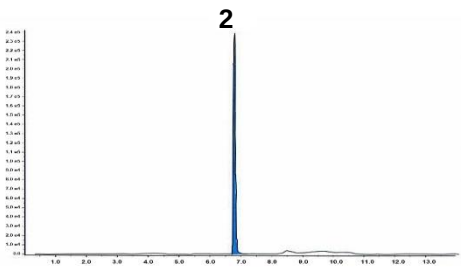
Conditions

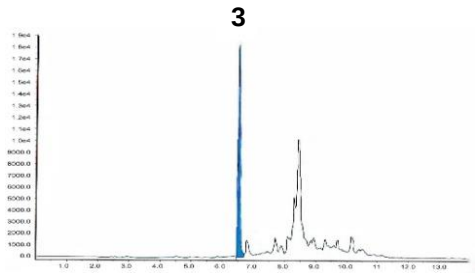
Column:	ACE Excel 2 C18
Dimensions:	100 x 2.1 mm
Part Number:	EXL-101-1002U
Mobile Phase:	A: 4 mM ammonium acetate in H_2O
	B: 0.2% (v/v) formic acid in MeOH

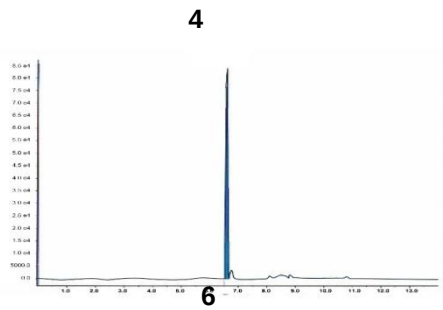
Time (mins)	%B
0.00	30
0.25	30
3.90	70
6.00	70
6.01	95
7.00	95
7.01	100

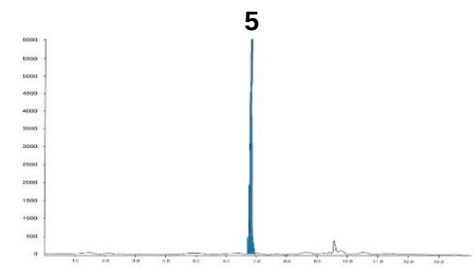
Flow Rate:	0.2 mL/min
Injection:	50 µL
Temperature:	50 °C
Detection:	Applied Biosystems 5000 MS/MS
	APCI in positive ion mode

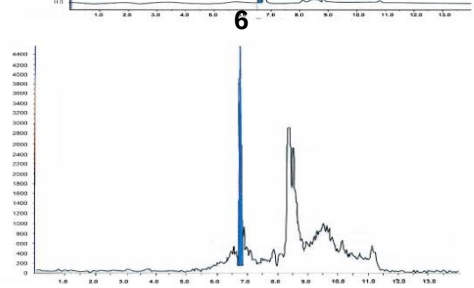


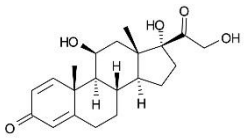




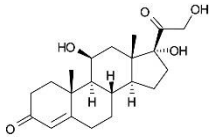




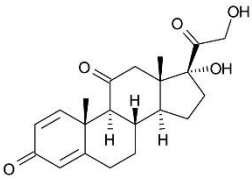




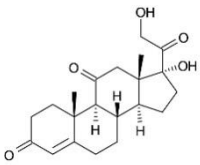
1. Prednisolone
(*m/z* 361.5 → 147.1)



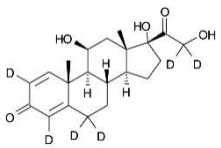
2. Cortisol
(*m/z* 363.5 → 121.3)



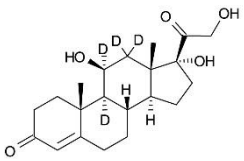
3. Prednisone
(*m/z* 359.4 → 147.1)



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

ACE® Ultra-inert UHPLC & HPLC Columns

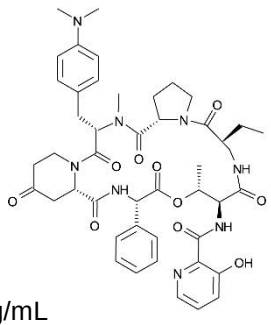
Application #**AN1360**

Conditions

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

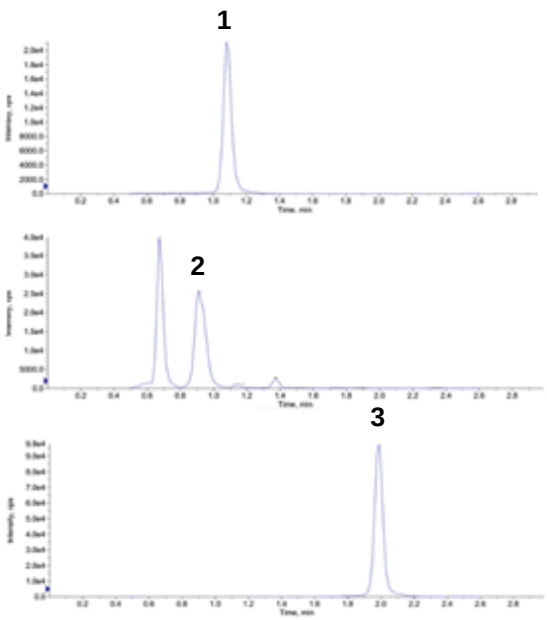
Time (mins)	%B
0.00	0
0.30	0
0.31	10
1.60	10
1.61	100
2.60	100
2.61	0
4.00	0

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

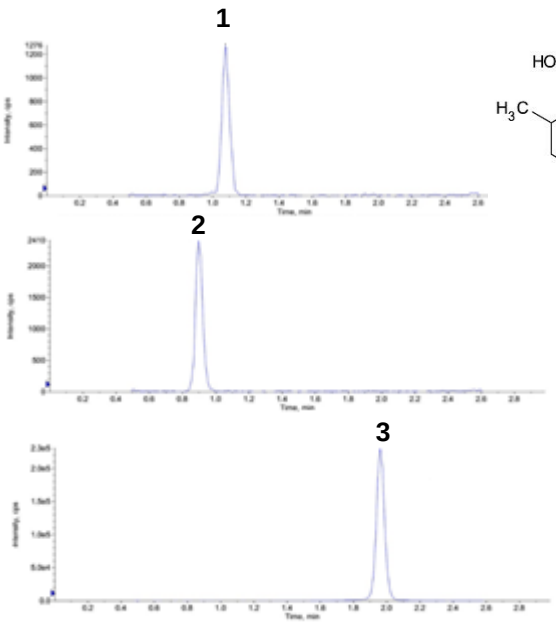


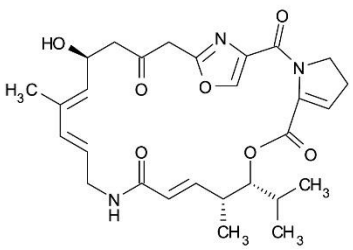
1. Pristinamycin IA (*m/z* 867.5 → 134.2)

Processed study sample containing pristinamycin IA and IIA



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





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

ACE®
Ultra-inert
UHPLC & HPLC Columns

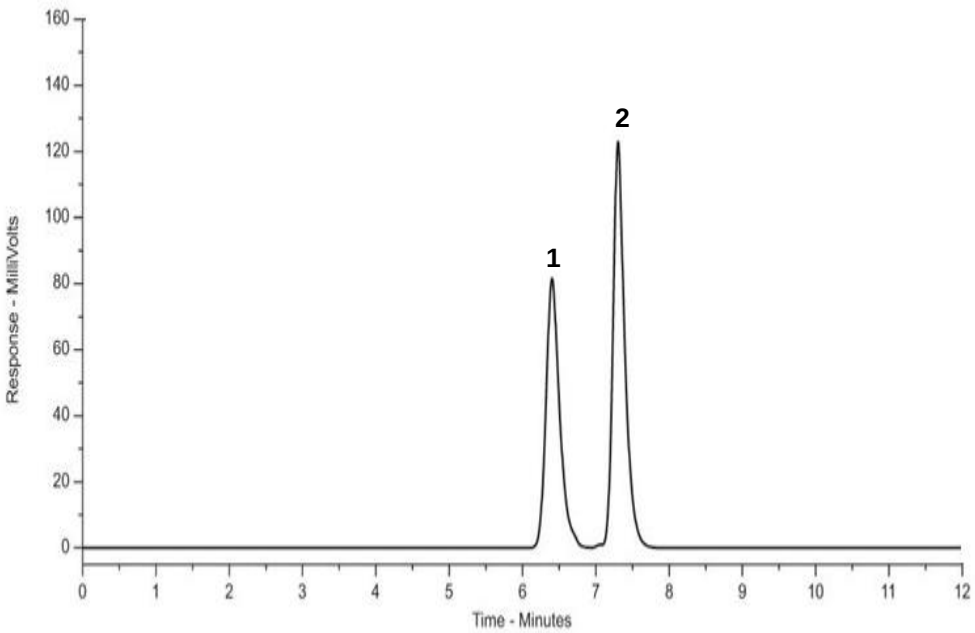
Application #AN3260

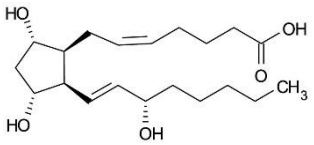
Conditions

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

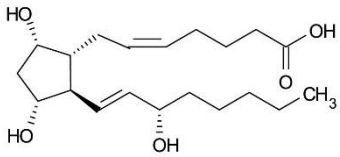
Time (mins)	%A	%B	%C
0	70	20	10
9	10	60	30
10	0.1	66.6	33.3

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





1. 8-iso-Prostaglandin $F_{2\alpha}$



2. Prostaglandin $F_{2\alpha}$

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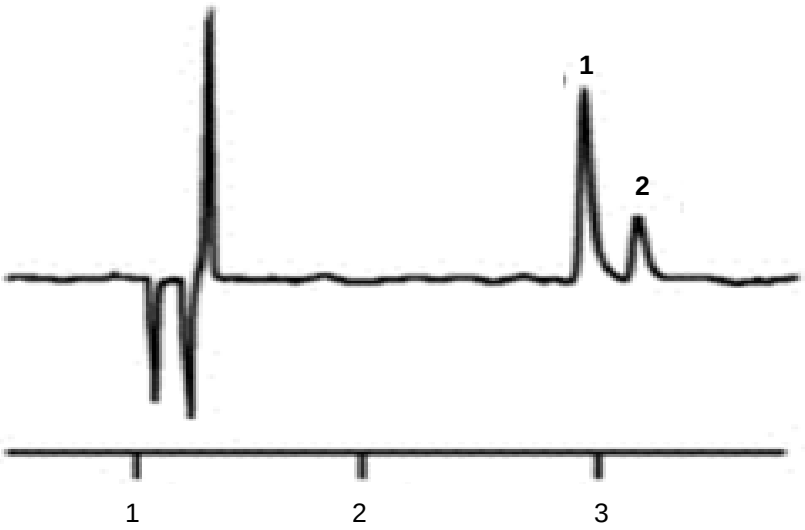
Psychoactive Substances in ‘Synthacaine’ by LC-UV

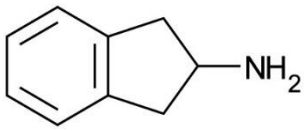
ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN3440

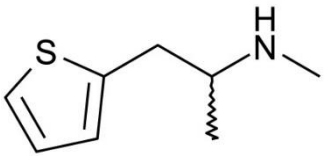
Conditions

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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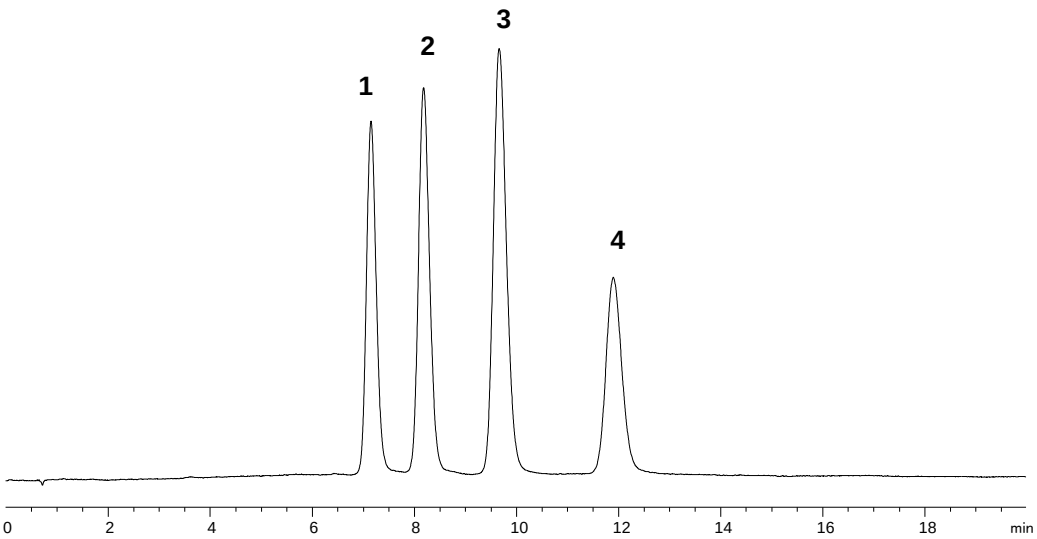
Quinidine, Quinine and their Hydroderivatives Separation

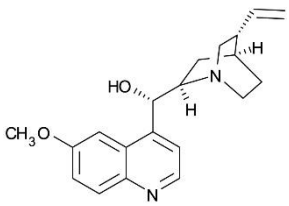
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN1600

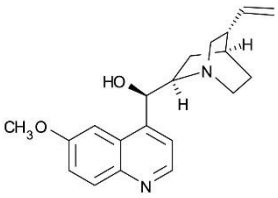
Conditions

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

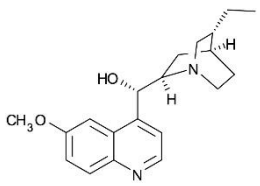




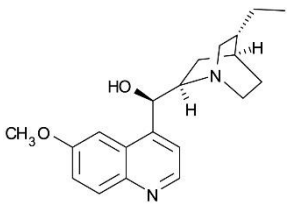
1. Quinidine



2. Quinine



3. Hydroquinidine



4. Hydroquinine

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Ranitidine Hydrochloride and Related Impurities

ACE® Ultra-inert UHPLC & HPLC Columns

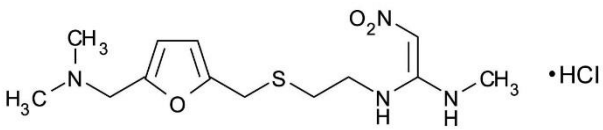
Application #AN3450

Conditions

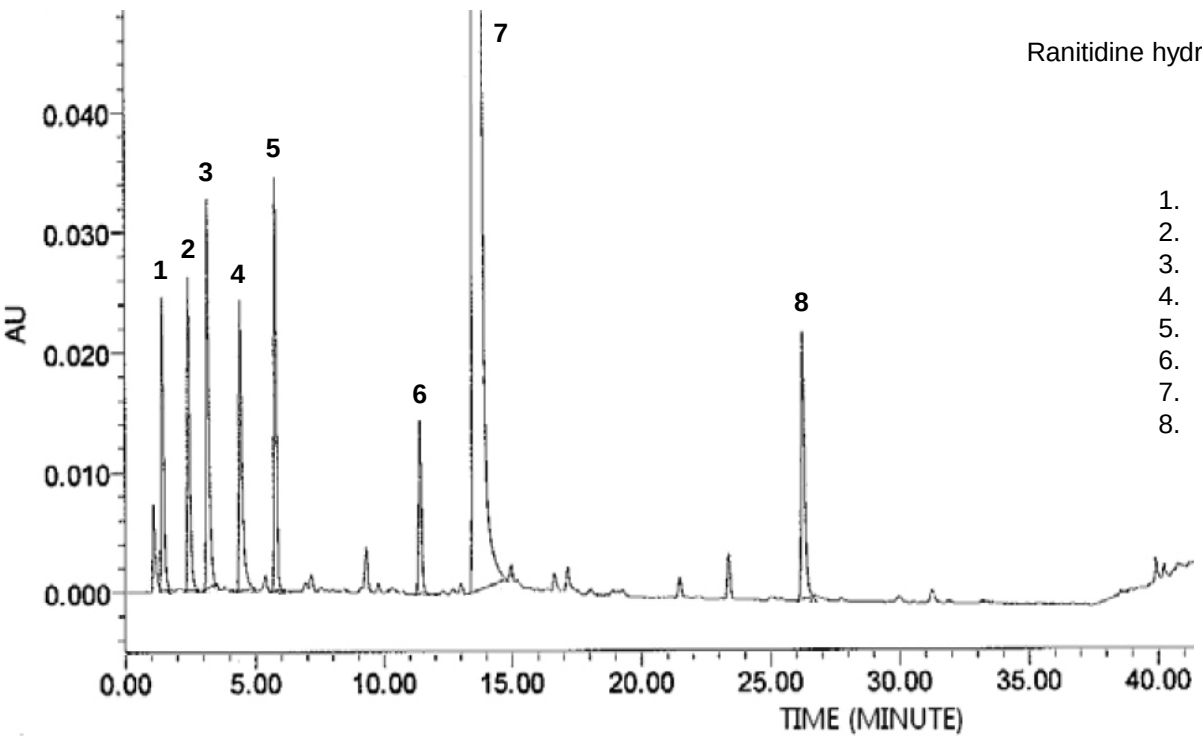
Column:	ACE 3 C18
Dimensions:	100 x 4.6 mm
Part Number:	ACE-111-1046
Mobile Phase:	A: 0.05 M KH_2PO_4 pH 6.5 in H_2O/MeCN (98:2 v/v) B: H_2O/MeCN (5:95 v/v)

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



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

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

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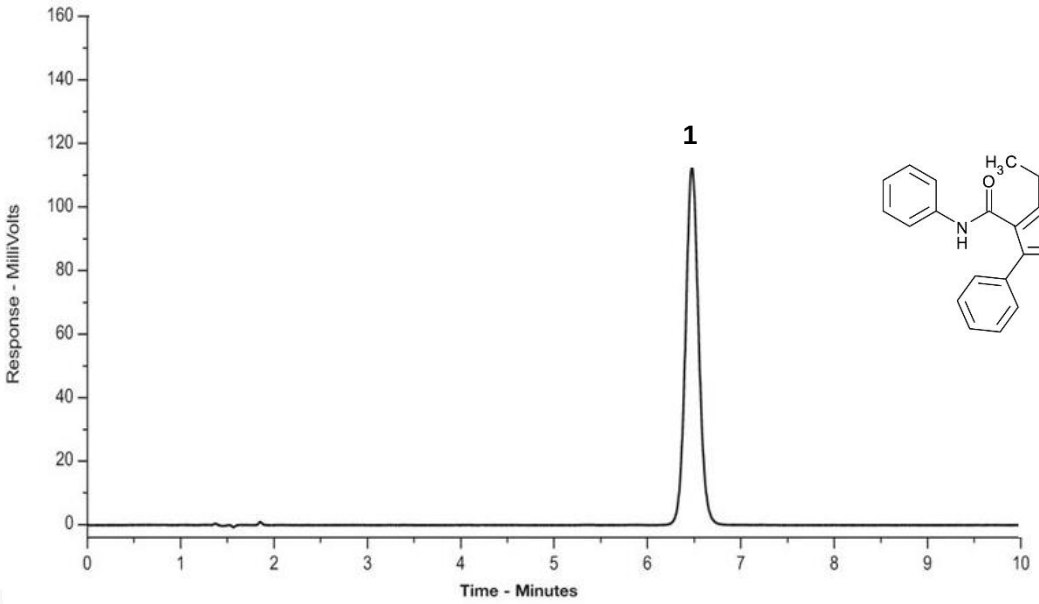
Statins - Atorvastatin

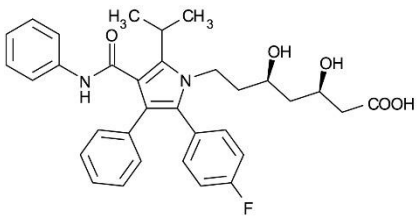
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN3310

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

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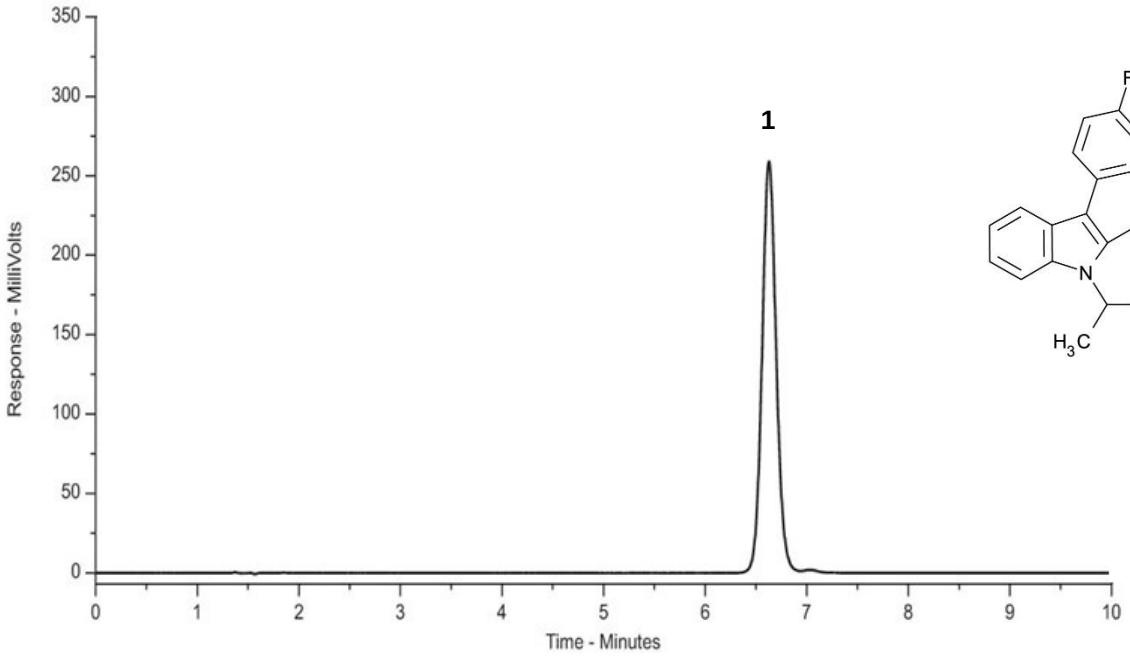
Statins - Fluvastatin

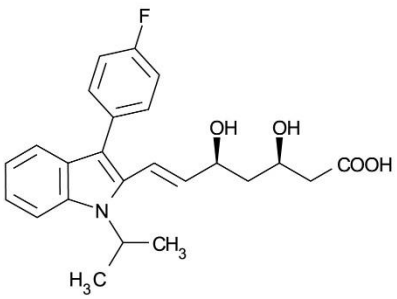
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN3320

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

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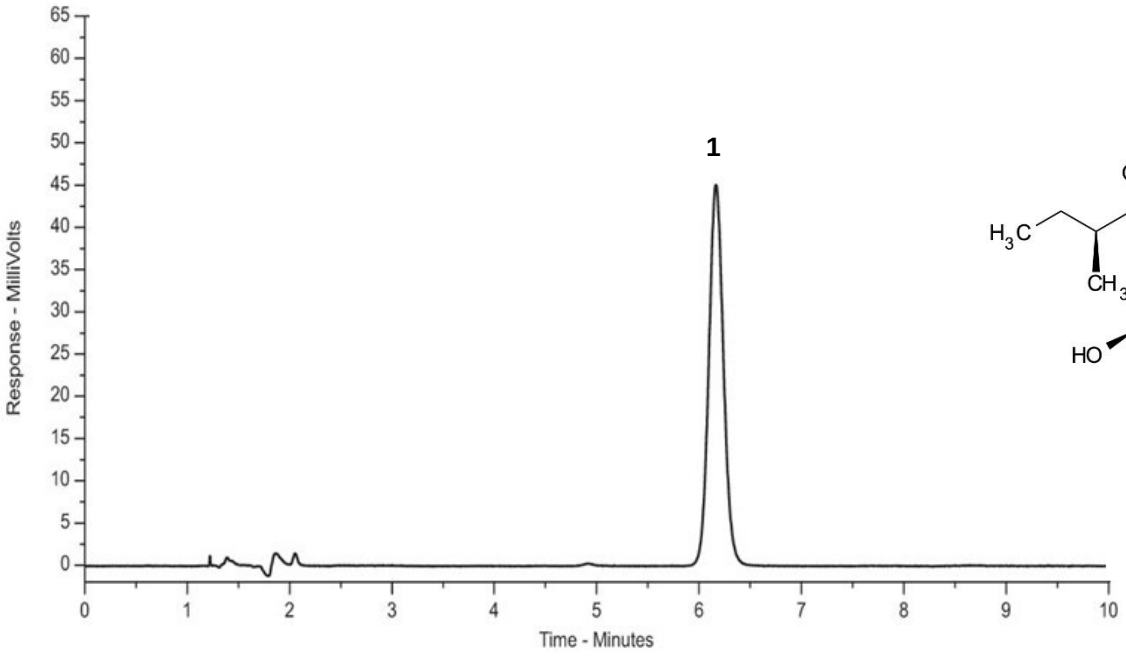
Statins - Pravastatin

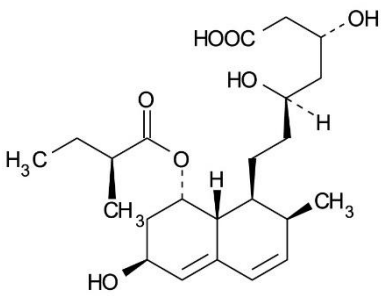
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN3330

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

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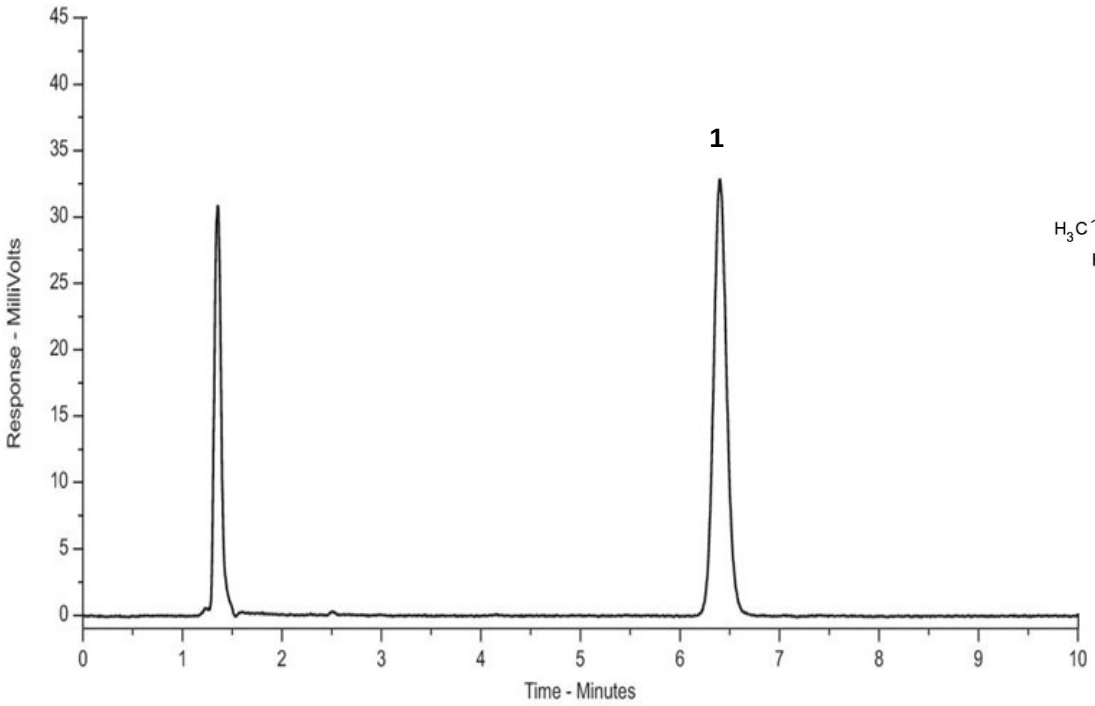
Statins - Simvastatin

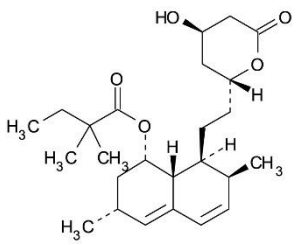
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN3340

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

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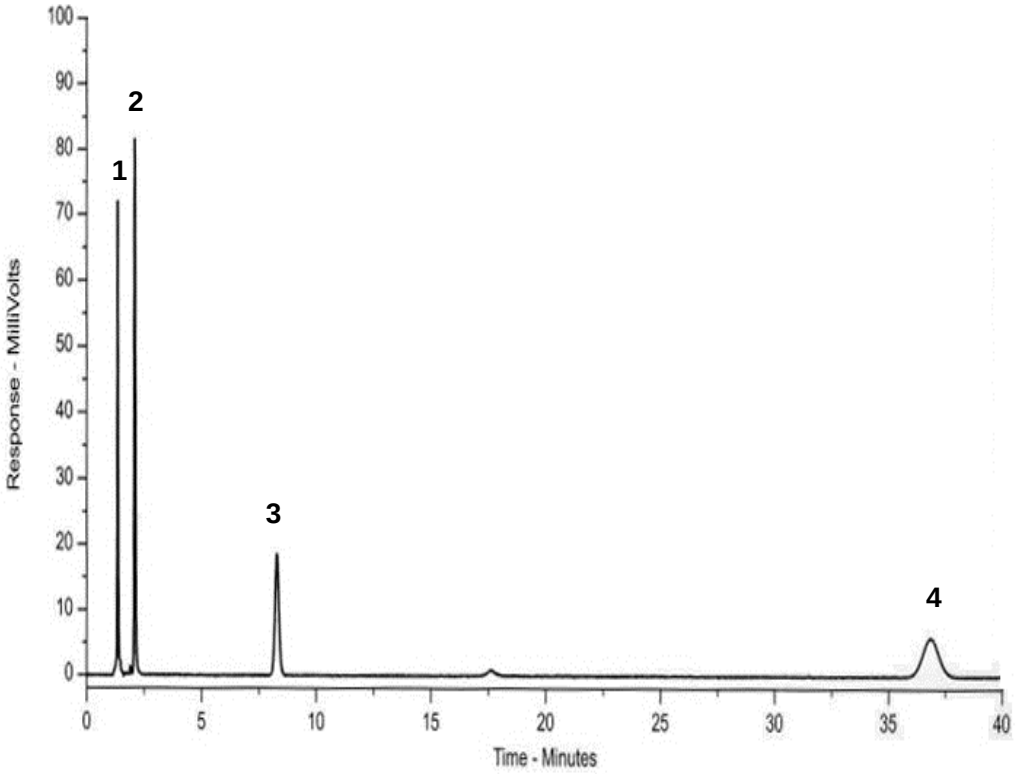
Statin Mixture

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN3410

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

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Steroid Hormones (Endogenous) by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

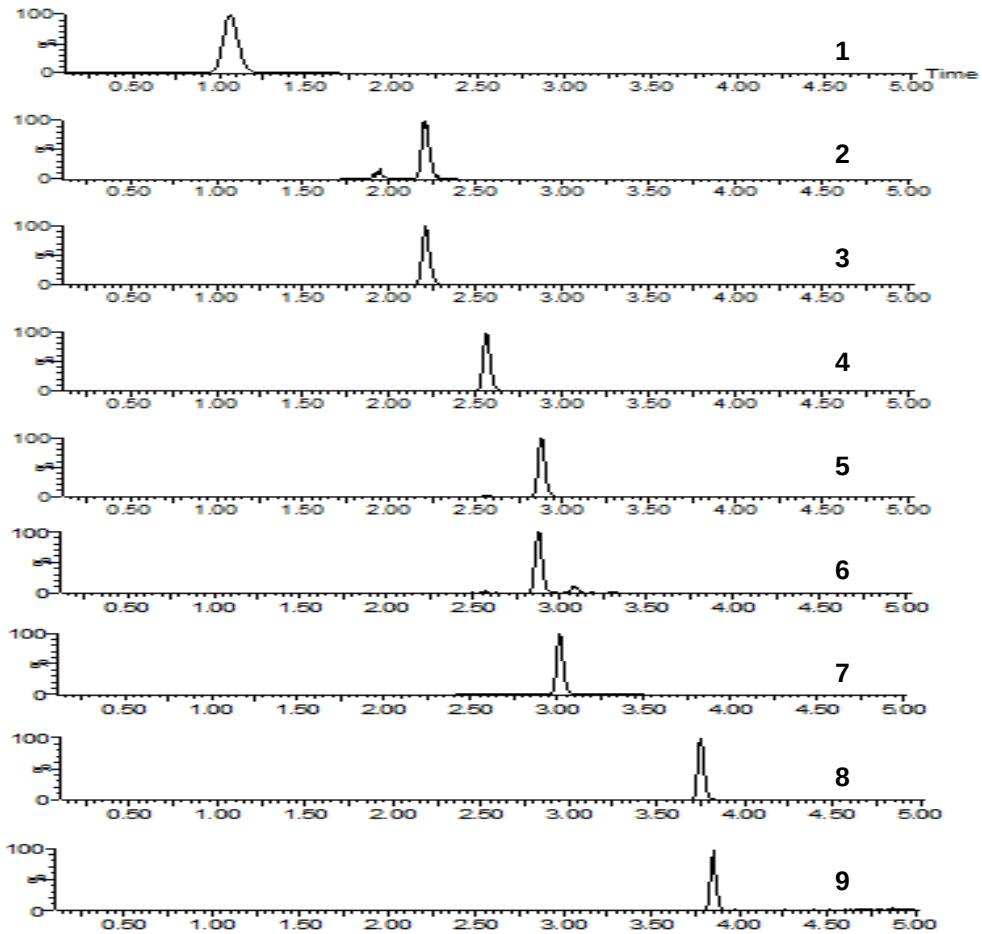
Application #**AN2640**

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 H_2O
	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. 17α-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)

ACE®
Ultra-inert
UHPLC & HPLC Columns

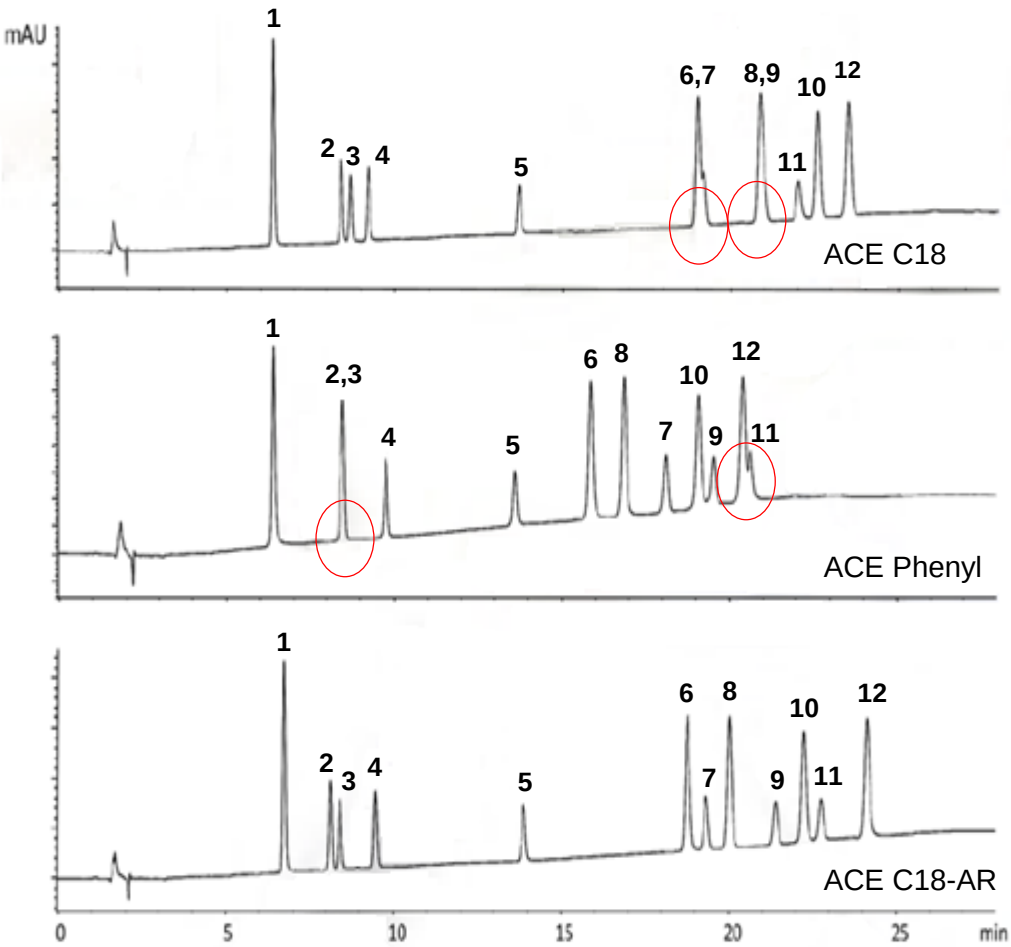
Application #**AN1060**

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: H_2O 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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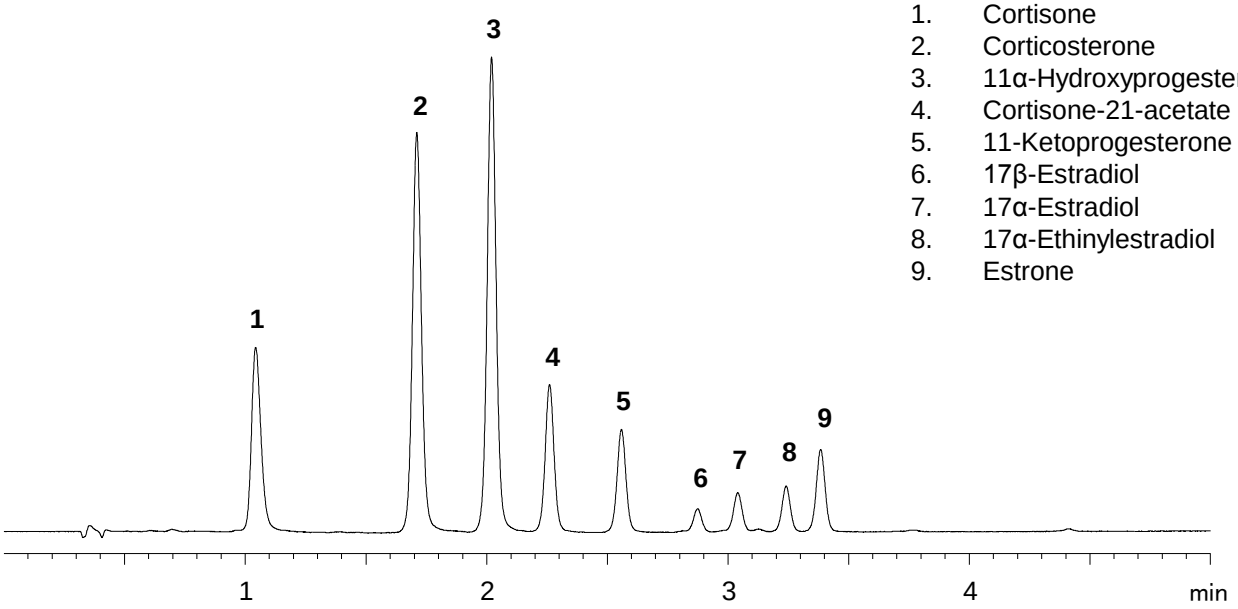
Steroid Mixture Separation (II)

ACE®
Ultra-inert
UHPLC & HPLC Columns

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 H_2O
	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



1. Cortisone
2. Corticosterone
3. 11α-Hydroxyprogesterone
4. Cortisone-21-acetate
5. 11-Ketoprogesterone
6. 17β-Estradiol
7. 17α-Estradiol
8. 17α-Ethinylestradiol
9. Estrone

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Steroids by LC-MS/MS

ACE®
Ultra-inert
UHPLC & HPLC Columns

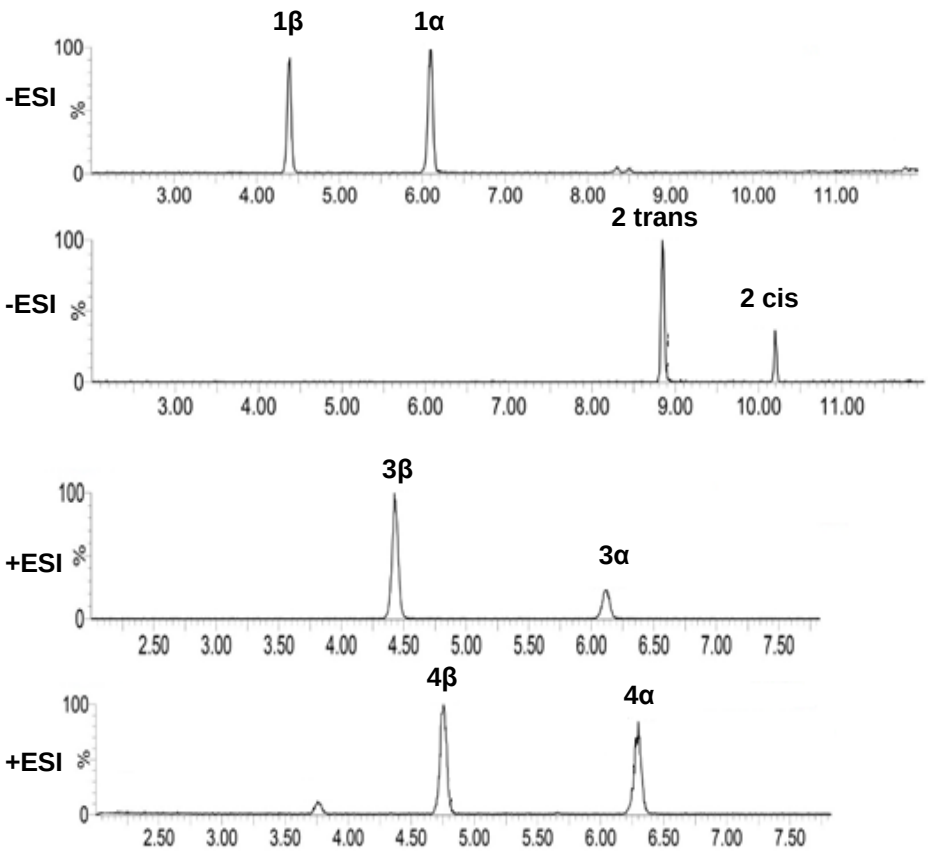
Application #AN1830

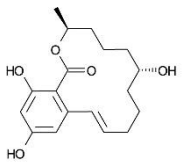
Conditions

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

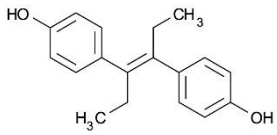
Time (mins)	%B
0.0	25
0.5	25
7.0	35
7.5	35
10.5	60
12.5	90

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



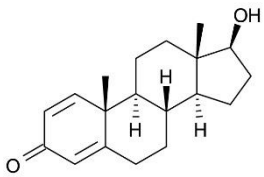


1. α- and β-Zearalenol
(*m/z* 319.17 → 275.12)

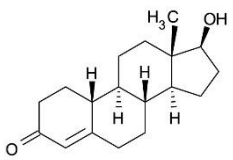


2. Diethylstilbestrol-d8
(*m/z* 275.23 → 245.09)

Also analysed in -ESI:
- Taleranol and zeranol-d4
- Taleranol and zeranol
- Zearalenone
- Hexestrol
- Diethylstilbestrol
- Dienesterol



3. α- and β-Boldenone
(*m/z* 287.17 → 121.12)



4. α- and β-Nortestosterone
(*m/z* 275.23 → 109.09)

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

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Steroids Separation using Enhanced Polar Selectivity

ACE®
Ultra-inert
UHPLC & HPLC Columns

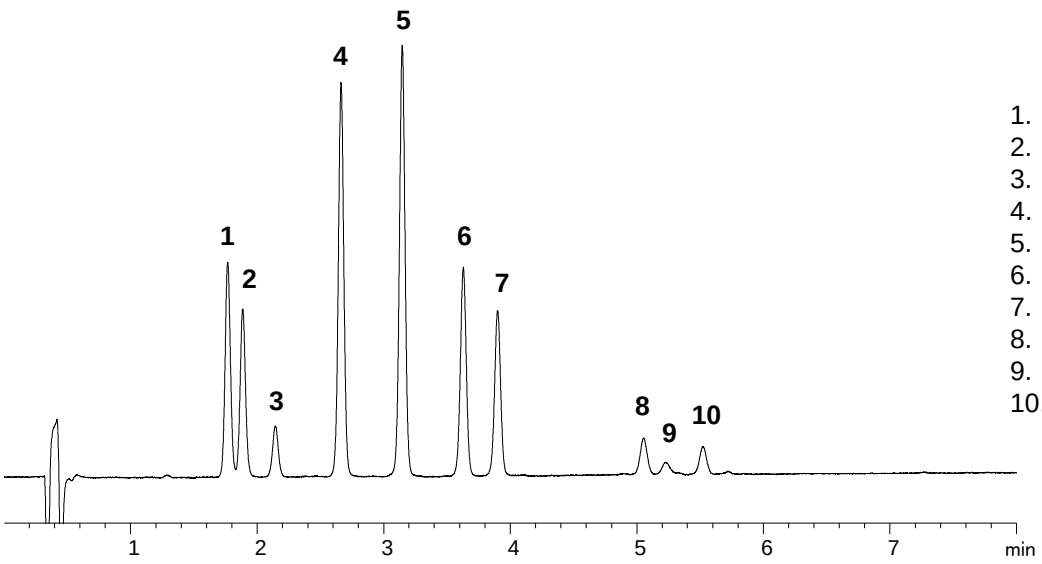
Application #AN2470

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 H_2O
	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. 11α-Hydroxyprogesterone
6. 11-Ketoprogesterone
7. 21-Hydroxyprogesterone
8. 17β-Estradiol
9. 17α-Estradiol
10. 17α-Ethinylestradiol

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Steroids UHPLC-UV Analysis and Comparison

ACE® Ultra-inert UHPLC & HPLC Columns

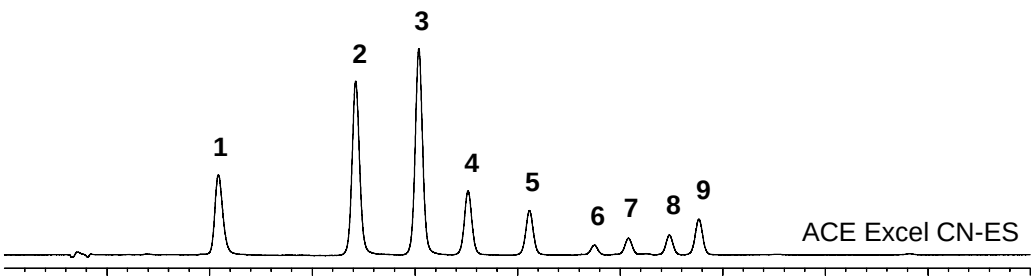
Application #**AN1640**

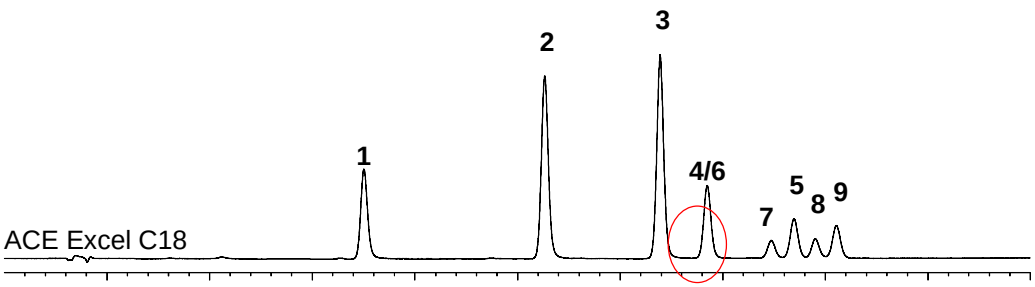
Conditions

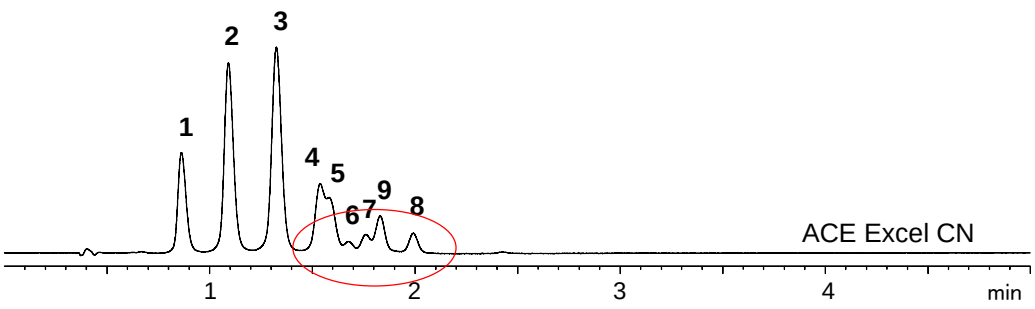
Column:	ACE Excel 2 CN-ES ACE Excel 2 C18 ACE Excel 2 CN
Dimensions:	50 x 2.1 mm
Part Number:	EXL-1013-0502U, EXL-101-0502U, EXL-104-0502U
Mobile Phase:	A: 0.1% formic acid in H_2O B: 0.1% formic acid in MeCN

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







1. Cortisone
2. Corticosterone
3. 11α-Hydroxyprogesterone
4. Cortisone-21-acetate
5. 11-Ketoprogesterone
6. 17β-Estradiol
7. 17α-Estradiol
8. 17α-Ethinylestradiol
9. Estrone

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Sulfonamides

ACE®
Ultra-inert
UHPLC & HPLC Columns

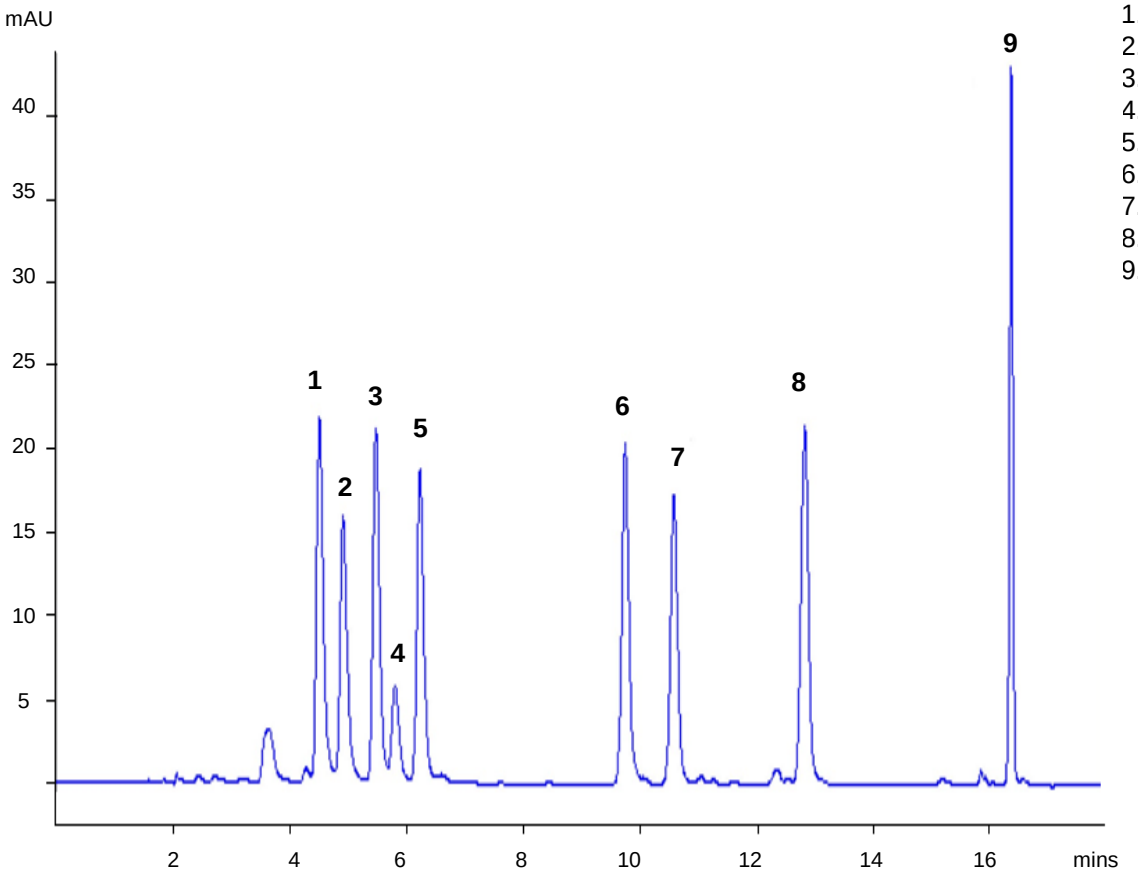
Application #**AN1610**

Conditions

Column:	ACE Excel 3 C18-PFP
Dimensions:	150 x 4.6 mm
Part Number:	EXL-1110-1546U
Mobile Phase:	A: H_2O
	B: MeCN
	C: 10% formic acid

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

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



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

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Sumatriptan and Promethazine by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

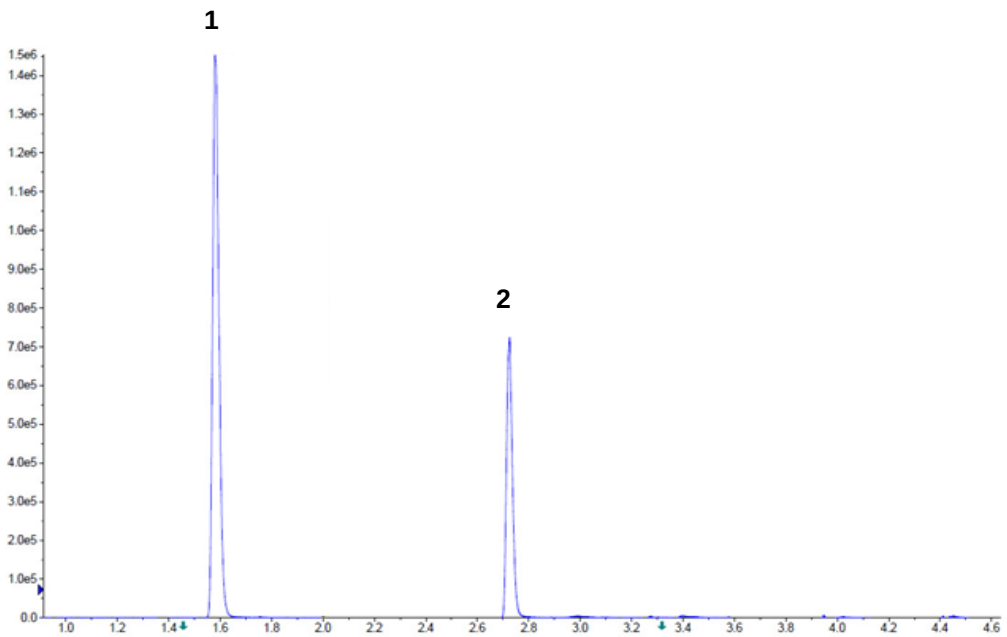
Application #**AN2530**

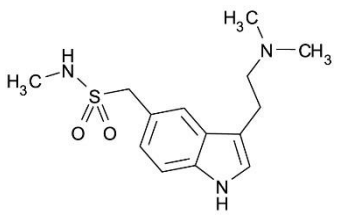
Conditions

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 H_2O
	B: 0.1% formic acid in MeOH

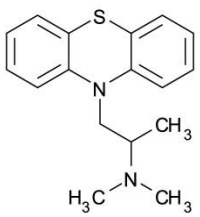
Time (min)	%B
0.0	15
0.5	15
2.5	90
3.5	90
5.5	15

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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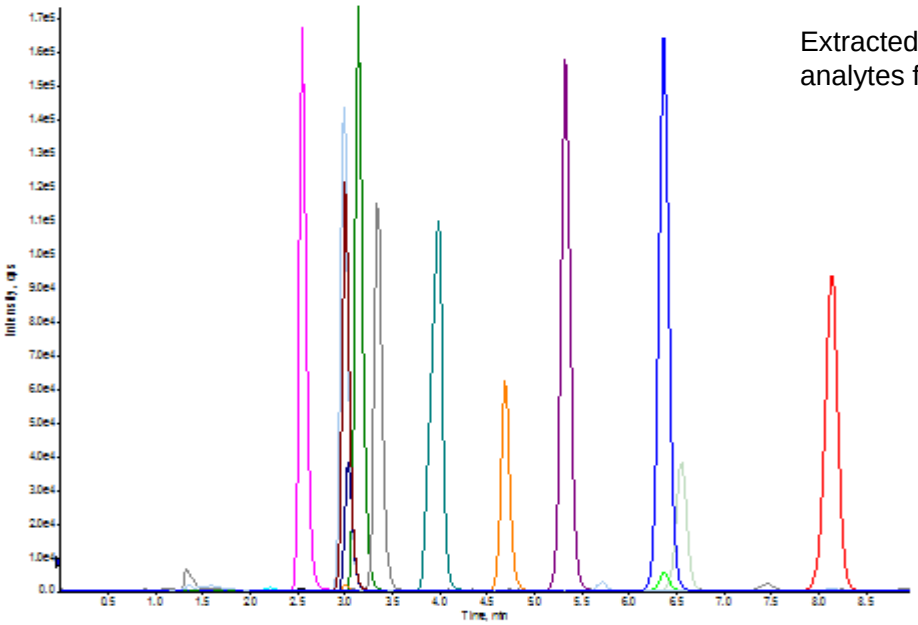
Synthetic Cannabinoids (SPICE) from Oral Fluid

ACE® Ultra-inert UHPLC & HPLC Columns

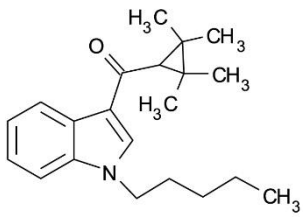
Application #AN1650

Conditions

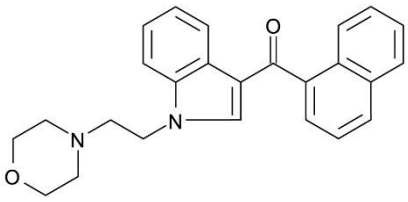
Column:	ACE Excel 2 C18-AR
Dimensions:	100 x 2.1 mm
Part Number:	EXL-109-1002U
Mobile Phase:	0.1% formic acid in MeOH/H_2O (85:15 v/v)
Flow Rate:	0.3 mL/min
Temperature:	Ambient
Detection:	Applied Biosystems/MDS Sciex 4000 Q-Trap Positive mode Turbo Ionspray



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	Declustering 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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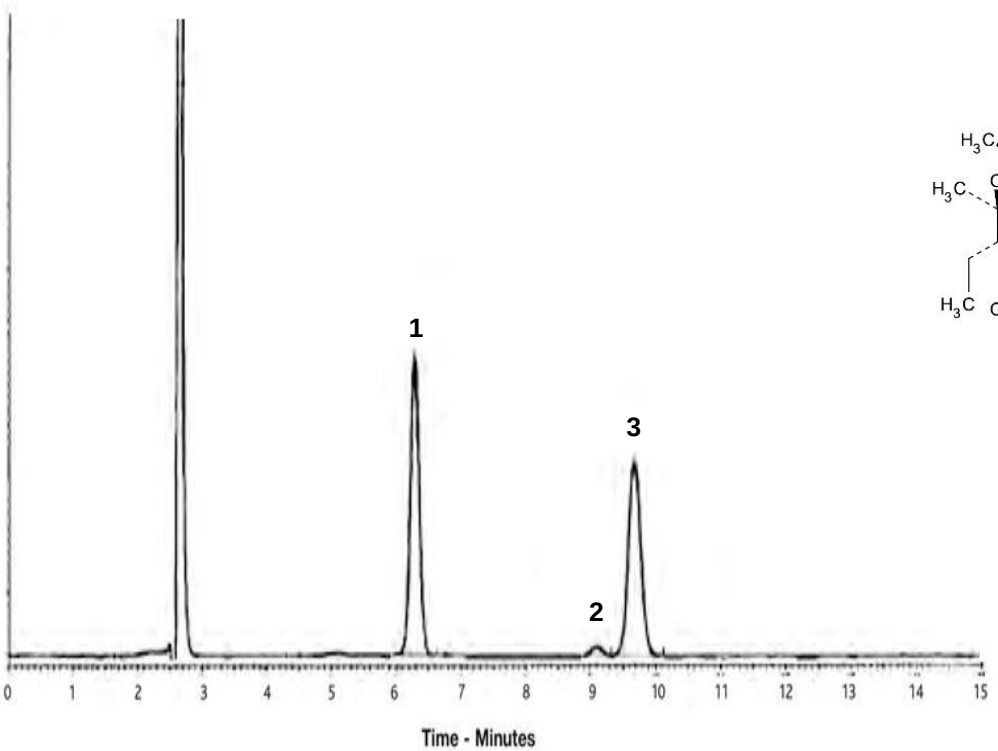
Telithromycin Analysis

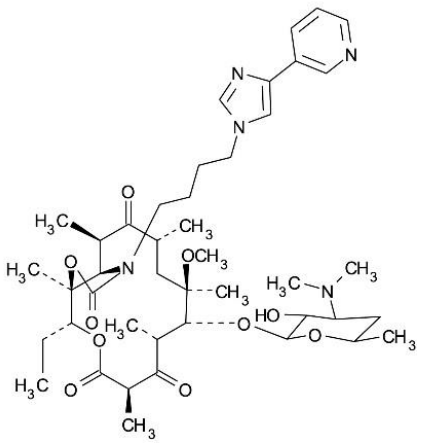
ACE®
Ultra-inert
UHPLC & HPLC Columns

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% H_2O_2 for 1 hour





1. Telithromycin
2. Degradant 1
3. Degradant 2

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Terfenadine and Fexofenadine in Rat Plasma

ACE®
Ultra-inert
UHPLC & HPLC Columns

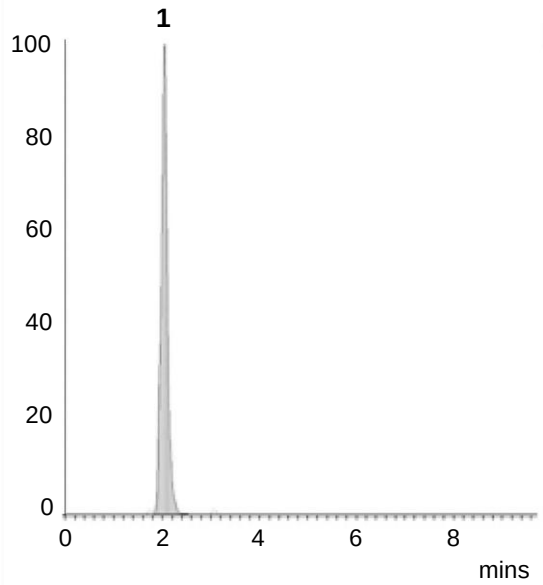
Application #**AN3290**

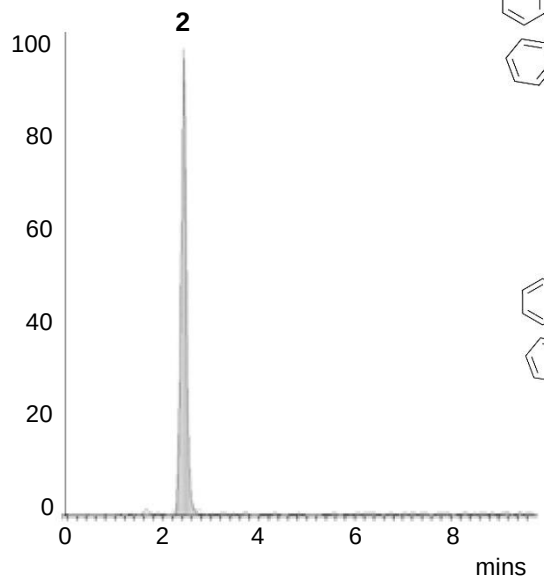
Conditions

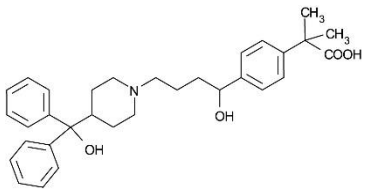
Column:	ACE 5 AQ
Dimensions:	50 x 3.0 mm
Part Number:	ACE-126-0503
Mobile Phase:	A: 0.1% formic acid in H_2O
	B: MeOH

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

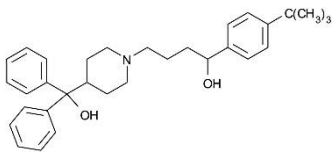
Flow Rate:	1 mL/min
Injection:	10 µL
Temperature:	Ambient
Detection:	Turbo IonSpray MS/MS
	Positive ion mode







1. Fexofenadine
(m/z 502.3 → 466.3)



2. Terfenadine
(m/z 472.3 → 436.3)

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Testosterone

ACE®
Ultra-inert
UHPLC & HPLC Columns

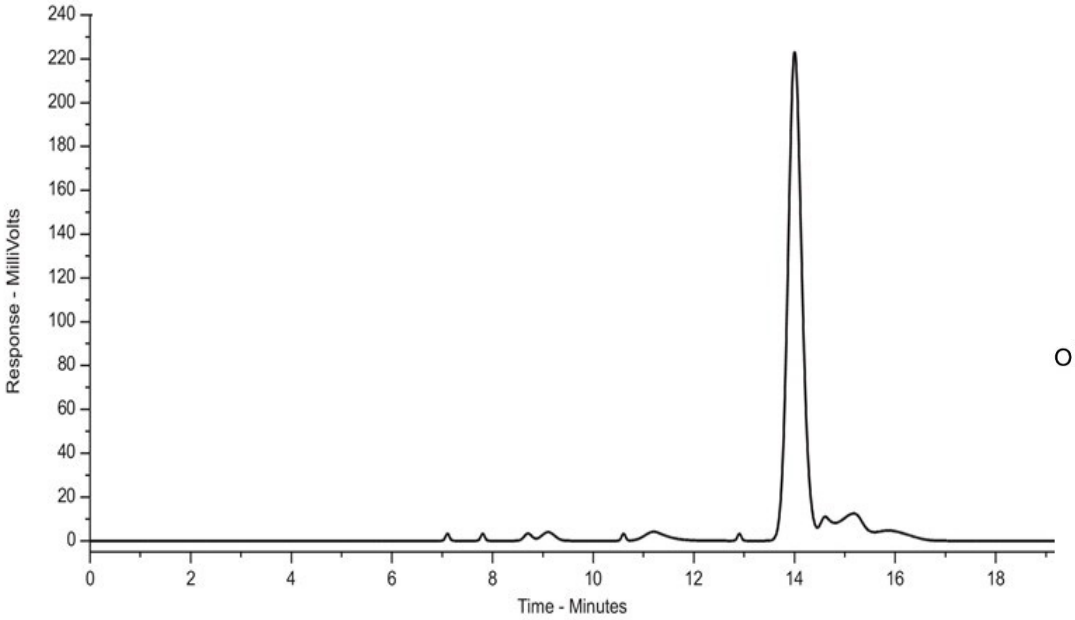
Application #AN3300

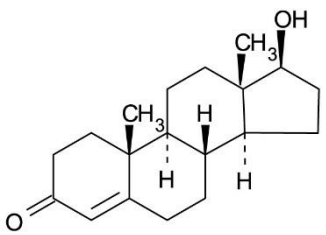
Conditions

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

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Thyroid Hormones by LC-MS/MS (I)

ACE®
Ultra-inert
UHPLC & HPLC Columns

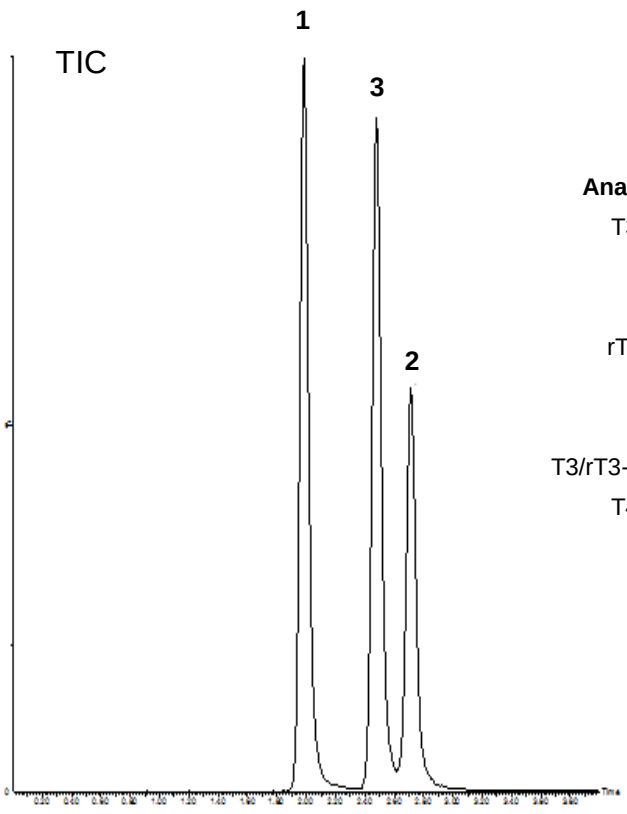
Application #AN2170

Conditions

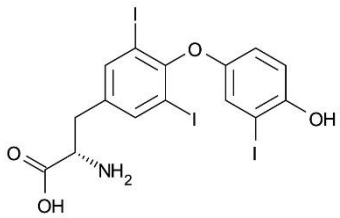
Column:	ACE Excel 2 C18-AR
Dimensions:	100 x 2.1 mm
Part Number:	EXL-109-1002U
Mobile Phase:	A: 2 mM ammonium acetate, 0.1% formic acid in H_2O B: 2 mM ammonium acetate, 0.1% formic acid in MeOH

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

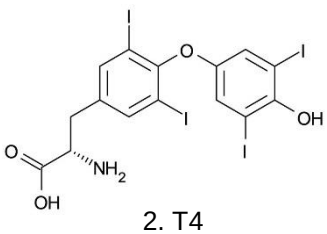
Flow Rate:	0.4 mL/min
Injection:	10 µL
Temperature:	40 °C
Detection:	XEVO TQS triple quad MS Desolvation temperature: 500 °C Ion source temperature: 150 °C Positive mode ESI, MRM



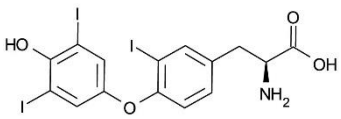
Analyte	Q1 (Da)	Q3 (Da)
T3	651.8	605.8
	(651.8)	(507.8)
	(651.8)	(478.9)
rT3	651.8	605.8
	(651.8)	(507.8)
	(651.8)	(478.9)
T3/rT3-d6 I.S.	657.8	611.8
T4	777.7	731.7
	(777.7)	(351)
	(777.7)	(633.8)



1. T3
(Tri-iodothyronine)



2. T4
(Thyroxine)



3. rT3
(Reversed tri-iodothyronine)

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Thyroid Hormones by LC-MS/MS (II)

ACE® Ultra-inert UHPLC & HPLC Columns

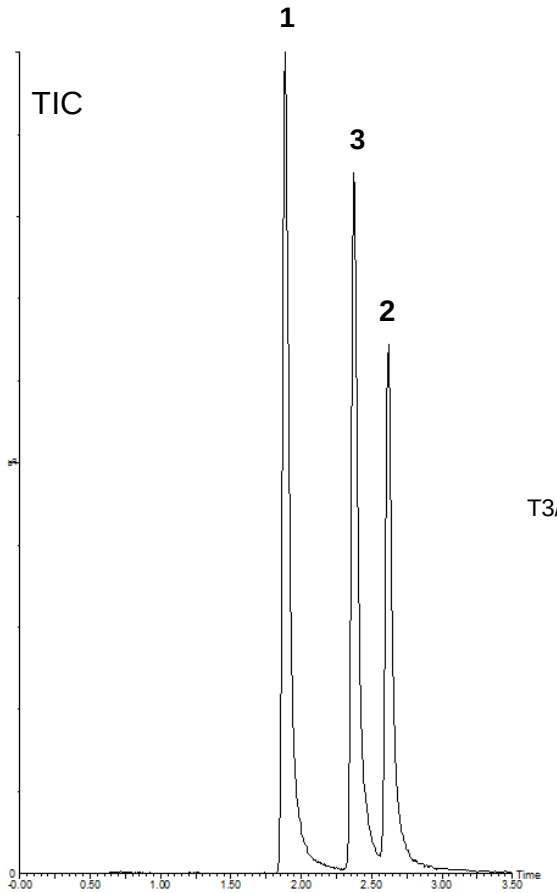
Application #AN2180

Conditions

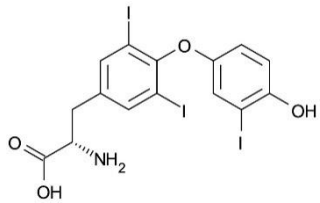
Column:	ACE Excel 1.7 C18-AR
Dimensions:	100 x 2.1 mm
Part Number:	EXL-179-1002U
Mobile Phase:	A: 2 mM ammonium acetate, 0.1% formic acid in H_2O
	B: 2 mM ammonium acetate, 0.1% formic acid in MeOH

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

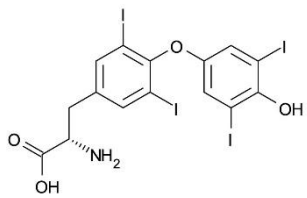
Flow Rate:	0.4 mL/min
Injection:	10 µL
Temperature:	40 °C
Detection:	XEVO TQS triple quad MS
	Desolvation temperature: 500 °C
	Ion source temperature: 150 °C
	Positive mode ESI, MRM



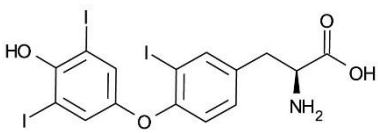
Analyte	Q1 (Da)	Q3 (Da)
T3	651.8	605.8
	(651.8)	(507.8)
	(651.8)	(478.9)
rT3	651.8	605.8
	(651.8)	(507.8)
	(651.8)	(478.9)
T3/rT3-d6 I.S.	657.8	611.8
T4	777.7	731.7
	(777.7)	(351)
	(777.7)	(633.8)



1. T3
(Tri-iodothyronine)



2. T4
(Thyroxine)



3. rT3
(Reversed tri-iodothyronine)

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Tocopherol Mixture Separation

ACE®
Ultra-inert
UHPLC & HPLC Columns

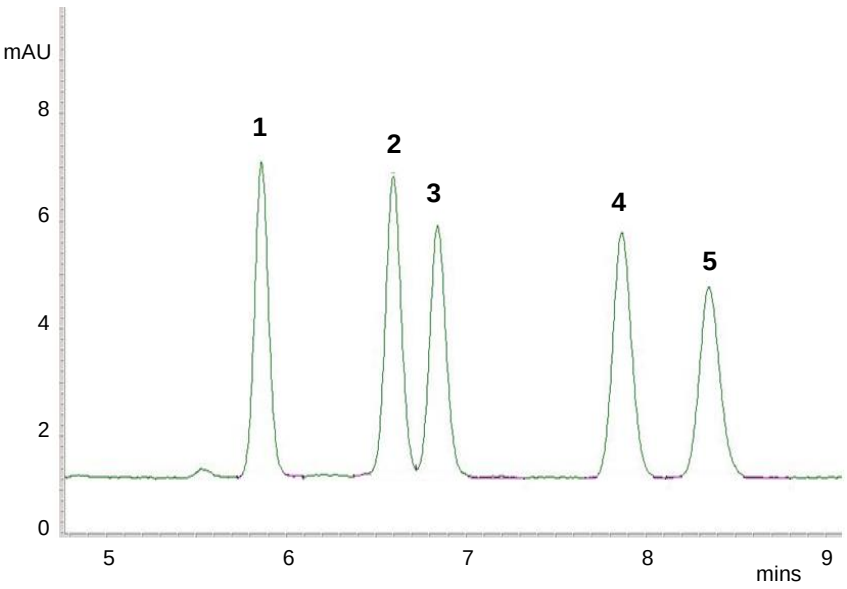
Application #**AN3390**

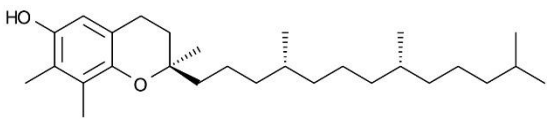
Conditions

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

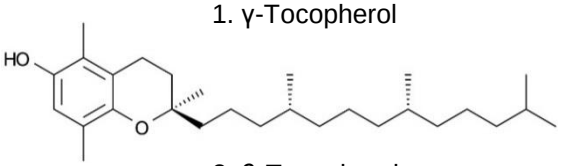
Time (mins)	%B
0.00	0
0.10	0
0.11	80
8.00	80
8.01	100
12.00	100
12.01	0
14.00	0

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

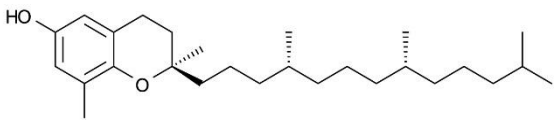




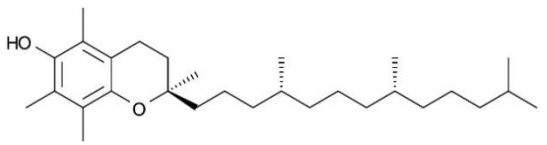
1. γ-Tocopherol



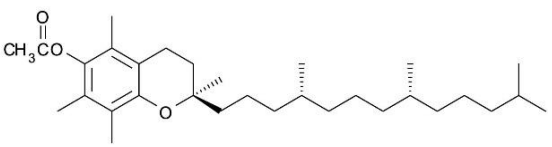
2. β-Tocopherol



3. δ-Tocopherol



4. α-Tocopherol



5. α-Tocopherol acetate

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Tricyclic Antidepressants (Gradient)

ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1690**

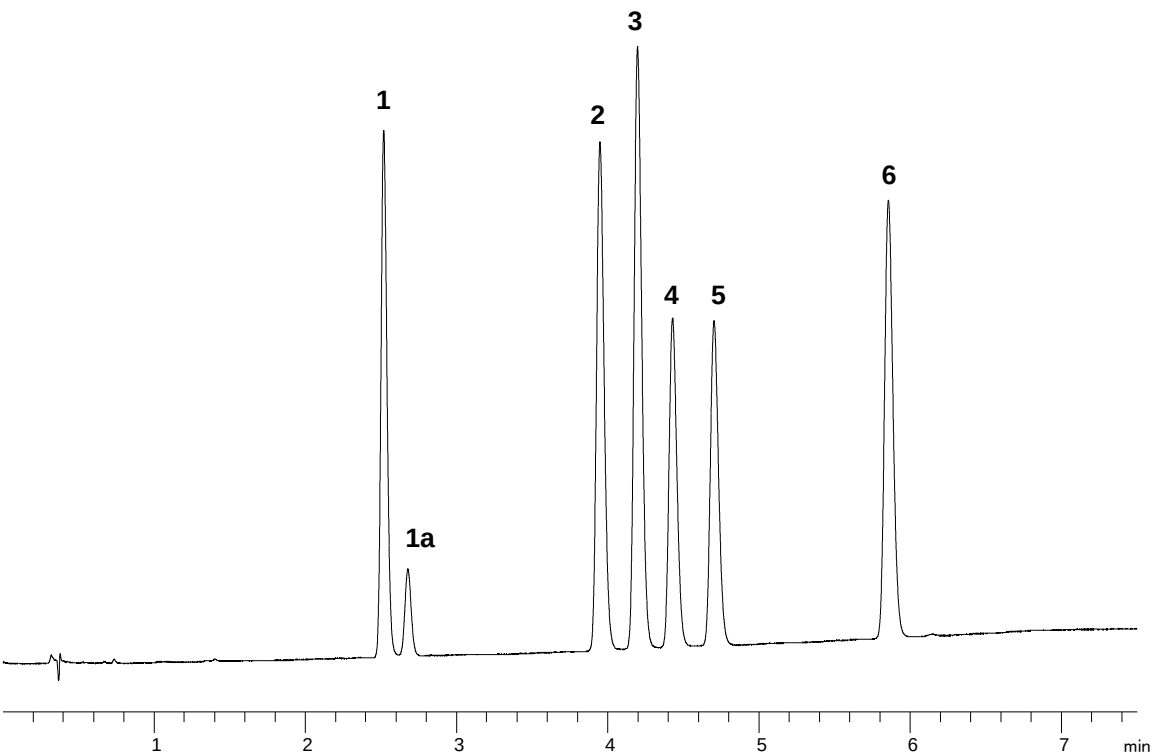
Conditions

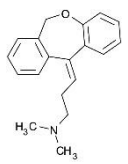
Column:	ACE Excel 2 SuperC18
Dimensions:	100 x 3.0 mm
Part Number:	EXL-1011-1003U
Mobile Phase:	A 20 mM ammonium formate pH 3.0 in H_2O
	B 20 mM ammonium formate pH 3.0 in MeOH/H_2O (9:1 v/v)

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

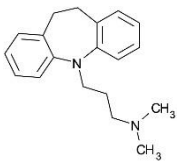
Post time 10 minutes

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

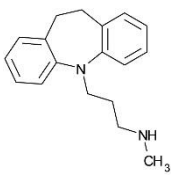




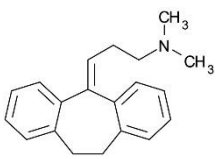
1. Doxepin + isomer



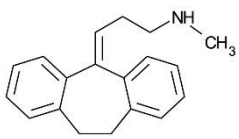
2. Imipramine



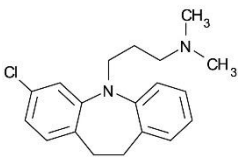
3. Desipramine



4. Amitriptyline



5. Nortriptyline



6. Clomipramine

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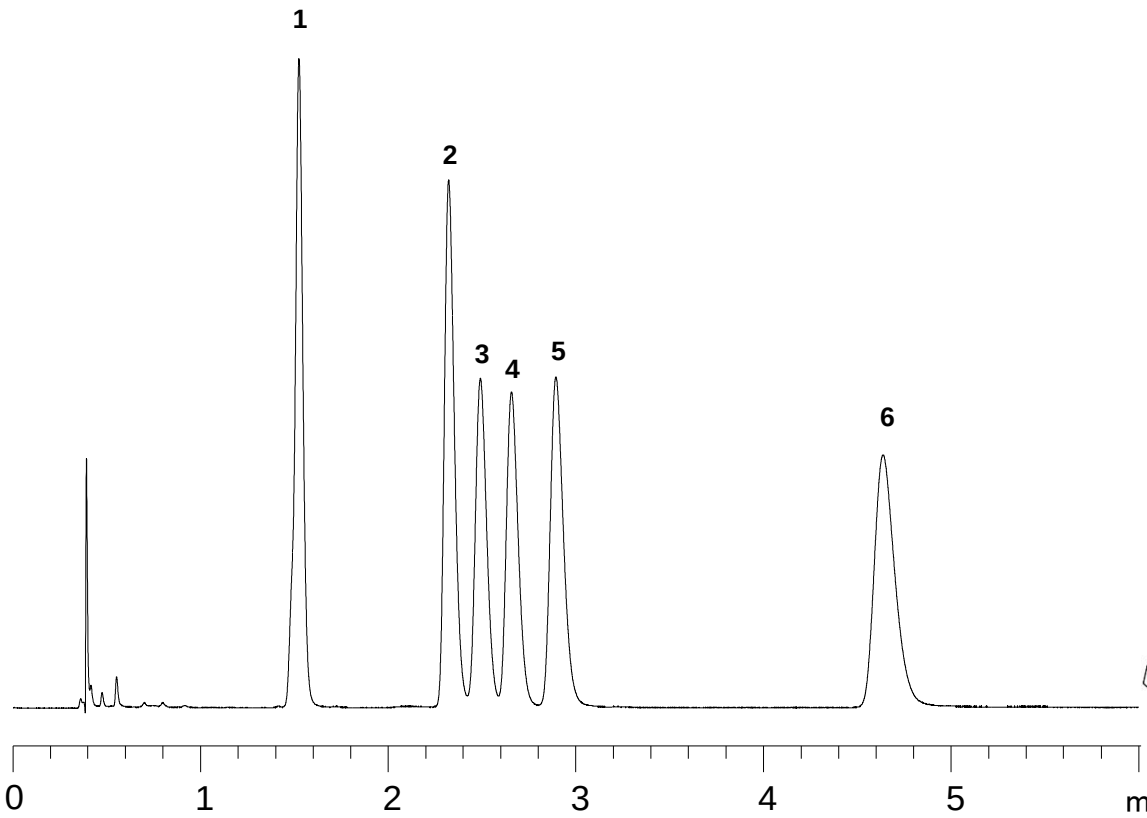
Tricyclic Antidepressants (Isocratic)

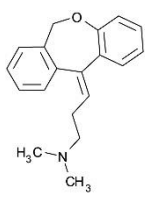
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1680**

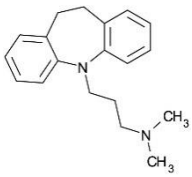
Conditions

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/H_2O (54:46 v/v)
Flow Rate:	1.2 mL/min
Injection:	2 µL
Temperature:	40 °C
Detection:	UV, 260 nm

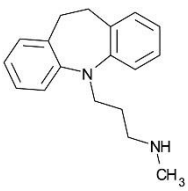




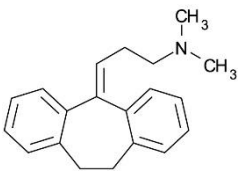
1. Doxepin



2. Imipramine



3. Desipramine



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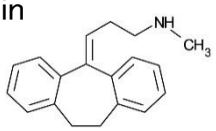
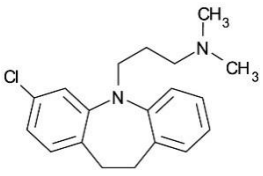


5. Nortriptyline



6. Clomipramine

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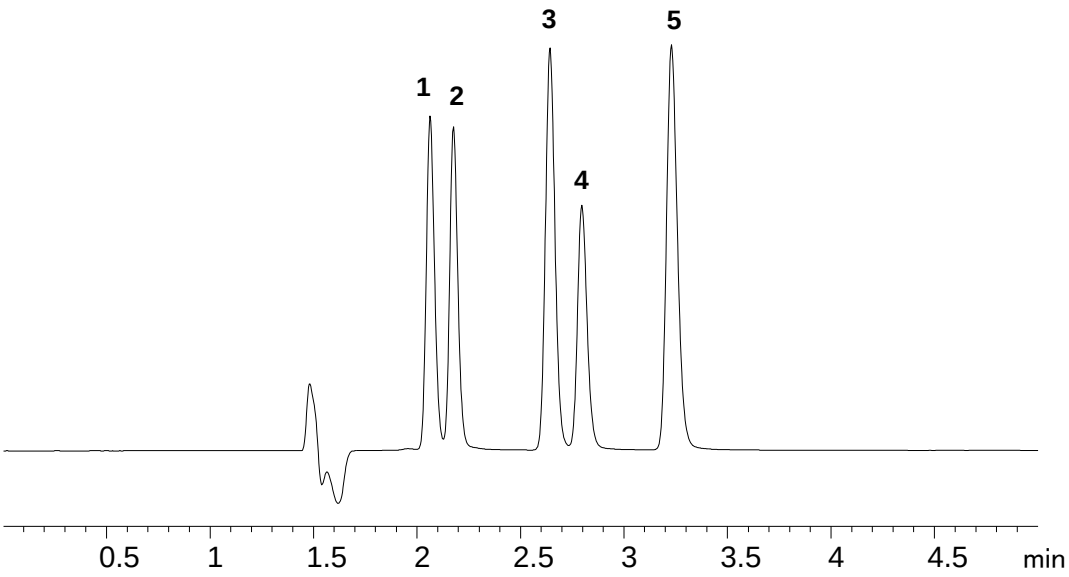
Tricyclic Antidepressants (Isocratic Rapid Analysis)

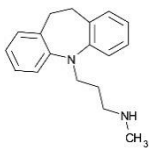
ACE® Ultra-inert UHPLC & HPLC Columns

Application #AN1700

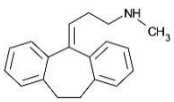
Conditions

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/H_2O (65:35 v/v)
Flow Rate:	1.5 mL/min
Injection:	10 µL
Temperature:	60 °C
Detection:	UV, 215 nm

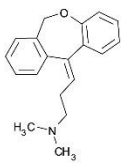




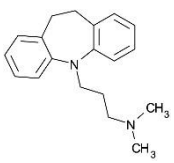
1. Desipramine



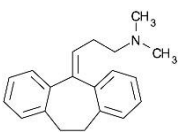
2. Nortriptyline



3. Doxepin



4. Imipramine



5. Amitriptyline

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

ACE® Ultra-inert UHPLC & HPLC Columns

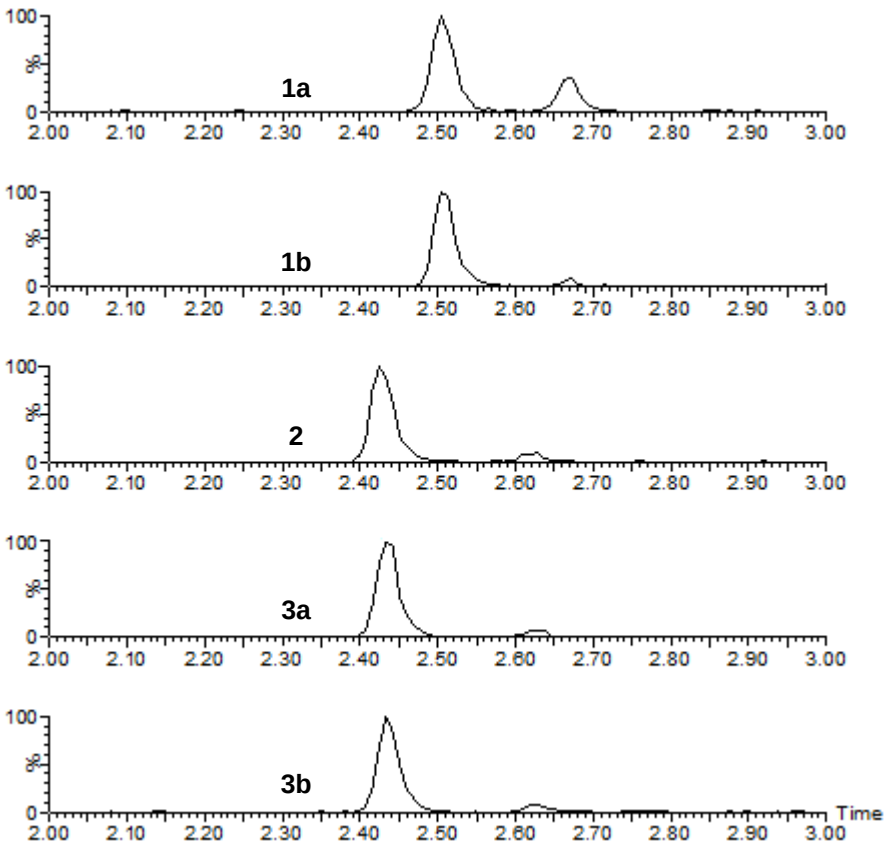
Application #AN2390

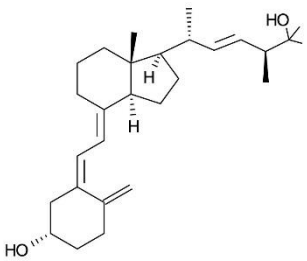
Conditions

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

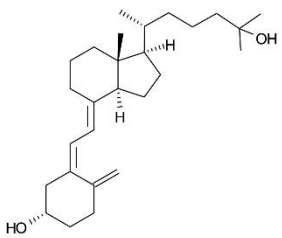
Time (mins)	%B
0.0	75
3.0	100
4.0	100

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





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



3a. 25-OH Vitamin D3 (*m/z* 383.5 → 257.5)
3b. 25-OH Vitamin D3 (*m/z* 383.5 → 107.2)

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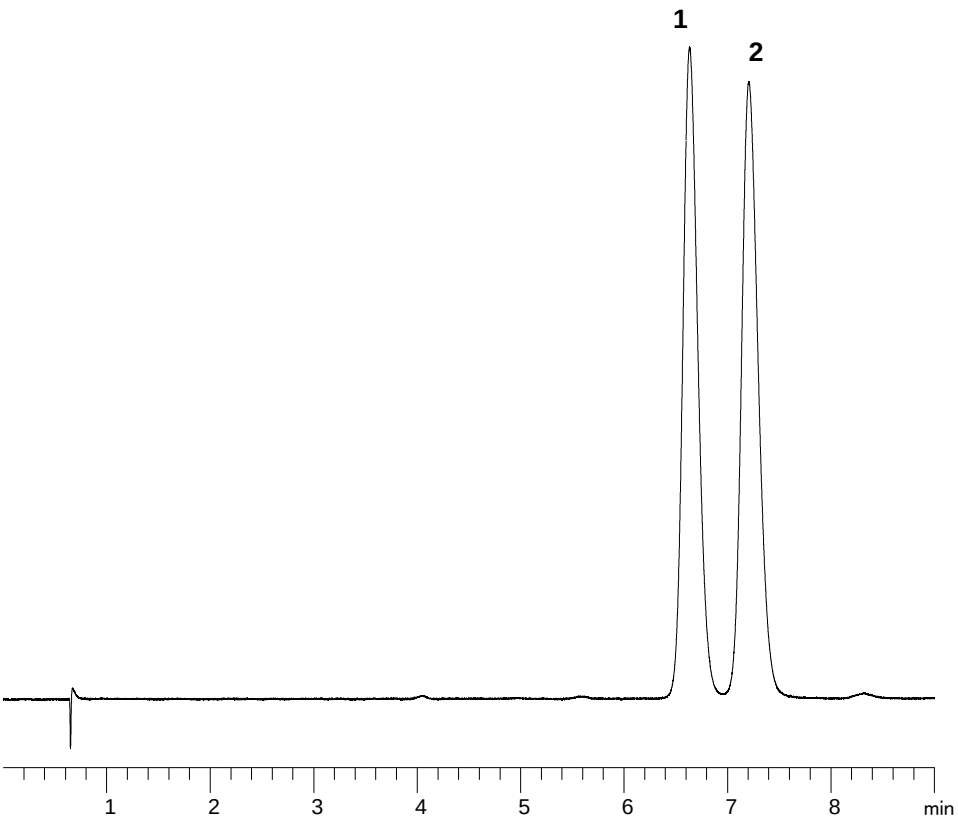
Vitamin D2/D3

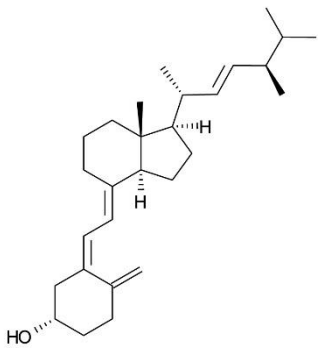
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #**AN1840**

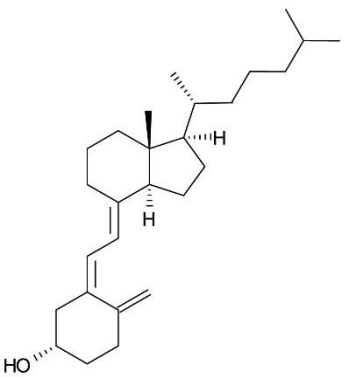
Conditions

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





1. Ergocalciferol (D2)



2. Cholecalciferol (D3)

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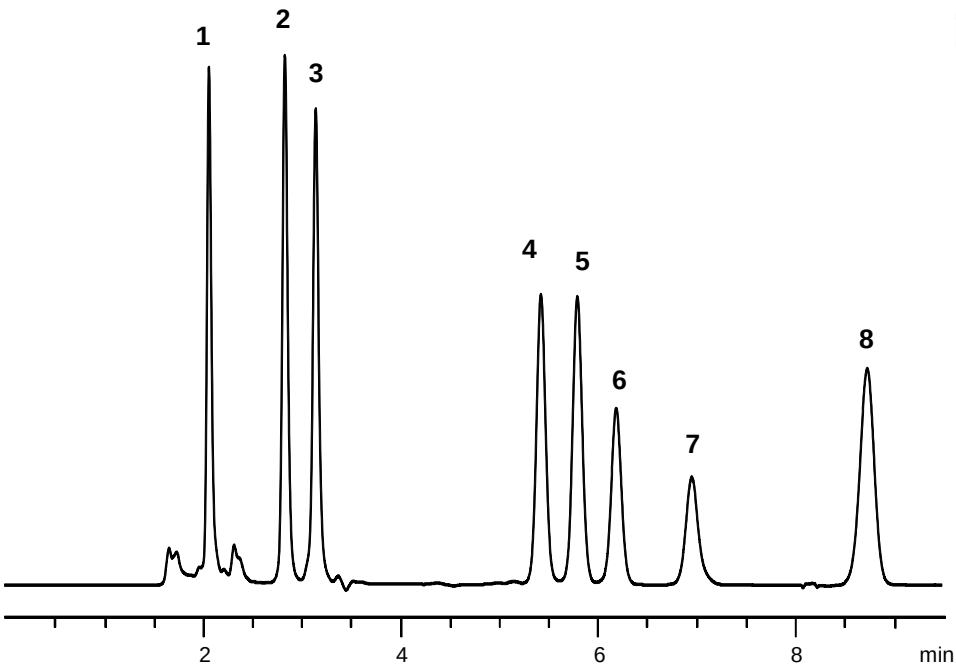
Vitamins – Fat Soluble

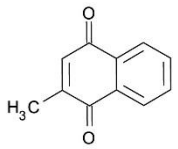
ACE®
Ultra-inert
UHPLC & HPLC Columns

Application #AN2420

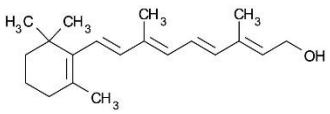
Conditions

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

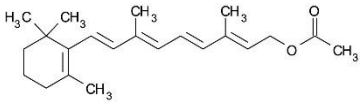




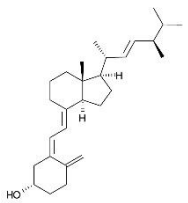
1. Menadione (Vitamin K3)



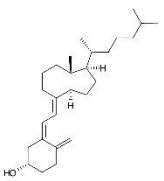
2. Retinol (Vitamin A)



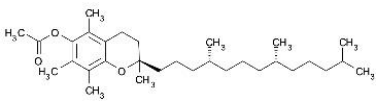
3. Vitamin A acetate



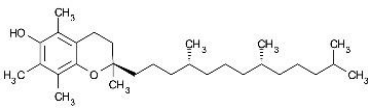
4. Ergocalciferol (Vitamin D2)



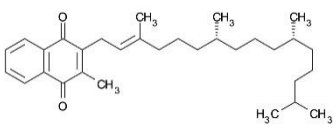
5. Cholecalciferol (Vitamin D3)



6. Vitamin E acetate



7. α-Tocopherol (Vitamin E)



8. Vitamin K1

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Water Soluble Vitamins (I)

ACE®
Ultra-inert
UHPLC & HPLC Columns

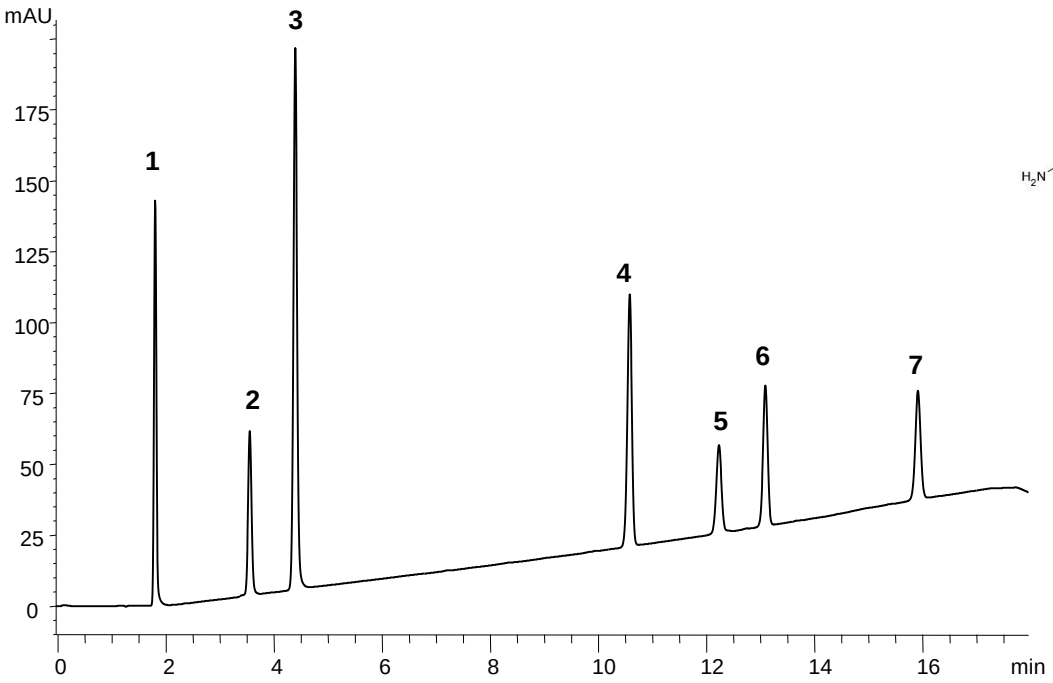
Application #AN1870

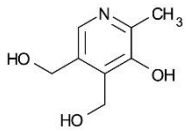
Conditions

Column:	ACE 3 C18-AR
Dimensions:	150 x 4.6 mm
Part Number:	ACE-119-1546
Mobile Phase:	A: 20 mM potassium phosphate pH 2.83 in H_2O B: 20 mM potassium phosphate pH 2.83 in MeOH/H_2O (50:50 v/v)

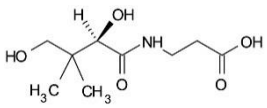
Time (mins)	%B
0	20
15	70

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

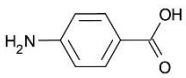




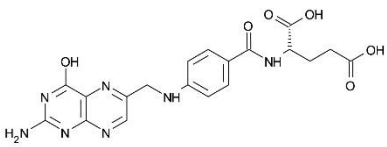
1. Pyridoxine (Vitamin B6)



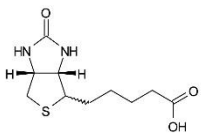
2. Pantothenic acid (Vitamin B5)



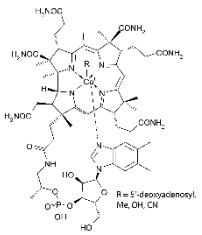
3. p-Aminobenzoic acid



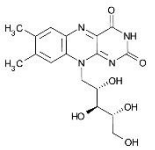
4. Folic acid (Vitamin B9/ Vitamin M)



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



6. Cyanocobalamin (Vitamin B12)



7. Riboflavin (Vitamin B2)

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